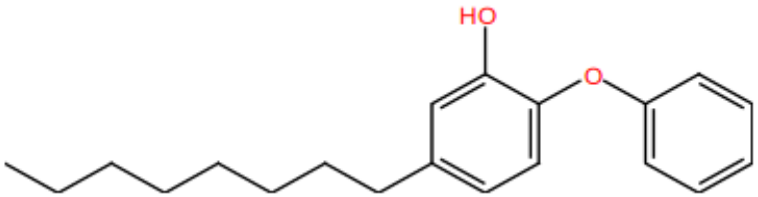
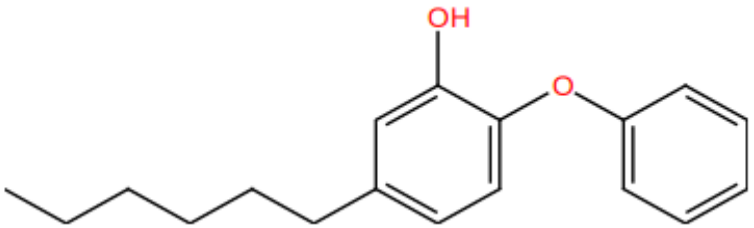
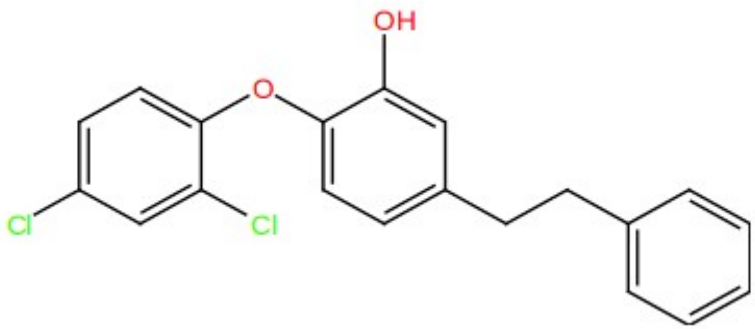
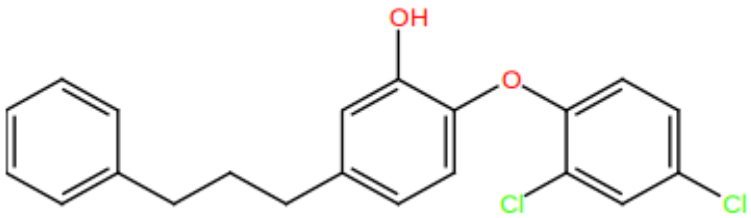
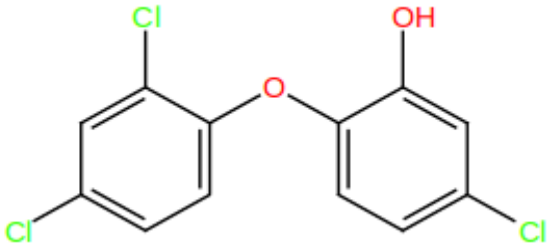
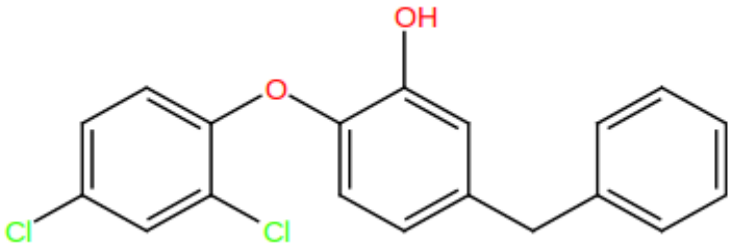
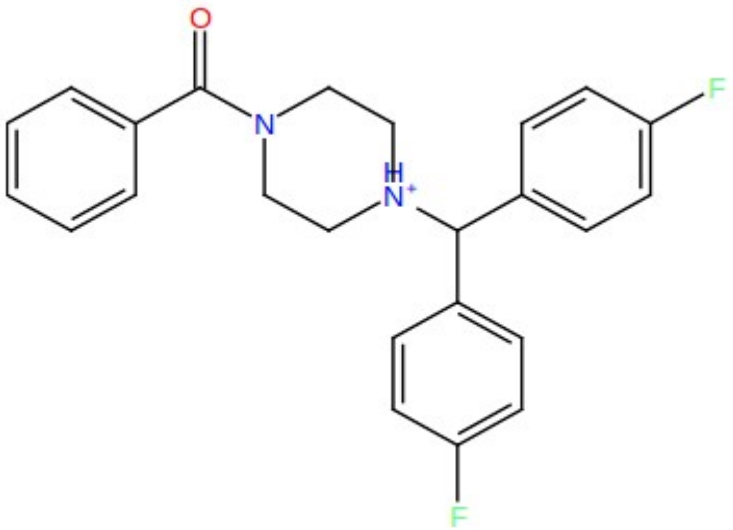
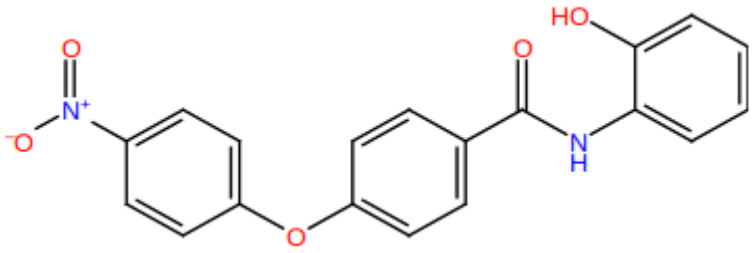
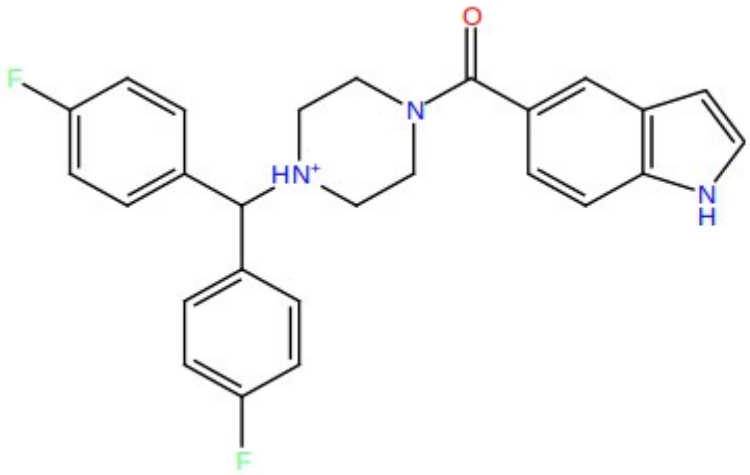
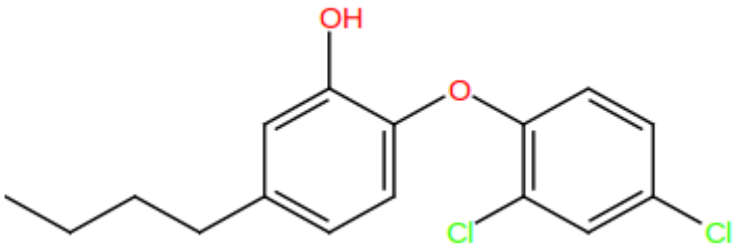
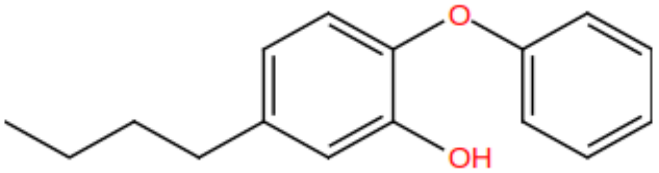
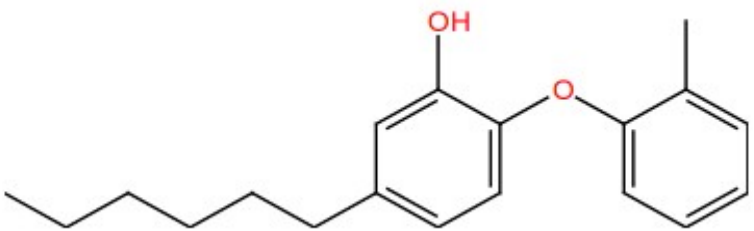
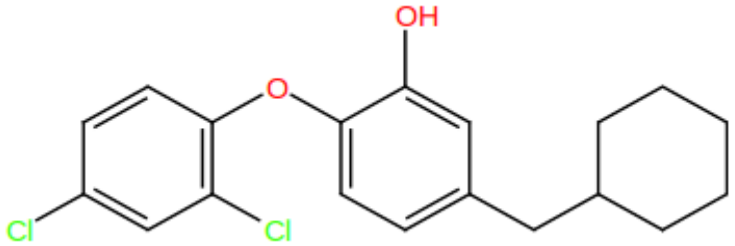
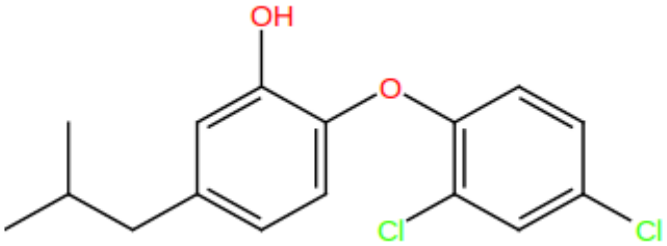
Supplement S2. MycPermCheck output for evaluation dataset of 19 InhA inhibitors and 21 impermeable compounds (sorted by probability), including an illustration of the compound structure. The coloring of the output values is assigned as described in the paper. For reasons of clarity only the represented isomeric form was considered by MycPermCheck in this table.

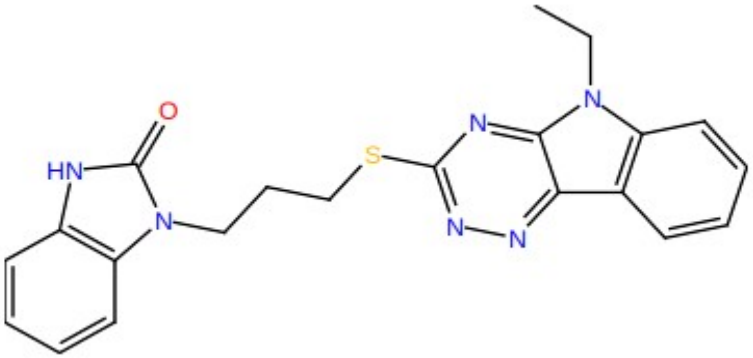
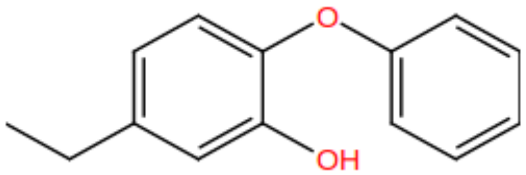
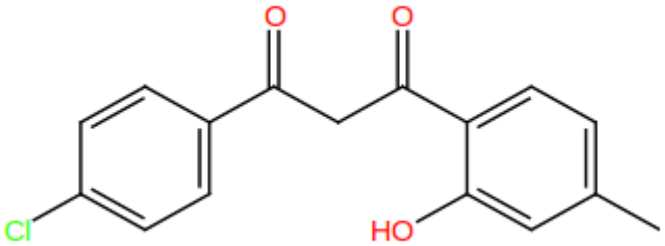
ID	Name	Structure	Prob.	FOSA	logP	PISA	accptHB	glob
P1	**8PP [1]**		**1.000**	325.953	5.951	297.640	1.25	0.794
P2	**6PP [1]**		**1.000**	260.549	5.175	297.639	1.25	0.817
P3	**Compound 25 [2]**		**1.000**	60.032	6.280	403.631	1.25	0.826

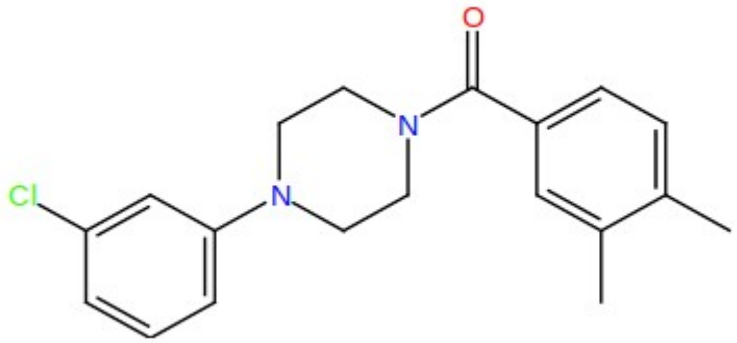
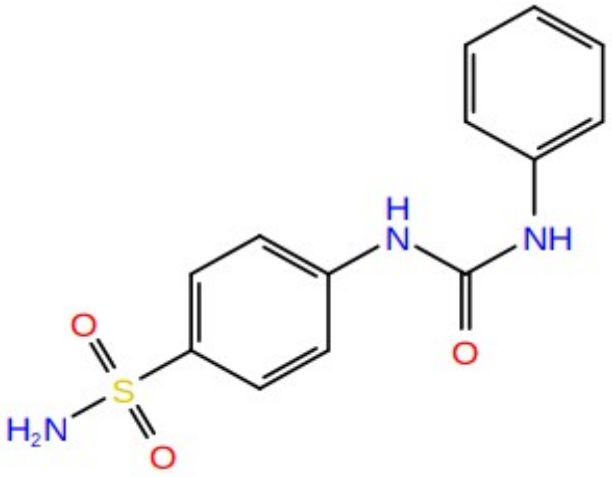
P4	**Compound 26 [2]**		**1.000**	90.908	6.676	407.062	1.25	0.812
P5	**Triclosan [1]**		**1.000**	0.000	4.738	225.618	1.25	0.898
P6	**Compound 24 [2]**		**1.000**	39.574	5.839	386.663	1.25	0.843

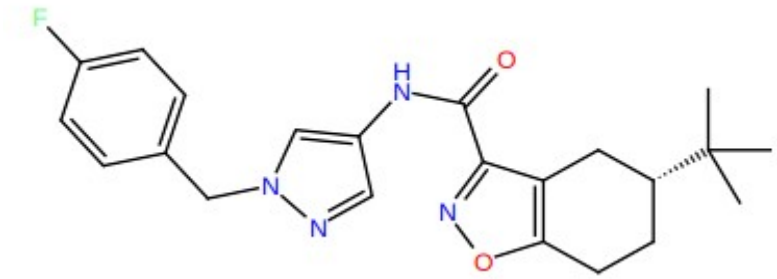
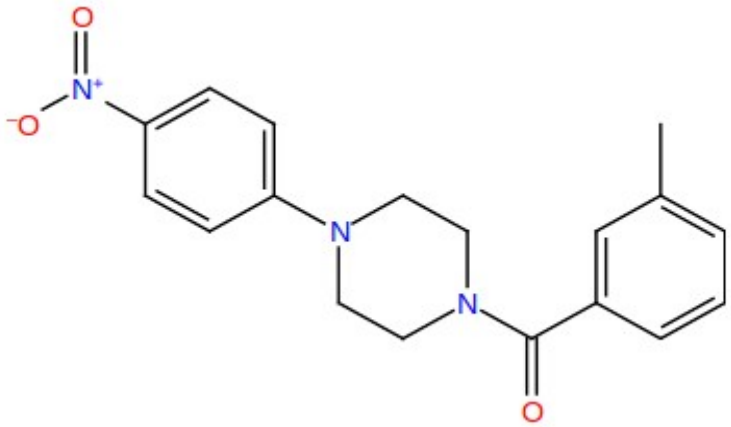
P7	**compound p6 [3]**		**1.000**	110.246	5.088	450.071	5.00	0.811
P8	**VH07 [4]**		**1.000**	0.000	3.180	451.793	4.75	0.812

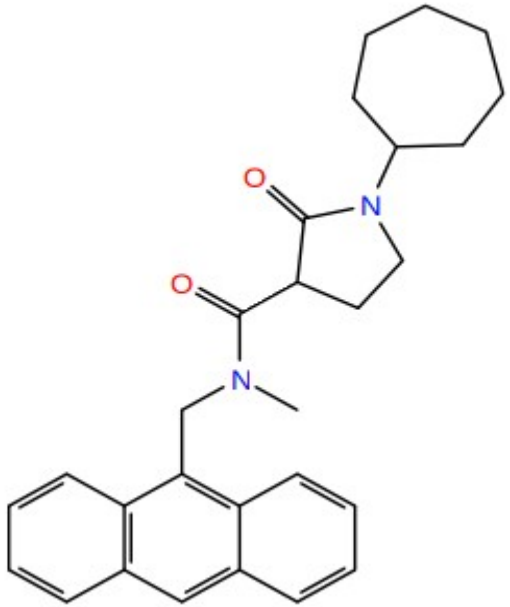
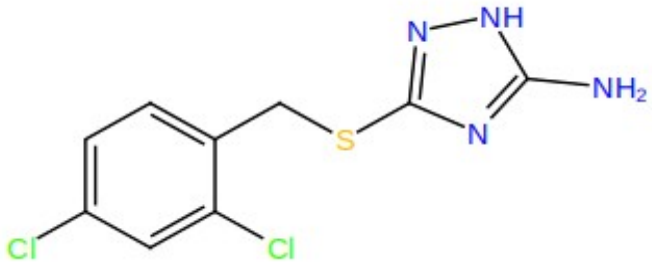
P9	**compound p4 [3]**		**1.000**	102.783	5.415	460.502	5.00	0.807
P10	**Compound 10 [2]**		**0.999**	195.669	5.383	206.906	1.25	0.827
P11	**4PP [1]**		**0.999**	195.624	4.402	297.640	1.25	0.843

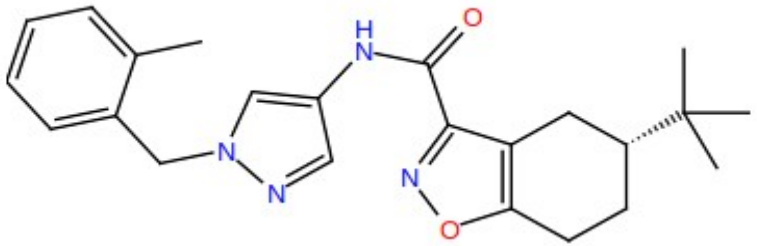
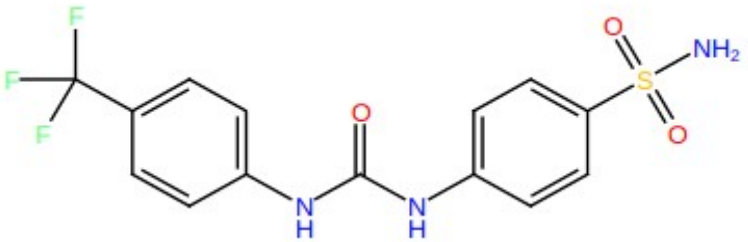
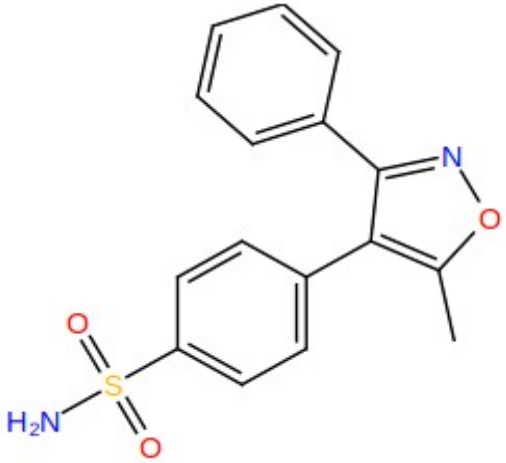
P12	**PT70 [5]**		**0.999**	320.707	5.424	254.594	1.25	0.824
P13	**Compound 7 [2]**		**0.999**	243.108	6.046	200.535	1.25	0.833
P14	**Compound 11 [2]**		**0.999**	190.289	5.296	200.893	1.25	0.836

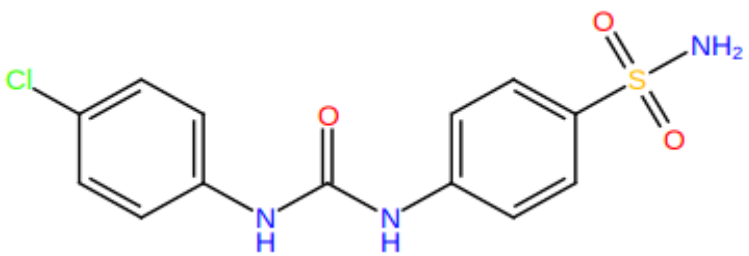
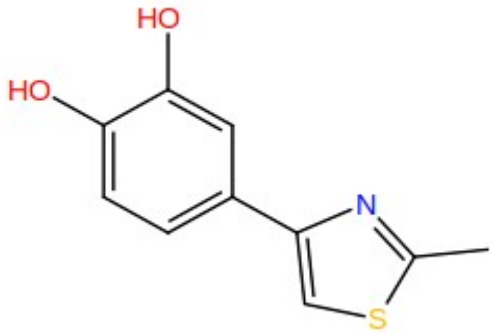
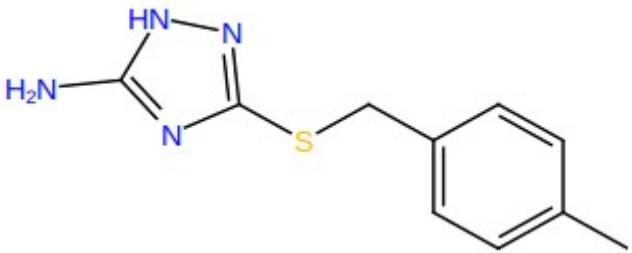
IM1	**CHEMBL589101**		**0.999**	202.630	4.755	349.535	5.00	0.785
P15	**2PP [1]**		**0.998**	130.198	3.522	297.899	1.25	0.872
P16	**VH04 [4]**		**0.970**	110.862	3.313	255.572	3.75	0.838

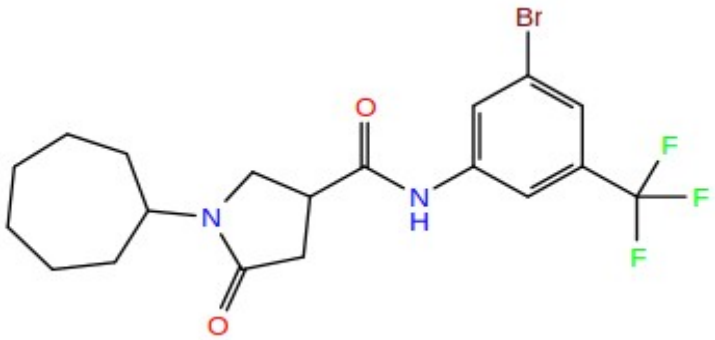
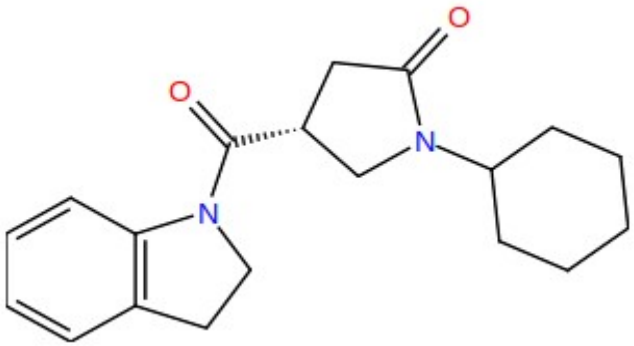
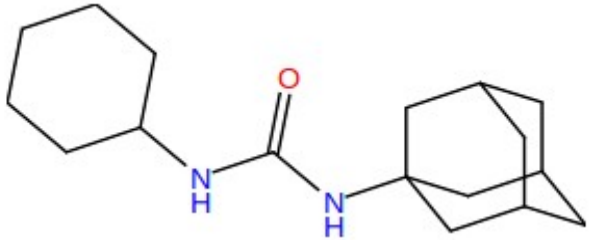
IM2	**CHEMBL239673**		**0.929**	280.710	4.636	222.903	4.00	0.825
IM3	**CHEMBL25600**		**0.800**	0.000	1.435	324.607	6.00	0.833

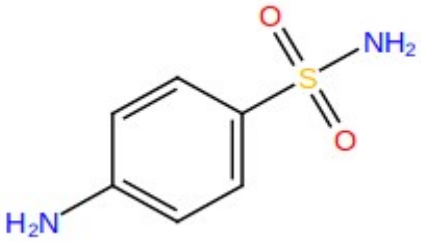
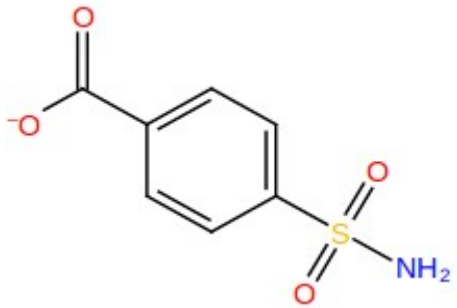
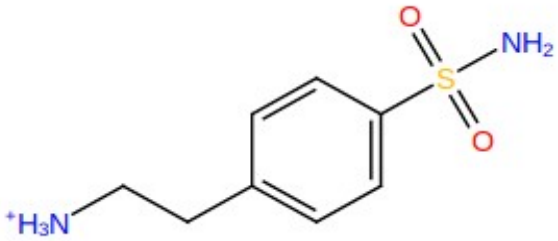
IM4	**CHEMBL259507**		**0.791**	317.104	4.606	231.036	5.50	0.798
P17	**compound a6 [3]**		**0.708**	219.506	3.158	258.913	5.00	0.819

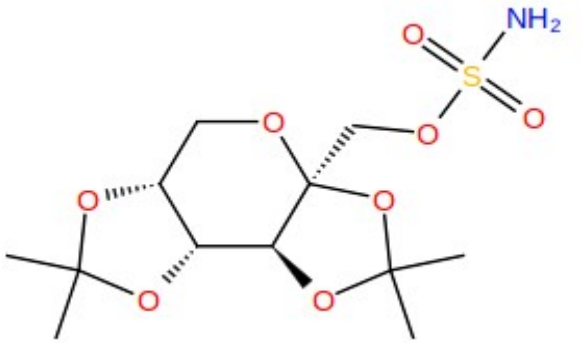
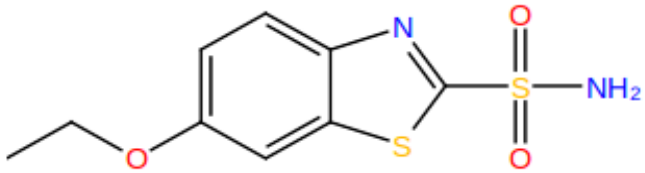
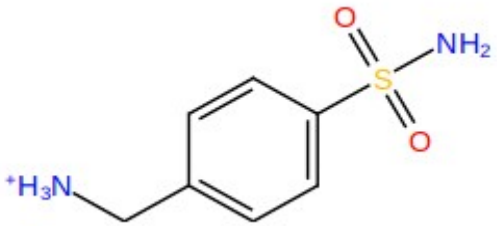
P18	**compound p67 [6]**		**0.685**	373.945	4.182	313.602	6.00	0.815
IM5	**CHEMBL569750**		**0.609**	25.619	2.222	140.881	3.00	0.858

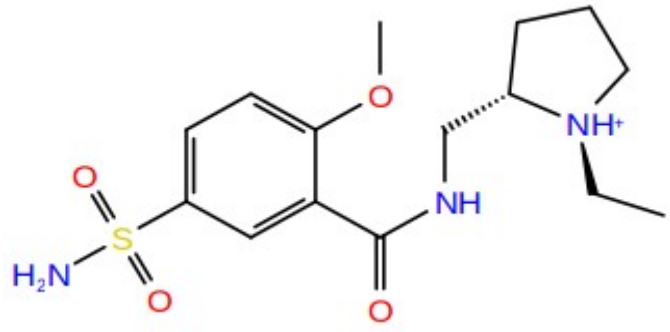
IM6	**CHEMBL412059**		**0.472**	371.394	4.539	221.566	5.50	0.811
IM7	**CHEMBL1337519**		**0.416**	0.301	1.152	271.776	6.50	0.812
IM8	**CHEMBL865**		**0.364**	80.488	1.669	287.397	6.00	0.847

IM9	**CHEMBL1446150**		**0.269**	0.000	0.667	289.682	6.50	0.822
IM10	**CHEMBL495123**		**0.190**	93.797	1.690	167.577	3.00	0.882
IM11	**CHEMBL568651**		**0.187**	118.214	1.622	165.437	3.00	0.858

P19	**compound d12 [6]**		**0.048**	321.497	4.212	89.257	5.50	0.811
IM12	**CHEMBL217499**		**0.002**	375.372	2.439	163.761	6.00	0.842
IM13	**CHEMBL242255**		**0.001**	533.944	3.469	0.000	2.00	0.830

IM14	**CHEMBL1875592**		**0.000**	0.000	-0.799	149.874	5.50	0.914
IM15	**CHEMBL1894686**		**0.000**	0.000	-0.579	132.673	6.50	0.904
IM16	**CHEMBL7087**		**0.000**	83.520	-0.795	127.201	5.50	0.886
IM17	**CHEMBL1884503**		**0.000**	77.398	-0.950	10.155	7.50	0.886

IM18	**CHEMBL220492**		**0.000**	373.113	0.762	0.000	8.25	0.884
IM19	**CHEMBL1410342**		**0.000**	139.412	0.460	132.217	6.75	0.852
IM20	**CHEMBL419**		**0.000**	48.934	-1.122	132.942	5.50	0.900

IM21	**CHEMBL196677**		**0.000**	349.105	0.685	77.555	8.25	0.818

References:

[1] Sullivan *et al.* (2006)
[2] Freundlich *et al.* (2009)
[3] He *et al.* (2007)
[4] Muddassar *et al. (2010)*
[5] Luckner *et al.* (2010)
[6] He *et al.* (2006)