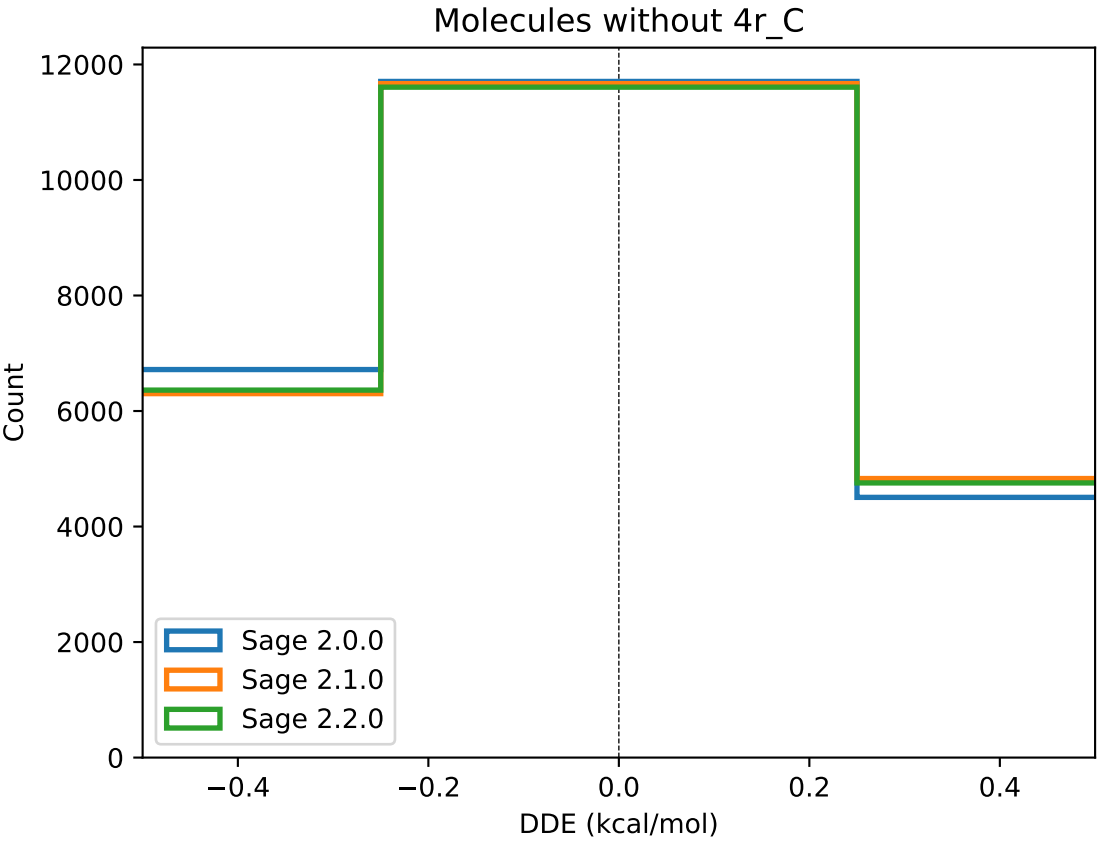
Molecules without 4r_C
12000
10000
8000
6000
4000
2000
0
Count
−0.4
−0.2
0.0
0.2
0.4
DDE (kcal/mol)
Sage 2.0.0
Sage 2.1.0
Sage 2.2.0