

# NATHAN MANCHEUN LUI, PH.D.

Eli Lilly and Company, Indianapolis, Indiana, USA | [nathan.lui@lilly.com](mailto:nathan.lui@lilly.com) | [thisisntnathan.github.io](https://thisisntnathan.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

*Advisor:* Professor David B. Collum

*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

*Advisors:* Professors Wael Rabeh and Panče Naumov

## RESEARCH EXPERIENCE

### Eli Lilly and Company

Indianapolis, IN, USA

Postdoctoral Scientist, Reaction Informatics

Aug 2023 – Present

- 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 reactions from internal chemistry data
- Reduced cycle times and increased design adoptions by triaging molecules from generative design teams in small-molecule discovery campaigns in the hit-to-lead and lead-optimization stages
- Planned and executed benchmarking efforts for upgrade of onsite computing hardware leading to substantial savings in infrastructure costs
- Maintained, optimized, and expanded internal cheminformatics and generative design tools

### Exscientia

Miami, FL, USA

Ph.D. Intern, Cheminformatics

Feb 2023 – May 2023

- 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*

- Structural and mechanistic study of the alkylation of Oppolzer enolates
- Designed, optimized, and executed multi-step synthetic routes to chiral and isotopically labeled substrates
- Determined structure of organometallic complexes through low-temperature heteronuclear NMR spectroscopy and small molecule X-ray crystallography
- Uncovered reaction mechanisms using *in situ* IR and rapid-inject NMR spectroscopy
- Revealed the origin of stereoselectivity through density functional theory calculations (DFT)

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

- Methods development project that pushes the boundaries of organosodium chemistry
- Computationally screened a library of monosilyl sodium amides using DFT and MD calculations
- Targeted high pKa amides to design easily adoptable sodium reagents for synthetic chemists

**MoFlowGAN: a tandem generative model for targeted molecular graph generation**

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

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

Lilly Postdoc Summit Lead Organizer

Apr 2024 – Present

- Led Agile team of 11 in organizing a two-day in-person summit with speakers and attendees across Lilly departments and business units; managed team kanban board; led team retrospectives
- Coordinated abstract submission and review process for seminar and poster session with 47 speakers
- Managed catering contracts, logistics, and travel funding

**Cornell University****Ithaca, NY, USA**

Senior Graduate Student

Jun 2021 – Jul 2023

- Distributed individual group duties, organized meeting schedules, and upkept lab material stock
- Troubleshoot and repaired capital equipment (e.g., glove boxes, spectrometers, chromatography systems)
- Mentored 2 junior graduate students teaching them air-free organometallic synthesis, traditional kinetic methods, and analytical IR and NMR spectroscopy
- Developed an open-source short course for computational chemistry used by graduate students both throughout and beyond the Cornell chemistry department

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

**SKILLS**

synthetic organic chemistry, IR and NMR spectroscopy, physical organic chemistry, preparative chromatography, high-performance computing, cloud computing (AWS), computational chemistry (QM/DFT/MD/FEP), cheminformatics (RDKit, OpenEye), structure-based drug design (SBDD), programming/scripting (bash, java, python (+jupyter), C++), git, machine learning (DL/RL), scikit-learn, pyTorch, data manipulation and visualization (NumPy/SciPy/Pandas/Plotly/Dash), learning agility, team leadership, project and people management (agile)

**PUBLICATIONS**

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.” *Chem. 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**; MacMillan, SN; Collum, DB “Lithiated Oppolzer Enolates: Solution Structures, Mechanism of Alkylation, and Origin of Stereoselectivity.” *Journal of the American Chemical Society* **2022**, 144, 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, 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, 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 5<sup>th</sup> 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 255<sup>th</sup> ACS General Meeting (top 20 abstracts in biological chemistry division)

## WORKING PAPERS & PREPRINTS

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." *Manuscript in Review*.

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