

ToxID 2.0 Configuration File

File Revision

2

m/z Window 0.6
RT Window (Second) 120
Laboratory Name Toxicology Unit
Company Name Kings College Hospital
Company Logo C:\Documents and Settings\All Users\Documents\My Pictures\logo_Foundation.jpg
Ion Ratio Window(%) 20
MS2 Search Library MS2_KCH MSMSLIB KCH_Library
MS3 Search Library ms3_kch
Exact Mass Window(ppm) 30

Compound Name	Parent Ion m	Analyte Type	Expected R	MS2 Produ	Intensity Tl	SI	RSI	SRM Fragment Ions
6-Acetylcodeine	342	metabolite of codeine	9.4	225	1	300	350	
6-Acetylmorphine	328.2	parent drug	6.47	211.1	1	300	350	
7-Amino-Clonazepam	286.2	parent drug	13	250	1	200	250	
7-Amino-Flunitrazepam	284.1	parent drug	13	256	1	200	250	
alpha-Hydroxymidazolam	342.1	metabolite of midazolam	13	203	10	200	250	
alpha-Hydroxymidazolam-glucuronide	518.1	metabolite of midazolam	13	342.1	10	200	250	
Alprazolam	309.1	parent drug	12.3	274	100	500	500	
Amisulpride	370.6	parent drug	8.11	242.1	1	300	400	
Amitriptyline	278	parent drug	12.3	233	10	500	500	
Amphetamine	136	parent drug	6.9	91.1	1	300	400	
Anhydroecgonine	168.1	parent drug	6	137	5	300	400	
AnhydroecgonineMethylEster	182.1	parent drug	2.4	91.3	5000	500	500	
Aripiprazole	448.5	parent drug	13.5	285.2	1	300	400	
Atropine	290.1	parent drug	7.5	124	10	500	500	
Benzocaine	166.2	parent drug	5.1	166.2	5000	500	500	
BenzoylEcgonine	290.2	metabolite of cocaine	7.4	168.2	25	300	400	
Buprenorphine	468.3	parent drug	5.28	414	1	300	400	
Buprenorphine2	468.3	parent drug	5.28	396	1	300	400	

Buprenorphine-Glucuronide	644 metabolite of buprenorphine	9.2	468	1	300	400
Caffeine	195 parent drug	5	138	100	500	500
Cathinone	150 parent drug	3.01	117.1	5000	500	500
Chlordiazepoxide	300.2 parent drug	5.8	227.1	5000	500	500
Citalopram	326.2 parent drug	11.45	262	100	400	500
Clonazepam	316.2 parent drug	13	269.8	100	500	500
Clozapine	327.2 parent drug	10.8	270.1	5000	500	500
Cocaethylene	318.2 metabolite of cocaine	9.4	196.1	1	300	400
Cocaine	304.1 parent drug	9	182.1	1	300	400
Codeine	300.1 parent drug	7.2	215	15	300	400
Codeine-Glucuronide	476 metabolite of codeine	5.6	300	1	300	400
Cyclizine	267 parent drug	12	167	500	600	600
Dehydroaripiprazole	446 metabolite of aripiprazole	13.3	285	1	300	400
DesmethylCitalopram	312.2 metabolite of citalopram	11.1	262	100	400	500
Desmethylmeconine	182.1 metabolite of Noscapine	4	162	1	400	500
Dextromethorphan	272.2 parent drug	6	272.2	5000	500	500
Diazepam	285.1 parent drug	13	257	5	300	400
Dihydrocodeine	302.2 parent drug	6.4	245	50	400	400
Dihydrocodeine-glucuronide	478 metabolite of dihydrocodeine	6	302	1	400	400
DiHydrocotarnine	205 metabolite of Noscapine	3.8	205	1	500	500
Dihydroxypapaverine	312 metabolite of papaverine	4.2	188	1	400	500
Dihydroxypapaverine-glucuronide	488 metabolite of papaverine	7.1	312	1	400	500
Ecgonine	186 metabolite of cocaine	0.97	124	1	400	400
Ecgonine-Methyl-Ester	200.2 metabolite of cocaine	1.4	82	5000	300	400
EDDP	278.2 metabolite of methadone	12.8	249	25	300	400
EMDP	264.2 metabolite of methadone	10.8	220.1	1	500	500
Ephedrine	166.2 parent drug	4.2	148	1	500	500
Fentanyl	337.2 parent drug	6.3	188.2	5000	500	500
Heroin	370.1 parent drug	7.7	328.9	1	300	400
Hydrocodone	300.2 parent drug	4.4	300.2	5000	500	500
Hydrocotarnine	220 metabolite of Noscapine	3.9	220	100	500	500
Hydromorphone	286.2 parent drug	3.5	286.2	5000	500	500
Hydroxy-Alprazolam	325 metabolite of alprazolam	12.1	279.1	10	300	350

Hydroxy-Alprazolam-glucuronide	501 metabolite of alprazolam	13	325	10	300	350
Hydroxybenzoylecgonine	306.3 parent drug	3.8	168.2	5000	500	500
Hydroxypapaverine	326 metabolite of papaverine	8.2	188	10	300	400
HydroxyPapaverine-Glucuronide	502 metabolite of papaverine	7.4	326	1	400	500
9-OHRisperidone	427.1 metabolite of risperidone	9.7	207	1	300	400
Imipramine	281.1 parent drug	10.5	86	1	400	500
Ketamine	238.7 parent drug	7.3	207	10	350	500
Lorazepam	321.1 parent drug	5.2	274.9	5000	500	500
Lormetazepam-glucuronide	511.1 metabolite of Lormetazepam	13	335.1	10	300	300
MDA	180.2 parent drug	5.6	105	2500	300	400
MDEA	208.1 parent drug	6.1	163.1	200	300	400
MDMA	194.1 parent drug	8.4	163.1	200	300	400
Mebeverine	429.6 parent drug	5	308	50	300	400
Meconine	195 metabolite of Noscapine	4.8	162	1	400	500
Methadone	310 parent drug	13.8	265.1	2000	300	400
Methamphetamine	150.1 parent drug	7.9	119	10	300	400
Methaqualone	251 parent drug	13	251	1	500	500
MORPHINE	286.2 parent drug	4.6	211	1	300	400
Morphine D6	292 internal standard	2.4	204	1	200	200
Morphine3Glucuronide	462 metabolite of morphine	2.7	286.15	1	200	400
Nalbuphine	358.3 parent drug	4.4	340.2	5000	500	500
Nalorphine	312.2 parent drug	3.4	312.2	5000	500	500
Naloxone	328.1 parent drug	4	328.1	5000	500	500
Naltrexone	342.2 parent drug	4.2	324.2	5000	500	500
Nitrazepam	282.1 parent drug	12	236.08	100	500	500
Norbenzoylecgonine	276.1 parent drug	4.2	136.2	5000	500	500
Norbuprenorphine	414.3 metabolite of buprenorphine	9.57	379	1	300	400
Norbuprenorphine-Glucuronide	590 metabolite of buprenorphine	7	414.2	1	250	300
Norclomipramine	301.3 metabolite of clomipramine	12.8	270	1	400	500
Norclozapine	313 metabolite of norclozapine	10.1	270	1	300	400
Norcocaethylene	304.2 parent drug	5.7	136.2	5000	500	500
Norcocaine	290.1 metabolite of cocaine	5.4	168.2	5000	500	500
Norcodeine	286.2 metabolite of codeine	3.7	286.2	5000	500	500

Nordiazepam	271.1 metabolite of diazepam	13	243	100	500	500
Nordiazepam-glucuronide	447.7 metabolite of diazepam	13	271	100	500	500
Norephidrine	152 parent drug	1.4	117	1	300	400
Norketamine	224 metabolite of ketamine	6.5	179	1	300	400
Normorphine	272.2 metabolite of morphine	2	272.2	1	500	500
Noroxycodone	302.1 parent drug	4	302.1	5000	500	500
Noroxymorphone	288.1 parent drug	2.3	213.4	5000	500	500
Norpropoxyphene	308.1 metabolite of propoxyphene	10.7	100	1	350	400
Nortriptyline	264.2 metyabolite of amitriptyline	11.5	233	1	400	500
Noscapine	414 parent drug	10.6	220	100	300	300
Olanzapine	313 parent drug	7.2	256.2	1	300	400
Oxazepam	287.1 parent drug	12.75	241.1	100	500	500
Oxazepam-glucuronide	463 parent drug	12.75	287.7	10	500	500
Oxycodone	316.1 parent drug	4.2	298.1	5000	500	500
Oxymorphone	302.1 parent drug	2.8	284.1	5000	500	500
Papaverine	340.3 parent drug	9.2	202	1	200	200
Phentermine	150 parent drug	4.5	91	1	400	400
Pholcodine	399.1 parent drug	4.2	114	1	400	400
PMA	166.1 metabolite of mebeverine	4.4	121.3	50	500	500
PMMA	180.1 parent drug	4.4	121.2	50	500	500
Propoxyphene	340.2 parent drug	13.1	266	100	500	500
Protriptyline	264.3 parent drug	11.5	233	100000	400	500
Psuedephidrine	166.2 parent drug	4.25	148	2	500	500
Quetiapine	384.3 parent drug	11.1	253	1	300	400
Quinidine	325.3 parent drug	7.2	184	5000	500	500
Quinine	325.3 parent drug	7.3	184	5	500	500
Risperidone	411.2 parent drug	10.14	191	1	300	400
Sulpiride	342.2 parent drug	6.5	214	1	300	400
Temazepam	301.1 parent drug	12.6	255	10	300	350
Temazepam-glucuronide	478 metabolite of temazepam	12.6	301	10	300	350