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Combination of pharmacophore hypothesis and molecular docking to identify novel inhibitors of HCV NS5B polymerase

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Abstract

Hepatitis C virus (HCV) infection or HCV related liver diseases are now shown to cause more than 350,000 deaths every year. Adaptability of HCV genome to vary its composition and the existence of multiple strains makes it more difficult to combat the emergence of drug resistant HCV infections. Among the HCV polyprotein which has both the structural and non structural regions, the non structural protein NS5B RNA-dependent RNA polymerase (RdRP) mainly mediates the catalytic role of RNA replication in conjunction with its viral protein machinery as well as host chaperone proteins. Lack of such RNA dependent RNA polymerase enzyme in host had made it an attractive and hotly pursued target for drug discovery efforts. Recent drug discovery efforts targeting HCV RdRP have seen success with FDA approval for sofosbuvir as a direct-acting anti-viral (DAA) against HCV infection. However, variations in drug binding sites induce drug resistance and therefore targeting allosteric sites could delay the emergence of drug resistance. In this study, we focussed on allosteric thumb site II of the non-structural protein NS5B RNA-dependent RNA polymerase and developed a five feature pharmacophore hypothesis/model which estimated the experimental activity with a strong correlation of 0.971 & 0.944 for training and test set respectively. Further, the Güner-Henry score of 0.6 suggests that the model was able to discern the active and inactive compounds and enrich the true positives during a database search. Together, our database search and molecular docking, HCV 1b viral replication inhibition results suggested the ligands with best fitness to the pharmacophore model dock to the key residues involved in thumbs site II and inhibited the HCV 1b viral replication in sub-micro-molar range.

Keywords: HCV, NS5B polymerase, RDRP, Thumb site II inhibitor, pharmacophore modeling

Introduction

Hepatitis C virus (HCV) belongs to *Flaviridae* family and its genome consists of 9.6-kb, single-stranded RNA with positive polarity and encodes a large molecular mass precursor poly-protein. The precursor molecule upon proteolytic processing yields three structural proteins (C, E1 and E2) and seven non-structural proteins (p7, NS2, NS3, NS4A, NS4B, NS5A and NS5B) [1,2]. Among these proteins, non-structural protein 5B (NS5B) mediates HCV RNA-dependent RNA polymerase (RdRp) and terminal transferase activities and regulates HCV viral replication. Recent trends have shown that HCV infections have afflicted more than 150 million people worldwide, which is approximately 3% of the world population [3]. Every year, Hepatitis C-related liver diseases like liver cirrhosis and hepatocellular carcinoma kills more than 350,000 people [4]. The conventional HCV treatment during the past decade employed a combination of pegylated-interferon and ribavirin which had imparted only a 40%-50% sustained viral response (SVR) in HCV infected patients [5]. Though the introduction of direct-acting antiviral(s) (DAA) in combination with interferon and ribavirin had increased the SVR of the patients, but required a longer treatment regimen (48 weeks) and was often associated with concomitant adverse side effects on patients due to use of interferon [6]. Current DAA development was targeted on non-structural proteins such as NS3/4A serine protease, NS5A and NS5B RNA-dependent RNA polymerase (RdRp) which are shown to be essential for HCV replication [6]. More importantly, research efforts targeting NS5B polymerase led to the identification of sofosbuvir which has been recently approved by FDA for use in a HCV treatment that was free from interferon [7]. Adaptability of HCV virus to mutate key residues involved in drug binding and the ability to vary its composition to diverse HCV genetic strain populations as evidenced with the six strains such as 1a, 1b, 2, 4, and 3, 6 present the possibility of emergence of drug resistance. Therefore, continued efforts are needed to develop DAA that can overcome mutations at drug binding

sites and to obfuscate the emergence of drug resistance due viral mutations on drug binding sites [8, 9].

X-ray crystallographic studies have revealed that NS5B structure resembled a right hand and possessed a finger, thumb and palm domains [8-10]. Various studies have shown that there are at least four allosteric sites in NS5B polymerase for inhibitor binding, namely palm site I, palm site II, nucleoside or thumb site I and non-nucleoside or thumb site II besides the RNA binding site (Supplementary Figure 1) [1,11-14]. NS5B inhibitors are broadly classified as i) nucleoside inhibitor that competes with nucleotides at the active site and ii) non-nucleoside inhibitors that could bind either at the thumb site II or palm site (Chart 1). Non-nucleoside inhibitors are docked at the thumb site II are involved in interaction with key residues such as S476, Y477, L419, L482, L497 and W528 (Supplementary Figure 2) and allosterically inhibit the viral RNA polymerase activity. NS5B has been shown to interact with cyclophilin and share its cyclophilin binding region with that NS5A. It was indirectly inferred from NMR binding studies that NS5B thumb site region could be involved in its interaction with NS5A and ligand binding at thumb site prevented the NS5B and NS5A interactions [15]. A recent study had exemplified that ligand binding at the thumb site II induced the conformational changes, re-orient the C-terminal tail, β -loop structural elements into the palm site of NS5B polymerase. These conformational changes further stabilize the closed state and allosterically inhibit the RNA binding and NS5B polymerase activity [16]. In this study, using combined approaches of pharmacophore modeling and virtual screening methods, we present key features that are important for inhibition of RNA polymerase activity. Further our database screening and evaluation of molecular interactions at the thumb site II led us to identification of novel chemical entities that could bind to thumb site II of NS5B and inhibit NS5B polymerase activity [17].

Materials & Methods

Data Collection for Pharmacophore Generation

Three hundred and ten HCV NS5B thumb site II inhibitors were selected from literature [5, 18-46] with activity (IC_{50} , μM) determined from HCV genotype 1b NS5B RdRP inhibition assay [24]. Eighteen molecules [18, 24, 28, 29, 32-35, 37, 41, 42, 45, 46] with diverse structures (Figure 1) and a four-fold activity spread (0.002 μM to 92 μM) were used to develop a pharmacophore model. The remaining 292 compounds (Supplementary Data1) were used as test set for validation of the model. Most of the modeling simulation works were performed on linux workstation using Accelrys Discovery Studio 3.5 (DS3.5) modeling suite [47]. 2D structures for all the ligands were sketched in Accelrys Draw [48]. 3D coordinates were generated using 'Prepare Ligands' module and the obtained 3D conformations were energy minimized using smart minimizer for 2000 steps with CHARMM forcefield by using the 'Minimize Ligands' module. A maximum of 255 conformations were generated for each molecule using the BEST conformation method in the 'Generate Conformations' module. BEST search method employed a poling algorithm [49] that samples diverse low energy conformations which are far from local minimum.

Construction of Pharmacophore Model

'3D QSAR Pharmacophore Generation' module (Hypogen program) was used to generate a valid pharmacophore from 18 training set molecules with the following features: hydrogen bond acceptor (0-3), hydrogen bond donor (0-3), hydrophobic aliphatic (0-3), negative ionizable (1-2) and ring aromatic (0-3) and interfeature distance of 3 Å as input parameters. Each run of the module generates 10 best pharmacophore models ranked based on the correlation between the experimental activity and the estimated activity predicted by each model. Hypogen algorithm used in '3D QSAR pharmacophore generation' uses the user input data i.e., training set, diverse conformational models, chemical features, activity and above

mentioned parameters to generate top ten pharmacophore models. Hypogen builds simplest model that can correlate the estimated activities with measured activities. The pharmacophore generation generally involves three phases. 1) a constructive phase – which identifies the features that are associated with most active compounds and builds hypotheses (models) that are common among the most active compounds, 2) subtractive phase – where the features that are common among the inactive compounds are removed from the initial hypotheses, and 3) optimization phase – where an attempt is made to refine the initial hypotheses model with slight refinement by either rotation or translation of feature type or add / remove certain feature and retains changes that lower the error involved during regression of activity estimate. The final model contain an ensemble or a set of generalized chemical features in three dimensional space as well as regression information that helps to predict the measured activity basing on their fitness to these features [50]. In order for the model to be acceptable, the following control or cost metrics should be satisfied. Configuration cost should be always be less than 17. The configuration cost of the model represents the entropy involved with the training set employed. Whenever the configuration cost was more than 17, one can only proceed further by changing the training set data. Besides the configuration cost, three other costs, namely the null cost, fixed cost and total cost also determine the validity of the model [50]. The null cost represent the highest cost for the phamacophore run as the cost was computed on averaged value of activity of the training set molecules without the structural weight to activity. The fixed cost represents the cost from the simplest pharmacophore model that fits the training set molecules perfectly. Total cost refers to the cost computed by structural feature(s) contribution to activity for each of the compound in the training set. For a model to be significant, the null cost should be greater than the fixed cost by more than 40 bit units. A difference of 40 to 60 bit units correspond to a 75% to 90% probabilty for correlation between the experimental and estimated activity values. Further, the total cost (the cost of the

pharmacophore model generated) should be close to the fixed cost in order for the model to be significant. Furthermore, to ensure that the best run is not random or a chance correlation, a randomization test using the Fisher validation (catscramble) test with confidence level of 98% was carried out under the '3D QSAR Pharmacophore Generation' module. The program randomizes the activity data of the training set molecules and generates 49 random pharmacophore models. None of these random models should have a higher correlation or lower total cost than the best model. Next, the predictive ability of the model to estimate the activity of 293 compounds (test set) that were not involved in the training set was carried out using 'Ligand Pharmacophore Mapping' module. For the model to be robust for database search, there should be strong correlation between the estimated and the experimental activity of the test set compounds. The Güner-Henry (GH) score was also calculated for the best model to determine the quality of the database screen. It uses a scoring method that infers the quality of the yield and the coverage of active compounds during a database search. The score has a range of 0 to 1, with 0 being a null model and 1 being the ideal model.

Database and Virtual Screening

After the validation of the pharmacophore model, the model was used to screen Chemdiv [51] and Interbioscreen library [52] derived from natural products compounds. The database screening was done using 'Search 3D Database' module in Discovery Studio 3.5. The 'Ligand Pharmacophore Mapping'/'Screen Library' module was used to estimate the activity of the library. Thus obtained focused library or the best hits were further analysed with molecular docking studies to investigate the possible interaction with HCV NS5B at thumb site II.

Docking studies

The HCV NS5B crystal structure (PDB ID 4EO6) that has resolution of 1.79Å was used for molecular docking studies. The protein was prepared for simulation studies by deleting the hetero-atoms and charges and potentials were assigned by using CHARMM force field in Discovery Studio 3.5. The missing atoms / residues were corrected using the 'Build and Edit Protein' module. The protein structure was energy minimized for 5000 steps (with the heavy atoms constrained) using the conjugate gradient algorithm with the 'Minimization' module in DS3.5. Genetic Optimization for Ligand Docking (GOLD) 5.0 program [53,54] was employed for evaluation of protein-ligand interaction energies. The active site of 5Å from the co-crystallized ligand was defined as the binding site of thumb site II. The docking parameters were optimized by stimulating the binding mode of the co-crystallised ligand and the same parameters were used to dock the focused library. ChemPLP and GOLD scoring function(s) were used to evaluate the molecular interactions of the ligand-protein complexes.

Cell Culture and Transfection

Huh.7 cells that contains the HCV genotype 1b sub-genomic replicon[55] designated as Huh.8 cells was a generous gift from Prof. Charles M. Rice, The Rockefeller University, U.S.A. Huh.8 cells were grown on T75 cell culture flasks in a DMEM medium supplemented with 10% FBS. The cells were maintained in a humidified incubator with 5% CO₂ at 37°C. When the cells reached 80% to 90% confluency, total cell count was determined using the haemocytometer and 200,000 cells per well were seeded into 6-well cell culture plates. The presence of HCV genotype 1b genome was verified by treating Huh.8 cells with Cyclosporine A (CsA) (0-500 nM) as a control to monitor the HCV 1b viral replication. Cells were incubated with inhibitors (CsA, compound 1-5) for 3 days and then harvested for downstream application. Experiments were performed in triplicate.

RNA Extraction and RT-qPCR

Total RNA was extracted from treated cells using TRIZOL reagent (Ambion, Life Technologies) as previously described [56]. Briefly, cells were lysed using the appropriate amount of TRIZOL reagent. Chloroform was added to the TRIZOL solution and centrifuged to obtain three separate phases. RNA containing aqueous phase was isolated by precipitation with isopropanol. The RNA pellet was then washed with 75% ethanol and re-suspended in DEPC-treated water. Synthesis of total cDNA from total RNA was performed using the Transcriptor First Strand cDNA Synthesis Kit (Roche) according to manufacturer's instructions. Random hexamer primers were used for the reaction. Real Time quantitative PCR (RT-qPCR) was set up using SYBR® Select Master Mix (Applied Biosystems) according to the manufacturer's instructions on Applied Biosystems 7500 Real- Time PCR machine. A standardized amount of cDNA (400ng), HCV genotype 1b primers, Forward primer (5'-CGGTAGCTCTGAATCGTCGGCTGT-3'), Reverse primer (5'-CATCCTCACTAGCCTCTTCACTCACGG-3') which detects the NS5A gene was employed to evaluate the amount of HCV 1b viral replication.

Results & Discussion

Our best pharmacophore model had five features - one negative ionizable (blue), one hydrogen bond acceptor (green), one ring aromatic (orange) and two hydrophobic aliphatic (cyan) features and are spaced at specific distances from each other (Figure 2A). These features are necessary for binding to thumb site II of NS5B RdRP. The best pharmacophore model has a correlation (r) of 0.971 and a configuration cost of 10.4 bits. The configuration cost (10.4 bits) of the model is well within the specified 17 bits, indicating that the program was able to handle complexity involved with the training set. The null, fixed and total costs are 151, 72.1 and 78.2 bits respectively. The total cost of the pharmacophore run was closer

to the fixed cost and the cost difference (78.9) between the null cost and fixed costs indicates that there is a probability of more than 90% of true correlation. The Hypogen program (in 3D QSAR Pharmacophore Generation) computes a fitness score for each ligand based on geometric fit of each ligand (in the training set) to the centre of the feature spheres. It estimated the activity of the ligands by simple regression of the fitness score to the activity. The higher the fitness score, the higher was the predicted activity (Table 1). Our best model was able to predict the experimental activity of the training set molecules with a strong correlation of 0.971. Likewise, the best model was also able to predict the activity of the test set molecules with a good correlation of 0.941 (Figure 3). The most active compound **1** in the training set mapped to all the features in the best pharmacophore model (Figure 2B). In contrast, the most inactive ligand, compound **18**, missed three features such as the hydrogen bond acceptor (green) and the two hydrophobic aliphatic features (cyan) (Figure 2C), which explains its lack of activity. The Fisher validation or cat scramble test with 98% confidence limits verified that the best pharmacophore model was a statistically significant and was not a chance correlation. None of the 13 random models that were generated had a correlation that was higher than the best pharmacophore model and likewise none of the random models had a total cost value lower than the best model (Supplementary Figure 3A, 3B). Further the predictive ability of the best model was also verified by using 292 test set compounds. The best model was able to recognise the active and inactive compounds and estimate their experimental activities with a correlation of 0.944 (Figure 3). The ability of the best model to discern actives and in-actives was further quantified using GH scoring and our results (Table 2) indicate that the best model had a GH score of 0.65 and could differentiate between the actives (true positives) and the in-actives (false positives). 3D Database screening with an in-house virtual library prepared Interbioscreen natural product based collection gave a focused library of 321 molecules. Ligand pharmacophore mapping was done to evaluate the fitness of

focused library to the best model and provided an estimate of their activity on HCV RdRP. The best fitting molecules S1N-09906, S1N-54222 were predicted to have an IC_{50} of 0.0096 and 0.0053 μ M respectively. As shown in Figure 4A, 4B, the best hits were shown to map most of the features except the ring aromatic feature and are estimated to possess a sub-micro-molar activity. The lack of fitness to ring aromatic feature might not be that critical to the activity prediction in comparison to lack of fitness to aliphatic features which hindered the activity to a greater extent (Figure 3C, Supplementary Figure 4A, 4B).

Our molecular docking results with best fitting ligands had high interaction or fitness scores with thumb site residues of NS5B polymerase. The best fitting ligand (1, Stock1N-09906) bears a 4-butoxy-benzoylamino moiety linked to 2-amino-acetyl amino fragment via 4-methylsulfanyl butyric acid (Table 3). On one hand, the 4-butoxy-benzoylamino scaffold was predicted to orient into the thumb site II pocket and was engaged in hydrophobic interactions with residues L419, M423, I497, I482, V485, L489, P496 residues. Further its carbonyl group was also involved in hydrogen bonding interaction with R496 (Figure 5A). On the other hand, the carboxyl and carbonyl groups on the 2-amino-acetyl amino substitution were engaged in hydrogen bonded interactions with S472 side chain oxygen and main chain amide atoms. The 4-methylsulfanyl moiety on butyric acid could project into crevices between His475 and K533 and stabilise the ligand binding. Similarly, Stock1N-054222 (2, Table 3) bearing a '4-butyl-2-oxo-2H-chromen-7yloxy' nucleus was oriented into the hydrophobic groove (L419, M423, I497, I482, V485, L489, P496 residues) with strong hydrophobic interactions. Further, the 2-oxo group on chromene was also involved in hydrogen interaction with L497. While the 2-[2-acetylamino]-acetylamino-3-methyl butyric acid fragment on 7th position of chromene nucleus maintained the hydrogen bonding interactions at the thumb site. The carboxyl group on butyric acid was not only involved in hydrogen bonding interactions with R501 side chain atoms but also maintained close contacts with W528 main chain carbonyl

atoms respectively (Figure 5B). Likewise, the carbonyl moieties on 2-[2-acetylamino]-acetylamino-3-methyl butyric acid were engaged in hydrogen bonding interactions with R423 and S476 respectively. Other best fitting ligands belonging to this scaffold (3, 4, and 6, Table 3) also showed similar interactions at thumb site II.

In order to assess the efficacy of our top ranking ligands, HCV 1b viral replication inhibition studies using HCV 1b replicon assay system were carried out and our results showed that the compounds (1, 2) among the top five compounds tested (Table 3) were able to potently inhibit HCV 1b viral replication at 1 μ M concentration. Further dose response studies in comparison with cyclosporine have revealed that compounds 1, 2 inhibited the HCV 1b viral replication in nanomolar range with an IC_{50} of 272.8 ± 1.70 (SEM) nM, 36.00 ± 1.77 (SEM) nM respectively (Supplementary Figure 5). Recent studies have highlighted that the mutations (M423T or L419M) on thumb site of NS5B polymerase could lower the ligand binding affinity (1, 2) and are susceptible to drug resistance [57]. Our best compounds (1, 2) bear no structural similarity to the ligands (VX-222 and ANA598) that lacked sensitivity to thumb site mutations [58]. Further, both the compounds 1, 2 are not only involved in close van der Waals contacts with hydrophobic residues in the vicinity of M423 residue but also extend their hydrophobic interactions with additional hydrophobic cavities (His475 and K533). We speculate that these additional hydrophobic interactions could enable the compounds 1, 2 to overcome the effect of mutations such as M423T or L419M as shown in previous studies [57]. Further *in vitro* binding studies using the compounds 1, 2 on wild type and M423T HCV NS5B polymerase might provide further insights into effect of M423T mutation at HCV thumb site. Taken together, both the hydrophobic interactions as well as hydrogen bonding with residues (S476, R501) that are involved at thumb site II could firmly lock the ligand at thumb site II, stabilize the closed or inactive conformation and allosterically inhibit the RNA polymerase activity of NS5B.

Conclusions

Combined approaches of ligand and structure based drug development are often used to identify novel chemical entities in academia and industry. Our ligand based 3D QSAR pharmacophore profiling on thumb site II inhibitors enabled us to identify key features that are required to bind thumb site II and allosterically inhibit the HCV RdRP mediated viral replication. Our pharmacophore model not only predicted the experimental activity with good correlation but also enriched the probability of finding true positives. Together with virtual screening and viral replication inhibition studies, we are able to identify two diverse scaffolds (Table 3) that are predicted to bind at thumb site II of NS5B polymerase and inhibit the viral replication in nanomolar range.

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Table 1: Fitness scores and prediction of IC₅₀ of training set molecules

Name	Fitness	Est IC ₅₀	Exp IC ₅₀	Error
Compound1	9.53	1.30e-03	2.00e-03	-1.6
Compound2	9.0	4.40e-03	2.00e-03	2.2
Compound3	9.13	3.20e-03	3.00e-03	1.1
Compound4	8.88	5.70e-03	0.01	-1.8
Compound5	8.12	0.033	0.014	2.4
Compound6	8.09	0.035	0.02	1.7
Compound7	8.08	0.036	0.042	-1.2
Compound8	7.08	0.36	0.11	3.3
Compound9	6.37	1.9	0.25	7.4
Compound10	6.74	0.78	0.49	1.6
Compound11	7.03	0.41	0.73	-1.8
Compound12	6.98	0.45	1.6	-3.5
Compound13	5.92	5.2	5	1
Compound14	6.29	2.2	6	-2.7
Compound16	6.15	3.1	9.4	-3.1
Compound16	5.28	22	29	-1.3
Compound17	5.14	32	57	-1.8
Compound18	4.67	92	92	1

Table 2: Güner Henry Scoring

Sl. No	Parameter	No. of molecules
1	Total molecules in data set (D)	310
2	Total number of actives in data set (A)	55
3	Total hits (Ht)	11
4	Active hits (Ha)	9
5	Yield of actives in percentage [(Ha/Ht) x 100]	81.8
6	Coverage of actives in percentage [(Ha/A) x 100]	16.4
7	Enrichment factor (E) [(Ha x D)/(Ht x A)]	4.61
8	False negatives [A – Ht]	46
9	False positives [Ht – Ha]	2
10	Goodness of hit score [(Ha/4HtA)(3A+Ht) x (1–((Ht–Ha)/(D–A)))]	0.65

Table 3: Structures of 6 top ligands to the best fit to pharmacophore model and had good GOLD PLP scores

Sl. No	Structure	Estimate IC ₅₀ (μM)	Fitness	GOLD PLP Score	Vendor ID	HCV 1b replication inhibition IC ₅₀ ± SEM (nM)
1		0.0053	8.90	76.88	STOCK 1N-09906	272.8±1.70
2		0.0096	8.65	62.04	STOCK 1N-54222	36.00±1.77
3		0.024	8.25	69.8	STOCK 1N-40747	Not Determined
4		0.031	8.14	69.72	STOCK 1N-54416	Not Determined
5		0.039	8.04	68.3	STOCK 1N-47746	Not Determined
6		0.039	8.03	68.3	STOCK 1N-52245	Not Determined

Chart 1: Nucleoside and non-nucleoside inhibitors that inhibit HCV RdRP.

Nucleoside or Thumb site I

Sofosbuvir

Mericitabine

Non-Nucleoside or Thumb site II

Beclabuvir/ BMS-791325

Setrobuvir

VX-222

Deleobuvir

ABT333/Dosabuvir

Figure Legends

Figure 1: The 18 molecules used as training set that were to develop NS5B pharmacophore model.

Figure 2: Best NS5B thumb site II pharmacophore model and its mapping to active and inactive. **A)** Pharmacophore model with 5 features, 1 negative ionizable feature (blue), 1 hydrogen bond acceptor (green), 1 ring aromatic feature (orange) and 2 hydrophobic aliphatic features (cyan). The grey sphere represents the exclusion volume. The distances (in Å) between the features are also shown. **B)** All features in the pharmacophore model are mapped to the most active molecule in the training set (**1**, 0.002 µM). **C)** Only 2 out of 5 features in the pharmacophore model are mapped to the most inactive molecule (**18**, 92 µM).

Figure 3: Estimated pIC₅₀ against experimental pIC₅₀ for compounds in the training and test set. The best model had a correlation (r) of 0.971 for training set and 0.944 for test set.

Figure 4: Pharmacophore mapping of best fitting novel compounds from Interbioscreen (IBS) Library. Most of the important features except ring aromatic feature had fitting with corresponding features in the best pharmacophore model.

Figure 5: Binding mode of best ligands at thumb site II of NS5B RdRP. **A)** The 4-butoxy-benzoyl amino fragment of the scaffold was engaged in hydrophobic interactions with groove residues L419, M423, I497, I482, V485, L489, and P496. Further its carbonyl group was also involved in hydrogen bonding interaction with R501 residue. The carboxyl and carbonyl groups on '2-amino-acetyl amino' substituent were mainly involved in bonded interactions

with side chain oxygen and main chain amide atoms of S472. Furthermore, the 4-methylsulfanyl moiety on butyric acid could project into crevices between His475 and K533 and stabilise the ligand binding. B). Chromene nucleus in this ligand was docked at the hydrophobic groove lined by L419, M423, I497, I482, V485, L489, and P496 residues. Further 2-oxo group was also engaged in hydrogen bonding to P496 residue. The carbonyl moieties on 2-[2-acetylamino]-acetylamino-3-methyl butyric acid were mainly involved in bonding interactions with residues such as R501, W428, S476 and stabilised the ligand binding at thumb site and inhibition of the HCV RdRP activity and viral replication.

Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

Graphical Abstract

HCV non structural protein NS5B RNA-dependent RNA polymerase (RdRP) mediates the catalytic role of viral RNA replication.

Lack of host RNA dependent RNA polymerase enzyme had made it an attractive and hotly pursued target for drug discovery efforts.

In this study, we developed a five feature pharmacophore (3D QSAR) model for thumb site inhibitors of HCV RdRP, which estimated the experimental activity with a strong correlation of 0.971 & 0.944 for training and test sets respectively.

Our database search and molecular docking results suggested the compounds 1, 2 with best fitness to the pharmacophore model were predicted to interact with key residues involved in thumbs site II and could inhibit the HCV RdRP activity. Further, the compounds 1, 2 potently inhibited HCV 1b viral replication in sub-micro-molar range.

Supplementary Information

Supplementary Figure 1: Structural coordinates of HCV NS5B polymerase showing the different binding domain at NS5B polymerase. Highlighted are the different ligand(s) binding regions namely Thumb site I, Thumb site II (green) and palm domain (blue) and finger domain (magenta). Thumb site I bears the nucleoside inhibitors which prevent the terminal release of nucleotides during transcription. Thumb site II region ligands that are non-nucleoside and can allosterically inhibit the polymerase activity. The palm domain as well two or more sites where ligands bind and inhibit the RdRP activity

Supplementary Figure 2. Residues at thumb site II of NS5B that was shown to interact significantly with inhibitors.

Supplementary Figure 3: Comparison of cost parameters between the best model and random model 1 to 13. A) None of the 13 random models have a higher correlation than the best model. B) None of the 13 random models have a lower total cost than the best model.

Supplementary Figure 4: Pharmacophore mapping of less active molecules from InterBioscreen Library. A) Ligand mapping of (Stock1N-54530) to the best pharmacophore model shows lack of fitness to aliphatic hydrophobic and negative ionisable features in addition to ring aromatic features had reduced its estimated activity (0.37 μM). B) Mapping of ligand (Stock1N-62776) reveals that lack of fitness to acceptor, negative ionisable, aliphatic hydrophobic and ring aromatic features had drastically affected its estimated activity (16 μM).

[illegible]

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3	4	2	0		
2	3	1	0		
1	2	2	0		
1	6	1	0		
4	7	1	0		
7	8	1	0		
8	9	1	0		
13	14	2	0		
12	13	1	0		
11	12	2	0		
10	11	1	0		
14	9	1	0		
9	10	2	0		
12	15	1	0		
8	16	2	0		
8	17	2	0		
5	18	1	0		
18	19	2	0		
18	20	1	0		
1	21	1	0		
21	22	1	0		
26	27	2	0		
25	26	1	0		
24	25	2	0		

```

23 24 1 0
27 22 1 0
22 23 2 0
26 28 1 0
 2 29 1 0
 3 30 1 0
 6 31 1 0
 7 32 1 0
10 33 1 0
11 34 1 0
13 35 1 0
14 36 1 0
15 37 1 0
15 38 1 0
15 39 1 0
20 40 1 0
23 41 1 0
24 42 1 0
25 43 1 0
27 44 1 0
28 45 1 0
28 46 1 0
28 47 1 0

```

M END

> <Name>

Compound4

> <Activ>

0.47

> <DB_Ref_id>

1.04

\$\$\$\$

Compound5

SciTegic10081411483D

```

47 49 0 0 0 0          999 V2000
-2.2540    0.6430    1.7290 C    0  0
-2.1490   -0.0160    0.4940 C    0  0
-0.9770    0.0960   -0.2690 C    0  0
 0.1030    0.8710    0.1990 C    0  0
 0.0000    1.5350    1.4430 C    0  0
-1.1800    1.4160    2.2010 C    0  0
 1.2380    0.9630   -0.5680 N    0  0
 1.4590   -0.0510   -1.8140 S    0  0
 3.0620    0.0390   -2.4450 C    0  0
 3.2660    0.1050   -3.8340 C    0  0
 4.5700    0.1780   -4.3480 C    0  0
 5.6720    0.1840   -3.4730 C    0  0
 5.4670    0.1170   -2.0840 C    0  0
 4.1600    0.0450   -1.5680 C    0  0
 7.0550    0.2600   -4.0180 C    0  0
 1.2340   -1.4000   -1.3240 O    0  0
 0.5330    0.3400   -2.8630 O    0  0
 1.1230    2.3690    1.9820 C    0  0
 0.9060    3.4390    2.5000 O    0  0
 2.3360    1.8440    1.8440 O    0  0
-3.3580    0.5370    2.4430 O    0  0
-3.9850   -0.6230    2.4430 C    0  0
-3.2420   -1.8180    2.4430 C    0  0

```

-3.9010	-3.0590	2.4430	C	0	0
-5.3030	-3.1110	2.4430	C	0	0
-6.0490	-1.9200	2.4430	C	0	0
-5.3930	-0.6760	2.4430	C	0	0
-6.1920	0.5780	2.4430	C	0	0
-2.9730	-0.6110	0.1270	H	0	0
-0.9180	-0.4200	-1.2190	H	0	0
-1.2680	1.9220	3.1520	H	0	0
1.9300	1.6540	-0.3590	H	0	0
2.4200	0.1000	-4.5060	H	0	0
4.7230	0.2280	-5.4160	H	0	0
6.3090	0.1210	-1.4060	H	0	0
4.0020	-0.0060	-0.5020	H	0	0
7.7680	0.3010	-3.1930	H	0	0
7.2290	-0.5820	-4.6860	H	0	0
7.1640	1.1760	-4.6000	H	0	0
3.1030	2.3320	2.1720	H	0	0
-2.1620	-1.7830	2.4430	H	0	0
-3.3260	-3.9750	2.4430	H	0	0
-5.8110	-4.0650	2.4430	H	0	0
-7.1290	-1.9650	2.4430	H	0	0
-5.5960	1.4900	2.4430	H	0	0
-6.8340	0.6000	3.3240	H	0	0
-6.8340	0.6000	1.5630	H	0	0
5	6	2	0		
4	5	1	0		
3	4	2	0		
2	3	1	0		
1	2	2	0		
1	6	1	0		
4	7	1	0		
7	8	1	0		
8	9	1	0		
13	14	2	0		
12	13	1	0		
11	12	2	0		
10	11	1	0		
14	9	1	0		
9	10	2	0		
12	15	1	0		
8	16	2	0		
8	17	2	0		
5	18	1	0		
18	19	2	0		
18	20	1	0		
1	21	1	0		
21	22	1	0		
26	27	2	0		
25	26	1	0		
24	25	2	0		
23	24	1	0		
27	22	1	0		
22	23	2	0		
27	28	1	0		
2	29	1	0		
3	30	1	0		
6	31	1	0		
7	32	1	0		
10	33	1	0		
11	34	1	0		
13	35	1	0		

```

14 36 1 0
15 37 1 0
15 38 1 0
15 39 1 0
20 40 1 0
23 41 1 0
24 42 1 0
25 43 1 0
26 44 1 0
28 45 1 0
28 46 1 0
28 47 1 0

```

M END

> <Name>

Compound5

> <Activ>

0.53

> <DB_Ref_id>

1.05

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Compound6

SciTegic10081411483D

```

51 53 0 0 0 0          999 V2000
  1.5470  1.6640  1.7660 C  0  0
  0.4260  1.6740  0.9220 C  0  0
 -0.4710  0.5940  0.9200 C  0  0
 -0.2520 -0.5120  1.7680 C  0  0
  0.8770 -0.5250  2.6190 C  0  0
  1.7700  0.5650  2.6130 C  0  0
 -1.1450 -1.5530  1.7460 N  0  0
 -2.2310 -1.6660  0.5490 S  0  0
 -3.0370 -3.1890  0.5490 C  0  0
 -4.4420 -3.2380  0.5490 C  0  0
 -5.1000 -4.4800  0.5490 C  0  0
 -4.3540 -5.6740  0.5490 C  0  0
 -2.9470 -5.6210  0.5490 C  0  0
 -2.2890 -4.3790  0.5490 C  0  0
 -5.0490 -6.9860  0.5490 C  0  0
 -3.2210 -0.6230  0.7580 O  0  0
 -1.5120 -1.5290 -0.7070 O  0  0
  1.1520 -1.6760  3.5370 C  0  0
  1.5200 -1.4920  4.6740 O  0  0
  0.9650 -2.8810  3.0080 O  0  0
  2.3870  2.6800  1.7640 O  0  0
  2.6450  3.2660  0.6130 C  0  0
  2.8260  4.6580  0.5570 C  0  0
  3.1020  5.2870 -0.6700 C  0  0
  3.1970  4.5220 -1.8480 C  0  0
  3.0160  3.1270 -1.7930 C  0  0
  2.7400  2.5020 -0.5620 C  0  0
  3.4670  5.1310 -3.0450 N  0  0
  2.8140  4.7310 -4.1760 C  0  0
  3.1330  5.4220 -5.4750 C  0  0
  2.0020  3.8380 -4.1290 O  0  0
  0.2500  2.5180  0.2700 H  0  0
 -1.3280  0.6250  0.2620 H  0  0
  2.6350  0.5610  3.2600 H  0  0

```

-1.1250	-2.2440	2.4690	H	0	0
-5.0160	-2.3240	0.5490	H	0	0
-6.1800	-4.5140	0.5490	H	0	0
-2.3670	-6.5330	0.5490	H	0	0
-1.2090	-4.3420	0.5490	H	0	0
-4.3810	-7.8480	0.5490	H	0	0
-5.6880	-7.0610	-0.3320	H	0	0
-5.6880	-7.0610	1.4300	H	0	0
1.1250	-3.6660	3.5470	H	0	0
2.7540	5.2500	1.4570	H	0	0
3.2380	6.3600	-0.6930	H	0	0
3.0840	2.5220	-2.6860	H	0	0
2.6020	1.4320	-0.5250	H	0	0
4.1390	5.8710	-3.0880	H	0	0
4.1970	5.3300	-5.6930	H	0	0
2.5230	5.0040	-6.2750	H	0	0
2.8980	6.4850	-5.3970	H	0	0
5	6	2	0		
4	5	1	0		
3	4	2	0		
2	3	1	0		
1	2	2	0		
1	6	1	0		
4	7	1	0		
7	8	1	0		
8	9	1	0		
13	14	2	0		
12	13	1	0		
11	12	2	0		
10	11	1	0		
14	9	1	0		
9	10	2	0		
12	15	1	0		
8	16	2	0		
8	17	2	0		
5	18	1	0		
18	19	2	0		
18	20	1	0		
1	21	1	0		
21	22	1	0		
26	27	2	0		
25	26	1	0		
24	25	2	0		
23	24	1	0		
27	22	1	0		
22	23	2	0		
25	28	1	0		
28	29	1	0		
29	30	1	0		
29	31	2	0		
2	32	1	0		
3	33	1	0		
6	34	1	0		
7	35	1	0		
10	36	1	0		
11	37	1	0		
13	38	1	0		
14	39	1	0		
15	40	1	0		
15	41	1	0		
15	42	1	0		

```

20 43 1 0
23 44 1 0
24 45 1 0
26 46 1 0
27 47 1 0
28 48 1 0
30 49 1 0
30 50 1 0
30 51 1 0

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M END

> <Name>

Compound6

> <Activ>

0.29

> <DB_Ref_id>

1.06

\$\$\$\$

Compound7

SciTegic10081411483D

```

47 49 0 0 0 0          999 V2000
-1.9080  1.2910 -1.7070 C  0  0
-1.2970  1.5600 -0.4700 C  0  0
-0.7300  0.5180  0.2800 C  0  0
-0.7710 -0.8050 -0.2010 C  0  0
-1.3870 -1.0800 -1.4450 C  0  0
-1.9510 -0.0270 -2.1890 C  0  0
-0.2090 -1.8050  0.5550 N  0  0
 0.7520 -1.4320  1.8050 S  0  0
 1.5700 -2.8170  2.4260 C  0  0
 1.6230 -3.0370  3.8130 C  0  0
 2.2910 -4.1640  4.3210 C  0  0
 2.9060 -5.0720  3.4400 C  0  0
 2.8520 -4.8520  2.0510 C  0  0
 2.1840 -3.7230  1.5450 C  0  0
 3.6110 -6.2680  3.9750 C  0  0
 1.7460 -0.4880  1.3260 O  0  0
-0.0920 -0.8910  2.8580 O  0  0
-1.4550 -2.4710 -1.9960 C  0  0
-2.4670 -2.8890 -2.5080 O  0  0
-0.3380 -3.1840 -1.8750 O  0  0
-2.4390  2.2710 -2.4100 O  0  0
-1.8240  3.4370 -2.4100 C  0  0
-2.5680  4.6310 -2.4100 C  0  0
-1.9100  5.8750 -2.4100 C  0  0
-0.5060  5.9240 -2.4100 C  0  0
 0.2400  4.7320 -2.4100 C  0  0
-0.4180  3.4920 -2.4100 C  0  0
-2.7030  7.1410 -2.4100 C  0  0
-1.9860  8.2600 -2.4100 O  0  0
-3.9120  7.1150 -2.4100 O  0  0
-1.2620  2.5740 -0.0950 H  0  0
-0.2660  0.7520  1.2270 H  0  0
-2.4240 -0.2290 -3.1400 H  0  0
-0.3930 -2.7620  0.3320 H  0  0
 1.1500 -2.3400  4.4910 H  0  0
 2.3280 -4.3300  5.3870 H  0  0
 3.3220 -5.5450  1.3690 H  0  0

```


2.1430	-3.5530	0.4790	H	0	0
3.3130	-6.4320	5.0100	H	0	0
3.4100	-7.1250	3.3340	H	0	0
4.6880	-6.0880	3.9630	H	0	0
-0.3160	-4.0880	-2.2110	H	0	0
-3.6460	4.5860	-2.4100	H	0	0
0.0080	6.8750	-2.4100	H	0	0
1.3200	4.7710	-2.4100	H	0	0
0.1580	2.5780	-2.4100	H	0	0
-2.4390	9.1110	-2.4100	H	0	0
5	6	2		0	
4	5	1		0	
3	4	2		0	
2	3	1		0	
1	2	2		0	
1	6	1		0	
4	7	1		0	
7	8	1		0	
8	9	1		0	
13	14	2		0	
12	13	1		0	
11	12	2		0	
10	11	1		0	
14	9	1		0	
9	10	2		0	
12	15	1		0	
8	16	2		0	
8	17	2		0	
5	18	1		0	
18	19	2		0	
18	20	1		0	
1	21	1		0	
21	22	1		0	
26	27	2		0	
25	26	1		0	
24	25	2		0	
23	24	1		0	
27	22	1		0	
22	23	2		0	
24	28	1		0	
28	29	1		0	
28	30	2		0	
2	31	1		0	
3	32	1		0	
6	33	1		0	
7	34	1		0	
10	35	1		0	
11	36	1		0	
13	37	1		0	
14	38	1		0	
15	39	1		0	
15	40	1		0	
15	41	1		0	
20	42	1		0	
23	43	1		0	
25	44	1		0	
26	45	1		0	
27	46	1		0	
29	47	1		0	

M END

> <Name>

Compound7

> <Activ>

0.33

> <DB_Ref_id>

1.07

\$\$\$\$

Compound8

SciTegic10081411483D

47	49	0	0	0	0	999	V2000
-1.7910		1.5040		-1.7340	C	0	0
-1.1910		1.7870		-0.4960	C	0	0
-0.6270		0.7560		0.2700	C	0	0
-0.6600	-0.5740			-0.1970	C	0	0
-1.2640	-0.8630			-1.4430	C	0	0
-1.8260	0.1800			-2.2030	C	0	0
-0.1000	-1.5620			0.5720	N	0	0
0.8590	-1.1740			1.8180	S	0	0
1.6860	-2.5490			2.4510	C	0	0
1.1250	-3.2750			3.5180	C	0	0
1.7990	-4.3970			4.0330	C	0	0
3.0330	-4.7890			3.4830	C	0	0
3.5920	-4.0630			2.4180	C	0	0
2.9180	-2.9410			1.9000	C	0	0
3.7460	-5.9750			4.0290	C	0	0
1.8500	-0.2300			1.3300	O	0	0
0.0140	-0.6270			2.8650	O	0	0
-1.3220	-2.2600			-1.9800	C	0	0
-2.3260	-2.6840			-2.5060	O	0	0
-0.2070	-2.9710			-1.8360	O	0	0
-2.3200	2.4750			-2.4510	O	0	0
-1.7130	3.6450			-2.4510	C	0	0
-0.3090	3.7010			-2.4510	C	0	0
0.3500	4.9430			-2.4510	C	0	0
-0.3950	6.1330			-2.4510	C	0	0
-1.7990	6.0820			-2.4510	C	0	0
-2.4590	4.8400			-2.4510	C	0	0
-3.9450	4.7970			-2.4510	C	0	0
-4.3870	4.1950			-3.6020	F	0	0
-4.4400	6.0740			-2.3850	F	0	0
-4.3830	4.0820			-1.3650	F	0	0
-1.1620	2.8050			-0.1310	H	0	0
-0.1700	1.0000			1.2190	H	0	0
-2.2890	-0.0330			-3.1560	H	0	0
-0.2850	-2.5230			0.3630	H	0	0
0.1780	-2.9730			3.9400	H	0	0
1.3650	-4.9490			4.8520	H	0	0
4.5390	-4.3590			1.9900	H	0	0
3.3480	-2.3830			1.0820	H	0	0
4.6310	-6.1760			3.4240	H	0	0
3.9820	-5.8050			5.0800	H	0	0
3.0960	-6.8480			3.9710	H	0	0
-0.1800	-3.8790			-2.1600	H	0	0
0.2690	2.7890			-2.4510	H	0	0
1.4300	4.9830			-2.4510	H	0	0
0.1090	7.0880			-2.4510	H	0	0
-2.3670	7.0020			-2.4510	H	0	0
2	3	2	0				

1	2	1	0
1	6	2	0
4	7	1	0
7	8	1	0
8	9	1	0
13	14	2	0
12	13	1	0
11	12	2	0
10	11	1	0
14	9	1	0
9	10	2	0
12	15	1	0
8	16	2	0
8	17	2	0
5	18	1	0
18	19	2	0
18	20	1	0
1	21	1	0
21	22	1	0
26	27	2	0
25	26	1	0
24	25	2	0
23	24	1	0
27	22	1	0
22	23	2	0
27	28	1	0
5	6	1	0
4	5	2	0
3	4	1	0
28	31	1	0
28	30	1	0
28	29	1	0
2	32	1	0
3	33	1	0
6	34	1	0
7	35	1	0
10	36	1	0
11	37	1	0
13	38	1	0
14	39	1	0
15	40	1	0
15	41	1	0
15	42	1	0
20	43	1	0
23	44	1	0
24	45	1	0
25	46	1	0
26	47	1	0

M END

> <Name>

Compound8

> <Activ>

0.27

> <DB_Ref_id>

1.09

\$\$\$\$

Compound9

SciTegic10081411483D

48	50	0	0	0	0	999	V2000
-1.6350	1.4800	1.5190	C	0	0		
-1.6720	0.1600	1.9980	C	0	0		
-1.1070	-0.8810	1.2440	C	0	0		
-0.4980	-0.6090	0.0020	C	0	0		
-0.4590	0.7190	-0.4810	C	0	0		
-1.0270	1.7560	0.2810	C	0	0		
0.0450	-1.6490	-0.7130	N	0	0		
0.2930	-3.0800	0.0020	S	0	0		
1.2720	-4.1230	-0.9630	C	0	0		
0.6660	-5.0700	-1.8070	C	0	0		
1.4630	-5.9200	-2.5920	C	0	0		
2.8650	-5.8220	-2.5350	C	0	0		
3.4690	-4.8730	-1.6900	C	0	0		
2.6720	-4.0240	-0.9040	C	0	0		
3.7090	-6.7210	-3.3670	C	0	0		
0.9880	-2.8300	1.2520	O	0	0		
-1.0040	-3.7090	0.1840	O	0	0		
0.1780	1.0570	-1.7950	C	0	0		
-0.3500	1.8280	-2.5630	O	0	0		
1.3360	0.4490	-2.0350	O	0	0		
-2.1640	2.4570	2.2280	O	0	0		
-1.5530	3.6250	2.2280	C	0	0		
-0.1480	3.6800	2.2280	C	0	0		
0.5100	4.9200	2.2280	C	0	0		
-0.2360	6.1090	2.2280	C	0	0		
-1.6410	6.0590	2.2280	C	0	0		
-2.3010	4.8180	2.2280	C	0	0		
-3.6190	4.7770	2.2280	O	0	0		
-4.3180	5.8540	1.6230	C	0	0		
-5.5920	5.4510	1.3070	F	0	0		
-3.6660	6.2400	0.4820	F	0	0		
-4.3770	6.9080	2.4980	F	0	0		
-2.1370	-0.0550	2.9470	H	0	0		
-1.1500	-1.8890	1.6330	H	0	0		
-1.0020	2.7730	-0.0820	H	0	0		
0.2870	-1.5200	-1.6740	H	0	0		
-0.4100	-5.1470	-1.8520	H	0	0		
0.9940	-6.6470	-3.2400	H	0	0		
4.5450	-4.7930	-1.6410	H	0	0		
3.1370	-3.2950	-0.2560	H	0	0		
3.0720	-7.2930	-4.0430	H	0	0		
4.4590	-6.1310	-3.8930	H	0	0		
4.2310	-7.4280	-2.7230	H	0	0		
1.7990	0.6250	-2.8650	H	0	0		
0.4280	2.7660	2.2280	H	0	0		
1.5900	4.9590	2.2280	H	0	0		
0.2700	7.0640	2.2280	H	0	0		
-2.2110	6.9750	2.2280	H	0	0		
2	3	2	0				
1	2	1	0				
1	6	2	0				
4	7	1	0				
7	8	1	0				
8	9	1	0				
13	14	2	0				
12	13	1	0				
11	12	2	0				
10	11	1	0				
14	9	1	0				

```

  9 10  2  0
12 15  1  0
  8 16  2  0
  8 17  2  0
  5 18  1  0
18 19  2  0
18 20  1  0
  1 21  1  0
21 22  1  0
26 27  2  0
25 26  1  0
24 25  2  0
23 24  1  0
27 22  1  0
22 23  2  0
27 28  1  0
29 28  1  0
  5  6  1  0
  4  5  2  0
  3  4  1  0
29 32  1  0
29 31  1  0
29 30  1  0
  2 33  1  0
  3 34  1  0
  6 35  1  0
  7 36  1  0
10 37  1  0
11 38  1  0
13 39  1  0
14 40  1  0
15 41  1  0
15 42  1  0
15 43  1  0
20 44  1  0
23 45  1  0
24 46  1  0
25 47  1  0
26 48  1  0
M  END
> <Name>
Compound9

> <Activ>
0.37

> <DB_Ref_id>
1.1

$$$$
Compound10
  SciTegic10081411483D

47 49  0  0  0  0          999 V2000
  -2.2560   -0.0720    1.6870 C   0  0
  -1.6700   -0.9650    0.7750 C   0  0
  -0.5860   -0.5550   -0.0200 C   0  0
  -0.0800    0.7560    0.0940 C   0  0
  -0.6680    1.6560    1.0110 C   0  0
  -1.7540    1.2360    1.8030 C   0  0
    0.9800    1.1290   -0.6960 N   0  0

```

1.8380	0.0040	-1.4850	S	0	0
3.2850	0.6520	-2.1620	C	0	0
3.6450	0.3340	-3.4830	C	0	0
4.8240	0.8610	-4.0350	C	0	0
5.6450	1.7090	-3.2680	C	0	0
5.2810	2.0250	-1.9460	C	0	0
4.1040	1.4980	-1.3930	C	0	0
6.8910	2.2680	-3.8520	C	0	0
2.2050	-1.0200	-0.5220	O	0	0
1.0120	-0.4980	-2.5670	O	0	0
-0.1640	3.0590	1.1660	C	0	0
-0.9320	3.9880	1.2710	O	0	0
1.1600	3.1880	1.1760	O	0	0
-3.2720	-0.4590	2.4310	O	0	0
-4.0220	-1.5860	2.0020	C	0	0
-5.4490	-1.5250	2.5250	C	0	0
-5.9060	-2.9550	2.2630	C	0	0
-4.6990	-3.8110	2.6480	C	0	0
-3.4940	-2.8690	2.6370	C	0	0
-2.0530	-1.9710	0.6830	H	0	0
-0.1520	-1.2600	-0.7150	H	0	0
-2.2090	1.9180	2.5060	H	0	0
1.2210	2.0960	-0.7850	H	0	0
3.0160	-0.3160	-4.0750	H	0	0
5.0960	0.6130	-5.0510	H	0	0
5.9060	2.6760	-1.3500	H	0	0
3.8260	1.7420	-0.3770	H	0	0
7.3220	2.9920	-3.1620	H	0	0
7.5760	1.4550	-4.0920	H	0	0
6.6560	2.7890	-4.7820	H	0	0
1.5490	4.0660	1.2710	H	0	0
-3.9960	-1.6370	0.9220	H	0	0
-6.0530	-0.7950	2.0060	H	0	0
-5.4710	-1.2970	3.5820	H	0	0
-6.7930	-3.2130	2.8240	H	0	0
-6.1330	-3.0820	1.2130	H	0	0
-4.8280	-4.2400	3.6310	H	0	0
-4.5740	-4.6290	1.9530	H	0	0
-3.1660	-2.6780	3.6480	H	0	0
-2.6560	-3.2770	2.0900	H	0	0
5	6	2	0		
4	5	1	0		
3	4	2	0		
2	3	1	0		
1	2	2	0		
1	6	1	0		
4	7	1	0		
7	8	1	0		
8	9	1	0		
13	14	2	0		
12	13	1	0		
11	12	2	0		
10	11	1	0		
14	9	1	0		
9	10	2	0		
12	15	1	0		
8	16	2	0		
8	17	2	0		
5	18	1	0		
18	19	2	0		
18	20	1	0		

```

1 21 1 0
21 22 1 0
25 26 1 0
24 25 1 0
23 24 1 0
23 22 1 0
26 22 1 0
2 27 1 0
3 28 1 0
6 29 1 0
7 30 1 0
10 31 1 0
11 32 1 0
13 33 1 0
14 34 1 0
15 35 1 0
15 36 1 0
15 37 1 0
20 38 1 0
22 39 1 0
23 40 1 0
23 41 1 0
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25 45 1 0
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26 47 1 0
M END
> <Name>
Compound10

> <Activ>
0.21

> <DB_Ref_id>
1.11

$$$$
Compound11
SciTegic10081411483D

38 40 0 0 0 0 999 V2000
0.1350 -1.7810 1.6170 C 0 0
0.6870 -1.5040 0.3570 C 0 0
0.6910 -0.1840 -0.1270 C 0 0
0.1440 0.8610 0.6420 C 0 0
-0.4120 0.5760 1.9120 C 0 0
-0.4140 -0.7460 2.3910 C 0 0
0.1640 2.1390 0.1410 N 0 0
0.5470 2.3930 -1.4120 S 0 0
0.2850 4.0160 -1.8810 C 0 0
1.9610 2.0960 -1.5670 O 0 0
-0.3090 1.5410 -2.2190 O 0 0
-1.0080 1.6540 2.7680 C 0 0
-1.6040 2.5820 2.2710 O 0 0
-0.8260 1.5020 4.0760 O 0 0
-0.5490 4.5660 -3.2560 S 0 0
-0.2750 6.1930 -2.8500 C 0 0
0.4570 6.3280 -1.6580 C 0 0
0.7790 5.0740 -1.1000 C 0 0

```

-0.9240	7.5800	-3.9440	Br	0	0
1.2010	-2.4770	-0.3690	O	0	0
0.5860	-3.6410	-0.3690	C	0	0
-0.8200	-3.6950	-0.3690	C	0	0
-1.4790	-4.9380	-0.3690	C	0	0
-0.7320	-6.1290	-0.3690	C	0	0
0.6720	-6.0760	-0.3690	C	0	0
1.3280	-4.8340	-0.3690	C	0	0
0.1290	-2.7950	1.9940	H	0	0
1.1230	0.0140	-1.1000	H	0	0
-0.8360	-0.9770	3.3590	H	0	0
-0.0590	2.9120	0.7340	H	0	0
-1.1840	2.1620	4.6820	H	0	0
0.7400	7.2740	-1.2170	H	0	0
1.3400	4.9450	-0.1840	H	0	0
-1.3970	-2.7830	-0.3690	H	0	0
-2.5590	-4.9770	-0.3690	H	0	0
-1.2380	-7.0820	-0.3690	H	0	0
1.2460	-6.9920	-0.3690	H	0	0
2.4080	-4.7990	-0.3690	H	0	0
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4	5	1	0		
3	4	2	0		
2	3	1	0		
1	2	2	0		
1	6	1	0		
4	7	1	0		
7	8	1	0		
8	9	1	0		
8	10	2	0		
8	11	2	0		
5	12	1	0		
12	13	2	0		
12	14	1	0		
17	18	1	0		
16	17	2	0		
15	16	1	0		
15	9	1	0		
18	9	2	0		
16	19	1	0		
2	20	1	0		
20	21	1	0		
25	26	2	0		
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23	24	2	0		
22	23	1	0		
26	21	1	0		
21	22	2	0		
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7	30	1	0		
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17	32	1	0		
18	33	1	0		
22	34	1	0		
23	35	1	0		
24	36	1	0		
25	37	1	0		
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M END

> <Name>
Compound11

> <Activ>
0.61

> <DB_Ref_id>
1.12

\$\$\$\$
Compound12
SciTegic10081411483D

41	43	0	0	0	0	999	V2000
-0.6040	-2.5390	1.7970	C	0	0		
-0.5550	-1.2250	1.3060	C	0	0		
0.0700	-0.9630	0.0760	C	0	0		
0.6460	-2.0120	-0.6700	C	0	0		
0.5940	-3.3340	-0.1720	C	0	0		
-0.0330	-3.5900	1.0620	C	0	0		
1.2500	-1.7230	-1.8690	N	0	0		
0.8630	-0.3630	-2.6620	S	0	0		
-0.8240	-0.0920	-2.6860	C	0	0		
1.4940	0.7440	-1.9650	O	0	0		
1.3220	-0.5120	-4.0320	O	0	0		
1.1910	-4.4810	-0.9280	C	0	0		
1.2580	-4.4630	-2.1350	O	0	0		
1.6310	-5.4880	-0.1780	O	0	0		
-2.0370	-1.2070	-3.0960	S	0	0		
-3.2680	-0.0670	-2.8320	C	0	0		
-2.7600	1.1780	-2.4280	C	0	0		
-1.3500	1.1640	-2.3440	C	0	0		
-5.0740	-0.5240	-3.0820	Br	0	0		
-1.0920	-0.2400	2.0000	O	0	0		
-0.4750	0.9240	2.0000	C	0	0		
-1.2170	2.1170	2.0000	C	0	0		
-0.5610	3.3610	2.0000	C	0	0		
0.8440	3.4120	2.0000	C	0	0		
1.5900	2.2210	2.0000	C	0	0		
0.9320	0.9800	2.0000	C	0	0		
1.5410	4.7250	2.0000	C	0	0		
-1.0840	-2.7460	2.7440	H	0	0		
0.1020	0.0550	-0.2890	H	0	0		
-0.0780	-4.5980	1.4510	H	0	0		
1.9260	-2.3500	-2.2540	H	0	0		
2.0270	-6.2580	-0.6040	H	0	0		
-3.3650	2.0470	-2.2050	H	0	0		
-0.7520	2.0180	-2.0510	H	0	0		
-2.2970	2.0820	2.0000	H	0	0		
-1.1390	4.2730	2.0000	H	0	0		
2.6700	2.2540	2.0000	H	0	0		
1.5080	0.0660	2.0000	H	0	0		
2.6190	4.5660	2.0170	H	0	0		
1.2150	5.3090	1.1360	H	0	0		
1.2700	5.2790	2.8980	H	0	0		
5	6	2	0				
4	5	1	0				
3	4	2	0				
2	3	1	0				
1	2	2	0				
1	6	1	0				

```

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7  8  1  0
8  9  1  0
8 10  2  0
8 11  2  0
5 12  1  0
12 13  2  0
12 14  1  0
17 18  1  0
16 17  2  0
15 16  1  0
15  9  1  0
18  9  2  0
16 19  1  0
 2 20  1  0
20 21  1  0
25 26  2  0
24 25  1  0
23 24  2  0
22 23  1  0
26 21  1  0
21 22  2  0
24 27  1  0
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 3 29  1  0
 6 30  1  0
 7 31  1  0
14 32  1  0
17 33  1  0
18 34  1  0
22 35  1  0
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M  END
> <Name>
Compound12

> <Activ>
1.9

> <DB_Ref_id>
1.13

$$$$
Compound13
SciTegic10081411483D

41 43  0  0  0  0          999 V2000
  0.6270  0.2950  1.9360 C  0  0
  0.7150  0.9730  0.7090 C  0  0
 -0.3980  1.6840  0.2250 C  0  0
 -1.5990  1.7190  0.9630 C  0  0
 -1.6810  1.0350  2.1970 C  0  0
 -0.5640  0.3240  2.6780 C  0  0
 -2.6660  2.4220  0.4630 N  0  0
 -2.7400  2.7660 -1.1190 S  0  0
 -2.3440  1.4140 -2.0880 C  0  0

```

-4.1070	3.1560	-1.4180	O	0	0
-1.7730	3.8170	-1.3850	O	0	0
-2.9350	1.0430	3.0180	C	0	0
-4.0170	1.1740	2.4960	O	0	0
-2.7580	0.9010	4.3280	O	0	0
-2.7650	-0.2090	-1.8090	S	0	0
-1.9690	-0.7260	-3.2170	C	0	0
-1.3730	0.3400	-3.9120	C	0	0
-1.5900	1.5720	-3.2620	C	0	0
-1.9470	-2.5450	-3.6970	Br	0	0
1.8340	0.9440	0.0140	O	0	0
2.5330	-0.1740	0.0140	C	0	0
1.8770	-1.4180	0.0140	C	0	0
2.6230	-2.6110	0.0140	C	0	0
4.0280	-2.5580	0.0140	C	0	0
4.6840	-1.3160	0.0140	C	0	0
3.9380	-0.1270	0.0140	C	0	0
1.9260	-3.9240	0.0140	C	0	0
1.4790	-0.2520	2.3130	H	0	0
-0.3160	2.2010	-0.7210	H	0	0
-0.6150	-0.2010	3.6190	H	0	0
-3.3980	2.7230	1.0740	H	0	0
-3.5270	0.8990	4.9120	H	0	0
-0.8160	0.2350	-4.8340	H	0	0
-1.2170	2.5220	-3.6250	H	0	0
0.7970	-1.4550	0.0140	H	0	0
4.6060	-3.4710	0.0140	H	0	0
5.7640	-1.2770	0.0140	H	0	0
4.4460	0.8260	0.0140	H	0	0
2.6640	-4.7260	-0.0040	H	0	0
1.2620	-3.9820	0.8770	H	0	0
1.3150	-4.0120	-0.8850	H	0	0
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4	5	1	0		
3	4	2	0		
2	3	1	0		
1	2	2	0		
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7	8	1	0		
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8	10	2	0		
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16	17	2	0		
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18	9	2	0		
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2	20	1	0		
20	21	1	0		
25	26	2	0		
24	25	1	0		
23	24	2	0		
22	23	1	0		
26	21	1	0		
21	22	2	0		
23	27	1	0		

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1 28 1 0
3 29 1 0
6 30 1 0
7 31 1 0
14 32 1 0
17 33 1 0
18 34 1 0
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M END

> <Name>

Compound13

> <Activ>

1.1

> <DB_Ref_id>

1.14

\$\$\$\$

Compound14

SciTegic10081411483D

```

45 47 0 0 0 0          999 V2000
-1.4020 -3.1350  2.2540 C  0  0
-1.4080 -1.8260  1.7480 C  0  0
-0.8480 -1.5640  0.4840 C  0  0
-0.2810 -2.6070 -0.2750 C  0  0
-0.2790 -3.9240  0.2400 C  0  0
-0.8400 -4.1800  1.5040 C  0  0
 0.2580 -2.3180 -1.5040 N  0  0
 0.1470 -0.8180 -2.1060 S  0  0
 0.7790 -0.7130 -3.6900 C  0  0
-1.2640 -0.4690 -2.1520 O  0  0
 0.9220  0.0570 -1.2440 O  0  0
 0.3130 -5.0660 -0.5310 C  0  0
 0.1780 -5.1410 -1.7310 O  0  0
 0.9750 -5.9590  0.1970 O  0  0
 2.4080 -0.8500 -4.1540 S  0  0
 2.0270 -0.6210 -5.7950 C  0  0
 0.6490 -0.4380 -5.9980 C  0  0
-0.0700 -0.4900 -4.7850 C  0  0
 3.3730 -0.6290 -7.1080 Br  0  0
-1.9350 -0.8460  2.4530 O  0  0
-1.3180  0.3180  2.4530 C  0  0
-2.0620  1.5120  2.4530 C  0  0
-1.4060  2.7560  2.4530 C  0  0
 0.0000  2.8090  2.4530 C  0  0
 0.7460  1.6150  2.4530 C  0  0
 0.0860  0.3730  2.4530 C  0  0
 0.6430  4.0200  2.4530 N  0  0
 0.1680  5.0430  1.6840 C  0  0
 0.8950  6.3610  1.7070 C  0  0
-0.8180  4.8890  1.0020 O  0  0
-1.8320 -3.3420  3.2250 H  0  0
-0.8590 -0.5510  0.1070 H  0  0

```

-0.8440	-5.1840	1.9060	H	0	0
0.7190	-3.0330	-2.0290	H	0	0
1.0630	-5.8200	1.1500	H	0	0
0.1880	-0.2750	-6.9650	H	0	0
-1.1430	-0.3730	-4.7130	H	0	0
-3.1410	1.4770	2.4530	H	0	0
-1.9960	3.6620	2.4530	H	0	0
1.8280	1.6350	2.4530	H	0	0
0.6620	-0.5390	2.4530	H	0	0
1.4570	4.1520	3.0160	H	0	0
0.4180	7.0590	1.0180	H	0	0
0.9200	6.7540	2.7230	H	0	0
1.9260	6.2210	1.3790	H	0	0
5	6	2	0		
4	5	1	0		
3	4	2	0		
2	3	1	0		
1	2	2	0		
1	6	1	0		
4	7	1	0		
7	8	1	0		
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8	11	2	0		
5	12	1	0		
12	13	2	0		
12	14	1	0		
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25	26	2	0		
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28	29	1	0		
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6	33	1	0		
7	34	1	0		
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17	36	1	0		
18	37	1	0		
22	38	1	0		
23	39	1	0		
25	40	1	0		
26	41	1	0		
27	42	1	0		
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M END

> <Name>
Compound14

> <Activ>
2.9

> <DB_Ref_id>
1.16

\$\$\$\$
Compound15
SciTegic10081411483D

41	43	0	0	0	0	999	V2000
-1.5960	1.7170	1.9900	C	0	0		
-0.4820	1.1330	1.3630	C	0	0		
-0.6250	0.5450	0.0940	C	0	0		
-1.8770	0.5370	-0.5530	C	0	0		
-2.9940	1.1250	0.0820	C	0	0		
-2.8460	1.7130	1.3510	C	0	0		
-1.9820	-0.0450	-1.7910	N	0	0		
-0.6480	-0.3440	-2.6620	S	0	0		
0.3890	1.0140	-2.7310	C	0	0		
0.0630	-1.4310	-2.0140	O	0	0		
-1.0740	-0.6620	-4.0140	O	0	0		
-4.3460	1.1410	-0.5650	C	0	0		
-5.0080	2.1530	-0.6000	O	0	0		
-4.7400	-0.0190	-1.0820	O	0	0		
-0.0550	2.6330	-2.9920	S	0	0		
1.5570	3.1600	-2.8890	C	0	0		
2.4470	2.1000	-2.6510	C	0	0		
1.7730	0.8640	-2.5610	C	0	0		
1.9900	4.9810	-3.0820	Br	0	0		
0.6910	1.1370	1.9630	O	0	0		
1.3910	0.0200	1.9630	C	0	0		
2.7950	0.0690	1.9630	C	0	0		
3.5430	-1.1230	1.9630	C	0	0		
2.8870	-2.3650	1.9630	C	0	0		
1.4800	-2.4180	1.9630	C	0	0		
0.7340	-1.2240	1.9630	C	0	0		
0.7810	-3.7360	1.9630	C	0	0		
1.5780	-4.8010	1.9880	O	0	0		
-0.4260	-3.8010	1.9390	O	0	0		
-1.4900	2.1700	2.9650	H	0	0		
0.2420	0.1000	-0.3750	H	0	0		
-3.6930	2.1660	1.8480	H	0	0		
-2.8810	-0.2870	-2.1540	H	0	0		
-5.6000	-0.0740	-1.5200	H	0	0		
3.5200	2.2110	-2.5490	H	0	0		
2.2680	-0.0840	-2.3810	H	0	0		
3.3050	1.0220	1.9630	H	0	0		
4.6210	-1.0820	1.9630	H	0	0		
3.4670	-3.2750	1.9630	H	0	0		
-0.3460	-1.2580	1.9630	H	0	0		
1.1880	-5.6830	1.9920	H	0	0		
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3	4	2	0				
2	3	1	0				
1	2	2	0				
1	6	1	0				

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8 9 1 0
8 10 2 0
8 11 2 0
5 12 1 0
12 13 2 0
12 14 1 0
17 18 1 0
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22 23 1 0
26 21 1 0
21 22 2 0
25 27 1 0
27 28 1 0
27 29 2 0
1 30 1 0
3 31 1 0
6 32 1 0
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Compound15

> <Activ>
1.4

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1.17

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Compound16
SciTegic10081411483D

41 43 0 0 0 0 999 V2000
-1.9100 -2.4300 -1.8160 C 0 0
-0.8460 -1.6330 -1.3630 C 0 0
-0.9490 -0.9650 -0.1310 C 0 0
-2.1130 -1.0920 0.6520 C 0 0
-3.1840 -1.8950 0.1920 C 0 0
-3.0740 -2.5610 -1.0430 C 0 0
-2.1840 -0.4260 1.8520 N 0 0
-1.1020 0.7270 2.2030 S 0 0
0.4510 0.0760 2.5100 C 0 0

```

-1.0100	1.6050	1.0510	O	0	0
-1.5590	1.4020	3.4040	O	0	0
-4.4420	-2.0590	0.9900	C	0	0
-4.9670	-3.1410	1.1060	O	0	0
-4.9120	-0.9430	1.5410	O	0	0
0.8380	-1.5450	2.8400	S	0	0
2.4920	-1.1880	2.9830	C	0	0
2.7620	0.1760	2.7790	C	0	0
1.5840	0.9040	2.5060	C	0	0
3.7380	-2.5410	3.3730	Br	0	0
0.2460	-1.5120	-2.0920	O	0	0
0.8630	-0.3460	-2.0920	C	0	0
0.1210	0.8480	-2.0920	C	0	0
0.7770	2.0900	-2.0920	C	0	0
2.1820	2.1430	-2.0920	C	0	0
2.9280	0.9490	-2.0920	C	0	0
2.2700	-0.2910	-2.0920	C	0	0
2.8810	3.4610	-2.0920	C	0	0
4.2110	3.3980	-2.0900	O	0	0
2.2560	4.4960	-2.0940	O	0	0
-1.8340	-2.9430	-2.7640	H	0	0
-0.1210	-0.3560	0.2050	H	0	0
-3.8850	-3.1760	-1.4040	H	0	0
-2.9020	-0.6540	2.5080	H	0	0
-5.7290	-0.9790	2.0570	H	0	0
3.7480	0.6210	2.8220	H	0	0
1.5620	1.9710	2.3180	H	0	0
-0.9590	0.8120	-2.0920	H	0	0
0.1950	3.0000	-2.0920	H	0	0
4.0080	0.9800	-2.0920	H	0	0
2.8460	-1.2050	-2.0920	H	0	0
4.7230	4.2190	-2.0880	H	0	0
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3	4	2	0		
2	3	1	0		
1	2	2	0		
1	6	1	0		
4	7	1	0		
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12	13	2	0		
12	14	1	0		
17	18	1	0		
16	17	2	0		
15	16	1	0		
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18	9	2	0		
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2	20	1	0		
20	21	1	0		
25	26	2	0		
24	25	1	0		
23	24	2	0		
22	23	1	0		
26	21	1	0		
21	22	2	0		
24	27	1	0		


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27 28 1 0
27 29 2 0
1 30 1 0
3 31 1 0
6 32 1 0
7 33 1 0
14 34 1 0
17 35 1 0
18 36 1 0
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28 41 1 0

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M END

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Compound16

> <Activ>

2.2

> <DB_Ref_id>

1.18

\$\$\$\$

Compound17

SciTegic10081411483D

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41 43 0 0 0 0          999 V2000
-1.5260 -0.3630 -0.7330 C 0 0
-0.4730 0.4260 -1.2230 C 0 0
0.7230 0.5410 -0.4960 C 0 0
0.8750 -0.1350 0.7300 C 0 0
-0.1840 -0.9320 1.2260 C 0 0
-1.3790 -1.0390 0.4900 C 0 0
2.0550 -0.0040 1.4200 N 0 0
3.3830 0.5270 0.6600 S 0 0
4.5210 0.2360 1.5140 O 0 0
3.4470 -0.1430 -0.6270 O 0 0
-0.0690 -1.6680 2.5270 C 0 0
1.0020 -2.0720 2.9200 O 0 0
-1.2110 -1.8340 3.1870 O 0 0
-3.2640 -1.6350 -1.4160 C 0 0
-2.6470 -0.4690 -1.4160 O 0 0
-4.6700 -1.6890 -1.4160 C 0 0
-5.3280 -2.9300 -1.4160 C 0 0
-4.5820 -4.1210 -1.4160 C 0 0
-3.1780 -4.0700 -1.4160 C 0 0
-2.5220 -2.8280 -1.4160 C 0 0
3.3320 2.2310 0.3830 C 0 0
2.3400 4.4040 0.8480 C 0 0
3.2340 5.0080 -0.0570 C 0 0
4.1800 4.2170 -0.7400 C 0 0
4.2280 2.8300 -0.5200 C 0 0
2.3910 3.0180 1.0680 C 0 0
3.1660 6.8670 -0.3540 Br 0 0
5.1210 2.0880 -1.1700 F 0 0
-0.5820 0.9470 -2.1620 H 0 0
1.5190 1.1540 -0.8950 H 0 0
-2.1920 -1.6460 0.8630 H 0 0
2.0960 -0.2380 2.3920 H 0 0

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-1.2030	-2.3030	4.0330	H	0	0
-5.2460	-0.7750	-1.4160	H	0	0
-6.4080	-2.9690	-1.4160	H	0	0
-5.0880	-5.0760	-1.4160	H	0	0
-2.6040	-4.9840	-1.4160	H	0	0
-1.4420	-2.7930	-1.4160	H	0	0
1.6090	4.9960	1.3830	H	0	0
4.8730	4.6680	-1.4360	H	0	0
1.7030	2.5570	1.7620	H	0	0

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4	5	1	0
3	4	2	0
2	3	1	0
1	2	2	0
1	6	1	0
4	7	1	0
7	8	1	0
8	9	2	0
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0.34

> <DB_Ref_id>
1.22

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Compound18

SciTegic10081411483D

49	51	0	0	0	0	999	V2000
0.8420	-0.9530	-1.6330	C	0	0		
0.8870	0.3620	-2.1230	C	0	0		
0.3180	1.4120	-1.3830	C	0	0		
-0.3010	1.1550	-0.1450	C	0	0		
-0.3480	-0.1700	0.3490	C	0	0		
0.2270	-1.2150	-0.3990	C	0	0		
-0.9940	-0.4940	1.6620	C	0	0		
-0.6150	-1.4280	2.3300	O	0	0		
-1.9920	0.3110	2.0150	O	0	0		
0.7600	-3.1010	-2.3280	C	0	0		
1.3770	-1.9350	-2.3280	O	0	0		
-0.6450	-3.1560	-2.3280	C	0	0		
-1.3050	-4.3960	-2.3280	C	0	0		
-0.5590	-5.5880	-2.3280	C	0	0		
0.8460	-5.5370	-2.3280	C	0	0		
1.5040	-4.2950	-2.3280	C	0	0		
-0.3320	2.5510	1.7710	C	0	0		
-0.8630	3.4120	2.4310	O	0	0		
0.8950	1.8520	2.2610	C	0	0		
2.0210	1.7560	1.4260	C	0	0		
3.1800	1.0980	1.8750	C	0	0		
3.2150	0.5330	3.1620	C	0	0		
2.0900	0.6310	4.0000	C	0	0		
0.9300	1.2870	3.5530	C	0	0		
4.7680	-0.3490	3.7630	Br	0	0		
-1.9880	2.9500	0.0110	C	0	0		
-1.5490	4.3250	-0.4920	C	0	0		
-2.7190	2.1370	-1.0570	C	0	0		
-0.8480	2.1990	0.5560	N	0	0		
-0.1290	1.3690	4.3570	F	0	0		
1.3610	0.5690	-3.0730	H	0	0		
0.3670	2.4160	-1.7840	H	0	0		
0.1930	-2.2300	-0.0260	H	0	0		
-2.4530	0.1560	2.8490	H	0	0		
-1.2230	-2.2420	-2.3280	H	0	0		
-2.3830	-4.4350	-2.3280	H	0	0		
-1.0650	-6.5430	-2.3280	H	0	0		
1.4200	-6.4510	-2.3280	H	0	0		
2.5840	-4.2600	-2.3280	H	0	0		
2.0040	2.1860	0.4330	H	0	0		
4.0350	1.0350	1.2170	H	0	0		
2.1040	0.2030	4.9940	H	0	0		
-2.6000	3.0450	0.9080	H	0	0		
-1.0290	4.8930	0.2790	H	0	0		
-2.4100	4.9100	-0.8150	H	0	0		
-0.8770	4.2270	-1.3440	H	0	0		
-2.9710	1.1450	-0.6820	H	0	0		
-3.6350	2.6430	-1.3670	H	0	0		
-2.0940	2.0080	-1.9400	H	0	0		
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4	5	1	0				
3	4	2	0				
2	3	1	0				
1	2	2	0				
1	6	1	0				

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7 9 1 0
1 11 1 0
11 10 1 0
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12 13 1 0
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Compound18

> <Activ>
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1.23

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Compound19
SciTegic10081411483D

58 60 0 0 0 0 999 V2000
-2.7080 1.1290 0.3100 C 0 0

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-2.4370	0.3260	-0.8090	C	0	0				
-1.1930	0.4100	-1.4560	C	0	0				
-0.2080	1.3010	-0.9870	C	0	0				
-0.4790	2.1120	0.1400	C	0	0				
-1.7290	2.0200	0.7810	C	0	0				
0.5370	3.0750	0.6760	C	0	0				
0.6840	3.2250	1.8660	O	0	0				
1.2390	3.7280	-0.2460	O	0	0				
-4.4930	-0.1160	0.9150	C	0	0				
-3.8760	1.0480	0.9150	O	0	0				
-5.8980	-0.1710	0.9150	C	0	0				
-6.5570	-1.4130	0.9150	C	0	0				
-5.8110	-2.6040	0.9150	C	0	0				
-4.4070	-2.5520	0.9150	C	0	0				
-3.7490	-1.3100	0.9150	C	0	0				
2.1440	0.9990	-0.9900	C	0	0				
3.2200	1.3770	-1.3920	O	0	0				
2.0370	0.1190	0.2310	C	0	0	1	0	0	0
1.5670	-1.2980	-0.1440	C	0	0				
1.4860	-2.2150	1.0860	C	0	0				
2.8180	-2.2640	1.8520	C	0	0	1	0	0	0
3.2860	-0.8490	2.2290	C	0	0				
3.3680	0.0730	1.0030	C	0	0				
2.7170	-3.1630	3.0860	C	0	0				
1.0730	1.8180	-3.0340	C	0	0				
1.8410	3.1360	-3.1400	C	0	0				
1.6470	0.7260	-3.9370	C	0	0				
0.9980	1.3630	-1.6380	N	0	0				
-3.1860	-0.3610	-1.1760	H	0	0				
-1.0080	-0.2190	-2.3160	H	0	0				
-1.9430	2.6360	1.6430	H	0	0				
2.1060	4.0870	-0.0130	H	0	0				
-6.4750	0.7420	0.9150	H	0	0				
-7.6360	-1.4510	0.9150	H	0	0				
-6.3170	-3.5580	0.9150	H	0	0				
-3.8330	-3.4670	0.9150	H	0	0				
-2.6700	-1.2740	0.9150	H	0	0				
1.2840	0.5600	0.8850	H	0	0				
0.5920	-1.2540	-0.6310	H	0	0				
2.2540	-1.7360	-0.8700	H	0	0				
1.1970	-3.2200	0.7750	H	0	0				
0.6960	-1.8580	1.7480	H	0	0				
3.5690	-2.6990	1.1900	H	0	0				
4.2590	-0.8950	2.7180	H	0	0				
2.5960	-0.4170	2.9560	H	0	0				
4.1640	-0.2790	0.3450	H	0	0				
3.6520	1.0770	1.3200	H	0	0				
3.6640	-3.2270	3.6210	H	0	0				
2.4260	-4.1750	2.8030	H	0	0				
1.9680	-2.7830	3.7800	H	0	0				
0.0140	1.9720	-3.2410	H	0	0				
1.4370	3.8970	-2.4730	H	0	0				
1.7970	3.5270	-4.1570	H	0	0				
2.8910	2.9920	-2.8840	H	0	0				
1.0820	-0.2000	-3.8280	H	0	0				
1.6210	1.0370	-4.9820	H	0	0				
2.6840	0.5170	-3.6770	H	0	0				
5	6	2	0						
4	5	1	0						
3	4	2	0						
2	3	1	0						

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5	7	1	0
7	8	2	0
7	9	1	0
1	11	1	0
11	10	1	0
15	16	2	0
14	15	1	0
13	14	2	0
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M END

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Compound19

> <Activ>

0.67

> <DB_Ref_id>

1.24

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Compound20

SciTegic10081411483D

61	63	0	0	0	0	999	V2000				
-2.6110		1.9140		0.9710	C	0	0				
-1.5960		2.3260		0.0940	C	0	0				
-1.0700		1.4320		-0.8530	C	0	0				
-1.5590		0.1130		-0.9320	C	0	0				
-2.5840		-0.3050		-0.0490	C	0	0				
-3.1040		0.6000		0.8970	C	0	0				
-3.1370		-1.6970		-0.0960	C	0	0				
-2.4300		-2.6390		-0.3730	O	0	0				
-4.4320		-1.8030		0.1880	O	0	0				
-2.2720		3.5980		2.4360	C	0	0				
-3.1040		2.7540		1.8580	O	0	0				
-0.9650		3.1910		2.7620	C	0	0				
-0.0780		4.0920		3.3790	C	0	0				
-0.4960		5.4000		3.6720	C	0	0				
-1.8010		5.8110		3.3460	C	0	0				
-2.6880		4.9100		2.7290	C	0	0				
-0.0490		-1.6270		-1.5190	C	0	0				
0.3830		-2.4080		-2.3360	O	0	0				
0.4750		-1.6130		-0.1050	C	0	0	1	0	0	0
1.0350		-2.9900		0.2990	C	0	0				
2.3540		-3.3180		-0.4240	C	0	0				
3.4120		-2.2230		-0.2230	C	0	0	1	0	0	0
2.8570		-0.8480		-0.6350	C	0	0				
1.5390		-0.5160		0.0860	C	0	0				
3.9260		-2.2030		1.2230	C	0	0				
-1.5100		-0.7010		-3.2540	C	0	0				
-0.3850		-0.3160		-4.2150	C	0	0				
-2.1880		-2.0180		-3.6350	C	0	0				
-1.0270		-0.7380		-1.8650	N	0	0				
5.1880		-1.3560		1.3910	C	0	0				
-1.2150		3.3360		0.1490	H	0	0				
-0.2870		1.7750		-1.5160	H	0	0				
-3.8870		0.2870		1.5720	H	0	0				
-4.9630		-1.0000		0.2720	H	0	0				
-0.6410		2.1860		2.5390	H	0	0				
0.9240		3.7750		3.6290	H	0	0				
0.1840		6.0920		4.1450	H	0	0				
-2.1230		6.8160		3.5700	H	0	0				
-3.6900		5.2290		2.4810	H	0	0				
-0.3670		-1.3850		0.5470	H	0	0				
1.2110		-3.0000		1.3750	H	0	0				
0.2990		-3.7740		0.1090	H	0	0				
2.1560		-3.4360		-1.4900	H	0	0				
2.7340		-4.2810		-0.0820	H	0	0				
4.2640		-2.4510		-0.8630	H	0	0				
2.6880		-0.8380		-1.7110	H	0	0				
3.5940		-0.0680		-0.4390	H	0	0				
1.7400		-0.3970		1.1520	H	0	0				
1.1600		0.4470		-0.2560	H	0	0				
3.1430		-1.8690		1.9040	H	0	0				
4.0920		-3.2190		1.5860	H	0	0				

-2.2420	0.1030	-3.1800	H	0	0
0.1520	0.5700	-3.8790	H	0	0
-0.7790	-0.1090	-5.2090	H	0	0
0.3380	-1.1290	-4.3070	H	0	0
-2.9380	-2.3150	-2.9020	H	0	0
-1.4550	-2.8200	-3.7070	H	0	0
-2.6840	-1.9300	-4.6020	H	0	0
5.5740	-1.4400	2.4060	H	0	0
5.9590	-1.6720	0.6900	H	0	0
4.9730	-0.3050	1.1990	H	0	0
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4	5	1		0	
3	4	2		0	
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5	7	1		0	
7	8	2		0	
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24	48	1		0	
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M END

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Compound20

> <Activ>

1.3

> <DB_Ref_id>

1.25

\$\$\$\$

Compound21

SciTegic10081411483D

```

58 60 0 0 0 0          999 V2000
-2.5390 1.2000 0.6980 C 0 0
-2.4440 0.5730 -0.5550 C 0 0
-1.2740 0.6970 -1.3210 C 0 0
-0.1860 1.4500 -0.8390 C 0 0
-0.2780 2.0830 0.4230 C 0 0
-1.4560 1.9530 1.1830 C 0 0
0.8520 2.8950 0.9780 C 0 0
0.9550 3.0860 2.1670 O 0 0
1.7050 3.3710 0.0750 O 0 0
-4.2550 -0.0810 1.4150 C 0 0
-3.6380 1.0830 1.4150 O 0 0
-5.6600 -0.1360 1.4150 C 0 0
-6.3190 -1.3780 1.4150 C 0 0
-5.5730 -2.5690 1.4150 C 0 0
-4.1690 -2.5170 1.4150 C 0 0
-3.5110 -1.2750 1.4150 C 0 0
2.0970 0.9310 -1.2190 C 0 0
3.1410 1.1720 -1.7780 O 0 0
2.0350 -0.0580 -0.0820 C 0 0 1 0 0 0
1.1770 -1.2810 -0.4530 C 0 0
1.1330 -2.3130 0.6840 C 0 0
2.5430 -2.7450 1.1190 C 0 0 1 0 0 0
3.3990 -1.5240 1.4930 C 0 0
3.4460 -0.4880 0.3600 C 0 0
0.9330 2.3320 -2.8560 C 0 0
1.4470 3.7520 -2.6210 C 0 0
1.6960 1.6040 -3.9640 C 0 0
0.9460 1.5540 -1.6090 N 0 0
2.4850 -3.7560 2.2670 C 0 0
3.7540 -4.1790 2.5680 F 0 0
1.7220 -4.8310 1.8900 F 0 0
1.9270 -3.1640 3.3700 F 0 0
-3.2740 -0.0070 -0.9330 H 0 0
-1.2250 0.2040 -2.2830 H 0 0

```

-1.5340	2.4340	2.1480	H	0	0
2.5040	3.8250	0.3720	H	0	0
-6.2370	0.7770	1.4150	H	0	0
-7.3990	-1.4170	1.4150	H	0	0
-6.0790	-3.5230	1.4150	H	0	0
-3.5950	-3.4320	1.4150	H	0	0
-2.4320	-1.2400	1.4150	H	0	0
1.5580	0.4430	0.7610	H	0	0
0.1620	-0.9660	-0.6990	H	0	0
1.5780	-1.7560	-1.3500	H	0	0
0.5570	-3.1830	0.3670	H	0	0
0.6020	-1.8850	1.5360	H	0	0
3.0180	-3.2390	0.2710	H	0	0
4.4130	-1.8410	1.7420	H	0	0
2.9940	-1.0540	2.3910	H	0	0
3.9850	-0.9130	-0.4880	H	0	0
4.0190	0.3820	0.6840	H	0	0
-0.1370	2.3390	-3.0660	H	0	0
0.7580	4.3380	-2.0130	H	0	0
1.5820	4.2750	-3.5680	H	0	0
2.4100	3.7340	-2.1100	H	0	0
1.3250	0.5860	-4.0820	H	0	0
1.5950	2.1320	-4.9120	H	0	0
2.7580	1.5460	-3.7260	H	0	0
2	3	2	0		
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5	6	1	0		
4	5	2	0		
3	4	1	0		
29	32	1	0		
29	31	1	0		
29	30	1	0		
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3	34	1	0		
6	35	1	0		

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 12 37  1  0
 13 38  1  0
 14 39  1  0
 15 40  1  0
 16 41  1  0
 19 42  1  0
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 23 48  1  0
 23 49  1  0
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 24 51  1  0
 25 52  1  0
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 27 58  1  0

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M END

> <Name>

Compound21

> <Activ>

2

> <DB_Ref_id>

1.26

\$\$\$\$

Compound22

SciTegic10081411483D

```

41 43  0  0  0  0          999 V2000
   0.2340    2.0390    2.1970 C    0  0
  -0.4160    0.4750    0.4550 C    0  0
  -0.9980    1.5250   -0.2810 C    0  0
  -0.9590    2.8440    0.2310 C    0  0
  -0.3420    3.0920    1.4690 C    0  0
  -1.5900    1.2440   -1.4880 N    0  0
  -1.1560   -0.0800   -2.3120 S    0  0
  -1.7420   -1.2270   -1.6410 O    0  0
  -1.6250    0.0820   -3.6780 O    0  0
  -1.5620    3.9940   -0.5180 C    0  0
  -1.6620    3.9670   -1.7230 O    0  0
  -1.9670    5.0120    0.2360 O    0  0
   0.5570   -0.2890   -2.3500 C    0  0
   2.5160   -1.6600   -1.8890 C    0  0
   3.3480   -0.6450   -2.3960 C    0  0
   2.7790    0.5490   -2.8830 C    0  0
   1.3850    0.7270   -2.8590 C    0  0
   1.1210   -1.4820   -1.8630 C    0  0
   5.2170   -0.8810   -2.4260 Br   0  0
   0.8540    1.8570   -3.3200 F    0  0
   0.1990    0.7280    1.6930 C    0  0
   0.7400   -0.2580    2.3790 O    0  0
   0.1230   -1.4220    2.3790 C    0  0

```

-1.9390	-2.7190	2.3790	C	0	0
-1.2810	-1.4770	2.3790	C	0	0
-1.1950	-3.9100	2.3790	C	0	0
0.8670	-2.6150	2.3790	C	0	0
0.2090	-3.8580	2.3790	C	0	0
0.7070	2.2400	3.1490	H	0	0
-0.4350	-0.5390	0.0800	H	0	0
-0.3070	4.0960	1.8710	H	0	0
-2.2910	1.8550	-1.8550	H	0	0
-2.3650	5.7830	-0.1840	H	0	0
2.9340	-2.5820	-1.5120	H	0	0
3.4060	1.3360	-3.2790	H	0	0
0.4840	-2.2620	-1.4730	H	0	0
-3.0190	-2.7580	2.3790	H	0	0
-1.8590	-0.5650	2.3790	H	0	0
-1.7010	-4.8630	2.3790	H	0	0
1.9470	-2.5800	2.3790	H	0	0
0.7830	-4.7740	2.3790	H	0	0
4	5	2	0		
3	4	1	0		
2	3	2	0		
1	5	1	0		
3	6	1	0		
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14	18	1	0		
17	13	1	0		
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24	25	2	0		
26	24	1	0		
25	23	1	0		
23	27	2	0		
1	29	1	0		
2	30	1	0		
5	31	1	0		
6	32	1	0		
12	33	1	0		
14	34	1	0		
16	35	1	0		
18	36	1	0		
24	37	1	0		
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M END
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Compound22

> <Activ>
0.31

> <DB_Ref_id>
1.27

\$\$\$\$
Compound23
SciTegic10081411483D

49	51	0	0	0	0	999	V2000
-1.2850	-1.2790	-0.8360	C	0	0		
-1.4020	-0.6270	0.4020	C	0	0		
-0.3340	0.1460	0.8890	C	0	0		
0.8540	0.2710	0.1410	C	0	0		
0.9690	-0.3870	-1.1050	C	0	0		
-0.1030	-1.1600	-1.5860	C	0	0		
2.2110	-0.2850	-1.9350	C	0	0		
2.1560	-0.3070	-3.1430	O	0	0		
3.3440	-0.1700	-1.2480	O	0	0		
2.2540	2.1820	0.0020	C	0	0		
3.2150	2.8070	0.3850	O	0	0		
1.4530	2.6430	-1.1720	C	0	0		
0.0610	2.7870	-1.0510	C	0	0		
-0.7030	3.2190	-2.1480	C	0	0		
-0.0760	3.5080	-3.3750	C	0	0		
1.3200	3.3630	-3.4960	C	0	0		
2.0840	2.9320	-2.3980	C	0	0		
2.5800	0.6290	1.8690	C	0	0		
2.1600	1.5000	3.0550	C	0	0		
2.3970	-0.8630	2.1390	C	0	0		
1.8790	1.0350	0.6430	N	0	0		
-2.5120	-0.7400	1.1060	O	0	0		
-3.1290	-1.9040	1.1060	C	0	0		
-4.5330	-1.9590	1.1060	C	0	0		
-5.1930	-3.2010	1.1060	C	0	0		
-4.4470	-4.3910	1.1060	C	0	0		
-3.0430	-4.3400	1.1060	C	0	0		
-2.3850	-3.0980	1.1060	C	0	0		
3.4020	2.7990	-2.5310	F	0	0		
-1.1000	4.0840	-4.8480	Br	0	0		
-2.1030	-1.8750	-1.2130	H	0	0		
-0.4410	0.6430	1.8440	H	0	0		
-0.0270	-1.6680	-2.5370	H	0	0		
4.1820	-0.1020	-1.7250	H	0	0		
-0.4320	2.5680	-0.1150	H	0	0		
-1.7730	3.3260	-2.0350	H	0	0		
1.8150	3.5840	-4.4320	H	0	0		
3.6100	0.8460	1.5800	H	0	0		
2.2910	2.5610	2.8460	H	0	0		
2.7500	1.2580	3.9400	H	0	0		
1.1110	1.3360	3.2990	H	0	0		
2.6230	-1.4470	1.2480	H	0	0		
3.0430	-1.1910	2.9530	H	0	0		
1.3670	-1.0800	2.4260	H	0	0		
-5.1110	-1.0450	1.1060	H	0	0		
-6.2720	-3.2400	1.1060	H	0	0		

-4.9530	-5.3460	1.1060	H	0	0
-2.4690	-5.2560	1.1060	H	0	0
-1.3050	-3.0630	1.1060	H	0	0

5	6	2	0
4	5	1	0
3	4	2	0
2	3	1	0
1	2	2	0
1	6	1	0
5	7	1	0
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7	9	1	0
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M  END
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Compound23

> <Activ>
1.4

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> <DB_Ref_id>
1.28
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\$\$\$

Compound24

SciTegic10081411483D

58	60	0	0	0	0			999	v2000						
-0.6860				2.0080		-2.8460	C	0	0						
-1.1000				2.2990		-1.5350	C	0	0						
-0.2750				1.9590		-0.4510	C	0	0						
0.9670				1.3260		-0.6680	C	0	0						
1.3790				1.0350		-1.9900	C	0	0						
0.5490				1.3790		-3.0720	C	0	0						
2.6900				0.3630		-2.2710	C	0	0						
3.5040				0.2010		-1.3940	O	0	0						
2.8690				-0.0230		-3.5310	O	0	0						
1.8870				-0.2990		0.7930	C	0	0						
2.6780				-0.6010		1.6560	O	0	0						
1.0370				-1.3440		0.1170	C	0	0	1	0	0	0		
1.6700				-2.7400		0.2370	C	0	0						
0.8010				-3.8180		-0.4280	C	0	0						
-0.6370				-3.8160		0.1210	C	0	0	1	0	0	0		
-1.2680				-2.4200		0.0100	C	0	0						
-0.3960				-1.3440		0.6760	C	0	0						
2.4430				2.0570		1.1700	C	0	0						
2.0650				2.0060		2.6510	C	0	0						
3.9530				1.9880		0.9450	C	0	0						
1.7480				1.0060		0.4120	N	0	0						
-2.2600				2.8910		-1.3260	O	0	0						
-2.9770				2.4960		-0.2930	C	0	0						
-3.6600				3.4400		0.4960	C	0	0						
-4.4260				3.0180		1.5960	C	0	0						
-4.5100				1.6510		1.9120	C	0	0						
-3.8280				0.7050		1.1250	C	0	0						
-3.0630				1.1290		0.0260	C	0	0						
-1.4980				-4.8730		-0.5760	C	0	0						
-1.3160				2.2680		-3.6830	H	0	0						
-0.6070				2.1900		0.5510	H	0	0						
0.8540				1.1600		-4.0860	H	0	0						
3.6860				-0.4780		-3.7730	H	0	0						
0.9840				-1.0880		-0.9410	H	0	0						
2.6620				-2.7420		-0.2170	H	0	0						
1.8110				-2.9940		1.2870	H	0	0						
0.7810				-3.6500		-1.5060	H	0	0						
1.2540				-4.7990		-0.2790	H	0	0						
-0.5900				-4.0800		1.1800	H	0	0						
-2.2600				-2.4200		0.4630	H	0	0						
-1.4080				-2.1640		-1.0410	H	0	0						
-0.8550				-0.3630		0.5350	H	0	0						
-0.3750				-1.5190											

-3.8930	-0.3460	1.3670	H	0	0
-2.5410	0.3990	-0.5760	H	0	0
-2.5100	-4.9040	-0.1700	H	0	0
-1.0620	-5.8650	-0.4610	H	0	0
-1.5740	-4.6640	-1.6420	H	0	0
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M END

> <Name>

Compound24

> <Activ>

0.74

> <DB_Ref_id>

1.29

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Compound25

SciTegic10081411483D

61	63	0	0	0	0	999	V2000				
-3.3650	-1.7130	1.5370	C	0	0						
-3.2300	-0.3460	1.2400	C	0	0						
-2.4200	0.0590	0.1660	C	0	0						
-1.7400	-0.8990	-0.6150	C	0	0						
-1.8770	-2.2740	-0.3120	C	0	0						
-2.6910	-2.6720	0.7660	C	0	0						
-1.1760	-3.3260	-1.1130	C	0	0						
-1.1150	-3.2540	-2.3180	O	0	0						
-0.6410	-4.3170	-0.4020	O	0	0						
0.2990	0.0190	-1.4280	C	0	0						
0.9690	0.4320	-2.3460	O	0	0						
0.8220	0.0350	-0.0140	C	0	0	1	0	0	0		
1.3830	-1.3420	0.3910	C	0	0						
2.7010	-1.6720	-0.3320	C	0	0						
3.7600	-0.5740	-0.1290	C	0	0	1	0	0	0		
3.2050	0.7990	-0.5430	C	0	0						
1.8870	1.1310	0.1780	C	0	0						
-1.4650	-0.5370	-3.0350	C	0	0						
-1.9940	0.8240	-3.4900	C	0	0						
-0.4080	-1.1060	-3.9820	C	0	0						
-0.9570	-0.4710	-1.6560	N	0	0						
-3.8630	0.5530	1.9670	O	0	0						
-3.2500	1.6930	2.2130	C	0	0						
-1.8710	1.7090	2.4820	C	0	0						
-1.2150	2.9260	2.7440	C	0	0						
-1.9410	4.1290	2.7360	C	0	0						
-3.3200	4.1150	2.4670	C	0	0						
-3.9730	2.9000	2.2050	C	0	0						
4.2740	-0.5570	1.3150	C	0	0						
5.5180	0.3140	1.4880	C	0	0						
-3.9860	-2.0290	2.3630	H	0	0						
-2.3280	1.1130	-0.0510	H	0	0						
-2.8030	-3.7190	1.0060	H	0	0						
-0.6820	-4.2810	0.5630	H	0	0						
-0.0190	0.2620	0.6390	H	0	0						
1.5590	-1.3540	1.4670	H	0	0						
0.6470	-2.1250	0.2010	H	0	0						
2.5040	-1.7870	-1.3980	H	0	0						
3.0820	-2.6330	0.0100	H	0	0						
4.6110	-0.8030	-0.7710	H	0	0						
3.0350	0.8090	-1.6190	H	0	0						
3.9420	1.5780	-0.3480	H	0	0						

2.0880	1.2500	1.2440	H	0	0
1.5080	2.0960	-0.1620	H	0	0
-2.2830	-1.2440	-2.9020	H	0	0
-2.7560	1.2110	-2.8130	H	0	0
-2.4360	0.7520	-4.4840	H	0	0
-1.1870	1.5550	-3.5370	H	0	0
0.2620	-1.7990	-3.4730	H	0	0
0.1990	-0.3070	-4.4060	H	0	0
-0.8790	-1.6430	-4.8070	H	0	0
-1.3110	0.7850	2.4880	H	0	0
-0.1560	2.9340	2.9490	H	0	0
-1.4370	5.0640	2.9380	H	0	0
-3.8770	5.0410	2.4610	H	0	0
-5.0330	2.8950	2.0000	H	0	0
3.4840	-0.2420	2.0000	H	0	0
4.4590	-1.5700	1.6700	H	0	0
5.9180	0.2170	2.4980	H	0	0
6.2890	0.0310	0.7720	H	0	0
5.2810	1.3650	1.3240	H	0	0
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3	4	2	0		
2	3	1	0		
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30 61 1 0

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M END

> <Name>

Compound25

> <Activ>

4.3

> <DB_Ref_id>

1.3

\$\$\$\$

Compound26

SciTegic10081411483D

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58 60 0 0 0 0          999 V2000
-0.8300  2.0880 -2.7340 C  0  0
-1.1950  2.3260 -1.4000 C  0  0
-0.3160  1.9730 -0.3610 C  0  0
 0.9300  1.3830 -0.6500 C  0  0
 1.2950  1.1440 -1.9980 C  0  0
 0.4100  1.5000 -3.0310 C  0  0
 2.6090  0.5190 -2.3550 C  0  0
 3.4750  0.3730 -1.5230 O  0  0
 2.7330  0.1500 -3.6270 O  0  0
 1.9470 -0.2620  0.7230 C  0  0
 2.7760 -0.5700  1.5490 O  0  0
 1.0960 -1.3070  0.0470 C  0  0  1  0  0  0
 1.7310 -2.7050  0.1660 C  0  0
 0.8590 -3.7830 -0.4980 C  0  0
-0.5760 -3.7810  0.0510 C  0  0  1  0  0  0
-1.2070 -2.3830 -0.0610 C  0  0
-0.3380 -1.3070  0.6060 C  0  0
 2.4730  2.0940  1.1430 C  0  0
 2.1600  1.9960  2.6350 C  0  0
 3.9730  2.0620  0.8500 C  0  0
 1.7660  1.0510  0.3850 N  0  0
-2.3590  2.8790 -1.1210 O  0  0
-3.0490  2.3930 -0.1090 C  0  0
-3.7090  3.2640  0.7770 C  0  0
-4.4430  2.7460  1.8590 C  0  0

```

-4.5200	1.3570	2.0570	C	0	0
-3.8590	0.4840	1.1720	C	0	0
-3.1270	1.0040	0.0920	C	0	0
-1.4370	-4.8360	-0.6460	C	0	0
-2.6950	-4.8320	-0.1000	F	0	0
-0.8710	-6.0720	-0.4780	F	0	0
-1.5210	-4.5490	-1.9840	F	0	0
-1.5020	2.3570	-3.5350	H	0	0
-0.6110	2.1620	0.6620	H	0	0
0.6780	1.3220	-4.0640	H	0	0
3.5470	-0.2810	-3.9160	H	0	0
1.0450	-1.0510	-1.0120	H	0	0
2.7230	-2.7070	-0.2870	H	0	0
1.8710	-2.9570	1.2170	H	0	0
0.8400	-3.6130	-1.5760	H	0	0
1.3150	-4.7620	-0.3500	H	0	0
-0.5290	-4.0430	1.1090	H	0	0
-2.1990	-2.3850	0.3930	H	0	0
-1.3500	-2.1270	-1.1110	H	0	0
-0.7950	-0.3260	0.4650	H	0	0
-0.3140	-1.4830	1.6840	H	0	0
2.0160	2.9840	0.7110	H	0	0
1.0960	1.8590	2.8200	H	0	0
2.4750	2.9000	3.1540	H	0	0
2.6880	1.1520	3.0840	H	0	0
4.1660	2.2810	-0.2010	H	0	0
4.5020	2.7870	1.4670	H	0	0
4.3870	1.0760	1.0650	H	0	0
-3.6520	4.3320	0.6290	H	0	0
-4.9490	3.4160	2.5370	H	0	0
-5.0840	0.9590	2.8870	H	0	0
-3.9180	-0.5820	1.3240	H	0	0
-2.6210	0.3300	-0.5860	H	0	0
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1	6	2	0		
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27	28	2	0		
26	27	1	0		
25	26	2	0		
24	25	1	0		
28	23	1	0		
23	24	2	0		
15	29	1	0		

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4 5 2 0
3 4 1 0
29 30 1 0
29 31 1 0
29 32 1 0
1 33 1 0
3 34 1 0
6 35 1 0
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14 40 1 0
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15 42 1 0
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16 44 1 0
17 45 1 0
17 46 1 0
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19 48 1 0
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26 56 1 0
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28 58 1 0
M END
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Compound26

> <Activ>
1.3

> <DB_Ref_id>
1.31

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Compound27
SciTegic10081411483D

61 63 0 0 0 0          999 V2000
1.4630 0.6330 -2.1720 C 0 0
2.2270 0.1820 -1.0820 C 0 0
1.9260 0.6150 0.2190 C 0 0
0.8570 1.5040 0.4430 C 0 0
0.0860 1.9610 -0.6520 C 0 0
0.3950 1.5210 -1.9530 C 0 0
-1.0610 2.9060 -0.4650 C 0 0
-1.9530 2.9710 -1.2770 O 0 0
-1.0100 3.6470 0.6410 O 0 0
1.7460 0.2270 -3.3930 O 0 0
-0.5530 1.4880 2.3500 C 0 0
-0.8650 1.9450 3.4240 O 0 0
-1.4020 0.4410 1.6740 C 0 0 1 0 0 0
-0.7700 -0.9550 1.7930 C 0 0

```

-1.6390	-2.0330	1.1290	C	0	0				
-3.0760	-2.0310	1.6780	C	0	0	1	0	0	0
-3.7070	-0.6330	1.5660	C	0	0				
-2.8360	0.4410	2.2320	C	0	0				
-3.9380	-3.0880	0.9800	C	0	0				
1.5140	2.8010	2.4390	C	0	0				
0.8960	4.1860	2.6430	C	0	0				
1.9820	2.1660	3.7500	C	0	0				
0.5860	1.9100	1.7270	N	0	0				
2.3140	-1.0660	-3.5490	C	0	0				
2.3440	-1.4770	-5.0140	C	0	0				
2.6270	-2.9690	-4.8810	C	0	0				
1.7620	-3.4120	-3.7010	C	0	0				
1.4240	-2.1370	-2.9280	C	0	0				
3.0470	-0.5000	-1.2460	H	0	0				
2.5290	0.2540	1.0410	H	0	0				
-0.1890	1.8650	-2.7950	H	0	0				
-1.6970	4.3070	0.7990	H	0	0				
-1.4550	0.6990	0.6150	H	0	0				
0.2230	-0.9570	1.3400	H	0	0				
-0.6270	-1.2090	2.8460	H	0	0				
-1.6580	-1.8630	0.0530	H	0	0				
-1.1860	-3.0140	1.2790	H	0	0				
-3.0290	-2.2950	2.7360	H	0	0				
-4.6990	-0.6350	2.0200	H	0	0				
-3.8480	-0.3790	0.5160	H	0	0				
-3.2950	1.4220	2.0920	H	0	0				
-2.8130	0.2660	3.3110	H	0	0				
-4.9470	-3.1210	1.3910	H	0	0				
-3.4980	-4.0780	1.0940	H	0	0				
-4.0180	-2.8770	-0.0860	H	0	0				
2.3280	2.8440	1.7190	H	0	0				
0.7870	4.7230	1.7010	H	0	0				
1.5180	4.7910	3.3010	H	0	0				
-0.0920	4.1040	3.0980	H	0	0				
2.2850	1.1330	3.5900	H	0	0				
2.8220	2.7230	4.1680	H	0	0				
1.1800	2.1680	4.4880	H	0	0				
3.3050	-1.0720	-3.1150	H	0	0				
1.3890	-1.3030	-5.4900	H	0	0				
3.1070	-0.9590	-5.5760	H	0	0				
2.3980	-3.5120	-5.7870	H	0	0				
3.6720	-3.1270	-4.6560	H	0	0				
0.8550	-3.8910	-4.0450	H	0	0				
2.2910	-4.1230	-3.0860	H	0	0				
0.3810	-1.8850	-3.0680	H	0	0				
1.5960	-2.2400	-1.8650	H	0	0				
5	6	2	0						
4	5	1	0						
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7	8	2	0						
7	9	1	0						
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13 14 1 0
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M END
> <Name>
Compound27

> <Activ>
0.46

> <DB_Ref_id>
1.36

$$$$
Compound28
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SciTegic10081411483D

61	63	0	0	0	0	999	V2000				
2.4920	1.0720	0.6840	C	0	0						
2.2700	-0.0430	-0.1410	C	0	0						
1.1520	-0.0840	-0.9900	C	0	0						
0.2480	0.9960	-1.0250	C	0	0						
0.4690	2.1210	-0.1950	C	0	0						
1.5900	2.1500	0.6520	C	0	0						
-0.4670	3.2910	-0.1970	C	0	0						
-1.6540	3.1370	-0.3630	O	0	0						
0.1070	4.4750	-0.0060	O	0	0						
3.5390	1.1070	1.4810	O	0	0						
-2.0530	0.5390	-1.3850	C	0	0						
-3.0230	0.5410	-2.1030	O	0	0						
-2.1560	0.1090	0.0590	C	0	0	1	0	0	0		
-3.5780	0.3300	0.6090	C	0	0						
-4.5940	-0.6540	0.0060	C	0	0						
-4.1620	-2.1190	0.1930	C	0	0	1	0	0	0		
-2.7420	-2.3440	-0.3590	C	0	0						
-1.7250	-1.3570	0.2400	C	0	0						
-4.2580	-2.5450	1.6620	C	0	0						
-0.6990	1.2730	-3.2890	C	0	0						
-1.0410	0.0760	-4.1780	C	0	0						
-1.5200	2.5180	-3.6330	C	0	0						
-0.8340	0.9300	-1.8670	N	0	0						
3.9260	-0.0200	2.0470	C	0	0						
2.9610	-0.9410	2.4900	C	0	0						
5.2950	-0.3090	2.2090	C	0	0						
3.3590	-2.1470	3.0960	C	0	0						
4.7250	-2.4320	3.2580	C	0	0						
5.6920	-1.5140	2.8150	C	0	0						
6.3260	0.6580	1.7460	C	0	0						
6.3010	1.7720	2.5430	F	0	0						
6.0650	1.0180	0.4490	F	0	0						
7.5650	0.0720	1.8160	F	0	0						
2.9590	-0.8750	-0.1210	H	0	0						
1.0040	-0.9530	-1.6150	H	0	0						
1.7660	3.0080	1.2890	H	0	0						
1.0720	4.5410	-0.0140	H	0	0						
-1.4710	0.7380	0.6310	H	0	0						
-3.9020	1.3550	0.4300	H	0	0						
-3.5640	0.2050	1.6910	H	0	0						
-4.7070	-0.4470	-1.0590	H	0	0						
-5.5760	-0.4920	0.4510	H	0	0						
-4.8500	-2.7520	-0.3710	H	0	0						
-2.4220	-3.3670	-0.1720	H	0	0						
-2.7580	-2.2270	-1.4430	H	0	0						
-1.6150	-1.5660	1.3050	H	0	0						
-0.7400	-1.5230	-0.2010	H	0	0						
-3.9920	-3.5940	1.8010	H	0	0						
-5.2720	-2.4060	2.0370	H	0	0						
-3.5900	-1.9470	2.2810	H	0	0						
0.3670	1.4920	-3.3320	H	0	0						
-0.5330	-0.8300	-3.8520	H	0	0						
-0.7500	0.2680	-5.2110	H	0	0						
-2.1130	-0.1170	-4.1640	H	0	0						
-1.2990	3.3280	-2.9370	H	0	0						
-1.3050	2.8520	-4.6460	H	0	0						
-2.5860	2.3050	-3.5700	H	0	0						
1.9100	-0.7250	2.3690	H	0	0						

2.6150	-2.8520	3.4360	H	0	0
5.0330	-3.3570	3.7210	H	0	0
6.7420	-1.7380	2.9420	H	0	0
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7	8	2	0		
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1	10	1	0		
11	12	2	0		
13	11	1	0		
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4	5	2	0		
3	4	1	0		
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0.19

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1.38

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Compound29

SciTegic10081411483D

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2.4860	1.1110	0.6560	C	0	0						
2.2500	0.0840	-0.2710	C	0	0						
1.1150	0.1230	-1.0960	C	0	0						
0.2030	1.1930	-0.9980	C	0	0						
0.4400	2.2310	-0.0640	C	0	0						
1.5800	2.1820	0.7560	C	0	0						
-0.5020	3.3890	0.0740	C	0	0						
-1.0170	3.6450	1.1370	O	0	0						
-0.7110	4.0840	-1.0390	O	0	0						
3.5550	1.0720	1.4280	O	0	0						
-2.1310	0.9120	-1.3090	C	0	0						
-3.1150	0.9960	-2.0040	O	0	0						
-2.2340	0.4820	0.1350	C	0	0	1	0	0	0		
-3.6560	0.7030	0.6860	C	0	0						
-4.6740	-0.2830	0.0820	C	0	0						
-4.2400	-1.7480	0.2700	C	0	0	1	0	0	0		
-2.8220	-1.9710	-0.2830	C	0	0						
-1.8050	-0.9860	0.3160	C	0	0						
-4.3380	-2.1740	1.7380	C	0	0						
-0.7670	1.5330	-3.2440	C	0	0						
-0.8550	0.2720	-4.1050	C	0	0						
-1.7790	2.6020	-3.6580	C	0	0						
-0.8980	1.2050	-1.8180	N	0	0						
3.9570	-0.1020	1.8670	C	0	0						
3.0160	-1.0780	2.2340	C	0	0						
5.3320	-0.3850	1.9690	C	0	0						
3.4440	-2.3320	2.7030	C	0	0						
4.8170	-2.6130	2.8030	C	0	0						
5.7620	-1.6410	2.4360	C	0	0						
7.2150	-1.9360	2.5430	C	0	0						
7.3890	-3.2170	2.9940	F	0	0						
7.7970	-1.0590	3.4200	F	0	0						
7.8010	-1.8030	1.3090	F	0	0						
2.9450	-0.7400	-0.3530	H	0	0						
0.9550	-0.6800	-1.8030	H	0	0						
1.7680	2.9690	1.4730	H	0	0						
-0.1620	3.9140	-1.8140	H	0	0						
-1.5490	1.1090	0.7070	H	0	0						
-3.9800	1.7290	0.5060	H	0	0						
-3.6430	0.5780	1.7680	H	0	0						
-4.7870	-0.0740	-0.9820	H	0	0						

-5.6560	-0.1210	0.5270	H	0	0
-4.9280	-2.3790	-0.2950	H	0	0
-2.5020	-2.9960	-0.0960	H	0	0
-2.8360	-1.8540	-1.3670	H	0	0
-1.6930	-1.1950	1.3810	H	0	0
-0.8200	-1.1520	-0.1250	H	0	0
-4.0680	-3.2210	1.8770	H	0	0
-5.3520	-2.0370	2.1130	H	0	0
-3.6700	-1.5720	2.3590	H	0	0
0.2460	1.9360	-3.2560	H	0	0
-0.1090	-0.4690	-3.8180	H	0	0
-0.6970	0.5120	-5.1580	H	0	0
-1.8380	-0.1890	-4.0140	H	0	0
-1.9940	3.2720	-2.8240	H	0	0
-1.4000	3.1880	-4.4960	H	0	0
-2.7190	2.1450	-3.9690	H	0	0
1.9590	-0.8670	2.1580	H	0	0
6.0550	0.3650	1.6860	H	0	0
2.7190	-3.0820	2.9840	H	0	0
5.1430	-3.5800	3.1640	H	0	0
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0.47

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1.4

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Compound30

SciTegic10081411483D

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62 64 0 0 0 0          999 V2000
  1.1600    0.6090   -1.9390 C    0  0
  1.8420   -0.0450   -0.8980 C    0  0
  1.6170    0.3260    0.4360 C    0  0
  0.7070    1.3570    0.7420 C    0  0
  0.0200    2.0160   -0.3030 C    0  0
  0.2520    1.6370   -1.6390 C    0  0
 -0.9590    3.1170   -0.0250 C    0  0
 -1.1210    4.0180   -0.8160 O    0  0
 -1.6070    3.0220    1.1310 O    0  0
  1.3730    0.2580   -3.1910 O    0  0
 -0.4920    1.1020    2.7730 C    0  0
 -0.6840    1.4100    3.9260 O    0  0
 -1.3420    0.0570    2.0980 C    0  0  1  0  0  0
 -0.7090   -1.3420    2.2170 C    0  0
 -1.5780   -2.4200    1.5530 C    0  0
 -3.0160   -2.4180    2.1020 C    0  0  1  0  0  0
 -3.6470   -1.0200    1.9900 C    0  0
 -2.7750    0.0570    2.6560 C    0  0
 -3.8770   -3.4730    1.4040 C    0  0
  1.3590    2.7050    2.7070 C    0  0
  2.6780    2.8770    1.9510 C    0  0
  0.6070    4.0240    2.8910 C    0  0
  0.5080    1.6990    2.0570 N    0  0
  1.5880   -1.0160   -3.4490 C    0  0

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0.8610	-2.0020	-2.7580	C	0	0
2.5390	-1.3950	-4.4160	C	0	0
1.0820	-3.3630	-3.0270	C	0	0
2.0330	-3.7400	-3.9900	C	0	0
2.7600	-2.7580	-4.6840	C	0	0
3.2270	-0.4780	-5.0680	O	0	0
2.5020	0.5230	-5.7680	C	0	0
3.1620	0.8400	-6.9260	F	0	0
2.3990	1.6430	-4.9810	F	0	0
1.2500	0.0570	-6.0680	F	0	0
2.5410	-0.8360	-1.1250	H	0	0
2.1540	-0.1910	1.2190	H	0	0
-0.2700	2.1370	-2.4410	H	0	0
-2.2520	3.6990	1.3690	H	0	0
-1.3950	0.3130	1.0390	H	0	0
0.2830	-1.3440	1.7640	H	0	0
-0.5660	-1.5960	3.2680	H	0	0
-1.5980	-2.2500	0.4750	H	0	0
-1.1230	-3.4000	1.7010	H	0	0
-2.9690	-2.6800	3.1600	H	0	0
-4.6390	-1.0210	2.4430	H	0	0
-3.7870	-0.7640	0.9390	H	0	0
-3.2340	1.0350	2.5160	H	0	0
-2.7520	-0.1210	3.7320	H	0	0
-4.8890	-3.5040	1.8110	H	0	0
-3.4410	-4.4650	1.5220	H	0	0
-3.9530	-3.2660	0.3380	H	0	0
1.5270	2.2210	3.6680	H	0	0
3.3480	3.5720	2.4570	H	0	0
2.4980	3.2560	0.9450	H	0	0
3.1950	1.9220	1.8590	H	0	0
-0.3440	3.8580	3.3950	H	0	0
1.2010	4.7270	3.4730	H	0	0
0.3970	4.4840	1.9260	H	0	0
0.1290	-1.7130	-2.0180	H	0	0
0.5230	-4.1170	-2.4960	H	0	0
2.2030	-4.7870	-4.1990	H	0	0
3.4900	-3.0530	-5.4240	H	0	0
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Compound31
SciTegic10081411483D

58 60 0 0 0 0 999 V2000
-0.6330 1.9630 -1.9940 C 0 0
-1.0230 2.2360 -0.6740 C 0 0
-0.1840 1.8890 0.3990 C 0 0
1.0570 1.2660 0.1560 C 0 0
1.4510 0.9900 -1.1740 C 0 0

```

0.6020	1.3400	-2.2400	C	0	0				
2.7600	0.3280	-1.4820	C	0	0				
2.8010	-0.8070	-1.9000	O	0	0				
3.8380	1.0740	-1.2620	O	0	0				
-1.4240	2.2870	-2.9980	O	0	0				
2.0140	-0.3690	1.5820	C	0	0				
2.8180	-0.6760	2.4300	O	0	0				
1.1620	-1.4140	0.9040	C	0	0	1	0	0	0
1.7970	-2.8110	1.0220	C	0	0				
0.9260	-3.8910	0.3590	C	0	0				
-0.5120	-3.8890	0.9080	C	0	0	1	0	0	0
-1.1430	-2.4900	0.7970	C	0	0				
-0.2710	-1.4140	1.4630	C	0	0				
-1.3730	-4.9420	0.2070	C	0	0				
2.5510	1.9860	1.9840	C	0	0				
2.1250	1.9690	3.4530	C	0	0				
4.0670	1.8770	1.8090	C	0	0				
1.8570	0.9390	1.2210	N	0	0				
-2.7250	2.1640	-2.8260	C	0	0				
-3.2230	1.0510	-2.1250	C	0	0				
-3.6250	3.1270	-3.3340	C	0	0				
-4.6040	0.8930	-1.9280	C	0	0				
-5.4960	1.8500	-2.4340	C	0	0				
-5.0100	2.9650	-3.1350	C	0	0				
-3.0000	4.6370	-4.2790	Br	0	0				
-1.9730	2.7130	-0.4780	H	0	0				
-0.5060	2.1110	1.4060	H	0	0				
0.8970	1.1330	-3.2600	H	0	0				
3.7330	2.0210	-1.1050	H	0	0				
1.1090	-1.1560	-0.1560	H	0	0				
2.7870	-2.8130	0.5660	H	0	0				
1.9400	-3.0650	2.0740	H	0	0				
0.9080	-3.7250	-0.7190	H	0	0				
1.3790	-4.8710	0.5120	H	0	0				
-0.4690	-4.1540	1.9670	H	0	0				
-2.1330	-2.4920	1.2520	H	0	0				
-1.2870	-2.2340	-0.2540	H	0	0				
-0.7300	-0.4340	1.3200	H	0	0				
-0.2480	-1.5900	2.5390	H	0	0				
-2.3830	-4.9730	0.6150	H	0	0				
-0.9360	-5.9340	0.3240	H	0	0				
-1.4510	-4.7360	-0.8610	H	0	0				
2.1680	2.8750	1.4830	H	0	0				
1.0410	1.9370	3.5610	H	0	0				
2.4860	2.8590	3.9690	H	0	0				
2.5350	1.0980	3.9630	H	0	0				
4.3710	2.2770	0.8420	H	0	0				
4.5860	2.4220	2.5980	H	0	0				
4.3870	0.8360	1.8540	H	0	0				
-2.5390	0.3110	-1.7320	H	0	0				
-4.9790	0.0350	-1.3890	H	0	0				
-6.5610	1.7290	-2.2850	H	0	0				
-5.7150	3.6910	-3.5160	H	0	0				
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Compound31

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1.42

Compound 32

Compound 32

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1.0370		0.2890	-1.6480	C	0	0
1.7360		-0.1450	-0.5100	C	0	0
1.3810		0.3340	0.7620	C	0	0
0.3220		1.2520	0.9040	C	0	0
-0.3810		1.6910	-0.2420	C	0	0
-0.0200		1.2050	-1.5120	C	0	0
-1.5140		2.6680	-0.1410	C	0	0
-2.3930		2.6890	-0.9710	O	0	0
-1.4690		3.4800	0.9120	O	0	0
1.3730		-0.1620	-2.8420	O	0	0
-1.2170		1.3940	2.7030	C	0	0
-1.5960		1.9510	3.7070	O	0	0
-2.0660		0.3480	2.0270	C	0	0
-1.4340		-1.0490	2.1470	C	0	0
-2.3030		-2.1270	1.4820	C	0	0
-3.7400		-2.1250	2.0310	C	0	0
-4.3710		-0.7270	1.9200	C	0	0
-3.5000		0.3480	2.5860	C	0	0
-4.6020		-3.1820	1.3340	C	0	0
0.9470		2.5190	2.9300	C	0	0
0.4390		3.9530	3.0800	C	0	0
1.2680		1.8630	4.2740	C	0	0
-0.0020		1.7030	2.1600	N	0	0
2.6520		-0.3590	-3.0920	C	0	0
3.6070		0.5410	-2.5900	C	0	0
3.0700		-1.4650	-3.8570	C	0	0
4.9750		0.3420	-2.8500	C	0	0
5.3890		-0.7620	-3.6130	C	0	0
4.4380		-1.6660	-4.1170	C	0	0
2.0630		-2.4380	-4.4000	C	0	0
0.9920		-1.9490	-5.3560	C	0	0
2.1130		-2.8300	-5.8630	C	0	0
2.5490		-0.8500	-0.6110	H	0	0
1.9340		-0.0160	1.6230	H	0	0
-0.5510		1.5350	-2.3910	H	0	0
-2.1060		4.2030	0.9790	H	0	0
-2.1190		0.6050	0.9690	H	0	0
-0.4410		-1.0510	1.6930	H	0	0
-1.2930		-1.3030	3.1970	H	0	0
-2.3240		-1.9570	0.4040	H	0	0
-1.8500		-3.1080	1.6310	H	0	0
-3.6930		-2.3890	3.0900	H	0	0
-5.3630		-0.7290	2.3730	H	0	0
-4.5140		-0.4730	0.8690	H	0	0
-3.9590		1.3280	2.4450	H	0	0
-3.4790		0.1720	3.6620	H	0	0
-5.6110		-3.2170	1.7440	H	0	0
-4.1620		-4.1720	1.4430	H	0	0
-4.6840		-2.9690	0.2680	H	0	0
1.8110		2.4840	2.2680	H	0	0
0.3590		4.4590	2.1170	H	0	0
1.1130		4.5370	3.7090	H	0	0
-0.5470		3.9670	3.5450	H	0	0
1.5820		0.8300	4.1330	H	0	0
2.0610		2.4080	4.7870	H	0	0

0.3910	1.8610	4.9200	H	0	0
3.2930	1.3930	-2.0020	H	0	0
5.7050	1.0370	-2.4630	H	0	0
6.4400	-0.9160	-3.8150	H	0	0
4.7640	-2.5120	-4.7030	H	0	0
1.7620	-3.2210	-3.7030	H	0	0
0.9960	-0.8990	-5.6520	H	0	0
0.0000	-2.3930	-5.2720	H	0	0
1.8690	-3.8610	-6.1150	H	0	0
2.8710	-2.3710	-6.4980	H	0	0
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4	5	1		0	
3	4	2		0	
2	3	1		0	
1	2	2		0	
1	6	1		0	
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7	8	2		0	
7	9	1		0	
1	10	1		0	
11	12	2		0	
13	11	1		0	
17	18	1		0	
16	17	1		0	
15	16	1		0	
14	15	1		0	
18	13	1		0	
13	14	1		0	
16	19	1		0	
20	21	1		0	
20	22	1		0	
20	23	1		0	
11	23	1		0	
4	23	1		0	
10	24	1		0	
24	25	2		0	
24	26	1		0	
25	27	1		0	
27	28	2		0	
28	29	1		0	
29	26	2		0	
26	30	1		0	
31	32	1		0	
31	30	1		0	
30	32	1		0	
2	33	1		0	
3	34	1		0	
6	35	1		0	
9	36	1		0	
13	37	1		0	
14	38	1		0	
14	39	1		0	
15	40	1		0	
15	41	1		0	
16	42	1		0	
17	43	1		0	
17	44	1		0	
18	45	1		0	
18	46	1		0	
19	47	1		0	
19	48	1		0	

```

19 49 1 0
20 50 1 0
21 51 1 0
21 52 1 0
21 53 1 0
22 54 1 0
22 55 1 0
22 56 1 0
25 57 1 0
27 58 1 0
28 59 1 0
29 60 1 0
30 61 1 0
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31 63 1 0
32 64 1 0
32 65 1 0

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M END

> <Name>

Compound32

> <Activ>

0.33

> <DB_Ref_id>

1.43

\$\$\$\$

Compound33

SciTegic10081411483D

```

64 66 0 0 0 0          999 V2000
  2.4510   0.3750   0.3320 C   0 0
  2.2440  -0.7690  -0.4550 C   0 0
  1.1390  -0.8460  -1.3180 C   0 0
  0.2280   0.2270  -1.4000 C   0 0
  0.4340   1.3810  -0.6090 C   0 0
  1.5450   1.4470   0.2520 C   0 0
 -0.5080   2.5450  -0.6620 C   0 0
 -0.1090   3.6740  -0.4960 O   0 0
 -1.7790   2.2360  -0.9000 O   0 0
  3.4880   0.4430   1.1390 O   0 0
 -2.0510  -0.3100  -1.7830 C   0 0
 -3.0120  -0.3480  -2.5140 O   0 0
 -2.1540  -0.7400  -0.3400 C   0 0 1 0 0 0
 -3.5760  -0.5190   0.2090 C   0 0
 -4.5920  -1.5060  -0.3930 C   0 0
 -4.1600  -2.9710  -0.2050 C   0 0 1 0 0 0
 -2.7420  -3.1930  -0.7600 C   0 0
 -1.7230  -2.2070  -0.1580 C   0 0
 -4.2560  -3.3950   1.2640 C   0 0
 -0.7070   0.4810  -3.6720 C   0 0
 -0.9650  -0.7320  -4.5680 C   0 0
 -1.5960   1.6740  -4.0250 C   0 0
 -0.8440   0.1250  -2.2520 N   0 0
  3.3200   1.0180   2.3140 C   0 0
  2.1170   0.8280   3.0180 C   0 0
  4.3380   1.8160   2.8730 C   0 0
  1.9280   1.4340   4.2720 C   0 0
  2.9410   2.2330   4.8260 C   0 0
  4.1460   2.4240   4.1290 C   0 0

```

5.6150	2.0270	2.1430	C	0	0
6.2830	3.0940	2.6880	F	0	0
5.3520	2.2790	0.8220	F	0	0
6.4800	0.7720	2.2600	C	0	0
2.9370	-1.5960	-0.3980	H	0	0
1.0020	-1.7380	-1.9140	H	0	0
1.7090	2.3240	0.8610	H	0	0
-2.4340	2.9430	-0.9670	H	0	0
-1.4690	-0.1130	0.2320	H	0	0
-3.9010	0.5060	0.0310	H	0	0
-3.5630	-0.6440	1.2930	H	0	0
-4.7050	-1.2970	-1.4570	H	0	0
-5.5760	-1.3440	0.0530	H	0	0
-4.8480	-3.6020	-0.7700	H	0	0
-2.4200	-4.2190	-0.5700	H	0	0
-2.7560	-3.0760	-1.8440	H	0	0
-1.6130	-2.4180	0.9060	H	0	0
-0.7380	-2.3730	-0.6000	H	0	0
-3.9860	-4.4410	1.4020	H	0	0
-5.2720	-3.2620	1.6390	H	0	0
-3.5920	-2.7930	1.8850	H	0	0
0.3460	0.7620	-3.6970	H	0	0
-0.3750	-1.5980	-4.2600	H	0	0
-0.7110	-0.5080	-5.6040	H	0	0
-2.0160	-1.0180	-4.5370	H	0	0
-1.4040	2.5080	-3.3520	H	0	0
-1.4160	1.9960	-5.0510	H	0	0
-2.6490	1.4100	-3.9400	H	0	0
1.3360	0.2150	2.5940	H	0	0
1.0020	1.2850	4.8090	H	0	0
2.7970	2.6970	5.7910	H	0	0
4.9220	3.0370	4.5610	H	0	0
5.9790	-0.1070	1.8540	H	0	0
6.7230	0.5660	3.3030	H	0	0
7.4180	0.8990	1.7190	H	0	0
5	6	2	0		
4	5	1	0		
3	4	2	0		
2	3	1	0		
1	2	2	0		
1	6	1	0		
5	7	1	0		
7	8	2	0		
7	9	1	0		
1	10	1	0		
11	12	2	0		
13	11	1	0		
17	18	1	0		
16	17	1	0		
15	16	1	0		
14	15	1	0		
18	13	1	0		
13	14	1	0		
16	19	1	0		
20	21	1	0		
20	22	1	0		
20	23	1	0		
11	23	1	0		
4	23	1	0		
10	24	1	0		
24	25	2	0		

```

24 26 1 0
25 27 1 0
27 28 2 0
28 29 1 0
29 26 2 0
30 33 1 0
30 32 1 0
30 31 1 0
26 30 1 0
2 34 1 0
3 35 1 0
6 36 1 0
9 37 1 0
13 38 1 0
14 39 1 0
14 40 1 0
15 41 1 0
15 42 1 0
16 43 1 0
17 44 1 0
17 45 1 0
18 46 1 0
18 47 1 0
19 48 1 0
19 49 1 0
19 50 1 0
20 51 1 0
21 52 1 0
21 53 1 0
21 54 1 0
22 55 1 0
22 56 1 0
22 57 1 0
25 58 1 0
27 59 1 0
28 60 1 0
29 61 1 0
33 62 1 0
33 63 1 0
33 64 1 0

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M END

> <Name>

Compound33

> <Activ>

0.3

> <DB_Ref_id>

1.44

\$\$\$\$

Compound34

SciTegic10081411483D

```

61 63 0 0 0 0          999 V2000
   1.2400   0.7050  -2.1410 C   0  0
   1.9080   0.0350  -1.1020 C   0  0
   1.6560   0.3790   0.2360 C   0  0
   0.7300   1.3940   0.5470 C   0  0
   0.0570   2.0700  -0.4960 C   0  0
   0.3160   1.7190  -1.8360 C   0  0

```

-0.9360	3.1560	-0.2170	C	0	0				
-1.8690	2.9690	0.5290	O	0	0				
-0.7050	4.3090	-0.8380	O	0	0				
1.4790	0.3810	-3.3950	O	0	0				
-0.6520	1.3120	2.4730	C	0	0				
-0.9820	1.7930	3.5310	O	0	0				
-1.5040	0.2660	1.7970	C	0	0	1	0	0	0
-0.8690	-1.1310	1.9140	C	0	0				
-1.7400	-2.2090	1.2500	C	0	0				
-3.1760	-2.2070	1.8010	C	0	0	1	0	0	0
-3.8070	-0.8110	1.6870	C	0	0				
-2.9380	0.2660	2.3550	C	0	0				
-4.0390	-3.2640	1.1030	C	0	0				
1.4980	2.4710	2.6350	C	0	0				
1.0020	3.8890	2.9180	C	0	0				
1.9000	1.7210	3.9040	C	0	0				
0.5040	1.7090	1.8650	N	0	0				
1.6950	-0.8890	-3.6780	C	0	0				
0.9610	-1.8870	-3.0120	C	0	0				
2.6580	-1.2540	-4.6390	C	0	0				
1.1860	-3.2420	-3.3030	C	0	0				
2.1450	-3.6060	-4.2620	C	0	0				
2.8810	-2.6130	-4.9300	C	0	0				
3.4430	-0.2110	-5.3520	C	0	0				
4.7770	-0.3950	-5.1020	F	0	0				
3.2130	-0.3090	-6.6990	F	0	0				
2.6190	-0.7440	-1.3300	H	0	0				
2.1840	-0.1500	1.0190	H	0	0				
-0.1950	2.2300	-2.6390	H	0	0				
-1.3400	5.0310	-0.7500	H	0	0				
-1.5550	0.5230	0.7380	H	0	0				
0.1230	-1.1330	1.4610	H	0	0				
-0.7290	-1.3850	2.9670	H	0	0				
-1.7600	-2.0390	0.1740	H	0	0				
-1.2850	-3.1900	1.4000	H	0	0				
-3.1290	-2.4710	2.8570	H	0	0				
-4.7990	-0.8110	2.1410	H	0	0				
-3.9490	-0.5550	0.6370	H	0	0				
-3.3970	1.2460	2.2130	H	0	0				
-2.9140	0.0900	3.4320	H	0	0				
-5.0470	-3.3010	1.5160	H	0	0				
-3.5980	-4.2540	1.2110	H	0	0				
-4.1210	-3.0510	0.0370	H	0	0				
2.3220	2.4860	1.9200	H	0	0				
0.5840	4.3570	2.0270	H	0	0				
1.8160	4.5180	3.2750	H	0	0				
0.2290	3.8790	3.6860	H	0	0				
2.2600	0.7190	3.6640	H	0	0				
2.6840	2.2600	4.4380	H	0	0				
1.0490	1.6170	4.5760	H	0	0				
0.2230	-1.6110	-2.2740	H	0	0				
0.6190	-4.0060	-2.7890	H	0	0				
2.3160	-4.6490	-4.4860	H	0	0				
3.6170	-2.8990	-5.6660	H	0	0				
3.1390	0.7750	-5.0000	H	0	0				
5	6	2	0						
4	5	1	0						
3	4	2	0						
2	3	1	0						
1	2	2	0						
1	6	1	0						

```
5 7 1 0
7 8 2 0
7 9 1 0
1 10 1 0
11 12 2 0
13 11 1 0
17 18 1 0
16 17 1 0
15 16 1 0
14 15 1 0
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13 14 1 0
16 19 1 0
20 21 1 0
20 22 1 0
20 23 1 0
11 23 1 0
4 23 1 0
10 24 1 0
24 25 2 0
24 26 1 0
25 27 1 0
27 28 2 0
28 29 1 0
29 26 2 0
26 30 1 0
30 31 1 0
30 32 1 0
2 33 1 0
3 34 1 0
6 35 1 0
9 36 1 0
13 37 1 0
14 38 1 0
14 39 1 0
15 40 1 0
15 41 1 0
16 42 1 0
17 43 1 0
17 44 1 0
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18 46 1 0
19 47 1 0
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19 49 1 0
20 50 1 0
21 51 1 0
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22 54 1 0
22 55 1 0
22 56 1 0
25 57 1 0
27 58 1 0
28 59 1 0
29 60 1 0
30 61 1 0
M END
> <Name>
Compound34
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> <Activ>
0.2

> <DB_Ref_id>
1.45

\$\$\$\$

Compound35

SciTegic10081411483D

60	62	0	0	0	0	999	V2000				
1.1820	0.5760	-2.0940	C	0	0						
1.9120	0.0800	-1.0020	C	0	0						
1.6210	0.5160	0.3010	C	0	0						
0.5940	1.4550	0.5210	C	0	0						
-0.1450	1.9550	-0.5760	C	0	0						
0.1540	1.5120	-1.8790	C	0	0						
-1.2460	2.9550	-0.3910	C	0	0						
-2.1580	3.0270	-1.1820	O	0	0						
-1.1350	3.7260	0.6850	O	0	0						
1.4550	0.1640	-3.3150	O	0	0						
-0.7660	1.3850	2.4650	C	0	0						
-1.0430	1.7930	3.5660	O	0	0						
-1.6170	0.3380	1.7870	C	0	0	1	0	0	0		
-0.9820	-1.0590	1.9060	C	0	0						
-1.8540	-2.1370	1.2420	C	0	0						
-3.2890	-2.1350	1.7910	C	0	0	1	0	0	0		
-3.9200	-0.7380	1.6800	C	0	0						
-3.0510	0.3380	2.3480	C	0	0						
-4.1500	-3.1920	1.0940	C	0	0						
1.2210	2.8160	2.4840	C	0	0						
2.0780	2.1130	3.5350	C	0	0						
2.0550	3.6030	1.4730	C	0	0						
0.3300	1.8630	1.8050	N	0	0						
1.7170	-1.1150	-3.4940	C	0	0						
0.9980	-2.0410	-2.7930	N	0	0						
2.7250	-1.5140	-4.3970	C	0	0						
1.2500	-3.3710	-2.9590	C	0	0						
2.2440	-3.8220	-3.8480	C	0	0						
2.9920	-2.8830	-4.5760	C	0	0						
3.5060	-0.5020	-5.1580	C	0	0						
3.0550	0.7540	-4.8420	F	0	0						
3.3460	-0.7190	-6.5020	F	0	0						
4.8320	-0.6080	-4.8320	F	0	0						
2.7010	-0.6410	-1.1620	H	0	0						
2.1970	0.1210	1.1250	H	0	0						
-0.4040	1.8890	-2.7230	H	0	0						
-1.8070	4.3980	0.8550	H	0	0						
-1.6680	0.5960	0.7300	H	0	0						
0.0100	-1.0610	1.4530	H	0	0						
-0.8420	-1.3130	2.9590	H	0	0						
-1.8730	-1.9670	0.1660	H	0	0						
-1.3980	-3.1170	1.3920	H	0	0						
-3.2420	-2.3990	2.8500	H	0	0						
-4.9120	-0.7380	2.1330	H	0	0						
-4.0630	-0.4830	0.6290	H	0	0						
-3.5080	1.3180	2.2050	H	0	0						
-3.0270	0.1620	3.4240	H	0	0						
-5.1620	-3.2230	1.5020	H	0	0						
-3.7150	-4.1840	1.2090	H	0	0						
-4.2290	-2.9830	0.0270	H	0	0						

0.4810	3.4630	2.9590	H	0	0
1.4690	1.5980	4.2770	H	0	0
2.7070	2.8300	4.0620	H	0	0
2.7310	1.3750	3.0680	H	0	0
2.6170	4.3940	1.9690	H	0	0
2.7500	2.9450	0.9510	H	0	0
1.4140	4.0700	0.7240	H	0	0
0.6720	-4.0920	-2.3970	H	0	0
2.4300	-4.8790	-3.9670	H	0	0
3.7600	-3.2130	-5.2620	H	0	0
2	3	2		0	
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1	6	2		0	
5	7	1		0	
7	8	2		0	
7	9	1		0	
1	10	1		0	
11	12	2		0	
13	11	1		0	
17	18	1		0	
16	17	1		0	
15	16	1		0	
14	15	1		0	
18	13	1		0	
13	14	1		0	
16	19	1		0	
20	21	1		0	
20	22	1		0	
20	23	1		0	
11	23	1		0	
4	23	1		0	
10	24	1		0	
24	25	2		0	
24	26	1		0	
25	27	1		0	
27	28	2		0	
28	29	1		0	
29	26	2		0	
26	30	1		0	
5	6	1		0	
4	5	2		0	
3	4	1		0	
30	33	1		0	
30	32	1		0	
30	31	1		0	
2	34	1		0	
3	35	1		0	
6	36	1		0	
9	37	1		0	
13	38	1		0	
14	39	1		0	
14	40	1		0	
15	41	1		0	
15	42	1		0	
16	43	1		0	
17	44	1		0	
17	45	1		0	
18	46	1		0	
18	47	1		0	
19	48	1		0	
19	49	1		0	

```

19 50 1 0
20 51 1 0
21 52 1 0
21 53 1 0
21 54 1 0
22 55 1 0
22 56 1 0
22 57 1 0
27 58 1 0
28 59 1 0
29 60 1 0

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M END

> <Name>

Compound35

> <Activ>

0.08

> <DB_Ref_id>

1.46

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Compound36

SciTegic10081411483D

```

60 62 0 0 0 0          999 V2000
  2.5160   1.0390   0.8300 C   0 0
  2.2890  -0.0980   0.0370 C   0 0
  1.1780  -0.1520  -0.8200 C   0 0
  0.2830   0.9340  -0.8930 C   0 0
  0.5120   2.0800  -0.0980 C   0 0
  1.6270   2.1250   0.7600 C   0 0
 -0.4120   3.2600  -0.1410 C   0 0
  0.0040   4.3830   0.0310 O   0 0
 -1.6890   2.9730  -0.3770 O   0 0
  3.5590   1.0880   1.6330 O   0 0
 -1.9900   0.3810  -1.2810 C   0 0
 -2.9430   0.3110  -2.0220 O   0 0
 -2.0940  -0.0490   0.1620 C   0 0 1 0 0 0
 -3.5160   0.1720   0.7110 C   0 0
 -4.5310  -0.8140   0.1090 C   0 0
 -4.1000  -2.2790   0.2950 C   0 0 1 0 0 0
 -2.6800  -2.5020  -0.2580 C   0 0
 -1.6620  -1.5180   0.3420 C   0 0
 -4.1950  -2.7050   1.7660 C   0 0
 -0.6740   1.2720  -3.1450 C   0 0
 -1.3960   2.5980  -3.3850 C   0 0
  0.7910   1.3110  -3.5820 C   0 0
 -0.7930   0.8540  -1.7400 N   0 0
  4.4180   0.0880   1.5920 C   0 0
  5.3750   0.0180   0.5640 C   0 0
  4.4010  -0.9260   2.5680 C   0 0
  6.2850  -1.0570   0.5370 C   0 0
  6.2600  -2.0330   1.4880 N   0 0
  5.3360  -1.9770   2.4920 C   0 0
  3.4080  -0.8950   3.6760 C   0 0
  3.5450   0.2730   4.3810 F   0 0
  3.6230  -1.9590   4.5120 F   0 0
  2.1410  -0.9710   3.1560 F   0 0
  2.9690  -0.9360   0.0880 H   0 0
  1.0260  -1.0390  -1.4200 H   0 0

```

1.8070	2.9980	1.3710	H	0	0
-2.3360	3.6900	-0.4180	H	0	0
-1.4080	0.5780	0.7320	H	0	0
-3.8400	1.1970	0.5330	H	0	0
-3.5020	0.0470	1.7950	H	0	0
-4.6450	-0.6050	-0.9550	H	0	0
-5.5140	-0.6520	0.5530	H	0	0
-4.7850	-2.9100	-0.2700	H	0	0
-2.3590	-3.5270	-0.0700	H	0	0
-2.6950	-2.3850	-1.3420	H	0	0
-1.5530	-1.7270	1.4060	H	0	0
-0.6780	-1.6840	-0.0980	H	0	0
-3.9280	-3.7520	1.9040	H	0	0
-5.2090	-2.5660	2.1410	H	0	0
-3.5270	-2.1050	2.3850	H	0	0
-1.1990	0.4510	-3.6330	H	0	0
-1.4260	2.8570	-4.4430	H	0	0
-0.8960	3.4100	-2.8560	H	0	0
-2.4240	2.5470	-3.0250	H	0	0
1.2640	0.3400	-3.4320	H	0	0
0.8730	1.5860	-4.6330	H	0	0
1.3480	2.0470	-3.0000	H	0	0
5.4120	0.7810	-0.1990	H	0	0
7.0200	-1.1070	-0.2540	H	0	0
5.3280	-2.7580	3.2380	H	0	0
2	3	2	0		
1	2	1	0		
1	6	2	0		
5	7	1	0		
7	8	2	0		
7	9	1	0		
1	10	1	0		
11	12	2	0		
13	11	1	0		
17	18	1	0		
16	17	1	0		
15	16	1	0		
14	15	1	0		
18	13	1	0		
13	14	1	0		
16	19	1	0		
20	21	1	0		
20	22	1	0		
20	23	1	0		
11	23	1	0		
4	23	1	0		
10	24	1	0		
24	25	2	0		
24	26	1	0		
25	27	1	0		
27	28	2	0		
28	29	1	0		
29	26	2	0		
26	30	1	0		
5	6	1	0		
4	5	2	0		
3	4	1	0		
30	33	1	0		
30	32	1	0		
30	31	1	0		
2	34	1	0		

```

3 35 1 0
6 36 1 0
9 37 1 0
13 38 1 0
14 39 1 0
14 40 1 0
15 41 1 0
15 42 1 0
16 43 1 0
17 44 1 0
17 45 1 0
18 46 1 0
18 47 1 0
19 48 1 0
19 49 1 0
19 50 1 0
20 51 1 0
21 52 1 0
21 53 1 0
21 54 1 0
22 55 1 0
22 56 1 0
22 57 1 0
25 58 1 0
27 59 1 0
29 60 1 0

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M END

> <Name>

Compound36

> <Activ>

0.19

> <DB_Ref_id>

1.47

\$\$\$\$

Compound37

SciTegic10081411483D

```

30 32 0 0 0 0          999 V2000
  4.1990 -0.0060  0.8930 C  0 0
  1.8550 -0.5310  0.4980 C  0 0
  3.1990 -0.5510  0.0660 C  0 0
  1.5140  0.0080  1.7070 N  0 0
  3.8320  0.5430  2.1330 C  0 0
  2.4760  0.5370  2.5160 C  0 0
  0.9080 -1.0370 -0.2660 O  0 0
 -0.2870 -0.4360 -0.3380 C  0 0
 -2.7230 -0.5740 -0.5370 C  0 0
 -1.4630 -1.2130 -0.4610 C  0 0
 -2.8130  0.8480 -0.4900 C  0 0
 -0.3710  0.9770 -0.2930 C  0 0
 -1.6290  1.6190 -0.3690 C  0 0
 -5.1990  0.6480 -0.6870 C  0 0
 -5.1640 -0.6480 -0.7340 N  0 0
 -3.9850 -1.3730 -0.6680 C  0 0
 -4.0690 -2.5780 -0.7210 O  0 0
 -4.0450  1.4160 -0.5660 N  0 0
  3.5640 -1.1390 -1.2500 C  0 0
  3.1970 -2.4590 -1.2770 F  0 0

```

4.9180	-1.0350	-1.4360	F	0	0
2.9140	-0.4630	-2.2480	F	0	0
5.2340	-0.0100	0.5840	H	0	0
4.5800	0.9670	2.7850	H	0	0
2.1910	0.9590	3.4670	H	0	0
-1.3930	-2.2910	-0.4940	H	0	0
0.5290	1.5660	-0.2010	H	0	0
-1.6740	2.6990	-0.3320	H	0	0
-6.1560	1.1450	-0.7460	H	0	0
-4.1410	2.4120	-0.5350	H	0	0
1	5	2	0		
4	2	1	0		
3	1	1	0		
2	7	1	0		
7	8	1	0		
13	11	2	0		
12	13	1	0		
9	10	2	0		
11	9	1	0		
10	8	1	0		
8	12	2	0		
15	16	1	0		
14	15	2	0		
9	16	1	0		
16	17	2	0		
3	19	1	0		
14	18	1	0		
11	18	1	0		
6	4	2	0		
5	6	1	0		
2	3	2	0		
19	22	1	0		
19	21	1	0		
19	20	1	0		
1	23	1	0		
5	24	1	0		
6	25	1	0		
10	26	1	0		
12	27	1	0		
13	28	1	0		
14	29	1	0		
18	30	1	0		

M END

> <Name>

Compound37

> <Activ>

4.4

> <DB_Ref_id>

2.11

\$\$\$\$

Compound38

SciTegic10081411483D

46	49	0	0	0	0	999	V2000
5.8580	-1.4160	0.3500	C	0	0		
3.5160	-1.9450	-0.0410	C	0	0		
4.8580	-1.9610	-0.4750	C	0	0		
3.1740	-1.4060	1.1660	N	0	0		

5.4900	-0.8650	1.5900	C	0	0
4.1370	-0.8750	1.9750	C	0	0
2.5680	-2.4530	-0.8050	O	0	0
1.3710	-1.8510	-0.8770	C	0	0
-1.0640	-1.9920	-1.0760	C	0	0
0.1970	-2.6290	-0.9980	C	0	0
-1.1620	-0.5680	-1.0290	C	0	0
1.2850	-0.4410	-0.8320	C	0	0
0.0270	0.2010	-0.9080	C	0	0
-3.5530	-0.7950	-1.2280	C	0	0
-3.5040	-2.0900	-1.2730	N	0	0
-2.3180	-2.8010	-1.2070	C	0	0
-2.3930	-4.0080	-1.2580	O	0	0
-2.4080	-0.0100	-1.1070	N	0	0
-2.5920	1.4570	-1.0660	C	0	0
-2.5250	1.9750	0.3650	C	0	0
-3.7480	1.5710	1.1840	C	0	0
-3.5960	2.4630	2.4080	C	0	0
-3.1430	3.8050	1.8360	C	0	0
-2.5960	3.4980	0.4400	C	0	0
5.2230	-2.5490	-1.7910	C	0	0
6.5780	-2.4450	-1.9780	F	0	0
4.5700	-1.8750	-2.7890	F	0	0
4.8600	-3.8710	-1.8180	F	0	0
6.8930	-1.4180	0.0390	H	0	0
6.2400	-0.4410	2.2400	H	0	0
3.8520	-0.4530	2.9260	H	0	0
0.2720	-3.7070	-1.0330	H	0	0
2.1840	0.1530	-0.7400	H	0	0
-0.0040	1.2790	-0.8710	H	0	0
-4.5200	-0.3140	-1.2870	H	0	0
-3.5470	1.7110	-1.5250	H	0	0
-1.8300	1.9320	-1.6840	H	0	0
-1.6250	1.6210	0.8460	H	0	0
-4.6660	1.7890	0.6540	H	0	0
-3.7440	0.5200	1.4400	H	0	0
-4.5140	2.5450	2.9730	H	0	0
-2.8380	2.0630	3.0670	H	0	0
-3.9690	4.4980	1.7680	H	0	0
-2.3930	4.2580	2.4690	H	0	0
-3.2730	3.8830	-0.3090	H	0	0
-1.6310	3.9550	0.2720	H	0	0
1	5	2	0		
4	2	1	0		
3	1	1	0		
2	7	1	0		
7	8	1	0		
13	11	2	0		
12	13	1	0		
9	10	2	0		
11	9	1	0		
10	8	1	0		
8	12	2	0		
15	16	1	0		
14	15	2	0		
9	16	1	0		
16	17	2	0		
3	25	1	0		
14	18	1	0		
11	18	1	0		
18	19	1	0		

```

20 19 1 0
23 24 1 0
22 23 1 0
21 22 1 0
21 20 1 0
24 20 1 0
6 4 2 0
5 6 1 0
2 3 2 0
25 28 1 0
25 27 1 0
25 26 1 0
1 29 1 0
5 30 1 0
6 31 1 0
10 32 1 0
12 33 1 0
13 34 1 0
14 35 1 0
19 36 1 0
19 37 1 0
20 38 1 0
21 39 1 0
21 40 1 0
22 41 1 0
22 42 1 0
23 43 1 0
23 44 1 0
24 45 1 0
24 46 1 0

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M END

> <Name>

Compound38

> <Activ>

2.4

> <DB_Ref_id>

2.14

\$\$\$\$

Compound39

SciTegic10081411483D

```

43 46 0 0 0 0          999 V2000
5.4550 -1.1860 0.3460 C 0 0
3.1130 -1.7030 -0.0630 C 0 0
4.4590 -1.7270 -0.4880 C 0 0
2.7680 -1.1660 1.1430 N 0 0
5.0840 -0.6370 1.5820 C 0 0
3.7270 -0.6390 1.9570 C 0 0
2.1680 -2.2070 -0.8340 O 0 0
0.9730 -1.6060 -0.9060 C 0 0
-1.4630 -1.7460 -1.1060 C 0 0
-0.2010 -2.3830 -1.0270 C 0 0
-1.5610 -0.3240 -1.0590 C 0 0
0.8870 -0.1950 -0.8610 C 0 0
-0.3710 0.4450 -0.9380 C 0 0
-2.8070 0.2360 -1.1370 N 0 0
-3.9510 -0.5490 -1.2580 C 0 0
-3.9020 -1.8440 -1.3030 N 0 0

```

-2.7170	-2.5550	-1.2340	C	0	0
-2.7910	-3.7620	-1.2870	O	0	0
-2.9900	1.7030	-1.0960	C	0	0
-2.9300	2.2230	0.2970	C	0	0
-1.8730	3.6350	1.9750	C	0	0
-1.9300	3.1450	0.6600	C	0	0
-2.8120	3.2070	2.9280	C	0	0
-3.8690	1.7930	1.2500	C	0	0
-3.8110	2.2850	2.5660	C	0	0
4.8300	-2.3130	-1.8030	C	0	0
6.1880	-2.2150	-1.9810	F	0	0
4.1880	-1.6350	-2.8050	F	0	0
4.4610	-3.6330	-1.8340	F	0	0
6.4920	-1.1910	0.0410	H	0	0
5.8300	-0.2150	2.2400	H	0	0
3.4360	-0.2170	2.9080	H	0	0
-0.1270	-3.4610	-1.0630	H	0	0
1.7850	0.3980	-0.7680	H	0	0
-0.4020	1.5250	-0.8980	H	0	0
-4.9180	-0.0680	-1.3160	H	0	0
-3.9550	1.9550	-1.5350	H	0	0
-2.2150	2.1780	-1.6950	H	0	0
-1.1050	4.3440	2.2540	H	0	0
-1.2050	3.4790	-0.0680	H	0	0
-2.7680	3.5840	3.9390	H	0	0
-4.6390	1.0860	0.9780	H	0	0
-4.5310	1.9550	3.2990	H	0	0
1	5	2	0		
4	2	1	0		
3	1	1	0		
2	7	1	0		
7	8	1	0		
13	11	2	0		
12	13	1	0		
9	10	2	0		
11	9	1	0		
10	8	1	0		
8	12	2	0		
16	17	1	0		
15	16	2	0		
14	15	1	0		
11	14	1	0		
9	17	1	0		
17	18	2	0		
3	26	1	0		
14	19	1	0		
19	20	1	0		
25	23	2	0		
24	25	1	0		
21	22	2	0		
23	21	1	0		
22	20	1	0		
20	24	2	0		
6	4	2	0		
5	6	1	0		
2	3	2	0		
26	29	1	0		
26	28	1	0		
26	27	1	0		
1	30	1	0		
5	31	1	0		


```

6 32 1 0
10 33 1 0
12 34 1 0
13 35 1 0
15 36 1 0
19 37 1 0
19 38 1 0
21 39 1 0
22 40 1 0
23 41 1 0
24 42 1 0
25 43 1 0

```

M END

> <Name>

Compound39

> <Activ>

1.6

> <DB_Ref_id>

2.15

\$\$\$\$

Compound40

SciTegic10081411483D

```

49 52 0 0 0 0          999 V2000
-4.1760    0.6110    4.8830 C    0 0
-3.1640   -0.6680    3.0760 C    0 0
-3.2360   -0.3400    4.4470 C    0 0
-3.9940   -0.0740    2.1700 N    0 0
-5.0210    1.2130    3.9380 C    0 0
-4.9080    0.8500    2.5820 C    0 0
-2.2870   -1.5570    2.6540 O    0 0
-1.6850   -1.3940    1.4690 C    0 0
-0.7910   -2.3420   -0.6050 C    0 0
-1.4280   -2.5160    0.6480 C    0 0
-0.4100   -1.0410   -1.0490 C    0 0
-1.3090   -0.1000    1.0390 C    0 0
-0.6740    0.0780   -0.2130 C    0 0
 0.4450   -2.0530   -3.0610 C    0 0
 0.1130   -3.2500   -2.6910 N    0 0
-0.5120   -3.5200   -1.4860 C    0 0
-0.7750   -4.6760   -1.2460 O    0 0
 0.2010   -0.9320   -2.2700 N    0 0
 0.6250    0.3810   -2.7990 C    0 0
 3.1130   -0.0590   -2.6250 C    0 0
 4.4550    0.4000   -2.0350 C    0 0
 4.7270    1.8810   -2.3360 C    0 0
 1.9450    0.8280   -2.1620 C    0 0
 2.2270    2.3130   -2.4530 C    0 0
 3.5680    2.7720   -1.8610 C    0 0
-2.3280   -0.9880    5.4320 C    0 0
-2.5940   -0.5060    6.6880 F    0 0
-1.0250   -0.7170    5.1040 F    0 0
-2.5290   -2.3460    5.4140 F    0 0
-4.2500    0.8790    5.9280 H    0 0
-5.7520    1.9450    4.2480 H    0 0
-5.5590    1.3110    1.8540 H    0 0
-1.7190   -3.5020    0.9820 H    0 0
-1.5060    0.7560    1.6660 H    0 0

```

-0.4000	1.0800	-0.5120	H	0	0
0.9300	-1.9260	-4.0200	H	0	0
-0.1600	1.1130	-2.6130	H	0	0
0.7230	0.3150	-3.8810	H	0	0
2.9300	-1.0980	-2.3480	H	0	0
3.1760	-0.0350	-3.7150	H	0	0
5.2640	-0.2130	-2.4340	H	0	0
4.4510	0.2440	-0.9550	H	0	0
5.6560	2.1950	-1.8630	H	0	0
4.8650	2.0120	-3.4100	H	0	0
1.8440	0.7110	-1.0820	H	0	0
1.4220	2.9300	-2.0550	H	0	0
2.2360	2.4750	-3.5310	H	0	0
3.5140	2.7460	-0.7730	H	0	0
3.7600	3.8090	-2.1390	H	0	0
1	5	2	0		
4	2	1	0		
3	1	1	0		
2	7	1	0		
7	8	1	0		
13	11	2	0		
12	13	1	0		
9	10	2	0		
11	9	1	0		
10	8	1	0		
8	12	2	0		
15	16	1	0		
14	15	2	0		
9	16	1	0		
16	17	2	0		
3	26	1	0		
14	18	1	0		
11	18	1	0		
18	19	1	0		
20	21	1	0		
21	22	1	0		
20	23	1	0		
23	24	1	0		
22	25	1	0		
25	24	1	0		
23	19	1	0		
6	4	2	0		
5	6	1	0		
2	3	2	0		
26	29	1	0		
26	28	1	0		
26	27	1	0		
1	30	1	0		
5	31	1	0		
6	32	1	0		
10	33	1	0		
12	34	1	0		
13	35	1	0		
14	36	1	0		
19	37	1	0		
19	38	1	0		
20	39	1	0		
20	40	1	0		
21	41	1	0		
21	42	1	0		
22	43	1	0		

22 44 1 0
23 45 1 0
24 46 1 0
24 47 1 0
25 48 1 0
25 49 1 0

M END

> <Name>

Compound40

> <Activ>

4.3

> <DB_Ref_id>

2.13

\$\$\$\$

Compound41

SciTegic10081411483D

43	46	0	0	0	0	999	V2000
6.1500	-1.1720	0.8590	C	0	0		
3.8140	-1.6410	0.3590	C	0	0		
5.1740	-1.6780	-0.0180	C	0	0		
3.4360	-1.1190	1.5640	N	0	0		
5.7440	-0.6410	2.0940	C	0	0		
4.3750	-0.6270	2.4220	C	0	0		
2.8890	-2.1110	-0.4510	O	0	0		
1.6930	-1.5100	-0.5250	C	0	0		
-0.7440	-1.6500	-0.7230	C	0	0		
0.5180	-2.2870	-0.6470	C	0	0		
-0.8420	-0.2280	-0.6780	C	0	0		
-2.0880	0.3320	-0.7560	N	0	0		
-3.2330	-0.4530	-0.8770	C	0	0		
-3.1840	-1.7480	-0.9220	N	0	0		
-1.9980	-2.4590	-0.8540	C	0	0		
-2.0720	-3.6660	-0.9040	O	0	0		
-5.8690	2.9770	-0.3730	C	0	0		
-5.0200	2.4200	1.8400	C	0	0		
-6.0630	2.8730	1.0160	C	0	0		
-3.7790	2.0670	1.2750	C	0	0		
-4.6310	2.6250	-0.9400	C	0	0		
-3.5840	2.1700	-0.1150	C	0	0		
-7.2360	3.2070	1.5510	F	0	0		
-2.2720	1.7990	-0.7130	C	0	0		
-4.4630	2.7270	-2.2560	F	0	0		
0.3480	0.5410	-0.5550	C	0	0		
1.6070	-0.1000	-0.4810	C	0	0		
-2.7990	1.6350	2.0680	F	0	0		
5.5800	-2.2460	-1.3300	C	0	0		
5.1890	-3.5590	-1.4020	F	0	0		
6.9430	-2.1700	-1.4610	F	0	0		
4.9840	-1.5370	-2.3400	F	0	0		
7.1970	-1.1910	0.5920	H	0	0		
6.4750	-0.2460	2.7830	H	0	0		
4.0610	-0.2170	3.3710	H	0	0		
0.5920	-3.3650	-0.6800	H	0	0		
-4.1990	0.0270	-0.9360	H	0	0		
-6.6720	3.3240	-1.0060	H	0	0		
-5.1660	2.3400	2.9060	H	0	0		
-1.4670	2.2440	-0.1290	H	0	0		

-2.2090	2.1950	-1.7270	H	0	0
0.3160	1.6210	-0.5180	H	0	0
2.5040	0.4940	-0.3870	H	0	0

1	5	2	0
4	2	1	0
3	1	1	0
2	7	1	0
7	8	1	0
9	10	2	0
11	9	1	0
10	8	1	0
8	27	2	0
14	15	1	0
13	14	2	0
12	13	1	0
11	12	1	0
9	15	1	0
15	16	2	0
3	29	1	0
12	24	1	0
22	20	2	0
21	22	1	0
18	19	2	0
20	18	1	0
19	17	1	0
17	21	2	0
19	23	1	0
21	25	1	0
27	26	1	0
11	26	2	0
20	28	1	0
24	22	1	0
6	4	2	0
5	6	1	0
2	3	2	0
29	32	1	0
29	31	1	0
29	30	1	0
1	33	1	0
5	34	1	0
6	35	1	0
10	36	1	0
13	37	1	0
17	38	1	0
18	39	1	0
24	40	1	0
24	41	1	0
26	42	1	0
27	43	1	0

M END

> <Name>
Compound41

> <Activ>
0.1

> <DB_Ref_id>
2.3

\$\$\$\$
Compound42

SciTegic10081411483D

46	49	0	0	0	0	999	V2000
		3.9790	-4.8520	-0.1580	C	0	0
		2.9470	-2.6640	-0.4300	C	0	0
		3.8520	-3.6500	-0.8790	C	0	0
		2.1950	-2.8610	0.6950	N	0	0
		3.1990	-5.0390	0.9960	C	0	0
		2.3130	-4.0230	1.4000	C	0	0
		2.8170	-1.5330	-1.0940	O	0	0
		1.6210	-0.9340	-1.1680	C	0	0
		-0.8160	-1.0720	-1.3650	C	0	0
		0.4470	-1.7110	-1.2890	C	0	0
		-0.9140	0.3500	-1.3200	C	0	0
		1.5350	0.4790	-1.1210	C	0	0
		0.2750	1.1190	-1.1970	C	0	0
		-2.1600	0.9100	-1.3980	N	0	0
		-3.3030	0.1230	-1.5180	C	0	0
		-3.2560	-1.1720	-1.5640	N	0	0
		-2.0700	-1.8830	-1.4960	C	0	0
		-2.1430	-3.0900	-1.5470	O	0	0
		-2.3440	2.3750	-1.3550	C	0	0
		-2.3010	2.8930	0.0370	C	0	0
		-1.2710	4.3070	1.7320	C	0	0
		-1.3120	3.8170	0.4160	C	0	0
		-2.2230	3.8730	2.6740	C	0	0
		-3.2520	2.4590	0.9790	C	0	0
		-3.2110	2.9470	2.2950	C	0	0
		-2.1800	4.3910	4.0670	C	0	0
		4.6660	-3.4320	-2.1040	C	0	0
		5.4550	-2.3220	-1.9340	F	0	0
		3.8360	-3.2400	-3.1780	F	0	0
		5.4590	-4.5270	-2.3260	F	0	0
		4.6640	-5.6210	-0.4820	H	0	0
		3.2790	-5.9510	1.5660	H	0	0
		1.7130	-4.1640	2.2870	H	0	0
		0.5200	-2.7890	-1.3220	H	0	0
		2.4340	1.0700	-1.0290	H	0	0
		0.2440	2.1990	-1.1600	H	0	0
		-4.2700	0.6040	-1.5780	H	0	0
		-1.5590	2.8520	-1.9450	H	0	0
		-3.3010	2.6290	-1.8110	H	0	0
		-0.5100	5.0160	2.0180	H	0	0
		-0.5780	4.1540	-0.3030	H	0	0
		-4.0140	1.7480	0.6950	H	0	0
		-3.9450	2.6090	3.0140	H	0	0
		-2.9980	3.9530	4.6410	H	0	0
		-1.2030	4.1840	4.5020	H	0	0
		-2.3200	5.4710	4.0570	H	0	0
1	5	2	0				
4	2	1	0				
3	1	1	0				
2	7	1	0				
7	8	1	0				
13	11	2	0				
12	13	1	0				
9	10	2	0				
11	9	1	0				
10	8	1	0				
8	12	2	0				
16	17	1	0				

```

15 16 2 0
14 15 1 0
11 14 1 0
9 17 1 0
17 18 2 0
3 27 1 0
14 19 1 0
19 20 1 0
25 23 2 0
24 25 1 0
21 22 2 0
23 21 1 0
22 20 1 0
20 24 2 0
23 26 1 0
6 4 2 0
5 6 1 0
2 3 2 0
27 30 1 0
27 29 1 0
27 28 1 0
1 31 1 0
5 32 1 0
6 33 1 0
10 34 1 0
12 35 1 0
13 36 1 0
15 37 1 0
19 38 1 0
19 39 1 0
21 40 1 0
22 41 1 0
24 42 1 0
25 43 1 0
26 44 1 0
26 45 1 0
26 46 1 0
M END
> <Name>
Compound42

> <Activ>
0.45

> <DB_Ref_id>
2.16

$$$$
Compound43
SciTegic10081411483D

40 43 0 0 0 0 999 V2000
3.9920 -0.8730 1.8500 C 0 0
3.4590 -1.9040 -0.2110 C 0 0
3.0670 -1.3710 0.9840 N 0 0
5.3650 -0.8910 1.5430 C 0 0
5.7890 -1.4340 0.3180 C 0 0
2.5330 -2.3750 -1.0220 O 0 0
1.3360 -1.7750 -1.0940 C 0 0
-1.1000 -1.9140 -1.2930 C 0 0
0.1620 -2.5530 -1.2170 C 0 0

```

-1.1970	-0.4920	-1.2480	C	0	0
-2.4430	0.0680	-1.3260	N	0	0
-3.5880	-0.7170	-1.4450	C	0	0
-3.5390	-2.0140	-1.4920	N	0	0
-2.3540	-2.7250	-1.4240	C	0	0
-2.4280	-3.9300	-1.4750	O	0	0
-3.4100	2.2210	2.3730	C	0	0
-1.3630	3.3950	1.7710	C	0	0
-2.3380	3.0570	2.7290	C	0	0
-1.4630	2.8960	0.4630	C	0	0
-3.5120	1.7210	1.0620	C	0	0
-2.5350	2.0590	0.1050	C	0	0
-2.2420	3.5270	3.9710	F	0	0
-2.6270	1.5330	-1.2830	C	0	0
-4.5330	0.9320	0.7380	F	0	0
-0.0080	0.2770	-1.1250	C	0	0
1.2520	-0.3630	-1.0490	C	0	0
4.8280	-1.9470	-0.5700	C	0	0
5.3830	-2.6820	-2.2190	Br	0	0
3.6660	-0.4550	2.7910	H	0	0
6.0860	-0.4900	2.2400	H	0	0
6.8440	-1.4490	0.0780	H	0	0
0.2360	-3.6310	-1.2500	H	0	0
-4.5550	-0.2380	-1.5040	H	0	0
-4.1580	1.9630	3.1090	H	0	0
-0.5390	4.0390	2.0390	H	0	0
-0.7110	3.1580	-0.2680	H	0	0
-1.8650	2.0080	-1.9020	H	0	0
-3.6020	1.7850	-1.7030	H	0	0
-0.0390	1.3570	-1.0880	H	0	0
2.1490	0.2280	-0.9570	H	0	0
4	5	2	0		
2	3	1	0		
1	4	1	0		
3	1	2	0		
2	6	1	0		
6	7	1	0		
8	9	2	0		
10	8	1	0		
9	7	1	0		
7	26	2	0		
13	14	1	0		
12	13	2	0		
11	12	1	0		
10	11	1	0		
8	14	1	0		
14	15	2	0		
11	23	1	0		
21	19	2	0		
20	21	1	0		
17	18	2	0		
19	17	1	0		
18	16	1	0		
16	20	2	0		
18	22	1	0		
20	24	1	0		
26	25	1	0		
10	25	2	0		
23	21	1	0		
5	27	1	0		
27	2	2	0		

```

27 28 1 0
1 29 1 0
4 30 1 0
5 31 1 0
9 32 1 0
12 33 1 0
16 34 1 0
17 35 1 0
19 36 1 0
23 37 1 0
23 38 1 0
25 39 1 0
26 40 1 0

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M END

> <Name>

Compound43

> <Activ>

0.86

> <DB_Ref_id>

2.44

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Compound44

SciTegic10081411483D

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43 46 0 0 0 0          999 V2000
  3.2580  4.3400  -2.3220 C  0  0
  2.4530  2.4610  -1.0000 C  0  0
  3.2340  3.6330  -1.1070 C  0  0
  1.7230  2.0080  -2.0610 N  0  0
  2.5000  3.8600  -3.4020 C  0  0
  1.7400  2.6880  -3.2440 C  0  0
  2.4220  1.7890   0.1330 O  0  0
  1.3090  1.1330   0.4920 C  0  0
 -1.1330  1.0430   0.6620 C  0  0
  0.0450  1.7350   0.2870 C  0  0
 -1.0570 -0.2540   1.2480 C  0  0
  1.3960 -0.1540   1.0740 C  0  0
  0.2210 -0.8460   1.4510 C  0  0
 -2.2290 -0.8730   1.5920 N  0  0
 -3.4610 -0.2630   1.3770 C  0  0
 -3.5700  0.9160   0.8500 N  0  0
 -2.4790  1.6660   0.4510 C  0  0
 -2.6990  2.7540  -0.0310 O  0  0
 -2.2330 -2.2190   2.2010 C  0  0
 -2.0200 -3.2830   1.1860 C  0  0
 -2.7600 -4.5120  -0.7850 C  0  0
 -2.9750 -3.5060   0.1740 C  0  0
 -1.5960 -5.2990  -0.7320 C  0  0
 -0.8560 -4.0700   1.2340 C  0  0
 -0.6450 -5.0780   0.2770 C  0  0
 -4.0820 -2.7690   0.1130 F  0  0
 -1.3930 -6.2500  -1.6410 F  0  0
  2.5860 -0.7210   1.2680 F  0  0
  4.0290  4.1230   0.0510 C  0  0
  4.9360  3.1640   0.4220 F  0  0
  3.1890  4.3910   1.1020 F  0  0
  4.6950  5.2680  -0.3030 F  0  0
  3.8480  5.2400  -2.4280 H  0  0

```


2.5020	4.3850	-4.3460	H	0	0
1.1560	2.3150	-4.0720	H	0	0
-0.0140	2.7170	-0.1580	H	0	0
0.3160	-1.8260	1.8950	H	0	0
-4.3650	-0.7850	1.6620	H	0	0
-1.4450	-2.2730	2.9550	H	0	0
-3.1860	-2.3810	2.7050	H	0	0
-3.4920	-4.6830	-1.5610	H	0	0
-0.1210	-3.9060	2.0100	H	0	0
0.2520	-5.6800	0.3220	H	0	0
1	5	2	0		
4	2	1	0		
3	1	1	0		
2	7	1	0		
7	8	1	0		
13	11	2	0		
12	13	1	0		
9	10	2	0		
11	9	1	0		
10	8	1	0		
8	12	2	0		
16	17	1	0		
15	16	2	0		
14	15	1	0		
11	14	1	0		
9	17	1	0		
17	18	2	0		
3	29	1	0		
14	19	1	0		
19	20	1	0		
25	23	2	0		
24	25	1	0		
21	22	2	0		
23	21	1	0		
22	20	1	0		
20	24	2	0		
22	26	1	0		
23	27	1	0		
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6	4	2	0		
5	6	1	0		
2	3	2	0		
29	32	1	0		
29	31	1	0		
29	30	1	0		
1	33	1	0		
5	34	1	0		
6	35	1	0		
10	36	1	0		
13	37	1	0		
15	38	1	0		
19	39	1	0		
19	40	1	0		
21	41	1	0		
24	42	1	0		
25	43	1	0		

M END

> <Name>

Compound44

> <Activ>

0.24

> <DB_Ref_id>

2.37

\$\$\$\$

Compound45

SciTegic10081411483D

49	52	0	0	0	0	999	V2000
3.7600	-5.1880	2.1820	C	0	0		
2.7770	-2.9710	1.9730	C	0	0		
3.6370	-3.9750	1.4790	C	0	0		
2.0660	-3.1580	3.1230	N	0	0		
3.0220	-5.3650	3.3630	C	0	0		
2.1800	-4.3300	3.8130	C	0	0		
2.6500	-1.8300	1.3220	O	0	0		
1.4550	-1.2290	1.2500	C	0	0		
-0.9820	-1.3690	1.0510	C	0	0		
0.2810	-2.0080	1.1290	C	0	0		
-1.0780	0.0530	1.0980	C	0	0		
1.3690	0.1820	1.2950	C	0	0		
0.1110	0.8220	1.2190	C	0	0		
-3.4690	-0.1720	0.8980	C	0	0		
-3.4200	-1.4670	0.8540	N	0	0		
-2.2360	-2.1800	0.9220	C	0	0		
-2.3090	-3.3850	0.8690	O	0	0		
-2.3240	0.6130	1.0200	N	0	0		
-2.5080	2.0780	1.0610	C	0	0		
-2.2290	2.7030	-0.2580	C	0	0		
-2.7300	2.9390	-2.6310	C	0	0		
-2.9960	2.3500	-1.3830	C	0	0		
-1.6990	3.8850	-2.7580	C	0	0		
-1.1950	3.6480	-0.3850	C	0	0		
-0.9320	4.2380	-1.6330	C	0	0		
-1.4180	4.5100	-4.0780	C	0	0		
-0.4100	3.6910	-4.8850	C	0	0		
4.4080	-3.7640	0.2250	C	0	0		
5.2070	-2.6580	0.3590	F	0	0		
3.5410	-3.5760	-0.8200	F	0	0		
5.1880	-4.8650	-0.0230	F	0	0		
4.4120	-5.9710	1.8220	H	0	0		
3.1000	-6.2870	3.9220	H	0	0		
1.6110	-4.4650	4.7210	H	0	0		
0.3560	-3.0840	1.0940	H	0	0		
2.2680	0.7750	1.3890	H	0	0		
0.0780	1.9020	1.2580	H	0	0		
-4.4360	0.3090	0.8400	H	0	0		
-3.5330	2.3030	1.3590	H	0	0		
-1.8420	2.5020	1.8130	H	0	0		
-3.3240	2.6620	-3.4900	H	0	0		
-3.7910	1.6230	-1.2930	H	0	0		
-0.6030	3.9260	0.4750	H	0	0		
-0.1370	4.9650	-1.7250	H	0	0		
-2.3520	4.6250	-4.6290	H	0	0		
-1.0590	5.5270	-3.9280	H	0	0		
0.5390	3.6150	-4.3540	H	0	0		
-0.7910	2.6880	-5.0740	H	0	0		
-0.2150	4.1620	-5.8480	H	0	0		
1	5	2	0				
4	2	1	0				

3	1	1	0
2	7	1	0
7	8	1	0
13	11	2	0
12	13	1	0
9	10	2	0
11	9	1	0
10	8	1	0
8	12	2	0
15	16	1	0
14	15	2	0
9	16	1	0
16	17	2	0
3	28	1	0
14	18	1	0
11	18	1	0
18	19	1	0
20	19	1	0
21	22	2	0
21	23	1	0
20	22	1	0
20	24	2	0
23	25	2	0
24	25	1	0
23	26	1	0
26	27	1	0
6	4	2	0
5	6	1	0
2	3	2	0
28	31	1	0
28	30	1	0
28	29	1	0
1	32	1	0
5	33	1	0
6	34	1	0
10	35	1	0
12	36	1	0
13	37	1	0
14	38	1	0
19	39	1	0
19	40	1	0
21	41	1	0
22	42	1	0
24	43	1	0
25	44	1	0
26	45	1	0
26	46	1	0
27	47	1	0
27	48	1	0
27	49	1	0

M END

> <Name>

Compound45

> <Activ>

1.1

> <DB_Ref_id>

2.18

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Compound46
SciTegic10081411483D

43	46	0	0	0	0	999	V2000
3.8440	-0.5060	1.8830	C	0	0		
3.1250	-1.7010	-0.1000	C	0	0		
2.8090	-1.0570	1.1090	C	0	0		
5.1720	-0.6090	1.4300	C	0	0		
2.1680	-2.2250	-0.8400	O	0	0		
0.9730	-1.6230	-0.9140	C	0	0		
-1.4650	-1.7640	-1.1110	C	0	0		
-0.2010	-2.4000	-1.0350	C	0	0		
-1.5610	-0.3420	-1.0670	C	0	0		
-2.8070	0.2190	-1.1450	N	0	0		
-3.9510	-0.5660	-1.2640	C	0	0		
-3.9020	-1.8610	-1.3110	N	0	0		
-2.7170	-2.5720	-1.2420	C	0	0		
-2.7910	-3.7790	-1.2930	O	0	0		
-1.5740	3.7710	1.7400	C	0	0		
-3.2230	2.2300	2.6520	C	0	0		
-2.2810	3.2580	2.8420	C	0	0		
-3.4550	1.7170	1.3650	C	0	0		
-1.8050	3.2600	0.4530	C	0	0		
-2.7460	2.2290	0.2620	C	0	0		
-2.0630	3.7440	4.0610	F	0	0		
-2.9900	1.6860	-1.1020	C	0	0		
-1.1250	3.7560	-0.5800	F	0	0		
-0.3710	0.4280	-0.9430	C	0	0		
0.8870	-0.2130	-0.8690	C	0	0		
4.4770	-1.7750	-0.5040	C	0	0		
5.4750	-1.2360	0.2560	N	0	0		
-4.3520	0.7440	1.2010	F	0	0		
4.8360	-2.4510	-1.7790	C	0	0		
4.2130	-1.8180	-2.8240	F	0	0		
4.4320	-3.7600	-1.7330	F	0	0		
6.1930	-2.3990	-1.9570	F	0	0		
3.6210	-0.0080	2.8140	H	0	0		
1.7810	-0.9860	1.4390	H	0	0		
5.9690	-0.1880	2.0210	H	0	0		
-0.1270	-3.4790	-1.0680	H	0	0		
-4.9180	-0.0860	-1.3240	H	0	0		
-0.8500	4.5630	1.8850	H	0	0		
-3.7660	1.8340	3.4980	H	0	0		
-2.3050	2.1520	-1.8090	H	0	0		
-4.0080	1.9280	-1.4140	H	0	0		
-0.4040	1.5080	-0.9060	H	0	0		
1.7850	0.3810	-0.7750	H	0	0		
2	5	1	0				
5	6	1	0				
7	8	2	0				
9	7	1	0				
8	6	1	0				
6	25	2	0				
12	13	1	0				
11	12	2	0				
10	11	1	0				
9	10	1	0				
7	13	1	0				
13	14	2	0				
10	22	1	0				
20	18	2	0				

```

19 20 1 0
16 17 2 0
18 16 1 0
17 15 1 0
15 19 2 0
17 21 1 0
19 23 1 0
25 24 1 0
9 24 2 0
22 20 1 0
26 2 2 0
26 29 1 0
4 27 2 0
27 26 1 0
18 28 1 0
2 3 1 0
1 4 1 0
3 1 2 0
29 32 1 0
29 31 1 0
29 30 1 0
1 33 1 0
3 34 1 0
4 35 1 0
8 36 1 0
11 37 1 0
15 38 1 0
16 39 1 0
22 40 1 0
22 41 1 0
24 42 1 0
25 43 1 0

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M END

> <Name>

Compound46

> <Activ>

0.06

> <DB_Ref_id>

2.47

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Compound47

SciTegic10081411483D

```

43 46 0 0 0 0          999 V2000
  5.4570 -1.1920  0.3300 C  0 0
  3.1150 -1.7090 -0.0760 C  0 0
  4.4610 -1.7310 -0.5020 C  0 0
  2.7680 -1.1680  1.1290 N  0 0
  5.0840 -0.6410  1.5680 C  0 0
  3.7290 -0.6430  1.9430 C  0 0
  2.1700 -2.2110 -0.8460 O  0 0
  0.9750 -1.6100 -0.9200 C  0 0
 -1.4630 -1.7500 -1.1190 C  0 0
 -0.1990 -2.3890 -1.0410 C  0 0
 -1.5600 -0.3280 -1.0720 C  0 0
  0.8890 -0.1990 -0.8750 C  0 0
 -0.3710  0.4410 -0.9510 C  0 0
 -3.9490 -0.5530 -1.2710 C  0 0

```

-3.9020	-1.8480	-1.3160	N	0	0
-2.7170	-2.5610	-1.2480	C	0	0
-2.7890	-3.7660	-1.3010	O	0	0
-2.8070	0.2320	-1.1500	N	0	0
-2.9900	1.6970	-1.1090	C	0	0
-2.9320	2.2170	0.2830	C	0	0
-1.8750	3.6250	1.9670	C	0	0
-1.9320	3.1350	0.6500	C	0	0
-2.8200	3.1990	2.9180	C	0	0
-3.8770	1.7930	1.2320	C	0	0
-3.8200	2.2830	2.5490	C	0	0
-2.7500	3.7970	4.5260	Cl	0	0
4.8320	-2.3200	-1.8160	C	0	0
6.1880	-2.2230	-1.9940	F	0	0
4.1900	-1.6410	-2.8180	F	0	0
4.4610	-3.6390	-1.8460	F	0	0
6.4940	-1.1970	0.0270	H	0	0
5.8320	-0.2190	2.2250	H	0	0
3.4380	-0.2190	2.8930	H	0	0
-0.1270	-3.4650	-1.0740	H	0	0
1.7870	0.3940	-0.7810	H	0	0
-0.4020	1.5210	-0.9120	H	0	0
-4.9160	-0.0720	-1.3300	H	0	0
-3.9530	1.9510	-1.5510	H	0	0
-2.2130	2.1740	-1.7070	H	0	0
-1.1010	4.3320	2.2340	H	0	0
-1.2010	3.4650	-0.0740	H	0	0
-4.6480	1.0900	0.9570	H	0	0
-4.5550	1.9470	3.2700	H	0	0
1	5	2	0		
4	2	1	0		
3	1	1	0		
2	7	1	0		
7	8	1	0		
13	11	2	0		
12	13	1	0		
9	10	2	0		
11	9	1	0		
10	8	1	0		
8	12	2	0		
15	16	1	0		
14	15	2	0		
9	16	1	0		
16	17	2	0		
3	27	1	0		
14	18	1	0		
11	18	1	0		
18	19	1	0		
20	19	1	0		
21	22	2	0		
21	23	1	0		
20	22	1	0		
20	24	2	0		
23	25	2	0		
24	25	1	0		
23	26	1	0		
6	4	2	0		
5	6	1	0		
2	3	2	0		
27	30	1	0		
27	29	1	0		

```

27 28 1 0
1 31 1 0
5 32 1 0
6 33 1 0
10 34 1 0
12 35 1 0
13 36 1 0
14 37 1 0
19 38 1 0
19 39 1 0
21 40 1 0
22 41 1 0
24 42 1 0
25 43 1 0

```

M END

> <Name>

Compound47

> <Activ>

1.1

> <DB_Ref_id>

2.19

\$\$\$\$

Compound48

SciTegic10081411483D

```

47 50 0 0 0 0          999 V2000
  2.8610 -4.8750   1.8480 C   0  0
  2.9180 -2.8090   0.5630 C   0  0
  2.7850 -3.4730   1.8030 C   0  0
  3.1190 -3.5100  -0.5900 N   0  0
  3.0680 -5.5820   0.6510 C   0  0
  3.1950 -4.8730  -0.5570 C   0  0
  2.8500 -1.4940   0.5060 O   0  0
  1.6560 -0.8870   0.4340 C   0  0
 -0.7810 -1.0240   0.2350 C   0  0
  0.4810 -1.6640   0.3130 C   0  0
 -0.8770  0.3980   0.2810 C   0  0
  1.5720  0.5250   0.4790 C   0  0
  0.3130  1.1660   0.4020 C   0  0
 -2.1230  0.9590   0.2030 N   0  0
 -3.2680  0.1760   0.0820 C   0  0
 -3.2210 -1.1190   0.0370 N   0  0
 -2.0370 -1.8320   0.1060 C   0  0
 -2.1110 -3.0390   0.0530 O   0  0
 -2.3050  2.4260   0.2440 C   0  0
 -2.6110  2.9780  -1.1010 C   0  0
 -1.8750  3.8070  -3.2710 C   0  0
 -1.5720  3.2870  -2.0020 C   0  0
 -3.2130  4.0180  -3.6460 C   0  0
 -3.9490  3.1910  -1.4780 C   0  0
 -4.2500  3.7110  -2.7480 C   0  0
 -0.2990  3.0940  -1.6580 F   0  0
 -3.5000  4.5060  -4.8520 F   0  0
  2.6880  1.2600   0.5940 O   0  0
  2.5470  2.6620   0.7700 C   0  0
  2.5670 -2.7010   3.0550 C   0  0
  3.3850 -1.6020   3.0650 F   0  0
  2.8580 -3.4940   4.1350 F   0  0

```

1.2580	-2.2990	3.1210	F	0	0
2.7640	-5.4050	2.7830	H	0	0
3.1310	-6.6600	0.6600	H	0	0
3.3540	-5.4140	-1.4780	H	0	0
0.5530	-2.7400	0.2770	H	0	0
0.2790	2.2460	0.4420	H	0	0
-4.2340	0.6560	0.0240	H	0	0
-1.3960	2.8890	0.6290	H	0	0
-3.1170	2.6660	0.9300	H	0	0
-1.0780	4.0430	-3.9630	H	0	0
-4.7520	2.9570	-0.7930	H	0	0
-5.2810	3.8730	-3.0310	H	0	0
2.1290	3.0800	-0.1460	H	0	0
1.9790	2.8360	1.6840	H	0	0
3.5410	3.0900	0.9080	H	0	0
1	5	2	0		
4	2	1	0		
3	1	1	0		
2	7	1	0		
7	8	1	0		
13	11	2	0		
12	13	1	0		
9	10	2	0		
11	9	1	0		
10	8	1	0		
8	12	2	0		
16	17	1	0		
15	16	2	0		
14	15	1	0		
11	14	1	0		
9	17	1	0		
17	18	2	0		
3	30	1	0		
14	19	1	0		
19	20	1	0		
25	23	2	0		
24	25	1	0		
21	22	2	0		
23	21	1	0		
22	20	1	0		
20	24	2	0		
22	26	1	0		
23	27	1	0		
12	28	1	0		
28	29	1	0		
6	4	2	0		
5	6	1	0		
2	3	2	0		
30	33	1	0		
30	32	1	0		
30	31	1	0		
1	34	1	0		
5	35	1	0		
6	36	1	0		
10	37	1	0		
13	38	1	0		
15	39	1	0		
19	40	1	0		
19	41	1	0		
21	42	1	0		
24	43	1	0		

25 44 1 0
29 45 1 0
29 46 1 0
29 47 1 0

M END

> <Name>

Compound48

> <Activ>

2.4

> <DB_Ref_id>

2.38

\$\$\$\$

Compound49

SciTegic10081411483D

43	46	0	0	0	0	999	V2000
5.3460	-1.3070	1.8520	C	0	0		
3.0080	-1.7640	1.3610	C	0	0		
4.3670	-1.8200	0.9840	C	0	0		
2.6330	-1.2190	2.5550	N	0	0		
4.9450	-0.7500	3.0760	C	0	0		
3.5760	-0.7170	3.4040	C	0	0		
2.0780	-2.2420	0.5570	O	0	0		
0.8810	-1.6410	0.4840	C	0	0		
-1.5550	-1.7810	0.2850	C	0	0		
-0.2930	-2.4180	0.3630	C	0	0		
-1.6520	-0.3590	0.3320	C	0	0		
0.7970	-0.2300	0.5290	C	0	0		
-0.4630	0.4120	0.4530	C	0	0		
-2.8980	0.2010	0.2540	N	0	0		
-4.0430	-0.5840	0.1330	C	0	0		
-3.9940	-1.8790	0.0880	N	0	0		
-2.8090	-2.5900	0.1560	C	0	0		
-2.8830	-3.7970	0.1040	O	0	0		
-3.0820	1.6680	0.2950	C	0	0		
-2.8380	2.2870	-1.0330	C	0	0		
-1.5840	3.8260	-2.4430	C	0	0		
-1.8140	3.2400	-1.1880	C	0	0		
-2.3750	3.4610	-3.5470	C	0	0		
-3.6290	1.9220	-2.1370	C	0	0		
-3.3970	2.5080	-3.3930	C	0	0		
-2.1540	4.0160	-4.7360	F	0	0		
4.7680	-2.4160	-0.3180	C	0	0		
4.3650	-3.7260	-0.3650	F	0	0		
6.1310	-2.3510	-0.4490	F	0	0		
4.1780	-1.7190	-1.3420	F	0	0		
6.3930	-1.3400	1.5840	H	0	0		
5.6800	-0.3480	3.7600	H	0	0		
3.2660	-0.2890	4.3440	H	0	0		
-0.2190	-3.4960	0.3280	H	0	0		
1.6930	0.3630	0.6230	H	0	0		
-0.4940	1.4900	0.4920	H	0	0		
-5.0100	-0.1030	0.0740	H	0	0		
-4.0980	1.8930	0.6190	H	0	0		
-2.3970	2.0940	1.0270	H	0	0		
-0.7970	4.5590	-2.5590	H	0	0		
-1.2030	3.5260	-0.3440	H	0	0		
-4.4160	1.1920	-2.0250	H	0	0		

```

-4.0080      2.2250    -4.2380 H    0    0
 1  5  2  0
 4  2  1  0
 3  1  1  0
 2  7  1  0
 7  8  1  0
13 11  2  0
12 13  1  0
 9 10  2  0
11  9  1  0
10  8  1  0
 8 12  2  0
16 17  1  0
15 16  2  0
14 15  1  0
11 14  1  0
 9 17  1  0
17 18  2  0
 3 27  1  0
14 19  1  0
19 20  1  0
25 23  2  0
24 25  1  0
21 22  2  0
23 21  1  0
22 20  1  0
20 24  2  0
23 26  1  0
 6  4  2  0
 5  6  1  0
 2  3  2  0
27 30  1  0
27 29  1  0
27 28  1  0
 1 31  1  0
 5 32  1  0
 6 33  1  0
10 34  1  0
12 35  1  0
13 36  1  0
15 37  1  0
19 38  1  0
19 39  1  0
21 40  1  0
22 41  1  0
24 42  1  0
25 43  1  0
M   END
> <Name>
Compound49

> <Activ>
1.2

> <DB_Ref_id>
2.2

$$$$
Compound50
SciTegic10081411483D

```

47	50	0	0	0	0	999	V2000
3.3010	-0.4770	-1.4080	C	0	0		
2.3750	-1.6820	0.4040	C	0	0		
2.2270	-1.0590	-0.8030	N	0	0		
4.5760	-0.5000	-0.8140	C	0	0		
1.3220	-2.2380	0.9690	O	0	0		
0.1270	-1.6370	0.8970	C	0	0		
-2.3110	-1.7750	0.6970	C	0	0		
-1.0470	-2.4140	0.7760	C	0	0		
-2.4060	-0.3540	0.7420	C	0	0		
-3.6520	0.2050	0.6660	N	0	0		
-4.7970	-0.5800	0.5450	C	0	0		
-4.7480	-1.8750	0.5000	N	0	0		
-3.5630	-2.5860	0.5670	C	0	0		
-3.6370	-3.7930	0.5160	O	0	0		
-3.9750	2.6230	-2.9730	C	0	0		
-2.1110	3.7890	-1.9280	C	0	0		
-2.8870	3.5080	-3.0640	C	0	0		
-2.4240	3.1860	-0.6970	C	0	0		
-4.2890	2.0180	-1.7420	C	0	0		
-3.5140	2.3010	-0.6010	C	0	0		
-2.5920	4.0800	-4.2300	F	0	0		
-3.8360	1.6720	0.7070	C	0	0		
-5.3220	1.1800	-1.6680	F	0	0		
-1.2170	0.4160	0.8650	C	0	0		
0.0410	-0.2250	0.9420	C	0	0		
3.6350	-1.7340	1.0430	C	0	0		
4.7500	-1.1350	0.4280	C	0	0		
3.7810	-2.4160	2.3580	C	0	0		
4.7790	-1.8130	3.0760	F	0	0		
4.0960	-3.7340	2.1540	F	0	0		
2.6020	-2.3280	3.0510	F	0	0		
5.9380	-1.1660	0.9960	O	0	0		
7.0290	-0.5900	0.2930	C	0	0		
3.1660	0.0140	-2.3610	H	0	0		
5.4140	-0.0310	-1.3080	H	0	0		
-0.9730	-3.4920	0.7400	H	0	0		
-5.7640	-0.1000	0.4870	H	0	0		
-4.5700	2.4060	-3.8480	H	0	0		
-1.2730	4.4670	-1.9940	H	0	0		
-1.8240	3.4060	0.1740	H	0	0		
-3.1930	2.0920	1.4810	H	0	0		
-4.8690	1.8970	0.9730	H	0	0		
-1.2500	1.4940	0.9030	H	0	0		
0.9400	0.3670	1.0330	H	0	0		
7.1640	-1.1410	-0.6390	H	0	0		
6.8500	0.4800	0.2010	H	0	0		
7.9300	-0.7270	0.8930	H	0	0		
7	8	2	0				
9	7	1	0				
8	6	1	0				
6	25	2	0				
12	13	1	0				
11	12	2	0				
10	11	1	0				
9	10	1	0				
7	13	1	0				
13	14	2	0				
10	22	1	0				
20	18	2	0				
19	20	1	0				

```

16 17 2 0
18 16 1 0
17 15 1 0
15 19 2 0
17 21 1 0
19 23 1 0
25 24 1 0
9 24 2 0
22 20 1 0
26 2 2 0
26 28 1 0
4 27 2 0
27 26 1 0
27 32 1 0
2 3 1 0
1 4 1 0
3 1 2 0
28 31 1 0
28 30 1 0
28 29 1 0
2 5 1 0
5 6 1 0
33 32 1 0
1 34 1 0
4 35 1 0
8 36 1 0
11 37 1 0
15 38 1 0
16 39 1 0
18 40 1 0
22 41 1 0
22 42 1 0
24 43 1 0
25 44 1 0
33 45 1 0
33 46 1 0
33 47 1 0
M END
> <Name>
Compound50

> <Activ>
0.23

> <DB_Ref_id>
2.45

$$$$
Compound51
SciTegic10081411483D

43 46 0 0 0 0 999 V2000
5.3500 -1.3070 1.8530 C 0 0
3.0100 -1.7620 1.3650 C 0 0
4.3690 -1.8200 0.9880 C 0 0
2.6370 -1.2110 2.5570 N 0 0
4.9490 -0.7440 3.0760 C 0 0
3.5800 -0.7110 3.4040 C 0 0
2.0800 -2.2400 0.5620 O 0 0
0.8830 -1.6390 0.4900 C 0 0
-1.5530 -1.7790 0.2910 C 0 0

```

-0.2910	-2.4160	0.3670	C	0	0
-1.6500	-0.3570	0.3360	C	0	0
0.7990	-0.2290	0.5350	C	0	0
-0.4610	0.4120	0.4590	C	0	0
-2.8960	0.2030	0.2580	N	0	0
-4.0410	-0.5820	0.1390	C	0	0
-3.9920	-1.8770	0.0940	N	0	0
-2.8070	-2.5880	0.1600	C	0	0
-2.8810	-3.7950	0.1090	O	0	0
-3.0800	1.6700	0.3010	C	0	0
-2.8340	2.2890	-1.0270	C	0	0
-1.5760	3.8260	-2.4380	C	0	0
-1.8090	3.2400	-1.1820	C	0	0
-2.3670	3.4630	-3.5430	C	0	0
-3.6250	1.9260	-2.1330	C	0	0
-3.3950	2.5120	-3.3890	C	0	0
-2.1410	4.0230	-4.7290	F	0	0
-4.1480	2.1640	-4.4300	F	0	0
4.7700	-2.4200	-0.3130	C	0	0
4.1820	-1.7270	-1.3380	F	0	0
4.3650	-3.7310	-0.3580	F	0	0
6.1330	-2.3590	-0.4440	F	0	0
6.3970	-1.3400	1.5860	H	0	0
5.6840	-0.3420	3.7600	H	0	0
3.2700	-0.2790	4.3440	H	0	0
-0.2170	-3.4940	0.3340	H	0	0
1.6950	0.3650	0.6270	H	0	0
-0.4920	1.4920	0.4960	H	0	0
-5.0080	-0.1020	0.0800	H	0	0
-4.0960	1.8950	0.6230	H	0	0
-2.3950	2.0960	1.0330	H	0	0
-0.7890	4.5570	-2.5490	H	0	0
-1.1970	3.5230	-0.3380	H	0	0
-4.4120	1.1950	-2.0160	H	0	0
1	5	2	0		
4	2	1	0		
3	1	1	0		
2	7	1	0		
7	8	1	0		
13	11	2	0		
12	13	1	0		
9	10	2	0		
11	9	1	0		
10	8	1	0		
8	12	2	0		
16	17	1	0		
15	16	2	0		
14	15	1	0		
11	14	1	0		
9	17	1	0		
17	18	2	0		
3	28	1	0		
14	19	1	0		
19	20	1	0		
25	23	2	0		
24	25	1	0		
21	22	2	0		
23	21	1	0		
22	20	1	0		
20	24	2	0		
23	26	1	0		

```

25 27 1 0
6 4 2 0
5 6 1 0
2 3 2 0
28 31 1 0
28 30 1 0
28 29 1 0
1 32 1 0
5 33 1 0
6 34 1 0
10 35 1 0
12 36 1 0
13 37 1 0
15 38 1 0
19 39 1 0
19 40 1 0
21 41 1 0
22 42 1 0
24 43 1 0

```

M END

> <Name>

Compound51

> <Activ>

4

> <DB_Ref_id>

2.22

\$\$\$\$

Compound52

SciTegic10081411483D

```

34 36 0 0 0 0          999 V2000
  3.4840 -2.6110 -0.7130 O 0 0
  2.2890 -2.0100 -0.7850 C 0 0
 -0.1480 -2.1500 -0.9840 C 0 0
  1.1130 -2.7870 -0.9060 C 0 0
 -0.2460 -0.7280 -0.9370 C 0 0
  2.2030 -0.5990 -0.7400 C 0 0
  0.9430 0.0430 -0.8160 C 0 0
 -1.4920 -0.1680 -1.0160 N 0 0
 -2.6370 -0.9530 -1.1370 C 0 0
 -2.5880 -2.2480 -1.1820 N 0 0
 -1.4020 -2.9590 -1.1130 C 0 0
 -1.4770 -4.1660 -1.1660 O 0 0
 -1.6760 1.2990 -0.9750 C 0 0
 -1.5570 1.8260 0.4120 C 0 0
 -2.3690 1.9650 2.7050 C 0 0
 -2.4940 1.4610 1.3990 C 0 0
 -1.3110 2.8320 3.0290 C 0 0
 -0.5000 2.6960 0.7360 C 0 0
 -0.3770 3.1970 2.0430 C 0 0
 -3.5020 0.6410 1.1040 F 0 0
 -1.1930 3.3070 4.2660 F 0 0
  4.6390 -1.7890 -0.6390 C 0 0
  1.1880 -3.8650 -0.9410 H 0 0
  3.1000 -0.0060 -0.6480 H 0 0
  0.9120 1.1210 -0.7790 H 0 0
 -3.6040 -0.4720 -1.1950 H 0 0
 -2.6580 1.5490 -1.3750 H 0 0

```

-0.9260	1.7720	-1.6090	H	0	0
-3.0880	1.6840	3.4630	H	0	0
0.2210	2.9810	-0.0160	H	0	0
0.4360	3.8650	2.2870	H	0	0
5.5120	-2.4330	-0.5270	H	0	0
4.6410	-1.1230	-1.5020	H	0	0
4.5650	-1.1720	0.2580	H	0	0

1	2	1	0
7	5	2	0
6	7	1	0
3	4	2	0
5	3	1	0
4	2	1	0
2	6	2	0
10	11	1	0
9	10	2	0
8	9	1	0
5	8	1	0
3	11	1	0
11	12	2	0
8	13	1	0
13	14	1	0
19	17	2	0
18	19	1	0
15	16	2	0
17	15	1	0
16	14	1	0
14	18	2	0
16	20	1	0
17	21	1	0
1	22	1	0
4	23	1	0
6	24	1	0
7	25	1	0
9	26	1	0
13	27	1	0
13	28	1	0
15	29	1	0
18	30	1	0
19	31	1	0
22	32	1	0
22	33	1	0
22	34	1	0

M END

> <Name>

Compound52

> <Activ>

64

> <DB_Ref_id>

2.41

\$\$\$\$

Compound53

SciTegic10081411483D

43	46	0	0	0	0	999	V2000
5.3670	-1.1910	0.3400	C	0	0		
3.0220	-1.7150	-0.0510	C	0	0		
4.3670	-1.7400	-0.4820	C	0	0		

2.6820	-1.1680	1.1520	N	0	0
5.0000	-0.6330	1.5760	C	0	0
3.6450	-0.6350	1.9570	C	0	0
2.0740	-2.2250	-0.8130	O	0	0
0.8790	-1.6230	-0.8850	C	0	0
-1.5590	-1.7640	-1.0840	C	0	0
-0.2950	-2.4000	-1.0080	C	0	0
-1.6560	-0.3400	-1.0390	C	0	0
0.7930	-0.2130	-0.8400	C	0	0
-0.4670	0.4300	-0.9160	C	0	0
-2.9020	0.2190	-1.1150	N	0	0
-4.0450	-0.5660	-1.2360	C	0	0
-3.9980	-1.8610	-1.2810	N	0	0
-2.8130	-2.5720	-1.2150	C	0	0
-2.8850	-3.7790	-1.2660	O	0	0
-3.0860	1.6860	-1.0740	C	0	0
-2.8460	2.2290	0.2910	C	0	0
-1.9140	3.9060	1.7970	C	0	0
-2.1190	3.4240	0.4900	C	0	0
-2.4300	3.2030	2.9000	C	0	0
-3.3590	1.5310	1.3980	C	0	0
-3.1520	2.0160	2.6990	C	0	0
-2.2340	3.6640	4.1330	F	0	0
-1.4730	4.3090	-0.8360	C1	0	0
4.7310	-2.3360	-1.7950	C	0	0
4.3610	-3.6560	-1.8140	F	0	0
6.0860	-2.2380	-1.9800	F	0	0
4.0820	-1.6660	-2.7990	F	0	0
6.4020	-1.1990	0.0310	H	0	0
5.7500	-0.2070	2.2250	H	0	0
3.3590	-0.2050	2.9060	H	0	0
-0.2230	-3.4780	-1.0410	H	0	0
1.6910	0.3810	-0.7480	H	0	0
-0.4980	1.5080	-0.8790	H	0	0
-5.0120	-0.0860	-1.2950	H	0	0
-2.3970	2.1520	-1.7770	H	0	0
-4.1000	1.9280	-1.3910	H	0	0
-1.3610	4.8200	1.9650	H	0	0
-3.9180	0.6170	1.2540	H	0	0
-3.5510	1.4730	3.5450	H	0	0
1	5	2	0		
4	2	1	0		
3	1	1	0		
2	7	1	0		
7	8	1	0		
13	11	2	0		
12	13	1	0		
9	10	2	0		
11	9	1	0		
10	8	1	0		
8	12	2	0		
16	17	1	0		
15	16	2	0		
14	15	1	0		
11	14	1	0		
9	17	1	0		
17	18	2	0		
3	28	1	0		
14	19	1	0		
19	20	1	0		
25	23	2	0		

24 25 1 0
21 22 2 0
23 21 1 0
22 20 1 0
20 24 2 0
23 26 1 0
22 27 1 0
6 4 2 0
5 6 1 0
2 3 2 0
28 31 1 0
28 30 1 0
28 29 1 0
1 32 1 0
5 33 1 0
6 34 1 0
10 35 1 0
12 36 1 0
13 37 1 0
15 38 1 0
19 39 1 0
19 40 1 0
21 41 1 0
24 42 1 0
25 43 1 0

M END

> <Name>

Compound53

> <Activ>

0.8

> <DB_Ref_id>

2.24

\$\$\$\$

Compound54

SciTegic10081411483D

43	46	0	0	0	0	999	V2000
3.7230	-0.4750	1.9530	N	0	0		
3.0640	-1.6740	-0.0430	C	0	0		
2.7520	-1.0330	1.1720	C	0	0		
5.0270	-0.5370	1.5600	C	0	0		
2.1060	-2.2030	-0.7780	O	0	0		
0.9080	-1.6020	-0.8500	C	0	0		
-1.5270	-1.7420	-1.0490	C	0	0		
-0.2660	-2.3790	-0.9730	C	0	0		
-1.6250	-0.3200	-1.0040	C	0	0		
-2.8710	0.2400	-1.0820	N	0	0		
-4.0160	-0.5450	-1.2010	C	0	0		
-3.9670	-1.8400	-1.2460	N	0	0		
-2.7810	-2.5510	-1.1800	C	0	0		
-2.8560	-3.7580	-1.2310	O	0	0		
-1.6330	3.7950	1.8010	C	0	0		
-3.2770	2.2520	2.7170	C	0	0		
-2.3380	3.2810	2.9020	C	0	0		
-3.5140	1.7380	1.4290	C	0	0		
-1.8650	3.2810	0.5110	C	0	0		
-2.8070	2.2520	0.3240	C	0	0		
-2.1150	3.7660	4.1210	F	0	0		

-3.0550	1.7070	-1.0390	C	0	0
-1.1890	3.7790	-0.5220	F	0	0
-0.4360	0.4490	-0.8810	C	0	0
0.8240	-0.1910	-0.8050	C	0	0
4.4080	-1.7400	-0.4570	C	0	0
5.4000	-1.1640	0.3570	C	0	0
-4.4100	0.7660	1.2670	F	0	0
4.7830	-2.4100	-1.7310	C	0	0
4.3950	-3.7230	-1.6900	F	0	0
6.1410	-2.3400	-1.9030	F	0	0
4.1580	-1.7810	-2.7780	F	0	0
1.7230	-0.9790	1.4920	H	0	0
5.7870	-0.0940	2.1850	H	0	0
-0.1910	-3.4570	-1.0060	H	0	0
-4.9820	-0.0640	-1.2600	H	0	0
-0.9100	4.5860	1.9430	H	0	0
-3.8200	1.8550	3.5620	H	0	0
-2.3710	2.1740	-1.7480	H	0	0
-4.0720	1.9490	-1.3500	H	0	0
-0.4670	1.5290	-0.8440	H	0	0
1.7210	0.4020	-0.7130	H	0	0
6.4420	-1.2010	0.0660	H	0	0
2	5	1	0		
5	6	1	0		
7	8	2	0		
9	7	1	0		
8	6	1	0		
6	25	2	0		
12	13	1	0		
11	12	2	0		
10	11	1	0		
9	10	1	0		
7	13	1	0		
13	14	2	0		
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19	20	1	0		
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17	15	1	0		
15	19	2	0		
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4	27	2	0		
27	26	1	0		
18	28	1	0		
2	3	1	0		
1	4	1	0		
3	1	2	0		
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29	31	1	0		
29	30	1	0		
3	33	1	0		
4	34	1	0		
8	35	1	0		
11	36	1	0		

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16 38 1 0
22 39 1 0
22 40 1 0
24 41 1 0
25 42 1 0
27 43 1 0

M END

> <Name>

Compound54

> <Activ>

0.11

> <DB_Ref_id>

2.46

\$\$\$\$

Compound55

SciTegic10081411483D

43	46	0	0	0	0	999	V2000
3.8240	-4.4980	0.2520	C	0	0		
2.7680	-2.3360	-0.1070	C	0	0		
3.6840	-3.3280	-0.5160	C	0	0		
2.0180	-2.4940	1.0230	N	0	0		
3.0450	-4.6470	1.4120	C	0	0		
2.1490	-3.6270	1.7750	C	0	0		
2.6270	-1.2340	-0.8160	O	0	0		
1.4300	-0.6330	-0.8910	C	0	0		
-1.0060	-0.7730	-1.0880	C	0	0		
0.2560	-1.4100	-1.0120	C	0	0		
-1.1030	0.6480	-1.0430	C	0	0		
1.3460	0.7770	-0.8460	C	0	0		
0.0860	1.4180	-0.9200	C	0	0		
-2.3500	1.2090	-1.1210	N	0	0		
-3.4940	0.4240	-1.2420	C	0	0		
-3.4450	-0.8710	-1.2870	N	0	0		
-2.2600	-1.5820	-1.2190	C	0	0		
-2.3340	-2.7890	-1.2720	O	0	0		
-2.5330	2.6760	-1.0800	C	0	0		
-2.4320	3.2010	0.3090	C	0	0		
-3.2750	3.3440	2.5900	C	0	0		
-3.3850	2.8420	1.2810	C	0	0		
-2.2170	4.2050	2.9320	C	0	0		
-1.3750	4.0630	0.6500	C	0	0		
-1.2660	4.5650	1.9570	C	0	0		
-2.0860	4.8160	4.5270	Cl	0	0		
-4.3910	2.0250	0.9730	F	0	0		
4.4980	-3.1500	-1.7480	C	0	0		
5.2740	-2.0270	-1.6230	F	0	0		
3.6660	-3.0120	-2.8300	F	0	0		
5.3030	-4.2440	-1.9280	F	0	0		
4.5180	-5.2740	-0.0410	H	0	0		
3.1350	-5.5370	2.0180	H	0	0		
1.5490	-3.7380	2.6660	H	0	0		
0.3300	-2.4880	-1.0450	H	0	0		
2.2420	1.3710	-0.7520	H	0	0		
0.0550	2.4980	-0.8830	H	0	0		
-4.4610	0.9040	-1.3010	H	0	0		
-1.7770	3.1480	-1.7030	H	0	0		

-3.5120	2.9260	-1.4920	H	0	0
-4.0120	3.0630	3.3300	H	0	0
-0.6410	4.3440	-0.0920	H	0	0
-0.4470	5.2270	2.2030	H	0	0

1	5	2	0
4	2	1	0
3	1	1	0
2	7	1	0
7	8	1	0
13	11	2	0
12	13	1	0
9	10	2	0
11	9	1	0
10	8	1	0
8	12	2	0
16	17	1	0
15	16	2	0
14	15	1	0
11	14	1	0
9	17	1	0
17	18	2	0
3	28	1	0
14	19	1	0
19	20	1	0
25	23	2	0
24	25	1	0
21	22	2	0
23	21	1	0
22	20	1	0
20	24	2	0
23	26	1	0
22	27	1	0
6	4	2	0
5	6	1	0
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28	31	1	0
28	30	1	0
28	29	1	0
1	32	1	0
5	33	1	0
6	34	1	0
10	35	1	0
12	36	1	0
13	37	1	0
15	38	1	0
19	39	1	0
19	40	1	0
21	41	1	0
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25	43	1	0

M END

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Compound55

> <Activ>

0.4

> <DB_Ref_id>

2.25

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Compound56
SciTegic10081411483D

43	46	0	0	0	0	999	V2000
3.9020	-0.4980	1.8690	C	0	0		
3.1860	-1.6930	-0.1130	C	0	0		
2.8670	-1.0490	1.0960	C	0	0		
5.2330	-0.6020	1.4160	C	0	0		
5.5330	-1.2280	0.2420	N	0	0		
2.2290	-2.2170	-0.8540	O	0	0		
1.0310	-1.6150	-0.9260	C	0	0		
-1.4040	-1.7560	-1.1250	C	0	0		
-0.1430	-2.3930	-1.0490	C	0	0		
-1.5020	-0.3340	-1.0800	C	0	0		
-2.7480	0.2270	-1.1580	N	0	0		
-3.8930	-0.5590	-1.2770	C	0	0		
-3.8440	-1.8530	-1.3220	N	0	0		
-2.6580	-2.5640	-1.2560	C	0	0		
-2.7320	-3.7710	-1.3070	O	0	0		
-3.5740	2.3480	2.5740	C	0	0		
-1.6150	3.6130	1.8810	C	0	0		
-2.5270	3.2330	2.8810	C	0	0		
-1.7520	3.1090	0.5760	C	0	0		
-3.7130	1.8420	1.2690	C	0	0		
-2.7990	2.2230	0.2670	C	0	0		
-2.3970	3.7090	4.1170	F	0	0		
-2.9320	1.6930	-1.1150	C	0	0		
-4.7130	1.0060	0.9920	F	0	0		
-0.3130	0.4360	-0.9570	C	0	0		
0.9470	-0.2050	-0.8810	C	0	0		
4.5350	-1.7680	-0.5180	C	0	0		
4.8950	-2.4430	-1.7930	C	0	0		
4.4900	-3.7520	-1.7460	F	0	0		
6.2520	-2.3910	-1.9710	F	0	0		
4.2720	-1.8110	-2.8360	F	0	0		
3.6820	0.0020	2.8010	H	0	0		
1.8420	-0.9780	1.4260	H	0	0		
6.0290	-0.1800	2.0080	H	0	0		
-0.0680	-3.4710	-1.0820	H	0	0		
-4.8590	-0.0780	-1.3360	H	0	0		
-4.2750	2.0550	3.3440	H	0	0		
-0.8090	4.2950	2.1090	H	0	0		
-1.0470	3.4060	-0.1880	H	0	0		
-2.1890	2.1660	-1.7580	H	0	0		
-3.9180	1.9410	-1.5080	H	0	0		
-0.3440	1.5160	-0.9200	H	0	0		
1.8440	0.3890	-0.7890	H	0	0		
3	1	2	0				
2	6	1	0				
6	7	1	0				
8	9	2	0				
10	8	1	0				
9	7	1	0				
7	26	2	0				
13	14	1	0				
12	13	2	0				
11	12	1	0				
10	11	1	0				
8	14	1	0				
14	15	2	0				
11	23	1	0				

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21 19 2 0
20 21 1 0
17 18 2 0
19 17 1 0
18 16 1 0
16 20 2 0
18 22 1 0
20 24 1 0
26 25 1 0
10 25 2 0
23 21 1 0
5 27 1 0
27 2 2 0
27 28 1 0
4 5 2 0
2 3 1 0
1 4 1 0
28 31 1 0
28 30 1 0
28 29 1 0
1 32 1 0
3 33 1 0
4 34 1 0
9 35 1 0
12 36 1 0
16 37 1 0
17 38 1 0
19 39 1 0
23 40 1 0
23 41 1 0
25 42 1 0
26 43 1 0

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M END

> <Name>

Compound56

> <Activ>

0.12

> <DB_Ref_id>

2.42

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Compound57

SciTegic10081411483D

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43 46 0 0 0 0          999 V2000
   3.8240 -4.5000   0.2480 C   0 0
   2.7680 -2.3360 -0.1110 C   0 0
   3.6840 -3.3300 -0.5200 C   0 0
   2.0180 -2.4960   1.0200 N   0 0
   3.0450 -4.6490   1.4080 C   0 0
   2.1470 -3.6270   1.7720 C   0 0
   2.6250 -1.2360 -0.8200 O   0 0
   1.4300 -0.6350 -0.8950 C   0 0
  -1.0080 -0.7750 -1.0920 C   0 0
   0.2560 -1.4120 -1.0160 C   0 0
  -1.1030  0.6480 -1.0470 C   0 0
   1.3440  0.7750 -0.8500 C   0 0
   0.0860  1.4180 -0.9240 C   0 0
  -2.3500  1.2070 -1.1250 N   0 0

```

-3.4940	0.4220	-1.2460	C	0	0
-3.4450	-0.8730	-1.2910	N	0	0
-2.2600	-1.5840	-1.2230	C	0	0
-2.3340	-2.7910	-1.2730	O	0	0
-2.5330	2.6740	-1.0820	C	0	0
-2.4320	3.1990	0.3050	C	0	0
-3.2770	3.3440	2.5860	C	0	0
-3.3850	2.8400	1.2770	C	0	0
-2.2170	4.2050	2.9280	C	0	0
-1.3750	4.0610	0.6460	C	0	0
-1.2660	4.5630	1.9530	C	0	0
-2.0700	4.8750	4.6840	Br	0	0
-4.3910	2.0250	0.9690	F	0	0
4.4980	-3.1500	-1.7520	C	0	0
5.2740	-2.0270	-1.6270	F	0	0
3.6660	-3.0140	-2.8320	F	0	0
5.3030	-4.2460	-1.9300	F	0	0
4.5180	-5.2740	-0.0450	H	0	0
3.1350	-5.5370	2.0160	H	0	0
1.5470	-3.7380	2.6620	H	0	0
0.3300	-2.4900	-1.0490	H	0	0
2.2420	1.3690	-0.7560	H	0	0
0.0530	2.4960	-0.8870	H	0	0
-4.4610	0.9020	-1.3050	H	0	0
-1.7770	3.1480	-1.7070	H	0	0
-3.5120	2.9240	-1.4960	H	0	0
-4.0160	3.0610	3.3240	H	0	0
-0.6410	4.3420	-0.0960	H	0	0
-0.4470	5.2250	2.1970	H	0	0
1	5	2	0		
4	2	1	0		
3	1	1	0		
2	7	1	0		
7	8	1	0		
13	11	2	0		
12	13	1	0		
9	10	2	0		
11	9	1	0		
10	8	1	0		
8	12	2	0		
16	17	1	0		
15	16	2	0		
14	15	1	0		
11	14	1	0		
9	17	1	0		
17	18	2	0		
3	28	1	0		
14	19	1	0		
19	20	1	0		
25	23	2	0		
24	25	1	0		
21	22	2	0		
23	21	1	0		
22	20	1	0		
20	24	2	0		
23	26	1	0		
22	27	1	0		
6	4	2	0		
5	6	1	0		
2	3	2	0		
28	31	1	0		

```

28 30 1 0
28 29 1 0
1 32 1 0
5 33 1 0
6 34 1 0
10 35 1 0
12 36 1 0
13 37 1 0
15 38 1 0
19 39 1 0
19 40 1 0
21 41 1 0
24 42 1 0
25 43 1 0

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M END

> <Name>

Compound57

> <Activ>

0.31

> <DB_Ref_id>

2.26

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Compound58

SciTegic10081411483D

```

44 47 0 0 0 0          999 V2000
  3.6800 -0.4710  1.8980 C  0  0
  2.9830 -1.6740 -0.1060 C  0  0
  2.6640 -1.0390  1.1090 C  0  0
  5.0180 -0.5370  1.4740 C  0  0
  2.0240 -2.2030 -0.8380 O  0  0
  0.8260 -1.6020 -0.9100 C  0  0
 -1.6090 -1.7420 -1.1100 C  0  0
 -0.3470 -2.3790 -1.0330 C  0  0
 -1.7070 -0.3200 -1.0650 C  0  0
 -2.9530  0.2400 -1.1410 N  0  0
 -4.0980 -0.5450 -1.2620 C  0  0
 -4.0490 -1.8400 -1.3070 N  0  0
 -2.8630 -2.5510 -1.2400 C  0  0
 -2.9370 -3.7580 -1.2910 O  0  0
 -1.7170  3.7950  1.7420 C  0  0
 -3.3630  2.2520  2.6560 C  0  0
 -2.4240  3.2790  2.8420 C  0  0
 -3.5990  1.7380  1.3690 C  0  0
 -1.9490  3.2810  0.4530 C  0  0
 -2.8900  2.2520  0.2640 C  0  0
 -2.2030  3.7660  4.0620 F  0  0
 -3.1370  1.7070 -1.1000 C  0  0
 -1.2710  3.7770 -0.5800 F  0  0
 -0.5170  0.4490 -0.9420 C  0  0
  0.7420 -0.1910 -0.8650 C  0  0
  4.3260 -1.7380 -0.5270 C  0  0
  5.3400 -1.1680  0.2640 C  0  0
 -4.4940  0.7660  1.2050 F  0  0
  4.6780 -2.4040 -1.8090 C  0  0
  4.2870 -3.7170 -1.7640 F  0  0
  6.0350 -2.3380 -2.0000 F  0  0
  4.0390 -1.7730 -2.8460 F  0  0

```


3.4300	0.0140	2.8300	H	0	0
1.6370	-0.9860	1.4370	H	0	0
5.7970	-0.1000	2.0820	H	0	0
-0.2730	-3.4570	-1.0670	H	0	0
-5.0640	-0.0640	-1.3200	H	0	0
-0.9940	4.5840	1.8850	H	0	0
-3.9060	1.8560	3.5020	H	0	0
-2.4510	2.1740	-1.8070	H	0	0
-4.1520	1.9490	-1.4100	H	0	0
-0.5490	1.5290	-0.9040	H	0	0
1.6390	0.4020	-0.7740	H	0	0
6.3710	-1.2150	-0.0570	H	0	0

2	5	1	0
5	6	1	0
7	8	2	0
9	7	1	0
8	6	1	0
6	25	2	0
12	13	1	0
11	12	2	0
10	11	1	0
9	10	1	0
7	13	1	0
13	14	2	0
10	22	1	0
20	18	2	0
19	20	1	0
16	17	2	0
18	16	1	0
17	15	1	0
15	19	2	0
17	21	1	0
19	23	1	0
25	24	1	0
9	24	2	0
22	20	1	0
26	2	2	0
26	29	1	0
4	27	2	0
27	26	1	0
18	28	1	0
2	3	1	0
1	4	1	0
3	1	2	0
29	32	1	0
29	31	1	0
29	30	1	0
1	33	1	0
3	34	1	0
4	35	1	0
8	36	1	0
11	37	1	0
15	38	1	0
16	39	1	0
22	40	1	0
22	41	1	0
24	42	1	0
25	43	1	0
27	44	1	0


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M  END
> <Name>

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Compound58

> <Activ>

0.075

> <DB_Ref_id>

2.48

\$\$\$\$

Compound59

SciTegic10081411483D

46	49	0	0	0	0	999	V2000
3.9690	-4.8070	-0.0350	C	0	0		
2.9060	-2.6480	-0.4060	C	0	0		
3.8260	-3.6410	-0.8080	C	0	0		
2.1520	-2.8090	0.7210	N	0	0		
3.1860	-4.9550	1.1210	C	0	0		
2.2810	-3.9360	1.4770	C	0	0		
2.7620	-1.5510	-1.1210	O	0	0		
1.5660	-0.9490	-1.1930	C	0	0		
-0.8710	-1.0900	-1.3920	C	0	0		
0.3920	-1.7270	-1.3140	C	0	0		
-0.9670	0.3320	-1.3460	C	0	0		
1.4800	0.4610	-1.1480	C	0	0		
0.2230	1.1020	-1.2240	C	0	0		
-2.2130	0.8930	-1.4240	N	0	0		
-3.3580	0.1080	-1.5450	C	0	0		
-3.3090	-1.1870	-1.5900	N	0	0		
-2.1230	-1.8980	-1.5210	C	0	0		
-2.1970	-3.1050	-1.5740	O	0	0		
-2.3970	2.3590	-1.3830	C	0	0		
-2.2970	2.8850	0.0060	C	0	0		
-3.1510	3.0330	2.2850	C	0	0		
-3.2560	2.5290	0.9750	C	0	0		
-2.0900	3.8910	2.6270	C	0	0		
-1.2380	3.7420	0.3520	C	0	0		
-1.1330	4.2440	1.6600	C	0	0		
-4.2660	1.7190	0.6620	F	0	0		
-1.9790	4.4200	4.0120	C	0	0		
4.6450	-3.4610	-2.0370	C	0	0		
5.4160	-2.3360	-1.9120	F	0	0		
3.8180	-3.3300	-3.1230	F	0	0		
5.4550	-4.5550	-2.2090	F	0	0		
4.6660	-5.5800	-0.3240	H	0	0		
3.2750	-5.8420	1.7310	H	0	0		
1.6800	-4.0470	2.3650	H	0	0		
0.4670	-2.8050	-1.3490	H	0	0		
2.3790	1.0550	-1.0550	H	0	0		
0.1890	2.1820	-1.1850	H	0	0		
-4.3240	0.5880	-1.6030	H	0	0		
-1.6390	2.8320	-2.0060	H	0	0		
-3.3730	2.6090	-1.7970	H	0	0		
-3.8870	2.7600	3.0280	H	0	0		
-0.4980	4.0180	-0.3870	H	0	0		
-0.3160	4.9010	1.9160	H	0	0		
-1.0960	5.0550	4.0880	H	0	0		
-2.8990	4.9450	4.2740	H	0	0		
-1.8580	3.5940	4.7110	H	0	0		
1	5	2	0				
4	2	1	0				

3	1	1	0
2	7	1	0
7	8	1	0
13	11	2	0
12	13	1	0
9	10	2	0
11	9	1	0
10	8	1	0
8	12	2	0
16	17	1	0
15	16	2	0
14	15	1	0
11	14	1	0
9	17	1	0
17	18	2	0
3	28	1	0
14	19	1	0
19	20	1	0
25	23	2	0
24	25	1	0
21	22	2	0
23	21	1	0
22	20	1	0
20	24	2	0
22	26	1	0
23	27	1	0
6	4	2	0
5	6	1	0
2	3	2	0
28	31	1	0
28	30	1	0
28	29	1	0
1	32	1	0
5	33	1	0
6	34	1	0
10	35	1	0
12	36	1	0
13	37	1	0
15	38	1	0
19	39	1	0
19	40	1	0
21	41	1	0
24	42	1	0
25	43	1	0
27	44	1	0
27	45	1	0
27	46	1	0

M END

> <Name>

Compound59

> <Activ>

0.26

> <DB_Ref_id>

2.27

\$\$\$\$

Compound60

SciTegic10081411483D

43	46	0	0	0	0	999	V2000
6.1450	-1.1720	0.8610	C	0	0		
3.8090	-1.6390	0.3610	C	0	0		
5.1680	-1.6780	-0.0160	C	0	0		
3.4300	-1.1170	1.5660	N	0	0		
5.7380	-0.6390	2.0960	C	0	0		
4.3690	-0.6250	2.4240	C	0	0		
2.8830	-2.1090	-0.4490	O	0	0		
1.6880	-1.5080	-0.5230	C	0	0		
-0.7500	-1.6480	-0.7210	C	0	0		
0.5140	-2.2850	-0.6450	C	0	0		
-0.8460	-0.2270	-0.6760	C	0	0		
-2.0920	0.3340	-0.7540	N	0	0		
-3.2360	-0.4510	-0.8730	C	0	0		
-3.1880	-1.7460	-0.9200	N	0	0		
-2.0040	-2.4570	-0.8520	C	0	0		
-2.0760	-3.6640	-0.9020	O	0	0		
-3.5880	2.1720	-0.1130	C	0	0		
-5.8730	2.9790	-0.3690	C	0	0		
-4.6370	2.6270	-0.9360	C	0	0		
-6.0680	2.8730	1.0200	C	0	0		
-3.7850	2.0660	1.2790	C	0	0		
-5.0240	2.4160	1.8420	C	0	0		
-4.4690	2.7310	-2.2540	F	0	0		
-2.2750	1.7990	-0.7110	C	0	0		
-2.8030	1.6390	2.0700	F	0	0		
0.3440	0.5430	-0.5530	C	0	0		
1.6020	-0.0980	-0.4770	C	0	0		
5.5740	-2.2460	-1.3280	C	0	0		
4.9790	-1.5350	-2.3380	F	0	0		
5.1840	-3.5570	-1.4000	F	0	0		
6.9380	-2.1680	-1.4590	F	0	0		
7.1920	-1.1890	0.5940	H	0	0		
6.4690	-0.2440	2.7850	H	0	0		
4.0550	-0.2150	3.3710	H	0	0		
0.5880	-3.3630	-0.6780	H	0	0		
-4.2030	0.0290	-0.9340	H	0	0		
-6.6780	3.3320	-0.9980	H	0	0		
-7.0200	3.1430	1.4530	H	0	0		
-5.1780	2.3360	2.9080	H	0	0		
-1.4710	2.2460	-0.1270	H	0	0		
-2.2130	2.1970	-1.7250	H	0	0		
0.3110	1.6230	-0.5160	H	0	0		
2.5000	0.4960	-0.3850	H	0	0		
1	5	2	0				
4	2	1	0				
3	1	1	0				
2	7	1	0				
7	8	1	0				
9	10	2	0				
11	9	1	0				
10	8	1	0				
8	27	2	0				
14	15	1	0				
13	14	2	0				
12	13	1	0				
11	12	1	0				
9	15	1	0				
15	16	2	0				
3	28	1	0				
12	24	1	0				

```

24 17 1 0
22 20 2 0
21 22 1 0
18 19 2 0
20 18 1 0
19 17 1 0
17 21 2 0
19 23 1 0
21 25 1 0
27 26 1 0
11 26 2 0
6 4 2 0
5 6 1 0
2 3 2 0
28 31 1 0
28 30 1 0
28 29 1 0
1 32 1 0
5 33 1 0
6 34 1 0
10 35 1 0
13 36 1 0
18 37 1 0
20 38 1 0
22 39 1 0
24 40 1 0
24 41 1 0
26 42 1 0
27 43 1 0

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M END

> <Name>

Compound60

> <Activ>

0.2

> <DB_Ref_id>

2.28

\$\$\$\$

Compound61

SciTegic10081411483D

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47 50 0 0 0 0          999 V2000
   3.2370  -0.4830  -1.4320 C   0  0
   2.3150  -1.6920   0.3770 C   0  0
   2.1620  -1.0650  -0.8260 N   0  0
   4.5140  -0.5100  -0.8420 C   0  0
   1.2620  -2.2460   0.9430 O   0  0
   0.0650  -1.6470   0.8710 C   0  0
  -2.3710  -1.7850   0.6720 C   0  0
  -1.1090  -2.4240   0.7500 C   0  0
  -2.4690  -0.3630   0.7190 C   0  0
  -3.7150   0.1950   0.6410 N   0  0
  -4.8590  -0.5900   0.5190 C   0  0
  -4.8100  -1.8850   0.4750 N   0  0
  -3.6250  -2.5960   0.5430 C   0  0
  -3.6990  -3.8030   0.4900 O   0  0
  -3.5410   2.4940  -3.0100 C   0  0
  -2.0640   3.9510  -1.7360 C   0  0
  -2.5880   3.5250  -2.9710 C   0  0

```

-2.4920	3.3420	-0.5430	C	0	0
-3.9710	1.8830	-1.8180	C	0	0
-3.4450	2.3070	-0.5820	C	0	0
-2.1820	4.1020	-4.1000	F	0	0
-3.8980	1.6620	0.6820	C	0	0
-4.8730	0.9060	-1.8710	F	0	0
-1.2790	0.4060	0.8400	C	0	0
-0.0190	-0.2340	0.9160	C	0	0
3.5740	-1.7480	1.0140	C	0	0
4.6900	-1.1500	0.3980	C	0	0
-1.9860	3.7540	0.6190	F	0	0
3.7210	-2.4340	2.3260	C	0	0
4.7460	-1.8560	3.0310	F	0	0
4.0000	-3.7600	2.1190	F	0	0
2.5550	-2.3180	3.0370	F	0	0
5.8790	-1.1840	0.9650	O	0	0
6.9590	-0.5610	0.2870	C	0	0
3.1020	0.0100	-2.3850	H	0	0
5.3520	-0.0430	-1.3360	H	0	0
-1.0350	-3.5020	0.7150	H	0	0
-5.8260	-0.1090	0.4610	H	0	0
-3.9450	2.1680	-3.9570	H	0	0
-1.3340	4.7460	-1.7050	H	0	0
-3.3340	2.0700	1.5210	H	0	0
-4.9510	1.8870	0.8480	H	0	0
-1.3100	1.4840	0.8790	H	0	0
0.8770	0.3570	1.0080	H	0	0
7.1170	-1.0840	-0.6560	H	0	0
6.7480	0.5060	0.2170	H	0	0
7.8580	-0.6840	0.8910	H	0	0
7	8	2	0		
9	7	1	0		
8	6	1	0		
6	25	2	0		
12	13	1	0		
11	12	2	0		
10	11	1	0		
9	10	1	0		
7	13	1	0		
13	14	2	0		
10	22	1	0		
20	18	2	0		
19	20	1	0		
16	17	2	0		
18	16	1	0		
17	15	1	0		
15	19	2	0		
17	21	1	0		
19	23	1	0		
25	24	1	0		
9	24	2	0		
22	20	1	0		
26	2	2	0		
4	27	2	0		
27	26	1	0		
18	28	1	0		
26	29	1	0		
27	33	1	0		
2	3	1	0		
1	4	1	0		
3	1	2	0		

```

29 30 1 0
29 31 1 0
29 32 1 0
2 5 1 0
5 6 1 0
34 33 1 0
1 35 1 0
4 36 1 0
8 37 1 0
11 38 1 0
15 39 1 0
16 40 1 0
22 41 1 0
22 42 1 0
24 43 1 0
25 44 1 0
34 45 1 0
34 46 1 0
34 47 1 0

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M END

> <Name>

Compound61

> <Activ>

0.1

> <DB_Ref_id>

2.5

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Compound62

SciTegic10081411483D

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43 46 0 0 0 0          999 V2000
  3.8220 -4.4960  0.2580 C  0 0
  2.7680 -2.3320 -0.1000 C  0 0
  3.6840 -3.3260 -0.5100 C  0 0
  2.0200 -2.4920  1.0310 N  0 0
  3.0450 -4.6450  1.4180 C  0 0
  2.1480 -3.6230  1.7830 C  0 0
  2.6270 -1.2310 -0.8090 O  0 0
  1.4320 -0.6290 -0.8810 C  0 0
 -1.0060 -0.7700 -1.0800 C  0 0
  0.2560 -1.4080 -1.0040 C  0 0
 -1.1040  0.6520 -1.0350 C  0 0
  1.3460  0.7810 -0.8360 C  0 0
  0.0860  1.4220 -0.9120 C  0 0
 -2.3500  1.2130 -1.1110 N  0 0
 -3.4920  0.4280 -1.2330 C  0 0
 -3.4450 -0.8670 -1.2770 N  0 0
 -2.2600 -1.5800 -1.2110 C  0 0
 -2.3340 -2.7850 -1.2620 O  0 0
 -2.5330  2.6780 -1.0700 C  0 0
 -2.4300  3.2050  0.3160 C  0 0
 -3.2730  3.3460  2.6000 C  0 0
 -3.3830  2.8440  1.2910 C  0 0
 -2.2130  4.2070  2.9370 C  0 0
 -1.3730  4.0660  0.6580 C  0 0
 -1.2660  4.5680  1.9670 C  0 0
 -4.3930  2.0310  0.9820 F  0 0
 -2.1090  4.6800  4.1780 F  0 0

```

4.4960	-3.1470	-1.7420	C	0	0
3.6640	-3.0080	-2.8220	F	0	0
5.3010	-4.2420	-1.9220	F	0	0
5.2740	-2.0250	-1.6170	F	0	0
4.5180	-5.2720	-0.0370	H	0	0
3.1350	-5.5350	2.0230	H	0	0
1.5490	-3.7360	2.6740	H	0	0
0.3300	-2.4840	-1.0370	H	0	0
2.2440	1.3750	-0.7440	H	0	0
0.0550	2.5020	-0.8750	H	0	0
-4.4590	0.9080	-1.2910	H	0	0
-1.7750	3.1520	-1.6950	H	0	0
-3.5100	2.9300	-1.4830	H	0	0
-4.0020	3.0680	3.3460	H	0	0
-0.6390	4.3480	-0.0840	H	0	0
-0.4490	5.2310	2.2210	H	0	0
1	5	2	0		
4	2	1	0		
3	1	1	0		
2	7	1	0		
7	8	1	0		
13	11	2	0		
12	13	1	0		
9	10	2	0		
11	9	1	0		
10	8	1	0		
8	12	2	0		
16	17	1	0		
15	16	2	0		
14	15	1	0		
11	14	1	0		
9	17	1	0		
17	18	2	0		
3	28	1	0		
14	19	1	0		
19	20	1	0		
25	23	2	0		
24	25	1	0		
21	22	2	0		
23	21	1	0		
22	20	1	0		
20	24	2	0		
22	26	1	0		
23	27	1	0		
6	4	2	0		
5	6	1	0		
2	3	2	0		
28	31	1	0		
28	30	1	0		
28	29	1	0		
1	32	1	0		
5	33	1	0		
6	34	1	0		
10	35	1	0		
12	36	1	0		
13	37	1	0		
15	38	1	0		
19	39	1	0		
19	40	1	0		
21	41	1	0		
24	42	1	0		

25 43 1 0

M END

> <Name>

Compound62

> <Activ>

0.51

> <DB_Ref_id>

2.29

\$\$\$\$

Compound63

SciTegic10081411483D

63	66	0	0	0	0	999	V2000
1.4260	-2.2690	1.0100	C	0	0		
0.1720	-3.0570	0.8240	C	0	0		
-1.0680	-2.2580	0.6620	C	0	0		
-1.0100	-0.9060	0.6850	C	0	0		
0.1700	-0.2030	0.8590	N	0	0		
0.0720	-4.2640	0.7930	O	0	0		
-2.3670	-2.9280	0.4750	C	0	0		
-2.5040	-3.7660	-0.3870	O	0	0		
-3.5020	-2.5530	1.3690	C	0	0		
-3.2600	-1.8140	2.5410	C	0	0		
-4.3300	-1.4610	3.3830	C	0	0		
-5.6410	-1.8440	3.0550	C	0	0		
-5.8830	-2.5840	1.8830	C	0	0		
-4.8140	-2.9370	1.0410	C	0	0		
-6.7720	-1.4710	3.9450	C	0	0		
3.8540	-2.2030	1.3530	C	0	0		
3.8110	-0.7910	1.3730	C	0	0		
5.0220	-2.8440	1.5080	O	0	0		
6.1880	-2.2460	0.9630	C	0	0		
4.9400	-0.0880	1.5490	O	0	0		
4.8420	1.3280	1.5880	C	0	0		
1.3690	-0.8420	1.0230	C	0	0		
2.5800	-0.1150	1.2090	C	0	0		
2.6640	-2.9410	1.1720	C	0	0		
0.0740	1.2720	0.8590	C	0	0		
0.2170	1.8300	-0.5100	C	0	0		
1.4140	2.4610	-0.8950	C	0	0		
1.5470	2.9880	-2.1900	C	0	0		
0.4840	2.8870	-3.1060	C	0	0		
-0.7130	2.2580	-2.7210	C	0	0		
-0.8460	1.7290	-1.4260	C	0	0		
0.6270	3.4450	-4.4750	C	0	0		
0.7210	2.3400	-5.5270	C	0	0		
-0.4730	4.4630	-4.7850	C	0	0		
-1.9410	-0.3710	0.5590	H	0	0		
-2.2560	-1.5140	2.8030	H	0	0		
-4.1370	-0.8920	4.2830	H	0	0		
-6.8890	-2.8830	1.6250	H	0	0		
-5.0100	-3.5060	0.1430	H	0	0		
-7.7460	-1.8240	3.6070	H	0	0		
-6.8220	-0.3850	4.0310	H	0	0		
-6.5980	-1.8770	4.9410	H	0	0		
6.0570	-1.6660	0.0490	H	0	0		
6.9120	-3.0330	0.7580	H	0	0		
6.6150	-1.5860	1.7170	H	0	0		

4.4790	1.6720	0.6190	H	0	0
4.2440	1.6060	2.4550	H	0	0
5.8440	1.7340	1.7300	H	0	0
2.5880	0.9650	1.2280	H	0	0
2.7050	-4.0210	1.1600	H	0	0
0.8560	1.6800	1.5020	H	0	0
-0.8890	1.5680	1.2750	H	0	0
2.2340	2.5410	-0.1950	H	0	0
2.4710	3.4710	-2.4790	H	0	0
-1.5330	2.1760	-3.4200	H	0	0
-1.7700	1.2460	-1.1390	H	0	0
1.5880	3.9440	-4.3540	H	0	0
-0.2070	1.7760	-5.6080	H	0	0
1.5180	1.6390	-5.2770	H	0	0
0.9410	2.7600	-6.5080	H	0	0
-0.5550	5.2210	-4.0060	H	0	0
-1.4390	3.9690	-4.8750	H	0	0
-0.2710	4.9730	-5.7270	H	0	0
3	2	1	0		
4	3	2	0		
5	4	1	0		
1	2	1	0		
2	6	2	0		
3	7	1	0		
7	8	2	0		
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11	10	2	0		
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9	14	2	0		
12	15	1	0		
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18	19	1	0		
17	20	1	0		
20	21	1	0		
23	22	2	0		
22	1	1	0		
1	24	2	0		
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17	23	1	0		
22	5	1	0		
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29	32	1	0		
32	33	1	0		
32	34	1	0		
4	35	1	0		
10	36	1	0		
11	37	1	0		
13	38	1	0		
14	39	1	0		
15	40	1	0		

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19 43 1 0
19 44 1 0
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24 50 1 0
25 51 1 0
25 52 1 0
27 53 1 0
28 54 1 0
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M END

> <Name>

Compound63

> <Activ>

1.15

> <DB_Ref_id>

3.01

\$\$\$\$

Compound64

SciTegic10081411483D

```

54 57 0 0 0 0          999 V2000
   3.6820   -0.7110   -0.8630 C   0  0
   1.2540   -0.7770   -1.2070 C   0  0
   3.6390    0.7010   -0.8440 C   0  0
  -0.0020    1.2890   -1.3600 N   0  0
  -1.1820    0.5860   -1.5330 C   0  0
  -1.2400   -0.7660   -1.5570 C   0  0
    0.0000   -1.5650   -1.3950 C   0  0
  -0.1000   -2.7720   -1.4240 O   0  0
  -2.5390   -1.4360   -1.7420 C   0  0
  -3.1150   -1.3690   -2.8030 O   0  0
  -3.1230   -2.1950   -0.5980 C   0  0
  -3.0720   -2.8460    1.7500 C   0  0
  -2.5210   -2.1310    0.6720 C   0  0
  -4.2250   -3.6290    1.5580 C   0  0
  -4.2770   -2.9790   -0.7870 C   0  0
  -4.8260   -3.6930    0.2890 C   0  0
  -4.8090   -4.3850    2.6990 C   0  0
   4.8500   -1.3520   -0.7110 O   0  0
   4.8380   -2.7720   -0.7380 C   0  0
   4.7680    1.4040   -0.6700 O   0  0
   4.6860    2.8200   -0.7250 C   0  0
   2.4920   -1.4490   -1.0450 C   0  0
   2.4080    1.3770   -1.0100 C   0  0

```

1.1970	0.6500	-1.1950	C	0	0
-0.0980	2.7640	-1.3580	C	0	0
-0.0530	3.3140	0.0210	C	0	0
0.9710	4.2050	0.3920	C	0	0
1.0140	4.7270	1.6970	C	0	0
0.0350	4.3550	2.6370	C	0	0
-0.9900	3.4630	2.2660	C	0	0
-1.0330	2.9430	0.9610	C	0	0
0.0880	4.9860	4.2300	C1	0	0
-2.1130	1.1210	-1.6580	H	0	0
-2.6050	-2.7930	2.7230	H	0	0
-1.6350	-1.5330	0.8260	H	0	0
-4.7460	-3.0350	-1.7600	H	0	0
-5.7130	-4.2930	0.1370	H	0	0
-5.6990	-4.9590	2.4470	H	0	0
-5.0720	-3.6920	3.4980	H	0	0
-4.0640	-5.0780	3.0920	H	0	0
5.7990	-3.2700	-0.6110	H	0	0
4.4200	-3.0920	-1.6920	H	0	0
4.1740	-3.1230	0.0530	H	0	0
5.6760	3.2280	-0.5240	H	0	0
4.2350	3.1000	-1.6780	H	0	0
4.0200	3.1560	0.0700	H	0	0
2.5330	-2.5290	-1.0590	H	0	0
2.4160	2.4590	-0.9900	H	0	0
-1.0290	3.0640	-1.8380	H	0	0
0.7270	3.1760	-1.9420	H	0	0
1.7270	4.4940	-0.3240	H	0	0
1.8050	5.4120	1.9670	H	0	0
-1.7480	3.1680	2.9760	H	0	0
-1.8220	2.2600	0.6820	H	0	0
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6	7	1	0		
5	6	2	0		
4	5	1	0		
2	7	1	0		
7	8	2	0		
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2	22	2	0		
22	1	1	0		
3	23	1	0		
24	4	1	0		
15	16	1	0		
4	25	1	0		
25	26	1	0		
30	31	2	0		
29	30	1	0		

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28 29 2 0
27 28 1 0
31 26 1 0
26 27 2 0
29 32 1 0
5 33 1 0
12 34 1 0
13 35 1 0
15 36 1 0
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17 39 1 0
17 40 1 0
19 41 1 0
19 42 1 0
19 43 1 0
21 44 1 0
21 45 1 0
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M END

> <Name>

Compound64

> <Activ>

1.1

> <DB_Ref_id>

03.02b

\$\$\$\$

Compound65

SciTegic10081411483D

```

60 63 0 0 0 0          999 V2000
   3.8070 -2.0610   1.1950 C   0 0
   1.3790 -2.1270   0.8520 C   0 0
   3.7640 -0.6480   1.2150 C   0 0
   0.1230 -0.0620   0.7010 N   0 0
  -1.0570 -0.7640   0.5270 C   0 0
  -1.1150 -2.1150   0.5040 C   0 0
   0.1250 -2.9160   0.6660 C   0 0
   0.0250 -4.1210   0.6370 O   0 0
  -2.4140 -2.7870   0.3160 C   0 0
  -2.5210 -3.7070  -0.4610 O   0 0
  -3.5860 -2.3070   1.1050 C   0 0
  -4.4940 -1.1540   3.0510 C   0 0
  -3.3890 -1.6070   2.3090 C   0 0
  -5.7990 -1.4000   2.5900 C   0 0
  -4.8930 -2.5530   0.6450 C   0 0
  -5.9980 -2.1000   1.3870 C   0 0
  -6.9690 -0.9240   3.3750 C   0 0
   4.9750 -2.7030   1.3500 O   0 0
   6.1330 -2.1250   0.7680 C   0 0

```

4.8930	0.0550	1.3910	O	0	0
4.7990	1.4710	1.3980	C	0	0
2.6170	-2.8010	1.0160	C	0	0
2.5330	0.0270	1.0510	C	0	0
1.3220	-0.6990	0.8650	C	0	0
0.0270	1.4140	0.7010	C	0	0
0.0940	1.9670	-0.6760	C	0	0
-0.9430	2.7910	-1.1540	C	0	0
-0.8810	3.3150	-2.4570	C	0	0
0.2170	3.0140	-3.2810	C	0	0
1.2520	2.1910	-2.8070	C	0	0
1.1910	1.6680	-1.5040	C	0	0
0.2910	3.6560	-4.8810	S	0	0
1.7360	3.0040	-5.7090	C	0	0
0.4160	5.1000	-4.7870	O	0	0
-0.8950	3.2290	-5.6020	O	0	0
-1.9880	-0.2280	0.4000	H	0	0
-4.3340	-0.6190	3.9750	H	0	0
-2.3890	-1.4120	2.6700	H	0	0
-5.0570	-3.0880	-0.2790	H	0	0
-6.9980	-2.2930	1.0270	H	0	0
-7.9360	-1.1720	2.9380	H	0	0
-6.9180	0.1600	3.4790	H	0	0
-6.9360	-1.3540	4.3750	H	0	0
5.9900	-1.5660	-0.1580	H	0	0
6.8480	-2.9240	0.5660	H	0	0
6.5820	-1.4510	1.4980	H	0	0
4.4790	1.7990	0.4100	H	0	0
4.1640	1.7680	2.2340	H	0	0
5.7950	1.8770	1.5780	H	0	0
2.6580	-3.8810	1.0020	H	0	0
2.5410	1.1070	1.0700	H	0	0
0.8440	1.8240	1.2970	H	0	0
-0.9100	1.7130	1.1700	H	0	0
-1.7890	3.0240	-0.5230	H	0	0
-1.6780	3.9450	-2.8220	H	0	0
2.0960	1.9610	-3.4410	H	0	0
1.9900	1.0370	-1.1430	H	0	0
1.8570	3.3480	-6.7360	H	0	0
1.6880	1.9160	-5.7250	H	0	0
2.6330	3.2890	-5.1560	H	0	0
1	3	2	0		
6	7	1	0		
5	6	2	0		
4	5	1	0		
2	7	1	0		
7	8	2	0		
6	9	1	0		
9	10	2	0		
9	11	1	0		
16	14	2	0		
12	13	2	0		
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13	11	1	0		
11	15	2	0		
14	17	1	0		
1	18	1	0		
18	19	1	0		
3	20	1	0		
20	21	1	0		
23	24	2	0		

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  3 23  1  0
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32 35  2  0
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M END

> <Name>

Compound65

> <Activ>

0.5

> <DB_Ref_id>

3.02

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Compound66

SciTegic10081411483D

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66 69  0  0  0  0          999 V2000
   3.8480   -2.2270   -1.6040 C   0  0
   1.4200   -2.2910   -1.9470 C   0  0
   3.8050   -0.8140   -1.5840 C   0  0

```

0.1640	-0.2270	-2.0980	N	0	0
-1.0160	-0.9300	-2.2720	C	0	0
-1.0740	-2.2810	-2.2950	C	0	0
0.1660	-3.0800	-2.1330	C	0	0
0.0660	-4.2850	-2.1640	O	0	0
-2.3730	-2.9510	-2.4820	C	0	0
-2.6170	-3.5350	-3.5120	O	0	0
-3.3750	-2.8930	-1.3770	C	0	0
-5.6210	-3.3260	-0.5390	C	0	0
-4.6780	-3.3810	-1.5800	C	0	0
-5.2640	-2.7810	0.7070	C	0	0
-3.0180	-2.3480	-0.1310	C	0	0
-3.9610	-2.2910	0.9100	C	0	0
-6.2600	-2.7230	1.8090	C	0	0
5.0160	-2.8670	-1.4490	O	0	0
6.1780	-2.2790	-2.0140	C	0	0
4.9340	-0.1110	-1.4080	O	0	0
4.8710	1.2990	-1.5680	C	0	0
2.6580	-2.9650	-1.7850	C	0	0
2.5740	-0.1370	-1.7480	C	0	0
1.3630	-0.8630	-1.9340	C	0	0
0.0680	1.2480	-2.0980	C	0	0
0.0780	1.7970	-0.7150	C	0	0
-0.9370	1.4410	0.1890	C	0	0
-0.9300	1.9590	1.4960	C	0	0
0.0940	2.8340	1.9000	C	0	0
1.1090	3.1890	0.9960	C	0	0
1.1020	2.6720	-0.3110	C	0	0
0.1040	3.3830	3.2830	C	0	0
-0.7110	4.6250	2.9180	C	0	0
1.5220	3.7210	3.7460	C	0	0
-0.6330	2.4630	4.2580	C	0	0
-1.9470	-0.3930	-2.3980	H	0	0
-6.6190	-3.7030	-0.7010	H	0	0
-4.9610	-3.8030	-2.5330	H	0	0
-2.0190	-1.9690	0.0350	H	0	0
-3.6800	-1.8710	1.8650	H	0	0
-5.8870	-2.2750	2.7290	H	0	0
-6.6040	-3.7310	2.0430	H	0	0
-7.1250	-2.1430	1.4840	H	0	0
6.0430	-1.7210	-2.9390	H	0	0
6.9030	-3.0720	-2.2050	H	0	0
6.6120	-1.6040	-1.2750	H	0	0
5.8710	1.7030	-1.4140	H	0	0
4.4080	1.5140	-2.5330	H	0	0
4.2250	1.7030	-0.7910	H	0	0
2.6990	-4.0450	-1.7970	H	0	0
2.5820	0.9430	-1.7290	H	0	0
-0.8500	1.5490	-2.6020	H	0	0
0.9080	1.6620	-2.6560	H	0	0
-1.7270	0.7700	-0.1130	H	0	0
-1.7130	1.6820	2.1880	H	0	0
1.8990	3.8610	1.2990	H	0	0
1.8850	2.9490	-1.0020	H	0	0
-0.8790	5.2680	3.7790	H	0	0
-1.6840	4.3440	2.5160	H	0	0
-0.1950	5.2130	2.1580	H	0	0
2.2090	2.8910	3.5820	H	0	0
1.5330	3.9590	4.8090	H	0	0
1.9060	4.5860	3.2070	H	0	0
-0.2990	1.4280	4.1700	H	0	0

-1.7050	2.4820	4.0720 H	0	0
-0.4670	2.7790	5.2870 H	0	0
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5	6	2	0	
4	5	1	0	
2	7	1	0	
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31 57 1 0
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M END

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Compound66

> <Activ>

0.68

> <DB_Ref_id>

03.02c

\$\$\$\$

Compound67

SciTegic10081411483D

60	64	0	0	0	0	999	V2000
-1.3300	1.4940	-0.4450	C	0	0		
-0.1740	2.4380	-0.4360	C	0	0		
1.1660	1.8070	-0.3260	C	0	0		
1.2730	0.4610	-0.2400	C	0	0		
0.1820	-0.3870	-0.2500	N	0	0		
-0.2230	3.6450	-0.5080	O	0	0		
2.3810	2.6390	-0.3110	C	0	0		
2.7090	3.2620	-1.2950	O	0	0		
-3.7540	1.1210	-0.5590	C	0	0		
-3.5410	-0.2790	-0.4730	C	0	0		
-1.0980	0.0880	-0.3520	C	0	0		
-2.2210	-0.7890	-0.3670	C	0	0		
-2.6490	2.0020	-0.5450	C	0	0		
0.4610	-1.8360	-0.1470	C	0	0		
0.7190	-2.4390	-1.4810	C	0	0		
1.9080	-3.1500	-1.7110	C	0	0		
2.1520	-3.7230	-2.9730	C	0	0		
1.2070	-3.5840	-4.0060	C	0	0		
0.0160	-2.8710	-3.7720	C	0	0		
-0.2290	-2.3010	-2.5100	C	0	0		
1.5060	-4.2770	-5.5450	Cl	0	0		
3.0610	2.6490	0.8320	O	0	0		
4.2150	3.4730	0.7680	C	0	0		
4.9060	3.4610	2.0840	C	0	0		
5.5820	2.3070	2.5140	C	0	0		
6.2360	2.2930	3.7580	C	0	0		
6.2150	3.4380	4.5760	C	0	0		
5.5370	4.5940	4.1450	C	0	0		
4.8850	4.6060	2.9000	C	0	0		
7.0080	3.4240	6.0960	Cl	0	0		
-4.9830	1.6310	-0.6560	F	0	0		
-4.5760	-1.1350	-0.4860	N	0	0		
-4.5350	-2.4020	-1.2560	C	0	0		
-5.1020	-3.5780	-0.4320	C	0	0		
-6.3650	-3.2400	0.1290	O	0	0		
-6.3220	-2.1210	1.0080	C	0	0		

-5.8260	-0.8610	0.2680	C	0	0
2.2710	0.0510	-0.1600	H	0	0
-2.0760	-1.8590	-0.3010	H	0	0
-2.8180	3.0670	-0.6110	H	0	0
-0.3930	-2.3320	0.3180	H	0	0
1.3280	-1.9880	0.4960	H	0	0
2.6410	-3.2600	-0.9240	H	0	0
3.0720	-4.2680	-3.1350	H	0	0
-0.7210	-2.7560	-4.5550	H	0	0
-1.1470	-1.7580	-2.3380	H	0	0
3.8960	4.4880	0.5350	H	0	0
4.8810	3.0700	0.0040	H	0	0
5.6020	1.4240	1.8910	H	0	0
6.7540	1.3990	4.0740	H	0	0
5.5120	5.4810	4.7640	H	0	0
4.3690	5.4980	2.5740	H	0	0
-3.5180	-2.6330	-1.5780	H	0	0
-5.1270	-2.2670	-2.1620	H	0	0
-4.4260	-3.8510	0.3790	H	0	0
-5.2330	-4.4610	-1.0590	H	0	0
-7.3240	-1.9650	1.4100	H	0	0
-5.6700	-2.3650	1.8480	H	0	0
-5.6860	-0.0450	0.9780	H	0	0
-6.5840	-0.5290	-0.4430	H	0	0
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Compound67

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0.02

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3.17

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Compound68

SciTegic10081411483D

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  1.7660 -1.8950 -1.4730 C 0 0
  0.5120 -2.6840 -1.6580 C 0 0
 -0.7290 -1.8830 -1.8200 C 0 0
 -0.6700 -0.5310 -1.7970 C 0 0
  0.5080  0.1700 -1.6230 N 0 0
  0.4120 -3.8890 -1.6880 O 0 0
 -2.0270 -2.5550 -2.0080 C 0 0
 -2.2520 -3.1820 -3.0160 O 0 0
 -3.0530 -2.4410 -0.9280 C 0 0
 -2.7110 -1.8750  0.3120 C 0 0
 -3.6780 -1.7700  1.3280 C 0 0
 -4.9860 -2.2300  1.1050 C 0 0
 -5.3280 -2.7970 -0.1350 C 0 0
 -4.3630 -2.9020 -1.1500 C 0 0
 -6.0080 -2.1190  2.1820 C 0 0
  4.1910 -1.8280 -1.1290 C 0 0
  4.1500 -0.4160 -1.1090 C 0 0
  5.3590 -2.4710 -0.9750 O 0 0
  6.5240 -1.8810 -1.5370 C 0 0

```

5.2770	0.2870	-0.9340	O	0	0
5.2050	1.7010	-1.0390	C	0	0
1.7070	-0.4670	-1.4590	C	0	0
2.9180	0.2600	-1.2730	C	0	0
3.0020	-2.5680	-1.3090	C	0	0
0.4140	1.6470	-1.6230	C	0	0
0.0740	2.1720	-0.2730	C	0	0
1.0450	2.1800	0.7440	C	0	0
0.7250	2.6760	2.0180	C	0	0
-0.5680	3.1640	2.2750	C	0	0
-1.5390	3.1580	1.2600	C	0	0
-1.2190	2.6600	-0.0140	C	0	0
-0.9610	3.7750	3.8400	S	0	0
-2.5780	4.3990	4.0040	N	0	0
-0.0720	4.8850	4.1350	O	0	0
-0.8540	2.6860	4.7950	O	0	0
-1.6020	0.0040	-1.9240	H	0	0
-1.7070	-1.5180	0.4940	H	0	0
-3.4080	-1.3340	2.2790	H	0	0
-6.3340	-3.1520	-0.3130	H	0	0
-4.6370	-3.3400	-2.1000	H	0	0
-6.9880	-2.5120	1.9100	H	0	0
-6.1350	-1.0700	2.4550	H	0	0
-5.6640	-2.6560	3.0640	H	0	0
6.3890	-1.3260	-2.4650	H	0	0
7.2500	-2.6720	-1.7230	H	0	0
6.9510	-1.2010	-0.8010	H	0	0
4.8090	1.9490	-2.0240	H	0	0
4.6450	2.0780	-0.1860	H	0	0
6.2170	2.1000	-0.9770	H	0	0
2.9280	1.3400	-1.2540	H	0	0
3.0450	-3.6480	-1.3220	H	0	0
-0.3500	1.9570	-2.3360	H	0	0
1.3650	2.0660	-1.9470	H	0	0
2.0410	1.8050	0.5510	H	0	0
1.4710	2.6820	2.7990	H	0	0
-2.5330	3.5330	1.4590	H	0	0
-1.9690	2.6580	-0.7910	H	0	0
-2.7190	5.1660	3.3320	H	0	0
-3.2560	3.6540	3.7890	H	0	0
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Compound68

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0.85

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03.02f

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Compound69
SciTegic10081411483D

57 60 0 0 0 0 999 V2000
-1.9400 0.7200 -0.4700 C 0 0
-1.3410 2.0750 -0.6530 C 0 0
0.1040 2.1840 -0.3350 C 0 0
0.7880 1.0960 0.0870 C 0 0
0.2040 -0.1480 0.2470 N 0 0

```

-1.9120	3.0740	-1.0300	O	0	0
0.8020	3.4740	-0.4750	C	0	0
0.9650	3.9660	-1.5670	O	0	0
1.3000	4.1570	0.7560	C	0	0
2.1260	5.2900	0.6490	C	0	0
2.5950	5.9330	1.8080	C	0	0
2.2380	5.4440	3.0770	C	0	0
1.4120	4.3110	3.1850	C	0	0
0.9430	3.6680	2.0260	C	0	0
2.7330	6.1230	4.3030	C	0	0
-3.8900	-0.7640	-0.5730	C	0	0
-3.0940	-1.8390	-0.1180	C	0	0
-5.1900	-0.9530	-0.8390	O	0	0
-5.5720	-2.1680	-1.4690	C	0	0
-3.6380	-3.0520	0.0530	O	0	0
-2.7780	-4.1250	0.4090	C	0	0
-1.1220	-0.3590	-0.0130	C	0	0
-1.7220	-1.6400	0.1590	C	0	0
-3.3150	0.5140	-0.7490	C	0	0
1.0810	-1.2430	0.7150	C	0	0
1.4350	-2.1720	-0.3930	C	0	0
1.2460	-3.5600	-0.2490	C	0	0
1.5830	-4.4280	-1.3040	C	0	0
2.1100	-3.9120	-2.5010	C	0	0
2.2980	-2.5260	-2.6430	C	0	0
1.9610	-1.6580	-1.5910	C	0	0
0.7480	-4.0610	0.8800	F	0	0
2.4660	-4.8300	-3.6150	C	0	0
2.9590	-4.1020	-4.6670	F	0	0
1.3500	-5.5160	-4.0170	F	0	0
3.4190	-5.7180	-3.1870	F	0	0
1.8400	1.2270	0.3040	H	0	0
2.4050	5.6730	-0.3220	H	0	0
3.2290	6.8030	1.7180	H	0	0
1.1340	3.9300	4.1580	H	0	0
0.3090	2.7980	2.1190	H	0	0
2.4000	5.6660	5.2350	H	0	0
2.4000	7.1610	4.3030	H	0	0
3.8230	6.1230	4.3030	H	0	0
-6.4740	-2.1390	-2.0790	H	0	0
-5.7160	-2.9220	-0.6950	H	0	0
-4.7500	-2.4960	-2.1050	H	0	0
-3.3850	-5.0220	0.5340	H	0	0
-1.9800	-4.1820	-0.3310	H	0	0
-2.3240	-3.8930	1.3720	H	0	0
-1.1460	-2.4860	0.5050	H	0	0
-3.9320	1.3300	-1.0980	H	0	0
0.5740	-1.7960	1.5050	H	0	0
1.9920	-0.8180	1.1370	H	0	0
1.4380	-5.4930	-1.1920	H	0	0
2.7020	-2.1230	-3.5610	H	0	0
2.1090	-0.5940	-1.7080	H	0	0
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Compound69

> <Activ>
0.41

> <DB_Ref_id>
3.03
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Compound70

SciTegic10081411483D

60	63	0	0	0	0	999	V2000
4.1990	-2.0180	0.1350	C	0	0		
1.7720	-2.0820	-0.2090	C	0	0		
4.1560	-0.6030	0.1540	C	0	0		
0.5160	-0.0180	-0.3590	N	0	0		
-0.6640	-0.7210	-0.5350	C	0	0		
-0.7230	-2.0720	-0.5570	C	0	0		
0.5180	-2.8710	-0.3950	C	0	0		
0.4180	-4.0760	-0.4260	O	0	0		
-2.0210	-2.7420	-0.7440	C	0	0		
-2.3380	-3.1700	-1.8300	O	0	0		
-2.9300	-2.8810	0.4320	C	0	0		
-3.3730	-2.5660	2.8070	C	0	0		
-2.5160	-2.4360	1.6990	C	0	0		
-4.6460	-3.1430	2.6480	C	0	0		
-4.2030	-3.4570	0.2730	C	0	0		
-5.0600	-3.5880	1.3810	C	0	0		
-5.5530	-3.2810	3.8180	C	0	0		
5.3670	-2.6580	0.2890	O	0	0		
6.5300	-2.0680	-0.2720	C	0	0		
5.2850	0.1000	0.3300	O	0	0		
5.1900	1.5160	0.3570	C	0	0		
3.0100	-2.7560	-0.0470	C	0	0		
2.9260	0.0720	-0.0100	C	0	0		
1.7150	-0.6540	-0.1970	C	0	0		
0.4200	1.4590	-0.3590	C	0	0		
0.8360	2.0350	-1.7130	C	0	0		
0.8090	3.5630	-1.7360	C	0	0		
-0.5700	4.0880	-1.5550	C	0	0		
-2.2600	5.1370	-0.1490	C	0	0		
-0.9550	4.6410	-0.3180	C	0	0		
-3.1780	5.0820	-1.2090	C	0	0		
-1.4900	4.0350	-2.6170	C	0	0		
-2.7930	4.5310	-2.4430	C	0	0		
-1.5960	-0.1840	-0.6600	H	0	0		
-3.0490	-2.2210	3.7770	H	0	0		
-1.5410	-1.9900	1.8320	H	0	0		
-4.5310	-3.8030	-0.6970	H	0	0		
-6.0370	-4.0330	1.2520	H	0	0		
-6.5120	-3.7440	3.5900	H	0	0		
-5.7500	-2.2970	4.2440	H	0	0		
-5.0640	-3.8830	4.5860	H	0	0		
6.3950	-1.5040	-1.1950	H	0	0		
7.2520	-2.8590	-0.4690	H	0	0		
6.9630	-1.3960	0.4690	H	0	0		
4.8440	1.8540	-0.6190	H	0	0		
4.5760	1.7990	1.2130	H	0	0		
6.1900	1.9220	0.5160	H	0	0		
3.0510	-3.8360	-0.0590	H	0	0		
2.9340	1.1520	0.0100	H	0	0		
1.0470	1.8580	0.4390	H	0	0		
-0.5990	1.7520	-0.1130	H	0	0		
0.2190	1.6250	-2.5120	H	0	0		
1.8190	1.6620	-2.0040	H	0	0		
1.2210	3.9420	-2.6720	H	0	0		
1.4590	3.9730	-0.9630	H	0	0		
-2.5550	5.5610	0.8010	H	0	0		

-0.2540	4.6860	0.5000 H	0	0
-4.1800	5.4650	-1.0780 H	0	0
-1.1990	3.6110	-3.5680 H	0	0
-3.5000	4.4900	-3.2600 H	0	0
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M END

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Compound70

> <Activ>

2.2

> <DB_Ref_id>

3.08

\$\$\$\$

Compound71

SciTegic10081411483D

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1.1020	-0.8140	-0.0840	C	0	0		
-0.1520	-1.6020	-0.2690	C	0	0		
-1.3930	-0.8030	-0.4330	C	0	0		
-1.3340	0.5490	-0.4100	C	0	0		
-0.1560	1.2500	-0.2360	N	0	0		
-0.2520	-2.8090	-0.3010	O	0	0		
-2.6920	-1.4750	-0.6190	C	0	0		
-3.2540	-1.4320	-1.6890	O	0	0		
-3.2930	-2.2030	0.5350	C	0	0		
-2.6820	-2.1470	1.8010	C	0	0		
-3.2500	-2.8340	2.8890	C	0	0		
-4.4280	-3.5780	2.7130	C	0	0		
-5.0410	-3.6350	1.4490	C	0	0		
-4.4750	-2.9490	0.3610	C	0	0		
-5.0270	-4.3050	3.8630	C	0	0		
3.5270	-0.7480	0.2600	C	0	0		
3.4860	0.6640	0.2790	C	0	0		
4.6950	-1.3910	0.4140	O	0	0		
4.6840	-2.8090	0.3870	C	0	0		
4.6130	1.3670	0.4550	O	0	0		
4.5310	2.7830	0.3950	C	0	0		
1.0430	0.6130	-0.0720	C	0	0		
2.2540	1.3400	0.1130	C	0	0		
2.3380	-1.4880	0.0780	C	0	0		
-0.2500	2.7270	-0.2340	C	0	0		
0.1660	3.3030	-1.5390	C	0	0		
1.2440	4.2010	-1.6000	C	0	0		
1.6460	4.7540	-2.8320	C	0	0		
0.9550	4.3970	-4.0180	C	0	0		
-0.1230	3.4940	-3.9470	C	0	0		
-0.5160	2.9470	-2.7150	C	0	0		
2.9750	5.8500	-2.8320	Cl	0	0		
1.3830	5.0290	-5.5610	Cl	0	0		
-2.2660	1.0840	-0.5350	H	0	0		
-1.7750	-1.5760	1.9450	H	0	0		
-2.7740	-2.7850	3.8580	H	0	0		
-5.9470	-4.2070	1.3090	H	0	0		
-4.9510	-2.9980	-0.6070	H	0	0		
-5.9400	-4.8520	3.6230	H	0	0		
-5.2640	-3.5960	4.6580	H	0	0		

-4.3050	-5.0200	4.2580	H	0	0
5.6450	-3.3090	0.5120	H	0	0
4.2660	-3.1290	-0.5680	H	0	0
4.0200	-3.1600	1.1760	H	0	0
5.5210	3.1910	0.6000	H	0	0
4.0840	3.0610	-0.5580	H	0	0
3.8630	3.1190	1.1880	H	0	0
2.2620	2.4200	0.1350	H	0	0
2.3810	-2.5660	0.0650	H	0	0
0.3830	3.1250	0.5590	H	0	0
-1.2790	3.0200	-0.0190	H	0	0
1.7600	4.4670	-0.6870	H	0	0
-0.6620	3.2070	-4.8380	H	0	0
-1.3440	2.2560	-2.6740	H	0	0
3	2	1	0		
4	3	2	0		
5	4	1	0		
1	2	1	0		
2	6	2	0		
3	7	1	0		
7	8	2	0		
7	9	1	0		
11	10	2	0		
12	11	1	0		
13	12	2	0		
10	9	1	0		
9	14	2	0		
12	15	1	0		
16	17	2	0		
16	18	1	0		
18	19	1	0		
17	20	1	0		
20	21	1	0		
23	22	2	0		
22	1	1	0		
1	24	2	0		
24	16	1	0		
17	23	1	0		
22	5	1	0		
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11	36	1	0		
13	37	1	0		
14	38	1	0		
15	39	1	0		
15	40	1	0		
15	41	1	0		
19	42	1	0		
19	43	1	0		
19	44	1	0		

```

21 45 1 0
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21 47 1 0
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M END

> <Name>

Compound71

> <Activ>

1.1

> <DB_Ref_id>

3.04

\$\$\$\$

Compound72

SciTegic10081411483D

```

61 64 0 0 0 0          999 V2000
  1.7400 -1.2170  2.1030 C  0  0
  0.4860 -2.0060  1.9180 C  0  0
 -0.7540 -1.2050  1.7540 C  0  0
 -0.6950  0.1460  1.7770 C  0  0
  0.4820  0.8480  1.9510 N  0  0
  0.3870 -3.2110  1.8870 O  0  0
 -2.0530 -1.8770  1.5680 C  0  0
 -2.7170 -2.2010  2.5230 O  0  0
  4.1660 -1.1500  2.4470 C  0  0
  4.1250  0.2620  2.4670 C  0  0
  1.6820  0.2110  2.1150 C  0  0
  2.8930  0.9370  2.3010 C  0  0
  2.9770 -1.8910  2.2660 C  0  0
  0.3890  2.3240  1.9530 C  0  0
  0.4260  2.8770  0.5720 C  0  0
 -0.7600  3.2950 -0.0630 C  0  0
 -0.7090  3.8160 -1.3690 C  0  0
  0.5210  3.9180 -2.0410 C  0  0
  1.7030  3.5000 -1.4060 C  0  0
  1.6560  2.9780 -0.1040 C  0  0
 -2.4180 -2.0860  0.3070 O  0  0
 -3.6620 -2.7660  0.2090 C  0  0
 -3.9790 -3.0180 -1.2210 C  0  0
 -3.1150 -3.8050 -2.0040 C  0  0
 -3.4140 -4.0430 -3.3560 C  0  0
 -5.4420 -2.7090 -3.1450 C  0  0
 -5.1410 -2.4710 -1.7910 C  0  0
  5.3340 -1.7930  2.6020 O  0  0
  6.4860 -1.2360  1.9820 C  0  0
  5.2520  0.9650  2.6430 O  0  0
  5.1890  2.3750  2.4920 C  0  0
 -1.9300  3.2030  0.5640 F  0  0
 -4.5760 -3.4960 -3.9260 C  0  0
 -6.6700 -2.1310 -3.7480 C  0  0
  0.5720  4.4690 -3.4220 C  0  0
  1.8610  4.4220 -3.8850 F  0  0

```

0.1370	5.7700	-3.4120	F	0	0
-0.2360	3.7230	-4.2420	F	0	0
-1.6270	0.6820	1.6520	H	0	0
2.9020	2.0180	2.3200	H	0	0
3.0200	-2.9710	2.2520	H	0	0
1.2150	2.7360	2.5310	H	0	0
-0.5410	2.6230	2.4390	H	0	0
-1.6190	4.1370	-1.8560	H	0	0
2.6520	3.5740	-1.9180	H	0	0
2.5680	2.6580	0.3790	H	0	0
-4.4340	-2.1310	0.6460	H	0	0
-3.5720	-3.7170	0.7340	H	0	0
-2.2190	-4.2270	-1.5700	H	0	0
-2.7500	-4.6470	-3.9570	H	0	0
-5.8050	-1.8670	-1.1900	H	0	0
7.2770	-1.9340	1.7090	H	0	0
6.9120	-0.4960	2.6600	H	0	0
6.1720	-0.7190	1.0780	H	0	0
6.1880	2.7810	2.6540	H	0	0
4.7290	2.5960	1.5290	H	0	0
4.5370	2.7710	3.2710	H	0	0
-4.8010	-3.6840	-4.9670	H	0	0
-6.8150	-2.3830	-4.7990	H	0	0
-6.6390	-1.0450	-3.6660	H	0	0
-7.5430	-2.4830	-3.1990	H	0	0
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30	31	1	0		
16	32	1	0		
18	35	1	0		
25	33	2	0		
33	26	1	0		
26	34	1	0		
3	2	1	0		

```

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5 4 1 0
35 38 1 0
35 37 1 0
35 36 1 0
4 39 1 0
12 40 1 0
13 41 1 0
14 42 1 0
14 43 1 0
17 44 1 0
19 45 1 0
20 46 1 0
22 47 1 0
22 48 1 0
24 49 1 0
25 50 1 0
27 51 1 0
29 52 1 0
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29 54 1 0
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34 61 1 0

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M END

> <Name>

Compound72

> <Activ>

0.06

> <DB_Ref_id>

3.21

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Compound73

SciTegic10081411483D

```

61 64 0 0 0 0          999 V2000
  2.4470 -1.2150  1.5860 C  0 0
  1.1930 -2.0020  1.4000 C  0 0
 -0.0470 -1.2030  1.2380 C  0 0
  0.0120  0.1480  1.2600 C  0 0
  1.1890  0.8520  1.4360 N  0 0
  1.0940 -3.2090  1.3690 O  0 0
 -1.3460 -1.8730  1.0510 C  0 0
 -2.0160 -2.1880  2.0060 O  0 0
  4.8730 -1.1480  1.9300 C  0 0
  4.8320  0.2640  1.9490 C  0 0
  2.3890  0.2130  1.5980 C  0 0
  3.6000  0.9390  1.7850 C  0 0
  3.6840 -1.8870  1.7480 C  0 0
  1.0960  2.3260  1.4360 C  0 0
 -0.0780  2.8010  0.6520 C  0 0
 -1.2500  3.2250  1.3070 C  0 0
 -2.3540  3.6700  0.5570 C  0 0
 -2.2850  3.6930 -0.8480 C  0 0

```

-1.1150	3.2720	-1.5020	C	0	0
-0.0140	2.8240	-0.7520	C	0	0
-1.7050	-2.0960	-0.2110	O	0	0
-3.0020	-2.6680	-0.3110	C	0	0
-3.3560	-2.8460	-1.7440	C	0	0
-2.3610	-3.2400	-2.6580	C	0	0
-2.6780	-3.4140	-4.0160	C	0	0
-4.9870	-2.7970	-3.5550	C	0	0
-4.6720	-2.6230	-2.1950	C	0	0
6.0410	-1.7890	2.0840	O	0	0
7.1870	-1.2520	1.4400	C	0	0
5.9590	0.9670	2.1250	O	0	0
5.8830	2.3830	2.0390	C	0	0
-1.3260	3.2050	2.6370	F	0	0
-3.9920	-3.1910	-4.4650	C	0	0
-5.7380	-2.2050	-1.2460	C	0	0
-3.4510	4.1660	-1.6410	C	0	0
-3.4380	3.5660	-2.8750	F	0	0
-3.3810	5.5270	-1.7930	F	0	0
-4.6120	3.8400	-0.9880	F	0	0
-0.9200	0.6840	1.1350	H	0	0
3.6090	2.0200	1.8050	H	0	0
3.7260	-2.9670	1.7360	H	0	0
2.0080	2.7440	1.0120	H	0	0
1.0120	2.6800	2.4630	H	0	0
-3.2520	3.9940	1.0590	H	0	0
-1.0570	3.2870	-2.5800	H	0	0
0.8830	2.5020	-1.2600	H	0	0
-3.7110	-1.9860	0.1560	H	0	0
-2.9850	-3.6390	0.1840	H	0	0
-1.3500	-3.4120	-2.3200	H	0	0
-1.9140	-3.7170	-4.7150	H	0	0
-5.9940	-2.6270	-3.9060	H	0	0
7.9690	-1.9590	1.1620	H	0	0
7.6310	-0.5060	2.1000	H	0	0
6.8610	-0.7420	0.5330	H	0	0
6.8710	2.7910	2.2460	H	0	0
5.4450	2.6430	1.0740	H	0	0
5.2070	2.7360	2.8160	H	0	0
-4.2370	-3.3240	-5.5080	H	0	0
-5.8520	-2.8590	-0.3810	H	0	0
-6.6970	-2.1740	-1.7660	H	0	0
-5.5260	-1.2010	-0.8790	H	0	0
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11	5	1	0		
5	14	1	0		
14	15	1	0		
17	16	2	0		
18	17	1	0		
19	18	2	0		
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23 24 2 0
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25 50 1 0
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M END

> <Name>

Compound73

> <Activ>

0.015

> <DB_Ref_id>

3.2

\$\$\$\$

Compound74

SciTegic10081411483D

61 64 0 0 0 0

999 V2000

1.6020	-1.5220	2.0700	C	0	0
0.3480	-2.3090	1.8850	C	0	0
-0.8930	-1.5100	1.7230	C	0	0
-0.8340	-0.1580	1.7440	C	0	0
0.3440	0.5430	1.9200	N	0	0
0.2480	-3.5160	1.8530	O	0	0
-2.1920	-2.1820	1.5350	C	0	0
-2.6800	-2.8320	2.4300	O	0	0
4.0270	-1.4550	2.4140	C	0	0
3.9860	-0.0430	2.4340	C	0	0
1.5430	-0.0940	2.0820	C	0	0
2.7540	0.6330	2.2690	C	0	0
2.8380	-2.1950	2.2320	C	0	0
0.2500	2.0200	1.9200	C	0	0
0.7150	2.6000	0.6310	C	0	0
0.0410	2.3070	-0.5700	C	0	0
0.4920	2.8610	-1.7810	C	0	0
1.6130	3.7070	-1.7950	C	0	0
2.2870	3.9980	-0.5960	C	0	0
1.8380	3.4450	0.6150	C	0	0
-2.7620	-2.0160	0.3440	O	0	0
-3.9980	-2.7050	0.2360	C	0	0
-4.5800	-2.4690	-1.1110	C	0	0
-4.8850	-3.5590	-1.9470	C	0	0
-5.4360	-3.3360	-3.2210	C	0	0
-5.3810	-0.9340	-2.8240	C	0	0
-4.8300	-1.1560	-1.5510	C	0	0
5.1950	-2.0980	2.5680	O	0	0
6.3460	-1.5430	1.9470	C	0	0
5.1130	0.6600	2.6090	O	0	0
5.0250	2.0760	2.5880	C	0	0
-1.0240	1.5060	-0.5680	F	0	0
-5.6840	-2.0230	-3.6620	C	0	0
-6.2660	-1.7870	-5.0100	C	0	0
2.0900	4.2930	-3.0760	C	0	0
3.4390	4.5220	-3.0020	F	0	0
1.4370	5.4770	-3.3090	F	0	0
1.8300	3.4200	-4.1020	F	0	0
-1.7660	0.3770	1.6190	H	0	0
2.7620	1.7130	2.2890	H	0	0
2.8810	-3.2730	2.2210	H	0	0
0.8520	2.4160	2.7360	H	0	0
-0.7850	2.3130	2.0980	H	0	0
-0.0270	2.6350	-2.7030	H	0	0
3.1500	4.6490	-0.6000	H	0	0
2.3590	3.6740	1.5330	H	0	0
-4.6740	-2.3140	0.9980	H	0	0
-3.8090	-3.7700	0.3690	H	0	0
-4.6950	-4.5680	-1.6150	H	0	0
-5.6660	-4.1760	-3.8580	H	0	0
-5.5690	0.0760	-3.1580	H	0	0
-4.5980	-0.3160	-0.9140	H	0	0
7.1370	-2.2420	1.6720	H	0	0
6.7750	-0.8050	2.6230	H	0	0
6.0290	-1.0230	1.0430	H	0	0
6.0120	2.4840	2.8120	H	0	0
4.5860	2.3770	1.6370	H	0	0
4.3480	2.3890	3.3810	H	0	0
-6.4220	-0.7360	-5.2520	H	0	0
-7.2290	-2.2930	-5.0820	H	0	0
-5.6100	-2.2110	-5.7680	H	0	0

1	2	1	0
2	6	2	0
3	7	1	0
7	8	2	0
9	10	2	0
12	11	2	0
11	1	1	0
1	13	2	0
13	9	1	0
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13	41	1	0
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34 61 1 0

M END

> <Name>

Compound74

> <Activ>

0.008

> <DB_Ref_id>

3.19

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Compound75

SciTegic10081411483D

65	69	0	0	0	0	999	V2000
-0.4380	1.2310	-1.3950	C	0	0		
0.7170	2.1760	-1.3850	C	0	0		
2.0610	1.5430	-1.2750	C	0	0		
2.1700	0.1950	-1.1890	C	0	0		
1.0760	-0.6500	-1.1990	N	0	0		
0.6560	3.3830	-1.4570	O	0	0		
3.1950	2.3150	-1.2620	N	0	0		
3.2230	3.4750	-0.5410	C	0	0		
-2.8590	0.8540	-1.5100	C	0	0		
-2.6470	-0.5470	-1.4220	C	0	0		
-4.0900	1.3610	-1.6050	F	0	0		
-0.2030	-0.1760	-1.3010	C	0	0		
-1.3260	-1.0550	-1.3180	C	0	0		
-1.7580	1.7340	-1.4940	C	0	0		
1.3540	-2.1000	-1.0960	C	0	0		
1.0250	-2.6250	0.2560	C	0	0		
1.5800	-2.0210	1.3980	C	0	0		
1.2700	-2.5160	2.6760	C	0	0		
0.4060	-3.6190	2.8140	C	0	0		
-0.1480	-4.2230	1.6700	C	0	0		
0.1600	-3.7250	0.3930	C	0	0		
0.0290	-4.2270	4.3730	Cl	0	0		
4.4820	4.2990	-0.5470	C	0	0		
4.7480	4.9240	0.7750	C	0	0		
2.2520	3.8260	0.0860	O	0	0		
-3.6820	-1.4020	-1.4360	N	0	0		
-3.6290	-2.6740	-2.1950	C	0	0		
-4.1410	-3.8540	-1.3420	C	0	0		
-5.4490	-3.5590	-0.7380	N	0	0		
-5.4000	-2.3540	0.1040	C	0	0		
-4.9340	-1.1190	-0.6950	C	0	0		
-5.9710	-4.7050	-0.0040	C	0	0		
4.5530	6.8200	2.2890	C	0	0		
4.3010	6.2290	1.0390	C	0	0		
5.2540	6.1080	3.2790	C	0	0		
5.4490	4.2090	1.7640	C	0	0		
5.7010	4.7990	3.0140	C	0	0		
5.5650	6.8300	4.8030	Cl	0	0		
3.1620	-0.2280	-1.1090	H	0	0		
4.0000	2.0230	-1.7810	H	0	0		
-1.1800	-2.1250	-1.2500	H	0	0		
-1.9280	2.8010	-1.5630	H	0	0		
2.4060	-2.2790	-1.3110	H	0	0		

0.7660	-2.6330	-1.8440	H	0	0
2.2440	-1.1760	1.2990	H	0	0
1.7010	-2.0410	3.5470	H	0	0
-0.8140	-5.0680	1.7620	H	0	0
-0.2700	-4.1910	-0.4800	H	0	0
4.4160	5.0740	-1.3090	H	0	0
5.3320	3.6760	-0.8300	H	0	0
-2.6150	-2.8830	-2.5470	H	0	0
-4.2520	-2.5630	-3.0820	H	0	0
-3.4220	-4.0860	-0.5550	H	0	0
-4.2230	-4.7440	-1.9670	H	0	0
-6.3890	-2.1620	0.5210	H	0	0
-4.7290	-2.5270	0.9470	H	0	0
-5.6970	-0.8400	-1.4220	H	0	0
-4.8110	-0.2680	-0.0230	H	0	0
-6.9020	-4.4280	0.4880	H	0	0
-6.0880	-5.5490	-0.6840	H	0	0
-5.2600	-4.9940	0.7700	H	0	0
4.2010	7.8240	2.4790	H	0	0
3.7640	6.7830	0.2850	H	0	0
5.7930	3.2030	1.5680	H	0	0
6.2400	4.2380	3.7640	H	0	0
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4	3	2	0		
5	4	1	0		
1	2	1	0		
2	6	2	0		
3	7	1	0		
7	8	1	0		
9	10	2	0		
9	11	1	0		
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16	21	2	0		
19	22	1	0		
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23	24	1	0		
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31	26	1	0		
26	27	1	0		
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36	37	1	0		
33	34	2	0		
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35 38 1 0
4 39 1 0
7 40 1 0
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15 43 1 0
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Compound75

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2

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03.15b

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Compound76

SciTegic10081411483D

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  3.9840 -0.2720 -0.4550 C 0 0
  3.9410  1.1410 -0.4360 C 0 0
  2.7110  1.8160 -0.6020 C 0 0
  1.5000  1.0920 -0.7870 C 0 0
  1.5570 -0.3380 -0.8010 C 0 0
  2.7950 -1.0100 -0.6370 C 0 0
  0.2990  1.7280 -0.9510 N 0 0
 -0.8790  1.0270 -1.1250 C 0 0
 -0.9340 -0.3240 -1.1480 C 0 0
  0.3030 -1.1250 -0.9860 C 0 0
  0.2010 -2.3320 -1.0160 O 0 0
  0.2050  3.2050 -0.9490 C 0 0
  0.2500  3.7540  0.4300 C 0 0
 -0.7170  3.3670  1.3750 C 0 0
 -0.6760  3.8870  2.6800 C 0 0
  0.3340  4.7990  3.0430 C 0 0

```

1.3030	5.1840	2.0980	C	0	0
1.2600	4.6620	0.7930	C	0	0
0.3850	5.4360	4.6350	C1	0	0
5.1520	-0.9120	-0.3030	O	0	0
6.3010	-0.3610	-0.9280	C	0	0
5.0700	1.8440	-0.2620	O	0	0
4.9770	3.2620	-0.2460	C	0	0
-2.2190	-0.9880	-1.3320	C	0	0
-3.4140	-0.3570	-1.4960	N	0	0
-4.3400	-1.2700	-1.6330	O	0	0
-3.7330	-2.4790	-1.5570	C	0	0
-2.4080	-2.3280	-1.3690	N	0	0
-4.4320	-3.8170	-1.6640	C	0	0
-4.4610	-4.4690	-0.3280	C	0	0
-3.5020	-5.4440	0.0000	C	0	0
-4.5160	-5.7030	2.1970	C	0	0
-5.4750	-4.7290	1.8710	C	0	0
-3.5290	-6.0610	1.2640	C	0	0
-5.4470	-4.1110	0.6070	C	0	0
2.7190	2.8980	-0.5820	H	0	0
2.8360	-2.0900	-0.6500	H	0	0
-1.8130	1.5590	-1.2520	H	0	0
-0.7270	3.5040	-1.4300	H	0	0
1.0290	3.6170	-1.5330	H	0	0
-1.4960	2.6700	1.1020	H	0	0
-1.4240	3.5800	3.3950	H	0	0
2.0840	5.8830	2.3630	H	0	0
2.0080	4.9630	0.0720	H	0	0
7.0880	-1.0630	-1.2070	H	0	0
6.7360	0.3750	-0.2520	H	0	0
5.9820	0.1600	-1.8300	H	0	0
4.6270	3.5900	-1.2250	H	0	0
4.3650	3.5550	0.6070	H	0	0
5.9770	3.6680	-0.0960	H	0	0
-3.8930	-4.4510	-2.3670	H	0	0
-5.4510	-3.6640	-2.0180	H	0	0
-2.7400	-5.7230	-0.7150	H	0	0
-4.5370	-6.1780	3.1680	H	0	0
-6.2330	-4.4530	2.5900	H	0	0
-2.7930	-6.8090	1.5140	H	0	0
-6.1880	-3.3630	0.3630	H	0	0
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8	9	2	0		
7	8	1	0		
4	7	1	0		
5	10	1	0		
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15	16	2	0		
14	15	1	0		
18	13	1	0		
13	14	2	0		
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2	22	1	0		
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27 28  2  0
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Compound76

> <Activ>
0.041

> <DB_Ref_id>
4.05

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Compound77
  SciTegic10081411483D

69 74  0  0  0  0          999 V2000
   -3.6190    0.9000   -0.7950 C    0  0
   -3.4060   -0.5000   -0.7070 C    0  0
   -2.0860   -1.0080   -0.6040 C    0  0
   -0.9630   -0.1310   -0.5860 C    0  0
   -1.1970    1.2750   -0.6800 C    0  0

```


-2.5160	1.7830	-0.7790	C	0	0
0.3170	-0.6080	-0.4840	N	0	0
1.4080	0.2400	-0.4750	C	0	0
1.2970	1.5860	-0.5610	C	0	0
-0.0390	2.2190	-0.6700	C	0	0
-0.0840	3.4260	-0.7420	O	0	0
0.5960	-2.0570	-0.3810	C	0	0
0.7230	-2.4880	1.0350	C	0	0
1.9940	-2.7310	1.5860	C	0	0
2.1170	-3.1390	2.9240	C	0	0
0.9670	-3.3070	3.7170	C	0	0
-0.3050	-3.0650	3.1680	C	0	0
-0.4260	-2.6560	1.8280	C	0	0
2.4960	2.4080	-0.5470	C	0	0
4.5840	2.9610	-0.4590	O	0	0
2.5220	3.7580	-0.6390	N	0	0
3.7720	1.9390	-0.4380	N	0	0
3.8260	4.0780	-0.5840	C	0	0
4.3600	5.4920	-0.6500	C	0	0
5.5510	5.5310	-1.5390	C	0	0
5.4300	6.0140	-2.8560	C	0	0
7.8010	5.6050	-3.2250	C	0	0
7.9220	5.1230	-1.9100	C	0	0
6.5550	6.0510	-3.6970	C	0	0
6.7970	5.0860	-1.0680	C	0	0
-4.8480	1.4100	-0.8910	F	0	0
-4.4430	-1.3560	-0.7210	N	0	0
-5.6890	-1.0680	0.0330	C	0	0
-6.1970	-2.3190	0.7810	C	0	0
-6.2700	-3.4880	-0.1070	N	0	0
-4.9530	-3.8030	-0.6800	C	0	0
-4.3910	-2.6210	-1.4940	C	0	0
-6.8520	-4.6410	0.5700	C	0	0
1.0960	-3.7380	5.1350	C	0	0
-0.1500	-3.8480	5.6930	F	0	0
1.8300	-2.8130	5.8300	F	0	0
1.7270	-4.9550	5.1860	F	0	0
-1.9410	-2.0780	-0.5350	H	0	0
-2.6850	2.8480	-0.8480	H	0	0
2.4080	-0.1660	-0.3950	H	0	0
1.5180	-2.2830	-0.9160	H	0	0
-0.2130	-2.6110	-0.8570	H	0	0
2.8830	-2.6040	0.9820	H	0	0
3.0960	-3.3240	3.3400	H	0	0
-1.1910	-3.1920	3.7720	H	0	0
-1.4060	-2.4710	1.4120	H	0	0
4.6430	5.8200	0.3500	H	0	0
3.5900	6.1540	-1.0450	H	0	0
4.4750	6.3570	-3.2250	H	0	0
8.6660	5.6330	-3.8710	H	0	0
8.8810	4.7790	-1.5470	H	0	0
6.4610	6.4220	-4.7070	H	0	0
6.8970	4.7130	-0.0590	H	0	0
-5.5410	-0.2520	0.7420	H	0	0
-6.4470	-0.7330	-0.6780	H	0	0
-5.5370	-2.5430	1.6230	H	0	0
-7.1840	-2.1150	1.1990	H	0	0
-4.2620	-4.0690	0.1230	H	0	0
-5.0350	-4.6800	-1.3240	H	0	0
-3.3690	-2.8460	-1.8090	H	0	0
-4.9750	-2.4880	-2.4040	H	0	0

-6.1840	-4.9690	1.3650	H	0	0
-7.8480	-4.3850	0.9320	H	0	0
-6.9550	-5.4630	-0.1390	H	0	0
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M END

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Compound77

> <Activ>

0.024

> <DB_Ref_id>

4.15

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Compound78

SciTegic10081411483D

69	74	0	0	0	0	999	V2000
-3.6410	2.0590	0.1660	C	0	0		
-3.4280	0.6580	0.2540	C	0	0		
-2.1070	0.1480	0.3570	C	0	0		
-0.9840	1.0250	0.3730	C	0	0		
-1.2170	2.4320	0.2810	C	0	0		
-2.5370	2.9390	0.1800	C	0	0		
0.2950	0.5510	0.4750	N	0	0		
1.3890	1.3980	0.4860	C	0	0		
1.2750	2.7420	0.3980	C	0	0		
-0.0600	3.3750	0.2890	C	0	0		
-0.1050	4.5840	0.2190	O	0	0		
0.5740	-0.8980	0.5780	C	0	0		
0.4080	-1.5840	-0.7320	C	0	0		
1.0350	-1.0570	-1.8750	C	0	0		
0.8850	-1.6950	-3.1190	C	0	0		
0.1090	-2.8630	-3.2210	C	0	0		
-0.5180	-3.3910	-2.0780	C	0	0		
-0.3690	-2.7520	-0.8340	C	0	0		
2.4790	3.5660	0.4140	C	0	0		
4.0080	5.0840	0.4040	N	0	0		
3.6740	2.8910	0.5160	O	0	0		
2.6930	4.8910	0.3460	N	0	0		
4.6290	3.8910	0.5080	C	0	0		
6.1270	3.6910	0.5980	C	0	0		
6.4200	2.2700	0.9140	C	0	0		
6.1720	1.2700	-0.0450	C	0	0		
6.9750	-0.4240	1.5100	C	0	0		
7.2210	0.5740	2.4690	C	0	0		
6.4490	-0.0760	0.2540	C	0	0		
6.9440	1.9200	2.1720	C	0	0		

-4.8690	2.5680	0.0700	F	0	0
-4.4630	-0.1970	0.2380	N	0	0
-4.3950	-1.4240	-0.6060	C	0	0
-5.4880	-2.4690	-0.2950	C	0	0
-5.9530	-2.4220	1.0920	N	0	0
-6.5940	-1.1270	1.3260	C	0	0
-5.6680	0.0900	1.0800	C	0	0
-4.9060	-2.7320	2.0640	C	0	0
-0.9690	-3.2620	0.2400	F	0	0
-0.0490	-3.5390	-4.5370	C	0	0
0.7520	-2.9240	-5.4650	F	0	0
-1.3570	-3.4570	-4.9380	F	0	0
0.3130	-4.8560	-4.4200	F	0	0
-1.9630	-0.9220	0.4240	H	0	0
-2.7070	4.0040	0.1130	H	0	0
2.3870	0.9920	0.5660	H	0	0
-0.1030	-1.3420	1.3090	H	0	0
1.5920	-1.0430	0.9370	H	0	0
1.6330	-0.1600	-1.8050	H	0	0
1.3690	-1.2850	-3.9920	H	0	0
-1.1150	-4.2870	-2.1560	H	0	0
6.5290	4.3280	1.3850	H	0	0
6.5860	3.9550	-0.3540	H	0	0
5.7700	1.5310	-1.0140	H	0	0
7.1880	-1.4570	1.7400	H	0	0
7.6230	0.3070	3.4360	H	0	0
6.2600	-0.8420	-0.4840	H	0	0
7.1370	2.6820	2.9120	H	0	0
-4.4710	-1.1270	-1.6540	H	0	0
-3.4100	-1.8950	-0.4920	H	0	0
-5.1500	-3.4750	-0.5350	H	0	0
-6.3460	-2.2790	-0.9450	H	0	0
-7.4430	-1.0510	0.6460	H	0	0
-7.0160	-1.1020	2.3300	H	0	0
-5.3550	0.5020	2.0430	H	0	0
-6.2420	0.8770	0.5860	H	0	0
-5.3010	-2.6150	3.0740	H	0	0
-4.5200	-3.7340	1.8770	H	0	0
-4.0800	-2.0290	1.9470	H	0	0
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12	13	1	0		
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18	13	1	0		
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19	22	2	0		
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23	20	2	0
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Compound78

> <Activ>

0.038

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4.18

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Compound79

SciTegic10081411483D

54	58	0	0	0	0	999	V2000
4.9380	-1.0390	0.6940	C	0	0		
4.8950	0.3730	0.7130	C	0	0		
3.6620	1.0470	0.5490	C	0	0		
2.4530	0.3200	0.3640	C	0	0		
2.5120	-1.1090	0.3500	C	0	0		
3.7500	-1.7810	0.5140	C	0	0		
1.2520	0.9570	0.1990	N	0	0		
0.0740	0.2520	0.0260	C	0	0		
0.0210	-1.1000	0.0020	C	0	0		
1.2600	-1.8990	0.1640	C	0	0		
1.1580	-3.1040	0.1350	O	0	0		
1.1560	2.4320	0.1990	C	0	0		
1.5900	3.0100	-1.0990	C	0	0		
2.6600	3.9180	-1.1420	C	0	0		
3.0700	4.4650	-2.3710	C	0	0		
2.4080	4.1050	-3.5600	C	0	0		
1.3360	3.1930	-3.5150	C	0	0		
0.9280	2.6460	-2.2870	C	0	0		
2.9060	4.7730	-5.0580	C1	0	0		
6.1070	-1.6760	0.8480	O	0	0		
7.2810	-0.8890	0.9790	C	0	0		
-1.2640	-1.7660	-0.1830	C	0	0		
-2.9320	-3.0920	-0.4290	C	0	0		
-2.3200	-0.9140	-0.3180	O	0	0		
-1.5920	-3.0840	-0.2440	N	0	0		
-3.3650	-1.7660	-0.4720	C	0	0		
-4.7850	-1.2810	-0.6620	C	0	0		
-5.5630	-1.5230	0.5840	C	0	0		
-5.5800	-0.5530	1.6000	C	0	0		
-7.0290	-1.9810	2.9380	C	0	0		
-7.0120	-2.9510	1.9220	C	0	0		
-6.3150	-0.7810	2.7780	C	0	0		
-6.2770	-2.7230	0.7440	C	0	0		
5.8030	0.9390	0.8540	H	0	0		
3.6720	2.1270	0.5690	H	0	0		
3.7930	-2.8590	0.5000	H	0	0		
-0.8590	0.7830	-0.1010	H	0	0		
1.7770	2.8320	1.0000	H	0	0		
0.1250	2.7230	0.4010	H	0	0		
3.1720	4.2010	-0.2340	H	0	0		
3.8980	5.1600	-2.3900	H	0	0		
0.8180	2.9080	-4.4200	H	0	0		
0.1030	1.9490	-2.2600	H	0	0		
8.1230	-1.5590	1.1550	H	0	0		
7.3560	-0.2380	0.1080	H	0	0		
7.1720	-0.2540	1.8600	H	0	0		
-3.5270	-3.9900	-0.5210	H	0	0		
-5.2460	-1.8220	-1.4880	H	0	0		
-4.7790	-0.2150	-0.8850	H	0	0		
-5.0330	0.3710	1.4830	H	0	0		
-7.5940	-2.1560	3.8420	H	0	0		
-7.5610	-3.8730	2.0450	H	0	0		
-6.3280	-0.0350	3.5590	H	0	0		
-6.2680	-3.4730	-0.0330	H	0	0		

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8 9 2 0
7 8 1 0
4 7 1 0
5 10 1 0
10 11 2 0
7 12 1 0
12 13 1 0
17 18 2 0
16 17 1 0
15 16 2 0
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18 13 1 0
13 14 2 0
16 19 1 0
1 20 1 0
20 21 1 0
9 22 1 0
23 25 1 0
22 25 2 0
22 24 1 0
24 26 1 0
26 23 2 0
26 27 1 0
27 28 1 0
5 6 1 0
4 5 2 0
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2 3 2 0
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> <Activ>

1.8

> <DB_Ref_id>

4.08

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Compound80

SciTegic10081411483D

66	71	0	0	0	0	999	V2000
-3.5510	0.7930	-0.5290	C	0	0		
-3.3380	-0.6070	-0.4410	C	0	0		
-2.0180	-1.1170	-0.3380	C	0	0		
-0.8940	-0.2400	-0.3200	C	0	0		
-1.1290	1.1680	-0.4140	C	0	0		
-2.4470	1.6740	-0.5160	C	0	0		
0.3850	-0.7150	-0.2190	N	0	0		
1.4790	0.1330	-0.2090	C	0	0		
1.3650	1.4770	-0.2950	C	0	0		
0.0290	2.1110	-0.4040	C	0	0		
-0.0160	3.3180	-0.4770	O	0	0		
0.6640	-2.1640	-0.1150	C	0	0		
0.3990	-2.6760	1.2540	C	0	0		
-0.5350	-3.7090	1.4530	C	0	0		
-0.7850	-4.1930	2.7480	C	0	0		
-0.1050	-3.6430	3.8500	C	0	0		
0.8280	-2.6070	3.6500	C	0	0		
1.0800	-2.1270	2.3550	C	0	0		
-0.4140	-4.2290	5.4320	Cl	0	0		
2.5670	2.2990	-0.2810	C	0	0		
4.6530	2.8540	-0.1970	O	0	0		
2.5900	3.6500	-0.3690	N	0	0		
3.8400	1.8300	-0.1760	N	0	0		
3.8950	3.9690	-0.3140	C	0	0		
4.4280	5.3850	-0.3790	C	0	0		
-4.7790	1.3030	-0.6250	F	0	0		
-4.3730	-1.4630	-0.4550	N	0	0		
-4.4180	-2.6410	0.4470	C	0	0		
-4.8910	-3.9060	-0.2950	C	0	0		
-6.1310	-3.6600	-1.0450	N	0	0		
-5.9510	-2.5920	-2.0370	C	0	0		
-5.5250	-1.2660	-1.3730	C	0	0		
-6.6390	-4.8830	-1.6580	C	0	0		
5.9140	5.3560	-0.3200	C	0	0		
6.6680	5.5820	-1.4840	C	0	0		
8.7230	5.3050	-0.2090	C	0	0		
7.9690	5.0780	0.9570	C	0	0		
8.0720	5.5550	-1.4280	C	0	0		
6.5650	5.1060	0.9000	C	0	0		
-1.8730	-2.1880	-0.2720	H	0	0		
-2.6170	2.7380	-0.5820	H	0	0		
2.4770	-0.2730	-0.1290	H	0	0		
1.7050	-2.3500	-0.3770	H	0	0		
0.0390	-2.7010	-0.8300	H	0	0		
-1.0620	-4.1350	0.6110	H	0	0		
-1.5040	-4.9880	2.8850	H	0	0		
1.3590	-2.1760	4.4880	H	0	0		
1.7990	-1.3340	2.2090	H	0	0		
4.0410	5.9570	0.4650	H	0	0		
4.1110	5.8520	-1.3110	H	0	0		

-3.4410	-2.8240	0.9000	H	0	0
-5.1040	-2.4160	1.2660	H	0	0
-4.1130	-4.2480	-0.9820	H	0	0
-5.0510	-4.7110	0.4240	H	0	0
-5.2010	-2.8980	-2.7700	H	0	0
-6.8830	-2.4390	-2.5840	H	0	0
-5.2910	-0.5290	-2.1430	H	0	0
-6.3550	-0.8610	-0.7950	H	0	0
-7.6000	-4.6800	-2.1330	H	0	0
-5.8980	-5.2730	-2.3560	H	0	0
-6.8010	-5.6350	-0.8870	H	0	0
6.1740	5.7760	-2.4260	H	0	0
9.8030	5.2830	-0.1660	H	0	0
8.4690	4.8870	1.8950	H	0	0
8.6530	5.7290	-2.3240	H	0	0
5.9900	4.9320	1.8010	H	0	0
1 6 2 0					
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8 9 2 0					
7 8 1 0					
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5 10 1 0					
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32 27 1 0					
27 28 1 0					
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5 6 1 0					
4 5 2 0					
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37 39 2 0					
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34 39 1 0					
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3 40 1 0					

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6 41 1 0
8 42 1 0
12 43 1 0
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14 45 1 0
15 46 1 0
17 47 1 0
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M END

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Compound80

> <Activ>

0.023

> <DB_Ref_id>

4.11

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Compound81

SciTegic10081411483D

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69 74 0 0 0 0          999 V2000
-3.0330  0.7620 -1.4410 C  0  0
-2.8200 -0.6390 -1.3540 C  0  0
-1.5000 -1.1470 -1.2500 C  0  0
-0.3770 -0.2700 -1.2340 C  0  0
-0.6110  1.1370 -1.3260 C  0  0
-1.9300  1.6450 -1.4280 C  0  0
 0.9020 -0.7460 -1.1330 N  0  0
 1.9960  0.1040 -1.1210 C  0  0
 1.8830  1.4470 -1.2090 C  0  0
 0.5470  2.0800 -1.3180 C  0  0
 0.5020  3.2870 -1.3890 O  0  0
 1.1820 -2.1930 -1.0290 C  0  0
 0.7250 -2.7480  0.2750 C  0  0
 1.0410 -2.0700  1.4670 C  0  0
 0.6150 -2.5820  2.7030 C  0  0
-0.1250 -3.7750  2.7540 C  0  0
-0.4410 -4.4550  1.5640 C  0  0
-0.0180 -3.9430  0.3240 C  0  0
 3.0840  2.2700 -1.1930 C  0  0
 5.0490  3.1480 -1.1410 N  0  0

```

2.8850	3.6290	-1.2910	O	0	0
4.3930	1.9920	-1.1040	N	0	0
4.1600	4.1580	-1.2540	C	0	0
4.5180	5.6290	-1.3280	C	0	0
5.1210	6.0570	-0.0390	C	0	0
4.3070	6.2500	1.0920	C	0	0
6.2660	6.8670	2.4000	C	0	0
7.0800	6.6740	1.2710	C	0	0
4.8770	6.6540	2.3110	C	0	0
6.5100	6.2700	0.0530	C	0	0
-4.2620	1.2720	-1.5370	F	0	0
-3.8570	-1.4920	-1.3690	N	0	0
-5.1170	-1.1910	-0.6450	C	0	0
-5.6370	-2.4240	0.1210	C	0	0
-5.6950	-3.6110	-0.7420	N	0	0
-4.3690	-3.9400	-1.2830	C	0	0
-3.7910	-2.7750	-2.1130	C	0	0
-6.2890	-4.7500	-0.0510	C	0	0
-0.3220	-4.5960	-0.7950	F	0	0
6.8050	7.2500	3.5550	F	0	0
-0.5740	-4.3180	4.0630	C	0	0
-0.1540	-3.4900	5.0700	F	0	0
-0.0410	-5.5680	4.2480	F	0	0
-1.9430	-4.3990	4.0800	F	0	0
-1.3550	-2.2170	-1.1840	H	0	0
-2.1000	2.7090	-1.4940	H	0	0
2.9940	-0.3030	-1.0430	H	0	0
2.2520	-2.3630	-1.1410	H	0	0
0.6740	-2.7150	-1.8420	H	0	0
1.6090	-1.1520	1.4360	H	0	0
0.8610	-2.0570	3.6150	H	0	0
-1.0120	-5.3730	1.6020	H	0	0
3.6170	6.2110	-1.5180	H	0	0
5.2330	5.7890	-2.1350	H	0	0
3.2400	6.0880	1.0270	H	0	0
8.1470	6.8360	1.3380	H	0	0
4.2480	6.8010	3.1760	H	0	0
7.1410	6.1210	-0.8110	H	0	0
-4.9810	-0.3590	0.0510	H	0	0
-5.8610	-0.8710	-1.3730	H	0	0
-4.9940	-2.6310	0.9800	H	0	0
-6.6310	-2.2130	0.5180	H	0	0
-3.6910	-4.1880	-0.4630	H	0	0
-4.4410	-4.8300	-1.9100	H	0	0
-2.7640	-3.0080	-2.4040	H	0	0
-4.3590	-2.6640	-3.0350	H	0	0
-6.3770	-5.5900	-0.7400	H	0	0
-5.6950	-4.9900	0.8320	H	0	0
-7.2930	-4.4880	0.2850	H	0	0
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1	2	1	0		
1	6	2	0		
9	10	1	0		
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5	10	1	0		
10	11	2	0		
7	12	1	0		
12	13	1	0		
17	18	2	0		

16	17	1	0
15	16	2	0
14	15	1	0
18	13	1	0
13	14	2	0
9	19	1	0
20	22	1	0
19	22	2	0
19	21	1	0
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23	20	2	0
2	32	1	0
36	37	1	0
35	36	1	0
34	35	1	0
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37	32	1	0
32	33	1	0
35	38	1	0
23	21	1	0
16	41	1	0
18	39	1	0
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41	44	1	0
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41	42	1	0
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6	46	1	0
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33	59	1	0
33	60	1	0
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M END

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Compound81

> <Activ>

0.045

> <DB_Ref_id>

4.19

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Compound82

SciTegic10081411483D

66	71	0	0	0	0	999	V2000
-2.4530	0.3180	-0.6910	C	0	0		
-2.2400	-1.0820	-0.6030	C	0	0		
-0.9200	-1.5900	-0.5000	C	0	0		
0.2030	-0.7130	-0.4840	C	0	0		
-0.0290	0.6930	-0.5760	C	0	0		
-1.3500	1.1990	-0.6780	C	0	0		
1.4820	-1.1890	-0.3830	N	0	0		
2.5760	-0.3420	-0.3710	C	0	0		
2.4630	1.0040	-0.4590	C	0	0		
1.1270	1.6370	-0.5680	C	0	0		
1.0820	2.8440	-0.6390	O	0	0		
1.7620	-2.6390	-0.2790	C	0	0		
1.4450	-3.1600	1.0760	C	0	0		
2.0820	-2.6190	2.2070	C	0	0		
1.7830	-3.1110	3.4880	C	0	0		
0.8460	-4.1500	3.6430	C	0	0		
0.2090	-4.6910	2.5120	C	0	0		
0.5080	-4.1970	1.2310	C	0	0		
0.4840	-4.7560	5.2050	C1	0	0		
3.6660	1.8280	-0.4430	C	0	0		
5.6310	2.7050	-0.3910	N	0	0		
3.4670	3.1880	-0.5390	O	0	0		
4.9770	1.5490	-0.3550	N	0	0		
4.7440	3.7170	-0.5020	C	0	0		
5.1020	5.1860	-0.5740	C	0	0		
-3.6820	0.8280	-0.7870	F	0	0		
-3.2750	-1.9370	-0.6190	N	0	0		
-3.3090	-3.0920	0.3110	C	0	0		
-3.9320	-4.3480	-0.3300	C	0	0		
-5.1800	-4.0610	-1.0490	N	0	0		
-4.9650	-3.0620	-2.1040	C	0	0		
-4.4080	-1.7280	-1.5590	C	0	0		
-6.2950	-3.7230	-0.1540	C	0	0		
3.8750	6.0040	-0.3730	C	0	0		
3.0800	6.3630	-1.4770	C	0	0		
1.5590	7.5510	0.0080	C	0	0		
2.3520	7.1920	1.1090	C	0	0		
1.9220	7.1370	-1.2850	C	0	0		
3.5120	6.4180	0.9200	C	0	0		
-0.7750	-2.6600	-0.4340	H	0	0		
-1.5200	2.2660	-0.7440	H	0	0		
3.5740	-0.7480	-0.2910	H	0	0		
2.8130	-2.8180	-0.5000	H	0	0		
1.1680	-3.1720	-1.0210	H	0	0		
2.8030	-1.8220	2.0960	H	0	0		

2.2790	-2.6860	4.3480	H	0	0
-0.5140	-5.4900	2.6150	H	0	0
0.0140	-4.6170	0.3650	H	0	0
5.5290	5.4080	-1.5510	H	0	0
5.8260	5.4220	0.2050	H	0	0
-2.2970	-3.3420	0.6470	H	0	0
-3.8690	-2.7970	1.2010	H	0	0
-4.1210	-5.1020	0.4300	H	0	0
-3.2210	-4.7890	-1.0270	H	0	0
-4.2620	-3.4650	-2.8360	H	0	0
-5.8950	-2.8830	-2.6390	H	0	0
-5.1880	-1.1640	-1.0370	H	0	0
-4.0880	-1.1070	-2.4080	H	0	0
-7.1700	-3.4590	-0.7500	H	0	0
-6.4830	-4.5550	0.5230	H	0	0
-6.0290	-2.8530	0.4470	H	0	0
3.3550	6.0490	-2.4730	H	0	0
0.6680	8.1450	0.1540	H	0	0
2.0720	7.5100	2.1040	H	0	0
1.3120	7.4120	-2.1330	H	0	0
4.1170	6.1470	1.7720	H	0	0
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8	9	2	0		
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18	13	1	0		
13	14	2	0		
16	19	1	0		
9	20	1	0		
21	23	1	0		
20	23	2	0		
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30	33	1	0		
24	22	1	0		
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37	39	2	0		
38	36	2	0		

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34 39 1 0
36 37 1 0
34 35 2 0
 3 40 1 0
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Compound82

> <Activ>

0.115

> <DB_Ref_id>

4.12

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Compound83

SciTegic10081411483D

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-3.4710  0.9610 -0.9380 C  0  0
-3.2580 -0.4390 -0.8500 C  0  0
-1.9380 -0.9470 -0.7460 C  0  0
-0.8160 -0.0700 -0.7290 C  0  0
-1.0490  1.3360 -0.8220 C  0  0
-2.3670  1.8420 -0.9220 C  0  0
 0.4650 -0.5470 -0.6270 N  0  0
 1.5570  0.3010 -0.6170 C  0  0
 1.4430  1.6470 -0.7030 C  0  0
 0.1070  2.2790 -0.8130 C  0  0
 0.0620  3.4860 -0.8850 O  0  0
 0.7420 -1.9960 -0.5240 C  0  0
 0.4280 -2.5180  0.8340 C  0  0
 0.9450 -1.8630  1.9670 C  0  0
 0.6540 -2.3500  3.2540 C  0  0

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-0.1520	-3.4880	3.4120	C	0	0
-0.6700	-4.1430	2.2790	C	0	0
-0.3810	-3.6600	0.9920	C	0	0
2.6450	2.4690	-0.6900	C	0	0
4.7310	3.0220	-0.6100	O	0	0
2.6680	3.8180	-0.7720	N	0	0
3.9200	1.9980	-0.5900	N	0	0
3.9730	4.1390	-0.7210	C	0	0
4.5080	5.5530	-0.7790	C	0	0
5.8710	5.5920	-0.1920	C	0	0
6.0410	5.5270	1.2030	C	0	0
8.4550	5.6680	0.9200	C	0	0
8.2870	5.7330	-0.4750	C	0	0
7.3320	5.5650	1.7580	C	0	0
6.9960	5.6950	-1.0310	C	0	0
-4.7010	1.4710	-1.0330	F	0	0
-4.2950	-1.2950	-0.8630	N	0	0
-4.3360	-2.4750	0.0370	C	0	0
-4.8110	-3.7380	-0.7090	C	0	0
-6.0530	-3.4900	-1.4550	N	0	0
-5.8750	-2.4180	-2.4450	C	0	0
-5.4470	-1.0960	-1.7780	C	0	0
-6.5630	-4.7110	-2.0700	C	0	0
-0.8750	-4.2890	-0.0720	F	0	0
9.6780	5.7030	1.4450	F	0	0
-0.4590	-4.0000	4.7730	C	0	0
0.1480	-3.2030	5.7090	F	0	0
0.0080	-5.2850	4.8940	F	0	0
-1.8150	-3.9880	4.9730	F	0	0
-1.7930	-2.0180	-0.6780	H	0	0
-2.5370	2.9080	-0.9900	H	0	0
2.5570	-0.1050	-0.5370	H	0	0
1.7930	-2.1760	-0.7480	H	0	0
0.1460	-2.5290	-1.2660	H	0	0
1.5660	-0.9880	1.8530	H	0	0
1.0550	-1.8420	4.1190	H	0	0
-1.2910	-5.0200	2.4000	H	0	0
3.8500	6.2130	-0.2130	H	0	0
4.5490	5.8830	-1.8170	H	0	0
5.1820	5.4490	1.8530	H	0	0
9.1490	5.8110	-1.1230	H	0	0
7.4550	5.5140	2.8300	H	0	0
6.8730	5.7460	-2.1020	H	0	0
-3.3580	-2.6580	0.4860	H	0	0
-5.0200	-2.2520	0.8570	H	0	0
-4.0350	-4.0780	-1.3990	H	0	0
-4.9710	-4.5450	0.0080	H	0	0
-5.1290	-2.7250	-3.1800	H	0	0
-6.8090	-2.2660	-2.9880	H	0	0
-5.2170	-0.3550	-2.5450	H	0	0
-6.2770	-0.6910	-1.1950	H	0	0
-7.5240	-4.5060	-2.5410	H	0	0
-5.8240	-5.1000	-2.7720	H	0	0
-6.7230	-5.4670	-1.3010	H	0	0
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4.17

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Compound84

SciTegic10081411483D

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-3.5390 0.7910 -0.3770 C 0 0
-3.3260 -0.6090 -0.2890 C 0 0
-2.0080 -1.1170 -0.1860 C 0 0
-0.8850 -0.2400 -0.1680 C 0 0
-1.1170 1.1660 -0.2620 C 0 0
-2.4360 1.6740 -0.3610 C 0 0
0.3960 -0.7170 -0.0660 N 0 0
1.4880 0.1330 -0.0570 C 0 0
1.3750 1.4770 -0.1430 C 0 0
0.0390 2.1090 -0.2520 C 0 0
-0.0060 3.3170 -0.3240 O 0 0
0.6740 -2.1640 0.0370 C 0 0
0.4240 -2.6720 1.4120 C 0 0
-0.5060 -3.7070 1.6210 C 0 0
-0.7440 -4.1880 2.9200 C 0 0
-0.0530 -3.6330 4.0140 C 0 0
0.8790 -2.6000 3.8030 C 0 0
1.1170 -2.1210 2.5040 C 0 0
-0.3440 -4.2170 5.6000 Cl 0 0
2.5760 2.2990 -0.1290 C 0 0
4.6620 2.8520 -0.0470 O 0 0
2.6000 3.6510 -0.2130 N 0 0
3.8520 1.8300 -0.0270 N 0 0
3.9040 3.9690 -0.1600 C 0 0
4.4390 5.3850 -0.2210 C 0 0
5.8710 5.3580 -0.6230 C 0 0
6.2210 5.5780 -1.9670 C 0 0
8.5740 5.3050 -1.4060 C 0 0
8.2270 5.0860 -0.0610 C 0 0
7.5700 5.5530 -2.3570 C 0 0
6.8770 5.1110 0.3320 C 0 0
-4.7700 1.3030 -0.4730 F 0 0
-4.3630 -1.4630 -0.3030 N 0 0
-4.4080 -2.6390 0.6040 C 0 0
-4.8810 -3.9060 -0.1390 C 0 0
-6.1190 -3.6620 -0.8910 N 0 0
-5.9380 -2.5960 -1.8850 C 0 0
-5.5140 -1.2690 -1.2230 C 0 0
-6.6270 -4.8850 -1.5020 C 0 0
9.8520 5.2790 -1.7770 F 0 0

6.5610	4.9040	1.6090	F	0	0
-1.8630	-2.1870	-0.1170	H	0	0
-2.6060	2.7380	-0.4300	H	0	0
2.4880	-0.2730	0.0230	H	0	0
1.7130	-2.3520	-0.2360	H	0	0
0.0430	-2.7030	-0.6700	H	0	0
-1.0410	-4.1350	0.7870	H	0	0
-1.4590	-4.9820	3.0660	H	0	0
1.4180	-2.1640	4.6330	H	0	0
1.8320	-1.3260	2.3480	H	0	0
4.3460	5.8500	0.7600	H	0	0
3.8670	5.9570	-0.9510	H	0	0
5.4530	5.7680	-2.7050	H	0	0
8.9980	4.8970	0.6720	H	0	0
7.8320	5.7230	-3.3930	H	0	0
-3.4340	-2.8200	1.0570	H	0	0
-5.0960	-2.4120	1.4200	H	0	0
-4.1020	-4.2500	-0.8220	H	0	0
-5.0430	-4.7090	0.5820	H	0	0
-5.1880	-2.9040	-2.6150	H	0	0
-6.8670	-2.4450	-2.4340	H	0	0
-5.2780	-0.5330	-1.9940	H	0	0
-6.3460	-0.8630	-0.6460	H	0	0
-7.5920	-4.6860	-1.9670	H	0	0
-5.8890	-5.2720	-2.2070	H	0	0
-6.7780	-5.6410	-0.7300	H	0	0
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4.14

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Compound85

SciTegic10081411483D

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4.0200		-0.2230		1.1680	C	0	0
3.9770		1.1890		1.1870	C	0	0
2.7460		1.8650		1.0230	C	0	0
1.5350		1.1390		0.8380	C	0	0
1.5920		-0.2890		0.8240	C	0	0
2.8300		-0.9630		0.9880	C	0	0
0.3360		1.7750		0.6740	N	0	0
-0.8440		1.0740		0.5000	C	0	0
-0.9020		-0.2770		0.4770	C	0	0
0.3380		-1.0780		0.6390	C	0	0

0.2380	-2.2830	0.6090	O	0	0				
0.2400	3.2520	0.6740	C	0	0				
0.6600	3.8280	-0.6290	C	0	0				
1.7520	4.7110	-0.6900	C	0	0				
2.1510	5.2580	-1.9220	C	0	0				
1.4550	4.9200	-3.1000	C	0	0				
0.3630	4.0350	-3.0370	C	0	0				
-0.0330	3.4880	-1.8050	C	0	0				
1.9380	5.5880	-4.6040	C1	0	0				
5.1880	-0.8650	1.3220	O	0	0				
6.3340	-0.3200	0.6890	C	0	0				
5.1060	1.8930	1.3630	O	0	0				
5.0330	3.3070	1.2540	C	0	0				
-2.1950	-0.9450	0.2910	C	0	0				
-2.9550	-0.6700	-0.6990	N	0	0				
-4.1580	-1.4820	-0.6350	C	0	0	2	0	0	0
-3.9650	-2.2420	0.6930	C	0	0	2	0	0	0
-2.6560	-1.8750	1.1290	O	0	0				
-4.3140	-2.3300	-1.8970	C	0	0				
-4.0740	-3.7230	0.6150	C	0	0				
-2.9730	-4.4860	0.1910	C	0	0				
-4.2790	-6.5240	0.4690	C	0	0				
-5.3790	-5.7600	0.8930	C	0	0				
-3.0740	-5.8870	0.1170	C	0	0				
-5.2770	-4.3590	0.9670	C	0	0				
2.7540	2.9450	1.0430	H	0	0				
2.8710	-2.0430	0.9750	H	0	0				
-1.7750	1.6090	0.3730	H	0	0				
0.8710	3.6500	1.4690	H	0	0				
-0.7870	3.5450	0.8870	H	0	0				
2.2890	4.9770	0.2110	H	0	0				
2.9920	5.9340	-1.9530	H	0	0				
-0.1800	3.7660	-3.9340	H	0	0				
-0.8710	2.8090	-1.7660	H	0	0				
7.1190	-1.0230	0.4120	H	0	0				
6.7740	0.4220	1.3570	H	0	0				
6.0140	0.1950	-0.2170	H	0	0				
6.0260	3.7150	1.4450	H	0	0				
4.5900	3.5510	0.2870	H	0	0				
4.3630	3.6760	2.0310	H	0	0				
-5.0120	-0.8240	-0.5530	H	0	0				
-4.6680	-1.8830	1.4320	H	0	0				
-4.4280	-1.7130	-2.7870	H	0	0				
-5.1910	-2.9730	-1.8240	H	0	0				
-3.4430	-2.9690	-2.0430	H	0	0				
-2.0450	-4.0040	-0.0800	H	0	0				
-4.3570	-7.6000	0.4120	H	0	0				
-6.3050	-6.2480	1.1620	H	0	0				
-2.2280	-6.4750	-0.2090	H	0	0				
-6.1270	-3.7770	1.2930	H	0	0				
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4.04

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Compound86

SciTegic10081411483D

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1.4900	-2.5510	-0.3420	C	0	0		
1.4410	-1.1230	-0.3220	C	0	0		
0.2010	-0.4530	-0.4880	C	0	0		
-1.0080	-1.1780	-0.6740	C	0	0		
-0.9490	-2.6040	-0.6880	C	0	0		
0.2850	-3.2750	-0.5240	C	0	0		
-2.2090	-0.5410	-0.8380	N	0	0		
-3.3870	-1.2440	-1.0120	C	0	0		
-3.4450	-2.5960	-1.0350	C	0	0		
-2.2030	-3.3930	-0.8730	C	0	0		
-2.3010	-4.6000	-0.9020	O	0	0		
-4.7420	-3.2680	-1.2230	C	0	0		
-4.9670	-3.8950	-2.2330	O	0	0		
-5.6110	-3.1310	-0.2270	O	0	0		
-6.8750	-3.7030	-0.5310	C	0	0		
-7.8150	-3.5290	0.6640	C	0	0		
-2.3070	0.9360	-0.8380	C	0	0		
-2.6640	1.4590	0.5080	C	0	0		
-1.6970	1.4960	1.5270	C	0	0		
-2.0350	1.9920	2.7990	C	0	0		
-3.3420	2.4490	3.0530	C	0	0		
-4.3090	2.4120	2.0310	C	0	0		
-3.9690	1.9180	0.7600	C	0	0		
-3.7560	3.0510	4.6050	C1	0	0		
2.6350	-3.2480	-0.1910	N	0	0		
2.5470	-0.3670	-0.1500	N	0	0		
3.7600	-0.5570	-0.9860	C	0	0		
4.2720	0.7790	-1.5680	C	0	0		
4.3320	1.8500	-0.5390	N	0	0		
3.1230	2.0350	0.3070	C	0	0		
2.6110	0.6970	0.8850	C	0	0		
5.4490	2.6270	-0.3750	C	0	0		
6.6680	2.1110	-0.7150	N	0	0		
7.7930	2.8690	-0.5610	C	0	0		
7.7310	4.1800	-0.0530	C	0	0		
6.4850	4.7230	0.3030	C	0	0		
5.3300	3.9380	0.1390	C	0	0		
0.1860	0.6290	-0.4730	H	0	0		
0.2990	-4.3570	-0.5410	H	0	0		
-4.3180	-0.7070	-1.1390	H	0	0		
-7.2750	-3.1990	-1.4120	H	0	0		
-6.7290	-4.7600	-0.7520	H	0	0		
-8.7930	-3.9570	0.4490	H	0	0		
-7.4020	-4.0080	1.5510	H	0	0		
-7.9570	-2.4730	0.8910	H	0	0		
-3.0610	1.2440	-1.5610	H	0	0		
-1.3520	1.3570	-1.1500	H	0	0		
-0.6930	1.1450	1.3400	H	0	0		
-1.2810	2.0160	3.5740	H	0	0		
-5.3150	2.7600	2.2110	H	0	0		
-4.7150	1.8930	-0.0220	H	0	0		
3.4900	-2.8090	0.0840	H	0	0		
2.6470	-4.2320	-0.3590	H	0	0		
3.5720	-1.2640	-1.7950	H	0	0		

4.5330	-1.0020	-0.3570	H	0	0
3.6020	1.1150	-2.3610	H	0	0
5.2500	0.6290	-2.0310	H	0	0
3.3180	2.7360	1.1190	H	0	0
2.3480	2.4860	-0.3150	H	0	0
3.2850	0.3570	1.6720	H	0	0
1.6370	0.8480	1.3550	H	0	0
8.7500	2.4490	-0.8340	H	0	0
8.6330	4.7640	0.0620	H	0	0
6.4120	5.7270	0.6930	H	0	0
4.3650	4.3460	0.4100	H	0	0
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6	39	1	0		
8	40	1	0		
15	41	1	0		
15	42	1	0		
16	43	1	0		
16	44	1	0		
16	45	1	0		
17	46	1	0		


```

17 47 1 0
19 48 1 0
20 49 1 0
22 50 1 0
23 51 1 0
25 52 1 0
25 53 1 0
27 54 1 0
27 55 1 0
28 56 1 0
28 57 1 0
30 58 1 0
30 59 1 0
31 60 1 0
31 61 1 0
34 62 1 0
35 63 1 0
36 64 1 0
37 65 1 0

```

M END

> <Name>

Compound86

> <Activ>

3.06

> <DB_Ref_id>

5.27

\$\$\$\$

Compound87

SciTegic10081411483D

```

55 58 0 0 0 0          999 V2000
-2.9880 -2.2540 0.1540 C 0 0
-1.5680 -2.7130 0.2090 C 0 0
-0.5470 -1.6720 -0.0680 C 0 0
-0.9320 -0.4060 -0.3520 C 0 0
-2.2580 -0.0120 -0.3950 N 0 0
-1.1780 -3.8340 0.4510 O 0 0
0.8870 -2.0100 -0.0370 C 0 0
1.3590 -2.7480 -0.8690 O 0 0
-5.3890 -2.7600 0.3670 C 0 0
-5.6900 -1.3980 0.0640 C 0 0
-3.2770 -0.8910 -0.1500 C 0 0
-4.6390 -0.4820 -0.1930 C 0 0
-4.0330 -3.1740 0.4080 C 0 0
-2.5210 1.4060 -0.7190 C 0 0
-1.3960 2.0140 -1.4810 C 0 0
-0.4710 2.8570 -0.8360 C 0 0
0.5880 3.4240 -1.5670 C 0 0
0.7270 3.1500 -2.9400 C 0 0
-0.1990 2.3090 -3.5820 C 0 0
1.5900 -1.4530 0.9450 O 0 0
2.9670 -1.7950 0.8850 C 0 0
3.7110 -1.0430 1.9320 C 0 0
4.3070 -1.7420 2.9940 C 0 0
5.0140 -1.0470 3.9900 C 0 0
4.5310 1.0550 2.8630 C 0 0
3.8220 0.3610 1.8650 C 0 0
5.1250 0.3520 3.9240 C 0 0

```

-1.2580	1.7420	-2.8540	C	0	0
-0.5900	3.1230	0.4630	F	0	0
-6.3480	-3.6700	0.6170	N	0	0
3.1990	1.1210	0.7480	C	0	0
-7.3090	-0.8070	-0.0060	C1	0	0
1.8460	3.7520	-3.7090	C	0	0
1.7720	3.3440	-5.0160	F	0	0
3.0410	3.3460	-3.1720	F	0	0
1.7600	5.1190	-3.6510	F	0	0
-0.1500	0.3140	-0.5470	H	0	0
-4.8950	0.5430	-0.4220	H	0	0
-3.7850	-4.2030	0.6350	H	0	0
-2.6780	1.9630	0.2050	H	0	0
-3.4380	1.4750	-1.3090	H	0	0
1.2990	4.0700	-1.0700	H	0	0
-0.1000	2.0960	-4.6350	H	0	0
3.0610	-2.8650	1.0720	H	0	0
3.3440	-1.5200	-0.1000	H	0	0
4.2250	-2.8180	3.0530	H	0	0
5.4710	-1.5880	4.8070	H	0	0
4.6210	2.1310	2.8180	H	0	0
5.6680	0.8870	4.6890	H	0	0
-1.9650	1.0960	-3.3540	H	0	0
-7.3180	-3.4340	0.6010	H	0	0
-6.0980	-4.6150	0.8260	H	0	0
3.4300	2.1820	0.8570	H	0	0
3.5370	0.7130	-0.2030	H	0	0
2.1150	1.0100	0.7930	H	0	0
1	2	1	0		
2	6	2	0		
3	7	1	0		
7	8	2	0		
9	10	2	0		
12	11	2	0		
11	1	1	0		
1	13	2	0		
13	9	1	0		
10	12	1	0		
11	5	1	0		
5	14	1	0		
14	15	1	0		
17	16	2	0		
18	17	1	0		
19	18	2	0		
16	15	1	0		
7	20	1	0		
20	21	1	0		
21	22	1	0		
25	26	2	0		
23	24	1	0		
26	22	1	0		
22	23	2	0		
18	33	1	0		
24	27	2	0		
27	25	1	0		
19	28	1	0		
15	28	2	0		
16	29	1	0		
9	30	1	0		
26	31	1	0		
10	32	1	0		

```

3  2  1  0
4  3  2  0
5  4  1  0
33 36  1  0
33 35  1  0
33 34  1  0
4  37  1  0
12 38  1  0
13 39  1  0
14 40  1  0
14 41  1  0
17 42  1  0
19 43  1  0
21 44  1  0
21 45  1  0
23 46  1  0
24 47  1  0
25 48  1  0
27 49  1  0
28 50  1  0
30 51  1  0
30 52  1  0
31 53  1  0
31 54  1  0
31 55  1  0

```

M END

> <Name>

Compound87

> <Activ>

1.41

> <DB_Ref_id>

5.03

\$\$\$\$

Compound88

SciTegic10081411483D

```

75 81  0  0  0  0          999 V2000
-1.0860 -1.7420 -1.1800 C  0  0
-2.3380 -2.5330 -1.3650 C  0  0
-3.5800 -1.7340 -1.5290 C  0  0
-3.5220 -0.3830 -1.5060 C  0  0
-2.3440  0.3180 -1.3320 N  0  0
-2.4360 -3.7380 -1.3960 O  0  0
-4.8770 -2.4080 -1.7170 C  0  0
-5.2700 -2.6820 -2.8260 O  0  0
 1.3530 -1.6910 -0.8340 C  0  0
 1.3070 -0.2620 -0.8160 C  0  0
-1.1430 -0.3180 -1.1680 C  0  0
 0.0660  0.4060 -0.9820 C  0  0
 0.1500 -2.4140 -1.0170 C  0  0
-2.4420  1.7950 -1.3300 C  0  0
-2.3830  2.3460  0.0490 C  0  0
-3.3320  1.9470  1.0080 C  0  0
-3.2780  2.4690  2.3110 C  0  0
-2.2740  3.3930  2.6600 C  0  0
-1.3240  3.7910  1.7010 C  0  0
-5.5530 -2.6780 -0.6030 O  0  0
-6.7850 -3.3320 -0.8650 C  0  0

```

-7.4850	-3.6060	0.4180	C	0	0
-8.5610	-2.7950	0.8200	C	0	0
-9.2230	-3.0510	2.0330	C	0	0
-7.7310	-4.9320	2.4450	C	0	0
-7.0710	-4.6760	1.2330	C	0	0
-8.8070	-4.1210	2.8500	C	0	0
-1.3790	3.2680	0.3970	C	0	0
2.4980	-2.3870	-0.6850	N	0	0
-9.6120	-4.4340	4.3320	C1	0	0
-2.2090	4.0310	4.2500	C1	0	0
2.4100	0.4920	-0.6420	N	0	0
3.0960	0.4960	0.6900	C	0	0
3.9860	1.7230	0.9200	C	0	0
4.7790	2.0250	-0.2750	N	0	0
3.9760	2.3610	-1.4570	C	0	0
2.9550	1.2620	-1.8120	C	0	0
6.2600	2.0210	-0.2790	C	0	0
7.0310	1.7210	0.8610	N	0	0
8.3650	1.7930	0.5630	C	0	0
8.5060	2.1370	-0.7620	C	0	0
7.1760	2.3930	-1.7130	S	0	0
9.4710	1.5640	1.4140	C	0	0
10.7750	1.6950	0.8850	C	0	0
10.9490	2.0490	-0.4740	C	0	0
9.8140	2.2680	-1.2950	C	0	0
-4.4530	0.1520	-1.6310	H	0	0
0.0490	1.4900	-0.9670	H	0	0
0.1640	-3.4960	-1.0350	H	0	0
-3.3770	2.0920	-1.8010	H	0	0
-1.6250	2.2090	-1.9220	H	0	0
-4.1060	1.2400	0.7460	H	0	0
-4.0120	2.1520	3.0370	H	0	0
-0.5470	4.4980	1.9530	H	0	0
-6.5730	-4.2750	-1.3690	H	0	0
-7.3990	-2.6740	-1.4800	H	0	0
-8.8830	-1.9710	0.1990	H	0	0
-10.0490	-2.4200	2.3280	H	0	0
-7.4010	-5.7580	3.0630	H	0	0
-6.2460	-5.3030	0.9280	H	0	0
-0.6470	3.5760	-0.3340	H	0	0
2.4730	-3.3850	-0.6230	H	0	0
3.3750	-1.9060	-0.6390	H	0	0
2.3240	0.4800	1.4830	H	0	0
3.6720	-0.4360	0.7970	H	0	0
4.6210	1.5980	1.8070	H	0	0
3.3480	2.5900	1.1190	H	0	0
3.4320	3.2830	-1.2170	H	0	0
4.6150	2.6070	-2.3140	H	0	0
3.3920	0.5530	-2.5250	H	0	0
2.1190	1.7440	-2.3320	H	0	0
9.3260	1.2970	2.4510	H	0	0
11.6370	1.5270	1.5160	H	0	0
11.9410	2.1480	-0.8870	H	0	0
9.9490	2.5390	-2.3320	H	0	0
3	2	1	0		
4	3	2	0		
5	4	1	0		
1	2	1	0		
2	6	2	0		
3	7	1	0		
7	8	2	0		

9	10	2	0
12	11	2	0
11	1	1	0
1	13	2	0
13	9	1	0
10	12	1	0
11	5	1	0
5	14	1	0
14	15	1	0
17	16	2	0
18	17	1	0
19	18	2	0
16	15	1	0
7	20	1	0
20	21	1	0
21	22	1	0
25	26	2	0
23	24	1	0
26	22	1	0
22	23	2	0
24	27	2	0
27	25	1	0
19	28	1	0
15	28	2	0
9	29	1	0
27	30	1	0
18	31	1	0
10	32	1	0
36	37	1	0
35	36	1	0
34	35	1	0
33	34	1	0
37	32	1	0
32	33	1	0
35	38	1	0
41	42	1	0
39	40	1	0
39	38	2	0
42	38	1	0
40	41	1	0
40	43	2	0
43	44	1	0
44	45	2	0
45	46	1	0
41	46	2	0
4	47	1	0
12	48	1	0
13	49	1	0
14	50	1	0
14	51	1	0
16	52	1	0
17	53	1	0
19	54	1	0
21	55	1	0
21	56	1	0
23	57	1	0
24	58	1	0
25	59	1	0
26	60	1	0
28	61	1	0
29	62	1	0

```

29 63 1 0
33 64 1 0
33 65 1 0
34 66 1 0
34 67 1 0
36 68 1 0
36 69 1 0
37 70 1 0
37 71 1 0
43 72 1 0
44 73 1 0
45 74 1 0
46 75 1 0

```

M END

> <Name>

Compound88

> <Activ>

0.138

> <DB_Ref_id>

5.09

\$\$\$\$

Compound89

SciTegic10081411483D

```

55 58 0 0 0 0          999 V2000
-1.6890 -0.8110 -0.7560 C 0 0
-0.2710 -1.2700 -0.7030 C 0 0
 0.7500 -0.2310 -0.9800 C 0 0
 0.3650  1.0370 -1.2620 C 0 0
-0.9590  1.4300 -1.3070 N 0 0
 0.1190 -2.3910 -0.4590 O 0 0
 2.1840 -0.5670 -0.9490 C 0 0
 2.8560 -0.3010  0.0210 O 0 0
-4.0920 -1.3180 -0.5450 C 0 0
-4.3920  0.0430 -0.8480 C 0 0
-1.9800  0.5510 -1.0630 C 0 0
-3.3420  0.9590 -1.1040 C 0 0
-2.7360 -1.7310 -0.5040 C 0 0
-1.2240  2.8480 -1.6310 C 0 0
-1.6420  3.6170 -0.4280 C 0 0
-0.7750  3.7480  0.6740 C 0 0
-1.1810  4.4770  1.8070 C 0 0
-2.4530  5.0740  1.8400 C 0 0
-3.3180  4.9430  0.7400 C 0 0
 2.6600 -1.1660 -2.0370 O 0 0
 4.0220 -1.5450 -1.8930 C 0 0
 4.1270 -2.6410 -0.8930 C 0 0
 3.4140 -3.8380 -1.0820 C 0 0
 3.5140 -4.8730 -0.1370 C 0 0
 5.0410 -3.5180  1.1880 C 0 0
 4.9420 -2.4830  0.2420 C 0 0
 4.3280 -4.7150  0.9980 C 0 0
-2.9140  4.2170 -0.3910 C 0 0
 0.4320  3.1850  0.6540 F 0 0
-5.0510 -2.2290 -0.2950 N 0 0
-6.0120  0.6370 -0.9180 C1 0 0
 4.4340 -5.8110  1.9980 C 0 0
-2.8830  5.8460  3.0370 C 0 0

```

-4.2190	6.1330	2.9410	F	0	0
-2.1680	7.0140	3.1090	F	0	0
-2.6540	5.1020	4.1660	F	0	0
1.1470	1.7580	-1.4590	H	0	0
-3.5960	1.9860	-1.3320	H	0	0
-2.4880	-2.7600	-0.2750	H	0	0
-2.0080	2.9020	-2.3870	H	0	0
-0.3220	3.2950	-2.0510	H	0	0
-0.5150	4.5760	2.6500	H	0	0
-4.2970	5.4020	0.7600	H	0	0
4.3810	-1.8990	-2.8590	H	0	0
4.5820	-0.6780	-1.5430	H	0	0
2.7870	-3.9670	-1.9510	H	0	0
2.9630	-5.7910	-0.2870	H	0	0
5.6680	-3.3890	2.0570	H	0	0
5.4920	-1.5650	0.3950	H	0	0
-3.5840	4.1190	-1.2320	H	0	0
-4.8340	-3.1800	-0.0820	H	0	0
-6.0140	-1.9590	-0.3180	H	0	0
5.1640	-5.5370	2.7600	H	0	0
3.4490	-6.0200	2.4140	H	0	0
4.7870	-6.7170	1.5080	H	0	0
1	2	1	0		
2	6	2	0		
3	7	1	0		
7	8	2	0		
9	10	2	0		
12	11	2	0		
11	1	1	0		
1	13	2	0		
13	9	1	0		
10	12	1	0		
11	5	1	0		
5	14	1	0		
14	15	1	0		
17	16	2	0		
18	17	1	0		
19	18	2	0		
16	15	1	0		
7	20	1	0		
20	21	1	0		
21	22	1	0		
25	26	2	0		
23	24	1	0		
26	22	1	0		
22	23	2	0		
18	33	1	0		
24	27	2	0		
27	25	1	0		
19	28	1	0		
15	28	2	0		
16	29	1	0		
9	30	1	0		
10	31	1	0		
27	32	1	0		
3	2	1	0		
4	3	2	0		
5	4	1	0		
33	36	1	0		
33	35	1	0		
33	34	1	0		

```

4 37 1 0
12 38 1 0
13 39 1 0
14 40 1 0
14 41 1 0
17 42 1 0
19 43 1 0
21 44 1 0
21 45 1 0
23 46 1 0
24 47 1 0
25 48 1 0
26 49 1 0
28 50 1 0
30 51 1 0
30 52 1 0
32 53 1 0
32 54 1 0
32 55 1 0

```

M END

> <Name>

Compound89

> <Activ>

0.154

> <DB_Ref_id>

5.04

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Compound90

SciTegic10081411483D

```

72 77 0 0 0 0          999 V2000
-0.1620 -2.6440 0.2130 C 0 0
-1.4160 -3.4340 0.0270 C 0 0
-2.6560 -2.6370 -0.1350 C 0 0
-2.6000 -1.2850 -0.1130 C 0 0
-1.4200 -0.5820 0.0630 N 0 0
-1.5140 -4.6410 -0.0020 O 0 0
-3.9530 -3.3090 -0.3220 C 0 0
-4.0200 -4.5160 -0.3460 O 0 0
2.2770 -2.5920 0.5590 C 0 0
2.2300 -1.1640 0.5780 C 0 0
-0.2190 -1.2190 0.2270 C 0 0
0.9900 -0.4940 0.4120 C 0 0
1.0720 -3.3160 0.3750 C 0 0
-1.5180 0.8950 0.0630 C 0 0
-1.0800 1.4710 -1.2340 C 0 0
-0.0160 2.3890 -1.2750 C 0 0
0.3980 2.9360 -2.5020 C 0 0
-0.2560 2.5680 -3.6930 C 0 0
-1.3220 1.6500 -3.6520 C 0 0
-5.0060 -2.5060 -0.4590 O 0 0
-6.2170 -3.2280 -0.6350 C 0 0
-7.3460 -2.2710 -0.7790 C 0 0
-8.6550 -2.7520 -0.9670 C 0 0
-9.7230 -1.8500 -1.1040 C 0 0
-8.1740 0.0160 -0.8670 C 0 0
-7.1080 -0.8870 -0.7290 C 0 0
-9.4850 -0.4630 -1.0550 C 0 0

```


-1.7330	1.1020	-2.4260	C	0	0
3.4220	-3.2890	0.7070	N	0	0
-10.7870	0.6390	-1.2270	Cl	0	0
0.2460	3.2360	-5.1900	Cl	0	0
3.3300	-0.4120	0.7500	N	0	0
4.2580	-0.6330	1.8910	C	0	0
4.5880	0.6820	2.6330	C	0	0
4.9340	1.7790	1.6930	N	0	0
4.0060	2.0000	0.5530	C	0	0
3.6820	0.6860	-0.1890	C	0	0
6.0530	2.5470	1.8670	C	0	0
6.0740	3.8790	1.4000	C	0	0
7.2320	4.6560	1.5860	C	0	0
8.3380	4.0820	2.2360	C	0	0
8.2620	2.7480	2.6820	C	0	0
7.1350	2.0020	2.4960	N	0	0
-3.5290	-0.7500	-0.2380	H	0	0
0.9730	0.5880	0.4280	H	0	0
1.0860	-4.3980	0.3590	H	0	0
-0.8990	1.2930	0.8650	H	0	0
-2.5490	1.1860	0.2620	H	0	0
0.4880	2.6760	-0.3630	H	0	0
1.2190	3.6370	-2.5180	H	0	0
-1.8320	1.3580	-4.5590	H	0	0
-6.3750	-3.8480	0.2480	H	0	0
-6.1290	-3.8260	-1.5410	H	0	0
-8.8440	-3.8140	-1.0060	H	0	0
-10.7230	-2.2320	-1.2440	H	0	0
-7.9770	1.0780	-0.8280	H	0	0
-6.1040	-0.5140	-0.5840	H	0	0
-2.5510	0.3970	-2.4000	H	0	0
3.3950	-4.2850	0.7910	H	0	0
4.2990	-2.8090	0.7360	H	0	0
3.8460	-1.3590	2.5940	H	0	0
5.1760	-1.0700	1.4960	H	0	0
3.7230	1.0000	3.2170	H	0	0
5.3960	0.5100	3.3460	H	0	0
3.0860	2.4360	0.9470	H	0	0
4.4160	2.7290	-0.1480	H	0	0
2.8790	0.8580	-0.9100	H	0	0
4.5510	0.3670	-0.7680	H	0	0
5.2190	4.3130	0.9020	H	0	0
7.2700	5.6760	1.2360	H	0	0
9.2380	4.6580	2.3910	H	0	0
9.1110	2.3070	3.1800	H	0	0
3	2	1		0	
4	3	2		0	
5	4	1		0	
1	2	1		0	
2	6	2		0	
3	7	1		0	
7	8	2		0	
9	10	2		0	
12	11	2		0	
11	1	1		0	
1	13	2		0	
13	9	1		0	
10	12	1		0	
11	5	1		0	
5	14	1		0	
14	15	1		0	

17	16	2	0
18	17	1	0
19	18	2	0
16	15	1	0
7	20	1	0
20	21	1	0
21	22	1	0
25	26	2	0
23	24	1	0
26	22	1	0
22	23	2	0
24	27	2	0
27	25	1	0
19	28	1	0
15	28	2	0
9	29	1	0
27	30	1	0
18	31	1	0
10	32	1	0
36	37	1	0
35	36	1	0
34	35	1	0
33	34	1	0
37	32	1	0
32	33	1	0
35	38	1	0
42	43	2	0
41	42	1	0
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36	65	1	0
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M END
> <Name>
Compound90

> <Activ>
0.069

> <DB_Ref_id>
5.08

\$\$\$\$
Compound91
SciTegic10081411483D

63	67	0	0	0	0	999	V2000
-0.9790	-1.3790	1.6210	C	0	0		
-0.3010	-2.6460	1.2150	C	0	0		
0.4450	-2.5900	-0.0660	C	0	0		
0.4780	-1.4410	-0.7790	C	0	0		
-0.1620	-0.2830	-0.3750	N	0	0		
-0.3010	-3.6930	1.8220	O	0	0		
1.1520	-3.7810	-0.5700	C	0	0		
1.1310	-4.8140	0.0570	O	0	0		
-2.3730	-0.1460	3.2380	C	0	0		
-2.2850	1.0140	2.4060	C	0	0		
-0.8810	-0.2260	0.7870	C	0	0		
-1.5430	0.9630	1.1970	C	0	0		
-1.7150	-1.3340	2.8300	C	0	0		
-0.0330	0.8950	-1.2620	C	0	0		
0.9570	1.8690	-0.7340	C	0	0		
0.5640	3.1900	-0.4530	C	0	0		
1.5000	4.1130	0.0450	C	0	0		
2.8340	3.7170	0.2620	C	0	0		
3.2270	2.3950	-0.0210	C	0	0		
1.7890	-3.6290	-1.7270	O	0	0		
2.4430	-4.8180	-2.1430	C	0	0		
3.1330	-4.5780	-3.4380	C	0	0		
3.8550	-5.6130	-4.0550	C	0	0		
4.5060	-5.3870	-5.2790	C	0	0		
3.7150	-3.0820	-5.2720	C	0	0		
3.0630	-3.3120	-4.0490	C	0	0		
4.4390	-4.1190	-5.8890	C	0	0		
2.2890	1.4730	-0.5180	C	0	0		
-3.0570	-0.1660	4.3990	N	0	0		
5.2360	-3.8400	-7.3810	Cl	0	0		
3.9790	4.8420	0.8650	Cl	0	0		
-2.8870	2.1760	2.7290	N	0	0		
-4.3380	2.2350	3.0390	C	0	0		
-5.0120	3.4420	2.3570	C	0	0		
-4.2790	4.6860	2.6150	N	0	0		
-2.9000	4.6020	2.1190	C	0	0		
-2.1250	3.4490	2.7890	C	0	0		
1.0370	-1.4490	-1.7050	H	0	0		
-1.4860	1.8520	0.5820	H	0	0		
-1.7700	-2.2230	3.4430	H	0	0		
-1.0040	1.3790	-1.3570	H	0	0		
0.2730	0.5650	-2.2540	H	0	0		
-0.4570	3.5000	-0.6170	H	0	0		
1.1840	5.1230	0.2580	H	0	0		
4.2460	2.0760	0.1410	H	0	0		
1.6890	-5.5960	-2.2710	H	0	0		

3.1800	-5.0880	-1.3850	H	0	0
3.9120	-6.5880	-3.5920	H	0	0
5.0570	-6.1930	-5.7420	H	0	0
3.6520	-2.1050	-5.7290	H	0	0
2.5080	-2.5120	-3.5800	H	0	0
2.5980	0.4590	-0.7300	H	0	0
-3.1900	-1.0270	4.8890	H	0	0
-3.4320	0.6840	4.7720	H	0	0
-4.8400	1.3150	2.7360	H	0	0
-4.4510	2.3130	4.1210	H	0	0
-5.0760	3.2780	1.2810	H	0	0
-6.0350	3.5470	2.7190	H	0	0
-4.7600	5.4630	2.1390	H	0	0
-2.9160	4.4670	1.0370	H	0	0
-2.3950	5.5490	2.3070	H	0	0
-1.1470	3.3440	2.3160	H	0	0
-1.9430	3.6880	3.8380	H	0	0
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5	4	1	0		
1	2	1	0		
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3	7	1	0		
7	8	2	0		
9	10	2	0		
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5	14	1	0		
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17	16	2	0		
18	17	1	0		
19	18	2	0		
16	15	1	0		
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20	21	1	0		
21	22	1	0		
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26	22	1	0		
22	23	2	0		
24	27	2	0		
27	25	1	0		
19	28	1	0		
15	28	2	0		
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27	30	1	0		
18	31	1	0		
10	32	1	0		
36	37	1	0		
35	36	1	0		
34	35	1	0		
33	34	1	0		
37	32	1	0		
32	33	1	0		
4	38	1	0		
12	39	1	0		
13	40	1	0		

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14 41 1 0
14 42 1 0
16 43 1 0
17 44 1 0
19 45 1 0
21 46 1 0
21 47 1 0
23 48 1 0
24 49 1 0
25 50 1 0
26 51 1 0
28 52 1 0
29 53 1 0
29 54 1 0
33 55 1 0
33 56 1 0
34 57 1 0
34 58 1 0
35 59 1 0
36 60 1 0
36 61 1 0
37 62 1 0
37 63 1 0

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M END

> <Name>

Compound91

> <Activ>

0.067

> <DB_Ref_id>

5.06

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Compound92

SciTegic10081411483D

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66 70 0 0 0 0          999 V2000
  0.3300 -1.6310 -0.1030 C 0 0
 -0.9220 -2.4200 -0.2890 C 0 0
 -2.1640 -1.6230 -0.4530 C 0 0
 -2.1060 -0.2720 -0.4300 C 0 0
 -0.9280 0.4320 -0.2560 N 0 0
 -1.0200 -3.6270 -0.3200 O 0 0
 -3.4610 -2.2950 -0.6390 C 0 0
 -3.8630 -2.5530 -1.7500 O 0 0
  2.7700 -1.5800 0.2420 C 0 0
  2.7230 -0.1500 0.2600 C 0 0
  0.2730 -0.2070 -0.0920 C 0 0
  1.4820 0.5200 0.0940 C 0 0
  1.5660 -2.3030 0.0590 C 0 0
 -1.0250 1.9060 -0.2540 C 0 0
 -0.5780 2.4860 -1.5490 C 0 0
  0.4820 3.4060 -1.5780 C 0 0
  0.9060 3.9550 -2.8030 C 0 0
  0.2660 3.5820 -4.0000 C 0 0
 -0.7970 2.6600 -3.9690 C 0 0
 -4.1290 -2.5840 0.4750 O 0 0
 -5.3650 -3.2310 0.2110 C 0 0
 -6.0550 -3.5220 1.4960 C 0 0
 -5.8730 -4.7640 2.1270 C 0 0

```

-6.5240	-5.0410	3.3420	C	0	0
-7.5430	-2.8300	3.2950	C	0	0
-6.8910	-2.5550	2.0820	C	0	0
-7.3610	-4.0740	3.9280	C	0	0
-1.2170	2.1110	-2.7440	C	0	0
3.9160	-2.2750	0.3910	N	0	0
-8.1600	-4.4120	5.4060	C1	0	0
0.7790	4.2540	-5.4920	C1	0	0
3.8220	0.6020	0.4320	N	0	0
3.8930	1.6370	1.4940	C	0	0
4.5220	2.9430	0.9690	C	0	0
5.7910	2.6910	0.2720	N	0	0
5.6000	1.7870	-0.8710	C	0	0
5.0200	0.4280	-0.4280	C	0	0
6.4380	3.9360	-0.1290	C	0	0
-3.0370	0.2640	-0.5550	H	0	0
1.4650	1.6020	0.1090	H	0	0
1.5800	-3.3850	0.0410	H	0	0
-0.4120	2.3070	0.5530	H	0	0
-2.0590	2.1970	-0.0620	H	0	0
0.9790	3.6970	-0.6640	H	0	0
1.7250	4.6600	-2.8100	H	0	0
-1.2970	2.3650	-4.8790	H	0	0
-5.1600	-4.1640	-0.3100	H	0	0
-5.9810	-2.5570	-0.3870	H	0	0
-5.2310	-5.5120	1.6820	H	0	0
-6.3730	-6.0000	3.8150	H	0	0
-8.1840	-2.0760	3.7350	H	0	0
-7.0330	-1.5960	1.6020	H	0	0
-2.0330	1.4040	-2.7280	H	0	0
4.7790	-1.8300	0.6230	H	0	0
3.9160	-3.2680	0.2700	H	0	0
2.9020	1.8460	1.9040	H	0	0
4.4960	1.2440	2.3150	H	0	0
3.8260	3.4450	0.2890	H	0	0
4.6910	3.6250	1.8030	H	0	0
4.9340	2.2580	-1.6000	H	0	0
6.5530	1.6290	-1.3750	H	0	0
4.7850	-0.1740	-1.3080	H	0	0
5.7700	-0.1230	0.1390	H	0	0
7.4120	3.7130	-0.5660	H	0	0
5.7850	4.4820	-0.8100	H	0	0
6.6040	4.5590	0.7480	H	0	0
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4	3	2	0		
5	4	1	0		
1	2	1	0		
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7	8	2	0		
9	10	2	0		
12	11	2	0		
11	1	1	0		
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13	9	1	0		
10	12	1	0		
11	5	1	0		
5	14	1	0		
14	15	1	0		
17	16	2	0		
18	17	1	0		

19	18	2	0
16	15	1	0
7	20	1	0
20	21	1	0
21	22	1	0
25	26	2	0
23	24	1	0
26	22	1	0
22	23	2	0
24	27	2	0
27	25	1	0
19	28	1	0
15	28	2	0
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27	30	1	0
18	31	1	0
10	32	1	0
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35	36	1	0
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33	34	1	0
37	32	1	0
32	33	1	0
35	38	1	0
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14	42	1	0
14	43	1	0
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17	45	1	0
19	46	1	0
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34	58	1	0
34	59	1	0
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36	61	1	0
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38	66	1	0

M END

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Compound92

> <Activ>

0.04

> <DB_Ref_id>

5.07

\$\$\$\$

Compound93

SciTegic10081411483D

30	31	0	0	0	0	999	V2000
0.2270		2.9510		-2.4880	C	0	0
-1.0450		2.4320		-2.7930	C	0	0
-1.3380		1.0800		-2.5530	C	0	0
-0.3590		0.2380		-2.0040	C	0	0
0.9140		0.7460		-1.6950	C	0	0
1.2170		2.1000		-1.9330	C	0	0
-0.7190		-1.4220		-1.7050	S	0	0
-0.1310		-1.9260		-0.2810	N	0	0
-0.0900		-2.2210		-2.7420	O	0	0
-2.1620		-1.5760		-1.6600	O	0	0
-0.2480		-1.1270		0.8300	C	0	0
0.4400		-0.4710		3.0780	C	0	0
0.5880		-1.3070		1.9570	C	0	0
-0.5370		0.5430		3.0840	C	0	0
-1.2230		-0.1110		0.8420	C	0	0
-1.3670		0.7210		1.9630	C	0	0
1.6390		-2.3750		1.9920	C	0	0
2.1780		-2.7500		0.9770	O	0	0
1.9160		-2.8580		3.1990	O	0	0
-0.7300		1.6580		4.5920	Br	0	0
2.7970		2.6580		-1.5350	Cl	0	0
0.5200		4.6190		-2.8060	Cl	0	0
-1.8140		3.0640		-3.2170	H	0	0
-2.3160		0.6870		-2.7910	H	0	0
1.6540		0.0820		-1.2710	H	0	0
0.3180		-2.8170		-0.2130	H	0	0
1.0800		-0.6090		3.9380	H	0	0
-1.8710		0.0450		-0.0100	H	0	0
-2.1230		1.4940		1.9510	H	0	0
2.5860		-3.5490		3.2910	H	0	0
5	6	2	0				
4	5	1	0				
3	4	2	0				
2	3	1	0				
1	2	2	0				
1	6	1	0				
4	7	1	0				
7	8	1	0				
7	9	2	0				
7	10	2	0				
8	11	1	0				
16	14	2	0				
15	16	1	0				
12	13	2	0				
14	12	1	0				
13	11	1	0				
11	15	2	0				
13	17	1	0				
17	18	2	0				
17	19	1	0				
14	20	1	0				
6	21	1	0				
1	22	1	0				
2	23	1	0				
3	24	1	0				

5 25 1 0
8 26 1 0
12 27 1 0
15 28 1 0
16 29 1 0
19 30 1 0

M END

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Compound93

> <Activ>

8.4

> <DB_Ref_id>

06.06b

\$\$\$\$

Compound94

SciTegic10081411483D

37 39 0 0 0 0 999 V2000

-0.9880	-1.8950	0.1850	C	0	0
0.1480	-1.6990	-0.6170	C	0	0
0.8070	-0.4570	-0.6150	C	0	0
0.3340	0.5980	0.1890	C	0	0
-0.8110	0.4020	0.9980	C	0	0
-1.4650	-0.8440	0.9920	C	0	0
-1.3480	1.4960	1.8690	C	0	0
-1.8790	1.0940	3.0190	O	0	0
1.0000	1.7990	0.1680	N	0	0
2.0760	2.1090	-1.0020	S	0	0
2.5470	3.7520	-1.0200	C	0	0
1.6000	5.0960	-0.5960	S	0	0
2.8690	6.1780	-0.9240	C	0	0
4.0270	5.5180	-1.3610	C	0	0
3.8440	4.1190	-1.4180	C	0	0
2.6390	8.0290	-0.6930	Br	0	0
3.2520	1.2990	-0.7380	O	0	0
1.4410	1.8010	-2.2720	O	0	0
-1.2890	2.6520	1.5210	O	0	0
-1.6700	-3.1800	0.1850	C	0	0
-3.7340	-4.4770	0.1850	C	0	0
-3.0780	-3.2340	0.1850	C	0	0
-2.9880	-5.6680	0.1850	C	0	0
-0.9240	-4.3750	0.1850	C	0	0
-1.5840	-5.6150	0.1850	C	0	0
0.5270	-2.4960	-1.2420	H	0	0
1.6800	-0.3300	-1.2420	H	0	0
-2.3400	-0.9880	1.6110	H	0	0
-2.2440	1.7500	3.6270	H	0	0
0.8200	2.4830	0.8770	H	0	0
4.9530	6.0120	-1.6250	H	0	0
4.6070	3.4200	-1.7310	H	0	0
-4.8150	-4.5160	0.1850	H	0	0
-3.6660	-2.3280	0.1850	H	0	0
-3.4940	-6.6210	0.1850	H	0	0
0.1560	-4.3540	0.1850	H	0	0
-1.0100	-6.5310	0.1850	H	0	0

5 6 2 0

4 5 1 0

3 4 2 0

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2 3 1 0
1 2 2 0
1 6 1 0
5 7 1 0
7 8 1 0
4 9 1 0
9 10 1 0
10 11 1 0
14 15 1 0
13 14 2 0
12 13 1 0
12 11 1 0
15 11 2 0
13 16 1 0
10 17 2 0
10 18 2 0
7 19 2 0
25 23 2 0
24 25 1 0
21 22 2 0
20 24 2 0
23 21 1 0
22 20 1 0
20 1 1 0
2 26 1 0
3 27 1 0
6 28 1 0
8 29 1 0
9 30 1 0
14 31 1 0
15 32 1 0
21 33 1 0
22 34 1 0
23 35 1 0
24 36 1 0
25 37 1 0
M END
> <Name>
Compound94

> <Activ>
3.7

> <DB_Ref_id>
6.09

$$$$
Compound95
SciTegic10081411483D

30 31 0 0 0 0 999 V2000
-2.8090 1.4770 -2.2190 C 0 0
-3.2310 0.1740 -1.8790 C 0 0
-2.2780 -0.8340 -1.6430 C 0 0
-0.9060 -0.5450 -1.7460 C 0 0
-0.4830 0.7500 -2.0860 C 0 0
-1.4320 1.7600 -2.3220 C 0 0
0.2520 -1.7910 -1.4510 S 0 0
1.3570 -1.3440 -0.3550 N 0 0
0.9530 -2.0670 -2.6910 O 0 0
-0.4470 -2.9470 -0.9180 O 0 0

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0.9670	-0.7010	0.7930	C	0	0
1.4350	0.7320	2.7130	C	0	0
1.8730	0.0860	1.5410	C	0	0
0.1030	0.5980	3.1450	C	0	0
-0.3670	-0.8320	1.2290	C	0	0
-0.7970	-0.1860	2.4000	C	0	0
3.3010	0.2540	1.1190	C	0	0
3.6090	0.2190	-0.0490	O	0	0
4.1680	0.4390	2.1090	O	0	0
-0.4730	1.4650	4.7150	Br	0	0
0.8160	1.0250	-2.1860	F	0	0
-4.5260	-0.1290	-1.7750	F	0	0
-4.0590	2.8550	-2.5390	Br	0	0
-2.5960	-1.8320	-1.3830	H	0	0
-1.0920	2.7520	-2.5820	H	0	0
2.3260	-1.5370	-0.5140	H	0	0
2.1310	1.3340	3.2810	H	0	0
-1.0760	-1.4280	0.6720	H	0	0
-1.8240	-0.3010	2.7170	H	0	0
5.1030	0.5550	1.9020	H	0	0

5	6	2	0
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3	4	2	0
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1	2	2	0
1	6	1	0
4	7	1	0
7	8	1	0
7	9	2	0
7	10	2	0
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16	14	2	0
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11	15	2	0
13	17	1	0
17	18	2	0
17	19	1	0
14	20	1	0
5	21	1	0
2	22	1	0
1	23	1	0
3	24	1	0
6	25	1	0
8	26	1	0
12	27	1	0
15	28	1	0
16	29	1	0
19	30	1	0

M END

> <Name>

Compound95

> <Activ>

4.5

> <DB_Ref_id>

06.06c

\$\$\$

Compound96

SciTegic10081411483D

27 28 0 0 0 0 999 V2000

-1.0220	1.1150	-0.1600	S	0	0
-0.0390	-0.1680	-0.2810	N	0	0
-0.6410	1.8460	1.0350	O	0	0
-0.8770	1.8930	-1.3790	O	0	0
1.3180	-0.0060	-0.1580	C	0	0
3.5620	-0.9040	0.1800	C	0	0
2.1760	-1.1090	0.0590	C	0	0
4.1010	0.3930	0.0900	C	0	0
1.8630	1.2910	-0.2480	C	0	0
3.2480	1.4900	-0.1250	C	0	0
1.6440	-2.5060	0.1620	C	0	0
0.5620	-2.7250	0.6560	O	0	0
2.4410	-3.4530	-0.3240	O	0	0
5.9590	0.6560	0.2560	Br	0	0
-2.6620	0.6520	-0.0100	C	0	0
-3.2830	-0.9280	0.0310	S	0	0
-4.8790	-0.3650	0.1900	C	0	0
-4.9470	1.0370	0.2130	C	0	0
-3.6700	1.6250	0.0980	C	0	0
-6.3170	-1.5720	0.3130	Br	0	0
-0.4200	-1.0760	-0.4450	H	0	0
4.2150	-1.7520	0.3420	H	0	0
1.2260	2.1500	-0.4120	H	0	0
3.6420	2.4920	-0.1950	H	0	0
2.1560	-4.3750	-0.2870	H	0	0
-5.8650	1.6060	0.3090	H	0	0
-3.4920	2.6920	0.0920	H	0	0

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1	4	2	0
2	5	1	0
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6	7	2	0
8	6	1	0
7	5	1	0
5	9	2	0
7	11	1	0
11	12	2	0
11	13	1	0
8	14	1	0
1	15	1	0
18	19	1	0
17	18	2	0
16	17	1	0
16	15	1	0
19	15	2	0
17	20	1	0
2	21	1	0
6	22	1	0
9	23	1	0
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19	27	1	0

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Compound96

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6.1

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06.06d

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Compound97
SciTegic10081411483D

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1.8830	-1.4750	-1.7290	C	0	0		
0.7540	-1.6780	-0.9140	C	0	0		
0.2810	-0.6330	-0.0980	C	0	0		
0.9360	0.6170	-0.0940	C	0	0		
2.0700	0.8160	-0.9140	C	0	0		
2.5350	-0.2310	-1.7270	C	0	0		
2.7950	2.1270	-0.9410	C	0	0		
4.1060	2.0430	-1.1430	O	0	0		
0.4510	1.6170	0.7130	N	0	0		
-1.0410	1.5060	1.3320	S	0	0		
-1.5740	2.9880	1.9940	C	0	0		
-1.7620	3.3690	3.6410	S	0	0		
-2.2910	4.9430	3.2830	C	0	0		
-2.3280	5.1890	1.9000	C	0	0		
-1.9160	4.0640	1.1580	C	0	0		
-2.7480	6.1410	4.6580	Br	0	0		
-1.9380	1.1430	0.2460	O	0	0		
-1.0020	0.5180	2.3960	O	0	0		
2.2030	3.1720	-0.7910	O	0	0		
0.0720	-2.9630	-0.9140	C	0	0		
-1.9920	-4.2600	-0.9140	C	0	0		
-1.3340	-3.0180	-0.9140	C	0	0		
-1.2460	-5.4510	-0.9140	C	0	0		
0.8180	-4.1580	-0.9140	C	0	0		
0.1580	-5.4010	-0.9140	C	0	0		
2.2580	-2.2660	-2.3610	H	0	0		
-0.5860	-0.7930	0.5270	H	0	0		
3.4020	-0.0880	-2.3580	H	0	0		
4.6330	2.8520	-1.1760	H	0	0		
1.0200	2.4120	0.9220	H	0	0		
-2.6330	6.1270	1.4510	H	0	0		
-1.8690	4.0350	0.0780	H	0	0		
-3.0700	-4.2990	-0.9140	H	0	0		
-1.9240	-2.1110	-0.9140	H	0	0		
-1.7520	-6.4040	-0.9140	H	0	0		
1.8980	-4.1370	-0.9140	H	0	0		
0.7320	-6.3150	-0.9140	H	0	0		
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4	5	1	0				
3	4	2	0				
2	3	1	0				
1	2	2	0				
1	6	1	0				
5	7	1	0				
7	8	1	0				
4	9	1	0				
9	10	1	0				

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14 15 1 0
13 14 2 0
12 13 1 0
12 11 1 0
15 11 2 0
13 16 1 0
10 17 2 0
10 18 2 0
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20 2 1 0
1 26 1 0
3 27 1 0
6 28 1 0
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Compound97

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6.7

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6.1

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Compound98

SciTegic10081411483D

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27 28 0 0 0 0          999 V2000
  0.9490 -1.3140 -0.0120 S 0 0
 -0.0410 -0.0450  0.1800 N 0 0
  1.7380 -1.0740 -1.2070 O 0 0
  1.7540 -1.4280  1.1910 O 0 0
  0.4550  1.2300  0.0900 C 0 0
  0.1430  3.6370 -0.1780 C 0 0
 -0.4020  2.3420 -0.0920 C 0 0
  1.5310  3.8300 -0.0880 C 0 0
  1.8480  1.4320  0.1780 C 0 0
  2.3850  2.7270  0.0880 C 0 0
 -1.8890  2.1780 -0.1910 C 0 0
 -2.3710  1.1910 -0.6950 O 0 0
 -2.6030  3.1820  0.3050 O 0 0
  0.0860 -2.7750 -0.2210 C 0 0
 -0.0960 -3.6620 -1.6580 S 0 0
 -1.0410 -4.8440 -0.8870 C 0 0
 -1.2230 -4.5680  0.4790 C 0 0

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-0.5740	-3.3750	0.8610	C	0	0
-1.7150	-6.3150	-1.8460	Br	0	0
4.0800	2.9630	0.1950	Cl	0	0
-1.0120	-0.1930	0.3650	H	0	0
-0.5020	4.4920	-0.3160	H	0	0
1.9300	4.8320	-0.1560	H	0	0
2.5120	0.5880	0.3150	H	0	0
-3.5680	3.1370	0.2720	H	0	0
-1.7910	-5.1900	1.1600	H	0	0
-0.5860	-2.9770	1.8670	H	0	0
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1	3	2	0		
1	4	2	0		
2	5	1	0		
10	8	2	0		
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10	20	1	0		
2	21	1	0		
6	22	1	0		
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Compound98

> <Activ>

4.6

> <DB_Ref_id>

06.07d

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Compound99

SciTegic10081411483D

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-0.0450	0.5680	1.2130	S	0	0		
0.4550	-0.1330	-0.1580	N	0	0		
-0.6760	-0.4590	2.0230	O	0	0		
1.1170	1.1660	1.8480	O	0	0		
1.1680	-1.3050	-0.1090	C	0	0		
2.0840	-3.3030	-1.1700	C	0	0		
1.3440	-2.1090	-1.2600	C	0	0		
2.6470	-3.6990	0.0530	C	0	0		

1.7350	-1.7090	1.1170	C	0	0
2.4730	-2.9040	1.1990	C	0	0
0.7600	-1.7210	-2.5840	C	0	0
-0.2970	-1.1390	-2.6500	O	0	0
1.4850	-2.0640	-3.6470	O	0	0
-1.2030	1.8140	0.9180	C	0	0
-0.7790	3.1090	0.5780	C	0	0
-2.5740	1.5250	1.0210	C	0	0
-1.7280	4.1170	0.3420	C	0	0
-3.5270	2.5310	0.7850	C	0	0
-3.1050	3.8360	0.4450	C	0	0
0.5200	3.3850	0.4770	F	0	0
-4.8220	2.2310	0.8870	F	0	0
-4.3550	5.2130	0.1250	Br	0	0
3.1560	-3.3890	2.6950	Cl	0	0
0.2440	0.2870	-1.0410	H	0	0
2.2250	-3.9240	-2.0430	H	0	0
3.2130	-4.6190	0.1010	H	0	0
1.6060	-1.1020	2.0020	H	0	0
1.1620	-1.8440	-4.5290	H	0	0
-2.8920	0.5270	1.2810	H	0	0
-1.3890	5.1110	0.0820	H	0	0

1	2	1	0
1	3	2	0
1	4	2	0
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19	22	1	0
10	23	1	0
2	24	1	0
6	25	1	0
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Compound99

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6.8

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06.07c

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Compound100

SciTegic10081411483D

38	40	0	0	0	0	999	V2000
1.0270	-0.2620	-1.6270	C	0	0		
0.4140	-0.5330	-0.3930	C	0	0		
-0.1480	0.5080	0.3630	C	0	0		
-0.1010	1.8340	-0.1110	C	0	0		
0.5140	2.1110	-1.3540	C	0	0		
1.0740	1.0610	-2.1040	C	0	0		
0.5880	3.5040	-1.9010	C	0	0		
1.6800	3.7790	-2.6080	O	0	0		
-0.6600	2.8320	0.6480	N	0	0		
-1.6850	2.4610	1.8460	S	0	0		
-0.8770	1.8010	3.2010	C	0	0		
0.7990	1.7360	3.4650	S	0	0		
0.6000	0.9610	4.9650	C	0	0		
-0.7540	0.7460	5.2730	C	0	0		
-1.6050	1.2300	4.2580	C	0	0		
2.0900	0.4880	6.0100	Br	0	0		
-2.3400	3.6910	2.2580	O	0	0		
-2.6110	1.4650	1.3360	O	0	0		
-0.2990	4.3010	-1.6940	O	0	0		
1.5530	-1.2400	-2.3340	O	0	0		
0.9360	-2.4040	-2.3340	C	0	0		
-1.1290	-3.7010	-2.3340	C	0	0		
-0.4690	-2.4590	-2.3340	C	0	0		
-0.3830	-4.8930	-2.3340	C	0	0		
1.6800	-3.5980	-2.3340	C	0	0		
1.0220	-4.8400	-2.3340	C	0	0		
0.3750	-1.5470	-0.0220	H	0	0		
-0.6130	0.2730	1.3100	H	0	0		
1.5470	1.2640	-3.0550	H	0	0		
1.7870	4.6600	-2.9870	H	0	0		
-0.4320	3.7870	0.4630	H	0	0		
-1.1070	0.2690	6.1780	H	0	0		
-2.6850	1.1660	4.2910	H	0	0		
-2.2070	-3.7400	-2.3340	H	0	0		
-1.0470	-1.5470	-2.3340	H	0	0		
-0.8890	-5.8460	-2.3340	H	0	0		
2.7600	-3.5630	-2.3340	H	0	0		
1.5960	-5.7560	-2.3340	H	0	0		
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3	4	2	0				
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9	10	1	0				
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14	15	1	0				
13	14	2	0				
12	13	1	0				
12	11	1	0				
15	11	2	0				

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10 18 2 0
7 19 2 0
1 20 1 0
20 21 1 0
26 24 2 0
25 26 1 0
22 23 2 0
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06.11a

$$$$
Compound101
SciTegic10081411483D

69 73 0 0 1 0 999 V2000
1.4960 -1.8220 -0.7390 C 0 0
2.0180 -0.1770 0.9970 C 0 0
2.3600 -0.7110 -0.1920 C 0 0
0.8300 -0.6750 1.7310 C 0 0
0.0350 -1.6510 -0.2830 C 0 0 3 0 0 0
-0.0340 -1.5230 1.1430 O 0 0
3.4200 -0.2750 -0.8710 O 0 0
2.8500 0.9340 1.5890 C 0 0
4.1250 0.3560 2.1650 C 0 0
0.6690 -0.3050 2.8710 O 0 0
-0.6470 -0.4410 -0.9340 C 0 0
-0.7740 -2.8710 -0.7090 C 0 0
-1.5770 0.3000 0.0270 C 0 0
-2.2060 -2.8230 -0.1900 C 0 0
-2.6650 -4.2510 -0.4540 C 0 0
-1.4600 -5.1080 -0.0690 C 0 0
-0.2580 -4.1620 -0.0790 C 0 0
-2.4200 1.2960 -0.6850 C 0 0
-1.8830 2.5440 -1.0470 C 0 0
-2.6790 3.4850 -1.7210 C 0 0
-4.0160 3.1820 -2.0350 C 0 0
-4.5550 1.9320 -1.6730 C 0 0

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-3.7560	0.9910	-0.9990	C	0	0
-5.8200	1.6320	-1.9650	F	0	0
-4.8500	4.1870	-2.7490	C	0	0
-4.0500	5.4450	-3.0860	C	0	0
-6.1390	4.4930	-1.9860	C	0	0
4.4670	-0.9940	2.3140	C	0	0
5.6850	-0.9650	2.8670	N	0	0
6.1190	0.2940	3.0700	C	0	0
5.1450	1.1440	2.6310	N	0	0
7.4420	0.5900	3.6750	C	0	0
8.2140	-0.4650	4.0220	C	0	0
7.7250	-1.8550	3.7910	C	0	0
6.5080	-2.0810	3.2340	C	0	0
-5.1420	3.4270	-3.9610	C	0	0
-5.3750	2.8240	-4.9250	N	0	0
1.8910	-2.7760	-0.3880	H	0	0
1.5600	-1.8360	-1.8280	H	0	0
4.0320	0.3400	-0.4470	H	0	0
2.2900	1.4360	2.3780	H	0	0
3.0970	1.6630	0.8180	H	0	0
0.0940	0.2390	-1.3550	H	0	0
-1.1840	-0.7390	-1.8350	H	0	0
-0.7730	-2.9560	-1.7870	H	0	0
-2.2170	-0.4010	0.5620	H	0	0
-1.0040	0.8020	0.8070	H	0	0
-2.8120	-2.0960	-0.7100	H	0	0
-2.2340	-2.5970	0.8680	H	0	0
-3.5520	-4.5080	0.1070	H	0	0
-2.8920	-4.3780	-1.5040	H	0	0
-1.5880	-5.5360	0.9150	H	0	0
-1.3330	-5.9250	-0.7640	H	0	0
0.0730	-3.9840	0.9340	H	0	0
0.5780	-4.5730	-0.6270	H	0	0
-0.8570	2.7840	-0.8090	H	0	0
-2.2590	4.4410	-1.9950	H	0	0
-4.1710	0.0330	-0.7220	H	0	0
-3.1710	5.2190	-3.6890	H	0	0
-3.7120	5.9410	-2.1760	H	0	0
-4.6630	6.1540	-3.6430	H	0	0
-6.8040	3.6290	-1.9900	H	0	0
-5.9190	4.7670	-0.9540	H	0	0
-6.6710	5.3260	-2.4460	H	0	0
3.9050	-1.8820	2.0560	H	0	0
7.7730	1.6060	3.8300	H	0	0
9.1840	-0.3020	4.4670	H	0	0
8.3480	-2.6920	4.0700	H	0	0
6.1880	-3.1030	3.0820	H	0	0
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15	16	1	0		
14	15	1	0		

14	12	1	0
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18	19	2	0
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15	51	1	0
16	52	1	0
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27	62	1	0
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M END
> <Name>

70	73	0	0	1	0	999	V2000				
-1.4900				-1.0250		1.5630	C	0	0		
-1.0000				1.3520		1.2560	C	0	0		
-0.8380				0.2560		2.0230	C	0	0		
-1.7950				1.2870		0.0080	C	0	0		
-1.5660				-1.0780		0.0250	C	0	0	3	0 0 0
-2.2010				0.1020		-0.4840	O	0	0		
-0.1250				0.2910		3.1470	O	0	0		
-0.3710				2.6600		1.6740	C	0	0		
-1.1000				3.2950		2.8050	C	0	0		
-2.0720				2.3260		-0.5470	O	0	0		
-0.1850				-1.2340		-0.6270	C	0	0		
-2.3730				-2.2970		-0.4000	C	0	0		
-0.2130				-0.9790		-2.1350	C	0	0		
-3.8070				-2.2500		0.1170	C	0	0		
-4.2660				-3.6780		-0.1460	C	0	0		
-3.0600				-4.5330		0.2380	C	0	0		
-1.8570				-3.5880		0.2290	C	0	0		
1.1520				-1.0060		-2.7190	C	0	0		
1.9730				0.1350		-2.6450	C	0	0		
3.2660				0.1090		-3.1970	C	0	0		
3.7420				-1.0550		-3.8260	C	0	0		
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5.1120				-1.0700		-4.4080	C	0	0		
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-0.4140				3.6210		3.9880	C	0	0		
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-1.5270	-3.4100	1.2420	H	0	0
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1.6150	1.0330	-2.1640	H	0	0
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0.9980	-3.0470	-3.4060	H	0	0
5.8970	0.5000	-3.1110	H	0	0
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6.8540	0.2110	-4.5610	H	0	0
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-2.0020	4.5610	7.5080	H	0	0
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SciTegic10081411483D

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-0.6820 1.2480 0.8380 C 0 0
-0.5140 0.1500 1.6020 C 0 0
-1.4810 1.1850 -0.4080 C 0 0
-1.2480 -1.1800 -0.3980 C 0 0 3 0 0 0
-1.8870 0.0000 -0.9020 O 0 0
0.2030 0.1840 2.7230 O 0 0
-0.0530 2.5550 1.2580 C 0 0
-0.8500 3.1560 2.3950 C 0 0
-1.7620 2.2250 -0.9570 O 0 0
0.1290 -1.3320 -1.0570 C 0 0
-2.0570 -2.3990 -0.8240 C 0 0

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-3.4900	-2.3520	-0.3050	C	0	0
-3.9490	-3.7790	-0.5680	C	0	0
-2.7440	-4.6350	-0.1840	C	0	0
-1.5410	-3.6900	-0.1930	C	0	0
1.4360	-1.2400	-3.1780	C	0	0
2.4140	-0.2380	-3.0490	C	0	0
3.6800	-0.4100	-3.6330	C	0	0
3.9750	-1.5860	-4.3480	C	0	0
2.9960	-2.5900	-4.4770	C	0	0
1.7290	-2.4160	-3.8930	C	0	0
3.2620	-3.7070	-5.1520	F	0	0
5.3180	-1.7560	-4.9610	C	0	0
-0.3480	3.5310	3.6020	N	0	0
-1.3460	4.0140	4.3340	N	0	0
-2.4790	3.9490	3.6090	C	0	0
-2.2130	3.4140	2.3810	N	0	0
-3.8400	4.3870	4.0430	N	0	0
-3.8730	4.8670	5.2460	C	0	0
-2.6740	4.9730	6.1150	C	0	0
-1.4750	4.5590	5.6560	C	0	0
-0.2500	4.6600	6.5290	C	0	0
-5.1950	5.3400	5.7890	C	0	0
6.2360	-0.5740	-4.6450	C	0	0
6.0100	-3.0240	-4.4570	C	0	0
5.1880	-1.8500	-6.3610	O	0	0
-2.1660	-1.1900	1.5720	H	0	0
-0.6070	-1.9860	1.5220	H	0	0
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0.9730	2.3850	1.5820	H	0	0
-0.0430	3.2480	0.4160	H	0	0
0.5470	-2.3170	-0.8520	H	0	0
0.8630	-0.6930	-0.5640	H	0	0
-2.0570	-2.4840	-1.9020	H	0	0
-0.2620	-0.0490	-2.7620	H	0	0
-0.6230	-1.7110	-3.0550	H	0	0
-4.0960	-1.6230	-0.8240	H	0	0
-3.5180	-2.1250	0.7520	H	0	0
-4.8360	-4.0350	-0.0080	H	0	0
-4.1760	-3.9060	-1.6190	H	0	0
-2.8710	-5.0650	0.8010	H	0	0
-2.6170	-5.4530	-0.8790	H	0	0
-1.2110	-3.5120	0.8200	H	0	0
-0.7050	-4.1020	-0.7420	H	0	0
2.1950	0.6660	-2.5020	H	0	0
4.4260	0.3650	-3.5290	H	0	0
0.9790	-3.1880	-3.9920	H	0	0
-2.7640	5.3810	7.1110	H	0	0
0.5350	3.9550	6.2640	H	0	0
-0.5220	4.4800	7.5700	H	0	0
0.1680	5.6660	6.4630	H	0	0
-5.8300	5.6800	4.9730	H	0	0
-5.6680	4.5430	6.3610	H	0	0
-5.0390	6.1840	6.4610	H	0	0
5.8300	0.3650	-5.0160	H	0	0
7.2170	-0.7170	-5.0980	H	0	0
6.3770	-0.4750	-3.5680	H	0	0
5.5160	-3.9260	-4.8180	H	0	0
6.0100	-3.0570	-3.3690	H	0	0
7.0470	-3.0570	-4.7930	H	0	0
4.8090	-2.7210	-6.5550	H	0	0

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8.15

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Compound104

SciTegic10081411483D

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  1.1040 -0.1890  0.8010 C  0 0
  1.4510 -0.7270 -0.3850 C  0 0
 -0.0900 -0.6820  1.5290 C  0 0
 -0.8750 -1.6640 -0.4860 C  0 0 3 0 0 0
 -0.9510 -1.5290  0.9390 O  0 0
  2.5160 -0.2970 -1.0590 O  0 0
  1.9340  0.9220  1.3930 C  0 0
  3.2230  0.3500  1.9450 C  0 0
 -0.2560 -0.3070  2.6680 O  0 0
 -1.5510 -0.4550 -1.1450 C  0 0
 -1.6840 -2.8830 -0.9120 C  0 0
 -2.4900  0.2890 -0.1930 C  0 0
 -3.1150 -2.8360 -0.3930 C  0 0
 -3.5760 -4.2640 -0.6560 C  0 0
 -2.3710 -5.1190 -0.2720 C  0 0
 -1.1680 -4.1740 -0.2810 C  0 0
 -3.3130  1.2970 -0.9120 C  0 0
 -4.5080  0.9080 -1.5410 C  0 0
 -5.2850  1.8610 -2.2210 C  0 0
 -4.8690  3.2050 -2.2740 C  0 0
 -3.6700  3.5940 -1.6450 C  0 0
 -2.8950  2.6390 -0.9650 C  0 0
  4.4770  0.7730  1.6310 N  0 0
  5.3440  0.0350  2.3110 N  0 0
  4.6620 -0.8570  3.0550 C  0 0
  3.3200 -0.6930  2.8540 N  0 0
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-5.7050	4.2010	-2.9980	C	0	0
-3.2130	5.0100	-1.6900	C	0	0
-2.0490	5.1930	-2.6640	C	0	0
-5.0960	4.6600	-4.2420	C	0	0
-4.6110	5.0250	-5.2310	N	0	0
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0.6580	-1.8570	-2.0200	H	0	0
3.0570	0.4100	-0.6860	H	0	0
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2.1640	1.6620	0.6270	H	0	0
-0.8070	0.2250	-1.5610	H	0	0
-2.0800	-0.7540	-2.0510	H	0	0
-1.6840	-2.9690	-1.9880	H	0	0
-3.1450	-0.4100	0.3260	H	0	0
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	0.1840		-0.7870		1.7400	C	0	0						
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	-0.6700		-1.6390		1.1430	O	0	0						
	2.8650		-0.4770		-0.7790	O	0	0						
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	3.4490		0.2110		2.3070	C	0	0						
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	-2.7950		-2.9730		-0.1840	C	0	0						
	-3.2560		-4.4010		-0.4490	C	0	0						
	-2.0510		-5.2560		-0.0620	C	0	0						
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	-3.0020		1.1210		-0.8400	C	0	0						
	-4.3950		0.9340		-0.8950	C	0	0						
	-5.1950		1.8280		-1.6250	C	0	0						
	-4.6070		2.9140		-2.3010	C	0	0						
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	-2.4120		2.2050		-1.5140	C	0	0						
	4.7400		0.5430		2.0350	N	0	0						
	5.5270		-0.1740		2.8260	N	0	0						
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	3.4400		-0.7500		3.3070	N	0	0						
	5.2290		-1.9280		4.6390	N	0	0						
	6.5180		-1.9730		4.7600	C	0	0						
	7.4420		-1.1430		3.9470	C	0	0						
	6.9430		-0.2890		3.0270	C	0	0						
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	-5.4750		3.8550		-3.0740	C	0	0						
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-1.6020	0.7230	0.6950	H	0	0
-3.4020	-2.2440	-0.7050	H	0	0
-2.8240	-2.7460	0.8730	H	0	0
-4.1410	-4.6560	0.1130	H	0	0
-3.4820	-4.5270	-1.4980	H	0	0
-2.1780	-5.6840	0.9220	H	0	0
-1.9220	-6.0740	-0.7580	H	0	0
-0.5160	-4.1330	0.9390	H	0	0
-0.0120	-4.7210	-0.6210	H	0	0
-4.8540	0.1030	-0.3790	H	0	0
-6.2640	1.6760	-1.6620	H	0	0
-1.3420	2.3480	-1.4710	H	0	0
8.5080	-1.2270	4.0940	H	0	0
7.4530	0.8510	1.2360	H	0	0
8.7990	0.0120	2.0040	H	0	0
8.1310	1.4670	2.7400	H	0	0
6.4300	-3.1390	6.6020	H	0	0
8.0140	-2.4830	6.1970	H	0	0
7.3730	-3.8560	5.2990	H	0	0
-4.6130	3.3830	-4.8790	H	0	0
-5.9550	4.8770	-6.2720	H	0	0
-6.0140	5.8790	-4.8240	H	0	0
-7.1990	4.5980	-5.0570	H	0	0
-2.0800	3.8810	-3.8590	H	0	0
-3.3340	4.9300	-3.3070	H	0	0
-1.2190	5.8870	-2.5270	H	0	0
-2.0160	5.2110	-1.0920	H	0	0
-0.6930	4.3420	-1.8650	H	0	0
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2	3	2	0		
1	5	1	0		
4	2	1	0		
3	7	1	0		
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24	25	1	0		
24	9	2	0		
27	9	1	0		
30	31	2	0		
29	30	1	0		
28	29	2	0		
26	28	1	0		

25	31	1	0
31	32	1	0
29	33	1	0
22	38	1	0
21	34	1	0
34	35	1	0
34	36	2	0
35	37	1	0
6	4	1	0
38	39	1	0
1	40	1	0
1	41	1	0
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Compound105

> <Activ>

0.006

> <DB_Ref_id>

8.19

\$\$\$\$

Compound106

SciTegic10081411483D

[illegible]

6.6930	-2.5270	5.5100	H	0	0
8.2130	-1.7450	5.0860	H	0	0
7.6090	-3.0830	4.1120	H	0	0
-6.4830	2.6680	-4.0370	H	0	0
-6.5800	1.2090	-3.1200	H	0	0
-8.6100	2.6550	-2.7520	H	0	0
-7.7180	2.4290	-1.2340	H	0	0
-7.5810	3.9410	-2.1280	H	0	0
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2	3	2	0		
1	5	1	0		
4	2	1	0		
3	7	1	0		
2	8	1	0		
8	9	1	0		
4	10	2	0		
5	11	1	0		
5	12	1	0		
11	13	1	0		
16	17	1	0		
15	16	1	0		
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14	12	1	0		
17	12	1	0		
13	18	1	0		
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13	44	1	0		
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14	47	1	0		
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15	49	1	0		

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17 53 1 0
19 54 1 0
21 55 1 0
23 56 1 0
30 57 1 0
32 58 1 0
32 59 1 0
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Compound106

> <Activ>

0.008

> <DB_Ref_id>

8.21

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Compound107

SciTegic10081411483D

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68 72 0 0 1 0          999 V2000
  0.2260 -1.5160 -1.1860 C 0 0
  0.7370  0.1370  0.5440 C 0 0
  1.0890 -0.4040 -0.6390 C 0 0
 -0.4580 -0.3520  1.2710 C 0 0
 -1.2390 -1.3380 -0.7450 C 0 0 3 0 0 0
 -1.3200 -1.2010  0.6800 O 0 0
  2.1560  0.0230 -1.3100 O 0 0
  1.5680  1.2490  1.1370 C 0 0
  2.8410  0.6730  1.7170 C 0 0
 -0.6290  0.0250  2.4070 O 0 0
 -1.9110 -0.1300 -1.4090 C 0 0
 -2.0470 -2.5580 -1.1710 C 0 0
 -2.8270  0.6350 -0.4540 C 0 0
 -3.4790 -2.5100 -0.6520 C 0 0
 -3.9390 -3.9380 -0.9160 C 0 0
 -2.7340 -4.7950 -0.5310 C 0 0
 -1.5310 -3.8490 -0.5410 C 0 0
 -3.6520  1.6400 -1.1740 C 0 0
 -4.8510  1.2620 -1.8020 C 0 0
 -5.6120  2.2360 -2.4770 C 0 0
 -5.2090  3.5390 -2.5330 N 0 0
 -4.0460  3.9170 -1.9270 C 0 0
 -3.2450  2.9840 -1.2370 C 0 0
  4.1050  1.0580  1.3920 N 0 0
  4.9560  0.3290  2.1030 N 0 0
  4.2520 -0.5180  2.8800 C 0 0
  2.9150 -0.3350  2.6670 N 0 0

```

4.8080	-1.5180	3.8410	N	0	0
6.1030	-1.5280	3.8900	C	0	0
6.9560	-0.6330	3.0700	C	0	0
6.3840	0.2470	2.2220	C	0	0
7.2430	1.1610	1.3850	C	0	0
6.7730	-2.4970	4.8260	C	0	0
-3.6220	5.3390	-1.9980	C	0	0
-3.0580	5.6900	-3.3750	C	0	0
0.6150	-2.4690	-0.8260	H	0	0
0.3000	-1.5370	-2.2740	H	0	0
2.7130	0.7110	-0.9230	H	0	0
1.0060	1.7520	1.9240	H	0	0
1.8160	1.9780	0.3660	H	0	0
-1.1650	0.5360	-1.8430	H	0	0
-2.4550	-0.4350	-2.3030	H	0	0
-2.0460	-2.6430	-2.2480	H	0	0
-3.4800	-0.0510	0.0860	H	0	0
-2.2450	1.1320	0.3230	H	0	0
-4.0850	-1.7830	-1.1720	H	0	0
-3.5080	-2.2840	0.4060	H	0	0
-4.8250	-4.1950	-0.3540	H	0	0
-4.1660	-4.0650	-1.9660	H	0	0
-2.8620	-5.2230	0.4540	H	0	0
-2.6060	-5.6120	-1.2250	H	0	0
-1.2000	-3.6710	0.4730	H	0	0
-0.6950	-4.2600	-1.0890	H	0	0
-5.1890	0.2360	-1.7700	H	0	0
-6.5340	1.9480	-2.9600	H	0	0
-2.3270	3.2990	-0.7620	H	0	0
8.0320	-0.6890	3.1540	H	0	0
6.7500	1.5110	0.4780	H	0	0
8.1560	0.6440	1.0900	H	0	0
7.5290	2.0370	1.9670	H	0	0
6.1390	-2.8090	5.6560	H	0	0
7.6730	-2.0460	5.2450	H	0	0
7.0720	-3.3930	4.2810	H	0	0
-4.4670	5.9830	-1.7520	H	0	0
-2.8870	5.5390	-1.2180	H	0	0
-2.7640	6.7390	-3.4150	H	0	0
-2.1920	5.0700	-3.6060	H	0	0
-3.8040	5.5230	-4.1510	H	0	0
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2	3	2	0		
1	5	1	0		
4	2	1	0		
3	7	1	0		
2	8	1	0		
8	9	1	0		
4	10	2	0		
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5	12	1	0		
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14	15	1	0		
14	12	1	0		
17	12	1	0		
13	18	1	0		
22	23	2	0		
21	22	1	0		
20	21	2	0		

19	20	1	0
23	18	1	0
18	19	2	0
3	1	1	0
26	27	2	0
25	26	1	0
24	25	1	0
24	9	2	0
27	9	1	0
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M END

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Compound107

> <Activ>
0.01

> <DB_Ref_id>
8.22

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Compound108

SciTegic10081411483D

74	78	0	0	1	0	999	V2000				
2.3200	-2.9850	0.0120	C	0	0						
2.8360	-1.3320	1.7440	C	0	0						
3.1760	-1.8610	0.5510	C	0	0						
1.6640	-1.8460	2.4920	C	0	0						
0.8630	-2.8300	0.4880	C	0	0	3	0	0	0		
0.8110	-2.7130	1.9140	O	0	0						
4.2250	-1.4140	-0.1370	O	0	0						
3.6600	-0.2090	2.3260	C	0	0						
3.3070	1.0880	1.6310	C	0	0						
1.5060	-1.4690	3.6290	O	0	0						
0.1680	-1.6210	-0.1500	C	0	0						
0.0550	-4.0510	0.0590	C	0	0						
-0.7110	-0.8560	0.8400	C	0	0						
-1.3770	-4.0020	0.5780	C	0	0						
-1.8380	-5.4300	0.3150	C	0	0						
-0.6330	-6.2870	0.6990	C	0	0						
0.5700	-5.3420	0.6900	C	0	0						
-1.7170	-0.0120	0.1410	C	0	0						
-1.3360	1.1990	-0.4610	C	0	0						
-2.3100	1.9780	-1.1170	C	0	0						
-3.6150	1.5800	-1.1780	N	0	0						
-3.9940	0.4040	-0.5960	C	0	0						
-3.0620	-0.4140	0.0740	C	0	0						
4.0470	1.6950	0.6660	N	0	0						
3.4180	2.8070	0.3010	N	0	0						
2.2850	2.9160	1.0220	C	0	0						
2.1760	1.8530	1.8750	N	0	0						
1.2740	4.0140	0.9340	N	0	0						
1.5700	4.9240	0.0610	C	0	0						
2.7950	4.8850	-0.7750	C	0	0						
3.6640	3.8610	-0.6420	C	0	0						
4.9120	3.8100	-1.4860	C	0	0						
0.6210	6.0780	-0.1130	C	0	0						
-5.4180	-0.0120	-0.6720	C	0	0						
-6.2600	0.6540	0.4180	C	0	0						
-1.9180	3.2620	-1.7580	C	0	0						
-2.3570	3.3180	-3.2210	C	0	0						
2.7310	-3.9340	0.3610	H	0	0						
2.3730	-2.9940	-1.0780	H	0	0						
4.4340	-1.8130	-0.9920	H	0	0						
4.7210	-0.4180	2.1900	H	0	0						
3.4570	-0.1170	3.3930	H	0	0						
0.8990	-0.9550	-0.6090	H	0	0						
-0.4080	-1.9220	-1.0230	H	0	0						
0.0550	-4.1370	-1.0170	H	0	0						
-1.2210	-1.5450	1.5140	H	0	0						
-0.1010	-0.2310	1.4920	H	0	0						
-1.9840	-3.2760	0.0590	H	0	0						
-1.4060	-3.7780	1.6350	H	0	0						
-2.7230	-5.6880	0.8750	H	0	0						
-2.0640	-5.5570	-0.7340	H	0	0						
-0.7600	-6.7150	1.6840	H	0	0						
-0.5040	-7.1040	0.0060	H	0	0						
0.9020	-5.1620	1.7010	H	0	0						
1.4060	-5.7520	0.1410	H	0	0						

-0.3080	1.5290	-0.4220	H	0	0
-3.3790	-1.3420	0.5290	H	0	0
2.9880	5.6740	-1.4860	H	0	0
5.4240	4.7710	-1.5620	H	0	0
4.6640	3.4840	-2.4960	H	0	0
5.6150	3.0920	-1.0660	H	0	0
0.3910	6.3010	-1.1560	H	0	0
1.0450	6.9780	0.3320	H	0	0
-0.3180	5.8670	0.3970	H	0	0
-5.4820	-1.0980	-0.6000	H	0	0
-5.8120	0.2230	-1.6600	H	0	0
-5.8910	0.4200	1.4160	H	0	0
-7.2970	0.3240	0.3590	H	0	0
-6.2480	1.7380	0.3050	H	0	0
-2.3420	4.0940	-1.1950	H	0	0
-0.8380	3.3920	-1.6740	H	0	0
-1.9920	2.4490	-3.7680	H	0	0
-3.4450	3.3510	-3.2950	H	0	0
-1.9610	4.2090	-3.7090	H	0	0
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4	2	1	0		
3	7	1	0		
2	8	1	0		
8	9	1	0		
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20	36	1	0		
6	4	1	0		
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Compound108

> <Activ>
0.007

> <DB_Ref_id>
8.24

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Compound109
SciTegic10081411483D

56 59 0 0 1 0          999 V2000
-1.6610 2.8030 -2.5270 C 0 0
-2.5970 2.3060 -3.4510 C 0 0
-2.7030 0.9130 -3.6560 C 0 0
-1.8710 0.0330 -2.9390 C 0 0
-0.8320 1.9230 -1.8120 C 0 0
-0.0580 -0.3940 -1.2630 C 0 0
-0.4270 -0.4390 0.2200 C 0 0
0.1930 -1.6380 0.9480 C 0 0 3 0 0 0
0.0520 -1.4580 2.3620 O 0 0
1.6720 -1.8510 0.5860 C 0 0

```

2.5220	-0.7350	1.1440	C	0	0
2.1380	-0.1400	2.2910	C	0	0
0.9020	-0.6050	2.9650	C	0	0
3.6250	-0.3420	0.5110	O	0	0
0.6890	-0.1960	4.0830	O	0	0
-0.9360	0.5370	-2.0180	C	0	0
-0.6160	-2.8580	0.5230	C	0	0
-2.0480	-2.8110	1.0420	C	0	0
-2.5070	-4.2390	0.7770	C	0	0
-1.3020	-5.0950	1.1630	C	0	0
-0.1000	-4.1500	1.1520	C	0	0
-3.8400	0.2740	-4.7750	Cl	0	0
-3.3640	3.1500	-4.1130	O	0	0
-3.3270	4.5190	-3.7390	C	0	0
3.0560	1.1120	2.9590	S	0	0
2.8950	2.3400	1.8100	C	0	0
3.5290	3.5050	1.8010	N	0	0
3.1460	4.2370	0.7210	N	0	0
2.2250	3.4700	0.0350	N	0	0
2.1100	2.3200	0.7450	N	0	0
4.5040	3.9450	2.8090	C	0	0
-1.5770	3.8680	-2.3640	H	0	0
-1.9440	-1.0350	-3.0900	H	0	0
-0.1160	2.3170	-1.1050	H	0	0
0.9830	-0.0970	-1.3920	H	0	0
-0.1180	-1.3890	-1.7050	H	0	0
-1.5100	-0.4280	0.3480	H	0	0
-0.1550	0.4940	0.7130	H	0	0
2.0290	-2.7980	0.9940	H	0	0
1.7990	-1.9060	-0.4960	H	0	0
4.2140	0.2940	0.9380	H	0	0
-0.6150	-2.9430	-0.5550	H	0	0
-2.6530	-2.0830	0.5210	H	0	0
-2.0760	-2.5850	2.0990	H	0	0
-3.3940	-4.4950	1.3390	H	0	0
-2.7340	-4.3660	-0.2720	H	0	0
-1.4300	-5.5230	2.1470	H	0	0
-1.1750	-5.9120	0.4680	H	0	0
0.2320	-3.9710	2.1660	H	0	0
0.7360	-4.5600	0.6040	H	0	0
-4.0240	5.0660	-4.3750	H	0	0
-3.5010	4.5850	-2.6650	H	0	0
-2.3250	4.9000	-3.9380	H	0	0
4.9180	4.9380	2.6290	H	0	0
5.3340	3.2400	2.8450	H	0	0
4.0320	3.9550	3.7920	H	0	0
3	4	2	0		
2	3	1	0		
1	2	2	0		
1	5	1	0		
6	7	1	0		
7	8	1	0		
8	9	1	0		
8	10	1	0		
10	11	1	0		
12	13	1	0		
13	9	1	0		
11	14	1	0		
13	15	2	0		
11	12	2	0		
5	16	2	0		


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 16  6  1  0
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 27 28  1  0
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> <Name>
Compound109

> <Activ>
0.28

> <DB_Ref_id>
9.37

$$$$
Compound110
  SciTegic10081411483D

58 61  0  0  1  0          999 V2000
   -2.5290    2.7910   -1.2970 C    0  0
   -3.8960    2.4810   -1.1950 C    0  0

```

-4.3050	1.3610	-0.4380	C	0	0				
-3.3420	0.5650	0.2090	C	0	0				
-1.5700	1.9940	-0.6490	C	0	0				
-0.9630	0.0350	0.7870	C	0	0				
-0.0430	-0.6620	-0.2150	C	0	0				
0.6740	-1.8790	0.3850	C	0	0	3	0	0	0
0.6520	-1.7830	1.8140	O	0	0				
2.1210	-2.0230	-0.1150	C	0	0				
2.9840	-0.9120	0.4320	C	0	0				
2.6860	-0.3960	1.6430	C	0	0				
1.5270	-0.9390	2.3910	C	0	0				
4.0160	-0.4470	-0.2700	O	0	0				
1.4020	-0.6010	3.5450	O	0	0				
-1.9770	0.8790	0.1030	C	0	0				
-0.1350	-3.1000	-0.0410	C	0	0				
-1.5680	-3.0530	0.4780	C	0	0				
-2.0270	-4.4800	0.2150	C	0	0				
-0.8220	-5.3360	0.6000	C	0	0				
0.3810	-4.3910	0.5900	C	0	0				
-5.9690	0.9570	-0.2930	C1	0	0				
-4.7790	3.2400	-1.8150	O	0	0				
-4.3120	4.4160	-2.4590	C	0	0				
3.6250	0.8460	2.3010	S	0	0				
3.5530	2.0350	1.1030	C	0	0				
4.6560	2.8730	0.8460	C	0	0				
4.6020	3.8650	-0.1490	C	0	0				
3.4320	4.0330	-0.9040	C	0	0				
2.3220	3.2090	-0.6640	C	0	0				
2.3870	2.2210	0.3340	C	0	0				
-2.2110	3.6470	-1.8730	H	0	0				
-3.6460	-0.2950	0.7910	H	0	0				
-0.5210	2.2420	-0.7330	H	0	0				
-1.4670	-0.6950	1.4220	H	0	0				
-0.3850	0.6490	1.4780	H	0	0				
0.6800	0.0430	-0.6290	H	0	0				
-0.5920	-0.9430	-1.1130	H	0	0				
2.5370	-2.9780	0.2030	H	0	0				
2.1520	-2.0120	-1.2050	H	0	0				
4.6470	0.1470	0.1560	H	0	0				
-0.1350	-3.1840	-1.1170	H	0	0				
-2.1740	-2.3240	-0.0410	H	0	0				
-1.5960	-2.8260	1.5370	H	0	0				
-2.9140	-4.7360	0.7750	H	0	0				
-2.2540	-4.6070	-0.8360	H	0	0				
-0.9490	-5.7640	1.5840	H	0	0				
-0.6950	-6.1540	-0.0960	H	0	0				
0.7110	-4.2130	1.6030	H	0	0				
1.2170	-4.8010	0.0410	H	0	0				
-5.1620	4.9080	-2.9300	H	0	0				
-3.7560	5.0060	-1.7330	H	0	0				
-3.6210	4.1190	-3.2480	H	0	0				
5.5610	2.7520	1.4220	H	0	0				
5.4590	4.4960	-0.3300	H	0	0				
3.3850	4.7950	-1.6700	H	0	0				
1.4180	3.3340	-1.2420	H	0	0				
1.5270	1.5920	0.5120	H	0	0				
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2	3	1	0						
1	2	2	0						
1	5	1	0						
6	7	1	0						

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13	9	1	0
11	14	1	0
13	15	2	0
11	12	2	0
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M END

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Compound110

> <Activ>

[illegible]

-2.3540	-3.4530	-2.1060 H	0	0
-0.6000	-3.3540	-2.2520 H	0	0

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M END

> <Name>

Compound111

> <Activ>
0.53

> <DB_Ref_id>
9.33

\$\$\$\$

Compound112

SciTegic10081411483D

50	52	0	0	1	0	999	V2000							
-0.4960				3.1500		-1.7680	C	0	0					
-1.8690				3.1290		-2.0720	C	0	0					
-2.5940				1.9300		-1.9360	C	0	0					
-1.9470				0.7600		-1.4980	C	0	0					
0.1500				1.9820		-1.3280	C	0	0					
0.1090				-0.4490		-0.7300	C	0	0					
0.4490				-0.3810		0.7580	C	0	0					
1.2460				-1.6000		1.2420	C	0	0	3	0	0	0	
1.3360				-1.5840		2.6700	O	0	0					
2.6540				-1.6840		0.6210	C	0	0					
3.5550				-0.5920		1.1470	C	0	0					
3.0860				0.1600		2.3710	C	0	0					
2.1760				-0.6950		3.2270	C	0	0					
4.6070				-0.3320		0.6090	O	0	0					
2.2360				-0.5650		4.4280	O	0	0					
-0.5740				0.7850		-1.1930	C	0	0					
0.4380				-2.8200		0.8160	C	0	0					
-0.9940				-2.7720		1.3340	C	0	0					
-1.4530				-4.1990		1.0700	C	0	0					
-0.2480				-5.0570		1.4550	C	0	0					
0.9530				-4.1110		1.4450	C	0	0					
-3.8950				1.8960		-2.2210	F	0	0					
-2.4690				4.2290		-2.4820	O	0	0					
-1.6890				5.4080		-2.6020	C	0	0					
-2.5740				6.5570		-3.0880	C	0	0					
0.0660				4.0660		-1.8690	H	0	0					
-2.5060				-0.1600		-1.3950	H	0	0					
1.2050				2.0080		-1.0980	H	0	0					
1.0080				-0.6110		-1.3240	H	0	0					
-0.5210				-1.3150		-0.9410	H	0	0					
-0.4530				-0.2480		1.3550	H	0	0					
0.9800				0.5430		0.9880	H	0	0					
3.1090				-2.6490		0.8540	H	0	0					
2.5960				-1.6170		-0.4670	H	0	0					
3.9490				0.4840		2.9530	H	0	0					
2.5530				1.0610		2.0630	H	0	0					
0.4380				-2.9040		-0.2620	H	0	0					
-1.6000				-2.0450		0.8140	H	0	0					
-1.0230				-2.5470		2.3930	H	0	0					
-2.3400				-4.4570		1.6330	H	0	0					
-1.6820				-4.3280		0.0210	H	0	0					
-0.3770				-5.4840		2.4390	H	0	0					
-0.1210				-5.8750		0.7620	H	0	0					
1.2850				-3.9320		2.4590	H	0	0					
1.7890				-4.5220		0.8960	H	0	0					
-1.2660				5.6370		-1.6230	H	0	0					
-0.8850				5.2150		-3.3090	H	0	0					
-1.9960				7.4770		-3.1780	H	0	0					
-3.0160				6.3180		-4.0550	H	0	0					
-3.3870				6.7400		-2.3870	H	0	0					

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1	5	1	0
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8	9	1	0
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M END

> <Name>
Compound112

> <Activ>
0.79

> <DB_Ref_id>
9.32

Compound113
SciTegic10081411483D

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13 9 1 0
11 14 2 0
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11 12 1 0
5 16 2 0
4 16 1 0
16 6 1 0
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19 20 1 0
17 18 1 0
18 19 1 0
17 8 1 0
2 22 1 0
22 23 1 0
23 24 1 0
23 25 1 0
1 26 1 0
3 27 1 0
4 28 1 0
5 29 1 0
6 30 1 0
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7 32 1 0
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M END
> <Name>
Compound113

> <Activ>
1.7

> <DB_Ref_id>
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SciTegic10081411483D

50	52	0	0	1	0				999	V2000						
-0.4940				3.1560		-1.7580	C		0	0						
-1.8650				3.1330		-2.0720	C		0	0						
-2.5880				1.9340		-1.9450	C		0	0						
-1.9450				0.7620		-1.5080	C		0	0						
0.1500				1.9860		-1.3200	C		0	0						
0.1060				-0.4490		-0.7320	C		0	0						
0.4410				-0.3830		0.7560	C		0	0						
1.2400				-1.6040		1.2380	C		0	0	3	0	0	0		
1.3300				-1.5900		2.6660	O		0	0						
2.6470				-1.6880		0.6170	C		0	0						
3.5470				-0.5940		1.1410	C		0	0						
3.0800				0.1580		2.3670	C		0	0						
2.1720				-0.7010		3.2230	C		0	0						
4.6000				-0.3340		0.6050	O		0	0						
2.2320				-0.5680		4.4240	O		0	0						
-0.5740				0.7870		-1.1950	C		0	0						
0.4320				-2.8220		0.8120	C		0	0						
-1.0020				-2.7750		1.3320	C		0	0						
-1.4610				-4.2030		1.0660	C		0	0						
-0.2560				-5.0610		1.4530	C		0	0						
0.9470				-4.1150		1.4410	C		0	0						
-2.4690				4.2300		-2.4820	O		0	0						
-1.6950				5.4160		-2.5920	C		0	0						
-2.5840				6.5610		-3.0800	C		0	0						
0.0660				4.0740		-1.8520	H		0	0						
-3.6410				1.9080		-2.1860	H		0	0						
-2.5080				-0.1540		-1.4140	H		0	0						
1.2030				2.0120		-1.0820	H		0	0						
1.0080				-0.6110		-1.3240	H		0	0						
-0.5230				-1.3130		-0.9490	H		0	0						
-0.4630				-0.2560		1.3520	H		0	0						
0.9710				0.5390		0.9920	H		0	0						
3.1020				-2.6500		0.8480	H		0	0						
2.5880				-1.6190		-0.4710	H		0	0						
3.9430				0.4800		2.9490	H		0	0						
2.5470				1.0570		2.0590	H		0	0						
0.4320				-2.9080		-0.2660	H		0	0						
-1.6070				-2.0470		0.8110	H		0	0						
-1.0290				-2.5490		2.3890	H		0	0						
-2.3480				-4.4610		1.6290	H		0	0						
-1.6870				-4.3300		0.0180	H		0	0						

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8	9	1	0
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10	11	1	0
12	13	1	0
13	9	1	0
11	14	2	0
13	15	2	0
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M END

> <Name>

Compound114

> <Activ>

2.9

> <DB_Ref_id>

9.23

\$\$\$\$

Compound115

SciTegic10081411483D

47	49	0	0	1	0	999	v2000				
	0.1310			2.5410		-3.5210	C	0	0		
	-0.7020			2.0460		-4.5400	C	0	0		
	-1.6950			1.1010		-4.2290	C	0	0		
	-1.8560			0.6520		-2.9070	C	0	0		
	-1.0210			1.1480		-1.8900	C	0	0		
	-0.0270			2.0940		-2.1980	C	0	0		
	-1.1900			0.6750		-0.4910	C	0	0		
	-0.4480			-0.6400		-0.2490	C	0	0		
	-0.4400			-1.0520		1.2300	C	0	0	3	0 0 0
	-0.4900			-2.4810		1.3130	O	0	0		
	-1.6350			-0.4520		1.9940	C	0	0		
	-2.9510			-1.0200		1.5220	C	0	0		
	-2.9030			-2.2930		0.7100	C	0	0		
	-1.6480			-3.0900		0.9990	C	0	0		
	-4.0010			-0.4790		1.7850	O	0	0		
	-1.7210			-4.2960		0.9510	O	0	0		
	-0.5530			2.4660		-5.7800	O	0	0		
	0.8780			-0.6050		1.8660	C	0	0		
	2.0480			-1.4910		1.4020	C	0	0		
	3.3890			-1.0320		1.9920	C	0	0		
	3.6600			0.4490		1.6910	C	0	0		
	2.5020			1.3380		2.1650	C	0	0		
	1.1600			0.8790		1.5740	C	0	0		
	0.8960			3.2680		-3.7530	H	0	0		
	-2.3390			0.7160		-5.0070	H	0	0		
	-2.6220			-0.0750		-2.6770	H	0	0		
	0.6170			2.4800		-1.4210	H	0	0		
	-2.2520			0.5640		-0.2710	H	0	0		
	-0.8440			1.4450		0.1970	H	0	0		
	0.5680			-0.5870		-0.6400	H	0	0		
	-0.8620			-1.4360		-0.8690	H	0	0		
	-1.5340			-0.6570		3.0600	H	0	0		
	-1.6470			0.6340		1.8850	H	0	0		
	-3.7830			-2.8980		0.9310	H	0	0		
	-2.9410			-2.0490		-0.3520	H	0	0		
	-1.1320			2.1180		-6.4700	H	0	0		
	0.7780			-0.7210		2.9460	H	0	0		
	1.8620			-2.5290		1.6800	H	0	0		
	2.1100			-1.4690		0.3130	H	0	0		
	4.1980			-1.6450		1.5940	H	0	0		
	3.3850			-1.1890		3.0710	H	0	0		
	4.5900			0.7630		2.1640	H	0	0		
	3.7990			0.5800		0.6170	H	0	0		
	2.4470			1.3140		3.2540	H	0	0		
	2.6920			2.3750		1.8880	H	0	0		
	0.3550			1.4980		1.9730	H	0	0		
	1.1710			1.0420		0.4950	H	0	0		
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> <Activ>
52

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9.2

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Compound116
SciTegic10081411483D

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3.8090 -0.2500 -4.0960 C 0 0
4.3690 -1.4650 -4.5230 C 0 0
3.6370 -2.6640 -4.4020 C 0 0
2.3440 -2.6370 -3.8500 C 0 0
2.5160 -0.2270 -3.5450 C 0 0
0.4160 -1.3950 -2.8360 C 0 0
0.4450 -1.6460 -1.3280 C 0 0
-0.9350 -1.4920 -0.6760 C 0 0 3 0 0 0
-1.5680 -0.3120 -1.1850 O 0 0

```

-0.8590	-1.4390	0.8610	C	0	0
-0.2070	-0.1580	1.3220	C	0	0
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1.7830	-1.4200	-3.4200	C	0	0
-1.7420	-2.7110	-1.1010	C	0	0
-3.1760	-2.6640	-0.5840	C	0	0
-3.6350	-4.0920	-0.8480	C	0	0
-2.4300	-4.9470	-0.4630	C	0	0
-1.2260	-4.0020	-0.4730	C	0	0
4.3070	-4.1560	-4.9220	C1	0	0
5.9630	-1.4610	-5.1930	S	0	0
6.5960	0.2130	-5.1930	C	0	0
0.2600	2.2460	0.9730	C	0	0
-0.5370	2.8480	2.1100	C	0	0
-0.0410	3.1950	3.3280	N	0	0
-1.8940	3.1390	2.0820	N	0	0
-1.0370	3.6880	4.0550	N	0	0
-2.1640	3.6620	3.3170	C	0	0
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-1.1720	4.2150	5.3830	C	0	0
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-4.8730	5.0820	5.4850	C	0	0
5.8830	-1.9320	-6.5640	O	0	0
6.8150	-2.2830	-4.3530	O	0	0
4.3690	0.6680	-4.1910	H	0	0
1.7720	-3.5490	-3.7500	H	0	0
2.0920	0.7110	-3.2190	H	0	0
-0.0550	-0.4370	-3.0570	H	0	0
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0.8650	-2.6290	-1.1110	H	0	0
1.1760	-1.0000	-0.8440	H	0	0
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-0.3030	-2.2950	1.2480	H	0	0
0.8950	0.7150	2.7330	H	0	0
-1.7420	-2.7970	-2.1800	H	0	0
-3.7810	-1.9360	-1.1030	H	0	0
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-3.8610	-4.2190	-1.8960	H	0	0
-2.5570	-5.3750	0.5220	H	0	0
-2.3030	-5.7660	-1.1560	H	0	0
-0.8960	-3.8240	0.5410	H	0	0
-0.3910	-4.4120	-1.0190	H	0	0
7.6040	0.3110	-5.6000	H	0	0
6.6100	0.5960	-4.1740	H	0	0
5.9360	0.8520	-5.7810	H	0	0
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0.2700	2.9380	0.1310	H	0	0
-2.4610	5.0470	6.8360	H	0	0
0.8200	3.5650	6.0000	H	0	0
-0.2420	4.0780	7.3070	H	0	0
0.4810	5.2750	6.2370	H	0	0
-5.5000	5.4260	4.6620	H	0	0
-5.3610	4.2930	6.0570	H	0	0
-4.7070	5.9280	6.1530	H	0	0

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10.19

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Compound117

SciTegic10081411483D

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-3.5440 3.6450 -1.9480 C 0 0
-4.8570 3.3190 -2.3320 C 0 0
-5.3780 2.0430 -2.0260 C 0 0
-4.5800 1.1050 -1.3430 C 0 0
-2.7510 2.7080 -1.2660 C 0 0
-2.4280 0.4450 -0.2440 C 0 0
-1.4970 -0.3030 -1.1990 C 0 0
-0.8210 -1.5130 -0.5410 C 0 0 3 0 0 0
-0.8960 -1.3790 0.8850 O 0 0
0.6430 -1.6870 -0.9880 C 0 0
1.5060 -0.5760 -0.4410 C 0 0
1.1580 -0.0370 0.7450 C 0 0
-0.0330 -0.5310 1.4750 C 0 0
2.5700 -0.1450 -1.1160 O 0 0
-0.2000 -0.1560 2.6130 O 0 0
-3.2680 1.4370 -0.9640 C 0 0
-1.6290 -2.7320 -0.9660 C 0 0
-3.0610 -2.6850 -0.4470 C 0 0
-3.5210 -4.1130 -0.7120 C 0 0
-2.3160 -4.9690 -0.3260 C 0 0
-1.1130 -4.0240 -0.3370 C 0 0
-6.9800 1.6160 -2.4780 Cl 0 0
-5.5850 4.2130 -2.9740 O 0 0
-4.9970 5.4750 -3.2540 C 0 0
1.9900 1.0740 1.3370 C 0 0
3.2670 0.4980 1.9090 C 0 0
4.5270 0.7790 1.4770 N 0 0
3.3490 -0.4040 2.9600 N 0 0
5.3830 0.0880 2.2190 N 0 0
4.6870 -0.6320 3.1210 C 0 0
5.2510 -1.5500 4.1570 N 0 0
6.5450 -1.6220 4.1380 C 0 0
7.3890 -0.8670 3.1790 C 0 0
6.8100 -0.0550 2.2710 C 0 0
7.6600 0.7170 1.2930 C 0 0

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7.2230	-2.5180	5.1390	C	0	0
-6.0020	6.3510	-4.0030	C	0	0
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-4.9710	0.1250	-1.1060	H	0	0
-1.7430	2.9700	-0.9770	H	0	0
-3.0700	-0.2530	0.2930	H	0	0
-1.8560	0.9490	0.5350	H	0	0
-0.7530	0.3730	-1.6200	H	0	0
-2.0310	-0.6040	-2.1010	H	0	0
1.0350	-2.6410	-0.6320	H	0	0
0.7130	-1.7050	-2.0760	H	0	0
3.0850	0.5940	-0.7650	H	0	0
-1.6280	-2.8170	-2.0440	H	0	0
-3.6670	-1.9570	-0.9680	H	0	0
-3.0900	-2.4590	0.6100	H	0	0
-4.4070	-4.3690	-0.1500	H	0	0
-3.7480	-4.2400	-1.7610	H	0	0
-2.4430	-5.3970	0.6580	H	0	0
-2.1880	-5.7870	-1.0210	H	0	0
-0.7820	-3.8450	0.6770	H	0	0
-0.2770	-4.4340	-0.8850	H	0	0
-4.7120	5.9360	-2.3080	H	0	0
-4.1050	5.3090	-3.8580	H	0	0
1.4310	1.5730	2.1280	H	0	0
2.2340	1.8050	0.5670	H	0	0
8.4640	-0.9690	3.2120	H	0	0
7.1140	1.0490	0.4100	H	0	0
8.4930	0.0990	0.9570	H	0	0
8.0750	1.6000	1.7790	H	0	0
6.6010	-2.7540	6.0030	H	0	0
8.1330	-2.0430	5.5040	H	0	0
7.5050	-3.4580	4.6650	H	0	0
-5.5730	7.3290	-4.2200	H	0	0
-6.3030	5.8780	-4.9380	H	0	0
-6.8990	6.5060	-3.4030	H	0	0
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10.18

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Compound118

SciTegic10081411483D

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-4.8160				3.4640		-2.5830	C	0	0		
-5.3880				2.2960		-2.0400	C	0	0		
-4.5880				1.3860		-1.3270	C	0	0		
-2.6430				2.8040		-1.6930	C	0	0		
-2.3710				0.6770		-0.3980	C	0	0		
-1.4210				-0.0840		-1.3230	C	0	0		
-0.7650				-1.2900		-0.6370	C	0	0	3	0 0 0
-0.8660				-1.1380		0.7850	O	0	0		
0.7050				-1.4800		-1.0550	C	0	0		
1.5660				-0.3670		-0.5050	C	0	0		
1.1990				0.1890		0.6670	C	0	0		
-0.0100				-0.2880		1.3800	C	0	0		
2.6450				0.0490		-1.1650	O	0	0		
-0.1950				0.1020		2.5100	O	0	0		
-3.2160				1.6400		-1.1530	C	0	0		
-1.5730				-2.5090		-1.0630	C	0	0		
-3.0060				-2.4620		-0.5440	C	0	0		
-3.4650				-3.8900		-0.8080	C	0	0		
-2.2600				-4.7460		-0.4230	C	0	0		
-1.0580				-3.8010		-0.4330	C	0	0		
-6.8380				2.0180		-2.2180	C	0	0		
-5.5570				4.3240		-3.2530	O	0	0		
-4.9610				5.5500		-3.6510	C	0	0		
2.0270				1.3020		1.2610	C	0	0		
3.2880				0.7240		1.8670	C	0	0		
4.5590				1.0930		1.5530	N	0	0		
3.3390				-0.2690		2.8350	N	0	0		
5.3940				0.3690		2.2880	N	0	0		
4.6720				-0.4590		3.0690	C	0	0		
5.2070				-1.4480		4.0530	N	0	0		
6.5000				-1.4680		4.1200	C	0	0		
7.3720				-0.5930		3.2970	C	0	0		
6.8200				0.2780		2.4280	C	0	0		
7.6970				1.1710		1.5880	C	0	0		
7.1500				-2.4270		5.0810	C	0	0		
-3.0000				4.6070		-2.8200	H	0	0		
-5.0280				0.4910		-0.9110	H	0	0		
-1.5900				3.0050		-1.5630	H	0	0		
-3.0100				-0.0150		0.1510	H	0	0		
-1.8140				1.2090		0.3730	H	0	0		
-0.6640				0.5840		-1.7330	H	0	0		
-1.9350				-0.3920		-2.2340	H	0	0		
1.0840				-2.4310		-0.6790	H	0	0		
0.7950				-1.5110		-2.1410	H	0	0		
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-1.5730				-2.5940		-2.1410	H	0	0		
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-3.0340				-2.2360		0.5140	H	0	0		
-4.3510				-4.1460		-0.2470	H	0	0		
-3.6920				-4.0170		-1.8580	H	0	0		
-2.3880				-5.1740							

-4.5280	6.0210	-2.7680	H	0	0
-4.1480	5.3260	-4.3410	H	0	0
1.4550	1.8160	2.0340	H	0	0
2.2920	2.0200	0.4860	H	0	0
8.4460	-0.6560	3.3970	H	0	0
7.2170	1.5160	0.6720	H	0	0
8.6070	0.6400	1.3080	H	0	0
7.9890	2.0500	2.1630	H	0	0
6.5000	-2.7240	5.9040	H	0	0
8.0440	-1.9750	5.5080	H	0	0
7.4530	-3.3320	4.5530	H	0	0
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Compound118

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10.17

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Compound119

SciTegic10081411483D

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-5.6560	2.2910	-2.2400	C	0	0						
-4.8490	1.3530	-1.5710	C	0	0						
-3.1000	3.0290	-1.3320	C	0	0						
-2.7170	0.7310	-0.4100	C	0	0						
-1.7920	-0.0070	-1.3780	C	0	0						
-1.1050	-1.2180	-0.7330	C	0	0	3	0	0	0		
-1.1670	-1.0940	0.6930	O	0	0						
0.3550	-1.3850	-1.1960	C	0	0						
1.2200	-0.2740	-0.6500	C	0	0						
0.8820	0.2560	0.5420	C	0	0						
-0.3020	-0.2460	1.2810	C	0	0						
2.2760	0.1650	-1.3320	O	0	0						
-0.4590	0.1200	2.4220	O	0	0						
-3.5700	1.7220	-1.1170	C	0	0						
-1.9130	-2.4370	-1.1590	C	0	0						
-3.3450	-2.3900	-0.6400	C	0	0						
-3.8050	-3.8180	-0.9050	C	0	0						
-2.6000	-4.6740	-0.5190	C	0	0						
-1.3970	-3.7290	-0.5300	C	0	0						
-6.8650	1.9340	-2.6670	F	0	0						

-5.9380	4.4840	-3.0820	O	0	0
-5.4520	5.8140	-3.1920	C	0	0
1.7150	1.3660	1.1340	C	0	0
3.0030	0.7920	1.6830	C	0	0
4.2540	1.0730	1.2290	N	0	0
3.1040	-0.1090	2.7340	N	0	0
5.1240	0.3840	1.9570	N	0	0
4.4450	-0.3360	2.8710	C	0	0
5.0280	-1.2530	3.8970	N	0	0
6.3210	-1.3230	3.8550	C	0	0
7.1480	-0.5680	2.8820	C	0	0
6.5520	0.2430	1.9830	C	0	0
7.3840	1.0150	0.9900	C	0	0
7.0180	-2.2180	4.8460	C	0	0
-3.5400	4.9680	-2.1620	H	0	0
-5.2120	0.3490	-1.4060	H	0	0
-2.1180	3.3180	-0.9850	H	0	0
-3.3500	0.0260	0.1300	H	0	0
-2.1410	1.2350	0.3660	H	0	0
-1.0530	0.6750	-1.8000	H	0	0
-2.3320	-0.3040	-2.2770	H	0	0
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0.4140	-1.3960	-2.2850	H	0	0
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-1.9120	-2.5230	-2.2370	H	0	0
-3.9510	-1.6620	-1.1600	H	0	0
-3.3740	-2.1640	0.4170	H	0	0
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-4.0320	-3.9450	-1.9540	H	0	0
-2.7280	-5.1020	0.4650	H	0	0
-2.4720	-5.4920	-1.2140	H	0	0
-1.0660	-3.5500	0.4840	H	0	0
-0.5610	-4.1400	-1.0780	H	0	0
-6.1820	6.3980	-3.7530	H	0	0
-5.2130	6.1730	-2.1910	H	0	0
-4.5270	5.7930	-3.7690	H	0	0
1.1640	1.8550	1.9370	H	0	0
1.9450	2.1050	0.3670	H	0	0
8.2240	-0.6690	2.8960	H	0	0
6.8270	1.3290	0.1070	H	0	0
8.2220	0.4040	0.6550	H	0	0
7.7910	1.9090	1.4630	H	0	0
6.4070	-2.4640	5.7140	H	0	0
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10.16
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Compound120

SciTegic10081411483D

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-5.1990				3.6770		-2.2970	C	0	0		
-5.7340				2.4750		-1.7850	C	0	0		
-4.8850				1.5350		-1.1700	C	0	0		
-2.9750				2.9890		-1.5700	C	0	0		
-2.6140				0.7970		-0.4140	C	0	0		
-1.7800				0.0330		-1.4440	C	0	0		
-1.0650				-1.1830		-0.8410	C	0	0	3	0 0 0
-1.0880				-1.0860		0.5890	O	0	0		
0.3830				-1.3270		-1.3470	C	0	0		
1.2520				-0.2180		-0.8050	C	0	0		
0.9430				0.2870		0.4060	C	0	0		
-0.2150				-0.2400		1.1670	C	0	0		
2.2850				0.2440		-1.5080	O	0	0		
-0.3430				0.1030		2.3200	O	0	0		
-3.5070				1.7910		-1.0630	C	0	0		
-1.8730				-2.4020		-1.2670	C	0	0		
-3.3050				-2.3550		-0.7480	C	0	0		
-3.7650				-3.7830		-1.0130	C	0	0		
-2.5590				-4.6390		-0.6270	C	0	0		
-1.3570				-3.6940		-0.6380	C	0	0		
-7.4150				2.1410		-1.9030	C1	0	0		
-5.9750				4.5710		-2.8790	O	0	0		
-5.4210				5.8460		-3.1690	C	0	0		
1.7820				1.3940		0.9950	C	0	0		
3.0180				0.8030		1.6380	C	0	0		
4.2700				0.8140		1.1070	N	0	0		
3.0620				0.1600		2.8670	N	0	0		
5.0860				0.2050		1.9580	N	0	0		
4.3710				-0.1960		3.0270	C	0	0		
4.8910				-0.9210		4.2270	N	0	0		
6.1630				-1.1610		4.1780	C	0	0		
7.0260				-0.7580		3.0400	C	0	0		
6.4880				-0.1050		1.9890	C	0	0		
7.3560				0.3090		0.8280	C	0	0		
6.7950				-1.8870		5.3350	C	0	0		
-3.4060				4.8470		-2.5720	H	0	0		
-5.2860				0.6110		-0.7760	H	0	0		
-1.9170				3.1930		-1.4900	H	0	0		
-3.2100				0.1100		0.1860	H	0	0		
-1.9690				1.3020		0.3050	H	0	0		
-1.0670				0.6970		-1.9320	H	0	0		
-2.3960				-0.2640		-2.2930	H	0	0		
0.8000				-2.2840		-1.0290	H	0	0		
0.4120				-1.3170		-2.4370	H	0	0		
2.9170				0.8390		-1.0840	H	0	0		
-1.8720				-2.4880		-2.3450	H	0	0		
-3.9110				-1.6270		-1.2680	H	0	0		
-3.3340				-2.1290		0.3100	H	0	0		
-4.6510				-4.0400		-0.4510	H	0	0		
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-2.6870				-5.068							

-2.4320	-5.4570	-1.3220	H	0	0
-1.0260	-3.5150	0.3760	H	0	0
-0.5210	-4.1050	-1.1850	H	0	0
-6.2000	6.4630	-3.6170	H	0	0
-4.9620	6.2340	-2.2600	H	0	0
-4.6320	5.7150	-3.9100	H	0	0
1.2060	1.9360	1.7450	H	0	0
2.0780	2.0910	0.2110	H	0	0
8.0810	-0.9880	3.0570	H	0	0
6.8120	0.4010	-0.1120	H	0	0
8.1520	-0.4210	0.6820	H	0	0
7.8210	1.2720	1.0390	H	0	0
6.2600	-1.7550	6.2760	H	0	0
7.8160	-1.5330	5.4800	H	0	0
6.8390	-2.9550	5.1230	H	0	0
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0.02

> <DB_Ref_id>

10.06

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Compound121

SciTegic10081411483D

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65 69 0 0 1 0          999 V2000
  5.8650   -0.0020   -1.8850 C   0  0
  6.1990   -1.3570   -1.7110 C   0  0
  5.2250   -2.2620   -1.2360 C   0  0
  3.9280   -1.8010   -0.9370 C   0  0
  4.5700    0.4530   -1.5880 C   0  0
  2.2310    0.0370   -0.7970 C   0  0
  1.2720   -0.1890   -1.9650 C   0  0
 -0.0680    0.5350   -1.7750 C   0  0  3  0  0  0
 -0.2340    0.8710   -0.3930 O   0  0
 -1.2640   -0.3010   -2.2640 C   0  0
 -1.4750   -1.4980   -1.3690 C   0  0
 -1.1500   -1.3970   -0.0640 C   0  0
 -0.6040   -0.1150    0.4450 C   0  0
 -1.9670   -2.6330   -1.8590 O   0  0
 -0.5060    0.0120    1.6450 O   0  0
  3.6000   -0.4450   -1.1130 C   0  0
  0.0250    1.8200   -2.5920 C   0  0
  1.1270    2.7400   -2.0760 C   0  0
  0.7190    4.0700   -2.6950 C   0  0
 -0.7700    4.1190   -2.3770 C   0  0
 -1.2460    2.6700   -2.5020 C   0  0

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5.6000	-3.9240	-1.0160	Cl	0	0
7.4220	-1.7640	-1.9940	O	0	0
8.2950	-0.8520	-2.6410	C	0	0
-1.3750	-2.7070	0.9820	S	0	0
-2.5060	-2.1110	2.0840	C	0	0
-2.7640	-2.6970	3.2770	N	0	0
-3.2620	-0.9820	1.8630	N	0	0
-3.6990	-1.9360	3.8400	N	0	0
-4.0080	-0.9060	3.0080	C	0	0
-5.0080	0.1740	3.2640	N	0	0
-5.6090	0.0680	4.4060	C	0	0
-5.3360	-1.0230	5.3730	C	0	0
-4.4200	-1.9690	5.0800	C	0	0
-4.1390	-3.0780	6.0610	C	0	0
-6.6390	1.1070	4.7680	C	0	0
6.6060	0.6930	-2.2500	H	0	0
3.1740	-2.4860	-0.5740	H	0	0
4.3260	1.4980	-1.7250	H	0	0
2.2700	1.0940	-0.5290	H	0	0
1.8690	-0.4630	0.1020	H	0	0
1.1170	-1.2540	-2.1370	H	0	0
1.7340	0.1040	-2.9060	H	0	0
-2.1740	0.3010	-2.2660	H	0	0
-1.1040	-0.6350	-3.2890	H	0	0
-2.1950	-2.6840	-2.7970	H	0	0
0.2210	1.5760	-3.6270	H	0	0
2.1090	2.4220	-2.3930	H	0	0
1.1210	2.8030	-0.9960	H	0	0
0.8850	4.0610	-3.7640	H	0	0
1.2580	4.9060	-2.2750	H	0	0
-1.3050	4.7850	-3.0390	H	0	0
-0.9220	4.4730	-1.3670	H	0	0
-1.8520	2.4060	-1.6460	H	0	0
-1.8570	2.5310	-3.3810	H	0	0
9.2460	-1.3550	-2.8160	H	0	0
7.7870	-0.4590	-3.5210	H	0	0
8.4810	-0.0180	-1.9630	H	0	0
-5.8730	-1.0570	6.3110	H	0	0
-3.7290	-3.9750	5.5960	H	0	0
-5.0570	-3.3590	6.5760	H	0	0
-3.4260	-2.7360	6.8130	H	0	0
-6.5040	2.0530	4.2440	H	0	0
-6.6000	1.3110	5.8380	H	0	0
-7.6370	0.7360	4.5330	H	0	0
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10.05

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Compound122

SciTegic10081411483D

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-1.1700	0.1520	-0.0140	C	0	0		
-2.5310	0.5530	-0.0700	C	0	0		
-3.6250	-0.4670	-0.1700	C	0	0		
-3.2790	-1.8200	-0.2030	N	0	0		
-1.9510	-2.2540	-0.1480	C	0	0		
0.4880	-1.6450	0.0020	C	0	0		
1.5250	-0.6890	0.0900	C	0	0		
1.2400	0.6990	0.1290	C	0	0		
-0.1250	1.1290	0.0780	C	0	0		
-0.4810	2.5080	0.1170	C	0	0		
-2.8580	1.9300	-0.0290	C	0	0		
-1.8360	2.9020	0.0640	C	0	0		
-4.2870	-2.7660	-0.2950	C	0	0		
-5.3930	-2.7030	0.5760	C	0	0		
-6.4180	-3.6660	0.4840	C	0	0		
-6.3340	-4.6890	-0.4790	C	0	0		
-5.2310	-4.7480	-1.3480	C	0	0		
-4.2070	-3.7910	-1.2560	C	0	0		
3.5610	1.1070	0.7830	C	0	0		
4.1990	2.2110	1.6500	C	0	0		
-1.7380	-3.4490	-0.1800	O	0	0		
-4.8030	-0.1760	-0.2230	O	0	0		
4.7320	3.3850	0.8130	C	0	0		
-7.8970	-3.5840	1.6480	Br	0	0		
5.6950	2.9100	-0.2850	C	0	0		
5.0630	1.8220	-1.1640	C	0	0		
4.5330	0.6480	-0.3240	C	0	0		
2.2770	1.5570	0.2110	N	0	0		
0.7420	-2.6950	-0.0230	H	0	0		
2.5470	-1.0450	0.1290	H	0	0		
0.2690	3.2830	0.1880	H	0	0		
-3.8890	2.2520	-0.0680	H	0	0		
-2.0940	3.9510	0.0960	H	0	0		
-5.4590	-1.9180	1.3160	H	0	0		
-7.1110	-5.4360	-0.5640	H	0	0		
-5.1680	-5.5330	-2.0880	H	0	0		
-3.3670	-3.8540	-1.9340	H	0	0		
3.3380	0.2520	1.4220	H	0	0		
5.0310	1.7790	2.2110	H	0	0		
3.4940	2.5720	2.3980	H	0	0		
5.2340	4.1060	1.4590	H	0	0		
3.8970	3.9180	0.3540	H	0	0		
6.0040	3.7540	-0.9000	H	0	0		
6.6020	2.5160	0.1780	H	0	0		
5.7930	1.4590	-1.8890	H	0	0		
4.2460	2.2560	-1.7460	H	0	0		
4.0610	-0.0920	-0.9690	H	0	0		
5.3810	0.1450	0.1410	H	0	0		
2.1620	2.4920	-0.1170	H	0	0		
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17	18	1	0
16	17	2	0
15	16	1	0
19	14	1	0
14	15	2	0
20	21	1	0
6	22	2	0
4	23	2	0
21	24	1	0
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26	44	1	0
26	45	1	0
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28	49	1	0
29	50	1	0

M END

> <Name>
Compound122

> <Activ>
0.066

> <DB_Ref_id>
11.16

\$\$\$
Compound123

SciTegic10081411483D

46	49	0	0	0	0	999	V2000
-0.4790	-0.7110	0.1210	C	0	0		
-0.7850	0.6720	0.1580	C	0	0		
-2.1470	1.0700	0.1020	C	0	0		
-3.2400	0.0510	0.0020	C	0	0		
-2.8950	-1.3030	-0.0310	N	0	0		
-1.5660	-1.7360	0.0240	C	0	0		
0.8730	-1.1250	0.1740	C	0	0		
1.9100	-0.1720	0.2620	C	0	0		
1.6250	1.2190	0.3010	C	0	0		
0.2600	1.6490	0.2500	C	0	0		
-0.0960	3.0270	0.2890	C	0	0		
-2.4730	2.4490	0.1430	C	0	0		
-1.4530	3.4200	0.2360	C	0	0		
-3.9020	-2.2460	-0.1230	C	0	0		
-5.0000	-2.1950	0.7600	C	0	0		
-6.0240	-3.1580	0.6680	C	0	0		
-5.9490	-4.1700	-0.3090	C	0	0		
-4.8560	-4.2190	-1.1870	C	0	0		
-3.8320	-3.2600	-1.0960	C	0	0		
2.6620	2.0740	0.3830	N	0	0		
3.9670	1.6040	0.8670	C	0	0		
4.8750	1.2130	-0.2990	C	0	0		
-1.3540	-2.9300	-0.0080	O	0	0		
-4.4180	0.3420	-0.0530	O	0	0		
5.3340	2.4180	-1.1190	C	0	0		
-7.4900	-3.0900	1.8480	Br	0	0		
6.0350	0.3150	0.1330	C	0	0		
1.1270	-2.1760	0.1490	H	0	0		
2.9320	-0.5270	0.2990	H	0	0		
0.6540	3.8030	0.3580	H	0	0		
-3.5040	2.7720	0.1020	H	0	0		
-1.7090	4.4690	0.2680	H	0	0		
-5.0590	-1.4180	1.5080	H	0	0		
-6.7270	-4.9160	-0.3920	H	0	0		
-4.8010	-4.9960	-1.9370	H	0	0		
-2.9980	-3.3160	-1.7830	H	0	0		
2.5430	3.0310	0.1150	H	0	0		
4.4300	2.3850	1.4690	H	0	0		
3.8160	0.7580	1.5390	H	0	0		
4.3870	0.4750	-0.9370	H	0	0		
5.9980	2.1270	-1.9340	H	0	0		
5.8710	3.1290	-0.4920	H	0	0		
4.4810	2.9360	-1.5550	H	0	0		
6.6230	0.0040	-0.7320	H	0	0		
6.6860	0.8360	0.8360	H	0	0		
5.6660	-0.5840	0.6250	H	0	0		
5	6	1	0				
4	5	1	0				
3	4	1	0				
2	3	2	0				
1	2	1	0				
1	6	1	0				
9	10	1	0				
8	9	2	0				
7	8	1	0				
1	7	2	0				
2	10	1	0				
10	11	2	0				

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3 12 1 0
12 13 2 0
11 13 1 0
5 14 1 0
18 19 2 0
17 18 1 0
16 17 2 0
15 16 1 0
19 14 1 0
14 15 2 0
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20 21 1 0
21 22 1 0
6 23 2 0
4 24 2 0
22 25 1 0
16 26 1 0
22 27 1 0
7 28 1 0
8 29 1 0
11 30 1 0
12 31 1 0
13 32 1 0
15 33 1 0
17 34 1 0
18 35 1 0
19 36 1 0
20 37 1 0
21 38 1 0
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22 40 1 0
25 41 1 0
25 42 1 0
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27 45 1 0
27 46 1 0
M END
> <Name>
Compound123

> <Activ>
0.13

> <DB_Ref_id>
11.15

$$$$
Compound124
SciTegic10081411483D

44 47 0 0 0 0 999 V2000
-0.0140 -0.8340 -0.0760 C 0 0
-0.3200 0.5490 -0.0390 C 0 0
-1.6820 0.9470 -0.0940 C 0 0
-2.7750 -0.0720 -0.1950 C 0 0
-2.4300 -1.4260 -0.2290 N 0 0
-1.1020 -1.8590 -0.1720 C 0 0
1.3380 -1.2500 -0.0210 C 0 0
2.3750 -0.2950 0.0660 C 0 0
2.0920 1.0940 0.1040 C 0 0

```


0.7270	1.5230	0.0530	C	0	0
0.3690	2.9040	0.0920	C	0	0
-2.0080	2.3260	-0.0550	C	0	0
-0.9860	3.2970	0.0390	C	0	0
-3.4380	-2.3690	-0.3180	C	0	0
-4.5490	-2.3010	0.5430	C	0	0
-5.5720	-3.2640	0.4510	C	0	0
-5.4850	-4.2930	-0.5040	C	0	0
-4.3750	-4.3590	-1.3650	C	0	0
-3.3520	-3.4020	-1.2730	C	0	0
-0.8890	-3.0530	-0.2050	O	0	0
-3.9510	0.2190	-0.2480	O	0	0
-7.0590	-3.1720	1.6050	Br	0	0
3.1270	1.9510	0.1880	N	0	0
4.1500	1.7700	1.2270	C	0	0
5.4920	1.3690	0.6130	C	0	0
3.2580	3.0740	-0.7520	C	0	0
6.4060	1.1410	1.6620	O	0	0
1.5920	-2.2990	-0.0490	H	0	0
3.3960	-0.6500	0.1040	H	0	0
1.1190	3.6800	0.1620	H	0	0
-3.0370	2.6480	-0.0940	H	0	0
-1.2440	4.3460	0.0720	H	0	0
-4.6190	-1.5100	1.2770	H	0	0
-6.2600	-5.0410	-0.5880	H	0	0
-4.3090	-5.1510	-2.0980	H	0	0
-2.5060	-3.4710	-1.9430	H	0	0
3.8090	1.0140	1.9360	H	0	0
4.2480	2.6930	1.7990	H	0	0
5.8850	2.1720	-0.0120	H	0	0
5.3930	0.4450	0.0430	H	0	0
2.4730	3.0060	-1.5040	H	0	0
3.2460	4.0120	-0.1930	H	0	0
4.2170	3.0040	-1.2640	H	0	0
7.2500	0.8890	1.2560	H	0	0
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4	5	1	0		
3	4	1	0		
2	3	2	0		
1	2	1	0		
1	6	1	0		
9	10	1	0		
8	9	2	0		
7	8	1	0		
1	7	2	0		
2	10	1	0		
10	11	2	0		
3	12	1	0		
12	13	2	0		
11	13	1	0		
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17	18	1	0		
16	17	2	0		
15	16	1	0		
19	14	1	0		
14	15	2	0		
6	20	2	0		
4	21	2	0		
16	22	1	0		
9	23	1	0		

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23 24 1 0
24 25 1 0
23 26 1 0
25 27 1 0
7 28 1 0
8 29 1 0
11 30 1 0
12 31 1 0
13 32 1 0
15 33 1 0
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M END

> <Name>

Compound124

> <Activ>

0.5

> <DB_Ref_id>

11.08

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Compound125

SciTegic10081411483D

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45 47 0 0 1 0          999 V2000
  0.0690    2.7270   -1.7540 C    0  0
  2.4680    3.0250   -2.0990 C    0  0
  1.1980    3.5660   -1.8280 C    0  0
  2.6110    1.6410   -2.2990 C    0  0
  0.2160    1.3350   -1.9520 C    0  0
  1.4880    0.8000   -2.2260 C    0  0
 -0.9560    0.4090   -1.8790 C    0  0
 -1.1490   -0.3180   -0.7380 N    0  0
 -2.2840   -1.2490   -0.6590 C    0  0
 -0.2470   -0.1930    0.4160 C    0  0  1  0  0  0
 -0.9010    0.6130    1.5380 C    0  0
 -1.7230    0.3010   -2.8080 O    0  0
 -1.4660    3.4300   -1.4210 Cl    0  0
  3.8390    4.0510   -2.1870 Cl    0  0
 -2.1040   -2.4270   -1.5910 C    0  0
 -2.8230   -2.6990   -2.7670 C    0  0
 -2.3880   -3.8900   -3.3870 C    0  0
 -1.3460   -4.4970   -2.6690 C    0  0
 -0.9300   -3.6150   -1.2770 S    0  0
 -0.4470   -6.0900   -3.1010 Br    0  0
  0.2430   -1.5370    0.8840 C    0  0
  1.3500   -1.9740    0.2910 O    0  0
 -0.3500   -2.1510    1.7410 O    0  0
  0.0490    0.8730    2.6510 C    0  0
  1.0640    1.8350    2.5010 C    0  0

```

1.8460	1.3640	4.7580	C	0	0
0.8320	0.4020	4.9090	C	0	0
1.9620	2.0800	3.5540	C	0	0
-0.0660	0.1570	3.8560	C	0	0
1.0900	4.6320	-1.6750	H	0	0
3.5790	1.2110	-2.5100	H	0	0
1.6120	-0.2620	-2.3810	H	0	0
-3.2010	-0.7190	-0.9150	H	0	0
-2.3810	-1.6080	0.3660	H	0	0
0.6830	0.2770	0.0950	H	0	0
-1.7800	0.0950	1.9230	H	0	0
-1.2840	1.5610	1.1590	H	0	0
-3.6160	-2.0720	-3.1530	H	0	0
-2.8100	-4.2820	-4.3040	H	0	0
1.7160	-2.8310	0.5470	H	0	0
1.1580	2.3880	1.5780	H	0	0
2.5370	1.5520	5.5670	H	0	0
0.7430	-0.1480	5.8340	H	0	0
2.7410	2.8180	3.4370	H	0	0
-0.8440	-0.5830	3.9790	H	0	0
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4	2	1	0		
3	1	1	0		
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11	36	1	0		
11	37	1	0		
16	38	1	0		
17	39	1	0		

	48	50	0	0	1	0	999	v2000								
	1.	0720			2.	4100	-1.8210	C	0	0						
	3.	4710			2.	7090	-2.1660	C	0	0						
	2.	2010			3.	2500	-1.8950	C	0	0						
	3.	6130			1.	3240	-2.3670	C	0	0						
	1.	2210			1.	0200	-2.0200	C	0	0						
	2.	4920			0.	4850	-2.2930	C	0	0						
	0.	0470			0.	0920	-1.9470	C	0	0						
	0.	0350			-0.	8750	-0.9830	N	0	0						
	1.	1070			-0.	9820	0.0150	C	0	0						
	-1.	0760			-1.	8360	-0.9400	C	0	0	1	0	0	0		
	1.	3300			0.	3070	0.7210	C	0	0						
	0.	2360			1.	0120	1.2580	C	0	0						
	0.	4470			2.	2330	1.9240	C	0	0						
	1.	7480			2.	7460	2.0570	C	0	0						
	2.	8400			2.	0430	1.5210	N	0	3						
	2.	6310			0.	8220	0.8530	C	0	0						
	-2.	3930			-1.	1390	-0.5940	C	0	0						
	-0.	8750			0.	1930	-2.7230	O	0	0						
	-0.	4630			3.	1130	-1.4880	c1	0	0						
	4.	8440			3.	7350	-2.2540	c1	0	0						
	4.	0430			2.	5200	1.6440	O	0	5						
	-1.	1680			-2.	6370	-2.2130	C	0	0						
	-0.	3440			-3.	6780	-2.2850	O	0	0						
	-1.	9430			-2.	3280	-3.0860	O	0	0						
	-2.	7580			-1.	3360	0.8320	C	0	0						
	-2.	7700			-2.	6290	1.3850	C	0	0						
	-3.	4510			-1.	7090	3.5330	C	0	0						
	-3.	4410			-0.	4160	2.9820	C	0	0						
	-3.	1150			-2.	8140	2.7340	C	0	0						
	-3.	0940			-0.	2280	1.6330	C	0	0						
	2.	0940			4.	3150	-1.7420	H	0	0						
	4.	5840			0.	8950	-2.5780	H	0	0						
	2.	6150			-0.	5780	-2.4470	H	0	0						
	0.	8480			-1.	7540	0.7420	H	0	0						
	2.	0290			-1.	2890	-0.4790	H	0	0						
	-0.	8500			-2.	6150	-0.2110	H	0	0						
	-0.	7660			0.	6210	1.1580	H	0	0						
	-0.	3930			2.	7740	2.3360	H	0	0						
	1.	9040			3.	6840	2.5700	H	0	0						
	3.	4730			0.	2830	0.4410	H	0	0						

-3.1990	-1.5000	-1.2310	H	0	0
-2.3300	-0.0700	-0.8110	H	0	0
-0.3540	-4.2320	-3.0760	H	0	0
-2.5140	-3.4840	0.7750	H	0	0
-3.7190	-1.8510	4.5700	H	0	0
-3.6990	0.4360	3.5960	H	0	0
-3.1250	-3.8090	3.1560	H	0	0
-3.0880	0.7680	1.2150	H	0	0

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17	41	1	0
17	42	1	0
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27	45	1	0
28	46	1	0
29	47	1	0
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M	CHG	2	15	1	21	-1
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M	END
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>	<Name>
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49	51	0	0	1	0		999	v2000						
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	2.5240			3.8400	1.0100	C	0	0						
	3.3910			3.4260	-0.0200	C	0	0						
	1.2210			3.3160	1.0800	C	0	0						
	1.6470			1.9650	-0.9040	C	0	0						
	0.7850			2.3830	0.1270	C	0	0						
	1.1470			0.9730	-1.9060	C	0	0						
	0.7850			-0.2710	-1.4710	N	0	0						
	0.1680			-1.2150	-2.4160	C	0	0						
	0.9960			-0.6930	-0.0800	C	0	0	1	0	0	0		
	-1.3090			-1.0430	-2.4750	C	0	0						
	-2.1540			-2.0330	-1.9410	C	0	0						
	-3.5510			-1.8730	-1.9960	C	0	0						
	-4.0940			-0.7190	-2.5880	C	0	0						
	-3.2540			0.2750	-3.1210	C	0	0						
	-1.8590			0.1110	-3.0640	C	0	0						
	-0.3380			-0.8960	0.6410	C	0	0						
	1.0630			1.2580	-3.0760	O	0	0						
	4.0490			2.0080	-2.2170	C1	0	0						
	3.0550			4.9810	2.1740	C1	0	0						
	1.8850			-1.9060	0.0040	C	0	0						
	3.1900			-1.6520	0.0000	O	0	0						
	1.4140			-3.0180	0.0660	O	0	0						
	-0.1620			-0.9360	2.1170	C	0	0						
	-0.1640			0.2600	2.8570	C	0	0						
	0.1700			-1.0080	4.9080	C	0	0						
	0.1720			-2.2030	4.1680	C	0	0						
	0.0020			0.2230	4.2520	C	0	0						
	0.0060			-2.1680	2.7730	C	0	0						
	-5.5220			-0.5530	-2.6450	C	0	0						
	-6.6740			-0.4180	-2.6930	N	0	0						
	4.3930			3.8300	-0.0700	H	0	0						
	0.5450			3.6230	1.8650	H	0	0						
	-0.2190			1.9880	0.1930	H	0	0						
	0.4020			-2.2340	-2.1090	H	0	0						
	0.5920			-1.0590	-3.4080	H	0	0						
	1.6020			0.0550	0.4340	H	0	0						
	-1.7380			-2.9200	-1.4860	H	0	0						
	-4.1890			-2.6410	-1.5840	H	0	0						
	-3.6660			1.1660	-3.5760	H	0	0						
	-1.2170			0.8750	-3.4750	H	0	0						
	-0.8180			-1.8160	0.3090	H	0	0						
	-1.0410			-0.1050	0.3790	H	0	0						
	3.4940			-0.7420	-0.1000	H	0	0						
	-0.2930			1.2110										

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    0.0100    -3.0900    2.2110 H    0    0
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 15 16  2  0
 14 15  1  0
 13 14  2  0
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 16 11  1  0
 11 12  2  0
 10 17  1  0
  7 18  2  0
 10 21  1  0
 17 24  1  0
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  2 20  1  0
 14 30  1  0
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  5  6  1  0
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 27 29  2  0
 28 26  2  0
 25 28  1  0
 24 29  1  0
 26 27  1  0
 24 25  2  0
  8  9  1  0
  8 10  1  0
 30 31  3  0
  3 32  1  0
  4 33  1  0
  6 34  1  0
  9 35  1  0
  9 36  1  0
 10 37  1  0
 12 38  1  0
 13 39  1  0
 15 40  1  0
 16 41  1  0
 17 42  1  0
 17 43  1  0
 22 44  1  0
 25 45  1  0
 26 46  1  0
 27 47  1  0
 28 48  1  0
 29 49  1  0
M  END
> <Name>
Compound127

> <Activ>
8

> <DB_Ref_id>
12.17

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11 12 2 0
10 17 1 0
7 18 2 0
10 21 1 0
17 24 1 0
1 19 1 0
2 20 1 0
15 30 1 0
6 4 2 0
5 6 1 0
21 23 2 0
21 22 1 0
2 3 2 0
1 5 2 0
4 2 1 0
3 1 1 0
5 7 1 0
7 8 1 0
27 29 2 0
28 26 2 0
25 28 1 0
24 29 1 0
26 27 1 0
24 25 2 0
8 9 1 0
8 10 1 0
30 31 3 0
3 32 1 0
4 33 1 0
6 34 1 0
9 35 1 0
9 36 1 0
10 37 1 0
12 38 1 0
13 39 1 0
14 40 1 0
16 41 1 0
17 42 1 0
17 43 1 0
22 44 1 0
25 45 1 0
26 46 1 0
27 47 1 0
28 48 1 0
29 49 1 0
M END
> <Name>
Compound128

> <Activ>
0.8

> <DB_Ref_id>
12.15

$$$$
Compound129
SciTegic10081411483D

50 52 0 0 1 0 999 V2000
0.7420 2.4220 1.7750 C 0 0

```

3.1430	2.7190	1.4300	C	0	0				
1.8710	3.2600	1.7010	C	0	0				
3.2850	1.3360	1.2300	C	0	0				
0.8910	1.0290	1.5780	C	0	0				
2.1620	0.4940	1.3050	C	0	0				
-0.2830	0.1040	1.6500	C	0	0				
-0.7280	-0.4840	0.5000	N	0	0				
-0.0960	-0.2110	-0.7990	C	0	0				
-1.8690	-1.4100	0.5580	C	0	0	1	0	0	0
-0.4980	1.1150	-1.3360	C	0	0				
-1.8050	1.3130	-1.8200	C	0	0				
-2.1860	2.5660	-2.3300	C	0	0				
-1.2620	3.6270	-2.3540	C	0	0				
0.0390	3.4240	-1.8670	C	0	0				
0.4280	2.1740	-1.3580	C	0	0				
-1.4820	-2.7110	1.2640	C	0	0				
-0.8280	-0.1250	2.7050	O	0	0				
-0.7930	3.1230	2.1090	C1	0	0				
4.5140	3.7440	1.3440	C1	0	0				
-3.0800	-0.7600	1.1740	C	0	0				
-3.6760	0.1560	0.4160	O	0	0				
-3.4590	-1.0700	2.2790	O	0	0				
-0.4100	-3.4320	0.5310	C	0	0				
-0.6480	-3.9200	-0.7660	C	0	0				
1.6210	-4.7990	-0.8560	C	0	0				
1.8590	-4.3110	0.4410	C	0	0				
0.3670	-4.6040	-1.4590	C	0	0				
0.8460	-3.6290	1.1350	C	0	0				
0.9550	4.4770	-1.8910	N	0	3				
2.0820	4.2440	-1.4550	O	0	5				
0.5680	5.5310	-2.3380	O	0	0				
1.7640	4.3260	1.8530	H	0	0				
4.2540	0.9060	1.0190	H	0	0				
2.2850	-0.5680	1.1480	H	0	0				
0.9860	-0.2440	-0.6840	H	0	0				
-0.3810	-0.9900	-1.5060	H	0	0				
-2.2210	-1.6090	-0.4530	H	0	0				
-2.5180	0.5020	-1.8050	H	0	0				
-3.1870	2.7150	-2.7010	H	0	0				
-1.5530	4.5920	-2.7440	H	0	0				
1.4320	2.0310	-0.9860	H	0	0				
-2.3500	-3.3610	1.3710	H	0	0				
-1.1560	-2.5140	2.2850	H	0	0				
-4.4590	0.6110	0.7540	H	0	0				
-1.6110	-3.7730	-1.2370	H	0	0				
2.4010	-5.3220	-1.3890	H	0	0				
2.8240	-4.4610	0.9040	H	0	0				
0.1820	-4.9770	-2.4550	H	0	0				
1.0350	-3.2560	2.1310	H	0	0				
15 16	2	0							
14 15	1	0							
13 14	2	0							
12 13	1	0							
16 11	1	0							
11 12	2	0							
10 17	1	0							
7 18	2	0							
10 21	1	0							
17 24	1	0							
1 19	1	0							
2 20	1	0							

```

15 30 1 0
6 4 2 0
5 6 1 0
21 23 2 0
21 22 1 0
2 3 2 0
1 5 2 0
4 2 1 0
3 1 1 0
5 7 1 0
7 8 1 0
27 29 2 0
28 26 2 0
25 28 1 0
24 29 1 0
26 27 1 0
24 25 2 0
8 9 1 0
8 10 1 0
9 11 1 0
30 32 2 0
30 31 1 0
3 33 1 0
4 34 1 0
6 35 1 0
9 36 1 0
9 37 1 0
10 38 1 0
12 39 1 0
13 40 1 0
14 41 1 0
16 42 1 0
17 43 1 0
17 44 1 0
22 45 1 0
25 46 1 0
26 47 1 0
27 48 1 0
28 49 1 0
29 50 1 0
M CHG 2 30 1 31 -1
M END
> <Name>
Compound129

> <Activ>
0.7

> <DB_Ref_id>
12.14

$$$$
Compound130
SciTegic10081411483D

51 53 0 0 1 0 999 V2000
0.3820 3.1900 -1.1960 C 0 0
2.7810 3.4880 -1.5410 C 0 0
1.5110 4.0290 -1.2700 C 0 0
2.9240 2.1040 -1.7410 C 0 0
0.5290 1.7980 -1.3940 C 0 0

```

1.8010	1.2630	-1.6680	C	0	0				
-0.6430	0.8710	-1.3210	C	0	0				
-0.7850	0.0780	-0.2180	N	0	0				
-1.8850	-0.8960	-0.1670	C	0	0				
0.1370	0.1730	0.9230	C	0	0	1	0	0	0
-1.7900	-1.8880	-1.2700	C	0	0				
-0.8570	-2.9370	-1.1940	C	0	0				
-0.7670	-3.8750	-2.2370	C	0	0				
-1.6090	-3.7650	-3.3560	C	0	0				
-2.5430	-2.7160	-3.4340	C	0	0				
-2.6330	-1.7780	-2.3900	C	0	0				
-0.5700	0.7450	2.1520	C	0	0				
-1.4530	0.8210	-2.2170	O	0	0				
-1.1530	3.8920	-0.8630	Cl	0	0				
4.1520	4.5130	-1.6290	Cl	0	0				
0.8050	-1.1460	1.2070	C	0	0				
1.9260	-1.3700	0.5280	O	0	0				
0.3310	-1.9250	2.0000	O	0	0				
0.3790	0.9640	3.2760	C	0	0				
1.3120	2.0140	3.2150	C	0	0				
2.1730	1.3780	5.4020	C	0	0				
1.2400	0.3280	5.4630	C	0	0				
2.2090	2.2200	4.2780	C	0	0				
0.3430	0.1210	4.4010	C	0	0				
-3.4340	-2.6010	-4.6180	C	0	0				
-3.1640	-3.6200	-5.4950	F	0	0				
-3.2180	-1.3960	-5.2370	F	0	0				
-4.7420	-2.6790	-4.2150	F	0	0				
1.4030	5.0940	-1.1170	H	0	0				
3.8930	1.6740	-1.9520	H	0	0				
1.9250	0.2010	-1.8230	H	0	0				
-2.8360	-0.3670	-0.2340	H	0	0				
-1.8600	-1.4150	0.7920	H	0	0				
0.9890	0.7920	0.6440	H	0	0				
-0.2060	-3.0270	-0.3360	H	0	0				
-0.0490	-4.6800	-2.1780	H	0	0				
-1.5350	-4.4890	-4.1550	H	0	0				
-3.3510	-0.9720	-2.4490	H	0	0				
-1.3730	0.0850	2.4780	H	0	0				
-1.0660	1.6840	1.9080	H	0	0				
2.4040	-2.1980	0.6650	H	0	0				
1.3450	2.6650	2.3540	H	0	0				
2.8620	1.5360	6.2180	H	0	0				
1.2120	-0.3200	6.3270	H	0	0				
2.9260	3.0270	4.2300	H	0	0				
-0.3710	-0.6880	4.4540	H	0	0				
14	15	2	0						
13	14	1	0						
12	13	2	0						
16	11	2	0						
11	12	1	0						
10	17	1	0						
7	18	2	0						
10	21	1	0						
17	24	1	0						
1	19	1	0						
2	20	1	0						
15	30	1	0						
6	4	2	0						
5	6	1	0						
21	23	2	0						

```

21 22 1 0
 2 3 2 0
 1 5 2 0
 4 2 1 0
 3 1 1 0
 5 7 1 0
 7 8 1 0
27 29 2 0
28 26 2 0
25 28 1 0
24 29 1 0
26 27 1 0
24 25 2 0
 8 9 1 0
 8 10 1 0
 9 11 1 0
15 16 1 0
30 33 1 0
30 32 1 0
30 31 1 0
 3 34 1 0
 4 35 1 0
 6 36 1 0
 9 37 1 0
 9 38 1 0
10 39 1 0
12 40 1 0
13 41 1 0
14 42 1 0
16 43 1 0
17 44 1 0
17 45 1 0
22 46 1 0
25 47 1 0
26 48 1 0
27 49 1 0
28 50 1 0
29 51 1 0
M END
> <Name>
Compound130

> <Activ>
1.7

> <DB_Ref_id>
12.13

$$$$
Compound131
SciTegic10081411483D

51 53 0 0 1 0          999 V2000
 0.7620 2.1860 1.8280 C 0 0
 3.1600 2.4840 1.4820 C 0 0
 1.8910 3.0250 1.7540 C 0 0
 3.3030 1.1000 1.2830 C 0 0
 0.9080 0.7950 1.6310 C 0 0
 2.1820 0.2600 1.3570 C 0 0
-0.2640 -0.1330 1.7030 C 0 0
-0.7750 -0.6370 0.5410 N 0 0

```

-0.2030	-0.2910	-0.7680	C	0	0				
-1.9260	-1.5510	0.5980	C	0	0	1	0	0	0
-0.5960	1.0780	-1.1900	C	0	0				
-1.9240	1.3460	-1.5670	C	0	0				
-2.2970	2.6390	-1.9670	C	0	0				
-1.3400	3.6700	-1.9920	C	0	0				
-0.0120	3.4060	-1.6150	C	0	0				
0.3610	2.1090	-1.2150	C	0	0				
-1.5120	-2.9220	1.1310	C	0	0				
-0.7540	-0.4320	2.7680	O	0	0				
-0.7730	2.8890	2.1620	Cl	0	0				
4.5310	3.5100	1.3960	Cl	0	0				
0.9980	4.4960	-1.6430	C	0	0				
-3.0700	-0.9530	1.3710	C	0	0				
-3.6780	0.0720	0.7830	O	0	0				
-3.3910	-1.3970	2.4490	O	0	0				
-0.4240	-3.5220	0.3160	C	0	0				
-0.6560	-3.8650	-1.0270	C	0	0				
1.6390	-4.6540	-1.2250	C	0	0				
1.8730	-4.3110	0.1170	C	0	0				
0.3730	-4.4320	-1.7970	C	0	0				
0.8420	-3.7440	0.8890	C	0	0				
1.7830	4.0900	1.9060	H	0	0				
4.2720	0.6700	1.0720	H	0	0				
2.3050	-0.8030	1.2010	H	0	0				
0.8830	-0.3560	-0.7110	H	0	0				
-0.5430	-1.0120	-1.5100	H	0	0				
-2.3610	-1.6410	-0.3990	H	0	0				
-2.6640	0.5570	-1.5490	H	0	0				
-3.3160	2.8440	-2.2560	H	0	0				
-1.6330	4.6640	-2.3010	H	0	0				
1.3810	1.9060	-0.9260	H	0	0				
-2.3650	-3.6000	1.1520	H	0	0				
-1.1910	-2.8500	2.1700	H	0	0				
0.5290	5.4180	-1.9830	H	0	0				
1.4550	4.5920	-0.6580	H	0	0				
1.7870	4.2420	-2.3520	H	0	0				
-4.4200	0.5020	1.2280	H	0	0				
-1.6270	-3.6970	-1.4730	H	0	0				
2.4300	-5.0900	-1.8170	H	0	0				
2.8440	-4.4810	0.5570	H	0	0				
0.1930	-4.6970	-2.8280	H	0	0				
1.0290	-3.4810	1.9200	H	0	0				
8	9	1	0						
8	10	1	0						
9	11	1	0						
15	16	2	0						
14	15	1	0						
13	14	2	0						
12	13	1	0						
16	11	1	0						
11	12	2	0						
10	17	1	0						
7	18	2	0						
10	22	1	0						
17	25	1	0						
1	19	1	0						
2	20	1	0						
15	21	1	0						
6	4	2	0						
5	6	1	0						

```

22 24 2 0
22 23 1 0
2 3 2 0
1 5 2 0
4 2 1 0
3 1 1 0
5 7 1 0
7 8 1 0
28 30 2 0
29 27 2 0
26 29 1 0
25 30 1 0
27 28 1 0
25 26 2 0
3 31 1 0
4 32 1 0
6 33 1 0
9 34 1 0
9 35 1 0
10 36 1 0
12 37 1 0
13 38 1 0
14 39 1 0
16 40 1 0
17 41 1 0
17 42 1 0
21 43 1 0
21 44 1 0
21 45 1 0
23 46 1 0
26 47 1 0
27 48 1 0
28 49 1 0
29 50 1 0
30 51 1 0
M END
> <Name>
Compound131

> <Activ>
1.8

> <DB_Ref_id>
12.12

$$$$
Compound132
SciTegic10081411483D

48 50 0 0 1 0          999 V2000
1.8220 1.3440 2.0680 C 0 0
4.2230 1.6420 1.7230 C 0 0
2.9530 2.1840 1.9940 C 0 0
4.3650 0.2580 1.5210 C 0 0
1.9710 -0.0490 1.8690 C 0 0
3.2420 -0.5820 1.5960 C 0 0
0.7990 -0.9750 1.9430 C 0 0
0.1760 -1.3400 0.7830 N 0 0
-0.9180 -2.3200 0.8280 C 0 0
0.5720 -0.7740 -0.5160 C 0 0 1 0 0 0
-2.2130 -1.6820 1.1800 C 0 0

```

-2.6410	-1.6470	2.5180	C	0	0
-3.8650	-1.0430	2.8500	C	0	0
-4.6640	-0.4730	1.8440	C	0	0
-4.2380	-0.5080	0.5040	C	0	0
-3.0120	-1.1110	0.1720	C	0	0
0.1970	0.7070	-0.6060	C	0	0
0.4040	-1.3970	3.0040	O	0	0
0.2890	2.0470	2.4000	Cl	0	0
5.5940	2.6680	1.6350	Cl	0	0
-4.9940	0.0330	-0.4470	F	0	0
2.0290	-1.0160	-0.8030	C	0	0
2.4300	-2.2780	-0.6720	O	0	0
2.7580	-0.1080	-1.1290	O	0	0
-0.1780	1.0940	-1.9900	C	0	0
0.8140	1.2050	-2.9830	C	0	0
-0.8850	1.8240	-4.6110	C	0	0
-1.8770	1.7130	-3.6210	C	0	0
0.4590	1.5700	-4.2930	C	0	0
-1.5230	1.3480	-2.3110	C	0	0
2.8460	3.2480	2.1460	H	0	0
5.3340	-0.1720	1.3110	H	0	0
3.3670	-1.6450	1.4410	H	0	0
-0.6800	-3.0880	1.5640	H	0	0
-1.0040	-2.8070	-0.1450	H	0	0
0.0960	-1.3400	-1.3150	H	0	0
-2.0310	-2.0840	3.2970	H	0	0
-4.1910	-1.0160	3.8790	H	0	0
-5.6040	-0.0100	2.1040	H	0	0
-2.6860	-1.1370	-0.8570	H	0	0
1.0210	1.3340	-0.2620	H	0	0
-0.6250	0.9370	0.0720	H	0	0
3.3540	-2.5000	-0.8480	H	0	0
1.8500	1.0120	-2.7440	H	0	0
-1.1580	2.1050	-5.6190	H	0	0
-2.9100	1.9080	-3.8670	H	0	0
1.2210	1.6560	-5.0550	H	0	0
-2.2890	1.2640	-1.5530	H	0	0
8	9	1	0		
8	10	1	0		
9	11	1	0		
15	16	2	0		
14	15	1	0		
13	14	2	0		
12	13	1	0		
16	11	1	0		
11	12	2	0		
10	17	1	0		
7	18	2	0		
10	22	1	0		
17	25	1	0		
1	19	1	0		
2	20	1	0		
15	21	1	0		
6	4	2	0		
5	6	1	0		
22	24	2	0		
22	23	1	0		
2	3	2	0		
1	5	2	0		
4	2	1	0		
3	1	1	0		


```

5 7 1 0
7 8 1 0
28 30 2 0
29 27 2 0
26 29 1 0
25 30 1 0
27 28 1 0
25 26 2 0
3 31 1 0
4 32 1 0
6 33 1 0
9 34 1 0
9 35 1 0
10 36 1 0
12 37 1 0
13 38 1 0
14 39 1 0
16 40 1 0
17 41 1 0
17 42 1 0
23 43 1 0
26 44 1 0
27 45 1 0
28 46 1 0
29 47 1 0
30 48 1 0

```

M END

> <Name>

Compound132

> <Activ>

3.2

> <DB_Ref_id>

12.11

\$\$\$\$

Compound133

SciTegic10081411483D

```

48 50 0 0 1 0          999 V2000
  0.2410  2.9070  -1.5520 C  0  0
  2.6400  3.2050  -1.8980 C  0  0
  1.3700  3.7460  -1.6260 C  0  0
  2.7820  1.8210  -2.0970 C  0  0
  0.3880  1.5150  -1.7510 C  0  0
  1.6600  0.9800  -2.0240 C  0  0
 -0.7850  0.5890  -1.6770 C  0  0
 -0.9780 -0.1360  -0.5360 N  0  0
 -2.1050 -1.0770  -0.4610 C  0  0
 -0.0860  0.0010   0.6240 C  0  0  1  0  0  0
 -2.0360 -2.1010  -1.5360 C  0  0
 -1.0740 -3.1250  -1.4710 C  0  0
 -1.0100 -4.0940  -2.4870 C  0  0
 -1.9050 -4.0410  -3.5690 C  0  0
 -2.8670 -3.0150  -3.6370 C  0  0
 -2.9310 -2.0460  -2.6190 C  0  0
 -0.8060  0.6730   1.7940 C  0  0
 -1.5490  0.4790  -2.6070 O  0  0
 -1.2940  3.6090  -1.2190 Cl  0  0
  4.0110  4.2310  -1.9850 Cl  0  0

```

-3.9580	-2.9470	-4.9580	C1	0	0
0.5280	-1.3190	1.0100	C	0	0
1.6480	-1.6320	0.3640	O	0	0
0.0170	-2.0210	1.8490	O	0	0
0.1250	0.9640	2.9150	C	0	0
1.0300	2.0360	2.8190	C	0	0
1.8860	1.5140	5.0380	C	0	0
0.9820	0.4420	5.1340	C	0	0
1.9100	2.3110	3.8800	C	0	0
0.1020	0.1670	4.0740	C	0	0
1.2620	4.8120	-1.4740	H	0	0
3.7510	1.3910	-2.3080	H	0	0
1.7840	-0.0820	-2.1790	H	0	0
-3.0400	-0.5240	-0.5460	H	0	0
-2.0970	-1.5700	0.5110	H	0	0
0.7950	0.5740	0.3330	H	0	0
-0.3830	-3.1720	-0.6420	H	0	0
-0.2710	-4.8800	-2.4360	H	0	0
-1.8450	-4.7930	-4.3420	H	0	0
-3.6680	-1.2550	-2.6640	H	0	0
-1.6240	0.0480	2.1530	H	0	0
-1.2860	1.5960	1.4710	H	0	0
2.0920	-2.4660	0.5650	H	0	0
1.0530	2.6520	1.9320	H	0	0
2.5630	1.7260	5.8530	H	0	0
0.9640	-0.1700	6.0240	H	0	0
2.6040	3.1350	3.8060	H	0	0
-0.5900	-0.6590	4.1550	H	0	0
8	9	1	0		
8	10	1	0		
9	11	1	0		
15	16	2	0		
14	15	1	0		
13	14	2	0		
12	13	1	0		
16	11	1	0		
11	12	2	0		
10	17	1	0		
7	18	2	0		
10	22	1	0		
17	25	1	0		
1	19	1	0		
2	20	1	0		
15	21	1	0		
6	4	2	0		
5	6	1	0		
22	24	2	0		
22	23	1	0		
2	3	2	0		
1	5	2	0		
4	2	1	0		
3	1	1	0		
5	7	1	0		
7	8	1	0		
28	30	2	0		
29	27	2	0		
26	29	1	0		
25	30	1	0		
27	28	1	0		
25	26	2	0		
3	31	1	0		

```

4 32 1 0
6 33 1 0
9 34 1 0
9 35 1 0
10 36 1 0
12 37 1 0
13 38 1 0
14 39 1 0
16 40 1 0
17 41 1 0
17 42 1 0
23 43 1 0
26 44 1 0
27 45 1 0
28 46 1 0
29 47 1 0
30 48 1 0

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M END

> <Name>

Compound133

> <Activ>

1.4

> <DB_Ref_id>

12.1

\$\$\$\$

Compound134

SciTegic10081411483D

```

48 50 0 0 1 0          999 V2000
  0.9140   2.3220   2.3670 C   0 0
  3.3140   2.6210   2.0220 C   0 0
  2.0450   3.1620   2.2930 C   0 0
  3.4570   1.2360   1.8220 C   0 0
  1.0620   0.9320   2.1680 C   0 0
  2.3340   0.3960   1.8970 C   0 0
 -0.1090   0.0040   2.2420 C   0 0
 -0.5290  -0.6150   1.1000 N   0 0
 -1.6640  -1.5510   1.1600 C   0 0
  0.1270  -0.3730  -0.1930 C   0 0 1 0 0 0
 -2.9590  -0.8520   0.9510 C   0 0
 -3.4920  -0.0410   1.9690 C   0 0
 -4.7190   0.6190   1.7740 C   0 0
 -5.4100   0.4710   0.5590 C   0 0
 -4.8770  -0.3400  -0.4590 C   0 0
 -3.6520  -1.0000  -0.2630 C   0 0
  0.9530  -1.5860  -0.6230 C   0 0
 -0.6800  -0.1950   3.2890 O   0 0
 -0.6190   3.0250   2.7010 Cl  0 0
  4.6860   3.6460   1.9360 Cl  0 0
 -0.8630   0.0490  -1.2460 C   0 0
 -1.3810   1.2620  -1.0800 O   0 0
 -1.1470  -0.6860  -2.1640 O   0 0
  1.7600  -1.2930  -1.8380 C   0 0
  2.8240  -0.3750  -1.7730 C   0 0
  3.2870  -0.7400  -4.1350 C   0 0
  2.2230  -1.6580  -4.2010 C   0 0
  3.5860  -0.1000  -2.9220 C   0 0
  1.4610  -1.9360  -3.0530 C   0 0

```

1.9370	4.2270	2.4460	H	0	0
4.4260	0.8070	1.6120	H	0	0
2.4590	-0.6660	1.7400	H	0	0
-1.6700	-2.0450	2.1310	H	0	0
-1.5370	-2.3170	0.3970	H	0	0
0.7540	0.5140	-0.1150	H	0	0
-2.9670	0.0780	2.9050	H	0	0
-5.1270	1.2420	2.5550	H	0	0
-6.3520	0.9760	0.4060	H	0	0
-5.4080	-0.4550	-1.3920	H	0	0
-3.2480	-1.6210	-1.0490	H	0	0
0.3110	-2.4430	-0.8120	H	0	0
1.6130	-1.9060	0.1820	H	0	0
-1.0940	1.8010	-0.3320	H	0	0
3.0610	0.1210	-0.8420	H	0	0
3.8730	-0.5290	-5.0170	H	0	0
1.9920	-2.1510	-5.1350	H	0	0
4.4020	0.6050	-2.8710	H	0	0
0.6450	-2.6410	-3.1110	H	0	0
8	9	1	0		
8	10	1	0		
9	11	1	0		
15	16	2	0		
14	15	1	0		
13	14	2	0		
12	13	1	0		
16	11	1	0		
11	12	2	0		
10	17	1	0		
7	18	2	0		
10	21	1	0		
17	24	1	0		
1	19	1	0		
2	20	1	0		
6	4	2	0		
5	6	1	0		
21	23	2	0		
21	22	1	0		
2	3	2	0		
1	5	2	0		
4	2	1	0		
3	1	1	0		
5	7	1	0		
7	8	1	0		
27	29	2	0		
28	26	2	0		
25	28	1	0		
24	29	1	0		
26	27	1	0		
24	25	2	0		
3	30	1	0		
4	31	1	0		
6	32	1	0		
9	33	1	0		
9	34	1	0		
10	35	1	0		
12	36	1	0		
13	37	1	0		
14	38	1	0		
15	39	1	0		
16	40	1	0		

48	50	0	0	1	0	999	V2000				
1.0840				2.1350		2.1180	C	0	0		
3.4830				2.4330		1.7720	C	0	0		
2.2130				2.9740		2.0440	C	0	0		
3.6260				1.0490		1.5720	C	0	0		
1.2320				0.7430		1.9190	C	0	0		
2.5040				0.2080		1.6460	C	0	0		
0.0590				-0.1840		1.9920	C	0	0		
-0.4570				-0.6840		0.8300	N	0	0		
-1.6270				-1.5710		0.8830	C	0	0		
0.1300				-0.3550		-0.4770	C	0	0	1	0 0 0
-2.8290				-0.8630		1.3960	C	0	0		
-3.2090				-1.0040		2.7420	C	0	0		
-4.3450				-0.3330		3.2280	C	0	0		
-5.1050				0.4810		2.3670	C	0	0		
-4.7240				0.6210		1.0190	C	0	0		
-3.5870				-0.0500		0.5350	C	0	0		
0.6950				-1.6050		-1.1530	C	0	0		
4.8550				3.4580		1.6850	Cl	0	0		
-0.4510				2.8370		2.4500	Cl	0	0		
-0.4270				-0.4880		3.0570	O	0	0		
-6.6280				1.3800		3.0170	Br	0	0		
-0.8470				0.3800		-1.3540	C	0	0		
-1.2530				1.5570		-0.8860	O	0	0		
-1.2170				-0.0910		-2.4040	O	0	0		
1.5050				-1.2600		-2.3510	C	0	0		
2.6760				-0.4920		-2.2120	C	0	0		
3.0380				-0.6070		-4.6170	C	0	0		
1.8680				-1.3750		-4.7560	C	0	0		
3.4410				-0.1660		-3.3450	C	0	0		
1.1020				-1.7010		-3.6240	C	0	0		
2.1060				4.0390		2.1960	H	0	0		
4.5950				0.6190		1.3620	H	0	0		
2.6280				-0.8540		1.4910	H	0	0		
-1.4040				-2.4210		1.5290	H	0	0		
-1.8310				-1.9560		-0.1160	H	0	0		
0.9090				0.3950		-0.3420	H	0	0		
-2.6310				-1.6280		3.4080	H	0	0		
-4.6220				-0.4530		4.2660	H	0	0		

-5.2960	1.2400	0.3430	H	0	0
-3.3000	0.0630	-0.5000	H	0	0
-0.1070	-2.2840	-1.4400	H	0	0
1.3050	-2.1780	-0.4550	H	0	0
-1.8770	2.0820	-1.4040	H	0	0
2.9910	-0.1500	-1.2370	H	0	0
3.6260	-0.3570	-5.4870	H	0	0
1.5580	-1.7130	-5.7340	H	0	0
4.3400	0.4230	-3.2380	H	0	0
0.2040	-2.2910	-3.7380	H	0	0
8	9	1	0		
8	10	1	0		
9	11	1	0		
15	16	2	0		
14	15	1	0		
13	14	2	0		
12	13	1	0		
16	11	1	0		
11	12	2	0		
10	17	1	0		
2	18	1	0		
1	19	1	0		
7	20	2	0		
10	22	1	0		
17	25	1	0		
14	21	1	0		
6	4	2	0		
5	6	1	0		
22	24	2	0		
22	23	1	0		
2	3	2	0		
1	5	2	0		
4	2	1	0		
3	1	1	0		
5	7	1	0		
7	8	1	0		
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29	27	2	0		
26	29	1	0		
25	30	1	0		
27	28	1	0		
25	26	2	0		
3	31	1	0		
4	32	1	0		
6	33	1	0		
9	34	1	0		
9	35	1	0		
10	36	1	0		
12	37	1	0		
13	38	1	0		
15	39	1	0		
16	40	1	0		
17	41	1	0		
17	42	1	0		
23	43	1	0		
26	44	1	0		
27	45	1	0		
28	46	1	0		
29	47	1	0		
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M END

> <Name>
Compound135

> <Activ>
9.1

> <DB_Ref_id>
12.04

\$\$\$\$
Compound136
SciTegic10081411483D

48	50	0	0	1	0	999	V2000				
0.9080	2.3880	2.0750	C	0	0						
3.3070	2.6860	1.7290	C	0	0						
2.0370	3.2270	2.0010	C	0	0						
3.4500	1.3020	1.5300	C	0	0						
1.0550	0.9960	1.8760	C	0	0						
2.3270	0.4610	1.6030	C	0	0						
-0.1180	0.0690	1.9500	C	0	0						
-0.5170	-0.5750	0.8130	N	0	0						
-1.6350	-1.5280	0.8790	C	0	0						
0.1430	-0.3390	-0.4790	C	0	0	1	0	0	0		
-2.8820	-0.8760	1.3570	C	0	0						
-3.5870	-0.0010	0.5120	C	0	0						
-4.7670	0.6140	0.9640	C	0	0						
-5.2440	0.3560	2.2610	C	0	0						
-4.5400	-0.5200	3.1100	C	0	0						
-3.3580	-1.1340	2.6560	C	0	0						
0.9250	-1.5740	-0.9270	C	0	0						
4.6780	3.7110	1.6420	Cl	0	0						
-0.6270	3.0900	2.4070	Cl	0	0						
-0.7040	-0.1100	2.9910	O	0	0						
-5.1770	-0.8680	4.8480	Br	0	0						
-0.8340	0.1320	-1.5220	C	0	0						
-0.9700	1.4520	-1.6150	O	0	0						
-1.4360	-0.6570	-2.2120	O	0	0						
1.7130	-1.3050	-2.1590	C	0	0						
2.8930	-0.5420	-2.0870	C	0	0						
3.2040	-0.7960	-4.4890	C	0	0						
2.0250	-1.5580	-4.5610	C	0	0						
3.6380	-0.2880	-3.2520	C	0	0						
1.2800	-1.8130	-3.3970	C	0	0						
1.9290	4.2930	2.1530	H	0	0						
4.4180	0.8720	1.3190	H	0	0						
2.4510	-0.6010	1.4480	H	0	0						
-1.3710	-2.3440	1.5520	H	0	0						
-1.8030	-1.9520	-0.1100	H	0	0						
0.8020	0.5240	-0.3920	H	0	0						
-3.2270	0.2010	-0.4860	H	0	0						
-5.3070	1.2860	0.3140	H	0	0						
-6.1530	0.8370	2.5920	H	0	0						
-2.8090	-1.8070	3.2990	H	0	0						
0.2530	-2.4140	-1.1020	H	0	0						
1.5930	-1.9150	-0.1360	H	0	0						
-1.5820	1.8190	-2.2660	H	0	0						
3.2310	-0.1490	-1.1400	H	0	0						
3.7760	-0.6000	-5.3840	H	0	0						
1.6920	-1.9480	-5.5110	H	0	0						
4.5430	0.2980	-3.1960	H	0	0						

```

      0.3750   -2.3990   -3.4590 H    0    0
  8  9  1  0
  8 10  1  0
  9 11  1  0
15 16  2  0
14 15  1  0
13 14  2  0
12 13  1  0
16 11  1  0
11 12  2  0
10 17  1  0
  2 18  1  0
  1 19  1  0
  7 20  2  0
10 22  1  0
17 25  1  0
15 21  1  0
  6  4  2  0
  5  6  1  0
22 24  2  0
22 23  1  0
  2  3  2  0
  1  5  2  0
  4  2  1  0
  3  1  1  0
  5  7  1  0
  7  8  1  0
28 30  2  0
29 27  2  0
26 29  1  0
25 30  1  0
27 28  1  0
25 26  2  0
  3 31  1  0
  4 32  1  0
  6 33  1  0
  9 34  1  0
  9 35  1  0
10 36  1  0
12 37  1  0
13 38  1  0
14 39  1  0
16 40  1  0
17 41  1  0
17 42  1  0
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26 44  1  0
27 45  1  0
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29 47  1  0
30 48  1  0
M  END
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Compound136

> <Activ>
3.5

> <DB_Ref_id>
12.03

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Compound137

[illegible]

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2 18 1 0
1 19 1 0
7 20 2 0
10 22 1 0
17 25 1 0
16 21 1 0
6 4 2 0
5 6 1 0
22 24 2 0
22 23 1 0
2 3 2 0
1 5 2 0
4 2 1 0
3 1 1 0
5 7 1 0
7 8 1 0
28 30 2 0
29 27 2 0
26 29 1 0
25 30 1 0
27 28 1 0
25 26 2 0
3 31 1 0
4 32 1 0
6 33 1 0
9 34 1 0
9 35 1 0
10 36 1 0
12 37 1 0
13 38 1 0
14 39 1 0
15 40 1 0
17 41 1 0
17 42 1 0
23 43 1 0
26 44 1 0
27 45 1 0
28 46 1 0
29 47 1 0
30 48 1 0
M END
> <Name>
Compound137

> <Activ>
8

> <DB_Ref_id>
12.02

$$$$
Compound138
SciTegic10081411483D

54 57 0 0 1 0 999 V2000
2.4180 3.3670 2.6580 C 0 0
4.8170 3.6660 2.3130 C 0 0
3.5470 4.2070 2.5840 C 0 0
4.9610 2.2810 2.1130 C 0 0

```

2.5660	1.9750	2.4590	C	0	0				
3.8380	1.4410	2.1880	C	0	0				
1.3930	1.0490	2.5330	C	0	0				
0.5220	1.0100	1.4830	N	0	0				
0.7910	1.8220	0.2890	C	0	0				
-0.6860	0.1700	1.5140	C	0	0	1	0	0	0
0.3950	1.1150	-0.9570	C	0	0				
1.1780	0.0550	-1.4450	C	0	0				
0.8030	-0.6130	-2.6230	C	0	0				
-0.3570	-0.2230	-3.3160	C	0	0				
-1.1410	0.8400	-2.8280	C	0	0				
-0.7660	1.5080	-1.6480	C	0	0				
-0.7540	-0.9260	-4.5570	C	0	0				
-2.1310	-0.5370	-5.4780	S	0	0				
-1.8110	-1.7500	-6.6070	C	0	0				
-0.6450	-2.4380	-6.2560	C	0	0				
-0.0570	-1.9710	-5.1070	N	0	0				
-0.3220	-1.3150	1.4510	C	0	0				
6.1900	4.6910	2.2250	Cl	0	0				
0.8830	4.0700	2.9900	Cl	0	0				
1.2150	0.3480	3.5020	O	0	0				
-1.5570	0.4980	2.6970	C	0	0				
-2.2710	1.6130	2.5820	O	0	0				
-1.5840	-0.2230	3.6680	O	0	0				
-1.5270	-2.1640	1.2640	C	0	0				
-2.0020	-2.9550	2.3260	C	0	0				
-3.8070	-3.7740	0.9120	C	0	0				
-3.3340	-2.9840	-0.1500	C	0	0				
-3.1410	-3.7600	2.1510	C	0	0				
-2.1930	-2.1800	0.0250	C	0	0				
3.4400	5.2710	2.7360	H	0	0				
5.9300	1.8520	1.9020	H	0	0				
3.9610	0.3790	2.0310	H	0	0				
1.8560	2.0590	0.2500	H	0	0				
0.2440	2.7620	0.3630	H	0	0				
-1.3340	0.4430	0.6840	H	0	0				
2.0700	-0.2500	-0.9180	H	0	0				
1.4100	-1.4280	-2.9920	H	0	0				
-2.0330	1.1440	-3.3530	H	0	0				
-1.3710	2.3200	-1.2790	H	0	0				
-2.4260	-1.9530	-7.4710	H	0	0				
-0.2170	-3.2620	-6.8120	H	0	0				
0.2030	-1.6210	2.3540	H	0	0				
0.3850	-1.5040	0.6430	H	0	0				
-2.1870	2.1480	1.7810	H	0	0				
-1.4940	-2.9490	3.2790	H	0	0				
-4.6840	-4.3910	0.7770	H	0	0				
-3.8440	-2.9940	-1.1010	H	0	0				
-3.5060	-4.3650	2.9650	H	0	0				
-1.8340	-1.5740	-0.7950	H	0	0				
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8	10	1	0						
9	11	1	0						
15	16	2	0						
14	15	1	0						
13	14	2	0						
12	13	1	0						
16	11	1	0						
11	12	2	0						
14	17	1	0						
20	21	1	0						

```

19 20 2 0
18 19 1 0
18 17 1 0
21 17 2 0
10 22 1 0
2 23 1 0
1 24 1 0
7 25 2 0
10 26 1 0
22 29 1 0
6 4 2 0
5 6 1 0
26 28 2 0
26 27 1 0
2 3 2 0
1 5 2 0
4 2 1 0
3 1 1 0
5 7 1 0
7 8 1 0
32 34 2 0
33 31 2 0
30 33 1 0
29 34 1 0
31 32 1 0
29 30 2 0
3 35 1 0
4 36 1 0
6 37 1 0
9 38 1 0
9 39 1 0
10 40 1 0
12 41 1 0
13 42 1 0
15 43 1 0
16 44 1 0
19 45 1 0
20 46 1 0
22 47 1 0
22 48 1 0
27 49 1 0
30 50 1 0
31 51 1 0
32 52 1 0
33 53 1 0
34 54 1 0
M END
> <Name>
Compound138

> <Activ>
5.7

> <DB_Ref_id>
12.01

$$$$
Compound139
SciTegic10081411483D

48 50 0 0 1 0          999 V2000

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-0.9540	-0.1980	-0.5370	N	0	0				
-2.0010	-1.2300	-0.5230	C	0	0				
-0.0790	-0.0540	0.6350	C	0	0	1	0	0	0
-0.8820	0.3470	1.8730	C	0	0				
0.0060	0.7610	2.9910	C	0	0				
0.6160	2.0280	2.9720	C	0	0				
1.6850	1.5450	5.1060	C	0	0				
1.0750	0.2790	5.1250	C	0	0				
1.4560	2.4190	4.0300	C	0	0				
0.2360	-0.1130	4.0680	C	0	0				
0.7490	-1.2900	0.8640	C	0	0				
1.8260	-1.4010	0.0910	O	0	0				
0.4320	-2.1060	1.6970	O	0	0				
-0.8170	0.6020	-1.6350	C	0	0				
0.2810	1.6180	-1.6520	C	0	0				
-1.5720	0.4870	-2.5730	O	0	0				
0.0270	2.9850	-1.3930	C	0	0				
1.5920	1.1930	-1.9340	C	0	0				
2.6480	2.1180	-1.9580	C	0	0				
1.0900	3.9080	-1.4170	C	0	0				
-1.8390	-2.1900	-1.6460	C	0	0				
-0.6600	-4.0570	-2.6710	C	0	0				
-0.8120	-3.1500	-1.6090	C	0	0				
-1.5340	-4.0070	-3.7710	C	0	0				
-2.7130	-2.1380	-2.7470	C	0	0				
-2.5620	-3.0470	-3.8110	C	0	0				
-3.7350	-2.9780	-5.2850	Br	0	0				
2.3990	3.4770	-1.6990	C	0	0				
3.6900	4.6050	-1.7280	Cl	0	0				
-1.8680	3.6710	-0.9770	I	0	0				
-2.9780	-0.7510	-0.5920	H	0	0				
-1.9600	-1.7690	0.4240	H	0	0				
0.6910	0.6860	0.4190	H	0	0				
-1.5200	-0.4740	2.2000	H	0	0				
-1.5730	1.1570	1.6380	H	0	0				
0.4440	2.7050	2.1480	H	0	0				
2.3300	1.8460	5.9180	H	0	0				
1.2520	-0.3930	5.9520	H	0	0				
1.9240	3.3920	4.0150	H	0	0				
-0.2300	-1.0880	4.0880	H	0	0				
2.4010	-2.1710	0.1890	H	0	0				
1.7970	0.1510	-2.1340	H	0	0				
3.6480	1.7720	-2.1770	H	0	0				
0.9010	4.9540	-1.2190	H	0	0				
0.1300	-4.7940	-2.6420	H	0	0				
-0.1380	-3.1950	-0.7660	H	0	0				
-1.4030	-4.7130	-4.5790	H	0	0				
-3.4990	-1.3960	-2.7680	H	0	0				
1	2	1	0						
1	3	1	0						
3	4	1	0						
8	10	2	0						
9	7	2	0						
6	9	1	0						
5	10	1	0						
7	8	1	0						
5	6	2	0						
4	5	1	0						
3	11	1	0						
11	12	1	0						
11	13	2	0						

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1 14 1 0
14 15 1 0
14 16 2 0
15 17 2 0
15 18 1 0
18 19 2 0
20 17 1 0
2 21 1 0
26 24 2 0
25 26 1 0
22 23 2 0
24 22 1 0
23 21 1 0
21 25 2 0
26 27 1 0
19 28 1 0
28 20 2 0
28 29 1 0
17 30 1 0
2 31 1 0
2 32 1 0
3 33 1 0
4 34 1 0
4 35 1 0
6 36 1 0
7 37 1 0
8 38 1 0
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10 40 1 0
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24 47 1 0
25 48 1 0
M END
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Compound139

> <Activ>
2.7

> <DB_Ref_id>
13.16

$$$$
Compound140
SciTegic10081411483D

48 50 0 0 1 0 999 V2000
-1.0010 -0.1280 -0.5140 N 0 0
-2.0710 -1.1350 -0.4890 C 0 0
-0.0810 -0.0370 0.6290 C 0 0 1 0 0 0
-0.8090 0.4550 1.8800 C 0 0
0.1380 0.7270 2.9930 C 0 0
0.9930 1.8430 2.9330 C 0 0
1.9310 1.2420 5.0980 C 0 0
1.0770 0.1270 5.1580 C 0 0
1.8890 2.1000 3.9850 C 0 0

```

0.1810	-0.1310	4.1060	C	0	0
0.6450	-1.3350	0.8600	C	0	0
1.7590	-1.4950	0.1510	O	0	0
0.2210	-2.1550	1.6410	O	0	0
-0.8830	0.6990	-1.5950	C	0	0
0.2560	1.6690	-1.6380	C	0	0
-1.6860	0.6440	-2.4970	O	0	0
0.0620	3.0520	-1.4140	C	0	0
1.5470	1.1800	-1.9100	C	0	0
2.6430	2.0570	-1.9590	C	0	0
1.1660	3.9270	-1.4630	C	0	0
-1.9610	-2.0800	-1.6310	C	0	0
-0.8750	-3.9800	-2.6990	C	0	0
-0.9790	-3.0860	-1.6190	C	0	0
-1.7530	-3.8700	-3.7910	C	0	0
-2.8390	-1.9680	-2.7240	C	0	0
-2.7370	-2.8630	-3.8060	C	0	0
-3.9150	-2.7140	-5.2690	Br	0	0
2.4540	3.4320	-1.7350	C	0	0
3.7930	4.5010	-1.7940	Cl	0	0
-1.6480	3.7690	-1.0460	Br	0	0
-3.0380	-0.6320	-0.5270	H	0	0
-2.0200	-1.6890	0.4480	H	0	0
0.7420	0.6300	0.3740	H	0	0
-1.5520	-0.2730	2.2050	H	0	0
-1.3820	1.3560	1.6620	H	0	0
0.9650	2.5060	2.0800	H	0	0
2.6190	1.4400	5.9070	H	0	0
1.1100	-0.5320	6.0140	H	0	0
2.5450	2.9560	3.9390	H	0	0
-0.4720	-0.9890	4.1590	H	0	0
2.2720	-2.3070	0.2530	H	0	0
1.7070	0.1260	-2.0830	H	0	0
3.6260	1.6630	-2.1700	H	0	0
1.0280	4.9860	-1.2920	H	0	0
-0.1200	-4.7520	-2.6880	H	0	0
-0.3010	-3.1770	-0.7820	H	0	0
-1.6590	-4.5660	-4.6120	H	0	0
-3.5900	-1.1910	-2.7260	H	0	0
1	2	1	0		
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8	10	2	0		
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1	14	1	0		
14	15	1	0		
14	16	2	0		
15	17	2	0		
15	18	1	0		
18	19	2	0		
20	17	1	0		
2	21	1	0		
26	24	2	0		

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25 26 1 0
22 23 2 0
24 22 1 0
23 21 1 0
21 25 2 0
26 27 1 0
19 28 1 0
28 20 2 0
28 29 1 0
17 30 1 0
2 31 1 0
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3 33 1 0
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6 36 1 0
7 37 1 0
8 38 1 0
9 39 1 0
10 40 1 0
12 41 1 0
18 42 1 0
19 43 1 0
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23 46 1 0
24 47 1 0
25 48 1 0

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M END

> <Name>

Compound140

> <Activ>

5

> <DB_Ref_id>

13.15

\$\$\$\$

Compound141

SciTegic10081411483D

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54 56 0 0 1 0          999 V2000
  0.1390 -0.1910 -0.1890 N 0 0
 -1.2870 -0.0610 0.1430 C 0 0
  0.7380 -1.5310 -0.2480 C 0 0 1 0 0 0
  0.7640 -2.1800 1.1370 C 0 0
  1.5550 -3.4390 1.1370 C 0 0
  2.9590 -3.3890 1.1370 C 0 0
  3.0470 -5.8220 1.1370 C 0 0
  1.6430 -5.8730 1.1370 C 0 0
  3.7050 -4.5800 1.1370 C 0 0
  0.8970 -4.6820 1.1370 C 0 0
  0.0630 -2.3980 -1.2750 C 0 0
  0.5940 -2.3540 -2.4920 O 0 0
 -0.8960 -3.0760 -0.9820 O 0 0
  0.8750 0.9340 -0.4370 C 0 0
  0.2150 2.2700 -0.2990 C 0 0
  2.0350 0.8440 -0.7640 O 0 0
  0.0200 2.8480 0.9730 C 0 0
 -0.2130 2.9530 -1.4510 C 0 0

```


-0.8340	4.2090	-1.3380	C	0	0
-0.5990	4.1040	1.0820	C	0	0
-2.0410	0.6270	-0.9370	C	0	0
-2.6330	0.8400	-3.2890	C	0	0
-1.9200	0.1890	-2.2680	C	0	0
-3.4690	1.9280	-2.9820	C	0	0
-2.8750	1.7170	-0.6290	C	0	0
-3.5920	2.3690	-1.6500	C	0	0
-4.7090	3.8260	-1.2360	Br	0	0
-1.0270	4.7870	-0.0720	C	0	0
-1.7810	6.3200	0.0680	Cl	0	0
0.4630	2.1430	2.2070	C	0	0
1.7720	2.7210	2.7460	C	0	0
-1.3890	0.5000	1.0720	H	0	0
-1.7090	-1.0530	0.3050	H	0	0
1.7460	-1.4570	-0.6560	H	0	0
-0.2480	-2.3850	1.4840	H	0	0
1.1760	-1.4920	1.8770	H	0	0
3.4710	-2.4380	1.1370	H	0	0
3.6210	-6.7380	1.1370	H	0	0
1.1370	-6.8280	1.1370	H	0	0
4.7850	-4.5410	1.1370	H	0	0
-0.1830	-4.7290	1.1370	H	0	0
0.2050	-2.8870	-3.1990	H	0	0
-0.0660	2.5180	-2.4300	H	0	0
-1.1580	4.7190	-2.2340	H	0	0
-0.7460	4.5430	2.0610	H	0	0
-2.5390	0.5040	-4.3110	H	0	0
-1.2810	-0.6460	-2.5120	H	0	0
-4.0100	2.4160	-3.7790	H	0	0
-2.9610	2.0470	0.3970	H	0	0
-0.3240	2.2010	2.9590	H	0	0
0.5690	1.0780	1.9980	H	0	0
2.0880	2.1880	3.6430	H	0	0
2.5590	2.6560	1.9960	H	0	0
1.6490	3.7720	3.0100	H	0	0
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1	3	1	0		
3	4	1	0		
8	10	2	0		
9	7	2	0		
6	9	1	0		
5	10	1	0		
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15	17	2	0		
15	18	1	0		
18	19	2	0		
20	17	1	0		
2	21	1	0		
26	24	2	0		
25	26	1	0		
22	23	2	0		
24	22	1	0		

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21 25 2 0
26 27 1 0
19 28 1 0
28 20 2 0
28 29 1 0
17 30 1 0
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8 39 1 0
9 40 1 0
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12 42 1 0
18 43 1 0
19 44 1 0
20 45 1 0
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31 53 1 0
31 54 1 0

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M END

> <Name>

Compound141

> <Activ>

5.6

> <DB_Ref_id>

13.13

\$\$\$\$

Compound142

SciTegic10081411483D

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51 53 0 0 1 0          999 V2000
-0.1250 1.0920 0.5860 N 0 0
0.4200 2.4490 0.4390 C 0 0
0.8030 -0.0450 0.6600 C 0 0 1 0 0 0
1.5080 -0.2680 -0.6780 C 0 0
2.2970 -1.5270 -0.6780 C 0 0
3.7030 -1.4770 -0.6780 C 0 0
3.7910 -3.9100 -0.6780 C 0 0
2.3870 -3.9610 -0.6780 C 0 0
4.4490 -2.6680 -0.6780 C 0 0
1.6390 -2.7710 -0.6780 C 0 0
1.7730 0.1080 1.8010 C 0 0
1.2680 -0.1170 3.0100 O 0 0
2.9260 0.4140 1.6020 O 0 0
-1.4790 0.9160 0.6460 C 0 0
-2.0220 -0.4760 0.6860 C 0 0

```

-2.2190	1.8730	0.6700	O	0	0
-2.7360	-0.9390	1.8110	C	0	0
-1.8140	-1.3320	-0.4120	C	0	0
-2.3180	-2.6430	-0.3910	C	0	0
-3.2400	-2.2520	1.8280	C	0	0
-0.1500	3.1430	-0.7460	C	0	0
-1.5920	4.8630	-1.6900	C	0	0
-1.0530	4.2070	-0.5700	C	0	0
-1.2290	4.4590	-2.9860	C	0	0
0.2130	2.7360	-2.0410	C	0	0
-0.3240	3.3930	-3.1640	C	0	0
0.1640	2.8480	-4.9010	Br	0	0
-3.0330	-3.1050	0.7280	C	0	0
-3.6500	-4.7050	0.7540	Cl	0	0
-2.9670	-0.0570	2.9840	C	0	0
1.5040	2.3910	0.3380	H	0	0
0.1970	3.0240	1.3380	H	0	0
0.2540	-0.9370	0.9610	H	0	0
2.1620	0.5700	-0.9140	H	0	0
0.7850	-0.2910	-1.4940	H	0	0
4.2150	-0.5250	-0.6780	H	0	0
4.3630	-4.8260	-0.6780	H	0	0
1.8810	-4.9160	-0.6780	H	0	0
5.5270	-2.6290	-0.6780	H	0	0
0.5590	-2.8160	-0.6780	H	0	0
1.8380	-0.0350	3.7850	H	0	0
-1.2700	-0.9860	-1.2770	H	0	0
-2.1500	-3.2870	-1.2420	H	0	0
-3.7890	-2.6020	2.6930	H	0	0
-2.2850	5.6800	-1.5550	H	0	0
-1.3360	4.5260	0.4220	H	0	0
-1.6500	4.9750	-3.8360	H	0	0
0.9060	1.9160	-2.1680	H	0	0
-3.5370	-0.5960	3.7400	H	0	0
-2.0100	0.3070	3.3590	H	0	0
-3.5530	0.8110	2.6800	H	0	0
1	2	1	0		
1	3	1	0		
3	4	1	0		
8	10	2	0		
9	7	2	0		
6	9	1	0		
5	10	1	0		
7	8	1	0		
5	6	2	0		
4	5	1	0		
3	11	1	0		
11	12	1	0		
11	13	2	0		
1	14	1	0		
14	15	1	0		
14	16	2	0		
15	17	2	0		
15	18	1	0		
18	19	2	0		
20	17	1	0		
2	21	1	0		
26	24	2	0		
25	26	1	0		
22	23	2	0		
24	22	1	0		

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23 21 1 0
21 25 2 0
26 27 1 0
19 28 1 0
28 20 2 0
28 29 1 0
17 30 1 0
2 31 1 0
2 32 1 0
3 33 1 0
4 34 1 0
4 35 1 0
6 36 1 0
7 37 1 0
8 38 1 0
9 39 1 0
10 40 1 0
12 41 1 0
18 42 1 0
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M END

> <Name>

Compound142

> <Activ>

3.7

> <DB_Ref_id>

13.12

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Compound143

SciTegic10081411483D

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54 56 0 0 1 0          999 V2000
  0.6370  0.2090  -1.1670 N  0 0
 -0.2100 -0.9560  -0.8700 C  0 0
  1.1680  0.3760  -2.5270 C  0 0 1 0 0 0
  0.4980  1.5540  -3.2360 C  0 0
 -0.9790  1.3950  -3.2850 C  0 0
 -1.5460  0.2680  -3.9070 C  0 0
 -3.7740  1.0940  -3.3780 C  0 0
 -3.2080  2.2200  -2.7550 C  0 0
 -2.9420  0.1180  -3.9540 C  0 0
 -1.8120  2.3710  -2.7090 C  0 0
  2.6690  0.4840  -2.5270 C  0 0
  3.3200 -0.6760  -2.5270 O  0 0
  3.2150  1.5630  -2.5260 O  0 0
  0.9110  1.1080  -0.1760 C  0 0
  0.2680  0.9220  1.1620 C  0 0
  1.6600  2.0340  -0.3820 O  0 0
  1.0440  0.6080  2.2970 C  0 0
 -1.1260  1.0640  1.2850 C  0 0

```

-1.7460	0.8940	2.5340	C	0	0
0.4210	0.4370	3.5460	C	0	0
0.3730	-1.7950	0.2100	C	0	0
2.2690	-2.9880	1.1620	C	0	0
1.7190	-2.1960	0.1410	C	0	0
1.4760	-3.3810	2.2540	C	0	0
-0.4220	-2.1880	1.3010	C	0	0
0.1280	-2.9810	2.3260	C	0	0
-0.9370	-3.5060	3.7890	Br	0	0
-0.9730	0.5800	3.6650	C	0	0
-1.6290	0.3990	4.9870	C	0	0
2.5210	0.4520	2.1910	C	0	0
-0.3250	-1.5550	-1.7730	H	0	0
-1.1990	-0.6130	-0.5690	H	0	0
1.0160	-0.5470	-3.0870	H	0	0
0.8860	1.6640	-4.2490	H	0	0
0.7460	2.4930	-2.7410	H	0	0
-0.9120	-0.4860	-4.3520	H	0	0
-4.8470	0.9780	-3.4130	H	0	0
-3.8470	2.9700	-2.3130	H	0	0
-3.3770	-0.7470	-4.4320	H	0	0
-1.3830	3.2390	-2.2290	H	0	0
4.2860	-0.6760	-2.5270	H	0	0
-1.7290	1.3060	0.4210	H	0	0
-2.8180	1.0040	2.6200	H	0	0
1.0140	0.1960	4.4160	H	0	0
3.3030	-3.2960	1.1080	H	0	0
2.3340	-1.8970	-0.6950	H	0	0
1.9160	-3.9900	3.0320	H	0	0
-1.4560	-1.8770	1.3460	H	0	0
-2.7040	0.5390	4.8810	H	0	0
-1.3690	-0.5800	5.3900	H	0	0
-1.2600	1.1540	5.6820	H	0	0
2.8870	0.3260	1.1730	H	0	0
2.8370	-0.4160	2.7690	H	0	0
3.0090	1.3300	2.6140	H	0	0
1	2	1	0		
1	3	1	0		
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8	10	2	0		
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5	10	1	0		
7	8	1	0		
5	6	2	0		
4	5	1	0		
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11	13	2	0		
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15	17	2	0		
15	18	1	0		
18	19	2	0		
20	17	1	0		
2	21	1	0		
26	24	2	0		
25	26	1	0		
22	23	2	0		
24	22	1	0		

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23 21 1 0
21 25 2 0
26 27 1 0
19 28 1 0
28 20 2 0
28 29 1 0
17 30 1 0
2 31 1 0
2 32 1 0
3 33 1 0
4 34 1 0
4 35 1 0
6 36 1 0
7 37 1 0
8 38 1 0
9 39 1 0
10 40 1 0
12 41 1 0
18 42 1 0
19 43 1 0
20 44 1 0
22 45 1 0
23 46 1 0
24 47 1 0
25 48 1 0
29 49 1 0
29 50 1 0
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30 52 1 0
30 53 1 0
30 54 1 0
M END
> <Name>
Compound143

> <Activ>
5.9

> <DB_Ref_id>
13.1

$$$$
Compound144
SciTegic10081411483D

42 45 0 0 0 0 999 V2000
2.8960 3.5660 -1.4100 C 0 0
4.8610 4.7340 -0.5740 C 0 0
3.8110 4.6290 -1.5000 C 0 0
5.0040 3.7730 0.4430 C 0 0
3.0310 2.6030 -0.3920 C 0 0
4.0880 2.7070 0.5350 C 0 0
2.1350 1.5600 -0.3030 N 0 0
0.7600 1.8160 -0.4340 C 0 0
-0.2560 0.7030 -0.3400 C 0 0
0.1210 -0.6580 -0.1150 C 0 0
1.4920 -0.8870 0.0080 N 0 0
2.4160 0.1170 -0.0740 C 0 0
-1.6290 1.0140 -0.4780 C 0 0
-2.6080 0.0000 -0.3940 C 0 0
-2.2400 -1.3500 -0.1700 C 0 0

```

-0.8630	-1.6990	-0.0250	C	0	0
0.4340	2.9690	-0.6250	O	0	0
6.2890	3.8980	1.5700	Cl	0	0
2.1700	-2.0740	0.2230	C	0	0
3.6430	-0.4000	0.0840	N	0	0
3.4800	-1.7170	0.2600	N	0	0
-3.2150	-2.2760	-0.0980	N	0	0
-4.4920	-1.9490	0.5530	C	0	0
-5.2560	-3.2190	0.9280	C	0	0
-6.4650	-2.8400	1.5450	O	0	0
-0.5270	-3.1210	0.2090	C	0	0
2.0920	3.5020	-2.1310	H	0	0
5.5570	5.5590	-0.6560	H	0	0
3.7030	5.3650	-2.2810	H	0	0
4.1990	1.9710	1.3180	H	0	0
-1.9470	2.0310	-0.6520	H	0	0
-3.6470	0.2770	-0.5060	H	0	0
1.8300	-3.0900	0.3440	H	0	0
-3.0570	-3.1820	-0.4880	H	0	0
-5.0860	-1.3260	-0.1170	H	0	0
-4.2990	-1.3400	1.4360	H	0	0
-4.6860	-3.8170	1.6390	H	0	0
-5.4960	-3.8010	0.0370	H	0	0
-6.9380	-3.6560	1.7760	H	0	0
-1.4450	-3.6940	0.3480	H	0	0
0.0800	-3.4900	-0.6150	H	0	0
0.0620	-3.2090	1.1230	H	0	0
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Compound144

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0.38

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14.11a

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Compound145

SciTegic10081411483D

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6.8280	3.2950	-0.3910	C	0	0	
7.5710	5.5100	0.3010	C	0	0	
7.7480	4.3540	-0.4790	C	0	0	
6.4730	5.6080	1.1760	C	0	0	
5.7270	3.3910	0.4800	C	0	0	
5.5510	4.5470	1.2640	C	0	0	
4.8280	2.3590	0.5640	N	0	0	
3.4510	2.6470	0.5270	C	0	0	
2.4280	1.5450	0.6170	C	0	0	
2.8130	0.1840	0.7440	C	0	0	
4.1720	-0.0680	0.7770	N	0	0	
5.1120	0.8950	0.6990	C	0	0	
1.0430	1.8480	0.5780	C	0	0	
0.0820	0.8090	0.6640	C	0	0	
0.4850	-0.5490	0.7910	C	0	0	
1.8650	-0.8710	0.8320	C	0	0	
3.1310	3.8130	0.4200	O	0	0	
6.2580	7.0140	2.1310	Cl	0	0	
4.8030	-1.2600	0.8910	C	0	0	
6.3690	0.3850	0.7560	N	0	0	
6.1800	-0.9670	0.8750	C	0	0	
-0.4370	-1.5180	0.8710	N	0	0	
-1.8630	-1.1700	1.0270	C	0	0	
-2.6330	-2.2890	1.7500	C	0	0	
-4.1370	-1.9710	1.8340	C	0	0	
-2.5160	-0.8650	-0.3320	C	0	0	
-4.0230	-0.5920	-0.1820	C	0	0	
-4.7090	-1.6930	0.5100	N	0	0	
-4.8090	-2.8930	-0.3160	C	0	0	
-5.6250	-2.6480	-1.5350	C	0	0	
-5.7790	-2.3770	-3.9510	C	0	0	
-5.0080	-2.6050	-2.7990	C	0	0	
-7.1680	-2.1910	-3.8420	C	0	0	
-7.0160	-2.4630	-1.4280	C	0	0	
-7.7850	-2.2340	-2.5800	C	0	0	

6.9810	2.4160	-1.0000	H	0	0
8.2870	6.3170	0.2210	H	0	0
8.5920	4.2790	-1.1480	H	0	0
4.7050	4.6270	1.9360	H	0	0
0.7090	2.8690	0.4820	H	0	0
-0.9650	1.0720	0.6310	H	0	0
2.1700	-1.9040	0.9280	H	0	0
4.3440	-2.2360	0.9730	H	0	0
6.9960	-1.6740	0.9470	H	0	0
-0.1460	-2.4730	0.8220	H	0	0
-1.9100	-0.2700	1.6410	H	0	0
-2.4960	-3.2380	1.2250	H	0	0
-2.2340	-2.4380	2.7540	H	0	0
-4.6740	-2.7990	2.2990	H	0	0
-4.2930	-1.1040	2.4750	H	0	0
-2.0330	-0.0060	-0.8010	H	0	0
-2.3710	-1.7050	-1.0140	H	0	0
-4.1740	0.3280	0.3830	H	0	0
-4.4780	-0.4320	-1.1600	H	0	0
-5.2580	-3.6970	0.2660	H	0	0
-3.8100	-3.2190	-0.6070	H	0	0
-5.3050	-2.3440	-4.9220	H	0	0
-3.9390	-2.7480	-2.8890	H	0	0
-7.7600	-2.0160	-4.7290	H	0	0
-7.4960	-2.4940	-0.4610	H	0	0
-8.8540	-2.0900	-2.4960	H	0	0
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Compound145

> <Activ>

0.84

> <DB_Ref_id>

14.10b

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Compound146

SciTegic10081411483D

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60 64 0 0 0 0          999 V2000
-3.4510 4.3010 -1.9220 C 0 0
-5.1560 5.8260 -1.0900 C 0 0
-4.7420 4.8460 -2.0080 C 0 0
-4.2750 6.2680 -0.0860 C 0 0
-2.5660 4.7380 -0.9180 C 0 0
-2.9810 5.7230 0.0000 C 0 0
-1.2970 4.2030 -0.8320 N 0 0
-0.1930 5.0430 -0.6800 C 0 0
1.1540 4.3890 -0.5960 C 0 0
1.2620 2.9690 -0.6720 C 0 0
0.1210 2.2400 -0.8200 N 0 0
-1.1370 2.8170 -0.9010 C 0 0
2.3160 5.1880 -0.4400 C 0 0
3.5880 4.5780 -0.3610 C 0 0
3.7070 3.1740 -0.4360 C 0 0

```

2.5550	2.3670	-0.5900	C	0	0
-0.3770	6.2400	-0.6250	O	0	0
-2.0940	2.0860	-1.0330	O	0	0
-4.7790	7.4670	1.0310	Cl	0	0
2.7230	0.8950	-0.6660	C	0	0
3.2050	0.2310	-1.5530	O	0	0
2.2420	0.2930	0.4630	N	0	0
2.3160	-1.1760	0.5880	C	0	0
2.1760	-1.6170	2.0550	C	0	0
1.2440	-1.8610	-0.2770	C	0	0
1.2520	-3.3850	-0.0780	C	0	0
1.1000	-3.7320	1.3420	N	0	0
2.1540	-3.1480	2.1800	C	0	0
1.0020	-5.1740	1.5310	C	0	0
-0.2230	-5.7290	0.8960	C	0	0
-1.2720	-7.2030	-0.7350	C	0	0
-0.1130	-6.6800	-0.1330	C	0	0
-2.5410	-6.7750	-0.3050	C	0	0
-1.4940	-5.3010	1.3240	C	0	0
-2.6500	-5.8240	0.7240	C	0	0
-3.1500	3.5470	-2.6370	H	0	0
-6.1540	6.2360	-1.1680	H	0	0
-5.4200	4.5100	-2.7790	H	0	0
-2.3070	6.0650	0.7750	H	0	0
0.1720	1.2420	-0.8750	H	0	0
2.2400	6.2640	-0.3810	H	0	0
4.4710	5.1900	-0.2420	H	0	0
4.6880	2.7210	-0.3750	H	0	0
1.8460	0.8500	1.1930	H	0	0
3.2990	-1.4820	0.2260	H	0	0
1.2540	-1.2150	2.4800	H	0	0
2.9940	-1.2150	2.6520	H	0	0
1.4020	-1.6330	-1.3320	H	0	0
0.2540	-1.4750	-0.0240	H	0	0
0.4390	-3.8340	-0.6520	H	0	0
2.1840	-3.8090	-0.4590	H	0	0
3.1230	-3.5610	1.8870	H	0	0
1.9900	-3.4300	3.2210	H	0	0
0.9920	-5.4000	2.5980	H	0	0
1.8810	-5.6580	1.1050	H	0	0
-1.1880	-7.9340	-1.5240	H	0	0
0.8570	-7.0120	-0.4670	H	0	0
-3.4320	-7.1780	-0.7660	H	0	0
-1.5840	-4.5700	2.1150	H	0	0
-3.6250	-5.4960	1.0530	H	0	0
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Compound146

> <Activ>

0.076

> <DB_Ref_id>

14.09b

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Compound147

SciTegic10081411483D

50	54	0	0	0	0	999	V2000
4.8260	-2.0620	-0.2170	C	0	0		
5.8400	-4.2070	-0.7710	C	0	0		
5.9180	-2.9450	-0.1580	C	0	0		
4.6660	-4.5880	-1.4490	C	0	0		
3.6490	-2.4410	-0.8910	C	0	0		
3.5720	-3.7050	-1.5080	C	0	0		
2.5740	-1.5760	-0.9470	N	0	0		
2.7790	-0.2400	-1.2890	C	0	0		
1.5700	0.6450	-1.3340	C	0	0		
0.2790	0.1020	-1.0660	C	0	0		
0.1820	-1.2170	-0.7050	N	0	0		
1.2970	-2.0530	-0.6520	C	0	0		
1.7230	2.0180	-1.6430	C	0	0		
0.5920	2.8580	-1.7010	C	0	0		
-0.6970	2.3300	-1.4770	C	0	0		
-0.8770	0.9490	-1.1780	C	0	0		
3.9080	0.1350	-1.5270	O	0	0		
1.1410	-3.2150	-0.3380	O	0	0		
4.5700	-6.1270	-2.2010	Cl	0	0		
-1.1580	-1.7700	-0.3260	C	0	0		
-2.1310	0.4380	-1.0120	N	0	0		
-2.3280	-1.0330	-1.0080	C	0	0		
-3.3240	1.2950	-0.8480	C	0	0		
-3.3070	2.0160	0.4510	C	0	0		
-3.2640	1.9770	2.8890	C	0	0		
-3.2810	1.2930	1.6580	C	0	0		
-3.2700	3.3830	2.9100	C	0	0		
-3.3130	3.4220	0.4770	C	0	0		
-3.2950	4.1040	1.7050	C	0	0		
-3.2360	1.2090	4.1700	C	0	0		
-3.2210	1.9510	5.2740	O	0	0		
-3.2300	0.0000	4.1700	O	0	0		
4.9060	-1.0960	0.2620	H	0	0		
6.6880	-4.8750	-0.7170	H	0	0		
6.8190	-2.6520	0.3590	H	0	0		
2.6700	-4.0020	-2.0270	H	0	0		
2.7010	2.4320	-1.8320	H	0	0		
0.7150	3.9080	-1.9220	H	0	0		
-1.5370	3.0060	-1.5430	H	0	0		
-1.2580	-1.6910	0.7580	H	0	0		
-1.2210	-2.8300	-0.5680	H	0	0		
-2.4240	-1.3650	-2.0410	H	0	0		
-3.2660	-1.2830	-0.5100	H	0	0		
-3.3610	2.0180	-1.6640	H	0	0		
-4.2210	0.6780	-0.9080	H	0	0		
-3.2750	0.2130	1.6370	H	0	0		
-3.2560	3.9160	3.8500	H	0	0		
-3.3320	3.9830	-0.4470	H	0	0		
-3.3010	5.1840	1.7230	H	0	0		
-3.2030	1.5160	6.1350	H	0	0		
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14.08b

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Compound148
  SciTegic10081411483D

68 73  0  0  0  0          999 V2000
   4.1910   -5.7440   -1.4750 C   0  0

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6.2680	-6.7270	-0.6660	C	0	0
5.2210	-6.6930	-1.6040	C	0	0
6.2850	-5.8130	0.4040	C	0	0
4.2070	-4.8260	-0.4060	C	0	0
5.2540	-4.8630	0.5330	C	0	0
3.1970	-3.8930	-0.2810	N	0	0
3.5140	-2.5570	-0.0470	C	0	0
2.3730	-1.5980	0.0740	C	0	0
1.0310	-2.0630	-0.0430	C	0	0
0.8120	-3.3980	-0.2700	N	0	0
1.8690	-4.3050	-0.3910	C	0	0
2.6390	-0.2280	0.3070	C	0	0
1.5780	0.6910	0.4160	C	0	0
0.2340	0.2640	0.2970	C	0	0
-0.0470	-1.1210	0.0780	C	0	0
4.6840	-2.2440	0.0430	O	0	0
1.6150	-5.4730	-0.5980	O	0	0
-0.7400	1.1820	0.3940	N	0	0
-0.4810	2.4650	1.0760	C	0	0
-1.7250	2.9470	1.8440	C	0	0
-2.8320	3.4510	0.9020	C	0	0
7.5610	-5.8570	1.5510	C1	0	0
-0.5820	-3.9260	-0.4040	C	0	0
-1.4590	-1.5960	-0.0330	C	0	0
-1.6020	-3.0700	0.3530	C	0	0
-1.1880	4.0350	-0.8150	C	0	0
-0.0310	3.5450	0.0760	C	0	0
-2.3240	4.4900	-0.0020	N	0	0
-3.3870	5.0390	-0.8360	C	0	0
-4.4180	5.7340	-0.0220	C	0	0
-4.1020	6.9420	0.6310	C	0	0
-5.7070	5.1880	0.1000	C	0	0
-6.3650	7.0510	1.5210	C	0	0
-6.6820	5.8460	0.8710	C	0	0
-5.0760	7.5980	1.4020	C	0	0
5.2010	-7.6660	-2.7360	C	0	0
6.3930	-8.1270	-3.1060	O	0	0
4.1620	-7.9900	-3.2600	O	0	0
3.3910	-5.7250	-2.2010	H	0	0
7.0570	-7.4570	-0.7700	H	0	0
5.2710	-4.1600	1.3570	H	0	0
3.6560	0.1250	0.4040	H	0	0
1.8160	1.7320	0.5920	H	0	0
-1.6390	0.9840	0.0000	H	0	0
0.3260	2.2850	1.7870	H	0	0
-1.4340	3.7620	2.5100	H	0	0
-2.1110	2.1600	2.4940	H	0	0
-3.2360	2.6250	0.3160	H	0	0
-3.6560	3.8560	1.4920	H	0	0
-0.6450	-4.9490	-0.0330	H	0	0
-0.8380	-3.9550	-1.4650	H	0	0
-1.7910	-1.4510	-1.0630	H	0	0
-2.1310	-1.0140	0.6000	H	0	0
-2.6130	-3.4180	0.1430	H	0	0
-1.4530	-3.1860	1.4280	H	0	0
-0.8400	4.8540	-1.4450	H	0	0
-1.5140	3.2360	-1.4830	H	0	0
0.7930	3.1840	-0.5430	H	0	0
0.3670	4.3950	0.6310	H	0	0
-3.8560	4.2340	-1.4020	H	0	0
-2.9610	5.7360	-1.5570	H	0	0

-3.1130	7.3650	0.5430 H	0	0
-5.9550	4.2620	-0.3990 H	0	0
-7.1140	7.5570	2.1150 H	0	0
-7.6720	5.4260	0.9630 H	0	0
-4.8340	8.5260	1.9020 H	0	0
7.1910	-7.6800	-2.7970 H	0	0
2	3	2	0	
1	5	2	0	
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3	1	1	0	
5	7	1	0	
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10	11	1	0	
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4	23	1	0	
11	24	1	0	
16	25	1	0	
25	26	1	0	
24	26	1	0	
27	28	1	0	
20	28	1	0	
22	29	1	0	
29	27	1	0	
29	30	1	0	
30	31	1	0	
31	32	2	0	
31	33	1	0	
34	35	1	0	
35	33	2	0	
32	36	1	0	
36	34	2	0	
3	37	1	0	
6	4	2	0	
5	6	1	0	
37	39	2	0	
37	38	1	0	
1	40	1	0	
2	41	1	0	
6	42	1	0	
13	43	1	0	
14	44	1	0	
19	45	1	0	
20	46	1	0	
21	47	1	0	
21	48	1	0	
22	49	1	0	
22	50	1	0	


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24 51 1 0
24 52 1 0
25 53 1 0
25 54 1 0
26 55 1 0
26 56 1 0
27 57 1 0
27 58 1 0
28 59 1 0
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M END

> <Name>

Compound148

> <Activ>

0.16

> <DB_Ref_id>

14.07d

\$\$\$\$

Compound149

SciTegic10081411483D

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56 60 0 0 0 0          999 V2000
-5.1190 -3.1410 -0.3930 C 0 0
-6.2810 -5.1210 0.4200 C 0 0
-6.2690 -3.9470 -0.3540 C 0 0
-5.1410 -5.4880 1.1580 C 0 0
-3.9760 -3.5060 0.3440 C 0 0
-3.9880 -4.6800 1.1190 C 0 0
-2.8460 -2.7130 0.3030 N 0 0
-2.9610 -1.3360 0.4710 C 0 0
-1.6970 -0.5350 0.4140 C 0 0
-0.4470 -1.1850 0.2030 C 0 0
-0.4300 -2.5510 0.0490 N 0 0
-1.6010 -3.3090 0.0940 C 0 0
-1.7580 0.8670 0.5700 C 0 0
-0.5800 1.6390 0.5140 C 0 0
0.6780 1.0240 0.3030 C 0 0
0.7520 -0.3960 0.1560 C 0 0
-4.0620 -0.8610 0.6500 O 0 0
-1.5250 -4.5100 -0.0550 O 0 0
1.7700 1.8050 0.2440 N 0 0
1.7190 3.1900 0.7620 C 0 0 1 0 0 0
3.1080 3.6370 1.2540 C 0 0
4.1390 3.7780 0.1150 C 0 0
-5.1560 -6.9180 2.1060 Cl 0 0
0.8630 -3.2680 -0.1840 C 0 0
2.0720 -1.0640 -0.0490 C 0 0
2.0570 -2.5210 0.4180 C 0 0
2.2130 5.0530 -0.9630 C 0 0
1.1430 4.1720 -0.2890 C 0 0

```

3.5390	4.3110	-1.2090	C	0	0	2	0	0	0
3.3580	3.2170	-2.2320	C	0	0				
4.4630	2.5430	-2.5430	O	0	0				
2.2740	2.9920	-2.7190	O	0	0				
-5.1310	-2.2420	-0.9940	H	0	0				
-7.1720	-5.7320	0.4390	H	0	0				
-7.1450	-3.6660	-0.9180	H	0	0				
-3.1130	-4.9670	1.6890	H	0	0				
-2.7030	1.3610	0.7340	H	0	0				
-0.6600	2.7110	0.6330	H	0	0				
2.6170	1.4490	-0.1480	H	0	0				
1.0410	3.1660	1.6150	H	0	0				
3.4880	2.9630	2.0230	H	0	0				
2.9980	4.6060	1.7420	H	0	0				
4.9300	4.4490	0.4530	H	0	0				
4.6350	2.8200	-0.0530	H	0	0				
1.0020	-3.3890	-1.2600	H	0	0				
0.8300	-4.2710	0.2440	H	0	0				
2.8690	-0.5470	0.4840	H	0	0				
2.3190	-1.0190	-1.1110	H	0	0				
2.0040	-2.5620	1.5080	H	0	0				
2.9880	-3.0180	0.1390	H	0	0				
2.4160	5.9120	-0.3220	H	0	0				
1.8240	5.4690	-1.8950	H	0	0				
0.4240	4.8320	0.1970	H	0	0				
0.5650	3.6450	-1.0510	H	0	0				
4.2480	5.0220	-1.6350	H	0	0				
4.4140	1.8300	-3.1930	H	0	0				
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1	5	2	0						
4	2	1	0						
3	1	1	0						
5	7	1	0						
11	12	1	0						
10	11	1	0						
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16	25	1	0						
25	26	1	0						
24	26	1	0						
27	28	1	0						
20	28	1	0						
22	29	1	0						
29	27	1	0						
29	30	1	0						
6	4	2	0						

```

5 6 1 0
30 32 2 0
30 31 1 0
1 33 1 0
2 34 1 0
3 35 1 0
6 36 1 0
13 37 1 0
14 38 1 0
19 39 1 0
20 40 1 0
21 41 1 0
21 42 1 0
22 43 1 0
22 44 1 0
24 45 1 0
24 46 1 0
25 47 1 0
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27 52 1 0
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28 54 1 0
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M END

> <Name>

Compound149

> <Activ>

1.1

> <DB_Ref_id>

14.07c

\$\$\$\$

Compound150

SciTegic10081411483D

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45 47 0 0 0 0          999 V2000
-4.8220 2.1830 0.6930 C 0 0
-6.9900 2.3280 -0.4060 C 0 0
-6.1070 2.7400 0.6070 C 0 0
-6.5860 1.3510 -1.3360 C 0 0
-4.4120 1.2070 -0.2340 C 0 0
-5.2970 0.7910 -1.2500 C 0 0
-3.1580 0.6640 -0.1520 N 0 0
-2.0490 1.4980 0.0000 C 0 0
-0.7090 0.8360 0.0840 C 0 0
-0.6090 -0.5840 0.0060 C 0 0
-1.7520 -1.3190 -0.1430 N 0 0
-3.0080 -0.7230 -0.2210 C 0 0
0.4570 1.6250 0.2400 C 0 0
1.7270 1.0100 0.3180 C 0 0
1.8460 -0.3990 0.2420 C 0 0
0.6780 -1.1880 0.0880 C 0 0
-2.2270 2.6970 0.0570 O 0 0
-3.9820 -1.4340 -0.3540 O 0 0
3.0530 -0.9790 0.3160 N 0 0

```

4.2580	-0.1530	0.4610	C	0	0
5.5160	-1.0200	0.4980	C	0	0
5.8280	-1.6660	-0.8520	C	0	0
-7.6620	0.8440	-2.5700	Cl	0	0
-1.6890	-2.7990	-0.2250	C	0	0
6.7210	-0.2870	1.0920	C	0	0
-4.1580	2.5150	1.4800	H	0	0
-7.9750	2.7670	-0.4610	H	0	0
-6.4200	3.4900	1.3200	H	0	0
-4.9880	0.0410	-1.9670	H	0	0
0.3870	2.7010	0.2990	H	0	0
2.6020	1.6330	0.4360	H	0	0
0.7790	-2.2640	0.0310	H	0	0
3.1310	-1.9750	0.2710	H	0	0
4.3050	0.5600	-0.3630	H	0	0
4.1760	0.4470	1.3670	H	0	0
5.4400	-1.7760	1.2790	H	0	0
6.7270	-2.2800	-0.8110	H	0	0
5.9770	-0.9060	-1.6190	H	0	0
5.0040	-2.3050	-1.1720	H	0	0
-0.9670	-3.2640	0.4470	H	0	0
-1.4340	-3.0900	-1.2420	H	0	0
-2.6700	-3.2130	0.0040	H	0	0
7.5740	-0.9590	1.1800	H	0	0
6.9980	0.5640	0.4710	H	0	0
6.4880	0.0880	2.0900	H	0	0
6	4	2	0		
5	6	1	0		
2	3	2	0		
1	5	2	0		
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7	8	1	0		
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13	14	2	0		
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8	17	2	0		
12	18	2	0		
15	19	1	0		
19	20	1	0		
20	21	1	0		
21	22	1	0		
4	23	1	0		
11	24	1	0		
21	25	1	0		
1	26	1	0		
2	27	1	0		
3	28	1	0		
6	29	1	0		
13	30	1	0		
14	31	1	0		
16	32	1	0		
19	33	1	0		

[illegible]

-0.1150	1.8110	1.9080	H	0	0
-1.9980	0.4490	2.4390	H	0	0
-3.0370	-1.1110	0.2030	H	0	0
-2.1150	-2.5660	2.7260	H	0	0
-1.4390	-2.7560	1.1250	H	0	0
-3.0160	-4.5980	1.6890	H	0	0
-3.5430	-3.7010	0.2850	H	0	0
1.7010	2.8320	2.5160	H	0	0
1.0490	4.0100	1.3810	H	0	0
2.7850	3.9420	1.6800	H	0	0
-4.5880	-3.3610	3.1250	H	0	0
-5.5180	-1.9220	0.6050	H	0	0
-6.1930	-1.7340	2.2070	H	0	0
-4.6270	0.1150	1.6420	H	0	0
-4.0980	-0.7790	3.0490	H	0	0
-6.7110	-4.2480	2.2520	H	0	0
-5.9820	-4.4510	0.6440	H	0	0
-5.4100	-5.4100	2.0080	H	0	0
6	4	2	0		
5	6	1	0		
2	3	2	0		
1	5	2	0		
4	2	1	0		
3	1	1	0		
5	7	1	0		
11	12	1	0		
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7	8	1	0		
15	16	2	0		
14	15	1	0		
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12	18	2	0		
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21	22	1	0		
4	23	1	0		
11	24	1	0		
22	25	1	0		
25	26	1	0		
26	27	1	0		
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25	28	1	0		
1	29	1	0		
2	30	1	0		
3	31	1	0		
6	32	1	0		
13	33	1	0		
14	34	1	0		
16	35	1	0		
19	36	1	0		
20	37	1	0		
21	38	1	0		
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22	40	1	0		

22 41 1 0
24 42 1 0
24 43 1 0
24 44 1 0
25 45 1 0
26 46 1 0
26 47 1 0
27 48 1 0
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M END

> <Name>

Compound151

> <Activ>

5.2

> <DB_Ref_id>

14.06d

\$\$\$\$

Compound152

SciTegic10081411483D

61	65	0	0	0	999	V2000
-7.1480	2.2210	-1.3650	C	0	0	
-9.4900	2.2350	-0.6970	C	0	0	
-8.4360	2.7760	-1.4510	C	0	0	
-9.2560	1.1350	0.1490	C	0	0	
-6.9100	1.1190	-0.5210	C	0	0	
-7.9670	0.5760	0.2360	C	0	0	
-5.6460	0.5720	-0.4370	N	0	0	
-4.5390	1.4040	-0.2850	C	0	0	
-3.1970	0.7420	-0.2030	C	0	0	
-3.1000	-0.6780	-0.2790	C	0	0	
-4.2400	-1.4120	-0.4280	N	0	0	
-5.4960	-0.8160	-0.5080	C	0	0	
-2.0310	1.5310	-0.0470	C	0	0	
-0.7640	0.9180	0.0310	C	0	0	
-0.6420	-0.4920	-0.0450	C	0	0	
-1.8100	-1.2810	-0.1990	C	0	0	
-4.7150	2.6040	-0.2300	O	0	0	
-6.4710	-1.5270	-0.6410	O	0	0	
0.5630	-1.0720	0.0290	N	0	0	
1.7850	-0.2480	-0.0510	C	0	0	
2.9570	-1.0510	-0.6440	C	0	0	
4.2580	-0.2340	-0.6330	C	0	0	
-10.5410	0.4750	1.0720	C1	0	0	
-4.1780	-2.8910	-0.5100	C	0	0	
4.5610	0.2520	0.7190	N	0	0	
3.4900	1.0880	1.2740	C	0	0	
2.1620	0.3180	1.3280	C	0	0	
5.8520	0.9300	0.7680	C	0	0	
6.9790	-0.0290	0.6350	C	0	0	
6.9100	-1.2890	1.2580	C	0	0	
7.9770	-2.1950	1.1310	C	0	0	
9.1140	-1.8420	0.3850	C	0	0	
9.1860	-0.5840	-0.2360	C	0	0	
8.1170	0.3220	-0.1110	C	0	0	

-6.3500	2.6520	-1.9550	H	0	0
-10.4750	2.6720	-0.7750	H	0	0
-8.6150	3.6210	-2.1000	H	0	0
-7.7910	-0.2690	0.8870	H	0	0
-2.1010	2.6100	0.0140	H	0	0
0.1130	1.5410	0.1500	H	0	0
-1.7090	-2.3570	-0.2560	H	0	0
0.6210	-2.0640	0.1390	H	0	0
1.5700	0.5880	-0.7190	H	0	0
2.7290	-1.3590	-1.6660	H	0	0
3.1130	-1.9690	-0.0740	H	0	0
5.0800	-0.8510	-0.9920	H	0	0
4.1720	0.6150	-1.3120	H	0	0
-5.1740	-3.3030	-0.3460	H	0	0
-3.7400	-3.1780	-1.4670	H	0	0
-3.5270	-3.2660	0.2790	H	0	0
3.3790	1.9860	0.6620	H	0	0
3.7660	1.4160	2.2770	H	0	0
1.3750	0.9790	1.6990	H	0	0
2.2540	-0.4880	2.0570	H	0	0
5.9420	1.4710	1.7090	H	0	0
5.9040	1.6660	-0.0350	H	0	0
6.0370	-1.5640	1.8320	H	0	0
7.9220	-3.1620	1.6090	H	0	0
9.9340	-2.5390	0.2890	H	0	0
10.0590	-0.3140	-0.8100	H	0	0
8.1780	1.2890	-0.5920	H	0	0
6	4	2	0		
5	6	1	0		
2	3	2	0		
1	5	2	0		
4	2	1	0		
3	1	1	0		
5	7	1	0		
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10	11	1	0		
9	10	2	0		
8	9	1	0		
12	7	1	0		
7	8	1	0		
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13	14	2	0		
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25	26	1	0		
26	27	1	0		
20	27	1	0		
33	34	2	0		
32	33	1	0		
31	32	2	0		
30	31	1	0		


```

29 30 2 0
29 34 1 0
28 29 1 0
25 28 1 0
1 35 1 0
2 36 1 0
3 37 1 0
6 38 1 0
13 39 1 0
14 40 1 0
16 41 1 0
19 42 1 0
20 43 1 0
21 44 1 0
21 45 1 0
22 46 1 0
22 47 1 0
24 48 1 0
24 49 1 0
24 50 1 0
26 51 1 0
26 52 1 0
27 53 1 0
27 54 1 0
28 55 1 0
28 56 1 0
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32 59 1 0
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34 61 1 0
M END
> <Name>
Compound152

> <Activ>
0.075

> <DB_Ref_id>
14.06c

$$$$
Compound153
SciTegic10081411483D

44 46 0 0 1 0          999 V2000
-2.1060 -0.4140 -3.1700 C 0 0
-2.4730 0.0060 -1.8180 C 0 0
-1.1580 -0.1290 -0.7890 S 0 0
-0.1780 -0.6990 -2.0510 C 0 0
-0.7540 -0.8030 -3.1990 N 0 0
-3.6970 0.4400 -1.4670 C 0 0
-4.0020 0.8440 -0.1020 C 0 0
-5.2050 1.3200 0.4200 C 0 0
-4.9430 1.5550 1.7700 C 0 0
-3.6040 1.2030 1.9710 C 0 0
-3.0060 0.7620 0.8240 O 0 0
-2.8480 1.2810 3.2810 C 0 0
-1.4040 0.8050 3.1170 C 0 0
-2.8260 -0.4370 -4.1410 O 0 0
1.1410 -1.0470 -1.9550 N 0 0

```

1.8220	-0.9360	-0.6580	C	0	0	1	0	0	0
2.2270	-2.3120	-0.1290	C	0	0				
2.9900	-0.0140	-0.7300	C	0	0				
5.3850	0.2910	-1.0780	C	0	0				
4.2620	-0.5490	-1.0040	C	0	0				
5.2420	1.6760	-0.8770	C	0	0				
2.8440	1.3790	-0.5310	C	0	0				
3.9710	2.2170	-0.6050	C	0	0				
1.0510	-3.0920	0.3960	C	0	0				
1.3340	-4.3140	0.8360	O	0	0				
-0.0590	-2.6130	0.4080	O	0	0				
6.6130	2.7010	-0.9650	Cl	0	0				
1.3070	2.0740	-0.1990	Cl	0	0				
-4.4790	0.4880	-2.2110	H	0	0				
-6.1390	1.4770	-0.1070	H	0	0				
-5.6370	1.9320	2.5100	H	0	0				
-2.8750	2.3050	3.6560	H	0	0				
-3.3670	0.6900	4.0350	H	0	0				
-0.8670	0.8750	4.0630	H	0	0				
-1.3770	-0.2270	2.7680	H	0	0				
-0.8770	1.4180	2.3870	H	0	0				
1.6290	-1.3750	-2.7640	H	0	0				
1.1680	-0.4280	0.0510	H	0	0				
2.9390	-2.1290	0.6740	H	0	0				
2.7340	-2.8870	-0.9020	H	0	0				
6.3540	-0.1390	-1.2890	H	0	0				
4.3810	-1.6110	-1.1580	H	0	0				
3.8630	3.2830	-0.4530	H	0	0				
0.6230	-4.8670	1.1880	H	0	0				
5	1	1	0						
4	5	2	0						
3	4	1	0						
1	2	1	0						
2	3	1	0						
2	6	2	0						
6	7	1	0						
10	11	1	0						
9	10	2	0						
8	9	1	0						
8	7	2	0						
11	7	1	0						
10	12	1	0						
12	13	1	0						
1	14	2	0						
4	15	1	0						
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18	22	2	0						
17	24	1	0						
24	25	1	0						
24	26	2	0						
21	27	1	0						
22	28	1	0						
6	29	1	0						
8	30	1	0						

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9 31 1 0
12 32 1 0
12 33 1 0
13 34 1 0
13 35 1 0
13 36 1 0
15 37 1 0
16 38 1 0
17 39 1 0
17 40 1 0
19 41 1 0
20 42 1 0
23 43 1 0
25 44 1 0

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M END

> <Name>

Compound153

> <Activ>

9

> <DB_Ref_id>

15.38

\$\$\$\$

Compound154

SciTegic10081411483D

```

44 46 0 0 1 0          999 V2000
-1.1330 -1.1000 3.4780 C 0 0
-1.8610 -0.4450 2.3940 C 0 0
-0.8850 -0.3010 1.0410 S 0 0
0.4040 -1.0590 1.8420 C 0 0
0.1700 -1.4140 3.0570 N 0 0
-3.1370 -0.0230 2.4840 C 0 0
-3.8090 0.6210 1.3670 C 0 0
-5.0960 1.1620 1.3140 C 0 0
-5.2290 1.6490 0.0150 C 0 0
-4.0160 1.3710 -0.6290 C 0 0
-3.1270 0.7360 0.1930 O 0 0
-3.6680 1.7110 -2.0630 C 0 0
-2.2620 1.2310 -2.4220 C 0 0
-1.5530 -1.3500 4.5860 O 0 0
1.6410 -1.3120 1.3180 N 0 0
1.9320 -0.9180 -0.0680 C 0 0 2 0 0 0
2.1290 -2.1460 -0.9570 C 0 0
3.1000 0.0040 -0.1410 C 0 0
5.4940 0.3070 -0.4880 C 0 0
4.3710 -0.5330 -0.4140 C 0 0
5.3520 1.6920 -0.2870 C 0 0
2.9530 1.3950 0.0580 C 0 0
4.0820 2.2330 -0.0160 C 0 0
0.8320 -2.8500 -1.2600 C 0 0
0.9470 -3.9630 -1.9810 O 0 0
-0.2210 -2.4100 -0.8650 O 0 0
6.7230 2.7170 -0.3750 Cl 0 0
1.4160 2.0900 0.3900 Cl 0 0
-3.6800 -0.1660 3.4060 H 0 0
-5.8320 1.1950 2.1070 H 0 0
-6.0920 2.1430 -0.4100 H 0 0
-4.4080 1.2680 -2.7310 H 0 0

```

-3.7600	2.7850	-2.2150	H	0	0
-2.0290	1.4610	-3.4610	H	0	0
-1.5200	1.6990	-1.7780	H	0	0
-2.1800	0.1500	-2.2930	H	0	0
2.3340	-1.7660	1.8790	H	0	0
1.1190	-0.2970	-0.4430	H	0	0
2.7910	-2.8140	-0.4060	H	0	0
2.6290	-1.8730	-1.8870	H	0	0
6.4630	-0.1230	-0.6990	H	0	0
4.4900	-1.5960	-0.5690	H	0	0
3.9730	3.2990	0.1370	H	0	0
0.1520	-4.4610	-2.2090	H	0	0

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2	3	1	0
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16	17	1	0
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13	35	1	0
13	36	1	0
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25	44	1	0

M END

> <Name>

Compound154

Compound155
SciTegic10081411483D

	43	45	0	0	1	0		999	V	2000	
	-1.2420				-1.1620		3.5840	C	0	0	
	-1.9790				-1.0900		2.3240	C	0	0	
	-0.9750				-0.5530		1.0960	S	0	0	
	0.3380				-0.4340		2.1620	C	0	0	
	0.0900				-0.7620		3.3850	N	0	0	
	-3.2770				-1.4120		2.1860	C	0	0	
	-3.9550				-1.3180		0.9020	C	0	0	
	-5.2850				-1.6130		0.5940	C	0	0	
	-5.4020				-1.3500		-0.7710	C	0	0	
	-4.1390				-0.9140		-1.1930	C	0	0	
	-3.2320				-0.8890		-0.1700	O	0	0	
	-3.7600				-0.5060		-2.6000	C	0	0	
	-2.2910				-0.0860		-2.6800	C	0	0	
	-1.6780				-1.5100		4.6580	O	0	0	
	1.6020				-0.0270		1.8440	N	0	0	
	1.9120				0.3440		0.4570	C	0	0	3 0 0 0
	2.0940				-0.8710		-0.4140	C	0	0	
	1.8970				-0.7480		-1.7600	N	0	0	
	2.4080				-1.9360		0.0630	O	0	0	
	3.0800				1.2660		0.3830	C	0	0	
	5.4730				1.5700		0.0370	C	0	0	
	4.3520				0.7300		0.1090	C	0	0	
	5.3300				2.9550		0.2360	C	0	0	
	2.9320				2.6560		0.5820	C	0	0	
	4.0610				3.4960		0.5080	C	0	0	
	6.7030				3.9810		0.1490	C1	0	0	
	1.3970				3.3540		0.9140	C1	0	0	
	2.0590				-1.8550		-2.5940	O	0	0	
	-3.8360				-1.7500		3.0470	H	0	0	
	-6.0570				-1.9670		1.2640	H	0	0	
	-6.2890				-1.4570		-1.3810	H	0	0	
	-3.9610				-1.3300		-3.2850	H	0	0	
	-4.4100				0.3030		-2.9320	H	0	0	
	-2.0270				0.2010		-3.6970	H	0	0	
	-2.0940				0.7520		-2.0100	H	0	0	
	-1.6410				-0.9080		-2.3850	H	0	0	
	2.3050				0.0160		2.5550	H	0	0	
	1.1070				0.9650		0.0630	H	0	0	
	1.6370				0.1370		-2.1480	H	0	0	
	6.4420				1.1410		-0.1740	H	0	0	
	4.4710				-0.3320		-0.0450	H	0	0	
	3.9530				4.5630		0.6600	H	0	0	
	1.8910				-1.6480		-3.5250	H	0	0	
5	1	1	0								
4	5	2	0								
3	4	1	0								
1	2	1	0								
2	3	1	0								
2	6	2	0								

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10 11  1  0
  9 10  2  0
  8  9  1  0
  8  7  2  0
11  7  1  0
10 12  1  0
12 13  1  0
  1 14  2  0
  4 15  1  0
15 16  1  0
16 17  1  0
17 18  1  0
17 19  2  0
16 20  1  0
25 23  2  0
24 25  1  0
21 22  2  0
23 21  1  0
22 20  1  0
20 24  2  0
23 26  1  0
24 27  1  0
18 28  1  0
  6 29  1  0
  8 30  1  0
  9 31  1  0
12 32  1  0
12 33  1  0
13 34  1  0
13 35  1  0
13 36  1  0
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18 39  1  0
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22 41  1  0
25 42  1  0
28 43  1  0
M  END
> <Name>
Compound155

> <Activ>
5.5

> <DB_Ref_id>
15.28

$$$$
Compound156
  SciTegic10081411483D

41 43  0  0  1  0          999 V2000
  -1.8420    1.0560   -3.1590 C    0  0
  -2.2350    0.1150   -2.1130 C    0  0
  -1.0800    0.0760   -0.9010 S    0  0
  -0.1350    1.2290   -1.7080 C    0  0
  -0.6110    1.6500   -2.8300 N    0  0
  -3.3690   -0.6110   -2.1340 C    0  0
  -3.7060   -1.5330   -1.0590 C    0  0

```

-4.8310	-2.3500	-0.9310	C	0	0				
-4.6490	-3.0220	0.2780	C	0	0				
-3.4300	-2.5660	0.7960	C	0	0				
-2.8340	-1.6450	-0.0180	O	0	0				
-2.7950	-3.0040	2.0980	C	0	0				
-1.4520	-2.3070	2.3220	C	0	0				
-2.4550	1.3130	-4.1700	O	0	0				
1.0600	1.7360	-1.2810	N	0	0				
1.6250	1.2720	-0.0060	C	0	0	1	0	0	0
3.0980	1.4660	0.0420	C	0	0				
0.9320	1.9040	1.1710	C	0	0				
0.3190	1.0540	1.9900	O	0	0				
0.9490	3.1020	1.3330	O	0	0				
5.3440	0.5370	0.2120	C	0	0				
3.9510	0.3540	0.1670	C	0	0				
5.8860	1.8320	0.1320	C	0	0				
3.6410	2.7610	-0.0380	C	0	0				
5.0340	2.9440	0.0080	C	0	0				
7.2050	2.0060	0.1750	F	0	0				
-4.0490	-0.5100	-2.9670	H	0	0				
-5.6620	-2.4430	-1.6170	H	0	0				
-5.3150	-3.7490	0.7250	H	0	0				
-3.4780	-2.7980	2.9230	H	0	0				
-2.6710	-4.0870	2.0960	H	0	0				
-1.0070	-2.6210	3.2650	H	0	0				
-0.7610	-2.5320	1.5100	H	0	0				
-1.5820	-1.2250	2.3580	H	0	0				
1.5380	2.4160	-1.8360	H	0	0				
1.5380	0.1870	0.0520	H	0	0				
-0.1450	1.3960	2.7650	H	0	0				
5.9950	-0.3190	0.3080	H	0	0				
3.5410	-0.6430	0.2290	H	0	0				
2.9920	3.6190	-0.1340	H	0	0				
5.4460	3.9410	-0.0540	H	0	0				
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1	2	1	0						
2	3	1	0						
2	6	2	0						
6	7	1	0						
10	11	1	0						
9	10	2	0						
8	9	1	0						
8	7	2	0						
11	7	1	0						
10	12	1	0						
12	13	1	0						
1	14	2	0						
4	15	1	0						
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16	18	1	0						
18	19	1	0						
18	20	2	0						
25	23	2	0						
24	25	1	0						
21	22	2	0						
23	21	1	0						
22	17	1	0						
17	24	2	0						

```

23 26 1 0
6 27 1 0
8 28 1 0
9 29 1 0
12 30 1 0
12 31 1 0
13 32 1 0
13 33 1 0
13 34 1 0
15 35 1 0
16 36 1 0
19 37 1 0
21 38 1 0
22 39 1 0
24 40 1 0
25 41 1 0

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M END

> <Name>

Compound156

> <Activ>

3

> <DB_Ref_id>

15.01

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Compound157

SciTegic10081411483D

```

41 43 0 0 1 0          999 V2000
-2.0880 -1.6860 2.7740 C 0 0
-1.6860 -0.3400 2.3710 C 0 0
-1.0980 -0.3540 0.8030 S 0 0
-1.3670 -2.0220 0.6720 C 0 0
-1.8650 -2.5880 1.7170 N 0 0
-1.7770 0.7460 3.1600 C 0 0
-1.3570 2.0630 2.7030 C 0 0
-1.4160 3.2810 3.3810 C 0 0
-0.8890 4.2130 2.4860 C 0 0
-0.5490 3.4940 1.3320 C 0 0
-0.8340 2.1640 1.4490 O 0 0
0.0630 4.0680 0.0700 C 0 0
0.3590 2.9690 -0.9490 C 0 0
-2.5490 -2.0140 3.8420 O 0 0
-1.1070 -2.7970 -0.4220 N 0 0
-0.5410 -2.1780 -1.6290 C 0 0 3 0 0 0
0.9260 -1.9670 -1.4980 C 0 0
-0.8940 -2.9530 -2.8690 C 0 0
-1.4040 -2.2310 -3.8610 O 0 0
-0.7170 -4.1470 -2.9280 O 0 0
3.1640 -2.8650 -1.1620 C 0 0
1.7770 -3.0640 -1.2850 C 0 0
3.7010 -1.5680 -1.2520 C 0 0
1.4610 -0.6700 -1.5900 C 0 0
2.8460 -0.4710 -1.4670 C 0 0
5.5590 -1.3010 -1.0880 Br 0 0
-2.1740 0.6450 4.1620 H 0 0
-1.7870 3.4670 4.3790 H 0 0
-0.7660 5.2750 2.6500 H 0 0
-0.6090 4.8150 -0.3520 H 0 0

```


0.9710	4.6150	0.3240	H	0	0
0.7790	3.3930	-1.8610	H	0	0
1.0590	2.2400	-0.5390	H	0	0
-0.5550	2.4380	-1.2210	H	0	0
-1.3030	-3.7770	-0.3940	H	0	0
-0.9100	-1.1540	-1.7130	H	0	0
-1.6520	-2.6680	-4.6880	H	0	0
3.8050	-3.7210	-1.0000	H	0	0
1.3710	-4.0630	-1.2150	H	0	0
0.8110	0.1780	-1.7560	H	0	0
3.2420	0.5330	-1.5390	H	0	0

5	1	1	0
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3	4	1	0
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M END

> <Name>

Compound157

> <Activ>

6

> <DB_Ref_id>
15.16

\$\$\$\$

Compound158

SciTegic10081411483D

57	60	0	0	1	0	999	V2000				
-3.2170	-1.8280	1.8960	O	0	0						
-4.4880	-1.4510	1.5700	C	0	0						
-5.4430	-2.3830	1.9980	C	0	0						
-4.7320	-3.4040	2.6290	C	0	0						
-3.3930	-3.0160	2.5370	C	0	0						
-4.7700	-0.1600	0.8320	C	0	0						
-3.4730	0.5640	0.4710	C	0	0						
-2.2110	-3.7090	3.0290	C	0	0						
-0.9770	-3.1950	2.8750	C	0	0						
0.2460	-3.8400	3.3460	C	0	0						
1.3610	-3.0450	3.0230	N	0	0						
1.0410	-1.9610	2.4040	C	0	0						
-0.6170	-1.7400	2.1250	S	0	0						
2.0410	-1.1050	2.0350	N	0	0						
1.7050	0.1390	1.3320	C	0	0	2	0	0	0		
1.1110	-0.1330	-0.0250	C	0	0						
1.8690	-0.7950	-0.9490	N	0	0						
1.2320	-1.0880	-2.4100	S	0	0						
0.7340	0.3610	-3.2030	C	0	0						
2.8710	1.0630	1.2600	C	0	0						
5.2660	1.3650	0.9120	C	0	0						
4.1430	0.5250	0.9860	C	0	0						
5.1230	2.7500	1.1110	C	0	0						
2.7250	2.4530	1.4570	C	0	0						
3.8540	3.2910	1.3850	C	0	0						
-0.8960	1.5760	-4.5390	C	0	0						
-0.4900	0.3950	-3.8950	C	0	0						
-0.0740	2.7150	-4.4900	C	0	0						
1.5550	1.5020	-3.1540	C	0	0						
1.1480	2.6840	-3.8010	C	0	0						
2.2620	-1.7190	-3.2170	O	0	0						
0.0630	-1.9280	-2.2170	O	0	0						
6.4940	3.7750	1.0250	C1	0	0						
-0.0120	0.2230	-0.2970	O	0	0						
0.3300	-4.8970	3.9280	O	0	0						
1.1880	3.1480	1.7890	C1	0	0						
-0.4780	3.8870	-5.1310	N	0	3						
0.2790	4.8540	-5.0550	O	0	5						
-1.5390	3.8590	-5.7110	O	0	0						
-6.5160	-2.3220	1.8650	H	0	0						
-5.1330	-4.2990	3.0860	H	0	0						
-5.3540	-0.3730	-0.0630	H	0	0						
-5.4100	0.4770	1.4430	H	0	0						
-2.8300	-0.0720	-0.1370	H	0	0						
-3.6840	1.4820	-0.0780	H	0	0						
-2.9200	0.8360	1.3690	H	0	0						
-2.3320	-4.6580	3.5310	H	0	0						
2.9920	-1.3340	2.2460	H	0	0						
1.0000	0.7130	1.9360	H	0	0						
2.7990	-1.0960	-0.7400	H	0	0						
6.2350	0.9360	0.7010	H	0	0						
4.2620	-0.5370	0.8320	H	0	0						
3.7440	4.3570	1.5370	H	0	0						

-1.8380	1.6050	-5.0720 H	0	0
-1.1190	-0.4820	-3.9300 H	0	0
2.4940	1.4730	-2.6230 H	0	0
1.7770	3.5630	-3.7660 H	0	0
3	4	1	0	
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15	20	1	0	
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24	25	1	0	
21	22	2	0	
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30	28	2	0	
29	30	1	0	
26	27	2	0	
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27	19	1	0	
19	29	2	0	
18	31	2	0	
18	32	2	0	
23	33	1	0	
16	34	2	0	
10	35	2	0	
24	36	1	0	
28	37	1	0	
5	1	1	0	
4	5	2	0	
37	39	2	0	
37	38	1	0	
3	40	1	0	
4	41	1	0	
6	42	1	0	
6	43	1	0	
7	44	1	0	
7	45	1	0	
7	46	1	0	
8	47	1	0	
14	48	1	0	
15	49	1	0	
17	50	1	0	
21	51	1	0	
22	52	1	0	
25	53	1	0	
26	54	1	0	

```

27 55 1 0
29 56 1 0
30 57 1 0
M CHG 2 37 1 38 -1
M END

```

```

> <Name>
Compound158

```

```

> <Activ>
6.6

```

```

> <DB_Ref_id>
16.09

```

```

$$$$
Compound159
SciTegic10081411483D

```

```

57 60 0 0 1 0          999 V2000
-2.0840 -4.3610 -1.3360 O 0 0
-2.4410 -5.5430 -0.7500 C 0 0
-3.3850 -6.2480 -1.5080 C 0 0
-3.6370 -5.4670 -2.6370 C 0 0
-2.8260 -4.3400 -2.4810 C 0 0
-1.8500 -5.9820 0.5700 C 0 0
-0.8480 -4.9550 1.1000 C 0 0
-2.6840 -3.1910 -3.3630 C 0 0
-1.8500 -2.1760 -3.0720 C 0 0
-1.6640 -0.9980 -3.9160 C 0 0
-0.7320 -0.1270 -3.3240 N 0 0
-0.2730 -0.5700 -2.2030 C 0 0
-0.8850 -2.0720 -1.7070 S 0 0
0.6430 0.1900 -1.5330 N 0 0
1.2130 -0.3120 -0.2750 C 0 0 2 0 0 0
0.5240 0.2830 0.9240 C 0 0
0.3440 1.6370 0.9710 N 0 0
-0.3960 2.2790 2.2600 S 0 0
-0.4530 4.0020 2.1820 C 0 0
2.6880 -0.1190 -0.2270 C 0 0
4.9320 -1.0470 -0.0570 C 0 0
3.5390 -1.2300 -0.1020 C 0 0
5.4750 0.2480 -0.1370 C 0 0
3.2290 1.1760 -0.3070 C 0 0
4.6210 1.3590 -0.2620 C 0 0
-1.7360 6.0710 2.2090 C 0 0
-1.6890 4.6680 2.2710 C 0 0
-0.5450 6.7990 2.0550 C 0 0
0.7360 4.7350 2.0270 C 0 0
0.6910 6.1390 1.9630 C 0 0
-1.7600 1.7770 2.2750 O 0 0
0.3650 1.9010 3.4360 O 0 0
6.7930 0.4220 -0.0940 F 0 0
0.1350 -0.4160 1.8280 O 0 0
-2.2110 -0.7670 -4.9710 O 0 0
-0.5900 8.1940 1.9900 N 0 3
0.4820 8.7810 1.8550 O 0 5
-1.6800 8.7110 2.0740 O 0 0
-3.8300 -7.2050 -1.2680 H 0 0
-4.3120 -5.6860 -3.4510 H 0 0
-2.6500 -6.1460 1.2930 H 0 0
-1.3750 -6.9570 0.4490 H 0 0

```

-0.4320	-5.2790	2.0550	H	0	0
-0.0350	-4.8090	0.3890	H	0	0
-1.3300	-3.9920	1.2560	H	0	0
-3.2640	-3.1600	-4.2740	H	0	0
0.9160	1.0780	-1.9000	H	0	0
1.1270	-1.3980	-0.2500	H	0	0
0.6600	2.2290	0.2280	H	0	0
5.5840	-1.9040	0.0390	H	0	0
3.1290	-2.2260	-0.0410	H	0	0
2.5800	2.0350	-0.4020	H	0	0
5.0330	2.3580	-0.3220	H	0	0
-2.6840	6.5840	2.2770	H	0	0
-2.6020	4.1020	2.3910	H	0	0
1.6860	4.2230	1.9570	H	0	0
1.6060	6.7050	1.8460	H	0	0
3	4	1	0		
1	2	1	0		
2	3	2	0		
2	6	1	0		
6	7	1	0		
5	8	1	0		
8	9	2	0		
12	13	1	0		
11	12	2	0		
10	11	1	0		
10	9	1	0		
13	9	1	0		
12	14	1	0		
14	15	1	0		
15	16	1	0		
16	17	1	0		
17	18	1	0		
18	19	1	0		
15	20	1	0		
25	23	2	0		
24	25	1	0		
21	22	2	0		
23	21	1	0		
22	20	1	0		
20	24	2	0		
30	28	2	0		
29	30	1	0		
26	27	2	0		
28	26	1	0		
27	19	1	0		
19	29	2	0		
18	31	2	0		
18	32	2	0		
23	33	1	0		
16	34	2	0		
10	35	2	0		
28	36	1	0		
5	1	1	0		
4	5	2	0		
36	38	2	0		
36	37	1	0		
3	39	1	0		
4	40	1	0		
6	41	1	0		
6	42	1	0		
7	43	1	0		

```

7 44 1 0
7 45 1 0
8 46 1 0
14 47 1 0
15 48 1 0
17 49 1 0
21 50 1 0
22 51 1 0
24 52 1 0
25 53 1 0
26 54 1 0
27 55 1 0
29 56 1 0
30 57 1 0

```

```
M CHG 2 36 1 37 -1
```

```
M END
```

```
> <Name>
```

```
Compound159
```

```
> <Activ>
```

```
7
```

```
> <DB_Ref_id>
```

```
16.13
```

```
$$$$
```

```
Compound160
```

```
SciTegic10081411483D
```

```

39 41 0 0 0 0          999 V2000
  0.5350 -3.5160 -1.8680 C  0  0
 -0.3810 -1.8110 -0.1660 S  0  0
  0.2850 -3.2790  0.3550 C  0  0
  0.7130 -4.0590 -0.5800 N  0  0
  0.8690 -4.0880 -2.8790 O  0  0
  0.4020 -3.6970  1.6500 N  0  0
 -0.1290 -2.7290  2.8340 S  0  0
  0.6780 -1.2030  2.8340 C  0  0
 -1.5450 -2.4940  2.6030 O  0  0
  0.1430 -3.3890  4.0970 O  0  0
 -0.0700 -0.0140  2.8340 C  0  0
  0.5880  1.2280  2.8340 C  0  0
  2.0820 -1.1540  2.8340 C  0  0
  1.9940  1.2790  2.8340 C  0  0
  2.7400  0.0880  2.8340 C  0  0
  2.6890  2.5940  2.8340 C  0  0
 -0.4000 -1.4260 -2.8270 C  0  0
 -0.0960 -2.2030 -1.7700 C  0  0
 -1.0350 -0.1090 -2.6820 C  0  0
 -1.3220  0.6350 -3.7600 C  0  0
 -1.9530  1.9370 -3.5960 C  0  0
 -2.2270  2.6580 -4.7190 O  0  0
 -2.7990  3.7990 -4.2290 C  0  0
 -2.8830  3.7930 -2.8300 C  0  0
 -2.3300  2.5820 -2.4160 C  0  0
  0.8130 -4.5860  1.8570 H  0  0
 -1.1500 -0.0530  2.8340 H  0  0
  0.0080  2.1390  2.8340 H  0  0
  2.6560 -2.0700  2.8340 H  0  0
  3.8200  0.1190  2.8340 H  0  0
  3.7540  2.4410  3.0150 H  0  0

```

2.4920	3.1090	1.8920 H	0	0
2.2990	3.2110	3.6400 H	0	0
-0.1740	-1.7720	-3.8270 H	0	0
-1.3010	0.3300	-1.7310 H	0	0
-1.1090	0.3120	-4.7700 H	0	0
-3.1450	4.6050	-4.8620 H	0	0
-3.2910	4.5720	-2.2020 H	0	0
-2.2210	2.2210	-1.4030 H	0	0

4	1	1	0
3	4	2	0
2	3	1	0
1	5	2	0
3	6	1	0
6	7	1	0
7	8	1	0
7	9	2	0
7	10	2	0
8	11	2	0
11	12	1	0
8	13	1	0
14	15	1	0
15	13	2	0
12	14	2	0
14	16	1	0
17	18	2	0
2	18	1	0
1	18	1	0
17	19	1	0
19	20	2	0
20	21	1	0
24	25	1	0
23	24	2	0
22	23	1	0
22	21	1	0
25	21	2	0
6	26	1	0
11	27	1	0
12	28	1	0
13	29	1	0
15	30	1	0
16	31	1	0
16	32	1	0
16	33	1	0
17	34	1	0
19	35	1	0
20	36	1	0
23	37	1	0
24	38	1	0
25	39	1	0


```

M  END
> <Name>
Compound160

> <Activ>
5

> <DB_Ref_id>
17.53

$$$$
Compound161

```

SciTegic10081411483D

50	53	0	0	0	0	999	V2000
-1.5630	-4.3460	1.7540	C	0	0		
-1.8400	-1.9530	0.8380	S	0	0		
-3.0800	-3.0940	0.6640	C	0	0		
-2.8360	-4.2600	1.1600	N	0	0		
-1.1390	-5.3510	2.2750	O	0	0		
-4.2890	-2.8890	0.0610	N	0	0		
-4.6060	-1.4300	-0.5660	S	0	0		
-3.4710	-0.9880	-1.7870	C	0	0		
-5.9260	-1.4920	-1.1720	O	0	0		
-4.5180	-0.4610	0.5120	O	0	0		
-3.2440	-1.8460	-2.8770	C	0	0		
-2.3180	-1.4860	-3.8730	C	0	0		
-2.7730	0.2290	-1.6890	C	0	0		
-1.6190	-0.2690	-3.7750	C	0	0		
-1.8480	0.5880	-2.6840	C	0	0		
-0.6390	0.1110	-4.8280	C	0	0		
0.3670	-2.8300	2.1070	C	0	0		
1.0200	-1.4960	1.9550	C	0	0		
2.3930	-1.4120	1.6680	C	0	0		
3.0080	-0.1560	1.5230	C	0	0		
2.2480	1.0220	1.6680	C	0	0		
0.8710	0.9360	1.9550	C	0	0		
0.2600	-0.3200	2.1000	C	0	0		
2.8460	2.2480	1.5270	N	0	0		
2.1130	3.5000	1.5510	C	0	0		
3.1430	4.5370	1.0900	C	0	0		
4.4880	3.9280	1.5200	C	0	0		
4.2740	2.4220	1.3420	C	0	0		
-0.8710	-3.0640	1.6350	C	0	0		
-4.9590	-3.6290	0.0100	H	0	0		
-3.7810	-2.7790	-2.9530	H	0	0		
-2.1480	-2.1480	-4.7090	H	0	0		
-2.9470	0.8870	-0.8500	H	0	0		
-1.3130	1.5240	-2.6040	H	0	0		
-0.2130	1.0860	-4.5920	H	0	0		
0.1170	-0.6680	-4.9200	H	0	0		
-1.1500	0.1940	-5.7870	H	0	0		
0.9140	-3.6150	2.6110	H	0	0		
2.9840	-2.3080	1.5570	H	0	0		
4.0650	-0.1110	1.3030	H	0	0		
0.2710	1.8280	2.0700	H	0	0		
-0.7970	-0.3770	2.3200	H	0	0		
1.7810	3.7050	2.5590	H	0	0		
1.2520	3.4710	0.8980	H	0	0		
3.1110	4.6350	0.0140	H	0	0		
2.9710	5.5140	1.5180	H	0	0		
4.6800	4.1560	2.5590	H	0	0		
5.3180	4.3010	0.9390	H	0	0		
4.8440	1.8480	2.0590	H	0	0		
4.5490	2.1080	0.3460	H	0	0		
4	1	1	0				
3	4	2	0				
2	3	1	0				
1	5	2	0				
3	6	1	0				
6	7	1	0				
7	8	1	0				
7	9	2	0				


```

7 10 2 0
8 11 2 0
11 12 1 0
8 13 1 0
14 15 1 0
15 13 2 0
12 14 2 0
14 16 1 0
17 18 1 0
22 23 2 0
21 22 1 0
20 21 2 0
19 20 1 0
23 18 1 0
18 19 2 0
28 24 1 0
27 28 1 0
26 27 1 0
24 25 1 0
25 26 1 0
24 21 1 0
17 29 2 0
2 29 1 0
1 29 1 0
6 30 1 0
11 31 1 0
12 32 1 0
13 33 1 0
15 34 1 0
16 35 1 0
16 36 1 0
16 37 1 0
17 38 1 0
19 39 1 0
20 40 1 0
22 41 1 0
23 42 1 0
25 43 1 0
25 44 1 0
26 45 1 0
26 46 1 0
27 47 1 0
27 48 1 0
28 49 1 0
28 50 1 0
M END
> <Name>
Compound161

> <Activ>
1.4

> <DB_Ref_id>
17.5

$$$$
Compound162
SciTegic10081411483D

56 59 0 0 0 0 999 V2000
2.1070 5.3790 -1.1000 C 0 0

```

2.1390	2.9730	-0.1800	S	0	0
3.3440	4.0820	0.2560	C	0	0
3.2300	5.2560	-0.2620	N	0	0
1.8220	6.3990	-1.6840	O	0	0
4.3980	3.8420	1.0920	N	0	0
4.5490	2.3690	1.7500	S	0	0
3.1840	1.9490	2.7190	C	0	0
4.6480	1.4120	0.6620	O	0	0
5.7250	2.3910	2.6040	O	0	0
2.7380	2.8280	3.7210	C	0	0
1.6270	2.4880	4.5080	C	0	0
2.5200	0.7310	2.5020	C	0	0
0.9590	1.2680	4.2930	C	0	0
1.4060	0.3910	3.2890	C	0	0
-0.2170	0.9060	5.1270	C	0	0
0.2560	3.9160	-1.8610	C	0	0
-0.4430	2.5960	-1.8610	C	0	0
-1.8500	2.5430	-1.8610	C	0	0
-2.5080	1.3010	-1.8610	C	0	0
-1.7620	0.1090	-1.8610	C	0	0
-0.3560	0.1600	-1.8610	C	0	0
0.3030	1.4020	-1.8610	C	0	0
-2.4550	-1.2010	-1.8610	C	0	0
-4.1470	-1.3850	-1.8610	S	0	0
-4.0370	-3.0680	-1.8610	C	0	0
-2.6950	-3.4670	-1.8610	C	0	0
-1.8150	-2.4120	-1.8610	N	0	0
1.3770	4.1150	-1.1420	C	0	0
-2.1900	-4.8930	-1.8610	C	0	0
-2.0590	-4.9880	-3.3810	C	0	0
-3.2360	-5.8520	-1.2970	C	0	0
-0.8420	-5.0020	-1.1440	C	0	0
5.0610	4.5650	1.2870	H	0	0
3.2500	3.7660	3.8850	H	0	0
1.2870	3.1660	5.2780	H	0	0
2.8610	0.0570	1.7310	H	0	0
0.8980	-0.5490	3.1190	H	0	0
-0.6720	-0.0060	4.7400	H	0	0
0.0900	0.8150	6.1700	H	0	0
-0.9630	1.7010	5.0690	H	0	0
-0.1580	4.7190	-2.4550	H	0	0
-2.4300	3.4530	-1.8610	H	0	0
-3.5880	1.2680	-1.8610	H	0	0
0.2230	-0.7520	-1.8610	H	0	0
1.3830	1.4340	-1.8610	H	0	0
-4.8910	-3.7340	-1.8610	H	0	0
-1.3500	-4.2580	-3.7750	H	0	0
-3.0200	-4.8130	-3.8630	H	0	0
-1.7130	-5.9790	-3.6760	H	0	0
-4.1620	-5.8240	-1.8710	H	0	0
-3.4770	-5.5980	-0.2660	H	0	0
-2.8670	-6.8770	-1.3100	H	0	0
-0.9060	-4.6760	-0.1050	H	0	0
-0.0920	-4.3870	-1.6410	H	0	0
-0.4860	-6.0310	-1.1480	H	0	0
4	1	1	0		
3	4	2	0		
2	3	1	0		
1	5	2	0		
3	6	1	0		
6	7	1	0		

7	8	1	0
7	9	2	0
7	10	2	0
8	11	2	0
11	12	1	0
8	13	1	0
14	15	1	0
15	13	2	0
12	14	2	0
14	16	1	0
17	18	1	0
22	23	2	0
21	22	1	0
20	21	2	0
19	20	1	0
23	18	1	0
18	19	2	0
28	24	2	0
27	28	1	0
26	27	2	0
24	25	1	0
25	26	1	0
24	21	1	0
17	29	2	0
2	29	1	0
1	29	1	0
27	30	1	0
30	31	1	0
30	32	1	0
30	33	1	0
6	34	1	0
11	35	1	0
12	36	1	0
13	37	1	0
15	38	1	0
16	39	1	0
16	40	1	0
16	41	1	0
17	42	1	0
19	43	1	0
20	44	1	0
22	45	1	0
23	46	1	0
26	47	1	0
31	48	1	0
31	49	1	0
31	50	1	0
32	51	1	0
32	52	1	0
32	53	1	0
33	54	1	0
33	55	1	0
33	56	1	0

M END

> <Name>

Compound162

> <Activ>

4.9

> <DB_Ref_id>

17.47

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Compound163

SciTegic10081411483D

40	42	0	0	0	0	999	V2000
3.9770	0.4620	-0.0040	C	0	0		
3.0210	1.5670	-0.0010	C	0	0		
1.4530	0.9790	-0.0050	S	0	0		
2.0090	-0.6220	-0.0050	C	0	0		
3.2900	-0.7650	-0.0050	N	0	0		
5.1840	0.5490	-0.0040	O	0	0		
3.3670	2.8680	0.0050	C	0	0		
2.3660	3.9250	0.0070	C	0	0		
1.0530	3.5590	0.0040	O	0	0		
0.3920	4.7550	0.0080	C	0	0		
1.2700	5.8470	0.0130	C	0	0		
2.5570	5.3080	0.0130	C	0	0		
1.2320	-1.7460	-0.0050	N	0	0		
-0.3790	-1.5800	-0.0050	S	0	0		
-1.1870	-3.1040	-0.0050	C	0	0		
-0.7450	-0.8690	1.2080	O	0	0		
-0.7450	-0.8690	-1.2170	O	0	0		
-3.2520	-4.3940	-0.0050	C	0	0		
-2.5920	-3.1520	-0.0050	C	0	0		
-2.4990	-5.5800	-0.0050	C	0	0		
-0.4370	-4.2940	-0.0050	C	0	0		
-1.0940	-5.5370	-0.0050	C	0	0		
-1.1200	4.8270	0.0050	C	0	0		
-1.7410	3.4290	-0.0030	C	0	0		
-3.1520	-6.8130	-0.0050	N	0	3		
-2.4450	-7.8200	-0.0050	O	0	5		
-4.3620	-6.7940	-0.0050	O	0	0		
4.4120	3.1400	0.0070	H	0	0		
1.0040	6.8960	0.0170	H	0	0		
3.4960	5.8460	0.0170	H	0	0		
1.6410	-2.6590	-0.0050	H	0	0		
-4.3310	-4.4340	-0.0050	H	0	0		
-3.1660	-2.2370	-0.0050	H	0	0		
0.6420	-4.2550	-0.0050	H	0	0		
-0.5210	-6.4530	-0.0050	H	0	0		
-1.4580	5.3930	0.8730	H	0	0		
-1.4550	5.4020	-0.8570	H	0	0		
-2.8290	3.4910	0.0060	H	0	0		
-1.4230	2.8720	-0.8850	H	0	0		
-1.4320	2.8650	0.8770	H	0	0		
3	4	1	0				
1	2	1	0				
2	3	1	0				
1	6	2	0				
2	7	2	0				
7	8	1	0				
11	12	1	0				
10	11	2	0				
9	10	1	0				
9	8	1	0				
12	8	2	0				
4	13	1	0				
13	14	1	0				
14	15	1	0				

```

14 16 2 0
14 17 2 0
22 20 2 0
21 22 1 0
18 19 2 0
20 18 1 0
19 15 1 0
15 21 2 0
10 23 1 0
23 24 1 0
20 25 1 0
5 1 1 0
4 5 2 0
25 27 2 0
25 26 1 0
7 28 1 0
11 29 1 0
12 30 1 0
13 31 1 0
18 32 1 0
19 33 1 0
21 34 1 0
22 35 1 0
23 36 1 0
23 37 1 0
24 38 1 0
24 39 1 0
24 40 1 0
M CHG 2 25 1 26 -1
M END
> <Name>
Compound163

> <Activ>
3.2

> <DB_Ref_id>
17.4

$$$$
Compound164
SciTegic10081411483D

41 43 0 0 0 0 999 V2000
3.5670 1.1860 -1.8580 C 0 0
2.1270 1.0270 -2.0430 C 0 0
1.3340 1.1620 -0.5720 S 0 0
2.7990 1.4140 0.2420 C 0 0
3.8540 1.4060 -0.5000 N 0 0
4.4160 1.1390 -2.7190 O 0 0
1.5330 0.8090 -3.2310 C 0 0
0.0900 0.6600 -3.3500 C 0 0
-0.6580 0.7910 -2.2190 O 0 0
-1.9370 0.6020 -2.6640 C 0 0
-1.9880 0.3550 -4.0430 C 0 0
-0.6680 0.3950 -4.4900 C 0 0
2.9510 1.6210 1.5840 N 0 0
1.6330 1.6330 2.5250 S 0 0
0.8260 0.1070 2.5250 C 0 0
2.0680 1.9200 3.8810 O 0 0
0.7250 2.6310 1.9920 O 0 0

```

-1.2360	-1.1820	2.5250	C	0	0
-0.5780	0.0610	2.5250	C	0	0
-0.4900	-2.3750	2.5250	C	0	0
1.5740	-1.0800	2.5250	C	0	0
0.9160	-2.3220	2.5250	C	0	0
-3.1210	0.6600	-1.7230	C	0	0
-2.6720	0.8960	-0.2810	C	0	0
-1.1860	-3.6880	2.5250	C	0	0
-0.2620	-4.6950	2.6230	F	0	0
-1.8950	-3.8300	1.3590	F	0	0
-2.0450	-3.7500	3.5920	F	0	0
2.1410	0.7380	-4.1210	H	0	0
-2.8730	0.1740	-4.6390	H	0	0
-0.3120	0.2500	-5.5020	H	0	0
3.8560	1.7660	1.9860	H	0	0
-2.3160	-1.2150	2.5250	H	0	0
-1.1520	0.9750	2.5250	H	0	0
2.6540	-1.0430	2.5250	H	0	0
1.4960	-3.2340	2.5250	H	0	0
-3.8050	1.4450	-2.0490	H	0	0
-3.6950	-0.2640	-1.8030	H	0	0
-2.1450	1.8460	-0.1940	H	0	0
-3.5290	0.9020	0.3920	H	0	0
-1.9960	0.1070	0.0470	H	0	0
1	2	1	0		
2	3	1	0		
1	6	2	0		
2	7	2	0		
7	8	1	0		
11	12	1	0		
10	11	2	0		
9	10	1	0		
9	8	1	0		
12	8	2	0		
4	13	1	0		
13	14	1	0		
14	15	1	0		
14	16	2	0		
14	17	2	0		
22	20	2	0		
21	22	1	0		
18	19	2	0		
20	18	1	0		
19	15	1	0		
15	21	2	0		
10	23	1	0		
23	24	1	0		
20	25	1	0		
5	1	1	0		
4	5	2	0		
3	4	1	0		
25	28	1	0		
25	27	1	0		
25	26	1	0		
7	29	1	0		
11	30	1	0		
12	31	1	0		
13	32	1	0		
18	33	1	0		
19	34	1	0		
21	35	1	0		

5.2700	2.5250	-5.8980 H	0	0
5.0370	3.9570	-4.8730 H	0	0
5.2720	2.3710	-4.1420 H	0	0

5	1	1	0
4	5	2	0
3	4	1	0
1	2	1	0
2	3	1	0
1	6	2	0
2	7	1	0
7	8	1	0
10	11	1	0
9	8	1	0
11	8	2	0
4	12	1	0
12	13	1	0
13	14	1	0
13	15	2	0
13	16	2	0
21	19	2	0
20	21	1	0
17	18	2	0
19	17	1	0
18	14	1	0
14	20	2	0
19	22	1	0
9	23	1	0
23	10	2	0
23	24	1	0
24	25	1	0
2	26	1	0
7	27	1	0
7	28	1	0
10	29	1	0
11	30	1	0
12	31	1	0
17	32	1	0
18	33	1	0
20	34	1	0
21	35	1	0
22	36	1	0
22	37	1	0
22	38	1	0
24	39	1	0
24	40	1	0
25	41	1	0
25	42	1	0
25	43	1	0

M END

> <Name>

Compound165

> <Activ>

7.3

> <DB_Ref_id>

17.23

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Compound166

SciTegic10081411483D

41	43	0	0	0	0	999	V2000
0.6010	-3.5330	-2.0820	C	0	0		
-0.0330	-2.2250	-1.9710	C	0	0		
-0.2970	-1.8400	-0.3610	S	0	0		
0.3850	-3.3090	0.1430	C	0	0		
0.8010	-4.0800	-0.8030	N	0	0		
0.9220	-4.0980	-3.1030	O	0	0		
-0.3580	-1.4450	-3.0210	C	0	0		
-0.9880	-0.1480	-2.8200	C	0	0		
-1.2380	0.2460	-1.5410	O	0	0		
-1.8200	1.4730	-1.6970	C	0	0		
-1.9340	1.8400	-3.0450	C	0	0		
-1.3910	0.7830	-3.7770	C	0	0		
0.5230	-3.7300	1.4340	N	0	0		
0.0040	-2.7680	2.6290	S	0	0		
0.8120	-1.2440	2.6290	C	0	0		
-1.4140	-2.5330	2.4160	O	0	0		
0.2930	-3.4380	3.8850	O	0	0		
0.7230	1.1880	2.6290	C	0	0		
0.0640	-0.0550	2.6290	C	0	0		
2.1290	1.2400	2.6290	C	0	0		
2.2170	-1.1950	2.6290	C	0	0		
2.8750	0.0470	2.6290	C	0	0		
2.8240	2.5530	2.6290	C	0	0		
-2.2700	2.2910	-0.5060	C	0	0		
-2.5220	3.1210	-3.5980	C	0	0		
-0.1470	-1.7810	-4.0250	H	0	0		
-1.3030	0.7070	-4.8530	H	0	0		
0.9390	-4.6190	1.6310	H	0	0		
0.1420	2.1000	2.6290	H	0	0		
-1.0160	-0.0940	2.6290	H	0	0		
2.7910	-2.1090	2.6290	H	0	0		
3.9550	0.0800	2.6290	H	0	0		
3.8910	2.3990	2.7910	H	0	0		
2.6110	3.0760	1.6970	H	0	0		
2.4470	3.1640	3.4490	H	0	0		
-2.0880	1.8180	0.4590	H	0	0		
-3.3400	2.4880	-0.5840	H	0	0		
-1.7540	3.2520	-0.5080	H	0	0		
-2.5040	3.1900	-4.6850	H	0	0		
-1.9730	3.9750	-3.1990	H	0	0		
-3.5590	3.2130	-3.2750	H	0	0		
5	1	1	0				
4	5	2	0				
3	4	1	0				
1	2	1	0				
2	3	1	0				
1	6	2	0				
2	7	2	0				
7	8	1	0				
11	12	1	0				
10	11	2	0				
9	10	1	0				
9	8	1	0				
12	8	2	0				
4	13	1	0				
13	14	1	0				
14	15	1	0				
14	16	2	0				
14	17	2	0				

```

22 20 2 0
21 22 1 0
18 19 2 0
20 18 1 0
19 15 1 0
15 21 2 0
20 23 1 0
10 24 1 0
11 25 1 0
7 26 1 0
12 27 1 0
13 28 1 0
18 29 1 0
19 30 1 0
21 31 1 0
22 32 1 0
23 33 1 0
23 34 1 0
23 35 1 0
24 36 1 0
24 37 1 0
24 38 1 0
25 39 1 0
25 40 1 0
25 41 1 0

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M END

> <Name>

Compound166

> <Activ>

3.2

> <DB_Ref_id>

17.15

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Compound167

SciTegic10081411483D

```

41 43 0 0 0 0          999 V2000
-0.7580 3.4240 2.2850 C 0 0
-0.1210 2.1110 2.2180 C 0 0
0.1920 1.6970 0.6270 S 0 0
-0.4670 3.1580 0.0720 C 0 0
-0.9120 3.9470 0.9880 N 0 0
-1.1130 4.0080 3.2830 O 0 0
0.1680 1.3530 3.2930 C 0 0
0.8050 0.0530 3.1620 C 0 0
1.1040 -0.3870 1.9080 O 0 0
1.6780 -1.6080 2.1290 C 0 0
1.7350 -1.9280 3.4920 C 0 0
1.1660 -0.8480 4.1660 C 0 0
-0.5600 3.5590 -1.2310 N 0 0
-0.0020 2.5740 -2.3890 S 0 0
-0.8100 1.0510 -2.3890 C 0 0
-0.2480 3.2230 -3.6660 O 0 0
1.4080 2.3460 -2.1250 O 0 0
-2.8730 -0.2400 -2.3890 C 0 0
-2.2150 1.0020 -2.3890 C 0 0
-2.1250 -1.4320 -2.3890 C 0 0
-0.0620 -0.1390 -2.3890 C 0 0

```

-0.7210	-1.3810	-2.3890	C	0	0
-2.8220	-2.7460	-2.3890	C	0	0
2.1720	-2.4710	0.9880	C	0	0
3.3690	-1.8260	0.2870	C	0	0
-0.0780	1.7190	4.2810	H	0	0
2.1390	-2.8300	3.9310	H	0	0
1.0370	-0.7350	5.2340	H	0	0
-0.9650	4.4390	-1.4730	H	0	0
-3.9510	-0.2740	-2.3890	H	0	0
-2.7890	1.9160	-2.3890	H	0	0
1.0180	-0.1000	-2.3890	H	0	0
-0.1400	-2.2930	-2.3890	H	0	0
-2.1540	-3.6080	-2.3890	H	0	0
-3.4590	-2.8190	-3.2700	H	0	0
-3.4590	-2.8190	-1.5100	H	0	0
2.4340	-3.4590	1.3670	H	0	0
1.3600	-2.6430	0.2830	H	0	0
3.7310	-2.4630	-0.5220	H	0	0
3.0980	-0.8540	-0.1210	H	0	0
4.1920	-1.6780	0.9860	H	0	0
5	1	1	0		
4	5	2	0		
3	4	1	0		
1	2	1	0		
2	3	1	0		
1	6	2	0		
2	7	2	0		
7	8	1	0		
11	12	1	0		
10	11	2	0		
9	10	1	0		
9	8	1	0		
12	8	2	0		
4	13	1	0		
13	14	1	0		
14	15	1	0		
14	16	2	0		
14	17	2	0		
22	20	2	0		
21	22	1	0		
18	19	2	0		
20	18	1	0		
19	15	1	0		
15	21	2	0		
20	23	1	0		
10	24	1	0		
24	25	1	0		
7	26	1	0		
11	27	1	0		
12	28	1	0		
13	29	1	0		
18	30	1	0		
19	31	1	0		
21	32	1	0		
22	33	1	0		
23	34	1	0		
23	35	1	0		
23	36	1	0		
24	37	1	0		
24	38	1	0		
25	39	1	0		

25 40 1 0
25 41 1 0

M END

> <Name>

Compound167

> <Activ>

1.4

> <DB_Ref_id>

17.13

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Compound168

SciTegic10081411483D

35 37 0 0 0 0 999 V2000

0.0160	-2.9820	2.5000	C	0	0
-0.4980	-1.6270	2.3300	C	0	0
-0.7090	-1.2830	0.7030	S	0	0
-0.1580	-2.8260	0.2660	C	0	0
0.1780	-3.5960	1.2440	N	0	0
0.2720	-3.5330	3.5470	O	0	0
-0.7600	-0.7810	3.3440	C	0	0
-1.2710	0.5570	3.0860	C	0	0
-1.4430	0.9320	1.7870	O	0	0
-1.9220	2.2070	1.8970	C	0	0
-2.0490	2.6290	3.2250	C	0	0
-1.6250	1.5510	4.0040	C	0	0
-0.0430	-3.3110	-1.0080	N	0	0
-0.5140	-2.3730	-2.2420	S	0	0
0.2950	-0.8500	-2.2420	C	0	0
-0.1760	-3.0700	-3.4710	O	0	0
-1.9370	-2.1350	-2.0920	O	0	0
0.2050	1.5820	-2.2420	C	0	0
-0.4530	0.3400	-2.2420	C	0	0
1.6110	1.6330	-2.2420	C	0	0
1.6990	-0.8010	-2.2420	C	0	0
2.3580	0.4410	-2.2420	C	0	0
2.3070	2.9470	-2.2420	C	0	0
-2.3360	3.2050	0.3580	Br	0	0
-0.5920	-1.0940	4.3650	H	0	0
-2.4020	3.5880	3.5800	H	0	0
-1.5780	1.4980	5.0820	H	0	0
0.3260	-4.2270	-1.1660	H	0	0
-0.3750	2.4940	-2.2420	H	0	0
-1.5330	0.3010	-2.2420	H	0	0
2.2740	-1.7150	-2.2420	H	0	0
3.4380	0.4750	-2.2420	H	0	0
3.3670	2.7970	-2.0370	H	0	0
2.1290	3.4530	-3.1910	H	0	0
1.9000	3.5740	-1.4490	H	0	0

5 1 1 0

4 5 2 0

3 4 1 0

1 2 1 0

2 3 1 0

1 6 2 0

2 7 2 0

7 8 1 0

11 12 1 0

```

10 11 2 0
9 10 1 0
9 8 1 0
12 8 2 0
4 13 1 0
13 14 1 0
14 15 1 0
14 16 2 0
14 17 2 0
22 20 2 0
21 22 1 0
18 19 2 0
20 18 1 0
19 15 1 0
15 21 2 0
20 23 1 0
10 24 1 0
7 25 1 0
11 26 1 0
12 27 1 0
13 28 1 0
18 29 1 0
19 30 1 0
21 31 1 0
22 32 1 0
23 33 1 0
23 34 1 0
23 35 1 0

```

M END

> <Name>

Compound168

> <Activ>

2.7

> <DB_Ref_id>

17.12

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Compound169

SciTegic10081411483D

```

35 37 0 0 0 0          999 V2000
  0.0120 -2.9880  2.5040 C  0 0
 -0.4980 -1.6290  2.3340 C  0 0
 -0.7070 -1.2870  0.7070 S  0 0
 -0.1580 -2.8300  0.2700 C  0 0
  0.1760 -3.6000  1.2480 N  0 0
  0.2680 -3.5390  3.5510 O  0 0
 -0.7580 -0.7830  3.3480 C  0 0
 -1.2660  0.5550  3.0900 C  0 0
 -1.4390  0.9320  1.7910 O  0 0
 -1.9140  2.2070  1.9000 C  0 0
 -2.0390  2.6270  3.2310 C  0 0
 -1.6150  1.5490  4.0080 C  0 0
 -0.0430 -3.3120 -1.0040 N  0 0
 -0.5140 -2.3770 -2.2380 S  0 0
  0.2930 -0.8510 -2.2380 C  0 0
 -0.1760 -3.0720 -3.4670 O  0 0
 -1.9390 -2.1390 -2.0880 O  0 0
  0.2030  1.5780 -2.2380 C  0 0

```

-0.4550	0.3380	-2.2380	C	0	0
1.6090	1.6310	-2.2380	C	0	0
1.6970	-0.8030	-2.2380	C	0	0
2.3560	0.4400	-2.2380	C	0	0
2.3050	2.9440	-2.2380	C	0	0
-2.3630	3.2970	0.2250	I	0	0
-0.5900	-1.0980	4.3690	H	0	0
-2.3910	3.5880	3.5840	H	0	0
-1.5680	1.4960	5.0880	H	0	0
0.3240	-4.2280	-1.1620	H	0	0
-0.3750	2.4900	-2.2380	H	0	0
-1.5330	0.2990	-2.2380	H	0	0
2.2720	-1.7190	-2.2380	H	0	0
3.4360	0.4710	-2.2380	H	0	0
3.3650	2.7930	-2.0330	H	0	0
2.1270	3.4490	-3.1880	H	0	0
1.8990	3.5700	-1.4450	H	0	0

5	1	1	0
4	5	2	0
3	4	1	0
1	2	1	0
2	3	1	0
1	6	2	0
2	7	2	0
7	8	1	0
11	12	1	0
10	11	2	0
9	10	1	0
9	8	1	0
12	8	2	0
4	13	1	0
13	14	1	0
14	15	1	0
14	16	2	0
14	17	2	0
22	20	2	0
21	22	1	0
18	19	2	0
20	18	1	0
19	15	1	0
15	21	2	0
20	23	1	0
10	24	1	0
7	25	1	0
11	26	1	0
12	27	1	0
13	28	1	0
18	29	1	0
19	30	1	0
21	31	1	0
22	32	1	0
23	33	1	0
23	34	1	0
23	35	1	0

M END

> <Name>

Compound169

> <Activ>

2.8

> <DB_Ref_id>
17.11

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Compound170

SciTegic10081411483D

37	40	0	0	0	0	999	V2000
-0.5980	1.6660	1.6310	S	0	0		
-1.0960	2.3400	3.1270	C	0	0		
-1.2850	1.2950	3.9650	N	0	0		
-1.0510	0.0720	3.4510	N	0	0		
-0.6560	0.0370	2.1600	C	0	0		
-0.3360	-1.1580	1.3550	N	0	0		
0.0410	-1.1380	0.1230	C	0	0		
0.1840	0.0780	-0.5920	N	0	0		
0.6000	-0.1620	-1.9100	C	0	0		
0.7620	-1.5970	-2.1580	C	0	0		
0.4060	-2.5120	-0.7950	S	0	0		
0.7910	0.7250	-2.7110	O	0	0		
-1.2810	3.7740	3.4380	C	0	0		
-1.0410	4.7440	2.4490	C	0	0		
-1.2170	6.1080	2.7420	C	0	0		
-1.6350	6.5040	4.0270	C	0	0		
-1.8730	5.5320	5.0180	C	0	0		
-1.6970	4.1700	4.7210	C	0	0		
-1.8510	8.1660	4.3850	Cl	0	0		
1.1510	-2.1010	-3.3460	C	0	0		
1.3050	-3.5800	-3.5590	C	0	0		
0.3260	-5.8140	-3.6840	C	0	0		
0.1740	-4.4300	-3.4840	C	0	0		
1.5920	-6.3550	-3.9570	C	0	0		
2.5780	-4.1310	-3.8320	C	0	0		
2.7130	-5.5170	-4.0290	C	0	0		
-1.3980	-3.8140	-3.1560	Cl	0	0		
3.9850	-3.1460	-3.9300	Cl	0	0		
0.0160	0.9940	-0.2230	H	0	0		
-0.7190	4.4480	1.4610	H	0	0		
-1.0310	6.8420	1.9730	H	0	0		
-2.1910	5.8210	6.0080	H	0	0		
-1.8830	3.4280	5.4860	H	0	0		
1.3600	-1.4390	-4.1740	H	0	0		
-0.5270	-6.4760	-3.6290	H	0	0		
1.7010	-7.4200	-4.1090	H	0	0		
3.6800	-5.9530	-4.2420	H	0	0		
5	1	1	0				
4	5	2	0				
3	4	1	0				
1	2	1	0				
2	3	2	0				
5	6	1	0				
6	7	2	0				
10	11	1	0				
9	10	1	0				
8	9	1	0				
8	7	1	0				
11	7	1	0				
9	12	2	0				
2	13	1	0				
17	18	2	0				
16	17	1	0				

```

15 16 2 0
14 15 1 0
18 13 1 0
13 14 2 0
16 19 1 0
10 20 2 0
20 21 1 0
26 24 2 0
25 26 1 0
22 23 2 0
24 22 1 0
23 21 1 0
21 25 2 0
23 27 1 0
25 28 1 0
8 29 1 0
14 30 1 0
15 31 1 0
17 32 1 0
18 33 1 0
20 34 1 0
22 35 1 0
24 36 1 0
26 37 1 0
M END
> <Name>
Compound170

> <Activ>
5.6

> <DB_Ref_id>
18.24

$$$$
Compound171
SciTegic10081411483D

37 40 0 0 0 0 999 V2000
1.9690 1.3710 -0.5680 S 0 0
2.8090 2.8650 -0.6520 C 0 0
1.8630 3.8150 -0.8240 N 0 0
0.5900 3.3850 -0.8810 N 0 0
0.4080 2.0530 -0.7620 C 0 0
-0.8650 1.3200 -0.7870 N 0 0
-1.0820 0.1890 -0.2070 C 0 0
-0.0700 -0.4710 0.5370 N 0 0
-0.5490 -1.6800 1.0660 C 0 0
-1.9490 -1.9000 0.6930 C 0 0
-2.5530 -0.6450 -0.2460 S 0 0
0.1330 -2.4200 1.7380 O 0 0
4.2720 3.0680 -0.5570 C 0 0
4.8110 4.3630 -0.6460 C 0 0
6.1990 4.5590 -0.5550 C 0 0
7.0550 3.4550 -0.3790 C 0 0
6.5160 2.1580 -0.2890 C 0 0
5.1250 1.9650 -0.3790 C 0 0
8.7500 3.6900 -0.2710 C1 0 0
-2.6500 -2.9880 1.0680 C 0 0
-4.0760 -3.1700 0.6660 C 0 0
-5.8910 -4.6170 -0.0800 C 0 0

```


-4.5470	-4.4450	0.2970	C	0	0
-6.7640	-3.5160	-0.0920	C	0	0
-4.9510	-2.0700	0.6540	C	0	0
-6.2950	-2.2420	0.2750	C	0	0
-6.3340	-5.8220	-0.4300	F	0	0
0.8630	-0.1370	0.6780	H	0	0
4.1580	5.2150	-0.7830	H	0	0
6.5980	5.5610	-0.6230	H	0	0
7.1600	1.3010	-0.1520	H	0	0
4.7190	0.9670	-0.3090	H	0	0
-2.1840	-3.7520	1.6720	H	0	0
-3.8770	-5.2950	0.3050	H	0	0
-7.7970	-3.6450	-0.3810	H	0	0
-4.6000	-1.0880	0.9360	H	0	0
-6.9650	-1.3970	0.2680	H	0	0

5	1	1	0
4	5	2	0
3	4	1	0
1	2	1	0
2	3	2	0
5	6	1	0
6	7	2	0
10	11	1	0
9	10	1	0
8	9	1	0
8	7	1	0
11	7	1	0
9	12	2	0
2	13	1	0
17	18	2	0
16	17	1	0
15	16	2	0
14	15	1	0
18	13	1	0
13	14	2	0
16	19	1	0
10	20	2	0
20	21	1	0
26	24	2	0
25	26	1	0
22	23	2	0
24	22	1	0
23	21	1	0
21	25	2	0
22	27	1	0
8	28	1	0
14	29	1	0
15	30	1	0
17	31	1	0
18	32	1	0
20	33	1	0
23	34	1	0
24	35	1	0
25	36	1	0
26	37	1	0


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M  END
> <Name>
Compound171

> <Activ>
48.2

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> <DB_Ref_id>
18.19

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Compound172

SciTegic10081411483D

37	40	0	0	0	0	999	V2000
1.9650	1.3670	-0.5700	S	0	0		
2.8030	2.8600	-0.6540	C	0	0		
1.8580	3.8110	-0.8260	N	0	0		
0.5860	3.3810	-0.8830	N	0	0		
0.4020	2.0470	-0.7640	C	0	0		
-0.8710	1.3170	-0.7910	N	0	0		
-1.0880	0.1860	-0.2090	C	0	0		
-0.0740	-0.4750	0.5350	N	0	0		
-0.5550	-1.6850	1.0640	C	0	0		
-1.9530	-1.9040	0.6910	C	0	0		
-2.5590	-0.6480	-0.2480	S	0	0		
0.1290	-2.4240	1.7360	O	0	0		
4.2680	3.0650	-0.5610	C	0	0		
4.8050	4.3600	-0.6490	C	0	0		
6.1940	4.5530	-0.5570	C	0	0		
7.0490	3.4510	-0.3810	C	0	0		
6.5100	2.1520	-0.2910	C	0	0		
5.1210	1.9610	-0.3810	C	0	0		
8.7440	3.6860	-0.2730	Cl	0	0		
-2.6540	-2.9920	1.0660	C	0	0		
-4.0820	-3.1760	0.6640	C	0	0		
-5.9060	-4.6020	-0.0960	C	0	0		
-4.5610	-4.4450	0.2810	C	0	0		
-6.7730	-3.4980	-0.0900	C	0	0		
-4.9530	-2.0700	0.6680	C	0	0		
-6.2970	-2.2320	0.2910	C	0	0		
-3.7500	-5.5020	0.2710	F	0	0		
0.8590	-0.1420	0.6740	H	0	0		
4.1540	5.2110	-0.7850	H	0	0		
6.5940	5.5570	-0.6250	H	0	0		
7.1550	1.2970	-0.1540	H	0	0		
4.7130	0.9630	-0.3110	H	0	0		
-2.1890	-3.7560	1.6700	H	0	0		
-6.2770	-5.5740	-0.3890	H	0	0		
-7.8070	-3.6210	-0.3790	H	0	0		
-4.5960	-1.0940	0.9590	H	0	0		
-6.9650	-1.3830	0.2950	H	0	0		
5	1	1	0				
4	5	2	0				
3	4	1	0				
1	2	1	0				
2	3	2	0				
5	6	1	0				
6	7	2	0				
10	11	1	0				
9	10	1	0				
8	9	1	0				
8	7	1	0				
11	7	1	0				
9	12	2	0				
2	13	1	0				
17	18	2	0				

```

16 17 1 0
15 16 2 0
14 15 1 0
18 13 1 0
13 14 2 0
16 19 1 0
10 20 2 0
20 21 1 0
26 24 2 0
25 26 1 0
22 23 2 0
24 22 1 0
23 21 1 0
21 25 2 0
23 27 1 0
8 28 1 0
14 29 1 0
15 30 1 0
17 31 1 0
18 32 1 0
20 33 1 0
22 34 1 0
24 35 1 0
25 36 1 0
26 37 1 0

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M END

> <Name>

Compound172

> <Activ>

56.2

> <DB_Ref_id>

18.18

\$\$\$\$

Compound173

SciTegic10081411483D

```

37 40 0 0 0 0          999 V2000
-0.6950 2.3360 0.4140 S 0 0
-1.1520 3.6230 1.4530 C 0 0
-1.7870 3.0510 2.5000 N 0 0
-1.8940 1.7110 2.4690 N 0 0
-1.3550 1.0960 1.3950 C 0 0
-1.3320 -0.3520 1.1110 N 0 0
-0.4390 -0.9510 0.3980 C 0 0
0.6370 -0.2400 -0.1930 N 0 0
1.4710 -1.1090 -0.9160 C 0 0
0.9810 -2.4880 -0.8480 C 0 0
-0.4180 -2.6110 0.0760 S 0 0
2.4570 -0.7340 -1.5080 O 0 0
-0.9000 5.0640 1.2420 C 0 0
-1.3420 6.0040 2.1930 C 0 0
-1.1030 7.3730 1.9920 C 0 0
-0.4220 7.8090 0.8420 C 0 0
0.0200 6.8710 -0.1090 C 0 0
-0.2210 5.5000 0.0900 C 0 0
-0.1950 9.1080 0.6520 F 0 0
1.5940 -3.5220 -1.4570 C 0 0
1.0610 -4.9160 -1.3610 C 0 0

```

1.3770	-7.3200	-1.0960	C	0	0
1.9200	-6.0240	-1.1840	C	0	0
-0.0100	-7.5160	-1.1860	C	0	0
-0.3300	-5.1190	-1.4510	C	0	0
-0.8630	-6.4160	-1.3630	C	0	0
3.6270	-5.8300	-1.0720	C1	0	0
0.7990	0.7440	-0.1170	H	0	0
-1.8650	5.6760	3.0780	H	0	0
-1.4430	8.0900	2.7270	H	0	0
0.5410	7.2010	-0.9960	H	0	0
0.1210	4.7850	-0.6450	H	0	0
2.4920	-3.3540	-2.0330	H	0	0
2.0200	-8.1800	-0.9590	H	0	0
-0.4220	-8.5120	-1.1150	H	0	0
-0.9960	-4.2810	-1.5900	H	0	0
-1.9320	-6.5650	-1.4340	H	0	0
5	1	1	0		
4	5	2	0		
3	4	1	0		
1	2	1	0		
2	3	2	0		
5	6	1	0		
6	7	2	0		
10	11	1	0		
9	10	1	0		
8	9	1	0		
8	7	1	0		
11	7	1	0		
9	12	2	0		
2	13	1	0		
17	18	2	0		
16	17	1	0		
15	16	2	0		
14	15	1	0		
18	13	1	0		
13	14	2	0		
16	19	1	0		
10	20	2	0		
20	21	1	0		
26	24	2	0		
25	26	1	0		
22	23	2	0		
24	22	1	0		
23	21	1	0		
21	25	2	0		
23	27	1	0		
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15	30	1	0		
17	31	1	0		
18	32	1	0		
20	33	1	0		
22	34	1	0		
24	35	1	0		
25	36	1	0		
26	37	1	0		

M END

> <Name>

Compound173

> <Activ>

61	64	0	0	1	0	999	V2000				
	0.0250			1.9490		-1.4590	C	0	0		
	0.4940			2.4390		-2.6910	C	0	0		
	1.1350			3.6890		-2.7620	C	0	0		
	1.3070			4.4530		-1.5940	C	0	0		
	0.8400			3.9710		-0.3610	C	0	0		
	0.1990			2.7190		-0.2850	C	0	0		
	-0.6480			0.6110		-1.4280	C	0	0		
	-1.7660			0.4900		-0.9820	O	0	0		
	-0.2460			2.2710		0.9340	N	0	0		
	1.7620			4.3380		-4.4180	Br	0	0		
	0.0230			-0.4790		-1.9160	N	0	0		
	1.4530			-0.3810		-2.3010	C	0	0		
	2.2810			-1.5310		-1.6970	C	0	0	1	0 0 0
	1.6310			-2.8990		-1.9750	C	0	0		
	0.1780			-2.9340		-1.4690	C	0	0	1	0 0 0
	-0.6560			-1.7870		-2.0720	C	0	0		
	3.7270			-1.4920		-2.1990	C	0	0		
	-0.4730			-4.2930		-1.7420	C	0	0		
	0.1680			1.0600		1.4100	C	0	0		
	0.9260			0.3770		0.7640	O	0	0		
	-0.3380			0.5980		2.7560	C	0	0	1	0 0 0
	-1.2970			-0.4840		2.6070	N	0	0		
	-0.7910			-1.7740		3.0410	C	0	0		
	0.7070			-1.5160		3.2500	C	0	0	1	0 0 0
	0.7680			-0.0200		3.6210	C	0	0		
	-2.5940			-0.3050		2.1020	C	0	0		
	-3.0940			1.0390		1.8500	C	0	0		
	-3.2950			-1.2640		1.8750	O	0	0		
	1.2340			-2.3240		4.2810	O	0	0		
	-2.8540			1.9960		2.7910	O	0	0		
	-3.4400			3.1110		2.2620	C	0	0		
	-4.0330			2.8630		1.0180	C	0	0		
	-3.8090			1.5140		0.7460	C	0	0		
	0.3590			1.8500		-3.5880	H	0	0		
	1.7970			5.4160		-1.6310	H	0	0		
	0.9820			4.5760		0.5230	H	0	0		
	-0.8730			2.8360		1.4710	H	0	0		
	1.5120			-0.4100		-3.3910	H	0	0		
	1.8630			0.5800		-1.9900	H	0	0		
	2.3110			-1.3930		-0.6150	H	0	0		
	1.6520			-3.1040		-3.0470	H	0	0		
	2.2110			-3.6900		-1.4940	H	0	0		
	0.2030			-2.7990		-0.3850	H	0	0		
	-1.6430			-1.7560		-1.6070	H	0	0		
	-0.8140			-1.9610		-3.1370	H	0	0		
	4.3340			-2.2810		-1.7520	H	0	0		
	4.1930			-0.5370		-1.9570	H	0	0		
	3.7640			-1.6150		-3.2810	H	0	0		
	0.1070			-5.0960		-1.2890	H	0	0		
	-1.4880			-4.3180		-1.3460	H	0	0		
	-0.5270			-4.4850		-2.8130	H	0	0		

-0.7950	1.4340	3.2660	H	0	0
-0.9690	-2.5350	2.2950	H	0	0
-1.2930	-2.0590	3.9570	H	0	0
1.2580	-1.7030	2.3400	H	0	0
0.5310	0.1250	4.6680	H	0	0
1.7420	0.4140	3.4470	H	0	0
2.1720	-2.1000	4.3710	H	0	0
-3.4360	4.0720	2.7600	H	0	0
-4.5570	3.5740	0.3950	H	0	0
-4.1210	0.9570	-0.1270	H	0	0
5	6	2		0	
4	5	1		0	
3	4	2		0	
2	3	1		0	
1	2	2		0	
1	6	1		0	
1	7	1		0	
7	8	2		0	
6	9	1		0	
3	10	1		0	
15	16	1		0	
14	15	1		0	
13	14	1		0	
12	13	1		0	
11	12	1		0	
11	16	1		0	
11	7	1		0	
13	17	1		0	
15	18	1		0	
9	19	1		0	
19	20	2		0	
21	19	1		0	
24	25	1		0	
23	24	1		0	
22	23	1		0	
22	21	1		0	
25	21	1		0	
22	26	1		0	
26	27	1		0	
26	28	2		0	
24	29	1		0	
32	33	1		0	
31	32	2		0	
30	31	1		0	
30	27	1		0	
33	27	2		0	
2	34	1		0	
4	35	1		0	
5	36	1		0	
9	37	1		0	
12	38	1		0	
12	39	1		0	
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15	43	1		0	
16	44	1		0	
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17	46	1		0	
17	47	1		0	
17	48	1		0	

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18 49 1 0
18 50 1 0
18 51 1 0
21 52 1 0
23 53 1 0
23 54 1 0
24 55 1 0
25 56 1 0
25 57 1 0
29 58 1 0
31 59 1 0
32 60 1 0
33 61 1 0

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M END

> <Name>

Compound174

> <Activ>

0.15

> <DB_Ref_id>

19.11

\$\$\$\$

Compound175

SciTegic10081411483D

```

62 65 0 0 1 0          999 V2000
-1.2750  0.0390  1.7710 C  0  0
-2.4560 -0.3810  2.4100 C  0  0
-3.7100  0.0490  1.9400 C  0  0
-3.7840  0.9030  0.8250 C  0  0
-2.6080  1.3260  0.1840 C  0  0
-1.3500  0.8980  0.6500 C  0  0
 0.0410 -0.4430  2.3020 C  0  0
 0.8780  0.3380  2.6890 O  0  0
-0.2190  1.3280  0.0010 N  0  0
-5.2860 -0.5200  2.8030 Br  0  0
 0.2810 -1.7910  2.3420 N  0  0
-0.6830 -2.7550  1.7570 C  0  0
 0.0240 -3.7800  0.8480 C  0  0  1  0  0  0
 1.2270 -4.4260  1.5580 C  0  0
 2.2120 -3.3540  2.0590 C  0  0  1  0  0  0
 1.5120 -2.3280  2.9710 C  0  0
-0.9600 -4.8420  0.3470 C  0  0
 3.4130 -3.9910  2.7660 C  0  0
-0.1370  2.6150 -0.4490 C  0  0
-1.0350  3.3950 -0.2340 O  0  0
 1.0920  3.0380 -1.2170 C  0  0  1  0  0  0
 0.7960  3.9170 -2.3350 N  0  0
 1.6510  5.0860 -2.3920 C  0  0
 2.7670  4.7750 -1.3940 C  0  0
 2.0760  3.8560 -0.3710 C  0  0
-0.2110  3.6620 -3.2830 C  0  0
-0.8870  2.3310 -3.2830 C  0  0
-2.2950  2.2470 -3.2830 C  0  0
-2.9350  1.0400 -3.2830 N  0  0
-2.2050 -0.1130 -3.2830 C  0  0
-0.7960 -0.0880 -3.2830 C  0  0
-0.1270  1.1480 -3.2830 C  0  0
-0.5170  4.5150 -4.0820 O  0  0

```

-2.3940	-1.0370	3.2680	H	0	0
-4.7390	1.2420	0.4510	H	0	0
-2.6900	1.9840	-0.6710	H	0	0
0.5430	0.6960	-0.1400	H	0	0
-1.1880	-3.2670	2.5760	H	0	0
-1.4530	-2.2240	1.1950	H	0	0
0.4020	-3.2500	-0.0280	H	0	0
0.8780	-5.0260	2.3990	H	0	0
1.7370	-5.1090	0.8770	H	0	0
2.5950	-2.8230	1.1860	H	0	0
2.1970	-1.5140	3.2140	H	0	0
1.2330	-2.7960	3.9160	H	0	0
-0.4830	-5.5500	-0.3300	H	0	0
-1.7890	-4.3770	-0.1870	H	0	0
-1.3760	-5.4060	1.1810	H	0	0
3.9230	-4.6910	2.1030	H	0	0
4.1200	-3.2270	3.0880	H	0	0
3.0910	-4.5430	3.6490	H	0	0
1.5880	2.1580	-1.6020	H	0	0
1.0870	5.9560	-2.0880	H	0	0
2.0320	5.2490	-3.3900	H	0	0
3.1830	5.6640	-0.9430	H	0	0
3.5710	4.2430	-1.8840	H	0	0
2.7780	3.2360	0.1700	H	0	0
1.5480	4.4630	0.3530	H	0	0
-2.8870	3.1500	-3.2830	H	0	0
-2.7190	-1.0630	-3.2830	H	0	0
-0.2360	-1.0110	-3.2830	H	0	0
0.9530	1.1800	-3.2830	H	0	0
5	6	2	0		
4	5	1	0		
3	4	2	0		
2	3	1	0		
1	2	2	0		
1	6	1	0		
1	7	1	0		
7	8	2	0		
6	9	1	0		
3	10	1	0		
15	16	1	0		
14	15	1	0		
13	14	1	0		
12	13	1	0		
11	12	1	0		
11	16	1	0		
11	7	1	0		
13	17	1	0		
15	18	1	0		
9	19	1	0		
19	20	2	0		
21	19	1	0		
24	25	1	0		
23	24	1	0		
22	23	1	0		
22	21	1	0		
25	21	1	0		
22	26	1	0		
26	27	1	0		
31	32	2	0		
30	31	1	0		
29	30	2	0		


```

28 29 1 0
32 27 1 0
27 28 2 0
26 33 2 0
 2 34 1 0
 4 35 1 0
 5 36 1 0
 9 37 1 0
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31 61 1 0
32 62 1 0

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M END

> <Name>

Compound175

> <Activ>

1.28

> <DB_Ref_id>

19.11d

\$\$\$\$

Compound176

SciTegic10081411483D

```

53 55 0 0 1 0          999 V2000
  0.3980  1.3590  -2.5000 C  0  0
  0.2280  0.9430  -3.8340 C  0  0
 -1.0450  0.9770  -4.4320 C  0  0
 -2.1520  1.4280  -3.6910 C  0  0
 -1.9880  1.8420  -2.3590 C  0  0
 -0.7170  1.8130  -1.7560 C  0  0
  1.7710  1.3110  -1.9020 C  0  0
  2.5660  2.2010  -2.0960 O  0  0
 -0.5880  2.2250  -0.4530 N  0  0
 -1.2640  0.4200  -6.2170 Br  0  0
  2.1150  0.2340  -1.1270 N  0  0
  3.4530  0.1410  -0.4980 C  0  0
  4.1470 -1.2150  -0.7690 C  0  0  1  0  0  0

```

3.1580	-2.3980	-0.8960	C	0	0				
1.8110	-2.0940	-0.2300	C	0	0	1	0	0	0
1.1480	-0.8710	-0.9060	C	0	0				
5.0840	-1.1430	-1.9780	C	0	0				
0.8810	-3.3110	-0.2480	C	0	0				
-1.5230	1.8650	0.4730	C	0	0				
-2.4690	1.1840	0.1520	O	0	0				
-1.3540	2.3340	1.8930	C	0	0				
-2.4380	1.8460	2.7580	N	0	0				
-2.4220	0.5470	3.1860	C	0	0				
-3.4940	0.0610	4.0410	C	0	0				
-1.5250	-0.1930	2.8540	O	0	0				
-3.4450	-1.2400	4.4460	O	0	0				
-4.5650	-1.3730	5.2170	C	0	0				
-5.3030	-0.1840	5.2930	C	0	0				
-4.6060	0.7520	4.5280	C	0	0				
1.0820	0.5980	-4.3980	H	0	0				
-3.1390	1.4590	-4.1330	H	0	0				
-2.8560	2.1840	-1.8080	H	0	0				
0.1930	2.7890	-0.1850	H	0	0				
3.3030	0.2560	0.5760	H	0	0				
4.0860	0.9770	-0.8050	H	0	0				
4.7770	-1.4120	0.0980	H	0	0				
2.9710	-2.6070	-1.9510	H	0	0				
3.6020	-3.3030	-0.4840	H	0	0				
2.0000	-1.8480	0.8170	H	0	0				
0.7320	-1.1660	-1.8710	H	0	0				
0.3180	-0.5040	-0.3010	H	0	0				
5.5940	-2.0900	-2.1540	H	0	0				
5.8460	-0.3770	-1.8300	H	0	0				
4.5290	-0.8910	-2.8830	H	0	0				
1.3460	-4.1560	0.2600	H	0	0				
-0.0660	-3.0800	0.2400	H	0	0				
0.6640	-3.6150	-1.2710	H	0	0				
-1.3340	3.4220	1.9240	H	0	0				
-0.3980	1.9860	2.2850	H	0	0				
-3.1800	2.4570	3.0330	H	0	0				
-4.8400	-2.2990	5.7050	H	0	0				
-6.2250	-0.0230	5.8360	H	0	0				
-4.8690	1.7850	4.3520	H	0	0				
5	6	2	0						
4	5	1	0						
3	4	2	0						
2	3	1	0						
1	2	2	0						
1	6	1	0						
1	7	1	0						
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11	16	1	0						
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13	17	1	0						
15	18	1	0						
9	19	1	0						
19	20	2	0						

```

19 21 1 0
21 22 1 0
22 23 1 0
23 24 1 0
23 25 2 0
28 29 1 0
27 28 2 0
26 27 1 0
26 24 1 0
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4 31 1 0
5 32 1 0
9 33 1 0
12 34 1 0
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16 41 1 0
17 42 1 0
17 43 1 0
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M END

> <Name>

Compound176

> <Activ>

1.02

> <DB_Ref_id>

19.11c

\$\$\$\$

Compound177

SciTegic10081411483D

```

55 57 0 0 1 0          999 V2000
  0.5760   -0.6020    1.5490 C   0  0
  0.7850   -1.4570    2.6470 C   0  0
 -0.2910   -2.1620    3.2130 C   0  0
 -1.5840   -2.0080    2.6840 C   0  0
 -1.8010   -1.1540    1.5880 C   0  0
 -0.7250   -0.4470    1.0160 C   0  0
  1.7500    0.1290    0.9710 C   0  0
  1.9980    1.2660    1.2990 O   0  0
 -0.9670    0.3790   -0.0550 N   0  0
  0.0000   -3.3070    4.6820 Br  0  0
  2.5450   -0.5180    0.0630 N   0  0
  2.2520   -1.9100   -0.3550 C   0  0

```

3.5040	-2.8070	-0.2690	C	0	0	1	0	0	0
4.7130	-2.1500	-0.9670	C	0	0				
4.9860	-0.7250	-0.4510	C	0	0	1	0	0	0
3.7250	0.1560	-0.5370	C	0	0				
3.8220	-3.1890	1.1820	C	0	0				
5.5700	-0.7340	0.9670	C	0	0				
-1.8050	-0.0250	-1.0550	C	0	0				
-2.3360	-1.1090	-1.0040	O	0	0				
-2.0490	0.9040	-2.2130	C	0	0				
-2.9940	1.9750	-1.8590	N	0	0				
-4.3180	1.6760	-1.7090	C	0	0				
-5.2660	2.7740	-1.3500	C	0	0				
-4.7110	0.5430	-1.8670	O	0	0				
-6.4900	2.4790	-0.7150	C	0	0				
-7.3710	3.4670	-0.3790	N	0	0				
-7.0660	4.7680	-0.6560	C	0	0				
-5.8570	5.1190	-1.2870	C	0	0				
-4.9430	4.1110	-1.6410	C	0	0				
1.7810	-1.5700	3.0510	H	0	0				
-2.4240	-2.5410	3.1080	H	0	0				
-2.8030	-1.0510	1.1990	H	0	0				
-0.5270	1.2770	-0.0980	H	0	0				
1.8950	-1.8810	-1.3850	H	0	0				
1.4400	-2.3260	0.2420	H	0	0				
3.2810	-3.7340	-0.7950	H	0	0				
4.5120	-2.1020	-2.0390	H	0	0				
5.6020	-2.7730	-0.8550	H	0	0				
5.7460	-0.2790	-1.0940	H	0	0				
3.4960	0.3630	-1.5820	H	0	0				
3.8970	1.1230	-0.0600	H	0	0				
4.8610	-3.4960	1.3010	H	0	0				
3.1920	-4.0180	1.5080	H	0	0				
3.6410	-2.3500	1.8520	H	0	0				
6.1530	-1.6390	1.1390	H	0	0				
6.2090	0.1350	1.1270	H	0	0				
4.7760	-0.7030	1.7130	H	0	0				
-2.4410	0.3440	-3.0610	H	0	0				
-1.1070	1.3500	-2.5350	H	0	0				
-2.6700	2.9120	-1.7280	H	0	0				
-6.7440	1.4530	-0.4880	H	0	0				
-7.7700	5.5430	-0.3850	H	0	0				
-5.6350	6.1540	-1.5000	H	0	0				
-4.0140	4.3670	-2.1250	H	0	0				
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4	5	1	0						
3	4	2	0						
2	3	1	0						
1	2	2	0						
1	6	1	0						
1	7	1	0						
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3	10	1	0						
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11	16	1	0						
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13	17	1	0						

```

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9 19 1 0
19 20 2 0
19 21 1 0
21 22 1 0
22 23 1 0
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17 44 1 0
17 45 1 0
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```

M END

> <Name>

Compound177

> <Activ>

0.57

> <DB_Ref_id>

19.11b

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Compound178

SciTegic10081411483D

```

56 58 0 0 1 0          999 V2000
-1.4550    0.4280    2.0820 C    0  0
-2.5530    0.5140    2.9590 C    0  0
-3.8630    0.5700    2.4530 C    0  0
-4.0800    0.5430    1.0640 C    0  0
-2.9880    0.4570    0.1840 C    0  0
-1.6720    0.4000    0.6850 C    0  0
-0.0740    0.3670    2.6620 C    0  0

```

0.7250	1.2500	2.4530	O	0	0				
-0.6270	0.3160	-0.1990	N	0	0				
-5.3260	0.6840	3.6370	Br	0	0				
0.2680	-0.7090	3.4370	N	0	0				
1.6070	-0.8010	4.0640	C	0	0				
2.2990	-2.1580	3.7950	C	0	0	1	0	0	0
1.3110	-3.3420	3.6680	C	0	0				
-0.0370	-3.0350	4.3340	C	0	0	1	0	0	0
-0.6970	-1.8140	3.6580	C	0	0				
3.2360	-2.0860	2.5860	C	0	0				
-0.9650	-4.2540	4.3160	C	0	0				
-0.6270	1.0800	-1.3320	C	0	0				
-1.5470	1.8300	-1.5630	O	0	0				
0.5350	0.9650	-2.2830	C	0	0				
0.2950	1.7130	-3.5260	N	0	0				
1.2500	1.7190	-4.5000	C	0	0				
0.9900	2.4840	-5.7560	C	0	0				
2.2850	1.1130	-4.3440	O	0	0				
-0.2210	3.1820	-5.9180	C	0	0				
-0.4650	3.9000	-7.1000	C	0	0				
0.5020	3.9260	-8.1210	C	0	0				
1.7110	3.2310	-7.9590	C	0	0				
1.9570	2.5100	-6.7780	C	0	0				
-2.3830	0.5370	4.0270	H	0	0				
-5.0800	0.5840	0.6580	H	0	0				
-3.1780	0.4380	-0.8810	H	0	0				
0.1350	-0.3050	-0.0120	H	0	0				
1.4570	-0.6880	5.1390	H	0	0				
2.2380	0.0350	3.7600	H	0	0				
2.9320	-2.3560	4.6620	H	0	0				
1.1250	-3.5510	2.6130	H	0	0				
1.7560	-4.2460	4.0800	H	0	0				
0.1520	-2.7890	5.3790	H	0	0				
-1.1150	-2.1090	2.6930	H	0	0				
-1.5290	-1.4450	4.2640	H	0	0				
3.7460	-3.0330	2.4080	H	0	0				
3.9980	-1.3200	2.7340	H	0	0				
2.6820	-1.8340	1.6820	H	0	0				
-0.5000	-5.1000	4.8240	H	0	0				
-1.9120	-4.0220	4.8050	H	0	0				
-1.1840	-4.5570	3.2930	H	0	0				
0.7130	-0.0840	-2.5240	H	0	0				
1.4390	1.3400	-1.8070	H	0	0				
-0.5610	2.2150	-3.6560	H	0	0				
-0.9690	3.1680	-5.1390	H	0	0				
-1.3950	4.4360	-7.2250	H	0	0				
0.3140	4.4790	-9.0300	H	0	0				
2.4530	3.2480	-8.7440	H	0	0				
2.8910	1.9770	-6.6640	H	0	0				
5	6	2	0						
4	5	1	0						
3	4	2	0						
2	3	1	0						
1	2	2	0						
1	6	1	0						
1	7	1	0						
7	8	2	0						
6	9	1	0						
3	10	1	0						
15	16	1	0						
14	15	1	0						

13 14 1 0
12 13 1 0
11 12 1 0
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11 7 1 0
13 17 1 0
15 18 1 0
9 19 1 0
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M END

> <Name>

Compound178

> <Activ>

0.54

> <DB_Ref_id>

19.11a

\$\$\$\$

Compound179

SciTegic10081411483D

57 59 0 0 1 0

999 V2000

-1.4200	1.2970	-1.8120	C	0	0				
-2.5040	1.0470	-2.6760	C	0	0				
-3.6560	0.3980	-2.1990	C	0	0				
-3.7270	-0.0080	-0.8530	C	0	0				
-2.6460	0.2360	0.0120	C	0	0				
-1.4900	0.8890	-0.4590	C	0	0				
-0.2110	1.9940	-2.3590	C	0	0				
0.1720	3.0370	-1.8830	O	0	0				
-0.4530	1.1150	0.4100	N	0	0				
-5.1030	0.0700	-3.3610	Br	0	0				
0.4550	1.4260	-3.4120	N	0	0				
0.0960	0.0780	-3.9120	C	0	0				
1.3360	-0.8320	-4.0310	C	0	0	1	0	0	0
2.4750	-0.1330	-4.7990	C	0	0				
2.8200	1.2500	-4.2110	C	0	0	1	0	0	0
1.5650	2.1390	-4.0920	C	0	0				
1.7990	-1.3300	-2.6560	C	0	0				
3.5530	1.1330	-2.8690	C	0	0				
-0.0660	0.1350	1.2810	C	0	0				
-0.6350	-0.9320	1.2910	O	0	0				
0.9690	0.3750	2.1410	N	0	0				
1.3850	-0.6780	3.0780	C	0	0				
0.3520	-0.9000	4.1600	C	0	0				
-0.3010	-2.0610	4.3630	N	0	0				
-1.1520	-1.9590	5.3890	N	0	0				
-1.0920	-0.7130	5.9040	C	0	0				
-0.1370	-0.0100	5.1390	C	0	0				
-2.0180	-3.0470	5.8730	C	0	0				
-1.9160	-0.2270	7.0780	C	0	0				
-2.4450	1.3590	-3.7090	H	0	0				
-4.6030	-0.5080	-0.4710	H	0	0				
-2.7230	-0.0840	1.0410	H	0	0				
0.0180	1.9960	0.4020	H	0	0				
-0.3670	0.1970	-4.8930	H	0	0				
-0.6560	-0.3810	-3.2680	H	0	0				
1.0430	-1.7170	-4.6000	H	0	0				
2.1680	-0.0060	-5.8380	H	0	0				
3.3630	-0.7680	-4.8240	H	0	0				
3.5080	1.7420	-4.9000	H	0	0				
1.2190	2.4240	-5.0860	H	0	0				
1.8010	3.0660	-3.5680	H	0	0				
2.8400	-1.6500	-2.6700	H	0	0				
1.1950	-2.1780	-2.3280	H	0	0				
1.7030	-0.5450	-1.9080	H	0	0				
4.1510	0.2210	-2.8360	H	0	0				
4.2050	1.9900	-2.7110	H	0	0				
2.8440	1.0960	-2.0430	H	0	0				
1.4320	1.2600	2.1250	H	0	0				
2.3340	-0.3960	3.5350	H	0	0				
1.5410	-1.6050	2.5290	H	0	0				
0.1620	1.0220	5.2770	H	0	0				
-1.9180	-3.9800	5.3200	H	0	0				
-3.0600	-2.7340	5.8150	H	0	0				
-1.7910	-3.2520	6.9200	H	0	0				
-1.7340	0.8130	7.3560	H	0	0				
-1.7050	-0.8460	7.9510	H	0	0				
-2.9750	-0.3280	6.8460	H	0	0				
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4	5	1	0						
3	4	2	0						
2	3	1	0						

1	2	2	0
1	6	1	0
1	7	1	0
7	8	2	0
6	9	1	0
3	10	1	0
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13	14	1	0
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13	17	1	0
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19	21	1	0
21	22	1	0
22	23	1	0
26	27	2	0
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M END
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Compound179

> <Activ>
0.37

SciTegic10081411483D

-2.6250	3.7360	-7.5200 H	0	0
-1.3690	2.5040	-7.5980 H	0	0
-0.9320	4.1930	-7.3630 H	0	0
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4	5	1	0	
3	4	2	0	
2	3	1	0	
1	2	2	0	
1	6	1	0	
1	7	1	0	
7	8	2	0	
6	9	1	0	
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19	21	1	0	
21	22	1	0	
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14	38	1	0	
15	39	1	0	
16	40	1	0	
16	41	1	0	
17	42	1	0	
17	43	1	0	
17	44	1	0	
18	45	1	0	
18	46	1	0	
18	47	1	0	
21	48	1	0	
22	49	1	0	
22	50	1	0	
25	51	1	0	
26	52	1	0	
29	53	1	0	
29	54	1	0	
29	55	1	0	
M	END			

> <Name>
Compound180

> <Activ>
0.35

> <DB_Ref_id>
19.10c

\$\$\$\$
Compound181
SciTegic10081411483D

62	64	0	0	1	0	999	V2000				
-0.0330				2.5220		-2.9790	C	0	0		
0.4400				3.0200		-4.2070	C	0	0		
1.0840				4.2680		-4.2680	C	0	0		
1.2560				5.0240		-3.0940	C	0	0		
0.7850				4.5330		-1.8650	C	0	0		
0.1390				3.2830		-1.7990	C	0	0		
-0.7130				1.1880		-2.9570	C	0	0		
-1.8340				1.0670		-2.5200	O	0	0		
-0.3100				2.8300		-0.5840	N	0	0		
1.7170				4.9260		-5.9160	Br	0	0		
-0.0390				0.0980		-3.4450	N	0	0		
1.3890				0.1930		-3.8300	C	0	0		
2.2170				-0.9570		-3.2270	C	0	0	1	0 0 0
1.5680				-2.3240		-3.5040	C	0	0		
0.1150				-2.3570		-2.9980	C	0	0	1	0 0 0
-0.7210				-1.2110		-3.6020	C	0	0		
3.6640				-0.9160		-3.7290	C	0	0		
-0.5370				-3.7170		-3.2720	C	0	0		
0.1470				1.6430		-0.0860	C	0	0		
0.9430				0.9840		-0.7130	O	0	0		
-0.3100				1.2030		1.1250	N	0	0		
0.1800				-0.0740		1.6600	C	0	0		
-0.3910				-0.3590		3.0020	C	0	0		
-1.5680				-1.1210		3.1190	C	0	0		
-2.1090				-1.3910		4.3870	C	0	0		
-1.4730				-0.9000		5.5450	C	0	0		
-0.2950				-0.1390		5.4260	C	0	0		
0.2440				0.1310		4.1560	C	0	0		
-2.0000				-1.1640		6.7810	N	0	0		
-1.2380				-0.8730		8.0060	C	0	0		
-3.3440				-1.7440		6.9000	C	0	0		
0.3050				2.4360		-5.1070	H	0	0		
1.7500				5.9870		-3.1210	H	0	0		
0.9280				5.1330		-0.9770	H	0	0		
-0.9710				3.3730		-0.0640	H	0	0		
1.4470				0.1660		-4.9200	H	0	0		
1.7990				1.1560		-3.5200	H	0	0		
2.2460				-0.8180		-2.1450	H	0	0		
1.5880				-2.5290		-4.5760	H	0	0		
2.1470				-3.1130		-3.0250	H	0	0		
0.1390				-2.2230		-1.9140	H	0	0		
-1.7070				-1.1820		-3.1390	H	0	0		
-0.8790				-1.3850		-4.6660	H	0	0		
4.2720				-1.7010		-3.2770	H	0	0		
4.1270				0.0410		-3.4920	H	0	0		
3.6990				-1.0470		-4.8090	H	0	0		
0.0410				-4.5200		-2.8130	H	0	0		

-1.5550	-3.7420	-2.8810	H	0	0
-0.5880	-3.9100	-4.3420	H	0	0
-0.9710	1.7540	1.6350	H	0	0
1.2680	-0.0430	1.7270	H	0	0
-0.0900	-0.8770	0.9730	H	0	0
-2.0600	-1.5000	2.2340	H	0	0
-3.0160	-1.9760	4.4570	H	0	0
0.2090	0.2460	6.3010	H	0	0
1.1490	0.7150	4.0700	H	0	0
-0.1850	-1.1500	7.9650	H	0	0
-1.6890	-1.4040	8.8440	H	0	0
-1.2950	0.1930	8.2190	H	0	0
-4.0980	-1.2890	6.2580	H	0	0
-3.6860	-1.6500	7.9320	H	0	0
-3.2990	-2.8070	6.6580	H	0	0
5	6	2	0		
4	5	1	0		
3	4	2	0		
2	3	1	0		
1	2	2	0		
1	6	1	0		
1	7	1	0		
7	8	2	0		
6	9	1	0		
3	10	1	0		
15	16	1	0		
14	15	1	0		
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12	13	1	0		
11	12	1	0		
11	16	1	0		
11	7	1	0		
13	17	1	0		
15	18	1	0		
9	19	1	0		
19	20	2	0		
19	21	1	0		
21	22	1	0		
22	23	1	0		
27	28	2	0		
26	27	1	0		
25	26	2	0		
24	25	1	0		
28	23	1	0		
23	24	2	0		
26	29	1	0		
29	30	1	0		
29	31	1	0		
2	32	1	0		
4	33	1	0		
5	34	1	0		
9	35	1	0		
12	36	1	0		
12	37	1	0		
13	38	1	0		
14	39	1	0		
14	40	1	0		
15	41	1	0		
16	42	1	0		
16	43	1	0		
17	44	1	0		

```

17 45 1 0
17 46 1 0
18 47 1 0
18 48 1 0
18 49 1 0
21 50 1 0
22 51 1 0
22 52 1 0
24 53 1 0
25 54 1 0
27 55 1 0
28 56 1 0
30 57 1 0
30 58 1 0
30 59 1 0
31 60 1 0
31 61 1 0
31 62 1 0

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M END

> <Name>

Compound181

> <Activ>

0.8

> <DB_Ref_id>

19.10b

\$\$\$\$

Compound182

SciTegic10081411483D

```

54 55 0 0 1 0          999 V2000
-0.5550 2.5660 -1.7130 C 0 0
-0.0700 3.0640 -2.9370 C 0 0
 0.5780 4.3130 -2.9920 C 0 0
 0.7400 5.0660 -1.8160 C 0 0
 0.2580 4.5760 -0.5920 C 0 0
-0.3910 3.3260 -0.5310 C 0 0
-1.2360 1.2320 -1.6970 C 0 0
-2.3590 1.1130 -1.2660 O 0 0
-0.8500 2.8730 0.6800 N 0 0
 1.2230 4.9690 -4.6350 Br 0 0
-0.5620 0.1450 -2.1850 N 0 0
 0.8650 0.2400 -2.5720 C 0 0
 1.6930 -0.9100 -1.9670 C 0 0 1 0 0 0
 1.0450 -2.2770 -2.2440 C 0 0
-0.4080 -2.3130 -1.7380 C 0 0 1 0 0 0
-1.2440 -1.1660 -2.3420 C 0 0
 3.1410 -0.8710 -2.4690 C 0 0
-1.0610 -3.6700 -2.0120 C 0 0
-0.4160 1.6740 1.1700 C 0 0
 0.3730 1.0080 0.5430 O 0 0
-0.8810 1.2360 2.3770 N 0 0
-0.4160 -0.0550 2.9060 C 0 0
-1.0370 -0.3630 4.2400 C 0 0
-1.8180 0.4020 4.7560 O 0 0
-0.7030 -1.5310 4.8650 N 0 0
-1.2730 -1.8980 6.1700 C 0 0
 0.2480 -2.4470 4.2210 C 0 0
-0.1990 2.4810 -3.8380 H 0 0

```

1.2360	6.0270	-1.8400	H	0	0
0.3950	5.1740	0.2990	H	0	0
-1.5020	3.4240	1.2010	H	0	0
0.9240	0.2130	-3.6600	H	0	0
1.2750	1.2030	-2.2600	H	0	0
1.7230	-0.7710	-0.8850	H	0	0
1.0650	-2.4820	-3.3160	H	0	0
1.6230	-3.0680	-1.7660	H	0	0
-0.3850	-2.1760	-0.6560	H	0	0
-2.2300	-1.1350	-1.8790	H	0	0
-1.4020	-1.3380	-3.4080	H	0	0
3.7460	-1.6600	-2.0230	H	0	0
3.6060	0.0840	-2.2250	H	0	0
3.1760	-0.9920	-3.5510	H	0	0
-0.4800	-4.4750	-1.5590	H	0	0
-2.0760	-3.6970	-1.6150	H	0	0
-1.1150	-3.8610	-3.0840	H	0	0
-1.5330	1.7950	2.8910	H	0	0
0.6700	-0.0310	3.0000	H	0	0
-0.6580	-0.8420	2.1940	H	0	0
-1.9710	-1.1700	6.5860	H	0	0
-0.4650	-2.0330	6.8890	H	0	0
-1.8010	-2.8480	6.0780	H	0	0
0.6270	-2.1090	3.2560	H	0	0
-0.2320	-3.4140	4.0690	H	0	0
1.1020	-2.6000	4.8790	H	0	0
5	6	2	0		
4	5	1	0		
3	4	2	0		
2	3	1	0		
1	2	2	0		
1	6	1	0		
1	7	1	0		
7	8	2	0		
6	9	1	0		
3	10	1	0		
15	16	1	0		
14	15	1	0		
13	14	1	0		
12	13	1	0		
11	12	1	0		
11	16	1	0		
11	7	1	0		
13	17	1	0		
15	18	1	0		
9	19	1	0		
19	20	2	0		
19	21	1	0		
21	22	1	0		
22	23	1	0		
23	24	2	0		
23	25	1	0		
25	26	1	0		
25	27	1	0		
2	28	1	0		
4	29	1	0		
5	30	1	0		
9	31	1	0		
12	32	1	0		
12	33	1	0		
13	34	1	0		

```

14 35 1 0
14 36 1 0
15 37 1 0
16 38 1 0
16 39 1 0
17 40 1 0
17 41 1 0
17 42 1 0
18 43 1 0
18 44 1 0
18 45 1 0
21 46 1 0
22 47 1 0
22 48 1 0
26 49 1 0
26 50 1 0
26 51 1 0
27 52 1 0
27 53 1 0
27 54 1 0

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M END

> <Name>

Compound182

> <Activ>

0.46

> <DB_Ref_id>

19.10a

\$\$\$\$

Compound183

SciTegic10081411483D

```

56 58 0 0 1 0          999 V2000
-0.6820  2.7660 -1.8670 C  0 0
-0.1950  3.2620 -3.0920 C  0 0
 0.4530  4.5100 -3.1470 C  0 0
 0.6130  5.2660 -1.9730 C  0 0
 0.1290  4.7770 -0.7480 C  0 0
-0.5200  3.5290 -0.6860 C  0 0
-1.3630  1.4320 -1.8520 C  0 0
-2.4840  1.3130 -1.4180 O  0 0
-0.9820  3.0780  0.5250 N  0 0
 1.1020  5.1620 -4.7910 Br 0 0
-0.6890  0.3440 -2.3380 N  0 0
 0.7380  0.4390 -2.7250 C  0 0
 1.5660 -0.7110 -2.1190 C  0 0 1 0 0 0
 0.9180 -2.0780 -2.3990 C  0 0
-0.5350 -2.1110 -1.8910 C  0 0 1 0 0 0
-1.3690 -0.9650 -2.4960 C  0 0
 3.0140 -0.6720 -2.6210 C  0 0
-1.1880 -3.4710 -2.1640 C  0 0
-0.5450  1.8830  1.0190 C  0 0
 0.2480  1.2150  0.3960 O  0 0
-1.0700  1.4160  2.3520 C  0 0
-0.4730  0.0740  2.7770 C  0 0
-0.9900 -0.3850  4.1130 C  0 0
-1.8150  0.2600  4.7190 O  0 0
-0.4550 -1.6620  4.6740 C  0 0
-0.9140 -2.1460  5.9160 C  0 0

```


-0.4390	-3.3110	6.4450	N	0	0
0.5020	-4.0290	5.7660	C	0	0
0.9980	-3.5940	4.5210	C	0	0
0.5160	-2.3960	3.9650	C	0	0
-0.3220	2.6760	-3.9920	H	0	0
1.1070	6.2270	-1.9960	H	0	0
0.2620	5.3790	0.1410	H	0	0
-1.6370	3.6270	1.0430	H	0	0
0.7970	0.4120	-3.8130	H	0	0
1.1500	1.4020	-2.4120	H	0	0
1.5960	-0.5720	-1.0370	H	0	0
0.9370	-2.2830	-3.4690	H	0	0
1.4960	-2.8670	-1.9180	H	0	0
-0.5120	-1.9770	-0.8090	H	0	0
-2.3570	-0.9360	-2.0310	H	0	0
-1.5270	-1.1390	-3.5610	H	0	0
3.6190	-1.4610	-2.1760	H	0	0
3.4800	0.2830	-2.3790	H	0	0
3.0490	-0.7930	-3.7030	H	0	0
-0.6070	-4.2750	-1.7130	H	0	0
-2.2010	-3.4980	-1.7700	H	0	0
-1.2420	-3.6620	-3.2360	H	0	0
-0.7950	2.1290	3.1290	H	0	0
-2.1600	1.3610	2.3200	H	0	0
0.6030	0.2290	2.8300	H	0	0
-0.6640	-0.6890	2.0230	H	0	0
-1.6600	-1.5900	6.4650	H	0	0
0.8730	-4.9490	6.1910	H	0	0
1.7420	-4.1760	3.9980	H	0	0
0.8870	-2.0530	3.0120	H	0	0
5	6	2	0		
4	5	1	0		
3	4	2	0		
2	3	1	0		
1	2	2	0		
1	6	1	0		
1	7	1	0		
7	8	2	0		
6	9	1	0		
3	10	1	0		
15	16	1	0		
14	15	1	0		
13	14	1	0		
12	13	1	0		
11	12	1	0		
11	16	1	0		
11	7	1	0		
13	17	1	0		
15	18	1	0		
9	19	1	0		
19	20	2	0		
19	21	1	0		
21	22	1	0		
22	23	1	0		
23	24	2	0		
23	25	1	0		
29	30	2	0		
28	29	1	0		
27	28	2	0		
26	27	1	0		
30	25	1	0		

```

25 26 2 0
2 31 1 0
4 32 1 0
5 33 1 0
9 34 1 0
12 35 1 0
12 36 1 0
13 37 1 0
14 38 1 0
14 39 1 0
15 40 1 0
16 41 1 0
16 42 1 0
17 43 1 0
17 44 1 0
17 45 1 0
18 46 1 0
18 47 1 0
18 48 1 0
21 49 1 0
21 50 1 0
22 51 1 0
22 52 1 0
26 53 1 0
28 54 1 0
29 55 1 0
30 56 1 0

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M END

> <Name>

Compound183

> <Activ>

1.04

> <DB_Ref_id>

19.09c

\$\$\$\$

Compound184

SciTegic10081411483D

```

56 58 0 0 1 0          999 V2000
-0.6510 2.7930 -1.9380 C 0 0
-0.1640 3.2890 -3.1620 C 0 0
0.4820 4.5370 -3.2170 C 0 0
0.6420 5.2930 -2.0430 C 0 0
0.1580 4.8050 -0.8190 C 0 0
-0.4900 3.5570 -0.7580 C 0 0
-1.3320 1.4590 -1.9220 C 0 0
-2.4550 1.3400 -1.4880 O 0 0
-0.9510 3.1060 0.4550 N 0 0
1.1310 5.1900 -4.8620 Br 0 0
-0.6600 0.3710 -2.4080 N 0 0
0.7690 0.4670 -2.7950 C 0 0
1.5980 -0.6840 -2.1900 C 0 0 1 0 0 0
0.9470 -2.0510 -2.4690 C 0 0
-0.5060 -2.0860 -1.9610 C 0 0 1 0 0 0
-1.3400 -0.9390 -2.5670 C 0 0
3.0430 -0.6450 -2.6920 C 0 0
-1.1560 -3.4430 -2.2370 C 0 0
-0.5160 1.9100 0.9490 C 0 0

```

0.2770	1.2420	0.3260	O	0	0
-1.0410	1.4430	2.2810	C	0	0
-0.4430	0.1020	2.7070	C	0	0
-0.9610	-0.3570	4.0430	C	0	0
-1.7810	0.2890	4.6500	O	0	0
-0.4320	-1.6390	4.5980	C	0	0
0.5000	-2.3360	3.8850	N	0	0
0.9940	-3.5100	4.3790	C	0	0
0.5640	-4.0220	5.6170	C	0	0
-0.3930	-3.3110	6.3610	C	0	0
-0.8970	-2.1050	5.8460	C	0	0
-0.2910	2.7030	-4.0630	H	0	0
1.1370	6.2540	-2.0690	H	0	0
0.2930	5.4060	0.0700	H	0	0
-1.6080	3.6560	0.9710	H	0	0
0.8280	0.4390	-3.8850	H	0	0
1.1800	1.4300	-2.4830	H	0	0
1.6250	-0.5450	-1.1080	H	0	0
0.9670	-2.2560	-3.5390	H	0	0
1.5270	-2.8420	-1.9880	H	0	0
-0.4810	-1.9490	-0.8790	H	0	0
-2.3260	-0.9080	-2.1020	H	0	0
-1.4980	-1.1110	-3.6310	H	0	0
3.6500	-1.4340	-2.2460	H	0	0
3.5100	0.3110	-2.4490	H	0	0
3.0800	-0.7680	-3.7760	H	0	0
-0.5760	-4.2480	-1.7830	H	0	0
-2.1720	-3.4710	-1.8400	H	0	0
-1.2130	-3.6370	-3.3070	H	0	0
-0.7660	2.1560	3.0590	H	0	0
-2.1290	1.3890	2.2500	H	0	0
0.6350	0.2560	2.7600	H	0	0
-0.6350	-0.6620	1.9530	H	0	0
1.7300	-4.0530	3.8050	H	0	0
0.9670	-4.9510	5.9920	H	0	0
-0.7360	-3.6860	7.3140	H	0	0
-1.6330	-1.5470	6.4040	H	0	0
5	6	2	0		
4	5	1	0		
3	4	2	0		
2	3	1	0		
1	2	2	0		
1	6	1	0		
1	7	1	0		
7	8	2	0		
6	9	1	0		
3	10	1	0		
15	16	1	0		
14	15	1	0		
13	14	1	0		
12	13	1	0		
11	12	1	0		
11	16	1	0		
11	7	1	0		
13	17	1	0		
15	18	1	0		
9	19	1	0		
19	20	2	0		
19	21	1	0		
21	22	1	0		
22	23	1	0		

```

23 24 2 0
23 25 1 0
29 30 2 0
28 29 1 0
27 28 2 0
26 27 1 0
30 25 1 0
25 26 2 0
2 31 1 0
4 32 1 0
5 33 1 0
9 34 1 0
12 35 1 0
12 36 1 0
13 37 1 0
14 38 1 0
14 39 1 0
15 40 1 0
16 41 1 0
16 42 1 0
17 43 1 0
17 44 1 0
17 45 1 0
18 46 1 0
18 47 1 0
18 48 1 0
21 49 1 0
21 50 1 0
22 51 1 0
22 52 1 0
27 53 1 0
28 54 1 0
29 55 1 0
30 56 1 0

```

M END

> <Name>

Compound184

> <Activ>

1.85

> <DB_Ref_id>

19.09b

\$\$\$\$

Compound185

SciTegic10081411483D

```

54 56 0 0 1 0          999 V2000
-0.6210 2.6580 -1.7480 C 0 0
-0.1350 3.1540 -2.9730 C 0 0
0.5120 4.4020 -3.0270 C 0 0
0.6720 5.1580 -1.8540 C 0 0
0.1870 4.6700 -0.6290 C 0 0
-0.4610 3.4220 -0.5660 C 0 0
-1.3030 1.3240 -1.7320 C 0 0
-2.4260 1.2050 -1.2990 O 0 0
-0.9220 2.9710 0.6450 N 0 0
1.1620 5.0550 -4.6720 Br 0 0
-0.6310 0.2360 -2.2190 N 0 0
0.7990 0.3320 -2.6060 C 0 0

```

1.6270	-0.8180	-2.0000	C	0	0	1	0	0	0
0.9760	-2.1860	-2.2790	C	0	0				
-0.4770	-2.2210	-1.7720	C	0	0	1	0	0	0
-1.3110	-1.0740	-2.3750	C	0	0				
3.0720	-0.7790	-2.5020	C	0	0				
-1.1270	-3.5780	-2.0450	C	0	0				
-0.4860	1.7740	1.1390	C	0	0				
0.3070	1.1080	0.5160	O	0	0				
-1.0120	1.3090	2.4710	C	0	0				
-0.4140	-0.0330	2.8970	C	0	0				
-0.9320	-0.4940	4.2320	C	0	0				
-1.7420	0.1600	4.8460	O	0	0				
-0.4420	-1.7480	4.7830	C	0	0				
0.6990	-2.7440	4.0080	S	0	0				
0.6910	-3.8950	5.2560	C	0	0				
-0.1900	-3.5250	6.2850	C	0	0				
-0.8340	-2.3010	6.0140	C	0	0				
-0.2620	2.5680	-3.8730	H	0	0				
1.1660	6.1190	-1.8770	H	0	0				
0.3220	5.2720	0.2600	H	0	0				
-1.5780	3.5200	1.1620	H	0	0				
0.8570	0.3050	-3.6930	H	0	0				
1.2090	1.2950	-2.2930	H	0	0				
1.6540	-0.6800	-0.9180	H	0	0				
0.9960	-2.3910	-3.3500	H	0	0				
1.5550	-2.9770	-1.7990	H	0	0				
-0.4510	-2.0840	-0.6890	H	0	0				
-2.2990	-1.0430	-1.9120	H	0	0				
-1.4690	-1.2460	-3.4410	H	0	0				
3.6800	-1.5680	-2.0570	H	0	0				
3.5390	0.1760	-2.2600	H	0	0				
3.1090	-0.9020	-3.5840	H	0	0				
-0.5470	-4.3830	-1.5920	H	0	0				
-2.1430	-3.6050	-1.6500	H	0	0				
-1.1840	-3.7710	-3.1170	H	0	0				
-0.7360	2.0220	3.2480	H	0	0				
-2.1000	1.2520	2.4390	H	0	0				
0.6640	0.1210	2.9490	H	0	0				
-0.6040	-0.7970	2.1430	H	0	0				
1.2930	-4.7950	5.2480	H	0	0				
-0.3560	-4.1090	7.1800	H	0	0				
-1.5530	-1.8420	6.6840	H	0	0				
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4	5	1	0						
3	4	2	0						
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13	14	1	0						
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11	7	1	0						
13	17	1	0						
15	18	1	0						

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19 20  2  0
19 21  1  0
21 22  1  0
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23 24  2  0
23 25  1  0
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  9 33  1  0
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16 40  1  0
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29 54  1  0
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> <Name>
Compound185

> <Activ>
0.97

> <DB_Ref_id>
19.09a

$$$$
Compound186
  SciTegic10081411483D

49 50  0  0  1  0          999 V2000
  -0.6150    2.2700   -1.1170 C    0  0
  -0.1290    2.7660   -2.3420 C    0  0
    0.5200    4.0140   -2.3980 C    0  0
    0.6800    4.7700   -1.2230 C    0  0
    0.1950    4.2810    0.0020 C    0  0
  -0.4530    3.0330    0.0630 C    0  0
  -1.2970    0.9360   -1.1010 C    0  0
  -2.4180    0.8160   -0.6680 O    0  0
  -0.9140    2.5820    1.2740 N    0  0

```

1.1680	4.6660	-4.0410	Br	0	0				
-0.6230	-0.1520	-1.5900	N	0	0				
0.8050	-0.0570	-1.9750	C	0	0				
1.6350	-1.2070	-1.3710	C	0	0	1	0	0	0
0.9840	-2.5740	-1.6480	C	0	0				
-0.4690	-2.6090	-1.1430	C	0	0	1	0	0	0
-1.3030	-1.4630	-1.7460	C	0	0				
3.0800	-1.1680	-1.8730	C	0	0				
-1.1210	-3.9670	-1.4160	C	0	0				
-0.4780	1.3850	1.7700	C	0	0				
0.3140	0.7190	1.1450	O	0	0				
-1.0040	0.9200	3.1000	C	0	0				
-0.4080	-0.4220	3.5260	C	0	0				
-0.9260	-0.8850	4.8610	C	0	0				
-0.4630	-2.0620	5.3730	N	0	0				
-1.7380	-0.2300	5.4730	O	0	0				
-0.2560	2.1800	-3.2420	H	0	0				
1.1740	5.7310	-1.2480	H	0	0				
0.3300	4.8830	0.8910	H	0	0				
-1.5700	3.1310	1.7910	H	0	0				
0.8650	-0.0840	-3.0640	H	0	0				
1.2170	0.9060	-1.6640	H	0	0				
1.6620	-1.0680	-0.2890	H	0	0				
1.0040	-2.7790	-2.7210	H	0	0				
1.5630	-3.3650	-1.1700	H	0	0				
-0.4450	-2.4730	-0.0600	H	0	0				
-2.2910	-1.4320	-1.2830	H	0	0				
-1.4610	-1.6350	-2.8110	H	0	0				
3.6860	-1.9570	-1.4280	H	0	0				
3.5470	-0.2130	-1.6310	H	0	0				
3.1150	-1.2910	-2.9550	H	0	0				
-0.5390	-4.7710	-0.9630	H	0	0				
-2.1350	-3.9940	-1.0190	H	0	0				
-1.1760	-4.1600	-2.4880	H	0	0				
-0.7280	1.6310	3.8770	H	0	0				
-2.0920	0.8650	3.0700	H	0	0				
0.6700	-0.2680	3.5800	H	0	0				
-0.5960	-1.1850	2.7720	H	0	0				
-0.7750	-2.4120	6.2560	H	0	0				
0.2090	-2.6020	4.8650	H	0	0				
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4	5	1	0						
3	4	2	0						
2	3	1	0						
1	2	2	0						
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11	16	1	0						
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13	17	1	0						
15	18	1	0						
9	19	1	0						
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21 22 1 0
22 23 1 0
23 24 1 0
23 25 2 0
2 26 1 0
4 27 1 0
5 28 1 0
9 29 1 0
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14 33 1 0
14 34 1 0
15 35 1 0
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17 38 1 0
17 39 1 0
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M END

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Compound186

> <Activ>

4.3

> <DB_Ref_id>

19.08j

\$\$\$\$

Compound187

SciTegic10081411483D

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55 56 0 0 1 0          999 V2000
-0.9220 0.1250 2.5170 C 0 0
-0.8970 -0.3380 3.8460 C 0 0
-2.0080 -1.0120 4.3870 C 0 0
-3.1510 -1.2230 3.5940 C 0 0
-3.1820 -0.7640 2.2670 C 0 0
-2.0720 -0.0880 1.7210 C 0 0
0.2830 0.8360 1.9800 C 0 0
0.5530 1.9570 2.3380 O 0 0
-2.1330 0.3500 0.4220 N 0 0
-1.9630 -1.6290 6.1660 Br 0 0
1.0780 0.1890 1.0700 N 0 0
0.7850 -1.2030 0.6520 C 0 0
2.0350 -2.1000 0.7380 C 0 0 1 0 0 0
3.2440 -1.4430 0.0410 C 0 0
3.5200 -0.0180 0.5580 C 0 0 1 0 0 0
2.2560 0.8610 0.4730 C 0 0
2.3530 -2.4840 2.1890 C 0 0

```


4.1040	-0.0270	1.9760	C	0	0
-2.6860	-0.4450	-0.5430	C	0	0
-3.1250	-1.5350	-0.2560	O	0	0
-2.7360	0.0620	-1.9570	C	0	0
-1.3670	0.0390	-2.6350	C	0	0
-1.4060	0.6030	-4.0310	C	0	0
-1.3050	1.9550	-4.1960	N	0	0
-1.5270	-0.1210	-4.9900	O	0	0
-1.1150	2.8570	-3.0510	C	0	0
-1.3830	2.5270	-5.5470	C	0	0
-0.0160	-0.1720	4.4510	H	0	0
-4.0120	-1.7380	3.9920	H	0	0
-4.0700	-0.9360	1.6780	H	0	0
-1.7700	1.2500	0.1830	H	0	0
0.4260	-1.1760	-0.3770	H	0	0
-0.0270	-1.6190	1.2500	H	0	0
1.8140	-3.0290	0.2150	H	0	0
3.0450	-1.3950	-1.0290	H	0	0
4.1330	-2.0660	0.1520	H	0	0
4.2770	0.4280	-0.0860	H	0	0
2.0270	1.0700	-0.5740	H	0	0
2.4280	1.8280	0.9490	H	0	0
3.4060	-2.7360	2.3200	H	0	0
1.7640	-3.3460	2.4980	H	0	0
2.1210	-1.6620	2.8650	H	0	0
4.7110	-0.9180	2.1370	H	0	0
4.7170	0.8570	2.1460	H	0	0
3.3070	-0.0290	2.7210	H	0	0
-3.3810	-0.5780	-2.5590	H	0	0
-3.1580	1.0680	-1.9750	H	0	0
-1.0650	-1.0080	-2.6680	H	0	0
-0.6330	0.5800	-2.0390	H	0	0
-1.8830	2.7870	-2.2790	H	0	0
-1.0920	3.8890	-3.4060	H	0	0
-0.1520	2.6460	-2.5820	H	0	0
-2.2520	2.2130	-6.1250	H	0	0
-0.4920	2.2460	-6.1080	H	0	0
-1.4040	3.6130	-5.4770	H	0	0
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3	4	2	0		
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11	7	1	0		
13	17	1	0		
15	18	1	0		
9	19	1	0		
19	20	2	0		
19	21	1	0		
21	22	1	0		

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23 24 1 0
23 25 2 0
24 26 1 0
24 27 1 0
2 28 1 0
4 29 1 0
5 30 1 0
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13 34 1 0
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27 55 1 0
M END
> <Name>
Compound187

> <Activ>
0.4

> <DB_Ref_id>
19.08h

$$$$
Compound188
SciTegic10081411483D

51 52 0 0 1 0 999 V2000
-0.7770 1.7250 2.2190 C 0 0
-1.1860 1.7290 3.5660 C 0 0
-2.5450 1.6040 3.8980 C 0 0
-3.5060 1.4730 2.8790 C 0 0
-3.1060 1.4690 1.5330 C 0 0
-1.7440 1.5940 1.1930 C 0 0
0.6820 1.8590 1.9080 C 0 0
1.2600 2.9060 2.0820 O 0 0
-1.3850 1.5860 -0.1310 N 0 0
-3.0800 1.6070 5.7050 Br 0 0
1.3530 0.7700 1.4200 N 0 0
2.7830 0.8670 1.0330 C 0 0
3.6110 -0.2830 1.6390 C 0 0 1 0 0 0

```

2.9610	-1.6500	1.3610	C	0	0				
1.5080	-1.6860	1.8670	C	0	0	1	0	0	0
0.6740	-0.5390	1.2640	C	0	0				
5.0570	-0.2440	1.1370	C	0	0				
0.8570	-3.0430	1.5940	C	0	0				
-1.9690	0.7010	-0.9920	C	0	0				
-2.8050	-0.0760	-0.5940	O	0	0				
-1.5530	0.7190	-2.4400	C	0	0				
-2.3240	-0.2990	-3.2790	C	0	0				
-1.9160	-0.2730	-4.7290	C	0	0				
-2.5690	-1.1250	-5.5140	O	0	0				
-1.0530	0.4780	-5.1190	O	0	0				
-2.1390	-1.0510	-6.8650	C	0	0				
-0.4430	1.8300	4.3480	H	0	0				
-4.5550	1.3750	3.1170	H	0	0				
-3.8620	1.3690	0.7660	H	0	0				
-0.6930	2.2290	-0.4650	H	0	0				
2.8420	0.8380	-0.0550	H	0	0				
3.1930	1.8300	1.3460	H	0	0				
3.6410	-0.1450	2.7210	H	0	0				
2.9820	-1.8560	0.2890	H	0	0				
3.5410	-2.4410	1.8400	H	0	0				
1.5330	-1.5490	2.9490	H	0	0				
-0.3130	-0.5080	1.7270	H	0	0				
0.5160	-0.7110	0.1990	H	0	0				
5.6660	-1.0250	1.5900	H	0	0				
5.5200	0.7150	1.3710	H	0	0				
5.0940	-0.3770	0.0570	H	0	0				
-0.1580	-3.0940	1.9840	H	0	0				
1.4320	-3.8460	2.0570	H	0	0				
0.8100	-3.2400	0.5230	H	0	0				
-1.7680	1.6950	-2.8750	H	0	0				
-0.4790	0.5490	-2.5180	H	0	0				
-3.3770	-0.0290	-3.1880	H	0	0				
-2.2010	-1.3050	-2.8770	H	0	0				
-2.6580	-1.8220	-7.4320	H	0	0				
-2.2770	-0.0250	-7.2110	H	0	0				
-1.0720	-1.2720	-6.8990	H	0	0				
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3	4	2	0						
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11	7	1	0						
13	17	1	0						
15	18	1	0						
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19	20	2	0						
19	21	1	0						
21	22	1	0						

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23 24 1 0
23 25 2 0
24 26 1 0
2 27 1 0
4 28 1 0
5 29 1 0
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26 51 1 0

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M END

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Compound188

> <Activ>

2.1

> <DB_Ref_id>

19.08g

\$\$\$\$

Compound189

SciTegic10081411483D

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48 49 0 0 1 0          999 V2000
-0.6110 2.2150 -1.0120 C 0 0
-0.1250 2.7110 -2.2360 C 0 0
0.5210 3.9590 -2.2910 C 0 0
0.6820 4.7150 -1.1170 C 0 0
0.1970 4.2270 0.1070 C 0 0
-0.4490 2.9790 0.1680 C 0 0
-1.2930 0.8810 -0.9960 C 0 0
-2.4160 0.7620 -0.5620 O 0 0
-0.9120 2.5260 1.3790 N 0 0
1.1720 4.6110 -3.9360 Br 0 0
-0.6210 -0.2090 -1.4840 N 0 0
0.8090 -0.1110 -1.8690 C 0 0
1.6370 -1.2620 -1.2660 C 0 0 1 0 0 0
0.9860 -2.6290 -1.5430 C 0 0
-0.4670 -2.6640 -1.0370 C 0 0 1 0 0 0
-1.3010 -1.5180 -1.6410 C 0 0
3.0820 -1.2230 -1.7680 C 0 0

```

-1.1170	-4.0210	-1.3110	C	0	0
-0.4770	1.3300	1.8750	C	0	0
0.3160	0.6640	1.2520	O	0	0
-1.0020	0.8630	3.2050	C	0	0
-0.4040	-0.4780	3.6310	C	0	0
-0.9240	-0.9390	4.9670	C	0	0
-0.4340	-2.1000	5.3930	O	0	0
-1.7290	-0.2810	5.5820	O	0	0
-0.2520	2.1250	-3.1370	H	0	0
1.1780	5.6760	-1.1410	H	0	0
0.3320	4.8280	0.9960	H	0	0
-1.5680	3.0760	1.8970	H	0	0
0.8670	-0.1410	-2.9590	H	0	0
1.2190	0.8520	-1.5590	H	0	0
1.6660	-1.1230	-0.1840	H	0	0
1.0080	-2.8340	-2.6150	H	0	0
1.5660	-3.4200	-1.0640	H	0	0
-0.4410	-2.5270	0.0450	H	0	0
-2.2870	-1.4860	-1.1780	H	0	0
-1.4590	-1.6890	-2.7050	H	0	0
3.6890	-2.0120	-1.3220	H	0	0
3.5490	-0.2680	-1.5250	H	0	0
3.1190	-1.3460	-2.8500	H	0	0
-0.5370	-4.8260	-0.8570	H	0	0
-2.1330	-4.0490	-0.9140	H	0	0
-1.1720	-4.2150	-2.3830	H	0	0
-0.7270	1.5760	3.9830	H	0	0
-2.0900	0.8090	3.1760	H	0	0
0.6740	-0.3220	3.6880	H	0	0
-0.5940	-1.2400	2.8750	H	0	0
-0.7270	-2.4530	6.2420	H	0	0
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12 31 1 0
13 32 1 0
14 33 1 0
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M END

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Compound189

> <Activ>

1

> <DB_Ref_id>

19.08

\$\$\$\$

Compound190

SciTegic10081411483D

```

43 45 0 0 1 0          999 V2000
-5.1840    1.8570    1.8790 F    0  0
-3.7890   -1.4200   -1.4590 C    0  0
 2.0940    0.8690   -3.5000 C    0  0
 1.6190    0.8460   -2.0470 C    0  0
 4.1700   -1.6110    1.6420 O    0  0
 3.8320   -2.8010   -0.2270 O    0  0
 3.4300   -2.0490    0.7930 C    0  0
 2.0290   -0.4320   -1.3150 C    0  0
 1.9510   -1.7640    0.8320 C    0  0
 1.5940   -0.4360    0.1520 C    0  0  1  0  0  0
 2.3260    0.6150    0.7970 O    0  0
 1.8870    0.9650    2.1170 C    0  0
 0.4340    1.5290    2.1190 C    0  0
-2.8320    1.4200    1.6520 C    0  0
-4.1890    1.1990    1.2830 C    0  0
-4.5020    0.2620    0.2600 C    0  0
-3.4690   -0.4510   -0.3970 C    0  0
-2.1290   -0.2150   -0.0080 C    0  0
-1.8070    0.6880    0.9860 C    0  0
-0.4610    0.7320    1.1820 C    0  0
 0.1000   -0.1680    0.2730 C    0  0
-0.9410   -0.7620   -0.4730 N    0  0
-2.2810    3.1490    3.5210 N    0  0
-2.5230    2.3790    2.6870 C    0  0
-2.9960   -2.1390   -1.6660 H    0  0
-4.0040   -0.8850   -2.3850 H    0  0
-4.6840   -1.9790   -1.1840 H    0  0

```

1.7660	1.7810	-3.9980	H	0	0
3.1820	0.8090	-3.5510	H	0	0
1.6880	0.0230	-4.0530	H	0	0
0.5410	0.9920	-1.9920	H	0	0
1.9730	1.7270	-1.5120	H	0	0
4.7700	-3.0210	-0.3110	H	0	0
3.1040	-0.5960	-1.3970	H	0	0
1.6490	-1.3120	-1.8300	H	0	0
1.4100	-2.5350	0.2870	H	0	0
1.6000	-1.7750	1.8630	H	0	0
2.5780	1.7030	2.5190	H	0	0
1.9630	0.0800	2.7500	H	0	0
0.4340	2.5680	1.7890	H	0	0
0.0390	1.5040	3.1330	H	0	0
-5.5310	0.0920	-0.0220	H	0	0
-0.8380	-1.4410	-1.1920	H	0	0
15	1	1	0		
17	2	1	0		
4	3	1	0		
8	4	1	0		
7	5	2	0		
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9	7	1	0		
10	8	1	0		
10	9	1	0		
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21	10	1	0		
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11	12	1	0		
12	13	1	0		
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19	14	2	0		
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19	18	1	0		
20	19	1	0		
21	20	2	0		
22	21	1	0		
14	24	1	0		
24	23	3	0		
2	25	1	0		
2	26	1	0		
2	27	1	0		
3	28	1	0		
3	29	1	0		
3	30	1	0		
4	31	1	0		
4	32	1	0		
6	33	1	0		
8	34	1	0		
8	35	1	0		
9	36	1	0		
9	37	1	0		
12	38	1	0		
12	39	1	0		
13	40	1	0		
13	41	1	0		
16	42	1	0		
22	43	1	0		

Compound191
SciTegic10081411483D

[illegible]


```

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7  6  1  0
8  7  2  0
9  8  1  0
5  9  1  0
8 10  1  0
10 11  1  0
11 12  1  0
12 13  1  0
7 13  1  0
10 14  1  0
14 15  1  0
15 16  1  0
15 17  2  0
10 18  1  0
18 19  1  0
19 20  1  0
6  1  1  0
4 21  1  0
2 22  1  0
1 24  1  0
24 23  3  0
3 25  1  0
9 26  1  0
12 27  1  0
12 28  1  0
13 29  1  0
13 30  1  0
14 31  1  0
14 32  1  0
16 33  1  0
18 34  1  0
18 35  1  0
19 36  1  0
19 37  1  0
20 38  1  0
20 39  1  0
20 40  1  0
21 41  1  0
21 42  1  0
21 43  1  0
M  END
> <Name>
Compound191

> <Activ>
0.08

> <DB_Ref_id>
22.3

$$$$
Compound192
  SciTegic10081411483D

43 45  0  0  1  0          999 V2000
  -0.6450    0.1760    1.1820 N    0  0
  -1.8990    0.6370    0.8050 C    0  0
  -1.8300    0.9710   -0.5330 C    0  0
  -0.5820    0.7520   -1.0250 C    0  0

```

0.1760	0.2500	0.0350	C	0	0				
1.6460	-0.1330	-0.0780	C	0	0	1	0	0	0
2.0060	-0.2640	-1.4590	O	0	0				
1.6000	0.8130	-2.3150	C	0	0				
0.0490	0.9380	-2.3970	C	0	0				
2.5270	0.9530	0.5510	C	0	0				
3.9960	0.6860	0.3550	C	0	0				
4.5180	1.1910	-0.7580	O	0	0				
4.6270	0.0530	1.1700	O	0	0				
1.9020	-1.4980	0.5680	C	0	0				
1.0100	-2.6000	-0.0060	C	0	0				
1.2710	-3.9630	0.6330	C	0	0				
-2.9830	1.4650	-1.2090	C	0	0				
-4.1930	1.6270	-0.4820	C	0	0				
-4.2440	1.2870	0.8960	C	0	0				
-3.0920	0.7850	1.5530	C	0	0				
-3.1450	0.4240	2.9800	C	0	0				
-2.9590	1.8030	-2.6110	C	0	0				
-2.9400	2.0680	-3.7400	N	0	0				
-0.3710	-0.1450	2.0820	H	0	0				
2.0200	0.6370	-3.3050	H	0	0				
2.0470	1.7340	-1.9400	H	0	0				
-0.2150	1.9140	-2.8030	H	0	0				
-0.3570	0.1780	-3.0650	H	0	0				
2.2890	0.9530	1.6150	H	0	0				
2.2710	1.9340	0.1520	H	0	0				
5.4570	1.0570	-0.9430	H	0	0				
2.9530	-1.7720	0.4880	H	0	0				
1.7910	-1.4380	1.6520	H	0	0				
-0.0410	-2.3280	0.0800	H	0	0				
1.1170	-2.6540	-1.0900	H	0	0				
0.6130	-4.7210	0.2090	H	0	0				
2.3070	-4.2680	0.4820	H	0	0				
1.0900	-3.9260	1.7070	H	0	0				
-5.0840	2.0060	-0.9630	H	0	0				
-5.1660	1.4140	1.4470	H	0	0				
-2.2030	0.0490	3.3810	H	0	0				
-3.9020	-0.3440	3.1330	H	0	0				
-3.4320	1.2990	3.5640	H	0	0				
3	2	2	0						
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5	4	2	0						
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11	13	2	0						
6	14	1	0						
14	15	1	0						
15	16	1	0						
3	17	1	0						
17	18	2	0						
18	19	1	0						
19	20	2	0						
2	20	1	0						
20	21	1	0						

```

17 22 1 0
2 1 1 0
22 23 3 0
1 24 1 0
8 25 1 0
8 26 1 0
9 27 1 0
9 28 1 0
10 29 1 0
10 30 1 0
12 31 1 0
14 32 1 0
14 33 1 0
15 34 1 0
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16 37 1 0
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18 39 1 0
19 40 1 0
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21 43 1 0

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M END

> <Name>

Compound192

> <Activ>

2.4

> <DB_Ref_id>

22.27

\$\$\$\$

Compound193

SciTegic10081411483D

```

39 41 0 0 1 0          999 V2000
  0.9830   -0.7420   -0.4380 N   0  0
  2.1660   -0.0080   -0.4630 C   0  0
  1.9080    1.2150    0.1310 C   0  0
  0.6020    1.2890    0.5140 C   0  0
  0.0160    0.0740    0.1870 C   0  0
 -1.4390   -0.2290    0.5140 C   0  0  2  0  0  0
 -2.2710    0.9300    0.3510 O   0  0
 -1.7190    2.2440    0.5680 C   0  0
 -0.2830    2.3360    1.1600 C   0  0
 -1.5530   -0.6480    1.9820 C   0  0
 -0.7520   -1.8850    2.2890 C   0  0
  0.5080   -1.6660    2.6560 O   0  0
 -1.2460   -2.9840    2.1990 O   0  0
 -2.0140   -1.3130   -0.4040 C   0  0
 -2.0550   -0.8830   -1.8710 C   0  0
 -2.5250   -2.0000   -2.8010 C   0  0
  2.9460    2.1860    0.2750 C   0  0
  4.2370    1.8710   -0.2270 C   0  0
  4.4870    0.6230   -0.8480 C   0  0
  3.4490   -0.3360   -0.9710 C   0  0
  3.7660   -1.8500   -1.7170 Cl  0  0
  2.7310    3.7130    1.0330 Cl  0  0
  0.8400   -1.6600   -0.7890 H   0  0

```

-2.4260	2.8110	1.1760	H	0	0
-1.7170	2.7210	-0.4120	H	0	0
-0.3030	2.1580	2.2360	H	0	0
0.0880	3.3440	1.0020	H	0	0
-2.6110	-0.8400	2.1580	H	0	0
-1.2460	0.1640	2.6410	H	0	0
1.0760	-2.4200	2.8690	H	0	0
-1.4630	-2.2460	-0.2910	H	0	0
-3.0040	-1.6170	-0.0650	H	0	0
-2.6720	0.0080	-1.9940	H	0	0
-1.0840	-0.5020	-2.1880	H	0	0
-2.5530	-1.6560	-3.8340	H	0	0
-1.8650	-2.8650	-2.7310	H	0	0
-3.5290	-2.3280	-2.5310	H	0	0
5.0470	2.5820	-0.1430	H	0	0
5.4790	0.4100	-1.2250	H	0	0
2	1	1	0		
3	2	1	0		
4	3	1	0		
5	4	2	0		
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14	32	1	0		
15	33	1	0		
15	34	1	0		
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16	36	1	0		
16	37	1	0		
18	38	1	0		
19	39	1	0		

M END

> <Name>

Compound193

45	47	0	0	1	0	999	v2000				
-1.1390				-0.9610		-1.0550	N	0	0		
-1.9980				-0.0900		-0.3870	C	0	0		
-1.2070				0.8170		0.2870	C	0	0		
0.1110				0.5670		0.0880	C	0	0		
0.1800				-0.5450		-0.7540	C	0	0		
1.4900				-1.1660		-1.2260	C	0	0	2	0 0 0
2.5740				-0.2580		-0.9820	O	0	0		
2.6150				0.3360		0.3240	C	0	0		
1.3790				1.2440		0.5800	C	0	0		
1.4670				-1.4180		-2.7360	C	0	0		
1.1640				-0.1700		-3.5210	C	0	0		
1.0980				-0.3320		-4.8400	O	0	0		
0.9980				0.8910		-2.9650	O	0	0		
1.7700				-2.4630		-0.4590	C	0	0		
0.9960				-2.5490		0.8580	C	0	0		
1.5060				-3.6640		1.7700	C	0	0		
-1.7810				1.8540		1.0700	C	0	0		
-3.1950				1.9340		1.1520	C	0	0		
-4.0080				0.9960		0.4610	C	0	0		
-3.4140				-0.0290		-0.3200	C	0	0		
-4.4040				-1.1560		-1.1540	C1	0	0		
-0.9590				2.8400		1.7910	C	0	0		
-1.7750				4.0700		2.1900	C	0	0		
-1.3960				-1.7270		-1.6330	H	0	0		
3.5330				0.9200		0.4020	H	0	0		
2.6780				-0.4590		1.0680	H	0	0		
1.3030				1.4670		1.6450	H	0	0		
1.4900				2.1920		0.0550	H	0	0		
0.6860				-2.1580		-2.9040	H	0	0		
2.4100				-1.8460		-3.0700	H	0	0		
0.9080				0.4300		-5.4000	H	0	0		
1.5650				-3.3320		-1.0840	H	0	0		
2.8380				-2.5860		-0.2850	H	0	0		
1.0080				-1.5900		1.3750	H	0	0		
-0.0720				-2.6640		0.6680	H	0	0		
0.9410				-3.6870		2.7030	H	0	0		
1.4200				-4.6330		1.2790	H	0	0		
2.5550				-3.5080		2.0200	H	0	0		
-3.6620				2.7090		1.7400	H	0	0		
-5.0840				1.0740		0.5370	H	0	0		
-0.1070				3.1250		1.1740	H	0	0		
-0.5160				2.3710		2.6700	H	0	0		
-1.1390				4.8830		2.5430	H	0	0		
-2.4790				3.8260		2.9850	H	0	0		
-2.3480				4.4440		1.3400	H	0	0		
2	1	1	0								
3	2	1	0								
4	3	1	0								
5	4	2	0								
1	5	1	0								

```

5 6 1 0
6 7 1 0
7 8 1 0
8 9 1 0
4 9 1 0
6 10 1 0
10 11 1 0
11 12 1 0
11 13 2 0
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18 19 2 0
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2 20 2 0
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22 23 1 0
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8 26 1 0
9 27 1 0
9 28 1 0
10 29 1 0
10 30 1 0
12 31 1 0
14 32 1 0
14 33 1 0
15 34 1 0
15 35 1 0
16 36 1 0
16 37 1 0
16 38 1 0
18 39 1 0
19 40 1 0
22 41 1 0
22 42 1 0
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23 45 1 0
M END
> <Name>
Compound194

> <Activ>
2

> <DB_Ref_id>
22.23

$$$$
Compound195
SciTegic10081411483D

43 45 0 0 1 0 999 V2000
-5.4400 -0.3710 1.9570 F 0 0
-3.3980 2.0920 -1.7290 C 0 0
2.8220 3.1080 0.3790 C 0 0
2.0720 1.7870 0.5630 C 0 0

```

3.8830	-1.1270	-2.5490	O	0	0				
3.5350	-2.9020	-1.2270	O	0	0				
3.1520	-1.7950	-1.8550	C	0	0				
2.2680	0.8320	-0.6170	C	0	0				
1.7130	-1.4060	-1.6480	C	0	0				
1.5220	-0.4920	-0.4320	C	0	0	3	0	0	0
2.1060	-1.1350	0.7090	O	0	0				
1.3910	-2.2660	1.2250	C	0	0				
-0.0140	-1.8670	1.7640	C	0	0				
-3.1000	-0.7190	1.5370	C	0	0				
-4.3500	-0.1020	1.2400	C	0	0				
-4.4450	0.8200	0.1620	C	0	0				
-3.3030	1.1310	-0.6170	C	0	0				
-2.0760	0.5000	-0.3050	C	0	0				
-1.9650	-0.4020	0.7340	C	0	0				
-0.6930	-0.8770	0.8300	C	0	0				
0.0410	-0.2480	-0.1800	C	0	0				
-0.8220	0.6150	-0.8910	N	0	0				
-2.9360	-2.3890	3.5290	N	0	0				
-3.0080	-1.6450	2.6410	C	0	0				
-2.4610	2.2560	-2.2600	H	0	0				
-3.7420	3.0550	-1.3520	H	0	0				
-4.1330	1.7360	-2.4510	H	0	0				
2.6540	3.7660	1.2320	H	0	0				
3.8930	2.9320	0.2710	H	0	0				
2.4770	3.6270	-0.5160	H	0	0				
1.0140	1.9670	0.7420	H	0	0				
2.3590	1.3090	1.4980	H	0	0				
4.4470	-3.2070	-1.3180	H	0	0				
3.3260	0.6560	-0.7990	H	0	0				
1.9770	1.3110	-1.5530	H	0	0				
1.3540	-0.8400	-2.5080	H	0	0				
1.0960	-2.3010	-1.5590	H	0	0				
1.3070	-3.0120	0.4320	H	0	0				
1.9880	-2.7150	2.0160	H	0	0				
0.0800	-1.4000	2.7460	H	0	0				
-0.6230	-2.7620	1.8810	H	0	0				
-5.3930	1.2870	-0.0640	H	0	0				
-0.5740	1.1910	-1.6600	H	0	0				
15	1	1	0						
17	2	1	0						
4	3	1	0						
8	4	1	0						
7	5	2	0						
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21	10	1	0						
10	11	1	0						
11	12	1	0						
12	13	1	0						
18	17	2	0						
19	14	2	0						
14	15	1	0						
15	16	2	0						
16	17	1	0						
18	22	1	0						
19	18	1	0						
20	19	1	0						

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21 20 2 0
22 21 1 0
14 24 1 0
24 23 3 0
2 25 1 0
2 26 1 0
2 27 1 0
3 28 1 0
3 29 1 0
3 30 1 0
4 31 1 0
4 32 1 0
6 33 1 0
8 34 1 0
8 35 1 0
9 36 1 0
9 37 1 0
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12 39 1 0
13 40 1 0
13 41 1 0
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22 43 1 0

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M END

> <Name>

Compound195

> <Activ>

0.12

> <DB_Ref_id>

22.22

\$\$\$\$

Compound196

SciTegic10081411483D

```

45 47 0 0 1 0          999 V2000
-0.5270 1.7520 -0.0570 N 0 0
0.5040 0.7870 -0.1330 C 0 0
-0.0760 -0.4650 -0.3440 C 0 0
-1.4140 -0.2640 -0.3930 C 0 0
-1.7310 1.0680 -0.2230 C 0 0
-3.0760 1.5180 -0.2380 C 0 0
-4.1040 0.5610 -0.4320 C 0 0
-2.4300 -1.2380 -0.5940 C 0 0
-3.7810 -0.8110 -0.6070 C 0 0
2.0080 1.0120 -0.0040 C 0 0 3 0 0 0
2.7130 -0.1410 -0.4860 O 0 0
2.2460 -1.4100 -0.0080 C 0 0
0.7930 -1.7050 -0.4750 C 0 0
2.4610 2.1910 -0.8650 C 0 0
2.3870 1.2250 1.4650 C 0 0
2.1230 2.0060 -2.3200 C 0 0
2.5640 2.9630 -3.1310 O 0 0
1.4940 1.0430 -2.6930 O 0 0
-3.4750 3.1760 -0.0270 Cl 0 0
-2.1170 -2.6660 -0.7830 C 0 0
-3.2890 -3.4180 -1.4160 C 0 0
1.3300 0.6930 2.4320 C 0 0
1.8220 0.6470 3.8790 C 0 0

```


-0.4100	2.7290	0.0880	H	0	0
-5.1410	0.8630	-0.4450	H	0	0
-4.5740	-1.5290	-0.7540	H	0	0
2.3160	-1.4200	1.0800	H	0	0
2.9240	-2.1820	-0.3770	H	0	0
0.3770	-2.5250	0.1090	H	0	0
0.7910	-2.0160	-1.5210	H	0	0
3.5430	2.2560	-0.7420	H	0	0
2.0290	3.1230	-0.5000	H	0	0
3.3610	0.7850	1.6800	H	0	0
2.5920	2.2770	1.6600	H	0	0
2.3810	2.9020	-4.0780	H	0	0
-1.8440	-3.1090	0.1740	H	0	0
-1.2210	-2.7640	-1.3960	H	0	0
-2.9980	-4.4140	-1.7520	H	0	0
-3.6760	-2.8750	-2.2770	H	0	0
-4.1020	-3.5330	-0.6990	H	0	0
0.4100	1.2740	2.3580	H	0	0
0.9760	-0.2890	2.1150	H	0	0
1.0410	0.2730	4.5410	H	0	0
2.6990	0.0060	3.9670	H	0	0
2.1020	1.6430	4.2230	H	0	0
5	1	1	0		
4	5	1	0		
3	4	1	0		
1	2	1	0		
2	3	2	0		
9	7	2	0		
8	9	1	0		
7	6	1	0		
4	8	2	0		
5	6	2	0		
12	13	1	0		
11	12	1	0		
10	11	1	0		
2	10	1	0		
3	13	1	0		
10	14	1	0		
10	15	1	0		
14	16	1	0		
16	17	1	0		
16	18	2	0		
6	19	1	0		
8	20	1	0		
20	21	1	0		
15	22	1	0		
22	23	1	0		
1	24	1	0		
7	25	1	0		
9	26	1	0		
12	27	1	0		
12	28	1	0		
13	29	1	0		
13	30	1	0		
14	31	1	0		
14	32	1	0		
15	33	1	0		
15	34	1	0		
17	35	1	0		
20	36	1	0		
20	37	1	0		

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22 41 1 0
22 42 1 0
23 43 1 0
23 44 1 0
23 45 1 0

M END

> <Name>

Compound196

> <Activ>

3

> <DB_Ref_id>

22.05

\$\$\$\$

Compound197

SciTegic10081411483D

42	44	0	0	1	0	999	V2000				
-4.3460		0.9730		0.8920	C	0	0				
-3.0150		1.2890		1.2830	C	0	0				
-1.9350		0.5470		0.7190	C	0	0				
-2.1620	-0.4690			-0.2110	C	0	0				
-0.8220	-1.3120			-0.8580	S	0	0				
0.0920	-0.2520			0.1760	C	0	0				
-0.5760	0.6950			0.9760	C	0	0				
0.1940	1.6410			1.8890	C	0	0				
1.6820	1.2270			2.0080	C	0	0				
2.2130	0.7930			0.7540	O	0	0				
1.6100	-0.3790			0.1950	C	0	0	2	0	0	0
2.1430	-0.5000			-1.2350	C	0	0				
1.6860	0.6500			-2.1350	C	0	0				
2.2310	0.5390			-3.5570	C	0	0				
2.0240	-1.5920			1.0350	C	0	0				
3.5180	-1.7190			1.1600	C	0	0				
4.0550	-1.0780			2.1950	O	0	0				
4.1560	-2.3650			0.3630	O	0	0				
-3.4880	-0.7770			-0.6020	C	0	0				
-3.7340	-1.8460			-1.5840	C	0	0				
-4.5760	-0.0600			-0.0490	C	0	0				
-5.3890	1.6330			1.3960	F	0	0				
-2.7910	2.3540			2.2340	C	0	0				
-2.6130	3.2110			2.9960	N	0	0				
0.1130	2.6470			1.4780	H	0	0				
-0.2540	1.6540			2.8810	H	0	0				
2.2800	2.0700			2.3550	H	0	0				
1.8110	0.4260			2.7360	H	0	0				
3.2290	-0.5800			-1.2360	H	0	0				
1.8650	-1.4610			-1.6700	H	0	0				
0.5980	0.7230			-2.1430	H	0	0				
1.9490	1.6110			-1.6940	H	0	0				
1.8790	1.3670			-4.1720	H	0	0				
3.3230	0.5390			-3.5530	H	0	0				
1.9010	-0.3870			-4.0260	H	0	0				
1.6190	-2.4650			0.5230	H	0	0				
1.5710	-1.5450			2.0250	H	0	0				
5.0100	-1.1210			2.3340	H	0	0				

-2.8320	-2.3360	-1.9490	H	0	0
-4.2600	-1.4340	-2.4450	H	0	0
-4.3710	-2.6090	-1.1390	H	0	0
-5.5860	-0.3050	-0.3480	H	0	0

2 23 1 0
 3 2 2 0
 4 3 1 0
 4 5 1 0
 6 5 1 0
 7 6 2 0
 3 7 1 0
 7 8 1 0
 9 8 1 0
 10 9 1 0
 11 10 1 0
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 13 14 1 0
 11 15 1 0
 15 16 1 0
 16 17 1 0
 16 18 2 0
 6 11 1 0
 19 4 2 0
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 21 19 1 0
 1 21 2 0
 1 22 1 0
 1 2 1 0
 23 24 3 0
 8 25 1 0
 8 26 1 0
 9 27 1 0
 9 28 1 0
 12 29 1 0
 12 30 1 0
 13 31 1 0
 13 32 1 0
 14 33 1 0
 14 34 1 0
 14 35 1 0
 15 36 1 0
 15 37 1 0
 17 38 1 0
 20 39 1 0
 20 40 1 0
 20 41 1 0
 21 42 1 0

M END
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 Compound197

 > <Activ>
 5.36

 > <DB_Ref_id>
 23.33

 \$\$\$\$
 Compound198
 SciTegic10081411483D

[illegible]

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20 19 1 0
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20 21 1 0
21 22 1 0
1 21 2 0
19 7 2 0
1 2 1 0
22 23 3 0
1 24 1 0
2 25 1 0
4 26 1 0
4 27 1 0
4 28 1 0
9 29 1 0
9 30 1 0
12 31 1 0
13 32 1 0
13 33 1 0
14 34 1 0
14 35 1 0
15 36 1 0
15 37 1 0
15 38 1 0
17 39 1 0
17 40 1 0
18 41 1 0
18 42 1 0
M END
> <Name>
Compound198

> <Activ>
2.85

> <DB_Ref_id>
23.32

$$$$
Compound199
SciTegic10081411483D

42 44 0 0 1 0          999 V2000
-3.6520 2.2230 0.0820 C 0 0
-2.5430 1.7710 0.8260 C 0 0
-1.4780 1.0980 0.1680 C 0 0
-1.5160 0.8530 -1.2070 C 0 0
-2.6370 1.3220 -1.9750 C 0 0
-3.7050 2.0020 -1.3180 C 0 0
-0.2230 -0.0250 -1.9020 S 0 0
-0.3030 0.5980 0.7480 C 0 0
0.4280 -0.0450 -0.2730 C 0 0
0.2950 0.6620 2.1500 C 0 0
1.8320 0.7440 1.9980 C 0 0
2.3200 -0.4550 1.3280 O 0 0
1.7790 -0.7250 0.0230 C 0 0 1 0 0 0
1.6080 -2.2620 0.0160 C 0 0
2.8240 -0.2660 -1.0040 C 0 0
2.9920 1.2300 -1.0250 C 0 0
4.0000 1.6970 -0.2930 O 0 0
2.2460 1.9320 -1.6700 O 0 0
0.5450 -2.7420 1.0060 C 0 0

```

0.3650	-4.2600	0.9880	C	0	0
-2.7210	1.1090	-3.4300	C	0	0
-2.5680	2.0020	2.2560	C	0	0
-2.5980	2.1840	3.4060	N	0	0
-4.4690	2.7360	0.5780	H	0	0
-4.5760	2.3460	-1.8480	H	0	0
-0.0740	1.5210	2.7250	H	0	0
0.0270	-0.2460	2.6970	H	0	0
2.1130	1.6620	1.4530	H	0	0
2.2790	0.7930	2.9900	H	0	0
1.3850	-2.6190	-0.9900	H	0	0
2.5610	-2.7580	0.2030	H	0	0
2.4650	-0.6110	-1.9730	H	0	0
3.7850	-0.7420	-0.8140	H	0	0
4.1600	2.6500	-0.2640	H	0	0
0.7720	-2.3930	2.0140	H	0	0
-0.4060	-2.2400	0.8240	H	0	0
-0.3920	-4.5680	1.7070	H	0	0
0.0720	-4.6020	-0.0060	H	0	0
1.2970	-4.7620	1.2520	H	0	0
-1.8570	0.6030	-3.8590	H	0	0
-2.8300	2.0700	-3.9320	H	0	0
-3.6050	0.5120	-3.6580	H	0	0
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4	3	1	0		
5	4	2	0		
6	5	1	0		
1	6	2	0		
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4	7	1	0		
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13	12	1	0		
9	13	1	0		
8	10	1	0		
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15	16	1	0		
16	17	1	0		
16	18	2	0		
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10	27	1	0		
11	28	1	0		
11	29	1	0		
14	30	1	0		
14	31	1	0		
15	32	1	0		
15	33	1	0		
17	34	1	0		
19	35	1	0		
19	36	1	0		

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20 38 1 0
20 39 1 0
21 40 1 0
21 41 1 0
21 42 1 0

M END

> <Name>

Compound199

> <Activ>

0.17

> <DB_Ref_id>

23.31

\$\$\$\$

Compound200

SciTegic10081411483D

42	44	0	0	1	0	999	V2000				
-4.2660	1.4920	-0.3750	C	0	0						
-4.2730	1.2990	1.0250	C	0	0						
-3.0900	0.8870	1.6930	C	0	0						
-1.8980	0.6780	0.9570	C	0	0						
-1.8960	0.8810	-0.4220	C	0	0						
-3.0740	1.2830	-1.1150	C	0	0						
-0.4510	0.1740	1.7150	S	0	0						
-0.6370	0.6410	-0.9650	C	0	0						
0.1930	0.2460	0.1020	C	0	0						
1.6620	-0.1130	-0.1210	C	0	0	3	0	0	0		
1.9360	-0.3300	-1.5120	O	0	0						
1.4450	0.6740	-2.4040	C	0	0						
-0.1000	0.7270	-2.3870	C	0	0						
1.9960	-1.4240	0.5960	C	0	0						
2.5630	1.0230	0.3770	C	0	0						
4.0180	0.7700	0.0940	C	0	0						
4.4510	1.2170	-1.0820	O	0	0						
4.7190	0.1990	0.8980	O	0	0						
1.0550	-2.5660	0.2070	C	0	0						
1.4060	-3.8830	0.9000	C	0	0						
-3.1050	0.6880	3.1470	C	0	0						
-3.1050	1.4770	-2.5430	C	0	0						
-3.1310	1.6270	-3.6930	N	0	0						
-5.1780	1.8030	-0.8690	H	0	0						
-5.1860	1.4590	1.5860	H	0	0						
1.8050	0.4450	-3.4040	H	0	0						
1.8710	1.6330	-2.1210	H	0	0						
-0.4340	1.6450	-2.8670	H	0	0						
-0.5120	-0.1050	-2.9590	H	0	0						
3.0350	-1.7050	0.4220	H	0	0						
2.0020	-1.2830	1.6760	H	0	0						
2.4010	1.0880	1.4530	H	0	0						
2.2600	1.9750	-0.0610	H	0	0						
5.3770	1.0840	-1.3240	H	0	0						
0.0180	-2.2930	0.3980	H	0	0						
1.0330	-2.6950	-0.8750	H	0	0						
0.7110	-4.6680	0.6090	H	0	0						
2.4200	-4.1930	0.6500	H	0	0						
1.3500	-3.7730	1.9840	H	0	0						
-2.1500	0.3710	3.5670	H	0	0						

-3.8480	-0.0680	3.4020	H	0	0
-3.3940	1.6170	3.6390	H	0	0

4	5	2	0
3	4	1	0
2	3	2	0
1	2	1	0
1	6	2	0
9	7	1	0
8	9	2	0
4	7	1	0
5	8	1	0
12	13	1	0
11	12	1	0
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8	13	1	0
10	14	1	0
10	15	1	0
15	16	1	0
16	17	1	0
16	18	2	0
14	19	1	0
19	20	1	0
3	21	1	0
6	22	1	0
5	6	1	0
22	23	3	0
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2	25	1	0
12	26	1	0
12	27	1	0
13	28	1	0
13	29	1	0
14	30	1	0
14	31	1	0
15	32	1	0
15	33	1	0
17	34	1	0
19	35	1	0
19	36	1	0
20	37	1	0
20	38	1	0
20	39	1	0
21	40	1	0
21	41	1	0
21	42	1	0

M END

> <Name>
Compound200

> <Activ>
0.32

> <DB_Ref_id>
23.3

\$\$\$\$

Compound201
SciTegic10081411483D

41	43	0	0	1	0	999	V2000
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-4.1170	2.1010	0.3650	C	0	0				
-4.5370	0.7790	0.6350	C	0	0				
-3.5860	-0.2620	0.7130	C	0	0				
-2.2110	0.0170	0.5290	C	0	0				
-1.7970	1.3280	0.2720	C	0	0				
-2.7420	2.3980	0.1740	C	0	0				
-1.0370	-1.2230	0.6130	S	0	0				
-0.4080	1.3910	0.1350	C	0	0				
0.0740	0.0740	0.2910	C	0	0				
1.5620	-0.2480	0.1880	C	0	0	3	0	0	0
2.2730	0.8100	-0.4610	O	0	0				
2.0330	2.1210	0.0570	C	0	0				
0.5530	2.5430	-0.1390	C	0	0				
1.7730	-1.4940	-0.6740	C	0	0				
2.1560	-0.4490	1.5860	C	0	0				
3.6450	-0.6760	1.5510	C	0	0				
4.3850	0.4260	1.6230	O	0	0				
4.1040	-1.7910	1.4630	O	0	0				
1.1250	-1.3730	-2.0530	C	0	0				
1.3550	-2.6120	-2.9220	C	0	0				
-4.0310	-1.6390	0.9860	C	0	0				
-2.2970	4.1950	-0.2050	Br	0	0				
-4.8670	2.8790	0.3090	H	0	0				
-5.5880	0.5700	0.7790	H	0	0				
2.3090	2.1390	1.1110	H	0	0				
2.6950	2.8160	-0.4590	H	0	0				
0.3480	3.3750	0.5330	H	0	0				
0.3960	2.8890	-1.1600	H	0	0				
2.8360	-1.7230	-0.7660	H	0	0				
1.4180	-2.3850	-0.1560	H	0	0				
1.6580	-1.3260	2.0020	H	0	0				
1.9260	0.4000	2.2290	H	0	0				
5.3480	0.3510	1.6060	H	0	0				
0.0610	-1.1600	-1.9610	H	0	0				
1.4690	-0.4750	-2.5640	H	0	0				
0.8710	-2.4940	-3.8930	H	0	0				
2.4200	-2.7810	-3.0740	H	0	0				
0.9390	-3.4980	-2.4470	H	0	0				
-3.2250	-2.3710	1.0290	H	0	0				
-4.7310	-1.9550	0.2130	H	0	0				
-4.5570	-1.6660	1.9410	H	0	0				
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4	5	1	0						
3	4	2	0						
2	3	1	0						
1	2	2	0						
1	6	1	0						
9	7	1	0						
8	9	2	0						
4	7	1	0						
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11	12	1	0						
10	11	1	0						
9	10	1	0						
8	13	1	0						
10	14	1	0						
10	15	1	0						
15	16	1	0						
16	17	1	0						
16	18	2	0						

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14 19 1 0
19 20 1 0
3 21 1 0
6 22 1 0
1 23 1 0
2 24 1 0
12 25 1 0
12 26 1 0
13 27 1 0
13 28 1 0
14 29 1 0
14 30 1 0
15 31 1 0
15 32 1 0
17 33 1 0
19 34 1 0
19 35 1 0
20 36 1 0
20 37 1 0
20 38 1 0
21 39 1 0
21 40 1 0
21 41 1 0

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M END

> <Name>

Compound201

> <Activ>

0.19

> <DB_Ref_id>

23.29

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Compound202

SciTegic10081411483D

```

41 43 0 0 1 0          999 V2000
-4.1370    1.9940    0.4160 C    0  0
-4.6520    0.7850   -0.1040 C    0  0
-3.8070   -0.3400   -0.2620 C    0  0
-2.4380   -0.2500    0.1030 C    0  0
-1.9340    0.9510    0.6110 C    0  0
-2.7720    2.0940    0.7870 C    0  0
-1.3730   -1.5820   -0.0630 S    0  0
-0.5740    0.8440    0.9020 C    0  0
-0.1950   -0.4770    0.5840 C    0  0
 1.2360   -0.9650    0.7890 C    0  0  3  0  0  0
 1.9610   -0.0860    1.6560 O    0  0
 1.8890    1.3050    1.3280 C    0  0
 0.4370    1.8360    1.4610 C    0  0
 1.9690   -1.0310   -0.5570 C    0  0
 1.2360   -2.3320    1.4710 C    0  0
 0.5230   -2.3140    2.7950 C    0  0
 0.5190   -3.4710    3.4530 O    0  0
 0.0000   -1.3050    3.2070 O    0  0
-4.4470   -1.7990   -0.8910 Cl   0  0
-2.2270    3.5960    1.4260 Cl   0  0
 1.3070   -0.1700   -1.6330 C    0  0
 2.1290   -0.0960   -2.9180 C    0  0
 1.4650    0.7600   -3.9960 C    0  0

```

-4.8030	2.8380	0.5290	H	0	0
-5.6950	0.7310	-0.3790	H	0	0
2.2680	1.4490	0.3160	H	0	0
2.5530	1.8480	2.0000	H	0	0
0.3690	2.7870	0.9340	H	0	0
0.1990	2.0200	2.5100	H	0	0
3.0180	-0.7620	-0.4380	H	0	0
2.0610	-2.0640	-0.8930	H	0	0
2.2830	-2.5960	1.6170	H	0	0
0.7910	-3.0880	0.8200	H	0	0
0.0780	-3.5250	4.3110	H	0	0
0.2950	-0.5210	-1.8400	H	0	0
1.1000	0.8300	-1.2500	H	0	0
3.1390	0.2600	-2.7110	H	0	0
2.3400	-1.0960	-3.2970	H	0	0
2.0820	0.7970	-4.8950	H	0	0
0.4820	0.3610	-4.2560	H	0	0
1.3260	1.7830	-3.6450	H	0	0
5	6	2	0		
4	5	1	0		
3	4	2	0		
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8	9	2	0		
4	7	1	0		
5	8	1	0		
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9	10	1	0		
8	13	1	0		
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10	15	1	0		
15	16	1	0		
16	17	1	0		
16	18	2	0		
3	19	1	0		
6	20	1	0		
14	21	1	0		
21	22	1	0		
22	23	1	0		
1	24	1	0		
2	25	1	0		
12	26	1	0		
12	27	1	0		
13	28	1	0		
13	29	1	0		
14	30	1	0		
14	31	1	0		
15	32	1	0		
15	33	1	0		
17	34	1	0		
21	35	1	0		
21	36	1	0		
22	37	1	0		
22	38	1	0		
23	39	1	0		
23	40	1	0		
23	41	1	0		

```

M  END
> <Name>
Compound202

> <Activ>
0.75

> <DB_Ref_id>
23.26

```

```

$$$$
Compound203
SciTegic10081411483D

```

```

32 34 0 0 1 0          999 V2000
-4.4020 0.9140 -0.6290 C 0 0
-4.6620 -0.4720 -0.5290 C 0 0
-3.5920 -1.3860 -0.3770 C 0 0
-2.2560 -0.9100 -0.3200 C 0 0
-2.0100 0.4630 -0.4140 C 0 0
-3.0720 1.4030 -0.5780 C 0 0
-0.9260 -1.9720 -0.1450 S 0 0
-0.6440 0.7350 -0.3340 C 0 0
0.0080 -0.5080 -0.1970 C 0 0
1.5290 -0.5990 -0.0920 C 0 0 3 0 0 0
2.1500 0.6150 -0.5250 O 0 0
1.6230 1.8170 0.0450 C 0 0
0.1490 2.0350 -0.3750 C 0 0
2.0570 -1.7030 -1.0120 C 0 0
1.9430 -0.8610 1.3610 C 0 0
3.4380 -0.8710 1.5390 C 0 0
3.9790 0.3070 1.8360 O 0 0
4.0740 -1.8900 1.4140 O 0 0
-3.9240 -3.0660 -0.2600 Cl 0 0
-2.8400 3.1000 -0.7250 Cl 0 0
-5.2340 1.5940 -0.7480 H 0 0
-5.6840 -0.8200 -0.5700 H 0 0
2.2400 2.6510 -0.2890 H 0 0
1.7190 1.7620 1.1310 H 0 0
0.1020 2.4340 -1.3910 H 0 0
-0.2950 2.7740 0.2930 H 0 0
1.7070 -1.5540 -2.0310 H 0 0
3.1490 -1.7170 -1.0080 H 0 0
1.7110 -2.6790 -0.6780 H 0 0
1.5330 -1.8380 1.6190 H 0 0
1.4940 -0.1250 2.0270 H 0 0
4.9360 0.3690 1.9630 H 0 0

5 6 2 0
4 5 1 0
3 4 2 0
2 3 1 0
1 2 2 0
1 6 1 0
9 7 1 0
8 9 2 0
4 7 1 0
5 8 1 0
12 13 1 0
11 12 1 0
10 11 1 0
9 10 1 0

```

```

8 13 1 0
10 14 1 0
10 15 1 0
15 16 1 0
16 17 1 0
16 18 2 0
3 19 1 0
6 20 1 0
1 21 1 0
2 22 1 0
12 23 1 0
12 24 1 0
13 25 1 0
13 26 1 0
14 27 1 0
14 28 1 0
14 29 1 0
15 30 1 0
15 31 1 0
17 32 1 0

```

M END

> <Name>

Compound203

> <Activ>

17.6

> <DB_Ref_id>

23.23

\$\$\$\$

Compound204

SciTegic10081411483D

```

42 44 0 0 1 0          999 V2000
-3.9980 2.1680 0.3550 C 0 0
-2.6510 2.2230 0.8090 C 0 0
-1.6990 1.3120 0.2600 C 0 0
-2.0700 0.3650 -0.6970 C 0 0
-0.8830 -0.7030 -1.3070 S 0 0
0.1680 0.1620 -0.2270 C 0 0
-0.3420 1.2150 0.5630 C 0 0
0.5530 1.9860 1.5200 C 0 0
2.0530 1.6600 1.2790 C 0 0
2.2540 0.2670 1.0270 O 0 0
1.6370 -0.2400 -0.1580 C 0 0 1 0 0 0
1.7540 -1.7620 -0.0840 C 0 0
0.9630 -2.3580 1.0820 C 0 0
1.0920 -3.8790 1.1640 C 0 0
2.3850 0.3120 -1.3770 C 0 0
3.8730 0.0980 -1.2850 C 0 0
4.3180 -1.0240 -1.8460 O 0 0
4.5840 0.9020 -0.7320 O 0 0
-3.4120 0.3100 -1.1450 C 0 0
-3.8110 -0.6840 -2.1540 C 0 0
-4.3710 1.2110 -0.6210 C 0 0
-4.9220 3.0040 0.8320 F 0 0
-2.2810 3.1930 1.8130 C 0 0
-1.9900 3.9750 2.6210 N 0 0
0.3960 3.0590 1.3980 H 0 0
0.2690 1.7170 2.5390 H 0 0

```

2.4470	2.2250	0.4340	H	0	0
2.6460	1.9390	2.1520	H	0	0
1.4530	-2.2190	-1.0270	H	0	0
2.7990	-2.0670	-0.0370	H	0	0
1.2580	-1.8950	2.0230	H	0	0
-0.0840	-2.0610	1.0290	H	0	0
0.5230	-4.2680	2.0100	H	0	0
0.7280	-4.3480	0.2480	H	0	0
2.1330	-4.1720	1.2990	H	0	0
2.1660	1.3810	-1.4060	H	0	0
2.0040	-0.1310	-2.2970	H	0	0
5.2640	-1.2210	-1.8200	H	0	0
-3.0120	-1.3590	-2.4570	H	0	0
-4.1700	-0.1720	-3.0450	H	0	0
-4.6290	-1.2890	-1.7640	H	0	0
-5.3930	1.1660	-0.9710	H	0	0
2	23	1	0		
3	2	2	0		
4	3	1	0		
4	5	1	0		
6	5	1	0		
7	6	2	0		
3	7	1	0		
7	8	1	0		
9	8	1	0		
10	9	1	0		
11	10	1	0		
11	12	1	0		
12	13	1	0		
13	14	1	0		
11	15	1	0		
15	16	1	0		
16	17	1	0		
16	18	2	0		
6	11	1	0		
19	4	2	0		
19	20	1	0		
21	19	1	0		
1	21	2	0		
1	22	1	0		
1	2	1	0		
23	24	3	0		
8	25	1	0		
8	26	1	0		
9	27	1	0		
9	28	1	0		
12	29	1	0		
12	30	1	0		
13	31	1	0		
13	32	1	0		
14	33	1	0		
14	34	1	0		
14	35	1	0		
15	36	1	0		
15	37	1	0		
17	38	1	0		
20	39	1	0		
20	40	1	0		
20	41	1	0		
21	42	1	0		

M END

Compound205
SciTegic10081411483D

42	44	0	0	1	0	999 V2000			
-4.2680				0.8030		1.3220	C	0	0
-4.3670				-0.6070		1.2230	C	0	0
-3.2290				-1.3830		0.8930	C	0	0
-3.3420				-2.8460		0.7850	C	0	0
-1.9800				-0.7520		0.6700	C	0	0
-0.5860				-1.6540		0.2720	S	0	0
0.1780				-0.0900		0.2520	C	0	0
1.6660				-0.0100		-0.0680	C	0	0
2.4880				-0.4390		1.1510	C	0	0
3.9690				-0.2670		0.9340	C	0	0
4.6350				-1.1580		0.4610	O	0	0
4.4610				0.9140		1.2970	O	0	0
1.9820				-0.8850		-1.2830	C	0	0
1.1310				-0.5330		-2.5040	C	0	0
1.4590				-1.3960		-3.7210	C	0	0
2.0410				1.3260		-0.4220	O	0	0
1.6110				2.3460		0.4810	C	0	0
0.0640				2.4450		0.5250	C	0	0
-0.5780				1.0650		0.5350	C	0	0
-1.8810				0.6390		0.7750	C	0	0
-3.0180				1.4400		1.0920	C	0	0
-5.3580				1.5100		1.6310	F	0	0
-2.9300				2.8790		1.1820	C	0	0
-2.8630				4.0370		1.2480	N	0	0
-5.3150				-1.0960		1.3990	H	0	0
-2.4120				-3.3500		0.5250	H	0	0
-4.0820				-3.0980		0.0240	H	0	0
-3.6900				-3.2560		1.7340	H	0	0
2.2580				-1.4920		1.3130	H	0	0
2.1800				0.1110		2.0370	H	0	0
5.4040				1.0880		1.1840	H	0	0
3.0430				-0.8360		-1.5270	H	0	0
1.8790				-1.9410		-1.0330	H	0	0
0.0700				-0.5940		-2.2620	H	0	0
1.2230				0.5260		-2.7440	H	0	0
0.8280				-1.1250		-4.5660	H	0	0
2.5060				-1.2790		-4.0060	H	0	0
1.2890				-2.4510		-3.5040	H	0	0
2.0470				3.2930		0.1640	H	0	0
2.0200				2.1250		1.4690	H	0	0
-0.3030				2.9850		-0.3500	H	0	0
-0.2320				3.0040		1.4120	H	0	0
2	3	2	0						
3	4	1	0						
3	5	1	0						
5	6	1	0						
7	6	1	0						

```

7 8 1 0
8 9 1 0
9 10 1 0
10 11 2 0
10 12 1 0
8 13 1 0
13 14 1 0
14 15 1 0
8 16 1 0
16 17 1 0
17 18 1 0
19 18 1 0
20 19 1 0
5 20 2 0
20 21 1 0
21 23 1 0
1 21 2 0
19 7 2 0
1 22 1 0
1 2 1 0
23 24 3 0
2 25 1 0
4 26 1 0
4 27 1 0
4 28 1 0
9 29 1 0
9 30 1 0
12 31 1 0
13 32 1 0
13 33 1 0
14 34 1 0
14 35 1 0
15 36 1 0
15 37 1 0
15 38 1 0
17 39 1 0
17 40 1 0
18 41 1 0
18 42 1 0
M END
> <Name>
Compound205

> <Activ>
0.13

> <DB_Ref_id>
23.18

$$$$
Compound206
SciTegic10081411483D

37 39 0 0 1 0 999 V2000
4.1640 0.4220 -0.4460 C 0 0
4.2070 -0.9280 -0.0060 C 0 0
3.0040 -1.6370 0.2440 C 0 0
1.7750 -0.9650 0.0530 C 0 0
1.7090 0.3420 -0.3650 C 0 0
2.9080 1.0630 -0.6330 C 0 0
0.4760 -1.3770 0.2200 N 0 0

```


0.4470	0.8500	-0.4900	C	0	0				
-0.2950	-0.2540	-0.1040	C	0	0				
3.0450	-3.0350	0.6910	C	0	0				
-1.7720	0.0450	-0.1350	C	0	0	3	0	0	0
-3.8850	0.1310	1.2360	C	0	0				
-4.2050	1.1270	2.0780	C	0	0				
-2.4530	-0.3300	1.1790	C	0	0				
-2.3850	-0.6780	-1.3090	C	0	0				
-1.7660	1.6060	-0.3520	C	0	0				
-0.3580	2.0570	-0.8540	C	0	0				
-3.0670	-1.6600	-1.1470	O	0	0				
-2.1130	-0.1520	-2.5000	O	0	0				
5.3070	1.0720	-0.6640	F	0	0				
2.8590	2.4340	-1.0940	C	0	0				
2.8240	3.5330	-1.4630	N	0	0				
5.1540	-1.4200	0.1440	H	0	0				
0.1500	-2.2680	0.5080	H	0	0				
4.0780	-3.3770	0.7190	H	0	0				
2.5450	-3.1230	1.6540	H	0	0				
2.5060	-3.6600	-0.0220	H	0	0				
-4.7050	-0.2660	0.6540	H	0	0				
-5.1820	1.5630	2.2280	H	0	0				
-3.3850	1.5220	2.6600	H	0	0				
-1.8770	0.1560	1.9650	H	0	0				
-2.4030	-1.4060	1.3460	H	0	0				
-2.5510	1.9360	-1.0220	H	0	0				
-1.9530	2.0960	0.5960	H	0	0				
0.0000	2.9450	-0.3480	H	0	0				
-0.3280	2.2050	-1.9280	H	0	0				
-2.4750	-0.5680	-3.2930	H	0	0				
4	5	2	0						
3	4	1	0						
2	3	2	0						
1	2	1	0						
1	6	2	0						
9	7	1	0						
8	9	2	0						
4	7	1	0						
5	8	1	0						
3	10	1	0						
9	11	1	0						
12	13	2	0						
12	14	1	0						
11	14	1	0						
11	15	1	0						
11	16	1	0						
16	17	1	0						
15	18	2	0						
15	19	1	0						
8	17	1	0						
6	21	1	0						
1	20	1	0						
5	6	1	0						
21	22	3	0						
2	23	1	0						
7	24	1	0						
10	25	1	0						
10	26	1	0						
10	27	1	0						
12	28	1	0						
13	29	1	0						

13 30 1 0
14 31 1 0
14 32 1 0
16 33 1 0
16 34 1 0
17 35 1 0
17 36 1 0
19 37 1 0

M END

> <Name>

Compound206

> <Activ>

6.3

> <DB_Ref_id>

24.35

\$\$\$\$

Compound207

SciTegic10081411483D

42	44	0	0	1	0	999	V2000				
-4.3340		0.0170		-1.7320	C	0	0				
-4.2620		-1.1700		-0.9570	C	0	0				
-3.0350		-1.5670		-0.3670	C	0	0				
-1.8970		-0.7520		-0.5720	C	0	0				
-1.9400		0.4020		-1.3180	C	0	0				
-3.1660		0.8120		-1.9160	C	0	0				
-0.5980		-0.8730		-0.1370	N	0	0				
-0.7560		1.0780		-1.4220	C	0	0				
0.0590		0.2500		-0.6700	C	0	0				
-2.9590		-2.7990		0.4360	C	0	0				
1.4670		0.7690		-0.6090	C	0	0	3	0	0	0
2.2560		-0.0590		1.6060	C	0	0				
2.6620		0.2710		3.0430	C	0	0				
1.8220		1.1780		0.8160	C	0	0				
2.4160		-0.2830		-1.1290	C	0	0				
1.3870		2.0410		-1.5370	C	0	0				
-0.0860		2.2790		-2.0020	C	0	0				
3.5000		0.0190		-1.5700	O	0	0				
1.9670		-1.5310		-1.0590	O	0	0				
-5.5000		0.3690		-2.2750	F	0	0				
3.0940		-0.9650		3.8320	C	0	0				
-3.2340		2.0190		-2.7010	C	0	0				
-3.2890		2.9900		-3.3340	N	0	0				
-5.1470		-1.7760		-0.8180	H	0	0				
-0.2070		-1.5900		0.4300	H	0	0				
-1.9690		-3.0080		0.8420	H	0	0				
-3.2560		-3.6510		-0.1760	H	0	0				
-3.6540		-2.7290		1.2740	H	0	0				
1.4750		-0.8180		1.5920	H	0	0				
3.0590		-0.5840		1.0900	H	0	0				
3.4450		1.0290		3.0570	H	0	0				
1.8590		0.7990		3.5590	H	0	0				
0.9770		1.6660		1.3010	H	0	0				
2.6090		1.9320		0.8180	H	0	0				
2.0140		1.9160		-2.4100	H	0	0				
1.7620		2.9220		-1.0330	H	0	0				
-0.5040		3.1820		-1.5840	H	0	0				
-0.1800		2.2990		-3.0780	H	0	0				

2.5250	-2.2540	-1.3730	H	0	0
3.3850	-0.6920	4.8480	H	0	0
2.2850	-1.6930	3.8790	H	0	0
3.9490	-1.4470	3.3590	H	0	0

4 5 2 0
 3 4 1 0
 2 3 2 0
 1 2 1 0
 1 6 2 0
 9 7 1 0
 8 9 2 0
 4 7 1 0
 5 8 1 0
 3 10 1 0
 9 11 1 0
 12 13 1 0
 12 14 1 0
 11 14 1 0
 11 15 1 0
 11 16 1 0
 16 17 1 0
 15 18 2 0
 15 19 1 0
 8 17 1 0
 6 22 1 0
 1 20 1 0
 13 21 1 0
 5 6 1 0
 22 23 3 0
 2 24 1 0
 7 25 1 0
 10 26 1 0
 10 27 1 0
 10 28 1 0
 12 29 1 0
 12 30 1 0
 13 31 1 0
 13 32 1 0
 14 33 1 0
 14 34 1 0
 16 35 1 0
 16 36 1 0
 17 37 1 0
 17 38 1 0
 19 39 1 0
 21 40 1 0
 21 41 1 0
 21 42 1 0

M END
 > <Name>
 Compound207

 > <Activ>
 1.5

 > <DB_Ref_id>
 24.34

 \$\$\$\$
 Compound208
 SciTegic10081411483D

[illegible]

```

6 21 1 0
1 20 1 0
5 6 1 0
21 22 3 0
2 23 1 0
7 24 1 0
10 25 1 0
10 26 1 0
10 27 1 0
12 28 1 0
12 29 1 0
13 30 1 0
13 31 1 0
13 32 1 0
14 33 1 0
14 34 1 0
16 35 1 0
16 36 1 0
17 37 1 0
17 38 1 0
19 39 1 0

```

M END

> <Name>

Compound208

> <Activ>

1.8

> <DB_Ref_id>

24.33

\$\$\$\$

Compound209

SciTegic10081411483D

```

39 41 0 0 1 0          999 V2000
  4.9870    0.8260   -1.4590 C    0  0
  5.2540   -0.4410   -0.8750 C    0  0
  4.2350   -1.1450   -0.1840 C    0  0
  2.9450   -0.5550   -0.1170 C    0  0
  2.6600    0.6600   -0.6970 C    0  0
  3.6860    1.3870   -1.3630 C    0  0
  1.7810   -0.9770    0.4730 N    0  0
  1.3610    1.0760   -0.5690 C    0  0
  0.8440    0.0310    0.1810 C    0  0
  4.4860   -2.3260    0.3830 F    0  0
 -0.6110    0.2420    0.5080 C    0  0  3  0  0  0
 -2.9260   -0.6970    0.4880 C    0  0
 -3.8480   -1.8670    0.1400 C    0  0
 -1.4630   -0.9750    0.1390 C    0  0
 -0.7090    0.5860    1.9670 C    0  0
 -0.9410    1.4860   -0.3990 C    0  0
  0.3790    2.1480   -0.9120 C    0  0
 -0.9940    1.7050    2.3240 O    0  0
 -0.4630   -0.4180    2.8050 O    0  0
 -5.3110   -1.5900    0.4900 C    0  0
  3.4320    2.6890   -1.9200 C    0  0
  3.2330    3.7380   -2.3730 N    0  0
  5.7700    1.3480   -1.9850 H    0  0
  6.2420   -0.8690   -0.9590 H    0  0
  1.6290   -1.8070    0.9880 H    0  0

```

-3.0270	-0.4280	1.5390	H	0	0
-3.2690	0.2190	0.0080	H	0	0
-3.7480	-2.1390	-0.9100	H	0	0
-3.5040	-2.7850	0.6190	H	0	0
-1.1070	-1.8670	0.6540	H	0	0
-1.3590	-1.2130	-0.9200	H	0	0
-1.5660	2.2130	0.1010	H	0	0
-1.5100	1.1580	-1.2580	H	0	0
0.6230	3.0720	-0.3990	H	0	0
0.3540	2.3220	-1.9850	H	0	0
-0.5080	-0.2620	3.7560	H	0	0
-5.9370	-2.4410	0.2240	H	0	0
-5.4200	-1.3850	1.5550	H	0	0
-5.6800	-0.7230	-0.0570	H	0	0

4	5	2	0
3	4	1	0
2	3	2	0
1	2	1	0
1	6	2	0
9	7	1	0
8	9	2	0
4	7	1	0
5	8	1	0
3	10	1	0
9	11	1	0
12	13	1	0
12	14	1	0
11	14	1	0
11	15	1	0
11	16	1	0
16	17	1	0
15	18	2	0
15	19	1	0
8	17	1	0
6	21	1	0
13	20	1	0
5	6	1	0
21	22	3	0
1	23	1	0
2	24	1	0
7	25	1	0
12	26	1	0
12	27	1	0
13	28	1	0
13	29	1	0
14	30	1	0
14	31	1	0
16	32	1	0
16	33	1	0
17	34	1	0
17	35	1	0
19	36	1	0
20	37	1	0
20	38	1	0
20	39	1	0

M END

> <Name>

Compound209

> <Activ>

5.4

[illegible]

```

16 17 1 0
15 18 2 0
15 19 1 0
8 17 1 0
6 20 1 0
5 6 1 0
20 21 3 0
1 22 1 0
2 23 1 0
7 24 1 0
12 25 1 0
12 26 1 0
13 27 1 0
13 28 1 0
13 29 1 0
14 30 1 0
14 31 1 0
16 32 1 0
16 33 1 0
17 34 1 0
17 35 1 0
19 36 1 0

```

M END

> <Name>

Compound210

> <Activ>

8.1

> <DB_Ref_id>

24.3

\$\$\$\$

Compound211

SciTegic10081411483D

```

37 39 0 0 1 0          999 V2000
-4.0960 -0.6130 0.8010 C 0 0
-4.2580 0.6370 0.1460 C 0 0
-3.1370 1.3030 -0.4180 C 0 0
-1.8650 0.6950 -0.2970 C 0 0
-1.6800 -0.5060 0.3520 C 0 0
-2.7990 -1.1910 0.8960 C 0 0
-0.6250 1.0940 -0.7290 N 0 0
-0.3850 -0.9360 0.4140 C 0 0
0.2420 0.0860 -0.2790 C 0 0
-3.3100 2.5940 -1.1070 C 0 0
1.7210 -0.1520 -0.3850 C 0 0 3 0 0 0
4.0100 0.7890 0.1070 C 0 0
4.5900 0.8200 1.3180 C 0 0
2.5350 1.0800 0.0120 C 0 0
2.0280 -0.5800 -1.8030 C 0 0
1.9120 -1.3480 0.6250 C 0 0
0.5260 -2.0080 0.9160 C 0 0
2.6550 0.1370 -2.5470 O 0 0
1.5630 -1.7770 -2.1450 O 0 0
-2.6400 -2.4730 1.5410 C 0 0
-2.5170 -3.5060 2.0510 N 0 0
-4.9610 -1.1090 1.2170 H 0 0
-5.2420 1.0840 0.0780 H 0 0
-0.3920 1.9040 -1.2440 H 0 0

```


-4.3670	2.8610	-1.1210	H	0	0
-2.6890	3.3500	-0.6250	H	0	0
-2.9780	2.5020	-2.1430	H	0	0
4.6660	0.5510	-0.7150	H	0	0
5.6310	0.6350	1.5450	H	0	0
3.9340	1.0570	2.1410	H	0	0
2.1550	1.3930	0.9840	H	0	0
2.3650	1.8960	-0.6910	H	0	0
2.3090	-0.9670	1.5550	H	0	0
2.6290	-2.0760	0.2680	H	0	0
0.3730	-2.1970	1.9690	H	0	0
0.3710	-2.9140	0.3520	H	0	0
1.7250	-2.1110	-3.0370	H	0	0

4	5	2	0
3	4	1	0
2	3	2	0
1	2	1	0
1	6	2	0
9	7	1	0
8	9	2	0
4	7	1	0
5	8	1	0
3	10	1	0
9	11	1	0
12	13	2	0
12	14	1	0
11	14	1	0
11	15	1	0
11	16	1	0
16	17	1	0
15	18	2	0
15	19	1	0
8	17	1	0
6	20	1	0
5	6	1	0
20	21	3	0
1	22	1	0
2	23	1	0
7	24	1	0
10	25	1	0
10	26	1	0
10	27	1	0
12	28	1	0
13	29	1	0
13	30	1	0
14	31	1	0
14	32	1	0
16	33	1	0
16	34	1	0
17	35	1	0
17	36	1	0
19	37	1	0


```

M  END
> <Name>
Compound211

> <Activ>
11

> <DB_Ref_id>
24.29

```

SciTegic10081411483D

[illegible]

```

11 14 1 0
11 15 1 0
11 16 1 0
16 17 1 0
15 18 2 0
15 19 1 0
8 17 1 0
6 21 1 0
13 20 1 0
5 6 1 0
21 22 3 0
1 23 1 0
2 24 1 0
7 25 1 0
10 26 1 0
10 27 1 0
10 28 1 0
12 29 1 0
12 30 1 0
13 31 1 0
13 32 1 0
14 33 1 0
14 34 1 0
16 35 1 0
16 36 1 0
17 37 1 0
17 38 1 0
19 39 1 0
20 40 1 0
20 41 1 0
20 42 1 0

```

M END

> <Name>

Compound212

> <Activ>

4.6

> <DB_Ref_id>

24.28

\$\$\$\$

Compound213

SciTegic10081411483D

```

39 41 0 0 1 0          999 V2000
-4.3650 -0.8300  0.8910 C  0  0
-4.5270  0.4220  0.2360 C  0  0
-3.4080  1.0860 -0.3280 C  0  0
-2.1350  0.4800 -0.2070 C  0  0
-1.9490 -0.7210  0.4400 C  0  0
-3.0680 -1.4080  0.9860 C  0  0
-0.8960  0.8770 -0.6390 N  0  0
-0.6540 -1.1520  0.5020 C  0  0
-0.0270 -0.1310 -0.1910 C  0  0
-3.5800  2.3790 -1.0190 C  0  0
 1.4510 -0.3690 -0.2950 C  0  0  3  0  0  0
 3.7560  0.5210  0.0740 C  0  0
 4.6390  1.6990  0.4840 C  0  0
 2.2660  0.8630  0.1020 C  0  0
 1.7580 -0.7970 -1.7130 C  0  0

```

1.6410	-1.5650	0.7130	C	0	0
0.2560	-2.2250	1.0040	C	0	0
1.9810	-1.9550	-1.9780	O	0	0
1.7600	0.1840	-2.6110	O	0	0
-2.9120	-2.6900	1.6310	C	0	0
-2.7870	-3.7230	2.1410	N	0	0
-5.2320	-1.3260	1.3070	H	0	0
-5.5120	0.8670	0.1680	H	0	0
-0.6620	1.6890	-1.1540	H	0	0
-2.6580	2.8010	-1.4180	H	0	0
-4.0080	3.1050	-0.3280	H	0	0
-4.2770	2.2580	-1.8480	H	0	0
3.9610	-0.3500	0.6950	H	0	0
4.0450	0.1440	-0.9060	H	0	0
5.6920	1.4180	0.4590	H	0	0
4.4830	2.5490	-0.1820	H	0	0
4.4040	2.0230	1.4980	H	0	0
1.9690	1.2210	1.0880	H	0	0
2.0490	1.6990	-0.5660	H	0	0
2.0390	-1.1840	1.6450	H	0	0
2.3580	-2.2930	0.3580	H	0	0
0.1040	-2.4140	2.0570	H	0	0
0.1020	-3.1310	0.4400	H	0	0
1.9490	-0.0230	-3.5350	H	0	0
4	5	2	0		
3	4	1	0		
2	3	2	0		
1	2	1	0		
1	6	2	0		
9	7	1	0		
8	9	2	0		
4	7	1	0		
5	8	1	0		
3	10	1	0		
9	11	1	0		
12	13	1	0		
12	14	1	0		
11	14	1	0		
11	15	1	0		
11	16	1	0		
16	17	1	0		
15	18	2	0		
15	19	1	0		
8	17	1	0		
6	20	1	0		
5	6	1	0		
20	21	3	0		
1	22	1	0		
2	23	1	0		
7	24	1	0		
10	25	1	0		
10	26	1	0		
10	27	1	0		
12	28	1	0		
12	29	1	0		
13	30	1	0		
13	31	1	0		
13	32	1	0		
14	33	1	0		
14	34	1	0		
16	35	1	0		

[illegible]

```

1  2  2  0
1  6  1  0
9  7  1  0
8  9  2  0
4  7  1  0
5  8  1  0
9 10  1  0
11 12  1  0
11 13  1  0
10 13  1  0
10 14  1  0
10 15  1  0
15 16  1  0
8 17  1  0
16 17  1  0
6 18  1  0
14 19  1  0
14 20  2  0
3 21  1  0
1 22  1  0
2 23  1  0
7 24  1  0
11 25  1  0
11 26  1  0
12 27  1  0
12 28  1  0
12 29  1  0
13 30  1  0
13 31  1  0
15 32  1  0
15 33  1  0
16 34  1  0
16 35  1  0
17 36  1  0
17 37  1  0
19 38  1  0
M  END
> <Name>
Compound214

> <Activ>
3.2

> <DB_Ref_id>
24.26

$$$$
Compound215
SciTegic10081411483D

41 43  0  0  1  0          999 V2000
-3.5330  2.4840  0.5000 C  0  0
-4.2050  1.2460  0.6820 C  0  0
-3.4710  0.0350  0.7290 C  0  0
-2.0610  0.0960  0.5840 C  0  0
-1.4030  1.2930  0.4060 C  0  0
-2.1210  2.5210  0.3650 C  0  0
-1.0920 -0.9000  0.5820 N  0  0
-0.0610  1.1170  0.2890 C  0  0
0.1600 -0.2640  0.4000 C  0  0
1.5250 -0.9430  0.3200 C  0  0  3  0  0  0

```

2.6390	0.1250	0.5000	C	0	0
2.3790	1.4120	-0.3160	C	0	0
1.0660	2.1210	0.0860	C	0	0
1.6520	-1.6270	-1.0430	C	0	0
1.6330	-1.9880	1.4040	C	0	0
0.5620	-2.6740	-1.2830	C	0	0
0.9220	-3.6540	-2.3980	C	0	0
-4.2910	-1.4570	0.9550	C1	0	0
2.2260	-3.0260	1.2130	O	0	0
1.0370	-1.6780	2.5530	O	0	0
-1.4510	3.8200	0.1860	C	0	0
-2.3600	4.8320	0.3610	F	0	0
-0.9240	3.8940	-1.0780	F	0	0
-0.4460	3.9450	1.1090	F	0	0
-4.1060	3.3980	0.4670	H	0	0
-5.2820	1.2420	0.7850	H	0	0
-1.2420	-1.8770	0.6900	H	0	0
3.6050	-0.2970	0.2250	H	0	0
2.7240	0.4020	1.5530	H	0	0
2.3420	1.1580	-1.3770	H	0	0
3.2170	2.1000	-0.1990	H	0	0
0.7990	2.8500	-0.6780	H	0	0
1.2090	2.6660	1.0220	H	0	0
1.6600	-0.8910	-1.8460	H	0	0
2.6400	-2.0680	-1.1620	H	0	0
0.3300	-3.2050	-0.3590	H	0	0
-0.3950	-2.1920	-1.4860	H	0	0
0.1250	-4.3850	-2.5390	H	0	0
1.0900	-3.1270	-3.3360	H	0	0
1.8320	-4.1990	-2.1520	H	0	0
1.0700	-2.3050	3.2870	H	0	0
2	3	2	0		
1	2	1	0		
1	6	2	0		
9	7	1	0		
8	9	2	0		
4	7	1	0		
5	8	1	0		
12	13	1	0		
11	12	1	0		
10	11	1	0		
9	10	1	0		
8	13	1	0		
10	14	1	0		
10	15	1	0		
14	16	1	0		
16	17	1	0		
3	18	1	0		
6	21	1	0		
15	19	2	0		
15	20	1	0		
5	6	1	0		
4	5	2	0		
3	4	1	0		
21	24	1	0		
21	23	1	0		
21	22	1	0		
1	25	1	0		
2	26	1	0		
7	27	1	0		
11	28	1	0		

```

11 29 1 0
12 30 1 0
12 31 1 0
13 32 1 0
13 33 1 0
14 34 1 0
14 35 1 0
16 36 1 0
16 37 1 0
17 38 1 0
17 39 1 0
17 40 1 0
20 41 1 0

```

M END

> <Name>

Compound215

> <Activ>

5.8

> <DB_Ref_id>

24.25

\$\$\$\$

Compound216

SciTegic10081411483D

```

43 45 0 0 1 0          999 V2000
-4.1090    2.1660    1.6480 C    0  0
-4.6620    0.9280    1.2320 C    0  0
-3.8160   -0.0700    0.6850 C    0  0
-2.4260    0.1840    0.5680 C    0  0
-1.8770    1.3810    0.9800 C    0  0
-2.7130    2.4020    1.5250 C    0  0
-1.3870   -0.5960    0.0760 N    0  0
-0.5270    1.4000    0.7850 C    0  0
-0.2030    0.1660    0.2030 C    0  0
 1.1970   -0.2750   -0.2130 C    0  0  3  0  0  0
 2.1330    0.9650   -0.2500 C    0  0
 1.9530    1.8930    0.9710 C    0  0
 0.5210    2.4670    1.0840 C    0  0
 1.1520   -0.9320   -1.5960 C    0  0
 1.7050   -1.2870    0.8180 C    0  0
 0.9340   -2.5800    0.7830 C    0  0
 1.3810   -3.4810   -0.0860 O    0  0
-0.0200   -2.7540    1.5040 O    0  0
 2.5370   -1.3440   -2.0980 C    0  0
 2.4860   -2.0590   -3.4490 C    0  0
-2.1890    3.6760    1.9510 C    0  0
-1.7750    4.7070    2.2910 N    0  0
-4.3750   -1.3260    0.2580 C    0  0
-4.8220   -2.3380   -0.0900 N    0  0
-4.7660    2.9200    2.0640 H    0  0
-5.7250    0.7600    1.3360 H    0  0
-1.4550   -1.5160   -0.2950 H    0  0
 3.1720    0.6390   -0.3150 H    0  0
 1.9510    1.5470   -1.1540 H    0  0
 2.6720    2.7090    0.9300 H    0  0
 2.1890    1.3300    1.8750 H    0  0
 0.3950    3.2870    0.3790 H    0  0
 0.3830    2.8690    2.0860 H    0  0

```


0.4750	-1.7850	-1.5960	H	0	0
0.6600	-0.2790	-2.3170	H	0	0
1.5860	-0.8110	1.7910	H	0	0
2.7680	-1.4860	0.6740	H	0	0
0.9300	-4.3320	-0.1580	H	0	0
3.2030	-0.4830	-2.1430	H	0	0
3.0490	-1.9590	-1.3580	H	0	0
3.4900	-2.3260	-3.7810	H	0	0
1.8790	-2.9610	-3.3870	H	0	0
2.0470	-1.4120	-4.2090	H	0	0
2	3	2	0		
1	2	1	0		
1	6	2	0		
9	7	1	0		
8	9	2	0		
4	7	1	0		
5	8	1	0		
12	13	1	0		
11	12	1	0		
10	11	1	0		
9	10	1	0		
8	13	1	0		
10	14	1	0		
10	15	1	0		
15	16	1	0		
16	17	1	0		
16	18	2	0		
14	19	1	0		
19	20	1	0		
6	21	1	0		
3	23	1	0		
5	6	1	0		
21	22	3	0		
4	5	2	0		
3	4	1	0		
23	24	3	0		
1	25	1	0		
2	26	1	0		
7	27	1	0		
11	28	1	0		
11	29	1	0		
12	30	1	0		
12	31	1	0		
13	32	1	0		
13	33	1	0		
14	34	1	0		
14	35	1	0		
15	36	1	0		
15	37	1	0		
17	38	1	0		
19	39	1	0		
19	40	1	0		
20	41	1	0		
20	42	1	0		
20	43	1	0		

M END

> <Name>

Compound216

> <Activ>

2.3


```

 4  7  1  0
 5  8  1  0
12 13  1  0
11 12  1  0
10 11  1  0
 9 10  1  0
 8 13  1  0
10 14  1  0
10 15  1  0
15 16  1  0
16 17  1  0
16 18  2  0
14 19  1  0
19 20  1  0
 3 21  1  0
 6 22  1  0
 5  6  1  0
22 23  3  0
 1 24  1  0
 2 25  1  0
 7 26  1  0
11 27  1  0
11 28  1  0
12 29  1  0
12 30  1  0
13 31  1  0
13 32  1  0
14 33  1  0
14 34  1  0
15 35  1  0
15 36  1  0
17 37  1  0
19 38  1  0
19 39  1  0
20 40  1  0
20 41  1  0
20 42  1  0
21 43  1  0
21 44  1  0
21 45  1  0
M  END
> <Name>
Compound217

> <Activ>
2.1

> <DB_Ref_id>
24.13

$$$$
Compound218
  SciTegic10081411483D

60 63  0  0  1  0          999 V2000
  -2.3830   1.2330   1.3500 C   0  0
  -2.4860   0.7580   0.0160 C   0  0
  -1.4080   0.0470  -0.5740 C   0  0
  -0.2380  -0.1680   0.1950 C   0  0
  -0.1230   0.2930   1.4900 C   0  0
  -1.1970   1.0020   2.1020 C   0  0

```

1.0880	-0.0310	2.0160	C	0	0				
1.7750	-0.7320	1.0220	C	0	0				
0.9470	-0.8180	-0.1190	N	0	0				
3.1860	-1.2870	1.1900	C	0	0	1	0	0	0
3.5230	-1.3240	2.5820	O	0	0				
3.2560	-0.1270	3.3260	C	0	0				
1.7360	0.2130	3.3690	C	0	0				
3.2680	-2.7300	0.6840	C	0	0	2	0	0	0
3.4820	-2.8120	-0.8280	C	0	0				
3.1290	-4.1860	-1.4000	C	0	0				
4.1950	-0.3850	0.4730	C	0	0				
3.8400	1.0740	0.5820	C	0	0				
2.7170	1.4320	-0.0350	O	0	0				
4.5450	1.8420	1.1950	O	0	0				
-1.5040	-0.4570	-1.9570	C	0	0				
-3.6110	0.9840	-0.6820	O	0	0				
-4.5760	1.8610	-0.1190	C	0	0				
-5.6880	2.1130	-1.1390	C	0	0				
-5.1580	2.7600	-2.3480	N	0	0				
-4.6700	4.0020	-2.4000	N	0	0				
-4.2600	4.3110	-3.6470	C	0	0				
-4.5200	3.1620	-4.4200	C	0	0				
-5.0920	2.1900	-3.5680	C	0	0				
2.0960	-3.5900	1.1600	C	0	0				
-1.1230	1.4900	3.4590	C	0	0				
-1.0700	1.8850	4.5470	N	0	0				
-3.2130	1.7700	1.7850	H	0	0				
1.1740	-1.2620	-0.9780	H	0	0				
3.8220	0.6900	2.8790	H	0	0				
3.6390	-0.2620	4.3400	H	0	0				
1.6040	1.2500	3.6720	H	0	0				
1.2320	-0.4120	4.1080	H	0	0				
4.2170	-3.1840	0.9630	H	0	0				
2.9280	-2.0270	-1.3400	H	0	0				
4.5060	-2.5390	-1.0860	H	0	0				
3.3890	-4.2420	-2.4570	H	0	0				
3.6560	-4.9750	-0.8630	H	0	0				
2.0610	-4.3770	-1.3090	H	0	0				
4.1840	-0.6910	-0.5720	H	0	0				
5.2010	-0.5510	0.8570	H	0	0				
2.4340	2.3540	-0.0040	H	0	0				
-0.6230	-1.0000	-2.2990	H	0	0				
-1.6640	0.3810	-2.6370	H	0	0				
-2.3610	-1.1250	-2.0410	H	0	0				
-4.0780	2.7930	0.1470	H	0	0				
-4.9790	1.3950	0.7810	H	0	0				
-6.4360	2.7600	-0.6780	H	0	0				
-6.1800	1.1800	-1.4120	H	0	0				
-3.8280	5.2580	-3.9430	H	0	0				
-4.3180	3.0450	-5.4770	H	0	0				
-5.4200	1.1880	-3.8110	H	0	0				
2.2910	-4.6540	1.0220	H	0	0				
1.1870	-3.3420	0.6110	H	0	0				
1.9020	-3.4240	2.2210	H	0	0				
26 25	1	0							
28 29	2	0							
27 28	1	0							
26 27	2	0							
6 31	1	0							
24 25	1	0							
23 24	1	0							

```
22 23 1 0
 2 22 1 0
 3 21 1 0
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17 18 1 0
10 17 1 0
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> <Name>
Compound218

> <Activ>
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0.003

> <DB_Ref_id>

25.02

\$\$\$\$

Compound219

SciTegic10081411483D

60	63	0	0	1	0	999	V2000							
-1.5590				1.5980		1.0760	C	0	0					
-1.6640				1.1210		-0.2600	C	0	0					
-0.5860				0.4100		-0.8500	C	0	0					
0.5840				0.1970		-0.0800	C	0	0					
0.6990				0.6580		1.2170	C	0	0					
-0.3750				1.3650		1.8260	C	0	0					
1.9100				0.3320		1.7400	C	0	0					
2.5980				-0.3690		0.7480	C	0	0					
1.7700				-0.4550		-0.3940	N	0	0					
4.0080				-0.9220		0.9160	C	0	0	1	0	0	0	
4.3460				-0.9610		2.3090	O	0	0					
4.0780				0.2360		3.0530	C	0	0					
2.5590				0.5760		3.0960	C	0	0					
4.0900				-2.3650		0.4080	C	0	0					
3.1410				-3.3070		1.1520	C	0	0					
3.1680				-4.7300		0.5960	C	0	0					
5.0180				-0.0190		0.1990	C	0	0					
4.8670				-0.0640		-1.2990	C	0	0					
4.0880				0.8810		-1.8160	O	0	0					
5.4260				-0.9120		-1.9550	O	0	0					
-0.6820				-0.0920		-2.2300	C	0	0					
-2.7870				1.3480		-0.9550	O	0	0					
-3.8090				2.1210		-0.3400	C	0	0					
-4.9670				2.3070		-1.3200	C	0	0	1	0	0	0	
-5.5160				1.0100		-1.7400	N	0	0					
-6.1070				0.1290		-0.9280	N	0	0					
-6.5040				-0.9650		-1.6050	C	0	0					
-6.1230				-0.7360		-2.9430	C	0	0					
-5.4960				0.5270		-3.0000	C	0	0					
-6.0680				3.2130		-0.7670	C	0	0					
-0.3010				1.8540		3.1840	C	0	0					
-0.2480				2.2500		4.2740	N	0	0					
-2.3890				2.1350		1.5100	H	0	0					
1.9960				-0.8960		-1.2540	H	0	0					
4.6450				1.0550		2.6060	H	0	0					
4.4610				0.1040		4.0650	H	0	0					
2.4260				1.6150		3.3970	H	0	0					
2.0550				-0.0470		3.8320	H	0	0					
3.9100				-2.4060		-0.6660	H	0	0					
5.1150				-2.7320		0.4590	H	0	0					
3.3580				-3.3050		2.2210	H	0	0					
2.1250				-2.9100		1.1510	H	0	0					
2.4900				-5.3750		1.1560	H	0	0					
2.8810				-4.7400		-0.4550	H	0	0					
4.1700				-5.1540		0.6720	H	0	0					
6.0040				-0.3870		0.4830	H	0	0					
4.9320				1.0100		0.5490	H	0	0					
3.9510				0.9060		-2.7730	H	0	0					
-0.2300				-1.0720		-2.3830	H	0	0					
-0.1910				0.6090		-2.9060	H	0	0					
-1.7300				-0.1580		-2.5210	H	0	0					

-3.3830	3.0860	-0.0580	H	0	0
-4.1410	1.5980	0.5550	H	0	0
-4.6050	2.6800	-2.2790	H	0	0
-7.0080	-1.8200	-1.1720	H	0	0
-6.2830	-1.4080	-3.7770	H	0	0
-5.0760	1.0370	-3.8570	H	0	0
-6.8890	3.3320	-1.4730	H	0	0
-5.6740	4.2050	-0.5450	H	0	0
-6.4790	2.8030	0.1540	H	0	0
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28	29	2	0		
27	28	1	0		
26	27	2	0		
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24	25	1	0		
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8	10	1	0		
4	9	1	0		
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2	3	1	0		
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16	44	1	0		
16	45	1	0		
17	46	1	0		
17	47	1	0		
19	48	1	0		
21	49	1	0		

M END

Compound219

0.003

25.24

Compound 220

56	59	0	0	1	0	999	V2000				
-3.1050				1.0700		-1.3050	O	0	0		
-0.9980				-0.3690		-2.5800	C	0	0		
5.1060				-1.1910		-2.3030	O	0	0		
3.7720				0.6060		-2.1660	O	0	0		
4.5490				-0.3420		-1.6460	C	0	0		
4.7010				-0.2990		-0.1500	C	0	0		
2.8580				-5.0120		0.2540	C	0	0		
2.8240				-3.5840		0.8050	C	0	0		
3.7720				-2.6430		0.0610	C	0	0		
2.2420				0.2990		2.7460	C	0	0		
3.7620				-0.0410		2.7030	C	0	0		
4.0290				-1.2380		1.9590	O	0	0		
3.6900				-1.2010		0.5670	C	0	0	1	0 0 0
1.4510				-0.7320		-0.7420	N	0	0		
2.2810				-0.6460		0.3990	C	0	0		
1.5940				0.0550		1.3930	C	0	0		
-0.6930				1.0880		1.4790	C	0	0		
0.3810				0.3790		0.8670	C	0	0		
0.2660				-0.0820		-0.4280	C	0	0		
-0.9020				0.1330		-1.1970	C	0	0		
-1.9800				0.8440		-0.6070	C	0	0		
-1.8770				1.3180		0.7270	C	0	0		
-4.1450				1.8010		-0.6720	C	0	0		
-5.3180				1.9590		-1.6390	C	0	0		
-6.4530				2.7320		-1.0020	C	0	0		
-6.3480				3.1950		0.2870	N	0	0		
-7.4730				3.8690		0.6800	C	0	0		
-8.6500				3.9240		-0.5450	S	0	0		
-7.6740				3.0530		-1.6090	C	0	0		
-0.6190				1.5760		2.8340	C	0	0		
-0.5660				1.9710		3.9240	N	0	0		
-0.3050				-1.1780		-2.8120	H	0	0		
-0.8050				0.4450		-3.2770	H	0	0		
-2.0100				-0.7340		-2.7660	H	0	0		
3.6350				0.6330		-3.1210	H	0	0		

5.6860	-0.6660	0.1330	H	0	0
4.6150	0.7310	0.2010	H	0	0
2.1800	-5.6560	0.8130	H	0	0
2.5740	-5.0250	-0.7990	H	0	0
3.8600	-5.4320	0.3340	H	0	0
3.0350	-3.5800	1.8730	H	0	0
1.8070	-3.1930	0.7970	H	0	0
3.5920	-2.6860	-1.0140	H	0	0
4.7970	-3.0120	0.1090	H	0	0
2.1090	1.3360	3.0470	H	0	0
1.7360	-0.3260	3.4850	H	0	0
4.3280	0.7750	2.2560	H	0	0
4.1430	-0.1760	3.7150	H	0	0
1.6800	-1.1760	-1.6010	H	0	0
-2.7070	1.8570	1.1600	H	0	0
-3.7520	2.7750	-0.3810	H	0	0
-4.4510	1.2540	0.2210	H	0	0
-5.6840	0.9840	-1.9650	H	0	0
-5.0020	2.4630	-2.5510	H	0	0
-7.5740	4.3090	1.6640	H	0	0
-7.9630	2.7850	-2.6150	H	0	0
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29	25	2	0		
21	1	1	0		
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6	37	1	0		

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8 41 1 0
8 42 1 0
9 43 1 0
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29 56 1 0

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M END

> <Name>

Compound220

> <Activ>

0.022

> <DB_Ref_id>

25.23

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Compound221

SciTegic10081411483D

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60 63 0 0 1 0          999 V2000
-2.5490    0.7770   -1.3990 O    0  0
-0.4410   -0.6640   -2.6740 C    0  0
 5.6620   -1.4840   -2.3990 O    0  0
 4.3300    0.3130   -2.2600 O    0  0
 5.1050   -0.6350   -1.7400 C    0  0
 5.2560   -0.5920   -0.2440 C    0  0
 3.4120   -5.3030    0.1560 C    0  0
 3.3810   -3.8790    0.7090 C    0  0
 4.3280   -2.9380   -0.0330 C    0  0
 2.7990    0.0040    2.6520 C    0  0
 4.3160   -0.3340    2.6090 C    0  0
 4.5860   -1.5310    1.8650 O    0  0
 4.2460   -1.4940    0.4730 C    0  0  1  0  0  0
 2.0080   -1.0250   -0.8360 N    0  0
 2.8360   -0.9410    0.3050 C    0  0
 2.1500   -0.2400    1.2990 C    0  0
-0.1370    0.7950    1.3850 C    0  0
 0.9370    0.0860    0.7730 C    0  0
 0.8220   -0.3750   -0.5220 C    0  0
-0.3460   -0.1600   -1.2930 C    0  0
-1.4240    0.5490   -0.7010 C    0  0
-1.3200    1.0250    0.6330 C    0  0
-3.5900    1.5040   -0.7640 C    0  0
-4.7640    1.6600   -1.7310 C    0  0
-5.8790    2.3770   -1.0940 N    0  0
-5.8220    2.9810    0.0980 N    0  0
-7.0040    3.5470    0.4040 C    0  0

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-7.8580	3.2720	-0.6840	C	0	0
-7.1130	2.5230	-1.6230	C	0	0
-7.2810	4.3110	1.6800	C	0	0
-0.0630	1.2830	2.7400	C	0	0
-0.0100	1.6780	3.8300	N	0	0
0.2540	-1.4690	-2.9080	H	0	0
-0.2540	0.1520	-3.3710	H	0	0
-1.4510	-1.0310	-2.8580	H	0	0
4.1910	0.3400	-3.2150	H	0	0
6.2420	-0.9590	0.0390	H	0	0
5.1720	0.4380	0.1070	H	0	0
2.7340	-5.9470	0.7170	H	0	0
3.1270	-5.3160	-0.8950	H	0	0
4.4140	-5.7250	0.2360	H	0	0
3.5920	-3.8730	1.7770	H	0	0
2.3630	-3.4840	0.7030	H	0	0
4.1500	-2.9790	-1.1080	H	0	0
5.3540	-3.3050	0.0160	H	0	0
2.6660	1.0430	2.9530	H	0	0
2.2930	-0.6190	3.3910	H	0	0
4.8850	0.4820	2.1620	H	0	0
4.6990	-0.4690	3.6210	H	0	0
2.2340	-1.4690	-1.6950	H	0	0
-2.1500	1.5630	1.0660	H	0	0
-3.1970	2.4790	-0.4730	H	0	0
-3.8970	0.9550	0.1270	H	0	0
-5.0960	0.6680	-2.0310	H	0	0
-4.4550	2.1950	-2.6290	H	0	0
-8.8910	3.5740	-0.7790	H	0	0
-7.4300	2.1310	-2.5800	H	0	0
-6.4320	4.3750	2.3590	H	0	0
-8.1020	3.8340	2.2170	H	0	0
-7.5900	5.3280	1.4360	H	0	0
20	2	1	0		
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19	18	1	0		
20	19	2	0		
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11 49 1 0
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Compound221

> <Activ>
0.03

> <DB_Ref_id>
25.22

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Compound222
SciTegic10081411483D

60 62 0 0 1 0 999 V2000
-5.3190 3.0100 1.2680 C 0 0
-4.0220 2.7930 1.8070 C 0 0
-3.1330 1.9060 1.1350 C 0 0
-1.8600 1.5630 1.4670 C 0 0
-0.9340 1.9630 2.6070 C 0 0
0.5230 1.4920 2.3300 C 0 0
0.5600 0.1660 1.7830 O 0 0
-0.0490 0.0080 0.4920 C 0 0 2 0 0 0
-1.4300 0.6520 0.4960 C 0 0
-3.5310 1.2620 -0.0200 C 0 0
-5.2250 0.7680 -1.8130 C 0 0

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-4.8190	1.4610	-0.5780	C	0	0				
-5.7130	2.3460	0.0760	C	0	0				
-2.4750	0.4650	-0.4360	N	0	0				
-0.1490	-1.5000	0.2400	C	0	0				
-1.0680	-2.2050	1.2360	C	0	0				
-1.1640	-3.7110	0.9880	C	0	0				
0.8500	0.6820	-0.5510	C	0	0	2	0	0	0
2.2680	0.3930	-0.2930	N	0	0				
2.8960	-0.5800	-1.0160	C	0	0				
4.1780	-0.7830	-0.7230	O	0	0				
2.2930	-1.1990	-1.8590	O	0	0				
4.7600	-1.8050	-1.5180	C	0	0				
6.1760	-1.7750	-0.9430	C	0	0				
4.7110	-1.3940	-2.9900	C	0	0				
4.0430	-3.1290	-1.2500	C	0	0				
-3.6490	3.4750	3.0210	C	0	0				
-3.3580	4.0240	4.0020	N	0	0				
0.5960	2.1620	-0.6560	C	0	0				
1.6390	2.9360	-0.3730	O	0	0				
-0.4900	2.5860	-0.9790	O	0	0				
-6.0160	3.6780	1.7500	H	0	0				
-0.9420	3.0450	2.7420	H	0	0				
-1.3050	1.5160	3.5290	H	0	0				
1.0230	2.1660	1.6330	H	0	0				
1.1050	1.4980	3.2500	H	0	0				
-4.4590	0.1170	-2.2340	H	0	0				
-5.4940	1.5020	-2.5700	H	0	0				
-6.1080	0.1580	-1.6110	H	0	0				
-6.7010	2.5140	-0.3280	H	0	0				
-2.4470	-0.1230	-1.2360	H	0	0				
-0.4650	-1.6990	-0.7830	H	0	0				
0.8420	-1.9570	0.2380	H	0	0				
-0.7540	-2.0040	2.2620	H	0	0				
-2.0590	-1.7500	1.2360	H	0	0				
-1.8180	-4.1820	1.7210	H	0	0				
-1.5470	-3.9120	-0.0120	H	0	0				
-0.1820	-4.1780	1.0680	H	0	0				
0.5920	0.3460	-1.5550	H	0	0				
2.7680	0.9040	0.4060	H	0	0				
6.1860	-1.9900	0.1250	H	0	0				
6.6290	-0.7950	-1.0900	H	0	0				
6.8090	-2.5120	-1.4380	H	0	0				
3.7660	-1.6700	-3.4570	H	0	0				
5.5120	-1.8750	-3.5510	H	0	0				
4.8320	-0.3160	-3.0940	H	0	0				
3.1600	-3.2480	-1.8790	H	0	0				
3.7210	-3.1890	-0.2110	H	0	0				
4.7050	-3.9730	-1.4430	H	0	0				
1.5430	3.8970	-0.4200	H	0	0				
3	4	1	0						
4	9	2	0						
4	5	1	0						
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8	7	1	0						
9	8	1	0						
12	10	1	0						
12	11	1	0						
13	12	2	0						
10	14	1	0						
9	14	1	0						

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15	16	1	0
16	17	1	0
8	18	1	0
18	19	1	0
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20	22	2	0
21	23	1	0
23	24	1	0
23	25	1	0
23	26	1	0
1	13	1	0
27	28	3	0
1	2	2	0
3	2	1	0
10	3	2	0
29	31	2	0
29	30	1	0
1	32	1	0
5	33	1	0
5	34	1	0
6	35	1	0
6	36	1	0
11	37	1	0
11	38	1	0
11	39	1	0
13	40	1	0
14	41	1	0
15	42	1	0
15	43	1	0
16	44	1	0
16	45	1	0
17	46	1	0
17	47	1	0
17	48	1	0
18	49	1	0
19	50	1	0
24	51	1	0
24	52	1	0
24	53	1	0
25	54	1	0
25	55	1	0
25	56	1	0
26	57	1	0
26	58	1	0
26	59	1	0
30	60	1	0

M END

> <Name>

Compound222

> <Activ>

18

> <DB_Ref_id>

26.261

\$\$\$\$

Compound223
SciTegic10081411483D

55	57	0	0	1	0	999	V2000				
-5.0020				2.8630		1.0720	C	0	0		
-3.7050				2.6470		1.6110	C	0	0		
-2.8170				1.7600		0.9390	C	0	0		
-1.5430				1.4160		1.2710	C	0	0		
-0.6170				1.8160		2.4120	C	0	0		
0.8400				1.3460		2.1350	C	0	0		
0.8770				0.0200		1.5880	O	0	0		
0.2680				-0.1390		0.2970	C	0	0	2	0 0 0
-1.1130				0.5060		0.3030	C	0	0		
-3.2150				1.1150		-0.2150	C	0	0		
-4.9080				0.6210		-2.0060	C	0	0		
-4.5020				1.3140		-0.7740	C	0	0		
-5.3970				2.1990		-0.1190	C	0	0		
-2.1580				0.3180		-0.6310	N	0	0		
0.1680				-1.6470		0.0450	C	0	0		
-0.7520				-2.3520		1.0410	C	0	0		
-0.8460				-3.8570		0.7950	C	0	0		
1.1660				0.5350		-0.7460	C	0	0	2	0 0 0
2.5840				0.2460		-0.4880	N	0	0		
3.2110				-0.7290		-1.2090	C	0	0		
4.4940				-0.9300		-0.9180	O	0	0		
2.6070				-1.3480		-2.0530	O	0	0		
5.0720				-1.9570		-1.7090	C	0	0		
6.5180				-2.1310		-1.3260	C	0	0		
7.1540				-3.2500		-1.7110	C	0	0		
-3.3320				3.3280		2.8260	C	0	0		
-3.0410				3.8770		3.8070	N	0	0		
0.9120				2.0160		-0.8520	C	0	0		
1.9550				2.7890		-0.5660	O	0	0		
-0.1720				2.4390		-1.1740	O	0	0		
-5.6990				3.5310		1.5550	H	0	0		
-0.6250				2.8980		2.5470	H	0	0		
-0.9880				1.3690		3.3340	H	0	0		
1.3400				2.0200		1.4370	H	0	0		
1.4220				1.3520		3.0570	H	0	0		
-4.1410				-0.0250		-2.4320	H	0	0		
-5.1820				1.3550		-2.7640	H	0	0		
-5.7870				0.0080		-1.8070	H	0	0		
-6.3830				2.3670		-0.5240	H	0	0		
-2.1310				-0.2700		-1.4320	H	0	0		
-0.1490				-1.8460		-0.9790	H	0	0		
1.1580				-2.1040		0.0430	H	0	0		
-0.4380				-2.1480		2.0660	H	0	0		
-1.7420				-1.8980		1.0390	H	0	0		
-1.5000				-4.3280		1.5270	H	0	0		
-1.2290				-4.0610		-0.2070	H	0	0		
0.1370				-4.3240		0.8770	H	0	0		
0.9080				0.1990		-1.7500	H	0	0		
3.0840				0.7580		0.2110	H	0	0		
5.0000				-1.6620		-2.7560	H	0	0		
4.5270				-2.8810		-1.5240	H	0	0		
7.1150											

```
4 5 1 0
6 5 1 0
7 6 1 0
8 7 1 0
9 8 1 0
12 10 1 0
12 11 1 0
13 12 2 0
10 14 1 0
9 14 1 0
8 15 1 0
2 26 1 0
15 16 1 0
16 17 1 0
8 18 1 0
18 19 1 0
18 28 1 0
19 20 1 0
20 21 1 0
20 22 2 0
21 23 1 0
23 24 1 0
24 25 2 0
1 13 1 0
26 27 3 0
1 2 2 0
3 2 1 0
10 3 2 0
28 30 2 0
28 29 1 0
1 31 1 0
5 32 1 0
5 33 1 0
6 34 1 0
6 35 1 0
11 36 1 0
11 37 1 0
11 38 1 0
13 39 1 0
14 40 1 0
15 41 1 0
15 42 1 0
16 43 1 0
16 44 1 0
17 45 1 0
17 46 1 0
17 47 1 0
18 48 1 0
19 49 1 0
23 50 1 0
23 51 1 0
24 52 1 0
25 53 1 0
25 54 1 0
29 55 1 0
M END
> <Name>
Compound223

> <Activ>
5.9
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SciTegic10081411483D

61	64	0	0	1	0	999	V2000				
-5.8750				3.0470		1.1130	C	0	0		
-4.5780				2.8280		1.6520	C	0	0		
-3.6900				1.9410		0.9800	C	0	0		
-2.4160				1.5980		1.3120	C	0	0		
-1.4920				1.9980		2.4530	C	0	0		
-0.0330				1.5270		2.1760	C	0	0		
0.0020				0.2030		1.6290	O	0	0		
-0.6060				0.0430		0.3380	C	0	0	2	0 0 0
-1.9860				0.6890		0.3440	C	0	0		
-4.0900				1.2970		-0.1740	C	0	0		
-5.7830				0.8030		-1.9650	C	0	0		
-5.3750				1.4980		-0.7330	C	0	0		
-6.2700				2.3810		-0.0780	C	0	0		
-3.0310				0.5020		-0.5900	N	0	0		
-0.7050				-1.4650		0.0860	C	0	0		
-1.6230				-2.1700		1.0840	C	0	0		
-1.7230				-3.6760		0.8340	C	0	0		
0.2930				0.7170		-0.7050	C	0	0	2	0 0 0
1.7110				0.4300		-0.4450	N	0	0		
2.3400				-0.5430		-1.1700	C	0	0		
3.6210				-0.7460		-0.8770	O	0	0		
1.7360				-1.1620		-2.0160	O	0	0		
4.2030				-1.7700		-1.6720	C	0	0		
5.6290				-1.9410		-1.2930	C	0	0		
7.7700				-3.0640		-1.5860	C	0	0		
6.4200				-2.9040		-1.9450	C	0	0		
8.3300				-2.2660		-0.5740	C	0	0		
6.1900				-1.1410		-0.2810	C	0	0		
7.5390				-1.3030		0.0780	C	0	0		
-4.2050				3.5120		2.8670	C	0	0		
-3.9140				4.0590		3.8480	N	0	0		
0.0390				2.1970		-0.8110	C	0	0		
1.0820				2.9730		-0.5250	O	0	0		
-1.0470				2.6210		-1.1330	O	0	0		
-6.5720				3.7150		1.5980	H	0	0		
-1.4980				3.0800		2.5880	H	0	0		
-1.8610				1.5510		3.3770	H	0	0		
0.4670				2.2030		1.4780	H	0	0		
0.5490				1.5330		3.0980	H	0	0		
-5.0160				0.1540		-2.3870	H	0	0		
-6.0510				1.5390		-2.7250	H	0	0		
-6.6640				0.1930		-1.7660	H	0	0		
-7.2580				2.5510		-0.4830	H	0	0		
-3.0040				-0.0880		-1.3910	H	0	0		
-1.0230				-1.6620		-0.9380	H	0	0		
0.2850				-1.9220		0.0840	H	0	0		
-1.3070				-1.9690		2.1070	H	0	0		
-2.6130				-1.7150		1.0860	H	0	0		
-2.3770				-4.1450		1.5660	H	0	0		
-2.1060				-3.8750		-0.1680	H	0	0		
-0.7420				-4.1450		0.9140	H	0	0		
0.0350											

2.2110	0.9390	0.2540	H	0	0
4.1390	-1.4690	-2.7170	H	0	0
3.6620	-2.6970	-1.4810	H	0	0
8.3770	-3.8050	-2.0880	H	0	0
5.9960	-3.5220	-2.7230	H	0	0
9.3670	-2.3890	-0.2990	H	0	0
5.5880	-0.3980	0.2250	H	0	0
7.9710	-0.6870	0.8530	H	0	0
0.9840	3.9320	-0.5740	H	0	0
3	4	1	0		
4	9	2	0		
4	5	1	0		
6	5	1	0		
7	6	1	0		
8	7	1	0		
9	8	1	0		
12	10	1	0		
12	11	1	0		
13	12	2	0		
10	14	1	0		
9	14	1	0		
8	15	1	0		
2	30	1	0		
15	16	1	0		
16	17	1	0		
8	18	1	0		
18	19	1	0		
18	32	1	0		
19	20	1	0		
20	21	1	0		
20	22	2	0		
21	23	1	0		
23	24	1	0		
29	27	2	0		
28	29	1	0		
25	26	2	0		
27	25	1	0		
26	24	1	0		
24	28	2	0		
1	13	1	0		
30	31	3	0		
1	2	2	0		
3	2	1	0		
10	3	2	0		
32	34	2	0		
32	33	1	0		
1	35	1	0		
5	36	1	0		
5	37	1	0		
6	38	1	0		
6	39	1	0		
11	40	1	0		
11	41	1	0		
11	42	1	0		
13	43	1	0		
14	44	1	0		
15	45	1	0		
15	46	1	0		
16	47	1	0		
16	48	1	0		
17	49	1	0		

```

17 50 1 0
17 51 1 0
18 52 1 0
19 53 1 0
23 54 1 0
23 55 1 0
25 56 1 0
26 57 1 0
27 58 1 0
28 59 1 0
29 60 1 0
33 61 1 0

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M END

> <Name>

Compound224

> <Activ>

0.72

> <DB_Ref_id>

26.24

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Compound225

SciTegic10081411483D

```

58 61 0 0 1 0          999 V2000
-5.0210 2.0100 -1.4450 C 0 0
-3.8120 1.8480 -2.1740 C 0 0
-2.6600 1.3520 -1.4960 C 0 0
-1.4100 1.1350 -1.9880 C 0 0
-0.7790 1.3200 -3.3590 C 0 0
 0.7720 1.1950 -3.2770 C 0 0
 1.1780 0.1190 -2.4220 O 0 0
 0.8180 0.2480 -1.0410 C 0 0 2 0 0 0
-0.6520 0.6330 -0.9280 C 0 0
-2.7270 1.0200 -0.1580 C 0 0
-3.9730 0.8070 2.0160 C 0 0
-3.9220 1.1660 0.5880 C 0 0
-5.0720 1.6700 -0.0660 C 0 0
-1.4730 0.5590 0.2190 N 0 0
 1.6990 1.3340 -0.4120 C 0 0
 0.9810 2.6800 -0.2910 C 0 0
 1.9340 3.8280 0.0390 C 0 0
 1.0720 -1.1150 -0.3950 C 0 0 2 0 0 0
 2.4450 -1.5350 -0.6210 N 0 0
 2.9690 -3.0330 0.0940 S 0 0
 2.8260 -3.1130 1.8130 C 0 0
 2.1270 -4.0680 -0.4820 O 0 0
 4.3710 -3.1760 -0.2560 O 0 0
 3.6970 -2.5980 4.0250 C 0 0
 3.8150 -2.5310 2.6250 C 0 0
 2.5940 -3.2440 4.6090 C 0 0
 1.7230 -3.7620 2.3950 C 0 0
 1.6080 -3.8260 3.7950 C 0 0
-3.7870 2.1860 -3.5740 C 0 0
-3.7680 2.4510 -4.7030 N 0 0
 0.1190 -2.1700 -0.8850 C 0 0
-0.6890 -2.6780 0.0410 O 0 0
 0.1110 -2.5120 -2.0450 O 0 0
-5.9120 2.3890 -1.9260 H 0 0

```

-1.0430	2.2970	-3.7680	H	0	0
-1.1850	0.5610	-4.0270	H	0	0
1.1900	1.0200	-4.2700	H	0	0
1.2190	2.1150	-2.9040	H	0	0
-3.0270	0.4490	2.4240	H	0	0
-4.7170	0.0250	2.1680	H	0	0
-4.2790	1.6760	2.6000	H	0	0
-5.9940	1.7970	0.4820	H	0	0
-1.2010	0.2380	1.1190	H	0	0
2.0760	1.0120	0.5590	H	0	0
2.6310	1.4430	-0.9670	H	0	0
0.4140	2.8960	-1.1950	H	0	0
0.1780	2.6230	0.4430	H	0	0
1.3890	4.7700	0.1150	H	0	0
2.4530	3.6410	0.9790	H	0	0
2.6860	3.9410	-0.7400	H	0	0
0.9180	-0.9410	0.6700	H	0	0
3.0700	-0.7750	-0.3180	H	0	0
4.4550	-2.1500	4.6500	H	0	0
4.6600	-2.0330	2.1780	H	0	0
2.5060	-3.2950	5.6860	H	0	0
0.9650	-4.2090	1.7700	H	0	0
0.7620	-4.3240	4.2440	H	0	0
-1.3260	-3.3590	-0.2090	H	0	0
3	4	1	0		
4	9	2	0		
4	5	1	0		
6	5	1	0		
7	6	1	0		
8	7	1	0		
9	8	1	0		
12	10	1	0		
12	11	1	0		
13	12	2	0		
10	14	1	0		
9	14	1	0		
8	15	1	0		
2	29	1	0		
15	16	1	0		
16	17	1	0		
8	18	1	0		
18	19	1	0		
18	31	1	0		
19	20	1	0		
20	21	1	0		
20	22	2	0		
20	23	2	0		
28	26	2	0		
27	28	1	0		
24	25	2	0		
26	24	1	0		
25	21	1	0		
21	27	2	0		
1	13	1	0		
29	30	3	0		
1	2	2	0		
3	2	1	0		
10	3	2	0		
31	33	2	0		
31	32	1	0		
1	34	1	0		

```

5 35 1 0
5 36 1 0
6 37 1 0
6 38 1 0
11 39 1 0
11 40 1 0
11 41 1 0
13 42 1 0
14 43 1 0
15 44 1 0
15 45 1 0
16 46 1 0
16 47 1 0
17 48 1 0
17 49 1 0
17 50 1 0
18 51 1 0
19 52 1 0
24 53 1 0
25 54 1 0
26 55 1 0
27 56 1 0
28 57 1 0
32 58 1 0

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M END

> <Name>

Compound225

> <Activ>

4

> <DB_Ref_id>

26.26f

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Compound226

SciTegic10081411483D

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51 53 0 0 1 0          999 V2000
-4.5650 1.6110 -0.9380 C 0 0
-3.3560 1.4490 -1.6660 C 0 0
-2.2030 0.9530 -0.9900 C 0 0
-0.9550 0.7360 -1.4820 C 0 0
-0.3220 0.9220 -2.8540 C 0 0
1.2280 0.7950 -2.7720 C 0 0
1.6350 -0.2810 -1.9160 O 0 0
1.2730 -0.1500 -0.5330 C 0 0 2 0 0 0
-0.1950 0.2340 -0.4220 C 0 0
-2.2720 0.6210 0.3480 C 0 0
-3.5160 0.4080 2.5230 C 0 0
-3.4650 0.7680 1.0960 C 0 0
-4.6170 1.2720 0.4390 C 0 0
-1.0180 0.1600 0.7250 N 0 0
2.1540 0.9360 0.0960 C 0 0
1.5180 2.3240 0.0270 C 0 0
1.0510 2.8260 1.3950 C 0 0
1.5290 -1.5140 0.1110 C 0 0 2 0 0 0
2.9140 -1.9120 -0.0700 N 0 0
3.4040 -3.4690 0.5330 S 0 0
3.1190 -3.6930 2.2850 C 0 0
2.6170 -4.4470 -0.1970 O 0 0

```

4.8300	-3.5680	0.2730	O	0	0
-3.3300	1.7870	-3.0680	C	0	0
-3.3110	2.0530	-4.1970	N	0	0
0.6090	-2.5800	-0.4160	C	0	0
-0.1410	-3.1860	0.5000	O	0	0
0.5760	-2.8480	-1.5960	O	0	0
-5.4550	1.9900	-1.4200	H	0	0
-0.5880	1.8970	-3.2600	H	0	0
-0.7290	0.1620	-3.5220	H	0	0
1.6460	0.6210	-3.7620	H	0	0
1.6740	1.7170	-2.3970	H	0	0
-2.5680	0.0570	2.9320	H	0	0
-4.2560	-0.3790	2.6740	H	0	0
-3.8280	1.2750	3.1050	H	0	0
-5.5370	1.3980	0.9900	H	0	0
-0.7440	-0.1620	1.6250	H	0	0
2.4100	0.6780	1.1230	H	0	0
3.1430	0.9430	-0.3630	H	0	0
2.1990	3.0390	-0.4340	H	0	0
0.6950	2.3380	-0.6880	H	0	0
1.9020	2.9960	2.0530	H	0	0
0.4880	3.7540	1.2930	H	0	0
0.4000	2.0940	1.8730	H	0	0
1.3360	-1.3480	1.1720	H	0	0
3.5160	-1.1820	0.3360	H	0	0
3.4020	-4.6740	2.6620	H	0	0
2.0620	-3.5450	2.5020	H	0	0
3.6840	-2.9450	2.8420	H	0	0
-0.0470	-2.9340	1.4300	H	0	0
3	4	1	0		
4	9	2	0		
4	5	1	0		
6	5	1	0		
7	6	1	0		
8	7	1	0		
9	8	1	0		
12	10	1	0		
12	11	1	0		
13	12	2	0		
10	14	1	0		
9	14	1	0		
8	15	1	0		
2	24	1	0		
15	16	1	0		
16	17	1	0		
8	18	1	0		
18	19	1	0		
18	26	1	0		
19	20	1	0		
20	21	1	0		
20	22	2	0		
20	23	2	0		
1	13	1	0		
24	25	3	0		
1	2	2	0		
3	2	1	0		
10	3	2	0		
26	28	2	0		
26	27	1	0		
1	29	1	0		
5	30	1	0		

```

5 31 1 0
6 32 1 0
6 33 1 0
11 34 1 0
11 35 1 0
11 36 1 0
13 37 1 0
14 38 1 0
15 39 1 0
15 40 1 0
16 41 1 0
16 42 1 0
17 43 1 0
17 44 1 0
17 45 1 0
18 46 1 0
19 47 1 0
21 48 1 0
21 49 1 0
21 50 1 0
27 51 1 0

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M END

> <Name>

Compound226

> <Activ>

6

> <DB_Ref_id>

26.26d

\$\$\$\$

Compound227

SciTegic10081411483D

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57 60 0 0 1 0          999 V2000
-5.6580 1.7010 -0.9040 C 0 0
-4.4490 1.5390 -1.6330 C 0 0
-3.2970 1.0450 -0.9570 C 0 0
-2.0470 0.8260 -1.4490 C 0 0
-1.4160 1.0120 -2.8180 C 0 0
0.1350 0.8870 -2.7380 C 0 0
0.5410 -0.1890 -1.8830 O 0 0
0.1800 -0.0590 -0.5000 C 0 0 2 0 0 0
-1.2890 0.3240 -0.3890 C 0 0
-3.3650 0.7110 0.3810 C 0 0
-4.6090 0.5000 2.5570 C 0 0
-4.5590 0.8590 1.1290 C 0 0
-5.7110 1.3630 0.4730 C 0 0
-2.1090 0.2500 0.7580 N 0 0
1.0610 1.0270 0.1290 C 0 0
0.3440 2.3730 0.2460 C 0 0
1.2970 3.5200 0.5860 C 0 0
0.4360 -1.4220 0.1450 C 0 0 2 0 0 0
1.8560 -1.7950 0.0470 N 0 0
2.6250 -1.8070 1.1760 C 0 0
4.0650 -2.1870 1.0610 C 0 0
2.1430 -1.5160 2.2460 O 0 0
6.0980 -3.0820 2.0590 C 0 0
4.7420 -2.7250 2.1680 C 0 0
6.7760 -2.9020 0.8400 C 0 0

```

4.7440	-2.0080	-0.1580	C	0	0
6.0980	-2.3650	-0.2680	C	0	0
-4.4240	1.8770	-3.0350	C	0	0
-4.4040	2.1450	-4.1640	N	0	0
-0.4570	-2.4980	-0.4100	C	0	0
-1.4800	-2.8420	0.3670	O	0	0
-0.2360	-2.9940	-1.4900	O	0	0
-6.5490	2.0820	-1.3870	H	0	0
-1.6800	1.9880	-3.2270	H	0	0
-1.8220	0.2540	-3.4880	H	0	0
0.5530	0.7130	-3.7290	H	0	0
0.5800	1.8090	-2.3630	H	0	0
-3.6620	0.1490	2.9650	H	0	0
-5.3480	-0.2890	2.7070	H	0	0
-4.9240	1.3650	3.1390	H	0	0
-6.6310	1.4880	1.0230	H	0	0
-1.8380	-0.0700	1.6580	H	0	0
1.4380	0.7030	1.1000	H	0	0
1.9940	1.1350	-0.4260	H	0	0
-0.2150	2.5920	-0.6620	H	0	0
-0.4650	2.3150	0.9750	H	0	0
0.7520	4.4610	0.6620	H	0	0
1.8090	3.3280	1.5290	H	0	0
2.0550	3.6350	-0.1880	H	0	0
0.1390	-1.4140	1.1930	H	0	0
2.2540	-2.0350	-0.8360	H	0	0
6.6170	-3.4940	2.9100	H	0	0
4.2310	-2.8670	3.1090	H	0	0
7.8170	-3.1780	0.7560	H	0	0
4.2310	-1.5960	-1.0160	H	0	0
6.6190	-2.2270	-1.2030	H	0	0
-1.5820	-2.4180	1.2290	H	0	0
3	4	1	0		
4	9	2	0		
4	5	1	0		
6	5	1	0		
7	6	1	0		
8	7	1	0		
9	8	1	0		
12	10	1	0		
12	11	1	0		
13	12	2	0		
10	14	1	0		
9	14	1	0		
8	15	1	0		
2	28	1	0		
15	16	1	0		
16	17	1	0		
8	18	1	0		
18	19	1	0		
18	30	1	0		
19	20	1	0		
20	21	1	0		
20	22	2	0		
27	25	2	0		
26	27	1	0		
23	24	2	0		
25	23	1	0		
24	21	1	0		
21	26	2	0		
1	13	1	0		


```

28 29 3 0
1 2 2 0
3 2 1 0
10 3 2 0
30 32 2 0
30 31 1 0
1 33 1 0
5 34 1 0
5 35 1 0
6 36 1 0
6 37 1 0
11 38 1 0
11 39 1 0
11 40 1 0
13 41 1 0
14 42 1 0
15 43 1 0
15 44 1 0
16 45 1 0
16 46 1 0
17 47 1 0
17 48 1 0
17 49 1 0
18 50 1 0
19 51 1 0
23 52 1 0
24 53 1 0
25 54 1 0
26 55 1 0
27 56 1 0
31 57 1 0

```

M END

> <Name>

Compound227

> <Activ>

4.5

> <DB_Ref_id>

26.26c

\$\$\$\$

Compound228

SciTegic10081411483D

```

59 61 0 0 1 0          999 V2000
-5.4340 3.0140 1.2130 C 0 0
-4.1370 2.7970 1.7540 C 0 0
-3.2480 1.9100 1.0800 C 0 0
-1.9750 1.5640 1.4140 C 0 0
-1.0510 1.9670 2.5530 C 0 0
0.4080 1.4960 2.2770 C 0 0
0.4450 0.1700 1.7280 O 0 0
-0.1640 0.0100 0.4390 C 0 0 2 0 0 0
-1.5450 0.6560 0.4430 C 0 0
-3.6470 1.2640 -0.0720 C 0 0
-5.3400 0.7710 -1.8650 C 0 0
-4.9340 1.4650 -0.6310 C 0 0
-5.8280 2.3480 0.0230 C 0 0
-2.5900 0.4690 -0.4900 N 0 0
-0.2640 -1.4960 0.1850 C 0 0

```

-1.1840	-2.2030	1.1840	C	0	0				
-1.2770	-3.7090	0.9350	C	0	0				
0.7340	0.6850	-0.6060	C	0	0	2	0	0	0
2.1520	0.3960	-0.3460	N	0	0				
2.7810	-0.5780	-1.0670	C	0	0				
4.2320	-0.8610	-0.7870	C	0	0				
2.1780	-1.1990	-1.9100	O	0	0				
4.8030	-1.9450	-1.7010	C	0	0				
6.2790	-2.2310	-1.4320	C	0	0				
6.8480	-3.3170	-2.3440	C	0	0				
-3.7640	3.4780	2.9670	C	0	0				
-3.4730	4.0250	3.9470	N	0	0				
0.4800	2.1640	-0.7110	C	0	0				
1.5230	2.9390	-0.4240	O	0	0				
-0.6060	2.5880	-1.0330	O	0	0				
-6.1310	3.6820	1.6970	H	0	0				
-1.0570	3.0470	2.6890	H	0	0				
-1.4200	1.5190	3.4770	H	0	0				
0.9080	2.1700	1.5800	H	0	0				
0.9900	1.5000	3.1970	H	0	0				
-4.5720	0.1250	-2.2890	H	0	0				
-5.6130	1.5060	-2.6230	H	0	0				
-6.2190	0.1580	-1.6640	H	0	0				
-6.8170	2.5180	-0.3810	H	0	0				
-2.5630	-0.1210	-1.2890	H	0	0				
0.7260	-1.9530	0.1850	H	0	0				
-0.5800	-1.6950	-0.8380	H	0	0				
-2.1740	-1.7480	1.1820	H	0	0				
-0.8690	-2.0000	2.2070	H	0	0				
-1.9380	-4.1970	1.6520	H	0	0				
-0.2950	-4.1740	1.0140	H	0	0				
-1.6640	-3.9100	-0.0630	H	0	0				
0.4760	0.3480	-1.6090	H	0	0				
2.6580	0.9040	0.3500	H	0	0				
4.8260	0.0330	-0.9770	H	0	0				
4.3630	-1.1330	0.2600	H	0	0				
4.2150	-2.8610	-1.6270	H	0	0				
4.6440	-1.6900	-2.7500	H	0	0				
6.8670	-1.3150	-1.5100	H	0	0				
6.4370	-2.4850	-0.3850	H	0	0				
7.9040	-3.4850	-2.1310	H	0	0				
6.3050	-4.2520	-2.2130	H	0	0				
6.7620	-3.0260	-3.3910	H	0	0				
1.4260	3.9000	-0.4730	H	0	0				
3	4	1	0						
4	9	2	0						
4	5	1	0						
6	5	1	0						
7	6	1	0						
8	7	1	0						
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13	12	2	0						
10	14	1	0						
9	14	1	0						
8	15	1	0						
2	26	1	0						
15	16	1	0						
16	17	1	0						
8	18	1	0						

```

18 19 1 0
18 28 1 0
19 20 1 0
20 21 1 0
20 22 2 0
21 23 1 0
23 24 1 0
24 25 1 0
1 13 1 0
26 27 3 0
1 2 2 0
3 2 1 0
10 3 2 0
28 30 2 0
28 29 1 0
1 31 1 0
5 32 1 0
5 33 1 0
6 34 1 0
6 35 1 0
11 36 1 0
11 37 1 0
11 38 1 0
13 39 1 0
14 40 1 0
15 41 1 0
15 42 1 0
16 43 1 0
16 44 1 0
17 45 1 0
17 46 1 0
17 47 1 0
18 48 1 0
19 49 1 0
21 50 1 0
21 51 1 0
23 52 1 0
23 53 1 0
24 54 1 0
24 55 1 0
25 56 1 0
25 57 1 0
25 58 1 0
29 59 1 0

```

M END

> <Name>

Compound228

> <Activ>

5

> <DB_Ref_id>

26.26b

\$\$\$\$

Compound229

SciTegic10081411483D

```

50 52 0 0 1 0          999 V2000
  -4.3070    2.5140    0.8520 C    0  0
  -3.0080    2.2970    1.3910 C    0  0

```

-2.1210	1.4100	0.7190	C	0	0				
-0.8480	1.0650	1.0510	C	0	0				
0.0780	1.4670	2.1910	C	0	0				
1.5370	0.9960	1.9140	C	0	0				
1.5720	-0.3300	1.3670	O	0	0				
0.9650	-0.4880	0.0760	C	0	0	2	0	0	0
-0.4160	0.1560	0.0820	C	0	0				
-2.5190	0.7660	-0.4360	C	0	0				
-4.2130	0.2720	-2.2270	C	0	0				
-3.8070	0.9650	-0.9940	C	0	0				
-4.6990	1.8500	-0.3400	C	0	0				
-1.4610	-0.0310	-0.8520	N	0	0				
0.8650	-1.9960	-0.1760	C	0	0				
-0.0550	-2.7010	0.8200	C	0	0				
-0.1500	-4.2070	0.5720	C	0	0				
1.8630	0.1860	-0.9670	C	0	0	2	0	0	0
3.2810	-0.1030	-0.7070	N	0	0				
3.9080	-1.0780	-1.4300	C	0	0				
5.3620	-1.3590	-1.1520	C	0	0				
3.3050	-1.6970	-2.2730	O	0	0				
-2.6350	2.9790	2.6060	C	0	0				
-2.3440	3.5270	3.5860	N	0	0				
1.6100	1.6660	-1.0720	C	0	0				
2.6530	2.4400	-0.7870	O	0	0				
0.5240	2.0900	-1.3950	O	0	0				
-5.0040	3.1820	1.3360	H	0	0				
0.0700	2.5490	2.3260	H	0	0				
-0.2910	1.0200	3.1150	H	0	0				
2.0370	1.6700	1.2190	H	0	0				
2.1190	1.0020	2.8360	H	0	0				
-3.4430	-0.3750	-2.6520	H	0	0				
-4.4860	1.0060	-2.9840	H	0	0				
-5.0900	-0.3420	-2.0250	H	0	0				
-5.6870	2.0180	-0.7440	H	0	0				
-1.4350	-0.6190	-1.6500	H	0	0				
0.5490	-2.1950	-1.1990	H	0	0				
1.8540	-2.4530	-0.1760	H	0	0				
0.2580	-2.4980	1.8460	H	0	0				
-1.0470	-2.2480	0.8180	H	0	0				
-0.8050	-4.6780	1.3070	H	0	0				
-0.5330	-4.4100	-0.4280	H	0	0				
0.8320	-4.6740	0.6560	H	0	0				
1.6060	-0.1500	-1.9710	H	0	0				
3.7810	0.4080	-0.0100	H	0	0				
5.7780	-2.1500	-1.7750	H	0	0				
5.4880	-1.6540	-0.1090	H	0	0				
5.9510	-0.4590	-1.3180	H	0	0				
2.5550	3.4000	-0.8360	H	0	0				
3	4	1	0						
4	9	2	0						
4	5	1	0						
6	5	1	0						
7	6	1	0						
8	7	1	0						
9	8	1	0						
12	10	1	0						
12	11	1	0						
13	12	2	0						
10	14	1	0						
9	14	1	0						
8	15	1	0						

```

  2 23  1  0
15 16  1  0
16 17  1  0
  8 18  1  0
18 19  1  0
18 25  1  0
19 20  1  0
20 21  1  0
20 22  2  0
  1 13  1  0
23 24  3  0
  1  2  2  0
  3  2  1  0
10  3  2  0
25 27  2  0
25 26  1  0
  1 28  1  0
  5 29  1  0
  5 30  1  0
  6 31  1  0
  6 32  1  0
11 33  1  0
11 34  1  0
11 35  1  0
13 36  1  0
14 37  1  0
15 38  1  0
15 39  1  0
16 40  1  0
16 41  1  0
17 42  1  0
17 43  1  0
17 44  1  0
18 45  1  0
19 46  1  0
21 47  1  0
21 48  1  0
21 49  1  0
26 50  1  0

```

M END

> <Name>

Compound229

> <Activ>

1.7

> <DB_Ref_id>

26.26a

\$\$\$\$

Compound230

SciTegic10081411483D

```

40 42  0  0  1  0          999 V2000
  -3.3220    2.4740    0.5980 C    0  0
  -2.0250    2.2600    1.1370 C    0  0
  -1.1350    1.3710    0.4650 C    0  0
    0.1390    1.0290    0.7990 C    0  0
    1.0630    1.4280    1.9390 C    0  0
    2.5200    0.9570    1.6660 C    0  0
    2.5570   -0.3670    1.1150 O    0  0

```

1.9530	-0.5240	-0.1760	C	0	0	2	0	0	0
0.5700	0.1210	-0.1740	C	0	0				
-1.5350	0.7280	-0.6880	C	0	0				
-3.2270	0.2320	-2.4830	C	0	0				
-2.8220	0.9280	-1.2480	C	0	0				
-3.7170	1.8100	-0.5940	C	0	0				
-0.4760	-0.0690	-1.1060	N	0	0				
1.8560	-2.0300	-0.4360	C	0	0				
0.9630	-2.7460	0.5780	C	0	0				
0.8610	-4.2500	0.3180	C	0	0				
-1.6540	2.9410	2.3520	C	0	0				
-1.3590	3.4880	3.3320	N	0	0				
2.8090	0.1370	-1.2290	C	0	0				
2.4770	1.3900	-1.5220	O	0	0				
3.7250	-0.4570	-1.7500	O	0	0				
-4.0190	3.1420	1.0800	H	0	0				
1.0570	2.5100	2.0740	H	0	0				
0.6900	0.9860	2.8650	H	0	0				
3.0200	1.6270	0.9670	H	0	0				
3.1020	0.9650	2.5860	H	0	0				
-2.4370	-0.3690	-2.9360	H	0	0				
-3.5550	0.9630	-3.2210	H	0	0				
-4.0680	-0.4260	-2.2700	H	0	0				
-4.7030	1.9780	-0.9980	H	0	0				
-0.4510	-0.6580	-1.9040	H	0	0				
1.5160	-2.2250	-1.4530	H	0	0				
2.8480	-2.4830	-0.4610	H	0	0				
1.3030	-2.5530	1.5960	H	0	0				
-0.0290	-2.2930	0.6070	H	0	0				
0.2290	-4.7290	1.0660	H	0	0				
0.4490	-4.4420	-0.6720	H	0	0				
1.8460	-4.7150	0.3650	H	0	0				
2.9860	1.8710	-2.1880	H	0	0				
3	4	1	0						
4	9	2	0						
4	5	1	0						
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8	7	1	0						
9	8	1	0						
12	10	1	0						
12	11	1	0						
13	12	2	0						
10	14	1	0						
9	14	1	0						
8	15	1	0						
2	18	1	0						
15	16	1	0						
16	17	1	0						
8	20	1	0						
1	13	1	0						
18	19	3	0						
1	2	2	0						
3	2	1	0						
10	3	2	0						
20	22	2	0						
20	21	1	0						
1	23	1	0						
5	24	1	0						
5	25	1	0						
6	26	1	0						

```

6 27 1 0
11 28 1 0
11 29 1 0
11 30 1 0
13 31 1 0
14 32 1 0
15 33 1 0
15 34 1 0
16 35 1 0
16 36 1 0
17 37 1 0
17 38 1 0
17 39 1 0
21 40 1 0

```

M END

> <Name>

Compound230

> <Activ>

0.7

> <DB_Ref_id>

26.18

\$\$\$\$

Compound231

SciTegic10081411483D

```

44 47 0 0 1 0          999 V2000
-4.0680 2.1910 0.3810 C 0 0
-2.8830 1.9590 1.1330 C 0 0
-1.8070 1.2500 0.5230 C 0 0
-0.5940 0.9260 1.0490 C 0 0
0.0570 1.1700 2.4020 C 0 0
1.5740 0.8300 2.3610 C 0 0
1.8380 -0.3670 1.6150 O 0 0
1.7010 1.1840 -2.6290 O 0 0
3.2250 -0.4570 -2.5200 O 0 0
2.4340 0.4710 -1.9860 C 0 0
2.5080 0.5880 -0.4860 C 0 0
1.5020 -0.3280 0.2210 C 0 0 2 0 0 0
0.0920 0.2250 0.0550 C 0 0
-1.9220 0.7910 -0.7710 C 0 0
-3.1930 0.5040 -2.9200 C 0 0
-3.0920 1.0040 -1.5390 C 0 0
-4.1680 1.7150 -0.9530 C 0 0
-0.7360 0.1390 -1.0860 N 0 0
1.5740 -1.7680 -0.2730 C 0 0
0.7890 -2.7750 0.5920 C 0 0
2.8850 -2.4980 0.0900 C 0 0
2.1040 -3.4650 0.9980 C 0 0
-2.8090 2.4470 2.4880 C 0 0
-2.7500 2.8420 3.5780 N 0 0
-4.9000 2.7290 0.8110 H 0 0
-0.0740 2.2090 2.7070 H 0 0
-0.4490 0.5470 3.1430 H 0 0
2.1450 1.6460 1.9160 H 0 0
1.9590 0.6890 3.3710 H 0 0
3.2250 -0.5820 -3.4790 H 0 0
3.4920 0.2770 -0.1390 H 0 0
2.3590 1.6250 -0.1880 H 0 0

```

-4.1720	0.7580	-3.3280	H	0	0
-2.3710	0.9060	-3.5140	H	0	0
-3.1030	-0.5820	-2.9200	H	0	0
-5.0700	1.8930	-1.5200	H	0	0
-0.5080	-0.3050	-1.9450	H	0	0
1.3300	-1.8420	-1.3340	H	0	0
0.2170	-2.3500	1.4180	H	0	0
0.0900	-3.4060	0.0430	H	0	0
3.6410	-1.8970	0.5980	H	0	0
3.3970	-2.9670	-0.7500	H	0	0
2.1800	-4.5200	0.7290	H	0	0
2.3520	-3.4040	2.0590	H	0	0

1	2	2	0
3	2	1	0
14	3	2	0
3	4	1	0
4	13	2	0
4	5	1	0
6	5	1	0
7	6	1	0
12	7	1	0
10	8	2	0
10	9	1	0
11	10	1	0
12	11	1	0
13	12	1	0
16	14	1	0
16	15	1	0
17	16	2	0
14	18	1	0
13	18	1	0
12	19	1	0
22	20	1	0
22	21	1	0
20	19	1	0
21	19	1	0
2	23	1	0
1	17	1	0
23	24	3	0
1	25	1	0
5	26	1	0
5	27	1	0
6	28	1	0
6	29	1	0
9	30	1	0
11	31	1	0
11	32	1	0
15	33	1	0
15	34	1	0
15	35	1	0
17	36	1	0
18	37	1	0
19	38	1	0
20	39	1	0
20	40	1	0
21	41	1	0
21	42	1	0
22	43	1	0
22	44	1	0


```

M  END
>  <Name>

```


[illegible]

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12  7  1  0
10  8  2  0
10  9  1  0
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12 11  1  0
13 12  1  0
16 14  2  0
16 15  1  0
17 16  1  0
14 18  1  0
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 2 19  1  0
12 20  1  0
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21 22  1  0
22 23  1  0
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 6 27  1  0
 6 28  1  0
 9 29  1  0
11 30  1  0
11 31  1  0
17 32  1  0
18 33  1  0
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M  END
> <Name>
Compound232

> <Activ>
3.7

> <DB_Ref_id>
26.08s

$$$$
Compound233
SciTegic10081411483D

37 39  0  0  1  0          999 V2000
-4.6090  1.2850 -0.2580 C  0  0
-3.2890  1.8090 -0.2190 C  0  0
-2.2050  0.8990 -0.0370 C  0  0
-0.8730  1.1720  0.0390 C  0  0
-0.0640  2.4590 -0.0310 C  0  0
 1.4120  2.2210  0.4000 C  0  0
 1.9320  0.9940 -0.1270 O  0  0
 3.7990 -1.4960  1.8950 O  0  0
 3.7270  0.7150  2.2540 O  0  0
 3.1740 -0.4650  1.9840 C  0  0
 1.6820 -0.4450  1.7870 C  0  0
 1.2870 -0.2050  0.3260 C  0  0  3  0  0  0

```

-0.2250	-0.0550	0.2030	C	0	0
-2.4360	-0.4590	0.0860	C	0	0
-4.0330	-2.6850	0.1970	C1	0	0
-3.7460	-0.9980	0.0450	C	0	0
-4.8380	-0.1090	-0.1270	C	0	0
-1.1990	-1.0760	0.2400	N	0	0
-3.0860	3.5080	-0.3970	C1	0	0
1.8010	-1.3360	-0.5680	C	0	0
1.2250	-1.1250	-2.2770	S	0	0
1.9960	-2.5960	-3.0120	C	0	0
-5.4570	1.9420	-0.3890	H	0	0
-0.1020	2.8360	-1.0530	H	0	0
-0.5000	3.2190	0.6170	H	0	0
2.0430	3.0350	0.0430	H	0	0
1.5020	2.2010	1.4860	H	0	0
4.6800	0.7700	2.3910	H	0	0
1.2600	-1.4120	2.0590	H	0	0
1.2340	0.3090	2.4360	H	0	0
-5.8520	-0.4820	-0.1620	H	0	0
-1.0250	-2.0470	0.3530	H	0	0
2.8910	-1.3750	-0.5550	H	0	0
1.4730	-2.3050	-0.1910	H	0	0
1.7230	-2.6620	-4.0650	H	0	0
3.0760	-2.5530	-2.8590	H	0	0
1.6230	-3.4880	-2.5140	H	0	0
1	17	2	0		
1	2	1	0		
3	2	2	0		
14	3	1	0		
3	4	1	0		
4	13	2	0		
4	5	1	0		
6	5	1	0		
7	6	1	0		
12	7	1	0		
10	8	2	0		
10	9	1	0		
11	10	1	0		
12	11	1	0		
13	12	1	0		
16	14	2	0		
16	15	1	0		
17	16	1	0		
14	18	1	0		
13	18	1	0		
2	19	1	0		
12	20	1	0		
20	21	1	0		
21	22	1	0		
1	23	1	0		
5	24	1	0		
5	25	1	0		
6	26	1	0		
6	27	1	0		
9	28	1	0		
11	29	1	0		
11	30	1	0		
17	31	1	0		
18	32	1	0		
20	33	1	0		
20	34	1	0		

[illegible]

```

14  3  1  0
  3  4  1  0
  4 13  2  0
  4  5  1  0
  6  5  1  0
  7  6  1  0
12  7  1  0
10  8  2  0
10  9  1  0
11 10  1  0
12 11  1  0
13 12  1  0
16 14  2  0
16 15  1  0
17 16  1  0
14 18  1  0
13 18  1  0
  2 19  1  0
12 20  1  0
20 21  1  0
22 23  1  0
22 21  1  0
21 23  1  0
  1 24  1  0
  5 25  1  0
  5 26  1  0
  6 27  1  0
  6 28  1  0
  9 29  1  0
11 30  1  0
11 31  1  0
17 32  1  0
18 33  1  0
20 34  1  0
20 35  1  0
21 36  1  0
22 37  1  0
22 38  1  0
23 39  1  0
23 40  1  0
M  END
> <Name>
Compound234

> <Activ>
1.9

> <DB_Ref_id>
26.08n

$$$$
Compound235
  SciTegic10081411483D

43 46  0  0  1  0          999 V2000
  -4.8300    1.3440   -0.0740 C    0  0
  -3.5100    1.8690   -0.0350 C    0  0
  -2.4260    0.9590    0.1470 C    0  0
  -1.0940    1.2350    0.2210 C    0  0
  -0.2830    2.5220    0.1520 C    0  0
    1.1930    2.2830    0.5800 C    0  0

```

1.7130	1.0570	0.0510	O	0	0				
-0.2090	-1.7650	2.9100	O	0	0				
1.7520	-2.7400	2.4360	O	0	0				
0.9200	-1.7030	2.4830	C	0	0				
1.4800	-0.4100	1.9570	C	0	0				
1.0660	-0.1400	0.5060	C	0	0	3	0	0	0
-0.4450	0.0080	0.3850	C	0	0				
-2.6560	-0.3960	0.2680	C	0	0				
-4.2520	-2.6250	0.3790	C1	0	0				
-3.9670	-0.9370	0.2270	C	0	0				
-5.0590	-0.0490	0.0570	C	0	0				
-1.4180	-1.0130	0.4200	N	0	0				
-3.3090	3.5690	-0.2130	C1	0	0				
1.5940	-1.2890	-0.3440	C	0	0				
0.9530	-1.2930	-1.7280	C	0	0				
1.6430	-0.1270	-2.4240	C	0	0				
3.0900	-0.2130	-1.9450	C	0	0				
3.0680	-1.0920	-0.6930	C	0	0				
-5.6780	2.0000	-0.2050	H	0	0				
-0.3220	2.9010	-0.8710	H	0	0				
-0.7210	3.2800	0.8010	H	0	0				
1.8240	3.1000	0.2250	H	0	0				
1.2850	2.2580	1.6680	H	0	0				
2.6540	-2.6070	2.1190	H	0	0				
1.0920	0.4260	2.5410	H	0	0				
2.5660	-0.4080	2.0550	H	0	0				
-6.0700	-0.4240	0.0220	H	0	0				
-1.2440	-1.9860	0.5310	H	0	0				
1.4320	-2.2260	0.1700	H	0	0				
1.1720	-2.2210	-2.2420	H	0	0				
-0.1190	-1.1790	-1.6930	H	0	0				
1.5610	-0.1830	-3.5000	H	0	0				
1.2010	0.8090	-2.1110	H	0	0				
3.7210	-0.6560	-2.7030	H	0	0				
3.4840	0.7720	-1.7340	H	0	0				
3.5180	-2.0490	-0.9160	H	0	0				
3.6310	-0.6600	0.1230	H	0	0				
1 17	2	0							
1 2	1	0							
3 2	2	0							
14 3	1	0							
3 4	1	0							
4 13	2	0							
4 5	1	0							
6 5	1	0							
7 6	1	0							
12 7	1	0							
10 8	2	0							
10 9	1	0							
11 10	1	0							
12 11	1	0							
13 12	1	0							
16 14	2	0							
16 15	1	0							
17 16	1	0							
14 18	1	0							
13 18	1	0							
2 19	1	0							
12 20	1	0							
23 24	1	0							
22 23	1	0							

```

21 22 1 0
21 20 1 0
24 20 1 0
1 25 1 0
5 26 1 0
5 27 1 0
6 28 1 0
6 29 1 0
9 30 1 0
11 31 1 0
11 32 1 0
17 33 1 0
18 34 1 0
20 35 1 0
21 36 1 0
21 37 1 0
22 38 1 0
22 39 1 0
23 40 1 0
23 41 1 0
24 42 1 0
24 43 1 0

```

M END

> <Name>

Compound235

> <Activ>

3.3

> <DB_Ref_id>

26.081

\$\$\$\$

Compound236

SciTegic10081411483D

```

39 41 0 0 1 0          999 V2000
-4.5020    1.4000   -0.4220 C    0  0
-3.1820    1.9260   -0.3810 C    0  0
-2.0980    1.0160   -0.1990 C    0  0
-0.7670    1.2890   -0.1250 C    0  0
 0.0430    2.5760   -0.1930 C    0  0
 1.5200    2.3380    0.2360 C    0  0
 2.0390    1.1090   -0.2910 O    0  0
 1.9880   -2.6520    2.0220 O    0  0
 0.1110   -1.6450    2.7150 O    0  0
 1.3110   -1.6580    2.1390 C    0  0
 1.7890   -0.3280    1.6250 C    0  0
 1.3950   -0.0880    0.1620 C    0  0  3  0  0  0
-0.1170    0.0630    0.0410 C    0  0
-2.3280   -0.3420   -0.0760 C    0  0
-3.9260   -2.5680    0.0350 Cl   0  0
-3.6410   -0.8810   -0.1170 C    0  0
-4.7300    0.0080   -0.2910 C    0  0
-1.0920   -0.9590    0.0760 N    0  0
-2.9780    3.6250   -0.5610 Cl   0  0
 1.9080   -1.2190   -0.7320 C    0  0
 1.4790   -1.0590   -2.1910 C    0  0
 3.4100   -1.4550   -0.5820 C    0  0
-5.3500    2.0590   -0.5530 H    0  0
 0.0060    2.9530   -1.2170 H    0  0

```

-0.3940	3.3360	0.4530	H	0	0
2.1510	3.1500	-0.1210	H	0	0
1.6090	2.3180	1.3240	H	0	0
-0.2540	-2.4670	3.0640	H	0	0
1.3280	0.4790	2.1950	H	0	0
2.8690	-0.2500	1.7500	H	0	0
-5.7440	-0.3650	-0.3240	H	0	0
-0.9180	-1.9320	0.1890	H	0	0
1.5960	-2.1890	-0.3440	H	0	0
1.8380	-1.8790	-2.8130	H	0	0
1.8690	-0.1290	-2.6070	H	0	0
0.3930	-1.0310	-2.2720	H	0	0
3.7420	-2.2580	-1.2400	H	0	0
3.9690	-0.5490	-0.8160	H	0	0
3.6560	-1.7420	0.4410	H	0	0
1	17	2	0		
1	2	1	0		
3	2	2	0		
14	3	1	0		
3	4	1	0		
4	13	2	0		
4	5	1	0		
6	5	1	0		
7	6	1	0		
12	7	1	0		
10	8	2	0		
10	9	1	0		
11	10	1	0		
12	11	1	0		
13	12	1	0		
16	14	2	0		
16	15	1	0		
17	16	1	0		
14	18	1	0		
13	18	1	0		
2	19	1	0		
12	20	1	0		
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20	22	1	0		
1	23	1	0		
5	24	1	0		
5	25	1	0		
6	26	1	0		
6	27	1	0		
9	28	1	0		
11	29	1	0		
11	30	1	0		
17	31	1	0		
18	32	1	0		
20	33	1	0		
21	34	1	0		
21	35	1	0		
21	36	1	0		
22	37	1	0		
22	38	1	0		
22	39	1	0		

M END

> <Name>

Compound236

> <Activ>


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> <DB_Ref_id>
26.08g
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\$\$\$\$

Compound237

SciTeGic10081411483D

[illegible]

```

18 17 1 0
15 19 1 0
14 19 1 0
2 20 1 0
1 21 1 0
5 22 1 0
5 23 1 0
6 24 1 0
6 25 1 0
8 26 1 0
8 27 1 0
8 28 1 0
10 29 1 0
12 30 1 0
12 31 1 0
18 32 1 0
19 33 1 0

```

M END

> <Name>

Compound237

> <Activ>

27

> <DB_Ref_id>

26.08a

\$\$\$\$

Compound238

SciTegic10081411483D

```

60 63 0 0 1 0          999 V2000
  0.2180    0.4040   -2.1010 C    0  0
 -0.6010   -0.7520   -1.9820 C    0  0
 -0.9360   -1.2260   -0.6810 C    0  0
 -1.7000   -2.2960   -0.3360 C    0  0
 -2.4510   -3.3430   -1.1440 C    0  0
 -3.4030   -4.1710   -0.2310 C    0  0
 -2.7980   -4.5010    1.0280 O    0  0
 -3.7180   -0.4350    2.4080 O    0  0
 -4.7510   -1.4650    0.7080 O    0  0
 -4.0720   -1.4480    1.8510 C    0  0
 -3.7600   -2.8010    2.4310 C    0  0
 -2.4610   -3.3920    1.8710 C    0  0  2  0  0  0
 -1.7140   -2.3400    1.0600 C    0  0
 -0.4620   -0.5770    0.4410 C    0  0
  0.8490    1.2480    1.5660 C    0  0
  0.3580    0.5750    0.3500 C    0  0
  0.6950    1.0650   -0.9380 C    0  0
 -0.9400   -1.2640    1.5490 N    0  0
 -1.5740   -3.9490    2.9880 C    0  0
 -0.2710   -4.5510    2.4610 C    0  0
  0.6280   -5.0830    3.5790 C    0  0
  1.4670    2.1550   -1.0680 O    0  0
  1.6840    2.6670   -2.3750 C    0  0
  2.4900    3.9450   -2.2890 C    0  0
  2.9230    4.4950   -1.1390 N    0  0
  3.6070    5.6190   -1.3750 N    0  0
  3.6490    5.8530   -2.7050 C    0  0
  2.9410    4.7960   -3.3190 C    0  0
  4.3380    7.0370   -3.3490 C    0  0

```

4.2170	6.4650	-0.3370	C	0	0
-1.0640	-1.4080	-3.1820	C	0	0
-1.4340	-1.9300	-4.1500	N	0	0
0.4860	0.7890	-3.0740	H	0	0
-3.0290	-2.8680	-1.9360	H	0	0
-1.7200	-3.9980	-1.6180	H	0	0
-4.3260	-3.6230	-0.0360	H	0	0
-3.6850	-5.1000	-0.7280	H	0	0
-4.9840	-0.6290	0.2830	H	0	0
-3.6120	-2.7180	3.5080	H	0	0
-4.5960	-3.4790	2.2610	H	0	0
0.5160	0.7910	2.4970	H	0	0
0.5160	2.2860	1.5660	H	0	0
1.9390	1.2480	1.5660	H	0	0
-0.7730	-1.0460	2.5030	H	0	0
-1.3690	-3.1830	3.7360	H	0	0
-2.1200	-4.6770	3.5870	H	0	0
-0.4750	-5.3310	1.7280	H	0	0
0.2660	-3.8290	1.8460	H	0	0
1.5400	-5.5140	3.1670	H	0	0
0.8920	-4.2850	4.2730	H	0	0
0.1170	-5.8620	4.1450	H	0	0
0.7140	2.8780	-2.8240	H	0	0
2.2420	1.9230	-2.9440	H	0	0
2.7770	4.6670	-4.3800	H	0	0
4.2680	7.0610	-4.4370	H	0	0
5.3950	7.0310	-3.0840	H	0	0
3.9050	7.9620	-2.9670	H	0	0
4.0700	6.1030	0.6800	H	0	0
3.7990	7.4700	-0.3970	H	0	0
5.2900	6.5390	-0.5130	H	0	0
1	2	2	0		
3	2	1	0		
14	3	2	0		
3	4	1	0		
4	13	2	0		
4	5	1	0		
6	5	1	0		
7	6	1	0		
12	7	1	0		
10	8	2	0		
10	9	1	0		
11	10	1	0		
12	11	1	0		
13	12	1	0		
16	14	1	0		
16	15	1	0		
17	16	2	0		
14	18	1	0		
13	18	1	0		
12	19	1	0		
19	20	1	0		
20	21	1	0		
2	31	1	0		
17	22	1	0		
22	23	1	0		
23	24	1	0		
27	28	2	0		
26	27	1	0		
25	26	1	0		
25	24	2	0		

```

28 24 1 0
27 29 1 0
26 30 1 0
1 17 1 0
31 32 3 0
1 33 1 0
5 34 1 0
5 35 1 0
6 36 1 0
6 37 1 0
9 38 1 0
11 39 1 0
11 40 1 0
15 41 1 0
15 42 1 0
15 43 1 0
18 44 1 0
19 45 1 0
19 46 1 0
20 47 1 0
20 48 1 0
21 49 1 0
21 50 1 0
21 51 1 0
23 52 1 0
23 53 1 0
28 54 1 0
29 55 1 0
29 56 1 0
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30 58 1 0
30 59 1 0
30 60 1 0

```

M END

> <Name>

Compound238

> <Activ>

0.03

> <DB_Ref_id>

27.12m

\$\$\$\$

Compound239

SciTegic10081411483D

```

56 59 0 0 1 0          999 V2000
  0.5350    0.8890   -2.1110 C    0  0
 -0.2840   -0.2670   -1.9920 C    0  0
 -0.6190   -0.7410   -0.6910 C    0  0
 -1.3830   -1.8110   -0.3460 C    0  0
 -2.1340   -2.8580   -1.1540 C    0  0
 -3.0860   -3.6860   -0.2410 C    0  0
 -2.4810   -4.0150    1.0180 O    0  0
 -3.4010    0.0500    2.3980 O    0  0
 -4.4350   -0.9800    0.6980 O    0  0
 -3.7550   -0.9630    1.8410 C    0  0
 -3.4430   -2.3160    2.4210 C    0  0
 -2.1440   -2.9060    1.8610 C    0  0  2  0  0  0
 -1.3970   -1.8550    1.0490 C    0  0

```

-0.1450	-0.0920	0.4310	C	0	0
1.1660	1.7330	1.5550	C	0	0
0.6750	1.0600	0.3400	C	0	0
1.0120	1.5500	-0.9480	C	0	0
-0.6230	-0.7790	1.5390	N	0	0
-1.2570	-3.4640	2.9780	C	0	0
0.0460	-4.0660	2.4510	C	0	0
0.9440	-4.5980	3.5690	C	0	0
1.7840	2.6400	-1.0780	O	0	0
2.0010	3.1520	-2.3850	C	0	0
2.8060	4.4300	-2.2990	C	0	0
3.2260	4.9520	-1.1110	N	0	0
3.8960	6.0570	-1.3570	O	0	0
3.9180	6.2590	-2.7010	C	0	0
3.2320	5.2430	-3.3460	C	0	0
4.6080	7.4440	-3.3410	C	0	0
-0.7480	-0.9230	-3.1920	C	0	0
-1.1170	-1.4450	-4.1600	N	0	0
0.8030	1.2750	-3.0840	H	0	0
-2.7120	-2.3830	-1.9460	H	0	0
-1.4030	-3.5130	-1.6280	H	0	0
-4.0090	-3.1380	-0.0460	H	0	0
-3.3680	-4.6150	-0.7380	H	0	0
-4.6670	-0.1440	0.2730	H	0	0
-3.2960	-2.2330	3.4980	H	0	0
-4.2790	-2.9940	2.2510	H	0	0
0.8330	1.2760	2.4870	H	0	0
0.8330	2.7710	1.5550	H	0	0
2.2560	1.7330	1.5550	H	0	0
-0.4560	-0.5610	2.4930	H	0	0
-1.0520	-2.6980	3.7260	H	0	0
-1.8030	-4.1920	3.5770	H	0	0
-0.1590	-4.8460	1.7180	H	0	0
0.5830	-3.3440	1.8360	H	0	0
1.8570	-5.0290	3.1570	H	0	0
1.2090	-3.8000	4.2630	H	0	0
0.4340	-5.3770	4.1350	H	0	0
1.0310	3.3630	-2.8340	H	0	0
2.5590	2.4080	-2.9540	H	0	0
3.0670	5.1120	-4.4070	H	0	0
5.0860	8.1210	-2.6330	H	0	0
3.8820	8.0210	-3.9150	H	0	0
5.3730	7.0900	-4.0320	H	0	0
1	2	2	0		
3	2	1	0		
14	3	2	0		
3	4	1	0		
4	13	2	0		
4	5	1	0		
6	5	1	0		
7	6	1	0		
12	7	1	0		
10	8	2	0		
10	9	1	0		
11	10	1	0		
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27.121

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Compound240
SciTegic10081411483D

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-2.2890 1.0390 -0.9980 C 0 0
-1.1070 0.8200 -1.7580 C 0 0
0.0490 0.3120 -1.1000 C 0 0
1.2730 0.0370 -1.6230 C 0 0
1.8590 0.1560 -3.0240 C 0 0

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3.4060	-0.0200	-2.9920	C	0	0				
3.8140	-1.0760	-2.1130	O	0	0				
2.0200	-3.0800	-1.4240	O	0	0				
2.9510	-4.4980	0.0410	O	0	0				
2.8180	-3.3130	-0.5470	C	0	0				
3.7480	-2.2400	-0.0430	C	0	0				
3.5060	-0.8890	-0.7250	C	0	0	3	0	0	0
2.0530	-0.4510	-0.5720	C	0	0				
0.0160	0.0310	0.2520	C	0	0				
-1.1560	-0.0630	2.4750	C	0	0				
-1.1500	0.2400	1.0310	C	0	0				
-2.3110	0.7500	0.3930	C	0	0				
1.2700	-0.4530	0.6030	N	0	0				
4.4470	0.1890	-0.1700	C	0	0				
3.7750	1.5570	-0.0490	C	0	0				
4.7700	2.6800	0.2380	C	0	0				
-3.4340	0.9670	1.0960	O	0	0				
-4.0430	-0.1450	1.7360	C	0	0				
-5.5140	0.0610	1.7850	C	0	0				
-7.6950	-0.7460	2.4360	N	0	0				
-6.3420	-0.9180	2.3810	C	0	0				
-8.2330	0.3910	1.9040	C	0	0				
-6.0530	1.1950	1.2540	N	0	0				
-7.4060	1.3670	1.3110	C	0	0				
-1.1230	1.1130	-3.1700	C	0	0				
-1.1410	1.3520	-4.3070	N	0	0				
-3.1800	1.4240	-1.4710	H	0	0				
1.6110	1.1230	-3.4590	H	0	0				
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3.7790	-0.2380	-3.9920	H	0	0				
3.8910	0.9020	-2.6740	H	0	0				
2.3830	-5.2290	-0.2360	H	0	0				
3.5800	-2.0740	1.0210	H	0	0				
4.7830	-2.5570	-0.1720	H	0	0				
-0.1660	-0.1110	2.9280	H	0	0				
-1.6470	-1.0220	2.6430	H	0	0				
-1.7270	0.6990	3.0040	H	0	0				
1.5660	-0.7440	1.5060	H	0	0				
4.8650	-0.1210	0.7890	H	0	0				
5.3540	0.2560	-0.7730	H	0	0				
3.1890	1.7770	-0.9430	H	0	0				
2.9880	1.5330	0.7070	H	0	0				
4.2560	3.6390	0.3140	H	0	0				
5.3070	2.4900	1.1680	H	0	0				
5.5040	2.7600	-0.5630	H	0	0				
-3.6500	-0.2110	2.7500	H	0	0				
-3.8200	-1.0390	1.1540	H	0	0				
-5.9060	-1.8130	2.7990	H	0	0				
-9.3010	0.5410	1.9390	H	0	0				
-7.8480	2.2600	0.8950	H	0	0				
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Compound240

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$$$$
Compound241
SciTegic10081411483D
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-0.1910				1.5450		1.5080	C	0	0		
0.7970				0.7660		0.8400	C	0	0		
2.0760				0.5160		1.2170	C	0	0		
2.9200				0.9590		2.4000	C	0	0		
4.4260				0.6860		2.1110	C	0	0		
4.6290				-0.6270		1.5660	O	0	0		
3.4280				1.5980		-1.3590	O	0	0		
5.4710				2.1680		-0.6350	O	0	0		
4.5250				1.2890		-0.9530	C	0	0		
4.9060				-0.1560		-0.7750	C	0	0		
4.0450				-0.8630		0.2770	C	0	0	3	0 0 0
2.6190				-0.3260		0.2440	C	0	0		
0.5040				0.1410		-0.3540	C	0	0		
-1.0390				-0.4040		-2.2580	C	0	0		
-0.7600				0.2700		-0.9790	C	0	0		
-1.7460				1.0680		-0.3440	C	0	0		
1.6370				-0.5660		-0.7380	N	0	0		
4.0430				-2.3790		0.0760	C	0	0		
3.3500				-3.1250		1.2190	C	0	0		
1.8280				-3.1410		1.0760	C	0	0		
-2.9510				1.2310		-0.9120	O	0	0		
-3.8930				2.0630		-0.2520	C	0	0		
-5.1820				2.1290		-1.0720	C	0	0		
-5.8340				0.7990		-1.1720	C	0	0		
-7.0060				-1.0720		-0.1580	C	0	0		
-6.3930				0.1900		-0.0350	C	0	0		
-7.0700				-1.7170		-1.3610	N	0	0		
-5.9060				0.1270		-2.4060	C	0	0		
-6.5310				-1.1330		-2.4710	C	0	0		
0.0590				2.1720		2.7830	C	0	0		
0.2540				2.6680		3.8150	N	0	0		
-2.2320				2.3010		1.3670	H	0	0		
2.7680				2.0220		2.5980	H	0	0		
2.5920				0.4020		3.2810	H	0	0		
4.8220				1.4200		1.4060	H	0	0		
5.0080				0.7790		3.0290	H	0	0		
6.3380				1.8480		-0.3550	H	0	0		
4.7500				-0.6990		-1.7070	H	0	0		
5.9650				-0.2300		-0.5210	H	0	0		
-0.2320				-1.0450		-2.6130	H	0	0		
-1.2360				0.3420		-3.0270	H	0	0		
-1.9340				-1.0190		-2.1540	H	0	0		
1.7380				-1.1310		-1.5490	H	0	0		
3.5960				-2.6410		-0.8810	H	0	0		
5.0590				-2.7500		-0.0660	H	0	0		
3.7380				-4.1410		1.3070	H	0	0		
3.6430				-2.7110		2.1840	H	0	0		
1.3890				-3.9100		1.7090	H	0	0		
1.4060				-2.1720		1.3480	H	0	0		
1.5390				-3.3520		0.0450	H	0	0		
-3.4550				3.0550							

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Compound242
SciTegic10081411483D

54	56	0	0	1	0	999	V2000				
-2.4590				1.1450		-1.0040	C	0	0		
-1.2790				0.9260		-1.7640	C	0	0		
-0.1230				0.4200		-1.1050	C	0	0		
1.1020				0.1430		-1.6290	C	0	0		
1.6900				0.2620		-3.0270	C	0	0		
3.2340				0.0880		-2.9980	C	0	0		
3.6430				-0.9690		-2.1190	O	0	0		
1.8400				-2.9710		-1.4220	O	0	0		
2.7810				-4.3910		0.0350	O	0	0		
2.6450				-3.2050		-0.5490	C	0	0		
3.5760				-2.1350		-0.0490	C	0	0		
3.3360				-0.7830		-0.7300	C	0	0	3	0 0 0
1.8810				-0.3460		-0.5780	C	0	0		
-0.1560				0.1390		0.2460	C	0	0		
-1.3280				0.0430		2.4690	C	0	0		
-1.3220				0.3480		1.0250	C	0	0		
-2.4820				0.8560		0.3870	C	0	0		
1.0980				-0.3460		0.6000	N	0	0		
4.2770				0.2950		-0.1760	C	0	0		
3.6040				1.6620		-0.0550	C	0	0		
4.5980				2.7870		0.2320	C	0	0		
-3.6050				1.0720		1.0900	O	0	0		
-4.2360				-0.0450		1.6970	C	0	0		
-5.7460				0.1890		1.7500	C	0	0		
-6.3460				-0.9320		2.3560	O	0	0		
-7.7480				-0.8240		2.4570	C	0	0		
-1.2930				1.2210		-3.1760	C	0	0		
-1.3110				1.4570		-4.3120	N	0	0		
-3.3500				1.5310		-1.4770	H	0	0		
1.4410				1.2290		-3.4650	H	0	0		
1.2380				-0.5040		-3.6600	H	0	0		
3.6090				-0.1330		-3.9960	H	0	0		
3.7210				1.0080		-2.6800	H	0	0		
2.2110				-5.1210		-0.2420	H	0	0		
3.4120				-1.9690		1.0160	H	0	0		
4.6110				-2.4530		-0.1820	H	0	0		
-0.3380				0.0160		2.9260	H	0	0		
-1.7970				-0.9260		2.6350	H	0	0		
-1.9160				0.7930		2.9960	H	0	0		
1.3970				-0.6390		1.5020	H	0	0		
4.6950				-0.0160		0.7830	H	0	0		
5.1820				0.3630		-0.7790	H	0	0		
3.0180				1.8830		-0.9470	H	0	0		
2.8180				1.6390		0.7030	H	0	0		
4.0840				3.7440		0.3110	H	0	0		
5.1370				2.5960		1.1600	H	0	0		

5.3320	2.8650	-0.5680 H	0	0
-3.8300	-0.1620	2.7010 H	0	0
-4.0040	-0.9320	1.1080 H	0	0
-6.1560	0.2910	0.7440 H	0	0
-5.9810	1.0680	2.3520 H	0	0
-8.2740	-1.6620	2.9180 H	0	0
-8.1520	-0.6890	1.4550 H	0	0
-7.9790	0.0720	3.0330 H	0	0
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Compound242

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0.04

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27.12f

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Compound243

SciTegic10081411483D

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-2.7680	1.0920	-0.7620	C	0	0						
-1.5880	0.8730	-1.5200	C	0	0						
-0.4300	0.3650	-0.8630	C	0	0						
0.7930	0.0900	-1.3870	C	0	0						
1.3810	0.2090	-2.7850	C	0	0						
2.9280	0.0330	-2.7560	C	0	0						
3.3360	-1.0220	-1.8750	O	0	0						
1.5330	-3.0240	-1.1780	O	0	0						
2.4880	-4.4510	0.2620	O	0	0						
2.3420	-3.2600	-0.3130	C	0	0						
3.2700	-2.1880	0.1930	C	0	0						
3.0270	-0.8360	-0.4860	C	0	0	3	0	0	0		
1.5740	-0.3990	-0.3340	C	0	0						
-0.4630	0.0840	0.4880	C	0	0						
-1.6350	-0.0100	2.7130	C	0	0						
-1.6290	0.2930	1.2700	C	0	0						
-2.7890	0.8030	0.6290	C	0	0						
0.7890	-0.4000	0.8420	N	0	0						
3.9690	0.2420	0.0680	C	0	0						
3.3160	1.6230	0.1270	C	0	0						
4.3340	2.7500	0.2890	C	0	0						
-3.9120	1.0190	1.3320	O	0	0						
-4.8260	-0.0570	1.4770	C	0	0						
-5.9630	0.3590	2.4120	C	0	0						
-5.3260	-0.4880	0.0980	C	0	0						
-1.6020	1.1660	-2.9320	C	0	0						
-1.6190	1.4040	-4.0680	N	0	0						
-3.6580	1.4780	-1.2320	H	0	0						
1.1330	1.1760	-3.2230	H	0	0						
0.9320	-0.5590	-3.4160	H	0	0						
3.3010	-0.1860	-3.7540	H	0	0						
3.4120	0.9550	-2.4360	H	0	0						
1.9240	-5.1840	-0.0200	H	0	0						
3.1000	-2.0240	1.2580	H	0	0						
4.3050	-2.5040	0.0660	H	0	0						
-0.6450	-0.0630	3.1640	H	0	0						
-2.1290	-0.9670	2.8790	H	0	0						
-2.2030	0.7540	3.2420	H	0	0						
1.0880	-0.6910	1.7440	H	0	0						
4.3500	-0.0470	1.0470	H	0	0						
4.8950	0.2770	-0.5080	H	0	0						
2.6890	1.7910	-0.7500	H	0	0						
2.5680	1.6620	0.9200	H	0	0						

3.8360	3.7190	0.3200	H	0	0
4.9140	2.6190	1.2010	H	0	0
5.0310	2.7640	-0.5510	H	0	0
-4.2230	-0.8440	1.9300	H	0	0
-5.5900	0.6780	3.3850	H	0	0
-6.6520	-0.4690	2.5720	H	0	0
-6.5290	1.1870	1.9840	H	0	0
-4.5180	-0.8690	-0.5270	H	0	0
-5.7850	0.3500	-0.4260	H	0	0
-6.0760	-1.2750	0.1880	H	0	0
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Compound243

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27.12

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Compound244

SciTegic10081411483D

53	55	0	0	1	0	999	V2000				
-2.6000				0.7050		-0.7110	C	0	0		
-1.4200				0.4860		-1.4690	C	0	0		
-0.2620				-0.0190		-0.8110	C	0	0		
0.9630				-0.2970		-1.3360	C	0	0		
1.5490				-0.1780		-2.7340	C	0	0		
3.0960				-0.3510		-2.7030	C	0	0		
3.5040				-1.4080		-1.8240	O	0	0		
1.6760				-3.4020		-1.1020	O	0	0		
2.6390				-4.8300		0.3320	O	0	0		
2.4940				-3.6410		-0.2440	C	0	0		
3.4380				-2.5740		0.2440	C	0	0		
3.1950				-1.2230		-0.4360	C	0	0	3	0 0 0
1.7420				-0.7850		-0.2830	C	0	0		
-0.2950				-0.3010		0.5390	C	0	0		
-1.4670				-0.3960		2.7640	C	0	0		
-1.4610				-0.0920		1.3200	C	0	0		
-2.6210				0.4160		0.6800	C	0	0		
0.9570				-0.7850		0.8930	N	0	0		
4.1370				-0.1440		0.1190	C	0	0		
3.4840				1.2360		0.1780	C	0	0		
4.5020				2.3630		0.3670	C	0	0		
-3.7440				0.6330		1.3830	O	0	0		
-4.8730				1.1490		0.6930	C	0	0		
-6.0390				1.3070		1.6700	C	0	0		
-7.2990				1.8600		1.0020	C	0	0		
-1.4340				0.7810		-2.8810	C	0	0		
-1.4510				1.0180		-4.0180	N	0	0		
-3.4900				1.0920		-1.1820	H	0	0		
1.3010				0.7890		-3.1720	H	0	0		
1.1000				-0.9430		-3.3650	H	0	0		
3.4690				-0.5720		-3.7030	H	0	0		
3.5800				0.5680		-2.3850	H	0	0		
2.0640				-5.5590		0.0630	H	0	0		
3.2850				-2.4040		1.3110	H	0	0		
4.4690				-2.8960		0.1040	H	0	0		
-2.4160				-0.1970		3.2600	H	0	0		
-0.6990				0.1950		3.2620	H	0	0		
-1.2270				-1.4490		2.9140	H	0	0		
1.2560				-1.0780		1.7950	H	0	0		
5.0630				-0.1090		-0.4570	H	0	0		
4.5180				-0.4330		1.0980	H	0	0		
2.7230				1.2700		0.9570	H	0	0		

2.8750	1.4120	-0.7090	H	0	0
4.0220	3.3400	0.4060	H	0	0
5.2190	2.3770	-0.4550	H	0	0
5.0590	2.2270	1.2930	H	0	0
-4.6000	2.1110	0.2620	H	0	0
-5.1330	0.4530	-0.1050	H	0	0
-6.2520	0.3630	2.1720	H	0	0
-5.7480	1.9280	2.5180	H	0	0
-8.1090	1.9490	1.7230	H	0	0
-7.1040	2.8400	0.5630	H	0	0
-7.6330	1.1970	0.2030	H	0	0
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3	4	1	0		
4	13	2	0		
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16	15	1	0		
17	16	2	0		
14	18	1	0		
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Compound244

> <Activ>

0.07

> <DB_Ref_id>

27.12d

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Compound245

SciTegic10081411483D

47	49	0	0	1	0	999	V2000				
-3.5470	1.0920	-0.6680	C	0	0						
-2.3650	0.8730	-1.4280	C	0	0						
-1.2090	0.3670	-0.7700	C	0	0						
0.0160	0.0900	-1.2930	C	0	0						
0.6010	0.2090	-2.6920	C	0	0						
2.1480	0.0350	-2.6620	C	0	0						
2.5570	-1.0210	-1.7810	O	0	0						
0.7810	-3.0330	-1.1130	O	0	0						
1.6910	-4.4430	0.3730	O	0	0						
1.5660	-3.2600	-0.2230	C	0	0						
2.4900	-2.1880	0.2870	C	0	0						
2.2480	-0.8360	-0.3930	C	0	0	3	0	0	0		
0.7950	-0.3980	-0.2400	C	0	0						
-1.2420	0.0860	0.5820	C	0	0						
-2.4140	-0.0100	2.8050	C	0	0						
-2.4080	0.2950	1.3630	C	0	0						
-3.5690	0.8030	0.7230	C	0	0						
0.0120	-0.3980	0.9350	N	0	0						
3.1890	0.2420	0.1620	C	0	0						
2.5290	1.6190	0.2440	C	0	0						
3.5310	2.7380	0.5250	C	0	0						
-4.6920	1.0200	1.4260	O	0	0						
-5.3540	-0.1040	1.9880	C	0	0						
-2.3810	1.1680	-2.8400	C	0	0						
-2.3990	1.4040	-3.9750	N	0	0						
-4.4380	1.4790	-1.1390	H	0	0						
0.3530	1.1760	-3.1290	H	0	0						
0.1520	-0.5570	-3.3220	H	0	0						
2.5210	-0.1840	-3.6600	H	0	0						
2.6330	0.9550	-2.3420	H	0	0						
1.1270	-5.1760	0.0920	H	0	0						
2.3160	-2.0230	1.3520	H	0	0						
3.5270	-2.5000	0.1640	H	0	0						
-1.4280	0.0020	3.2710	H	0	0						
-2.8460	-0.9960	2.9670	H	0	0						
-3.0370	0.7170	3.3280	H	0	0						
0.3080	-0.6910	1.8380	H	0	0						
3.5860	-0.0550	1.1330	H	0	0						
4.1070	0.2910	-0.4260	H	0	0						
1.9610	1.8280	-0.6620	H	0	0						
1.7320	1.6190	0.9880	H	0	0						

3.0250	3.7030	0.5740 H	0	0
4.0510	2.5630	1.4670 H	0	0
4.2790	2.7930	-0.2640 H	0	0
-6.4340	-0.0230	2.1130 H	0	0
-4.9180	-0.3010	2.9670 H	0	0
-5.1550	-0.9690	1.3550 H	0	0

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14	3	2	0
3	4	1	0
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Compound245

> <Activ>
0.36

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27.12b

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Compound246

SciTegic10081411483D

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-2.1860				0.1580		-0.9630	C	0	0		
-1.0020				-0.0570		-1.7210	C	0	0		
0.1560				-0.5530		-1.0630	C	0	0		
1.3830				-0.8220		-1.5860	C	0	0		
1.9650				-0.7070		-2.9860	C	0	0		
3.5140				-0.8710		-2.9510	C	0	0		
3.9320				-1.9220		-2.0670	O	0	0		
2.9650				1.0640		0.2730	O	0	0		
4.6680				1.5410		-1.1040	O	0	0		
3.9790				0.7380		-0.2990	C	0	0		
4.5530				-0.6450		-0.1310	C	0	0		
3.6250				-1.7320		-0.6820	C	0	0	3	0 0 0
2.1660				-1.3030		-0.5350	C	0	0		
0.1250				-0.8340		0.2910	C	0	0		
-1.0330				-0.9450		2.5140	C	0	0		
-1.0390				-0.6350		1.0740	C	0	0		
-2.2010				-0.1310		0.4320	C	0	0		
1.3830				-1.3090		0.6430	N	0	0		
3.8710				-3.0740		0.0080	C	0	0		
2.9710				-4.1880		-0.5310	C	0	0		
3.2050				-5.5270		0.1680	C	0	0		
-3.4430				0.1000		1.2070	C	0	0		
-3.9650				-0.6110		2.0330	O	0	0		
-4.0080				1.3010		0.8770	N	0	0		
-5.2520				1.7190		1.5370	C	0	0		
-5.7310				3.0680		1.0020	C	0	0		
-4.7790				4.1820		1.3930	C	0	0		
-3.8520				4.7250		0.5620	N	0	0		
-3.2190				5.6740		1.2870	C	0	0		
-3.7750				5.6970		2.5620	C	0	0		
-4.7480				4.7620		2.6230	N	0	0		
-1.0180				0.2360		-3.1310	C	0	0		
-1.0390				0.4710		-4.2680	N	0	0		
-3.0760				0.5410		-1.4380	H	0	0		
1.7110				0.2580		-3.4240	H	0	0		
1.5200				-1.4810		-3.6090	H	0	0		
3.8890				-1.0940		-3.9510	H	0	0		
3.9940				0.0590		-2.6370	H	0	0		
4.3520				2.4410		-1.2560	H	0	0		
5.4830				-0.7310		-0.6930	H	0	0		
4.7790				-0.8260		0.9200	H	0	0		
-0.0490				-1.1780		2.9180	H	0	0		
-1.6820				-1.8010		2.7050	H	0	0		
-1.4300				-0.0960		3.0680	H	0	0		
1.6820				-1.5980		1.5490	H	0	0		
4.9200				-3.3590		-0.0660	H	0	0		
3.7600				-2.9810		1.0880	H	0	0		
1.9220				-3.8990		-0.4710	H	0	0		
3.0900				-4.2910		-1.6110	H	0	0		
2.5450				-6.2930		-0.2380	H	0	0		
4.2380				-5.8480		0.0490	H	0	0		
3.0020				-5.4430		1.2360	H	0	0		

-3.5700	1.8850	0.1930 H	0	0
-5.0880	1.7680	2.6150 H	0	0
-6.0120	0.9530	1.3870 H	0	0
-6.7290	3.2990	1.3710 H	0	0
-5.8280	3.0390	-0.0820 H	0	0
-3.6720	4.4790	-0.3830 H	0	0
-2.4180	6.2910	0.9000 H	0	0
-3.5040	6.3360	3.3930 H	0	0
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> <Name>

Compound246

> <Activ>

0.86

> <DB_Ref_id>

27.09g

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Compound247

SciTegic10081411483D

62	65	0	0	1	0	999	V2000				
-0.5290	-1.6760	-0.4320	C	0	0						
0.8500	-1.8050	-0.1110	C	0	0						
1.5640	-0.6520	0.3260	C	0	0						
2.8710	-0.5510	0.6860	C	0	0						
4.0120	-1.5550	0.7640	C	0	0						
5.2270	-0.9490	1.5270	C	0	0						
5.4730	0.4200	1.1700	O	0	0						
2.3810	0.4430	3.5060	O	0	0						
4.2250	-0.2710	4.5590	O	0	0						
3.5680	0.5200	3.7150	C	0	0						
4.4140	1.5450	3.0100	C	0	0						
4.4280	1.3480	1.4880	C	0	0	3	0	0	0		
3.0860	0.7870	1.0220	C	0	0						
0.9280	0.5680	0.4220	C	0	0						
-1.0880	2.0530	0.2210	C	0	0						
-0.4450	0.7310	0.1060	C	0	0						
-1.1740	-0.4120	-0.3240	C	0	0						
1.8710	1.4920	0.8570	N	0	0						
4.7640	2.6490	0.7580	C	0	0						
4.8050	2.4770	-0.7620	C	0	0						
4.8590	3.8130	-1.5040	C	0	0						
-2.6110	-0.2970	-0.6640	C	0	0						
-3.1720	0.5570	-1.3110	O	0	0						
-3.3220	-1.3360	-0.1330	N	0	0						
-4.7740	-1.4060	-0.3550	C	0	0						
-5.0880	-1.8400	-1.7870	C	0	0						
-6.5510	-1.8930	-2.0350	C	0	0						
-8.5450	-0.9630	-3.0660	C	0	0						
-7.1600	-0.9080	-2.8380	C	0	0						
-9.2890	-2.0060	-2.4880	C	0	0						
-7.2830	-2.9020	-1.4770	N	0	0						
-8.6290	-2.9650	-1.6950	C	0	0						
1.4770	-3.0980	-0.2380	C	0	0						
1.9750	-4.1410	-0.3440	N	0	0						
-1.0960	-2.5350	-0.7600	H	0	0						
3.6860	-2.4650	1.2620	H	0	0						

4.3030	-1.8200	-0.2520	H	0	0
5.0700	-1.0040	2.6060	H	0	0
6.1290	-1.5270	1.3130	H	0	0
5.1620	-0.1070	4.7290	H	0	0
4.0060	2.5410	3.1780	H	0	0
5.4280	1.5290	3.4080	H	0	0
-0.5180	2.7790	0.7990	H	0	0
-2.0650	1.9420	0.6930	H	0	0
-1.2440	2.4690	-0.7750	H	0	0
1.7270	2.4610	1.0250	H	0	0
4.0660	3.4380	1.0370	H	0	0
5.7010	3.0650	1.1250	H	0	0
5.6370	1.8380	-1.0550	H	0	0
3.9590	1.8810	-1.1050	H	0	0
4.9200	3.6520	-2.5800	H	0	0
3.9790	4.4140	-1.2810	H	0	0
5.7380	4.3850	-1.2010	H	0	0
-2.8520	-2.0370	0.4020	H	0	0
-5.2170	-0.4340	-0.1410	H	0	0
-5.2130	-2.1000	0.3610	H	0	0
-4.6470	-2.8140	-2.0000	H	0	0
-4.6210	-1.1640	-2.5060	H	0	0
-9.0290	-0.2170	-3.6800	H	0	0
-6.5720	-0.1130	-3.2750	H	0	0
-10.3540	-2.0700	-2.6500	H	0	0
-9.1970	-3.7660	-1.2480	H	0	0
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3	2	1	0		
14	3	2	0		
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26	27	1	0		
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M END

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Compound247

> <Activ>

1.2

> <DB_Ref_id>

27.09f

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Compound248

SciTegic10081411483D

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-1.2640 1.2270 -0.3220 C 0 0
-0.0800 1.0080 -1.0760 C 0 0
1.0720 0.5020 -0.4160 C 0 0
2.2970 0.2250 -0.9390 C 0 0
2.8790 0.3420 -2.3380 C 0 0
4.4260 0.1740 -2.3090 C 0 0
4.8380 -0.8830 -1.4300 O 0 0
3.1520 -2.9710 -0.8420 O 0 0
3.6330 -4.1350 1.0120 O 0 0
3.7690 -3.0980 0.1890 C 0 0
4.7680 -2.0610 0.6290 C 0 0
4.5310 -0.7030 -0.0410 C 0 0 3 0 0 0
3.0780 -0.2620 0.1090 C 0 0
1.0370 0.2210 0.9360 C 0 0
-0.1270 0.1170 3.1580 C 0 0
-0.1290 0.4280 1.7170 C 0 0

```

-1.2850	0.9380	1.0720	C	0	0
2.2950	-0.2620	1.2890	N	0	0
5.4710	0.3670	0.5200	C	0	0
6.9410	0.0700	0.2320	C	0	0
7.5680	1.0740	-0.7360	C	0	0
-2.5290	1.1780	1.8460	C	0	0
-2.6560	1.6760	2.9410	O	0	0
-3.6250	0.7500	1.1520	N	0	0
-4.9590	0.8990	1.7480	C	0	0
-6.0100	0.3670	0.8650	C	0	0
-7.5880	0.6910	-1.0040	C	0	0
-6.5760	1.1840	-0.1390	C	0	0
-8.0350	-0.6270	-0.8570	C	0	0
-6.4590	-0.9590	1.0120	C	0	0
-7.4670	-1.4470	0.1520	C	0	0
-8.9790	-0.8690	-1.7680	O	0	0
-8.2540	1.2680	-2.0040	O	0	0
-9.1860	0.3160	-2.5660	C	0	0
-0.0940	1.3010	-2.4880	C	0	0
-0.1080	1.5350	-3.6230	N	0	0
-2.1520	1.6150	-0.7990	H	0	0
2.6250	1.3070	-2.7790	H	0	0
2.4340	-0.4320	-2.9610	H	0	0
4.7970	-0.0450	-3.3130	H	0	0
4.9120	1.1000	-1.9920	H	0	0
3.0080	-4.8360	0.7870	H	0	0
4.6720	-1.8870	1.7010	H	0	0
5.7790	-2.4140	0.4360	H	0	0
-0.0760	0.9940	3.8050	H	0	0
0.7260	-0.5180	3.3930	H	0	0
-1.0310	-0.4340	3.4140	H	0	0
2.5920	-0.5530	2.1910	H	0	0
5.1950	1.3540	0.1470	H	0	0
5.3070	0.5020	1.5900	H	0	0
7.5140	0.0220	1.1580	H	0	0
7.0640	-0.9470	-0.1370	H	0	0
8.6520	0.9690	-0.7540	H	0	0
7.1800	0.9300	-1.7460	H	0	0
7.3380	2.0960	-0.4360	H	0	0
-3.5100	0.3400	0.2480	H	0	0
-5.1490	1.9530	1.9450	H	0	0
-4.9860	0.3710	2.7010	H	0	0
-6.2380	2.2030	-0.2580	H	0	0
-6.0410	-1.6020	1.7720	H	0	0
-7.8150	-2.4630	0.2640	H	0	0
-8.9400	0.1190	-3.6020	H	0	0
-10.1990	0.6720	-2.4590	H	0	0
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Compound248

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0.54

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27.09

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Compound249

SciTegic10081411483D

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-1.7560				1.3550		-0.5230	C	0	0		
-0.5700				1.1370		-1.2790	C	0	0		
0.5820				0.6310		-0.6170	C	0	0		
1.8050				0.3530		-1.1430	C	0	0		
2.3870				0.4710		-2.5410	C	0	0		
3.9360				0.3030		-2.5120	C	0	0		
4.3480				-0.7540		-1.6330	O	0	0		
2.5140				-2.7640		-0.9140	O	0	0		
3.2230				-4.0530		0.7750	O	0	0		
3.2480				-2.9550		0.0250	C	0	0		
4.2750				-1.9320		0.4260	C	0	0		
4.0410				-0.5740		-0.2440	C	0	0	3	0 0 0
2.5880				-0.1330		-0.0920	C	0	0		
0.5470				0.3500		0.7320	C	0	0		
-0.6170				0.2460		2.9570	C	0	0		
-0.6190				0.5570		1.5140	C	0	0		
-1.7770				1.0660		0.8690	C	0	0		
1.8050				-0.1350		1.0860	N	0	0		
4.9810				0.4960		0.3160	C	0	0		
6.4510				0.2010		0.0270	C	0	0		
7.0390				1.1210		-1.0410	C	0	0		
-3.0200				1.3070		1.6430	C	0	0		
-3.1580				1.8980		2.6890	O	0	0		
-4.0980				0.7520		1.0160	N	0	0		
-5.4320				0.8770		1.6250	C	0	0		
-6.4670				0.1760		0.8220	C	0	0		
-8.0740				0.1720		-1.0080	C	0	0		
-7.0960				0.8360		-0.2480	C	0	0		
-8.4280				-1.1520		-0.6950	C	0	0		
-6.8200				-1.1490		1.1330	C	0	0		
-7.8010				-1.8130		0.3750	C	0	0		
-0.5860				1.4300		-2.6890	C	0	0		
-0.5980				1.6640		-3.8260	N	0	0		
-2.6430				1.7440		-1.0000	H	0	0		
2.1350				1.4360		-2.9820	H	0	0		
1.9430				-0.3030		-3.1640	H	0	0		
4.3070				0.0840		-3.5140	H	0	0		
4.4200				1.2280		-2.1950	H	0	0		
2.5840				-4.7500		0.5700	H	0	0		
4.2210				-1.7500		1.5000	H	0	0		
5.2750				-2.3030		0.2030	H	0	0		
-0.5760				1.1230		3.6040	H	0	0		
0.2420				-0.3810		3.1930	H	0	0		
-1.5180				-0.3130		3.2090	H	0	0		
2.1000				-0.4240		1.9900	H	0	0		
4.7050				1.4820		-0.0550	H	0	0		
4.8160				0.6310		1.3870	H	0	0		
7.0410				0.2480		0.9430	H	0	0		
6.5880				-0.8460		-0.2460	H	0	0		
8.1250				1.0310		-1.0740	H	0	0		
6.6330				0.8790		-2.0230	H	0	0		
6.7970				2.1620		-0.8300	H	0	0		
-3.9750				0.2640		0.1520	H	0	0		
-5.6880				1.9340		1.7070	H	0	0		

-5.4060	0.4610	2.6310 H	0	0
-8.5570	0.6800	-1.8300 H	0	0
-6.8280	1.8530	-0.4940 H	0	0
-9.1800	-1.6620	-1.2770 H	0	0
-6.3420	-1.6620	1.9550 H	0	0
-8.0700	-2.8300	0.6150 H	0	0
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Compound249

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0.98

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27.09d

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Compound250

SciTegic10081411483D

48	50	0	0	0	0	999	V2000
1.0180	-0.5760	1.8580	C	0	0		
0.1580	0.1720	-0.3010	C	0	0		
1.0740	-0.5900	0.4510	C	0	0		
-0.8130	0.9490	0.3600	C	0	0		
0.0450	0.2030	2.5160	C	0	0		
-0.8670	0.9610	1.7620	C	0	0		
0.2130	0.1580	-1.6700	N	0	0		
-1.1480	-0.0060	-2.5310	S	0	0		
-2.1880	-1.2210	-1.8770	C	0	0		
1.5060	0.2910	-2.3550	C	0	0		
2.4100	1.2440	-1.6420	C	0	0		
4.4940	1.6970	-0.4550	C	0	0		
3.6480	0.7950	-1.1250	C	0	0		
4.1170	3.0390	-0.2990	C	0	0		
2.0330	2.5960	-1.4820	C	0	0		
2.8890	3.4880	-0.8100	C	0	0		
4.1520	-0.8400	-1.2990	Cl	0	0		
0.5370	3.1880	-2.0900	Cl	0	0		
-2.4770	-3.3560	-0.7600	C	0	0		
-1.6350	-2.3710	-1.2890	C	0	0		
-3.8730	-3.1990	-0.8120	C	0	0		
-3.5840	-1.0490	-1.9390	C	0	0		
-4.4200	-2.0430	-1.4040	C	0	0		
-1.8480	1.2660	-2.4900	O	0	0		
-0.7680	-0.4060	-3.8750	O	0	0		
-0.0200	0.2250	3.8340	O	0	0		
-0.9790	1.0780	4.4400	C	0	0		
1.9940	-1.3890	2.6430	C	0	0		
1.8630	-1.3110	3.9650	O	0	0		
2.8340	-2.0610	2.0880	O	0	0		
-5.8460	-1.8590	-1.4730	C	0	0		
-6.9960	-1.7130	-1.5250	N	0	0		
1.8240	-1.1890	-0.0450	H	0	0		
-1.5240	1.5410	-0.2010	H	0	0		
-1.6130	1.5590	2.2640	H	0	0		
1.3380	0.6450	-3.3730	H	0	0		
1.9840	-0.6860	-2.4140	H	0	0		
5.4430	1.3690	-0.0530	H	0	0		

4.7720	3.7290	0.2170	H	0	0
2.6150	4.5250	-0.6820	H	0	0
-2.0550	-4.2340	-0.3100	H	0	0
-0.5650	-2.4880	-1.2500	H	0	0
-4.5160	-3.9630	-0.4020	H	0	0
-3.9860	-0.1500	-2.3980	H	0	0
-0.9320	0.9320	5.5200	H	0	0
-0.8090	2.0940	4.0820	H	0	0
-1.9690	0.7700	4.1040	H	0	0
2.4650	-1.8130	4.5290	H	0	0
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Compound250

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0.9

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28.01

\$\$\$\$
Compound251
SciTegic10081411483D

48	51	0	0	1	0	999	V2000				
-2.8460				0.2270		-1.6050	S	0	0		
-1.3930				-0.5250		-2.0840	C	0	0		
-0.7290				-1.1740		-1.0270	C	0	0		
-1.4880				-1.0000		0.1430	C	0	0		
-2.6760				-0.2620		0.0180	C	0	0		
-0.7400				-0.5990		-3.4100	C	0	0		
-0.0660				-1.7710		-3.8010	C	0	0		
0.5530				-1.8400		-5.0610	C	0	0		
0.5000				-0.7380		-5.9320	C	0	0		
-0.1720				0.4340		-5.5430	C	0	0		
-0.7930				0.5040		-4.2830	C	0	0		
-1.0450				-1.5720		1.4380	C	0	0		
-1.7640				-2.6390		2.0060	C	0	0		
-1.3340				-3.1740		3.2330	C	0	0		
-0.1990				-2.6310		3.8610	C	0	0		
0.4940				-1.5960		3.3050	N	0	0		
0.0900				-1.0660		2.1130	C	0	0		
2.9610				1.2150		0.9260	C	0	0		
2.2210				0.0390		1.5160	C	0	0		
0.1760				1.2790		0.9530	C	0	0		
0.8360				2.5940		1.4140	C	0	0		
0.8730				0.0670		1.5330	C	0	0		
2.3870				2.5610		1.4160	C	0	0	3	0 0 0
2.9450				2.9120		2.8010	C	0	0		
-3.6250				0.0530		1.0780	C	0	0		
-4.7110				0.7290		0.7090	O	0	0		
-3.4040				-0.2990		2.2130	O	0	0		
0.2070				-1.7170		-1.0920	H	0	0		
-0.0220				-2.6210		-3.1350	H	0	0		
1.0700				-2.7400		-5.3590	H	0	0		
0.9770				-0.7910		-6.8990	H	0	0		
-0.2130				1.2790		-6.2110	H	0	0		
-1.3070				1.4060		-3.9900	H	0	0		
-2.6350				-3.0450		1.5120	H	0	0		
-1.8710				-3.9920		3.6880	H	0	0		
0.1330				-3.0390		4.8030	H	0	0		
2.8830				1.1620		-0.1600	H	0	0		
4.0250				1.1390		1.1560	H	0	0		
2.7770				-0.7970		1.9140	H	0	0		
0.2170				1.2150		-0.1350	H	0	0		
-0.8830				1.2810		1.2230	H	0	0		
0.4800				3.4120		0.7890	H	0	0		
0.4730				2.8200		2.4180	H	0	0		
2.7420				3.3340		0.7320	H	0	0		
2.5820				3.8890		3.1270	H	0	0		
2.6520				2.1620		3.5350	H	0	0		
4.0330				2.9510		2.7790	H	0	0		

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29.13b

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Compound252

SciTegic10081411483D

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1.3650		0.1090		-3.4510	S	0	0				
-0.1210		0.8260		-3.0530	C	0	0				
-0.5100		0.5450		-1.7320	C	0	0				
0.4410		-0.2660		-1.0720	C	0	0				
1.5350		-0.5900		-1.9060	C	0	0				
2.6780		-1.4160		-1.5330	C	0	0				
2.6740		-2.0240		-0.4880	O	0	0				
3.6860		-1.4420		-2.4020	O	0	0				
0.2950		-0.7170		0.3200	N	0	0				
0.1950		0.2400		1.3730	N	0	0				
0.2580		-2.0510		0.6080	C	0	0				
0.3070		-2.8670		-0.2830	O	0	0				
0.1540		-2.4810		2.0510	C	0	0	2	0	0	0
0.5860		-3.9490		2.2310	C	0	0				
-0.4340		-4.9340		1.6310	C	0	0				
-1.8520		-4.7110		2.1840	C	0	0	2	0	0	0
-2.2850		-3.2460		1.9980	C	0	0				
-1.2680		-2.2620		2.6000	C	0	0				
-1.9470		-5.1370		3.6540	C	0	0				
-0.9550		1.6430		-3.8890	C	0	0				
-1.6450		2.3160		-4.5840	C	0	0				
-2.4980		3.1440		-5.4300	C	0	0				
-2.0100		4.5940		-5.3440	C	0	0				
-2.3950		2.6370		-6.8690	C	0	0				
-3.9410		3.0370		-4.9280	C	0	0				
-1.0230		1.0140		1.2090	C	0	0				
1.3610		1.1150		1.3480	C	0	0				
2.6190		0.3480		1.7810	C	0	0				
3.8400		1.2830		1.8730	C	0	0				
3.5780		2.4320		2.7520	N	0	0				
2.4040		3.2110		2.3320	C	0	0				
1.1410		2.3360		2.2540	C	0	0				
3.5180		2.0510		4.1600	C	0	0				
-1.4160		0.8980		-1.2620	H	0	0				
3.6560		-0.8670		-3.1780	H	0	0				
0.8400		-1.8540		2.6210	H	0	0				
0.6950		-4.1580		3.2950	H	0	0				
1.5680		-4.1150		1.7910	H	0	0				
-0.1110		-5.9590		1.8180	H	0	0				
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-2.5390		-5.3420		1.6190	H	0	0				
-2.3970		-3.0370		0.9340	H	0	0				
-3.2680		-3.0840		2.4420	H	0	0				
-1.5920		-1.2340		2.4220	H	0	0				
-1.2540		-2.3850		3.6840	H	0	0				
-2.9630		-5.0000		4.0270	H	0	0				
-1.6620		-6.1820		3.7740	H	0	0				
-1.2810		-4.5350		4.2740	H	0	0				
-2.0470		4.9770		-4.3240	H	0	0				
-2.6250		5.2440		-5.9670	H	0	0				
-0.9810		4.6760		-5.6910	H	0	0				
-2.7150		1.6000		-6.9570	H	0	0				
-1.3670		2.7010		-7.2290	H	0	0				
-3.0180		3.2360		-7.5330	H	0	0				
-4.3070		2.0100		-4.9570	H	0	0				

-4.6080	3.6450	-5.5410 H	0	0
-4.0200	3.3910	-3.9000 H	0	0
-1.8830	0.4320	0.8710 H	0	0
-0.8560	1.8090	0.4830 H	0	0
-1.2890	1.4800	2.1560 H	0	0
1.5020	1.4630	0.3240 H	0	0
2.4530	-0.1230	2.7500 H	0	0
2.8300	-0.4590	1.0780 H	0	0
4.7130	0.7360	2.2340 H	0	0
4.0980	1.6500	0.8790 H	0	0
2.6050	3.6520	1.3560 H	0	0
2.2500	4.0410	3.0220 H	0	0
0.3050	2.9320	1.8870 H	0	0
0.8650	2.0080	3.2600 H	0	0
3.3890	2.8890	4.8460 H	0	0
4.4360	1.5330	4.4360 H	0	0
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0.063

> <DB_Ref_id>

30.12

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Compound253

SciTegic10081411483D

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-2.3670 1.4940 0.3650 S 0 0
-1.5000 1.3070 -1.0820 C 0 0
-0.2440 0.7150 -0.8730 C 0 0
-0.0250 0.4240 0.4920 C 0 0
-1.1190 0.8070 1.2990 C 0 0
-1.2070 0.6540 2.7480 C 0 0
-2.2660 0.8160 3.3110 O 0 0
-0.0780 0.3340 3.3730 O 0 0
1.2070 -0.2010 1.0020 N 0 0
2.4440 0.5040 0.9380 N 0 0
1.1640 -1.4570 1.5370 C 0 0
1.7970 -1.7190 2.5310 O 0 0
0.3130 -2.5020 0.8610 C 0 0 2 0 0 0
-1.1210 -2.5020 1.4200 C 0 0
-1.9900 -3.5780 0.7540 C 0 0
-1.3590 -4.9770 0.8650 C 0 0 2 0 0 0

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0.0760	-4.9790	0.3140	C	0	0
0.9470	-3.9000	0.9790	C	0	0
-2.2230	-6.0310	0.1680	C	0	0
-1.9120	1.6740	-2.4060	C	0	0
-2.2540	1.9790	-3.5040	C	0	0
-2.6660	2.3500	-4.8520	C	0	0
-3.4940	1.2050	-5.4410	C	0	0
-3.5100	3.6230	-4.7700	C	0	0
-1.4140	2.5940	-5.6990	C	0	0
3.5410	-0.4240	1.1430	C	0	0
2.4610	1.5470	1.9570	C	0	0
1.7170	2.7970	1.4610	C	0	0
1.8260	3.9530	2.4730	C	0	0
3.2270	4.2500	2.7950	N	0	0
3.9490	3.0860	3.3220	C	0	0
3.9060	1.9040	2.3380	C	0	0
0.4770	0.4960	-1.6480	H	0	0
-0.0840	0.2230	4.3320	H	0	0
0.2620	-2.2460	-0.1970	H	0	0
-1.5800	-1.5230	1.2770	H	0	0
-1.0980	-2.6800	2.4960	H	0	0
-2.9820	-3.5800	1.2050	H	0	0
-2.1330	-3.3240	-0.2990	H	0	0
-1.3120	-5.2380	1.9220	H	0	0
0.0570	-4.8090	-0.7620	H	0	0
0.5310	-5.9590	0.4650	H	0	0
1.9400	-3.9020	0.5250	H	0	0
1.0880	-4.1540	2.0310	H	0	0
-1.7830	-7.0240	0.2790	H	0	0
-3.2300	-6.0390	0.5800	H	0	0
-2.3010	-5.8220	-0.8980	H	0	0
-2.9260	0.2770	-5.4960	H	0	0
-3.8280	1.4490	-6.4510	H	0	0
-4.3810	1.0180	-4.8360	H	0	0
-2.9530	4.4530	-4.3360	H	0	0
-4.3960	3.4590	-4.1540	H	0	0
-3.8460	3.9280	-5.7600	H	0	0
-0.7970	3.3950	-5.2910	H	0	0
-1.6870	2.8710	-6.7190	H	0	0
-0.8030	1.6930	-5.7520	H	0	0
4.5260	-0.0100	0.9220	H	0	0
3.3990	-1.2990	0.5080	H	0	0
3.5450	-0.7600	2.1800	H	0	0
1.9510	1.1660	2.8420	H	0	0
2.1310	3.1210	0.5060	H	0	0
0.6660	2.5660	1.2810	H	0	0
1.3520	4.8500	2.0720	H	0	0
1.2950	3.6990	3.3910	H	0	0
3.7030	4.5840	1.9430	H	0	0
3.5100	2.7950	4.2770	H	0	0
4.9830	3.3690	3.5250	H	0	0
4.4060	1.0410	2.7770	H	0	0
4.4710	2.1680	1.4410	H	0	0
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Compound253

> <Activ>

0.138

> <DB_Ref_id>

30.12d

\$\$\$\$

Compound254

SciTegic10081411483D

61	62	0	0	0	0	999	V2000				
-1.2990	2.8030	0.6620	S	0	0						
0.2190	2.0920	0.9220	C	0	0						
0.4900	1.0680	-0.0020	C	0	0						
-0.5740	0.8960	-0.9140	C	0	0						
-1.6410	1.7870	-0.6660	C	0	0						
-2.8890	1.8630	-1.4180	C	0	0						
-3.2460	0.9280	-2.0940	O	0	0						
-3.5720	2.9980	-1.3030	O	0	0						
-0.5640	-0.1060	-1.9940	N	0	0						
-0.6820	0.3120	-3.3540	N	0	0						
-0.4430	-1.4320	-1.6950	C	0	0						
-0.2580	-2.2420	-2.5740	O	0	0						
-0.5470	-1.8610	-0.2520	C	0	0	2	0	0	0		
-0.1170	-3.3280	-0.0720	C	0	0						
-1.1350	-4.3150	-0.6720	C	0	0						
-2.5530	-4.0920	-0.1170	C	0	0	2	0	0	0		
-2.9860	-2.6270	-0.3050	C	0	0						
-1.9690	-1.6410	0.2970	C	0	0						
-2.6500	-4.5160	1.3520	C	0	0						
1.1820	2.4220	1.9320	C	0	0						
1.9800	2.6970	2.7700	C	0	0						
2.9650	3.0290	3.7930	C	0	0						
3.8260	4.1890	3.2870	C	0	0						
2.2210	3.4390	5.0670	C	0	0						
3.8340	1.7950	4.0590	C	0	0						
0.6130	0.2070	-4.0040	C	0	0						
-1.6620	-0.5200	-4.0310	C	0	0						
1.5640	1.2850	-3.4840	C	0	0						
2.7730	1.1910	-4.2030	O	0	0						
1.3970	0.4780	-0.0290	H	0	0						
-3.2210	3.7090	-0.7500	H	0	0						
0.1370	-1.2340	0.3180	H	0	0						
-0.0080	-3.5390	0.9920	H	0	0						
0.8670	-3.4960	-0.5120	H	0	0						
-0.8140	-5.3400	-0.4840	H	0	0						
-1.1500	-4.1970	-1.7560	H	0	0						
-3.2400	-4.7230	-0.6820	H	0	0						
-3.1000	-2.4180	-1.3690	H	0	0						
-3.9690	-2.4650	0.1390	H	0	0						
-2.2930	-0.6150	0.1190	H	0	0						
-1.9550	-1.7660	1.3810	H	0	0						
-3.6640	-4.3770	1.7270	H	0	0						
-2.3670	-5.5630	1.4690	H	0	0						
-1.9800	-3.9180	1.9710	H	0	0						

4.3540	3.9340	2.3670	H	0	0
4.5700	4.4710	4.0310	H	0	0
3.2090	5.0660	3.0840	H	0	0
1.5800	2.6410	5.4400	H	0	0
1.5940	4.3110	4.8810	H	0	0
2.9260	3.6990	5.8580	H	0	0
3.2420	0.9470	4.4040	H	0	0
4.5860	2.0100	4.8180	H	0	0
4.3560	1.4900	3.1500	H	0	0
0.4860	0.2930	-5.0840	H	0	0
1.0270	-0.7870	-3.8320	H	0	0
-2.4860	-0.8460	-3.3980	H	0	0
-1.1720	-1.4080	-4.4280	H	0	0
-2.0840	0.0310	-4.8710	H	0	0
1.7830	1.1290	-2.4280	H	0	0
1.1470	2.2790	-3.6500	H	0	0
3.3630	1.8830	-3.8610	H	0	0
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0.052

> <DB_Ref_id>

30.12a

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Compound255

SciTegic10081411483D

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  0.0720   1.3500  -2.3130 S   0  0
  1.2210   0.4670  -1.4280 C   0  0
  1.1460   0.7300  -0.0490 C   0  0
  0.1290   1.6680   0.2460 C   0  0
 -0.5490   2.1020  -0.9140 C   0  0
 -1.6410   3.0680  -0.9570 C   0  0
 -2.0590   3.5550   0.0680 O   0  0
 -2.1170   3.3590  -2.1640 O   0  0
 -0.1760   2.1310   1.6090 N   0  0
  0.6860   3.0680   2.2520 N   0  0
 -1.2830   1.6640   2.2580 C   0  0
 -1.5700   2.0840   3.3540 O   0  0
 -2.1350   0.6190   1.5780 C   0  0  2  0  0  0
 -3.5680   0.6190   2.1390 C   0  0
 -4.4380  -0.4570   1.4730 C   0  0
 -3.8070  -1.8560   1.5840 C   0  0  2  0  0  0
 -2.3690  -1.8580   1.0350 C   0  0
 -1.5000  -0.7770   1.6970 C   0  0
 -4.6700  -2.9080   0.8810 C   0  0
  2.1890  -0.4650  -1.9300 C   0  0
  2.9940  -1.2340  -2.3480 C   0  0
  3.9820  -2.1820  -2.8520 C   0  0
  3.3220  -3.5590  -2.9750 C   0  0
  4.4590  -1.7010  -4.2230 C   0  0
  5.1540  -2.2380  -1.8670 C   0  0
  1.9920   2.4670   2.4510 C   0  0
  0.7930   4.2660   1.4380 C   0  0
  1.7750   0.2810   0.7050 H   0  0

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-2.8400	3.9940	-2.2460	H	0	0
-2.1860	0.8770	0.5200	H	0	0
-4.0250	1.6000	1.9960	H	0	0
-3.5450	0.4430	3.2150	H	0	0
-5.4300	-0.4610	1.9280	H	0	0
-4.5820	-0.2010	0.4220	H	0	0
-3.7640	-2.1210	2.6430	H	0	0
-2.3890	-1.6920	-0.0430	H	0	0
-1.9160	-2.8380	1.1880	H	0	0
-0.5080	-0.7790	1.2420	H	0	0
-1.3570	-1.0310	2.7500	H	0	0
-4.2290	-3.9010	0.9920	H	0	0
-5.6760	-2.9200	1.3010	H	0	0
-4.7540	-2.6990	-0.1860	H	0	0
2.9490	-3.9180	-2.0140	H	0	0
4.0330	-4.2930	-3.3520	H	0	0
2.4800	-3.5220	-3.6660	H	0	0
4.9140	-0.7110	-4.1700	H	0	0
3.6270	-1.6490	-4.9240	H	0	0
5.2010	-2.3870	-4.6350	H	0	0
5.6310	-1.2660	-1.7460	H	0	0
5.9140	-2.9400	-2.2150	H	0	0
4.8180	-2.5700	-0.8850	H	0	0
1.9730	1.5060	2.9630	H	0	0
2.6190	3.1430	3.0350	H	0	0
2.4750	2.3180	1.4840	H	0	0
-0.1600	4.7500	1.2250	H	0	0
1.2600	4.0160	0.4840	H	0	0
1.4320	4.9900	1.9410	H	0	0
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17 36 1 0
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18 38 1 0
18 39 1 0
19 40 1 0
19 41 1 0
19 42 1 0
23 43 1 0
23 44 1 0
23 45 1 0
24 46 1 0
24 47 1 0
24 48 1 0
25 49 1 0
25 50 1 0
25 51 1 0
26 52 1 0
26 53 1 0
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27 55 1 0
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27 57 1 0

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M END

> <Name>

Compound255

> <Activ>

0.088

> <DB_Ref_id>

30.06a

\$\$\$\$

Compound256

SciTegic10081411483D

```

58 59 0 0 0 0          999 V2000
  -0.4450   1.0180  -2.5100 S   0  0
    0.4530   1.5510  -1.1740 C   0  0
  -0.2170   1.3240   0.0410 C   0  0
  -1.4710   0.7070  -0.1640 C   0  0
  -1.7350   0.4810  -1.5330 C   0  0
  -2.9420  -0.1310  -2.0820 C   0  0
  -3.8360  -0.4750  -1.3460 O   0  0
  -2.9750  -0.2710  -3.4040 O   0  0
  -2.3890   0.3500   0.9300 N   0  0
  -3.1580   1.3890   1.6290 C   0  0
  -2.5310  -0.9570   1.3030 C   0  0
  -3.3260  -1.2620   2.1600 O   0  0
  -1.6820  -2.0000   0.6230 C   0  0  2  0  0  0
  -2.3150  -3.3980   0.7400 C   0  0
  -1.4450  -4.4770   0.0780 C   0  0
  -0.0080  -4.4750   0.6270 C   0  0  2  0  0  0
    0.6230  -3.0760   0.5160 C   0  0
  -0.2460  -2.0000   1.1820 C   0  0
    0.8550  -5.5290  -0.0740 C   0  0
    1.7480   2.1660  -1.1760 C   0  0

```

2.8220	2.6800	-1.1800	C	0	0
4.1390	3.3070	-1.1760	C	0	0
5.2050	2.2070	-1.1910	C	0	0
4.2640	4.1840	-2.4240	C	0	0
4.2730	4.1600	0.0900	C	0	0
-2.5880	1.6470	3.0250	C	0	0
-3.2540	2.6600	0.7870	C	0	0
0.1660	1.5800	1.0200	H	0	0
-3.7520	-0.6700	-3.8180	H	0	0
-4.1290	0.8970	1.6930	H	0	0
-1.6290	-1.7420	-0.4360	H	0	0
-3.3070	-3.4000	0.2850	H	0	0
-2.4590	-3.6520	1.7910	H	0	0
-1.4260	-4.3110	-1.0000	H	0	0
-1.8990	-5.4570	0.2300	H	0	0
-0.0510	-4.7400	1.6860	H	0	0
1.6150	-3.0800	0.9710	H	0	0
0.7670	-2.8220	-0.5350	H	0	0
0.2110	-1.0210	1.0390	H	0	0
-0.2700	-2.1760	2.2580	H	0	0
1.8650	-5.5610	0.3360	H	0	0
0.9340	-5.3240	-1.1410	H	0	0
0.4180	-6.5220	0.0430	H	0	0
5.1250	1.5510	-0.3240	H	0	0
6.2050	2.6410	-1.1910	H	0	0
5.1070	1.5900	-2.0860	H	0	0
3.5020	4.9630	-2.4510	H	0	0
4.1580	3.5820	-3.3260	H	0	0
5.2380	4.6680	-2.4570	H	0	0
3.5120	4.9400	0.1390	H	0	0
5.2480	4.6450	0.1270	H	0	0
4.1740	3.5430	0.9840	H	0	0
-2.5510	0.7360	3.6230	H	0	0
-3.1970	2.3730	3.5610	H	0	0
-1.5760	2.0430	2.9590	H	0	0
-3.6370	2.4360	-0.2090	H	0	0
-3.9080	3.3910	1.2640	H	0	0
-2.2740	3.1210	0.6700	H	0	0
5	1	1	0		
4	5	2	0		
3	4	1	0		
1	2	1	0		
2	3	2	0		
5	6	1	0		
6	7	2	0		
6	8	1	0		
4	9	1	0		
9	10	1	0		
9	11	1	0		
11	12	2	0		
13	11	1	0		
17	18	1	0		
16	17	1	0		
15	16	1	0		
14	15	1	0		
18	13	1	0		
13	14	1	0		
16	19	1	0		
2	20	1	0		
20	21	3	0		
21	22	1	0		

```

22 23 1 0
22 24 1 0
22 25 1 0
10 26 1 0
10 27 1 0
3 28 1 0
8 29 1 0
10 30 1 0
13 31 1 0
14 32 1 0
14 33 1 0
15 34 1 0
15 35 1 0
16 36 1 0
17 37 1 0
17 38 1 0
18 39 1 0
18 40 1 0
19 41 1 0
19 42 1 0
19 43 1 0
23 44 1 0
23 45 1 0
23 46 1 0
24 47 1 0
24 48 1 0
24 49 1 0
25 50 1 0
25 51 1 0
25 52 1 0
26 53 1 0
26 54 1 0
26 55 1 0
27 56 1 0
27 57 1 0
27 58 1 0
M END
> <Name>
Compound256

> <Activ>
0.086

> <DB_Ref_id>
30.03

$$$$
Compound257
SciTegic10081411483D

46 48 0 0 0 0 999 V2000
2.5740 -0.7360 1.8180 S 0 0
1.1740 -1.2440 1.0120 C 0 0
0.6050 -0.2340 0.2230 C 0 0
1.3550 0.9610 0.3070 C 0 0
2.4750 0.8300 1.1560 C 0 0
0.9940 2.1910 -0.4160 N 0 0
-0.3010 2.2110 -1.3870 S 0 0
-0.5960 3.7810 -2.0430 C 0 0
-0.0350 1.3010 -2.4860 O 0 0
-1.4510 1.8260 -0.5900 O 0 0

```

-1.3980	6.0670	-1.7890	C	0	0
-1.1640	4.7910	-1.2420	C	0	0
-1.0660	6.3300	-3.1290	C	0	0
-0.2640	4.0470	-3.3830	C	0	0
-0.5000	5.3220	-3.9260	C	0	0
0.4800	-2.5530	1.0120	C	0	0
-1.5840	-3.8480	1.0120	C	0	0
-0.9260	-2.6050	1.0120	C	0	0
-0.8360	-5.0370	1.0120	C	0	0
1.2270	-3.7460	1.0120	C	0	0
0.5680	-4.9880	1.0120	C	0	0
3.4410	1.8790	1.4490	C	0	0
4.4510	1.5390	2.2460	O	0	0
3.3010	2.9830	0.9760	O	0	0
-1.5160	4.5180	0.1760	C	0	0
-1.6450	-6.5610	1.0120	S	0	0
-0.7580	-7.6970	2.0700	C	0	0
-1.6370	-7.0820	-0.3440	O	0	0
-2.9810	-6.3690	1.5430	O	0	0
-0.2910	-0.3400	-0.3770	H	0	0
1.5510	3.0160	-0.3050	H	0	0
-1.8340	6.8480	-1.1820	H	0	0
-1.2480	7.3110	-3.5470	H	0	0
0.1720	3.2720	-3.9960	H	0	0
-0.2440	5.5260	-4.9550	H	0	0
-2.6640	-3.8850	1.0120	H	0	0
-1.5060	-1.6930	1.0120	H	0	0
2.3070	-3.7130	1.0120	H	0	0
1.1430	-5.9020	1.0120	H	0	0
5.1210	2.1990	2.4690	H	0	0
-1.6480	5.4630	0.7050	H	0	0
-2.4020	3.8870	0.2150	H	0	0
-0.7010	3.9790	0.6560	H	0	0
0.2480	-7.9400	1.7280	H	0	0
-1.3160	-8.6310	2.1500	H	0	0
-0.6760	-7.2720	3.0700	H	0	0
5	1	1	0		
4	5	2	0		
3	4	1	0		
1	2	1	0		
2	3	2	0		
4	6	1	0		
6	7	1	0		
7	8	1	0		
7	9	2	0		
7	10	2	0		
15	13	2	0		
14	15	1	0		
11	12	2	0		
13	11	1	0		
12	8	1	0		
8	14	2	0		
21	19	2	0		
20	21	1	0		
17	18	2	0		
16	20	2	0		
19	17	1	0		
18	16	1	0		
16	2	1	0		
5	22	1	0		
22	23	1	0		

```

22 24 2 0
12 25 1 0
19 26 1 0
26 27 1 0
26 28 2 0
26 29 2 0
3 30 1 0
6 31 1 0
11 32 1 0
13 33 1 0
14 34 1 0
15 35 1 0
17 36 1 0
18 37 1 0
20 38 1 0
21 39 1 0
23 40 1 0
25 41 1 0
25 42 1 0
25 43 1 0
27 44 1 0
27 45 1 0
27 46 1 0

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M END

> <Name>

Compound257

> <Activ>

1.8

> <DB_Ref_id>

31.12

\$\$\$\$

Compound258

SciTegic10081411483D

```

48 50 0 0 0 0          999 V2000
  3.2150   -1.6310   -0.2200 S   0  0
  2.5960   -0.0530   -0.2200 C   0  0
  1.1950   -0.0200   -0.2200 C   0  0
  0.6540   -1.3240   -0.2200 C   0  0
  1.6560   -2.3190   -0.2200 C   0  0
 -0.7930   -1.6000   -0.2200 N   0  0
 -1.8500   -0.3710   -0.1830 S   0  0
 -3.4840   -0.9260   -0.1110 C   0  0
 -1.5780    0.4040    1.0140 O   0  0
 -1.6800    0.3890   -1.4100 O   0  0
 -5.2400   -2.1970    0.9950 C   0  0
 -3.9080   -1.7520    0.9480 C   0  0
 -6.1490   -1.8190   -0.0110 C   0  0
 -4.3890   -0.5470   -1.1170 C   0  0
 -5.7210   -0.9940   -1.0680 C   0  0
  3.2910    1.2560   -0.2200 C   0  0
  3.2030    3.6890   -0.2200 C   0  0
  2.5450    2.4470   -0.2200 C   0  0
  4.6070    3.7420   -0.2200 C   0  0
  4.6950    1.3080   -0.2200 C   0  0
  5.3540    2.5510   -0.2200 C   0  0
  1.4220   -3.7580   -0.2200 C   0  0
  2.5060   -4.5260   -0.2530 O   0  0

```

0.2930	-4.1880	-0.1890	O	0	0
-2.9550	-2.1560	2.0140	C	0	0
5.3070	5.0620	-0.2200	C	0	0
6.8130	5.0660	-0.2160	C	0	0
4.6820	6.0960	-0.2220	O	0	0
-7.5570	-2.2890	0.0420	C	0	0
0.5920	0.8810	-0.2200	H	0	0
-1.1230	-2.5430	-0.2420	H	0	0
-5.5680	-2.8300	1.8070	H	0	0
-4.0630	0.0860	-1.9290	H	0	0
-6.4120	-0.6990	-1.8430	H	0	0
2.6210	4.6020	-0.2200	H	0	0
1.4650	2.4140	-0.2200	H	0	0
5.2750	0.3960	-0.2200	H	0	0
6.4340	2.5800	-0.2200	H	0	0
2.4060	-5.4870	-0.2550	H	0	0
-2.3150	-1.3500	2.3740	H	0	0
-2.3110	-2.9530	1.6430	H	0	0
-3.5080	-2.5450	2.8680	H	0	0
7.1760	6.0940	-0.2140	H	0	0
7.1840	4.5080	0.6430	H	0	0
7.1900	4.5800	-1.1170	H	0	0
-8.1780	-1.9420	-0.7850	H	0	0
-8.0180	-1.9530	0.9690	H	0	0
-7.5760	-3.3790	0.0340	H	0	0
5	1	1	0		
4	5	2	0		
3	4	1	0		
1	2	1	0		
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7	9	2	0		
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19	17	1	0		
18	16	1	0		
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22	23	1	0		
22	24	2	0		
12	25	1	0		
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26	27	1	0		
26	28	2	0		
13	29	1	0		
3	30	1	0		
6	31	1	0		
11	32	1	0		
14	33	1	0		
15	34	1	0		

```

17 35 1 0
18 36 1 0
20 37 1 0
21 38 1 0
23 39 1 0
25 40 1 0
25 41 1 0
25 42 1 0
27 43 1 0
27 44 1 0
27 45 1 0
29 46 1 0
29 47 1 0
29 48 1 0

```

M END

> <Name>

Compound258

> <Activ>

0.39

> <DB_Ref_id>

31.11

\$\$\$\$

Compound259

SciTegic10081411483D

```

45 47 0 0 0 0          999 V2000
-0.1640 2.1190 -2.6820 S 0 0
 0.4470 0.9180 -1.6580 C 0 0
 0.3500 1.2580 -0.3010 C 0 0
-0.2420 2.5290 -0.1370 C 0 0
-0.5800 3.1270 -1.3730 C 0 0
-0.4750 3.1480 1.1800 N 0 0
-0.1910 2.3050 2.5310 S 0 0
-1.0120 0.7850 2.5310 C 0 0
 1.2380 2.0530 2.5980 O 0 0
-0.6850 3.0920 3.6490 O 0 0
-3.0740 -0.5060 2.5310 C 0 0
-2.4180 0.7380 2.5310 C 0 0
-2.3280 -1.6970 2.5310 C 0 0
-0.2660 -0.4040 2.5310 C 0 0
-0.9240 -1.6470 2.5310 C 0 0
 1.0530 -0.3980 -1.9670 C 0 0
 1.3500 -2.2790 -3.4860 C 0 0
 0.7750 -1.0290 -3.1930 C 0 0
 2.2050 -2.8990 -2.5570 C 0 0
 1.9080 -1.0180 -1.0370 C 0 0
 2.4830 -2.2660 -1.3300 C 0 0
-1.2030 4.4340 -1.5390 C 0 0
-1.8200 4.9260 -0.4690 O 0 0
-1.1390 5.0040 -2.6010 O 0 0
-3.2150 1.9920 2.5310 C 0 0
 2.8150 -4.2250 -2.8690 C 0 0
 3.6490 -4.8890 -1.8050 C 0 0
 2.6450 -4.7480 -3.9430 O 0 0
 0.6780 0.6390 0.5240 H 0 0
-0.8070 4.0900 1.2360 H 0 0
-4.1540 -0.5530 2.5310 H 0 0
-2.8340 -2.6520 2.5310 H 0 0

```

0.8150	-0.3670	2.5310	H	0	0
-0.3500	-2.5630	2.5310	H	0	0
1.1310	-2.7580	-4.4300	H	0	0
0.1210	-0.5610	-3.9120	H	0	0
2.1250	-0.5370	-0.0940	H	0	0
3.1370	-2.7340	-0.6090	H	0	0
-2.2500	5.7890	-0.5270	H	0	0
-2.8340	2.7660	3.2010	H	0	0
-4.2400	1.7710	2.8280	H	0	0
-3.2400	2.4060	1.5240	H	0	0
3.9650	-5.8750	-2.1460	H	0	0
4.5000	-4.2580	-1.5530	H	0	0
3.0550	-5.0260	-0.9000	H	0	0
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23	39	1	0		
25	40	1	0		
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25	42	1	0		
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27	45	1	0		

M END

> <Name>
Compound259

> <Activ>
1.4

> <DB_Ref_id>
31.1

\$\$\$\$
Compound260
SciTegic10081411483D

43	45	0	0	0	0	999	V2000
-1.4920		1.5200		2.9510	S	0	0
-1.0610		0.0410		2.2440	C	0	0
0.1580		0.1030		1.5550	C	0	0
0.7190		1.3980		1.6290	C	0	0
-0.0880		2.2890		2.3710	C	0	0
1.9980		1.7620		0.9960	N	0	0
2.7660		0.6950		0.0470	S	0	0
1.7810		0.1800		-1.2750	C	0	0
3.9430		1.3530		-0.4880	O	0	0
3.0780		-0.4670		0.8610	O	0	0
0.5720		0.6720		-3.3300	C	0	0
1.3730		1.1020		-2.2580	C	0	0
0.1800		-0.6760		-3.4220	C	0	0
1.3890		-1.1660		-1.3650	C	0	0
0.5880		-1.5960		-2.4370	C	0	0
-1.7540		-1.2680		2.2440	C	0	0
-3.8160		-2.5630		2.2440	C	0	0
-3.1600		-1.3200		2.2440	C	0	0
-3.0700		-3.7540		2.2440	C	0	0
-1.0080		-2.4610		2.2440	C	0	0
-1.6660		-3.7030		2.2440	C	0	0
0.2150		3.6910		2.6270	C	0	0
1.1470		4.2380		1.8500	O	0	0
-0.3650		4.2850		3.5040	O	0	0
-0.6680		-1.1310		-4.5550	C	0	0
1.7850		2.5270		-2.1680	C	0	0
0.6230		-0.7230		1.0310	H	0	0
2.3950		2.6660		1.1520	H	0	0
0.2580		1.3770		-4.0860	H	0	0
1.7030		-1.8730		-0.6110	H	0	0
0.2890		-2.6310		-2.5020	H	0	0
-4.8970		-2.6020		2.2440	H	0	0
-3.7380		-0.4080		2.2440	H	0	0
-3.5760		-4.7070		2.2440	H	0	0
0.0720		-2.4280		2.2440	H	0	0
-1.0920		-4.6170		2.2440	H	0	0
1.3830		5.1660		1.9810	H	0	0
-0.8030		-2.2110		-4.4980	H	0	0
-1.6130		-0.5860		-4.5430	H	0	0
-0.1660		-0.9060		-5.4960	H	0	0
2.8180		2.6780		-1.8570	H	0	0
1.1450		3.0470		-1.4550	H	0	0
1.6560		3.0060		-3.1390	H	0	0
5	1	1	0				
4	5	2	0				
3	4	1	0				
1	2	1	0				

```

2  3  2  0
4  6  1  0
6  7  1  0
7  8  1  0
7  9  2  0
7 10  2  0
15 13  2  0
14 15  1  0
11 12  2  0
13 11  1  0
12  8  1  0
 8 14  2  0
21 19  2  0
20 21  1  0
17 18  2  0
16 20  2  0
19 17  1  0
18 16  1  0
16  2  1  0
 5 22  1  0
22 23  1  0
22 24  2  0
13 25  1  0
12 26  1  0
 3 27  1  0
 6 28  1  0
11 29  1  0
14 30  1  0
15 31  1  0
17 32  1  0
18 33  1  0
19 34  1  0
20 35  1  0
21 36  1  0
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26 42  1  0
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M  END
> <Name>
Compound260

> <Activ>
1

> <DB_Ref_id>
31.09

$$$$
Compound261
  SciTegic10081411483D

40 42  0  0  0  0          999 V2000
   -2.5980    2.1800   -1.2420 S    0  0
   -2.1540    0.6930   -0.5590 C    0  0
   -0.9220    0.7500    0.1090 C    0  0
   -0.3630    2.0450    0.0370 C    0  0
   -1.1840    2.9430   -0.6820 C    0  0

```

0.9280	2.4020	0.6480	N	0	0
1.7260	1.3160	1.5470	S	0	0
2.4490	0.0820	0.5780	C	0	0
2.7830	2.0220	2.2500	O	0	0
0.7640	0.6930	2.4380	O	0	0
3.6700	-2.0180	0.3870	C	0	0
3.0860	-1.0160	1.1860	C	0	0
3.6170	-1.9200	-1.0160	C	0	0
2.3940	0.1800	-0.8220	C	0	0
2.9780	-0.8200	-1.6190	C	0	0
-2.8480	-0.6150	-0.5590	C	0	0
-4.9100	-1.9080	-0.5590	C	0	0
-4.2540	-0.6660	-0.5590	C	0	0
-4.1640	-3.1000	-0.5590	C	0	0
-2.1020	-1.8070	-0.5590	C	0	0
-2.7600	-3.0490	-0.5590	C	0	0
-0.8850	4.3480	-0.9300	C	0	0
-1.8010	5.0270	-1.6150	O	0	0
0.1420	4.8320	-0.5180	O	0	0
4.3260	-3.1430	-1.9880	Cl	0	0
3.1480	-1.1250	2.6680	C	0	0
-0.4470	-0.0820	0.6150	H	0	0
1.3100	3.3150	0.5100	H	0	0
4.1580	-2.8590	0.8570	H	0	0
1.9040	1.0220	-1.2870	H	0	0
2.9320	-0.7320	-2.6950	H	0	0
-5.9900	-1.9470	-0.5590	H	0	0
-4.8320	0.2440	-0.5590	H	0	0
-4.6700	-4.0550	-0.5590	H	0	0
-1.0220	-1.7750	-0.5590	H	0	0
-2.1860	-3.9630	-0.5590	H	0	0
-1.6510	5.9610	-1.8070	H	0	0
3.6870	-2.0310	2.9430	H	0	0
3.6020	-0.2230	3.0800	H	0	0
2.1370	-1.2030	3.0680	H	0	0
5	1	1	0		
4	5	2	0		
3	4	1	0		
1	2	1	0		
2	3	2	0		
4	6	1	0		
6	7	1	0		
7	8	1	0		
7	9	2	0		
7	10	2	0		
15	13	2	0		
14	15	1	0		
11	12	2	0		
13	11	1	0		
12	8	1	0		
8	14	2	0		
21	19	2	0		
20	21	1	0		
17	18	2	0		
16	20	2	0		
19	17	1	0		
18	16	1	0		
16	2	1	0		
5	22	1	0		
22	23	1	0		
22	24	2	0		

```

13 25 1 0
12 26 1 0
3 27 1 0
6 28 1 0
11 29 1 0
14 30 1 0
15 31 1 0
17 32 1 0
18 33 1 0
19 34 1 0
20 35 1 0
21 36 1 0
23 37 1 0
26 38 1 0
26 39 1 0
26 40 1 0

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M END

> <Name>

Compound261

> <Activ>

0.75

> <DB_Ref_id>

31.08

\$\$\$\$

Compound262

SciTegic10081411483D

```

40 42 0 0 0 0          999 V2000
-1.2950 1.4300 -3.0760 S 0 0
-1.0060 0.0270 -2.1720 C 0 0
0.0740 0.1640 -1.2890 C 0 0
0.6500 1.4510 -1.3830 C 0 0
-0.0060 2.2620 -2.3340 C 0 0
1.8030 1.8810 -0.5740 N 0 0
2.7150 0.7790 0.1850 S 0 0
2.1040 0.4020 1.7540 C 0 0
2.6950 -0.4320 -0.6150 O 0 0
4.0450 1.3440 0.3380 O 0 0
2.4730 -0.3710 4.0310 C 0 0
2.9750 -0.0650 2.7560 C 0 0
1.1040 -0.2130 4.3090 C 0 0
0.7320 0.5610 2.0270 C 0 0
0.2320 0.2540 3.3070 C 0 0
-1.6990 -1.2810 -2.1720 C 0 0
-3.7620 -2.5760 -2.1720 C 0 0
-3.1040 -1.3340 -2.1720 C 0 0
-3.0160 -3.7680 -2.1720 C 0 0
-0.9530 -2.4750 -2.1720 C 0 0
-1.6110 -3.7150 -2.1720 C 0 0
0.3480 3.6370 -2.6620 C 0 0
1.5740 4.0210 -2.3200 O 0 0
-0.4550 4.3540 -3.2130 O 0 0
-1.2150 0.4220 3.6000 C 0 0
0.4340 -0.6070 -0.6170 H 0 0
2.0220 2.8540 -0.4920 H 0 0
3.1410 -0.7290 4.8010 H 0 0
4.0250 -0.1860 2.5450 H 0 0
0.7250 -0.4490 5.2910 H 0 0

```

0.0700	0.9200	1.2540	H	0	0
-4.8420	-2.6150	-2.1720	H	0	0
-3.6840	-0.4220	-2.1720	H	0	0
-3.5220	-4.7210	-2.1720	H	0	0
0.1270	-2.4410	-2.1720	H	0	0
-1.0370	-4.6310	-2.1720	H	0	0
1.8570	4.9240	-2.5160	H	0	0
-1.4220	0.0800	4.6130	H	0	0
-1.5000	1.4610	3.4350	H	0	0
-1.7970	-0.1950	2.9140	H	0	0

5	1	1	0
4	5	2	0
3	4	1	0
1	2	1	0
2	3	2	0
4	6	1	0
6	7	1	0
7	8	1	0
7	9	2	0
7	10	2	0
15	13	2	0
14	15	1	0
11	12	2	0
13	11	1	0
12	8	1	0
8	14	2	0
21	19	2	0
20	21	1	0
17	18	2	0
16	20	2	0
19	17	1	0
18	16	1	0
16	2	1	0
5	22	1	0
22	23	1	0
22	24	2	0
15	25	1	0
3	26	1	0
6	27	1	0
11	28	1	0
12	29	1	0
13	30	1	0
14	31	1	0
17	32	1	0
18	33	1	0
19	34	1	0
20	35	1	0
21	36	1	0
23	37	1	0
25	38	1	0
25	39	1	0
25	40	1	0


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M  END
> <Name>
Compound262

> <Activ>
7.4

> <DB_Ref_id>
31.05

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\$\$\$\$

Compound263

SciTegic10081411483D

43	45	0	0	0	0	999	V2000
-1.1700		1.5290		3.0510	S	0	0
-0.8540		0.1130		2.1780	C	0	0
0.2520		0.2340		1.3260	C	0	0
0.8240		1.5240		1.4160	C	0	0
0.1410		2.3500		2.3340	C	0	0
2.0020		1.9410		0.6350	N	0	0
2.6890		0.9080		-0.4080	S	0	0
1.5960		0.4160		-1.6510	C	0	0
3.8070		1.5980		-1.0300	O	0	0
3.0880		-0.2690		0.3420	O	0	0
0.0450		0.9610		-3.4440	C	0	0
0.9320		1.3750		-2.4360	C	0	0
-0.1840		-0.4100		-3.6700	C	0	0
1.3710		-0.9510		-1.8710	C	0	0
0.4820		-1.3710		-2.8770	C	0	0
1.1640		2.8260		-2.2050	C	0	0
0.2670		-2.8300		-3.0840	C	0	0
-1.2740		-0.8810		-4.9140	C1	0	0
-1.5470		-1.1950		2.1780	C	0	0
-3.6110		-2.4900		2.1780	C	0	0
-2.9530		-1.2480		2.1780	C	0	0
-2.8630		-3.6820		2.1780	C	0	0
-0.8010		-2.3890		2.1780	C	0	0
-1.4590		-3.6310		2.1780	C	0	0
0.4840		3.7290		2.6500	C	0	0
-0.2600		4.3180		3.5820	O	0	0
1.4000		4.2720		2.0780	O	0	0
0.6310		-0.5470		0.6780	H	0	0
2.3750		2.8610		0.7480	H	0	0
-0.4610		1.7050		-4.0450	H	0	0
1.8870		-1.6820		-1.2620	H	0	0
2.2110		3.0960		-2.0670	H	0	0
0.6170		3.1450		-1.3170	H	0	0
0.7830		3.3950		-3.0530	H	0	0
0.9160		-3.3930		-2.4100	H	0	0
-0.7890		-3.0640		-2.9460	H	0	0
0.5350		-3.0960		-4.1060	H	0	0
-4.6900		-2.5290		2.1780	H	0	0
-3.5330		-0.3360		2.1780	H	0	0
-3.3690		-4.6370		2.1780	H	0	0
0.2790		-2.3550		2.1780	H	0	0
-0.8870		-4.5450		2.1780	H	0	0
-0.0720		5.2350		3.8280	H	0	0
5	1	1	0				
4	5	2	0				
3	4	1	0				
1	2	1	0				
2	3	2	0				
4	6	1	0				
6	7	1	0				
7	8	1	0				
7	9	2	0				
7	10	2	0				
15	13	2	0				
14	15	1	0				

```

11 12 2 0
13 11 1 0
12 8 1 0
8 14 2 0
12 16 1 0
15 17 1 0
13 18 1 0
24 22 2 0
23 24 1 0
20 21 2 0
19 23 2 0
22 20 1 0
21 19 1 0
19 2 1 0
5 25 1 0
25 26 1 0
25 27 2 0
3 28 1 0
6 29 1 0
11 30 1 0
14 31 1 0
16 32 1 0
16 33 1 0
16 34 1 0
17 35 1 0
17 36 1 0
17 37 1 0
20 38 1 0
21 39 1 0
22 40 1 0
23 41 1 0
24 42 1 0
26 43 1 0

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M END

> <Name>

Compound263

> <Activ>

5.4

> <DB_Ref_id>

31.02

\$\$\$\$

Compound264

SciTegic10081411483D

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44 46 0 0 0 0          999 V2000
-1.1470 1.4320 2.9570 S 0 0
-0.8300 0.0140 2.0840 C 0 0
0.2770 0.1370 1.2320 C 0 0
0.8500 1.4260 1.3220 C 0 0
0.1640 2.2520 2.2400 C 0 0
2.0250 1.8420 0.5410 N 0 0
2.7110 0.8130 -0.5040 S 0 0
1.6130 0.3240 -1.7460 C 0 0
3.8280 1.5020 -1.1270 O 0 0
3.1090 -0.3670 0.2420 O 0 0
0.0590 0.8770 -3.5350 C 0 0
0.9490 1.2870 -2.5270 C 0 0
-0.1720 -0.4940 -3.7660 C 0 0

```

1.3870	-1.0430	-1.9690	C	0	0
0.4940	-1.4570	-2.9750	C	0	0
1.1840	2.7360	-2.2950	C	0	0
0.2750	-2.9160	-3.1840	C	0	0
-1.2660	-0.9610	-5.0080	C1	0	0
-1.5240	-1.2950	2.0840	C	0	0
-3.5880	-2.5880	2.0840	C	0	0
-2.9300	-1.3460	2.0840	C	0	0
-2.8400	-3.7790	2.0840	C	0	0
-0.7770	-2.4860	2.0840	C	0	0
-1.4360	-3.7290	2.0840	C	0	0
0.5080	3.6310	2.5570	C	0	0
-0.1950	4.2970	3.5190	N	0	0
1.4100	4.1820	1.9690	O	0	0
0.6560	-0.6450	0.5840	H	0	0
2.4020	2.7620	0.6580	H	0	0
-0.4450	1.6210	-4.1330	H	0	0
1.9000	-1.7750	-1.3630	H	0	0
2.2300	3.0040	-2.1560	H	0	0
0.6390	3.0550	-1.4040	H	0	0
0.8030	3.3070	-3.1410	H	0	0
0.9240	-3.4810	-2.5140	H	0	0
-0.7790	-3.1480	-3.0430	H	0	0
0.5410	-3.1800	-4.2070	H	0	0
-4.6660	-2.6270	2.0840	H	0	0
-3.5080	-0.4360	2.0840	H	0	0
-3.3460	-4.7340	2.0840	H	0	0
0.3030	-2.4550	2.0840	H	0	0
-0.8630	-4.6430	2.0840	H	0	0
0.0140	5.2440	3.7640	H	0	0
-0.9420	3.8420	4.0060	H	0	0
5	1	1	0		
4	5	2	0		
3	4	1	0		
1	2	1	0		
2	3	2	0		
4	6	1	0		
6	7	1	0		
7	8	1	0		
7	9	2	0		
7	10	2	0		
15	13	2	0		
14	15	1	0		
11	12	2	0		
13	11	1	0		
12	8	1	0		
8	14	2	0		
12	16	1	0		
15	17	1	0		
13	18	1	0		
24	22	2	0		
23	24	1	0		
20	21	2	0		
19	23	2	0		
22	20	1	0		
21	19	1	0		
19	2	1	0		
5	25	1	0		
25	26	1	0		
25	27	2	0		
3	28	1	0		


```

6 29 1 0
11 30 1 0
14 31 1 0
16 32 1 0
16 33 1 0
16 34 1 0
17 35 1 0
17 36 1 0
17 37 1 0
20 38 1 0
21 39 1 0
22 40 1 0
23 41 1 0
24 42 1 0
26 43 1 0
26 44 1 0

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M END

> <Name>

Compound264

> <Activ>

14

> <DB_Ref_id>

31.01

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Compound265

SciTegic10081411483D

```

45 47 0 0 0 0          999 V2000
-2.0020    0.9120   -1.7440 S    0  0
-1.4980   -0.6060   -1.1850 C    0  0
-0.2070   -0.5800   -0.6390 C    0  0
 0.3460    0.7190   -0.6970 C    0  0
-0.5370    1.6480   -1.2850 C    0  0
 1.6910    1.0470   -0.1970 N    0  0
-2.1920   -1.9140   -1.1850 C    0  0
-4.2540   -3.2090   -1.1850 C    0  0
-3.5980   -1.9670   -1.1850 C    0  0
-3.5080   -4.3990   -1.1850 C    0  0
-1.4450   -3.1060   -1.1850 C    0  0
-2.1040   -4.3480   -1.1850 C    0  0
-0.2620    3.0660   -1.4880 C    0  0
-0.9770    3.6700   -2.4330 O    0  0
 0.5740    3.6230   -0.8160 O    0  0
 1.9900    0.8690    1.1250 C    0  0
 0.8870    0.5210    2.0720 C    0  0
-1.3110    1.0490    2.9920 C    0  0
-0.2560    1.3420    2.1130 C    0  0
-1.2290   -0.0720    3.8380 C    0  0
 0.9690   -0.6060    2.9200 C    0  0
-0.0900   -0.8970    3.8010 C    0  0
 2.7230    1.5660   -1.1070 C    0  0
-2.5160   -0.4300    4.9140 Cl   0  0
 3.3200    2.8670   -0.5720 C    0  0
 3.7830    0.5040   -1.3960 C    0  0
 2.3420   -1.6430    2.9050 Cl   0  0
 3.1290    0.9900    1.5140 O    0  0
 0.3120   -1.4360   -0.2240 H    0  0
-5.3340   -3.2480   -1.1850 H    0  0

```

-4.1760	-1.0550	-1.1850	H	0	0
-4.0140	-5.3540	-1.1850	H	0	0
-0.3650	-3.0740	-1.1850	H	0	0
-1.5290	-5.2640	-1.1850	H	0	0
-0.8320	4.6090	-2.6070	H	0	0
-2.1800	1.6890	3.0080	H	0	0
-0.3300	2.2070	1.4670	H	0	0
-0.0310	-1.7580	4.4530	H	0	0
2.1170	1.7560	-1.9920	H	0	0
2.5920	3.4450	-0.0040	H	0	0
3.6780	3.4920	-1.3900	H	0	0
4.1660	2.6600	0.0840	H	0	0
3.3220	-0.4100	-1.7710	H	0	0
4.5020	0.8670	-2.1310	H	0	0
4.3340	0.2520	-0.4880	H	0	0
5	1	1	0		
4	5	2	0		
3	4	1	0		
1	2	1	0		
2	3	2	0		
4	6	1	0		
12	10	2	0		
11	12	1	0		
8	9	2	0		
7	11	2	0		
10	8	1	0		
9	7	1	0		
7	2	1	0		
5	13	1	0		
13	14	1	0		
13	15	2	0		
6	16	1	0		
16	17	1	0		
22	20	2	0		
21	22	1	0		
18	19	2	0		
20	18	1	0		
19	17	1	0		
17	21	2	0		
6	23	1	0		
20	24	1	0		
23	25	1	0		
23	26	1	0		
21	27	1	0		
16	28	2	0		
3	29	1	0		
8	30	1	0		
9	31	1	0		
10	32	1	0		
11	33	1	0		
12	34	1	0		
14	35	1	0		
18	36	1	0		
19	37	1	0		
22	38	1	0		
23	39	1	0		
25	40	1	0		
25	41	1	0		
25	42	1	0		
26	43	1	0		
26	44	1	0		

26 45 1 0

M END

> <Name>

Compound265

> <Activ>

1.2

> <DB_Ref_id>

32.15

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Compound266

SciTegic10081411483D

48	50	0	0	0	0	999	V2000
-1.9980	1.2910	-1.8890	S	0	0		
-1.4760	-0.2360	-1.3710	C	0	0		
-0.1680	-0.2210	-0.8670	C	0	0		
0.3830	1.0800	-0.9200	C	0	0		
-0.5190	2.0220	-1.4650	C	0	0		
1.7440	1.4000	-0.4570	N	0	0		
-2.1700	-1.5450	-1.3710	C	0	0		
-4.2320	-2.8380	-1.3710	C	0	0		
-3.5740	-1.5960	-1.3710	C	0	0		
-3.4860	-4.0290	-1.3710	C	0	0		
-1.4240	-2.7360	-1.3710	C	0	0		
-2.0820	-3.9790	-1.3710	C	0	0		
-0.2500	3.4400	-1.6530	C	0	0		
-1.0270	4.0720	-2.5280	O	0	0		
0.6390	3.9770	-1.0310	O	0	0		
2.1560	0.9940	0.7810	C	0	0		
1.2030	0.2340	1.6420	C	0	0		
-0.8980	0.1130	2.8690	C	0	0		
0.0000	0.8300	2.0580	C	0	0		
-0.5940	-1.2010	3.2660	C	0	0		
1.5080	-1.0820	2.0390	C	0	0		
0.6120	-1.7970	2.8490	C	0	0		
2.6680	2.1540	-1.3150	C	0	0		
-1.5430	-1.9590	4.1230	C	0	0		
3.2890	3.3260	-0.5550	C	0	0		
3.7170	1.2310	-1.9360	C	0	0		
3.2740	1.2500	1.1660	O	0	0		
0.3630	-1.0820	-0.4830	H	0	0		
-5.3120	-2.8770	-1.3710	H	0	0		
-4.1540	-0.6860	-1.3710	H	0	0		
-3.9920	-4.9840	-1.3710	H	0	0		
-0.3440	-2.7050	-1.3710	H	0	0		
-1.5080	-4.8950	-1.3710	H	0	0		
-0.8890	5.0140	-2.6880	H	0	0		
-1.8220	0.5760	3.1850	H	0	0		
-0.2440	1.8380	1.7580	H	0	0		
2.4300	-1.5470	1.7240	H	0	0		
0.8520	-2.8070	3.1520	H	0	0		
1.9730	2.5140	-2.0740	H	0	0		
-1.2130	-2.9670	4.3750	H	0	0		
-2.5040	-2.0390	3.6170	H	0	0		
-1.6990	-1.4180	5.0570	H	0	0		
2.6960	3.6060	0.3160	H	0	0		
3.3730	4.2010	-1.1970	H	0	0		
4.2910	3.0700	-0.2050	H	0	0		

3.2400	0.4080	-2.4690	H	0	0
4.3540	1.7810	-2.6270	H	0	0
4.3560	0.8010	-1.1640	H	0	0

5	1	1	0
4	5	2	0
3	4	1	0
1	2	1	0
2	3	2	0
4	6	1	0
12	10	2	0
11	12	1	0
8	9	2	0
7	11	2	0
10	8	1	0
9	7	1	0
7	2	1	0
5	13	1	0
13	14	1	0
13	15	2	0
6	16	1	0
16	17	1	0
22	20	2	0
21	22	1	0
18	19	2	0
20	18	1	0
19	17	1	0
17	21	2	0
6	23	1	0
20	24	1	0
23	25	1	0
23	26	1	0
16	27	2	0
3	28	1	0
8	29	1	0
9	30	1	0
10	31	1	0
11	32	1	0
12	33	1	0
14	34	1	0
18	35	1	0
19	36	1	0
21	37	1	0
22	38	1	0
23	39	1	0
24	40	1	0
24	41	1	0
24	42	1	0
25	43	1	0
25	44	1	0
25	45	1	0
26	46	1	0
26	47	1	0
26	48	1	0

M END

> <Name>

Compound266

> <Activ>

3

> <DB_Ref_id>

32.14

\$\$\$\$

Compound267

SciTegic10081411483D

45	47	0	0	0	0	999	V2000
-1.5570		1.2760		-2.1780	S	0	0
-1.0740		-0.2300		-1.5660	C	0	0
0.1910		-0.1930		-0.9670	C	0	0
0.7480		1.1060		-1.0310	C	0	0
-0.1110		2.0220		-1.6760	C	0	0
2.0720		1.4440		-0.4820	N	0	0
-1.7700		-1.5390		-1.5660	C	0	0
-3.8320		-2.8340		-1.5660	C	0	0
-3.1740		-1.5920		-1.5660	C	0	0
-3.0860		-4.0230		-1.5660	C	0	0
-1.0210		-2.7300		-1.5660	C	0	0
-1.6820		-3.9730		-1.5660	C	0	0
0.1740		3.4340		-1.8980	C	0	0
-0.6600		4.0780		-2.7090	O	0	0
1.1230		3.9530		-1.3590	O	0	0
2.3380		1.2330		0.8400	C	0	0
1.2480		0.7090		1.7170	C	0	0
-0.9800		0.9340		2.6780	C	0	0
0.0450		1.4280		1.8520	C	0	0
-0.8070		-0.2770		3.3690	C	0	0
1.4200		-0.5040		2.4100	C	0	0
0.3950		-0.9960		3.2350	C	0	0
3.1170		2.0120		-1.3480	C	0	0
-1.8930		-0.7990		4.2420	C	0	0
4.2870		1.0410		-1.4980	C	0	0
3.4360		1.4670		1.2870	O	0	0
0.6930		-1.0390		-0.5120	H	0	0
-4.9120		-2.8730		-1.5660	H	0	0
-3.7540		-0.6800		-1.5660	H	0	0
-3.5920		-4.9780		-1.5660	H	0	0
0.0570		-2.6990		-1.5660	H	0	0
-1.1070		-4.8890		-1.5660	H	0	0
-0.5160		5.0160		-2.8890	H	0	0
-1.9020		1.4920		2.7760	H	0	0
-0.0980		2.3600		1.3240	H	0	0
2.3400		-1.0620		2.3130	H	0	0
0.5330		-1.9280		3.7640	H	0	0
2.6860		2.2520		-2.3180	H	0	0
3.4530		2.9590		-0.9280	H	0	0
-1.6580		-1.7420		4.7330	H	0	0
-2.7950		-0.9450		3.6490	H	0	0
-2.1170		-0.0660		5.0180	H	0	0
5.1040		1.5040		-2.0550	H	0	0
4.6580		0.7270		-0.5230	H	0	0
3.9810		0.1470		-2.0410	H	0	0
5	1	1	0				
4	5	2	0				
3	4	1	0				
1	2	1	0				
2	3	2	0				
4	6	1	0				
12	10	2	0				
11	12	1	0				
8	9	2	0				

```

7 11 2 0
10 8 1 0
9 7 1 0
7 2 1 0
5 13 1 0
13 14 1 0
13 15 2 0
6 16 1 0
16 17 1 0
22 20 2 0
21 22 1 0
18 19 2 0
20 18 1 0
19 17 1 0
17 21 2 0
6 23 1 0
20 24 1 0
23 25 1 0
16 26 2 0
3 27 1 0
8 28 1 0
9 29 1 0
10 30 1 0
11 31 1 0
12 32 1 0
14 33 1 0
18 34 1 0
19 35 1 0
21 36 1 0
22 37 1 0
23 38 1 0
23 39 1 0
24 40 1 0
24 41 1 0
24 42 1 0
25 43 1 0
25 44 1 0
25 45 1 0

```

M END

> <Name>

Compound267

> <Activ>

2

> <DB_Ref_id>

32.13

\$\$\$\$

Compound268

SciTegic10081411483D

```

45 47 0 0 0 0          999 V2000
-1.4100    1.1540   -2.4340 S   0  0
-0.9120   -0.3610   -1.8600 C   0  0
 0.3730   -0.3340   -1.3010 C   0  0
 0.9260    0.9650   -1.3600 C   0  0
 0.0490    1.8930   -1.9630 C   0  0
 2.2680    1.2970   -0.8480 N   0  0
-1.6060   -1.6700   -1.8600 C   0  0
-3.6680   -2.9650   -1.8600 C   0  0

```

-3.0120	-1.7210	-1.8600	C	0	0
-2.9220	-4.1540	-1.8600	C	0	0
-0.8590	-2.8610	-1.8600	C	0	0
-1.5180	-4.1030	-1.8600	C	0	0
0.3280	3.3090	-2.1720	C	0	0
-0.6060	3.9980	-2.8240	O	0	0
1.3550	3.7910	-1.7600	O	0	0
2.5000	1.3010	0.4980	C	0	0
1.3590	1.0410	1.4280	C	0	0
-0.8320	1.6760	2.2890	C	0	0
0.2500	1.9060	1.4220	C	0	0
-0.8090	0.5780	3.1660	C	0	0
1.3830	-0.0600	2.3060	C	0	0
0.2990	-0.2890	3.1740	C	0	0
3.3610	1.6230	-1.7720	C	0	0
-1.9510	0.3340	4.0820	C	0	0
2.5450	-0.9900	2.3320	C	0	0
3.6110	1.5140	0.9240	O	0	0
0.8890	-1.1850	-0.8750	H	0	0
-4.7480	-3.0040	-1.8600	H	0	0
-3.5900	-0.8100	-1.8600	H	0	0
-3.4280	-5.1090	-1.8600	H	0	0
0.2210	-2.8300	-1.8600	H	0	0
-0.9430	-5.0200	-1.8600	H	0	0
-0.4690	4.9400	-2.9870	H	0	0
-1.6800	2.3480	2.2770	H	0	0
0.2230	2.7540	0.7500	H	0	0
0.3160	-1.1330	3.8490	H	0	0
4.0210	0.7600	-1.8670	H	0	0
2.9430	1.9570	-2.7210	H	0	0
3.9470	2.4430	-1.3580	H	0	0
-2.7580	1.0630	3.9960	H	0	0
-1.6000	0.3460	5.1130	H	0	0
-2.3710	-0.6520	3.8850	H	0	0
3.2890	-0.8010	1.5580	H	0	0
2.1930	-2.0160	2.2110	H	0	0
3.0430	-0.9220	3.2990	H	0	0
5	1	1	0		
4	5	2	0		
3	4	1	0		
1	2	1	0		
2	3	2	0		
4	6	1	0		
12	10	2	0		
11	12	1	0		
8	9	2	0		
7	11	2	0		
10	8	1	0		
9	7	1	0		
7	2	1	0		
5	13	1	0		
13	14	1	0		
13	15	2	0		
6	16	1	0		
16	17	1	0		
22	20	2	0		
21	22	1	0		
18	19	2	0		
20	18	1	0		
19	17	1	0		
17	21	2	0		

```

6 23 1 0
20 24 1 0
21 25 1 0
16 26 2 0
3 27 1 0
8 28 1 0
9 29 1 0
10 30 1 0
11 31 1 0
12 32 1 0
14 33 1 0
18 34 1 0
19 35 1 0
22 36 1 0
23 37 1 0
23 38 1 0
23 39 1 0
24 40 1 0
24 41 1 0
24 42 1 0
25 43 1 0
25 44 1 0
25 45 1 0

```

M END

> <Name>

Compound268

> <Activ>

1.4

> <DB_Ref_id>

32.12

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Compound269

SciTegic10081411483D

```

39 41 0 0 0 0          999 V2000
-0.6060  0.7600  2.4490 S  0  0
-0.3810 -0.6090  1.4770 C  0  0
 0.6370 -0.4390  0.5280 C  0  0
 1.2190  0.8440  0.6290 C  0  0
 0.6290  1.6190  1.6530 C  0  0
 2.3120  1.3050 -0.2420 N  0  0
-1.0740 -1.9180  1.4770 C  0  0
-3.1390 -3.2130  1.4770 C  0  0
-2.4810 -1.9710  1.4770 C  0  0
-2.3910 -4.4020  1.4770 C  0  0
-0.3280 -3.1090  1.4770 C  0  0
-0.9860 -4.3510  1.4770 C  0  0
 1.0060  2.9810  2.0040 C  0  0
 0.4120  3.4920  3.0780 O  0  0
 1.8160  3.5780  1.3340 O  0  0
 2.1090  1.4320 -1.5860 C  0  0
 0.7360  1.2010 -2.1290 C  0  0
-1.6250  1.7910 -2.2170 C  0  0
-0.3340  2.0080 -1.7050 C  0  0
-1.8500  0.7640 -3.1520 C  0  0
 0.5140  0.1760 -3.0660 C  0  0
-0.7780 -0.0430 -3.5760 C  0  0
 3.6310  1.6310  0.3220 C  0  0

```


-3.4260	0.4980	-3.7730	Cl	0	0
3.0250	1.7270	-2.3180	O	0	0
0.9470	-1.1850	-0.1950	H	0	0
-4.2170	-3.2520	1.4770	H	0	0
-3.0610	-1.0580	1.4770	H	0	0
-2.8970	-5.3570	1.4770	H	0	0
0.7520	-3.0780	1.4770	H	0	0
-0.4140	-5.2670	1.4770	H	0	0
0.6270	4.3930	3.3540	H	0	0
-2.4380	2.4200	-1.8830	H	0	0
-0.1720	2.7990	-0.9860	H	0	0
1.3300	-0.4490	-3.3980	H	0	0
-0.9360	-0.8340	-4.2950	H	0	0
4.3730	0.9420	-0.0780	H	0	0
3.8570	2.6780	0.1230	H	0	0
3.6010	1.4960	1.4040	H	0	0
5	1	1	0		
4	5	2	0		
3	4	1	0		
1	2	1	0		
2	3	2	0		
4	6	1	0		
12	10	2	0		
11	12	1	0		
8	9	2	0		
7	11	2	0		
10	8	1	0		
9	7	1	0		
7	2	1	0		
5	13	1	0		
13	14	1	0		
13	15	2	0		
6	16	1	0		
16	17	1	0		
22	20	2	0		
21	22	1	0		
18	19	2	0		
20	18	1	0		
19	17	1	0		
17	21	2	0		
6	23	1	0		
20	24	1	0		
16	25	2	0		
3	26	1	0		
8	27	1	0		
9	28	1	0		
10	29	1	0		
11	30	1	0		
12	31	1	0		
14	32	1	0		
18	33	1	0		
19	34	1	0		
21	35	1	0		
22	36	1	0		
23	37	1	0		
23	38	1	0		
23	39	1	0		

M END

> <Name>

Compound269

> <Activ>

1.2

> <DB_Ref_id>

32.07

\$\$\$\$

Compound270

SciTegic10081411483D

42	44	0	0	0	0	999	V2000
1.2270	-0.0410	2.6080	S	0	0		
-0.1480	-0.5630	1.7660	C	0	0		
-0.6930	0.4360	0.9450	C	0	0		
0.0550	1.6310	1.0310	C	0	0		
1.1490	1.5140	1.9180	C	0	0		
-0.2830	2.8500	0.2790	N	0	0		
-0.8440	-1.8710	1.7660	C	0	0		
-2.9060	-3.1660	1.7660	C	0	0		
-2.2480	-1.9240	1.7660	C	0	0		
-2.1600	-4.3560	1.7660	C	0	0		
-0.0960	-3.0630	1.7660	C	0	0		
-0.7560	-4.3050	1.7660	C	0	0		
2.1060	2.5680	2.2230	C	0	0		
3.0020	2.2890	3.1660	O	0	0		
2.0570	3.6210	1.6310	O	0	0		
-0.2990	2.8260	-1.0860	C	0	0		
0.1190	1.5760	-1.7890	C	0	0		
-0.2770	-0.1230	-3.4880	C	0	0		
-0.6720	1.0550	-2.8280	C	0	0		
0.9060	-0.7790	-3.1110	C	0	0		
1.3030	0.9200	-1.4100	C	0	0		
1.6970	-0.2580	-2.0720	C	0	0		
1.3220	-2.0230	-3.8090	C	0	0		
-0.6050	4.1000	0.9850	C	0	0		
-0.6460	3.8030	-1.7090	O	0	0		
-1.5700	0.3200	0.3200	H	0	0		
-3.9860	-3.2050	1.7660	H	0	0		
-2.8280	-1.0120	1.7660	H	0	0		
-2.6660	-5.3110	1.7660	H	0	0		
0.9820	-3.0310	1.7660	H	0	0		
-0.1820	-5.2210	1.7660	H	0	0		
3.6580	2.9550	3.4040	H	0	0		
-0.8910	-0.5180	-4.2870	H	0	0		
-1.5840	1.5530	-3.1250	H	0	0		
1.9160	1.3130	-0.6130	H	0	0		
2.6080	-0.7580	-1.7750	H	0	0		
2.2540	-2.4550	-3.4410	H	0	0		
1.4470	-1.8200	-4.8730	H	0	0		
0.5410	-2.7770	-3.7050	H	0	0		
-1.6740	4.2930	0.8990	H	0	0		
-0.2560	4.0310	2.0140	H	0	0		
-0.0780	4.9260	0.5080	H	0	0		
5	1	1	0				
4	5	2	0				
3	4	1	0				
1	2	1	0				
2	3	2	0				
4	6	1	0				
12	10	2	0				
11	12	1	0				

```

8 9 2 0
7 11 2 0
10 8 1 0
9 7 1 0
7 2 1 0
5 13 1 0
13 14 1 0
13 15 2 0
6 16 1 0
16 17 1 0
22 20 2 0
21 22 1 0
18 19 2 0
20 18 1 0
19 17 1 0
17 21 2 0
20 23 1 0
6 24 1 0
16 25 2 0
3 26 1 0
8 27 1 0
9 28 1 0
10 29 1 0
11 30 1 0
12 31 1 0
14 32 1 0
18 33 1 0
19 34 1 0
21 35 1 0
22 36 1 0
23 37 1 0
23 38 1 0
23 39 1 0
24 40 1 0
24 41 1 0
24 42 1 0

```

M END

> <Name>

Compound270

> <Activ>

2

> <DB_Ref_id>

32.04

\$\$\$\$

Compound271

SciTegic10081411483D

```

55 57 0 0 0 0          999 V2000
-5.1680 -0.2830 -0.4490 C 0 0
-3.8340 1.8690 -0.2280 C 0 0
-2.6010 0.9840 -0.1030 C 0 0
-2.6740 -0.4060 -0.0040 C 0 0
-3.9880 -1.1720 0.0100 C 0 0
-1.0490 1.7130 -0.0920 S 0 0
-1.3890 -0.9360 0.0860 C 0 0
-0.4470 0.1050 0.0490 C 0 0
-1.0780 -2.3770 0.2030 C 0 0
0.0120 -2.7910 -0.1130 O 0 0

```

-2.0580	-3.1500	0.6660	O	0	0
-1.6780	-4.5160	0.7460	C	0	0
-2.8480	-5.3400	1.2830	C	0	0
1.0040	-0.1430	0.1250	N	0	0
1.8830	0.8830	-0.0740	C	0	0
3.2250	0.6390	-0.0020	N	0	0
1.4770	1.9960	-0.3160	O	0	0
4.2540	1.8670	-0.2420	S	0	0
3.9960	2.8610	0.7850	O	0	0
4.0350	2.3630	-1.5880	O	0	0
-5.1390	1.1330	0.1740	C	0	0
-5.2340	1.0270	1.7030	C	0	0
-6.3460	1.9360	-0.3220	C	0	0
5.9530	1.4980	-0.1350	N	0	0
6.9100	2.5920	-0.1850	C	0	0
8.2390	1.9840	-0.6230	C	0	0
7.7500	0.9550	-1.6350	C	0	0
6.4940	0.4200	-0.9530	C	0	0
-5.1410	-0.1950	-1.5350	H	0	0
-6.1070	-0.7850	-0.2130	H	0	0
-3.8920	2.1930	-1.2680	H	0	0
-3.6950	2.7700	0.3730	H	0	0
-3.9140	-2.0550	-0.6270	H	0	0
-4.1640	-1.5250	1.0250	H	0	0
-1.3960	-4.8520	-0.2520	H	0	0
-0.8160	-4.5920	1.4100	H	0	0
-2.5800	-6.3950	1.3460	H	0	0
-3.1440	-4.9900	2.2720	H	0	0
-3.7130	-5.2540	0.6270	H	0	0
1.3400	-1.0630	0.3240	H	0	0
3.5740	-0.2750	0.1970	H	0	0
-5.2770	2.0080	2.1760	H	0	0
-4.3690	0.5000	2.1080	H	0	0
-6.1270	0.4770	1.9960	H	0	0
-6.3630	2.9410	0.0940	H	0	0
-7.2770	1.4430	-0.0450	H	0	0
-6.3260	2.0250	-1.4100	H	0	0
6.5780	3.3240	-0.9060	H	0	0
6.9810	3.0780	0.7750	H	0	0
8.7350	1.5040	0.2090	H	0	0
8.9120	2.7130	-1.0530	H	0	0
7.5000	1.4360	-2.5700	H	0	0
8.4810	0.1860	-1.8340	H	0	0
6.7350	-0.4160	-0.3120	H	0	0
5.7640	0.0860	-1.6740	H	0	0
4	5	1	0		
3	4	2	0		
2	3	1	0		
1	5	1	0		
8	6	1	0		
7	8	2	0		
3	6	1	0		
4	7	1	0		
7	9	1	0		
9	10	2	0		
9	11	1	0		
11	12	1	0		
12	13	1	0		
8	14	1	0		
14	15	1	0		
15	16	1	0		

```

15 17 2 0
16 18 1 0
18 19 2 0
18 20 2 0
1 21 1 0
21 2 1 0
21 22 1 0
21 23 1 0
18 24 1 0
27 28 1 0
26 27 1 0
25 26 1 0
25 24 1 0
28 24 1 0
1 29 1 0
1 30 1 0
2 31 1 0
2 32 1 0
5 33 1 0
5 34 1 0
12 35 1 0
12 36 1 0
13 37 1 0
13 38 1 0
13 39 1 0
14 40 1 0
16 41 1 0
22 42 1 0
22 43 1 0
22 44 1 0
23 45 1 0
23 46 1 0
23 47 1 0
25 48 1 0
25 49 1 0
26 50 1 0
26 51 1 0
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28 55 1 0

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M END

> <Name>

Compound271

> <Activ>

0.4

> <DB_Ref_id>

33.07f

\$\$\$\$

Compound272

SciTegic10081411483D

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62 65 0 0 0 0          999 V2000
  -5.4360    3.2730    0.8670 C    0  0
  -3.1040    4.2700    0.6760 C    0  0
  -2.6000    2.8360    0.5840 C    0  0
  -3.4260    1.7280    0.7730 C    0  0
  -4.9060    1.8440    1.1110 C    0  0

```

-0.9450	2.5550	0.2210	S	0	0
-2.6840	0.5600	0.6170	C	0	0
-1.3520	0.8850	0.3200	C	0	0
-3.2320	-0.8090	0.7460	C	0	0
-2.6230	-1.7500	0.2990	O	0	0
-4.4020	-0.9120	1.3710	O	0	0
-4.8540	-2.2560	1.4510	C	0	0
-6.1990	-2.2990	2.1780	C	0	0
-0.3200	-0.1450	0.0980	N	0	0
0.9140	0.2130	-0.3630	C	0	0
1.8590	-0.7520	-0.5640	N	0	0
1.1680	1.3730	-0.5900	O	0	0
3.3200	-0.3110	-1.1110	S	0	0
3.9100	0.5700	-0.1190	O	0	0
3.1270	0.3260	-2.4020	O	0	0
-4.4770	4.3730	1.3890	C	0	0
-4.2950	4.2230	2.9040	C	0	0
-5.0860	5.7520	1.1170	C	0	0
4.4790	-1.5840	-1.3730	N	0	0
5.8610	-1.1880	-1.6740	C	0	0
6.8340	-2.3090	-1.7950	C	0	0
6.3850	-3.6560	-1.9000	C	0	0
4.9360	-3.9630	-1.8610	C	0	0
4.0470	-2.7400	-2.1600	C	0	0
8.2250	-2.0310	-1.8110	C	0	0
9.1600	-3.0840	-1.9370	C	0	0
8.7130	-4.4200	-2.0550	C	0	0
7.3300	-4.7050	-2.0350	C	0	0
-5.5900	3.4140	-0.2030	H	0	0
-6.4180	3.3770	1.3280	H	0	0
-3.1820	4.6480	-0.3440	H	0	0
-2.3570	4.8850	1.1800	H	0	0
-5.0350	1.5740	2.1600	H	0	0
-5.4790	1.1230	0.5270	H	0	0
-4.9510	-2.6450	0.4380	H	0	0
-4.1060	-2.8360	1.9900	H	0	0
-6.5700	-3.3220	2.2420	H	0	0
-6.1080	-1.8890	3.1840	H	0	0
-6.9430	-1.7070	1.6450	H	0	0
-0.5290	-1.1060	0.2850	H	0	0
1.6640	-1.7150	-0.3810	H	0	0
-3.6820	5.0210	3.3200	H	0	0
-3.8150	3.2750	3.1430	H	0	0
-5.2600	4.2440	3.4120	H	0	0
-4.4410	6.5570	1.4690	H	0	0
-6.0490	5.8540	1.6170	H	0	0
-5.2480	5.8980	0.0490	H	0	0
6.1970	-0.5000	-0.8960	H	0	0
5.8670	-0.6230	-2.6070	H	0	0
4.6990	-4.7600	-2.5680	H	0	0
4.6990	-4.3480	-0.8670	H	0	0
4.0780	-2.4860	-3.2210	H	0	0
3.0100	-2.9730	-1.9220	H	0	0
8.5760	-1.0140	-1.7250	H	0	0
10.2190	-2.8650	-1.9470	H	0	0
9.4300	-5.2210	-2.1560	H	0	0
6.9940	-5.7290	-2.1230	H	0	0
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2	3	1	0		
1	5	1	0		

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> <Activ>
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> <DB_Ref_id>
33.07g

\$\$\$\$
Compound273
SciTegic10081411483D

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-6.3070	-0.3500	-0.8560	C	0	0		
-4.9730	1.8030	-0.6350	C	0	0		
-3.7400	0.9200	-0.5100	C	0	0		
-3.8130	-0.4710	-0.4100	C	0	0		
-5.1290	-1.2360	-0.3990	C	0	0		
-2.1880	1.6470	-0.4980	S	0	0		
-2.5270	-1.0000	-0.3200	C	0	0		
-1.5860	0.0410	-0.3580	C	0	0		
-2.2190	-2.4430	-0.2030	C	0	0		
-1.1350	-2.8590	-0.5390	O	0	0		
-3.1900	-3.2110	0.2810	O	0	0		
-2.8090	-4.5760	0.3590	C	0	0		
-3.9710	-5.3970	0.9240	C	0	0		
-0.1350	-0.2070	-0.2810	N	0	0		
0.7440	0.8220	-0.4710	C	0	0		
2.0860	0.5760	-0.3970	N	0	0		
0.3380	1.9360	-0.7010	O	0	0		
3.1150	1.8070	-0.6250	S	0	0		
2.8400	2.8010	0.3960	O	0	0		
2.9120	2.3030	-1.9750	O	0	0		
-6.2770	1.0680	-0.2330	C	0	0		
-6.3730	0.9630	1.2950	C	0	0		
-7.4840	1.8710	-0.7310	C	0	0		
4.8130	1.4430	-0.4960	N	0	0		
5.7580	2.5200	-0.8220	C	0	0		
7.1840	1.9860	-1.0720	C	0	0		
7.6250	1.0940	0.0210	N	0	0		
6.6560	0.0820	0.5000	C	0	0		
5.2540	0.6910	0.6850	C	0	0		
8.8770	1.1970	0.5660	C	0	0		
9.2640	0.2560	1.6760	C	0	0		
9.6520	2.0310	0.1600	O	0	0		
-6.2790	-0.2600	-1.9430	H	0	0		
-7.2460	-0.8500	-0.6190	H	0	0		
-5.0310	2.1290	-1.6740	H	0	0		
-4.8340	2.7030	-0.0350	H	0	0		
-5.0530	-2.1190	-1.0330	H	0	0		
-5.3030	-1.5900	0.6190	H	0	0		
-2.5470	-4.9180	-0.6430	H	0	0		
-1.9360	-4.6500	1.0060	H	0	0		
-3.7030	-6.4530	0.9820	H	0	0		
-4.2440	-5.0430	1.9160	H	0	0		
-4.8480	-5.3110	0.2830	H	0	0		
0.2010	-1.1290	-0.0920	H	0	0		
2.4360	-0.3400	-0.2070	H	0	0		
-6.4080	1.9430	1.7680	H	0	0		

-5.5120	0.4300	1.6990	H	0	0
-7.2700	0.4180	1.5880	H	0	0
-7.5000	2.8790	-0.3170	H	0	0
-8.4160	1.3790	-0.4490	H	0	0
-7.4670	1.9570	-1.8170	H	0	0
5.4060	3.0450	-1.7090	H	0	0
5.7620	3.2480	-0.0120	H	0	0
7.2130	1.4240	-2.0060	H	0	0
7.8770	2.8220	-1.1840	H	0	0
6.6190	-0.7270	-0.2310	H	0	0
7.0000	-0.3550	1.4390	H	0	0
4.5350	-0.1050	0.8890	H	0	0
5.2360	1.3500	1.5550	H	0	0
10.2950	0.3750	2.0080	H	0	0
9.1350	-0.7750	1.3480	H	0	0
8.6170	0.4140	2.5390	H	0	0
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3	4	2	0		
2	3	1	0		
1	5	1	0		
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7	8	2	0		
3	6	1	0		
4	7	1	0		
7	9	1	0		
9	10	2	0		
9	11	1	0		
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2	35	1	0		
2	36	1	0		
5	37	1	0		
5	38	1	0		
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13	41	1	0		
13	42	1	0		
13	43	1	0		

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16 45 1 0
22 46 1 0
22 47 1 0
22 48 1 0
23 49 1 0
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25 52 1 0
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M END

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Compound273

> <Activ>

0.6

> <DB_Ref_id>

33.07

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Compound274

SciTegic10081411483D

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60 62 0 0 0 0          999 V2000
-5.9940 -0.3380 -0.7090 C 0 0
-4.6600 1.8140 -0.4880 C 0 0
-3.4280 0.9300 -0.3630 C 0 0
-3.5000 -0.4590 -0.2640 C 0 0
-4.8160 -1.2250 -0.2520 C 0 0
-1.8750 1.6580 -0.3510 S 0 0
-2.2170 -0.9880 -0.1740 C 0 0
-1.2730 0.0510 -0.2110 C 0 0
-1.9060 -2.4320 -0.0570 C 0 0
-0.8140 -2.8440 -0.3710 O 0 0
-2.8870 -3.2050 0.4020 O 0 0
-2.5060 -4.5700 0.4830 C 0 0
-3.6780 -5.3950 1.0180 C 0 0
0.1760 -0.1950 -0.1350 N 0 0
1.0550 0.8300 -0.3320 C 0 0
2.3970 0.5860 -0.2580 N 0 0
0.6500 1.9450 -0.5680 O 0 0
3.4280 1.8140 -0.4920 S 0 0
3.1560 2.8130 0.5270 O 0 0
3.2210 2.3050 -1.8440 O 0 0
-5.9650 1.0800 -0.0860 C 0 0
-6.0610 0.9750 1.4420 C 0 0
-7.1720 1.8810 -0.5840 C 0 0
5.1250 1.4510 -0.3670 N 0 0
6.0680 2.5080 -0.7460 C 0 0
7.4980 1.9610 -0.9100 C 0 0
7.9300 1.2640 0.3050 N 0 0

```

7.0020	0.1870	0.6620	C	0	0
5.5720	0.7320	0.8280	C	0	0
9.3030	0.7810	0.1930	C	0	0
-5.9690	-0.2480	-1.7970	H	0	0
-6.9360	-0.8380	-0.4730	H	0	0
-4.7190	2.1390	-1.5270	H	0	0
-4.5240	2.7150	0.1110	H	0	0
-4.7400	-2.1090	-0.8870	H	0	0
-4.9920	-1.5800	0.7660	H	0	0
-2.2210	-4.9040	-0.5140	H	0	0
-1.6470	-4.6470	1.1490	H	0	0
-3.4080	-6.4490	1.0780	H	0	0
-3.9750	-5.0450	2.0060	H	0	0
-4.5410	-5.3090	0.3590	H	0	0
0.5140	-1.1170	0.0610	H	0	0
2.7480	-0.3300	-0.0620	H	0	0
-6.1170	1.9550	1.9140	H	0	0
-5.1900	0.4590	1.8480	H	0	0
-6.9470	0.4120	1.7340	H	0	0
-7.1900	2.8890	-0.1680	H	0	0
-8.1040	1.3910	-0.3050	H	0	0
-7.1540	1.9710	-1.6700	H	0	0
5.7380	2.9590	-1.6820	H	0	0
6.0470	3.2950	0.0080	H	0	0
7.5450	1.2790	-1.7620	H	0	0
8.1820	2.7830	-1.1210	H	0	0
7.0240	-0.5880	-0.1070	H	0	0
7.3260	-0.2790	1.5940	H	0	0
4.8870	-0.0920	1.0260	H	0	0
5.5180	1.3980	1.6900	H	0	0
9.6780	0.2870	1.0900	H	0	0
9.9650	1.6170	-0.0290	H	0	0
9.3730	0.0720	-0.6310	H	0	0
4	5	1	0		
3	4	2	0		
2	3	1	0		
1	5	1	0		
8	6	1	0		
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7	9	1	0		
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12	13	1	0		
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18	24	1	0		
28	29	1	0		
27	28	1	0		
26	27	1	0		

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29 24 1 0
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27 30 1 0
1 31 1 0
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2 34 1 0
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23 47 1 0
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M END

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Compound274

> <Activ>

2

> <DB_Ref_id>

33.07d

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Compound275

SciTegic10081411483D

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61 63 0 0 0 0          999 V2000
   3.8850   -2.7250   -3.6860 C   0  0
   2.5630   -3.9160   -1.8710 C   0  0
   2.0000   -2.5490   -1.5120 C   0  0
   2.4590   -1.3650   -2.0880 C   0  0
   3.5820   -1.3220   -3.1150 C   0  0
   0.7360   -2.4430   -0.3560 S   0  0
   1.7480   -0.2850   -1.5700 C   0  0
   0.8050   -0.7460   -0.6390 C   0  0
   1.9650    1.1270   -1.9530 C   0  0
   1.1210    1.9570   -1.7090 O   0  0
   3.1150    1.3960   -2.5650 O   0  0
   3.2420    2.7710   -2.8950 C   0  0

```

4.5820	3.0080	-3.5900	C	0	0
-0.1040	0.1640	0.0800	N	0	0
-1.1190	-0.3440	0.8400	C	0	0
-1.9510	0.5140	1.5020	N	0	0
-1.2790	-1.5370	0.9260	O	0	0
-3.1520	-0.1020	2.3980	S	0	0
-2.5470	-0.9260	3.4320	O	0	0
-4.0240	-0.8500	1.5080	O	0	0
3.9300	-3.8240	-2.5980	C	0	0
5.0430	-3.5100	-1.5900	C	0	0
4.2480	-5.1760	-3.2480	C	0	0
-4.1760	1.0350	3.2290	N	0	0
-5.4450	0.5410	3.7730	C	0	0
-6.3670	1.6170	4.3770	C	0	0
-3.5410	2.1460	3.9360	C	0	0
-6.5160	2.8960	3.5370	C	0	0
-4.0040	3.4960	3.3610	C	0	0
-5.4080	3.9260	3.8120	C	0	0
3.1190	-2.9810	-4.4200	H	0	0
4.8260	-2.6930	-4.2350	H	0	0
1.8300	-4.4080	-2.5120	H	0	0
2.6450	-4.5240	-0.9670	H	0	0
4.4710	-0.9180	-2.6290	H	0	0
3.3240	-0.6350	-3.9220	H	0	0
2.4140	3.0430	-3.5510	H	0	0
3.1780	3.3520	-1.9750	H	0	0
4.6970	4.0570	-3.8630	H	0	0
5.4100	2.7170	-2.9430	H	0	0
4.6520	2.4160	-4.5040	H	0	0
0.0290	1.1520	0.0120	H	0	0
-1.8320	1.5060	1.4410	H	0	0
5.1520	-4.2990	-0.8460	H	0	0
4.8300	-2.5800	-1.0610	H	0	0
6.0000	-3.3930	-2.0960	H	0	0
4.2890	-5.9810	-2.5140	H	0	0
5.2110	-5.1410	-3.7580	H	0	0
3.4880	-5.4360	-3.9860	H	0	0
-5.2340	-0.2190	4.5270	H	0	0
-5.9790	0.0290	2.9710	H	0	0
-7.3540	1.1700	4.5140	H	0	0
-6.0290	1.8750	5.3810	H	0	0
-2.4610	2.0640	3.8070	H	0	0
-3.7230	2.0780	5.0080	H	0	0
-7.4690	3.3610	3.7870	H	0	0
-6.5670	2.6560	2.4750	H	0	0
-3.2990	4.2680	3.6720	H	0	0
-3.9570	3.4730	2.2710	H	0	0
-5.3910	4.1540	4.8770	H	0	0
-5.6620	4.8610	3.3120	H	0	0
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1	5	1	0		
8	6	1	0		
7	8	2	0		
3	6	1	0		
4	7	1	0		
7	9	1	0		
9	10	2	0		
9	11	1	0		
11	12	1	0		

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14 15 1 0
15 16 1 0
15 17 2 0
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18 19 2 0
18 20 2 0
 1 21 1 0
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Compound275

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1.1

> <DB_Ref_id>
33.07c
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Compound276

SciTegic10081411483D

58	60	0	0	0	0	999	V2000
-3.1500	4.5960	1.0510	C	0	0		
-3.7770	2.7130	-0.5390	C	0	0		
-2.4510	2.0720	-0.1560	C	0	0		
-1.5000	2.7150	0.6370	C	0	0		
-1.6860	4.1250	1.1780	C	0	0		
-2.1020	0.4840	-0.7070	S	0	0		
-0.4040	1.8770	0.8220	C	0	0		
-0.6190	0.6620	0.1500	C	0	0		
0.7990	2.2270	1.6110	C	0	0		
1.5530	1.3580	1.9840	O	0	0		
0.9750	3.5200	1.8650	O	0	0		
2.1480	3.7660	2.6250	C	0	0		
2.2850	5.2680	2.8790	C	0	0		
0.3690	-0.4300	0.1600	N	0	0		
0.0430	-1.6500	-0.3550	C	0	0		
0.9690	-2.6540	-0.3380	N	0	0		
-1.0550	-1.8420	-0.8240	O	0	0		
0.5660	-4.0980	-0.9550	S	0	0		
0.2300	-3.8960	-2.3530	O	0	0		
-0.5390	-4.6150	-0.1680	O	0	0		
-3.7830	4.2480	-0.3200	C	0	0		
-2.9980	4.9420	-1.4410	C	0	0		
-5.2270	4.7600	-0.3630	C	0	0		
1.7930	-5.3320	-0.9300	N	0	0		
1.3850	-6.6910	-1.3090	C	0	0		
2.4160	-7.7400	-0.8590	C	0	0		
3.8150	-7.4100	-1.3870	C	0	0		
4.1930	-5.9770	-1.0040	C	0	0		
3.1170	-4.9750	-1.4510	C	0	0		
-3.7400	4.1310	1.8420	H	0	0		
-3.2010	5.6700	1.2310	H	0	0		
-4.5510	2.2460	0.0740	H	0	0		
-4.0120	2.4690	-1.5760	H	0	0		
-1.0310	4.7910	0.6150	H	0	0		
-1.3650	4.1700	2.2190	H	0	0		
2.0660	3.2230	3.5670	H	0	0		
3.0040	3.3910	2.0650	H	0	0		
3.1780	5.4790	3.4690	H	0	0		
2.3460	5.8150	1.9380	H	0	0		
1.4240	5.6470	3.4300	H	0	0		
1.2770	-0.2730	0.5470	H	0	0		
1.8810	-2.5120	0.0450	H	0	0		
-3.4530	4.7780	-2.4180	H	0	0		
-1.9750	4.5670	-1.4840	H	0	0		
-2.9510	6.0180	-1.2710	H	0	0		
-5.7090	4.5350	-1.3120	H	0	0		
-5.2560	5.8420	-0.2210	H	0	0		
-5.8200	4.3050	0.4300	H	0	0		
1.2480	-6.7340	-2.3910	H	0	0		
0.4180	-6.9120	-0.8590	H	0	0		
2.4410	-7.7790	0.2310	H	0	0		
2.1110	-8.7310	-1.1970	H	0	0		
3.8280	-7.5140	-2.4730	H	0	0		
4.5470	-8.1150	-0.9940	H	0	0		
5.1560	-5.7130	-1.4430	H	0	0		
4.3220	-5.9120	0.0780	H	0	0		

	3.3790	-3.9750	-1.1030 H	0	0
	3.0720	-4.9280	-2.5390 H	0	0
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Compound276

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1

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33.07b

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Compound277

SciTegic10081411483D

56	58	0	0	0	0	999	V2000
-5.3160	-0.2600	-0.5530	C	0	0		
-3.9820	1.8930	-0.3300	C	0	0		
-2.7500	1.0080	-0.2050	C	0	0		
-2.8220	-0.3810	-0.1070	C	0	0		
-4.1390	-1.1470	-0.0940	C	0	0		
-1.1970	1.7360	-0.1930	S	0	0		
-1.5370	-0.9100	-0.0180	C	0	0		
-0.5960	0.1290	-0.0550	C	0	0		
-1.2280	-2.3540	0.1000	C	0	0		
-0.1350	-2.7660	-0.2130	O	0	0		
-2.2090	-3.1270	0.5590	O	0	0		
-1.8280	-4.4920	0.6390	C	0	0		
-3.0000	-5.3170	1.1720	C	0	0		
0.8560	-0.1170	0.0210	N	0	0		
1.7340	0.9080	-0.1740	C	0	0		
3.0760	0.6640	-0.1000	N	0	0		
1.3280	2.0230	-0.4100	O	0	0		
4.1060	1.8930	-0.3340	S	0	0		
3.8560	2.8770	0.7050	O	0	0		
3.8770	2.4040	-1.6740	O	0	0		
-5.2870	1.1560	0.0700	C	0	0		
-5.3830	1.0530	1.6000	C	0	0		
-6.4940	1.9590	-0.4260	C	0	0		
5.8050	1.5210	-0.2460	N	0	0		
6.7440	2.6460	-0.2850	C	0	0		
8.1720	2.2070	0.0960	C	0	0		
8.5760	1.1290	-0.7320	O	0	0		
7.7270	-0.0040	-0.6480	C	0	0		
6.2910	0.3930	-1.0430	C	0	0		
-5.2910	-0.1700	-1.6390	H	0	0		
-6.2560	-0.7600	-0.3160	H	0	0		
-4.0410	2.2170	-1.3690	H	0	0		
-3.8440	2.7930	0.2700	H	0	0		
-4.0620	-2.0310	-0.7290	H	0	0		
-4.3120	-1.5020	0.9220	H	0	0		
-1.5430	-4.8260	-0.3570	H	0	0		
-0.9690	-4.5680	1.3070	H	0	0		
-2.7320	-6.3710	1.2320	H	0	0		
-3.2990	-4.9690	2.1600	H	0	0		
-3.8630	-5.2310	0.5120	H	0	0		
1.1910	-1.0390	0.2170	H	0	0		
3.4260	-0.2520	0.0960	H	0	0		
-5.4340	2.0330	2.0720	H	0	0		
-4.5140	0.5330	2.0040	H	0	0		
-6.2720	0.4940	1.8930	H	0	0		

-6.5120	2.9670	-0.0100	H	0	0
-7.4260	1.4690	-0.1460	H	0	0
-6.4770	2.0470	-1.5120	H	0	0
6.4040	3.4200	0.4000	H	0	0
6.7350	3.0860	-1.2850	H	0	0
8.2190	1.8890	1.1390	H	0	0
8.8790	3.0250	-0.0330	H	0	0
7.7620	-0.3970	0.3690	H	0	0
8.1150	-0.7750	-1.3130	H	0	0
6.2440	0.6540	-2.1020	H	0	0
5.6250	-0.4590	-0.9020	H	0	0
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3	4	2	0		
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Compound277

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2.5

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33.07a

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Compound278

SciTegic10081411483D

53	55	0	0	0	0	999	V2000
-4.0220	1.1680	-0.7090	C	0	0		
-2.0000	2.7090	-0.6190	C	0	0		
-1.1520	1.4450	-0.5800	C	0	0		
-1.6890	0.1680	-0.7440	C	0	0		
-3.1700	-0.0860	-1.0020	C	0	0		
0.5350	1.5800	-0.3100	S	0	0		
-0.6760	-0.7810	-0.6460	C	0	0		
0.5510	-0.1390	-0.4160	C	0	0		
-0.8770	-2.2420	-0.7690	C	0	0		
-0.0590	-3.0080	-0.3140	O	0	0		
-1.9840	-2.6310	-1.3960	O	0	0		
-2.0920	-4.0430	-1.4800	C	0	0		
-3.3930	-4.4140	-2.1930	C	0	0		
1.8150	-0.8830	-0.2680	N	0	0		
2.9430	-0.2320	0.1390	C	0	0		
4.1080	-0.9360	0.2720	N	0	0		
2.9140	0.9510	0.3790	O	0	0		
5.4400	-0.1520	0.7560	S	0	0		
6.4920	-1.1390	0.9200	O	0	0		
5.7480	0.8500	-0.2480	O	0	0		
-3.3930	2.4730	-1.2580	C	0	0		
-3.2620	2.3790	-2.7850	C	0	0		
-4.3070	3.6580	-0.9320	C	0	0		
5.2090	0.6430	2.2540	C	0	0		
4.8200	0.0180	3.3970	N	0	0		
4.7580	0.9880	4.3340	C	0	0		
5.1110	2.2010	3.7400	C	0	0		
5.3930	1.9750	2.4380	N	0	0		
4.5310	-1.4140	3.5800	C	0	0		
-4.1500	1.2640	0.3710	H	0	0		
-5.0220	1.0270	-1.1170	H	0	0		
-2.1150	3.0510	0.4100	H	0	0		
-1.4570	3.4920	-1.1480	H	0	0		
-3.5160	-0.9260	-0.3980	H	0	0		
-3.2850	-0.3770	-2.0470	H	0	0		
-1.2280	-4.4180	-2.0330	H	0	0		
-2.0780	-4.4490	-0.4690	H	0	0		
-3.4040	-4.0120	-3.2070	H	0	0		

-3.5120	-5.4960	-2.2380	H	0	0
-4.2520	-4.0060	-1.6640	H	0	0
1.8400	-1.8610	-0.4670	H	0	0
4.1490	-1.9160	0.0760	H	0	0
-2.8650	3.2990	-3.2150	H	0	0
-4.2320	2.1880	-3.2440	H	0	0
-2.5940	1.5660	-3.0640	H	0	0
-3.8970	4.6000	-1.2930	H	0	0
-4.4490	3.7480	0.1470	H	0	0
-5.2890	3.5250	-1.3870	H	0	0
4.4750	0.8160	5.3630	H	0	0
5.1640	3.1760	4.2050	H	0	0
3.4710	-1.6470	3.6760	H	0	0
5.0350	-1.7750	4.4770	H	0	0
4.9180	-1.9750	2.7290	H	0	0
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Compound278

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0.15

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33.05j

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Compound279

SciTegic10081411483D

53	55	0	0	0	0	999	V2000
-4.2270	0.9490	-0.5610	C	0	0		
-2.2050	2.4880	-0.4690	C	0	0		
-1.3570	1.2250	-0.4300	C	0	0		
-1.8940	-0.0510	-0.5960	C	0	0		
-3.3750	-0.3050	-0.8540	C	0	0		
0.3300	1.3590	-0.1620	S	0	0		
-0.8810	-1.0000	-0.4980	C	0	0		
0.3460	-0.3590	-0.2680	C	0	0		
-1.0820	-2.4630	-0.6210	C	0	0		
-0.2710	-3.2270	-0.1520	O	0	0		
-2.1820	-2.8500	-1.2620	O	0	0		
-2.2950	-4.2640	-1.3340	C	0	0		
-3.5780	-4.6330	-2.0800	C	0	0		
1.6080	-1.1020	-0.1190	N	0	0		
2.7460	-0.4450	0.2540	C	0	0		
3.9100	-1.1490	0.3890	N	0	0		
2.7250	0.7440	0.4650	O	0	0		
5.2520	-0.3580	0.8320	S	0	0		
6.3380	-1.3200	0.8590	O	0	0		
5.4630	0.7170	-0.1230	O	0	0		
-3.5980	2.2540	-1.1090	C	0	0		
-3.4670	2.1600	-2.6350	C	0	0		
-4.5120	3.4390	-0.7810	C	0	0		
5.1040	0.3320	2.3910	C	0	0		
5.9180	1.2560	2.9360	N	0	0		
5.4750	1.5430	4.1640	N	0	0		
4.3710	0.8280	4.4710	C	0	0		
4.1040	0.0290	3.3360	C	0	0		
7.0960	1.8530	2.2890	C	0	0		
-4.3550	1.0450	0.5200	H	0	0		
-5.2270	0.8080	-0.9690	H	0	0		
-2.3200	2.8320	0.5590	H	0	0		
-1.6640	3.2730	-1.0000	H	0	0		
-3.7210	-1.1450	-0.2500	H	0	0		
-3.4900	-0.5960	-1.8990	H	0	0		
-1.4200	-4.6490	-1.8570	H	0	0		
-2.3120	-4.6560	-0.3180	H	0	0		

-3.5680	-4.2210	-3.0900	H	0	0
-3.6890	-5.7150	-2.1410	H	0	0
-4.4510	-4.2370	-1.5650	H	0	0
1.6290	-2.0860	-0.2930	H	0	0
3.9450	-2.1330	0.2170	H	0	0
-3.0800	3.0820	-3.0660	H	0	0
-4.4360	1.9590	-3.0940	H	0	0
-2.7910	1.3510	-2.9160	H	0	0
-4.1020	4.3810	-1.1450	H	0	0
-4.6540	3.5290	0.2950	H	0	0
-5.4940	3.3070	-1.2380	H	0	0
3.8320	0.8870	5.4080	H	0	0
3.2910	-0.6740	3.2170	H	0	0
7.6490	2.5490	2.9200	H	0	0
6.7850	2.3930	1.3930	H	0	0
7.7810	1.0640	1.9820	H	0	0
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Compound279

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0.26

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33.05i

\$\$\$\$

Compound280

SciTegic10081411483D

51	53	0	0	0	0	999	V2000
-4.6600	-0.0510	-0.6720	C	0	0		
-3.3260	2.1020	-0.4510	C	0	0		
-2.0940	1.2190	-0.3260	C	0	0		
-2.1660	-0.1720	-0.2270	C	0	0		
-3.4830	-0.9370	-0.2150	C	0	0		
-0.5410	1.9450	-0.3150	S	0	0		
-0.8830	-0.7010	-0.1370	C	0	0		
0.0610	0.3380	-0.1740	C	0	0		
-0.5720	-2.1450	-0.0200	C	0	0		
0.5200	-2.5570	-0.3340	O	0	0		
-1.5530	-2.9160	0.4390	O	0	0		
-1.1720	-4.2810	0.5190	C	0	0		
-2.3440	-5.1070	1.0530	C	0	0		
1.5100	0.0920	-0.0980	N	0	0		
2.3890	1.1190	-0.2910	C	0	0		
3.7300	0.8750	-0.2170	N	0	0		
1.9840	2.2340	-0.5240	O	0	0		
4.7620	2.1040	-0.4470	S	0	0		
6.4060	1.6040	-0.3170	C	0	0		
4.5430	2.6090	-1.7910	O	0	0		
4.5000	3.0920	0.5840	O	0	0		
-4.6310	1.3670	-0.0490	C	0	0		
-4.7270	1.2620	1.4780	C	0	0		
-5.8380	2.1700	-0.5470	C	0	0		
8.6820	2.1560	-0.3870	C	0	0		
7.3770	2.5490	-0.4900	N	0	0		
9.0040	0.8110	-0.1080	C	0	0		
6.6520	0.2850	-0.0450	N	0	0		
7.9550	-0.1150	0.0600	C	0	0		
-4.6350	0.0390	-1.7600	H	0	0		
-5.6020	-0.5510	-0.4360	H	0	0		
-3.3850	2.4280	-1.4900	H	0	0		
-3.1900	3.0020	0.1480	H	0	0		
-3.4080	-1.8200	-0.8500	H	0	0		
-3.6580	-1.2910	0.8030	H	0	0		
-0.8870	-4.6170	-0.4790	H	0	0		

-0.3130	-4.3570	1.1850	H	0	0
-2.0760	-6.1620	1.1150	H	0	0
-2.6430	-4.7580	2.0410	H	0	0
-3.2070	-5.0220	0.3940	H	0	0
1.8480	-0.8300	0.0960	H	0	0
4.0820	-0.0410	-0.0260	H	0	0
-4.7790	2.2420	1.9510	H	0	0
-3.8580	0.7420	1.8850	H	0	0
-5.6150	0.7030	1.7710	H	0	0
-5.8560	3.1780	-0.1310	H	0	0
-6.7700	1.6780	-0.2680	H	0	0
-5.8200	2.2580	-1.6330	H	0	0
9.4710	2.8810	-0.5200	H	0	0
10.0350	0.4980	-0.0260	H	0	0
8.1800	-1.1500	0.2750	H	0	0
4	5	1	0		
3	4	2	0		
2	3	1	0		
1	5	1	0		
8	6	1	0		
7	8	2	0		
3	6	1	0		
4	7	1	0		
7	9	1	0		
9	10	2	0		
9	11	1	0		
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Compound280

> <Activ>

0.3

> <DB_Ref_id>

33.05h

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Compound281

SciTegic10081411483D

59	62	0	0	0	0	999	V2000
-1.0720	5.3570	1.7600	C	0	0		
-1.5760	4.5100	-0.5840	C	0	0		
-1.0880	3.1520	-0.0980	C	0	0		
-0.5020	2.9630	1.1520	C	0	0		
-0.2730	4.0940	2.1460	C	0	0		
-1.2680	1.7850	-1.1190	S	0	0		
-0.1700	1.6190	1.3140	C	0	0		
-0.5350	0.9020	0.1640	C	0	0		
0.4690	1.0490	2.5210	C	0	0		
0.3730	-0.1330	2.7580	O	0	0		
1.1310	1.9060	3.2930	O	0	0		
1.7110	1.2790	4.4260	C	0	0		
2.4530	2.3220	5.2640	C	0	0		
-0.3110	-0.5470	0.0350	N	0	0		
-0.8180	-1.2250	-1.0370	C	0	0		
-0.6020	-2.5680	-1.1450	N	0	0		
-1.4510	-0.6390	-1.8850	O	0	0		
-1.2090	-3.3580	-2.4220	S	0	0		
-0.6090	-2.7830	-3.6150	O	0	0		
-2.6520	-3.2110	-2.3790	O	0	0		
-0.9960	5.6840	0.2480	C	0	0		
0.4610	5.9430	-0.1540	C	0	0		
-1.8030	6.9550	-0.0430	C	0	0		
-0.8790	-4.9450	-2.4280	N	0	0		
-1.8750	-6.0260	-2.3240	C	0	0		
-1.0900	-7.3600	-2.3520	C	0	0		
0.3400	-6.8930	-2.4880	C	0	0		
0.4710	-5.4980	-2.5330	C	0	0		
1.5530	-7.6270	-2.5760	C	0	0		
2.8090	-6.9790	-2.7030	C	0	0		
1.6910	-4.8030	-2.6580	C	0	0		
2.8790	-5.5650	-2.7440	C	0	0		
-2.1170	5.2170	2.0410	H	0	0		
-0.7150	6.2030	2.3480	H	0	0		
-2.6640	4.5040	-0.5140	H	0	0		
-1.3340	4.6250	-1.6410	H	0	0		
0.7930	4.3180	2.1640	H	0	0		
-0.5470	3.7700	3.1500	H	0	0		
0.9140	0.8140	5.0060	H	0	0		

2.3980	0.5080	4.0740	H	0	0
2.8980	1.8610	6.1450	H	0	0
3.2360	2.8010	4.6760	H	0	0
1.7680	3.0980	5.6040	H	0	0
0.2150	-1.0330	0.7340	H	0	0
-0.0780	-3.0660	-0.4510	H	0	0
0.5490	6.2440	-1.1970	H	0	0
1.0640	5.0450	-0.0160	H	0	0
0.8950	6.7320	0.4590	H	0	0
-1.7750	7.2210	-1.1000	H	0	0
-1.4080	7.7990	0.5230	H	0	0
-2.8460	6.8220	0.2420	H	0	0
-2.4380	-5.9180	-1.4100	H	0	0
-2.5660	-5.9610	-3.1510	H	0	0
-1.2210	-7.9240	-1.4400	H	0	0
-1.3710	-7.9790	-3.1940	H	0	0
1.5180	-8.7070	-2.5470	H	0	0
3.7150	-7.5650	-2.7680	H	0	0
1.7230	-3.7230	-2.6880	H	0	0
3.8340	-5.0700	-2.8420	H	0	0
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2	3	1	0		
1	5	1	0		
8	6	1	0		
7	8	2	0		
3	6	1	0		
4	7	1	0		
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30	29	2	0		
28	31	1	0		
27	29	1	0		
1	33	1	0		
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2	35	1	0		
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5	37	1	0		
5	38	1	0		

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13 41 1 0
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14 44 1 0
16 45 1 0
22 46 1 0
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Compound281

> <Activ>

0.26

> <DB_Ref_id>

33.07h

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Compound282

SciTegic10081411483D

```

55 57 0 0 0 0          999 V2000
-5.3600 -0.3010 -0.6250 C 0 0
-4.0260 1.8520 -0.4040 C 0 0
-2.7930 0.9670 -0.2790 C 0 0
-2.8650 -0.4240 -0.1820 C 0 0
-4.1820 -1.1890 -0.1680 C 0 0
-1.2400 1.6950 -0.2680 S 0 0
-1.5820 -0.9530 -0.0920 C 0 0
-0.6390 0.0880 -0.1290 C 0 0
-1.2720 -2.3950 0.0250 C 0 0
-0.1800 -2.8090 -0.2870 O 0 0
-2.2520 -3.1680 0.4840 O 0 0
-1.8710 -4.5330 0.5660 C 0 0
-3.0430 -5.3590 1.1000 C 0 0
0.8100 -0.1600 -0.0510 N 0 0
1.6890 0.8670 -0.2440 C 0 0
3.0310 0.6230 -0.1700 N 0 0
1.2850 1.9820 -0.4790 O 0 0
4.0620 1.8520 -0.4020 S 0 0
5.7070 1.3520 -0.2700 C 0 0
3.8440 2.3570 -1.7460 O 0 0
3.8010 2.8400 0.6310 O 0 0
-5.3300 1.1150 -0.0040 C 0 0
-5.4260 1.0100 1.5250 C 0 0
-6.5370 1.9180 -0.5000 C 0 0
7.2850 -0.3630 0.1070 C 0 0

```

5.9840	0.0430	0.0000	N	0	0
8.3520	0.5410	-0.0570	C	0	0
6.7320	2.3010	-0.4430	C	0	0
8.0740	1.8910	-0.3360	C	0	0
9.1800	2.8670	-0.5160	C	0	0
-5.3340	-0.2130	-1.7130	H	0	0
-6.3010	-0.8030	-0.3910	H	0	0
-4.0840	2.1760	-1.4430	H	0	0
-3.8890	2.7520	0.1950	H	0	0
-4.1080	-2.0720	-0.8030	H	0	0
-4.3580	-1.5430	0.8480	H	0	0
-1.5860	-4.8690	-0.4320	H	0	0
-1.0120	-4.6090	1.2320	H	0	0
-2.7760	-6.4140	1.1600	H	0	0
-3.3420	-5.0100	2.0880	H	0	0
-3.9060	-5.2720	0.4390	H	0	0
1.1480	-1.0820	0.1410	H	0	0
3.3830	-0.2930	0.0210	H	0	0
-5.4790	1.9900	1.9980	H	0	0
-4.5570	0.4920	1.9300	H	0	0
-6.3150	0.4510	1.8180	H	0	0
-6.5550	2.9260	-0.0840	H	0	0
-7.4690	1.4260	-0.2210	H	0	0
-6.5200	2.0060	-1.5860	H	0	0
7.4980	-1.4000	0.3200	H	0	0
9.3730	0.1950	0.0310	H	0	0
6.4900	3.3320	-0.6580	H	0	0
8.8500	3.8850	-0.7290	H	0	0
9.8200	2.5450	-1.3380	H	0	0
9.7890	2.8970	0.3890	H	0	0
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3	6	1	0		
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1	22	1	0		
22	2	1	0		
22	23	1	0		
22	24	1	0		
29	27	2	0		
28	29	1	0		
25	26	2	0		
27	25	1	0		
26	19	1	0		
19	28	2	0		

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29 30 1 0
1 31 1 0
1 32 1 0
2 33 1 0
2 34 1 0
5 35 1 0
5 36 1 0
12 37 1 0
12 38 1 0
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13 40 1 0
13 41 1 0
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16 43 1 0
23 44 1 0
23 45 1 0
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M END

> <Name>

Compound282

> <Activ>

0.2

> <DB_Ref_id>

33.05g

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Compound283

SciTegic10081411483D

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52 54 0 0 0 0          999 V2000
-4.8070 -0.1170 -0.6600 C 0 0
-3.4730 2.0350 -0.4380 C 0 0
-2.2400 1.1500 -0.3130 C 0 0
-2.3120 -0.2380 -0.2150 C 0 0
-3.6290 -1.0040 -0.2010 C 0 0
-0.6870 1.8790 -0.3010 S 0 0
-1.0290 -0.7680 -0.1250 C 0 0
-0.0860 0.2710 -0.1620 C 0 0
-0.7190 -2.2110 -0.0080 C 0 0
0.3730 -2.6230 -0.3200 O 0 0
-1.6990 -2.9840 0.4510 O 0 0
-1.3180 -4.3500 0.5330 C 0 0
-2.4900 -5.1740 1.0660 C 0 0
1.3630 0.0250 -0.0860 N 0 0
2.2420 1.0530 -0.2770 C 0 0
3.5840 0.8090 -0.2030 N 0 0
1.8380 2.1660 -0.5120 O 0 0
4.6150 2.0370 -0.4340 S 0 0
6.2600 1.5350 -0.3030 C 0 0
4.3970 2.5430 -1.7790 O 0 0

```

4.3540	3.0250	0.5980	O	0	0
-4.7770	1.3010	-0.0370	C	0	0
-4.8730	1.1950	1.4920	C	0	0
-5.9840	2.1020	-0.5330	C	0	0
7.8360	-0.1800	0.0740	C	0	0
6.5370	0.2270	-0.0330	N	0	0
8.9050	0.7250	-0.0900	C	0	0
7.2870	2.4840	-0.4770	C	0	0
8.6270	2.0740	-0.3690	C	0	0
-4.7810	-0.0270	-1.7460	H	0	0
-5.7480	-0.6170	-0.4240	H	0	0
-3.5310	2.3610	-1.4790	H	0	0
-3.3360	2.9360	0.1620	H	0	0
-3.5530	-1.8890	-0.8360	H	0	0
-3.8050	-1.3590	0.8140	H	0	0
-1.0330	-4.6840	-0.4650	H	0	0
-0.4590	-4.4260	1.1990	H	0	0
-2.2230	-6.2290	1.1270	H	0	0
-2.7890	-4.8240	2.0550	H	0	0
-3.3530	-5.0880	0.4060	H	0	0
1.7010	-0.8970	0.1070	H	0	0
3.9360	-0.1090	-0.0120	H	0	0
-4.9260	2.1760	1.9630	H	0	0
-4.0040	0.6760	1.8970	H	0	0
-5.7620	0.6350	1.7850	H	0	0
-6.0020	3.1090	-0.1170	H	0	0
-6.9160	1.6110	-0.2540	H	0	0
-5.9670	2.1910	-1.6190	H	0	0
8.0490	-1.2170	0.2870	H	0	0
9.9260	0.3850	-0.0020	H	0	0
7.0510	3.5160	-0.6910	H	0	0
9.4300	2.7830	-0.4980	H	0	0
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18	20	2	0		
18	21	2	0		
1	22	1	0		
22	2	1	0		
22	23	1	0		
22	24	1	0		
29	27	2	0		
28	29	1	0		
25	26	2	0		
27	25	1	0		

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26 19 1 0
19 28 2 0
1 30 1 0
1 31 1 0
2 32 1 0
2 33 1 0
5 34 1 0
5 35 1 0
12 36 1 0
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14 41 1 0
16 42 1 0
23 43 1 0
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23 45 1 0
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29 52 1 0

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M END

> <Name>

Compound283

> <Activ>

0.15

> <DB_Ref_id>

33.05f

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Compound284

SciTegic10081411483D

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54 56 0 0 0 0          999 V2000
-5.1370 -0.0960 -0.6330 C 0 0
-3.8030 2.0560 -0.4120 C 0 0
-2.5700 1.1720 -0.2870 C 0 0
-2.6420 -0.2190 -0.1870 C 0 0
-3.9570 -0.9850 -0.1740 C 0 0
-1.0150 1.9000 -0.2750 S 0 0
-1.3570 -0.7480 -0.0980 C 0 0
-0.4160 0.2930 -0.1350 C 0 0
-1.0470 -2.1900 0.0200 C 0 0
0.0450 -2.6020 -0.2910 O 0 0
-2.0290 -2.9630 0.4750 O 0 0
-1.6480 -4.3280 0.5570 C 0 0
-2.8220 -5.1550 1.0860 C 0 0
1.0350 0.0450 -0.0580 N 0 0
1.9140 1.0720 -0.2560 C 0 0
3.2560 0.8280 -0.1830 N 0 0
1.5080 2.1850 -0.4960 O 0 0
4.2850 2.0550 -0.4200 S 0 0
5.9320 1.5430 -0.3480 C 0 0
4.0310 2.5880 -1.7480 O 0 0
4.0630 3.0230 0.6390 O 0 0

```

-5.1070	1.3200	-0.0100	C	0	0
-5.2010	1.2150	1.5180	C	0	0
-6.3140	2.1230	-0.5080	C	0	0
8.1600	1.4690	-1.3260	C	0	0
6.8190	1.8870	-1.3830	C	0	0
8.6080	0.7090	-0.2280	C	0	0
6.3810	0.7830	0.7460	C	0	0
7.7210	0.3630	0.8090	C	0	0
9.9790	0.2790	-0.1680	C	0	0
11.0860	-0.0650	-0.1190	N	0	0
-5.1090	-0.0080	-1.7190	H	0	0
-6.0760	-0.5960	-0.3960	H	0	0
-3.8610	2.3810	-1.4510	H	0	0
-3.6640	2.9570	0.1900	H	0	0
-3.8830	-1.8670	-0.8100	H	0	0
-4.1330	-1.3380	0.8420	H	0	0
-1.3610	-4.6620	-0.4410	H	0	0
-0.7910	-4.4050	1.2250	H	0	0
-2.5550	-6.2090	1.1450	H	0	0
-3.1230	-4.8070	2.0720	H	0	0
-3.6830	-5.0670	0.4240	H	0	0
1.3710	-0.8750	0.1390	H	0	0
3.6060	-0.0880	0.0140	H	0	0
-5.2540	2.1950	1.9900	H	0	0
-4.3340	0.6950	1.9240	H	0	0
-6.0920	0.6560	1.8130	H	0	0
-6.3300	3.1310	-0.0920	H	0	0
-7.2460	1.6330	-0.2260	H	0	0
-6.2970	2.2090	-1.5940	H	0	0
8.8320	1.7400	-2.1290	H	0	0
6.4730	2.4710	-2.2230	H	0	0
5.6980	0.5190	1.5410	H	0	0
8.0530	-0.2210	1.6560	H	0	0
3	4	2	0		
2	3	1	0		
1	5	1	0		
8	6	1	0		
7	8	2	0		
3	6	1	0		
4	7	1	0		
7	9	1	0		
9	10	2	0		
9	11	1	0		
11	12	1	0		
12	13	1	0		
8	14	1	0		
14	15	1	0		
15	16	1	0		
15	17	2	0		
16	18	1	0		
18	19	1	0		
18	20	2	0		
18	21	2	0		
1	22	1	0		
22	2	1	0		
22	23	1	0		
22	24	1	0		
29	27	2	0		
28	29	1	0		
25	26	2	0		
27	25	1	0		


```

26 19 1 0
19 28 2 0
27 30 1 0
4 5 1 0
30 31 3 0
1 32 1 0
1 33 1 0
2 34 1 0
2 35 1 0
5 36 1 0
5 37 1 0
12 38 1 0
12 39 1 0
13 40 1 0
13 41 1 0
13 42 1 0
14 43 1 0
16 44 1 0
23 45 1 0
23 46 1 0
23 47 1 0
24 48 1 0
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24 50 1 0
25 51 1 0
26 52 1 0
28 53 1 0
29 54 1 0

```

M END

> <Name>

Compound284

> <Activ>

0.4

> <DB_Ref_id>

33.05

\$\$\$\$

Compound285

SciTegic10081411483D

```

57 59 0 0 0 0          999 V2000
-5.6520 1.1310 -0.0100 C 0 0
-4.3180 3.2830 0.2110 C 0 0
-3.0860 2.4000 0.3360 C 0 0
-3.1580 1.0100 0.4360 C 0 0
-4.4750 0.2440 0.4470 C 0 0
-1.5330 3.1270 0.3480 S 0 0
-1.8750 0.4800 0.5250 C 0 0
-0.9320 1.5210 0.4880 C 0 0
-1.5640 -0.9630 0.6430 C 0 0
-2.3110 -1.7830 0.1620 O 0 0
-0.4450 -1.2680 1.2910 O 0 0
-0.2250 -2.6700 1.3590 C 0 0
1.0720 -2.9450 2.1190 C 0 0
0.5180 1.2730 0.5650 N 0 0
1.1070 0.3960 -0.3010 C 0 0
2.4530 0.1780 -0.2170 N 0 0
0.4450 -0.1820 -1.1310 O 0 0
3.1390 -0.8670 -1.2500 S 0 0

```

4.8150	-1.1090	-0.9100	C	0	0
2.4530	-2.1390	-1.1020	O	0	0
3.0200	-0.3050	-2.5840	O	0	0
-5.6230	2.5490	0.6130	C	0	0
-5.7190	2.4430	2.1410	C	0	0
-6.8300	3.3520	0.1150	C	0	0
7.0820	-1.5350	-1.6720	C	0	0
5.7210	-1.3400	-1.9610	C	0	0
7.5370	-1.5000	-0.3420	C	0	0
5.2660	-1.0740	0.4200	C	0	0
6.6270	-1.2700	0.7050	C	0	0
5.3010	-1.3730	-3.2090	O	0	0
6.0060	-2.1920	-4.1290	C	0	0
7.1350	-1.5370	-4.5510	F	0	0
5.2070	-2.4610	-5.2090	F	0	0
6.3610	-3.3650	-3.5180	F	0	0
-5.6270	1.2210	-1.0980	H	0	0
-6.5940	0.6310	0.2270	H	0	0
-4.3770	3.6090	-0.8280	H	0	0
-4.1820	4.1840	0.8110	H	0	0
-4.3990	-0.6390	-0.1870	H	0	0
-4.6500	-0.1090	1.4650	H	0	0
-1.0740	-3.1230	1.8690	H	0	0
-0.1640	-3.0550	0.3420	H	0	0
1.2830	-4.0140	2.1470	H	0	0
1.9100	-2.4300	1.6500	H	0	0
0.9980	-2.5940	3.1490	H	0	0
1.0680	1.7500	1.2500	H	0	0
3.0160	0.6460	0.4650	H	0	0
-6.6040	1.8910	2.4550	H	0	0
-5.7660	3.4340	2.5940	H	0	0
-4.8460	1.9340	2.5470	H	0	0
-6.8480	4.3590	0.5310	H	0	0
-7.7620	2.8590	0.3970	H	0	0
-6.8130	3.4390	-0.9710	H	0	0
7.7850	-1.7130	-2.4750	H	0	0
8.5840	-1.6500	-0.1250	H	0	0
4.5660	-0.8970	1.2270	H	0	0
6.9750	-1.2420	1.7270	H	0	0
1	5	1	0		
8	6	1	0		
7	8	2	0		
3	6	1	0		
4	7	1	0		
7	9	1	0		
9	10	2	0		
9	11	1	0		
11	12	1	0		
12	13	1	0		
8	14	1	0		
14	15	1	0		
15	16	1	0		
15	17	2	0		
16	18	1	0		
18	19	1	0		
18	20	2	0		
18	21	2	0		
1	22	1	0		
22	2	1	0		
22	23	1	0		
22	24	1	0		

```

29 27 2 0
28 29 1 0
25 26 2 0
27 25 1 0
26 19 1 0
19 28 2 0
26 30 1 0
31 30 1 0
4 5 1 0
3 4 2 0
2 3 1 0
31 34 1 0
31 33 1 0
31 32 1 0
1 35 1 0
1 36 1 0
2 37 1 0
2 38 1 0
5 39 1 0
5 40 1 0
12 41 1 0
12 42 1 0
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13 44 1 0
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14 46 1 0
16 47 1 0
23 48 1 0
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27 55 1 0
28 56 1 0
29 57 1 0
M END
> <Name>
Compound285

> <Activ>
0.4

> <DB_Ref_id>
33.05d

$$$$
Compound286
SciTegic10081411483D

56 58 0 0 0 0 999 V2000
-4.6020 0.9750 0.6520 C 0 0
-2.5820 2.5140 0.7440 C 0 0
-1.7340 1.2500 0.7830 C 0 0
-2.2710 -0.0250 0.6170 C 0 0
-3.7500 -0.2790 0.3590 C 0 0
-0.0450 1.3850 1.0510 S 0 0
-1.2580 -0.9750 0.7150 C 0 0
-0.0290 -0.3340 0.9450 C 0 0
-1.4570 -2.4380 0.5920 C 0 0

```

-0.5210	-3.1900	0.7210	O	0	0
-2.7010	-2.8360	0.3380	O	0	0
-2.8070	-4.2500	0.2580	C	0	0
-4.2580	-4.6370	-0.0310	C	0	0
1.2330	-1.0760	1.0940	N	0	0
2.4200	-0.4020	1.1350	C	0	0
3.5840	-1.1060	1.2740	N	0	0
2.4420	0.8030	1.0510	O	0	0
4.9850	-0.2930	1.3220	S	0	0
5.2350	0.6520	-0.1010	C	0	0
4.9300	0.6050	2.4610	O	0	0
6.0550	-1.2720	1.4140	O	0	0
-3.9750	2.2790	0.1040	C	0	0
-3.8420	2.1860	-1.4220	C	0	0
-4.8890	3.4650	0.4320	C	0	0
5.9260	0.8320	-2.4300	C	0	0
5.7270	0.0510	-1.2770	C	0	0
5.6350	2.2070	-2.4080	C	0	0
4.9440	2.0270	-0.0800	C	0	0
5.1430	2.8050	-1.2340	C	0	0
6.0350	-1.4020	-1.3070	C	0	0
5.0140	-2.1000	-0.7150	F	0	0
7.2030	-1.6350	-0.6250	F	0	0
6.1780	-1.8130	-2.6070	F	0	0
-4.7300	1.0700	1.7330	H	0	0
-5.6040	0.8340	0.2440	H	0	0
-2.6950	2.8570	1.7720	H	0	0
-2.0390	3.2990	0.2130	H	0	0
-4.0960	-1.1190	0.9630	H	0	0
-3.8650	-0.5700	-0.6850	H	0	0
-2.1500	-4.5980	-0.5390	H	0	0
-2.4780	-4.6720	1.2070	H	0	0
-4.3610	-5.7190	-0.1110	H	0	0
-4.9180	-4.2740	0.7580	H	0	0
-4.5940	-4.1990	-0.9710	H	0	0
1.2170	-2.0740	1.1620	H	0	0
3.5820	-2.1040	1.3440	H	0	0
-3.4590	3.1090	-1.8530	H	0	0
-4.8110	1.9800	-1.8810	H	0	0
-3.1640	1.3790	-1.7030	H	0	0
-4.4770	4.4060	0.0680	H	0	0
-5.0310	3.5550	1.5080	H	0	0
-5.8690	3.3320	-0.0250	H	0	0
6.3030	0.3810	-3.3360	H	0	0
5.7870	2.8070	-3.2950	H	0	0
4.5670	2.4860	0.8200	H	0	0
4.9200	3.8610	-1.2170	H	0	0
1	5	1	0		
8	6	1	0		
7	8	2	0		
3	6	1	0		
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9	11	1	0		
11	12	1	0		
12	13	1	0		
8	14	1	0		
14	15	1	0		
15	16	1	0		
15	17	2	0		

```

16 18 1 0
18 19 1 0
18 20 2 0
18 21 2 0
1 22 1 0
22 2 1 0
22 23 1 0
22 24 1 0
29 27 2 0
28 29 1 0
25 26 2 0
27 25 1 0
26 19 1 0
19 28 2 0
26 30 1 0
4 5 1 0
3 4 2 0
2 3 1 0
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30 32 1 0
30 31 1 0
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13 44 1 0
14 45 1 0
16 46 1 0
23 47 1 0
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29 56 1 0

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M END

> <Name>

Compound286

> <Activ>

0.2

> <DB_Ref_id>

33.05c

\$\$\$\$

Compound287

SciTegic10081411483D

```

53 55 0 0 0 0          999 V2000
-4.9240 -0.1070 -0.6780 C 0 0
-3.5900 2.0450 -0.4570 C 0 0

```

-2.3570	1.1600	-0.3320	C	0	0
-2.4300	-0.2290	-0.2340	C	0	0
-3.7440	-0.9940	-0.2210	C	0	0
-0.8030	1.8890	-0.3200	S	0	0
-1.1450	-0.7580	-0.1450	C	0	0
-0.2010	0.2810	-0.1820	C	0	0
-0.8340	-2.2010	-0.0270	C	0	0
0.2660	-2.6090	-0.3130	O	0	0
-1.8260	-2.9790	0.4000	O	0	0
-1.4430	-4.3440	0.4840	C	0	0
-2.6270	-5.1740	0.9800	C	0	0
1.2480	0.0350	-0.1040	N	0	0
2.1270	1.0640	-0.2830	C	0	0
3.4690	0.8200	-0.2110	N	0	0
1.7210	2.1820	-0.5060	O	0	0
4.4980	2.0530	-0.4260	S	0	0
6.1430	1.5590	-0.2560	C	0	0
4.3070	2.5510	-1.7750	O	0	0
4.2130	3.0450	0.5980	O	0	0
-4.8950	1.3110	-0.0550	C	0	0
-4.9880	1.2050	1.4730	C	0	0
-6.1000	2.1130	-0.5530	C	0	0
8.4240	1.5100	-1.1020	C	0	0
7.0840	1.9120	-1.2380	C	0	0
8.8220	0.7540	0.0180	C	0	0
6.5370	0.8050	0.8610	C	0	0
7.8770	0.4020	0.9980	C	0	0
10.0900	0.3730	0.1460	F	0	0
-4.8970	-0.0180	-1.7660	H	0	0
-5.8630	-0.6070	-0.4410	H	0	0
-3.6480	2.3710	-1.4960	H	0	0
-3.4510	2.9450	0.1430	H	0	0
-3.6700	-1.8770	-0.8560	H	0	0
-3.9200	-1.3500	0.7950	H	0	0
-1.1310	-4.6720	-0.5080	H	0	0
-0.6040	-4.4220	1.1740	H	0	0
-2.3590	-6.2290	1.0430	H	0	0
-2.9550	-4.8320	1.9630	H	0	0
-3.4730	-5.0860	0.2990	H	0	0
1.5860	-0.8890	0.0780	H	0	0
3.8180	-0.0980	-0.0270	H	0	0
-5.0650	2.1860	1.9430	H	0	0
-4.1090	0.7070	1.8790	H	0	0
-5.8650	0.6270	1.7660	H	0	0
-6.1250	3.1150	-0.1270	H	0	0
-7.0310	1.6150	-0.2830	H	0	0
-6.0760	2.2110	-1.6390	H	0	0
9.1470	1.7810	-1.8570	H	0	0
6.7810	2.4920	-2.0980	H	0	0
5.8150	0.5330	1.6150	H	0	0
8.1780	-0.1780	1.8590	H	0	0
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3	4	2	0		
2	3	1	0		
1	5	1	0		
8	6	1	0		
7	8	2	0		
3	6	1	0		
4	7	1	0		
7	9	1	0		
9	10	2	0		

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12 13  1  0
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15 17  2  0
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18 20  2  0
18 21  2  0
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22  2  1  0
22 23  1  0
22 24  1  0
29 27  2  0
28 29  1  0
25 26  2  0
27 25  1  0
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19 28  2  0
27 30  1  0
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12 37  1  0
12 38  1  0
13 39  1  0
13 40  1  0
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14 42  1  0
16 43  1  0
23 44  1  0
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23 46  1  0
24 47  1  0
24 48  1  0
24 49  1  0
25 50  1  0
26 51  1  0
28 52  1  0
29 53  1  0
M  END
> <Name>
Compound287

> <Activ>
0.5

> <DB_Ref_id>
33.05b

$$$$
Compound288
  SciTegic10081411483D

53 55  0  0  0  0          999 V2000
  -4.2210  -0.5660  0.0000 C  0  0

```

-2.8870	1.5860	0.2210	C	0	0
-1.6540	0.7010	0.3460	C	0	0
-1.7270	-0.6880	0.4450	C	0	0
-3.0410	-1.4550	0.4590	C	0	0
-0.1020	1.4300	0.3570	S	0	0
-0.4420	-1.2170	0.5350	C	0	0
0.5000	-0.1780	0.4980	C	0	0
-0.1330	-2.6600	0.6520	C	0	0
0.9590	-3.0720	0.3380	O	0	0
-1.1110	-3.4320	1.1130	O	0	0
-0.7310	-4.7970	1.1930	C	0	0
-1.9020	-5.6230	1.7280	C	0	0
1.9490	-0.4260	0.5740	N	0	0
2.8280	0.6010	0.3790	C	0	0
4.1700	0.3570	0.4530	N	0	0
2.4240	1.7170	0.1440	O	0	0
5.2010	1.5860	0.2210	S	0	0
5.0390	2.2750	-1.3540	C	0	0
4.8890	2.6090	1.2030	O	0	0
6.5470	1.0590	0.3510	O	0	0
-4.1920	0.8500	0.6230	C	0	0
-4.2870	0.7440	2.1520	C	0	0
-5.3990	1.6520	0.1250	C	0	0
4.2280	4.0570	-2.7990	C	0	0
4.3590	3.4960	-1.5180	C	0	0
4.7770	3.4000	-3.9160	C	0	0
5.5880	1.6170	-2.4670	C	0	0
5.4550	2.1800	-3.7480	C	0	0
-4.1940	-0.4770	-1.0880	H	0	0
-5.1600	-1.0660	0.2360	H	0	0
-2.9450	1.9100	-0.8180	H	0	0
-2.7480	2.4860	0.8200	H	0	0
-2.9670	-2.3380	-0.1780	H	0	0
-3.2170	-1.8090	1.4750	H	0	0
-0.4470	-5.1330	0.1950	H	0	0
0.1290	-4.8730	1.8570	H	0	0
-2.7700	-5.5290	1.0740	H	0	0
-1.6290	-6.6740	1.8070	H	0	0
-2.1940	-5.2790	2.7210	H	0	0
2.2870	-1.3460	0.7690	H	0	0
4.5210	-0.5590	0.6460	H	0	0
-4.3400	1.7270	2.6250	H	0	0
-3.4180	0.2260	2.5570	H	0	0
-5.1760	0.1850	2.4450	H	0	0
-5.4140	2.6600	0.5410	H	0	0
-6.3300	1.1600	0.4040	H	0	0
-5.3810	1.7420	-0.9610	H	0	0
3.7070	4.9940	-2.9280	H	0	0
3.9390	4.0020	-0.6620	H	0	0
4.6760	3.8320	-4.9010	H	0	0
6.1090	0.6800	-2.3420	H	0	0
5.8770	1.6760	-4.6060	H	0	0
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3	4	2	0		
2	3	1	0		
1	5	1	0		
8	6	1	0		
7	8	2	0		
3	6	1	0		
4	7	1	0		
7	9	1	0		


```

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  9 11  1  0
11 12  1  0
12 13  1  0
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14 15  1  0
15 16  1  0
15 17  2  0
16 18  1  0
18 19  1  0
18 20  2  0
18 21  2  0
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22  2  1  0
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22 24  1  0
29 27  2  0
28 29  1  0
25 26  2  0
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24 46  1  0
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M  END
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Compound288

> <Activ>
0.2

> <DB_Ref_id>
33.05a

$$$$
Compound289
  SciTegic10081411483D

56 58  0  0  0  0          999 V2000

```

-5.4960	-0.1150	-0.6760	C	0	0
-4.1620	2.0370	-0.4550	C	0	0
-2.9300	1.1520	-0.3300	C	0	0
-3.0020	-0.2360	-0.2310	C	0	0
-4.3180	-1.0040	-0.2190	C	0	0
-1.3770	1.8810	-0.3190	S	0	0
-1.7190	-0.7680	-0.1430	C	0	0
-0.7750	0.2730	-0.1780	C	0	0
-1.4080	-2.2090	-0.0240	C	0	0
-0.3160	-2.6230	-0.3380	O	0	0
-2.3890	-2.9820	0.4350	O	0	0
-2.0080	-4.3480	0.5150	C	0	0
-3.1800	-5.1720	1.0490	C	0	0
0.6740	0.0250	-0.1020	N	0	0
1.5530	1.0550	-0.2930	C	0	0
2.8950	0.8110	-0.2190	N	0	0
1.1480	2.1700	-0.5260	O	0	0
3.9260	2.0390	-0.4470	S	0	0
5.5700	1.5410	-0.2970	C	0	0
3.7190	2.5350	-1.7970	O	0	0
3.6520	3.0330	0.5760	O	0	0
-5.4670	1.3010	-0.0530	C	0	0
-5.5630	1.1950	1.4740	C	0	0
-6.6740	2.1040	-0.5510	C	0	0
7.7910	1.2910	-1.2580	C	0	0
6.4510	1.6950	-1.3810	C	0	0
8.2500	0.7320	-0.0510	C	0	0
6.0250	0.9840	0.9100	C	0	0
7.3650	0.5780	1.0310	C	0	0
9.6660	0.3030	0.0780	C	0	0
-5.4710	-0.0270	-1.7640	H	0	0
-6.4380	-0.6150	-0.4400	H	0	0
-4.2210	2.3610	-1.4940	H	0	0
-4.0260	2.9380	0.1440	H	0	0
-4.2440	-1.8870	-0.8540	H	0	0
-4.4940	-1.3570	0.7990	H	0	0
-1.7230	-4.6820	-0.4830	H	0	0
-1.1490	-4.4240	1.1810	H	0	0
-2.9120	-6.2270	1.1110	H	0	0
-3.4790	-4.8240	2.0370	H	0	0
-4.0430	-5.0860	0.3900	H	0	0
1.0120	-0.8950	0.0900	H	0	0
3.2460	-0.1070	-0.0280	H	0	0
-5.6150	2.1780	1.9470	H	0	0
-4.6940	0.6780	1.8790	H	0	0
-6.4510	0.6370	1.7670	H	0	0
-6.6920	3.1110	-0.1350	H	0	0
-7.6060	1.6130	-0.2700	H	0	0
-6.6580	2.1910	-1.6370	H	0	0
8.4650	1.4100	-2.0940	H	0	0
6.1000	2.1250	-2.3090	H	0	0
5.3480	0.8670	1.7420	H	0	0
7.7110	0.1500	1.9610	H	0	0
9.9220	-0.1150	1.0530	H	0	0
10.3220	1.1560	-0.0980	H	0	0
9.8890	-0.4490	-0.6780	H	0	0
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3	4	2	0		
2	3	1	0		
1	5	1	0		
8	6	1	0		

7	8	2	0
3	6	1	0
4	7	1	0
7	9	1	0
9	10	2	0
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12	13	1	0
8	14	1	0
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Compound289

> <Activ>

0.4

> <DB_Ref_id>

33.04d

\$\$\$\$

Compound290

SciTegic10081411483D

45	47	0	0	0	0	999	V2000
0.4140	3.2540	-2.2830	S	0	0		
1.1020	2.7660	-0.8180	C	0	0		
0.7580	1.4770	-0.4040	C	0	0		
-0.1110	0.8910	-1.3530	C	0	0		
-0.3890	1.7560	-2.4410	C	0	0		
-0.6580	-0.4690	-1.2090	N	0	0		
-0.3070	-1.3500	0.1040	S	0	0		
-1.1290	-2.8690	0.1040	C	0	0		
1.1230	-1.6020	0.0920	O	0	0		
-0.7460	-0.5940	1.2660	O	0	0		
-3.1910	-4.1600	0.1040	C	0	0		
-2.5350	-2.9160	0.1040	C	0	0		
-2.4430	-5.3520	0.1040	C	0	0		
-0.3810	-4.0590	0.1040	C	0	0		
-1.0390	-5.3010	0.1040	C	0	0		
-1.2480	1.4340	-3.5740	C	0	0		
-1.3540	2.3730	-4.5100	O	0	0		
-1.8140	0.3670	-3.6210	O	0	0		
-3.3300	-1.6600	0.1040	C	0	0		
-3.1410	-6.6660	0.1040	C	0	0		
2.0100	3.6330	-0.0170	C	0	0		
2.3540	4.9220	-0.4310	C	0	0		
3.2210	5.5000	0.5220	C	0	0		
3.4980	4.6390	1.6080	C	0	0		
2.6970	3.1410	1.4480	S	0	0		
4.3590	4.9750	2.7310	C	0	0		
4.5860	3.9470	3.8090	C	0	0		
4.8830	6.0650	2.7910	O	0	0		
1.1040	1.0020	0.5040	H	0	0		
-1.2460	-0.8500	-1.9240	H	0	0		
-4.2720	-4.2010	0.1040	H	0	0		
0.6990	-4.0220	0.1040	H	0	0		
-0.4590	-6.2130	0.1040	H	0	0		
-1.9100	2.2090	-5.2810	H	0	0		
-3.0100	-0.9280	0.8440	H	0	0		
-4.3770	-1.8930	0.2990	H	0	0		
-3.2700	-1.1910	-0.8770	H	0	0		
-2.4710	-7.5280	0.1040	H	0	0		
-3.7770	-6.7400	-0.7750	H	0	0		
-3.7770	-6.7400	0.9850	H	0	0		
2.0120	5.4020	-1.3380	H	0	0		
3.6290	6.4980	0.4240	H	0	0		
5.3090	4.3220	4.5320	H	0	0		
3.6370	3.6950	4.2830	H	0	0		
4.9920	3.0370	3.3710	H	0	0		
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4	5	2	0				
3	4	1	0				
1	2	1	0				
2	3	2	0				
4	6	1	0				
6	7	1	0				
7	8	1	0				
7	9	2	0				

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12  8  1  0
  8 14  2  0
  5 16  1  0
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16 18  2  0
12 19  1  0
13 20  1  0
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24 25  1  0
23 24  2  0
21 22  2  0
22 23  1  0
21  2  1  0
24 26  1  0
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Compound290

> <Activ>
0.3073

> <DB_Ref_id>
35.03

$$$$
Compound291
  SciTegic10081411483D

41 43  0  0  0  0          999 V2000
  -0.0220    1.7420   -3.1410 S    0  0
  -1.2290    1.3260   -2.0270 C    0  0
  -0.7150    0.7210   -0.8710 C    0  0
   0.6930    0.6150   -0.9360 C    0  0
   1.2150    1.1410   -2.1370 C    0  0
   1.5080    0.0220    0.1390 N    0  0
   0.7930   -0.5550    1.4750 S    0  0
   1.9370   -1.2090    2.5900 C    0  0

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0.1110	0.5550	2.1170	O	0	0
-0.1060	-1.6190	1.0620	O	0	0
3.4900	-2.9670	3.2440	C	0	0
2.5610	-2.4430	2.3260	C	0	0
3.7950	-2.2580	4.4180	C	0	0
2.2420	-0.5000	3.7640	C	0	0
3.1720	-1.0250	4.6800	C	0	0
-2.6990	1.4960	-2.0860	C	0	0
-4.6450	2.8150	-2.7330	C	0	0
-3.2500	2.6490	-2.6760	C	0	0
-5.4850	1.8200	-2.1970	C	0	0
-3.5430	0.5060	-1.5530	C	0	0
-4.9400	0.6660	-1.6070	C	0	0
2.6250	1.1800	-2.5020	C	0	0
2.9080	1.7230	-3.6820	O	0	0
3.4590	0.7320	-1.7500	O	0	0
2.2420	-3.1990	1.0860	C	0	0
-6.9120	1.9860	-2.2560	C	0	0
-8.0650	2.1190	-2.3050	N	0	0
-1.3050	0.3770	-0.0310	H	0	0
2.5020	-0.0250	0.0450	H	0	0
3.9730	-3.9120	3.0510	H	0	0
4.5100	-2.6600	5.1210	H	0	0
1.7640	0.4470	3.9670	H	0	0
3.4060	-0.4800	5.5820	H	0	0
-5.0550	3.7050	-3.1880	H	0	0
-2.6040	3.4120	-3.0860	H	0	0
-3.1250	-0.3810	-1.1000	H	0	0
-5.5780	-0.1030	-1.1930	H	0	0
3.8280	1.7720	-3.9710	H	0	0
1.2480	-3.6390	1.1740	H	0	0
2.3360	-2.5390	0.2250	H	0	0
2.9570	-4.0120	0.9630	H	0	0
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3	4	1	0		
1	2	1	0		
2	3	2	0		
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18	16	1	0		
16	2	1	0		
5	22	1	0		
22	23	1	0		
22	24	2	0		
12	25	1	0		
19	26	1	0		
5	1	1	0		

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3 28 1 0
6 29 1 0
11 30 1 0
13 31 1 0
14 32 1 0
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M END

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Compound291

> <Activ>

0.2663

> <DB_Ref_id>

35.02

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Compound292

SciTegic10081411483D

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42 44 0 0 1 0          999 V2000
-4.3010 1.0650 -1.1190 C 0 0
-2.9810 1.5860 -1.0840 C 0 0
-1.8970 0.6740 -0.9100 C 0 0
-0.5640 0.9470 -0.8400 C 0 0
0.2480 2.2330 -0.9080 C 0 0
1.7270 1.9880 -0.4900 C 0 0
2.2380 0.7620 -1.0270 O 0 0
1.0550 -0.4120 -3.2560 O 0 0
2.0880 -2.3420 -3.7400 O 0 0
1.6930 -1.3790 -2.9120 C 0 0
2.1000 -1.5660 -1.4750 C 0 0
1.5960 -0.4360 -0.5720 C 0 0 3 0 0 0
0.0840 -0.2810 -0.6860 C 0 0
-2.1290 -0.6820 -0.7910 C 0 0
-3.7270 -2.9080 -0.6740 Cl 0 0
-3.4400 -1.2210 -0.8260 C 0 0
-4.5290 -0.3300 -0.9900 C 0 0
-0.8910 -1.3030 -0.6480 N 0 0
-2.7750 3.2850 -1.2580 Cl 0 0
1.9980 -0.6780 0.8870 C 0 0
0.9240 -0.2270 1.8770 C 0 0
1.4340 -0.1760 3.3180 C 0 0
0.3610 0.2750 4.3090 C 0 0
-5.1490 1.7210 -1.2440 H 0 0
0.2050 2.6170 -1.9280 H 0 0
-0.1840 2.9900 -0.2520 H 0 0
2.3560 2.8050 -0.8460 H 0 0
1.8260 1.9610 0.5960 H 0 0
1.8610 -2.2810 -4.6780 H 0 0
1.6600 -2.4820 -1.0820 H 0 0
3.1840 -1.6600 -1.4040 H 0 0

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-5.5450	-0.7010	-1.0180	H	0	0
-0.7170	-2.2750	-0.5410	H	0	0
2.2540	-1.7250	1.0470	H	0	0
2.9530	-0.1990	1.1070	H	0	0
0.5100	0.7380	1.5820	H	0	0
0.0410	-0.8590	1.8030	H	0	0
1.8500	-1.1390	3.6130	H	0	0
2.3180	0.4570	3.3930	H	0	0
0.7560	0.2890	5.3240	H	0	0
-0.0020	1.2720	4.0550	H	0	0
-0.4900	-0.4040	4.2890	H	0	0

1	17	2	0
1	2	1	0
3	2	2	0
14	3	1	0
3	4	1	0
4	13	2	0
4	5	1	0
6	5	1	0
7	6	1	0
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M END

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Compound292

> <Activ>

0.76


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> <DB_Ref_id>  
26.08
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