

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.

Qualifications

- 2018** PhD, School of Physics, Faculty of Science, University of Sydney
- 2013** BSc. Hons. 1st class, Research School of Biology, Australian National University

Prizes and Presentations

- 2019** *Predictive modelling of cannabinoid-protein interactions with machine learning and molecular*

dynamics

Featured postdoc 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 international journal

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)