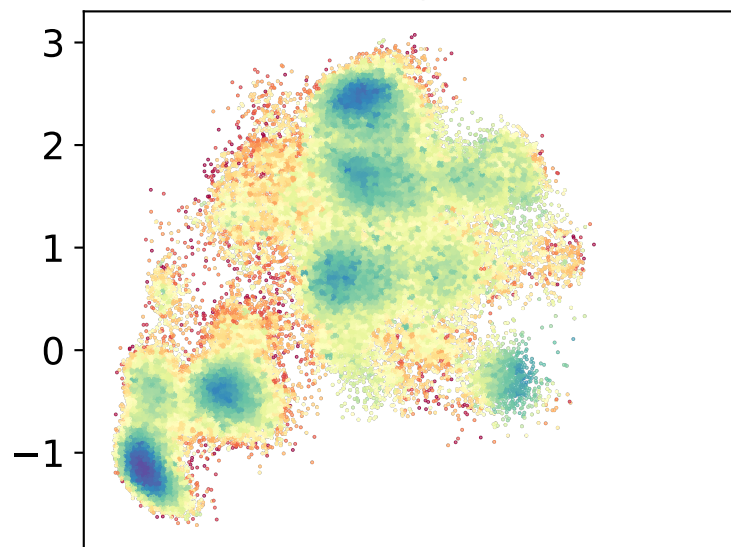
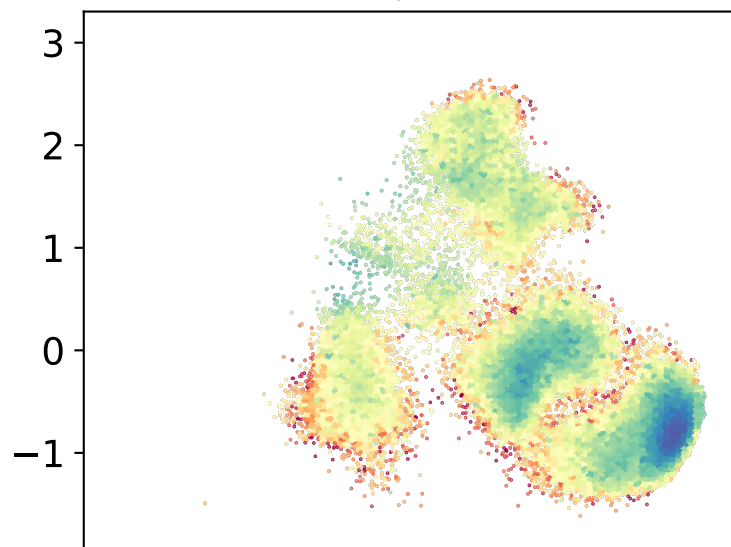
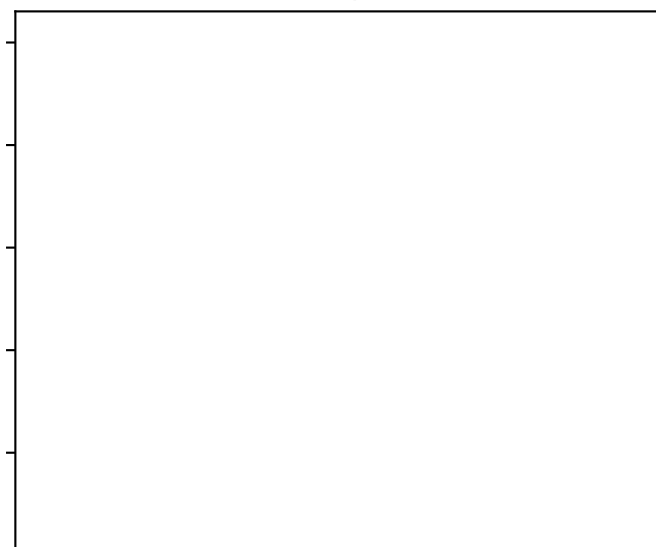
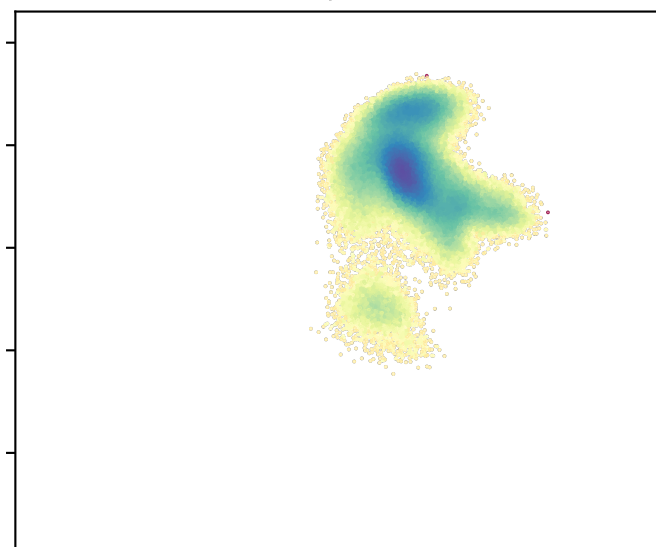


AGaMD: 2000 ns
H2O, cisGaMD: 2000 ns
H2O, trans

PC 1

BcMD: 2000 ns
H2O, ciscMD: 2000 ns
H2O, trans

PC 1

Energy [kcal/mol]

