

# NATHAN MANCHEUN LUI

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## EDUCATION

### Cornell University

Doctor of Philosophy in Chemistry

Master of Science in Chemistry

*Advisor:* Professor David B. Collum

*Minor:* Computer science (Anticipated)

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

## MAJOR RESEARCH PROJECTS

### 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 *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 on policy 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 metrics

## LEADERSHIP ROLES

### CS Project Team Leader

Aug 2022 – Present

- Directed a team of 3 students from diverse backgrounds through project proposal, presentation, and execution of a project on developing normalizing 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

### Senior Graduate Student

Jun 2021 – Present

- Distributed individual group duties, organized meeting schedules, and upkeep 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

## SKILLS

synthetic organic and organometallic chemistry, IR and NMR spectroscopy, physical organic chemistry, preparative chromatography, high-performance computing, computational chemistry (QM/DFT/MD), chemoinformatics (RDKit), unix, java, python, machine learning (DL/RL), scikit-learn, pyTorch, team mentorship, problem-solving

## SELECT HONORS AND AWARDS

**ACS General Meeting Technical Session Chair 2022 • Simon Bauer Scholarship Award 2022 • ACS/Covestro Graduate Teaching Award 2020**

## PUBLICATIONS

**Lui, N.M.**; MacMillan, S.N.; Collum, D.B. "Lithiated Oppolzer Enolates: Solution Structures, Mechanism of Alkylation, and Origin of Stereoselectivity." *Journal of the American Chemical Society* **2022**, article in press.

– Selected for an oral presentation at the 2022 ACS Fall General Meeting

Ma, Y., **Lui, N.M.**, Keresztes, I., Woltornist, R.A., Collum, D.B. "Sodium Isopropyl(trimethylsilyl)amide (NaPTA): A Stable and Highly Soluble Lithium Diisopropylamide Mimic." *Journal of Organic Chemistry* **2022**, 87 (21), 14223.

– 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, M.B.; Polavaram, S.; Kurlevskaya, A.; Commins, P.; Schramm, S.; Carrasco-López, C.; **Lui, N.M.**; Solntsev, K. M.; Laptinok, S.P.; Navizet, I.; Naumov, P. "Spectrochemistry of Firefly Bioluminescence." *Chemical Reviews* **2022**, 122 (16), 13207.

– Featured on the cover of the late August 2022 issue of *Chemical Reviews*.

Carrasco-López, C.; **Lui, N.M.**; Schramm, S.; Naumov, P. "The elusive relationship between structure and colour emission in beetle luciferases." *Nature Reviews Chemistry* **2021**, 5 (1), 4.

– Featured on the cover of the January 2021 issue of *Nature Reviews Chemistry*.

Schramm, S.; Karothu, D.P.; **Lui, N.M.**; Commins, P.; Ahmed, E.; Catalano, L.; Li, L.; Weston, J.; Moriwaki, T.; Solntsev, K. M.; Naumov, P. "Thermochemiluminescent Peroxide Crystals." *Nature Communications* **2019**, 10 (1), 997.

**Lui, N.M.**; Schramm S.; Naumov P. "pH-dependent fluorescence from firefly oxyluciferin in agarose thin films." *New Journal of Chemistry* **2019**, 43 (3), 1122.

– Selected for an oral presentation at the 5<sup>th</sup> UAE Undergraduate Research Competition

Carrasco-López, C.; Ferreira, J.; **Lui, N.M.**; 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 (4), e201800072.

– 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 MANUSCRIPTS

Gambrill, Y.; Commins, P.; Schramm, S.; AlNeyadi, S.S.; **Lui, N.M.**; Naumov, P. "Natural product isolation of the extract of *Cleome rupicola* fruits exhibiting antioxidant activity." *Manuscript in submission at the Journal of Natural Products*.

\***Lui, N.M.**; Li, M.; Ford, M. "MoFlowGAN: Combining adversarial and likelihood learning to enable targeted *de novo* molecular generation." *Manuscript in preparation*. Open-access Code.

\* Corresponding author