



At the level of the binding site, we use machine learning, big data, and docking to predict the poses and affinities of pocket-bound ligands.



At the level of the protein, we use molecular dynamics simulations to study how target motions impact binding.



At the level of the subcellular environment, we use large-scale modelling and simulation to study binding in the context of the whole microcosm.

Computational Biology and Computer-Aided Drug Discovery

The molecular universe within each of our cells is ruled by active proteins that determine subcellular functions in health or sickness. **Computer-aided drug design** (CADD) seeks to intelligently identify small-molecule ligands that disrupt or enhance the critical interactions these “drug targets” form with other microscopic partners, with the ultimate goal of probing molecular mechanisms and curing disease.

Opportunities for Students and Collaborators

We develop and apply cutting-edge CADD methods by simulating ligand-target interactions at multiple scales. Both programmers interested in methods development and non-programmers interested in methods applications are welcome! Possible projects include those related to molecular visualization, Zika-virus drug discovery, machine-learning-based binding-affinity prediction, and online tool development.

Please send Dr. Durrant an email at durrantj@pitt.edu if you'd like to discuss future interactions as an undergraduate, rotating first-year graduate student, PhD candidate, post-doctoral researcher, or collaborator! You can learn more about our research at <https://durrantlab.com>



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