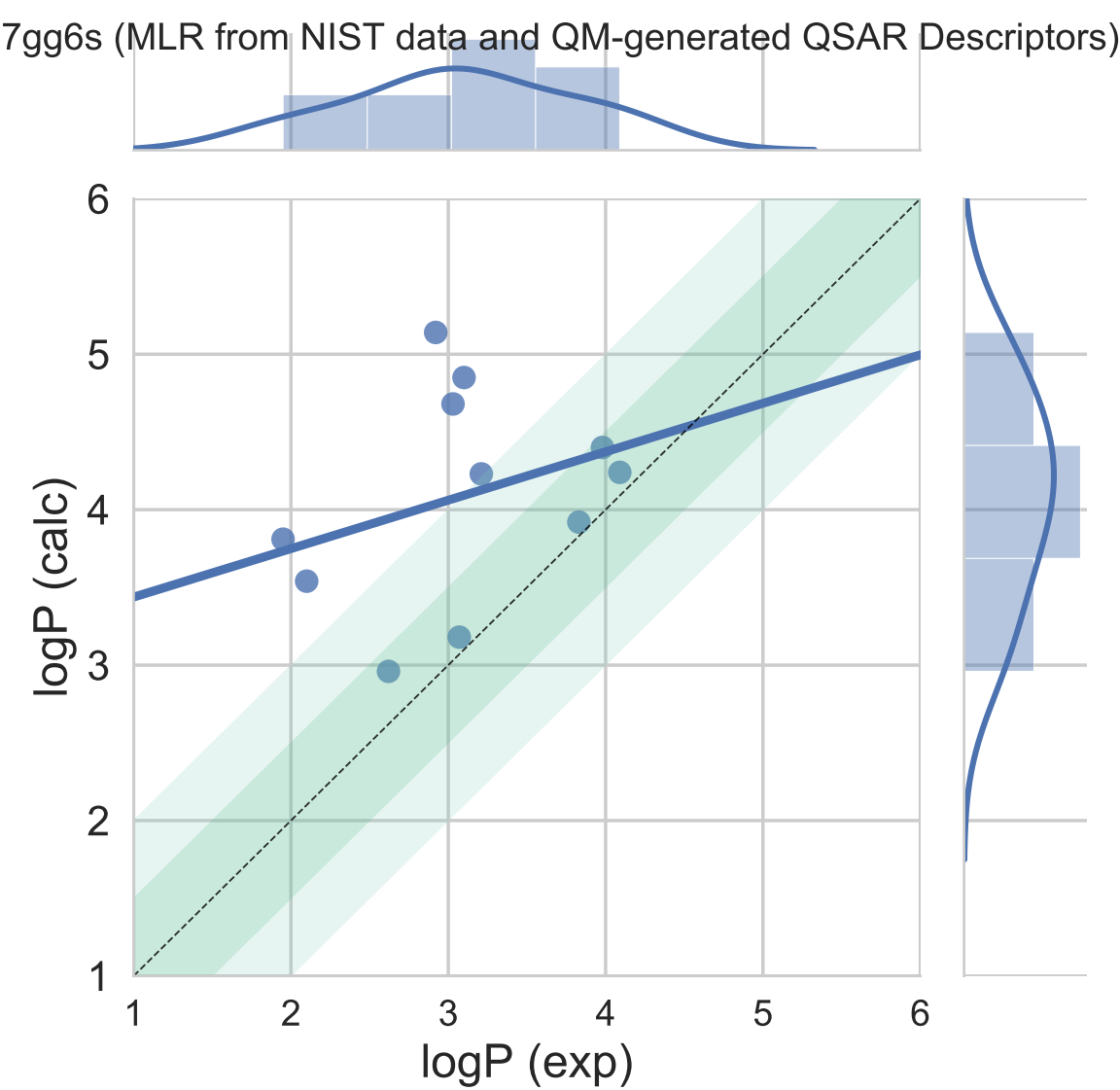
7gg6s (MLR from NIST data and QM-generated QSAR Descriptors)
logP (calc)
logP (exp)
1
2
3
4
5
6