NATHAN MANCHEUN LUI, PH.D.

Eli Lilly and Company, Indianapolis, IN, USA | nathanlui95@gmail.com | 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

Eli Lilly and Company **Indianapolis, IN, USA**
Postdoctoral Scientist, Reaction Informatics Aug 2023 – Present
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 **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

- 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 multi-dimensional NMR spectroscopy and small molecule X-ray crystallography
- 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 & OUTREACH

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

Co-Chair, Indianapolis Postdoc Group Jun 2024 – Present

- 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 upkept lab material stock
- Troubleshot 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 spotlight talk at the 2024 Lilly Postdoc Summit (top 3 abstracts of 50)

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

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; 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; Laptenok, 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 | computational chemistry (QM/DFT), cheminformatics (RDKit, OpenEye), structure-based drug design (SBDD), programming/scripting (bash, java, python (+jupyter), C++), git, machine learning (DL/RL), scikit-learn, pyTorch, Keras, HuggingFace, data manipulation and visualization (NumPy/SciPy/Pandas/Plotly/Dash), high-performance computing, cloud computing (AWS), 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