BA 85-4012-1

4/12-85

IKU
SINTEF-GRUPPEN

Håkon Magnussonsgt 1 B
P.O.Box 1883 Jarlesletta
N-7001 Trondheim, Norway
Tel.: +47 7 92 06 11

REG. NO.
22.153

ACCESSIBILITY
Confidential

REPORT TITLE/ TITTEL

DATA REPORT

ANALYSIS OF BIOMARKERS IN EXTRACTS

Åpen kontrakt T-4533, Job no. 19

CLIENT/ OPPDRAGSGIVER
Statoil

PROJECT MANAGER/ PROSJEKTANSVARLIG
L. Schou

AUTHORS/ FORFATTERE
L. Schou

DATE/ DATO	REPORT NO./ RAPPORT NR.	NO. OF PAGES/ ANT. SIDER	NO. OF ENCLOSURES/ ANT. BILAG
85.11.12	22.1811.00/01/85	53	-

SUMMARY/ SAMMENDRAG

This data report contains mass chromatograms and tabulated data representative of saturated steranes and terpanes. Six extracts supplied by Statoil were analysed by GC-MS.

KEY WORDS
Biomarkers
GC-MS
Extracts

STIKKORD

149/r/jbl/1

CONTENTS

IKU SINTEF-GRUPPEN

INTRODUCTION

Six extracts were supplied by Statoil for analysis of biomarkers. The weights of some of the samples were reported by Statoil to be very low, and these samples could then be expected to give poor chromatograms. The results of all samples seem, however, to be satisfactory. The sample identities are given below.

IKU Code	Statoil code
C-2888	S-1236
C-2889	S-1237
C-2890	S-1238
C-2891	S-1239
C-2892	S-1240
C-2893	S-1241

The analyses were performed under the Open Contract T-4533, Job no. 19 and the IKU project code 22.1811.

Ten copies of this data report have been sent to Statoil (Att. T. Meyer) and ten copies are stored at IKU.

EXPERIMENTAL

The extracts diluted in n-hexane and analysed on a VG 70-70H mass spectrometer with a DS-11/250 data system. A Varian 3700 GC is interfaced to the mass spectrometer and the GC is equipped with a fused silica capillary column coated with DB no. 5 (30mx0.3 mm i.d.). Split injections were performed (split ratio 1:10) and hydrogen was used as carrier gas. The temperature program was 120°C (2 min.) to 280°C at 4°C/min. The mass spectrometer was operated in EI with 70eV electron energy and an ion source temperature of 200°C. Multiple ion detection (MID) was applied with 80 msec. dwell time per ion.

COMMENTS TO CHROMATOGRAMS AND TABLES

The terpane mass chromatograms (m/z 163, 177, 191) were seen to contain peaks in addition to the commonly seen 17α(H),21β(H)-hopanes. These peaks (U,V,W) have tentatively been identified as C_{27}-C_{29} 25-norhopanes according to Volkman et al (1983). Peak W (25-norhopane) can easily be mistaken for the 28,39-bisnorhopane (Z in m/z 191) from retention time, and thus it is important also to compare both the m/z 163, 177 and the 191 mass chromatograms.

In the sterane mass chromatogram m/z 217 the high intensity of C29 20R 14α(H),17α(H) sterane (t in m/z 217) may be due to coelution with some unknown compound. However, it is possible that the low values of %20S are real, but they seem low compared to the other maturity ratios. This is not possible to verify since the sample amounts are too low for any decent spectra to be acquired.

IKU SINTEF-GRUPPEN

REFERENCE

VOLKMAN, J.K., ALEXANDER, R., KAGI, R.I., RULLKOTTER, J., 1983: GC-MS characterisation of C_{27} and C_{28} triterpanes in sediments and petroleums. Geochim. Cosmochim. Acta., 47, pp. 1033-1040.

Table 1: Molecular ratios calculated from terpane and sterane mass chromatograms. Maturity ratios.

IKU no.	Code	αβ/αβ+βα[1)]	%22S[2)]	%ββ[3)]	%20S[4)]
C-2888	S-1236	0.83	60.9	55.6	18.8
C-2889	S-1237	0.78	56.1	66.0	22.9
C-2890	S-1238	0.91	60.4	80.6	48.0
C-2891	S-1239	0.90	59.1	69.9	34.3
C-2892	S-1240	0.85	57.4	72.1	22.4
C-2893	S-1241	0.89	58.7	68.3	23.0

1) E/E+F in m/z 191
2) % distribution between first and second eluting isomers of doublet G and H (m/z 191)
3) 2(r+s)/(q+t+2(r+s)) in m/z 217
4) q/q+t in m/z 217

Table 2 Molecular ratios calculated from terpane and sterane mass chromatograms. Source characteristic and maturity ratios.

IKU no.	Code	Q/E[1)]	Tm/Ts[2)]	X/E[3)]	a/a+j[4)]	Z/E[5)]
C-2888	S-1236	0.27	3.00	0.02	-	0.40
C-2889	S-1237	0.21	2.50	0.00	-	0.72
C-2890	S-1238	0.18	0.87	0.15	0.91	0.07
C-2891	S-1239	0.02	1.57	0.16	0.57	0.08
C-2892	S-1240	0.19	1.59	0.05	1.00	0.37
C-2893	S-1241	0.14	1.65	0.03	0.61	0.19

1) Relative abundance of tricyclic terpanes (Q/E in m/z 191)
2) B/A in m/z 191
3) Relative abundance of unknown (X/E in m/z 191)
4) Relative abundance of C_{27} rearranged steranes (a/a+j in m/z 217)
5) Relative abundance of bisnorhopane (Z/E in m/z 191)

Table 3 Molecular ratios from terpane mass chromatograms (m/z 191)

IKU no.	Code	U/E[1)]	V/E[2)]	W/E[3)]
C-2888	S-1236	0.22	0.13	0.40
C-2889	S-1237	0.21	0.18	0.69
C-2890	S-1238	0.04	0.12	0.76
C-2891	S-1239	0.02	0.15	0.38
C-2892	S-1240	0.07	0.36	0.36
C-2893	S-1241	0.06	0.18	0.30

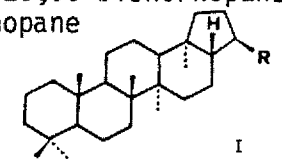
1) Relative intensity of 17α(H),18α(H),21β(H)-25,28,30-trisnorhopane (U/E)
2) Relative intensity of 17α(H)-25,30-bisnorhopane (V/E)
3) Relative intensity of 25-norhopane (W/E)

IKU SINTEF-GRUPPEN

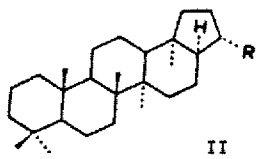
Figure 1a.

Mass chromatograms representing terpanes (m/z 191)

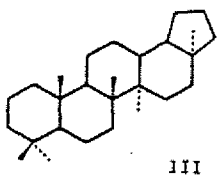
A	T_s, 18α(H)-trisnorneohopane	$C_{27}H_{46}$	(III)
B	T_m, 17α(H)-trisnorhopane	$C_{27}H_{46}$	(I,R=H)
C	17α(H)-norhopane	$C_{29}H_{50}$	(I,R=C_2H_5)
D	17β(H)-normoretane	$C_{29}H_{50}$	(II,R=C_2H_5)
E	17α(H)-hopane	$C_{30}H_{52}$	(I,R=C_3H_7)
F	17β(H)-moretane	$C_{30}H_{52}$	(II,R=C_3H_7)
G	17α(H)-homohopane (22S)	$C_{31}H_{54}$	(I,R=C_4H_9)
H	17α(H)-homohopane (22R) + unknown triterpane (gammacerane?)	$C_{31}H_{54}$	(I,R=C_4H_9)
I	17β(H)-homomoretane	$C_{31}H_{54}$	(II,R=C_4H_9)
J	17α(H)-bishomohopane (22S,22R)	$C_{32}H_{56}$	(I,R=C_5H_{11})
K	17α(H)-trishomohopane (22S,22R)	$C_{33}H_{58}$	(I,R=C_6H_{13})
L	17α(H)-tetrakishomohopane (22S,22R)	$C_{34}H_{60}$	(I,R,=C_7H_{15})
M	17α(H)-pentakishomohopane (22S,22R)	$C_{35}H_{62}$	(I,R=C_8H_{17})
Z	bisnorhopane	$C_{28}H_{48}$	
X	unknown triterpane	$C_{30}H_{52}$	
P	tricyclic terpane	$C_{23}H_{42}$	(IV,R=C_4H_9)
Q	tricyclic terpane	$C_{24}H_{44}$	(IV,R=C_5H_{11})
R	tricyclic terpane (17R,17S)	$C_{25}H_{46}$	(IV,R=C_6H_{13})
S	tetracyclic terpane	$C_{24}H_{42}$	(V)
T	tricyclic terpane (17R,17S)	$C_{26}H_{48}$	(IV,R=C_7H_{15})
U	17α(H), 18α(H),21β(H)-25,28,30-trisnorhopane		
V	17α(H)-25,30-bisnorhopane		
W	25-norhopane		



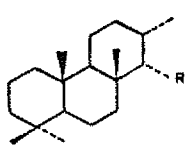
I

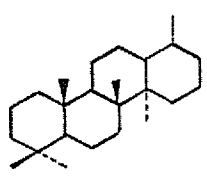


II



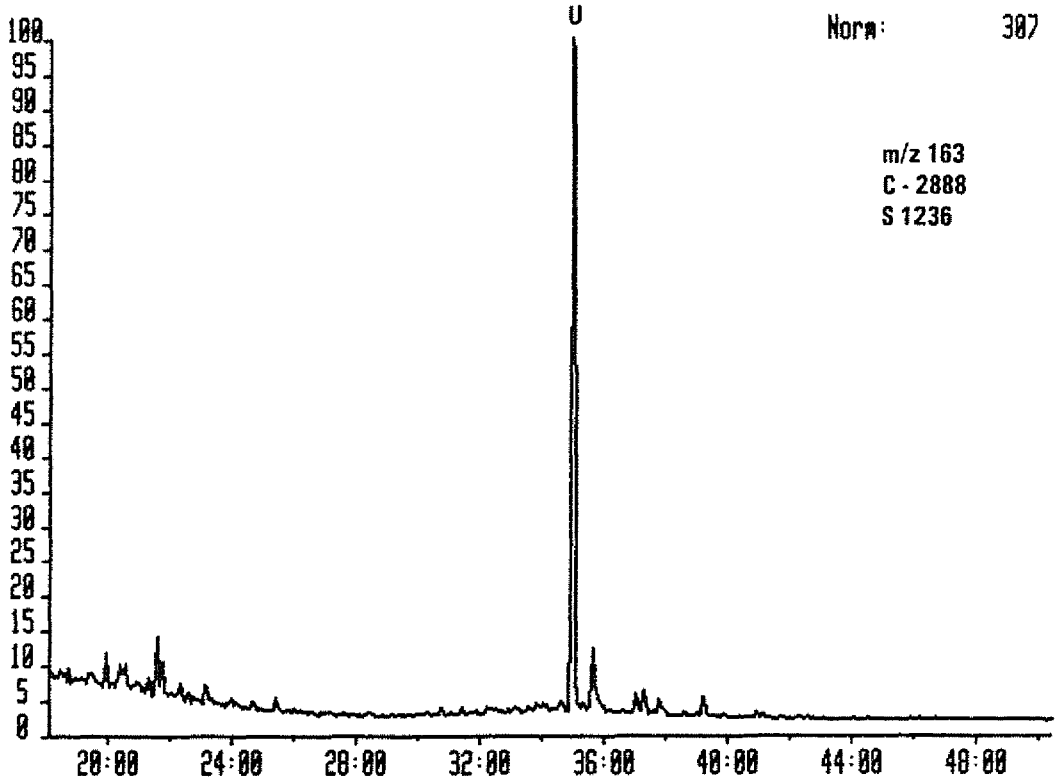
III



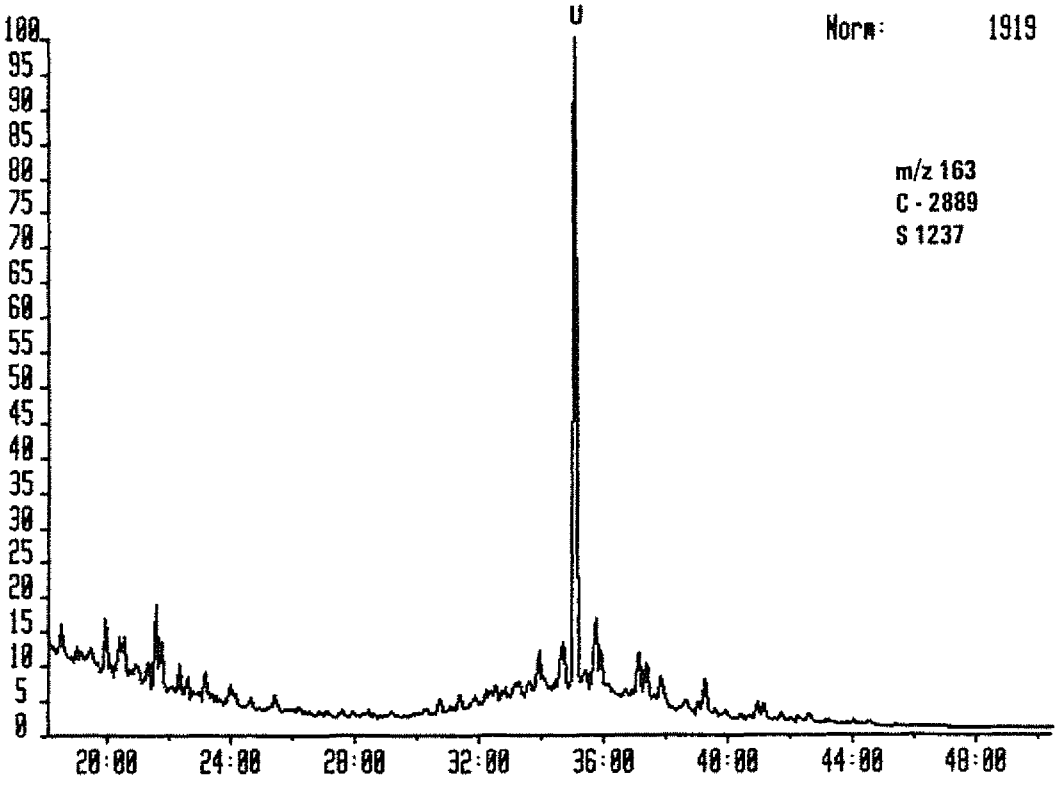


IKU

C2888SAT 30-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 163.1000
Text:

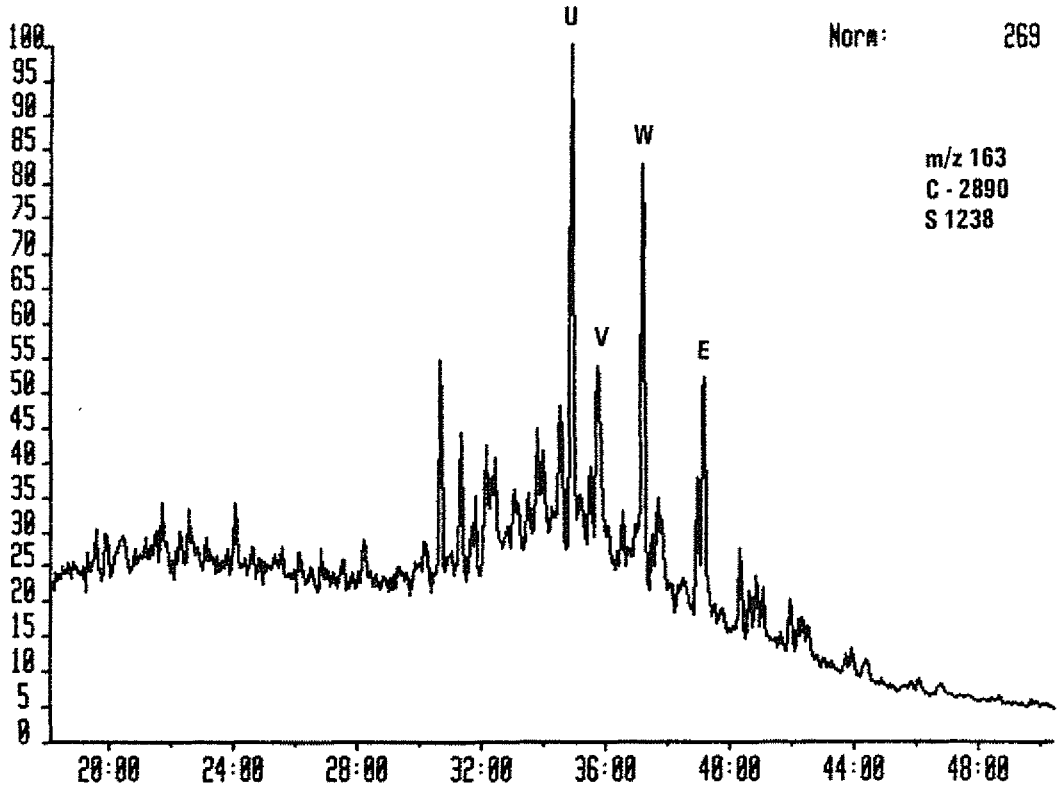


C2889SAT 29-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 163.1000
Text:

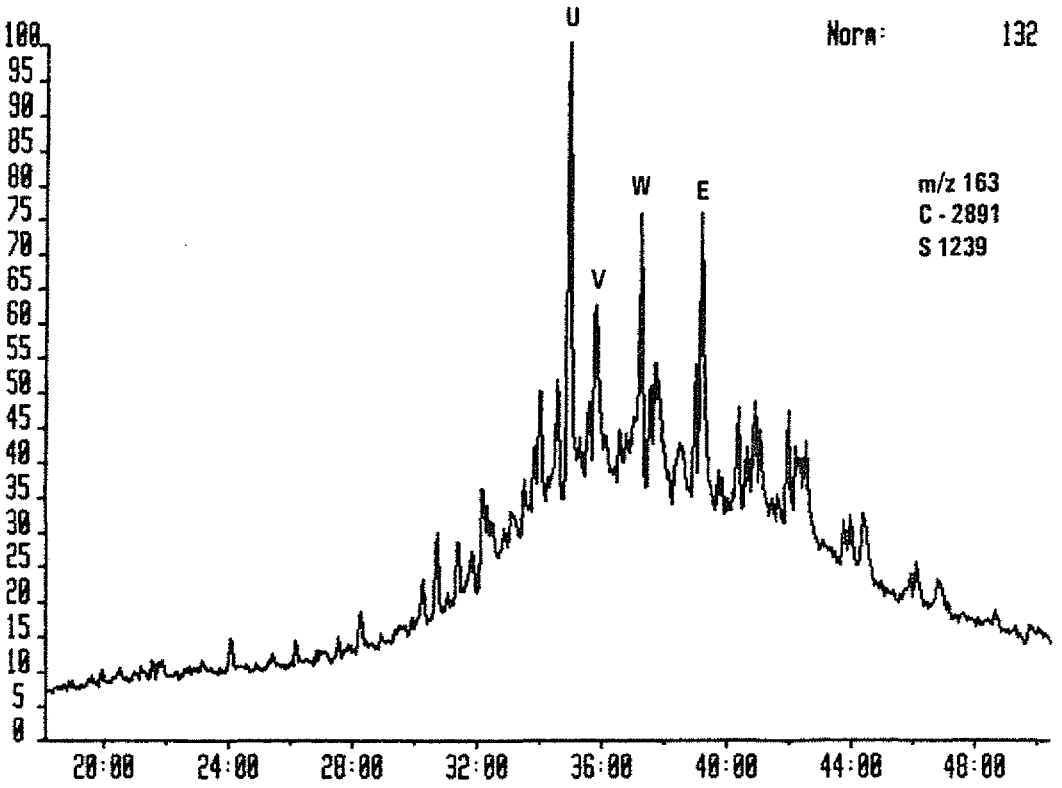


IKU

C2890SAT 29-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 163.1000
Text:

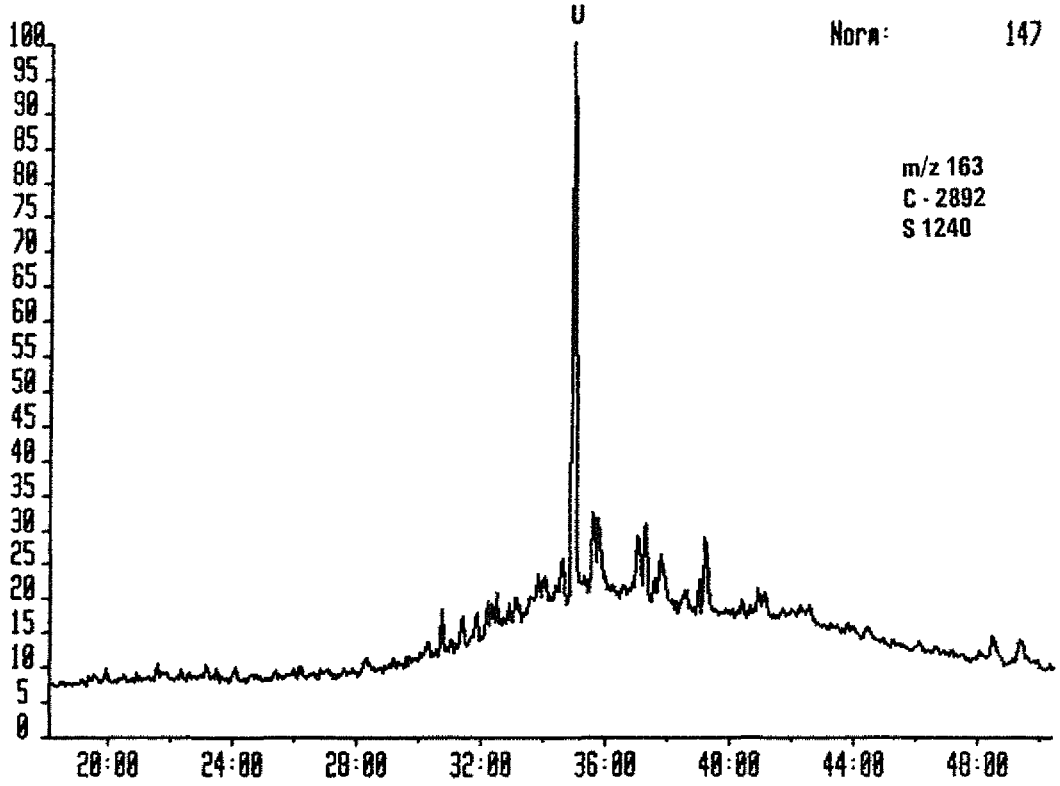


C2891SAT 29-OCT-85 Sir:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 163.1000
Text:

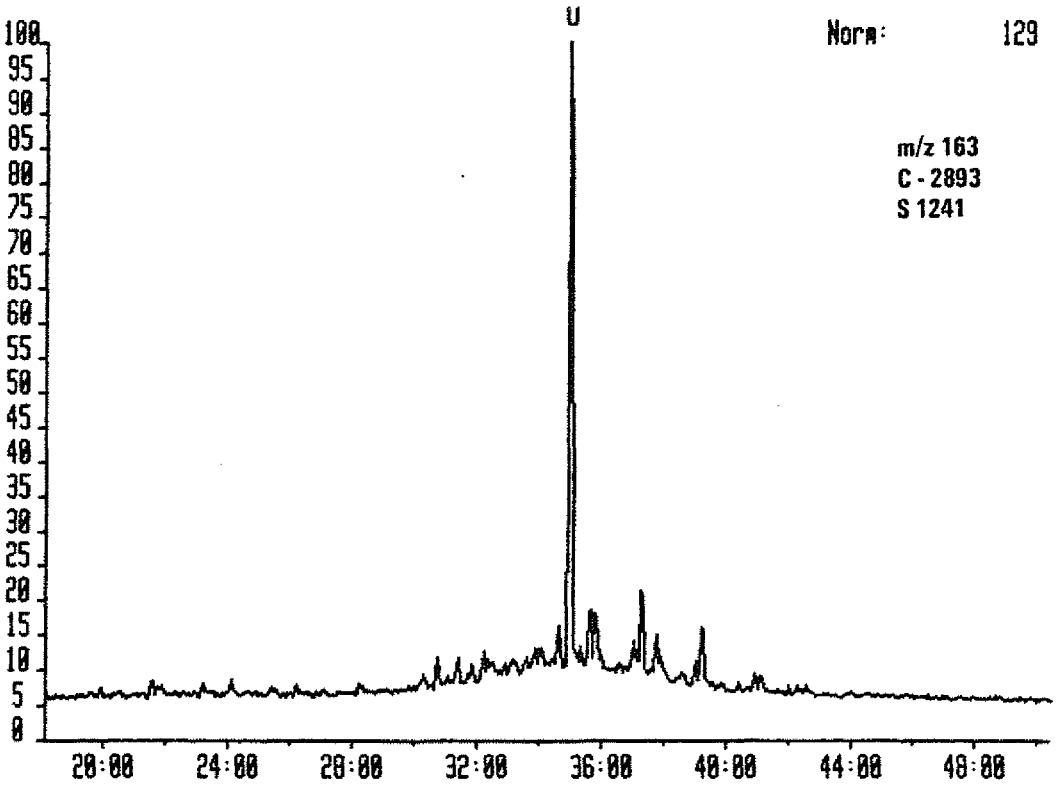


IKU

C2892SAT 29-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 163.1000
Text:

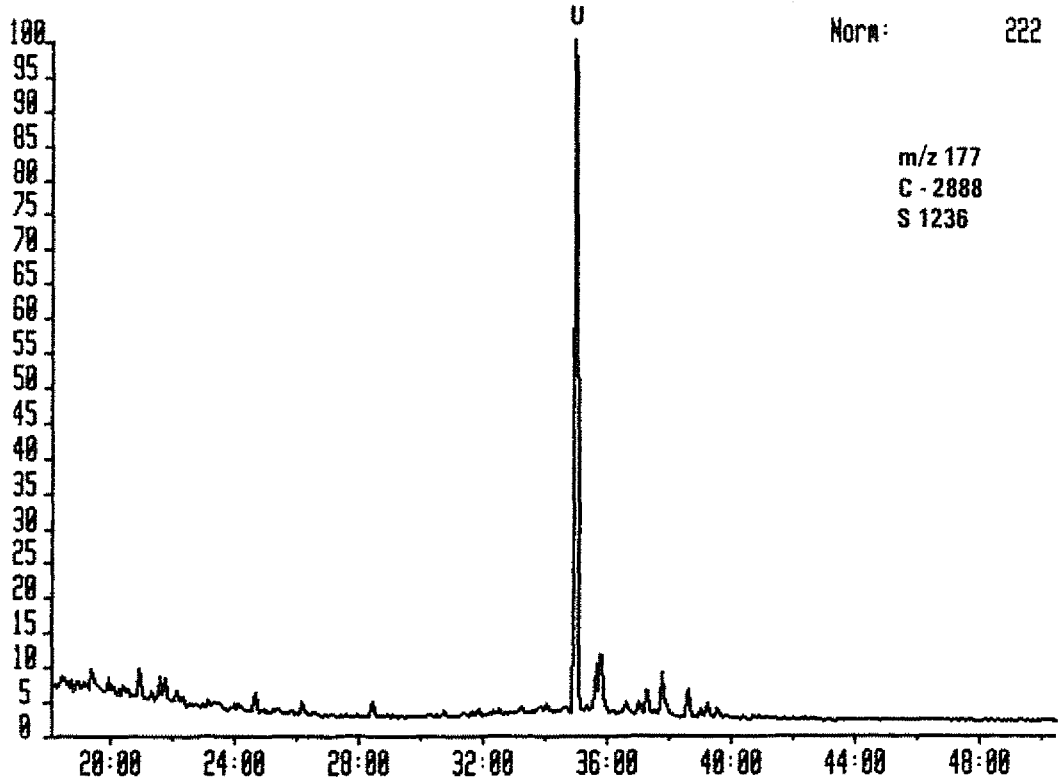


C2893SAT 30-OCT-85 Sir:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 163.1000
Text:

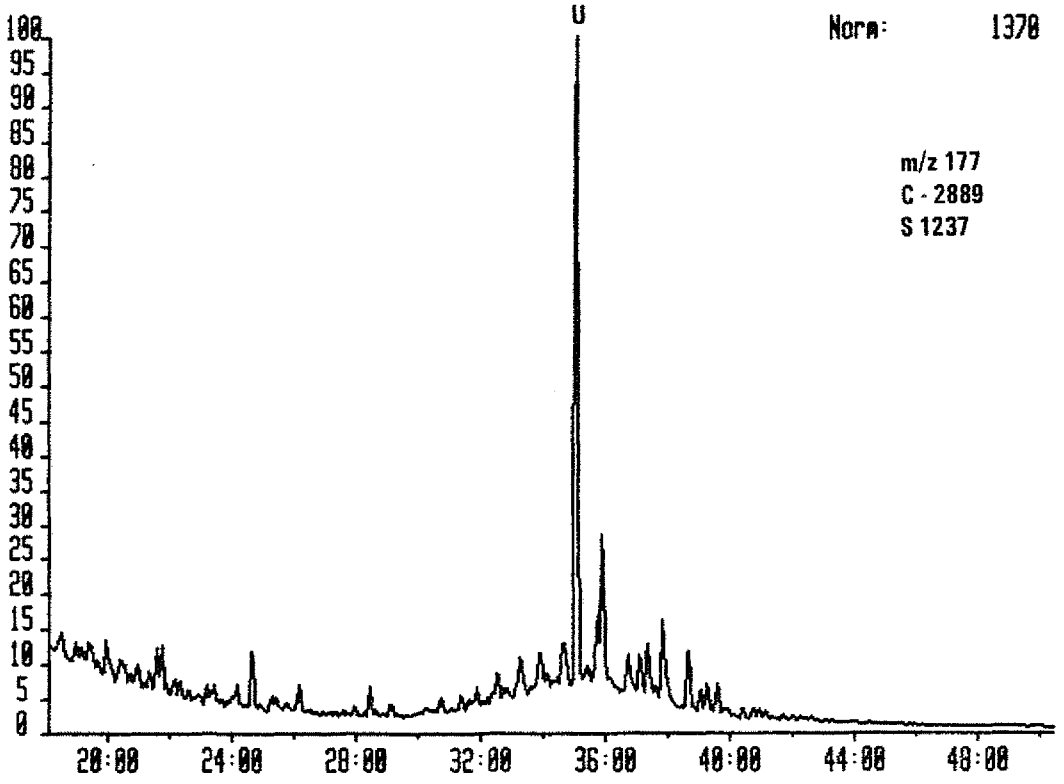


IKU

C2888SAT 30-OCT-85 Sir:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 177.1000
Text:

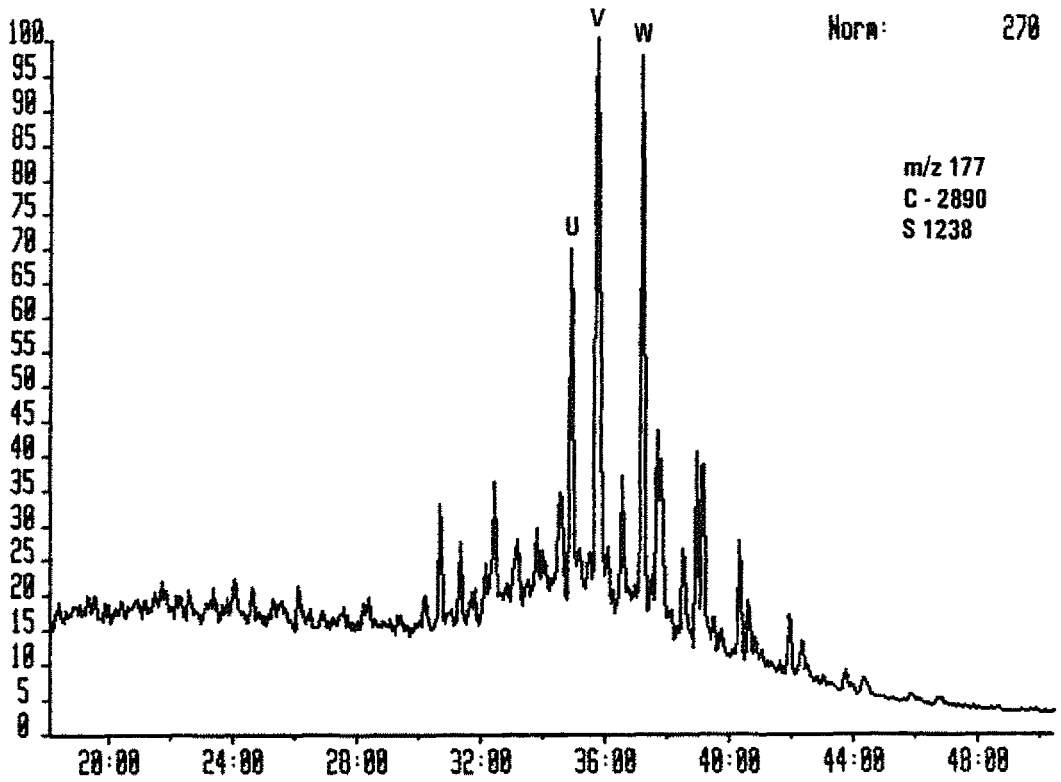


C2889SAT 29-OCT-85 Sir:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 177.1000
Text:

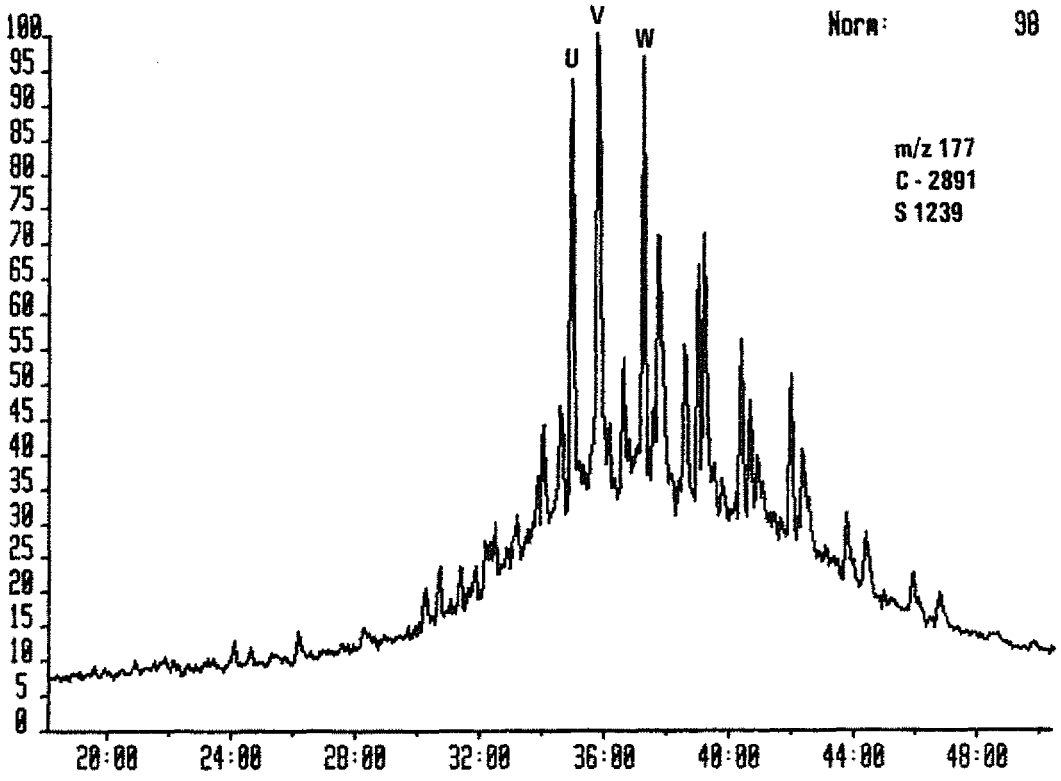


IKU

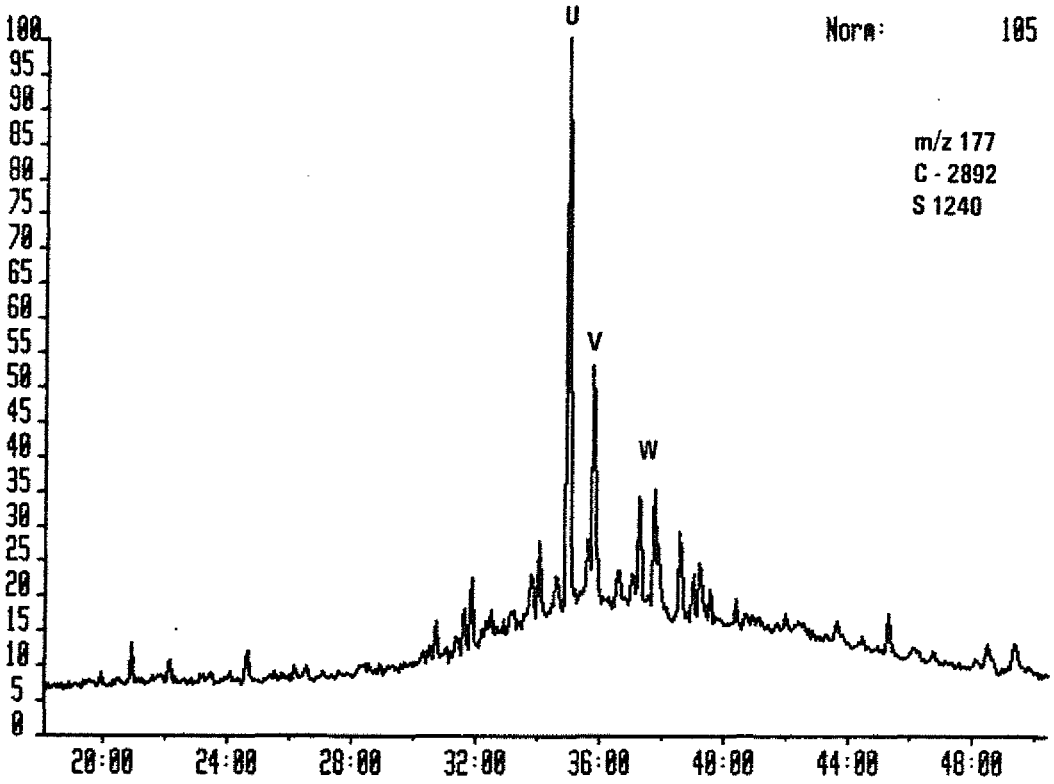
C2890SAT 29-OCT-85 Slr:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 177.1000
Text:



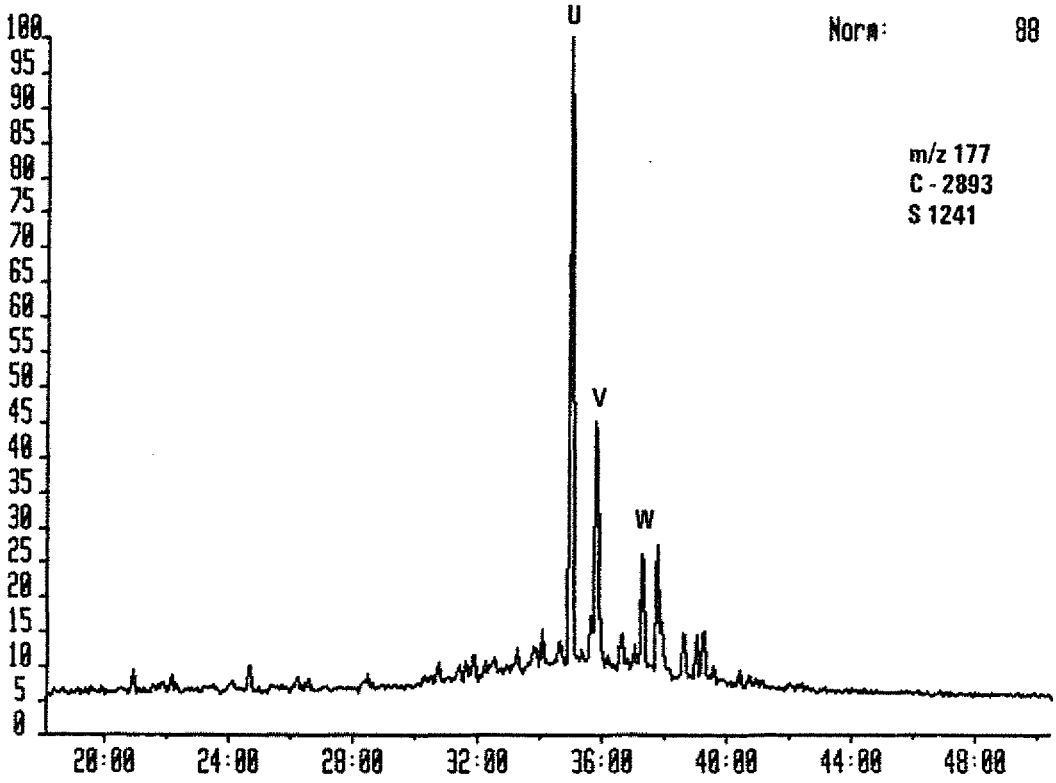
C2891SAT 29-OCT-85 Slr:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 177.1000
Text:



C2892SAT 29-OCT-85 Slr:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 177.1000
Text:

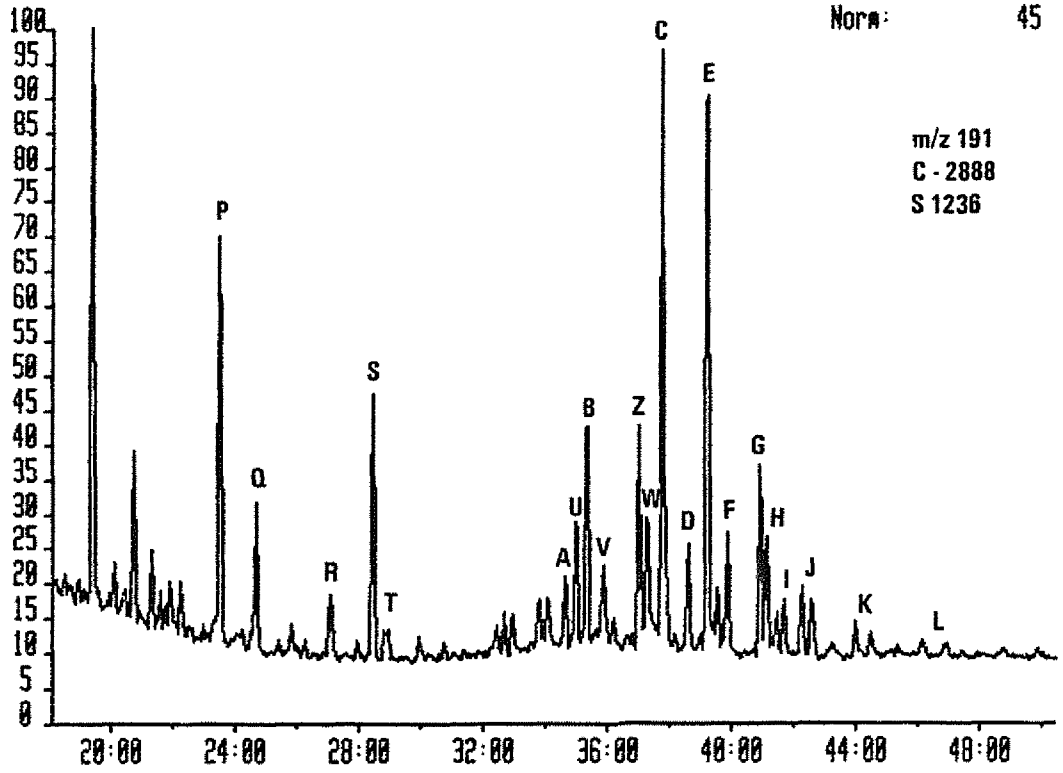


C2893SAT 30-OCT-85 Slr:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 177.1000
Text:

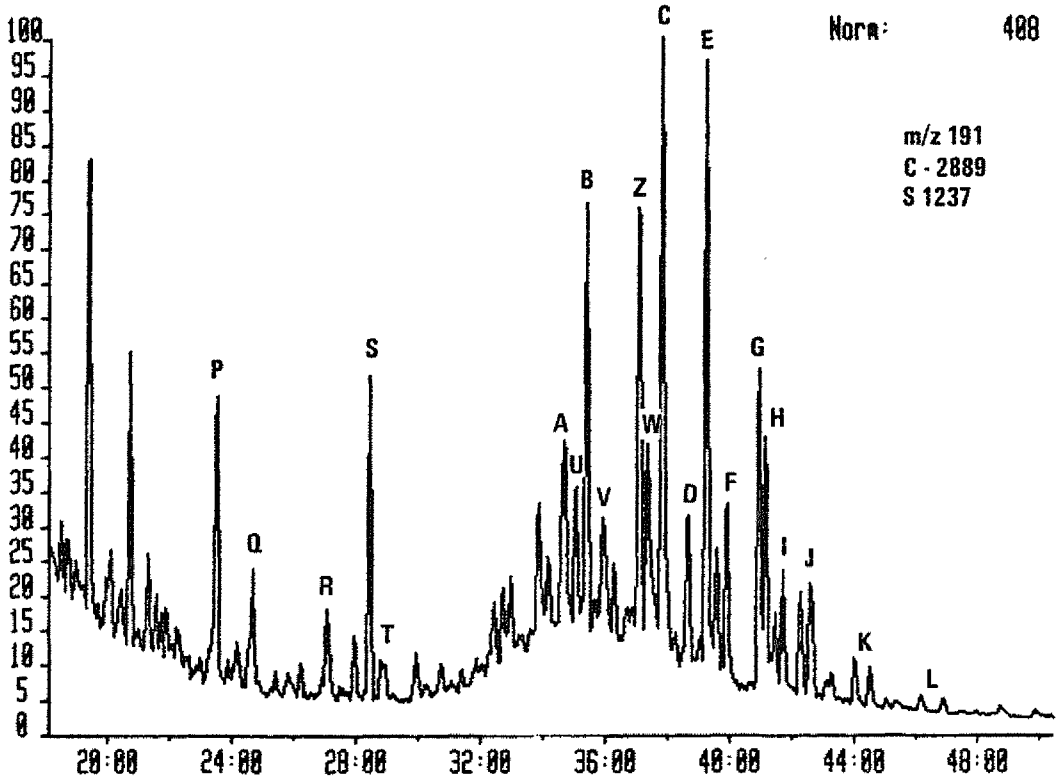


IKU

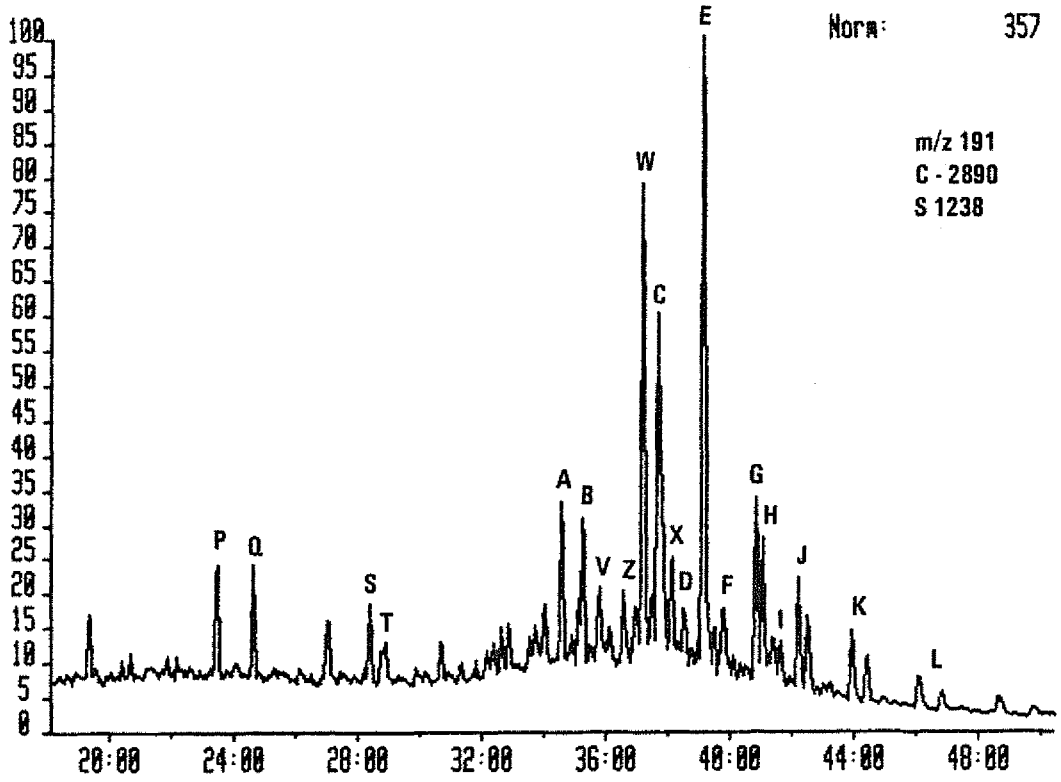
C2888SAT 30-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 191.1000
Text:



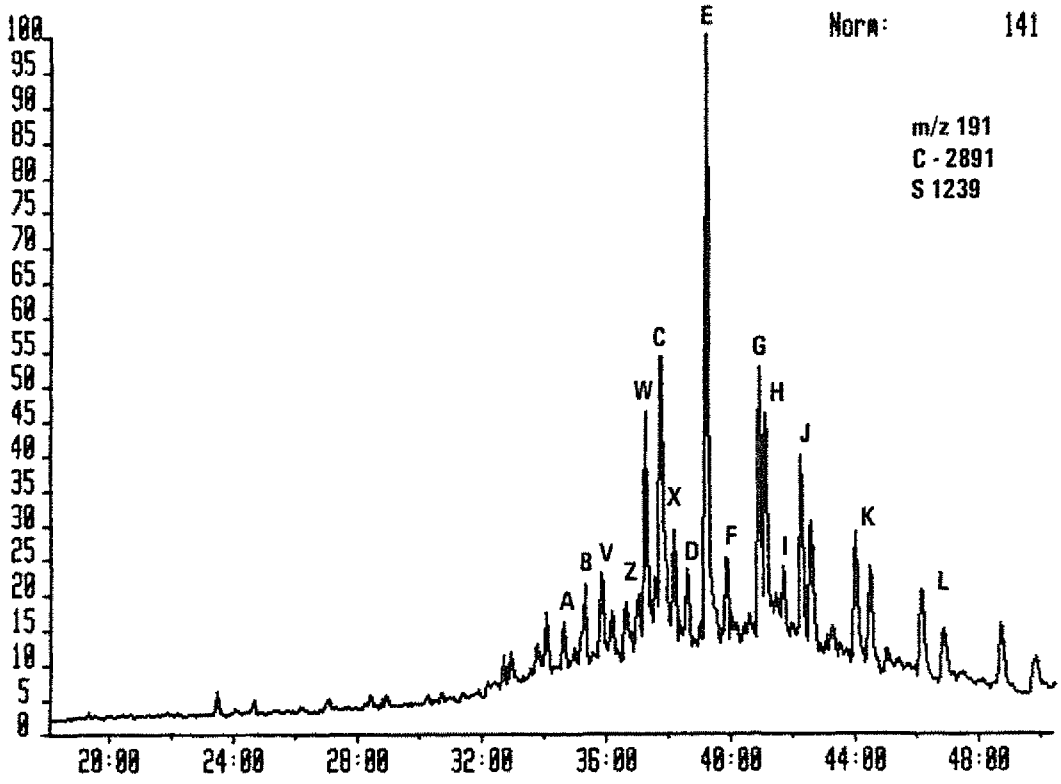
C2889SAT 29-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 191.1000
Text:



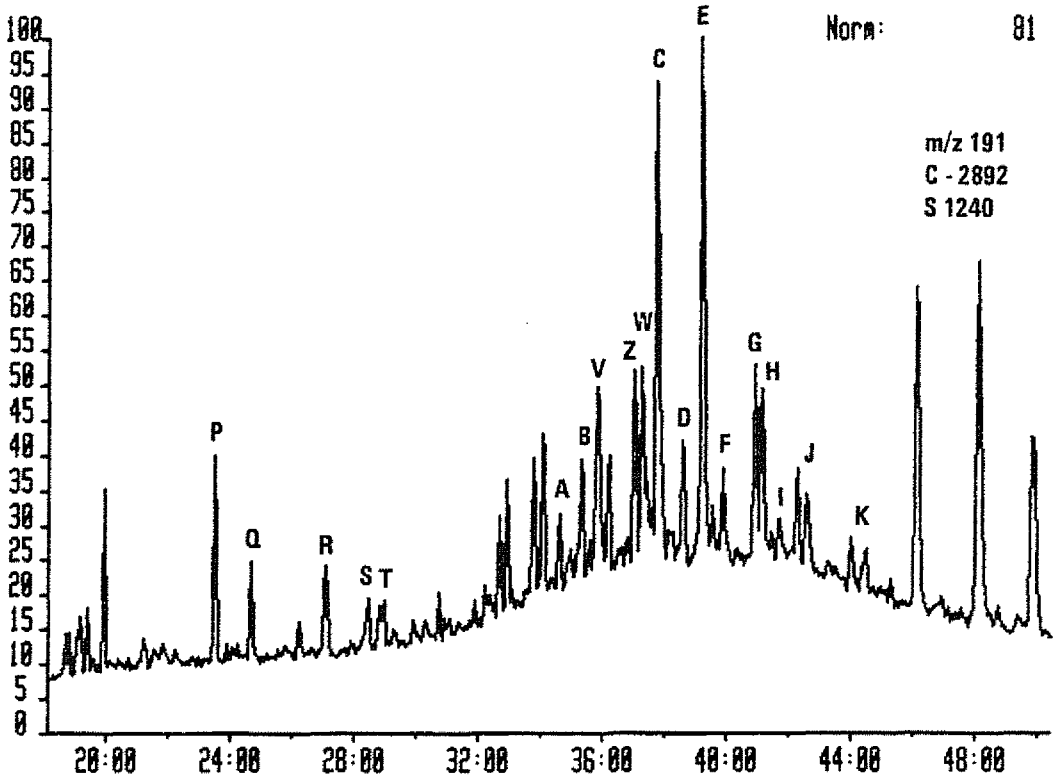
C2890SAT 29-OCT-85 Sir:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 191.1000
Text:



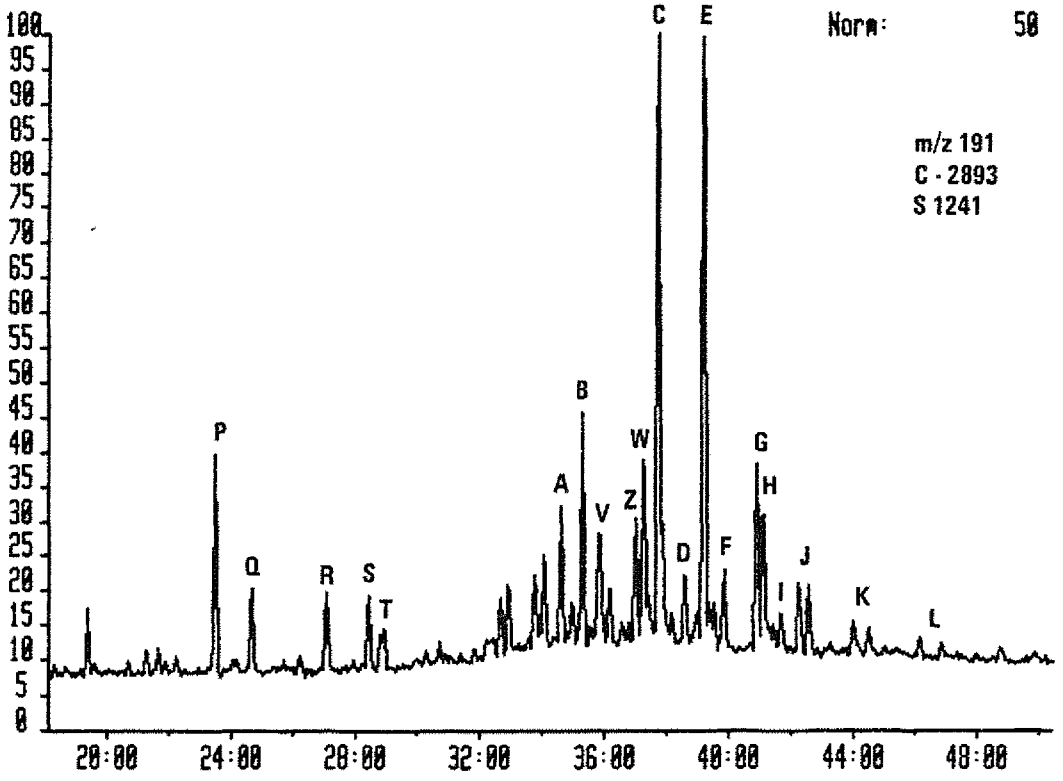
C2891SAT 29-OCT-85 Sir:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 191.1000
Text:



C2892SAT 29-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 191.1000
Text:



C2893SAT 30-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 191.1000
Text:

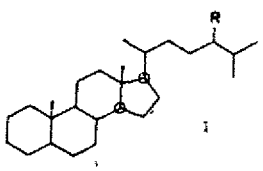


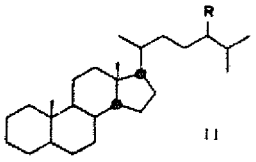
IKU SINTEF-GRUPPEN

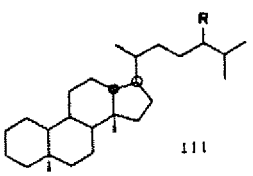
Figure 1b.

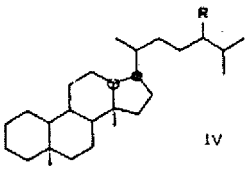
Mass chromatograms representing steranes (m/z 217 and 218)

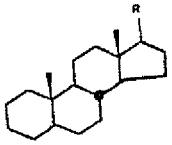
a	13β(H),17α(H)-diasterane (20S)	$C_{27}H_{48}$	(III,R=H)
b	13β(H),17α(H)-diasterane (20R)	$C_{27}H_{48}$	(III,R=H)
c	13α(H),17β(H)-diasterane (20S)	$C_{27}H_{48}$	(IV,R=H)
d	13α(H),17β(H)-diasterane (20R)	$C_{27}H_{48}$	(IV,R=H)
e	13β(H),17α(H)-diasterane (20S)	$C_{28}H_{50}$	(III,R=CH_3)
f	13β(H),17α(H)-diasterane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



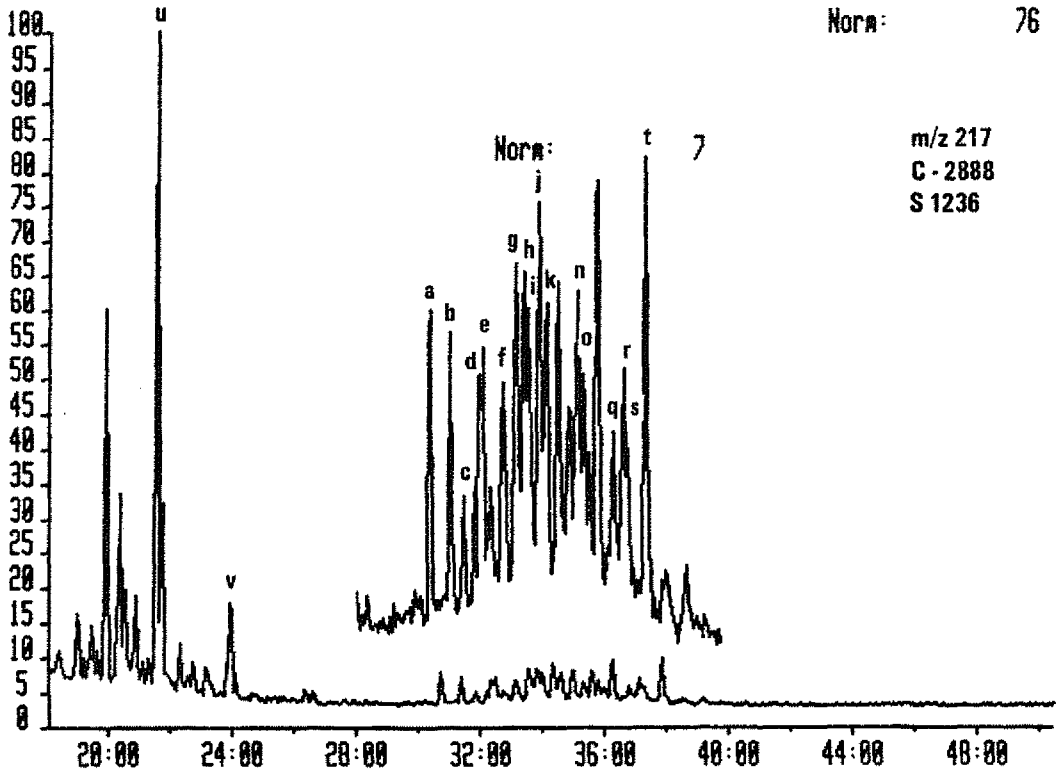




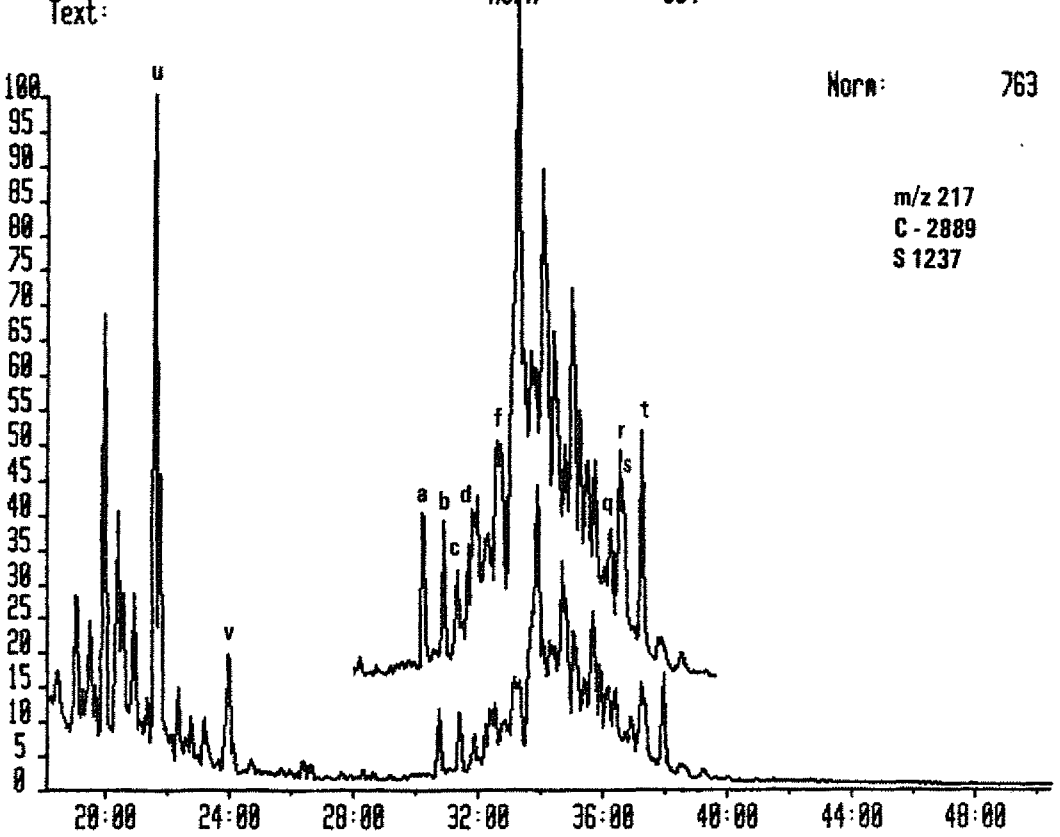




C2888SAT 30-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 217.1000
Text:

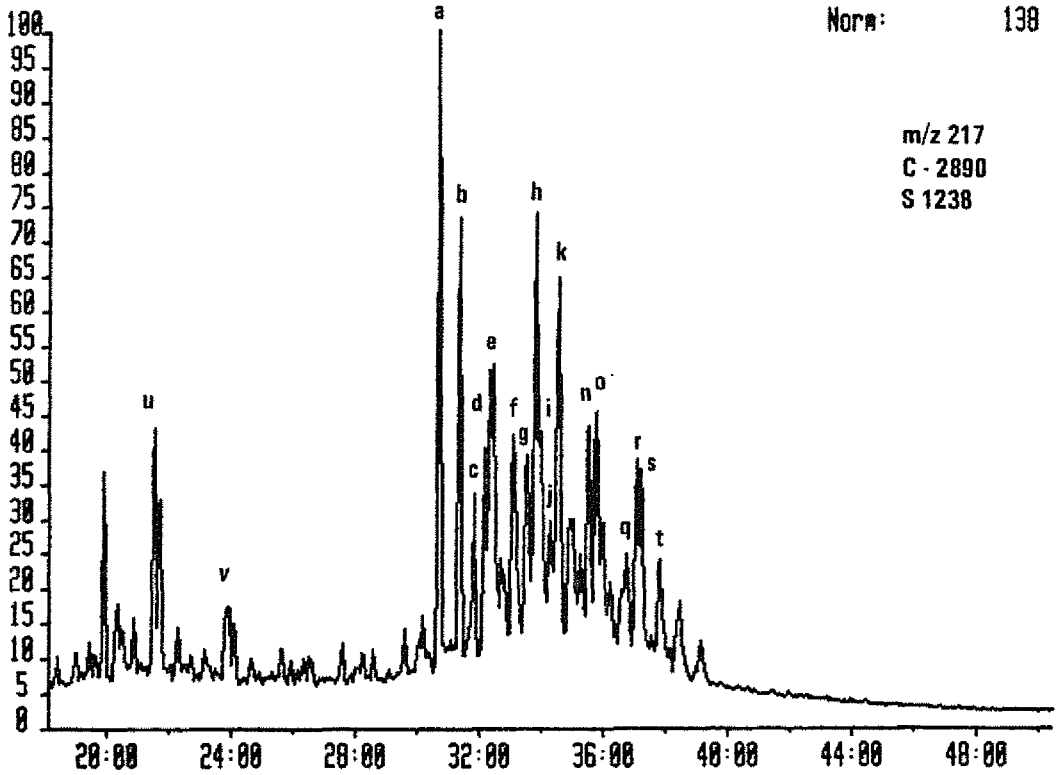


C2889SAT 29-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1
Text:

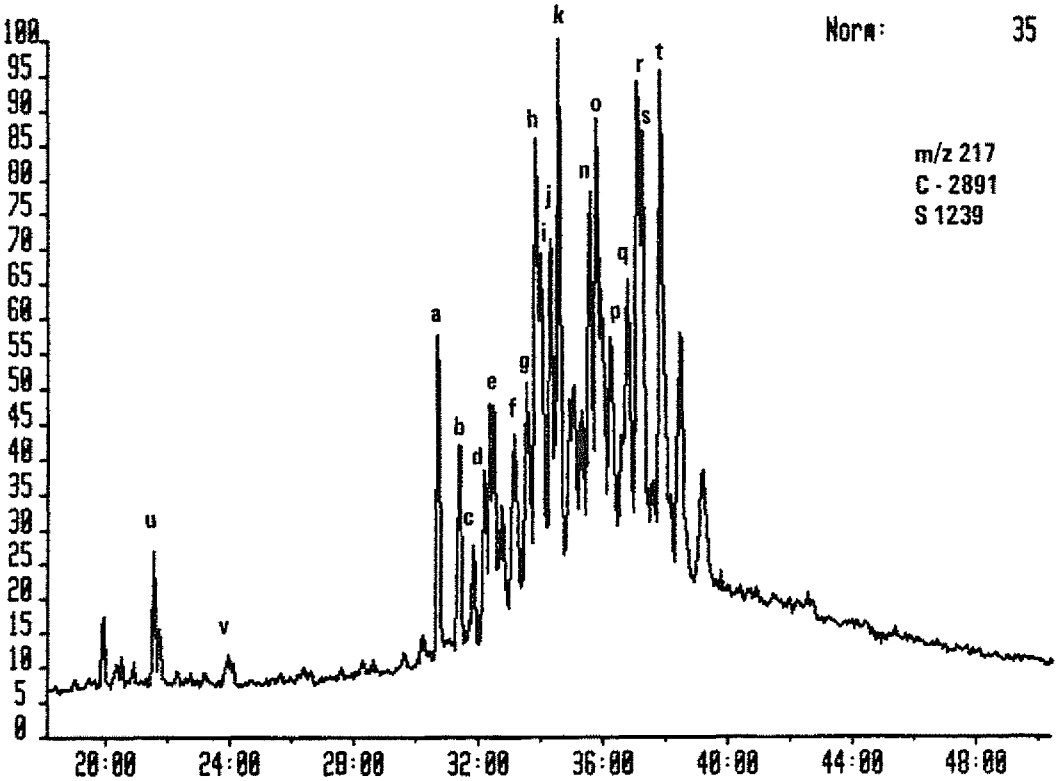


IKU

C2890SAT 29-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 217.1000
Text:

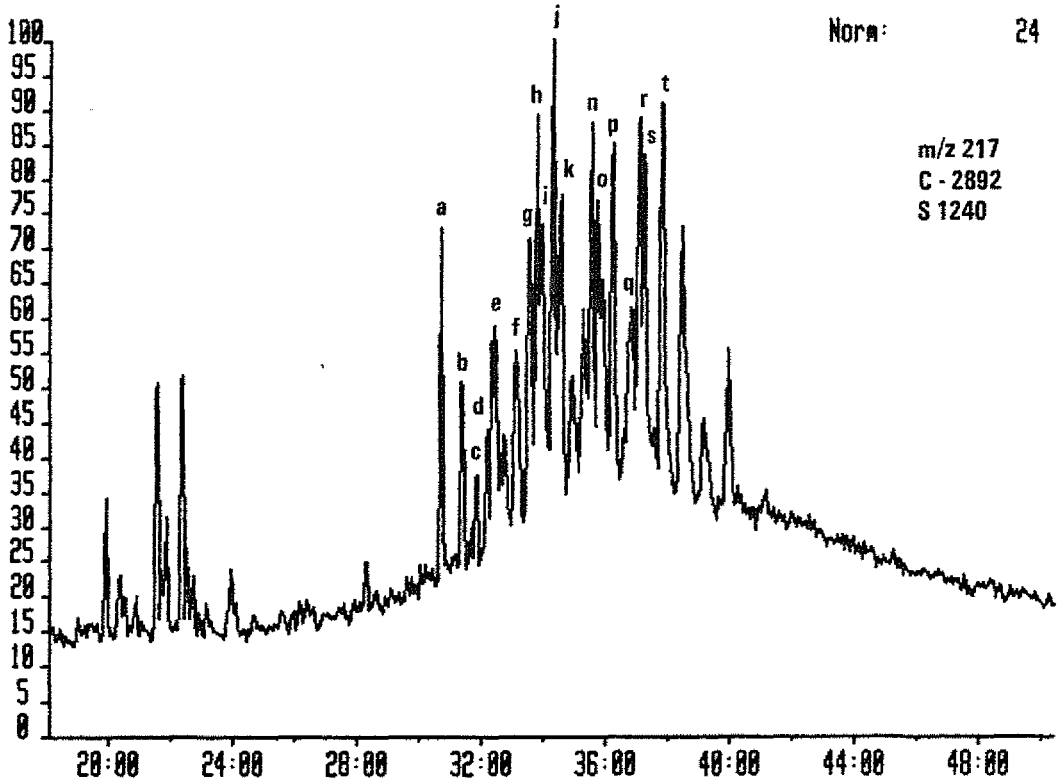


C2891SAT 29-OCT-85 Stir:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 217.1000
Text:

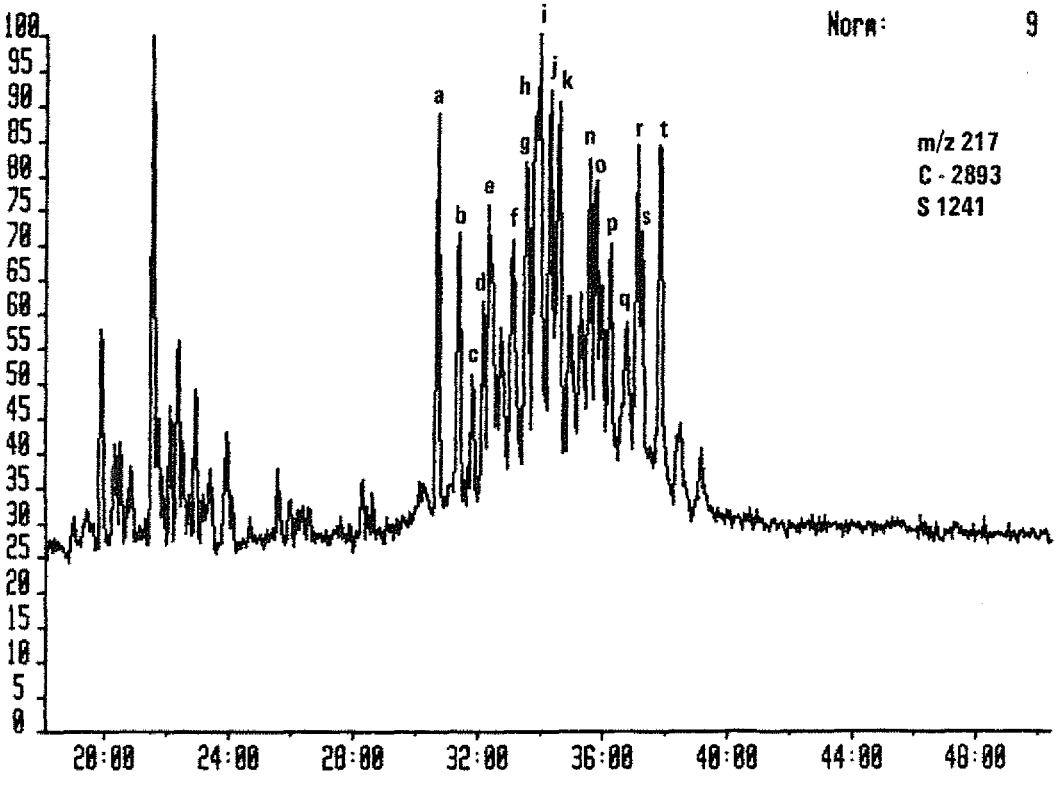


IKU

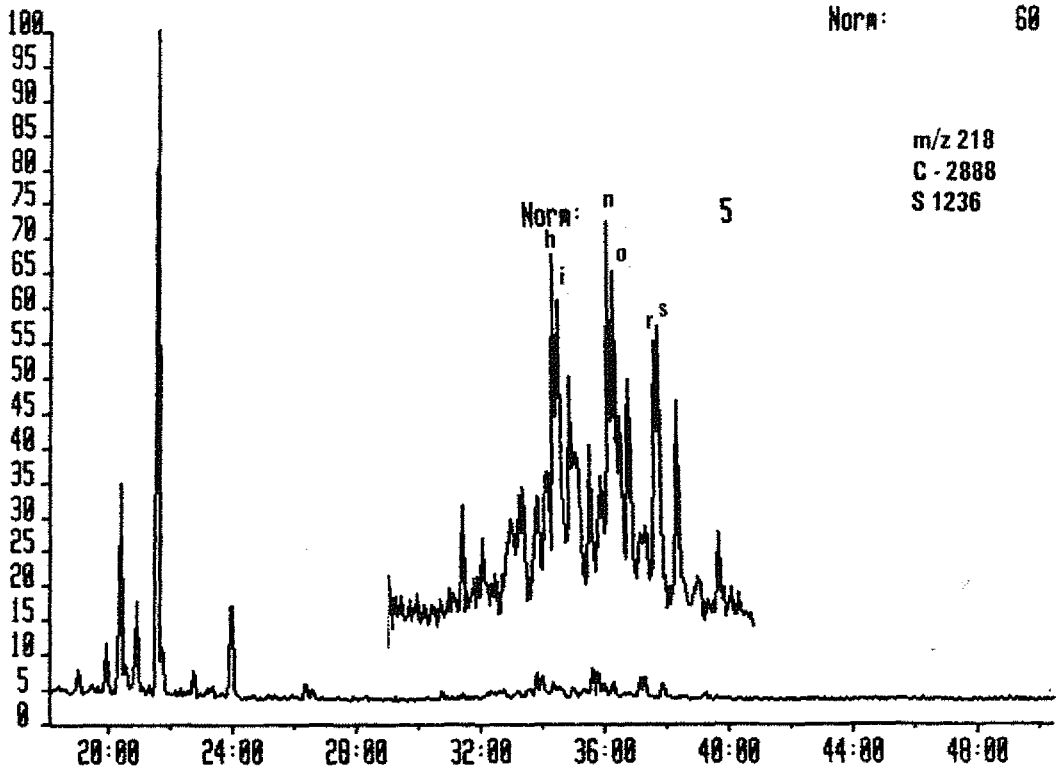
C2892SAT 29-OCT-85 Sir:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 217.1000
Text:



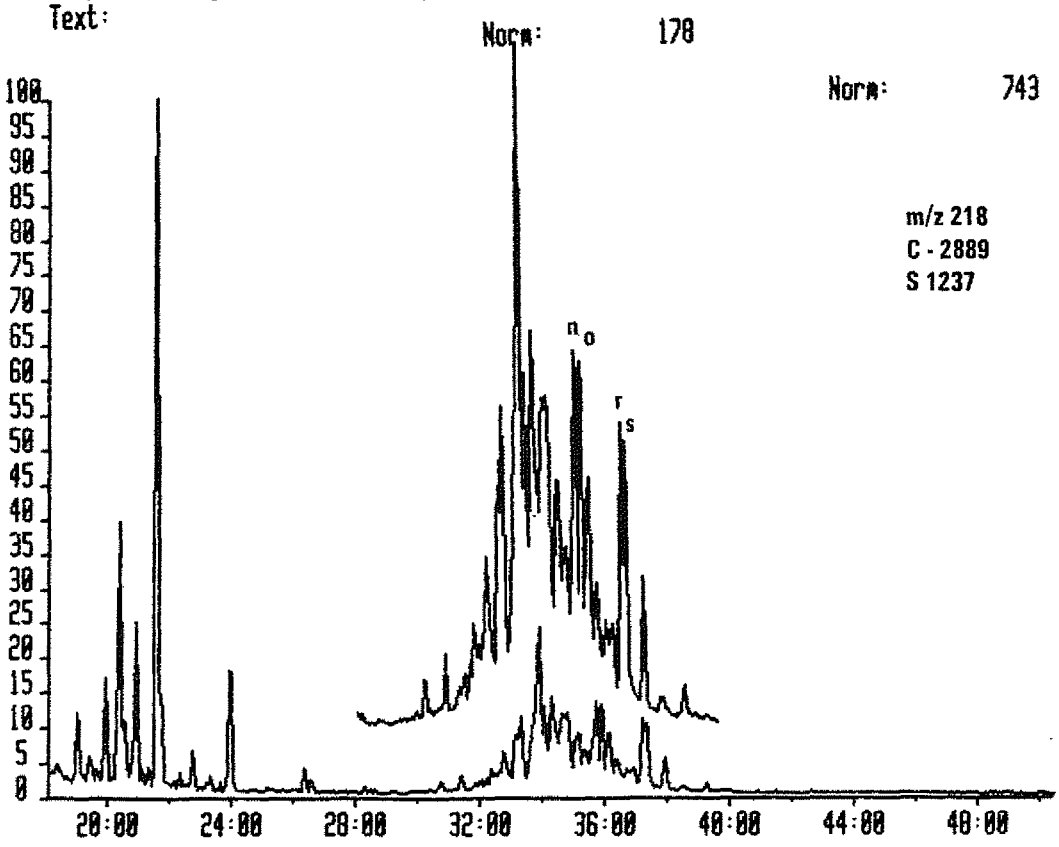
C2893SAT 30-OCT-85 Sir:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 217.1000
Text:



C2888SAT 30-OCT-85 Sir:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 218.1000
Text:

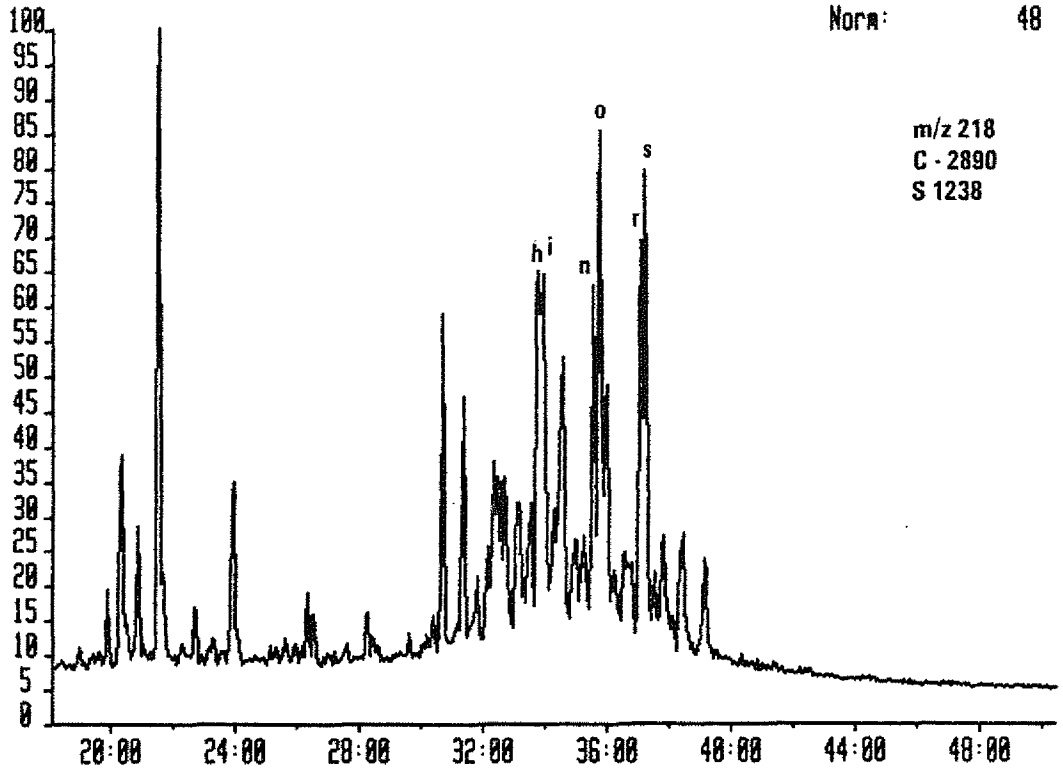


C2889SAT 29-OCT-85 Sir:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 218.1000
Text:

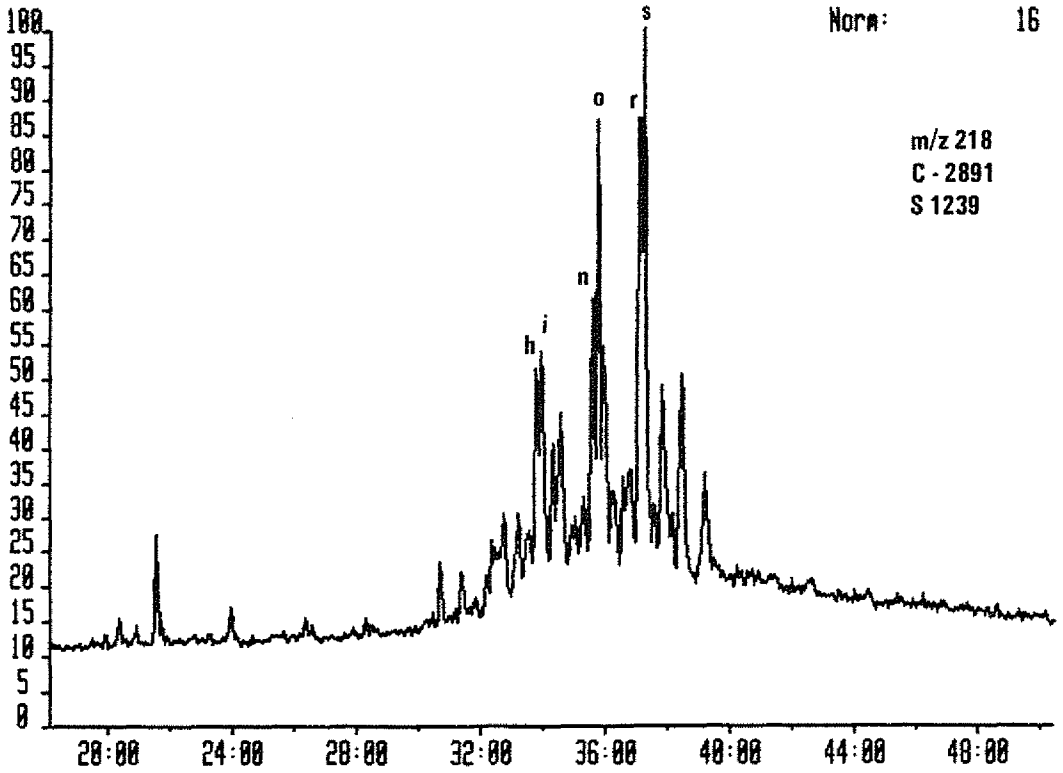


IKU GRUPPEN

C2890SAT 29-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 218.1000
Text:

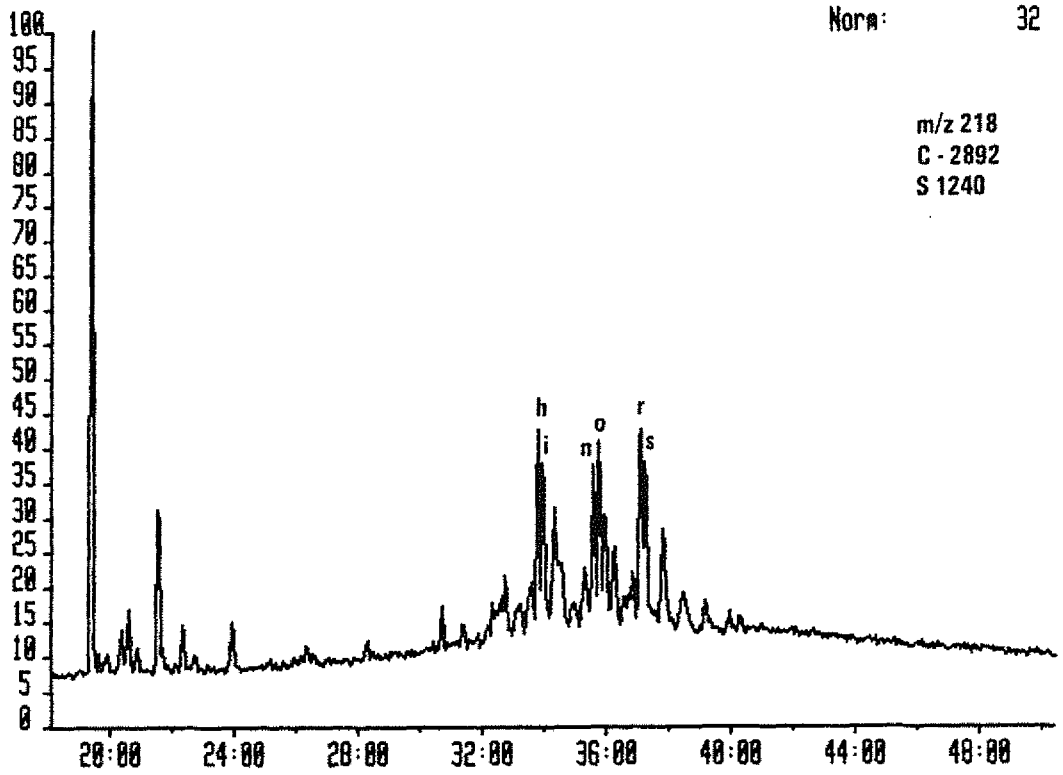


C2891SAT 29-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 218.1000
Text:

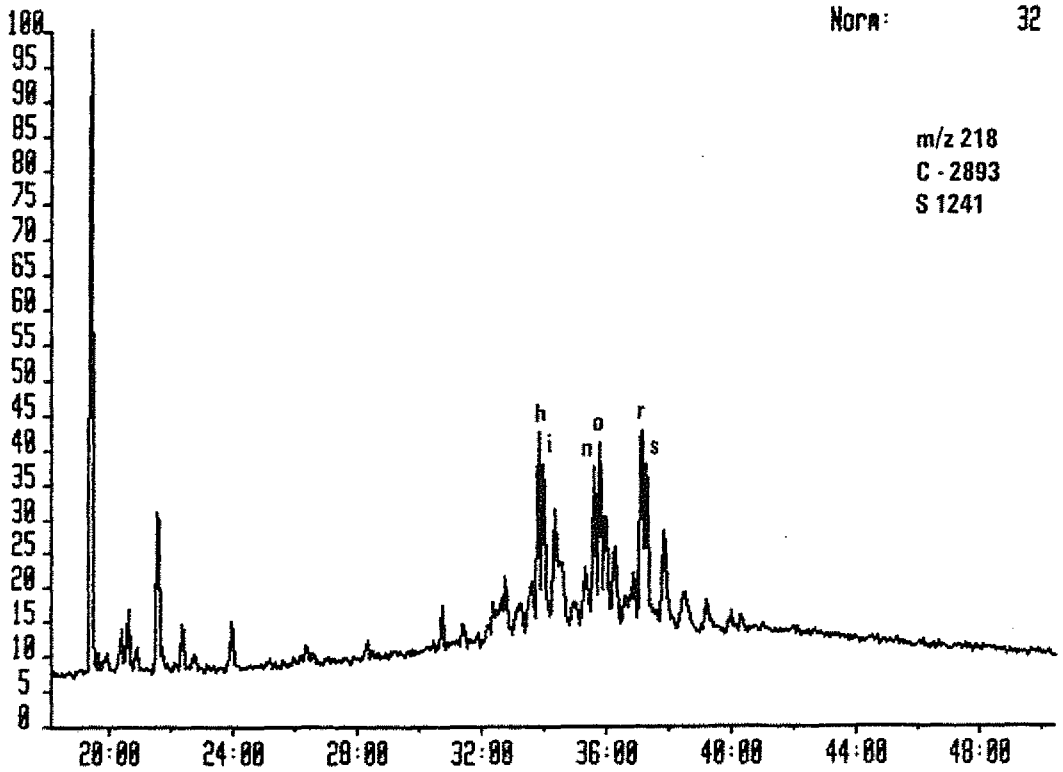


IKU

C2892SAT 29-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 218.1000
Text:



C2892SAT 29-OCT-85 Str:Voltage 7070H Acnt:IKU System:TRIT
Sample 1 Injection 1 Group 1 Mass 218.1000
Text:



APPENDIX I

Lists of peak heights and peak areas from mass chromatograms.

IKU
SINTEF-GRUPPEN

Peak heights in m/z 191
mass chromatograms

C-2888

SINTEF-GRUPPEN

SAMPLE 1 INJECTION 1 GROUP 1 CHANNEL 191.10

	HEIGHT	RETENTION TIME	PEAK IDENTITIES IN CHROMATOGRAM
1	3.842363E+01	0:19:21	
2	1.164414E+01	0:20:40	
3	5.511907E+00	0:21:15	
4	2.567983E+01	0:23:25	P
5	9.580173E+00	0:24:35	Q
6	4.358986E+00	0:26:57	R
7	1.763266E+01	0:28:19	S
8	3.027444E+00	0:33:51	
9	4.541677E+00	0:34:25	A
10	8.398349E+00	0:34:45	U
11	1.419145E+01	0:35:07	B
12	4.567662E+00	0:35:37	V
13	1.459837E+01	0:36:46	Z
14	7.665018E+00	0:37:00	W
15	3.860538E+01	0:37:29	C
16	6.620533E+00	0:38:19	D
17	3.602670E+01	0:38:56	E
18	4.035387E+00	0:39:15	
19	7.841376E+00	0:39:35	F
20	1.241880E+01	0:40:36	G
21	7.415856E+00	0:40:48	H
22	3.813873E+00	0:41:23	I
23	4.558738E+00	0:41:57	J
24	3.825885E+00	0:42:15	
	1.37 +00		T

SAMPLE 1 INJECTION 1 GROUP 1 CHANNEL 191.10

	HEIGHT	RETENTION TIME	PEAK IDENTITIES IN CHROMATOGRAM
1	2.666291E+02	0:19:22	
2	1.804318E+02	0:20:41	
3	1.544551E+02	0:23:26	P
4	1.900208E+02	0:28:18	S
5	1.089436E+02	0:34:27	A
6	7.926045E+01	0:34:50	U
7	2.492147E+02	0:35:11	B
8	2.553266E+02	0:36:51	Z
9	1.070944E+02	0:37:06	W
10	3.478789E+02	0:37:34	C
11	8.443674E+01	0:38:23	D
12	3.532689E+02	0:38:57	E
13	1.001318E+02	0:39:38	F
14	1.842505E+02	0:40:38	G
15	1.416408E+02	0:40:51	H
16	6.896042E+01	0:41:23	I

SAMPLE 1 INJECTION 1 GROUP 1 CHANNEL 191.10

	HEIGHT	RETENTION TIME	PEAK IDENTITIES IN CHROMATOGRAM
1	3.698156E+01	0:19:19	
2	1.553334E+01	0:20:38	
3	1.556695E+01	0:22:07	
4	5.537069E+01	0:23:23	P
5	5.888925E+01	0:24:32	Q
6	3.196645E+01	0:26:53	R
7	4.119510E+01	0:28:15	S
8	1.729196E+01	0:28:36	T
9	2.157383E+01	0:28:45	
10	2.172428E+01	0:30:31	
11	2.507000E+01	0:32:26	
12	2.631199E+01	0:32:40	
13	1.508704E+01	0:33:19	
14	1.994378E+01	0:33:30	
15	2.782380E+01	0:33:49	
16	8.369632E+01	0:34:21	A
17	3.258189E+01	0:34:54	
18	7.364905E+01	0:35:02	B
19	1.154505E+01	0:35:15	
20	3.952330E+01	0:35:33	V
21	1.838710E+01	0:35:52	
22	3.780998E+01	0:36:19	
23	2.746008E+01	0:36:43	Z
24	2.403201E+02	0:36:57	W
25	2.624194E+01	0:37:15	
26	1.442342E+02	0:37:27	C
27	4.931495E+01	0:37:33	
28	5.404697E+01	0:37:52	X
29	1.020784E+01	0:38:03	
30	2.611126E+01	0:38:15	D
31	3.210918E+02	0:38:51	E
32	2.327979E+01	0:39:13	
33	8.372820E+00	0:39:23	
34	3.091372E+01	0:39:31	F
35	9.389077E+01	0:40:33	G
36	7.038952E+01	0:40:46	H
37	1.820329E+01	0:41:04	
38	2.141061E+01	0:41:19	I
39	5.704962E+01	0:41:54	J
40	3.864245E+01	0:42:11	
41	3.567935E+01	0:43:35	K
42	2.338444E+01	0:44:04	
43	1.486269E+01	0:45:42	

SAMPLE 1 INJECTION 1 GROUP 1 CHANNEL 191.10

	HEIGHT	RETENTION TIME	PEAK IDENTITIES IN CHROMATOGRAM
1	6.732518E+00	0:32:28	
2	7.069357E+00	0:32:43	
3	7.310350E+00	0:33:31	
4	1.191799E+01	0:33:50	
5	9.905501E+00	0:34:23	A
6	4.965319E+00	0:34:56	
7	1.523297E+01	0:35:03	B
8	1.743441E+01	0:35:36	V
9	1.000813E+01	0:35:55	
10	1.090449E+01	0:36:21	
11	1.144009E+01	0:36:46	Z
12	4.524121E+01	0:36:59	W
13	1.123068E+01	0:37:17	
14	5.663803E+01	0:37:28	C
15	2.200592E+01	0:37:54	X
16	1.354061E+01	0:38:18	D
17	5.339470E+00	0:38:43	
18	1.215025E+02	0:38:54	E
19	5.894163E+00	0:39:12	
20	1.589946E+01	0:39:33	F
21	6.055915E+00	0:39:43	
22	4.943310E+00	0:40:16	
23	5.376565E+01	0:40:35	G
24	4.196775E+01	0:40:47	H
25	7.375901E+00	0:41:07	
26	1.457313E+01	0:41:20	I
27	4.014484E+00	0:41:38	
28	3.798244E+01	0:41:55	J
29	2.660407E+01	0:42:14	
30	6.478352E+00	0:42:56	
31	2.663924E+01	0:43:38	K
32	1.914973E+01	0:44:07	
33	5.009979E+00	0:44:39	
34	1.784487E+01	0:45:45	L
35	1.002779E+01	0:46:28	
36	1.278243E+01	0:48:18	M
37	6.692955E+00	0:49:23	

SAMPLE 1 INJECTION 1 GROUP 1 CHANNEL 191.10

	HEIGHT	RETENTION TIME	PEAK IDENTITIES IN CHROMATOGRAM
1	4.867727E+00	0:18:39	
2	8.108655E+00	0:19:20	
3	2.189321E+01	0:19:54	
4	2.418984E+01	0:23:24	P
5	1.211314E+01	0:24:34	Q
6	1.057180E+01	0:26:55	R
7	5.840993E+00	0:28:18	
8	5.553166E+00	0:28:38	
9	1.279562E+01	0:32:28	
10	1.603557E+01	0:32:43	
11	1.641914E+01	0:33:32	
12	1.835642E+01	0:33:51	
13	9.892118E+00	0:34:23	A
14	1.514101E+01	0:35:06	B
15	2.029283E+01	0:35:36	V
16	1.322519E+01	0:35:57	
17	2.331520E+01	0:36:46	Z
18	2.091486E+01	0:37:00	W
19	5.437740E+01	0:37:29	C
20	1.387161E+01	0:38:19	D
21	5.970354E+01	0:38:55	E
22	7.238535E+00	0:39:15	
23	1.078189E+01	0:39:35	F
24	2.180974E+01	0:40:35	G
25	1.865193E+01	0:40:49	H
26	1.051578E+01	0:41:57	J
27	8.042413E+00	0:42:14	
28	3.672392E+01	0:45:44	
29	4.114494E+01	0:47:42	
30	2.244116E+01	0:49:24	

SAMPLE 1 INJECTION 1 GROUP 1 CHANNEL 191.10

	HEIGHT	RETENTION TIME	PEAK IDENTITIES IN CHROMATOGRAM
1	4.964254E+00	0:19:20	
2	1.584480E+01	0:23:24	P
3	6.281731E+00	0:24:35	Q
4	6.023384E+00	0:26:56	R
5	5.636175E+00	0:28:17	S
6	2.684829E+00	0:28:39	
7	3.063471E+00	0:28:47	
8	4.551309E+00	0:32:28	
9	5.328942E+00	0:32:43	
10	5.194431E+00	0:33:33	
11	6.331896E+00	0:33:51	
12	1.060779E+01	0:34:23	A
13	3.080585E+00	0:34:45	U
14	1.690334E+01	0:35:05	B
15	7.997736E+00	0:35:36	V
16	4.194225E+00	0:35:57	
17	9.120937E+00	0:36:46	Z
18	1.263796E+01	0:37:00	W
19	4.360502E+01	0:37:28	C
20	5.094389E+00	0:38:19	D
21	4.307097E+01	0:38:55	E
22	3.236423E+00	0:39:15	
23	5.941565E+00	0:39:35	F
24	1.390018E+01	0:40:36	G
25	9.781236E+00	0:40:48	H
26	2.839387E+00	0:41:21	I
27	5.443304E+00	0:41:55	J
28	5.245508E+00	0:42:13	
29	2.423725E+00	0:43:39	

Peak areas in m/z 191
mass chromatograms

SAMPLE 1 INJECTION 1 GROUP 1 CHANNEL 191.10

	AREA	RETENTION TIME	PEAK IDENTITIES IN CHROMATOGRAM
1	1.333930E+02	0:19:21	
2	4.646515E+01	0:20:40	
3	2.250738E+01	0:21:15	
4	8.846336E+01	0:23:25	P
5	2.927474E+01	0:24:35	Q
6	2.857452E+01	0:26:57	R
7	6.745936E+01	0:28:19	S
8	1.537407E+01	0:33:51	
9	1.833397E+01	0:34:25	A
10	3.966684E+01	0:34:45	U
11	6.717570E+01	0:35:07	B
12	2.885178E+01	0:35:37	V
13	7.529726E+01	0:36:46	Z
14	3.851594E+01	0:37:00	W
15	1.744136E+02	0:37:29	C
16	2.633488E+01	0:38:19	D
17	1.575480E+02	0:38:56	E
18	1.933428E+01	0:39:15	
19	3.330369E+01	0:39:35	F
20	4.857187E+01	0:40:36	G
21	3.443699E+01	0:40:48	H
22	1.771478E+01	0:41:23	I
23	1.979450E+01	0:41:57	J
24	2.407168E+01	0:42:15	
	9.86 +00		T

SAMPLE 1 INJECTION 1 GROUP 1 CHANNEL 191.10

	AREA	RETENTION TIME	PEAK IDENTITIES IN CHROMATOGRAM
1	1.236709E+03	0:19:22	
2	6.574001E+02	0:20:41	
3	5.828009E+02	0:23:26	
4	7.233092E+02	0:28:18	S
5	9.007651E+02	0:34:27	A
6	3.617166E+02	0:34:50	U
7	1.092378E+03	0:35:11	B
8	1.280746E+03	0:36:51	Z
9	6.963051E+02	0:37:06	W
10	1.690305E+03	0:37:34	C
11	4.946623E+02	0:38:23	D
12	1.884712E+03	0:38:57	E
13	4.747780E+02	0:39:38	F
14	7.822448E+02	0:40:38	G
15	5.843466E+02	0:40:51	H
16	3.263539E+02	0:41:23	I
	5.84 +02		P
	2.37 +02		Q

SAMPLE 1 INJECTION 1 GROUP 1 CHANNEL 191.10

	AREA	RETENTION TIME	PEAK IDENTITIES IN CHROMATOGRAM
1	1.503176E+02	0:19:19	
2	5.615181E+01	0:20:38	
3	1.070652E+02	0:22:07	
4	2.218134E+02	0:23:23	P
5	2.230405E+02	0:24:32	Q
6	2.177733E+02	0:26:53	R
7	1.783548E+02	0:28:15	S
8	7.417242E+01	0:28:36	T
9	9.594053E+01	0:28:45	
10	9.424936E+01	0:30:31	
11	8.947199E+01	0:32:26	
12	1.129566E+02	0:32:40	
13	5.977645E+01	0:33:19	
14	7.565035E+01	0:33:30	
15	1.268142E+02	0:33:49	
16	4.136698E+02	0:34:21	A
17	1.418945E+02	0:34:54	
18	2.828611E+02	0:35:02	B
19	4.937150E+01	0:35:15	
20	3.213185E+02	0:35:33	V
21	8.570124E+01	0:35:52	
22	2.294102E+02	0:36:19	
23	2.105658E+02	0:36:43	Z
24	9.784868E+02	0:36:57	W
25	1.269234E+02	0:37:15	
26	5.689664E+02	0:37:27	C
27	2.094654E+02	0:37:33	
28	2.597186E+02	0:37:52	X
29	4.080163E+01	0:38:03	
30	1.375193E+02	0:38:15	D
31	1.469595E+03	0:38:51	E
32	1.077302E+02	0:39:13	
33	2.324329E+01	0:39:23	
34	1.540405E+02	0:39:31	F
35	4.302323E+02	0:40:33	G
36	2.938777E+02	0:40:46	H
37	1.183068E+02	0:41:04	
38	1.137153E+02	0:41:19	I
39	3.122970E+02	0:41:54	J
40	2.555917E+02	0:42:11	
41	2.176534E+02	0:43:35	K
42	1.335738E+02	0:44:04	
43	9.575076E+01	0:45:42	

SAMPLE 1 INJECTION 1 GROUP 1 CHANNEL 191.10

	AREA	RETENTION TIME	PEAK IDENTITIES IN CHROMATOGRAM
1	2.802736E+01	0:32:28	
2	4.054810E+01	0:32:43	
3	5.072815E+01	0:33:31	
4	7.048597E+01	0:33:50	
5	5.387862E+01	0:34:23	A
6	2.026295E+01	0:34:56	
7	6.462321E+01	0:35:03	B
8	1.190595E+02	0:35:36	V
9	5.779029E+01	0:35:55	
10	5.994465E+01	0:36:21	
11	8.804472E+01	0:36:46	Z
12	2.054039E+02	0:36:59	W
13	4.789659E+01	0:37:17	
14	4.274446E+02	0:37:28	C
15	1.063966E+02	0:37:54	X
16	6.438873E+01	0:38:18	D
17	2.496852E+01	0:38:43	
18	5.978458E+02	0:38:54	E
19	3.188449E+01	0:39:12	
20	6.550329E+01	0:39:33	F
21	2.093247E+01	0:39:43	
22	2.118837E+01	0:40:16	
23	2.526917E+02	0:40:35	G
24	1.982624E+02	0:40:47	H
25	5.228154E+01	0:41:07	
26	7.634562E+01	0:41:20	I
27	1.668024E+01	0:41:38	
28	2.061864E+02	0:41:55	J
29	2.083575E+02	0:42:14	
30	4.960265E+01	0:42:56	
31	1.980103E+02	0:43:38	K
32	1.216976E+02	0:44:07	
33	3.579723E+01	0:44:39	
34	1.438668E+02	0:45:45	L
35	8.650456E+01	0:46:28	
36	1.060116E+02	0:48:18	M
37	6.852428E+01	0:49:23	

SINTEF-GRUPPEN

SAMPLE 1 INJECTION 1 GROUP 1 CHANNEL 191.10

	AREA	RETENTION TIME	PEAK IDENTITIES IN CHROMATOGRAM
1	2.811179E+01	0:18:39	
2	2.840873E+01	0:19:20	
3	5.901306E+01	0:19:54	
4	9.480635E+01	0:23:24	P
5	4.572141E+01	0:24:34	Q
6	6.867270E+01	0:26:55	R
7	2.527112E+01	0:28:18	
8	2.591698E+01	0:28:38	
9	6.049055E+01	0:32:28	
10	5.952407E+01	0:32:43	
11	7.834198E+01	0:33:32	
12	8.184762E+01	0:33:51	
13	4.672408E+01	0:34:23	A
14	7.292049E+01	0:35:06	B
15	1.514392E+02	0:35:36	V
16	5.226744E+01	0:35:57	
17	1.489974E+02	0:36:46	Z
18	7.432457E+01	0:37:00	W
19	3.302052E+02	0:37:29	C
20	7.180888E+01	0:38:19	D
21	3.399252E+02	0:38:55	E
22	3.384306E+01	0:39:15	
23	5.311832E+01	0:39:35	F
24	1.059107E+02	0:40:35	G
25	1.023258E+02	0:40:49	H
26	5.007357E+01	0:41:57	J
27	5.516251E+01	0:42:14	
28	2.513331E+02	0:45:44	
29	3.027868E+02	0:47:42	
30	2.310363E+02	0:49:24	

SAMPLE 1 INJECTION 1 GROUP 1 CHANNEL 191.10

	AREA	RETENTION TIME	PEAK IDENTITIES IN CHROMATOGRAM
1	1.857270E+01	0:19:20	
2	5.691336E+01	0:23:24	P
3	2.360108E+01	0:24:35	Q
4	3.591525E+01	0:26:56	R
5	2.470567E+01	0:28:17	S
6	1.107112E+01	0:28:39	
7	1.107778E+01	0:28:47	
8	2.172445E+01	0:32:28	
9	2.558685E+01	0:32:43	
10	2.337787E+01	0:33:33	
11	2.646343E+01	0:33:51	
12	4.489793E+01	0:34:23	A
13	1.588017E+01	0:34:45	U
14	6.117847E+01	0:35:05	B
15	5.280344E+01	0:35:36	V
16	2.031586E+01	0:35:57	
17	4.732031E+01	0:36:46	Z
18	6.314855E+01	0:37:00	W
19	2.106418E+02	0:37:28	C
20	2.791349E+01	0:38:19	D
21	1.759976E+02	0:38:55	E
22	1.333962E+01	0:39:15	
23	2.452152E+01	0:39:35	F
24	6.184600E+01	0:40:36	G
25	4.733942E+01	0:40:48	H
26	1.471668E+01	0:41:21	I
27	3.111090E+01	0:41:55	J
28	2.723969E+01	0:42:13	
29	1.535653E+01	0:43:39	

Peak areas and peak heights from
m/z 217 mass chromatograms

Peak identification in chromatograms	Retention time	Area	Height
C-2888			
a	30.34	11.0	2.5
b	31.13	10.6	2.3
c	31.39	3.4	0.9
g	33.20	19.5	2.5
h	33.37	15.0	2.3
i	33.47	13.9	1.9
j	34.08	17.9	2.9
k	-	22.6	2.3
l	-	15.2	1.7
m	-	9.8	2.1
n	35.20	13.9	1.3
o	35.32	6.7	0.5
p	35.59	23.8	3.3
q	36.32	4.4	1.1
r	36.50	11.4	1.7
s	36.02	8.0	1.2
t	37.36	20.3	3.7
u	21.32	247.5	56.5
v	23.52	33.4	7.0

Peak identification in chromatograms	Retention time	Area	Height
C-2889			
a	30.33	234.9	49.5
b	31.12	221.2	46.4
c		109.4	23.5
g			
h	33.31		
i	33.40	poor resolution	
j	33.51		
k			
l			
m			
n	35.24	840.4	93.9
o	35.49	293.4	52.1
p	36.10	289.5	42.9
q	36.39	202.3	26.7
r		417.6	60.7
s	36.57	319.6	44.0
t	37.40	428.0	80.7
u	21.32	2753.6	561.6
v	23.52	469.5	87.2

Peak identification in chromatograms	Retention time	Area	Height
C-2890			
a	30.31	445.6	98.9
b	31.12	335.7	68.1
c	31.38	96.5	23.8
g	33.19	227.2	26.0
h	33.36	437.7	61.5
i	33.45	210.8	25.8
j	34.04	60.1	11.0
k	34.19	412.4	52.1
l	-	-	-
m	-	-	-
n	35.18	213.7	29.8
o	35.30	226.1	30.3
p	35.57	-	-
q	36.30	65.6	9.4
r	36.48	191.3	28.1
s	36.57	151.2	26.8
t	37.32	81.9	14.0
u	21.28	202.6	37.8
v	23.51	47.5	9.1

Peak identification in chromatograms	Retention time	Area	Height
C-2891			
a	30.32	49.7	12.4
b	31.12	49.2	8.0
c	31.39	17.2	3.4
g	33.20	78.6	7.8
h	33.37	145.7	16.8
i	33.47	87.3	11.3
j	34.05	56.0	11.4
k	34.21	159.6	20.1
l	-	-	-
m	-	-	-
n	35.20	106.5	13.0
o	35.32	122.0	15.7
p	35.59	54.9	7.0
q	36.32	67.3	8.5
r	36.51	136.9	16.9
s	36.59	93.7	14.7
t	37.34	106.1	17.6
u	21.29	22.3	5.3
v	23.50	6.1	1.1

Peak identification in chromatograms	Retention time	Area	Height
C-2892			
a	30.32	33.2	9.5
b	31.12	27.7	5.1
c	31.40	10.4	2.3
g	33.20	68.3	7.1
h	33.36	55.1	9.3
i	33.45	38.8	6.2
j	34.07	61.3	11.5
k	34.23	57.7	7.8
l	-	-	-
m	-	-	-
n	35.21	62.1	9.0
o	35.32	48.1	6.5
p	36.00	75.6	8.6
q	36.36	23.1	2.8
r	36.52	45.0	8.4
s	37.00	43.1	7.4
t	37.35	76.5	10.0
u	21.31	30.0	6.8
v	23.50	6.7	1.4

Peak identification in chromatograms	Retention time	Area	Height
C-2893			
a	30.34	19.8	4.2
b	31.13	16.2	2.9
c	31.40	7.2	1.3
g	33.35	14.7	3.2
h	33.40	12.7	3.4
i	33.45	18.7	4.2
j	34.07	15.7	3.3
k	34.23	26.9	3.3
l	-	-	-
m	-	-	-
n	35.20	22.1	3.0
o	35.33	16.5	2.7
p	36.00	14.1	2.1
q	36.32	2.8	0.9
r	36.52	18.7	3.4
s	37.00	13.4	2.4
t	37.34	17.9	3.4
u	21.30	20.6	5.3
v	23.51	6.9	1.2

Peak areas and peak heights in
m/z 218 mass chromatograms

Peak identification in chromatograms	Retention time	Area	Height
C-2888			
h	33.36	8.0	1.5
i	33.47	5.6	1.1
n	35.23	8.3	1.7
o	35.33	8.0	1.5
r	37.00	4.9	1.2
s	37.00	8.7	1.3
C-2889			
h	33.31	-	-
i	33.39	-	-
n	35.28	329.1	54.1
o	35.39	263.2	52.1
r	36.57	286.6	52.0
s	37.04	273.6	48.1
C-2890			
h	33.31	90.5	15.3
i	33.42	121.4	17.3
n	35.30	90.1	17.3
o	35.45	150.3	25.7
r	36.48	121.3	21.4
s	36.56	148.8	24.1
C-2891			
h	33.33	26.0	3.7
i	33.44	39.6	4.0
n	35.21	26.7	4.5
o	35.32	39.3	7.5
r	36.51	44.8	7.8
s	36.59	69.1	9.4

Peak identification in chromatograms	Retention time	Area	Height
C-2892			
h	33.35	36.7	7.1
i	33.44	22.4	5.0
n	35.22	35.9	5.7
o	35.32	36.0	6.0
r	36.52	36.4	6.0
s	37.00	35.2	5.5
C-2893			
h	33.35	15.4	2.8
i	33.45	14.0	3.8
n	35.22	11.6	2.2
o	35.32	13.0	2.3
r	36.52	13.9	2.3
s	37.00	10.1	2.1

APPENDIX II

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

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

Source characteristic parameters

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

Maturity dependant parameters

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

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

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

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

Migration and weathering

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