Dillon R. McCarthy

Denver, Colorado
Google Scholar · Github · Linkedin

Research Experience

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

- Establish a physics based platform for the design and selection of modified small interfering RNA (siRNA) and evaluate efficacy of molecular dynamics for siRNA prediction.
  - Developed and implemented novel tools for rapid generation of siRNA duplexes and protein-bound complexes, providing a starting point for any structural modeling.
  - Demonstrated the limitations of atomistic simulations as a predictive method for exploring the relationship between chemical modifications and the biophysical properties, stability, and binding free energy of siRNA duplexes.

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

- (Computational) Modeling of oganofunctionalized DNA-nanocages for use in nanomedicine.
  - Elucidated the essential atomistic interactions which govern the formation of stable human serum albumin, dendridic-DNA nanocage complexes, pore-forming abilities, and stability of cholesterol decorated DNA-nanocages in POPC lipid bilayers.
  - Developed customized molecular dynamics simulation protocols 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.

Technical Expertise

Molecular modeling, simulation, and scientific computing.

Simulation Tools Schrödiner Software Suites (Desmond/Macromodel/Jaguar), Amber/AmberTools, CCG Moe, ORCA and Gaussian for QM and QM/MM, VMD, and Pymol.

Programming Python, Bash, and Tcl, with some experience in R.

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

Workflows Working within HPC and cloud-based compute environments alongside Slurm/Torque queuing, and git (Bitbucket and GitHub) for code management.

Organic and macromolecular synthesis.

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

Analysis NMR (^{1}H, ^{13}C, NOESY/ROESY, COSY, HSQC/HMBC, ^{1}H-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.

Education

2016 – 2022 **The University of Vermont**, Burlington, VT
Ph.D. in Chemistry, with a focus in 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.