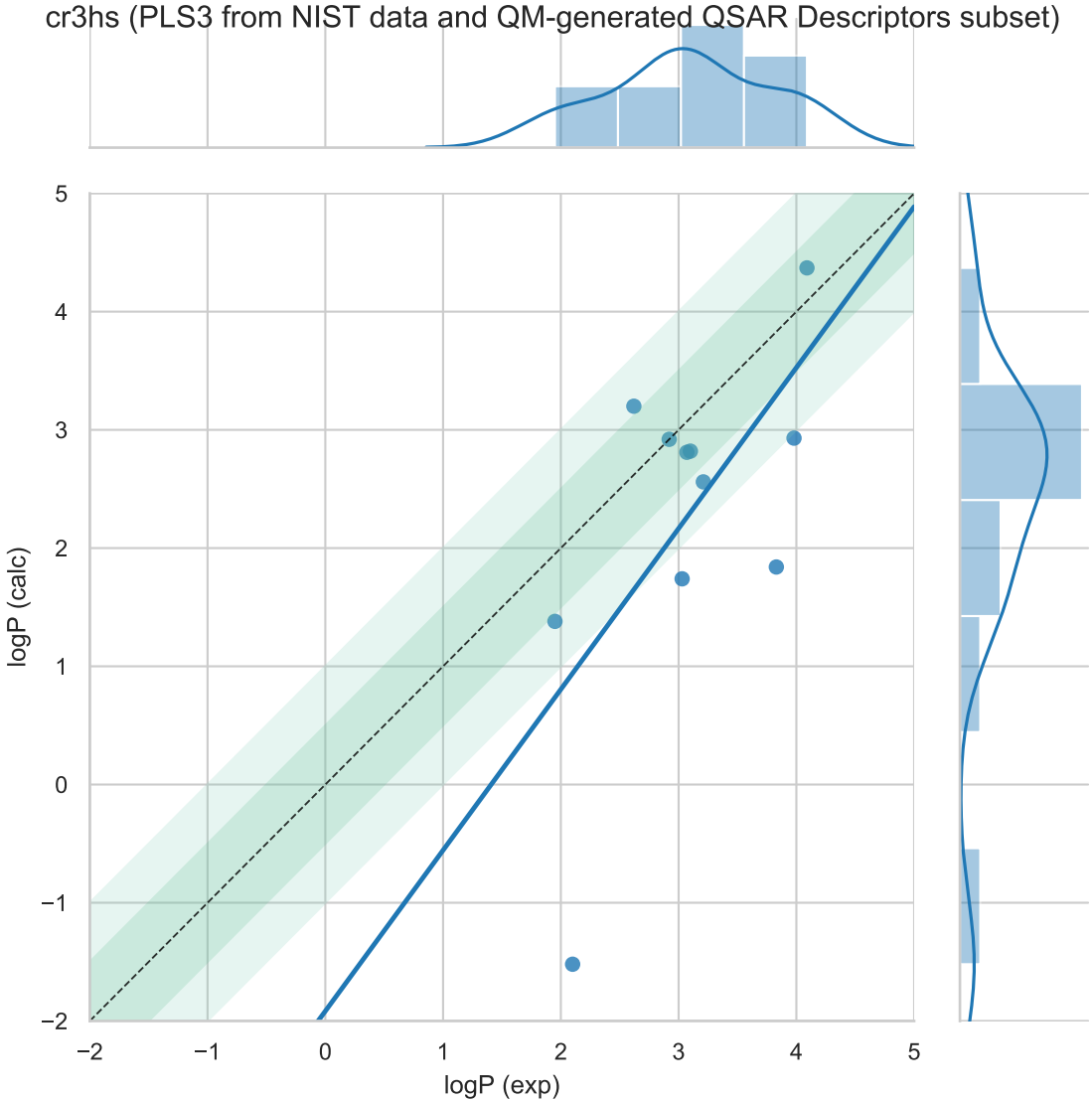
cr3hs (PLS3 from NIST data and QM-generated QSAR Descriptors subset)
logP (calc)
logP (exp)
5
4
3
2
1
0
−1
−2
−2
−1
0
1
2
3
4
5