Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting Information

Thermodynamics-informed calculation and blind prediction of apparent pK_a values submitted to the euroSAMPL 1 challenge

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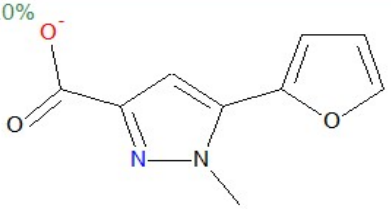
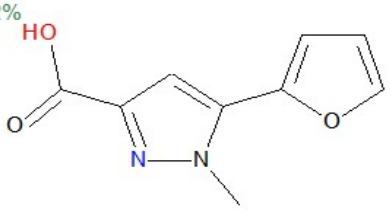
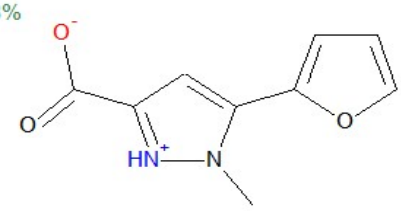
Detailed microscopic ionization patterns for each of the 35 euroSAMPL compounds. The first column contains S+pKa predicted macroscopic pK_a values. The corresponding macrostate transitions are in the second columns. Third column contains structures of all microstates with relative contributions to their respective macrostates in %. The latter are determined from Boltzmann distribution of microstates relative to each macrostate.

euroSAMPL-01

pKa	Macrostates	Microstates
	M^-	100.0% 
3.50		
	HM	99.2%  0.8% 
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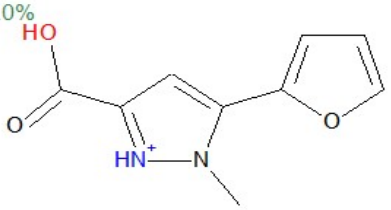
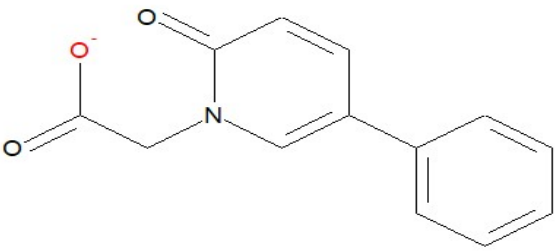
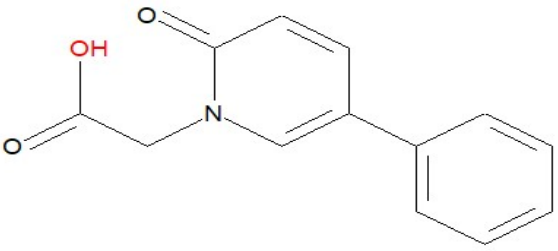
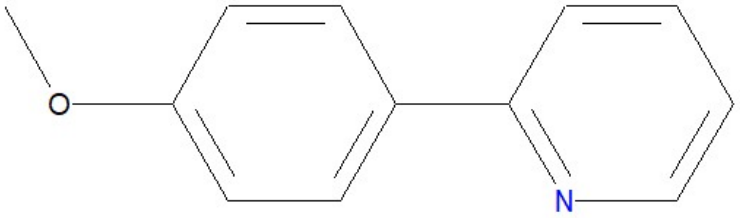
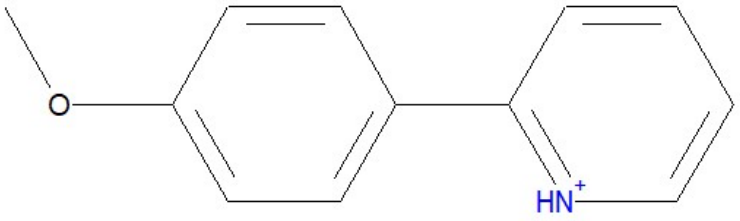
	H_2M^+	100.0% 

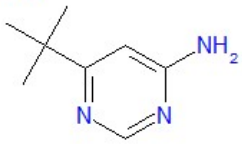
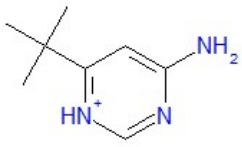
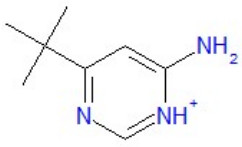
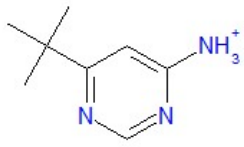
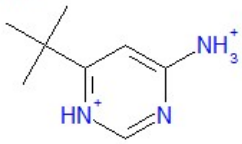
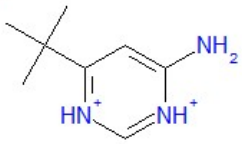
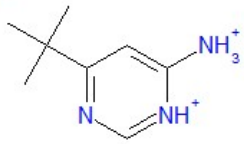
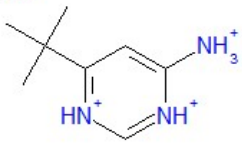
euroSAMPL-02

pKa	Macrostates	Microstates
	M^-	100.0% 
3.49		
	HM	100.0% 

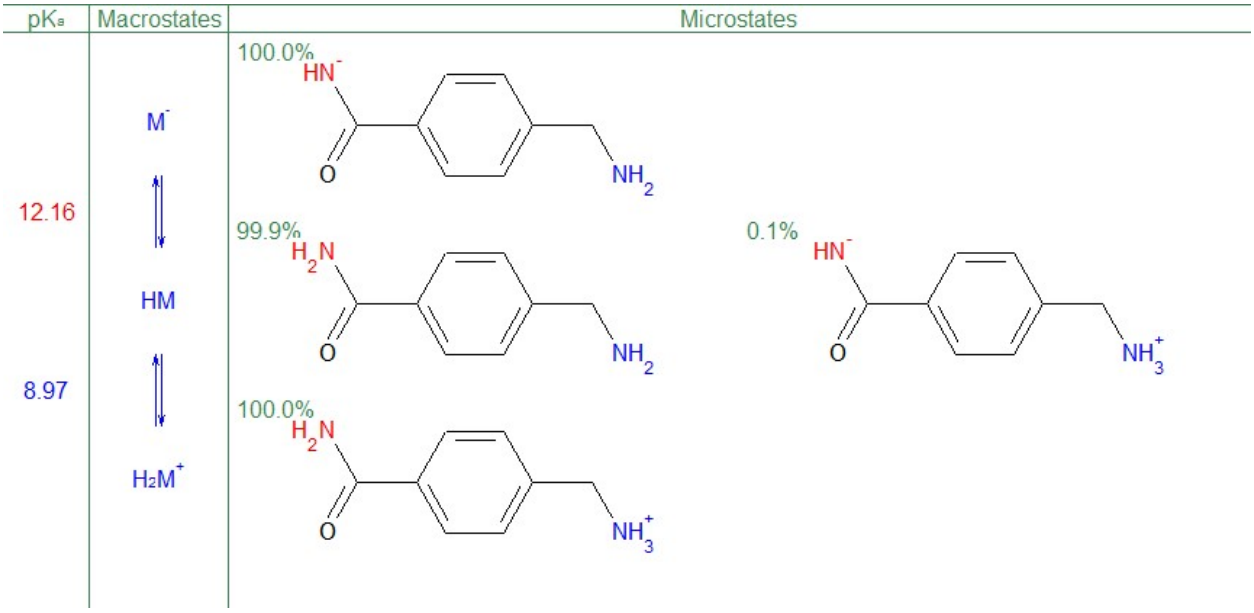
euroSAMPL-03

pKa	Macrostates	Microstates
	M	100.0% 
5.13	⇕	
	HM^+	100.0% 

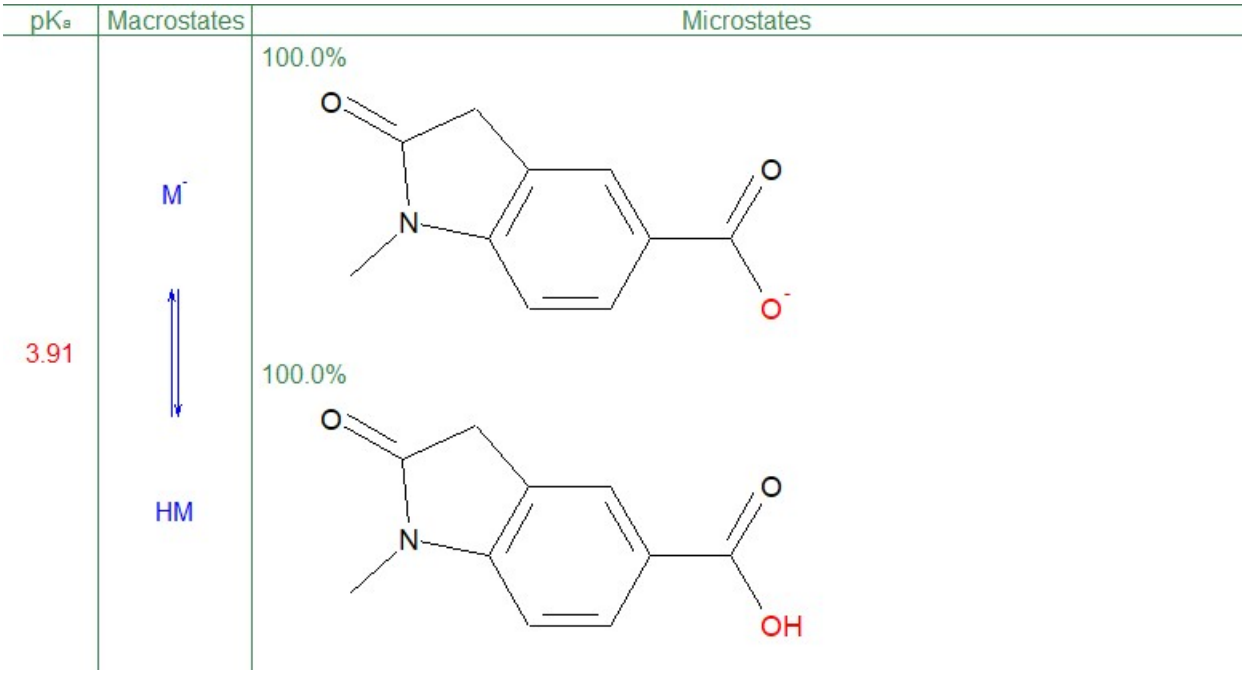
euroSAMPL-04

pKa	Macrostates	Microstates		
	M	100.0% 		
6.54	⇕			
	HM^+	99.8% 	0.2% 	0.0% 
-1.09	⇕			
	H_2M^{+2}	100.0% 	0.0% 	0.0% 
-7.72	⇕			
	H_3M^{+3}	100.0% 		

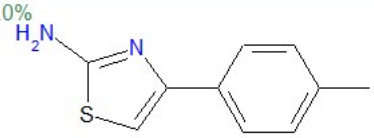
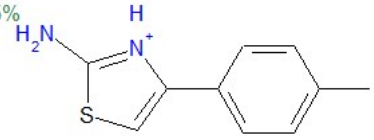
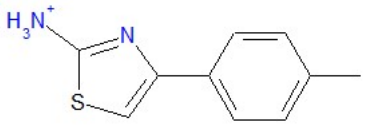
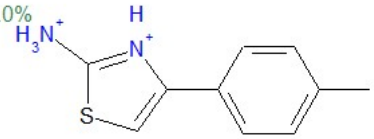
euroSAMPL-05



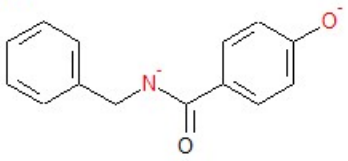
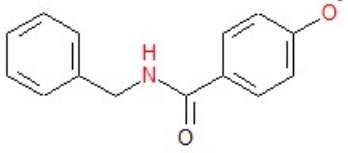
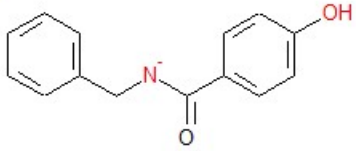
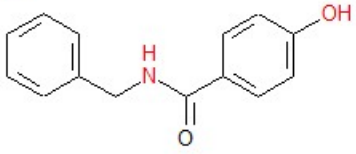
euroSAMPL-06



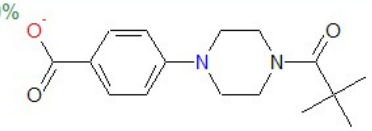
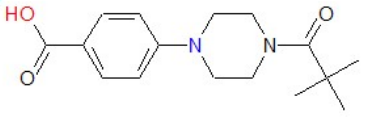
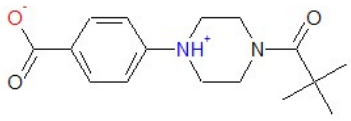
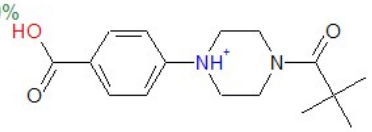
euroSAMPL-07

pKa	Macrostates	Microstates
	M	100.0% 
4.68	⇕	
	HM^+	99.5%  0.5% 
-0.54	⇕	
	H_2M^{+2}	100.0% 

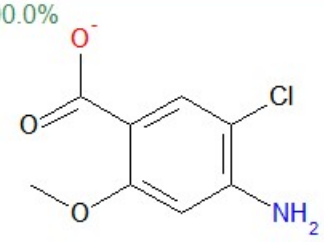
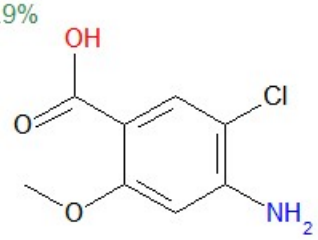
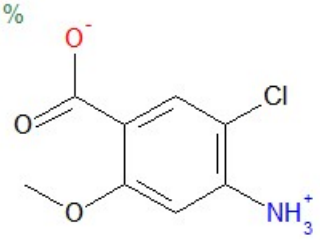
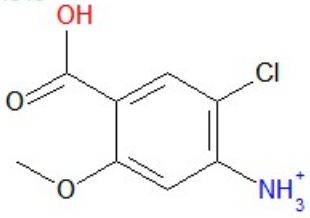
euroSAMPL-08

pKa	Macrostates	Microstates
	M^{-2}	100.0% 
11.65	⇕	
	HM^-	99.6%  0.4% 
8.91	⇕	
	H_2M	100.0% 

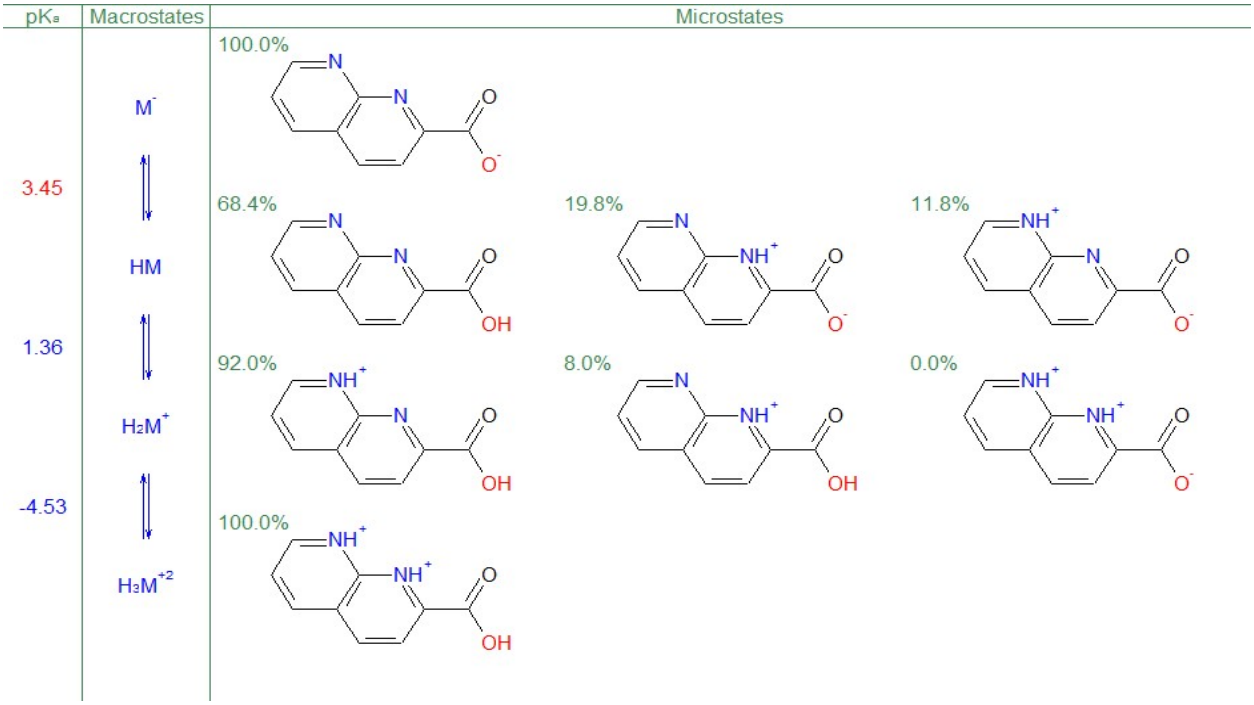
euroSAMPL-09

pKa	Macrostates	Microstates
	M^-	100.0% 
4.41		
	HM	95.0%  5.0% 
2.62		
	H_2M^+	100.0% 

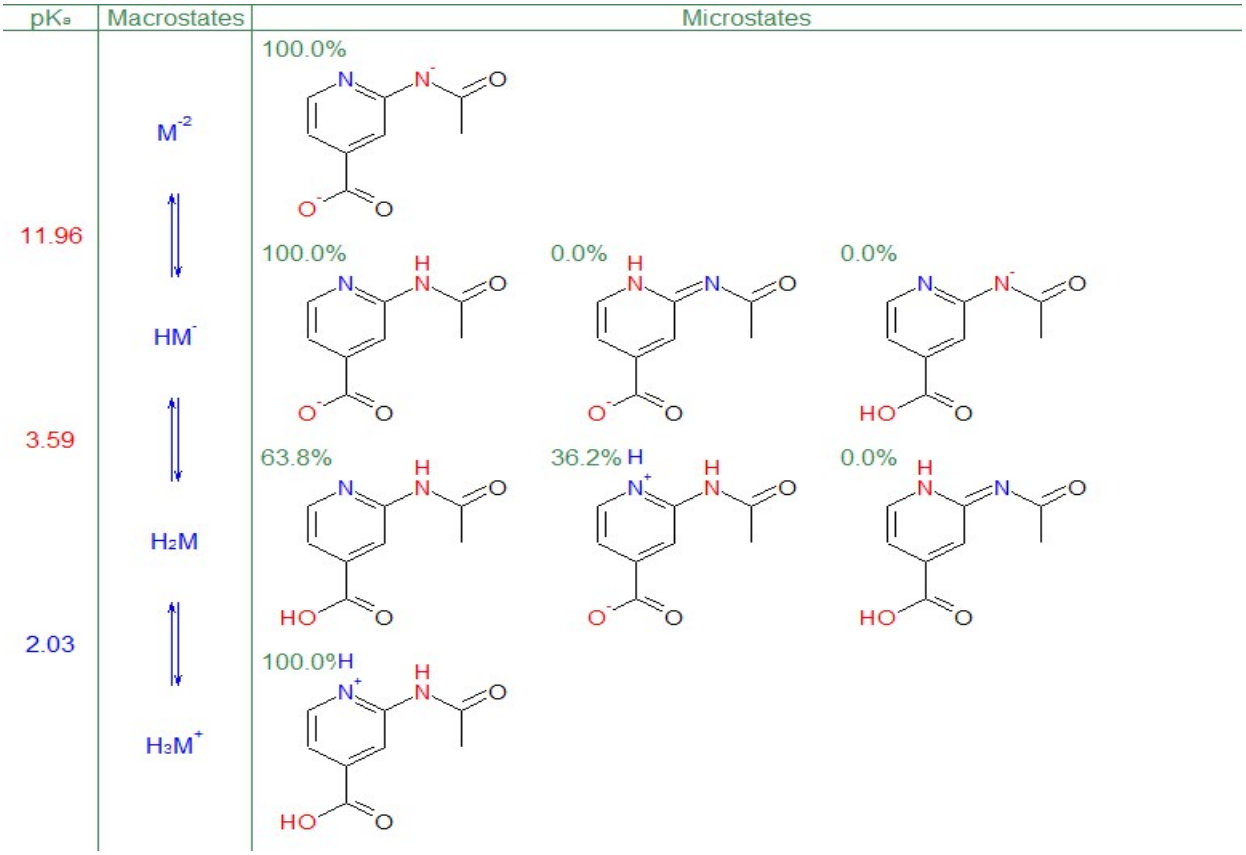
euroSAMPL-10

pKa	Macrostates	Microstates
	M^-	100.0% 
4.84		
	HM	99.9%  0.1% 
1.18		
	H_2M^+	100.0% 

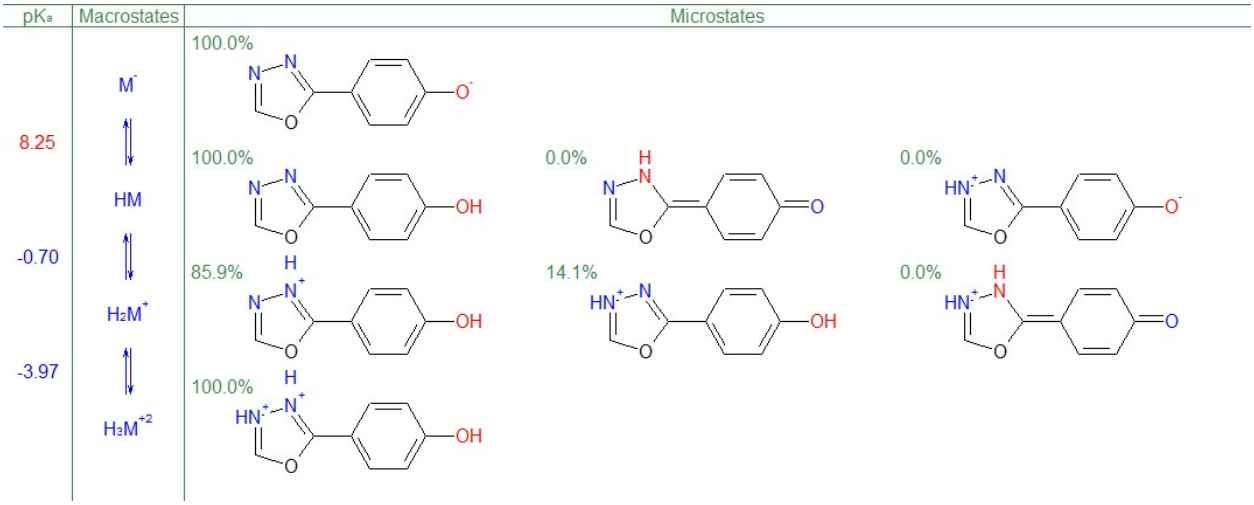
euroSAMPL-11



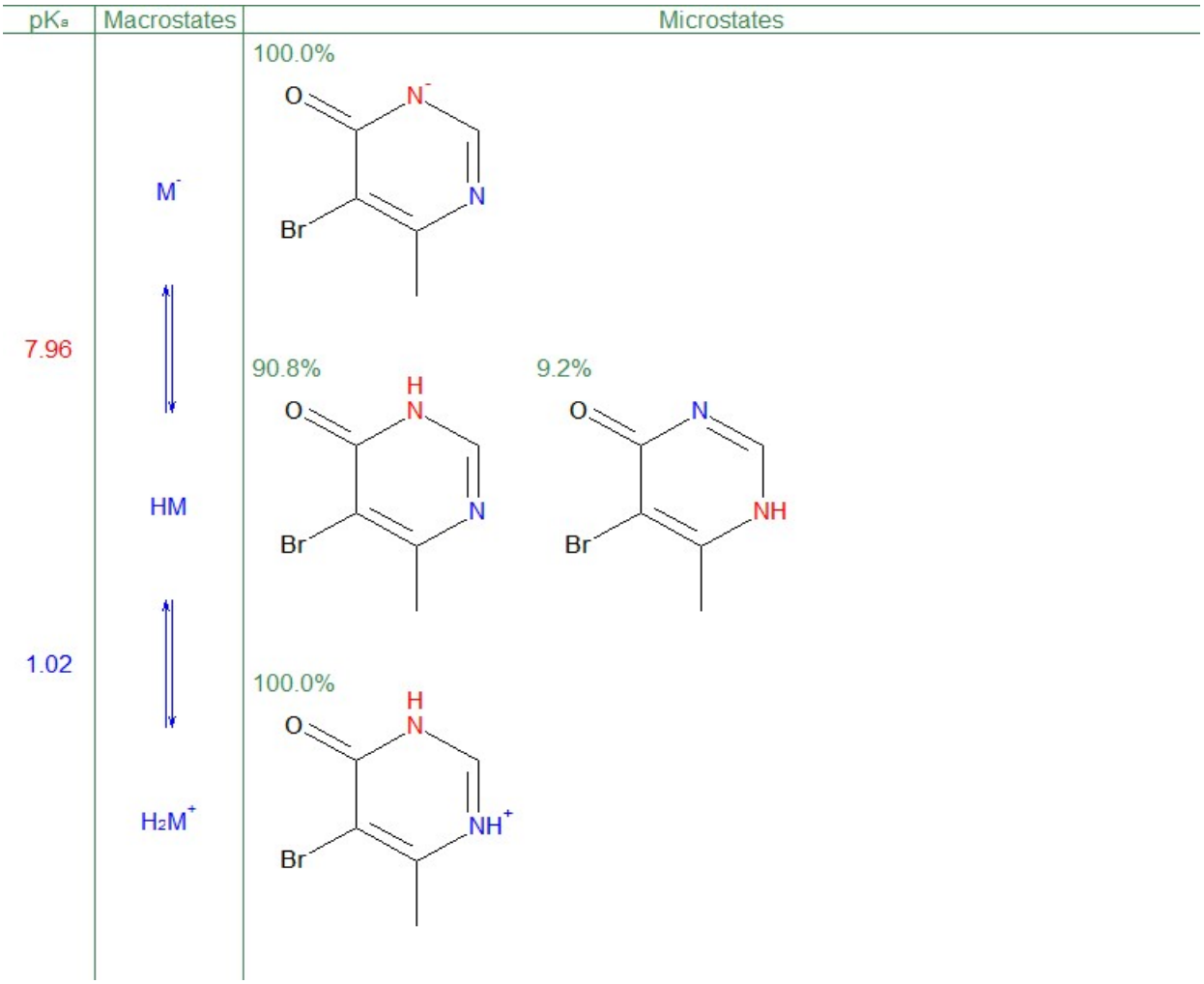
euroSAMPL-12



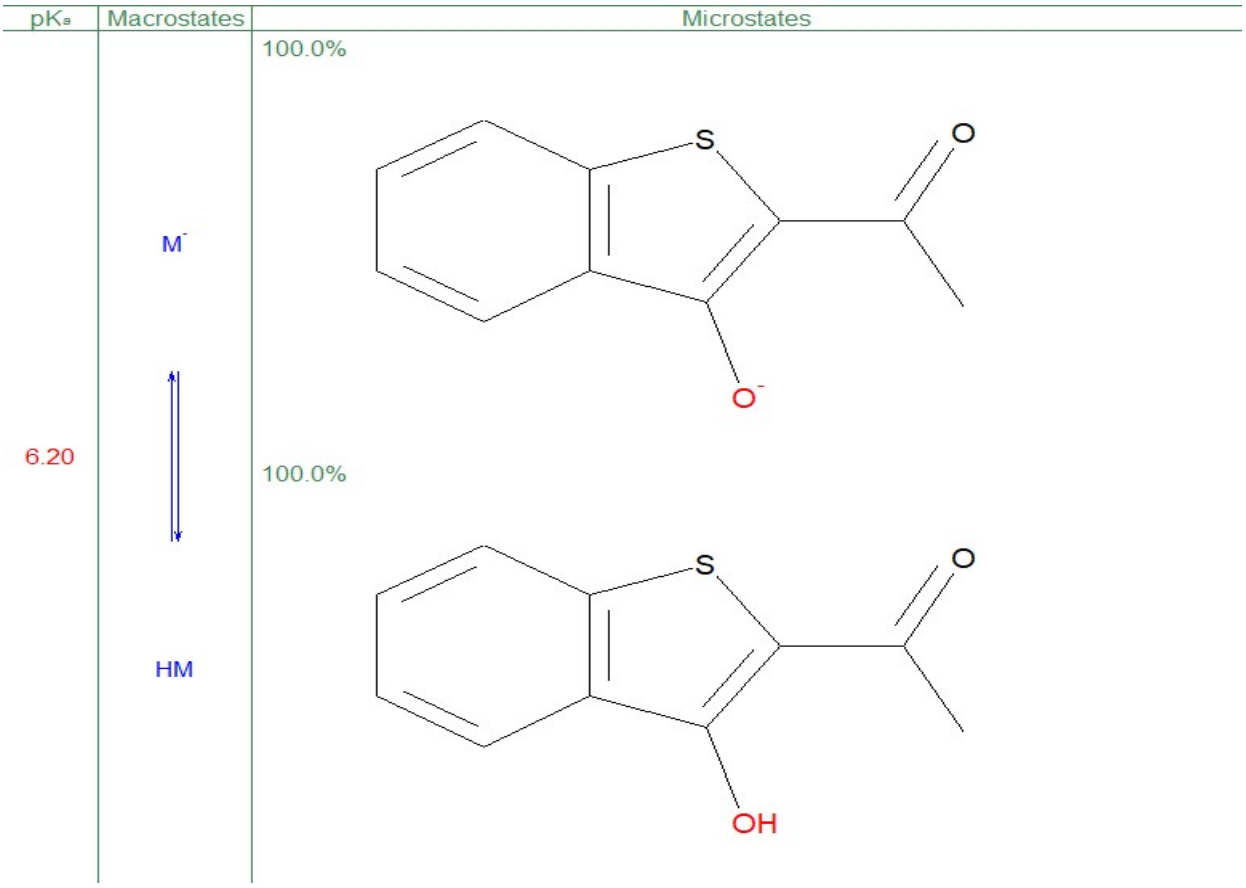
euroSAMPL-13



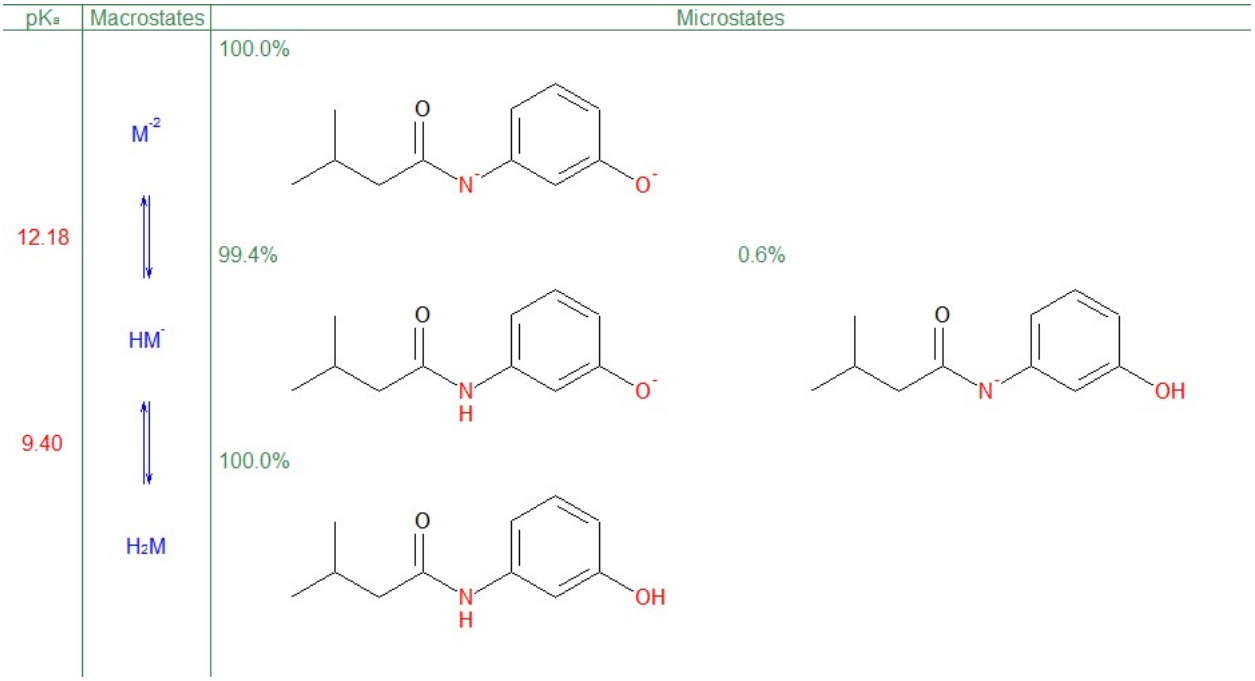
euroSAMPL-14



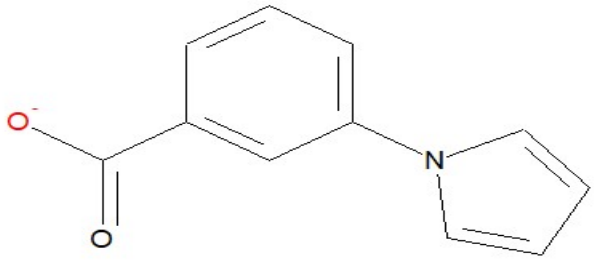
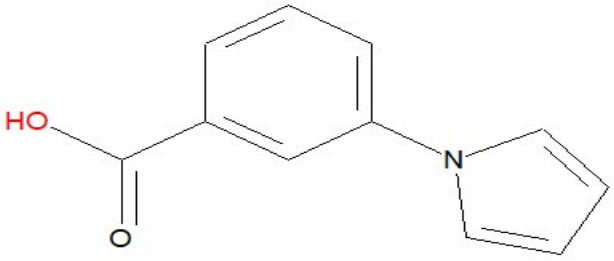
euroSAMPL-15



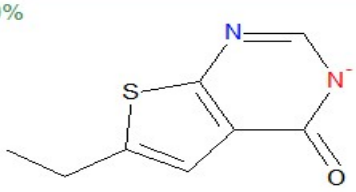
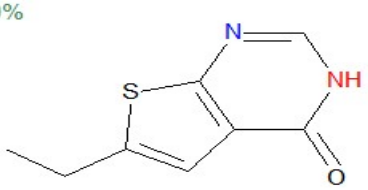
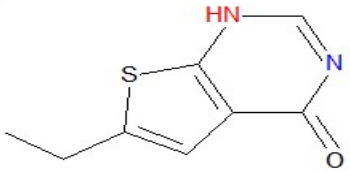
euroSAMPL-16



euroSAMPL-17

pKa	Macrostates	Microstates
	M^-	100.0% 
3.83		
	HM	100.0% 

euroSAMPL-18

pKa	Macrostates	Microstates
	M^-	100.0% 
9.46		
	HM	100.0%  0.0% 
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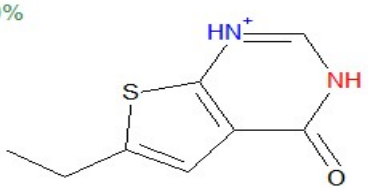
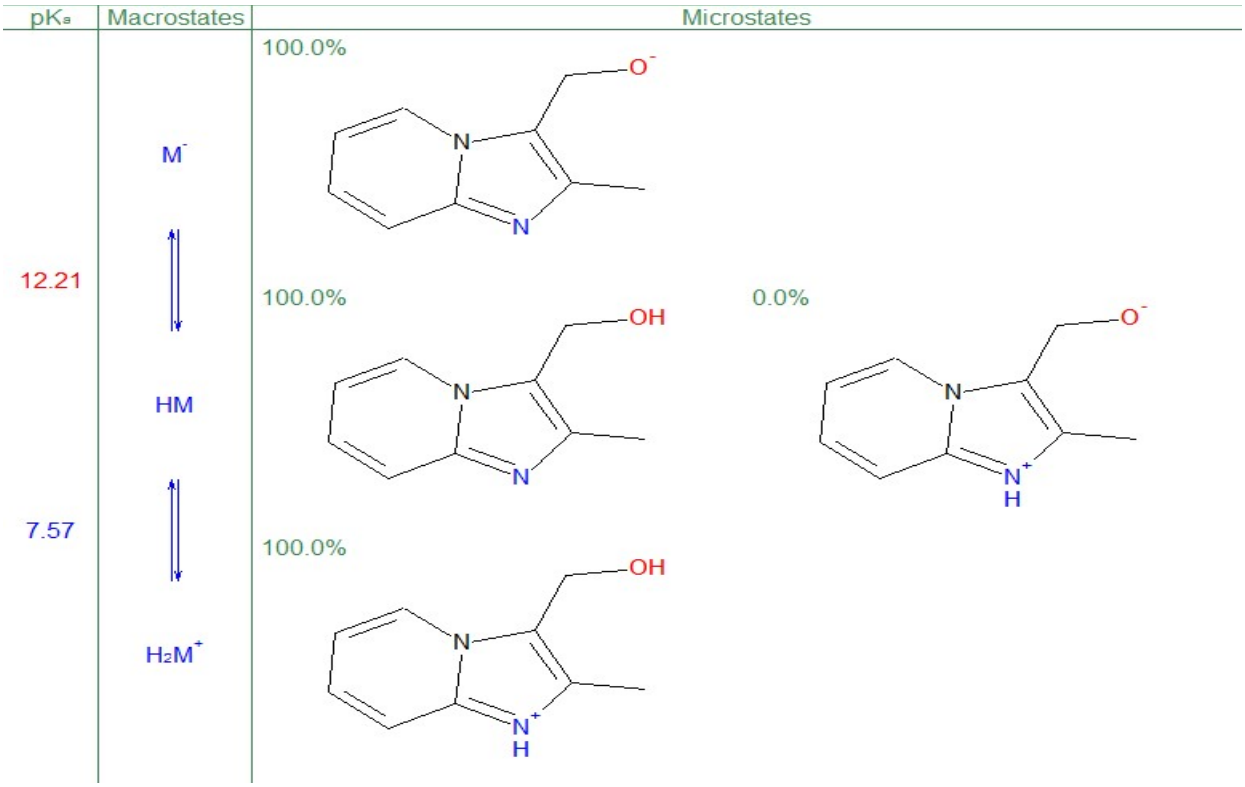
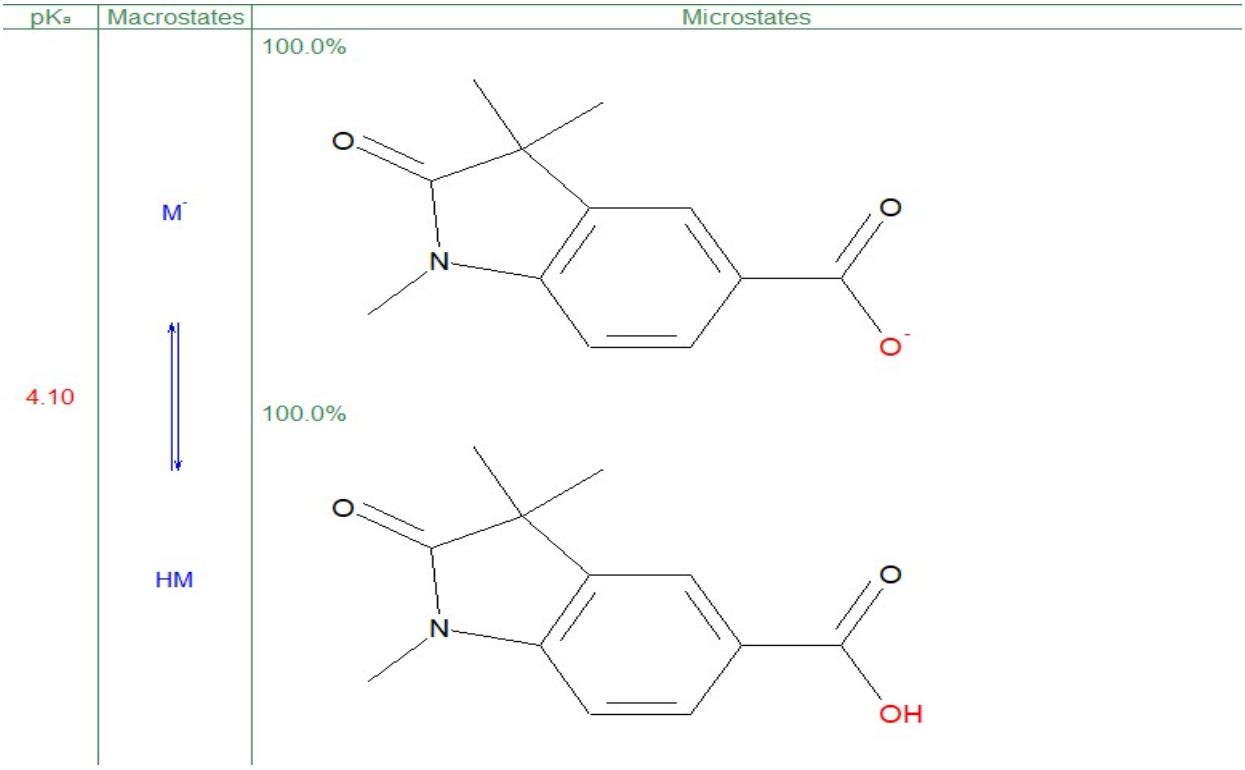
	H_2M^+	100.0% 

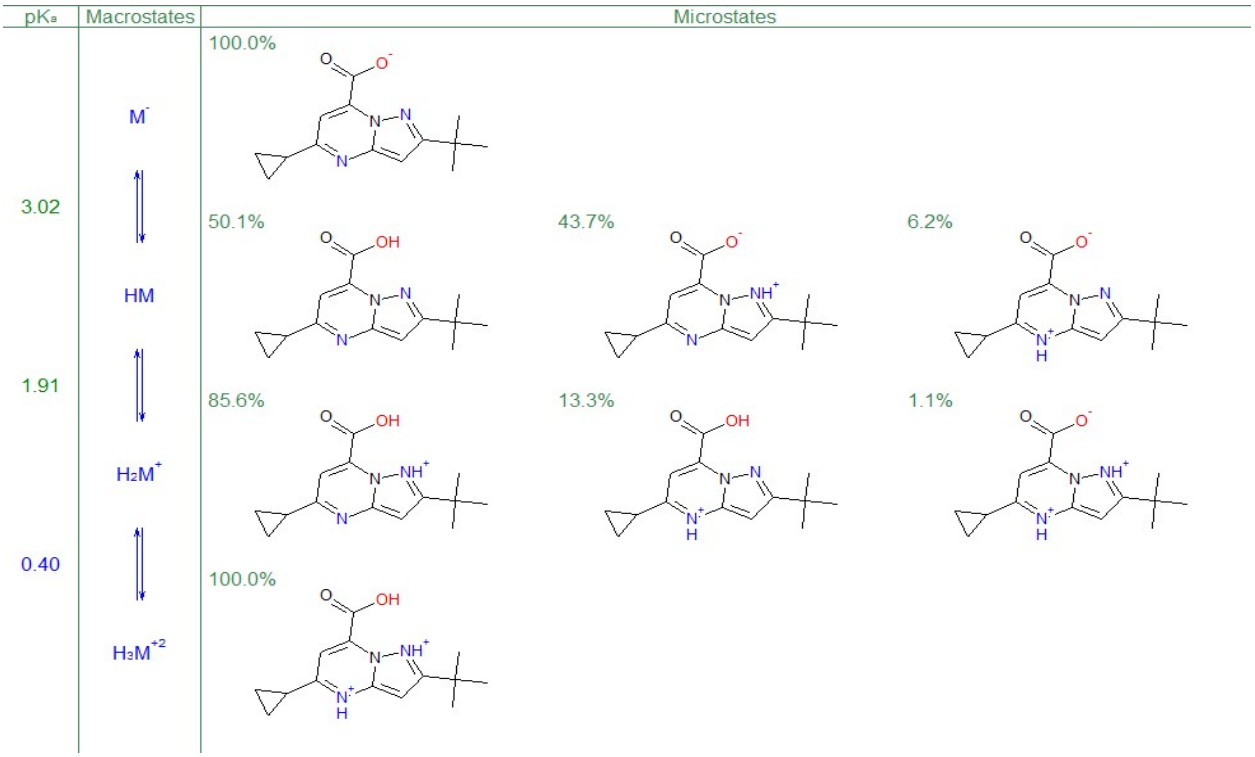
euroSAMPL-19



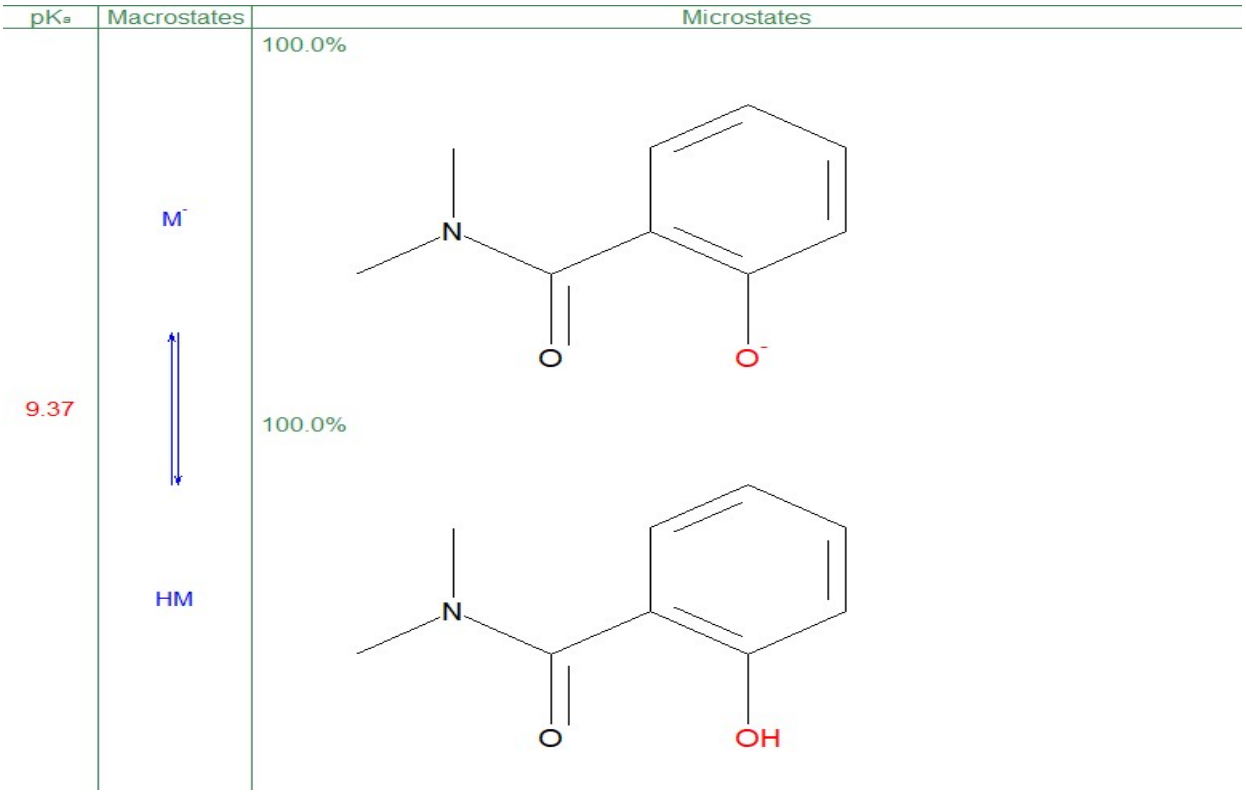
euroSAMPL-20



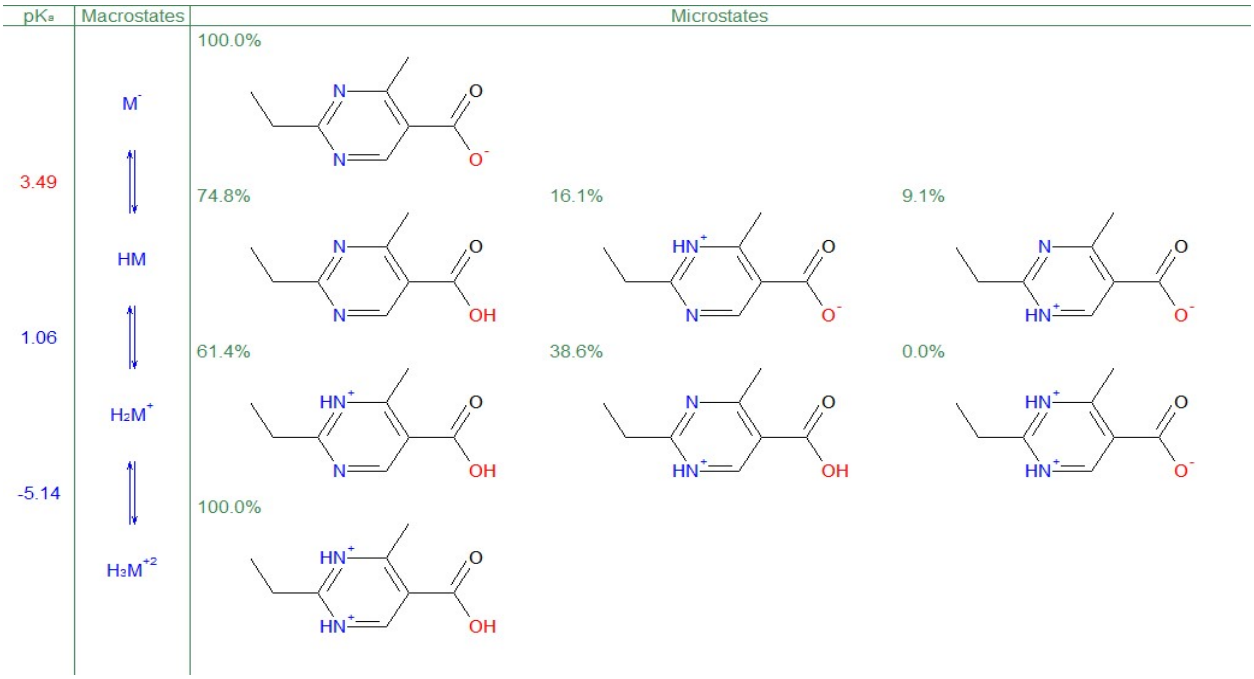
euroSAMPL-21



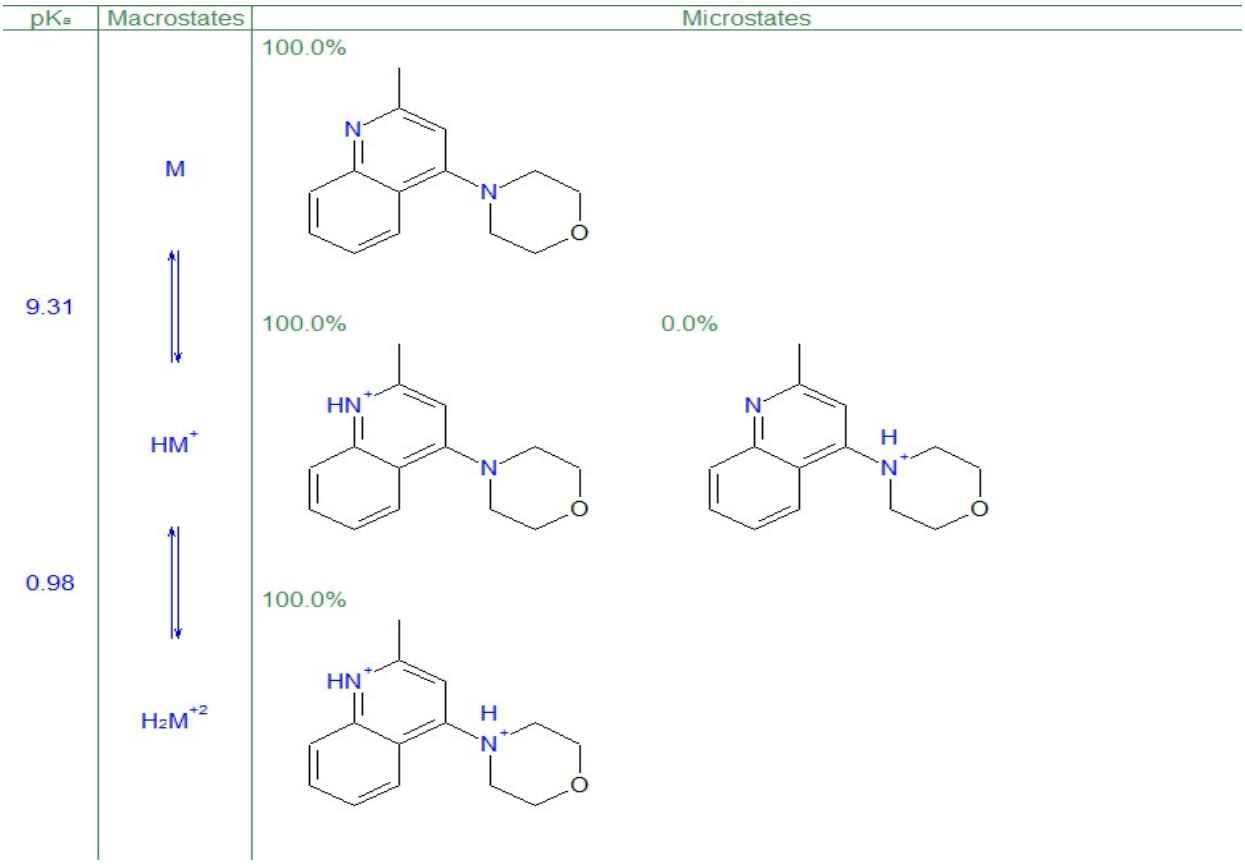
euroSAMPL-22



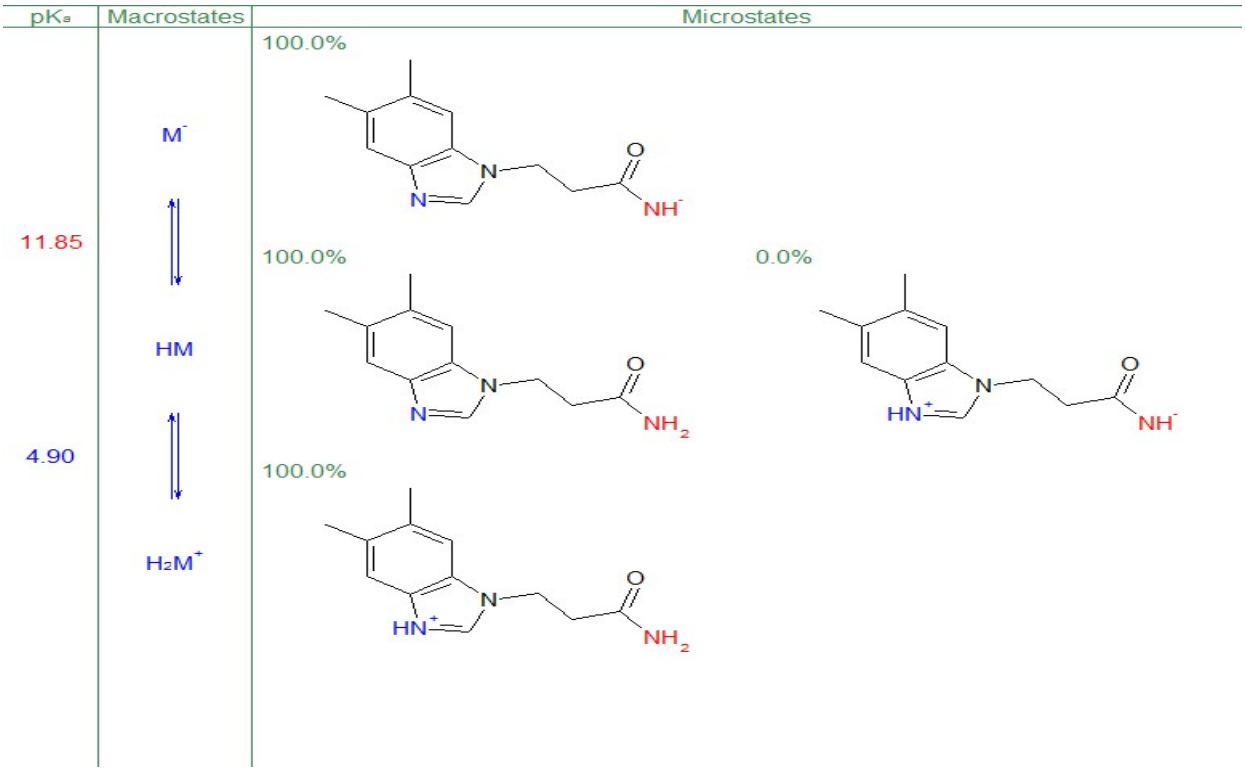
euroSAMPL-23



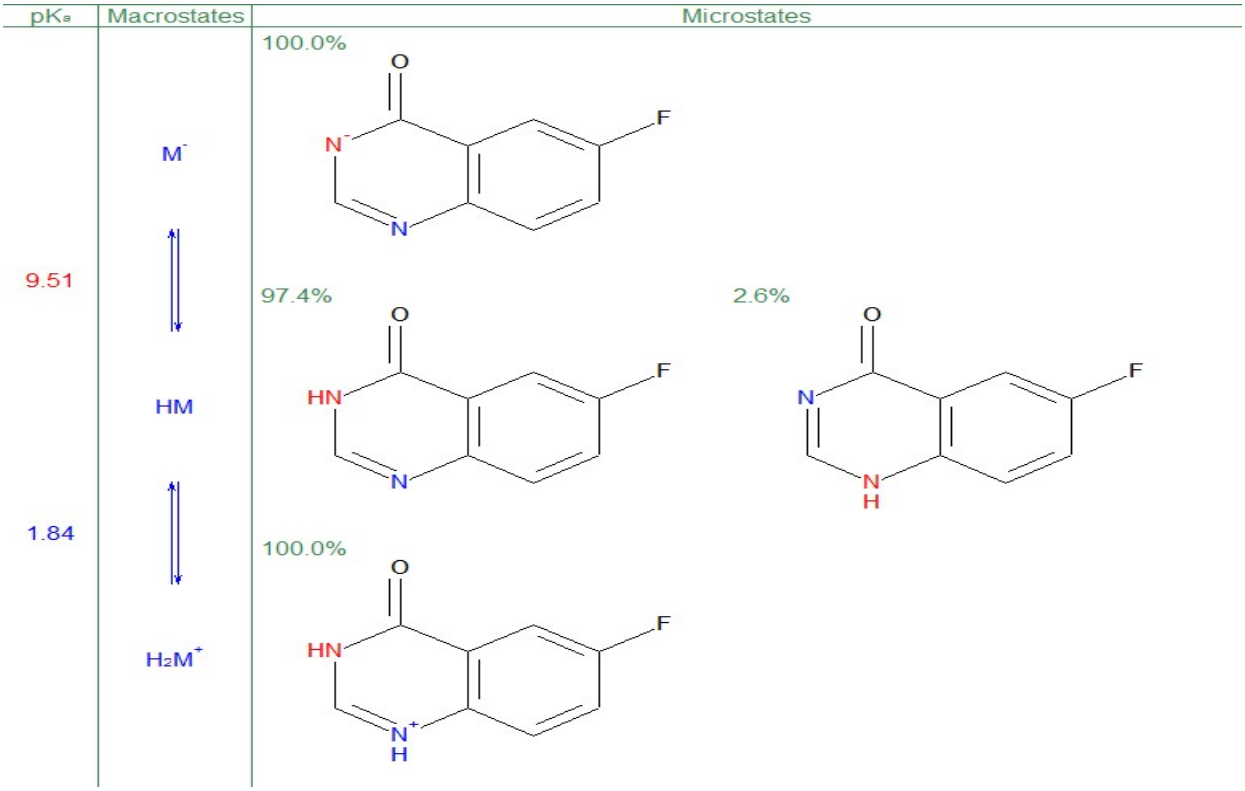
euroSAMPL-24



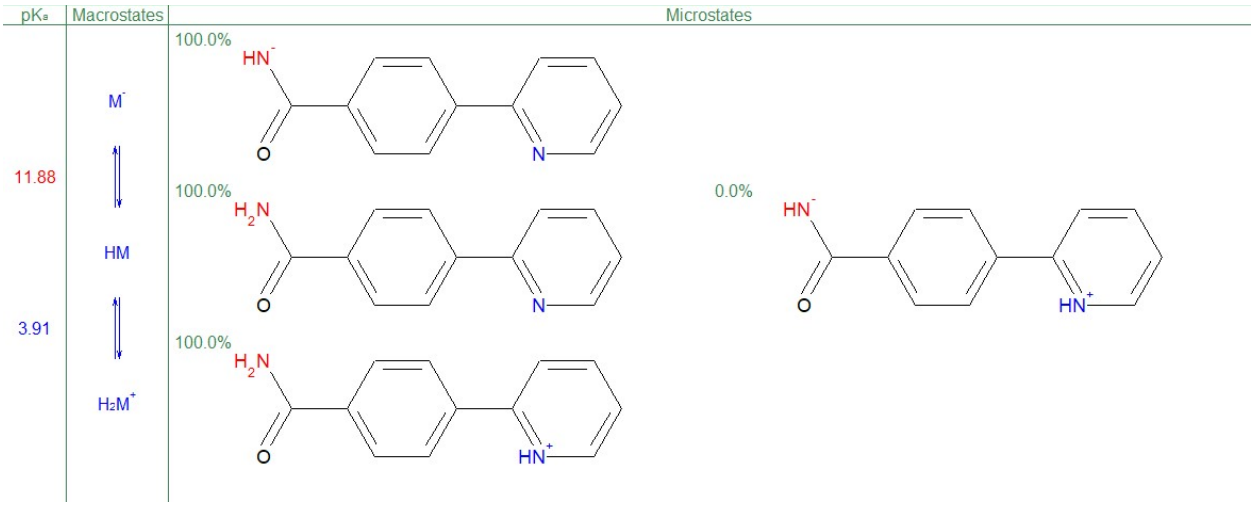
euroSAMPL-25



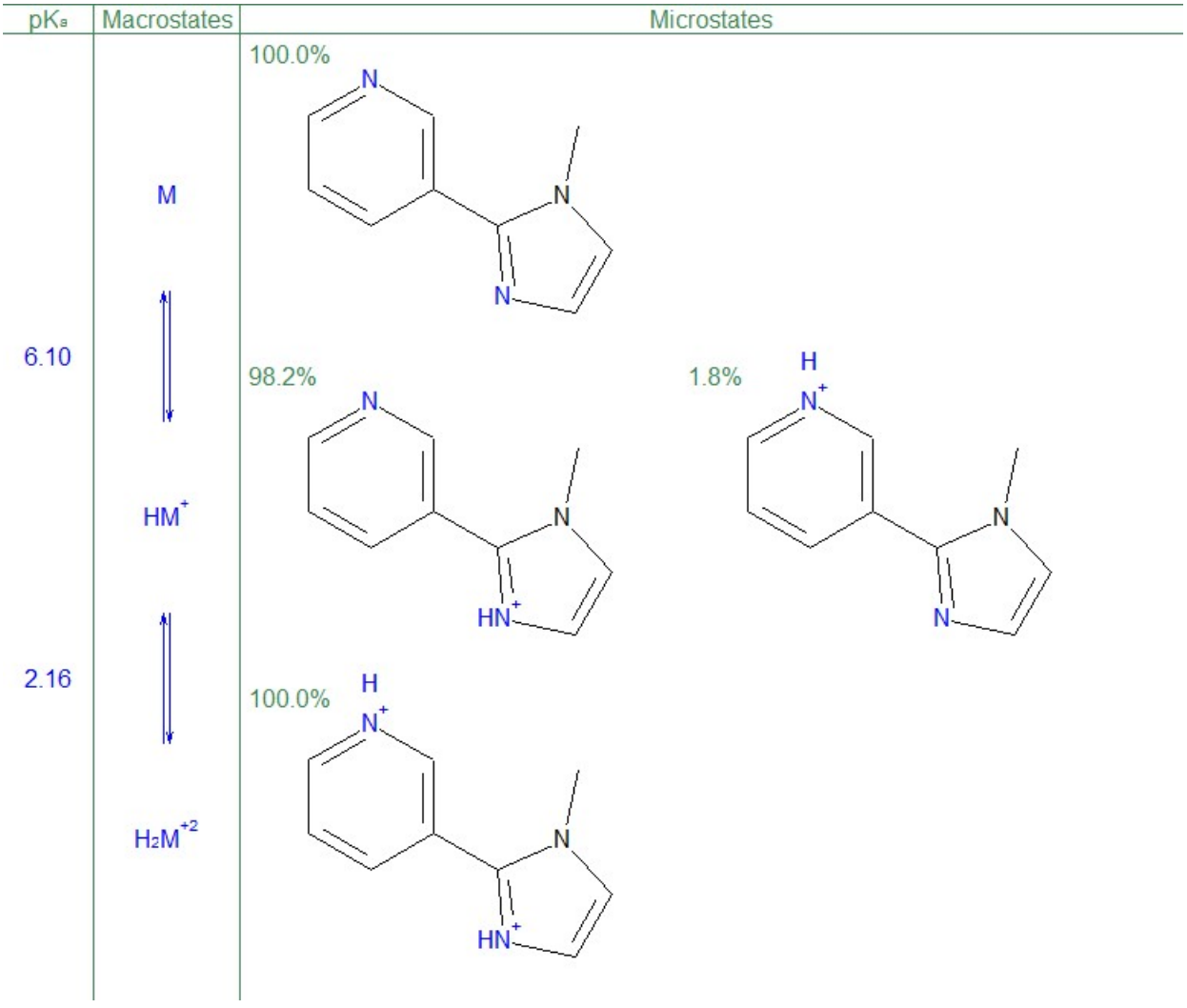
euroSAMPL-26



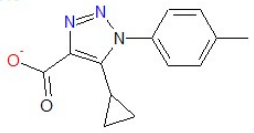
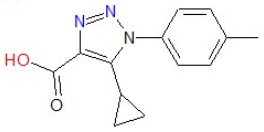
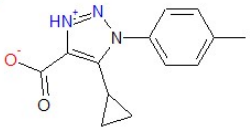
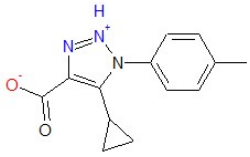
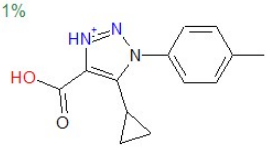
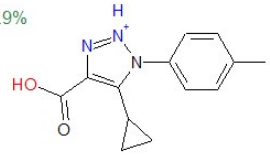
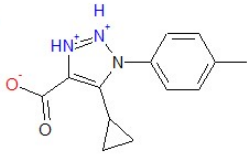
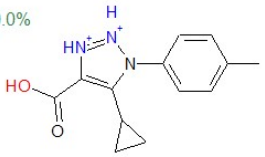
euroSAMPL-27



euroSAMPL-28



euroSAMPL-29

pKa	Macrostates	Microstates		
	M^-	100.0% 		
3.63				
	HM	99.8% 	0.2% 	0.0% 
-0.19				
	H_2M^+	66.1% 	33.9% 	0.0% 
-2.12				
	H_3M^{+2}	100.0% 		

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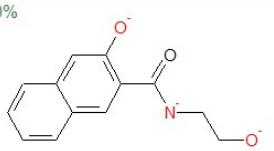
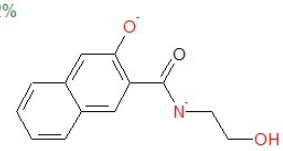
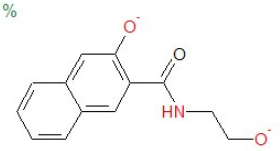
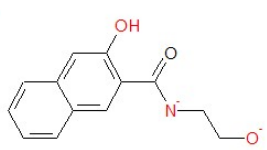
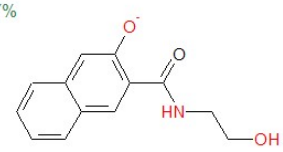
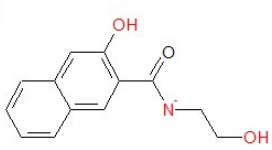
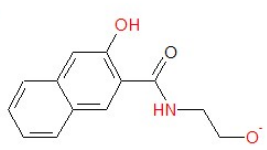
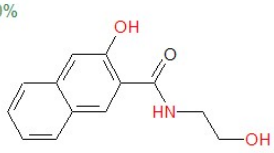
pKa	Macrostates	Microstates		
	M^{-3}	100.0% 		
12.77				
	HM^{-2}	79.2% 	20.1% 	0.7% 
11.68				
	H_2M^-	95.7% 	4.2% 	0.1% 
9.06				
	H_3M	100.0% 		

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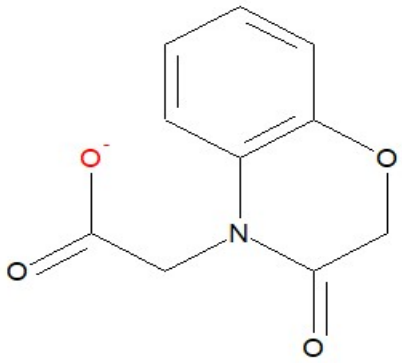
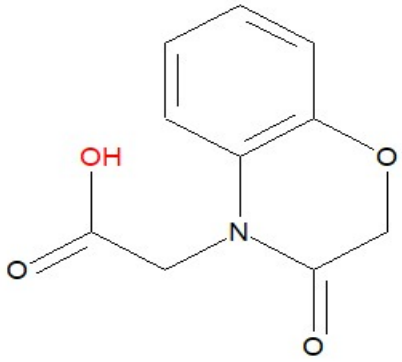
pKa	Macrostates	Microstates
		100.0%
	M⁻	
3.35		100.0%
	HM	

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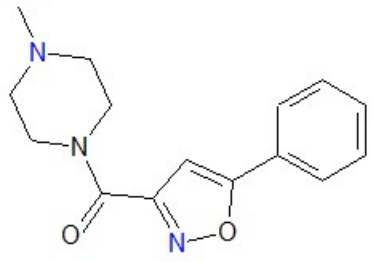
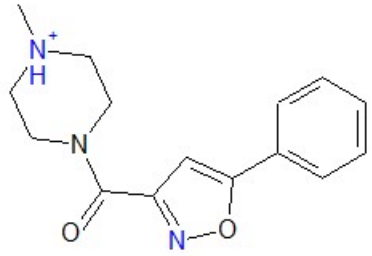
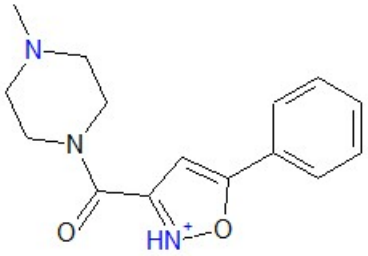
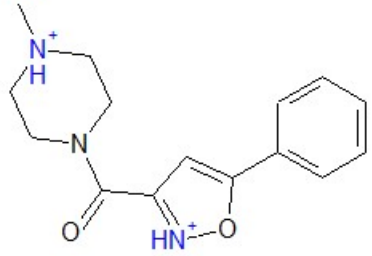
pKa	Macrostates	Microstates
	M	100.0% 
7.27	⇕	
	HM^+	100.0%  0.0% 
-3.77	⇕	
	H_2M^{+2}	100.0% 

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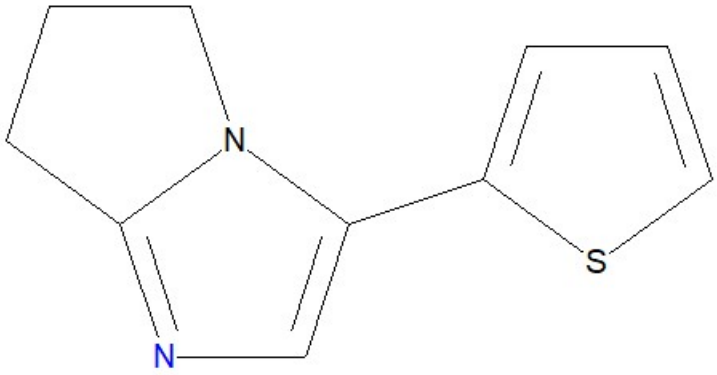
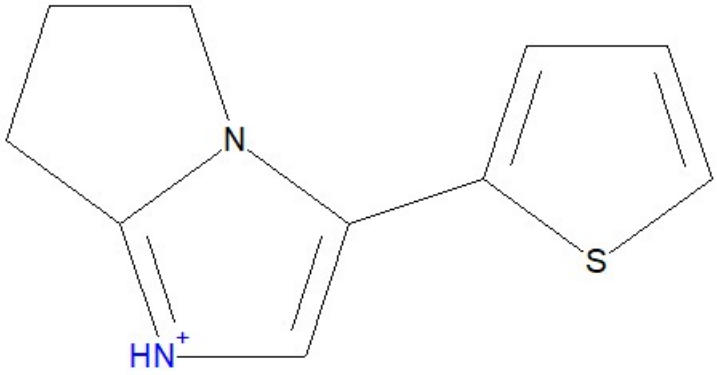
pK_a	Macrostates	Microstates
	M	100.0% 
6.39		
	HM^+	100.0% 

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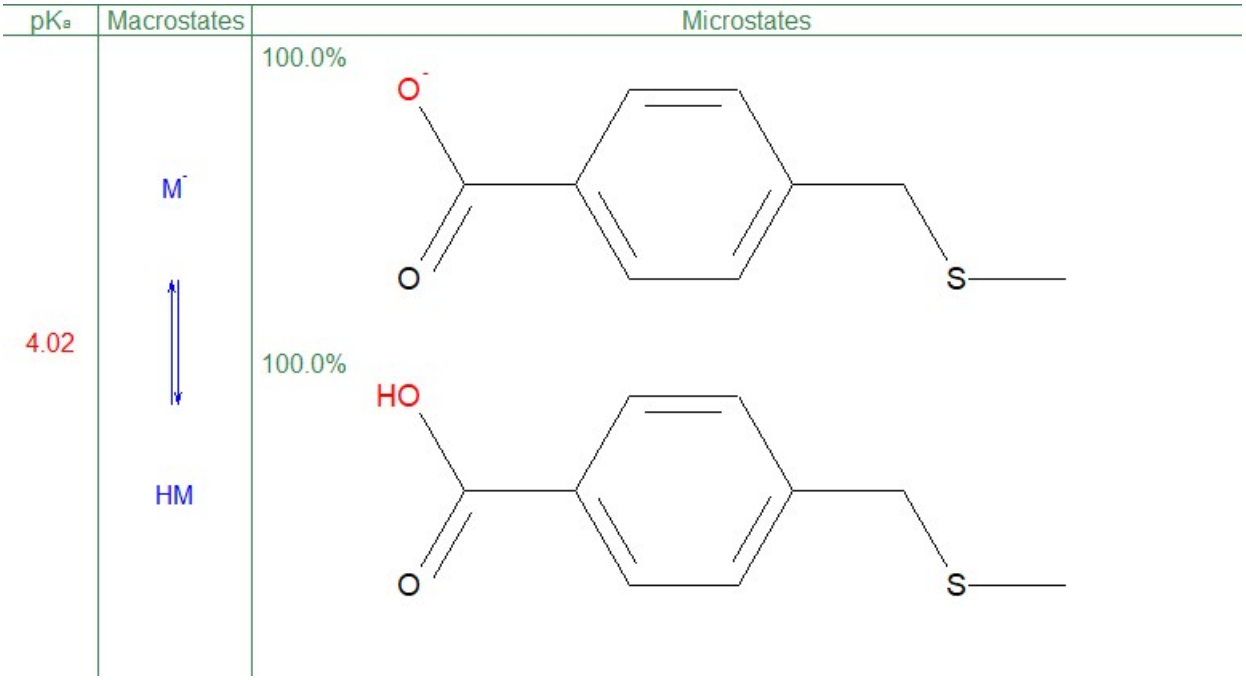

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