The Tentative Identification of Volatilizable Organic Compounds by Linear Temperature Programmed Gas Chromatographic Retention Indices with Notes on Other Methods for Identifying Organic Substances; 1988

Methods for the Examination of Waters and Associated Materials

Her Majesty's Stationery Office

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1988

Note, the use of the word 'Tentative' in the title refers to the identification and not, as is usual in this series, to the degree of testing.

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The Tentative Identification of Volatilizable Organic Compounds by Linear Temperature Programmed Gas Chromatographic Retention Indices (LTPRI), with an Inventory of Indices, with Notes on other Methods for Identifying Organic Substances; 1988.

This procedure for tentatively identifying volatilizable organic compounds is based on the WRC Final Report and Inventories of Indices compiled under DOE Contract PECD 7/7/188–4/84. LTPRI is often suitable for tentative identification and for rapid screening of samples when GCMS is not practicable.

Contents

About This Series

This booklet is part of a series intended to provide both recommended methods for the determination of water quality, and in addition, short reviews of the more important analytical techniques of interest to the water and sewage industries.

In the past, the Department of the Environment and its predecessors, in collaboration with various learned societies, have issued volumes of methods for the analysis of water and sewage culminating in 'Analysis of Raw, Potable and Waste Waters'. These volumes inevitably took some years to prepare, so that they were often partially out of date before they appeared in print. The present series will be published as series of booklets on single or related topics; thus allowing for the replacement or addition of methods as quickly as possible without need of waiting for the next edition. The rate of publication will also be related to the urgency of requirements for that particular method, tentative methods and notes being issued when necessary.

The aim is to provide as complete and up to date a collection of methods and reviews as is practicable, which will, as far as possible, take into account the analytical facilities available in different parts of the Kingdom, and the quality criteria of interest to those responsible for the various aspects of the water cycle. Because both needs and equipment vary widely, where necessary, a selection of methods may be recommended for a single determinand. It will be the responsibility of the users—the senior technical staff—to decide which of these methods to use for the determination in hand. Whilst the attention of the user is drawn to any special known hazards which may occur with the use of any particular method, responsibility for proper supervision and the provision of safe working conditions must remain with the user.

The preparation of this series and its continuous revision is the responsibility of the Standing Committee of Analysts (to review Standard Methods for Quality Control of the Water Cycle). The Standing Committee of Analysts is a committee of the Department of the Environment set up in 1972. Currently it has 9 Working Groups, each responsible for one section or aspect of water cycle quality analysis. They are as follows:

1.0 General principles of sampling and accuracy of results
2.0 Microbiological methods
3.0 Empirical and physical methods
4.0 Metals and metalloids
5.0 General nonmetallic substances
6.0 Organic impurities
7.0 Biological monitoring
8.0 Sewage Works Control Methods
9.0 Radiochemical methods

The actual methods and reviews are produced by smaller panels of experts in the appropriate field, under the overall supervision of the appropriate working group and the main committee.

The names of those associated with this method are listed inside the back cover. Publication of new or revised methods will be notified to the technical press, whilst a list of Methods in Print is given in the current HMSO Sectional Publication List No 5.

Whilst an effort is made to prevent errors from occurring in the published text, a few errors have been found in booklets in this series. Correction notes and minor additions to published booklets not warranting a new booklet in this series will be issued periodically as the need arises. Should an error be found affecting the operation of a method, the true sense not being obvious, or an error in the printed text be discovered prior to sale, a separate correction note will be issued for inclusion in that booklet.

L R PITTWELL
Secretary and Chairman

11 August 1988

Warning to Users

The analytical procedures given in this booklet should only be carried out by competent trained persons, with adequate supervision when necessary.

Local Safety Regulations must be observed.

Laboratory procedures should be carried out only in properly equipped laboratories.

Field Operations should be conducted with due regard to possible local hazards, and portable safety equipment should be carried.

Care should be taken against creating hazards for one's self, one's colleagues, those outside the laboratory or work place, or subsequently for maintenance or waste disposal workers. Where the Committee have considered that a special unusual hazard exists, attention has been drawn to this in the text so that additional care might be taken beyond that which should be exercised at all times when carrying out analytical procedures. Reagents of adequate purity must be used, along with properly maintained apparatus and equipment of correct specifications. Specifications for reagents, apparatus and equipment are given in manufacturers' catalogues and various published standards. If contamination is suspected, reagent purity should be checked before use. Lone working, whether in the laboratory or field, should be discouraged.

The best safeguard is a thorough consideration of hazards and the consequent safety precautions and remedies well in advance. Without intending to give a complete checklist, points that experience has shown are often forgotten include: laboratory tidiness, stray radiation leaks (including ultra violet), use of correct protective clothing and goggles, removal of toxic fumes and wastes, containment in the event of breakage, access to taps, escape routes, and the accessibility of the correct and properly maintained first-aid, fire-fighting, and rescue equipment. Hazardous reagents and solutions should always be stored in plain sight and below face level. Attention should also be given to potential vapour and fire risks. If in doubt, it is safer to assume that the hazard may exist and take reasonable precautions, rather than to assume that no hazard exists until proved otherwise.

There are numerous handbooks on first aid and laboratory safety. Among such publications are: 'Guide to Safe Practices in Chemical Laboratories' and 'Hazards in the Chemical Laboratory', issued by the Royal Society of Chemistry, London: 'Safety in Biological Laboratories' (Editors Hartree and Booth), Biochemical Society Special Publication No 5. The Biochemical Society, London, which includes biological hazards; and 'The Prevention of Laboratory Acquired Infection', Public Health Laboratory Service Monograph 6, HMSO, London.

It cannot be too strongly emphasised that prompt first aid, decontamination, or administration of the correct antidote can save life; but that incorrect treatment can make matters worse. It is suggested that both supervisors and operators be familiar with emergency procedures before starting even a slightly hazardous operation, and that doctors consulted after any accident involving chemical contamination, ingestion, or inhalation, be made familiar with the chemical nature of the injury, as some chemical injuries require specialist treatment not normally encountered by most doctors. Similar warning should be given if a biological or radiochemical injury is suspected. Some very unusual parasites, viruses and other micro-organisms are occasionally encountered in samples and when sampling in the field. In the latter case, all equipment including footwear should be disinfected by appropriate methods if contamination is suspected. If an ambulance is called or a hospital notified of an incoming patient give information on the type of injury, especially if poisoning is suspected, as the patient may be taken directly to a specialised hospital.

Identification of Unknown Organic Substances

In the past, organic substances were identified by their chemical and physical properties, usually, but not always, after separation. This was aided by the preparation of derivatives and whether these derivatives had the expected properties.

The use of chemical and physical properties should not be entirely excluded even now. It is useful to know whether a substance is acidic or basic and in what it is soluble. Plenty of reference works are available. There are a number of additional techniques which have been developed, these include Mass Spectrometry, infra red and ultra violet absorptiomety, nuclear magnetic resonance spectrometry, as well as various techniques based on chromatographic elution times and electrophoretic separation. All have their own special uses and limitations. Specialist texts should be consulted. A brief summary follows:

Mass Spectrometry

This is one of the most favoured methods, usually with prior separation by G C or HPLC.

The mass spectrum of a single substance is dependent to a large extent on the type of ion source used and also on the spectrometer. Occasionally, compounds, some quite unusual, can be formed in the instrument and cause interference. Several good atlases of spectra exist (see Ref 16); but care is necessary when identifying an unknown substance. Some inorganic compounds can be detected even without the use of plasma sources.

IR and UV Absorptiometry

These techniques are only useful if a high concentration or some solid is available. IR can be used in a reflectance mode for examining insoluble material. Instruments are subdivided by wavelength range used. The absorption bands are indicative of structural groups, but the molecular vibrations involved are also affected by the surrounding parts of the molecule. This can cause quite marked frequency variations for a single radical. Thus the cyanide frequency depends on the adjacent bonding or coordination, and the carbonate frequency depends on the pH. Water can only be used as a solvent for a very limited part of the IR spectrum due to its own strong IR absorption bands. Several good spectral indexes are available (see Ref 17).

NMR

This form of spectrometry is rarely used except for special problems and requires a relatively high concentration of sample. The spectrum varies markedly with the resolution of the instrument. It is chiefly used for elucidating bonding and structure.

Electrophoresis

This technique is used to separate and identify charged ions, especially amino acids and peptides.

CG and Other Chromatographic Indexes

These can often be used for tentative identification of trace components. The index is dependent on the column used and on the eluent. The more indices obtained for a substance (using columns of different polarity etc), the smaller the number of substances that need to be considered in the final identification. These techniques can sometimes be used to show that a substance is not present at above the chromatographic limit of detection. This booklet gives details of one method, the Linear Temperature Programmed Gas Chromatographic Retention Index (or LTPRI). See also Refs 13, 15 and 20.

Introduction to LTPRI

While Gas Chromatography coupled to a Mass Spectrometer is usually the method of choice for the identification of unknown compounds detected by gas chromatography, there are laboratories which lack such facilities and also investigations where the use of an alternative method of identification is required or additional confirmation is needed. The procedure outlined in this booklet provides such an alternative (1–3).

Unknown compounds found in water may be tentatively identified from their gas chromatographic linear temperature programmed retention indices (LTPRIs). Normally, retention indices are calculated for isothermal conditions and related to the retention times of members of a homologous series of n-alkane standards and quoted in terms of carbon number × 100 (Kovat's Indices); but environmental samples usually contain organic compounds with a wide range of boiling points which cannot be eluted from a gas chromatograph at one single temperature. Hence in this procedure, the equivalent carbon number or retention index is calculated using a linear temperature programmed gradient. The measured LTPRI values are compared with these in a central computer library or table containing data for relevant compounds, generated under 'ideal' conditions, thus enabling tentative identifications to be made.

Retention times vary with the type of column used (including method of preparation) and also with its age and prior usage. In addition they also vary with the elution conditions. Hence, it is essential that the columns and conditions used be as identical as is possible with those used when compiling the inventory, and that frequent recalibrations be made (as experience dictates) in order to allow for the effects of ageing and use. Examples of the effects of column variation and age are included in the test data.

This procedure is intended to fit in with other laboratory operations, and so may in part, but not in its entirety, be very flexible. Hence, the usual method format has been modified, and only those parts of the method requiring rigid standardization have been given in detail. All other steps are only given in outline. When seeking to identify a compound, users should take into account the effects of any preliminary steps which may eliminate some possible substances. Blanks have not been mentioned, but must not be forgotten. It would not be helpful, having identified a substance, to find that it originated from a reagent and not from the original sample.

While intended as a means of reducing the list of possibilities which must be checked when identifying an unknown Gas Chromatographic peak, there is the possibility of using the procedure to confirm the absence of a substance in identifiable amounts by noting whether there are any peaks present which, within analytical error, might be attributable to that substance.

Using an electron-capture detector (ECD), peaks may be seen in the chromatograms which are due to compounds present at a concentration too low to be identified by GC-MS. Whilst ECD does not respond well to n-alkanes, LTPRIs can be calculated and tentative identifications obtained, provided the n-alkane standards or a series of other EC responsive compounds such as the n-chloralkanes, etc are run at sufficiently high concentrations. (Refs 18 and 20)

Recently, commercial instruments have been developed using a variety of detectors—ECD, FID, ATD, FPD, PID and MS. In addition homologous series of compounds for use as retention index standards with such detectors are also available (Ref 19).

See also published Health and Safety Executive Work (Ref 20)

Measurement of Linear Temperature Programmed Retention Indices

1 Performance Characteristics of the Procedure

1.1	Substances Identified	Substances, soluble in organic solvents, giving recognizable gas chromatographic peaks with either non-polar (polydimethylsiloxane) or polar (polyethyleneglycol or similar), coated columns (for example OV1 or Carbowax 20M).
1.2	Sample Types	Waters, soils and sediments.
1.3	Basis of the Procedure	Extraction of the substances to be identified into a suitable organic solvent, followed by gas chromatography with either a polar or non-polar column or on both types of column, followed by location of the GC peak for the substance relative to the peaks of n-alkanes obtained under the same standard conditions. Other markers may be used instead of alkanes.
1.4	Range of Application	Substances with gas chromatographic peaks lying between n-C_6H_{14} and n-$C_{40}H_{82}$ see also Section 10.
1.5	Typical Standard Deviation	See Tables 1, 2 and 3.
1.6	Limiting Lower Concentration	Dependent on sensitivity of the substance to a Flame Ionization Detector, or other detector if used.
1.7	Interferences	Substances with similar Retention Indices and solubilities may cause confusion of identity. Some substances decompose. The decomposition products may give anomalous peaks. Large amounts of substances, especially the solvent, may cause imprecision. A few compounds give diffuse peaks which may not register on some automatic computing instruments. Ageing of the column may cause slight migration of the peaks, especially for polar compounds. This phenomenon is use dependent. With non-polar columns the shift is small, 1 to 2 units gradually increasing to about 10; but with polar the shift will increase more rapidly to 10 to 50 units. The degree of shift is also compound dependent, see Ref 3.
1.8	Time for analysis	About one hour per sample, but very dependent on computer facilities available.

2 Outline Procedure

2.1 Sample Preparation

Samples are extracted into a suitable solvent which should, if possible, be more volatile than the substance to be identified, or whose presence is sought. Acidic compounds should be extracted from acid solution, bases should be extracted from alkaline solution; this may preclude some solvents—ethers are soluble in acids.

2.2 Gas Chromatography

The extract either has a reference mixture of n-alkanes (spread uniformly over the probable range of LTPRI values), or a series of easily detected compounds with accurately known RI, such as n.chloroalkanes or n-alkylbis (trifluoromethyl) phosphine sulphides (Ref 19), coinjected with it or added to it. Alternatively, a few substances of known LTPRI with values close to that of the substance suspected may be used as standards. If necessary for clarity, the n-alkane plot can be run as a separate external standard provided adequate control substances are added to each run to ensure accurate correlation.

The amount of standard used must be based on experience, but should be just sufficient to give clear markers on the chromatogram. The amount of sample used will depend on the amount of material available and on the size of the peaks produced in the chromatogram (See Introduction, last paragraph and Section 5.1 first paragraph).

2.1 The extract is examined by gas chromatography with flame ionization or any other suitable detector using either or both of two standard columns which have been precalibrated using a mixture of n-alkanes. (See Sections 3 and 4).

2.3 Calculation of the Index

The GC/FID chromatogram for the extract is compared with the calibration chromatogram (or the plot of the retention times for the n-alkanes added to the sample). Figs 1–5 show typical curves for various column types.

2.3.1 The LTPRI of the peak (or peaks) to be tentatively identified is calculated first by noting the two closest n-alkanes, one on either side of the peak to be identified, and then by measuring the distance (time) that the mid point of the peak to be identified is along a smooth curve passing through the elution times for the various alkanes, measurement being from the nearest alkane peak below the peak to be identified.

2.3.2 The first two numbers of the LTPRI are the number of carbon atoms in the lower reference n-alkane (the first number is zero for nonane and below); the second two numbers are the percentage time (or chart trace distance) between the n-alkane peak designated and the n-alkane peak next above it, corrected for the slight variation of retention time with carbon number. (This curve is slightly S-shaped).

2.3.3 If reference substances other than n-alkanes are used (as is now commonly the case), calculations are made so that the index obtained is still n-alkane based.

2.4 Analytical Quality Assurance

Because columns deteriorate, periodic quality checks are essential using either a reference n-alkane mixture or a selection of known substances.

It is advisable, if the substances are available, to compare the peak from the sample with peaks of the probable substances obtained under identical conditions. Good correspondence does not guarantee identification, but it does greatly limit the number of probable compounds. The presence of a hitherto unlisted compound can occur.

3 Standard Columns

3.1 Non-Polar

A non-polar polydimethylsiloxane PS 255 capillary column or similar OVI column. (See Fig 1 for a typical chromatogram) (Note that in Tables 4 and 5 most non polar column data are listed as OV1, data for PS 255 are identical within normal variations).

3.2 Polar

(The performance of both these columns changes more rapidly with use than does that of the non-polar column above. Regular checking of performance and, if necessary, replacement are essential).

EITHER

3.2.1 A polar Carbowax 20M column
(Figs 2–4 show the effects of various methods of coating on the curves obtained)

OR

3.2.2 A polar Superox 0.6 column
(See Fig 5 for a typical curve).

3.3 Dimensions— approximately 50 m of 0.2 mm bore, coating thickness 0.2 μm.

3.4 Availability— all three columns are available commercially, but preparational details, which are very intricate, are given in Ref 3, a copy, of which is deposited in the Department of the Environment Library.

Commercial instruments with twin columns and built in computers for retention index calculations are available.

4 Chromatographic Conditions

Chromatograph: The test data given in this booklet were obtained using an Erba Science 4160 chromatograph, columns being changed as required.

Data processing: the peaks given as illustration were acquired and retention times measured using a Hewlett Packard 3390A reporting integrator fitted with input/output board (option 100) and interfaced with a Digital Equipment Corporation VAX 11/780 computer which was used for both data storage and calculation of LTPRIs using a polynomial curve fitting technique.

Any other equivalent equipment giving a comparable or better performance may be used. Note that information is given for manual calculation or use of other data processing equipment. The operating conditions which follow were those used to obtain the test data. If other equipment is used, follow the manufacturer's instructions and optimize conditions to achieve comparable indices.

Comparable results have been obtained on several other makes of gas chromatograph.

4.1 Operating conditions used to obtain the test data with the non-polar column.

Carrier gas:	Hydrogen; head pressure set such that at ambient temperature the elution time for methane (column hold-up time) is 120 s. (See Section 9)
Injection:	Split; injector vent flow rate approximately 30 ml/min (split ratio approximately 15:1), injector temperature 200°C. Volume injected: 1 μl of sample. Standard coinjection 1.8 μl. Recommended concentrations are 400 μg/ml for dissolved solid samples and 0.4 μl/ml for liquid extract samples.
Detection:	Flame ionization; detector temperature 350°C; detector gas pressures: hydrogen 0.4 kg/cm², air 1.5 kg/cm². Note some commercial instruments use electron capture detector (usually with chloroalkane, n-alkylbis (trifluoromethyl) phosphine sulphides or similar standards). Other detectors may be used for special substances (see Introduction to LTPRI, final paragraph).
Oven temperature:	30°C for injection then programmed immediately to rise to 330°C at 4°C/min and then held at 330°C until no further n-alkanes eluted. See also 4.3.

4.2 Operating conditions used to obtain the test data with the Polar columns

	Carrier gas: Hydrogen; head pressure set such that at 60°C the elution time for methane (column hold-up time) is 120 s. (See Section 9).
Injection:	Split; injector vent flow rate approximately 30 ml/min (split ratio approx 15:1); injector temperature 200°C. Recommended

concentrations are 400 μg/ml for dissolved solid samples and 0.4 μl/ml for liquid extract samples.

Detection: Flame ionization; detector temperature 250°C; detector gas pressures; hydrogen 0.4 kg/cm², air 1.5 kg/cm². Note some commercial instruments use electron capture detectors (usually with chloroalkane or similar standards). Other detectors may be used for special substances.

Oven temperature: 60°C for injection then programmed immediately to 220°C at 4°C min and held for 20 min.

Carbowax 20M columns are not usable below 60°C and not reliable above 220°C. However, their stronger absorptive capacity makes them viable for many substances eluting at <40°C on other columns. The range for Superox 0.6 is 40–270°C.

4.3 Variant Oven Temperature Programmes. Often, the same heating programme is used with both columns, and commercial instruments are available with both columns in the same furnace operated simultaneously; however, for many substances it is better to operate each column separately with different heating programmes, as for instance in Sections 4.1 and 4.2 above. Whatever the variation chosen, standards and samples must be treated in exactly the same way when determining indices.

5 Calculation of Indices

Indices may be calculated manually if necessary, but more accurate indices can be calculated, provided adequate computor facilities are available, see the Appendix and Section 5.2.

5.1 Manual Calculation using a Spline

The initial GC plot of alkane number against retention time will probably be a flattened S shape. The degree of curvature is dependent on the instrument used, and the heating programme chosen. A few are almost linear. It is this non-linearity which makes it necessary to take the shape of the curve into account when calculating a retention index from retention time data. Occasionally, overloading may occur, especially with the Carbowax column, making peaks hard to locate. If this happens, either resort to a differential plot to locate the peaks, or dilute the sample and rerun the chromatogram.

If the data cannot be fed to a suitably programmed computer for curve fitting and determination of the LTPRI; it should be plotted as a graph. Use of a very large sheet of graph paper is recommended (eg 1 m×2 m) so that it is possible to subdivide the space between alkane carbon numbers sufficiently to estimate the unknown substance peak location to an accuracy of +5% or preferably even +1%. Plot the graph of the number of carbons in the standard alkanes versus their elution times, using a plastic spline ruler held by many spline weights. The flexibility of the spline will make good allowance for the overall curvature of the graph and the effect of remote points on the section of main interest. The weights should be located at points corresponding to alkane elution times and, when obtaining a smooth curve, should not be moved more than the experimental error would allow. Superimpose the plot from the sample, using either the control additions or the n-alkane additions to align the curves. Identify the pair of alkanes between which the peak to be indexed falls and measure the percentage distance along the curve from the lower of the two alkanes to the peak intercept. This is best done either by having a fine calibrated scale on the side of the spline itself or by use of a planimeter (as used for measuring distances on maps). Then calculate the distance along the curve that the peak to be identified is beyond the lower alkane peak as a percentage of the distance between the two alkane peaks. (See Section 2.4.2 for how to express the index).

The LPTRI so obtained may then be compared with data in Tables 4 and 5, or in the library of compounds held in the WRC data system, and a list of identifications produced in probability order.

If substances other than n-alkanes are used (see Ref 19, or other suitable materials of known index), use the appropriate Retention Index numbers instead.

5.2 See Ref 7 for yet another alternative approximate calculation technique. See Ref 21 for a general reference to the cubic spline technique with a listing of available FORTRAN discs.

6 Substance Identification

6.1 Tentative Identification

6.1.1 Identification of an unknown

Consult tables 4 and 6 which list already determined indices for methyl silicone and polyethylene glycol columns respectively. Always compare data only with that obtained using the same column. (See also 6.3 below)

6.1.2 Verification of the presence or absence of a known substance.

Tables 5 and 7 give Retention Indexes for a list of known substances listed by column type as above.

6.2 Corroboration of Data

Prepare solutions of suspected compounds in the same solvent and spike the sample with them and rerun on the same column to see if the elution peaks coincide.

6.3 New Data

The Water Research Centre collect data on newly measured substances. For enquiries on additions to the tables and new indices contact the address given below. If giving or enquiring about indices, always state the column used.

Water Research Centre
Stevenage Laboratory
Elder Way
Stevenage, Herts, SG1 1TH
United Kingdom
(Stevenage (0438) 312444)

or Medmenham Laboratory
PO Box 16, Marlow
SL7 2HD
United Kingdom
(Henley on Thames (0491) 571531)

WRC also keep a record of data from a variety of non-standard columns.

7 Commonly Used Extraction Solvents

The following are the most commonly used solvents for extracting samples:

n-Pentane
Dichloromethane
Diethyl ether
n-Hexane and Carbon disulphide may also be used for some compounds

8 Standard Substances

The original standards on which the indices are based are normal alkanes from pentane or hexane to $C_{40}H_{82}$. Above $C_{26}H_{54}$ alternate alkanes may be used.

8.1 A series of other commonly encountered substances with a useful range of volatilities eg n-chloroalkanes or another homologous series, such as n-alkylbis (trifluoromethyl) phosphine sulphides, with better detection characteristics than n-alkanes may be used provided their retention indices are accurately known. Readily detected substances with accurately known RI may also be added as internal standards. See also Ref 19.

9 Hazards

Hydrogen is flammable and mixtures with air etc are potentially explosive. If released into air as a high pressure jet it can be self igniting. A good safety guide is given in Ref 14. Alternatively, helium or other gas may be used, but the effect on index measurement should be checked.

All the solvents are flammable and volatile, some are narcotic and toxic. Ethers tend to form explosive peroxides on storage (see Ref 12). Ensure good ventilation, absence of flames and sparks and check the hazard specific to the chosen solvent before use.

10 Extension of the Method

Provided columns and conditions are standardised, other columns than those given here can be used. WRC has list of Indexes for many compounds on a variety of columns.

If high temperature capillary column chromatographs are used, it has been shown that the n-alkanes provide a useful series of peaks up to C_{70} and even to C_{80}; though at such temperatures and molecular weights many compounds will decompose and give confused multiple peaks due to the fragments; charring may also occur.

Other detectors than FID can be used with other homologous series of compounds with known LTPRI than n-alkanes. (See Ref 19).

Appendix

A.1 Rigorous Calculation of Linear Temperature Programmed Retention Indices

The Kovats method of assigning retention indices calculates the logarithmeic retention of a solute interpolated between those of two standard compounds (4). The standard compounds can be comprised of any homologous series of organic compounds. The standards most commonly adopted are the n-alkane series. The logarithmic relationship which prevails under isothermal gas chromatographic operating conditions is replaced, under linear temperature programmed elution, by a near-linear relationship expressed by the equation of Van Den Dool and Kratz (5)

$$I = 100z + 100 \frac{[t_{Rx} - t_{Rz}]}{[t_{Rz+1} - t_{Rz}]}$$

where I = linear temperature programmed retention index
t_{Rx} = retention time of unknown
t_{Rz} = retention time of the n-alkane (with Z carbon atoms) eluting immediately before the unknown
t_{Rz+1} = retention time of the n-alkane eluting immediately after the unknown

However, it has been clearly demonstrated that the linear relationship between retention data for the n-alkane series does not strictly hold true especially at the low molecular weight end of the series (6). Thus other approaches to the fitting of a mathematical function to retention time data have been explored. These have included the application of polynomial fits and various cubic spline techniques (6,7,8).

The method used when calculating the linear programmed retention indices given in Tables 1–5 was a computerized polynomial routine which used the Water Research Centre in-house computer—a DEC VAX 11/780. It utilized two Fortran sub-routines which are derived from the DEC VAX NAG library and which is not generally accessible. However the following text provides references which give the information on which these sub-routines are based and from which users may work out their own programme.

The method employed is due to Forsythe (9) and is based upon the generation of a set of polynomials orthogonal with respect to summation over the normalized data set. The extensions due to Clenshaw (10) to represent these polynomials as well as the approximating polynomials in their Chebyshev-series forms are incorporated. The modifications suggested by Reimsch and Gentleman (11) to the method originally employed by Clenshaw for evaluating the orthogonal polynomials from the Chebysev-series representations are used to give greater numerical stability.

The routine determines the least squares polynomial approximations of degrees 0, 1 ..... K to the set of data points (X(R), Y(R)) with weights W(R) (R = 1,2,....M). The value of K + 1 when K is the maximum degree required is specified by the user.

The approximation of degree I has the property that it minimizes SIGMA (I), the sum of the squares of the weighted residuals EPS (R) (R = 1,2, ...M), where

$$EPS(R) = W(R)\ X\ (Y(R) - F(R))$$

and F(R) is the value of the polynomial of degree I at the Rth data point.

Each polynomial is represented in the Chebyshev-series form with normalized argument X. This argument lies in the range −1 to +1 and is related to the original variable X by the linear transformation

$$X = (2 \times X - XMAX - XMIN)/(XMAX - XMIN).$$

Here XMAX and XMIN are respectively the largest and smallest values of X(R). The polynomial approximation of degree I is represented as

$$0.5 \times A\ (I+1,1) \times T_0(\overline{X}) + A\ (I+1,2) \times T_1\ (\overline{X})$$
$$+ A\ (I+1,3) \times T_2\ (\overline{X}) + ... + A\ (I+1,I+1) \times TI\ (\overline{X})$$

where TJ (X) is the Chebyshev polynomial of the first kind of degree J with argument ($\overline{X}$).

For each value of I (I = 0,1,...K) the routine produces the values of A(I + 1, J + 1) (J = 0, 1...I), together with the value of the root mean square residual S (I + 1) defined by the square root of SIGMA (I)/(M − I − 1). In the case M = I + 1 the routine sets the value of S (I + 1) to zero.

A further routine evaluates the polynomial:

$$0.5 \times A(1) \times T_0(\overline{X}) + A(2) \times T_1(\overline{X}) + A(3) \times T_2(\overline{X}) + \ldots + A(\text{NPLUS } 1) \times T_N(\overline{X})$$

for any value of $\overline{X}$ satisfying $-1 \leqslant X \leqslant 1$. Here Tj (X) denotes the Chebyshev polynomial of the first kind of degree J with argument $\overline{X}$. The value of NPLUS1 = N + 1 is prescribed by the user.

While the mathematics of this system of calculation appears complex it is nevertheless simple in operation and provides reliable 'best fit' data.

A.2 Examples of Computer Calculation Programmes

The following examples shows how such a programme was developed for use on computers using IBM and BBC 'BASIC'. They employ a cubic spline approach.

BBC users see Section A2.1. IBM users see either A2.2 or A2.1 plus A2.3.

For more information, using Fortran, see also Ref 21. It is known that other suitable programmes also exist. It is suggested that new users of this method check the suitability of their chosen programme.

A2.1 Using BBC 'BASIC'

```
1REM
2REM
3REM
4REM
5REM
6REM
7REM
9
10ONERROR:REPORT:END
11
90GOSUB 1000: REM initialise variables
99
100FORTT%=0 TO 1
110GOSU 2000: REM input-data
120GOSU 1500: REM Test spline against existing routines
186NEXT
900END
999
1000REM Subroutine to initialise variables
1010
1100 DIMx(40,.y(400, knots(40),U(40)
1110 DIM Unknown X(40), Old-calc(40)
1490RETURN
1499
1500REM Subroutine to test spline against existing progam
1509
1510PRINT' 'titles':@%=&20306: REM Change to PRINT USING ££.£££
1519                          : REM
1520TIME=0:dydx1=1E26:dydxn=1E26:GOSUB10000:T%=TIME
1530PRINT"Time taken to calculate 2nd order derivatives="T%/100;" secs." '
1540TIME=0: FORI%=TOM%:X=UnknownX(I%):GOSUB11000:NEXT:T%=TIME
1550PRINT"Time taken to calculate interpolated value="T%/100*M%);" secs"
1559
1560PRINT' ' " Retention  Calculated indices"
1570PRINT" time/min       new     old" ' '
1600FORJ%=1TOM%
1610@%=&20306:PRINT" "UnknownX(J%):"          ";
1620@%=&20106:X=UnknownX(J%):GOSUB11000: PRINTspline"          "
```

```
1630@% = &20106: PRINTOld-calc(J%)
1650NEXT
1990RETURN
1999
2000REM Subroutine input-data
2010
2050REM     Routine to input test data from DATA statements
2099
2100 READ N%                        : REM Input number of x & y values
2105 READ titles                    : REM Input file title
2109
2110 FOR I% = 1 TO N%
2120 READ y(I%),x(I%)               : REM Input N% pairs of x,y values
2130 NEXT I%
2149
2150 READ M%                        : REM Input number of unknown values
2159
2160 FOR I% = 1 TO M%
2170 READ Old-cal (I%)              : REM Input original calculated values
2180 READ UnknownX(I%)              : REM Input unknown x values
2190 NEXT I%
2199
2290RETURN
2299
2500rem          **** Test Data ****
2509
2510DATA 25."Non-Polar Column (24 standards)"
2519
2520DATA    700.   4.319
2530DATA    800.   6.448
2540DATA    900.   9.629
2550DATA   1000.  13.455
2560DATA   1100.  17.439
2570DATA   1200.  21.340
2580DATA   1300.  25.062
2590DATA   1400.  28.578
2600DATA   1500.  31.897
2610DATA   1600.  35.049
2620DATA   1700.  38.037
2630DATA   1800.  40.899
2640DATA   1900.  43.640
2650DATA   2000.  46.283
2660DATA   2100.  48.828
2670DATA   2200.  51.288
2680DATA   2300.  53.659
2690DATA   2400.  55.937
2700DATA   2500.  58.123
2710DATA   2600.  60.220
2720DATA   2800.  64.149
2730DATA   3000.  67.823
2740DATA   3200.  71.298
2750DATA   3600.  78.863
2799
2800DATA    8
2809
2810DATA    849.   8.018
2820DATA    975.  12.709
2830DATA   1148.  19.378
2840DATA   1248.  23.167
2850DATA   1252.  23.306
2860DATA   1312.  25.477
2870DATA   1913.  44.021
2880DATA   2505.  58.228
2999
```

```
3010DATA  20. "Polar Column (20 standards)"
3019
3020DATA  1000.  5.014
3030DATA  1100.  7.262
3040DATA  1200. 10.211
3050DATA  1300. 13.541
3060DATA  1400. 16.981
3070DATA  1500. 20.361
3080DATA  1600. 23.621
3090DATA  1700. 26.736
3100DATA  1800. 29.720
3110DATA  1900. 32.580
3120DATA  2000. 35.325
3130DATA  2100. 37.957
3140DATA  2200. 40.493
3150DATA  2300. 42.936
3160DATA  2400. 45.298
3170DATA  2500. 47.595
3180DATA  2600. 49.825
3190DATA  2800. 54.104
3200DATA  3000. 58.143
3210DATA  3200. 62.658
3219
3300DATA   6
3309
3310DATA  1009.  5.174
3320DATA  1234. 11.339
3330DATA  1265. 12.378
3340DATA  1474. 19.473
3350DATA  2636. 50.480
3360DATA  3104. 60.591
9999
10000 REM Subroutine to calculate spline
10010
10050REM Given two arrays x( ) and y( ) this procedure
10060REM calculates the second derivatives of the
10070REM interpolating function at the tabulated points x( ).
10099
10100REM     **** Arguments ****
10109
10110REM  Global      x( )  x values
10120REM              y( )  y values
10130REM         knots( )  second derivatives of the
10140REM                   interpolating function
10150REM             U( )  working array
10199
10200REM           N%      number of points
10210REM         dydxl     dy/dx at first point
10220REM                   (signals natural spline if > 1E25)
10230REM         dydxn     dy/dx at last point
10240REM                   (signals natural spline if > 1E25)
10250REM     On.Un.sig.p   working variables
10299
10300REM     **** Set lower end point condition ****
10309
10310REM      Set condition to be a natural spline
10319
10320 If dydx1 > 1E25 knots(1)=0
10330 If dydx1 >          U(1)=0
10339
10340REM     Set to specified first derivative
10349
10350 If dydx1 < 1E25 knots(1)=-0.5
10360 If dydx1 < 1E25      U(1)=(3/(x(2)-x(1))*((y(2)-y(1))/(x(2)-x(1))-dydx1)
```

```
10399
10400REM      **** Decomposition loop of triangonal matrix ****
10409
10450  For I% = 2 To N%
10460          sig  =  (x(I%) - x(I% - 1))/(x(I% + 1) - x(I% - 1))
10470            p  =  sig*knots (I% - 1) + 2
10480 knots (I%)  =  (sig - 1)/p
10489
10490      U(I%)  =  (y(I% + 1) - y(I%))/(xI% + 1) - x(I%))
10500      U(I%)  =  U(I%) - (y(I%) - y(I% - 1))/(x(I%) - x(I% - 1))
10510      U(I%)  =  (6*U(I%)/(xI% + 1) - x(I% - 1)) - sig*U(I% - 1))/p
10520NEXT I%
10549
10550REM  **** Set higher end point condition ****
10559
10560REM  Set condition to be a natural spline
10569
10570 If dydxn > 1E25 Qn = 0
10580 If dynxn > 1E25 Un = 0
10589
10590REM  Set to specified first derivative
10599
10600 If dydxn < 1E25     Qn =  - 0.5
10610 If dydxn < 1E25     Un = (3/(xN%) - x(N% - 1))
10620 If dydxn < 1E25     Un - Un*(dydxn - (y(N%) - y(N% - 1))/(x N%) - x(N% - 1)))
10629
10630 knots (N%) = (Un - Qn*U (N% - 1))/(Qn*knots (N% - 1) + 1)
10639
10650REM  **** Backsubstitution loop of tridiagonal algorithm ****
10659
10660 For I% = N% - 1 TO 1 STEP  - 1
10670 knots(I%) = knots (I%) *knots (I% + 1) + U(I%)
10680 NEXT I%
10689
10690 RETURN
10699
11000REM Subroutine Function spline
11010
11050REM  Given two arrays x( ) and y( ) and a value of x
11060REM  this procedure calculates a cubic-spline interpolated
11070REM  value y
11099
11100REM                  **** Arguments *****
11109
11110REM  Global      x( )   x values
1120REM             y( )   y values
1130REM        knots ( )   second derivatives of the
1140REM                    interpolating function
11199
11200REM              N%   number of points
11210REM              X    x values for which calculated y value
11220REM                   is required
11230REM  Local       Y    Calculated y value, interpolated using
11240REM                   cubic spine
11250REM              a,b,h working variables
11260REM            low,high
11299
11300REM    ****   Find the appropriate spline using    ****
11310REM    ****         a bisection routine             ****
11319
11350  low = 1
11360  high = N%
11370  K% = (high + low)/2
11380  If (x(K%)>X) high = K% ELSE low = K%
```

```
11390  If (high-low)>=2 GOTO 11370
11399
11400REM      **** Interpolate using cubic between 'low' and 'high'; ****
11409
11410  h=x(high)-x(low)
11450  a=(x(high)-X)/h
11460  b=(X-x(low))/h
11470  Y=a*y(low) +b*y(high)
11480 spline=Y+(a 3-a)*knots (low)+(b 3-b)*knots(high))*h 2/6
11490RETURN
```

A2.2 Using IBM (GW Basic Compatible)

```
1 REM
2 REM
3 REM
4 REM
5 REM
6 REM
7 REM
9 REM
10 REM ONERROR:REPORT:END
11 REM
90 GOSUB 1000   :REM initialise variables
99 REM
100 FOR TT%=0 TO 1
110 GOSUB 2000   :REM inputdata
120 GOSUB 1500   :REM Test spline against existing routines
186 NEXT
900 END
999 REM
1000 REM Subroutine to initialise variables
1010 REM
1100 DIM X(40),Y(40),KNOTS(40),(U)(40)
1110 DIM UNKNOWNX(40),OLDCALC(40)
1490 RETURN
1499 REM
1500 REM Subroutine to test spline against existing program
1509 REM
1519 REM                              :REM
1520 TIME=0:DYDX1=1E+26:DYDXN=1E+26:GOSUB 10000:T%=TIME
1530 PRINT"Time taken to calculate 2nd order derivatives="T%/100;" secs." '
1540 TIME=0: FOR I%=1 TO M%:X=UNKNOWNX(I%):GOSUB 11000:NEXT:T%=TIME
1550 PRINT"Time taken to calculate interpolated value      ="T%/(100*M%);" secs"
1559 REM
1560 PRINT' ' "  Retention      Calculated indices"
1570 PRINT"   time/min          new        old" ' '
1600 FOR J%=1 TO M%
1610 PRINT"      ";UNKNOWNX(J%);"         ";
1620 X=UNKNOWNX(J%):GOSUB 11000:PRINT SPLINE"     ";
1630 PRINT OLDCALC(J%)
1650 NEXT
1990 RETURN
1999 REM
2000 REM Subroutine inputdata
2010 REM
2050 REM      Routine to input test data from DATA statements
2099 REM
2100 READ N%                    : REM Input number of x & y values
2105 READ TITLES                : REM Input file title
2109 REM
2110 FOR I%=1 TO N%
2120 READ Y(I%),X(I%)           : REM Input N% pairs of x,y values
2130 NEXT I%
```

```
2149 REM
2150 READ M%                    : REM Input number of unknown values
2159 REM
2160 FOR I% = 1 TO M%
2170 READ OLDCALC(I%)          : REM Input original calculated values
2180 READ UNKNOWNX(I%)         : REM Input unknown x values
2190 NEXT I%
2199 REM
2290 RETURN
2299 REM
2500 REM        **** Test Data ****
2509 REM
2510 DATA 24,"Non-Polar Column ( 24 standards )"
2519 REM
2520 DATA  700,  4.319
2530 DATA  800,  6.448
2540 DATA  900,  9.629
2550 DATA 1000, 13.455
2560 DATA 1100, 17.439
2570 DATA 1200, 21.340
2580 DATA 1300, 25.062
2590 DATA 1400, 28.578
2600 DATA 1500, 31.897
2610 DATA 1600, 35.049
2620 DATA 1700, 38.037
2630 DATA 1800, 40.899
2640 DATA 1900, 43.640
2650 DATA 2000, 46.283
2660 DATA 2100, 48.828
2670 DATA 2200, 51.288
2680 DATA 2300, 53.659
2690 DATA 2400, 55.937
2700 DATA 2500, 58.123
2710 DATA 2600, 60.220
2720 DATA 2800, 64.149
2730 DATA 3000, 67.823
2740 DATA 3200, 71.298
2750 DATA 3600, 78.863
2799 REM
2800 DATA 8
2809 REM
2810 DATA  849,  8.018
2820 DATA  975, 12.709
2830 DATA 1148, 19.378
2840 DATA 1248, 23.167
2850 DATA 1252, 23.306
2860 DATA 1312, 25.477
2870 DATA 1913, 44.021
2880 DATA 2505, 58.228
2999 REM
3010 DATA 20, "Polar Column ( 20 standards )"
3019 REM
3020 DATA 1000,  5.014
3030 DATA 1100,  7.262
3040 DATA 1200, 10.211
3050 DATA 1300, 13.541
3060 DATA 1400, 16.981
3070 DATA 1500, 20.361
3080 DATA 1600, 23.621
3090 DATA 1700, 26.736
3100 DATA 1800, 29.720
3110 DATA 1900, 32.580
3120 DATA 2000, 35.325
3130 DATA 2100, 37.957
```

```
3140 DATA 2200, 40.493
3150 DATA 2300, 42.936
3160 DATA 2400, 45.298
3170 DATA 2500, 47.595
3180 DATA 2600, 49.825
3190 DATA 2800, 54.104
3200 DATA 3000, 58.143
3210 DATA 3200, 62.658
3219 REM
3300 DATA 6
3309 REM
3310 DATA 1009,  5.174
3320 DATA 1234, 11.339
3330 DATA 1265, 12.378
3340 DATA 1474, 19.473
3350 DATA 2636, 50.480
3360 DATA 3104, 60.591
9999 REM
10000 REM Subroutine to calculate spline
10010 REM
10050 REM      Given two arrays x( ) and y( ) this procedure
10060 REM      calculates the second derivatives of the
10070 REM      interpolating function at the tabulated points x( ).
10099 REM
10100 REM              **** Arguments ****
10109 REM
10110 REM  Global     x( )     x values
10120 REM             y( )     y values
10130 REM         knots( )     Second derivatives of the
10140 REM                      interpolating function
10150 REM            U( )     working array
10199 REM
10200 REM           N%        number of points
10210 REM         dydx1       dy/dx at first point
10220 REM                     (signals natural spline if > 1E25)
10230 REM         dydxn       dy/dx at last point
10240 REM                     (signals natural spline if > 1E25)
10250 REM   Qn,Un,sig,p       working variables
10299 REM
10300 REM      ****   Set lower end point condition   ****
10309 REM
10310 REM      Set condition to be a natural spline
10319 REM
10320 IF DYDX1 > 9.999999E+24 THEN KNOTS(1)=0
10330 IF DYDX1 > 9.999999E+24  THEN U(1)=0
10339 REM
10340 REM      Set to specified first derivative
10349 REM
10350 IF DYDX1 < 9.999999E+24 THEN KNOTS(1)= -.5
10360 IF DYDX1 < 9.999999E+24 THEN U(1)=(3/(X(2)-X(1)))*((Y(2)-Y(1))/(X(2)-X(1))-DYDX
10399 REM
10400 REM      ****   Decomposition loop of triangonal matrix   ****
10409 REM
10450  FOR I%=2 TO N%
10460         SIG  =  (X(I%)-X(I%-1))/(X(I%+1)-X(I%-1))
10470           P  =  SIG*KNOTS(I%-1)+2
10480 KNOTS(I%)  =  (SIG-1)/P
10489 REM
10490       U(I%)  =  (Y(I%+1)-Y(I%))/(X(I%+1)-X(I%))
10500       U(I%)  =  U(I%)-(Y(I%)-Y(I%-1))/(X(I%)-X(I%-1))
10510       U(I%)  =  (6*U(I%)/(X(I%+1)-X(I%-1))-SIG*U(I%-1))/P
10520 NEXT I%
10549 REM
10550 REM      ****   Set higher end point condition   ****
```

```
10559 REM
10560 REM    Set condition to be a natural spline
10569 REM
10570 IF DYDXN > 9.999999E+24  THEN QN=0
10580 IF DYDYN > 9.999999E+24  THEN UN=0
10589 REM
10590 REM      Set to specified first derivative
10599 REM
10600 IF DYDXN < 9.999999E+24  THEN QN= -0.5
10610 IF DYDXN < 9.999999E+24  THEN UN=(3/(X(N%)-X(N%-1)))
10620 IF DYDXN < 9.999999E+24  THEN UN=UN*(DYDXN-(Y(N%)-Y(N%-1))/(X(N%)-X(N%-1)))
10629 REM
10630 KNOTS(N%)=(UN-QN*U(N%-1))/(QN*KNOTS(N%-1)+1)
10639 REM
10650 REM      ****    Backsubstitution loop of tridiagonal algorithm    ****
10659 REM
10660 FOR I%=N%-1 TO 1 STEP -1
10670 KNOTS(I%)=KNOTS(I%) * KNOTS(I%+1)+U(I%)
10680 NEXT I%
10689 REM
10690 RETURN
10699 REM
11000 REM Subroutine Function spline
11010 REM
11050 REM      Given two arrays x( ) and y( ) and a value of X
11060 REM      this procedure calculates a cubic-spline interpolated
11070 REM      value Y.
11099 REM
11100 REM              **** Arguments *****
11109 REM
11110 REM  Global     x( )   x values
11120 REM             y( )   y values
11130 REM         knots( )   Second derivatives of the
11140 REM                    interpolating function
11199 REM
11200 REM             N%    number of points
11210 REM             X     x value for which calculated y value
11220 REM                   is required.
11230 REM  Local      Y     Calculate y value, interpolated using
11240 REM                   cubic spine.
11250 REM          a,b,h    working variables
11260 REM        low,high
11299 REM
11300 REM     ****    Find the appropriate spline using    ****
11310 REM     ****          a bisection routine.           ****
11319 REM
11350 LOW=1
11360 HIGH=N%
11370 K%=(HIGH+LOW)/2
11380 IF (X(K%)>X)THEN HIGH=K% ELSE LOW=K%
11390 IF (HIGH-LOW)>=2 GOTO 11370
11399 REM
11400 REM      ****    Interpolate using cubic between 'low' and 'high'    ****
11409 REM
11410 H=X(HIGH)-X(LOW)
11450 A=(X(HIGH)-X)/H
11460 B=(X-X(LOW))/H
11470 Y=A*Y(LOW) +B*Y(HIGH)
11480 SPLINE=Y+((A^3-A)*KNOTS(LOW)+(B^3-B)*KNOTS(HIGH))*H^2/6
11490 RETURN
```

Comparison of Methods of Calculation

(i) Non Polar Column with 24 standards and 8 unknown samples (as in 5.1.3)

Retention time/min	Calculated by A.2	Indices by A.1	A.2–A.1	Calculated using the Van den Dool and Katz equation*
8.018	855.0	849.0	6.0	849.4
12.709	980.9	975.0	5.9	980.5
19.378	1149.2	1148.0	1.2	1149.7
23.167	1248.4	1248.0	0.4	1249.1
23.306	1252.2	1252.0	0.2	1252.8
25.477	1311.5	1312.0	−0.5	1311.8
44.021	1914.2	1913.0	1.2	1914.4
58.228	2504.9	2505.0	−0.1	2505.0

(ii) Polar Column with 20 standards and 6 unknown samples (as in 5.1.3).

Retention time/min	Calculated by A.2	Indices by A.1	A.2–A.1	Calculated using the Van den Dool and Katz equation*
5.174	1007.5	1009.0	−1.5	1007.1
11.339	1234.3	1234.0	−0.3	1233.9
12.378	1265.5	1265.0	0.5	1265.1
19.473	1473.4	1474.0	−0.6	1473.7
50.480	2629.7	2636.0	−6.3	2630.6
60.591	3111.1	3104.0	7.1	3108.4

Note if manual plotting were used using a calibrated spline (as in Section 5.1), the indices obtained would not be as accurate and would be partly dependent on the degree of time scale enlargement obtainable from the recorder.

* Calculated by British Gas plc London Research Station

A2.3 Note M Tech Computer Services (4 Church Hill, Reepham Norfolk, 0603, 870620) have an inexpensive computer programme available for translating BBC Basic to IBM compatible MSDGS (IBM information).

References

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Address for Correspondence

(See also section 6 above for queries about Index Values).

However thoroughly a procedure may be tested, there is always the possibility of a user discovering a hitherto unknown problem. Users with information on this procedure are requested to write to:

The Secretary
The Standing Committee of Analysts
The Department of the Environment
Romney House
43 Marsham Street
LONDON SW1P 3PY
England

Table 1 Typical Standard Deviations for LTPRI determined with the non polar polydimethylsiloxane PS225 column. (data to nearest whole number, all repeat measurements determined on different columns of the same type).

Substance	LTPRI	Standard Deviation*	Degrees of Freedom
n butanol	0661	±1	2
Benzene	0662	±7	12
2 pentanone	0674	±1	2
1.4 dioxane	0692	±1	2
1 nitropropane	0708	±1	2
2 methyl 2 pentanol	0723	±1	2
Pyridine	0732	±6	1
1.iodobutane	0797	±1	2
2 octyne	0869	–	2
Hydrindane	0976	±2	12
Octanol	1056	±0.4	4
2.6 dimethylphenol	1079	±1	4
2 ethylhexanoic acid	1117	±1	3
2.6 dimethyl aniline	1130	±0.5	4
Naphthalene	1155	±2	9
Methyl decanoate	1308	±1	4
Dicyclohexylamine	1400	–	1
Methyl undecanoate	1408	±1	4
Methyl dodecanoate	1508	±1	4
Diethylphthalate	1548	±1	9
Pristane	1710	±1	9
Pyrene	2059	±6	9
Di(2-ethylhexyl) phthalate	2504	±1	9
Perylene	2811	±11	9
Cholesterol	3091	±7	9

*based on the percentage section of the LTPRI (also Tables 2 and 3)

Table 2 Typical Standard Deviations for LTPRI determined with the polar polyethyleneglycol Carbowax 20M column

Substance	LTPRI	Standard Deviation*	Degrees of Freedom
o-Xylene	1181	±4	7
Anisole	1331	±4	7
Furfural	1447	±5	7
Pristane	1674	±4	7
Naphthalene	1710	±4	7
B-Ionone	1910	±6	7
Acenapthene	2092	±6	7
Diethyl phthalate	2335	±6	7

Table 3 Typical Standard Deviations for LTPRI determined with a polar Superox 0.6 column

Substance	LTPRI	Standard Deviation*	Degrees of Freedom
o-Xylene	1173	±2	3
Anisole	1324	±2	3
Furfural	1431	±2	3
Pristane	1667	±2	3
Naphthalene	1706	±2	3
B-Ionone	1909	±1	3
Acenapthene	2092	±2	3
Diethyl phthalate	2316	±2	3

Table 4 Linear Temperature Programmed Retention Indices Truncated Version in Retention Index Order—Methyl Silicone Columns

Retention index	Compound name	Stationary phase
0661	butanol, 1-	OV-1
0669	benzene	OV-1
0674	pentanone, 2-	OV-1
0692	dioxane, 1, 4-	OV-1
0707	propane, 1-nitro	OV-1
0723	pentanol, 2-methyl-2-	OV-1
0732	pyridine	OV-1
0768	methane, dibromochloro	OV-1
0797	butane, 1-iodo	OV-1
0827	benzene, chloro	OV-1
0832	picoline, beta (3-methylpyridine)	OV-1
0832	picoline, gamma (4-methylpyridine)	OV-1
0846	benzene, ethyl	OV-1
0852	methane, tribromo	OV-1
0860	methane, bis-(methylthio)	OV-1
0869	disulphide, ethylmethyl	OV-1
0869	disulphide, ethylmethyl	OV-1
0876	ethane, 1, 1, 2, 2-tetrachloro	OV-1
0923	heptanone, 5-methyl-3-	OV-1
0931	toluene, 2-chloro	OV-1
0932	toluene, 3-chloro	OV-1
0936	toluene, 4-chloro	OV-1
0959	phenol	OV-1
0962	hepten-2-one, 6-methyl-5-	OV-1
0965	phenol, 2-chloro	OV-1
0975	hydrindane, cis- (hexahydroindane)	OV-1
0981	benzene, 1, 3-dichloro	OV-1
0983	toluene, alpha-chloro (benzyl chloride)	OV-1
0985	benzene, 1, 4-dichloro	OV-1
1007	benzene, 1, 2-dichloro	OV-1
1046	benzene, nitro	OV-1
1051	triazine, 2, 4, 6-trichloro-1, 3, 5- (cyanuric chloride)	OV-1
1055	ethane, hexachloro	OV-1
1056	octanol, 1-	OV-1
1076	pyrazine, 2-isopropyl-3-methoxy	OV-1
1079	phenol, 2, 6-dimethyl	OV-1
1094	aniline, 2-chloro	OV-1
1106	toluene, alpha, alpha-dichloro (benzal chloride)	OV-1
1117	hexanoic acid, 2-ethyl	OV-1
1123	phenol, 2, 4-dimethyl (m-xylenol)	OV-1
1125	phenol, 2, 5-dimethyl (2, 5-xylenol)	OV-1

Retention index	Compound name	Stationary phase
1130	aniline, 2, 6-dimethyl	OV-1
1140	phenol, 2, 4-dichloro	OV-1
1150	benzene, 1, 2, 4-trichloro	OV-1
1155	naphthalene	OV-1
1156	naphthalene	OV-1
1158	aniline, 3-chloro	OV-1
1160	pyrazine, 2-isobutyl-3-methoxy	OV-1
1161	aniline, 4-chloro	OV-1
1161	thianaphthene	OV-1
1164	borneol, 2-methyliso	OV-1
1167	phenol, 3, 4-dimethyl (3, 4-xylenol)	OV-1
1171	phenol, 4-chloro	OV-1
1173	phenol, 3-chloro	OV-1
1182	toluidine, 3-chloro-o-	OV-1
1185	benzene, 1-chloro-3-nitro	OV-1
1193	benzene, 1-chloro-4-nitro	OV-1
1195	aniline, 2-chloro-4-methyl	OV-1
1199	benzene, 1-chloro-2-nitro	OV-1
1201	toluidine, 6-chloro-m-	OV-1
1202	benzene, hexachloro (HCB)	OV-1
1202	butadiene, hexachloro	OV-1
1204	aniline, 2, 6-dichloro	OV-1
1249	toluidine, 6-chloro-o-	OV-1
1252	toluidine, 2-chloro-p-	OV-1
1253	aniline, 2-chloro-4-methyl	OV-1
1256	toluidine, 4-chloro-o-	OV-1
1256	toluidine, 5-chloro-o-	OV-1
1259	toluene, 6-chloro-2-nitro	OV-1
1260	phenol, 4-chloro-3-methyl	OV-1
1268	toluene, 4-chloro-2-nitro	OV-1
1287	aniline, 2, 4-dichloro	OV-1
1288	aniline, 2, 5-dichloro	OV-1
1288	benzene, 3, 5-dichloronitro	OV-1
1290	benzonitrile, 2, 6-dichloro (dichlobenil)	OV-1
1301	benzene, 1, 2, 4, 5-tetrachloro	OV-1
1302	anisole, 2, 4, 6-trichloro	OV-1
1304	phenol, 2, 3, 5-trichloro	OV-1
1306	aniline, 2, 3-dichloro	OV-1
1308	decanoic acid, methyl ester	OV-1
1312	toluene, 4-chloro-3-nitro	OV-1
1315	benzene, 2, 5-dichloronitro	OV-1
1316	toluene, 2-chloro-4-nitro	OV-1
1318	cyclopentadiene, hexachloro	OV-1
1322	benzene, 2, 4-dichloronitro	OV-1
1327	phenol, 2, 4, 5-trichloro	OV-1
1332	phenol, 2, 3, 4-trichloro	OV-1
1339	benzene, 3, 4-dichloronitro	OV-1
1341	anisole, 2, 3, 6-trichloro	OV-1
1344	benzene, 2, 3-dichloronitro	OV-1
1346	phenol, 2, 3, 6-trichloro	OV-1
1348	biphenyl	OV-1
1348	naphthalene, 1-chloro	OV-1
1348	naphthalene, 2-chloro	OV-1
1352	aniline, 3, 5-dichloro	OV-1
1377	aniline, 3, 4-dichloro	OV-1
1384	decalol, trans-1, 10-dimethyl-trans-9- (geosmin)	OV-1
1392	toluene, 2, 6-dinitro	OV-1
1400	dicyclohexylamine	OV-1
1408	undecanoic acid, methyl ester	OV-1
1412	acenaphthylene	OV-1
1415	phenol, 2-amino-4-chloro	OV-1

Retention index	Compound name	Stationary phase
1435	phenol, 2, 4-dinitro	OV-1
1465	anisole, 2, 3, 4-trichloro	OV-1
1468	toluene, 2, 4-dinitro	OV-1
1490	benzene, 1-chloro-2, 4-dinitro	OV-1
1494	anisole, 2, 3, 5, 6-tetrachloro	OV-1
1494	anisole, 2, 4, 5-trichloro	OV-1
1507	dodecanoic acid, methyl ester	OV-1
1538	aniline, 4-chloro-2-nitro	OV-1
1548	phthalic acid, diethyl ester	OV-1
1575	aniline, N-phenyl	OV-1
1588	acetic acid, methyl ester, 2, 4-dichlorophenoxy (2, 4-D methyl ester)	OV-1
1588	hydrazine, 1, 2-diphenyl	OV-1
1589	phenol, 3, 4, 5-trichloro	OV-1
1610	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H- (chlordane)	OV-1
1614	phosphoric acid, tributyl ester	OV-1
1645	cyclohexane, alpha-hexachloro (alpha-BHC)	OV-1
1645	cyclohexane, hexachloro (BHC)	OV-1
1652	ether, 4-bromophenyl phenyl	OV-1
1660	toluidine, alpha, alpha, alpha-trifluoro-2, 6-dinitro-N, N-dipropyl-p- (trifluralin)	OV-1
1672	cyclohexane, beta-hexachloro (beta-BHC)	OV-1
1680	benzene, hexachloro (HCB)	OV-1
1689	anisole, pentachloro	OV-1
1699	triazine-2, 4-diamine, 2-chloro-N-ethyl-N′-(1-methylethyl)-1, 3, 5- (atrazine)	OV-1
1704	cyclohexane, gamma-hexachloro (gamma-BHC, lindane)	OV-1
1709	pentadecane, 2, 6, 10, 14-tetramethyl (pristane)	OV-1
1713	triazine-2, 4-diamine, 6-chloro-N, N′-bis (1-methylethyl)-1, 3, 5- (propazine)	OV-1
1715	phenol, pentachloro	OV-1
1721	benzene, n-butyl, sulphonamide	OV-1
1752	anthracene	OV-1
1766	phosphorothioic acid, OO-diethyl O-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester (diazinon)	OV-1
1771	phenol, 2-sec-butyl-4, 6-dinitro (dinoseb)	OV-1
1816	propionanilide, 3′, 4′-dichloro (propanil)	OV-1
1834	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H- (chlordane)	OV-1
1841	acetic acid, butyl ester, 2, 4-dichlorophenoxy (2, 4-D butyl ester)	OV-1
1873	indene, 1, 4, 5, 6, 7, 8, 8-heptachloro-3a, 4, 7, 7a-tetrahydro-4, 7-methano-1H- (heptachlor)	OV-1
1874	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H- (chlordane)	OV-1
1903	urea, 3-(3, 4-dichlorophenyl)-1-methyoxy-1-methyl (linuron)	OV-1
1915	parathion oxygen analog	OV-1
1920	phosphorodithioic acid, OO-dimethyl S-1, 2-dicarbethoxyethyl ester (malathion)	OV-1
1931	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H (chlordane)	OV-1
1939	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H- (chlordane)	OV-1
1941	phosphorothioic acid, OO-diethyl O-4-nitrophenyl ester (parathion)	OV-1
1946	naphthalene, 1, 2, 3, 4, 10, 10-hexachloro-1, 4, 4, 5, 8, 8-hexahydro-exo-1, 4-endo-5, 8-dimethano (aldrin)	OV-1
1989	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H- (chlordane)	OV-1

Retention index	Compound name	Stationary phase
2012	indane, 1, 4, 5, 6, 7, 8, 8-heptachloro-2, 3-epoxy-3a, 4, 7, 7a-tetrahydro-4, 7-methano-1H- (heptachlor epoxide)	OV-1
2036	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H- (chlordane)	OV-1
2042	benzidine	OV-1
2042	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H- (chlordane)	OV-1
2061	pyrene	OV-1
2063	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H- (chlordane)	OV-1
2072	ethene, 1, 1-dichloro-2- (2-chlorophenyl)-2-(4-chlorophenyl) (o, p′-DDE)	OV-1
2073	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H- (chlordane)	OV-1
2086	benzodioxathiepin 3-oxide, 6, 7, 8, 9, 10, 10-hexachloro 1, 5,5a,6,9, 9a-hexahydro-6,9-methano-2, 4, 3- (endosulfan I)	OV-1
2086	norbornene-2, 3-dimethanol, 1, 4, 5, 6, 7, 7-hexachloro, cyclic sulphite, 5- (endosulphan)	OV-1
2097	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H- (chlordane)	OV-1
2116	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H- (chlordane)	OV-1
2139	naphthalene, 1, 2, 3, 4, 10, 10-hexachloro-6, 7-epoxy-1, 4, 4a, 5, 6, 7, 8, 8a-octahydro-exo-1, 4:5, 8-dimethano (dieldrin)	OV-1
2146	ethane, 1, 1-dichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl) (o, p′-TDE)	OV-1
2146	ethane, 2-(2-chlorophenyl)-2-(4-chlorophenyl)-1, 1-dichloro (2, 4′ DDD)	OV-1
2163	acetic acid, iso-octyl ester, 2, 4-dichlorophenoxy (2, 4-D iso-octyl ester)	OV-1
2183	benzodioxathiepin 3-oxide, 6, 7, 8, 9, 10, 10-hexachloro 1, 5, 5a, 6, 9, 9a-hexahydro-6, 9-methano-2, 4, 3- (endosulfan II)	OV-1
2213	ethane, 1, 1-dichloro-2, 2-bischlorophenyl (TDE)	OV-1
2232	ethane, 1, 1, 1-trichloro-2, 2-bis (chlorophenyl) (DDT)	OV-1
2234	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H- (chlordane)	OV-1
2249	indene, 1, 2, 4, 5, 6, 7, 8, 8-octachloro-2, 3, 3a, 4, 7, 7a-hexahydro-4, 7-methano-1H- (chlordane)	OV-1
2287	phthalic acid, butyl benzyl ester	OV-1
2300	ethane, 1, 1, 1-trichloro-2, 2-bis (4-chlorophenyl) (p, p′-DDT)	OV-1
2410	acetic acid, 4-chloro-2-methylphenoxy (MCPA)	OV-1
2419	diazepam	OV-1
2464	phosphorodithioic acid, O, O-dimethyl S-[(4-oxo-1, 2, 3-benzotriazin-3 (4H)-yl) methyl] ester (azinphos-methyl)	OV-1
2504	phthalic acid, di (2-ethylhexyl) ester	OV-1
2505	phthalic acid, di (2-ethylhexyl) ester	OV-1
2506	phthalic acid, di (2-ethylhexyl) ester	OV-1
2506	phthalic acid, dioctyl ester	OV-1
2553	phosphorodithioic acid, O, O-diethyl S-[(4-oxo-1, 2, 3-benzotriazin-3 (4H)-yl) methyl] ester (azinphos-ethyl)	OV-1
2654	phosphorothioic acid, O, O-diethyl O- (3-chloro-4-methyl-2-oxo-2H-1-benzopyran-7-yl) ester (coumaphos)	OV-1
2657	cyclopropanecarboxylic acid, 3-(2, 2-dichlorovinyl)-2, 2-dimethyl-, (3-phenoxyphenyl) methyl ester (permethrin)	OV-1
2676	benzacridine, dimethyl	OV-1
2814	perylene	OV-1
3093	cholesterol	OV-1

Table 5 Linear Temperature Programmed Retention Indices Full Version in Alphabetical Order of Compound Name—Methyl Silicone Columns

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
acenaphthylene									
cas no. 208-96-8									
1412	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
acetic acid, 4-chloro-2-methylphenoxy (MCPA)									
cas no. 94-74-6									
2410	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
acetic acid, butyl ester, 2,4-dichlorophenoxy (2,4-D butyl ester)									
cas no. 94-80-4									
1841	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
acetic acid, iso-octyl ester, 2,4-dichlorophenoxy (2,4-D iso-octyl ester)									
cas no. 25168-26-7									
2163	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
acetic acid, methyl ester, 2,4-dichlorophenoxy (2,4-D methyl ester)									
cas no. 1928-38-7									
1588	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 2,3-dichloro									
cas no. 608-27-5									
1306	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 2,4-dichloro									
cas no. 554-00-7									
1287	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 2,5-dichloro									
cas no. 95-82-9									
1288	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 2,6-dichloro									
cas no. 608-31-1									
1204	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 2,6-dimethyl									
cas no. 87-62-7									
1130	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 2-chloro									
cas no. 95-51-2									
1094	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 2-chloro-4-methyl									
cas no. 615-65-6									
1195	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1253	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 3,4-dichloro									
cas no. 95-76-1									
1377	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 3,5-dichloro									
cas no. 626-43-7									
1352	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 3-chloro									
cas no. 108-42-9									
1158	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 4-chloro									
cas no. 106-47-8									
1161	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 4-chloro-2-nitro									
cas no. 89-63-4									
1538	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, N-phenyl									
cas no. 122-39-4									
1575	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
anisole, 2,3,4-trichloro									
cas no. 54135-80-7									
1465	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
anisole, 2,3,5,6-tetrachloro									
cas no. 6936-40-9									
1494	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
anisole, 2,3,6-trichloro									
cas no. 50375-10-5									
1341	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
anisole, 2,4,5-trichloro									
cas no. 6130-75-2									
1494	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
anisole, 2,4,6-trichloro									
cas no. 87-40-1									
1302	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
anisole, pentachloro									
cas no. 1825-21-4									
1689	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
anthracene									
cas no. 120-12-7									
1752	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzacridine, dimethyl									
cas no. 2381-40-0									
2676	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene									
cas no. 71-43-2									
0669	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1,2,4,5-tetrachloro									
cas no. 95-94-3									
1301	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1,2,4-trichloro									
cas no. 120-82-1									
1150	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1,2-dichloro									
cas no. 95-50-1									
1007	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1,3-dichloro									
cas no. 541-73-1									
0981	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1,4-dichloro									
cas no. 106-46-7									
0985	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1-chloro-2,4-dinitro									
cas no. 121-86-8									
1490	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1-chloro-2-nitro									
cas no. 89-21-4									
1199	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1-chloro-3-nitro									
cas no. 88-73-3									
1185	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1-chloro-4-nitro									
cas no. 121-73-3									
1193	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 2,3-dichloronitro									
cas no. 3209-22-1									
1344	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 2,4-dichloronitro									
cas no. 611-06-3									
1322	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 2,5-dichloronitro									
cas no. 89-61-2									
1315	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
benzene, 3,4-dichloronitro									
cas no. 99-54-7									
1339	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 3,5-dichloronitro									
cas no. 618-62-2									
1288	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, chloro									
cas no. 108-90-7									
0827	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, ethyl									
cas no. 100-41-4									
0846	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, hexachloro (HCB)									
cas no. 118-74-1									
1202	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1680	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, n-butyl, sulphonamide									
cas no. 3622-84-2									
1721	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, nitro									
cas no. 98-95-3									
1046	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzidine									
cas no. 92-87-5									
2042	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzodioxathiepin 3-oxide, 6,7,8,9,10,10-hexachloro 1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3- (endosulfan I)									
cas no. 959-98-8									
2056	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzodioxathiepin 3-oxide, 6,7,8,9,10,10-hexachloro 1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3- (endosulfan II)									
cas no. 33213-65-9									
2183	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzonitrile, 2,6-dichloro (dichlobenil)									
cas no. 1194-65-6									
1290	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
biphenyl									
cas no. 92-52-4									
1348	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
borneol, 2-methyliso									
cas no. 2371-42-8									
1164	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
butadiene, hexacloro									
cas no. 87-68-3									
1202	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
butane, 1-iodo									
cas no. 542-69-8									
0797	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
butanol, 1-									
cas no. 71-36-3									
0661	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
cholesterol									
cas no. 57-88-5									
3093	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
cyclohexane, alpha-hexachloro (alpha-BHC)									
cas no. 319-84-6									
1645	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
cyclohexane, beta-hexacloro (beta-BHC)									
cas no. 319-85-7									
1672	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
cyclohexane, gamma-hexachloro (gamma-BHC, lindane)									
cas no. 58-89-9									
1704	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
cyclohexane, hexachloro (BHC)									
cas no. 608-73-1									
1645	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
cyclopentadiene, hexachloro									
cas no. 77-47-4									
1318	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
cyclopropanecarboxylic acid, 3-(2,2-dichlorovinyl)-2,2-dimethyl-, (3-phenoxyphenyl)methyl ester (permethrin)									
cas no. 52645-53-1									
2657	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
decalol, trans-1,10-dimethyl-trans-9- (geosmin)									
cas no. 19700-21-1									
1384	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
decanoic acid, methyl ester									
cas no. 110-42-9									
1308	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
diazepam									
cas no. 52357-79-6									
2419	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
dicyclohexylamine									
cas no. 101-83-7									
1400	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
dioxane, 1,4-									
cas no. 123-91-1									
0692	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
disulphide, ethylmethyl									
cas no. 2033-39-5									
0869	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
dodecanoic acid, methyl ester									
cas no. 111-82-0									
1507	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,1,1-trichloro-2,2-bis(4-chlorophenyl) (p,p'-DDT)									
cas no. 50-29-3									
2300	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,1,1-trichloro-2,2-bis(chlorophenyl) (DDT)									
cas no. 50-29-3									
2232	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,1,2,2-tetrachloro									
cas no. 79-34-5									
0876	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,1-dichloro-2,2-bischlorophenyl (TDE)									
cas no. 72-54-8									
2213	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,1-dichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl) (o,p'-TDE)									
cas no. 53-19-0									
2146	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 2-(2-chlorophenyl)-2-(4-chlorophenyl)-1,1-dichloro (2,4'DDD)									
cas no. 53-19-0									
2146	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, hexachloro									
cas no. 67-72-1									
1055	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,1-dichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl) (o,p'-DDE)									
cas no. 3424-82-6									
2072	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ether, 4-bromophenyl phenyl									
cas no. 101-55-3									
1652	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
heptanone, 5-methyl-3-									
cas no. 541-85-5									
0923	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
hepten-2-one, 6-methyl-5-									
cas no. 110-93-0									
0962	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
hexanoic acid, 2-ethyl									
cas no. 149-57-5									
1117	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
hydrazine, 1,2-diphenyl									
cas no. 122-66-7									
1588	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
hydrindane, cis- (hexahydroindane)									
cas no. 496-10-6									
0975	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
indane, 1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3a,4,7,7a-tetrahydro-4,7-methano-1H- (heptachlor epoxide)									
cas no. 1024-57-3									
2012	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H- (chlordane)									
cas no. 57-74-9									
1610	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1834	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1874	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1931	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1939	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1989	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2036	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2042	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2063	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2073	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2097	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2116	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2234	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2249	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
indene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-4,7-methano-1H- (heptachlor)									
cas no. 76-44-8									
1873	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
methane, bis-(methylthio)									
cas no. 1618-26-4									
0860	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
methane, dibromochloro									
cas no. 124-48-1									
0768	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
methane, tribromo									
cas no. 75-25-2									
0852	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
naphthalene									
cas no. 91-20-3									
1155	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1156	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
naphthalene, 1,2,3,4,10,10-hexachloro-1,4,4,5,8,8-hexahydro-exo-1,4-endo-5,8-dimethano (aldrin)									
cas no. 309-00-2									
1946	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
naphthalene, 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-exo-1,4:5,8-dimethano (dieldrin)									
cas no. 60-57-1									
2139	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
naphthalene, 1-chloro									
cas no. 90-13-1									
1348	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
naphthalene, 2-chloro									
cas no. 91-58-7									
1348	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro, cyclic sulphite, 5- (endosulphan)									
cas no. 115-29-7									
2086	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
octanol, 1-									
cas no. 111-87-5									
1056	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
pentadecane, 2,6,10,14-tetramethyl (pristane)									
cas no. 1921-70-6									
1709	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
pentanol, 2-methyl-2-									
cas no. 590-36-3									
0723	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
pentanone, 2-									
cas no. 107-87-9									
0674	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
perylene									
cas no. 198-55-0									
2814	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol									
cas no. 108-95-2									
0959	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2,3,4-trichloro									
cas no. 15950-66-0									
1332	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2,3,5-trichloro									
cas no. 933-78-8									
1304	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2,3,6-trichloro									
cas no. 933-75-5									
1346	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2,4,5-trichloro									
cas no. 95-95-4									
1327	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2,4-dichloro									
cas no. 120-83-2									
1140	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2,4-dimethyl (m-xylenol)									
cas no. 105-67-9									
1123	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2,4-dinitro									
cas no. 51-28-5									
1435	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2,5-dimethyl (2,5-xylenol)									
cas no. 95-87-4									
1125	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2,6-dimethyl									
cas no. 576-26-1									
1079	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2-amino-4-chloro									
cas no. 95-85-2									
1415	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2-chloro									
cas no. 95-57-8									
0965	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2-sec-butyl-4,6-dinitro (dinoseb)									
cas no. 88-85-7									
1771	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 3,4,5-trichloro									
cas no. 609-19-8									
1589	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
phenol, 3,4-dimethyl (3,4-xylenol)									
cas no. 95-65-8									
1167	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 3-chloro									
cas no. 108-43-0									
1173	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 4-chloro									
cas no. 106-48-9									
1171	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 4-chloro-3-methyl									
cas no. 59-50-7									
1260	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, pentachloro									
cas no. 87-86-5									
1715	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phosphoric acid, tributyl ester									
cas no. 126-73-8									
1614	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phosphorodithioic acid, O,O-diethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] ester (azinphos-ethyl)									
cas no. 2642-71-9									
2553	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phosphorodithioic acid, O,O-dimethyl S-[(4-oxo-1,2,3-benzotriazin-3 (4H)-yl)methyl] ester (azinphos-methyl)									
cas no. 86-50-0									
2464	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phosphorodithioic acid, OO-dimethyl S-1,2-dicarbethoxylethyl ester (malathion)									
cas no. 121-75-5									
1920	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phosphorothioic acid, O,O-diethyl O-(3-chloro-4-methyl-2-oxo-2H-1-benzopyran-7-yl) ester (coumaphos)									
cas no. 56-72-4									
2654	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phosphorothioic acid, OO-diethyl O-4-nitrophenyl ester (parathion)									
cas no. 56-38-2									
1941	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phosphorothioic acid, OO-diethyl O-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester (diazinon)									
cas no. 333-41-5									
1766	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phthalic acid, butyl benzyl ester									
cas no. 85-68-7									
2287	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phthalic acid, di(2-ethylhexyl) ester									
cas no. 117-81-7									
2504	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2505	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2506	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phthalic acid, diethyl ester									
cas no. 84-66-2									
1548	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phthalic acid, dioctyl ester									
cas no. 117-81-7									
2506	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
picoline, beta (3-methylpyridine)									
cas no. 108-99-6									
0832	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
picoline, gamma (4-methylpyridine)									
cas no. 108-89-4									
0832	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
propane, 1-nitro									
cas no. 108-03-2									
0707	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
propionanilide, 3',4'-dichloro (propanil)									
cas no. 709-98-8									
1816	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
pyrazine, 2-isobutyl-3-methoxy									
cas no. 2468-3-00-9									
1160	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
pyrzine, 2-isopropyl-3-methoxy									
cas no. 25773-40-4									
1076	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
pyrene									
cas no. 129-00-0									
2061	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
pyridine									
cas no. 110-86-1									
0732	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
thianaphthene									
cas no. 95-15-8									
1161	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 2,4-dinitro									
cas no. 121-14-2									
1468	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 2,6-dinitro									
cas no. 606-20-2									
1392	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 2-chloro									
cas no. 95-49-8									
0931	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 2-chloro-4-nitro									
cas no. 121-86-8									
1316	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 3-chloro									
cas no. 108-41-8									
0932	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 4-chloro									
cas no. 106-43-4									
0936	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 4-chloro-2-nitro									
cas no. 89-59-8									
1268	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
tolunen, 4-chloro-3-nitro									
cas no. 89-60-1									
1312	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 6-chloro-2-nitro									
cas no. 83-42-1									
1259	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, alpha,alpha-dichloro (benzal chloride)									
cas no. 98-87-3									
1106	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, alpha-chloro (benzyl chloride)									
cas no. 100-44-7									
0983	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluidine, 2-chloro-p-									
cas no. 615-65-6									
1252	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluidine, 3-chloro-o-									
cas no. 87-60-5									
1182	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluidine, 4-chloro-o									
cas no. 95-69-2									
1256	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
toluidine, 5-chloro-o- cas no. 95-79-4									
1256	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluidine, 6-chloro-m- cas no. 95-81-8									
1201	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluidine, 6-chloro-o- cas no. 87-63-8									
1249	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluidine, alpha,alpha,alpha-trifluoro-2,6-dinitro-N,N-dipropyl-p- (trifluralin) cas no. 1582-09-8									
1660	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
triazine, 2,4,6-trichloro-1,3,5- (cyanuric chloride) cas no. 108-77-0									
1051	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
triazine-2,4-diamine, 2-chloro-N-ethyl-N'-(1-methylethyl)-1,3,5- (atrazine) cas no. 1912-24-9									
1699	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
trizine-2,4-diamine, 6-chloro-N,N'-bis(1-methylethyl)-1,3,5- (propazine) cas no. 139-40-2									
1713	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
undecanoic acid, methyl ester cas no. 111-81-9									
1408	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
urea, 3-(3,4-dichlorophenyl)-1-methyoxy-1-methyl (linuron) cas no. 330-55-2									
1903	SAC	OV-1	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

Table 6 Linear Temperature Programmed Retention Indices Truncated Version in Retention Index Order—Polyethylene Glycol Columns

Retention index	Compound name	Stationary phase
1000	methane, trichloro	Superox 0.6
1012	ethene, tetrachloro	Superox 0.6
1026	propane, 1,2-dichloro	Superox 0.6
1027	benzene, methyl, (toluene)	Superox 0.6
1028	ethene, trichloro	Superox 0.6
1045	ethane, 1,2-dichloro	Superox 0.6
1066	propene, 2,3-dichloro	Superox 0.6
1110	benzene, ethyl	Superox 0.6
1112	propene, trans-1,3-dichloro	Superox 0.6
1132	methane, bromodichloro	Superox 0.6
1158	ether, 2,2-dichloroethyl methyl	Superox 0.6
1169	propane, 1-chloro-2,3-epoxy (epichlorohydrin)	Superox 0.6
1172	heptanone, 5-methyl-2-	Superox 0.6
1180	benzene, 1,2-dimethyl, (o-xylene)	Carbowax 20M
1180	picoline, alpha (2-methylpyridine)	Superox 0.6
1183	propene, cis-1,3-dichloro	Superox 0.6
1188	benzene, chloro	Superox 0.6
1190	benzene, 1,2-dimethyl, (o-xylene)	Carbowax 20M
1205	benzene, chloro	Carbowax 20M
1226	ethane, 1,2-dibromo	Superox 0.6
1236	ethane, 1,1,2-trichloro	Superox 0.6
1252	picoline, beta (3-methylpyridine)	Superox 0.6
1256	methane, bis-(methylthio)	Superox 0.6
1257	picoline, gamma (4-methylpyridine)	Superox 0.6

Retention index	Compound name	Stationary phase
1267	methane, dibromochloro	Superox 0.6
1276	formamide, N, N-dimethyl	Superox 0.6
1277	toluene, 2-chloro	Superox 0.6
1288	toluene, 3-chloro	Superox 0.6
1291	toluene, 2-chloro	Carbowax 20M
1291	toluene, 4-chloro	Superox 0.6
1301	toluene, 3-chloro	Carbowax 20M
1304	toluene, 4-chloro	Carbowax 20M
1314	hepten-2-one, 6-methyl-5-	Superox 0.6
1329	ethanol, 2-chloro	Superox 0.6
1330	anisole	Carbowax 20M
1341	anisole	Carbowax 20M
1357	ethanol, 2-chloro	Carbowax 20M
1384	benzene, 1,3-dichloro	Superox 0.6
1400	ethane, hexachloro	Superox 0.6
1407	methane, tribromo	Superox 0.6
1410	pyrazine, 2-isopropyl-3-methoxy	Superox 0.6
1411	benzene, 1,4-dichloro	Superox 0.6
1446	furfuraldehyde	Carbowax 20M
1452	benzene, 1,2-dichloro	Superox 0.6
1457	furfuraldehyde	Carbowax 20M
1475	ethane, 1,1,2,2-tetrachloro	Superox 0.6
1478	toluene, alpha-chloro (benzyl chloride)	Superox 0.6
1480	butadiene, hexachloro	Superox 0.6
1481	propanoic acid (propionic acid)	Superox 0.6
1497	toluene, alpha-chloro (benzyl chloride)	Carbowax 20M
1514	propanoic acid, 2-methyl	Superox 0.6
1528	phosphonium, (3,4-dichlorobenzyl) triphenyl, chloride (Eulan)	Superox 0.6
1552	ethane, 1,2-dihydroxy (ethylene glygol)	Superox 0.6
1562	borneol, 2-methyliso	Superox 0.6
1603	benzene, 1,2,4-trichloro	Superox 0.6
1664	pentadecane, 2,6,10,14-tetramethyl (pristane)	Carbowax 20M
1672	toluene, alpha,alpha-dichloro (benzal chloride)	Superox 0.6
1675	pentadecane, 2,6,10,14-tetramethyl (pristane)	Carbowax 20M
1683	benzene, nitro	Superox 0.6
1690	naphthalene	Superox 0.6
1690	toluene, alpha,alpha-dichloro (benzal chloride)	Carbowax 20M
1709	naphthalene	Carbowax 20M
1720	naphthalene	Carbowax 20M
1749	benzene, 1-methyl-2-iodo	Superox 0.6
1750	benzene 1,2,4,5-tetrachloro	Superox 0.6
1750	phenol, 2-nitro	Superox 0.6
1751	thianaphthene	Superox 0.6
1768	anisole, 2,4,6-trichloro	Superox 0.6
1788	phenol, 2-chloro	Superox 0.6
1789	decalol, trans-1,10-dimethyl-trans-9- (geosmin)	Superox 0.6
1815	phenol, 2-chloro	Carbowax 20M
1847	benzene, 1-chloro-3-nitro	Superox 0.6
1862	benzene, 1-chloro-3-nitro	Carbowax 20M
1879	aniline, 2-chloro	Superox 0.6
1887	anisole, 2,3,6-trichloro	Superox 0.6
1887	benzene, 1-chloro-4-nitro	Superox 0.6
1887	benzene, 3,5-dichloronitro	Superox 0.6
1893	toluidine, 3-chloro-o-	Superox 0.6
1896	toluene, 6-chloro-2-nitro	Superox 0.6
1901	aniline, 2-chloro	Carbowax 20M
1901	toluene, 4-chloro-2-nitro	Superox 0.6
1902	benzene, 1-chloro-4-nitro	Carbowax 20M
1905	aniline, 2,6-dichloro	Superox 0.6

Retention index	Compound name	Stationary phase
1909	ionone, beta-	Carbowax 20M
1915	toluene, 4-chloro-2-nitro	Carbowax 20M
1922	ionone, beta-	Carbowax 20M
1932	phenol	Superox 0.6
1936	biphenyl	Superox 0.6
1946	benzene, 1-chloro-2-nitro	Superox 0.6
1948	biphenyl	Carbowax 20M
1957	toluidine, 3-chloro-p-	Superox 0.6
1961	phenol	Carbowax 20M
1962	naphthalene, 1-chloro	Superox 0.6
1964	benzene, 1-chloro-2-nitro	Carbowax 20M
1965	toluene, 2-chloro-4-nitro	Superox 0.6
1973	naphthalene, 2-chloro	Carbowax 20M
1975	toluidine, 6-chloro-m-	Superox 0.6
1977	aniline, 2-chloro-4-methyl	Carbowax 20M
2010	phenol, 2,5-dimethyl (2,5-xylenol)	Superox 0.6
2014	methenamine	Superox 0.6
2014	phenol, 2,4-dimethyl (m-xylenol)	Superox 0.6
2031	anisole, 2,3,5,6-tetrachloro	Superox 0.6
2039	toluene, 4-chloro-3-nitro	Superox 0.6
2040	benzene, 3,4-dichloronitro	Superox 0.6
2053	benzene, 2,5-dichloronitro	Superox 0.6
2064	benzene, 2,4-dichloronitro	Superox 0.6
2079	phosphoric acid, tributyl ester	Superox 0.6
2084	benzonitrile, 2,6-dichloro (dichlobenil)	Superox 0.6
2092	acenaphthene	Carbowax 20M
2093	indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H (chlordane)	Carbowax 20M
2098	phenol, 2,4-dichloro	Superox 0.6
2100	aniline, 4-chloro	Superox 0.6
2103	acenaphthene	Carbowax 20M
2110	aniline, 3-chloro	Superox 0.6
2123	acenaphthylene	Superox 0.6
2127	toluidine, 6-chloro-o-	Superox 0.6
2130	aniline, 4-chloro	Carbowax 20M
2137	benzene, 2,3-dichloronitro	Superox 0.6
2140	aniline, 3-chloro	Carbowax 20M
2144	phenol, 3,4-dimethyl (3,4-xylenol)	Superox 0.6
2145	toluidine, 5-chloro-o-	Superox 0.6
2155	toluidine, 4-chloro-o-	Superox 0.6
2160	aniline, 2-chloro-4-methyl	Superox 0.6
2164	toluidine, 2-chloro-p-	Superox 0.6
2183	anisole, 2,3,4-trichloro	Superox 0.6
2193	benzene, hexachloro (HCB)	Superox 0.6
2203	aniline, 2,4-dichloro	Superox 0.6
2212	indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-4, 7-methano-1H- (chlordane)	Carbowax 20M
2226	aniline, 2,3-dichloro	Superox 0.6
2261	aniline, 2,3-dichloro	Superox 0.6
2287	indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H- (chlordane)	Carbowax 20M
2299	hydrazine, 1,2-diphenyl	Superox 0.6
2322	toluene, 2,6-dinitro	Superox 0.6
2326	phenol, 2,3,6-trichloro	Superox 0.6
2333	phthalic acid, diethyl ester	Carbowax 20M
2342	phenol, 4-chloro	Superox 0.6
2345	phenol, 3-chloro	Superox 0.6
2346	phthalic acid, diethyl ester	Carbowax 20M
2376	phenol, 4-chloro	Carbowax 20M
2378	phenol, 3-chloro	Carbowax 20M

Retention index	Compound name	Stationary phase
2382	phosphorothioic acid, 00-diethyl 0-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl]ester (diazinon)	Superox 0.6
2394	ether, 4-bromophenyl phenyl	Superox 0.6
2410	phenol, 4-chloro-3-methyl	Superox 0.6
2420	toluene, 2,4-dinitro	Superox 0.6
2429	indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-4, 7-methano-1H- (chlordane)	Carbowax 20M
2438	phenol, 4-chloro-3-methyl	Carbowax 20M
2452	cyclohexane, alpha-hexachloro (alpha-BHC)	Superox 0.6
2465	acetic acid, methyl ester, 2,4-dichlorophenoxy (2,4-D methyl ester)	Superox 0.6
2469	aniline, 3,5-dichloro	Superox 0.6
2505	indene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-4,7-methano-1H- (heptachlor)	Superox 0.6
2510	indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H- (chlordane)	Carbowax 20M
2519	aniline, 3,4-dichloro	Superox 0.6
2521	aniline, N-phenyl	Superox 0.6
2526	benzene, 1-chloro-2,4-dinitro	Superox 0.6
2530	indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H- (Chlordane)	Carbowax 20M
2536	naphthalene, 1,2,3,4,10,10-hexachloro-1,4,4,5,8,8-hexa-hydro-exo-1,4-endo-5,8-dimethano (aldrin)	Superox 0.6
2537	naphthalene, 1,2,3,4,10,10-hexachloro-1,4,4,5,8,8-hexa-hydro-exo-1,4-endo-5,8-dimethano (aldrin)	Carbowax 20M
2542	indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H- (chlordane)	Carbowax 20M
2543	phenol, 2-amino-4-chloro	Carbowax 20M
2545	benzene, 1-chloro-2,4-dinitro	Carbowax 20M
2596	indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H- (chlordane)	Carbowax 20M
2634	anthracene	Superox 0.6
2641	acetic acid, butyl ester, 2,4-dichlorophenoxy (2,4-D butyl ester)	Superox 0.6
2682	triazine-2,4-diamine, 6-chloro-N,N′-bis(1-methylethyl)-1,3,5- (propazine)	Superox 0.6
2776	triazine-2,4-diamine, 2-chloro-N-ethyl-N′-(1-methylethyl)-1,3,5- (atrazine)	Superox 0.6
2828	indane, 1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3a,4,7,7a-tetrahydro-4,7-methano-1H- (heptachlor epoxide)	Superox 0.6
2856	cyclohexane, beta-hexachloro (beta-BHC)	Superox 0.6
2872	triazine-2,4-diamine, 6-chloro-N,N′diethyl-1,3,5-(simazine)	Superox 0.6
2879	norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro, cyclic sulphite, 5- (endosulphan)	Superox 0.6
2880	benzodioxathiepin 3-oxide, 6,7,8,9,10,10-hexachloro 1,5,5a,6,9,9a-hexahydro-6, 9-methano-2,4,3-(endosulfan I)	Superox 0.6
2904	ethene,1,1-dichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl) (o,p′-DDE)	Superox 0.6
2911	acetic acid, iso-octyl ester, 2,4-dichlorophenoxy (2,4-D iso-octyl ester)	Superox 0.6
2956	benzene, n-butyl, sulphonamide	Superox 0.6
3103	ethane, 1,1,1-trichloro-2,2-bis(4-chlorophenyl) (p,p′-DDT)	Superox 0.6
3103	naphthalene, 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a, 5,6,7,8,8a-octahydro-exo-1,4:5,8-dimethano (dieldrin)	Superox 0.6
3106	ethane, 1,1,1-trichloro-2,2-bis (chlorophenyl) (DDT)	Superox 0.6
3106	phthalic acid, di(2-ethylhexyl) ester	Superox 0.6

Retention index	Compound name	Stationary phase
3106	phthalic acid, dioctyl ester	Superox 0.6
3120	ethane, 1,1-dichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl) (o,p'-TDE)	Superox 0.6
3123	ethane, 2-(2-chlorophenyl)-2-(4-chlorophenyl)-1, 1-dichloro (2,4'DDD)	Superox 0.6
3197	propionanilide, 3',4'-dichloro (propanil)	Superox 0.6

Table 7 Linear Temperature Programmed Retention Indices Full Version in Alphabetical Order of Compound Name—Polyethylene Glycol Columns

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
acenaphthene									
cas no. 83-32-9									
2092	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
2103	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
acenaphthylene									
cas no. 208-96-8									
2123	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
acetic acid, butyl ester, 2,4-dichlorophenoxy (2,4-D butyl ester)									
cas no. 94-80-4									
2641	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
acetic acid, iso-octyl ester, 2,4-dichlorophenoxy (2,4-D iso-octyl ester)									
cas no. 25168-26-7									
2911	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
acetic acid, methyl ester, 2,4-dichlorophenoxy (2,4-D methyl ester)									
cas no. 1928-38-7									
2465	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 2,3-dichloro									
cas no. 608-27-5									
2261	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 2,4-dichloro									
cas no. 554-00-7									
2203	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 2,5-dichloro									
cas no. 95-28-9									
2226	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 2,6-dichloro									
cas no. 608-31-1									
1905	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 2-chloro									
cas no. 95-51-2									
1879	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1901	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
aniline, 2-chloro-4-methyl									
cas no. 615-65-6									
1977	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2160	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 3,4-dichloro									
cas no. 95-76-1									
2519	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 3,5-dichloro									
cas no. 626-43-7									
2469	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 3-chloro									
cas no. 108-42-9									
2110	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2140	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, 4-chloro									
cas no. 106-47-8									
2100	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2130	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
aniline, N-phenyl									
cas no. 122-39-4									
2521	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
anisole									
cas no. 100-66-3									
1330	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
1341	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
anisole, 2,3,4-trichloro									
cas no. 54135-80-7									
2183	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
anisole, 2,3,5,6-tetrachloro									
cas no. 6936-40-9									
2031	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
anisole, 2,3,6-trichloro									
cas no. 50375-10-5									
1887	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
anisole, 2,4,6-trichloro									
cas no. 87-40-1									
1768	SAC	Superox 0.6	quartz glass	bondend phase	0.32	50	hydrogen	standard	28
anthracene									
cas no. 120-12-7									
2634	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1,2,4,5-tetrachloro									
cas no. 95-94-3									
1750	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
benzene, 1,2,4-trichloro									
cas no. 120-82-1									
1603	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1,2-dichloro									
cas no. 95-50-1									
1452	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1,2-dimethyl (o-xylene)									
cas no. 95-47-6									
1180	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
1190	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1,3-dichloro									
cas no. 541-73-1									
1384	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1,4-dichloro									
cas no. 106-46-7									
1411	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1-chloro-2,4-dinitro									
cas no. 121-86-8									
2526	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2545	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1-chloro-2-nitro									
cas no. 89-21-4									
1946	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1964	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1-chloro-3-nitro									
cas no. 88-73-3									
1847	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1862	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1-chloro-4-nitro									
cas no. 121-73-3									
1887	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1902	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 1-methyl-2-iodo									
cas no. 615-37-2									
1749	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 2,3-dichloronitro									
cas no. 3209-22-1									
2137	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 2,4-dichloronitro									
cas no. 611-06-3									
2064	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
benzene, 2,5-dichloronitro									
cas no. 89-61-2									
2053	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	*28*
benzene, 3,4-dichloronitro									
cas no. 99-54-7									
2040	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, 3,5-dichloronitro									
cas no. 618-62-2									
1887	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, chloro									
cas no. 108-90-7									
1188	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1205	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, ethyl									
cas no. 100-41-4									
1110	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, hexachloro (HCB)									
cas no. 118-74-1									
2193	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, methyl, (toluene)									
cas no. 108-88-3									
1027	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, n-butyl, sulphonamide									
cas no. 3622-84-2									
2956	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzene, nitro									
cas no. 98-95-3									
1683	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzodioxathiepin 3-oxide, 6,7,8,9,10,10-hexachloro 1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3-(endosulfan I)									
cas no. 959-98-8									
2880	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
benzonitrile, 2,6-dichloro (dichlobenil)									
cas no. 1194-65-6									
2084	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
biphenyl									
cas no. 92-52-4									
1936	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1948	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
borneol, 2-methyliso									
cas no. 2371-42-8									
1562	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
butadiene, hexachloro									
cas no. 87-68-3									
1480	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
cyclohexane, alpha-hexachloro (alpha-BHC)									
cas no. 319-84-6									
2452	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
cyclohexane, beta-hexachloro (beta-BHC)									
cas no. 319-85-7									
2856	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
cyclohexane, hexachloro (BHC)									
cas no. 608-73-1									
2452	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
decalol, trans-1,10-dimethyl-trans-9-(geosmin)									
cas no. 19700-21-1									
1789	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,1,1-trichloro-2,2-bis (4-chlorophenyl) (p,p'-DDT)									
cas no. 50-29-3									
3103	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,1,1-trichloro-2,2-bis(chlorophenyl) (DDT)									
cas no. 50-29-3									
3106	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,1,2,2-tetrachloro									
cas no. 79-34-5									
1475	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,1,2-trichloro									
cas no. 79-00-5									
1236	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,1-dichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl) (o,p'-TDE)									
cas no. 53-19-0									
3120	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,2-dibromo									
cas no. 106-93-4									
1226	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,2-dichloro									
cas no. 107-06-2									
1045	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 1,2-dihydroxy (ethylene glygol)									
cas no. 107-21-1									
1552	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, 2-(2-chlorophenyl)-2-(4-chlorophenyl)-1,1-dichloro (2,4'DDD)									
cas no. 53-19-0									
3123	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethane, hexachloro									
cas no. 67-72-1									
1400	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethanol, 2-chloro									
cas no. 107-07-3									
1329	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
1357	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethene, 1,1-dichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl) (o,p'-DDE)									
cas no. 3424-82-6									
2904	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethene, tetrachloro									
cas no. 127-18-4									
1012	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ethene, trichloro									
cas no. 79-01-6									
1028	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ether, 2,2-dichloroethyl methyl									
cas no. 34862-07-2									
1158	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ether, 4-bromophenyl phenyl									
cas no. 101-55-3									
2394	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
formamide, N,N-dimethyl									
cas no. 68-12-2									
1276	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
furfuraldehyde									
cas no. 98-01-1									
1446	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
1457	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
heptanone, 5-methyl-3-									
cas no. 541-85-5									
1172	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
hepten-2-one, 6-methyl-5-									
cas no. 110-93-0									
1314	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
hydrazine, 1,2-diphenyl									
cas no. 122-66-7									
2299	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
indane, 1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3a,4,7,7a-tetrahydro-4,7-methano-1H-(heptachlor epoxide)									
cas no. 1024-57-3									
2828	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
indene, 1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-(chlordane)									
cas no. 57-74-9									
2093	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
2212	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
2287	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
2429	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
2510	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
2530	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
2542	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
2596	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
indene, 1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-4,7-methano-1H-(heptachlor)									
cas no. 76-44-8									
2505	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
ionone, beta-									
cas no. 14901-07-6									
1909	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
1922	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
methane, bis-(methylthio)									
cas no. 1618-26-4									
1256	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
methane, bromodichloro									
cas no. 75-27-4									
1132	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
methane, dibromochloro									
cas no. 124-48-1									
1267	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
methane, tribromo									
cas no. 75-25-2									
1407	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
methane, trichloro									
cas no. 67-66-3									
1000	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
methenamine									
cas no. 100-97-0									
2014	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
naphthalene									
cas no. 91-20-3									
1690	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1709	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
1720	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
naphthalene, 1,2,3,4,10,10-hexachloro-1,4,4,5,8,8-hexahydro-exo-1,4-endo-5,8-dimethano (aldrin)									
cas no. 309-00-2									
2536	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2537	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
naphthalene, 1,2,3,4,10,10-hexachloro-6,7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-exo-1,4:5,8-dimethano (dieldrin)									
cas no. 60-57-1									
3103	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
naphthalene, 1-chloro									
cas no. 90-13-1									
1962	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
naphthalene, 2-chloro									
cas no. 91-58-7									
1973	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro, cyclic sulphite, 5-(endosulphan)									
cas no. 115-29-7									
2879	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
pentadecane, 2,6,10,14-tetramethyl (pristane)									
cas no. 1921-70-6									
1664	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1675	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
phenol									
cas no. 108-95-2									
1932	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1961	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2,3,6-trichloro									
cas no. 933-75-5									
2326	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2,4-dichloro									
cas no. 120-83-2									
2098	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2,4-dimethyl (m-xylenol)									
cas no. 105-67-9									
2014	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2,5-dimethyl (2,5-xylenol)									
cas no. 95-87-4									
2010	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
pehnol, 2-amino-4-chloro									
cas no. 95-85-2									
2543	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2-chloro									
cas no. 95-57-8									
1788	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1815	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 2-nitro									
cas no. 88-75-5									
1750	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 3,4-dimethyl (3,4-xylenol)									
cas no. 95-65-8									
2144	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
phenol, 3-chloro									
cas no. 108-43-0									
2345	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2378	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 4-chloro									
cas no. 106-48-9									
2342	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2376	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phenol, 4-chloro-3-methyl									
cas no. 59-50-7									
2410	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2438	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phosphonium, (3,4-dichlorobenzyl)triphenyl, chloride (Eulan)									
cas no. 4386-40-7									
1528	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phosphoric acid, tributyl ester									
cas no. 126-73-8									
2079	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phosphorothioic acid, OO-diethyl O-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester (diazinon)									
cas no. 333-41-5									
2382	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phthalic acid, di(2-ethylhexyl) ester									
cas no. 117-81-7									
3106	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phthalic acid, diethyl ester									
cas no. 84-66-2									
2333	SAC	Carbowax 20M	quartz glass	wall-coated open tubular	0.32	50	hydrogen	standard	28
2346	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
phthalic acid, dioctyl ester									
cas no. 117-71-7									
3106	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
picoline, alpha (2-methylpyridine)									
cas no. 109-96-8									
1180	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
picoline, beta (3-methylpyridine)									
cas no. 108-99-6									
1252	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
picoline, gamma (4-methylpyridine)									
cas no. 108-89-4									
1257	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
propane, 1,2-dichloro									
cas no. 78-87-5									
1026	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

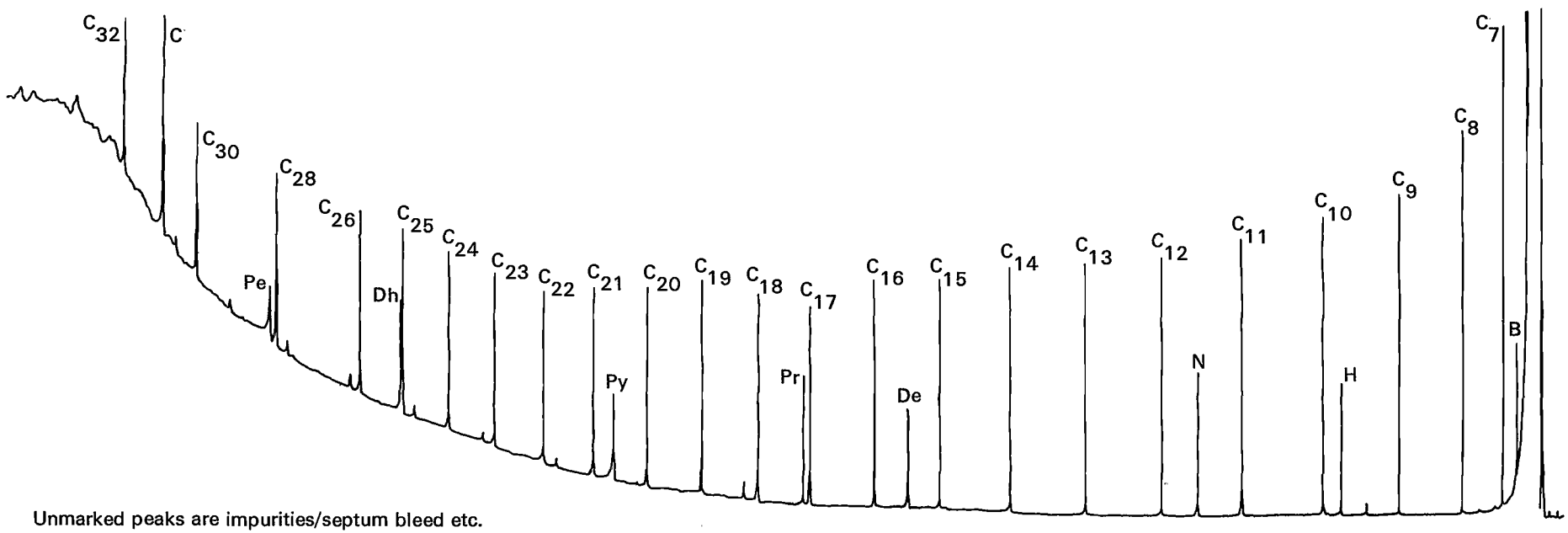
LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
propane, 1-chloro-2,3-epoxy (epichlorohydrin)									
cas no. 106-89-8									
1169	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
propanoic acid (propionic acid)									
cas no. 79-09-4									
1481	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
propanoic acid, 2-methyl									
cas no. 79-31-2									
1514	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
propene, 2,3-dichloro									
cas no. 78-88-6									
1066	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
propene, cis-1,3-dichloro									
cas no. 542-75-6									
1183	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
propene, trans-1,3-dichloro									
cas no. 542-75-6									
1112	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
propionanilide, 3′,4′-dichloro (propanil)									
cas no. 709-98-8									
3197	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
pyrazine, 2-isopropyl-3-methoxy									
cas no. 25773-40-4									
1410	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
thianaphthene									
cas no. 95-15-8									
1751	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 2,4-dinitro									
cas no. 121-14-2									
2420	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 2,6-dinitro									
cas no. 606-20-2									
2322	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 2-chloro									
cas no. 95-49-8									
1277	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1291	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 2-chloro-4-nitro									
cas no. 121-86-8									
1965	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 3-chloro									
cas no. 108-41-8									
1288	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1301	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
toluene, 4-chloro									
cas no. 106-43-4									
1291	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1304	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 4-chloro-2-nitro									
cas no. 89-59-8									
1901	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1915	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 4-chloro-3-nitro									
cas no. 89-60-1									
2039	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, 6-chloro-2-nitro									
cas no. 83-42-1									
1896	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, alpha, alpha-dichloro (benzal chloride)									
cas no. 98-87-3									
1672	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1690	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluene, alpha-chloro (benzyl chloride)									
cas no. 100-44-7									
1478	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
1497	SAC	Carbowax 20M	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluidine, 2-chloro-p-									
cas no. 615-61-6									
2164	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluidine, 3-chloro-o-									
cas no. 87-60-5									
1893	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluidine, 3-chloro-p-									
cas no. 95-74-9									
1957	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluidine, 4-chloro-o-									
cas no. 95-69-2									
2155	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluidine, 5-chloro-o-									
cas no. 95-79-4									
2145	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluidine, 6-chloro-m-									
cas no. 95-81-8									
1975	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
toluidine, 6-chloro-o-									
cas no. 87-63-8									
2127	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

LTP Index	Column Origin	Stationary Phase	Column Material	Column Type	ID (mm)	LEN (m)	Carrier Gas	Sample Type	LIT Ref
triazine-2,4-diamine, 2-chloro-N-ethyl-N′-(1-methylethyl)-1,3,5- (atrazine) cas no. 1912-24-9									
2776	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
triazine-2,4-diamine, 6-chloro-N,N′-bis (1-methylethyl)-1-3,5- (propazine) cas no. 139-40-2									
2682	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
2682	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28
triazine-2,4-diamine, 6-chloro-N,N′-diethyl-1-3,5- (simazine) cas no. 122-34-9									
2872	SAC	Superox 0.6	quartz glass	bonded phase	0.32	50	hydrogen	standard	28

Figure 1 LTPRI test mixture chromatographed on PS 255

C - cholesterol
B - benzene (not used in final mix)
H - cis-hydrindane
N - naphthalene
De - diethyl phthalate
Pr - pristane
Py - pyrene
Dh - di-(2-ethylhexyl) phthalate
Pe - perylene



Unmarked peaks are impurities/septum bleed etc.

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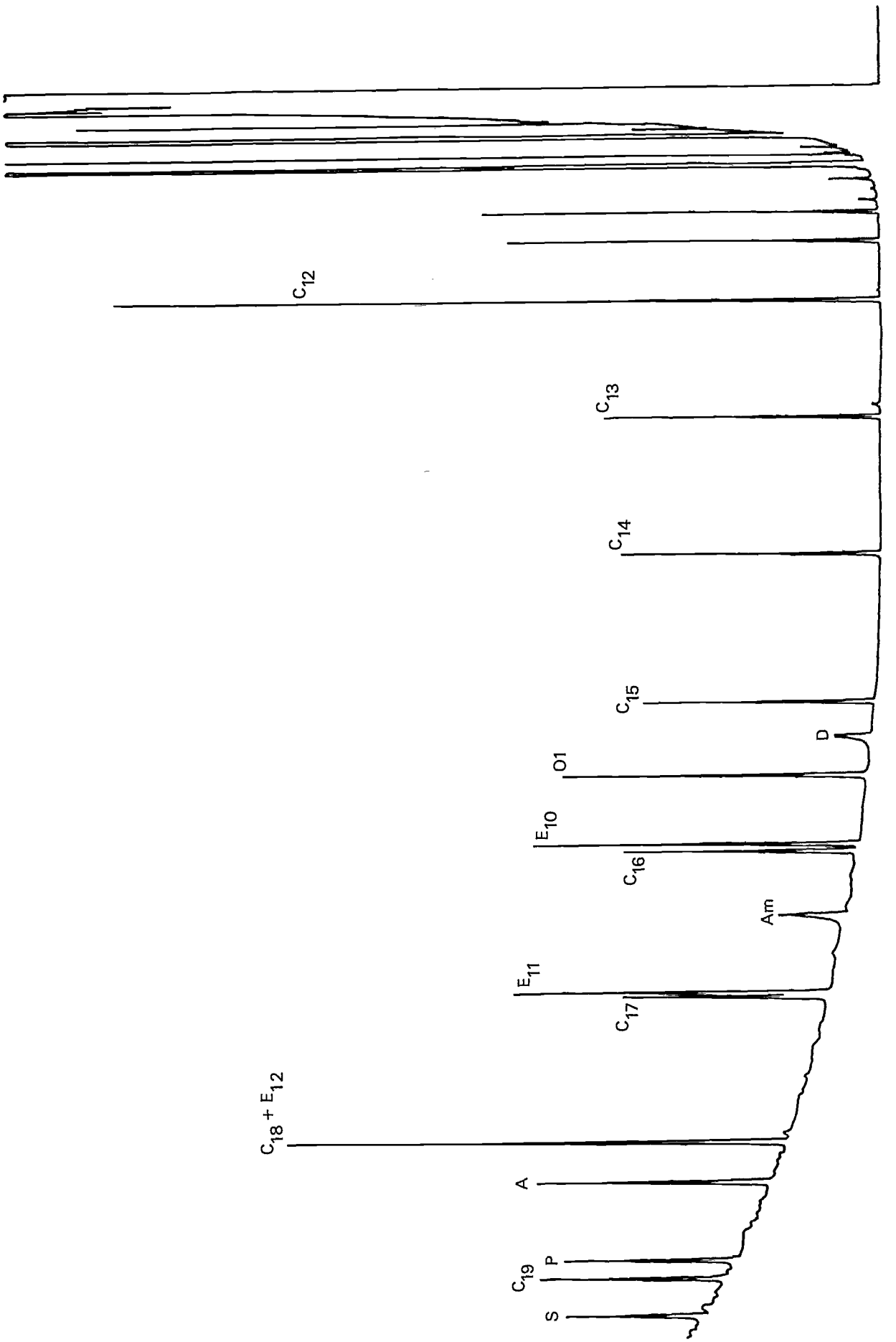

Figure 2 Grob test mix and n-alkanes chromatographed on statically coated Carbowax 20M column

Figure 3 Grob test mixture and n-alkanes chromatographed on immobilised Carbowax 20M column

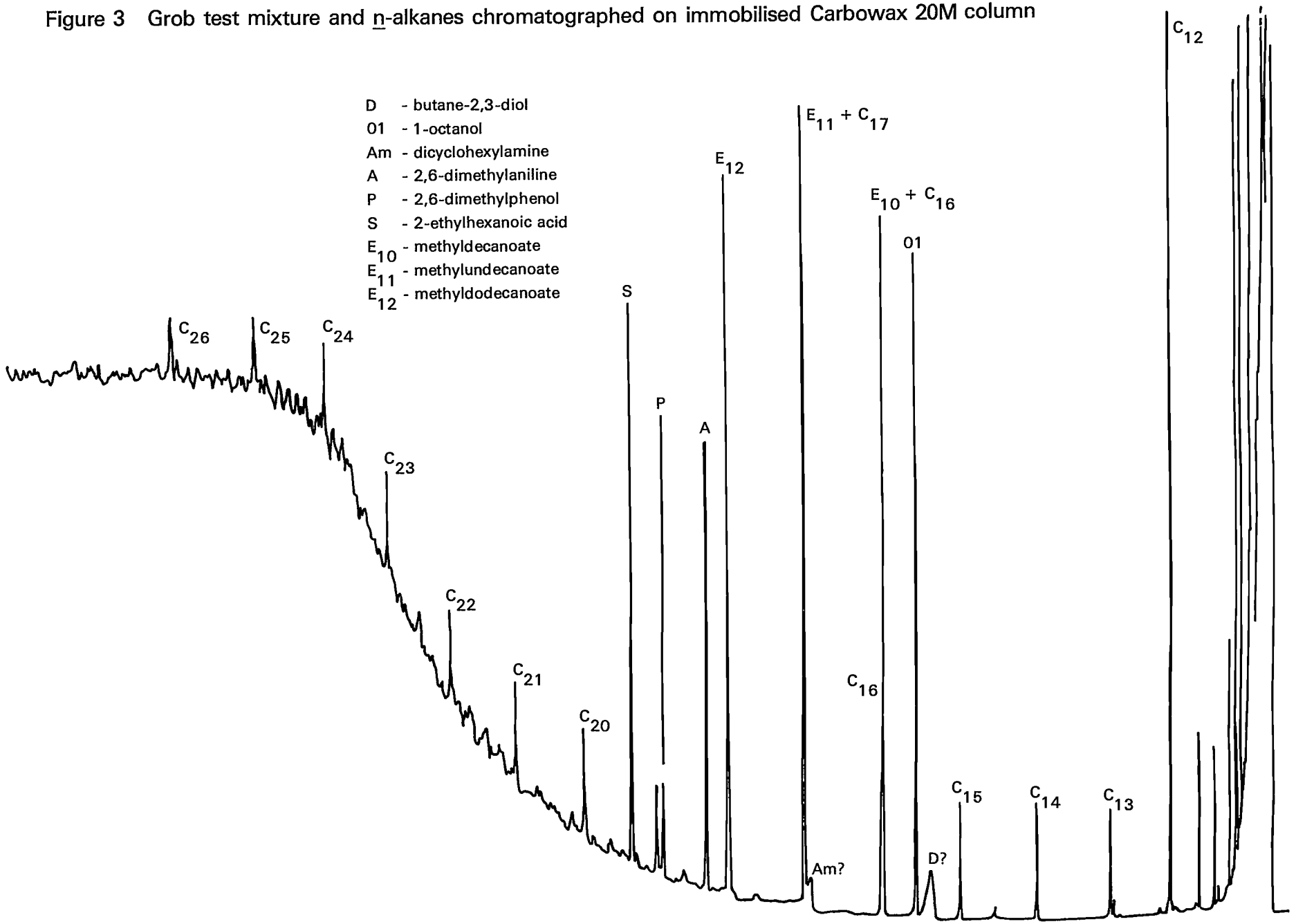

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Figure 4 LTPRI test mixture chromatographed on non-immobilised Carbowax 20M column

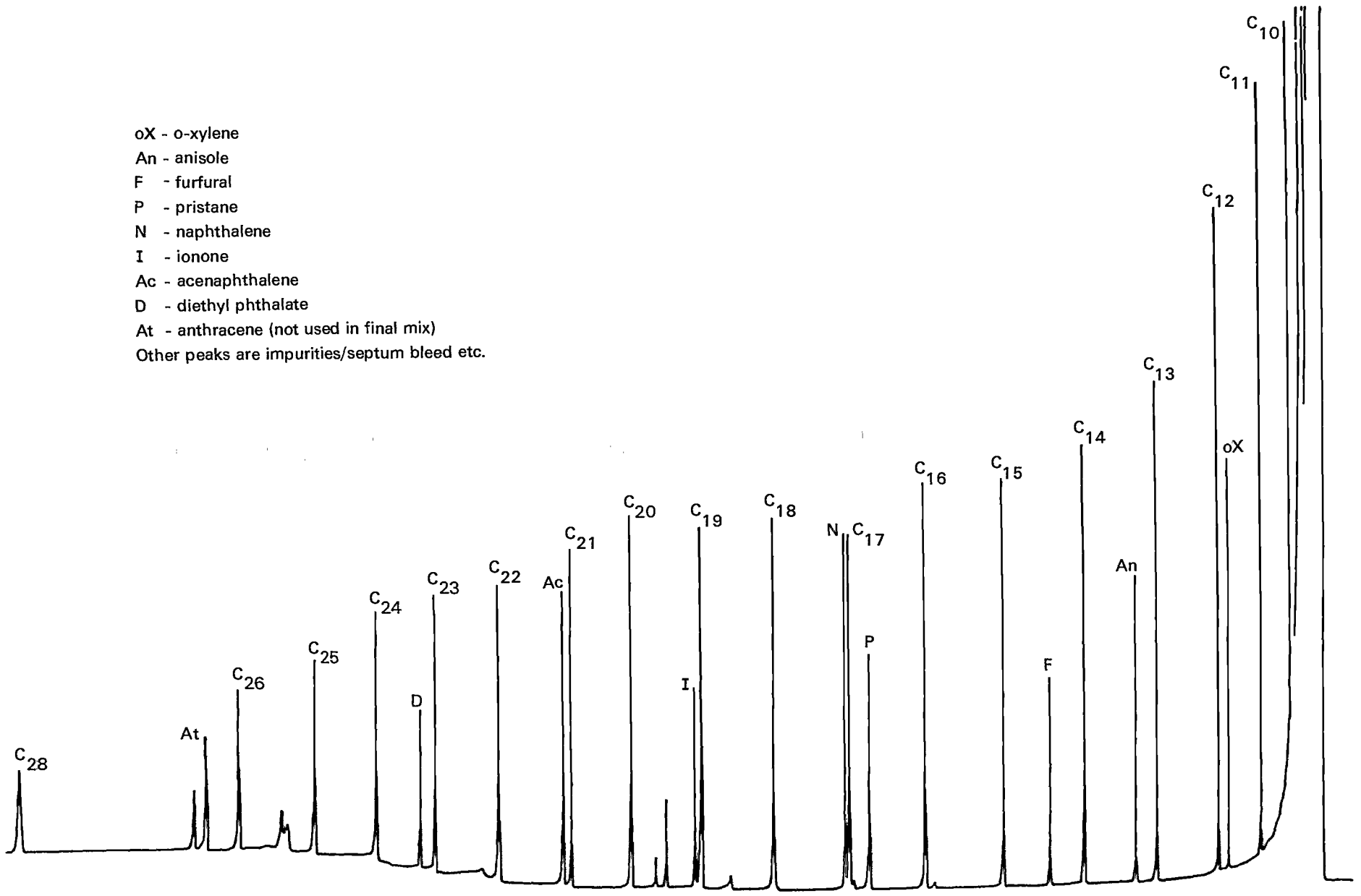
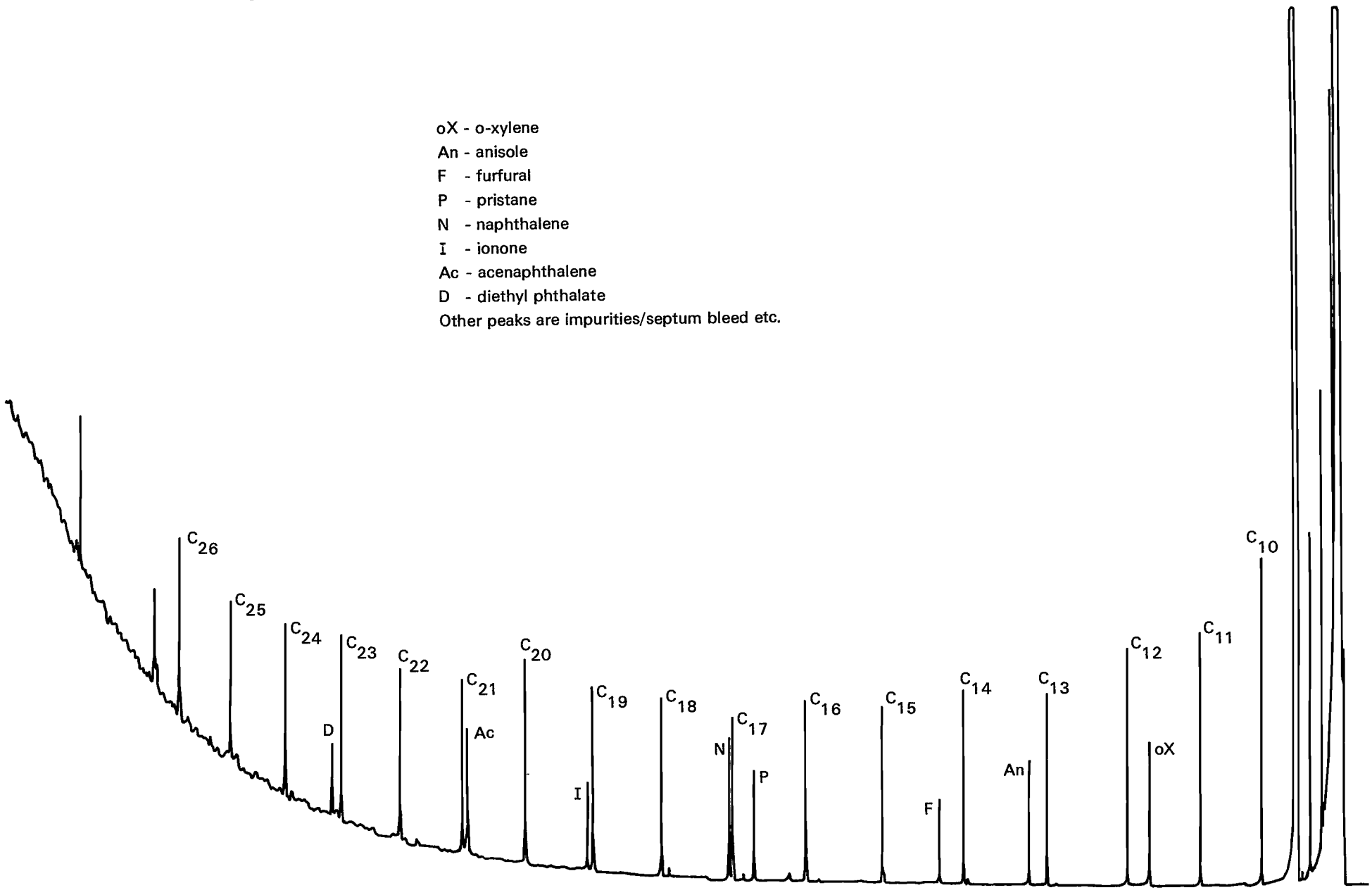


Figure 5 LTPRI test mixture chromatographed on immobilised Superox 0.6 column



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