

ToxID 1.0 Configuration File

Global intensity cutoff 1
 m/z window 0.4
 RT window in secs 30
 SI threshold 100
 RSI threshold 100
 Laboratory Toxicology Unit
 Company Name Kings College Hospital
 Company Logo C:\Documents and Settings\All Users\Documents\My Pictures\logo_Foundation.jpg

Compound name	Parent ion	Analyte Type	Expected R	product ion	product ion SI	RSI	RSI
6-Acetylcodeine	342.3	metabolite of codeine	4.7	342.3	1	200	200
6-Acetylmorphine	328.2	parent drug	3.4	211.1	1	200	200
Alprazolam	309.1	parent drug	4.9	281	5000	200	200
Amphetamine	136	parent drug	3.8	91.1	1	200	200
Anhydroecgonine	168.1	parent drug	1	91.4	5000	200	200
AnhydroecgonineMethylEster	182.1	parent drug	1.9	91.3	5000	200	200
Benzocaine	166.2	parent drug	4.6	166.2	5000	200	200
Benzoylecgonine	290.2	parent drug	3.8	168.2	1	200	200
Buprenorphine	468.3	parent drug	4.78	414	1	200	200
Buprenorphine-D4	472.3	internal standard	4.78	310	1	200	200
Cathinone	150	parent drug	2.51	117.1	5000	200	200
Chlordiazepoxide	300.2	parent drug	5.3	227.1	5000	200	200
Clonazepam	316.2	parent drug	6.4	269.8	5000	200	200
Clozapine	327.2	parent drug	5.5	270.1	5000	200	200
Cocaethylene	318.2	parent drug	5.5	196.1	50000	200	200
Cocaine	304.1	parent drug	5	182.1	1	200	200
Codeine	300.1	parent drug	4	215	1	200	200
Dextromethorphan	272.2	parent drug	5.5	272.2	5000	200	200
Diazepam	285.2	parent drug	5.2	285.2	1	200	200
Dihydrocodeine	302.2	parent drug	4.6	201.2	1	200	200

Ecgonine-Methyl-Ester	200.2	metabolite of morphine	1.2	182.1	5000	200	200
EDDP	278.2	parent drug	10.6	249	1	200	200
EMDP	264.2	parent drug	5.8	220.1	1	200	200
Ephedrine	166.2	parent drug	3.2	166.2	5000	200	200
Fentanyl	337.2	parent drug	5.8	188.2	5000	200	200
Heroin	370.1	parent drug	4.7	328.9	1	200	200
Hydrocodone	300.2	parent drug	3.9	300.2	5000	200	200
Hydromorphone	286.2	parent drug	3	286.2	5000	200	200
Hydroxy-Alprazolam	325	metabolite of alprazolam	4.6	279.1	5000	200	200
Hydroxybenzoylecgonine	306.3	parent drug	3.3	168.2	5000	200	200
Lorazepam	321.1	parent drug	4.7	274.9	5000	200	200
MDA	180.2	parent drug	4.1	105	1	200	200
MDEA	208.1	parent drug	5	163.1	1	200	200
MDMA	194.1	parent drug	4.2	163.1	1	200	200
Methadone	310.1	parent drug	11.9	265.1	1	200	200
Methamphetamine	150.1	parent drug	4.1	119	1	200	200
Morphine	286.2	parent drug	1.8	286	0.2	200	200
MORPHINE	286.2	parent drug	1.8	211.1	0.2	200	200
Morphine D6	292	internal standard	4	202	1	200	200
Nalbuphine	358.3	parent drug	3.9	340.2	5000	200	200
Nalorphine	312.2	parent drug	2.9	312.2	5000	200	200
Naloxone	328.1	parent drug	3.5	328.1	5000	200	200
Naltrexone	342.2	parent drug	3.7	324.2	5000	200	200
Nitrazepam	282.1	parent drug	5	236.08	5000	200	200
Norbenzoylecgonine	276.1	parent drug	3.7	136.2	5000	200	200
Norbuprenorphine	414.3	parent drug	4.8	414.3	5000	200	200
Norcocaethylene	304.2	parent drug	5.2	136.2	5000	200	200
Norcocaine	290.1	parent drug	4.9	168.2	5000	200	200
Norcodeine	286.2	metabolite of codeine	3.2	286.2	5000	200	200
Nordiazepam	271.1	parent drug	4.83	271.1	5000	200	200
Normorphine	272.2	metabolite of morphine	1.5	272.2	5000	200	200
Noroxycodone	302.1	parent drug	3.5	302.1	5000	200	200
Noroxymorphone	288.1	parent drug	1.8	213.4	5000	200	200

Norpropoxyphene	308.1 parent drug	6.9	308.1	5000	200	200
Noscapine	414.3 parent drug	5.2	219.9	1	200	200
Oxazepam	287.1 parent drug	4.6	241.1	5000	200	200
Oxycodone	316.1 parent drug	3.7	298.1	5000	200	200
Oxymorphone	302.1 parent drug	2.3	284.1	5000	200	200
Papaverine	340.3 parent drug	5.1	340.3	1	200	200
PMA	166.1 parent drug	3.9	121.3	5000	200	200
PMMA	180.1 parent drug	3.9	121.2	5000	200	200
Propoxyphene	340.2 parent drug	4.9	266	1	200	200
Quinidine	325.3 parent drug	4.9	325.3	5000	200	200
Quinine	325.3 parent drug	4.8	325.3	5000	200	200
Temazepam	301.1 parent drug	4.9	301.1	5000	200	200