

**AutoDock: docking, virtual screening and drug design.**

Instructors: Prof. Arthur J. Olson, Dr. Stefano Forli

**(Mon, Dec. 12th) Introduction to docking: AutoDock Suite**

- Introduction to docking methods
- AutoDock and AutoDock Vina
- AutoDockTools

**(Tue, Dec. 13th) Virtual screening tools**

- Introduction to virtual screening
- Virtual screening input preparation
- Virtual screening post-processing

**(Wed, Dec. 14th) Advanced docking methods**

- Docking with flexible residues
- Relaxed-complex docking
- Grid maps and AutoLigand for drug design
- Covalent docking

**(Thu, Dec. 15th) PMV, advanced visualization tools**

- Design publication-quality images
- Secondary structure, molecular surfaces and coloring schemes
- Ambient occlusion, depth cueing, clipping planes