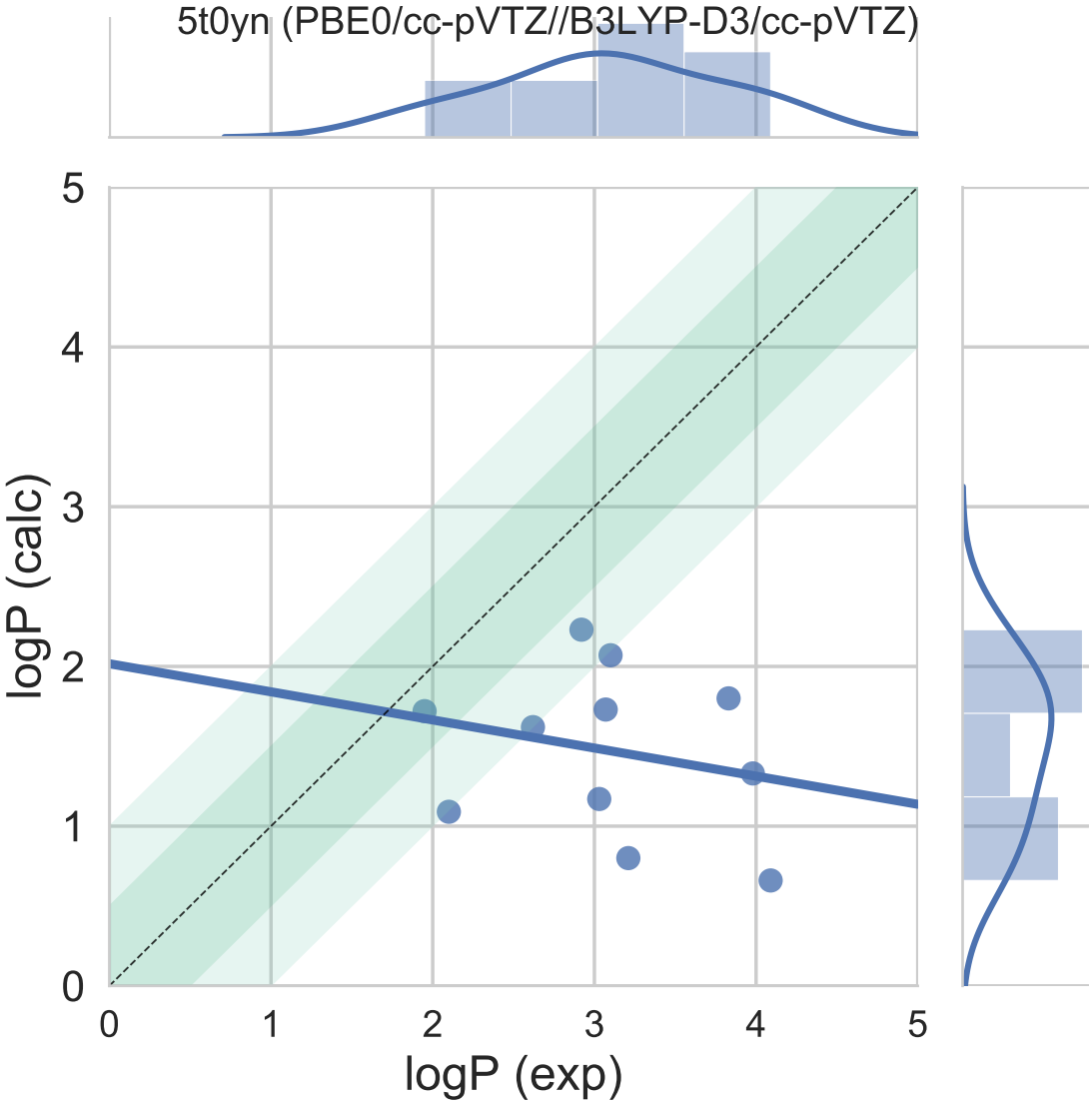
5t0yn (PBE0/cc-pVTZ//B3LYP-D3/cc-pVTZ)
logP (calc)
logP (exp)
0
1
2
3
4
5