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Identification of Drugs by Chemical Ionization Mass Spectroscopy—Part II*

Forensic scientists are currently actively evaluating new instrumental techniques to determine their potential application for solving some of the problems that are unique to their field. Liquid chromatography, flameless atomic absorption, electron scanning microscopy, and thermal analysis offer fertile areas for research and development. Mass spectroscopy is by no means a new instrumental technique; its application to analytical organic chemistry has been well documented since the early 1960's [*1–4*]. Unfortunately, its utilization in the forensic sciences has been minimal up to the present. A major limitation has been the cost and complexity of the instrument. However, with increased fundings becoming available to many laboratories and with the improved engineering and reliability of the latest generation of mass spectrometers, this technique is becoming feasible for many forensic laboratories. Its application to forensic drug identification has been demonstrated in previous publications [*5–8*].

Since the spectra that are generated by conventional electron impact (EI) mass spectroscopy are frequently quite complex, materials must be introduced into the mass spectrometer's source in a relatively pure state. This requirement is usually accomplished by the separation of a material's components on a gas chromatograph that has been interfaced to the mass spectrometer. The practical effect of this process is that the analyst must have some prior information regarding the material's composition in order to select the proper chromatographic conditions. Consequently, mass spectroscopy has been limited to a confirmatory role in forensic drug identification, supplementing chromatographic and spectrophotometric techniques.

The recent development of a new mass spectral ionization process known as chemical ionization (CI) offers the potential of making the mass spectrometer a versatile instrument that is capable of participating in all facets of forensic drug identification. Basically, a combined EI/CI source provides the analyst with the option of identifying multicomponent mixtures without prior chromatographic separation, as well as by the more conventional EI mass spectral techniques. As a result of the work that has been conducted at the New Jersey State Police Laboratory, it is apparent that CI represents a major advancement in the utilization of analytical instrumentation for drug identification. This paper presents a compilation of CI spectral data for 303 drugs and common diluents, and discusses various applications that CI offers for the identification of drug mixtures.

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Experimental

All CI spectra were taken on a Dupont 21-490 single focusing mass spectrometer. The instrument was fitted with a dual EI/CI source and a differential pumping system. The unit has a resolution of 600 with a 10 percent valley. The reagent gas was isobutane (99.9 percent pure) at a source pressure of 0.5–1.0 torr. The source temperature was 200° ± 10°C. The ionizing voltage was 300 eV in the CI mode. All materials analyzed were admitted into the source through the direct probe. When pure standards were available they were analyzed in their salt form; otherwise the materials were extracted into chloroform as a free acid or base and examined as such. The temperatures selected varied with the volatility of the compound. A probe temperature at either 100, 200, or 300°C was found adequate for all materials analyzed. Spectra of unknown substances were taken at all three temperatures.

Five cubic centimetres of urine were made acid at a pH of 2 and extracted into chloroform. The chloroform was evaporated to near dryness and 10 μl transferred to a ½-in. capillary tube closed at one end. The chloroform was taken to dryness and placed into the direct probe of the mass spectrometer. Spectra were taken at probe temperatures of 100, 200, and 300°C. Counting isobutane CI spectra presented no difficulty, because at high gain ions from the sample and background are observed at every mass unit. This eliminates the need for a mass marker in CI analysis.

Discussion and Results

Chemical ionization mass spectroscopy was first developed by Munson and Field in 1966 at Esso Research Laboratories [*9*]. Whereas conventional EI spectra are generated by the direct impact of high energy electrons (70 eV) with the sample molecules at a source pressure of 10^{-7} torr, the CI process uses high energy electrons (300 eV) to first ionize a reagent gas at a source pressure of 0.5–1.0 torr; the sample is then in turn ionized by these reagent gas ions. An EI source must be modified in order to accommodate the high pressures required for CI; several authors have described the necessary modifications that were made [*10–12*]. Several CI mass spectrometers are currently available commercially with more manufacturers planning to include CI as an option in their line of commercial mass spectrometers in the near future.

The selection of a reagent gas will determine the complexity of the spectrum that is produced. The analyst is therefore provided with enormous latitude in determining the characteristics and complexity of the CI spectrum. Ionized helium and nitrogen gases, through a charge-transfer process, produce spectra quite comparable to that of EI spectra. In the presence of methane or isobutane gases, the sample molecule will be ionized through a proton-transfer reaction. The *tert*-butyl ion ($t\text{-}C_4H_9^+$) is produced in highest concentration when isobutane is ionized. The proton-transfer reaction of this ion with the sample molecules will produce protonated molecular ions (MH^+) which undergo little decomposition [*13*]. Hence, spectra generated by isobutane CI usually display a predominant MH^+ with little or no fragmentation. Ionized methane will produce comparable spectra displaying more fragmentation than isobutane. The majority of drugs for which isobutane CI spectral data has been collected generally show fewer than four ions in abundances greater than 10 percent. The comparison of the EI and isobutane CI spectra of heroin illustrates the simplicity of the latter (see Fig. 1).

A good deal of research remains to be done in determining the CI characteristics of other potential reagent gases. Dimethylamine has been found to react preferentially with carbonyl compounds, thus offering the possibility that CI could eventually be

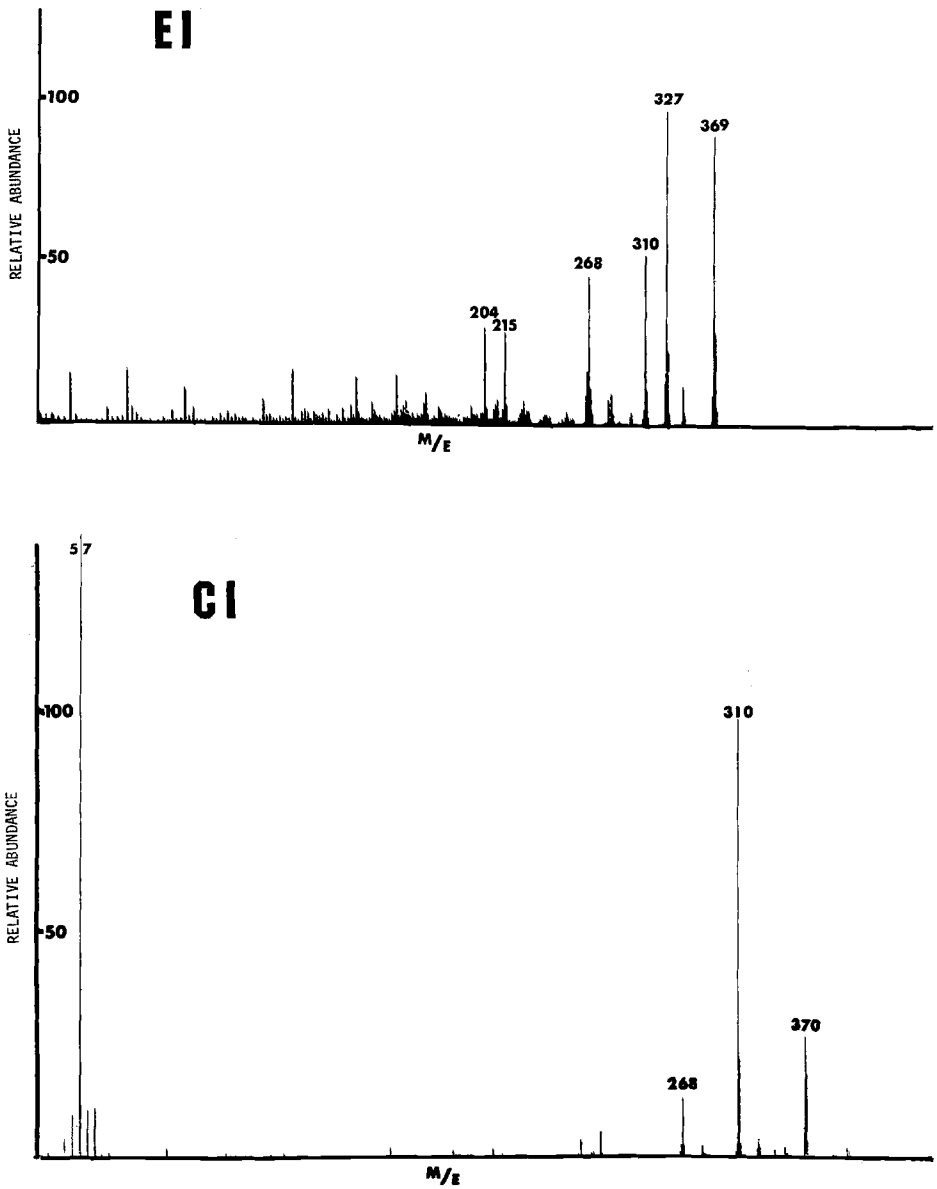

FIG. 1—*Mass spectra of heroin (EI and CI).*

applied for function group analysis [*14*]. Hunt and Ryan have demonstrated that an argon-water mixture reagent gas will generate spectra that exhibit the combined characteristics of methane and EI spectra [*15*].

The primary advantage of isobutane CI is that it permits the analyst to rapidly identify the components of a complex organic mixture without having to resort to any prior chromatographic separation techniques. This is best accomplished by placing the material in the spectrometer's source through the direct probe; each component of the

mixture would then be expected to produce a predominant MH^+ peak for identification. Published isobutane CI drug spectra have already demonstrated the applicability of this technique to forensic drug identification [*16–18*]. The isobutane CI drug spectra collection has now been expanded to include 303 drugs and common diluents (see Tables 1 and 2). While the simplicity of these spectra would not allow them to be used as a specific means of identification, examination of Table 1 reveals that drug identification can still be made with a high degree of certainty by this technique. Of the 303 compounds listed, 14 pairs showed indistinguishable isobutane CI spectra; three drugs—phentermine, phenylpropylmethylamine and methamphetamine—were also found indistinguishable from one another. The monosaccharide and disaccharide sugars examined all have similar CI spectra.

Interestingly, the fragmentation of MH^+ can be described by mechanisms that are analogous to those used in solution carbonium ion chemistry [*16*]. The loss of neutral fragments such as H_2O, RCOOH, and NH_3 from MH^+ are common occurrences, and are suggestive of the presence of nonphenolic hydroxy groups, esters, and amines, respectively. This type of fragmentation is exemplified by the loss of water at the C-6 position from the protonated morphine ion (see Fig. 2). All morphine derivatives having a free C-6 hydroxy group show an ion corresponding to the loss of water from MH^+ in the isobutane CI spectrum.

A major advantage of the isobutane CI drug collection is that it can easily accommodate a manual search system. Experience indicates that it is not necessary to resort to an expensive computerized data retrieval system; a simple arrangement of spectral data on index cards is found to be most convenient. Data can be retrieved from either alphabetically arranged cards as shown in Table 1, or from cards that are arranged numerically according to the major ion present in each spectrum (Table 2). The compilation of a molecular weight index for most drugs listed in the Merck Index (8th edition) supplements such a data collection [*19*].

As illicit drugs are generally received in combination with mixtures of organic diluents, the CI technique has been successfully applied for their direct analysis without prior chromatographic separation or solvent extraction [*16,18*]. It has already been shown that identical mass spectra are produced by drugs in both their salt and free acid or base forms [*18,20*]. This observation precludes the necessity of any sample preparation prior to the insertion of the illicit powder in the direct probe of the mass spectrometer. Figure 3 illustrates an isobutane CI spectrum of approximately one microgram of Amesec®, a common prescription drug. The four components of Amesec®, amobarbital, aminophylline (a mixture of theophylline and ethylenediamine), and ephedrine, are identifiable

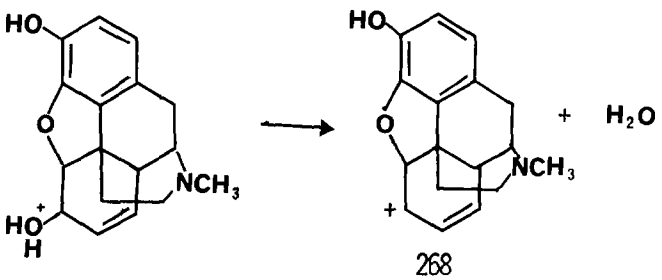

FIG. 2—*Mechanism for the fragmentation of morphine.*

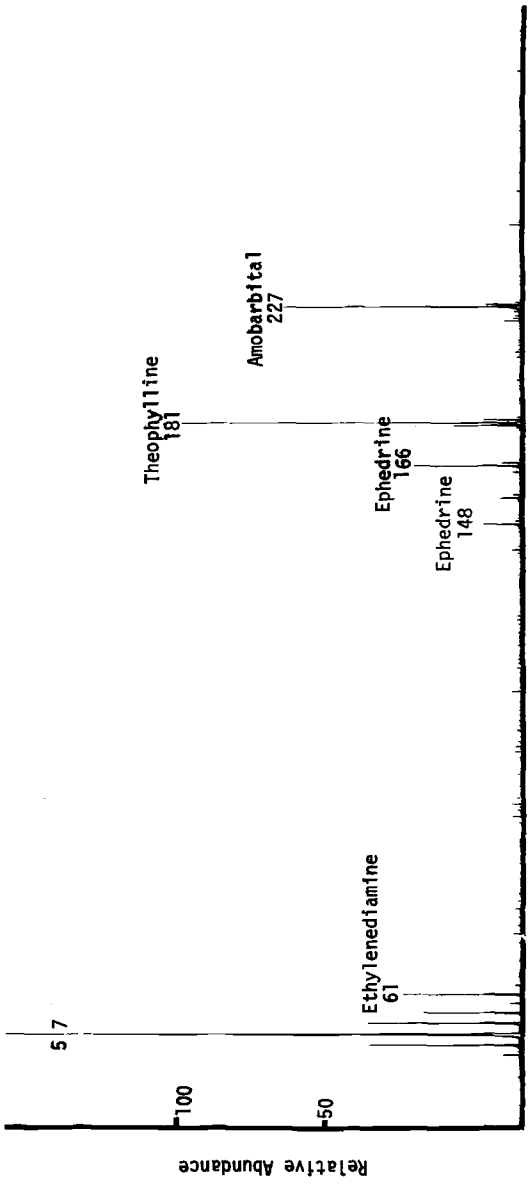

FIG. 3—*CI mass spectrum of Amesec®.*

TABLE 1—*Alphabetical index of isobutane CI mass spectra*[a,b].

Compounds	Molecular Weight	Mass Spectral Peaks in Order of Abundance						
		1	2	3	4	5	6	7
Acetaminophen	151	152						
Acetazolamide	222	223	207 (18%)					
Acetophenazine	411	117	99 (80%)	412 (55%)				
Acetylcarbromal	278	279	281 (98%)					
Acetylcodeine	341	282	342 (15%)					
n-Acetylcysteine	163	164						
Acetylsalicylic acid	180	121	139 (20%)	163 (18%)	181 (17%)	138 (17%)	180 (10%)	
Acetylethylmorphine	355	296	356 (27%)					
Adiphenine	311	312	100 (65%)	86 (20%)				
Adrenaline	183	166	184 (25%)					
Allylbarbital	224	225	185 (17%)					
Alphaprodine	261	188	187 (50%)	172 (35%)	262 (26%)			
Alphenal	244	245	113 (43%)	205 (14%)				
Alverine	281	282	176 (30%)					
Allobarbital	208	209	169 (11%)					
Amantadine	151	152	135 (48%)	151 (32%)	150 (15%)			
Aminoantipyrine	203	204	203 (50%)	84 (42%)				
Aminophenol	109	110	109 (40%)					
p-Aminosalycylate	153	154	153 (28%)	135 (13%)	136 (12%)			
Amitriptyline	277	278						
Amobarbital	226	227						
Amphetamine	135	136						
Anileridine	352	353	351 (25%)	212 (24%)	246 (14%)	234 (10%)		
Anthracene	178	179	178 (14%)					
Apomorphine	267	268	267 (22%)	266 (20%)				
Aprobarbital	210	211	171 (13%)					
Ascorbic acid	176	177						
Atrolactic acid	166	167	149 (58%)	107 (37%)	166 (30%)			
Atropine	289	124	290 (17%)					
Barbital	184	185						
Barbituric acid	128	129						
Benactyzine	327	328	310 (74%)	183 (20%)				
Bendroflumethiazide	421	422	320 (38%)					
Benzocaine	165	166						
Benzopyrene	252	253	252 (59%)					
Benzphetamine	239	240	148 (85%)					
Biperiden	311	312						

Bishydroxycoumarin	336	337	163 (32%)					
Brompheniramine	318	319	321 (98%)	166 (15%)				
Brucine	394	395						
Bufotenine	204	205	198 (11%)					
Butabarbital	212	213						
Butacaine	306	307	263 (20%)					
Butethal	212	213						
Caffeine	194	195						
Cannabidiol	314	315						
Cannabinol	311	312						
Cantharidin	196	197						
Carbinoxamine	290	291	293 (30%)					
Carbromal	236	237	239 (98%)					
Chloramphenicol	322	323	325 (65%)	305 (34%)	307 (18%)	289 (18%)	291 (10%)	327 (10%)
Chlordiazepoxide	299	284	286 (33%)	300 (33%)	283 (30%)	285 (30%)	302 (10%)	
Chloroacetophenone	154	155	157 (35%)	139 (20%)	154 (17%)			
Chlorophenylalanine	199	200	202 (35%)	154 (30%)				
Chlorpheniramine	274	275	277 (30%)	230 (22%)	203 (10%)			
Chlorphentermine	183	184	186 (30%)					
Chlorpromazine	318	319	318 (32%)	234 (30%)				
Chlorpropamide	276	192	194 (35%)					
Chlorprothixene	315	316	318 (30%)					
Chlortetracycline	478	479	481 (40%)	461 (20%)				
Chlorzoxazone	169	170	172 (35%)	118 (20%)	136 (10%)			
Cholesterol	386	369	212 (67%)	385 (32%)				
Cinchonidine	294	295	296 (20%)					
Clofibrate	242	243	115 (55%)	245 (30%)	128 (13%)	169 (12%)		
Cocaine	303	304	182 (33%)					
Codeine	299	282	300 (22%)					
Colchicine	399	400	399 (25%)	372 (20%)	386 (15%)	371 (15%)		
Coniine	127	128	126 (24%)					
Coranine	178	179						
Cotarmine	255	204	118 (40%)					
Cyclandelate	276	125	277 (30%)	107 (20%)	135 (18%)			
Cyclophosphamide	260	261	211 (30%)	225 (25%)	213 (11%)	227 (10%)		
Cyproheptadine	287	288	287 (30%)					
Desipramine	266	267	222 (21%)					
Diacetylmorphine	360	310	370 (33%)	268 (14%)				
Dianisidine	244	245						
Diazepam	284	285	287 (30%)					
Dibucaine	343	344						
Dicyclomine	309	310	100 (55%)	86 (48%)	69 (35%)			

(*Continued*)

TABLE 1—Continued.

Compounds	Molecular Weight	Mass Spectral Peaks in Order of Abundance						
		1	2	3	4	5	6	7
Diethylpropion	205	206	204 (30%)	100 (28%)	135 (15%)			
Diethylstillbestrol	268	269	268 (35%)					
Diethyltryptamine	216	217						
Dihydrocodeine	301	302	284 (25%)	301 (20%)				
Dihydrocodeinone	299	300						
Dihydrodiacetylmorphine	371	372	312 (15%)	330 (12%)				
Dihydromorphine	287	288	287 (18%)					
2,5-Dimethoxy-4-methylamphetamine	209	210						
Dimethyldihydroresorcinol	140	141						
2,6-Dimethyl-4-isopropylbenzaldehyde thiosemicarbazone	249	250	174 (18%)	158 (15%)				
Dimethylgloxime	116	117	116 (16%)					
Dimethyltryptamine	188	189						
Dioxyline	367	368						
Diphenhydramine	255	256	167 (25%)					
Diphenylhydantoin	252	253						
Doxepine	279	280						
Doxycycline hyclate	444	445	444 (12%)	427 (10%)				
1-Dromoran	257	258	256 (50%)	257 (25%)				
Dydrogesterone	312	313	312 (72%)	268 (33%)	207 (15%)			
Dyphylline	254	255	254 (40%)					
Emetine	480	481	479 (60%)	480 (48%)				
Ephedrine	165	166	148 (50%)					
Ergonovine	325	326	268 (35%)	308 (12%)	325 (12%)			
Ethacrynic acid	302	303	305 (65%)	285 (10%)				
Ethchlorvynol	144	127	129 (34%)	109 (10%)				
Ethinamate	167	125	107 (66%)	163 (13%)				
Ethionamide	166	167	166 (25%)					
Ethosuximide	141	142						
Ethoxazene	256	257	256 (45%)	138 (15%)	133 (15%)			
5-Ethyl-5-(3 hydroxy-1-methylbutyl)-barbituric acid	242	225	243 (40%)	157 (23%)				
Ethylenediamine	60	61						
Ethylmorphine	313	296	314 (11%)					

5-Ethyl-2 thiobarbital	172	173					
Ethynylestrodiol	296	279	297 (50%)	296 (32%)	280 (21%)	295 (19%)	213 (12%)
Fenfluramine	231	232	72 (68%)	212 (25%)			
Fructose	180	163	145 (85%)	127 (25%)			
Furazolidone	225	226					
Galactose	180	163	145 (85%)	127 (25%)			
Gentisic acid	154	155					
Glucose	180	163	145 (85%)	127 (25%)			
Glutethimide	217	218					
Glyceryl Guaiacolate	198	199	198 (60%)	124 (50%)	125 (30%)		
Glycine	75	76					
Griseofulvin	352	353	355 (35%)	352 (30%)			
Hexachlorophene	404	407	409 (80%)	405 (50%)	411 (40%)		
Hexobarbital	236	237					
Hippuric acid	179	180	105 (54%)	135 (31%)	134 (21%)	162 (15%)	
Histamine	111	112					
Homatropine	275	124	107 (14%)	276 (10%)			
Hydralazine	160	161					
Hydromorphone	285	286					
p-Hydroxyamphetamine	151	152	135 (95%)				
Hydroxybenzoic acid	138	139	121 (35%)				
d-4-Hydroxynorephedrine	167	150	168 (50%)	123 (17%)			
B-Hydroxy-B-phenyl-ethylamine	137	138	120 (50%)				
4-Hydroxyphenylisopropyl-methylamine	165	166	135 (10%)				
Hydroxytyramine	153	154	137 (24%)	124 (24%)			
Hydroxyzine	374	375	377 (30%)				
Hyoscyamine	289	124	237 (20%)	290 (15%)			
Ibogaine	310	311					
Imipramine	280	281					
Indomethacin	357	358	357 (44%)	360 (38%)			
Isobarbituric acid	128	129					
Isoephedrine	165	166	107 (42%)	148 (15%)			
Isoniazide	137	138	137 (10%)				
Isoproterenol	211	194	212 (50%)	192 (30%)			
Isoxsuprine	301	302	178 (16%)	284 (12%)			
Lactose	342	163	145 (85%)	127 (25%)			
Levallorphan	283	284	282 (50%)	283 (25%)			
Lidocaine	234	235	86 (13%)				
Lysergic acid diethylamide	323	324					

(Continued)

TABLE 1—Continued.

Compounds	Molecular Weight	Mass Spectral Peaks in Order of Abundance						
		1	2	3	4	5	6	7
Mandelic acid	152	135	107 (65%)					
Mannitol	182	183	165 (20%)	147 (10%)	129 (10%)			
Mannose	180	163	145 (85%)	127 (25%)				
Mebutamate	232	233	172 (75%)					
Meclizine	390	391	393 (30%)	390 (18%)	189 (18%)	389 (11%)	243 (10%)	
Mecloqualone	270	235	271 (90%)	273 (32%)	118 (10%)			
Meperidine	247	248						
Mephensine	182	183	147 (30%)	109 (17%)	165 (15%)			
Mephenoxalone	223	224	223 (25%)	155 (25%)	125 (25%)	218 (15%)	124 (10%)	157 (10%)
Mephentermine	163	164						
Mephenytoin	218	219	189 (10%)					
Mephobarbital	246	247						
Meprobamate	218	219	158 (61%)					
Mescaline	211	212						
Metanephrine	197	198	180 (27%)					
Metaxalone	221	222						
Methacycline	442	443	198 (38%)	425 (10%)	400 (10%)			
Methadone	309	310						
Methallenestrill	286	199	287 (58%)	269 (25%)	229 (18%)			
Methamphetamine	149	150						
Methapyrilene	261	262	166 (27%)	191 (13%)				
Methaqualone	250	251	250 (30%)	235 (20%)				
Metharbital	198	199						
Methdilazine	296	297						
Methenamine	140	141	112 (45%)	140 (35%)				
Methocarbamol	241	242	199 (100%)	118 (83%)	124 (33%)	224 (10%)		
Methohexital	262	263						
d-Methorphan	271	272	270 (64%)	271 (21%)				
Methoxamine	211	212	194 (55%)	152 (20%)	168 (18%)	167 (15%)		
m-Methoxyamphetamine	165	166	149 (10%)	138 (10%)				
p-Methoxyamphetamine	165	166	149 (45%)	122 (15%)				
Methsuximide	203	204						
p-Methylamphetamine	149	150	133 (49%)					
Methylenedioxy-amphetamine	179	180	136 (10%)					
n-Methylephedrine	179	72	180 (50%)	162 (20%)				
Methylergonovine	339	340	322 (26%)	339 (15%)				

Methylphenidate	233	234	84 (70%)	151 (10%)				
Methylsalicylamide	151	152	151 (73%)	121 (25%)	120 (13%)			
Methylsalicylate	152	153	152 (35%)	120 (35%)	121 (20%)			
3-Methylsalicylate	152	135	134 (82%)	153 (80%)	152 (70%)	105 (42%)	106 (34%)	78 (25%)
Methyltryptamine	174	175	158 (50%)	131 (40%)				
Methylprylone	183	184						
Methysergide	353	354	353 (15%)					
Metronidazole	171	172						
Metyrapone	226	227	226 (36%)	120 (12%)				
O^6-Monoacetylmorphine	327	328	268 (55%)	327 (30%)				
Morphine	285	268	286 (20%)					
Naphazoline	210	211	210 (20%)	209 (18%)				
Nicotinamide	122	123						
Nicotire	162	163						
Nitrofurantoin	238	239	238 (20%)					
Nortriptyline	263	264						
Noscapine	413	221	222 (15%)					
Orphenadrine	269	181	270 (80%)	224 (11%)	198 (10%)			
Oxanamide	157	158	131 (10%)					
Oxazepam	286	269						
Oxycodone	315	316						
Oxymorphone	301	302						
Oxyphenbutazone	324	325	324 (70%)	199 (35%)				
Oxytetracycline	460	461	443 (30%)	198 (30%)	460 (16%)			
Palmitic acid	256	257	256 (90%)	239 (85%)				
Papaverine	339	340						
Pentanediamine	102	103	86 (39%)					
Pentazocine	285	286	284 (50%)	285 (40%)	217 (16%)	230 (10%)		
Pentobarbital	226	227						
Pentylenetrazole	138	139						
Perhenazine	403	404	406 (30%)	234 (19%)				
Phenacaine	298	299	262 (18%)					
Phenacetin	179	180	179 (12%)					
Phenaglycodol	214	197	155 (45%)	199 (35%)	157 (18%)	198 (15%)	156 (15%)	
Phenazopyridine	213	214	213 (11%)	105 (15%)				
Phencyclidine	243	244	242 (63%)					
Phendimethrazine	191	192						
Phenelzine	136	137	135 (34%)	122 (22%)	105 (12%)			
Phenethylamine	121	122	105 (45%)	91 (22%)				
Phenindamine	261	262						
Pheniramine	240	241						

(*Continued*)

TABLE 1—Continued.

Compounds	Molecular Weight	Mass Spectral Peaks in Order of Abundance						
		1	2	3	4	5	6	7
Phenmetrazine	177	178						
Phenobarbital	232	233						
Phenothiazine	199	199	200 (45%)					
Phentermine	149	150						
Phenylbutazone	308	309	190 (50%)					
Phenylephrine	167	168	150 (33%)	123 (10%)				
Phenylpropanolamine	151	152	134 (50%)	107 (25%)				
Phenylpropylmethylamine	149	150						
Phenyltoloxamine	255	256						
Phenyramidol	214	107	215 (65%)	95 (23%)	108 (13%)	197 (10%)		
Physostigmine salicylate	275	276	139 (38%)	219 (18%)				
Pilocarpine	208	209	208 (15%)					
Piperidolate	323	112	111 (40%)	324 (37%)				
Prilocaine	220	221						
Primidone	218	219	164 (13%)	181 (12%)				
Probarbital	198	199						
Probenecid	285	286						
Procaine	236	237	100 (16%)	99 (12%)				
Procaine amide	235	236	99 (18%)	136 (12%)				
Prochlorperazine	373	374	376 (30%)	373 (27%)	234 (20%)			
Promazine	284	285	284 (15%)					
Promethazine	284	285	284 (27%)					
Propranolol	259	260	72 (60%)					
Protriptyline	263	264						
Putrescine	88	89	72 (60%)	73 (30%)				
3-Pyridinemethanol	109	110	92 (14%)					
Pyridoxine	169	170	152 (15%)					
Pyrilamine	285	286	241 (10%)					
Quinidine	324	325	136 (18%)					
Quinine	324	325	136 (20%)					
Resorcinol	110	111	110 (100%)					
Saccharine	183	184						
Salicylamide	137	138	137 (11%)					
Salicylic acid	138	139						
Sarcosine	89	90						
Scopolamine	303	138	304 (16%)					
Secobarbital	238	239	199 (36%)					

Sorbitol	182	183	165 (20%)	147 (10%)	129 (10%)		
Stearic acid	284	285	284 (70%)	267 (45%)	283 (26%)		
Strychnine	334	335	334 (25%)				
Sucrose	342	163	145 (85%)	127 (25%)			
Sulfachlorpyritazine	284	285	220 (60%)	287 (40%)	251 (20%)		
Sulfadiazine	250	251	186 (60%)				
Sulfameter	280	281	216 (10%)				
Sulfamethizole	270	271					
Sulfamethoxazole	253	254					
Sulfapyridine	249	250	185 (20%)				
Sulfinpyrazone	404	279	278 (55%)	405 (35%)	280 (20%)		
Sulfisomidine	278	279	214 (40%)				
Sulfisoxazole	267	268					
Sulfosalicylic acid	218	219	218 (65%)	201 (25%)	200 (20%)		
Talbutal	224	225	185 (22%)				
Tetracaine	264	265	194 (14%)				
Tetracycline	444	427	445 (40%)	428 (30%)	426 (28%)	257 (25%)	
Tetrahydrocannabinol	314	315					
Theobromine	180	181	180 (10%)				
Theophylline	180	181	180 (12%)				
Thiethylperazine	399	400	401 (95%)	402 (25%)			
Thioacetamide	75	76	75 (80%)				
Thiobarbituric acid	200	145					
Thioridazine	370	371	370 (77%)				
Tolazoline	160	161					
Tolbutamide	270	172	271 (32%)	198 (25%)			
Tranylcypromine	133	134	132 (25%)	133 (20%)			
Trifluoperazine	407	408	407 (30%)	278 (13%)	302 (10%)	279 (10%)	
Triflupromazine	352	353					
Trihexyphenidyl	301	302	300 (12%)				
Trimeprazine	298	299	200 (55%)	298 (50%)	240 (42%)	239 (20%)	199 (20%)
Trimethadione	143	144					
Tropine	141	124	142 (60%)	140 (50%)	141 (20%)		
Tybamate	274	275	232 (40%)	158 (30%)	176 (30%)	214 (20%)	
Tyramine	137	138	121 (50%)	108 (30%)	107 (10%)		
Vinbarbital	224	225					
Violuric acid	157	158	142 (33%)				
Warfarin	308	309	251 (15%)	291 (10%)			
Yohimbine	354	355	354 (75%)	353 (40%)	352 (10%)	337 (10%)	

[a] Only those peaks with abundances 10 percent or greater are shown. Abundances are indicated in parentheses.
[b] The M+2 ion is not recorded.

TABLE 2—*Base peak index of isobutane CI mass spectra*[a,b].

Compounds	Molecular Weight	Mass Spectral Peaks in Order of Abundance						
		1	2	3	4	5	6	7
Ethylenediamine	60	61						
n-Methylephedrine	179	72	180 (50%)	162 (20%)				
Thioacetamide	75	76	75 (80%)					
Glycine	75	76						
Putrescine	88	89	72 (60%)	73 (30%)				
Sarcosine	89	90						
Pentanediamine	102	103	86 (39%)					
Phenyramidol	214	107	215 (65%)	95 (23%)	108 (13%)	197 (10%)		
3-Pyridinemethanol	109	110	92 (14%)					
Aminophenol	109	110	109 (40%)					
Resorcinol	110	111	110 (100%)					
Histamine	111	112						
Piperidolate	323	112	111 (40%)	324 (37%)				
Acetophenazine	411	117	99 (80%)	412 (55%)				
Dimethylglyoxime	116	117	116 (16%)					
Acetylsalicylic acid	180	121	139 (20%)	163 (18%)	181 (17%)	138 (17%)	180 (10%)	
Phenethylamine	121	122	105 (45%)	91 (22%)				
Nicotinamide	122	123						
Atropine	289	124	290 (17%)					
Hyoscyamine	289	124	237 (20%)	290 (15%)				
Homatropine	279	124	107 (14%)	275 (10%)				
Tropine	141	124	142 (60%)	140 (50%)	141 (20%)			
Ethinamate	167	125	107 (66%)	163 (13%)				
Cyclandelate	276	125	277 (30%)	107 (20%)	135 (18%)			
Ethchlorvynol	144	127	129 (34%)	109 (10%)				
Coniine	127	128	126 (24%)					
Barbituric acid	128	129						
Isobarbituric acid	128	129						
Tranylcypromine	133	134	132 (25%)	133 (20%)				
Mandelic acid	152	135	107 (65%)					
3-Methylsalicylate	152	135	134 (82%)	153 (80%)	152 (70%)	105 (42%)	106 (34%)	78 (25%)
Amphetamine	135	136						
Phenelzine	136	137	135 (34%)	122 (22%)	105 (12%)			
B-Hydroxy-B-phenylethylamine	137	138	120 (50%)					
Tyramine	137	138	121 (50%)	108 (30%)	107 (10%)			
Salicylamide	137	138	137 (11%)					

Isoniazide	137	138	137 (10%)		
Scopolamine	303	138	304 (16%)		
Salicylic acid	138	139			
Pentylenete trazole	138	139			
Hydroxybenzoic acid	138	139	121 (35%)		
Dimethyldihydroresocinol	140	141			
Methenamine	140	141	112 (45%)	140 (35%)	
Ethosuximide	141	142			
Trimethadione	143	144			
Thiobarbituric acid	144	145			
Phentermine	149	150			
Phenylpropylmethylamine	149	150			
Methamphetamine	149	150			
p-Methylamphetamine	149	150	133 (49%)		
d-4-Hydroxynorephedrine	167	150	168 (50%)	123 (17%)	
Acetaminophen	151	152			
Phenylpropanolamine	151	152	134 (50%)	107 (25%)	
1-Hydroxyamphetamine	151	152	135 (95%)		
Amantadine	151	152	135 (48%)	151 (32%)	150 (15%)
Methylsalicylamide	151	152	151 (73%)	121 (25%)	120 (13%)
Methylsalicylate	152	153	152 (35%)	120 (35%)	121 (20%)
p-Aminosalicylate	153	154	153 (28%)	135 (13%)	136 (12%)
Hydroxytyramine	153	154	137 (24%)	124 (24%)	
Gentisic acid	154	155			
Chloroacetophenone	154	155	157 (35%)	139 (20%)	154 (17%)
Oxanamide	157	158	131 (10%)		
Violuric acid	157	158	142 (33%)		
Tolazoline	160	161			
Hydralazine	160	161			
Nicotine	162	163			
Lactose	342	163	145 (85%)	127 (25%)	
Sucrose	342	163	145 (85%)	127 (25%)	
Glucose	180	163	145 (85%)	127 (25%)	
Fructose	180	163	145 (85%)	127 (25%)	
Mannose	180	163	145 (85%)	127 (25%)	
Galactose	180	163	145 (85%)	127 (25%)	
Acetylcysteine	163	164			
Mephentermine	163	164			
Ephedrine	165	166	148 (50%)		
Isoephedrine	165	166	107 (42%)	148 (15%)	
4-Hydroxyphenylisopropyl methylamine	165	166	135 (10%)		

(*Continued*)

TABLE 2—Continued.

Compounds	Molecular Weight	Mass Spectral Peaks in Order of Abundance						
		1	2	3	4	5	6	7
Benzocaine	165	166						
p-Methoxyamphetamine	165	166	149 (45%)	122 (15%)				
m-Methoxyamphetamine	165	166	149 (10%)	138 (10%)				
Adrenaline	183	166	184 (25%)					
Atrolactic acid	166	167	149 (58%)	107 (37%)	166 (30%)			
Ethionamide	166	167	166 (25%)					
Phenylephrine	167	168	150 (33%)	123 (10%)				
Chlorzoxazone	169	170	172 (35%)	118 (20%)	136 (10%)			
Pyridoxine	169	170	162 (15%)					
Metronidazole	171	172						
Tolbutamide	270	172	271 (32%)	198 (25%)				
5-Ethyl-2-thiobarbital	172	173						
Methyltryptamine	174	175	158 (50%)	131 (40%)				
Ascorbic acid	176	177						
Phenmetrazine	177	178						
Coramine	178	179						
Anthracene	178	179	178 (14%)					
Hippuric acid	179	180	105 (54%)	135 (31%)	134 (21%)	162 (15%)		
Methylenedioxyamphetamine	179	180	136 (10%)					
Phenacetine	179	180						
Theophylline	180	181	180 (12%)					
Threobromine	180	181	180 (10%)					
Orphenadrine	269	182	270 (80%)	224 (11%)	198 (10%)			
Mannitol	182	183	165 (20%)	147 (10%)	129 (10%)			
Sorbitol	182	183	165 (20%)	147 (10%)	129 (10%)			
Mephensine	182	183	147 (30%)	109 (17%)	165 (15%)			
Chlorphentermine	183	184	186 (35%)	167 (12%)				
Methyprylone	183	184						
Saccharine	183	184						
Barbital	184	185						
Alphaprodine	261	188	187 (50%)	172 (35%)	262 (26%)			
Dimethyltryptamine	188	189						
Phendimetrazine	191	192						
Chlorpropamide	276	192	194 (35%)					
Isoproterenol	211	194	212 (50%)	192 (30%)				
Caffeine	194	195						
Cantharidin	196	197						

Phenaglycodol	214	197	155 (45%)	199 (35%)	157 (35%)	156 (15%)	198 (15%)	
Metanephrine	197	198	180 (27%)					
Metharbital	198	199						
Probarbital	198	199						
Phenothiazine	199	199	200 (45%)					
Glyceryl guaiacolate	198	199	198 (60%)	124 (50%)	125 (30%)			
Methallenestrill	286	199	287 (58%)	269 (25%)	229 (18%)			
Chlorophenylalanine	199	200	202 (35%)	154 (30%)				
Methsuximide	203	204						
Cotarnine	255	204	118 (40%)					
Aminoantipyrine	203	204	203 (53%)	84 (42%)				
Bufotenine	204	205	198 (11%)					
Diethylpropion	205	206	204 (30%)	100 (28%)	135 (15%)			
Pilocarpine	208	209	208 (15%)					
Allobarbital	208	209	169 (11%)					
2.5-Dimethoxy-4-methyl amphetamine	209	210						
Aprobarbital	210	211	171 (13%)					
Naphazoline	210	211	210 (20%)	209 (18%)				
Mescaline	211	212						
Methoxamine	211	212	194 (55%)	152 (20%)	168 (18%)	167 (15%)		
Butethal	212	213						
Butabarbital	212	213						
Phenazopyridine	213	214	105 (15%)	213 (11%)				
Diethyltryptamine	216	217						
Gluthethimide	217	218						
Meprobamate	218	219	158 (51%)					
Primidone	218	219	164 (13%)	181 (12%)				
Mephenytoin	218	219	189 (10%)					
Sulfosalicylic acid	218	219	218 (65%)	201 (25%)	200 (20%)			
Prilocaine	220	221						
Noscapine	413	221	222 (15%)					
Metaxalone	221	222						
Acetazolamide	222	223	207 (18%)	123 (18%)				
Mephenoxalone	223	224	223 (25%)	125 (25%)	155 (25%)	218 (15%)	157 (10%)	124 (10%)
Talbutal	224	225	185 (22%)					
Vinbarbital	224	225						
Allylbarbital	224	225	185 (17%)					
5-Ethyl-5-(3-hydroxy-1-methylbutyl-barbituric acid	242	225	243 (40%)	157 (23%)				
Furazolidone	225	226						

(*Continued*)

TABLE 2—Continued.

Compounds	Molecular Weight	Mass Spectral Peaks in Order of Abundance						
		1	2	3	4	5	6	7
Amobarbital	226	227						
Pentobarbital	226	227						
Metyrapone	226	227	226 (36%)	120 (12%)				
Fenfluramine	231	232	72 (68%)	212 (25%)				
Phenobarbital	232	233						
Mebutamate	232	233	172 (75%)					
Methylphenidate	233	234	84 (70%)	151 (10%)				
Lidocaine	234	235	86 (13%)					
Mecloqualone	270	235	271 (90%)	273 (32%)	118 (10%)			
Procaine amide	235	236	99 (18%)	136 (12%)				
Hexobarbital	236	237						
Procaine	236	237	100 (15%)	99 (12%)				
Carbromal	236	237	239 (98%)					
Secobarbital	238	239	199 (36%)					
Nitrofurantoin	238	239	238 (20%)					
Benzphetamine	239	240	148 (85%)					
Pheniramine	240	241						
Methocarbamol	241	242	199 (100%)	118 (83%)	124 (33%)	224 (10%)		
Clofibrate	242	243	245 (30%)	115 (55%)	128 (13%)	169 (12%)		
Phencylidine	243	244	242 (63%)					
Dianisidine	244	245						
Alphenal	244	245	113 (43%)	205 (14%)				
Mephobarbital	246	247						
Meperidine	247	248						
2,6-Dimethyl-4-isopropyl-benzaldehyde thiosemicarbazone	249	250	174 (18%)	158 (15%)				
Sulfapyridine	249	250	185 (20%)					
Methaqualone	250	251	250 (30%)	235 (20%)				
Sulfadiazine	250	251	186 (60%)					
Diphenylhydantoin	252	253						
Benzopyrene	252	253	252 (59%)					
Sulfamethoxazole	253	254						
Dyphylline	254	255	254 (40%)					
Diphenhydramine	255	256	167 (25%)					
Phenyltoloxamine	255	256						
Ethoxazene	256	257	256 (45%)	133 (15%)	138 (15%)			

Palmitic acid	256	257	256 (90%)	239 (85%)			
1-Dromoran	257	258	256 (50%)	257 (25%)			
Propranolol	259	260	72 (60%)				
Cyclophosphamide	260	261	211 (30%)	225 (25%)	213 (11%)	227 (10%)	
Phenindamine	261	262					
Methapyrilene	261	262	166 (27%)	191 (13%)			
Methohexital	262	263					
Nortriptyline	263	264					
Protriptyline	263	264					
Tetracaine	264	265	194 (14%)				
Desipramine	266	267	222 (21%)				
Sulfisoxazole	267	268					
Apomorphine	267	268	267 (22%)	266 (20%)			
Morphine	285	268	286 (20%)	269 (20%)			
Diethylstillbestrol	268	269	268 (35%)				
Oxazepam	286	269					
Sulfamethizole	270	271					
d-Methorphan	271	272	270 (64%)	271 (21%)			
Chlorpheniramine	274	275	277 (30%)	230 (22%)	203 (10%)		
Tybamate	274	275	232 (40%)	176 (30%)	158 (30%)	214 (20%)	
Physostigmine salicylate	275	276	139 (38%)	219 (18%)			
Amitriptyline	277	278					
Sulfisomidine	278	279	214 (40%)				
Sulfinpyrazone	404	279	278 (55%)	405 (35%)	280 (20%)		
Ethynylestradiol	296	279	297 (50%)	296 (32%)	280 (21%)	295 (19%)	213 (12%)
Acetylcarbromal	278	279	281 (98%)				
Doxepine	279	280					
Sulfameter	280	281	216 (10%)				
Imipramine	280	281					
Alverine	281	282	176 (30%)				
Codeine	299	282	300 (22%)				
Acetylcodeine	341	282	342 (15%)				
Levallorphan	283	284	282 (50%)	283 (25%)			
Chlordiazepoxide	299	284	300 (33%)	287 (33%)	283 (30%)	285 (30%)	302 (10%)
Stearic acid	284	285	284 (70%)	267 (45%)	283 (26%)		
Promethazine	284	285	284 (27%)				
Promazine	284	285	284 (15%)				
Diazepam	284	285	287 (30%)				
Sulfachlorpyridazine	284	285	220 (50%)	287 (40%)	251 (20%)		
Hydromorphone	285	286					
Probenecid	285	286					

(*Continued*)

TABLE 2—Continued.

Compounds	Molecular Weight	Mass Spectral Peaks in Order of Abundance						
		1	2	3	4	5	6	7
Pyrilamine	285	286	241 (10%)					
Pentazocine	285	286	284 (50%)	285 (40%)	217 (16%)	230 (10%)		
Dihydromorphine	287	288	287 (18%)					
Cyproheptadine	287	288	287 (30%)					
Carbinoxamine	290	291	293 (30%)					
Cinchonidine	294	295	296 (25%)					
Ethylmorphine	313	296	314 (11%)					
Acetylethylmorphine	355	296	356 (27%)					
Methdilazine	296	297						
Trimeprazine	298	299	200 (55%)	298 (50%)	240 (42%)	239 (20%)	199 (20%)	
Phenacaine	298	299	262 (18%)					
Dihydrocodeinone	299	300						
Oxymorphone	301	302						
Isoxsuprine	301	302	178 (16%)	284 (12%)				
Dihydrocodeine	301	302	284 (25%)	301 (20%)				
Trihexyphenidyl	301	302	300 (12%)					
Ethacynic acid	302	303	305 (65%)	285 (10%)				
Cocaine	303	304	182 (33%)					
Butacaine	306	307	263 (20%)					
Phenylbutazone	308	309	190 (50%)					
Warfarin	308	309	251 (15%)	291 (10%)				
Methadone	309	310						
Dicyclomine	309	310	100 (55%)	86 (48%)	99 (35%)			
Diacetylmorphine	369	310	370 (33%)	268 (14%)				
Ibogaine	310	311						
Adiphenine	311	312	100 (65%)	86 (20%)				
Biperiden	311	312						
Cannabinol	311	312						
Dydrogesterone	312	313	312 (72%)	268 (33%)	207 (15%)			
Cannabidiol	314	315						
Tetrahydrocannabinal	314	315						
Oxycodone	315	316						
Chlorprothixene	315	316	318 (30%)					
Brompheniramine	318	319	321 (98%)	166 (15%)				
Chlorpromazine	318	319	318 (30%)	321 (30%)	234 (30%)			
Chloramphenical	322	323	325 (65%)	305 (34%)	307 (18%)	289 (18%)	291 (10%)	327 (10%)

Lysergic acid diethylamide	323	324				
Oxyphenbutazone	324	325	324 (70%)	199 (35%)		
Quinine	324	325	136 (20%)			
Quinidine	324	325	136 (18%)			
Ergonovine	325	326	268 (35%)	325 (12%)	308 (12%)	
O^6-Monoacetylmorphine	327	328	268 (55%)	327 (30%)		
Benactyzine	327	328	310 (74%)	183 (20%)		
Strychnine	334	335	334 (25%)			
Bishydroxycoumarin	336	337	163 (32%)			
Methylergonovine	339	340	322 (26%)	339 (15%)		
Papaverine	339	340				
Dibucaine	343	344				
Anileridine	352	353	351 (25%)	212 (24%)	246 (14%)	234 (10%)
Triflupromazine	352	353				
Griseofulvin	352	353	355 (35%)	352 (30%)		
Methysergide	353	354	353 (15%)			
Yohimbine	354	355	354 (75%)	353 (40%)	352 (10%)	337 (10%)
Indomethacin	357	358	357 (44%)	360 (38%)		
Dioxyline	367	368				
Cholesterol	386	369	385 (32%)	212 (67%)		
Thioridazine	370	371	370 (77%)			
Dihydrodiacetylmorphine	371	372	312 (15%)	330 (12%)		
Prochlorperazine	373	374	376 (30%)	373 (27%)	234 (20%)	
Hydroxzine	374	375	377 (30%)			
Meclizine	390	391	390 (18%)	189 (18%)	389 (11%)	243 (10%)
Brucine	394	395				
Thiethylperazine	399	400	401 (95%)	402 (25%)		
Colchicine	399	400	399 (25%)	372 (20%)	386 (15%)	371 (15%)
Perphenazine	403	404	406 (30%)	234 (19%)		
Hexachlorophene	404	407	409 (80%)	405 (50%)	411 (40%)	
Trifluperazine	407	408	407 (30%)	278 (13%)	302 (10%)	279 (10%)
Bendroflumethiazide	421	422	420 (38%)			
Tetracycline	444	427	445 (40%)	428 (30%)	426 (28%)	257 (25%)
Methacycline	442	443	198 (38%)	425 (10%)	400 (10%)	
Doxycycline hyclate	444	445	444 (12%)	427 (10%)		
Oxytetracycline	460	461	443 (30%)	198 (30%)	460 (16%)	
Chlortetracycline	478	479	481 (40%)	461 (20%)		
Emetine	480	481	479 (60%)	480 (48%)		

[a] Only those peaks with abundances 10 percent or greater are shown. Abundances are indicated in parentheses.
[b] The M+2 ion is not recorded.

from their MH^+ peaks at m/e (mass per unit charge) 227, 181, 61, and 166, respectively. Additionally, ephedrine shows a fragmentation ion at m/e 148 due to the loss of H_2O from the MH^+ ion.

The identification of an unknown drug substance can be facilitated with CI data. Recently, an unknown white powder yielded a spectrum consisting only of an ion at m/e 192. Hence, the assumption was made that the material had a molecular weight of 191 and may therefore contain an odd number of nitrogens. Using the natural abundance of C^{13}, the substance was calculated by the $(MH + 1)^+$ to MH^+ ratio to have a maximum of twelve carbons. This data yielded a probable empirical formula of $C_{12}H_{17}NO$. Wet chemical analysis showed the presence of a tertiary amine. Phendimetrazine was considered to be a most reasonable possibility and its presence was later confirmed by both infrared spectrophotometry and EI mass spectroscopy.

Perhaps CI's greatest potential lies in the area of forensic toxicology. The simplicity of the isobutane CI spectrum seems ideally suited for the identification of drugs and their metabolites present in the complex biological matrixes that comprise human tissues and organs. The toxicologist's potential ability to directly analyze the extracts of biological matter, without prior chromatographic treatment at the high levels of sensitivity offered by the mass spectrometer, represents a significant advancement to analytical toxicology. CI's utilization for making rapid preliminary identifications of drugs present in the gastric contents of overdose cases has already been demonstrated [*14,17*]. Isobutane CI has been successfully utilized in our laboratory for both the screening and confirmation of drugs present in the extracts of blood, urine and body organs. Figure 4 shows the isobutane CI spectrum of an acid extract of a urine that had been spiked with 5 μg/ml of secobarbital. The MH^+ for secobarbital is clearly identifiable at m/e 239.

The application of isobutane CI to other areas of the forensic sciences offers much promise. The combination of pyrolysis gas chromatography and isobutane CI for fiber and paint identification, and the detection and characterization of organic explosive residues, are areas worthy of exploration.

The versatility of the CI mass spectrometer is enhanced by the operator's ability to convert it to a conventional EI mode of operation. This can be accomplished by either substituting helium or nitrogen as the reagent gas, or by simply excluding the reagent gas from the spectrometer's source.

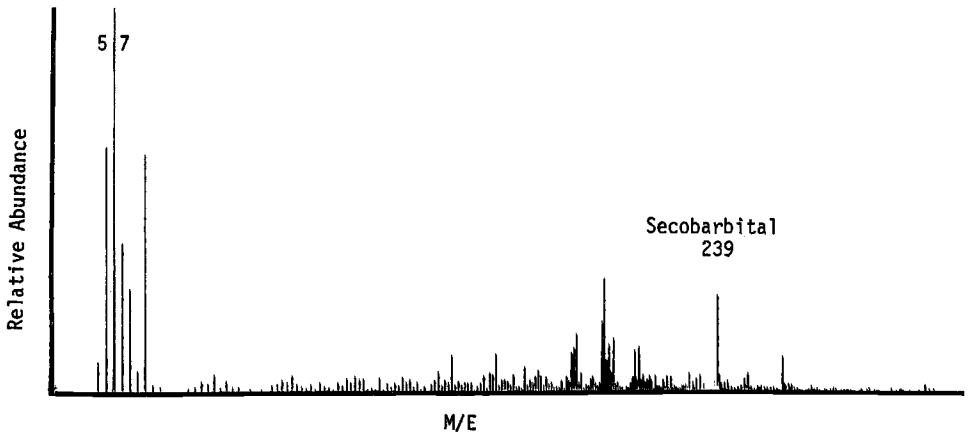

FIG. 4—*CI mass spectrum of urine sample containing secobarbital (5 μg/ml).*

Summary

The application of isobutane chemical ionization mass spectroscopy to the forensic identification of drugs has been discussed. CI spectral data for 303 drugs and common diluents have been compiled and presented. These spectra are characterized by their relative simplicity. The majority of the compounds analyzed show an MH^+ peak with four or less fragmentation ions in abundances greater than 10 percent. A relatively simple and inexpensive search system is suggested for the identification of drugs and diluents by CI.

The advent of this new technique as a supplement for conventional EI spectroscopy promises to expand the versatility of the mass spectrometer in the forensic sciences. The analyst now has the option of either performing a direct analysis on a suspect drug without prior chromatographic treatment, or alternatively utilizing the unit in a CI or conventional EI mode with a gas chromatograph interface. A variety of reagent gases are now known, so that the analyst can control the complexity and characteristics of the CI spectrum produced.

Isobutane CI has successfully been applied for the identification of drug mixtures in powders and pills as well as to the detection of drugs present in gastric contents, urine, and blood.

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Announcement

The American Board of Forensic Toxicology (ABFT) is pleased to announce that the following persons, having successfully passed the Board's Qualifying Examination and met all other requirements, have been granted Certificates of Qualification in Forensic Toxicology, thereby becoming the initial group of diplomates of ABFT:

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Erratum

Richard Saferstein, Jew-Ming Chao, and John Manura, "Identification of Drugs by Chemical Ionization Mass Spectroscopy—Part II," *Journal of Forensic Sciences,* Vol. 19, No. 3, July 1974, pp. 463-485. In Table 1, p. 469, the molecular weight of cannabinol should be 310, and the first mass spectral peak should be 311. On p. 473, Table 1, the correct information for noscapine should be a first mass spectral peak at 220 and a second mass spectral peak at 221 (15%).

Note

Reference is made to the presentation at the Plenary Session, Ethics and the Forensic Sciences, 28th Annual Meeting of the AAFS, Washington, D.C., 19 Feb. 1976, by Leo Dal Cortivo, Ph.D., entitled, "Ethical Practices as They Pertain to the Discipline of Toxicology." The title of Dr. Dal Cortivo's presentation appeared in the October 1976 issue of *JOFS* along with the manuscripts of the other participants of this session with the statement, "Manuscript Not Submitted at Time of Publication." The language of this statement in no way implies tardiness or lack of reliability on the part of the speaker.

—The Editor