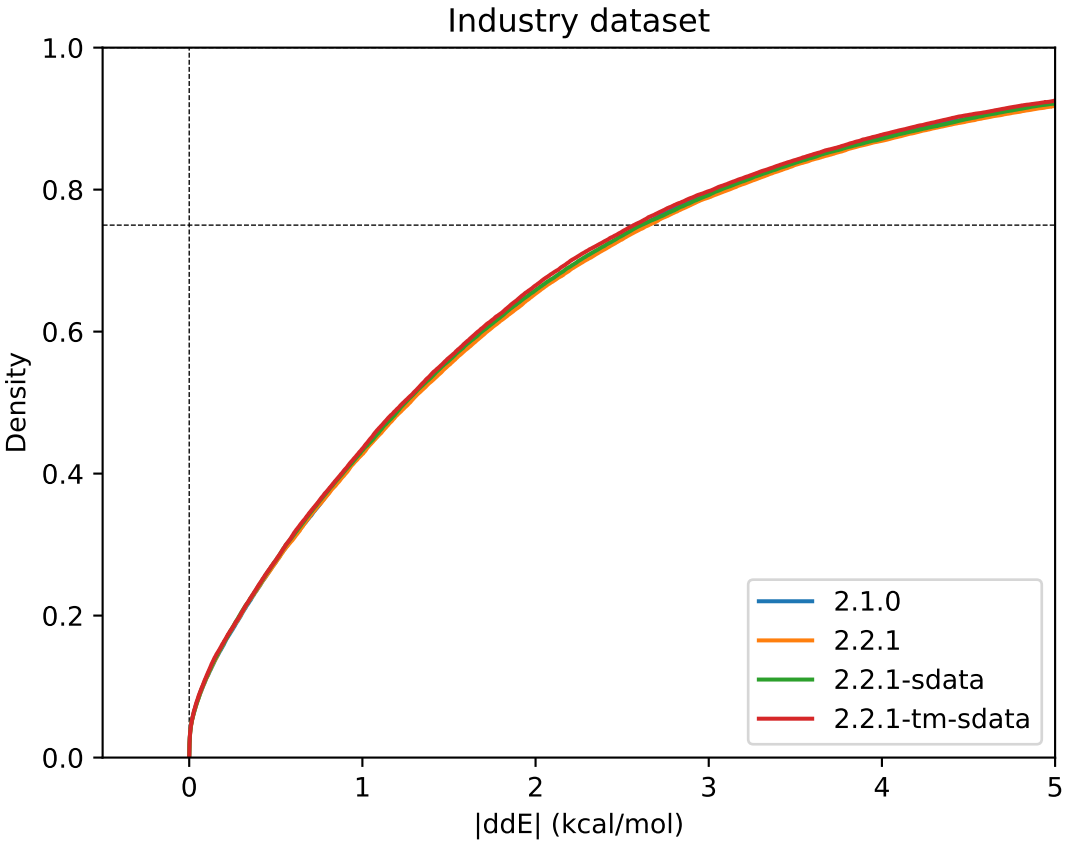
Industry dataset
1.0
0.8
0.6
0.4
0.2
0.0
Density
0
1
2
3
4
5
|ddE| (kcal/mol)
2.1.0
2.2.1
2.2.1-sdata
2.2.1-tm-sdata