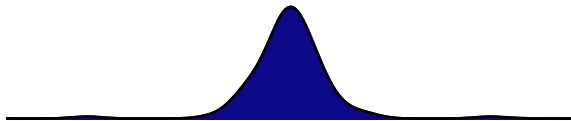
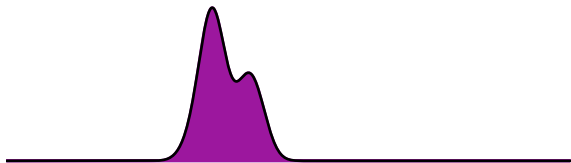


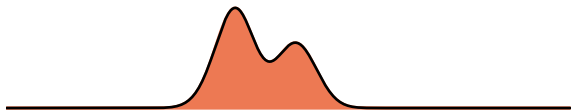
QM



QM+LEC



QSPR/ML



-20

-10

0

10

20

$\Delta pK_a$  error (calc - exp)