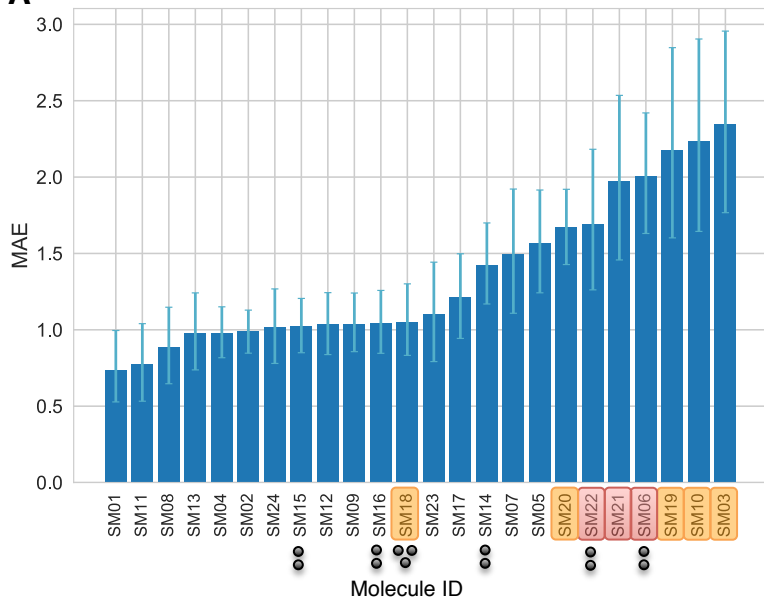
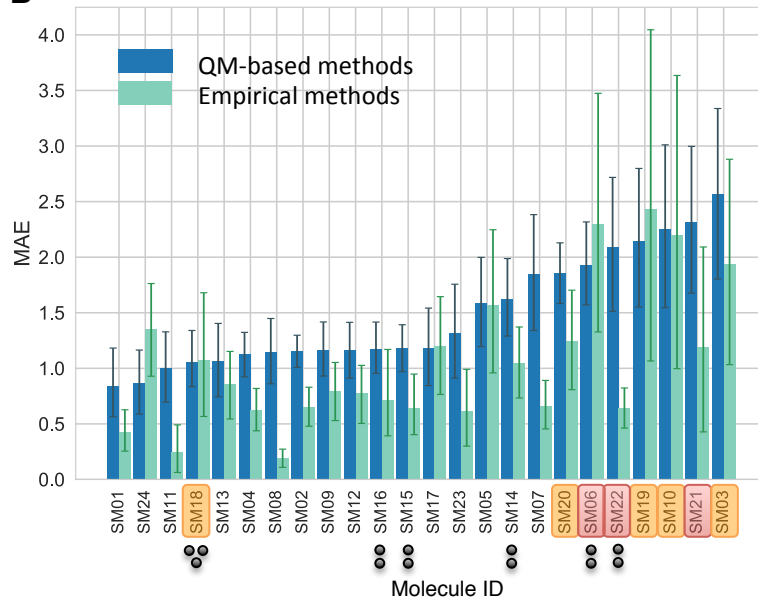
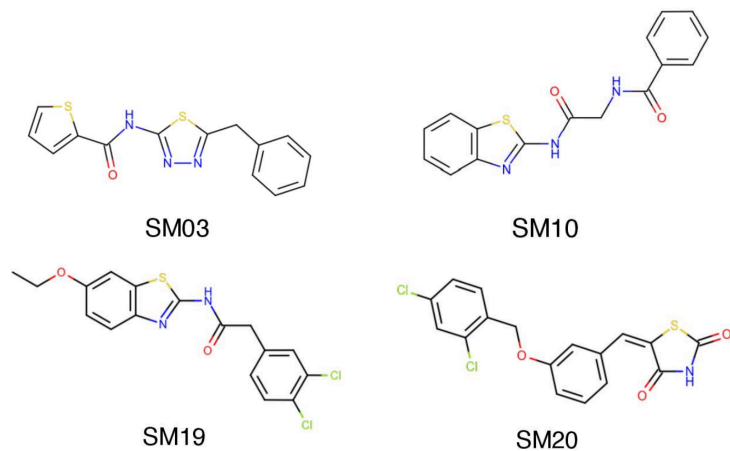


A**B****C** SAMPL6 molecules with sulfur-containing heterocycles
 3 experimental pK_a values

 2 experimental pK_a values

Sulfur-containing heterocycles

Bromo and iodo groups

D SAMPL6 molecules with bromo and iodo groups