WOOJIN LEE

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EDUCATION

UNIVERSITY OF CALIFORNIA, LOS ANGELES Los Angeles, CA

Doctor of Philosophy, Chemistry

- Research Advisors: Prof. Kendall N. Houk and Prof. Hosea M. Nelson
- Graduated: September 2023
- Thesis: Exploring Reaction Mechanisms of Short-Lived Carbocation and Radical Intermediates via Synergetic Modern Computational Methods and Collaborative Experiments

UNIVERSITY OF CALIFORNIA, BERKELEY Berkeley, CA

Bachelor of Science, Chemistry

- Research Advisor: Prof. F. Dean Toste
- Graduated: May 2016

RESEARCH EXPERIENCE

UNIVERSITY OF CALIFORNIA, LOS ANGELES Los Angeles, CA

Graduate Research Assistant Oct 2018 – Oct 2023

- Utilized Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations to understand the behavior and reactivities of short-lived carbocation and radical intermediates
- Enhanced the reliability and robustness of the computational findings through collaborative experiments
- Collaborated with Professor Isaac J. Krauss (Brandeis University), Professor Jiannan Zhao (Dalian University of Technology), and Professor Massimo Bietti (University of Rome, Tor Vergata)
- Designed experimental mechanistic studies for collaborators to corroborate the computational predictions
- Found the timing difference in non-classical carbocation formation from *exo*- and *endo*-2-norbornyl brosylates in the 'Molecular Dynamics of the Norbornyl Cation and Its Generation in Winstein-Trifan Solvolysis' project
- Investigated C–H insertion reactions of vinyl carbocations in the 'Computational Exploration of the Nature of Li^+-Ureide Anion Catalysis on Formation of Highly Reactive Vinyl Carbocations and Subsequent C–C Bond Forming Reactions' project
- Determined an oxidation potential through in silico modeling to provide support for further experimental studies in the 'Electrochemical Fluorination of Vinyl Boronates Through Donor-Stabilized Vinyl Carbocation Intermediates' project
- Uncovered the origin of the mechanistic switch from homoallylation to cyclopropylcarbinylation in the 'Mechanistic Switch from Homoallylation to Cyclopropylcarbinylation of Aldehydes' project
- Elucidated the full reaction pathway in the 'Diastereoselective Radical Aminoacylation of Olefins through N-Heterocyclic Carbene Catalysis' project and identified rate- and diastereoselectivity-determining steps
- Discovered evidence of divergent radical and cationic pathways in dioxirane oxygenation in the 'Interplay Between Radical and Cationic Pathways in C(sp^3)–H Bond Oxygenation of Bicyclic and Spirocyclic Hydrocarbons by Dioxiranes' project
- Conducted experimental research on vinyl cation C–H insertion reactions and Lewis-acid catalyst development
- Developed a lithium urea catalyst in the 'Urea-Catalyzed Vinyl Carbocation Formation Enables Mild Functionalization of Unactivated C–H Bonds' project and established a new substrate class, demonstrating vinyl cation compatibility with the Lewis basic and heteroatom-containing substrates
- Extended the use of QM modeling, molecular docking, and conformational analysis in biological applications

Graduate Teaching Assistant Oct 2018 – Dec 2022

- Coordinated with professors and fellow TAs to instruct, guide, and support +200 undergraduate students in chemistry courses
- Educated students on essential organic chemistry concepts, laboratory techniques, and safety practices
- TA Classes: Practical and Theoretical Introductory Organic Synthesis, Organic Chemistry Laboratory, General and Organic Chemistry Laboratory, Organic Reactions and Pharmaceuticals, Organic Structural Methods

CALIFORNIA INSTITUTE OF TECHNOLOGY Pasadena, CA

Visiting Student Researcher Oct 2021 – Sep 2022

- Performed computational experiments in the 'Cationic Claisen-Type Cascade Reactions Enabled by Vinyl Cation' project, finding cationic [3,3] and [1,3] rearrangements
- Conducted computational mechanistic studies in the 'Accessing Medium-sized Rings via Vinyl Carbocation Intermediates' project, revealing canonical Friedel–Crafts reactions involved in medium-sized ring formation of vinyl cations

UNIVERSITY OF CALIFORNIA, BERKELEY Berkeley, CA

Research Assistant in Professor F. Dean Toste's research group Jan 2016 – May 2017

- Investigated strategies for stabilizing Oxo-Re catalyst in the 'Hydrogen Gas-Mediated Deoxydehydration/Hydrogenation of Sugar Acids: Catalytic Conversion of Glucarates to Adipates' project, achieving 72% yield in the aqueous adipic acid synthesis

- Conducted mechanistic studies to reveal substrate selectivity determined by the electronic effects
- Developed laboratory skills in organic synthesis, purification, and characterization

WORK EXPERIENCE

UNIVERSITY OF SOUTHERN CALIFORNIA Los Angeles, CA

Postdoctoral Research Associate in Professor Vsevolod "Seva" Katritch research group Oct 2023 – Present

- Conducted computational drug discovery research to target prostaglandin D_2 receptor 1 (DP1) using structure-based virtual screening of 3 trillion make-on-demand compounds from the Enamine REAL database
- Prioritized 104 compounds for synthesis and in vitro validation through ligand property modeling, multi-parameter filtering (MPF), similarity deduplication, chemical novelty filter, diversity-based down-sampling, ultimately revealing 10 validated DP1 antagonists and agonists
- Performed GPCR homology modeling and molecular dynamics (MD) simulations to investigate receptor–ligand interactions and conformational dynamics of DP1
- Collaborate with Prof. Vadim Cherezov (University of Southern California) to integrate computational predictions with structural and pharmacological studies

GENENTECH, INC South San Francisco, CA

Medicinal Chemist Intern in the Small Molecule Discovery Chemistry Department May 2017 – Sep 2017

- Formulated a synthetic process for highly branched dendrimer drug conjugates
- Optimized a synthetic route to active pharmaceutical ingredient (API)
- Acquired comprehensive knowledge of pharmaceutical research, encompassing target synthesis, biologically-active molecule synthesis, and physicochemical analysis

REPUBLIC OF KOREA ARMY South Korea

Squad Leader & Operation Staff, 53rd Ammunition Battalion Headquarters Apr 2009 – Feb 2011

- Achieved the rank of Sergeant and received an honorable discharge in February 2011
- Led a team of 10 soldiers during training and field operations as a squad leader; ensured mission success and safety
- Coordinated logistical and operational support under high-pressure conditions

SKILLS

- Computational Chemistry and Biology: Proficient in molecular dynamics (GROMACS, Progdyn Suite), quantum mechanical atomistic simulations (Gaussian, ORCA), and molecular docking (Molsoft ICM-Pro, AutoDock Vina)
- Computer-Aided Drug Design: Skilled in high-throughput virtual ligand screening with a focus on structure-based drug discovery and early-stage hit identification (Molsoft ICM-Pro, V-SYNTHES)
- Data-Driven Drug Design: Skilled in Python, Jupyter Notebook, RDKit, and scikit-learn for predictive modeling, cheminformatics, and QSAR analysis using molecular descriptors and machine learning (XGBoost, CatBoost, LightGBM)
- Conformational and Energetic Analysis: Utilized Molsoft ICM-Pro, Spartan 18, and XTB-CREST to generate conformational ensembles and calculate relative energies, supporting structure–activity relationship (SAR) studies and ligand optimization strategies
- High-Performance Computing (HPC): Experienced with Linux-based HPC environments (UCLA IDRE, NSF XSEDE, USC CARC) to run large-scale simulations, manage resources, and perform parallelized workflows

AWARDS

- Hanwha TotalEnergies Industry-Academic Scholarship Nominee 2023
  (declined the offer due to its condition requiring post-graduation employment, which conflicts with my decision to pursue my career in computational chemistry)
- Excellence in Chemistry Fellowship 2018 – 2023
- UCLA Doctoral Student Travel Grant 2022
- Graduate Dean's Scholar Award 2018

PUBLICATIONS

[11] Davoudinasab, B.; Raskovalov, A.; **Lee, W.**; Han, G. W.; Katritch, V.; Cherezov, V. "Structural Insights into Mechanism of Activation and Inhibition of Prostaglandin Receptors," *Manuscript under review by Nature Portfolio*

[10] Williams, C. G.; Nistanaki, S.; Dong, K.; **Lee, W.**; Houk, K. N.; Nelson, H. M. "Main-Group Catalyzed Cationic Claisen Rearrangements via Vinyl Carbocations," *Org. Lett*., **2024**, *26,* 4847–4852.

[9] Zhao, Z.; Popov, S.; **Lee, W.**; Burch, J. E.; Delgadillo, D. A.; Kim, L. J.; Shahgholi, M.; Houk, K. N.; Nelson, H. M. "Accessing

Medium-sized Rings via Vinyl Carbocation Intermediates," *Org. Lett*., **2024**, *26,* 1000–1005.

[8] **Lee, W.**; Benton, T.; Sengupta, A.; Houk, K. N. "Molecular Dynamics of the Norbornyl Cation and Its Generation in Winstein–Trifan Solvolysis: The Timing of Sigma-Bridging," *J. Org. Chem.,* **2024**, *89*, 1140–1146.
[*Highlighted in ACS Editors' Choice, UCLA Chemistry & Biochemistry Newsroom, and CNSI Newsroom*]

[7] Galeotti, M.[#]; **Lee, W.**[#]; Sisti, S.; Casciotti, M.; Salamone, M.; Houk, K. N.; Bietti, M. "Radical and Cationic Pathways in C(sp^3)–H Bond Oxygenation by Dioxiranes of Bicyclic and Spirocyclic Hydrocarbons Bearing Cyclopropane Moieties," *J. Am. Chem. Soc.,* **2023**, *145*, 24021–24034.
[[#]*Authors contributed equally*]

[6] **Lee, W.**; Nelson, H. M.; Houk, K. N. "Computational Exploration of the Nature of Li^+-Ureide Anion Catalysis on Formation of Highly Reactive Vinyl Carbocations and Subsequent C–C Bond Forming Reactions," *J. Org. Chem.,* **2023**, *88*, 3403–3408.

[5] Liu, W.-D.[#]; **Lee, W.**[#]; Shu, H.; Xiao, C.; Chen, X.; Houk, K. N.; Zhao, J. "Diastereoselective Radical Aminoacylation of Olefins through *N*-Heterocyclic Carbene Catalysis," *J. Am. Chem. Soc.,* **2022**, *144*, 22767–22777.
[[#]*Authors contributed equally* | *Highlighted in Synfacts*]

[4] **Lee, W.**[#]; Polyak, D.[#]; Xu, B.; Houk, K. N.; Krauss, I. J. "A Mechanistic Switch from Homoallylation to Cyclopropylcarbinylation of Aldehydes," *Org. Lett*., **2022**, *24,* 4660–4664.
[[#]*Authors contributed equally*]

[3] Wigman, B.; **Lee, W.**; Wei, W.; Houk, K. N.; Nelson, H. M. "Electrochemical Fluorination of Vinyl Boronates Through Donor-Stabilized Vinyl Carbocation Intermediates," *Angew. Chem. Int. Ed.*, **2022**, e202113972.

[2] Bagdasarian, A. L.; Popov, S.; Wigman, B.; Wei, W.; **Lee, W.**; Nelson, H. M. "Urea-Catalyzed Vinyl Carbocation Formation Enables Mild Functionalization of Unactivated C–H Bonds," *Org. Lett*., **2020**, *22,* 7775–7779.
[*Highlighted in Synfacts*]

[1] Larson, R.; Samant, A.; Chen, J.; **Lee, W.**; Bohn, M.; Ohlmann, D.; Zuend, S.; Toste, F. D. "Hydrogen Gas-Mediated Deoxydehydration/Hydrogenation of Sugar Acids: Catalytic Conversion of Glucarates to Adipates," *J. Am. Chem. Soc.,* **2017**, *139*, 14001–14004.

PRESENTATIONS

THE THIRD DRUG DISCOVERY INNOVATION WORKSHOP — Los Angeles, CA
University of Southern California — Feb 2025
Title: Virtual Ligand Screening and Molecular Dynamics Simulations of the Prostaglandin D_2 Receptor 1

HOUK RESEARCH CONFERENCE POSTER PRESENTATION — Los Angeles, CA
University of California, Los Angeles — Aug 2022
Title: Diastereoselective Radical Iminoacylation of Olefins through N-Heterocyclic Carbene Catalysis

NATIONAL ORGANIC CHEMISTRY SYMPOSIUM POSTER PRESENTATION — San Diego, CA
American Chemical Society Division of Organic Chemistry — June 2022
Title: Diastereoselective Radical Iminoacylation of Olefins through N-Heterocyclic Carbene Catalysis

VIRTUAL CCHF ORAL PRESENTATION — Los Angeles, CA
Center for Selective C–H Functionalization (CCHF) — Dec 2021
Title: Selectivity in C–H Oxidation by Ethyl Trifluoromethyl Dioxirane

GENENTECH POSTER PRESENTATION — South San Francisco, CA
Genentech Inc. — Aug 2017
Title: Improving Poor Lung Retention of Inhaled Compounds

GENENTECH ORAL PRESENTATION — South San Francisco, CA
Small Molecule Discovery Chemistry Department, Genentech Inc. — July 2017
Title: Improving Poor Lung Retention of Inhaled Compounds