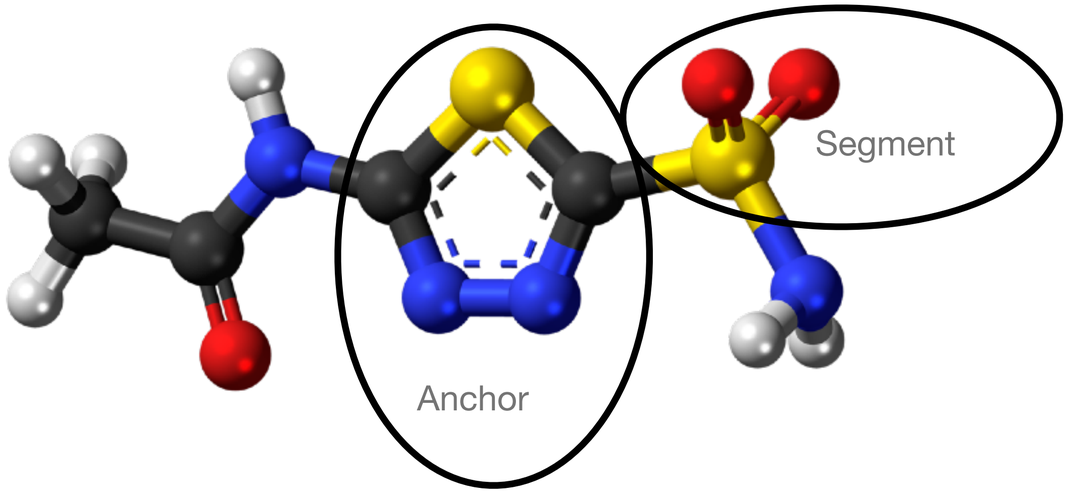
UCSF DOCK is based on anchor-and-grow



- Receptor spheres and rigid “anchor” in ligand
  - represented as graph of atoms separated by distances
  - docking is search for isomorphic subgraph
- Until the molecule is complete, segments are iteratively
  - added to the anchor and
  - pruned if the energy is too high
- Complete structures are locally minimized

AutoDock uses a genetic algorithm

- Population of structures
  - represented by torsions. bond length and angles assumed constant.
  - evolve over generations
- Generations iterate
  - mapping & fitness evaluation. mapping x and calculating E(x).
  - selection. fitter individuals reproduce more.
  - crossover. torsions swapped between individuals. enable global search.
  - mutation. small changes to individuals. permit local search.