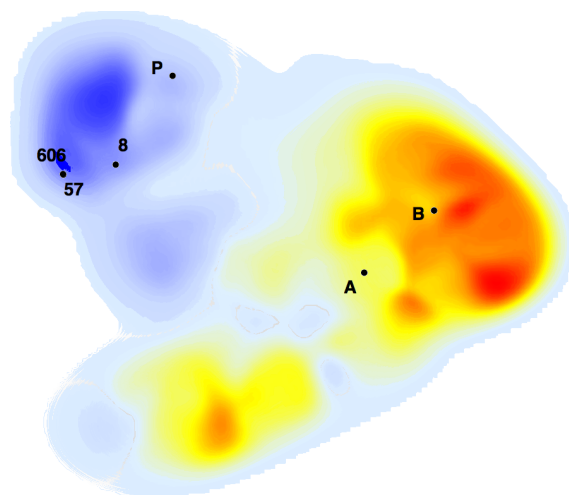
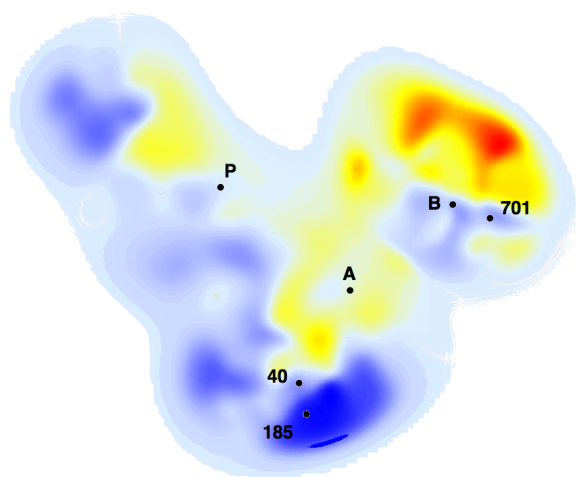


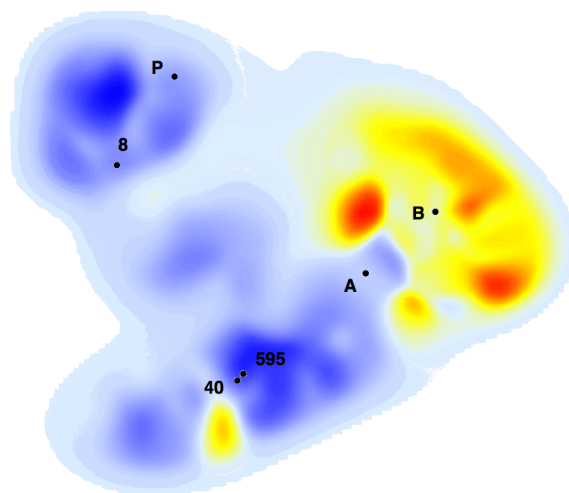
(a) AM1 conformations colored by DFT-D2 energies



(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 S5: **Smoothed principal components analysis visualizations with minimum energy conformations.** 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).