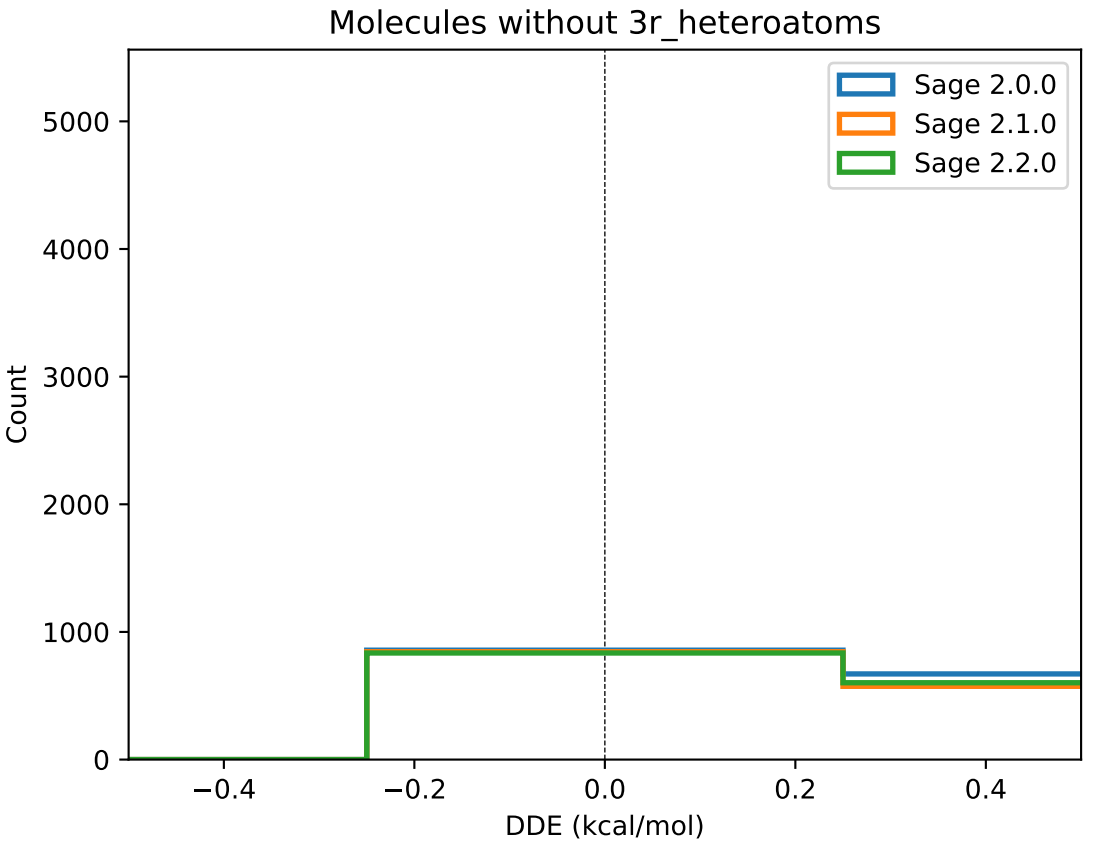
Molecules without 3r_heteroatoms
Sage 2.0.0
Sage 2.1.0
Sage 2.2.0
Count
5000
4000
3000
2000
1000
0
−0.4
−0.2
0.0
0.2
0.4
DDE (kcal/mol)