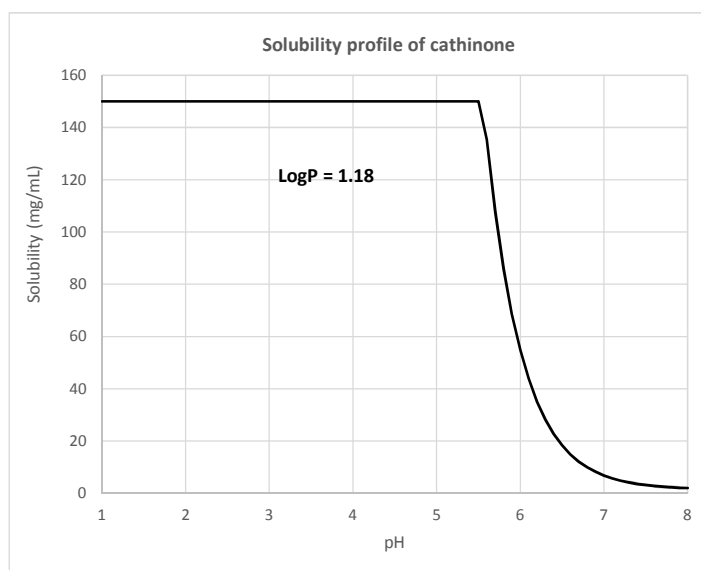
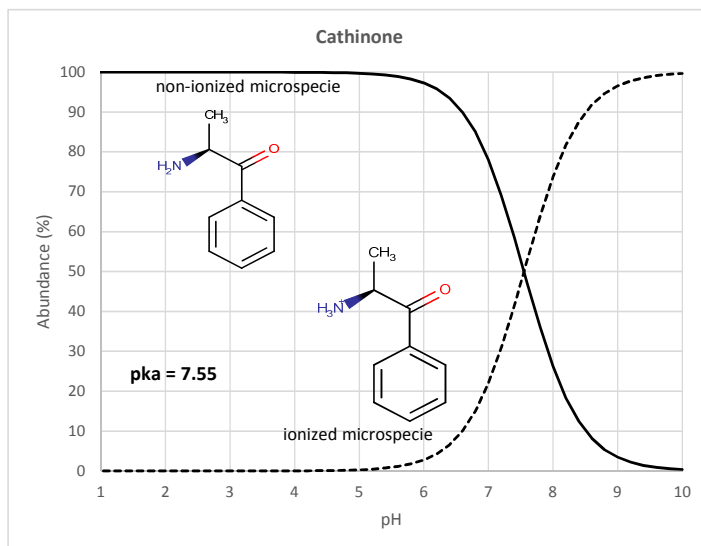


pH	Microspecies	
	1	2
0	0	100
0.2	0	100
0.4	0	100
0.6	0	100
0.8	0	100
1	0	100
1.2	0	100
1.4	0	100
1.6	0	100
1.8	0	100
2	0	100
2.2	0	100
2.4	0	100
2.6	0	100
2.8	0	100
3	0	100
3.2	0	100
3.4	0.01	99.99
3.6	0.01	99.99
3.8	0.02	99.98
4	0.03	99.97
4.2	0.04	99.96
4.4	0.07	99.93
4.6	0.11	99.89
4.8	0.18	99.82
5	0.28	99.72
5.2	0.44	99.56
5.4	0.7	99.3
5.6	1.11	98.89
5.8	1.74	98.26
6	2.74	97.26
6.2	4.27	95.73
6.4	6.6	93.4
6.6	10.08	89.92
6.8	15.08	84.92
7	21.96	78.04
7.2	30.85	69.15
7.4	41.41	58.59
7.6	52.84	47.16
7.8	63.97	36.03
8	73.78	26.22
8.2	81.69	18.31
8.4	87.61	12.39
8.6	91.81	8.19
8.8	94.67	5.33
9	96.57	3.43
9.2	97.81	2.19
9.4	98.61	1.39
9.6	99.12	0.88
9.8	99.44	0.56
10	99.65	0.35

pH	Solubility (mg/mL)
	1
1.1	150.01
1.2	150.01
1.3	150.01
1.4	150.01
1.5	150.01
1.6	150.01
1.7	150.01
1.8	150.01
1.9	150.01
2	150.01
2.1	150.01
2.2	150.01
2.3	150.01
2.4	150.01
2.5	150.01
2.6	150.01
2.7	150.01
2.8	150.01
2.9	150.01
3	150.01
3.1	150.01
3.2	150.01
3.3	150.01
3.4	150.01
3.5	150.01
3.6	150.01
3.7	150.01
3.8	150.01
3.9	150.01
4	150.01
4.1	150.01
4.2	150.01
4.3	150.01
4.4	150.01
4.5	150.01
4.6	150.01
4.7	150.01
4.8	150.01
4.9	150.01
5	150.01
5.1	150.01
5.2	150.01
5.3	150.01
5.4	150.01
5.5	150.01
5.6	135.39
5.7	107.86
5.8	85.98
5.9	68.61
6	54.8
6.1	43.84
6.2	35.13
6.3	28.22
6.4	22.72
6.5	18.36
6.6	14.89
6.7	12.14
6.8	9.95
6.9	8.21
7	6.83
7.1	5.73
7.2	4.86
7.3	4.17
7.4	3.62
7.5	3.19
7.6	2.84
7.7	2.56
7.8	2.34
7.9	2.17

Canonical smiles CC(C(=O)C1=CC=CC=C1)N

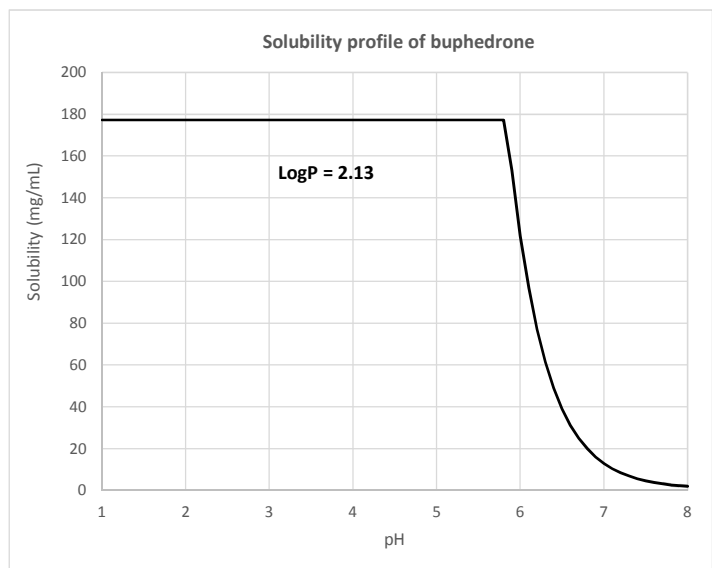
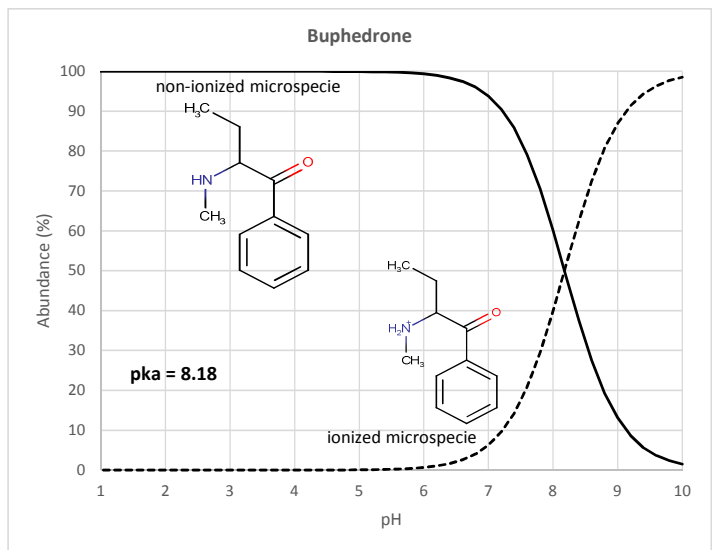


Cathinone

	Chemaxon	pkCSM		
Molecular weigh (g/mol)	149.193			
Intrinsic solubility (mg/ml)	1.5			
Solubility at pH 7.4 (mg/ml)	3.62			
pka	7.55			
LogP	1.18			
	pkCSM	pkCSM	Convert	
		other units	Peff (cm/h)	
Intrinsic solubility (log mol/L)	0.8	941.344191	6.309573	
LogP	1.8673			
Number of rotatable bonds	2			
Caco2 permeability (log Papp 10E-6 cm/s)	1.159			0.99697602
Intestinal absorption (human) (% Absorbed)	92.649			
Pgp substrate	No			
Pgp I inhibitor	No			
Pgp II inhibitor	No			
VDss (human) (log L/kg)	0.638	4.345	L/kg	
Fraction unbound (human)	0.733			
BBB permeability (log BB)	0.493			
CNS permeability (log PS)	-2.244			
CYP2D6 substrate	No			
CYP3A4 substrate	No			
CYP1A2 inhibitor	Yes			
CYP2C19 inhibitor	No			
CYP2C9 inhibitor	No			
CYP2D6 inhibitor	No			
CYP3A4 inhibitor	No			
Total clearance (log mL/min/kg)	0.894	0.470	L/h/kg	
Renal OCT2 substrate	No			

pH	Microspecies	
	1	2
0	0	100
0.2	0	100
0.4	0	100
0.6	0	100
0.8	0	100
1	0	100
1.2	0	100
1.4	0	100
1.6	0	100
1.8	0	100
2	0	100
2.2	0	100
2.4	0	100
2.6	0	100
2.8	0	100
3	0	100
3.2	0	100
3.4	0	100
3.6	0	100
3.8	0	100
4	0.01	99.99
4.2	0.01	99.99
4.4	0.02	99.98
4.6	0.03	99.97
4.8	0.04	99.96
5	0.07	99.93
5.2	0.11	99.89
5.4	0.17	99.83
5.6	0.26	99.74
5.8	0.42	99.58
6	0.66	99.34
6.2	1.04	98.96
6.4	1.64	98.36
6.6	2.58	97.42
6.8	4.02	95.98
7	6.23	93.77
7.2	9.52	90.48
7.4	14.3	85.7
7.6	20.91	79.09
7.8	29.53	70.47
8	39.91	60.09
8.2	51.28	48.72
8.4	62.52	37.48
8.6	72.56	27.44
8.8	80.73	19.27
9	86.91	13.09
9.2	91.32	8.68
9.4	94.34	5.66
9.6	96.36	3.64
9.8	97.67	2.33
10	98.52	1.48

pH	Solubility (mg/mL)
1.1	177.25
1.2	177.25
1.3	177.25
1.4	177.25
1.5	177.25
1.6	177.25
1.7	177.25
1.8	177.25
1.9	177.25
2	177.25
2.1	177.25
2.2	177.25
2.3	177.25
2.4	177.25
2.5	177.25
2.6	177.25
2.7	177.25
2.8	177.25
2.9	177.25
3	177.25
3.1	177.25
3.2	177.25
3.3	177.25
3.4	177.25
3.5	177.25
3.6	177.25
3.7	177.25
3.8	177.25
3.9	177.25
4	177.25
4.1	177.25
4.2	177.25
4.3	177.25
4.4	177.25
4.5	177.25
4.6	177.25
4.7	177.25
4.8	177.25
4.9	177.25
5	177.25
5.1	177.25
5.2	177.25
5.3	177.25
5.4	177.25
5.5	177.25
5.6	177.25
5.7	177.25
5.8	177.25
5.9	153.11
6	121.78
6.1	96.9
6.2	77.14
6.3	61.44
6.4	48.97
6.5	39.06
6.6	31.19
6.7	24.94
6.8	19.98
6.9	16.03
7	12.9
7.1	10.41
7.2	8.44
7.3	6.87
7.4	5.62
7.5	4.63
7.6	3.84
7.7	3.22
7.8	2.72
7.9	2.33
8	2.01



Buphedrone

	Chemaxon	pkCSM		
Molecular weigh (g/mol)	177.247			
Intrinsic solubility (mg/ml)	0.8			
Solubility at pH 7.4 (mg/ml)	5.62			
pka	8.18			
LogP	2.13			
	pkCSM	pkCSM	Convert	
		other units	Peff	
Intrinsic solubility (log mol/L)	0.8	1118.35296	6.309573	
LogP	1.8673			
Number of rotatable bonds	4			
Caco2 permeability (log Papp 10E-6 cm/s)	1.159			1.061776 cm/h
Intestinal absorption (human) (% Absorbed)	92.649			
Pgp substrate	No			
Pgp I inhibitor	No			
Pgp II inhibitor	No			
VDss (human) (log L/kg)	0.638	4.345		L/kg
Fraction unbound (human)	0.733			
BBB permeability (log BB)	0.493			
CNS permeability (log PS)	-2.244			
CYP2D6 substrate	No			
CYP3A4 substrate	No			
CYP1A2 inhibitor	Yes			
CYP2C19 inhibitor	No			
CYP2C9 inhibitor	No			
CYP2D6 inhibitor	No			
CYP3A4 inhibitor	No			
Total clearance (log mL/min/kg)	0.894	0.470		L/h/kg
Renal OCT2 substrate	No			