

NATHAN MANCHEUN LUI, PH.D.

Eli Lilly and Company, Indianapolis, IN, USA | thisisnathan.github.io

EDUCATION

Cornell University

Ithaca, NY, USA

Doctor of Philosophy in Chemistry

Aug 2023

Master of Science in Chemistry

Dec 2020

Dissertation: Structure-selectivity principles underlying alkylations of Oppolzer's camphorsultam enolates

Select awards: Simon Bauer Scholarship (2022), ACS Graduate Teaching Award (2020)

New York University Abu Dhabi

Abu Dhabi, AD, UAE

Bachelor of Science in Chemistry with specialization in Biochemistry

May 2018

Thesis: Conserved loops mediate the active site microenvironment and determine the color of bioluminescence in beetle luciferases

RESEARCH

Eli Lilly and Company

Indianapolis, IN, USA

Advisor – Frontier AI Research

Feb 2025 – Present

Building intelligent multi-agent systems to accelerate molecular discovery

Postdoctoral Scientist – Reaction Informatics

Aug 2023 – Jan 2025

Transfer learning approaches for reaction product prediction in the low-data regime

- Developed machine learning methods of reaction product and byproduct prediction using multi-task and transfer learning on graph-based transformer models
- Built ML-ready reaction datasets for niche reaction spaces
- Reduced cycle times and increased design adoptions by triaging molecules from generative design teams in small-molecule discovery campaigns
- Planned and executed benchmarking efforts for upgrade of onsite computing hardware leading to substantial savings in infrastructure costs

Exscientia (acquired by Recursion Pharmaceuticals)

Miami, FL, USA

Ph.D. Intern, Cheminformatics

Feb 2023 – May 2023

Identifying data-driven MPO weightings for computational drug design

- Leveraged machine learning on chemical and biological data to improve early-stage scoring, ranking, and selection strategies for small-molecule structure-based drug design projects
- Curated large (~5M), high-dimensional protein-ligand binding datasets for machine learning
- Built, validated, and packaged internal models for compound potency and multi-objective scoring
- Developed internal tools for identifying and optimizing small molecules in computational design cycles

Cornell University

Ithaca, NY, USA

Graduate Research Assistant and Ph.D. Candidate

Oct 2018 – July 2023

Oppolzer enolates: solution structures, mechanism of alkylation, and the origin of stereoselectivity

Monosilyl amides: highly soluble organosodium bases with wide-ranging synthetic applications

MoFlowGAN: a tandem generative model for targeted molecular graph generation

- A flow model that takes advantage of a hybrid objective to generate property-targeted molecular graphs
- Designed and implemented a normalizing flow model that can also be trained adversarially as well as on policy gradients for multi-parameter optimization
- Demonstrated that reinforcement learning on deep deterministic policy gradients (DDPG) enables models to generate samples that outperform the training set on key chemical parameters

LEADERSHIP & OUTREACH

Eli Lilly and Company**Indianapolis, IN, USA**

Co-Chair, Indianapolis Postdoc Group

Jun 2024 – Jan 2025

- Serve as the point-of-contact for postdocs in Indianapolis with Lilly leadership and elevating any individual concerns from Lilly postdocs about the program
- Organize monthly professional development and networking events with internal and external speakers
- Coordinate with San Diego and Boston Group co-chairs to foster inter-site synergy

Lead Organizer, 2024 Lilly Postdoc Summit

Apr 2024 – Oct 2024

- Organized a two-day conference attended by 57 postdocs from across 6 Lilly sites and 15 departments
- Implemented an Agile structure for organizing team across 3 Lilly sites; planned and oversaw sprints; managed kanban board, task assignments, and WIP limits
- Coordinated abstract submission and review process for poster session with 50 presenters and spotlight seminars session with 3 speakers
- Worked with leadership to secure budget, catering contracts, logistics support, and travel arrangements

Cornell University**Ithaca, NY, USA**

Senior Graduate Student

Jun 2021 – Jul 2023

- Managed individual group duties, organized meeting schedules, and upkeep lab material stock
- Troubleshoot and repaired capital equipment
- Mentored 2 junior graduate students
- Developed an open-source short course for computational chemistry ([link](#))

CS Project Team Leader

Aug 2022 – Jan 2023

- Led a team of 3 students from diverse backgrounds through project proposal, presentation, and execution of a project on developing FlowGANs for *de novo* molecular generation.
- Homogenized different project ideas incorporating individual goals and topic interests
- Organized project timeline, scheduled code reviews, and set progress checkpoints
- Re-evaluated project targets and redistributed tasks when team members and resources were in flux

MANUSCRIPTS & PREPRINTS

***Lui, NM**; Ghanekar, PG; Schiffler, MA “Transfer learning approaches for reaction product prediction in the low-data regime.” *Manuscript in preparation*. *Corresponding author

- Selected for oral presentation at the ACS Spring 2025 General Meeting
- Selected for spotlight talk at the 2024 Lilly Postdoc Summit (top 3 abstracts of 50)

PUBLICATIONS

You, Q; Ma, Y; Woltornist, RA; **Lui, NM**; Spivey, JA; Keresztes, I; Collum, DB “Sodium Alkyl(trimethylsilyl)amides: Substituent- and Solvent-Dependent Solution Structures and Reactivities.” *Journal of the American Chemical Society* **2024**, 146 (44), 30397. [Paper](#)

Gambrill, Y; Commins, P; Schramm, S; **Lui, NM**; AlNeyadi, SS; Naumov, P “Natural Product Isolation of the Extract of *Cleome rupicola* Fruits Exhibiting Antioxidant Activity.” *Chemistry & Biodiversity* **2024**, e202301382. [Paper](#)

Lui, NM; Collum, DB “Sodiated Oppolzer Enolates: Solution Structures and Mechanisms of Alkylation.” *Organic Chemistry Frontiers* **2023**, 10, 4750. [Paper](#)

- Featured in the 2023 HOT Articles collection of *Organic Chemistry Frontiers*.

***Lui, NM**; Li, MD; Ford, M “MoFlowGAN: Combining adversarial and likelihood learning to enable targeted molecular generation.” *ChemRxiv preprint* **2023**. [Paper](#) [Code](#) *Corresponding author

Lui, NM; MacMillan, SN; Collum, DB “Lithiated Oppolzer Enolates: Solution Structures, Mechanism of Alkylation, and Origin of Stereoselectivity.” *Journal of the American Chemical Society* **2022**, 144 (51), 23379. [Paper](#)
– Selected for oral presentation at the ACS Spring 2022 General Meeting
– Named session chair for Physical Organic Chemistry at ACS Spring 2022

Ma, Y; **Lui, NM**; Keresztes, I; Woltornist, RA; Collum, DB “Sodium Isopropyl(trimethylsilyl)amide (NaPTA): A Stable and Highly Soluble Lithium Diisopropylamide Mimic.” *The Journal of Organic Chemistry* **2022**, 87 (21), 14223. [Paper](#)
– Featured in the December 2022 installment of “[Some Items of Interest to Process R&D Chemists and Engineers](#)” in *Organic Process Research & Development*.

Al-Handawi, MB; Polavaram, S; Kurlevskaya, A; Commins, P; Schramm, S; Carrasco-López, C; **Lui, NM**; Solntsev, KM; Laptinok, SP; Navizet, I; Naumov, P “Spectrochemistry of Firefly Bioluminescence.” *Chemical Reviews* **2022**, 122 (16), 13207. [Paper](#)

Carrasco-López, C; **Lui, NM**; Schramm, S; Naumov, P “The elusive relationship between structure and colour emission in beetle luciferases.” *Nature Reviews Chemistry* **2021**, 5, 4. [Paper](#)

Schramm, S; Karothu, DP; **Lui, NM**; Commins, P; Ahmed, E; Catalano, L; Li, L; Weston, J; Moriwaki, T; Solntsev, KM; Naumov, P “Thermochemiluminescent Peroxide Crystals.” *Nature Communications* **2019**, 10, 997. [Paper](#)

Lui, NM; Schramm, S; Naumov, P “pH-dependent fluorescence from firefly oxyluciferin in agarose thin films.” *New Journal of Chemistry* **2019**, 43, 1122. [Paper](#)
– Selected for oral presentation at the 5th UAE Undergraduate Research Competition

Carrasco-López, C; Ferreira, J; **Lui, NM**; Schramm, S; Berraud-Pache, R; Navizet, I; Panjikar, S; Naumov, P; Rabeh, W “Beetle luciferases with naturally red- and blue-shifted emission.” *Life Science Alliance* **2018**, 1, e201800072. [Paper](#)
– Selected for spotlight talk at the 2018 ISBC General Meeting (best abstract in section)
– Selected for Sci-Mix at the 255th ACS General Meeting (top 20 abstracts in biological chemistry division)

SKILLS

Technical | machine learning (scikit-learn, pyTorch, Keras, HuggingFace), LLM agents and multi-agent systems (langchain/langgraph, swarm), cheminformatics (RDKit, OpenEye), programming/scripting (bash, java, python (+jupyter), C++), git, data manipulation and visualization (NumPy/SciPy/Pandas/Plotly/Dash), high-performance computing, cloud computing (AWS), computational chemistry (QM/DFT), structure-based drug design (SBDD), synthetic organic chemistry, physical organic chemistry

Professional | team leadership, project and people management (agile), event organization, inter-site coordination, learning agility, cross-functional collaboration, scientific communication