

Dillon R. McCarthy, PhD

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Professional Summary

Computational chemist with 2 years of industry postdoctoral experience applying computer-aided drug discovery methods to complex chemistry challenges in multidisciplinary teams. Skilled at developing discovery workflows that integrate molecular dynamics, free energy methods, and QM/MM, with working knowledge of docking and pharmacophore modeling. Applied molecular dynamics to rationally design DNA nanomaterials and developed a physics-based modeling platform for chemically modified siRNA, demonstrating ability to innovate predictive approaches in drug discovery. Implemented advanced simulation strategies to build predictive models and explore the conformational landscape of large biomolecules including nucleic acids and proteins. Detail-oriented and self-motivated researcher with strong experience in translating molecular modeling insights across cross-disciplinary teams, and eager to continue expanding into AI/ML methods for drug discovery.

Technical Expertise

Molecular modeling, simulation, and scientific computing.

Molecular Simulation Schrödinger Software Suites (Desmond/Macromodel/Jaguar/Prime), Amber/AmberTools, CCG Moe, ORCA and Gaussian for QM and QM/MM, VMD, and PyMOL.

Programming Python, Shell Scripting, Tcl, with experience in R.

Software and Packages Schrödinger's Python API, MDAnalysis, MDTraj, PyTorch, PyEMMA, MSMBuilder, NumPy, Scikit-learn, Numba, RDKit, Jupyter Notebooks, Pandas/Polars.

Workflows Linux, Unix, HPC and cloud-based compute environments, Slurm/Torque queuing, git (Bitbucket and GitHub) for codebase management, and L^AT_EX for scientific writing.

Drug Discovery Familiar with structure- and ligand-based design tools (Glide, AutoDock Vina, HTVS) and maintain working awareness of medicinal chemistry principles (SAR, ADMET, DMPK).

Organic and macromolecular synthesis.

Synthesis Macromolecular, polymer, and small molecule organic synthesis, solid-supported flow methods, and air-free techniques.

Analysis NMR (¹H, ¹³C, NOESY/ROESY, COSY, HSQC/HMBC, ¹H-qNMR), FTIR, UV-Vis spectroscopy, and reaction kinetics and binding studies.

Purification Chromatography (normal/reverse-phase HPLC, chiral HPLC, size-exclusion chromatography, gas chromatography/mass spectrometry).

Research Experience

2022 – 2024 **Postdoctoral Researcher** – Computer-Aided Drug Discovery
Johnson & Johnson Innovative Medicine, Spring House, PA

- Developed a physics-based modeling framework for chemically modified siRNA, applying molecular dynamics to evaluate stability, structural integrity, and binding free energies to guide molecular design strategies.
 - Developed and implemented novel computational tools for the rapid generation and analysis of siRNA duplexes and protein-bound complexes, enabling streamlined structural modeling and facilitating molecular design workflows.
 - Assessed the predictive limits of atomistic simulations for oligonucleotide drug discovery, providing strategic input on when physics-based methods could inform lead optimization decisions.

2016 – 2022 **Graduate Research Assistant** – The Schneebeli and Li Labs
The University of Vermont, Burlington, VT

- (Computational) Applied atomistic modeling to guide the rational design of organofunctionalized therapeutic DNA nanocages.

- Elucidated the essential atomistic interactions which govern the formation of stable human serum albumin, dendritic-DNA nanocage complexes, pore-forming abilities, and stability of cholesterol decorated DNA-nanocages in POPC lipid bilayers.
- Developed customized molecular dynamics workflow to explore long-timescale events in DNA-nanocage/protein supramolecular assemblies.
- (Synthetic & Computational) Design and investigation of catalytic pillar[5]arenes and [2]rotaxanes, towards the development and synthesis of novel [2]rotaxanes.
 - Utilized unbiased and free energy all-atom simulations to design and develop catalytic [2]rotaxanes, and coarse-grain modeling of polymeric rotaxanes to probe pillar[5]arene diffusion along a rotaxane axle.
 - Synthesized the first asymmetric, doubly directional [2]rotaxane capable of regioselective aminolysis at distal end-groups, providing a new synthetic route to otherwise challenging rotaxane diastereoisomers.

Education

- 2016 – 2022 **The University of Vermont**, Burlington, VT
 Ph.D. in Chemistry, with a focus on organic and computational chemistry
 Thesis: [Precision in Macromolecular and Supramolecular Design](#) [↗](#)
 Advisors: Prof. Jianing Li and Prof. Severin T. Schneebeli
- 2012 – 2016 **The University of Connecticut**, Storrs, CT
 B.S. in Chemistry

Published Work

7. **McCarthy, D. R.**, Ke, X., Schenkelberg, M., Balegamire, N. A., Liang, H., Li, J., Schneebeli, S. T. “Kinetically Controlled Synthesis of Rotaxane Geometric Isomers”, *Chem. Sci.* **2024**, *15*, 4860–4870. [↗](#)
6. **McCarthy, D. R.**, Remington, J. R., Ferrell J. B., Schneebeli, S. T., Li, J. “Nano-Bio Interactions between DNA Nanocages and Human Serum Albumin”, *J. Chem. Theory Comput.* **2023**, *19*(21), 7873–7881. (Supplemental Cover) [↗](#)
5. Rajappan, S. C., **McCarthy, D. R.**[†], Campbell, J. P., Ferrell, J. B., Sharafi, M., Li, J., Schneebeli, S. T. “Selective Monofunctionalization Enabled by Reaction-History-Dependent Communication in Catalytic Rotaxanes”, *Angew. Chem. Int. Ed.* **2020**, *59*(38), 16668–16674. (†Co-first Author) [↗](#)
4. Sharafi, M., McKay, K.T., Ivancic, M., **McCarthy, D. R.**, Dudkina, N., Murphy, K. E., Rajappan, S. C., Campbell, J. P., Shen, Y., Badireddy, A. R., Li, J., Schneebeli, S. T. “Size-Selective Catalytic Polymer Acylation with a Molecular Tetrahedron”, *Chem (Cell Press)* **2020**, *6*, 1469–1494. [↗](#)
3. Ferrell, J. B., Campbell, J. P., **McCarthy, D. R.**, McKay, K. T., Hensinger, M., Srinivasan, R., Zhao, X., Wurthmann, A., Li, J., Schneebeli, S. T. “Chemical Exploration with Virtual Reality in Organic Teaching Laboratories”, *J. Chem. Ed.* **2019**, *96*(9), 1961–1966. [↗](#)
2. Chidchob, P., Offenbartl-Stiegert, D., **McCarthy, D. R.**, Li, J., Howorka, S., Sleiman, H. “Spatial presentation of cholesterol units on a DNA cube as a determinant of membrane protein-mimicking functions”, *J. Am. Chem. Soc.* **2019**, *141*(2), 1100–1108. [↗](#)
1. Chan, S., **McCarthy, D. R.**, Li, J., Palczewski, K., Yuan, S. “Designing Safer Analgesics via μ -Opioid Receptor Pathways”, *Trends in Pharma. Sci.* **2017**, *38*, 1016. [↗](#)