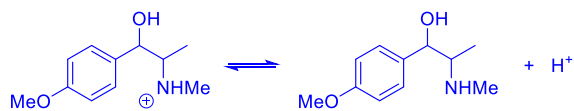
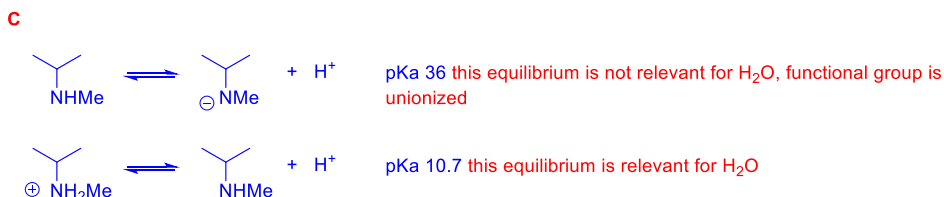
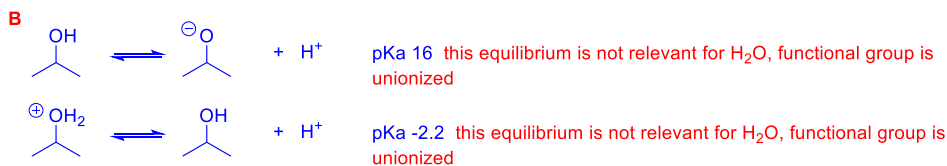
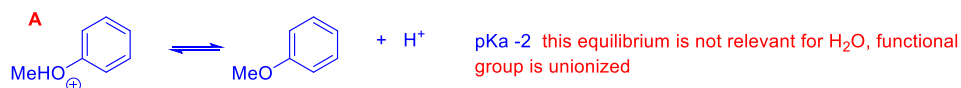
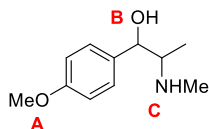


BPS 2110

Assignment 3 Answers Q 13

13. An analytical chemist must make a series of LogP measurements as part of the ADME effort at a major pharmaceutical company. For each of the molecules shown, predict the approximate pH at which each measurement should be made.

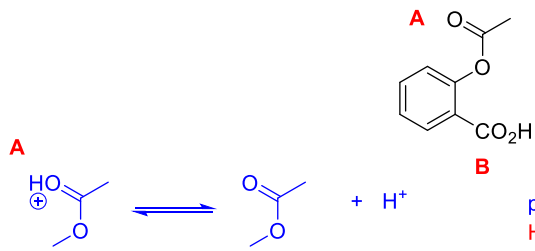


molecule is in this form when pH < 10.7

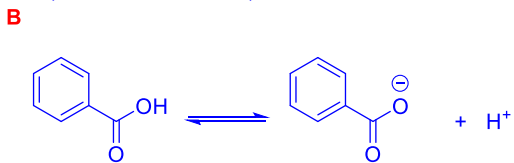
molecule is in this form when pH > 10.7

for LogP, Make the measurements at pH greater than 10.7

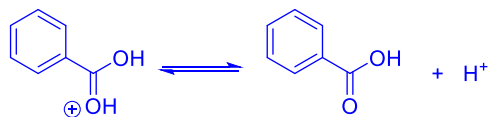
a.



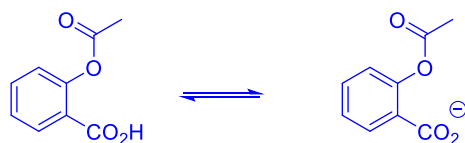
pKa -7.8 this equilibrium is not relevant for H₂O, functional group is unionized



pKa 4.2 this equilibrium is relevant for H₂O



pKa -7.8 this equilibrium is not relevant for H₂O, functional group is unionized

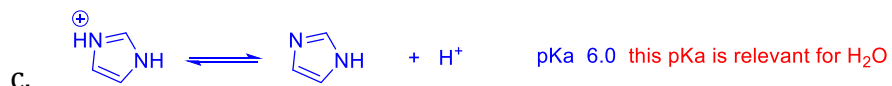
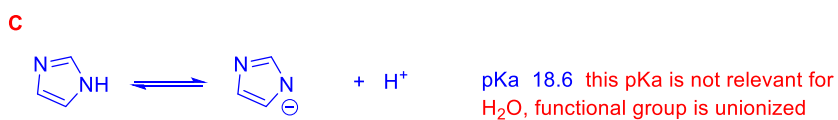
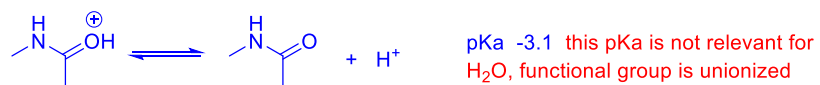
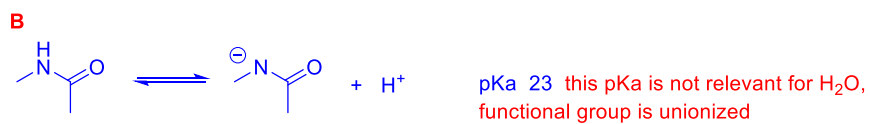
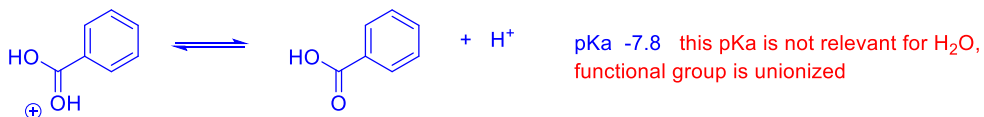
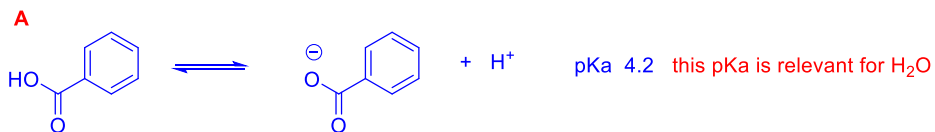
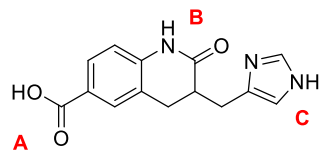


molecule is in this form when pH < 4.2

molecule is in this form when pH > 4.2

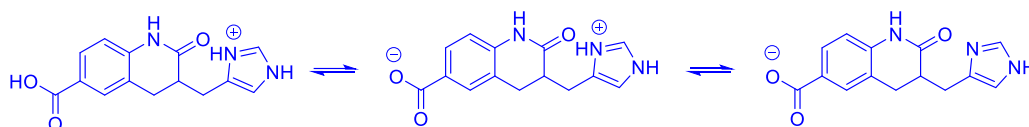
b.

measure LogP at pH less than 4.2



molecule will be in this form at pH < 4.2

molecule will be in this form at pH > 6.0



molecule will be in this form when pH is between 4.2 and 6.0
the overall charge on this form is 0
measure LogP when pH is between 4.2 and 6.0