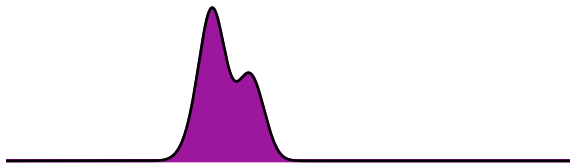


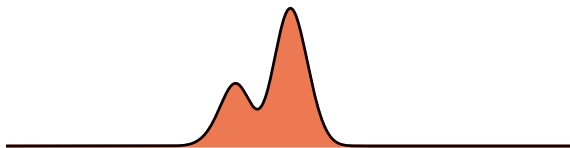
QM



QM+LEC



QSPR/ML



-20

-10

0

10

20

ΔpK_a error (calc - exp)