

ID	receipt_id	RMSE (kcal/mol)	MAE (kcal/mol)	ME (kcal/mol)	R ²	m	τ
SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/D	US/PMF/MT/MD_19	finzb 0.50 [0.29, 0.66]	0.40 [0.21, 0.61]	-0.24 [-0.54, 0.06]	0.93 [0.62, 0.99]	1.15 [0.72, 1.41]	0.57 [-0.17, 1.00]
	US/PMF/MT/MD_2	mknyd 0.60 [0.35, 0.81]	0.51 [0.29, 0.73]	-0.24 [-0.62, 0.14]	0.88 [0.23, 0.99]	1.15 [0.43, 1.43]	0.69 [0.08, 1.00]
	US/PMF/MT/MD_22	iyo2o 0.80 [0.45, 1.14]	0.67 [0.41, 1.00]	0.57 [0.19, 0.97]	0.83 [0.25, 0.99]	0.66 [0.24, 0.85]	0.71 [0.08, 1.00]
	US/PMF/MT/MD_20	ttmwo 0.94 [0.61, 1.21]	0.79 [0.45, 1.14]	0.11 [-0.55, 0.71]	0.75 [0.02, 0.97]	1.24 [0.08, 1.74]	0.57 [-0.09, 1.00]
	US/PMF/MT/MD_9	uui3y 1.06 [0.45, 1.51]	0.80 [0.37, 1.31]	0.77 [0.30, 1.29]	0.83 [0.23, 0.99]	1.20 [0.42, 1.55]	0.69 [0.00, 1.00]
	US/PMF/MT/MD_9	rkitq 1.15 [0.49, 1.79]	0.86 [0.43, 1.46]	-0.09 [-0.97, 0.60]	0.15 [0.00, 0.88]	0.15 [-0.07, 0.59]	0.36 [-0.36, 1.00]
	US/PMF/MT/MD_26	o3aiv 1.24 [0.75, 1.67]	1.05 [0.62, 1.53]	0.88 [0.28, 1.48]	0.65 [0.10, 0.96]	0.97 [-0.79, 1.43]	0.14 [-0.83, 0.83]
	US/PMF/MT/MD_7	8jxan 1.31 [0.72, 1.90]	1.09 [0.66, 1.66]	0.68 [-0.09, 1.49]	0.72 [0.02, 0.94]	1.33 [0.04, 2.16]	0.50 [-0.20, 1.00]
	FEP-MM	4ndha 1.46 [1.04, 1.85]	1.32 [0.89, 1.76]	1.27 [0.74, 1.75]	0.75 [0.13, 0.95]	0.49 [0.20, 0.82]	0.55 [-0.04, 1.00]
	US/PMF/MT/MD_12	w2q3q 1.48 [1.05, 1.83]	1.36 [0.95, 1.76]	-1.23 [-1.75, -0.62]	0.74 [0.47, 0.99]	1.09 [0.69, 1.98]	0.79 [0.33, 1.00]
SOMD/AM1BCC-GAFF-TIP3P/MBAR/D	US/PMF/MT/MD_12	emfe8 1.50 [1.04, 1.87]	1.31 [0.78, 1.80]	1.21 [0.55, 1.79]	0.70 [0.08, 0.95]	0.31 [0.07, 0.46]	0.57 [0.04, 1.00]
	US/PMF/MT/MD_23	7uted 1.54 [1.09, 1.88]	1.38 [0.90, 1.83]	-1.32 [-1.83, -0.77]	0.72 [0.02, 0.99]	0.99 [-0.27, 1.42]	0.43 [-0.36, 1.00]
	US/PMF/MT/MD_25	vgqcz 1.55 [1.01, 2.05]	1.40 [1.00, 1.90]	1.40 [1.00, 1.90]	0.72 [0.01, 0.99]	0.72 [-0.19, 1.04]	0.43 [-0.36, 1.00]
	US/PMF/MT/MD_21	ftout 1.64 [1.10, 2.11]	1.49 [1.04, 1.99]	1.49 [1.04, 1.99]	0.83 [0.22, 0.99]	1.16 [0.42, 1.51]	0.69 [0.00, 1.00]
	FEP-QM/MM	ahtcq 1.74 [1.31, 2.07]	1.59 [1.07, 2.04]	-1.59 [-2.04, -1.07]	0.81 [0.50, 1.00]	1.14 [0.76, 1.83]	0.79 [0.42, 1.00]
	US/PMF/MT/MD_24	aai8i 1.76 [1.23, 2.28]	1.62 [1.21, 2.13]	1.62 [1.21, 2.13]	0.72 [0.02, 0.99]	0.83 [-0.23, 1.19]	0.43 [-0.36, 1.00]
	SQM-opt	c8jfq 1.92 [1.00, 2.70]	1.57 [0.86, 2.40]	-0.29 [-1.51, 1.09]	0.18 [0.00, 0.92]	0.70 [-0.21, 2.80]	0.40 [-0.33, 0.98]
	US/PMF/MT/MD_11	7fk2x 1.94 [1.42, 2.35]	1.77 [1.19, 2.29]	1.77 [1.19, 2.29]	0.70 [0.09, 0.95]	0.43 [0.11, 0.65]	0.57 [0.08, 1.00]
	US/PMF/MT/MD_6	egmst 1.96 [1.51, 2.36]	1.85 [1.41, 2.28]	1.85 [1.41, 2.28]	0.75 [0.14, 0.95]	0.68 [0.24, 1.13]	0.55 [-0.04, 1.00]
	US/PMF/MT/MD_4	gt5n0 1.98 [1.37, 2.49]	1.77 [1.14, 2.38]	1.77 [1.14, 2.38]	0.58 [0.02, 0.92]	0.81 [-0.16, 1.28]	0.50 [-0.20, 1.00]
FS-DAM/GAFF2/TIP3P	gemch 2.00 [0.90, 2.85]	1.55 [0.75, 2.48]	1.55 [0.75, 2.48]	0.84 [0.28, 0.98]	0.84 [0.28, 0.98]	1.69 [0.38, 2.41]	0.71 [0.22, 1.00]
	US/PMF/MT/MD_27	8pxph 2.05 [1.49, 2.56]	1.91 [1.42, 2.43]	1.91 [1.42, 2.43]	0.65 [0.10, 0.96]	0.71 [-0.60, 1.06]	0.14 [-1.00, 0.84]
	US/PMF/MT/MD_17	iaz7f 2.19 [1.70, 2.57]	2.04 [1.44, 2.53]	2.04 [1.44, 2.53]	0.91 [0.80, 1.00]	0.37 [0.28, 0.54]	0.76 [0.22, 1.00]
	AMOEBa/BAR/Tinker	8fcb6 2.23 [1.03, 3.27]	1.77 [0.98, 2.82]	-0.77 [-2.31, 0.58]	0.23 [0.00, 0.96]	-0.46 [-0.98, 1.23]	-0.29 [-1.00, 0.44]
	DFT-opt	bjyua 2.23 [1.26, 3.08]	1.91 [1.19, 2.78]	-0.29 [-1.69, 1.36]	0.66 [0.01, 0.94]	2.03 [-0.21, 3.66]	0.43 [-0.26, 1.00]
	US/PMF/MT/MD_14	rc4qr 2.29 [1.93, 2.62]	2.22 [1.85, 2.58]	2.22 [1.85, 2.58]	0.86 [0.12, 0.99]	1.06 [0.14, 1.32]	0.57 [-0.17, 1.00]
	US/PMF/MT/MD_10	s78rs 2.40 [1.93, 2.82]	2.30 [1.82, 2.76]	2.30 [1.82, 2.76]	0.70 [0.08, 0.95]	0.63 [0.15, 0.94]	0.57 [0.05, 1.00]
	US/PMF/MT/MD_5	nb8jk 2.51 [2.00, 2.96]	2.41 [1.91, 2.90]	2.41 [1.91, 2.90]	0.75 [0.13, 0.95]	0.99 [0.36, 1.64]	0.55 [-0.04, 1.00]
	US/PMF/MT/MD_13	gkdce 2.68 [2.26, 3.06]	2.61 [2.19, 3.02]	2.61 [2.19, 3.02]	0.86 [0.11, 0.99]	1.16 [0.15, 1.44]	0.57 [-0.24, 1.00]
	SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/C	iv75a 2.70 [1.74, 3.44]	2.34 [1.40, 3.26]	2.30 [1.29, 3.26]	0.75 [0.02, 0.97]	1.65 [0.13, 2.34]	0.57 [-0.09, 1.00]
DDM/GAFF/AM1-BCC/TIP3P	yedi3 2.77 [1.44, 3.85]	2.21 [1.08, 3.45]	1.79 [0.35, 3.32]	0.41 [0.00, 0.89]	1.37 [-0.69, 2.51]	0.18 [-0.62, 0.92]	0.18 [-0.62, 0.92]
	US/PMF/MT/MD_18	xcuey 2.82 [2.52, 3.08]	2.78 [2.49, 3.06]	2.78 [2.49, 3.06]	0.93 [0.62, 0.99]	0.72 [0.45, 0.90]	0.57 [0.00, 1.00]
	US/PMF/MT/MD_16	ogd0g 2.99 [2.57, 3.33]	2.93 [2.44, 3.31]	2.93 [2.44, 3.31]	0.91 [0.83, 1.00]	0.52 [0.39, 0.75]	0.82 [0.36, 1.00]
	US/PMF/MT/MD_1	4ysuf 3.01 [2.24, 3.67]	2.83 [2.14, 3.54]	2.83 [2.14, 3.54]	0.88 [0.22, 0.99]	1.58 [0.60, 1.96]	0.69 [0.08, 1.00]
	US/PMF/MT/MD_3	widya 3.17 [2.56, 3.72]	3.05 [2.44, 3.66]	3.05 [2.44, 3.66]	0.58 [0.02, 0.92]	0.80 [-0.24, 1.27]	0.50 [-0.20, 1.00]
	SOMD/AM1BCC-GAFF-TIP3P/MBAR/C	ibhca 3.48 [2.21, 4.62]	3.05 [1.95, 4.25]	3.05 [1.95, 4.25]	0.72 [0.02, 0.94]	1.76 [0.02, 2.85]	0.50 [-0.25, 1.00]
	US/PMF/MT/MD_15	m0qdw 4.00 [3.70, 4.25]	3.98 [3.67, 4.24]	3.98 [3.67, 4.24]	0.91 [0.82, 1.00]	0.76 [0.57, 1.08]	0.79 [0.22, 1.00]
	SOMD/AM1BCC-GAFF-TIP3P-NOBUFFER/MBAR/A	bhns3 4.64 [3.63, 5.51]	4.41 [3.42, 5.41]	4.41 [3.42, 5.41]	0.77 [0.03, 0.97]	1.67 [0.19, 2.30]	0.57 [-0.08, 1.00]
	SOMD/AM1BCC-GAFF-TIP3P/MBAR/A	mdqkg 5.41 [4.21, 6.61]	5.14 [4.09, 6.33]	5.14 [4.09, 6.33]	0.74 [0.05, 0.95]	1.81 [0.23, 2.86]	0.57 [0.00, 1.00]
	NULL1	null3 5.98 [5.10, 6.91]	5.85 [5.06, 6.77]	-5.85 [-6.77, -5.06]	0.00 [0.00, 0.00]	0.00 [0.00, 0.00]	nan [nan, nan]
EKEN-DIAZ/MD/MMPBSA	US/PMF/MT/MD_8	e032m 6.26 [4.20, 8.00]	5.57 [3.65, 7.60]	5.57 [3.65, 7.60]	0.15 [0.00, 0.87]	0.96 [-0.45, 3.68]	0.36 [-0.36, 1.00]
	BSSE-corrected RI-B3PW91 (SMD)/CBS	8brzp 7.07 [5.63, 8.46]	6.80 [5.53, 8.23]	6.80 [5.53, 8.23]	0.84 [0.13, 0.97]	2.22 [0.59, 3.00]	0.64 [0.04, 1.00]
	BSSE-corrected RI-B3PW91 (SMD)/CBS	5r5n7 22.51 [11.38, 34.29]	17.86 [10.84, 28.41]	4.63 [-12.38, 14.87]	0.60 [0.00, 0.96]	-13.14 [-19.91, 3.50]	-0.21 [-1.00, 0.73]
	BSSE-corrected RI-B3PW91-D3 (SMD)/CBS	kuovg 36.41 [30.99, 40.13]	35.46 [28.94, 40.04]	31.73 [17.75, 40.04]	0.44 [0.15, 0.94]	-9.02 [-15.66, 4.60]	0.29 [-0.50, 1.00]