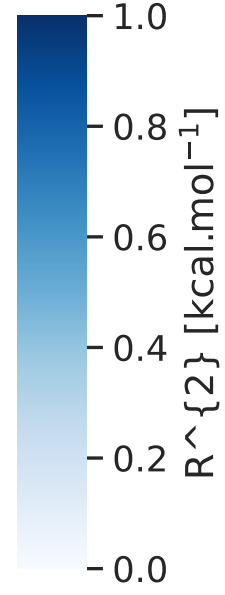


Testing Dataset

$$R^2(E_{int}^{EMLE}, E_{int}^{QM/MM})$$

$$R^2(E_{static}^{EMLE}, E_{static}^{QM/MM})$$

$$R^2(E_{ind}^{EMLE}, E_{ind}^{QM/MM})$$



| | | | | | | | | | | |
|-------|------|------|------|------|------|------|------|------|------|------|
| Iter0 | 0.94 | 0.94 | 0.97 | 0.97 | 0.97 | 0.97 | 0.99 | 0.99 | 0.99 | 0.99 |
| Iter1 | 0.95 | 0.95 | 0.98 | 0.98 | 0.98 | 0.98 | 0.99 | 0.99 | 0.99 | 0.99 |
| Iter2 | 0.95 | 0.95 | 0.98 | 0.98 | 0.98 | 0.98 | 0.99 | 0.99 | 0.99 | 0.99 |

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

| | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|
| 0.92 | 0.92 | 0.96 | 0.96 | 0.96 | 0.96 | 0.98 | 0.98 | 0.98 | 0.98 |
| 0.93 | 0.93 | 0.97 | 0.97 | 0.97 | 0.97 | 0.99 | 0.99 | 0.99 | 0.99 |
| 0.93 | 0.93 | 0.97 | 0.97 | 0.97 | 0.97 | 0.99 | 0.99 | 0.99 | 0.99 |

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

| | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|
| 0.91 | 0.94 | 0.94 | 0.97 | 0.95 | 0.97 | 0.97 | 0.99 | 0.97 | 0.99 |
| 0.89 | 0.92 | 0.96 | 0.98 | 0.96 | 0.98 | 0.97 | 0.99 | 0.98 | 0.99 |
| 0.90 | 0.92 | 0.96 | 0.98 | 0.96 | 0.98 | 0.97 | 0.99 | 0.98 | 0.99 |

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