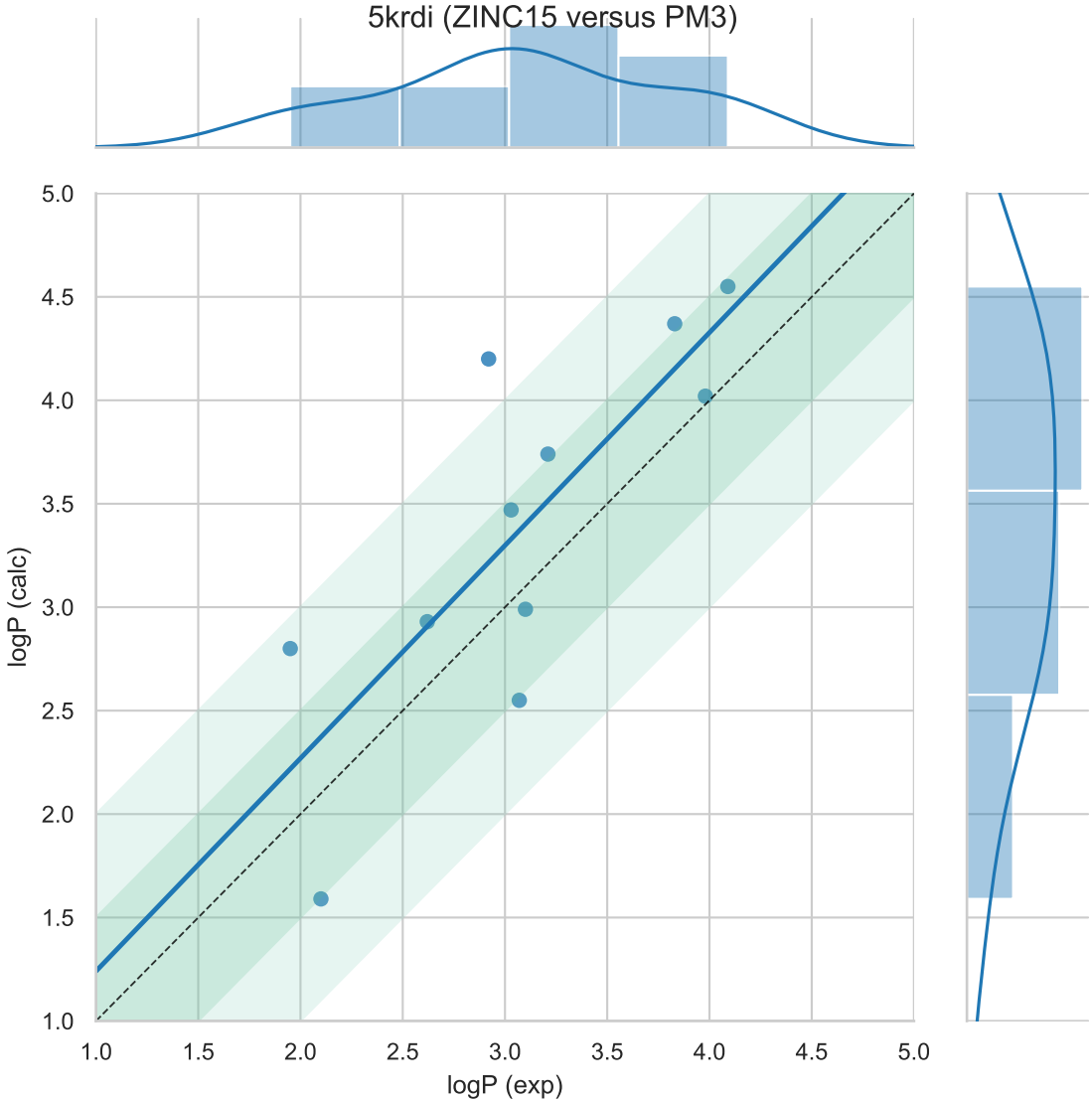
5krdi (ZINC15 versus PM3)
logP (calc)
logP (exp)
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0