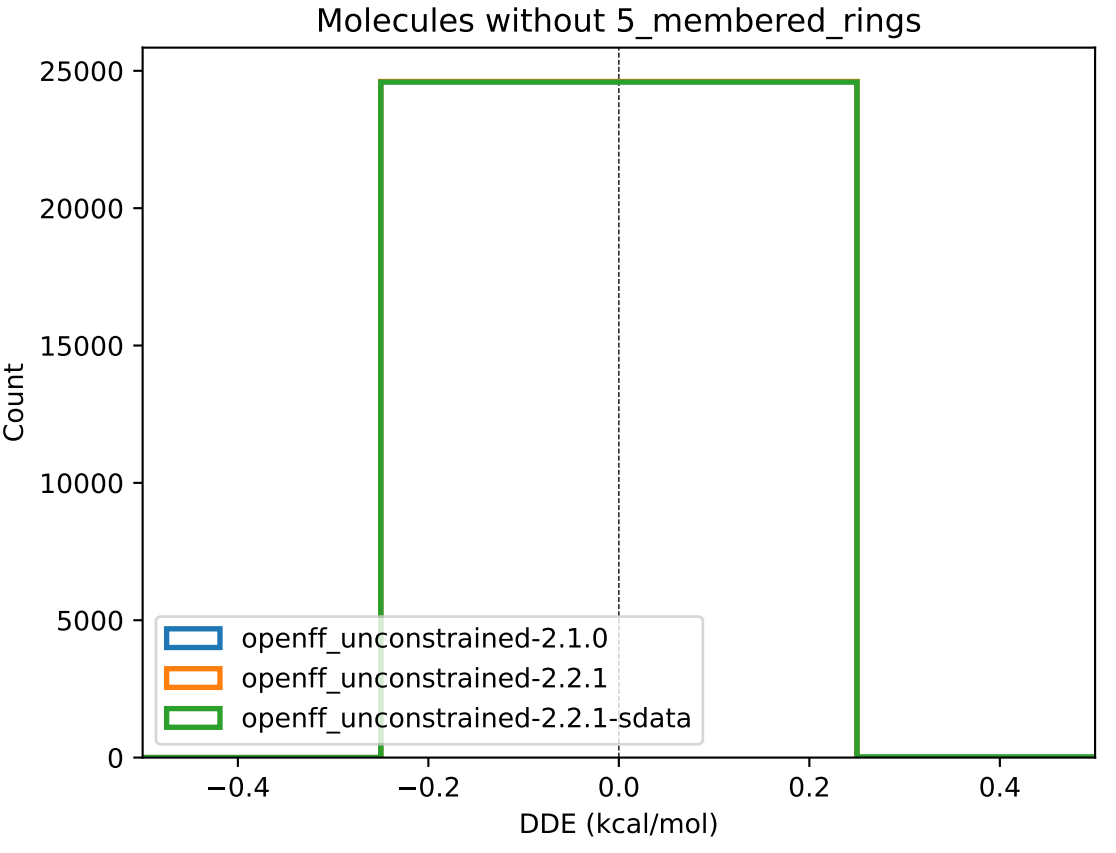
Molecules without 5_membered_rings
25000
20000
15000
10000
5000
0
Count
−0.4
−0.2
0.0
0.2
0.4
DDE (kcal/mol)
openff_unconstrained-2.1.0
openff_unconstrained-2.2.1
openff_unconstrained-2.2.1-sdata