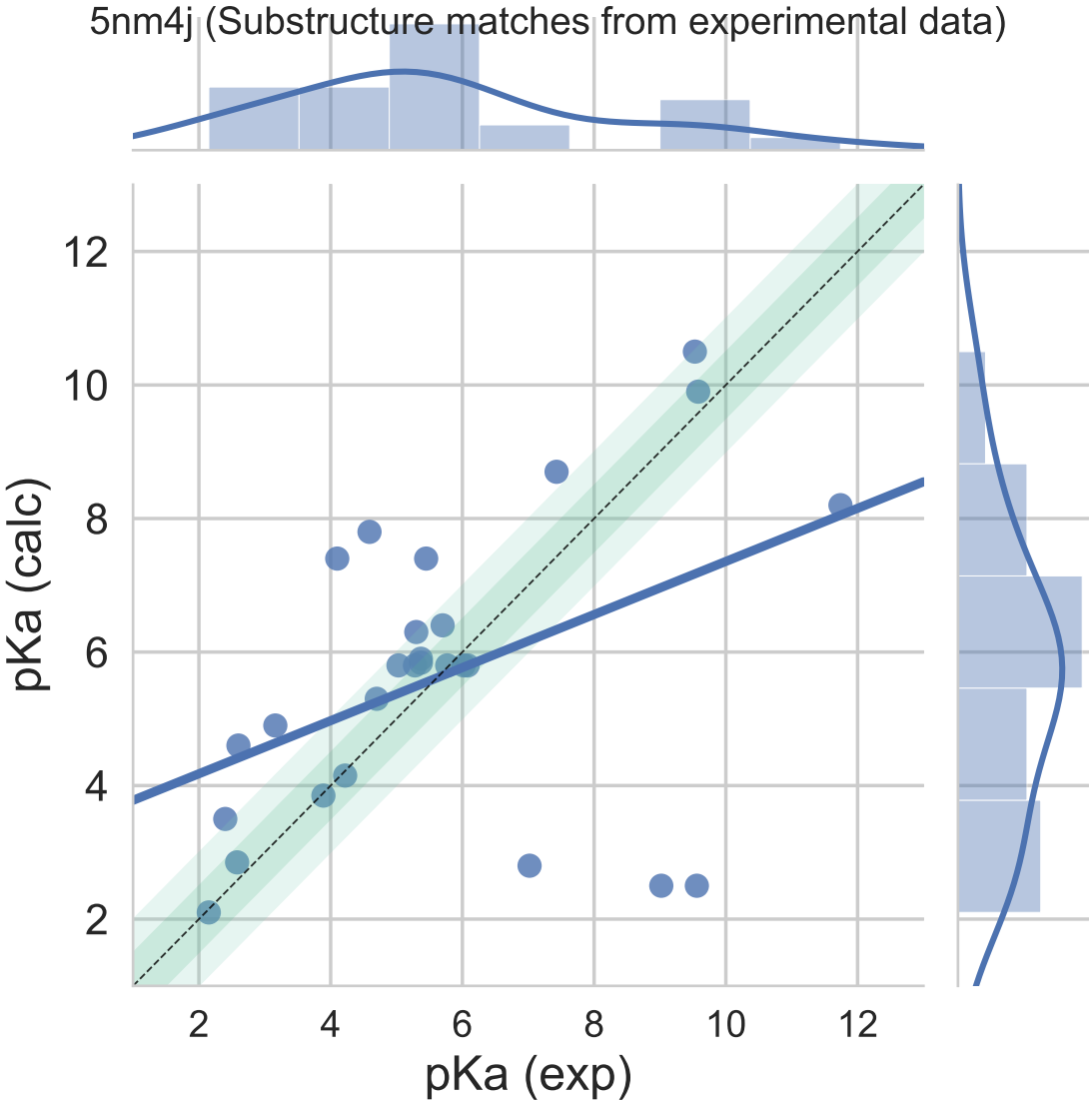
5nm4j (Substructure matches from experimental data)
pKa (calc)
pKa (exp)
2
4
6
8
10
12