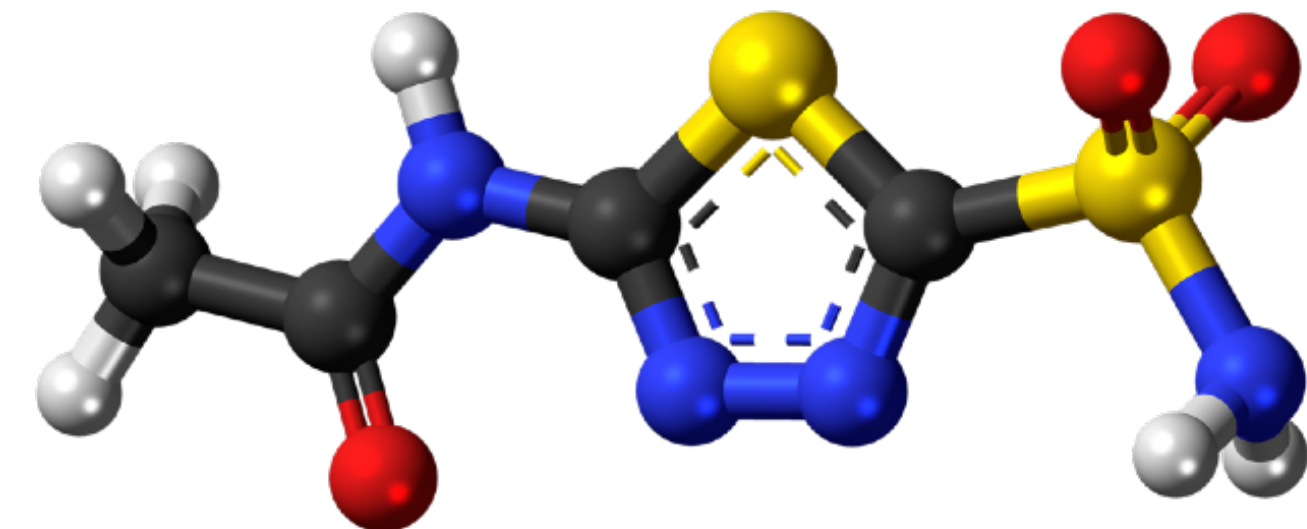
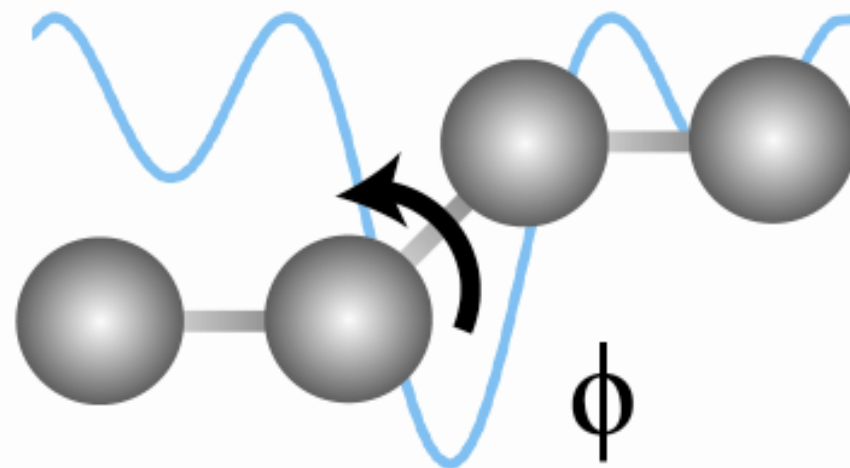
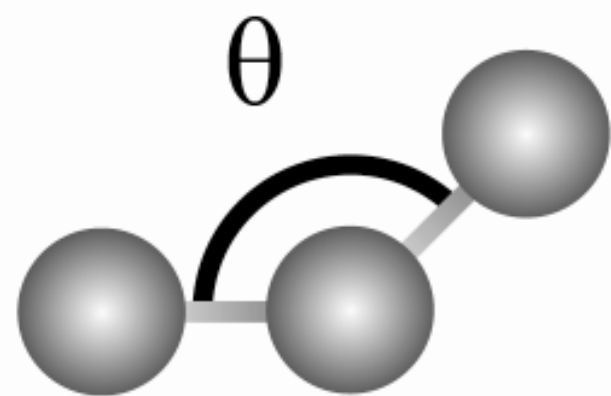
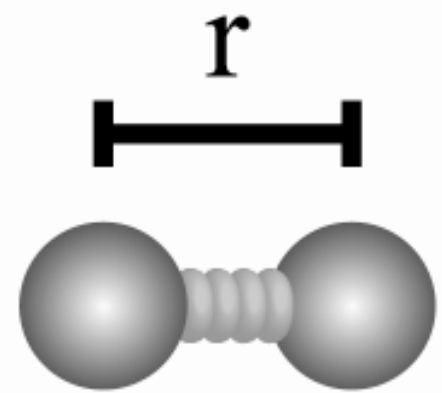


# AutoDock uses a genetic algorithm

- 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.



# Crossover

