

Section Two

Urine Toxicology

5.11 Identification of Compounds in Toxicology

5.11 Key Ions for Commonly Encountered Compounds in Blood and Urine Toxicology

5.11.1 BACKGROUND

This method was created to aide the analyst in the identification of the wide variety of commonly encountered compounds in blood and urine.

5.11.2 SCOPE

This method provides the key ions to be used to establish the presence of compounds of interest in blood and urine. In order to familiarize the analyst with Drug Recognition Examination (DRE), the compounds are arranged according to DRE categories. DRE categories include central nervous system (CNS) depressants, CNS stimulants, narcotic analgesics, PCP, hallucinogens and cannabis. Additional compound information includes drug class, intended use and examples of trade names.

5.11.3 EQUIPMENT AND REAGENTS

Refer to appropriate analytical method.

5.11.4 PROCEDURE

With the assistance of case history and screening results, use the following table to detect drug compounds and their metabolites in urine and blood. When the presence of a compound is supported by the listed ions, the analyst must analyze relevant reference material to establish the compound's retention time in order to complete the identification process.

5.11.5 DRE CATEGORIES

5.11.5.1 CNS Depressants

| Compound | Key Ions | | | | | | | Suggested Window | Class | Background Info. |
|--------------------------|----------|----------------|-----|-----|-----|-----|------------|------------------|---|--|
| | Base | Prominent Ions | | | | | MW | | | |
| Anticonvulsants | | | | | | | | | | |
| Carbamazepine | 193 | 192 | 236 | 191 | 165 | 44 | 236 | 250 | Ureas – Ethylene bridged 1,1-diphenylurea | Tegretol® (Novartis) Tonic-clonic and partial seizures |
| Carbamazepine-M/artifact | 193 | 165 | 96 | 83 | 139 | 177 | 193 | 210 | --- | Diphenylurea |
| Carbamazepine Epoxide | 180 | 193 | 207 | 252 | 152 | 223 | 252 | 280 | --- | Metabolite |
| Gabapentin | 153 | 81 | 67 | 110 | 96 | 68 | | 240 | Structurally related to GABA | Neurontin® (P-D), Excreted primarily unchanged |
| Phenytoin | 180 | 252 | 77 | 104 | 223 | | 252 | 280 | Hydantoins | Dilantin® Structurally related to barbiturates. All seizure types except absence |

| Compound | Key Ions | | | | | | | Suggested Window | Class | Background Info. |
|---------------------------|----------|----------------|-----|-----|-----|-----|------------|------------------|---|--|
| | Base | Prominent Ions | | | | | MW | | | |
| Anticonvulsants | | | | | | | | | | |
| Primidone | 146 | 190 | 117 | 161 | 103 | 91 | 218 | 230 | 5-Ethylidihydro-5-4,6-(1H,5H) pyrimidinedione | Mysoline® (Wyeth-Ayerst) 2-desoxy-phenobarbital, converts to phenobarbital & PEMA. Good for all types of seizures except absence. |
| Topiramate | 43 | 324 | 59 | 110 | 127 | 189 | 339 | 360 | Sulfamate-substituted monosaccharide | Topamax® (Ortho-McNeil) Has numerous other indications |
| Valproic Acid | 73 | 102 | 55 | 41 | 57 | 115 | 144 | 140 | 2-Propyl pentanoic acid | Depakote® / Depakene® (Abbott) Multiple seizure types including absence. Also for Mania |
| Antidepressants/-M | | | | | | | | | | |
| Amitriptyline | 58 | 202 | 215 | 189 | 178 | 165 | 277 | 300 | Tricyclic (TCA) Tertiary Amine | Elavil® (Zeneca) |
| Nortriptyline | 44 | 202 | 215 | 220 | 115 | 91 | 263 | 300 | TCA Secondary Amine | Pamelor® (Norvartis) Norpramin®, Pertofrane®. Parent <i>or</i> metabolite of amitriptyline |
| Citalopram | 58 | 238 | 208 | 42 | 190 | 221 | 324 | 340 | SSRI Bicyclic Phthalane Derivative | Celexa® (Racemic) Lexapro® (S-Citalopram) |
| Desmethylcitalopram | 44 | 238 | 310 | 138 | 208 | 57 | | 340 | -- | Citalopram metabolite |
| Amoxapine | 245 | 257 | 193 | 247 | 228 | 164 | 313 | 350 | TCA Secondary Amine | Asendin® (Lederle) Depression w/anxiety or agitation. |
| Loxepine | 257 | 70 | 83 | 193 | 228 | 259 | 327 | 350 | TCA | Loxitane® (antipsychotic), Parent <i>or</i> metabolite of amoxapine |
| Bupropion | 44 | 100 | 57 | 139 | 111 | 224 | 239 | 250 | Aminoketone | Wellbutrin® (GlaxoWellcome) |
| Imipramine | 234 | 235 | 58 | 193 | 195 | 220 | 280 | 300 | TCA Dimethylamine Tertiary amine | Tofranil® High 5-HT/NE uptake ratio Anticholinergic and sedative effects tend to be marked |
| Imipramine-N-Oxide | 194 | 41 | 42 | 235 | 193 | 192 | 296 | 310 | --- | Metabolite |
| Desipramine | 234 | 195 | 193 | 235 | 208 | 266 | 266 | 280 | TCA Secondary amine | Norpramin (Hoechst Marion Roussel®) Parent <i>or</i> metabolite of Imipramine Less sedative effects than imipramine Higher NE than 5-HT uptake blocking capacity |
| Clomipramine | 58 | 85 | 268 | 228 | 314 | 130 | 314 | 320 | TCA Tertiary amine | Anafranil® (Novartis) Obsessive-compulsive disorder (OCD) |
| Doxepine | 58 | 42 | 165 | 152 | 178 | 189 | 279 | 290 | TCA Tertiary amine | Sinequan® (Roerig) Also for anxiety. |
| Nordoxepine | 44 | 178 | 165 | 222 | 204 | 128 | 265 | 280 | --- | Metabolite of Doxepin |
| Fluoxetine | 44 | 104 | 91 | 59 | 309 | 148 | 309 | 320 | Unrelated to other Anti-depressants | Prozac® (Dista) Selective 5-HT reuptake inhibitor For OCD also. |
| Norfluoxetine | 134 | 104 | 191 | 162 | 77 | 251 | 295 | 300 | --- | Metabolite of Fluoxetine |
| Maprotiline | 44 | 203 | 202 | 277 | 189 | 59 | 277 | 300 | Tetracyclic | Ludiomil® (Novartis) |
| Mirtazapine | 195 | 194 | 208 | 196 | 180 | 167 | 265 | 280 | Tetracyclic | Remeron® |
| Paroxetine | 192 | 44 | 138 | 329 | 70 | 109 | 177 | 200 | | Paxil® Selective 5-HT reuptake inhibitor |

| Compound | Key Ions | | | | | | | Suggested Window | Class | Background Info. |
|-----------------------------|----------|----------------|-----|-----|-----|-----|------------|------------------|---|---|
| | base | Prominent Ions | | | | | MW | | | |
| Antidepressants/-M | | | | | | | | | | |
| Sertraline | 274 | 276 | 159 | 262 | 239 | 306 | 304 | 330 | | Zoloft® Low dose has no CNS depression Selective 5-HT reuptake inhibitor For OCD also. |
| Trazodone | 205 | 70 | 176 | 231 | 278 | 56 | 371 | 390 | Chemically unrelated to TCA or other ADs Inhibits 5-HT uptake | Desyrel® High temp GC/MS program |
| Venlafaxine | 58 | 134 | 179 | 91 | 119 | 121 | 202 | 290 | Phenethylamine | Effexor® Potent inhibitor of 5-HT and NE reuptake |
| O-Desmethyl Venlafaxine | 58 | 120 | 165 | 107 | 91 | 202 | --- | 270 | --- | Metabolite |
| Antihistamines | | | | | | | | | | |
| Brompheniramine | 247 | 249 | 167 | 58 | 72 | 168 | 318 | 260 | Propylamine Derivative | Dimetane® Produce Drowsiness |
| Chlorpheniramine | 203 | 205 | 202 | 167 | 58 | 139 | 274 | 290 | Propylamine Derivative | Chlor-Trimeton® Produce Drowsiness |
| Diphenhydramine | 58 | 73 | 165 | 152 | 42 | 227 | 255 | 260 | Aminoalkyl ether | Benadryl® Significant Anti-Chol. activity Produce Drowsiness |
| Doxylamine | 71 | 58 | 167 | 180 | 182 | 72 | 270 | 290 | Aminoalkyl ether | Unisom®, Decapryn® Produce Drowsiness |
| Promethazine | 72 | 284 | 180 | 198 | 213 | 152 | 284 | 310 | Phenothiazine Derivative | Phenergan® |
| Antiparkinson Agents | | | | | | | | | | |
| Trihexyphenidyl | 98 | 218 | 55 | 77 | 284 | 300 | 301 | 350 | Anticholinergics | Artane® |
| Antipsychotics | | | | | | | | | | |
| Clozapine | 243 | 256 | 192 | 227 | 326 | 70 | 326 | 350 | Dibenzapine Derivative | Clozaril® Severely ill schizophrenics |
| Haloperidol | 224 | 42 | 237 | 226 | 123 | 206 | 375 | 380 | Fluorobutyphenones | Haldol® |
| Olanzapine | 242 | 229 | 213 | 198 | 42 | 169 | 312 | 340 | Dibenzapine Derivative | Zyprexa® Psychotic disorders |
| Quetiapine | 210 | 144 | 239 | 209 | 251 | 321 | 383 | 400 | Dibenzothiazepines | Seroquel® |
| Quetiapine-M | 227 | 210 | 239 | 139 | 251 | 183 | 295 | 310 | --- | Metabolite |
| Thioridazine | 98 | 370 | 70 | 126 | 185 | 244 | 370 | 390 | Phenothiazine Derivative | Mellaril® |
| Antitussives | | | | | | | | | | |
| Dextromethorphan | 271 | 59 | 150 | 214 | 270 | 171 | 271 | 300 | d-isomer of levorphanol | Vicks Formula 44, Robitussin, Street name: DMX |
| Sedative/Hypnotic | | | | | | | | | | |
| Amobarbital | 156 | 141 | 157 | 142 | 197 | 98 | 226 | 220 | Barbiturate Alkyl-substituted barbituric acid | Amytal® |
| Butalbital | 168 | 167 | 124 | 141 | 153 | 209 | 224 | 220 | Barbiturate Alkyl-substituted barbituric acid | Fiorinal®, Esgic® |
| Eszopiclone | 143 | 245 | 99 | 217 | 112 | | | | | Lunesta® |
| | | | | | | | | | | |
| | | | | | | | | | | |
| Compound | Key Ions | | | | | | | Suggested Window | Class | Background Info. |

| | base | Prominent Ions | | | | | MW | | | |
|--|------|----------------|-----|-----|-----|-----|------------|-----|--|--|
| Pentobarbital | 156 | 141 | 157 | 98 | 197 | 69 | 226 | 230 | Barbiturate Alkyl-substituted barbituric acid | Nembutal® |
| Sedative/Hypnotic | | | | | | | | | | |
| Phenobarbital | 204 | 232 | 117 | 161 | 146 | 217 | 232 | 240 | Barbiturate Phenyl/alkyl-substituted barbituric acid | Luminal®, Phenalix®, Solfotin® Long-Acting Also – Anti-convulsant |
| Secobarbital | 168 | 167 | 195 | 97 | 153 | 124 | 238 | 220 | Barbiturate Alkyl-substituted barbituric acid | Seconal®, Tuinal® |
| Zaleplon | 248 | 305 | 263 | 262 | 43 | 249 | 305 | 380 | Pyrazolopyrim-idine | Sonata® |
| Zolpidem | 235 | 236 | 92 | 65 | 219 | 307 | 307 | 320 | Imidazopyridine | Ambien® |
| Miscellaneous Depressants | | | | | | | | | | |
| γ-Hydroxybutyric Acid (GHB) -TMS | 147 | 117 | 233 | 204 | 133 | 59 | --- | 260 | Lactone | Potential date rape drug Refer to method for detailed information |
| Propranolol | 72 | 115 | 144 | 100 | 215 | 259 | 259 | 270 | Alkylpropranol- amine | Cardinal β-Blocker |
| Fenfluramine | 72 | 159 | 44 | 109 | 216 | 56 | 231 | 250 | Sympatho-mimetic Phenethylamine | Anorexiant, Sedation and Drowsiness |
| Vortioxetine | 256 | 119 | 298 | 240 | 136 | 161 | | | | Atypical antidepressant |
| Benzodiazepines Anxiety/Hypnotic/Anticonvulsant | | | | | | | | | | |
| Alprazolam | 279 | 204 | 308 | 273 | 77 | 245 | 308 | 350 | Triazolo- benzodiazepine | Xanax® |
| α-Hydroxyalprazolam- TMS | 381 | 396 | 383 | 293 | 190 | 173 | | 420 | --- | Metabolite of alprazolam |
| Diazepam | 256 | 283 | 284 | 257 | 221 | 165 | 284 | 300 | 1,4- benzodiazepine | Valium® (Roche) Also – Muscle Relaxant |
| Midazolam | 310 | 312 | 311 | 163 | 325 | 75 | 325 | 340 | Fluorinated Triazolo benzodiazepine | Versed® |
| α-Hydroxymidazolam- TMS | 310 | 73 | 398 | 413 | 333 | 168 | | 460 | --- | Metabolite of midazolam |
| Nordiazepam | 242 | 241 | 269 | 270 | 214 | 151 | 270 | 290 | 1,4- benzodiazepine | Calmday®, Madar®, Stilny® Parent or metabolite of diazepam, prazepam, clorazepate, chlordiazepoxide |
| Nordiazepam-TMS | 347 | 342 | 343 | 327 | 227 | 269 | | 350 | 1,4- benzodiazepine | See above |
| Oxazepam | 205 | 239 | 267 | 177 | 151 | 104 | 286 | 280 | 1,4- benzodiazepine | Serax® (Wyeth-Ayerst) |
| Oxazepam-TMS | 429 | 430 | 313 | 147 | 401 | 415 | | 450 | 1,4- benzodiazepine | See above. |
| Temazepam | 271 | 255 | 300 | 165 | 193 | 228 | 300 | 320 | 1,4- benzodiazepine | Restoril |
| Temazepam-TMS | 343 | 257 | 345 | 283 | 357 | 372 | | 390 | 1,4- benzodiazepine | See above. |
| Lorazepam | 239 | 274 | 75 | 276 | 302 | 111 | 320 | 340 | Dichloro-1,4- benzodiazepine | Ativan® |
| Lorazepam-TMS | 429 | 431 | 147 | 347 | 177 | 449 | | 470 | Dichloro-1,4- benzodiazepine | Ativan® |
| Triazolam | 313 | 238 | 315 | 342 | 203 | 279 | 342 | 380 | Triazolo- benzodiazepine | Halcion® |
| α-Hydroxytriazolam | | | | | | | | | Triazolo- benzodiazepine | Metabolite of triazolam |
| Clonazepam | 280 | 314 | 286 | 315 | 234 | 288 | 315 | 350 | 7-Nitro benzodiazepine | Klonopin® (Roche) Akinetic and myoclonic seizures |
| 7-Aminoclonazepam | 285 | 256 | 257 | 258 | 44 | 287 | --- | 300 | 7-Nitro benzodiazepine | Metabolite |

| | | | | | | | | | | |
|----------|-----|-----|-----|-----|--|--|--|--|--|--|
| Etizolam | 342 | 313 | 266 | 224 | | | | | | |
|----------|-----|-----|-----|-----|--|--|--|--|--|--|

| Compound | Key Ions | | | | | | | Suggested Window | Class | Background Info. |
|--|----------|----------------|-----|-----|-----|-----|------------|------------------|---|--|
| | base | Prominent Ions | | | | | MW | | | |
| Benzodiazepines | | | | | | | | | | |
| Anxiety/Hypnotic/Anticonvulsant | | | | | | | | | | |
| Flurazepam | 86 | 99 | 87 | 183 | 58 | 315 | 387 | 400 | Fluoro-1,4-benzodiazepine | Dalmane® |
| Flunitrazepam | 312 | 286 | 285 | 313 | 266 | 238 | 313 | 360 | 7-Nitro benzodiazepine | Rohypnol® |
| Midazolam | | | | | | | | | | |
| Muscle Relaxants | | | | | | | | | | |
| Baclofen | 138 | 103 | 195 | 77 | 140 | 75 | 213 | 230 | 3-(p-Chloro phenyl)- γ aminobutyric acid | Lioresal®, GABA analog. Spasticity Depresses synaptic transmission |
| Carisoprodol | 55 | 58 | 158 | 97 | 104 | 83 | 260 | 270 | Dicarbamate | Soma® Major side effect is drowsiness |
| Meprobamate | 83 | 55 | 71 | 96 | 114 | 144 | 218 | 170 | Carbamate derivative | Miltown® (Wallace), Equanil® Parent or metabolite of carisoprodol |
| Meprobamate artifact (early R ₁) | 84 | 55 | 56 | 83 | 41 | 101 | | 120 | Carbamate | |
| Meprobamate artifact (mid R ₁) | 84 | 55 | 56 | 83 | 41 | 101 | | 120 | Carbamate | |
| Methocarbamol | 118 | 109 | 124 | 77 | 62 | 81 | 241 | 250 | Carbamate derivative | Robaxin® |
| Cyclobenzaprine | 58 | 215 | 202 | 216 | 213 | 189 | 275 | 360 | Very similar to amitriptyline (TCA). | Flexeril® (Merck) Note 202:215 ratio in MS. |
| Methaqualone | 235 | 233 | 250 | 91 | 143 | 132 | | | | Quaalude |

5.11.5.2 CNS Stimulants

| Compound | Key Ions | | | | | | | Suggested Window | Class | Background Info. |
|---------------------------|----------|----------------|-----|-----|-----|-----|------------|------------------|---|---|
| | base | Prominent Ions | | | | | MW | | | |
| Amphetamine | 44 | 91 | 65 | 120 | 115 | 134 | 135 | 145 | Sympathomimetic Phenethylamine | Dexedrine® |
| Methamphetamine | 58 | 91 | 65 | 56 | 134 | 115 | 149 | 160 | Sympathomimetic Phenethylamine | Desoxyn® |
| Phentermine | 58 | 91 | 134 | 65 | 115 | 117 | 149 | 160 | Sympathomimetic Phenethylamine | Ionamin®, Fastin® |
| Benzphetamine | 148 | 91 | 65 | 149 | 77 | 42 | 239 | 250 | Sympathomimetic Phenethylamine | Didrex® Methamphetamine as metabolite (-CH ₂ C ₆ H ₅) |
| Diethylpropion | 100 | 72 | 77 | 44 | 56 | | 205 | 220 | Anorexiant Sympathomimetic Phenethylamine | Tenuate®, Tepanil® Anorexiant |
| Methylphenidate | 84 | 91 | 150 | 56 | 115 | 118 | 233 | 250 | Sympathomimetic Phenethylamine | Ritalin® Attention Deficient Disorder (ADD) |
| Ephedrine/Pseudoephedrine | 58 | 77/71 | 51 | 79 | 105 | 131 | 165 | 180 | Sympathomimetic Phenethylamine | Numerous cold and sinus preparations. |
| Mazindol | 266 | 268 | 231 | 204 | 176 | 115 | 284 | 300 | Sympathomimetic Phenethylamine | Sanorex® Anorexiant |
| Pemoline | 176 | 107 | 77 | 89 | 147 | 248 | 176 | 370 | Sympathomimetic Phenethylamine | Cylert® ADD, Narcolepsy |
| Phenmetrazine | 71 | 56 | 42 | 77 | 177 | 105 | 177 | 190 | Sympathomimetic Phenethylamine | Preludin® |

| Phendimetrazine | 85 | 57 | 42 | 56 | 191 | 70 | 191 | 200 | Sympathomimetic Phenethylamine | Plegine® Anorexiant |
|---|-----------------|----------------|-----|-----|-----|-----|------------|-----------------------------|-----------------------------------|--|
| Cocaine | 82 | 182 | 77 | 94 | 105 | 303 | 303 | 320 | Benzoic acid derivative | Alkaloid obtained from <i>Erythroxylon coca</i> |
| <i>Compound</i> | <i>Key Ions</i> | | | | | | | <i>Suggested Window</i> | <i>Class</i> | <i>Background Info.</i> |
| | base | Prominent Ions | | | | | MW | | | |
| Ecgonine methyl ester Methylecgonine | 82 | 96 | 83 | 199 | 168 | 182 | 199 | 220 | --- | Cocaine-M (-benzoylester) |
| Benzoylecgonine | 124 | 168 | 82 | 77 | 105 | 94 | 289 | 300 | --- | Cocaine-M (-methylester)_ |
| Benzoylecgonine-TMS | 82 | 240 | 105 | 361 | 256 | 346 | 361 | 380 | --- | Cocaine-M (-methylester)_ |
| Cocaethylene Ethylcocaine | 82 | 196 | 94 | 105 | 317 | 272 | 317 | 330 | --- | Transesterification occurs with concurrent cocaine + EtOH use |
| Norcocaine | 168 | 136 | 68 | 108 | 77 | 289 | 289 | 320 | --- | Cocaine metabolite, Demethylation of ecgonine |
| Propylhexedrine | 58 | 140 | 55 | 44 | 155 | 67 | 155 | 170 | Aliphatic amine | Benzedrex® Used as an Decongestant. Inhaler, has abuse potential as an amphetamine substitute |

5.11.5.3 Narcotic Analgesics

| <i>Compound</i> | <i>Key Ions</i> | | | | | | | <i>Suggested Window</i> | <i>Class</i> | <i>Background Info.</i> |
|---------------------------|-----------------|----------------|-----|-----|-----|-----|------------|-----------------------------|---|--|
| | base | Prominent Ions | | | | | MW | | | |
| Buprenorphine | 378 | 55 | 43 | 57 | 410 | 379 | 467 | 480 | Thebaine derivative | Subutex®, moderate to severe pain, opiate addiction |
| Codeine-TMS | 371 | 178 | 196 | 234 | 146 | 313 | 371 | 390 | Alkaloid | Tylenol 3® |
| Codeine | 299 | 162 | 229 | 214 | 124 | 115 | 299 | 320 | Alkaloid Methyl-morphine | Mild to moderate pain. Alkaloid occurs naturally in opium |
| Norcodeine | 285 | 215 | 81 | 148 | 115 | 164 | 285 | 300 | --- | Codeine-M (-CH ₃) |
| Morphine-2TMS | 429 | 236 | 196 | 414 | 146 | 414 | 429 | 450 | Alkaloid | |
| Morphine | 285 | 162 | 215 | 115 | 268 | 174 | 285 | 320 | Alkaloid | Moderate to severe acute and chronic pain. <i>Papaver somniferum</i> poppy |
| 6-Monoacetylmorphine | 327 | 268 | 43 | 215 | 146 | 284 | 327 | 350 | Alkaloid | Heroin Metabolite |
| Dihydrocodeine | 301 | 164 | 244 | 284 | 115 | 128 | 301 | 320 | Reduction of Codeine | |
| Dihydrocodeine-TMS | 373 | 236 | 146 | 282 | 315 | | | | Reduction of Codeine | TMS |
| Hydrocodone-TMS | 371 | 234 | 356 | 313 | 282 | 184 | | 390 | Synthetic opiate | See below |
| Hydrocodone | 299 | 242 | 214 | 185 | 115 | 96 | 299 | 320 | Synthetic opiate. Catalytic rearrangement of codeine | Hycodan®, Vicodin®, Codone®, Lortab® Moderate to moderately severe pain |
| Levophanol | 257 | 256 | 59 | 200 | 150 | 157 | 257 | 270 | Morphinan | Dromoran® (Europe) Severe pain |
| Meperidine (Pethidine) | 71 | 247 | 172 | 218 | 103 | 232 | 247 | 260 | Phenyl-piperidine | Demerol® (Sanofi), Moderate to severe pain |
| Meperidine-M | 57 | 42 | 56 | 233 | 158 | 91 | 233 | 260 | --- | Metabolite |
| | | | | | | | | | | |
| | | | | | | | | | | |
| <i>Compound</i> | <i>Key Ions</i> | | | | | | | <i>Suggested Window</i> | <i>Class</i> | <i>Background Info.</i> |

| | | | | | | | | | | |
|---|-----------|-----------|------------|------------|------------|------------|------------|------------|--|--|
| Methadone | 72 | 294 | 165 | 223 | 57 | 91 | 309 | 320 | Diphenyl-alkylketone | Dolophine [®] , Methadose [®] Severe pain, detox and temp. maintenance treatment of narcotic addiction |
| Methadone-M (nor-) -H ₂ O | 277 | 276 | 262 | 220 | 165 | 200 | 277 | 300 | --- | Metabolite |
| Oxycodone | 315 | 230 | 201 | 258 | 115 | 140 | 315 | 330 | Catalytic reduction of hydroxy-codeinone. | Percolone [®] , Roxicodone [®] , Oxycontin [®] , OxyR [®] , Moderate to moderately severe pain |
| Pentazocine | 217 | 110 | 70 | 202 | 230 | 285 | 285 | 300 | Benzomorphan derivative | Talwin [®] |
| Propoxyphene | 58 | 91 | 105 | 178 | 250 | 265 | 339 | 280 | | Darvon [®] , Darvocet [®] Mild to moderate pain |
| Norpropoxyphene/-M | 44 220 | 220 44 | 205 205 | 100 100 | 129 129 | 307 307 | | 320 320 | --- | Propoxyphene metabolites |
| Propoxyphene-M | 44 | 100 | 234 | 88 | 105 | 57 | 325 | 320 | --- | Metabolite |
| Propoxyphene Artifact (2) | 115 | 208 | 193 | 130 | 179 | 91 | 208 | 220 | --- | Metabolite |
| Tramadol | 58 | 263 | 135 | 77 | 107 | 218 | | 280 | | Ultram [®] Moderate pain with chronic pain |
| Tramadol-M (NDT) N-Desmethyltramadol | 188 | 135 | 150 | 249 | 77 | 55 | | | --- | Metabolite |
| N-Desmethyltramadol Artifact | 73 | 189 | 121 | 135 | 261 | | | | Carbamate derivative of NDT | Injection port formed. |
| Tramadol-M (ODT) O-Desmethyltramadol | 58 | 249 | 121 | 77 | | | | | --- | Metabolite |
| Fentanyl | 245 | 146 | 189 | 105 | 207 | 253 | 336 | 340 | Opioid/ Anilide Derivative | Sublimaze [®] Duragesic Post-Op pain, Chronic pain (transdermal) |
| Hydromorphone | 285 | 162 | 229 | 214 | 124 | 115 | 299 | 320 | Alkaloid Methyl-morphine | Mild to moderate pain. Alkaloid occurs naturally in opium |

5.11.5.4 PCP

| Compound | Key Ions | | | | | | | Suggested Window | Class | Background Info. |
|---------------|----------|----------------|-----|-----|-----|-----|------------|---------------------|-------|--------------------|
| | base | Prominent Ions | | | | | MW | | | |
| Phencyclidine | 200 | 91 | 242 | 243 | 186 | 166 | 243 | 260 | | Dissociative agent |

5.11.5.5 Hallucinogens

| Compound | Key Ions | | | | | | | Suggested Window | Class | Background Info. |
|------------------------------|----------|----------------|-----|-----|-----|-----|------------|---------------------|--------------------|---------------------------------------|
| | base | Prominent Ions | | | | | MW | | | |
| Mescaline | 182 | 167 | 181 | 211 | 151 | 148 | 211 | 230 | 2-Phenylethylamine | Peyote cactus |
| Mescaline Formyl Artifact | 44 | 181 | 182 | 58 | 167 | 223 | | 240 | --- | Metabolite/ artifact |
| Psilocyn | 58 | 204 | 42 | 77 | 117 | 146 | 204 | 210 | Indolethylamine | <i>Psilocybe mexicana</i> mushroom |
| 3,4-MDA | 44 | 136 | 135 | 77 | 51 | 81 | 179 | 190 | | |
| 3,4-MDMA | 58 | 77 | 135 | 51 | 105 | 89 | 193 | 210 | | |

5.11.5.6 Cannabis

| Compound | Key Ions | | | | | | | Suggested Window | Class | Background Info. |
|-----------------|------------|----------------|------------|-----|-----|-----|------------|---------------------|-------|------------------|
| | base | Prominent Ions | | | | | MW | | | |
| Carboxy-THC-TMS | 371 | 473 | 488 | 474 | 489 | 297 | 488 | FS=500 | | |
| Δ9-THC | 371 | 386 | 306 | | | | | | | |

5.11.6 OTHER COMPOUNDS OF INTEREST

Miscellaneous Diluents, Ancillary Compounds

| Compound | Key Ions | | | | | | | Suggested Window | Class | Background Info. |
|---------------|----------|----------------|-----|-----|-----|-----|------------|------------------|----------------------------|--------------------------|
| | base | Prominent Ions | | | | | MW | | | |
| Acetaminophen | 109 | 151 | 43 | 80 | 53 | | 151 | 160 | Aniline derivative | Tylenol® |
| Aspirin | 120 | 138 | 92 | 43 | 63 | 121 | 180 | 190 | Acetylsalicylic Acid | |
| Caffeine | 194 | 109 | 67 | 82 | 55 | 193 | 194 | 210 | Methylxanthine | Nodoze® |
| Ibuprofen | 163 | 161 | 91 | 107 | 119 | 117 | 118 | 206 | Arylacetic acid derivative | Nuprin®, Motrin®, Advil® |
| Lidocaine | 86 | 58 | 234 | 72 | 120 | 77 | 234 | 250 | Anilides | Xylocaine® |
| Nicotine | 84 | 133 | 162 | 161 | 42 | 119 | 162 | 180 | Alkaloid | |
| Cotinine | 98 | 176 | 119 | 118 | 175 | 42 | 176 | 190 | --- | Nicotine-M |
| Guaifenesin | 124 | 109 | 198 | 81 | 95 | 167 | 198 | 210 | Methoxyphenoxypropane diol | Expectorant Robitussin® |
| Verapamil | 303 | 304 | 151 | 58 | 260 | 165 | 454 | 470 | Calcium channel blocker | Calan®, Isoptin® |

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Revision History

Section Five

Quality Assurance

5.11 Key Ions for Commonly Encountered Compounds

| Revision # | Issue Date | Revision |
|-------------------|-------------------|--|
| 0 | 05-07-2007 | Combined urine (2.5.2) and blood compounds, updated compounds, reformatting. |
| 1 | 04/22/2015 | Addition of new or more common compounds |

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