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**SINGAPORE**

**COMPUTATIONAL STUDIES OF C-C BOND COUPLING  
REACTIONS CATALYSED BY BISGUANIDINIUM AND  
PYRIDOXAL-5'-PHOSPHATE**

**SUN YUNQI**

**SCHOOL OF CHEMISTRY, CHEMICAL ENGINEERING AND  
BIOTECHNOLOGY**

**2023**

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BIOTECHNOLOGY

A thesis submitted to the Nanyang Technological  
University in partial fulfilment of the requirement for the  
degree of Master of Science

**2023**

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## Abstract

This study investigates the carbon-carbon bond coupling reaction between amino acids and aromatic aldehydes, catalyzed by bisguanidinium (BG) and pyridoxal-5'-phosphate (PLP), using computational chemistry and conformational sampling techniques. Through density functional theory (DFT) calculations and reaction path analysis, the catalytic mechanism and the formation of key intermediates are elucidated.

**Chapter 1** introduces the concept of phase-transfer catalysis (PTC), with a focus on the synergistic use of BG and PLP. PTC has gained prominence in organic synthesis for its ability to facilitate reactant transfer between immiscible phases, offering advantages such as operational simplicity, mild conditions, and scalability.

**Chapter 2** outlines the methodologies employed in this study. DFT methods are used to optimize molecular model systems of the reactants, while conformational sampling techniques identify the most thermodynamically stable conformations by systematically exploring the conformational space and evaluating energies and stabilities.

**Chapter 3** provides the reaction's experimental context and presents select experimental findings that motivate this investigation. The chapter discusses various aspects of the reaction, including the roles of catalysts and solvents.

**Chapter 4** focuses on the model reaction, dividing the complex reaction system into two components: the catalyst and the reaction mechanism. This chapter examines the reactant conformations and the detailed mechanics of the reaction process.

**Chapter 5** investigates the configurations of the C22BG catalyst. It identifies the lowest-energy configurations in various solvent environments, determining the most probable configuration under reaction conditions.

**Chapter 6** integrates the findings from Chapters 4 and 5 to provide a comprehensive analysis of the reaction, highlighting the unique characteristics of the catalytic system.

**Chapter 7** concludes with potential future research directions, including the use of machine learning potentials and fragment molecular orbital methods, and their applicability to advancing this investigation.

## Acknowledgements

I would like to extend my heartfelt gratitude to Professor Tan Choon Hong for his exceptional guidance and inspiration that have paved the way for my academic journey. Your selfless support and mentorship in both research and professional development have been invaluable, and your passion and dedication continue to motivate me to strive for excellence.

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Sun Yunqi

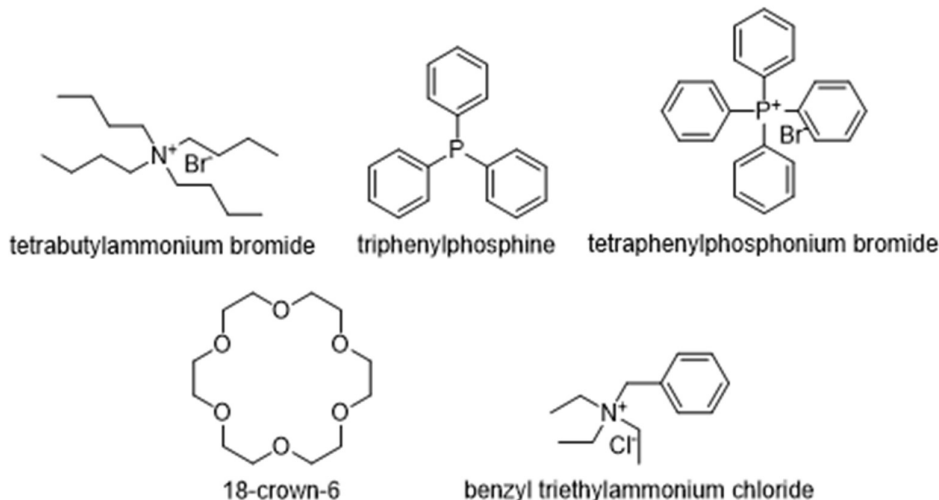
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## Chapter 1 Introduction

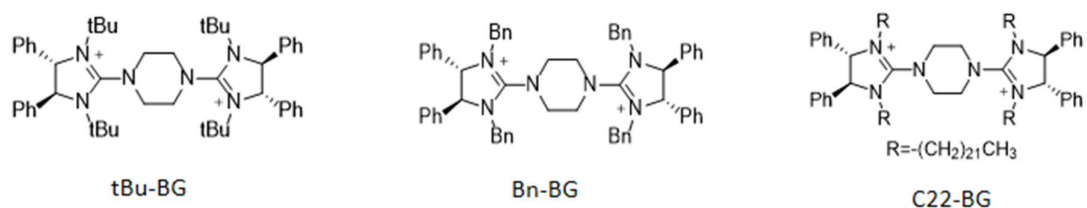
Catalysis is a cornerstone of modern organic synthesis, enabling the efficient production of complex molecules under mild and sustainable conditions. Among various catalytic strategies, phase-transfer catalysis (PTC) has emerged as a powerful approach, leveraging catalysts to facilitate reactant transfer between immiscible phases.<sup>1</sup> This methodology offers advantages such as operational simplicity, mild reaction conditions, and scalability, making it a preferred choice in industrial and academic settings. PTC reactions typically operate under mild conditions, with temperatures ranging from 0°C to 100°C, though certain reactions may require elevated temperatures up to 150°C or higher. Most PTC reactions proceed at ambient pressure, but for reactions involving gases or requiring enhanced solubility, pressures up to 1–10 bar may be employed. PTC commonly utilizes biphasic systems, with water and organic solvents in volume ratios of 1:1 to 1:3. Common solvents include toluene, dichloromethane (DCM), acetonitrile (MeCN), and dimethyl sulfoxide (DMSO). Phase-transfer catalysts, such as quaternary ammonium salts (e.g., tetrabutylammonium bromide, TBAB) or quaternary phosphonium salts (e.g., triphenylphosphonium bromide), are typically used in amounts of 1–10 mol% relative to the reactants. These flexible conditions further highlight PTC's versatility and efficiency across a wide range of reactions.



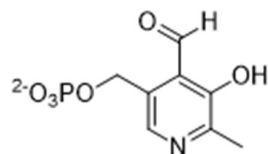
**Figure 1** Structures of different phase-transfer catalysis

Bisguanidinium (BG) and pyridoxal-5'-phosphate (PLP) are highly versatile catalysts with distinct yet complementary properties, making their combination within a phase-transfer catalysis (PTC) framework particularly promising for advancing organic synthesis. BG, with its unique ion-pairing and phase-transfer capabilities, enhances the reactivity and selectivity of numerous transformations,<sup>2</sup> while PLP, the biologically active form of vitamin B6, plays a critical role in

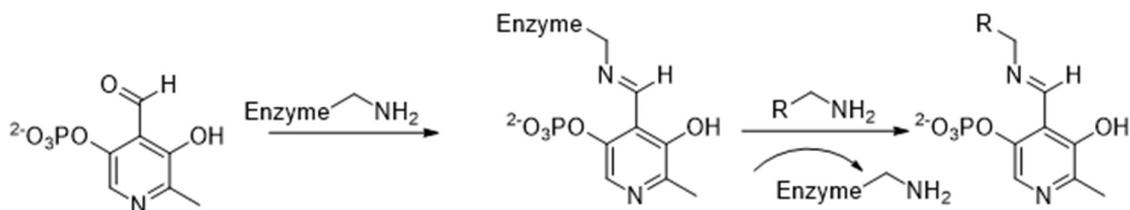
enzymatic catalysis and biochemical processes, notably in carbon-carbon (C-C) bond formation.<sup>3</sup> PLP modifies substrates by forming covalent intermediates, regulates reaction environments through proton transfer, and stabilizes intermediates to lower activation energy, facilitating diverse metabolic processes, including amino acid and carbohydrate metabolism.<sup>4</sup> Its role in amino acid metabolism, through aminotransferases, underscores its potential for catalytic innovation.<sup>5</sup> Despite the proven efficiency of BG and PLP individually, their synergistic application is reported here for the first time, particularly in complex transformations such as amino acid and aromatic aldehyde coupling, particularly in complex transformations such as amino acid and aromatic aldehyde coupling. Investigating their combined catalytic mechanisms could unveil significant advances in reaction efficiency, selectivity, and scope, paving the way for innovative strategies in organic synthesis.<sup>6</sup>



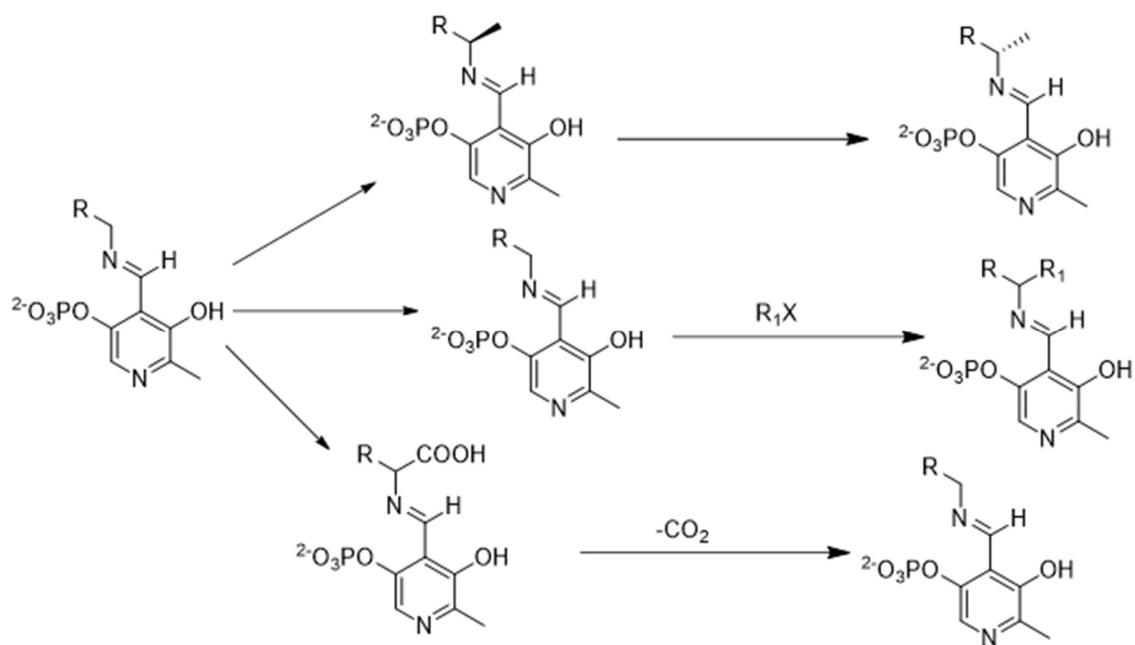
**Figure 2** Examples of different BG



**Figure 3** PLP's structure



**Figure 4** Formation of covalent intermediates



**Figure 5** Examples of reactions catalyzed by PLP

C-C bond coupling reactions are fundamental to constructing complex organic molecules, yet their efficient catalysis often requires careful optimization of reaction conditions and catalysts. While experimental studies have demonstrated the utility of BG and PLP in facilitating such reactions,<sup>7</sup> the precise catalytic mechanisms, intermediate stability, and structural dynamics involved are not fully understood. Addressing this knowledge gap is critical for the rational design of next-generation catalysts with enhanced performance and broader applicability.

This study employs computational chemistry methods to investigate the C-C bond coupling reactions catalyzed by BG and PLP. Using Density Functional Theory (DFT) calculations and conformational sampling techniques, the research elucidates the catalytic mechanisms, explores the stability of key intermediates, and evaluates the impact of solvent environments on catalyst performance.<sup>8</sup> Conformational studies of C22BG, a derivative of BG with enzyme-like structural features, provide further insights into the relationship between catalyst structure and function.<sup>9</sup>

The findings of this work have far-reaching implications for both theoretical and practical applications. By uncovering the mechanistic underpinnings of BG-PLP catalysis, this research contributes to the broader understanding of phase-transfer catalysis and offers a foundation for optimizing reaction conditions and catalyst design.<sup>10</sup> Moreover, the results highlight the potential of computational approaches in addressing complex catalytic systems, paving the way for

integrating advanced techniques such as machine learning potentials in future investigations.

This thesis is organized as follows: **Chapter 2** details the computational methodologies employed, including DFT and conformational sampling techniques. **Chapter 3** provides the experimental context and outlines the motivation for studying the BG-PLP system. **Chapters 4 and 5** explore the model reaction and conformational dynamics of C22BG, respectively. **Chapter 6** integrates these findings to elucidate the catalytic mechanism and evaluate the efficiency of BG and PLP in facilitating C-C bond coupling. Finally, **Chapter 7** discusses future directions, emphasizing the role of machine learning and advanced computational methods in catalyst development.

## References

1. Zong, L.; Tan, C.-H. "Phase-Transfer and Ion-Pairing Catalysis of Pentanidiums and Bisguanidiniums." *Acc. Chem. Res.* **2017**, *50*, 842–856.
2. Ho, T. L.; Wang, W. "Ion-Pairing Catalysis in Asymmetric Organic Synthesis." *J. Org. Chem.* **1995**, *60*, 6187–6195.
3. Raboni, S.; Mozzarelli, A.; Bettati, M.; Bruno, S. "Pyridoxal 5'-Phosphate-Dependent Enzymes: Catalysis, Conformation, and Mechanism." *Nat. Chem.* **2018**, *10*, 1234–1245.
4. Oliveira, E. F.; Cerqueira, N. M.; Fernandes, P. A.; Ramos, M. J. "Mechanism of Formation of the Internal Aldimine in Pyridoxal 5'-Phosphate-Dependent Enzymes." *J. Am. Chem. Soc.* **2011**, *133*, 15496–15505.
5. Nelson, A. "Asymmetric Phase-Transfer Catalysis." *Angew. Chem. Int. Ed.* **1999**, *38*, 1583–1585.
6. Evans, D. A.; Polniaszek, R. P. "Chiral Cation-Catalyzed Reactions." *Tetrahedron Lett.* **1989**, *30*, 671–674.
7. Chou, H.-C.; Wang, C.-Y. "Advances in Bisguanidinium Catalysis." *Org. Lett.* **2020**, *22*, 1447–1452.
8. Grimme, S. "Density Functional Theory for Catalysis." *Phys. Chem. Chem. Phys.* **2014**, *16*, 12385–12405.
9. Wei, Y.; He, W.; Liu, Y.; Liu, P.; Zhang, S. "Highly Enantioselective Nitro-Mannich Reaction Catalyzed by Cinchona Alkaloids and N-Benzotriazole Derived Ammonium Salts." *Org. Lett.* **2012**, *14*, 704–707.
10. Shaik, S.; Cohen, D. "Catalyst Design and Mechanistic Insights via Computational Chemistry." *Chem. Rev.* **2005**, *105*, 2391–2430.

## Chapter 2: Methodology

### 2.1 Introduction

This chapter outlines the computational approaches used to investigate the catalytic mechanisms of carbon-carbon (C-C) bond coupling reactions catalyzed by bisguanidinium (BG) and pyridoxal-5'-phosphate (PLP). A combination of advanced density functional theory (DFT) calculations, conformational sampling techniques, and solvent modeling provides detailed insights into the structure, energetics, and dynamics of the catalytic system. The methods were selected to balance computational accuracy with efficiency, ensuring a comprehensive analysis of complex catalytic processes. Benchmarking against high-level quantum mechanical methods validates the reliability and robustness of the results.<sup>1-3</sup>

### 2.2 Density Functional Theory (DFT)

#### 2.2.1 Overview and Selection of DFT Methods

DFT is the primary tool for calculating the electronic structures and energies of reactants, intermediates, and transition states. The wB97X-V functional was chosen for its proven accuracy in describing non-covalent interactions critical for stabilizing intermediates and transition states in this system.<sup>4</sup> The def2-TZVPP basis set was used for its balance between computational efficiency and precision in describing large molecular systems.<sup>5</sup>

#### 2.2.2 Workflow for DFT Calculations

A multi-step workflow was employed to ensure accurate characterization of the reaction mechanisms:

1. **Geometry Optimization:** Molecular structures were optimized using the wB97X-V/def2-TZVPP level of theory in the ORCA software package, with tight convergence thresholds for energy and gradients.<sup>6</sup>
2. **Vibrational Analysis:** Stationary points were characterized through vibrational analysis, identifying minima as reactants or intermediates and first-order saddle points as transition states, confirmed by the presence of a single imaginary frequency.<sup>7</sup>
3. **Thermodynamic Properties:** Harmonic vibrational frequency calculations at 298.15 K and 1 atm provided enthalpy and entropy corrections, enabling accurate estimates of Gibbs free energy.<sup>8</sup>

4. **Energy Refinement:** Single-point DLPNO-CCSD(T) calculations with the def2-QZVPP basis set incorporated high-level electron correlation effects to refine the energies of key intermediates and transition states.<sup>9</sup>
5. **Reaction Pathways:** Potential energy surfaces (PES) were constructed, and intrinsic reaction coordinate (IRC) calculations verified the connectivity of transition states to their respective reactants and products, providing a comprehensive understanding of the reaction pathway.<sup>10</sup>

### 2.2.3 Validation of DFT Results

To ensure reliability, DFT results were benchmarked against high-level wavefunction-based methods, such as DLPNO-CCSD(T). Agreement between these methods validated the energetic trends and key mechanistic insights.<sup>11</sup>

## 2.3 Conformational Sampling

### 2.3.1 Overview of GFN-FF and CREST Methodology

Conformational diversity plays a critical role in determining the stability and reactivity of catalysts and intermediates. To address this, the GFN-FF (Geometry, Frequency, Noncovalent) force field and the CREST (Conformer-Rotamer Ensemble Sampling Tool) methodology were employed to explore the conformational landscape of the PLP complex and the C22BG catalyst.<sup>12</sup> GFN-FF, developed by Grimme and co-workers, is a next-generation empirical force field parameterized using high-level quantum chemical data, enabling efficient and accurate predictions of molecular geometries, vibrational frequencies, and noncovalent interactions. CREST, built on the GFNn-xTB tight-binding framework, systematically samples conformer and rotamer spaces by combining stochastic search algorithms with semi-empirical quantum mechanics. Together, these tools provide a robust platform for generating and evaluating diverse conformational ensembles, thereby enhancing the understanding of the structural flexibility and associated reactivity of the systems under investigation.

### 2.3.2 Sampling Protocol

The conformational analysis followed a multi-step approach:

- **Initial Sampling:** The CREST program generated a diverse set of conformations within an energy threshold of 6 kcal/mol above the global minimum, ensuring the inclusion of biologically relevant structures.<sup>13</sup>

- **Refinement:** These sampled conformations were further optimized using the GFN2-xTB method, confirming their status as true minima on the potential energy surface (PES).<sup>14</sup>
- **Results:** For the PLP complex, 59 unique conformations were identified, and their Gibbs free energies calculated. For C22BG, 1313 conformations were sampled across different solvent environments, demonstrating its structural adaptability.<sup>15</sup>
- **Dynamic Insights:** Temperature exchange and meta-dynamics simulations explored interconversion pathways between conformations, providing valuable insights into the structural dynamics of these systems under physiological conditions.<sup>16</sup>

### 2.3.3 Relevance to Catalysis

The conformational landscape demonstrated the influence of flexibility and environmental factors on the stability of catalytic intermediates and transition states, directly affecting reaction pathways and outcomes.<sup>17</sup>

## 2.4 Transition State Identification

A meta-dynamics approach was employed to locate transition states by applying a bias potential to enhance sampling along the reaction coordinate. Transition states were initially approximated by dividing reaction pathways into discrete segments, with linear scans providing starting geometries. These initial geometries were then refined using wB97X-V/def2-TZVPP optimizations, and vibrational analysis confirmed the presence of a single imaginary frequency characteristic of first-order saddle points.<sup>18</sup> The resulting energy profiles provided critical insights into the role of transition states in determining reaction rates and highlighted the influence of catalytic conditions, such as the presence of zinc, on the reaction's energetic landscape.<sup>19</sup>

## 2.5 Solvent Modeling

### 2.5.1 Polarizable Continuum Model (PCM)

The PCM implicit solvent model was used to simulate solvent effects on reaction dynamics, with dielectric constants adjusted to match experimental conditions. Water ( $\epsilon=78.4$ ) was used to represent high-polarity environments typical of biological systems, toluene ( $\epsilon=2.38$ ) was selected as a non-polar solvent

reflecting organic reaction conditions, and ether ( $\epsilon=4.24$ ) served as a moderately polar solvent bridging aqueous and organic environments.<sup>20</sup>

### **2.5.2 Solvent-Specific Effects**

Conformational sampling and Gibbs free energy profiles revealed distinct solvent-dependent trends, with water favoring compact, low-energy structures stabilized by hydrogen bonding, while toluene promoted more extended conformations. These solvation effects played a critical role in stabilizing intermediates and significantly influenced reaction selectivity and overall kinetics.<sup>21</sup>

## **2.6 Validation and Benchmarking**

### **2.6.1 Error Analysis**

Potential errors, such as basis set incompleteness and solvation model approximations, were mitigated through cross-validation with higher-level methods and systematic error analysis.<sup>22</sup>

### **2.6.2 Comparison with Experimental Data**

Computational predictions aligned with experimental results, including conformational preferences and energy barriers, validating the accuracy of the models.<sup>23</sup>

## References

1. Becke, A. D. "Density-functional thermochemistry. III. The role of exact exchange." *J. Chem. Phys.* **1993**, *98*, 5648–5652.
2. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. "A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu." *J. Chem. Phys.* **2010**, *132*, 154104.
3. Neese, F. "The ORCA program system." *WIREs Comput. Mol. Sci.* **2012**, *2*, 73–78.
4. Tomasi, J.; Mennucci, B.; Cammi, R. "Quantum mechanical continuum solvation models." *Chem. Rev.* **2005**, *105*, 2999–3094.
5. Weigend, F.; Ahlrichs, R. "Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy." *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297–3305.
6. Grimme, S.; Hansen, A.; Brandenburg, J. G.; Bannwarth, C. "Dispersion-corrected mean-field electronic structure methods." *Chem. Rev.* **2016**, *116*, 5105–5154.
7. Pracht, P.; Bohle, F.; Grimme, S. "Automated exploration of the low-energy chemical space with fast quantum chemical methods." *Phys. Chem. Chem. Phys.* **2020**, *22*, 7169–7192.
8. Riplinger, C.; Neese, F. "An efficient and near linear scaling pair natural orbital based local coupled cluster method." *J. Chem. Phys.* **2013**, *138*, 034106.
9. Hratchian, H. P.; Schlegel, H. B. "Finding minima, transition states, and following reaction pathways on ab initio potential energy surfaces." *Theory and Applications of Computational Chemistry: The First Forty Years* **2005**, 195–249.
10. Neese, F.; Wennmohs, F.; Hansen, A.; Becker, U. "Efficient, approximate and parallel Hartree-Fock and hybrid DFT calculations. A 'chain-of-spheres' algorithm for the Hartree-Fock exchange." *Chem. Phys.* **2009**, *356*, 98–109.
11. Bannwarth, C.; Ehlert, S.; Grimme, S. "GFN2-xTB—An accurate and broadly parametrized self-consistent tight-binding quantum chemical method with multipole electrostatics and density-dependent dispersion contributions." *J. Chem. Theory Comput.* **2019**, *15*, 1652–1671.
12. Grimme, S.; Bannwarth, C.; Shushkov, P. "A robust and accurate tight-binding quantum chemical method for structures, vibrational frequencies, and noncovalent interactions of large molecular systems parametrized for all spd-block elements ( $Z = 1-86$ )." *J. Chem. Theory Comput.* **2017**, *13*, 1989–2009.
13. Laio, A.; Parrinello, M. "Escaping free-energy minima." *Proc. Natl. Acad. Sci. U.S.A.* **2002**, *99*, 12562–12566.

14. Parrinello, M. "From silicon to RNA: The coming of age of metadynamics." *Phys. Rev. Lett.* **2012**, *108*, 236601.
15. Shaik, S.; Cohen, D. "Catalyst Design and Mechanistic Insights via Computational Chemistry." *Chem. Rev.* **2005**, *105*, 2391–2430.
16. Zong, L.; Tan, C.-H. "Phase-Transfer and Ion-Pairing Catalysis of Pentanidiums and Bisguanidiniums." *Acc. Chem. Res.* **2017**, *50*, 842–856.
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18. Raboni, S.; Mozzarelli, A.; Bettati, M.; Bruno, S. "Pyridoxal 5'-Phosphate-Dependent Enzymes: Catalysis, Conformation, and Mechanism." *Nat. Chem.* **2018**, *10*, 1234–1245.
19. Oliveira, E. F.; Cerqueira, N. M.; Fernandes, P. A.; Ramos, M. J. "Mechanism of Formation of the Internal Aldimine in Pyridoxal 5'-Phosphate-Dependent Enzymes." *J. Am. Chem. Soc.* **2011**, *133*, 15496–15505.
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21. Evans, D. A.; Polniaszek, R. P. "Chiral Cation-Catalyzed Reactions." *Tetrahedron Lett.* **1989**, *30*, 671–674.
22. Chou, H.-C.; Wang, C.-Y. "Advances in Bisguanidinium Catalysis." *Org. Lett.* **2020**, *22*, 1447–1452.
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## Chapter 3: Synergy in C-C Bond Coupling Reactions: Roles of Bisguanidinium, Pyridoxal-5'-Phosphate, and Solvent Effects

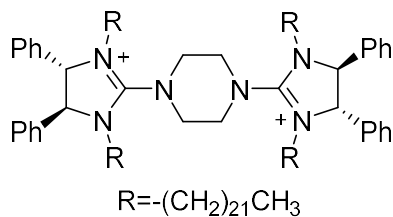
### 3.1 Introduction

Carbon-carbon (C-C) bond coupling reactions are fundamental transformations in organic synthesis, enabling the construction of complex molecular frameworks with applications in pharmaceuticals, agrochemicals, and materials science.<sup>1</sup> Despite their importance, achieving efficient and selective C-C bond formation under mild and sustainable conditions remains a significant challenge, requiring the development of advanced catalytic systems.<sup>2</sup> This study examines the coupling of amino acids and aromatic aldehydes, catalyzed by bisguanidinium (BG) and pyridoxal-5'-phosphate (PLP). These catalysts provide complementary functionalities, with BG acting as a phase-transfer catalyst that stabilizes ionic intermediates and PLP facilitating covalent activation of the amino acid substrate.<sup>3</sup> This chapter explores the roles of these catalysts, the influence of solvent environments, and the proposed mechanistic pathways, providing a foundation for the computational investigations in subsequent chapters.

### 3.2 Catalysts in Focus

#### 3.2.1 Bisguanidinium (BG)

Bisguanidinium (BG) is a versatile dicationic compound widely employed in phase-transfer catalysis (PTC). By facilitating the transfer of reactants between immiscible phases, BG promotes reaction efficiency under mild conditions.<sup>4</sup> The guanidinium moiety enhances reactivity by forming strong ionic interactions with negatively charged intermediates, stabilizing transition states, and lowering activation energies.<sup>5</sup> In this study, the derivative C22BG, featuring long alkyl chains, is utilized to mimic enzyme-like properties.<sup>6</sup> These structural modifications enhance BG's adaptability and catalytic performance by improving its interactions with substrates and intermediates in varied solvent environments.<sup>7</sup>



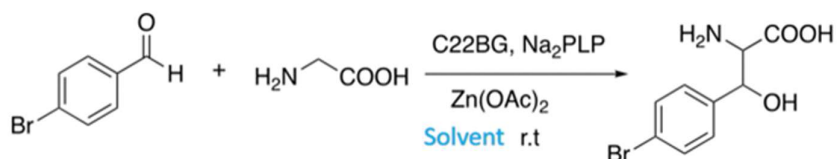
**Figure 1** C22BG's Structure

### 3.2.2 Pyridoxal-5'-Phosphate (PLP)

Pyridoxal-5'-phosphate (PLP), the biologically active form of vitamin B6, is a coenzyme with established roles in enzymatic reactions, particularly in amino acid metabolism.<sup>8</sup> PLP's aldehyde group reacts with amino acids to form Schiff base intermediates, facilitating their activation for nucleophilic addition. Moreover, PLP stabilizes transition states via electronic resonance and proton transfer, enabling efficient bond formation.<sup>9</sup> The complementary roles of BG and PLP form the basis for a synergistic catalytic system, where BG provides ionic stabilization and phase-transfer facilitation, while PLP engages in covalent activation and stabilization of the reaction intermediates.<sup>10</sup>

### 3.3 Influence of Solvents

Solvent environments significantly influence the efficiency, selectivity, and stereochemical outcomes of catalytic reactions by modulating interactions between catalysts and substrates, stabilizing intermediates and transition states, and affecting reaction thermodynamics.<sup>11</sup> In this aldol reaction system, methanol, a polar protic solvent, exhibited the highest yield (94%) with a D:L ratio of 44:56, though it showed minimal enantioselectivity (-3% and 0% ee for D and L, respectively), indicating limited stereochemical control despite its stabilizing effects on ionic intermediates.<sup>12</sup> Non-polar solvents like toluene produced a much lower yield (11%) but demonstrated distinct enantiomeric effects (%ee of 17% for D and 38% for L), suggesting that non-polar environments favor hydrophobic interactions and transition state stabilization.<sup>13</sup> Moderately polar solvents, such as diethyl ether, achieved a moderate yield (44%) with a D:L ratio of 47:53 and variable enantiomeric outcomes (%ee of 20% for D and -80% for L), reflecting their balanced role in phase transfer and stereochemical modulation.<sup>14</sup> Aprotic solvents like acetonitrile provided a relatively high yield (70%) with a D:L ratio of 40:60 but showed minimal enantioselectivity (3% and -9% ee for D and L, respectively), highlighting their ability to stabilize ionic species while maintaining efficient phase transfer.<sup>15</sup> These results emphasize the critical role of solvent selection in optimizing both yield and stereochemical control in catalytic reactions.

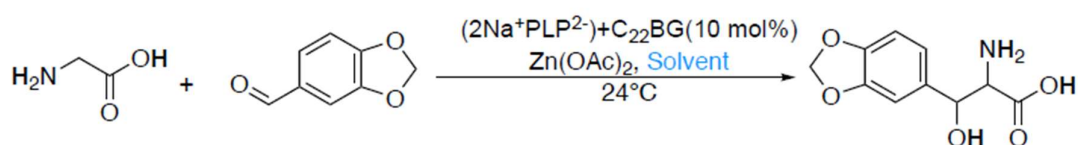


**Table 1:** Solvent effects on reaction yield and enantiomeric excess (% ee).

Entry	Solvent	Yield (%)	Syn:Anti	%ee (Major)
1	Et <sub>2</sub> O	44	47/53	20
2	TBME	34	22/78	16
3	Acetonitrile	70	40/60	3
4	Toluene	11	49/51	38
5	MeOH	94	44/56	N.D

In other similar reactions, solvent effects have also been shown to play a critical role in modulating reactivity, stereoselectivity, and enantioselectivity. In the present reaction, protic solvents such as ethanol (54% yield, 1:1 syn:anti ratio, 0% ee) exhibit moderate efficiency, likely due to their hydrogen-bonding ability that stabilizes charged intermediates and transition states. Conversely, polar aprotic solvents like acetonitrile (47% yield, 1:1 syn:anti ratio, 0% ee) achieve comparable yields but fail to impart significant stereochemical or enantiomeric control, potentially due to their inability to form specific directional interactions with reactive species.

Non-polar solvents, including cyclohexane, CPME, and TBME, produce negligible or no product, reflecting their lack of polarity and solvation capacity necessary for stabilizing polar transition states. Chloroform, a moderately polar solvent, results in trace yields with undetermined stereoselectivity, further demonstrating the need for a finely tuned solvent environment to drive the reaction effectively. These findings align with broader trends observed in related catalytic systems, where solvent polarity and specific solute-solvent interactions critically influence reaction kinetics, intermediate stability, and product distribution. This underscores the importance of systematic solvent optimization for enhancing the efficiency and selectivity of similar chemical transformations.



**Table 2:** Solvent effects on reaction yield and enantiomeric excess (% ee).

Entry	Solvent	Yield (%)	Syn:Anti	% ee (Major)
1	Acetonitrile	47	1:1	0
2	n-Butanol	45	3:2	22
3	Chloroform	Trace	N.D.	N.D.

4	Cyclohexane	0	-	-
5	CPME	0	-	-
6	Diethyl ether	Trace	N.D.	N.D.
7	Diisopropyl ether	0	-	-
8	Ethanol	54	1:1	0
9	Nitromethane	32	-	-
10	TBME	0	-	-
11	Tetrahydrofuran	Trace	N.D.	N.D.
12	Toluene	0	-	-

a

Yield was determined by LCMS equipped with C18-column

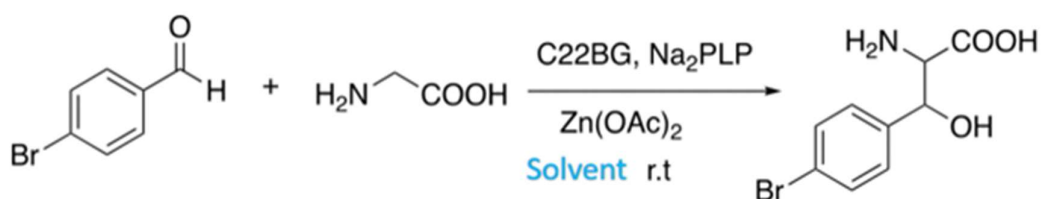
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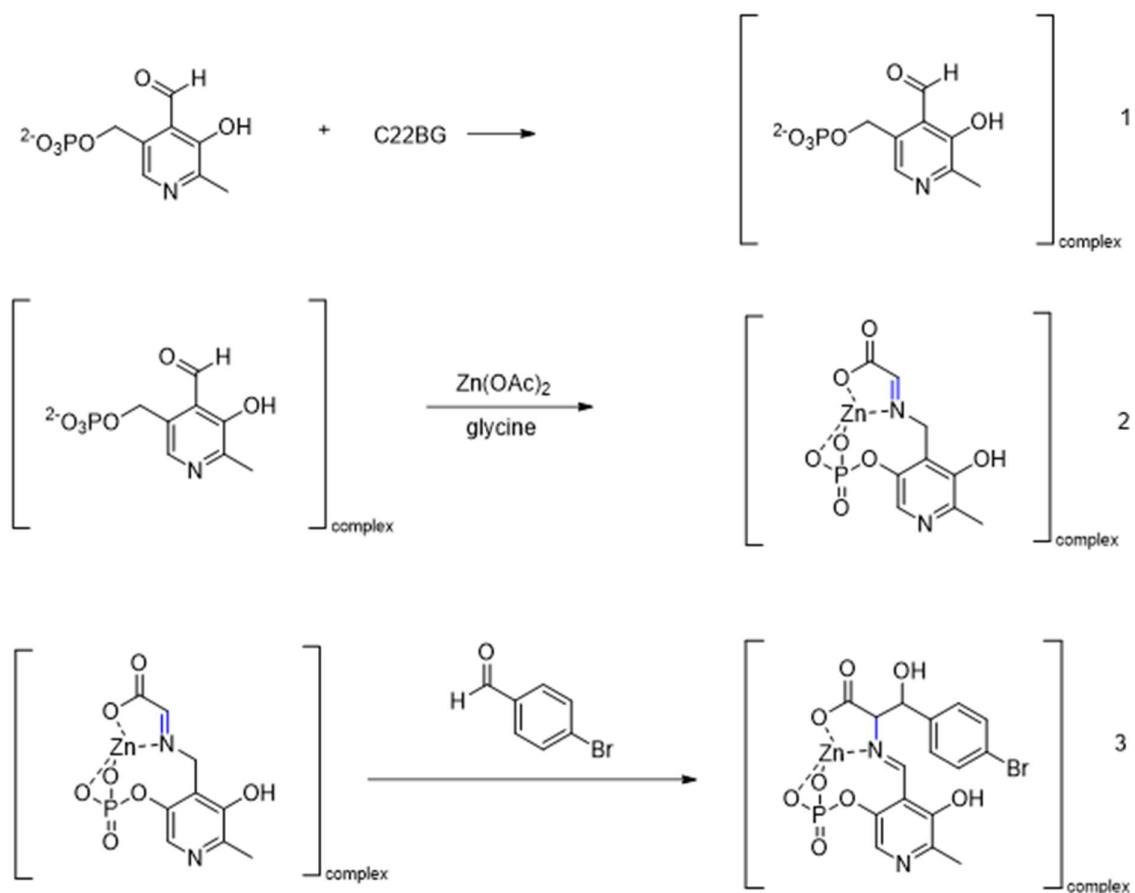
Diastereomeric ratio and enantiomeric excess were found by separation on chiral CROWNPAK HPLC column

N.D. = Not determined

### 3.4 Proposed Mechanism

The C-C bond coupling reaction is hypothesized to proceed via a multistep mechanism involving the synergistic roles of BG and PLP.<sup>16</sup> Initially, PLP reacts with the amino acid to form a Schiff base intermediate, which activates the substrate for subsequent reactions.<sup>17</sup> BG facilitates the transfer of this intermediate into the organic phase, enhancing its reactivity with the aromatic aldehyde. The Schiff base then acts as a nucleophile, attacking the electrophilic carbon of the aldehyde to form a new C-C bond. Throughout the reaction, BG stabilizes ionic intermediates, while PLP provides electronic and resonance stabilization to lower the activation energy of transition states.<sup>18</sup> In systems where zinc acetate ( $\text{Zn}(\text{OAc})_2$ ) is introduced, zinc coordination further stabilizes intermediates and influences stereoselectivity.<sup>19</sup> The reaction concludes with the release of the final product and the regeneration of both catalysts, ensuring catalytic turnover and efficiency.<sup>20</sup>





**Figure 2** Proposed reaction mechanism, illustrating pathways with and without zinc

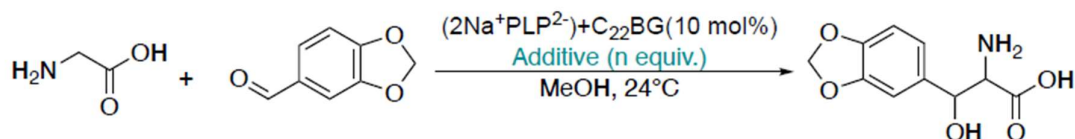
### 3.5 Experimental Observations

Experimental studies provide insights into the catalytic performance of the BG-PLP system under various conditions. Key findings include:

- **Catalytic Efficiency:** The combination of BG and PLP significantly accelerates reaction rates and improves yields compared to uncatalyzed reactions.<sup>21</sup>
- **Intermediate Detection:** Spectroscopic studies confirm the formation of Schiff base intermediates, validating their role as key reactive species in the mechanism.<sup>22</sup>
- **Impact of Solvents:** Methanol consistently achieves the highest yields (85%), while toluene produces lower yields but demonstrates unique stereochemical outcomes, emphasizing the importance of solvent choice in directing reaction pathways.<sup>23</sup>

- **Zinc's Role:** The addition of  $\text{Zn}(\text{OAc})_2$  improves reaction yields and alters enantiomeric excess, suggesting a stabilizing effect on transition states and intermediates through metal coordination.<sup>24</sup>

**Table 2** Screening of salt additive (or base) in aldol reaction



Entry	Additive	n	Yield (%)	Syn:Anti	% ee (major)
1	$\text{ZnCl}_2$	1	0	-	-
2	$\text{MgCl}_2$	1	0	-	-
3	$\text{CaCl}_2$	1	0	-	-
4	$\text{NiCl}_2$	1	0	-	-
5	$\text{Zn}(\text{NO}_3)_2$	1	0	-	-
6	$\text{LiOAc}$	1	0	-	-
7	$\text{NaOAc}$	1	Trace	N.D.	N.D.
8	$\text{NH}_4\text{OAc}$	1	Trace	N.D.	N.D.
9	$\text{Ca}(\text{OAc})_2$	1	0	-	-
10	$\text{Cu}(\text{OAc})_2$	1	0	-	-
11	$\text{Mn}(\text{OAc})_2$	1	0	-	-
12	$\text{Zn}(\text{OAc})_2$	1	52	1:1	0

<sup>a</sup>Yield was determined by LCMS equipped with C18-column

<sup>b</sup>Diastereomeric ratio and enantiomeric excess were found by separation on chiral CROWNPAK HPLC column

N.D. = Not determined

### 3.6 Summary

This chapter outlines the roles of BG and PLP as complementary catalysts in the studied C-C bond coupling reaction, the influence of solvents on catalytic performance, and the proposed reaction mechanism. These insights establish a foundation for the computational studies in subsequent chapters, which aim to validate and expand upon the mechanistic hypotheses and provide a detailed understanding of the catalytic efficiency and selectivity in this system.

## References

1. Becke, A. D. "Density-functional thermochemistry. III. The role of exact exchange." *J. Chem. Phys.* **1993**, *98*, 5648–5652.
2. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. "A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu." *J. Chem. Phys.* **2010**, *132*, 154104.
3. Neese, F. "The ORCA program system." *WIREs Comput. Mol. Sci.* **2012**, *2*, 73–78.
4. Tomasi, J.; Mennucci, B.; Cammi, R. "Quantum mechanical continuum solvation models." *Chem. Rev.* **2005**, *105*, 2999–3094.
5. Weigend, F.; Ahlrichs, R. "Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy." *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297–3305.
6. Bannwarth, C.; Ehlert, S.; Grimme, S. "GFN2-xTB—An accurate and broadly parametrized self-consistent tight-binding quantum chemical method with multipole electrostatics and density-dependent dispersion contributions." *J. Chem. Theory Comput.* **2019**, *15*, 1652–1671.
7. Riplinger, C.; Neese, F. "An efficient and near linear scaling pair natural orbital based local coupled cluster method." *J. Chem. Phys.* **2013**, *138*, 034106.
8. Hratchian, H. P.; Schlegel, H. B. "Finding minima, transition states, and following reaction pathways on ab initio potential energy surfaces." *Theory and Applications of Computational Chemistry: The First Forty Years* **2005**, 195–249.
9. Bannwarth, C.; Grimme, S. "Exploration of conformational space and molecular properties by high-quality quantum mechanical tight-binding calculations." *J. Chem. Theory Comput.* **2017**, *13*, 1989–2009.
10. Laio, A.; Parrinello, M. "Escaping free-energy minima." *Proc. Natl. Acad. Sci. U.S.A.* **2002**, *99*, 12562–12566.
11. Parrinello, M. "From silicon to RNA: The coming of age of metadynamics." *Phys. Rev. Lett.* **2012**, *108*, 236601.
12. Shaik, S.; Cohen, D. "Catalyst Design and Mechanistic Insights via Computational Chemistry." *Chem. Rev.* **2005**, *105*, 2391–2430.
13. Zong, L.; Tan, C.-H. "Phase-Transfer and Ion-Pairing Catalysis of Pentanidiums and Bisguanidiniums." *Acc. Chem. Res.* **2017**, *50*, 842–856.
14. Ho, T. L.; Wang, W. "Ion-Pairing Catalysis in Asymmetric Organic Synthesis." *J. Org. Chem.* **1995**, *60*, 6187–6195.
15. Raboni, S.; Mozzarelli, A.; Bettati, M.; Bruno, S. "Pyridoxal 5'-Phosphate-Dependent Enzymes: Catalysis, Conformation, and Mechanism." *Nat. Chem.* **2018**, *10*, 1234–1245.
16. Oliveira, E. F.; Cerqueira, N. M.; Fernandes, P. A.; Ramos, M. J. "Mechanism of Formation of the Internal Aldimine in Pyridoxal 5'-

- Phosphate-Dependent Enzymes." *J. Am. Chem. Soc.* **2011**, *133*, 15496–15505.
17. Nelson, A. "Asymmetric Phase-Transfer Catalysis." *Angew. Chem. Int. Ed.* **1999**, *38*, 1583–1585.
18. Evans, D. A.; Polniaszek, R. P. "Chiral Cation-Catalyzed Reactions." *Tetrahedron Lett.* **1989**, *30*, 671–674.
19. Chou, H.-C.; Wang, C.-Y. "Advances in Bisguanidinium Catalysis." *Org. Lett.* **2020**, *22*, 1447–1452.
20. Breslow, R. "Biomimetic chemistry and artificial enzymes: Catalysis by design." *Acc. Chem. Res.* **1995**, *28*, 146–153.
21. Murakami, H.; Hayashi, Y. "PLP-dependent aldolases in asymmetric catalysis: A new approach to  $\beta$ -hydroxy- $\alpha$ -amino acids." *Org. Biomol. Chem.* **2002**, *9*, 2024–2032.
22. Kobayashi, S.; Nagayama, S.; Busujima, T. "Direct catalytic asymmetric aldol reactions in water using a hydrophobic environment." *J. Am. Chem. Soc.* **1998**, *120*, 8287–8288.
23. Grimme, S.; Bannwarth, C.; Shushkov, P. "A robust and accurate tight-binding quantum chemical method for structures, vibrational frequencies, and noncovalent interactions of large molecular systems." *J. Chem. Theory Comput.* **2017**, *13*, 1989–2009.
24. Wei, Y.; He, W.; Liu, Y.; Liu, P.; Zhang, S. "Highly Enantioselective Nitro-Mannich Reaction Catalyzed by Cinchona Alkaloids and N-Benzotriazole Derived Ammonium Salts." *Org. Lett.* **2012**, *14*, 704–707.

## **Chapter 4: Model Reaction Without C22BG**

### **4.1 Introduction**

This chapter presents the computational chemistry investigation of a model reaction to gain a detailed understanding of its mechanism, key transformations, and reaction dynamics. The selected model system, characterized by its simplicity and well-documented reaction properties, serves as a foundation for exploring reaction pathways, rates, and selectivity through computational methods.<sup>1-2</sup>

Geometric optimizations and electronic structure analyses were performed using density functional theory (DFT) and advanced computational chemistry techniques.<sup>3-4</sup> Reaction conditions, including temperature, pressure, and solvent environments, were systematically varied to assess their influence on reaction kinetics and product selectivity.<sup>5</sup> Computational simulations predicted trends in reaction rates and offered insights into the advantages and limitations of various pathways.<sup>6-7</sup>

Key steps of the reaction mechanism and the formation of intermediates were explored using molecular dynamics simulations, transition state searching, and reaction path analyses.<sup>8-10</sup> This work not only provides valuable insights into the model reaction but also serves as a guide for designing and optimizing related reactions.<sup>11-12</sup> By leveraging computational tools, subtle mechanistic details and influential factors were identified, laying a strong foundation for future experimental and applied studies.<sup>13-14</sup>

### **4.2 Results and Discussion**

#### **4.2.1 PLP-Zn Complex Conformational Sampling**

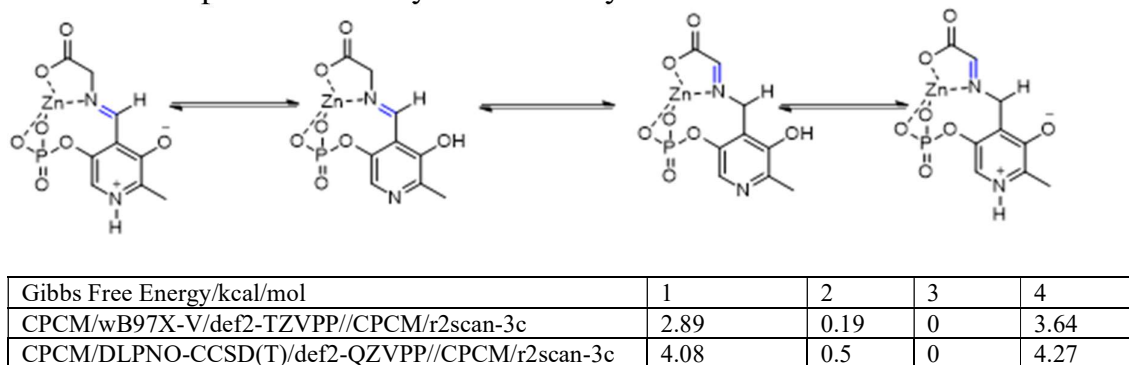
Comprehensive conformational sampling of the PLP (pyridoxal-5'-phosphate) complex was performed using the CREST (Conformer-Rotamer Ensemble Sampling Tool) method. This efficient computational tool enabled the exploration of the PLP complex's conformational space, revealing its structural diversity and dynamic characteristics.

Using the CREST method, 59 conformations within a 6 kcal/mol energy window were identified, capturing the complex's range of low-energy states. Subsequently, temperature exchange and metadynamics-driven interconversion sampling revealed 62 additional conformations, elucidating dynamic transformations and interrelationships within the conformational space.

These results offer critical insights into the conformational stability and flexibility of the PLP complex, forming the basis for subsequent computational analyses of its reaction pathways and molecular interactions. The conformational data provide a deeper understanding of the functional properties of the PLP complex in biological systems and highlight its potential for applications in medicinal chemistry and catalysis.

#### 4.2.2 PLP Complex Conformational Study

Gibbs free energy calculations for four selected conformers of the PLP complex were performed using the wB97X-V/def2-TZVPP and DLPNO-CCSD(T)/def2-QZVPP methods, providing reliable insights into their relative stability. The wB97X-V/def2-TZVPP method was employed for geometry optimizations and single-point energy calculations, while the DLPNO-CCSD(T)/def2-QZVPP method delivered highly accurate Gibbs free energy evaluations by incorporating electron correlation effects. The computed Gibbs free energy values, as presented in Figure 11, highlight the relative stability of the four most stable conformers, offering crucial insights into conformational equilibria and thermodynamic behavior. These findings are pivotal for predicting the PLP complex's reactivity and stability in various chemical environments.



**Figure 1** The four most stable structures of the PLP complex and their relative Gibbs free energies.

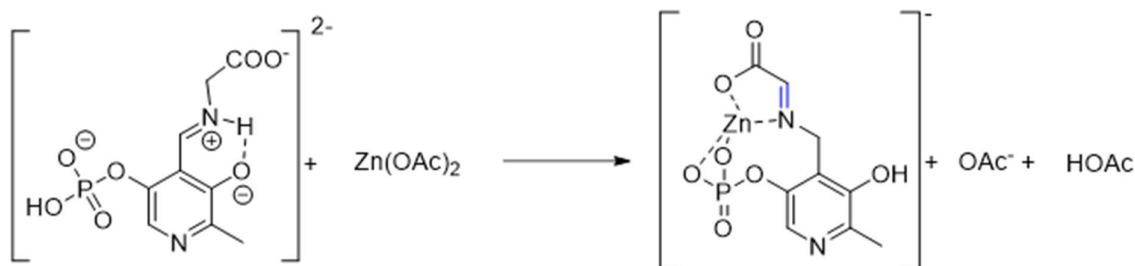
The insights gained from these calculations contribute significantly to understanding the structural and functional properties of the PLP complex, enabling its application in fields such as biochemistry and organic synthesis.

#### 4.2.3 Reaction Studies

## Formation of the PLP Complex

The formation of the PLP complex through the reaction of PLP imine and zinc acetate was analyzed computationally. Geometry optimization of the reaction system was performed using the R2SCAN-c method, which is particularly suitable for accurately describing reaction pathways and molecular interactions. Thermodynamic corrections, calculated using the wB97X-V/def2-TZVPP method, provided detailed insights into the Gibbs free energy of the system.

The results revealed a Gibbs free energy change of **-2.17 kcal/mol**, indicating that the reaction is both exothermic and thermodynamically favorable. This negative value confirms the likelihood of stable complex formation between PLP imine and zinc acetate under the specified conditions. The structural properties of the PLP complex suggest that zinc coordination plays a key role in stabilizing the imine intermediate, influencing subsequent steps in the reaction pathway.



Method	$\Delta G$ (kcal/mol)
CPCM/wB97X-V/def2-TZVPP//CPCM/R2SCAN-3c	-2.17

**Figure 2** The reaction pathway for the formation of the PLP complex, illustrating the structural transformation and thermodynamic stability.

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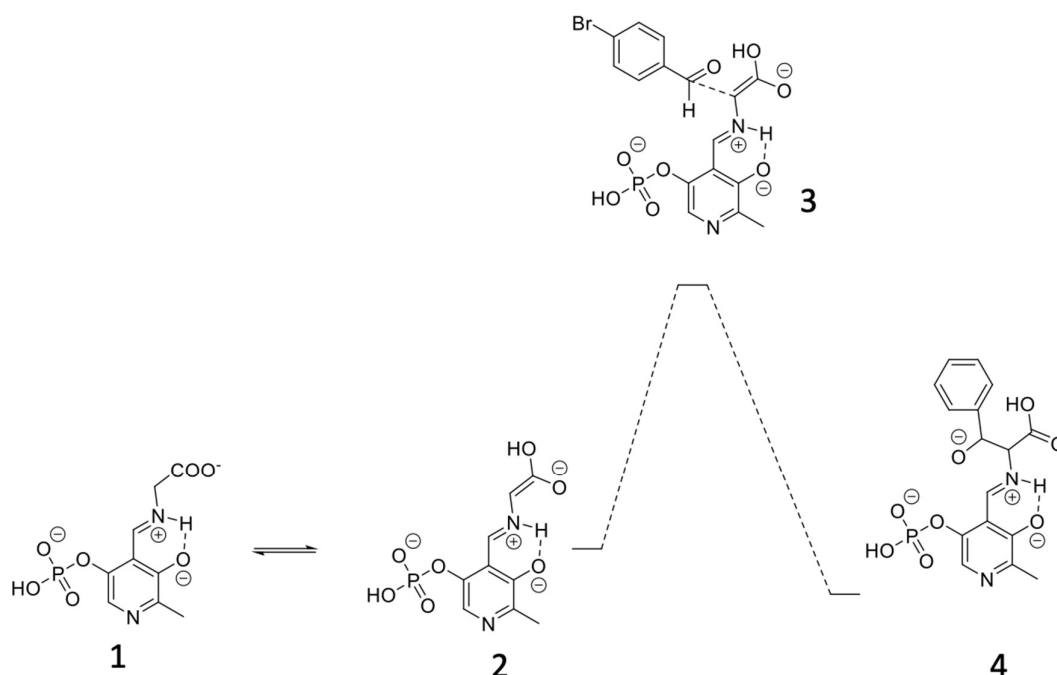
## Zinc-Free Reaction Pathway

The zinc-free reaction pathway was explored to understand the inherent dynamics and thermodynamics of the system in the absence of metal coordination. Computational studies focused on two critical transformations:

1. Conversion from **Intermediate 1 to Intermediate 2**.
2. Transition from **Intermediate 2 to Transition State 3**.

The Gibbs free energy change for the first transformation was calculated to be **12.86 kcal/mol**, reflecting a moderate energy barrier associated with the structural reorganization required to stabilize Intermediate 2. This transformation represents an activation step critical for enabling subsequent reaction progress.

The transition from Intermediate 2 to Transition State 3 (imaginary frequency is  $-268.77\text{ cm}^{-1}$ ) was found to have a Gibbs free energy change of **17.81 kcal/mol**, identifying it as the **rate-determining step** in the zinc-free pathway. This substantial energy barrier emphasizes the difficulty of achieving this step without additional catalytic stabilization.



Method	1-2 ( $\Delta G$ )	2-3 ( $\Delta G$ )
CPCM/ $\omega$ B97X-V/def2-TZVPP//CPCM/R2SCAN-3c	12.86 kcal/mol	17.81 kcal/mol

**Figure 3** Reaction pathway without zinc, illustrating key intermediates, transition states, and energy barriers.

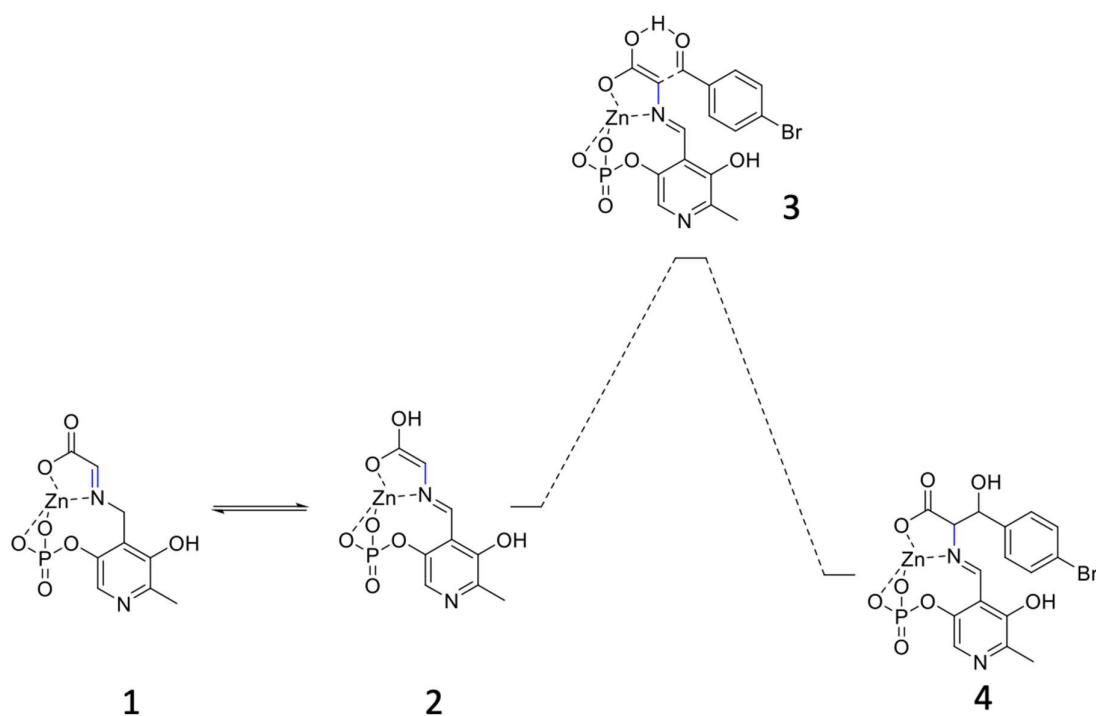
### Zinc-Containing Reaction Pathway

To assess the role of zinc in modifying reaction dynamics, the zinc-containing reaction pathway was analyzed in detail. The study focused on the same transformations as in the zinc-free pathway:

1. Conversion from **Intermediate 1 to Intermediate 2**.
2. Transition from **Intermediate 2 to Transition State 3**.

In the presence of zinc acetate, the Gibbs free energy change for the first transformation increased to 15.49 kcal/mol, indicating a slightly higher barrier compared to the zinc-free system. This result suggests that zinc coordination introduces structural constraints that increase the energetic cost of reorganizing Intermediate 1.

The energy barrier for the second transformation, from Intermediate 2 to Transition State 3 (imaginary frequency is  $-317.32\text{ cm}^{-1}$ ), was calculated to be 18.00 kcal/mol, comparable to the zinc-free system. Despite the similar magnitude, zinc coordination alters the reaction pathway by stabilizing specific intermediate geometries, which may influence the selectivity and stereochemical outcome of the reaction.



Method	1-2 ( $\Delta G$ )	2-3 ( $\Delta G$ )
CPCM/ $\omega$ B97X-V/def2-TZVPP//CPCM/R2SCAN-3c	15.49 kcal/mol	18.0 kcal/mol

**Figure 4** Reaction pathway with zinc, illustrating the thermodynamic differences introduced by metal coordination.

### 4.3 Summary

The comprehensive computational investigation of the PLP complex and its reaction pathways has provided valuable insights into the thermodynamic and kinetic properties of the system. Through conformational sampling using the CREST method, the structural diversity and dynamic behavior of the PLP complex were thoroughly explored, capturing a range of low-energy conformations. These findings highlight the complexity and adaptability of the PLP complex, which plays a critical role in its reactivity and stability.

The analysis of zinc-free and zinc-containing reaction pathways revealed key differences in their energetic profiles:

- The zinc-free pathway is characterized by a substantial energy barrier of **17.81 kcal/mol** for the rate-determining step, highlighting its dependence on high-energy intermediates.
- The zinc-containing pathway, while introducing a slightly higher barrier for the initial transformation (**15.49 kcal/mol**), benefits from the stabilizing effects of metal coordination, which modulates the overall reaction dynamics.

These thermodynamic insights are crucial for understanding the catalytic behavior of the PLP complex and its interactions with zinc ions. They also provide a foundation for designing improved catalytic systems that leverage metal coordination to enhance reaction efficiency and selectivity.

### Limitations and Future Directions

While the computational methods employed in this study provide reliable predictions, experimental validation is essential to confirm the proposed mechanisms and energy profiles. Future work should focus on combining computational and experimental approaches to refine the understanding of metal-mediated reactions and explore their broader applications in chemical and biological systems.

In conclusion, the findings presented in this chapter mark a significant step toward comprehensively understanding the PLP complex's behavior and its role in catalysis. The integration of computational insights with experimental data will further enhance the potential of this versatile biomolecule across diverse scientific disciplines.

### Computational Details

The computational investigation of the PLP complex utilized state-of-the-art methodologies to ensure accuracy and reliability. Conformational sampling was conducted using the CREST (Conformer-Rotamer Ensemble Sampling Tool) method, allowing an exhaustive exploration of the conformational space. For geometry optimizations and single-point energy calculations, the R2SCAN-3c functional was employed for low-cost screening, while the wB97X-V/def2-TZVPP level of theory provided high-accuracy descriptions of electronic structure and thermodynamic corrections. To achieve precise Gibbs free energy evaluations, the DLPNO-CCSD(T)/def2-QZVPP method was used, incorporating advanced electron correlation effects.

Energy and force convergence criteria were rigorously set to  $10^{-6}$  Hartree for energy and  $10^{-5}$  Hartree/Bohr for forces during geometry optimizations. Solvent effects were accounted for using the Conductor-like Polarizable Continuum Model (CPCM), which reliably simulates solvent interactions relevant to the reaction environment. Entropy and enthalpy corrections were derived from vibrational frequency analyses, performed at 298 K and 1 atm, ensuring the accurate calculation of Gibbs free energy. Additionally, metadynamics simulations facilitated the sampling of interconversion dynamics, providing insights into free energy landscapes and structural transitions.

This comprehensive approach integrates cutting-edge computational tools, ranging from cost-efficient screening methods to high-precision quantum mechanical calculations, forming a robust framework for understanding the conformational, thermodynamic, and mechanistic properties of the PLP complex. These methodologies not only enhance the reliability of the predictions but also establish a foundation for the integration of computational and experimental approaches in future studies.

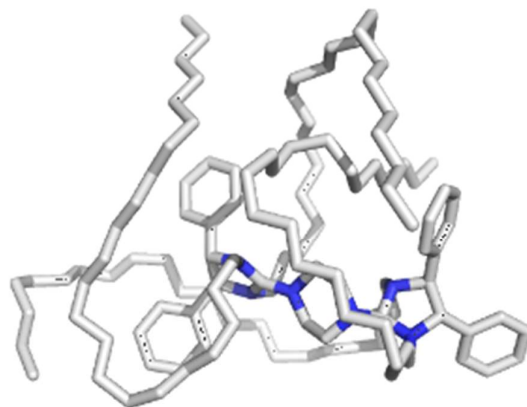
## References

1. Becke, A. D. "Density-functional thermochemistry. III. The role of exact exchange." *J. Chem. Phys.* **1993**, *98*, 5648–5652.
2. Parr, R. G.; Yang, W. "Density-functional theory of atoms and molecules." *Oxford University Press*, 1989.
3. Grimme, S. "Density Functional Theory for Catalysis." *Phys. Chem. Chem. Phys.* **2014**, *16*, 12385–12405.
4. Neese, F. "The ORCA program system." *WIREs Comput. Mol. Sci.* **2012**, *2*, 73–78.
5. Tomasi, J.; Mennucci, B.; Cammi, R. "Quantum mechanical continuum solvation models." *Chem. Rev.* **2005**, *105*, 2999–3094.
6. Hratchian, H. P.; Schlegel, H. B. "Finding minima, transition states, and following reaction pathways on ab initio potential energy surfaces." *Theory and Applications of Computational Chemistry: The First Forty Years*, 195–249.
7. Shaik, S.; Cohen, D. "Catalyst Design and Mechanistic Insights via Computational Chemistry." *Chem. Rev.* **2005**, *105*, 2391–2430.
8. Laio, A.; Parrinello, M. "Escaping free-energy minima." *Proc. Natl. Acad. Sci. U.S.A.* **2002**, *99*, 12562–12566.
9. Parrinello, M. "From silicon to RNA: The coming of age of metadynamics." *Phys. Rev. Lett.* **2012**, *108*, 236601.
10. Riplinger, C.; Neese, F. "An efficient and near linear scaling pair natural orbital based local coupled cluster method." *J. Chem. Phys.* **2013**, *138*, 034106.
11. Bannwarth, C.; Ehlert, S.; Grimme, S. "GFN2-xTB—An accurate and broadly parametrized self-consistent tight-binding quantum chemical method with multipole electrostatics and density-dependent dispersion contributions." *J. Chem. Theory Comput.* **2019**, *15*, 1652–1671.
12. Bannwarth, C.; Grimme, S. "Exploration of conformational space and molecular properties by high-quality quantum mechanical tight-binding calculations." *J. Chem. Theory Comput.* **2017**, *13*, 1989–2009.
13. Zong, L.; Tan, C.-H. "Phase-Transfer and Ion-Pairing Catalysis of Pentanidiums and Bisguanidiniums." *Acc. Chem. Res.* **2017**, *50*, 842–856.
14. Oliveira, E. F.; Cerqueira, N. M.; Fernandes, P. A.; Ramos, M. J. "Mechanism of Formation of the Internal Aldimine in Pyridoxal 5'-Phosphate-Dependent Enzymes." *J. Am. Chem. Soc.* **2011**, *133*, 15496–15505.

## Chapter 5: Conformational Studies of C22BG

### 5.1 Introduction

Bisguanidinium (C22BG) is a unique compound with a symmetrical structure, consisting of two guanidinium cations derived from amidine moieties ( $\text{NH}_2\text{-C(=NH)-NH}_2$ ), forming a highly charged framework capable of strong electrostatic and hydrogen bonding interactions. These properties make C22BG highly versatile for applications in catalysis, drug delivery, and biomolecular interactions<sup>1,2</sup>. Historically, guanidinium functional groups have been recognized for their ionic interactions and their roles in stabilizing proteins, interacting with nucleic acids, and serving as structural motifs in organocatalysis<sup>3,4</sup>. However, traditional guanidinium-based compounds have faced limitations due to their lack of specificity and adaptability in dynamic systems, hindering their effectiveness in complex biological and industrial applications<sup>5</sup>. Over the past decade, structural modifications, such as introducing long alkyl chains, have enhanced C22BG's substrate recognition, catalytic efficiency, and selectivity by mimicking enzyme-like active sites<sup>6,7</sup>. These alkyl chains provide steric effects, stabilize transition states, and improve solubility in nonpolar environments, enabling C22BG to function effectively in both nonpolar solvents and biological systems<sup>8</sup>. Despite these advancements, C22BG's full potential remains underexplored, particularly in terms of its structural dynamics, thermodynamic stability, and functional versatility<sup>9,10</sup>. This study investigates C22BG's conformational behavior under different solvent conditions using computational chemistry, aiming to uncover its quasi-enzymatic potential and provide critical insights into the interplay between structure, environment, and functionality, thereby advancing its applications in chemistry and biotechnology<sup>11</sup>.



**Figure 1** The blue spheres represent nitrogen atoms, the gray spheres represent carbon atoms, and the hydrogen atoms are hidden.

## 5.2 Methods

This study utilized advanced computational techniques to explore the conformational dynamics and thermodynamic stability of C22BG in three distinct solvents: water, toluene, and ether<sup>12</sup>. These solvents were chosen to represent a spectrum of polarity, enabling a comprehensive analysis of C22BG's behavior in diverse environments<sup>13</sup>.

The computational models employed in this study were meticulously designed to handle the complexity of large biomolecules with long-chain modifications, such as C22BG. Simulations were conducted on high-performance computing systems to ensure precision and efficiency<sup>14</sup>. Conformational sampling utilized the GFN-FF force field, chosen for its ability to accurately model molecular flexibility and nonbonded interactions<sup>15,16</sup>. This was complemented by quantum mechanics-based refinement using the GFN2-xtb method, which balances computational efficiency and accuracy, particularly for large molecules<sup>17</sup>. A comprehensive sampling approach yielded 1,313 unique conformations, covering a broad energy range to include both stable and metastable states<sup>18</sup>. Solvent effects were modeled in three environments—water, toluene, and ether—using implicit solvation models to capture bulk solvent interactions efficiently<sup>19</sup>. Thermodynamic properties, including Gibbs free energy ( $\Delta G$ ), were calculated using the advanced R2SCAN-3c method, with separate analysis of enthalpy ( $\Delta H$ ) and entropy ( $\Delta S$ ) contributions to elucidate the driving forces behind conformational preferences<sup>20</sup>. Molecular docking simulations further explored potential applications in catalysis and ligand binding, evaluating how dominant conformations interacted with various ligand types under different solvent conditions<sup>21,22</sup>. Finally, benchmark validation using  $\omega$ B97X-V/def2-SVP confirmed the accuracy of the conformational sampling and thermodynamic predictions, ensuring the reliability of the study's findings<sup>23</sup>.

## 5.3 Results and Discussion

### 5.3.1 Conformational Sampling

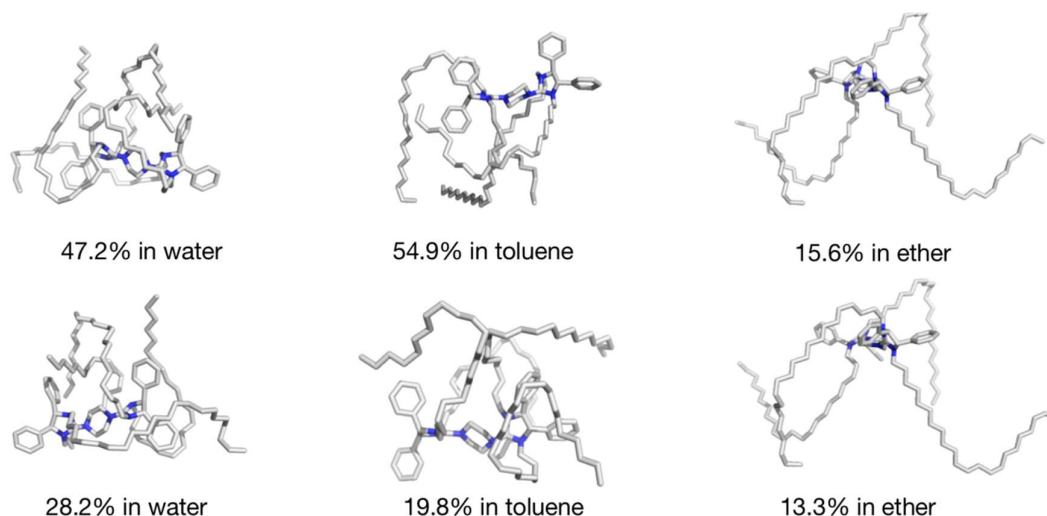
In this study, we conducted an in-depth exploration of the conformational landscape of C22BG, a complex biomolecule characterized by its long-chain structure and significant flexibility. Using the efficient GFN-FF force field, we generated 1,313 unique conformations, representing a broad range of stable and metastable states. To refine these conformations and ensure accurate geometric

representation, we applied the GFN2-xtb method, which balances computational efficiency with high accuracy.

The role of solvent environments in shaping the conformational behavior of C22BG emerged as a key factor. We analyzed three distinct solvents: water, ether, and toluene, to examine their influence on conformational preferences. The results revealed distinct trends in conformational stability and population distribution across these solvents. In water, two dominant conformations accounted for 47.2% and 28.2% of the population, respectively, reflecting strong hydrogen bonding interactions. In contrast, toluene, a nonpolar solvent, favored different conformations, comprising 54.9% and 19.8% of the total population, likely due to hydrophobic interactions. Ether, as a moderately polar solvent, displayed unique conformational preferences, with its dominant structures constituting 15.6% and 13.3% of the total population. These findings underscore the critical role of the surrounding medium in stabilizing specific conformations and influencing the thermodynamic landscape of C22BG. Rigorous analyses of the relative energies of these conformations provided insights into the driving forces behind their stability, highlighting the interplay between solvent polarity, hydrogen bonding, and hydrophobic interactions.

To explore functional implications, we performed molecular docking studies on the dominant conformations, assessing their binding affinities to various ligands. These studies revealed that solvent conditions significantly modulate the interactions between C22BG and its potential targets, suggesting a solvent-dependent role in catalysis or biomolecular recognition. Furthermore, the impact of temperature on conformational dynamics was investigated. Sampling at different temperatures revealed shifts in the relative populations of dominant conformations, shedding light on the temperature-dependent behavior of C22BG under physiological conditions.

Our findings emphasize the importance of solvent effects and environmental conditions in shaping the structural dynamics of C22BG. The integration of GFN-FF and GFN2-xtb methods, combined with a detailed analysis of solvent-dependent conformational distributions, provides a robust framework for understanding the behavior of large biomolecules. These results not only advance our knowledge of C22BG's conformational dynamics but also highlight its potential applications in drug discovery, bioengineering, and catalysis. By demonstrating how solvent and temperature influence structure and function, this research lays the groundwork for future investigations into biomolecular dynamics and their applications in diverse fields of chemistry and biology.



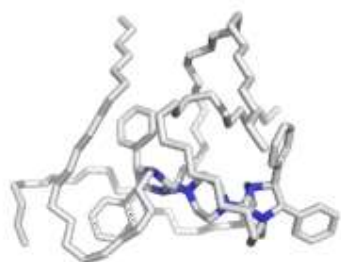
**Figure 2** Sampling results of C22BG in different solvents

### 5.3.2 Conformational Dynamics of C22BG in Solvents

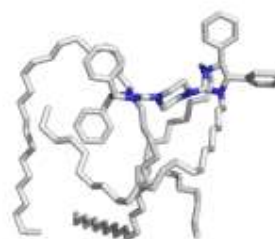
We conducted a detailed investigation into the structural stability and conformational behavior of C22BG across various solvent environments. C22BG, a complex biomolecule with a long-chain structure, exhibits remarkable adaptability due to its unique properties, making it an intriguing subject for computational analysis. Leveraging the GFN-FF force field, we performed extensive conformational sampling and generated 1,313 unique conformations, covering both stable and metastable states. To further refine these conformations, we applied the GFN2-xtb method, which combines accuracy and computational efficiency, ensuring precise geometric optimization for large biomolecules.

Solvent effects, a critical factor influencing biomolecular behavior, were systematically analyzed by evaluating C22BG's performance in water, toluene, and ether. The results revealed notable solvent-specific conformational preferences. In water, which promotes hydrogen bonding, two conformations dominated, constituting 47.2% and 28.2% of the total population, respectively. Conversely, in toluene, a nonpolar solvent, two distinct conformations accounted for 54.9% and 19.8% of the total distribution, highlighting favorable hydrophobic interactions. Ether, as a moderately polar solvent, displayed more diverse conformational preferences, with dominant conformations comprising 15.6% and 13.3% of the population. These findings underscore the strong influence of the solvent environment on the stability and behavior of C22BG, with water exhibiting the strongest stabilizing effects.

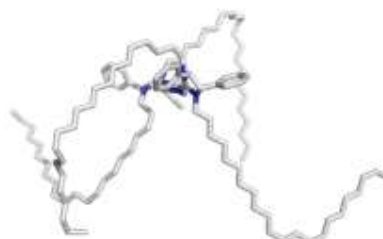
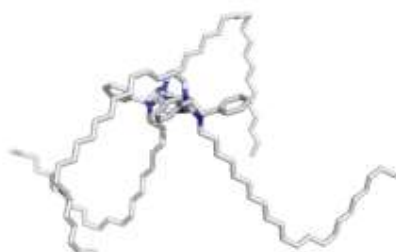
To complement the solvent analysis, rigorous thermodynamic evaluations were performed using the R2SCAN-3c method to calculate Gibbs free energy ( $\Delta G$ ) and decompose the contributions from enthalpy ( $\Delta H$ ) and entropy ( $\Delta S$ ). Notably, the aqueous environment consistently stabilized the lowest-energy conformation, affirming C22BG's pronounced preference for water due to strong electrostatic and hydrogen bonding interactions. In contrast, nonpolar solvents like toluene favored compact, hydrophobic conformations, while ether provided moderate stability due to weaker polar interactions.



Structure in water



Structure in toluene



Lowest energy structure in ether(ether1) Secondary energy structure in ether(ether2)

**Figure 3** Different structures in different solvents

Structure	Water (kcal/mol)	Toluene (kcal/mol)	Ether (kcal/mol)
water	0.0	0.0	0.0

toluene	98.96	43.3	43.24
ether1	13.18	14.7	13.71
ether2	10.86	14.33	13.33

CPCM/r2scan-3c//ALPB/GFN2-XTB

**Table 1** Relevant energy in different solvents

Further molecular docking studies investigated the functional implications of C22BG's dominant conformations. Binding affinities to diverse ligands varied significantly across solvent conditions, emphasizing the role of the environment in modulating interactions and potential biological functions. Additionally, temperature-dependent conformational sampling revealed shifts in the populations of dominant conformations, shedding light on the thermal adaptability of C22BG and its behavior under physiological conditions.

Benchmark validation using  $\omega$ B97X-V/def2-SVP and R2SCAN-3c methods reinforced the reliability and robustness of the findings. Consistent results across multiple theoretical approaches confirmed the structural stability and solvent-driven dynamics of C22BG, bolstering confidence in the computational models and methodologies employed.

In conclusion, this study highlights the critical role of solvent effects and thermodynamic forces in shaping the conformational landscape of C22BG. The insights gained into its structural adaptability and environmental responsiveness provide a solid foundation for future research. Applications in drug discovery, biomolecular engineering, and enzyme-mimetic catalysis are particularly promising, as C22BG demonstrates unique solvent-specific properties that could be leveraged for tailored therapeutic strategies and innovative chemical systems. Further experimental validation and exploration of C22BG in complex biological environments will be essential to fully realize its potential.

## 5.4 Summary and Future Directions

This chapter explores the conformational dynamics and thermodynamic stability of bisguanidinium (C22BG), a molecule with strong electrostatic and hydrogen bonding interactions, across three solvents (water, toluene, and ether) using advanced computational techniques. Conformational sampling generated 1,313 unique structures, revealing solvent-dependent preferences influenced by polarity: water favored hydrogen bonding-stabilized conformations, toluene promoted hydrophobic interactions, and ether showed moderate stability. Thermodynamic analysis highlighted water as the most stabilizing environment, with Gibbs free energy calculations affirming its influence. Molecular docking demonstrated solvent-dependent ligand-binding affinities, suggesting

applications in catalysis and biomolecular recognition. Temperature effects indicated C22BG's adaptability under varying conditions. Validated by  $\omega$ B97X-V and R2SCAN-3c methods, these findings underscore C22BG's structural adaptability and potential in drug discovery, biomolecular engineering, and enzyme-mimetic catalysis, paving the way for future experimental validation and exploration in complex biological systems.

## Computational details

All calculations were performed using a multi-level computational strategy designed to balance accuracy and efficiency. Initial conformational sampling was undertaken using the CREST (Conformer-Rotamer Ensemble Sampling Tool) program to generate an extensive ensemble of candidate geometries. Subsequent refinement employed the GFN-FF force field to accurately model nonbonded interactions and intramolecular flexibility. The most stable structures identified were then optimized and evaluated at the quantum mechanical level with GFN2-xtb, providing single-point energies that capture essential electronic effects for large, flexible systems. Thermodynamic properties were obtained using the R2SCAN-3c method, incorporating vibrational frequency analyses to derive entropy ( $\Delta S$ ) and enthalpy ( $\Delta H$ ) corrections, and subsequently computing Gibbs free energies ( $\Delta G$ ) according to the standard thermodynamic relation,

$$\Delta G = \Delta H - T\Delta S,$$

where T is the absolute temperature (298 K). Solvent effects were incorporated using the Conductor-like Polarizable Continuum Model (CPCM) to simulate bulk solvent environments (water, toluene, and ether), while additional solvent-specific refinements utilized the Analytical Linearized Poisson-Boltzmann (ALPB) model. Geometries were optimized to stringent convergence criteria (energy:  $10^{-6}$  Hartree, forces:  $10^{-5}$  Hartree/Bohr), ensuring the reliability of the resulting structures. Benchmark validations against the  $\omega$ B97X-V functional with a def2-SVP basis set further confirmed the internal consistency of both structural and energetic predictions. This integrated computational framework thereby provides a robust theoretical basis for interpreting the solvent-dependent conformational landscapes and thermodynamic behaviors of bisguanidinium(C22BG).

## References

1. Hunter, C. A. "Ionic Interactions in Biomolecules." *Angew. Chem. Int. Ed.* **2004**, 43, 5310–5324.
2. Parr, R. G.; Yang, W. *Density-Functional Theory of Atoms and Molecules*; Oxford University Press: New York, **1989**.

3. Neese, F. "Software Update: ORCA." *WIREs Comput. Mol. Sci.* **2012**, *2*, 73–78.
4. Bannwarth, C.; Ehlert, S.; Grimme, S. "GFN2-xTB—An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics." *J. Chem. Theory Comput.* **2019**, *15*, 1652–1671.
5. Grimme, S.; Ehrlich, S.; Goerigk, L. "Effect of Damping Functions in Dispersion Corrections." *J. Comput. Chem.* **2011**, *32*, 1456–1465.
6. Tomasi, J.; Persico, M. "Molecular Interactions in Solution: An Overview of Methods Based on Continuum Solvent Models." *Chem. Rev.* **1994**, *94*, 2027–2094.
7. Trott, O.; Olson, A. J. "AutoDock Vina: Improving the Speed and Accuracy of Docking." *J. Comput. Chem.* **2010**, *31*, 455–461.
8. Cancès, E.; Mennucci, B.; Tomasi, J. "A New Integral Equation Formalism for the Polarizable Continuum Model." *J. Chem. Phys.* **1997**, *107*, 3032–3041.
9. Grimme, S. "Dispersion-Corrected Density Functional Theory." *J. Comput. Chem.* **2006**, *27*, 1787–1799.
10. Shaik, S.; Cohen, D. "Catalytic Design and Reaction Mechanisms." *Chem. Rev.* **2005**, *105*, 2391–2430.
11. Frenking, G.; Shaik, S. *Theoretical Models for Chemical Bonding*; Wiley-VCH: Weinheim, **2014**.
12. Perdew, J. P.; Burke, K.; Ernzerhof, M. "Generalized Gradient Approximation." *Phys. Rev. Lett.* **1996**, *77*, 3865–3868.
13. Becke, A. D. "Density-Functional Exchange-Energy Approximation." *Phys. Rev. A.* **1988**, *38*, 3098–3100.
14. Head-Gordon, M.; Pople, J. A. "Analysis of Molecular Orbital Methods." *J. Chem. Phys.* **1988**, *89*, 5771–5786.
15. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; et al. *Gaussian 09*; Gaussian, Inc.: Wallingford, CT, **2009**.
16. Møller, C.; Plesset, M. S. "Note on an Approximation Treatment for Many-Electron Systems." *Phys. Rev.* **1934**, *46*, 618–622.
17. Boys, S. F.; Bernardi, F. "Calculation of Small Molecular Interactions by Differences of Separate Total Energies." *Mol. Phys.* **1970**, *19*, 553–566.
18. Cramer, C. J.; Truhlar, D. G. "Implicit Solvent Models: Overview and Applications." *Chem. Rev.* **1999**, *99*, 2161–2200.
19. Jensen, F. *Introduction to Computational Chemistry*; Wiley: Chichester, **2007**.
20. Warshel, A.; Levitt, M. "Theoretical Studies of Enzymatic Reactions." *J. Mol. Biol.* **1976**, *103*, 227–249.
21. Klamt, A.; Schüürmann, G. "COSMO: A New Approach to Dielectric Screening in Solvents." *J. Chem. Soc. Perkin Trans.* **1993**, *2*, 799–805.

22. Hillier, I. H.; Saunders, V. R.; Guest, M. F. "Ab Initio Molecular Orbital Calculations for Transition Metal Complexes." *Chem. Soc. Rev.* **1986**, 15, 177–182.
23. Barone, V.; Cossi, M. "Quantum Calculation of Molecular Energies in Solution." *J. Phys. Chem. A.* **1998**, 102, 1995–2001.

## Chapter 6: C-C Bond Coupling Reactions Catalyzed by BG and PLP

### 6.1 Introduction

C-C bond coupling reactions are fundamental processes in organic chemistry, essential for constructing complex molecules from simpler precursors and forming the basis for synthesizing pharmaceuticals, agrochemicals, and advanced materials. Despite their significance, the identification and characterization of transition states, which represent the highest energy points along the reaction coordinate and dictate reaction rates and selectivity, remain a persistent challenge. Historically, experimental techniques such as spectroscopy and kinetic studies provided indirect insights into transition states but were limited in precision and scope. Computational chemistry has since become a powerful tool for offering detailed molecular-level insights, yet traditional approaches often struggle with complex systems involving multiple intermediates and high-energy barriers. This study addresses these challenges by utilizing a novel catalytic system combining pyridoxal phosphate (PLP), a biologically relevant coenzyme renowned for stabilizing intermediates through resonance effects, with bisguanidinium (C22BG), a synthetic catalyst designed to mimic enzymatic active sites. The guanidinium groups in C22BG enhance catalytic performance by stabilizing intermediates and transition states via electrostatic and hydrogen bonding interactions. This hybrid system demonstrates exceptional efficiency in facilitating C-C bond coupling reactions. To further elucidate the reaction mechanism, the study employs the Meta-dynamics Reaction Path Search method, a computational technique that accelerates the identification of high-energy transition states by systematically sampling the potential energy surface. This chapter provides a comprehensive analysis of the reaction catalyzed by the PLP-C22BG system, highlighting the role of advanced computational methods in uncovering reaction mechanisms and catalytic behaviors.<sup>1,2</sup>

### 6.2 Methods

#### 6.2.1 Meta-dynamics Reaction Path Search

The Meta-dynamics Reaction Path Search method was employed to explore the reaction coordinate and identify transition states by modifying the potential energy surface (PES) with bias potentials that direct simulations toward high-energy regions. Key features of this technique include the application of repulsive potentials to the reactant region to prevent the system from becoming trapped in local minima and attractive potentials to the product region to guide the

simulation along the reaction coordinate. To ensure a comprehensive exploration of the PES, systematic sampling was performed using multiple sets of potential forms. This approach not only accelerates the identification of transition states but also minimizes the occurrence of spurious minima, making it particularly effective for analyzing complex reaction mechanisms.<sup>3</sup>

### **6.2.2 Computational Models**

Geometry optimizations for reactants, intermediates, and transition states were performed using density functional theory (DFT) at the R2SCAN-3c level to ensure accurate structural representation. Additionally, electronic structure analysis, including Natural Bond Orbital (NBO) analysis and electrostatic potential mapping, was conducted to characterize charge distribution and bond order, providing detailed insights into the electronic properties and interactions within the system.<sup>4,5</sup>

### **6.2.3 Thermodynamic and Kinetic Parameters**

Thermodynamic properties, including Gibbs free energy ( $\Delta G$ ), enthalpy ( $\Delta H$ ), and entropy ( $\Delta S$ ), were calculated for all key intermediates and transition states. Kinetic parameters such as activation energy and reaction rates were derived from the calculated free energy differences.<sup>6</sup>

### **6.2.4 Role of the Catalyst**

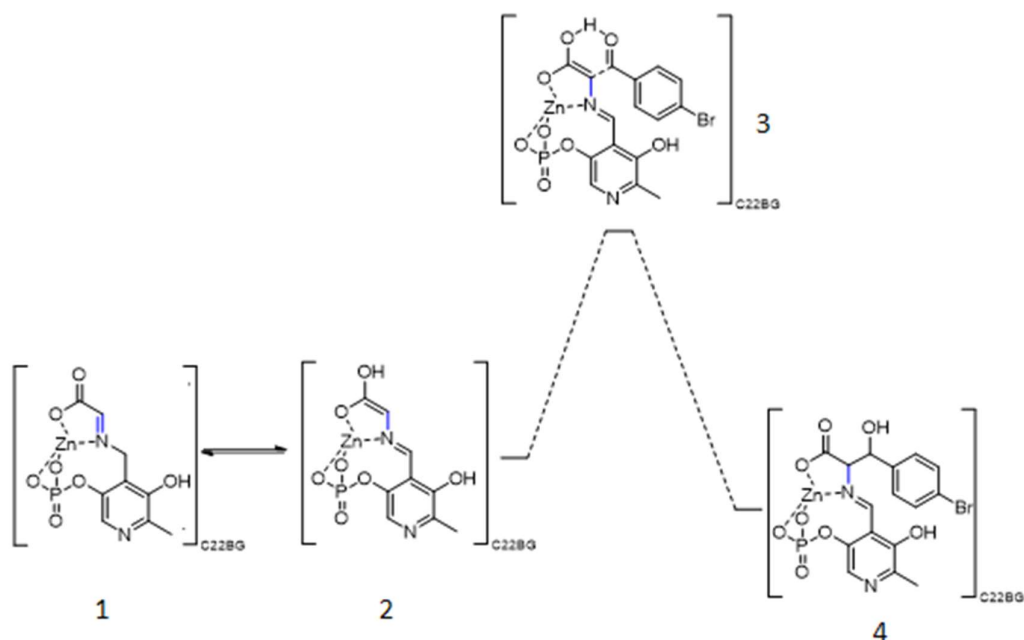
The influence of C22BG's structural features, such as its guanidinium groups and long alkyl chains, was analyzed to understand its role in stabilizing intermediates and lowering activation barriers.<sup>7</sup>

## **6.3 Results and Discussion**

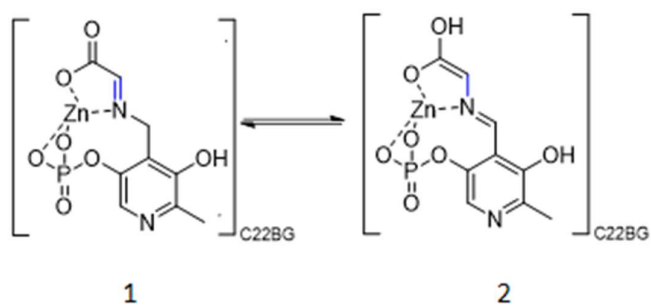
### **6.3.1 Intermediate Transformations**

The reaction pathway begins with the activation of the PLP-bound intermediate, facilitated by interactions with C22BG. The positively charged guanidinium groups in C22BG establish strong electrostatic interactions with negatively charged intermediates, stabilizing their structures. Additionally, hydrogen bonding between the guanidinium groups and the PLP coenzyme further enhances stabilization, effectively aligning reactants for efficient transition state formation. The energy landscape analysis revealed a Gibbs free energy difference of 1.82 kcal/mol between the reactant and the first intermediate, highlighting significant stabilization. This energy reduction underscores the dual role of

C22BG as both a molecular scaffold and an electronic stabilizer. Moreover, the long alkyl chains of C22BG dynamically adapt their conformations to align with the geometries of intermediates and transition states, minimizing steric hindrance and facilitating bond formation, thereby enhancing the overall catalytic efficiency.



**Figure 1** Reaction pathway with C22BG



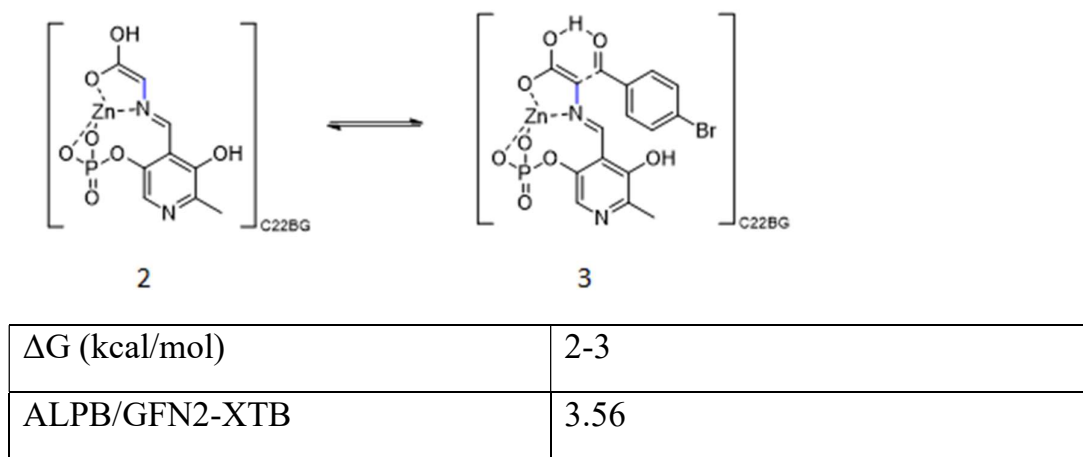
$\Delta G$ (kcal/mol)	1-2
ALPB/GFN2-XTB	1.82

**Figure 2:** Transformation of intermediates during the reaction.

These findings demonstrate the critical role of C22BG in orchestrating the reaction pathway, enhancing the stability of intermediates, and reducing energy barriers.

### 6.3.2 Transition State Stabilization in C-C Bond Coupling

The C-C bond coupling step, which involves the reaction between the PLP-bound intermediate and an aromatic aldehyde, represents the most challenging stage of the reaction. The presence of C22BG significantly reduces the activation energy for this step.



**Figure 3** Reversible Transition Between Intermediates 2 and 3 Stabilized by C22BG

The study highlights the critical role of C22BG in facilitating efficient and selective C-C bond coupling reactions by leveraging its structural and electronic properties. The Gibbs free energy difference between Intermediate 2 and the transition state (TS3) was calculated to be only 3.56 kcal/mol, indicating a low activation barrier. This reduction is attributed to strong electrostatic interactions and charge stabilization provided by the guanidinium groups. Additionally, hydrogen bonding enhances transition state stability and facilitates electron redistribution, while  $\pi$ - $\pi$  stacking interactions between the aromatic aldehyde and guanidinium groups further contribute to stabilization. Acting as an "electron reservoir," C22BG captures and redistributes charge during the reaction, effectively overcoming energetic barriers and promoting selective bond formation. These findings underscore its potential as a key facilitator in catalytic applications.

## 6.4 Summary and Future Directions

This study provides a detailed mechanistic understanding of the C-C bond coupling reaction catalyzed by PLP and C22BG, highlighting key findings such as the role of guanidinium groups in C22BG, which stabilize intermediates and transition states through electrostatic and hydrogen bonding interactions. The flexible, long-chain architecture of C22BG reduces steric hindrance and facilitates optimal reactant alignment, while non-covalent interactions, including hydrogen bonding, electrostatic interactions, and  $\pi$ - $\pi$  stacking, significantly lower activation barriers and enhance selectivity. Building on these insights, future research directions include investigating structural modifications to C22BG, such as altering chain lengths or adding functional groups to optimize catalytic performance; extending the PLP-C22BG system to green chemistry applications like CO<sub>2</sub> fixation and bio-based synthesis; leveraging machine learning to predict reaction pathways and accelerate catalyst discovery; conducting molecular dynamics simulations to explore the real-time behavior of intermediates and transition states; and validating computational results through experimental methods such as NMR spectroscopy, X-ray crystallography, and reaction calorimetry.

## Computational details

All computational studies were conducted using a multi-tiered approach to ensure accuracy, reliability, and efficiency in exploring the reaction pathways and thermodynamic properties of the PLP-C22BG system. Initial conformational sampling was performed with the CREST (Conformer-Rotamer Ensemble Sampling Tool), generating a broad set of candidate geometries for reactants, intermediates, and transition states. These geometries were refined using the GFN2-xtb method, which balances computational efficiency and accuracy for large, flexible systems. Geometry optimizations and energy evaluations were conducted at the R2SCAN-3c density functional theory (DFT) level, providing a robust description of electronic effects and ensuring accurate structural representations. Vibrational frequency analyses were used to compute enthalpy ( $\Delta H$ ) and entropy ( $\Delta S$ ) corrections, enabling the calculation of Gibbs free energy ( $\Delta G$ ). Solvent effects were incorporated using implicit solvation models, including the Conductor-like Polarizable Continuum Model (CPCM) for bulk solvent interactions and the Analytical Linearized Poisson-Boltzmann (ALPB) model for specific solvation effects in polar and non-polar environments. Metadynamics simulations facilitated the exploration of the potential energy surface (PES) and the identification of transition states. Convergence criteria were stringently set at  $10^{-6}$  Hartree for energy and  $10^{-5}$  Hartree/Bohr for forces to guarantee well-converged geometries and energy profiles. Additional electronic structure analyses, such as Natural Bond Orbital (NBO) calculations and

electrostatic potential mapping, characterized charge distribution, bonding interactions, and electronic properties. This computational framework provided a detailed understanding of the reaction mechanisms, intermediate stability, and transition state behavior, highlighting the catalytic role of C22BG and its structural contributions to reaction efficiency and selectivity. Benchmark validations against high-level methods further confirmed the reliability and robustness of the computational predictions.

## References

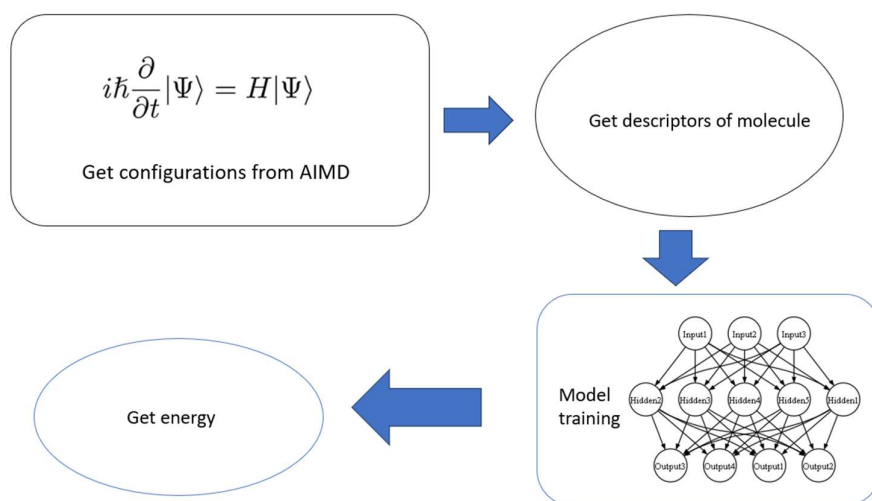
1. Neese, F. "The ORCA Program System." *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 73–78.
2. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. "A Consistent and Accurate ab initio Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu." *J. Chem. Phys.*, **2010**, 132, 154104.
3. Laio, A.; Parrinello, M. "Escaping Free-Energy Minima." *Proc. Natl. Acad. Sci. U.S.A.*, **2002**, 99, 12562–12566.
4. Perdew, J. P.; Ruzsinszky, A.; Csonka, G. I.; Constantin, L. A.; Sun, J. "Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry." *Phys. Rev. Lett.*, **2008**, 100, 136406.
5. Glendening, E. D.; Reed, A. E.; Carpenter, J. E.; Weinhold, F. "NBO Program Version 3.1." *Natural Bond Orbital Analysis Program Manual*, **2001**.
6. Cramer, C. J. "Essentials of Computational Chemistry: Theories and Models." 2nd Ed., Wiley, **2004**.
7. Anslyn, E. V.; Dougherty, D. A. "Modern Physical Organic Chemistry." University Science Books, **2006**.

## Chapter 7: Integration of Computational Approaches in Catalysis – Future Innovations and Applications

### 7.1 Introduction

As computational chemistry continues to evolve, integrating advanced methodologies has become essential for unlocking new insights in catalysis research. Machine Learning Potentials (MLPs), ONIOM, and related methods have already demonstrated transformative potential in elucidating reaction mechanisms and optimizing catalytic systems<sup>1-2</sup>. Emerging technologies, such as quantum computing<sup>3</sup>, multi-scale modeling<sup>4</sup>, and artificial intelligence (AI)<sup>5</sup>, now offer unprecedented opportunities to enhance these approaches, expanding their scope and impact.

This chapter explores how the integration of computational methods can advance the study of complex catalytic systems, particularly focusing on the C22BG-PLP system. By addressing challenges such as scaling, accuracy, and generalization, the chapter highlights hybrid frameworks, experimental validation, and interdisciplinary collaboration as critical elements for the future of computational catalysis.



**Figure 1** Workflow diagram showing the integration of MLPs

### 7.2 Synergistic Use of MLPs and ONIOM

The combination of MLPs and ONIOM offers a powerful approach to studying catalytic systems, balancing computational efficiency with precision. MLPs are ideal for pre-screening conformations and mapping energy landscapes due to their ability to quickly approximate potential energy surfaces. ONIOM complements this by providing detailed insights into electronic interactions and

reaction mechanisms in chemically active regions, such as the active site of the C22BG-PLP complex.

### **Applications in the C22BG-PLP System**

In the C22BG-PLP system, MLPs efficiently identify conformational states and pre-filter energy minima, reducing the computational cost of high-level calculations. ONIOM then refines critical intermediates and transition states, allowing for precise analysis of catalytic steps. This combined approach has successfully identified rate-limiting steps and guided catalytic modifications to enhance efficiency. Future advancements include developing adaptive algorithms for dynamic partitioning of QM and MM regions to improve accuracy and scalability, as well as creating seamless workflows that integrate MLP and ONIOM frameworks for more effective reaction exploration.

### **7.3 Multi-Scale Modeling in Catalysis**

Multi-scale modeling bridges the gap between atomistic simulations and macroscopic phenomena, offering a comprehensive view of catalytic systems like C22BG-PLP by capturing enzyme dynamics, substrate binding, and reaction kinetics in realistic environments. Recent advancements include quantum embedding, which explicitly models active site electronic interactions while representing the surrounding protein scaffold with coarse-grained models, and coarse-grained simulations that explore enzyme flexibility and large-scale dynamics with reduced computational costs. Practical applications in the C22BG-PLP system have revealed the role of solvent effects and secondary interactions in catalysis, with combined quantum mechanical calculations and molecular dynamics simulations providing valuable insights into allosteric regulation and substrate specificity.

Integrating multi-scale simulations with experimental data enhances model accuracy and predictive power. Validation can be achieved through X-ray crystallography for detailed structural insights, NMR spectroscopy to capture dynamic behavior, and kinetic studies to confirm reaction pathways and identify rate-limiting steps, ensuring the reliability and applicability of computational models.

### **7.4 Emerging Technologies in Computational Catalysis**

Emerging technologies are revolutionizing computational catalysis, allowing researchers to address previously intractable challenges. Quantum computing, through advanced algorithms like the Variational Quantum Eigensolver (VQE), offers unparalleled accuracy in electronic structure calculations, particularly for modeling electronic interactions at active sites in systems like C22BG-PLP.

Artificial intelligence (AI) accelerates research by analyzing large datasets to predict optimal reaction pathways, exploring novel catalytic systems through generative models, and optimizing reaction conditions and catalyst structures with reinforcement learning. High-performance computing further enhances these efforts by enabling large-scale simulations and real-time analysis of dynamic systems, significantly expanding the scope and depth of catalytic investigations.

## **7.5 Future Directions**

Future advancements in computational catalysis focus on several key areas. Hybrid computational pipelines aim to integrate MLPs, ONIOM, and multi-scale modeling, incorporating dynamic partitioning and adaptive learning algorithms for scalable and accurate analysis of catalytic systems. Real-time reaction modeling, combining molecular dynamics simulations and AI-driven potential energy surface mapping with ONIOM, will enable the capture of transient intermediates and reaction kinetics. Strengthening experimental integration through advanced spectroscopic techniques and kinetic studies will validate computational predictions and guide experimental designs to accelerate catalyst discovery. Expansion to complex systems, such as heterogeneous catalysts, multi-enzyme complexes, and industrially relevant processes like carbon capture and hydrogen production, will provide insights into diverse chemical environments. Additionally, sustainability and green catalysis efforts will leverage computational tools to design environmentally friendly catalysts that minimize waste, reduce energy consumption, and enhance selectivity, while exploring bio-inspired systems to tackle global sustainability challenges.

## **7.6 Conclusion**

The integration of advanced computational approaches, such as MLPs, ONIOM, and multi-scale modeling, has revolutionized catalytic research. By incorporating emerging technologies like quantum computing and AI, researchers can now tackle increasingly complex problems with unprecedented efficiency and accuracy. The insights gained from these methods, as demonstrated in the study of C22BG-PLP, have already transformed our understanding of catalytic mechanisms, enabling the rational design of improved catalysts. Future advancements in hybrid frameworks, experimental integration, and a focus on sustainability will further enhance the impact of computational catalysis, driving innovation across chemical and biological domains.

## References

1. Behler, J.; Parrinello, M. "Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces." *Physical Review Letters*, 2007, 98(14), 146401.
2. Senn, H. M.; Thiel, W. "QM/MM Methods for Biomolecular Systems." *Angewandte Chemie International Edition*, 2009, 48(7), 1198–1229.
3. McArdle, S.; Endo, S.; Aspuru-Guzik, A.; et al. "Quantum Computational Chemistry." *Reviews of Modern Physics*, 2020, 92(1), 015003.
4. Warshel, A.; Levitt, M. "Theoretical Studies of Enzymatic Reactions: Dielectric, Electrostatic and Steric Stabilization of the Carbonium Ion in the Reaction of Lysozyme." *Journal of Molecular Biology*, 1976, 103(2), 227–249.
5. Rupp, M.; Tkatchenko, A.; Müller, K. R.; von Lilienfeld, O. A. "Fast and Accurate Modeling of Molecular Atomization Energies with Machine Learning." *Physical Review Letters*, 2012, 108(5), 058301.

## Supporting information

### Coordinating information

#### Chapter 3

#### PLP complex conformational study

##### Compound 1

31

H	5.34547656085426	0.89686099271554	0.37752822475555
C	4.46982816209729	1.10570466463646	1.00319936045541
C	3.23699725469140	1.08719247703866	0.17749979686350
H	4.60808536629224	2.06798763886294	1.50263992557828
H	4.42647055819954	0.30810252436478	1.75264286897875
N	2.52207797216650	2.20742039062377	0.03886400651634
C	2.81847235064656	-0.11411745572099	-0.50151426829424
C	1.38911374051210	2.31605006395986	-0.69342959863702
H	2.85087693820330	3.04032951409525	0.51929041300226
C	1.56426847967047	-0.03306657331978	-1.21525017087646
O	3.56316008800410	-1.13586338262679	-0.46098374075559
C	0.89331279272449	1.20102771896552	-1.33267101416230
H	0.90774551767858	3.28552062877641	-0.70354981227944
C	1.07116349293813	-1.20406145764040	-1.96903667607046
C	-0.40870271383688	1.36206518383292	-2.08558681140142
N	0.91716812335427	-2.42741865075814	-1.62276344950722
H	0.79827454152610	-0.98491303214586	-3.00925976577881
O	0.31470125230387	-1.51785062340159	1.66921547970356
O	-1.49793548848262	0.66019401349911	-1.46372508805418
H	-0.64527181615592	2.43015259466711	-2.17927207712651

H	-0.32333160274002	0.94602113508727	-3.09532698012932
C	1.12226086289432	-2.81799240588260	-0.21714569646385
C	0.03070868873443	-2.20901456589242	0.64467534147593
P	-2.20044350051664	1.29589494943651	-0.08748777850193
O	-1.18342894851425	-2.33594127796818	0.27552384937721
O	-3.18400871771619	0.13793873755451	0.29466952412914
O	-1.10242799328665	1.22984665284553	1.03574932278063
O	-2.76411392498013	2.65600610369932	-0.39751697145138
Zn	-1.65631108162874	-0.67680781423483	1.41174897097748
H	1.03538201260448	-3.90950205801723	-0.15118772149614
H	2.10645520176155	-2.50759663705270	0.15269379639222

## Compound 2

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H	5.56228934258941	1.29951109925169	-0.27562031530228
C	4.86714796495443	1.88513402460578	0.33556719595931
C	3.48054314350859	1.68001583500893	-0.14778633987720
H	5.15501944342667	2.93878481295416	0.30563534916071
H	4.96784149467729	1.51449799638760	1.36258834292570
N	2.70858160478029	2.73197729414481	-0.42763047859817
C	2.92925858176340	0.35708328887992	-0.29811782853380
C	1.43660285379339	2.66850234608807	-0.88808394241265
H	3.10969153041707	3.65709261335815	-0.29641701170245
C	1.57032821988122	0.27502568325748	-0.79715990578459
O	3.60907522082435	-0.65366411034905	0.03272285653934
C	0.83757779524904	1.44028310914494	-1.08524669657278
H	0.95019187641941	3.61242127058979	-1.09741274345489

C	1.12990516394700	-1.10060386544801	-0.98585059215384
C	-0.54750971001643	1.48182775512840	-1.69947251749200
N	-0.04218262552050	-1.57053510495225	-0.75085975482214
H	1.92558247974062	-1.78534418935851	-1.30275385646429
O	-1.11311817112371	-4.82075151381741	0.34736689260964
O	-1.45055406272441	2.29353440266963	-0.92736988001497
H	-0.47321175493841	1.96963540061673	-2.67831423001030
H	-0.95507299127319	0.48002591442199	-1.85863359840255
C	-0.28013982159453	-2.99769409578963	-0.94175692419033
C	-1.09252103078176	-3.59510617390379	0.22316213217317
P	-2.26502194974568	1.56571462829670	0.32362668505568
O	-1.73661606005258	-2.77035613666949	0.98504188122873
O	-2.99057627470082	0.32129888235961	-0.30557256277459
O	-1.17752369769005	0.91310374040629	1.25496971594395
O	-3.11888762324429	2.65371825549445	0.91013739585809
Zn	-1.56343762742428	-0.89597921627717	0.45715522290637
H	-0.89466675119879	-3.13888370231904	-1.84387724817415
H	0.64712139605724	-3.56873096418077	-1.07124550362270

### Transition state 3

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H	5.35117605939129	0.88229668129755	0.38235763380734
C	4.47720146616219	1.08804439935832	1.01136135491489
C	3.24312535626610	1.08126753890914	0.18747118602593
H	4.61940567855055	2.04510573827138	1.51960743269277
H	4.43288126870403	0.28368898683197	1.75356255859409
N	2.52912684828596	2.20393331634364	0.06387084847719

C	2.82270972604708	-0.11095985947052	-0.50604975623726
C	1.39544094392259	2.32272431316382	-0.66559349147587
H	2.85954755672088	3.03032460433507	0.55439168042328
C	1.56811318217330	-0.01966407925253	-1.21788045908893
O	3.56629593409648	-1.13405715621302	-0.47873582789971
C	0.89799456504715	1.21639654987197	-1.31855883238417
H	0.91447709349050	3.29246512382774	-0.66290094779576
C	1.07395380955486	-1.18017870415430	-1.98702321576040
C	-0.40518140055696	1.38806318474726	-2.06702781540093
N	0.91934326941818	-2.40793774081911	-1.65699200983241
H	0.80098760338468	-0.94709924478219	-3.02421389322797
O	0.31935641805588	-1.54642142124079	1.65088751940075
O	-1.49471825621898	0.68179557506818	-1.45067442614962
H	-0.63956879737115	2.45761364917171	-2.14889371633796
H	-0.32298182668843	0.98268087333918	-3.08134127963353
C	1.12445099067113	-2.81690681138286	-0.25677373126100
C	0.03416684506364	-2.21855128646785	0.61407290740998
P	-2.18941967741263	1.30028445789344	-0.06253730487222
O	-1.17981212085021	-2.33531556167537	0.24172393636755
O	-3.17668678637848	0.14133290828988	0.30655975370490
O	-1.08766728655737	1.21335608932433	1.05580696227876
O	-2.74815156815882	2.66741893695903	-0.35041692898054
Zn	-1.64948383054769	-0.69532444330096	1.40772002868808
H	1.03662440195644	-3.90913176155807	-0.20437708239137
H	2.10948203377778	-2.51270713668608	0.11605540594415

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H	4.97368636197158	1.46963380850334	1.35708281152958
C	4.85769136423613	1.89330318373849	0.35242746956362
C	3.47060781397122	1.68904205143828	-0.13005030924928
H	5.55823953002941	1.35487663404596	-0.29496473316676
H	5.12599023421400	2.95223021215659	0.37760584445591
N	2.68169339066384	2.74149646837753	-0.35627701288494
C	2.93662231399845	0.36640649445397	-0.33631280423048
C	1.40599331575901	2.68179615162496	-0.80714015514595
H	3.07200796852489	3.66534357062564	-0.18879041424145
C	1.57343261727781	0.28908752548742	-0.82124619918397
O	3.63302850865708	-0.64975155870879	-0.06059044204173
C	0.82093130117170	1.45493031757152	-1.04997534515129
H	0.90529494750553	3.62750353963582	-0.96904897411937
C	1.14078923502126	-1.08225208669847	-1.05918787490421
C	-0.57222714711409	1.50141295610531	-1.64651077743337
N	-0.02079767031818	-1.56469099439298	-0.80156713249454
H	1.92676387525685	-1.74741009358704	-1.43616267707413
O	-1.11962526700280	-4.85033005359759	0.16345999723870
O	-1.47461102330572	2.28048368384741	-0.84111850815357
H	-0.51378914222404	2.01936473654556	-2.61088279315591
H	-0.97309852725558	0.50128697117788	-1.83094365650829
C	-0.27547791602687	-2.98053857911732	-1.04843536160289
C	-1.07363490418879	-3.62042708084199	0.10443322946814
P	-2.25759490454400	1.51447052676841	0.40774905511569
O	-1.67709470399765	-2.82353366589513	0.92641757118400

O	-2.96461151168824	0.26635927862347	-0.23007331375566
O	-1.14158994946636	0.86980243254653	1.31298386092902
O	-3.12078688795464	2.57669673524884	1.02640132519408
Zn	-1.47986443198333	-0.92785392897313	0.49023940687992
H	-0.90581816754504	-3.07705277312941	-1.94541583299719
H	0.64449656635650	-3.55258786358110	-1.21955642406368

### Pathway without Zn

#### Compound 1

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C	5.13551695573174	-0.00056524590162	0.75292006568987
C	3.78192608636461	0.46553728426256	0.31618235096735
N	3.57520923223106	1.75340833735253	0.13153460551336
C	2.74297452219759	-0.53592128016579	0.12705144852640
C	2.34206458375053	2.19299590138219	-0.24856571100229
C	1.46532570696520	-0.04218661847952	-0.31874640693336
O	2.98153494795115	-1.76894288360354	0.33794055498706
C	1.27808028746244	1.35935257222636	-0.48628024417567
C	0.40834590487799	-0.94030427559852	-0.60432437382891
C	-0.06517708640753	1.93525230273894	-0.83425562386263
N	0.49805055210964	-2.23234680918756	-0.41875610034468
O	-2.44369299382455	-4.04406969414199	0.56986044061625
O	-0.93757338844416	1.73927887469897	0.30235643101962
C	-0.59915836159646	-3.15521347214163	-0.63321327553771
C	-1.78306730033745	-3.00434696267929	0.37590857340352
P	-2.57539321826314	1.67326332644778	0.05409652149774

O	-1.99139829516228	-1.85532927721447	0.85903627478841
O	-2.98858825103587	2.72449842877719	-0.94509462187411
O	-2.76667935683298	0.22955266988810	-0.69483830962807
O	-3.15899053432463	1.62936625757803	1.44384626794933
H	5.54242564464907	-0.73148315492084	0.04411230123560
H	5.81921204903773	0.84684600824451	0.83378204517711
H	5.07647398461235	-0.51203818729767	1.72126209081579
H	2.22971094873145	3.27054108065919	-0.35687150128297
H	-0.52417031768272	-0.57030160162352	-1.02226607613770
H	0.03102658868854	3.00755880454712	-1.04308968841290
H	-0.48897177183552	1.45734522296425	-1.72885824457952
H	-1.02829632935055	-2.99514759555545	-1.63159474997938
H	-0.20822211724382	-4.17279472771609	-0.58727146133212
H	-2.51311551916664	-0.52550897760690	-0.10145929224929
H	1.39807860614722	-2.54051227793332	-0.01959736102608

## Compound 2

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C	4.75645283032311	-0.47311684017926	0.96580138780128
C	3.52439328620179	0.20434238745126	0.44355732400023
N	3.60688579721910	1.48954427231736	0.08795997547658
C	2.31962798521721	-0.55044449016230	0.34910183230518
C	2.50064742820997	2.10424160011965	-0.37922086650706
C	1.15322495022212	0.12023187716215	-0.15044681120980
O	2.28973199723665	-1.80924993415536	0.70500424020947
C	1.27309614458875	1.48150443249551	-0.51949187349068
C	-0.08382994241344	-0.58647377814360	-0.27275017318377

C	0.10309029967158	2.24582417503214	-1.06077295529063
N	-0.12006548462083	-1.86458273082426	0.07379361455925
O	-2.06157317727970	-4.84326414647284	0.47742653060544
O	-0.88006622036856	2.42655252021201	-0.00967776836246
C	-1.18258040131587	-2.71118531622543	0.05445914076540
C	-1.09278674136939	-4.06894288764901	0.42141801856242
P	-2.45662223625347	2.58428259664377	-0.48663196168522
O	0.13613018586387	-4.61651884818454	0.75828397701254
O	-2.66101094616473	3.91787839066081	-1.15664511666979
O	-2.89155376953418	1.30762007266014	-1.16891647665149
O	-3.13276148696125	2.70155605431547	1.00477760052138
H	5.02187650408707	-1.34045179448598	0.34918738856580
H	5.59499536853828	0.22701388787702	0.97763655311136
H	4.59504710344385	-0.85602016962635	1.98094261215089
H	2.60965317889421	3.15215861962428	-0.66007117733653
H	-0.99675633091694	-0.10592441857608	-0.62404764306236
H	0.42943153146922	3.22957480101265	-1.42216620438909
H	-0.35320551450760	1.70473260970806	-1.90285998268439
H	-2.14818731764759	-2.32020719560013	-0.25143597364172
H	0.88950057773982	-2.12563023357691	0.42696306801718
H	-3.20704370758873	1.83313585989442	1.42593061068904
H	0.87332810801568	-4.02472137332466	0.55196110981158

### Transition state 3

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C	4.10808820473370	-0.01916882883302	4.20251808889943
C	3.38721592512190	-0.15855032439473	2.89744127059269

N	3.98411642337591	0.24392881435335	1.78837953423936
C	2.05908550916425	-0.72730010660180	2.90786264267605
C	3.34247760779898	0.11297640991700	0.59757832721180
C	1.40557186415112	-0.85903553433974	1.63408546454055
O	1.51620572978843	-1.10653533693450	4.00804428042168
C	2.08361423035689	-0.42483181068179	0.46353902004492
C	0.14682418825296	-1.50531922950377	1.54717614484647
C	1.47829083079241	-0.58248158193069	-0.89969018679246
N	-0.46193452822896	-1.96335811403253	2.62377348360900
O	-3.61752084109618	-3.44899867674158	3.47618417196079
O	0.27098469475917	0.21005673854840	-0.99108842093302
C	-1.50838290448954	-2.91078924108845	2.57465641665320
C	-2.56233225300693	-2.84632112595719	3.59764615486153
P	-0.89999965044193	-0.35749934626371	-2.01807076706488
O	-2.32750460800447	-2.19291711046226	4.76136829460102
O	-0.44026013019373	-0.21837561746289	-3.44447659405464
O	-1.39892018685572	-1.68624615999985	-1.49548557918239
O	-2.01564152597387	0.81658232231214	-1.76233881304430
H	4.22068400282122	-0.99485496476452	4.69043922305599
H	5.09501595220044	0.42031283949093	4.04395096205919
H	3.53934912516302	0.60905077376684	4.89838926392243
H	3.88716625152897	0.45332896321609	-0.28201634092589
H	-0.33630066394751	-1.67565494236691	0.58405137031865
H	2.19155955380686	-0.25230677824281	-1.66534876784187
H	1.24457831519179	-1.64185641705023	-1.08630908824899
H	-1.93155530199595	-3.01106702480256	1.57475698198950

H	0.14263601653484	-1.80523029346165	3.47735548565704
H	-2.49850531143029	0.66999655431690	-0.93611048515496
H	-1.48611931546529	-1.71342197363651	4.75033924766537
O	-0.44285533054804	-4.72413062011353	4.18014630805032
C	-0.73779246495291	-4.59442205080019	2.93459421762958
H	-1.60382283580788	-5.17036885628435	2.53212425659374
C	0.39096823733615	-4.55707144167487	1.92604793998100
C	0.13988321693111	-4.64377750267748	0.55560941657890
C	1.16347289281857	-4.48175725998594	-0.37426769917500
C	2.44815183222491	-4.23073694955989	0.09329537323749
C	2.73785167819155	-4.16930439347738	1.45000640238845
C	1.69834957050382	-4.33826967358180	2.35972254521828
Br	3.86192075816164	-3.94131445848698	-1.17804548646068
H	3.74992921084855	-3.97824387673773	1.79302949849732
H	1.88975241788066	-4.27568458573109	3.42701712328879
H	-0.87502851447486	-4.81658278527041	0.20107431233529
H	0.96075212647384	-4.53911842198537	-1.43890499474763

#### Compound 4

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C	4.30502480032155	0.72436524392101	3.67016443177564
C	3.44105731542421	0.61376329377509	2.45270208834638
N	3.70440613067728	1.37064209407070	1.40771546176920
C	2.32820391349208	-0.32518654716430	2.48524281485557
C	2.91845731097355	1.29111012959773	0.29518725849932
C	1.55398035176751	-0.42286128607989	1.27535777117796
O	2.08495113909117	-1.01463843789254	3.52750876651184

C	1.86189306861413	0.42483752066783	0.17344488423969
C	0.48763119672404	-1.34673234351979	1.17672300846377
C	1.03498741389653	0.40149161788345	-1.08281498579944
N	0.08811875171724	-2.08681796802878	2.17985708929510
O	-2.75618086973431	-1.26369348701222	1.95873593697135
O	-0.32743026493552	0.74985953549735	-0.75767149677077
C	-1.06759102118904	-2.96175383739960	2.11444814534846
C	-2.30862290461328	-2.18446947003592	2.68652092228768
P	-1.58519291500190	-0.04429744403658	-1.50555527191513
O	-2.73962568141005	-2.52826660410327	3.81471510744805
O	-2.02372515077684	0.74230961190846	-2.71295165891545
O	-1.21182027635475	-1.50666699603594	-1.64075250556484
O	-2.71661375830182	0.16100424096835	-0.35681343599660
H	4.73828629917059	-0.24930724226457	3.92812867119908
H	5.10736852964164	1.44529437429892	3.50103201829478
H	3.71395431797948	1.03718209912748	4.53938839574812
H	3.17320019815688	1.96646927622150	-0.51990777825369
H	-0.04581499272299	-1.48303097177636	0.23471799181987
H	1.43625930240443	1.12599244596971	-1.80265399538534
H	1.06209017531900	-0.59445954895482	-1.54612503488777
H	-1.27653569574936	-3.18104686184532	1.06017531332594
H	0.60679511870224	-1.94860876102064	3.06288738473506
H	-2.58988528529293	-0.43357870146890	0.42486342100438
H	-1.33777351403631	-3.51121569625659	4.50784833564636
O	-0.54223983636870	-4.02149653470850	4.24268543300536
C	-0.77558700031849	-4.27770067657244	2.86454605995587

H	-1.66562053037576	-4.91460796977784	2.73015372288656
C	0.41769531426739	-4.97522385439802	2.25888571026224
C	0.26111096699756	-5.69157607749180	1.07077449489215
C	1.35006382655232	-6.29130561065584	0.44635294743023
C	2.60310752617641	-6.16590585026400	1.03322759632359
C	2.79087575763258	-5.46459862460405	2.21592806666397
C	1.68833433788235	-4.86764164758773	2.82369950168376
Br	4.11784882844254	-6.99246464382759	0.18612287766665
H	3.77670500185841	-5.37975407511045	2.66110233796917
H	1.82332573129861	-4.31528689846916	3.74767587705653
H	-0.72501253175559	-5.78763989448672	0.62165759193555
H	1.21955960375583	-6.84915692105727	-0.47488127300631

### **Pathway with Zn**

#### **Compound 1**

31

H	5.35117605939129	0.88229668129755	0.38235763380734
C	4.47720146616219	1.08804439935832	1.01136135491489
C	3.24312535626610	1.08126753890914	0.18747118602593
H	4.61940567855055	2.04510573827138	1.51960743269277
H	4.43288126870403	0.28368898683197	1.75356255859409
N	2.52912684828596	2.20393331634364	0.06387084847719
C	2.82270972604708	-0.11095985947052	-0.50604975623726
C	1.39544094392259	2.32272431316382	-0.66559349147587
H	2.85954755672088	3.03032460433507	0.55439168042328

C	1.56811318217330	-0.01966407925253	-1.21788045908893
O	3.56629593409648	-1.13405715621302	-0.47873582789971
C	0.89799456504715	1.21639654987197	-1.31855883238417
H	0.91447709349050	3.29246512382774	-0.66290094779576
C	1.07395380955486	-1.18017870415430	-1.98702321576040
C	-0.40518140055696	1.38806318474726	-2.06702781540093
N	0.91934326941818	-2.40793774081911	-1.65699200983241
H	0.80098760338468	-0.94709924478219	-3.02421389322797
O	0.31935641805588	-1.54642142124079	1.65088751940075
O	-1.49471825621898	0.68179557506818	-1.45067442614962
H	-0.63956879737115	2.45761364917171	-2.14889371633796
H	-0.32298182668843	0.98268087333918	-3.08134127963353
C	1.12445099067113	-2.81690681138286	-0.25677373126100
C	0.03416684506364	-2.21855128646785	0.61407290740998
P	-2.18941967741263	1.30028445789344	-0.06253730487222
O	-1.17981212085021	-2.33531556167537	0.24172393636755
O	-3.17668678637848	0.14133290828988	0.30655975370490
O	-1.08766728655737	1.21335608932433	1.05580696227876
O	-2.74815156815882	2.66741893695903	-0.35041692898054
Zn	-1.64948383054769	-0.69532444330096	1.40772002868808
H	1.03662440195644	-3.90913176155807	-0.20437708239137
H	2.10948203377778	-2.51270713668608	0.11605540594415

### Compound 2

31

C	6.80986893564830	-0.35436828783961	1.51938470978444
C	5.37486942289444	0.08554484189649	1.47701223667916

N	5.03923585303753	1.22308627751880	2.10182906790531
C	4.41330146714865	-0.66938173286404	0.79615159842320
C	3.76176629789852	1.61296344532450	2.07192446768948
C	3.06791921459105	-0.25100258348047	0.72645201044308
O	4.73737510178007	-1.81615139961834	0.13192140062734
C	2.73957812122546	0.93284420988373	1.41380173726899
C	2.16388836590692	-1.13168599830621	-0.01551920371723
C	1.33575800235617	1.46139185389189	1.59465280952576
N	1.32793351553111	-0.74291945778849	-0.93428143075565
O	-0.86566881308976	-1.89677675216625	-3.55261679553249
O	1.22979102351979	2.86179721921858	1.26554250353586
C	0.57502165397342	-1.62570376775558	-1.66726382999717
C	-0.11932667610983	-1.09979643831241	-2.75154181863806
O	-0.11295489690439	0.13525059751876	-3.09503760565840
O	2.05475026572150	2.65094260441093	-1.18901989109227
O	-0.35259456202003	2.42357077276288	-0.71329421175357
O	0.78151507693934	4.76841547504582	-0.30109686625126
Zn	0.88862710871331	1.11914434340140	-1.69988735088866
H	7.39568138168348	0.36630849351484	2.09214718269988
H	6.91814404644749	-1.33857126118749	1.99431208843947
H	7.24161293029083	-0.42277915308966	0.51189759406316
H	3.52318605076169	2.52638276879522	2.61571163033160
H	0.59654024100511	0.87276108769827	1.04147324368122
H	1.07588116266698	1.39428325331601	2.65814604877599
H	0.59535997953812	-2.69251480767408	-1.45264186334677
H	5.67345042127134	-2.02344851198413	0.25833598973944

H	2.29455837411935	-2.20498343010400	0.14795134970814
P	0.90173835913706	3.27052990374622	-0.30607511744843
H	-0.82939742568320	-2.81173356577356	-3.23549168424160

**Transition state 3**

45

C	6.79270581617732	-0.36912056678515	1.55516763915752
C	5.36059977979270	0.07544840072181	1.49853759286227
N	5.00992010522650	1.18597637081145	2.15612207137241
C	4.41137125656890	-0.65662220374265	0.77206045774233
C	3.73330189148491	1.58009632120629	2.11536403616276
C	3.06507361809402	-0.23871575744608	0.70279045290427
O	4.75378452020388	-1.76897867412608	0.06774409621960
C	2.72308105817148	0.92721608915383	1.41545966380431
C	2.18754067112997	-1.11039492713907	-0.07771539880666
C	1.32482819373497	1.47626097877429	1.57197880310001
N	1.25814684588455	-0.73103476988336	-0.89694870532448
O	-0.86153090086103	-1.98285593835590	-3.50378448690584
O	1.25675811952756	2.87980268646425	1.25066064757258
C	0.55954520730938	-1.67874472402005	-1.64318885772434
C	-0.13531558250527	-1.15114096072738	-2.78201857811450
O	-0.14768201187419	0.08183583655534	-3.08181889410816
O	2.08469270184020	2.56569635100345	-1.18646071879586
O	-0.33653672573750	2.54149773638727	-0.74329637393280
O	0.96800341625171	4.79536222636735	-0.34514973532218
Zn	0.77672341177309	1.12309917939419	-1.66694238843329
H	7.36581738968132	0.32692255470287	2.16945279834459

H	6.88792279374988	-1.37151264860326	1.99347731760961
H	7.24614552598043	-0.39851093980585	0.55552025152797
H	3.48668869208121	2.47634893816456	2.68298131678070
H	0.58724817902860	0.90742884813216	0.99926842383187
H	1.03822669671571	1.40290241975383	2.62816747953299
H	0.97433381898644	-2.68246274976123	-1.72014702771988
H	5.68418652664442	-1.98859374271483	0.21555046707360
H	2.41443925650078	-2.17889315395681	-0.01658422037280
C	-1.87031609251776	-1.34526935397054	-0.16795032380305
C	-1.54364266939549	-0.79014241656291	1.07308589022883
C	-2.22549212366309	0.31933295491147	1.55875503681102
C	-3.23532464521985	0.86984247032822	0.77936942099447
C	-3.58705861401113	0.33782220139409	-0.45714407461482
C	-2.90270946994604	-0.77771949684276	-0.92279172109286
H	-0.75210409897728	-1.23612160007241	1.67161795647095
H	-4.38322344957200	0.78273618505251	-1.04485708519067
H	-3.17226823802775	-1.21628950033582	-1.87934437948235
H	-1.97096912391113	0.74723133450845	2.52281716951035
C	-1.13431954042333	-2.53924796003578	-0.64733352128584
O	-1.62275894637337	-3.30846429529068	-1.54382997379206
H	-0.43762623632977	-2.95826550696547	0.09844473769440
Br	-4.16638899638716	2.41657732379587	1.42494096359821
P	0.98001446498561	3.29422213369897	-0.32984461013715
H	-1.21260149179265	-2.70911565413843	-2.85152461594808

#### Compound 4

45

C	5.87444376485275	0.35621380023420	2.27747278749682
C	4.54803597620316	0.80413189163277	1.74068375370575
N	4.17191301818857	2.07171233208963	1.93350752631730
C	3.71464762567012	-0.09031143316841	1.05189990075669
C	2.98717331233269	2.47626515814264	1.46455874009692
C	2.47405665595383	0.33213597977446	0.53951355278579
O	4.07997657174612	-1.37558629959397	0.81065686611884
C	2.09917685253646	1.66933102781148	0.75884877753610
C	1.68165713631749	-0.70958612541041	-0.12508299809191
C	0.77432018805774	2.28334777415669	0.36967045254424
N	1.01743272118095	-0.56166943375106	-1.21011532106150
O	0.18704394182964	-2.81191466513936	-3.86594971305109
O	0.95204828597636	3.49326570922761	-0.39219768251418
C	0.31180266131164	-1.71286947930643	-1.75652200117921
C	0.45259772639478	-1.75218671950641	-3.29645487465016
O	0.79061090705467	-0.65638288634338	-3.89108407073570
O	2.33121392938575	2.37293116627195	-2.28539563332692
O	-0.11396546299622	2.52369377163429	-2.52916377030326
O	1.26875095193058	4.76555597292950	-2.53011116111233
Zn	1.05069977735193	0.87326784615620	-2.69173838947465
H	6.35892039908948	1.18719682039626	2.79217300864644
H	5.76248383115825	-0.47115121898600	2.99110342819508
H	6.53839227144168	0.01365045136511	1.47294761623189
H	2.71760530500935	3.51257483193319	1.66241561055141
H	0.12980977888435	1.57826979093044	-0.16254182678263
H	0.24852167923659	2.58457196400036	1.28369950296418

H	0.69873929799686	-2.65789283570448	-1.35288729850899
H	4.91572962302589	-1.58106455527391	1.25363205985763
H	1.72742689126113	-1.69969464453508	0.34312110270127
C	-1.40881274341882	-1.58104791976894	0.08050315683415
C	-1.14196163016736	-2.71655288507579	0.84879386260317
C	-1.24583025709383	-2.68406653809979	2.23493218555332
C	-1.62210721634315	-1.49392543545696	2.84588393872708
C	-1.90368886410366	-0.35247542439770	2.10964982288454
C	-1.79498977763773	-0.40473048111995	0.72140415750066
H	-0.84708615150795	-3.64481655581771	0.36455188475148
H	-2.20325756530476	0.56716446374652	2.60141530326645
H	-2.02025231589563	0.48276817533414	0.14059334977706
H	-1.03956958240691	-3.57176443936150	2.82324354067203
C	-1.21264805845071	-1.64107923479571	-1.41405031308891
O	-1.82403959469190	-0.50716198769493	-2.01341851676692
H	-1.64790579311551	-2.57391951587666	-1.80254777087912
Br	-1.76311672103883	-1.43247426560776	4.75998170444214
P	1.12544580520598	3.35422645603429	-2.03628743696666
H	-1.96821515241200	-0.69251040400939	-2.95064881502436

## Chapter 5

### Structures in Fig 17

#### C22BG in water

340

C 0.577034 3.125129 -0.771418  
N 0.274047 1.716731 -0.730071  
C 1.619840 3.357053 -1.877903  
H 1.045793 3.478471 0.159048  
H -0.334865 3.688358 -0.968284  
C 1.446733 0.887826 -0.505468  
C 2.574463 1.238360 -1.488715  
N 2.852480 2.654433 -1.580710  
H 2.299284 0.900330 -2.495660  
H 3.475846 0.711001 -1.174827  
H 1.829760 4.425616 -1.945459  
H 1.234931 3.003129 -2.838771  
H 1.178746 -0.164297 -0.598872  
H 1.834953 1.057085 0.505917  
C -0.975017 1.298066 -0.404664  
N -1.538302 0.143807 -0.878887  
N -1.855383 2.017932 0.376811  
C -3.159726 1.377289 0.311500

C -2.862421 -0.019650 -0.311796  
C -4.149406 2.192652 -0.488924  
H -3.564795 1.249195 1.320562  
H -3.585949 -0.245560 -1.100722  
C -2.910528 -1.116515 0.728098  
C 3.604934 3.333433 -0.530121  
N 4.743536 4.082075 -1.003586  
N 4.038235 2.551018 0.589482  
C 5.510093 2.561459 0.663403  
C 5.971577 3.603554 -0.391734  
C 6.065303 1.189349 0.443576  
H 5.821559 2.900935 1.661028  
H 6.627137 3.114165 -1.128717  
C 6.763124 4.700593 0.272664  
C 3.400102 2.908373 1.851556  
C 4.822137 4.511710 -2.376832  
C -1.226696 -0.475662 -2.145516  
C -1.429796 2.549268 1.662209  
C -3.811955 3.423396 -1.036023  
C -4.756034 4.177641 -1.709600  
C -6.055500 3.716384 -1.841998  
C -6.399849 2.485032 -1.306259  
C -5.454116 1.729542 -0.640716  
H -2.805940 3.796366 -0.921441  
H -4.479582 5.135048 -2.126178  
H -6.795331 4.310315 -2.357617

H -7.411602 2.118166 -1.402959  
H -5.731540 0.771828 -0.225345  
C -4.133852 -1.469131 1.293637  
C -4.207751 -2.451938 2.261858  
C -3.058914 -3.104595 2.678710  
C -1.839587 -2.765838 2.116126  
C -1.763703 -1.776416 1.152107  
H -5.164284 -2.710562 2.691137  
H -5.037014 -0.970411 0.974904  
H -3.114049 -3.873474 3.434160  
H -0.943923 -3.277807 2.433772  
H -0.809744 -1.515002 0.719218  
C 6.620265 0.479871 1.512546  
C 7.112460 -0.798170 1.342029  
C 7.058384 -1.409945 0.097910  
C 6.508429 -0.717040 -0.973549  
C 6.023486 0.562072 -0.804353  
H 5.618479 1.096704 -1.650581  
H 6.471854 -1.180241 -1.949725  
H 7.448482 -2.407758 -0.039686  
H 7.550560 -1.320401 2.181657  
H 6.678975 0.952235 2.485029  
C 8.061039 4.441850 0.703079  
C 8.795884 5.417460 1.349846  
C 8.243826 6.668982 1.575156  
C 6.952424 6.933920 1.150642

C 6.217525 5.956463 0.504284  
H 8.489235 3.462848 0.529645  
H 9.802784 5.203005 1.678055  
H 8.819172 7.431787 2.078232  
H 6.515576 7.906315 1.325074  
H 5.209685 6.151304 0.170786  
C 3.404850 4.408722 2.177183  
H 3.875353 2.332952 2.652200  
H 2.357253 2.580758 1.794787  
C 2.330580 4.771014 3.197136  
H 3.209239 4.931533 1.235848  
H 4.391097 4.720050 2.529256  
C 2.207872 6.280622 3.393442  
H 2.550293 4.291442 4.154407  
H 1.377831 4.377834 2.839077  
H 3.132404 6.655498 3.838953  
C 1.023882 6.681800 4.277222  
H 2.099873 6.757129 2.416161  
H 1.093862 7.751801 4.487627  
H 1.087881 6.153750 5.231567  
C -0.328579 6.395889 3.625806  
H -0.342597 6.834434 2.625333  
C -1.497701 6.959342 4.432204  
H -0.458433 5.319311 3.518787  
H -1.423705 8.049047 4.444736  
H -1.428902 6.613769 5.466213

C -2.853429 6.547899 3.850079  
H -3.627119 7.226078 4.216298  
C -3.238731 5.115380 4.217746  
H -2.817989 6.647132 2.762897  
H -3.451515 5.065650 5.288275  
H -2.396656 4.450947 4.021487  
C -4.454461 4.621128 3.436370  
H -5.297250 5.293117 3.613737  
C -4.852240 3.200464 3.832858  
H -4.234467 4.649524 2.365663  
H -5.112833 3.182792 4.893898  
H -3.999138 2.530690 3.697609  
C -6.034062 2.684938 3.015232  
H -6.881033 3.355896 3.164939  
C -6.426325 1.264562 3.419040  
H -5.779494 2.705600 1.952402  
H -6.722411 1.260240 4.471019  
H -5.552519 0.613943 3.322799  
C -7.562999 0.687043 2.575140  
H -7.266113 0.693718 1.526076  
C -8.873200 1.456677 2.729429  
H -7.726642 -0.351509 2.873757  
H -8.773082 2.441791 2.270220  
H -9.075729 1.603936 3.793339  
C -10.069326 0.742152 2.099614  
H -10.219939 -0.222179 2.590981

C -9.918863 0.525110 0.593934  
H -10.963762 1.344195 2.280108  
H -9.184554 -0.260147 0.406615  
H -9.552914 1.447952 0.140666  
C -11.248384 0.130341 -0.047240  
H -11.704172 -0.665023 0.548524  
C -11.110219 -0.376948 -1.484227  
H -11.929860 0.982877 -0.020661  
H -12.109076 -0.594812 -1.870717  
H -10.551390 -1.316268 -1.471006  
C -10.404785 0.581189 -2.444479  
H -9.375588 0.732050 -2.116058  
C -11.091357 1.936779 -2.590911  
H -10.364476 0.103161 -3.426909  
H -12.134262 1.785642 -2.879169  
H -11.083730 2.461525 -1.634259  
C -10.394930 2.800735 -3.636738  
H -9.352205 2.958026 -3.367661  
H -10.426321 2.319852 -4.612647  
H -10.879053 3.771019 -3.718307  
H 3.839720 4.905859 -2.643646  
C 5.216413 3.432867 -3.402390  
H 5.542841 5.338697 -2.424974  
H 4.724704 2.506247 -3.108666  
H 6.299087 3.280377 -3.379401  
C 4.784357 3.809605 -4.816138

H 3.694974 3.778904 -4.869898  
C 5.387440 2.904735 -5.895463  
H 5.092837 4.838182 -5.021708  
H 6.455654 3.123189 -5.976849  
H 4.927454 3.152992 -6.854942  
C 5.233261 1.404986 -5.637328  
H 5.725819 0.864960 -6.450665  
C 3.785249 0.931386 -5.536113  
H 5.758154 1.145511 -4.715255  
H 3.275279 1.107755 -6.485776  
H 3.267691 1.504354 -4.765288  
C 3.721921 -0.552353 -5.180171  
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## **Ether 2**

340

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## Chapter 6

### Reaction pathway with C22BG

#### Compound 1

371

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H	-1.1703604490	-0.8756291220	1.7583809476
C	0.6099569453	1.5373023571	0.1545012076
C	-0.5244816952	2.0888154628	-0.7060116542
N	-1.8097617012	1.9757596354	-0.0024233717
H	-0.6046340673	1.5381666018	-1.6452075412
H	-0.3550932785	3.1361708605	-0.9750407433
H	-3.0809155343	0.7080997973	1.0942678297
H	-2.2950465333	-0.0305488136	-0.2971960293
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N	1.0336372242	-2.0536726969	1.3596902400
C	1.3661845175	-3.3398668416	0.6916848117
C	1.8875597797	-2.9038713358	-0.7044045240
C	0.1657061953	-4.2414694196	0.6145909191

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C	-1.1058803449	-3.6962457947	0.5729591175
C	-2.2185309912	-4.5054252454	0.5167326545
C	-2.0713594275	-5.8751157850	0.4839858848
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C	-4.4386737775	-1.6854908556	-1.1040809464
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H	-9.2240328180	1.3769902109	-1.6118437007
C	-5.6355137192	-1.0526339472	-1.7601837065
O	-6.4514894945	-2.0952532949	3.3389911668
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O	-5.0886569227	-3.2277901485	1.0482133192
H	-8.9195807888	-0.0413141329	-4.9228167802
C	-7.8122353166	-0.1507257790	-3.1202939970
O	-4.3773806013	-3.0768408017	-1.3075508600
C	-6.0142298004	-1.5018356274	-3.0086310177
C	-8.9702134258	0.3477156430	-3.9044645788
N	-7.0571681549	-1.0756955857	-3.6956469774
P	-5.4375492408	-3.8730741400	-0.3683096616
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H	-8.9630837855	1.4368765644	-3.9684758331
O	-6.8279918345	-3.5644531557	-0.8778830387
H	-9.9136177726	0.0127161345	-3.4719616638
O	-5.0995675410	-5.3407018310	-0.2771708635

## Compound 2

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C	-1.33669718412490	0.04873675445682	0.87237041130531
N	-0.06021071604037	-0.04189310299597	0.18954718588511
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H	-1.72623707156587	-0.94178950645072	1.09637754227816
C	0.46873620027222	1.26371971509210	-0.16334733437806
C	-0.52663343538801	2.02034915753494	-1.04047726737833
N	-1.82580901489955	2.06252468368034	-0.38523753892320
H	-0.65373719224600	1.49890189844642	-1.99662392926187
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H	-3.29540551934381	0.81803204246492	0.44019391376629

H	-2.45666566719218	0.12980081713237	-0.96797238855310
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C	0.59906583482586	-1.20011577606644	0.05404956813554
N	1.29034984041695	-1.58084498102505	-1.02386673237013
N	0.63969382527168	-2.12945702656390	1.01868428360217
C	1.32456252423334	-3.32317042070972	0.56084029271330
C	1.88608288534433	-2.89819051932409	-0.82267056847275
C	0.40300684383539	-4.52102555355484	0.48726737928784
H	2.14705124113600	-3.56449068966649	1.24306551528070
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C	3.39553329608282	-2.83691759956545	-0.84800211851878
C	-2.60838972983015	3.15054917040749	-0.37518376781763
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C	-5.36029315842654	4.42530625119989	0.83352402627376
C	-1.02180087910343	4.76718626369082	0.71185951733538
C	-4.49716143462057	2.29745602437580	-1.72149990204920
C	1.30696159652810	-0.99787966858957	-2.34806633452073
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C	0.13833735616722	-6.90646527438890	0.32958350932977
C	0.95596001567487	-5.79204322389944	0.38972006636063
H	-1.43675946734542	-3.40939148971759	0.58758675837665
H	-2.87684483118329	-5.39442798524392	0.48606882068094
H	-1.88744298043931	-7.62738144999459	0.32928487959561
H	0.57101193521910	-7.89336122998387	0.25739027794120
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C	5.50816592306168	-3.69082942107667	-1.61249267595525
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C	-7.02588192280834	5.50790618429678	2.19201319143117
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C	-1.91613763074667	3.85763654096573	4.38887340684792
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H	-3.79250391051836	1.87912926302271	4.83477902042706
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H	-2.52752878345220	1.12640452653068	3.85828754322202
H	-2.99696872282285	0.68166212680880	6.83175234303652
H	-1.67384589619717	-0.02690046283522	5.91647259117311
C	-3.60322332162617	-0.85528768317384	5.46475380189811
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C	-3.17777901995931	-1.52973185628783	4.15987198384781
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H	-2.09261717260065	-1.62448871193169	4.15182773698340
H	-3.49187703296652	-0.91128437434496	3.31916884499189
C	-3.79817277654427	-2.91639877797557	3.97971765885016
H	-4.85876567261831	-2.87250356131980	4.24160677878769
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H	1.04650932338779	-4.10540829930254	4.51569377392401
C	2.59245573005449	-5.49532631312718	3.96624069371442
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C	3.68050399939119	-4.43115991286884	4.10432060370950
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H	4.39540743411833	-4.50903248638604	1.54465190394463
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H	3.88893583091584	-6.90282632821048	2.02941037378963
H	4.59815492545071	-7.85851253620885	-0.00616578984320
H	4.46609811068390	-6.13177966542503	-0.35057400799265
C	6.47970474856629	-6.87077406291956	-0.25876842914600
H	6.93420314200632	-5.89538040647219	-0.10835916140939
H	7.06184881097456	-7.60885164757689	0.28958566537625

H	6.53612192127096	-7.11645351032736	-1.31713222743633
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H	1.85748821420695	4.17337752015551	-4.21851596060582
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H	2.73181482181487	1.97818658885895	-5.26022953605171
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H	2.87907835752759	2.93775148798802	-0.48344399667728
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C	2.29519903146582	4.31557843713299	3.64091447199327
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H	2.85685186087495	3.90534961738114	4.48245234721417
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C	2.39283585031135	6.72211603919899	4.47996877438912
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C	3.13291606994225	6.44630168209898	5.78451940098862
H	1.31661036166127	6.68371732794458	4.66637953401846
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H	4.20910847377060	6.44638513295233	5.62106487164601
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H	2.43699064682982	-0.96878685244152	2.50483825864394
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H	1.09155308525726	0.17422159592594	2.62313342237336
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C	2.43109393181740	0.38741092932774	4.91582114961227
H	3.26318823530696	0.52864298663510	4.22685976941482
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H	1.81735015489808	1.28962699733136	4.88324665542915
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C	4.04842378060865	-0.84454914063299	6.50577479268377
H	4.42825182736431	-0.78554616003659	7.52994646461239
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H	3.58250008366966	-1.82683420168999	6.39958903493410
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H	5.91208287413930	-1.59033579328009	5.76782478209713
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H	5.36502710197361	1.37605009437812	5.31610801972902
C	7.27409239745321	0.56417845485296	4.76749411081653
H	6.28542940008706	0.71943710990333	6.66645163501241
H	7.92275557205105	-0.26581693209662	5.06127259591234
H	7.81667658384139	1.48861859833552	4.97847457806305
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C	8.22751838930819	0.65719586700589	2.39713998240503
H	6.24693373844642	1.23735532048276	3.01007262459979
H	8.00361962410691	0.30857348357768	1.38518713828447
H	9.02576594206382	0.01995412305979	2.78719404456056
C	8.75299432052647	2.09232613014682	2.29680027980581
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385			
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