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Thin-Layer Chromatography and Mass Spectrometry for Screening of Biological Samples for Drugs and Metabolites

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Key Words:

Off-line TLC-MS

EI mass spectrometry

Drugs

Metabolites

Summary

This paper describes a method for off-line coupling of thin-layer chromatography (TLC) and electron-impact ionization mass spectrometry (EIMS) which is well suited for routine forensic and toxicological investigations of a large number of samples. The advantages and drawbacks of this approach are discussed. Several TLC systems for 493 compounds of forensic and toxicological interest are described and eight-peak mass spectra from full EI mass spectra are listed.

1 Introduction

The screening of biological samples for drugs in forensic chemistry and toxicology can be divided in two main areas of application:

- (i) the detection of known, well-investigated drugs and their metabolites using one or more appropriate analytical methods for purification, isolation, separation, and identification; and
- (ii) the identification of unknown, newly synthesized or isolated drugs or metabolites.

The identification of unknowns is the most difficult and interesting part of toxicological research and should be performed using all the analytical techniques available in the laboratory, e.g. ultraviolet spectroscopy (UV) [1,2], infrared spectroscopy (IR) [1,3], gas chromatography (GC) [4], GC-mass spectrometry (GC-MS) [5], GC-tandem mass spectrometry (GC-MS-MS) [6], high-performance liquid

chromatography (HPLC) as HPLC-UV [7-9], HPLC-MS [10], and HPLC-MS-MS [11], TLC-UV [12], high performance TLC-Fourier transform IR (HPTLC-FTIR) [13], TLC-MS [14], TLC-MS-MS [15], etc.

The detection of known drugs and metabolites is, in contrast, a rather routine procedure and can be performed by a tested method and use of the corresponding compilation (libraries) of analytical data for each technique [1,2,16,17].

As a simple, low cost method TLC is still of importance [18]. The batch nature of this method enables the simultaneous analysis of many samples [12,17,18] and, therefore, routine investigations – it is a less time-consuming procedure than, for example, HPLC. The variety of HPLC methods can be further used for comprehensive analysis of blood or plasma samples. Furthermore, because the whole chromatogram is obtained, the analyst has a much greater chance of observing the presence of unknowns that might be missed by column chromatography either as a result of nonelution from the column or migration with the solvent front. There is no doubt that the direct analysis of compounds from the TLC plate reduces losses of the substances analyzed. One suitable MS method, for example, is fast atom bombardment (FAB) [15].

In this paper we introduce the TLC systems used in our laboratory and the compilation of full EI mass spectra reduced to eight-peak mass spectra.

2 Experimental

2.1 Off-line TLC-EIMS

Silica P₂₅₄ (Merck, Darmstadt, Germany) TLC plates (20 cm × 10 cm) were used for R_F determination and for all forensic analyses of biological species. The compositions (v/v) of the mobile phases were:

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- (1) methanol–25% aqueous ammonia, 100 + 1.5;
 (2) cyclohexane–toluene–diethylamine, 75 + 15 + 10;
 (3) chloroform–methanol, 90 + 10;
 (4) chloroform–acetone, 80 + 20;
 (5) ethyl acetate–methanol–25% aq. ammonia, 85 + 10 + 5;
 (6) ethyl acetate, 100.

These mobile phases are comparable with those described elsewhere [19]. Experimentally determined $R_F \times 100$ values were converted into corrected $hR_F \times 100$ values by a graphical standardization procedure suggested elsewhere [19], in which a six-point correction graph is constructed from the $R_F \times 100$ values of four reference compounds (morphine, codeine, hydroxyzine, and trimipramine) and the points 0,0 and 100,100. The corrected $hR_F \times 100$ values of 493 drugs and metabolites are listed in **Tables 1** and **2**.

Table 1
 Eight-peak mass spectra, molecular weights, and hR_F (corrected $R_F \times 100$) values measured using mobile phases 1–3, for drugs and related compounds.

No.	Eight-peak mass spectrum								M^+	hR_F in mobile phase:			Compound name	Elemental composition
	a	b	c	d	e	f	g	h		1	2	3		
1	41	69	184	43	55	168	77	167	240	93	49	87	Buthalital	$C_{11}H_{16}N_2O_2S$
2	41	84	70	58	281	167	88	43	451	18	9	11	Homofenazine	$C_{23}H_{28}N_3OF_3S$
3	41	224	237	206	226	123	56	239	375	67	10	27	Haloperidol	$C_{21}H_{23}NO_2ClF$
4	43	42	157	58	59	41	44	70	157	79	89	75	Ethadion	$C_7H_{11}NO_3$
5	43	172	92	156	44	65	60	108	215	76	0	1	Sulfacarbamide	$C_7H_9N_3O_3S$
6	44	45	42	77	65	167	95	43	167	33	1	1	Phenylephrine	$C_9H_{13}NO_2$
7	44	45	58	202	91	203	220	191	263	34	27	16	Nortriptyline	$C_{19}H_{21}N$
8	44	45	77	95	123	42	65	121	167	25	4	1	Synephrine	$C_9H_{13}NO_2$
9	44	59	70	277	71	278	203	178	277	15	17	5	Maprotiline	$C_{20}H_{23}N$
10	44	77	76	58	65	95	51	121	167	42	1	1	Metaraminol	$C_9H_{13}NO_2$
11	44	77	79	45	51	91	105	107	151	42	25	5	Norpseudoephedrine	$C_9H_{13}NO$
12	44	83	180	182	143	41	55	137	222	80	6	71	Bromisoval	$C_6H_{11}N_2O_2Br$
13	44	91	65	42	45	51	92	120	135	43	15	9	Amphetamine	$C_9H_{13}N$
14	44	128	74	127	76	607	63	577	651	24	0	0	Liothyronine	$C_{15}H_{12}NO_4I_3$
15	44	166	151	57	135	43	71	91	209	51	16	17	2,5-Dimethoxy-4-methylamphetamine	$C_{12}H_{19}NO_2$
16	44	242	270	269	241	243	271	244	408	84	3	57	Dipotassium-chlorazepate	$C_{16}H_{11}N_2O_4ClK_2$
17	44	303	106	285	261	118	104	200	347	72	0	0	Cefalexin	$C_{16}H_{17}N_3O_4S$
18	45	217	41	70	69	110	285	202	285	61	15	12	Pentazocine	$C_{19}H_{27}NO$
19	56	83	217	42	57	123	216	98	311	84	0	1	Noramidopyrine-methansulfonic acid	$C_{13}H_{17}N_3O_4S$
20	56	83	308	106	107	78	79	202	308	57	0	32	Nifenazone	$C_{17}H_{16}N_4O_2$
21	56	100	138	110	237	57	70	58	237	42	7	23	Viloxazine	$C_{13}H_{19}NO_3$
22	56	118	119	91	162	55	77	44	162	92	3	3	Aminorex	$C_9H_{10}N_2O$
23	56	137	83	245	230	84	77	57	245	70	24	66	Isopropylamino-phenazone	$C_{14}H_{19}N_3O$
24	56	231	97	111	112	77	71	232	231	66	36	81	Aminophenazone	$C_{13}H_{17}N_3O$
25	57	82	95	99	125	96	116	111	252	54	0	9	Cimetidine	$C_{10}H_{16}N_6S$
26	57	155	181	195	41	196	83	237	252	84	6	92	Methylnealbarbital	$C_{13}H_{20}N_2O_3$
27	58	42	41	59	89	125	168	91	183	44	18	17	Chlorphentermine	$C_{10}H_{14}NCl$
28	58	55	89	90	118	42	71	41	291	57	27	39	Cyclopentolate	$C_{17}H_{25}NO_3$
29	58	59	42	72	77	103	161	88	303	53	47	36	Chlorphenoxamine	$C_{18}H_{22}NOCl$
30	58	59	42	165	44	77	103	43	225	65	82	59	Polycaine	$C_{16}H_{19}N$
31	58	59	42	202	203	91	115	43	277	51	55	32	Amitriptyline	$C_{20}H_{23}N$
32	58	59	165	57	42	43	55	178	279	51	52	37	Doxepin	$C_{19}H_{21}NO$
33	58	71	59	42	75	111	44	43	257	77	26	42	Meclofenoxate	$C_{12}H_{16}NO_3Cl$
34	58	71	72	208	59	57	42	44	294	53	43	35	Noxiptiline	$C_{19}H_{22}N_2O$
35	58	71	150	176	72	193	59	92	264	48	15	32	Tetracaine	$C_{15}H_{24}N_2O_2$
36	58	71	167	72	182	55	42	45	270	48	41	10	Doxylamine	$C_{17}H_{22}N_2O$
37	58	72	71	59	42	57	224	91	295	40	34	18	Normetadone	$C_{20}H_{25}NO$
38	58	73	45	57	43	44	167	165	333	54	44	43	Bromazine	$C_{17}H_{20}NOBr$
39	58	73	45	165	46	59	166	74	269	55	48	33	Orphenadrine	$C_{18}H_{23}NO$

Table 1 (Continued)

No.	Eight-peak mass spectrum								M^+	hR_F in mobile phase:			Compound name	Elemental composition
	a	b	c	d	e	f	g	h		1	2	3		
40	58	73	45	213	197	59	44	152	285	28	42	28	Medrylamine	$C_{18}H_{23}NO_2$
41	58	73	165	167	45	166	152	44	255	55	45	33	Diphenhydramine	$C_{17}H_{21}NO$
42	58	73	165	167	152	45	59	166	469	29	53	25	Dimenhydrinate*8- Chlortheophylline	$C_{17}H_{21}NO \cdot C_7H_7N_4O_2Cl$
43	58	77	59	56	51	79	50	43	165	30	5	5	Ephedrine	$C_{10}H_{15}NO$
44	58	77	59	95	65	42	51	56	181	41	3	2	Etilefrine	$C_{10}H_{15}NO_2$
45	58	84	200	86	213	85	214	285	301	47	45	23	Dominal-Sulfoxide	$C_{16}H_{19}N_3OS$
46	58	86	326	85	280	43	241	255	326	48	26	24	Acetopromazine	$C_{19}H_{22}N_2OS$
47	58	91	41	42	59	134	65	117	149	46	26	31	Phentermine	$C_{10}H_{15}N$
48	58	91	59	56	42	65	134	57	149	31	28	13	Methamphetamine	$C_{10}H_{15}N$
49	58	91	105	115	77	57	59	130	339	68	59	55	Dextropropoxyphene	$C_{22}H_{29}NO_2$
50	58	91	197	72	71	185	184	64	255	55	44	27	Tripelemamine	$C_{16}H_{21}N_3$
51	58	97	72	71	79	42	78	40	261	53	42	25	Thenylidiamine	$C_{14}H_{19}N_3S$
52	58	97	72	71	80	191	79	190	261	52	43	26	Methapyrilene	$C_{14}H_{19}N_3S$
53	58	105	42	88	47	59	45	46	162	78	6	74	Methomyl	$C_5H_{10}N_2O_2S$
54	58	126	141	59	69	56	41	44	141	20	32	10	Cyclopentamine	$C_9H_{19}N$
55	58	221	59	42	222	189	43	44	315	56	51	51	Chlorprothixene	$C_{18}H_{18}NCIS_6$
56	58	234	44	59	165	41	427	45	445	52	0	3	Narceine	$C_{23}H_{27}NO_8$
57	58	234	235	85	195	193	194	130	280	48	49	23	Imipramine	$C_{19}H_{24}N_2$
58	58	238	91	239	167	59	56	165	329	68	55	68	Prenylamine	$C_{24}H_{27}N$
59	58	242	229	243	344	210	74	282	344	34	57	29	Levomepromazine- S-oxide	$C_{19}H_{24}N_2O_2S$
60	58	249	208	99	234	294	193	248	294	55	62	54	Trimipramine	$C_{20}H_{26}N_2$
61	58	249	250	121	46	248	45	44	249	59	6	6	Tramadol- <i>O</i> -desmethyl	$C_{15}H_{23}NO_2$
62	58	250	130	120	59	65	92	42	250	47	10	21	Butamin	$C_{14}H_{22}N_2O_2$
63	58	253	59	193	165	72	44	115	253	51	52	32	Tolpropamine	$C_{18}H_{23}N$
64	58	254	44	42	73	77	59	72	289	52	41	37	Clofedanol	$C_{17}H_{26}NOCl$
65	58	255	40	72	71	42	59	210	255	53	39	48	Phenyltoloxamine	$C_{17}H_{21}NO$
66	58	263	59	45	44	57	41	42	263	44	65	24	Tramadol	$C_{16}H_{25}NO_2$
67	58	284	86	238	199	85	198	285	284	44	41	30	Promazine	$C_{17}H_{20}N_2S$
68	58	293	100	45	87	59	294	115	293	59	61	48	Butriptyline	$C_{21}H_{27}N$
69	58	298	100	180	59	198	199	212	298	58	55	39	Alimemazine	$C_{18}H_{22}N_2S$
70	58	318	86	320	272	85	319	273	318	49	49	35	Chlorpromazine	$C_{17}H_{19}N_2ClS$
71	58	328	100	229	329	242	282	283	328	57	49	38	Levomepromazine	$C_{19}H_{24}N_2OS$
72	59	43	129	41	42	58	70	40	129	79	79	0	Dimethadione	$C_5H_7NO_3$
73	59	257	150	256	42	200	76	157	257	35	13	7	Levorphanol	$C_{17}H_{23}NO$
74	59	271	270	150	214	171	213	203	271	34	44	17	Dextromethorphan	$C_{18}H_{25}NO$
75	70	43	71	269	153	244	144	223	611	66	1	48	Dihydroergocristine	$C_{35}H_{41}N_5O_5$
76	70	44	191	192	189	59	71	165	263	19	17	7	Protriptyline	$C_{19}H_{21}N$
77	70	71	44	190	42	247	57	119	247	47	2	9	Ketobemidone	$C_{15}H_{21}NO_2$
78	70	112	293	264	305	291	295	44	374	75	67	79	Bromhexine	$C_{14}H_{20}N_2Br_2$
79	70	113	141	409	43	71	283	128	409	53	24	37	Butaperazine	$C_{24}H_{31}N_3OS$
80	70	113	339	43	141	42	45	44	339	48	24	37	Perazine	$C_{20}H_{25}N_3S$
81	70	153	131	267	43	125	91	207	581	63	1	34	Ergotamine	$C_{33}H_{35}N_5O_5$
82	70	204	98	99	69	77	89	113	204	78	0	52	Fenozolone	$C_{11}H_{12}N_2O_2$
83	70	322	180	104	77	323	209	44	367	82	0	59	Phenytol-3-norvaline	$C_{20}H_{21}N_3O_4$
84	70	464	42	43	98	466	71	394	464	40	1	36	Loprazolam	$C_{23}H_{21}N_6O_3Cl$
85	71	42	56	43	177	77	70	72	177	50	14	21	Phenmetrazine	$C_{11}H_{15}NO$
86	71	43	78	149	106	51	79	84	207	71	43	81	Nicotafuryl	$C_{11}H_{13}NO_3$
87	71	70	247	57	42	246	91	172	247	52	37	34	Pethidine	$C_{15}H_{21}NO_2$
88	72	41	56	221	73	43	150	109	265	48	11	11	Oxprenolol	$C_{15}H_{23}NO_3$
89	72	43	73	111	41	65	69	93	211	48	1	3	Orciprenaline	$C_{11}H_{17}NO_3$
90	72	43	221	151	40	56	71	57	336	47	0	3	Acebutolol	$C_{18}H_{28}N_2O_4$
91	72	44	42	56	107	43	57	73	325	55	15	6	Bisoprolol	$C_{18}H_{31}NO_4$
92	72	44	43	56	148	45	60	207	207	1	0	0	Guanoxan	$C_{10}H_{13}N_3O_2$
93	72	44	43	124	123	58	70	41	211	40	0	1	Isoprenaline	$C_{11}H_{17}NO_3$

Table 1 (Continued)

No.	Eight-peak mass spectrum								M^+	hR_F in mobile phase:			Compound name	Elemental composition
	a	b	c	d	e	f	g	h		1	2	3		
94	72	44	56	107	73	223	43	58	267	49	8	8	Metoprolol	C ₁₅ H ₂₅ NO ₃
95	72	44	73	179	178	214	58	42	317	22	57	20	Mecloxamine	C ₁₉ H ₂₄ NOCl
96	72	56	73	43	222	107	41	58	266	45	0	2	Atenolol	C ₁₄ H ₂₂ N ₂ O ₃
97	72	56	73	43	249	58	41	100	249	52	11	12	Alprenolol	C ₁₅ H ₂₃ NO ₂
98	72	58	71	229	73	158	91	70	244	68	58	54	Isoaminile	C ₁₆ H ₂₄ N ₂
99	72	73	86	44	200	57	70	42	285	52	41	30	Isothipendyl	C ₁₆ H ₁₉ N ₃ S
100	72	73	284	42	44	198	213	56	284	50	37	35	Promethazine	C ₁₇ H ₂₀ N ₂ S
101	72	91	73	44	42	148	65	70	163	19	57	16	Dimetamfetamine	C ₁₁ H ₁₇ N
102	72	91	73	44	98	297	121	45	341	34	7	22	Propafenone	C ₂₁ H ₂₇ NO ₃
103	72	115	144	73	56	116	43	259	259	50	7	10	Propranolol	C ₁₆ H ₂₁ NO ₂
104	72	271	255	256	273	371	257	73	371	79	18	85	Camazepam	C ₁₉ H ₁₈ N ₃ O ₅ Cl
105	72	322	265	249	42	43	121	323	322	81	47	96	Cyclocoumarol	C ₂₀ H ₁₈ O ₄
106	78	106	122	51	79	107	123	50	152	68	0	17	Nicometamide	C ₇ H ₈ N ₂ O ₂
107	81	53	330	96	82	332	312	52	330	1	7	12	Furosemide	C ₁₂ H ₁₁ N ₂ O ₅ ClS
108	81	137	121	136	95	93	41	138	274	83	79	92	Salicylic acid bornyl ester	C ₁₇ H ₂₂ O ₃
109	83	70	257	42	193	71	43	228	327	52	39	53	Loxapine	C ₁₈ H ₁₈ N ₃ OCl
110	83	82	140	42	44	124	96	41	333	13	24	4	Deptropine	C ₂₃ H ₂₇ NO
111	84	85	56	91	55	82	57	77	233	57	34	34	Methylphenidate	C ₁₄ H ₁₉ NO ₂
112	84	91	182	85	77	55	104	65	265	31	7	7	Antazoline	C ₁₇ H ₁₉ N ₃
113	84	128	129	85	165	215	179	178	343	46	48	25	Clemastine	C ₂₁ H ₂₆ NOCl
114	84	133	42	162	161	51	119	41	162	54	39	35	Nicotine	C ₁₀ H ₁₄ N ₂
115	85	43	114	101	72	115	86	157	157	31	0	6	Buformin	C ₆ H ₁₅ N ₅
116	85	84	183	107	77	56	55	184	267	10	0	3	Azacyclonol	C ₁₈ H ₂₁ NO
117	85	86	58	91	84	70	225	309	309	44	36	22	Benzydamine	C ₁₉ H ₂₃ N ₃ O
118	86	44	57	41	87	77	84	43	209	55	4	6	Bamethan	C ₁₂ H ₁₉ NO ₂
119	86	57	41	192	87	111	70	58	225	47	1	1	Terbutaline	C ₁₂ H ₁₉ NO ₃
120	86	57	276	41	71	114	87	70	291	28	14	10	Penbutolol	C ₁₈ H ₂₉ NO ₂
121	86	58	41	42	56	87	319	99	319	38	14	4	Chloroquine	C ₁₈ H ₂₆ N ₃ Cl
122	86	58	87	72	42	56	77	84	234	70	35	73	Lidocaine	C ₁₄ H ₂₂ N ₂ O
123	86	58	279	294	280	193	97	42	294	26	61	36	Dimetacrine	C ₂₀ H ₂₆ N ₂
124	86	72	141	44	219	143	88	140	254	76	14	54	Butanilicaine	C ₁₃ H ₁₉ N ₂ OCl
125	86	87	120	58	278	92	65	73	343	49	6	10	Cinchocaine	C ₂₀ H ₂₉ N ₃ O ₂
126	86	99	43	58	41	57	71	42	299	47	1	7	Metoclopramide	C ₁₄ H ₂₂ ClN ₃ O ₂
127	86	99	58	87	387	56	42	43	387	62	30	48	Flurazepam	C ₂₁ H ₂₃ N ₃ OClF
128	86	99	60	71	44	87	58	84	312	48	46	53	Salverine	C ₁₉ H ₂₄ N ₂ O ₂
129	86	99	71	100	220	87	237	58	336	53	32	35	Prusocaine	C ₁₉ H ₃₂ N ₂ O ₃
130	86	99	91	87	58	191	71	100	263	69	59	57	Butetamate	C ₁₆ H ₂₅ NO ₂
131	86	99	100	58	87	167	168	71	328	47	71	38	Fencarbamide	C ₁₉ H ₂₄ N ₂ OS
132	86	99	106	77	87	58	73	44	327	66	40	53	Benactyzine	C ₂₀ H ₂₅ NO ₃
133	86	99	120	58	87	65	71	92	235	49	1	5	Procainamide	C ₁₃ H ₂₁ N ₃ O
134	86	99	120	58	87	71	65	92	236	54	6	31	Procaine	C ₁₃ H ₂₀ N ₂ O ₂
135	86	102	58	198	91	103	87	97	289	21	79	21	Bencyclan	C ₁₉ H ₃₁ NO
136	86	125	87	100	58	127	44	116	309	35	84	41	Clofenciclan	C ₁₈ H ₂₈ NOCl
137	86	130	57	74	56	114	128	41	316	52	6	11	Timolol	C ₁₃ H ₂₄ N ₄ O ₃ S
138	86	216	288	87	58	273	161	100	288	40	17	8	Phenglutarimide	C ₁₇ H ₂₄ N ₂ O ₂
139	86	298	180	198	87	212	299	58	298	58	57	51	Diethazine	C ₁₈ H ₂₂ N ₂ S
140	91	95	171	155	109	65	108	107	366	40	5	60	Glibornuride	C ₁₈ H ₂₆ N ₂ O ₄ S
141	91	106	44	78	51	177	79	107	298	70	2	25	Nialamid	C ₁₆ H ₁₈ N ₄ O ₂
142	91	106	127	110	57	92	104	65	231	71	17	74	Isocarboxazid	C ₁₂ H ₁₃ N ₃ O ₂
143	91	159	160	131	65	92	81	77	160	13	2	2	Tolazoline	C ₁₀ H ₁₂ N ₂
144	92	240	93	121	91	103	65	104	270	71	0	48	Pimetremide	C ₁₆ H ₁₈ N ₂ O ₂
145	93	77	183	264	43	137	322	105	322	86	0	51	Kebuzone	C ₁₉ H ₁₈ N ₂ O ₃
146	94	138	42	108	154	136	97	137	303	1	6	39	Scopolamine	C ₁₇ H ₂₁ NO ₄
147	94	151	57	95	58	41	108	77	151	23	19	7	Amantadine	C ₁₀ H ₁₇ N
148	95	96	208	109	42	41	54	82	208	53	0	32	Pilocarpine	C ₁₁ H ₁₆ N ₂ O ₂
149	96	97	105	77	216	98	218	42	337	61	17	35	Lobeline	C ₂₂ H ₂₇ NO ₂

Table 1 (Continued)

No.	Eight-peak mass spectrum								M^+	hR_F in mobile phase:			Compound name	Elemental composition
	a	b	c	d	e	f	g	h		1	2	3		
150	96	139	70	42	111	97	55	43	285	37	20	8	Piperylone	$C_{17}H_{23}N_3O$
151	97	58	202	40	98	99	77	260	260	54	46	42	Methaphenilene	$C_{15}H_{20}N_2S$
152	97	82	83	111	68	42	98	103	273	71	87	71	Tilidine	$C_{17}H_{23}NO_2$
153	97	98	55	82	199	198	180	296	296	29	32	15	Methdilazine	$C_{18}H_{26}N_2S$
154	97	99	70	98	43	188	96	71	286	50	38	44	Thenalidine	$C_{17}H_{22}N_2S$
155	98	70	42	99	96	41	40	44	246	65	27	62	Mepivacaine	$C_{15}H_{22}N_2O$
156	98	70	113	112	99	44	111	83	113	18	6	5	Nanofin	$C_7H_{15}N$
157	98	70	370	126	99	185	244	125	370	48	43	30	Thioridazine	$C_{21}H_{26}N_2S_2$
158	98	85	99	113	41	42	55	105	295	62	60	62	Pridinol	$C_{20}H_{25}NO$
159	98	99	218	85	131	219	84	69	287	66	67	61	Cycrimine	$C_{19}H_{29}NO$
160	98	111	99	288	44	200	41	199	399	47	15	13	Pipazethate	$C_{21}H_{25}N_3O_3S$
161	98	137	97	136	234	41	193	110	234	5	67	3	Sparteine	$C_{15}H_{26}N_2$
162	98	176	175	118	119	121	147	177	176	57	7	60	Cotinine	$C_{10}H_{12}N_2O$
163	98	218	99	55	41	42	85	70	311	64	68	64	Biperiden	$C_{21}H_{29}NO$
164	99	44	197	58	309	112	41	97	309	32	60	37	Metixene	$C_{20}H_{23}NS$
165	99	56	167	194	266	165	207	195	266	57	49	41	Cyclizine	$C_{18}H_{22}N_2$
166	99	72	165	300	228	229	242	241	300	57	42	46	Chlorcyclizine	$C_{18}H_{21}N_2Cl$
167	99	167	114	98	165	70	96	152	281	46	37	28	Diphenylpyraline	$C_{19}H_{23}NO$
168	100	44	72	101	77	42	56	105	205	76	62	63	Amfepramone	$C_{13}H_{19}NO$
169	100	86	44	101	226	72	198	312	312	67	64	47	Profenamine	$C_{19}H_{24}N_2S$
170	100	111	142	87	105	43	77	188	445	89	0	10	Tiemonium iodide	$C_{18}H_{24}NO_2SI$
171	100	113	378	101	87	264	194	347	378	64	20	70	Doxapram	$C_{24}H_{30}N_2O_2$
172	100	128	265	56	55	43	266	101	392	76	40	71	Dextromoramide	$C_{25}H_{32}N_2O_2$
173	105	77	106	421	128	52	419	423	419	74	52	79	Broxaldine	$C_{17}H_{11}NO_2Br_2$
174	105	91	104	77	133	92	51	65	136	77	37	12	Phenelzine	$C_8H_{12}N_2$
175	105	104	244	77	79	106	103	95	244	67	26	71	Etomidate	$C_{14}H_{16}N_2O_2$
176	106	78	137	51	107	79	50	52	137	47	1	11	Isoniazid	$C_6H_7N_3O$
177	106	78	177	178	51	107	149	79	178	59	15	56	Nicethamide	$C_{10}H_{14}N_2O$
178	106	211	78	212	104	107	91	51	296	82	6	67	Lytosin	$C_{19}H_{24}N_2O$
179	107	78	149	57	108	79	77	72	261	40	45	19	Ethoheptazine	$C_{16}H_{23}NO_2$
180	107	79	70	77	105	108	71	43	176	82	12	64	Centalun	$C_{11}H_{12}O_2$
181	107	91	79	77	108	92	51	65	242	85	19	86	Mandelic acid, benzyl ester	$C_{15}H_{14}O_3$
182	107	108	78	79	80	77	51	109	214	80	12	64	Fenylamidol	$C_{13}H_{14}N_2O$
183	107	176	90	70	89	42	77	105	176	60	0	23	Pemoline	$C_9H_8N_2O_2$
184	108	80	109	78	44	107	51	53	109	71	6	50	Nicomethanol	C_6H_7NO
185	108	109	137	209	45	136	81	80	209	83	3	46	Lactylphenetidin	$C_{11}H_{15}NO_3$
186	108	213	81	54	77	136	43	214	213	59	1	50	Phenazopyridine	$C_{11}H_{11}N_5$
187	108	232	78	77	57	176	107	189	232	87	0	34	Mofebutazone	$C_{13}H_{16}N_2O_2$
188	109	121	229	65	93	110	80	53	229	82	0	45	Osalmid	$C_{13}H_{11}NO_3$
189	109	124	81	53	52	51	110	125	124	81	16	83	Guajacol	$C_7H_8O_2$
190	109	180	194	181	43	193	44	42	375	44	0	3	Theodrenaline	$C_{17}H_{21}N_5O_5$
191	111	83	112	255	113	57	45	44	255	91	0	75	Thenitrazolum	$C_8H_5N_3O_3S_2$
192	112	98	111	55	491	448	110	128	591	59	4	35	Veratrine	$C_{32}H_{49}NO_9$
193	112	125	44	123	110	41	66	42	263	43	75	43	Melperone	$C_{16}H_{22}NOF$
194	112	161	85	163	113	45	114	65	161	64	44	69	Clomethiazole	C_6H_8NCIS
195	112	310	111	58	41	212	199	96	310	53	46	44	Pecazine	$C_{19}H_{22}N_2S$
196	113	42	144	216	77	103	130	51	374	86	0	66	Pesomin	$C_{12}H_{12}N_2O_2Br_2$
197	113	70	43	127	141	248	267	42	407	40	42	43	Trifluoroperazine	$C_{21}H_{24}N_3F_3S$
198	113	70	373	141	43	42	71	127	373	49	33	37	Prochlorperazine	$C_{20}H_{24}N_3ClS$
199	114	44	365	142	42	115	263	128	365	58	3	16	Periciazine	$C_{21}H_{23}N_3OS$
200	114	72	337	43	100	115	44	237	337	66	20	70	Propanidid	$C_{18}H_{27}NO_5$
201	114	99	42	70	43	96	98	193	307	22	44	22	Hepzidine	$C_{21}H_{25}NO$
202	114	100	42	56	115	70	101	55	398	36	3	18	Pholcodine	$C_{23}H_{30}N_2O_4$
203	118	203	117	119	103	204	78	77	203	76	51	92	Mesuximide	$C_{12}H_{13}NO_2$
204	120	92	105	150	148	121	65	133	165	64	3	59	Ethenzamide	$C_9H_{11}NO_2$

Table 1 (Continued)

No.	Eight-peak mass spectrum								M^+	hR_F in mobile phase:			Compound name	Elemental composition
	a	b	c	d	e	f	g	h		1	2	3		
205	120	92	152	44	121	65	93	64	152	93	64	93	Salicylic acid, methyl ester	$C_8H_8O_3$
206	120	92	163	64	63	121	93	62	163	98	0	75	Carsalam	$C_8H_5NO_3$
207	120	92	166	121	65	93	64	63	166	93	68	93	Salicylic acid, ethyl ester	$C_9H_{10}O_3$
208	120	137	43	92	121	65	179	64	179	90	0	77	Salacetamide	$C_9H_9NO_3$
209	120	152	43	121	92	91	146	65	194	93	61	84	Acetylsalicylic acid, methyl ester	$C_{10}H_{10}O_4$
210	120	165	92	137	65	121	166	93	165	67	6	57	Benzocaine	$C_9H_{11}NO_2$
211	121	58	72	71	98	122	215	214	285	51	39	25	Mepyramine	$C_{17}H_{23}N_3O$
212	121	58	72	78	71	215	122	77	286	55	38	28	Thonzylamine	$C_{16}H_{22}N_4O$
213	121	65	94	93	122	214	44	66	214	95	65	93	Salicylic acid, phenyl ester	$C_{13}H_{10}O_3$
214	121	109	151	65	93	43	271	80	271	86	0	30	Acetaminosalol	$C_{15}H_{13}NO_4$
215	121	152	138	244	93	122	475	65	475	69	4	59	Fluspirilene	$C_{29}H_{31}N_3OF_2$
216	122	123	221	107	105	91	77	79	221	78	0	78	Metaxalone	$C_{12}H_{15}NO_3$
217	123	95	77	121	124	65	107	78	153	14	0	0	Octopamine	$C_8H_{11}NO_2$
218	124	83	82	289	94	140	96	125	289	18	6	3	Atropine	$C_{17}H_{23}NO_3$
219	124	83	361	82	94	125	67	42	361	6	23	10	Cyheptropine	$C_{24}H_{27}NO_2$
220	124	95	77	123	121	65	153	125	153	14	0	0	Norfenefrine	$C_8H_{11}NO_2$
221	124	109	198	77	81	125	123	52	198	11	37	17	Guaifenesin	$C_{10}H_{14}O_4$
222	124	168	82	289	77	105	83	42	289	21	0	1	Benzoyllecgonine	$C_{16}H_{19}NO_4$
223	124	223	109	77	122	224	123	125	223	75	0	71	Mephenoxalone	$C_{11}H_{13}NO_4$
224	125	153	70	91	244	44	43	41	583	60	1	28	Dihydroergotamine	$C_{33}H_{37}N_5O_5$
225	126	127	91	174	55	41	42	70	217	50	66	32	Prolintane	$C_{15}H_{23}N$
226	132	133	56	115	77	51	116	91	133	54	33	33	Tranlylcypromine	$C_9H_{11}N$
227	136	81	137	42	41	79	55	82	324	51	3	11	Chinine	$C_{20}H_{24}N_2O_2$
228	136	324	189	137	81	173	82	138	324	51	3	11	Chinidin	$C_{20}H_{24}N_2O_2$
229	140	83	82	124	96	201	97	125	307	13	26	6	Benzatropine	$C_{21}H_{25}NO$
230	140	141	84	138	98	245	287	288	288	69	42	73	Bupivacaine	$C_{18}H_{28}N_2O$
231	141	41	98	167	45	169	168	43	226	92	0	32	Proxibarbal	$C_{10}H_{14}N_2O_4$
232	141	156	41	43	98	69	155	112	198	55	0	22	Ipral	$C_9H_{14}N_2O_3$
233	141	170	41	98	142	169	43	55	212	93	6	74	Propylbarbital	$C_{10}H_{16}N_2O_3$
234	143	70	100	98	144	56	43	99	400	56	7	32	Clopenthixol	$C_{22}H_{25}N_2OCIS$
235	143	70	100	99	56	41	144	44	434	62	5	33	Flupenthixol	$C_{23}H_{25}N_2OSF_3$
236	145	117	90	89	80	63	146	59	225	6-620	0		Cobaltoxane	$C_9H_7NO_4S$
237	145	130	64	161	89	48	90	146	190	55	36	2	Dihydralazine	$C_8H_{10}N_6$
238	147	165	201	167	166	105	203	117	432	75	61	83	Bucizine	$C_{28}H_{33}N_2Cl$
239	148	91	149	92	65	58	43	56	255	70	57	65	Benzylephedrine	$C_{17}H_{21}NO$
240	148	163	91	103	120	44	77	117	206	76	0	53	2-Ethyl-2-phenylmalonic acid, diamide	$C_{11}H_{14}N_2O_2$
241	152	42	98	154	153	174	69	56	273	66	1	63	Chlormezanone	$C_{11}H_{12}NO_3CIS$
242	153	166	83	55	84	98	41	138	181	82	7	66	Ethypicone	$C_{10}H_{15}NO_2$
243	154	97	96	138	167	41	56	110	321	22	61	28	Ethybenzatropine	$C_{22}H_{27}NO$
244	155	227	157	185	229	184	154	156	227	90	2	67	Buclosamide	$C_{11}H_{13}NO_2Cl$
245	156	92	108	65	341	157	93	64	341	92	0	35	Methyldisulfanilamide	$C_{15}H_{15}N_3O_4S_2$
246	156	93	281	125	43	157	55	63	281	78	2	32	Menazone	$C_6H_{12}N_5O_2PS_2$
247	167	43	237	41	124	55	166	168	316	83	3	87	Rectidon	$C_{12}H_{17}N_2O_3Br$
248	169	58	135	153	168	72	170	109	256	45	35	13	Pheniramine	$C_{16}H_{20}N_2O$
249	170	142	83	68	41	114	155	55	170	93	0	67	Propylthiouracil	$C_7H_{10}N_2OS$
250	172	157	173	41	55	113	43	242	242	89	6	85	Thioamobarbital	$C_{11}H_{18}N_2O_2S$
251	172	157	173	41	57	228	98	55	228	89	6	85	Thiobutobarbital	$C_{10}H_{16}N_2O_2S$
252	172	187	84	57	42	188	44	43	261	50	30	35	Alphaprodine	$C_{16}H_{23}NO_2$
253	173	174	146	230	105	57	89	41	230	89	0	85	Pivalylindandione	$C_{14}H_{14}O_3$
254	179	58	178	180	225	165	195	210	253	50	33	32	Nefopam	$C_{17}H_{19}NO$
255	180	55	109	67	82	137	42	181	180	57	3	37	Theobromine	$C_7H_8N_4O_2$
256	180	95	68	41	53	123	42	96	180	75	1	30	Theophylline	$C_7H_8N_4O_2$

Table 1 (Continued)

No.	Eight-peak mass spectrum								M^+	hR_F in mobile phase:			Compound name	Elemental composition
	a	b	c	d	e	f	g	h		1	2	3		
257	180	224	95	194	193	123	109	181	224	66	0	36	Etofylline	$C_9H_{12}N_4O_3$
258	180	264	193	109	181	194	42	247	264	55	6	66	Pentifylline	$C_{13}H_{20}N_4O_2$
259	181	194	109	193	42	67	137	238	238	66	0	45	Protheobromine	$C_{10}H_{14}N_4O_3$
260	181	223	124	43	41	138	224	182	302	94	7	85	Narcobarbital	$C_{11}H_{15}N_2O_3Br$
261	182	82	83	105	94	77	96	303	303	65	47	47	Cocaine	$C_{17}H_{21}NO_4$
262	189	105	285	201	190	164	148	390	390	76	58	79	Meclozine	$C_{25}H_{27}N_2Cl$
263	192	178	272	191	244	44	466	190	466	53	1	19	Cephaline	$C_{28}H_{38}N_2O_4$
264	192	205	272	244	190	273	270	480	480	54	9	34	Emetine	$C_{29}H_{40}N_2O_4$
265	193	236	192	191	194	165	190	237	236	60	4	56	Carbamazepine	$C_{15}H_{12}N_2O$
266	193	237	178	194	115	191	179	192	237	81	3	84	Cyheptamide	$C_{16}H_{15}NO$
267	193	264	72	43	71	220	192	265	264	58	39	58	Mianserin	$C_{18}H_{20}N_2$
268	194	109	55	193	195	67	82	137	194	52	3	58	Caffeine	$C_8H_{10}N_4O_2$
269	194	109	67	193	238	81	55	42	238	4	1	1	Acetylline	$C_9H_{10}N_4O_4$
270	194	180	109	193	238	95	137	81	238	60	3	38	Proxiphylline	$C_{10}H_{14}N_4O_3S$
271	194	195	238	193	72	178	45	196	238	56	8	29	Nomifensine	$C_{16}H_{18}N_2$
272	195	194	193	180	167	118	89	63	195	81	40	89	Iminodibenzyle	$C_{14}H_{13}N$
273	196	178	135	107	164	56	57	77	303	56	0	4	Fenoterol	$C_{17}H_{21}NO_4$
274	200	139	143	96	227	270	310	370	370	38	5	16	Oxypendyl	$C_{20}H_{26}N_4OS$
275	200	199	185	171	84	71	115	131	200	13	7	2	Tetryzoline	$C_{13}H_{16}N_2$
276	201	45	203	299	72	165	166	176	418	58	8	36	Etodroxizine	$C_{23}H_{31}N_2O_3Cl$
277	201	105	203	165	189	285	166	202	406	85	78	91	Meclozine-N-oxide	$C_{25}H_{27}N_2OCl$
278	201	167	117	202	251	115	165	368	368	76	51	78	Cinnarizine	$C_{26}H_{28}N_2$
279	201	175	176	259	202	70	84	242	259	19	13	5	Primaquine	$C_{15}H_{21}N_3O$
280	201	176	70	56	202	258	42	71	377	58	8	46	Morazone	$C_{23}H_{27}N_3O_2$
281	201	203	299	166	374	132	165	202	374	68	9	54	Hydroxyzine	$C_{21}H_{27}N_2O_2Cl$
282	202	187	133	172	201	203	44	144	202	14	10	7	Trimizoline	$C_{13}H_{18}N_2$
283	203	58	205	204	72	167	202	168	274	45	33	18	Chlorphenamine	$C_{16}H_{19}N_2Cl$
284	203	105	218	204	190	216	201	165	434	74	79	89	Chlorbenzoxamine	$C_{27}H_{31}N_2OCl$
285	205	70	231	44	176	56	209	42	371	63	9	58	Trazodone	$C_{19}H_{22}N_5OCl$
286	205	240	91	125	242	206	186	84	311	74	27	78	Quazepam	$C_{20}H_{22}NCl$
287	209	208	278	207	193	194	84	200	278	51	39	20	Tripolidine	$C_{19}H_{22}N_2$
288	209	210	141	208	115	153	152	195	210	14	3	6	Naphazoline	$C_{14}H_{14}N_2$
289	210	123	137	122	77	95	109	211	210	78	53	89	Guajakolethylglykolate	$C_{11}H_{14}O_4$
290	211	212	107	77	213	105	106	80	212	71	6	66	2,5-Diaminobenzo-phenone	$C_{13}H_{12}N_2O$
291	212	187	427	352	70	98	43	45	427	51	10	36	Dixyracine	$C_{24}H_{33}N_3O_3S$
292	214	129	68	216	157	131	41	67	214	88	0	57	8-Chlorotheophylline	$C_7H_7N_4O_2Cl$
293	220	205	221	147	77	178	42	148	413	64	22	74	Noscapine	$C_{22}H_{23}NO_7$
294	223	42	181	109	138	193	67	194	254	50	0	19	Dihydroxypropyl-theobromine	$C_{10}H_{14}N_4O_4$
295	223	194	180	254	109	193	166	95	254	48	0	12	Diprophylline	$C_{10}H_{14}N_4O_4$
296	224	58	225	223	209	195	71	196	295	54	20	35	Dibenzepin	$C_{18}H_{21}N_3O$
297	229	231	194	172	174	200	230	196	229	62	8	31	Clonidine	$C_9H_9N_3Cl_2$
298	230	231	58	105	44	42	173	158	321	68	16	39	Phenazocine	$C_{22}H_{27}NO$
299	230	231	77	232	105	233	154	195	231	93	25	87	2-Amino-5-chloro-benzophenone	$C_{13}H_{10}NOCl$
300	230	231	303	58	41	44	42	288	303	42	18	20	Pentazocine hydrate	$C_{19}H_{29}NO_2$
301	230	265	267	232	154	139	195	264	265	93	20	87	2-Amino-2',5-dichloro-benzophenone	$C_{13}H_9NOCl_2$
302	232	217	215	202	216	231	117	203	293	31	79	41	Amitriptyline oxide	$C_{20}H_{23}NO$
303	235	234	195	208	193	266	194	44	266	26	20	11	Desipramine	$C_{18}H_{22}N_2$
304	235	250	233	236	41	91	65	50	250	70	37	80	Methaqualone	$C_{16}H_{14}N_2O$
305	235	266	91	175	236	65	132	267	266	82	27	86	2-Hydroxymethyl-methaqualone	$C_{16}H_{14}N_2O_2$
306	236	77	78	315	317	51	63	90	315	61	12	41	Bromazepam	$C_{14}H_{10}N_3OBr$
307	240	175	132	242	241	176	88	90	240	76	52	92	Anetholtrithione	$C_{10}H_8OS_3$

Table 1 (Continued)

No.	Eight-peak mass spectrum								M^+	hR_F in mobile phase:			Compound name	Elemental composition
	a	b	c	d	e	f	g	h		1	2	3		
308	241	242	77	105	195	165	243	119	242	90	8	90	2-Amino-5-nitro-benzophenone	$C_{13}H_{10}N_2O_3$
309	241	276	139	195	111	165	119	242	276	90	7	84	2-Amino-5-nitro-2'-chlorobenzophenone	$C_{13}H_9N_2O_3Cl$
310	242	207	244	270	269	243	208	271	270	67	40	74	Medazepam	$C_{16}H_{15}ClN_2$
311	242	270	269	241	44	243	271	244	332	82	6	60	Chlorazepic acid	$C_{16}H_{13}N_2O_4Cl$
312	243	256	245	227	192	258	70	326	326	57	4	38	Clozapine	$C_{18}H_{19}N_4Cl$
313	244	229	44	173	243	245	230	214	244	13	8	5	Xylometazoline	$C_{16}H_{24}N_2$
314	245	189	146	246	42	202	57	44	336	70	45	74	Fentanyl	$C_{22}H_{28}N_2O$
315	246	42	247	377	91	172	47	115	452	74	42	81	Difenoxin	$C_{30}H_{32}N_2O_2$
316	246	403	143	43	70	248	113	405	403	55	7	29	Perphenazine	$C_{21}H_{26}N_3OClS$
317	246	445	70	185	153	125	98	87	445	61	35	53	Thiopropazate	$C_{23}H_{28}N_3O_2ClS$
318	247	248	249	250	219	212	221	232	248	54	55	37	Pyrobutamine	$C_{12}H_{13}N_4Cl$
319	247	248	249	250	219	212	221	232	248	61	2	31	Pyrimethamine	$C_{12}H_{13}N_4Cl$
320	249	247	58	72	167	248	168	250	318	45	33	16	Brompheniramine	$C_{16}H_{19}N_2Br$
321	249	248	95	123	154	75	126	250	249	93	19	87	2-Amino-5-chloro-2'-fluorobenzophenone	$C_{13}H_9NOClF$
322	250	70	221	41	180	44	42	68	389	20	0	0	Reproterol	$C_{18}H_{23}N_5O_5$
323	250	207	70	91	251	119	181	148	341	55	3	45	Fenetylline	$C_{18}H_{23}N_5O_2$
324	250	207	251	70	181	208	42	198	357	55	3	35	Cafedrine	$C_{18}H_{23}N_5O_3$
325	251	266	249	77	148	252	44	76	266	85	3	69	3'-Hydroxymethaqualone	$C_{16}H_{14}N_2O_2$
326	251	266	249	143	77	252	267	76	266	82	0	78	4'-Hydroxymethaqualone	$C_{16}H_{14}N_2O_2$
327	252	118	90	77	91	253	119	145	252	88	10	88	Phenopyrazone	$C_{15}H_{12}N_2O_2$
328	253	252	43	254	104	235	57	251	253	51	1	8	Triamterene	$C_{12}H_{11}N_7$
329	255	131	254	125	257	256	57	58	325	78	31	69	Clemizole	$C_{19}H_{20}N_3Cl$
330	256	283	284	221	257	285	258	255	368	66	8	64	Ketazolam	$C_{20}H_{17}N_2O_3Cl$
331	256	283	284	285	257	258	255	286	284	75	23	73	Diazepam	$C_{16}H_{13}N_2OCl$
332	257	77	259	51	241	75	229	151	286	56	0	40	Oxazepam	$C_{15}H_{11}N_2O_2Cl$
333	260	245	217	218	44	261	246	259	260	9	1	1	Oxymetazoline	$C_{16}H_{24}N_2O$
334	260	261	42	202	57	217	203	218	261	63	45	57	Phenindamine	$C_{19}H_{19}N$
335	260	288	259	287	261	262	289	102	288	75	2	60	Flurazepam-N1-dealkyl	$C_{15}H_{10}N_2OCIF$
336	265	308	121	266	187	43	145	131	308	92	0	74	Warfarin	$C_{19}H_{16}O_4$
337	266	160	235	251	247	77	146	267	266	82	12	61	2'-Hydroxymethyl-methaqualone	$C_{16}H_{14}N_2O_2$
338	266	267	224	268	250	220	111	125	267	83	0	21	Apomorphine	$C_{17}H_{17}NO_2$
339	266	268	267	255	231	102	88	176	284	70	12	20	Mazindol	$C_{16}H_{13}ClN_2O$
340	267	294	295	268	248	220	221	266	295	74	12	71	Nimetazepam	$C_{16}H_{13}N_3O_3$
341	268	143	425	55	70	43	42	269	425	54	5	27	Carfenazine	$C_{24}H_{31}N_3O_2S$
342	269	58	268	85	270	314	271	228	314	51	54	34	Clomipramine	$C_{19}H_{23}N_3Cl$
343	269	205	297	271	285	221	268	299	353	79	0	17	Butizid	$C_{11}H_{16}N_3O_4ClS_2$
344	271	254	116	145	89	64	80	117	350	56	0	5	Chiniofon	$C_9H_6NO_4SI$
345	271	273	300	255	77	256	272	193	300	53	8	59	3-Hydroxydiazepam	$C_{16}H_{13}N_2O_2Cl$
346	273	204	279	308	77	310	307	309	308	71	3	60	Alprazolam	$C_{17}H_{13}N_4Cl$
347	274	302	301	303	275	283	273	276	302	76	24	67	Fludiazepam	$C_{16}H_{12}N_2OCIF$
348	280	42	70	437	143	248	113	281	437	63	6	23	Fluphenazine	$C_{22}H_{26}N_3OF_3S$
349	280	253	281	234	206	264	254	252	281	68	0	36	Nitrazepam	$C_{15}H_{11}N_3O_3$
350	280	314	315	234	288	286	240	316	315	72	0	53	Clonazepam	$C_{15}H_{10}N_3O_3Cl$
351	281	120	280	122	282	160	91	65	281	32	1	3	Phentolamine	$C_{17}H_{19}N_2O$
352	282	281	236	263	237	145	235	264	282	90	0	21	Niflumic acid	$C_{13}H_9N_2O_2F_3$
353	282	299	284	283	241	77	247	56	299	62	2	50	Chlordiazepoxide	$C_{16}H_{14}N_3OCl$
354	283	255	282	254	284	264	256	106	283	74	1	52	7-Aminoflunitrazepam	$C_{16}H_{14}N_3OF$
355	283	282	256	176	157	43	41	57	283	67	22	24	Levallorphan	$C_{19}H_{25}NO$
356	285	42	229	228	96	59	58	44	285	23	3	9	Hydromorphone	$C_{17}H_{19}NO_3$
357	285	162	215	42	286	124	284	174	285	37	1	9	Morphine	$C_{17}H_{19}NO_3$
358	285	270	55	77	105	91	166	257	285	85	83	96	2-Cyclopropylmethyl-amino-5-chlorobenzophenone	$C_{17}H_{16}NOCl$

Table 1 (Continued)

No.	Eight-peak mass spectrum								M^+	hR_F in mobile phase:			Compound name	Elemental composition
	a	b	c	d	e	f	g	h		1	2	3		
	359	285	286	77	287	269	76	221		75	286	63		
360	286	244	288	218	217	216	287	77	286	76	0	54	Desmethyloclobazam	$C_{15}H_{11}N_2O_2Cl$
361	287	286	215	288	96	229	243	228	287	51	45	44	Cyproheptadine	$C_{21}H_{21}N$
362	288	255	41	107	105	91	93	203	288	86	17	81	Prasterone	$C_{19}H_{28}O_2$
363	288	273	287	290	332	289	304	245	332	74	2	54	N1-(2-Hydroxyethyl)-flurazepam	$C_{17}H_{14}N_2O_2ClF$
364	290	259	275	291	123	243	44	81	290	55	0	22	Trimethoprim	$C_{14}H_{18}N_4O_3$
365	291	239	293	274	75	276	275	138	320	52	1	36	Lorazepam	$C_{15}H_{10}N_2O_2Cl_2$
366	291	290	105	108	70	115	204	42	291	65	43	47	Butinoline	$C_{20}H_{21}NO$
367	294	259	293	205	77	295	296	137	294	71	2	44	Estazolam	$C_{16}H_{11}N_4Cl$
368	299	162	229	124	300	214	298	188	299	33	6	18	Codeine	$C_{18}H_{21}NO_3$
369	299	242	59	42	243	96	70	214	299	25	4	20	Hydrocodone	$C_{18}H_{21}NO_3$
370	299	271	300	224	272	252	270	280	299	76	0	52	Desmethylflunitrazepam	$C_{15}H_{10}N_2O_3F$
371	300	77	51	255	258	259	256	257	300	62	9	70	Clobazam	$C_{16}H_{13}N_2O_2Cl$
372	301	44	42	59	70	302	164	300	301	26	8	13	Dihydrocodeine	$C_{18}H_{23}NO_3$
373	302	246	313	211	273	289	304	274	331	75	2	60	Didesethylflurazepam	$C_{17}H_{15}N_3OClF$
374	303	301	305	115	194	196	304	58	301	51	0	6	Broxyquinoline	$C_9H_5NOBr_2$
375	303	304	58	151	43	260	165	57	454	59	23	70	Verapamil	$C_{27}H_{38}N_2O_4$
376	305	307	150	306	115	213	152	215	305	56	0	5	Clioquinol	C_9H_5NOCl
377	305	307	306	309	308	334	289	75	334	52	7	62	Lormetazepam	$C_{16}H_{12}N_2O_2Cl_2$
378	308	280	307	309	310	91	43	281	308	75	29	73	Pinazepam	$C_{18}H_{13}N_2OCl$
379	308	310	309	307	58	42	136	311	351	70	8	60	Adinazolam	$C_{19}H_{18}N_5Cl$
380	310	312	325	311	327	163	297	142	325	72	8	65	Midazolam	$C_{18}H_{13}N_3ClF$
381	311	188	41	81	70	241	43	56	311	59	1	23	Nalorphine	$C_{19}H_{21}NO_3$
382	311	296	42	44	255	312	310	253	311	45	23	37	Thebaine	$C_{19}H_{21}NO_3$
383	312	285	313	286	266	238	239	183	313	63	10	72	Flunitrazepam	$C_{16}H_{12}N_3O_3F$
384	312	399	297	281	371	43	313	298	399	55	0	37	Colchicine	$C_{22}H_{25}NO_6$
385	313	43	315	314	278	316	279	331	416	83	18	93	Cyproterone acetate	$C_{24}H_{29}O_4Cl$
386	314	67	56	222	77	121	105	315	314	76	15	75	Iodphenazone	$C_{11}H_{11}N_2OI$
387	315	70	230	44	42	316	140	258	315	50	23	51	Oxycodone	$C_{18}H_{21}NO_4$
388	318	289	320	291	319	290	317	275	318	79	35	88	Clotiazepam	$C_{16}H_{15}N_2OClS$
389	323	221	181	222	223	207	324	72	323	60	3	39	Lysergide	$C_{20}H_{25}N_3O$
390	324	91	269	55	296	295	323	326	324	65	36	74	Prazepam	$C_{19}H_{17}N_2OCl$
391	325	297	324	255	43	306	296	326	325	73	0	41	Flunitrazepam, 7-Acetamide	$C_{18}H_{16}N_3O_2F$
392	327	70	41	96	242	84	82	328	327	65	13	66	Naloxone	$C_{19}H_{21}NO_4$
393	327	268	42	43	44	215	162	285	327	46	6	19	Monoacetylmorphine	$C_{19}H_{21}NO_4$
394	327	369	268	43	310	215	42	204	369	47	15	38	Diacetylmorphine	$C_{21}H_{23}NO_5$
395	329	283	224	268	330	270	269	285	346	68	1	65	Nifedipine	$C_{17}H_{18}N_2O_6$
396	331	313	43	273	321	333	374	219	374	92	21	96	Cyproterone	$C_{22}H_{27}O_3Cl$
397	334	44	120	335	107	144	162	130	334	26	8	19	Strychnine	$C_{21}H_{22}N_2O_2$
398	338	339	324	340	154	325	308	293	339	61	10	65	Papaverine	$C_{20}H_{21}NO_4$
399	342	313	238	344	75	315	102	137	342	60	1	40	Triazolam	$C_{17}H_{12}N_4Cl_2$
400	353	354	355	169	184	170	156	144	354	63	5	38	Yohimbine	$C_{21}H_{26}N_2O_3$
401	354	252	353	267	295	253	355	224	354	64	41	54	Vincamine	$C_{21}H_{26}N_2O_3$
402	363	206	143	70	232	218	207	193	363	54	6	22	Opipramol	$C_{23}H_{29}N_3O$
403	365	221	195	366	212	197	364	351	578	72	3	77	Deserpidine	$C_{32}H_{38}N_2O_8$
404	378	449	467	410	55	435	434	450	467	76	9	68	Buprenorphine	$C_{29}H_{41}NO_4$
405	386	138	387	150	42	110	90	301	430	70	1	45	Piritramide	$C_{27}H_{34}N_4O$
406	386	359	323	245	388	303	387	361	386	88	92	94	Quintozene	$C_{17}H_{11}N_2ClF_4S$
407	394	392	396	245	318	316	395	393	392	75	8	66	Brotizolam	$C_{15}H_{10}N_4ClBrS$
408	394	395	379	107	120	380	392	203	394	16	2	17	Brucine	$C_{23}H_{26}N_2O_4$
409	399	113	70	141	43	72	400	71	399	51	30	41	Thiethylperazine	$C_{22}H_{29}N_3S_2$
410	405	53	278	51	44	78	50	127	405	81	0	3	Diodone	$C_7H_5NO_3I_2$
411	406	286	314	333	315	294	287	295	406	81	0	46	Floctafenine	$C_{20}H_{17}N_2O_4F_3$
412	424	173	264	426	422	423	425	279	422	88	0	81	Benzbromarone	$C_{17}H_{12}Br_2O_3$

Table 1 (Continued)

No.	Eight-peak mass spectrum								M^+	hR_F in mobile phase:			Compound name	Elemental composition
	a	b	c	d	e	f	g	h		1	2	3		
413	498	408	470	463	662	336	517	89	662	81	0	41	Iobenzaminic acid	$C_{16}H_{13}N_2O_3I_3$
414	504	429	473	84	505	41	474	42	504	68	0	37	Dipyridamole	$C_{24}H_{40}N_8O_4$
415	608	607	609	395	195	397	251	396	608	69	4	74	Reserpine	$C_{33}H_{40}N_2O_9$

Mobile phases: 1 Methanol–25% aqueous ammonia, 100 + 1.5; 2 cyclohexane–toluene–diethylamine, 75 + 15 + 10; 3 chloroform–methanol, 90 + 10.

Table 2

Eight-peak mass spectra, molecular weights, and hR_F (corrected $R_F \times 100$) values measured using mobile phases 4–6 for drugs and related compounds.

No.	Eight-peak mass spectrum								M^+	hR_F in mobile phase:			Compound name	Elemental composition
	a	b	c	d	e	f	g	h		1	2	3		
416	43	129	69	41	86	97	250	252	278	49	57	48	Acecarbromal	$C_9H_{15}N_2O_3Br$
417	55	83	82	113	70	97	41	127	155	52	68	53	Bemegride	$C_8H_{13}NO_2$
418	57	41	141	167	83	182	181	55	238	58	39	69	Nealbarbital	$C_{12}H_{18}N_2O_3$
419	67	193	169	66	192	168	41	150	234	50	37	64	Cyclopal	$C_{12}H_{14}N_2O_3$
420	69	43	55	83	44	53	41	51	98	49	74	62	Methylpentynol	$C_6H_{10}O$
421	77	278	109	78	218	51	110	65	404	4	16	4	Sulfinpyrazone	$C_{23}H_{20}N_2O_3S$
422	79	81	221	41	53	178	93	164	262	73	58	72	Methohexital	$C_{14}H_{18}N_2O_3$
423	81	91	106	95	79	78	68	67	167	49	74	59	Ethinamate	$C_9H_{13}NO_2$
424	83	55	71	96	44	84	81	114	218	9	60	34	Meprobamate	$C_9H_{18}N_2O_4$
425	92	156	65	108	191	93	55	255	255	9	9	20	Sulfathiazole	$C_9H_9N_3O_2S_2$
426	92	156	108	65	118	162	174	253	253	26	5	54	Sulfamethoxazole	$C_{10}H_{11}N_3O_3S$
427	92	214	65	108	172	156	42	43	214	1	25	6	Sulfaguanidine	$C_7H_{10}N_4O_2S$
428	93	199	324	109	77	205	162	135	324	52	7	62	Oxyphenbutazone	$C_{19}H_{20}N_2O_3$
429	97	58	55	158	104	83	62	71	260	36	73	53	Carisoprodol	$C_{12}H_{24}N_2O_4$
430	97	72	55	71	62	110	69	158	232	10	59	35	Mebutamate	$C_{10}H_{20}N_2O_4$
431	104	132	51	78	77	103	218	41	218	29	24	61	Phenylmethylbarbital	$C_{11}H_{10}N_2O_3$
432	108	109	176	43	137	81	80	53	179	38	68	38	Phenacetine	$C_{10}H_{13}NO_2$
433	109	151	43	80	81	108	110	54	151	15	45	34	Paracetamol	$C_8H_9NO_2$
434	113	55	70	42	41	85	69	114	141	50	57	56	Ethosuximide	$C_7H_{11}NO_2$
435	118	117	91	44	65	77	92	103	179	47	74	55	Phenprobamate	$C_{10}H_{13}NO_2$
436	120	92	138	64	63	65	121	93	138	7	11	25	Salicylic acid	$C_7H_6O_3$
437	120	137	92	65	121	64	63	93	137	38	46	55	Salicylamide	$C_7H_7NO_2$
438	120	138	92	121	43	57	69	63	180	18	16	30	Acetylsalicylic acid	$C_9H_8O_4$
439	121	362	241	57	65	120	93	363	408	4	24	32	Ethylbiscoumacetate	$C_{22}H_{16}O_8$
440	123	105	78	51	77	106	50	52	123	1	0	0	Nicotinic acid	$C_6H_5NO_2$
441	129	43	57	128	44	41	72	58	157	0	7	60	Paramethadione	$C_7H_{11}NO_3$
442	136	154	80	108	52	53	137	82	154	6	2	23	Gentisic acid	$C_7H_6O_4$
443	138	195	103	140	77	51	75	102	213	1	0	0	Baclofen	$C_{10}H_{12}NO_2Cl$
444	139	141	111	357	140	113	359	75	357	16	6	20	Indometacin	$C_{19}H_{16}NO_4Cl$
445	140	155	83	98	55	41	69	97	183	31	61	25	Methypylon	$C_{10}H_{17}NO_2$
446	141	156	55	98	53	157	142	69	240	53	44	67	Hexetal	$C_{12}H_{20}N_2O_3$
447	141	156	98	41	142	55	157	184	212	50	38	65	Butobarbital	$C_{10}H_{16}N_2O_3$
448	146	190	117	118	161	189	103	91	218	8	39	26	Primidone	$C_{12}H_{14}N_2O_2$
449	151	223	222	72	123	152	108	52	223	38	40	35	Etamivan	$C_{12}H_{17}NO_3$
450	155	170	112	169	55	82	41	39	198	66	53	67	Metharbital	$C_9H_{14}N_2O_3$
451	156	92	108	65	42	138	43	157	267	25	8	52	Sulfafurazole	$C_{11}H_{13}N_3O_3S$
452	156	141	41	57	157	98	55	69	212	50	44	63	Secbutabarbital	$C_{10}H_{16}N_2O_3$
453	156	141	43	41	157	55	71	155	226	55	45	66	Pentobarbital	$C_{11}H_{18}N_2O_3$
454	156	141	155	98	112	55	41	157	184	41	31	61	Barbital	$C_8H_{12}N_2O_3$
455	156	141	157	142	197	183	198	98	226	52	38	65	Amobarbital	$C_{11}H_{18}N_2O_3$
456	156	158	92	77	108	157	314	65	314	29	9	51	Sulfaphenazole	$C_{15}H_{14}N_4O_2S$

Table 2 (Continued)

No.	Eight-peak mass spectrum								M^+	hR_F in mobile phase:			Compound name	Elemental composition
	a	b	c	d	e	f	g	h		1	2	3		
457	161	163	91	119	107	206	117	164	206	46	7	54	Ibuprofen	$C_{13}H_{18}O_2$
458	167	124	80	41	166	165	106	141	208	50	31	66	Allobarbital	$C_{10}H_{12}N_2O_3$
459	167	168	41	97	124	195	153	53	224	53	41	67	Talbutal	$C_{11}H_{16}N_2O_3$
460	167	168	124	169	97	195	41	153	210	48	36	65	Aprobarbital	$C_{10}H_{14}N_2O_3$
461	167	209	43	124	41	53	210	168	288	50	31	67	Propallylonal	$C_{10}H_{13}N_2O_3Br$
462	168	167	41	43	97	124	195	169	238	50	41	67	Secobarbital	$C_{12}H_{18}N_2O_3$
463	168	167	41	124	181	97	141	169	224	54	38	67	Butalbital	$C_{11}H_{16}N_2O_3$
464	172	156	92	65	108	63	64	80	172	13	52	46	Sulfanilamide	$C_6H_8N_2O_2S$
465	172	157	173	43	41	242	55	69	242	77	49	74	Thiopental	$C_{11}H_{18}N_2O_2S$
466	180	77	104	209	223	252	51	181	252	33	36	53	Phenytoin	$C_{15}H_{12}N_2O_2$
467	183	77	184	308	105	93	252	91	308	78	66	68	Phenylbutazone	$C_{19}H_{20}N_2O_2$
468	184	185	92	65	108	186	66	183	249	16	24	42	Sulfapyridine	$C_{11}H_{11}N_3O_2S$
469	188	96	77	56	105	55	51	93	188	18	49	14	Phenazone	$C_{11}H_{12}N_2O$
470	189	104	190	77	105	51	218	132	218	62	76	58	Mephenytoin	$C_{12}H_{14}N_2O_2$
471	189	117	132	160	115	91	217	190	217	63	78	62	Glutethimide	$C_{13}H_{15}NO_2$
472	199	200	92	65	108	156	80	184	264	23	8	41	Sulfamerazine	$C_{11}H_{12}N_4O_2S$
473	199	200	92	65	108	156	80	184	278	23	13	45	Sulfadimidine	$C_{12}H_{14}N_4O_2S$
474	199	244	200	178	179	184	183	245	244	30	7	41	Flurbiprofen	$C_{15}H_{13}FO_2$
475	203	232	132	175	204	130	233	118	232	32	65	47	Aminoglutethimide	$C_{13}H_{16}N_2O_2$
476	204	232	117	146	77	118	161	51	232	47	28	65	Phenobarbital	$C_{12}H_{12}N_2O_3$
477	207	41	165	124	44	122	91	77	286	52	30	69	Brallobarbital	$C_{10}H_{11}N_2O_3Br$
478	207	141	67	81	79	208	59	80	236	50	35	64	Cyclobarbital	$C_{12}H_{16}N_2O_3$
479	210	208	69	44	165	167	41	71	236	53	74	56	Carbromal	$C_7H_{13}N_2O_2Br$
480	214	213	92	65	108	43	215	66	278	5	5	16	Sulfisomidine	$C_{12}H_{14}N_4O_2S$
481	214	242	295	216	215	297	244	179	295	25	13	40	Diclofenac	$C_{14}H_{11}Cl_2NO_2$
482	215	230	56	216	77	96	231	41	230	61	73	50	Propyphenazone	$C_{14}H_{18}N_2O$
483	218	117	118	146	77	103	115	91	246	70	43	69	Methylphenobarbital	$C_{13}H_{14}N_2O_3$
484	221	81	141	222	79	41	93	67	250	50	30	65	Heptabarb	$C_{13}H_{18}N_2O_3$
485	221	81	157	80	79	155	222	41	236	65	48	65	Hexobarbital	$C_{12}H_{16}N_2O_3$
486	239	52	158	303	64	62	81	159	331	7	40	47	Hydroflumethiazide	$C_8H_8N_3O_4F_3S_2$
487	251	280	91	121	118	189	252	119	280	62	21	56	Phenprocoumon	$C_{18}H_{16}O_3$
488	256	121	185	224	257	65	43	41	285	13	5	23	Probenecid	$C_{13}H_{19}NO_4S$
489	269	285	268	221	205	206	271	299	297	4	34	39	Hydrochlorothiazide	$C_7H_8N_3O_4ClS_2$
490	295	268	297	97	57	270	62	64	295	2	2	16	Chlorothiazide	$C_7H_6N_3O_4ClS_2$
491	310	64	312	42	43	63	62	56	359	19	53	50	Methylclothiazide	$C_9H_{11}N_3O_4Cl_2S_2$
492	310	121	43	311	353	120	92	65	353	52	15	51	Acenocoumarol	$C_{19}H_{15}NO_6$
493	354	131	113	228	43	41	355	147	780	1	33	5	Digoxin	$C_{41}H_{64}O_{14}$

Mobile phases: 4 chloroform-acetone, 80 + 20; 5 ethyl acetate-methanol-25% aqueous ammonia, 85 + 10 + 5; 6 ethyl acetate.

The reagents used for color reactions were [2]: *Marquis*, *Dragendorff* (modified), *Ludy Tenger*, potassium iodoplatinate, palladium chloride, ferric chloride-sulfuric acid, mercury nitrate-mercury sulfate, diphenylcarbazone, fast blue B, *Bratton-Marshall*.

EI mass spectra were obtained with a Finnigan MAT 212 (Bremen, Germany) instrument equipped with a spectro-system SS 300. The compounds were transferred in quartz crucibles to the direct inlet system of the instrument and evaporated by TIC controlled heating to 200°C. EI spectra were obtained at 100 eV ionization energy in full-scan mode. The eight-peak mass spectra are also tabulated (Tables 1 and 2).

2.2 Preparation of Biological Samples

The TLC plates were pretreated with a solution of methanol + 1.5% aqueous ammonia and reactivated for 2 h at 150°C in a clean heating oven and subsequently cooled in a clean closed system. The samples were obtained from biological species - urine, tissue (lung, liver, kidney) and stomach content - by liquid-liquid extraction at pH 3 and pH 9 or solid-phase extraction as described elsewhere [20]. For screening, extracts containing acidic and neutral or basic and neutral drugs, and compounds after conjugate cleavage, were applied to the TLC plate as spots. In this way ten extracts can be developed in parallel. If spots of any unknown compounds were detected, the extracts containing

these compounds were applied to a pretreated TLC plate as a band and developed with an appropriate mobile phase. One part of the TLC plate (approximately 2 cm) was used for detection of the substances by use of color reactions. One or more bands to be investigated by MS were marked, scratched from the plate, extracted with methanol-dichloromethane (1:1, v/v) under sonication for 5 min, and centrifuged. The supernatant was transferred to another clean tube and evaporated to dryness by means of a gentle stream of nitrogen. The residue was dissolved in methanol (20 μ L) and this solution (5 μ L) was transferred to a quartz MS crucible and the solvent again evaporated. The identification of compounds from their mass spectra was confirmed by TLC with reference compounds and the mobile phases mentioned above. An example is given in **Figure 1** – the EIMS of the unknown contained a prominent peak m/z 58 and a weak peak at m/z 91. Five candidates were selected as standards for TLC confirmation and the unknown was identified as amitriptyline.

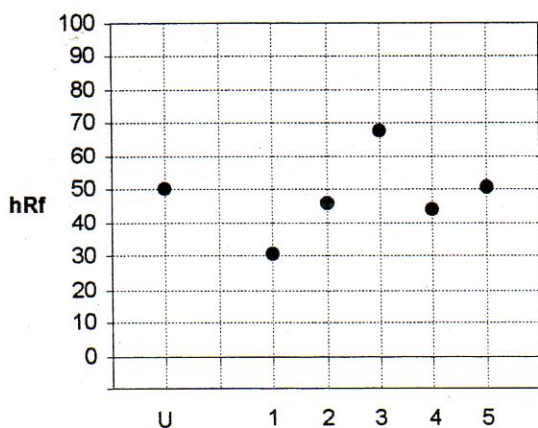


Figure 1

TLC confirmation of the unknown (U) using mobile phase 1 and five standards, selected upon MS investigation (prominent m/z 58 and weak peak at m/z 91). 1, methamphetamine; 2, phentermine; 3, dextropropoxyphene; 4, chlorphentermine; 5, amitriptyline. The unknown was identified as amitriptyline.

3 Results and Discussion

Libraries of corrected hR_F values and corresponding EI mass spectra were created for routine toxicological and forensic applications. To make the identification of unknowns easier corrected hR_F values were tabulated with the eight most intense mass spectrometric peaks. Important data for drugs and their metabolites are arranged in Tables 1 and 2.

3.1 Identification of the Unknowns by PC-Based Library Search

The compilation of corrected hR_F values, full and eight peak EI mass spectra, and the structures of the investigated substances are kept as a library in a PC-based searching system [21]. It aids the selection or rejection of possible candidates during the analysis of unknowns after each step of an investigation. **Figure 2** shows an example of the data placed in this library (optional mobile phases for further use are reserved).

4 Conclusion

A simple off-line TLC–EIMS approach for the screening of biological samples for drugs and their metabolites is described. Corrected hR_F values and eight-peak mass spectra for 493 drugs and metabolites are tabulated. This technique can be used in practice as an alternative screening method or together with HPLC–MS. The most important application is quick analysis in emergency clinical cases of intoxication. The library created from TLC and MS data can be used for identification by means of a PC-based library search.

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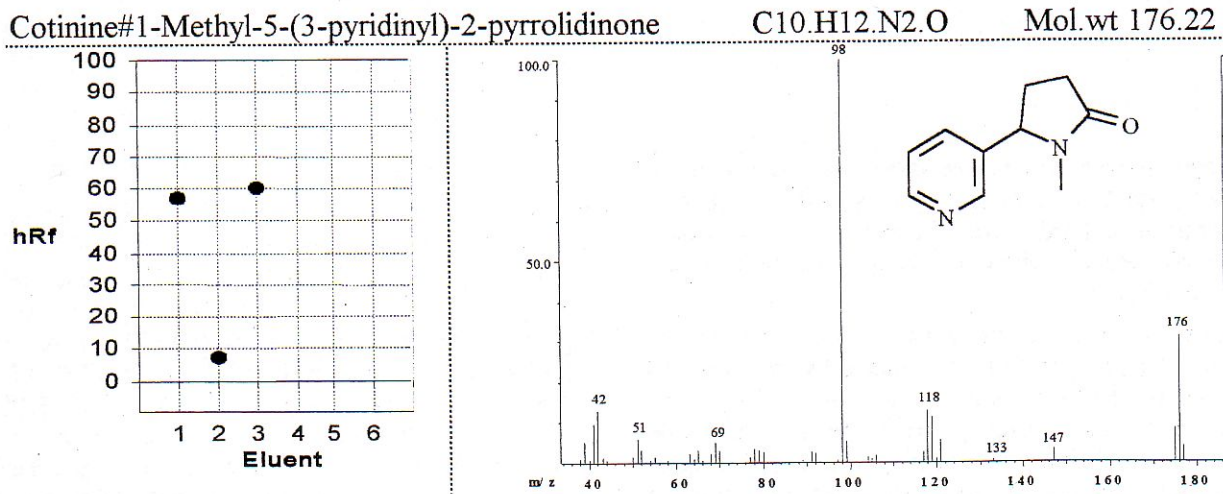


Figure 2

Corrected hR_F values, EI mass spectrum, and structure of cotinine.

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