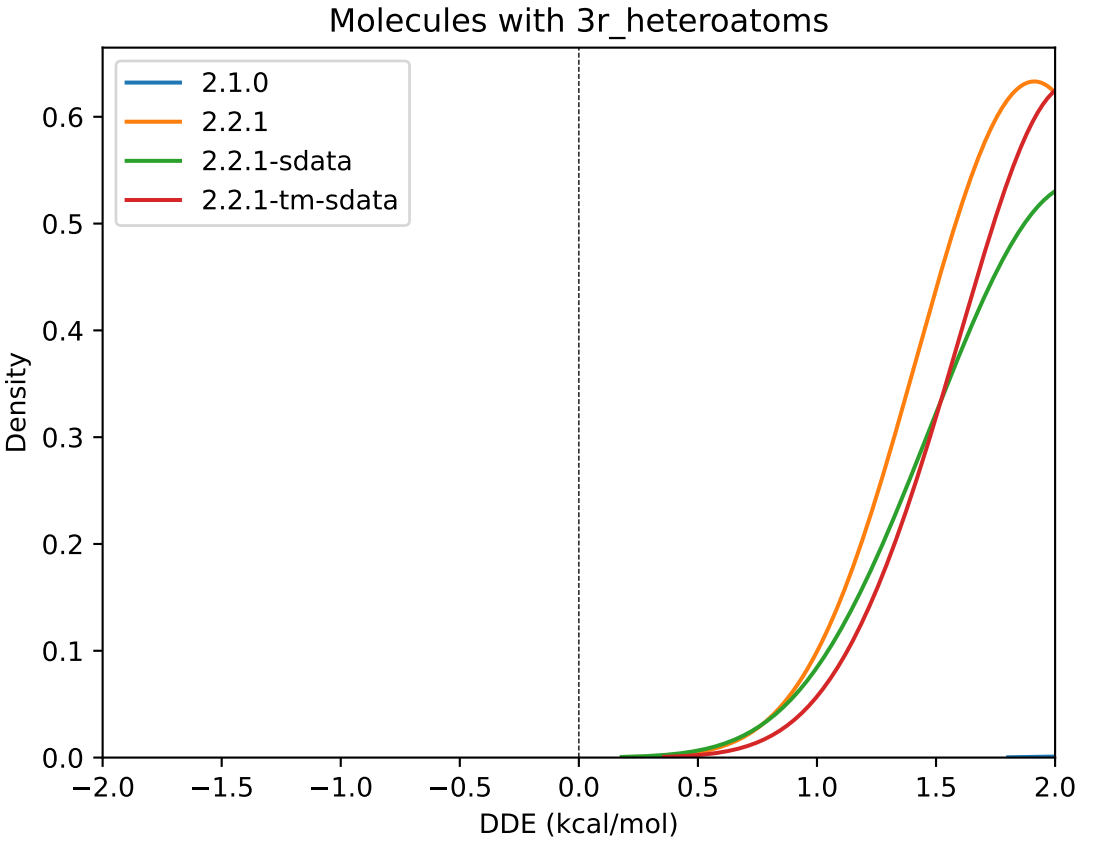
Molecules with 3r_heteroatoms
2.1.0
2.2.1
2.2.1-sdata
2.2.1-tm-sdata
Density
0.0
0.1
0.2
0.3
0.4
0.5
0.6
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
DDE (kcal/mol)