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USE OF SE-30 AS A STATIONARY PHASE FOR THE GAS–LIQUID CHROMATOGRAPHY OF DRUGS

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CONTENTS

1. INTRODUCTION

Gas–liquid chromatography (GLC) has for many years been chosen by numerous analysts as the method of choice for screening extracts of biological materials for the presence of drugs. The technique is reliable, highly selective and very sensitive, allowing qualitative analyses to be performed on submicrogram amounts of drugs. A large number of stationary phases have been advocated for use and over 300 different phases have been reported[1]. This makes the analyst's task very difficult when faced with a large amount of retention data in the literature — some in retention times, some in relative retention times to a number of different drugs and some in retention indices, all on numerous stationary phases. What is required is the standardisation not only on one or two stationary phases, but also on the retention parameters to be measured. When this is achieved, a comprehensive collection of retention data can be compiled which can be continuously and easily updated.

Fortunately, a large step forward has already been taken by the suggestion that a list of "preferred stationary phases" be designated and that all work should be carried out using them[1–4]. A previous study in this laboratory[5] compared eight different stationary phases and found that a low polarity phase, such as SE-30 or OV-17, is the "preferred liquid phase" for the identification of basic drugs. Of all the low-polarity phases in common use SE-30 is undoubtably the best choice since it was one of the first phases to be used[6], is probably the most extensively used for the analysis of drugs and is the stationary phase for which most data have been reported[7–11]. Chemically, SE-30 is a dimethyl silicone elastomer, with a useful temperature range of 80–300° and is often sold as the proprietary E-301 or OV-1 gum rubbers, the liquid silicone OV-101 being very similar.

The monographs concerning the GLC analysis of drugs[12,13], as well as the published collections of drug retention data using SE-30 (refs. 14–16), quote data as

retention times or relative retention times to a number of drugs. In the author's opinion retention indices provide the most reproducible GLC retention parameters for drug identification and this study has therefore been carried out using retention indices. The intention of this work was to convert literature retention data using SE-30 as the stationary phase for drugs and other commonly occurring chemicals such as plasticisers into retention indices and to compile these as a list for use in identification procedures for drugs. Naturally, variations between laboratories will occur with measurements of retention indices due to differences in chromatographic conditions such as temperature, sample size and column loading and the inter-laboratory variations of measurements of retention indices for drugs under normal operational conditions have been determined.

2. EXPERIMENTAL

Three drugs (amphetamine, diphenhydramine and dipipanone) were sent as aqueous solutions (1 mg/ml) to eleven laboratories. Each laboratory was asked to extract the drugs, chromatograph them on the normal SE-30 column used in their laboratory (Table 1) and report the results as retention indices for the three drugs.

Published data were used to accumulate a library of retention indices for drugs on SE-30 columns. Where collections of data were in retention times or relative retention times, the retention indices were calculated after calibration curves of retention times plotted against known retention indices had been constructed. For those commonly used drugs not included in the literature, or where two literature values for a drug differed by more than 50 retention index units, the retention indices were measured in this study using the conditions for laboratory 2 (Table 1).

3. RESULTS AND DISCUSSION

The individual retention indices obtained by each laboratory for each of the

TABLE 1

SE-30 GLC SYSTEMS USED

Mean temperatures used: amphetamine, 100°; diphenhydramine, 200°; dipipanone, 230°.

Laboratory	*Column*						
	Material	*Length (m)*	*I.D. (mm)*	*Phase*	*Support*	*Carrier*	*Flow-rate (ml/min)*
1	—	—	—	OV-1	—	—	—
2	Glass	2	4	2% SE-30	Chromosorb G	N_2	60
3	Glass	2	3	2.5% SE-30	Chromosorb G	N_2	44
4	Glass	2	4	2.5% SE-30	Chromosorb W	N_2	40
5	Glass	1.5	2	2.5% SE-30	Chromosorb G	N_2	60
6	Glass	2	4	2% SE-30	Chromosorb G	N_2	60
7	Glass	1.5	4	2.5% E-301	Chromosorb G	Ar	75
8	Glass	1.5	3	2.5% SE-30	Celite	N_2	60
9	Glass	1.5	4	2.5% SE-30	Diatomite CQ	N_2	50 and 25
10	Glass	2	3	3% E-301	Chromosorb W	N_2	18
11	Glass	1.5	4	2.5% SE-30	HP Chromosorb W	N_2	40

TABLE 2

SE-30 RETENTION INDICES

Laboratory	*Amphetamine*	*Diphenhydramine*	*Dipipanone*
1	1110	1855	
2			2467
3	1135	1880	2500
4	1170	1870	2480
5	1165	1895	2515
6	1148	1864	2496
7	1140	1870	2492
8	1168	1897	2492
9	1153	1897	2477
10	1170	1892	2502
11	1140	1850	2507
Mean	1150	1877	2492
Standard deviation	19.4	17.8	14.6
Coefficient of variation	1.7	0.95	0.58

drugs on the SE-30 columns, together with the respective means, standard deviations and coefficients of variation are given in Table 2. All the columns were made of glass and contained packing material of 2–3% SE-30 (Table 1). The support appeared to make little difference to the results, although there was a tendency to use Chromosorb G, acid washed, dimethyldichlorosilane treated, 80–100 mesh. The standard deviation decreased as the retention index increased, which supports earlier findings that SE-30 acts more satisfactorily and reproducibly at higher temperatures[5]. Each analyst can form his own decision as to the likely deviation of his results on his

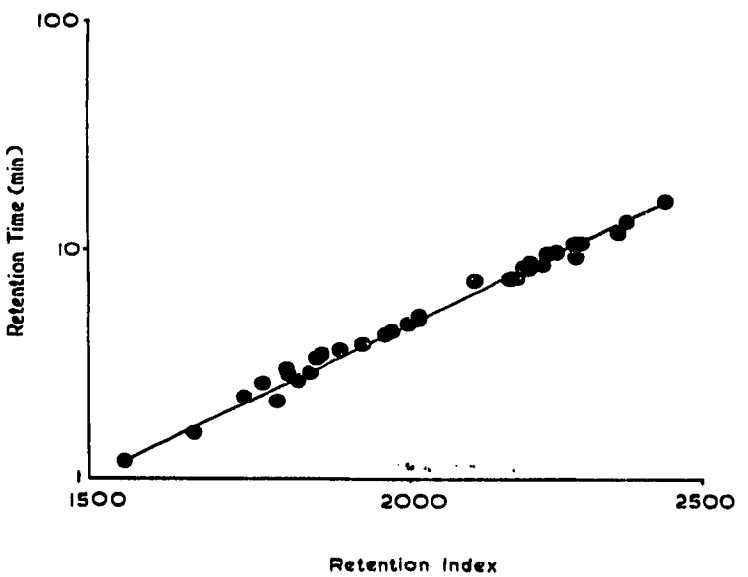

Fig. 1. Calibration graph of experimentally determined retention indices for a number of drugs against the retention time data of Beckett and Moffat[8] using SE-30 as the stationary phase.

TABLE 3

RETENTION INDICES OF 480 COMPOUNDS USING SE-30 AS THE STATIONARY PHASE, ARRANGED IN ALPHABETICAL ORDER OF DRUG NAME

Neg. = No peak between 1000 and 3500.

Drug	*Retention index*	*Reference*	
		Source	*Check*
Acenocoumarin	1900	10	
Acepromazine	2665	8, 10, 15	
Acetanilide	1365	10	
Acetophenazine	Neg.	This study	10
Acetyldihydrocodeinone	2450	15	
Acetylsalicylic acid	1295	10, 19	
Aconitine	2280	19	
Adiphenine	2190	19	10
Aldrin	1950	19	
Aletamine	1280	7, 10	
Allobarbitone	1600	10	15
Allylbarbituric acid	1670	10	15
Alphacetylmethadol	2160	15	
Alphameprodine	1840	15	
Alphamethadol	2150	15	
Alphaprodine	1895	10, 15	
Ametazole	1390	This study	
Amethocaine	2215	19	10, 15
Amidopyrine	1890	19	8, 10
p-Aminosalicylic acid	1330	10	
Amisometradine	2025	10	
Amitryptyline	2200	19	8, 10, 15
Amolanone	2210	10, 15	
Amphetamine	1110	19	7, 10
Amprotropine	2010	15	
Ampyrone	1950	19	
iso-Amylamine, *see* Isoamylamine			
Amylobarbitone	1725	19	10, 15
Amylocaine	1635	8, 10	
Anileridine	2845	19	10, 15
Aniline	1150	10	
Anisaldehyde	1230	10	
Anisinidione	2285	10	
Antazoline	2330	19	8, 10, 15
Anthracene	1790	10	
Apoatropine	2025	15	
Aprobarbitone	1620	10	15
Atropine	2175	19	10, 15
Azacyclonol	2210	19	10, 15
Azapetine	1925	15	
Barbitone	1495	19	10, 15
Bemegride	1390	10	
Benactyzine	2230	19	10
Benzethidine	2680	15	
Benzhexol	2230	19	10, 15
Benzocaine	1530	This study	8, 10
Benzphetamine	1850	7, 10	

TABLE 3 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Benztropine	2320	10, 15	
Betameprodine	1830	15	
Betaprodine	1790	15	
Biperiden	2280	15	
Bromodiphenhydramine	2150	19	10, 15
Bromopheniramine	2070	10, 15	
Brucine	3280	19	
Buclizine	3285	19	10
Bufotenine	2000	15	
Buphenine	2320	This study	15
	1270*	This study	
Bupivacaine	2270	8	15
Butabarbitone	1655	10	
Butacaine	2470	5	10
Butallylonal	2025	10	
Butanilicaine	2010	15	
Butethamate	1740	15	
Butethamine	2050	This study	10, 15
Butobarbitone	1660	10	15
Butriptyline	2155	15	
Butylphthalate	1880	10	
n-Butyric acid	1330	10	
Caffeine	1810	19	8, 10, 15
Camphor	1130	10	
Cantharidin	1490	19	
Capric acid	1485	10	
n-Caproic acid	1410	10	
Captodiame	2775	19	10, 15
Caramiphen	1950	15	
Carbamazepine	2290	15	
Carbaryl	1490	19	
Carbetapentane	2240	This study	10
Carbimazole	1670	15	
Carbinoxamine	2050	5	10, 15
Carbromal	1500	19	
Carisoprodol	1850	19	10
Carminic acid	1690	10	
Carphenazine	3590	19	
Chlophedianol	2070	15	
Chlorbenside	2050	19	
Chlorcyclizine	2215	19	8, 10, 15
Chlordane	2020	19	
Chlordiazepoxide	2790	This study	19
	2500*	This study	10, 15
	2460*	This study	
	2300*	This study	15
Chlormethiazole	1230	20	
Chlormezanone	2250	10	
Chloroprocaine	2200	10, 15	

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TABLE 3 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Chloropyrilene	2130	This study	10
Chloroquine	2575	19	8, 15
Chlorothymol	1510	10	
Chlorphenesin carbamate	1690	10	
Chlorpheniramine	2000	19	8, 10, 15
Chlorphenoxamine	2040	10, 15	
Chlorphentermine	1320	19	7, 10, 15
Chlorpromazine	2440	19	8, 10, 15
Chlorpropamide	1740	10	15
Chlorprothixene	2510	10	
Chlorzoxazone	1710	10, 15	
Cholesterol	3015	10	
Cinchocaine	2690	19	10, 15
Cinchonidine	2625	19	8, 15
Cinchonine	2575	19	8, 10, 15
Clemizole	2680	5	10, 15
Clofibrate	1560	10	
Cocaine	2180	19	8, 10
Codeine	2385	19	8, 10, 15
Cotarnine	1780	19	
Cotinine	1670	8	
Cyclandelate	1900	10	
Cyclizine	2010	19	8, 10, 15
Cyclobarbitone	1950	10	15
Cyclomethycaine	2225	10	
Cyclopentamine	1080	This study	7, 10
Cyclopentolate	2010	15	
Cypenamine	1345	7	
Cyproheptadine	2355	10, 15	
Dapsone	2860	19	10
Deptropine	2590	15	
Desipramine	2260	This study	10, 15
Desmethylchlorpromazine	2480	8	
Desomorphine	2275	15	
Dexamethasone	2950	10	
Dexoxadrol	2340	8	
Dextromethorphan	2115	8, 15	
Dextropropoxyphene	2180	19	8, 10, 15
Diamorphine	2615	19	8, 10, 15
Diazepam	2410	5	10, 15
Diazinon	1760	10	
Dibenzepin	2480	10	
Dicophane	2290	19	10, 15
Dicylomine	2100	This study	10
Didesmethylchlorpromazine	2480	8	
Dieldrin	2110	19	15
Diethazine	2280	15	
Diethylpropion	1480	19	7, 10
Diethylthiambutene	2000	15	
Diethyltryptamine	1900	10	
Dihydrocodeine	2365	8	10, 15

TABLE 3 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Dihydrocodeinone	2425	10	
Dihydroergotamine	2310	19	
Dihydromorphine	2440	15	
Dimenhydrinate	1840	10	
Dimethindene	2270	10, 15, 19	
Dimethoxanate	2030	This study	
3,4-Dimethoxyphenethylamine	1540	19	
Dimethrin	1210	19	
N,N-Dimethylamphetamine	1230	7	
N,N-Dimethylphenethylamine	1150	10	
Dimethylthiambutene	1870	15	
Dimethyltryptamine	1750	10, 15	
4,6-Dinitro-*o*-cresol	1620	10	
2,4-Dinitrophenol	1510	10	
Diphenadione	2910	10	
Diphenhydramine	1855	19	8, 10
Diphenylpyraline	2090	This study	10, 15
Dipipanone	2470	5	8, 15
Dopamine	2150	15	
Doxapram	2875	15	
Doxylamine	1925	10, 15	
Dyclonine	1640	10	
Ectylurea	1360	19	10
Embramine	2150	15	
Emcyclamate	1090	10	
Ephedrine	1350	19	7, 10, 15
Ergocristine	2500	10	
Ergocryptine	2180	10	
Ergotamine	2360	10	
Etafedrine	1460	7, 15	
Ethchlorvynol	1030	19	
Ethinamate	1360	19	10
Ethinyloestradiol	2710	10	
Ethoheptazine	1845	19	8, 10, 15
Ethomoxane	1975	15	
Ethopropazine	2350	This study	10, 15
Ethotoin	1800	10	
Ethoxyquin	2800	19	
Ethoxzolamide	2550	10	
N-Ethylamphetamine	1210	19	7, 10
N-Ethylbenzylamine	1010	10	
Ethylisobutrazine	2455	8	
Ethylmorphine	2415	19	10, 15
Ethylmethylthiambutene	1925	15	
Etoxeridine	2310	15	
Etryptamine	1850	8	
Eucatropine	2000	15	
Fenfluramine	1220	7, 10	
Fenmetramide	1765	8	

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TABLE 3 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Fentanyl	2700	15	
Fluopromazine	2175	15	
Fluphenazine	3045	19	
Gallamine	2700	15	
Gentisic acid	2350	10	
Glutethimide	1825	19	8, 10, 15
Guanethidine	Neg.	This study	
Haloperidol	2940	10	
Harmine	2280	This study	10
Heptabarbitone	2100	10	
Hexachlorophane	2795	10, 15	
Hexamine	1210	10	
Hexobarbitone	1850	10	
Hexoestrol	2400	10	
Hexylcaine	1950	15	
Hippuric acid	1730	10	
Histamine	1500	10	
Homatropine	2045	19	10, 15
Hydrallazine	1530	10	
Hydrastine	2975	19	10
Hydrastinine	1590	19	
Hydrocodone	2425	15	
Hydromorphone	2490	10	
Hydroxyamylobarbitone	1930	15	
Hydroxychloroquine	2860	19	10
Hydroxypethidine	2025	15	
Hydroxyphenamate	1740	19	10, 15
p-Hydroxyphenylpyruvic acid	1380	10	
Hydroxyquinidine	2780	15	
Hydroxyzine	2840	19	10, 15
Hyoscine	2285	19	10, 15
Hyoscyamine	2225	19	10
Imipramine	2220	19	8, 10, 15
Indomethacin	2690	10	
Iproniazid	1580	This study	10
Isoamylamine	1025	10	
Isocarboxazid	1960	19	10
Isomethadone	2125	8	
Isomethepten	1050	7, 10	
Isoniazid	1630	19	10
Isoprenaline	1720	10	
Isopropamide	2060	10	
Isopropylhexedrine	1140	7	
Isoquinoline	1440	10	
Isothipendyl	2260	This study	8, 10, 15
Ketamine	1830	10, 15	
Ketobemidone	2010	15	
Lachesine	1860	15	
Lauric acid	1600	10	

TABLE 3 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Leptazol	1535	This study	7, 10
Levallorphan	2340	5	10, 15
Levomethorphan	2230	15	
Levorphanol	2225	10, 15	
Lignocaine	1860	19	8, 10, 15
Lindane	1740	10	
cis-Linoleic acid	1330	10	
Linolenic acid	2175	10	
Lobeline	1780	19	
Lysergide	3445	19	
Malathion	1900	10	
Mandelic acid	1500	10	
MDA (Methylenedioxyamphetamine)	1470	19	10
Mebhydrolin	2450	15	
Mebutamate	1865	19	10
Meclofenoxate	1740	15	
Meclozine	3050	19	10, 15
Mefenamic acid	2185	10, 15	
Mephenesin	1550	10	
Mephenesin carbamate	1570	10	
Mephenoxalone	2120	19	10
Mephentermine	1240	19	7, 10
Mepivacaine	2075	This study	10, 15
Meprobamate	1790	19	8, 10, 15
Mepyramine	2205	5	8, 10, 15
Mescaline	1690	19	10, 15
Metabutoxycaine	2225	10	
Metaxalone	2180	10	
Methadone	2170	19	8, 10, 15
Methadone (cyclic metabolite)	2030	8	
Methaphenilene	1980	10	
Methapyrilene	1970	19	8, 15
Methaqualone	2180	10, 15	8
Metharbitone	1470	10	15
Methdilazine	2470	8, 10, 15	
Methimazole	1550	15	
Methixene	2490	10	
Methocarbamol	1510	10	
Methohexitone	1760	10	
Methoin	1795	19	10
Methotrimeprazine	2515	This study	8, 10, 15
Methoxamine	1720	10, 15	
Methoxychlor	2410	19	10
Methoxyphenamine	1360	7, 10	
Methoxypromazine	2500	19	10
Methsuximide	1595	19	
Methylaminomethylheptane	1000	7	
Methylamphetamine	1170	19	7, 10
Methyldesorphine	2290	15	

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TABLE 3 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Methyldihydromorphine	2375	15	
Methyldimethoxyamphetamine, *see* STP			
Methylenedioxyamphetamine, *see* MDA			
Methylephedrine	1400	7, 10	
Methylphenidate	1780	19	7, 10
Methylphenobarbitone	1920	19	15
Methylsalicylate	1200	10	
Methyltestosterone	2610	15	
Methyprylone	1505	19	10, 15
Methysergide	3050	10	
Metopon	2375	15	
Metronidazole	1590	10, 15	
Modaline	1420	7	
6-Monoacetylmorphine	2480	15	
Morpheridine	2500	15	
Morphine	2435	19	8, 10, 15
Myristic acid	1740	10	
Nalorphine	2570	19	10, 15
Naphazoline	2090	This study	10
Nialamide	1500*	This study	
Nicotinamide	1460	10	
Nicotine	1340	19	7, 10
Nicotinyl alcohol	1150	10, this study	
Nicoumalone	1770	10	
Nifenazone	1600	15	
Nikethamide	1500	19	7, 10
Nitrazepam	2675	5	15
p-Nitromethylamphetamine	1655	10	
Norethynodrel	2520	10	
Norfenfluramine	1130	7	
Normethadone	2080	8	
Norpethidine	1745	19	8
Norpseudoephedrine	1310	7	
Nortriptyline	2215	5	10, 15
Noscapine	3100	10	
Nystatin	1960	10	
Orphenadrine	1925	5	8, 10, 15
Oxazepam	2335	10	15
Oxycodone	2425	15	
Oxymetazoline	2170	10, 15	
Oxymorphone	2520	10, 15	
Oxypertine	2125	15	
Oxyphencyclimine	2540	10	
Pachycarpine	1765	19	
Palmitic acid	1975	10	
Papaverine	2805	5	10, 15
Paracetamol	1710	19	10
Parathion	1925	10	
Pargyline	1200	19	7, 10

TABLE 3 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Pecazine	2550	19	10, 15
Pentachlorophenol	1740	This study	10
Pentaquin	2540	15	
Pentazocine	2265	19	8, 10, 15
Pentobarbitone	1750	19	10, 15
Perphenazine	2200	19	
Pethidine	1740	19	8, 10, 15
Phenacaine	2615	10	
Phenacetin	1660	19	8, 10, 15
Phenadoxone	2510	8, 15	
Phenanthrene	1780	10	
Phenazocine	2670	8, 10	
Phenazone	1830	19	10
Phenazopyridine	2345	10	
Phencyclidine	1870	19	10, 15
Phendimetrazine	1440	19	7, 10, 15
Phenelzine	1340	This study	10
α-Phenethylamine	1010	19	10
β-Phenethylamine	1120	19	10
Pheneturide	1450	15	
Phenindamine	2160	This study	8, 10, 15
Pheniprazine	1410	10	
Pheniramine	1805	5	8, 15
Phenmetrazine	1430	19	7, 10
Phenobarbitone	1950	19	10, 15
Phenothiazine	2010	10, 15	
Phenoxybenzamine	2230	10, 15	
Phenoxypropazine	1465	7	
Phenprobamate	1520	15	
Phensuximide	1640	10	
Phentermine	1130	19	7, 10
Phenylbutazone	2370	10, 15	
Phenylpropanolamine	1310	19	7, 10
Phenylsalicylate	1740	10	
Phenyltoloxamine	1925	10, 15	
Phenyramidol	2000	This study	10
Phenytoin	2335	15, 19	
Pholcodine	2380	10	
Physostigmine	1810	19	10
Picrotoxin	2205	19	
Pilocarpine	2010	10	15
Pipamazine	3260	This study	
Pipazethate	2010	15	
Piperidolate	2325	This study	10, 15
Piperocaine	1955	This study	10
Piperoxan	1830	15	
Pipethanate	2470	10	
Pipobroman	2200	10	
Pipradrol	2150	19	8, 10, 15

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TABLE 3 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Pramoxine	2305	This study	10, 15
Prenylamine	2540	15	
Prilocaine	1845	8, 10	
Primaquine	2320	This study	10
Primidone	2250	19	8, 10, 15
Probarbital	1550	19	10, 15
Probenecid	2320	This study	10
Procainamide	2230	10, 15	
Procaine	1995	19	8, 10, 15
Procarbazine	1990	10	
Prochlorperazine	2935	10	
Procyclidine	2115	This study	10, 15
Progesterone	2785	10	
Promazine	2295	19	8, 10, 15
Promethazine	2260	19	8, 10, 15
Propantheline	2350	10	
Properidine	1740	15	
Propiomazine	2725	This study	15
Propoxycaine	2320	15	
Propranolol	2145	10, 15	
N-Propylamphetamine	1330	19	
Propylhexedrine	1170	19	7, 10
5-Propyl-5-isobutylbarbituric acid	1690	10	
Prothipendyl	2330	This study	10, 15
Protokylol	1500	10	
Protriptyline	2230	15	
Pseudoephedrine	1350	7	
Pyrathiazine	2520	8, 10	
Pyridoxamine	2000	19	
Pyrimethamine	2140	19	10
Pyrrobutamine	2430	19	8, 10, 15
Quinalbarbitone	1775	19	10, 15
Quinidine	2760	19	10, 15
Quinine	2755	19	10, 15
Quinoline	1440	10	
iso-Quinoline, see Isoquinoline			
Quinuronium	2100	15	
Resorcinol	1610	10	
Rotenone	3250	10	
Salicylamide	1460	19	10
Salicylic acid	1330	19	10
Sanguinarine	2880	19	
Santonin	2160	10, 15	
Secbutobarbitone	1780	19	
Sparteine	1770	10, 15	
Stearic acid	2175	10	
Stilboestrol	2300	This study	10, 15
STP (Methyldimethoxyamphetamine)	1620	19	10
Strychnine	3040	19	10, 15

TABLE 3 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Styramate	1670	10	
Sulphonal	1475	15	
Tacrine	2140	15	
Talbutal	1700	10	15
Tetrahydrocannabinol	2455	19	
Tetrahydrozoline	1960	8	
Thebacon	2500	15	
Thebaine	2525	19	10
Thenyldiamine	2010	This study	10
Theobromine	1840	10	
Theophylline	1485	10	
Thiabendazole	2010	10	
Thiamylal	1890	19	10
Thiantoin	2145	19	
Thiethylperazine	3260	10	
Thiopentone	1850	19	10
Thiopropazate	3450	This study	
Thioridazine	3110	19	10
Thiosalicylic acid	1500	10	
Thiothixene	3015	10	
Thonzylamine	2200	This study	10, 15
Thymol	1270	10	
Thymoxamine	1830	15	
Tolazamide	1650	10	
Tolazoline	1550	15	
Tolbutamide	1690	10	
Tranylcypromine	1210	19	7, 10
Triamcinolone	3070	10	
Trifluoperazine	2680	This study	8, 10, 15
Triflupromazine	2210	19	8, 10
Trimeperidine	1830	15	
Trimeprazine	2320	This study	8, 10, 15
Trimethoprim	2610	15	
Trimipramine	2200	15	
Tripelennamine	1960	19	8, 10, 15
Triprolidine	2250	19	8, 10, 15
Tropine	1200	10	
Troxidone	1100	19	
Tryptamine	1740	8, 10, 15, 19	
Tybamate	1700	10	
Tymazoline	1850	8	
Vinbarbitone	1750	10	15
Warfarin	1460	19	10, 15
Xenysalate	2440	15	
Xylometazoline	1920	10, 15	

(Continued on p. 82)

TABLE 3 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Yohimbine	3290	19	10
Zoxazolamine	1625	10	

* Major decomposition product.

column from those in Tables 3 and 4 by consideration of the standard deviations in Table 2 and this is discussed later.

Retention indices for 171 drugs were available from previously published data (Moffat *et al.*[5] and Kazyak and Permisohn[9]) and the retention indices for a further 43 drugs were measured for this study. The data for these 214 drugs were used to calibrate other published data (Beckett *et al.*[7], Beckett and Moffat[8], Finkle *et al.*[10] and Clarke[15]) to convert their retention times and relative retention times to retention indices. Fig. 1 shows such a calibration graph and all values were within ± 50 retention index units from the regression line. Tables 3 and 4 give the retention indices of 480 drugs and chemicals using SE-30 as the stationary phase arranged in alphabetical order of drug name and ascending order of retention index, respectively. No attempt has been made to separate particular chemical groups, so that the tables contain acidic, neutral and basic drugs as well as steroids, insecticides, plasticisers and other commonly encountered chemicals. They are named according to Martindale[17], or the Merck Index[18] if they are not included in the former's work. Some entries are for the parent drugs although the peaks actually observed were thermal decomposition products. These are indicated where known, but care must be exercised when using a linked GC–MS system because the peak observed may not be for the parent drug. For example, quinuronium is a quaternary ammonium compound and would not be expected to be eluted from a GC column although it gives a peak of retention index 2100.

The source of each retention index is included in the tables. In some cases the mean values obtained from several sources have been used. Often a check on the value finally included was made from another source and the results had to agree to within ± 50 retention index units. Where values obtained from different sources varied by more than ± 50 retention index units, the value finally used was determined experimentally. Only 9 out of 480 values needed to be re-determined.

Table 3 can be used to find the retention index of a drug, or if the drug is not in the table its probable retention index can be obtained by using the correlation graph of molecular weight *vs.* retention index (Fig. 2). Compounds with many polar functional groups will deviate to the largest extent from the regression line.

The reproducibility of retention indices will change with the temperature of the column (Table 2) and also with the nature of the drug being chromatographed. Those drugs containing alkyl, aryl, alkoxy, amide or tertiary amino groups will give nearly symmetrical peaks and the retention indices will be very reproducible. On the other hand, primary amino, alcoholic and especially phenolic groups will cause tailing peaks in the chromatogram. In these cases, and also where tailing peaks are obtained

TABLE 4

RETENTION INDICES OF 480 COMPOUNDS USING SE-30 AS THE STATIONARY PHASE, ARRANGED IN ASCENDING ORDER OF RETENTION INDEX

Neg. = No peak between 1000 and 3500.

Drug	*Retention index*	*Reference*	
		Source	*Check*
Acetophenazine	Neg.	This study	10
Guanethidine	Neg.	This study	
Methylaminomethylheptane	1000	7	
N-Ethylbenzylamine	1010	10	
α-Phenethylamine	1010	19	10
Isoamylamine	1025	10	
Ethchlorvynol	1030	19	
Isomethepten	1050	7, 10	
Cyclopentamine	1080	This study	7, 10
Emcylamate	1090	10	
Troxidone	1100	19	
Amphetamine	1110	19	7, 10
β-Phenethylamine	1120	19	10
Camphor	1130	10	
Norfenfluramine	1130	7	
Phentermine	1130	19	7, 10
Isopropylhexedrine	1140	7	
Aniline	1150	10	
N,N-Dimethylphenethylamine	1150	10	
Nicotinyl alcohol	1150	10, this study	
Methylamphetamine	1170	19	7, 10
Propylhexedrine	1170	19	7, 10
Methylsalicylate	1200	10	
Pargyline	1200	19	7, 10
Tropine	1200	10	
Dimethrin	1210	19	
N-Ethylamphetamine	1210	19	7, 10
Hexamine	1210	10	
Tranylcypromine	1210	19	7, 10
Fenfluramine	1220	7	10
Anisaldehyde	1230	10	
Chlormethiazole	1230	20	
N,N-Dimethylamphetamine	1230	7	
Mephentermine	1240	19	7, 10
Thymol	1270	10	
Buphenine	1270*	This study	
Aletamine	1280	7, 10	
Acetylsalicylic acid	1295	10, 19	
Norpseudoephedrine	1310	7	
Phenylpropanolamine	1310	19	7, 10
Chlorphentermine	1320	19	7, 10, 15
p-Aminosalicylic acid	1330	10	
n-Butyric acid	1330	10	
cis-Linoleic acid	1330	10	
N-Propylamphetamine	1330	19	

(Continued on p. 84)

TABLE 4 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Salicylic acid	1330	19	10
Nicotine	1340	19	7, 10
Phenelzine	1340	This study	10
Cypenamine	1345	7	
Ephedrine	1350	19	7, 10, 15
Pseudoephedrine	1350	7	
Ectylurea	1360	19	10
Ethinamate	1360	19	10
Methoxyphenamine	1360	7, 10	
Acetanilide	1365	10	
p-Hydroxyphenylpyruvic acid	1380	10	
Ametazole	1390	This study	
Bemegride	1390	10	
Methylephedrine	1400	7, 10	
n-Caproic acid	1410	10	
Pheniprazine	1410	10	
Modaline	1420	7	
Phenmetrazine	1430	19	7, 10
Phendimetrazine	1440	19	7, 10, 15
Quinoline	1440	10	
Isoquinoline	1440	10	
Pheneturide	1450	15	
Etafedrine	1460	7, 15	
Nicotinamide	1460	10	
Salicylamide	1460	19	10
Warfarin	1460	19	10, 15
Phenoxypropazine	1465	7	
MDA (Methylenedioxyamphetamine)	1470	19	10
Metharbitone	1470	10	15
Sulphonal	1475	15	
Diethylpropion	1480	19	7, 10
Capric acid	1485	10	
Theophylline	1485	10	
Cantharidin	1490	19	
Carbaryl	1490	19	
Barbitone	1495	19	10, 15
Carbromal	1500	19	
Histamine	1500	10	
Mandelic acid	1500	10	
Nialamide	1500*	This study	
Nikethamide	1500	19	7, 10
Protokylol	1500	10	
Thiosalicylic acid	1500	10	
Methyprylone	1505	19	10, 15
Chlorothymol	1510	10	
2,4-Dinitrophenol	1510	10	
Methocarbamol	1510	10	
Phenprobamate	1520	15	
Benzocaine	1530	This study	8, 10
Hydrallazine	1530	10	
Leptazol	1535	This study	7, 10

TABLE 4 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
3,4-Dimethoxyphenethylamine	1540	19	
Mephenesin	1550	10	
Methimazole	1550	15	
Probarbital	1550	19	10, 15
Tolazoline	1550	15	
Clofibrate	1560	10	
Mephenesin carbamate	1570	10	
Iproniazid	1580	This study	10
Hydrastinine	1590	19	
Metronidazole	1590	10, 15	
Methsuximide	1595	19	
Allobarbitone	1600	10	15
Lauric acid	1600	10	
Nifenazone	1600	15	
Resorcinol	1610	10	
Aprobarbitone	1620	10	15
4,6-Dinitro-*o*-cresol	1620	10	
STP (Methyldimethoxyamphetamine)	1620	19	10
Zoxazolamine	1625	10	
Isoniazid	1630	19	10
Amylocaine	1635	8, 10	
Dyclonine	1640	10	
Phensuximide	1640	10	
Tolazamide	1650	10	
Butabarbitone	1655	10	
p-Nitromethylamphetamine	1655	10	
Butobarbitone	1660	10	15
Phenacetin	1660	19	8, 10, 15
Allylbarbituric acid	1670	10	15
Carbimazole	1670	15	
Cotinine	1670	8	
Styramate	1670	10	
Chlorphenesin carbamate	1690	10	
Carminic acid	1690	10	
Mescaline	1690	19	10, 15
5-Propyl-5-isobutylbarbituric acid	1690	10	
Tolbutamide	1690	10	
Talbutal	1700	10	15
Tybamate	1700	10	
Chlorzoxazone	1710	10, 15	
Paracetamol	1710	19	10
Isoprenaline	1720	10	
Methoxamine	1720	10, 15	
Amylobarbitone	1725	19	10, 15
Hippuric acid	1730	10	
Butethamate	1740	15	
Chlorpropamide	1740	10, 15	
Hydroxyphenamate	1740	19	10, 15
Lindane	1740	10	

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TABLE 4 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Meclofenoxate	1740	15	
Myristic acid	1740	10	
Pentachlorophenol	1740	This study	10
Pethidine	1740	19	8, 10, 15
Phenylsalicylate	1740	10	
Properidine	1740	15	
Tryptamine	1740	8, 10, 15, 19	
Norpethidine	1745	19	8
Dimethyltryptamine	1750	10, 15	
Pentobarbitone	1750	19	10, 15
Vinbarbitone	1750	10, 15	
Diazinon	1760	10	
Methohexitone	1760	10	
Fenmetramide	1765	8	
Pachycarpine	1765	19	
Nicoumalone	1770	10	
Sparteine	1770	10, 15	
Quinalbarbitone	1775	19	10, 15
Cotarnine	1780	19	
Lobeline	1780	19	
Methylphenidate	1780	19	7, 10
Phenanthrene	1780	10	
Secbutobarbitone	1780	19	
Anthracene	1790	10	
Betaprodine	1790	15	
Meprobamate	1790	19	8, 10, 15
Methoin	1795	19	10
Ethotoin	1800	10	
Pheniramine	1805	5	8, 15
Caffeine	1810	19	8, 10, 15
Physostigmine	1810	19	10
Glutethimide	1825	19	8, 10, 15
Betameprodine	1830	15	
Ketamine	1830	10, 15	
Phenazone	1830	19	10
Piperoxan	1830	15	
Thymoxamine	1830	15	
Trimeperidine	1830	15	
Alphameprodine	1840	15	
Dimenhydrinate	1840	10	
Theobromine	1840	10	
Ethoheptazine	1845	19	8, 10, 15
Prilocaine	1845	8, 10	
Benzphetamine	1850	7, 10	
Carisoprodol	1850	19	10
Etryptamine	1850	8	
Hexobarbitone	1850	10	
Thiopentone	1850	19	10
Tymazoline	1850	8	
Diphenhydramine	1855	19	8, 10
Lachesine	1860	15	

TABLE 4 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Lignocaine	1860	19	8, 10, 15
Mebutamate	1865	19	10
Dimethylthiambutene	1870	15	
Phencyclidine	1870	19	10, 15
Butylphthalate	1880	10	
Amidopyrine	1890	19	8, 10
Thiamylal	1890	19	10
Alphaprodine	1895	10, 15	
Acenocoumarin	1900	10	
Cyclandelate	1900	10	
Diethyltryptamine	1900	10	
Malathion	1900	10	
Methylphenobarbitone	1920	19	15
Xylometazoline	1920	10, 15	
Azapetine	1925	15	
Doxylamine	1925	10, 15	
Ethylmethylthiambutene	1925	15	
Orphenadrine	1925	5	8, 10, 15
Parathion	1925	10	
Phenyltoloxamine	1925	10, 15	
Hydroxyamylobarbitone	1930	15	
Aldrin	1950	19	
Ampyrone	1950	19	
Caramiphen	1950	15	
Cyclobarbitone	1950	10	15
Hexylcaine	1950	15	
Phenobarbitone	1950	19	10, 15
Piperocaine	1955	This study	10
Isocarboxazid	1960	19	10
Nystatin	1960	10	
Tetrahydrozoline	1960	8	
Tripelennamine	1960	19	8, 10, 15
Methapyrilene	1970	19	8, 15
Ethomoxane	1975	15	
Palmitic acid	1975	10	
Methaphenilene	1980	10	
Procarbazine	1990	10	
Procaine	1995	19	8, 10, 15
Bufotenine	2000	15	
Chlorpheniramine	2000	19	8, 10, 15
Diethylthiambutene	2000	15	
Eucatropine	2000	15	
Phenyramidol	2000	This study	10
Pyridoxamine	2000	19	
Amprotropine	2010	15	
Butanilicaine	2010	15	
Cyclizine	2010	19	8, 10, 15
Cyclopentolate	2010	15	
Ketobemidone	2010	15	

(Continued on p. 88)

TABLE 4 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Phenothiazine	2010	10, 15	
Pilocarpine	2010	10	15
Pipazethate	2010	15	
Thenyldiamine	2010	This study	10
Thiabendazole	2010	10	
Chlordane	2020	19	
Amisometradine	2025	10	
Apoatropine	2025	15	
Butallylonal	2025	10	
Hydroxypethidine	2025	15	
Dimethoxanate	2030	This study	
Methadone (cyclic metabolite)	2030	8	
Chlorphenoxamine	2040	10, 15	
Homatropine	2045	19	10, 15
Butethamine	2050	This study	10, 15
Carbinoxamine	2050	5	10, 15
Chlorbenside	2050	19	
Isopropamide	2060	10	
Brompheniramine	2070	10, 15	
Chlophedianol	2070	15	
Mepivacaine	2075	This study	10, 15
Normethadone	2080	8	
Diphenylpyraline	2090	This study	10, 15
Naphazoline	2090	This study	10
Dicyclomine	2100	This study	10
Heptabarbitone	2100	10	
Quinuronium	2100	15	
Dieldrin	2110	19	15
Dextromethorphan	2115	8, 15	
Procyclidine	2115	This study	10, 15
Mephenoxalone	2120	19	10
Isomethadone	2125	8	
Oxypertine	2125	15	
Chloropyrilene	2130	This study	10
Pyrimethamine	2140	19	10
Tacrine	2140	15	
Propranolol	2145	10, 15	
Thiantoin	2145	19	
Alphamethadol	2150	15	
Bromodiphenhydramine	2150	19	10, 15
Dopamine	2150	15	
Embramine	2150	15	
Pipradrol	2150	19	8, 10, 15
Butriptyline	2155	15	
Alphacetylmethadol	2160	15	
Phenindamine	2160	This study	8, 10, 15
Santonin	2160	10, 15	
Methadone	2170	19	8, 10, 15
Oxymetazoline	2170	10, 15	
Atropine	2175	19	10, 15
Fluopromazine	2175	15	

TABLE 4 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Linolenic acid	2175	10	
Stearic acid	2175	10	
Cocaine	2180	19	8, 10
Dextropropoxyphene	2180	19	8, 10, 15
Ergocryptine	2180	10	
Metaxalone	2180	10	
Methaqualone	2180	10, 15	8
Mefenamic acid	2185	10, 15	
Adiphenine	2190	19	10
Amitriptyline	2200	19	8, 10, 15
Chloroprocaine	2200	10, 15	
Perphenazine	2200	19	
Pipobroman	2200	10	
Thonzylamine	2200	This study	10, 15
Trimipramine	2200	15	
Mepyramine	2205	5	8, 10, 15
Picrotoxin	2205	19	
Amölanone	2210	10, 15	
Azacyclonol	2210	19	10, 15
Triflupromazine	2210	19	8, 10
Amethocaine	2215	19	10, 15
Chlorcyclizine	2215	19	8, 10, 15
Nortriptyline	2215	5	10, 15
Imipramine	2220	19	8, 10, 15
Cyclomethycaine	2225	10	
Hyoscyamine	2225	19	10
Levorphanol	2225	10, 15	
Metabutoxycaine	2225	10	
Benactyzine	2230	19	10
Benzhexol	2230	19	10, 15
Levomethorphan	2230	15	
Phenoxybenzamine	2230	10, 15	
Procainamide	2230	10, 15	
Protriptyline	2230	15	
Carbetapentane	2240	This study	10
Chlormezanone	2250	10	
Primidone	2250	19	8, 10, 15
Triprolidine	2250	19	8, 10, 15
Desipramine	2260	This study	10, 15
Isothipendyl	2260	This study	8, 10, 15
Promethazine	2260	19	8, 10, 15
Pentazocine	2265	19	8, 10, 15
Bupivacaine	2270	8	15
Dimethindene	2270	10, 15, 19	
Desomorphine	2275	15	
Aconitine	2280	19	
Biperiden	2280	15	
Diethazine	2280	15	
Harmine	2280	This study	10

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TABLE 4 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Anisinidione	2285	10	
Hyoscine	2285	19	10, 15
Carbamazepine	2290	15	
Dicophane	2290	19	10, 15
Methyldesorphine	2290	15	
Promazine	2295	19	8, 10, 15
Chlordiazepoxide	2300*	This study	15
Stilboestrol	2300	This study	10, 15
Pramoxine	2305	This study	10, 15
Dihydroergotamine	2310	19	
Etoxeridine	2310	15	
Benztropine	2320	10, 15	
Buphenine	2320	This study	
Primaquine	2320	This study	10
Probenecid	2320	This study	10
Propoxycaine	2320	15	
Trimeprazine	2320	This study	8, 10, 15
Piperidolate	2325	This study	10, 15
Antazoline	2330	19	8, 10, 15
Prothipendyl	2330	This study	10, 15
Oxazepam	2335	10, 15	
Phenytoin	2335	15, 19	
Dexoxadrol	2340	8	
Levallorphan	2340	5	10, 15
Phenazopyridine	2345	10	
Ethopropazine	2350	This study	10, 15
Gentisic acid	2350	10	
Propantheline	2350	10	
Cyproheptadine	2355	10, 15	
Ergotamine	2360	10	
Dihydrocodeine	2365	8	10, 15
Phenylbutazone	2370	10, 15	
Methyldihydromorphine	2375	15	
Metopon	2375	15	
Pholcodine	2380	10	
Codeine	2385	19	8, 10, 15
Hexoestrol	2400	10	
Diazepam	2410	5	10, 15
Methoxychlor	2410	19	10
Ethylmorphine	2415	19	10, 15
Dihydrocodeinone	2425	10	
Hydrocodone	2425	15	
Oxycodone	2425	15	
Pyrrobutamine	2430	19	8, 10, 15
Morphine	2435	19	8, 10, 15
Chlorpromazine	2440	19	8, 10, 15
Dihydromorphine	2440	15	
Xenysalate	2440	15	
Acetyldihydrocodeine	2450	15	
Mebhydrolin	2450	15	
Ethylisobutrazine	2455	8	

TABLE 4 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Tetrahydrocannabinol	2455	19	
Chlordiazepoxide	2460*	This study	
Butacaine	2470	5	10
Dipipanone	2470	5	8, 15
Methdilazine	2470	8, 10, 15	
Pipethanate	2470	10	
Desmethylchlorpromazine	2480	8	
Dibenzepin	2480	10	
Didesmethylchlorpromazine	2480	8	
6-Monoacetylmorphine	2480	15	
Hydromorphone	2490	10	
Methixene	2490	10	
Chlordiazepoxide	2500*	This study	10, 15
Ergocristine	2500	10	
Methoxypromazine	2500	19	10
Morpheridine	2500	15	
Thebacon	2500	15	
Chlorprothixene	2510	10	
Phenadoxone	2510	8	15
Methotrimeprazine	2515	This study	8, 10, 15
Norethynodrel	2520	10	
Oxymorphone	2520	10, 15	
Pyrathiazine	2520	8	10
Thebaine	2525	19	10
Oxyphencyclimine	2540	10	
Pentaquin	2540	15	
Prenylamine	2540	15	
Ethoxzolamide	2550	10	
Pecazine	2550	19	10, 15
Nalorphine	2570	19	10, 15
Chloroquine	2575	19	8, 15
Cinchonine	2575	19	8, 10, 15
Deptropine	2590	15	
Methyltestosterone	2610	15	
Trimethoprim	2610	15	
Diamorphine	2615	19	8, 10, 15
Phenacaine	2615	10	
Cinchonidine	2625	19	8, 15
Acepromazine	2665	8, 10, 15	
Phenazocine	2670	8, 10	
Nitrazepam	2675	5	15
Benzethidine	2680	15	
Clemizole	2680	5	10, 15
Trifluoperazine	2680	This study	8, 10, 15
Cinchocaine	2690	19	10, 15
Indomethacin	2690	10	
Fentanyl	2700	15	
Gallamine	2700	15	
Ethinyloestradiol	2710	10	

(Continued on p. 92)

TABLE 4 *(continued)*

Drug	*Retention index*	*Reference*	
		Source	*Check*
Propiomazine	2725	This study	15
Quinine	2755	19	10, 15
Quinidine	2760	19	10, 15
Captodiame	2775	19	10, 15
Hydroxyquinidine	2780	15	
Progesterone	2785	10	
Chlordiazepoxide	2790	This study	19
Hexachlorophane	2795	10, 15	
Ethoxyquin	2800	19	
Papaverine	2805	5	10, 15
Hydroxyzine	2840	19	10, 15
Anileridine	2845	19	10, 15
Dapsone	2860	19	10
Hydroxychloroquine	2860	19	10
Doxapram	2875	15	
Sanguinarine	2880	19	
Diphenadione	2910	10	
Prochlorperazine	2935	10	
Haloperidol	2940	10	
Dexamethasone	2950	10	
Hydrastine	2975	19	10
Cholesterol	3015	10	
Thiothixene	3015	10	
Strychnine	3040	19	10, 15
Fluphenazine	3045	19	
Meclozine	3050	19	10, 15
Methysergide	3050	10	
Triamcinolone	3070	10	
Noscapine	3100	10	
Thioridazine	3110	19	10
Rotenone	3250	10	
Pipamazine	3260	This study	
Thiethylperazine	3260	10	
Brucine	3280	10	
Buclizine	3285	19	10
Yohimbine	3290	19	10
Lysergide	3445	19	
Thiopropazate	3450	This study	
Carphenazine	3590	19	

* Major decomposition product.

because of decomposition, the retention indices are much less reproducible and will decrease with increased amount of drug injected onto the column. A suitable factor to use for routine identification purposes is ± 50 retention index units when more than 99% of experimentally determined values will fall within this range from the mean value. An experienced analyst using isothermal conditions and obtaining good symmetrical chromatographic peaks will obviously be able to obtain better reproducibility and it is expected that most values obtained will fall in the range ± 20 from

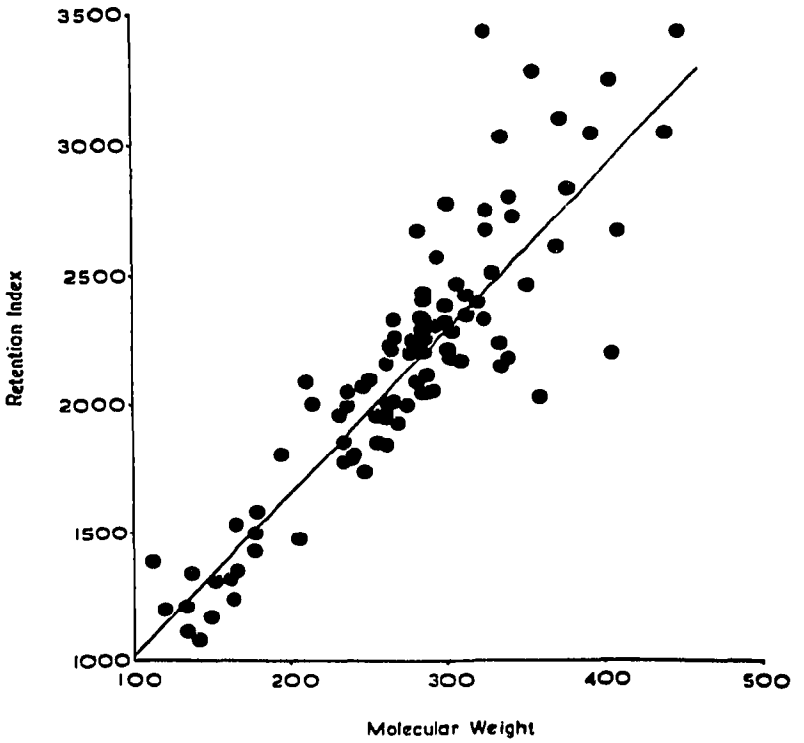

Fig. 2. Correlation of retention index and molecular weight for drugs chromatographed on an SE-30 column.

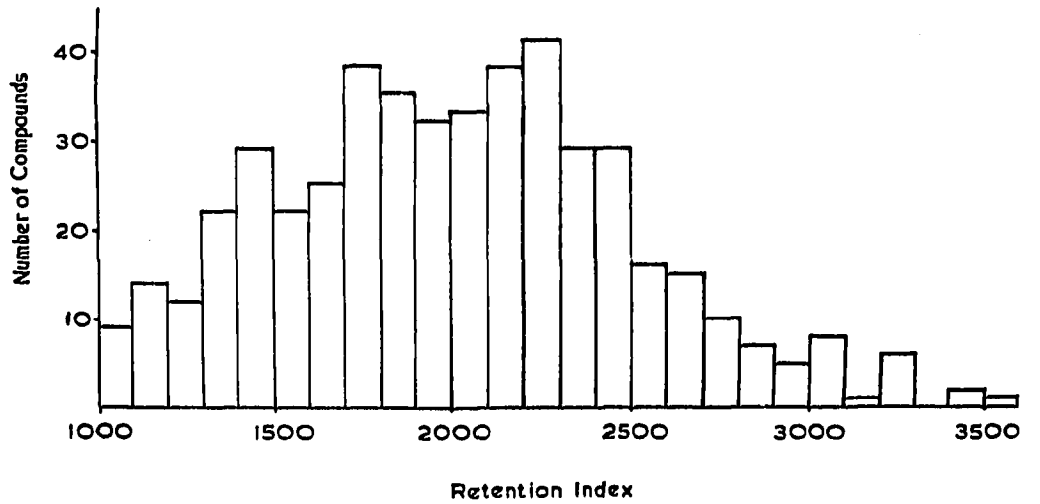

Fig. 3. Frequency histogram of retention indices of 478 drugs on an SE-30 column.

the values in Tables 3 and 4. It must be remembered that since the retention indices in Tables 3 and 4 were obtained from many sources, and each value is subject to some error, a drug with a smaller index than another may not necessarily be eluted first. For example, acetylsalicylic acid and phenylpropanolamine are quoted as having retention indices of 1295 and 1310, respectively, but under some conditions they may elute in the reverse order. The important feature to recognise is that they elute within the error factor of the value given in Tables 3 and 4.

Fig. 3 shows the histogram for the 478 drugs that gave peaks (two were not eluted between 1000 and 3500). Obviously, if a peak is obtained with a retention index of 2200, this information is far less useful for identification purposes than a value of 3500, where fewer compounds are possible identities. Thus, Fig. 3 may help in determining the usefulness of the retention index for an unknown drug for identification purposes.

It is hoped that by creating this unified collection of data for the GLC identification of drugs by measurement of their retention indices on an SE-30 column it will aid analysts to standardise on this single "preferred liquid phase" and that future analysis will be performed using this phase.

4. ACKNOWLEDGEMENT

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5. SUMMARY

The dimethyl silicone elastomer SE-30 has been chosen as the preferred liquid phase for the gas–liquid chromatographic analysis of drugs, and retention index data have been compiled for 480 drugs and commonly occurring chemicals such as plasticisers. The inter-laboratory variation in measurement of retention indices has been measured for three drugs in eleven laboratories and the standard deviations were between 20 and 15 retention index units.

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