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IDENTIFICATION OF ORGANIC MICROPOLLUTANTS IN RAW AND TREATED WATER BY APPLICATION OF GC-MS-DP

PART II : RESULTS

JANUARY 1978

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1. INTRODUCTION

In the last decade, concern has increased over the potential adverse health effects attributable to the organic matter present in drinking water. This concern has resulted, to a great extent, from the development of sophisticated analytical instrumentation capable of providing detailed information on the identity of the organic substances present, and growing evidence that long-term exposure to quite low concentrations of organic substances could lead to chronic disease (1). The increasing tendency in the UK to draw supplies from water sources known to be polluted with industrial and domestic effluent (2), containing a great variety of organic micropollutants, intensifies the general desire for information on the identity of the organic matter in the derived potable water in order that some assessment of the risk to public health may be attempted.

As virtually no information existed on the identity of such organic micropollutants in UK waters, a contract was awarded to the Water Research Association (now part of the Water Research Centre) by the Department of the Environment in 1971 for relevant research to be carried out. The broad objective of the research was "to apply the technique of mass spectrometry to the problem of characterising and measuring organic substances in water".

Much of the early research work was concerned with methodology. This extensive phase of the research has already been reported (Contract Report - "Identification of organic micropollutants in raw and treated water by application of GC-MS-DP. Part I: Method of Analysis", August 1977). Part II, this present report, is concerned with the data obtained by applying the techniques developed to the examination of selected raw and treated waters. All of the raw waters examined contained relatively high levels of wastewater.

The instrumentation employed, although the most appropriate available, has some limitations which have an important bearing on the data produced. Although very many compounds have been identified, and are listed in this report, they are all essentially volatile in nature (see Part I, Section 2).

This means that probably over 80% of the organic matter in the samples has not been analysed as it is non-volatile*. The technique is also essentially qualitative (see Section 3.4), although quantitative estimates have been made where possible. To obtain quantitative data for all of the substances identified would be exceedingly time-consuming and would, in many cases, probably be unnecessary. It is considered that any further effort on quantitative aspects should be devoted to any potentially hazardous compounds identified.

It is also important to stress the very time-consuming nature of the overall analysis. Thus in order to study in some detail five raw and treated waters duplicate sampling was not possible. A further, related, compromise was necessary between the time devoted to identifying components in a particular sample and the examination of other samples. It would have been quite possible, due to the complexity encountered in all samples, to have devoted all of the time available to the examination of just one sample. However, within an arbitary time, as many components as possible were identified. This left numerous "unknowns" which for various reasons were not positively identified.

A consequence of these unavoidable limitations is that this work can be considered only as the first step towards a comprehensive understanding of the nature of organic compounds in drinking water. It must also be emphasized that any attempt at this stage to draw conclusions from this or similar work about the safety of drinking water derived from polluted sources would be inappropriate. Analytical data is a vital element in such an assessment but this must be matched by suitable epidemiological and toxicological data which is not currently available. Work now proceeding under a new DOE contract which embraces all these aspects should enable further material progress to be made in this field.

The present work does however give for the first time some detailed information on the composition of the volatile organic components of some raw and treated waters.

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* Work on non-volatile chlorinated organic micropollutants is being carried out under a new DOE contract at the Water Research Centre.

2. ANALYSIS

2.1. SAMPLING

Grab samples of raw and treated water were taken at five water works treating lowland rivers which contained appreciable levels of wastewaters. The selected sites were:

Clapham (River Great Ouse)
Coppermills (River Lea)
Hampton (River Thames)
Staines (River Thames)
Langford (Rivers Chelmer and Blackwater)

Brief details of the processes are given in Table 1. Table 2 gives information on the point of sampling, the date and details of the samples themselves. Due to analytical limitations (see Part I, Section 9) samples of raw and treated water had to be taken on different occasions from any particular site. Similar limitations meant that duplicates could not be processed.

Table 3 gives information on the samples taken for GC-MS and supplementary analysis. Samples taken for GC-MS were always processed in the laboratory on the same day as they were taken.

2.2. OUTLINE OF OVERALL PROCEDURE

A full account of the experimental procedure has been given Part I, section 8.

A summary of the overall analytical technique is given here.

Solvent extration using successively petroleum ether and diethyl ether was used exclusively for the preparation of suitable extracts for GC-MS examination. Two separate solvent extracts, one petroleum ether extract and one diethyl ether extract, were obtained for each aqueous sample taken. After drying over anhydrous sodium sulphate each extract was concentrated to a volume of 1ml. The extracts were split into two 500 µl fractions, one of which was further reduced in volume to 100 µl, while the other was methylated using diazomethane. After methylation, the methylated extracts were reduced in volume to 100 µl.

Two solvent blanks, one petroleum ether and one diethyl ether, were treated in the same manner as the extracts, so that each sample gave rise to four solvent extracts and four solvent blanks.

Two GC-MS systems were used for this work. One was a Pye 104 GC coupled via a membrane separator to an AEI MS30 mass spectrometer, while the other was a Hewlett-Packard 5710A gas chromatograph coupled directly to a VG 16F mass spectrometer. Either SCOT or PLOT glass capillary columns were used for the GC separation, and each solvent extract and blank was run on two different columns, one of which had OV-1 as stationary phase while the other employed FFAP as stationary phase.

Both mass spectrometers were used in a cyclic scanning mode, with a mass range of 20 - 460 a.m.u. The scan speed used (1 sec /decade) resulted in one spectral scan being taken approximately every 3 secs. The mass spectrometer was coupled to a VG 2040 data system, and the data stored on a magnetic disc. After data acquisition had been completed, interpretation of the data i.e. inspection of the mass spectra produced by compounds eluting from the GC column, proceeded. Invariably, data interpretation was the rate-determining step of the total analysis.

Often, further work was necessary to confirm tentative identifications. This usually involved obtaining a pure standard of a compound believed to be present in a certain sample, and running this standard on the GC-MS system. Several hundred pure compounds were run for this reason, and they form the basis of the library of mass spectral data at WRC. A listing of these compounds is given in Appendix 1.

2.3. SUPPLEMENTARY ANALYSES

Although by far the main analytical task was the identification of the unknown organic micropollutants encountered, which required GC-MS-DP, certain other analytical techniques were utilised. These are outlined in more detail in Part I, Section 4, 7.1, 7.2 and 7.3 and involve capillary GC, total non-volatile organic carbon, trihalomethane determination and measurement of total organically bound halogens respectively. The analyses and results are discussed in Section 3.5 of this report.

3. RESULTS AND DISCUSSION

Tables 4 - 7 give listings of compounds positively identified, information on unknown compounds detected, the samples in which the compounds were identified or detected, and some quantitative estimates for certain of the identified micropollutants.

3.1. TOTAL ORGANIC MICROPOLLUTANTS POSITIVELY IDENTIFIED

Table 4 gives a listing in alphabetical order of the total number of organic compounds identified in the solvent extracts obtained from the samples, and indicate(by means of a √) whether these compounds were detected in raw or treated samples. Compounds which were detected only after methylation of the solvent extracts are indicated by a 'x' immediately before the compound name.

The molecular formula and molecular weight are also given. The molecular weight indicated is that calculated from integral values of the atomic weights of the most abundant isotope of each element present e.g. the molecular weight of chloroform, $CHCl_3$, is 118 (12 + 1 + (3 × 35)), rather than 119.38 (which takes into account the contribution of the ^{37}Cl isotope).

These identifications were based on the following criteria -

a) the mass spectrum matches that of a pure compound run on the equipment used for the GC-MS analysis of the extracts. This is referred to in Table 4 as MSs (used as an abbreviation for mass spectrometric standard).

b) the mass spectra of the detected compound matches a published mass spectrum of the pure compound. This corresponds to MSr (mass spectrometric reference).

c) the gas chromatographic retention time of the compound matched that of the pure compound run as a standard (RTs).

d) the gas chromatographic retention time was as given in reference tables of GC retention data (RTr).

One hundred and thirty six compounds are listed in Table 4. These have a range of molecular weight from 60 to 394 and many different chemical classes are represented. Approximately 40% of the compounds are hydrocarbons, (aliphatic, alicyclic, aromatic and polyaromatic) while halogenated compounds represent 30% of the total. The only other prominent groups are the carboxylic acids which make up 12% of the total, and the phthalates (7%).

Of the halogenated compounds, only eight occurred in both raw and treated samples, and only twelve were identified in the raw sample examined. In contrast, thirty-three halogenated compounds were identified in treated water samples. It is generally accepted that several halogenated compounds (i.e. the trihalomethanes or haloforms) are produced in the chlorination process during water treatment (see Section 2.3.2 and Part I, Section 7.2). It also appears likely that other halogenated compounds are produced during water treatment as several "non-haloform" halogenated compounds were detected several times in treated water samples but were not detected in any of the raw water samples.

Appendix 2 gives a comprehensive list of organic micropollutants identified in treated water and reported in the literature up to about March 1977.

3.2. COMPOUNDS DETECTED BUT NOT POSITIVELY IDENTIFIED

Table 5 lists compounds which were detected, and, although the mass spectral data appears to refer to a single component, no positive identifications have as yet been made. The full mass spectrum of each of the eight unknowns which were detected in more than one sample is given in Appendix 3.

Certain structural features which are obvious from the mass spectral data have been noted in Table 5, and the four most intense ions present in the mass spectrum listed. Also, ions which are obviously related isotopically have been noted e.g. the natural abundance ratio for $^{35}Cl : {}^{37}Cl$ is 3 : 1, so that the two ions at $m/_e$ 107 and 109 in a 3 : 1 ratio in the mass spectrum of the unknown compound 142 in Table 5, indicates that there is at least one chlorine atom in the compound.

No published mass spectral reference data is available which matches any of the mass spectra obtained for the compounds listed in Table 5. The use of computerised library search routines on the Mass Spectral Search System (3), which has a current file of 39 509 mass spectra, did not produce any positive identifications, although mass spectra from the US Environmental Protection Agency, the National Institutes of Health and the US Food and Drug Administration (National Bureau of Standards) are included in the MSSS files. Also the examination of many of the mass spectra referred to in Table 5 by other research workers involved in the mass spectral examination of organic micropollutants in water did not lead to any identifications.

Although the actual identities of the compounds in Table 5 are not known it is interesting to note that, as in Table 4, the number of apparently halogenated compounds in treated water samples is far greater than the number of such compounds in the raw water samples examined.

3.3. LOCATION OF ORGANIC MICROPOLLUTANTS DETECTED

Table 6 gives the sampling locations where the various organic compounds listed in Tables 4 and 5 were detected. It should be pointed out that the sample extracts from Hampton, Coppermills, and some of the extracts from Clapham were examined exclusively on the Pye 104 GC-AEI MS30 system, while the Hewlett Packard 5710 GC-VG16F system was also used for the remainder of the samples. (The reasons for this have been outlined in Part I (Section 8.7)). Due to the greater sensitivity of the latter system, it is inevitable that more compounds were detected in the Staines, Langford and Clapham samples. It should also be noted that the absence of a √ in this table means that a compound was not detected. This does not necessarily mean that the compound in question was not present.

In view of the above factors, a degree of caution should be exercised when attempting to draw conclusions from the data in this Table. However, some general observations can be made.

Of the one hundred and eighty compounds in Table 5 approximately half (92)

were only detected once, sixty eight compounds have been detected in samples from more than one sampling location, and of these, fifty have been detected in samples from more than two sampling locations. Only six compounds were detected in every sample examined. Of these, four are carboxylic acids (lauric, myristic, palmitic and stearic acids) which are naturally occurring compounds. The presence of toluene in most treated waters has been reported by many workers, but as far as is known, the presence of 2 - (p-chlorophenoxy) - methyl propionic acid has not been reported previously in treated waters although it is known to be present in some wastewaters (4). It is a metabolite of a drug, clofibrate, and the precise levels present obviously need to be determined.

3.4. QUANTITATIVE ESTIMATION OF ORGANIC MICROPOLLUTANTS IDENTIFIED

In Part I and in the introduction to this report the essentially qualitative nature of this type of study has been stressed. Although semi-quantitative estimates can often be made, more accurate data requires considerable effort. In order to produce such data the various potential losses during extraction, concentration, GC separation, derivatizations (if used), passage through the membrane separator and the production of mass spectral ions must be known. This information is usually produced by calibrating the overall process with the pure substances, or less accurately by assuming behaviour identical to that known for similar substances. Since in this work well over one hundred organic micropollutants have been identified calibration with pure substances would have involved a massive effort and many of the pure substances are not in fact available.

In this work order of magnitude of concentration has been determined for many compounds identified, by comparison to the known behaviour of various organic substances in the overall analytical process. Thus the extraction and concentration stages were calibrated with a range of organic substances (see Part I, Section 3.5.5.). Standard mixtures of calibrating substances, consisting of hydrocarbons, halogenated compounds and carboxylic acid methyl esters were run on the GC-MS systems.

The data relates to Staines and Langford and was produced entirely on the

VG16F based system. Data from this system was more amenable to quantitative treatment owing to the high GC resolution, high MS sensitivity, and direct GC-MS coupling. (i.e. no membrane separator to evaluate).

Some organic micropollutants in Table 7 could not be given even an order of magnitude quantification since insufficient information was available on their behaviour through the system, particularly in the extraction stage. These substances are indicated by a '*' in the table, although they must have been present above about 1 ng/litre in order to have been detected.

Four of the haloforms identified, chloroform, dichlorobromomethane, dibromochloromethane and bromoform, were accurately quantified by use of GC with electron capture detection (see Section 2.7.2.).

3.5. SUPPLEMENTARY ANALYSES

3.5.1. Capillary GC

Although GC-MS was used to obtain the identities of compounds present in the various extracts examined, capillary GC using wall-coated open tabular (WCOT) columns and a flame ionisation detector (FID) was used to ascertain the complexity of the solvent extracts (see Part I, Sections 4 and 5). The porous layer open tubular (PLOT) columns used for the GC-MS analysis did not have the resolving power of the WCOT columns, and when composite GC peaks were encountered using GC-MS it was often only possible to identify the major component present. (For the reasons given in Part I, Section 6, WCOT GC columns were not used for the GC-MS analyses). Also the overall detection limit for the GC-FID systems was roughly ten times lower than that for the more sensitive of the two GC-MS systems. Thus although, for example, seventy four compounds were detected by GC-MS using a PLOT GC column in the raw water sample from Staines, the GC-FID trace obtained using a WCOT GC column indicated that <u>at least</u> one hundred and seventy one compounds were present. The number of components indicated by high resolution GC in each sample is shown in Table 8.

3.5.2. Trihalomethane levels

As mentioned in Part I, Section 7, increasing concern has developed recently

about the levels of certain haloforms (trihalogenated methanes) which are formed during disinfection with chlorine at the treatment works (5) (6).

In this work many trihalomethanes (seven) were identified (compounds 12,14, 16,41,43,57 and 69, Table 4) and all appear to be produced during treatment. Four predominant haloforms (chloroform, bromodichloromethane, chlorodibromomethane and bromoform) were quantified by the GC-ECD method developed at the WRC (7). All of the treated waters were examined and three of the raw waters. The results are given in Table 9, which shows that although raw water contains very low levels, relatively high levels occur after treatment.

Coppermills was resampled and significantly lower levels were encountered but it is not known whether or not the variation was due to season or a change of treatment conditions.

3.5.3. Total organically bound halogens

The levels of total organically bound halogens (chlorine, bromine, iodine) in cyclohexane extracts of Staines raw and treated water as determined by the neutron activation analysis method (referred to in Part I, Section 7) are given below

Sample	Total organically bound halogens (µg/l)		
	chlorine	bromine	iodine
Staines raw	0.45	0.03	0.01
Staines treated	3.24	1.27	0.05

The levels show the considerable increase in essentially non-polar, non-volatile organically bound halogens after treatment. The increase in organic bromine compounds appears particularly pronounced.

3.5.4. Total non-volatile organic carbon

Total non-volatile organic carbon levels are given in Table 10 for all samples. This parameter indicates the total amount of organic matter present in the sample less volatile organic substances which would be removed during the purging process employed in the analytical method. An estimate of the total

concentration of organic compounds may be obtained by doubling the TOC level. It is important to realise that many of the compounds identified and reported in Table 4 would not be included in this parameter due to volatility.

The parameter therefore indicates mainly organic matter not amenable to identification by the GC-MS approach. Removal figures could not be calculated since the raw and treated samples were taken at different times except for Coppermills 7.2.77. where a removal of about 15% was found.

4. CONCLUSIONS AND RECOMMENDATIONS

Conclusions and recommendations for further studies in relation to the analytical approach were made in Part I of this report. Generally, the approach developed was successful in that a multitude of organic micropollutants could be detected and identified.

All of the raw and treated waters examined contained a complex mixture of organic compounds which constituted a wide range of chemical types and covered a broad molecular weight range.

Chlorinated substances and hydrocarbons formed two predominant classes. The former were much more numerous in the treated water samples which probably reflects their synthesis during chlorination.

From the quantitative point of view various haloforms (see Section 3.5.2.) were the most significant. Generally, however, the amounts of organic micropollutants found were exceedingly low.

More compounds were detected than were postively identified. For a considerable number of these unknown substances mass spectral data was produced but for various reasons identification was not possible.

Due to analytical limitations the data relates to volatile organic substances. This means in effect that most of the organic matter in water (not necessarily

most of the components) has not been studied because of its non-volatile nature.

The GC-MS analytical approach in this type of survey is essentially qualitative in nature and although semi-quantitative estimates are sometimes feasible the quantitative side is very time-consuming and laborious.

From the research some recommendations for further study can be made.

a. Techniques need to be developed which are suitable for the identifications of non-volatile organic matter in water.

b. The unknown substances detected for which mass spectral data has been produced need more detailed study in order that they may be identified.

c. The quantitative side to GC-MS survey of this type requires improvement in order that better estimates of the amount of substances identified can be made.

d. More data is needed on other raw waters containing wastewater and on the derived drinking water. Similarly more data is needed on the frequency of the pollutants and on variation with time (and season).

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TABLES

1. Treatment processes.
2. Location and description of samples.
3. Summary of samples taken.
4. Organic micropollutants postively identified.
5. Organic micropollutants detected by GC-MS but not positively identified.
6. Location of organic micropollutants identified.
7. Quantitative estimates of organic micropollutants identified.
8. Number of components in samples examined detected by high resolution capillary GC.
9. Levels of trihalomethanes found in treated and raw waters.
10. Levels of non-volatile total organic carbon found in raw and treated waters.

Table 1. Treatment Processes

	CLAPHAM	COPPERMILLS	HAMPTON	LANGFORD	STAINES
Source Water	River Great Ouse	River Lea (Chingford) River Thames (Hampton)	River Thames	Rivers Chelmer and Blackwater	River Thames
Abstraction Point	Clapham	Chingford	Ashford Common	Langford	Staines
Intake	Direct from river	Reservoir	Reservoir	Reservoir	Direct from river
Primary Filter Beds		√	√		
Slow Sand Filtration		√	√		
Primary Chlorination	√			√	√
Sedimentation Tanks	√			√	√
Activated Carbon (Powder)	√				√
Softening				√	
Rapid gravity filters	√			√	√
Chlorination	√	√	√	√	√
Fluoridation	√				
Other	SO_2	SO_2, NH_3	NH_3		SO_2

Table 2. Location and Description of Samples

	CLAPHAM	COPPERMILLS	HAMPTON	LANGFORD	STAINES
Raw Water Sampling Point	River up-stream of works	Primary Filter Bed	Primary Filter Bed	Tap, Pipeline to Works	Tap after Coarse Filter
Date	23.8.76	14.7.76	26.7.76	20.9.76	22.11.76
Size (Litres)	20	20	20	20	20
Colour	Yellowish	Slight	Slight	Yellowish	Slight
Odour	Earthy	Earthy	Earthy	Earthy	Earthy
Treated Water Sampling Point	Tap(Labs)	Tap Pumphouse	Tap Contact Reservoir	Tap Pumphouse	Tap (Labs)
Date	9.8.76	2.6.76	23.3.76	7.9.76	4.11.76
Size (Litres)	20	20	20	20	20
Colour	Clear	Clear	Clear	Clear	Clear
Odour	Chlorine	Chlorine	Chlorine	Chlorine	Chlorine

Location	SAMPLE SIZE FOR ANALYSIS (LITRES)				
	Total non-volatile organic carbon	Trihalomethane determination	Total organically bound haloforms	Solvent extraction for GC-MS-DP	Date
Clapham Raw	2 × 0.1	-	-	20	23.8.76
Clapham Treated	2 × 0.1	-	-	20	9.8.76
" "	-	2 × 1	-	-	23.8.76
Coppermills Raw	2 × 0.1	2 × 1	-	-	7.2.77
" "	2 × 0.1	-	-	20	14.7.76
" Treated	2 × 0.1	-	-	20	2.6.76
" "	2 × 0.1	2 × 1	-	-	7.2.77
	-	2 × 1	-	-	14.7.76
Hampton Raw	2 × 0.1	-	-	20	26.7.76
" "	2 × 0.1	2 × 1	-	-	14.2.77
" Treated	2 × 0.1	2 × 1	-	-	14.2.77
" "	-	-	-	20	23.3.76
Langford Raw	2 × 0.1	-	-	20	20.9.76
" Treated	2 × 0.1	2 × 1	-	20	7.9.76
Staines Raw	2 × 0.1	2 × 1	-	20	22.11.76
" "	-	-	10	-	13.8.75
" Treated	2 × 0.1	2 × 1	-	20	4.11.76
" "	-	-	10		13.8.75

TABLE 4. ORGANIC MICROPOLLUTANTS POSITIVELY IDENTIFIED

Compound Name	No	Formula	M. Wt. *	Identification +	Type of Sample	
					Raw	Treated
Acenaphthene	1	$C_{12}H_{10}$	154	MSs, RTs	√	
Acetic acid	2	$C_2H_4O_2$	60	MSs, RTr	√	
Acetone	3	C_3H_6O	58	MSr, RTr		√
Acetophenone	4	C_8H_8O	120	MSr	√	
Anthracene	5	$C_{14}H_{10}$	178	MSs, RTs	√	
Benzaldehyde	6	C_7H_6O	106	MSr		√
Benzene	7	C_6H_6	78	MSs, RTs	√	√
x Benzoic acid	8	$C_7H_6O_2$	122	MSr	√	√
Benzthiazole	9	C_7H_5NS	135	MSs, RTs	√	
Benzyl cyanide	10	C_8H_7N	117	MSs, RTs		√
Biphenyl	11	$C_{12}H_{10}$	154	MSs, RTs	√	
Bromochloroiodomethane	12	CH Cl BrI	254	MSr		√
Bromochloromethane	13	CH_2Cl Br	128	MSs, RTs		√
Bromodichloromethane	14	CH Cl_2Br	162	MSs, RTs		√
Bromoethychloroethyl ether	15	C_4H_8O Cl Br	186	MSr		√
Bromoform	16	CH Br_3	250	MSs, RTs		√
C_7 alkane isomer	17	C_7H_{16}	100	MSr	√	√
C_7 alkane isomer	18	C_7H_{16}	100	MSr		√
C_3 benzene isomer	19	C_9H_{12}	120	MSr, RTr	√	√
C_3 benzene isomer	20	C_9H_{12}	120	MSr, RTr	√	√
C_3 benzene isomer	21	C_9H_{12}	120	MSr, RTr	√	√
C_3 benzene isomer	22	C_9H_{12}	120	MSr, RTr	√	√
C_3 benzene isomer	23	C_9H_{12}	120	MSr, RTr	√	√
C_3 benzene isomer	24	C_9H_{12}	120	MSr, RTr	√	√
C_3 benzene isomer	25	C_9H_{12}	120	MSr, RTr	√	√
C_3 benzene isomer	26	C_9H_{12}	120	MSr, RTr	√	√
C_4 benzene isomer	27	$C_{10}H_{14}$	134	MSr, RTr	√	√
C_4 benzene isomer	28	$C_{10}H_{14}$	134	MSr, RTr	√	√
C_4 benzene isomer	29	$C_{10}H_{14}$	134	MSr, RTr	√	√
C_4 benzene isomer	30	$C_{10}H_{14}$	134	MSr, RTr	√	√
C_4 benzene isomer	31	$C_{10}H_{14}$	134	MSr, RTr	√	√

Compound Name	No	Formula	M.Wt.*	Identification+	Type of Sample	
					Raw	Treated
C_4 benzene isomer	32	$C_{10}H_{14}$	134	MSr, RTr	√	√
C_4 benzene isomer	33	$C_{10}H_{14}$	134	MSr,RTr	√	√
C_4 benzene isomer	34	$C_{10}H_{14}$	134	MS r,RTr	√	√
C_5 benzene isomer	35	$C_{11}H_{16}$	148	MSr,RTr	√	√
C_5 benzene isomer	36	$C_{11}H_{16}$	148	MSr,RTr	√	√
C_6 diene isomer	37	C_6H_{10}	82	MSr,RTr		√
Camphor	38	$C_{10}H_{16}O$	152	MSr	√	
Carbon tetrachloride	39	CCl_4	152	MSs,RTs		√
Chlorobenzene	40	C_6H_5Cl	112	MSs,RTs	√	√
Chlorodibromomethane	41	$CH\,Cl\,Br_2$	206	MSs,RTs		√
bis-Chloroethyl ether	42	$C_4H_8O\,Cl_2$	142	MSs,RTs	√	√
Chloroform	43	$CH\,Cl_3$	118	MSs,RTs		√
Chloromethylbutene isomer	44	C_5H_9Cl	104	MSr		√
Chloromethyl butene isomer	45	C_5H_9Cl	104	MSr		√
Chloromethyl butene isomer	46	C_5H_9Cl	104	MSr		√
Chloromethyl butene isomer	47	C_5H_9Cl	104	MSr		√
x p-Chlorophenoxy acetic acid	48	$C_8H_7O_3Cl$	186	MSs,RTs		√
x 2-(p-chlorophenoxy)-2 methyl propionic acid	49	$C_{10}H_{11}O_3Cl$	214	MSr	√	√
Cyanobenzene	50	C_7H_5N	103	MSr		√
Cyclohexane	51	C_6H_{12}	84	MSr,RTr	√	√
n-Decane	52	$C_{10}H_{22}$	142	MSr,RTr	√	
x n-Decanoic acid	53	$C_{10}H_{20}O_2$	172	MSr,RTr	√	√
x Dehydroabietic acid	54	$C_{20}H_{28}O_2$	300	MSr	√	
Diacetone alcohol	55	$C_6H_{13}O_2$	116	MSr	√	
Dibromoacetronitrile	56	$C_2HN\,Br_2$	197	MSr		√
Dibromoiodomethane	57	$CH\,Br_2I$	298	MSr		√
1,5-Dibromopentane	58	$C_5H_{10}Br_2$	228	MSs,RTs		√
Dibromopentane isomer	59	$C_5H_{10}Br_2$	228	MSr		√
Dibromopentane isomer	60	$C_5H_{10}Br_2$	228	MSr		√
Dibutylphthalate isomer	61	$C_{16}H_{22}O_4$	278	MSs,RTs	√	√

Compound Name	No	Formula	M.Wt*	Identification+	Type of Sample	
					Raw	Treated
Dibutylphthalate isomer	62	$C_{16}H_{22}O_4$	278	MSs,RTs	√	√
x Dichloroacetic acid	63	$C_2H_2O_2Cl_2$	128	MSr		√
Dichloroacetonitrile	64	$C_2HN\,Cl_2$	109	MSr		√
Dichlorobenzene isomer	65	$C_6H_4\,Cl_2$	146	MSs,RTs	√	√
Dichlorobenzene isomer	66	$C_6H_4Cl_2$	146	MSs,RTs	√	√
1,1-Dichloroethane	67	$C_2H_4Cl_2$	98	MSs,RTs	√	√
1,2-Dichloroethane	68	$C_2H_4Cl_2$	98	MSs,RTs	√	√
Dichloroiodomethane	69	$CH\,Cl_2I$	210	MSr		√
Dichloromethane	70	CH_2Cl_2	84	MSs,RTs	√	
x 3,6-Dichloro-2-methoxy benzoic acid	71	$C_8H_6Cl_2O_3$	220	MSs,RTs		√
Dichloropentane isomer	72	$C_5H_{10}Cl_2$	140	MSr		√
Diethylphthalate	73	$C_{12}H_{14}O_4$	222	MSs,RTs	√	√
x Dimethyl benzoic acid isomer	74	$C_9H_{10}O_2$	150	MSr	√	
Dimethylnaphthalene isomer	75	$C_{12}H_{12}$	156	MSs,RTr	√	
Dimethylnaphthalene isomer	76	$C_{12}H_{12}$	156	MSs,RTr	√	
Dimethylnaphthalene isomer	77	$C_{12}H_{12}$	156	MSs,RTr	√	
Dimethylphthalate	78	$C_{10}H_{10}O_4$	194	MSs,RTs	√	√
Dioctylphthalate isomer	79	$C_{24}H_{38}O_4$	390	MSs,RTr	√	√
Dioctylphthalate isomer	80	$C_{24}H_{38}O_4$	390	MSs,RTr	√	√
Dioctylphthalate isomer	81	$C_{24}H_{38}O_4$	390	MSs,RTr	√	√
Diphenylamine	82	$C_{12}H_{11}\,N$	169	MSs,RTs	√	√
Dipropyl phthalate isomer	83	$C_{14}H_{18}O_4$	250	MSs,RTs	√	√
Dipropyl phthalate isomer	84	$C_{14}H_{18}O_4$	250	MSs,RTs		√
n-Dodecane	85	$C_{12}H_{26}$	170	MSr,RTr	√	
n-Eicosane	86	$C_{20}H_{42}$	282	MSs,RTs	√	
Ethylbenzene	87	C_8H_{10}	106	MSs,RTs	√	√
Ethylstyrene isomer	88	$C_{10}H_{12}$	132	MSr	√	
Fluoranthene	89	$C_{16}H_{10}$	202	MSs,RTs	√	√
Fluorene	90	$C_{13}H_{10}$	166	MSs,RTs	√	√
n-Heptadecane	91	$C_{17}H_{36}$	240	MSr,RTr	√	√
x n-Heptadecanoic acid	92	$C_{17}H_{34}O_2$	270	MSr,RTr	√	√
n-Heptacosane	93	$C_{27}H_{56}$	380	MSs,RTs	√	
Hexachloroethane	94	C_2Cl_6	234	MSs,RTs		√

Compound Name	No	Formula	M.Wt.*	Identification+	Type of Sample	
					Raw	Treated
n-Hexacosane	95	$C_{26}H_{54}$	366	MSs,RTs	√	
n-Hexadecane	96	$C_{16}H_{34}$	226	MSr,RTr		√
x Lactic acid	97	$C_3H_6O_3$	90	MSr		√
x Lauric acid	98	$C_{12}H_{24}O_2$	200	MSs,RTs	√	√
Methylcyclohexane	99	C_7H_{14}	98	MSr		√
1-Methyl naphthalene	100	$C_{11}H_{10}$	142	MSs,RTs	√	√
2-Methylnaphthalene	101	$C_{11}H_{10}$	142	MSs,RTs	√	√
Methylstyrene isomer	102	C_9H_{10}	118	MSr	√	
Methylstyrene isomer	103	C_9H_{10}	118	MSr	√	
Methylstyrene isomer	104	C_9H_{10}	118	MSr	√	
x Myristic acid	105	$C_{14}H_{28}O_2$	228	MSs,RTs	√	√
Naphthalene	106	$C_{10}H_8$	128	MSs,RTs	√	√
n-Nonadecane	107	$C_{19}H_{40}$	268	MSs,RTs	√	
x n-Nonanoic acid	108	$C_9H_{18}O_2$	158	MSr,RTr	√	
n-Octacosane	109	$C_{28}H_{58}$	394	MSs,RTs	√	
x n-Octanoic acid	110	$C_8H_{16}O_2$	144	MSr,RTr	√	
x Palmitic acid	111	$C_{16}H_{32}O_2$	256	MSs,RTs	√	√
n-Pentadecane	112	$C_{15}H_{32}$	212	MSr,RTr		√
x Pentadecanoic acid	113	$C_{15}H_{30}O_2$	242	MSr,RTr	√	√
Phenanthrene	114	$C_{14}H_{10}$	178	MSs,RTs	√	√
Phenol	115	C_6H_6O	94	MSs,RTs		√
Pyrene	116	$C_{16}H_{10}$	202	MSs,RTs	√	
x Stearic acid	117	$C_{18}H_{36}O_2$	284	MS,RTs	√	√
Styrene	118	C_8H_8	104	MSr,RTr		√
x Succinic acid	119	$C_4H_6O_4$	118	MSr		√
α - Terpineol	120	$C_{10}H_{18}O$	154	MSr	√	
Tetrachlorobenzene isomer	121	$C_6H_2Cl_4$	214	MSr,RTr		√
Tetrachlorobenzene isomer	122	$C_6H_2Cl_4$	214	MSr,RTr		√
Tetrachloroethylene	123	C_2Cl_4	164	MSs,RTs	√	√
n-Tetradecane	124	$C_{14}H_{30}$	198	MSr,RTr	√	
Toluene	125	C_7H_8	92	MSs,RTs	√	√
x Toluic acid isomer	126	$C_8H_8O_2$	136	MSs,RTr		√
Tributylphosphate	127	$C_{12}H_{27}O_4P$	266	MSs,RTs	√	√
Trichlorobenzene isomer	128	$C_6H_3Cl_3$	180	MSs,RTr	√	
Trichloroethylene	129	C_2HCl_3	130	MSs,RTs	√	√
n-Tridecane	130	$C_{13}H_{28}$	184	MSr,RTr	√	
x n-Tridecanoic acid	131	$C_{13}H_{26}O_2$	214	MSr,RTr	√	√

Compound Name	No	Formula	M.Wt.*	Identification+	Type of Sample	
					Raw	Treated
n-Undecane	132	$C_{11}H_{24}$	156	MSr,RTr	√	
Vinyl chloride	133	C_2H_3Cl	62	MSr	√	
m-Xylene	134	C_8H_{10}	106	MSs,RTs,	√	√
o-Xylene	135	C_8H_{10}	106	MSs,RTs	√	√
p-Xylene	136	C_8H_{10}	106	MSs,RTs	√	√

+ MSs = corresponds to the mass spectrum of the pure compound run as a standard

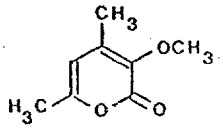
MSr = corresponds to mass spectral data published in reference works

RTs = GC retention time corresponds to standard. RTr = GC retention time corresponds to reference data.

* The molecular weight given is calculated from the integral values of the atomic weights of the most abundant isotope of each element present.

x Compound identified after methylation as its methyl ester.

TABLE 5. ORGANIC MICROPOLLUTANTS DETECTED BY GC-MS BUT NOT POSITIVELY IDENTIFIED.

Number	Structural information	Principal Masses	Where found	
			Raw	Treated
137	Brominated, oxygenated. Probably contains C_3H_6O Br fragment	43, 73, 41, 55 (137:139 = 1:1, 151:153 = 1:1)		√
138	Isomer of 140?	59, 43, 41, 31 (151:153 = 1:1)		√
139	Possibly 	155, 154, 67, 127, 126		√
140	Brominated, oxygenated	59, 57, 29, 41 (137:139 = 1:1)		√
141	Unsaturated carboxylic acid? (detected as methyl ester)	55, 41, 43, 69 (264, 265)	√	
142	Chlorinated, oxygenated. Probably contains C_4H_8OCl fragment	59, 43, 41, 107 (107:109 = 3:1)		√
143	Chlorinated polyaromatic compound? $C_{15}H_{13}Cl$?	228, 230, 106, 103 (228:230 = 3:1)	√	
144	Trialkyl phosphate	133, 99, 90, 155	√	
145	Nitrophenol	65, 139, 109, 39	√	
146	Dimethyl acridine?	194, 193, 192, 195	√	
147		143, 303, 187, 105	√	
148	Detected after methylation-suggests that this compound is a dichloro acid	130, 132, 103, 43 (165:167:169 = 9:6:1)		√
149	Unsaturated carboxylic acid (detected as methyl ester) - nomolog of 156?	43, 60, 57, 102 (228, 229)	√	
150	Alkyl substituted, nitrogenated polyaromatic compound?	196, 211, 197, 93	√	√
151	Dichlorinated	69, 41, 39, 27 (105:107:109 = 9:6:1)		√
152	Detected after methylation	169, 184, 41, 55	√	

Number	Structural information	Principal Masses	Where found	
			Raw	Treated
153	Unsaturated carboxylic acid (detected as methyl ester) - homolog of 149?	43, 102, 60, 57 (256, 257)	√	
154	Chlorinated alcohol? Possibly C_5H_9O Cl	57, 29, 27, 41 (120:122 = 3:1, 102:104 = 3:1)		√
155	Tetradecanediol?	69, 55, 83, 97	√	
156	Mono chloro compound?	41, 69, 27, 39 (77:79=3:1, 76:78=3:1)		√
157	Isomer of 156	41, 69, 76, 77 (77:79=3:1, 76:78=3:1)		√
158	C_5 or C_6 alcohol	45, 43, 27, 41		√
159	C_5 or C_6 alcohol	43, 45, 27, 41		√
160	C_5 or C_6 alcohol	59, 27, 31, 41		√
161	?	67, 53, 39, 68		√
162	Brominated compound	31, 43, 73, 55 (123:125 = 1:1)		√
163	Isomer of 162	73, 55, 43, 41 (123:125 = 1:1)		√
164	?	139, 67, 53, 43		√
165	?	68, 96, 39, 41		√
166	Chlorinated compound	58, 43, 68, 27 (173:175 = 3:1), 200:202 = 3:1, 215:217 = 3:1)		√
167	Butyl butyrate?	71, 56, 43, 89	√	
168	Methyl dihydroindene isomer?	117, 132, 131, 115	√	
169	Phenyl alkane?	91, 155, 184, 65	√	
170	Di-n-decyl ketone?	43, 57, 41, 169		√
171	Chlorinated compound	59, 31, 29, 57 (83:85:87 = 9:6:1, 123:125:127 = 9:6:1)		√

Number	Structural information	Principal Masses	Where found	
			Raw	Treated
172	Butyl butyrate?	71, 56, 43, 89	√	
173	Dibromomethoxymethyl benzene? (detected after methylation) - originally as a dibromomethyl phenol?	265, 280, 237, 263	√	
174	Mass spectrum indicative of dimethylformamide but GC retention time incorrect	73, 44, 42, 30	√	
175	Possibly an organic nitrate	46, 59, 29, 31	√	
176	Possibly an organic nitrate	46, 45, 30, 90	√	
177	A hexadecatetraene	79, 67, 41, 80	√	
178	Isopropyl disulphide?	43, 41, 108, 150		√
179	Dichloro compound	73, 29, 43, 93 (93:95 = 3:1, 117: 119:121 = 9:6:1)		√
180	Chlorinated	59, 41, 43, 93 (93:95 = 3:1)		√

TABLE 6. LOCATION OF ORGANIC MICROPOLLUTANTS IDENTIFIED

Number	Compound name	Hampton		Clapham		Coppermills		Langford		Staines	
		R	T	R	T	R	T	R	T	R	T
1	Acenaphthene			√							
2	Acetic acid							√			
3	Acetone		√								
4	Acetophenone			√							
5	Anthracene			√							
6	Benzaldehyde								√		√
7	Benzene	√	√	√		√	√	√	√	√	√
8	Benzoic acid	√		√	√				√		
9	Benzthiazole			√						√	
10	Benzyl cyanide				√				√	√	√
11	Biphenyl			√							
12	Bromochloroiodomethane				√		√		√		
13	Bromochloromethane								√		
14	Bromodichloromethane				√		√		√		√
15	Bromoethylchloroethyl ether								√		
16	Bromoform		√		√		√		√		√
17	C_7 alkane isomer		√	√			√				
18	C_7 alkane isomer						√				
19	C_3 benzene isomer			√			√	√	√	√	√
20	C_3 benzene isomer			√				√	√	√	
21	C_3 benzene isomer			√				√		√	
22	C_3 benzene isomer			√						√	
23	C_3 benzene isomer			√						√	
24	C_3 benzene isomer			√						√	
25	C_3 benzene isomer			√						√	
26	C_3 benzene isomer									√	
27	C_4 benzene isomer			√				√		√	
28	C_4 benzene isomer			√						√	
29	C_4 benzene isomer			√						√	
30	C_4 benzene isomer			√						√	
31	C_4 benzene isomer									√	
32	C_4 benzene isomer									√	

Number	Compound name	Hampton		Clapham		Coppermills		Langford		Staines	
		R	T	R	T	R	T	R	T	R	T
33	C_4 benzene isomer									√	
34	C_4 benzene isomer									√	
35	C_5 benzene isomer									√	
36	C_5 benzene isomer									√	
37	C_6 diene isomer						√				
38	Camphor									√	
39	Carbon tetrachloride								√		√
40	Chlorobenzene						√			√	
41	Chlorodibromomethane		√		√		√		√		√
42	bis-Chloroethyl ether							√	√		
43	Chloroform		√		√		√		√		√
44	Chloromethyl butene isomer				√						√
45	Chloromethyl butene isomer				√		√				
46	Chloromethylbutene isomer						√				
47	Chloromethylbutene isomer				√						
48	p-Chlorophenoxy acetic acid								√		
49	2-(p-chlorophenoxy)-2-methyl-propionic acid	√	√	√	√	√	√	√	√	√	√
50	Cyanobenzene										√
51	Cyclohexane	√	√	√		√		√			
52	n-Decane					√		√		√	
53	n-Decanoic acid	√		√	√	√					
54	Dehydroabietic acid									√	
55	Diacetone alcohol							√		√	
56	Dibromoacetonitrile								√		√
57	Dibromoiodomethane				√		√		√		
58	1,5-Dibromopentane						√		√		√
59	Dibromopentane isomer						√		√		√
60	Dibromopentane isomer								√		
61	Dibutyl phthalate isomer	√	√		√	√	√	√	√	√	√
62	Dibutyl phthalate isomer	√		√	√				√	√	√
63	Dichloroacetic acid								√	√	

Number	Compound name	Hampton		Clapham		Coppermills		Langford		Staines	
		R	T	R	T	R	T	R	T	R	T
64	Dichloroacetonitrile						√		√		√
65	Dichlorobenzene isomer			√	√		√	√	√	√	√
66	Dichlorobenzene isomer			√			√	√	√	√	√
67	1,1-Dichloroethane	√									
68	1,2-Dichloroethane			√	√				√		√
69	Dichloroiodomethane				√		√		√		
70	Dichloromethane	√		√		√					
71	3,6-Dichloro-2-methoxybenzoic acid								√		
72	Dichloropentane isomer						√		√		√
73	Diethyl phthalate	√		√	√	√	√	√	√	√	√
74	Dimethyl benzoic acid isomer	√									
75	Dimethyl naphthalene isomer			√		√				√	
76	Dimethylnaphthalene isomer			√							
77	Dimethylnaphthalene isomer			√							
78	Dimethyl phthalate	√									
79	Dioctyl phthalate isomer	√						√		√	√
80	Dioctyl phthalate isomer	√						√		√	√
81	Dioctyl phthalate isomer	√						√		√	√
82	Diphenylamine	√			√			√			√
83	Dipropyl phthalate isomer	√									√
84	Dipropyl phthalate isomer				√						
85	n-Dodecane				√					√	
86	n-Eicosane					√				√	
87	Ethylbenzene			√				√	√	√	
88	Ethyl styrene isomer									√	
89	Fluoranthene			√					√	√	
90	Fluorene			√							
91	n-Heptadecane					√					√
92	n-Heptadecanoic acid						√				
93	n-Heptacosane							√			
94	Hexachloroethane								√		
95	n-Hexacosane							√			
96	n-Hexadecane								√		√
97	Lactic acid				√						

Number	Compound name	Hampton		Clapham		Coppermills		Langford		Staines	
		R	T	R	T	R	T	R	T	R	T
98	Lauric acid	√	√	√	√	√	√	√	√	√	√
99	Methyl cyclohexane					√					
100	1-Methyl naphthalene			√				√	√	√	√
101	2-Methyl napthalene			√					√	√	√
102	Methyl styrene isomer									√	
103	Methyl styrene isomer									√	
104	Methyl styrene isomer									√	
105	Myristic acid	√	√	√	√	√	√	√	√	√	√
106	Naphthalene	√				√		√	√	√	√
107	n-Nonadecane									√	
108	n-Nonanoic acid	√									
109	n-Octacosane							√		√	
110	n-Octanoic acid	√		√							
111	Palmitic acid	√	√	√	√	√	√	√	√	√	√
112	n-Pentadecane	√						√		√	√
113	n-Pentadecanoic acid		√	√	√		√	√		√	√
114	Phenanthrene								√	√	
115	Phenol								√		
116	Pyrene									√	
117	Stearic acid	√	√	√	√	√	√	√	√	√	√
118	Styrene							√			
119	Succinic acid				√						
120	α - Terpineol									√	
121	Tetrachlorobenzene isomer						√				
122	Tetrachlorobenzene isomer						√				
123	Tetrachloroethylene						√			√	√
124	n-Tetradecane	√								√	
125	Toluene	√	√	√	√	√	√	√	√	√	√
126	Toluic acid isomer								√		
127	Tributyl phosphate	√		√	√				√	√	√
128	Trichlorobenzene isomer									√	
129	Trichloroethylene									√	√

Number	Compound name	Hampton		Clapham		Coppermills		Langford		Staines	
		R	T	R	T	R	T	R	T	R	T
130	n-Tridecane	√			√					√	
131	n-Tridecanoic acid					√		√	√		√
132	n-Undecane				√					√	
133	Vinyl chloride	√			√						√
134	m-Xylene	√	√	√			√	√	√	√	√
135	o-Xylene	√	√	√			√	√	√	√	√
136	p-Xylene	√	√	√			√	√	√	√	√
137									√		
138									√		
139									√		
140					√				√		
141		√				√	√	√			
142					√		√		√		√
143				√							
144				√							
145				√							
146		√									
147		√		√							
148					√				√		
149					√		√	√	√	√	
150		√						√			√
151								√	√		
152		√			√	√		√			
153										√	
154											√
155										√	
156											√
157											√
158											√
159											√
160											√
161											√
162									√		
163									√		
164									√		

Number	Compound name	Hampton		Clapham		Coppermills		Langford		Staines	
		R	T	R	T	R	T	R	T	R	T
165									✓		
166										✓	
167										✓	
168										✓	
169										✓	
170					✓						
171					✓						
172									✓		
173								✓		✓	
174											
175										✓	
176										✓	
177				✓							
178							✓				
179					✓						
180					✓						

TABLE 7. QUANTITATIVE ESTIMATES OF ORGANIC MICROPOLLUTANTS IDENTIFIED (ng/litre)

No.	Compound name	Staines		Langford	
		Raw	Treated	Raw	Treated
2	Acetic acid	-	-	*	-
6	Benzaldehyde	-	*	-	*
7	Benzene	150	60	50	50
8	Benzoic acid	-	-	-	*
9	Benzthiazole	20	-	-	-
10	Benzyl cyanide	*	*	-	*
12	Bromochloroiodomethane	-	-	-	200
13	Bromochloromethane	-	-	-	50
14	Bromodichloromethane	-	22×10^3	-	76×10^3
15	Bromoethyl chloroethyl ether	-	-	-	50
16	Bromoform	-	1.3×10^3	-	5×10^3
19	C_3 benzene isomer	100	20	20	20
20	C_3 benzene isomer	100	-	20	20
21	C_3 benzene isomer	50	-	10	-
22	C_3 benzene isomer	50	-	-	-
23	C_3 benzene isomer	50	-	-	-
24	C_3 benzene isomer	20	-	-	-
25	C_3 benzene isomer	20	-	-	-
26	C_3 benzene isomer	20	-	-	-
27	C_4 benzene isomer	50	-	20	-
28	C_4 benzene isomer	50	-	-	-
29	C_4 benzene isomer	50	-	-	-
30	C_4 benzene isomer	20	-	-	-
31	C_4 benzene isomer	20	-	-	-
32	C_4 benzene isomer	10	-	-	-
33	C_4 benzene isomer	10	-	-	-
34	C_4 benzene isomer	10	-	-	-
35	C_5 benzene isomer	20	-	-	-
36	C_5 benzene isomer	20	-	-	-
38	Camphor	*	-	-	-
39	Carbon tetrachloride	-	5	-	20

No	Compound name	Staines		Langford	
		Raw	Treated	Raw	Treated
40	Chlorobenzene	15	-	-	-
41	Chlorodibromomethane	-	5×10^3	-	40×10^3
42	bis-Chloroethyl ether	-	-	50	100
43	Chloroform	-	56×10^3	-	72×10^3
44	Chloromethyl butene isomer	-	5	-	-
48	p-chlorophenoxy acetic acid	-	-	-	10
49	2-(p-chlorophenoxy)-2-methyl propionic acid	40	20	50	20
50	Cyanobenzene	-	*	-	-
51	Cyclohexane	-	-	20	-
52	n-Decane	25	-	20	-
54	Dehydroabietic acid	*	-	-	-
55	Diacetone alcohol	*	-	*	-
56	Dibromoacetonitrile	-	*	-	*
57	Dibromoiodomethane	-	-	-	200
58	1,5-Dibromopentane	-	100	-	200
59	Dibromopentane isomer	-	50	-	100
60	Dibromopentane isomer	-	-	-	50
61	Dibutyl phthalate isomer	300	100	500	500
62	Dibutyl phthalate isomer	100	50	-	200
63	Dichloroacetic acid	*	-	-	*
64	Dichloroacetonitrile		*	-	*
65	Dichlorobenzene isomer	200	100	50	50
66	Dichlorobenzene isomer	50	20	10	20
68	1,2-Dichloroethane	-	20	-	20
69	Dichloroiodomethane	-	-	-	500
71	3,6-Dichloro-2-methoxybenzoic acid	-	-	-	20
72	Dichloropentane isomer	-	50	-	50
73	Diethyl phthalate	200	50	200	200
75	Dimethyl naphthalene isomer	25	-	-	-
79	Dioctyl phthalate isomer	1000	200	500	-
80	Dioctyl phthalate isomer				
81	Dioctyl phthalate isomer				

No.	Compound name	Staines		Langford	
		Raw	Treated	Raw	Treated
82	Diphenylamine	*	*	*	-
83	Dipropyl phthalate isomer	-	50	-	-
85	n-Dodecane	40	-	-	-
86	n-Eicosane	50	-	-	-
87	Ethyl benzene	100	-	50	50
88	Ethyl styrene isomer	50	-	-	-
89	Fluoranthene	50	-	-	20
91	n-Heptadecane	-	20	-	-
93	n-Heptacosane	-	-	50	-
94	Hexachloroethane	-	-	-	50
95	n-Hexacosane	-	-	50	-
96	n-Hexadecane	-	15	-	20
98	Lauric acid	100	50	100	300
100	1-Methyl naphthalene	50	5	20	10
101	2-Methyl napthalene	50	5	-	10
102	Methyl styrene isomer	20	-	-	-
103	Methyl styrene isomer	20	-	-	-
104	Methyl styrene isomer	10	-	-	-
105	Myristic acid	400	300	200	500
106	Naphthalene	100	20	50	30
107	n-Nonadecane	50	-	-	-
109	n-Octacosane	50	-	50	-
111	Palmitic acid	1000	800	600	2×10^3
112	n-Pentadecane	50	20	50	-
113	Pentadecanoic acid	100	100	50	-
114	Phenanthrene	30	-	-	10
115	Phenol	-	-	-	*
116	Pyrene	20	-	-	-
117	Stearic acid	300	300	200	400
118	Styrene	-	-	20	-
120	α-Terpineol	*	-	-	-
123	Tetrachloroethylene	100	20	-	-
124	n-Tetradecane	40	-	-	-
125	Toluene	100	80	50	60

No.	Compound name	Staines		Langford	
		Raw	Treated	Raw	Treated
126	Toluic acid isomer	-	-	-	*
127	Tributyl phosphate	*	*	-	*
128	Trichlorobenzene isomer	20	-	-	-
129	Trichloroethylene	70	50	-	-
130	n-Tridecane	50	-	-	-
131	n-Tridecanoic acid	-	50	50	50
132	n-Undecane	30	-	-	-
133	Vinyl chloride	-	10	-	-
134	m-Xylene	50	50	20	50
135	o-Xylene	20	10	10	10
136	p-Xylene	50	20	10	30

Table 8 Number of components in samples examined detected by high resolution capillary GC.

Sample	Minimum number of components present at levels of at least 0.1 ng./litre
Hampton Raw	157
Hampton Treated	107
Clapham Raw	149
Clapham Treated	139
Coppermills Raw	153
Coppermills Treated	92
Langford Raw	97
Langford Treated	118
Staines Raw	171
Staines Treated	137

Table 9. Levels of Trihalomethanes found in treated and raw waters

Location	Levels in µg/l				Date
	$CHCl_3$	$CHCl_2Br$	$CHClBr_2$	$CHBr_3$	
Clapham Treated	80	42	14	1.8	23.8.76
Coppermills Raw	0.2	0.04	<0.02	<0.02	7.2.77
Coppermills Treated	10.8	11.2	3.7	1.3	7.2.77
Coppermills Treated	30	32	36	8	14.7.76
Hampton Raw	0,2	0.03	<0.02	<0.02	14.2.77
Hampton Treated	8	10.8	4.6	0.6	14.2.77
Langford Treated	72	76	40	5	7.9.76
Staines Raw	2.3	0.03	<0.02	<0.02	22.11.76
Staines Treated	56	22	5	1.3	4.11.76

Table 10. Levels of Non-Volatile Total Organic Carbon found in Raw and Treated Waters

Location	Level mg C/l		% Removal	Date
	Raw	Treated		
Clapham	11.2	-	-	23.8.76
Clapham	-	8.5	-	9.8.76
Coppermills	5.5	-	-	14.7.76
"	-	3.3	-	2.6.76
"	5.2	4.4	15%	7.2.77
Hampton	4.3	-	-	26.7.76
"	4.8	4.0	-	14.2.77
Langford	6.75	-	-	20.9.76
"	-	5.3	-	7.9.76
Staines	5.5	-	-	22.11.76
"	-	4.5	-	4.11.76

APPENDICES

1. Mass spectral library
2. List of organic compounds identified in drinking water (international)
3. Mass spectra of unknown compounds occurring in more than one sample.

APPENDIX 1

MASS SPECTRAL LIBRARY

Classification

- Polyaromatic Hydrocarbons
- Bases
- Phenols
- Alcohols
- Halogenated (includes all chloro- and bromo-compounds except pesticides)
- Pesticides
- Phthalates
- Methyl esters
- Miscellaneous

. Fluoranthene
Anthracene
Phenanthrene
Acenaphthylene
Acenaphthene
1,2,5,6-Dibenzanthracene
1,2,3,4-Dibenzanthracene
Indeno(1,2,3-c.d)Pyrene
3,4-Benzfluoranthene
11,12-Benzfluoranthene
3,4-Benzpyrene
1,2-Benzanthracene
1,2-Benzfluorene
Naphthalene
Benzo(g.h.i.)Perylene
Perylene
Pyrene
Chrysene
2-Methyl Anthracene
9-Methyl Anthracene
1-Methyl Phenanthrene
1-Methyl Fluorene
9,10-Diphenyl Anthracene
9-Phenyl Anthracene
Triphenylene
1-Methyl Naphthalene
2-Methyl Naphthalene
1,4-Dimethyl Naphthalene
1,5-Dimethyl Naphthalene
1,6-Dimethyl Naphthalene
2,3-Dimethyl Naphthalene
2,6-Dimethyl Naphthalene
Fluorene
2,3,6-Trimethyl Naphthalene
Biphenyl
3,3'-Dimethyl Biphenyl
4,4'-Dimethyl Biphenyl

2. Pyridine
2-Methyl Pyridine
3-Methyl Pyridine
4-Methyl Pyridine
2-Ethyl Pyridine
3-Ethyl Pyridine
4-Ethyl Pyridine
2,3-Dimethyl Pyridine
2,4-Dimethyl Pyridine
2,5-Dimethyl Pyridine
2,6-Dimethyl Pyridine
3,4-Dimethyl Pyridine
3,5-Dimethyl Pyridine
2,4,6-Trimethyl Pyridine
iso-Quinoline
Quinoline
2-Methyl Quinoline
4-Methyl Quinoline
6-Methyl Quinoline
7-Methyl Quinoline
8-Methyl Quinoline
3-Methyl Quinoline
2,4-Dimethyl Quinoline
2,6-Dimethyl Quinoline
o-Ethyl Aniline
n-Ethyl Aniline
m-Toluidine
p'-Toluidine
5,6-Benzoquinoline
2-Phenyl Pyridine
N-Methyl-p-toluidine

3. Phenol
o-Cresol
m-Cresol
p-Cresol
2,3-Xylenol
2,4-Xylenol
2,5-Xylenol
2,6-Xylenol
3,4-Xylenol
3,5-Xylenol
1-Naphthol
Catechol
2-Hydroxy Biphenyl

4. Butan-1-ol
Butan-2-ol
Pentan-1-ol
Hexan-1-ol
Octan-1-ol
Octan-2-ol
2,5-Dimethyl-2,5- Hexanediol
Hexan-2-ol
Hexan-3-ol
Heptan-2-ol

5. Pentachlorophenol
2-Chlorophenol
3-Chlorophenol
4-Chlorophenol
2,4-Dichlorophenol
2,6-Dichlorophenol
2,4,5-Trichlorophenol
2,4,6-Trichlorophenol
2,4,6-Tribromophenol
Bromochloromethane
Bromodichloromethane
Bromoform
Chloroform
Dichloromethane
1,1-Dichloroethane
1,2-Dichloroethane
1,1,1-Trichloroethane
Trichloroethylene
Tetrachloroethylene
Carbon Tetrachloride
1,2-Dichloroethylene
1,1,2,2-Tetrabromoethane
1,3-Dibromopropane
Chlorobenzene
1,2-Dichlorobenzene
1,3-Dichlorobenzene

5. Continued:
1,4-Dichlorobenzene
1,2,4-Trichlorobenzene
1,2,3,4-Tetrachlorobenzene
1,2,3,5-Tetrachlorobenzene
1,2,4,5-Tetrachlorobenzene
2-Chlorotoluene
3-Chlorotoluene
4-Chlorotoluene
Dibromomethane
1,2-Dibromoethane
1,2-Dibromopropane
Chlorodibromomethane
Pentachlorobenzene
5-Chloro-2-methylaniline
3-Chloro-4-methylaniline
2,4-Dichloroaniline
2,6-Dichloroaniline
3,4-Dichloroaniline
2-Chloroaniline
3-Chloroaniline
4-Chloroaniline
1-Chloro-2-nitrobenzene
1-Chloro-4-nitrobenzene
4-Chloro-3,5-Xylenol
1-Chloro-2,4-Dinitrophenol
Hexachloroethane
2-Bromopropane
1,6-Dichlorohexane
Trans-1,2-Dibromocyclohexane
Bromocyclohexane
1-Bromobutane
Bis-2-Chloroethylether
2,2-Dichloroethyl Methyl ether
3-Chloroheptane
3-Bromohexane
Hexachloro-1,3-Butadiene
1,2-Dibromopentane
1-Chloro-3- hydroxypropane
1-Chloro-5- hydroxyhexane
1-Chloro-3-methyl-2-butene
1-Chlorobutane
1-Chlorohexane
p-Bromo-N,N-Diethylaniline
Tris(2-Chloroethyl)Phosphate
1,3-Dichlorobutane
1,4-Dibromo-2-butene
1,5-Dichloropentane
1,5-Dibromopentane
4,4'-Dichlorobiphenyl
2-Chlorobiphenyl

2,3,5-Trichlorobiphenyl
2,2',4,4'-Tetrachlorobiphenyl
Trans-1,4-Dichloro-2-butene
1,3-Dichloro-2-hydroxypropane

6. Aldrin
Dieldrin
Endrin
D. D. D.
D. D. E.
D. D. T.
Heptachlor
Heptachlor epoxide
Endosulfan
3,6-Dichloro-2-methoxymethyl benzoate (dicamba methyl ester)
4,Amino-3,5,6-Trichloromethyl picolinate (picloram methyl ester)
2,4-Dichlorophenoxy methyl propionate(2,4 DP methyl ester)
2,4-Dichlorophenoxy methyl acetate (2,4D methyl ester)
2-Methyl-4-chloro phenoxy methyl acetate (MCPA methyl ester)
2-Methyl-4-chloro phenoxy methyl propionate (mecoprop methyl ester)
2-Methyl-4-chloro phenoxy methyl butyrate (MCPB methyl ester)
2,3,6-Trichloro methyl benzoate
2,4-Dichlorophenol methyl ether

7. Dimethyl glycol phthalate
Dibutyl glycol phthalate
Di-n-butyl phthalate
Dimethyl phthalate
Diethyl phthalate
Dioctyl anthalate
Di-iso-octyl phthalate
Dinonyl phthalate
Diphenyl phthalate
Di-iso-propyl phthalate
Dimethyl-iso-phthalate
Diethyl terephthalate
Dibutyl terephthalate
Dipentyl phthalate
Di-iso-butyl phthalate
Dipropyl phthalate
Diallyl phthalate
Dicyclohexyl phthalate

8. Methyl octanoate
Methyl decanoate
Methyl laurate
Methyl myristate
Methyl palmitate
Methyl stearate
Methyl linoleate

9. Benzthiazole
Methyl Benzthiazole
Thianaphthene
Thiophen
Thiazole
Thiazolidine
2-Methyl thiophene
1-Butanethiol
Tetrahydrothiophene
Tetrahydrofuran
2-Nitroaniline
3-Nitroaniline
4-Nitroaniline
2-Nitrotoluene
6-Nitroquinoline
8-Nitroquinoline
Nitrobenzene
1-Nitronaphthalene
2-Nitro-m-xylene
4-Nitro-o-xylene
o-Anisidine
4-Nitrotoluene
Di-n-butyl ether
Nonadecane
Eicosane
Heneicosane
Docosane
Tricosane
Tetracosane
Pentacosane
Hexacosane
Haptacosane
Octacosane
Nonacosane
Triacontane
Hentriacontane
Dotriacontane
Tritriacontane
Mestranol
Ethynodiol diacetate
Lyndestranol
Cholestane
Cholesterol
Coprostanol
2,3,5-Trimethyl indole
Cumene
Pseudo cumene
Mesitylene
t-butyl benzene
n-butyl benzene
Ethyl benzene

9. Continued
Carbazole
Dibenzofuran
Durene
Hexamethyl benzene
p-tolyl ether
Diphenyl ether
Di-n-propyl ether
Di-n-pentyl ether
Isobutyl acetate
Dibutyl ketone
Acetyl tri-n-butyl citrate
Tri-o-cresyl phosphate
Tri-m-cresyl phosphate
Tri-p-cresyl phosphate
Limonene
Indane
Indene
Indole
Isopropyl disulphide
Trimethyl phosphate
Triethyl phosphate
Tributyl phosphate
2-ethoxyethylacetate
1-phenylhexane
1-phenyldecane
Tetradecane
Hexadecane
Octadecane
N-methyl-o-nitroaniline
2-methyl-4-nitroaniline
4-methyl-2-nitroaniline

APPENDIX 2

LIST OF ORGANIC COMPOUNDS IDENTIFIED IN DRINKING WATER* (INTERNATIONAL)

Classification

1. Polynuclear aromatic hydrocarbons and benzene
2. Alkyl substituted polynuclear aromatic hydrocarbons
3. Aliphatic amines and derivatives
4. Aromatic amines and derivatives
5. Cyanides and azo compounds
6. Nitro and nitroso compounds
7. Organo phosphorus compounds
8. Pesticides and herbicides
9. Aliphatic organo halogens excl. pesticides and herbicides
10. Aromatic organo halogens excl. pesticides and herbicides
12. Mercaptans and miscellaneous sulphur compounds
13. Phenols
14. Quinones
15. Heterocyclics
16. Surfactants
18. Ethers
19. Aldehydes
20. Ketones
21. Aliphatic acids
22. Aromatic acids
23. Esters
24. Alcohols
25. Arylalkanes
26. Alkanes
27. Alkenes
28. Amino acids and proteins
29. Carbohydrates

* The list is drawn from the computer-based data bank held at the Water Research Centre. Most of the data was compiled as a part of EUROCOP-COST 64B project 'Analysis of organic micropollutants in water' from international sources reported in the literature. It is important to note that the total data bank covers other sample types such as raw waters, waste waters, sediments, etc.

1: POLYNUCLEAR AROMATIC HYDROCARBONS AND BENZENE

Acenaphthene
Anthracene
Benzathracene (1,2-)
Benzene
Benzofluoranthene (11,12-)
Benzofluoranthene (3,4-)
Benzoperylene (1,12-)
Benzopyrene (3,4-)
Biphenyl
Fluoranthene
Fluorene
Indene
Indeno (1,2,3-cd) pyrene
Naphthalene
Perylene
Phenanthrene
Pyrene
Terphenyl (2-)

2: ALKYL SUBSTITUTED POLYNUCLEAR AROMATIC HYDROCARBONS

Dimethylnaphthalene isomers
Dimethylnaphthalene (2,6-)
Ethylnaphthalene isomers
Methylindane (3-)
Methylindene isomers
Methylnaphthalene (1-)
Methylnaphthalene (2-)

3: ALIPHATIC AMINES AND DERIVATIVES

Decyldimethylamine
Dimethyldodecylamine
Ethyl methyl maleimide
Ethylamine
Propylamine

4: AROMATIC AMINES AND DERIVATIVES

Aminomethylpyridine isomers
Atrazine
Butylbenzene sulphonamide
Chloroaniline isomers
Deethylatrazine
Diethylaniline (N,N-)

4: (CONT)

Propazine
Simazine
Toluidine (2-)

5: CYANIDES AND AZO COMPOUNDS

Isocyanic acid
Methylbenzonitrile isomers
Methylcyanobenzene isomers

6: NITRO AND NITROSO COMPOUNDS

Chloronitrobenzene isomers
Chloro-2-nitrobenzene (1-)
Chloro-3-nitrobenzene (1-)
Chloro-4-nitrobenzene (1-)
Dinitrotoluene isomers
Dinitrotoluene (2,4-)
Dinitrotoluene (2,6-)
Nitrobenzene
Nitrotoluene (2-)
Nitrotoluene (4-)
Nitrotrichloromethane

7: ORGANO PHOSPHORUS COMPOUNDS

Tributyl phosphate
Triethyl phosphate
Triphenyl phosphate

8: PESTICIDES AND HERBICIDES

Alachlor
Aldrin
Atrazine
BHC, (gamma-), (lindane)
BHC, (benzene hexachloride)
Butachlor
Chlordane
Chlordene
Chloroalachlor
Chlorophenylethyl sulphone
Cyanazine
DDE
DDE (p, p')
DDT (p, p')
Deethylatrazine

8 (CONT)

Dichloropropane
Dichloropropene
Dichloropropene (1,3-)
Dieldrin
Endosulfan
Endrin
Hexachlorobenzene
Heptachloronorbornene isomers
Heptachloronorbornene
Heptachlor
Heptachlor epoxide
ODB, o-dichlorobenzene
PDB, p-dichlorobenzene
Propazine
Simazine
TCB, (trichlorobenzene isomers)
Toxaphene, (octachlorocamphene)
Trichlorophenol isomers

9: ALIPHATIC ORGANO HALOGENS EXCL. PESTICIDES AND HERBICIDES

Bis-(chloroisopropyl) ether isomers
Bis-(2-chloroethyl) ether
Bis-(2-chloroisopropyl) ether
Bis-(2-chloropropyl) ether
Bis-(3-chloropropyl)ether
Bromo-2-chloroethane(1-)
Bromobutane isomers
Bromochloromethane
Bromodichloromethane
Bromoethane
Bromomethane
Chloroethyl ether isomers
Chloromethane
Chlorooctane isomers
Chloropropene (1-)
Chloropropyl propyl ether isomers
Chloro-3-methylbutane (1-)
Dibromochloromethane
Dibromodichloroethane isomers
Dibromoethane isomers
Dibromoethane (1,2-)
Dibromomethane
Dichlorodifluoroethane isomers
Dichloroethane isomers
Dichloroethane (1,2-)
Dichloroethyl ether isomers
Dichloroethyl ethyl ether (2,2-)

9 (CONT)

Dichloroethylene isomers
Dichloroethylene (1,2-)
Dichloromethane
Dichloropropane isomers
Dichloropropene isomers
Dichloropropene (1,3-)
Hexachlorobutadiene
Hexachloroethane
Iodoethane
Nitrotrichloromethane
Pentachloroethane
Tetrachloroacetone (1,1,3,3-)
Tetrachloroethane isomers
Tetrachloroethane (1,1,2,2-)
Tetrachloroethene
Tetrachloroethylene
Tetrachloromethane, (carbon tetrachloride)
Tribromométhane, (bromoform)
Trichloroacetaldehyde, (chloral)
Trichloroethane (1,1,2-)
Trichloroethylene
Trichlorofluoromethane
Trichloromethane, (chloroform)
Trichloropropane (1,1,1-)
Trichloropropane (1,2,3-)

10: AROMATIC ORGANO HALOGENS EXCL. PESTICIDES AND HERBICIDES

Bis-(4-chlorophenyl) sulphone
Bromobenzene
Bromochlorobenzene isomers
Bromophenylphenyl ether isomers
Butyldichlorobenzene (t-) isomers
Chloroaniline isomers
Chlorobenzene
Chlorocresol (4-)
Chlorohydroxybenzophenone isomers
Chloronitrobenzene isomers
Chlorophenol (2-)
Chlorophenylethyl sulphone
Chloropyridine isomers
Chlorotoluene isomers
Chlorotoluene (4-)
Chloro-2-nitrobenzene (1-)
Chloro-3-nitrobenzene (1-)
Chloro-4-nitrobenzene (1-)
Dibromobenzene isomers

10 (CONT)

Dichlorobenzene (1,2-)
Dichlorobenzene (1,3-)
Dichlorobenzene (1,4-)
Dichlorophenol (2,6-)
Hexachlorobenzene
Iodobenzene
Polychlorinated biphenyl isomers
Trichlorobenzene (1,2,4-)
Trichlorobenzene (1,3,5-)
Trichlorophenol isomers

12: MERCAPTANS AND MISCELLANEOUS SULPHUR COMPOUNDS

Bis-(4-chlorophenyl) sulphone
Butylbenzene sulphonamide
Chlorophenylethyl sulphone
Dimethyl disulphide
Endosulfan
Methylbenzothiazole (2-)
Methylthiobenzothiazole (2-)

13: PHENOLS

Chlorocresol (4-)
Chlorohydroxybenzophenone isomers
Chlorophenol (2-)
Chlorophenol (4-)
Dichlorophenol (2,6-)
Di-t-butyl-4-methylphenol (2,6-)
Hydroxybiphenyl (2-)
Hydroxytoluene (3-), (m-cresol)
Methoxyphenol (2-), (guaiacol)
Nonylphenol isomers
Trichlorophenol isomers

14: QUINONES

Di-t-butyl-1, 4-benzoquinone (2,6-)

15: HETEROCYCLICS

Aminomethylpyridine isomers
Atrazine
Chloropyridine isomers
Deethylatrazine
Diethylbarbituric acid, (barbital)
Dioxane (1,4-)
Methylbenzothiazole (2-)
Methylthiobenzothiazole (2-)
Paraldehyde

15 (CONT)

Piperidine
Propazine
Simazine
Tetramethyltetrahydrofuran
Trimethylcyanuric acid (1,3,5-)
Trimethylisocyanurate

16: SURFACTANTS

Alkyl benzene sulphonates
Linear alkyl sulphonates and alkyl benzene sulphonates

18: ETHERS

Bis-chloroethyl ether isomers
Bis-3-(chloropropyl)ether
Bis-(chloroisopropyl) ether isomers
Bis-(2-chloroethyl) ether
Bis-(2-chloroisopropyl) ether
Bis-(2-chloropropyl) ether
Bromophenyl phenyl ether isomers
Chloropropyl propyl ether isomers
Dichloroethyl ether isomers
Dichloroethyl ethyl ether (2,2-)
Dicyclohexyl ether
Diethoxyethane isomers
Diethyl ether
Dihexyl ether
Dimethoxyacetophenone isomers
Dimethoxybenzene isomers
Dimethoxybenzene (1,2-), (veratrole)
Dimethoxyisobutane (1,1-)
Diphenyl ether
Ethyl benzyl ether
Methoxyphenol (2-), (guaiacol)

19: ALDEHYDES

Benzaldehyde
Ethanal, (acetaldehyde)
Ethylbutanal (2-)
Isobutanal
Pentanal
Trichloroacetaldehyde, (chloral)

20: KETONES

Acetone
Acetophenone
Benzophenone
Butan-2-one
Butylacetophenone(4-t-)
Camphor
Chlorohydroxybenzophenone isomers
Cyclohexanone
Dihydrocarvone
Dimethoxyacetophenone isomers
Ethylacetophenone isomers
Isooctenone isomers
Isophorone
Methylhexa-3-ene-2-one(5-)
Pentanone(2-)
Tetrachloroacetone(1,1,3,3-)
Tetramethyl-3-pentanone (2,2,4,4-)
Trimethylcyanuric acid(1,3,5-)

21: ALIPHATIC ACIDS

Abietic acid

22: AROMATIC ACIDS

Fulvic acid
Humic acid
Phthalic acid anhydride

23: ESTERS

Benzylbutyl phthalate
Butyl acetate(sec-)
Butyl octyl maleate
Dialkyl phthalates
Dibutyl phthalate
Diethyl malonate
Diethyl phthalate
Dihexyl phthalate
Dimethyl phthalate
Dioctyl adipate
Dioctyl phthalate
Dipropyl phthalate
Di-(2-ethylhexyl)adipate
Di-(2-ethylhexyl)phthalate
Di-isobutyl phthalate
Ethyl acetate
Ethyl hexadecanoate, (ethyl palmitate)
Methyl benzoate
Methyl hexadecanoate, (methyl palmitate)

23 (CONT)

Methyl octadecandoate, (methyl stearate)
Octylbutyl fumarate
Phenyl benzoate
Tributyl phosphate
Triethyl phosphate
Triphenyl phosphate

24: ALCOHOLS

Butoxy-2-ethoxyethanol(1-)
Cyclohexanol
Dihydroxyethane (1,2-),(ethylene glycol)
Ethanol
Ethyl-1-hexanol(2-)
Geosmin
Hydroxyoctadecanoic acid (3-)
Isobutanol
Methylisoborneol (2-)
Pentanol (1-)
Propanol (1-)
Terpineol (4-) isomers

25: ARYLALKANES

Benzenes(C4-)
Benzenes(C5-)
Benzenes(C6-)
Butylbenzene isomers
Butylbenzene
Butylmethylbenzene(t-) isomers
Diethylbenzene isomers
Dimethylethylbenzene isomers
Diphenylheptane isomers
Diphenylmethane
Ethylbenzene
Ethylindane isomers
Ethylstyrene isomers
Ethyltoluene isomers
Ethyltoluene(2-)
Ethyltoluene(3- and 4-)
Ethyltoluene(3-)
Ethyltoluene(4-)
Ethylxylene isomers
Isobutylbenzene
Isopropylbenzene, (cumene)
Isopropylmethylbenzene isomers, (cymene isomers)

25 (CONT)

Isopropyltoluene isomers
Methylbiphenyl isomers
Methylpropylbenzene isomers
Pentylbenzene
Propylbenzene
Propyltoluene isomers
Styrene
Tetramethylbenzene isomers
Tetramethylbenzene(1,2,3,5-)
Tetramethylbenzene(1,2,4,5-)
Toluene
Trimethylbenzenes isomers
Trimethylbenzene(1,2,3-)
Trimethylbenzene(1,2,4-)
Trimethylbenzene(1,3,5-)
Xylene isomers, (dimethylbenzene isomers)
Xylene(1,2-)
Xylene(1,3-)
Xylene(1,4-)

26: ALKANES

Alkanes (C_{21}-C_{24})
Alkanes (C_9-C_{27})
Cyclohexane
Cyclopentane
Decane(n-)
Dodecane(n-)
Eicosane (n-)
Ethyl-5-methyl heptane(2-)
Heptadecane(n-)
Heptane(n-)
Hexadecane(n-)
Hydrocarbons (C_1-C_4)
Methylcyclobutane
Methylcyclohexane
Nonadecane(n-)
Nonane(n-)
Octadecane(n-)
Pentadecane(n-)
Propylcyclohexane
Tetradecane(n-)
Tridecane(n-)
Undecane isomers
Undecane(n-)

27: ALKENES

Cyclohexene
Cyclopentadiene
Cyclopentene
Methylcyclopentene
Heptadec-1-ene
Heptene isomers
Limonene
Pentene isomers

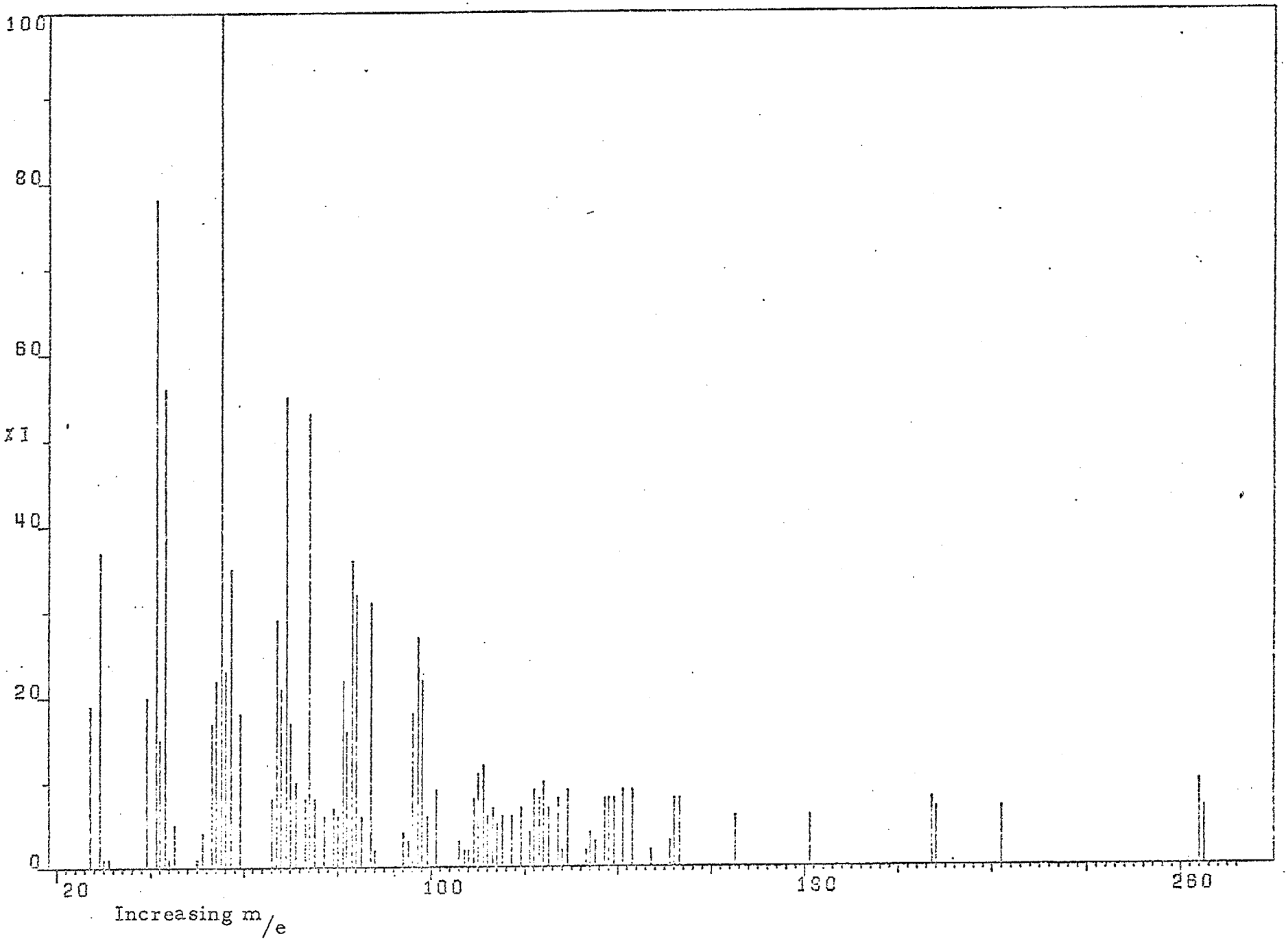
28: AMINO ACIDS AND PROTEINS

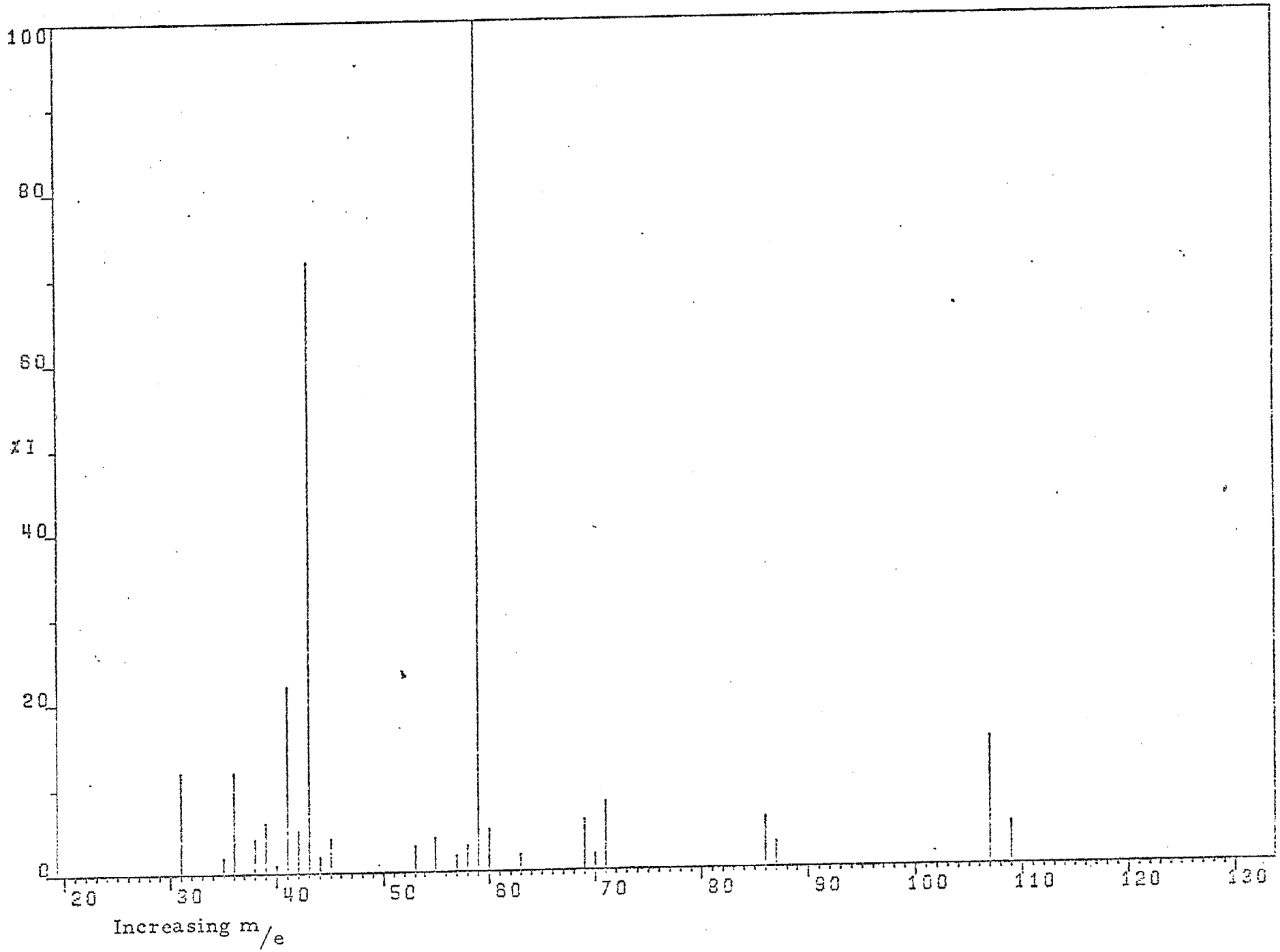
Total protein (as C)

29: CARBOHYDRATES

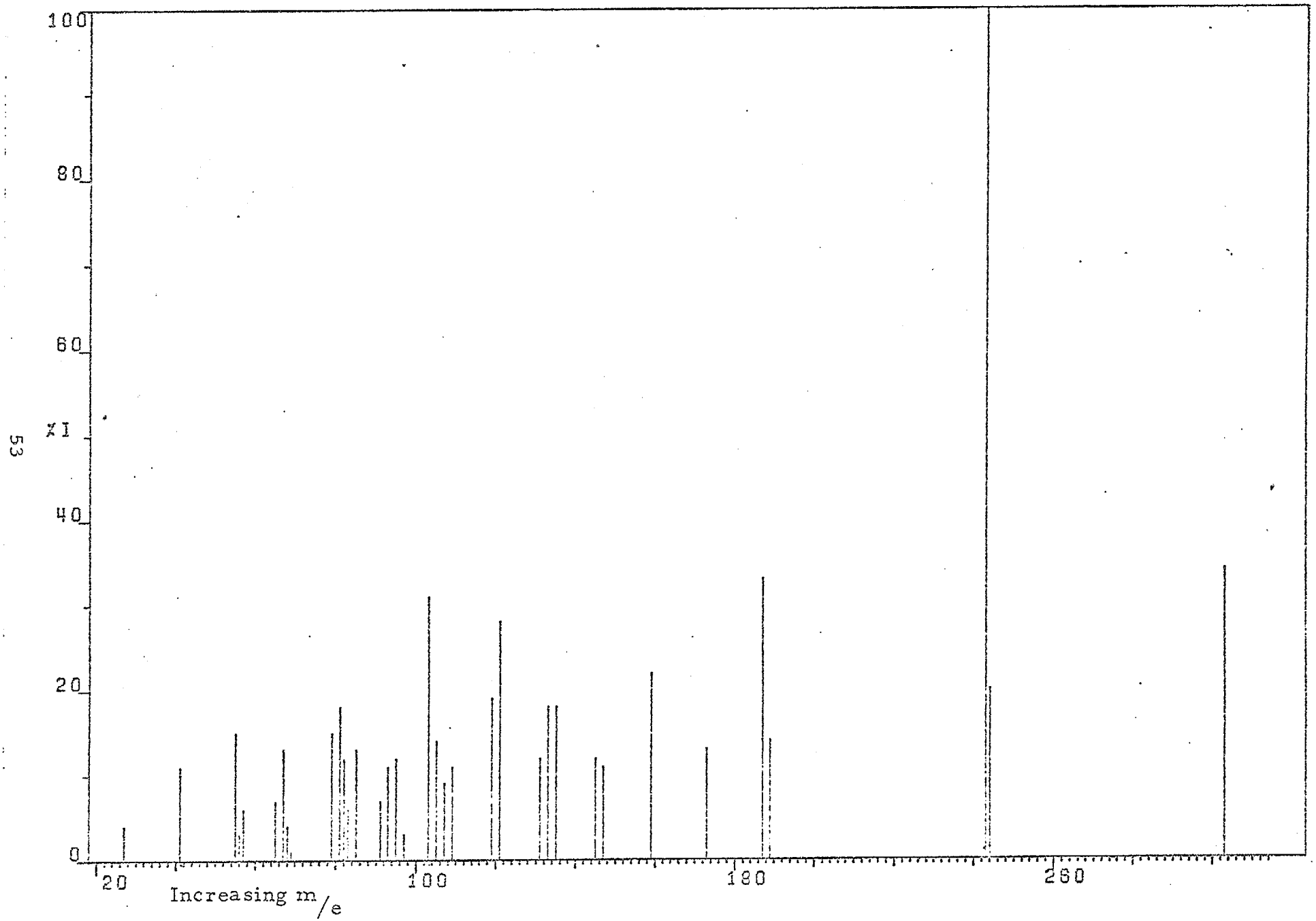
Total polysaccharides (as glucose)

APPENDIX 3. MASS SPECTRA OF UNIDENTIFIED COMPOUNDS OCCURRING IN MORE THAN ONE SAMPLE


100
80
60
40
20
0
X 1
20
100
180
260
Increasing m/e


100
80
60
40
20
0
% I
20
30
40
50
60
70
80
90
100
110
120
130
Increasing m/e

Unknown 147



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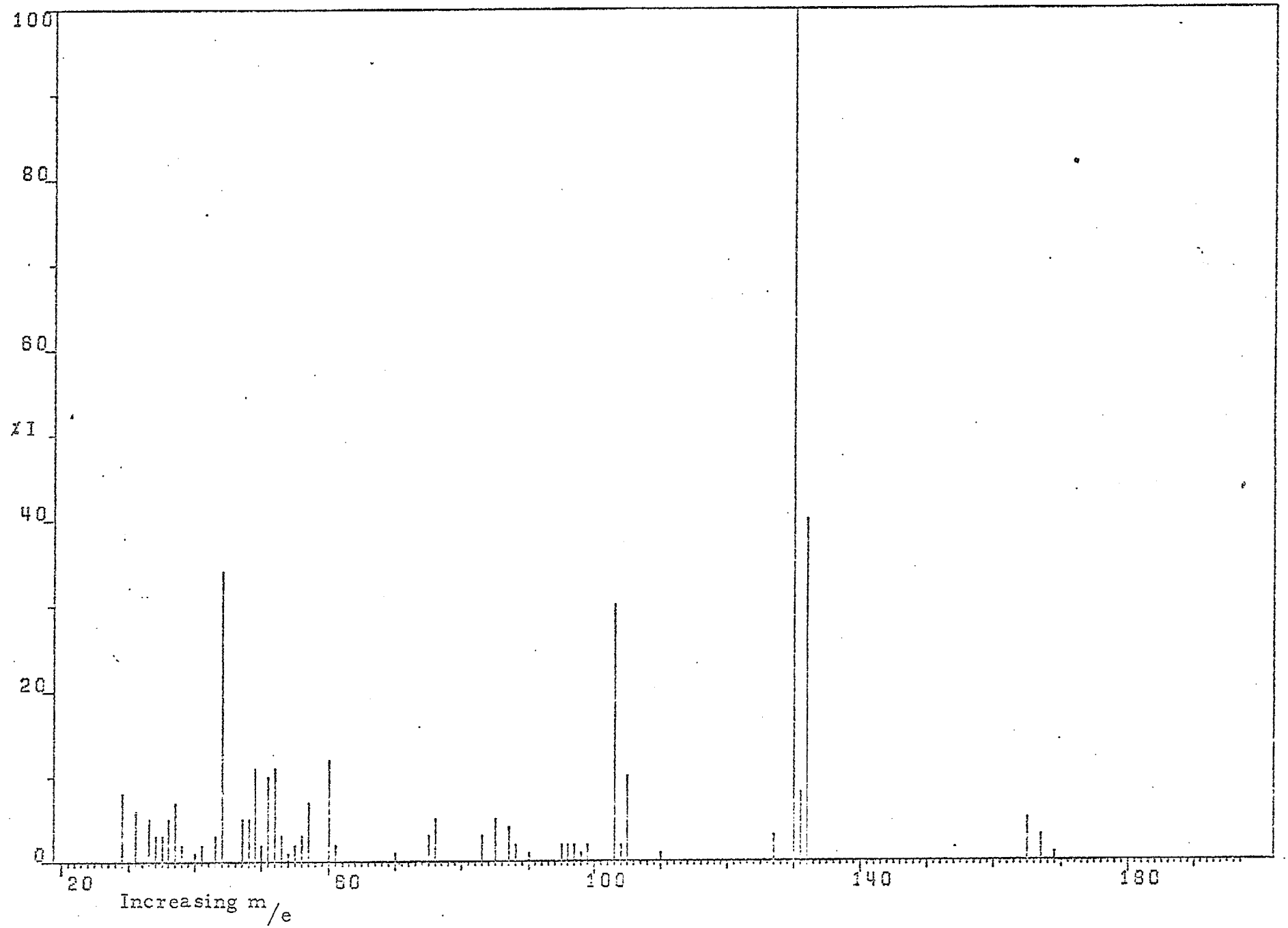

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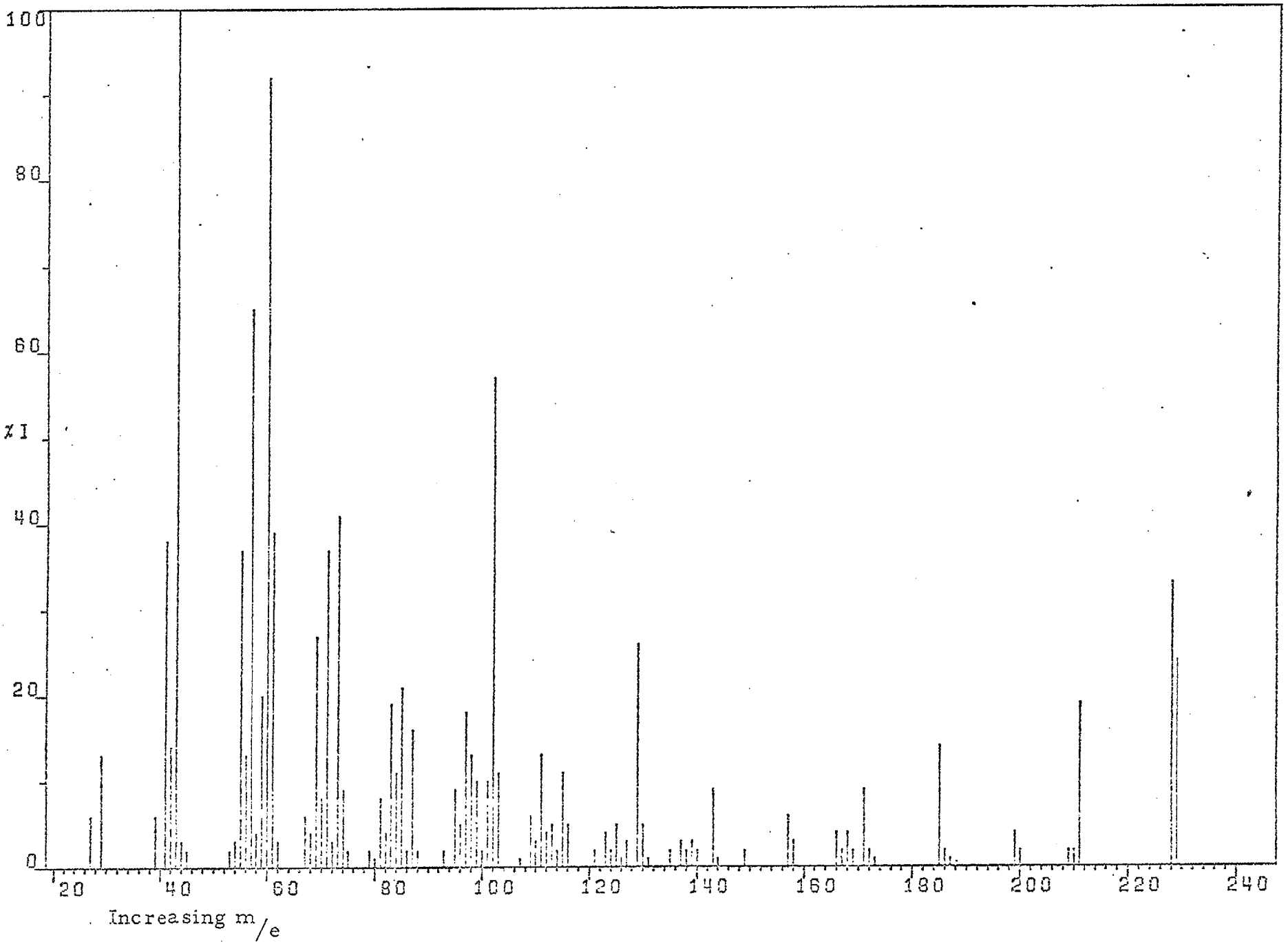
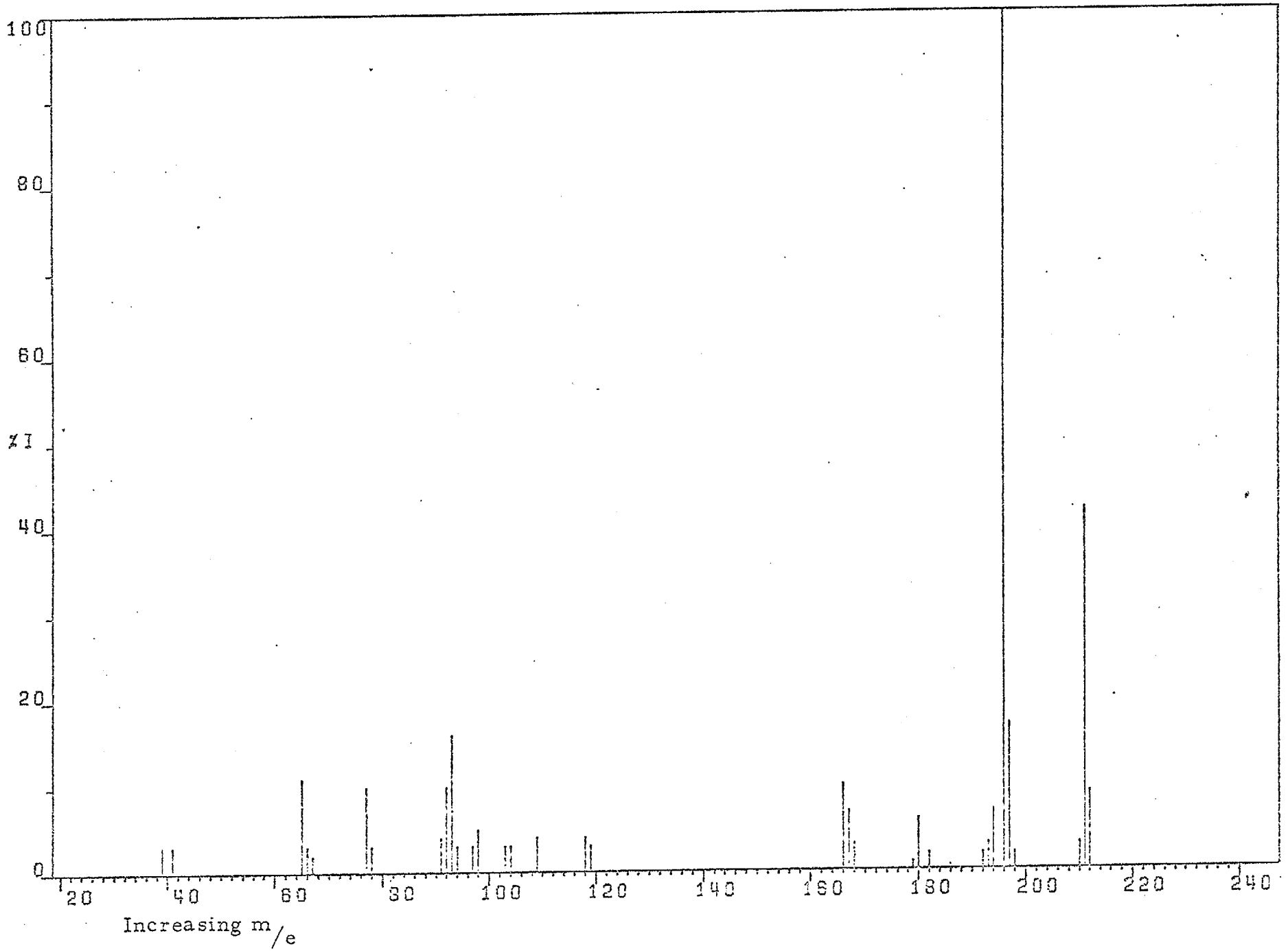

100
80
60
%I
40
20
0
20
40
60
80
100
120
140
160
180
200
220
240
Increasing m/e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80
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40
20
0
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40
60
80
100
120
140
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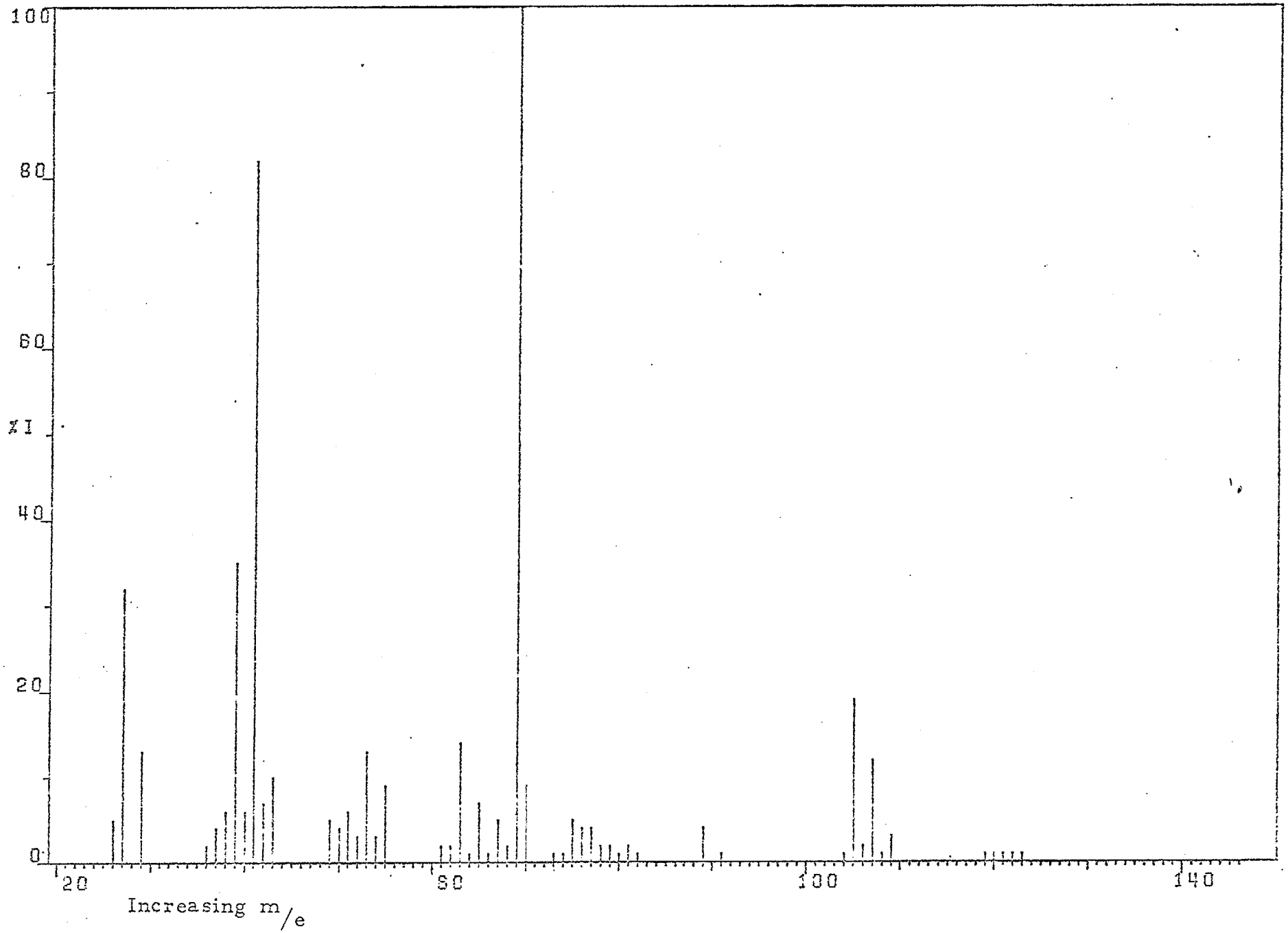
200
220
240
Increasing m/e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60
%I
40
20
0
20
80
100
140
Increasing m/e

Unknown 152