

NATHAN MANCHEUN LUI, PH.D.

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EDUCATION

Cornell University

Doctor of Philosophy in Chemistry

Master of Science in Chemistry

Dissertation: Structure-selectivity principles underlying alkylations of Oppolzer's camphorsultam enolates

Advisor: Professor David B. Collum

Ithaca, NY, USA

Aug 2023

Dec 2020

New York University Abu Dhabi

Bachelor of Science in Chemistry with specialization in Biochemistry

Thesis: Conserved loops mediate the active site microenvironment and determine the color of bioluminescence in beetle luciferases

Advisors: Professors Wael Rabeh and Panče Naumov

Minor: Urban Studies

Abu Dhabi, AD, UAE

May 2018

RESEARCH

Eli Lilly and Company

Advisor, Exploratory Discovery AI

Building intelligent multi-agent systems to accelerate drug discovery

Postdoctoral Scientist, Exploratory Discovery AI

Transfer learning approaches for reaction product prediction in the low-data regime

Indianapolis, IN, USA

Feb 2025 – Present

Aug 2023 – Jan 2025

Exscientia (acquired by Recursion Pharmaceuticals)

Ph.D. Intern, Cheminformatics

Identifying data-driven MPO weightings for computational drug design

Miami, FL, USA

Feb 2023 – May 2023

Cornell University

Graduate Research Assistant and Ph.D. Candidate

Oppolzer enolates: solution structures, mechanism of alkylation, and the origin of stereoselectivity

Sodium Alkyl(trimethylsilyl)amides: organosodium bases with broad synthetic applications

MoFlowGAN: a tandem generative model for targeted molecular graph generation | Independent project

Ithaca, NY, USA

Oct 2018 – July 2023

New York University Abu Dhabi

Undergraduate Research Assistant

Beetle luciferases with naturally red- and blue-shifted emission

Thermochemiluminescent peroxide crystals

pH-Dependent fluorescence from firefly oxyluciferin in agarose thin films

Natural product isolation of the extract of Cleome rupicola fruits

Abu Dhabi, UAE

July 2015 – May 2018

University of Puerto Rico – Río Piedras

NSF-REU Student

Hierarchical assembly of supramolecular G-quadruplexes via enzyme instructed self-assembly

San Juan, PR, USA

Jun 2017 – Aug 2017

LEADERSHIP & OUTREACH

Eli Lilly and Company

Co-Chair, Indianapolis Postdoc Group

Lead Organizer, 2024 Lilly Postdoc Summit

Indianapolis, IN, USA

Jun 2024 – Feb 2025

Apr 2024 – Oct 2024

Cornell University

Senior Graduate Student

CS Project Team Leader

Ithaca, NY, USA

Jun 2021 – Jul 2023

Aug 2022 – Jan 2023

New York University Abu Dhabi

President, American Chemical Society (ACS) International Student Chapter

Finance Director, Love Local Abu Dhabi

Class of 2018 Representative, The 2010 Fund

Abu Dhabi, UAE

Aug 2017 – May 2018

July 2014 – May 2016

Sep 2014 – Jun 2016

MANUSCRIPTS & PREPRINTS

- [2] ***Lui, NM**; Ghanekar, PG; Schiffler, MA; Harman, WD “Transfer learning approaches for reaction product prediction in the low-data regime.” *Manuscript in preparation*. *Corresponding author
– Selected for oral presentation at the ACS Spring 2025 General Meeting
– Selected for spotlight talk at the 2024 Lilly Postdoc Summit (top 3 abstracts of 50)
- [1] ***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

- [10] 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](#)
- [9] 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](#)
- [8] **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*.
- [7] **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
- [6] 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*.
- [5] Al-Handawi, MB; Polavaram, S; Kurlevskaya, A; Commins, P; Schramm, S; Carrasco-López, C; **Lui, NM**; Soltsev, KM; Laptinok, SP; Navizet, I; Naumov, P “Spectrochemistry of Firefly Bioluminescence.” *Chemical Reviews* **2022**, *122* (16), 13207. [Paper](#)
- [4] 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](#)
- [3] Schramm, S; Karothu, DP; **Lui, NM**; Commins, P; Ahmed, E; Catalano, L; Li, L; Weston, J; Moriwaki, T; Soltsev, KM; Naumov, P “Thermochemiluminescent Peroxide Crystals.” *Nature Communications* **2019**, *10*, 997. [Paper](#)
- [2] **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

- [1] 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)

PRESENTATIONS

- [15] "Transfer learning approaches for reaction product prediction in the low-data regime." Selected talk at American Chemical Society Spring National Meeting. San Diego, CA, Mar 2025.
- [14] "A deep learning approach to mechanism-aware reaction product prediction." Selected talk and poster at the Lilly Postdoc Summit. Indianapolis, IN, Oct 2024.
- [13] "A deep learning approach to mechanism-aware reaction product prediction." Research highlight at the Lilly Global Computational Chemistry Summit. San Diego, CA, Sep 2024.
- [12] "Structure-selectivity principles underlying the alkylation of Oppolzer's camphorsultam enolates." Doctoral dissertation defense at Cornell University. Ithaca, NY, July 2023.
- [11] "Structure and mechanism of the alkylation of Oppolzer's camphorsultam-derived enolates." Selected talk at the American Chemical Society Fall National Meeting. Chicago, IL, Aug 2022.
- [10] "Structure and Mechanism of Lithium Enolates of the Oppolzer Sultam." Seminar at Cornell University. Ithaca, NY, Apr 2022.
- [9] "The active site microenvironment determines the color of emission in beetle luciferases." Spotlight talk at the International Symposium on Bioluminescence and Chemiluminescence. Nantes, FR, May 2018.
- [8] "Approaching the color problem of bioluminescence: Contributions of the active site microenvironment to the emission of red and green luciferases." Sci-Mix poster presentation at the American Chemical Society Spring National Meeting. New Orleans, LA, Mar 2018.
- [7] "Bioluminescence in Nanotechnology: Characterization of two novel luciferases for applications in emerging nanobiotechnologies." Poster presentation at the UAE Environmental & Materials Science Symposium. Abu Dhabi, UAE, Dec 2017
- [6] "CellPlus: Paving the way for artificial organelles by the enzyme-instructed self-assembly of guanosine derivatives." Poster presentation at the American Chemical Society Asia-Pacific International Chapters Conference. Jeju, SK, Nov 2017.
- [5] "Structural insight into the mechanism of a blue-shifted green-emitting luciferase." Selected talk at the Middle East Molecular Biology Sources Annual Congress. Abu Dhabi, UAE, Nov 2017.
- [4] "CellPlus: Paving the way for artificial organelles by the enzyme-instructed self-assembly of guanosine derivatives." Poster presentation at the Puerto Rico - CLIMB Symposium. San Juan, PR, July 2017.
- [3] "Humidity responsive luminescent switching in oxyluciferin-agarose thin films as a basis for optical humidity sensors." Selected talk at the UAE Undergraduate Research Competition. Abu Dhabi, UAE, May 2017.
- [2] "Humidity responsive luminescent switching in oxyluciferin-agarose thin films as a basis for optical humidity sensors." Poster presentation at the International Workshop on Advanced Materials. Ras Al Khaimia, UAE, Feb 2017.
- [1] "Crystallization of NiSO₄ polymorphs: The importance of temperature, saturation, and solvent polarity in crystallization" Presentation at NYU Shanghai. Shanghai, CN, May 2016.

HONORS & AWARDS

Graduate Conference Travel Grant (Cornell)	2022
Simon Bauer Scholarship Award (Cornell)	2022
ACS Graduate Teaching Award (Cornell)	2020
International Undergraduate Student Chapter Travel Grant (ACS)	2018
Undergraduate Conference Travel Grants (NYU)	2017, 2018
Conference Travel Award (NSF/UPR)	2017
Research Experiences for Undergraduates Award (NSF)	2017
Undergraduate Research Grants (NYU)	2015, 2016, 2017
External Impact Grant for Student Activity Groups (NYU)	2014

TEACHING

CHEM 7650: Advanced Physical Organic Chemistry and Reaction Mechanisms (Cornell)	2023
CHEM 2510: Introduction to Experimental Organic Chemistry (Cornell)	2019 – 2020
CHEM 2070: General Chemistry I (Cornell)	2018