

Testing Dataset

$$RMSE(E_{int}^{EMLE} - E_{int}^{QM/MM})$$

$$RMSE(E_{static}^{EMLE} - E_{static}^{QM/MM})$$

$$RMSE(E_{ind}^{EMLE} - E_{ind}^{QM/MM})$$

RMSE [kcal.mol⁻¹]

2.5

2.0

1.5

1.0

Iter0	2.11	2.12	1.69	1.76	1.67	1.76	1.28	1.25	1.23	1.19
Iter1	2.41	2.40	2.00	2.09	2.11	2.25	1.66	1.59	1.45	1.34
Iter2	2.40	2.43	2.01	2.08	2.05	2.13	1.63	1.53	1.56	1.43

2.21	2.21	1.55	1.55	1.53	1.53	0.96	0.96	0.95	0.95
2.51	2.51	1.72	1.72	1.87	1.87	1.07	1.07	0.96	0.96
2.55	2.55	1.74	1.74	1.76	1.76	1.06	1.06	1.05	1.05

0.74	0.59	0.55	0.63	0.54	0.62	0.68	0.65	0.63	0.57
0.87	0.72	0.75	0.85	0.74	0.85	0.96	0.91	0.87	0.76
0.87	0.71	0.74	0.81	0.73	0.80	0.94	0.84	0.85	0.72

QM7-Species
QM7-Reference
Bespoke-Iter1-Species
Bespoke-Iter1-Reference
Bespoke-Iter2-Species
Bespoke-Iter2-Reference
Patched-Iter1-Species
Patched-Iter1-Reference
Patched-Iter2-Species
Patched-Iter2-Reference

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