

## Section Two

### Urine Toxicology

#### 5.11 Identification of Compounds in Urine

##### 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 services 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 compounds 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			
<b>Anticonvulsants</b>										
Carbamazepine	193	192	236	191	165	44	<b>236</b>	250	Ureas – Ethylene bridged 1,1-diphenylurea	Tegretol® (Novartis) Tonic-clonic and partial seizures
Carbamazepine-M/artifact	193	165	96	83	139	177	<b>193</b>	210	---	Diphenylurea
Carbamazepine Epoxide	180	193	207	252	152	223	<b>252</b>	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		<b>252</b>	280	Hydantoin	Dilantin® Structurally related to barbiturates. All seizure types except absence

Compound	Key Ions							Suggested Window	Class	Background Info.
	Base	Prominent Ions					MW			
<b>Anticonvulsants</b>										
Primidone	146	190	117	161	103	91	<b>218</b>	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	<b>339</b>	360	Sulfamate-substituted monosaccharide	Topamax® (Ortho-McNeil) Has numerous other indications
Valproic Acid	73	102	55	41	57	115	<b>144</b>	140	2-Propyl pentanoic acid	Depakote® / Depakene® (Abbott) Multiple seizure types including absence. Also for Mania
<b>Antidepressants/-M</b>										
Amitriptyline	58	202	215	189	178	165	<b>277</b>	300	Tricyclic (TGA) Tertiary Amine	Elavil® (Zeneca)
Nortriptyline	44	202	215	220	115	91	<b>263</b>	300	TCA Secondary Amine	Pamelor® (Novartis) Norpramin®, Pertofrane®. Parent <i>or</i> metabolite of amitriptyline
Citalopram	58	238	208	42	190	221	<b>324</b>	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	<b>313</b>	350	TCA Secondary Amine	Asendin® (Lederle) Depression w/anxiety or agitation.
Loxepine	257	70	83	193	228	259	<b>327</b>	350	TCA	Loxitane® (antipsychotic), Parent <i>or</i> metabolite of amoxapine
Bupropion	44	100	57	139	111	224	<b>239</b>	250	Aminoketone	Wellbutrin® (GlaxoWellcome)
Imipramine	234	235	58	193	195	220	<b>280</b>	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	<b>296</b>	310	---	Metabolite
Desipramine	234	195	193	235	208	266	<b>266</b>	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	<b>314</b>	320	TCA Tertiary amine	Anafranil® (Novartis) Obsessive-compulsive disorder (OCD)
Doxepine	58	42	165	152	178	189	<b>279</b>	290	TCA Tertiary amine	Sinequan® (Roerig) Also for anxiety.
Nordoxepine	44	178	165	222	204	128	<b>265</b>	280	---	Metabolite of Doxepin
Fluoxetine	44	104	91	59	309	148	<b>309</b>	320	Unrelated to other Anti-depressants	Prozac® (Dista) Selective 5-HT reuptake inhibitor For OCD also.
Norfluoxetine	134	104	191	162	77	251	<b>295</b>	300	---	Metabolite of Fluoxetine
Maprotiline	44	203	202	277	189	59	<b>277</b>	300	Tetracyclic	Ludiomil® (Novartis)
Mirtazapine	195	194	208	196	180	167	<b>265</b>	280	Tetracyclic	Remeron®
Paroxetine	192	44	138	329	70	109	<b>177</b>	200		Paxil® Selective 5-HT reuptake inhibitor

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

Pentobarbital	156	141	157	98	197	69	<b>226</b>	230	Barbiturate Alkyl-substituted barbituric acid	Nembutal <sup>®</sup>
<b>Compound</b>	<b>Key Ions</b>							<b>Suggested Window</b>	<b>Class</b>	<b>Background Info.</b>
	base	Prominent Ions					MW			
<b>Sedative/Hypnotic</b>										
Phenobarbital	204	232	117	161	146	217	<b>232</b>	240	Barbiturate Phenyl/alkyl-substituted barbituric acid	Luminal <sup>®</sup> , Phenalix <sup>®</sup> , Solfotin <sup>®</sup> Long-Acting Also – <b>Anti-convulsant</b>
Secobarbital	168	167	195	97	153	124	<b>238</b>	220	Barbiturate Alkyl-substituted barbituric acid	Secobarbital <sup>®</sup> , Tuinal <sup>®</sup>
Zaleplon	248	305	263	262	43	249	<b>305</b>	380	Pyrazolopyrim-idine	Sonata <sup>®</sup>
Zolpidem	235	236	92	65	219	307	<b>307</b>	320	Imidazopyridine	Ambien <sup>®</sup>
<b>Miscellaneous Depressants</b>										
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	<b>259</b>	270	Aryloxypropanol- amine	Inderal β-Blocker
Fenfluramine	72	159	44	109	216	56	<b>231</b>	250	Sympatho-mimetic Phenethylamine	Anorexiant, Sedation and Drowsiness
<b>Benzodiazepines Anxiety/Hypnotic/Anticonvulsant</b>										
Alprazolam	279	204	308	273	77	245	<b>308</b>	350	Triazolo- benzodiazepine	Xanax <sup>®</sup>
α-Hydroxyalprazolam- TMS	381	396	383	293	190	173	---	420	---	Metabolite of alprazolam
Diazepam	256	283	284	257	221	165	<b>284</b>	300	1,4- benzodiazepine	Valium <sup>®</sup> (Roche) Also – <b>Muscle Relaxant</b>
Midazolam	310	312	311	163	325	75	<b>325</b>	340	Fluorinated Triazolo benzodiazepine	Versed <sup>®</sup>
α-Hydroxymidazolam- TMS	310	73	398	413	383	168	---	460	---	Metabolite of midazolam
Nordiazepam	242	241	269	270	214	151	<b>270</b>	290	1,4- benzodiazepine	Calmday <sup>®</sup> , Madar <sup>®</sup> , Stilny <sup>®</sup> Parent or metabolite of diazepam, prazepam, clorazepate, chlordiazepoxide
Nordiazepam-TMS	341	342	343	327	227	269	---	350	1,4- benzodiazepine	See above
Oxazepam	205	239	267	177	151	104	<b>286</b>	280	1,4- benzodiazepine	Serax <sup>®</sup> (Wyeth-Ayerst)
Oxazepam-TMS	429	430	313	147	401	415	---	450	1,4- benzodiazepine	See above.
Temazepam	271	255	300	165	193	228	<b>300</b>	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	<b>320</b>	340	Dichloro-1,4- benzodiazepine	Ativan <sup>®</sup>
Lorazepam-TMS	429	431	147	347	177	449	---	470	Dichloro-1,4- benzodiazepine	Ativan <sup>®</sup>
Triazolam	313	238	315	342	203	279	<b>342</b>	380	Triazolo- benzodiazepine	Halcion <sup>®</sup>
α-Hydroxytriazolam							---		Triazolo- benzodiazepine	Metabolite of triazolam
Clonazepam	280	314	286	315	234	288	<b>315</b>	350	7-Nitro benzodiazepine	Klonopin <sup>®</sup> (Roche) Akinetic and myoclonic seizures

7-Aminoclonazepam	285	256	257	258	44	287	---	300	7-Nitro benzodiazepine	Metabolite
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Compound	Key Ions							Suggested Window	Class	Background Info.
	base	Prominent Ions					MW			
<b>Benzodiazepines</b> <i>Anxiety/Hypnotic/Anticonvulsant</i>										
Flurazepam	86	99	87	183	58	315	<b>387</b>	400	Fluoro-1,4-benzodiazepine	Dalmane®
Flunitrazepam	312	286	285	313	266	238	<b>313</b>	360	7-Nitro benzodiazepine	Rohypnol®
Midazolam										
<b>Muscle Relaxants</b>										
Baclofen	138	103	195	77	140	75	<b>213</b>	230	3-(p-Chloro phenyl)-γ aminobutyric acid	Lioresal®, GABA analog. Spasticity Depresses synaptic transmission
Carisoprodol	55	58	158	97	104	83	<b>260</b>	270	Dicarbamate	Soma® Major side effect is drowsiness
Meprobamate	83	55	71	96	114	144	<b>218</b>	170	Carbamate derivative	Miltown® (Wallace), Equanil® Parent or metabolite of carisoprodol
Meprobamate artifact (early R <sub>i</sub> )	84	55	56	83	41	101		120	Carbamate	
Meprobamate artifact (mid R <sub>i</sub> )	84	55	56	83	41	101		120	Carbamate	
Methocarbamol	118	109	124	77	62	81	<b>241</b>	250	Carbamate derivative	Robaxin®
Cyclobenzaprine	58	215	202	216	213	189	<b>275</b>	300	Very similar to amitriptyline (TCA).	Flexeril® (Merck) Note 202:215 ratio in MS.

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

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

## 5.11.5.3 Narcotic Analgesics

Compound	Key Ions							Suggested Window	Class	Background Info.
	base	Prominent Ions					MW			
Buprenorphine	378	55	43	57	410	379	<b>467</b>	480	Thebaine derivative	Subutex®, moderate to severe pain, opiate addiction
Codeine-TMS	371	178	196	234	146	313	<b>371</b>	390	Alkaloid	Tylenol 3®
Codeine	299	162	229	214	124	115	<b>299</b>	320	Alkaloid Methyl-morphine	Mild to moderate pain. Alkaloid occurs naturally in opium
Norcodeine	285	215	81	148	115	164	<b>285</b>	300	---	Codeine-M (-CH <sub>3</sub> )
Morphine-2TMS	429	236	196	414	146	414	<b>429</b>	450	Alkaloid	
Morphine	285	162	215	115	268	174	<b>285</b>	320	Alkaloid	Moderate to severe acute and chronic pain. <i>Papaver somniferum</i> poppy
6-Monoacetylmorphine	327	268	43	215	146	284	<b>327</b>	350	Alkaloid	Heroin Metabolite
Dihydrocodeine	301	164	244	284	115	128	<b>301</b>	320	Reduction of Codeine	
Hydrocodone-TMS	371	234	356	313	282	184		390	Synthetic opiate	See below
Hydrocodone	299	242	214	185	115	96	<b>299</b>	320	Synthetic opiate. Catalytic rearrangement of codeine	Hycodan®, Vicodin®, Codone®, Lortab® Moderate to moderately severe pain
Levophanol	257	256	59	200	150	157	<b>257</b>	270	Morphinan	Dromoran® (Europe) Severe pain
Meperidine (Pethidine)	71	247	172	218	103	232	<b>247</b>	260	Phenyl-piperidine	Demerol® (Sanofi), Moderate to severe pain
Meperidine-M	57	42	56	233	158	91	<b>233</b>	260	---	Metabolite
Methadone	72	294	165	223	57	91	<b>309</b>	320	Diphenyl-alkylketone	Dolophine®, Methadose® Severe pain, detox and temp. maintenance treatment of narcotic addiction
Methadone-M (nor-) -H <sub>2</sub> O	277	276	262	220	165	200	<b>277</b>	300	---	Metabolite

Oxycodone	315	230	201	258	115	140	<b>315</b>	330	Catalytic reduction of hydroxy-codeinone.	Percolone <sup>®</sup> , Roxicodone <sup>®</sup> , Oxycontin <sup>®</sup> , OxyR <sup>®</sup> , Moderate to moderately severe pain	
Pentazocine	217	110	70	202	230	285	<b>285</b>	300	Benzomorphan derivative	Talwin <sup>®</sup>	
Propoxyphene	58	91	105	178	250	265	<b>339</b>	280		Darvon <sup>®</sup> , Darvocet <sup>®</sup> Mild to moderate pain	
<b>Compound</b>	<b>Key Ions</b>							<b>Suggested Window</b>	<b>Class</b>	<b>Background Info.</b>	
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	<b>325</b>	320	---	Metabolite	
Propoxyphene Artifact (2)	115	208	193	130	179	91	<b>208</b>	220	---	Metabolite	
Tramadol	58	263	135	77	107	218		280		Ultram <sup>®</sup> 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	<b>336</b>	340	Opioid/ Anilide Derivative	Sublimaze <sup>®</sup> Duragesic Post-Op pain, Chronic pain (transdermal)	
Hydromorphone	285	162	229	214	124	115	<b>299</b>	320	Alkaloid Methyl-morphine	Mild to moderate pain. Alkaloid occurs naturally in opium	

5.11.5.4 PCP

<b>Compound</b>	<b>Key Ions</b>							<b>Suggested Window</b>	<b>Class</b>	<b>Background Info.</b>
	base	Prominent Ions					MW			
Phencyclidine	200	91	242	243	186	166	<b>243</b>	260		Dissociative agent

5.11.5.5 Hallucinogens

<b>Compound</b>	<b>Key Ions</b>							<b>Suggested Window</b>	<b>Class</b>	<b>Background Info.</b>
	base	Prominent Ions					MW			
Mescaline	182	167	181	214	151	148	<b>211</b>	230	2-Phenylethylamine	Peyote cactus
Mescaline Formyl Artifact	44	181	182	58	167	223		240	---	Metabolite/ artifact
Psilocyn	58	204	42	77	117	146	<b>204</b>	210	Indolethylamine	<i>Psilocybe mexicana</i> mushroom
3,4-MDA	44	136	135	77	51	81	<b>179</b>	190		
3,4-MDMA	58	77	135	51	105	89	<b>193</b>	210		

5.11.5.6 Cannabis

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

5.11.6 **OTHER COMPOUNDS OF INTEREST**  
Miscellaneous Diluents, Ancillary Compounds

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

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## ***Revision History***

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### Section Five

#### Quality Assurance

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#### **5.11 Key Ions for Commonly Encountered Compounds**

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<b>Revision #</b>	<b>Issue Date</b>	<b>Revision</b>
0	05-07-2007	Combined urine (2.5.2) and blood compounds, updated compounds, reformatting.

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