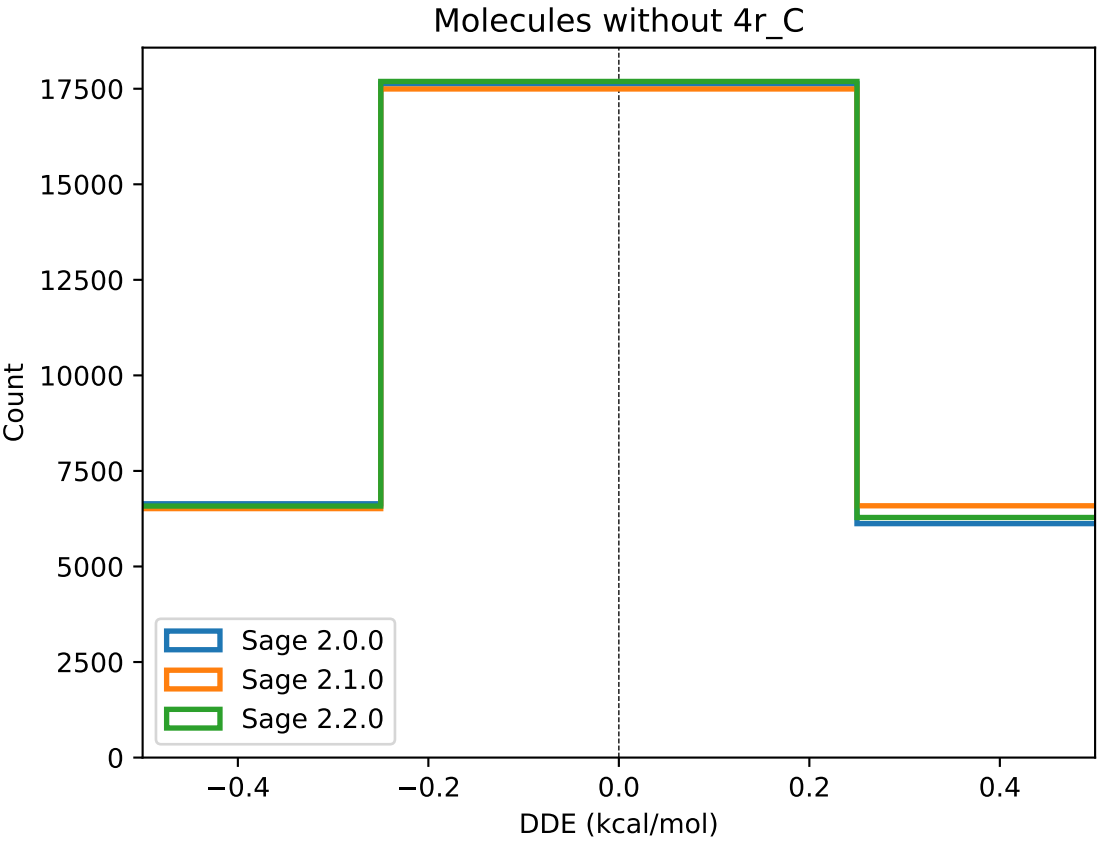
Molecules without 4r_C
Count
17500
15000
12500
10000
7500
5000
2500
0
−0.4
−0.2
0.0
0.2
0.4
DDE (kcal/mol)
Sage 2.0.0
Sage 2.1.0
Sage 2.2.0