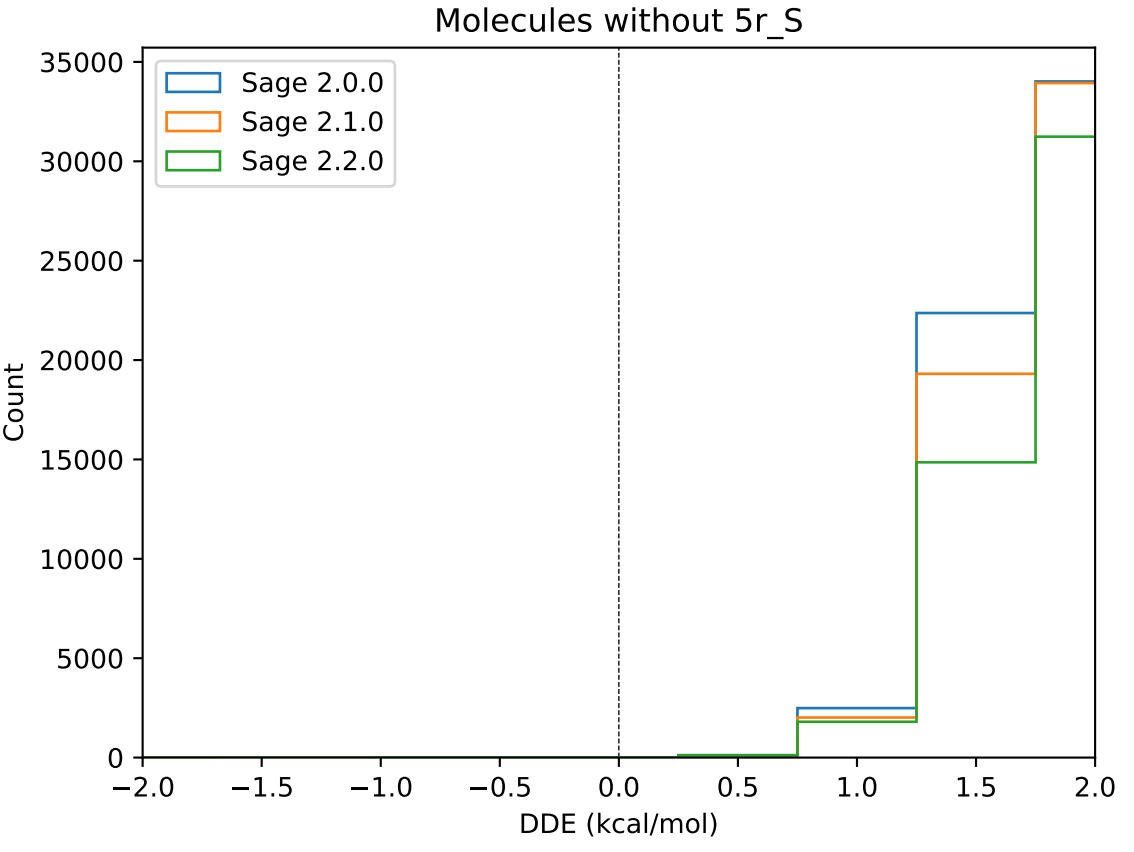
Molecules without 5r_S
Sage 2.0.0
Sage 2.1.0
Sage 2.2.0
Count
DDE (kcal/mol)
35000
30000
25000
20000
15000
10000
5000
0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0