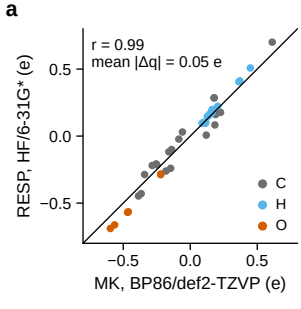
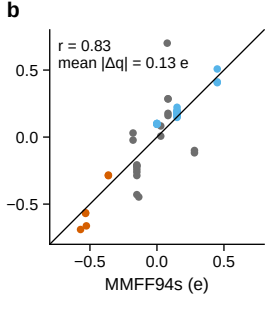
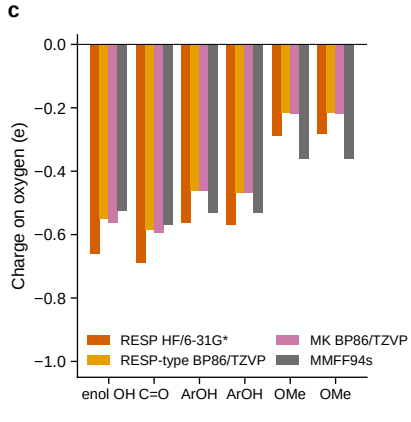






d

Fit	RRMS
MK BP86, 1 pt/Å²	0.102
MK BP86, 6 pt/Å²	0.098
RESP HF, 6 pt/Å²	0.087
Dipole (D)	
BP86/TZVP density	3.55
MK charges	3.51
HF/6-31G* density	3.01
RESP charges	2.94