Dillon R. McCarthy
Philadelphia, PA

Contact Me: Linkedin
Google Scholar · Github

TECHNICAL EXPERTISE

Computational

- Highly experienced in the simulation of functionalized nucleic acids and their interaction with proteins, especially using all-atom molecular dynamics (unbiased and enhanced sampling), DFT, and free-energy approaches (MM/GBSA, FEP).
- Development and implementation of custom software for the design, simulation, and analysis of molecular models.
- Experienced in various software suites including Schrödinger, ORCA, Amber, and MOE.
- Proficient in VMD, Pymol, MDAnalysis, MDTraj, and Schrödinger's Python API.
- Python, TCL/tk, and Bash for use in scientific applications.
- Building and maintaining GNU/Linux GPU workstations.

Synthetic

- Macromolecular and small molecule organic synthesis, solid-supported flow chemistry, and air-free techniques.
- Design and execution of NMR kinetics and binding studies, especially for macromolecular systems.
- NMR (^{1}H, ^{13}C, NOESY/ROESY, COSY, HSQC/HMBC, ^{1}H-qNMR), FTIR, and UV-Vis spectroscopy.
- Chromatography (normal/reverse-phase HPLC, chiral HPLC, size-exclusion chromatography, gas chromatography/mass spectrometry).

RESEARCH AND PROFESSIONAL EXPERIENCE

2022 – present **Postdoctoral Research Fellow** – Computer Aided Drug Design
Johnson & Johnson Innovative Medicine, Spring House, PA

- Developed a novel platform for building chemically-modified small interfering RNA's (siRNA) in Schrödinger and CCG-MOE environments, which enabled the rapid construction of siRNA models used in downstream workflows.
- Lead the computational investigation into the behavior of chemically modified siRNA to better understand the relationship between modification, modification pattern, sequence, and therapeutic knockdown.
- Prediction of changes to siRNA duplex stability using MM/GBSA and other free energy based approaches for modified siRNA backbones.
- Co-leader of the postdoc steering committee, responsible for guiding and implementing career development-oriented seminar sessions which met the interests of fellow postdocs.

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

- Multiscale modeling of oganofunctionalized DNA-nanocages for use in nanomedicine.
  - Elucidated the essential atomistic interactions which govern the formation of stable human serum albumin and dendridic-DNA nanocage complexes.
  - Investigated pore-forming abilities and stability of cholesterol decorated DNA-nanocages in POPC lipid bilayers.
- Computational design and investigation of catalytic pillar[5]arenes and [2]rotaxanes, towards the development and synthesis of novel [2]rotaxanes.
  - Utilizing 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 first asymmetric, doubly directional [2]rotaxane capable of regioselective aminolysis at distal end-groups.

Summer 2016 **Research Intern** – Nalas Engineering
Centerbrook, CT

- Synthesis of HBIW (intermediate for the energetic compound HNIW) under varying conditions to determine the optimal experimental parameters.
- Aided in scale-up production of pharmaceutically relevant intermediates.

SELECTED PUBLICATIONS

4. **McCarthy, D. R.**, Huiming, L., Bellino, S. A., Balegamire, N., Li, J., Schneebeli, S. T. "Efficient Synthesis of Doubly Directional Asymmetric [2]Rotaxanes", *Chem. Sci.* In Revision.
3. **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**. Articles ASAP. (Back Cover)
2. 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)
1. 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.

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

PRESENTATIONS

Oct. 2023 (Poster) "**Towards the Rational Design of siRNA Therapeutics**"
Global Fellowship Symposium, Beerse, BE

Oct. 2020 (Talk) "**Selective Monofunctionalization Enabled by Reaction-History-Dependent Communication in Catalytic Rotaxanes**"
Champlain Chemistry Symposium, Burlington, VT (Virtual)

Apr. 2018 (Poster) "**Towards Precise Molecular Shape Control**"
UVM Student Research Conference, Burlington, VT

Nov. 2017 (Talk) "**All-Atom Molecular Dynamics for the Study of DNA Cage Behavior**"
Sleiman/Li Group Collaborator Meeting, Montréal, QC