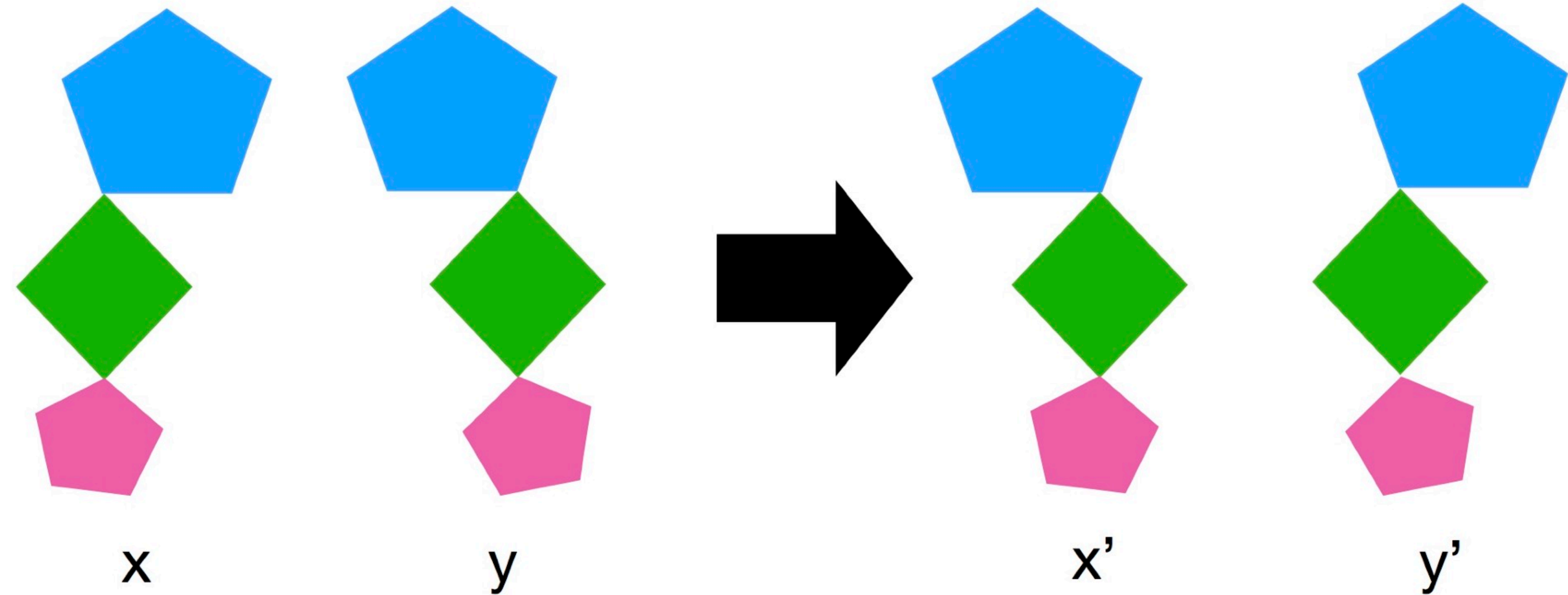


Crossover



FFT is common in docking

- Both molecules are represented by a 3D grid
- FFT correlation calculation
 - gives scores as molecules are translated relative to one another
 - is much faster than direct calculation
- Scores can be based on
 - shape complementarity [Katchalski-Katir et al, 1991]
 - van der Waals and electrostatics
- Strategy makes most sense for rigid binding

