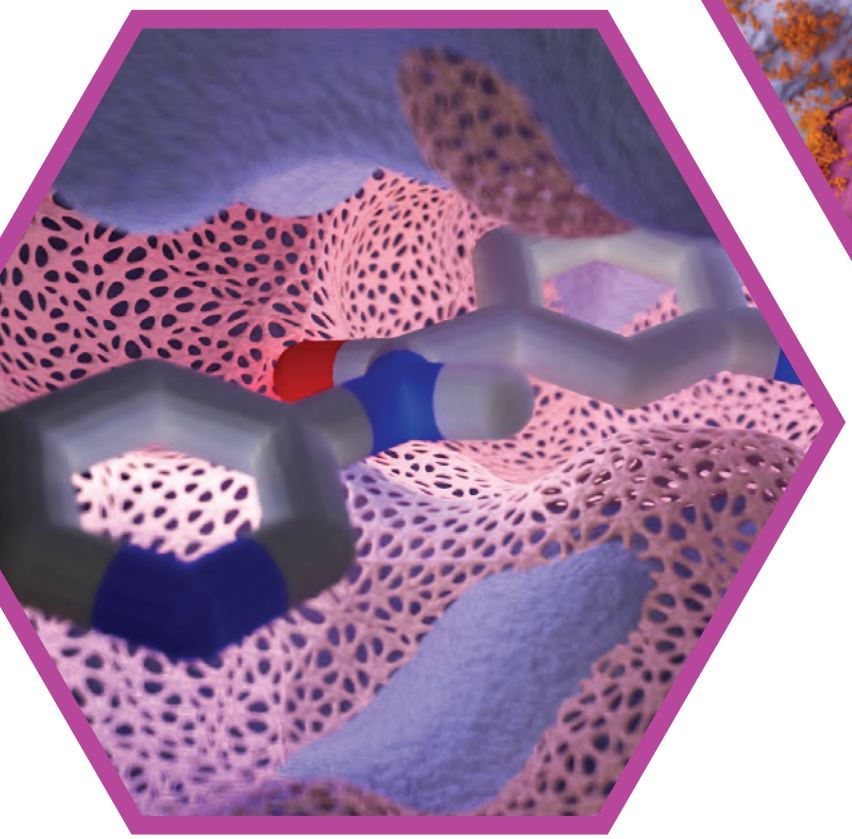
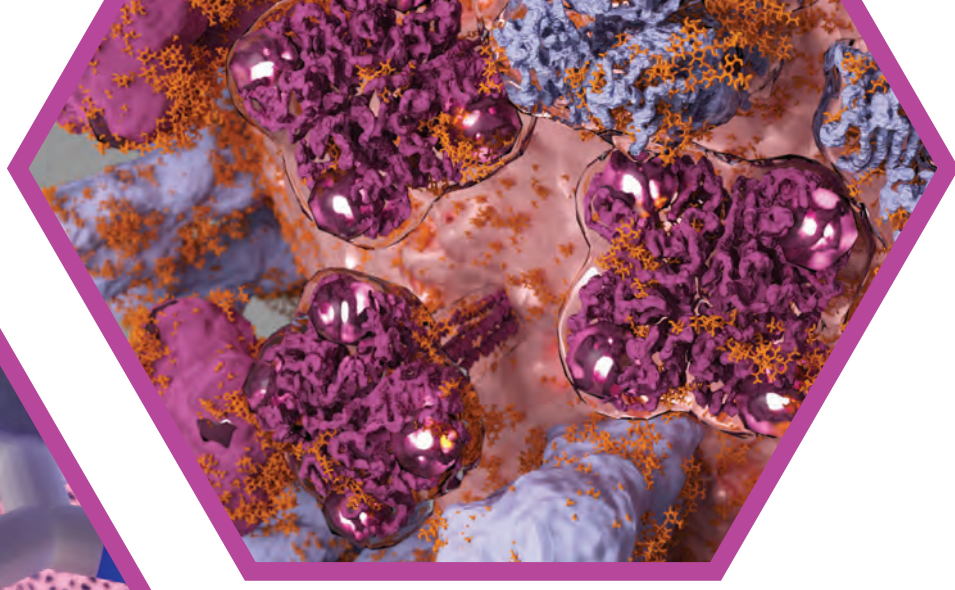
# DURRANT LAB





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

**At the level of the protein**, we use molecular dynamics simulations to study how receptor 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, 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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