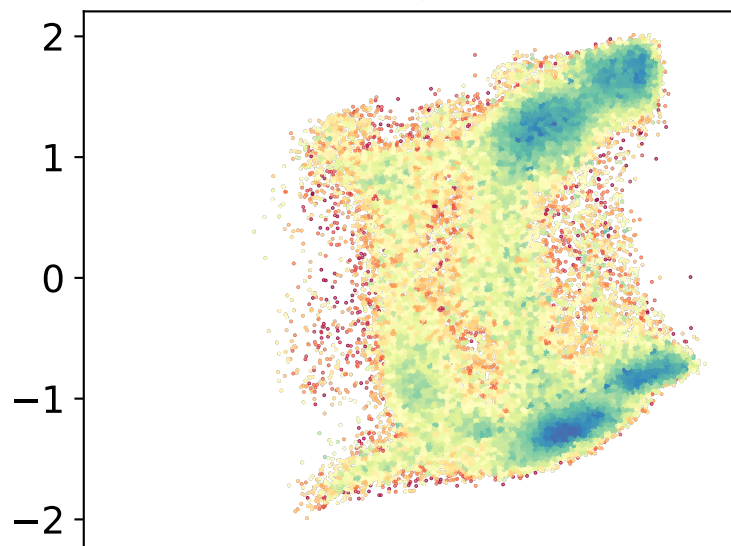
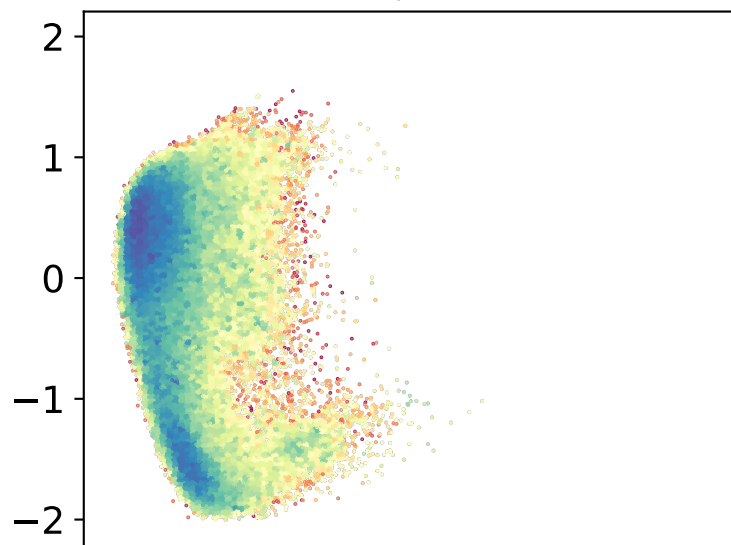


A

GaMD: 2000 ns
H2O, cis



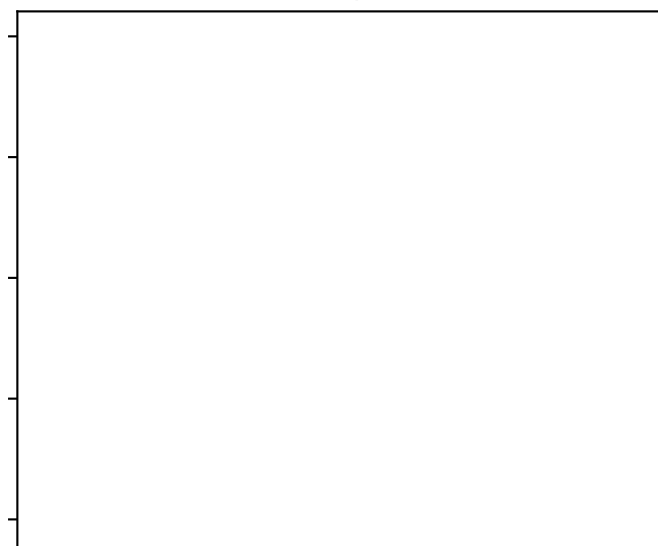
GaMD: 2000 ns
H2O, trans



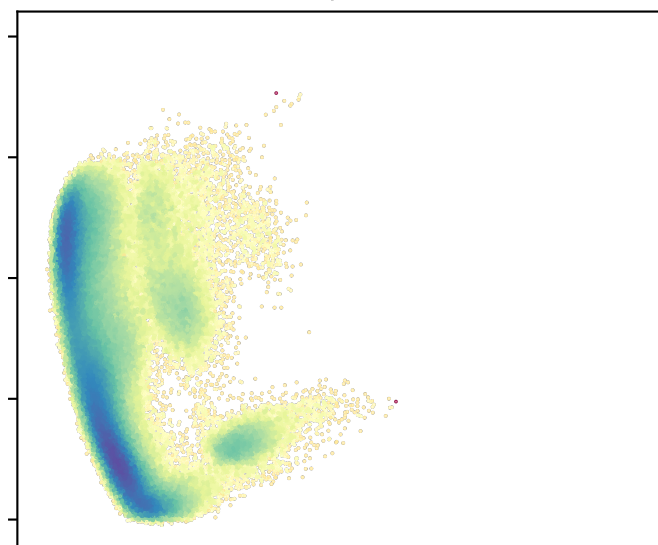
PC 1

B

cMD: 2000 ns
H2O, cis



cMD: 2000 ns
H2O, trans



PC 1

Energy [kcal/mol]

