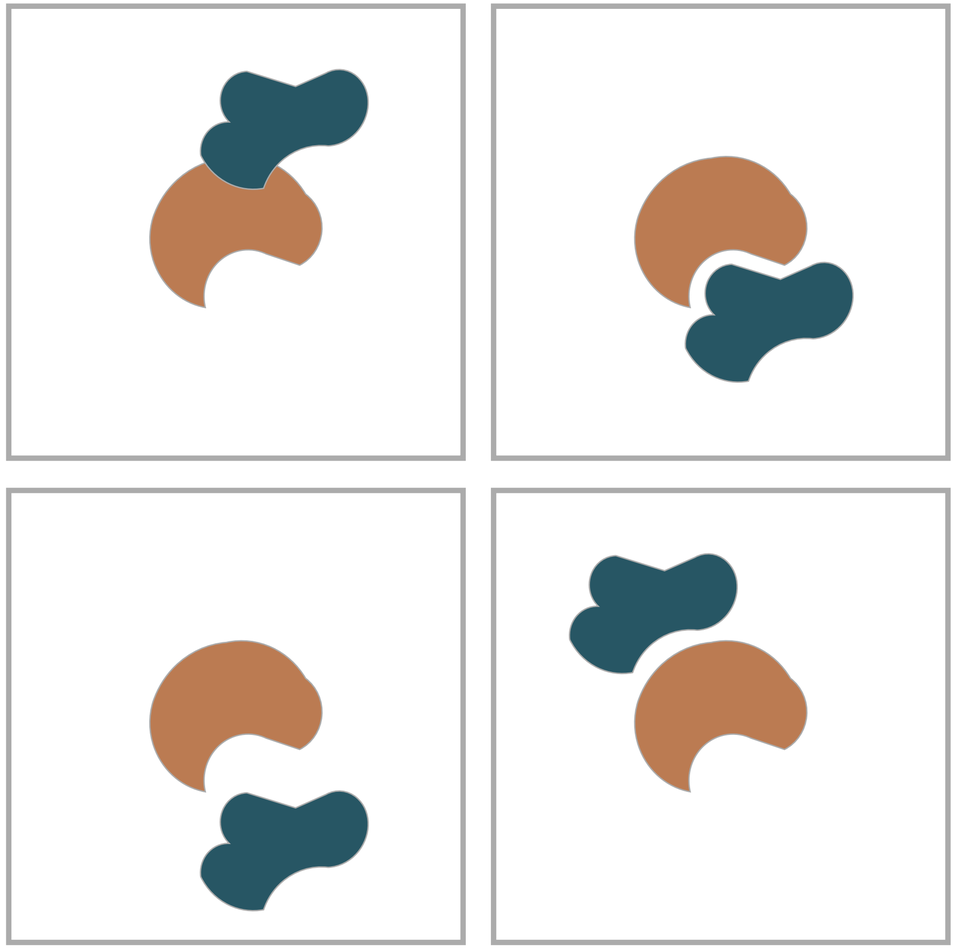
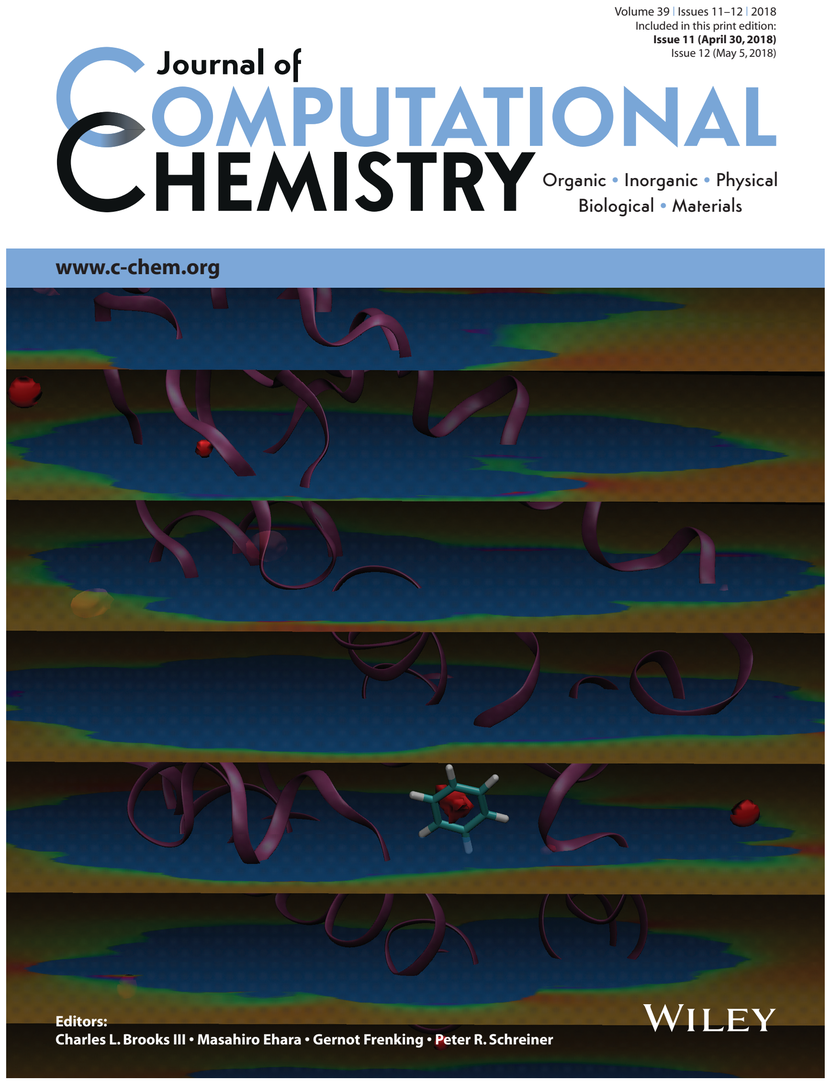
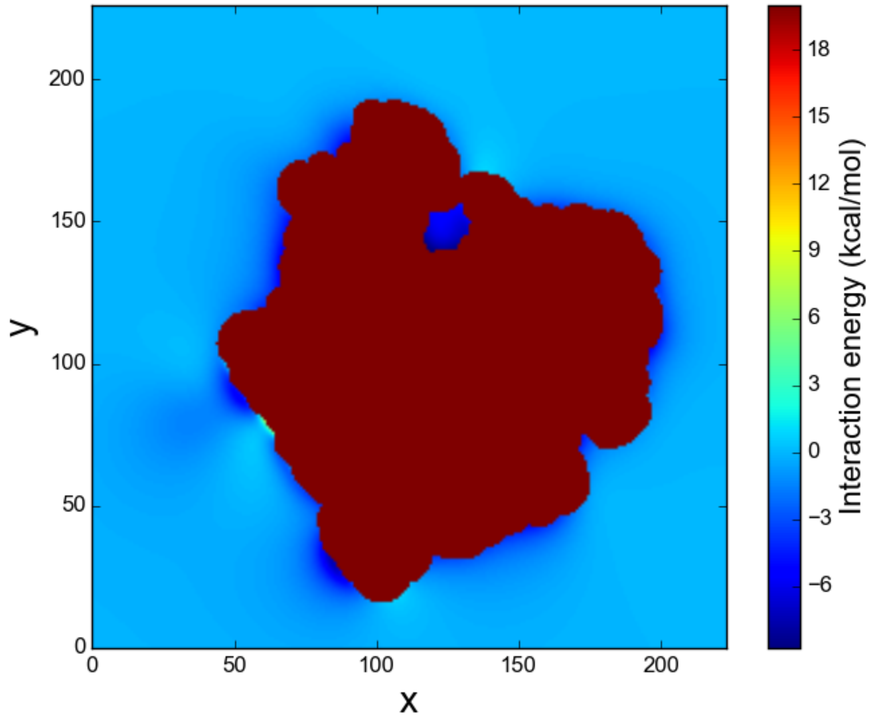
FFT is common in docking

- 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



FFT can also be used to estimate binding ΔG





2D cross section of the interaction energy

[Nguyen, Zhou, and Minh, 2018]