

NATHAN MANCHEUN LUI

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EDUCATION

Cornell University

Doctor of Philosophy in Chemistry (Minor: Computer Science)

Master of Science in Chemistry

Advisor: Professor David B. Collum

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

Ithaca, NY, USA

Candidate

Dec 2020

New York University Abu Dhabi

Bachelor of Science in Chemistry with specialization in Biochemistry

Advisors: Professors Wael Rabeh and Panče Naumov

Abu Dhabi, AD, UAE

May 2018

RESEARCH EXPERIENCE

Exscientia

Ph.D. Intern, Cheminformatics

Miami, FL, USA

Feb 2023 – Present

- Curated and analyzed high-dimensional protein-ligand binding data for machine learning
- Developed tools for hypertuning reward functions for multi-parameter optimization (MPO)
- Designed and implemented improved consensus scoring workflows for computational drug design

Cornell University

Ph.D. Candidate

Ithaca, NY, USA

Oct 2018 – Present

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 *de novo* 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

Cornell University

Senior Graduate Student

Ithaca, NY, USA

Jun 2021 – Present

- 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

Cornell University

CS Project Team Leader

Ithaca, NY, USA

Aug 2022 – Jan 2023

- Directed 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, computational chemistry (QM/DFT/MD), cheminformatics (RDKit, OpenEye), docking (GOLD, OEDock), programming/scripting (bash, java, python (+jupyter)), git, machine learning (DL/RL), scikit-learn, pyTorch, cloud computing (AWS), data manipulation and visualization (NumPy/SciPy/Pandas/Plotly/Dash)

PUBLICATIONS

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 263rd ACS General Meeting

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* (3), 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)

WORKING PAPERS

***Lui, NM**; Li, MD; Ford, MT “MoFlowGAN: Combining adversarial and likelihood learning to enable targeted *de novo* molecular generation.” *Preprint in submission*. [Manuscript Code](#) *Corresponding author

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.” *Manuscript in review*.

Lui, NM; Collum, DB “Sodiated Oppolzer Enolates: Solution Structures and Mechanisms of Alkylation.” *Manuscript in preparation*.