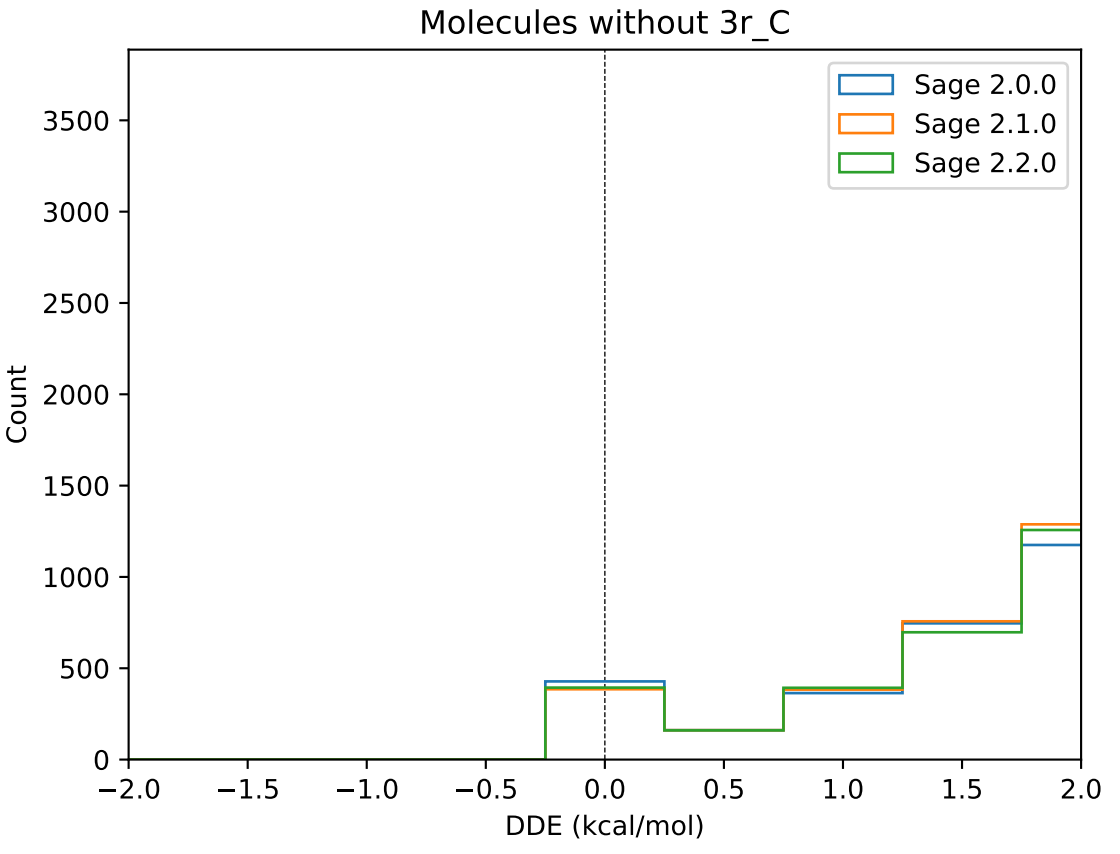
Molecules without 3r_C
Sage 2.0.0
Sage 2.1.0
Sage 2.2.0
Count
0
500
1000
1500
2000
2500
3000
3500
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
DDE (kcal/mol)