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SIMON-ROBERTSON

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**PETROLEUM GEOCHEMICAL ANALYSIS OF
HYDROCARBONS IN DRILLING FLUID
SAMPLES, N2/7-27S WELL,
EMBLA FIELD, NORWEGIAN NORTH SEA**

by

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1 SUMMARY

Petroleum geochemical analyses have been carried out on behalf of Phillips Petroleum Company Norway of hydrocarbons in four drilling fluid samples from the N2/7-27S well, Embla Field, drilled in the Norwegian North Sea.

The samples submitted for geochemical analyses comprised four sealed, canned drilling fluids corresponding to drilled depths 4966', 6181' and 7047' (two samples, corresponding to circulation at 00:00 hrs and 16:15 hrs) on 25 November 1991. Geochemical analyses were carried out in order to determine the nature and origin of hydrocarbons encountered while drilling and to compare the hydrocarbons with oils and extracts analysed previously from the Embla Field area. The analyses have been carried out on a rapid completion priority basis.

Headspace gaseous hydrocarbon (C_1-C_{6+}) yields for the four drilling fluid samples are relatively high, particularly for the two samples corresponding to circulation at 7047', whereas gasoline hydrocarbon (C_4-C_7) yields and solvent extraction yields are low. These data indicate that the hydrocarbon influx to the well bore is predominantly gas, derived from a deep, mature source rock. Gas chromatography analyses of the very small solvent extraction yields show oil-like distributions, indicating the presence of minor amounts of oil in the drilling fluid.

Gas chromatography-mass spectrometry (GC-MS) analysis of branched and cyclic alkane fractions of the two drilling fluid extracts corresponding to circulation at 7047' has been carried out. These data indicate that the hydrocarbons in the drilling fluid include a minor oil component, derived from a middle mature or later middle mature Kimmeridge Clay/Draupne Formation source rock. The oil component is comparable to oil staining in core samples analysed previously from the N2/7-20X and N2/7-21S wells (Report Number 6796/1c).

2 INTRODUCTION

This report describes the results of a petroleum geochemical analysis carried out on behalf of Phillips Petroleum Company Norway of hydrocarbons in four drilling fluid samples from the N2/7-27S well, Embla Field, Norwegian North Sea.

Following an initial telephone conversation on 27 November 1991 between Mr M Kingsley of Phillips Petroleum Company Norway and Mr M A Bastow of Simon-Robertson, a suggested analytical programme and costing for geochemical analyses of four drilling fluid samples were forwarded to the client on 28 November 1991 (fax reference 8329). Four sealed, canned drilling fluid samples were received at the North Wales laboratories of Simon-Robertson on 2 December 1991 (airway bill 117/2644-0886). Geochemical analysis have been carried out in accordance with proposal number Ic/91/060 and service order number 43862. The geochemical analyses were carried out on a rapid completion priority basis and preliminary results of analyses were forwarded to the client on 4 December 1991 (fax references 8459 and 8477), 6 December 1991 (fax reference 8515) and 16 December 1991 (fax reference 8717).

The total numbers of geochemical analyses carried out were as follows:

Headspace gaseous (C ₁ -C ₆₊) hydrocarbons	:	4
Gasoline range (C ₄ -C ₇) hydrocarbons	:	4
Quantitative solvent extraction	:	4
Non-quantitative solvent extraction	:	2
Whole extract gas chromatography	:	3
Alkane gas chromatography	:	2
Alkane gas chromatography-mass spectrometry	:	2

3 RESULTS AND INTERPRETATION

This section of the report describes the results of geochemical analyses of the drilling fluid samples and presents a detailed interpretation of the data.

The four drilling fluid samples were received for geochemical analyses in sealed cans. Documentation received with the samples indicated that the well was circulating gas at the time that one of the samples corresponding to a drilled depth of 7047' was collected, and therefore the samples were submitted for airspace gaseous hydrocarbon (C_1-C_{6+}) analysis. The results of these analyses are presented in Table 1. The total headspace gas yields are relatively high for drilling fluid samples, but consistent with the circulation of large amounts of gas in the drilling fluid system. The headspace gas yields of the two shallower samples at 4966' and 6181' are dominated by methane, with small proportions of the heavier C_2 to C_{6+} components. The two samples at 7047' contain significantly greater proportions of heavier gaseous hydrocarbons, particularly ethane and propane. The data suggest a significant increase in the rate of gas influx to the well bore at about 7047'. In each of the four samples analysed, the proportions of the heavier wet gas (C_2-C_{6+}) components and the iso-butane/normal butane ratios indicate that the gas is of thermogenic origin, rather than of shallow, biogenic origin. The headspace gaseous hydrocarbon analysis data therefore indicate the influx to the well bore of significant amounts of gas derived from a deep, mature source, at a rate which increases significantly at about 7047'.

Gasoline range (C_4-C_7) hydrocarbon chromatograms for the four samples are presented in Figure 1(1-4) and the gasoline range hydrocarbon data are given in Table 2. The total gasoline hydrocarbon yields, which reach a maximum of 3360 ppb at 7047' (16:15 hrs), are small in comparison to the headspace gaseous hydrocarbon yields, indicating that the influx to the well bore is predominantly gas rather than light oil or condensate. The ratios of the total headspace gas yields to the total gasoline hydrocarbon yields are smaller for the two samples at 7047' than the shallower samples 4966' and 6181', possibly indicating a slightly more significant heavier hydrocarbon component at 7047', compared to the shallower samples.

The distributions of gasoline range hydrocarbons in the two samples from 7047' are very similar to each other and in addition are broadly similar to oils analysed previously from the N2/7-20X and N2/7-21S wells, although the canned drilling fluid samples contain slightly higher proportions of the cyclic alkanes, mainly cyclopentane, methylcyclopentane and also methylcyclohexane. The reason for this enrichment in these cyclic alkane components is not apparent. The distribution of gasoline range hydrocarbons in the samples 4966' and 6181' are dissimilar to the samples at 7047'. In view of the very small gasoline hydrocarbon yields for the samples 4966' and 6181' (35 ppb and 135 ppb respectively), the possibility that minor hydrocarbon-based drilling fluid contaminants contributed to the gasoline range hydrocarbon data should be considered.

The gasoline range hydrocarbon analyses indicate that the two fluid samples at 7047' may contain minor amounts of oil, the light hydrocarbon fraction of which is broadly similar to oils analysed previously. The data for the samples at 4966' and 6181' is more equivocal, and any oil present in the mud is in very small amounts. The gasoline hydrocarbon data indicate that the hydrocarbon influx to the well bore is dominantly gas.

The results of quantitative solvent extraction of the four drilling fluid samples are given in Table 3. The solvent extraction yields are all very low. The extract weights obtained are as follows:

Depth (feet)	Extract (mg)	Extract (ppm)
4966	1.0	10
6181	0.6	5
7047 (16.15 hrs)	1.6	15
7047 (00.00 hrs)	1.9	15

The sample extract phials were noted to be clear, with no visible extract colouration.

These data indicate that the drilling fluid samples contain only very small amounts of heavier hydrocarbons and confirm that the influx to the well is dominantly gas. The very small amounts of extract obtained from the quantitative solvent extraction precluded the application of a number of geochemical techniques and also resulted in some difficulties in carrying out the gas chromatographic analyses, as described below.

Whole extract gas chromatograms for the samples at 6181' and 7047' are presented in Figure 2(1-3). Insufficient extract was available for whole extract gas chromatography analysis of the sample 4966'.

The whole extract gas chromatograms are dominated by the solvent peak, indicative of the small amount of extract available for analysis. The samples at 7047' show an oil-like distribution of normal alkanes. The normal alkanes decrease steadily in relative abundance from about $n\text{-C}_{15}$ upwards and minor amounts of longer carbon chain length normal alkanes up to about $n\text{-C}_{36}$ are apparent. The isoprenoid alkanes pristane and phytane are present, with pristane dominant over phytane.

The whole extract gas chromatogram of the sample 6181' shows a possible trace of an oil-like distribution of hydrocarbons, represented mainly by normal alkanes between $n\text{-C}_{13}$ and $n\text{-C}_{16}$, with very small traces of longer carbon chain length normal alkanes. However, the chromatogram appears to be dominated by contaminant peaks which may be derived from very small amounts of hydrocarbon-based substances in the drilling fluid system.

Alkane gas chromatograms of the two samples at 7047' are presented in Figure 3(1-2) and the alkane gas chromatography quantitative data are given in Table 4. Despite the small extract weights, the alkane gas chromatograms show good peak resolution and illustrate the distributions of alkane hydrocarbons in the extracts. The alkane gas chromatograms are very similar, indicating that the nature of the hydrocarbon influx had not changed significantly during circulation at 7047'. The chromatograms are dominated by normal alkanes at $n\text{-C}_{14}$ and $n\text{-C}_{15}$. Normal alkanes decrease steadily in relative abundance from $n\text{-C}_{16}$ up to $n\text{-C}_{35}$. There is no significant odd or even carbon number preference which, combined with the pristane/ $n\text{-C}_{17}$ and phytane/ $n\text{-C}_{18}$ ratios, indicates generation of the oil from a middle mature source. Polycyclic molecular biomarker peaks are not clearly apparent in the higher molecular weight range of the chromatograms, indicating that the steranes and triterpanes are in relatively low abundance, consistent with a mature source. The

chromatographic baselines are approximately flat, indicating that the extracts do not include a significant degraded oil component.

Due to the very small extract weight obtained from the initial, quantitative solvent extraction analyses, it was necessary to carry out further extractions in order to obtain sufficient hydrocarbon for more detailed alkane gas chromatography-mass spectrometry (GC-MS) analyses. The two samples at 7047' were selected for further analyses and as large a volume of the drilling mud as possible was extracted non-quantitatively. Sufficient extract was obtained from each of the two samples for alkane GC-MS analysis.

Alkane GC-MS analysis of branched and cyclic alkane fractions of the samples at 7047' was carried out. Selective removal of the normal alkanes generally improves the peak resolution, particularly in cases where the polycyclic molecular biomarkers are present in low abundance. Selected alkane GC-MS mass chromatograms are presented in Figures 4(1-2) to 8(1-2) and the calculated GC-MS ratios are given in Table 5. The results obtained are generally good, with good peak resolution, enabling the sterane and triterpane biomarkers to be identified. An index to the GC-MS peak assignments is given in Appendix 3 and the GC-MS quantitative data are given in Appendix 4(1-2).

The m/e 191 mass chromatograms (Figures 5(1-2) and 6(1-2)) show the distributions of the C₁₉ to C₃₀ tricyclic terpanes and the C₂₇ to C₃₅ pentacyclic triterpanes (hopanes). The moderately high ratio of the C₂₇ 18 α (H)-trisnorhopane (Ts) to C₂₇ 17 α (H)-trisnorhopane (Tm) (ratio 1, Table 5) indicates generation of the oil from a middle mature or late mature source rock. The other triterpane maturity parameters are consistent with the Ts/Tm ratios. It is noted that the Ts/Tm ratios are comparable to the core extracts analysed from the N2/7-20X and N2/7-21S wells, but are lower than the values obtained for the tested oils analysed from these wells. The data indicate that the oil present in the drilling fluid samples was generated at a lower level of maturity than the tested oils. The medium to light oils analysed (Report No. 6796/1c) were generated from a middle to late or late mature source.

The m/e 191 mass chromatograms do not show significant amounts of the C₂₈ 17 α (H)18 α (H)21 β (H)-28,30-bisnorhopane. Whereas bisnorhopane is a common constituent of Kimmeridge Clay/Draupne Formation source rocks, the relative abundance of this compound typically decreases markedly with increasing maturation and may be very minor or not distinguishable in hydrocarbons derived from middle to late mature source rocks. Low relative abundance of C₂₈ bisnorhopane was also noted in the oils and core extracts analysed from the N2/7-20X and N2/7-21S wells.

Demethylated hopanes (25-norhopanes), the presence of which would indicate biodegradation of the oil, are not apparent on the m/e 177 and m/e 191 mass chromatograms.

The m/e 191 mass chromatograms include an unidentified C₃₀ triterpane, which corresponds to the peak X of Philp and Gilbert (1986). This structurally unelucidated compound appears to be thermodynamically more stable than the hopanes, and is typically relatively abundant in late mature samples. The relative abundance of this peak in the drilling fluid extracts is comparable to the core extracts analysed previously, but less than the tested oil samples, indicating that the oils are derived from a more mature source.

The m/e 191 mass chromatogram of the sample corresponding to circulation at 16.15 hrs (Figure 6.1) includes an unidentified component, labelled UI, which

coelutes with the later eluting C_{29} tricyclic terpane isomer. This compound may also be present in the sample corresponding to circulation at 00.00 hrs. (Figure 6.2), but is less apparent. This component was noted in the core extracts analysed previously, but not in the tested oils. The origin and significance of this peak remains completely uncertain. The drilling fluid extracts also appear to contain minor amounts of three other unidentified components which were identified in the core extracts.

The C_{27} , C_{28} , and C_{29} steranes are shown on the m/e 217 and m/e 218 mass chromatograms (Figure 8(1-2)). The distributions of the steranes are consistent with generation of the oil from a mature source and do not show the effects of degradation. The sterane distributions are similar to the oils and core extracts analysed previously, indicating that these are derived from the same source. The data are also consistent with generation of the oil from source rocks in the Kimmeridge Clay/Draupne Formation.

The C_{27} , C_{28} and C_{29} rearranged steranes (diasteranes) are shown on the m/e 259 mass chromatograms (Figures 5(1-2) and 6(1-2)). These diasteranes are more thermally stable than the steranes and increase in relative abundance at later maturity. The relative abundances of the diasteranes compared to the steranes in the hydrocarbon extracted from the drilling fluid samples are comparable to the core extracts, indicating that these are representative of similar levels of maturity, whereas the diasteranes are relatively more abundant in the oils, indicating a higher level of maturity.

The m/e 259 mass chromatograms include an unidentified peak, labelled U2, the origin of which is uncertain. This peak is also present in the oils analysed previously and is particularly prominent in the N2/7-21S DST-3 sample (Figure 6.4, Report No. 6796/Ic), and is also present in the core extracts, particularly the sample at 15281.7' in the N2/7-21S well (Figure 13.3, Report No. 6796/Ic).

The m/e 217, m/e 218 and m/e 231 mass chromatograms indicate the presence of 4-methylsteranes, although the individual isomers are not readily apparent, a feature typical of mature samples. The C_{30} $4\alpha(H)$ -methyl- $5\alpha(H)14\alpha(H)17\alpha(H)$ 20R sterane and also the isomeric C_{30} $4\alpha(H)$ -methyl- $5\alpha(H)14\beta(H)17\beta(H)$ 20R and 20S isoosteranes are apparent on the m/e 217 mass chromatograms. The 4-methylsteranes are generally considered to indicate the contribution of the lipid constituents of dinoflagellates or comparable marine algae to the source rock kerogen and are common in Kimmeridge Clay/Draupne Formation source rocks and related oils.

4 REFERENCES

- ROBERTSON GROUP plc, 1988. A petroleum geochemical evaluation of Phillips well 2/7-20X and 2/7-20X sidetrack 2, Norwegian North Sea. Proprietary report number 6390/Ic, November 1988.
- ROBERTSON GROUP plc, 1990. A petroleum geochemical evaluation of the interval 13810' to 16351'TD of the N2/7-21S well, Norwegian North Sea. Proprietary report number 6708/Ic, June 1990.
- ROBERTSON GROUP plc, 1990. Petroleum geochemical analysis of tested oils and bitumen in core samples, N2/7-20X and N2/7-21S wells, Norwegian North Sea. Proprietary report number 6796/Ic, October 1990.

GENERAL DATA		AIRSPACE GASEOUS HYDROCARBON DATA														
SAMPLE DEPTH Feet	SAMPLE TYPE	TOC % OF ROCK	GAS ABUNDANCE, %								TOTAL ABUNDANCE (ppm)	SUM, %			RATIOS	
			C1	C2	C3	iC4	nC4	iC5	nC5	C6+		C1-C5	C1-C4	C2-C4	C2-C4/ C1-C4	i-C4/ n-C4
4966	Mud	-	88.6	3.5	2.4	0.4	1.3	0.6	0.8	2.4	5615	97.6	96.2	7.7	0.08	0.33
6181	Mud	-	71.0	2.6	4.2	1.5	3.8	2.6	4.0	10.3	10274	89.7	83.1	12.1	0.15	0.40
7047 (16.15 hrs.)	Mud	-	36.3	13.1	14.1	5.7	13.5	5.2	6.5	7.5	64694	92.5	80.8	44.5	0.55	0.50
7047 (00.00 hrs.)	Mud	-	38.6	14.7	14.5	4.4	9.6	4.1	5.5	8.6	40589	91.4	81.9	43.3	0.53	0.46

AIRSPACE GASEOUS HYDROCARBON DATA
TABLE 1

SAMPLE DATA						
SAMPLE DEPTH (Feet)	4966	6181	7047(16.15 hrs.)	7047(00.00 hrs.)		
SAMPLE TYPE	Mud	Mud	Mud	Mud		

COMPONENTS	GASOLINE RANGE COMPONENT ABUNDANCE (%)				
i-C4	1.384	1.259	4.016	3.045	
n-C4	16.854	4.114	11.909	8.866	
i-C5	4.237	2.919	5.294	4.619	
n-C5	8.958	8.301	13.941	12.732	
2,2,dmb	1.071	.139	.191	.198	
cp	1.677	.954	1.255	1.037	
2,3,dmb	.634	.537	.723	.717	
2,mp	4.660	4.815	5.312	5.482	
3,mp	4.784	3.366	3.232	3.319	
n-C6	8.473	9.617	10.693	11.244	
mcp+2,2,dmp	5.021	5.629	4.610	4.601	
2,4,dmp	.255	.374	.412	.476	
benz	3.480	5.225	1.943	2.144	
3,3,dmp	.246	.154	.086	.103	
ch	4.941	5.614	5.476	5.452	
2,mh	3.193	3.356	3.400	3.991	
1,1,dmcp	.372	.509	.454	.511	
3,mh	3.073	2.701	2.750	3.245	
cis,1,3,dmcp	1.070	1.001	.616	.709	
trans,1,3,dmcp	.859	.907	.600	.681	
trans,1,2,dmcp+3,ep	2.377	2.576	1.508	1.746	
n-C7	6.732	7.001	8.251	9.931	
mch+cis,1,2,dmcp	9.660	12.283	8.785	10.007	
ecp	1.012	1.089	.385	.483	
tol	4.980	15.563	4.160	4.663	

GENERAL DATA												
Total Abundance(ppb)	35			135			3360			1815		
TOC (% of Rock)												
Abundance at 1% TOC	*			*			*			*		
Alkane Composition	45	26	29	37	25	39	48	27	25	46	27	27
C7 Alkane Composition	17	17	65	16	15	69	22	18	60	24	19	58
Aromatic Composition	8.46			20.79			6.10			6.81		

RATIOS											
i/n-C4	.08			.31			.34			.34	
i/n-C5	.47			.35			.38			.36	
cp / 2,3,dmb	2.65			1.78			1.74			1.45	
n-C7 / mch	.70			.57			.94			.99	
2,mp / 3,mp	.97			1.43			1.64			1.65	
n-C6 / mcp +2,2,dmp	1.69			1.71			2.32			2.44	
mch / tol	1.94			.79			2.11			2.15	
Late Mature Index	.36			.43			.22			.21	
Aromaticity Index	.74			2.22			.50			.47	
Heptane Index	23.34			21.91			30.28			31.15	
Isoheptane Index	1.34			1.21			1.94			1.98	
Kerogen Type Index	14.44			14.77			13.58			13.68	

LEGEND					
i - iso	c - cyclo	m - methyl	b - butane	h - hexane	tol - toluene
n - normal	d - di	e - ethyl	p - pentane	benz - benzene	
Alkane Composition - % composition of normal, iso and cyclo alkanes					
C7 Alkane Composition - % composition of C7 normal, iso and cyclo alkanes					
Aromatic Composition - % composition of Benzene + Toluene					
For definition of indices - Late Mature, Aromaticity, Heptane, Isoheptane & Kerogen Type - see Appendix 2					

GASOLINE RANGE HYDROCARBON DATA

TABLE : 2

GENERAL DATA			CHEMICAL ANALYSIS DATA												
SAMPLE DEPTH (Feet)	SAMPLE TYPE	ANALYSED LITHOLOGY	TOC % OF ROCK	PYROLYSIS					SOLVENT EXTRACTION/FRACTIONATION						
				Tmax °C	HI	OI	PI	POT.YLD. (ppm)	EXTR. (ppm)	HC (ppm)	EXTR. % GC	HC %GC	ALK. %HC		
4966	Mud		-							10					
6181	Mud		-							5					
7047 (16.15 hrs.)	Mud		-							15					
7047 (00.00 hrs.)	Mud		-							15					

SUMMARY OF CHEMICAL ANALYSIS DATA

TABLE : 3

SAMPLE DATA						
SAMPLE DEPTH (Feet)	7047(16.15 hrs.)	7047(00.00 hrs.)				
SAMPLE TYPE	Mud	Mud				

COMPONENTS	QUANTIFIED NORMAL AND ISOPRENOID ALKANE ABUNDANCES (%)				
	n-C10				
n-C11	.22				
n-C12	1.22	.12			
n-C13	4.69	3.85			
n-C14	9.88	13.45			
n-C15	8.55	11.54			
n-C16	6.43	6.83			
n-C17	6.23	5.75			
n-C18	5.47	5.11			
n-C19	5.46	3.96			
n-C20	4.66	4.72			
n-C21	4.50	4.14			
n-C22	3.71	3.42			
n-C23	3.67	3.49			
n-C24	2.82	2.59			
n-C25	2.69	2.80			
n-C26	2.32	2.04			
n-C27	1.74	1.63			
n-C28	1.53	1.65			
n-C29	1.35	1.24			
n-C30	1.12	1.05			
n-C31	1.14	1.05			
n-C32	.85	.81			
n-C33	.88	.82			
n-C34	.86	.71			
n-C35	.61	.61			
n-C36					
i-C15 (Farnesane)	2.73	3.29			
i-C16	4.94	5.45			
i-C18 (Norpristane)	3.24	2.92			
i-C19 (Pristane)	3.82	3.25			
i-C20 (Phytane)	2.72	2.55			

GENERAL DATA						
Total Abundance(%)	100	100				
TOC (% of Rock)	.00	.00				
Extract (ppm)	15	15				
Hydrocarbons (ppm)						
Hydrocarbon(mg/gTOC)						
Alks(% Hydrocarbons)						
Rock-Eval HI						
Rock-Eval PI						

RATIOS						
CPI-1	1.04	1.07				
CPI-2	1.04	1.06				
CPI-3	.90	.88				
Bias	1.81	1.77				
i-C19 / n-C17	.61	.57				
i-C20 / n-C18	.50	.50				
i-C19 / i-C20	1.40	1.27				

LEGEND						
i - isoprenoid	n - normal	For definition of Ratios CPI-1,-2,-3 and Bias - see Appendix 2				

ALKANE GAS CHROMATOGRAPHY DATA

TABLE : 4

APPENDIX 1

Abbreviations used in analytical data sheets

APPENDIX 1
 ABBREVIATIONS USED IN ANALYTICAL DATA SHEETS

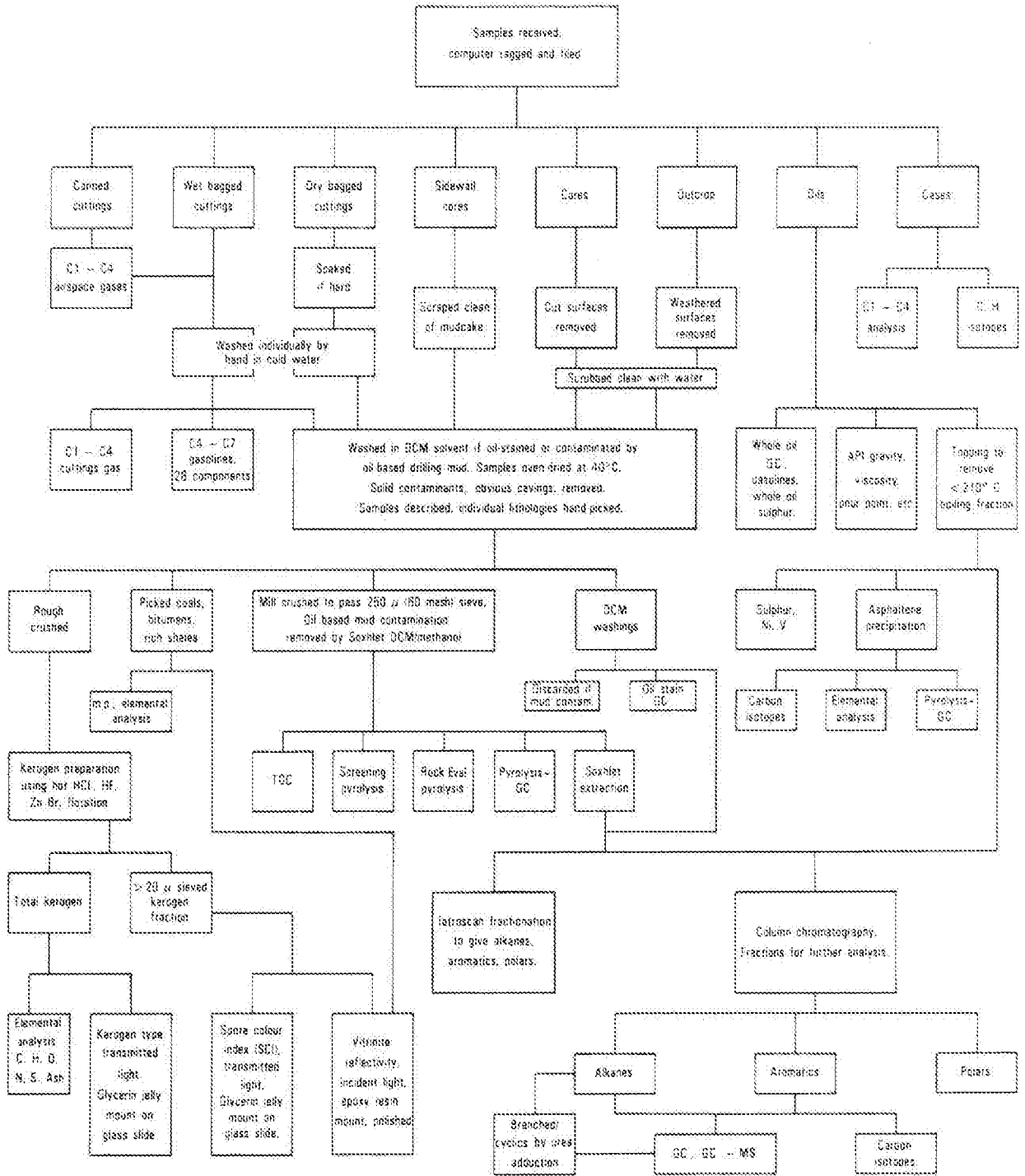
a/a	-	as above	MOST	-	mudstone
Ac	-	acritarchs	med	-	medium
ADD	-	mud additive	NET	-	metamorphic rocks
Al	-	algae	mic	-	mica/micaceous
Am	-	amorphous	micr	-	micritic
ang	-	angular	min	-	mineral
ARB	-	anhydrite	unr	-	minor
aren	-	arenaceous	mod	-	moderate
arg	-	argillaceous	ntl	-	mottled
BAS	-	basalt	n-	-	normal
bd	-	bedded/bedding	NA	-	not available
B(IT)	-	bitumen/bituminous	nod	-	nodule/nodular
bl	-	blue	NS	-	no sample
bl'd	-	bleached	occ	-	occasional
blk	-	black	ol	-	olive
bri	-	brilliant	ool	-	oolitic
brn	-	brown	orng	-	orange
calc	-	calcareous	OS	-	oil stain
CALT	-	calcite	P	-	picked lithology
carb	-	carbonaceous	pal	-	pale
COL	-	conglomerate	Ph	-	phytane
CHK	-	chalk	pink	-	pink
CHT	-	chert	por	-	porous/porosity
CLYST	-	claystone	pp	-	purple
CMT	-	cement	Pr	-	pristane
Comp	-	composite	pred	-	predominantly
crs	-	coarse	Prt	-	present
CSG	-	casing point/shoe	PYR/pyr	-	pyrite/pyritic
Ctgs	-	ditch cuttings	QTZ(T)	-	quartz(ite)
Cu	-	cuticle	Re	-	resin
C(vd)	-	caved	R(ew)	-	reworked
decarb	-	decarbonated	rnd	-	round(ed)
Di	-	dinocysts	Sap	-	sapropel
dk	-	dark	sbng	-	subangular
DLT	-	dolerite	sbrd	-	subrounded
DOL/dol	-	dolomite/dolomitic	SCI	-	spore colour index
dsk	-	dusky	Sf	-	semifusinite
Ex	-	exinite	sft	-	soft
Exs	-	exsudatinites	SH	-	shale
extr	-	extracted	shly	-	shaly
f	-	fine	sil	-	siliceous
Fel	-	feldspathic	skc	-	slickenside surface
fer	-	ferruginous	SLA	-	slate
Flu	-	fluorescence	SLI(ST)	-	silt(stone)
fm	-	formation	sily	-	silty
foss	-	fossils/fossiliferous	SND	-	sand
fr	-	friable	sndy	-	sandy
frac	-	fracture	Sp	-	spores
frags	-	fragments	SST	-	sandstone
Fu	-	fusinite	st	-	stained
GLC/glc	-	glaucconite/glauconitic	stks	-	streaks
gn	-	green	suc	-	sucrosic
grd	-	graded/grading to	suri	-	surface
grns	-	grains	SWC	-	side wall core
gy	-	grey	TD	-	total depth
GYP	-	gypsum	TGC	-	total organic carbon
HAL	-	halite	tr	-	trace(s)
hd	-	hard	trns	-	transparent
hor	-	horizontal	v	-	very
H(RV)	-	high reflecting vitrinite	vgt	-	variegated
i-	-	iso-	Vit	-	vitrinite
I/b	-	inter-bedded	vn	-	vein
IGN	-	igneous rocks	VOLC	-	volcanic rocks
inc	-	including	VR	-	vitrinite reflectivity
Inert	-	inertinite	wht	-	white
lam	-	laminae/laminated	xln	-	crystalline
LCM	-	lost circulation material	yel	-	yellow
LIG/lig	-	lignite/lignitic		-	
lms	-	lens(es)		-	no analysis carried out
L(RV)	-	low reflecting vitrinite	*	-	analysed but no data obtained
LST	-	limestone	gy-gn	-	grayish green
lt	-	light	gy/gn	-	grey-green (gradation)
mass	-	massive	gn-gy	-	greenish gray

Note: (Maturity data tables only). Number in brackets refers to number of reflectivity values averaged to give quoted result. Preferred values for indigenous phytoclasts are listed first.

APPENDIX 2

Analytical procedures and techniques

FLOW CHART FOR GEOCHEMICAL ANALYSIS



07/50N / 5214

APPENDIX FIGURE 1

APPENDIX 2

ANALYTICAL PROCEDURES AND TECHNIQUES

This appendix summarises the main steps in the analyses carried out in the Robertson Research International Ltd. petroleum geochemistry laboratories. Analytical pathways are shown on the flow chart (Appendix Figure 1) and details of laboratory procedures and techniques are given in the text. These may in certain circumstances be adapted to suit particular samples or conditions. Interpretation guidelines are also defined.

1. Sample Preparation

General

Samples are received into the laboratories in the forms of well-site canned ditch cuttings, bagged ditch cuttings in various stages of preparation from wet, unwashed to dried, washed; sidewall cores, conventional cores, outcrop samples, crude oil samples and gas samples. Each sample is assigned a number which is entered into a computer system to monitor sample selection and progress. Preparation techniques are directed towards obtaining clean samples, free of drilling mud and mud additives, obvious caving contamination and indeterminate fine material. Washing with cold water is standard but further washing with solvent (dichloromethane, DCM) is carried out if oil-based mud is present, after which samples are dried, described and individual lithologies hand-picked where practicable. Samples are rough crushed to approximately pea-sized fragments for kerogen preparation or finely milled for chemical analysis.

Kerogen Preparation

Kerogen concentrates for microscopic examination and elemental analysis are prepared using standard palynological procedures but omitting oxidation or acetolysis. Acid maceration involves the use of hot hydrochloric acid (HCl) to remove carbonates and hot 60% hydrofluoric acid (HF) to remove or break down silicates. Mineral residues are separated from the kerogen by a combination of ultrasonic vibration and zinc bromide flotation. Kerogen samples for spore colour and kerogen typing are mounted on glass slides in glycerin jelly, those for vitrinite reflectivity are dried and mounted in epoxy resin. Kerogen residues are stored in methanol.

2. Maturity Evaluation

The techniques employed for interpreting maturity and thermal history in these laboratories are based mainly on spore colouration and vitrinite reflectivity measurement, supplemented by data obtained from airspace gas and gasoline analysis, pyrolysis Tmax, and hydrocarbon analysis including gas chromatography and gas chromatography-mass spectrometry.

Spore Colouration

Sporomorph colour is assessed using a >20 μ sieved kerogen fraction viewed in transmitted light on a standard palynological microscope. Unusual hues are checked using incident blue/UV light fluorescence. Measurement is made by eye against reference sets of single grain spore mounts and trained operators achieve a high degree of accuracy and reproducibility. The 1 to 10 Spore Colour Index (SCI) scale was designed for linearity with increasing depth and temperature and correlates approximately with the following zones of oil generation: 1.0 to 3.5, immature; 3.5 to 5.0, early mature, generation of low gravity oils (28 to 35 °API); 5.0 to 7.0, middle mature, generation of medium gravity oils (35 to 42 °API); 7.0 to 8.5, late mature, generation of light oils (>42 °API) and condensates; 8.5 to 10, post mature, generation of condensate, wet gas and, ultimately, dry gas. Linearity of scale is of great value in prediction, by extrapolation, of the depth to any part of the oil generation sequence. The value of SCI measurement lies in the objective selection of measured grains, so minimising problems of caving and reworking, and in its more direct correlation against oil generation than vitrinite reflectivity measurement. Limitations in its use concern the difficulty of correlation against other colour scales and the insensitivity of the scale in the late to post mature region. Anomalous colours may result from bleaching or staining during deposition and diagenesis. The correlation of SCI against Thermal Alteration Index (TAI) given on the SCI versus depth plot in the reports was made by direct comparison of Staplin's standard slides with SCI standard slides.

Vitrinite Reflectivity

The majority of preparations examined under reflected light in these laboratories are made using >20 μ sieved kerogen, mounted in resin blocks and polished with carborundum and alumina although total kerogen may be used when sample size is

limited. Picked coals, organic-rich shales or limestones containing solid bitumen are mounted directly in resin blocks and polished in the usual way. Measurement is made on a Leitz Orthoplan microscope fitted with an MFV Compact photometer which feeds values direct to a desk top computer for data processing from each sample. The system is calibrated against glass standards and reflectance values are expressed as arithmetic means of measurements taken in oil immersion (R_o or $R_{m oil}$). R_{max} and R_{min} may be measured and quoted in certain circumstances but the difference is insignificant below about R_o 1.0%. Some operator selection of particles during measurement is essential and obvious contaminants or non-vitrinitic material are noted but not necessarily quoted. The value quoted on data tables is that which is interpreted as most appropriate, but other possibilities may also be given. Plotted figures assume a logarithmic increase of reflectance with depth. R_o 0.5% is a widely accepted threshold value for the onset of oil generation, although as the kinetics of oil generation may not be identical to those of vitrinite reflectivity development this must be seen only as a general guide. The floor for oil generation is characterised by a reflectance value of about 1.3%. Wet gas generation peaks at a value of about 1% and ceases at the 2% level. Dry gas generation peaks at a reflectance of about 1.5% and ceases at the 3% to 4% level. Correlation of reflectance values with other maturity parameters may not be universal because of time-temperature factors and is best made on a local basis.

Reflectivity measurement is a widely used and versatile tool which may be readily calibrated against easily obtained standards. It is applicable over a wide range of maturity stages from immature to post mature (0.2% to 5% R_o). High surface intercepts on plotted figures and discordances at faults and unconformities can give realistic estimates of the amount of section missing. It is of limited value in Early Palaeozoic sections where land plant material is absent, although a general guide to maturity may be obtained from chitinous organic matter. Even a skilled operator may have difficulty in distinguishing indigenous vitrinite from some forms of inertinite, anomalously reflecting "pseudovitrinite", cavings and reworked fragments.

Airspace Gas Analysis

Wet cuttings are collected at the well site and sealed in partly full cans containing bactericide. In the laboratory, the airspace (headspace) gas is extracted using a can piercer fitted with a septum and analysed by gas chromatography. The proportions of methane, ethane, propane, *iso*- and *n*-butane are calculated from integrated peak areas by comparison with a standard mixture of these gases. Methane is the dominant gas in immature and post mature sediments, comprising 90-100% of total gas, falling to 30-70% in mature sediments. The onset of maturity for oil generation (SCI 3.5) is characteristically marked by an increase in wet gas (C_2-C_4) to between 10 and 20% with further increases in maturity indicated by a decrease in the ratio of *iso*- to *n*-butane. Ratios of >1.0 are typical for immature sediments and <0.5 are usual in mature sediments. Departures from composition versus depth trends may be useful in indicating migrant gas at faults, unconformities or reservoir rocks but limit the method as a reliable maturity indicator. Airspace gas analysis is an inexpensive and rapidly executed method of screening samples for further maturity and hydrocarbon content determinations.

Gasoline Analysis and Cuttings Gas Analysis

Cuttings samples received wet, preferably in sealed containers, are suitable for gasoline and cuttings gas analysis. A portion of the washed cuttings sample is retained wet, pulverised in a sealed shaker and warmed to expel the C_1 to C_7 hydrocarbon components into the shaker airspace. A sample of this airspace gas is then removed and analysed by gas chromatography either for cuttings gas (C_1 to C_4) or gasolines (C_4 to C_7). Up to 28 hydrocarbon components are identified in the C_4 to C_7 range and their relative proportions calculated from integrated peak areas with reference to standard mixtures. Immature source rocks yield low total abundances and limited numbers of components whereas mature source rocks usually contain a full complement of identified hydrocarbons with the onset of maturity indicated by a rapid rise in total gasoline abundances with depth. Anomalous amounts of gasolines may mark the presence of oil stain. Gasolines may be used in oil to oil or oil to source rock correlations but the concentration of some of the measured components is not only a function of source but also depends on maturity, migration and alteration in the reservoir. Using the most stable compounds, pairs with similar chemical structure and boiling points are reduced to pair ratios and compared with the same pair ratios in other oils or possible source rocks. Gasoline analysis is a valuable tool in that it measures directly the hydrocarbons being generated from a sediment but its sensitivity in detecting traces of oil places constraints on its use as a maturity indicator.

Rock-Eval Pyrolysis, Gas Chromatography (GC) and Gas Chromatography-Mass Spectrometry (GC-MS) in Maturity Analysis

These three analytical processes measure parameters which are functions of both maturity and kerogen type. Data from them may give a general guide to maturity but if the kerogen types are known, more specific conclusions may be drawn. From Rock-Eval data, the temperature of maximum rate of pyrolysis, T_{max} , is the most useful datum; gas chromatograms of alkanes, separated from source rock extracts or oils, yield carbon preference indices (CPI) and isoprenoid ratios; GC-MS quantitative fragmentograms provide abundance ratios for specific compounds which are particularly useful in assessing the level of maturity at which source rock hydrocarbons or oils have been generated. All these supplementary data may be used to confirm results from visual analysis or supplant them if poor or unavailable.

3. Source Rock Evaluation

Total Organic Carbon Content (TOC)

Organic carbon values are obtained by treating 0.1g of crushed rock sample with hot, concentrated HCl to remove carbonates. The washed residue is filtered on to a glass fibre pad and ignited in a Leco carbon analyser. For screening purposes, samples are analysed singly but where further analyses, such as pyrolysis or solvent extraction are anticipated, a duplicate sample is run. Blanks and standards are run as routine and where values from duplicated samples do not concur within strict accuracy limits, they are rerun. Where samples are heavily stained with oil, either from natural deposits or drilling mud, TOC is repeated on the dried, solvent extracted sample.

TOC measurement is fundamental in assessing source rock quality since when combined with kerogen type and maturity, a full description of the potential to generate oil may be given. It is found in practice that sediments containing less than 0.3% TOC are unlikely to have any source potential, those containing between 0.3% and 1% may be marginal sources but the better quality sources contain in excess of 1% TOC. Screening by TOC is therefore an inexpensive and rapid method of selection of samples for further analysis in source potential evaluation.

Rock-Eval Pyrolysis

Pyrolysis data are obtained using the IFF-Fina Rock-Eval apparatus. 100 mg of crushed, whole rock either from bulk sample or picked lithology is weighed accurately into a crucible and introduced into a furnace at 250°C. Free hydrocarbons (roughly equivalent to solvent extractable hydrocarbons) are volatilised and quantified by flame ionisation detector (FID) to give Peak 1 (S_1 , ppm). The furnace temperature is increased to 350°C at 25°C/minute and within this range, kerogens crack to give hydrocarbons, measured by FID to give Peak 2 (S_2 , ppm) and carbon dioxide, measured by thermal conductivity detector (TCD) to give Peak 3 (S_3 , ppm). The temperature at the maximum rate of evolution of cracked volatiles (T_{max}) is measured automatically but can also be monitored visually. The instrument is calibrated daily using standards both at the beginning of the work period and at regular intervals thereafter and crucible blanks are run as routine. The tabulated data in reports comprise the following parameters:

- T_{max} °C - temperature of maximum rate of Peak 2 hydrocarbon evolution.
- Hydrogen Index (HI) - S_2/TOC (mg/g) or ratio of released hydrocarbon to organic carbon content. This is a measure of the hydrocarbon generating potential remaining in the kerogen as opposed to that of the whole rock.
- Oxygen Index (OI) - S_3/TOC (mg/g) or ratio of released carbon dioxide to organic carbon content.
- Production Index (PI) - $S_1/(S_1+S_2)$, or ratio of the amount of hydrocarbons released in the first stage of heating to the total amount of hydrocarbons released and cracked during pyrolysis.
- Potential Yield (PY) - S_2 (ppm) or total of hydrocarbons released during cracking of kerogen compared to original weight of rock.

T_{max} , hydrogen index and oxygen index are each functions of both maturity and kerogen type. Using published and empirical data, it has been possible to assemble a model to show the relationships of these factors to maturity as measured by spore colouration and vitrinite reflectivity for a selection of pure kerogen types. The kerogen types used are algal sapropel (type I), waxy sapropel (type II), vitrinite (type IIIA) and inertinite (type IIIB) and a computer program has been devised by which the amounts of these components may be calculated from the HI, OI, T_{max} and maturity

data for any sample. These are the values expressed in the "kerogen composition by calculation" columns tabulated in the reports.

The hydrogen index is a measure of the hydrocarbon generating potential of the kerogen and is analogous to the atomic H/C ratio. Immature, organically rich source rocks and oil shales give values above 500, mature oil source rocks give values between 200 and 550. For a given kerogen type, these values progressively diminish with increasing maturity.

The temperature of maximum rate of pyrolysis depends partly on the kerogen type but the transition from immature to mature organic matter is marked by temperatures between 415° and 435°C. The maturity transition from oil and wet gas generation to dry gas generation is marked by temperatures between 455° and 460°C. In practice, greater variation than these ideal temperature ranges may be seen, but they are nevertheless useful as general guides to the level of maturity attained by the sediment.

The production index increases with maturity from values near zero for immature organic matter to maximum values of 0.15 during the late stages of oil generation. Anomalously high values indicate the presence of oil or contaminants. The potential yield is an indication of the predicted yield of hydrocarbons from the source rock at optimum maturity and is a measure of the quality of the source rock. For immature sediments, values of 0 to 2000 ppm of hydrocarbon characterise a poor source rock, 2000 to 6000 ppm fair, 6000 to 20 000 ppm good and above 20 000 ppm very good.

Pyrolysis techniques have in recent years provided a major advance in the assessment of source rock quality and generating potential. Hydrocarbon yields from immature source beds examined on-structure may be translated into actual oil productivity from the same beds in mature basinal, off-structure situations. Models relating maturity and kerogen type may be used to define original source rock quality grades which are of great value in mapping organic facies. Amorphous kerogen types, indistinguishable in microscopic preparations over a wide range of chemical properties, may be readily differentiated by pyrolysis. The problem of analysing bulk samples containing mixed kerogens has been largely overcome by the kerogen type/maturity model and anomalous results arising from the presence of caving contamination and drilling mud additives can usually be explained by inspection. High oxygen indices sometimes occur as a result of the presence of metastable carbonates and in such cases the sample is acid decarbonated and re-run.

Visual Examination of Kerogen Concentrates

All palynological preparations on which SCI determinations are made are also examined for kerogen type. Visual estimations of the relative abundance of the broad groups vitrinite, inertinite and sapropel are made on the total kerogen slide mount but reference is also made to the >20µ sieved fraction to assist in identification. The scheme of identification is shown in Appendix Table 1. Full use is made of incident blue or UV light in distinguishing immature or early mature oil-prone kerogen from gas-prone kerogen.

Extract Analysis

The soluble organic materials present in rocks can be extracted with organic solvents, fractionated and analysed. The type and amount of material extracted depends largely upon the nature of the contained kerogen and its maturity, although the presence of migrant oil or drilling contamination may be the determining factors.

A maximum of 40g of crushed sample is extracted for a minimum of 12 hours in a Soxhlet apparatus using laboratory redistilled DCM. The solvent and the more volatile components (approximately up to n-C₁₅) are lost by evaporation in an air flow and the resulting total extract is weighed, dissolved in hexane and separated into alkanes (saturate) hydrocarbon, aromatic hydrocarbon, resene and asphaltene (polar) fractions by silica adsorption chromatography in the katroscan process.

Larger fractions, suitable for further analysis, are obtained by column chromatography. The extract is run through a short glass column packed with silica and alumina and eluted with hexane (to give the saturate fraction), (3:1 hexane: toluene mixture (to give the aromatic fraction) and methanol (to give the polar, or resene and asphaltene, fraction). A small proportion of non-eluted polar compounds usually remains on the column.

4. Oil Analysis

RRI laboratories offer a wide range of oil analyses both for geochemical purposes and industrial use. Physical property determinations are based mainly on IP methods and are available for lubricating oils, fuels and greases as well as crudes. Frequently measured properties of crude oils presented in geochemistry reports include: API gravity, pour point, viscosity and contents of water, sulphur, wax, asphaltene, nickel, vanadium and other metals. Chemical analysis of oils involves the following:

Whole oil gas chromatography - using split syringe injection and a temperature programme from -20°C or -30°C up to 270°C at 4°C/minute.

Associated gas - if oil has high gas/oil ratio.

Gasoline analysis - as for gasolines in rock samples but a weighed quantity of oil is used.

Topping of the oil - this is equivalent to the removal of the fraction boiling below about 210°C and gives a more standardised product for comparison of gas chromatograms of the C₁₅₊ fraction.

Column chromatography and gas chromatography - as for solvent extracts. Analysis is carried out on topped oil.

5. Gas Analysis

The hydrocarbon gases, C₁ to C₄, may be collected from the airspace of sealed canned samples or may be received from well-site tests in a special sealed gas cylinder (gas mouse). Chromatographic separation of the C₁ to C₄ gases is effected as described under airspace gas analysis. In addition, the separated gas components may be analysed for stable carbon and hydrogen isotope composition which may provide valuable clues to the origin of the gas.

6. Solid Bitumen Analysis

In some oil fields, problems are encountered where bitumen developments form continuous or patchy layers within reservoirs, dividing the pay zones and acting as barriers to natural fluid movement or inhibiting enhanced oil recovery techniques. Integrated geochemical and sedimentological studies aim to produce geological models capable of predicting the occurrence of bitumen layers and their likely thickness and ability to act as permeability barriers. Of further concern are the past or present relationships between the bitumen and reservoir oil, their source rocks and the timing of bitumen formation.

Analysis schemes involve screening of samples by assessing the amount of bitumen in polished core pieces using reflected light microscopy, followed by solvent extraction of control samples to estimate the proportion of solvent soluble bitumen. Different phases of bitumen formation are differentiated by reflectance measurement as described for vitrinite reflectance measurement. Soluble extracts are fractionated to give alkane, aromatics, asphaltene and resene components. Separated bitumens may be subjected to elemental analysis.

The data tabulated in reports comprise the following parameters:

Total extract - soluble organic matter, heavier than about $n-C_{15+}$, expressed as ppm of weight of rock.

Hydrocarbons - sum of alkane and aromatic hydrocarbons, expressed as ppm of weight of rock.

Extract % of organic carbon (EPOC) - $\frac{\text{total extract ppm}}{\text{TOC} \times 100}$; the extractability.

Hydrocarbons mg/g of organic carbon - total hydrocarbons normalised to 1g of organic carbon.

Hydrocarbons % extract - total hydrocarbons as a proportion of total extract.

Alkanes % hydrocarbons - the proportion of alkanes (saturates) in the total hydrocarbons. The proportion of aromatics is (100 minus this value) expressed as a percentage.

The extractability of oil-prone sapropelic organic matter increases rapidly in the oil generation zone and diminishes to very low values in post mature sediments. Overall the extractability of sapropelic organic matter is greater than that of gas-prone humic organic matter for similar levels of maturity. Samples with extractabilities of greater than 20% generally contain migrant oil or are contaminated with mud additives.

As maturation proceeds in the oil generation zone the proportion of hydrocarbons in the total extract increases from less than 20% to a maximum in the most productive horizons of around 60%. This trend is reversed as the oil-condensate zone is entered. The relative proportions of alkanes to aromatics can be used as a check for low levels of contamination. Fractions of the extract, separated by column chromatography are retained for further analysis by gas chromatography or for stable carbon isotope determination.

Capillary Gas Chromatography of C_{15+} Alkanes

A portion of the Soxhlet extract is eluted with hexane through a short silica column to yield the saturate hydrocarbon fraction. This fraction is evaporated in a stream of dry nitrogen at room temperature. A small portion of the fraction is then taken up in hexane and introduced into a 25 metre, wall-coated, open tubular glass capillary column coated with OV-1, or equivalent, mounted in a Carlo Erba gas chromatograph which is temperature programmed from 70°C to 270°C at 3°C/minute.

C_{15+} chromatograms are inspected for the distributions of n -alkanes, and the presence and abundance of isoprenoids (particularly pristane and phytane), steranes and triterpanes and unresolved envelopes of naphthenic compounds. The ratios pristane:phytane and pristane: $n-C_{17}$ are calculated. Carbon Preference Index (CPI) values quoted are those as defined by Philippi as the ratio $2C_{29}$ to $(C_{28}+C_{30})$ unless otherwise stated. Chromatography may reveal information about the kerogen type of the source rock, its maturity and condition of deposition and, if migrant oil is present, whether this has been water-flushed or biodegraded. Contaminant drilling mud additives may be identified.

Capillary Gas Chromatography of Aromatic and Branched/Cyclic Alkanes

The aromatic portion of the Soxhlet extract is eluted from a short silica/alumina column by a hexane/toluene mixture. The dried fraction is taken up in DCM and introduced into a 25 metre, wall-coated, open tubular glass capillary column coated with OV-1, or equivalent, mounted in a Carlo Erba gas chromatograph which is temperature programmed from 70°C to 270°C at 3°C/minute.

Branched chain alkanes are separated from normal alkanes by urea adduction and treated as for total alkanes.

Gas Chromatography-Mass Spectrometry

Mass spectrometry is a technique in which molecules are bombarded with high energy electrons causing ionisation and fragmentation of the molecules into ions of varying mass (m) and charge (z). The way in which a molecule fragments into ions of various m/z value is known as its fragmentation pattern, or mass spectrum and is unique. When linked to a gas chromatograph the mass spectrometer can be used in two different modes:

1. Full Scan Mode: A mass spectrum is obtained of each peak eluting from the gas chromatograph and a structural identification of the compound producing that peak can be made.
2. Multiple or Single Ion Monitoring Mode: The mass spectrometer is tuned to certain m/z values to detect whether a compound, eluting from the gas chromatograph, fragments to give an ion at that value. Certain fragmentations are indicative of specific compound types and the most commonly monitored fragment ions used in petroleum geochemistry are those with m/z values of 191, 217 and 259 which are the principal fragment ions obtained from groups of alkanes known as triterpanes, regular steranes and rearranged steranes respectively. These are compounds containing 27 to 35 carbon atoms arranged in a polycyclic, normally 4 or 5 ring, structure, occurring in the n - C_{26} to n - C_{35} region of a gas chromatogram. The basic molecular skeletons of these compounds are very similar to those of the original organic matter deposited in the sediment and so these 191, 217 and 259 distribution plots, known as mass fragmentograms or mass chromatograms, form a pattern characteristic of the source material. This technique of "fingerprinting" is also one of the more exact methods of correlating an oil to its source, or to another oil.

Carbon Isotope ($^{13}C/^{12}C$) Ratio Analysis

Carbon has two stable isotopes, the more abundant ^{12}C isotope and the heavier ^{13}C isotope, which in nature forms about 1% of carbon. Deviations from the $^{13}C/^{12}C$ ratio are extremely small and carbon isotope ratios, as measured by mass spectrometry, are expressed as deviations from a standard, the Pee Dee Belemnite carbonate (PDB standard) in parts per thousand (parts per mil; ‰). Positive deviations indicate ^{13}C enrichment and conversely, negative deviations indicate ^{13}C impoverishment.

While the carbon isotope ratios of oils and rock extracts can range from -20 to -32 ‰ depending on the source organic matter type, the difference between a specific oil and its source is small. Measurements are usually made on the C_{15+} alkane and aromatic hydrocarbon fractions separately and there should be no more than 1 ‰ difference between the oil and its source for either fraction. If there is any doubt that the source rock extracts are not indigenous to the source rock kerogen, the carbon isotope ratio of the extracted source rock kerogen can be measured.

Pyrolysis-Gas Chromatography

The hydrocarbon pyrolysate derived from thermal, anhydrous cracking of kerogen is analysed by capillary gas chromatography. A few mg of rock, kerogen or asphaltene is heated to 600°C for 20 seconds in the injector of a gas chromatograph. The chromatograph oven is kept at -30°C during pyrolysis and then raised to 300°C at a programmed rate of 7.5°C/minute. Chromatograms produced this way are often very different from those of source rock extracts or oils in that branched and cyclic isomers are generated freely giving numerous, closely spaced peaks, along with unsaturated, alkene (olefin) hydrocarbons. The "doublet" peaks often observed in these chromatograms comprise alkene-alkane pairs, the first eluting, and usually smaller peak, being the alkene. The chromatograms range from C_1 to C_{30} or above and although variable, are broadly characteristic of source rock type. Gas-prone kerogen cracks to give a more limited molecular weight range of products, concentrated towards the light ends, whereas oil-prone kerogen gives more prominent alkene-alkane doublets in the C_{12} to C_{30} region. The largest peak from both types is usually methane.

Elemental Analysis

Total (unsieved) kerogen is prepared as described in Section 1. The dried material is combusted in oxygen in an elemental analyser and the oxides of carbon, hydrogen, nitrogen and sulphur are measured. The unburnt residue is the ash content. Oxygen is usually calculated by difference but can be determined separately if required. Results are quoted as percentage weights of C, H, O, N, S and Ash with the atomic ratio H/C and O/C calculated and plotted on the standard van Krevelen diagram. The relative amounts of C, H and O present in organic matter are dependent on both source and maturity. At known maturity levels, some measure of source quality may be determined. Limitations of the method in source rock assessment involve the difficulty of obtaining pure kerogen (in particular, free from pyrite) and the lack of a simple, direct determination of oxygen content.

Kerogen Typing Scheme for Transmitted White and Incident Blue/U.V. Light

General Properties	RRI Report Data Tables	Type *
Sapropelic (Oil-prone gas-prone at high maturity)	Algal Sapropel	Type I
	Waxy Sapropel	Type II
Humic (Gas-prone)	Vitrinite	Type IIIA
	Inertinite	Type IIIB

Amorphous		Structured	
Non-Fluorescent	Fluorescent	Non-Fluorescent	Fluorescent
Type I/II at high maturity (SCI >7.5)	Type I Sapropel Type II (degraded spores) Soft bitumens	Vitrinite (Type IIIA) brown/black, woody tissue	Cuticle Spores Pollen Dinocysts (Type II)
Type IIIA/B			
Oil residues (bitumens) Mineral (undigested) Grease contamination Mud additives		Inertinite (Type IIIB) very dark brown/black, woody tissue	Resinite Algae (Tasmanites, Botryococcus etc.)
		Solid bitumen - brown/ black (oil residue) often with crystal imprints	(Type I)
		Microforaminifera, chitinozoa etc. (Not usually important)	
		Spores, cuticle etc. at high maturity levels	
		Mud Additives - walnut etc.	

* Types I, II, III approximately sensu Tissot et al but Type III subdivided into IIIA (vitrinite) and IIIB (inertinite)

APPENDIX TABLE 1

Alkane gas chromatography data - definition of ratios

CPI 1 (Bray and Evans):

$$\frac{1}{2} \times \left[\frac{C_{25} + C_{27} + C_{29} + C_{31} + C_{33}}{C_{24} + C_{26} + C_{28} + C_{30} + C_{32}} + \frac{C_{25} + C_{27} + C_{29} + C_{31} + C_{33}}{C_{25} + C_{27} + C_{29} + C_{31} + C_{33}} \right]$$

CPI 2 (Radke and Statoil):

$$\frac{1}{2} \times \left[\frac{C_{25} + C_{27} + C_{29} + C_{31}}{C_{24} + C_{26} + C_{28} + C_{30}} + \frac{C_{25} + C_{27} + C_{29} + C_{31}}{C_{25} + C_{27} + C_{29} + C_{31}} \right]$$

CPI 3 (Statoil and Philippi):

$$\frac{2 \times C_{27}}{C_{26} + C_{28}}$$

Bias:

$$\frac{C_{16} + C_{17} + C_{18} + C_{19} + C_{20} + C_{21} + C_{22}}{C_{23} + C_{24} + C_{25} + C_{26} + C_{27} + C_{28} + C_{29} + C_{30} + C_{31} + C_{32} + C_{33}}$$

Gasoline ratios - definition of indices

- Late mature index - Benzene/methyl cyclohexane
- Aromaticity index - Toluene/*n*-heptane
- Heptane index - *n*-Heptane/all C₇ compounds (%)
- Iso*-heptane index - Methyl hexanes (non-cyclic)/dimethyl cyclopentanes
- Kerogen type index - Heptane index-4/*Iso*-heptane index

APPENDIX 3

Index of alkane molecular biomarker
GC-MS peak assignments

STERANES

$5\beta(H)14\alpha(H)17\alpha(H)$ and $5\alpha(H)14\alpha(H)17\alpha(H)$ C_{27} , C_{28} and C_{29} regular (normal) steranes and $5\alpha(H)14\beta(H)17\beta(H)$ C_{27} , C_{28} and C_{29} isosteranes

Peak	Assignment
S27a	C_{27} $5\beta(H)14\alpha(H)17\alpha(H)$ 20R cholestane
S27c	C_{27} $5\alpha(H)14\alpha(H)17\alpha(H)$ 20S cholestane
S27d	C_{27} $5\alpha(H)14\beta(H)17\beta(H)$ 20R isocholestane
S27e	C_{27} $5\alpha(H)14\beta(H)17\beta(H)$ 20S isocholestane
S27b	C_{27} $5\alpha(H)14\alpha(H)17\alpha(H)$ 20R cholestane
S28a	C_{28} 24-methyl- $5\beta(H)14\alpha(H)17\alpha(H)$ 20R cholestane
S28c	C_{28} 24-methyl- $5\alpha(H)14\alpha(H)17\alpha(H)$ 20S cholestane
S28d	C_{28} 24-methyl- $5\alpha(H)14\beta(H)17\beta(H)$ 20R isocholestane
S28e	C_{28} 24-methyl- $5\alpha(H)14\beta(H)17\beta(H)$ 20S isocholestane
S28b	C_{28} 24-methyl- $5\alpha(H)14\alpha(H)17\alpha(H)$ 20R cholestane
S29a	C_{29} 24-ethyl- $5\beta(H)14\alpha(H)17\alpha(H)$ 20R cholestane
S29c	C_{29} 24-ethyl- $5\alpha(H)14\alpha(H)17\alpha(H)$ 20S cholestane
S29d	C_{29} 24-ethyl- $5\alpha(H)14\beta(H)17\beta(H)$ 20R isocholestane
S29e	C_{29} 24-ethyl- $5\alpha(H)14\beta(H)17\beta(H)$ 20S isocholestane
S29b	C_{29} 24-ethyl- $5\alpha(H)14\alpha(H)17\alpha(H)$ 20R cholestane

Configurations:

- a $5\beta(H)14\alpha(H)17\alpha(H)$ 20R (immature or biological configuration)
- b $5\alpha(H)14\alpha(H)17\alpha(H)$ 20R (regular or normal sterane)
- c $5\alpha(H)14\alpha(H)17\alpha(H)$ 20S (regular or normal sterane)
- d $5\alpha(H)14\beta(H)17\beta(H)$ 20R (isosterane)
- e $5\alpha(H)14\beta(H)17\beta(H)$ 20S (isosterane)

Notes:

All steranes listed are likely to be 24R and 24S epimers which cannot be separated with the chromatography conditions used.

The elution sequence of normal and isosteranes for each of the C_{27} , C_{28} and C_{29} groups is as shown in the above listing: $5\alpha(H)14\alpha(H)17\alpha(H)$ 20S, $5\alpha(H)14\beta(H)17\beta(H)$ 20R, $5\alpha(H)14\beta(H)17\beta(H)$ 20S, $5\alpha(H)14\alpha(H)17\alpha(H)$ 20R. The C_{27} , C_{28} and C_{29} $5\beta(H)14\alpha(H)17\alpha(H)$ 20R steranes approximately coelute with the respective C_{27} , C_{28} and C_{29} $5\alpha(H)14\beta(H)17\beta(H)$ 20R isosteranes. The order of thermal stability of the steranes is $5\alpha(H) > 5\beta(H)$, $5\alpha(H)$ 20S $>$ $5\alpha(H)$ 20R and $14\beta(H)17\beta(H) >$ $14\alpha(H)17\alpha(H)$.

C_{30} 4-desmethylsteranes have been identified and are considered to be biological markers for marine organic material; however, these compounds cannot be differentiated from C_{30} 4-methylsteranes without metastable ion monitoring (GC-MS-MS). C_{30} 4-desmethylsteranes occur with $5\alpha(H)14\alpha(H)17\alpha(H)$ 20R and 20S and $5\alpha(H)14\beta(H)17\beta(H)$ 20R and 20S (isosterane) configurations. C_{25} steranes have also been identified (Shi Ji-Yang *et al.*, 1982) but are rare.

METHYLSTERANES

4 α (H) and 4 β (H) C₂₈, C₂₉ and C₃₀ methylsteranes

Peak	Assignment
MS28d	C ₂₈ 4 α (H)-methyl-5 α (H)14 α (H)17 α (H) 20S cholestane
MS28b	C ₂₈ 4 α (H)-methyl-5 β (H)14 α (H)17 α (H) 20R cholestane
MS28e	C ₂₈ 4 α (H)-methyl-5 α (H)14 β (H)17 β (H) 20R cholestane
MS28f	C ₂₈ 4 α (H)-methyl-5 α (H)14 β (H)17 β (H) 20S cholestane
MS28c	C ₂₈ 4 α (H)-methyl-5 α (H)14 α (H)17 α (H) 20R cholestane
MS28a	C ₂₈ 4 β (H)-methyl-5 α (H)14 α (H)17 α (H) 20R cholestane
MS29d	C ₂₉ 4 α (H)-methyl-5 α (H)14 α (H)17 α (H) 20S methylcholestane
MS29b	C ₂₉ 4 α (H)-methyl-5 β (H)14 α (H)17 α (H) 20R methylcholestane
MS29e	C ₂₉ 4 α (H)-methyl-5 α (H)14 β (H)17 β (H) 20R methylcholestane
MS29f	C ₂₉ 4 α (H)-methyl-5 α (H)14 β (H)17 β (H) 20S methylcholestane
MS29c	C ₂₉ 4 α (H)-methyl-5 α (H)14 α (H)17 α (H) 20R methylcholestane
MS29a	C ₂₉ 4 β (H)-methyl-5 α (H)14 α (H)17 α (H) 20R methylcholestane
MS30d	C ₃₀ 4 α (H)-methyl-5 α (H)14 α (H)17 α (H) 20S ethylcholestane
MS30b	C ₃₀ 4 α (H)-methyl-5 β (H)14 α (H)17 α (H) 20R ethylcholestane
MS30e	C ₃₀ 4 α (H)-methyl-5 α (H)14 β (H)17 β (H) 20R ethylcholestane
MS30f	C ₃₀ 4 α (H)-methyl-5 α (H)14 β (H)17 β (H) 20S ethylcholestane
MS30c	C ₃₀ 4 α (H)-methyl-5 α (H)14 α (H)17 α (H) 20R ethylcholestane
MS30a	C ₃₀ 4 β (H)-methyl-5 α (H)14 α (H)17 α (H) 20R ethylcholestane

Configurations:

- a 4 β (H)5 α (H)14 α (H)17 α (H) 20R (immature)
- b 4 α (H)5 β (H)14 α (H)17 α (H) 20R (immature)
- c 4 α (H)5 α (H)14 α (H)17 α (H) 20R (regular or normal methylsterane)
- d 4 α (H)5 α (H)14 α (H)17 α (H) 20S (regular or normal methylsterane)
- e 4 α (H)5 α (H)14 β (H)17 β (H) 20R (isomethylsterane)
- f 4 α (H)5 α (H)14 β (H)17 β (H) 20S (isomethylsterane)

Notes:

The full stereochemistry of the methylsteranes, that is, either the 23,24-dimethyl (dinosterane) or the 24-ethyl configuration, cannot be determined without full scan GC-MS analysis and examination of mass spectra. Mass spectra of 23,24-dimethylsteranes (dinosteranes) show a significant ion at m/e 198 (Goodwin et al., 1988). The elution sequence of the C₂₈, C₂₉ and C₃₀ 4-methyl-14 α (H)17 α (H) 20R steranes is 4 α (H)5 β (H), 4 α (H)5 α (H) and 4 β (H)5 α (H). In synthetic mixtures of 4-methylsteranes, the 4 β (H)5 β (H) isomer elutes between the 4 α (H)5 β (H) and 4 α (H)5 α (H) (Goodwin et al., 1988) but does not appear to occur naturally.

The order of thermal stability of the naturally occurring 4-methylsteranes is 4 α (H) > 4 β (H) and 4 α (H)5 α (H) > 4 α (H)5 β (H) (Wolff et al., 1986). The elution sequence of 4 α (H)-methyl-5 α (H)14 α (H)17 α (H) and 4 α (H)-methyl-5 α (H)14 β (H)17 β (H) steranes for each of the C₂₇, C₂₈ and C₂₉ groups is similar to the desmethyl steranes and is as shown in the above listing: 4 α (H)-methyl-5 α (H)14 α (H)17 α (H) 20S, 4 α (H)-methyl-5 α (H)14 β (H)17 β (H) 20R, 4 α (H)-methyl-5 α (H)14 β (H)17 β (H) 20S, 4 α (H)-methyl-5 α (H)14 α (H)17 α (H) 20R. The order of thermal stability is presumed to be comparable to the desmethyl steranes.

Compounds identified as methylsteranes, but substituted at a position other than at C-4 on the A-ring, have been reported (Fowler and Douglas, 1987; Summons and Powell, 1987; Summons et al., 1987), but appear to be rare.

REARRANGED STERANES (DIASTERANES)

13 β (H)17 α (H) and 13 α (H)17 β (H) C₂₇, C₂₈ and C₂₉ rearranged steranes

Peak	Assignment
r27d	C ₂₇ 13 β (H)17 α (H) 20S diacholestane
r27c	C ₂₇ 13 β (H)17 α (H) 20R diacholestane
r27b	C ₂₇ 13 α (H)17 β (H) 20S diacholestane
r27a	C ₂₇ 13 α (H)17 β (H) 20R diacholestane
r28d	C ₂₈ 24-methyl-13 β (H)17 α (H) 20S diacholestane
r28c	C ₂₈ 24-methyl-13 β (H)17 α (H) 20R diacholestane
r28b	C ₂₈ 24-methyl-13 α (H)17 β (H) 20S diacholestane
r28a	C ₂₈ 24-methyl-13 α (H)17 β (H) 20R diacholestane
r29d	C ₂₉ 24-ethyl-13 β (H)17 α (H) 20S diacholestane
r29c	C ₂₉ 24-ethyl-13 β (H)17 α (H) 20R diacholestane
r29b	C ₂₉ 24-ethyl-13 α (H)17 β (H) 20S diacholestane
r29a	C ₂₉ 24-ethyl-13 α (H)17 β (H) 20R diacholestane

Configurations:

- a 13 α (H)17 β (H) 20R
- b 13 α (H)17 β (H) 20S
- c 13 β (H)17 α (H) 20R
- d 13 β (H)17 α (H) 20S

Notes:

All rearranged steranes listed are likely to be 24R and 24S epimers which, with the exception of C₂₈ 24-methyl-13 β (H)17 α (H) diacholestanes, cannot normally be separated with the chromatography conditions used.

The C₂₉ 24-ethyl-13 β (H)17 α (H) 20S diacholestane co-elutes with the C₂₇ 5 α (H)14 β (H)17 β (H) 20R isocholestane and the C₂₉ 24-ethyl-13 α (H)17 β (H) 20R diacholestane co-elutes with the C₂₈ 24-methyl-5 α (H)14 β (H)17 β (H) 20R isocholestane under normal chromatography conditions. The 13 α (H)17 β (H) configuration is less thermally stable than 13 β (H)17 α (H).

C₃₀ rearranged steranes also occur, with 13 β (H)17 α (H) 20R and 20S and 13 α (H)17 β (H) 20R and 20S configurations.

TRICYCLIC TERPANES

Peak	Assignment
t19	C ₁₉ tricyclic terpane
t20	C ₂₀ tricyclic terpane
t21	C ₂₁ tricyclic terpane
t22	C ₂₂ tricyclic terpane
t23	C ₂₃ tricyclic terpane
t24	C ₂₄ tricyclic terpane
t25	C ₂₅ tricyclic terpane
t26	C ₂₆ tricyclic terpanes
t27	C ₂₇ tricyclic terpanes
t28	C ₂₈ tricyclic terpanes
t29	C ₂₉ tricyclic terpanes
t30	C ₃₀ tricyclic terpanes

Notes:

C₂₆, C₂₈, C₂₉ and C₃₀ tricyclic terpanes occur as isomeric pairs (at C-22). C₂₂ and C₂₇ tricyclic terpanes are generally less abundant, suggesting branching at these positions. Tricyclic terpanes of higher molecular weight, up to C₄₀ and higher, have been identified (Moldowan et al., 1983), but are unusual. Mello et al. (1988) identified C₃₁, C₃₃, C₃₄ and C₃₅ tricyclic terpanes in Brazilian oils.

TETRACYCLIC TERPANES

Seco-17,21-hopanes

Peak	Assignment
t24	C ₂₄ tetracyclic terpane
t26	C ₂₆ tetracyclic terpane

Notes:

The tetracyclic terpanes are hopane related compounds and have the structure seco-17,21-hopane.

PENTACYCLIC TRITERPANES

C₂₇ and C₂₉ to C₃₅ 17 α (H)21 β (H) and 17 β (H)21 β (H) hopane and 17 β (H)21 α (H) moretane series

C₂₇ and C₂₉ to C₃₅ 17 α (H)21 β (H) hopane series:

Peak	Assignment
h27s	C ₂₇ 18 α (H)-22,29,30-trisnorneohopane (Ts)
h27m	C ₂₇ 17 α (H)-trisorhopane (Tm)
h29	C ₂₉ 17 α (H)21 β (H)-30-norhopane
h30	C ₃₀ 17 α (H)21 β (H)-30-hopane
h31S	C ₃₁ 17 α (H)21 β (H)-30,31-homohopane 22S
h31R	C ₃₁ 17 α (H)21 β (H)-30,31-homohopane 22R
h32S	C ₃₂ 17 α (H)21 β (H)-30,31-bishomohopane 22S
h32R	C ₃₂ 17 α (H)21 β (H)-30,31-bishomohopane 22R
h33S	C ₃₃ 17 α (H)21 β (H)-30,31-trishomohopane 22S
h33R	C ₃₃ 17 α (H)21 β (H)-30,31-trishomohopane 22R
h34S	C ₃₄ 17 α (H)21 β (H)-30,31-tetrakishomohopane 22S
h34R	C ₃₄ 17 α (H)21 β (H)-30,31-tetrakishomohopane 22R
h35S	C ₃₅ 17 α (H)21 β (H)-30,31-pentakishomohopane 22S
h35R	C ₃₅ 17 α (H)21 β (H)-30,31-pentakishomohopane 22R

C₂₇ and C₂₉ to C₃₅ 17 β (H)21 α (H) moretane series:

Peak	Assignment
m29	C ₂₉ 17 β (H)21 α (H)-30-normoretane
m30	C ₃₀ 17 β (H)21 α (H)-30-moretane
m31	C ₃₁ 17 β (H)21 α (H)-homomoretane
m32	C ₃₂ 17 β (H)21 α (H)-bishomomoretane

C₂₇ 17 β (H) and C₂₉ to C₃₅ 17 β (H)21 β (H) hopane series:

Peak	Assignment
b27	C ₂₇ 17 β (H) trisorhopane
b29	C ₂₉ 17 β (H)21 β (H) norhopane 22R
b30	C ₃₀ 17 β (H)21 β (H) hopane 22R
b31	C ₃₁ 17 β (H)21 β (H) homohopane 22R
b32	C ₃₂ 17 β (H)21 β (H)-30,31-bishomohopane 22R
b33	C ₃₃ 17 β (H)21 β (H)-30,31-trishomohopane 22R
b34	C ₃₄ 17 β (H)21 β (H)-30,31-tetrakishomohopane 22R
b35	C ₃₅ 17 β (H)21 β (H)-30,31-pentakishomohopane 22R

Notes:

The C₂₉ to C₃₅ pentacyclic triterpane (hopane) series of compounds have been identified with 17 α (H)21 β (H) (hopane), 17 β (H)21 α (H) (moretane) and 17 β (H)21 β (H) (hopane) configurations. C₂₇ trisorhopanes have no side-chain at C-21 and have either the 17 α (H) or the 17 β (H) configuration, the former being the more thermally stable and the latter form generally present in immature samples only. The C₂₇ 18 α (H)-trisnorneohopane (Ts) is more thermally stable than C₂₇ 17 α (H)-trisorhopane (Tm). 3-methylhopanes are rarely present and may be detected by use of m/e 205 mass chromatograms (McEvoy and Giger, 1986).

UNSATURATED PENTACYCLIC TRITERPENOIDS

Peak	Assignment
uh1	C ₂₇ 22,29,30-trisnorneohop-13(18)-ene
uh2	C ₂₇ trisnorhop-17-ene
uh3	C ₂₉ norhop-17(21)-ene
uh4	C ₂₉ 30-neonor-13(18)-ene
uh5	C ₃₀ hop-17(21)-ene
uh6	C ₃₀ neohop-13(18)-ene
uh7	C ₃₁ homohop-17(21)-ene (22R and 22S)

Notes:

Unsaturated pentacyclic compounds usually occur in thermally immature samples only.

OTHER PENTACYCLIC TRITERPENOIDS

Peak	Assignment
T	C ₂₇ 17 α (H)18 α (H)21 β (H)-25,28,30-trisnorhopane
Tnm	C ₂₇ 17 β (H)18 α (H)21 α (H)-25,28,30-trisnormoretane
B	C ₂₈ 17 α (H)18 α (H)21 β (H)-28,30-bisnorhopane
Bnm	C ₂₈ 17 β (H)18 α (H)21 α (H)-28,30-bisnormoretane
G	C ₃₀ gammacerane
O	C ₃₀ 18 α (H) oleanane
J	C ₃₀ 18 β (H) oleanane ("compound J")
L	C ₃₀ lupane
Y	C ₂₇ triterpane (structurally unelucidated)
X	C ₃₀ triterpane (structurally unelucidated)

Notes:

The C₃₀ 18 α (H) oleanane and 18 β (H) oleanane (formerly "compound J" of Grantham *et al.*, 1983) coelute on standard GC columns. The 18 β (H) oleanane is less thermally stable than 18 α (H) oleanane (Riva *et al.*, 1988).

The structurally unelucidated C₂₇ and C₃₀ pentacyclic triterpanes are peaks Y and X, respectively, of Philp and Gilbert (1986).

DEMETHYLATED HOPANES and DEMETHYLATED MORETANES

C₂₅ and C₂₈ to C₃₄ 17 α (H)21 β (H)-25-norhopanes and 17 β (H)21 α (H)-25-normoretanes

Peak	Assignment
dh26s	C ₂₆ 18 α (H)-22,25,29,30-tetrakisnorhopane
dh26m	C ₂₆ 17 α (H)-22,25,28,30-tetrakisnorhopane
dh2a	C ₂₆ 17 α (H)21 β (H)-25,30-bisnorhopane
dm2a	C ₂₆ 17 β (H)21 α (H)-25,30-bisnormoretane
dh29	C ₂₉ 17 α (H)21 β (H)-25-norhopane
dm29	C ₂₉ 17 β (H)21 α (H)-25-normoretane
dh30s	C ₃₀ 17 α (H)21 β (H)-25-norhomohopane 22S
dh30R	C ₃₀ 17 α (H)21 β (H)-25-norhomohopane 22R
dh31S	C ₃₁ 17 α (H)21 β (H)-25-norbishomohopane 22S
dh31R	C ₃₁ 17 α (H)21 β (H)-25-norbishomohopane 22R
dh32S	C ₃₂ 17 α (H)21 β (H)-25-nortrishomohopane 22S
dh32R	C ₃₂ 17 α (H)21 β (H)-25-nortrishomohopane 22R
dh33S	C ₃₃ 17 α (H)21 β (H)-25-nortetrakishomohopane 22S
dh33R	C ₃₃ 17 α (H)21 β (H)-25-nortetrakishomohopane 22R
dh34S	C ₃₄ 17 α (H)21 β (H)-25-norpentakishomohopane 22S
dh34R	C ₃₄ 17 α (H)21 β (H)-25-norpentakishomohopane 22R

Notes:

Nuclear demethylated hopanes are biological markers for severe bacterial degradation (Volkman *et al.*, 1983a and b). Demethylation involves the loss of the C-25 methyl group from the C-10 position on the A-ring (Rullkotter and Wendisch, 1982).

DEMETHYLATED TRICYCLIC TERPANES

Peak	Assignment
dt18	C ₁₈ tricyclic terpane
dt19	C ₁₉ tricyclic terpane
dt20	C ₂₀ tricyclic terpane
dt21	C ₂₁ tricyclic terpane
dt22	C ₂₂ tricyclic terpane
dt23	C ₂₃ tricyclic terpane
dt24	C ₂₄ tricyclic terpane
dt25	C ₂₅ tricyclic terpanes
dt26	C ₂₆ tricyclic terpanes
dt27	C ₂₇ tricyclic terpanes
dt28	C ₂₈ tricyclic terpanes
dt29	C ₂₉ tricyclic terpanes

Notes:

These compounds are relatively unusual and are indicative of the severest levels of biodegradation (Howell *et al.*, 1984). C₂₅, C₂₇, C₂₈ and C₂₉ demethylated tricyclic terpanes occur as isomeric (at C-22) pairs.

SECOHOPANES

Seco-8,14-hopanes

Peak	Assignment
sh1	C ₂₇ seco-8,14-hopane
sh2	C ₂₉ seco-8,14-hopane
sh3	C ₃₀ seco-8,14-hopane

Notes:

Tetracyclic terpanes in degraded oil stains from the Morondava Basin of Madagascar have been identified as Ring-C opened seco-8,14-hopanes by Rullkotter and Wendisch (1982). Stereochemistry at C-8 and C-14 gives rise to several isomers and higher and lower carbon numbers may also be present. Minor amounts of secohopanes were detected in Brazilian oils by Mello et al. (1988).

OTHER COMPOUNDS

Peak	Assignment
BC	C ₃₄ botryococcane
S	C ₃₀ squalane
β C	β -carotane

MIDMASC CHROMATOGRAMS

DATA: 91M08C #1

SCANS 700 TO 2000

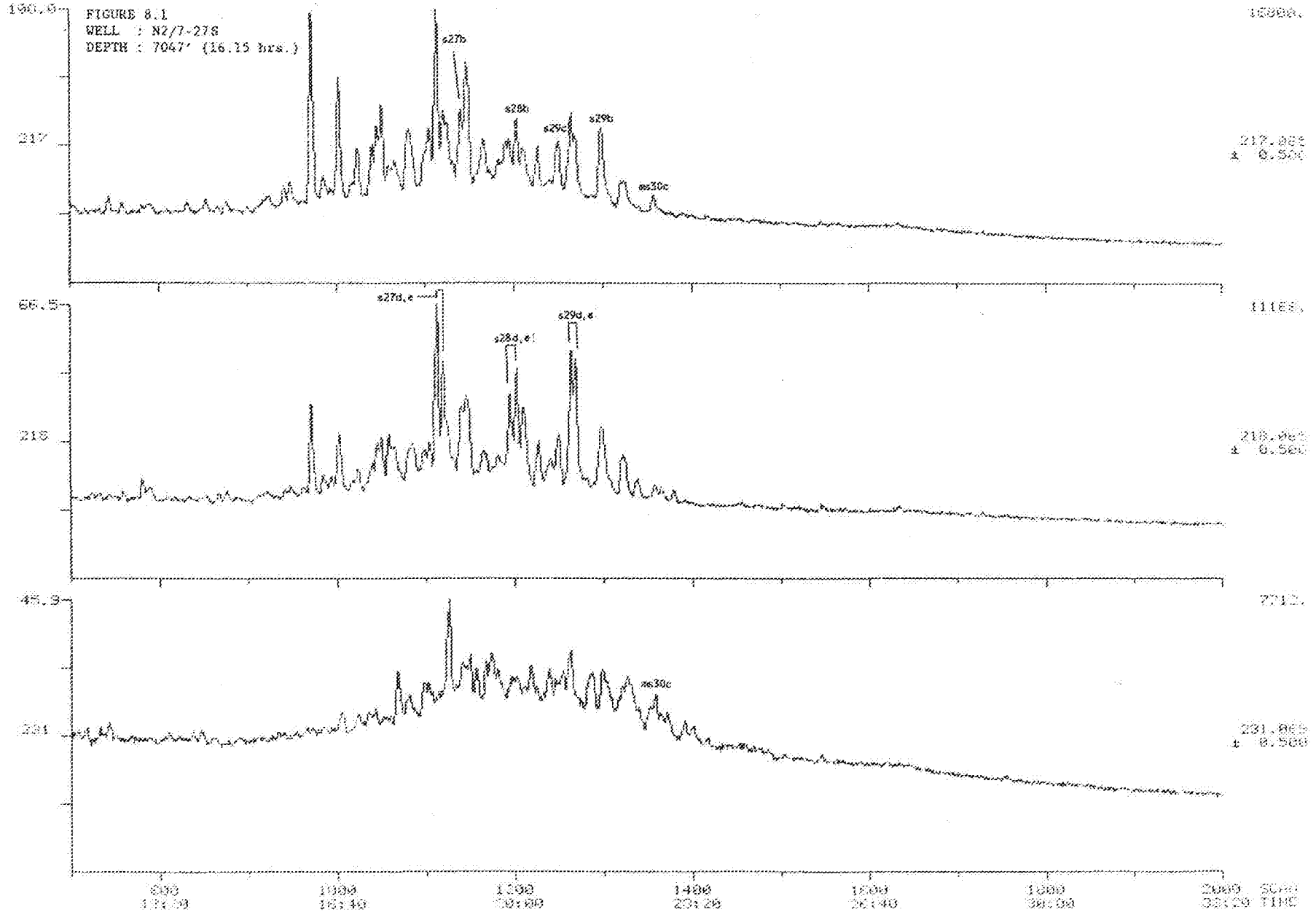
12/13/91 15:20:00

CALI: C131291 #2

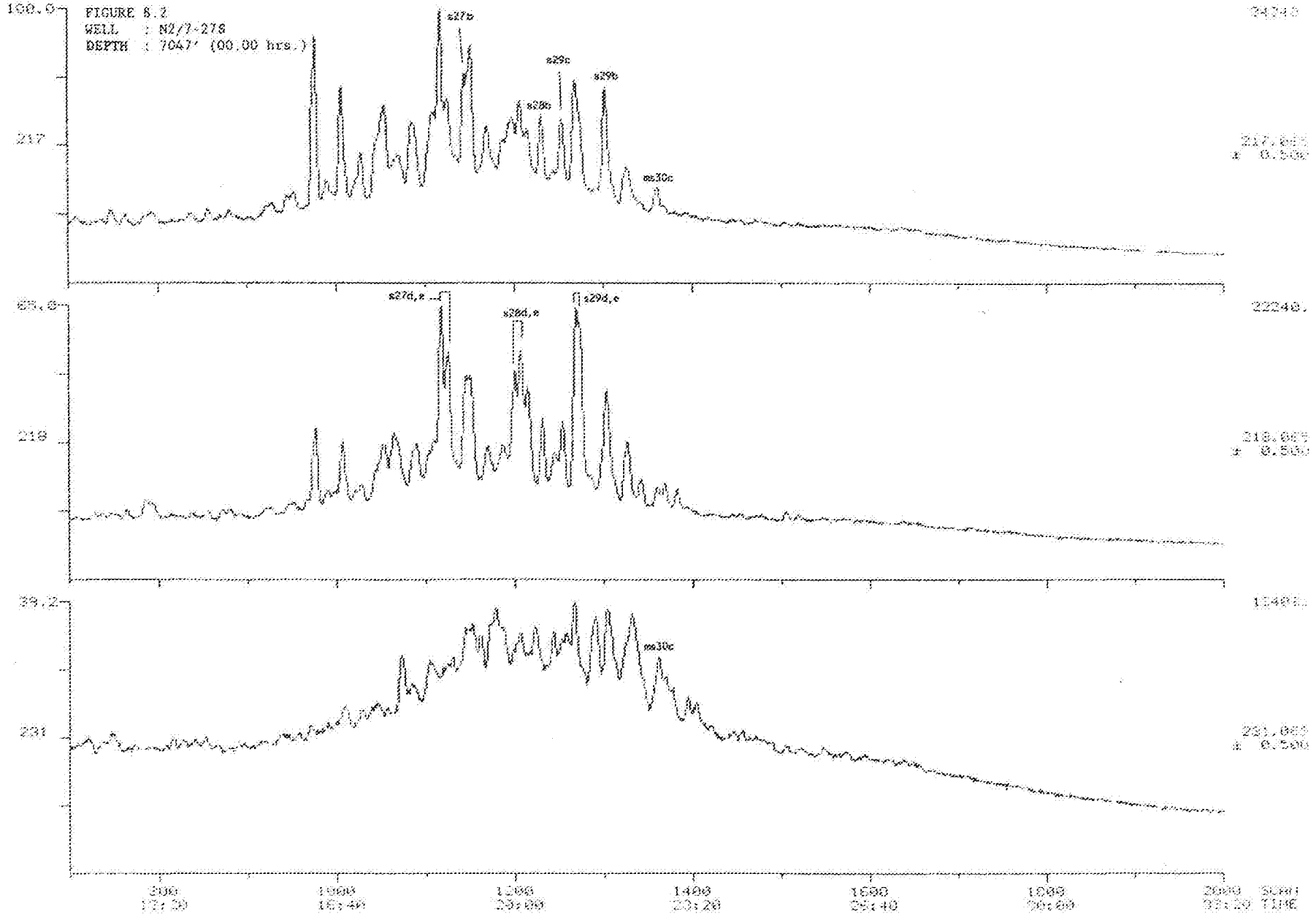
SAMPLE: 91M 3 BRANCH CYCLIC PHILLIPS 277-278

COND: 20.1 20.1 100.0 5.11 300.00

RANGE: 0 1.2000 LABEL: H 0. 1.0 J 0 BASE: U 20. 0



HYDRADE CHROMATOGRAMS DATA: 91R400 #1 SCANS 780 TO 2080
 12/13/81 16:10:00 CALI: C131291 #2
 SAMPLE: 91R 4 BRANCH CYCLIC PHILLIPS 2/7-275
 COND.S.: 20.1 30.7 130.0 5.8 300.33
 RAHLE: G 1.2000 LABEL: N 0. 4.0 QUANT: A 0. 1.0 0 0 BASE: U 00. 3



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APPENDIX 4(1-2)

Alkane GC-MS quantitative data

Appendix	Depth (feet)/Sample No.
4.1	7047 (16.15 hrs)
4.2	7047 (00.00 hrs)

APPENDIX 4.1

12/13/91 15:26:37
 CAN 1 OF 2000
 Acquisition started

Acquire Run 0 91M3RC ACQUIRING
 12/13/91 15:26:00 + 0:00 Pre sectors: 14000 Scan: 2 of 2000
 Sample: 91M 3 BRANCH CYCLIC PHILLIPS 277-278
 Conds: 20.1 30/M 130.0 37M 300.20
 Formula: ACQU @130 Instrument: 4000 Weight: 0.000
 Submitted by: MAB Analyst: PCH Acct. No: P21290

***** SCAN PARAMETERS *****
 **** Mode: Centroid positive non

MSD scan Desc: GC Mass intervals: 17
 Scan time: 1.000 s Samp. int.: 0.200 ms Master rates: 512

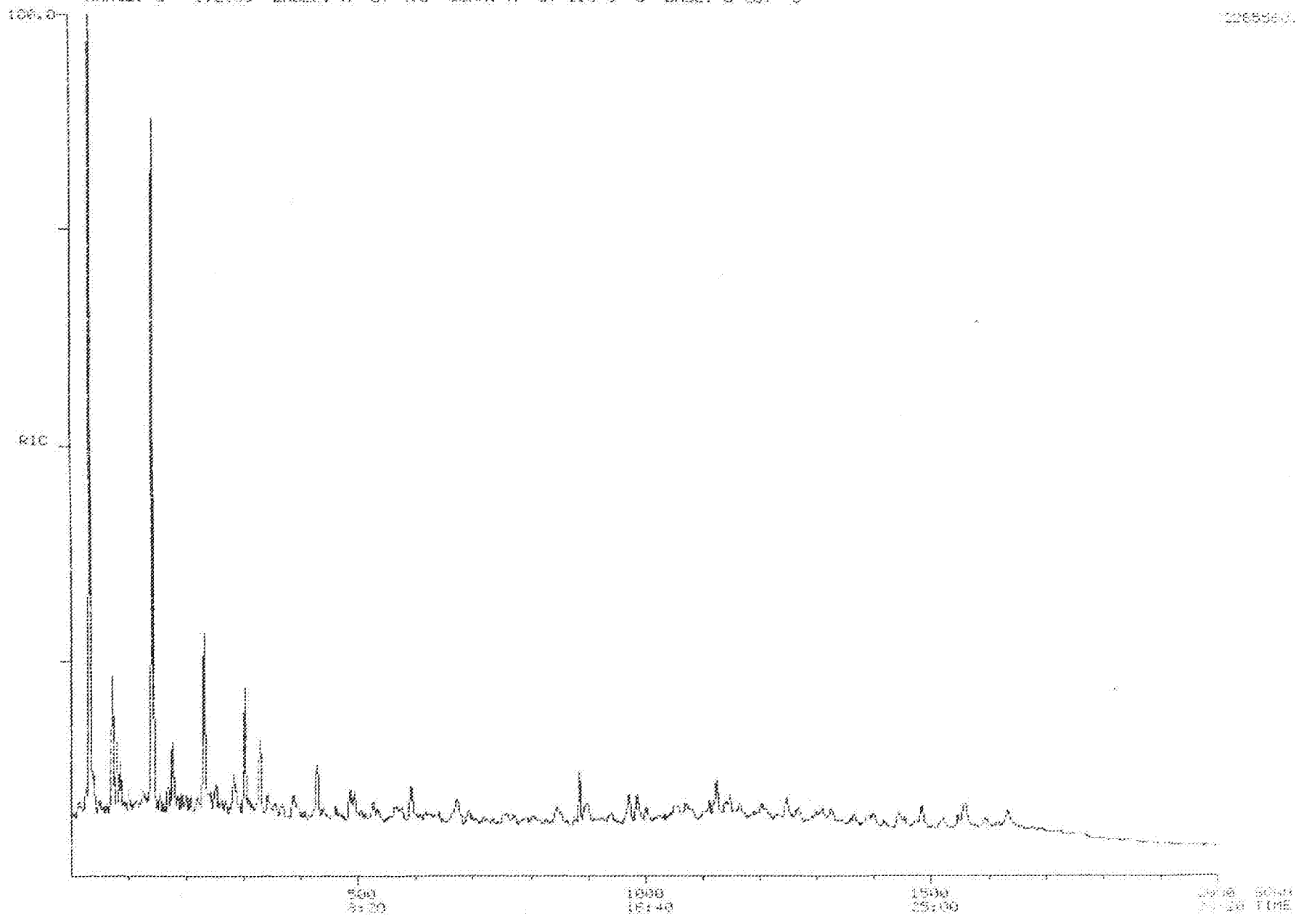
Int #	Lo mass	Hi mass	Time	MPW	MA	TH	BL	IGN
1	84.525	85.525	0.052	1	80	5	1	0 Pos
2	122.537	123.537	0.052	1	80	5	1	0 Pos
3	148.545	149.545	0.052	1	80	5	1	0 Pos
4	150.548	151.548	0.052	1	80	5	1	0 Pos
5	182.549	183.549	0.052	1	80	5	1	0 Pos
6	175.553	177.553	0.052	1	80	5	1	0 Pos
7	182.559	183.559	0.052	1	80	5	1	0 Pos
8	190.557	191.557	0.052	1	80	5	1	0 Pos
9	216.565	217.565	0.052	1	80	5	1	0 Pos
10	217.565	218.565	0.052	1	80	5	1	0 Pos
11	230.569	231.569	0.052	1	80	5	1	0 Pos
12	231.569	232.569	0.052	1	80	5	1	0 Pos
13	238.572	239.572	0.053	1	80	5	1	0 Pos
14	252.576	253.576	0.052	1	80	5	1	0 Pos
15	258.577	259.577	0.052	1	80	5	1	0 Pos
16	397.619	398.619	0.052	1	80	5	1	0 Pos
17	411.623	412.623	0.052	1	80	5	1	0 Pos

Interface number 0
 Sub-interface number 0
 # of acqu buffers 13
 Instrument type 0
 Full scale mass 1024 u
 Zero scale mass 1 u
 Intensity/ion 2
 Peak width 992. mmo
 Offset at low mass 0 mmu
 Offset at high mass 0 mmo
 Voltage settling time(MS) 4

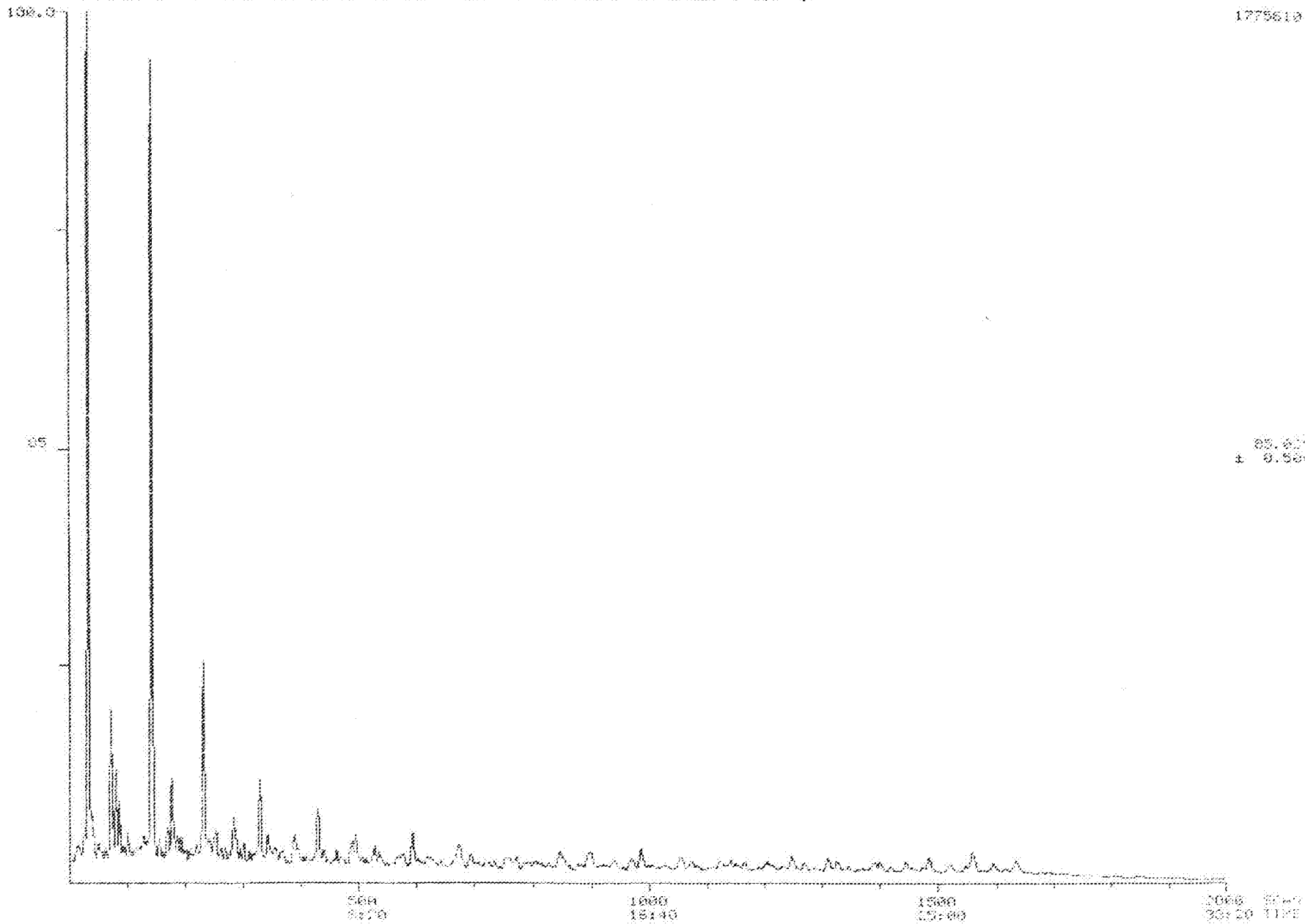
12/13/91 15:26:59
 ACQUISITION COMPLETED
 SCANS 1 TO 2000 Centroid

Mode	Scans	Secs	Out of	%	Peaks per scan	per sec
Centroid	2000	323.8	2000	0	39004	20

NIDRIC DATA: SIM300 #1 SCANS 1 TO 2000
12/18/81 15:25:00 CALI: C131351 #2
SAMPLE: 91M B BRANCH CYCLIC PHILLIPS Z-7-275
CONDS: 20.1 30 M 100.0 5.4 300.00
RANGE: 0 1.2000 LABEL: H 0. 4.0 QUAN: A 0. 1.0 0 0 BASE: D 20. 0



MICROASS CHROMATOGRAM DATA: 91M58C #1 SCANS 1 TO 2000
12/10/91 15:26:00 CALI: C131291 #2
SAMPLE: 91M 3 BRANCH CYCLIC PHILLIPS 277-279
CONDENS: 20.1 30.0 130.0 370.0
RANGE: G 1.2000 LABEL: N 0. 4.0 QUANT: A 0. 1.0 U 0. BASE: U 20. 3



NUMERICAL CHROMATOGRAMS

DATA: SIMSEC #1
CALI: C131251 #2

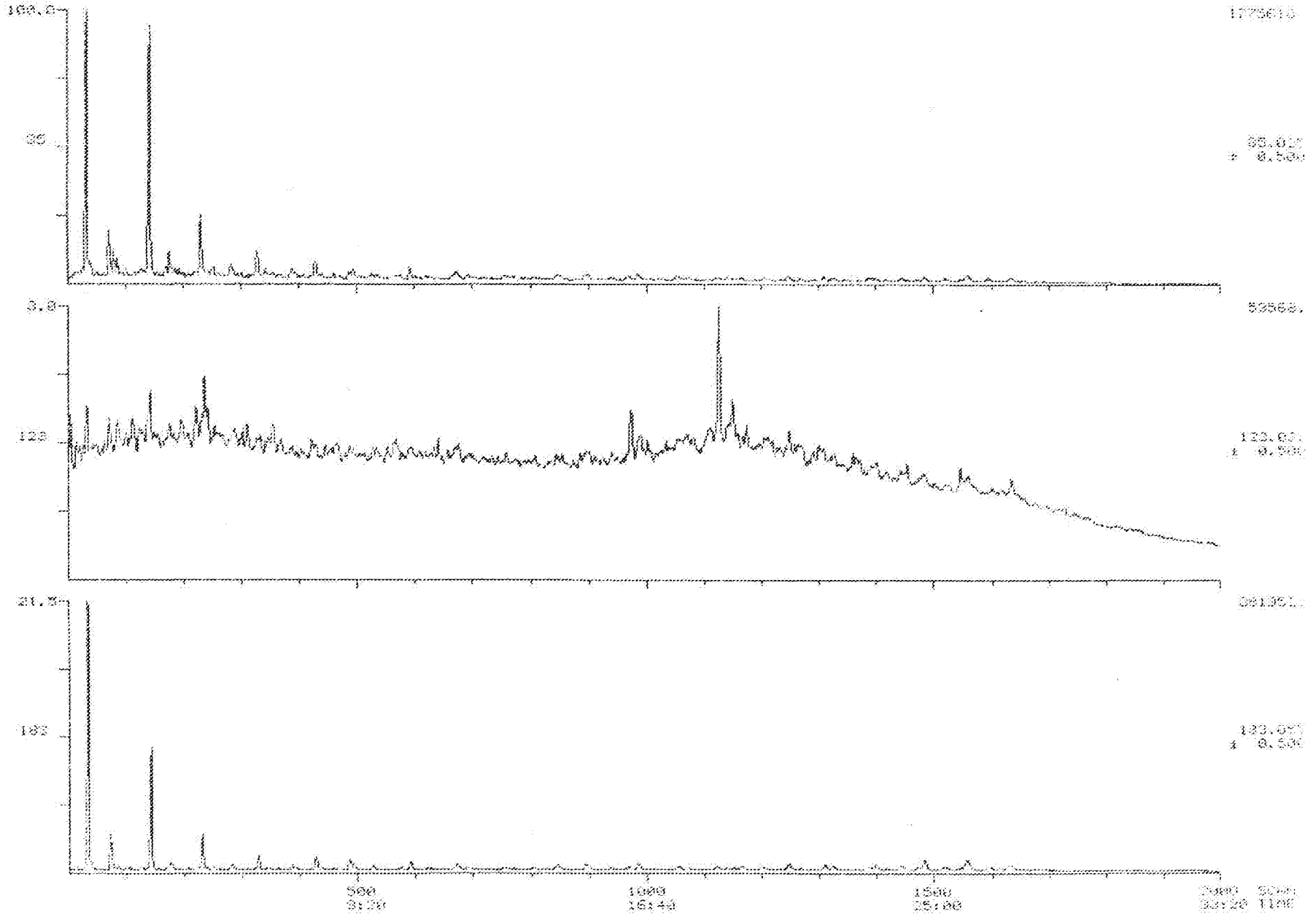
SCANS 1 TO 2000

10/13/91 15:26:00

SAMPLE: SIM 3 ERANCH CYCLIC PHILLIPS 277-275

COND: 25.1 30 M 130.0 0.1 300.20

RANGE: C 1.0000 LABEL: N 0. 4.0 QUAN: A 0. 1.0 J 0 BASE: U 00. 3



HIGH RES CHROMATOGRAMS

DATA: 31M38C #1

SCANS 1 TO 2000

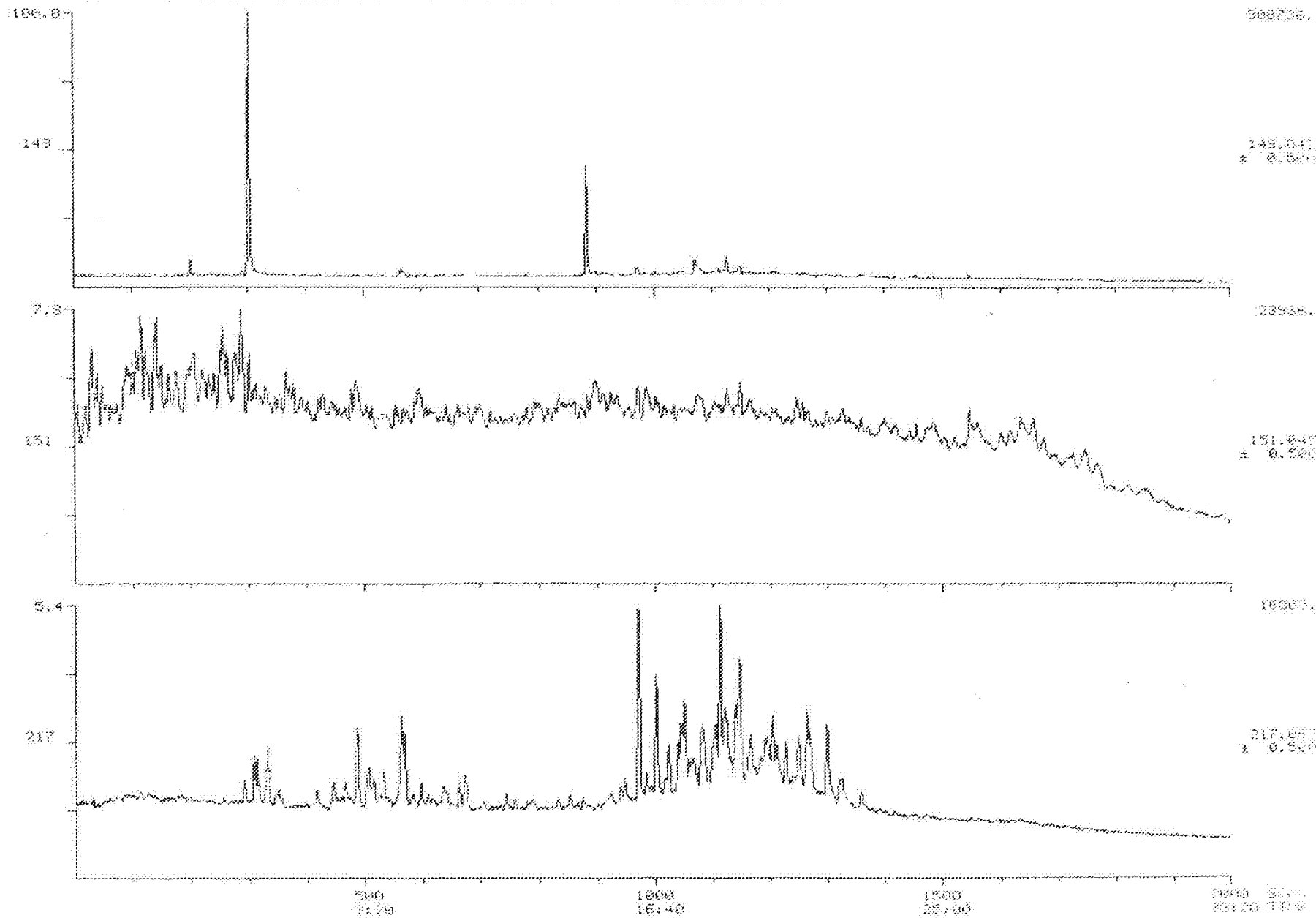
12/13/91 15:20:00

CH1: 0131291 #2

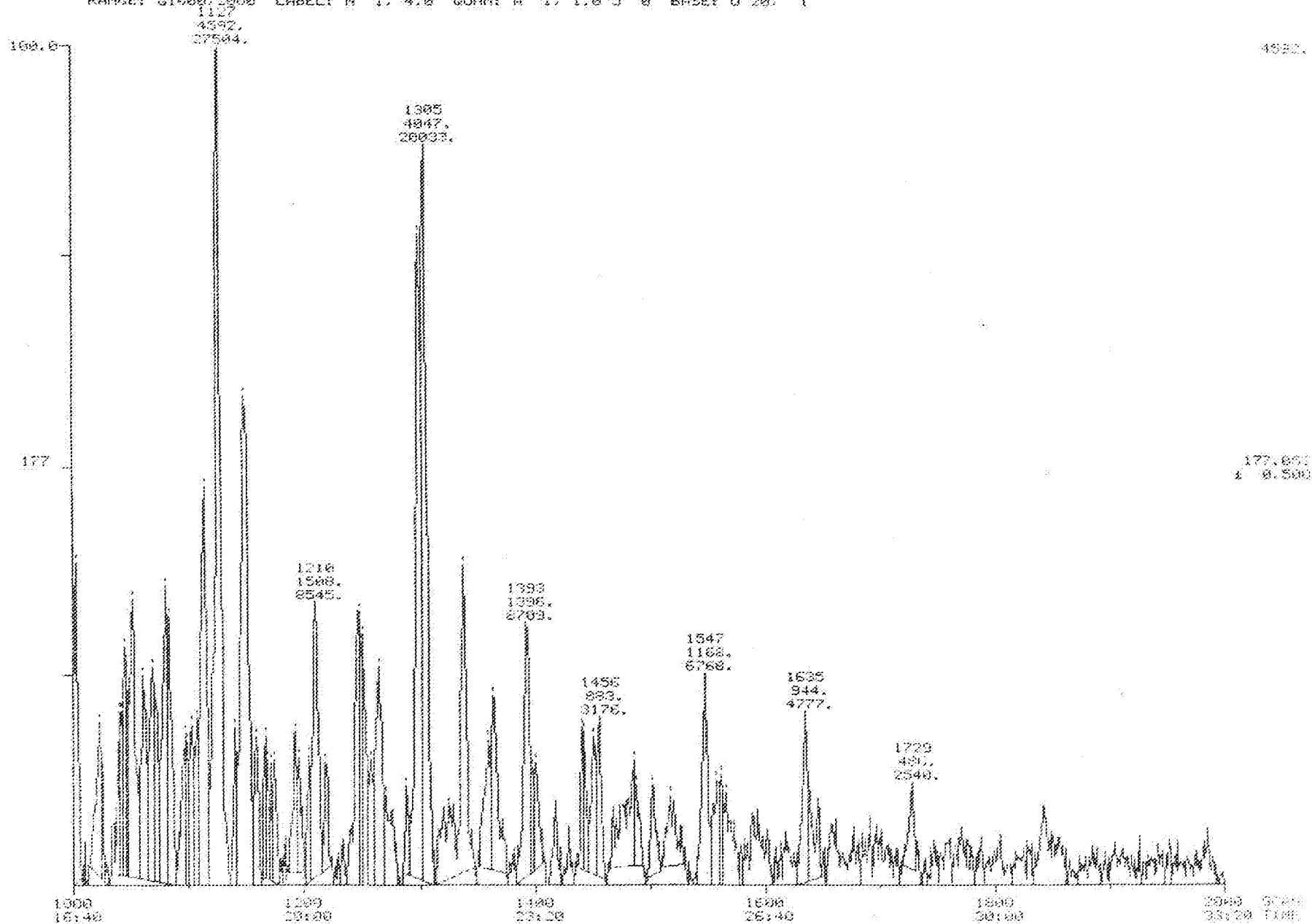
SAMPLE: 91M 3 BRANCH CYCLIC PHILLIPS 277-275

COND: 2001 307M 13010 5 M 000120

RANGE: G 1.0000 LABEL: H 0.4.0 QUAN: A 0.1.0 J 0.0 BASE: U 00. 0



HIDRAX CHROMATOGRAM DATA: 91NSEC #1 SCANS 1000 TO 2000
12/13/51 15:28:00 CALI: C131291 #2
SAMPLE: 91N S BRANCH CYCLIC PHILLIPS 2/7-275
CONCS.: 20.1 30.1 100.0 5.1 900.20
RANGE: 61000.0000 LABEL: H 1, 4.0 QUAN: H 1, 1.0 U 0 BRSE: U 20. 1



Reference retention time (min:s)		18:47							
No.	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num
1	176.55	177.55	1003	16:43	A BB	6728.	1758.	---	0.
2	176.55	177.55	1024	17:04	A BV	4581.	853.	---	0.
3	176.55	177.55	1026	17:06	A VB	891.	594.	---	0.
4	176.55	177.55	1040	17:20	A BV	2449.	904.	---	0.
5	176.55	177.55	1042	17:22	A VV	1554.	906.	---	0.
6	176.55	177.55	1045	17:25	A VV	3305.	1262.	---	0.
7	176.55	177.55	1047	17:27	A VV	2049.	1168.	---	0.
8	176.55	177.55	1052	17:32	A VV	8574.	1526.	---	0.
9	176.55	177.55	1061	17:41	A VV	6293.	1120.	---	0.
10	176.55	177.55	1069	17:49	A VV	5064.	1177.	---	0.
11	176.55	177.55	1071	17:51	A VV	4229.	1019.	---	0.
12	176.55	177.55	1081	18:01	A VV	8256.	1639.	---	0.
13	176.55	177.55	1083	18:03	A VB	5272.	1465.	---	0.
14	176.55	177.55	1097	18:17	A BV	4064.	832.	---	0.
15	176.55	177.55	1099	18:19	A VV	1920.	784.	---	0.
16	176.55	177.55	1103	18:23	A VV	2976.	880.	---	0.
17	176.55	177.55	1108	18:28	A VV	3312.	912.	---	0.
18	176.55	177.55	1114	18:34	A VV	12256.	2192.	---	0.
19	176.55	177.55	1127	18:47	A VB	27504.	4592.	---	0.
20	176.55	177.55	1141	19:01	A BV	2864.	864.	---	0.
21	176.55	177.55	1149	19:09	A VV	20288.	2688.	---	0.
22	176.55	177.55	1159	19:19	A VB	3248.	816.	---	0.
23	176.55	177.55	1167	19:27	A BV	2464.	778.	---	0.
24	176.55	177.55	1169	19:29	A VV	979.	656.	---	0.
25	176.55	177.55	1172	19:32	A VV	1405.	650.	---	0.
26	176.55	177.55	1176	19:35	A VB	2416.	675.	---	0.
27	176.55	177.55	1193	19:53	A BV	3040.	784.	---	0.
28	176.55	177.55	1196	19:56	A VB	2240.	640.	---	0.
29	176.55	177.55	1205	20:05	A BV	2459.	701.	---	0.
30	176.55	177.55	1210	20:10	A VV	8545.	1508.	---	0.
31	176.55	177.55	1219	20:19	A VB	2216.	584.	---	0.
32	176.55	177.55	1248	20:48	A BV	8160.	1504.	---	0.
33	176.55	177.55	1250	20:50	A VV	2512.	1328.	---	0.
34	176.55	177.55	1252	20:52	A VV	3808.	1376.	---	0.
35	176.55	177.55	1258	20:58	A VV	3568.	688.	---	0.
36	176.55	177.55	1265	21:05	A VV	7728.	1200.	---	0.
37	176.55	177.55	1271	21:11	A VB	3472.	496.	---	0.
38	176.55	177.55	1289	21:29	A BV	1876.	487.	---	0.
39	176.55	177.55	1300	21:40	A VV	18779.	3538.	---	0.
40	176.55	177.55	1305	21:45	A VB	20033.	4047.	---	0.
41	176.55	177.55	1339	22:19	A BB	14560.	1689.	---	0.
42	176.55	177.55	1360	22:40	A BV	4553.	715.	---	0.
43	176.55	177.55	1364	22:44	A VB	5847.	960.	---	0.
44	176.55	177.55	1393	23:13	A BV	8709.	1396.	---	0.
45	176.55	177.55	1398	23:18	A VV	1075.	572.	---	0.
46	176.55	177.55	1401	23:21	A VB	2648.	587.	---	0.
47	176.55	177.55	1441	24:01	A BV	1976.	779.	---	0.
48	176.55	177.55	1443	24:03	A VV	1904.	768.	---	0.
49	176.55	177.55	1451	24:11	A VV	4144.	737.	---	0.
50	176.55	177.55	1456	24:16	A VB	3176.	883.	---	0.
51	176.55	177.55	1484	24:46	A BV	6904.	586.	---	0.
52	176.55	177.55	1488	24:48	A VB	1532.	449.	---	0.
53	176.55	177.55	1502	25:02	A BB	2856.	500.	---	0.
54	176.55	177.55	1518	25:18	A BB	3608.	394.	---	0.
55	176.55	177.55	1547	25:47	A BV	6768.	1168.	---	0.

Reference retention time (min:s) 18:47

No.	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num
56	176.55	177.55	1558	25:58	A VV	3372.	576.	---	0.
57	176.55	177.55	1562	26:02	A VV	1504.	408.	---	0.
58	176.55	177.55	1566	26:06	A VB	3712.	512.	---	0.
59	176.55	177.55	1635	27:15	A BV	4777.	944.	---	0.
60	176.55	177.55	1638	27:18	A VB	3351.	537.	---	0.
61	176.55	177.55	1729	28:49	A BB	2540.	486.	---	0.

MIDRASS CHROMATOGRAM

DATA: SIMOBE #1

SCANS 300 TO 1100

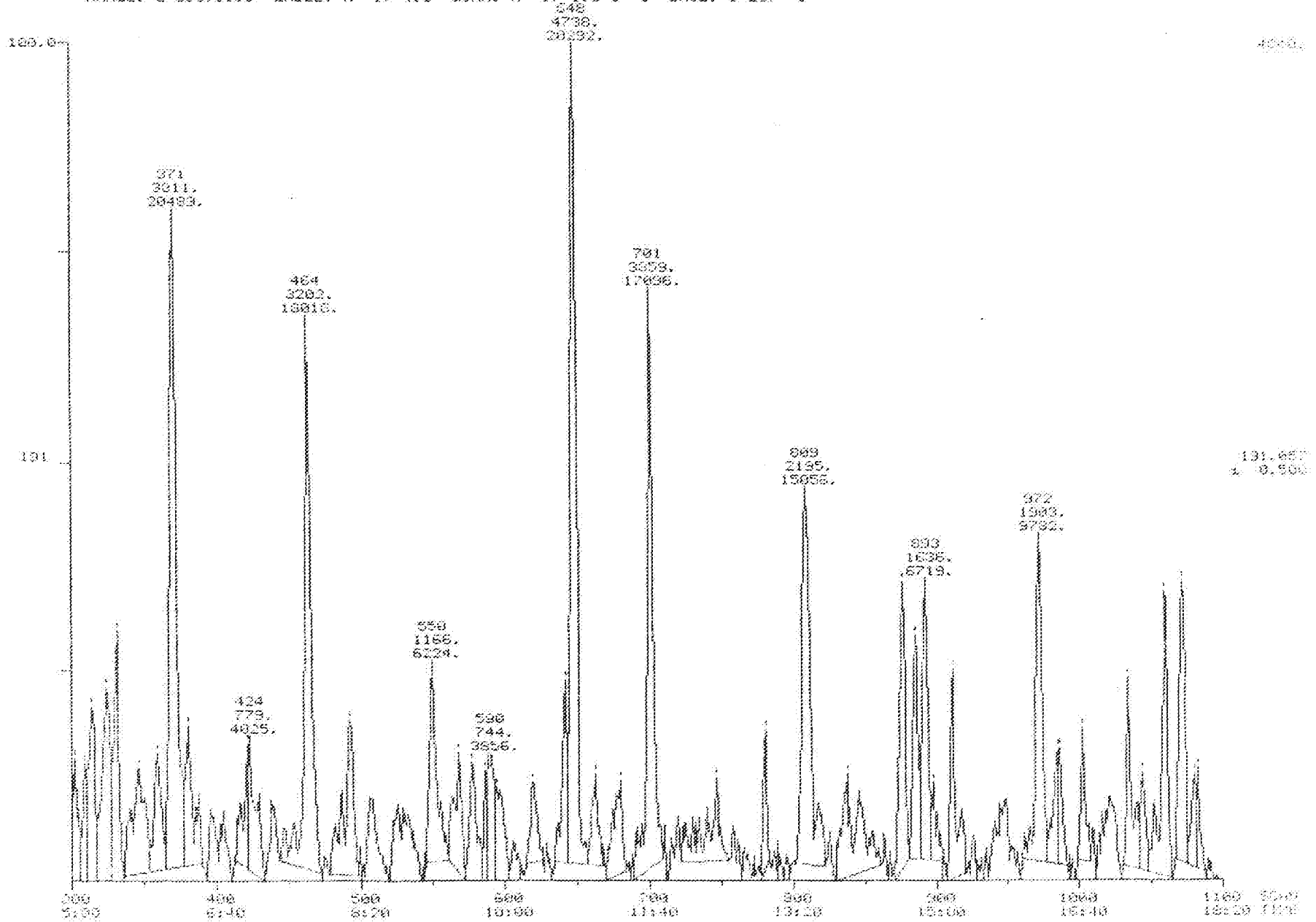
12-13-91 15:29:08

CALI: C131291 #2

SAMPLE: SIM O BRANCH CYCLIC PHILLIPS 247-275

COND5.: 20.1 20/M 130.0 3/M 300.00

RANGE: 0 300.1100 LABEL: N 1. 4.0 DURR: 0 1. 1.0 J 0 BASE: U 20. 1



Reference retention time (min.s)				6.11					
No.	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num
1	190.56	191.56	303	5:03	A BV	2488.	712.	---	0.
2	190.56	191.56	310	5:10	A VV	2528.	630.	---	0.
3	190.56	191.56	314	5:14	A VV	5008.	1008.	---	0.
4	190.56	191.56	325	5:25	A VV	7696.	1120.	---	0.
5	190.56	191.56	332	5:32	A VB	5952.	1440.	---	0.
6	190.56	191.56	347	5:47	A BV	6332.	611.	---	0.
7	190.56	191.56	360	6:00	A VV	4047.	681.	---	0.
8	190.56	191.56	371	6:11	A VV	20489.	3811.	---	0.
9	190.56	191.56	382	6:22	A VB	5104.	804.	---	0.
10	190.56	191.56	422	7:02	A BV	3631.	727.	---	0.
11	190.56	191.56	424	7:04	A VB	8025.	779.	---	0.
12	190.56	191.56	464	7:44	A BB	16016.	3202.	---	0.
13	190.56	191.56	493	8:13	A BB	7420.	894.	---	0.
14	190.56	191.56	550	9:10	A BB	6224.	1166.	---	0.
15	190.56	191.56	568	9:28	A BB	4276.	694.	---	0.
16	190.56	191.56	578	9:38	A BV	4232.	688.	---	0.
17	190.56	191.56	587	9:47	A VV	1672.	640.	---	0.
18	190.56	191.56	590	9:50	A VV	3856.	744.	---	0.
19	190.56	191.56	595	9:55	A VB	2896.	544.	---	0.
20	190.56	191.56	620	10:20	A BB	2572.	470.	---	0.
21	190.56	191.56	642	10:42	A BV	4834.	1053.	---	0.
22	190.56	191.56	648	10:48	A VV	20292.	4738.	---	0.
23	190.56	191.56	663	11:03	A VB	2470.	533.	---	0.
24	190.56	191.56	680	11:20	A BB	3904.	541.	---	0.
25	190.56	191.56	701	11:41	A BB	17096.	3359.	---	0.
26	190.56	191.56	747	12:27	A BB	5200.	482.	---	0.
27	190.56	191.56	781	13:01	A BB	2604.	804.	---	0.
28	190.56	191.56	809	13:29	A BB	15056.	2195.	---	0.
29	190.56	191.56	838	13:58	A BB	8120.	601.	---	0.
30	190.56	191.56	877	14:37	A BB	7528.	1672.	---	0.
31	190.56	191.56	886	14:46	A BV	6213.	1289.	---	0.
32	190.56	191.56	893	14:53	A VV	2719.	1636.	---	0.
33	190.56	191.56	899	14:59	A VB	1400.	445.	---	0.
34	190.56	191.56	912	15:12	A BB	5936.	1212.	---	0.
35	190.56	191.56	972	16:12	A BV	9782.	1903.	---	0.
36	190.56	191.56	985	16:25	A VV	3313.	671.	---	0.
37	190.56	191.56	987	16:27	A VB	1669.	682.	---	0.
38	190.56	191.56	1003	16:43	A BB	3088.	764.	---	0.
39	190.56	191.56	1034	17:14	A BV	5208.	1095.	---	0.
40	190.56	191.56	1048	17:25	A VV	2086.	575.	---	0.
41	190.56	191.56	1060	17:40	A VB	8858.	1655.	---	0.
42	190.56	191.56	1072	17:52	A BV	7291.	1635.	---	0.
43	190.56	191.56	1081	18:01	A VV	2046.	547.	---	0.
44	190.56	191.56	1084	18:04	A VB	1671.	593.	---	0.

MIDRANGE CHROMATOGRAM

DATA: 91H2BC #1

SCANS 1800 TO 2000

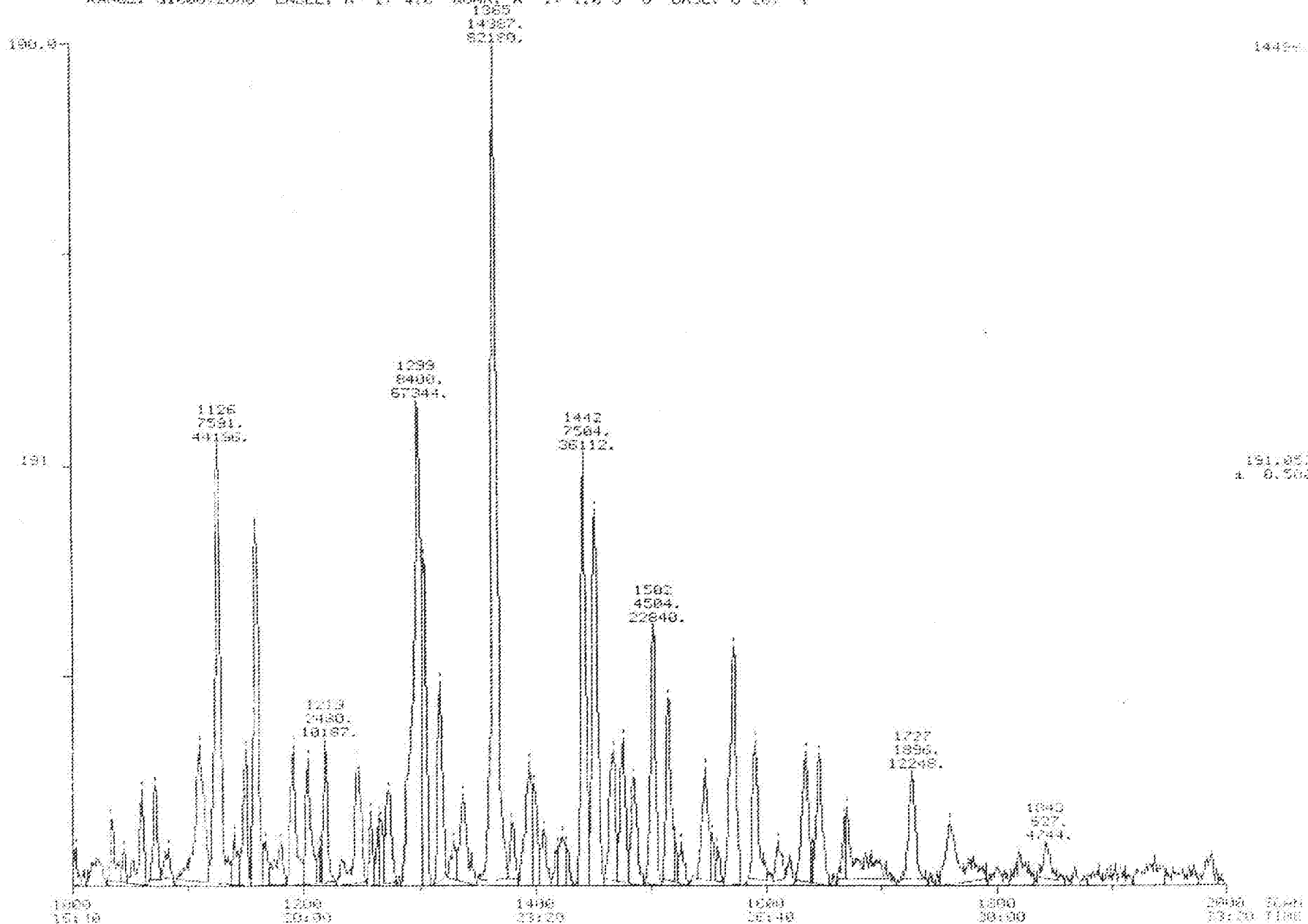
12-13-91 15:28:30

CALI: C131291 #2

SAMPLE: 91M 3 BRANCH CYCLIC PHILLIPS 2-7-273

COND: 1 20.1 33.8 139.8 578 300.20

RANGE: 01000-2000 LABEL: N-1: 4.0 QUAN: A 1: 1.0 J 0 BASE: U 20. 1



Reference retention time (min/s) 22:45

No.	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num
1	190.56	191.56	1003	16:43	A BV	2412	673	---	0.
2	190.56	191.56	1034	17:14	A BV	5208	1095	---	0.
3	190.56	191.56	1043	17:25	A VV	2036	573	---	0.
4	190.56	191.56	1060	17:40	A VB	8858	1655	---	0.
5	190.56	191.56	1070	17:50	A BV	7084	1612	---	0.
6	190.56	191.56	1084	18:04	A VB	2956	514	---	0.
7	190.56	191.56	1110	18:30	A BV	20760	2375	---	0.
8	190.56	191.56	1126	18:46	A VV	44196	7591	---	0.
9	190.56	191.56	1140	19:00	A VV	3688	900	---	0.
10	190.56	191.56	1150	19:10	A VB	9925	2344	---	0.
11	190.56	191.56	1159	19:19	A BV	30164	6381	---	0.
12	190.56	191.56	1167	19:27	A VV	3462	761	---	0.
13	190.56	191.56	1180	19:40	A VB	5958	739	---	0.
14	190.56	191.56	1191	19:51	A BV	13347	2454	---	0.
15	190.56	191.56	1204	20:04	A VV	11672	2189	---	0.
16	190.56	191.56	1213	20:13	A VV	1093	587	---	0.
17	190.56	191.56	1215	20:15	A VV	1292	683	---	0.
18	190.56	191.56	1219	20:19	A VB	10187	2480	---	0.
19	190.56	191.56	1247	20:47	A BB	16000	2134	---	0.
20	190.56	191.56	1258	20:58	A BV	4442	1289	---	0.
21	190.56	191.56	1265	21:05	A VV	3663	1218	---	0.
22	190.56	191.56	1267	21:07	A VV	3833	1101	---	0.
23	190.56	191.56	1274	21:14	A VB	8710	1588	---	0.
24	190.56	191.56	1299	21:39	A BV	67344	8400	---	0.
25	190.56	191.56	1304	21:44	A VB	19760	5664	---	0.
26	190.56	191.56	1318	21:58	A BB	17104	3478	---	0.
27	190.56	191.56	1330	22:10	A BV	3635	675	---	0.
28	190.56	191.56	1339	22:19	A VB	10605	1542	---	0.
29	190.56	191.56	1365	22:45	A BV	82180	14387	---	0.
30	190.56	191.56	1380	23:00	A VB	4715	997	---	0.
31	190.56	191.56	1396	23:16	A BV	14880	2144	---	0.
32	190.56	191.56	1399	23:19	A VV	7760	1776	---	0.
33	190.56	191.56	1408	23:28	A VB	5152	992	---	0.
34	190.56	191.56	1419	23:39	A BV	2976	688	---	0.
35	190.56	191.56	1424	23:44	A VV	4508	864	---	0.
36	190.56	191.56	1427	23:47	A VB	2304	704	---	0.
37	190.56	191.56	1442	24:02	A BV	36112	7504	---	0.
38	190.56	191.56	1452	24:12	A VB	35520	6512	---	0.
39	190.56	191.56	1468	24:28	A BV	13880	2254	---	0.
40	190.56	191.56	1476	24:36	A VV	14045	2508	---	0.
41	190.56	191.56	1485	24:45	A VB	11546	1886	---	0.
42	190.56	191.56	1502	25:02	A BB	22840	4504	---	0.
43	190.56	191.56	1515	25:15	A BV	16704	3165	---	0.
44	190.56	191.56	1521	25:21	A VV	2291	816	---	0.
45	190.56	191.56	1527	25:27	A VB	3053	723	---	0.
46	190.56	191.56	1547	25:47	A BV	12721	1962	---	0.
47	190.56	191.56	1554	25:54	A VV	2465	620	---	0.
48	190.56	191.56	1558	25:58	A VB	1962	602	---	0.
49	190.56	191.56	1572	26:12	A BB	25928	4135	---	0.
50	190.56	191.56	1590	26:30	A BB	14200	2421	---	0.
51	190.56	191.56	1610	26:50	A BB	3832	869	---	0.
52	190.56	191.56	1634	27:14	A BV	14621	2266	---	0.
53	190.56	191.56	1640	27:20	A VV	960	622	---	0.
54	190.56	191.56	1646	27:26	A VB	13971	2258	---	0.
55	190.56	191.56	1668	27:48	A BV	3728	1072	---	0.

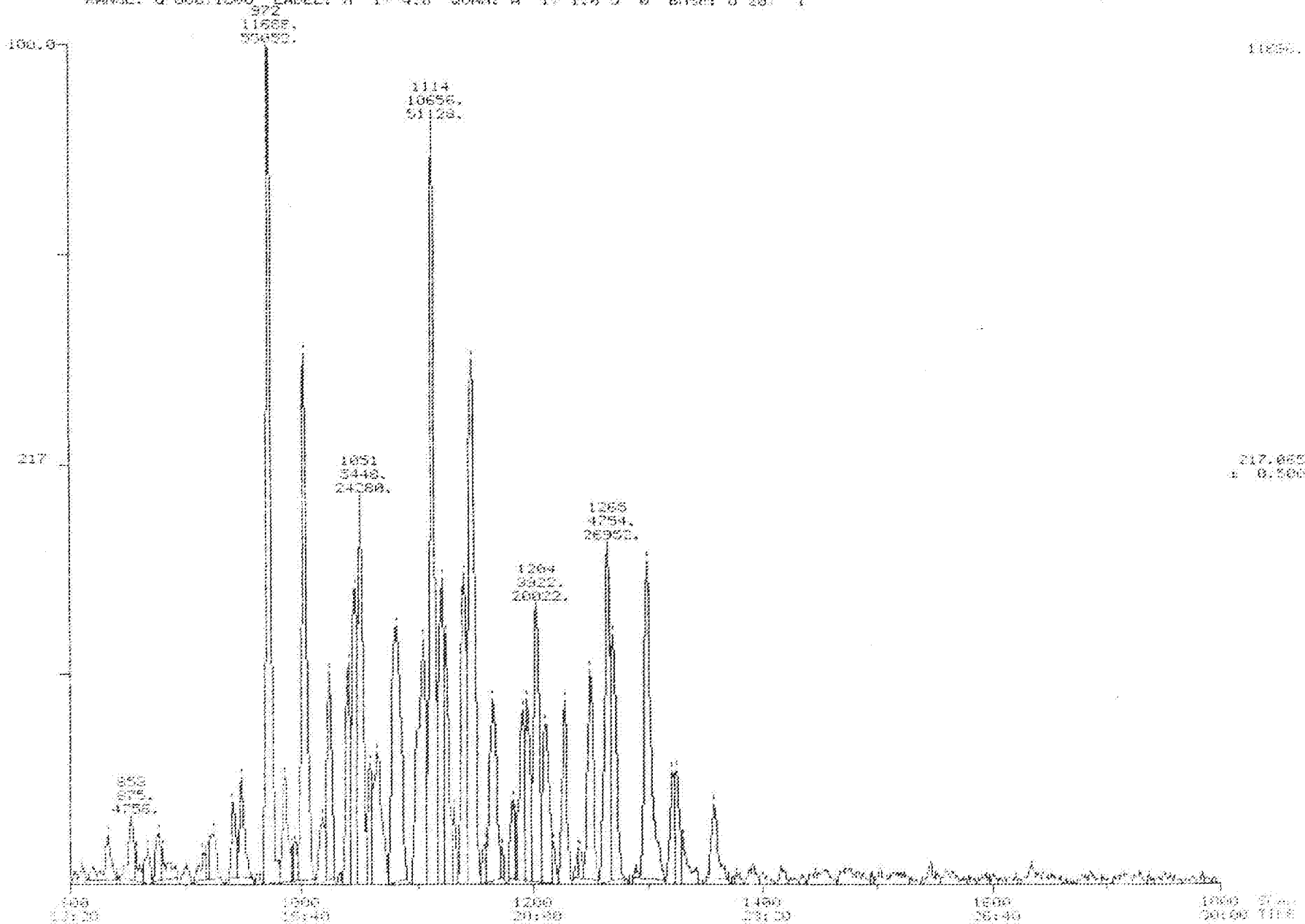
Reference retention time (min.s) 22.45									
No.	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num
56	190.56	191.56	1670	27.50	A VB	11504	1264	--	0.
57	190.56	191.56	1727	28.47	A BB	12248	1896	--	0.
58	190.56	191.56	1760	29.20	A BB	15706	1076	--	0.
59	190.56	191.56	1843	30.43	A BB	4744	627	--	0.

MS/MS CHROMATOGRAM

DATA: SIM88C #1
CALI: C131291 #2

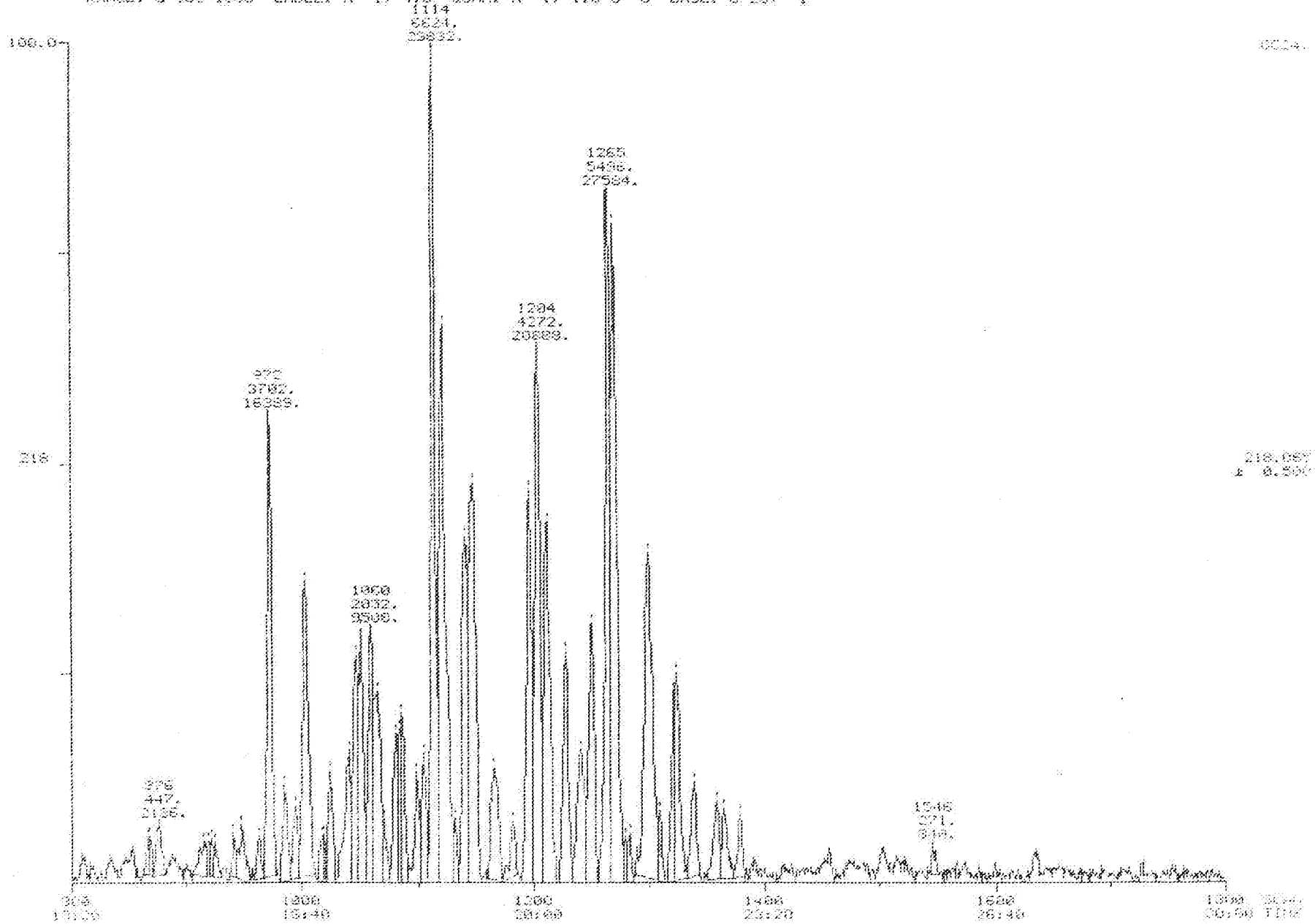
SCANS 800 TO 1800

12-13-91 15:25:40
SAMPLE: SIM 3 BRANCH CYCLIC PHILLIPS 2-7-275
COND.: 20.1 50.0 100.0 5/0 900.20
RANGE: Q 900.1000 LABEL: H 1-4.0 QUAN: 0 1- 1.0 U 0 BASE: U 20. 1



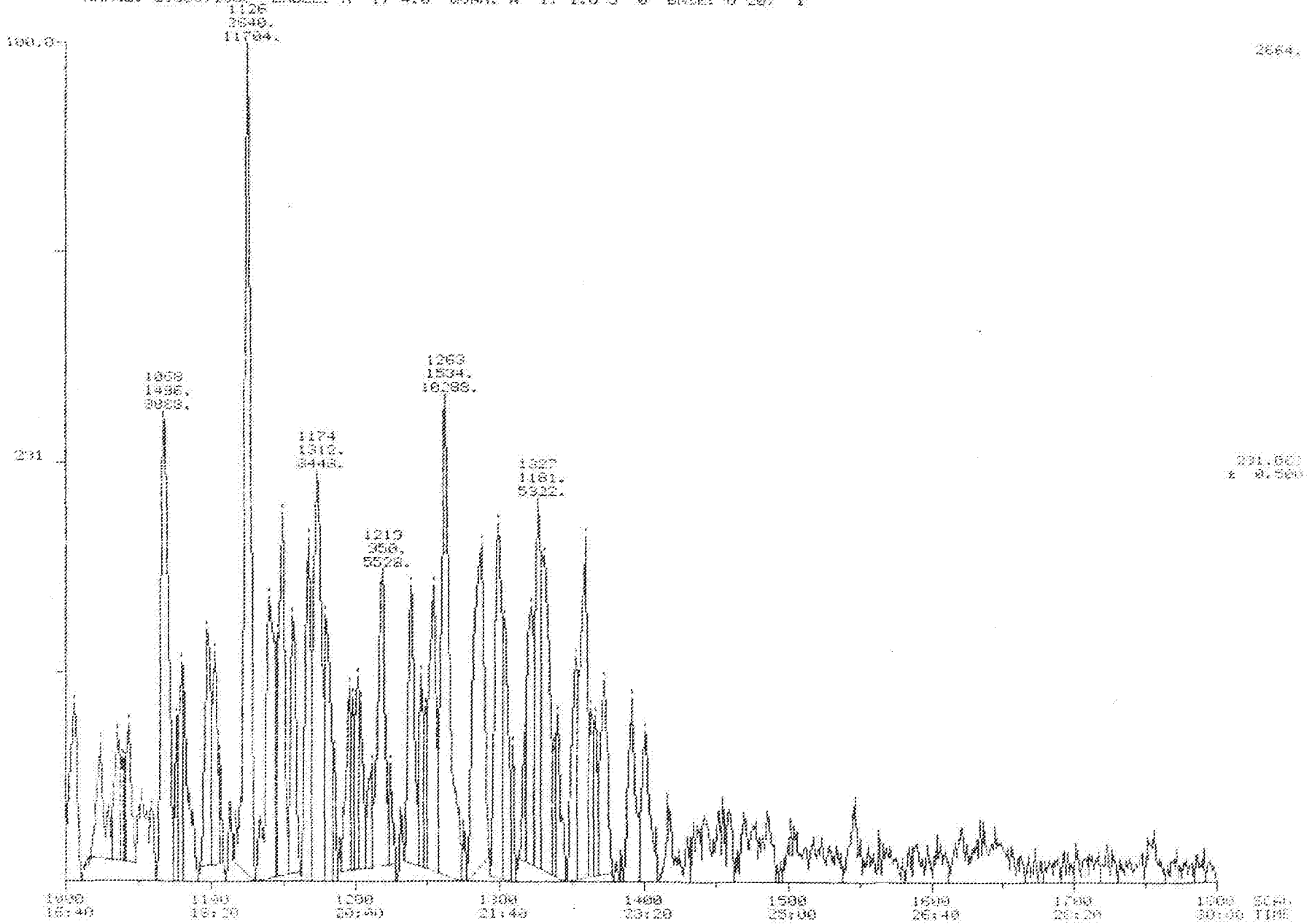
Reference retention time (min) at 15:12									
No.	Low	High	Scan	Time	Meth	Area	Height	Wave	Num
1	216.57	217.57	833	13.53	A BV	4864.	648.	--	0.
2	216.57	217.57	833	14.13	A BV	4755.	875.	--	0.
3	216.57	217.57	857	14.17	A VV	1471.	426.	--	0.
4	216.57	217.57	868	14.28	A VB	2300.	484.	--	0.
5	216.57	217.57	877	14.37	A BV	3281.	667.	--	0.
6	216.57	217.57	880	14.48	A VB	2517.	428.	--	0.
7	216.57	217.57	915	15.15	A BV	2238.	409.	--	0.
8	216.57	217.57	920	15.20	A VV	2812.	520.	--	0.
9	216.57	217.57	924	15.24	A VB	3583.	677.	--	0.
10	216.57	217.57	941	15.41	A BV	4388.	1063.	--	0.
11	216.57	217.57	945	15.45	A VB	6360.	1395.	--	0.
12	216.57	217.57	972	16.12	A BV	55032.	11688.	--	0.
13	216.57	217.57	986	16.26	A VV	8041.	1465.	--	0.
14	216.57	217.57	992	16.32	A VV	917.	495.	--	0.
15	216.57	217.57	994	16.34	A VV	1933.	636.	--	0.
16	216.57	217.57	1003	16.43	A VB	36901.	7387.	--	0.
17	216.57	217.57	1019	16.59	A BV	5325.	893.	--	0.
18	216.57	217.57	1023	17.05	A VB	13139.	2875.	--	0.
19	216.57	217.57	1041	17.21	A BV	14160.	3104.	--	0.
20	216.57	217.57	1047	17.27	A VV	20880.	4160.	--	0.
21	216.57	217.57	1051	17.31	A VV	24280.	5448.	--	0.
22	216.57	217.57	1060	17.40	A VV	7296.	1704.	--	0.
23	216.57	217.57	1066	17.46	A VB	14432.	3886.	--	0.
24	216.57	217.57	1083	18.03	A BV	31752.	6576.	--	0.
25	216.57	217.57	1105	18.35	A BV	28624.	6456.	--	0.
26	216.57	217.57	1114	18.34	A VV	51128.	10556.	--	0.
27	216.57	217.57	1122	18.42	A VV	21168.	4288.	--	0.
28	216.57	217.57	1125	18.45	A VV	14984.	3512.	--	0.
29	216.57	217.57	1132	18.52	A VB	3024.	1064.	--	0.
30	216.57	217.57	1141	19.01	A BV	23072.	4660.	--	0.
31	216.57	217.57	1148	19.08	A VB	41876.	7306.	--	0.
32	216.57	217.57	1159	19.17	A BV	2195.	574.	--	0.
33	216.57	217.57	1166	19.26	A VV	18095.	3534.	--	0.
34	216.57	217.57	1174	19.34	A VB	462.	422.	--	0.
35	216.57	217.57	1184	19.44	A BV	4291.	1120.	--	0.
36	216.57	217.57	1184	19.46	A VV	1817.	924.	--	0.
37	216.57	217.57	1192	19.52	A VV	13189.	2590.	--	0.
38	216.57	217.57	1196	19.56	A VV	11042.	2556.	--	0.
39	216.57	217.57	1204	20.04	A VV	20022.	3922.	--	0.
40	216.57	217.57	1211	20.11	A VV	14008.	2230.	--	0.
41	216.57	217.57	1218	20.18	A VB	1503.	577.	--	0.
42	216.57	217.57	1228	20.28	A BV	12360.	2568.	--	0.
43	216.57	217.57	1237	20.37	A BV	1383.	430.	--	0.
44	216.57	217.57	1241	20.41	A VV	1214.	393.	--	0.
45	216.57	217.57	1250	20.50	A VB	16195.	2935.	--	0.
46	216.57	217.57	1255	21.05	A BV	26952.	4754.	--	0.
47	216.57	217.57	1270	21.10	A VB	14988.	3451.	--	0.
48	216.57	217.57	1299	21.39	A BV	30056.	4445.	--	0.
49	216.57	217.57	1321	22.01	A BV	7496.	1576.	--	0.
50	216.57	217.57	1325	22.05	A VV	7504.	1600.	--	0.
51	216.57	217.57	1330	22.10	A VB	4024.	856.	--	0.
52	216.57	217.57	1358	22.38	A BV	6588.	1033.	--	0.

MICRAST CHROMATOGRAM DATA: 311350 #1 SCANS 900 TO 1080
 12/13/91 15:28:00 CALI: C131231 #2
 SAMPLE: 31M G BRANCH CYCLIC PHILIPS 277-175
 COND.: 28.1 28.11 136.9 5.4 300/20
 RANGE: G 900-1080 LABEL: N 1: 1.0 QUAN: A 1: 1.0 0 0 BASE: U 20. 1



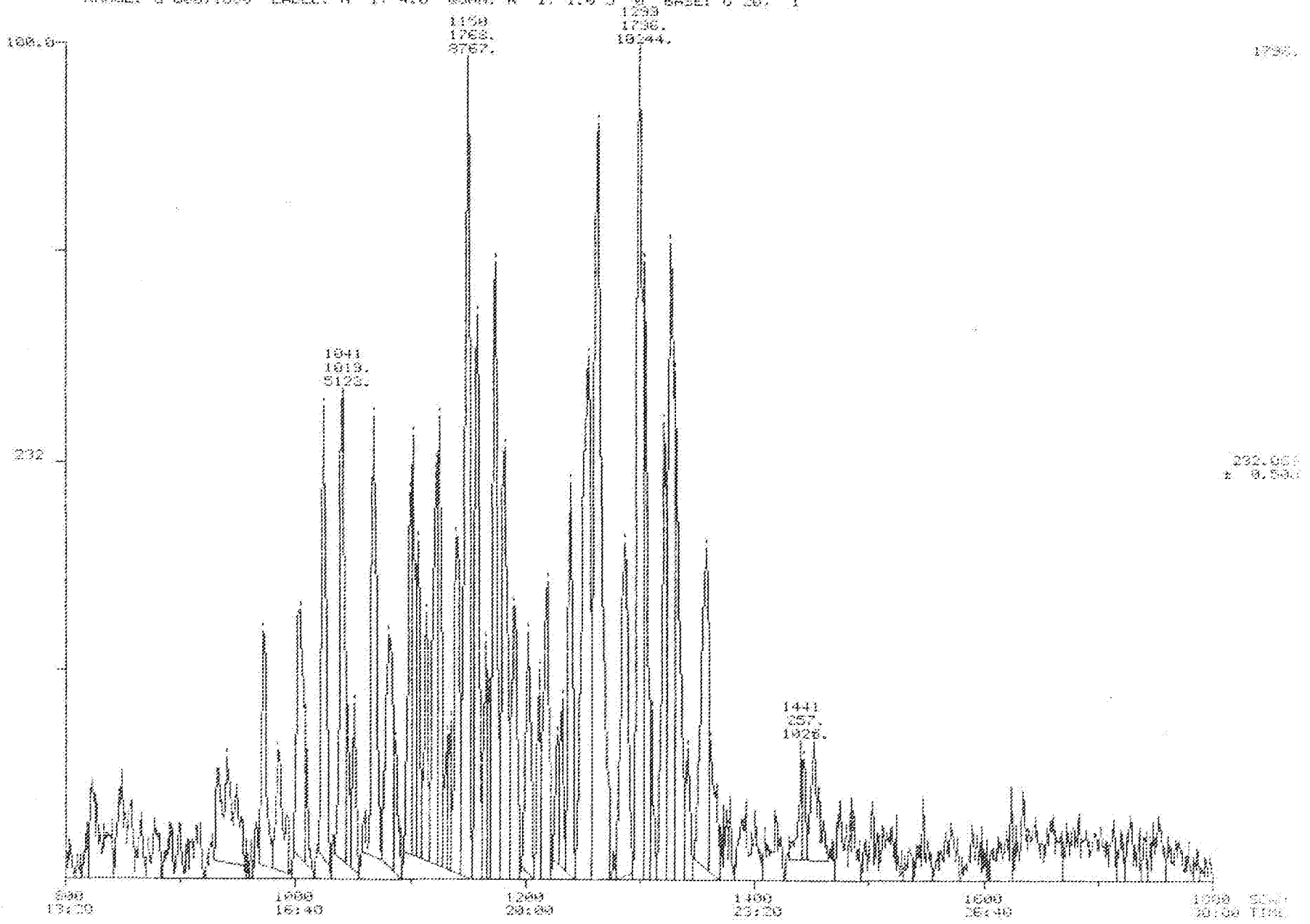
Reference retention time (min s) 18:34									
No.	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num
1	217.57	218.57	866	14:26	A BV	708	302	---	0
2	217.57	218.57	868	14:28	A VB	780	322	---	0
3	217.57	218.57	875	14:36	A BB	2136	447	---	0
4	217.57	218.57	915	15:15	A BV	1927	278	---	0
5	217.57	218.57	919	15:19	A VV	952	277	---	0
6	217.57	218.57	922	15:22	A VV	906	308	---	0
7	217.57	218.57	924	15:24	A VB	876	270	---	0
8	217.57	218.57	941	15:41	A BV	992	347	---	0
9	217.57	218.57	948	15:48	A VB	2512	438	---	0
10	217.57	218.57	963	16:03	A BV	1587	341	---	0
11	217.57	218.57	972	16:12	A VB	16389	3702	---	0
12	217.57	218.57	985	16:25	A BV	3868	783	---	0
13	217.57	218.57	995	16:35	A VV	2958	586	---	0
14	217.57	218.57	1003	16:43	A VB	13582	2346	---	0
15	217.57	218.57	1017	16:57	A BV	1224	362	---	0
16	217.57	218.57	1019	16:59	A VV	845	372	---	0
17	217.57	218.57	1021	17:01	A VV	712	370	---	0
18	217.57	218.57	1024	17:04	A VB	3555	888	---	0
19	217.57	218.57	1041	17:21	A BV	7104	1056	---	0
20	217.57	218.57	1047	17:27	A VV	8982	1808	---	0
21	217.57	218.57	1051	17:31	A VV	8376	2020	---	0
22	217.57	218.57	1060	17:40	A VV	9508	2032	---	0
23	217.57	218.57	1065	17:45	A VV	9444	1520	---	0
24	217.57	218.57	1071	17:51	A VB	1516	508	---	0
25	217.57	218.57	1082	18:02	A BV	5764	1184	---	0
26	217.57	218.57	1084	18:04	A VV	2368	1232	---	0
27	217.57	218.57	1086	18:06	A VV	4960	1344	---	0
28	217.57	218.57	1099	18:19	A VV	4200	880	---	0
29	217.57	218.57	1106	18:25	A VB	4448	1032	---	0
30	217.57	218.57	1114	18:34	A BV	29832	6624	---	0
31	217.57	218.57	1122	18:42	A VV	27808	4408	---	0
32	217.57	218.57	1132	18:52	A VB	1408	520	---	0
33	217.57	218.57	1141	19:01	A BV	15648	2752	---	0
34	217.57	218.57	1148	19:08	A VB	20176	3168	---	0
35	217.57	218.57	1166	19:26	A BB	6624	896	---	0
36	217.57	218.57	1182	19:42	A BB	2592	452	---	0
37	217.57	218.57	1197	19:57	A BV	15432	3120	---	0
38	217.57	218.57	1204	20:04	A VV	20888	4272	---	0
39	217.57	218.57	1212	20:12	A VB	17222	2864	---	0
40	217.57	218.57	1228	20:28	A BV	9576	1948	---	0
41	217.57	218.57	1241	20:41	A VV	8220	1068	---	0
42	217.57	218.57	1251	20:51	A VB	11568	2060	---	0
43	217.57	218.57	1265	21:05	A BV	27584	5496	---	0
44	217.57	218.57	1270	21:10	A VV	26148	5216	---	0
45	217.57	218.57	1279	21:19	A VV	1000	364	---	0
46	217.57	218.57	1283	21:23	A VB	1216	400	---	0
47	217.57	218.57	1299	21:39	A BV	22313	2588	---	0
48	217.57	218.57	1309	21:49	A VB	1437	560	---	0
49	217.57	218.57	1321	22:01	A BV	5633	1526	---	0
50	217.57	218.57	1324	22:04	A VB	7815	1655	---	0
51	217.57	218.57	1339	22:19	A BB	3932	751	---	0
52	217.57	218.57	1359	22:39	A BV	3770	616	---	0
53	217.57	218.57	1365	22:45	A VV	2783	565	---	0
54	217.57	218.57	1379	22:59	A VB	2342	514	---	0
55	217.57	218.57	1346	23:46	A BB	840	271	---	0

MICHAEL CHROMATOGRAM DATA: 31M30C #1 SCANS 1000 TO 1800
 12/12/91 13:25:00 COLI: C131391 #2
 SAMPLE: 31M 3 BRANCH CYCLIC PHILLIPS 2-7-27S
 CORDS.: 30.1 30.0 130.0 5.0 300.00
 RANGE: 01000.1000 LABEL: M 17 4.0 DUGH: A L 1.0 J 0 BRCE: U 20. 1



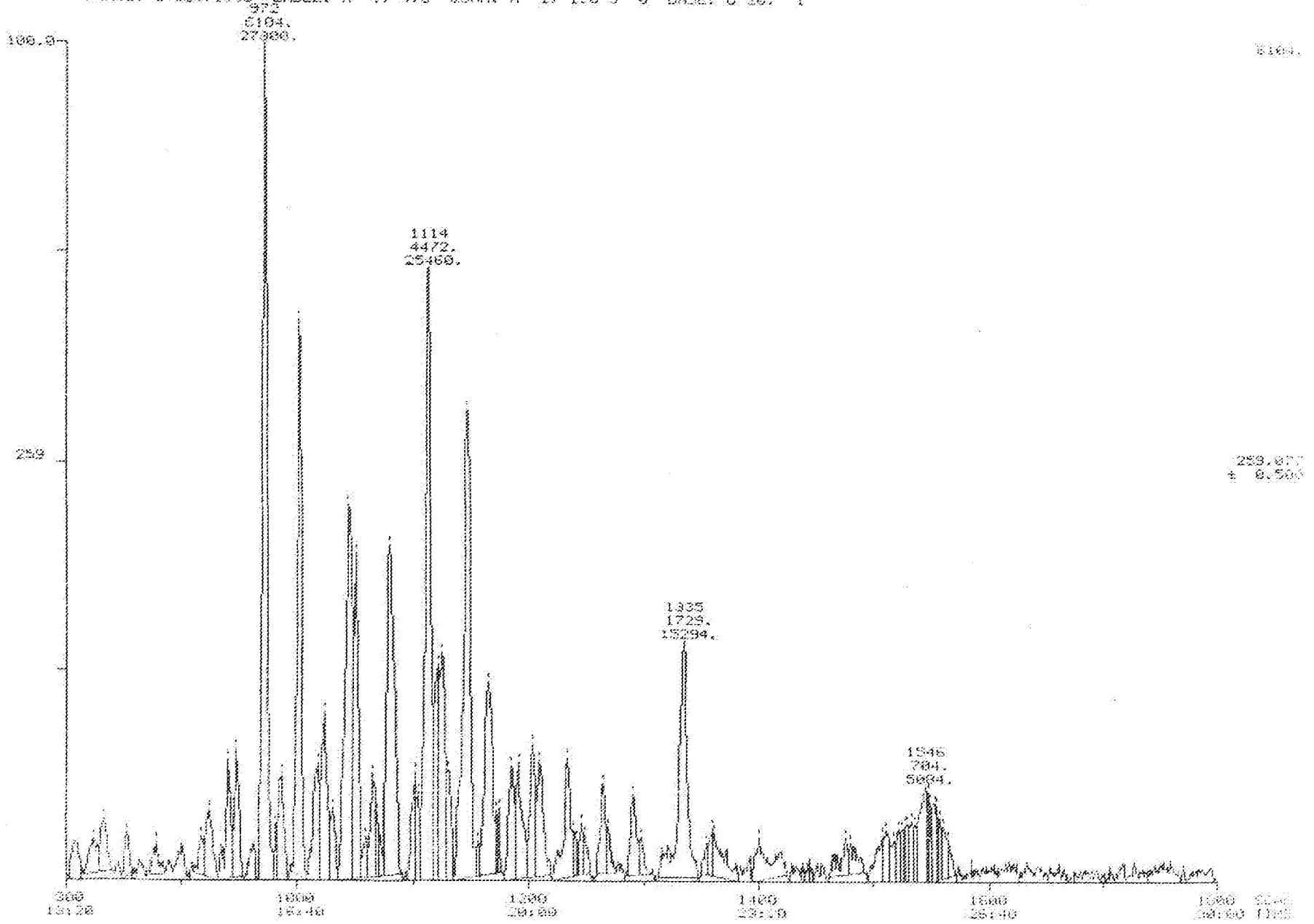
Reference retention time (min:s)				18:46						
No.	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num	
1	230.57	231.57	1008	16:46	A BV	2520	568	---	0	
2	230.57	231.57	1024	17:04	A BV	2402	372	---	0	
3	230.57	231.57	1038	17:16	A VV	1746	408	---	0	
4	230.57	231.57	1039	17:19	A VV	593	334	---	0	
5	230.57	231.57	1041	17:21	A VV	623	331	---	0	
6	230.57	231.57	1044	17:24	A VB	1478	445	---	0	
7	230.57	231.57	1068	17:48	A BV	8888	1496	---	0	
8	230.57	231.57	1077	17:57	A VV	1272	520	---	0	
9	230.57	231.57	1080	18:00	A VV	1920	704	---	0	
10	230.57	231.57	1082	18:02	A VB	2816	664	---	0	
11	230.57	231.57	1098	18:18	A BV	3862	757	---	0	
12	230.57	231.57	1103	18:23	A VV	2372	483	---	0	
13	230.57	231.57	1107	18:27	A VB	641	353	---	0	
14	230.57	231.57	1126	18:46	A BV	11704	2640	---	0	
15	230.57	231.57	1141	19:01	A BV	6183	902	---	0	
16	230.57	231.57	1146	19:06	A VV	1431	777	---	0	
17	230.57	231.57	1150	19:10	A VV	4586	1157	---	0	
18	230.57	231.57	1157	19:17	A VB	3566	821	---	0	
19	230.57	231.57	1163	19:23	A BV	4536	1096	---	0	
20	230.57	231.57	1174	19:34	A VV	8448	1312	---	0	
21	230.57	231.57	1130	19:40	A VV	3984	856	---	0	
22	230.57	231.57	1184	19:46	A VB	896	424	---	0	
23	230.57	231.57	1197	19:57	A BV	2558	593	---	0	
24	230.57	231.57	1199	19:59	A VV	1005	555	---	0	
25	230.57	231.57	1202	20:02	A VV	1691	617	---	0	
26	230.57	231.57	1204	20:04	A VV	1791	536	---	0	
27	230.57	231.57	1212	20:12	A VV	1303	330	---	0	
28	230.57	231.57	1219	20:19	A VV	5520	950	---	0	
29	230.57	231.57	1225	20:25	A VB	588	322	---	0	
30	230.57	231.57	1239	20:39	A BV	4456	888	---	0	
31	230.57	231.57	1246	20:46	A VV	1992	619	---	0	
32	230.57	231.57	1249	20:49	A VV	1002	520	---	0	
33	230.57	231.57	1255	20:55	A VV	5326	914	---	0	
34	230.57	231.57	1263	21:03	A VB	10288	1534	---	0	
35	230.57	231.57	1269	21:09	A BV	8732	1029	---	0	
36	230.57	231.57	1279	21:39	A BV	6720	1132	---	0	
37	230.57	231.57	1304	21:44	A VV	2805	633	---	0	
38	230.57	231.57	1309	21:49	A VB	923	437	---	0	
39	230.57	231.57	1317	21:57	A BV	1022	415	---	0	
40	230.57	231.57	1322	22:02	A VV	4277	826	---	0	
41	230.57	231.57	1327	22:07	A VV	5322	1181	---	0	
42	230.57	231.57	1331	22:11	A VV	5999	1006	---	0	
43	230.57	231.57	1338	22:18	A VV	814	414	---	0	
44	230.57	231.57	1340	22:20	A VB	1757	522	---	0	
45	230.57	231.57	1353	22:33	A BV	3607	714	---	0	
46	230.57	231.57	1359	22:39	A VV	6321	1088	---	0	
47	230.57	231.57	1365	22:43	A VV	1343	539	---	0	
48	230.57	231.57	1366	22:46	A VV	1587	612	---	0	
49	230.57	231.57	1372	22:52	A VB	3105	622	---	0	
50	230.57	231.57	1391	23:11	A BV	3700	583	---	0	
51	230.57	231.57	1400	23:20	A VB	3324	484	---	0	

MIDRASS CHROMATOGRAM DATA: 91M380 #1 SCANS 800 TO 1800
12/13/91 15:09:00 CALI: 0131291 #2
SAMPLE: 91M 3 BRANCH CYCLIC PHILLIPS 277-275
COND5.: 20.1 30 M 130.0 5.0 300.20
RANGE: 0 800.1800 LABEL: N 17 4.0 0600: A 1. 1.0 J 31 BASE: U 00. 1



Reference retention time (min:s)		21:03							
No.	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num
1	231.57	232.57	940	15:40	A BB	3320	227	---	0
2	231.57	232.57	972	15:12	A BV	2651	506	---	0
3	231.57	232.57	985	15:25	A VB	1991	250	---	0
4	231.57	232.57	1004	15:44	A BV	3668	533	---	0
5	231.57	232.57	1009	15:49	A VB	660	327	---	0
6	231.57	232.57	1024	17:04	A BB	4304	973	---	0
7	231.57	232.57	1041	17:21	A BV	5123	1019	---	0
8	231.57	232.57	1045	17:25	A VV	1005	399	---	0
9	231.57	232.57	1051	17:31	A VB	1300	350	---	0
10	231.57	232.57	1068	17:48	A BB	5292	949	---	0
11	231.57	232.57	1082	18:02	A BV	2394	501	---	0
12	231.57	232.57	1097	18:07	A VB	1264	285	---	0
13	231.57	232.57	1100	18:20	A BV	3048	782	---	0
14	231.57	232.57	1102	18:22	A VV	2770	908	---	0
15	231.57	232.57	1107	18:27	A VV	2142	685	---	0
16	231.57	232.57	1114	18:34	A VV	2200	536	---	0
17	231.57	232.57	1123	18:43	A VV	4381	869	---	0
18	231.57	232.57	1125	18:45	A VV	3045	971	---	0
19	231.57	232.57	1132	18:52	A VV	934	290	---	0
20	231.57	232.57	1135	18:55	A VV	699	325	---	0
21	231.57	232.57	1140	19:00	A VV	3744	726	---	0
22	231.57	232.57	1150	19:10	A VB	8767	1768	---	0
23	231.57	232.57	1158	19:18	A BV	4916	1216	---	0
24	231.57	232.57	1166	19:26	A VV	1940	516	---	0
25	231.57	232.57	1168	19:28	A VV	1060	416	---	0
26	231.57	232.57	1174	19:34	A VV	6400	1328	---	0
27	231.57	232.57	1182	19:42	A VV	5540	932	---	0
28	231.57	232.57	1190	19:50	A VB	3248	592	---	0
29	231.57	232.57	1202	20:02	A BB	2768	521	---	0
30	231.57	232.57	1212	20:12	A BV	1756	456	---	0
31	231.57	232.57	1219	20:19	A VB	2532	644	---	0
32	231.57	232.57	1228	20:28	A BV	1266	277	---	0
33	231.57	232.57	1232	20:32	A VV	1091	366	---	0
34	231.57	232.57	1239	20:39	A VB	3913	845	---	0
35	231.57	232.57	1255	20:55	A BV	9736	1128	---	0
36	231.57	232.57	1263	21:03	A VB	12072	1628	---	0
37	231.57	232.57	1287	21:27	A BB	5364	719	---	0
38	231.57	232.57	1299	21:39	A BV	10244	1796	---	0
39	231.57	232.57	1304	21:44	A VV	4344	1332	---	0
40	231.57	232.57	1310	21:50	A VB	924	368	---	0
41	231.57	232.57	1321	22:01	A BV	4548	968	---	0
42	231.57	232.57	1327	22:07	A VV	7764	1372	---	0
43	231.57	232.57	1331	22:11	A VV	4984	1096	---	0
44	231.57	232.57	1342	22:22	A VB	1220	284	---	0
45	231.57	232.57	1358	22:38	A BV	5250	689	---	0
46	231.57	232.57	1362	22:42	A VB	1590	281	---	0
47	231.57	232.57	1441	24:01	A BV	1025	257	---	0
48	231.57	232.57	1443	24:03	A VV	559	218	---	0
49	231.57	232.57	1462	24:12	A VB	1906	255	---	0

MICHAES CHROMATOGRAM DATA: 91H360 #1 SCANS 808 TO 1000
 12/13/91 15:26:06 CALI: C131291 #2
 SAMPLE: 91H 3 BRANCH CYCLIC PHILIPS 2-7-275
 COND5.: 20.1 38.0 100.0 5.0 300.20
 RANGE: G 000.1000 LABEL: N 1. 4.0 DUAN: A 1. 1.0 J 0 BASE: U 00. 1



Reference retention time (min:s)		18:12							
No.	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num
1	258.58	259.58	828	13:45	A BV	2093.	251.	---	0.
2	258.58	259.58	834	13:54	A VB	2511.	383.	---	0.
3	258.58	259.58	854	14:14	A BB	1456.	313.	---	0.
4	258.58	259.58	879	14:39	A BB	1400.	246.	---	0.
5	258.58	259.58	917	15:17	A BV	1433.	282.	---	0.
6	258.58	259.58	924	15:24	A VB	3319.	488.	---	0.
7	258.58	259.58	941	15:41	A BV	4667.	876.	---	0.
8	258.58	259.58	948	15:48	A VB	4125.	939.	---	0.
9	258.58	259.58	972	16:12	A BV	27800.	6104.	---	0.
10	258.58	259.58	982	16:22	A VV	1024.	416.	---	0.
11	258.58	259.58	987	16:27	A VB	4280.	784.	---	0.
12	258.58	259.58	1002	16:42	A BB	17920.	4052.	---	0.
13	258.58	259.58	1018	16:58	A BV	5464.	884.	---	0.
14	258.58	259.58	1024	17:04	A VV	6896.	1236.	---	0.
15	258.58	259.58	1032	17:12	A VB	2796.	532.	---	0.
16	258.58	259.58	1048	17:28	A BV	19616.	2743.	---	0.
17	258.58	259.58	1051	17:31	A VV	9577.	2382.	---	0.
18	258.58	259.58	1060	17:40	A VV	1436.	305.	---	0.
19	258.58	259.58	1066	17:46	A VV	3822.	755.	---	0.
20	258.58	259.58	1070	17:50	A VV	778.	463.	---	0.
21	258.58	259.58	1072	17:52	A VV	904.	325.	---	0.
22	258.58	259.58	1080	18:00	A VB	18673.	2410.	---	0.
23	258.58	259.58	1102	18:22	A BV	3336.	792.	---	0.
24	258.58	259.58	1105	18:25	A VV	2304.	648.	---	0.
25	258.58	259.58	1114	18:34	A VV	25460.	4472.	---	0.
26	258.58	259.58	1122	18:42	A VV	7128.	1580.	---	0.
27	258.58	259.58	1126	18:46	A VV	9400.	1672.	---	0.
28	258.58	259.58	1131	18:51	A VB	3140.	804.	---	0.
29	258.58	259.58	1147	19:07	A BV	23981.	3428.	---	0.
30	258.58	259.58	1157	19:17	A VV	473.	257.	---	0.
31	258.58	259.58	1165	19:25	A VV	11192.	1406.	---	0.
32	258.58	259.58	1173	19:33	A VV	862.	458.	---	0.
33	258.58	259.58	1175	19:35	A VB	700.	483.	---	0.
34	258.58	259.58	1186	19:46	A BV	4751.	842.	---	0.
35	258.58	259.58	1192	19:52	A VV	5311.	848.	---	0.
36	258.58	259.58	1204	20:04	A VV	4988.	984.	---	0.
37	258.58	259.58	1210	20:10	A VB	5210.	850.	---	0.
38	258.58	259.58	1234	20:34	A BV	6030.	874.	---	0.
39	258.58	259.58	1240	20:40	A VV	388.	342.	---	0.
40	258.58	259.58	1243	20:43	A VV	486.	264.	---	0.
41	258.58	259.58	1247	20:47	A VV	1256.	372.	---	0.
42	258.58	259.58	1250	20:50	A VB	872.	278.	---	0.
43	258.58	259.58	1265	21:05	A BV	3517.	655.	---	0.
44	258.58	259.58	1270	21:10	A VB	1199.	341.	---	0.
45	258.58	259.58	1291	21:31	A BV	3306.	590.	---	0.
46	258.58	259.58	1298	21:38	A VB	1086.	287.	---	0.
47	258.58	259.58	1335	22:15	A BB	15294.	1729.	---	0.
48	258.58	259.58	1335	22:15	A BV	878.	241.	---	0.
49	258.58	259.58	1350	22:40	A VV	1494.	358.	---	0.
50	258.58	259.58	1362	22:42	A VB	3196.	318.	---	0.
51	258.58	259.58	1401	23:21	A BB	4588.	310.	---	0.
52	258.58	259.58	1476	24:36	A BV	2286.	271.	---	0.
53	258.58	259.58	1480	24:40	A VB	1606.	232.	---	0.
54	258.58	259.58	1508	25:08	A BV	2688.	340.	---	0.
55	258.58	259.58	1512	25:12	A VV	1988.	376.	---	0.

Reference retention time (min): 16.12										
No.	Low	Mass	High	Scan	Time	Meth	Area	Height	Name	Num
56	258	58	259	1519	25:19	A VV	1400	312	---	0.
57	258	58	259	1523	25:23	A VV	1428	372	---	0.
58	258	58	259	1526	25:26	A VV	1112	384	---	0.
59	258	58	259	1528	25:28	A VV	832	420	---	0.
60	258	58	259	1530	25:30	A VV	1208	424	---	0.
61	258	58	259	1534	25:34	A VV	1700	448	---	0.
62	258	58	259	1537	25:37	A VV	800	416	---	0.
63	258	58	259	1546	25:46	A VV	5084	704	---	0.
64	258	58	259	1548	25:48	A VV	1228	660	---	0.
65	258	58	259	1550	25:50	A VB	584	584	---	0.
66	258	58	259	1554	25:54	A BV	2120	572	---	0.
67	258	58	259	1556	25:56	A VV	920	540	---	0.
68	258	58	259	1559	25:59	A VV	1174	445	---	0.
69	258	58	259	1561	26:01	A VV	1620	380	---	0.
70	258	58	259	1566	26:06	A VB	848	276	---	0.

APPENDIX 4.2

12/13/91 14:10:18 SCAN 1 OF 2000
Acquisition started

Acquire 12/13/91 14:10:00 + 0:02 Run 0:91M49C ACQUIRING
Free sectors: 13625 Scan: 2 of 2000
Sample: 9th & BRANCH CYCLIC PHILLIPS 2/7-27S
Conds.: 20.1 30/M 100.0 5/M 300.20
Formula: A000 0160 Instrument: 4000 Weight: 0.000
Submitted by: MAB Analyst: PCH Acct. No: P21290

***** SCAN PARAMETERS *****
**** Mode: Centroid positive ion

MID scan Desc: GC Mass intervals: 17
Scan time: 1.000 s Samp. int.: 0.200 ms Master rate: 512

Int #	Lo mass	Hi mass	Time	MPW	MPW	MA	TH	BL	ION
1	84.525	85.525	0.052	1	80	5	1	0	Pos
2	122.537	123.537	0.052	1	80	5	1	0	Pos
3	148.545	149.545	0.052	1	90	5	1	0	Pos
4	150.545	151.545	0.052	1	90	5	1	0	Pos
5	162.549	163.549	0.052	1	80	5	1	0	Pos
6	176.553	177.553	0.052	1	80	5	1	0	Pos
7	182.559	183.559	0.052	1	80	5	1	0	Pos
8	190.557	191.557	0.052	1	80	5	1	0	Pos
9	216.565	217.565	0.052	1	80	5	1	0	Pos
10	217.565	218.565	0.052	1	80	5	1	0	Pos
11	230.569	231.569	0.052	1	80	5	1	0	Pos
12	231.569	232.569	0.052	1	80	5	1	0	Pos
13	238.572	239.572	0.052	1	80	5	1	0	Pos
14	252.576	253.576	0.052	1	80	5	1	0	Pos
15	258.577	259.577	0.052	1	80	5	1	0	Pos
16	397.619	398.619	0.052	1	80	5	1	0	Pos
17	411.623	412.623	0.052	1	80	5	1	0	Pos

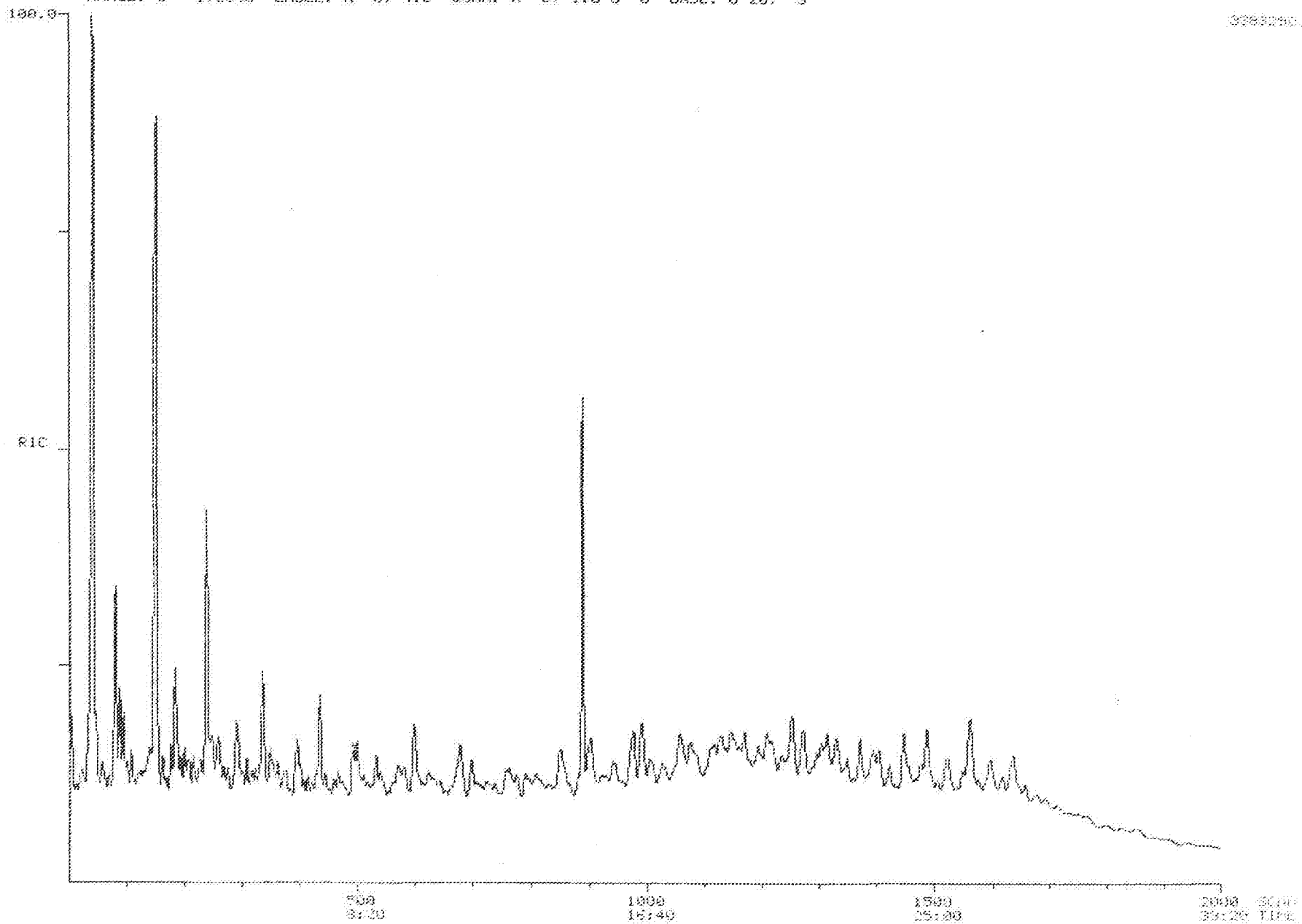
Interface number 0
Sub-interface number 0
of acqu buffers 16
Instrument type 0
Full scale mass 1024 u
Zero scale mass 1 u
Intensity/ion 2
Peak Width 972 mmu
Offset at low mass 0 mmu
Offset at high mass 0 mmu
Voltage settling time(MS) 4

12/13/91 14:38:40
ACQUISITION COMPLETED
SCANS 1 TO 2000 Centroid

Mode	Scans	Secs	Out of	%	Peaks per scan	per sec
Centroid	2000	352.8	2000.0	17.6	39001	20. 20.

HIDRIC DATA: 91M480 #1 SCANS 1 TO 2000
12/13/91 16:18:00 CALL: C131291 #2
SAMPLE: 91M 4 BRANCH CYCLIC PHILLIPS 2/7-275
CONDS.: 20.1 30.0 130.0 5.0 300.00
RANGE: 5 1.0000 LABEL: N 0. 4.0 QUAN: 4 0. 1.0 J 0 BASE: 0 20. 3

0000000



MIDMASS CHROMATOGRAM

DATA: 91HSDC #1
CALI: C101291 #2

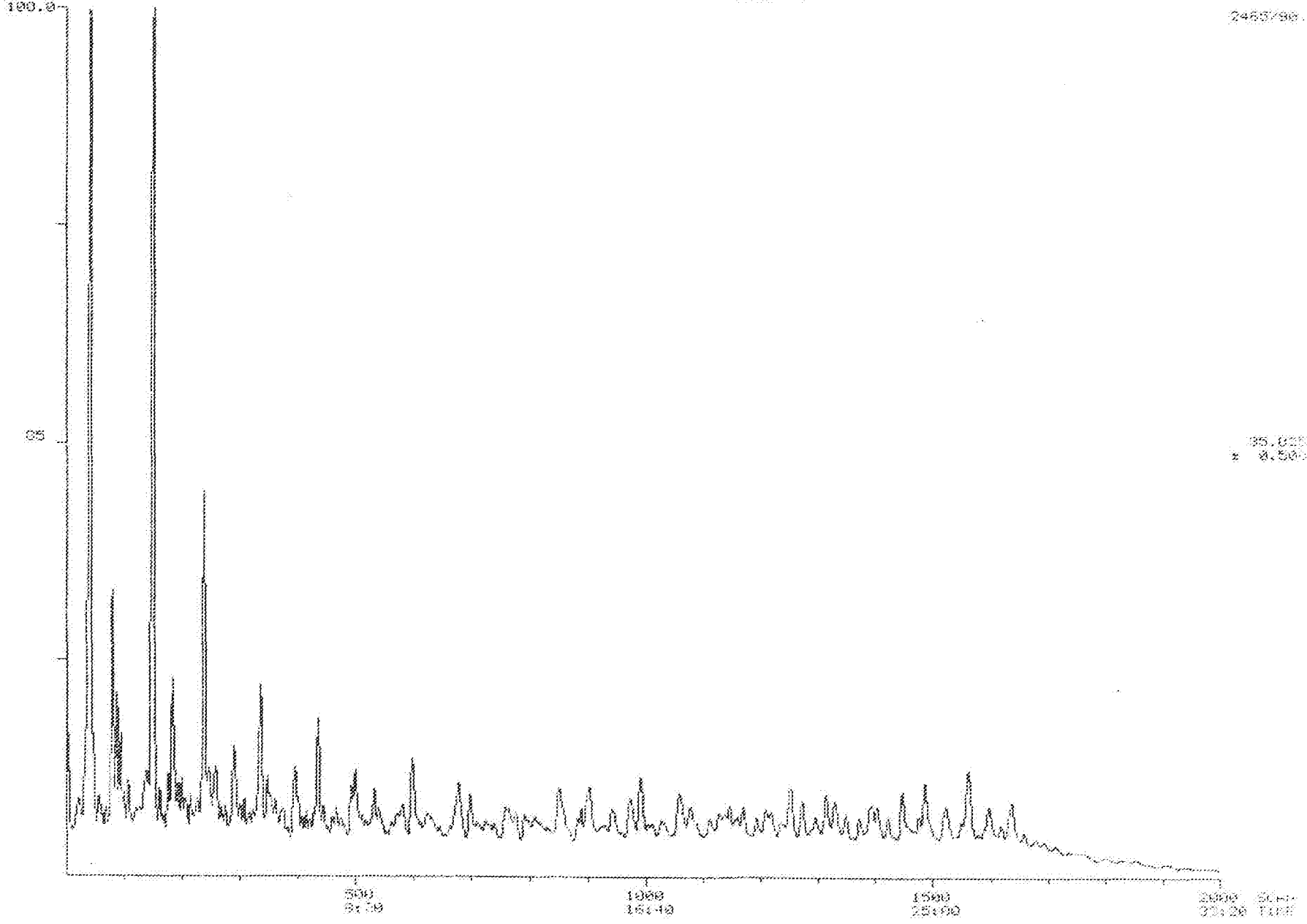
SCANS 1 TO 2000

12/13/91 16:18:00

SAMPLE: 91M 4 SPANCH CYCLIC PHILLIPS 2-7-275

CONDS.: 20.1 33/M 130.0 5/M 300.20

RANGE: G 1.2000 LABEL: N 9. 4.0 QUANT: R 9. 1.0 J 0 CASE: U 20. 3



HIGH-RES CHROMATOGRAMS

DATA: 91M4EC #1
CALL: C131291 #2

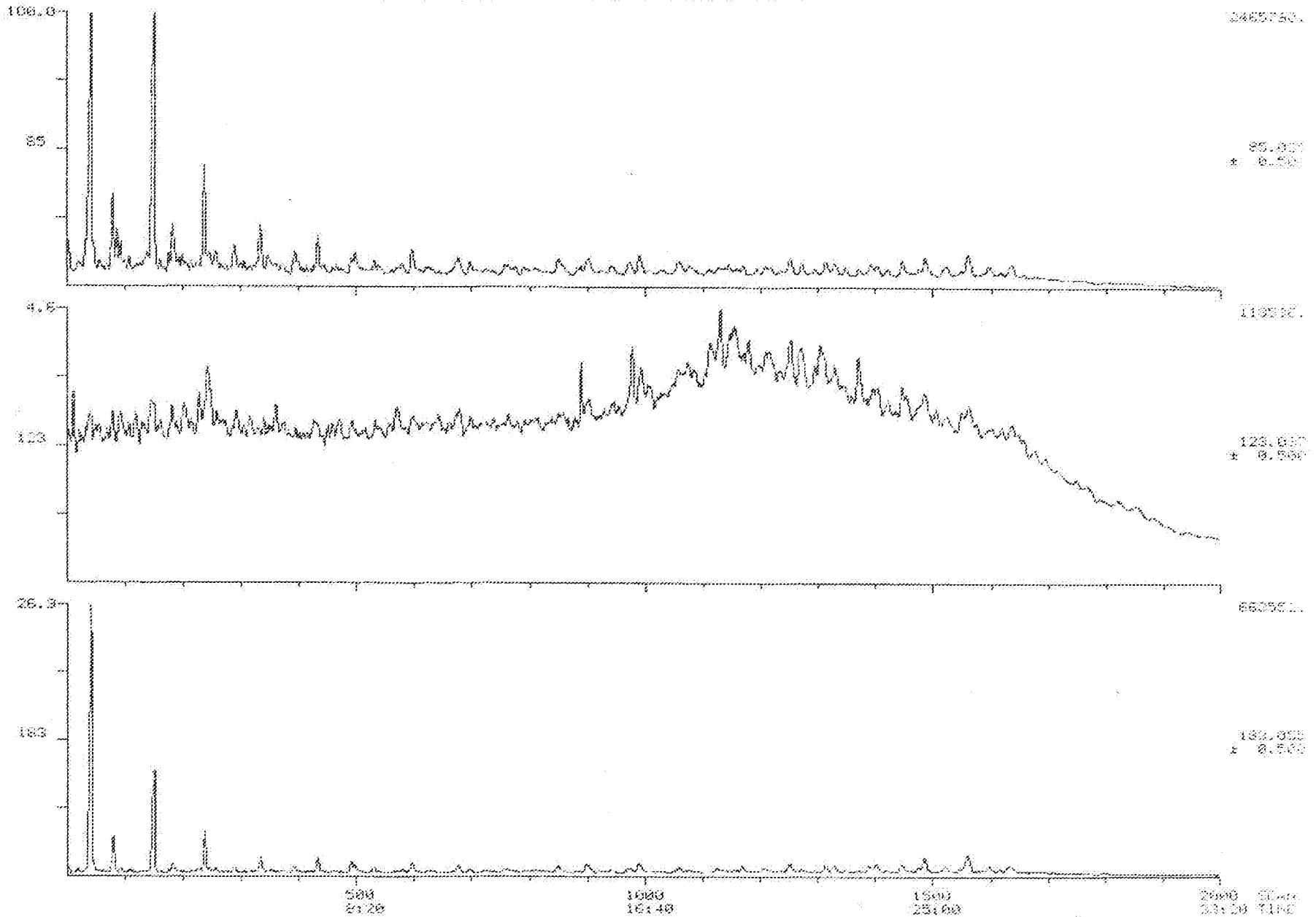
SCANS 1 TO 2000

12/13/91 16:18:00

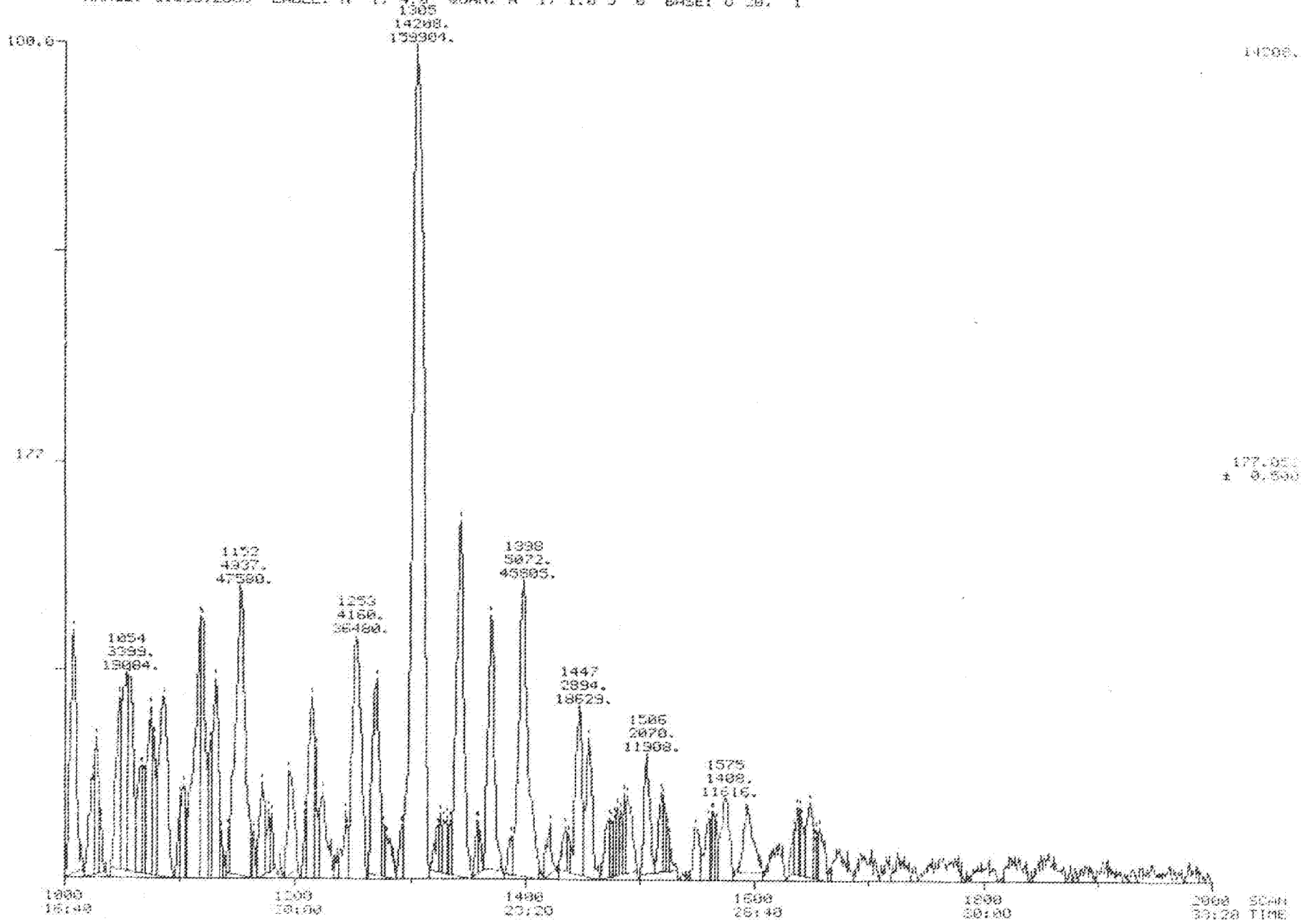
SAMPLE: 91M 4 BRANCH CYCLIC PHILLIPS 2/7-275

COND: 20.1 30/M 138.6 5/M 320.00

RANGE: C 1/2000 LABEL: H 0. 4.0 DURR: A 0. 1.0 J 0 BASE: J 20. 3



MICRASS CHROMATOGRAM DATA: 91M48C #1 SCANS 1000 TO 2000
 12/10/91 18:18:00 CALI: 0131291 #2
 SAMPLE: BIN 4 BRANCH CYCLO PHILLIPS 2/7-275
 COND.: 20.1 38.4 130.8 5.4M 300.20
 RANGE: 01000.2000 LABEL: N 1. 4. 9 QUAN: A 1. 1.0 J 0 BASE: U 00. 1



14005

177.020
± 0.500

1000 15:40 1000 20:00 1400 20:20 1500 25:40 1800 30:00 2000 SCAN 30:20 TIME

Reference No.	Retention time (min:s)	21:45	Low Mass	High Mass	Scan	Time	Meth	Area	Height	Name	Num
1	176.55	177.55	1058	16:48	A	BB	25888	4154	---	---	0.
2	176.55	177.55	1028	17:05	A	BV	9013	1752	---	---	0.
3	176.55	177.55	1028	17:08	A	VV	7635	2344	---	---	0.
4	176.55	177.55	1031	17:11	A	VB	3160	1431	---	---	0.
5	176.55	177.55	1048	17:28	A	BV	14507	2965	---	---	0.
6	176.55	177.55	1054	17:34	A	VV	19084	3399	---	---	0.
7	176.55	177.55	1054	17:36	A	VV	16593	3340	---	---	0.
8	176.55	177.55	1056	17:46	A	VV	7844	1834	---	---	0.
9	176.55	177.55	1068	17:48	A	VV	7122	1840	---	---	0.
10	176.55	177.55	1075	17:55	A	VV	11913	2885	---	---	0.
11	176.55	177.55	1077	17:57	A	VV	7336	2379	---	---	0.
12	176.55	177.55	1086	18:06	A	VB	26505	3077	---	---	0.
13	176.55	177.55	1100	18:20	A	BV	4032	1408	---	---	0.
14	176.55	177.55	1103	18:23	A	VV	4448	1600	---	---	0.
15	176.55	177.55	1105	18:25	A	VV	2400	1408	---	---	0.
16	176.55	177.55	1117	18:37	A	VV	30304	4480	---	---	0.
17	176.55	177.55	1119	18:39	A	VV	17920	4448	---	---	0.
18	176.55	177.55	1126	18:46	A	VV	3640	2368	---	---	0.
19	176.55	177.55	1131	18:51	A	VV	16896	3424	---	---	0.
20	176.55	177.55	1136	18:56	A	VB	1088	800	---	---	0.
21	176.55	177.55	1142	19:02	A	BV	1515	772	---	---	0.
22	176.55	177.55	1152	19:12	A	VV	47580	4937	---	---	0.
23	176.55	177.55	1162	19:22	A	VV	1567	846	---	---	0.
24	176.55	177.55	1164	19:24	A	VB	1834	789	---	---	0.
25	176.55	177.55	1171	19:31	A	BV	8749	1598	---	---	0.
26	176.55	177.55	1178	19:38	A	VV	3450	1090	---	---	0.
27	176.55	177.55	1180	19:40	A	VB	1338	1009	---	---	0.
28	176.55	177.55	1195	19:55	A	BB	11792	1803	---	---	0.
29	176.55	177.55	1209	20:09	A	BV	3552	1184	---	---	0.
30	176.55	177.55	1214	20:14	A	VV	17312	3104	---	---	0.
31	176.55	177.55	1218	20:18	A	VV	5440	2240	---	---	0.
32	176.55	177.55	1224	20:24	A	VB	10368	1904	---	---	0.
33	176.55	177.55	1245	20:45	A	BV	6112	1152	---	---	0.
34	176.55	177.55	1253	20:53	A	VB	36480	4160	---	---	0.
35	176.55	177.55	1271	21:11	A	BV	25176	3356	---	---	0.
36	176.55	177.55	1277	21:17	A	VV	2408	884	---	---	0.
37	176.55	177.55	1280	21:20	A	VB	4048	704	---	---	0.
38	176.55	177.55	1293	21:33	A	BV	3424	896	---	---	0.
39	176.55	177.55	1305	21:45	A	VB	159904	14208	---	---	0.
40	176.55	177.55	1324	22:04	A	BV	3277	784	---	---	0.
41	176.55	177.55	1327	22:07	A	VV	2488	1021	---	---	0.
42	176.55	177.55	1330	22:10	A	VV	3368	936	---	---	0.
43	176.55	177.55	1333	22:13	A	VV	1706	979	---	---	0.
44	176.55	177.55	1336	22:16	A	VV	2683	925	---	---	0.
45	176.55	177.55	1344	22:24	A	VB	43535	6075	---	---	0.
46	176.55	177.55	1358	22:38	A	BV	2418	917	---	---	0.
47	176.55	177.55	1360	22:40	A	VB	2126	889	---	---	0.
48	176.55	177.55	1370	22:50	A	BB	29056	4363	---	---	0.
49	176.55	177.55	1388	23:08	A	BV	2371	656	---	---	0.
50	176.55	177.55	1398	23:18	A	VB	45805	5072	---	---	0.
51	176.55	177.55	1422	23:42	A	BB	4352	873	---	---	0.
52	176.55	177.55	1435	23:55	A	BV	3008	759	---	---	0.
53	176.55	177.55	1438	23:58	A	VV	1915	648	---	---	0.
54	176.55	177.55	1447	24:07	A	VV	18629	2894	---	---	0.
55	176.55	177.55	1455	24:15	A	VB	15200	2386	---	---	0.

Reference retention time (min): 21.45

No	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num
56	176.55	177.55	1473	24:33	A BV	5830	1017	---	0
57	176.55	177.55	1475	24:35	A VV	1850	976	---	0
58	176.55	177.55	1478	24:38	A VV	2947	1057	---	0
59	176.55	177.55	1481	24:41	A VV	3159	1170	---	0
60	176.55	177.55	1484	24:44	A VV	2956	1092	---	0
61	176.55	177.55	1487	24:47	A VV	3648	1365	---	0
62	176.55	177.55	1489	24:49	A VB	7322	1324	---	0
63	176.55	177.55	1506	25:06	A BV	11908	2070	---	0
64	176.55	177.55	1519	25:19	A VV	5568	1372	---	0
65	176.55	177.55	1521	25:21	A VV	3892	1304	---	0
66	176.55	177.55	1525	25:25	A VV	1246	752	---	0
67	176.55	177.55	1527	25:27	A VB	1226	588	---	0
68	176.55	177.55	1549	25:49	A BV	5728	896	---	0
69	176.55	177.55	1561	26:01	A VV	6400	1056	---	0
70	176.55	177.55	1563	26:03	A VV	2272	1184	---	0
71	176.55	177.55	1565	26:05	A VV	2208	1184	---	0
72	176.55	177.55	1567	26:07	A VV	2560	1024	---	0
73	176.55	177.55	1575	26:15	A VB	11616	1408	---	0
74	176.55	177.55	1594	26:34	A BB	11040	1184	---	0
75	176.55	177.55	1634	27:14	A BV	2680	783	---	0
76	176.55	177.55	1638	27:18	A VV	4177	1182	---	0
77	176.55	177.55	1640	27:20	A VV	2159	1158	---	0
78	176.55	177.55	1642	27:22	A VV	2419	1005	---	0
79	176.55	177.55	1649	27:29	A VV	8141	1288	---	0
80	176.55	177.55	1653	27:33	A VV	1329	695	---	0
81	176.55	177.55	1655	27:35	A VV	1600	830	---	0
82	176.55	177.55	1658	27:38	A VB	4631	873	---	0

MIDRACS CHROMATOGRAM

DATA: 91M48C #1
CALI: C131291 #2

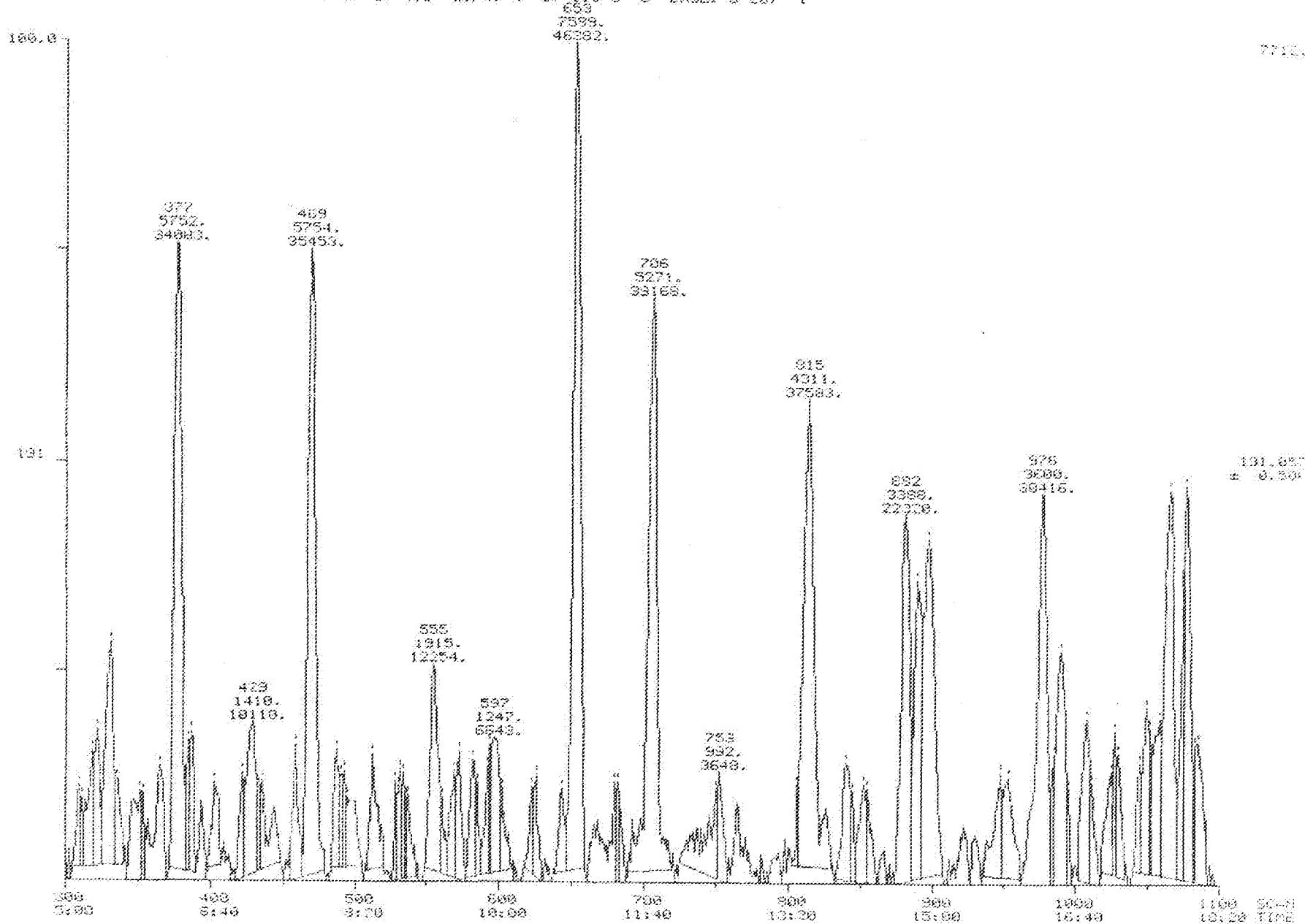
SCANS 300 TO 1100

12/13/91 16:16:00

SAMPLE: 91M 4 BRANCH CYCLIC PHILLIPS 2/7-27S

COND.: 20.1 30/N 130.0 5/M 300.20

RANGE: C 300.1100 LABEL: M 1, 4.2 QUAN: A 1, 1.0 J 0 BASE: U 20, 1



Reference retention time (min.s)				10:53					
No.	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num
1	190.56	191.56	310	5:10	A BV	2743	750	---	0
2	190.56	191.56	312	5:12	A VV	1301	637	---	0
3	190.56	191.56	319	5:19	A VV	5275	1066	---	0
4	190.56	191.56	322	5:22	A VV	5215	1256	---	0
5	190.56	191.56	331	5:31	A VV	12680	2052	---	0
6	190.56	191.56	336	5:36	A VB	2759	802	---	0
7	190.56	191.56	352	5:52	A BV	6576	832	---	0
8	190.56	191.56	354	5:54	A VV	1056	800	---	0
9	190.56	191.56	366	6:06	A VB	6800	1072	---	0
10	190.56	191.56	377	6:17	A BV	34023	5752	---	0
11	190.56	191.56	385	6:25	A VV	2349	1222	---	0
12	190.56	191.56	387	6:27	A VB	3535	1289	---	0
13	190.56	191.56	403	6:43	A BB	3920	777	---	0
14	190.56	191.56	423	7:03	A BV	4153	980	---	0
15	190.56	191.56	429	7:09	A VV	10110	1410	---	0
16	190.56	191.56	434	7:14	A VV	1525	773	---	0
17	190.56	191.56	438	7:16	A VB	4931	826	---	0
18	190.56	191.56	459	7:39	A BV	5155	1249	---	0
19	190.56	191.56	469	7:49	A VB	35453	5754	---	0
20	190.56	191.56	487	8:07	A BV	5217	1066	---	0
21	190.56	191.56	491	8:11	A VV	1635	859	---	0
22	190.56	191.56	493	8:13	A VV	1522	889	---	0
23	190.56	191.56	495	8:15	A VB	5008	648	---	0
24	190.56	191.56	513	8:33	A BB	6200	1072	---	0
25	190.56	191.56	529	8:49	A BV	2372	920	---	0
26	190.56	191.56	532	8:52	A VV	2669	1023	---	0
27	190.56	191.56	534	8:54	A VV	1744	985	---	0
28	190.56	191.56	536	8:56	A VV	1477	756	---	0
29	190.56	191.56	538	8:58	A VB	2106	766	---	0
30	190.56	191.56	555	9:15	A BV	12254	1915	---	0
31	190.56	191.56	561	9:21	A VV	2176	711	---	0
32	190.56	191.56	570	9:30	A VV	4679	992	---	0
33	190.56	191.56	573	9:33	A VB	3755	1182	---	0
34	190.56	191.56	582	9:42	A BV	4394	1094	---	0
35	190.56	191.56	585	9:45	A VV	2008	862	---	0
36	190.56	191.56	592	9:52	A VV	3032	1004	---	0
37	190.56	191.56	594	9:54	A VV	2363	1191	---	0
38	190.56	191.56	597	9:57	A VV	6443	1247	---	0
39	190.56	191.56	602	10:02	A VB	2824	770	---	0
40	190.56	191.56	623	10:23	A BV	2351	799	---	0
41	190.56	191.56	626	10:26	A VB	3089	945	---	0
42	190.56	191.56	644	10:44	A BV	3810	769	---	0
43	190.56	191.56	653	10:53	A VB	45382	7599	---	0
44	190.56	191.56	680	11:20	A BV	5272	928	---	0
45	190.56	191.56	682	11:22	A VV	1680	928	---	0
46	190.56	191.56	684	11:24	A VB	2096	784	---	0
47	190.56	191.56	706	11:46	A BB	39168	5271	---	0
48	190.56	191.56	751	12:31	A BV	9056	321	---	0
49	190.56	191.56	753	12:33	A VB	3648	992	---	0
50	190.56	191.56	807	13:27	A BV	1753	754	---	0
51	190.56	191.56	815	13:35	A VB	37583	4311	---	0
52	190.56	191.56	841	14:01	A BV	6799	1096	---	0
53	190.56	191.56	845	14:05	A VV	2121	829	---	0
54	190.56	191.56	853	14:13	A VV	4848	902	---	0
55	190.56	191.56	956	14:16	A VB	3064	873	---	0

Reference retention time (mins) 10.53									
No.	Low mass	High	Scan	Time	meth	Area	Height	Name	NUM
56	190.56	191.56	882	14.42	A BV	22320.	3388.	---	0.
57	190.56	191.56	890	14.50	A VV	15519.	2756.	---	0.
58	190.56	191.56	898	14.58	A VB	26029.	3117.	---	0.
59	190.56	191.56	948	15.48	A BV	5940.	958.	---	0.
60	190.56	191.56	953	15.53	A VB	7404.	932.	---	0.
61	190.56	191.56	976	16.16	A BV	30416.	3600.	---	0.
62	190.56	191.56	985	16.25	A VV	3200.	1200.	---	0.
63	190.56	191.56	990	16.30	A VV	14800.	2144.	---	0.
64	190.56	191.56	996	16.36	A VB	1228.	896.	---	0.
65	190.56	191.56	1008	16.48	A BV	9280.	1517.	---	0.
66	190.56	191.56	1012	16.52	A VB	2704.	932.	---	0.
67	190.56	191.56	1025	17.05	A BV	4868.	954.	---	0.
68	190.56	191.56	1028	17.08	A VV	3281.	1334.	---	0.
69	190.56	191.56	1030	17.10	A VB	3560.	1133.	---	0.
70	190.56	191.56	1045	17.25	A BV	3571.	1004.	---	0.
71	190.56	191.56	1049	17.29	A VV	6477.	1526.	---	0.
72	190.56	191.56	1052	17.32	A VV	2428.	1341.	---	0.
73	190.56	191.56	1058	17.38	A VV	7695.	1451.	---	0.
74	190.56	191.56	1065	17.45	A VV	26723.	3580.	---	0.
75	190.56	191.56	1075	17.55	A VV	11611.	3285.	---	0.
76	190.56	191.56	1077	17.57	A VV	13948.	3641.	---	0.
77	190.56	191.56	1083	18.03	A VV	2482.	1256.	---	0.
78	190.56	191.56	1086	18.06	A VB	6857.	1295.	---	0.

MIDRANGE CHROMATOGRAM

DATA: SIM480 #1
CALI: C131291 #2

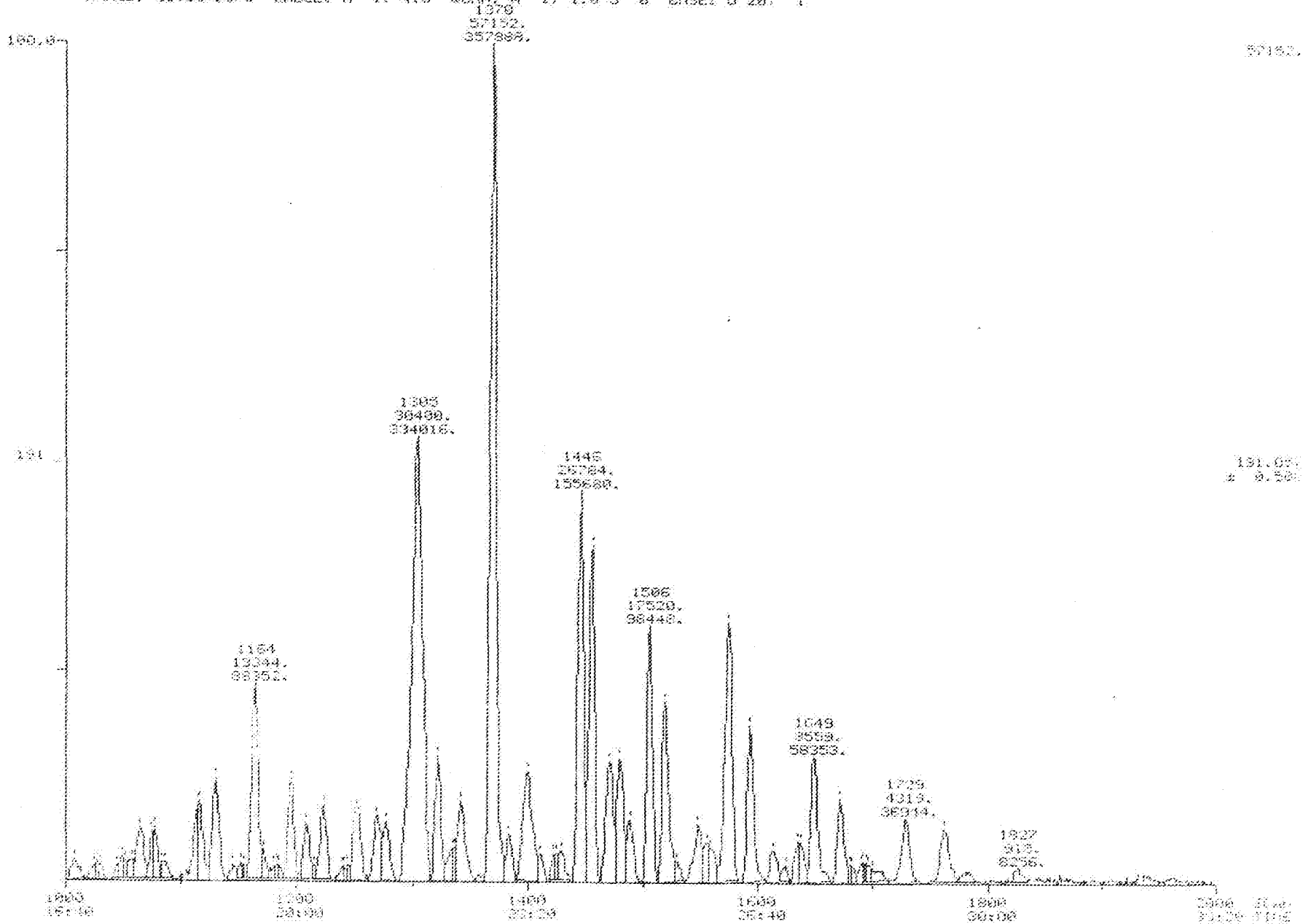
SCANS 1000 TO 2000

12/13/91 16:10:00

SAMPLE: 91M 4 BRANCH CYCLIC PHILIPS 2/7-2/8

COND.: 20.1 30.0 130.0 5/0 200.20

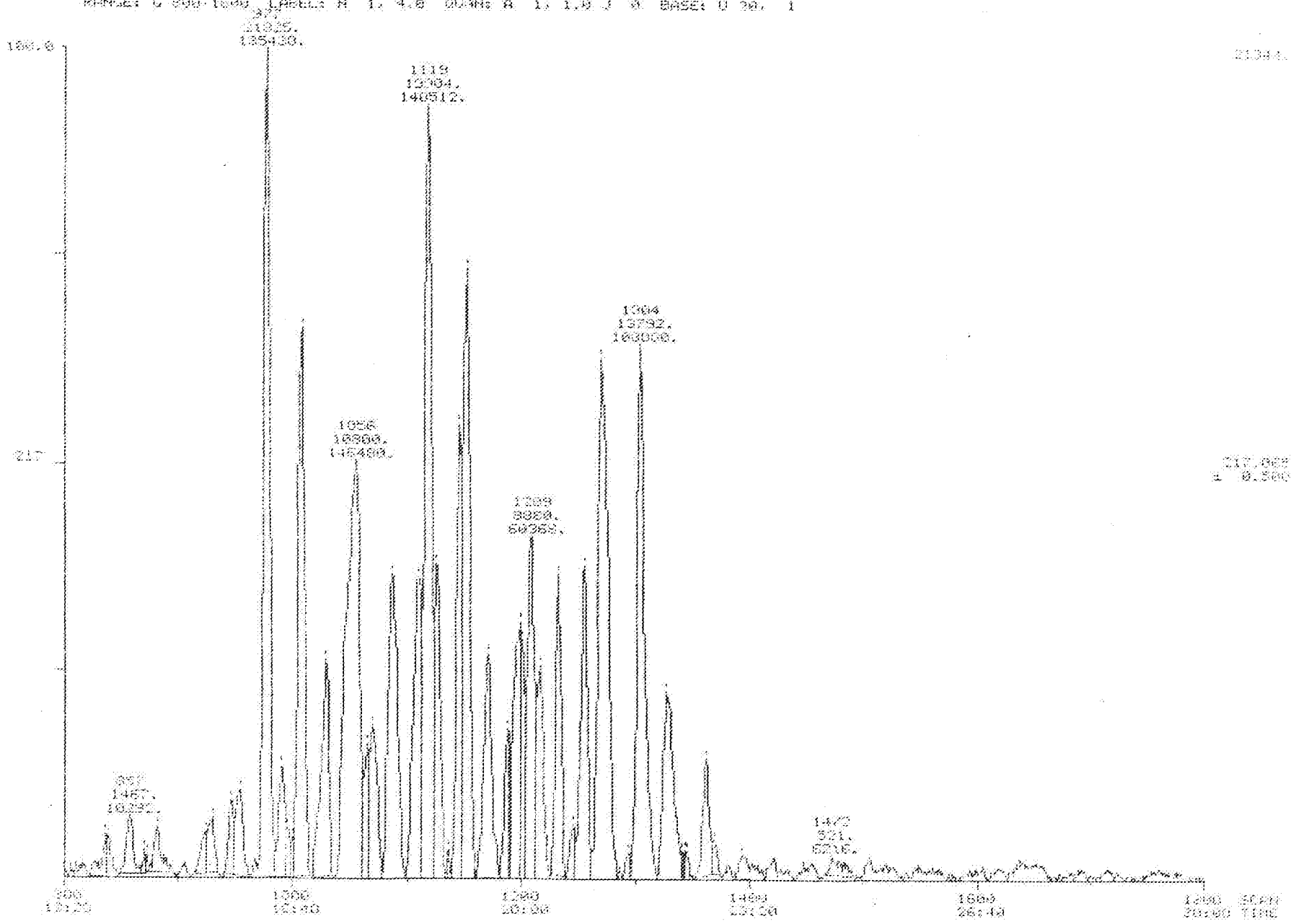
RANGE: 61000-2000 LABEL: N 1. 4.0 QUANT: A 1, 1.0 J 0 GASE: U 20. 1



Reference retention time (min): 22:50									
No.	Low Mass	High	Scan	Time	Math	Area	Height	Name	Num
1	190.56	191.56	1008	16.48	A BV	10092	1431	---	0
2	190.56	191.56	1025	17.05	A BV	4808	954	---	0
3	190.56	191.56	1028	17.08	A VV	2281	1004	---	0
4	190.56	191.56	1030	17.10	A VB	3560	1133	---	0
5	190.56	191.56	1045	17.25	A BV	2453	899	---	0
6	190.56	191.56	1049	17.29	A VV	5913	1413	---	0
7	190.56	191.56	1052	17.32	A VV	2190	1223	---	0
8	190.56	191.56	1058	17.38	A VV	4928	1323	---	0
9	190.56	191.56	1065	17.45	A VV	25016	3439	---	0
10	190.56	191.56	1075	17.55	A VV	10224	3125	---	0
11	190.56	191.56	1077	17.57	A VV	12785	3479	---	0
12	190.56	191.56	1083	18.03	A VV	2103	1082	---	0
13	190.56	191.56	1086	18.06	A VB	5390	1116	---	0
14	190.56	191.56	1114	18.34	A BV	27909	5301	---	0
15	190.56	191.56	1114	18.36	A VV	23852	5491	---	0
16	190.56	191.56	1130	18.50	A VB	45767	7047	---	0
17	190.56	191.56	1145	19.05	A BV	5459	1038	---	0
18	190.56	191.56	1152	19.12	A VV	3840	1166	---	0
19	190.56	191.56	1154	19.14	A VB	901	901	---	0
20	190.56	191.56	1164	19.24	A BV	88382	10344	---	0
21	190.56	191.56	1171	19.31	A VV	7104	1952	---	0
22	190.56	191.56	1180	19.40	A VV	3328	960	---	0
23	190.56	191.56	1183	19.43	A VV	2496	1088	---	0
24	190.56	191.56	1185	19.45	A VV	3040	928	---	0
25	190.56	191.56	1196	19.56	A VB	41216	6816	---	0
26	190.56	191.56	1209	20.09	A BV	22624	3776	---	0
27	190.56	191.56	1216	20.16	A VV	2432	864	---	0
28	190.56	191.56	1224	20.24	A VB	31872	4992	---	0
29	190.56	191.56	1240	20.40	A BV	3674	936	---	0
30	190.56	191.56	1242	20.42	A VV	2369	1034	---	0
31	190.56	191.56	1243	20.45	A VV	2850	1070	---	0
32	190.56	191.56	1252	20.52	A VB	39744	5398	---	0
33	190.56	191.56	1270	21.10	A BV	31680	4481	---	0
34	190.56	191.56	1278	21.18	A VB	26128	4031	---	0
35	190.56	191.56	1305	21.45	A BV	334016	30400	---	0
36	190.56	191.56	1320	22.03	A BV	50826	8496	---	0
37	190.56	191.56	1335	22.15	A VV	13251	2319	---	0
38	190.56	191.56	1337	22.17	A VV	4890	2292	---	0
39	190.56	191.56	1343	22.23	A VB	40873	5443	---	0
40	190.56	191.56	1370	22.50	A BV	357888	57152	---	0
41	190.56	191.56	1384	23.04	A VB	19456	3264	---	0
42	190.56	191.56	1401	23.21	A BV	70556	7386	---	0
43	190.56	191.56	1411	23.31	A VB	8900	1907	---	0
44	190.56	191.56	1423	23.43	A BV	6944	1824	---	0
45	190.56	191.56	1425	23.45	A VV	3520	1824	---	0
46	190.56	191.56	1429	23.49	A VB	12382	1984	---	0
47	190.56	191.56	1446	24.06	A BV	155680	26784	---	0
48	190.56	191.56	1456	24.16	A VB	133664	22072	---	0
49	190.56	191.56	1471	24.31	A BV	64192	8288	---	0
50	190.56	191.56	1480	24.40	A VV	55008	8448	---	0
51	190.56	191.56	1489	24.49	A VB	27360	4256	---	0
52	190.56	191.56	1506	25.06	A BV	98448	17520	---	0
53	190.56	191.56	1519	25.19	A BV	82938	12355	---	0
54	190.56	191.56	1529	25.29	A VB	5398	1341	---	0
55	190.56	191.56	1548	25.48	A BV	21467	3954	---	0

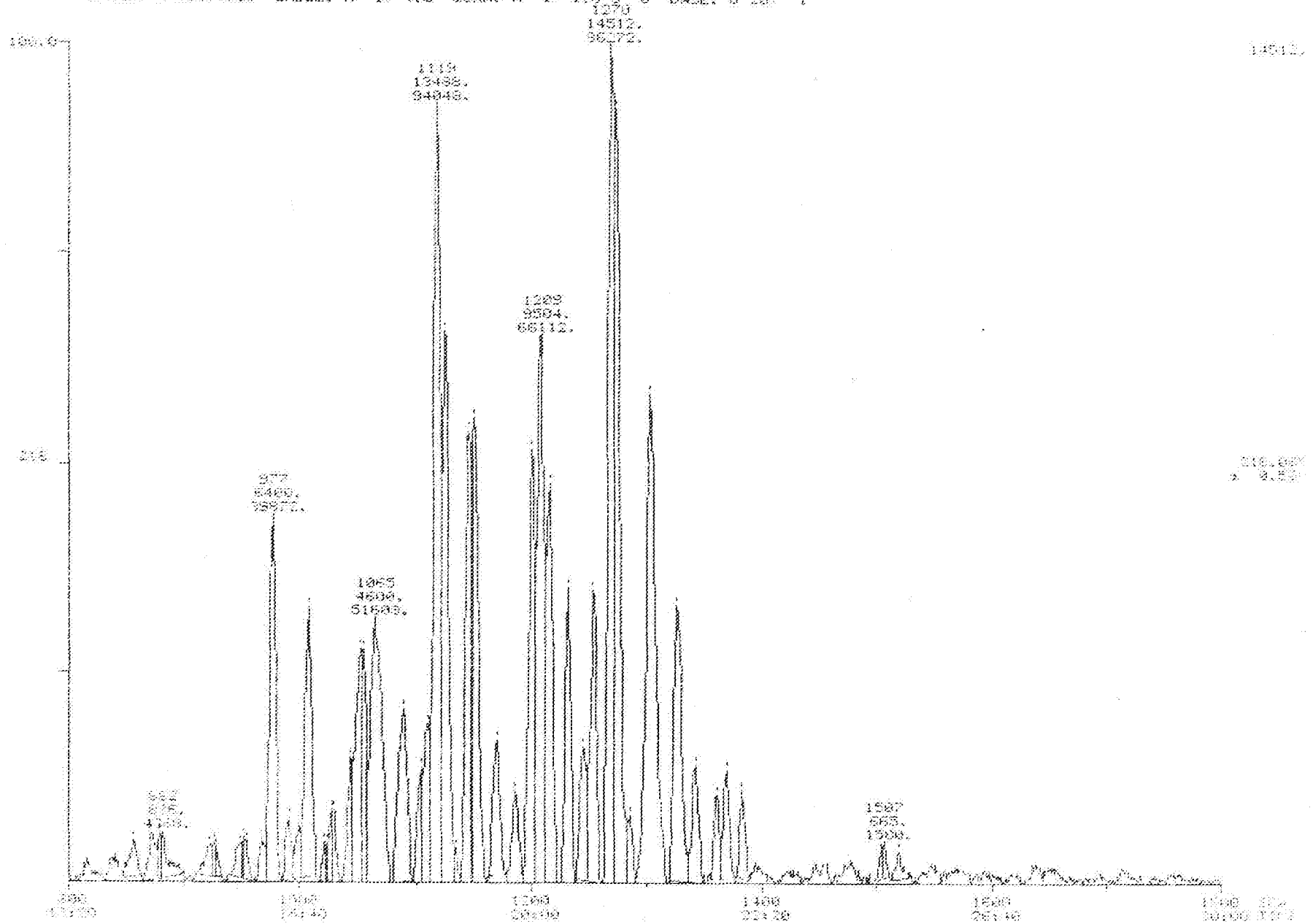
Reference retention time (min.s) 22.50									
No.	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num
56	190.56	191.56	1556	25:50	A VV	15131	2677	---	0.
57	190.56	191.56	1557	25:59	A VV	13030	2340	---	0.
58	190.56	191.56	1575	26:15	A VB	126206	17601	---	0.
59	190.56	191.56	1594	26:34	A BB	86080	10626	---	0.
60	190.56	191.56	1613	26:53	A BV	14833	2136	---	0.
61	190.56	191.56	1624	27:04	A VB	5371	1061	---	0.
62	190.56	191.56	1635	27:15	A BV	13954	2814	---	0.
63	190.56	191.56	1637	27:17	A VV	13261	2739	---	0.
64	190.56	191.56	1649	27:29	A VB	38353	3559	---	0.
65	190.56	191.56	1672	27:52	A BV	39824	3723	---	0.
66	170.56	171.56	1650	28:00	A VV	2235	1264	---	0.
67	190.56	191.56	1682	28:02	A VV	4069	1093	---	0.
68	190.56	191.56	1690	28:10	A VV	4896	1275	---	0.
69	190.56	191.56	1692	28:12	A VV	2587	1424	---	0.
70	190.56	191.56	1694	28:14	A VV	2373	1317	---	0.
71	190.56	191.56	1696	28:16	A VV	3803	1147	---	0.
72	190.56	191.56	1700	28:20	A VB	6931	869	---	0.
73	190.56	191.56	1729	28:49	A BB	38944	4319	---	0.
74	190.56	191.56	1763	29:23	A BB	32360	3512	---	0.
75	190.56	191.56	1827	30:27	A BB	8056	913	---	0.

HPLC CHROMATOGRAM DATA: 31M48C #1 SCANS 800 TO 1800
 12/13/81 16:10:00 CALI: C131291 #2
 SAMPLE: 31M 4 BRANCH CYCLO PHILLIPS 2-7-275
 CONDS.: 20.1 30.4 130.0 3.4 300.20
 RANGE: 0 999-1000 LABEL: H 1. 4.0 QUAN: A 1. 1.0 J 0. BASE: U 20. 1



Reference		Retention time (min:s)		17.D6						
No.	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num	
1	218.57	217.57	837	10:57	A BV	7030	1133	---	0.	
2	218.57	217.57	839	10:59	A VR	4827	1071	---	0.	
3	218.57	217.57	887	14:17	A BV	10292	1467	---	0.	
4	218.57	217.57	871	14:31	A VV	1872	609	---	0.	
5	218.57	217.57	873	14:33	A VV	508	312	---	0.	
6	218.57	217.57	882	14:42	A VB	8647	1202	---	0.	
7	218.57	217.57	924	15:24	A BV	8688	1094	---	0.	
8	218.57	217.57	930	15:30	A VB	9050	1434	---	0.	
9	218.57	217.57	948	15:46	A BV	10071	1686	---	0.	
10	218.57	217.57	954	15:54	A VB	18581	2239	---	0.	
11	218.57	217.57	977	16:17	A BV	135430	21325	---	0.	
12	218.57	217.57	990	16:30	A VV	18752	2873	---	0.	
13	218.57	217.57	996	16:36	A VV	4276	1263	---	0.	
14	218.57	217.57	1000	16:40	A VV	1793	1033	---	0.	
15	218.57	217.57	1038	16:48	A VB	92325	14109	---	0.	
16	218.57	217.57	1029	17:09	A BB	44736	5596	---	0.	
17	218.57	217.57	1056	17:36	A BV	148480	10800	---	0.	
18	218.57	217.57	1066	17:48	A VV	15600	3472	---	0.	
19	218.57	217.57	1070	17:50	A VR	28784	3952	---	0.	
20	218.57	217.57	1087	18:07	A BB	74416	7888	---	0.	
21	218.57	217.57	1110	18:30	A BV	67440	7808	---	0.	
22	218.57	217.57	1119	18:39	A VV	140512	15904	---	0.	
23	218.57	217.57	1126	18:48	A VB	44016	8128	---	0.	
24	218.57	217.57	1137	18:57	A BB	1416	660	---	0.	
25	218.57	217.57	1146	19:06	A BV	60832	11712	---	0.	
26	218.57	217.57	1152	19:12	A VB	102192	15712	---	0.	
27	218.57	217.57	1171	19:31	A BB	48208	9758	---	0.	
28	218.57	217.57	1188	19:48	A BV	15856	3856	---	0.	
29	218.57	217.57	1190	19:50	A VV	7024	3584	---	0.	
30	218.57	217.57	1199	19:59	A VV	49456	8656	---	0.	
31	218.57	217.57	1201	20:01	A VV	21232	6176	---	0.	
32	218.57	217.57	1209	20:09	A VV	60268	8880	---	0.	
33	218.57	217.57	1216	20:16	A VB	33808	5836	---	0.	
34	218.57	217.57	1232	20:32	A BB	42768	7768	---	0.	
35	218.57	217.57	1249	20:45	A BV	8896	1440	---	0.	
36	218.57	217.57	1255	20:55	A VV	56304	8096	---	0.	
37	218.57	217.57	1270	21:10	A VB	135200	13424	---	0.	
38	218.57	217.57	1294	21:34	A BV	2912	704	---	0.	
39	218.57	217.57	1275	21:36	A VV	1050	688	---	0.	
40	218.57	217.57	1304	21:44	A VB	108080	13792	---	0.	
41	218.57	217.57	1327	22:07	A BV	51760	4816	---	0.	
42	218.57	217.57	1341	22:21	A VV	1424	736	---	0.	
43	218.57	217.57	1343	22:23	A VV	1408	752	---	0.	
44	218.57	217.57	1345	22:25	A VB	1632	720	---	0.	
45	218.57	217.57	1362	22:42	A BV	19408	2990	---	0.	
46	218.57	217.57	1364	22:49	A VB	4368	894	---	0.	
47	218.57	217.57	1394	23:14	A BB	8576	615	---	0.	
48	218.57	217.57	1472	24:02	A BB	6216	521	---	0.	

HYDRASS CHROMATOGRAM DATA: SIM480 #1 SCANS 500 TO 1000
 12/10/91 16:10:30 CALI: 0131291 #2
 SAMPLE: 91A 4 BRANCH CYCLIC PHILLIPS 377-275
 COND: 20.1 100-H 130.0 5.0 300.20
 RANGE: 0 500 1000 LABEL: N 1 4.0 CURR: A 1 1.0 J 0 BASE: U 20 1



Reference retention time (min.s) 18.07

No	Low Mass	High	Scan	Time	Math	Area	Height	Name	Num
1	217.57	218.57	856	14.15	A BB	4608.	647.	---	0.
2	217.57	218.57	872	14.32	A BV	6279.	835.	---	0.
3	217.57	218.57	879	14.39	A VV	2581.	331.	---	0.
4	217.57	218.57	882	14.42	A VB	4368.	536.	---	0.
5	217.57	218.57	922	15.22	A BV	4090.	361.	---	0.
6	217.57	218.57	926	15.25	A VV	1575.	373.	---	0.
7	217.57	218.57	928	15.28	A VB	1395.	513.	---	0.
8	217.57	218.57	949	15.49	A BV	3828.	606.	---	0.
9	217.57	218.57	951	15.51	A VV	1335.	746.	---	0.
10	217.57	218.57	954	15.54	A VB	2539.	683.	---	0.
11	217.57	218.57	968	16.08	A BV	4504.	808.	---	0.
12	217.57	218.57	977	16.17	A VB	39872.	6400.	---	0.
13	217.57	218.57	991	16.31	A BV	6348.	1106.	---	0.
14	217.57	218.57	1000	16.40	A VV	4325.	946.	---	0.
15	217.57	218.57	1008	16.48	A VB	31970.	4671.	---	0.
16	217.57	218.57	1022	17.02	A BV	2548.	696.	---	0.
17	217.57	218.57	1024	17.04	A VV	1376.	499.	---	0.
18	217.57	218.57	1028	17.08	A VV	4440.	1267.	---	0.
19	217.57	218.57	1030	17.10	A VB	3780.	1271.	---	0.
20	217.57	218.57	1045	17.35	A BV	10656.	2168.	---	0.
21	217.57	218.57	1053	17.33	A VV	25652.	4056.	---	0.
22	217.57	218.57	1055	17.35	A VV	15038.	4040.	---	0.
23	217.57	218.57	1065	17.45	A VB	51608.	4800.	---	0.
24	217.57	218.57	1090	18.10	A BB	27216.	3006.	---	0.
25	217.57	218.57	1105	18.25	A BV	10096.	2000.	---	0.
26	217.57	218.57	1111	18.31	A VV	14576.	2768.	---	0.
27	217.57	218.57	1119	18.39	A VV	94048.	13486.	---	0.
28	217.57	218.57	1126	18.46	A VV	57104.	9552.	---	0.
29	217.57	218.57	1136	18.56	A VB	1536.	608.	---	0.
30	217.57	218.57	1147	19.07	A BV	42224.	7856.	---	0.
31	217.57	218.57	1149	19.09	A VV	15392.	7744.	---	0.
32	217.57	218.57	1151	19.11	A VB	38840.	8048.	---	0.
33	217.57	218.57	1171	19.31	A BB	16688.	2356.	---	0.
34	217.57	218.57	1187	19.47	A BB	10736.	1616.	---	0.
35	217.57	218.57	1201	20.01	A BV	45392.	7936.	---	0.
36	217.57	218.57	1209	20.09	A VV	66112.	9504.	---	0.
37	217.57	218.57	1216	20.16	A VB	39680.	6760.	---	0.
38	217.57	218.57	1232	20.32	A BB	28480.	5136.	---	0.
39	217.57	218.57	1245	20.45	A BV	17688.	2216.	---	0.
40	217.57	218.57	1254	20.54	A VB	30108.	5057.	---	0.
41	217.57	218.57	1270	21.10	A BV	86272.	14512.	---	0.
42	217.57	218.57	1273	21.13	A VV	71416.	13992.	---	0.
43	217.57	218.57	1286	21.26	A VB	5152.	1192.	---	0.
44	217.57	218.57	1304	21.44	A BB	82552.	8496.	---	0.
45	217.57	218.57	1327	22.07	A BV	38761.	4780.	---	0.
46	217.57	218.57	1343	22.23	A VB	14007.	2038.	---	0.
47	217.57	218.57	1362	22.42	A BV	8716.	1469.	---	0.
48	217.57	218.57	1376	22.50	A VB	11604.	1883.	---	0.
49	217.57	218.57	1384	22.64	A BB	7912.	1559.	---	0.
50	217.57	218.57	1505	25.05	A BV	2212.	631.	---	0.
51	217.57	218.57	1507	25.07	A VB	1580.	465.	---	0.
52	217.57	218.57	1520	25.20	A BB	3144.	477.	---	0.

MIDRANGE CHROMATOGRAM

DATE: 8/14/80 #1

SCANS 1000 TO 1800

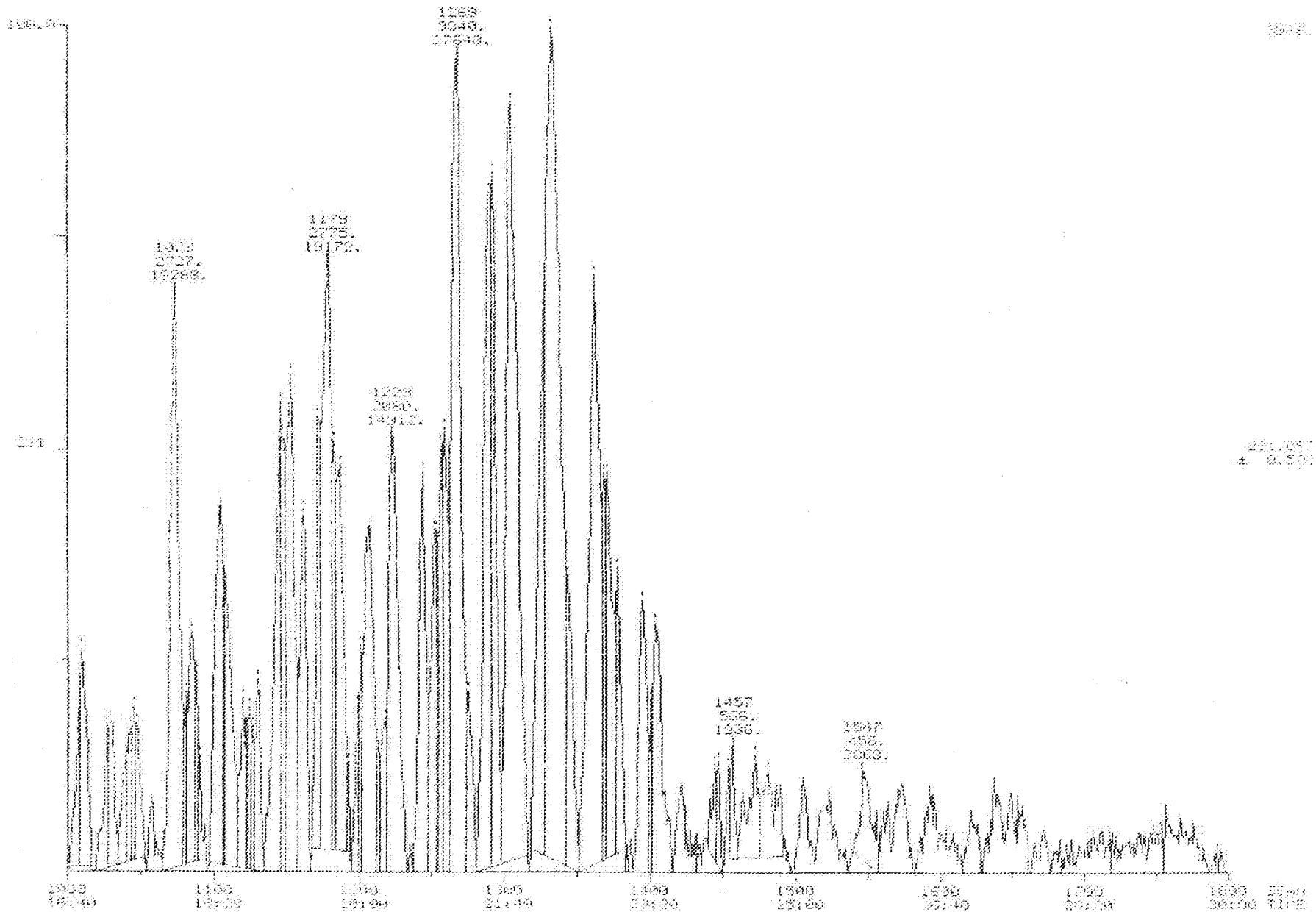
12-13-81 10:10:00

CAL: 0131291 #2

SAMPLE: 21M 4 BRANCH CYCLIC PHILIPS 2-7-275

COND.: 20.1 20.0 130.0 5.0 200.00

RANGE: 01000-1100 LABEL: H 1) 4.2 SUPP: A 1) 1.0 0 0 0002: 0 00: 1



Reference retention time (min): 22:12										
No.	Low Mass	High Mass	Scan	Time	Math	Area	Height	Name	Num	
1	230.57	231.57	1008	16.48	A BV	3400.	324.	---	0.	
2	230.57	231.57	1010	16.50	A VB	4224.	1024.	---	0.	
3	230.57	231.57	1027	17.07	A BV	2679.	673.	---	0.	
4	230.57	231.57	1029	17.09	A VV	2777.	684.	---	0.	
5	230.57	231.57	1040	17.20	A VV	2422.	644.	---	0.	
6	230.57	231.57	1043	17.23	A VV	1729.	630.	---	0.	
7	230.57	231.57	1046	17.25	A VV	1261.	721.	---	0.	
8	230.57	231.57	1047	17.27	A VB	2534.	637.	---	0.	
9	230.57	231.57	1073	17.53	A BV	17288.	2727.	---	0.	
10	230.57	231.57	1081	18.01	A VV	2026.	806.	---	0.	
11	230.57	231.57	1086	18.05	A VV	4795.	1077.	---	0.	
12	230.57	231.57	1088	18.08	A VV	1942.	679.	---	0.	
13	230.57	231.57	1091	18.11	A VB	901.	489.	---	0.	
14	230.57	231.57	1105	18.25	A BV	9721.	1706.	---	0.	
15	230.57	231.57	1107	18.27	A VV	2795.	1485.	---	0.	
16	230.57	231.57	1109	18.29	A VV	6702.	1311.	---	0.	
17	230.57	231.57	1120	18.40	A VV	2317.	797.	---	0.	
18	230.57	231.57	1123	18.43	A VV	1379.	705.	---	0.	
19	230.57	231.57	1125	18.45	A VV	1400.	755.	---	0.	
20	230.57	231.57	1127	18.47	A VV	1131.	678.	---	0.	
21	230.57	231.57	1130	18.50	A VB	3829.	890.	---	0.	
22	230.57	231.57	1146	19.06	A BV	12912.	2192.	---	0.	
23	230.57	231.57	1148	19.08	A VV	5768.	2048.	---	0.	
24	230.57	231.57	1153	19.13	A VV	13808.	2320.	---	0.	
25	230.57	231.57	1162	19.22	A VB	8992.	1896.	---	0.	
26	230.57	231.57	1172	19.32	A BV	6773.	2018.	---	0.	
27	230.57	231.57	1179	19.39	A VV	19172.	2775.	---	0.	
28	230.57	231.57	1183	19.43	A VV	3619.	1910.	---	0.	
29	230.57	231.57	1187	19.47	A VV	10517.	1804.	---	0.	
30	230.57	231.57	1193	19.53	A VB	415.	415.	---	0.	
31	230.57	231.57	1199	19.59	A BV	2160.	784.	---	0.	
32	230.57	231.57	1201	20.01	A VV	2043.	1056.	---	0.	
33	230.57	231.57	1208	20.08	A VV	12172.	1615.	---	0.	
34	230.57	231.57	1213	20.13	A VV	1744.	624.	---	0.	
35	230.57	231.57	1216	20.16	A VV	2888.	720.	---	0.	
36	230.57	231.57	1223	20.23	A VB	14912.	2080.	---	0.	
37	230.57	231.57	1244	20.44	A BV	11280.	1972.	---	0.	
38	230.57	231.57	1252	20.52	A VV	6592.	1600.	---	0.	
39	230.57	231.57	1254	20.54	A VV	2168.	1600.	---	0.	
40	230.57	231.57	1257	20.57	A VV	5520.	2000.	---	0.	
41	230.57	231.57	1259	20.59	A VV	6912.	2080.	---	0.	
42	230.57	231.57	1266	21.08	A VV	27648.	3840.	---	0.	
43	230.57	231.57	1276	21.15	A VB	3504.	848.	---	0.	
44	230.57	231.57	1290	21.30	A BV	18802.	3147.	---	0.	
45	230.57	231.57	1292	21.32	A VV	11664.	3239.	---	0.	
46	230.57	231.57	1305	21.45	A VB	33022.	3529.	---	0.	
47	230.57	231.57	1327	22.07	A BV	14955.	2543.	---	0.	
48	230.57	231.57	1332	22.12	A VV	41634.	2872.	---	0.	
49	230.57	231.57	1344	22.24	A VB	5553.	1368.	---	0.	
50	230.57	231.57	1362	22.42	A BV	24220.	2745.	---	0.	
51	230.57	231.57	1369	22.49	A VV	5137.	1901.	---	0.	
52	230.57	231.57	1371	22.51	A VV	9132.	1902.	---	0.	
53	230.57	231.57	1378	22.58	A VB	3644.	1337.	---	0.	
54	230.57	231.57	1395	23.15	A BV	7720.	1972.	---	0.	
55	230.57	231.57	1401	23.21	A VV	2192.	808.	---	0.	

Reference retention time (min.s) 22.12										
No.	Low	Mass	High	Scan	Time	Meth	Area	Height	Name	Num
56	230	57	231.57	1404	24.24	A VB	7544	1168	--	0
57	230	57	231.57	1445	24.08	A BV	1553	443	--	0
58	230	57	231.57	1447	24.07	A VB	1330	479	--	0
59	230	57	231.57	1454	24.14	A BV	1622	431	--	0
60	230	57	231.57	1457	24.17	A VB	1535	365	--	0
61	230	57	231.57	1472	24.32	A VB	4034	480	--	0
62	230	57	231.57	1481	24.41	A VB	4560	404	--	0
63	230	57	231.57	1547	25.47	A BB	3868	456	--	0

Reference retention time (min):		23.12									
No.	Low	High	Scan	Time	Path	Area	Height	Name	Num		
56	231.57	232.57	1405	23.26	A VB	3446	313	---	0		
57	231.57	232.57	1446	24.08	A BV	5155	602	---	0		
58	231.57	232.57	1454	24.14	A VV	2304	724	---	0		
59	231.57	232.57	1486	24.14	A VB	2652	717	---	0		
60	231.57	232.57	1575	25.15	A BV	2273	433	---	0		
61	231.57	232.57	1577	25.17	A VB	915	394	---	0		

Reference retention time (min's) 18:38									
No.	Low Mass	High	Scan	Time	Meth	Area	Height	Name	Num
56	258.58	259.58	1424	23.44	A VB	3742	459	---	0
57	258.58	259.58	1467	24.27	A BV	1830	448	---	0
58	258.58	259.58	1471	24.31	A VV	1560	460	---	0
59	258.58	259.58	1479	24.39	A VV	4632	696	---	0
60	258.58	259.58	1483	24.43	A VV	1584	584	---	0
61	258.58	259.58	1484	24.46	A VB	3552	576	---	0
62	258.58	259.58	1506	25.06	A BV	2067	396	---	0
63	258.58	259.58	1515	25.15	A VB	4341	455	---	0
64	258.58	259.58	1549	25.49	A BB	5424	360	---	0