

Dr. Lewis Martin

Postdoctoral Researcher specializing in computational chemistry, molecular dynamics, protein-ligand interactions and drug discovery

Skills

I use python libraries to study the interactions between molecules and proteins. This includes custom data visualization of large datasets, non-linear curve fitting with Bayesian estimation, clustering in high dimensions, predicting new drugs with new structures, and cost-benefit analyses to bring drug discovery to academics.

For examples see:

- molecular dynamics simulations of ligands bound to the active site of proteins ([cannabinoid1_scra](#))
- validating the best way to describe ligands to predict their activity with machine learning ([molecular_fingerprints](#))
- comparing frequentist and Bayesian confidence intervals ([timeseries_CI](#))

Publications

- 2020** Martin, Lewis James, and Michael T. Bowen. "Comparing fingerprints for ligand-based virtual screening: a fast, scalable approach for unbiased evaluation." *Journal of Chemical Information and Modeling* (2020).
- 2018** Martin, Lewis J., Behnam Akhavan, and Marcela MM Bilek. "Electric fields control the orientation of peptides irreversibly immobilized on radical-functionalized surfaces." *Nature communications* 9.1 (2018): 1-11.
- 2016** Martin, Lewis, et al. "Force fields for simulating the interaction of surfaces with biological molecules." *Interface Focus* 6.1 (2016): 20150045.
- 2014** Martin, Lewis J., and Ben Corry. "Locating the route of entry and binding sites of benzocaine and phenytoin in a bacterial voltage gated sodium channel." *PLoS Comput Biol* 10.7 (2014): e1003688.
- 2014** Martin, Lewis J., Rebecca Chao, and Ben Corry. "Molecular dynamics simulation of the partitioning of benzocaine and phenytoin into a lipid bilayer." *Biophysical Chemistry* 185 (2014): 98-107.

Supporting Publications

- 2020** Ametovski, Adam, et al. "Exploring Stereochemical and Conformational Requirements at Cannabinoid Receptors for Synthetic Cannabinoids Related to SDB-006, 5F-SDB-006, CUMYL-PICA, and 5F-CUMYL-PICA." *ACS Chemical Neuroscience* (2020).
- 2020** Benson, Melissa J., et al. "Medicinal Cannabis for Inflammatory Bowel Disease: A Survey of Perspectives, Experiences, and Current Use in Australian Patients." *Crohn's & Colitis* 360 2.2 (2020): otaa015.
- 2019** Anderson, Lyndsey L., et al. "Coadministered cannabidiol and clobazam: Preclinical evidence for both pharmacodynamic and pharmacokinetic interactions." *Epilepsia* 60.11 (2019): 2224-2234.
- 2019** Banister, Samuel D., et al. "The chemistry and pharmacology of putative synthetic cannabinoid receptor agonist (SCRA) new psychoactive substances (NPS) 5F-PY-PICA, 5F-PY-PINACA, and their analogs." *Drug testing and analysis* 11.7 (2019): 976-989.
- 2018** Akhavan, Behnam, et al. "Plasma activated coatings with dual action against fungi and bacteria." *Applied Materials Today* 12 (2018): 72-84.

Prizes and Presentations

- 2019** *Predictive modelling of cannabinoid-protein interactions with machine learning and molecular dynamics*
Presentation at the annual Brain and Mind Centre symposium
- 2018** *Canon Information Systems Research Australia (CiSRA) prize*
Awarded to the postgraduate student producing the best refereed publication in a leading

Teaching and education

2019

Predicting novel drug-protein interactions using recommender systems from Netflix

A one semester coding project for a Masters of Neuroscience student who was interested in psychopharmacology. (Manuscript in preparation)