Molecules without 3 membered rings 35000 openff_unconstrained-2.1.0 openff_unconstrained-2.2.1 openff_unconstrained-2.2.1-sdata 30000 25000 20000 -15000 10000 5000 0 -0.4-0.20.2 0.4 0.0 DDE (kcal/mol)