Nicolò **Tampellini**

Ph.D. Student · Organic Chemistry

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Education

Ph.D. - Yale University

New Haven, CT, USA

Doctoral Student

Sep 2021 - Feb 2026

- Advisor: Prof. Scott J. Miller

B.Sc. - University of Bologna

Bologna, IT

Bachelor of Science Degree

Sep 2017 - Jul 2020

- 110 with Honors / 110 (Italian GPA 29.43 / 30)
- Thesis advisor: Prof. Paolo Righi - Co-advisor: Prof. Giorgio Bencivenni

Publications

6. Peptide-Catalyzed Asymmetric Amination of Sulfenamides Enabled by DFT-Guided Catalyst Optimization
- **Tampellini, N.**; Choi, E. S.; Miller, S.* *J. Am. Chem. Soc.*, **2025**, *147*, 41122-41129 - Link
- Highlighted by The American Peptide Society - Link
- Highlighted by Thieme Synfacts - Link
- Highlighted by Yale Scientific Magazine - *(article in preparation)*

5. Exp.tal Lineage and Computational Analysis of a General Aminoxyl-based Oxidation Catalyst: Generality from Substrate-Specific Interactions
- Rozema, S. ‡; **Tampellini, N.‡**; Rein, J.; Sigman, M.; Lin, S.; Miller, S.* *ACS Catalysis* **2025**, 15, *20*, 17548–17557 - Link

‡ = equal contribution, listed in alphabetical order

4. Enantiocontrolled Cyclization to Form Chiral 7- and 8-Membered Rings Unified by the Same Catalyst Operating with Different Mechanisms
- **Tampellini, N.**, Mercado, B., and Miller, S.* *J. Am. Chem. Soc.* **2025**, 147, 5, 4624–4630 - Link

3. Catalytic Enantioselective Sulfoxidation of Functionalized Thioethers Mediated by Aspartic Acid-Containing Peptides
- Huth, S., **Tampellini, N.**, Guerrero, M. and Miller, S.* *Org. Lett.* **2024**, 26, 32, 6872–6877 - Link

2. Scaffold-Oriented Asymmetric Catalysis: Conformational Modulation of Transition State Multivalency during a Catalyst-Controlled Assembly of a Pharmaceutically Relevant Atropisomer
- **Tampellini, N.**; Mercado, B. and Miller, S.* *Chem. Eur. J.* **2024**, e202401109 - Link

1. Computational Investigation on the Origin of Atroposelectivity for the Cinchona Alkaloid Primary Amine-Catalyzed Vinylogous Desymmetrization of N-(2-t-Butylphenyl)maleimides
- **Tampellini, N.***; Righi, P. and Bencivenni, G.* *J. Org. Chem.* **2021**, 86, 17, 11782–11793 - Link

Awards

2024 Kenneth B. Wiberg Research Fellowship, Yale University - New Haven, CT - Link

2017 National Finalist, Italian Olympiads of Chemistry - Rome, IT - Link

2016 National Finalist, Italian Olympiads of Chemistry - Frascati, IT - Link

Personal Projects

FIRECODE - Filtering Refiner and Embedder for Conformationally Dense Ensembles

2021-present

- Open-source computational chemistry program for automated [constrained] conformational ensemble generation, processing and optimization. Interfaces with external calculators like XTB/TBLITE, ORCA, and Neural Network models via ASE (AIMNET2, UMA). Repository

PRISM - PRuning Interface for Similar Molecules (with Rowan)

2025-present

- Open-source computational chemistry program for molecular similarity pruning. Modular production-ready code to remove similar, rotameric and mirror image molecular duplicates from conformational ensembles. Adopted by Rowan as part of the company's pipeline. Repository

Conferences and Invited Talks

Rowan Seminar Series

Boston, MA, USA

Rowan Scientific Corporation - Host: Dr. Jonathon Vandezande

January 2026

- Presented my research work on "Atomistic Modeling to Understand and Design Flexible Asymmetric Catalysts - Link

National Organic Symposium 2025

Troy, NY, USA

Rensselaer Polytechnic Institute

July 2025

- Presented a poster about my research work on the "Stereocontrolled Cyclization of Inherently Chiral Medium-Sized Rings".

Pfizer Research Spotlight

Cambridge, MA, USA

Pfizer Kendall Square Site — *June 2025*

- Presented my research work on the ”Stereocontrolled Cyclization of Inherently Chiral Medium-Sized Rings” to an audience of Pfizer professionals and selected peers.

Indena Innovation Symposium 2024

Settala, IT

Indena S.p.A. - Host: Alessandro Brusa — *Dec. 2024*

- Presented my research work on the ”Stereocontrolled Cyclization of Inherently Chiral Medium-Sized Rings” to an audience of professionals working on the Research and Development branch of the company.

Yale Chemistry Symposium 2024

New Haven, CT, USA

Yale University - Host: Prof. Scott J. Miller — *Aug. 2024*

- Presented my research work to the department on the ”Stereocontrolled Cyclization of Inherently Chiral Medium-Sized Rings”

UTD Research Talk 2024

Richardson, TX, USA

University of Texas at Dallas - Host: Prof. Filippo Romiti — *June 2024*

- Presented my research work titled ”Atroposelective Synthesis of New Chiral Scaffolds with Flexible, Bifunctional Superbases”

Organic Chemistry Colloquium 2023

Bologna, IT

University of Bologna - Host: Prof. Paolo Righi — *Dec. 2023*

- Presented my research work on ”Catalyst Conformational Modulation - Enabling the Atroposelective Cyclization of Quinazolinediones with Flexible Bifunctional Superbases”