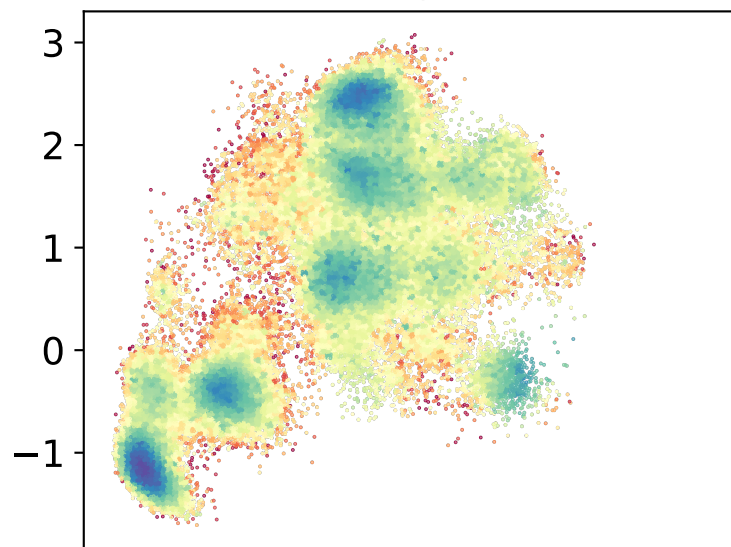
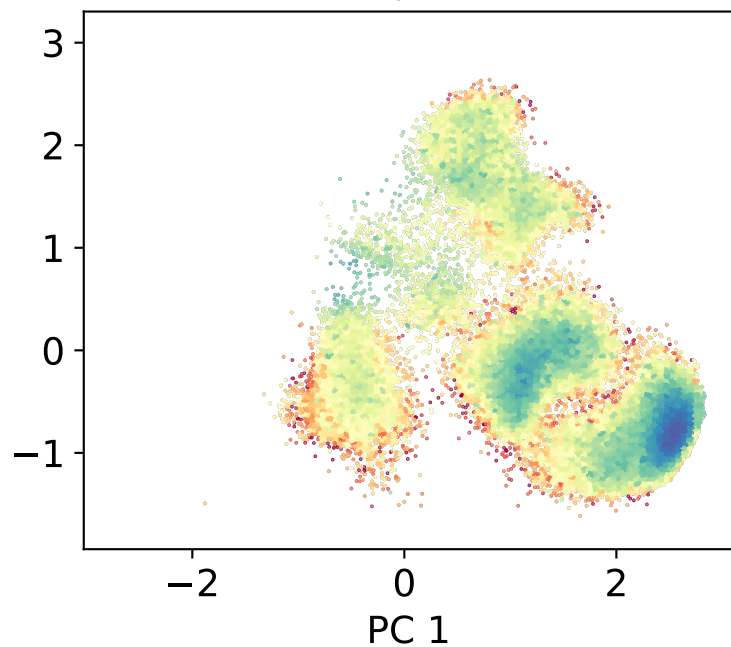


A

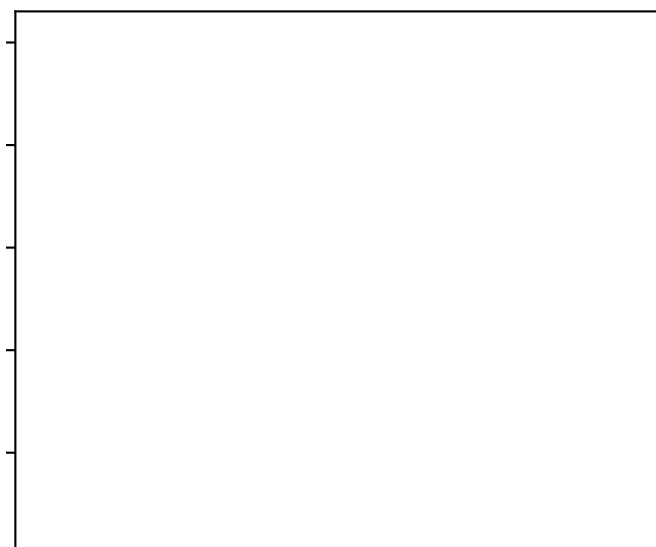
GaMD: 2000 ns
H2O, cis



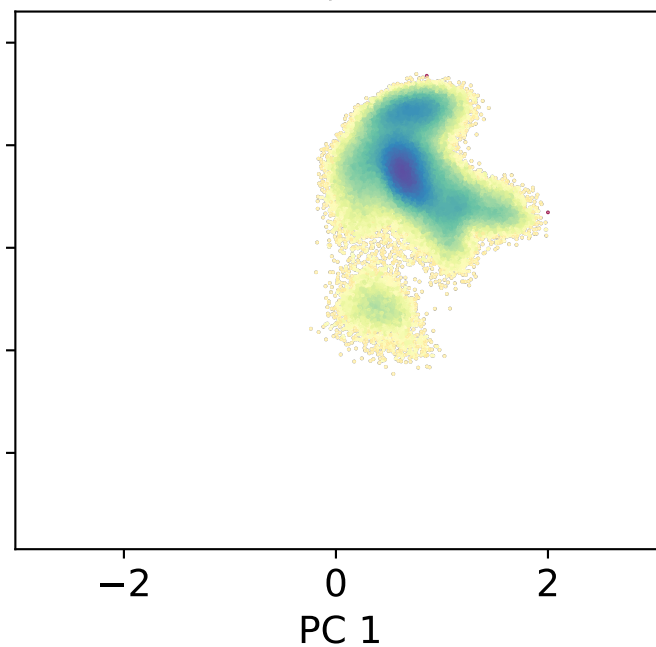
GaMD: 2000 ns
H2O, trans

**B**

cMD: 2000 ns
H2O, cis



cMD: 2000 ns
H2O, trans



Energy [kcal/mol]

