

CHREV. 148

## GAS-LIQUID CHROMATOGRAPHIC RETENTION INDICES OF 1318 SUBSTANCES OF TOXICOLOGICAL INTEREST ON SE-30 OR OV-1 STATIONARY PHASE\*

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### 1. INTRODUCTION

Gas-liquid chromatography (GLC) is one of the most widely used techniques, either alone or in combination with mass spectrometry, for the separation and identification of drugs, their metabolites and other endogenous materials present in solvent extracts of biological samples submitted for toxicological analysis. Many different stationary phases have been used and retention data have been expressed in a variety of ways such as retention times, retention times relative to arbitrary internal standards and retention indices. It has been proposed<sup>1</sup> that the low polarity dimethylsilicone stationary phases such as SE-30 and OV-1 should be used as the preferred liquid phases for the identification of drugs and that the most reproducible and useful GLC retention parameter is the retention index. As an aid to analysts wishing to standardise on these stationary phases, retention index data for either SE-30 or OV-1 have previously been provided for 480 drugs (see ref. 1) and 296 non-drug substances likely to be encountered in toxicological analyses (see ref. 2). A wealth of retention data using SE-30 and similar stationary phases is available both in the published literature and in private collections and some of this data has now been used in this compilation comprising 1318 compounds. These include not only drugs, but plasticizers, antioxidants, stabilisers, etc., so that the data provide a comprehensive list of retention indices of materials likely to be encountered in a wide variety of medicinal, toxicological and pharmacological analyses.

Data have been extracted from thirty-six sources and the multiplicity of data for a particular compound enables an estimate of the reproducibility of the retention index to be made. The determination of a mean value for the retention index of a

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compound has in many cases highlighted retention index values which differed greatly from the mean and these have been noted in the compilations.

## 2. COMPILATION OF DATA

This work lists retention index values from 1318 compounds on SE-30 or OV-1 stationary phases, being compiled from 4586 separate retention index values taken from thirty-six sources. These sources included the scientific literature and colleagues who generously donated their data<sup>1-36</sup>. Where the source gave a retention index it was used, otherwise retention times or relative retention times were converted to retention indices using appropriate calibration curves<sup>1</sup>. The names of the compounds used in this compilation were taken from Martindale<sup>37</sup> whenever possible or the Merck Index<sup>38</sup> or, for the economic poisons, the Nanogen Index<sup>39</sup>. For each compound the mean of all retention index values extracted from the sources was calculated. Values differing by more than  $\pm 50$  retention index units were then extracted and the mean recalculated. This procedure was repeated until all of the values used to calculate the mean retention index were within this  $\pm 50$  retention index unit window.

## 3. RESULTS AND DISCUSSION

Table 1 gives the retention index data for 1318 substances in alphabetical order of compound name. The contents of each column are: *RI*: mean retention index, 9999 indicates that no material was detected under the conditions used by the respective authors; (*n*): the number of values used to obtain the mean retention index; - +: these two columns show the range of the (*n*) retention index values about the mean; > 50: any values which differed by more than 50 retention index units from the mean and which were extracted during the calculation of the mean, are shown in this column. If a single reference contained multiple determinations in this category they are listed separately; [Ref]: the origin of the value cited in the previous column; Refs.: the origins of the (*n*) values used to calculate the mean retention index. Where a single reference contained multiple determinations it has only been cited once.

The retention index quoted for many of the compounds is that obtained from a single value quoted from one source and therefore the reliability and reproducibility of that value cannot be estimated. However, many are the mean of retention indices from several sources. These mean values enable an estimate to be made of both the reproducibility of measurement of the retention index of a particular compound and also the reliability with which a retention index was determined by the original author. For example, the retention index of barbitone in Table I is 1497, which is the mean of 20 determinations, the range of reported values being from 17 retention index units below this value (1480) to 33 above (1530). Thus, the measurement of the retention index of barbitone is very reproducible. Only one reported value differed from the mean by more than 50 retention index units, this being a value of 1560 reported in ref. 12. It is therefore likely that, on this occasion, these authors used conditions of measurement which were different to those of the other authors. On the other hand, the range of reported values for chlorpromazine (retention index 2486, mean 21 determinations) is much greater than for barbitone being from 46 retention index units below the mean (2440) to 49 retention index units above (2535) and five

TABLE 1

## RETENTION INDICES OF 1318 COMPOUNDS, USING SE-30 OR OV-1 AS THE STATIONARY PHASE, IN ALPHABETICAL ORDER OF COMPOUND

*RI* = Mean retention index from (*n*) values all of which were within  $\pm 50$  retention index units of the mean; 9999 = no peak observed; + - = range of values about the mean; > 50 = retention indices greater than 50 retention index units from the mean; [Ref.] = source of the value in the preceding column; Refs. = sources of the retention indices used to calculate the mean value.

<i>Compound name</i>	<i>RI</i>	<i>(n)</i>	-	+	> 50	[Ref.]	<i>Refs.</i>
Acepihylline	1000	(1)					7
Acepromazine	2694	(5)	28	41	2850	[14]	4, 10, 11, 15, 27
7-Acetamidoclonazepam	3263	(2)	8	7			32, 35
7-Acetamidoflunitrazepam	3115	(1)					32
7-Acetamidonitrazepam	3205	(1)					32
Acetanilide	1358	(1)					10
Acetophenazine	9999	(2)					1, 10
Acetylcarbromal	1215	(2)	15	16	1505	[35]	7, 10
Acetylcodeine	2510	(2)	15	15			14, 35
Acetylcysteine	1547	(1)					10
Acetyldihydrocodeine	2455	(1)					11
Acetylindole	1487	(1)					10
Acetylmethylamphetamine	1630	(1)					15
Acetyl- $\beta$ -phenethylamine	1524	(1)					33
Acetylprocaine	2340	(1)					15
Acetylsalicylic acid (aspirin)	1309	(6)	49	31	1400	[12]	5, 10, 14, 16, 17
					1410	[12]	35
Acetyltributyl citrate	2253	(1)					2
Acetyltriethyl citrate	1730	(1)					2
Acetyl-D-tryptophan	2184	(1)					10
Acetyl-L-tryptophan	2058	(1)					10
Aconitine					2280	[5]	
					2670	[11]	
					9999	[10]	
Adiphenine	2186	(12)	26	29	2250	[23]	5, 10, 12, 13, 15
Ajmaline	2705	(1)					35
Aldrin	1943	(5)	28	27			5, 7, 13
Aletamine	1293	(5)	16	27			3, 10, 11, 22, 29
Allobarbitone	1606	(11)	20	9			6, 7, 9, 10-12, 16, 18, 19, 26, 35
Allobarbitone metabolite	1785	(1)					35
Allopurinol	882	(1)					10
5-Allyl-5-butylbarbituric acid	1698	(1)					18
N-Allyl-3-hydroxymorphinan	2370	(1)					21
5-Allyl-5-(2-hydroxypropyl)-barbitone	1837	(3)	22	33			12
5-Allyl-5-phenylbarbituric acid					2003	[10]	
					2106	[10]	
Allylprodine	1929	(1)					30
Alphacetylmethadol	2187	(3)	7	13			11, 15, 20
Alphameprodine	1850	(1)					11
Alphamethadol	2180	(1)					11
Alphaprodine	1792	(4)	42	33	1895	[7]	10, 11, 20, 30
Alprenolol	1760	(2)	5	5	1840	[14]	12
Alverine	2142	(2)	2	3			7, 15

(Continued on p. 198)

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Amantadine	1257	(3)	7	13			7, 11, 35
Am̄ucetamide	2235	(2)	5	5			11
Ametazole	1390	(1)					1
Amethocaine	2219	(15)	29	26	2280	[14]	5, 7, 9-12
					2285	[11]	13, 15, 25, 28
Ametryne	1775	(2)	0	0			11
Amidephrine	9999	(1)					11
Amidopyrine	1903	(19)	25	32	2000	[28]	4, 5, 7, 9, 10, 12, 13, 15, 16, 25, 26, 35
Aminacrine	2240	(1)					7
<i>p</i> -Aminobenzoic acid	1547	(1)					10
2-Amino-5-chlorobenzophenone	2039	(6)	39	41	2125	[36]	7, 35, 36
2-Amino-5-chlorodiphenylamine	2078	(2)	3	3			36
2-Amino-5-chloro-2'-fluoro-benzophenone					1980	[7]	
					2045	[36]	
					2090	[36]	
2-Amino-5-chloro-3-hydroxy-benzophenone	2390	(2)	10	10			36
2-Amino-2'-chloro-5-nitrobenzophenone	2516	(4)	46	34			7, 35, 36
7-Aminoclonazepam	2900	(2)	5	5			32, 35
2-Amino-5,2'-dichlorobenzophenone					2120	[7]	
					2195	[36]	
					2240	[36]	
					2480	[36]	
7-Aminoflunitrazepam	2723	(2)	3	2			32
5-Amino-2'-fluoro-2-methylaminobenzophenone	2703	(2)	3	2			36
2-Amino-2'-fluoro-5-nitrobenzophenone	2363	(2)	18	17			36
Aminoglutethimide	2227	(1)					10
7-Amino-3-hydroxycyclonazepam	2890	(1)					35
7-Aminonitrazepam	2828	(2)	43	42			32
2-Amino-5-nitrobenzophenone	2388	(4)	38	47	2475	[36]	7, 35, 36
Aminonitrothiazole	9999	(1)					11
7-Aminonorflunitrazepam	2825	(1)					32
Aminoparathion	1885	(1)					35
<i>p</i> -Aminophenol	1265	(1)					10
Aminophylline					1970	[12]	
					1970	[12]	
					2083	[10]	
5-Aminoquinoline	1598	(1)					2
<i>p</i> -Aminosalicylic acid	1309	(1)					10
Aminotriazole	9999	(1)					11
Amisometradine	2021	(1)					10
Amitriptyline	2196	(25)	46	34			4-7, 9-16, 17, 25, 27, 28, 30, 35
Amodiaquine	9999	(1)					10
Amolanone	2226	(2)	10	9			10, 11
Amotriphene	9999	(1)					11
Amphetamine	1123	(17)	38	32	1090	[7]	3, 5-10
					1190	[13]	11, 13, 14, 16, 17
					1260	[13]	22, 25, 29, 35
					1265	[12]	

TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Amprotopine	2038	(1)					11
Ampyrone	1950	(1)					5
iso-Amylamine	1046	(1)					10
Amylobarbitone	1718	(25)	18	47			5-7, 9-16, 17-19, 24, 26, 35
Amylocaine	1600	(8)	38	25			4, 10, 12, 14, 34
Androsterone	2488	(2)	8	7			7, 11
Anethole	1284	(1)					2
Anhalonidine	1825	(1)					15
Anhalonine	1850	(1)					15
Anilazine	2010	(1)					2
Anileridine	2850	(4)	5	15			5, 7, 10, 15
Aniline	1158	(1)					10
Anisaldehyde	1246	(2)	19	19			10
Anisindione	2273	(2)	13	13			7, 10
Antazoline	2328	(9)	28	32			4, 5, 7, 9-11, 14, 15, 25
Anthracene	1754	(2)	43	42			2, 10
9,10-Anthracenedicarbonitrile	2288	(1)					2
Apoatropine	2050	(1)					11
Apomorphine	2530	(1)					11
Aprobarbitone	1622	(12)	22	33			7, 9-11, 15, 16, 18, 19, 26, 33, 35
Apronal					1231	[10]	
					1578	[19]	
Atrazine	1655	(3)	25	50			2, 11
Atropine	2199	(21)	49	46	2048	[34]	5-11
					2145	[12]	12-15, 17
					2250	[14]	22, 28
					2377	[23]	5, 10, 11, 14, 15
Azacyclonol	2243	(5)	33	22			11
Azaperone	2705	(1)					11
Azapetine	1939	(8)	14	28			7, 11, 12, 15
Azataidine	2415	(1)					11
Azinphos-methyl	2430	(1)					2
Azobenzene	1556	(1)					2
Bamipine	2211	(4)	21	14			12
Barbitone	1497	(20)	17	33	1560	[12]	5-7, 9-14, 16, 18, 19, 24, 26, 35
BBO (2,5-di(4-biphenyloxazole)	3710	(1)					2
BBOT (2,5-bis(5'-tert.-butyl-benzoxazolyl(2'))thiophene)	2745	(1)					2
	3750	(1)					2
Beclamide	1480	(1)					11
	1678	(1)					11
Bemegrade	1373	(2)	34	37			9, 10, 14
Benactyzine	2248	(13)	28	32			5, 7, 10, 12, 13, 15
Benethamine	1798	(3)	8	7			11, 15
Benorylate	1840	(2)	10	10			11
Benperidol					1471	[35]	
					2975	[11]	
Benzamine	1816	(3)	21	17			14, 15, 30
$\alpha$ -Benzenehexachloride	1690	(1)					2
$\beta$ -Benzenehexachloride	1710	(1)					2

(Continued on p. 200)

TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
$\delta$ -Benzenehexachloride	1755	(1)					2
$\gamma$ -Benzenehexachloride	1715	(1)					7
Benzene-sulphonamide	1525	(1)					10
Benzethidine	2695	(2)	15	15			7, 11
Benzhexol	2219	(11)	34	41	2275	[11]	5, 7, 10, 12, 13, 28
					2280	[13]	
2-Benzhydroxymethyl- 2-imidazoline	2210	(4)	15	15			12
Benzocaine	1555	(9)	25	45			1, 4, 7, 8, 10, 14
Benzocetamine	2082	(3)	12	23			11, 35
Benzoic acid	1180	(2)	11	10			10, 35
Benzonate	9999	(1)					11
Benzophenone	1610	(2)	0	1			2, 33
Benzoyllecgonine	2570	(1)					35
Benzphetamine	1760	(1)					25
Benzphetamine	1855	(8)	16	47			3, 7, 9-11, 14, 15, 29
Benzthiazide	2680	(1)					7
Benztropine	2314	(6)	24	41			7, 10, 11, 14, 15, 28
Benzylamine	2368	(5)	33	42			12, 14
Benzyl alcohol	1046	(1)					2
Benzylamine	995	(2)	10	10			10, 22
N-Benzylamphetamine	1784	(1)					29
Benzyl benzoate	1738	(1)					2
Benzylbutyl phthalate	2290	(1)					8
1-Benzyl-3-ethyl-6,7- dimethoxyisoquinoline	2488	(2)	3	2			12
Benzylmorphine	3015	(1)					11
$\alpha$ -Benzylphenethylamine	1800	(1)					15
Berberine	2070	(1)					11
Betahistine	1235	(1)					11
Betameprodine	1823	(1)					11
Betaprodine	1790	(1)					11
Bethanidine	1925	(1)					7
Bibenzonium bromide	1923	(2)	3	2			12
Biperiden	2266	(8)	41	34	2205	[12]	7, 11, 12, 14, 25, 35
Biphenyl	1389	(1)					2
4,4'-Bipyridyl dihydrate	1507	(1)					2
Bisacodyl	2820	( )					7
Bisnortilidine	1825	(1)					35
Brallobarbitone	1858	(5)	16	7			9, 16, 18, 26, 35
Brallobarbitone metabolite (5-(2-oxopropyl)-5- (2-propenyl)barbituric acid)	1795	(1)					35
Brallobarbitone metabolite (5-(2-hydroxypropyl)-5- (2-propenyl)barbituric acid)	1835	(1)					35
Brallobarbitone metabolite (5-(2-bromo-2-propenyl)- 5-acetylbarbituric acid)	2040	(1)					35
Brallobarbitone metabolite (5-(2-bromo-2-propenyl)- 5-(2-hydroxypropyl)barbituric acid)	2135	(1)					35

TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Brocresine	9999	(1)					11
Bromazepam	2663	(4)	17	37	2762	[9]	16, 32, 35
Bromazepam metabolite (3-hydroxybromazepam)	2500	(1)					35
Bromazepam metabolite (2-(2-amino-5-bromo- benzoyl)pyridine)	2243	(3)	48	32			35, 36
Bromazepam decomposition product	2255	(1)					35
Bromdiphenhydramine	2155	(10)	15	25			5, 7, 8, 10, 11, 14, 15, 28
Bromhexine					2295	[12]	
					2295	[12]	
					2330	[12]	
					2340	[12]	
					2380	[11]	
					2385	[11]	
1-Bromodecane	1326	(1)					2
Bromodiacetylurea	1567	(3)	17	13			12, 13
Bromodimethoxyamphetamine	1813	(2)	18	17			14, 15
Bromonaphthalene	1434	(1)					2
Bromo STP					1868	[30]	
					2195	[7]	
Brompheniramine	2096	(11)	26	34			4, 7, 10, 11, 12, 14, 15, 28
Bromvaletone					1212	[10]	
					1510	[35]	
Broxaldinc	2686	(2)	4	4			11
Brucine	3280	(2)	0	0	3560	[14]	5, 7
Buclizine	3286	(2)	1	1	3365	[11]	5, 10
Bufotenine	2030	(1)					10
Buflylline	2301	(1)					30
Bulan	2310	(1)					2
Bunamidine	9999	(1)					11
Buphenine	2314	(6)	29	36	2384	[10]	1, 4, 7, 11, 14, 25
					2613	[10]	
	1270	(1)					1
Bupivacaine	2273	(3)	33	27	2360	[14]	7, 11, 28
Butacaine	2457	(4)	27	20			7, 10, 15, 34
Butalamine	2490	(1)					11
Butalbital	1668	(12)	28	27			7, 9-12, 15, 16, 18, 19, 26, 35
Butalbital metabolite	1940	(1)					35
Butallylonal	1995	(6)	15	30			7, 9, 10, 16, 26, 35
Butanilcaine	2025	(1)					11
Butethamate	1754	(2)	4	4			8, 11
Butethamine	2061	(3)	11	14			1, 10, 11
Butobarbitone	1665	(12)	20	20			6, 7, 10-12, 14, 16-19, 35
Butoxyethyl nicotinate	1640	(1)					11
Butriptyline	2181	(4)	26	19			7, 11, 15
Butylamine	909	(1)					10
Butyl aminobenzoate	1742	(3)	7	8			7, 10, 15
N-2-Butylamphetamine	1365	(1)					29

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TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
<i>N-n</i> -Butylamphetamine	1422	(1)					29
Butylated hydroxyanisole	1462	(1)					2
Butylated hydroxytoluene	1490	(1)					2
Butylbenzyl phthalate	2327	(1)					2
Butylbenzyl sebacate	1585	(1)					2
	2130	(1)					2
	2520	(1)					2
Butylisodecyl phthalate	1950	(1)					2
Butyl PBD	3342	(1)					2
Butylsextyl phthalate	1940	(1)					2
	2235	(1)					2
Butyl stearate	2157	(1)					2
	2362	(1)					2
<i>n</i> -Butyric acid	1309	(1)					10
Cadaverine	1035	(1)					2
Caffeine	1810	(30)	30	25	1945	[28]	4-17, 22, 24, 25, 31, 35
Calusterone	2750	(1)					7
Camphor	1137	(2)	0	1			2, 10
Cannabidiol	2383	(2)	18	17	2190	[11]	15, 35
Cannabinol	2520	(3)	45	35			11, 15, 35
Cartharidin	1490	(1)					5
Capric acid	1473	(1)					10
<i>n</i> -Caproic acid	1249	(1)					10
	1399	(1)					10
Captan	2000	(1)					2
Captodiamide	2774	(7)	39	36			5, 9-11, 15, 23, 25
Carbamiphen	1971	(4)	6	4			11, 12
Carbamazepine	2290	(1)					7
Carbaryl	1490	(1)					5
Carbazole	1784	(1)					2
Carbetapentane	2232	(6)	32	32			1, 10, 12
Carbimazole	1678	(1)					11
Carbinoxamine	2080	(12)	28	30			8, 10-12, 14, 15, 34
Carbophenothion	2255	(1)					2
Carbromal	1513	(5)	13	12	1192	[10]	5-7, 16, 35
					1580	[12]	
Carbromal metabolite [2-bromo-2-ethyl- (butyric acid) amide]	1205	(1)					35
Carbromal metabolite [2-bromo-2-ethyl-3-hydroxy- (butyric acid)]	1340	(1)					35
Carbromal metabolite (diethylacetylcarbamide)	1380	(1)					35
Carisoprodol	1830	(7)	35	25	2135	[23]	5, 7, 10, 12, 15
Carminic acid	1507	(1)					10
	1702	(1)					10
Carphenazine	3590	(1)					5
CDEC (2-chloroallyldiethyl- dithiocarbamic acid)	1685	(1)					2
Chlophedianol	2080	(7)	20	15			7, 11, 12, 15
Chloral hydrate	9999	(1)					7



TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Chloramphenicol	2310	(1)					7
Chlorbenside	2045	(2)	5	5			2, 5
Chlorcyclizine	2225	(19)	50	30			4, 5, 7, 10-15, 23
Chlordane	2020	(1)					5
Chlordecone	2240	(1)					2
Chlordiazepoxide					2190	[25]	
	2453	(6)	28	22	2300	[1]	1, 11, 12
	2530	(9)	30	50	2660	[32]	1, 6, 7, 10, 14, 16, 28, 32, 35
	2799	(5)	19	16	2893	[9]	1, 7, 13
Chlormethiazole	1230	(3)	9	5			9, 16, 35
Chlormethiazole metabolite (dechlorchlormethiazole)	1185	(1)					35
Chlormethiazole metabolite (2-hydroxychlormethiazole)	1365	(1)					35
Chlornezanone	2238	(4)	18	17	2150	[12]	7, 10, 11, 28
					2165	[12]	
					2335	[23]	
<i>o</i> -Chlorobenzylidenemalonitrile	1516	(1)					2
5-Chloro-2-cyclopropylmethyl- aminobenzophenone	2407	(3)	37	43			36
2'-Chloro-2,5-diaminobenzophenone	2330	(1)					35
5-Chloro-2-diethylaminoethyl- amino-2'-fluorobenzophenone	2558	(2)	3	2			26
5-Chloro-2-fluoro-2-hydroxy- ethylaminobenzophenone	2472	(3)	47	28			36
5-Chloro-2-methylamino- diphenylamine	2250	(2)	20	20			36
Chloroprocaine	2229	(4)	39	46	2347	[30]	10, 11, 29
Chloropyrilene	2133	(6)	8	20	2058	[11]	1, 10, 12
Chloroquine	2590	(4)	15	20	2660	[14]	4, 5, 7, 10
Chlorothiazide					1720	[33]	
					9999	[7]	
Chlorothymol	1486	(2)	21	19			10
Chlorphenesin	1677	(4)	17	18	2113	[10]	7, 10, 11
Chlorpheniramine	2002	(20)	22	28			4-15, 28
Chlorphenoxamine	2072	(4)	41	23			7, 10, 11, 15
Chlorphentermine	1342	(12)	32	27			3, 5, 7, 9-11, 14, 16, 22, 25, 29, 35
2-Chloroprocaine	2290	(1)					28
Chlorproethazine	2617	(1)					27
Chlorproguanil	1621	(1)					30
Chlorpromazine	2486	(21)	46	49	2400	[12]	4-7, 10-17
					2410	[12]	
					2415	[28]	23, 25, 27, 30, 35
					2553	[9]	
					2685	[13]	
Chlorpropamide	1791	(4)	48	39	1720	[33]	6, 7, 10, 11
Chlorprothiazide	2510	(1)					7
Chlorprothixene	2487	(9)	37	38	2400	[12]	7, 10-12, 15, 25
					2410	[12]	27
					2542	[9]	

(Continued on p. 204)

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Chlorthalidone	2145	(1)					7
Chlorzoxazone	1728	(7)	17	17			10-12, 15
5- $\alpha$ -Cholestane	2852	(1)					2
Cholesterol	3086	(6)	26	29	3008 3020	[2] [17]	6, 7, 10, 11, 16, 35
Chromonar	2820	(1)					11
Cinchocaine	2701	(15)	41	39			5, 7, 9-15
Cinchonidine	2598	(6)	24	27			4, 5, 7, 10, 11, 14
Cinchonine	2583	(7)	9	22	2644	[10]	4, 5, 7, 10, 11, 14, 15
Cinchophen	9999	(1)					11
Cinnamylcocaine	2495	(1)					15
Cinnarizine	3065	(1)					11
Citral	1272	(1)					2
Citroflex A4	2224	(1)					2
Clemastine	2415	(3)	5	5			7, 11
Clemizole	2675	(4)	15	15	2585 2590	[12] [12]	10, 11, 14, 34
Clioquinide	9999	(1)					11
Clobazam					2645 2660 2777	[32] [32] [30]	
Clobutinol	1784	(4)	9	16			12
Clofazimine	9999	(1)					12
Clofibrate	1549	(3)	44	36			7, 10, 15
Clomiphene	2930	(1)					7
Clomipramine	2406	(7)	26	19	2335 2345	[12] [12]	7, 11, 12, 30, 35
Clonazepam	2885	(3)	25	35	2965	[32]	7, 14, 35
Clonazepam metabolite [7-(2-chlorophenyl)-1,3- dihydro-7-amino-2H-1,4- benzodiazepin-2-one]	2850	(1)					35
Clonazepam metabolite [7-acetamino-5-( <i>o</i> - chlorophenyl)-1,3- dihydro-1-methyl-2H- 1,4-benzodiazepin-2-one]	3105	(2)	20	20			35
Clonidine	2248	(1)					30
Clopendixol	2274	(1)					35
Cloponone	2011	(2)	4	4			11
Clorazepate	2457	(3)	8	18	2655 2760	[32] [14]	12, 15
Clorgyline	1883	(2)	8	7			11
Clorprenaline	1604	(2)	34	33			7, 30
Clotrimazole	2100	(1)					7
Clozapine					2915 3011	[35] [9]	
Cocaethylene	2330	(1)					15
Cocaine	2187	(24)	27	50	2240 2245	[14] [28]	4-10 11-13, 15-17, 25, 31, 35
Codeine	2376	(24)	41	37	2290 2295	[12] [12]	4-7, 9-11 12, 14-17, 20-22, 25, 28, 31, 35

TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Colchicine					2380	[7]	
					2490	[11]	
					2340	[34]	
					3466	[10]	
Coniine	9999	(1)					7
Cotarnine	1808	(4)	28	42			5, 7, 11, 15
Cotinine	1678	(2)	8	7			4, 35
Cropropamide	1738	(2)	2	3			9, 30
Crotamiton	1550	(1)					7
Crotethamide	1688	(2)	4	4			9, 30
Cyclandelate	1903	(4)	13	7			7, 10, 15
Cyclazocine					2065	[11]	
					2070	[11]	
					2195	[21]	
					2342	[30]	
Cyclizine	2020	(19)	20	30			4, 5, 8-15, 17
Cyclobarbitone	1963	(19)	23	25			7, 9-12, 14-16, 18, 19, 24, 26, 35
Cyclobarbitone metabolite (hydroxycyclobarbitone)	2170	(1)					35
Cyclobarbitone metabolite (3'-ketocyclobarbitone)	2190	(1)					35
Cyclododecanone	1524	(1)					2
Cyclohexylamine	917	(2)	15	15			10, 22
Cyclohexylisooctyl phthalate	2446	(1)					2
	2532	(1)					2
Cyclohexyltridecyl phthalate	2518	(1)					2
Cyclomethycaine					2225	[7]	
					2227	[10]	
					2515	[28]	
					2972	[30]	
Cyclopentamine	1087	(9)	14	22	1510	[12]	1, 3, 7, 8, 10, 11, 22
					1515	[12]	23
Cyclopentobarbitone	1862	(3)	4	3			10, 18, 19
Cyclopentolate	2020	(2)	10	10			7, 11
2-Cyclopropylmethylamino-5-chlorobenzophenone	2385	(1)					35
Cycrimine	2114	(6)	24	26			7, 12, 15
Cyheptamide	2265	(1)					15
Cypenamine	1345	(1)					3
Cyproheptadine	2366	(5)	16	34			7, 10, 11, 14, 15
2,4-D Butyl ester (2,4-dichlorophenoxyacetic acid)	1840	(1)					2
2,4-D Isobutyl ester	1805	(1)					2
2,4-D Isopropyl ester	1700	(1)					2
2,4-D Methyl ester	1605	(1)					2
Dapsone	2880	(2)	20	21			5, 10
DCPA (dimethyl-2,3,5,6-tetrachloroterephthalate)	1960	(1)					2
DDA methyl ester (2,2-bis-(4-chlorophenyl)acetic acid)	2085	(1)					2

(Continued on p. 206)

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
<i>o,p'</i> -DDE	2070	(1)					2
<i>p,p'</i> -DDE (1,1-dichloro-2,2-bis-(4-chlorophenyl)ethylene)	2130	(1)					2
Deanol	2539	(1)					10
Deanol acetamidobenzoate	2227	(1)					10
Debrisoquine	9999	(1)					7
Decoquinat	9999	(1)					11
Demeton S-methyl	1628	(1)					2
Demoxepam	2529	(4)	49	46			11, 15, 28, 32
Deptropine	2615	(1)					11
N1-Desalkylflurazepam	2471	(5)	41	39			7, 28, 32, 35
N1-Desalkyl-3-hydroxyflurazepam	2240	(1)					35
Desipramine	2242	(15)	46	39	2170	[12]	1, 4, 6, 7, 10-12, 14, 15, 27, 28, 30, 35
Desmethylchlordiazepoxide					2885	[32]	
					2930	[32]	
					3100	[7]	
Desmethylchlorpromazine	2480	(1)					4
Desmethyldiazepam	2496	(7)	16	14			6, 7, 11, 14, 17, 28, 35
Desmethylmedazepam					2275	[35]	
					2410	[28]	
Desmetryne	1795	(2)	5	5			11
Desomorphine	2295	(1)					11
Dexamethasone	2970	(1)					10
Dexbrompheniramine	2075	(1)					10
Dexoxadrol	2340	(1)					4
Dexpanthelol	1807	(2)	2	3			11
Dextromethorphan	2140	(6)	15	32			6, 7, 10, 11, 15, 28
Dextromoramide	2940	(2)	0	0			11, 14
Dextropropoxyphene	2188	(21)	33	32	1687	[11]	5-7, 10-12
					1940	[11]	13, 14, 16, 17, 20
					1964	[9]	25, 28, 35
					2074	[12]	
Dextropropoxyphene metabolite	2375	(1)					10
Dextropropoxyphene metabolite	2551	(1)					10
Dextropropoxyphene metabolite	2397	(1)					30
Diallyl phthalate	1712	(2)	14	13			2, 8
2,5-Diaminobenzophenone	2198	(2)	28	27	2300	[36]	36
2,5-Diamino-2'-chlorobenzophenone	2345	(2)	10	10			36
2,5-Diamino-2'-fluorobenzophenone	2188	(2)	38	37			36
Diamorphine	2614	(17)	49	33	2505	[12]	4-7, 10, 11, 15
					2510	[12]	14-16, 20, 35
					2510	[25]	
					2692	[9]	
Diampromide	2434	(1)					30
	1734	(1)					30
	1859	(1)					30
	2079	(1)					30
	2232	(1)					30
Diamyl phthalate	2127	(2)	13	13			2, 8

TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Diazepam	2425	(14)	20	35	2335	[12]	6, 7, 10-12, 14
					2345	[12]	15-17, 25, 28
					2490	[32]	34, 35
					2505	[9]	
					2510	[32]	
Diazinon	1758	(3)	13	11	1485	[12]	2, 7, 10
					1495	[12]	
Diazoxide	9999	(1)					11
Dibenzepin	2443	(7)	38	27	2505	[9]	10-12, 14, 27, 35
Dibenzyl phthalate	2690	(1)					2
Dibenzyl sebacate	2135	(1)					2
<i>m</i> -Dibromobenzene	1197	(1)					2
<i>o</i> -Dibromobenzene	1221	(1)					2
<i>p</i> -Dibromobenzene	1193	(1)					2
<i>p</i> -Dibutoxyethoxyethyl adipate	1285	(1)					2
Di(butoxyethyl) phthalate	2850	(1)					2
Di(butoxyethyl) sebacate	2700	(1)					2
Dibutyl adipate	1695	(2)	35	35			2, 8
N,N-Di- <i>n</i> -butylamphetamine	1689	(1)					29
Dibutyl maleate	1505	(1)					2
Dibutyl phthalate	1913	(3)	25	15			2, 8, 10
Dibutyl sebacate	2137	(2)	0	1			2, 8
Dibutyl terephthalate	2066	(1)					2
Dichlone	1760	(1)					2
Dichloroaniline	1323	(1)					10
<i>p</i> -Dichlorobenzene	1023	(1)					10
Dichlorophen	2140	(1)					7
Dichlorophenazone	1855	(1)					10
Diclofenac	2271	(1)					30
Dicophane ( <i>o,p'</i> -isomer)	2218	(2)	2	2			2, 10
Dicophane ( <i>p,p'</i> -isomer)	2299	(5)	9	10			2, 5, 7, 10, 11
Dicyclohexyl adipate	2282	(1)					2
Dicyclohexyl oxalate	1880	(1)					2
Dicyclohexyl phthalate	2461	(1)					2
Dicyclomine	1708	(2)	8	7			11, 15
	2097	(8)	48	18			1, 7, 10, 12, 14
Didesmethylchlorpromazine	2480	(1)					4
Dieldrin	2110	(7)	10	35	2170	[13]	2, 5, 12, 13
					2175	[11]	
					2215	[13]	
Diethadione	1490	(2)	5	5			12
Diethazine	2377	(6)	8	18			7-9, 11, 15, 27
Di(ethoxyethyl) adipate	1924	(2)	44	44			2, 8
Di(ethoxyethyl) phthalate	2103	(2)	33	32			2, 8
Di(ethoxyethyl) sebacate	2270	(1)					2
Diethyl adipate	1344	(2)	6	5			2, 8
Diethylaminoethyl diphenylpropionate	2292	(1)					30
N,N-Diethylamphetamine	1371	(1)					29
Di-(2-ethylhexyl) adipate	2381	(1)					2
Di-(2-ethylhexyl) isophthalate	2730	(1)					2

(Continued on p. 208)

TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Di-(2-ethylhexyl) phthalate	2507	(1)					2
Di-(2-ethylhexyl) sebacate	2792	(1)					2
Diethyl maleate	1081	(1)					2
Diethyl- <i>p</i> -nitrophenyl phosphate	1880	(1)					35
Diethyl phthalate	1564	(2)	4	4			2, 8
Diethylpropion	1486	(11)	43	41	1402	[25]	3, 5, 7, 9-11, 13
					1550	[12]	14, 22, 29
					1555	[12]	
					1555	[12]	
Diethyl sebacate	1745	(2)	0	1			2, 8
Diethylstilboestrol	2366	(1)					10
Diethylthiambutene	2008	(2)	8	9			7, 11
N,N-Diethyl- <i>m</i> -toluamide	1583	(2)	12	12	1490	[11]	2, 11
Diethyltryptamine	1910	(4)	10	15	1800	[28]	7, 10, 15
					1993	[11]	
Digitalin	1902	(1)					10
Digitoxin	1902	(1)					10
Diheptyl phthalate	2500	(1)					2
Dihexyverine	2315	(1)					7
9,10-Dihydroanthracene	1662	(1)					2
Dihydrocodeine	2363	(7)	23	17	2290	[12]	7, 10-12, 14, 15
					2295	[12]	
					2417	[9]	
					2660	[25]	
Dihydrodesoxymorphine	2232	(1)					10
Dihydroergotamine	2315	(3)	5	5	2385	[13]	5, 7, 13
Dihydromorphine	2451	(4)	11	19			7, 11, 15, 20
Diisobutyl adipate	1660	(1)					2
Diisobutyl phthalate	1853	(2)	11	10	1930	[35]	2, 8
Diisobutyl terephthalate	1972	(1)					2
Diisodecyl adipate	2745	(1)					2
Diisodecyl phthalate	2511	(1)					2
Diisooctyl adipate	2444	(1)					8
Diisooctyl phthalate	2525	(1)					8
Diisopropyl phthalate	1633	(1)					8
Diloxanide	2420	(2)	15	15			11
Dimelfine	2555	(2)	5	5			12
Dimenhydrinate	1844	(1)					10
Dimethindene	2258	(4)	38	22	2342	[10]	5, 7, 11, 15
Dimethisoquin	2030	(1)					7
Dimethoate	1725	(3)	5	10			2, 12
Dimethocaine	2108	(2)	13	12			11
Dimethothiazine	3078	(2)	18	17			7, 27
Dimethoxanate	2029	(2)	0	1	2160	[10]	1, 8
Dimethoxyethyl phthalate	1980	(1)					2
3,4-Dimethoxyphenethylamine	1551	(2)	11	11			5, 10
Dimethrin	1210	(1)					5
Dimethyl adipate	1213	(2)	10	10			2, 8
<i>p</i> -Dimethylaminobenzaldehyde	1528	(1)					2
N,N-Dimethylamphetamine	1236	(2)	6	7			3, 29
N,N-Dimethylaniline	1080	(3)	5	4	1010	[9]	5, 10, 22
Dimethyl isophthalate	1488	(1)					2

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Dimethylmescaline	1700	(1)					15
$\alpha,\alpha$ -Dimethyl- $\beta$ -methylsuccinamide	1195	(1)					2
N,N-Dimethylphenethylamine	1159	(3)	1	1			5, 10, 22
Dimethyl phthalate	1406	(3)	26	28			2, 7, 8
Dimethyl POPOP (POPOP = 1,4-bis-(5-phenyloxazolyl-2)benzene)	3618	(1)					2
2,4-Dimethylquinoline	1446	(1)					2
2,7-Dimethylquinoline	1425	(1)					2
Dimethyl sebacate	1634	(2)	12	13			2, 8
Dimethyl terephthalate	1475	(1)					2
Dimethylthiambutene	1885	(1)					2
Dimethyltryptamine					1745	[28]	
					1885	[11]	
Dimetridazole	1353	(1)					11
Dimophebumine	2300	(1)					11
4,6-Dinitro- <i>o</i> -cresol	1617	(1)					10
2,4-Dinitrophenol	1471	(2)	36	35			10
Dinonyl adipate	2484	(1)					2
Dinonyl phthalate	2649	(1)					2
Diocetyl adipate	2383	(1)					2
Diocetyl phthalate	2515	(2)	5	4			2, 35
Diocetyl sebacate	2782	(1)					2
Di-( <i>n</i> -decyl) adipate	2905	(1)					2
Dioxadrol	2323	(2)	3	2			15
Dioxaphetyl butyrate	2491	(1)					30
Dioxyamidopyrine	2018	(2)	3	2			11
Dioxyline	2895	(1)					10
Diperodon	2370	(1)					7
Diphenadione	2934	(1)					10
Diphenamid	1970	(2)	5	5			12
Diphenazoline	2275	(2)	5	5			11
Diphenhydramine	1873	(23)	23	47			4, 5, 7-17, 25, 28, 35
Diphenidol	2384	(3)	6	6			7, 10, 15
Diphenoxalate	2443	(1)					30
Diphenyl adipate	2397	(1)					2
Diphenylamine	1601	(2)	18	18	1520	[25]	9, 29
Diphenyl mercury	2397	(1)					2
Diphenyl phthalate	2550	(1)					2
Diphenylpyraline	2099	(8)	19	22			1, 7, 8, 10, 11, 15, 23
Dipipanone	2474	(4)	7	6			4, 11, 17, 34
Diprophylline					1285	[25]	
					2470	[7]	
Dipropyl adipate	1545	(1)					2
N,N-Di- <i>n</i> -propylamphetamine	1526	(1)					29
Dipropyl phthalate	1746	(2)	3	2			2, 8
Dipyramidole	1640	(1)					10
Dipyrene	1983	(6)	14	12	1916	[10]	9, 10, 12
Disextyl maleate	2116	(2)	0	0			2, 12
Disulfiram	2141	(2)	14	14			10, 35
Dofamium chloride	1676	(2)	9	9			11
	1898	(2)	8	7			11
	1974	(2)	9	8			11

(Continued on p. 210)

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Dorniphen	2310	(1)					15
Dopamine	2175	(1)					11
Dothiepin	2380	(1)					11
Doxapram	2906	(3)	29	44	3014	[30]	7, 10, 11
Doxepin	2217	(7)	12	13	2340	[14]	7, 10, 11, 15, 16, 28, 35
Doxylamine	1906	(7)	21	14	1968	[10]	11, 12, 15
Droperidol					3430	[10]	
					9999	[7]	
Dropropizine	2112	(2)	7	8			11
Dyclonine	1678	(2)	38	37			11, 15
Dyrene	2010	(1)					2
Ecgonine	9999	(1)					7
Ectylurea	1396	(6)	46	44			5, 10, 12, 13
Embramine	2185	(1)					11
Emeponium bromide	1973	(2)	8	7			11
Emetine	2505	(1)					11
Emylcamate	1105	(1)					10
Enallypropymal	1561	(2)	2	1			10, 18
Endosulphan I	2085	(1)					2
Endosulphan II	2175	(1)					2
Endrin	2183	(2)	3	2			2, 7
Ephedrine	1363	(17)	30	42	1440	[12]	3, 5-10
					1445	[12]	11, 13, 14, 16, 22, 25, 31, 35
Ergocristine	2495	(1)					10
Ergocryptine	2184	(1)					10
Ergosterol	1714	(1)					10
Ergotamine	2366	(1)					10
Etafedrine	1519	(7)	44	21	1460	[11]	3, 11, 12, 30
Etenzamide	1542	(1)					11
Ethacrynic acid	9999	(1)					10
Ethamivan					1740	[25]	
					1894	[9]	
					1930	[14]	
Ethanolamine	780	(1)					2
Ethchlorvynol	1023	(5)	13	7			5, 7, 10
Ethinamate	1363	(6)	5	7			5-7, 10, 16, 35
Ethinylloestradiol	2719	(1)					10
Ethion	2220	(1)					2
Ethionamide	1756	(5)	36	9			7, 12
Ethoheptazine	1857	(10)	13	30			4, 7, 8, 10, 11, 14, 15, 34
Ethomoxane	1975	(3)	15	18			11, 15
Ethopropazine	2357	(7)	17	33	2270	[14]	1, 7, 10, 11, 15, 23, 27
Ethosuximide	1206	(4)	16	14			6, 7, 10, 35
Ethosuximide metabolite (3-hydroxyethosuximide)	1320	(1)					35
Ethosuximide metabolite (1-hydroxyethyl- ethosuximide)	1370	(1)					35
Ethosuximide metabolite (3-ketoethosuximide)	1385	(1)					35
Ethotoin	1800	(4)	15	10	1875	[7]	7, 10, 12, 15
					1915	[9]	



TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Ethoxazene	9999	(1)					11
Ethoxyquin	2800	(1)					5
Ethoxzolamide	2578	(1)					10
Ethylallylbarbitone	1555	(1)					26
3-Ethylamino-3-phenylnorcamphane	1570	(1)					25
N-Ethylamphetamine	1228	(7)	18	22			3, 5, 9, 10, 22, 25, 29
Ethylan	2175	(1)					2
Ethyl benzoate	1227	(1)					2
N-Ethylbenzylamine	1031	(2)	8	7	1120	[5]	10, 22
N-Ethyl- <i>p</i> -chloroamphetamine	1434	(1)					29
Ethylene glycol	771	(1)					10
Ethylisobutrazine	2455	(1)					4
Ethylmethylthiambutene	1943	(1)					11
Ethylmorphine	2411	(19)	36	39	2335	[12]	1, 5, 7, 9-12
					2335	[12]	13-15, 20, 25
					2505	[11]	28, 31
Ethyl oleate	2175	(1)					2
Ethyl parathion	1953	(3)	8	7			12, 35
5-Ethyl-5-phenylhydantoin					1795	[12]	
					1810	[12]	
					1913	[26]	
5-Ethyl-5- <i>p</i> -tolylbarbituric acid	2085	(1)					2
Ethynodiol diacetate	2445	(1)					10
	2779	(1)					10
Etilefrine					1685	[35]	
					9999	[11]	
Etisazole	1668	(2)	33	32			11
Etodroxizine	3175	(1)					35
Etomidate	2008	(1)					30
Etoxidine	2325	(1)					11
Etryptamine	1848	(2)	8	7			4, 15
Eucatropine	2026	(3)	16	11			7, 11
Eugenol	1368	(1)					2
Famprofazone	3059	(1)					30
Fencamfamin	1677	(5)	22	20			9, 11, 29, 31
Fenethylline	2830	(5)	35	46			9, 15, 16, 25, 35
Fenfluramine	1222	(7)	10	14			3, 6, 7, 10, 11, 14, 29
Fenmetramide					1765	[4]	
					1915	[28]	
Fentanyl	2650	(3)	25	20	2720	[15]	11, 12
					2779	[9]	
Flavoxate	9999	(1)					11
Flufenamic acid	1950	(3)	20	40			11, 14
Flunitrazepam	2645	(3)	35	35	2535	[28]	32, 35
Flunitrazepam decomposition product	2410	(1)					35
Fluorene	1580	(1)					2
Fluorenone	1705	(1)					2
2'-Fluoro-2-methylamino-5-nitro-benzophenone	2430	(3)	45	40			36

(Continued on p. 212)

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Flupenthixol	9999	(1)					11
Fluphenazine	3065	(4)	20	20			5, 7, 16, 35
Flupromazine	2211	(15)	21	39			4, 7, 10, 12, 13, 15, 23, 27
Flurazepam	2785	(10)	39	23	2555	[28]	6, 7, 10, 11, 14, 15
					2858	[9]	17, 32, 35
Fluspirilene	1017	(1)					35
Folpet	2015	(1)					2
Fosazepam	2610	(2)	5	5			32
Furethidine	2637	(1)					30
Galantamine	2285	(3)	15	25			12
Gallamine					2625	[11]	
					9999	[10]	
Gelsemine	2850	(1)					11
Gentisic acid	2352	(1)					10
Geraniol	1192	(1)					10
Gitalin	9999	(1)					10
Glutethimide	1836	(24)	36	34	2165	[23]	4-7, 9-17, 19, 24, 26, 35
Glutethimide metabolite (hydroxyglutethimide)	1875	(1)					35
Glyceryl dibenzoate	2442	(1)					2
Glycopyrrolate	2120	(1)					10
Grisofulvin	2700	(1)					7
Guaiacol	1092	(1)					10
Guaiphenesin	1650	(1)					35
Guanethidine	9999	(1)					1
Haloperidol					2810	[12]	
					2835	[12]	
					2905	[7]	
					2965	[10]	
					2980	[35]	
					3020	[14]	
					3149	[30]	
Halopyramine	2234	(1)					30
Halquinol	1743	(2)	8	7			11
Harman	1952	(7)	32	48			2, 7, 12, 14
Harmine	2291	(3)	11	22			1, 10, 11
Heptabarbitalone	2058	(11)	33	48			6, 7, 9, 10, 12, 15, 16, 18, 26, 35
Heptabarbitalone metabolite [5-ethyl-5-(3-oxo- 1-cyclohepten-1-yl)- barbituric acid]	2320	(1)					35
Heptabarbitalone metabolite [5-ethyl-5-(3-hydroxy- 1-cyclohepten-1-yl)- barbituric acid]	2275	(1)					35
Heptachlor	1880	(2)	10	10			2, 7
Heptachlor epoxide	2015	(1)					2
Heptaminol	1118	(2)	22	22	1030	[25]	9, 11
Hexachlorophane	2807	(3)	12	18			7, 10, 11

TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Hexamine	1210	(2)	6	5			10, 11
Hexethal	1858	(3)	23	20			10, 18, 19
Hexobarbitone	1857	(19)	37	33			6, 7, 9-12, 14-16, 18, 19, 24, 26, 35
Hexobarbitone metabolite [1,5-dimethyl-5-(3-hydroxy-1-cyclohexen-1-yl)barbituric acid]	2080	(1)					35
Hexobarbitone metabolite [1,5-dimethyl-5-(3-oxo-1-cyclohexen-1-yl)-barbituric acid]	2050	(1)					35
Hexobendine	9999	(1)					11
Hexoestrol	2402	(1)					10
Hexylcaine	1965	(3)	10	8			11, 15
Hexylresorcinol	1777	(1)					10
Hippuric acid					1390	[35]	
					1735	[10]	
Histamine	1497	(2)	4	3			7, 10
Homarylamine	1519	(1)					9
Homatropine	2072	(13)	32	48			5, 7, 9-13
Hordeanine					1485	[12]	
					1490	[12]	
					1490	[12]	
					1495	[12]	
					2815	[7]	
Howflex GBP	1947	(1)					2
Hydrallazine	1528	(2)	3	2			7, 10
Hydrastine	2988	(3)	13	27	2500	[11]	5, 13
Hydrastinine	1590	(1)					5
Hydrochlorothiazide	9999	(2)					7, 10
Hydrocodone	2440	(9)	29	25	2325	[12]	7, 9-11, 15, 20
					2340	[12]	25, 35
					2340	[12]	
					2365	[4]	
					2380	[12]	
					2380	[12]	
					2390	[12]	
					2500	[11]	
Hydromorphone	2467	(7)	12	13	2580	[14]	7, 10, 11, 15, 20, 21
					2585	[11]	25
Hydroquinidine	2810	(2)	10	10			7, 11
Hydroquinine	1450	(1)					7
Hydroquinone	1220	(1)					7
Hydroxyamphetamine					1320	[7]	
					2763	[10]	
Hydroxyamylorbarbitone	1632	(1)					10
4-Hydroxyantipyrac	1874	(1)					10
Hydroxybenzoic acid	1565	(1)					35
3-Hydroxybromazepam	2555	(2)	15	15			32
1-Hydroxychloridene	1955	(1)					2

(Continued on p. 214)

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Hydroxychloroquine	2872	(2)	12	11			5, 10
Hydroxyephedrine	1682	(1)					9
N1-Hydroxyethylflurazepam	2688	(4)	38	42			7, 32, 35
$\beta$ -Hydroxyethyltheophylline	2090	(1)					25
1-Hydroxyharman	1920	(1)					2
	2015	(1)					2
	2290	(1)					2
2-Hydroxyiminodibenzyl	2265	(1)					35
3-Hydroxymorphinan	2237	(2)	7	6			20, 21
Hydroxypentobarbitone	1915	(1)					35
Hydroxypethidine	2045	(1)					11
Hydroxyphenamate	1724	(4)	34	21			5, 10, 11
4-Hydroxyphenobarbitone	2415	(1)					35
p-Hydroxyphenylpyruvic acid					1347	[10]	
					1365	[10]	
					1835	[35]	
3-Hydroxypirazepam	2860	(1)					32
$\beta$ -Hydroxypropyltheophylline	2090	(1)					25
Hydroxyzine	2849	(5)	14	21	2470	[25]	5, 9-11, 13
					2750	[12]	
					2760	[12]	
					2760	[13]	
					2980	[7]	
Hymecromone	2003	(2)	28	28			10
Hyoscine	2303	(14)	38	48	2240	[12]	5, 7, 9-12
					2245	[12]	13, 14, 25
					2365	[11]	
Hyoscyamine	2192	(15)	32	33			5, 7, 10-13, 15, 28
Ibogaine	2872	(2)	29	28	9999	[11]	7, 22
Ibomal	1883	(6)	17	8			9, 10, 16, 18, 19, 35
Ibomal metabolite [5-(1-methylethyl)-5- (2-oxopropyl)barbituric acid]	1770	(1)					35
Imidazole	1095	(1)					2
Imidocarb	9999	(1)					11
Iminodibenzyl	1920	(1)					35
Imipramine	2223	(23)	37	47	2165	[12]	4-7, 9-11
					2285	[13]	12-16
					2295	[13]	17, 23, 25, 27, 28, 30, 35
Indene	1062	(1)					2
Indole	1276	(1)					2
Indomethacin	2685	(2)	5	5			10, 14
Iprindole	2335	(2)	5	5			11, 15
Iproniazid	1593	(11)	23	37	1700	[5]	1, 7, 8, 10, 12, 14
					2060	[26]	
					2065	[23]	
Isatin	1712	(1)					2
Isoaminile	1830	(1)					11
Isobutyl aminobenzoate	1795	(1)					30
Isobutylcyclohexyl phthalate	1868	(1)					2
	2159	(1)					2
	2453	(1)					2

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
3-Isobutyl-1-methylxanthine	2150	(1)					2
Isocarboxazid	1949	(11)	19	25			5, 8, 10, 12-14
Isometamidium	9999	(1)					11
Isomethadone	2128	(2)	3	2			4, 15
Isomethheptene	1052	(5)	22	26			3, 10, 11, 22, 29
Isoniazid	1670	(4)	40	15	1515	[12]	5, 16, 30, 35
					1525	[12]	
					1525	[12]	
					1582	[10]	
Isooctylhydrocupreine	3103	(1)					10
Isoprenaline	1730	(1)					10
Isopropamide					2025	[12]	
					2058	[10]	
					2383	[10]	
					2430	[35]	
N-Isopropylamphetamine	1257	(1)					29
Isopropylhexedrine	1140	(1)					3
N-Isopropyl- $\alpha$ -methyl- $\beta$ -phenethylamine	1247	(2)	6	6			10, 22
Isopyrin	2024	(4)	14	16			12
Isoquinoline	1426	(1)					10
Isothipendyl	2267	(7)	7	23			1, 4, 10, 11, 15, 27
Isosuprine	2300	(3)	10	15	2398	[10]	7, 12
Ketamine	1843	(5)	20	17			7, 10, 11, 15, 28
Ketobemidone	2035	(3)	25	20			7, 11, 20
Ketobisnortilidine	2030	(1)					35
Kojic acid	1443	(1)					10
Lachesine	1852	(1)					11
Laudanine	2695	(1)					15
Laudanosine	2660	(1)					15
Lauric acid	1600	(1)					10
Lecithin	1945	(1)					10
	2147	(1)					10
Leptazol	1552	(9)	29	45	1475	[25]	1, 9-12, 14
					1490	[3]	15, 25, 29
					1705	[12]	
					1705	[12]	
Leucinocaine	2240	(1)					30
	2315	(1)					30
Levallorphan	2359	(7)	19	16			7, 9-11, 20, 34
Levamisole	1928	(2)	3	2			11
Levomethorphan					2130	[20]	
					2155	[30]	
					2230	[7]	
					2255	[11]	
Levomoramide	2980	(1)					30
Levophenacymorphan	3202	(1)					30
	2406	(1)					30
Levopropoxyphene	2185	(1)					7

(Continued on p. 216)

TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Levorphanol	2234	(6)	9	12			7, 9-11, 20, 31
Lidoflazine	9999	(1)					11
Lignocaine	1870	(24)	40	25			4-16, 25, 28, 35
Limonene	1053	(1)					2
Linalol	1100	(1)					10
Lindane	1745	(4)	15	12			2, 10, 12
<i>cis</i> -Linoleic acid	1309	(1)					10
	2179	(1)					10
Linolenic acid	2178	(1)					10
Lobeline					1780	[5]	
					2085	[12]	
Lophophorine	1850	(1)					15
Lorazepam	2402	(8)	37	38	2325	[12]	7, 11, 12, 14, 25
					2330	[12]	32, 35
					2478	[9]	
					2515	[32]	
Loxapine	2530	(2)	50	50			15, 28
Lysergide	3445	(1)					5
Mafenide	9999	(1)					11
Malathion	1917	(4)	17	18			2, 10, 12
Mandelic acid	1487	(1)					10
Maprotiline	2356	(2)	31	30			7, 9
Mazindol	2355	(1)					15
Mebenzazine	1240	(1)					11
Mebeverine	9999	(1)					11
Mebhydrolin	2465	(1)					11
Meboral	1894	(1)					10
Mebutamate	1889	(7)	24	36	1965	[13]	5, 10, 12, 13
Meclofenamic acid	2420	(1)					14
Meclofenoxate	1770	(2)	20	20			11, 14
Mecloqualone	2255	(1)					15
Meclozine	3033	(7)	28	17	2515	[12]	5, 7, 10, 13, 14, 23
Meconic acid	1466	(1)					10
Medazepam	2226	(11)	46	49	2285	[32]	9-12, 15
					2350	[32]	25, 28, 36
Mefenamic acid	2201	(2)	29	29	2480	[14]	10, 11
Melitracene	2268	(2)	48	48			9, 25
Mepenzolate	2327	(3)	17	29			10, 12
Mephenesin	1568	(7)	28	37			6, 7, 10, 12, 15
Mephenoqualone	2155	(3)	35	29			5, 10, 15
Mephentermine	1239	(10)	29	21	1295	[12]	3, 5, 7, 10, 11, 13
					1305	[12]	14, 22, 29
					1370	[12]	
					1375	[12]	
Mepivacaine	2071	(15)	41	29			1, 7, 8, 10-12, 14, 15, 28, 35
Meprobamate	1796	(17)	16	34	1850	[11]	4-7, 9, 10, 12
					2250	[14]	13, 14, 16, 26, 35
Mepyramine	2220	(12)	35	30			4, 6, 7, 10-12, 14, 15, 34
2-Mercaptobenzothiazole	1936	(1)					2
Mercumallylic acid	2074	(2)	25	24			10

TABLE I (continued)

<i>Compound name</i>	<i>RI</i>	<i>(n)</i>	-	+	>50	[ <i>Ref.</i> ]	<i>Refs.</i>
Mescaline	1688	(9)	28	12	1815	[11]	5-7, 10, 11, 14-16, 35
Mesoridazine	9999	(1)					11
Mestranol	2612	(1)					10
Metabutethamine	1988	(1)					15
Metabutoxycaine	2226	(2)	1	1			7, 10
Metamfepyraron	1372	(1)					9
Metaraminol	9999	(1)					7
Metaxalone	2163	(3)	18	21			7, 10, 15
Metazocine	1920	(1)					20
Metformin	9999	(1)					7
Methadone	2148	(29)	23	33			4-17, 20, 25, 28, 35
Methadone metabolite	2021	(2)	10	9			4, 10
Methallatal	1736	(1)					10
Methallibure	9999	(1)					11
Methandienone	2672	(1)					10
Methaphenilene	1966	(3)	23	22			10, 11
Methapyrilene	1981	(22)	19	29			4-16, 28, 35
Methaqualone	2125	(22)	35	25	2190	[17]	4, 6-11
					2190	[35]	12, 14-16, 24
					2235	[28]	26, 34, 35
Methaqualone metabolite [3-( <i>o</i> -tolyl)-4(3)- quinazolin]	2170	(1)					35
Methaqualone metabolite [4-oxo-3-( <i>o</i> -tolyl)- 3,4-dihydro-2- quinazolincarbaldehyde]	2240	(1)					35
Methaqualone metabolite [2-hydroxymethyl-3- ( <i>o</i> -tolyl)-4(3)quinazoline]	2360	(1)					35
Methaqualone metabolite [4-oxo-3-( <i>o</i> -tolyl)-3,4- dihydro-2-carboxyquinazoline]	2400	(1)					35
Methaqualone metabolite [3-(2'-hydroxymethylphenyl)- 2-methyl-4(3H)-quinazoline]	2410	(1)					35
Methaqualone metabolite [3-(3'-hydroxy-2'-methylphenyl)- 2-methyl-4(3H)-quinazoline]	2490	(1)					35
Methaqualone metabolite [3-(4'-hydroxy-2'-methylphenyl)- 2-methyl-4(3H)quinazoline]	2520	(1)					35
Methaqualone metabolite [3-(4'-hydroxy-5'-methoxy- 2'-methylphenyl)-4(3H)- quinazoline]	2560	(1)					35
Methaqualone metabolite [6-hydroxy-3-(3'-methylphenyl)- 4(3H)quinazoline]	2525	(1)					35
Metharbitone	1472	(6)	32	43			10-12, 18, 19
Methazolamide	2187	(3)	27	37			11, 15

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TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Methdilazine	2467	(3)	12	10			4, 10, 11
Methimazole	1550	(1)					11
Methiomeprazine	2685	(1)					27
Methixene	2461	(7)	31	39			10-12, 15, 27
Methiocarbamol					1507	[10]	
					2485	[23]	
Methiohexitene	1766	(4)	11	5			6, 10, 15, 18
Methoin	1791	(14)	41	17			5-10, 12, 13, 15, 26
Methoprotryne	2098	(2)	23	22			11
Methotrimeprazine	2514	(10)	29	36	2440	[12]	1, 4, 7, 10-12
					2445	[12]	15, 27, 35
					2588	[9]	
Methoxamine	1726	(2)	1	1			10, 11
Methoxsalen	1980	(1)					7
Methoxyamphetamine	1385	(1)					7
<i>p</i> -Methoxybenzophenone	1874	(1)					10
Methoxychlor	2417	(9)	12	23	2345	[12]	2, 5, 7, 10, 13
					2355	[12]	
3-Methoxymorphinan	2146	(2)	18	17			20, 21
Methoxyphenamine	1361	(5)	20	25	1455	[12]	7, 10, 11, 22, 29
					1470	[12]	
					1470	[12]	
Methoxypromazine	2542	(4)	42	38			5, 10, 15, 23
Methstyridone	1885	(1)					15
Methsuximide	1622	(9)	32	38			5, 7, 12, 13, 15, 33
Methylclothiazide	9999	(1)					7
2-Methylamino-5-chlorobenzo- phenone	2107	(6)	37	48			7, 35, 36
Methylaminomethylheptane	1000	(1)					3
Methylamphetamine	1176	(17)	41	31	1335	[12]	3, 5-11
					1340	[12]	13, 14, 16, 22
					1340	[12]	25, 29, 35
					1345	[12]	
Methylanhalonidine	1800	(1)					15
Methyl anthranilate	1343	(1)					2
Methylbenzylamine	1078	(2)	43	42			33, 35
<i>N</i> -Methyl- <i>N</i> - <i>n</i> -butylamphetamine	1486	(1)					29
Methyl caprylate	1130	(1)					2
Methyl decanoate	1305	(1)					2
Methyl-desorphine	2305	(1)					11
Methyldihydromorphine	2380	(1)					11
<i>N</i> -Methyl-2,3-dihydroxymorphinan	2500	(1)					21
4-Methyl-2,5-dimethoxy- amphetamine	1635	(1)					15
Methylenedioxyamphetamine	1472	(6)	15	23			5-7, 11, 22, 29
3,4-Methylenedioxy-2- methoxyamphetamine	1647	(1)					10
3,4-Methylenedioxy-4- methoxyamphetamine	1702	(1)					10
3,4-Methylenedioxy-5- methoxyamphetamine	1705	(1)					10
3,4-Methylenedioxyphentermine	1646	(1)					29



TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
N-Methylephedrine	1400	(5)	31	23			3, 10, 11, 22, 29
Methylergometrine	9999	(1)					10
Methyl hippurate	1675	(1)					35
Methyl <i>p</i> -hydroxybenzoate	1419	(1)					2
Methyl linoleate	2100	(1)					2
N-Methylmescaline	1700	(1)					15
N-Methyl-3,4-methylenedioxyamphetamine	1585	(1)					15
Methyl myristate	1715	(2)	5	5			33, 35
2-Methylnaphthalene	1313	(1)					2
Methyl nicotinate	1100	(1)					7
Methylnitrazepam	2570	(1)					28
Methyl nonanoate	1215	(1)					2
Methyl oleate	2086	(1)					2
Methyl palmitate	1889	(2)	22	21			2, 35
Methyl parathion	1851	(4)	6	9			2, 12, 35
$\alpha$ -Methylphenethylhydrazine					1400	[10]	
					2042	[23]	
Methyl phenidate	1737	(18)	46	43	1810	[14]	3, 5-7, 9-13, 15, 25, 31
Methylphenobarbitone	1891	(22)	39	29	1770	[14]	5, 6, 9, 11-13
					1988	[26]	15, 16, 18, 19, 24, 35
5-Methyl-5-phenylhydantoin	1866	(1)					2
5-( <i>p</i> -Methylphenyl)-5-phenylhydantoin	2584	(2)	37	36			2, 10
N-Methyl-N- <i>n</i> -propylamphetamine	1396	(1)					29
Methyl salicylate	1193	(3)	13	12			6, 7, 10
Methyl stearate	2115	(2)	0	1			2, 35
Methyltestosterone	2643	(2)	8	7			7, 11
5-Methyltryptamine	1795	(1)					11
$\alpha$ -Methyltryptamine	1740	(1)					11
N-Methyltryptamine	1770	(1)					11
Methyprylon	1529	(10)	29	29			5-7, 9-11, 15, 26, 35
Methysergide	3089	(1)					10
Metoclopramide	2630	(1)					7
Metofoline	2635	(1)					16
Metopon	2459	(3)	7	6	2380	[11]	10, 15, 20
Metronidazole	1592	(3)	32	33			7, 10, 11
Metyrapone	1860	(1)					7
Mevinphos	1450	(1)					2
Miconazole	2980	(1)					7
Mirex	2470	(1)					2
Modaline	1420	(1)					3
Molindone	2465	(1)					28
3-Monoacetylmorphine	2490	(1)					15
6-Monoacetylmorphine	2537	(6)	22	28	2402	[10]	6, 7, 11, 15, 20, 35
Monuron	1100	(1)					7
Morantel	9999	(1)					11
Morazone	1718	(2)	13	12			11
Morinamide	1906	(6)	16	14			11, 12
Morpheridine	2535	(1)					11

(Continued on p. 220)

TABLE 1 (continued)

Compound name	RJ	(n)	-	+	>50	[Ref.]	Refs.
Morphine	2454	(20)	44	41	2335	[12]	4-7, 9-11
					2340	[12]	13, 15-17, 20
					2380	[12]	21, 22, 25, 31, 35
					2390	[12]	
					2400	[14]	
					2510	[11]	
Morpholine	810	(1)					2
Myristic acid	1754	(2)	6	6			7, 35
Naftazone	1448	(1)					11
Nalorphine	2577	(9)	37	33	2643	[10]	5, 11, 13, 14, 16
					2680	[11]	20, 35
Naloxone	2640	(3)	0	0			7, 11, 20
Naphazoline	2057	(12)	47	43	1990	[25]	1, 7-12, 14, 15
Naphthalene	1186	(1)					2
1-Naphthonitrile	1489	(1)					2
2-Naphthyl acetate	1585	(1)					2
$\alpha$ -Naphthylamine	1531	(1)					9
Narcobarbital	1814	(2)	1	1			9, 26
Nealbarbitone	1720	(1)					18
Neocinchophen	2495	(1)					15
Neopine	2395	(2)	0	0			15, 22
Neostigmine bromide	1770	(3)	5	5	1850	[12]	12, 15
					1860	[12]	
					1500	[1]	
					9999	[10]	
Nialamide							
Nicametate	1608	(2)	8	7			11
Nicergoline	9999	(1)					11
Nicocodine	3408	(1)					30
Nicodicodine	3327	(1)					30
Nicotinamide	1459	(2)	16	16			2, 10
Nicotine	1348	(20)	43	37	1415	[12]	3, 5-9, 11
					1420	[12]	12-14, 16, 17
					1430	[11]	22, 25, 35
Nicotinic acid	1335	(1)					7
Nicotinic acid amide	1390	(1)					35
Nicotinyl alcohol	1215	(3)	15	31	1100	[7]	1, 8
					1119	[10]	
Nicoumalone	1779	(4)	4	1	1875	[10]	10, 12
Nifenazone	1608	(1)					11
Nifuratel	2590	(1)					11
Nifuroxime	2380	(1)					11
Nifursol	9999	(1)					11
Nikethamide	1525	(16)	25	35	1760	[25]	3, 5, 7-14, 22, 29
Nimorazole	1803	(2)	8	7			11
Nitrazepam	2750	(8)	45	30	1467	[25]	11, 12, 14-16
					2674	[35]	17, 35
					2690	[12]	
					2830	[32]	
					2913	[10]	
<i>p</i> -Nitromethylamphetamine	1658	(1)					10
Nitroxynil	1754	(2)	6	6			11

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Nomifensine	2122	(1)					35
Noracymethadol	2231	(1)					30
	2081	(1)					30
Noramidopyrine	1710	(1)					25
Norbormide	2050	(1)					11
Norclobazam					2695	[32]	
					2815	[32]	
Norcodeine	2388	(2)	13	12			20, 21
Nordiazepam	2570	(2)	15	15			32
Norethisterone	2625	(1)					10
Norethynodrel	2551	(1)					10
Norfenfluramine	1133	(2)	3	3			3, 29
Norflunitrazepam	2740	(2)	5	5			32
Norharman					1920	[7]	
					2005	[2]	
					2100	[1-4]	
Norlevorphanol	2244	(2)	0	1			21, 30
Normethadone	2091	(7)	11	14			4, 7, 9, 12
Normorphine	2438	(1)					20
Norpethidine	1745	(4)	5	5			4, 5, 14, 20
Norpipanone	2488	(1)					30
Norpropoxyphene	2395	(3)	30	45			7, 14, 28
Norpropoxyphene amide					2472	[14]	
					2580	[28]	
Norpropyphenazone	1780	(1)					35
Norpseudoephedrine	1302	(3)	24	17	1362	[11]	3, 25, 29
Nortilidate	1835	(1)					35
Nortriptyline	2210	(16)	40	30			6, 7, 10-12, 14, 15, 17, 27, 28, 30, 34, 35
Noscapine	3120	(2)	20	19	3240	[14]	7, 10
Noxyptiline	2267	(3)	12	8			11, 35
Noxythiolin	2370	(2)	10	10			11
Nystatin	1945	(1)					10
Obidoximè bromide	9999	(1)					11
Octacaine	1893	(2)	3	2			11
Octamylamine	1303	(1)					29
Octaphonium chloride	2013	(2)	8	7			11
Octyldecyl adipate	2540	(1)					2
	2745	(1)					2
	2940	(1)					2
4-tert.-Octyl-2-methylcyclohexyl acetate	1611	(1)					2
Oestradiol	2659	(1)					10
Oestriol	2970	(1)					10
Oestrone	2612	(1)					10
Orciprenaline	9999	(1)					7
Orphenadrine	1936	(16)	16	17	1875	[10]	4, 7, 8, 10-12, 14, 15, 28, 34
Orthocaine	1655	(1)					7
Oxanamide	1249	(1)					10

(Continued on p. 222)

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Oxazepam	2336	(12)	26	44	2260	[12]	6, 7, 10-12, 14
					2270	[12]	15, 17, 25, 32, 35
					2415	[28]	
					2425	[32]	
					2430	[16]	
Oxethazaine	2525	(1)					7
Oxomemazine	2725	(2)	5	5			15, 27
Oxprenolol	1870	(3)	30	40			11, 14
Oxybuprocaine	2471	(1)					30
Oxyclozanide	9999	(1)					11
Oxycodone	2524	(3)	23	26	2425	[7]	10, 20, 35
					2450	[25]	
Oxymetazoline	2168	(5)	23	32			7, 10, 11, 15, 35
Oxymetholone	2835	(1)					7
Oxymorphone	2532	(5)	12	13			7, 10, 11, 15, 20
Oxypertine	2355	(1)					11
Oxyphenbutazone					1630	[7]	
					9999	[10]	
Oxyphencyclimine	2550	(3)	10	21			7, 10, 14
	1661	(1)					10
Padimate	1964	(2)	4	4			11
Palmitic acid	1973	(4)	14	18			7, 10, 35
Panidazole	2065	(2)	0	0			11
Papaverine	2825	(11)	40	37	2770	[12]	7, 9-12, 14
					2900	[11]	15, 22, 25, 34, 35
Paracetamol	1687	(11)	27	28	1760	[6]	5, 10, 12, 14, 17, 33
					1760	[7]	35
					1780	[13]	
Paramethadione					1120	[10]	
					9999	[7]	
Parathion	1942	(5)	7	13			2, 10, 12, 35
Parbendazole	9999	(1)					11
Pargyline	1214	(7)	14	18			3, 5, 7, 10, 11, 22, 29
Pecazine	2524	(13)	39	36	2445	[12]	5, 10-12, 13, 15
					2445	[12]	23, 27
Pellotine	1825	(1)					15
Pemoline					2080	[30]	
					2240	[31]	
Penfluridol	3380	(1)					35
Pentachlorophenol	1749	(2)	9	8			1, 10
Pentapiperide	9999	(1)					11
Pentaquin	2555	(2)	15	15			7, 11
Pentazocine	2275	(20)	35	46			4-7, 9-16, 20, 28, 35
Pentifylline	2195	(1)					11
Pentobarbitone	1740	(26)	25	40			1, 5-7, 9-19, 24, 26, 35
Pentorex	1256	(1)					29
Perazine					2760	[27]	
					2930	[35]	
Perhexiline	2153	(2)	3	2			11
Perhydrophentermine	1167	(1)					29
Pericyazine					3230	[7]	
					3340	[14]	

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Perphenazine	2207	(3)	7	13			5, 7, 13
Perthane	2175	(1)					2
Pethidine	1751	(25)	26	28			4-17, 20, 25, 35
Pethidine intermediate A	1652	(1)					30
Pethidine intermediate B	1759	(2)	9	19			20, 30
Phenacaine	2617	(2)	27	27			7, 10
Phenacemide	1473	(1)					10
Phenacetin	1675	(21)	45	30	1755	[13]	4, 5, 7, 9-17, 24, 26, 35
Phenadoxone	2522	(3)	12	28			4, 7, 11
Phenamprovidine	2014	(1)					30
Phenanthrene	1786	(1)					10
Phenatine	2089	(2)	6	6			11
Phenazine	1703	(1)					2
Phenazocine	2684	(5)	34	36			4, 10, 11, 14, 20
Phenazone	1848	(8)	16	39			5, 7, 9, 10, 15, 16, 25, 35
Phenazone metabolite (1-phenyl-4-hydroxy- 2,3-dimethyl-3-pyrazolin- 5-one)	2730	(1)					35
Phenazopyridine	2245	(5)	35	25	2345	[7]	12, 15
					2346	[10]	
Phenbutrazate	2670	(1)					11
Phencyclidine	1904	(10)	34	28	1755	[28]	5-7, 9-11, 14, 15, 35
Phendimetrazine	1444	(13)	34	48	1555	[12]	3, 5, 7, 9-12
					1560	[12]	13, 22, 25, 29, 31
Phenelzine	1335	(3)	5	5	2135	[23]	1, 10, 14
Phenetamine	2213	(2)	8	7			12
$\alpha$ -Phenethylamine	1031	(4)	21	19			2, 5, 10, 22
$\beta$ -Phenethylamine	1111	(7)	21	9			2, 5, 7, 10, 14, 22, 35
Pheneturide	1465	(1)					11
Phenglutarimide	2321	(1)					30
Phenindamine	2167	(9)	17	38			1, 4, 8, 10, 11, 15, 28
Phenindione	2055	(1)					7
Pheniprazine	1400	(1)					10
Pheniramine	1804	(11)	49	36	1969	[10]	4, 7, 8, 11, 14, 15, 28, 34, 35
Phenmetrazine	1431	(16)	38	37	1495	[12]	3, 5-7, 9-11
					1495	[12]	13, 14, 16, 22, 25
					1495	[12]	29, 31, 35
Phenobarbitone	1957	(23)	27	33	2010	[13]	5-7, 9-12
					2034	[15]	13-17
					2065	[11]	18, 24, 26, 36
Phenol	981	(1)					10
Phenoperidine	2872	(1)					30
Phenothiazine	2024	(4)	14	11			7, 10, 11, 13
Phenoxybenzamine	2233	(4)	8	12			7, 10, 11, 15
Phenoxypropazine	1468	(3)	3	5			3, 7, 11
Phenprobamate	1520	(1)					11
Phensuximide	1634	(4)	14	16			6, 7, 10, 15
Phentermine	1147	(10)	18	26	1365	[12]	3, 5, 7, 9-11, 14
					1367	[12]	22, 25, 29

(Continued on p. 224)

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Phentolamine	9999	(1)					7
Phenylalanine	2205	(1)					7
Phenylbutazone	2365	(10)	25	32	2230	[12]	6, 7, 9-12
					2235	[12]	14, 17, 25
Phenylephrine					1660	[7]	
					2158	[34]	
					9999	[10]	
$\alpha$ -Phenyl- $\alpha$ -ethylglutaconamide	1842	(1)					10
$\alpha$ -Phenylglutarimide	1782	(1)					10
Phenylmethylbarbituric acid	1880	(2)	5	5			15, 18
Phenylpropanolamine	1313	(8)	27	45	1375	[8]	3, 5, 7, 10, 14, 22
					1415	[1]	
Phenylpropanone	1110	(2)	3	2			10, 22
1-Phenylpropylamine	1128	(3)	3	2			5, 10, 22
3-Phenylpropylamine	1205	(1)					35
Phenylpropylmethylamine	1176	(2)	1	1			10, 22
1-Phenyl-3-pyrazolidinone	1957	(1)					10
Phenyltoloxamine	1938	(13)	18	22	2010	[5]	7, 10-13
					2055	[13]	15, 28
Phenylramidol	2006	(6)	31	32	2485	[11]	1, 8, 10, 15
Phenytol	2330	(7)	15	14	2270	[12]	5, 9, 15-17, 35
					2270	[12]	
					2400	[14]	
					2460	[6]	
					2486	[10]	
Pholcodine					2381	[10]	
					3005	[12]	
					3030	[12]	
					3170	[14]	
Phorate	1675	(1)					2
Phthivazid	9999	(1)					11
Physostigmine	1804	(5)	24	10			5, 7, 10, 11
	2035	(1)					11
	2190	(3)	15	15			11, 12
Phytomenadione	3287	(1)					10
Picloxydine	9999	(1)					11
Picrotoxin					2205	[5]	
					2280	[10]	
					2356	[10]	
					2464	[10]	
					2545	[10]	
Pilocarpine	2014	(6)	13	26	2220	[28]	10, 12, 15
Piminodine					2020	[11]	
					2310	[11]	
					2885	[20]	
					2949	[9]	
Pimozide	9999	(2)					7, 11
Pindolol	2260	(1)					14
Pipamazine	3260	(1)					1
Pipamperone	3070	(1)					35
Pipazethate	2037	(1)					11
Piperacetazine	9999	(2)					10, 11

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Piperazine	813	(2)	23	22			2, 22
Piperidine	790	(1)					2
Piperidolate	2318	(7)	28	17			1, 10-12
Piperilate	2464	(1)					10
Piperocaine	1980	(8)	25	29			1, 8, 10, 15
Piperonal	1305	(1)					7
Piperoxan	1840	(2)	10	10			11, 15
Pipethanate					2205	[23]	
					2475	[11]	
Pipobroman	1811	(3)	16	17			10, 11
					2030	[11]	
					2050	[11]	
					2200	[10]	
Pipradrol	2145	(16)	50	50			5, 10-15, 23, 31
Piracetam	1640	(1)					35
Pivalylbenzhydrazine	1613	(1)					10
Pizotifen	2375	(1)					11
Polythiazide	2380	(1)					7
POPOP (1,4-bis(5-phenyl-oxazolyl-2)benzene)	3525	(1)					2
PPO (2,5-diphenyloxazole)	2050	(1)					2
Practolol	9999	(1)					11
Prajmalium bitartrate					2925	[35]	
					9999	[11]	
Pramoxine	2281	(5)	31	24			1, 7, 10, 11, 15
Prazepam	2641	(8)	31	14	2710	[9]	2, 7, 11, 15, 16
					2715	[32]	17, 25, 35
Prenylamine	2557	(3)	7	13			7, 11, 15
Prilocaine	1825	(6)	25	15			4, 7, 10, 14, 15
Primaquine	2314	(4)	8	6	2105	[5]	1, 7, 10
Primidone	2247	(13)	42	28	2165	[12]	4, 5, 7, 11-15
					2170	[12]	15-17, 35
Probarbital	1567	(7)	17	28			5, 10, 11, 15, 18, 19
Probenecid	2336	(2)	16	16			1, 10
Procainamide	2248	(3)	28	25			7, 10, 11
Procaine	2018	(20)	23	32	2105	[28]	4, 5, 7-15, 25
Procarbazine	1990	(2)	10	11			10
Prochlorperazine	2954	(4)	27	16	3120	[7]	10, 14, 23, 27
Procyclidine	2156	(13)	41	19	2220	[14]	1, 7-12, 35
Profadol	1748	(2)	8	7			11
Progesterone	2793	(1)					10
Proheptazine	1590	(1)					11
	1920	(1)					11
	1937	(1)					11
Prolan	2250	(1)					2
Prolintane	1634	(11)	49	21	1520	[25]	9, 11, 12, 14, 15, 29, 31
Promazine	2316	(17)	41	44			4, 5, 7, 9-11, 13-15, 23, 27, 28, 35
Promethazine	2259	(20)	39	41	2205	[12]	4, 5, 7, 10-12
					2328	[9]	13-15, 23, 25, 27, 28
Prometryne	1853	(2)	8	7			11

(Continued on p. 226)

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Promoxolane	1252	(1)					10
Propanidid	2433	(2)	8	7			12
Propantheline bromide					2180	[12]	
					2205	[12]	
					2215	[12]	
					2349	[10]	
Propelidone	1750	(1)					11
Propiomazine	2738	(5)	13	17			1, 11, 14, 15, 27
Propionylpromazine	2800	(1)					27
Propoxycaine	2335	(1)					11
Propranolol	2157	(5)	7	9			7, 10, 11, 14, 15
N-Propylamphetamine	1324	(3)	6	6			5, 22, 29
Propylhexedrine	1169	(7)	9	16			3, 5, 10, 11, 14, 22, 29
Propyl <i>p</i> -hydroxybenzoate	1567	(1)					2
Propyliodone	9999	(1)					10
5-Propyl-5-isobutylbarbituric acid	1693	(1)					10
N-Propyl- $\alpha$ -methyl- $\beta$ -phenethylamine	1318	(2)	29	29			10
Propyl myristate	1859	(1)					10
Propylparaben	1620	(2)	5	5			15, 35
Propyphenazone	1925	(1)					35
Proquamezine	2434	(3)	6	11			7, 11, 27
Prothipendyl	2339	(6)	19	34			1, 10, 11, 15, 27, 35
Protokylol	1487	(1)					10
Protoveratrine A	2465	(1)					7
Protoveratrine B	2465	(1)					7
Protriptyline	2261	(5)	31	39	2340	[15]	7, 11, 14, 28, 30
Proxymetacaine	2323	(2)	13	12			7, 15
Proxiphylline	2103	(1)					9
Pseudococaine	2180	(1)					15
Pseudoephedrine	1354	(8)	37	44	1418	[22]	3, 7, 9-11, 14, 25, 31
Pseudomorphine	2770	(1)					11
Psilocin	1980	(1)					7
Psilocybin	2059	(1)					30
Putrescine	930	(1)					2
Pyrantel	9999	(1)					10
Pyrazinazine	2536	(4)	16	18			4, 10, 15, 23
Pyrazinamide	1250	(1)					7
Pyrene	1983	(1)					2
Pyridbenzamine	1980	(1)					2
Pyridostigmine bromide	1515	(1)					12
Pyridoxamine	2000	(1)					5
Pyrimethamine	2138	(3)	4	2			5, 7, 10
Pyrithyldione	1557	(3)	27	18			12, 35
Pyrrobutamine	2419	(12)	34	28	2345	[12]	5, 10-14
					2360	[12]	15, 23
					2480	[4]	
					2515	[13]	
Pyrocaine	1968	(3)	3	7			11, 20
Pyrrolidine	695	(1)					2
Pyrroliphen	2396	(1)					10
Pyruvic acid	1249	(1)					10



TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Quinalbarbitone	1791	(24)	29	29			5-7, 9-19, 24, 26, 35
Quinalbarbitone metabolite [5-(1-methylbutyl)barbituric acid]	1660	(1)					35
Quinalbarbitone metabolite [5-(3-hydroxy-1-methylbutyl)- 5-(2-propenyl)barbituric acid]	1965	(1)					35
Quinidine	2784	(5)	24	26			5-7, 10, 13
Quinine	2803	(13)	48	47			5-7, 9-11, 13-16, 25, 35
Quinoline					1247	[2]	
					1427	[10]	
Quinone	1250	(1)					7
Racemethorphan	2124	(7)	19	24			11, 12, 20, 21
Racemoramide	2930	(1)					11
Racemorphan	2218	(2)	3	2			11, 21
Rafoxanide	9999	(1)					11
Rescinnamine	2180	(1)					7
Reserpine	9999	(2)					7, 10
Resorantel	9999	(1)					11
Resorcinol	1258	(2)	8	7			10, 35
Riconoleic acid	1991	(1)					10
Rimantadine	1388	(1)					11
Ritodrine	9999	(1)					11
Rolicypram	9999	(1)					11
Ronnel	1893	(4)	13	22			2, 12
Rotenone	3242	(1)					10
Rotoxamine	2049	(1)					10
Saccharin					1764	[10]	
					1875	[10]	
Salicylaldehyde	1072	(1)					10
Salicylamide	1455	(14)	20	45	1560	[24]	5-7, 9, 10, 14, 16, 24, 26, 33, 35
Salicylic acid	1308	(9)	28	22			5-7, 9, 10, 16, 17, 35
Salol					1650	[7]	
					1660	[6]	
					1745	[10]	
Sanctizer 141	2410	(1)					2
Sanguinarine	2880	(1)					5
Santonin	2174	(2)	4	4	1945	[5]	10, 11
Secbutobarbitone	1662	(7)	12	18	1780	[5]	7, 10, 11, 15, 16, 18, 35
Secbutobarbitone metabolite (hydroxysecbutobarbitone)	1928	(1)					35
Secergan	2310	(1)					15
Simazine	1690	(1)					2
Sitosterol	3193	(2)	39	39			10
SKF 525A	2326	(1)					2
Sparteine	1801	(12)	46	29			5, 7, 10-13, 15
Spirolactone	3280	(1)					10
Stearic acid	2174	(3)	4	4			7, 10, 35
Stigmasterol	3234	(1)					2

(Continued on p. 228)

TABLE 1 (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
<i>trans</i> -Stilbene	1755	(1)					2
Stilboestrol	2298	(2)	3	2			1, 11
STP	1616	(3)	8	4			5, 7, 10
Strychrine	3119	(8)	23	31	3020	[13]	6, 7, 9, 10, 13, 14
					3040	[5]	16, 35
					3060	[31]	
					3280	[25]	
Styramate	1667	(2)	2	1			10, 33
Succinylcholine chloride	9999	(1)					10
Sulphafurazole	1212	(1)					10
Sulphaguanidine	9999	(1)					10
Sulphamoxole	9999	(1)					11
Sulphanilamide	2166	(1)					10
Sulphathiazole	9999	(1)					10
Sulphonal	1478	(1)					11
Sulphosalicylic acid	1265	(1)					10
Sulpiride					2062	[35]	
					2832	[35]	
Symazine	9999	(1)					11
Synhexyl	2616	(1)					10
2,4,5-T Isopropyl ester (2,4,5-trichlorophenoxyacetic acid)	1825	(1)					2
2,4,5-T Methyl ester	1740	(1)					2
Tacrine	2165	(2)	5	5			11, 14
Talbutal	1701	(6)	28	19			10-12, 18, 19, 33
Tartaric acid	1249	(1)					10
Taurolin	9999	(1)					11
<i>o,p'</i> -TDE	2130	(1)					2
<i>p,p'</i> -TDE	2200	(1)					2
Temazepam					2470	[12]	
					2480	[12]	
					2525	[12]	
					2535	[12]	
					2595	[11]	
					2630	[32]	
					2675	[32]	
Terbutryne	1940	(2)	0	0			11
Terodiline	1908	(2)	8	7			11
<i>p</i> -Terphenyl	2208	(1)					2
Terpineol	1127	(1)					2
	1170	(1)					2
	1183	(1)					2
Testosterone	2620	(1)					7
Tetracaine	2215	(9)	35	25			10, 12, 13, 15
Tetrachlorvinphos <i>Z</i> -isomer	2430	(1)					2
Tetracycline	1950	(1)					7
$\Delta^9$ -Tetrahydrocannabinol	2473	(4)	20	17	2390	[11]	5, 15, 16, 35
Tetrahydrofurfuryl oleate	2290	(1)					2
	2480	(1)					2
	2660	(1)					2
Tetrahydrozoline	1833	(3)	11	19	1750	[25]	9, 11, 15
Tetraphenylethylene	2478	(1)					2
Thebacon	2533	(2)	3	2			11, 35

TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Thebaine	2517	(14)	32	18	2395 2400 2580	[12] [12] [11]	5, 7, 9, 10, 13, 14 15, 21, 22, 25
Thenalidine	2318	(1)					30
Thenylidiamine	1999	(11)	31	31			1, 8, 10, 12, 15, 28
Theobromine					1840 1847 1910 2250 2470 2845	[35] [10] [14] [25] [11] [7]	
Theophylline	1999	(7)	44	41	2105 2450	[7] [30]	12, 14, 15, 35
Thiabendazole	2040	(5)	39	40			7, 10, 14, 15
Thiacetazone	2038	(2)	3	2			11
Thialbarbitone	2116	(1)					18
Thiambutosine	1715	(1)					11
Thiamylal	1899	(5)	14	18			5, 10, 15, 19
Thianaphthene	1200	(1)					2
Thianthrene	1901	(1)					2
Thiantoin	2145	(1)					5
Thiazesim	2595	(1)					15
Thiethylperazine	3247	(1)					10
Thiobarbituric acid	738	(1)					18
Thiocartide	2005	(2)	5	5			11
Thiopentone	1859	(19)	24	31	1730 1740 1765 1765	[12] [12] [11] [12]	5, 7, 9, 10, 13, 15 16, 17, 18, 19, 24 26, 35
Thiopropazate	3465	(2)	15	15			1, 14
Thiopropazine	9999	(1)					7
Thioridazine	3114	(8)	34	31	3176 3180	[9] [6]	5, 10, 13, 14, 23 27, 28
Thiosalicylic acid	1494	(1)					10
Thiothixene	3060	(1)					10
Thonzylamine	2203	(7)	48	47	2045	[5]	1, 7, 10, 11, 15, 23
Thozalinone	2040	(1)					15
Thymol	1260	(1)					10
Thymoxamine	1832	(1)					11
Tigloidine	1687	(1)					30
Tiletamine					1695 1720 2195 2200	[15] [30] [11] [11]	
Tilidate	1840	(2)	0	0			16, 35
Tolazamide	1651	(1)					10
Tolazoline	1598	(6)	43	37	1490 1510	[7] [14]	11, 12, 30
Tolbutamide	1683	(2)	13	13			7, 10
<i>o</i> -Toluidine	2356	(1)					10
Tranylecypromine	1223	(12)	23	49	1290 1291	[8] [8]	3, 5, 7-11 13, 14, 22, 29, 35

(Continued on p. 230)

TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Triacetin	1282	(1)					2
Triamcinolone	2970	(1)					10
	3107	(1)					10
Tritenzylamine	2271	(1)					2
Tributyl citrate	2150	(1)					2
Tributyl phosphate	1690	(1)					2
Tributylin	1552	(1)					2
Tri-(2-chloroethyl) phosphate	1740	(1)					2
Tricresyl phosphate	2695	(1)					2
Triethyl citrate	1655	(1)					2
Tri-(2-ethylhexyl) phosphate	2463	(1)					2
Triethyl phosphate	1109	(1)					2
Triflubazam	2244	(1)					2
Trifluomeprazine	2250	(1)					11
Trifluoperazine	2683	(10)	18	37	2615	[12]	1, 4, 6, 10, 11, 14
					2625	[12]	15, 17, 23, 27
Trifluoperidol					2545	[12]	
					2545	[12]	
					2570	[12]	
					2590	[12]	
					2655	[36]	
					2797	[30]	
Triisobutyl phosphate	1483	(1)					2
Triisopropyl phosphate	1182	(1)					2
Trimecaine	1971	(2)	6	6			15, 28
Trimeperidine	1652	(1)					30
	1737	(1)					30
	1808	(1)					30
	1851	(2)	28	27			11, 30
Trimeprazine	2309	(10)	29	36	2230	[12]	1, 4, 6, 7, 10-12
					2245	[12]	23, 27
Trimethobenzamide					3287	[10]	
					9999	[11]	
Trimethoprim	2638	(1)					11
Trimethoxyamphetamine	1748	(1)					10
Trimethylamine	2215	(1)					7
Trimethyl citrate	1442	(1)					2
N,N- $\alpha$ -Trimethyl- $\beta$ -phenethylamine	1233	(2)	5	5			10, 22
Trimethyl phosphate	995	(1)					2
Trimetozine	2198	(3)	23	17			11, 15
Trimipramine	2201	(11)	36	49			6, 11, 12, 14, 15, 27, 30, 35
Triethyl phosphate	2445	(1)					2
Trioxsalen	2155	(1)					7
Tripelennamine	1980	(15)	20	30			1, 4-11, 14, 15, 25, 28
Triphenylamine	2055	(1)					2
Triphenyl phosphate	2363	(1)					2
Triprolidine	2253	(7)	8	11			4, 5, 7, 9-11, 14
Tripropyl phosphate	1372	(1)					2
Triptylene	2224	(1)					2
Tris(butoxyethyl) phosphate	2363	(1)					2
Tris(2,3-dichloropropyl) phosphate	2307	(1)					2
Trometamol	1645	(1)					11

TABLE I (continued)

Compound name	RI	(n)	-	+	>50	[Ref.]	Refs.
Tropacocaine	1952	(4)	17	25			12, 15
Tropicamide	2330	(2)	0	0			7, 15
Tropine	1193	(3)	13	9			7, 10, 22
Troxidone	1100	(1)					5
Tryptamine	1742	(13)	32	48	1800	[13]	2, 4, 5, 7, 10-12, 14, 15, 35
Tuaminoheptane	888	(4)	32	32	785	[9]	10, 11, 22, 25
Tubocurarine	2495	(1)					11
Tybamate					1708	[10]	
					1743	[9]	
					2015	[12]	
					2030	[12]	
Tymazoline	1850	(1)					4
Tyramine	1436	(4)	31	19	1525	[12]	2, 7, 12
					1530	[12]	
Umbelliferone	1828	(1)					10
Urea	9999	(1)					10
Urethane	838	(1)					10
Valnoctamide	1370	(2)	5	5			12
Vinbarbitone	1740	(9)	24	33			9-11, 15, 16, 18, 19, 26, 35
Vinbarbitone metabolite [5-(1-ethyl- <i>n</i> -propyl) barbituric acid]	1660	(1)					35
Vinbarbitone metabolite [5-hydroxy-5-(1-ethyl- <i>n</i> -propyl)barbituric acid]	1790	(1)					35
Vinbarbitone metabolite [5-(3-hydroxy-1-methylbutyl)- 5-vinylbarbituric acid]	1930	(1)					35
Vinylbitone	1720	(1)					16
Warfarin	1432	(3)	27	28	2625	[7]	5, 10, 11
Xenysalate	2443	(2)	3	2			7, 11
Xylometazoline	1940	(4)	21	17	2130	[4]	10, 11, 15
					2520	[25]	
Yohimbine	3269	(3)	13	21	2050	[11]	5, 10, 14
Zoxazolamine	1629	(1)					10
Zylofuramine	1665	(1)					15

values have been reported that differ from the mean by more than 50 retention index units. The determination of the retention index of barbitone is therefore far more reproducible than that for chlorpromazine. The factors affecting the reproducibility of retention indices have previously been discussed<sup>2</sup>.

Data concerning reproducibility have been summarised in Table 2 which shows the retention indices and associated standard deviations for twenty compounds for which more than ten values using SE-30 were available. Comparable data for retention indices measured on OV-17 have also been included for comparison but, because

much less OV-17 data were available, a lower limit of five determinations was set. The reproducibility, as measured by the standard deviation, is therefore marginally better using SE-30 than using OV-17. The mean standard deviation of 16.7 for SE-30 compares well with the standard deviations for inter-laboratory measurements of retention indices for basic drugs reported by Moffat<sup>1</sup> which were between 20 and 15 retention index units. The difference of 50 retention index units from the mean, used to identify unusual values, therefore corresponds to 3 standard deviations which would theoretically be expected to encompass 99% of experimentally determined values.

TABLE 2

RETENTION INDICES (*RI*), STANDARD DEVIATIONS (S.D.) AND RETENTION INDEX DIFFERENCES ( $\Delta RI$ ) FOR TWENTY COMPOUNDS FOR WHICH MULTIPLE DETERMINATIONS ON BOTH SE-30 AND OV-17 STATIONARY PHASES WERE AVAILABLE

<i>Compound</i>	<i>SE-30</i>		<i>OV-17</i>		$\Delta RI$
	<i>RI</i>	<i>S.D.</i>	<i>RI</i>	<i>S.D.</i>	
Amitriptyline	2196	22.13	2518	23.39	322
Amylobarbitone	1718	15.33	1988	10.97	270
Barbitone	1497	14.25	1796	13.01	299
Caffeine	1810	13.22	2246	23.82	436
Chlorpromazine	2486	31.56	2890	18.03	404
Cyclobarbitone	1963	12.30	2351	5.73	388
Dextropropoxyphene	2188	22.36	2455	25.53	267
Glutethimide	1836	17.62	2205	24.10	369
Lignocaine	1870	15.48	2164	26.19	294
Meprobamate	1796	14.51	2182	12.43	386
Methapyrilene	1981	11.70	2296	22.41	315
Methaqualone	2125	15.18	2580	19.85	455
Methylphenobarbitone	1891	16.05	2262	25.73	371
Nicotine	1348	18.65	1553	15.60	205
Pentazocine	2275	22.20	2607	19.35	332
Pentobarbitone	1740	13.46	2017	14.35	277
Pethidine	1751	12.90	1996	9.92	245
Phenacetin	1675	16.25	2040	8.02	365
Phenobarbitone	1957	13.22	2372	16.98	415
Salicylamide	1455	16.46	1802	16.19	347
	Mean S.D.		Mean S.D.		Mean $\Delta RI$
		16.74		17.58	338

Some compounds undergo on-column decomposition and therefore give multiple peaks. An example is chlordiazepoxide, which can give four peaks, and these are reported individually under the parent compound in Tables 1 and 3. Other compounds, such as propantheline bromide, would not be expected to elute as the parent compound, but nevertheless give a peak with a retention index around 2200 or 2350. In these cases the retention indices should be determined in the user's laboratory under specific experimental conditions and special care should be exercised if a mass spectrometer is being used as detector.

Table 3 has been generated from the data in Table 1 to aid the identification of an unknown compound and contains 1820 entries from 1318 compounds in as-

TABLE 3

1820 RETENTION INDICES OF 1318 COMPOUNDS, USING SE-30 OR OV-1 AS THE STATIONARY PHASE, ARRANGED IN ASCENDING ORDER OF RETENTION INDEX

Mean retention indices are given as well as each value which was greater than  $\pm 50$  retention index units from the mean (indicated by an asterisk).

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
695	Pyrrrolidine	1109	Triethyl phosphate
738	Thiobarbituric acid	1110	Phenylpropanone
771	Ethylene glycol	1111	$\beta$ -Phenethylamine
780	Ethanolamine	1118	Heptaminol
785*	Tuaminoheptane	1119	Nicotinyl alcohol
790	Piperidine	1120*	N-Ethylbenzylamine
810	Morpholine	1120*	Paramethadione
813	Piperazine	1123	Amphetamine
838	Urethane	1127	Terpineol
882	Allopurinol	1128	1-Phenylpropylamine
888	Tuaminoheptane	1130	Methyl caprylate
909	Butylamine	1133	Norfenfluramine
917	Cyclohexylamine	1137	Camphor
930	Putrescine	1140	Isopropylhexedrine
981	Phenol	1147	Phentermine
995	Benzylamine	1158	Aniline
995	Trimethyl phosphate	1159	N,N-Dimethylphenethylamine
1000	Acepifylline	1167	Perhydrophentermine
1000	Methylaminomethylheptane	1169	Propylhexedrine
1010*	Dimethylaniline	1170	Terpineol
1017	Fluspirilene	1176	Methylamphetamine
1023	Ethchlorvynol	1176	Phenylpropylmethylamine
1023	<i>p</i> -Dichlorobenzene	1180	Benzoic acid
1030*	Heptaminol	1182	Triisopropyl phosphate
1031	$\alpha$ -Phenethylamine	1183	Terpineol
1031	N-Ethylbenzylamine	1185	Chlormethiazole metabolite
1035	Cadaverine	1186	Naphthalene
1046	Benzyl alcohol	1190*	Amphetamine
1046	iso-Amylamine	1192*	Carbromal
1052	Isomethheptene	1192	Geraniol
1053	Limonene	1193	Methyl salicylate
1062	Indene	1193	<i>p</i> -Dibromobenzene
1072	Salicylaldehyde	1193	Tropine
1078	Methylbenzylamine	1195	$\alpha,\alpha$ -Dimethyl- $\beta$ -succinamide
1080	N,N-Dimethylaniline	1197	<i>m</i> -Dibromobenzene
1081	Diethyl maleate	1200	Thianaphthene
1087	Cyclopentamine	1205	3-Phenylpropylamine
1090*	Amphetamine	1205	Carbromal metabolite
1092	Guaiacol	1206	Ethosuximide
1095	Imidazole	1210	Dimethrin
1100	Linalol	1210	Hexamine
1100	Methyl nicotinate	1212*	Bromvaletone
1100	Monuron	1212	Sulphafurazole
1100*	Nicotinyl alcohol	1213	Dimethyl adipate
1100	Troxidone	1214	Pargyline
1105	Emylcamate	1215	Acetylcarbromal

(Continued on p. 234)

TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
1215	Methyl nonanoate	1309	<i>p</i> -Aminosalicylic acid
1215	Nicotinyl alcohol	1309	<i>n</i> -Butyric acid
1220	Hydroquinone	1309	<i>cis</i> -Linoleic acid
1221	<i>o</i> -Dibromobenzene	1313	2-Methylnaphthalene
1222	Fenfluramine	1313	Phenylpropanolamine
1223	Tranlylcypromine	1318	<i>n</i> -Propyl- $\alpha$ -methyl- $\beta$ -phenethylamine
1227	Ethyl benzoate	1320	Ethosuximide metabolite
1228	N-Ethylamphetamine	1320*	Hydroxyamphetamine
1230	Chlormethiazole	1323	Dichloroaniline
1231*	Apronal	1324	N-Propylamphetamine
1233	N,N, $\alpha$ -Trimethyl- $\beta$ -phenethylamine	1326	1-Bromodecane
1235	Betahistine	1335*	Methylamphetamine
1236	N,N-Dimethylamphetamine	1335	Nicotinic acid
1239	Mephentermine	1335	Phenelzine
1240	Mebenzazine	1340	Carbromal metabolite
1246	Anisaldehyde	1340*	Methylamphetamine
1247	N-Isopropyl- $\alpha$ -methyl- $\beta$ -phenethylamine	1340*	Methylamphetamine
1247*	Quinoline	1342	Chlorphentermine
1249	<i>n</i> -Caproic acid	1343	Methyl anthranilate
1249	Oxanamide	1344	Diethyl adipate
1249	Pyruvic acid	1345	Cypenamine
1249	Tartaric acid	1345*	Methylamphetamine
1250	Pyrazinamide	1347*	<i>p</i> -Hydroxyphenylpyruvic acid
1250	Quinone	1348	Nicotine
1252	Promoxolane	1353	Dimetridazole
1256	Pentorex	1354	Pseudoephedrine
1257	Amantadine	1358	Acetanilide
1257	N-Isopropylamphetamine	1361	Methoxyphenamine
1258	Resorcinol	1362*	Norpseudoephedrine
1260*	Amphetamine	1363	Ephedrine
1260	Thymol	1363	Ethinamate
1265	<i>p</i> -Aminophenol	1365	N-2-Butylamphetamine
1265*	Amphetamine	1365	Chlormethiazole metabolite
1265	Sulphosalicylic acid	1365*	<i>p</i> -Hydroxyphenylpyruvic acid
1270	Buphenine	1365*	Phentermine
1272	Citral	1367*	Phentermine
1276	Indole	1368	Eugenol
1282	Triacetin	1370	Ethosuximide metabolite
1284	Anethole	1370*	Mephentermine
1285*	Diprophylline	1370	Valnoctamide
1285	<i>p</i> -Dibutoxyethoxyethyl adipate	1371	N,N-Diethylamphetamine
1290*	Tranlylcypromine	1372	Metamfepyrmon
1291*	Tranlylcypromine	1372	Tripropyl phosphate
1293	Aletamine	1373	Bemcgride
1295*	Mephentermine	1375*	Mephentermine
1302	Norpseudoephedrine	1375*	Phenylpropanolamine
1303	Octamylamine	1380	Carbromal metabolite
1305*	Mephentermine	1385	Ethosuximide metabolite
1305	Methyl decanoate	1385	Methoxyamphetamine
1305	Piperonal	1388	Rimantadine
1308	Salicylic acid	1389	Biphenyl
1309	Acetylsalicylic acid	1390	Ametazole
		1390*	Hippuric acid



TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
1390	Nicotinic acid amide	1475	Dimethyl terephthalate
1396	Ectylurea	1475*	Leptazol
1396	N-Methyl-N- <i>n</i> -propylamphetamine	1478	Sulphonal
1399	<i>n</i> -Caproic acid	1480	Beclamide
1400*	Acetylsalicylic acid	1483	Triisobutyl phosphate
1400*	$\alpha$ -Methylphenethylhydrazine	1485*	Diazinon
1400	N-Methylephedrine	1485*	Hordeine
1400	Pheniprazine	1486	Chlorothymol
1402*	Diethylpropion	1486	Diethylpropion
1406	Dimethyl phthalate	1486	N-Methyl-N- <i>n</i> -butylamphetamine
1410*	Acetylsalicylic acid	1487	Acetylindole
1415*	Nicotine	1487	Mandelic acid
1415*	Phenylpropanolamine	1487	Protokylol
1418*	Pseudoephedrine	1488	Dimethyl isophthalate
1419	Methyl <i>p</i> -hydroxybenzoate	1489	1-Naphthonitrile
1420	Modaline	1490	Butylated hydroxytoluene
1420*	Nicotine	1490	Cantharidin
1422	N- <i>n</i> -Butylamphetamine	1490	Carbaryl
1425	2,7-Dimethylquinoline	1490	Diethadione
1426	Isoquinoline	1490*	Hordeine
1427*	Quinoline	1490*	Hordeine
1430*	Nicotine	1490*	Leptazol
1431	Phenmetrazine	1490*	N,N-Diethyl- <i>m</i> -toluamide
1432	Warfarin	1490*	Tolazoline
1434	Bromonaphthalene	1494	Thiosalicylic acid
1434	N-Ethyl- <i>p</i> -chloroamphetamine	1495*	Diazinon
1436	Tyramine	1495*	Hordeine
1440*	Ephedrine	1495*	Phenmetrazine
1442	Trimethyl citrate	1495*	Phenmetrazine
1443	Kojic acid	1495*	Phenmetrazine
1444	Phendimetrazine	1497	Barbitone
1445*	Ephedrine	1497	Histamine
1446	2,4-Dimethylquinoline	1500*	Nialamide
1448	Naftazone	1505*	Acetylcarbromal
1450	Hydroquinine	1505	Dibutyl maleate
1450	Mevinphos	1507	4,4'-Bipyridyl dihydrate
1455*	Methoxyphenamine	1507	Carminic acid
1455	Salicylamide	1507*	Methocarbamol
1459	Nicotinamide	1510*	Bromvalerone
1460*	Etafedrine	1510*	Cyclopentamine
1462	Butylated hydroxyanisole	1510*	Tolazoline
1465	Pheneturide	1513	Carbromal
1466	Meconic acid	1515*	Cyclopentamine
1467*	Nitrazepam	1515*	Isoniazid
1468	Phenoxypropazine	1515	Pyridostigmine bromide
1470*	Methoxyphenamine	1516	<i>o</i> -Chlorobenzylidenemalonitrile
1470*	Methoxyphenamine	1519	Etafedrine
1471*	Benperidol	1519	Homarylamine
1471	2,4-Dinitrophenol	1520*	Diphenylamine
1472	Metharbitone	1520	Phenprobamate
1472	Methylenedioxyamphetamine	1520*	Prolintane
1473	Capric acid	1524	Acetyl- $\beta$ -phenethylamine
1473	Phenacemide	1524	Cyclododecanone

(Continued on p. 236)

TABLE 3 (continued)

<i>Rf</i>	<i>Compound name</i>	<i>Rf</i>	<i>Compound name</i>
1525	Benzenesulphonamide	1598	5-Aminoquinoline
1525*	Isoniazid	1598	Tolazoline
1525*	Isoniazid	1600	Amylocaine
1525	Nikethamide	1600	Lauric acid
1525*	Tyramine	1601	Diphenylamine
1526	N,N-Di- <i>n</i> -propylamphetamine	1604	Clorprenaline
1528	<i>p</i> -Dimethylaminobenzaldehyde	1605	2,4-D Methyl ester
1528	Hydrallazine	1606	Allobarbitone
1529	Methypylon	1608	Nicametate
1530*	Tyramine	1608	Nifenazone
1531	$\alpha$ -Naphthylamine	1610	Benzophenone
1542	Etenzamide	1611	4- <i>tert.</i> -Octyl-2-methylcyclohexyl acetate
1545	Dipropyl adipate	1613	Pivalylbenzhydrazine
1547	Acetylcysteine	1616	STP
1547	<i>p</i> -Aminobenzoic acid	1617	4,6-Dinitro- <i>o</i> -cresol
1549	Clofibrate	1620	Propylparaben
1550	Crotamiton	1621	Chlorproguanil
1550*	Diethylpropion	1622	Aprobarbitone
1550	Methimazole	1622	Methsuximide
1551	3,4-Dimethoxyphenethylamine	1628	Demeton S-methyl
1552	Leptazol	1629	Zoxazolamine
1552	Tributyryn	1630	Acetylmethylamphetamine
1555	Benzocaine	1630*	Oxyphenbutazone
1555*	Diethylpropion	1632	Hydroxyamylobarbitone
1555*	Diethylpropion	1633	Diisopropyl phthalate
1555	Ethylallylbarbitone	1634	Dimethyl sebacate
1555*	Phendimetrazine	1634	Phensuximide
1556	Azobenzene	1634	Prolintane
1557	Pyrrithyldione	1635	4-Methyl-2,5-dimethoxyamphetamine
1560*	Barbitone	1640	Butoxyethyl nicotinate
1560*	Phendimetrazine	1640	Dipyramidole
1560*	Salicylamide	1640	Piracetam
1561	Enallylpropymal	1645	Trometamol
1564	Diethyl phthalate	1646	3,4-Methylenedioxyphentermine
1565	Hydroxybenzoic acid	1647	3,4-Methylenedioxy-2-methoxy-amphetamine
1567	Bromodiacetylurea	1650	Guaiphenesin
1567	Probarbital	1650*	Salol
1567	Propyl <i>p</i> -hydroxybenzoate	1651	Tolazamide
1568	Mephesisin	1652	Pethidine
1570	3-Ethylamino-3-phenylnorcamphane		intermediate A
1578*	Apronal	1652	Trimeperidine
1580*	Carbromal	1655	Atrazine
1580	Fluorene	1655	Orthocaine
1582*	Isoniazid	1655	Phenyl salicylate
1583	N,N-Diethyl- <i>m</i> -toluamide	1655	Triethyl citrate
1585	2-Naphthyl acetate	1658	<i>p</i> -Nitromethylamphetamine
1585	Butylbenzyl sebacate	1660	Diisobutyl adipate
1585	N-Methyl-3,4-methylene-dioxyamphetamine	1660*	Phenylephrine
1590	Hydrastinine	1660*	Salol
1590	Proheptazine	1660	Quinalbarbitone metabolite
1592	Metronidazole	1660	Vinbarbitone metabolite
1593	Iproniazid	1661	Oxyphencyclimine

TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
1662	9,10-Dihydroanthracene	1710	$\beta$ -Benzenehexachloride
1662	Secbutobarbitone	1710	Noramidopyrine
1665	Butobarbitone	1712	Diallyl phthalate
1665	Zylofuramine	1712	Isatin
1667	Styramate	1714	Ergosterol
1668	Butalbital	1715	$\gamma$ -Benzenehexachloride
1668	Etisazole	1715	Methyl myristate
1670	Isoniazid	1715	Thiambutosine
1675	Methyl hippurate	1718	Amylobarbitone
1675	Phenacetin	1718	Morazone
1675	Phorate	1720*	Chlorothiazide
1676	Dofamium chloride	1720*	Chlorpropamide
1677	Chlorphenesin	1720	Nealbarbitone
1677	Fencamfamin	1720*	Tiletamine
1678	Beclamide	1720	Vinylbitone
1678	Carbimazole	1724	Hydroxyphenamate
1678	Cotinine	1725	Dimethoate
1678	Dyclonine	1726	Methoxamine
1682	Hydroxyephedrine	1728	Chlorzoxazone
1683	Tolbutamide	1730	Acetyltriethyl citrate
1685	CDEC	1730	Isoprenaline
1685*	Etilefrine	1730*	Thiopentone
1687*	Dextropropoxyphene	1734	Diampromide
1687	Paracetamol	1735*	Hippuric acid
1687	Tigloidine	1736	Methallatal
1688	Crotethamide	1737	Methyl phenidate
1688	Mescaline	1737	Trimeperidine
1689	N,N-Di- <i>n</i> -butylamphetamine	1738	Benzyl benzoate
1690	$\alpha$ -Benzenehexachloride	1738	Cropropamide
1690	Simazine	1740	$\alpha$ -Methyltryptamine
1690	Tributyl phosphate	1740	2,4,5-T Methyl ester
1693	5-Propyl-5-isobutyl barbituric acid	1740*	Ethamivan
1695	Dibutyl adipate	1740	Pentobarbitone
1695*	Tiletamine	1740*	Thiopentone
1698	5-Allyl-5-butyl barbituric acid	1740	Tri-(2-chloroethyl) phosphate
1700	2,4-D Isopropyl ester	1740	Vinbarbitone
1700	Dimethylmescaline	1742	Butyl aminobenzoate
1700*	Iproniazid	1742	Tryptamine
1700	N-Methylmescaline	1743	Halquinol
1701	Talbutal	1743*	Tybamate
1702	3,4-Methylenedioxy-4-methoxy- amphetamine	1745	Diethyl sebacate
1702	Carminic acid	1745*	Dimethyltryptamine
1703	Phenazine	1745	Lindane
1705	3,4-Methylenedioxy-5-methoxy- amphetamine	1745*	Norpethidine
1705	Fluorenone	1745*	Salol
1705*	Leptazol	1746	Dipropyl phthalate
1705*	Leptazol	1748	Profadol
1708	Dicyclomine	1748	Trimethoxyamphetamine
1708*	Tybamate	1749	Pentachlorophenol
		1750	Propерidine
		1750*	Tetrahydrozoline

(Continued on p. 238)

TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
1751	Pethidine	1796	Meprobamate
1754	Anthracene	1798	Benethamine
1754	Butethamate	1800	$\alpha$ -Benzylphenethylamine
1754	Myristic acid	1800*	Diethyltryptamine
1754	Nitroxynil	1800	Ethotoin
1755	$\delta$ -Benzenhexachloride	1800	Methylanhalonidine
1755*	Phenacetin	1800*	Tryptamine
1755*	Phencyclidine	1801	Sparteine
1755	<i>trans</i> -Stilbene	1803	Nimorazole
1756	Ethionamide	1804	Pheniramine
1758	Diazinon	1804	Physostigmine
1759	Pethidine intermediate B	1805	2,4-D Isobutyl ester
1760	Alprenolol	1807	Dexpanthelol
1760	Benzphetamine	1808	Cotarnine
1760	Dichlone	1808	Trimeperidine
1760*	Nikethamide	1810	Caffeine
1760*	Paracetamol	1810*	5-Ethyl-5-phenylhydantoin
1760*	Paracetamol	1810*	Methyl phenidate
1764*	Saccharin	1811	Pipobroman
1765*	Fenmetramide	1813	Bromodimethoxyamphetamine
1765*	Thiopentone	1814	Narcobarbital
1765*	Thiopentone	1815*	Mescaline
1766	Methohexitone	1816	Benzamine
1770	Meclofenoxate	1823	Betameprodine
1770*	Methylphenobarbitone	1825	Anhalonidine
1770	N-Methyltryptamine	1825	Bisnortilidine
1770	Neostigmine bromide	1825	Pellotine
1770	Ibomal metabolite	1825	Prilocaine
1775	Ametryne	1825	2,4,5,-T Isopropyl ester
1777	Hexylresorcinol	1828	Umbelliferone
1779	Nicoumalone	1830	Carisoprodol
1780*	Lobeline	1830	Isoaminile
1780	Norpropyphenazone	1832	Thymoxamine
1780*	Paracetamol	1833	Tetrahydrozoline
1780*	Secbutobarbitone	1835	Brallobarbitone metabolite
1782	$\alpha$ -Phenylglutarimide	1835	Nortilidate
1784	N-Benzylamphetamine	1835*	<i>p</i> -Hydroxyphenylpyruvic acid
1784	Carbazole	1836	Glutethimide
1784	Clobutinol	1837	5-Allyl-5-(2-hydroxypropyl)barbitone
1785	Allobarbitone metabolite	1840*	Alprenolol
1786	Phenanthrene	1840	Benorylate
1790	Betaprodine	1840	2,4-D Butyl ester
1790	Secobarbitone	1840	Piperoxan
1790	Vinbarbitone metabolite	1840*	Theobromine
1791	Chlorpropamide	1840	Tilidate
1791	Methoin	1842	$\alpha$ -Phenyl- $\alpha$ -ethylglutaconamide
1791	Quinalbarbitone	1843	Ketamine
1792	Alphaprodine	1844	Dimenhydrinate
1795*	5-Ethyl-5-phenylhydantoin	1847*	Theobromine
1795	5-Methyltryptamine	1848	Etryptamine
1795	Brallobarbitone metabolite	1848	Phenazone
1795	Desmetryne	1850	Alphameprodine
1795	Isobutyl aminobenzoate	1850	Anhalonine

TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
1850	Lophophorine	1895*	Alphaprodine
1850*	Meprobamate	1898	Dofamium chloride
1850*	Neostigmine bromide	1899	Thiamylal
1850	Tymazoline	1901	Thianthrene
1851	Methyl parathion	1902	Digitalin
1851	Trimeperidine	1902	Digitoxin
1852	Lachesine	1903	Amidopyrine
1853	Diisobutyl phthalate	1903	Cyclandelate
1853	Prometryne	1904	Phencyclidine
1855	Benzphetamine	1906	Doxylamine
1855	Dichlorophenazone	1906	Morinamide
1857	Ethoheptazine	1908	Terodiline
1857	Hexobarbitone	1910	Diethyltryptamine
1858	Brallobarbitone	1910*	Theobromine
1858	Hexethal	1913*	5-Ethyl-5-phenylhydantoin
1859	Diampromide	1913	Dibutyl phthalate
1859	Propyl myristate	1915*	Ethotoin
1859	Thiopentone	1915*	Fenmetramide
1860	Metyrapone	1915	Hydroxypentobarbitone
1860*	Neostigmine bromide	1916*	Dipyron
1862	Cyclopentobarbitone	1917	Malathion
1866	5-Methyl-5-phenylhydantoin	1920	1-Hydroxyharman
1868*	Bromo STP	1920	Iminodibenzyl
1868	Isobutylcyclohexyl phthalate	1920	Metazocine
1870	Lignocaine	1920*	Norharman
1870	Oxprenolol	1920	Proheptazine
1873	Diphenhydramine	1923	Bibenzonium bromide
1874	4-Hydroxyantipyrine	1924	Di(ethoxyethyl) adipate
1874	<i>p</i> -Methoxybenzophenone	1925	Bethanidine
1875*	Ethotoin	1925	Propyphenazone
1875	Glutethimide metabolite	1928	Levamisole
1875	Nicoumalone	1928	Secbutobarbitone metabolite
1875*	Orphenadrine	1929	Allylprodine
1875*	Saccharin	1930*	Diisobutyl phthalate
1880	Dicyclohexyl oxalate	1930*	Ethamivan
1880	Diethyl- <i>p</i> -nitrophenyl phosphate	1930	Vinbarbitone metabolite
1880	Heptachlor	1936	2-Mercaptobenzothiazole
1880	Phenylmethylbarbituric acid	1936	Orphenadrine
1883	Clorgyline	1937	Proheptazine
1883	Ibomal	1938	Phenyltoloxamine
1885	Aminoparathion	1939	Azapetine
1885	Dimethylthiambutene	1940	Butalbital metabolite
1885*	Dimethyltryptamine	1940	Butylsxtyl phthalate
1885	Methstyridone	1940*	Dextropropoxyphene
1889	Mebutamate	1940	Terbutryne
1889	Methyl palmitate	1940	Xylometazoline
1891	Methylphenobarbitone	1942	Parathion
1893	Octacaine	1943	Aldrin
1893	Ronnel	1943	Ethylmethylthiambutene
1894*	Ethamivan	1945*	Caffeine
1894	Meboral	1945	Lecithin

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TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
1945	Nystatin	1999	Thenyldiamine
1945*	Santonin	1999	Theophylline
1947	Howflex GBP	2000*	Amidopyrine
1949	Isocarboxazid	2000	Captan
1950	Ampyrone	2000	Pyridoxamine
1950	Butylisodecyl phthalate	2002	Chlorpheniramine
1950	Flufenamic acid	2003*	5-Allyl-5-phenyl barbituric acid
1950	Tetracycline	2003	Hymecromonc
1952	Harman	2005*	Norharman
1952	Tropacocaine	2005	Thiocarlide
1953	Ethyl parathion	2006	Phenylramidol
1955	1-Hydroxychloridene	2008	Diethylthiambutene
1957	1-Phenyl-3-pyrazolidinone	2008	Etomidate
1957	Phenobarbitone	2010	Anilazine
1960	DCPA	2010	Dyrene
1963	Cyclobarbitone	2010*	Phenobarbitone
1964*	Dextropropoxyphene	2010*	Phenyltoloxamine
1964	Padimate	2011	Cloponone
1965	Hexylcaine	2013	Octaphonium chloride
1965*	Mebutamate	2014	Phenampromide
1965	Quinalbarbitone metabolite	2014	Pilocarpine
1966	Methaphenilene	2015	1-Hydroxyharman
1968*	Doxylamine	2015	Folpet
1968	Pyrocaine	2015	Heptachlor epoxide
1969*	Pheniramine	2015*	Tybamate
1970*	Aminophylline	2018	Dio.yamidopyrine
1970*	Aminophylline	2018	Procaine
1970	Diphenamid	2020	Chlordane
1971	Caramiphen	2020	Cyclizine
1971	Trimecaine	2020	Cyclopentolate
1972	Diisobutyl terephthalate	2020*	Piminodine
1973	Emepromium bromide	2021	Amisometradine
1973	Palmitic acid	2021	Methadone metabolite
1974	Dofamium chloride	2024	Isopyrin
1975	Ethomoxane	2024	Phenothiazine
1980*	2-Amino-5-chloro-2'- fluorobenzophenone	2025	Butanilcaine
1980	Dimethoxyethyl phthalate	2025*	Isopropamide
1980	Methoxsalen	2026	Eucatropine
1980	Piperocaine	2029	Dimethoxanate
1980	Psilocin	2030	Bufotenine
1980	Pyridbenzamine	2030	Dimethisoquin
1980	Tripeleennamine	2030	Ketobisnortilidine
1981	Methapyrilene	2030*	Pipobroman
1983	Dipyrone	2030*	Tybamate
1983	Pyrene	2034*	Phenobarbitone
1983*	Methylphenobarbitone	2035	Ketobemidone
1988	Metabutethamine	2035	Physostigmine
1988*	Ibomal	2037	Pipazethate
1990*	Naphazoline	2038	Amprotropine
1990	Procarbazine	2038	Thiacetazone
1991	Riconoleic acid	2039	2-Amino-5-chlorobenzophenone
1993*	Diethyltryptamine	2040	Brallobarbitone metabolite
1995	Butallylonal	2040	Thiazendazole
		2040	Thozalinone

TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
2042*	$\alpha$ -Methylphenethylhydrazine	2085	Endosulphan I
2045*	2-Amino-5-chloro-2'-fluorobenzophenone	2085*	Lobeline
2045	Chlorbenside	2086	Methyl oleate
2045	Hydroxypethidine	2089	Phenatine
2045*	Thonzylamine	2090*	2-Amino-5-chloro-2'-fluorobenzophenone
2048*	Atropine	2090	$\beta$ -Hydroxyethyltheophylline
2049	Rotoxamine	2090	$\beta$ -Hydroxypropyltheophylline
2050	Apoatropine	2091	Normethadone
2050	Hexobarbital metabolite	2096	Brompheniramine
2050	Norbormide	2097	Dicyclomine
2050*	Pipobroman	2098	Methoprotrolyne
2050	PPO	2099	Diphenylpyraline
2050*	Yohimbine	2100	Clotrimazole
2055	Phenindione	2100	Methyl linoleate
2055*	Phenyltoloxamine	2100*	Norharman
2055	Triphenylamine	2103	Di(ethoxyethyl)phthalate
2057	Naphazoline	2103	Proxiphylline
2058	Acetyl-L-tryptophan	2105*	Primaquine
2058*	Chloropyrilene	2105*	Procaine
2058	Heptabarbitalone	2105*	Theophylline
2058*	Isopropamide	2106*	5-Allyl-5-phenylbarbituric acid
2059	Psilocybin	2106*	Alphenal
2060*	Iproniazid	2107	2-Methylamino-5-chlorobenzophenone
2061	Butethamine	2108	Dimethocaine
2062*	Sulpiride	2110	Dieldrin
2065*	Cyclazocine	2112	Dropropizine
2065*	Iproniazid	2113*	Chlorphenesin
2065	Panidazole	2114	Cycrimine
2065*	Phenobarbitone	2115	Methyl stearate
2066	Dibutyl terephthalate	2116	Disethyl maleate
2070	Berberine	2116	Thialbarbitone
2070*	Cyclazocine	2120*	2-Amino-5,2'-dichlorobenzophenone
2070	<i>o,p'</i> -DDE	2120	Glycopyrrolate
2071	Mepivacaine	2122	Nomifensine
2072	Chlorphenoxamine	2124	Racemethorphan
2072	Homatropine	2125*	2-Amino-5-chlorobenzophenone
2074*	Dextropropoxyphene	2125	Methaqualone
2074	Mercumallylic acid	2127	Diamyl phthalate
2075	Dexbrompheniramine	2128	Isomethadone
2078	2-Amino-5-chlorodiphenylamine	2129	Chlorothenylpiramine
2079	Diampromide	2130	Butylbenzyl sebacate
2080	Carbinoxamine	2130*	Levomethorphan
2080	Chlophedianol	2130	<i>o,p'</i> -TDE
2080	Hexobarbitone metabolite	2130	<i>p,p'</i> -DDE
2080*	Pemoline	2130*	Xylometazoline
2081	Noracymethadol	2133	Chloropyrilene
2082	Benzocetamine	2135	Brallobarbitone metabolite
2083*	Aminophylline	2135*	Carisoprodol
2085	5-Ethyl-5- <i>p</i> -tolylbarbituric acid	2135	Dibenzyl sebacate
2085	DDA Methyl ester	2135*	Phenelzine

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TABLE 3 (continued)

<i>R<sub>I</sub></i>	<i>Compound name</i>	<i>R<sub>I</sub></i>	<i>Compound name</i>
2137	Dibutyl sebacate	2180*	Propranthaline bromide
2138	Pyrimethamine	2180	Pseudococaine
2140	Dextromethorphan	2180	Rescinnamine
2140	Dichlorophen	2181	Butriptyline
2141	Disulfiram	2183	Endrin
2142	Alverine	2184	Acetyl-D-tryptophan
2145*	Atropine	2184	Ergocryptine
2145	Chlorthalidone	2185	Embramine
2145	Pipradrol	2185	Levopropoxyphene
2145	Thiantoin	2186	Adiphenine
2146	3-Methoxymorphinan	2187	Alphacetylmethadol
2147	Lecithin	2187	Cocaine
2148	Methadone	2187	Methazolamide
2150	3-Isobutyl-1-methylxanthine	2188	2,5-Diamino-2'-fluorobenzophenone
2150*	Chlormezanone	2188	Dextropropoxyphene
2150	Tributyl citrate	2190*	Cannabidiol
2153	Chlorothen	2190*	Chlordiazepoxide
2153	Perhexiline	2190	Cyclobarbitone metabolite
2155	Bromdiphenhydramine	2190*	Methaqualone
2155*	Levomethorphan	2190*	Methaqualone
2155	Mephoxalone	2190	Physostigmine
2155	Trioxsalen	2192	Hyoscyamine
2156	Procyclidine	2195*	2-Amino-5,2'-dichlorobenzophenone
2157	Butyl stearate	2195*	Bromo STP
2157	Propranolol	2195*	Cyclazocine
2158*	Phenylephrine	2195	Pentifylline
2159	Isobutylcyclohexyl phthalate	2195*	Tiletamine
2160*	Dimethoxanate	2196	Amitriptyline
2163	Metaxalone	2198	2,5-Diaminobenzophenone
2165*	Chlormezanone	2198	Trimetozine
2165*	Glutethimide	2199	Atropine
2165*	Imipramine	2200	<i>p,p'</i> -TDE
2165*	Primidone	2200*	Pipobroman
2165	Tacrine	2200*	Tiletamine
2166	Sulphanilamide	2201	Mefenamic acid
2167	Phenindamine	2201	Trimipramine
2168	Oxymetazoline	2203	Thonzylamine
2170	Cyclobarbitone metabolite	2205*	Biperiden
2170*	Desipramine	2205	Phenylalanine
2170*	Dieldrin	2205*	Picrotoxin
2170	Methaqualone metabolite	2205*	Pipethanate
2170*	Primidone	2205*	Promethazine
2174	Santonin	2205*	Propranthaline bromide
2174	Stearic acid	2207	Perphenazine
2175*	Dieldrin	2208	<i>p</i> -Terphenyl
2175	Dopamine	2210	2-Benzhydroxymethyl-2-imidazoline
2175	Endosulphan II	2210	Nortriptyline
2175	Ethyl oleate	2211	Bamipine
2175	Ethylan	2211	Flupromazine
2175	Perthane	2213	Phenetamine
2178	Linolenic acid	2215*	Dieldrin
2179	<i>cis</i> -Linoleic acid	2215*	Propranthaline bromide
2180	Alphamethadol	2215	Trimethylamine



TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
2217	Doxepin	2245*	Cocaine
2218	Dicophane ( <i>o,p'</i> -isomer)	2245*	Hyoscine
2218	Racemorphan	2245	Phenazopyridine
2219	Amethocaine	2245*	Trimeperazine
2219	Benzhexol	2247	Primidone
2220	Ethion	2248	Benactyzine
2220	Mepyramine	2248	Clonidine
2220*	Pilocarpine	2248	Procaïnamide
2220*	Procyclidine	2250*	Adiphenine
2223	Imipramine	2250*	Atropine
2224	Citroflex A4	2250	5-Chloro-2-methylaminodiphenylamine
2224	Triptylene	2250*	Meprobamate
2225	Chlorcyclizine	2250	Prolan
2225*	Cyclomethycaine	2250*	Theobromine
2226	Amolanone	2250	Trifluomeprazine
2226	Medazepam	2253	Acetyltributyl citrate
2226	Metabutoxycaine	2253	Triprolidine
2227	Aminoglutethimide	2255	Bromazepam decomposition product
2227*	Cyclomethycaine		
2227	Deanol acetamidobenzoate	2255	Carbophenothion
2229	Chloroprocaine	2255*	Levomethorphan
2230*	Levomethorphan	2255	Mecloqualone
2230*	Phenylbutazone	2258	Dimethindene
2230*	Trimeprazine	2259	Promethazine
2231	Noracymethadol	2260*	Oxazepam
2232	Carbetapentane	2260	Pindolol
2232	Diampromide	2261	Protriptyline
2232	Dihydrodesoxymorphine	2265	2-Hydroxyiminodibenzyl
2233	Phenoxybenzamine	2265	Cyheptamide
2234	Halopyramine	2266	Biperiden
2234	Levorphanol	2267	Isothipendyl
2235	Ambucetamide	2267	Noxiptyline
2235	Butylsxytl phthalate	2268	Melitracene
2235*	Methaqualone	2270	Di(ethoxyethyl)sebacate
2235*	Phenylbutazone	2270*	Ethopropazine
2237	3-Hydroxymorphinan	2270*	Oxazepam
2238	Chlormezanone	2270*	Phenytoin
2240	Aminacrine	2270*	Phenytoin
2240*	2-Amino-5,2'-dichlorobenzophenone	2271	Diclofenac
2240	Chlordecone	2271	Tribenzylamine
2240*	Cocaine	2273	Anisindione
2240*	Hyoscine	2273	Bupivacaine
2240	Leucinocaine	2274	Clopenthixol
2240	Methaqualone metabolite	2275*	Benzhexol
2240	N1-Desalkyl-3-hydroxyflurazepam	2275*	Desmethylmedazepam
2240*	Pemoline	2275	Diphenazoline
2242	Desipramine	2275	Heptabarbital metabolite
2243	Azacyclonol	2275	Pentazocin�
2243	Bromazepam metabolite	2280*	Aconitine
2244	Norlevorphanol	2280*	Amethocaine
2244	Triflubazam	2280*	Benzhexol

(Continued on p. 244)

TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
2230*	Picrotoxin	2325*	Hydrocodone
2231	Pramoxine	2325*	Lorazepam
2232	Dicyclohexyl adipate	2326	SKF 525A
2285*	Amethocaine	2327	Butylbenzyl phthalate
2285	Galantamine	2327	Mepenzolate
2285*	Imipramine	2328	Antazoline
2285*	Medazepam	2328*	Promethazine
2288	9,10-Anthracene-dicarbonitrile	2330*	Bromhexine
2290	Benzylbutyl phthalate	2330	2'-Chloro-2,5-diaminobenzophenone
2290	Carbamazepine	2330	Cocaethylene
2290	2-Chloroprocaine	2330*	Lorazepam
2290*	Codeine	2330	Phenytoin
2290*	Dihydrocodeine	2330	Tropicamide
2290	1-Hydroxyharman	2335	Chlormezanone
2290	Tetrahydrofurfuryl oleate	2335*	Clomipramine
2291	Harmine	2335*	Diazepam
2292	Diethylaminoethyl diphenylpropionate	2335*	Ethylmorphine
2295*	Bromhexine	2335*	Ethylmorphine
2295*	Bromhexine	2335	Iprindole
2295*	Codeine	2335*	Morphine
2295	Desmorphine	2335	Propoxycaïne
2295*	Dihydrocodeine	2336	Oxazepam
2295*	Imipramine	2336	Probenecid
2298	Stilboestrol	2339	Prothipendyl
2299	Dicophane ( <i>p,p'</i> -isomer)	2340	Acetylprocaine
2300*	2,5-Diaminobenzophenone	2340*	Bromhexine
2300*	Chlordiazepoxide	2340	Dexoadrol
2300	Dimophebumine	2340*	Doxepin
2300	Isoxsuprine	2340*	Hydrocodone
2301	Bufliline	2340*	Hydrocodone
2303	Hyoscine	2340*	Morphine
2305	Methyldesorphine	2340*	Protriptyline
2307	Tris(2,3-dichloropropyl) phosphate	2342*	Cyclazocine
2309	Trimeprazine	2342*	Dimethindene
2310	Bulan	2345	2,5-Diamino-2'-chlorobenzophenone
2310	Chloramphenicol	2345*	Clomipramine
2310	Domiphen	2345*	Diazepam
2310*	Piminodine	2345*	Methoxychlor
2310	Secergan	2345*	Phenazopyridine
2314	Benztropine	2345*	Pyrrobutamine
2314	Buphenine	2346*	Phenazopyridine
2314	Primaquine	2347*	Chloroprocaine
2315	Dihexyverine	2349*	Propantheline bromide
2315	Dihydroergotamine	2350*	Medazepam
2315	Leucinocaine	2352	Gentisic acid
2316	Promazine	2355	Mazindol
2318	Piperidolate	2355*	Methoxychlor
2318	Thenalidine	2355	Oxypertine
2320	Heptabarbital metabolite	2356	Maprotiline
2321	Phenylglutarimide	2356	<i>o</i> -Toluidine
2323	Dioxadrol	2356*	Picrotoxin
2323	Proxymetacaine	2357	Ethopropazine
2325	Etoxidine	2359	Levallorphan

TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
2360*	Bupivacaine	2390*	Morphine
2360	Methaqualone metabolite	2395	Neopine
2360*	Pyrrbutamine	2395	Norpropoxyphene
2362	Butyl stearate	2395*	Thebaine
2363	2-Amino-2'-fluoro-5-nitrobenzophenone	2396	Pyrrloiphene
2363	Dihydrocodeine	2397	Dextrorphan
2363	Triphenyl phosphate	2397	Diphenyl adipate
2363	Tris(butoxyethyl) phosphâte	2397	Diphenyl mercury
2365*	Hydrocodone	2398*	Isoxsuprine
2365*	Hyoscine	2400*	Chlorpromazine
2365	Phenylbutazone	2400*	Chlorprothixene
2366	Cyproheptadine	2400	Methaqualone metabolite
2366	Diethylstilboestrol	2400*	Morphine
2366	Ergotamine	2400*	Phenytoin
2368	Benzydamine	2400*	Thebaine
2370	Diperodon	2402	Hexoestrol
2370	N-Allyl-3-hydroxymorphinan	2402	Lorazepam
2370	Noxythiolin	2402*	6-Monoacetylmorphine
2375	Dextropropoxyphene metabolite	2406	Clomipramine
2375	Pizotifen	2406	Levophenacetyl morphan
2376	Codeine	2407	5-Chloro-2-cyclopropylmethylamino-benzophenone
2377*	Azacyclonol	2410*	Chlorpromazine
2377	Diethazine	2410*	Chlorprothixene
2380*	Bromhexine	2410*	Desmethylmedazepam
2380*	Colchicine	2410	Flunitrazepam decomposition product
2380	Dothiepin	2410	Methaqualone metabolite
2380*	Hydrocodone	2410	Sancticer 141
2380*	Hydrocodone	2411	Ethylmorphine
2380	Methyl dihydro morphine	2415	Azatadine
2380*	Metopon	2415*	Chlorpromazine
2380*	Morphine	2415	Clemastine
2380	Nifuroxime	2415	4-Hydroxyphenobarbitone
2380	Polythiazide	2415*	Oxazepam
2381	Di-(2-ethylhexyl) adipate	2417*	Dihydrocodeine
2381*	Pholcodine	2417	Methoxychlor
2383	Cannabidiol	2419	Pyrrbutamine
2383	Diocetyl adipate	2420	Diloxanide
2383*	Isopropamide	2420	Meclofenamic acid
2384*	Buphenine	2425	Diazepam
2384	Diphenidol	2425*	Oxazepam
2385*	Bromhexine	2425*	Oxycodone
2385	2-Cyclopropylmethylamino-5-chloro-benzophenone	2430	Azinphos-methyl
2385*	Dihydroergotamine	2430	2'-Fluoro-2-methylamino-5-nitro-benzophenone
2388	2-Amino-5-nitrobenzophenone	2430*	Isopropamide
2388	Norcodeine	2430*	Oxazepam
2390	2-Amino-5-chloro-3-hydroxy benzophenone	2430	Tetrachlorvinphos (Z-isomer)
2390*	Hydrocodone	2433	Propanidid
2390*	$\Delta^9$ -Tetrahydrocannabinol	2434	Diampromide
		2434	Proquamezine

(Continued on p. 246)

TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
2438	Normorphine	2480*	2-Amino-5,2'-dichlorobenzophenone
2440	Hydrocodone	2480	Desmethylchlorpromazine
2440*	Methotrimeprazine	2480	Didesmethylchlorpromazine
2442	Glyceryl dibenzoate	2480*	Mefenamic acid
2443	Dibenzepin	2480*	Pyrrbutamine
2443	Diphenoxalate	2480*	Temazepam
2443	Xenysalate	2480	Tetrahydrofurfuryl oleate
2444	Diisooctyl adipate	2484	Dinonyl adipate
2445	Ethynodiol diacetate	2485*	Methocarbamol
2445*	Pecazine	2485	Oxycodone
2445*	Pecazine	2485*	Phenylramidol
2445*	Methotrimeprazine	2486	Chlorpromazine
2445	Trioctyl phosphate	2486*	Phenytoin
2446	Cyclohexylisooctyl phthalate	2487	Chlorprothixene
2450*	Oxycodone	2488	Androsterone
2450*	Theophylline	2488	1-Benzyl-3-ethyl-6,7-dimethoxy- isoquinoline
2451	Dihydromorphine	2488	Norpipanone
2453	Chlordiazepoxide	2490	Butalamine
2453	Isobutylcyclohexyl phthalate	2490*	Colchicine
2454	Morphine	2490*	Diazepam
2455	Acetyldihydrocodeine	2490	Methaqualone metabolite
2455	Ethylisobutrazine	2490	3-Monoacetylmorphine
2457	Butacaine	2491	Dioxaphetyl butyrate
2457	Clorazepate	2495	Cinnamylcocaine
2459	Metopon	2495	Ergocristine
2460*	Phenytoin	2495	Neocinchophen
2461	Dicyclohexyl phthalate	2495	Tubocurarine
2461	Methixene	2496	Desmethyldiazepam
2463	Tri-(2-ethylhexyl) phosphate	2500	Bromazepam metabolite
2464*	Picrotoxin	2500	Diheptyl phthalate
2464	Piperilate	2500*	Hydrastine
2465	Mebhydrolin	2500*	Hydrocodone
2465	Molindone	2500	N-Methyl-2,3-dihydroxymorphinan
2465	Protoveratrine A	2505*	Diamorphine
2465	Protoveratrine B	2505*	Diazepam
2467	Hydromorphone	2505*	Dibenzepin
2467	Methdilazine	2505	Emetine
2470*	Diprophylline	2505*	Ethylmorphine
2470*	Hydroxyzine	2507	Di-(2-ethylhexyl)phthalate
2470	Mirex	2510	Acetylcodeine
2470*	Temazepam	2510	Chlorprothiazide
2470*	Theobromine	2510*	Diamorphine
2471	N1-Desalkylflurazepam	2510*	Diamorphine
2471	Oxybuprocaine	2510*	Diazepam
2472	5-Chloro-2-fluoro-2-hydroxyethylamino- benzophenone	2510*	Morphine
2472*	Norpropoxyphene amide	2511	Diisodecyl phthalate
2473	$\Delta^9$ -Tetrahydrocannabinol	2514	Methotrimeprazine
2474	Dipipanone	2515*	Cyclomethycaine
2475*	2-Amino-5-nitrobenzophenone	2515	Dioctyl phthalate
2475*	Pipethanate	2515*	Lorazepam
2478*	Lorazepam	2515*	Meclozine
2478	Tetraphenylethylene	2515*	Pyrrbutamine

TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
2516	2-Amino-2'-chloro-5-nitrobenzophenone	2578	Ethoxzolamide
2517	Thebaine	2580*	Hydromorphone
2518	Cyclohexyltridecyl phthalate	2580*	Norpropoxyphene amide
2520	Butylbenzyl sebacate	2580*	Thebaine
2520	Cannabinol	2583	Cinchonine
2520	Methaqualone metabolite	2584	5-( <i>p</i> -Methylphenyl)-5-phenyl- hydantoin
2520*	Xylometazoline		
2522	Phenadoxone	2585*	Clemizole
2524	Oxycodone	2585*	Hydromorphone
2524	Pecazine	2588*	Methotrimeprazine
2525	Diisooctyl phthalate	2590	Chloroquine
2525	Methaqualone metabolite	2590*	Clemizole
2525	Oxethazaine	2590	Nifuratel
2525*	Temazepam	2590*	Trifluperidol
2529	Demoxepam	2595*	Temazepam
2530	Apomorphine	2595	Thiazesim
2530	Chlordiazepoxide	2598	Cinchonidine
2530	Loxapine	2610	Fosazepam
2532	Cyclohexylisooctyl phthalate	2612	Oestrone
2532	Oxymorphone	2612	Mestranol
2533	Thebacon	2613*	Buphenine
2535*	Flunitrazepam	2614	Diamorphine
2535	Morpheridine	2615	Deptropine
2535*	Temazepam	2615*	Trifluoperazine
2536	Pyrathiazine	2616	Synhexyl
2537	6-Monoacetylmorphine	2617	Chlorproctazine
2539	Deanol	2617	Phenacaine
2540	Octyldecyl adipate	2620	Testosterone
2542*	Chlorprothixene	2625*	Gallamine
2542	Methoxypropazine	2625	Norethisterone
2545*	Picrotoxin	2625*	Trifluoperazine
2545*	Trifluperidol	2625*	Warfarin
2545*	Trifluperidol	2630	Metoclopramide
2550	Diphenyl phthalate	2630*	Temazepam
2550	Oxyphencylimine	2635	Metofoline
2551	Dextropropoxyphene metabolite	2637	Furethidine
2551	Norethynodrel	2638	Trimethoprim
2553*	Chlorpromazine	2640	Naloxone
2555	3-Hydroxybromazepam	2641	Prazepam
2555	Dimelfine	2643	Methyltestosterone
2555*	Flurazepam	2643*	Nalorphine
2555	Pentaquin	2644*	Cinchonine
2557	Prenylamine	2645*	Clobazam
2558	5-Chloro-2-diethylaminoethylamino- 2'-fluorobenzophenone	2645	Flunitrazepam
		2649	Dinonyl phthalate
2560	Methaqualone metabolite	2650	Fentanyl
2570	Benzoylcegonine	2655*	Clorazepate
2570	Methylnitrazepam	2655*	Trifluperidol
2570	Nordiazepam	2659	Oestradiol
2570*	Trifluperidol	2660*	Chlordiazepoxide
2577	Nalorphine	2660*	Chloroquine

(Continued on p. 248)

TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
2660*	Clobazam	2760*	Hydroxyzine
2660*	Dihydrocodeine	2760*	Hydroxyzine
2660	Laudanosine	2760*	Perazine
2660	Tetrahydrofurfuryl oleate	2762*	Bromazepam
2663	Bromazepam	2763*	Hydroxyamphetamine
2670*	Aconitine	2770*	Papaverine
2670	Phenbutrazate	2770	Pseudomorphine
2672	Methandienone	2774	Captodiamine
2674*	Nitrazepam	2777*	Clobazam
2675	Clemizole	2779	Ethynodiol diacetate
2675*	Temazepam	2779*	Fentanyl
2680	Benzthiazide	2782	Diocetyl sebacate
2680*	Nalorphine	2784	Quinidine
2683	Trifluoperazine	2785	Flurazepam
2684	Phenazocine	2792	Di-(2-ethylhexyl) sebacate
2685*	Chlorpromazine	2793	Progesterone
2685	Indomethacin	2797*	Trifluoperidol
2685	Methiomeprazine	2799	Chlordiazepoxide
2686	Broxaldine	2800	Ethoxyquin
2688	N1-Hydroxyethylflurazepam	2800	Propionylpromazine
2690	Dibenzyl phthalate	2803	Quinine
2690*	Nitrazepam	2807	Hexachlorophane
2692*	Diamorphine	2810*	Haloperidol
2694	Accpromazine	2810	Hydroquinidine
2695	Benzethidine	2815*	Hordenine
2695	Laudanine	2815*	Norclobazam
2695*	Norclobazam	2820	Bisacodyl
2695	Tricresyl phosphate	2820	Chromonar
2700	Di(butoxyethyl) sebacate	2825	7-Aminonorfunitrazepam
2700	Griseofulvin	2825	Papaverine
2701	Cinchocaine	2828	7-Aminonitrazepam
2703	5-Amino-2'-fluoro-2-methylamino-benzophenone	2830	Fenethylamine
2705	Ajmaline	2830*	Nitrazepam
2705	Azaperone	2832*	Sulpiride
2710*	Prazepam	2835*	Haloperidol
2715*	Prazepam	2835	Oxymetholone
2719	Ethinylestradiol	2845*	Theobromine
2720*	Fentanyl	2849	Hydroxyzine
2723	7-Aminoflunitrazepam	2850*	Acepromazine
2725	Oxomemazine	2850	Anileridine
2730	Di(2-ethylhexyl) isophthalate	2850	Clonazepam metabolite
2730	Phenazone metabolite	2850	Di(butoxyethyl) phthalate
2738	Propiomazine	2850	Gelsemine
2740	Norfunitrazepam	2852	5- $\alpha$ -Cholestane
2745	BBOT	2858*	Flurazepam
2745	Diisodecyl adipate	2860	3-Hydroxyprazepam
2745	Octyldecyl adipate	2872	Hydroxychloroquine
2750	Calusterone	2872	Ibogaine
2750*	Hydroxyzine	2872	Phenoperidine
2750	Nitrazepam	2880	Dapsone
2760*	Clorazepate	2880	Sanguinarine
2760*	Hydroxyzine	2885	Clonazepam
		2885*	Desmethylchlordiazepoxide

TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
2885*	Piminodine	3086	Cholesterol
2890	7-Amino-3-hydroxyclonazepam	3089	Methysergide
2893*	Chlordiazepoxide	3100	Desmethylchlordiazepoxide
2895	Dioxyline	3103	Isooctylhydrocupreine
2900	7-Aminoclonazepam	3105	Clonazepam metabolite
2900*	Papaverine	3107	Triamcinolone
2905	Di( <i>n</i> -decyl) adipate	3114	Thioridazine
2905*	Haloperidol	3115	7-Acetamidoflunitrazepam
2906	Doxapram	3119	Strychnine
2913*	Nitrazepam	3120	Noscapine
2915*	Clozapine	3120*	Prochlorperazine
2925*	Prajmalium bitartrate	3149*	Haloperidol
2930	Clomiphene	3170*	Pholcodine
2930*	Desmethylchlordiazepoxide	3175	Etodroxizine
2930*	Perazine	3176*	Thioridazine
2930	Racemoramide	3180*	Thioridazine
2934	Diphenadione	3193	Sitosterol
2940	Dextromoramide	3202	Levophenacetylmorphan
2940	Octyldecyl adipate	3205	7-Acetamidonitrazepam
2949*	Piminodine	3230*	Pericyazine
2954	Prochlorperazine	3234	Stigmasterol
2965*	Clonazepam	3240*	Noscapine
2965*	Haloperidol	3242	Rotenone
2970	Dexamethasone	3247	Thiethylperazine
2970	Oestriol	3260	Pipamazine
2970	Triamcinolone	3263	7-Acetamidoclonazepam
2972*	Cyclomethycaine	3269	Yohimbine
2975*	Benperidol	3280	Brucine
2980*	Haloperidol	3280	Spirocholactone
2980*	Hydroxyzine	3280*	Strychnine
2980	Levomoramide	3286	Buclizine
2980	Miconazole	3287	Phytomenadione
2988	Hydrastine	3287*	Trimethobenzamide
3005*	Pholcodine	3327	Nicodicodine
3008*	Cholesterol	3340*	Colchicine
3011*	Clozapine	3340*	Pericyazine
3014*	Doxapram	3342	Butyl PBD
3015	Benzylmorphine	3365*	Buclizine
3020*	Cholesterol	3380	Penfluridol
3020*	Haloperidol	3408	Nicocodine
3020*	Strychnine	3430*	Droperidol
3030*	Pholcodine	3445	Lysergide
3033	Meclozine	3465	Thiopropazate
3040*	Strychnine	3466*	Colchicine
3059	Famprofazone	3525	POPOP
3060*	Strychnine	3560*	Brucine
3060	Thiothixene	3590	Carphenazine
3065	Cinnarizine	3618	Dimethyl POPOP
3065	Fluphenazine	3710	BBO
3070	Pipamperone	3750	BBOT
3078	Dimethothiazine	9999	Acetophenazine

(Continued on p. 250)

TABLE 3 (continued)

<i>RI</i>	<i>Compound name</i>	<i>RI</i>	<i>Compound name</i>
9999*	Aconitine	9999	Methalibure
9999	Amidephrine	9999	Methylclothiazide
9999	Aminonitrothiazole	9999	Methylergometrine
9999	Aminotriazole	9999	Morantel
9999	Amodiaquine	9999*	Nialamide
9999	Amotriphene	9999	Nicergoline
9999	Benzonate	9999	Nifursol
9999	Brocresine	9999	Obidoxime bromide
9999	Bunamidine	9999	Orciprenaline
9999	Chloral hydrate	9999	Oxyclozanide
9999*	Chlorothiazide	9999*	Oxyphenbutazone
9999	Cinchophen	9999*	Paramethadione
9999	Clixanide	9999	Parbendazole
9999	Clofazimine	9999	Pentapiperide
9999	Coniine	9999	Phentolamine
9999	Debrisoquine	9999*	Phenylephrine
9999	Decoquinat	9999	Phthivazid
9999	Diazoxide	9999	Picloxydine
9999*	Droperidol	9999	Pimozide
9999	Ecgonine	9999	Piperacetazine
9999	Ethacrynic acid	9999	Practolol
9999	Ethoxazene	9999*	Prajmalium bitartrate
9999*	Etilefrine	9999	Propylidone
9999	Flavoxate	9999	Pyrantel
9999	Flupenthixol	9999	Rafoxanide
9999*	Galamine	9999	Reserpine
9999	Gitalin	9999	Resorantel
9999	Guanethidine	9999	Ritodrine
9999	Hexobendine	9999	Rolicypram
9999	Hydrochlorothiazide	9999	Succinylcholine chloride
9999*	Ibogaine	9999	Sulphaguanidine
9999	Imidocarb	9999	Sulphamoxole
9999	Isometamidium	9999	Sulphathiazole
9999	Lidoflazine	9999	Symazine
9999	Mafenide	9999	Taurolin
9999	Mebeverine	9999	Thiopropazine
9999	Mesoridazine	9999*	Trimethobenzamide
9999	Metaraminol	9999	Urea
9999	Metformin		

cending order of retention index. The entries include not only the mean retention index, but also each of the values which were greater than  $\pm 50$  retention index units from the mean, these being indicated by an asterisk. Table 3 can therefore be used to obtain a tentative identification of an unknown compound before referring to Table 1 for more complete data.

The data in Table 3, excluding the 9999 entries, have been used to generate the histogram in Fig. 1. Thus, Fig. 1 may help in determining the usefulness of the retention index measurement for an unknown compound for identification purposes, e.g. a value of around 2200 is much less useful than one of around 3500.



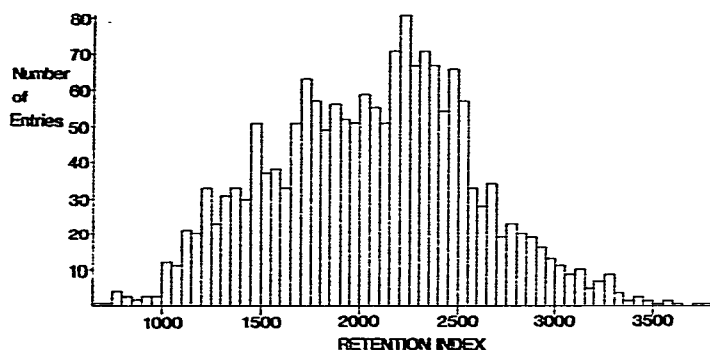


Fig. 1. Histogram of 1742 retention index values associated with 1318 compounds.

#### 4. CONCLUSIONS

It is hoped that this compilation will enable those involved with the analysis of drugs to identify more easily unknown compounds when using SE-30 or OV-1 stationary phases. Table 1 may be used to obtain the retention index of a compound together with an estimate of its reproducibility and Table 3 can be used with Fig. 1 to help identify an unknown compound. The retention indices quoted in this work may be easily converted to retention times or relative retention times, if they are considered more appropriate to particular needs, by the use of appropriate calibration graphs. Analysts' collections of retention parameters may therefore be supplemented and checked for unusual results regardless of the retention parameter used.

#### 5. ACKNOWLEDGEMENTS

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#### 6. SUMMARY

Retention indices associated with 1318 substances likely to be encountered in toxicological analyses are presented. They are listed in ascending order of retention index for identification purposes and also in alphabetical order of compound name. The 4586 values used in this collection have been extracted from 36 sources, many of which have not been previously published. In many cases, where the quoted retention index is the mean of several determinations, the reproducibility and reliability of this value may be assessed.

A histogram of the 1742 values listed is provided to help in determining the usefulness of a retention index for identification purposes.

The reproducibility of inter-laboratory retention index measurements for twenty compounds on both SE-30 and OV-17 are presented and show the former, on average, to give more reproducible results.

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