

ID	sid	RMSE [kcal/mol]	MAE [kcal/mol]	ME [kcal/mol]	R ²	m	τ
AMOEBA/DDM/BAR	6	2.76 [1.84, 3.97]	2.12 [1.36, 3.33]	-1.69 [-2.98, -0.43]	0.50 [0.13, 0.78]	1.25 [0.53, 2.05]	0.47 [0.12, 0.74]
FSDAM/GAFF2/OPC3	4	2.97 [2.05, 5.14]	2.24 [1.58, 4.22]	0.43 [-1.59, 2.39]	0.12 [0.00, 0.56]	0.60 [-0.53, 1.60]	0.24 [-0.22, 0.62]
MD/DOCKING/GAFF/xtb-GNF/	5	5.65 [3.90, 7.34]	4.51 [3.03, 6.39]	-4.23 [-6.18, -2.31]	0.00 [0.00, 0.26]	-0.10 [-1.01, 0.80]	-0.05 [-0.41, 0.34]