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FINAL REPORT

Hydrocarbon characterization of well 31/3-2, the Troll field.

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Norsk Hydro A/S

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SUMMARY/ SAMMENDRAG

One oil and ten sandstone cores were analysed by organic geochemical methods. All the samples were seen to contain the same type of organic matter, with high abundances of mature hydrocarbons. The richness is very high from 1567.80 down to 1593.50m, where it starts decreasing slightly.

KEY WORDS/ STIKKORD

Hydrocarbons	Correlation
Troll field	GC-MS

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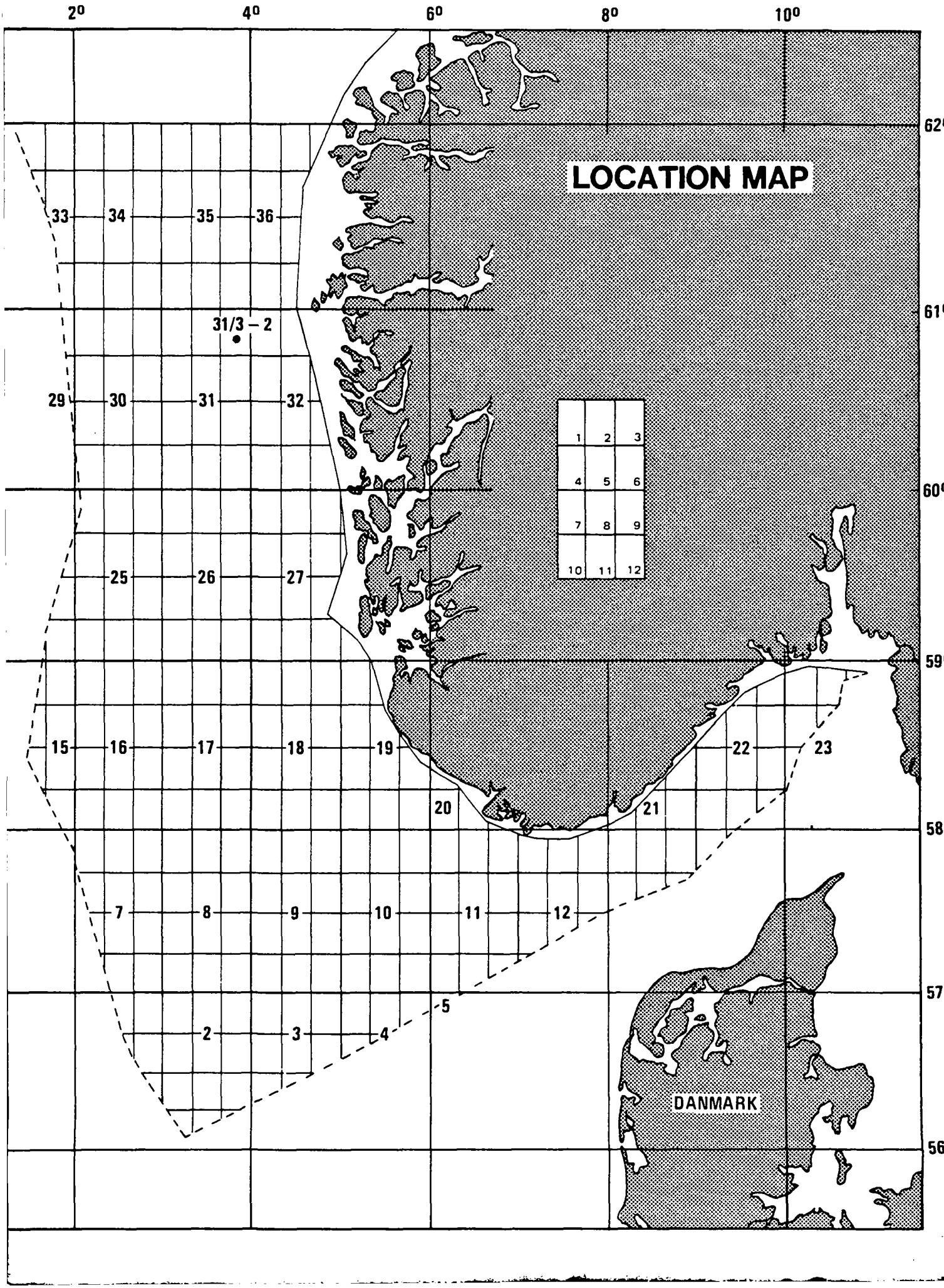
1. INTRODUCTION

Ten sandstone cores and an oil from well 31/3-2 in the Troll field (Location Map) were analysed for hydrocarbon characterisation and correlation purposes. The samples were taken from the depth interval listed below:

IKU no.	Sample Type	Depth (m)
B-4681	Oil	
B-4682	Core, sst	1567.80
B-4683	"	1571.50
B-4684	"	1573.95
B-4685	"	1581.65
B-4686	"	1586.40
B-4687	"	1587.50
B-4688	"	1590.50
B-4689	"	1593.50
B-4690	"	1595.50
B-4691	"	1628.00

Common organic geochemical methods were applied. In addition to extraction and GC analyses, GC-MS and $\delta^{13}C$ isotope data were used in the correlation.


LOCATION MAP
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31/3 – 2
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2. EXPERIMENTAL

2.1 Extractable Organic Matter

Powdered rock was extracted by flowblending for 3 minutes using dichloromethane (DCM) as solvent. The DCM used was of organic geochemical grade and blank analyses showed the occurrence of negligible amounts of contaminating hydrocarbons.

Activated copper fillings were used to remove any free sulphur from the samples.

After extraction the solvent was removed on a Buchi Rotavapor and the amount of extractable organic matter (EOM) was determined.

2.2 Evaporation of the light components in fluid samples

Prior to chromatographic separation of oil/condensate sample, the fraction boiling below 210°C were removed by heating the sample until constant weight at 210°C is obtained. The heating is performed at atmospheric pressure.

The fraction of light components is determined as the weight difference between the original sample and the amount that is left after the heating.

2.3 Chromatographic Separation

The extractable organic matter (EOM) was separated into saturated fraction, aromatic fraction and non hydrocarbon fraction using a MPLC system with hexane as eluant (Radke et al., Anal. Chem., 1980). The various fractions were evaporated on a Buchi Rotavapor and transferred to glass vials and dried in stream of nitrogen.

The same separation procedure was applied to the fractions of oil/condensate samples boiling above 210°C.

2.4 Molecular Sieve Adsorption

The sample containing 2mg of n-alkanes was dissolved in 35ml of cyclohexane and 1g of Molecular Sieve pellets (5Å) which had been activated at 300°C in 24 hours, were added. This mixture was then refluxed for about 24 hours. While the solution was still hot, the sieve pellets were removed from the solution by filtering. The solvent was then removed on a Buchi Rotavapor. GC analysis was performed on the samples, using the same conditions as for the other GC analysis.

The normal alkanes were recovered from the Molecular Sieve pellets by destruction of the pellets with hydrofluoric acid. The solution was extracted with boric acid and hexane, and the solvent was then removed on a Buchi Rotavapor. GC analysis were performed on the samples, using the same conditions as for the other GC analysis.

2.5 Gas Chromatographic Analysis

The C_2-C_8 hydrocarbon fractions were determined by hydrogen stripping on a Carlo Erba Fractovap GC. The column used was a 30m fused silica capillary column coated with SE-54. The temperature program applied was 50°C (2 min.) to 180°C at 4°C/min.

The saturated and the branched/cyclic hydrocarbon fractions were each diluted with n-hexane and analysed on a HP 5730A. The GC is equipped with a 15m DB-1 fused silica column and hydrogen (ca. 2.5 ml/min.) is used as carrier gas. Injections are performed in split mode (split ratio 1:10). The temperature program applied is 80°C (2 min.) to 280°C at 4°C/min.

The total aromatic fractions were, after dilution with n-hexane, analysed on a Carlo Erba Fractovap Series 2150 GC. The GC is equipped with a 30m DB-5 fused silica column, and hydrogen (2.5 ml/min.) is used as carrier gas. The temperature program applied is 80°C (2 min.) to 280°C at 4°C/min. and injections are performed splitless.

The data processing for all the GC analyses was performed on a VG Multichrom lab data system.

2.6 Gas chromatography - mass spectrometry (GC-MS)

GC-MS analyses were performed on a VG Micromass 70-70H GC-MS-DS system. The Varian Series 3700 GC was fitted with a fused silica OV-1 capillary column (30m x 0.3mm i.d.). Helium (0.7kg/cm^2) was used as carrier gas and the injections were performed in split mode (1.5µl, split ratio 1:15). The GC oven was programmed from 70°C to 280°C at 4°C/min. after an initial isothermal period of 2 minutes for the aromatic hydrocarbons, while an initial temperature of 120°C was applied for the saturated fractions.

The saturated hydrocarbons were analysed in multiple ion mode (MID) at a scan cycle time of approximately 2 secs. Full data collection was applied for the aromatic hydrocarbons at a scan time of 1 sec/decade. The mass spectrometer operated at 70eV electron energy and an ion source temperature of 200°C. Data acquisition was done by VG data systems.

Peak identification was performed applying knowledge of elution patterns in certain mass chromatograms. Calculation of peak ratios was done from peak height in the appropriate mass chromatograms.

2.7 δ^{13}C isotope analysis

The δ^{13}C isotope analysis was performed by mass spectrometry at Institute for Energy Technology (IFE) in Oslo according to their method. Their reference value for the standard NBS-22 is -29.8.

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3. RESULTS AND DISCUSSION

3.1 API gravity

The API gravity of the oil was determined to 28.1°API (Table 1), indicating it to be a relatively high gravity oil, of low maturity and/or possibly biodegraded.

3.2 GC of C_2-C_8 hydrocarbons

Gas chromatogram of C_2-C_8 hydrocarbons in the oil is shown in Figure 1, while the relative distribution of the compounds is given in Table 2. The main compounds are seen to be cyclic, and thus the oil has probably undergone some degree of biodegradation. Very low amounts of n-alkanes are detected.

3.3 Amount of C_{15}+ EOM and hydrocarbons

The oil sample was topped to 210°C prior to separation of asphaltenes and chromatographic separation. Approximately 85% of the crude oil was left after the treatment (Table 3), implying the oil to be relatively heavy.

The amounts of asphaltenes (Table 4) are fairly similar in the oil and all the extracts with very rich hydrocarbon content (0.7-5.0% of EOM). The two deepest cores show relatively higher asphaltene content.

Eight of the ten sandstone cores were seen to be very rich both in extractable organic matter, EOM (4771-18027ppm, average 10979ppm) and in hydrocarbons (2000-10827ppm, average 6076ppm). The two deepest cores contain less organic material, but are still rich in EOM (1311-2267ppm, average 1789ppm) and fair-rich in hydrocarbon content (119-535ppm, average 327ppm). The amounts of the EOM and the various chromatographic fractions are presented in Table 5.1-5.3.

3.4 Gas chromatography of C_{15}+ saturated hydrocarbons

Gas chromatograms of saturated hydrocarbons are given in Figure 2, and data from the chromatograms are presented in Table 6.

The oil is seen to exhibit a unimodal n-alkane distribution with maximum at nC_{17}. Isoprenoids are relatively abundant ($Pr/n\text{-}C_{17}$ = 1.0) and the pristane/phytane ratio of 2.0 is high compared to most North Sea oils and Upper Jurassic source rocks (Cornford et al., 1983). The abundant isoprenoids suggest that mild biodegradation might have taken place.

All the extracts from the sandstone cores show the same general distribution of saturated hydrocarbons as the oil, except that the cores have lost most of the low molecular weight compounds ($<n\text{-}C_{17}$). Abundant isoprenoids are seen in all the samples ($Pr/n\text{-}C_{17}$ varies between 1.1 and 1.6), and the pristane/phytane ratios are in the range 1.7-2.5. From the relative amounts of the internal standard (S in Figure 2) the two deepest samples are seen to contain less hydrocarbons than the rest, supporting what was seen in the discussion on the chromatographic separation.

The data discussed so far suggest that the hydrocarbons in the extracted sandstones originate from the same source rock as the oil.

3.5 Branched/cyclic and n-alkanes

The oil and two of the cores were treated with molecular sieve to separate the n-alkanes from the branched and cyclic alkanes. The gas chromatograms are shown in Figure 3a and b, and the amounts are given in Table 7.

Even with the slightly higher intensity of n-alkanes in the $C_{20}\text{-}C_{35}$ range seen in the cores the general distributions in the GC's show that both the n-alkanes and the branched/cyclic hydrocarbons can be siad to be of the same type in the three samples.

A quantitative comparison is presented in Table 7. The quantitative results were obtained in two different ways; by simple gravimetry and by integration of the gas chromatograms.

The gravimetric results give approximately 100% recovery for the two core samples, while the oil seems to have lost approximately 50%. This could be due to the difference seen in the GC traces of these three samples. The saturated HC fraction of the oil contained relatively more than the cores of low molecular weight compounds. Thus the weight loss

of the oil may be due to further loss of these compounds. All three samples were seen to have approximately the same ratio of n-alkanes and branched/cyclic hydrocarbons (0.29-0.35).

The results from the GC-integration are lower than the gravimetric. This would be expected since the chromatographic fraction contain higher molecular weight compounds that will not elute through a GC column. A relatively higher proportion in the n-alkane fractions is lost. However, the ratio of n-alkanes to branched/cyclic hydrocarbons is the same for all three samples.

3.6 Gas chromatography of C_{15}+ aromatic hydrocarbons

Gas chromatograms are given in Figure 4, while certain aromatic ratios used in maturity estimation (Radke et al., 1983) are presented in Table 8.

Except for the oil and one sandstone core sample from 1590.5m, the rest of the samples (all sandstone cores) have lost much of the low molecular weight material, i.e. mainly alkyl naphthalenes. This makes the alkylnaphthalene ratios less accurate. Apart from loss of the alkyl naphthalenes the general aromatic hydrocarbon distribution appears to be similar in all samples including the oil.

Maturity based on MPI 1 appears to be fairly low compared with the alkyl naphthalene ratios. The MPI 1 value varies from 0.59-0.76. The average value is therefore 0.69 ($\pm$0.05 S.D.). The oil has an MPI 1 of 0.71. The estimated vitrinite reflectance of the source for these aromatic hydrocarbons is between 0.7-0.9% with a spot value based on the average MPI 1 equal to 0.8% approximately. This is based on the graph in the aromatics report no. 05.6260.00/01/84 (Hall and Schou, 1984). The methyl naphthalene ratios average 2 for the samples down to 1593.5m (but excluding this sample). It was felt that the methyl naphthalenes peaks were too small to be accurately measured below 1590.5m. The oil had a value of 2.1, whereas the most suitable sandstone core (i.e. the one with most alkyl naphthalenes) gave a value of 1.89. These values are considered to be high relative to the MPI 1 indicated maturity level. A value above 1.5 may be expected for condensates. Similarly values for DMNR (which roughly average 3.3) are not

those seen during the main phase of oil generation (which range from 1.0-2.0 - from aromatics report, Hall and Schou, 1984). Furthermore biphenyl and methyl-biphenyls (figure 4) have been tentatively identified as prominent components of all samples. These compounds are considered to become prominent only in very highly mature oil-prone source rocks (i.e. greater than 1% Ro). This may be an indication of a high maturity source for these hydrocarbons, however coals also appear to have large amounts of these compounds at lower maturities than type II marine source rocks.

The evidence suggests that there may be two sources for the aromatic hydrocarbons in these sandstone cores and the oil. One highly mature yielding mostly wet gas-condensate range hydrocarbons (i.e. mainly alkyl naphthalenes or lower molecular weight hydrocarbons), the second source being oil window mature and yielding a 'normal' oil. The latter has both alkyl naphthalenes and phenanthrenes in which the alkyl naphthalene pattern is marked by the higher maturity source hydrocarbons. There is no indication from the aromatics whether the two sources had similar organic matter (i.e. whether the hydrocarbons are from the same source rock horizon buried to different depths).

3.7 GC-MS analysis of saturated terpane and sterane

Mass chromatograms representing terpanes (m/z 191) and steranes (m/z 217 and 218) are shown in Figure 5. Molecular ratios calculated from the chromatograms are given in Table 9 and 10.

The same overall profiles are seen for steranes and terpanes in both the oil and the ten sandstone cores. All the applied molecular ratios suggest that the hydrocarbons are of oil window maturity. The deepest core shows somewhat different chromatograms, a fact that is probably due to generally much lower abundance of hydrocarbons in this sample. One compound elutes at the same retention time as bisnorhopane (Z) in the m/z 191 mass chromatograms. It is, however, not possible from the chromatograms to verify this very tentative determination. The relative abundance of this compound and the other two eluting immediately before and after the C_{29} 17α(H),21β(H)-hopane is similar in all the samples.

The triangular plot in Figure 6 shows the molecular weight distribution of the C_{27}-C_{29} regular 14β,17β-steranes to be nearly identical for all the samples.

From the sterane and terpane mass chromatograms the hydrocarbons extracted from the sandstone cores can be said to originate from the same or at least a very similar source rock as the oil.

3.8 GC-MS analysis of aromatic hydrocarbons

The data obtained from the analysis of aromatic hydrocarbons support what was seen from other parameters (Figure 7). The total ion chromatograms (TIC) are similar to the GC traces, apart from one abundant peak representing elemental sulfur (S_8). This peak partly masks an interesting part of the TIC's. Mass chromatograms representing alkylated homologs of benzene (m/z 92, 106), naphthalene (m/z 142, 156, 170), phenanthrene (m/z 178, 192, 206) and dibenzothiophene (m/z 184, 198, 212) in addition to mono- and tri-aromatic steranes (m/z 253 and 231) are presented.

Only minor differences are detected from inspection of mass chromatograms and in the maturity data in Table 11.

3.9 $\delta^{13}C$ isotope ratios

Saturated and aromatic hydrocarbon fractions were analysed for their $\delta^{13}C$ isotope ratios. The data are presented in Table 12.

The results vary from -29.5 to -28.3°/oo (i.e. 1.2°/oo) for the saturated and from -27.9 to -27.1°/oo (i.e. 0.8o/oo) for the aromatic hydrocarbons.

More than 1°/oo variation in the saturated hydrocarbon fractions may be due to generation from different type of source rocks. However, the two samples with the most different values for saturated hydrocarbons (B-4682 and B-4690) gave exactly the same value for the aromatic hydrocarbons. Based on this and on the similarities of the results from the other analyses, the hydrocarbons in the cores and the oil are believed to originate from the same source rock or source rocks.

4. CONCLUSION

All the performed analyses suggest that the oil and the hydrocarbons in the cores have been generated from the same source rock. The amount of hydrocarbons is very high down to 1593.50m where it starts decreasing.

Some of the parameters indicate that more than one source rock, or different maturity stages of the same source rock, may have been responsible for the generation of the hydrocarbons.

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Table 1. API gravity of oil sample.

IKU no.	^{o}API
B-4681	28.1

IKU

Table 2. Relative distribution of C_2-C_8 hydrocarbons in the oil sample.

	B-4681 % of total oil
nC_2	-
nC_3	-
MC_3	-
nC_4	-
MC_4	0.2
nC_5	0.1
CyC_5+2,3DMC_4	0.7
$2MC_5$	-
$3MC_5$	0.2
nC_6	0.4
$MCyC_5$	1.4
benzene	-
C_yC_6	2.2
$2MC_6$	-
2,3DMC_5	0.3
$3MC_6$	0.4
$DMCyC_5$ (1,3; 1,2)	0.7
2,2,4 TMC_5	0.5
nC_7	-
$MCyC_6$	3.3
2,4DMC_6	0.2
Toluene	-
$2MC_7$	<0.1
$3MC_7$	<0.1
$DMCyC_6$ (1,2)	0.7
nC_8	0.3
M/P-xylene	0.5
O-xylene	-

List of C_2-C_8 hydrocarbons in Table 2 and Figure 1.

nC_2	ethane
nC_3	propane
MC_3	methyl-propane
nC_4	butane
MC_4	methyl-butane
nC_5	pentane
CyC_5+2,3DMC_4	cyclopentane + 2,3-dimethyl-butane
$2MC_5$	2-methyl-pentane
$3MC_5$	3-methyl-pentane
nC_6	hexane
$MCyC_5$	methyl-cyclopentane
	benzene
CyC_6	cyclohexane
$2MC_6$	2-methyl-hexane
2,3DMC_5	2,3-dimethyl-pentane
$3MC_6$	3-methyl-hexane
$DMCyC_5$	dimethyl-cyclopentane
2,2,4TMC_5	2,2,4-trimethyl-pentane
nC_7	heptane
$MCyC_6$	methyl-cyclohexane
2,4DMC_6	2,4-dimethyl-hexane
	toluene
$2MC_7$	2-methyl-heptane
$3MC_7$	3-methyl-heptane
$DMCyC_6$	dimethyl-cyclohexane
nC_8	octane
	m/p-xylene
	o-xylene

IKU

Table 3. Amount of light components in oil sample.

IKU no.	Crude oil (mg)	>210°C (mg)	Light components (mg)	(%)
B-4681	212.0	180.9	31.1	14.7

Table 4. Asphaltenes and EOM.

IKU No.	Depth (m)	Asphaltenes (mg)	EOM (mg)
B-4681	Oil	7.9	180.9
B-4682	1567.80	6.0	321.9
B-4683	1571.50	14.4	285.8
B-4684	1573.95	7.6	201.2
B-4685	1581.65	6.5	445.5
B-4686	1586.40	13.0	476.2
B-4687	1587.50	5.4	781.3
B-4688	1590.60	5.8	186.1
B-4689	1593.50	15.2	461.1
B-4690	1595.50	2.4	36.3
B-4691	1628.00	8.0	42.4

TABLE : 5.1

CONCENTRATION OF EOM AND CHROMATOGRAPHIC FRACTIONS

IKU-No	DEPTH (m)	Rock Extr. (g)	EOM (mg)	Sat. (mg)	Aro. (mg)	HC (mg)	Non HC (mg)
B 4681	OIL	0.2	180.9	40.2	22.4	62.6	118.3
B 4682	1567.80	33.2	321.1	135.7	57.3	193.0	128.1
B 4683	1571.50	33.3	285.8	105.4	45.0	150.4	135.4
B 4684	1573.95	42.2	201.2	57.6	26.7	84.3	116.9
B 4685	1581.65	45.1	445.5	168.0	81.2	249.2	196.3
B 4686	1586.40	29.8	476.2	215.6	107.1	322.6	153.6
B 4687	1587.50	43.3	781.3	235.5	117.5	353.0	428.3
B 4688	1590.60	28.0	186.1	56.1	32.8	88.9	97.2
B 4689	1593.50	32.3	461.1	193.0	85.0	278.0	183.1
B 4690	1595.50	36.3	82.3	12.8	6.6	19.4	62.9
B 4691	1628	32.3	42.4	2.6	1.2	3.8	38.6

DATE : 16 - 8 - 84.

TABLE : 5.2

WEIGHT OF EOM AND CHROMATOGRAPHIC FRACTIONS

(Weight ppm OF rock)

IKU-No	DEPTH (m)	EOM	Sat.	Aro.	HC	Non HC
B 4681	OIL					
B 4682	1567.80	9675	4088	1726	5814	3861
B 4683	1571.50	8575	3162	1350	4512	4062
B 4684	1573.95	4771	1367	633	2000	2772
B 4685	1581.65	9871	3723	1799	5522	4350
B 4686	1586.40	15980	7233	3594	10827	5153
B 4687	1587.50	18027	5434	2711	8145	9882
B 4688	1590.60	6635	2000	1171	3171	3463
B 4689	1593.50	14298	5984	2636	8620	5678
B 4690	1595.50	2267	354	182	535	1731
B 4691	1628	1311	82	37	119	1193

DATE : 16 - 8 - 84.

TABLE : 5.3

COMPOSITION IN % OF MATERIAL EXTRACTED FROM THE ROCK

IKU-No	DEPTH (m)	Sat / EOM	Aro / EOM	HC / EOM	SAT / Aro	Non HC / EOM	HC / Non HC
B 4681	OIL	22.2	12.4	34.6	179.5	65.4	52.9
B 4682	1567.80	42.3	17.8	60.1	236.9	39.9	150.6
B 4683	1571.50	36.9	15.7	52.6	234.2	47.4	111.1
B 4684	1573.95	28.6	13.3	41.9	215.9	58.1	72.1
B 4685	1581.65	37.7	18.2	55.9	206.9	44.1	126.9
B 4686	1586.40	45.3	22.5	67.8	201.3	32.2	210.1
B 4687	1587.50	30.1	15.0	45.2	200.4	54.8	82.4
B 4688	1590.60	30.1	17.7	47.8	170.8	52.2	91.6
B 4689	1593.50	41.9	18.4	60.3	227.1	39.7	151.8
B 4690	1595.50	15.6	8.0	23.6	194.5	76.4	30.9
B 4691	1628	6.2	2.8	9.1	220.0	90.9	10.0

DATE : 16 - 8 - 84.

T A B L E 6.

TABULATION OF DATA FROM THE GASCHROMATOGRAMS

IKU No.	DEPTH (m)	PRISTANE / n-C17	PRISTANE / PHYTANE	CPI
B 4681	OIL	1.0	2.0	1.0
B 4682	1567.80	1.3	1.8	1.1
B 4683	1571.50	1.2	1.8	1.1
B 4684	1573.95	1.6	1.7	1.1
B 4685	1581.65	1.3	2.0	1.0
B 4686	1586.40	1.2	1.9	1.0
B 4687	1587.50	1.1	1.9	1.0
B 4688	1590.60	1.2	2.2	1.0
B 4689	1593.50	1.1	1.9	1.0
B 4690	1595.50	1.3	2.0	1.0
B 4691	1628	1.3	2.5	1.1

DATE : 16 - 8 - 84.

Table 7. Amounts of n-alkanes and branched/cyclic hydrocarbons.

a) Gravimetric results.

IKU no.	Sample type	Depth (m)	SAT (mg)	N-alkanes (mg)	B/C (mg)	N-alkanes+B/C (mg)	N-alkanes+B/C (% of SAT)	N-alkanes / B+C
B-4681	Oil	-	11.1	1.3	4.5	5.8	52.3	0.29
B-4682	Core, sst	1567.80	10.2	2.6	7.4	10.0	98.0	0.35
B-4684	Core, sst	1573.95	8.9	2.3	7.1	9.4	105.6	0.32

b) Results from integration of gas chromatograms.

IKU No.	Depth (m)	SAT (mg)	SAT (% of grav.)	N-alkanes (mg)	N-alkanes (% of grav.)	B/C (mg)	B/C (% of grav)	N-alkanes / B+C
B-4681	Oil	4.5	40.5	0.3	24.6	2.3	50.8	0.13
B-4682	1567.80	3.3	32.4	0.9	32.7	4.9	66.2	0.17
B-4684	1573.95	2.9	32.6	0.6	25.2	4.7	66.2	0.12

Table 8. Aromatic hydrocarbon ratios.

IKU No.	Depth (m)	MNR	MPI 1
B-4681	Oil	2.14	0.71
B-4682	1567.80	1.75	0.69
B-4683	1571.50	2.50	0.73
B-4684	1573.95	2.11	0.70
B-4685	1581.65	2.10	0.72
B-4686	1586.40	1.63	0.64
B-4687	1587.50	1.91	0.73
B-4688	1590.60	1.89	0.62
B-4689	1593.50	1.43	0.76
B-4690	1595.50	∿1.00	0.72
B-4691	1628.00	1.67	0.59

MNR = 2/1 MN

MPI 1 = 1.5(3-MP+2-MP/P+9-MP+1-MP)

Table 9. Maturity ratios calculated from peak heights in sterane and terpane mass chromatograms.

IKU code	Depth (m)	Sample type	m/z 191		m/z 217	
			$\alpha\beta/\alpha\beta+\beta\alpha$ [1]	%22S [2]	%20S [3]	$\%\beta\beta$ [4]
B-4681	-	Oil	0.91	58.4	49.0	75.6
B-4682	1567.80	Core, sst	0.90	54.8	47.1	76.9
B-4683	1571.50	"	0.90	62.0	42.1	74.7
B-4684	1573.95	"	0.91	55.6	47.9	71.7
B-4685	1581.65	"	0.90	59.1	50.8	76.1
B-4686	1586.40	"	0.90	57.1	50.8	74.9
B-4687	1587.50	"	0.91	56.5	53.2	73.2
B-4688	1590.50	"	0.91	59.1	47.1	73.0
B-4689	1593.50	"	0.91	60.2	53.1	73.6
B-4690	1595.50	"	0.91	61.9	52.3	69.4
B-4691	1628.00	"	0.90	59.1	61.6	73.5

1) E/E+F in m/z 191.
2) J_1/J_1+J_2 in m/z 191.
3) q/q+t in m/z 217.
4) 2(r+s)/(2(r+s)+q+t) in m/z 217.

Table 10. Molecular ratios calculated from sterane and terpane mass chromatograms.

IKU code	Depth (m)	Sample type	m/z 191 Tm/Ts[1]	m/z 191 TRI/E[2]	m/z 191 Z/E	m/z 191 X/E	m/z 217 a/a+j[3]
B-4681	-	Oil	0.52	0.07	0.17	0.18	0.85
B-4682	1567.80	Core, sst	0.72	0.06	0.18	0.14	0.85
B-4683	1571.50	"	0.53	0.07	0.18	0.17	0.83
B-4684	1573.95	"	0.83	0.05	0.16	0.18	0.83
B-4685	1581.65	"	0.76	0.06	0.19	0.20	0.83
B-4686	1586.40	"	0.76	0.06	0.18	0.17	0.83
B-4687	1587.50	"	0.63	0.08	0.22	0.18	0.86
B-4688	1590.50	"	0.61	0.05	0.23	0.20	0.85
B-4689	1593.50	"	0.70	0.05	0.17	0.16	0.85
B-4690	1595.50	"	0.75	0.05	0.19	0.18	0.82
B-4691	1628.00	"	1.00	0.06	0.17	0.14	0.61

1) B/A in m/z 191.
2) Q/E in m/z 191.
3) Relative amounts of C_{27} rearranged steranes (a/a+j in m/z 217).

Table 11. Maturity ratios from aromatic sterane mass chromatograms.

IKU no.	Depth (m)	Sample type	$C_{21}/C_{21}+C_{28,29}$	$C_{20}/C_{20}+C_{26,27}$	TRI/TRI+MONO
B-4681	-	Oil	50.0	35.3	70.5
B-4682	1567.80	Core, sst	41.2	35.3	60.5
B-4683	1571.50	"	44.4	50.0	59.8
B-4684	1573.95	"	37.5	35.3	57.9
B-4685	1581.65	"	47.1	36.8	62.4
B-4686	1586.40	"	41.2	31.3	61.3
B-4687	1587.50	"	39.8	40.2	55.2
B-4688	1590.50	"	41.2	37.5	55.1
B-4689	1593.50	"	46.0	35.3	58.2
B-4690	1595.50	"	44.4	36.8	63.2
B-4691	1628.00	"	33.3	33.3	49.5

Table 12. $\delta^{13}C$ isotope ratios of hydrocarbon fractions.

IKU no.	Depth (m)	Sample type	SAT	ARO
B-4681	-	Oil	-29.1	-
B-4682	1567.80	Core, sst	-29.5	-27.6
B-4683	1571.50	"	-28.7	-27.7
B-4684	1573.95	"	-28.5	-27.6
B-4685	1581.65	"	-28.5	-27.9
B-4686	1586.40	"	-28.7	-27.2
B-4687	1587.50	"	-28.8	-27.1
B-4688	1590.50	"	-28.9	-27.4
B-4689	1593.50	"	-28.9	-27.2
B-4690	1595.50	"	-28.3	-27.6
B-4691	1628.00	"	not sufficient material	

FIGURE 1

C_2-C_8 hydrocarbon gas chromatogram

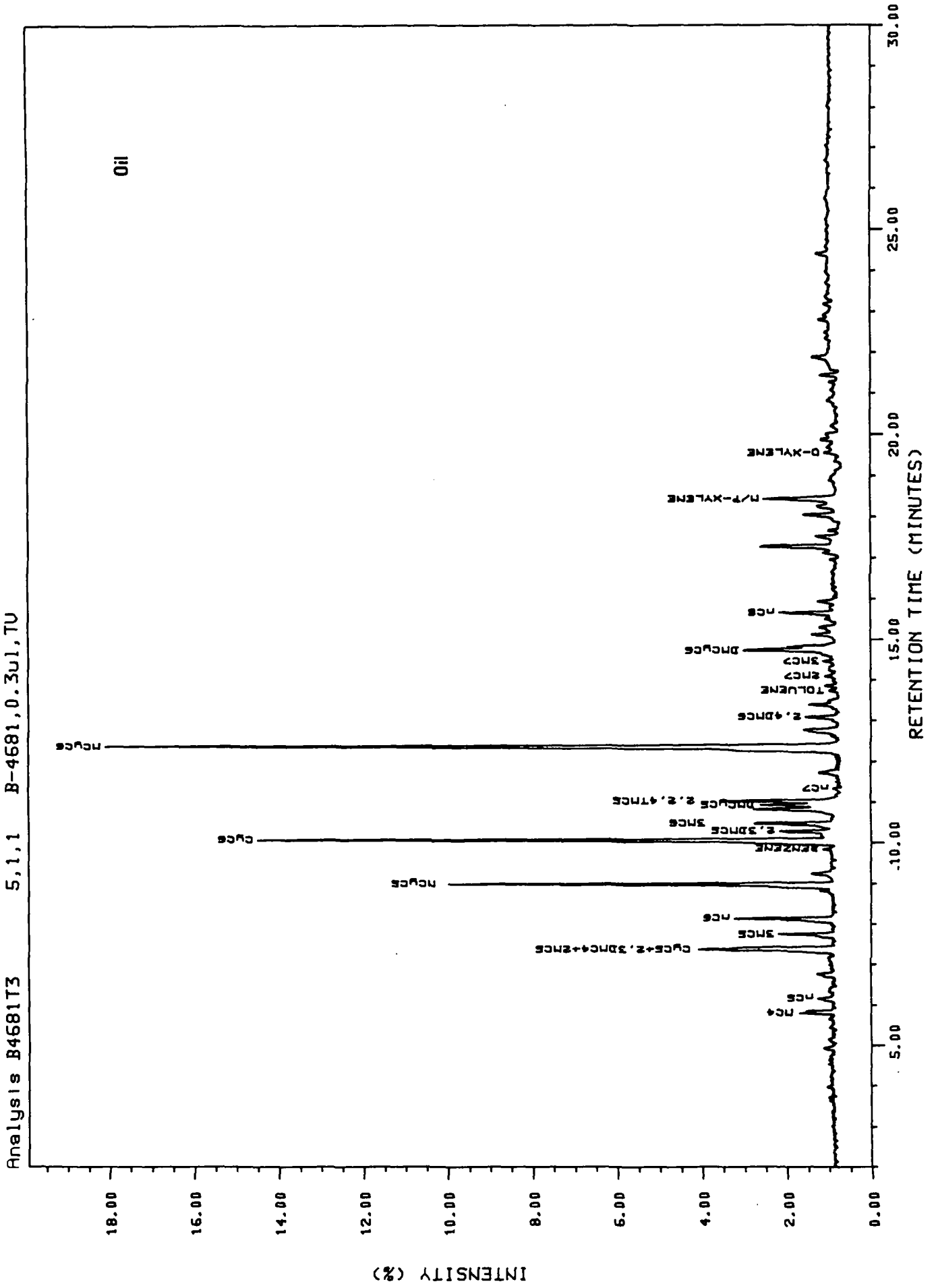
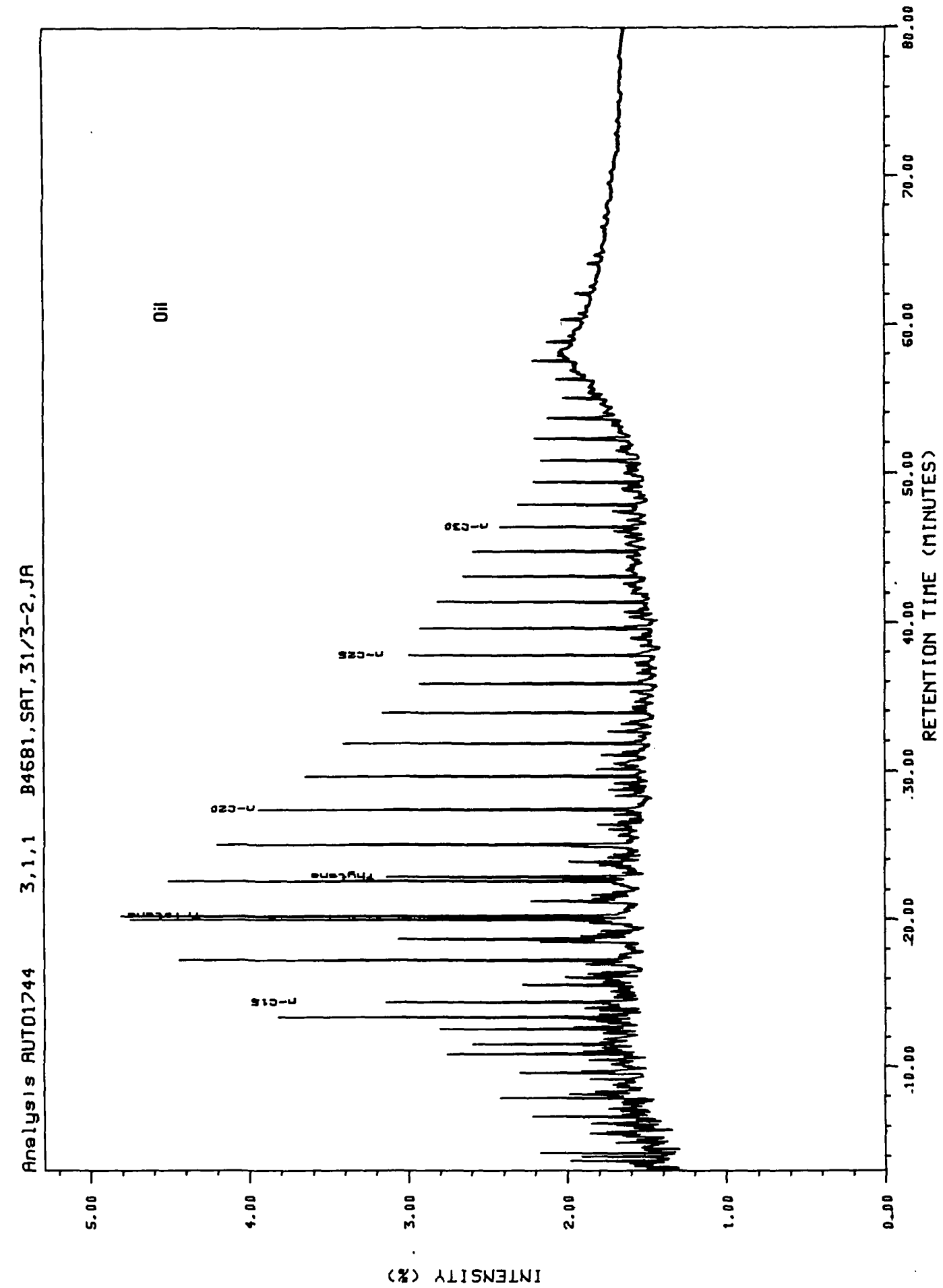
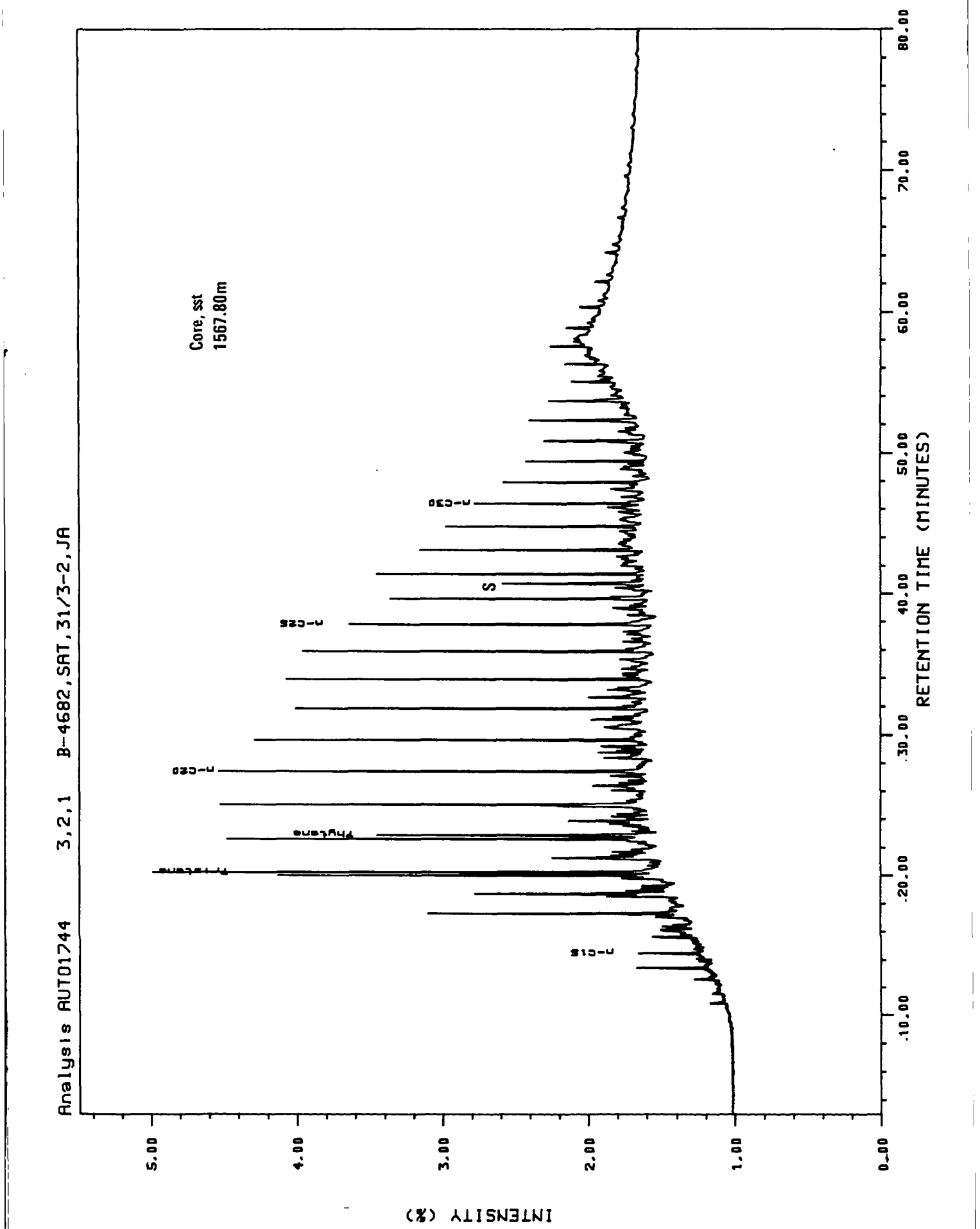

Analysis B4681T3 5,1,1 B-4681,0.3ul,TU
Oil
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
2.00
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
5.00
10.00
15.00
20.00
25.00
30.00
nC4
nC5
CyC5+2,3DMC4+2MC5
3MC5
nC6
nCyC5
BENZENE
2,3DMC5
3MC6
DMCyC5
2,2,4TMC5
nC7
nCyC6
2,4DMC6
TOLUENE
2MC7
3MC7
DMCyC6
nC8
m/p-XYLENE
o-XYLENE

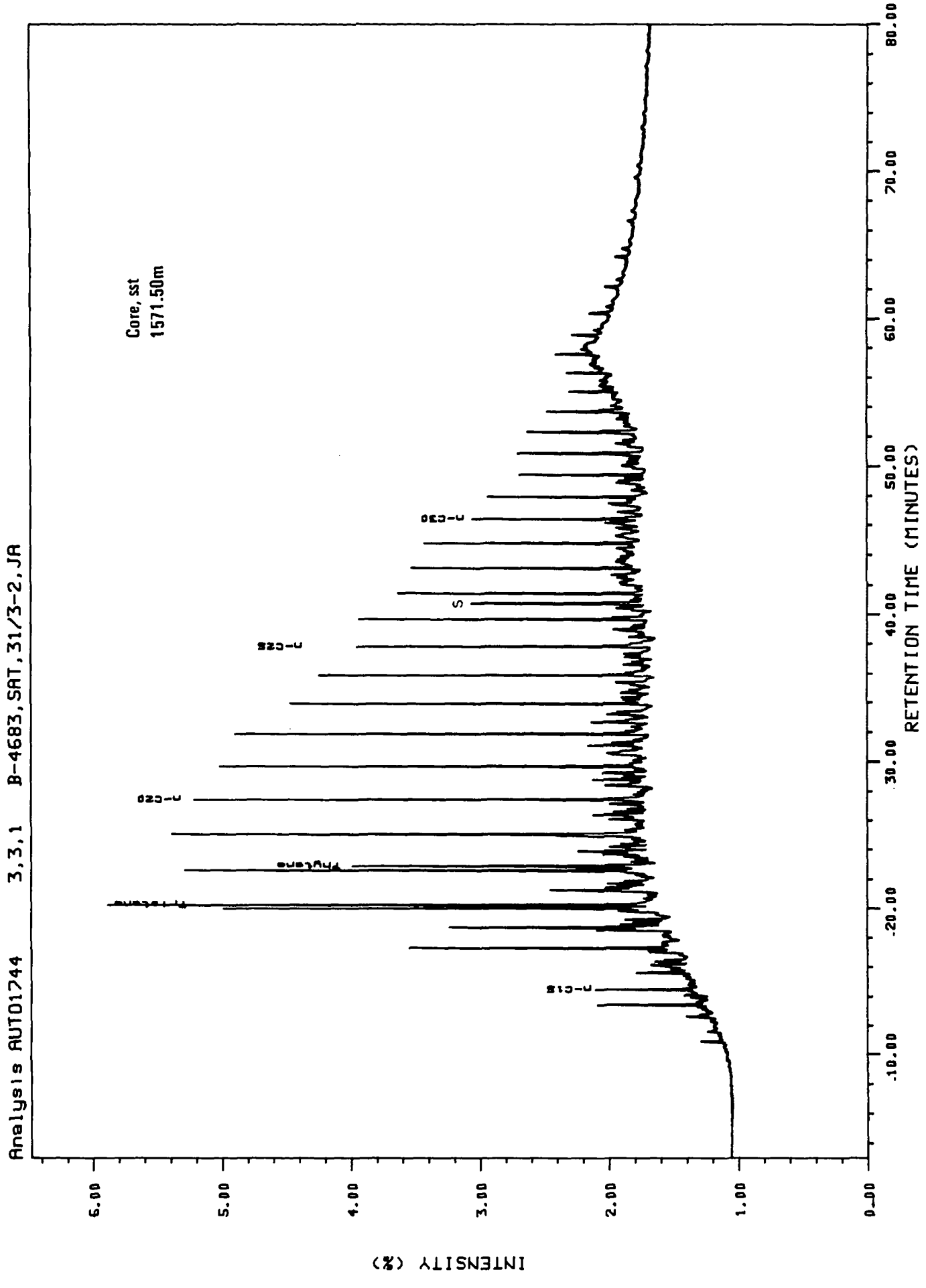
FIGURE 2

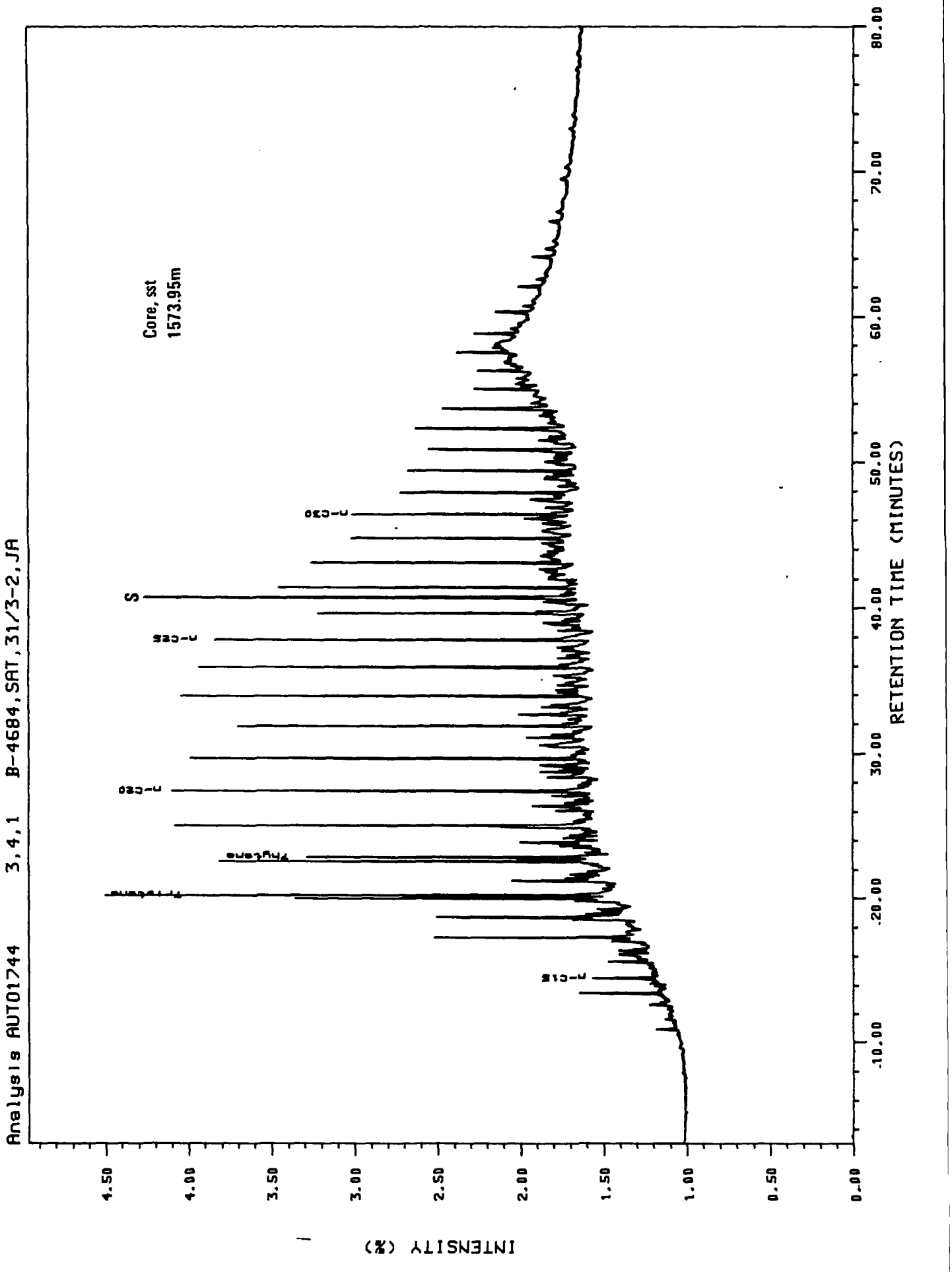
Saturated hydrocarbon gas chromatograms

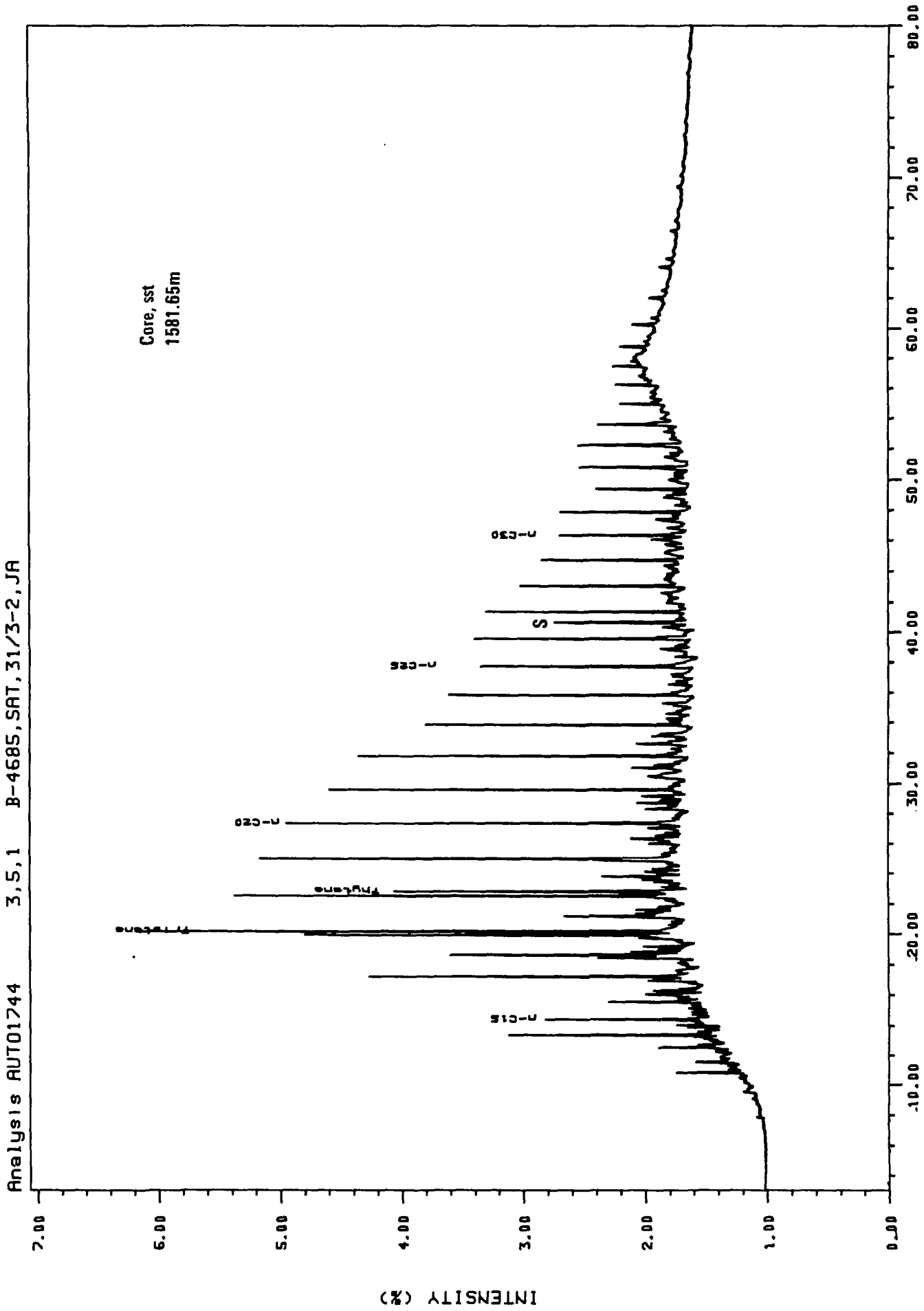
$n\text{-}C_{15}$ etc. - n-alkanes
Pr - pristane
Ph - phytane
* - acyclic isoprenoids
S - squalane (internal standard)

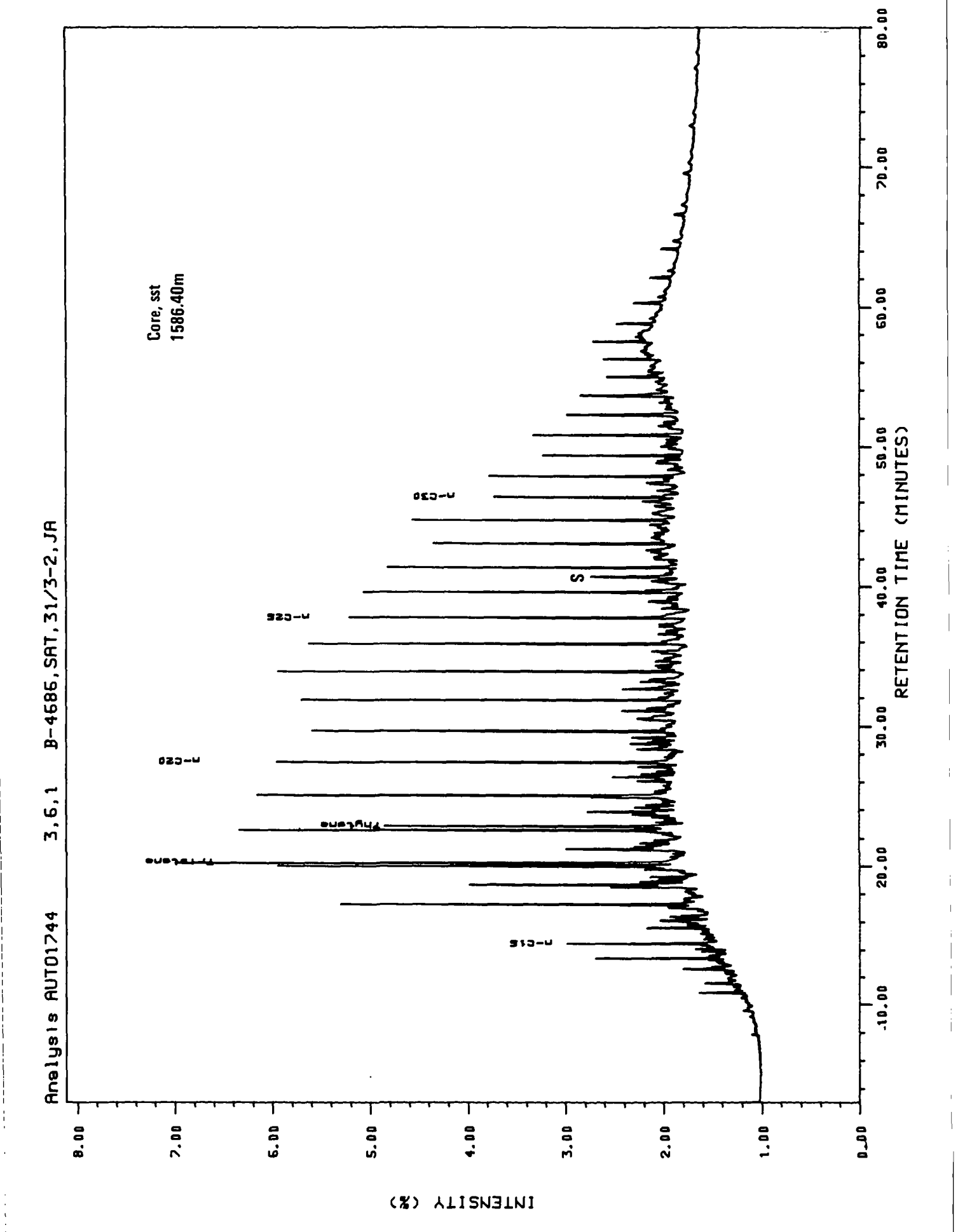

Analysis AUT01744 3,1,1 B4681,SAT,31/3-2,JA
Oil
n-C15
n-C20
n-C25
n-C30
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
1.00
2.00
3.00
4.00
5.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00

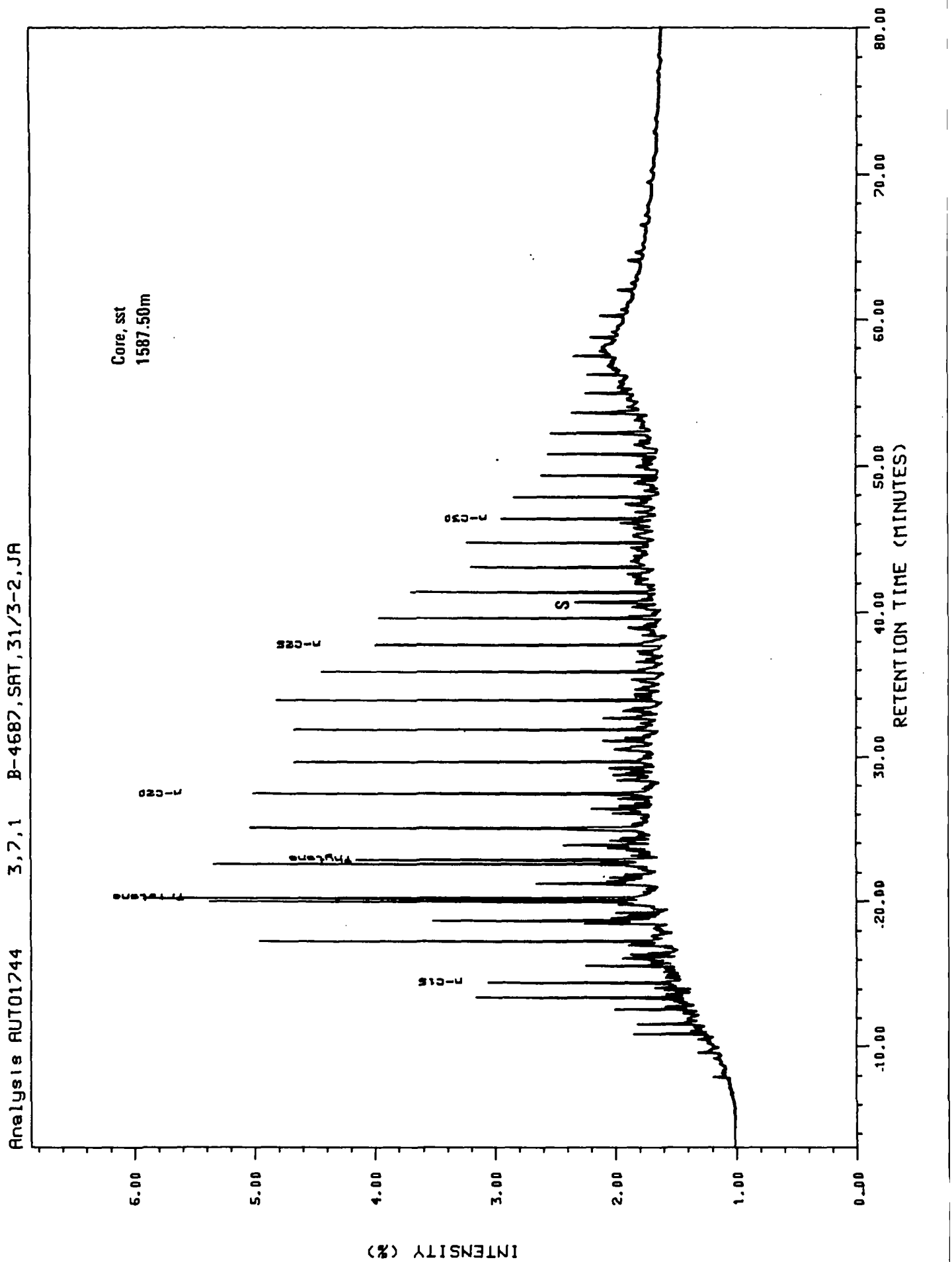

Analysis AUTO1744 3,2,1 B-4682,SAT,31/3-2,JA
Core, sst
1567.80m
n-C18
Pristane
Phytane
n-C20
n-C25
S
n-C30
INTENSITY (%)
5.00
4.00
3.00
2.00
1.00
0.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00
RETENTION TIME (MINUTES)

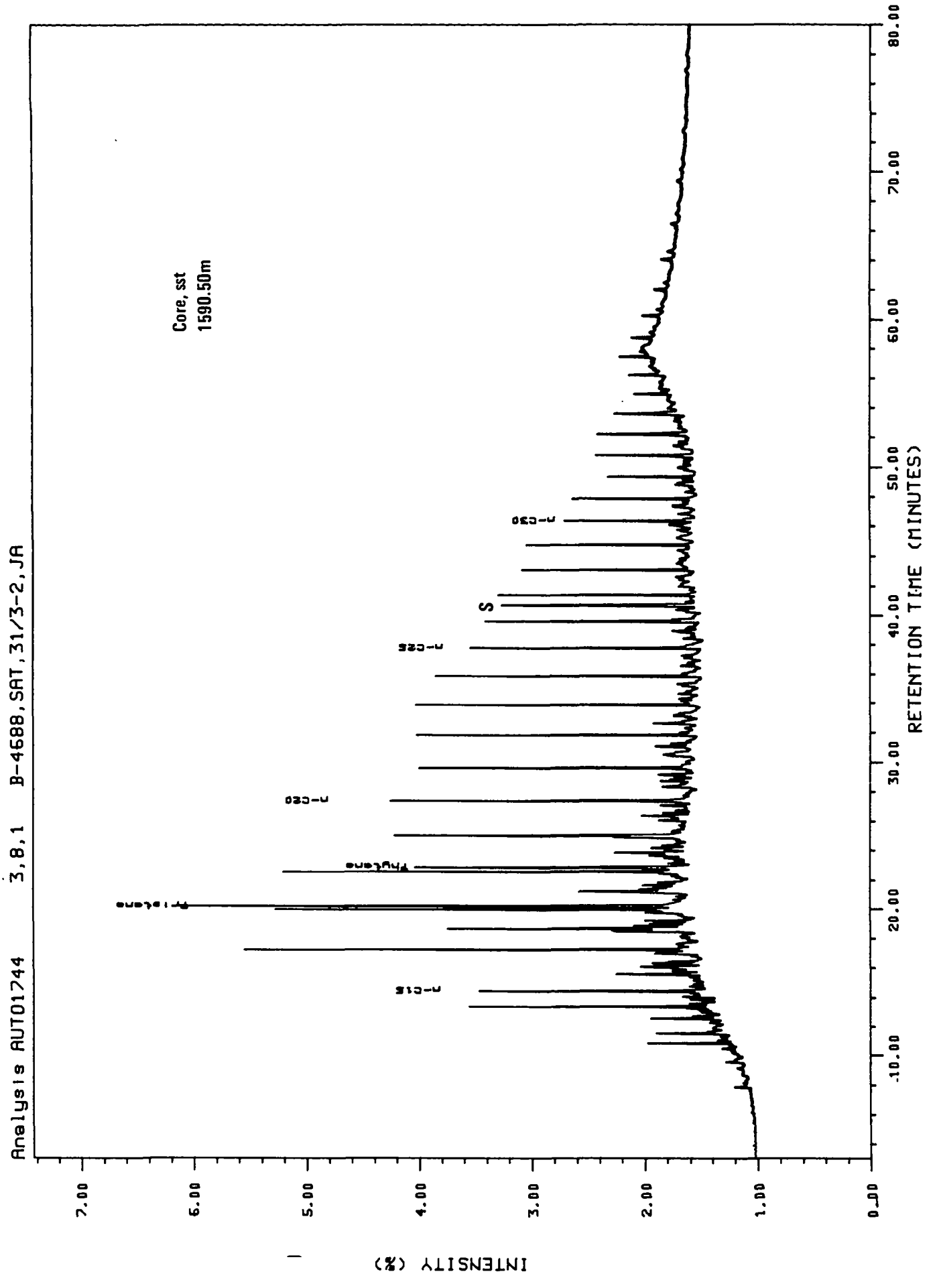

Analysis AUTO1744 3,3,1 B-4683,SAT,31/3-2,JR
Core, sst
1571.50m
n-C18
Phytane
n-C29
n-C28
S
n-C30
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
1.00
2.00
3.00
4.00
5.00
6.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00

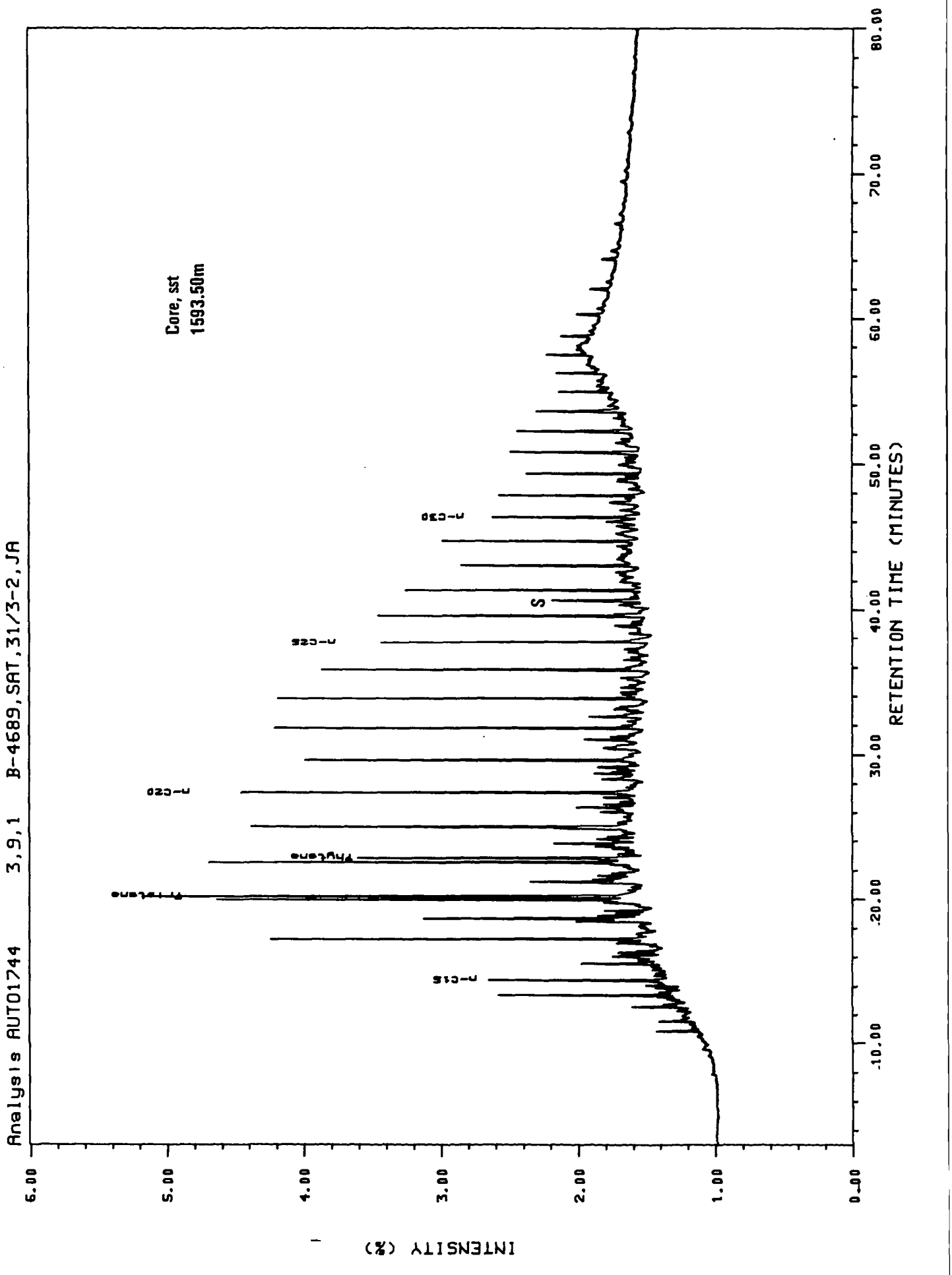

Analysis AUTO1744 3,4,1 B-4684,SAT,31/3-2,JA
Core, sst
1573.95m
n-C15
Pristane
Phytane
n-C20
n-C25
S
n-C30
INTENSITY (%)
4.50
4.00
3.50
3.00
2.50
2.00
1.50
1.00
0.50
0.00
-10.00
.20.00
30.00
40.00
50.00
60.00
70.00
80.00
RETENTION TIME (MINUTES)

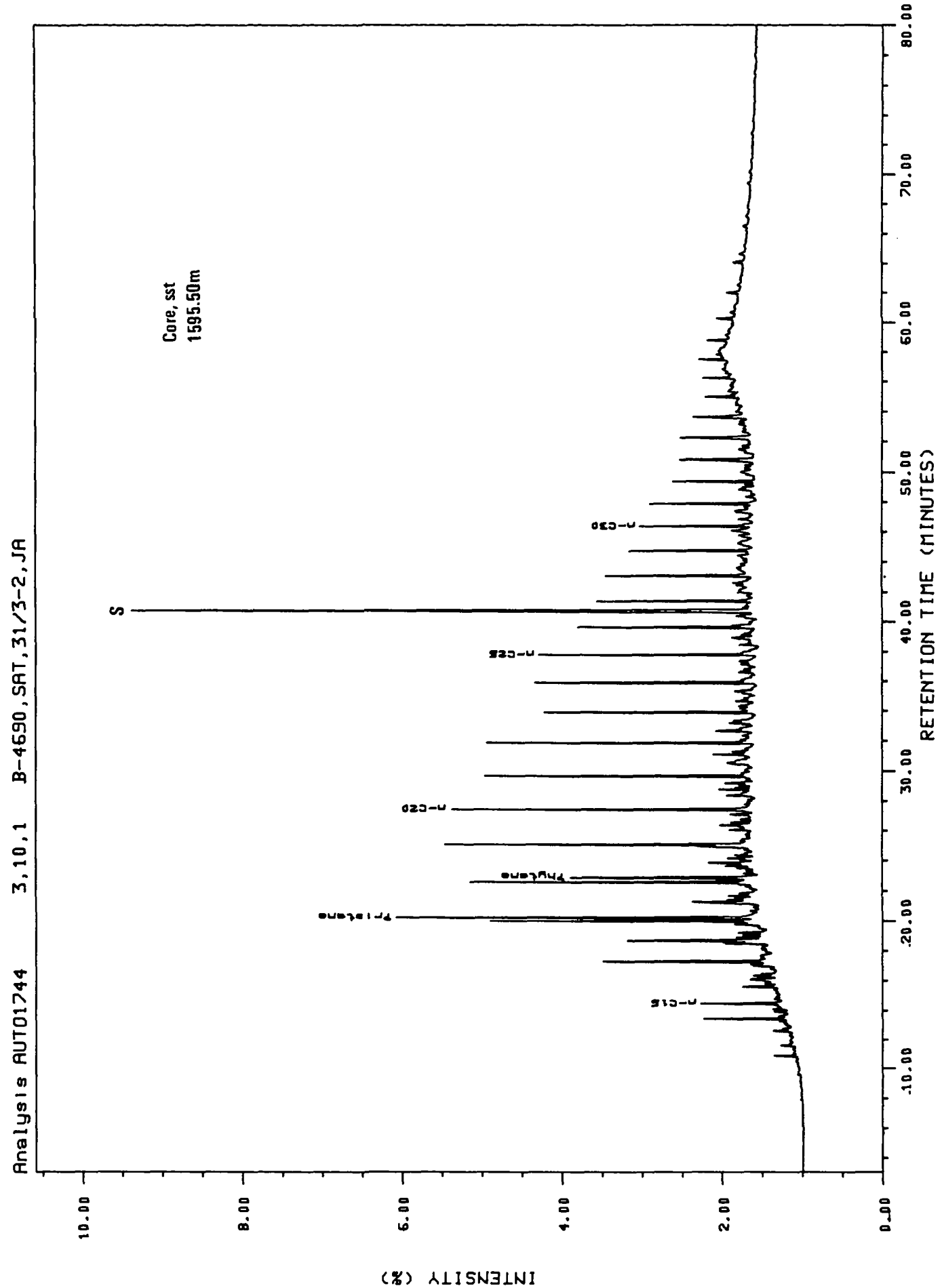

Analysis AUT01744 3,5,1 B-4685,SAT,31/3-2,JA
Core, sst
1581.65m
n-C15
n-C20
n-C25
S
n-C30
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00


Analysis AUTO1744 3,6,1 B-4686,SAT,31/3-2,JA
Core, sst
1586.40m
n-C15
Pristane
n-C20
Phytane
n-C25
S
n-C30
INTENSITY (%)
RETENTION TIME (MINUTES)
8.00
7.00
6.00
5.00
4.00
3.00
2.00
1.00
0.00
-10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00


Analysis AUTO1744 3,7,1 B-4687,SAT,31/3-2,JA
Core, sst
1587.50m
n-C15
Pristane
Phytane
n-C20
n-C25
S
n-C30
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
1.00
2.00
3.00
4.00
5.00
6.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00


Analysis AUT01744 3,8,1 B-4688,SAT,31/3-2,JA
Core, sst
1590.50m
n-C18
Pristane
Phytane
n-C29
n-C25
S
n-C30
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
-10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00


Analysis AUTO1744 3,9,1 B-4689,SAT,31/3-2,JA
Core, sst
1593.50m
n-C15
Pristane
Phytane
n-C20
n-C25
S
n-C30
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
1.00
2.00
3.00
4.00
5.00
6.00
10.00
20.00
30.00
40.00
50.00
60.00
80.00


Analysis AUTO1744 3,10,1 B-4690,SAT,31/3-2,JA
Core, sst
1595.50m
S
n-C18
Pristane
Phytane
n-C29
n-C28
n-C30
INTENSITY (%)
RETENTION TIME (MINUTES)
10.00
8.00
6.00
4.00
2.00
0.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00

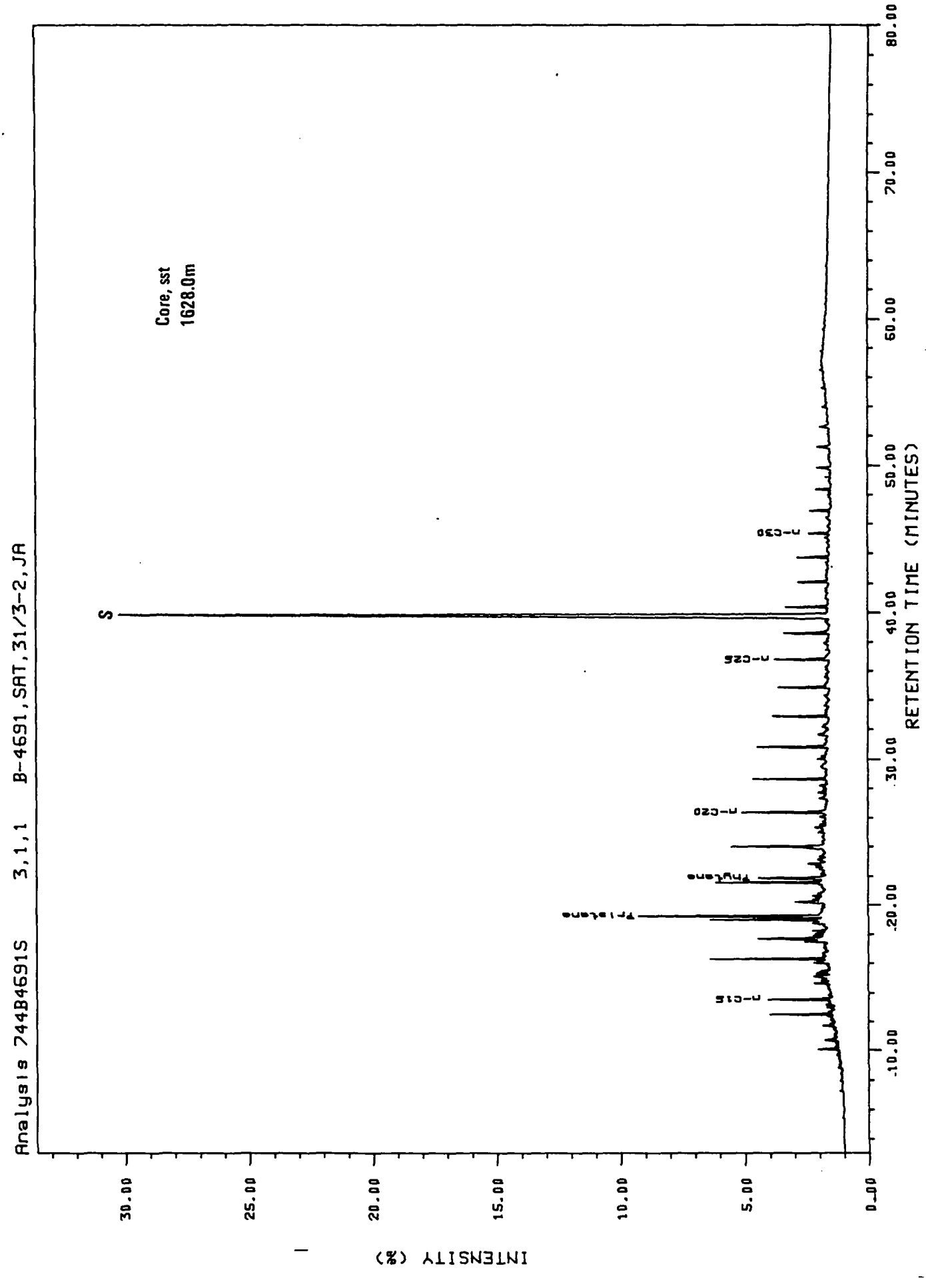
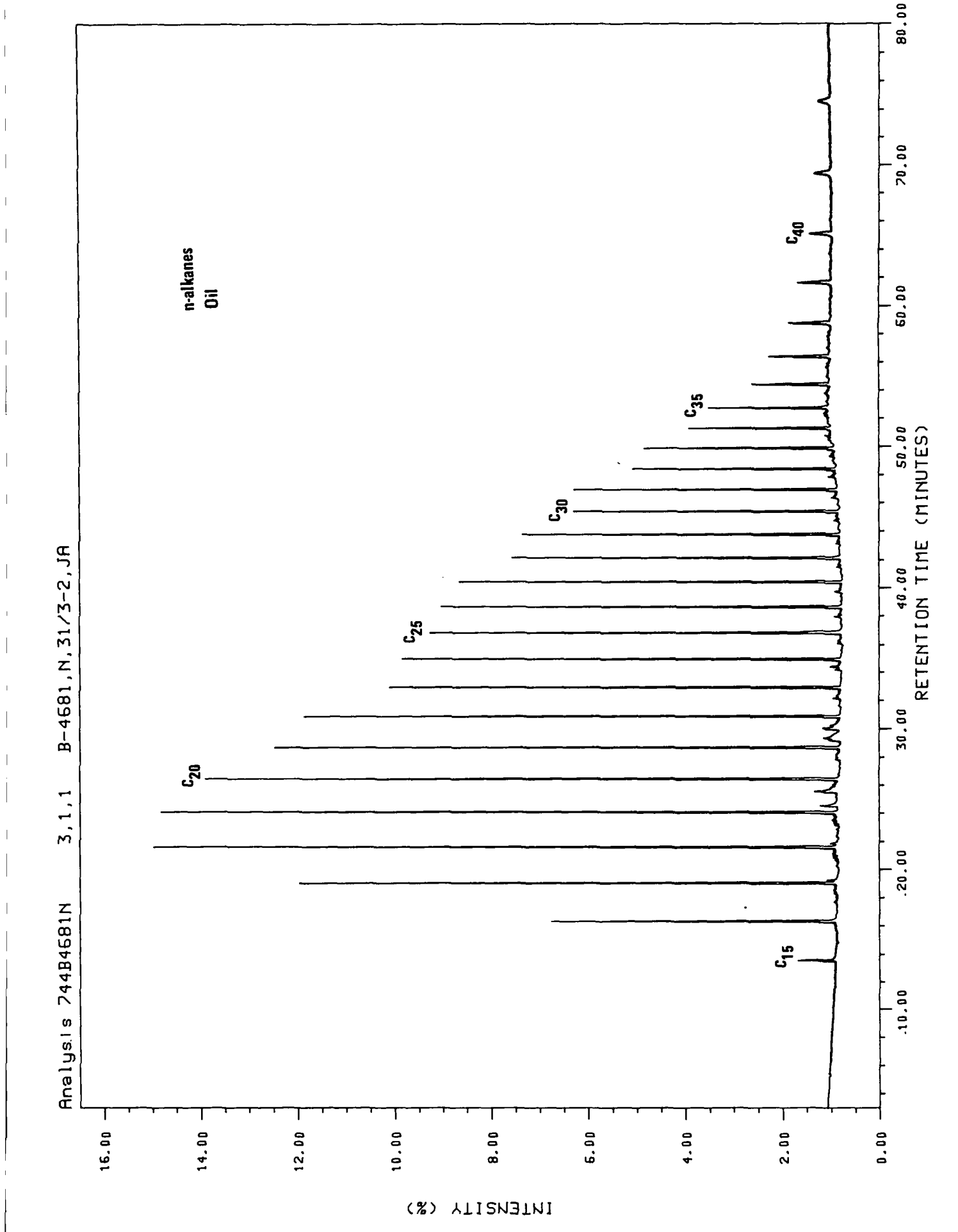
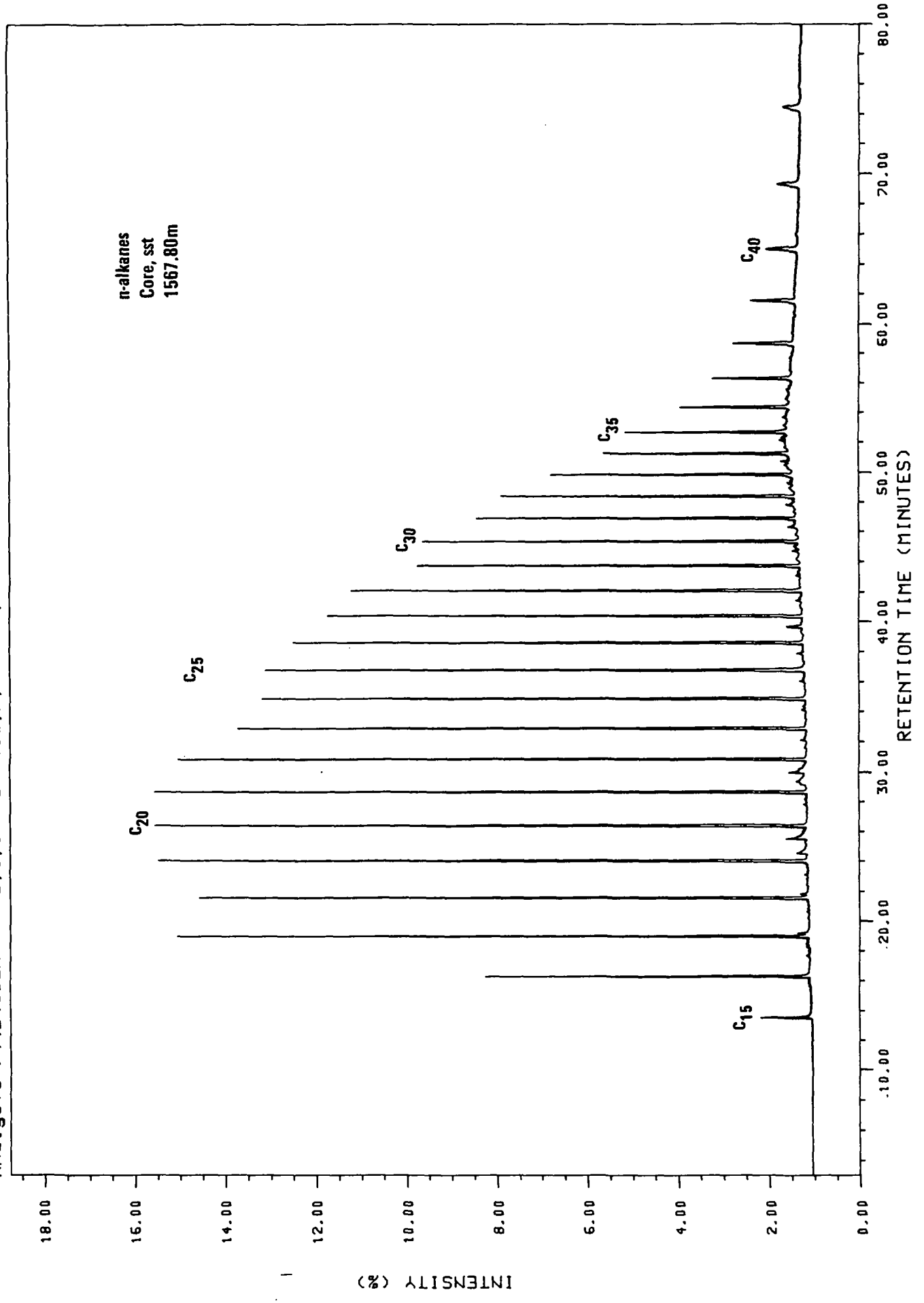

Analysis 244B4691S 3,1,1 B-4691,SAT,31/3-2,JA
Core, sst
1628.0m
S
n-C15
Tricyclane
Phytane
n-C20
n-C25
n-C30
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
5.00
10.00
15.00
20.00
25.00
30.00
-10.00
.20.00
30.00
40.00
50.00
60.00
20.00
80.00

FIGURE 3a

n-alkanes after separation with
molecular sieve


Analysis 244B4681N 3,1,1 B-4681,N,31/3-2,JA
n-alkanes
Oil
C_{15}
C_{20}
C_{25}
C_{30}
C_{35}
C_{40}
INTENSITY (%)
16.00
14.00
12.00
10.00
8.00
6.00
4.00
2.00
0.00
RETENTION TIME (MINUTES)
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00


Analysis 744B4682N 3,1,1 B-4682,N,31/3-2,JA
n-alkanes
Core, sst
1567,80m
C15
C20
C25
C30
C35
C40
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
2.00
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00

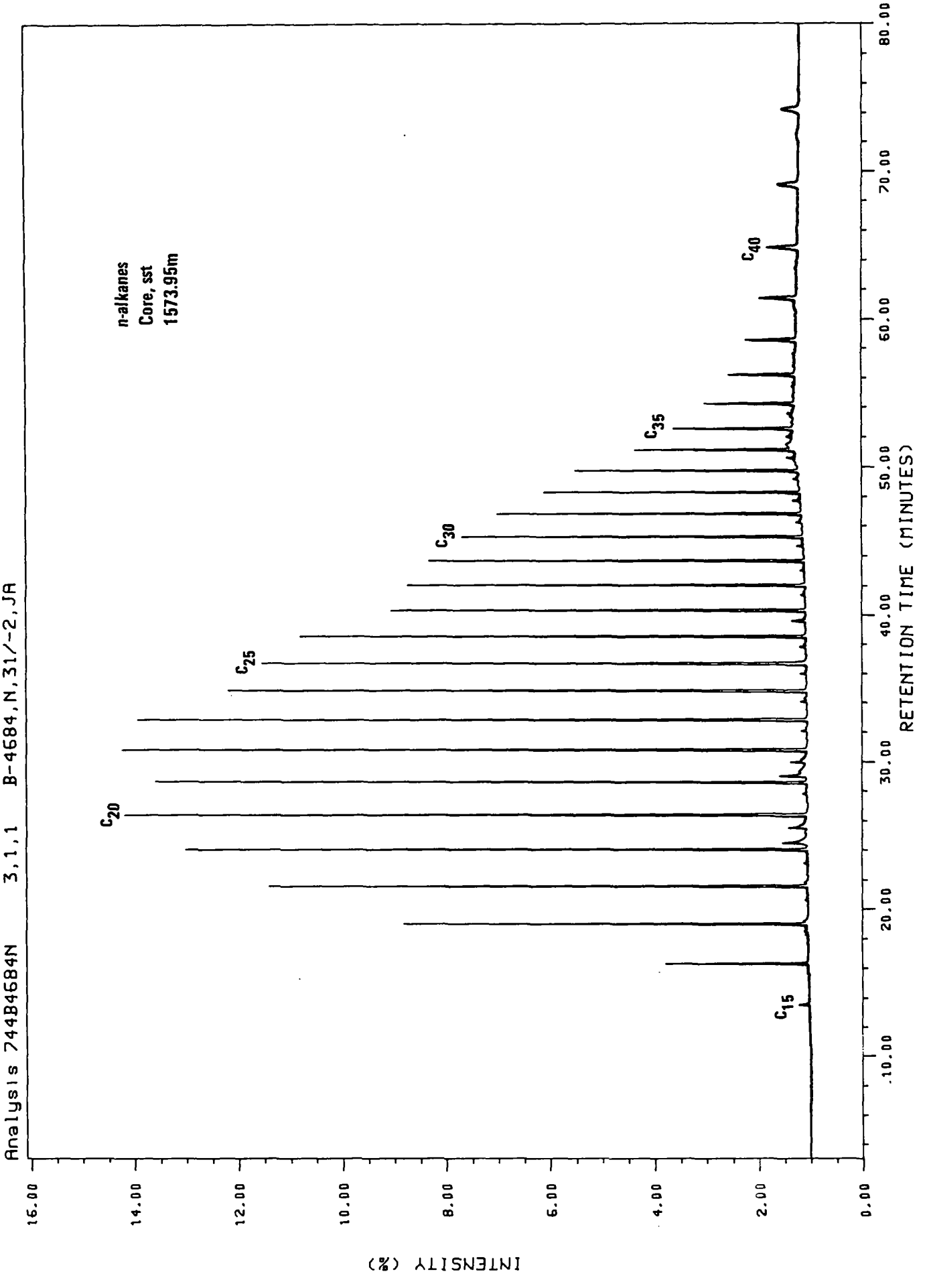
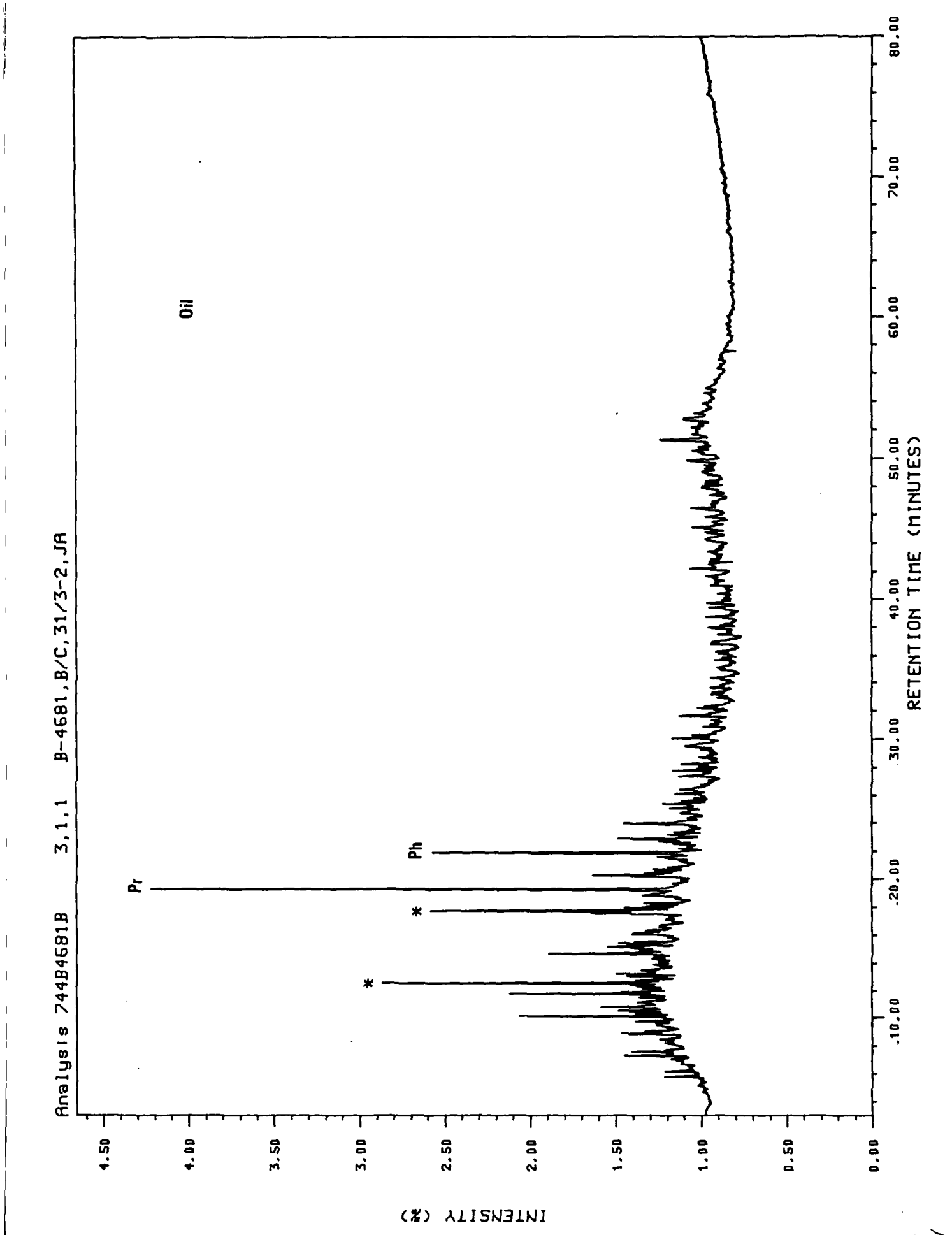
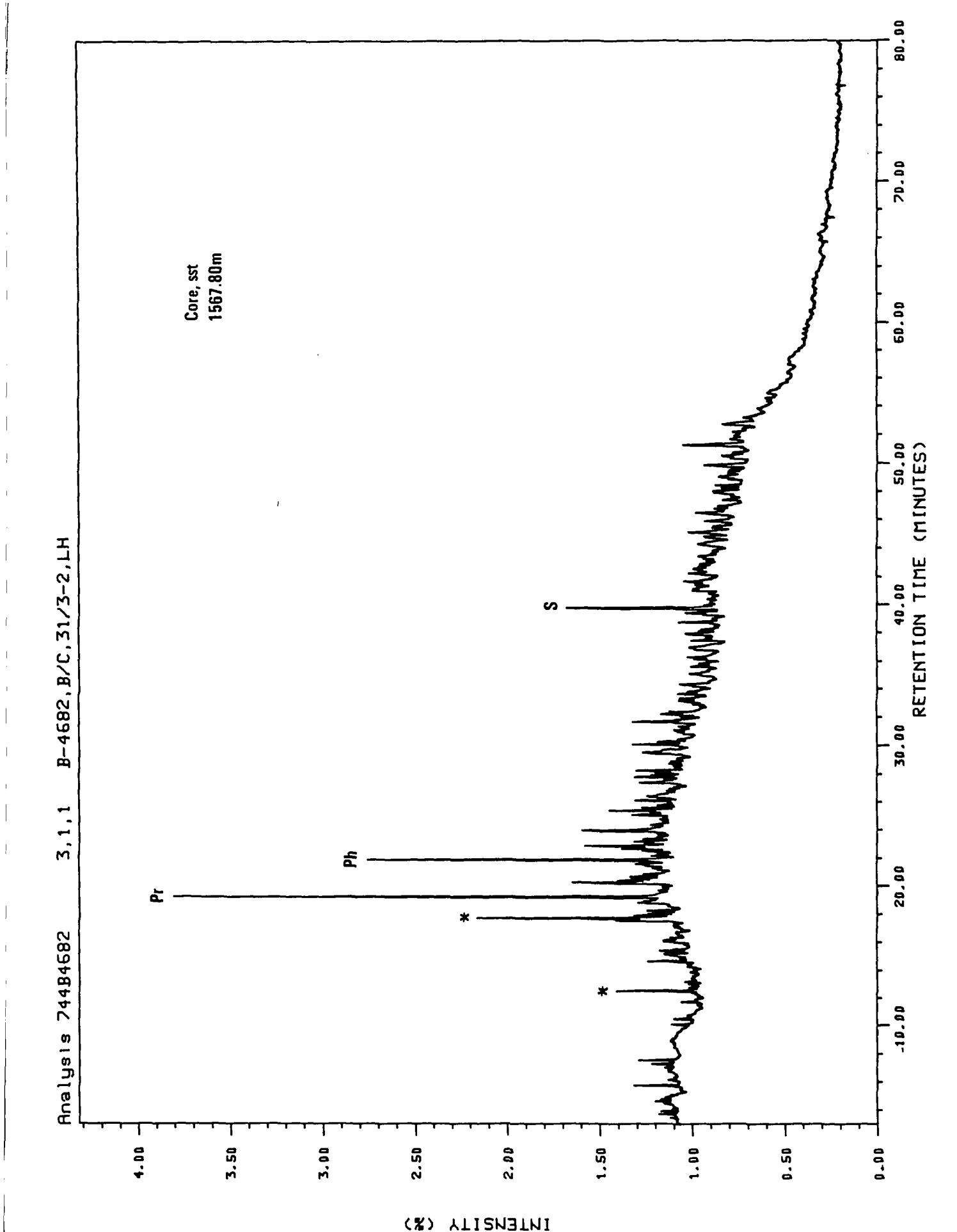

Analysis 744B4684N 3,1,1 B-4684,N,31/-2,JA
n-alkanes
Core, sst
1573.95m
C15
C20
C25
C30
C35
C40
INTENSITY (%)
16.00
14.00
12.00
10.00
8.00
6.00
4.00
2.00
0.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00
RETENTION TIME (MINUTES)

FIGURE 3b

Branched/cyclic hydrocarbons after
removal of n-alkanes with molecular sieve


Analysis 74B4681B 3,1,1 B-4681,B/C,31/3-2,JA
Oil
Pr
Ph
*
*
INTENSITY (%)
4.50
4.00
3.50
3.00
2.50
2.00
1.50
1.00
0.50
0.00
-10.00
.20.00
30.00
40.00
50.00
60.00
70.00
80.00
RETENTION TIME (MINUTES)


Analysis 744B4682 3,1,1 B-4682,B/C,31/3-2,LH
Core, sst
1567.80m
Pr
Ph
S
*
*
INTENSITY (%)
RETENTION TIME (MINUTES)
4.00
3.50
3.00
2.50
2.00
1.50
1.00
0.50
0.00
-10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00

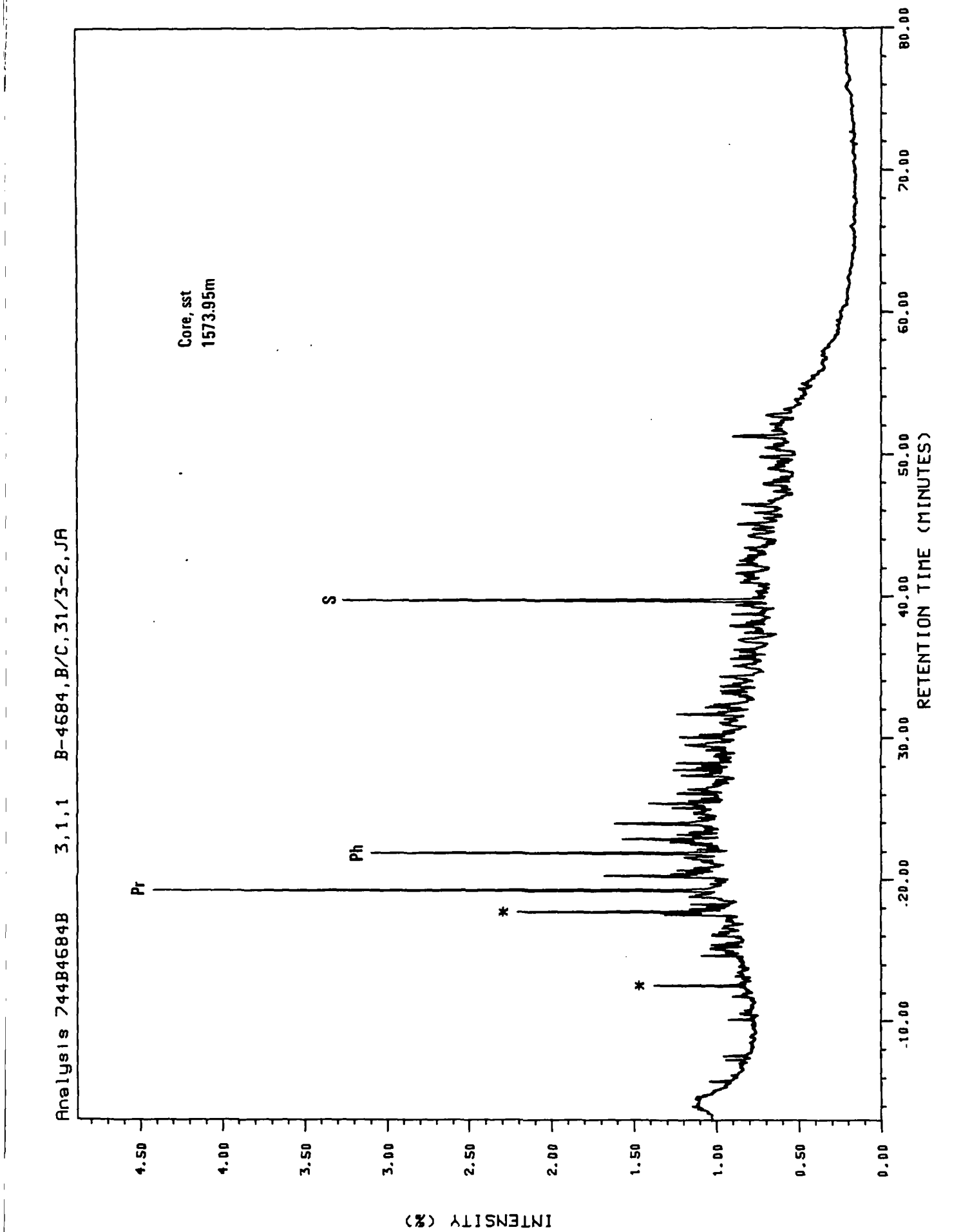
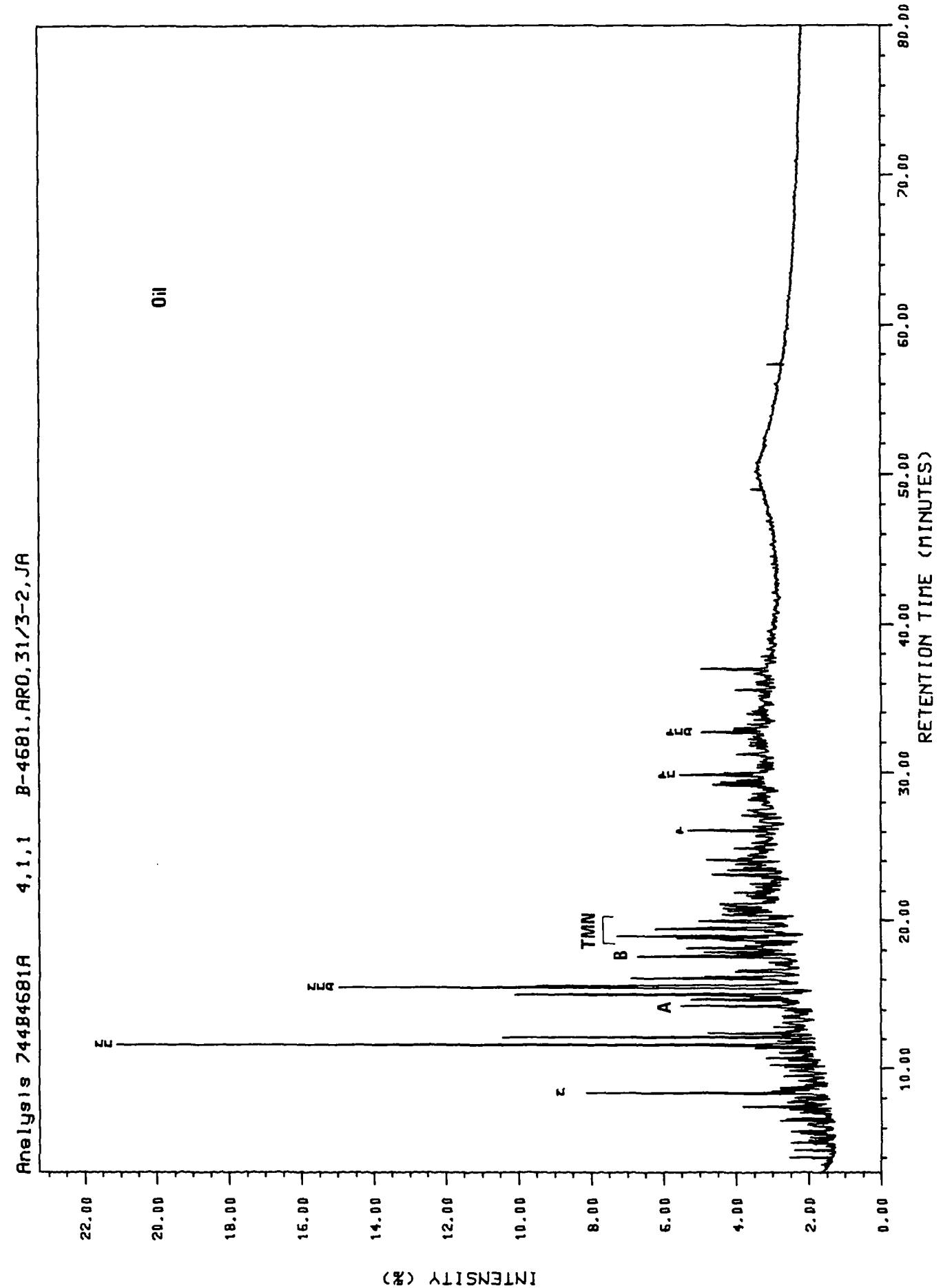
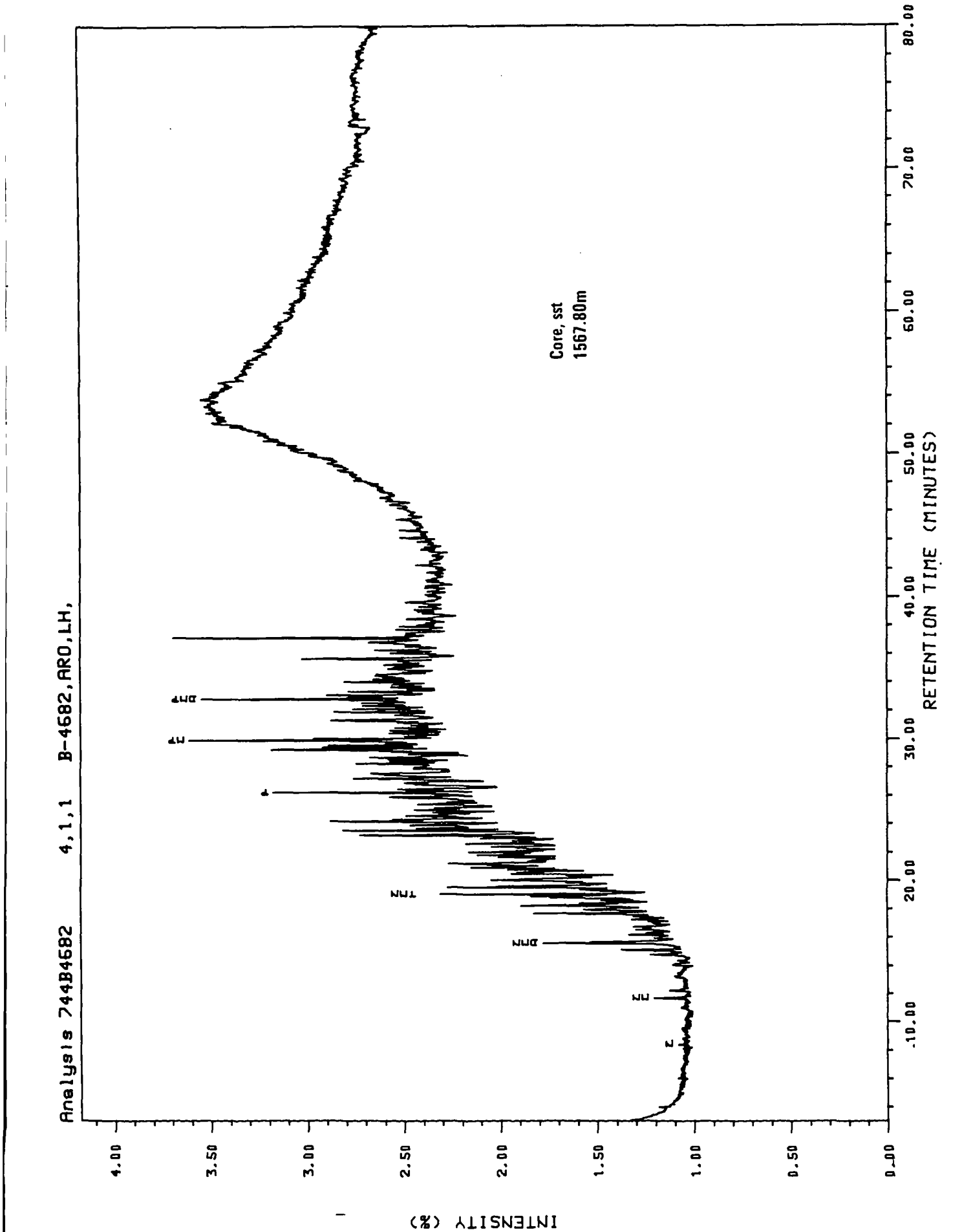

Analysis 744B4684B 3,1,1 B-4684,B/C,31/3-2,JA
Core, sst
1573.95m
Pr
Ph
S
*
*
INTENSITY (%)
4.50
4.00
3.50
3.00
2.50
2.00
1.50
1.00
0.50
0.00
-10.00
.20.00
30.00
40.00
50.00
60.00
70.00
80.00
RETENTION TIME (MINUTES)

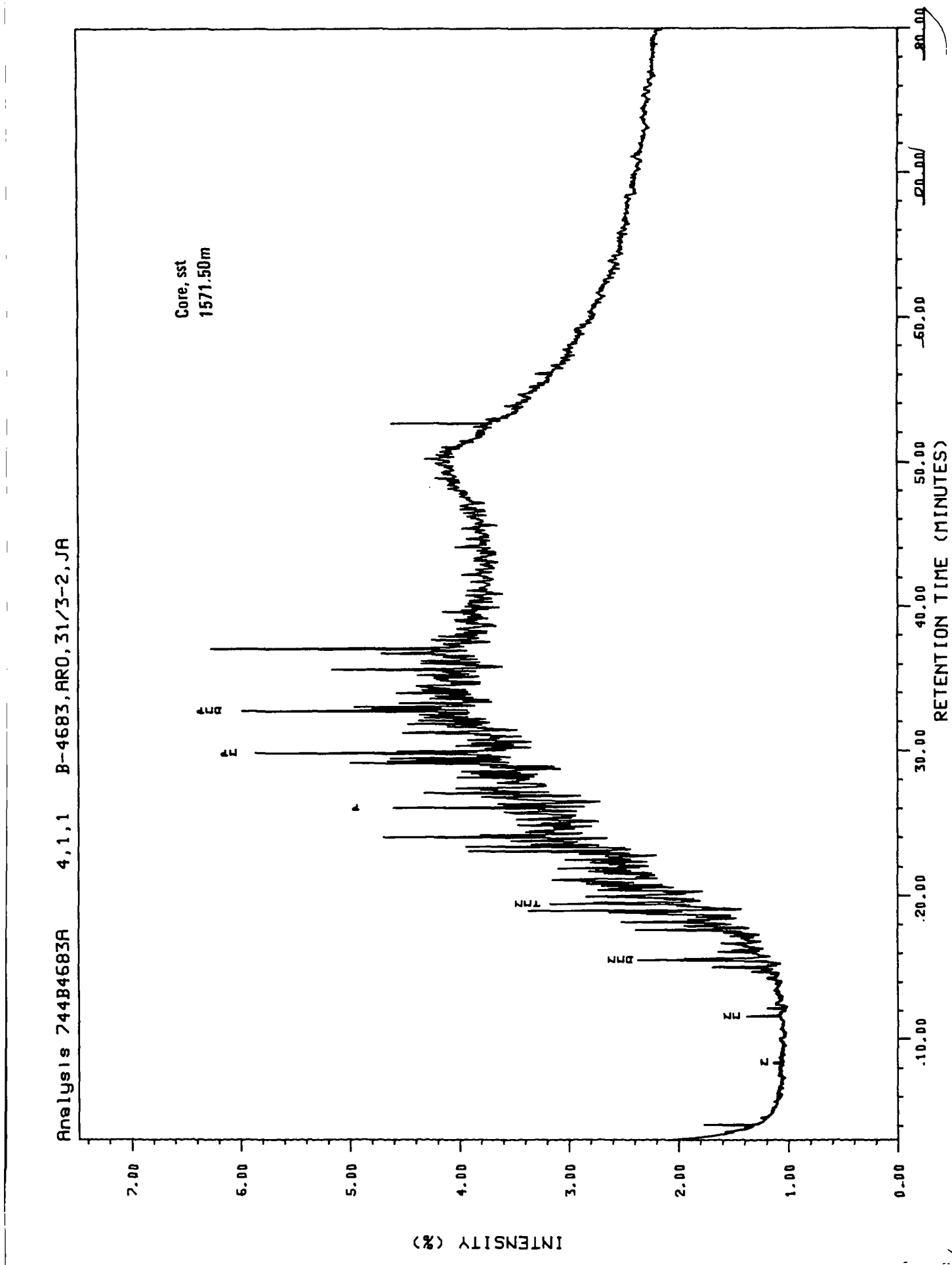
FIGURE 4

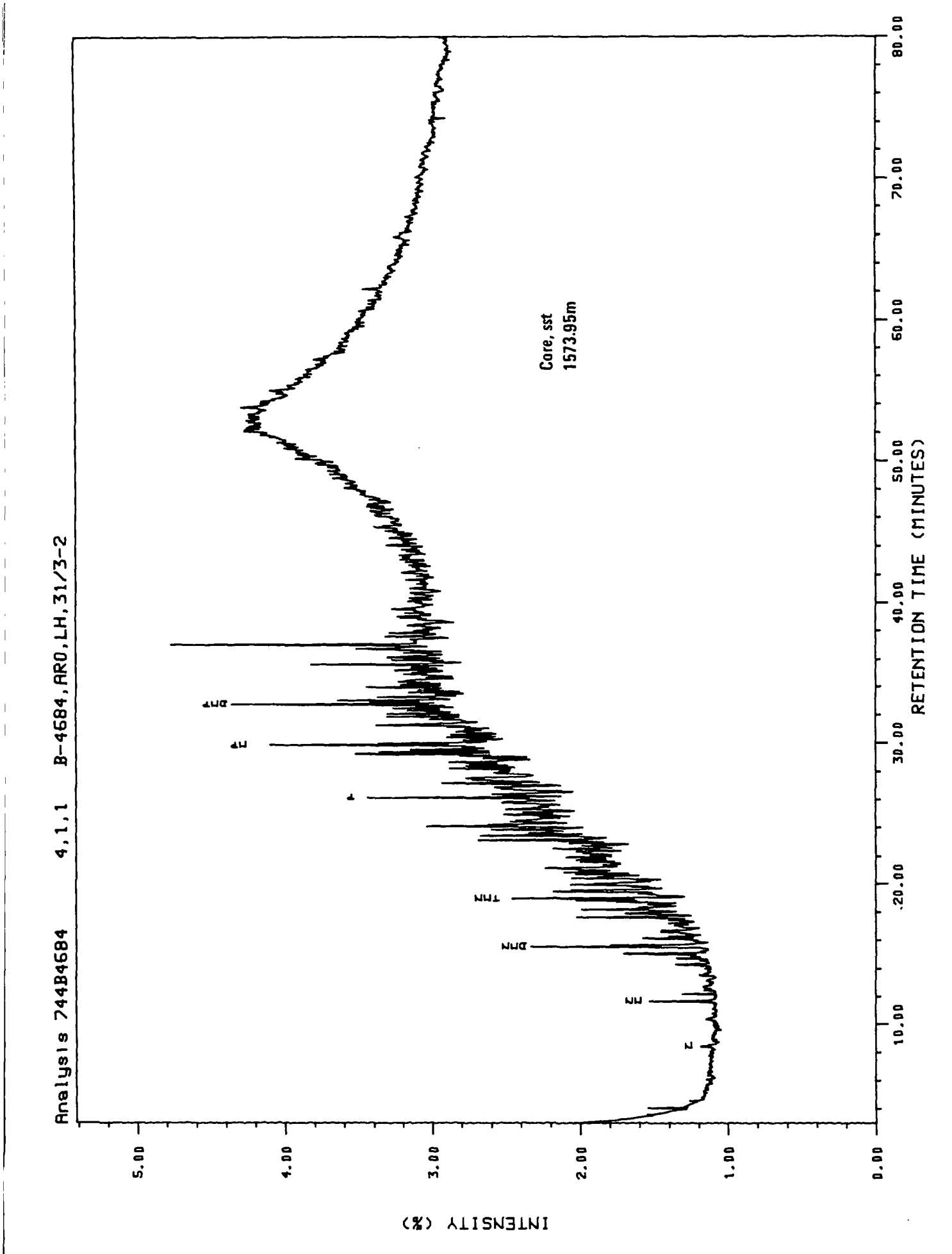
Aromatic hydrocarbon gas chromatograms

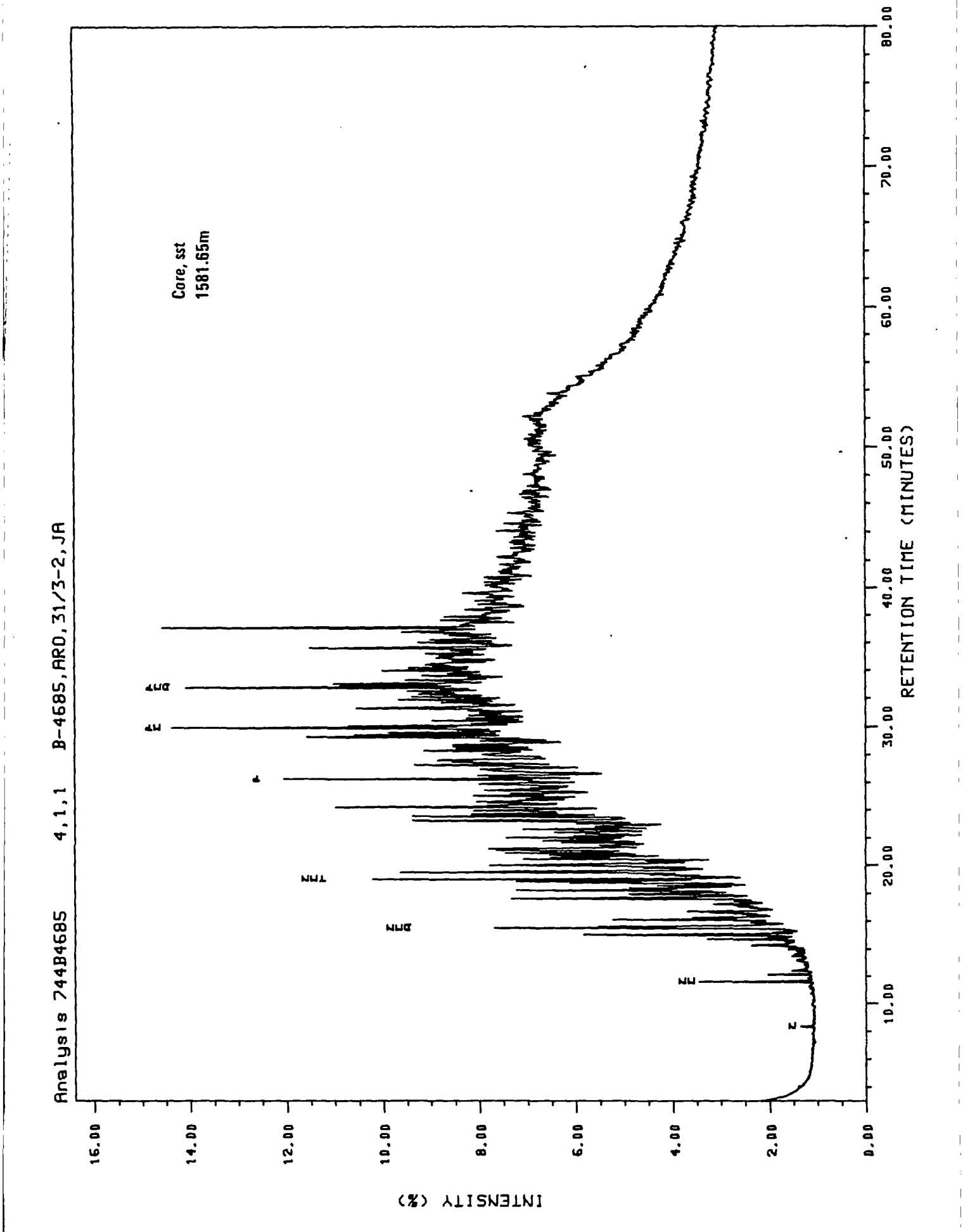
N - naphthalene
MN - methylnaphthalenes
DMN - dimethylnaphthalenes
TMN - trimethylnaphthalenes
P - phenanthrene
MP - methylphenanthrenes
DMP - dimethylphenanthrenes

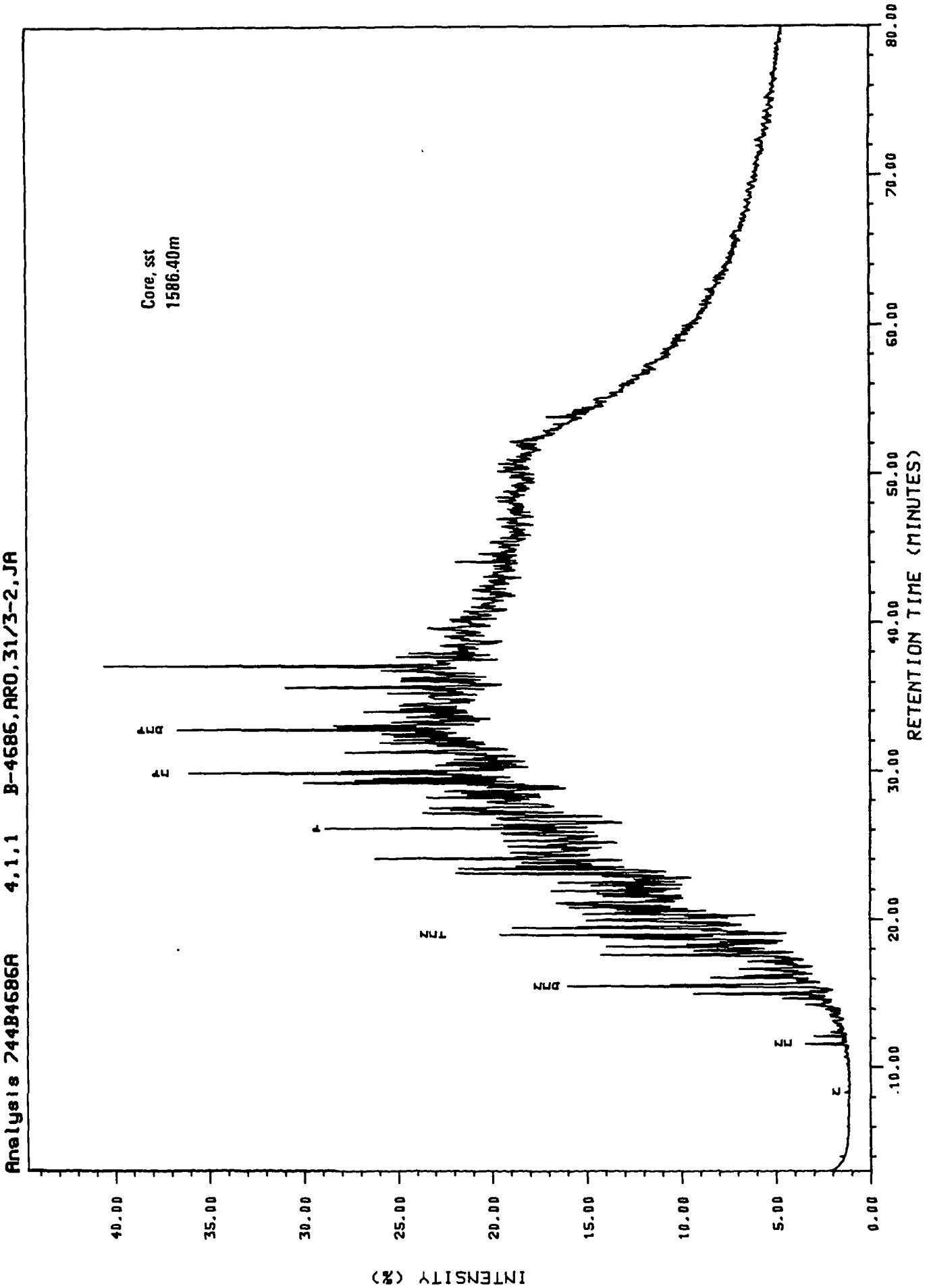

Analysis 74484681A 4,1,1 B-4681,ARO,31/3-2,JA
Oil
TMN
B
A
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
2.00
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00

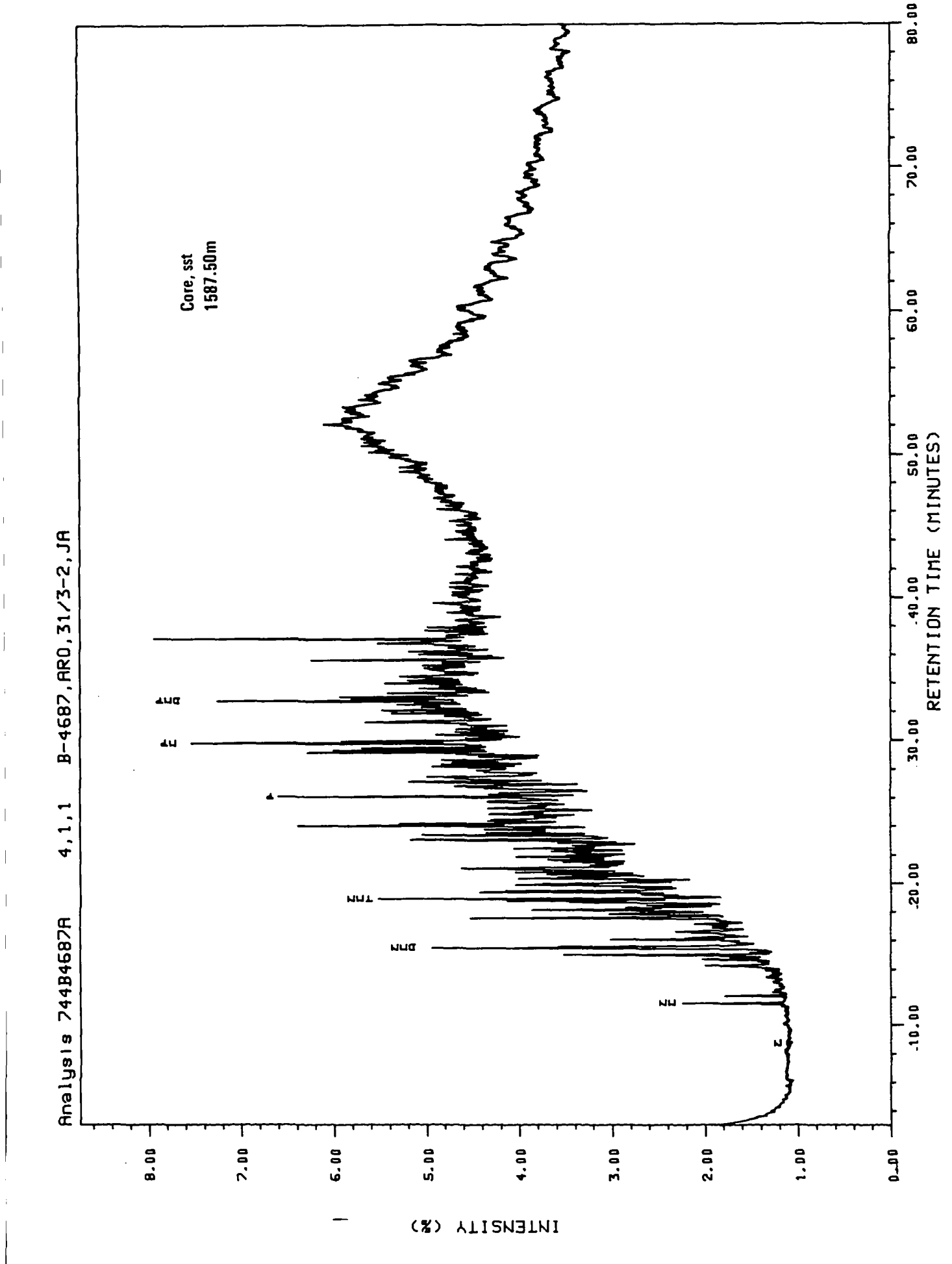

Analysis 244B4682 4,1,1 B-4682,ARO,LH,
Core, sst
1567.80m
INTENSITY (%)
RETENTION TIME (MINUTES)
4.00
3.50
3.00
2.50
2.00
1.50
1.00
0.50
0.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00

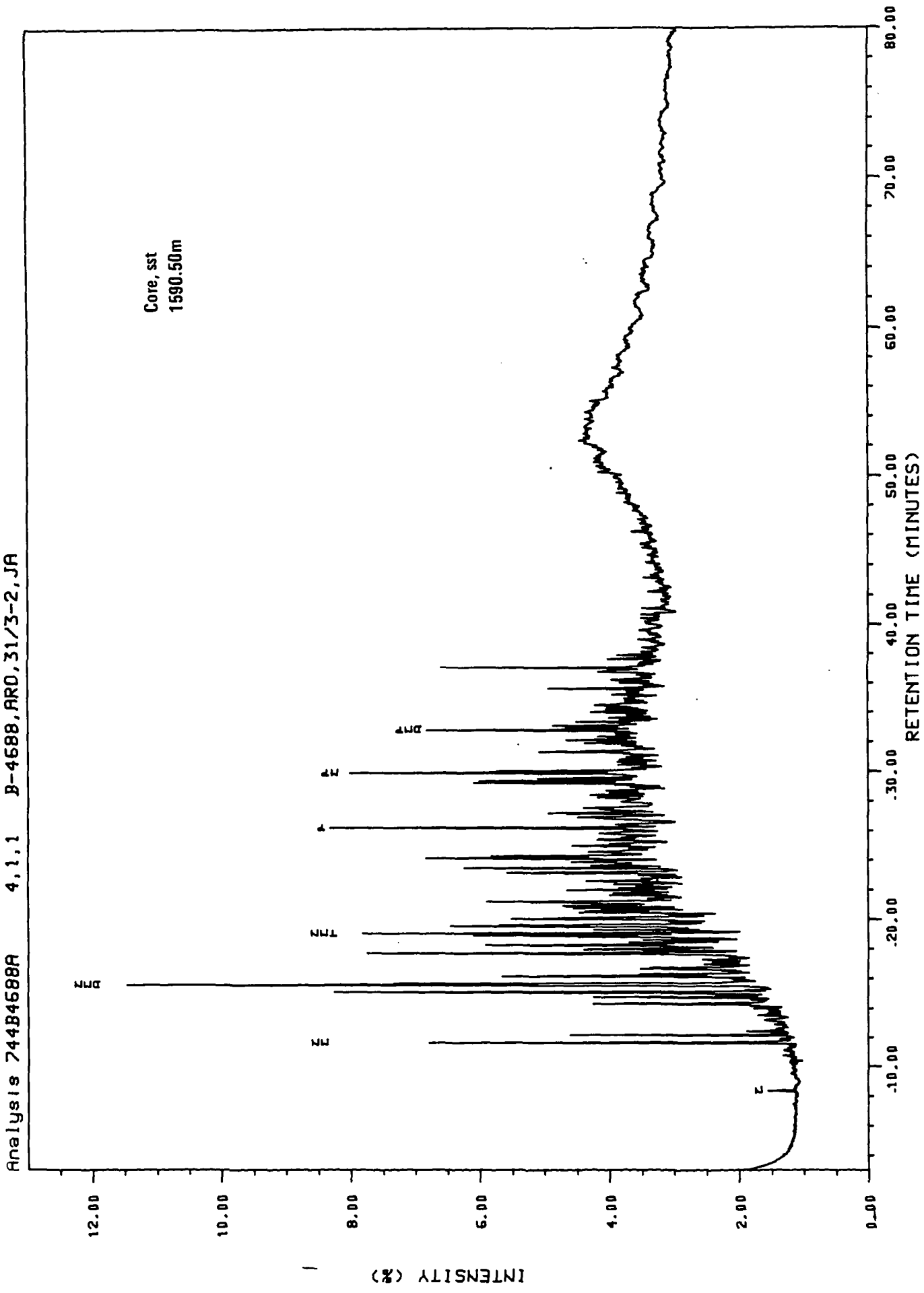

Analysis 244B4683A 4,1,1 B-4683,ARO,31/3-2,JA
Core, sst
1571.50m
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
10.00
20.00
30.00
40.00
50.00
60.00
80.00

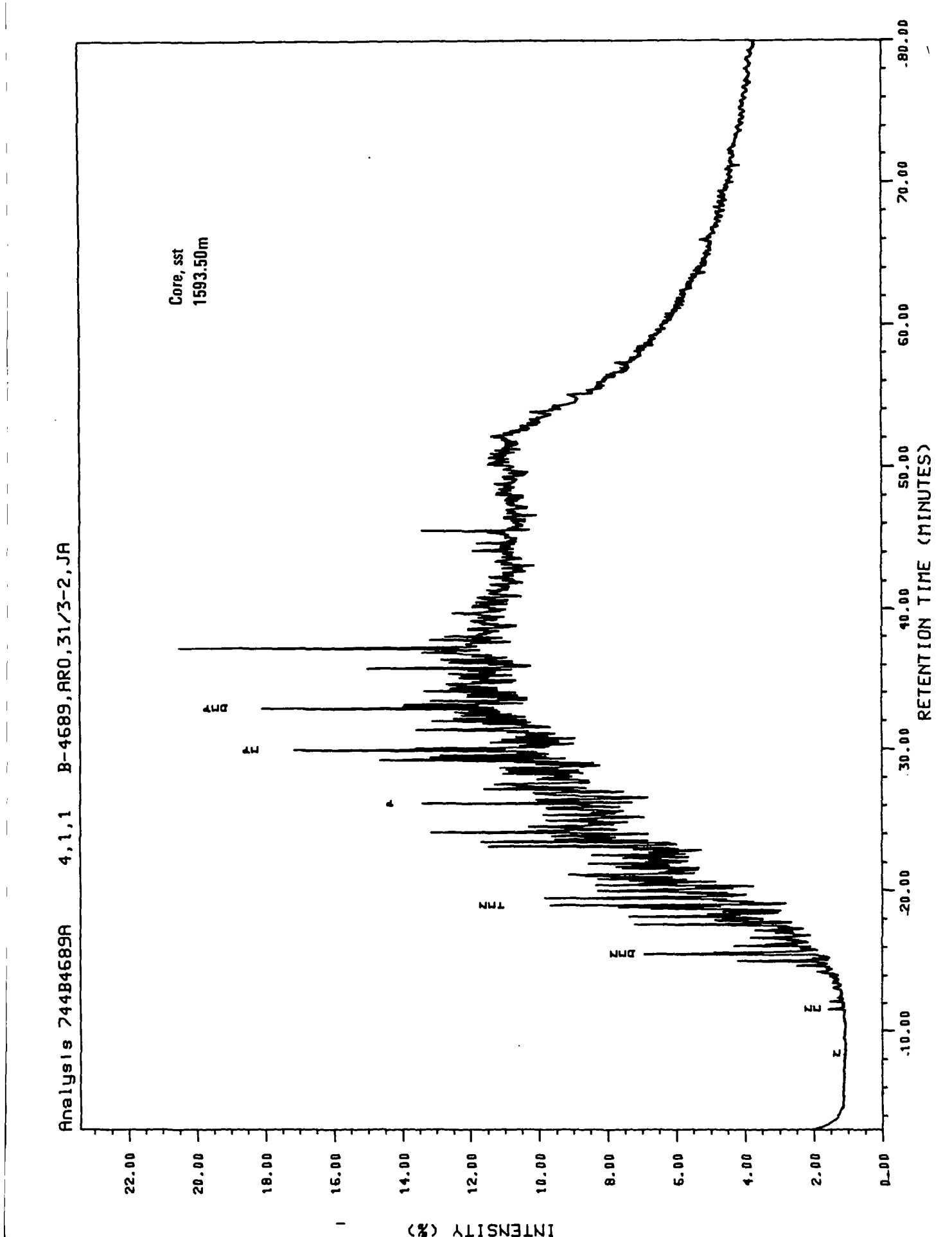

Analysis 244B4684 4,1,1 B-4684,AR0,LH,31/3-2
Core, sst
1573.95m
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
1.00
2.00
3.00
4.00
5.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00

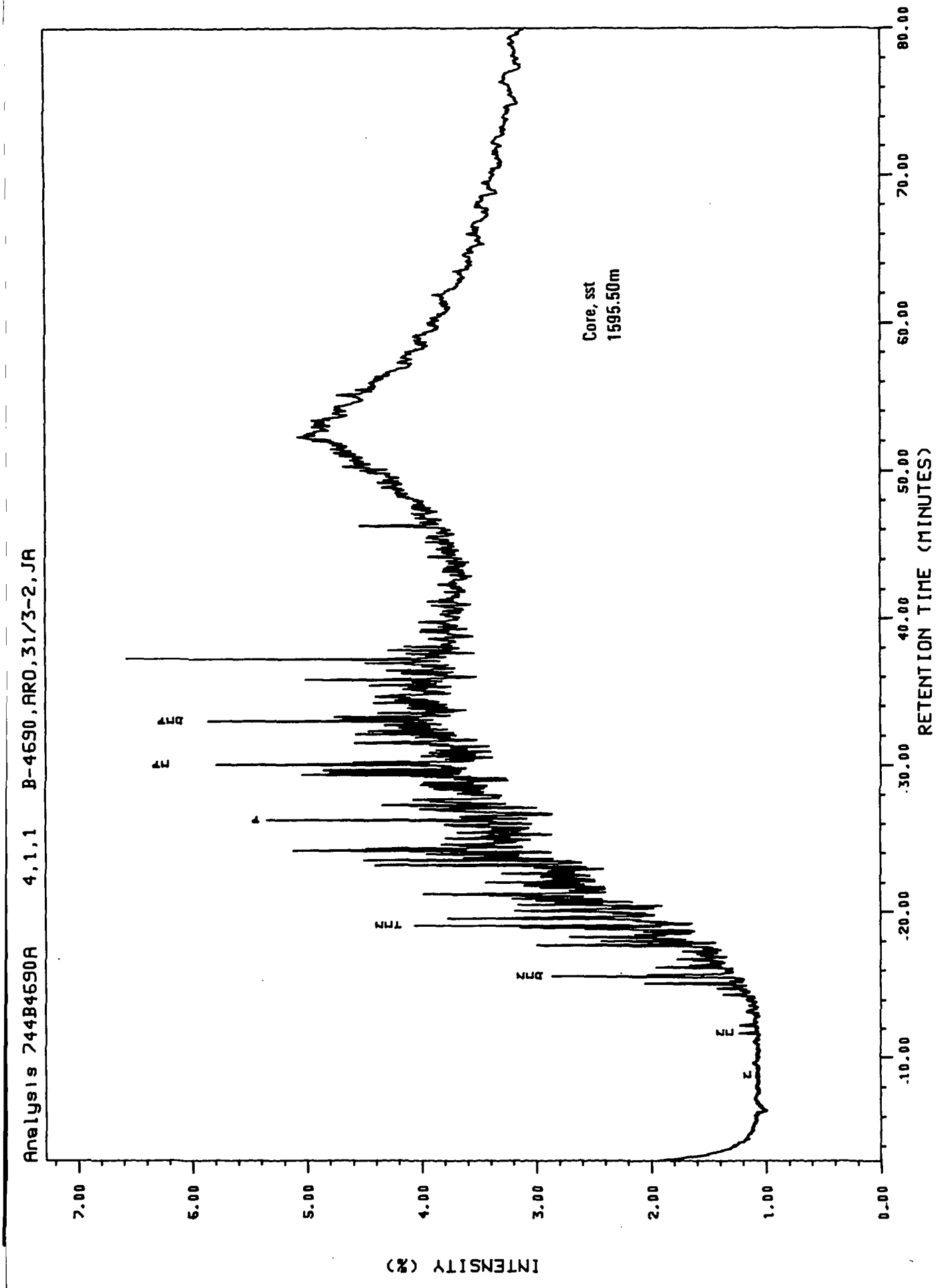

Analysis 744B4685 4,1,1 B-4685,ARO,31/3-2,JA
Core, sst
1581.65m
INTENSITY (%)
RETENTION TIME (MINUTES)
16.00
14.00
12.00
10.00
8.00
6.00
4.00
2.00
0.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00


Analysis 24B4686A 4,1,1 B-4686,ARO,31/3-2,JA
Core, sst
1586.40m
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
5.00
10.00
15.00
20.00
25.00
30.00
35.00
40.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00


Analysis 744B4687A 4,1,1 B-4687,ARO,31/3-2,JA
Core, sst
1587.50m
INTENSITY (%)
RETENTION TIME (MINUTES)
8.00
7.00
6.00
5.00
4.00
3.00
2.00
1.00
0.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00


Analysis 744B4688A 4,1,1 B-4688,ARO,31/3-2,JA
Core, sst
1590.50m
RETENTION TIME (MINUTES)
INTENSITY (%)
0.00
2.00
4.00
6.00
8.00
10.00
12.00
-10.00
-20.00
-30.00
40.00
50.00
60.00
70.00
80.00


Analysis 744B4689A 4,1,1 B-4689,ARO,31/3-2,JA
Core, sst
1593.50m
DMN
TMN
DMT
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
2.00
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
20.00
22.00
-10.00
-20.00
-30.00
-40.00
-50.00
-60.00
-70.00
-80.00


Analysis 244B4690A 4,1,1 B-4690,ARO,31/3-2,JA
Core, sst
1595.50m
INTENSITY (%)
RETENTION TIME (MINUTES)
0.00
1.00
2.00
3.00
4.00
5.00
6.00
7.00
10.00
20.00
30.00
40.00
50.00
60.00
70.00
80.00

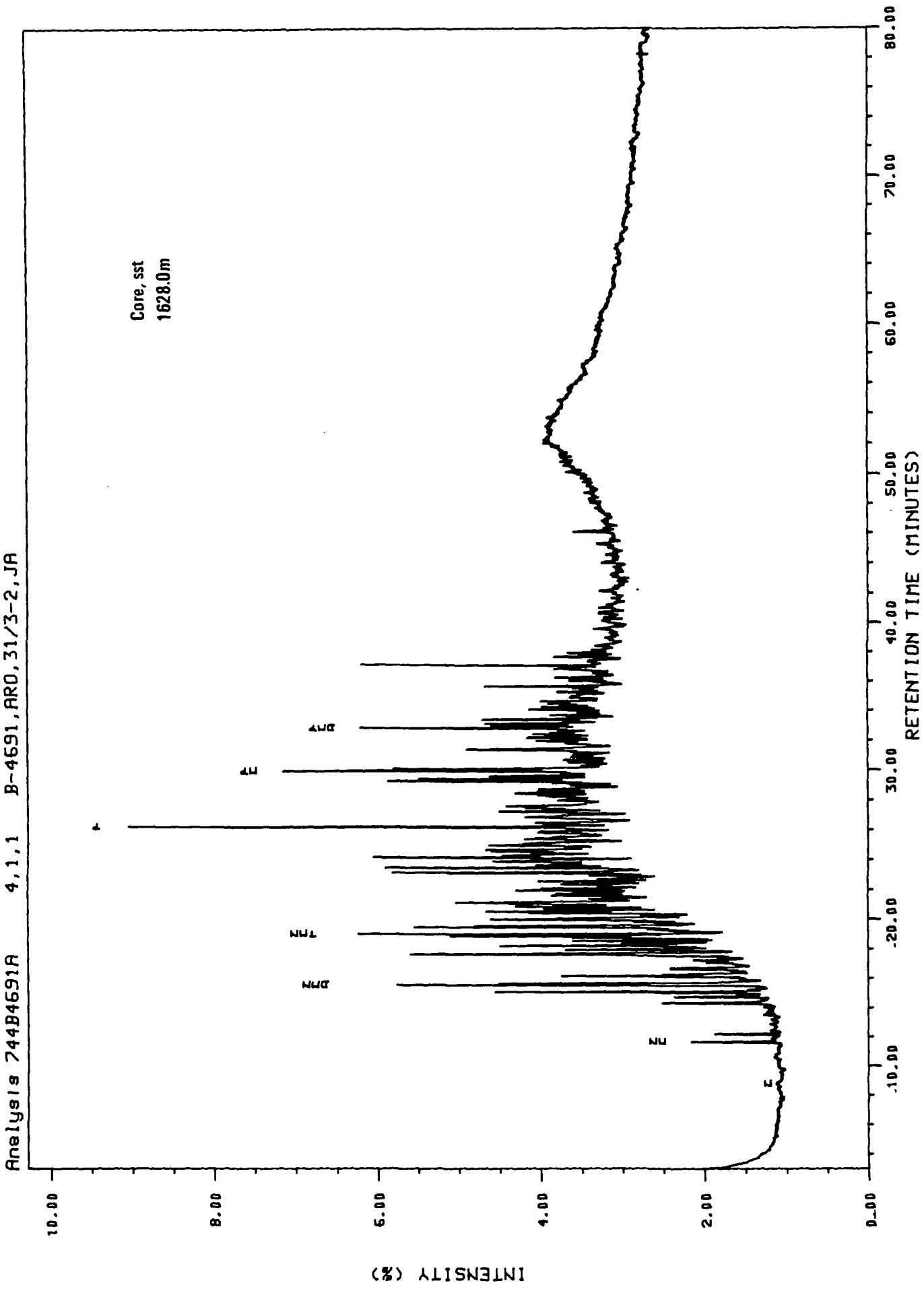
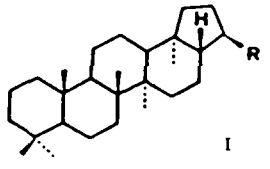

Analysis 244B4691A 4,1,1 B-4691,ARD,31/3-2,JA
Core, sst
1628.0m
INTENSITY (%)
RETENTION TIME (MINUTES)
10.00
8.00
6.00
4.00
2.00
0.00
-10.00
-20.00
30.00
40.00
50.00
60.00
70.00
80.00

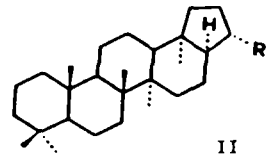
Figure 5

Mass chromatograms representing terpanes (m/z 191)

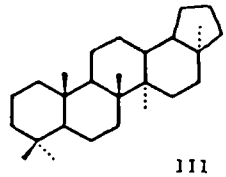
A	T_s, 18α(H)-trisnorneohopane	$C_{27}H_{46}$	(III)
B	T_m, 17α(H)-trisnorhopane	$C_{27}H_{46}$	(I,R=H)
C	17α(H)-norhopane	$C_{29}H_{50}$	(I,R=C_2H_5)
D	17β(H)-normoretane	$C_{29}H_{50}$	(II,R=C_2H_5)
E	17α(H)-hopane	$C_{30}H_{52}$	(I,R=C_3H_7)
F	17β(H)-moretane	$C_{30}H_{52}$	(II,R=C_3H_7)
G	17α(H)-homohopane (22S)	$C_{31}H_{54}$	(I,R=C_4H_9)
H	17α(H)-homohopane (22R)	$C_{31}H_{54}$	(I,R=C_4H_9)
	+ unknown triterpane (gammacerane?)		
I	17β(H)-homomoretane	$C_{31}H_{54}$	(II,R=C_4H_9)
J	17α(H)-bishomohopane (22S,22R)	$C_{32}H_{56}$	(I,R=C_5H_{11})
K	17α(H)-trishomohopane (22S,22R)	$C_{33}H_{58}$	(I,R=C_6H_{13})
L	17α(H)-tetrakishomohopane (22S,22R)	$C_{34}H_{60}$	(I,R,=C_7H_{15})
M	17α(H)-pentakishomohopane (22S,22R)	$C_{35}H_{62}$	(I,R=C_8H_{17})
Z	bisnorhopane	$C_{28}H_{48}$	
X	unknown triterpane	$C_{30}H_{52}$	
P	tricyclic terpane	$C_{23}H_{42}$	(IV,R=C_4H_9)
Q	tricyclic terpane	$C_{24}H_{44}$	(IV,R=C_5H_{11})
R	tricyclic terpane (17R,17S)	$C_{25}H_{46}$	(IV,R=C_6H_{13})
S	tetracyclic terpane	$C_{24}H_{42}$	(V)
T	tricyclic terpane (17R,17S)	$C_{26}H_{48}$	(IV,R=C_7H_{15})



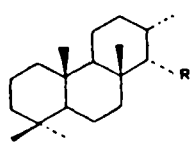
I

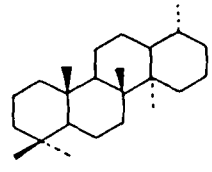


II

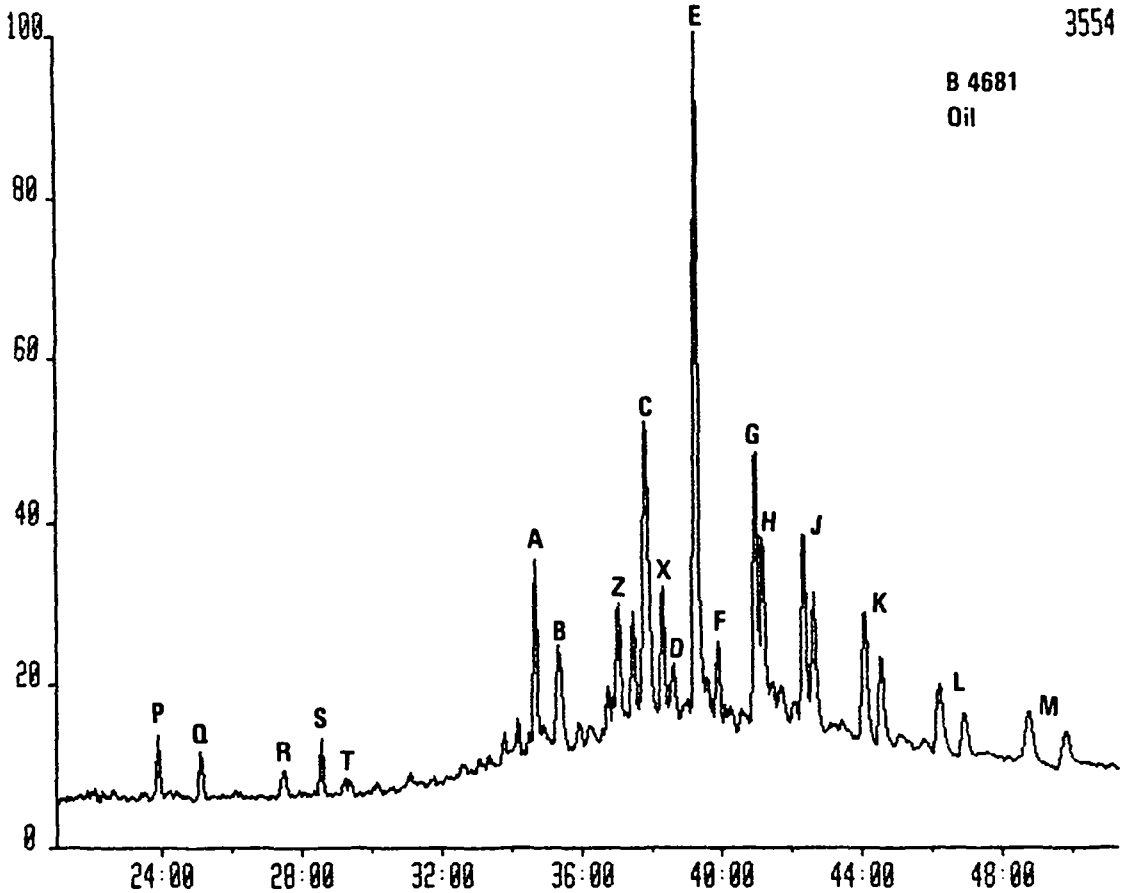


III

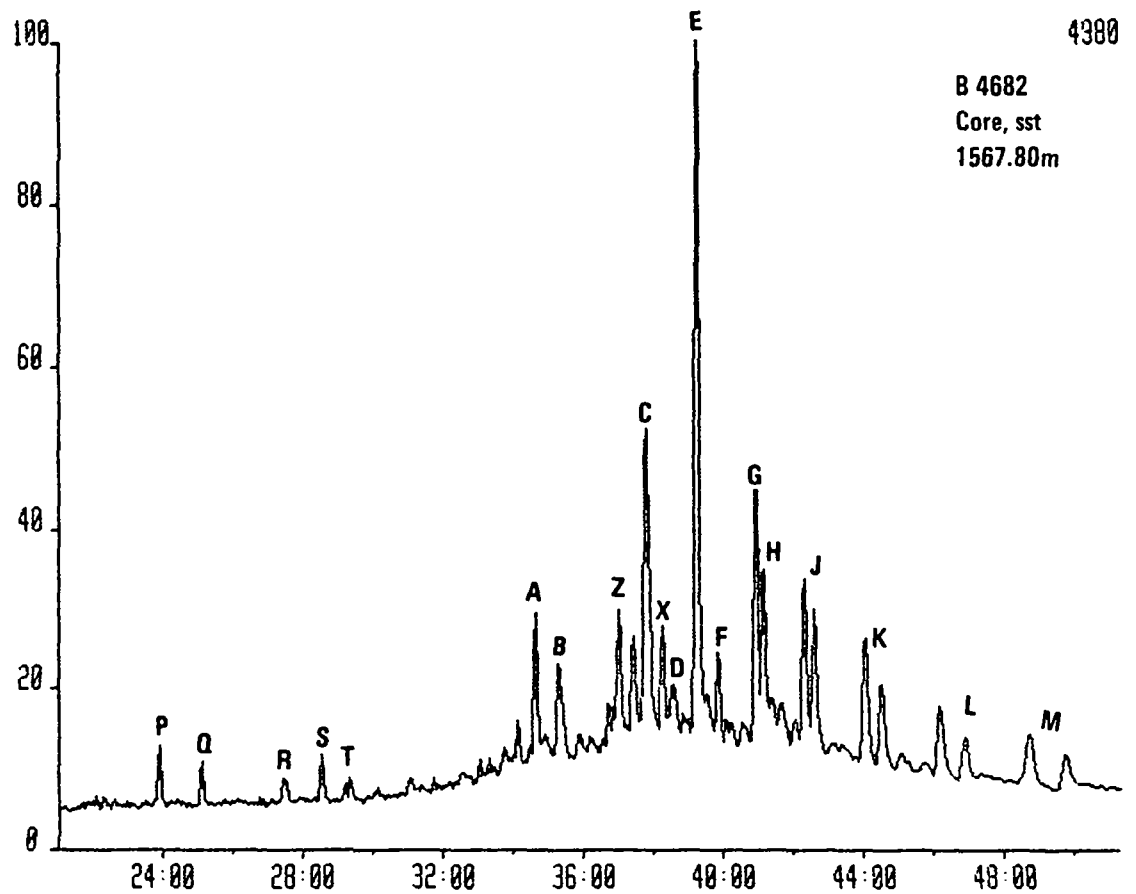




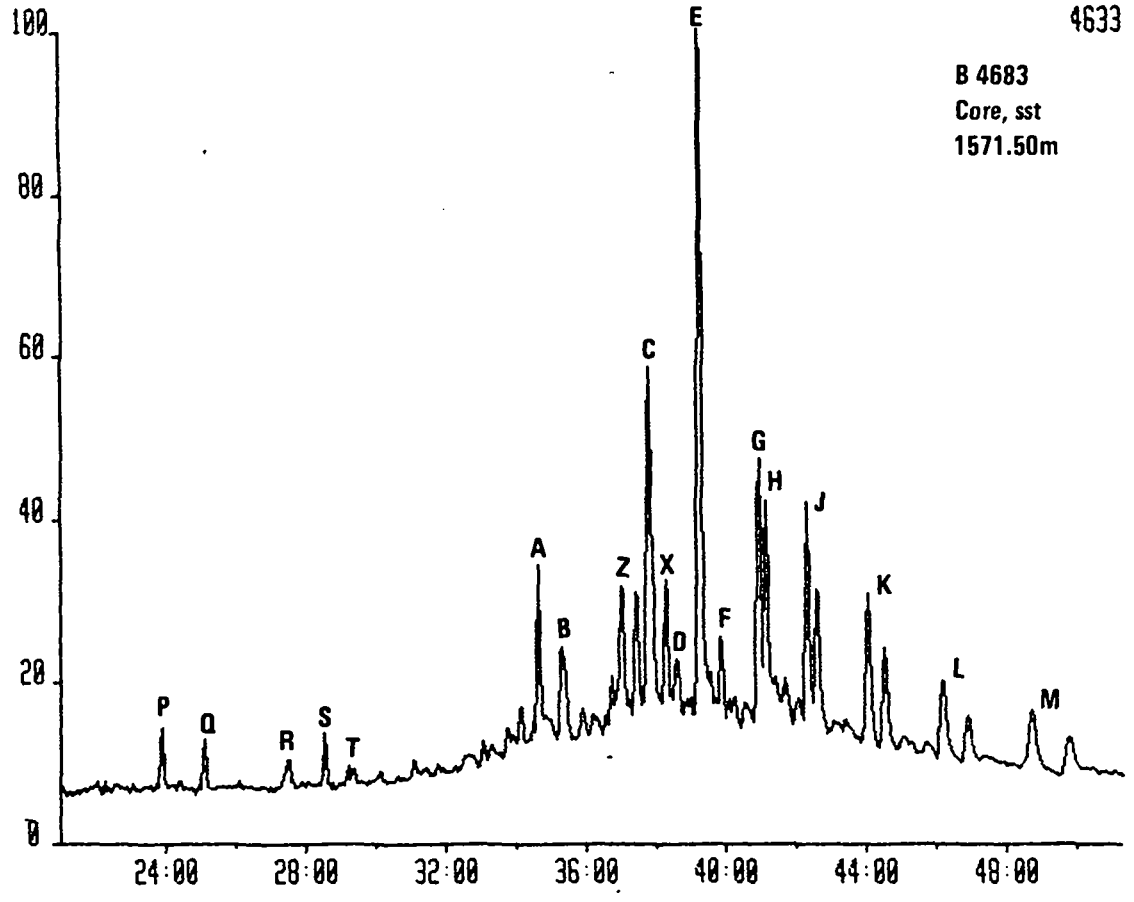
IKU



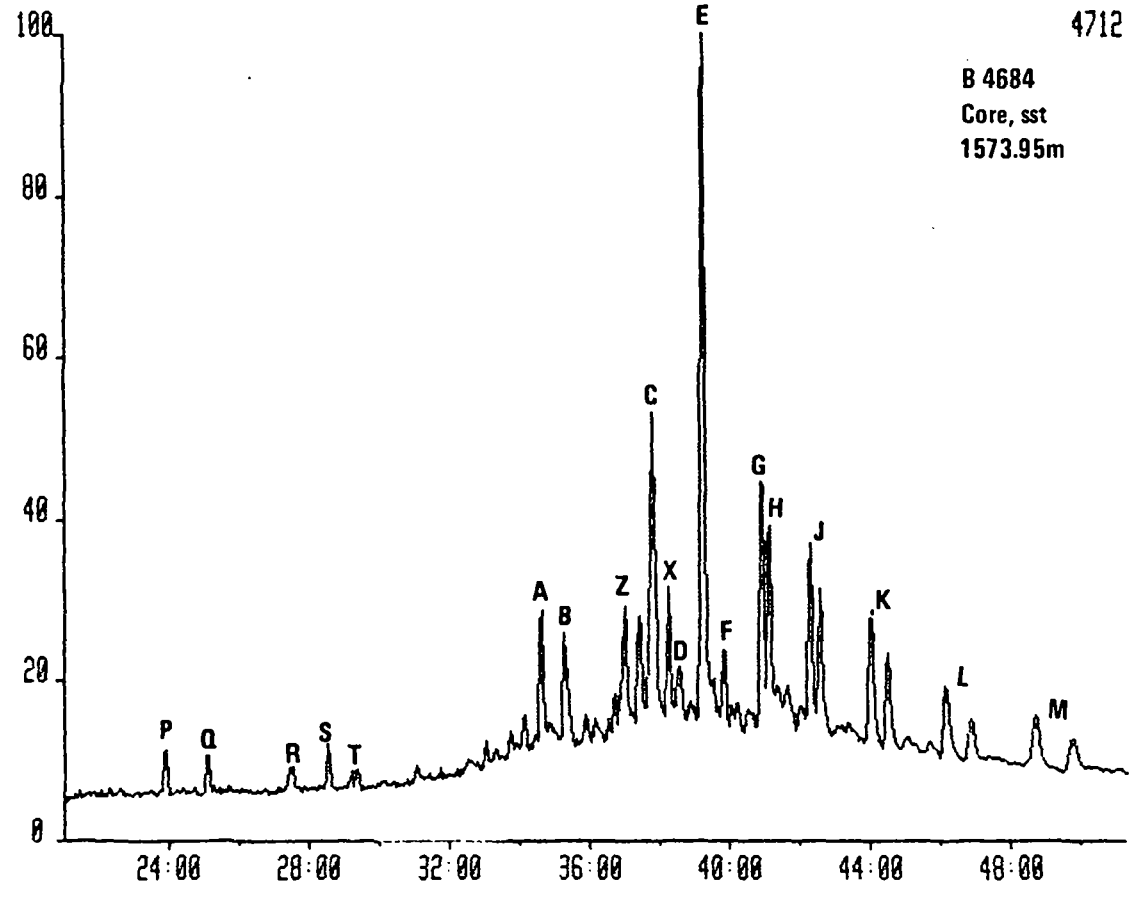
744TROL1 191.1000 G1 I1 S2



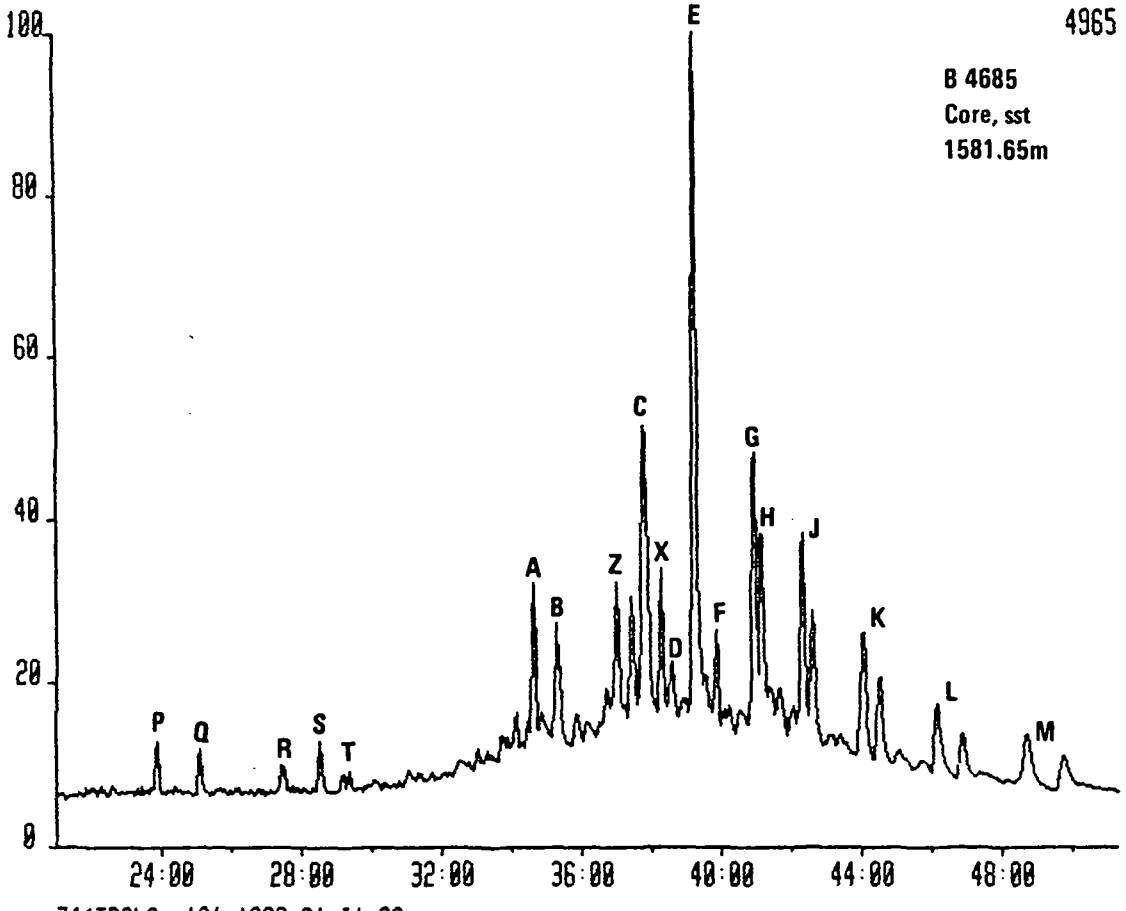
IKU



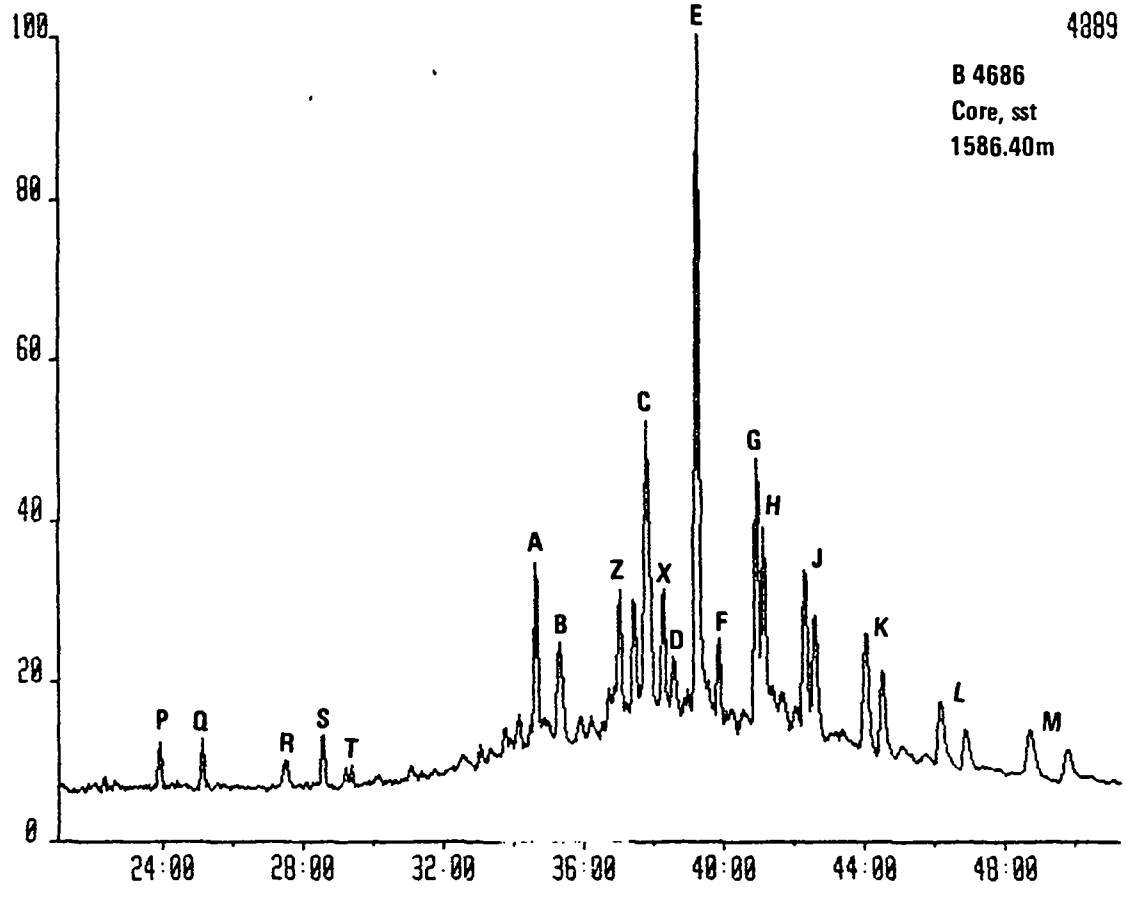
744TROL1 191.1000 G1 I1 S4



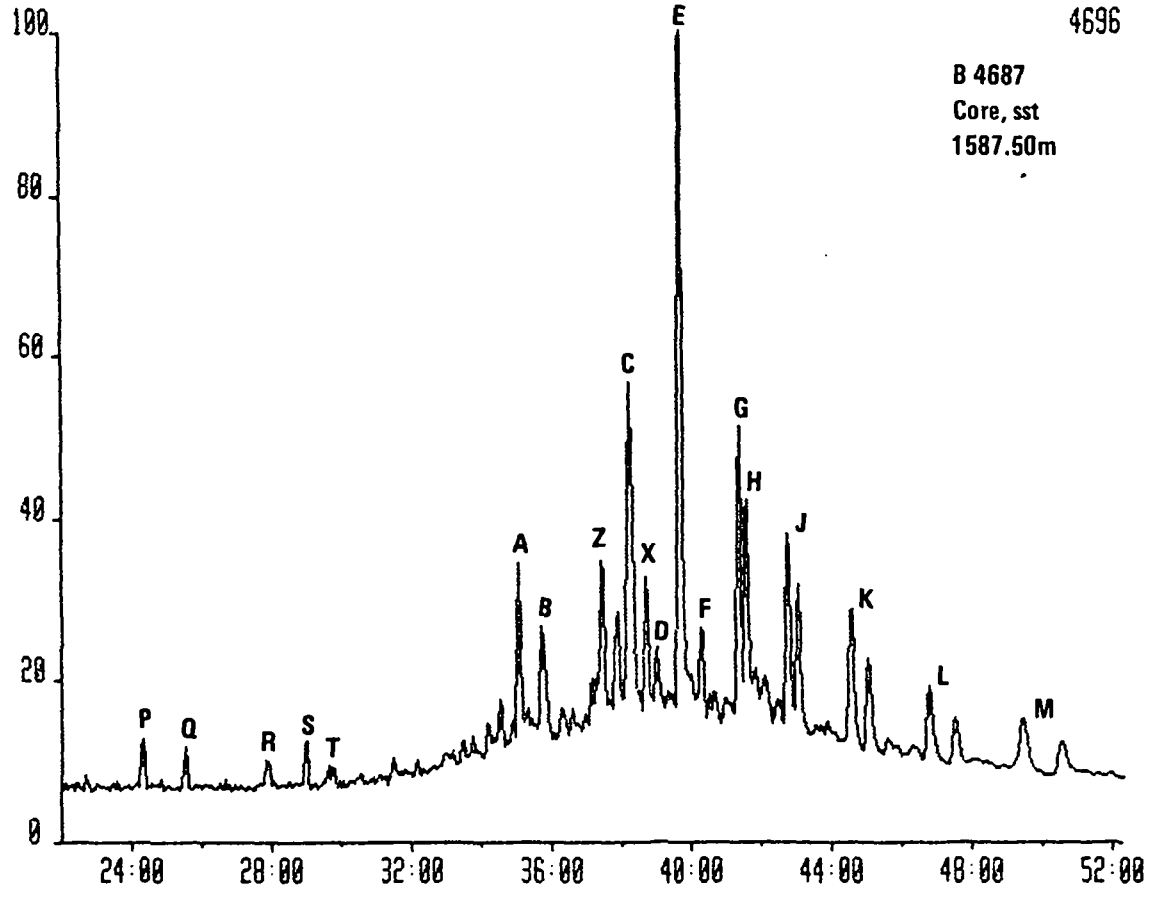
IKU



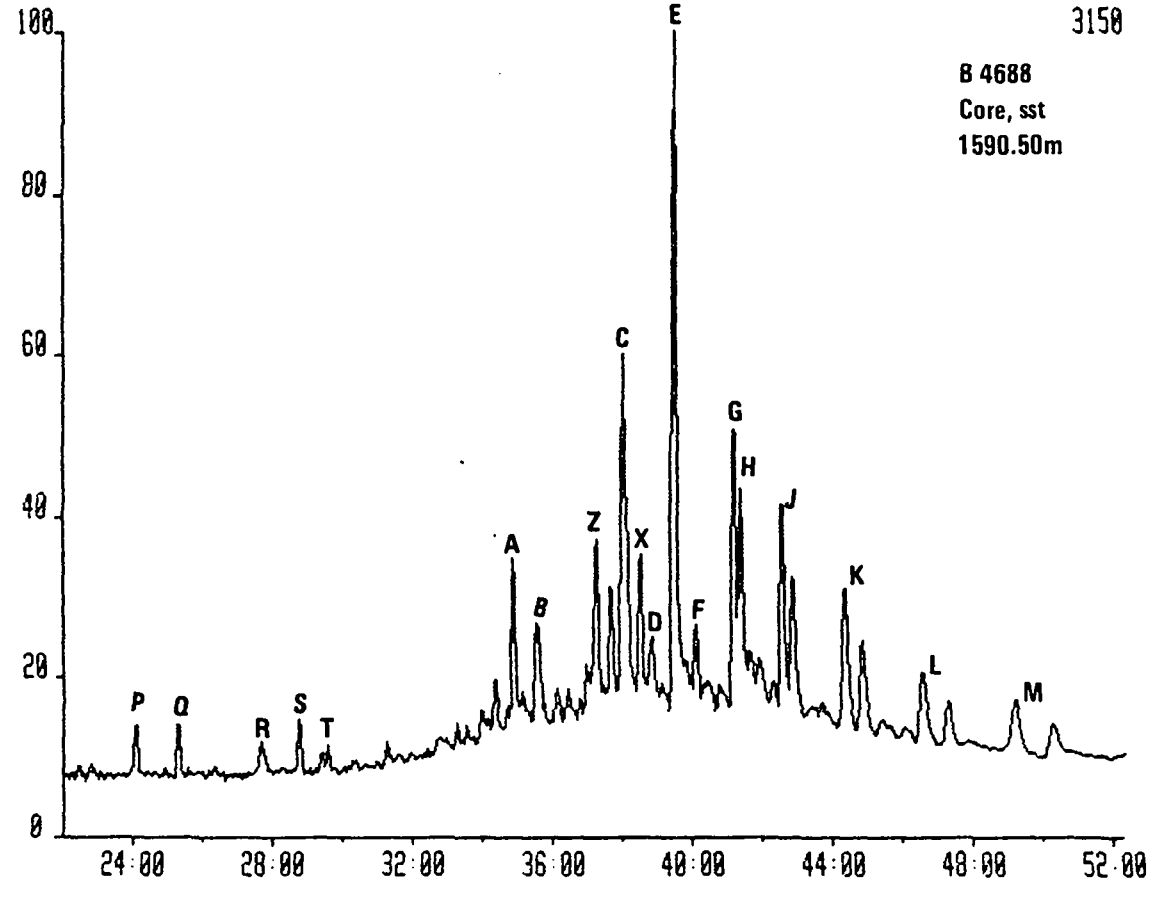
744TROL2 191.1000 G1 I1 S2



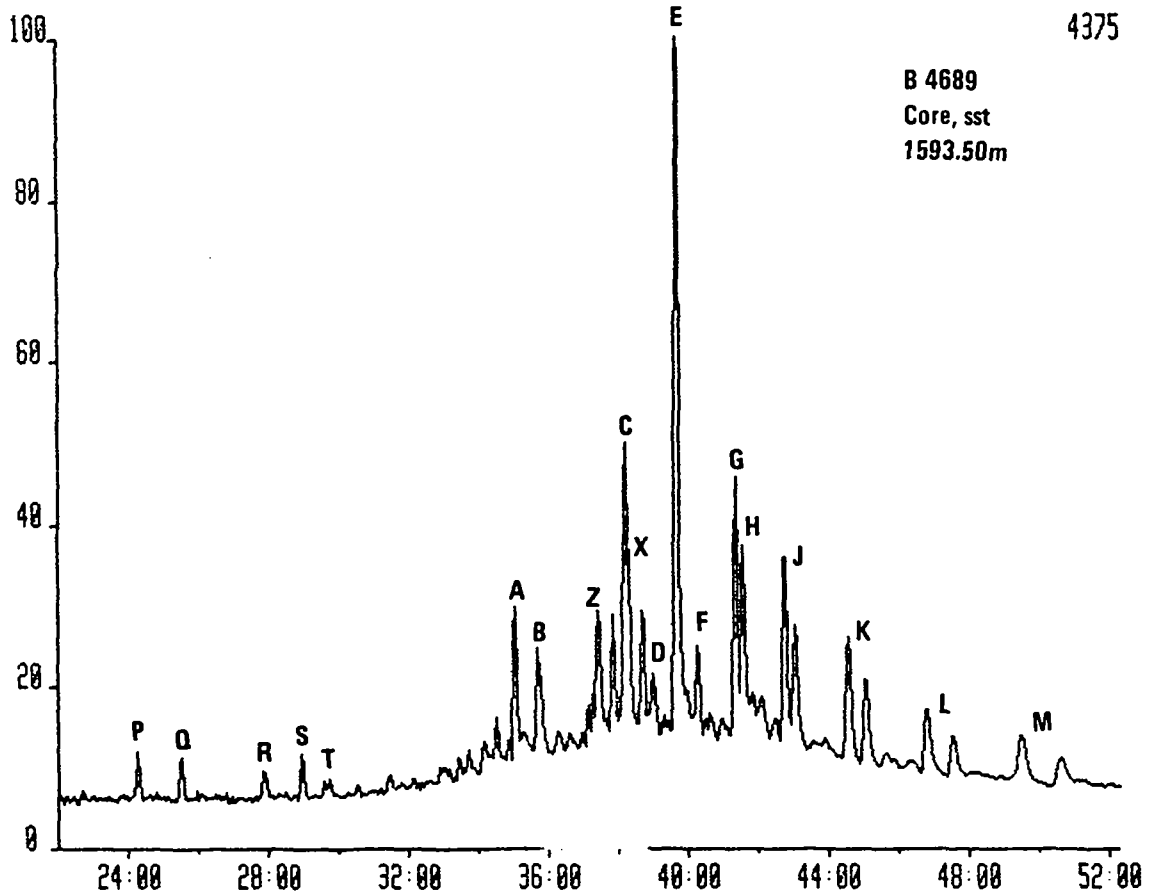
IKU



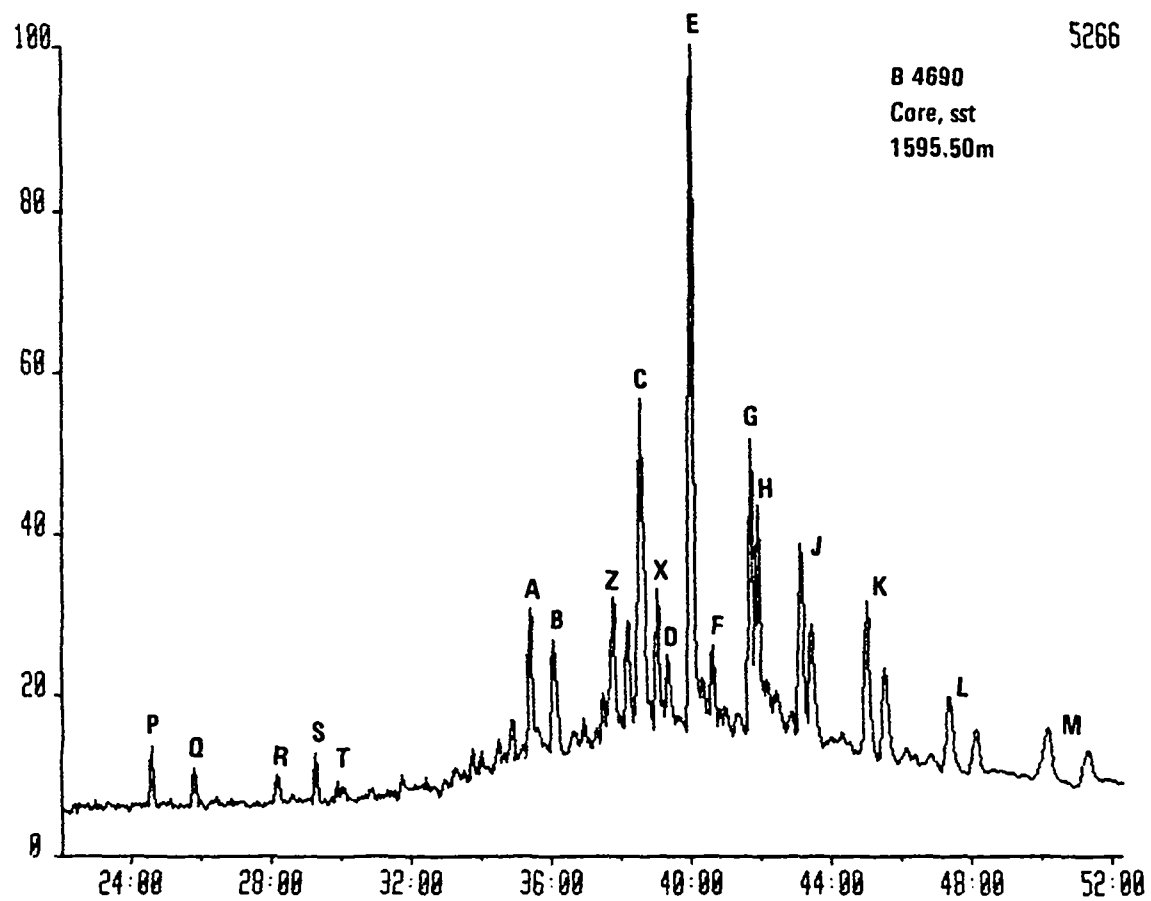
744TROL3 191.1000 G1 I1 S2



IKU



744TROL3 191.1000 G1 I1 S4



IKU

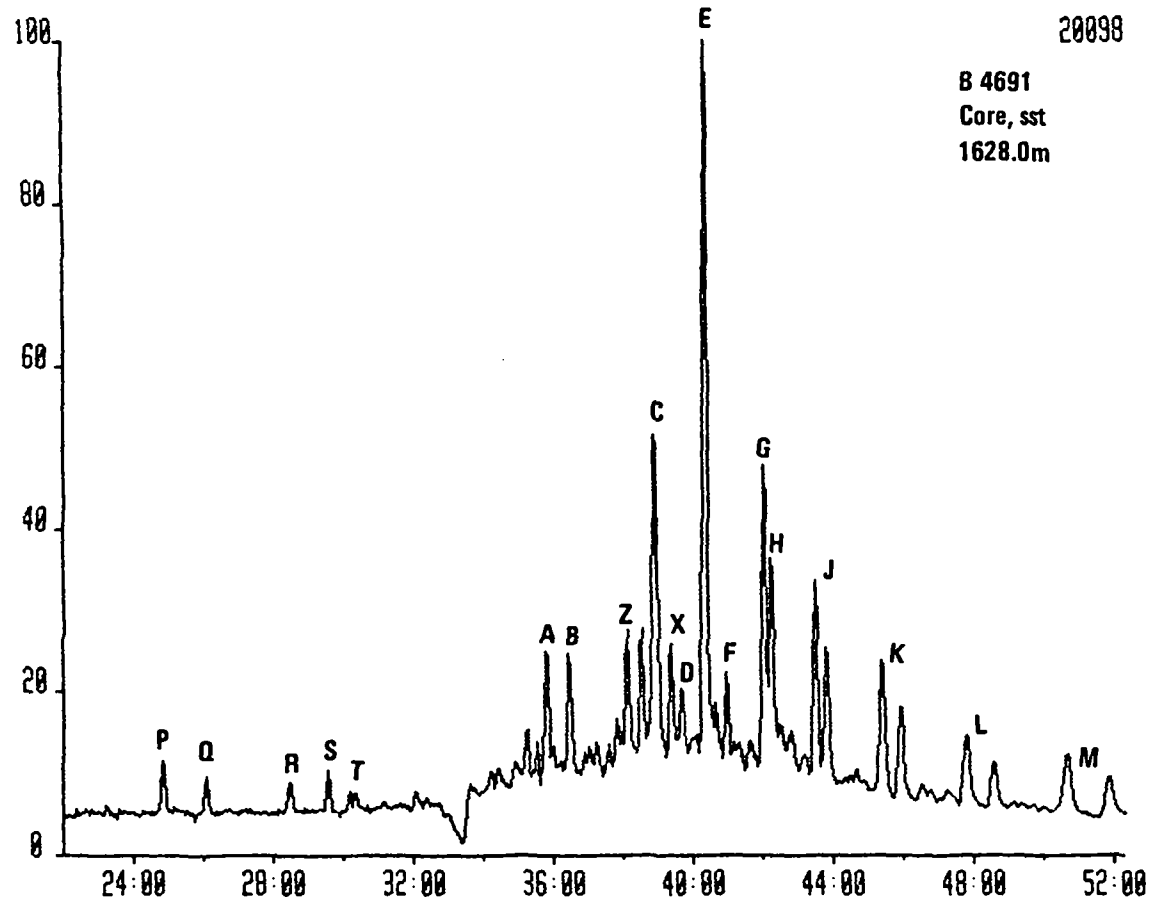
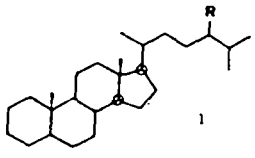

100
80
60
40
20
0
20098
B 4691
Core, sst
1628.0m
P
Q
R
S
T
A
B
Z
C
X
D
E
F
G
H
J
K
L
M
24:00
28:00
32:00
36:00
40:00
44:00
48:00
52:00

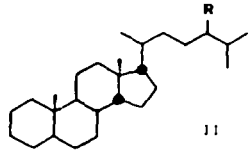
Figure 5

Mass chromatograms representing steranes (m/z 217 and 218)

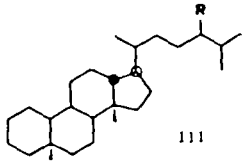
a	13β(H),17α(H)-diasterane (20S)	$C_{27}H_{48}$	(III,R=H)
b	13β(H),17α(H)-diasterane (20R)	$C_{27}H_{48}$	(III,R=H)
c	13α(H),17β(H)-diasterane (20S)	$C_{27}H_{48}$	(IV,R=H)
d	13α(H),17β(H)-diasterane (20R)	$C_{27}H_{48}$	(IV,R=H)
e	13β(H),17α(H)-diasterane (20S)	$C_{28}H_{50}$	(III,R=CH_3)
f	13β(H),17α(H)-diasterane (20R)	$C_{28}H_{50}$	(III,R=CH_3)
g	13α(H),17β(H)-diasterane (20S)	$C_{28}H_{50}$	(IV,R=CH_3)
	+ 14α(H),17α(H)-sterane (20S)	$C_{27}H_{48}$	(I,R=H)
h	13β(H),17α(H)-diasterane (20S)	$C_{29}H_{52}$	(III,R=C_2H_5)
	+ 14β(H),17β(H)-sterane (20R)	$C_{27}H_{48}$	(II,R=H)
i	14β(H),17β(H)-sterane (20S)	$C_{27}H_{48}$	(II,R=H)
	+ 13α(H),17β(H)-diasterane (20R)	$C_{28}H_{50}$	(IV,R=CH_3)
j	14α(H),17α(H)-sterane (20R)	$C_{27}H_{48}$	(I,R=H)
k	13β(H),17α(H)-diasterane (20R)	$C_{29}H_{52}$	(III,R=C_2H_5)
l	13α(H),17β(H)-diasterane (20S)	$C_{29}H_{52}$	(III,R=C_2H_5)
m	14α(H),17α(H)-sterane (20S)	$C_{28}H_{50}$	(I,R=CH_3)
n	13α(H),17β(H)-diasterane (20R)	$C_{29}H_{52}$	(III,R=C_2H_5)
	+ 14β (H),17β (H)-sterane (20R)	$C_{28}H_{50}$	(II,R=CH_3)
o	14β(H),17β(H)-sterane (20S)	$C_{28}H_{50}$	(II,R=CH_3)
p	14α(H),17α(H)-sterane (20R)	$C_{28}H_{50}$	(I,R=CH_3)
q	14α(H),17α(H)-sterane (20S)	$C_{29}H_{52}$	(I,R=C_2H_5)
r	14β(H),17β(H)-sterane (20R)	$C_{29}H_{52}$	(II,R=C_2H_5)
	+ unknown sterane		
s	14β(H),17β(H)-sterane (20S)	$C_{29}H_{52}$	(II,R=C_2H_5)
t	14β(H),17β(H)-sterane (20R)	$C_{29}H_{52}$	(I,R=C_2H_5)
u	5α(H)-sterane	$C_{21}H_{36}$	(V,R=C_2H_5)
v	5α(H)-sterane	$C_{22}H_{38}$	(IV,R=C_3H_7)



I



II



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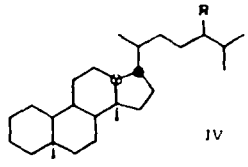

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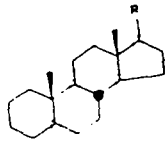

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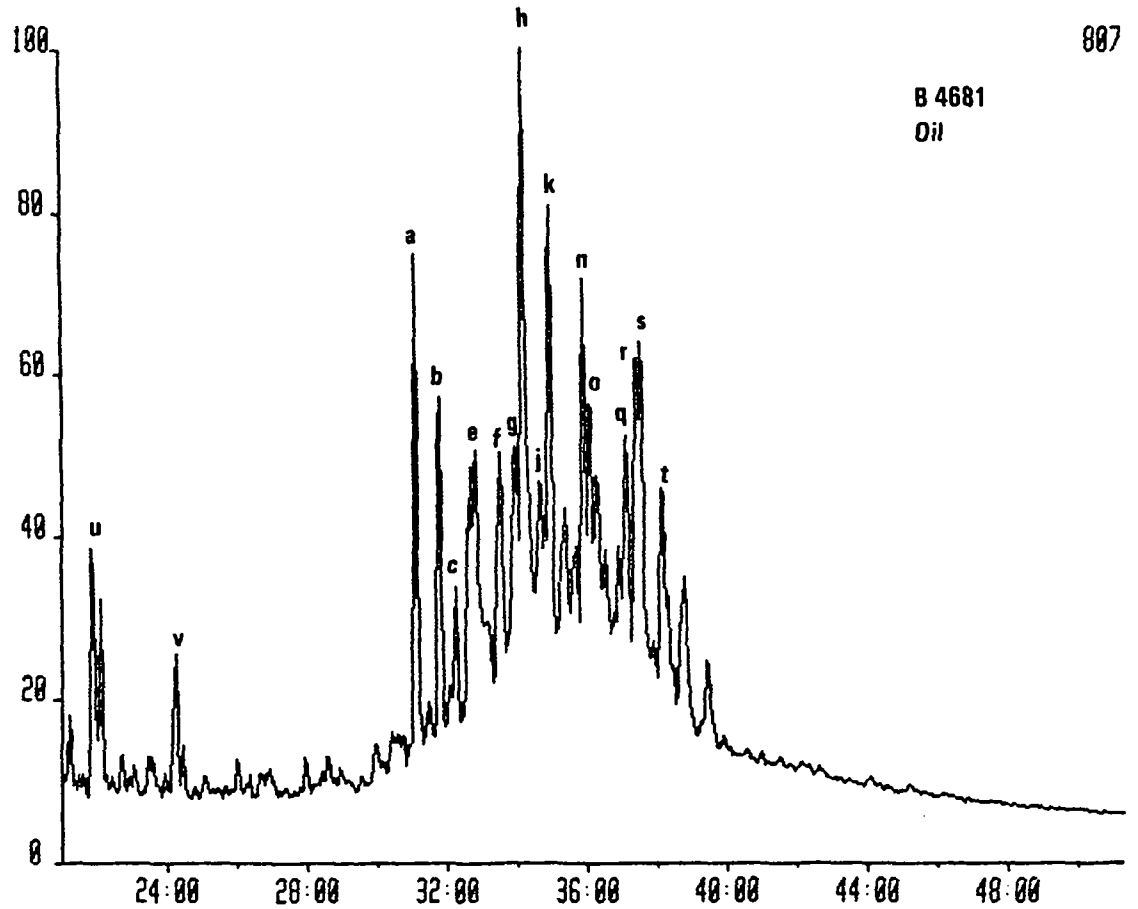
807
B 4681
Oil
100
80
60
40
20
0
24:00
28:00
32:00
36:00
40:00
44:00
48:00
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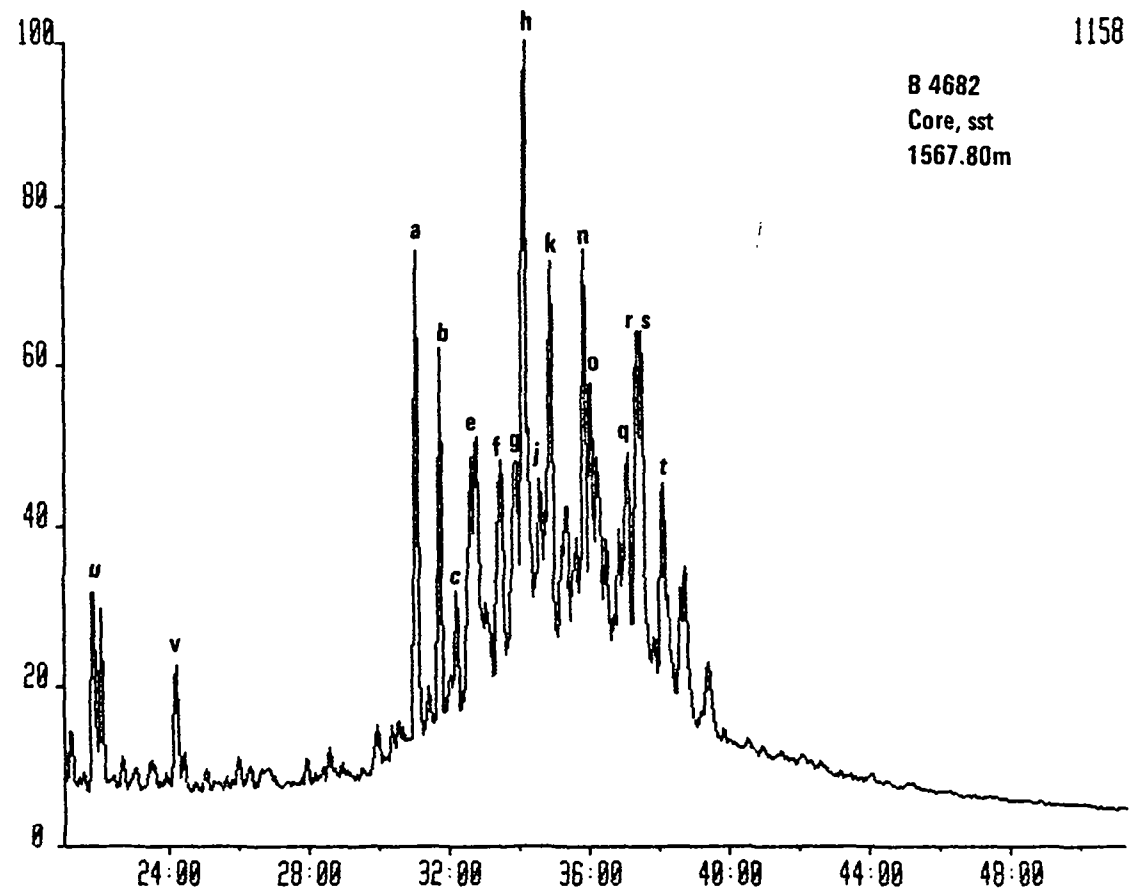
b
c
e
f
g
h
i
k
n
o
q
r
s
t
u
v


1158
B 4682
Core, sst
1567.80m
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80
60
40
20
0
24:00
28:00
32:00
36:00
40:00
44:00
48:00
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f
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j
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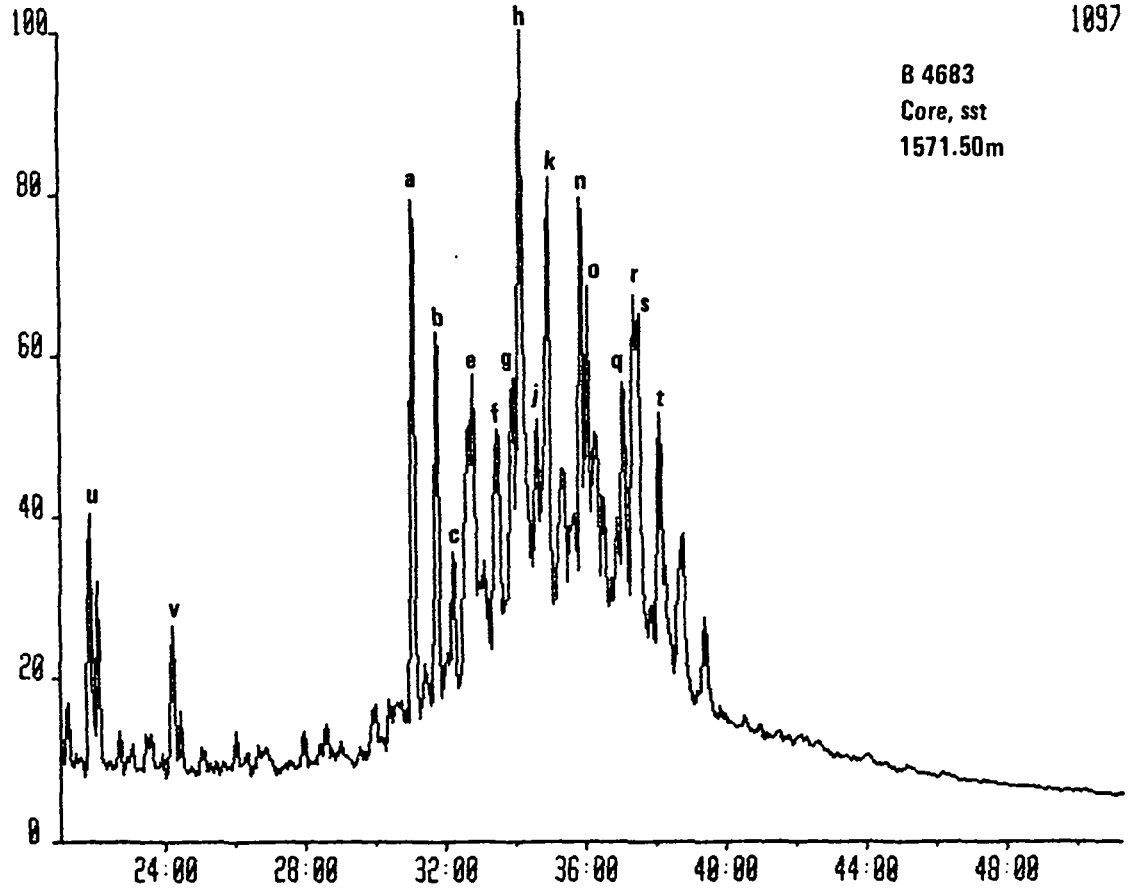
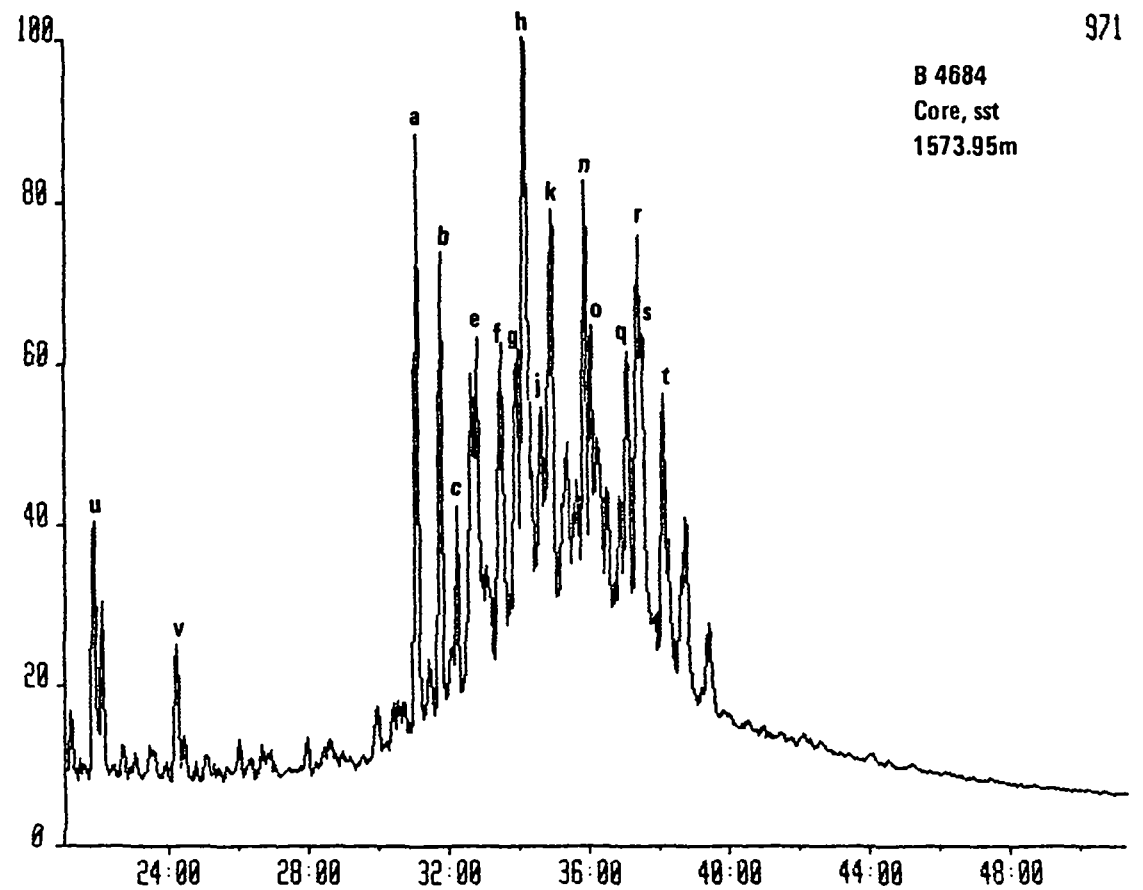
o
q
r
s
t
u
v

IKU



744TROL1 217.1000 G1 I1 S4



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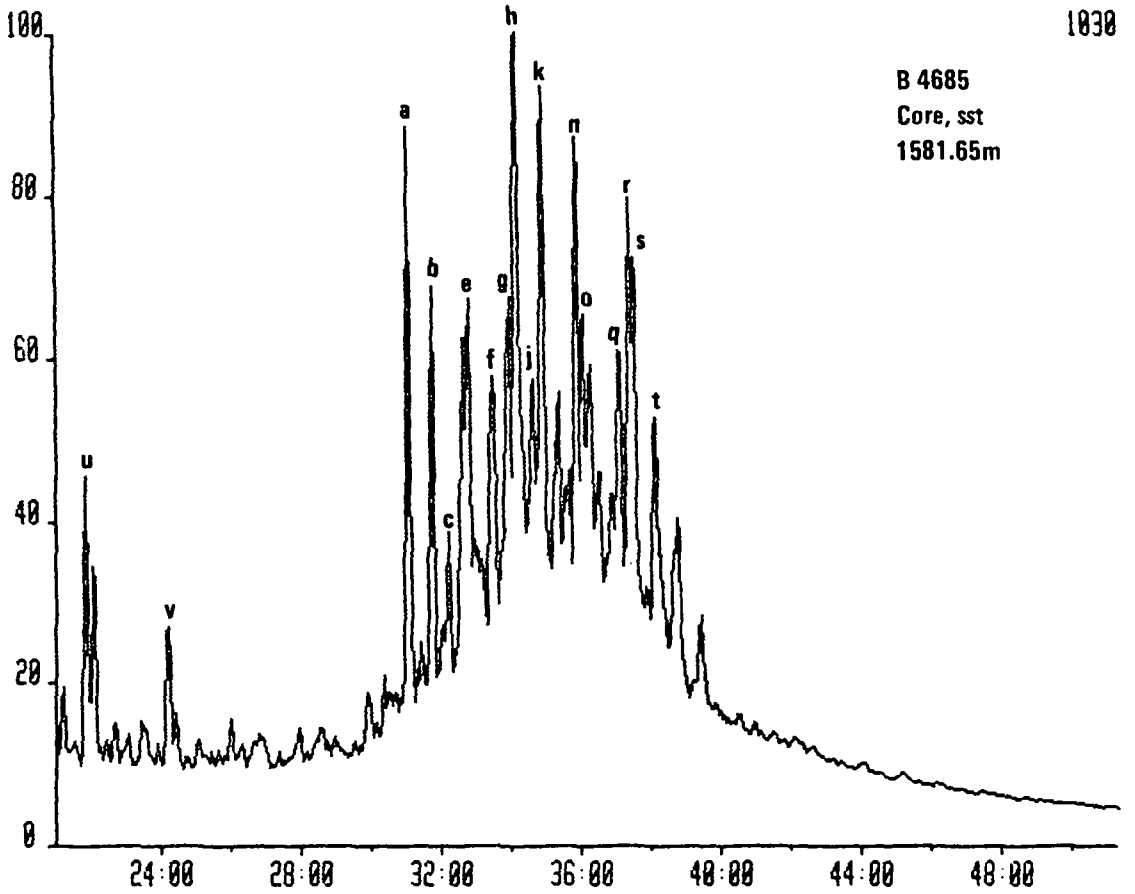
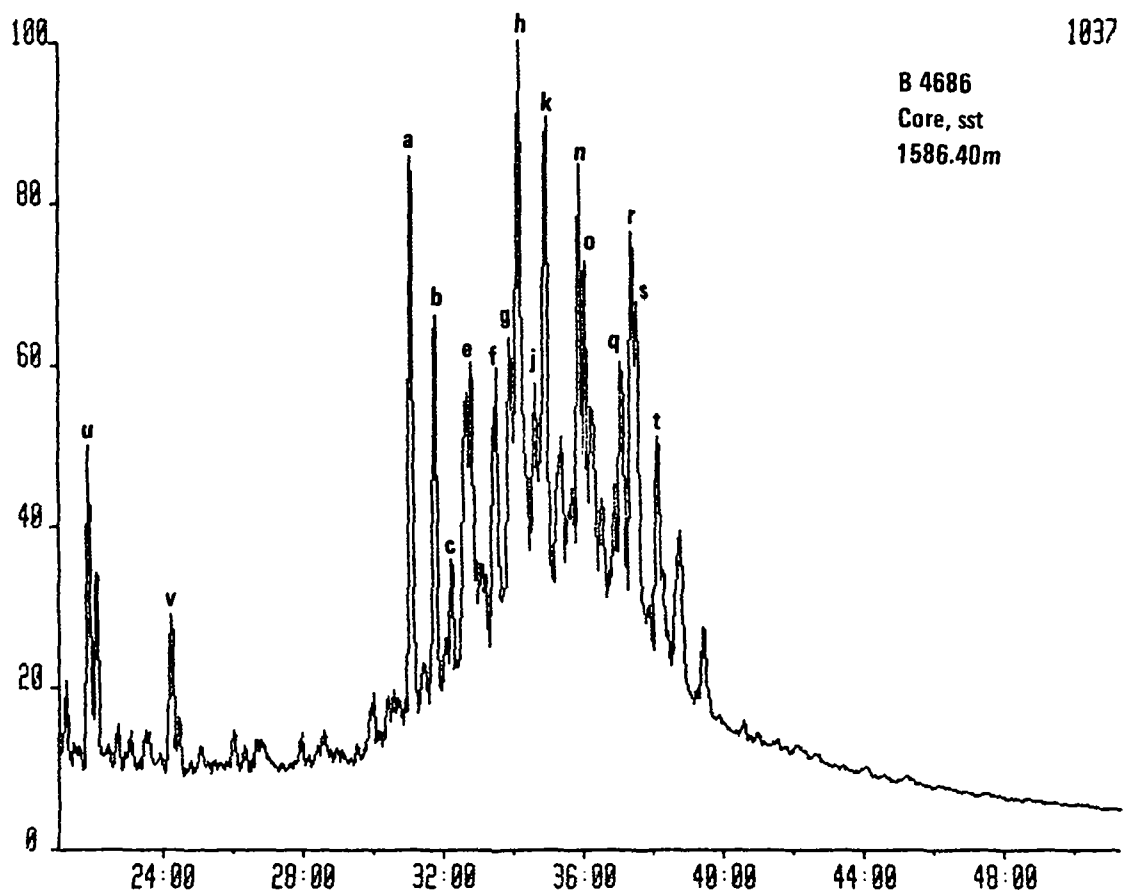
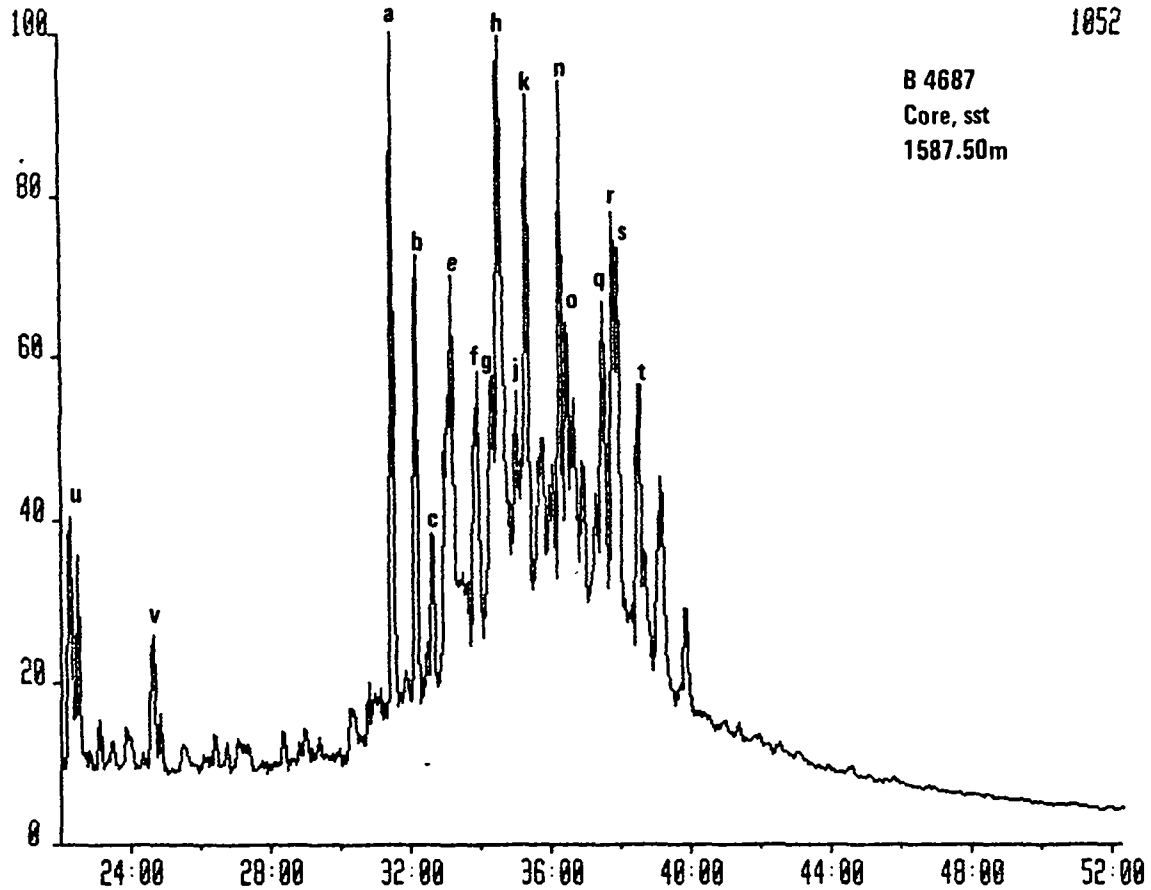


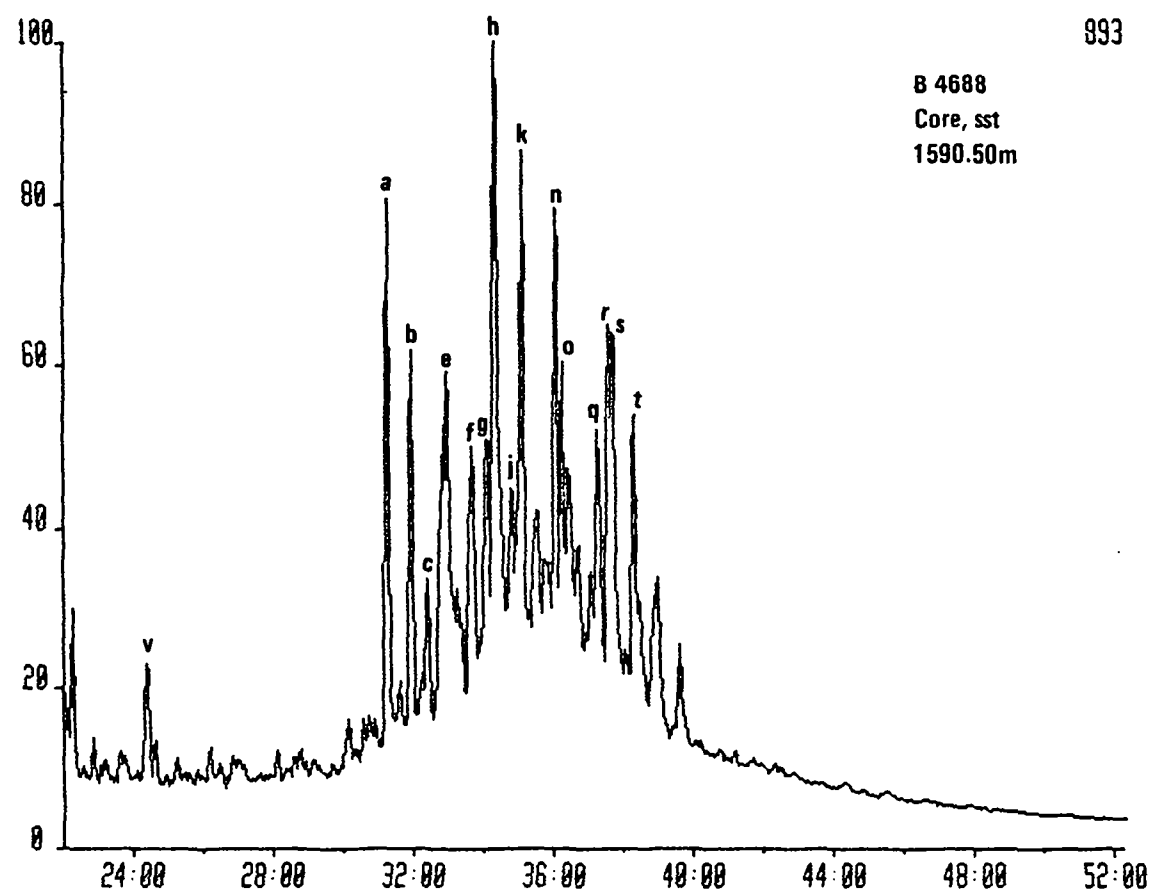
744TROL2 217.1000 G1 I1 S2



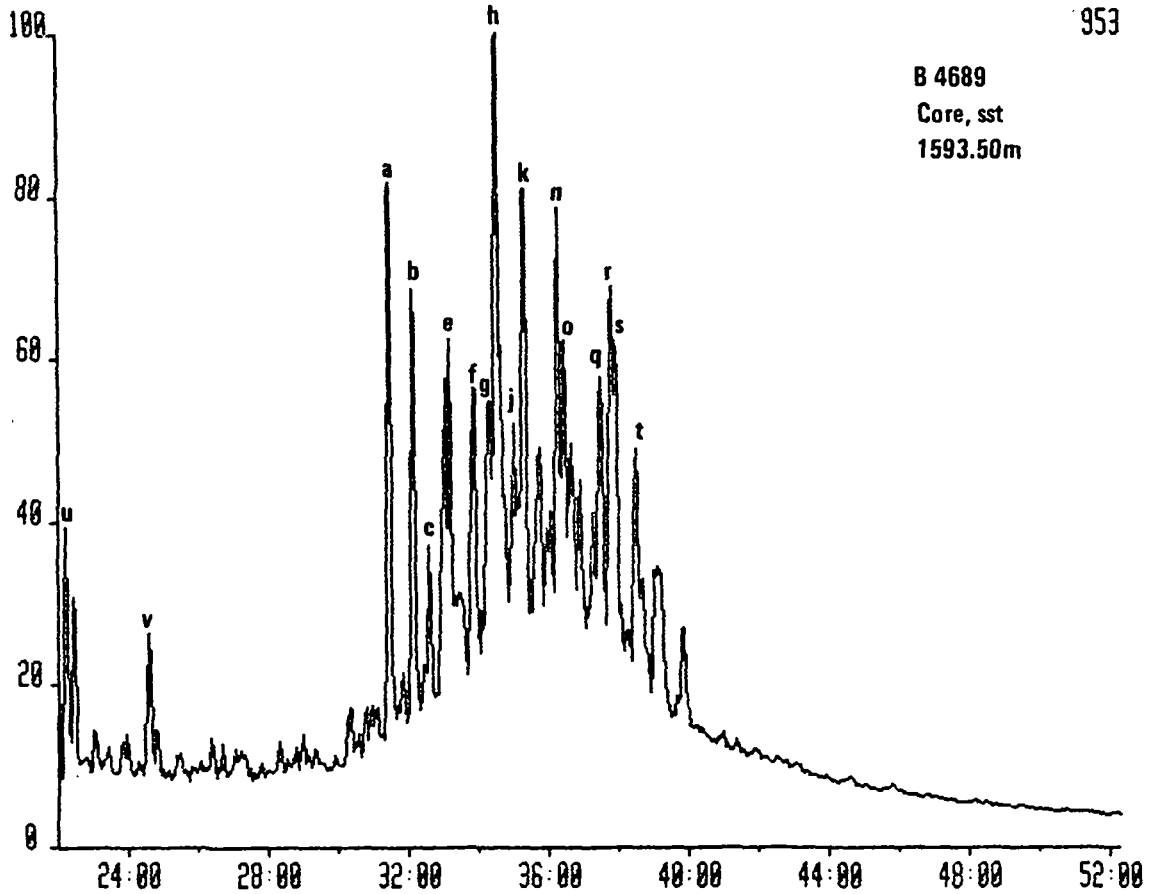
IKU



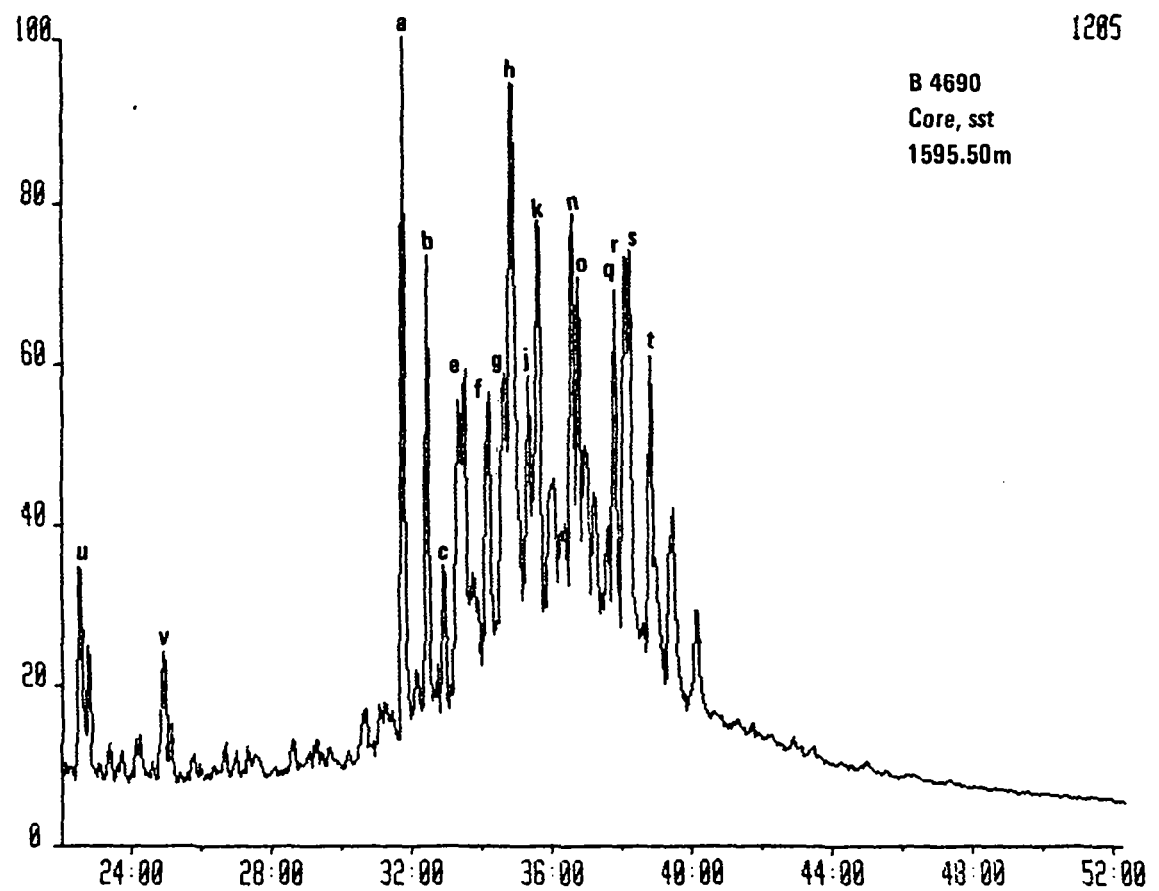
744TROL3 217.1000 G1 I1 S2



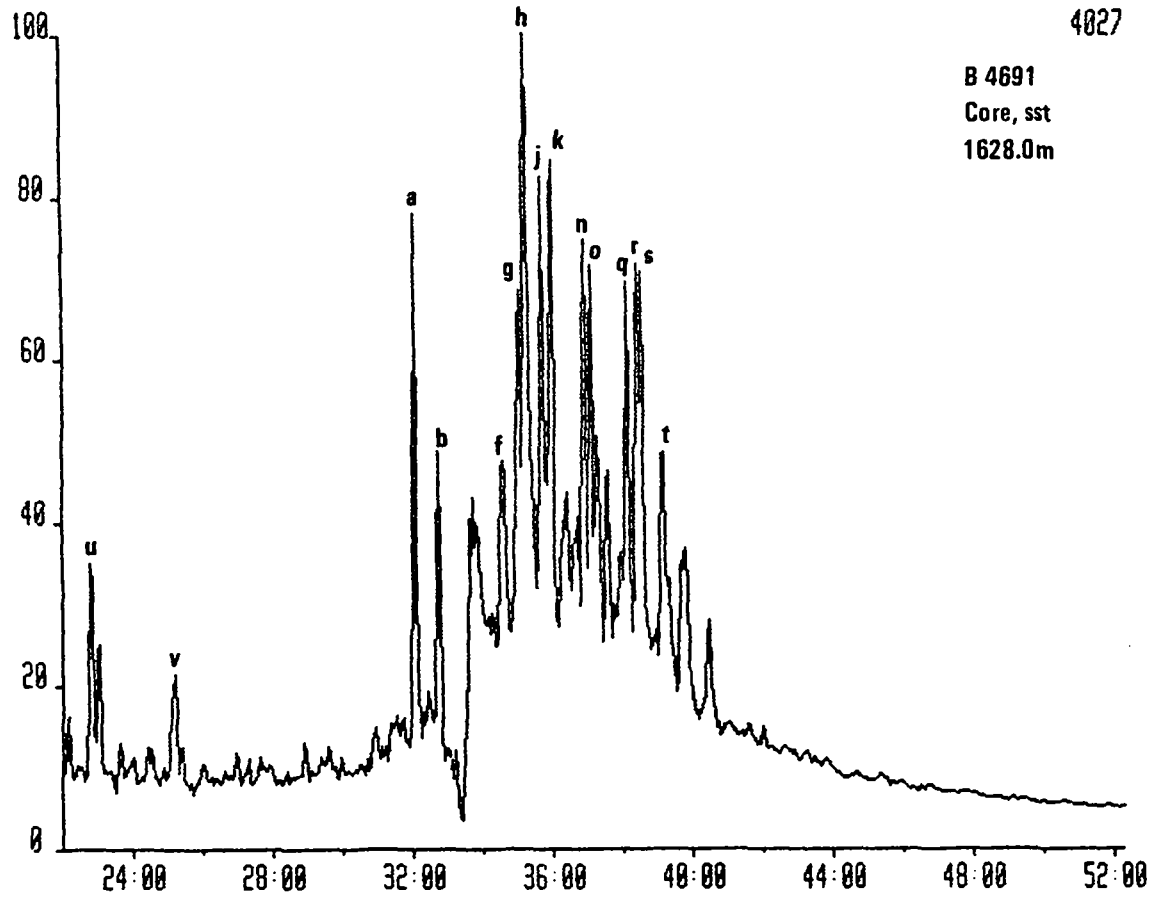
IKU



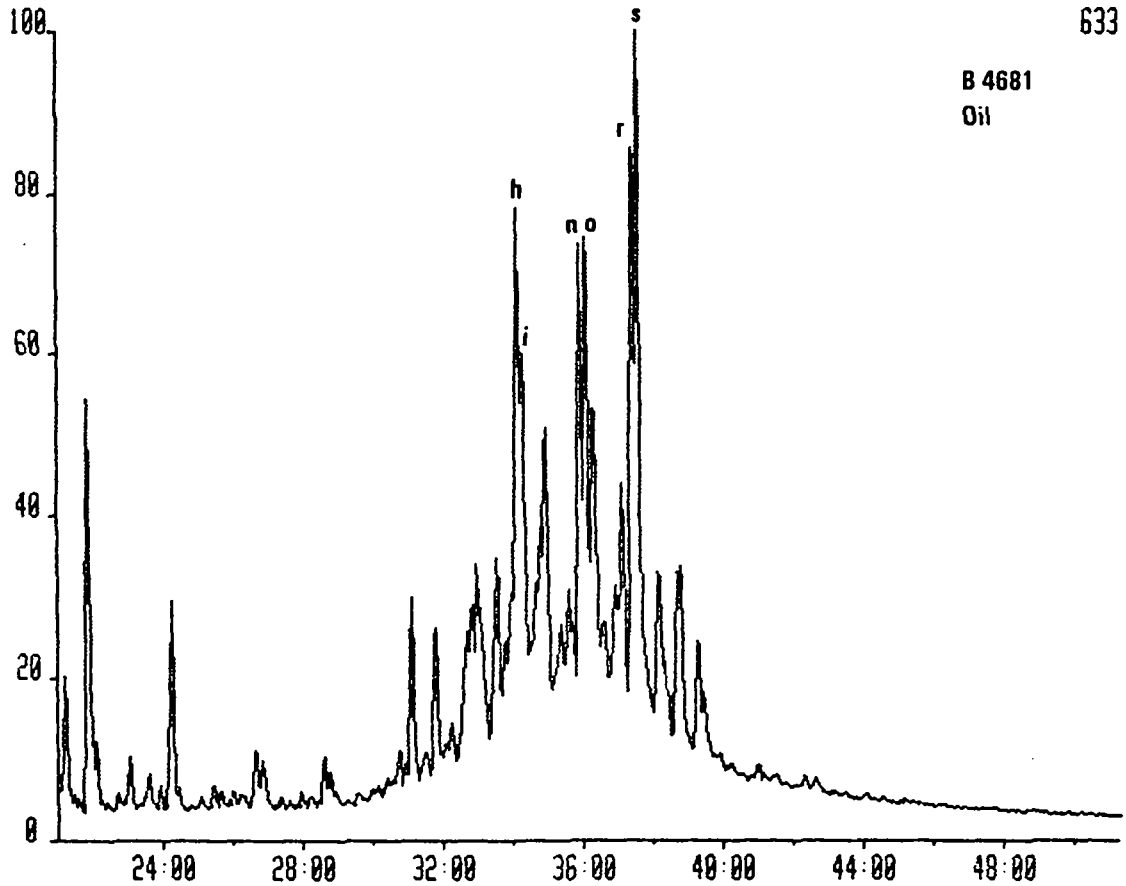
744TROL3 217.1000 G1 I1 S4



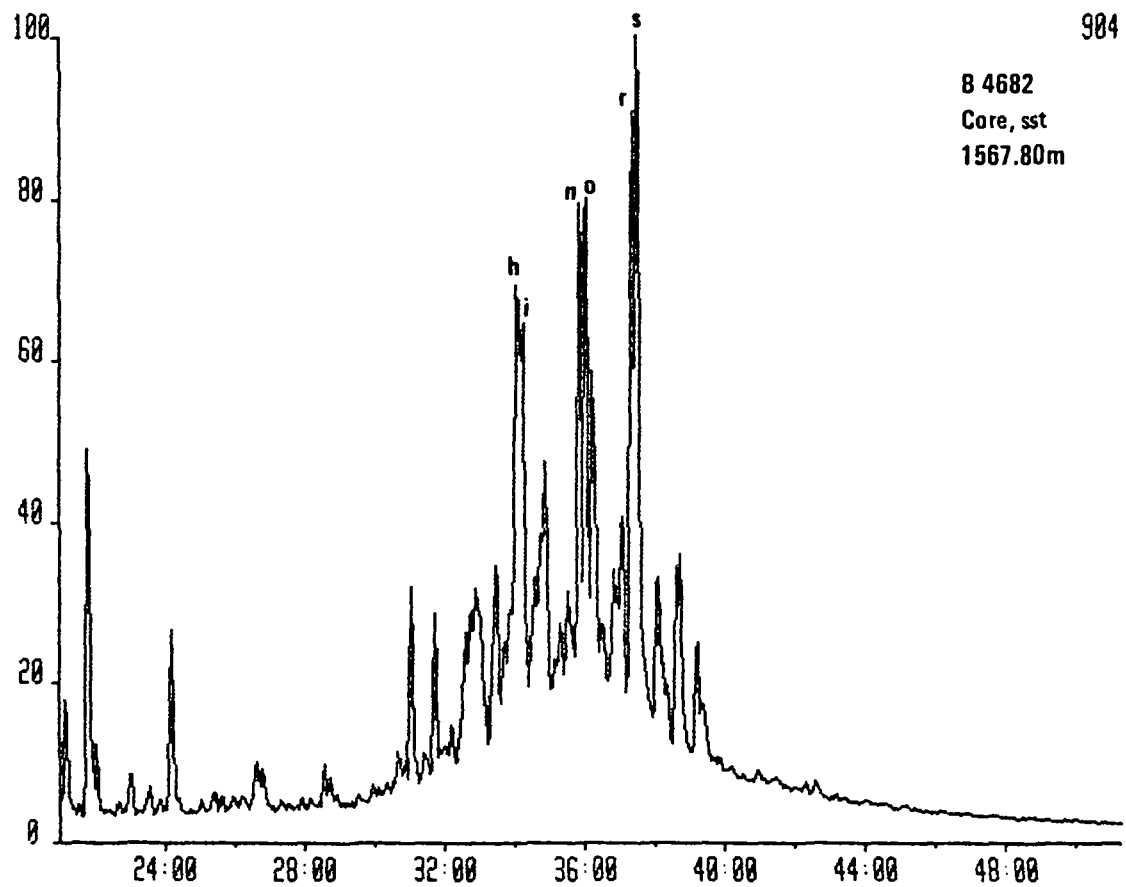
IKU

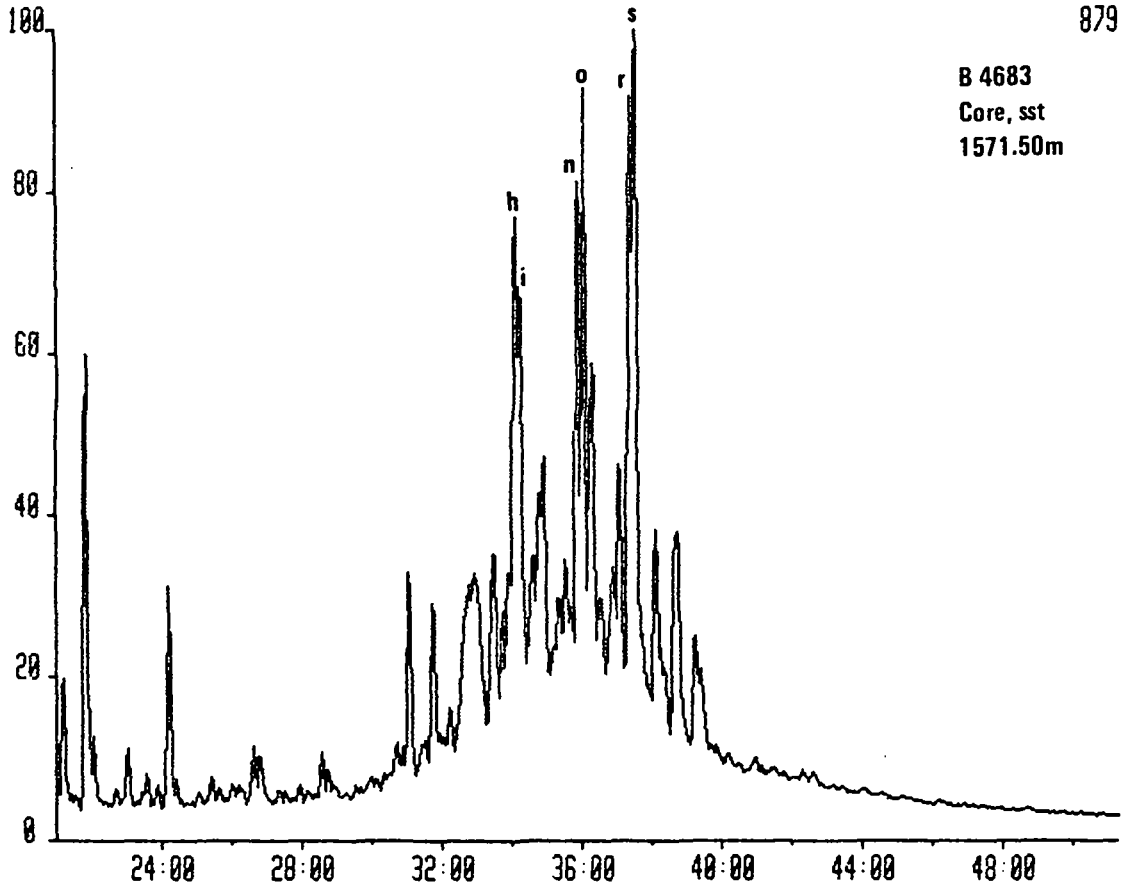

4027
B 4691
Core, sst
1628.0m
100
80
60
40
20
0
u
v
a
b
f
g
h
j
k
n
o
q
r
s
t
24:00
28:00
32:00
36:00
40:00
44:00
48:00
52:00

IKU

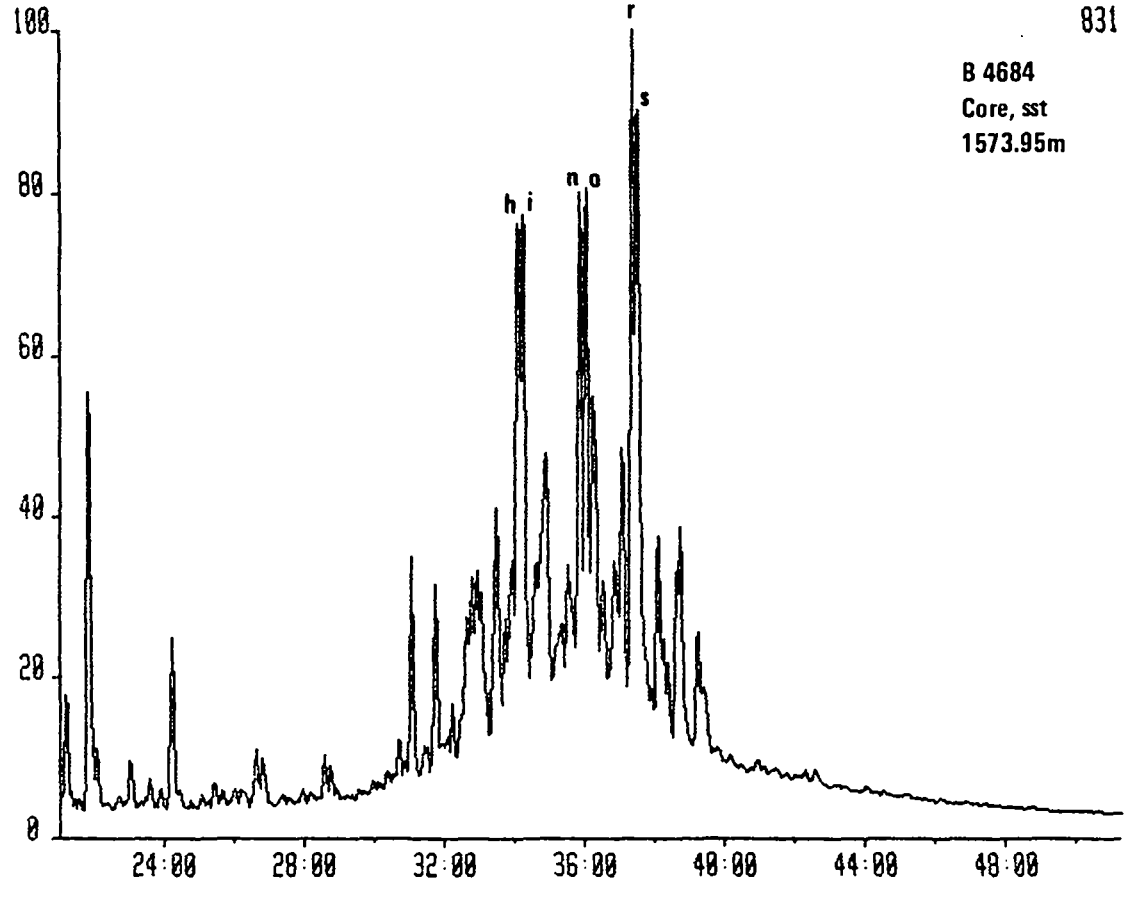


744TROL1 218.1000 G1 I1 S2

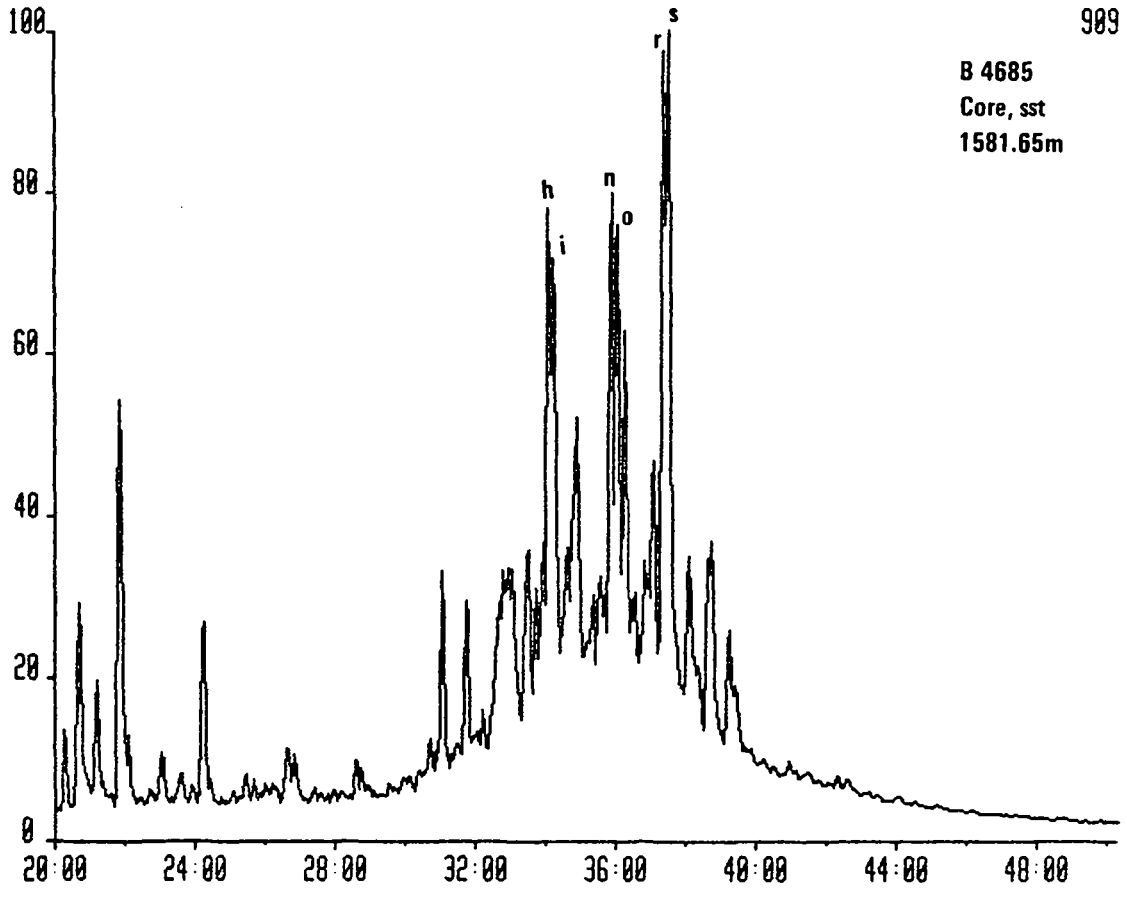




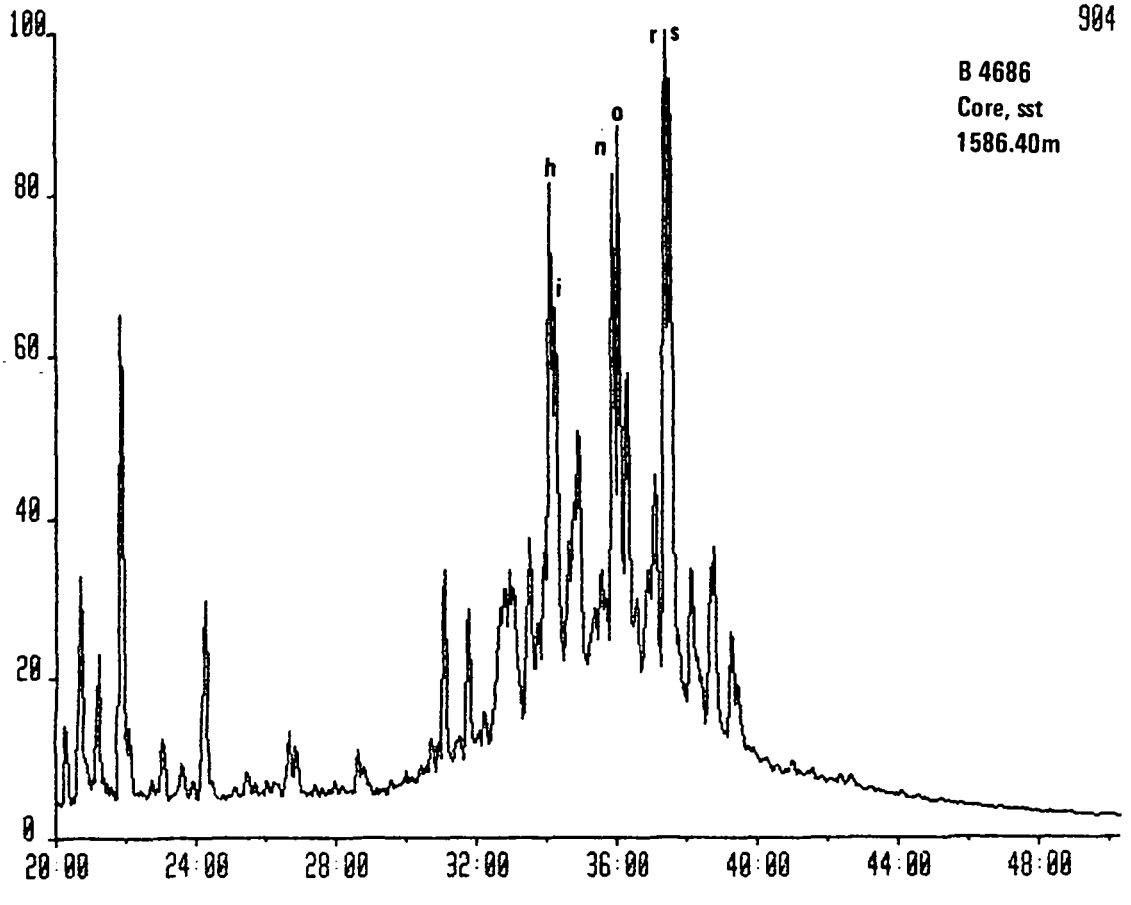
744TROL1 218.1000 G1 I1 S4



744TROL2 218.1000 G1 I1 S1



744TROL2 218.1000 G1 I1 S2



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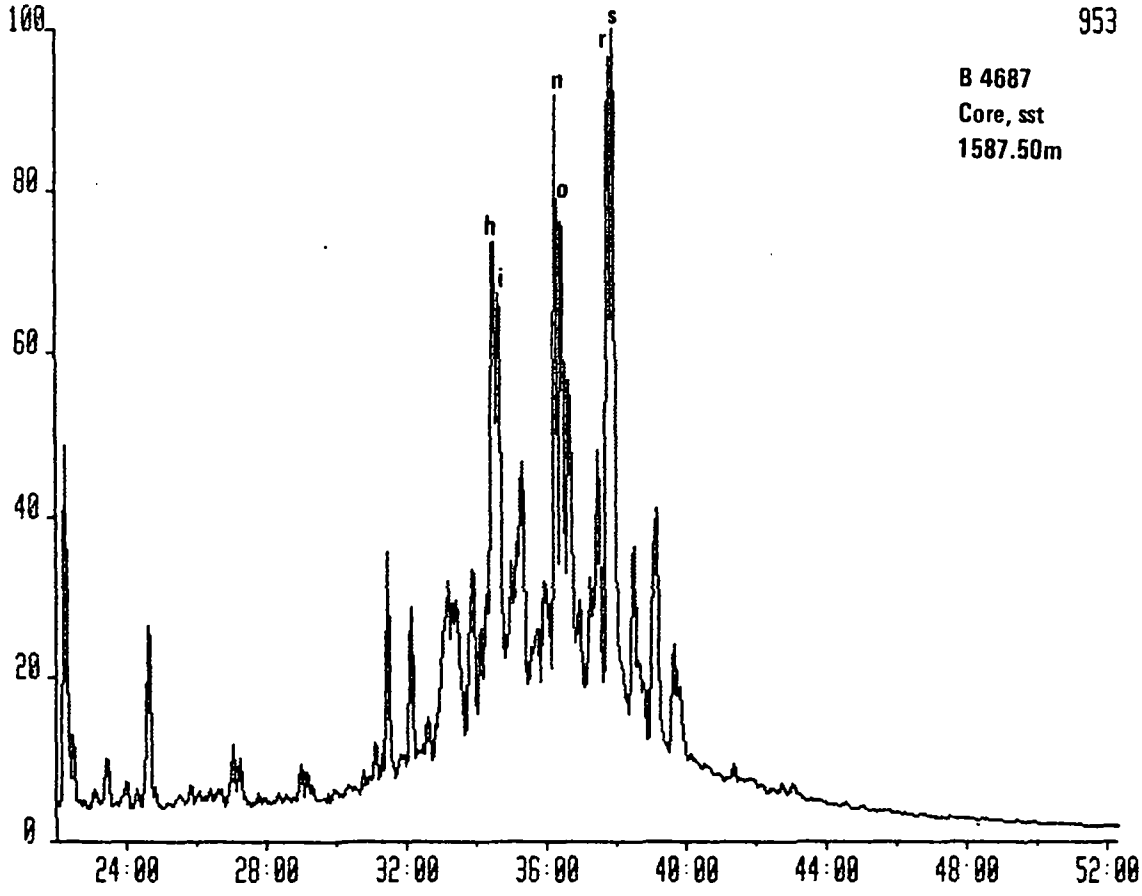
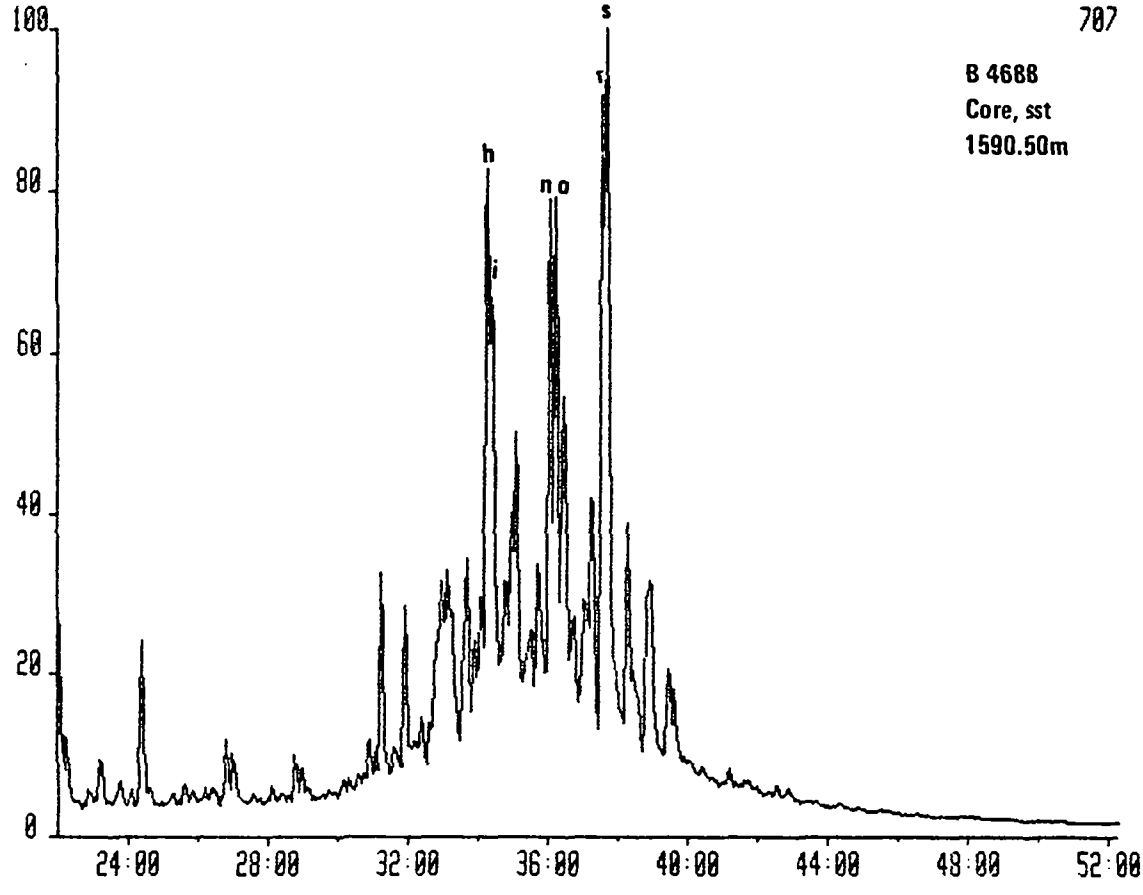
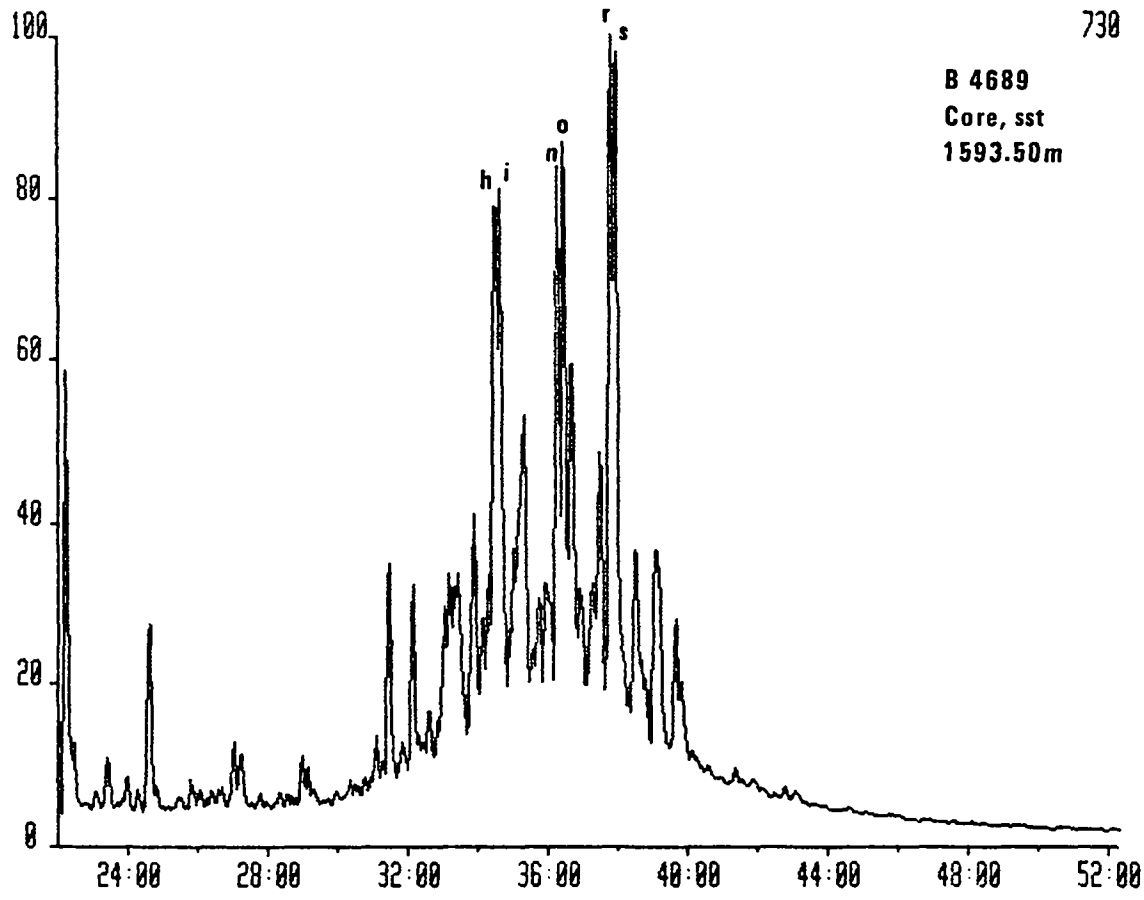
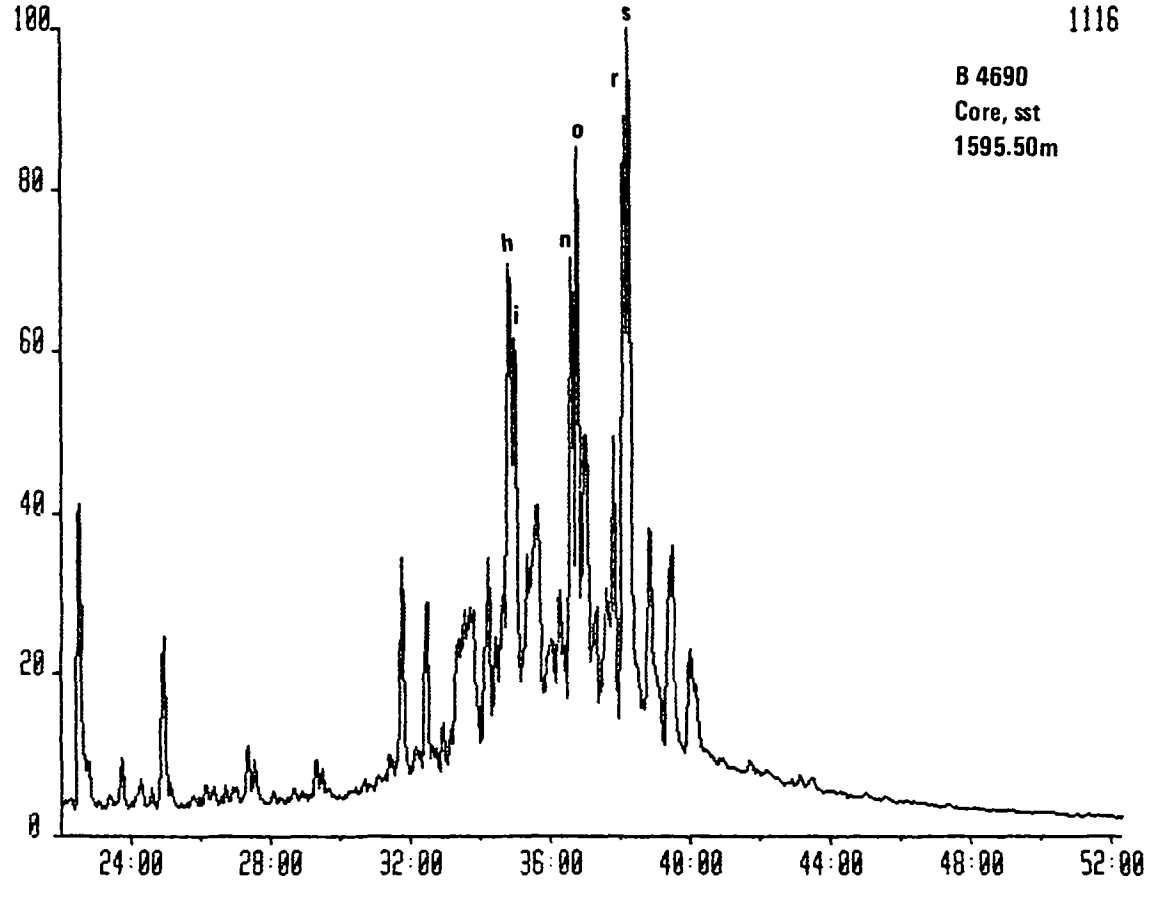


744TROL3 218.1000 G1 I1 S2





744TROL3 218.1000 G1 I1 S4



IKU

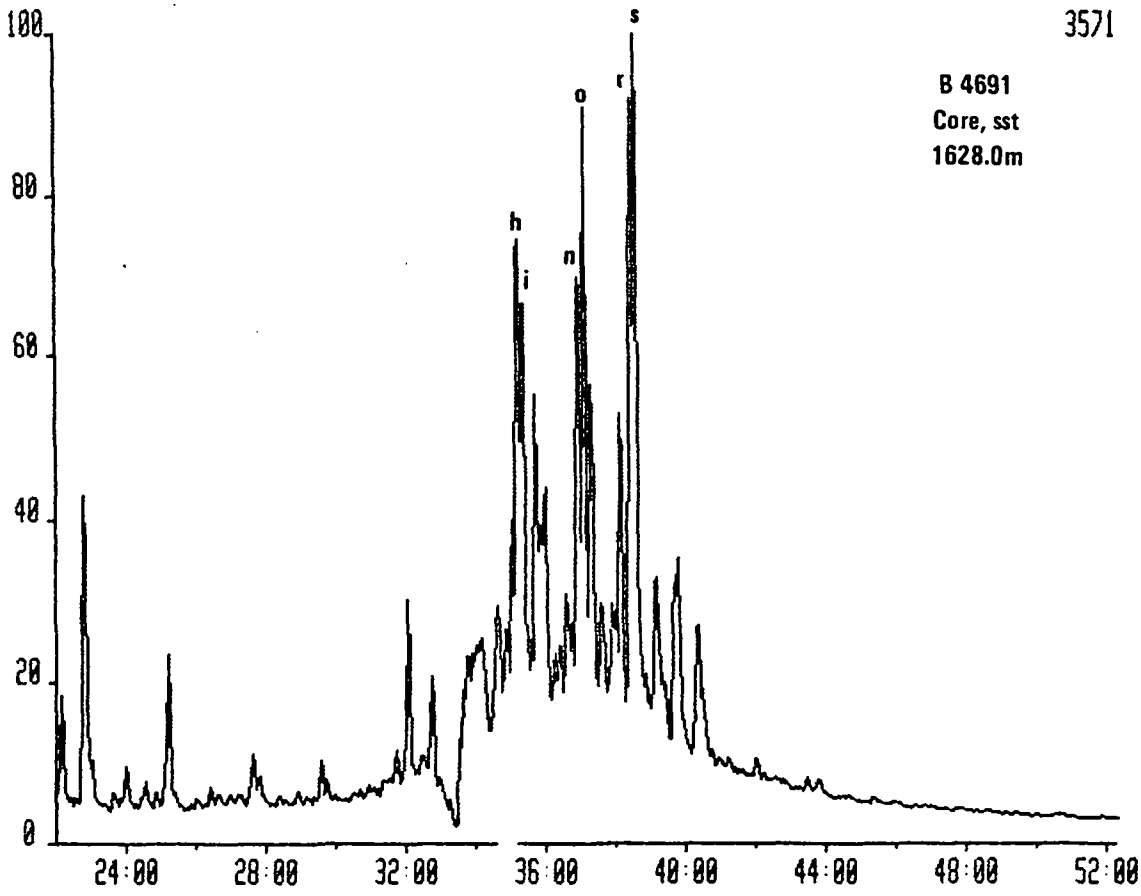
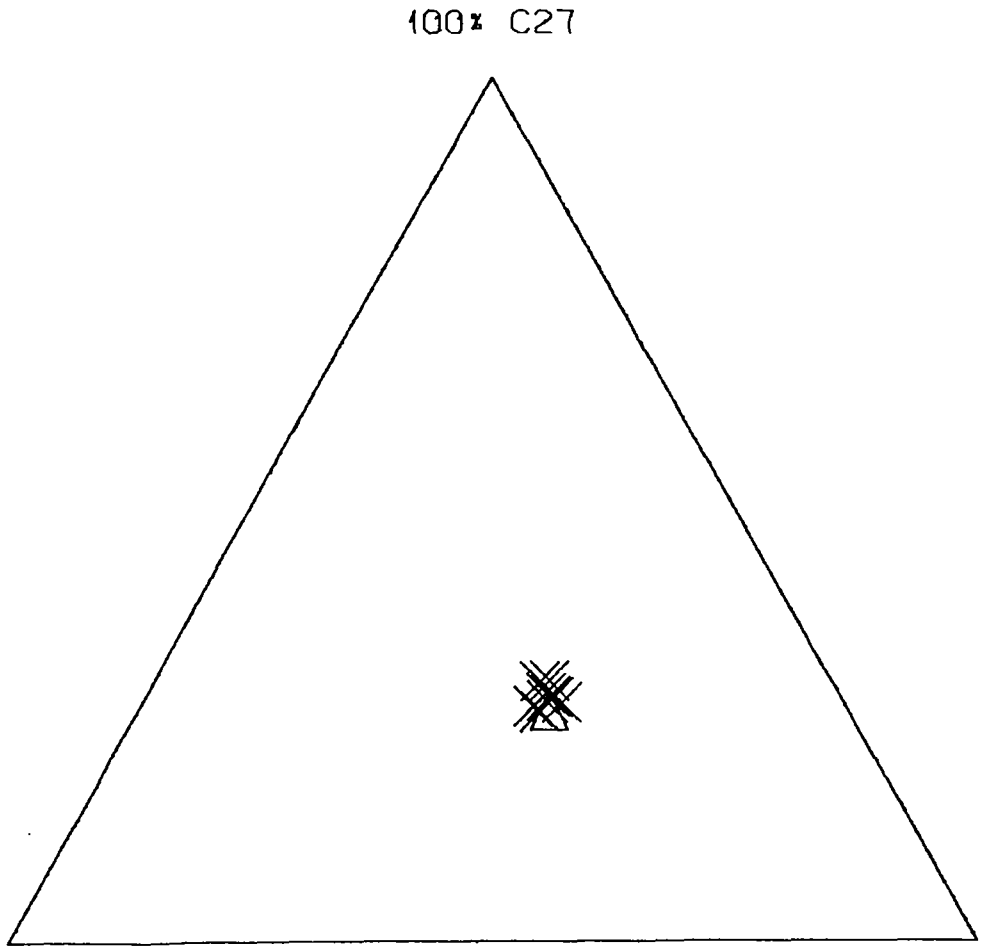
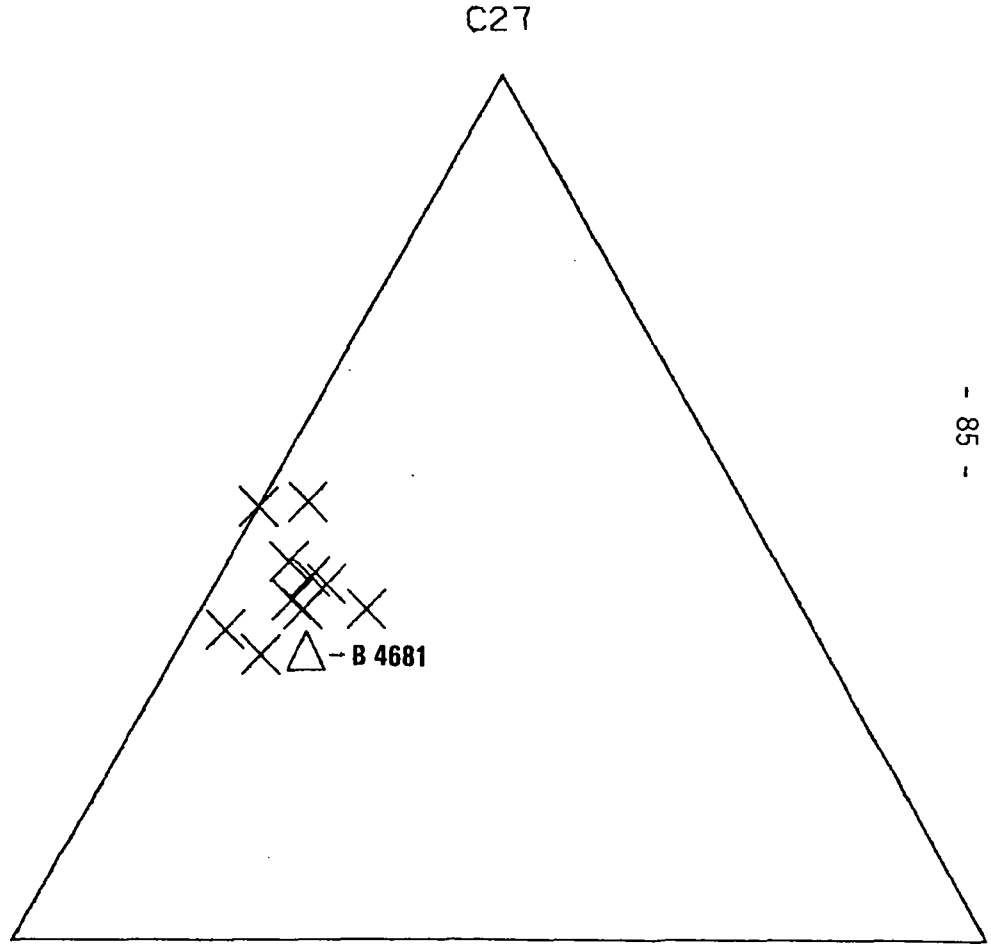

3571
B 4691
Core, sst
1628.0m
h
i
n
o
r
s
100
80
60
40
20
0
24:00
28:00
32:00
36:00
40:00
44:00
48:00
52:00

FIGURE 6

Triangular plots of molecular weight distribution of C_{27}-C_{29} regular 14β,17β-steranes

TROLL 31/3-2





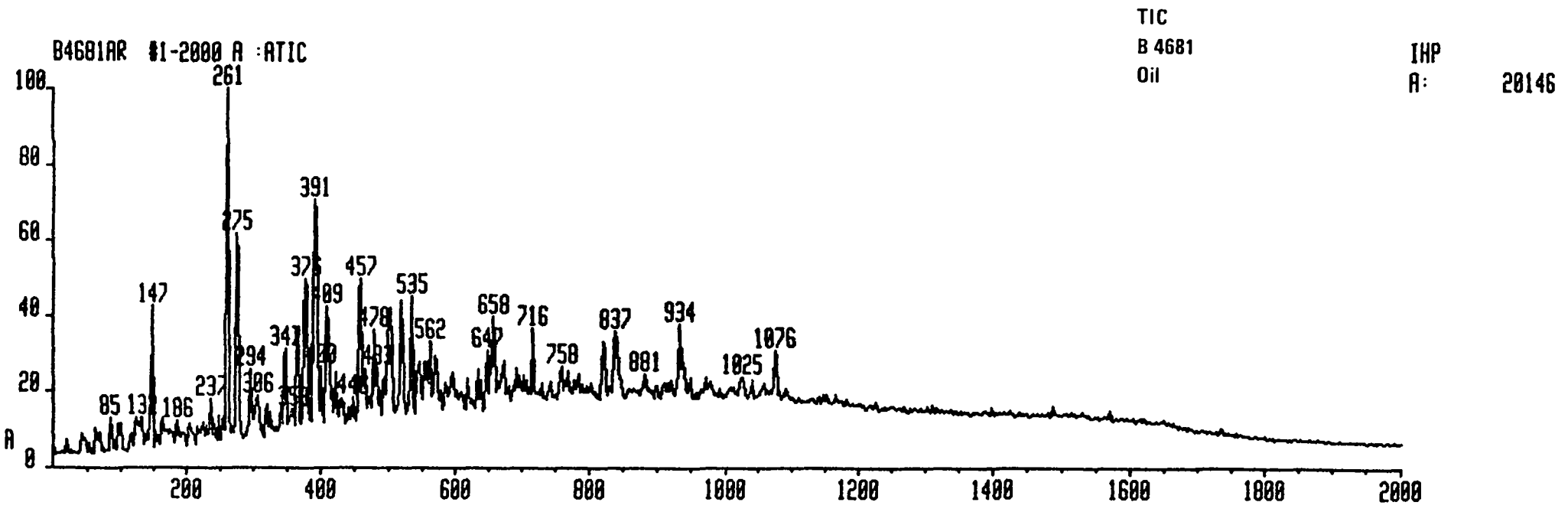
100% C29 C28

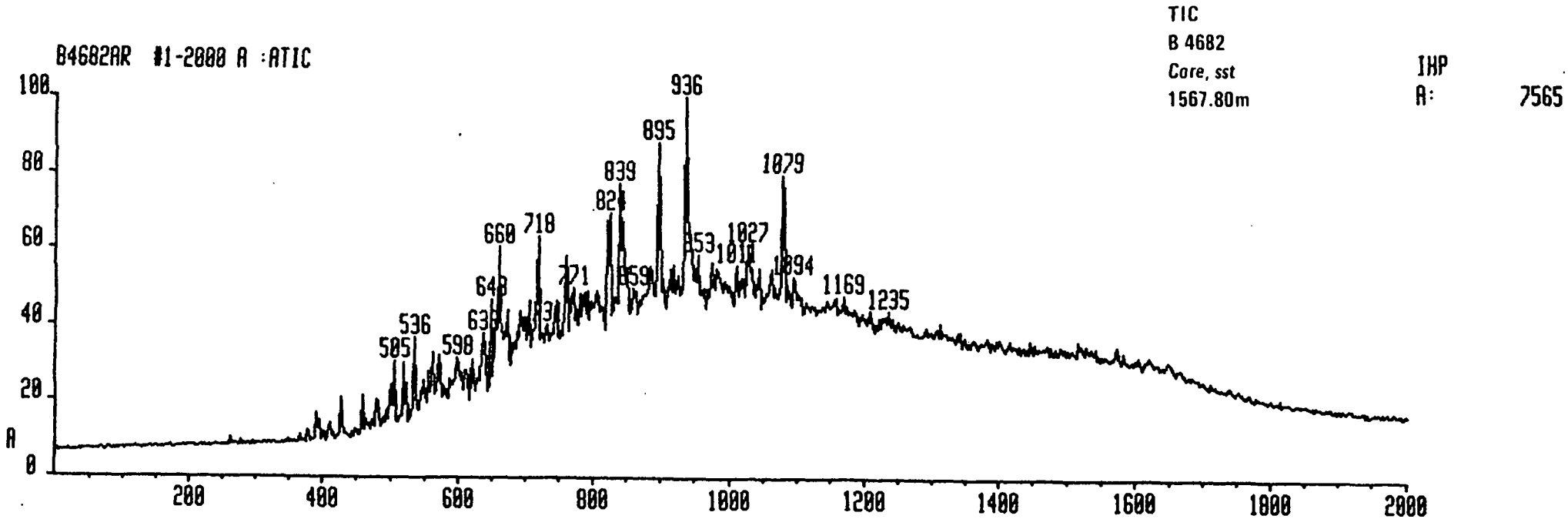
C27 (20-40%)
C28 (20-40%)
C29 (40-60%)

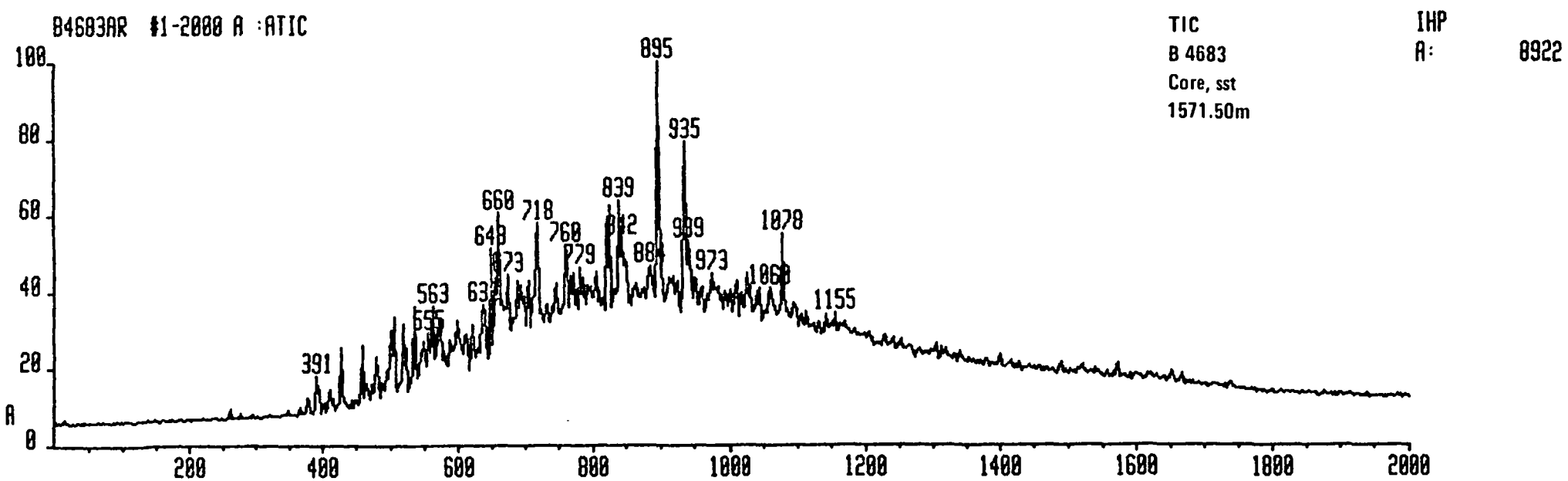
FIGURE 7

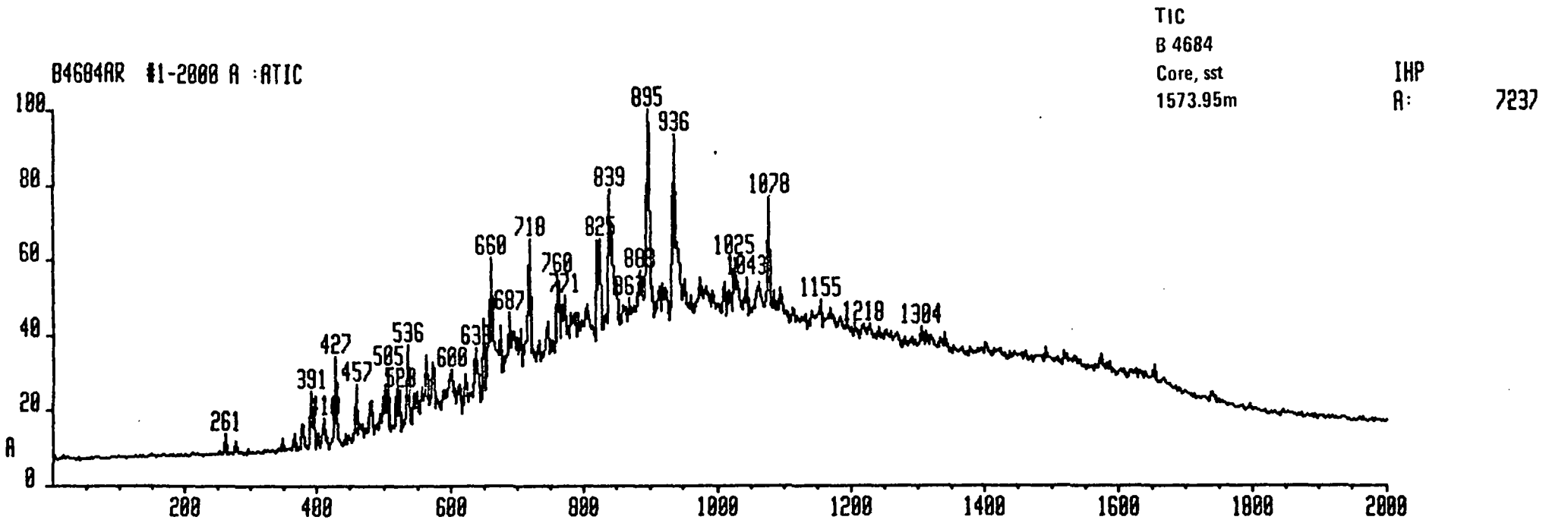
Mass chromatograms of aromatic hydrocarbons

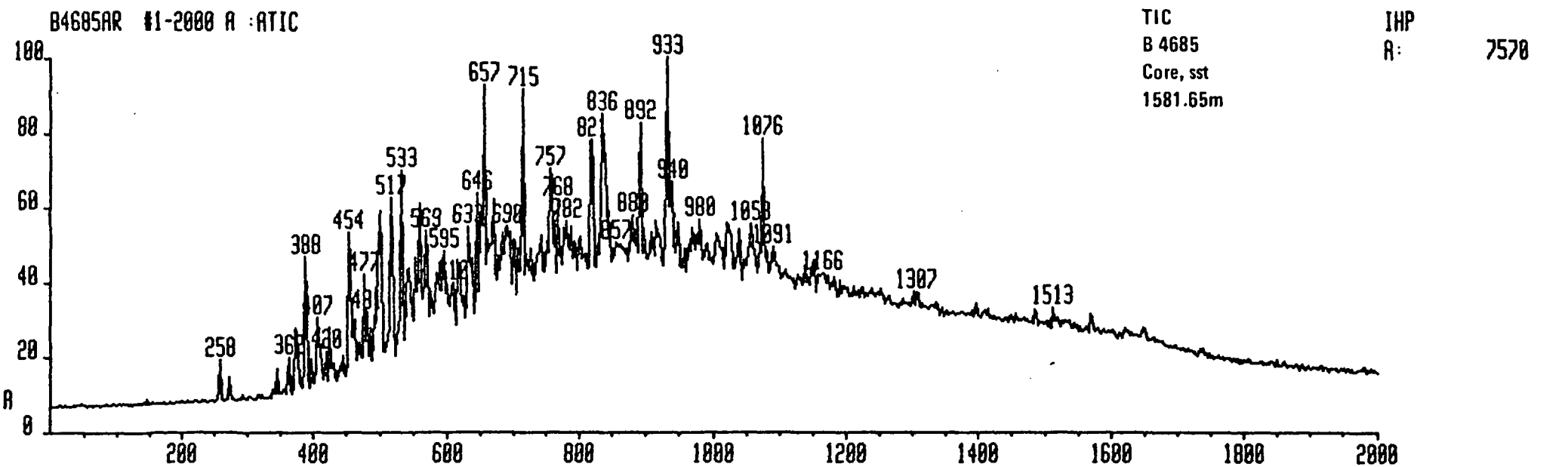
TIC	-	total ion chromatogram
m/z 92, 106	-	alkylated benzenes
m/z 142, 156, 170	-	alkylated naphthalenes
m/z 178, 192, 206	-	alkylated phenanthrenes
m/z 184, 198, 212	-	alkylated dibenzothiophenes
m/z 231	-	triaromatic steranes
m/z 253	-	monoaromatic steranes

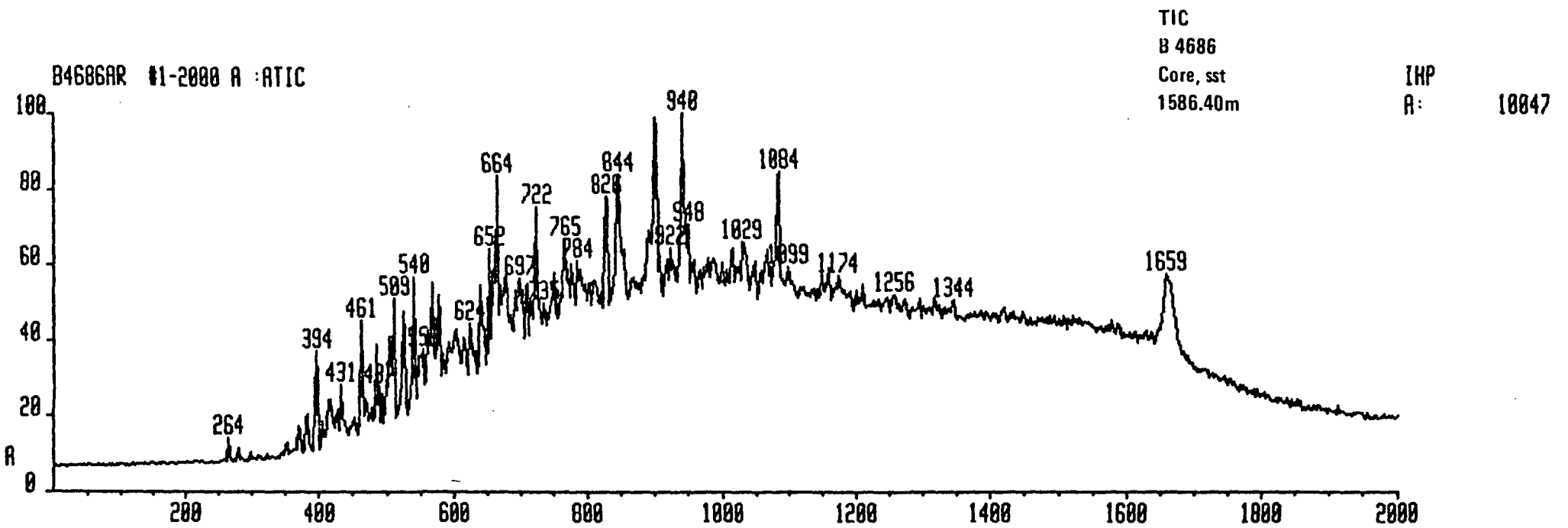

B4681AR #1-2000 A :ATIC
TIC
B 4681
Oil
IHP
A: 20146
A
100
80
60
40
20
0
200
400
600
800
1000
1200
1400
1600
1800
2000
261
275
391
147
457
535
658
716
837
934
1076
562
758
881
1025
294
306
237
186
85

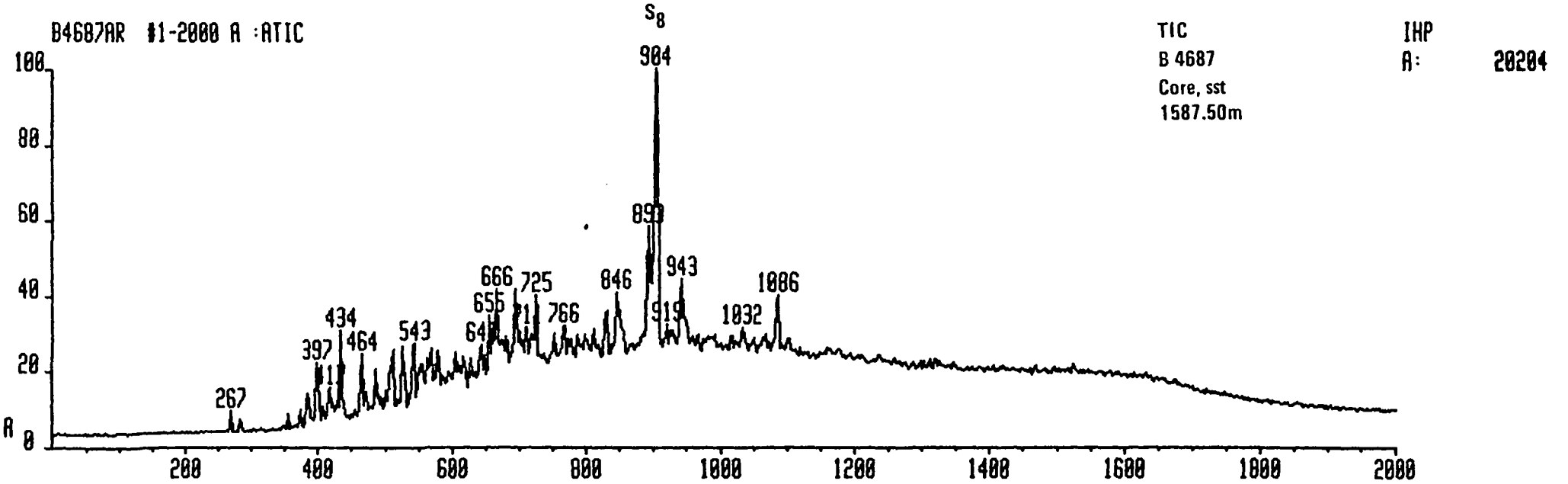

B4682AR #1-2000 A :ATIC
TIC
B 4682
Core, sst
1567.80m
IHP
A: 7565
936
895
839
1079
660
718
1027
1169
1235
536
505
598
A
0
20
40
60
80
100
200
400
600
800
1000
1200
1400
1600
1800
2000

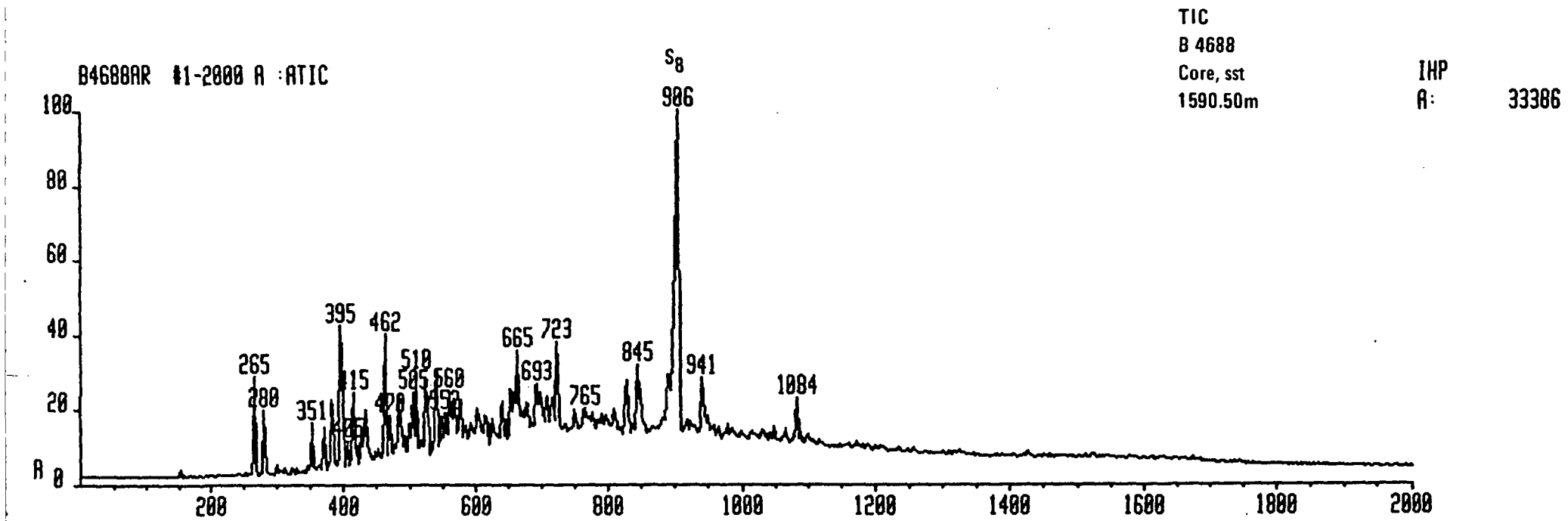

B4683AR #1-2000 A :ATIC
TIC
B 4683
Core, sst
1571.50m
IHP
A: 8922
895
935
839
660
718
760
1078
973
563
391
1155
A
0
20
40
60
80
100
200
400
600
800
1000
1200
1400
1600
1800
2000

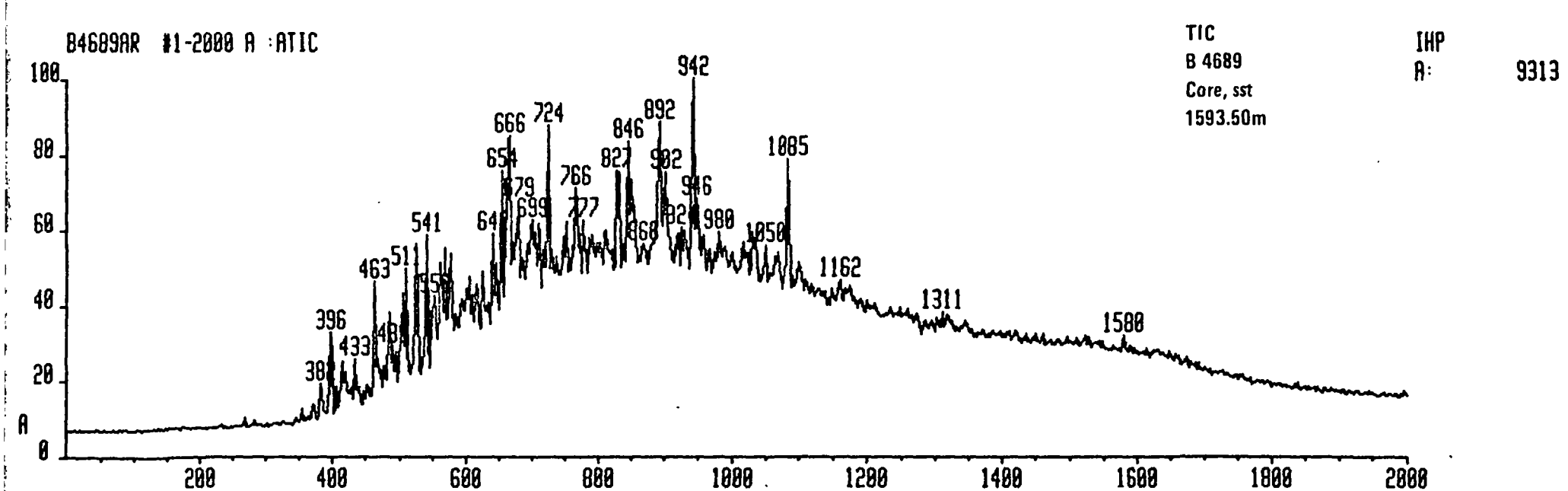

B4684AR #1-2000 A :ATIC
TIC
B 4684
Core, sst
1573.95m
IHP
A: 7237
A
100
80
60
40
20
0
200
400
600
800
1000
1200
1400
1600
1800
2000
895
936
839
1078
718
825
660
760
1025
1043
1155
1218
1304
687
536
427
505
600
391
457
261


B4685AR #1-2000 A :ATIC
TIC
B 4685
Core, sst
1581.65m
IHP
A: 7570
A
100
80
60
40
20
0
200
400
600
800
1000
1200
1400
1600
1800
2000
933
657
715
836
892
1076
533
757
940
980
454
388
595
1166
1307
1513
258


B4686AR #1-2000 A :ATIC
TIC
B 4686
Core, sst
1586.40m
IHP
A: 10047
100
80
60
40
20
A
0
264
394
431
461
509
540
624
664
722
765
844
940
948
1029
1084
1174
1256
1344
1659
200
400
600
800
1000
1200
1400
1600
1800
2000


B4687AR #1-2000 A :ATIC
S_8
TIC
B 4687
Core, sst
1587.50m
IHP
A: 20204
100
80
60
40
20
A
0
267
397
434
464
543
666
725
846
904
943
1032
1086
200
400
600
800
1000
1200
1400
1600
1800
2000


B4688AR #1-2000 A :ATIC
TIC
B 4688
Core, sst
1590.50m
IHP
A: 33386
S8
906
265
280
351
395
462
665
723
693
765
845
941
1084
A
0
20
40
60
80
100
200
400
600
800
1000
1200
1400
1600
1800
2000


B4689AR #1-2000 A :ATIC
TIC
B 4689
Core, sst
1593.50m
IHP
A: 9313
942
666
724
892
846
827
902
1085
766
541
463
396
433
1162
1311
1580
A
0
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40
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80
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200
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600
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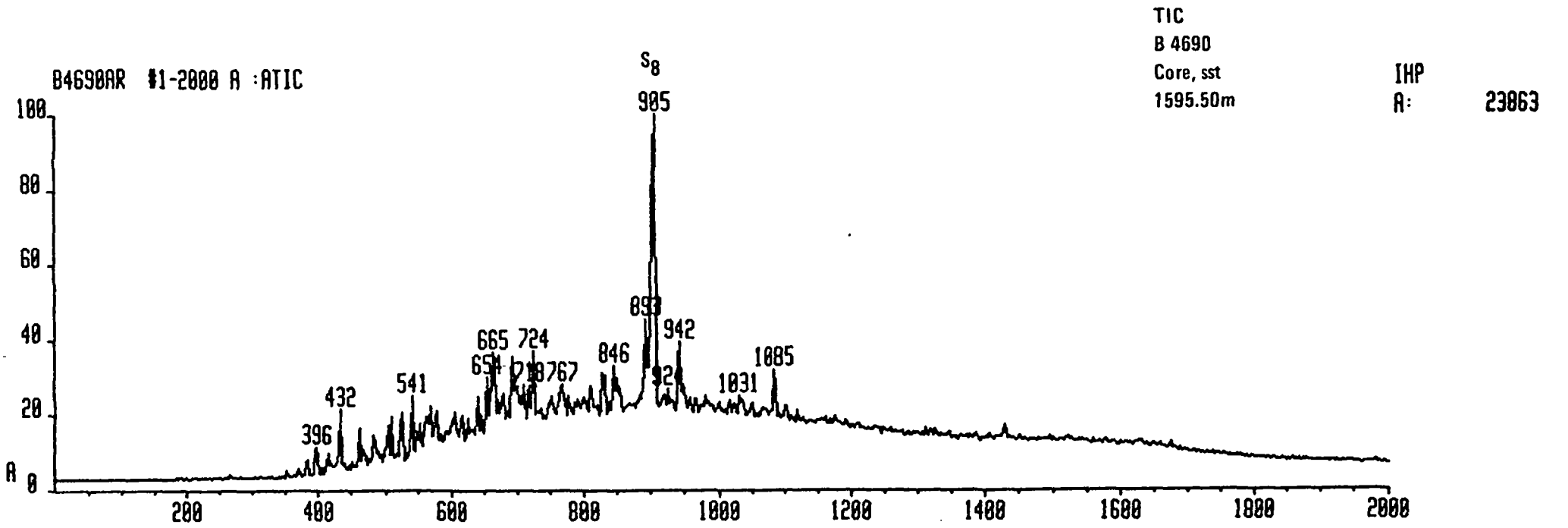
1200
1400
1600
1800
2000


B4690AR #1-2000 A :ATIC
TIC
B 4690
Core, sst
1595.50m
IHP
A: 23863
S_8
985
100
80
60
40
20
A 0
396
432
541
665
724
767
846
893
942
1031
1085
200
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600
800
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1200
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1600
1800
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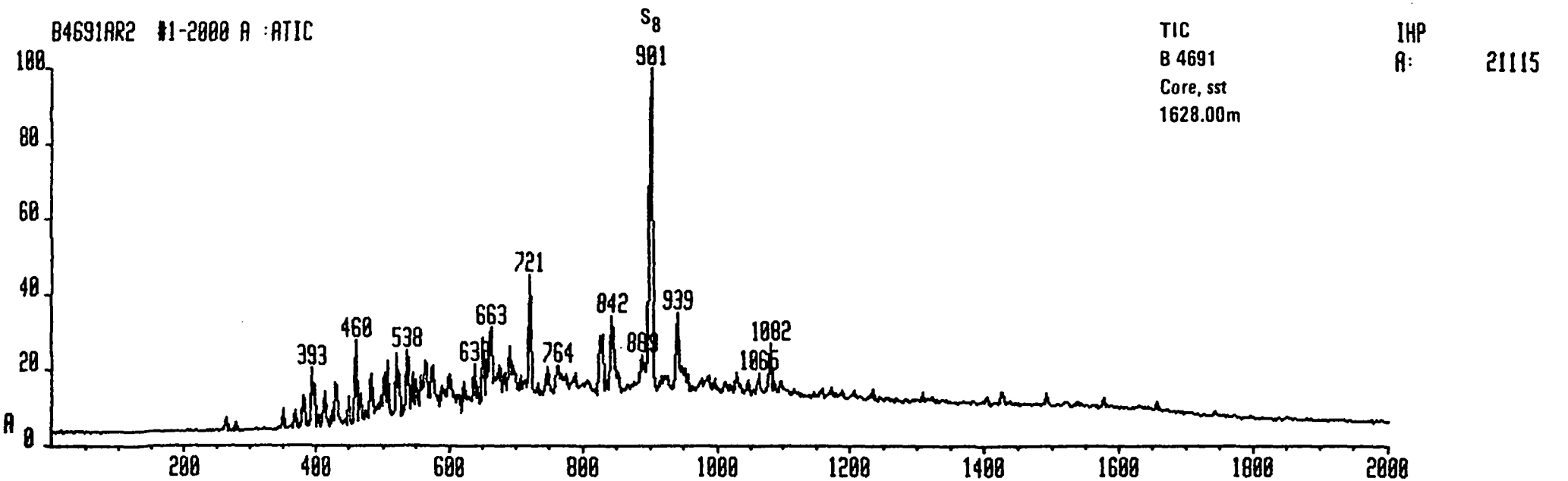
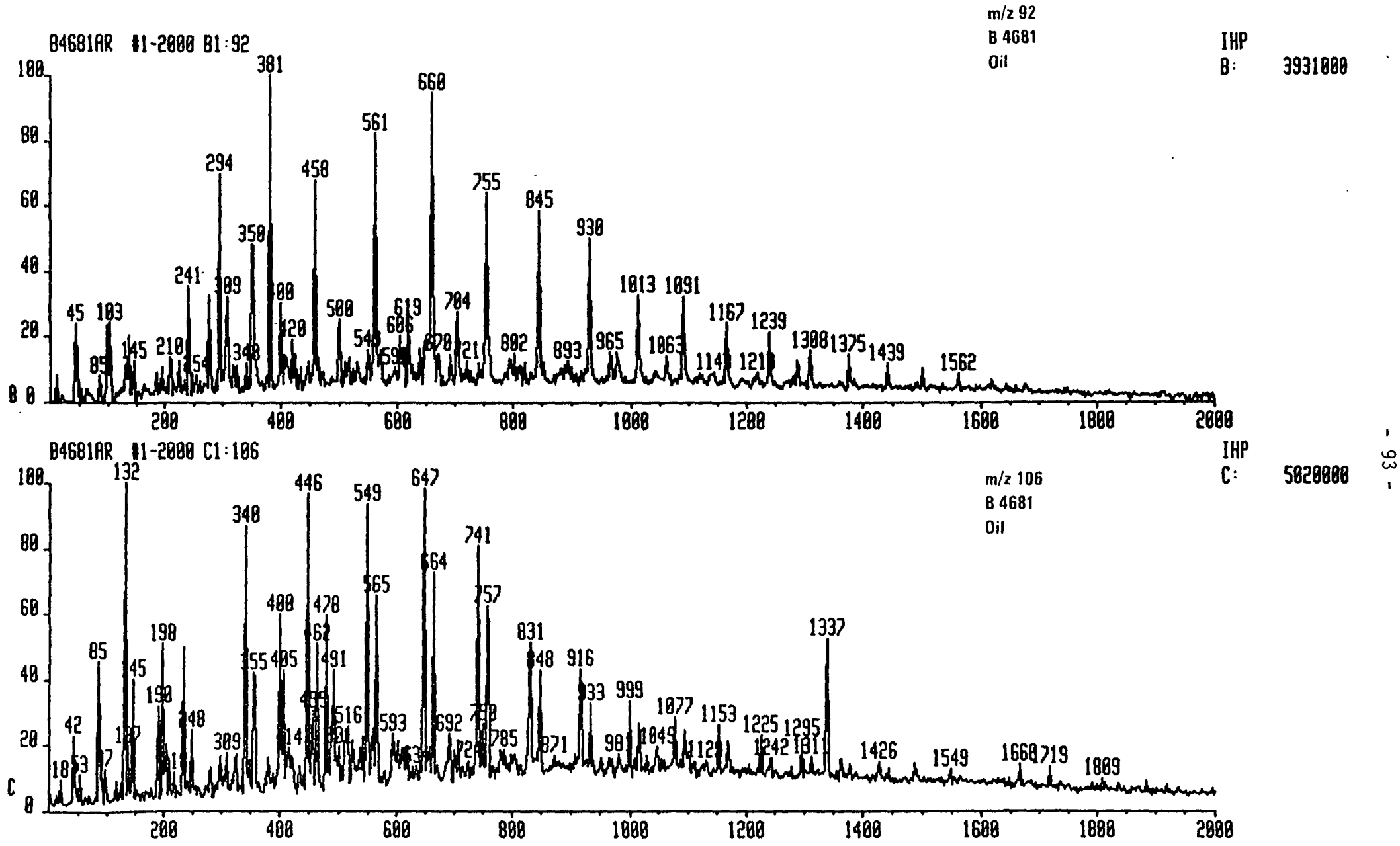
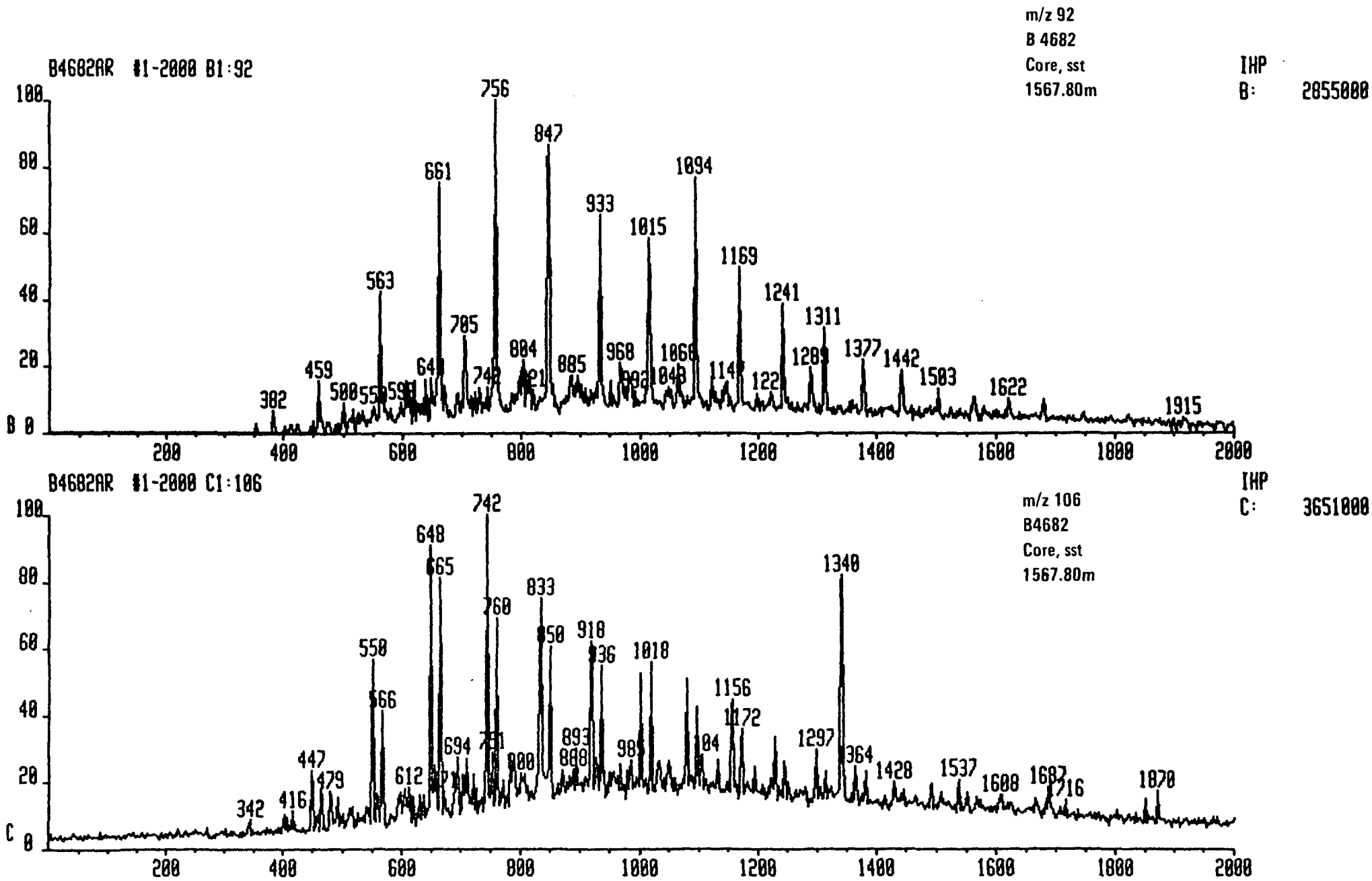

B4691AR2 #1-2000 A :ATIC
TIC
B 4691
Core, sst
1628.00m
IHP
A: 21115
S_8
981
100
80
60
40
20
A 0
393
460
538
663
721
764
842
939
1066
1082
200
400
600
800
1000
1200
1400
1600
1800
2000


B4681AR #1-2000 B1:92
m/z 92
B 4681
Oil
IHP
B: 3931000
B 0
B4681AR #1-2000 C1:106
m/z 106
B 4681
Oil
IHP
C: 5020000
C 0
200
400
600
800
1000
1200
1400
1600
1800
2000


B4682AR #1-2000 B1:92
m/z 92
B 4682
Core, sst
1567.80m
IHP
B: 2855000
B 0
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459
500
563
661
756
785
847
884
885
933
968
1015
1066
1094
1122
1169
1241
1289
1311
1377
1442
1503
1622
1915
B4682AR #1-2000 C1:106
m/z 106
B4682
Core, sst
1567.80m
IHP
C: 3651000
C 0
342
416
447
479
550
566
612
648
665
694
742
760
800
833
850
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893
918
936
988
1018
1156
1172
1184
1297
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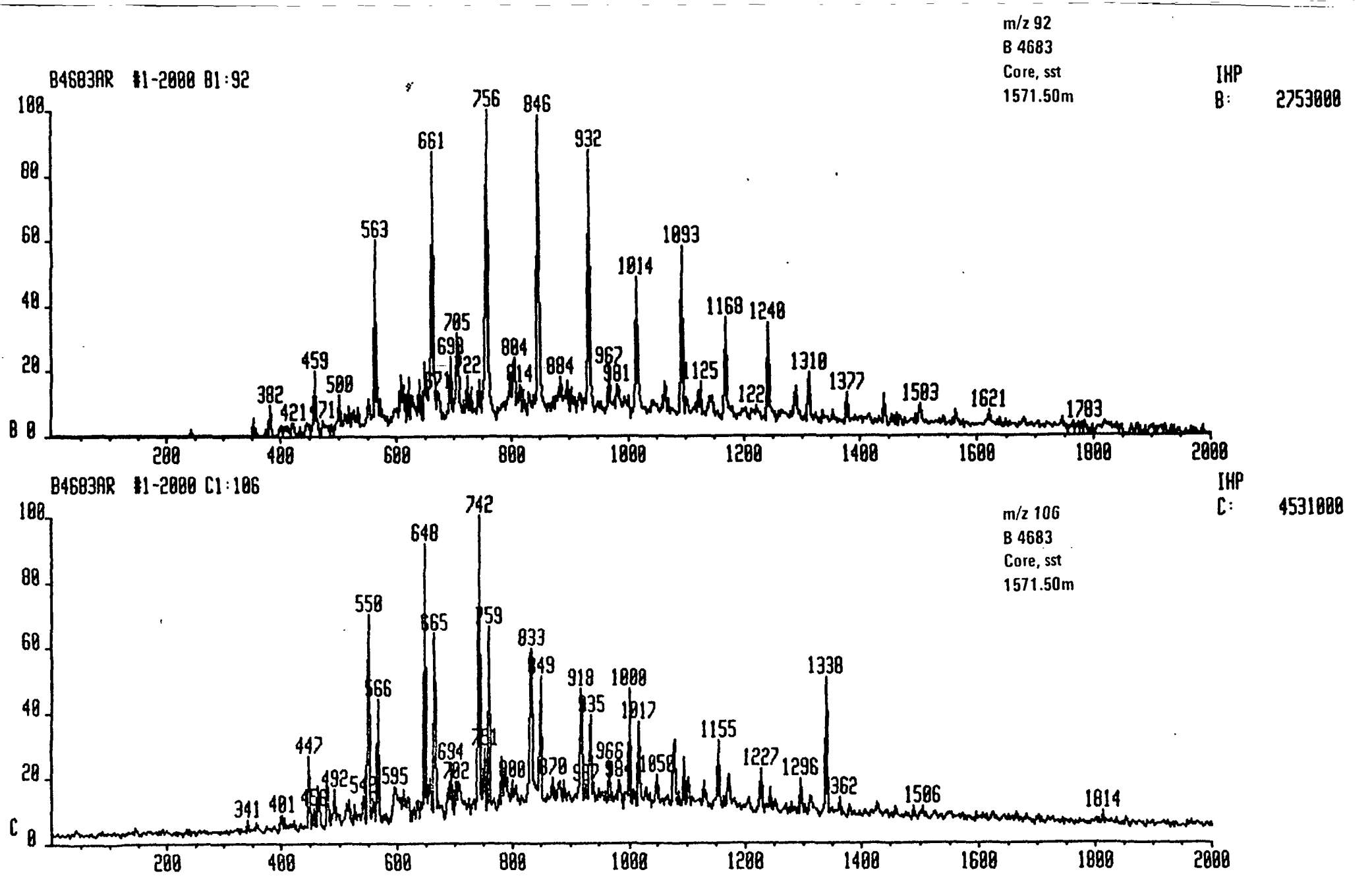
B4683AR #1-2000 B1:92
m/z 92
B 4683
Core, sst
1571.50m
IHP
B: 2753000
B 0
B4683AR #1-2000 C1:106
m/z 106
B 4683
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IHP
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1800
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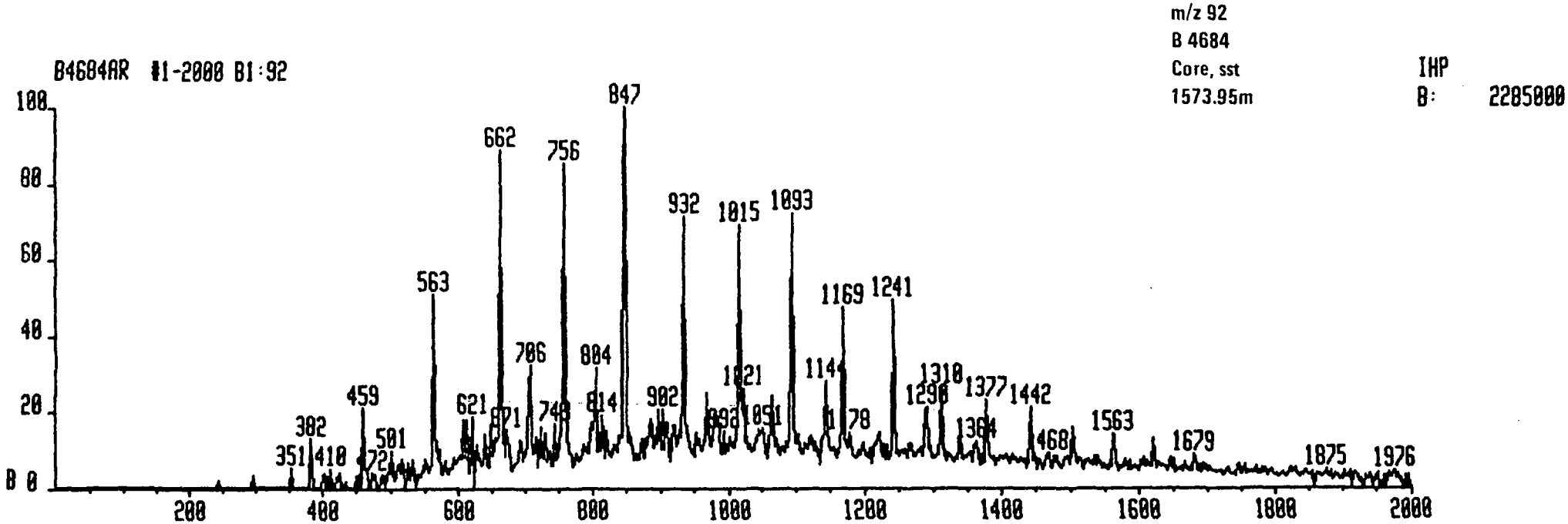
B4684AR #1-2000 B1:92
m/z 92
B 4684
Core, sst
1573.95m
IHP
B: 2285000
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200
400
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800
1000
1200
1400
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1800
2000
847
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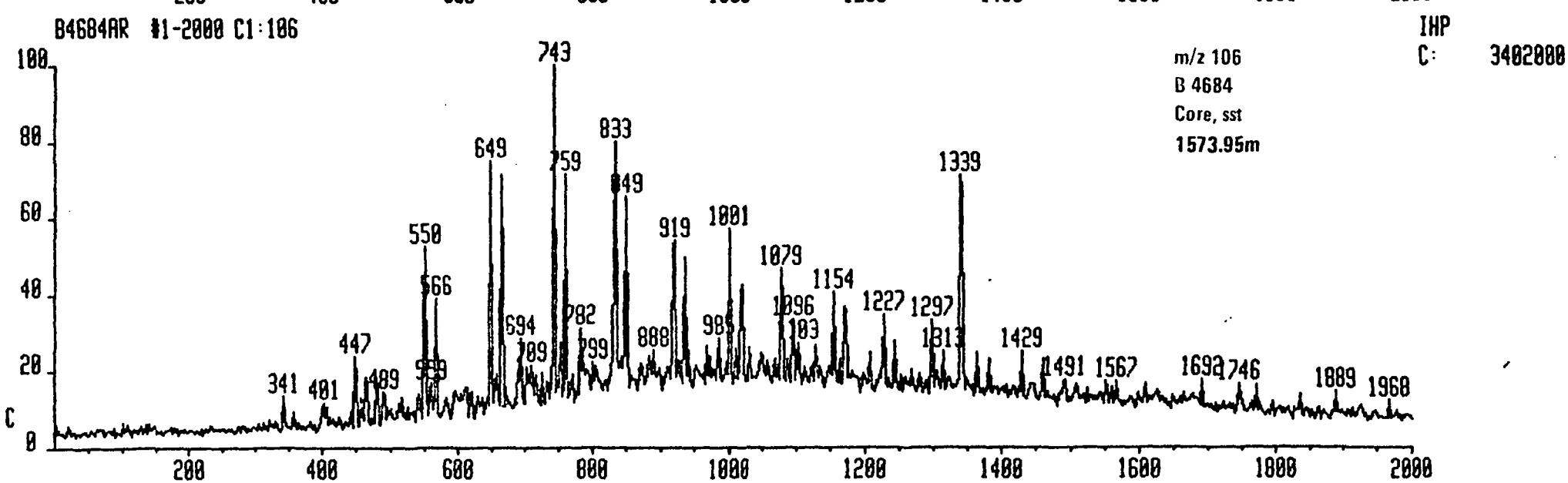
B4684AR #1-2000 C1:106
m/z 106
B 4684
Core, sst
1573.95m
IHP
C: 3402000
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60
40
20
200
400
600
800
1000
1200
1400
1600
1800
2000
743
833
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1339
550
919
1001
1079
1154
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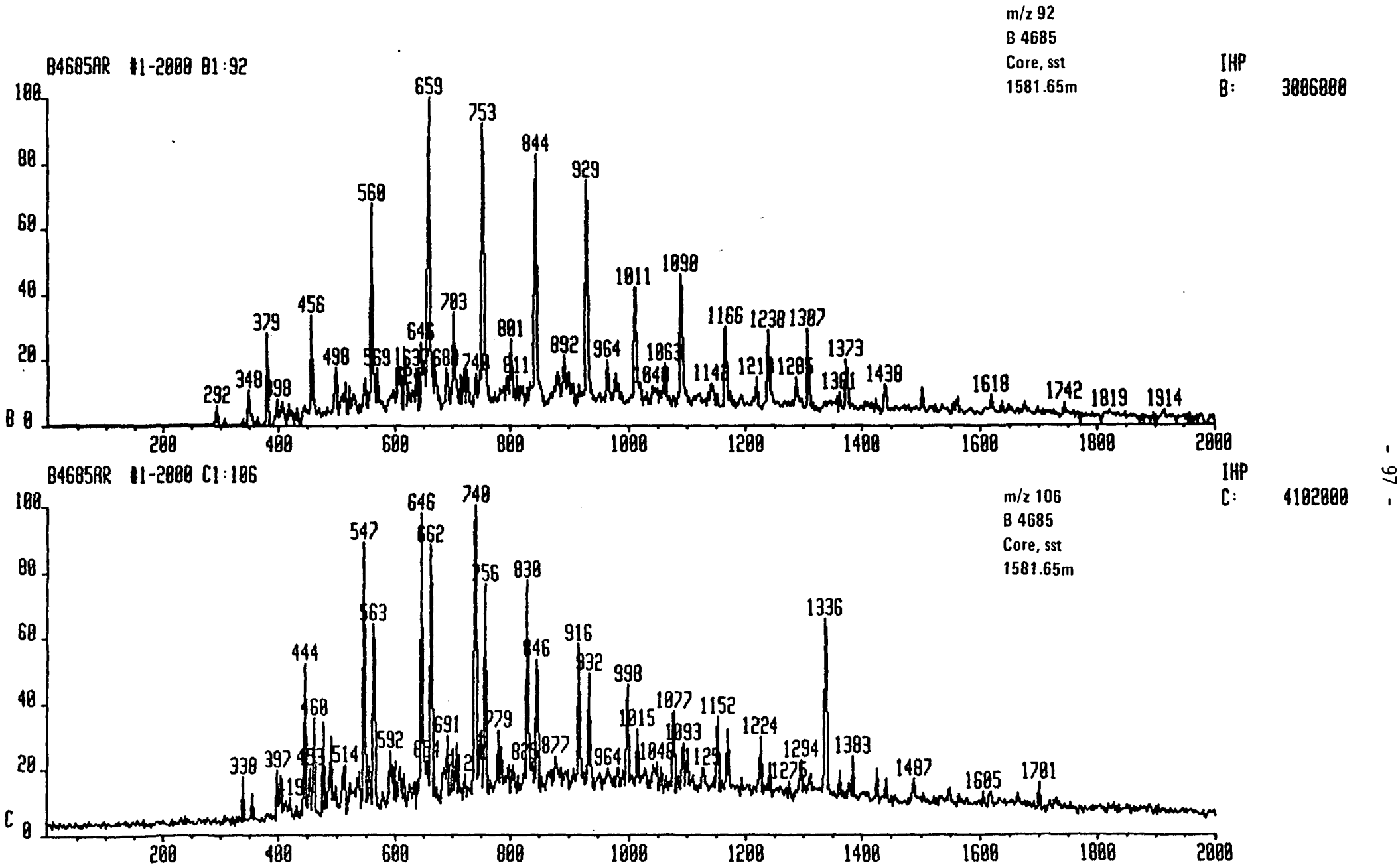
1968


B4685AR #1-2000 B1:92
m/z 92
B 4685
Core, sst
1581.65m
IHP
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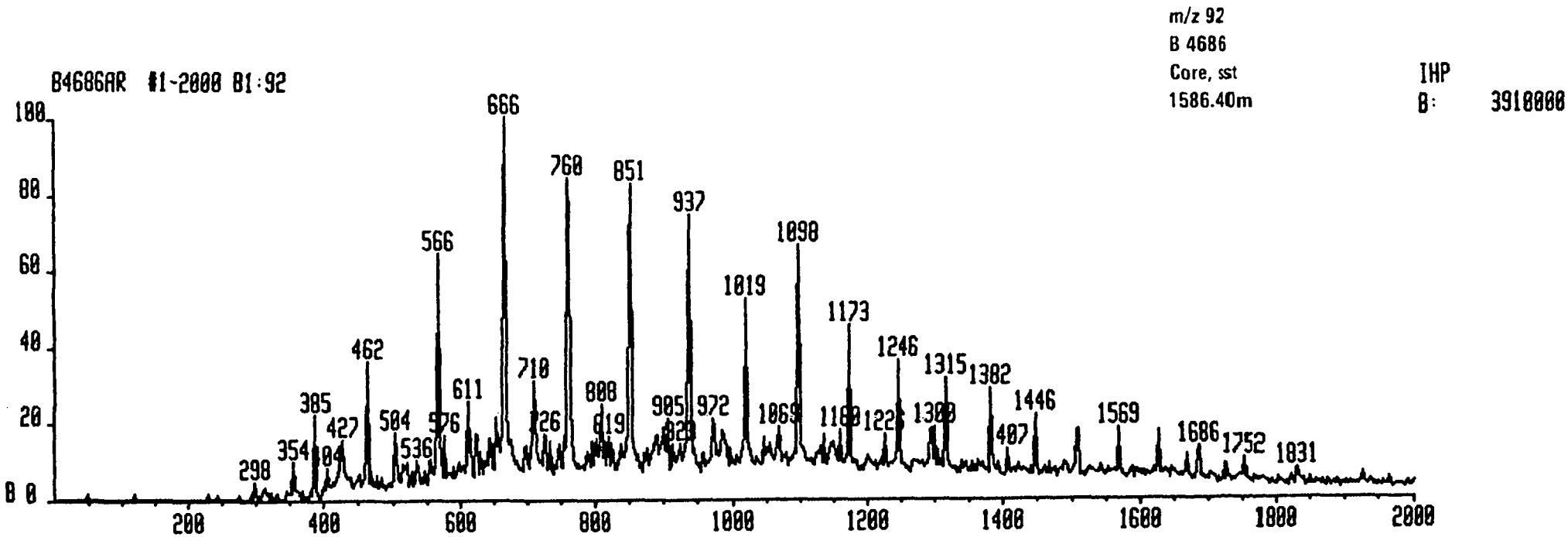
B4685AR #1-2000 C1:106
m/z 106
B 4685
Core, sst
1581.65m
IHP
C: 4102000


B4686AR #1-2000 B1:92
m/z 92
B 4686
Core, sst
1586.40m
IHP
B: 3910000
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60
40
20
200
400
600
800
1000
1200
1400
1600
1800
2000
666
760
851
937
566
1098
1019
1173
462
1246
1315
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354
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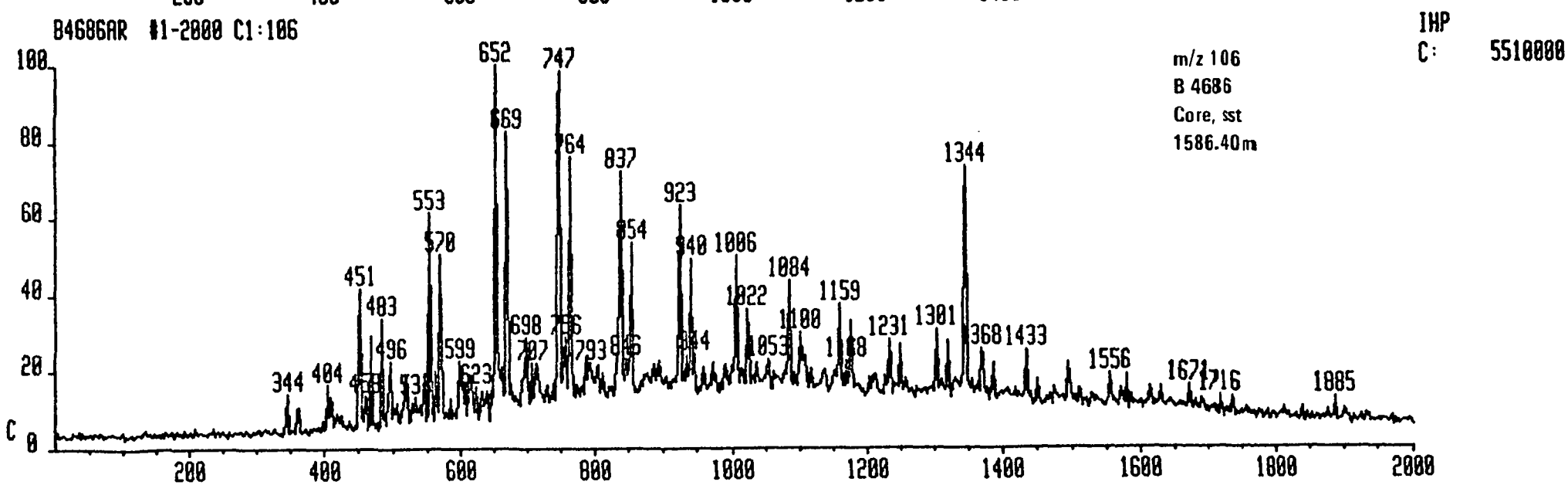
B4686AR #1-2000 C1:106
IHP
C: 5510000
m/z 106
B 4686
Core, sst
1586.40m
C 0
100
80
60
40
20
200
400
600
800
1000
1200
1400
1600
1800
2000
652
747
669
764
837
1344
553
923
570
854
1006
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1100
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1301
496
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793
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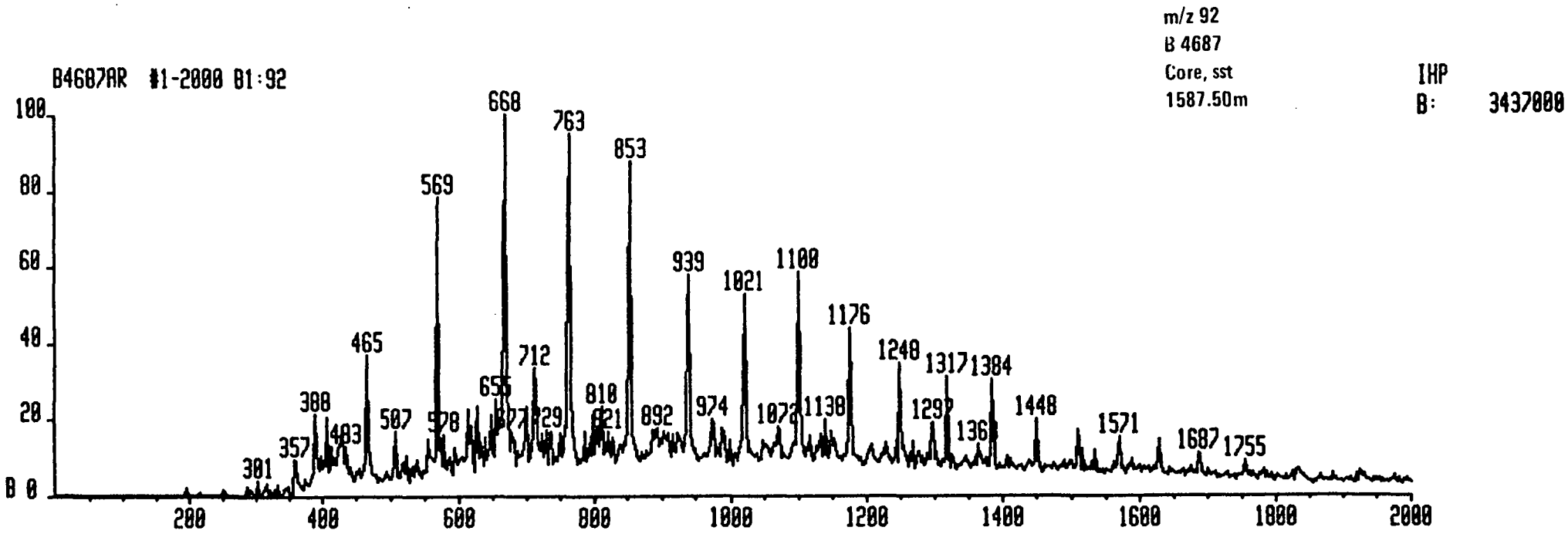
344
404
1556
1716
1885


B4687AR #1-2000 B1:92
m/z 92
B 4687
Core, sst
1587.50m
IHP
B: 3437000
B
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40
20
0
200
400
600
800
1000
1200
1400
1600
1800
2000
668
763
853
569
939
1021
1100
1176
465
712
1248
1317
1384
388
810
892
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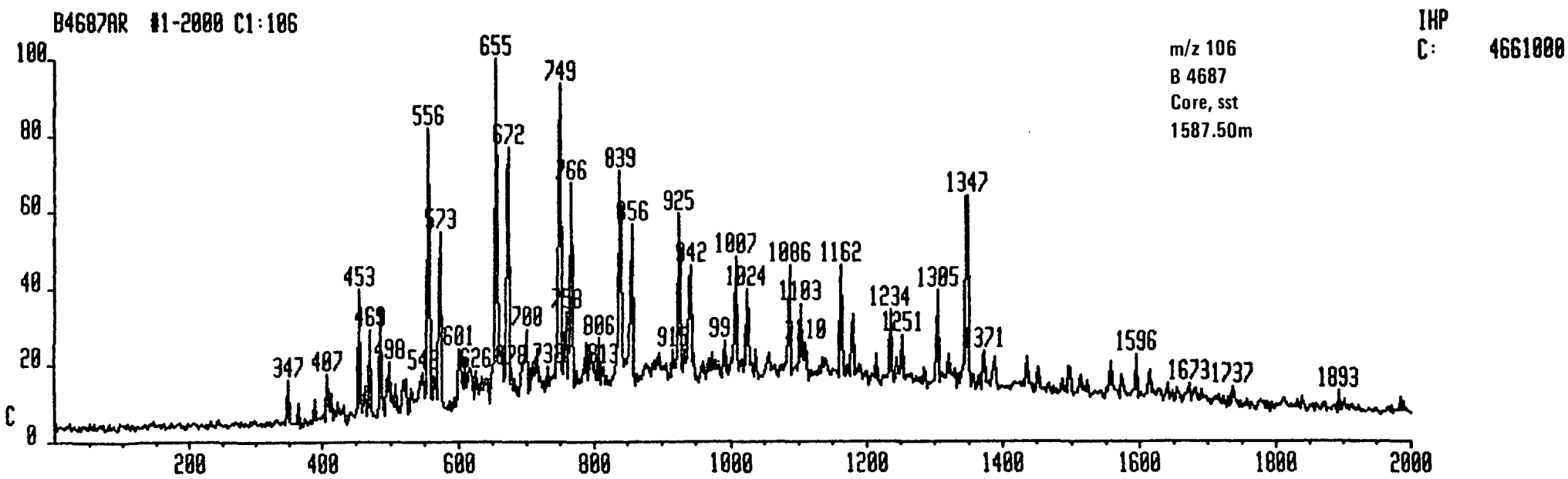
B4687AR #1-2000 C1:106
m/z 106
B 4687
Core, sst
1587.50m
IHP
C: 4661000
C
100
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40
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0
200
400
600
800
1000
1200
1400
1600
1800
2000
655
749
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672
839
766
925
1347
573
856
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1024
1103
1305
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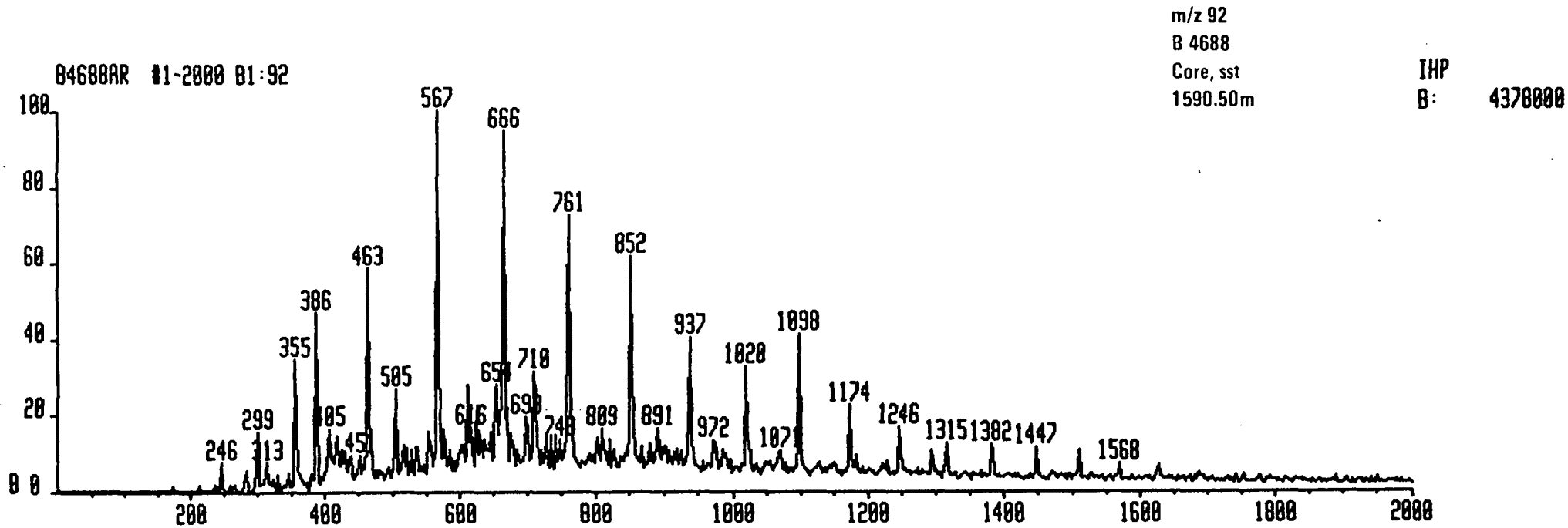
B4688AR #1-2000 B1:92
m/z 92
B 4688
Core, sst
1590.50m
IHP
B: 4378000
B 0
100
80
60
40
20
200
400
600
800
1000
1200
1400
1600
1800
2000
567
666
761
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386
355
505
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937
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1020
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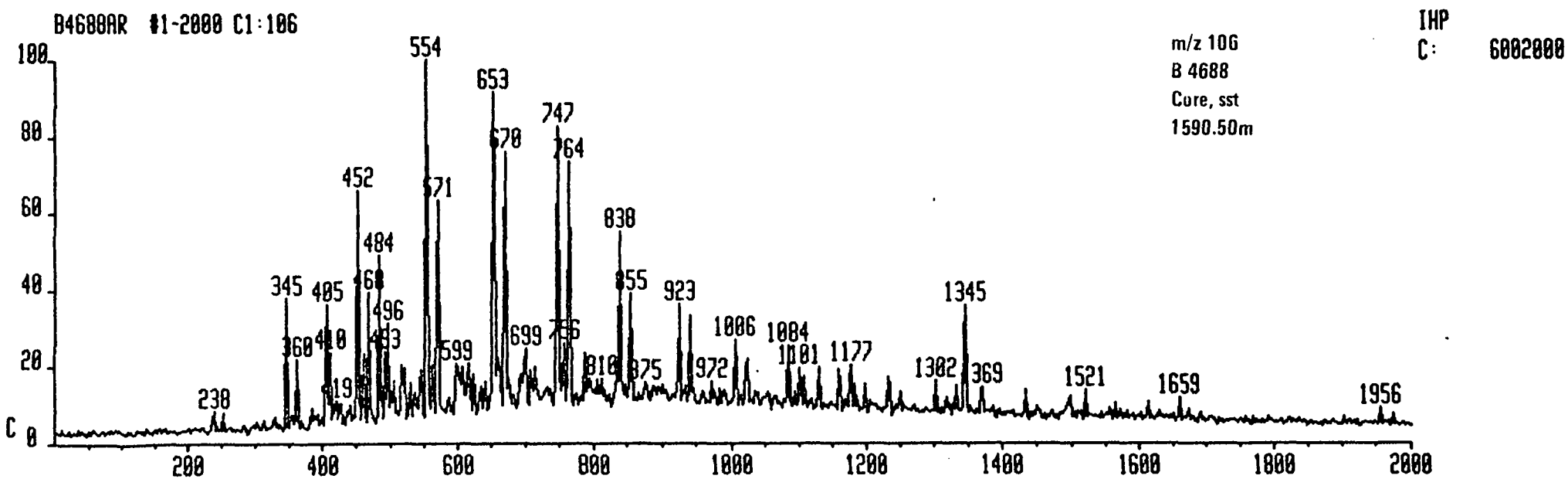
B4688AR #1-2000 C1:106
m/z 106
B 4688
Core, sst
1590.50m
IHP
C: 6002000
C 0
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60
40
20
200
400
600
800
1000
1200
1400
1600
1800
2000
554
653
747
670
764
452
571
838
484
855
923
1345
345
405
468
496
1006
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810
875
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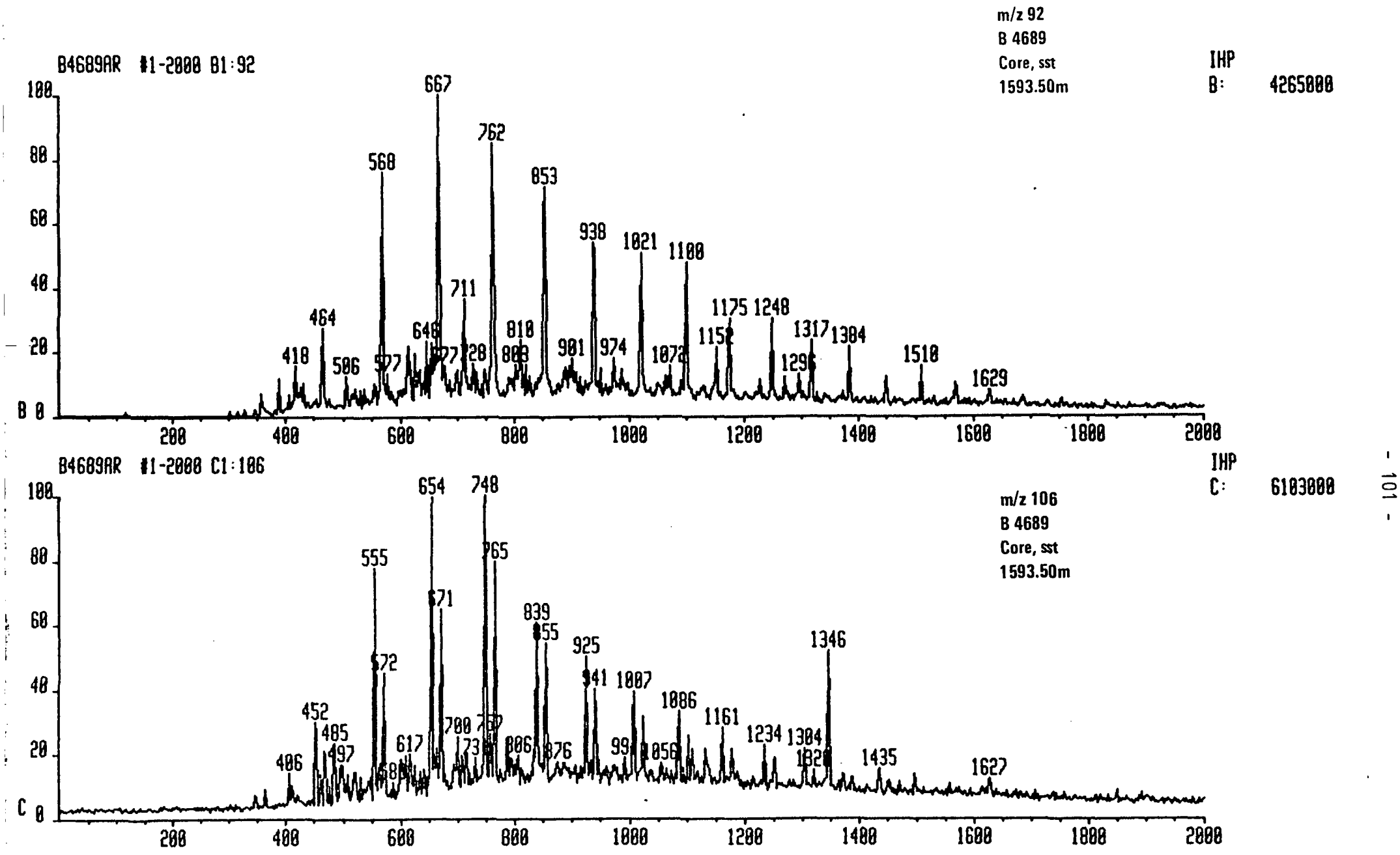
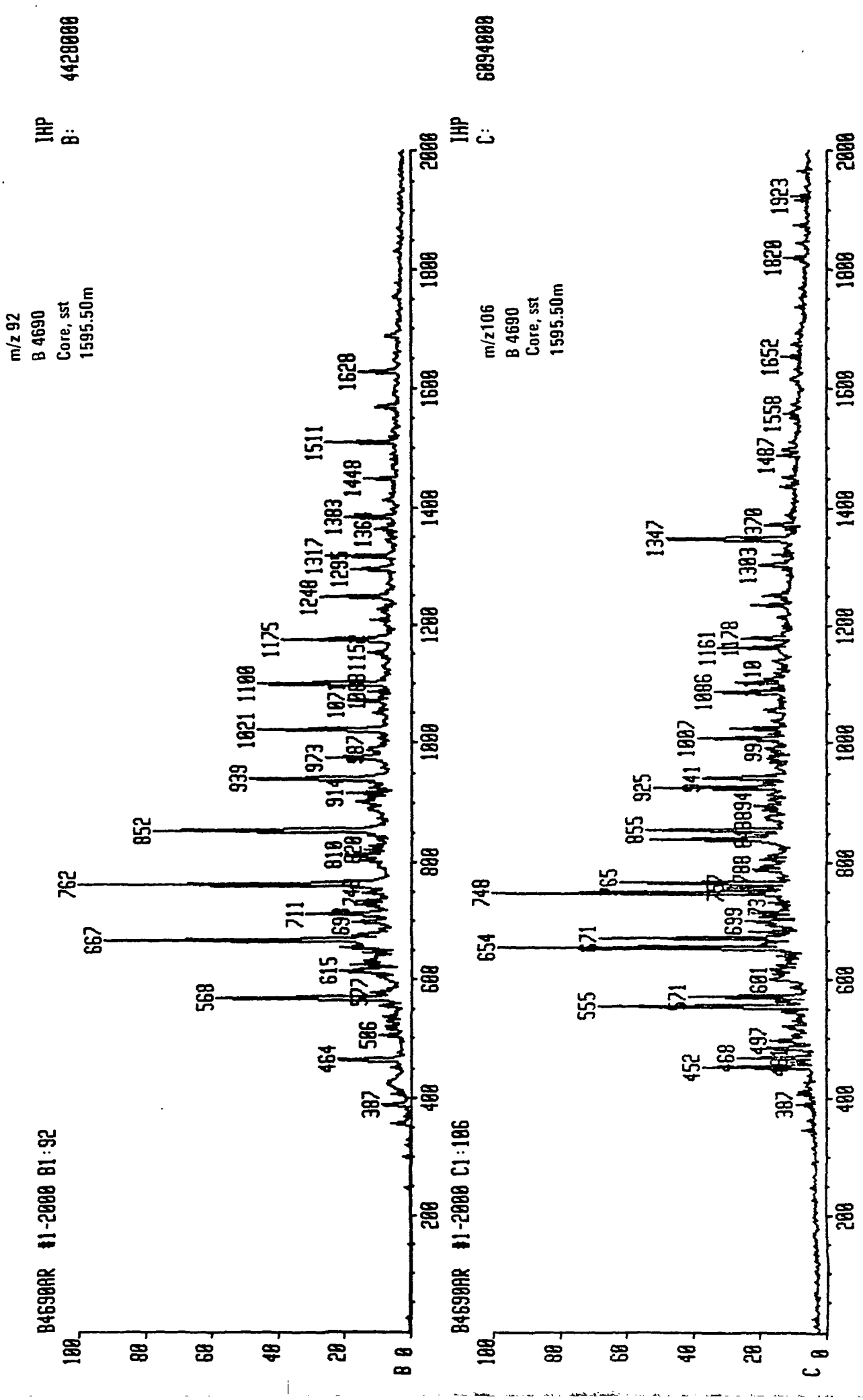
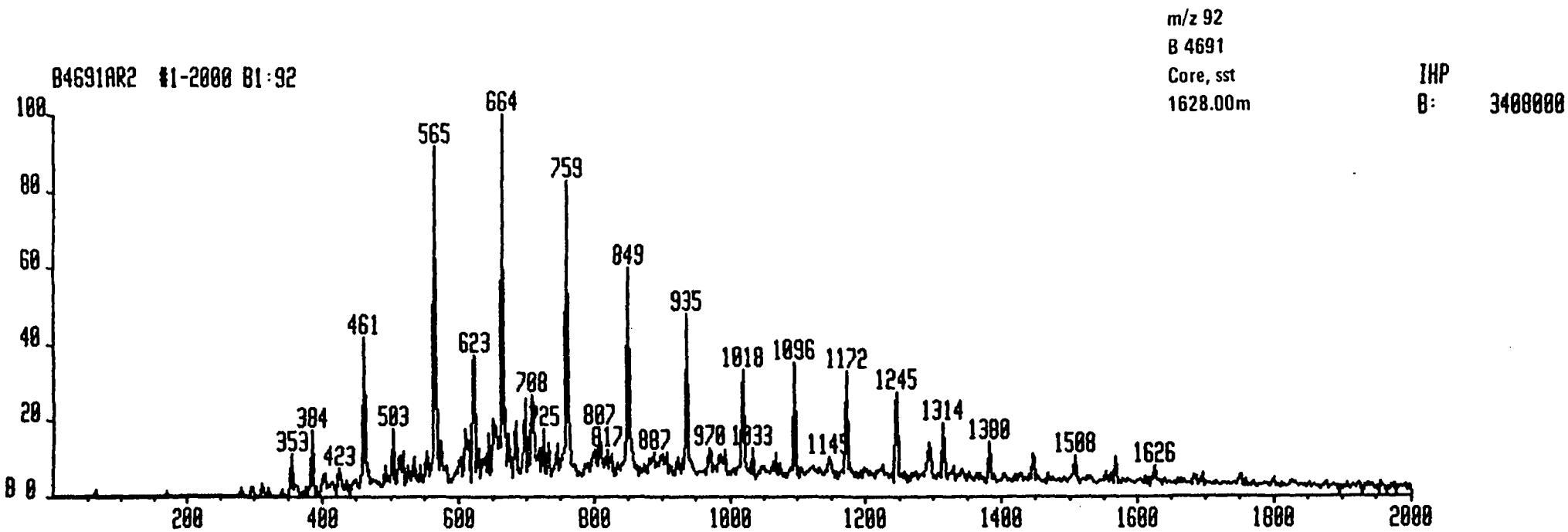

B4689AR #1-2000 B1:92
m/z 92
B 4689
Core, sst
1593.50m
IHP
B: 4265000
B4689AR #1-2000 C1:106
m/z 106
B 4689
Core, sst
1593.50m
IHP
C: 6103000


B4690AR #1-2000 B1:92
m/z 92
B 4690
Core, sst
1595.50m
IHP
B: 4428000
B 0
C1:106
m/z106
C: 6894000
C 0


B4691AR2 #1-2000 B1:92
m/z 92
B 4691
Core, sst
1628.00m
IHP
B: 3408000
B
100
80
60
40
20
0
200
400
600
800
1000
1200
1400
1600
1800
2000
353
384
423
461
503
565
623
664
708
725
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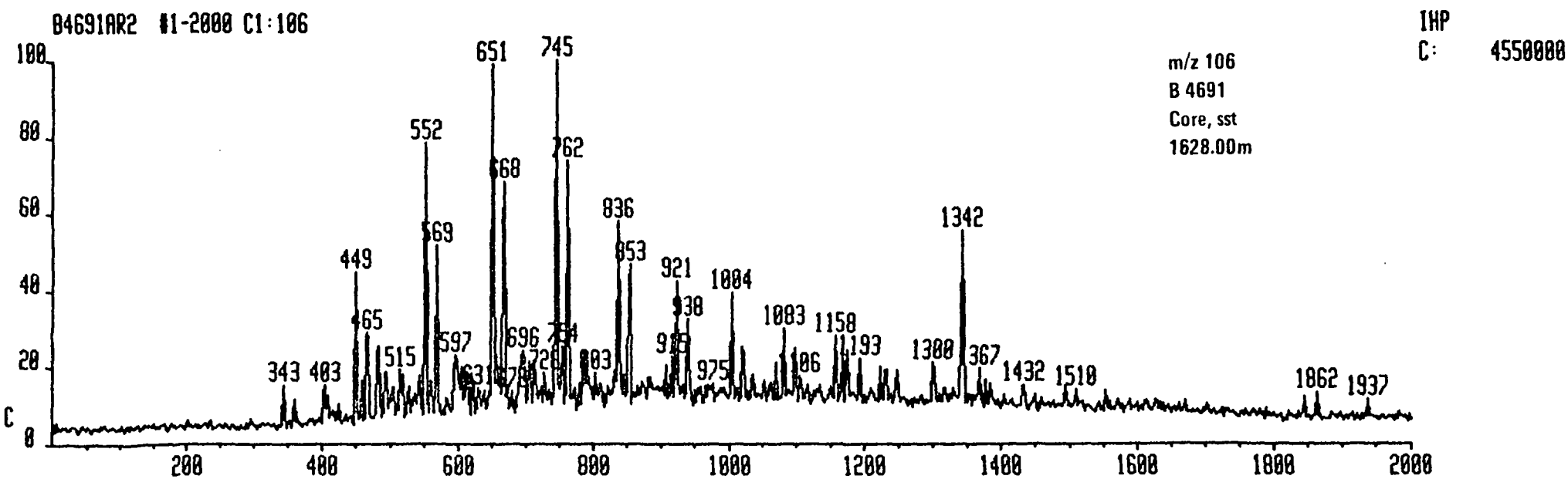
B4691AR2 #1-2000 C1:106
m/z 106
B 4691
Core, sst
1628.00m
IHP
C: 4550000
C
100
80
60
40
20
0
200
400
600
800
1000
1200
1400
1600
1800
2000
343
403
449
465
515
552
569
597
631
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762
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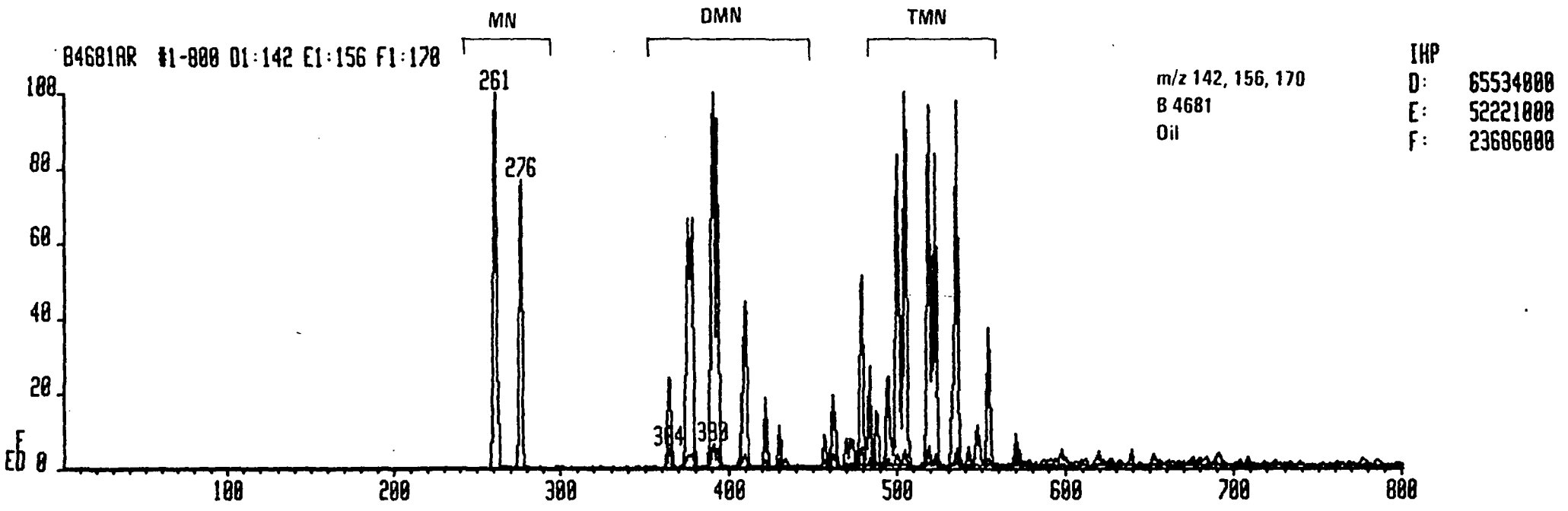
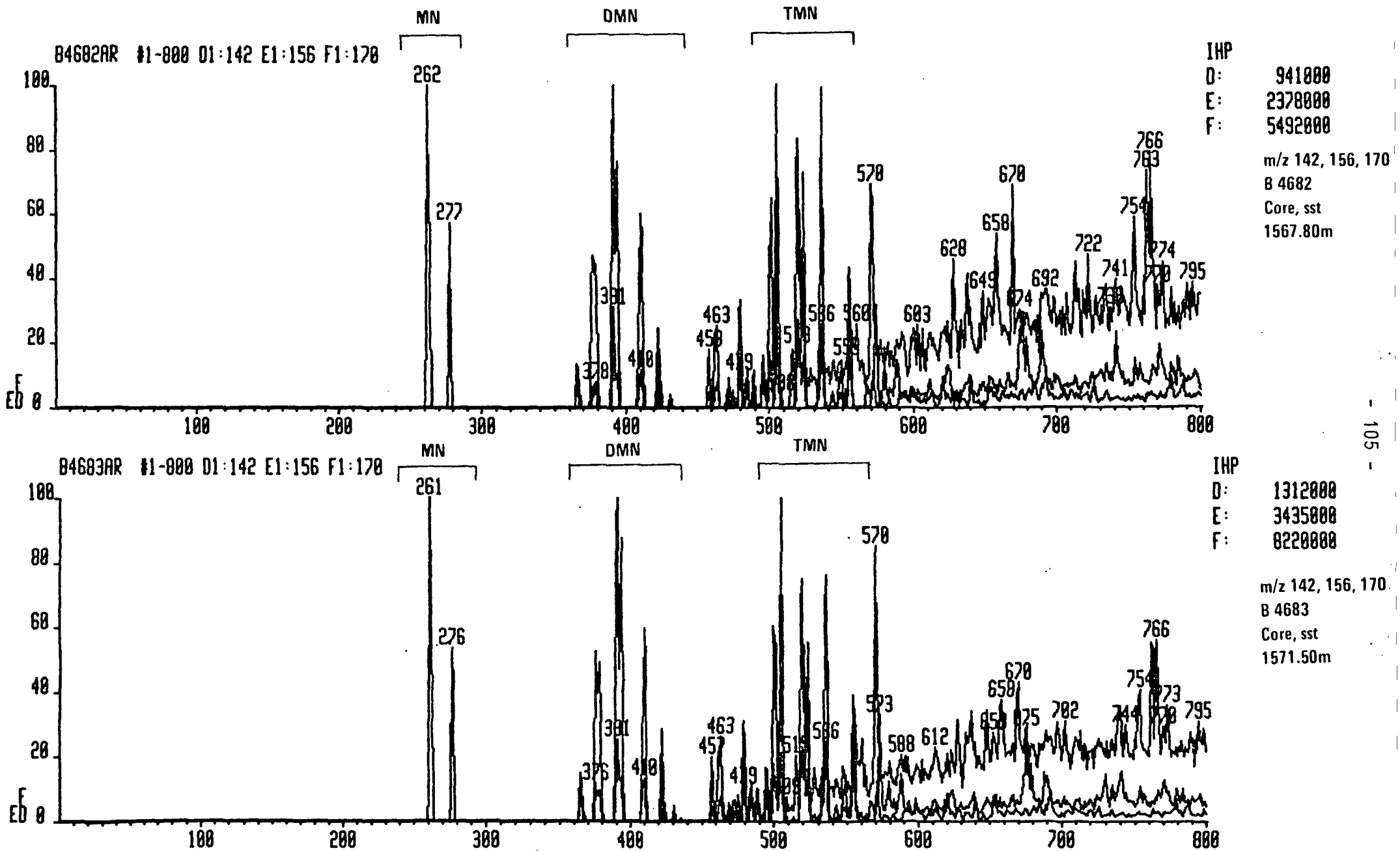
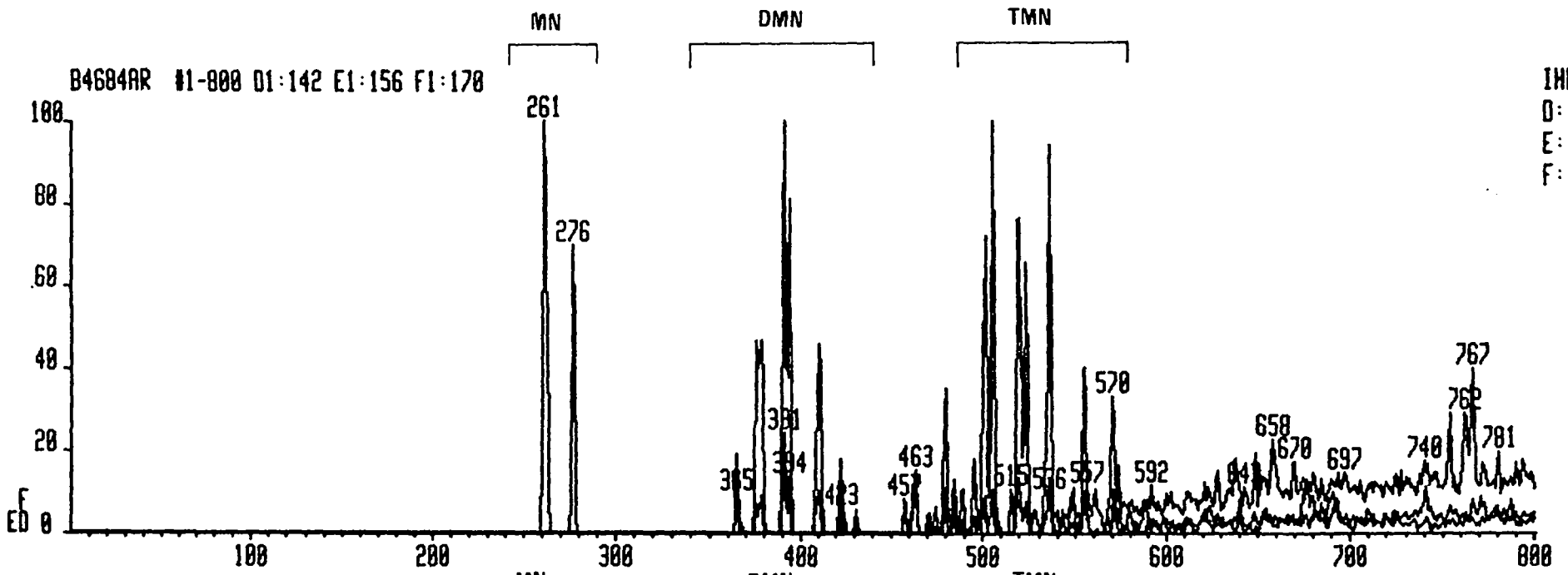
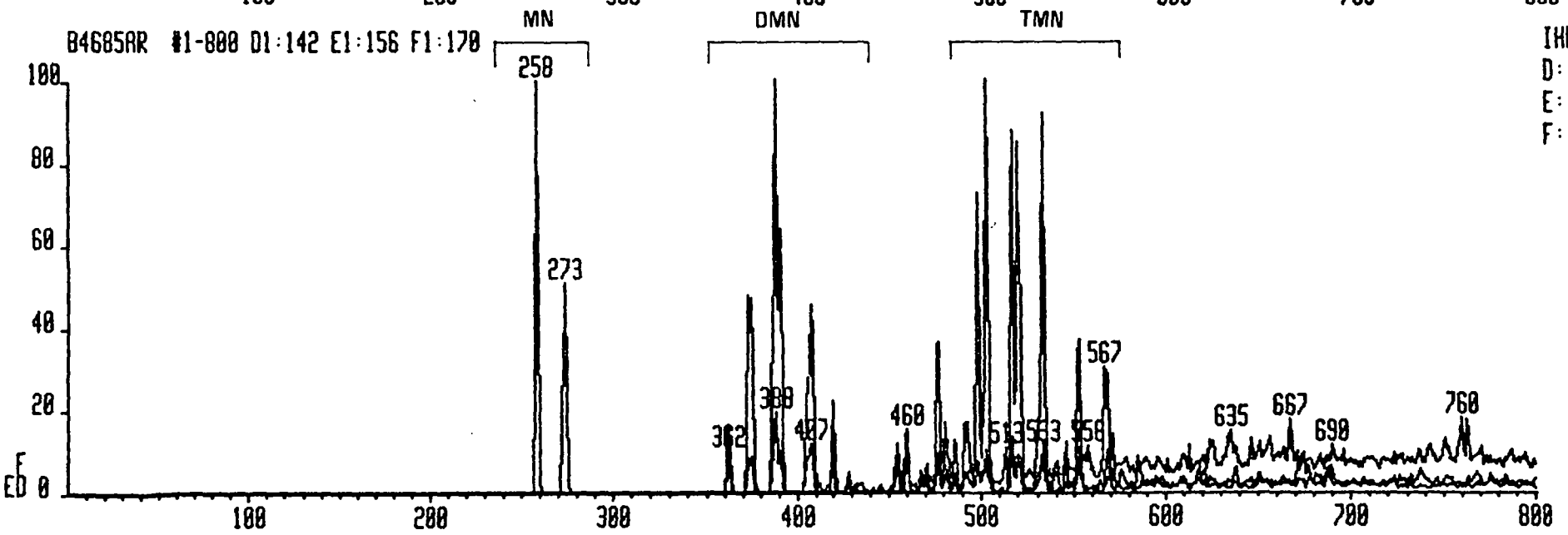

MN
DMN
TMN
B4681AR #1-800 D1:142 E1:156 F1:170
261
276
384
388
100
80
60
40
20
0
E
F
100
200
300
400
500
600
700
800
m/z 142, 156, 170
B 4681
Oil
IHP
D: 65534000
E: 52221000
F: 23686000


MN
DMN
TMN
B4682AR #1-800 D1:142 E1:156 F1:170
IHP
D: 941000
E: 2378000
F: 5492000
m/z 142, 156, 170
B 4682
Core, sst
1567.80m
B4683AR #1-800 D1:142 E1:156 F1:170
IHP
D: 1312000
E: 3435000
F: 8220000
m/z 142, 156, 170
B 4683
Core, sst
1571.50m



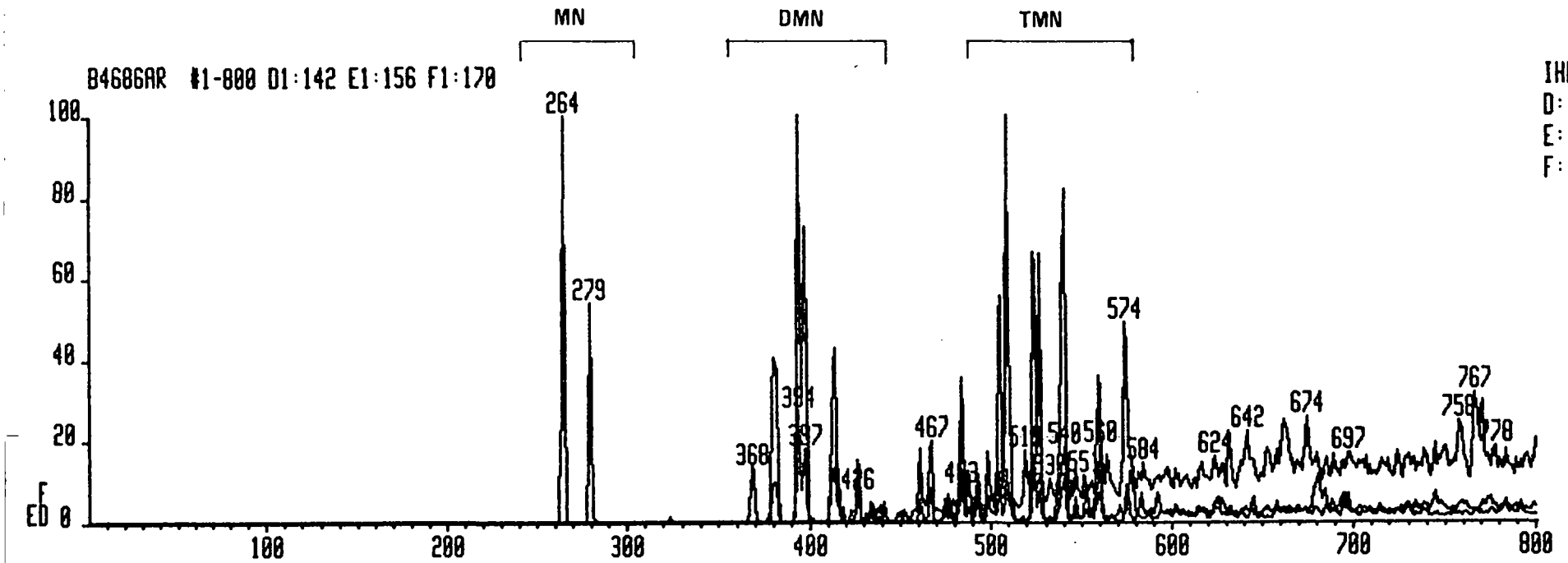
IHP
D: 2003000
E: 4655000
F: 5721000

m/z 142, 156, 170
B 4684
Core, sst
1573.95m



IHP
D: 4682000
E: 11676000
F: 13197000

m/z 142, 156, 170
B 4685
Core, sst
1581.65m


MN
DMN
TMN
B4686AR #1-800 D1:142 E1:156 F1:170
IHP
D: 3355000
E: 11199000
F: 14606000
m/z 142, 156, 170
B 4686
Core, sst
1586.40m
264
279
368
394
397
426
467
574
584
624
642
674
697
767
758
778
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100
200
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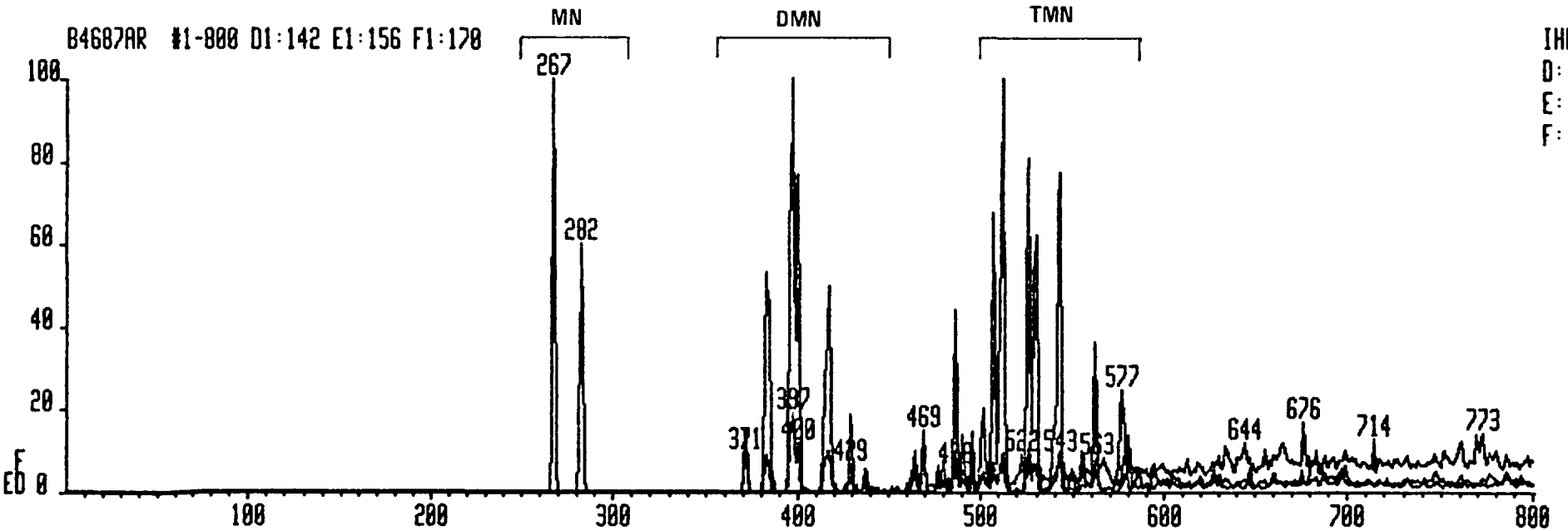
500
600
700
800


MN
DMN
TMN
B4687AR #1-800 D1:142 E1:156 F1:170
IHP
D: 5644000
E: 13065000
F: 13781000
m/z 142, 156, 170
B 4687
Core, sst
1587.50m
267
282
371
397
400
429
469
577
644
676
714
773
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80
60
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100
200
300
400
500
600
700
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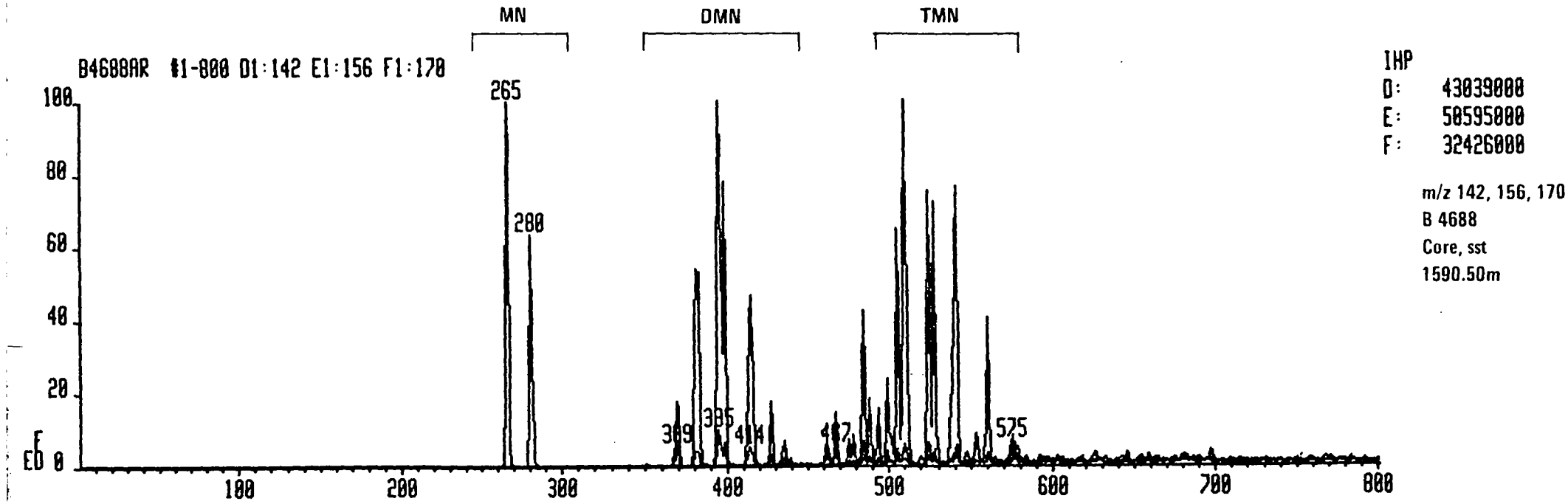
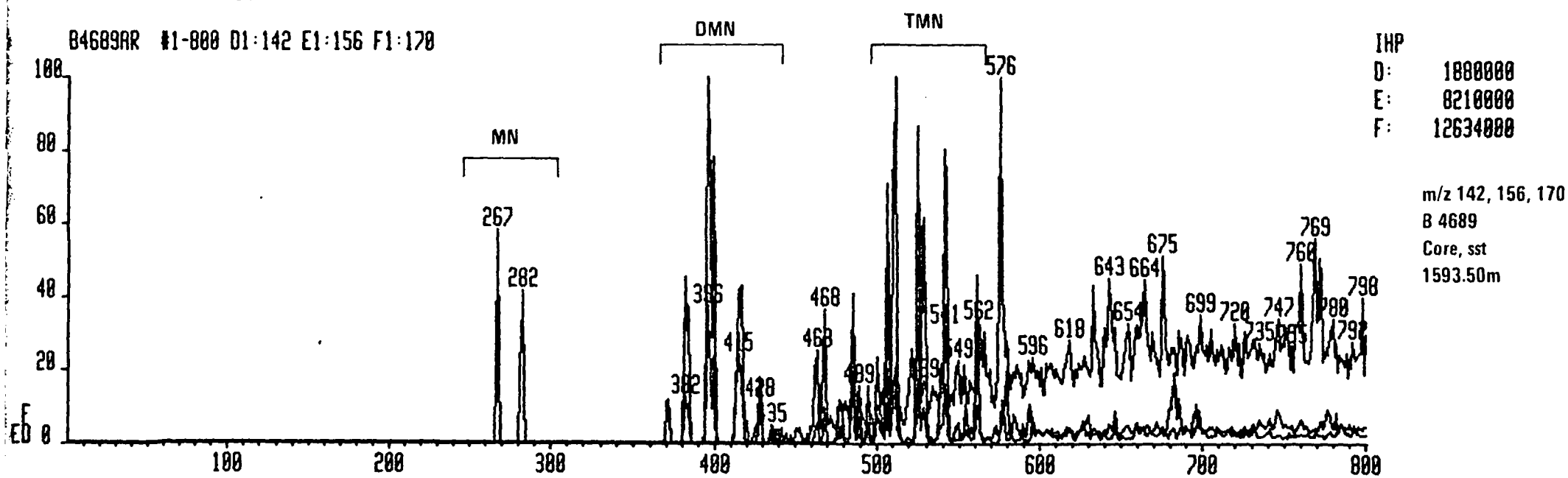

B4688AR #1-800 D1:142 E1:156 F1:170
MN
DMN
TMN
IHP
D: 43039000
E: 50595000
F: 32426000
m/z 142, 156, 170
B 4688
Core, sst
1590.50m
265
280
389
395
414
467
575
100
80
60
40
20
0
100
200
300
400
500
600
700
800


B4689AR #1-800 D1:142 E1:156 F1:170
MN
DMN
TMN
IHP
D: 1880000
E: 8210000
F: 12634000
m/z 142, 156, 170
B 4689
Core, sst
1593.50m
267
282
382
386
415
428
435
468
468
489
489
541
549
562
576
596
618
643
654
664
675
699
720
735
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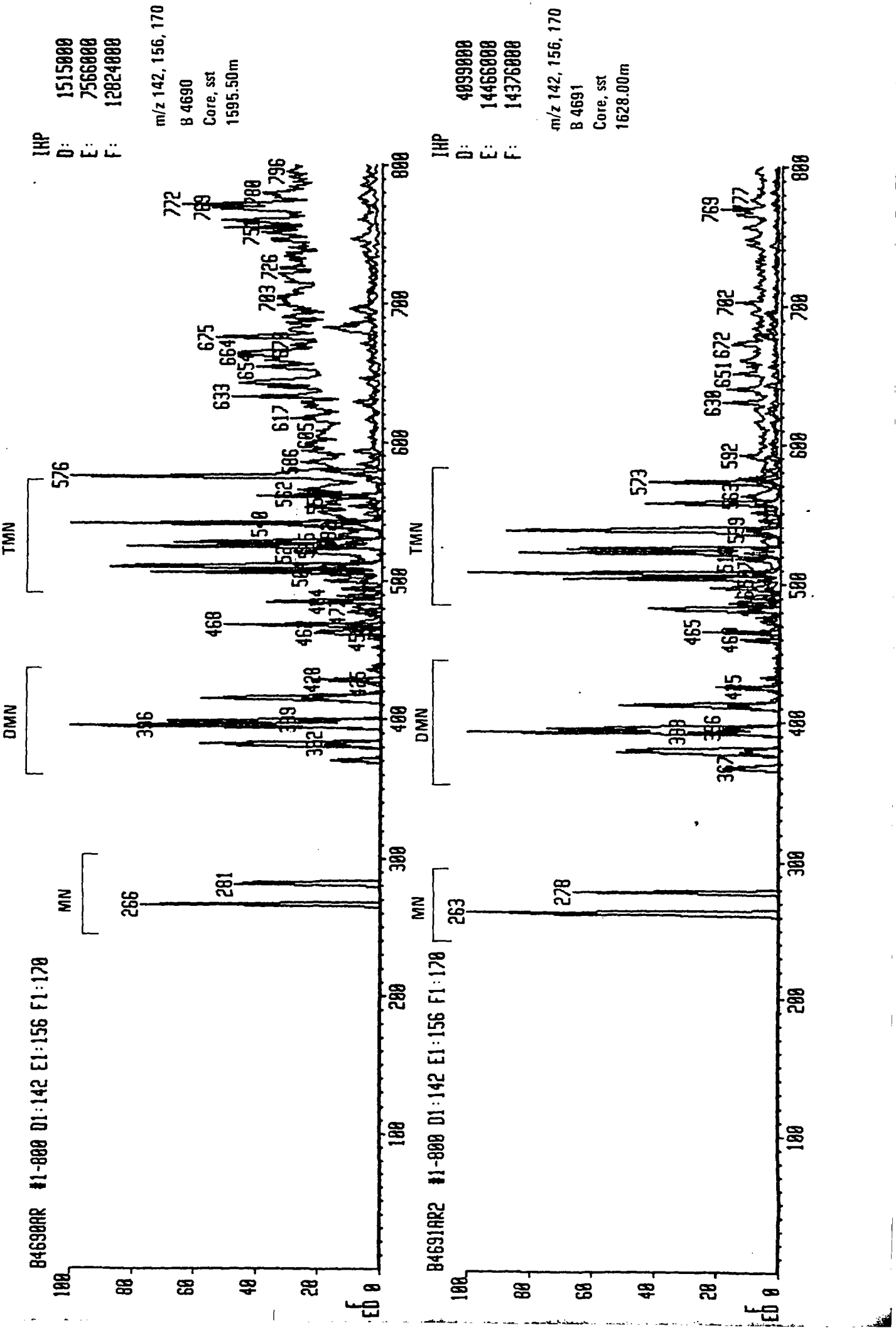
B4690AR #1-800 D1:142 E1:156 F1:170
MN
DMN
TMN
m/z 142, 156, 170
B 4690
Core, sst
1595.50m
IHP
D: 1515000
E: 7566000
F: 12824000
B4691AR2 #1-800 D1:142 E1:156 F1:170
MN
DMN
TMN
m/z 142, 156, 170
B 4691
Core, sst
1628.00m
IHP
D: 4099000
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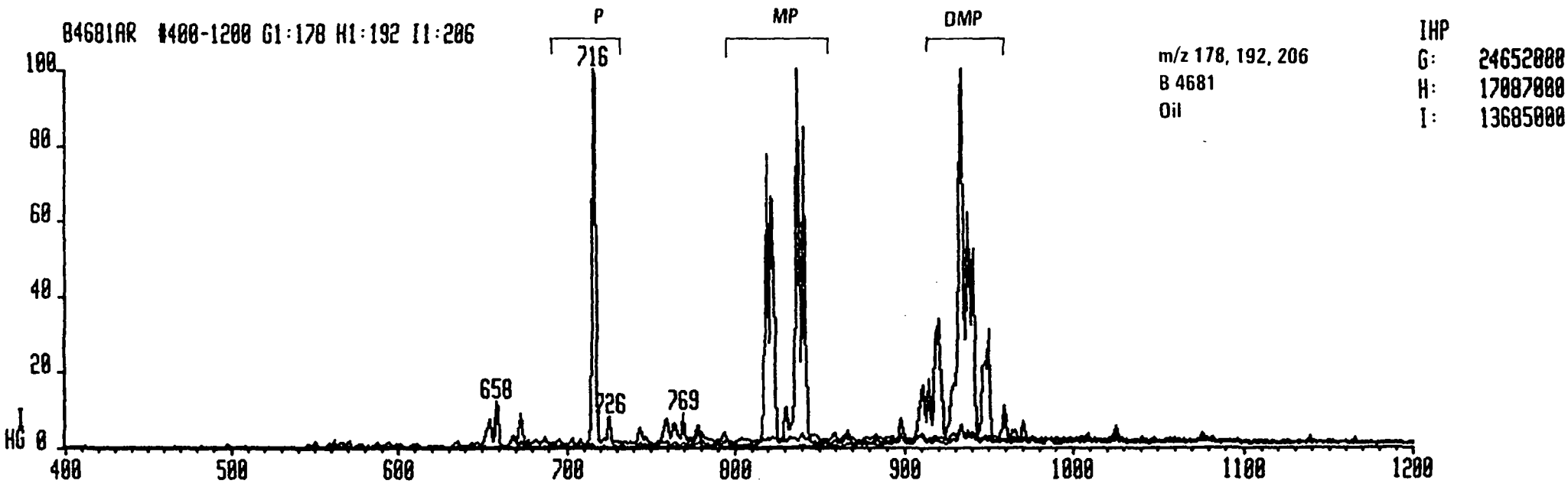
F: 14376000


B4681AR #400-1200 G1:178 H1:192 I1:206
P
MP
DMP
716
658
726
769
m/z 178, 192, 206
B 4681
Oil
IHP
G: 24652000
H: 17007000
I: 13685000
100
80
60
40
20
I
HG 0
400
500
600
700
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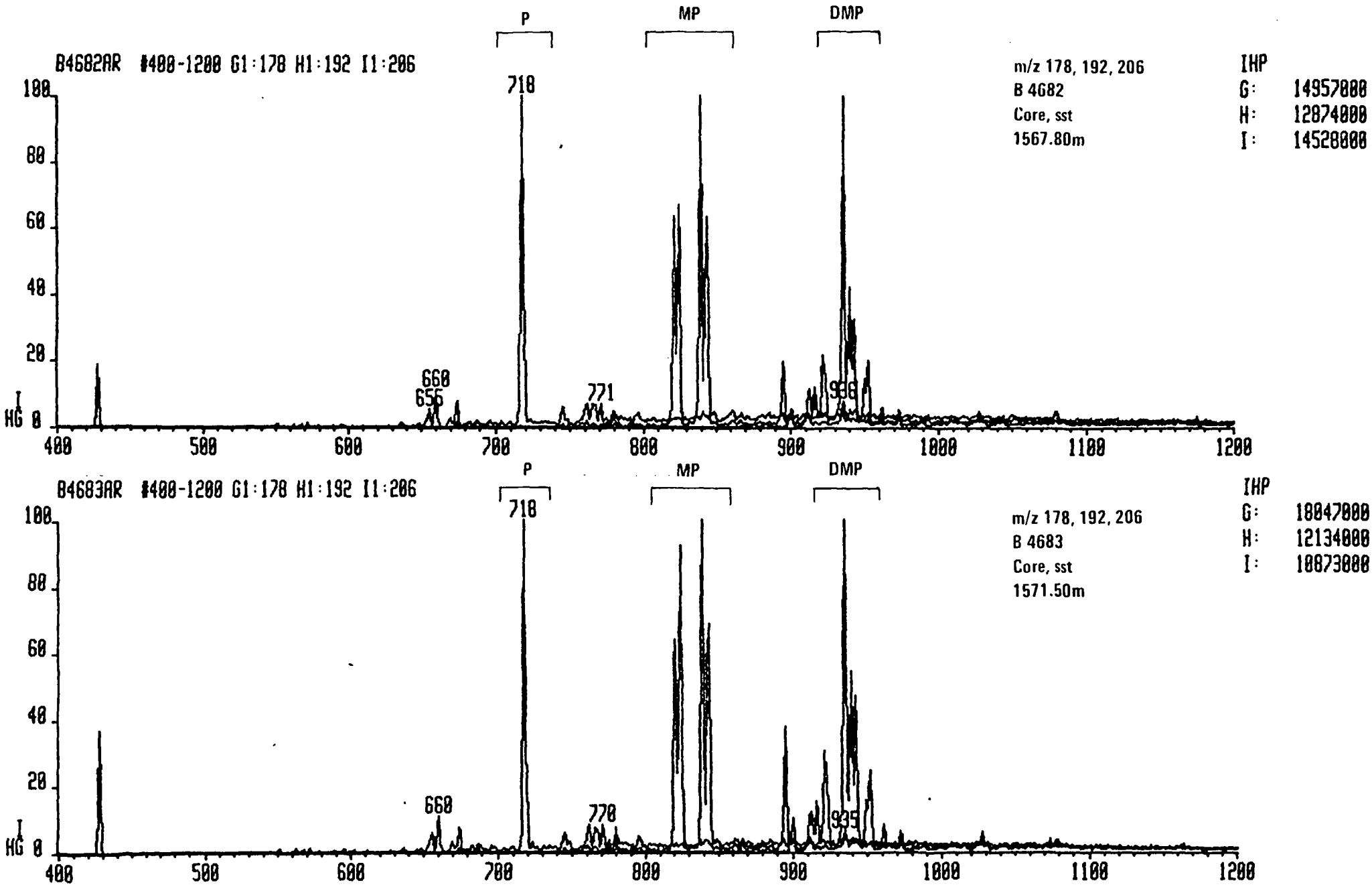
1100
1200


B4682AR #400-1200 G1:178 H1:192 I1:206
P
MP
DMP
718
660
656
771
908
m/z 178, 192, 206
B 4682
Core, sst
1567.80m
IHP
G: 14957000
H: 12874000
I: 14528000
B4683AR #400-1200 G1:178 H1:192 I1:206
718
660
770
935
m/z 178, 192, 206
B 4683
Core, sst
1571.50m
IHP
G: 18047000
H: 12134000
I: 18073000
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20
0
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500
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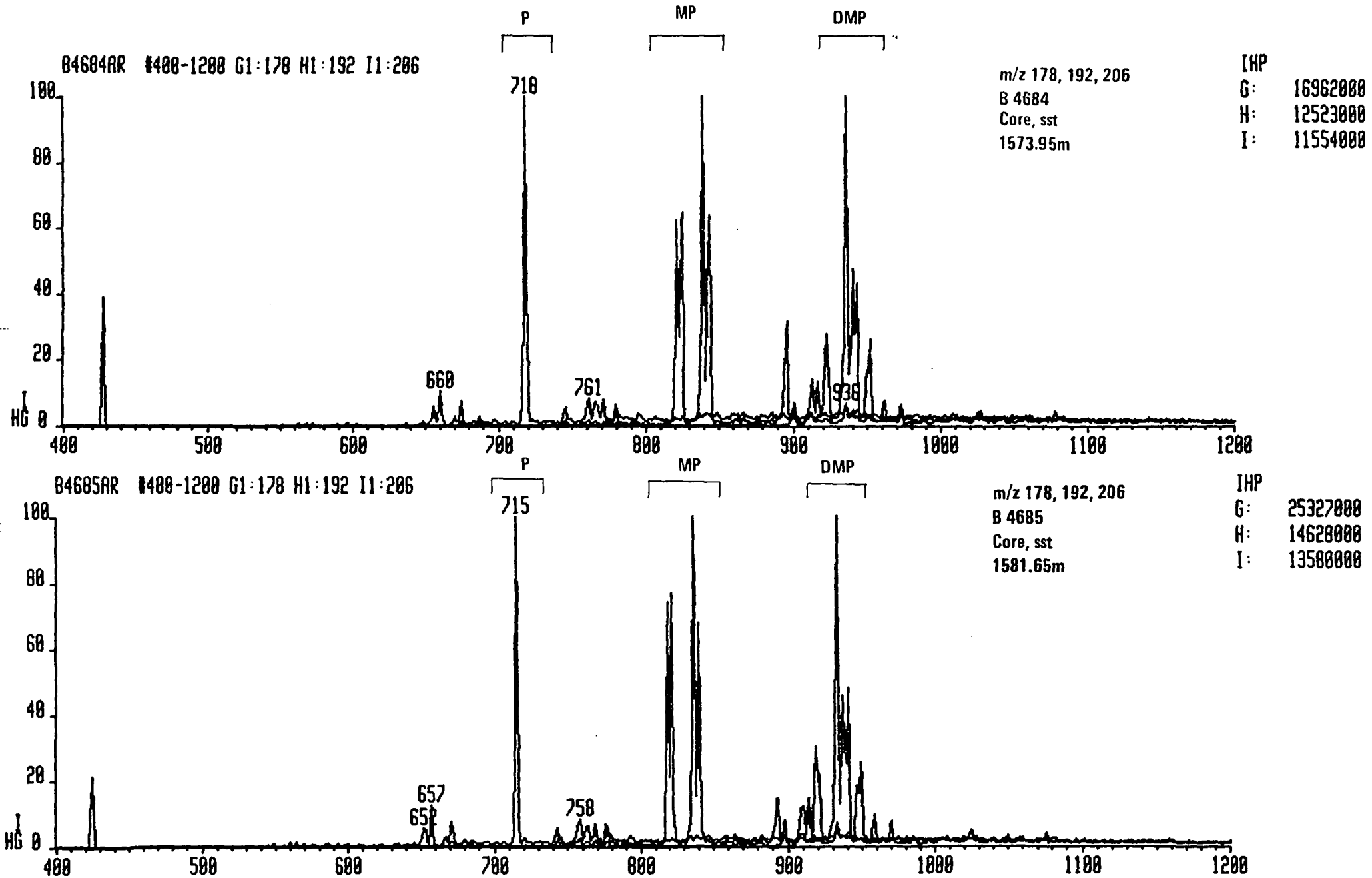
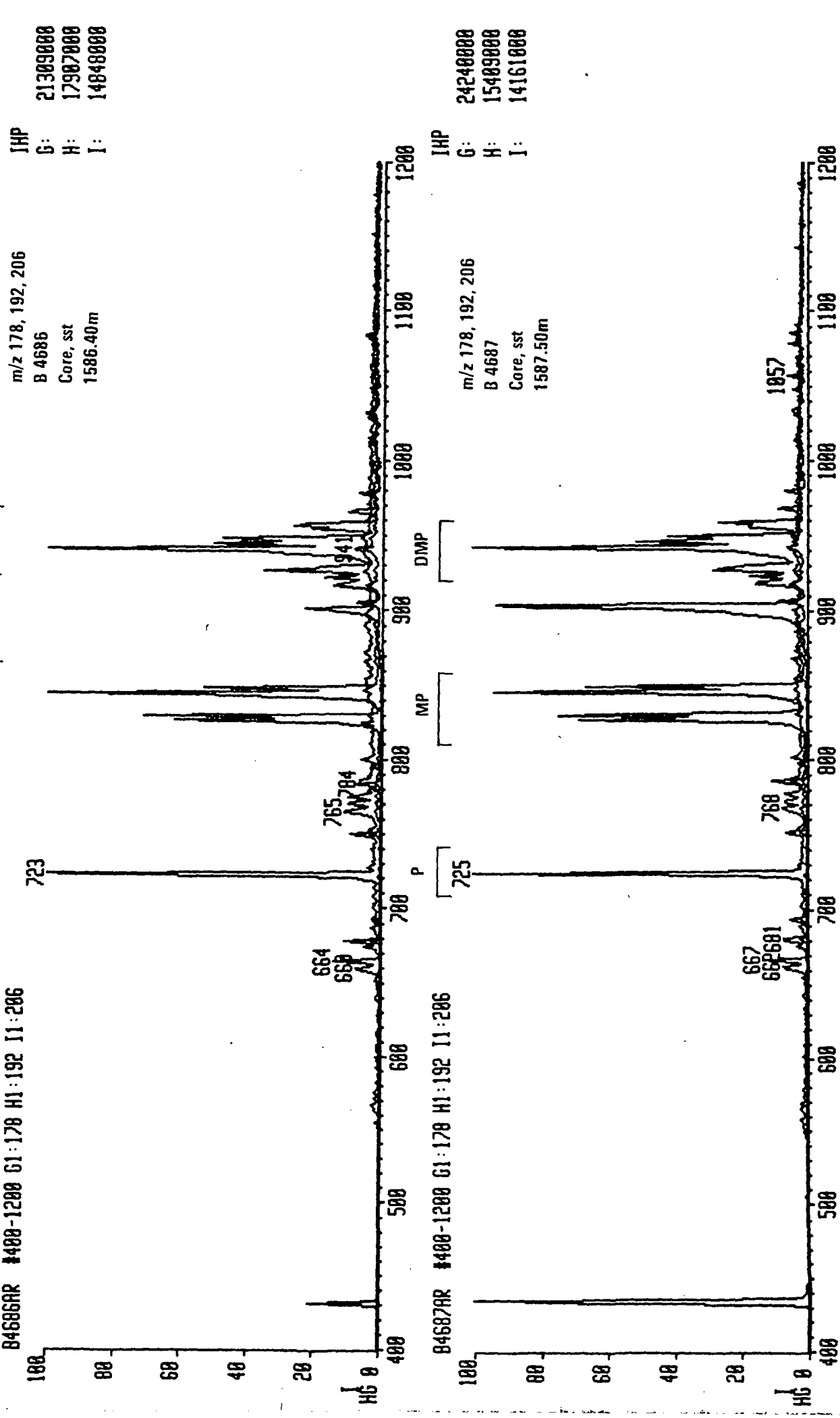

P
MP
DMP
B4684AR #400-1200 G1:178 H1:192 I1:206
718
660
761
936
m/z 178, 192, 206
B 4684
Core, sst
1573.95m
IHP
G: 16962000
H: 12523000
I: 11554000
B4685AR #400-1200 G1:178 H1:192 I1:206
715
657
658
758
m/z 178, 192, 206
B 4685
Core, sst
1581.65m
IHP
G: 25327000
H: 14628000
I: 13580000
100
80
60
40
20
HG 0
400
500
600
700
800
900
1000
1100
1200


B4686AR #400-1200 G1:178 H1:192 I1:206
m/z 178, 192, 206
B 4686
Core, sst
1586.40m
IHP
G: 21309000
H: 17987000
I: 14848000
P
MP
DMP
723
765
784
941
664
669
B4687AR #400-1200 G1:178 H1:192 I1:206
m/z 178, 192, 206
B 4687
Core, sst
1587.50m
IHP
G: 24240000
H: 15409000
I: 14161000
725
768
1057
667
681
HC
100
80
60
40
20
0
400
500
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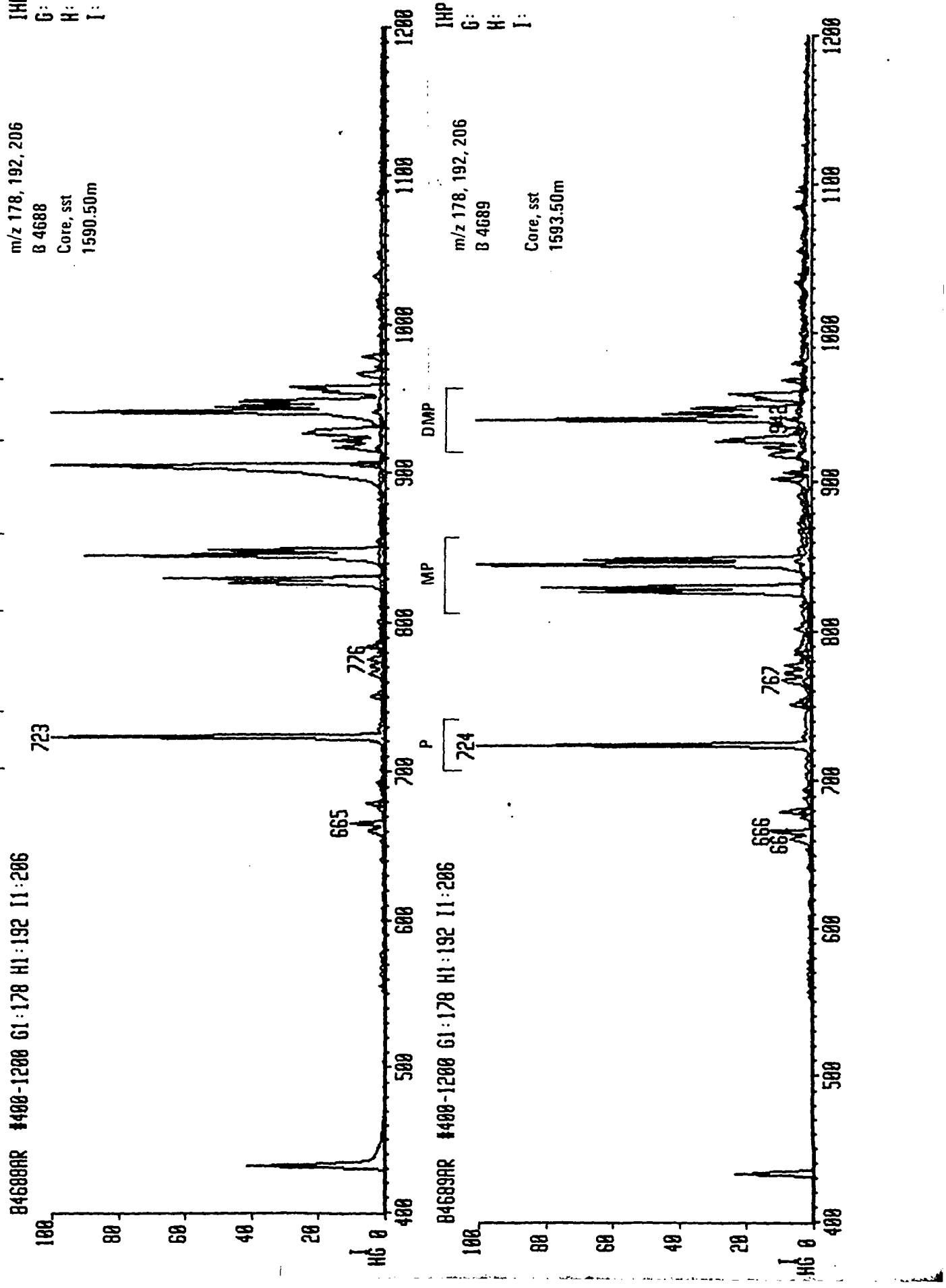
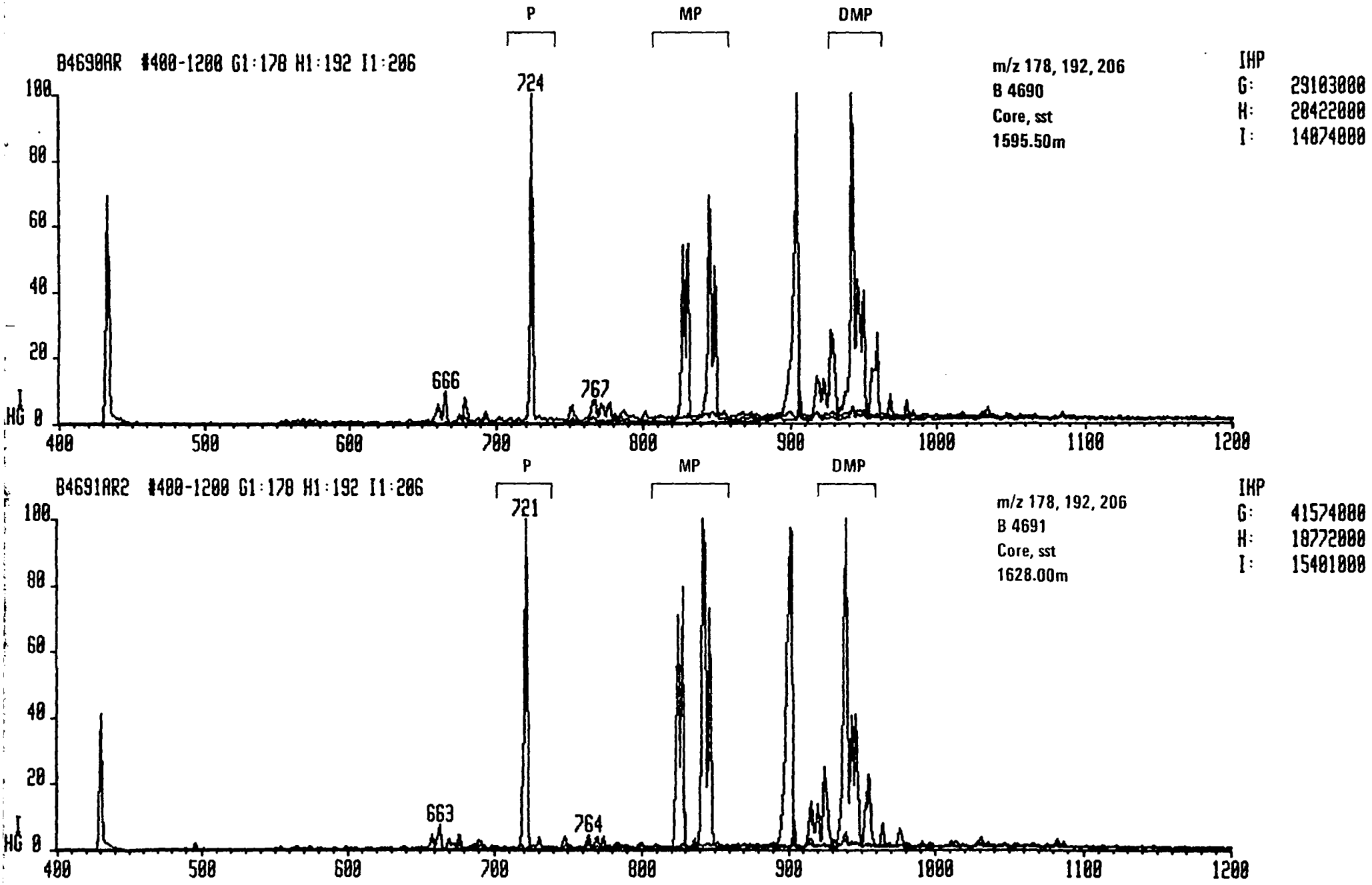
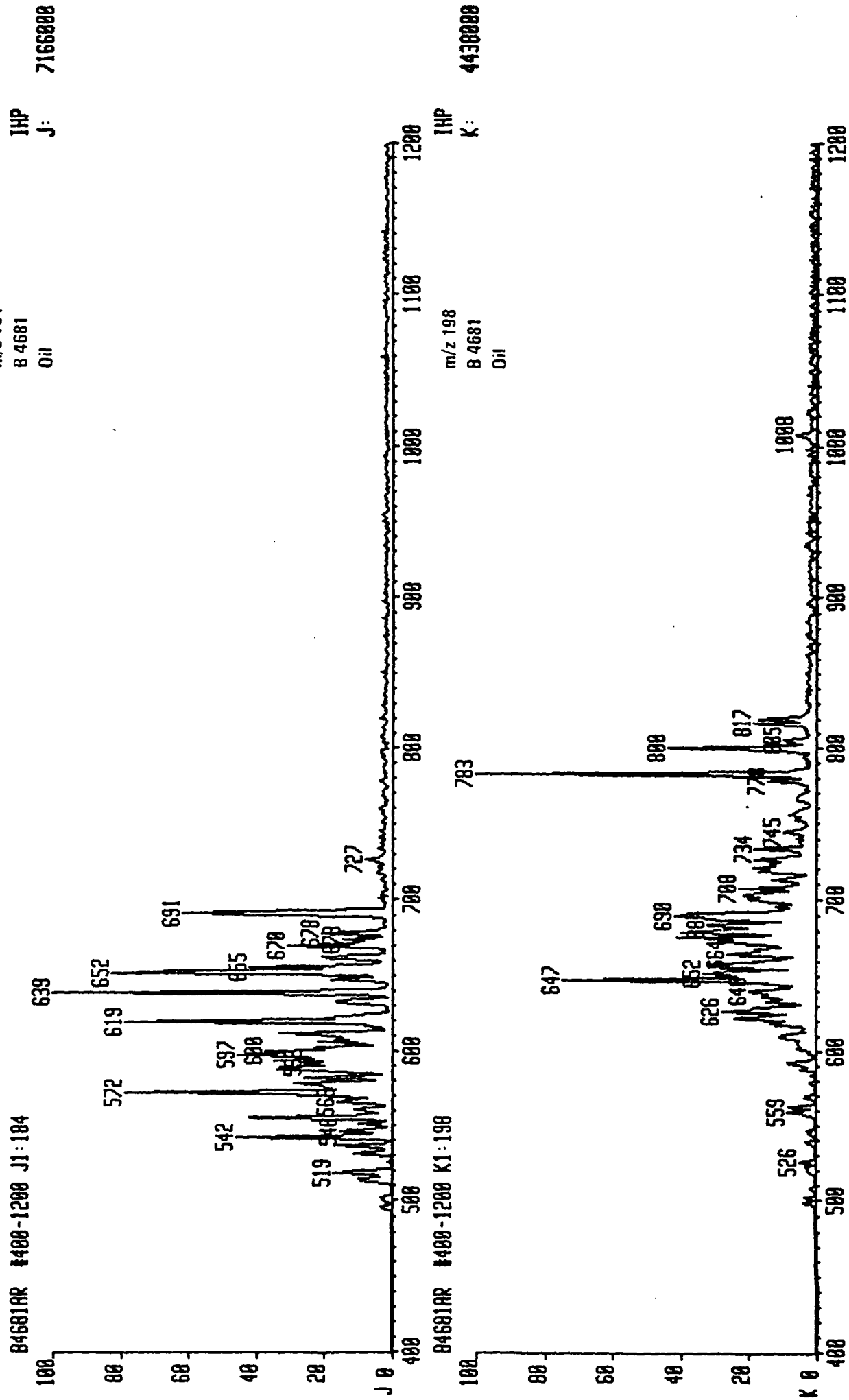
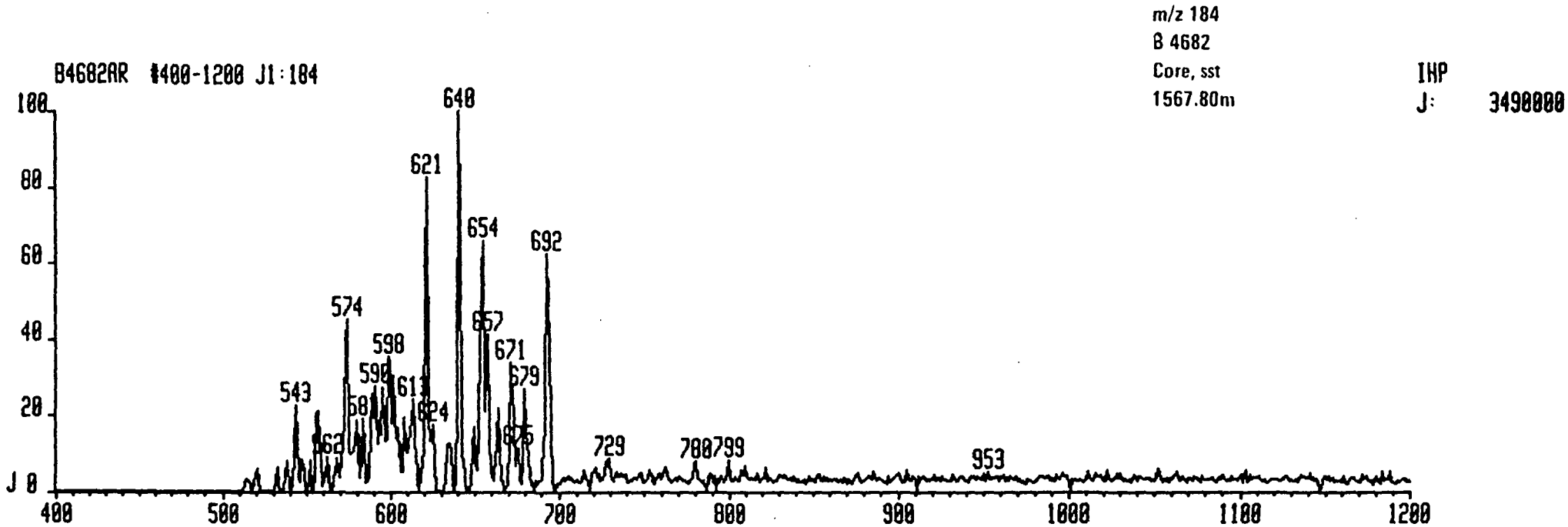
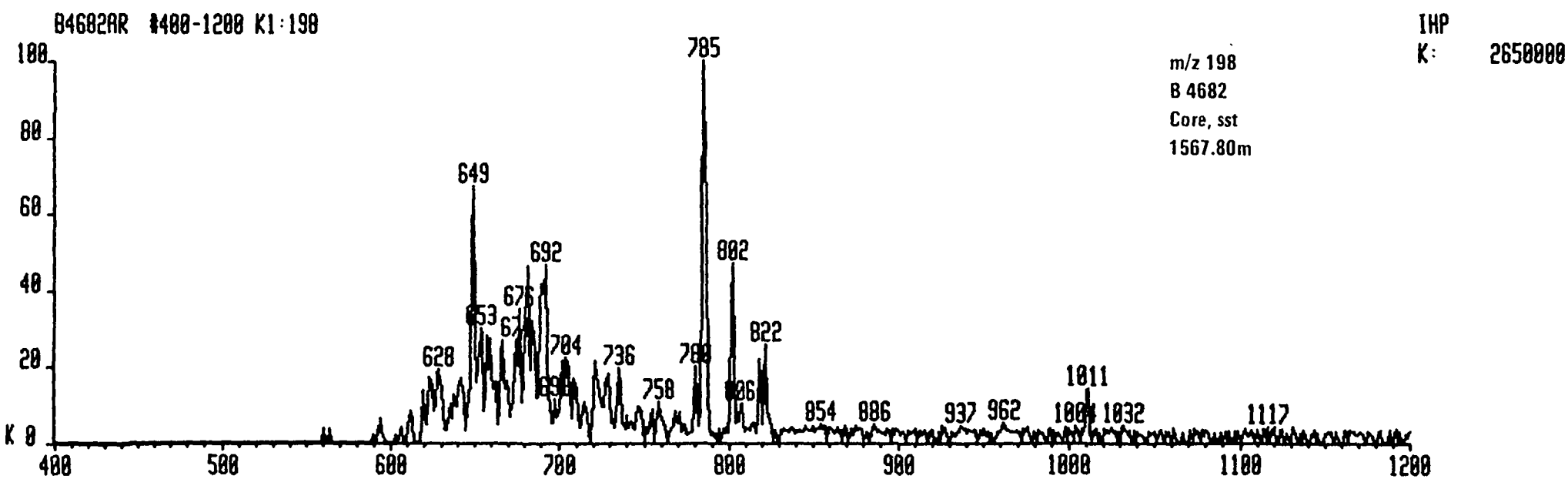
800
900
1000
1100
1200

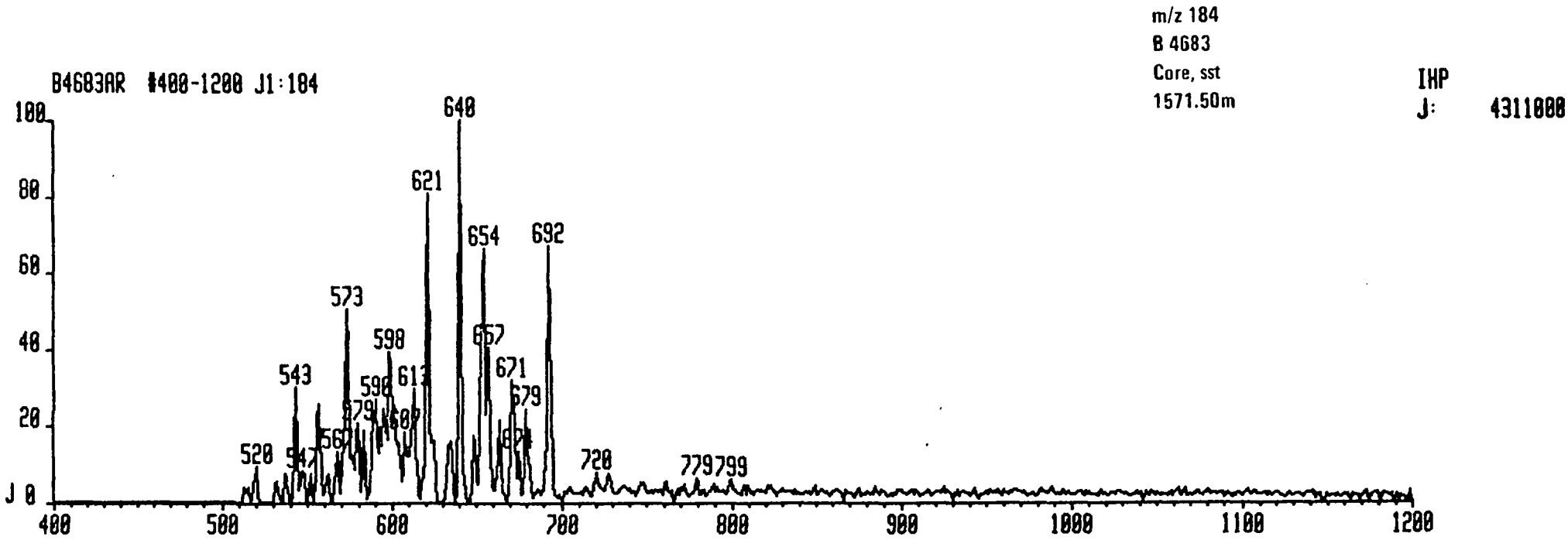

B4688AR #400-1200 G1:178 H1:192 I1:206
m/z 178, 192, 206
B 4688
Core, sst
1590.50m
IHP
G: 49536000
H: 33966000
I: 18494000
P
MP
DMP
723
665
776
B4689AR #400-1200 G1:178 H1:192 I1:206
m/z 178, 192, 206
B 4689
Core, sst
1593.50m
IHP
G: 25164000
H: 14176000
I: 14633000
724
666
767
944


P
MP
DMP
B4690AR #400-1200 G1:178 H1:192 I1:206
724
666
767
m/z 178, 192, 206
B 4690
Core, sst
1595.50m
IHP
G: 29103000
H: 20422000
I: 14074000
100
80
60
40
20
0
HG
400
500
600
700
800
900
1000
1100
1200
P
MP
DMP
B4691AR2 #400-1200 G1:178 H1:192 I1:206
721
663
764
m/z 178, 192, 206
B 4691
Core, sst
1628.00m
IHP
G: 41574000
H: 18772000
I: 15401000
100
80
60
40
20
0
HG
400
500
600
700
800
900
1000
1100
1200


B4681AR #400-1200 J1:184
m/z 184
B 4681
Oil
IHP
J: 7166000
B4681AR #400-1200 K1:198
m/z 198
B 4681
Oil
IHP
K: 4430000


m/z 184
B 4682
Core, sst
1567.80m
B4682AR #400-1200 J1:184
IHP
J: 3490000
640
621
654
692
574
657
598
671
590
679
543
613
624
729
780
799
953
J 0
100
80
60
40
20
400
500
600
700
800
900
1000
1100
1200


B4682AR #400-1200 K1:198
IHP
K: 2650000
m/z 198
B 4682
Core, sst
1567.80m
785
649
692
802
676
653
822
704
736
628
758
854
886
937
962
1011
1032
1117
K 0
100
80
60
40
20
400
500
600
700
800
900
1000
1100
1200


B4683AR #400-1200 J1:184
m/z 184
B 4683
Core, sst
1571.50m
IHP
J: 4311000
640
621
654
692
573
598
657
543
671
679
520
720
779
799
J 0
100
80
60
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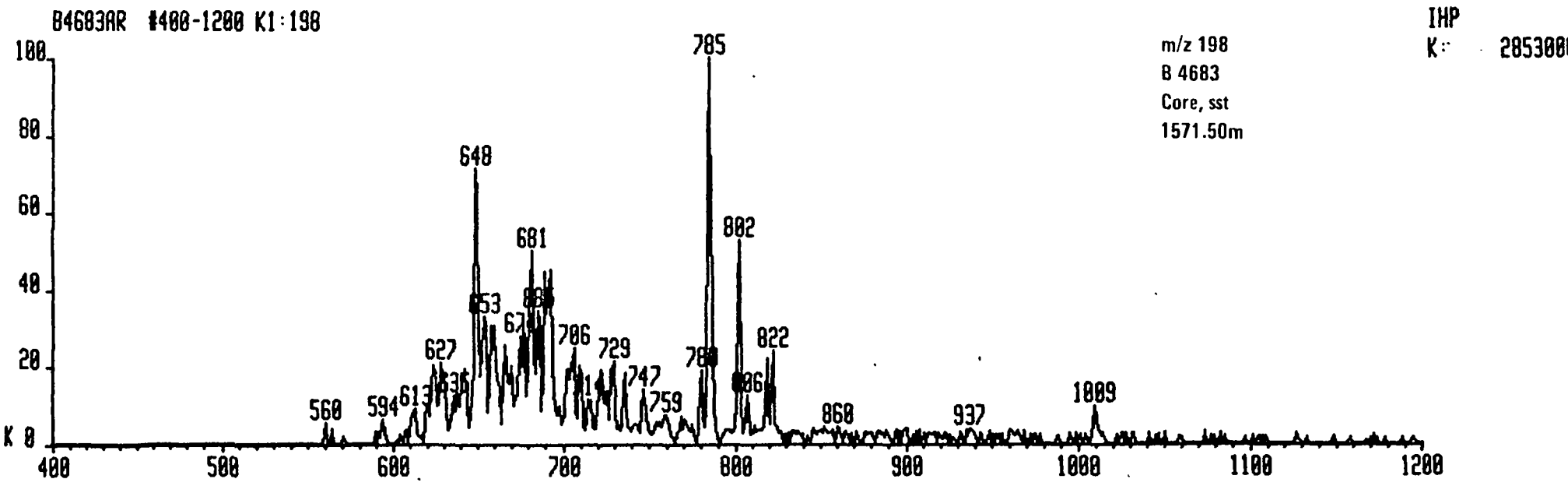
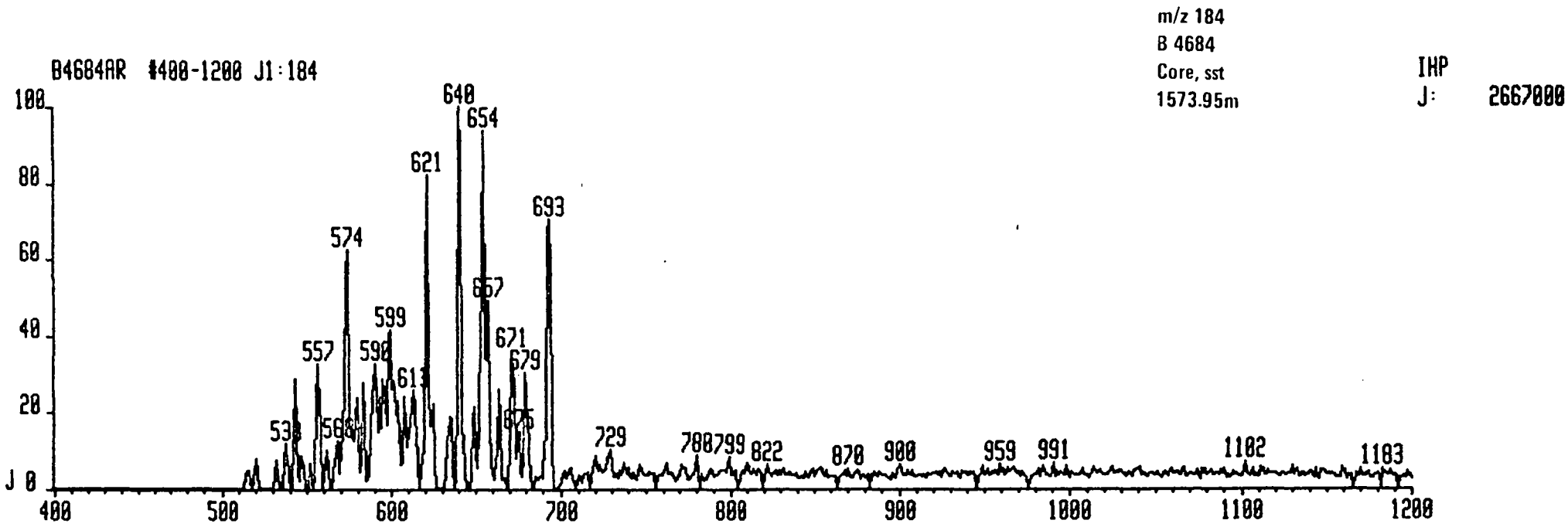
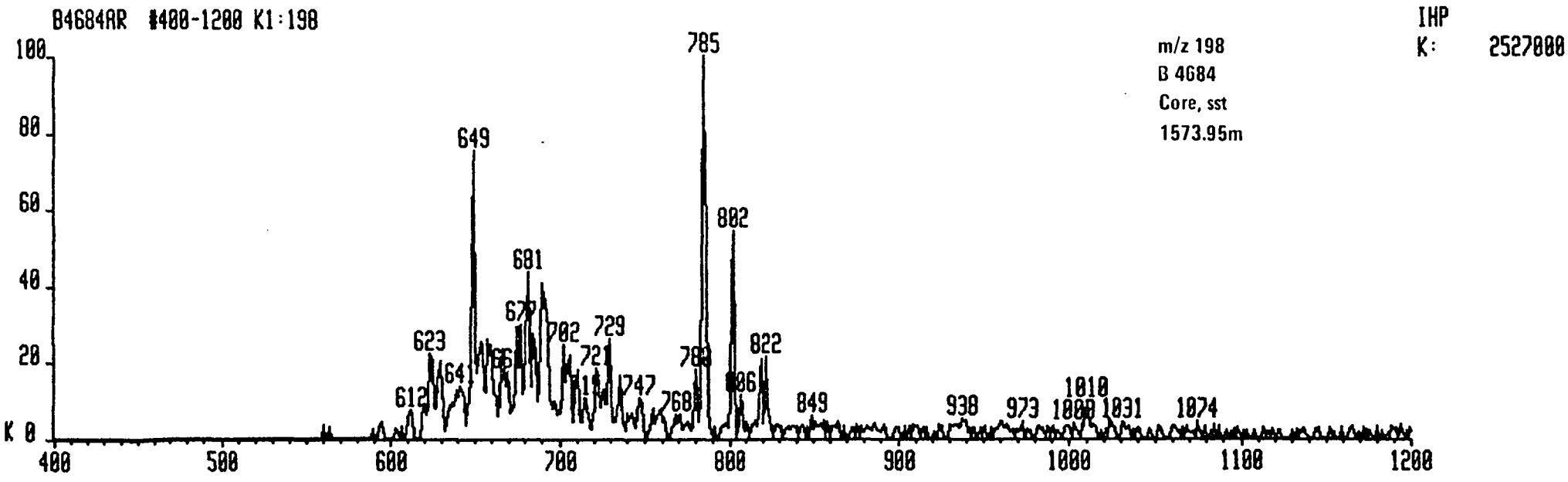
20
400
500
600
700
800
900
1000
1100
1200


B4683AR #400-1200 K1:198
m/z 198
B 4683
Core, sst
1571.50m
IHP
K: 2853000
785
648
681
802
627
706
729
822
747
759
560
594
860
937
1009
K 0
100
80
60
40
20
400
500
600
700
800
900
1000
1100
1200


B4684AR #400-1200 J1:184
m/z 184
B 4684
Core, sst
1573.95m
IHP
J: 2667000
640
654
621
693
574
657
599
671
557
590
679
613
538
566
675
729
780
799
822
870
900
959
991
1102
1183
J 0
100
80
60
40
20
400
500
600
700
800
900
1000
1100
1200


B4684AR #400-1200 K1:198
m/z 198
B 4684
Core, sst
1573.95m
IHP
K: 2527000
785
649
802
681
677
702
729
623
721
822
612
641
747
768
849
938
973
1010
1031
1074
K 0
100
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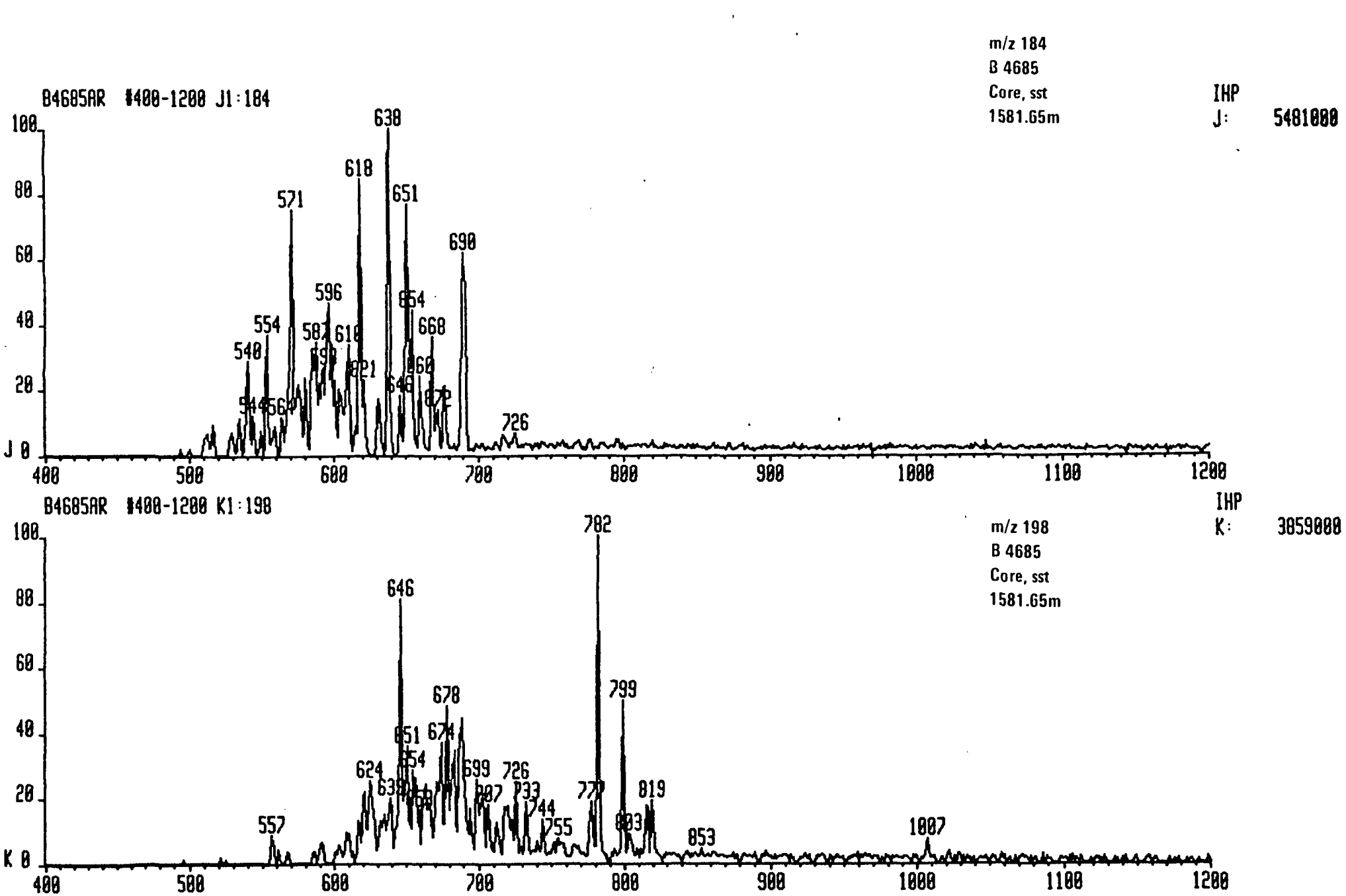
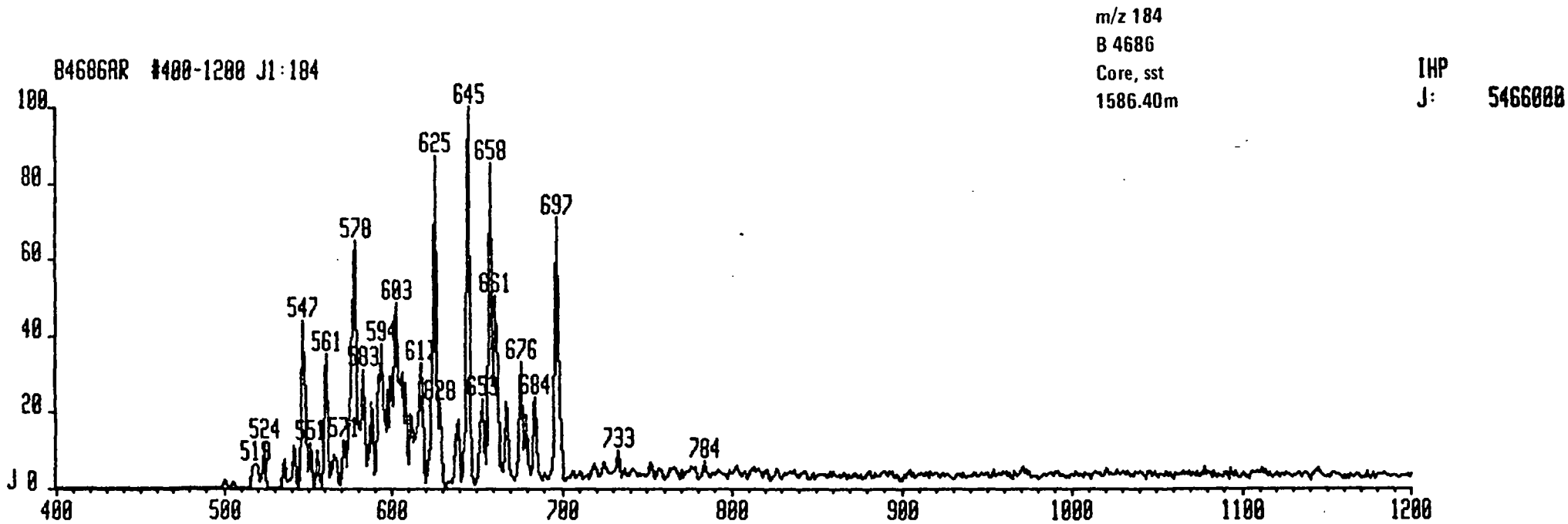
400
500
600
700
800
900
1000
1100
1200


B4685AR #400-1200 J1:184
m/z 184
B 4685
Core, sst
1581.65m
IHP
J: 5481000
J 0
100
80
60
40
20
400
500
600
700
800
900
1000
1100
1200
638
618
571
651
690
596
654
554
668
540
726
B4685AR #400-1200 K1:198
m/z 198
B 4685
Core, sst
1581.65m
IHP
K: 3859000
K 0
782
646
799
678
674
624
699
726
819
557
853
1007


B4686AR #400-1200 J1:184
m/z 184
B 4686
Core, sst
1586.40m
IHP
J: 5466000
645
625
658
697
578
603
661
547
561
594
676
684
524
733
784
J 0
100
80
60
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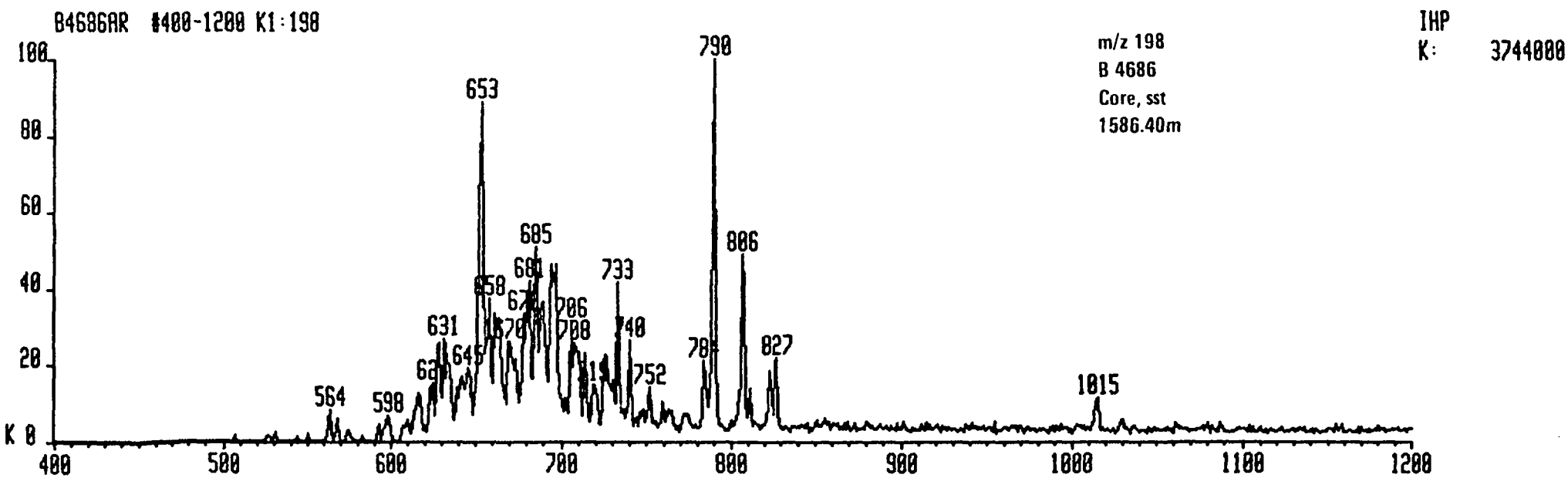
20
400
500
600
700
800
900
1000
1100
1200


B4686AR #400-1200 K1:198
m/z 198
B 4686
Core, sst
1586.40m
IHP
K: 3744000
790
653
685
806
733
631
706
740
827
752
564
598
1015
K 0
100
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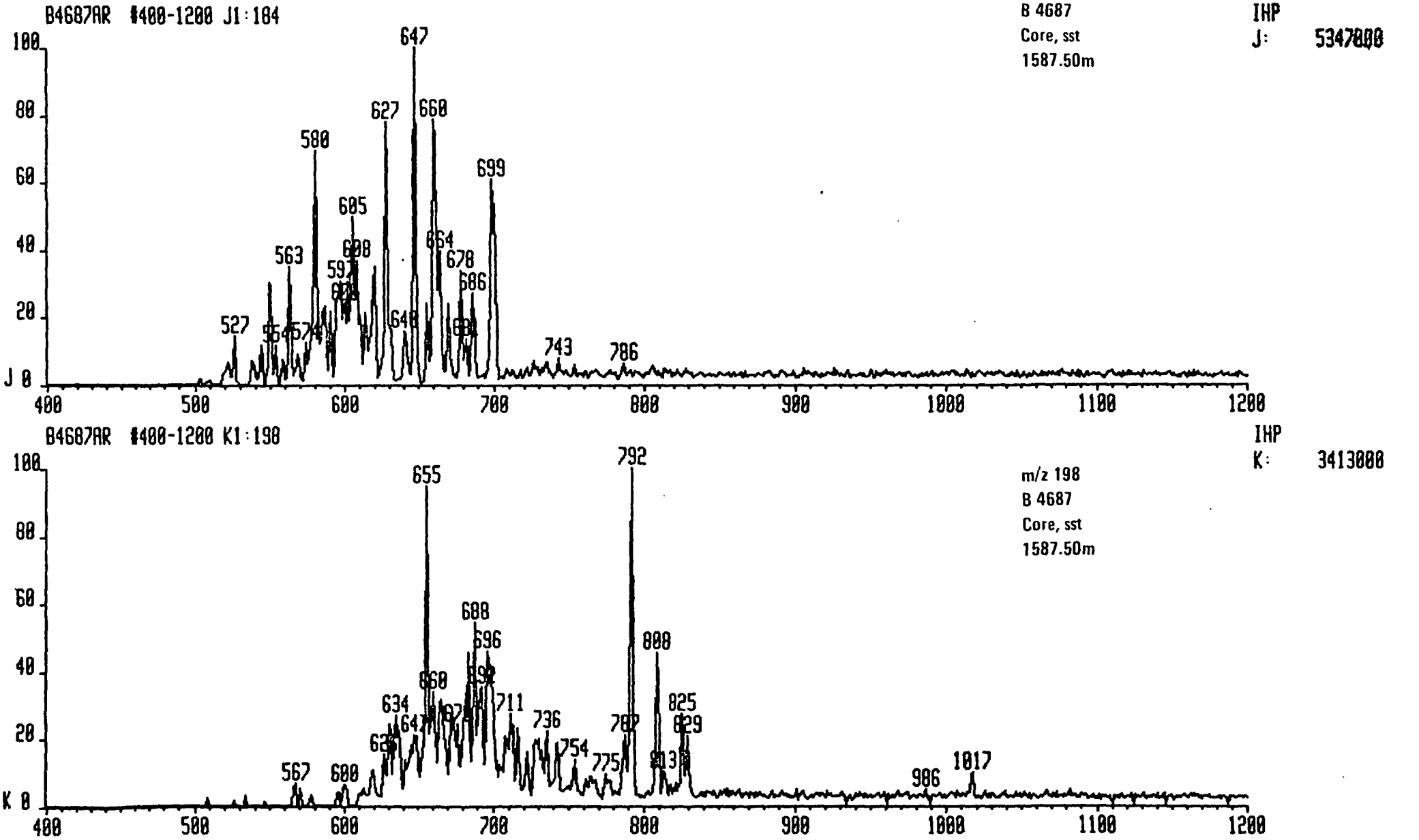
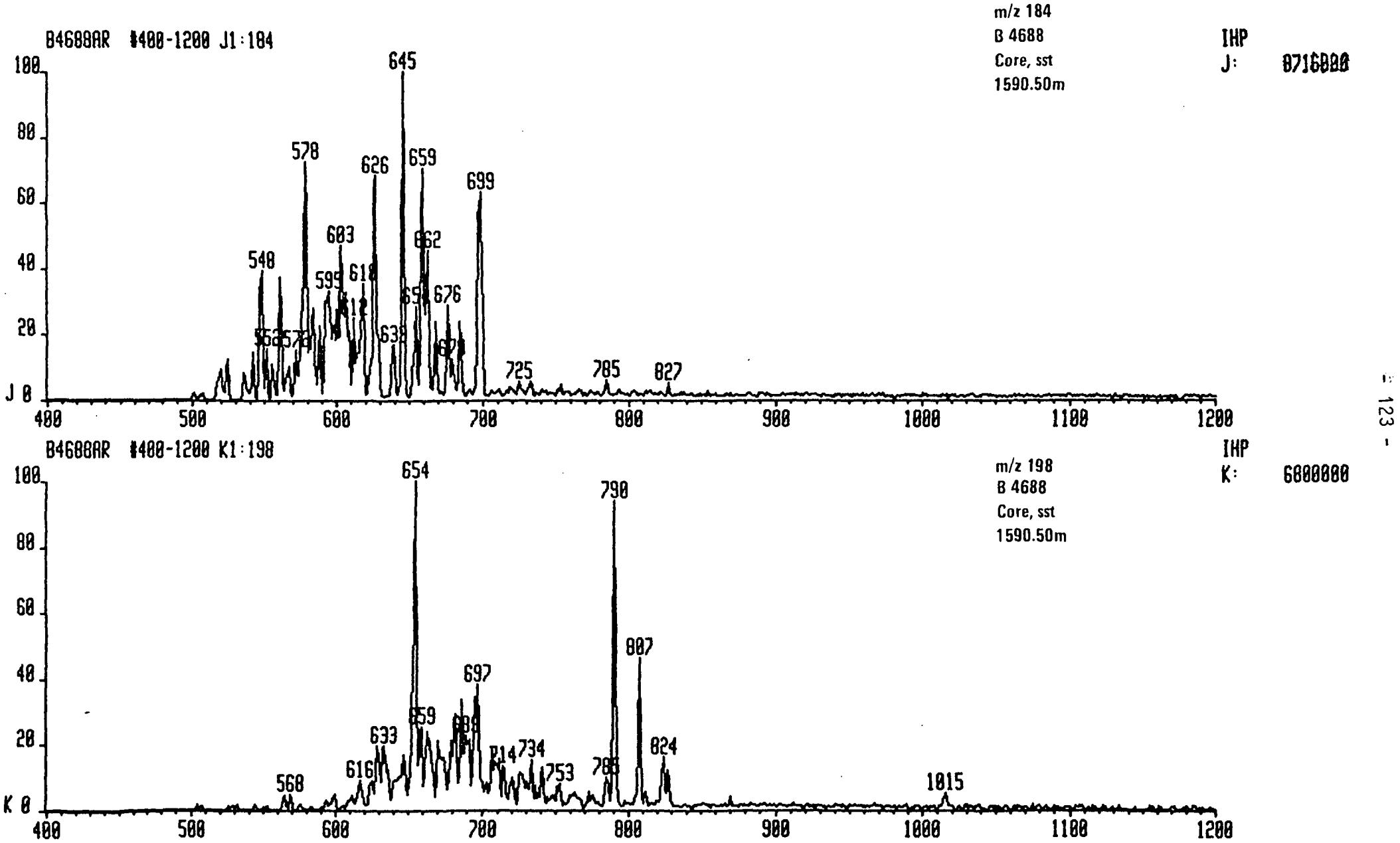
1000
1100
1200


B4687AR #400-1200 J1:184
m/z 184
B 4687
Core, sst
1587.50m
IHP
J: 5347000
B4687AR #400-1200 K1:198
m/z 198
B 4687
Core, sst
1587.50m
IHP
K: 3413000


B4688AR #400-1200 J1:184
m/z 184
B 4688
Core, sst
1590.50m
IHP
J: 8716800
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40
20
J 0
645
578
626
659
699
603
662
548
618
676
725
785
827
400
500
600
700
800
900
1000
1100
1200
B4688AR #400-1200 K1:198
m/z 198
B 4688
Core, sst
1590.50m
IHP
K: 6800000
100
80
60
40
20
K 0
654
790
807
697
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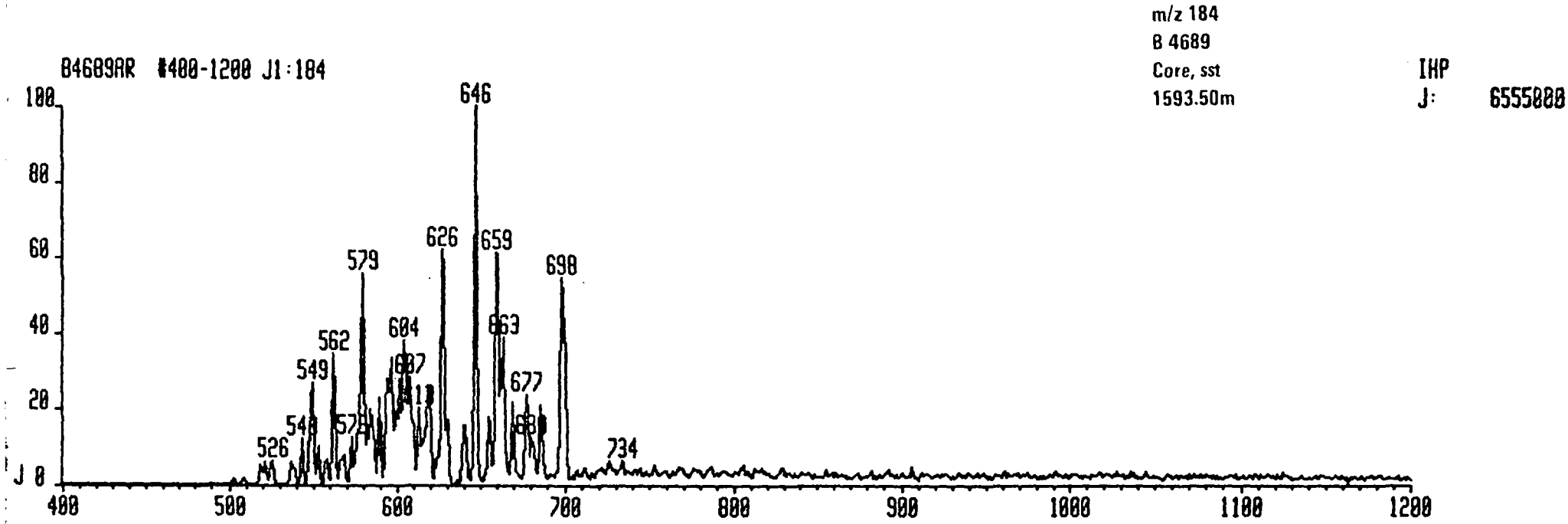
B4689AR #400-1200 J1:184
m/z 184
B 4689
Core, sst
1593.50m
IHP
J: 6555000
646
626
659
579
698
604
663
562
549
677
526
734
J 0
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60
40
20
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700
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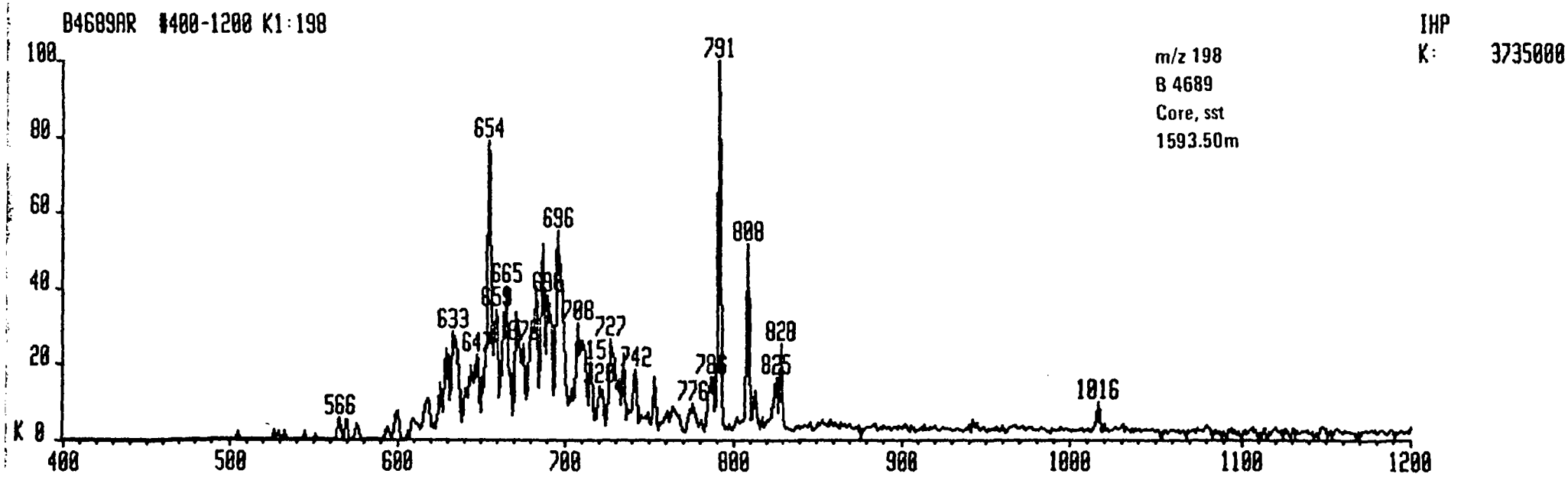
1000
1100
1200


B4689AR #400-1200 K1:198
m/z 198
B 4689
Core, sst
1593.50m
IHP
K: 3735000
791
654
696
808
665
633
727
742
828
825
566
1016
K 0
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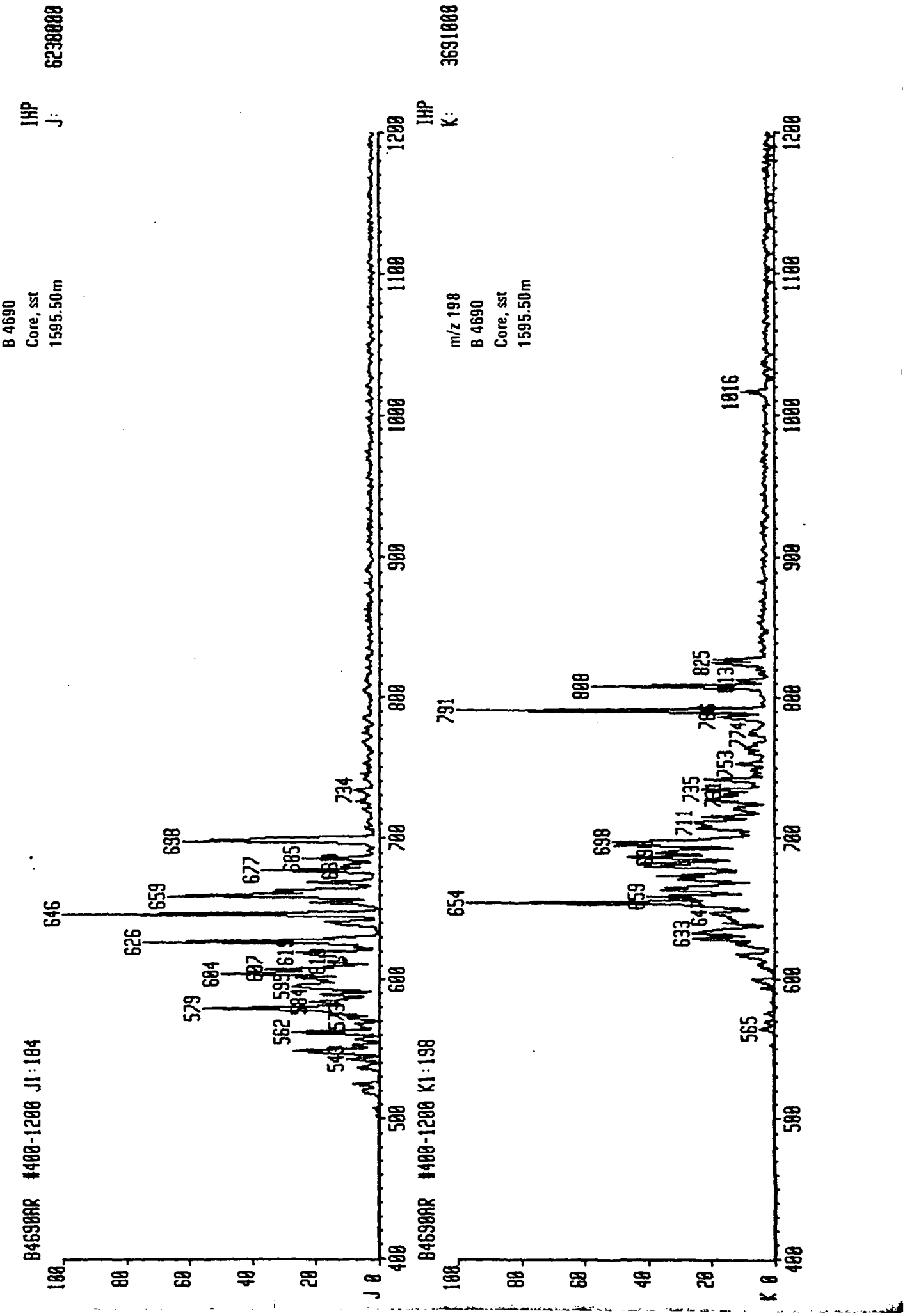
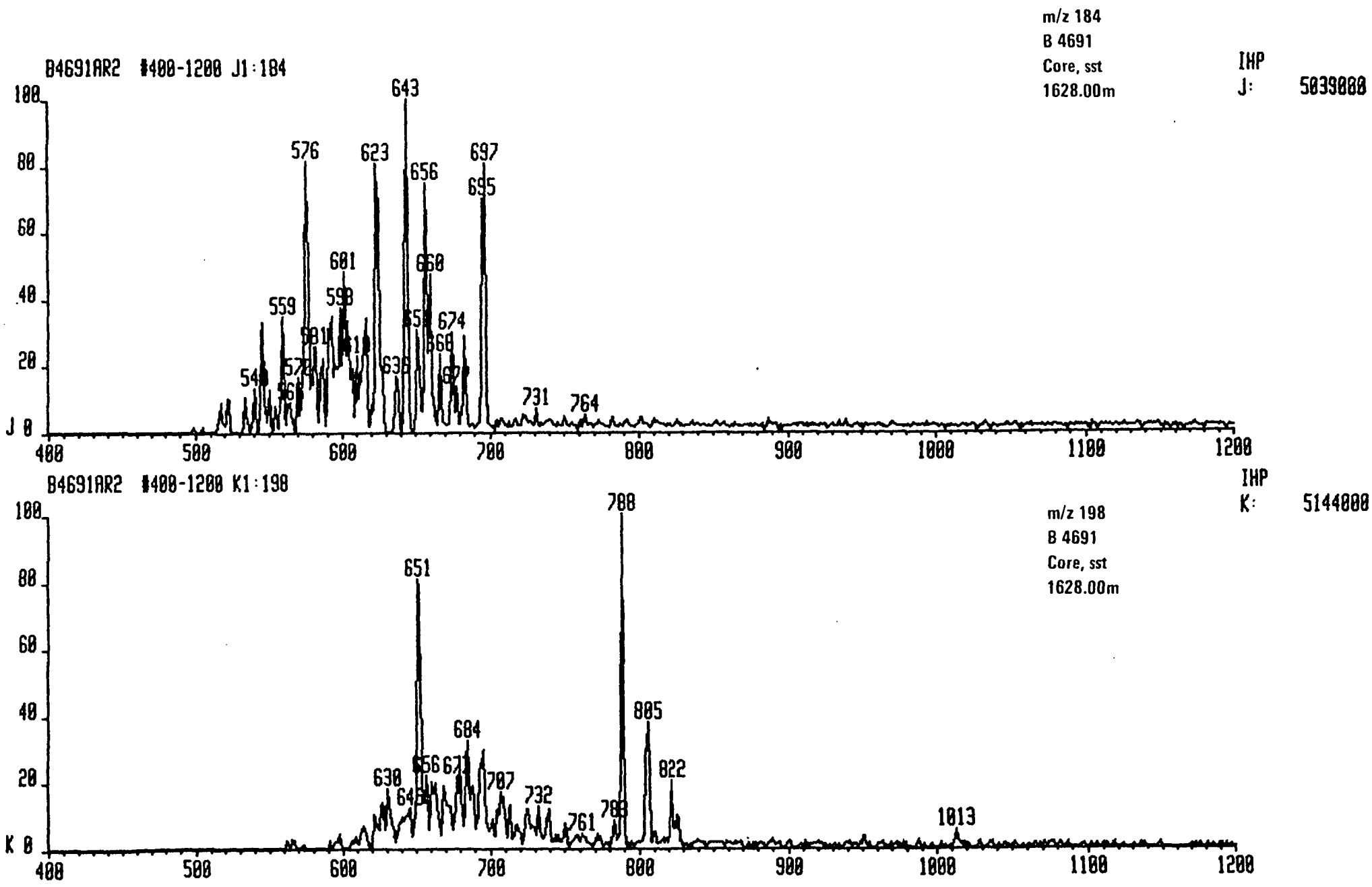
1100
1200


B4690AR #400-1200 J1:184
m/z 184
B 4690
Core, sst
1595.50m
IHP
J: 6230000
J 0
B4690AR #400-1200 K1:198
m/z 198
B 4690
Core, sst
1595.50m
IHP
K: 3691000
K 0


B4691AR2 #400-1200 J1:184
m/z 184
B 4691
Core, sst
1628.00m
IHP
J: 5039000
643
576
623
697
656
695
601
660
559
674
731
764
J 0
B4691AR2 #400-1200 K1:198
IHP
K: 5144000
m/z 198
B 4691
Core, sst
1628.00m
788
651
805
684
822
630
707
732
761
1013
K 0
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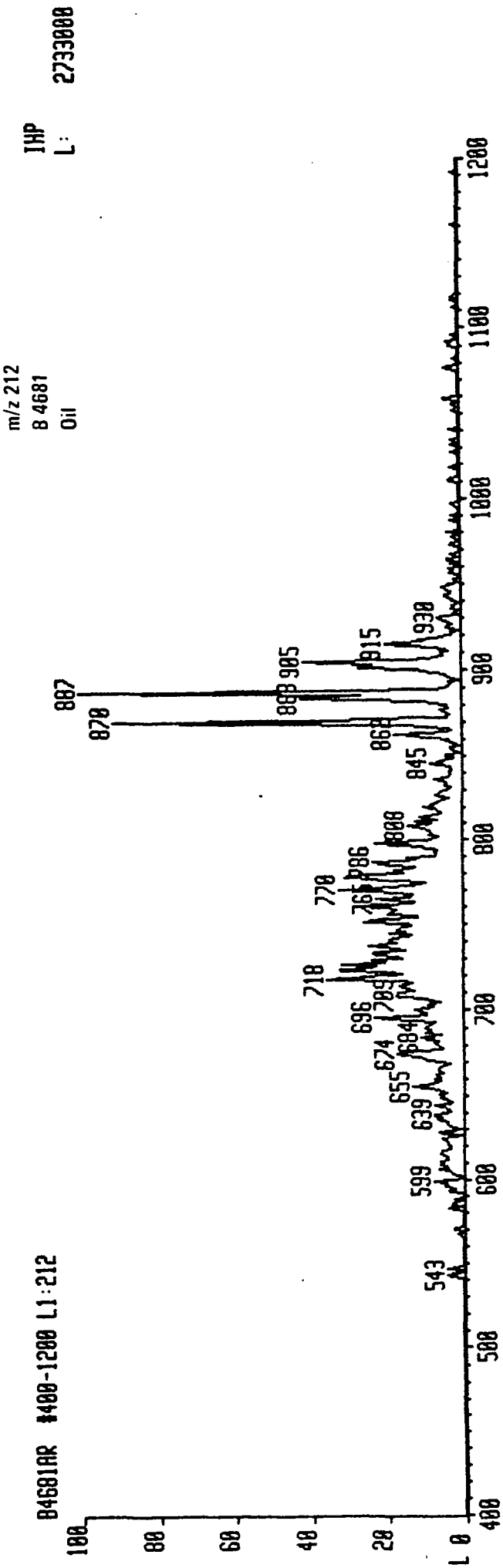
B4681AR #400-1200 L1:212
m/z 212
B 4681
Oil
IHP
L: 2733000
100
80
60
40
20
L 0
400
500
600
700
800
900
1000
1100
1200
543
599
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674
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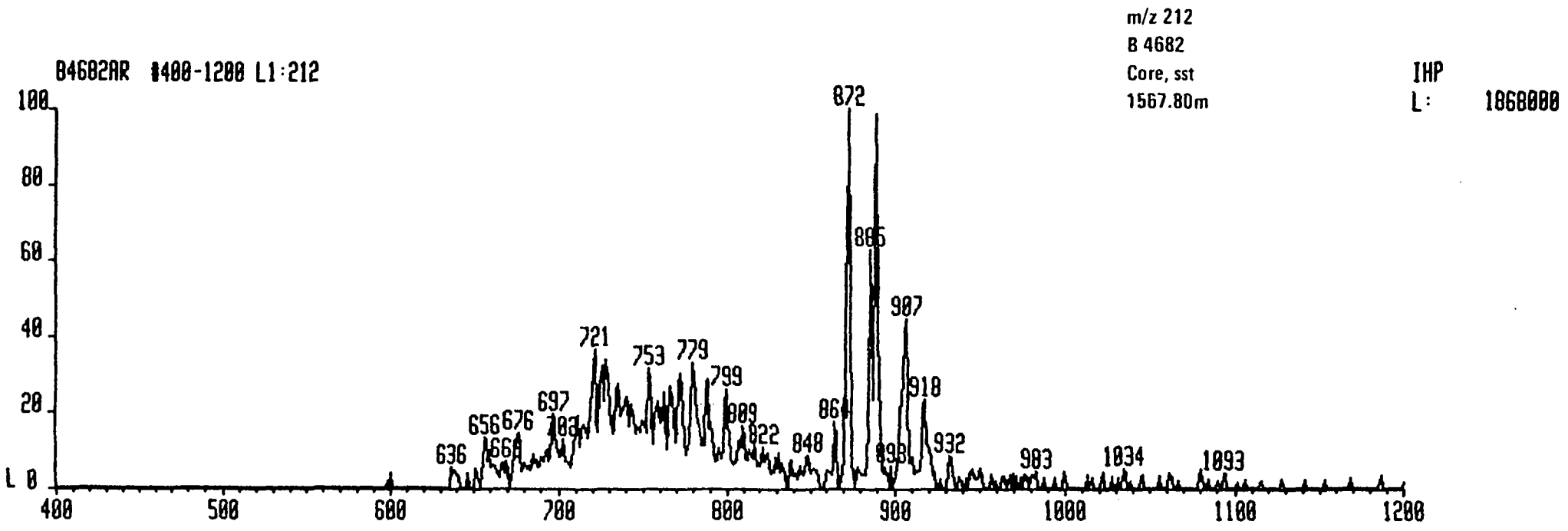
B4682AR #400-1200 L1:212
m/z 212
B 4682
Core, sst
1567.80m
IHP
L: 1868000
100
80
60
40
20
L 0
400
500
600
700
800
900
1000
1100
1200
872
885
907
918
932
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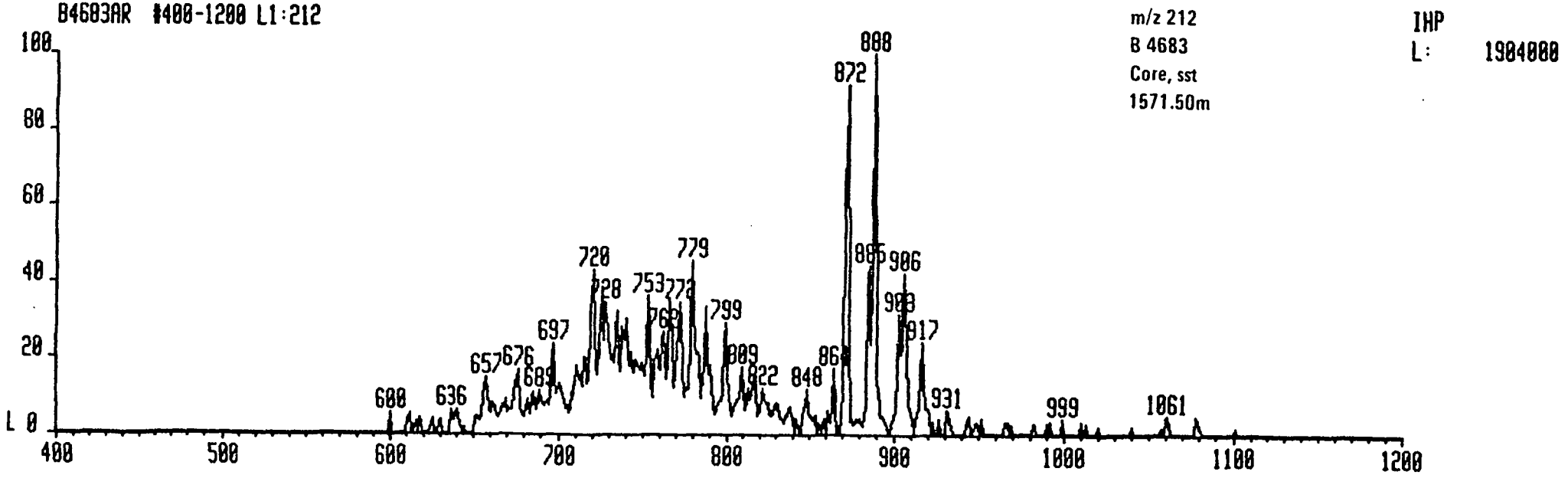
B4683AR #400-1200 L1:212
m/z 212
B 4683
Core, sst
1571.50m
IHP
L: 1904000
100
80
60
40
20
L 0
400
500
600
700
800
900
1000
1100
1200
888
872
885
906
908
917
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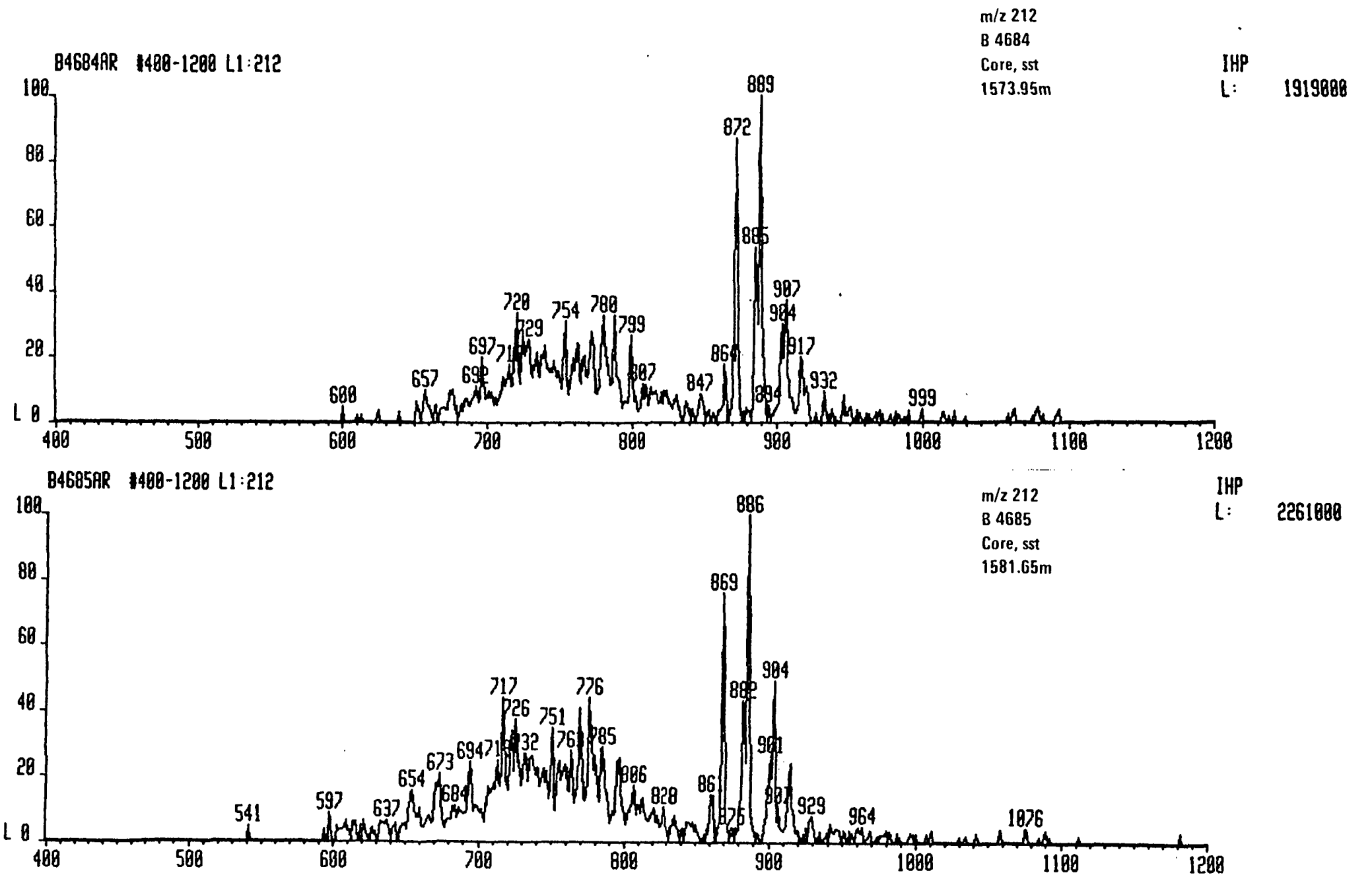
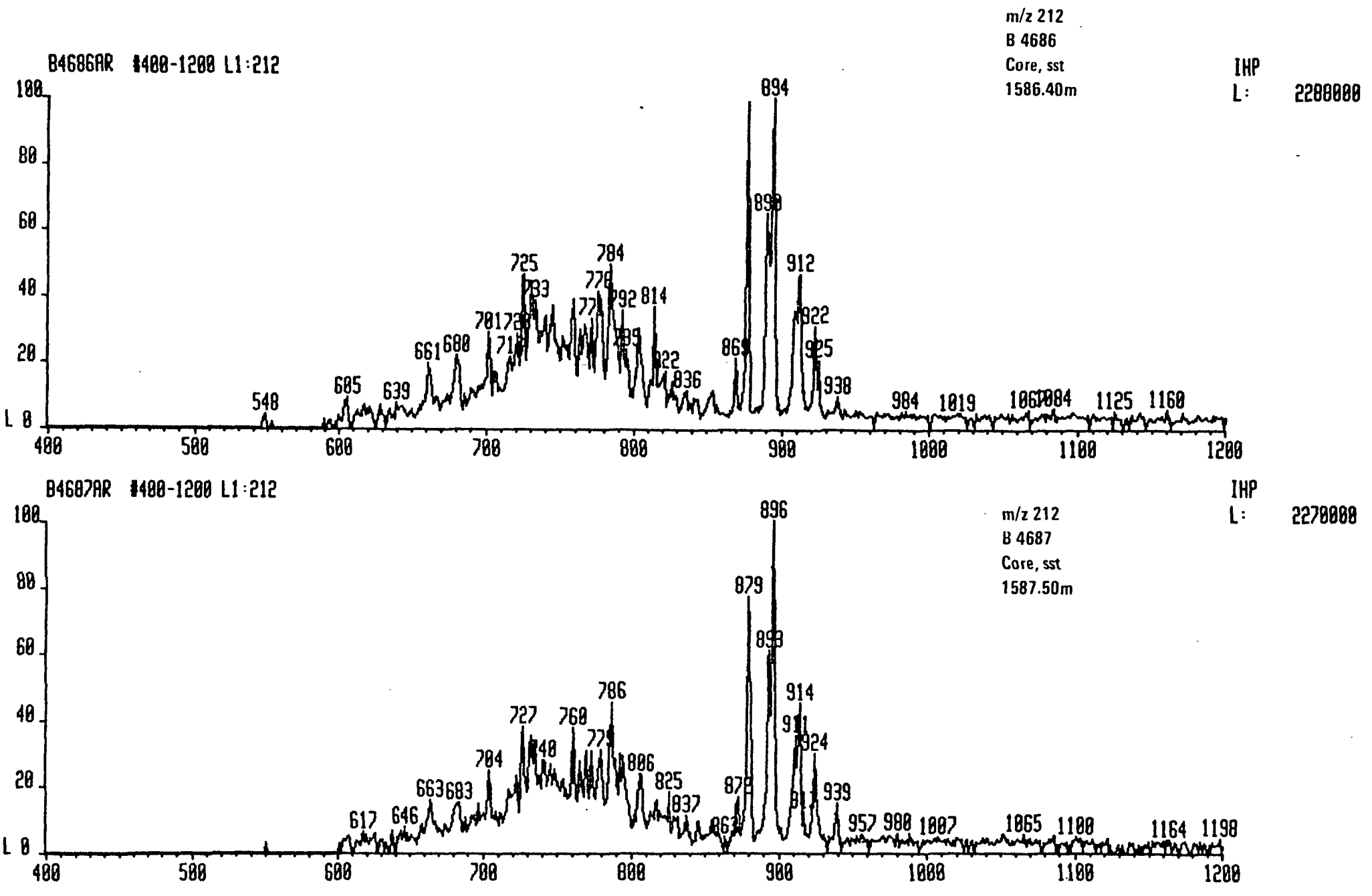
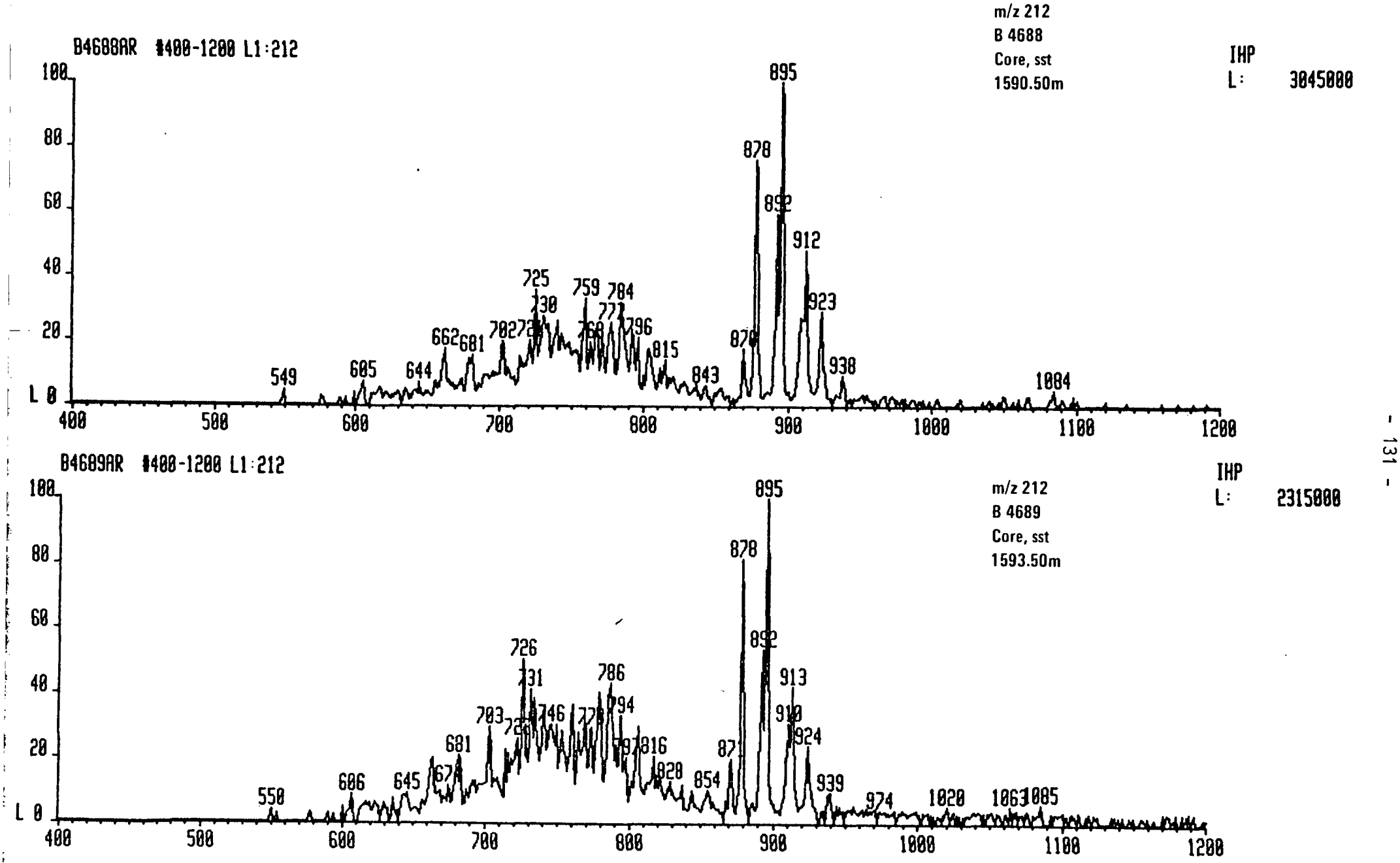

B4684AR #400-1200 L1:212
m/z 212
B 4684
Core, sst
1573.95m
IHP
L: 1919000
B4685AR #400-1200 L1:212
m/z 212
B 4685
Core, sst
1581.65m
IHP
L: 2261000


B4686AR #400-1200 L1:212
m/z 212
B 4686
Core, sst
1586.40m
IHP
L: 2280000
B4687AR #400-1200 L1:212
m/z 212
B 4687
Core, sst
1587.50m
IHP
L: 2270000


B4688AR #400-1200 L1:212
m/z 212
B 4688
Core, sst
1590.50m
IHP
L: 3045000
100
80
60
40
20
L 0
400
500
600
700
800
900
1000
1100
1200
549
605
644
662
681
702
725
730
759
784
796
815
843
878
895
912
923
938
1084
B4689AR #400-1200 L1:212
m/z 212
B 4689
Core, sst
1593.50m
IHP
L: 2315000
550
606
645
681
703
726
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924
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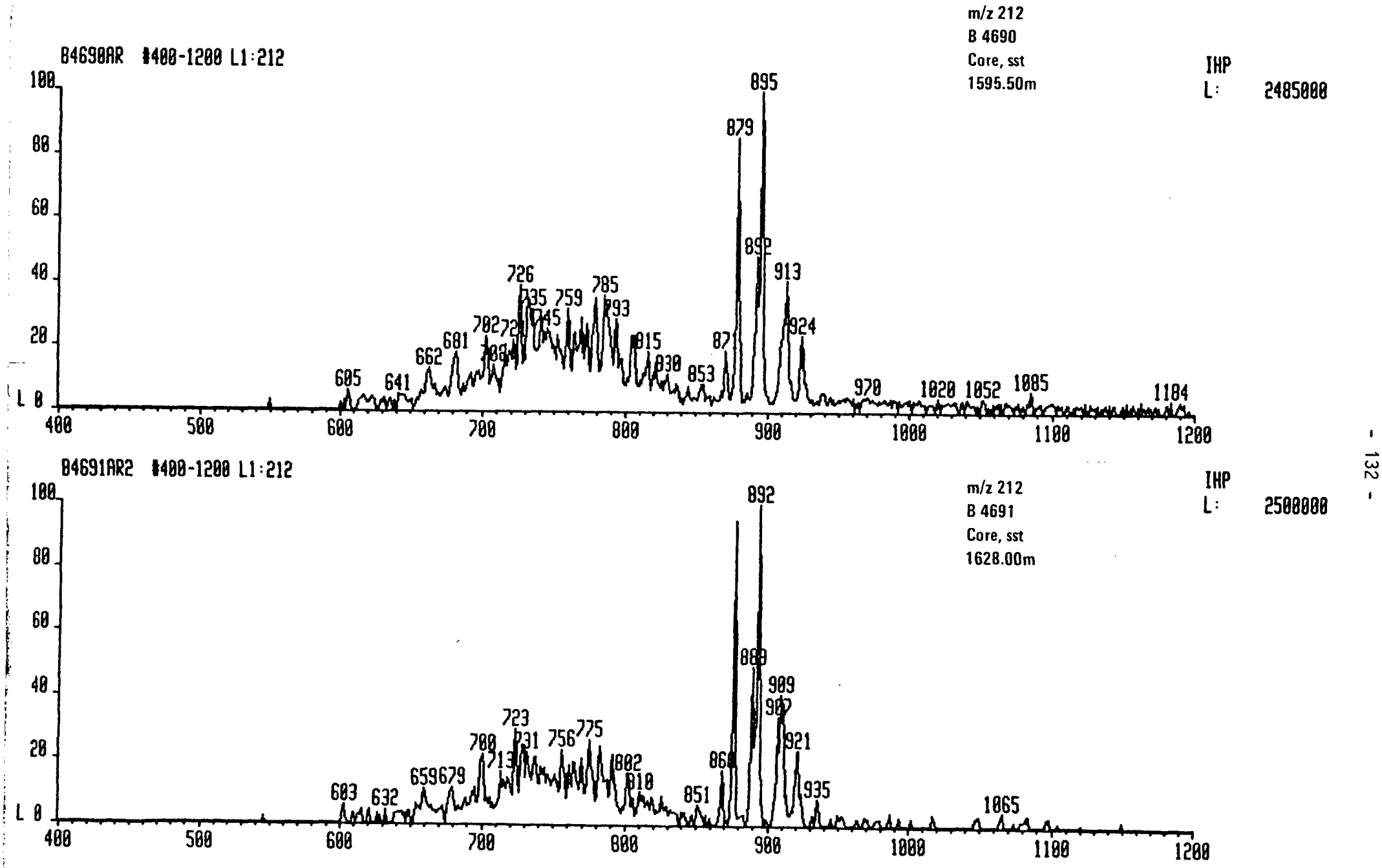
B4690AR #400-1200 L1:212
m/z 212
B 4690
Core, sst
1595.50m
IHP
L: 2485000
100
80
60
40
20
L 0
400
500
600
700
800
900
1000
1100
1200
605
641
662
681
702
726
735
759
785
793
815
830
853
879
895
892
913
924
970
1020
1052
1085
1184
B4691AR2 #400-1200 L1:212
m/z 212
B 4691
Core, sst
1628.00m
IHP
L: 2500000
603
632
659
679
700
723
731
756
775
802
810
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892
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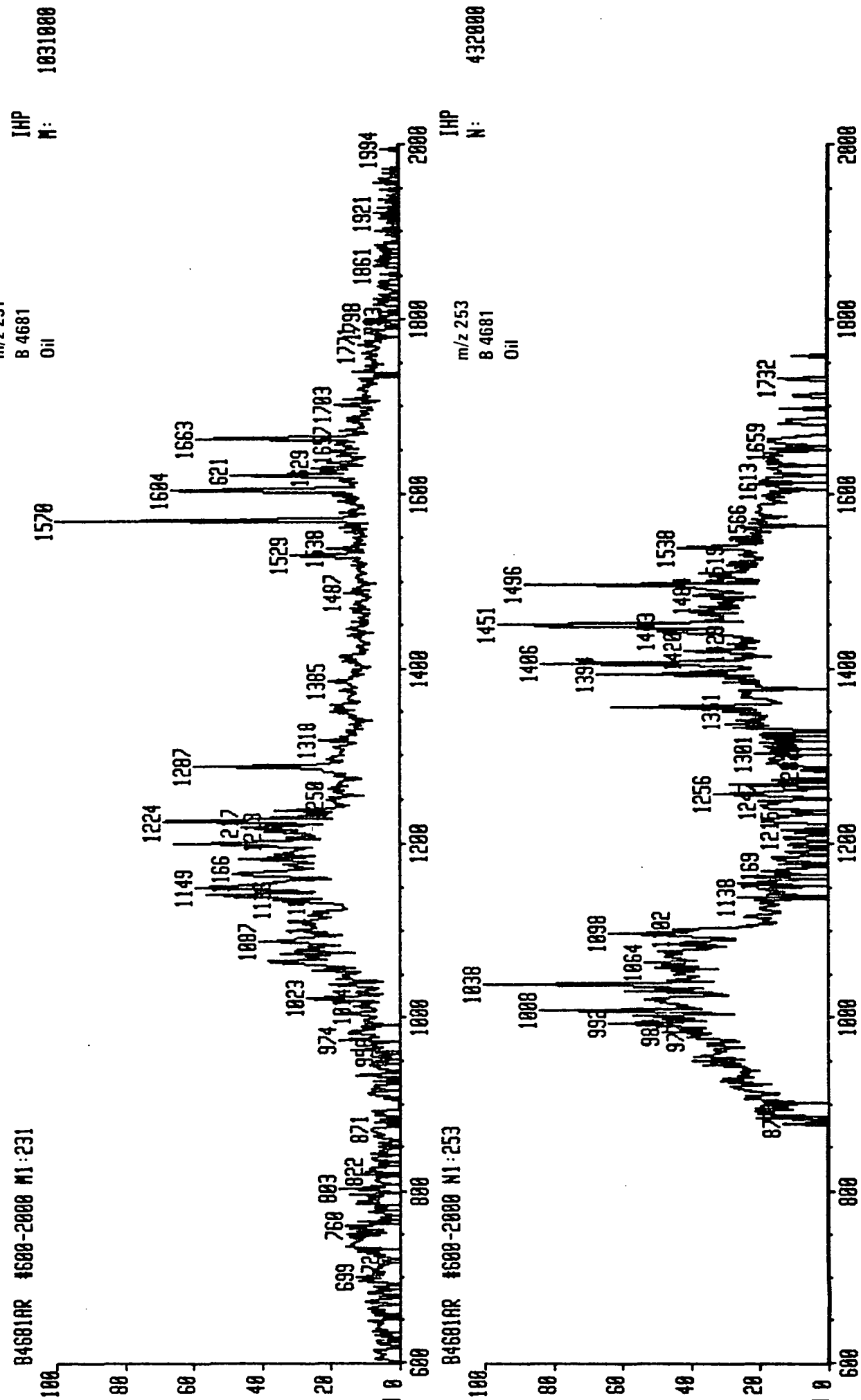
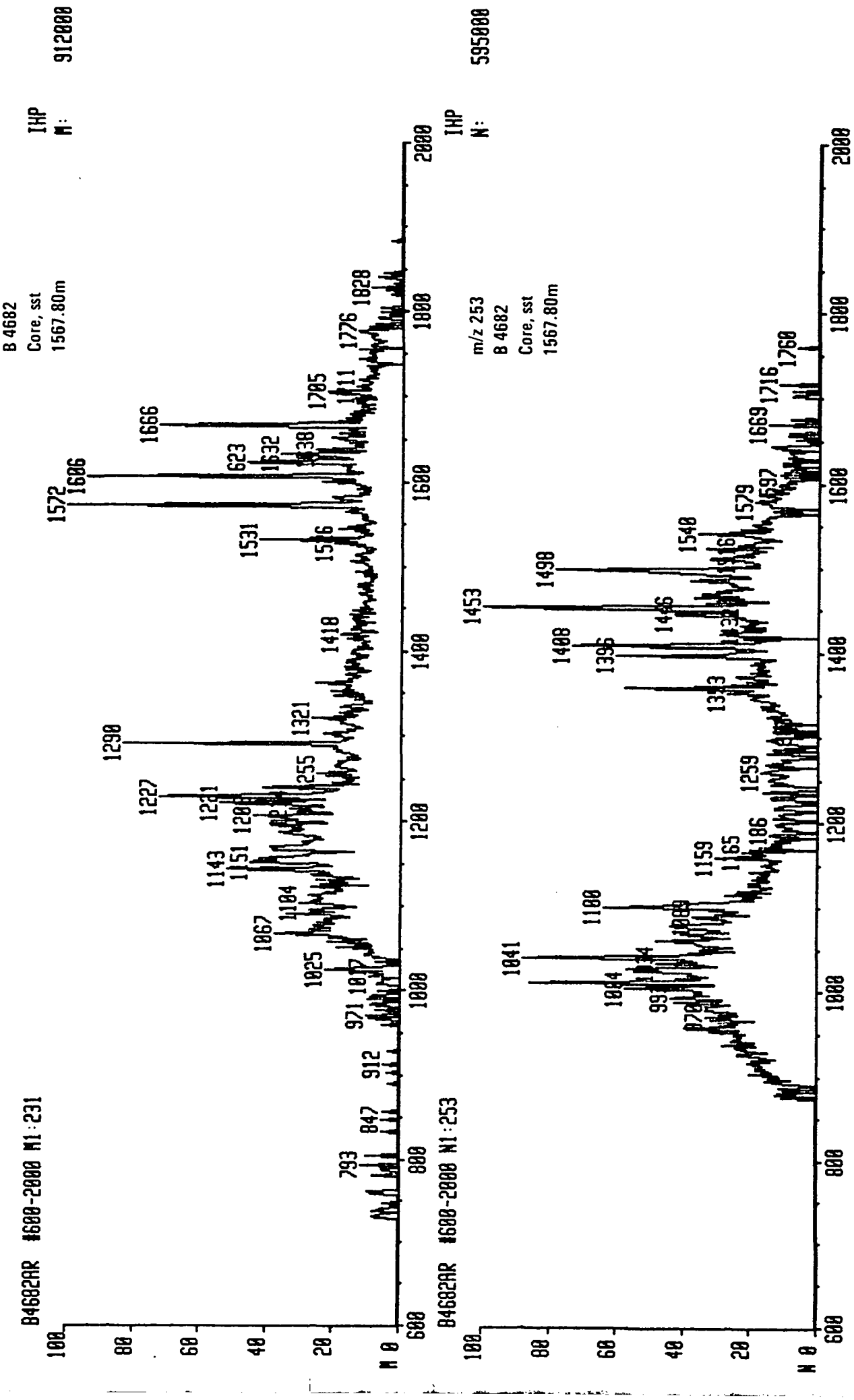

B4681AR #600-2000 N1:231
m/z 231
B 4681
Oil
IHP
M: 1031000
B4681AR #600-2000 N1:253
m/z 253
B 4681
Oil
IHP
N: 432000


B4682AR #600-2000 N1:231
m/z 231
B 4682
Core, sst
1567.80m
IHP
N: 912000
B4682AR #600-2000 N1:253
m/z 253
B 4682
Core, sst
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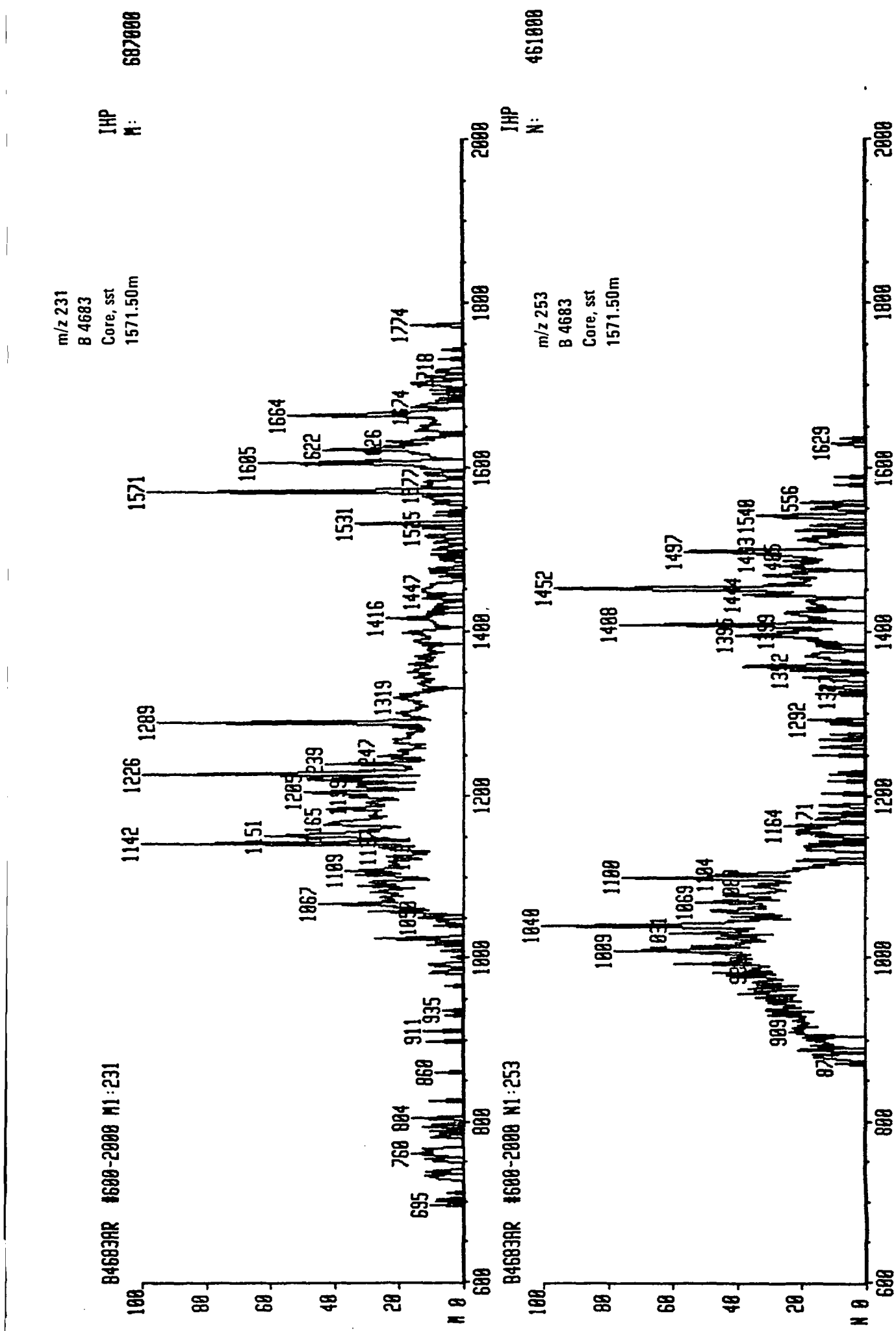
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m/z 253
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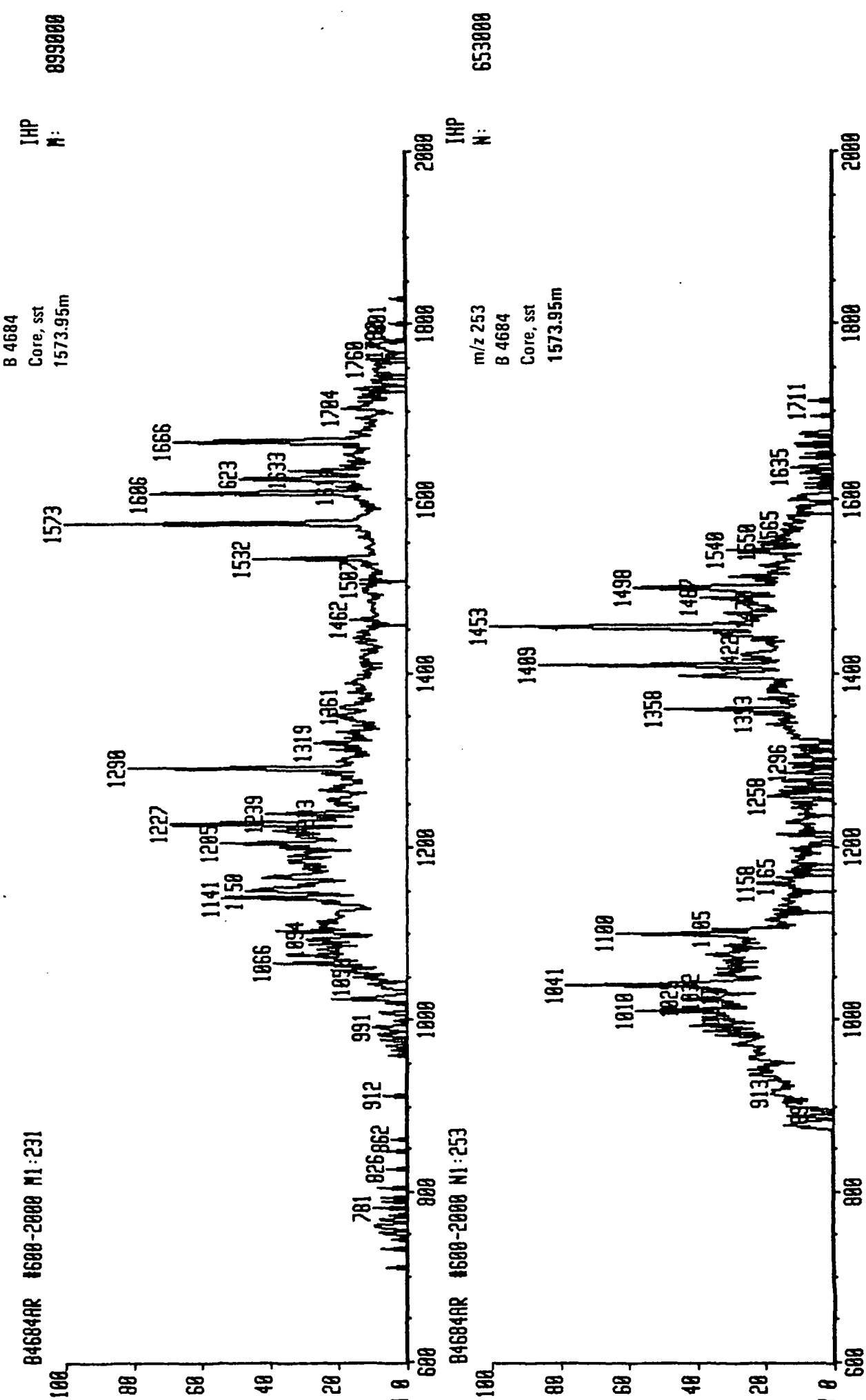
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m/z 253
B 4684
Core, sst
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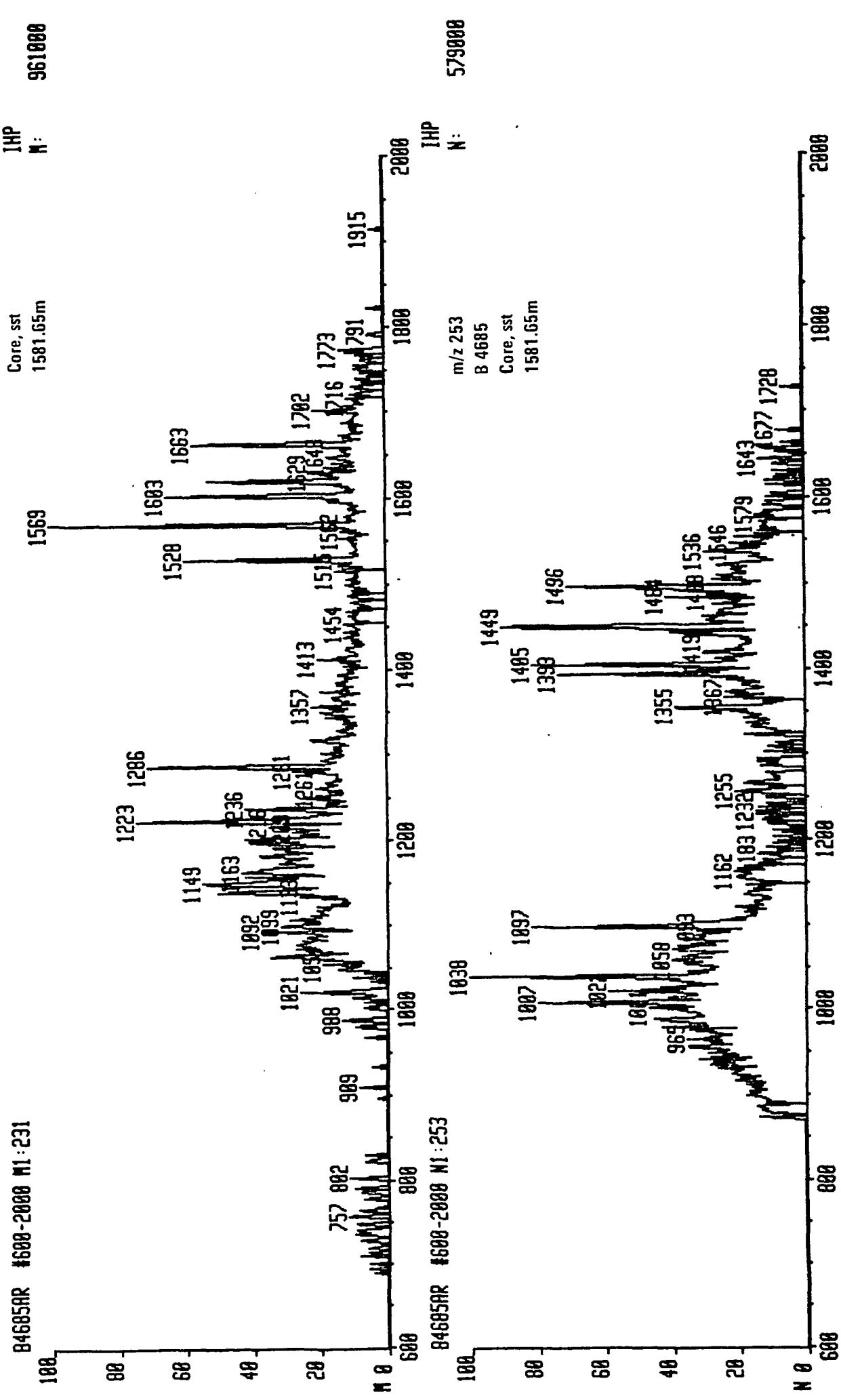
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m/z 253
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Core, sst
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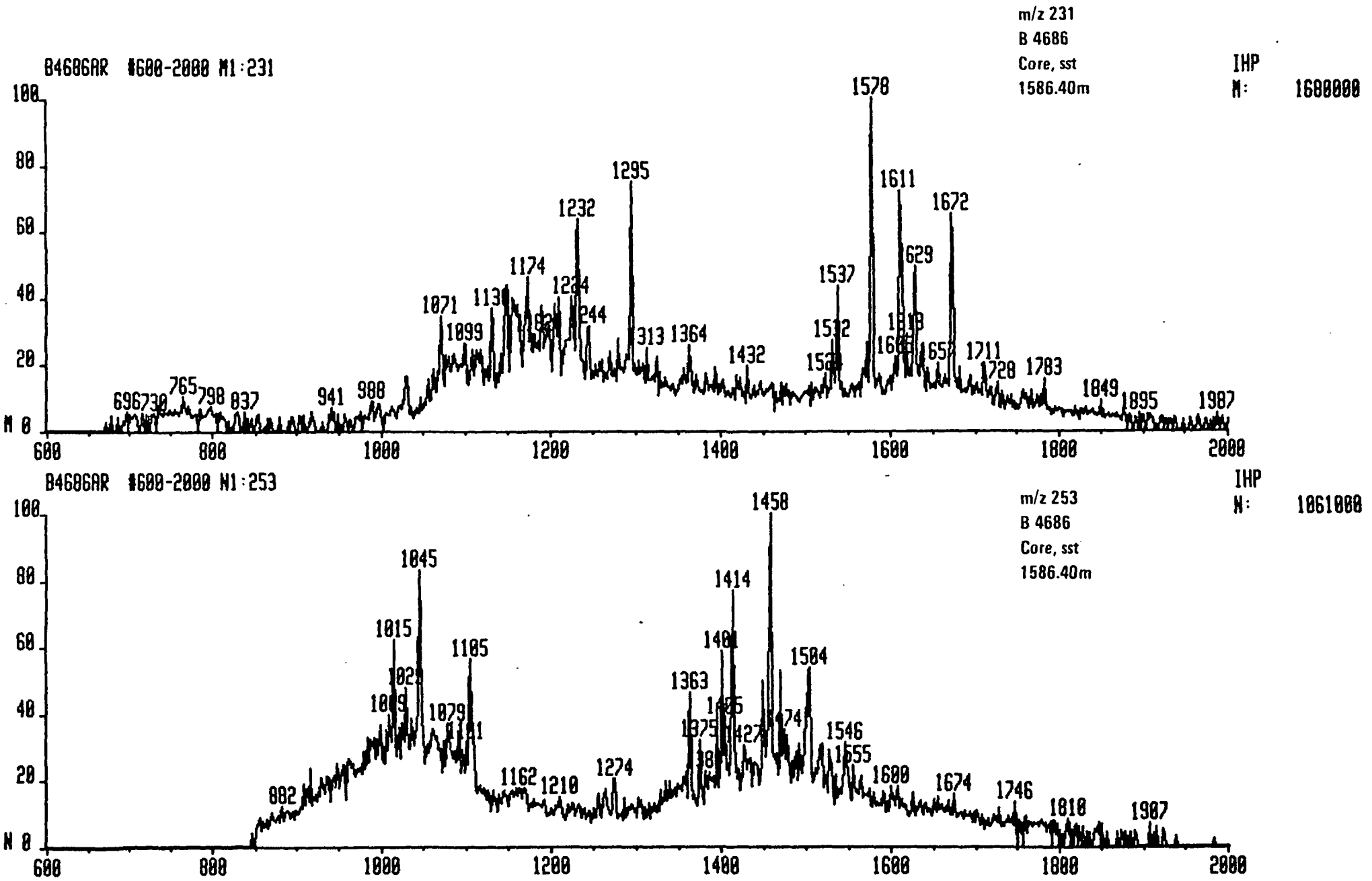
N: 579000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M 0
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800
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1400
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1800
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1578
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1611
1672
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629
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1071
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313
1364
1432
1512
1711
1728
1783
1849
1895
1987
765
798
837
941
988
B4686AR $600-2000 M1:253
m/z 253
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Core, sst
1586.40m
IHP
M: 1061000
1458
1045
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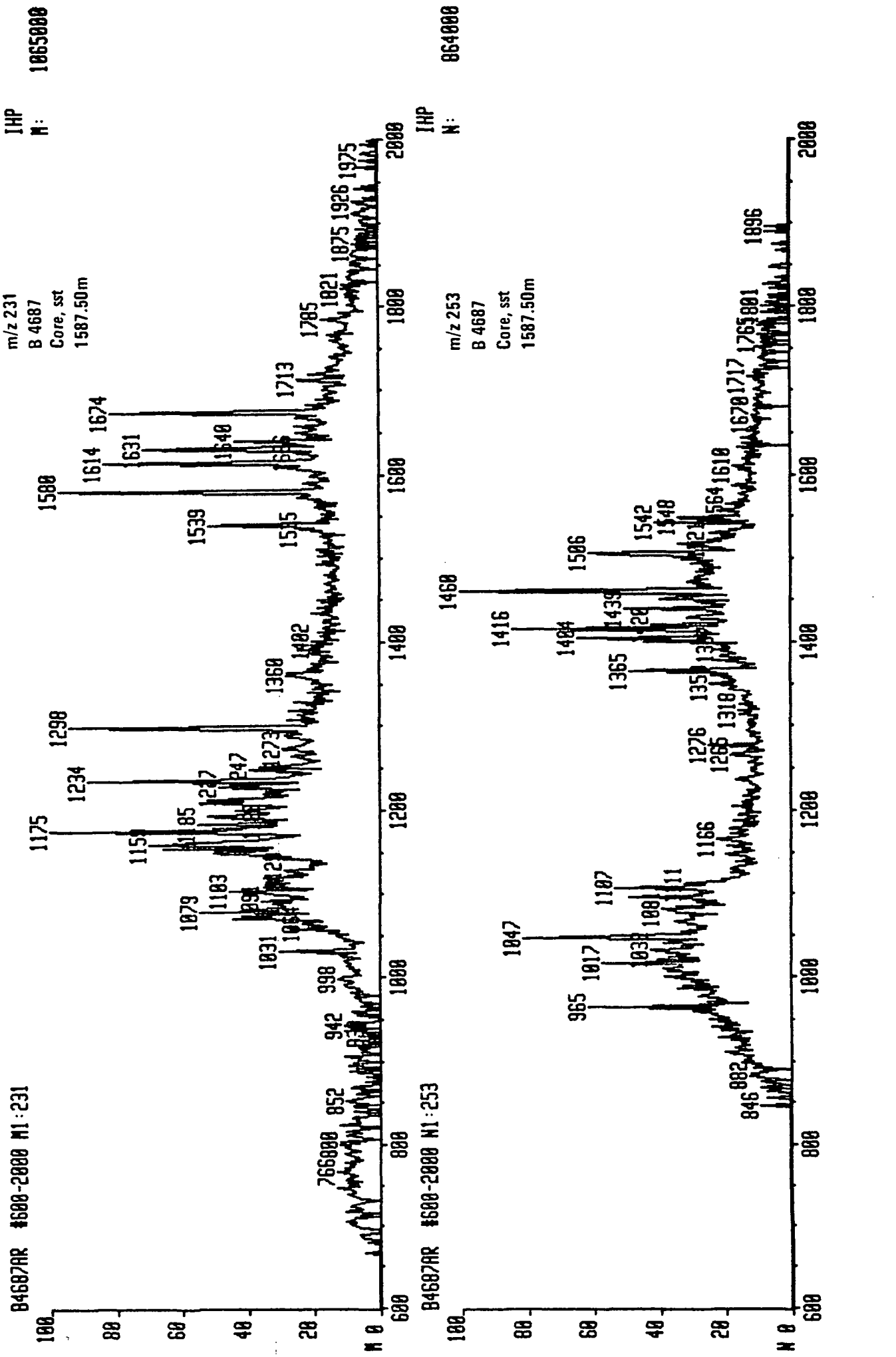
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m/z 253
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Core, sst
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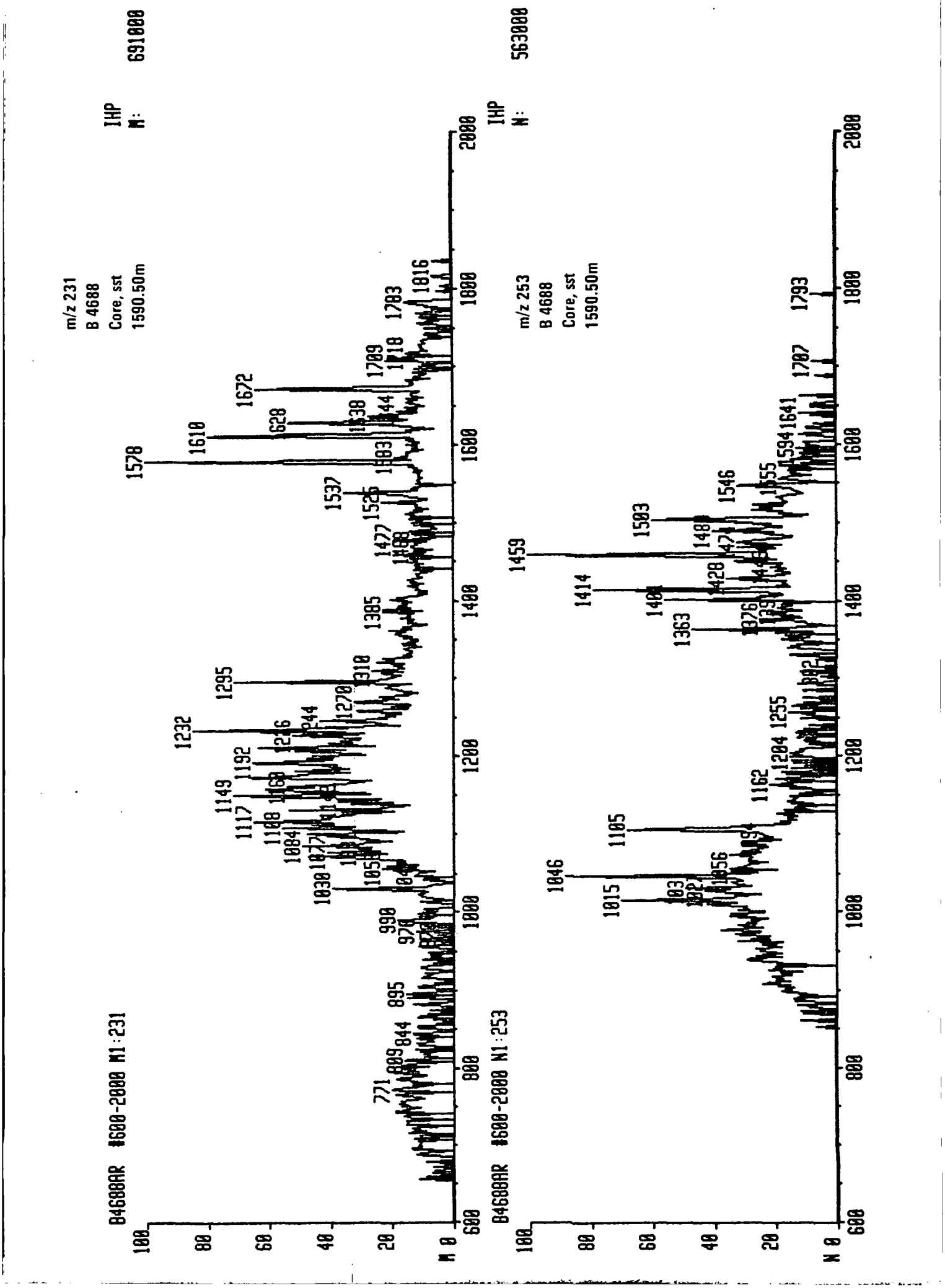
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B 4688
Core, sst
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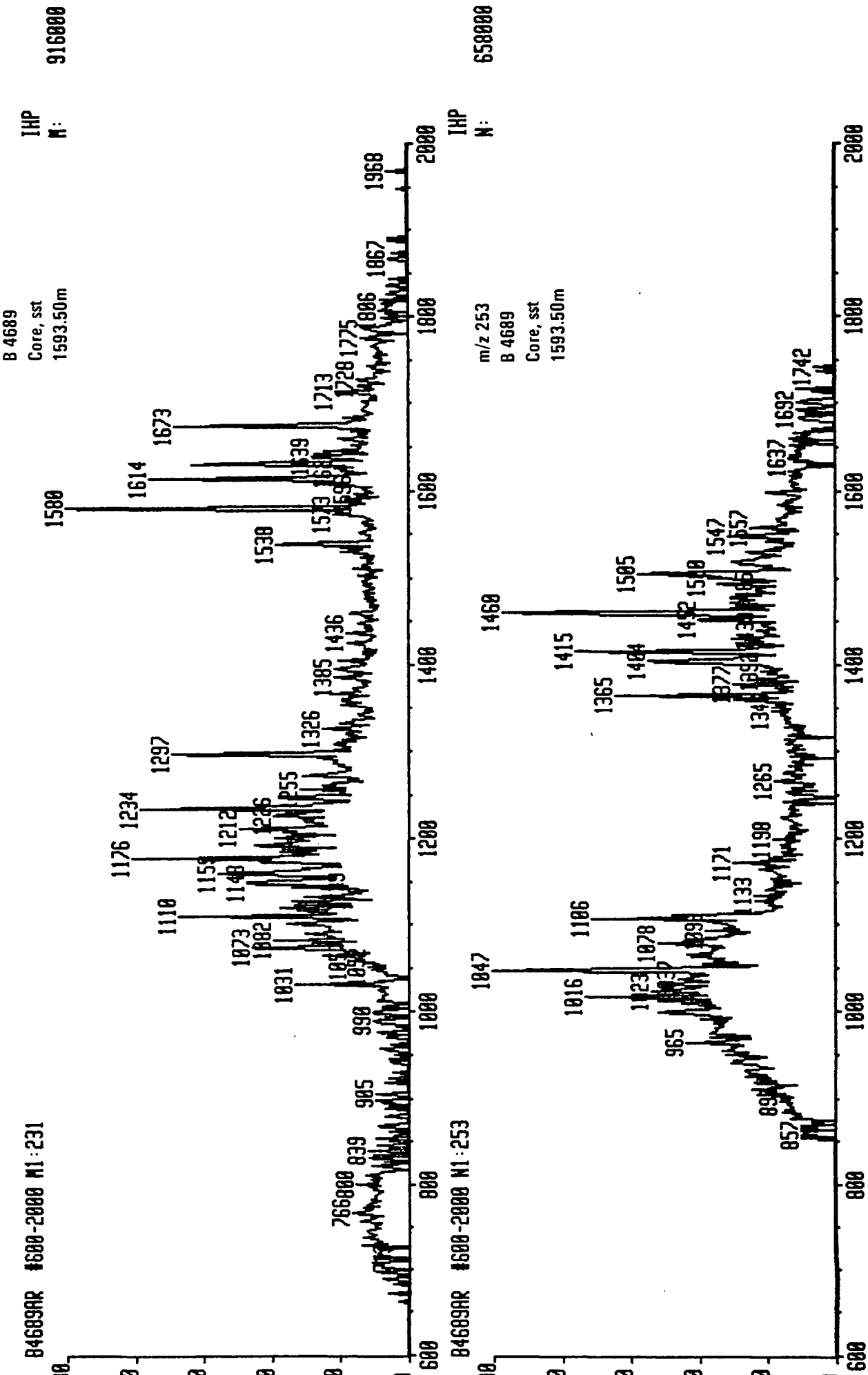
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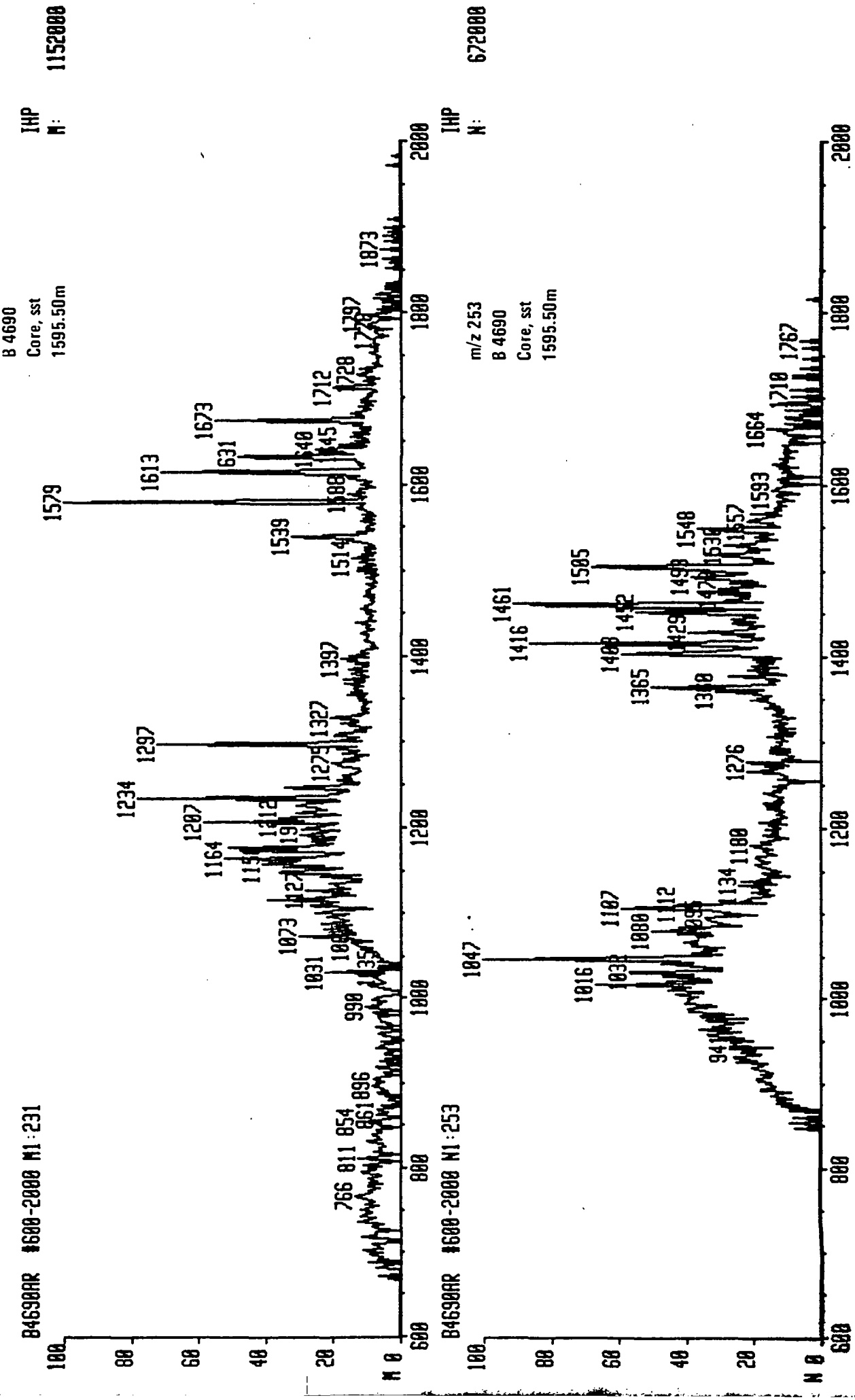
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IHP
N: 1152000
B4690AR #600-2000 N1:253
m/z 253
B 4690
Core, sst
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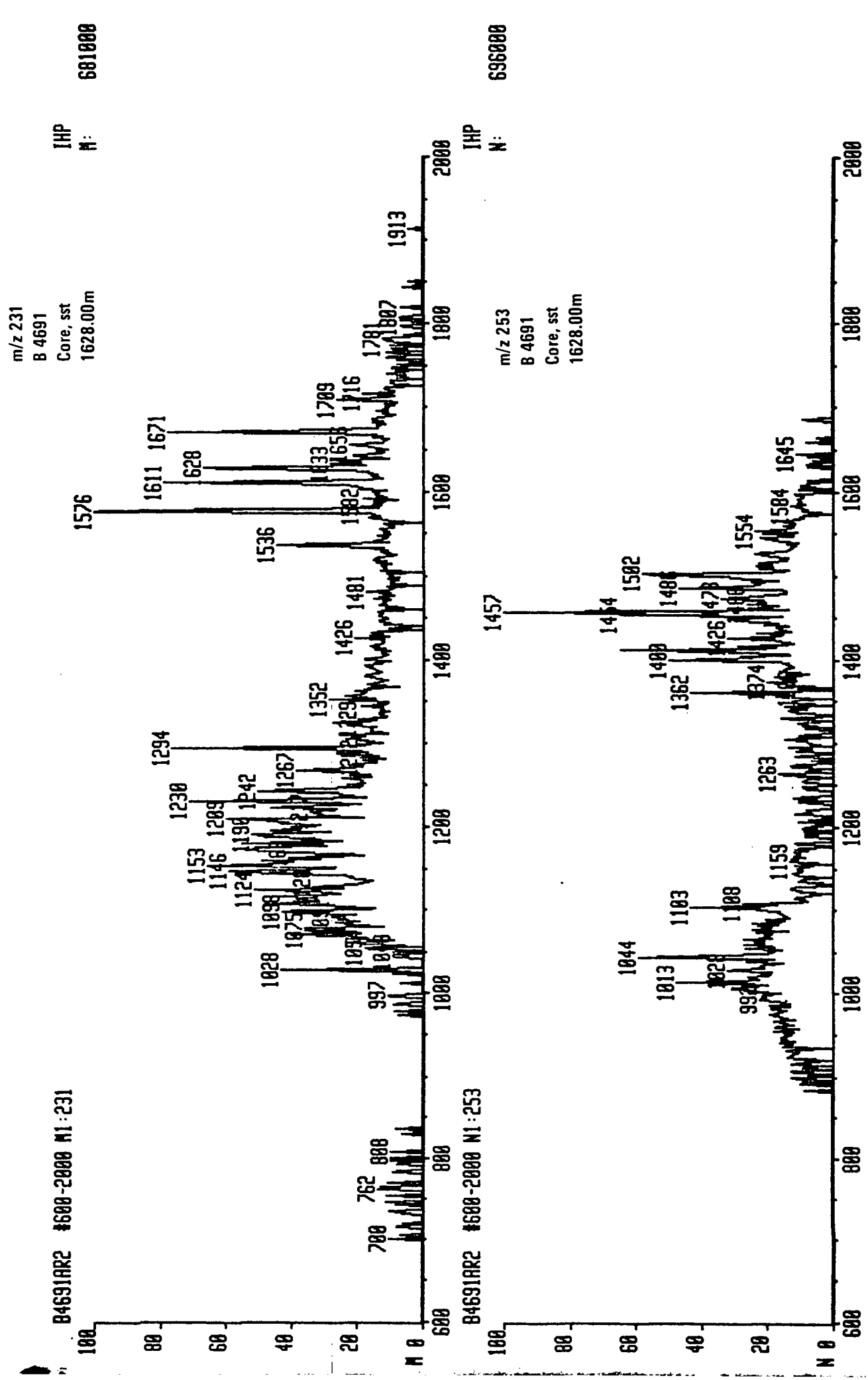
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B 4691
Core, sst
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IHP
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m/z 253
B 4691
Core, sst
1628.00m
IHP
N: 696000
100
80
60
40
20
0
600
800
1000
1200
1400
1600
1800
2000

APPENDIX

Molecular ratios from terpane and sterane mass chromatograms applied as maturity and source characteristic parameters

Geochemical fossils or biological marker components are characteristic of the type of organic matter present at the time the sediments were deposited. The biological isomers of these components undergo changes due to increased maturity in particular, but also to a certain degree caused by migration and weathering processes.

1.2.1 Source characteristic parameters

In the m/z 191 mass chromatograms, representing terpanes, the hopanes and moretanes are the major components in most extracts and oils. Of the hopanes the C_{27} and C_{29}-C_{35} homologs are ubiquitous, while the C_{28} bisnorhopane is believed to be typical of certain types of source rocks. This is also the case for the component, probably gammacerane, sometimes seen to coelute with the 22S isomer of the C_{31} 17α(H)-hopanes (H). In the sterane mass chromatograms, m/z 217 and m/z 218, the molecular weight distribution of the C_{27}-C_{29} regular steranes is believed to be representative of the original input of organic matter. The highest molecular weight compounds, the C_{29} steranes, represent organic matter of terrestrial origin, while the lower molecular weight analogs originate from more marine type environments.

1.2.2 Maturity dependant parameters

The biological isomers of the hopanes, the 17β(H), 21β(H)-hopanes, undergo structural changes during the maturation process. The isomerisation reactions are thought to be produced via the 17β(H), 21α(H)-hopanes (moretanes) to the most stable 17α(H), 21β(H)-hopanes. At equilibrium 100% of the 17α(H)-hopanes are seen. The ratio αβ/αβ+βα is used to describe this reaction. In the extended hopanes ($\geq C_{31}$), the thermally stable S configurations at C-22 become increasingly more abundant as compared to the biological preferred R configurations at increased maturity level. The equilibrium ratio is approximately 60% of the 22S configuration. Another ratio that is known to change with maturity is the Tm/Ts (Seifert et al., 1978) of the C_{27} hopanes. The maturable 18α(H)-trisnorneohopane (Tm) is reduced in intensity relative to the more stable

17α(H)-trisnorneohopane (Ts), causing the Tm/Ts to decrease at increased maturity. This ratio is also believed to be source dependant, and this should be born in mind when applying the ratio for maturity comparison. The amount of tricyclic terpanes is also to a certain extent seen to be maturity dependant.

Two isomerisation reactions taking place in the steranes are most commonly applied for maturity assignments from the m/z 217 mass chromatograms. The biologically preferred 14α(H), 17α(H)-isomers of the regular steranes is transformed to the thermally stable 14β(H), 17β(H)-steranes, the %ββ approaching 75% at equilibrium. An equilibrium concentration of 50% is seen of the stable S configuration at C-20 as opposed to the 100% of the biological 20R epimer (Mackenzie et al., 1980). The abundance of rearranged steranes increased with increasingly maturity.

One of the reactions taking place at an early stage of diagenesis is the aromatisation of steranes, leading to the formation of mono- and tri-aromatic analogs. This process is measured as the abundance of tri-aromatic relative to mono-aromatic compounds (% tri/tri + mono) in the m/z 231 and 253 mass chromatograms, respectively. In addition the degree of side chain cracking, as $\%C_{20}/C_{26,\ 27}$ and $\%C_{21}/C_{28,29}$ respectively, is applied. These cracking processes are also taking place during early diagenesis, and are used for maturity assignment together with the previously mentioned ratios.

Migration and weathering

The effect on the geochemical fossils of migration and weathering, is less apparent than the maturity induced changes. Migration is believed to cause an increase in the relative amounts of rearranged and 14β(H), 17β(H) regular steranes (Seifert and Moldowan, 1978, 1981). Severe biological alteration leads to the formation of desmethyl-hopanes (Seifert and Moldowan, 1979).