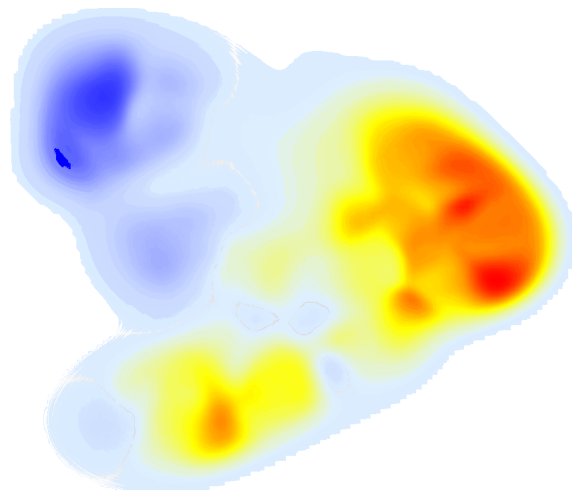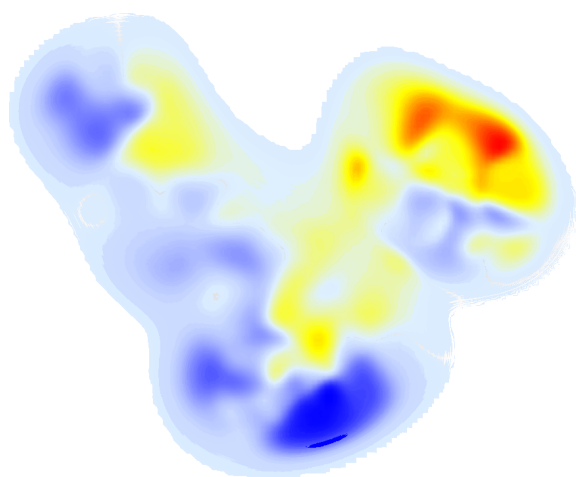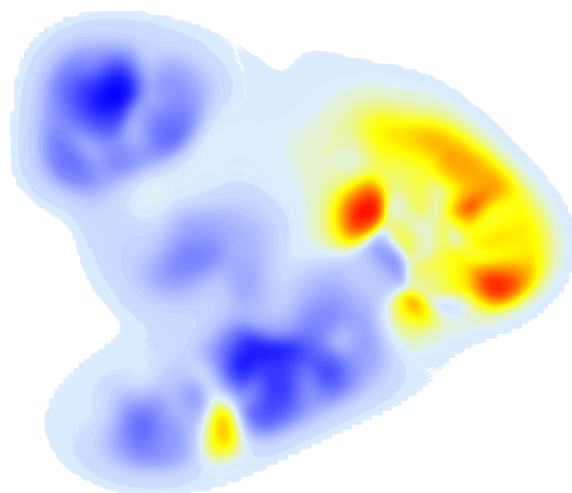(a) AM1 conformations colored by DFT-D2 energies

(b) DFT-D2 conformations colored by DFT-D2 energies

(c) AM1 conformations colored by DFT-D3 energies

(d) DFT-D2 conformations colored by DFT-D3 energies

Figure S3: **Smoothed principal components analysis visualizations.** Shown are projections to the first two principal components smoothed by Lisard using conformations relaxed by AM1 (a,c) and DFT-D2 (b,d), colored by DFT-D2 (a,b) and DFT-D3 energies (c,d).