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Cooper Stergis Jamieson, PhD
Structural Biology & Chemistry
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Executive Summary

Accomplished scientist who leverages interdisciplinary expertise in computational chemistry, biochemistry, and machine learning to enable hit identification and accelerate lead optimization across virology, oncology, and inflammation. In the past year, conducted key experiments that have: terminated projects, identified hit material, and developed lead series. Passionate about developing and implementing computational methodologies and AI/ML to drive scientific breakthroughs.

Award-winning doctoral research uncovered and characterized a novel family of enzymes named the "pericyclases." These enzymes catalyze pericyclic reactions and exist in all walks of life. The pericyclases are critical for aromatic amino acid biosynthesis and in the construction of structurally diverse natural products that possess inspiration for drug discovery. Post-PhD research with Nobel Laureate Frances Arnold integrated computational chemistry and machine learning with directed evolution to accelerate the generation of novel biocatalysts. A PhD and post-PhD fellowship on enzymatic reactions yielded a deep understanding of biocatalysis and protein-ligand interactions, perfectly positioning me for success in identifying and optimizing novel drug candidates.

Work Experience

April 2023 – Current
Research Scientist at **Gilead Sciences**
Leverages computational chemistry, AI/ML, and structure-based drug design to enable hit identification, lead optimization, and drug discovery across Gilead's virology, oncology, and inflammation therapeutic areas.

- Pioneered methodologies for ultra-large (>1B compound) virtual screens utilizing physics-based and machine learning approaches.
- Developed simple and interpretable computational models to accelerate hit-to-lead and lead optimization campaigns through efficient computational prioritization and design triage.
- Collaborated cross-functionally with medicinal chemists, biologists, and DMPK scientists on drug discovery initiatives.

Expertise in cross-departmental collaboration & communication, structure-based modeling, ligand-based modeling, molecular docking, free energy calculations, and AI/ML.

November 2018 – July 2022
Artificial Intelligence & Computational Chemist at **Ro5**
Strategic development and deployment of machine learning models at an AI/ML drug discovery startup that accelerated molecular docking, affinity prediction, and property prediction.

- Developed & patented modern architecture machine learning models for physicochemical property prediction and lead optimization.
- Communication skills bridged the knowledge gap between chemists and computer scientists.

Expertise in Python, JavaScript, high-performance computing, and database management.

Education

July 2022 – April 2023
Caltech, **Post-PhD**, advised by **Frances H. Arnold**
National Institute of Health, R. L. Kirschstein National Research Service Award Fellow
Worked as a hybrid scientist in the laboratory and as a computational chemist.

- Engineered enzymes to catalyze new-to-nature transformations, including diastereoselective cyclopropanation & sp^2-amination reactions.
- Developed computational workflows (leveraging molecular docking & quantum mechanical calculations) to accelerate directed evolution and enzyme engineering.
- Led molecular modeling seminars to showcase strategies for structure-based enzyme design.

Expertise in directed evolution, site directed mutagenesis, enzyme engineering, high-throughput experimentation, and encoding small molecules and proteins as graphs.

December 2021 – July 2022
UCLA, **Post-PhD**, advised by **Kendall N. Houk** & **Yi Tang**
UCLA Distinguished Research Fellow
Learned wet-laboratory skills to validate computational predictions and led to multiple publications including a unifying biosynthetic strategy for the construction of all fungal pyridone natural products.

- Discovered the first natural examples of enzyme-catalyzed pericyclic reactions.
- Leveraged computational chemistry to elucidate enzymatic functional & reaction mechanisms.
- Validated theoretical predictions with *in vivo* and *in vitro* experiments.

Expertise in heterologous expression systems, large-scale fermentation, protein purification, and general biochemistry laboratory techniques.

September 2017 – December 2021
UCLA, **PhD** in **Theoretical and Computational Chemistry**, advised by **Kendall N. Houk** & **Yi Tang**
"Fungal pericyclases & pericyclic reactions in nature."
Graduated early with more than 20 papers, led two research subgroups (biosynthesis & reaction dynamics), and received recognition for both research and teaching excellence.

- Published first-author papers in Nature describing the first reported Alder-ene reaction in biology.
- Selected by K. N. Houk to co-teach his graduate-level physical organic chemistry course.
- Received multiple awards for teaching & research excellence, including the inaugural Royal Society of Chemistry Horizon Prize.

Expertise in pericyclic reactions, genome mining, biosynthetic gene clusters, retrobiosynthesis, density functional theory, ab initio molecular dynamics, QM/MM and methodologies for benchmarking.

September 2012 – May 2016
Lewis & Clark College, **BA** in **Chemistry** (honors), **BA** in **Art**
Chemistry Thesis: “Molybdenum-catalyzed phosphine oxidation reactions”, advised by Louis Y. Kuo
Double major focusing on organometallic catalysis & ceramic sculpture. Received Kent Swanson Memorial Scholarship for award-winning ceramic works.

Skilled in glove box and Schlenk line techniques and glaze and clay body formulation.

Selected Awards, Fellowships, Scholarships, Service, Outreach & Professional Associations

2023 Ambassador of Gilead Sciences Science Day
2023 Master of Ceremonies of COMP Together Conference
2022 Invited Young Scientist at the 71st Lindau Nobel Laureate Meeting in Chemistry
2021 Guest Lecture at Lewis & Clark College, “The Diels–Alder Reaction In Nature”
2021 Royal Society of Chemistry Horizon Prize
2021 Saul and Sylvia Winstein Dissertation Award
2020–2021 UCLA Graduate Education Dissertation Year Fellowship
2020 American Chemical Society Reviewer Lab Certificate
2020 Don C. Atkins Excellence in Research Award
2020 Michael E. Jung Excellence in Teaching Award
2020 UCLA Chemistry & Biochemistry Excellence in Research Fellowship
2019–2021 Senior Foote Graduate Fellow
2019 Saul Winstein Fellowship
2019 Volunteer at UCLA’s Exploring Your Universe Science Festival
2019 Stanford’s CQMD/Pulse Quantum Molecular Design Summer School
2018 Sequoia & Kings Canyon National Park Citizen Science Volunteer
2017 Read Marfa Volunteer
2014–2016 Kent Swanson Memorial Scholarship
2015–2016 Lewis & Clark College Presidential Grant
2013–2014 Mellon Funds Research Grant

Patents

System and method for prediction of protein-ligand bioactivity using point-cloud machine learning.
Alwin Bucher, Alvaro Prat, Orestis Bastas, Aurimas Pabrinkis, Gintautas Kamuntavičius, Mikhail Demtchenko, Sam C. Macer, Zeyu Yang, **Cooper S. Jamieson**, Žygimantas Jočys, Roy Tal, Charles D. Knuff. Ro5. USA. 2022-02-22. US11256995B1.

System and method for prediction of protein-ligand bioactivity and pose propriety.
Alwin Bucher, Aurimas Pabrinkis, Orestis Bastas, Mikhail Demtchenko, Zeyu Yang, **Cooper S. Jamieson**, Žygimantas Jočys, Roy Tal, Charles D. Knuff. Ro5. USA. 2022-02-22. US11256994B1

System and method for prediction of protein-ligand interactions and their bioactivity.
Orestis Bastas, Alwin Bucher, Aurimas Pabrinkis, Mikhail Demtchenko, Zeyu Yang, **Cooper S. Jamieson**, Žygimantas Joĉys, Roy Tal, Charles D. Knuff. Ro5. USA. 2021-11-16. US11176462B1.

Publications

‡co-authors; *corresponding author

Tandem intermolecular [4+ 2] cycloadditions are catalysed by glycosylated enzymes for natural product biosynthesis.
Jiawang Liu, Jiayan Lu, Chen Zhang, Qingyang Zhou, **Cooper S. Jamieson**, Changhui Shang, K. N. Houk, Jiahai Zhou, Youcai Hu. *Nat. Chem.* 2023, 15, 1083–1090.

***Enantio*- and diastereoenriched enzymatic synthesis of 1,2,3-polysubstituted cyclopropanes from (*Z*/*E*)-trisubstituted enol acetates.**
Runze Mao, Daniel J. Wackelin, **Cooper S. Jamieson**, Torben Rogge, Shilong Gao, Anuvab Das, Doris M. Taylor, K. N. Houk, Frances H. Arnold. *J. Am. Chem. Soc.* 2023, 145, 29, 16176–16185.

Biosynthesis of polycyclic natural products from conjugated polyenes via tandem isomerization and pericyclic reactions.
Kanji Niwa, Masao Ohashi,* Kaili Xie, Chen-Yu Chiang, **Cooper S. Jamieson**, Michio Sato, Kenji Watanabe, Fang Liu, K. N. Houk,* Yi Tang.* *J. Am. Chem. Soc.* 2023, 145, 25, 13520–13525.

Computational design of a tetrapericyclic cycloaddition and the nature of potential energy surfaces with multiple bifurcations.
Ana Martin-Somer,* Xiao-Song Xue, **Cooper S. Jamieson**, Yike Zou, K. N. Houk.* *J. Am. Chem. Soc.* 2023, 145, 7, 4221–4230.

Enzymatic *cis*-decalin formation in natural product biosynthesis.
Masao Ohashi,‡ Dan Tan,‡ Jiayan Lu,‡ **Cooper S. Jamieson**, Daiki Kanayama, Jiahai Zhou,* K. N. Houk,* Yi Tang.* *J. Am. Chem. Soc.* 2023, 145, 6, 3301–3305.

Discovery and characterization of a terpene biosynthetic pathway featuring a norbornene-forming Diels-Alderase.
Zuodong Sun, **Cooper S. Jamieson**, Masao Ohashi, K. N. Houk,* Yi Tang.* *Nat. Commun.* 2022, 13, 2568.

Computational prediction and experimental validation of a bridged cation intermediate in akanthomycin biosynthesis.
Cooper S. Jamieson, Masao Ohashi, K. N. Houk,* Yi Tang.* *J. Am. Chem. Soc.* 2022, 144, 12, 5280–5283.

Computations on pericyclic reactions reveal the richness of ambimodal transition states and pericyclases.
K. N. Houk,* Xiao-Song Xue, Fang Liu, Yu Chen, Xiangyang Chen, **Cooper S. Jamieson**. *Isr. J. Chem.* 2022, 62, e202100071.

Ambimodal transition states in Diels–Alder cycloadditions of tropolone and tropolonate with N-methylmaleimide
Hong Zhang,* Mathias K. Thøgersen, **Cooper S. Jamieson**, Xiao-Song Xue, Karl A. Jørgensen,* K. N. Houk.* *Angew. Chem. Int. Ed.* 2021, 60, 24991.

Sulfide oxidation by 2,6-bis[hydroxyl(methyl)amino]-4-morpholino-1,3,5-triazinatodioxomolybdenum (VI): mechanistic implications with DFT calculations for a new class of molybdenum(VI) complex.
Cayden X. Bullock, **Cooper S. Jamieson**, Pierre Moënne-Loccoz, Buck Taylor, Jordan A.M. Gonzalez, Ellie A. Draves, Louis Y. Kuo.* *Inorg. Chem*. 2021, 60, 11, 7762–7772.

Computational exploration of the mechanism of critical steps in the biomimetic synthesis of preuisolactone A, and discovery of new ambimodal (5 + 2)/(4 + 2) cycloadditions.
Hong Zhang,* Alexander J. E. Novak, **Cooper S. Jamieson**, Xiao-Song Xue, Shuming Chen, Dirk Trauner,* K. N. Houk.* *J. Am. Chem. Soc*. 2021, 143, 17, 6601–6608.

Biosynthesis of *para*-cyclophane-containing hirsutellone family of fungal natural products.
Masao Ohashi,‡ Thomas B. Kakule,‡ Man-Cheng Tang, **Cooper S. Jamieson**, Mengting Liu, Yi-Lei Zhao, K. N. Houk,* Yi Tang.* *J. Am. Chem. Soc.* 2021, 143, 15, 5605–5609.

Total synthesis and computational investigations of sesquiterpene-tropolones ameliorate stereochemical inconsistencies and resolve an ambiguous biosynthetic relationship.
Christopher Y. Bemis, Chad N. Ungarean, Alexander S. Shved, **Cooper S. Jamieson**, Taehwan Hwang, Ken S. Lee, K. N. Houk,* David Sarlah.* *J. Am. Chem. Soc.* 2021, 143, 15, 6006–6017.

Fungal dioxygenase AsqJ is promiscuous and bimodal: substrate-directed formation of quinolones versus quinazolinones.
Manuel Einsiedler, **Cooper S. Jamieson**,‡ Mark A. Maskeri,‡ K. N. Houk,* Tobias A. M. Gulder.* *Angew. Chem. Int. Ed.* 2021, 60, 8297.

Cycloadditions of cyclopentadiene and cycloheptatriene with tropones: all *endo*-[6+4] cycloadditions are ambimodal.
Cooper S. Jamieson, Arkajyoti Sengupta, K. N. Houk.* *J. Am. Chem. Soc.* 2021, 143, 10, 3918–3926.

Catalytic mechanism and *endo*-to-*exo* selectivity reversion of an octalin-forming natural Diels–Alderase.
Michio Sato, Shinji Kishimoto, Mamoru Yokoyama, **Cooper S. Jamieson**, Kazuto Narita, Naoya Maeda, Kodai Hara, Hiroshi Hashimoto, Yuta Tsunematsu, K. N. Houk, Yi Tang, Kenji Watanabe.* *Nat. Catal.* 2021, 4, 223–232.

Biosynthesis and synthetic biology of psychoactive natural products.
Cooper S. Jamieson,‡ Joshua Misa,‡ Yi Tang,* John M. Billingsley.* *Chem. Soc. Rev.* 2021, 50, 6950-7008.

Library construction of stereochemically diverse isomers of spirooliganin: their total synthesis and antiviral activity.
Ru-Bing Wang,‡ Shuang-Gang Ma,‡,* **Cooper S. Jamieson**,‡ Rong-Mei Gao, Yun-Bao Liu, Yong Li, Xiao-Jing Wang, Yu-Huan Li, K. N. Houk,* Jing Qu,* Shi-Shan Yu.* *Chem. Sci.* 2021, 12, 7003-7011.

A polyketide cyclase that forms medium-ring lactones.
De-Wei Gao,‡ **Cooper S. Jamieson**,‡ Gaoqian Wang,‡ Yan Yan, Jiahai Zhou, K. N. Houk,* Yi Tang.* *J. Am. Chem. Soc.* 2021, 143, 1, 80–84.

An enzymatic Alder-ene reaction.
Masao Ohashi,‡ **Cooper S. Jamieson**,‡ Yujuan Cai,‡ Dan Tan, Daiki Kanayama, Man-Cheng Tang, Sarah M. Anthony, Jason V. Chari, Joyann S. Barber, Elias Picazo, Thomas B. Kakule, Shugeng Cao, Neil K. Garg,* Jiahai Zhou,* K. N. Houk,* Yi Tang.* *Nature*. 586, 64–69.

Bioinspired synthesis of (–)-PF-1018.
Hugo Quintela-Varela, **Cooper S. Jamieson**, Qianzhen Shao, K. N. Houk,* Dirk Trauner.* *Angew. Chem. Int. Ed.* 2020, 59, 5263.

Biosynthesis of the fungal glyceraldehyde-3-phosphate dehydrogenase inhibitor heptelidic acid and mechanism of self-resistance.
Yan Yan, Xin Zang, **Cooper S. Jamieson**, Hsiao-Ching Lin, K. N. Houk,* Jiahai Zhou,* Yi Tang.* *Chem. Sci*. 2020, 11, 9554-9562.

Expanding the frontiers of higher-order cycloadditions.
David McLeod, Mathias Kirk Thøgersen, Nicolaj Inunnguaq Jessen, Karl A. Jørgensen,* **Cooper S. Jamieson**, Xiao-Song Xue, K. N. Houk,* Fang Liu,* Roald Hoffmann.* *Acc. Chem. Res.* 2019, 52, 12, 3488–3501.

Structural basis for stereoselective dehydration and hydrogen-bonding catalysis by the SAM-dependent pericyclase LepI.
Yujuan Cai,‡ Yang Hai,‡ Masao Ohashi,‡ **Cooper S. Jamieson**, Marc Garcia-Borras, K. N. Houk,* Jiahai Zhou,* Yi Tang.* *Nat. Chem.* 2019, 11, 812–820.

Enzymatic intermolecular hetero-Diels–Alder reaction in the biosynthesis of tropolonic sesquiterpenes.
Qibin Chen,‡ Jie Gao,‡ **Cooper S. Jamieson**, Jiawang Liu, Masao Ohashi, Jian Bai, Daojian Yan, Bingyu Liu, Yongsheng Che, Yanan Wang, K. N. Houk,* Youcai Hu.* *J. Am. Chem. Soc*. 2019, 141, 36, 14052–14056.

Mechanisms and dynamics of reactions involving entropic intermediates.
Zhongyue Yang, **Cooper S. Jamieson**, Xiao-Song Xue, Marc Garcia-Borràs, Tyler Benton, Xiaofei Dong, Fang Liu, K. N. Houk.* *Trends Chem*. 2019, 1, 1, 22 - 34.

Enzyme-catalyzed inverse-electron demand Diels–Alder reaction in the biosynthesis of antifungal ilicicolin H.
Zhuan Zhang, **Cooper S. Jamieson**, Yi-Lei Zhao, Dehai Li, Masao Ohashi, K. N. Houk,* Yi Tang.* *J. Am. Chem. Soc*. 2019, 141, 14, 5659–5663.

Ambimodal trispericyclic transition state and dynamic control of periselectivity.
Xiao-Song Xue,‡ **Cooper S. Jamieson**,‡ Marc Garcia-Borràs,‡ Xiaofei Dong,‡ Zhongyue Yang, K. N. Houk.* *J. Am. Chem. Soc.* 2019, 141, 3, 1217–1221.

Genome-mined diels–alderase catalyzes formation of the *cis*-octahydrodecalins of varicidin A and B.
Dan Tan,‡ **Cooper S. Jamieson**,‡ Masao Ohashi, Man-Cheng Tang,* K. N. Houk,* Yi Tang.* *J. Am. Chem. Soc.* 2019, 141, 2, 769–773.

The expanding world of biosynthetic pericyclases: cooperation of experiment and theory for discovery.
Cooper S. Jamieson,‡ Masao Ohashi,‡ Fang Liu, Yi Tang,* K. N. Houk.* *Nat. Prod. Rep.* 2019, 36, 698-713.

Relationships between product ratios in ambimodal pericyclic reactions and bond lengths in transition structures.
Zhongyue Yang, Xiaofei Dong, Yanmin Yu, Peiyuan Yu, Yingzi Li, **Cooper S. Jamieson**, K. N. Houk.* *J. Am. Chem. Soc.* 2018, 140, 8, 3061–3067.

CASSCF calculations reveal competitive chair (pericyclic) and boat (pseudopericyclic) transition states for the [3,3] sigmatropic rearrangement of allyl esters.
Henry W. Kreiman, Mackenzie E. Batali, **Cooper S. Jamieson**, Molly A. Lyon, James A. Duncan.* *J. Org. Chem*. 2018, 83, 4, 1717–1726.