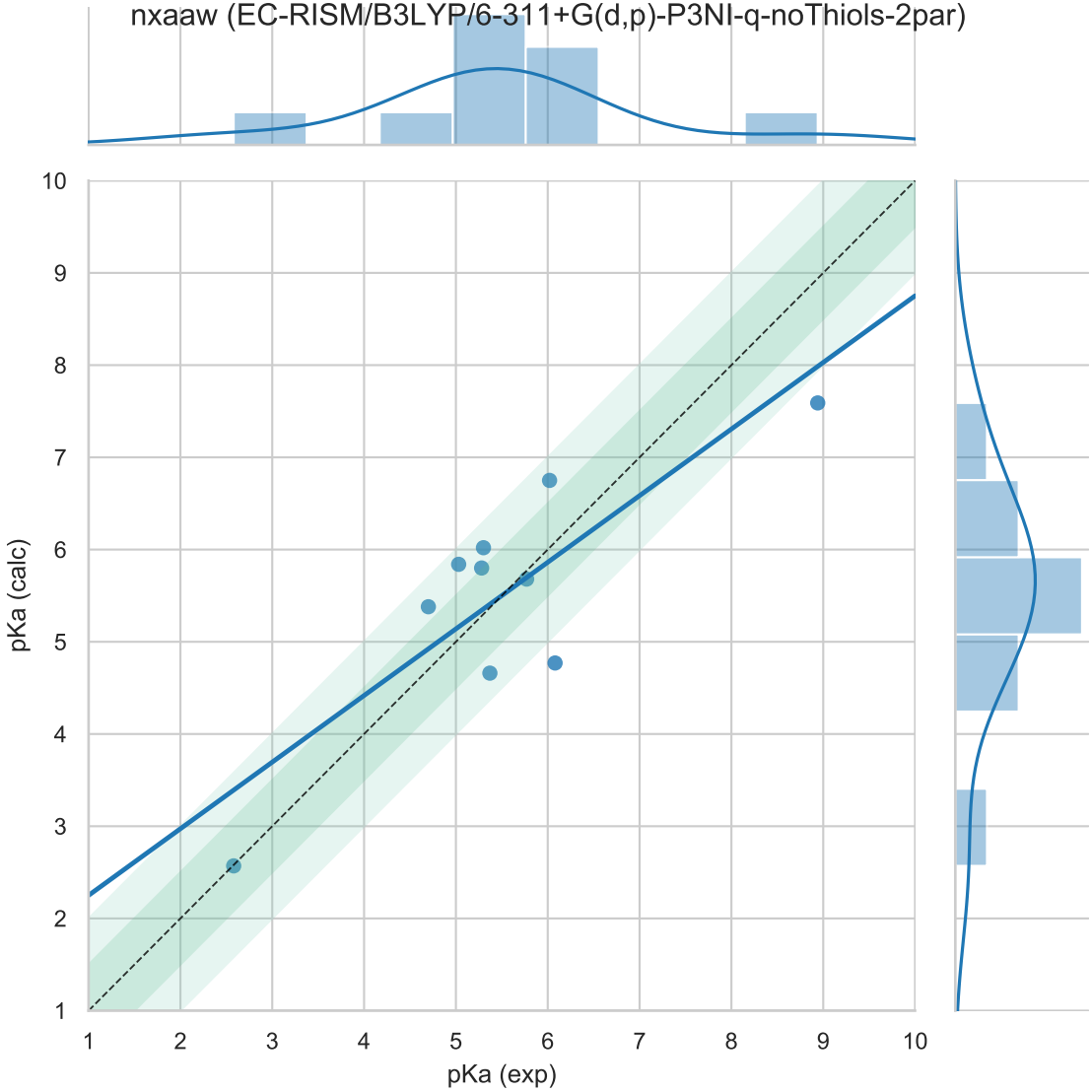
nxaaw (EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par)
pKa (calc)
pKa (exp)
1
2
3
4
5
6
7
8
9
10