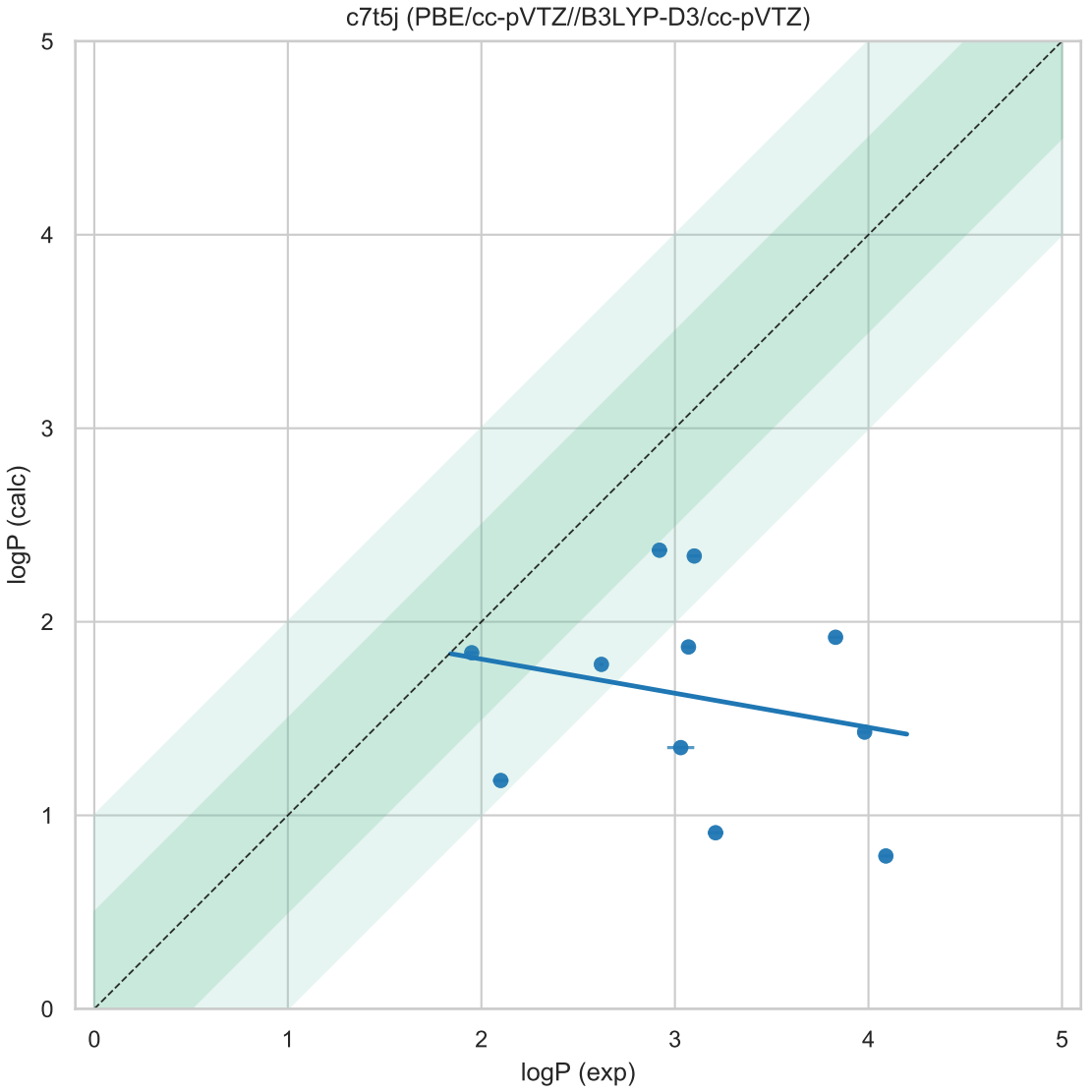
c7t5j (PBE/cc-pVTZ//B3LYP-D3/cc-pVTZ)
logP (calc)
logP (exp)
0
1
2
3
4
5