NATHAN MANCHEUN LUI

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EDUCATION

Cornell University **Ithaca, NY, USA**
Doctor of Philosophy in Chemistry (Minor: Computer Science) Candidate
Master of Science in Chemistry Dec 2020
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
Advisors: Professors Wael Rabeh and Panče Naumov

RESEARCH EXPERIENCE

Exscientia **Miami, FL, USA**
Ph.D. Intern, Cheminformatics Feb 2023 – Present
- Curated and analyzed large, high-dimensional protein-ligand binding datasets for machine learning
- Developed tools for identifying and optimizing small molecules in computational design cycles
- Explored improved consensus scoring strategies for structure-based drug design

Cornell University **Ithaca, NY, USA**
Ph.D. Candidate 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 **Ithaca, NY, USA**
Senior Graduate Student Jun 2021 – Present
- Distributed individual group duties, organized meeting schedules, and upkept lab material stock
- Troubleshot 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 **Ithaca, NY, USA**
CS Project Team Leader 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), molecular docking, 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; Laptenok, 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 preparation.* 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.*