

Testing Dataset

Pearson's  $\rho(E_{int}^{EMLE}, E_{int}^{QM/MM})$ Pearson's  $\rho(E_{static}^{EMLE}, E_{static}^{QM/MM})$ Pearson's  $\rho(E_{ind}^{EMLE}, E_{ind}^{QM/MM})$ Pearson's  $\rho$ 

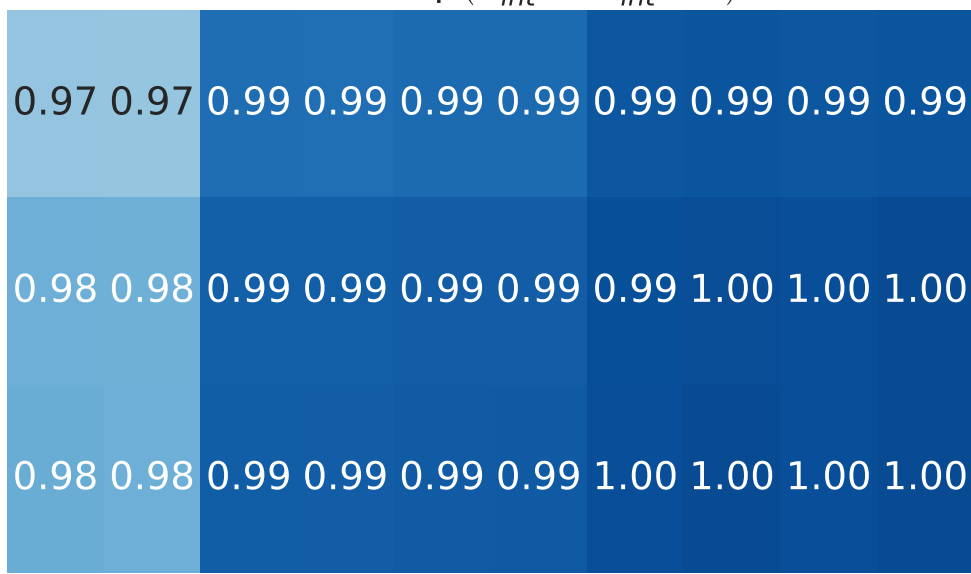
1.00

0.99

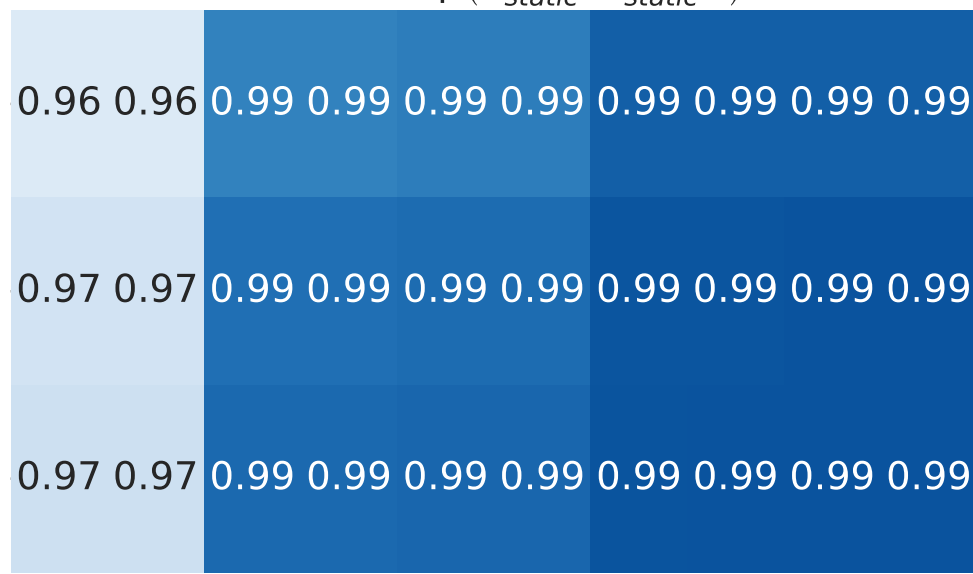
0.98

0.97

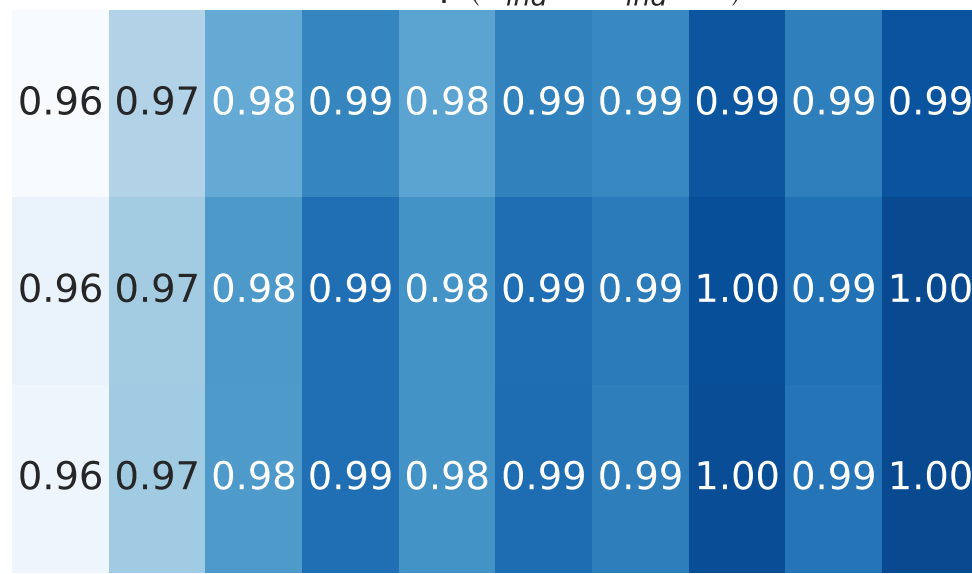
0.96

Iter0  
Iter1  
Iter2

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



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



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