

NGS NSO-1

Appendix A3.3a

Whole oil GC chromatograms

Explanations

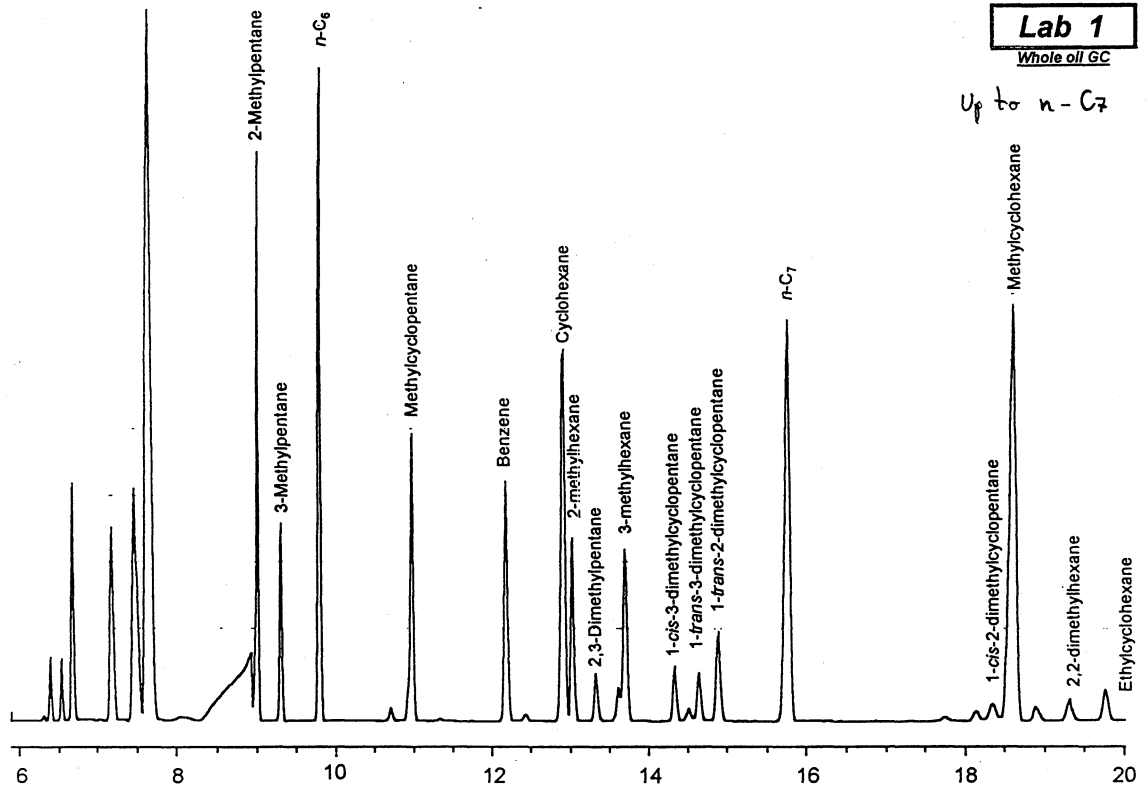
Some laboratories quantified light and heavy constituents in separate runs. These are:

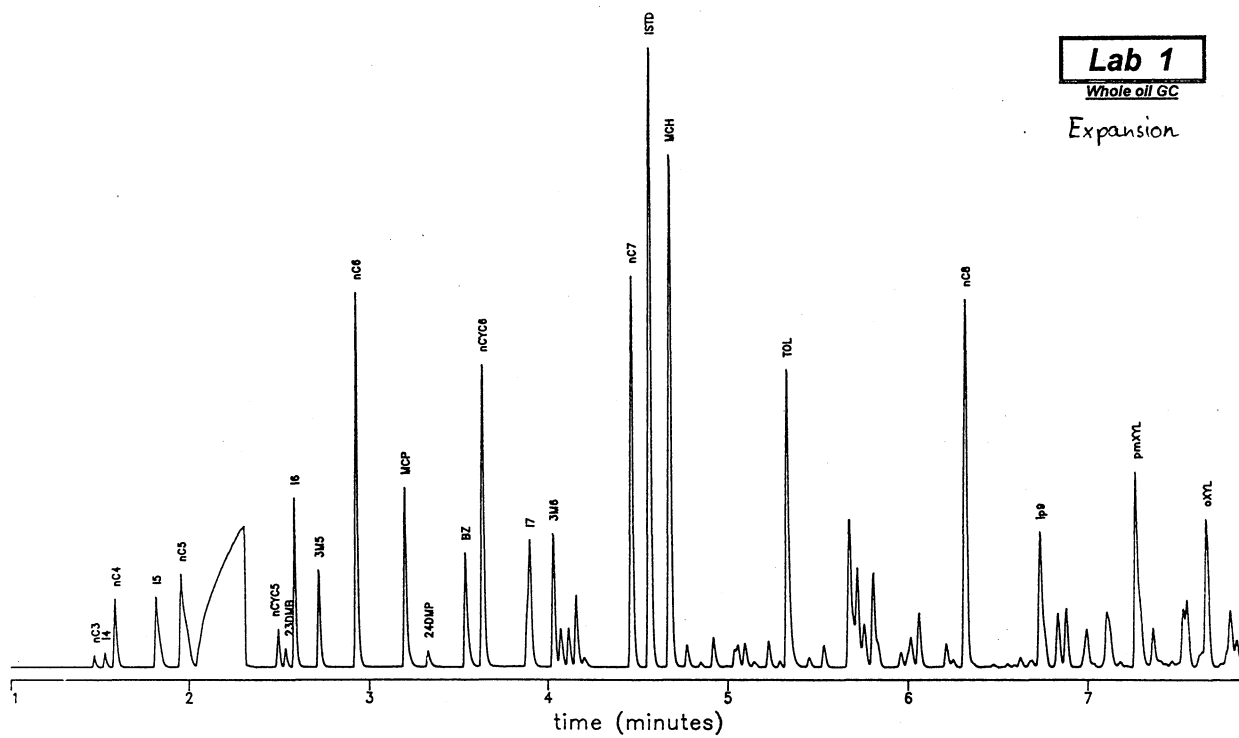
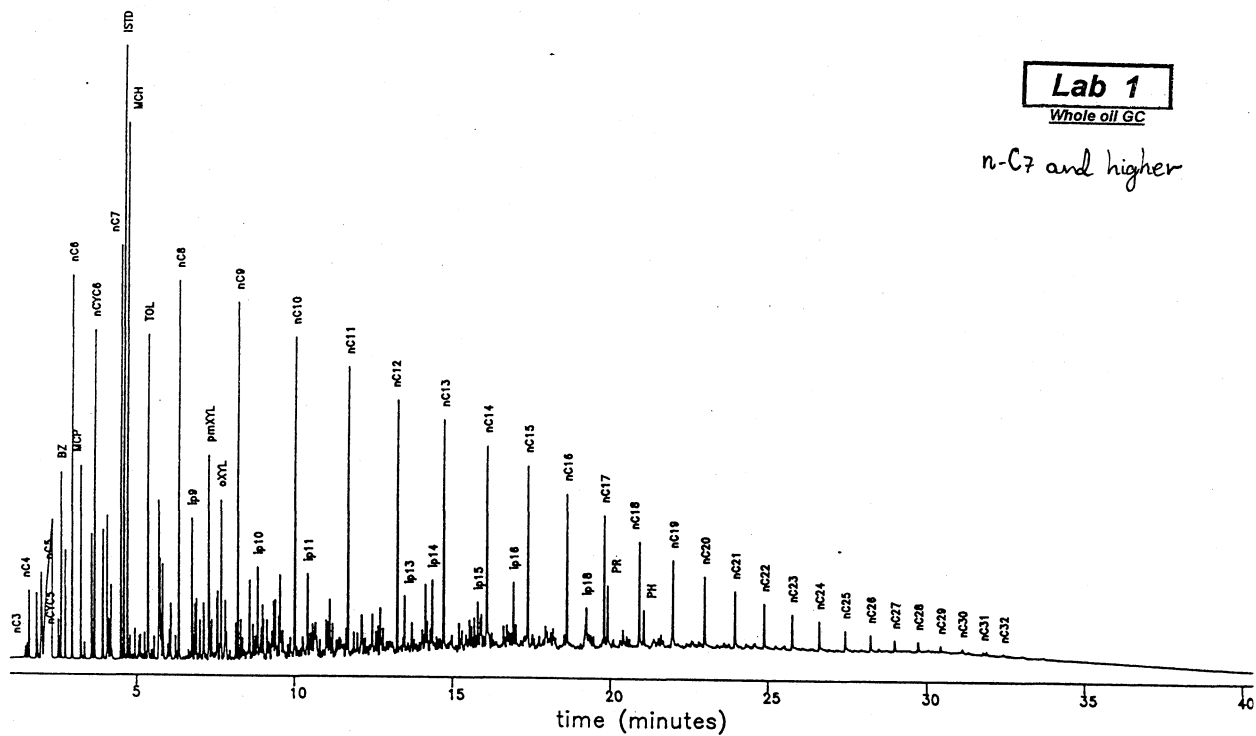
1. Lab 1 analysed the light constituents up to but not including n-C7 in one run and the n-C7+ constituents in another.
2. Lab 2 analysed all constituents in one run, but did an additional analysis that was used to quantify the light constituents up to toluene.
3. Lab 38 analysed the constituents up to toluene in one run and the higher constituents in another.
4. Lab 55 analysed the constituents up to xylene in one run and the C10+ constituents in another.
5. Lab 72 analysed up but not including n-C9 in one run and above n-C9 in another.
6. Lab 92 analysed up but not including n-C9 in one run and above n-C9 in another.

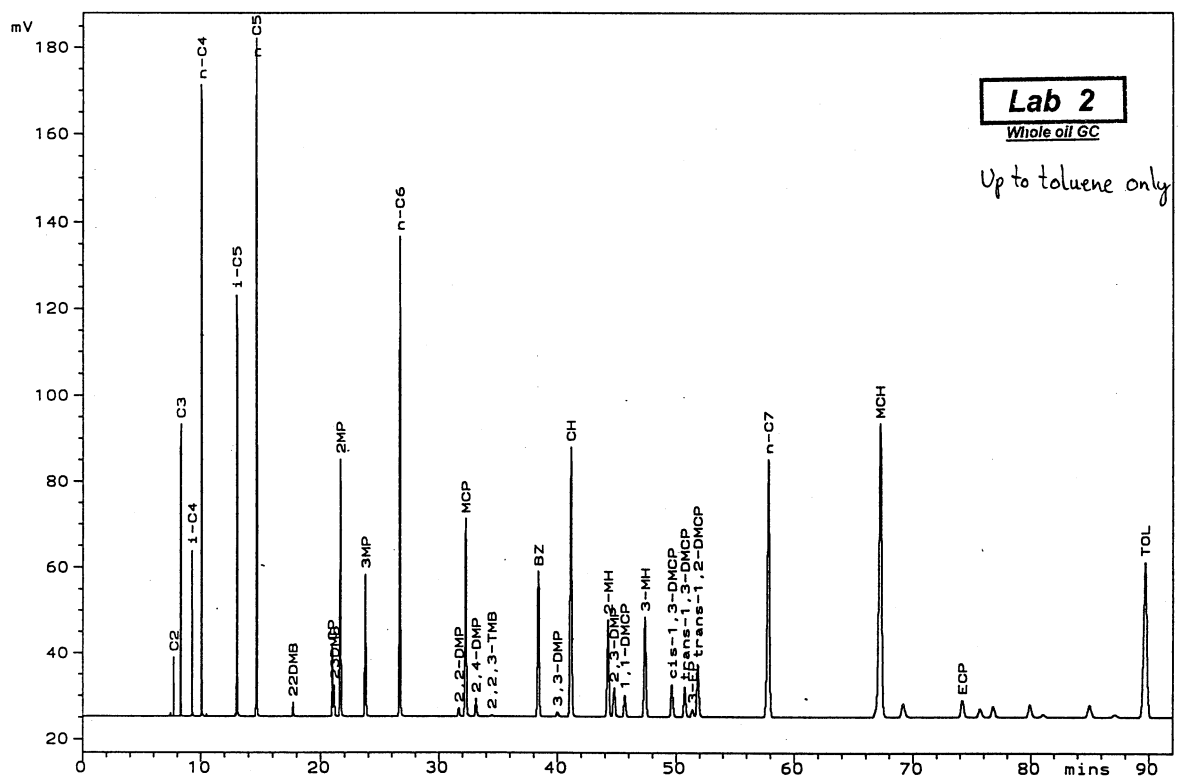
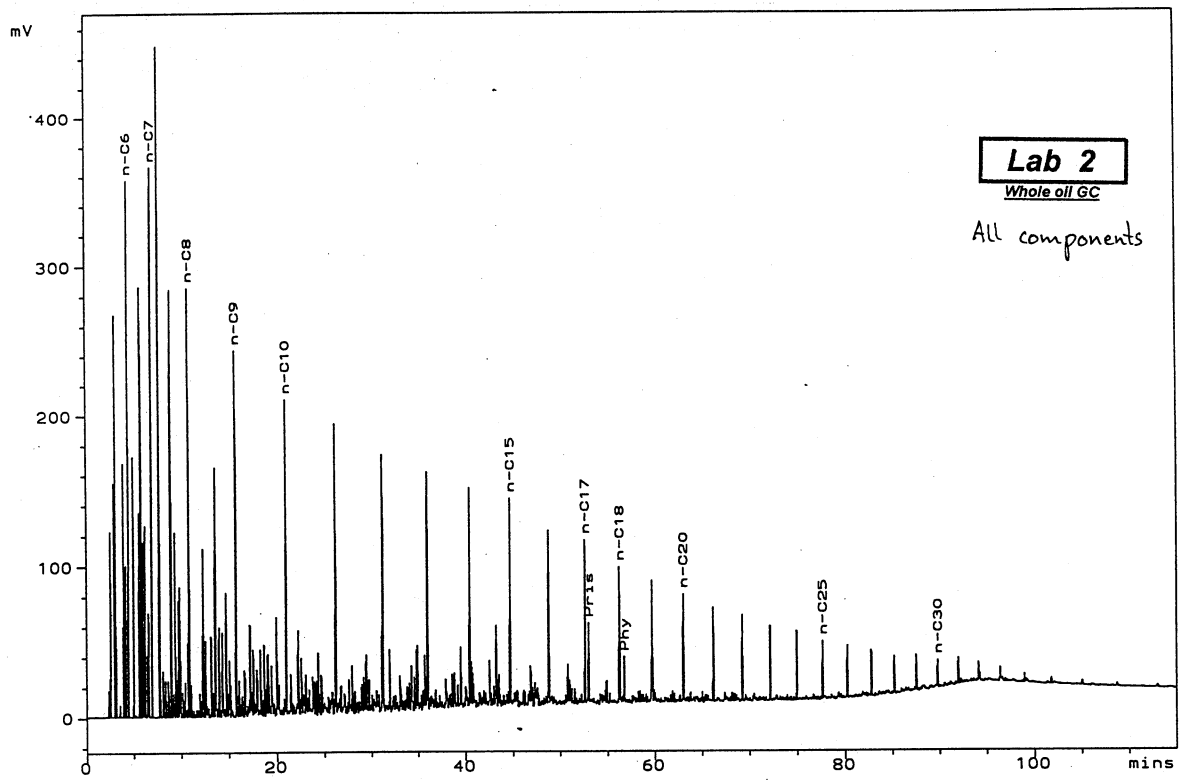
The other laboratories analysed all constituents in one run. Most of these laboratories produced an expansion of the light end of the chromatogram in addition to the total chromatogram.

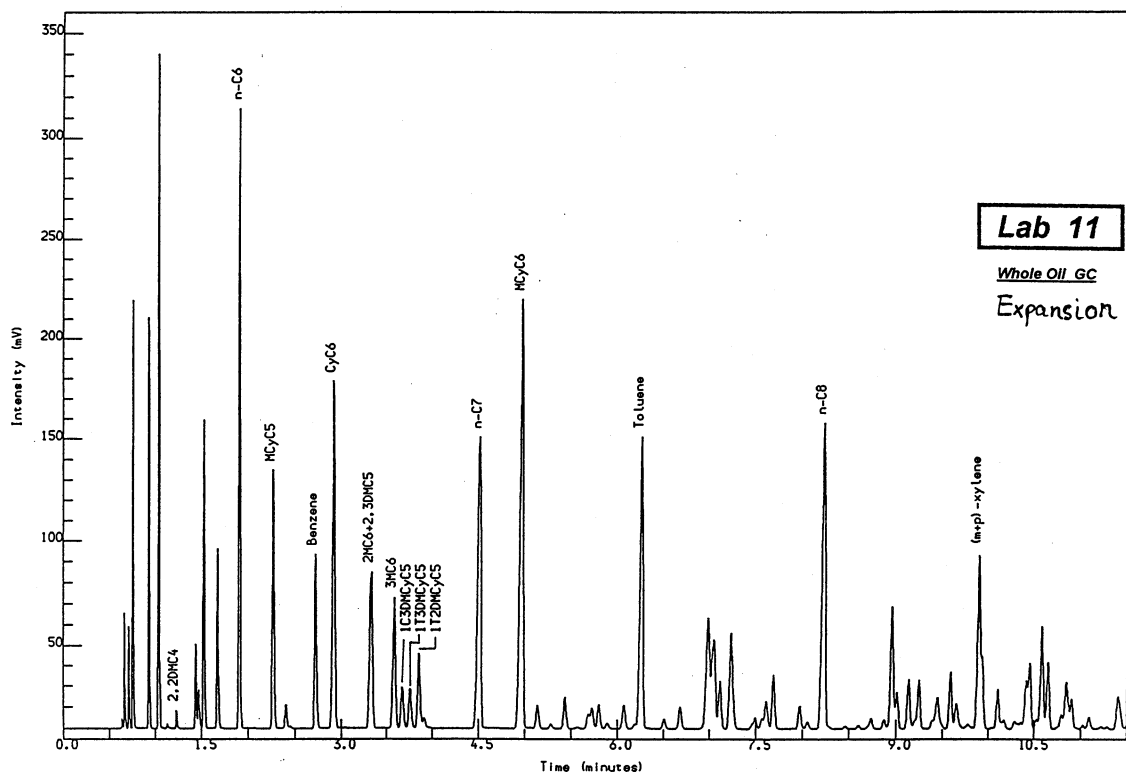
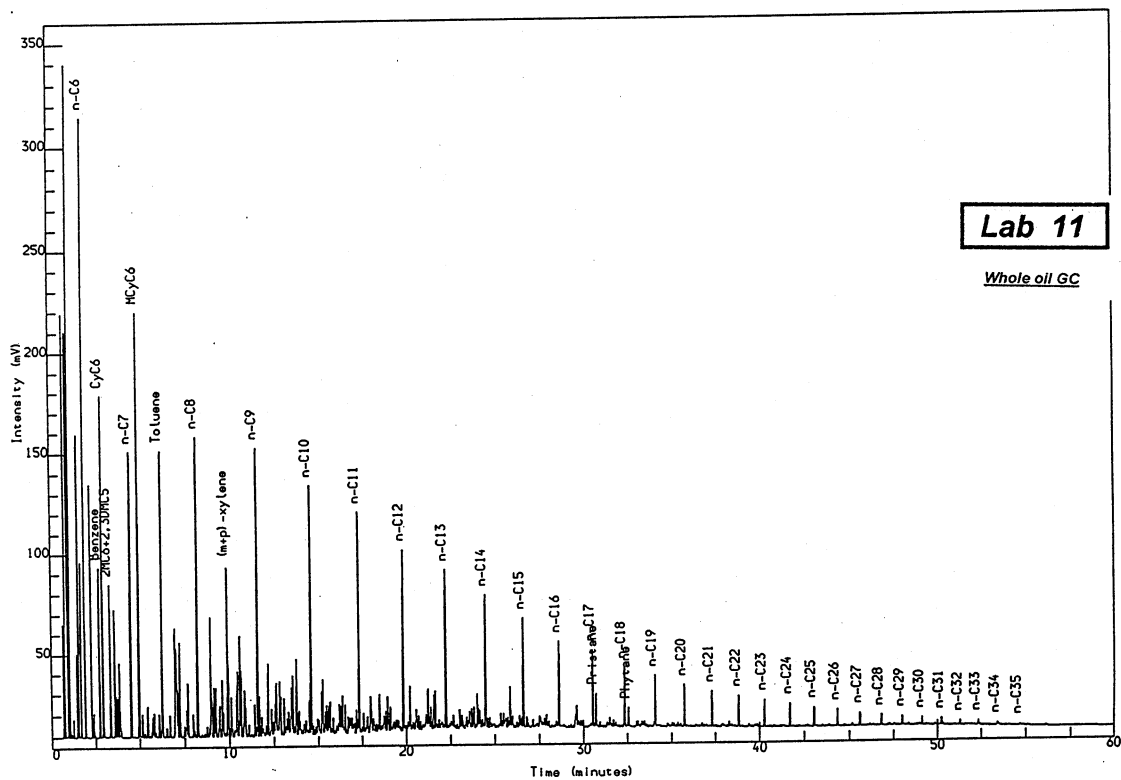
Lab 1

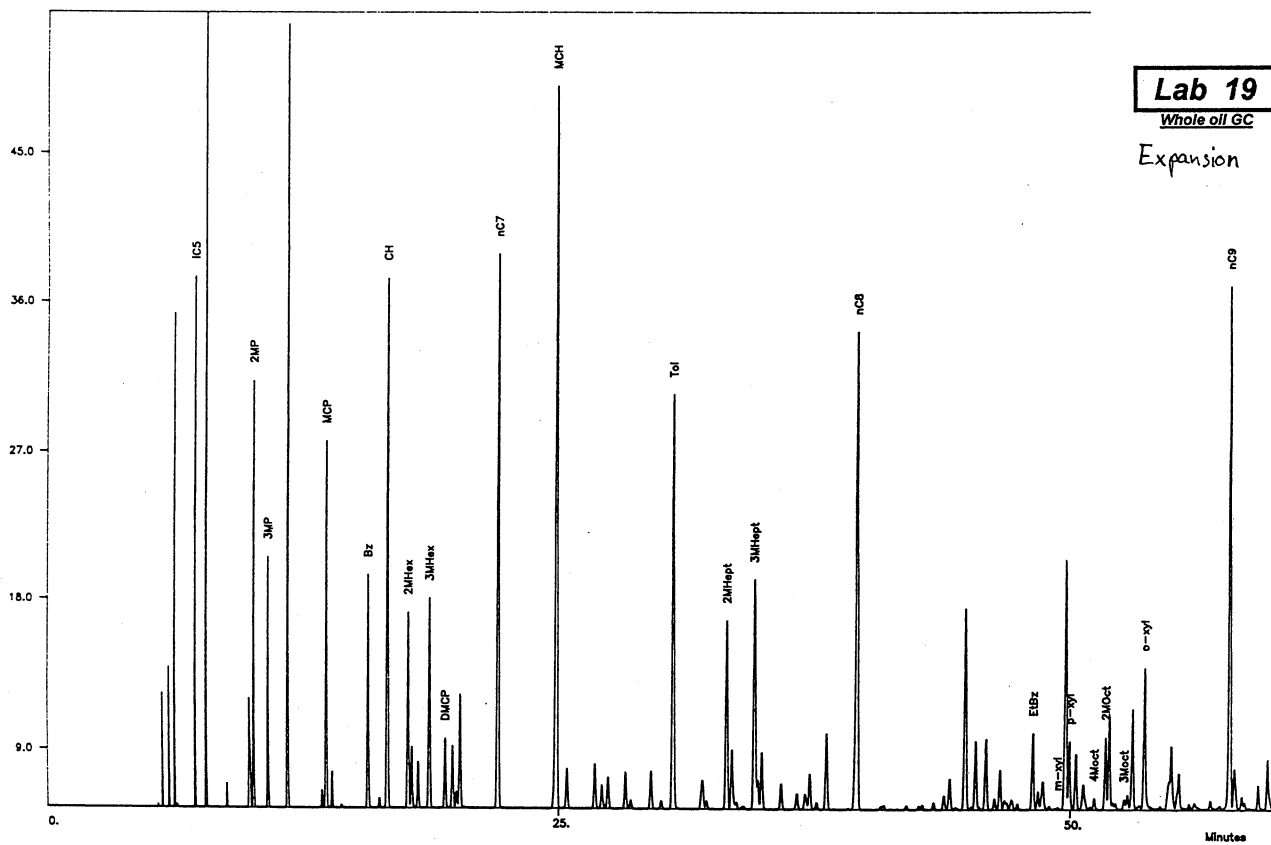
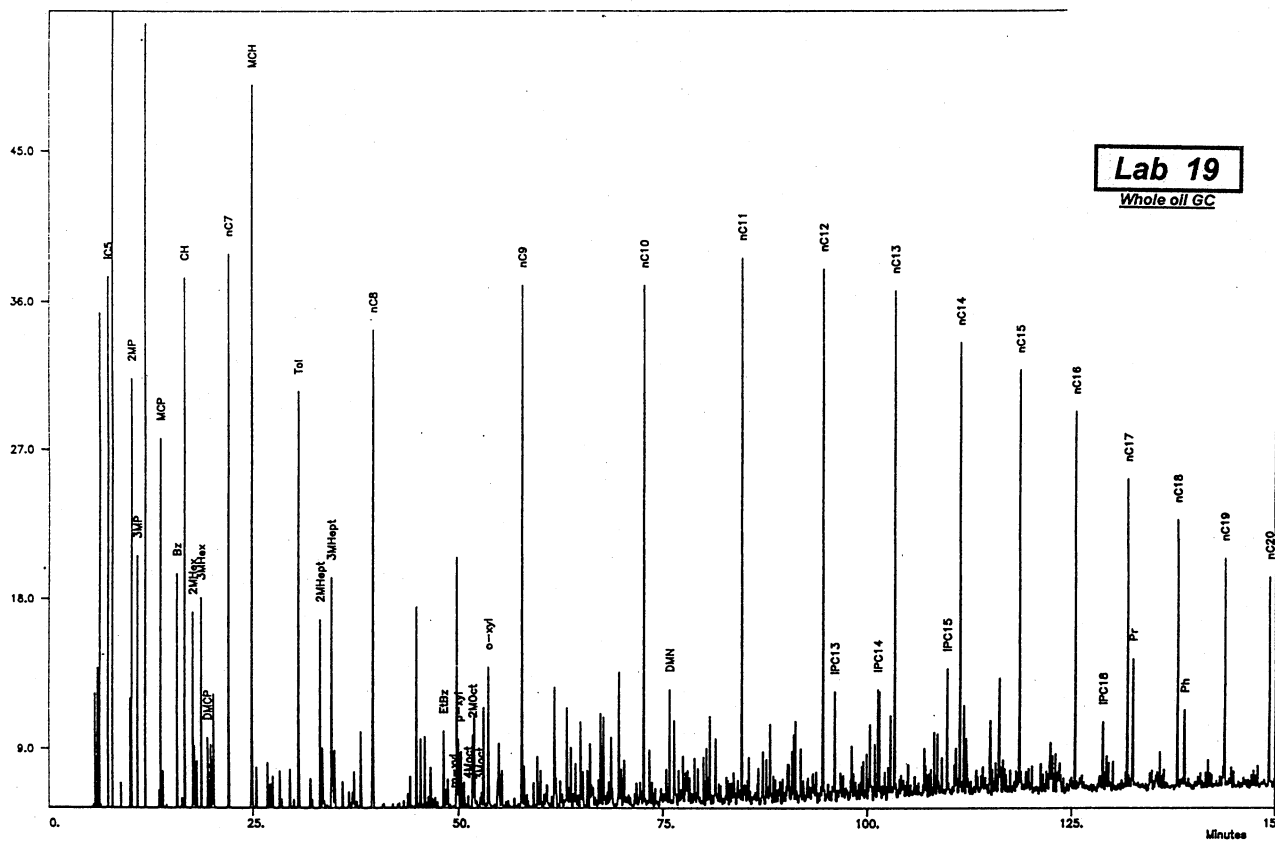
Whole oil GC

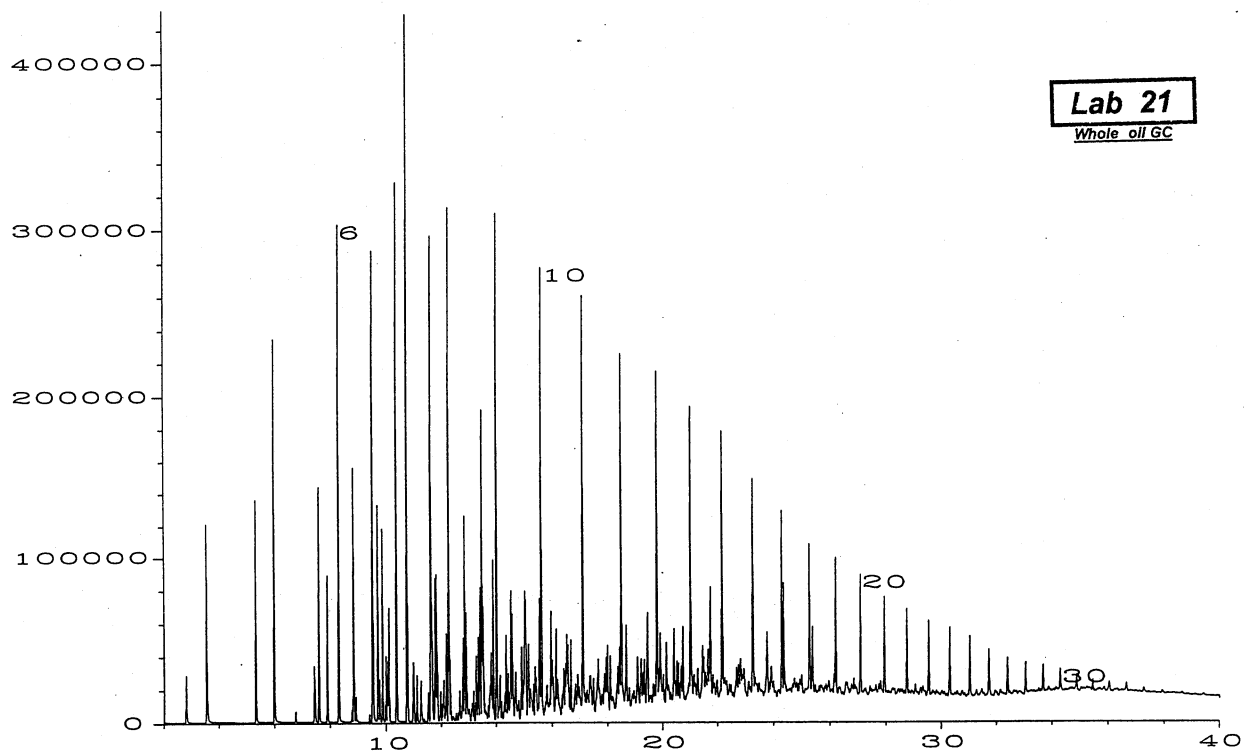
Up to n-C₇

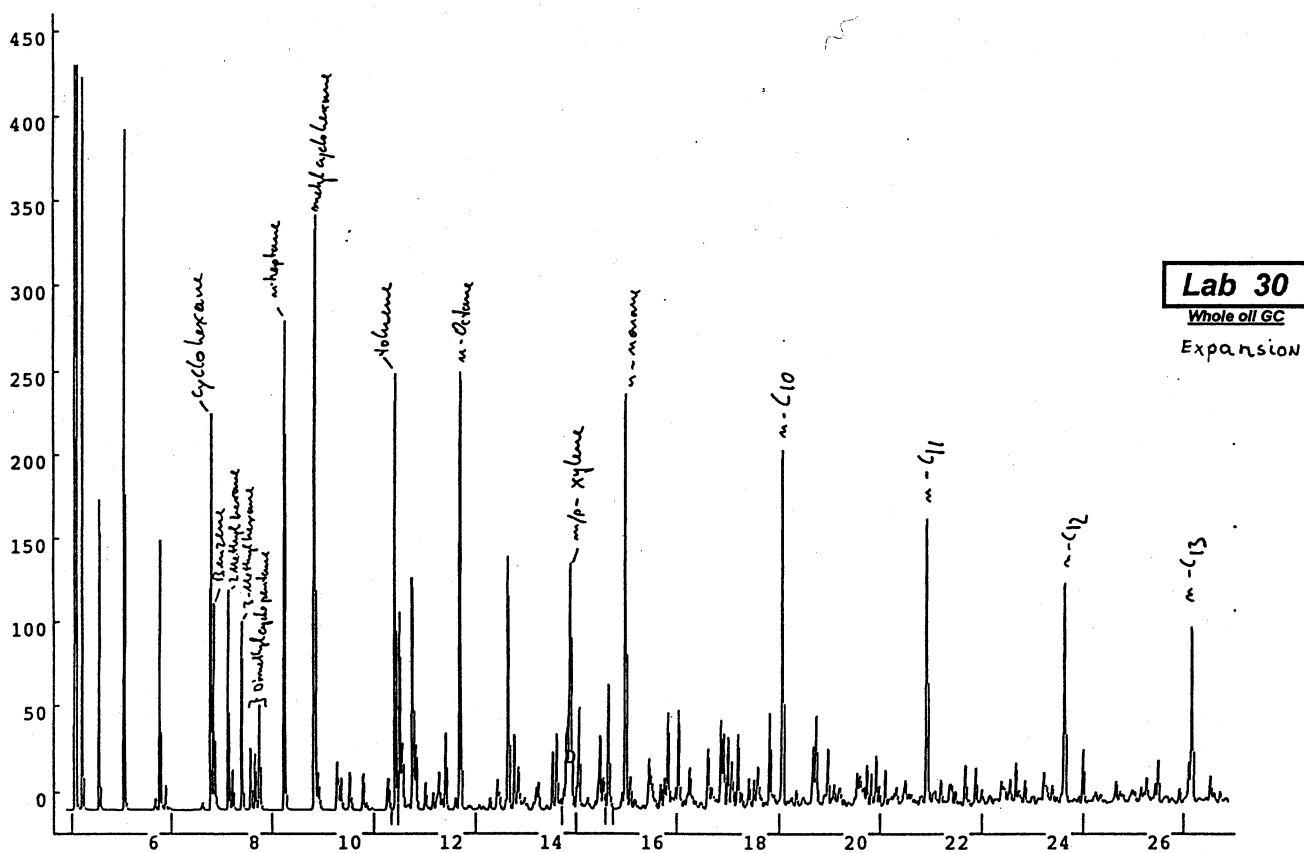
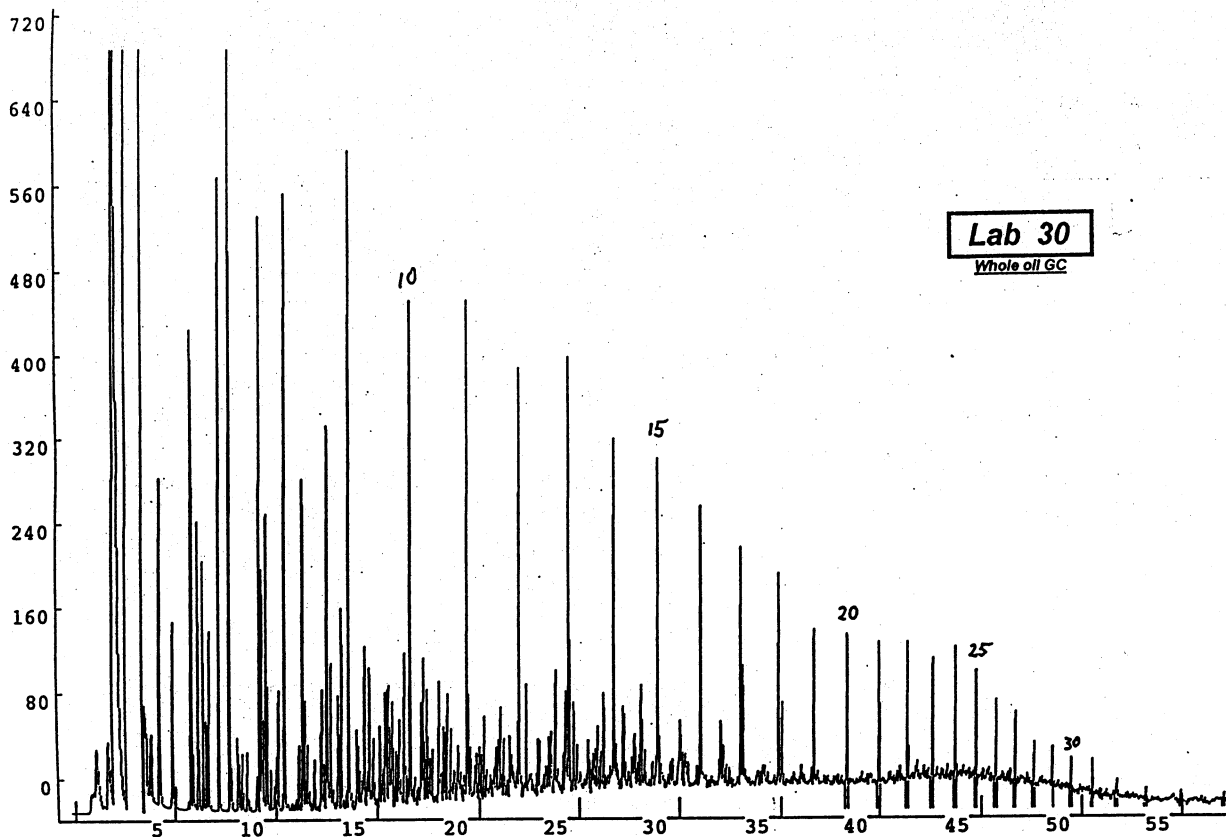


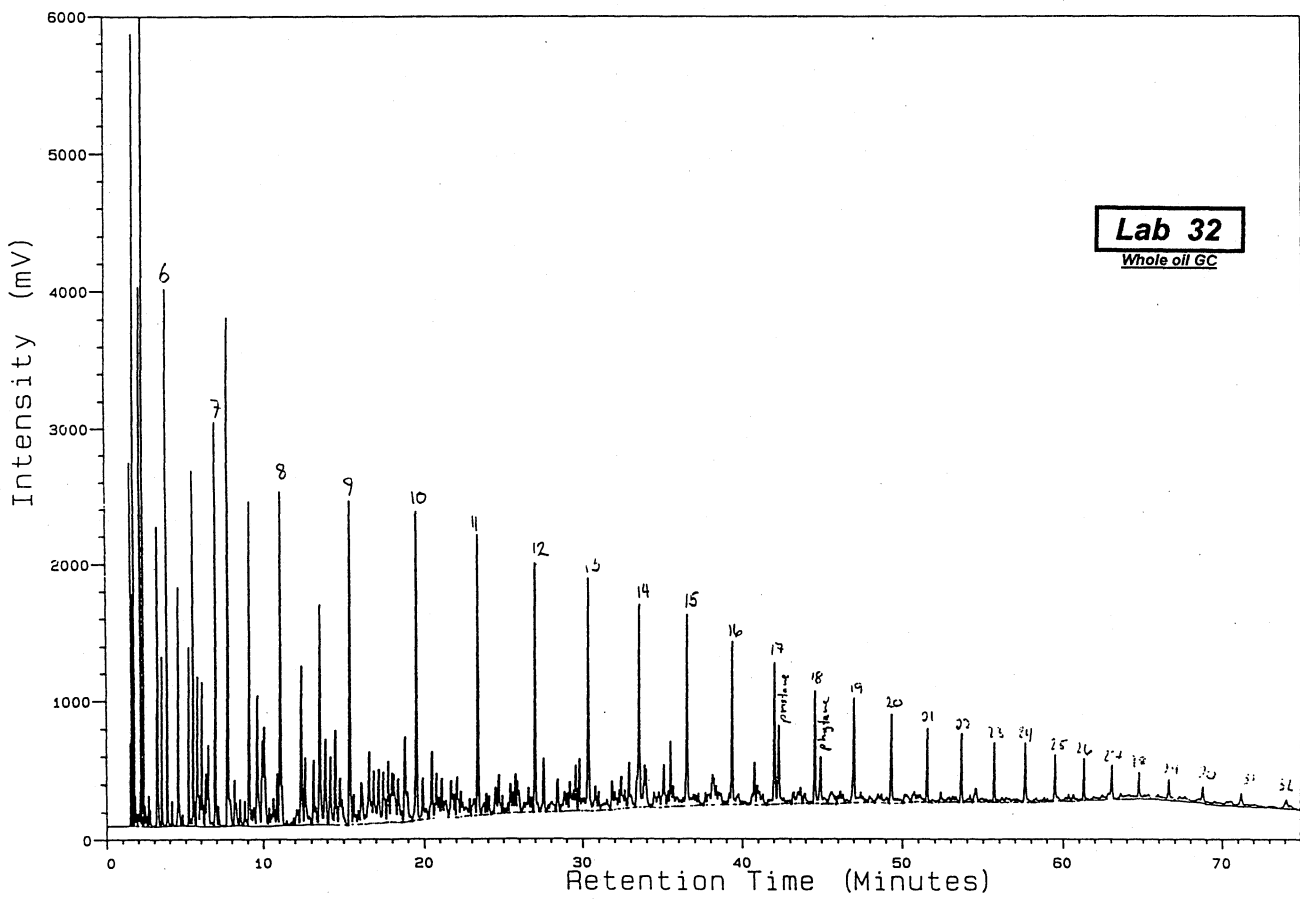


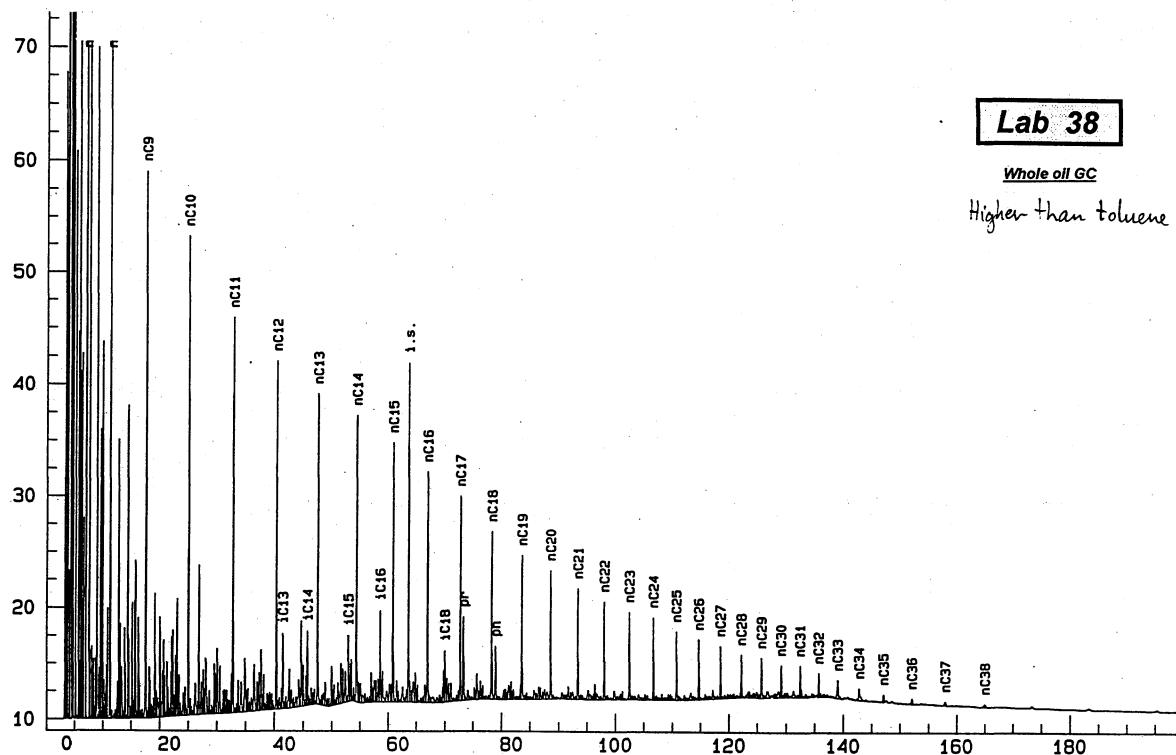




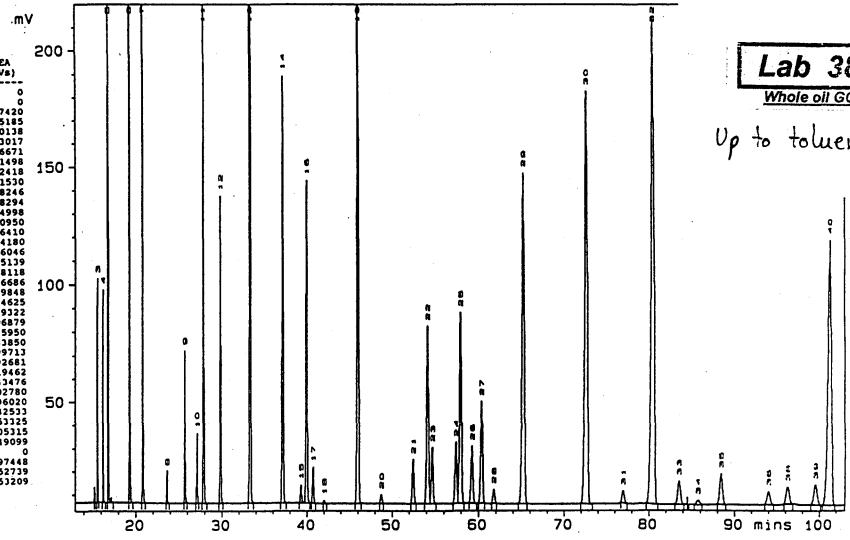


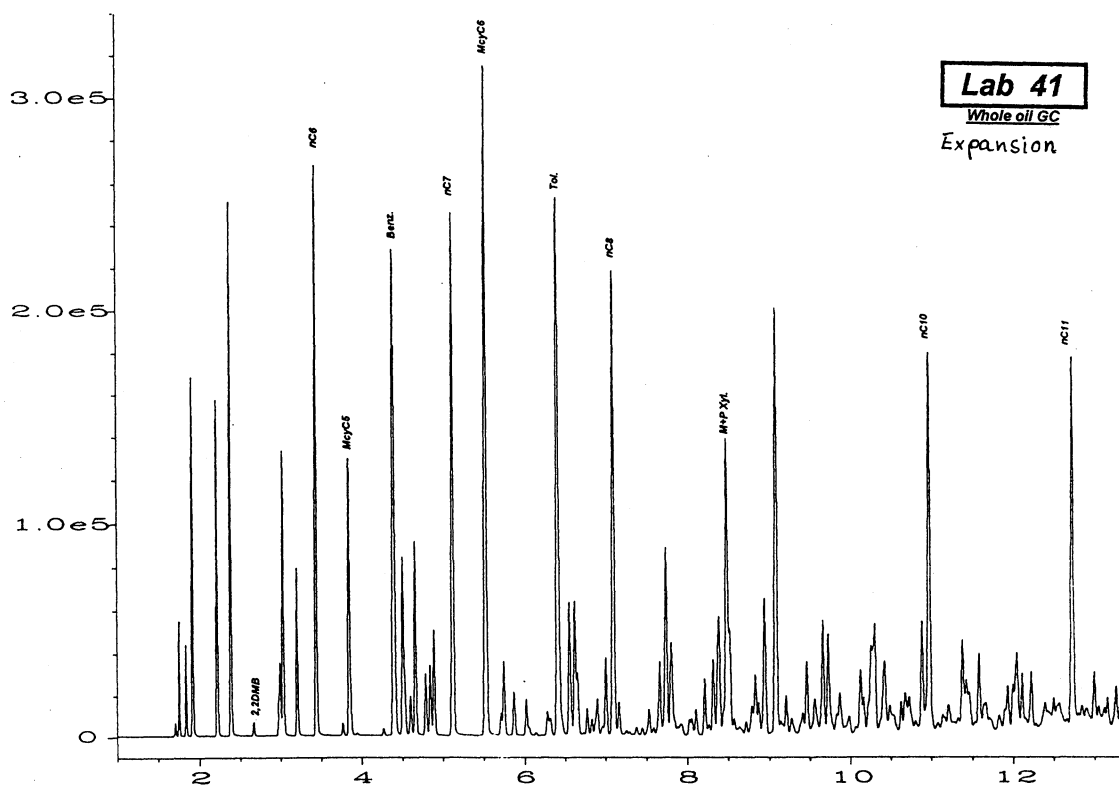
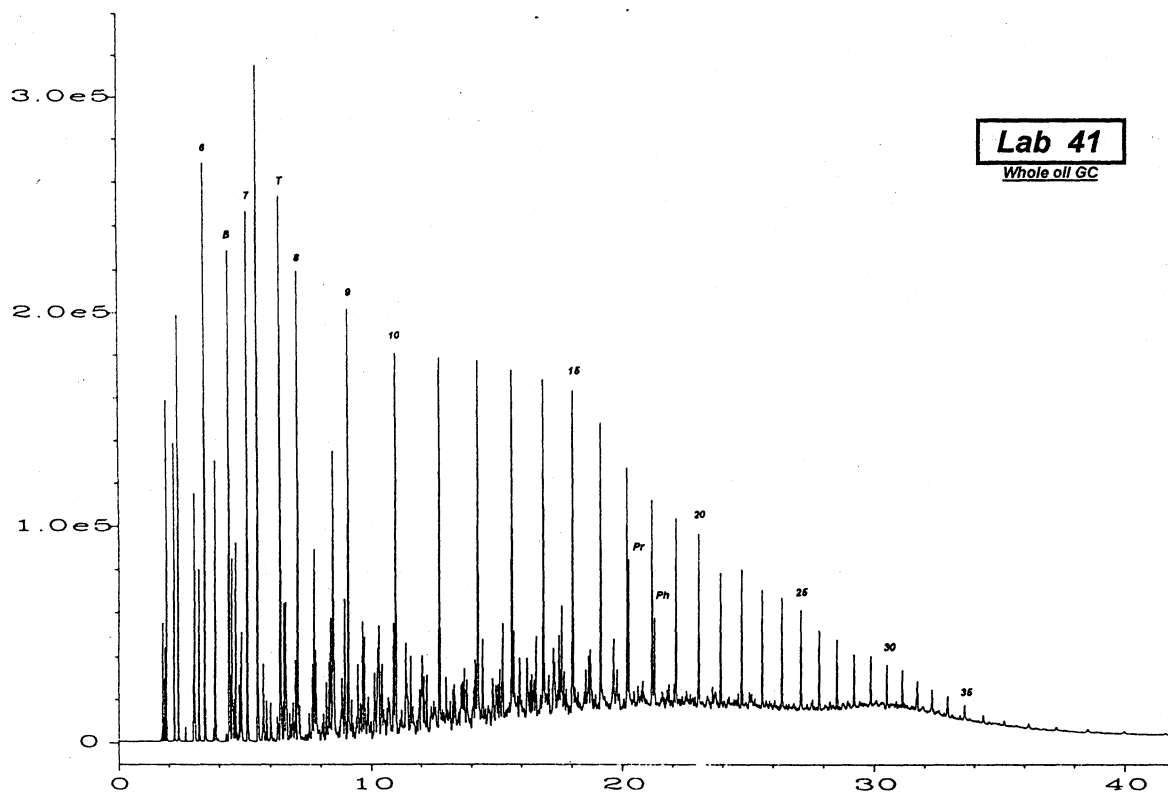


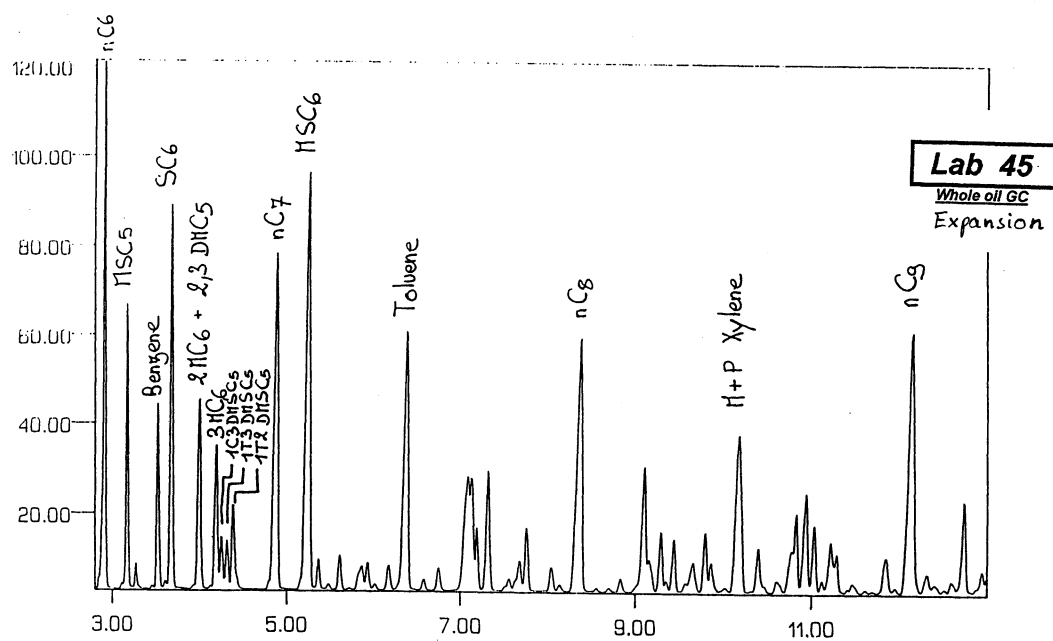
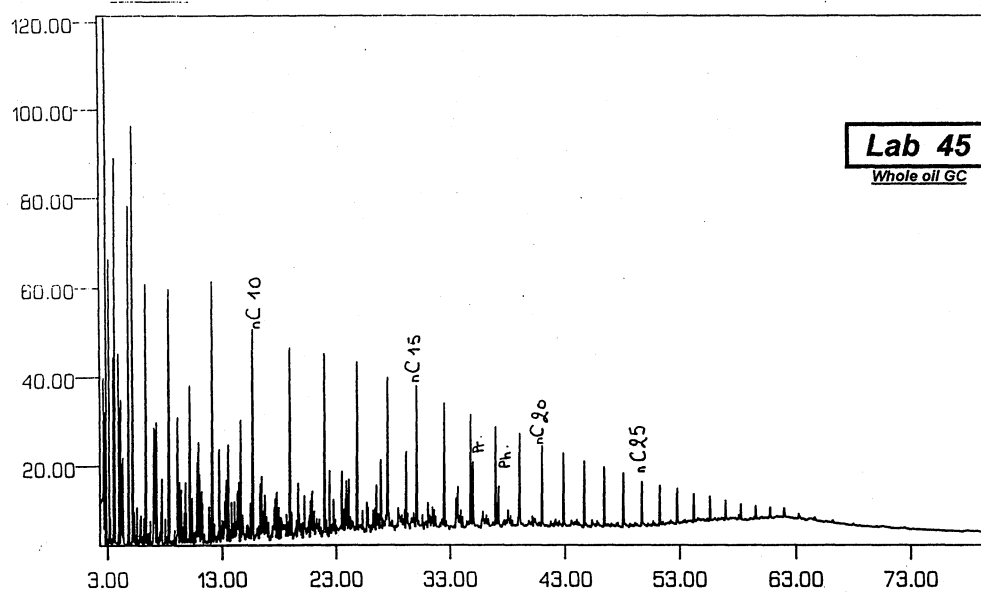


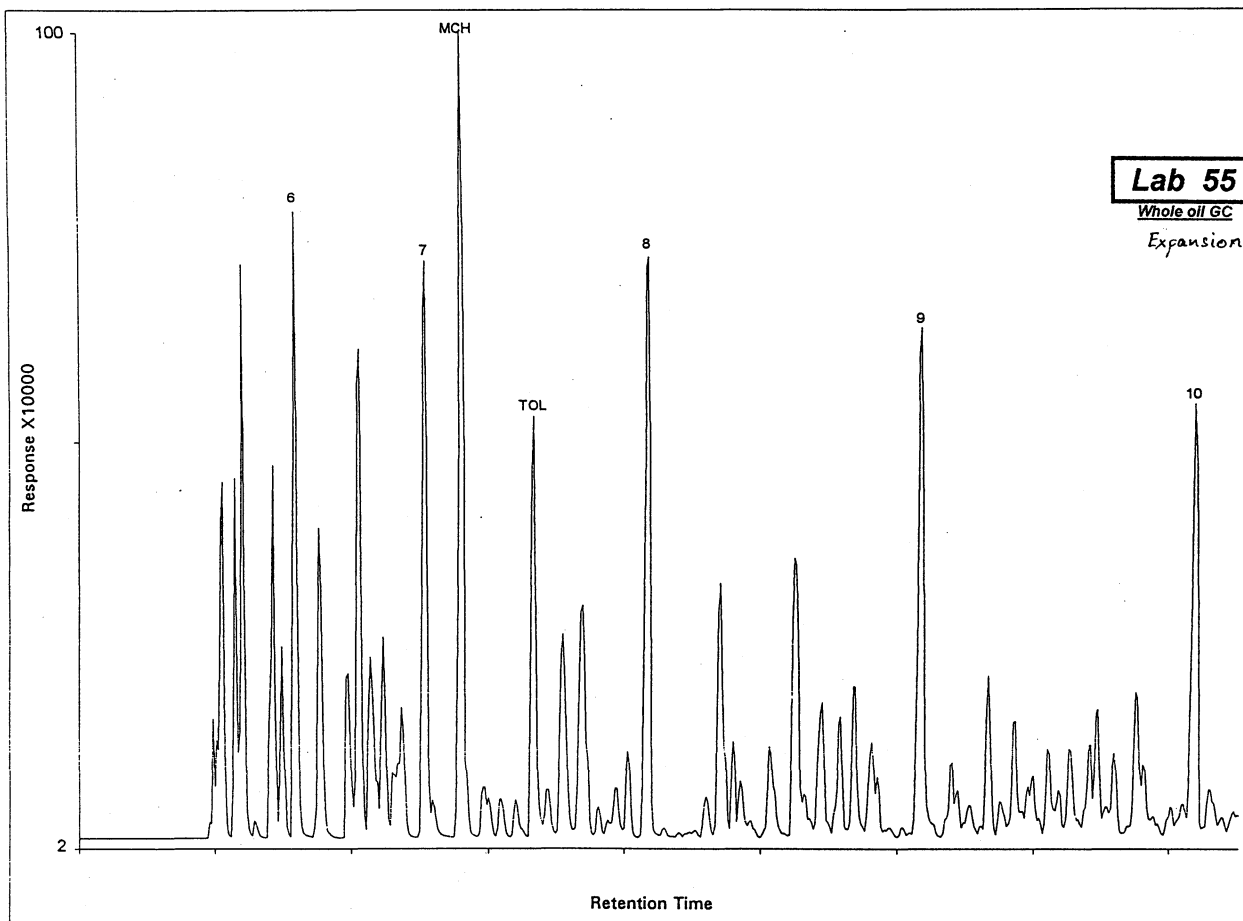
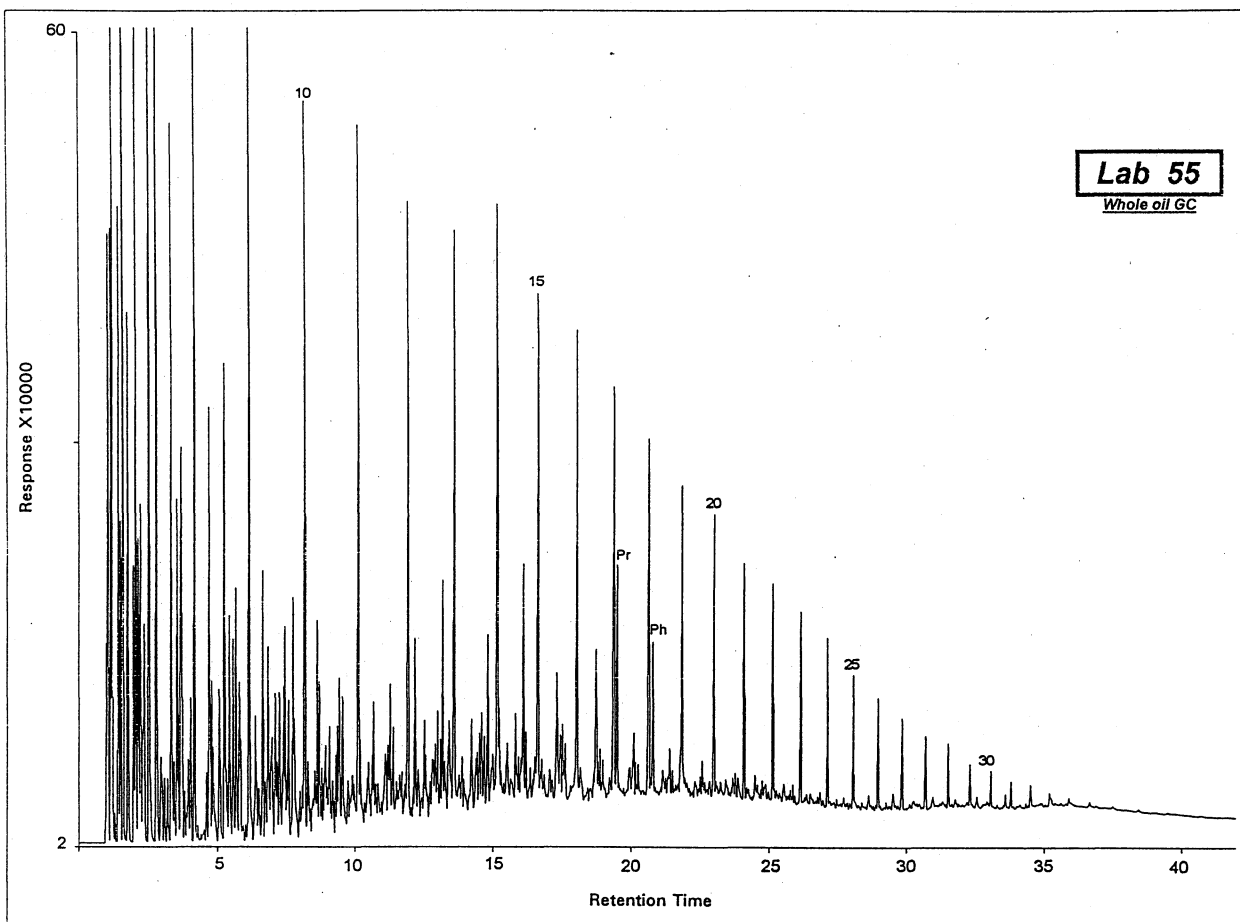


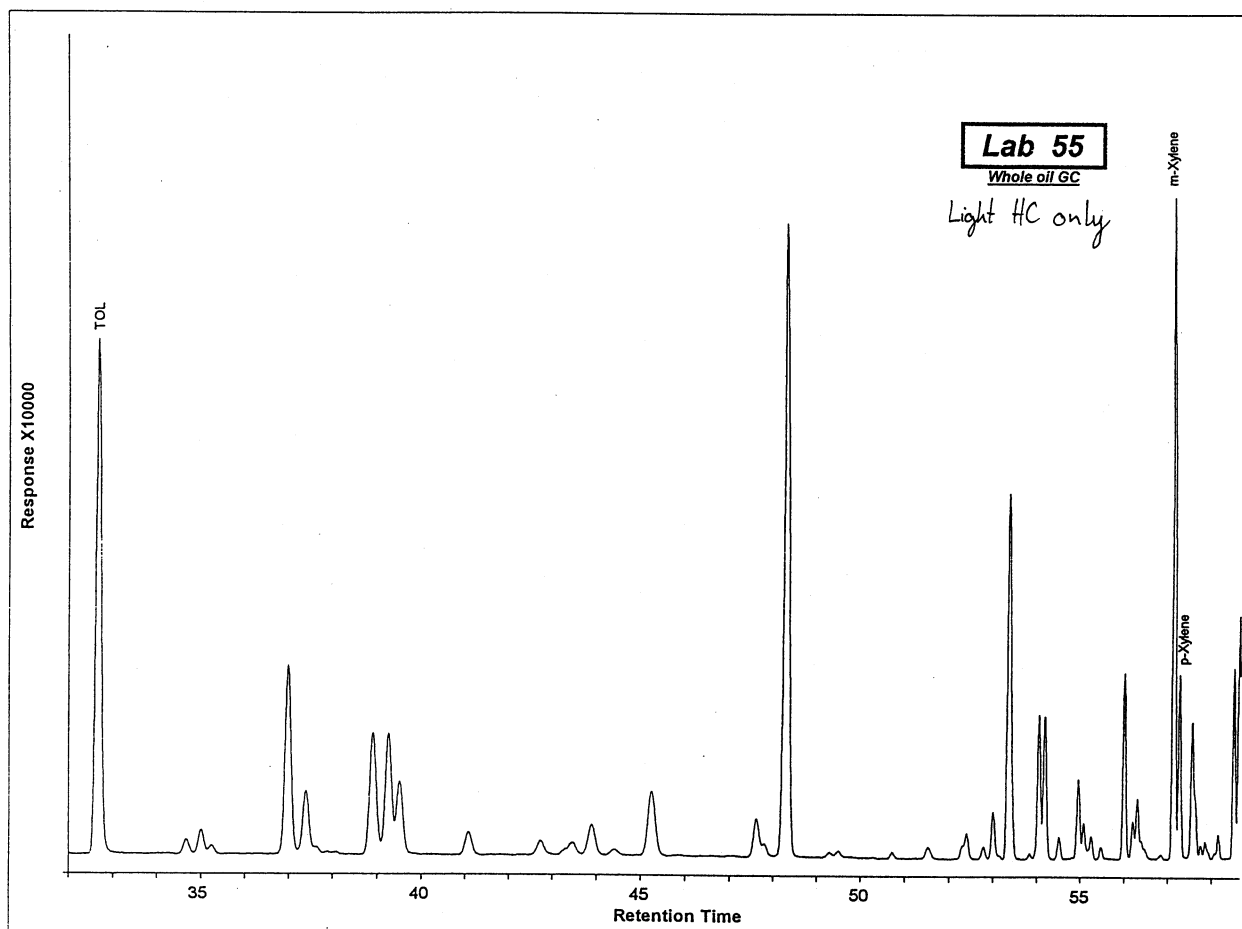
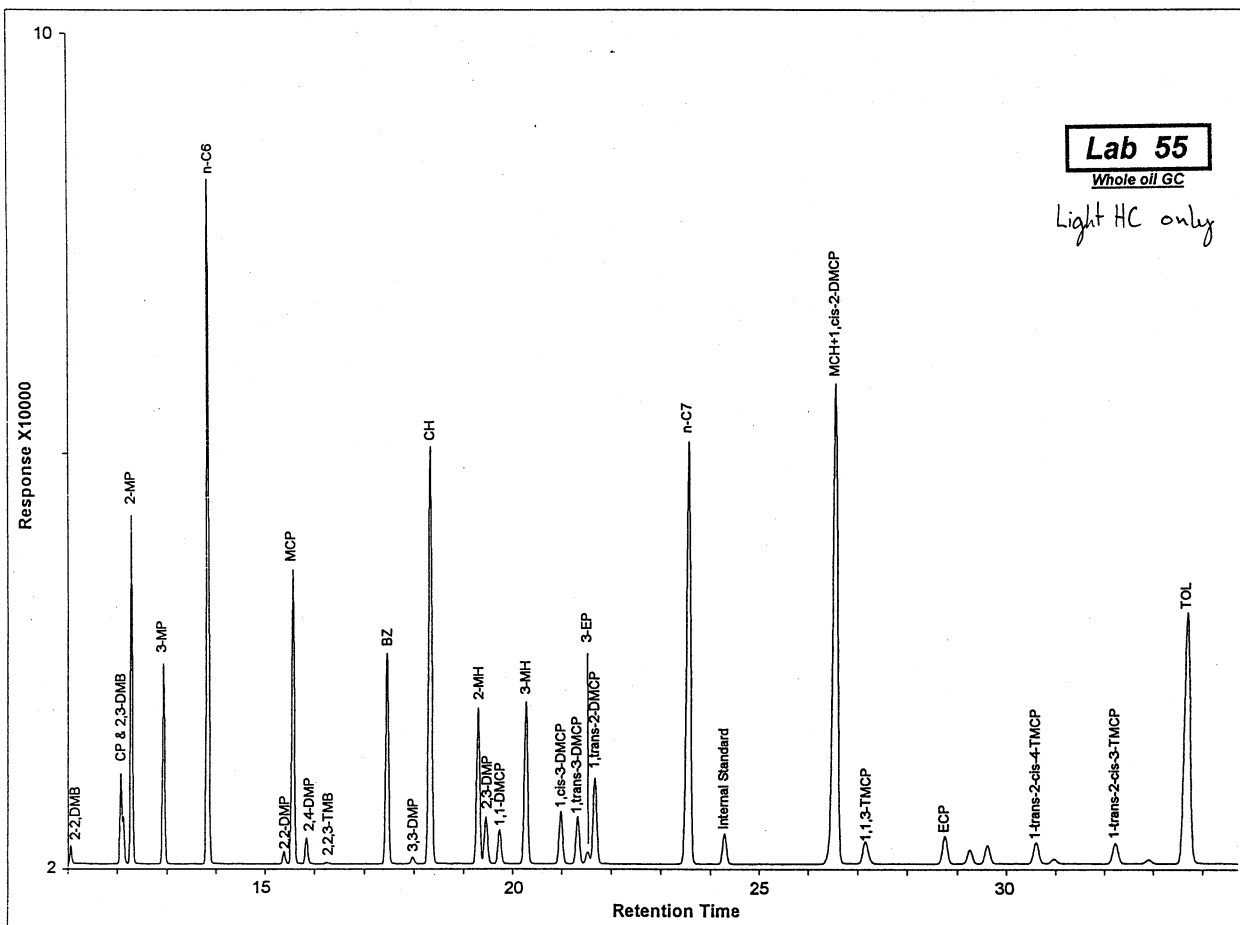
COMPONENT No. Name	RET. TIME (min)	HEIGHT (uV)	AREA (uVs)
1 methane	0.00	0	0
2 ethane	0.00	0	0
3 propane	15.59	95887	277420
4 i-butane	16.22	91183	275185
5 n-butane	16.82	366004	1170138
6 i-pentane	19.28	353802	1341017
7 n-pentane	20.79	550039	2284671
8 2,3-dimethylbutane	23.62	13905	71498
9 cyclopentane	25.71	65817	362418
10 2,3-dimethylbutane	27.10	30108	181520
11 2-methylpentane	27.87	212991	1458246
12 3-methylpentane	29.83	131378	898294
13 n-hexane	33.33	404219	1114098
14 methylcyclopentane	37.16	182920	1620950
15 2,2-dimethylpentane	39.30	7567	76410
16 benzene	39.98	137907	1284180
17 2,4-dimethylpentane	40.72	15401	156046
18 2,2,3-trimethylbutane	42.02	1422	15139
19 cyclohexane	46.03	241643	2828118
20 3,3-dimethylpentane	48.74	3867	46886
21 1,1-dimethylcyclopentane	52.43	19098	259848
22 2-methylhexane	54.13	76483	1114625
23 2,3-dimethylpentane	54.66	24484	349322
24 1-c-3-dimethylcyclopentane	57.40	26427	406879
25 3-methylhexane	57.94	82121	1235950
26 1-tr-3-dimethylcyclopentane	59.25	24831	383850
27 1-tr-2-dimethylcyclopentane	60.37	44001	699713
28 3-ethylpentane	61.77	6002	92681
29 reference peak	65.23	141649	2618462
30 n-heptane	72.66	177074	3743476
31 1-c-2-dimethylcyclopentane	76.98	3157	102780
32 methylcyclohexane	80.52	207924	4996020
33 1,1,3-trimethylcyclopentane	83.53	10046	232532
34 2,2-dimethylhexane	85.70	2052	51125
35 ethylcyclopentane	88.44	13243	305315
36 2,5-dimethylhexane	94.00	5785	149089
37 not present	0.00	0	0
38 2,2,3-trimethylpentane	96.25	7442	197448
39 1-tr-2-c-4-trimethylcyclopentane	99.51	8886	252739
40 toluene	101.29	113688	2253209

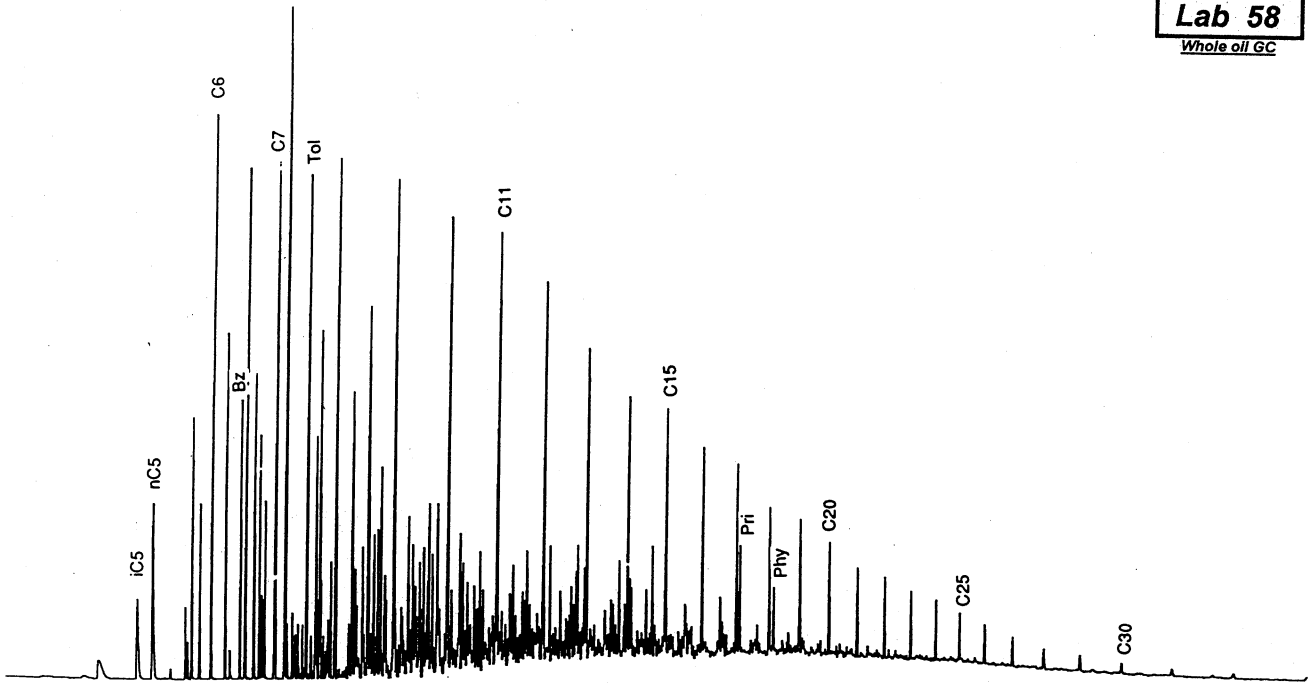


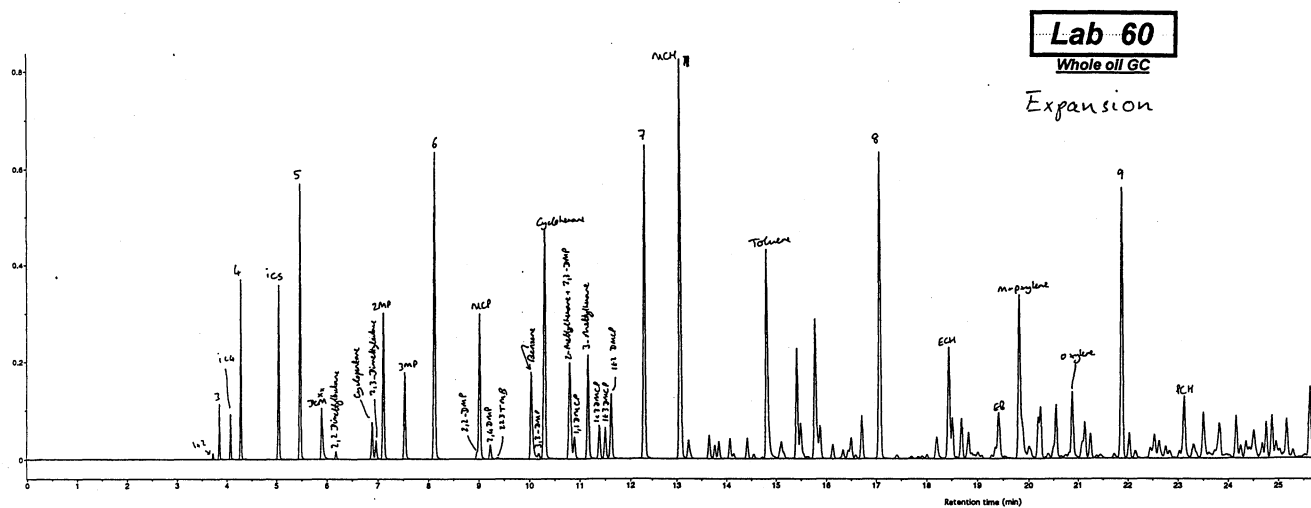
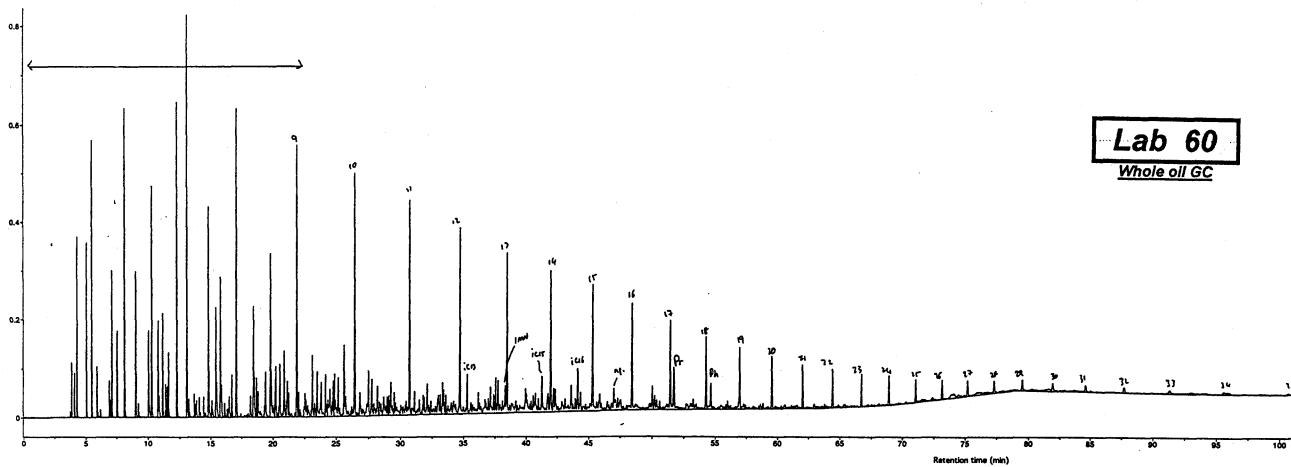


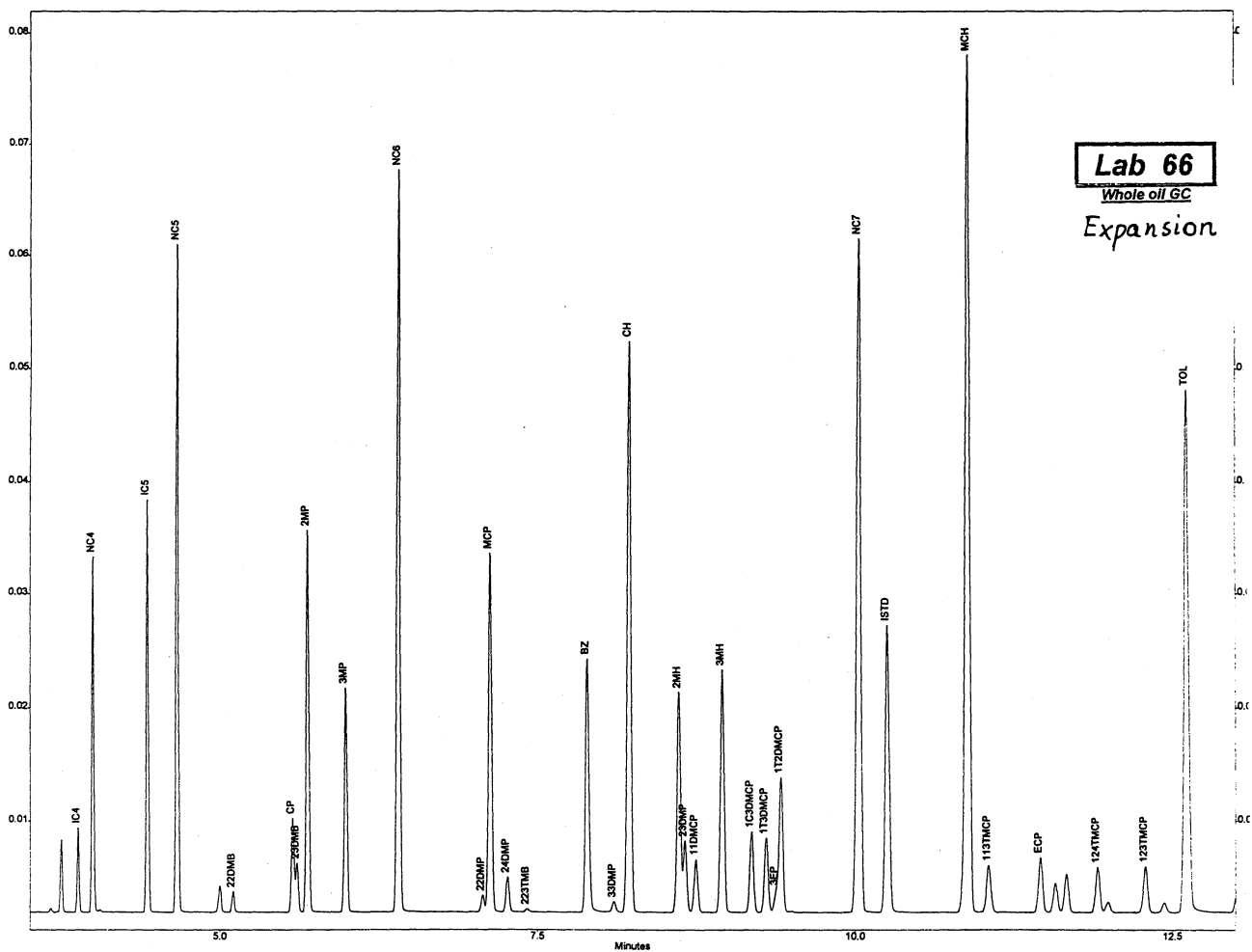
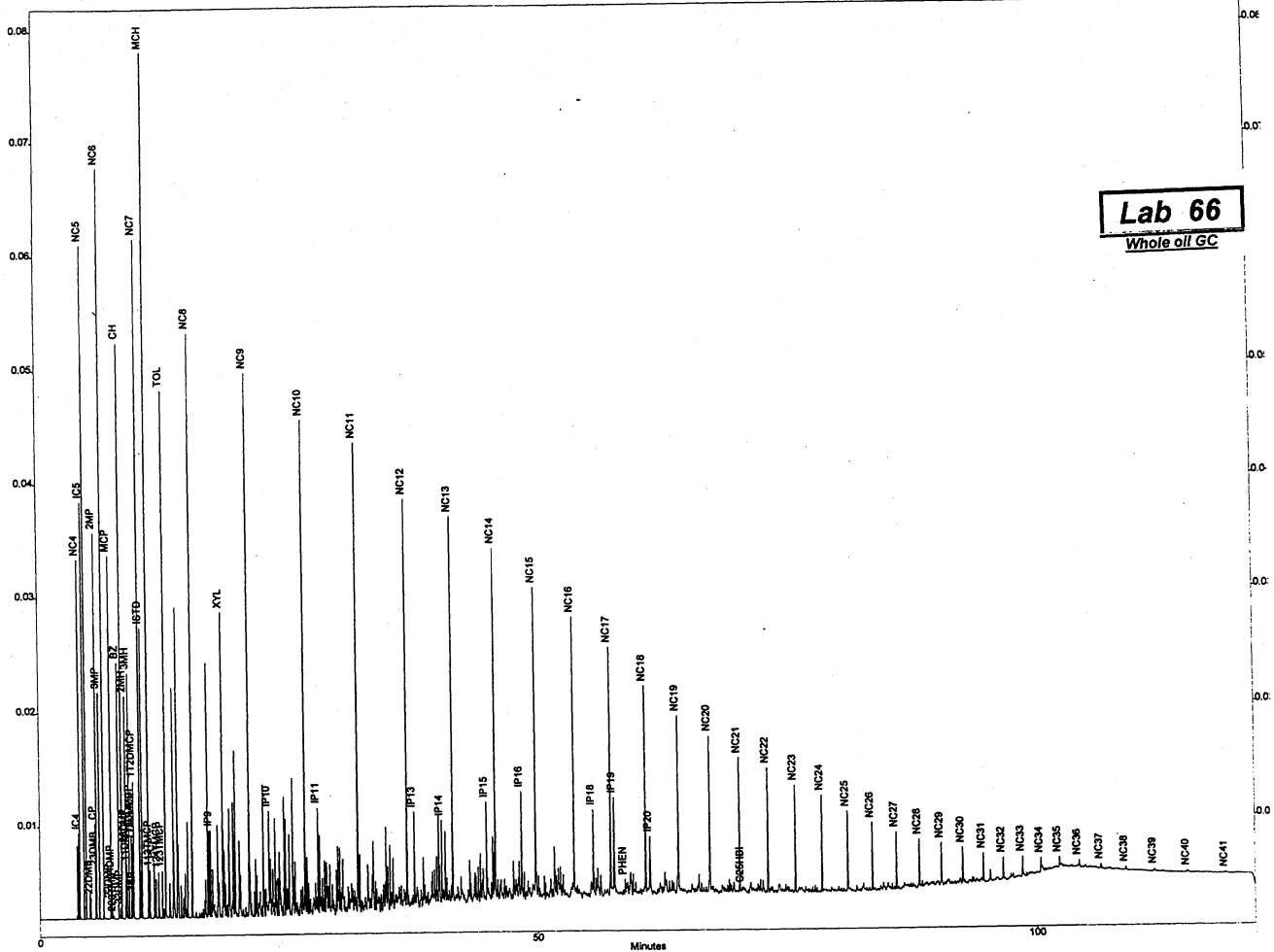


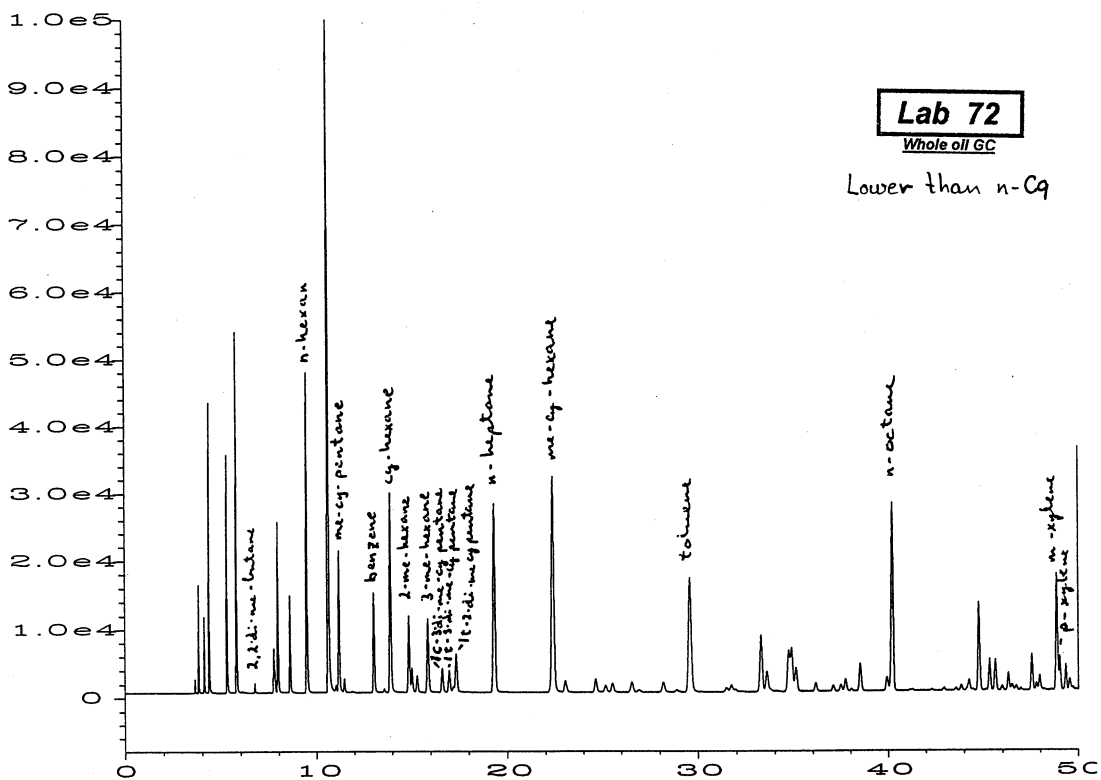
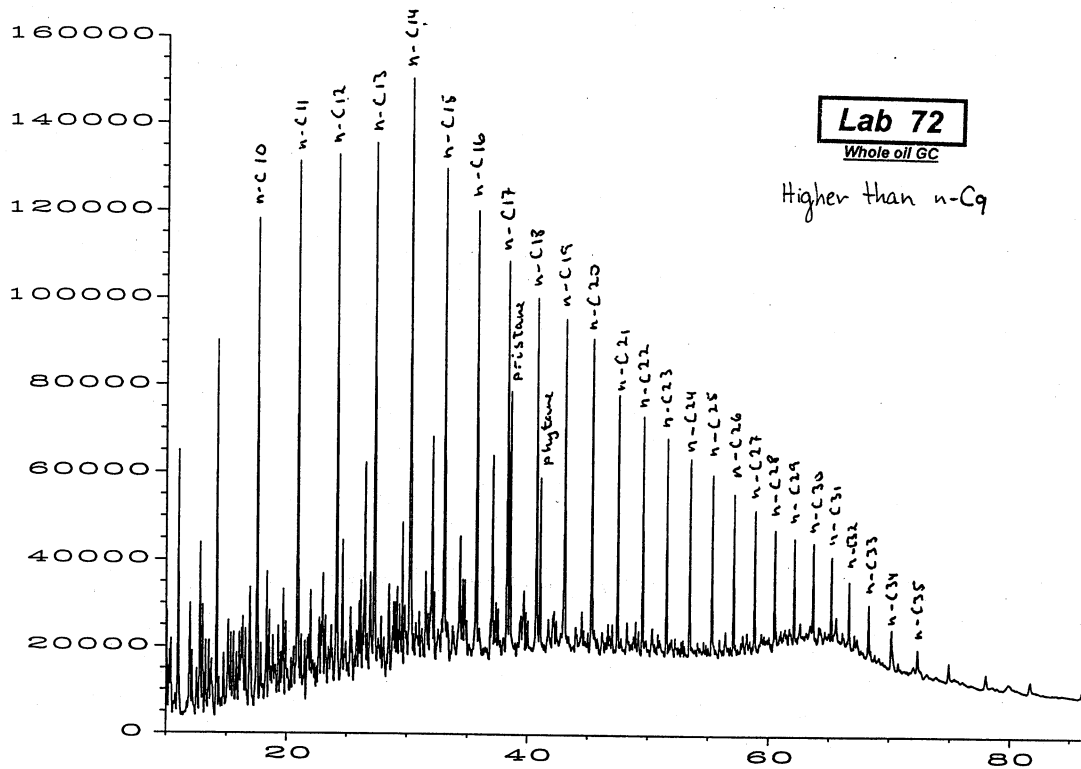


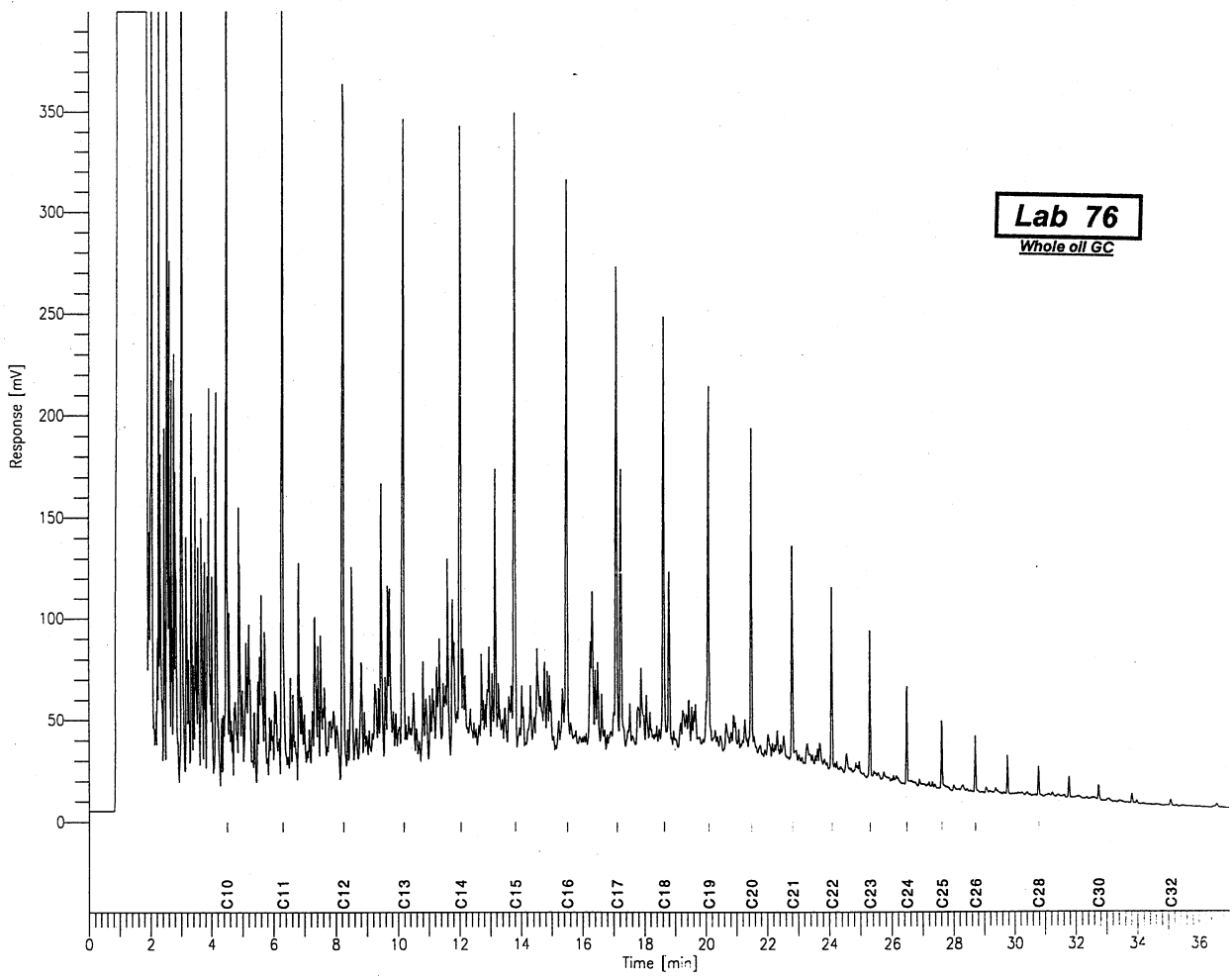


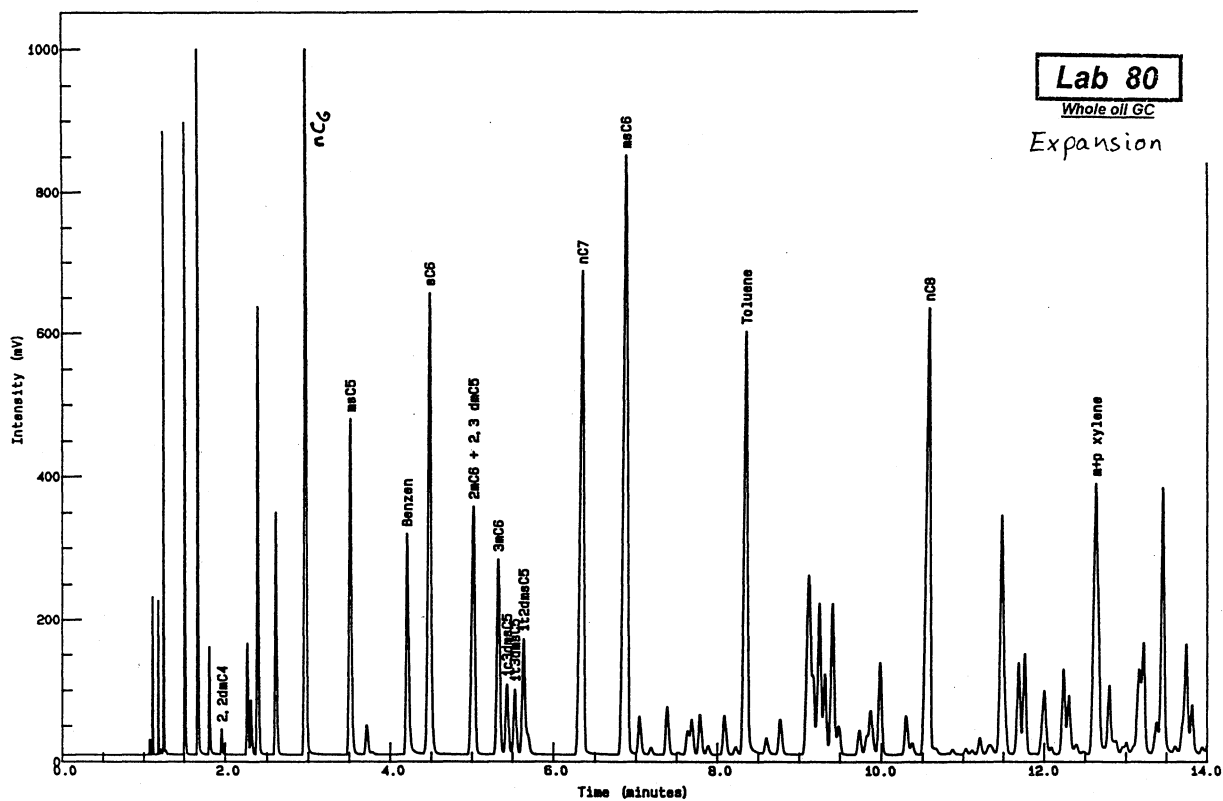
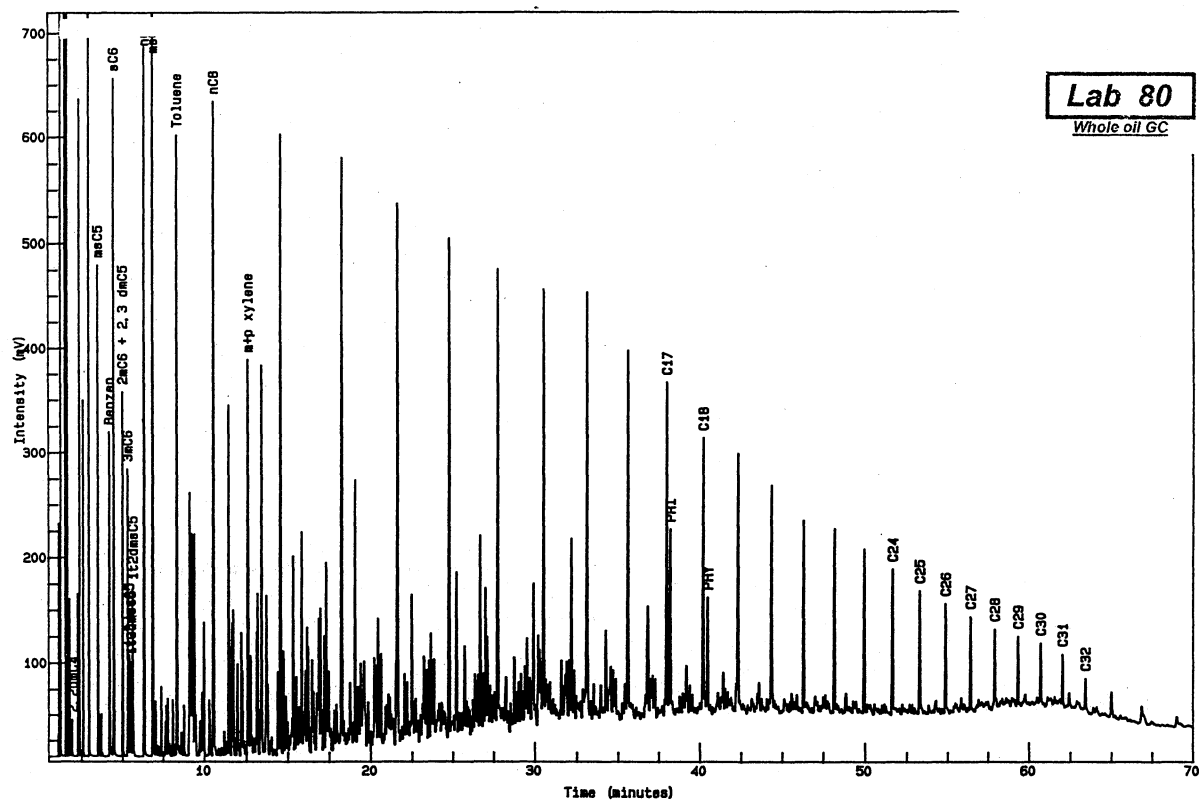


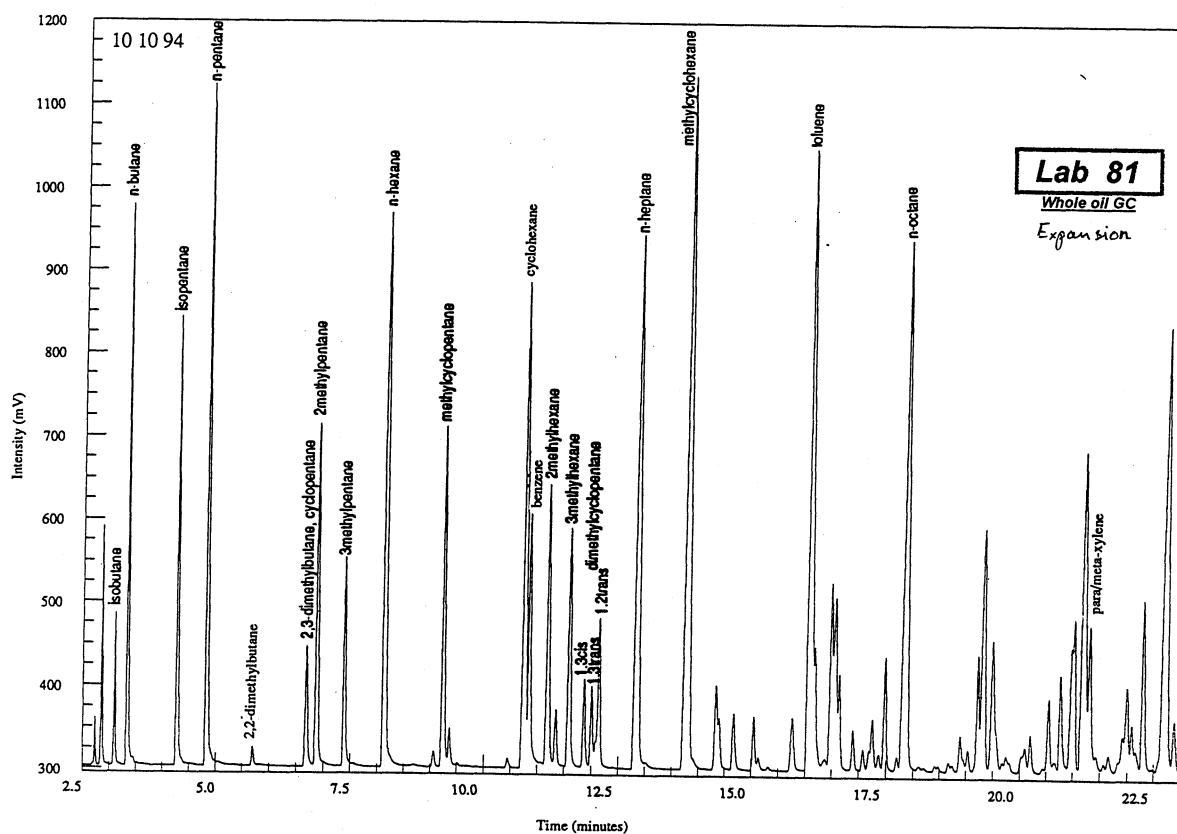
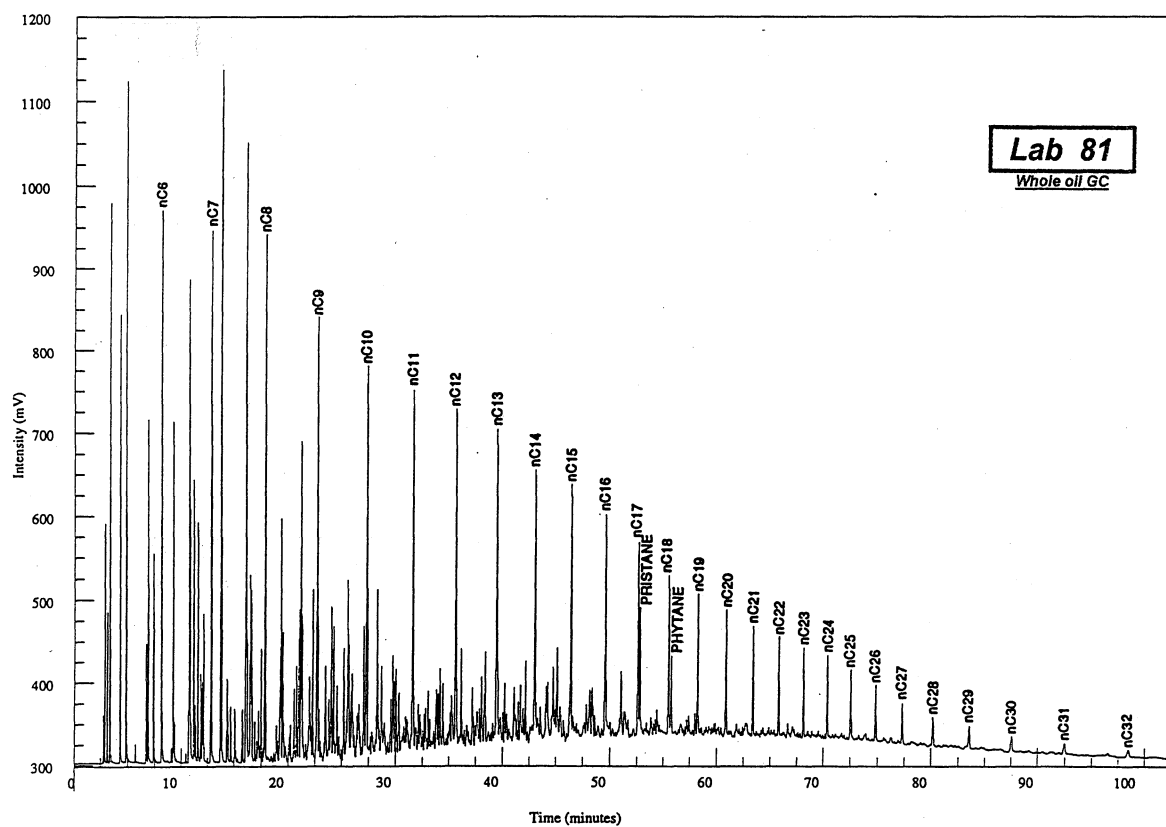


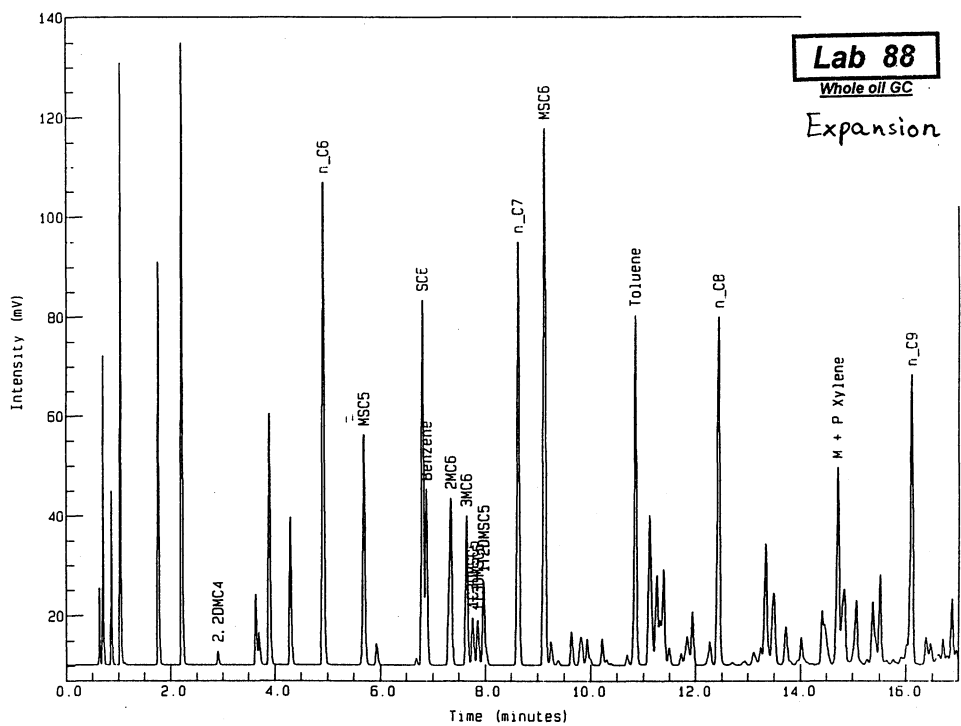
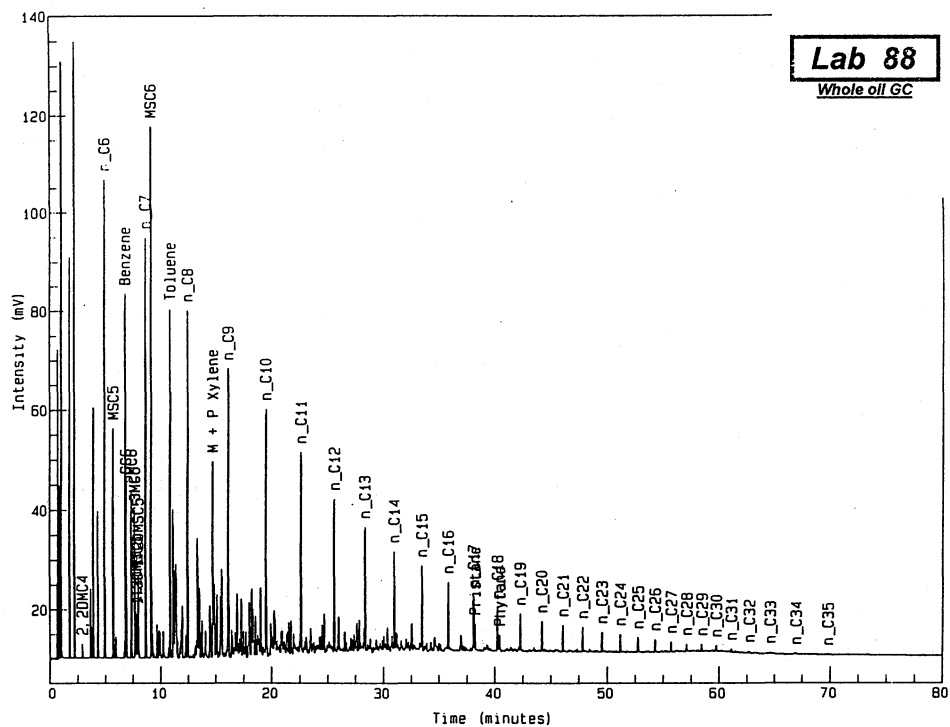






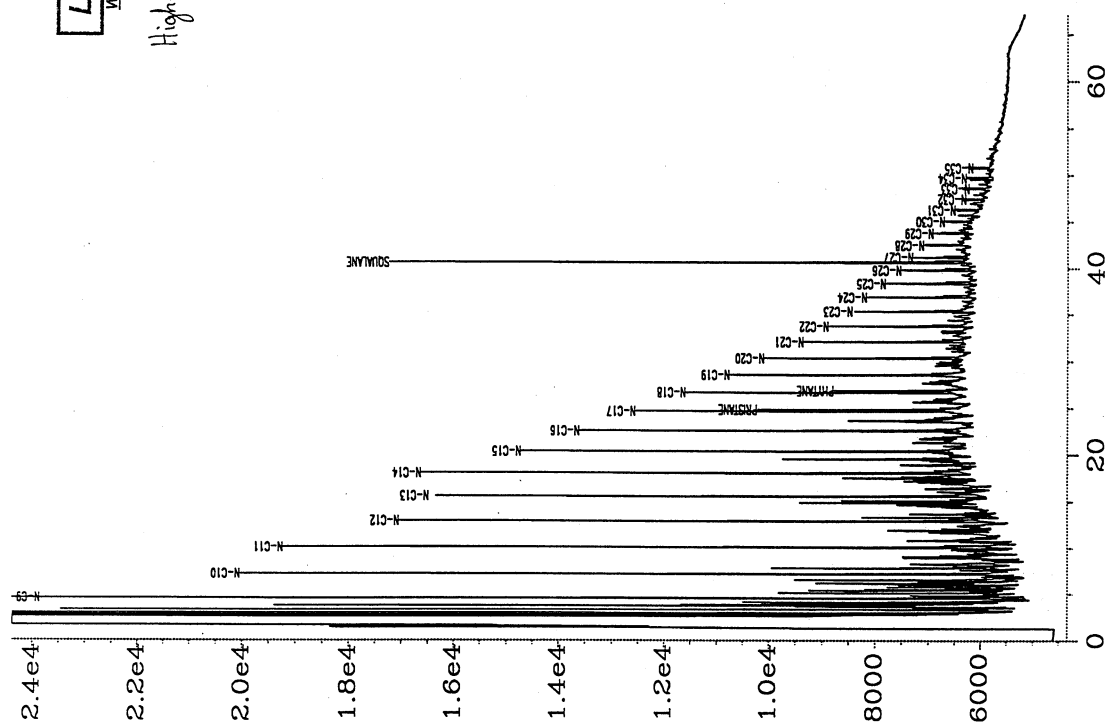






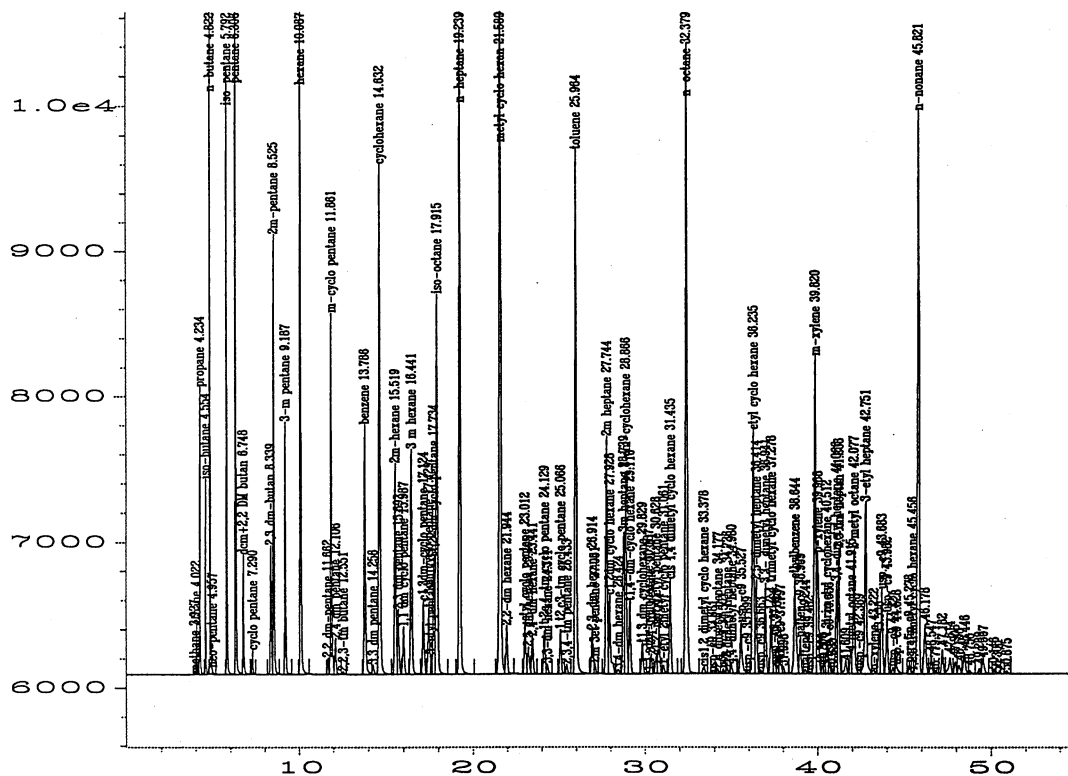
Whole oil GC

Higher than n-C9

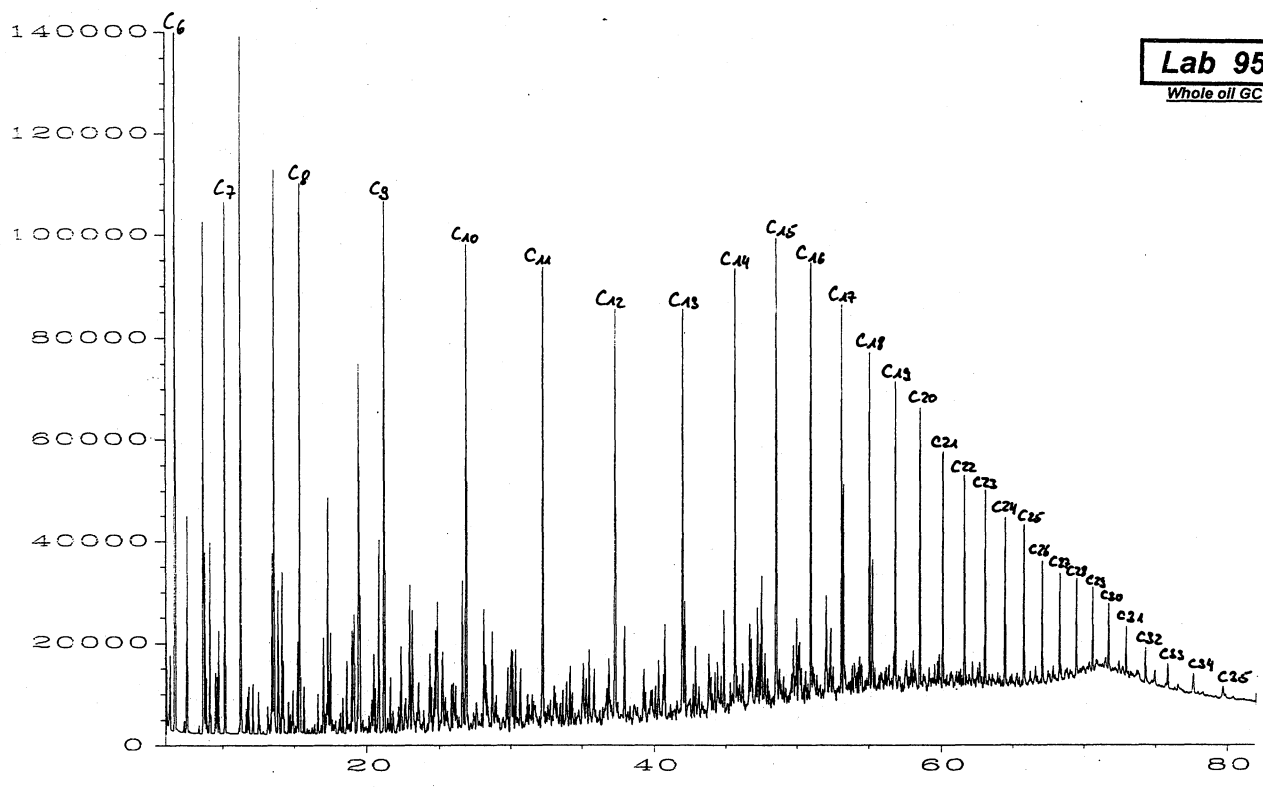


Whole oil GC

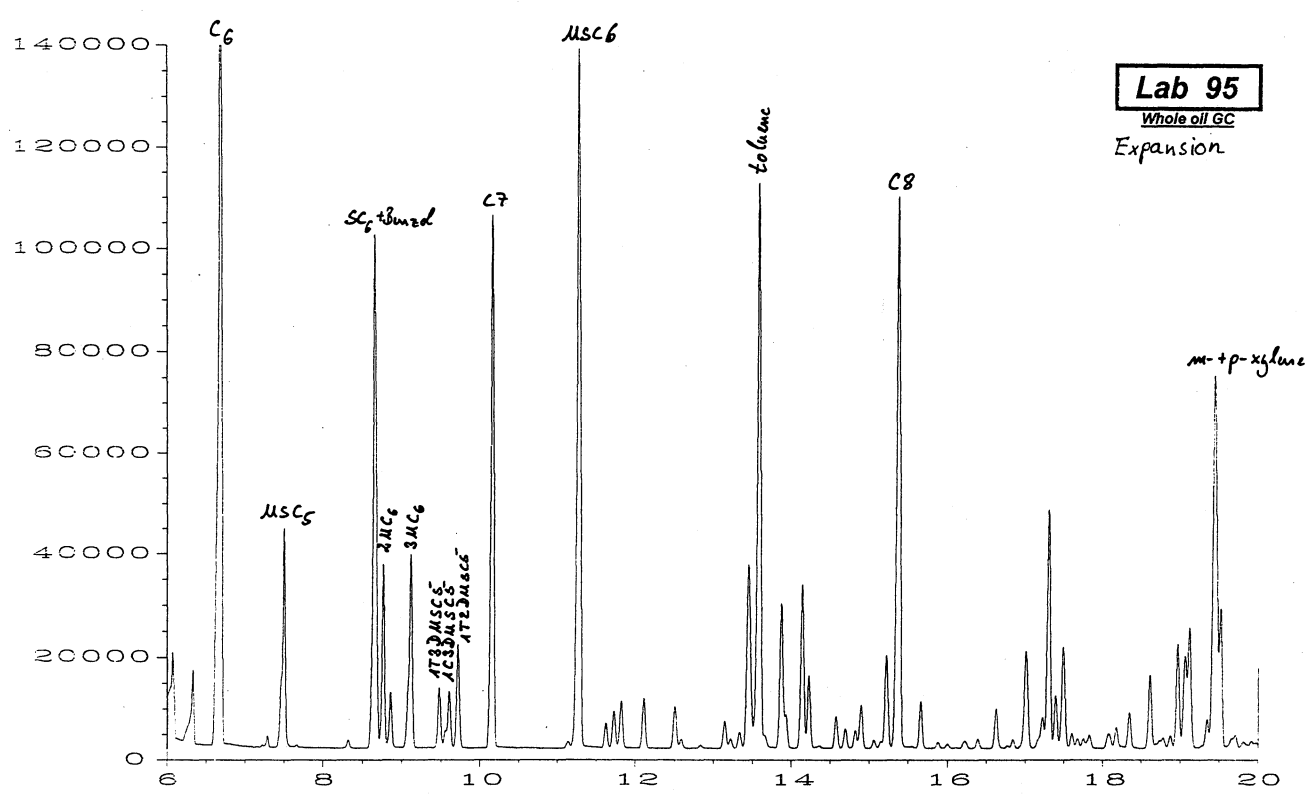
Lower than n-Cg

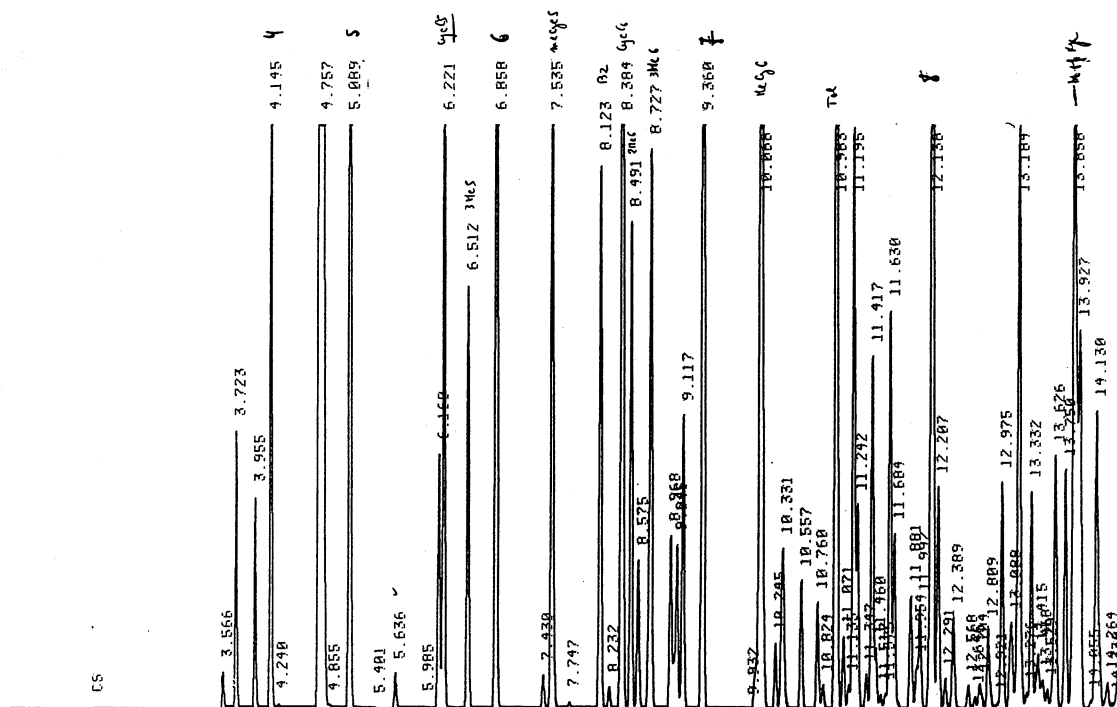
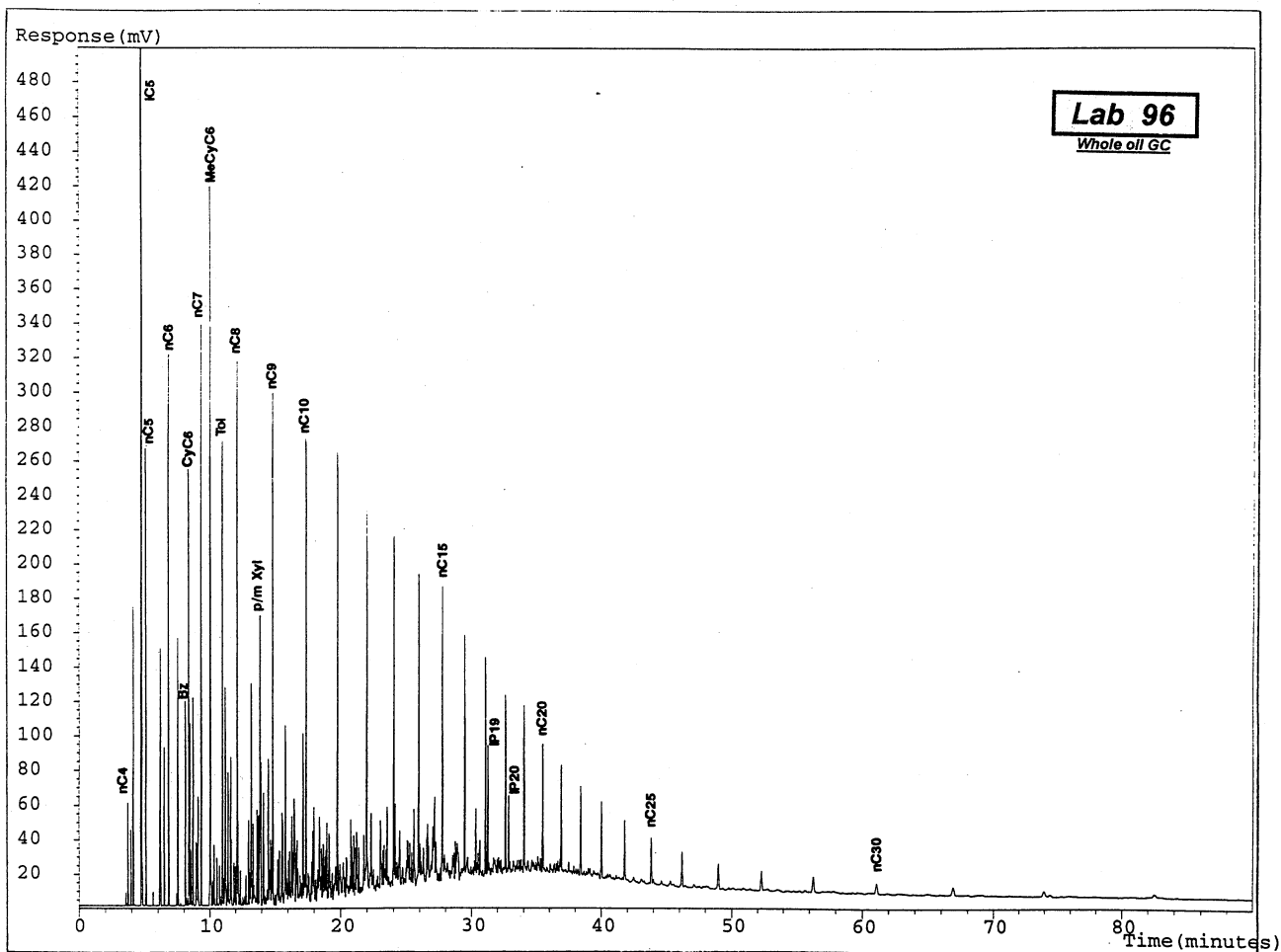


Lab 95
Whole oil GC



Lab 95
Whole oil GC
Expansion



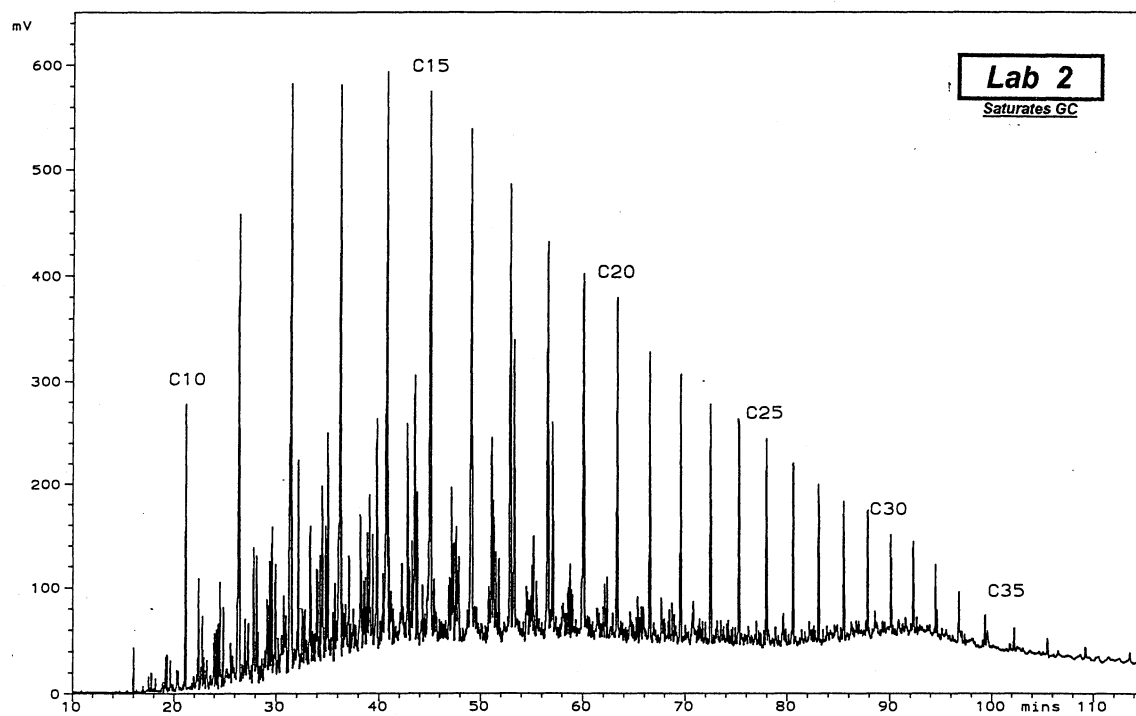
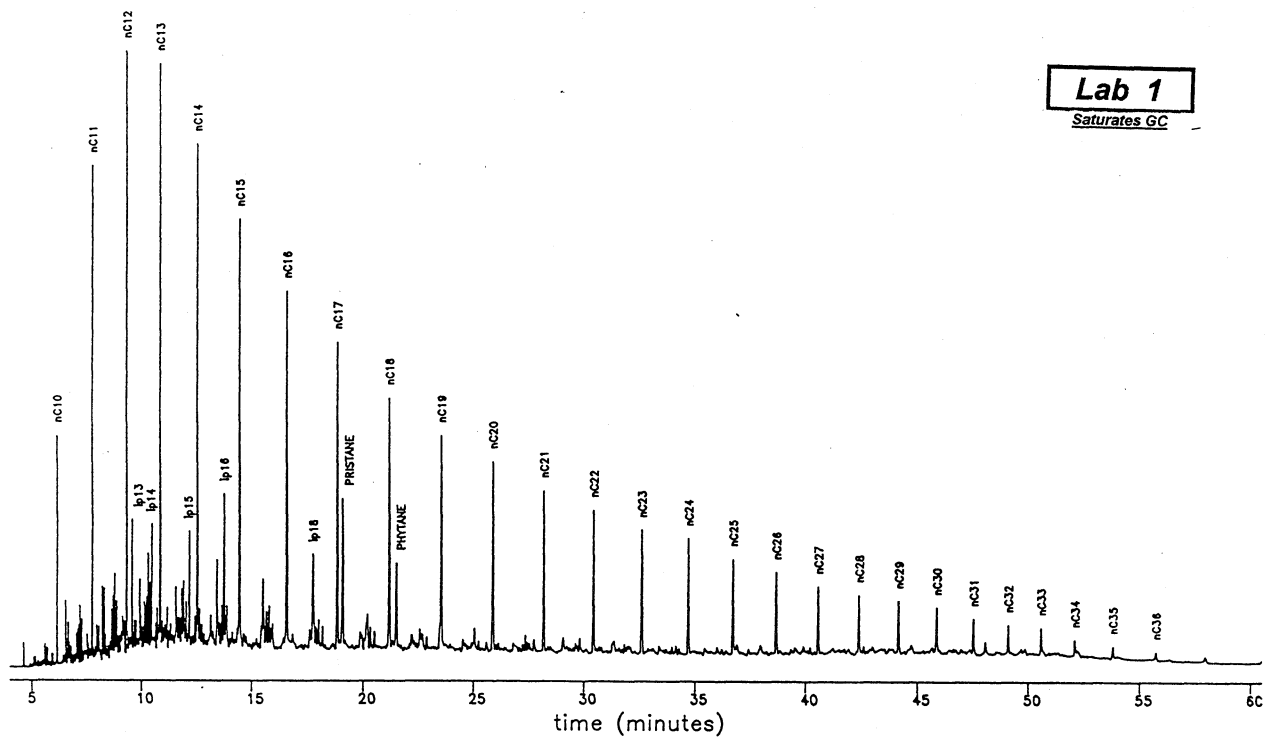


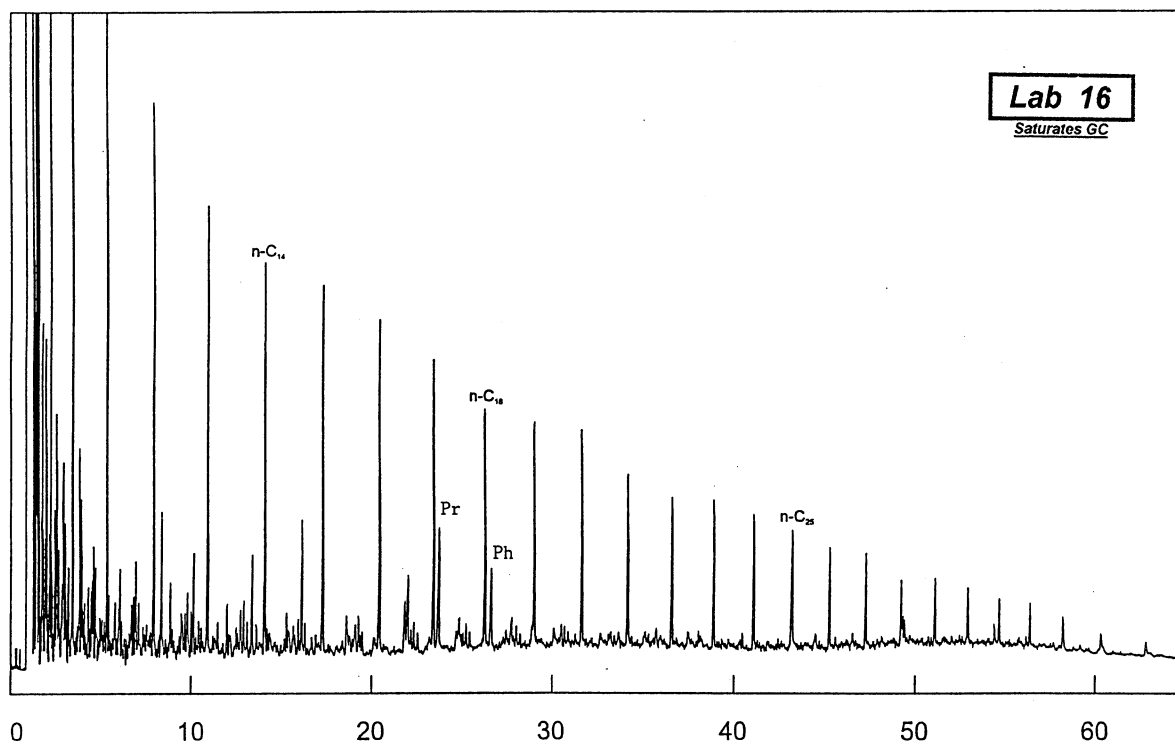
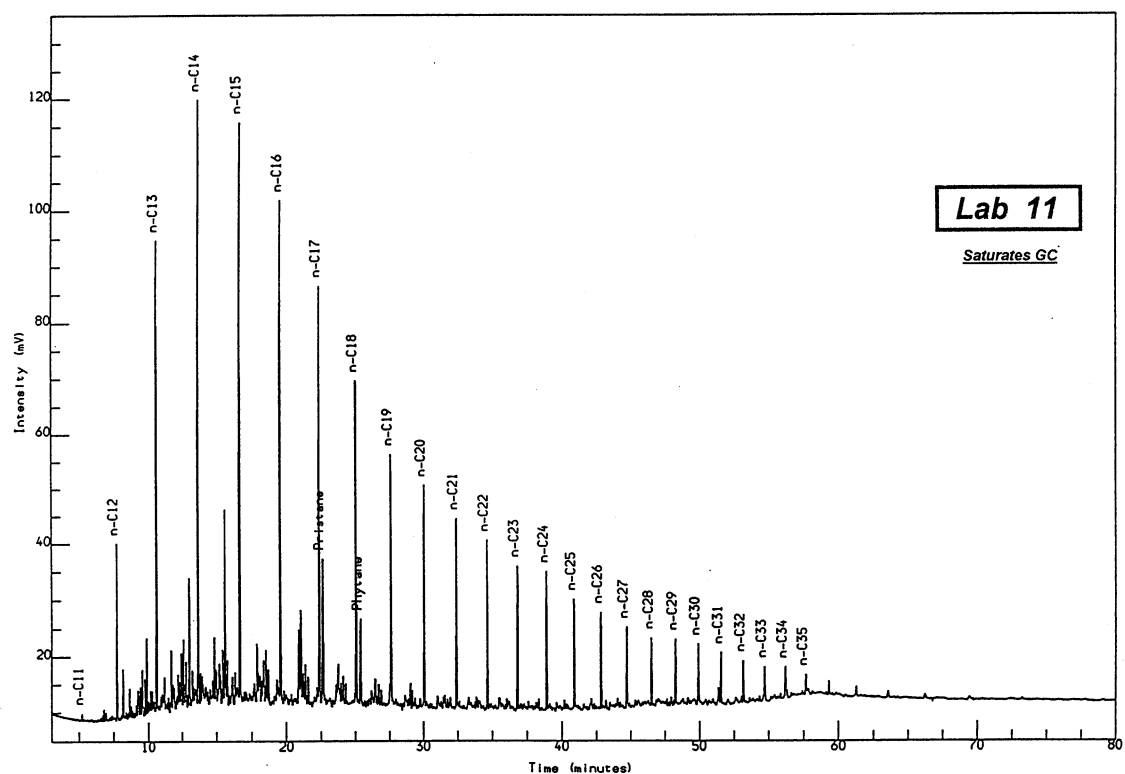
Lab 96
Whole oil GC
Expansion

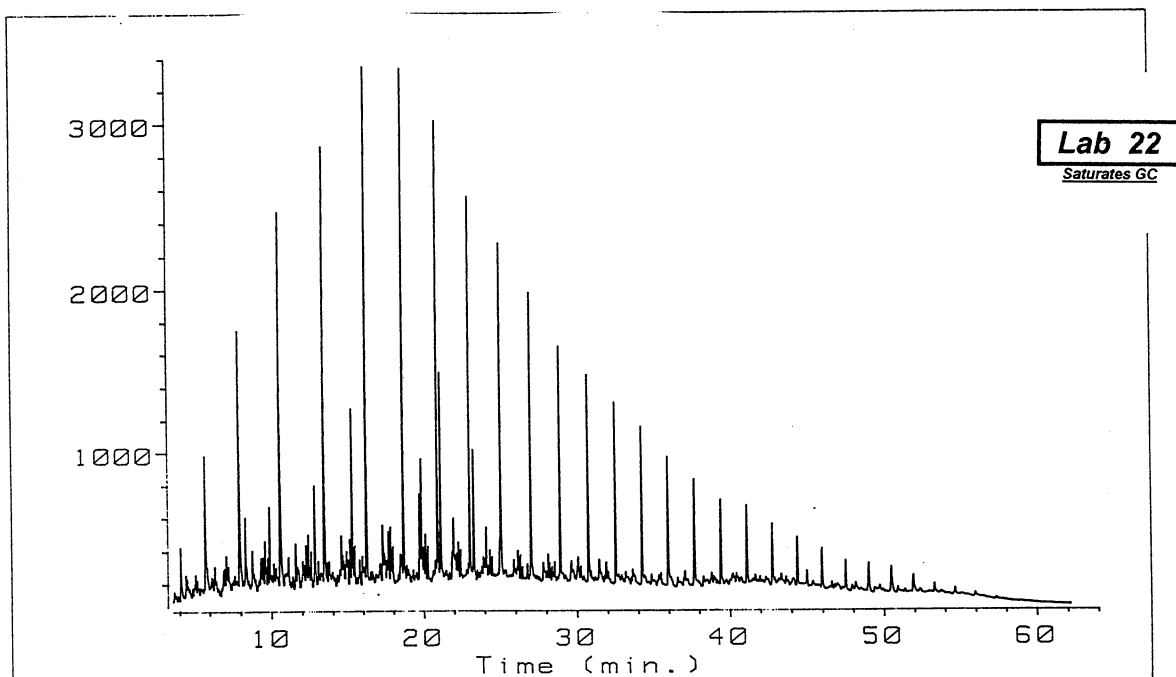
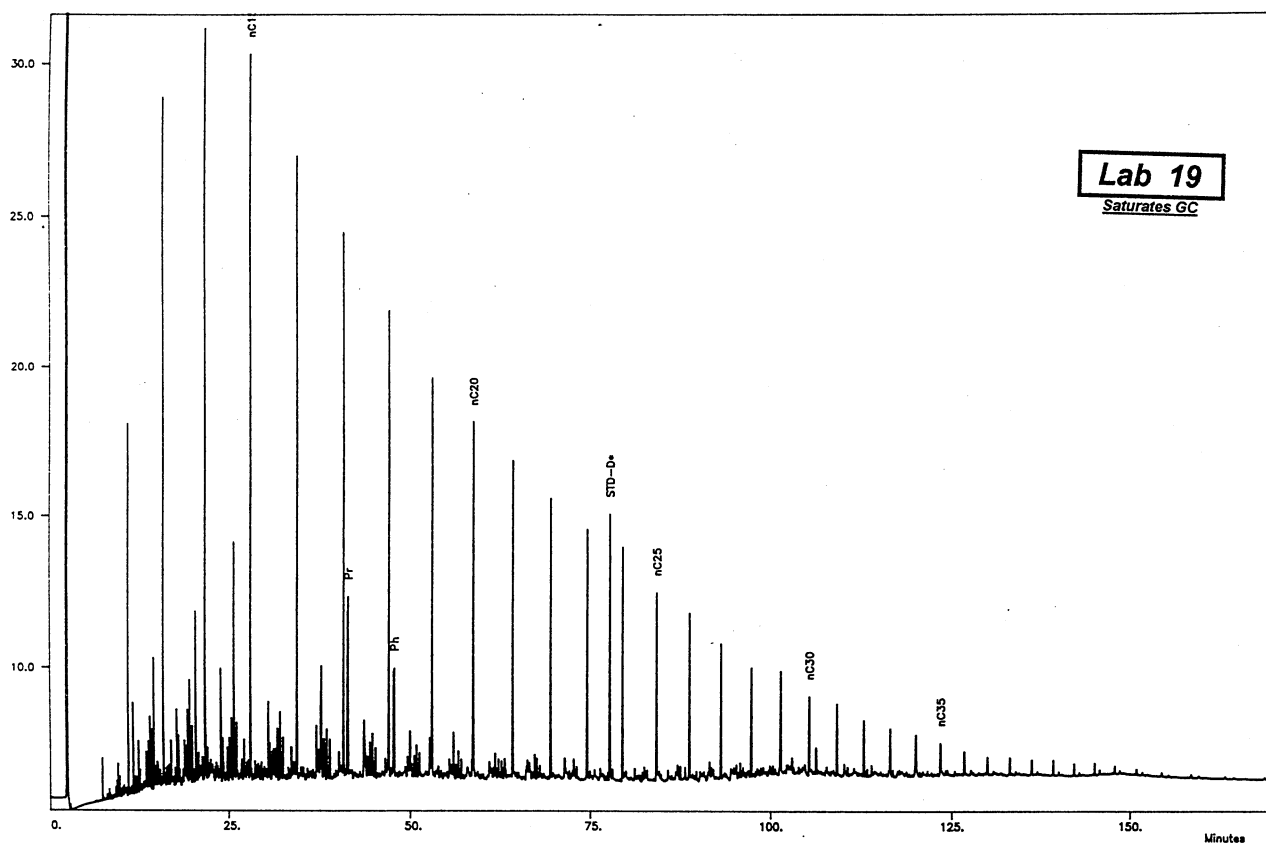
NGS NSO-1

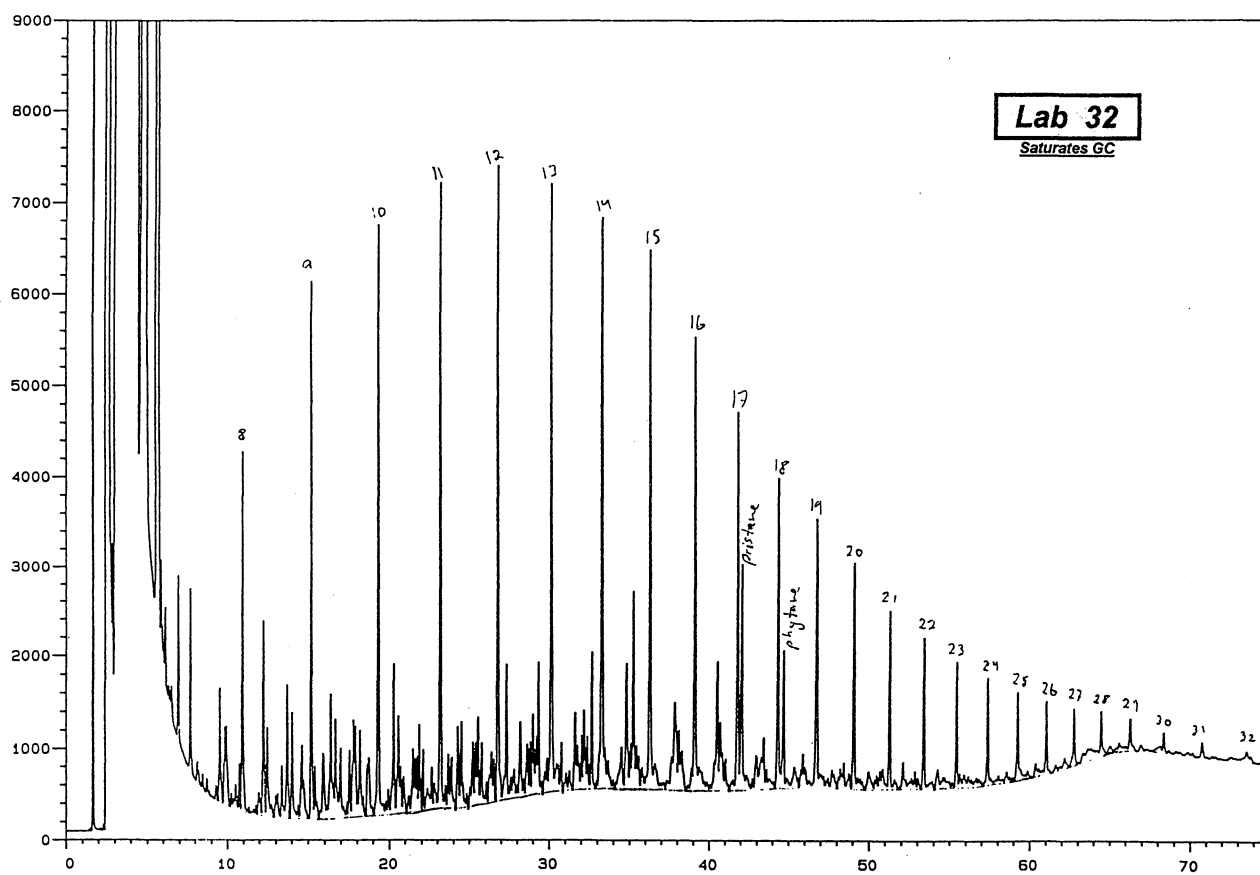
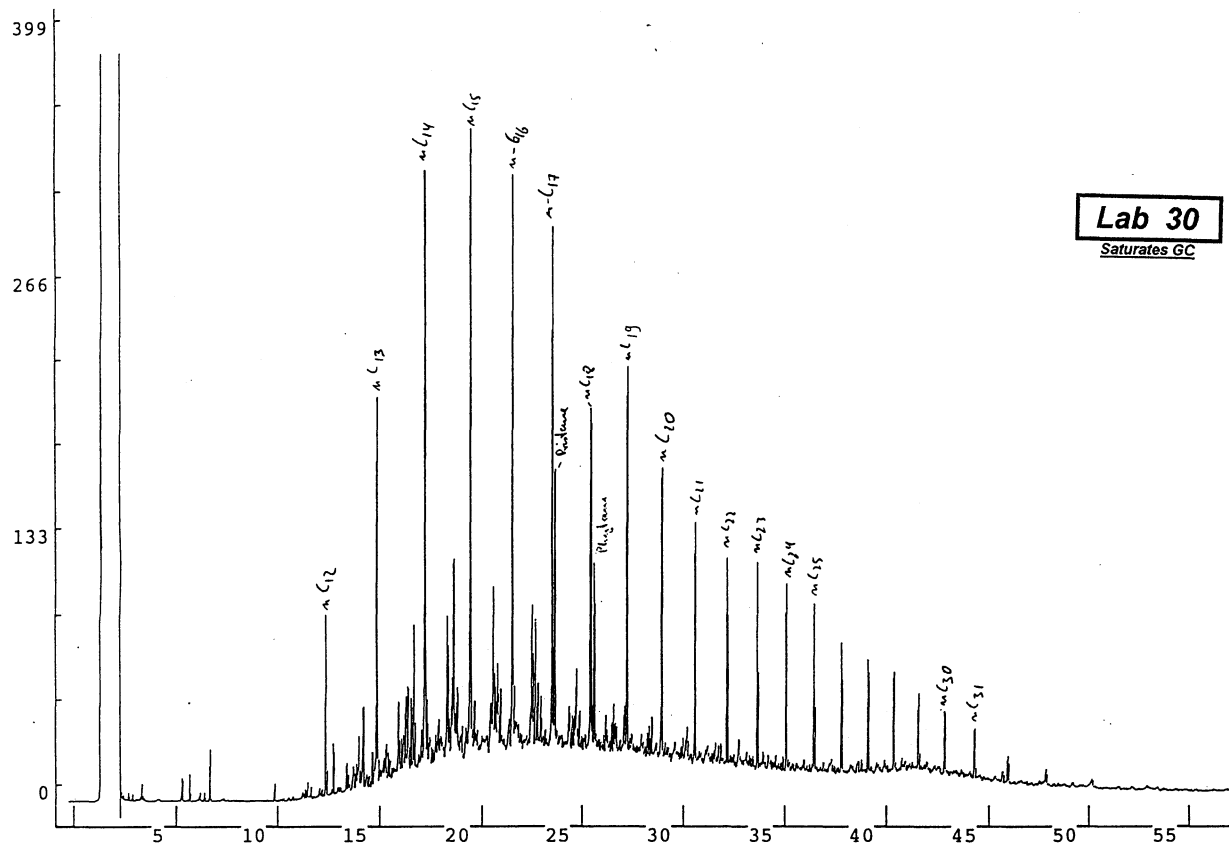
Appendix A3.3b

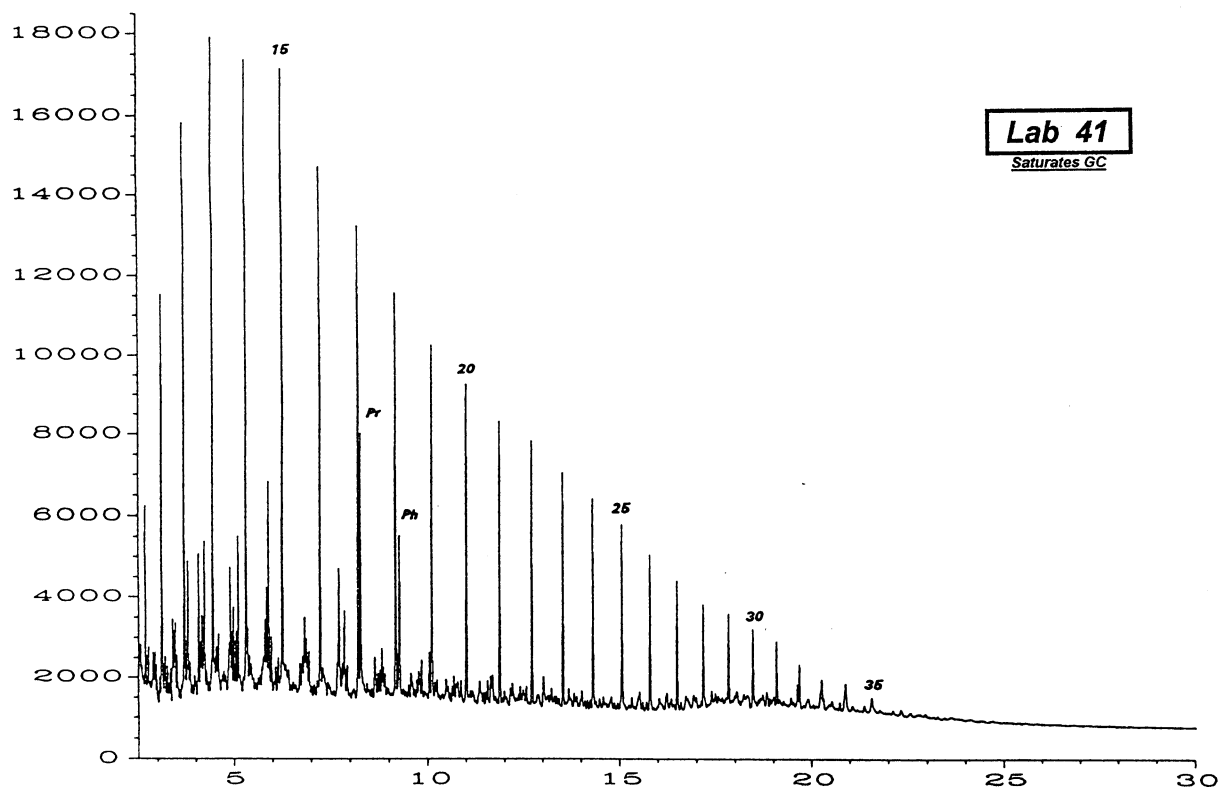
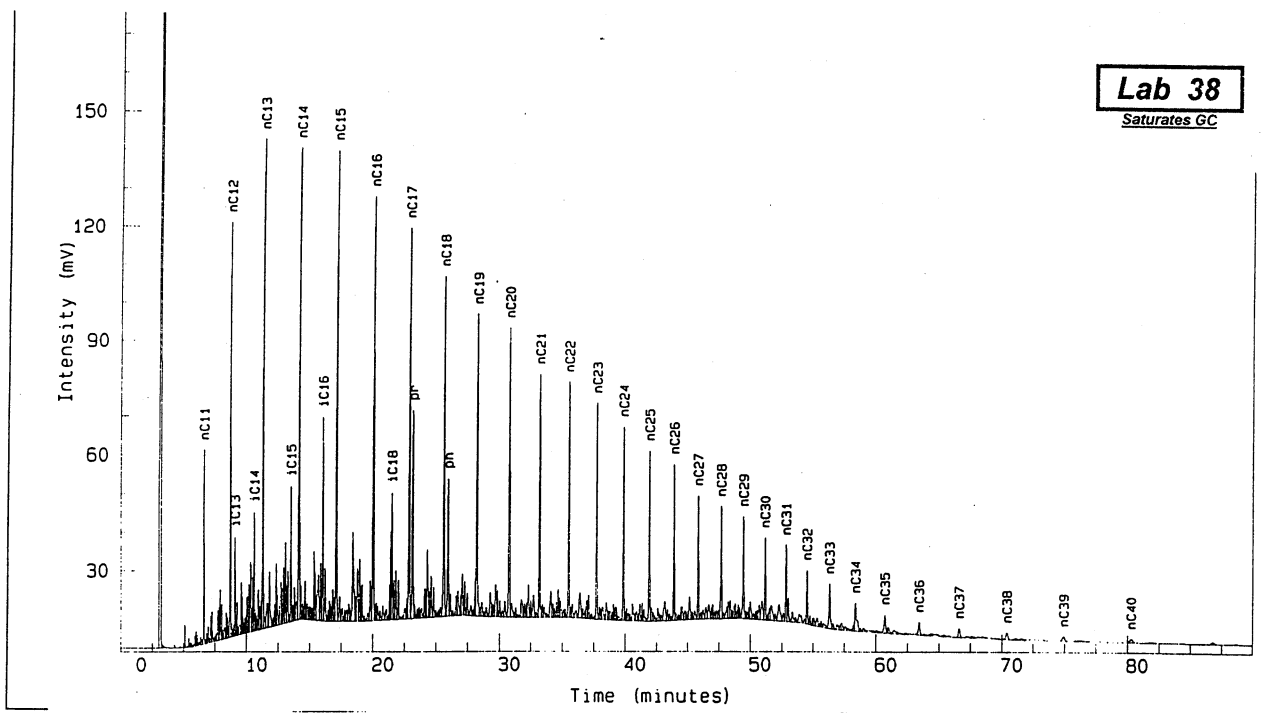
Saturates fraction GC chromatograms

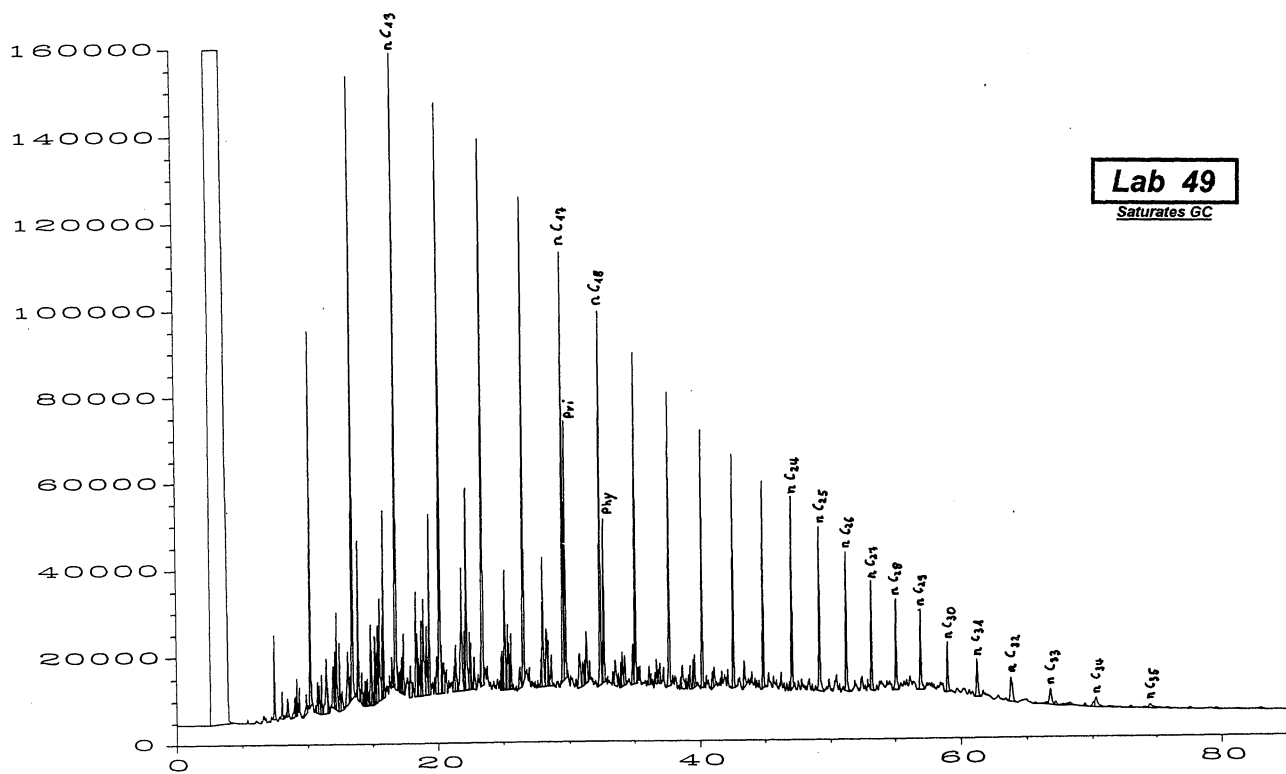
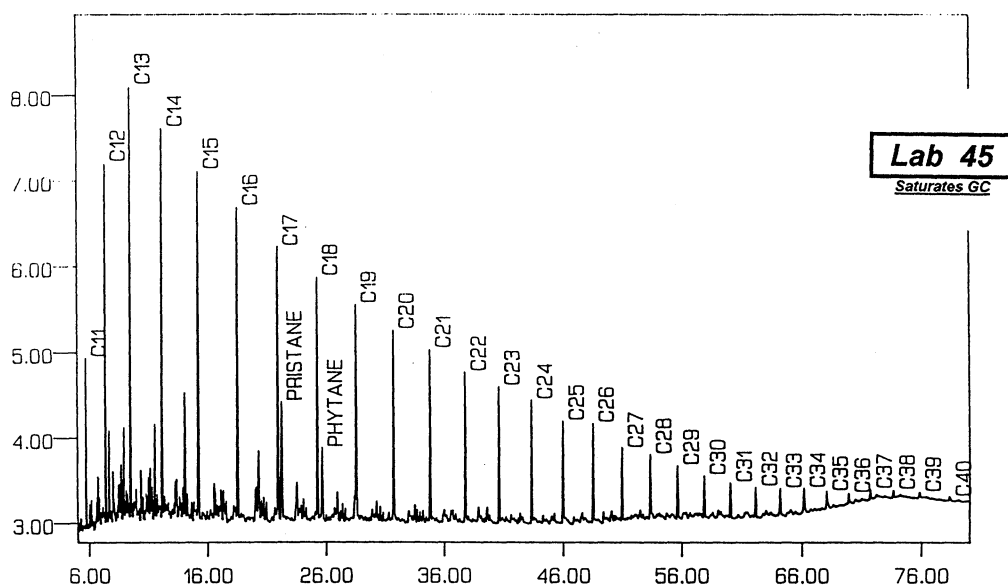


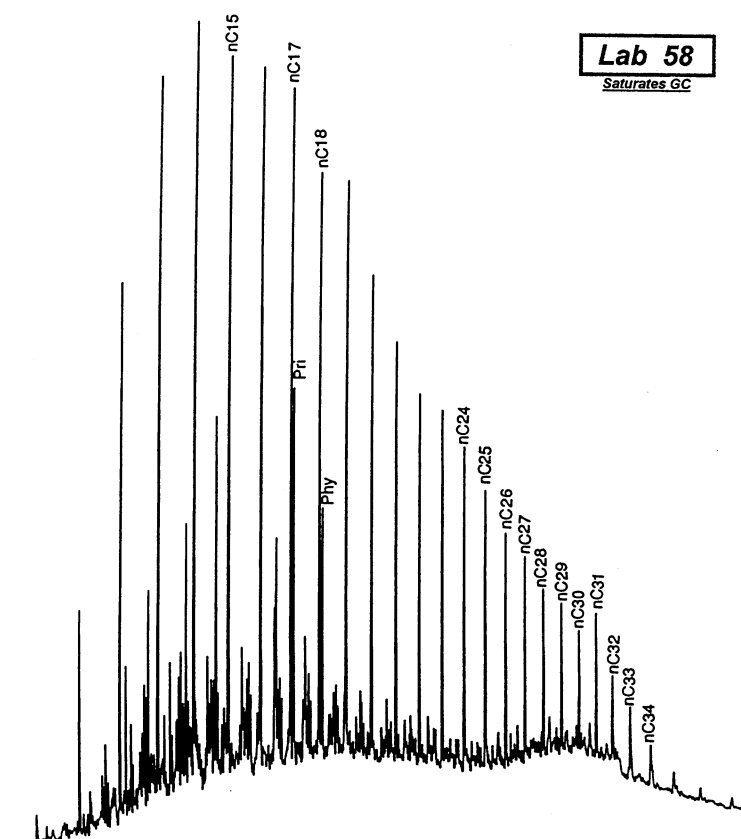
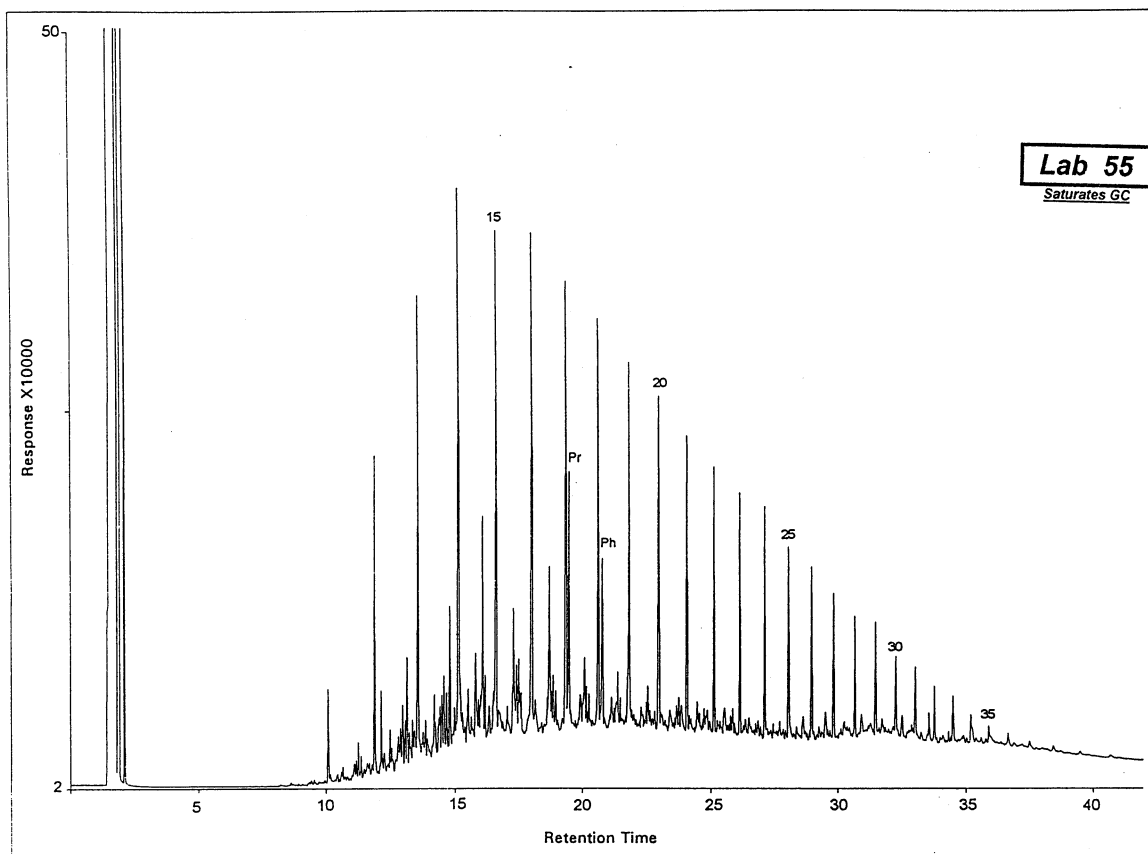


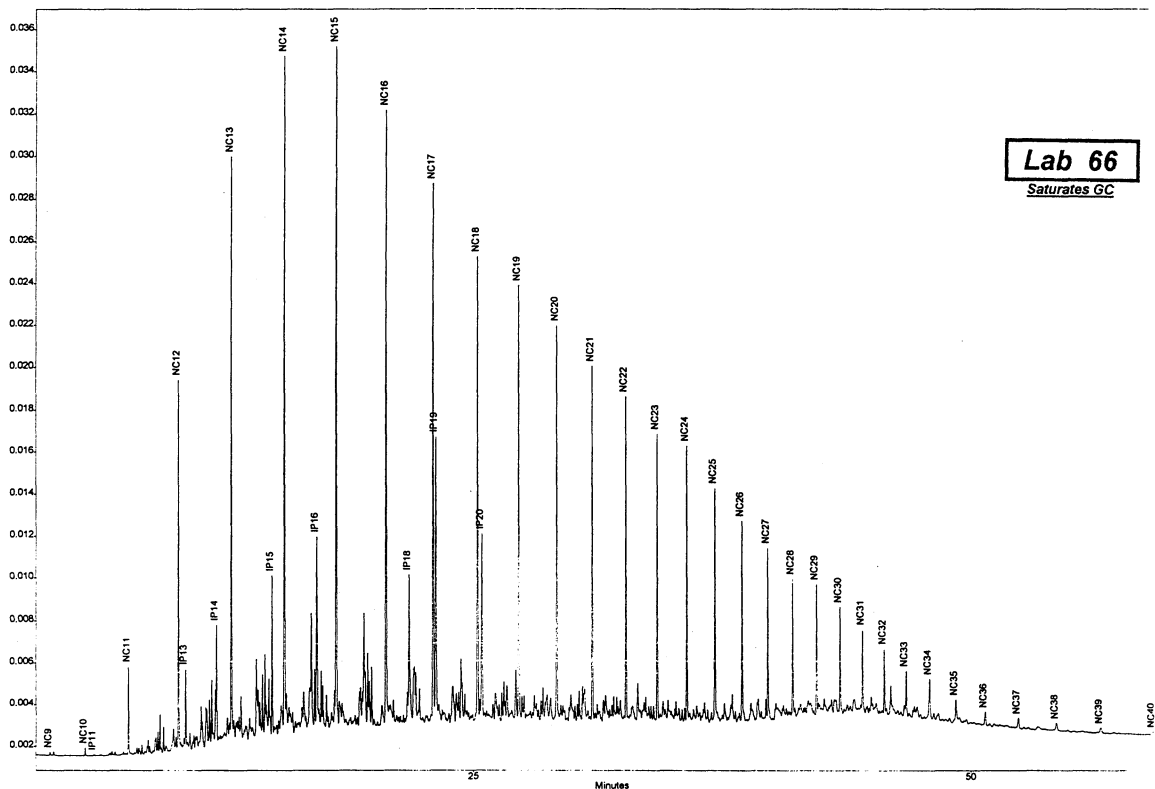
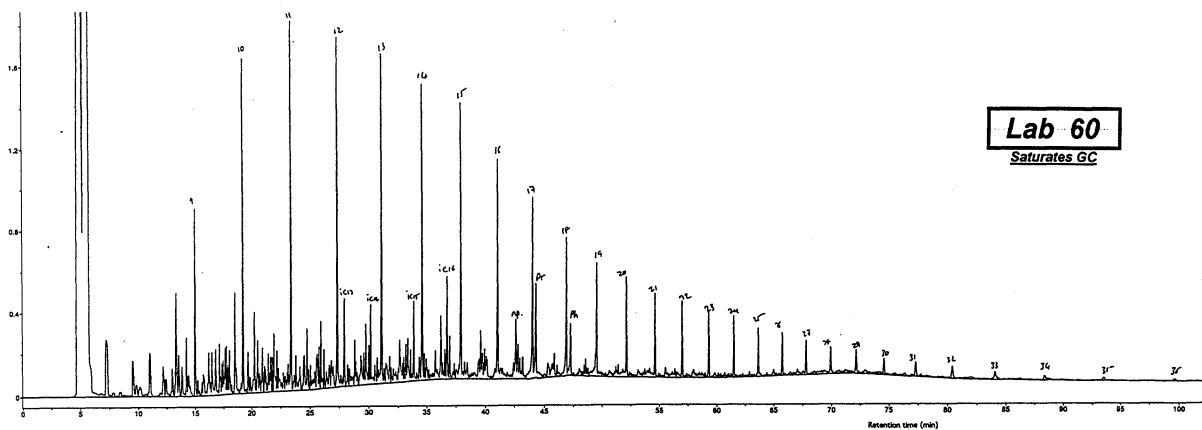


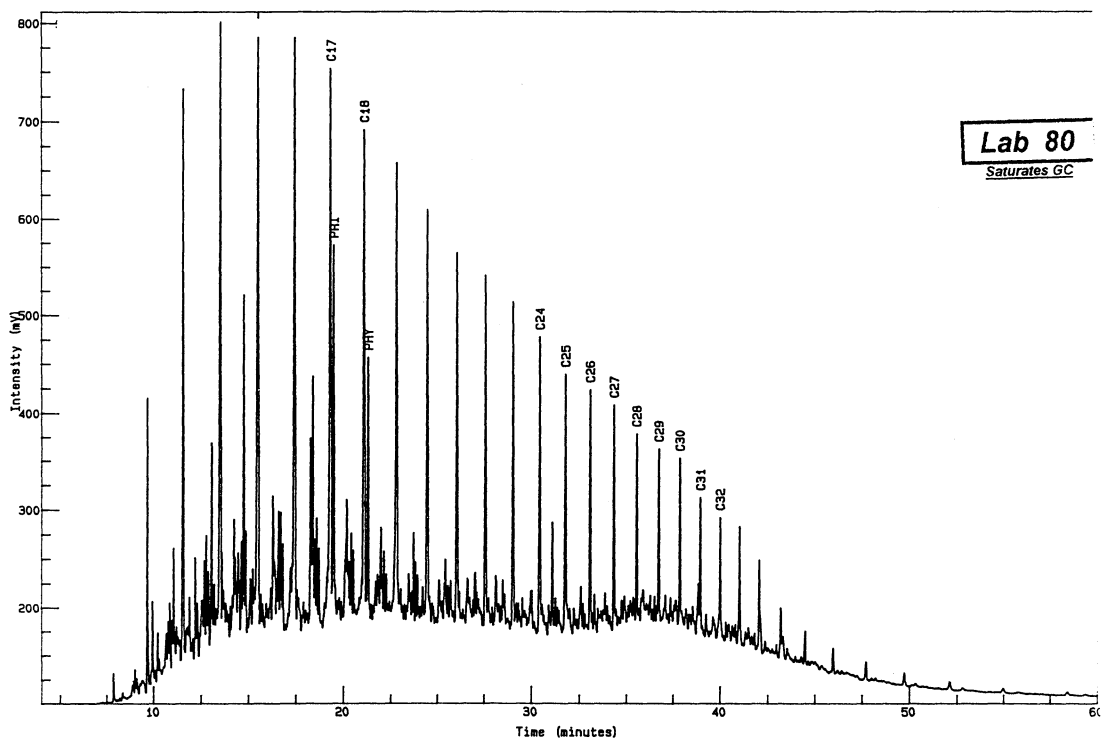
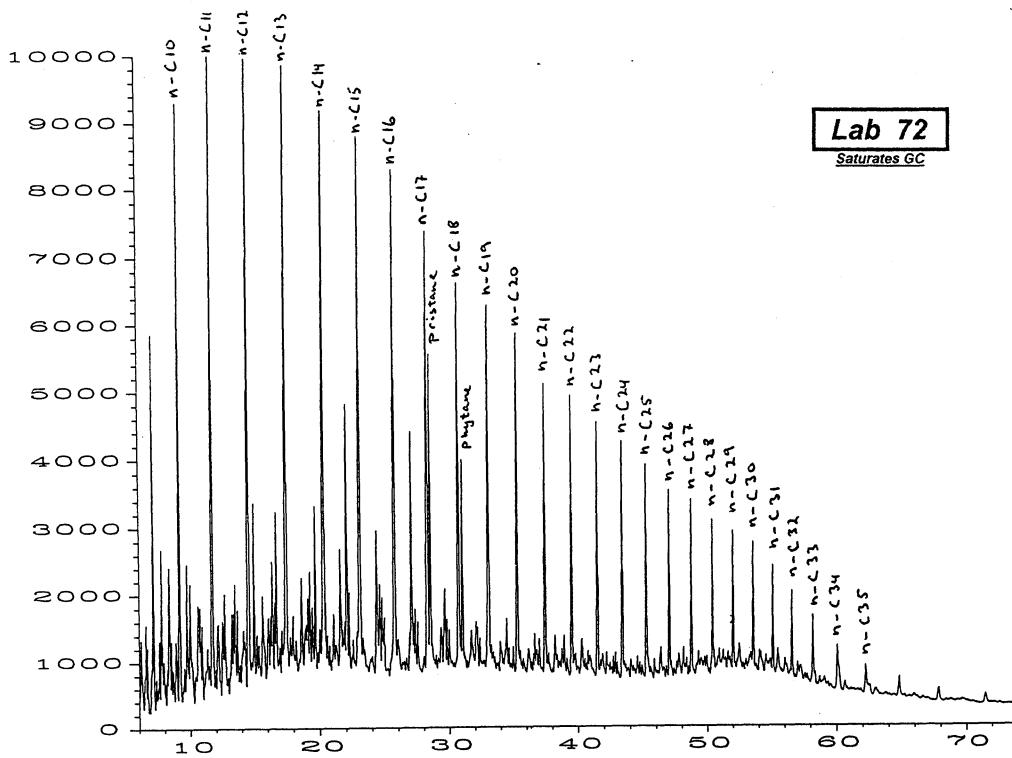


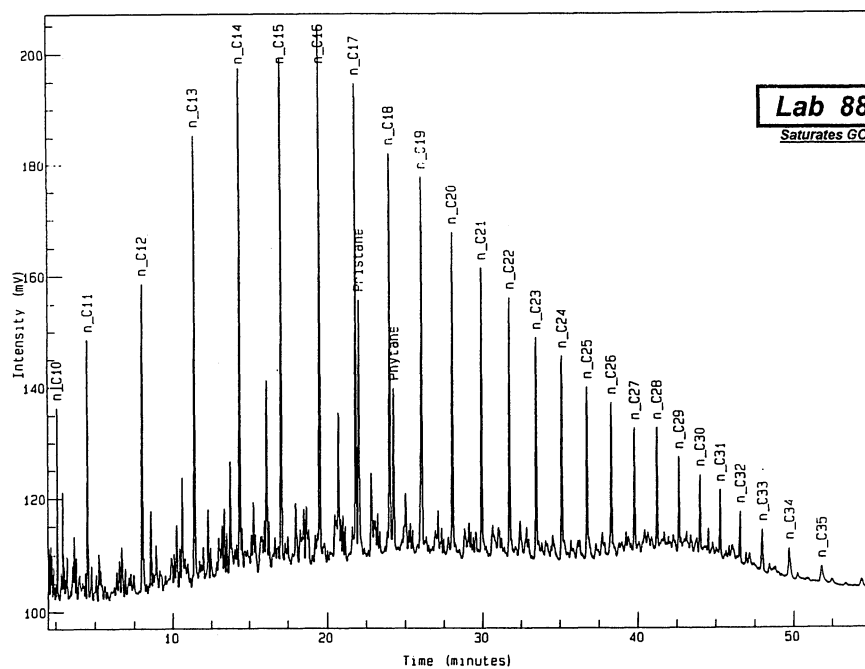
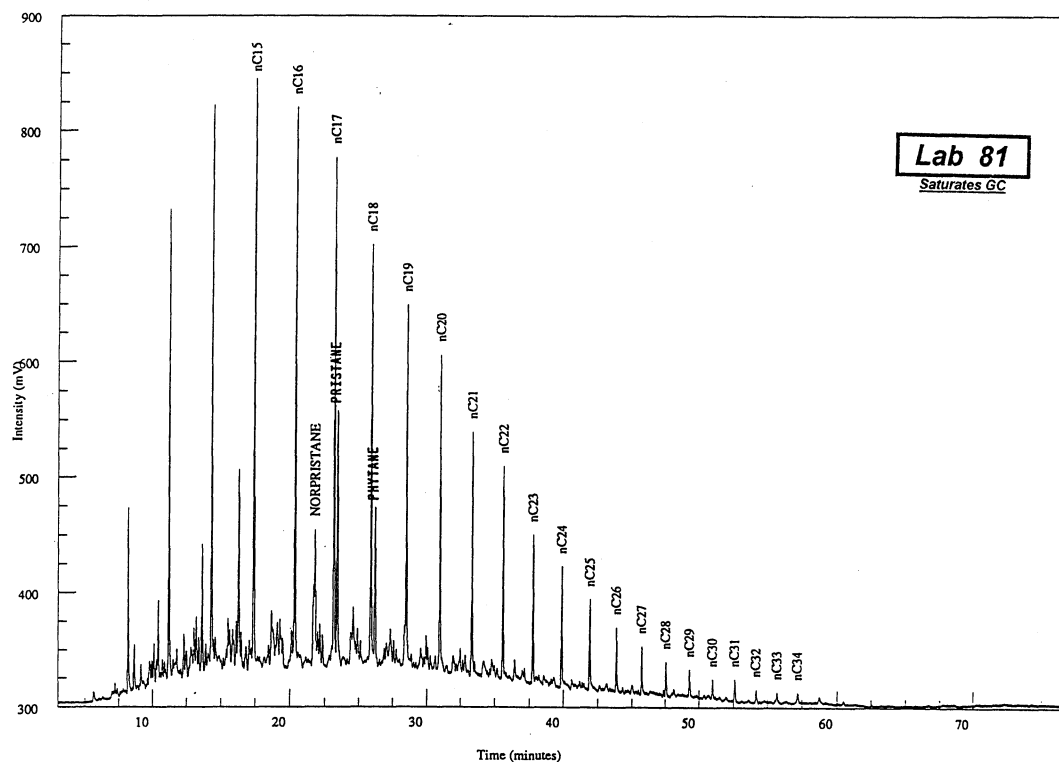


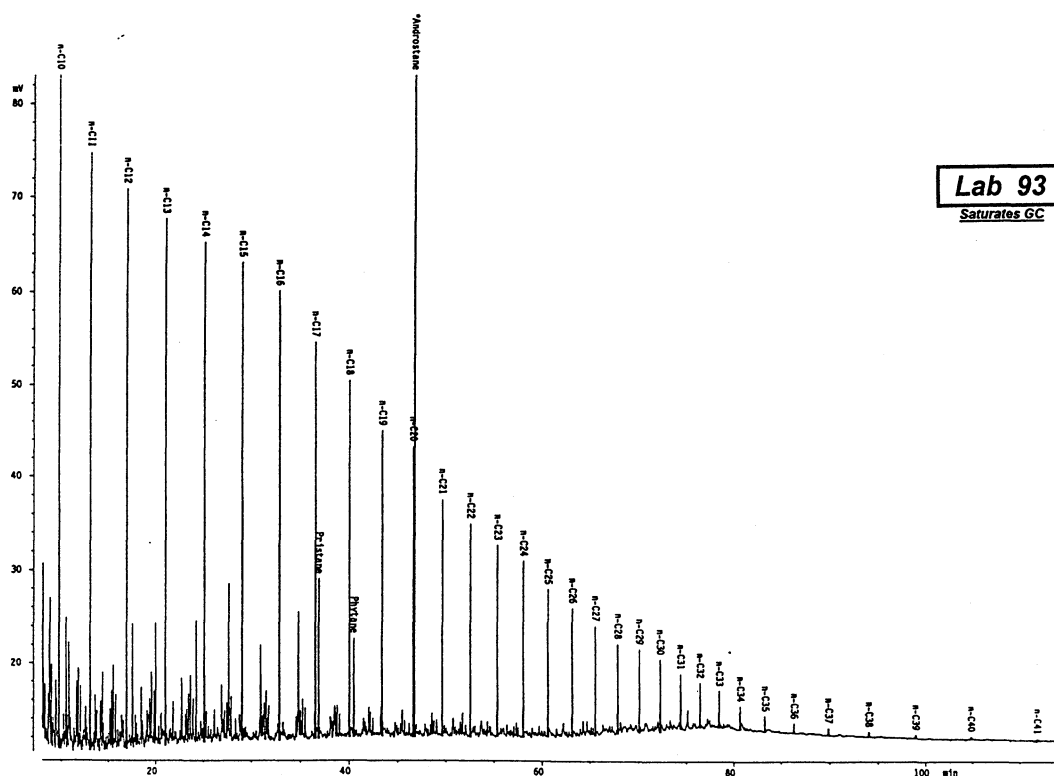
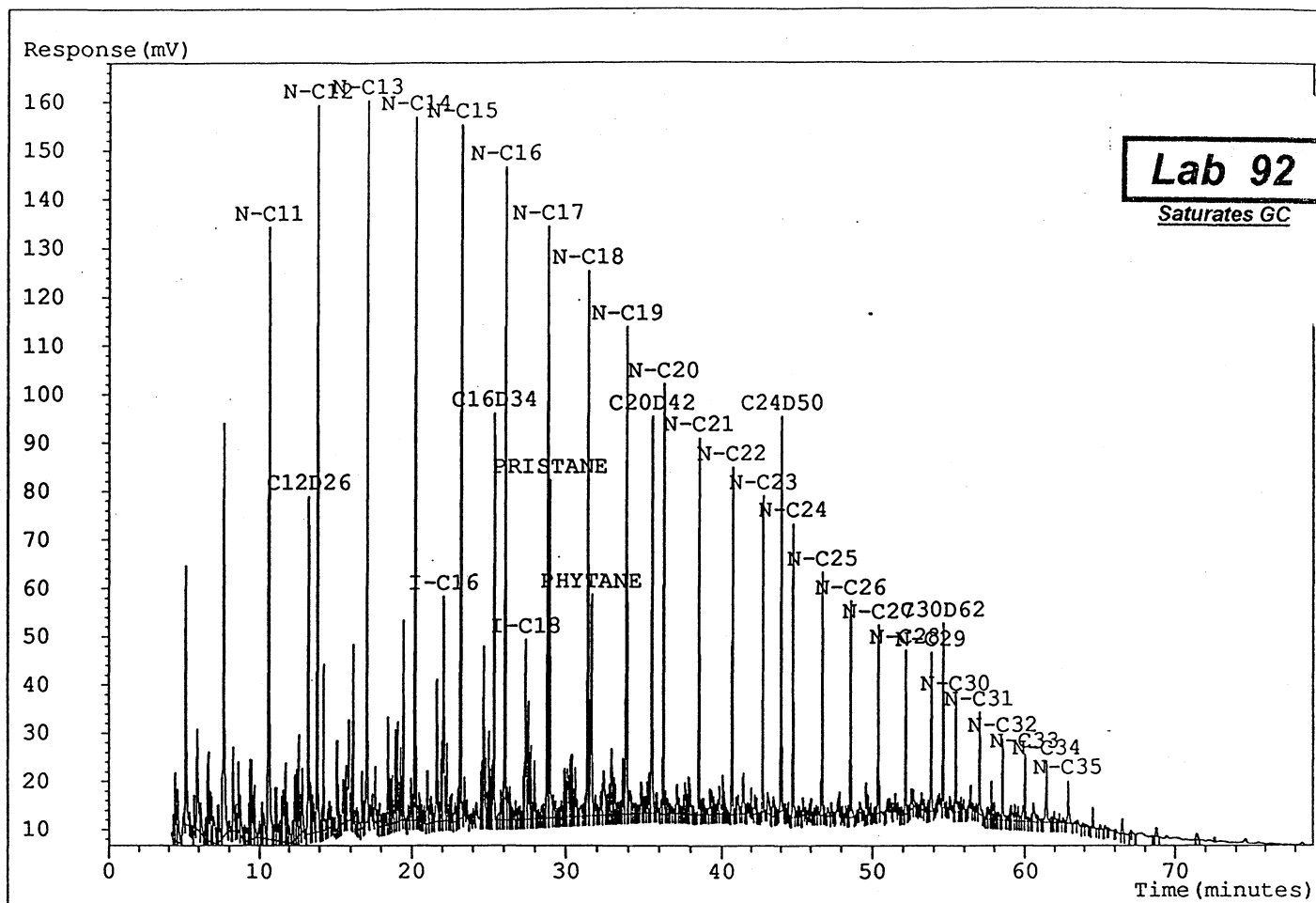


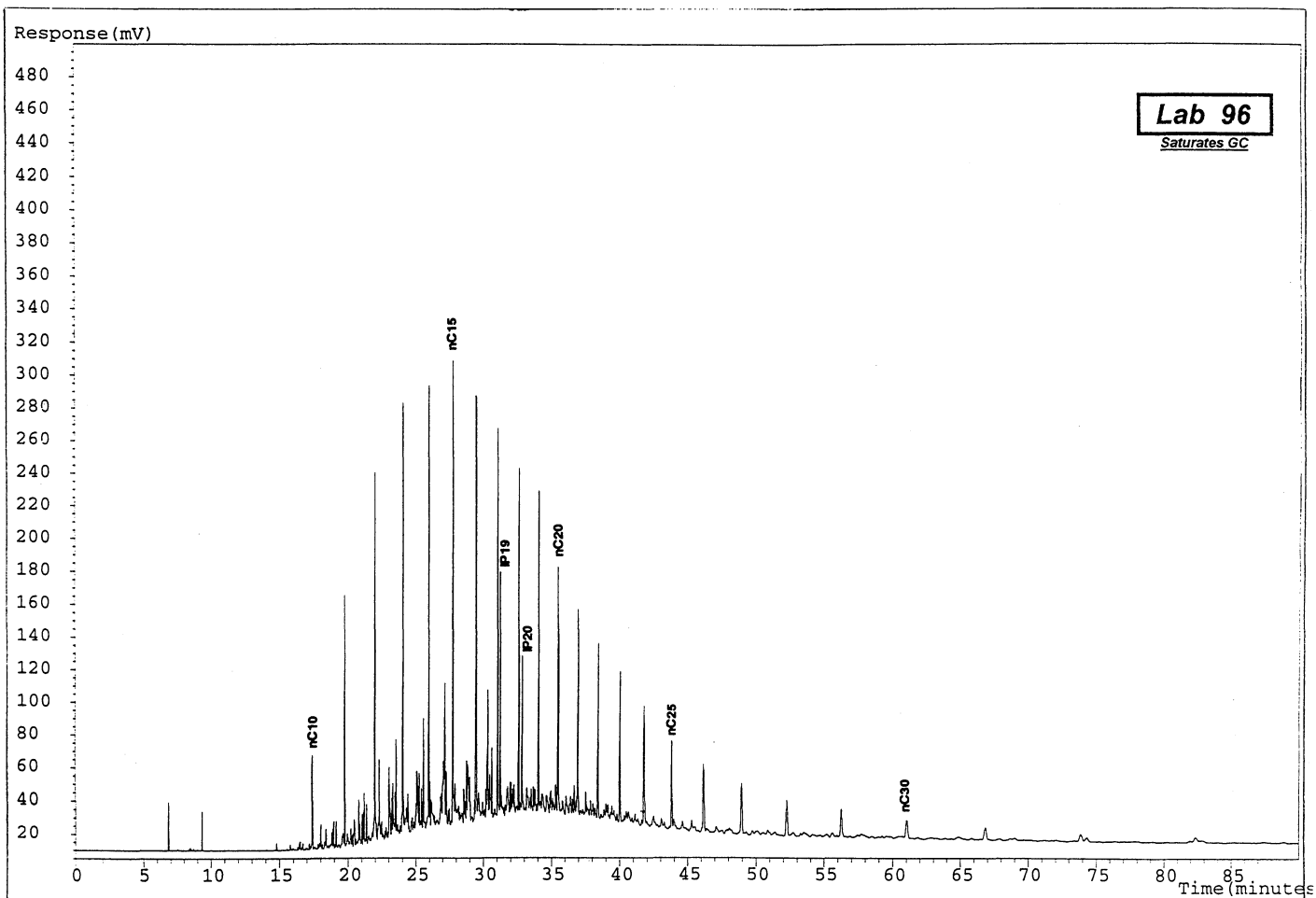
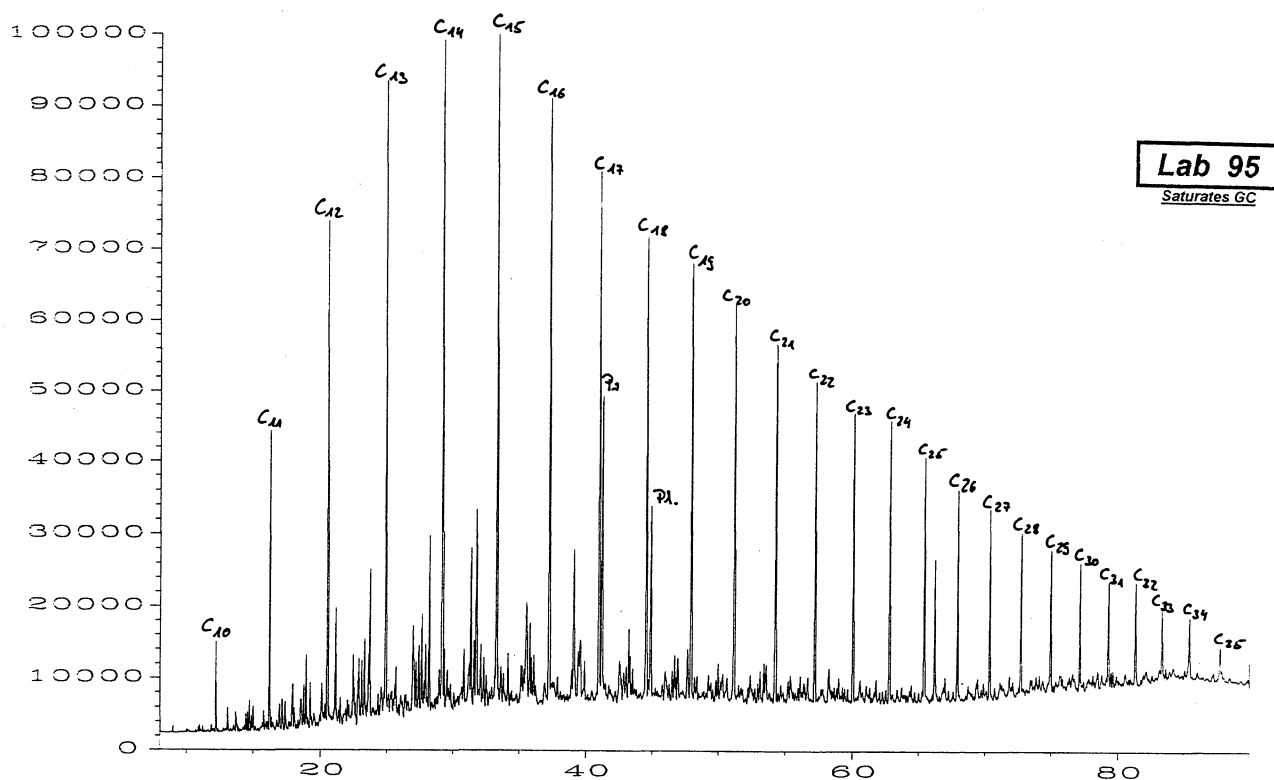








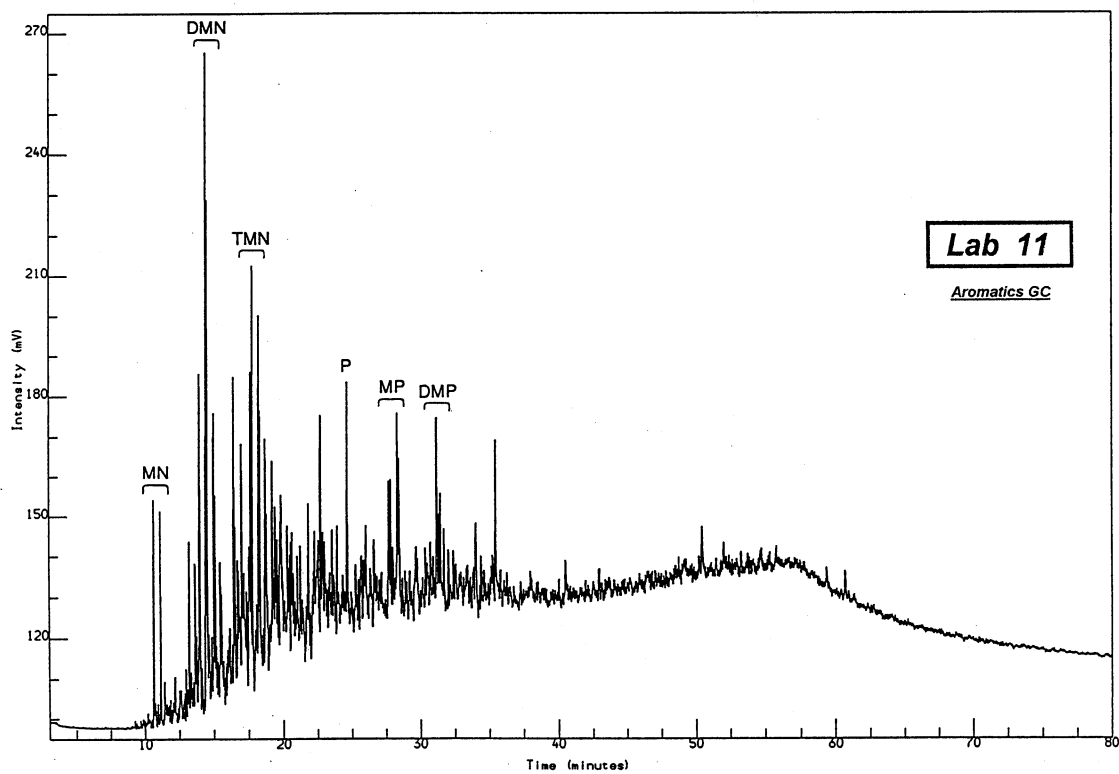
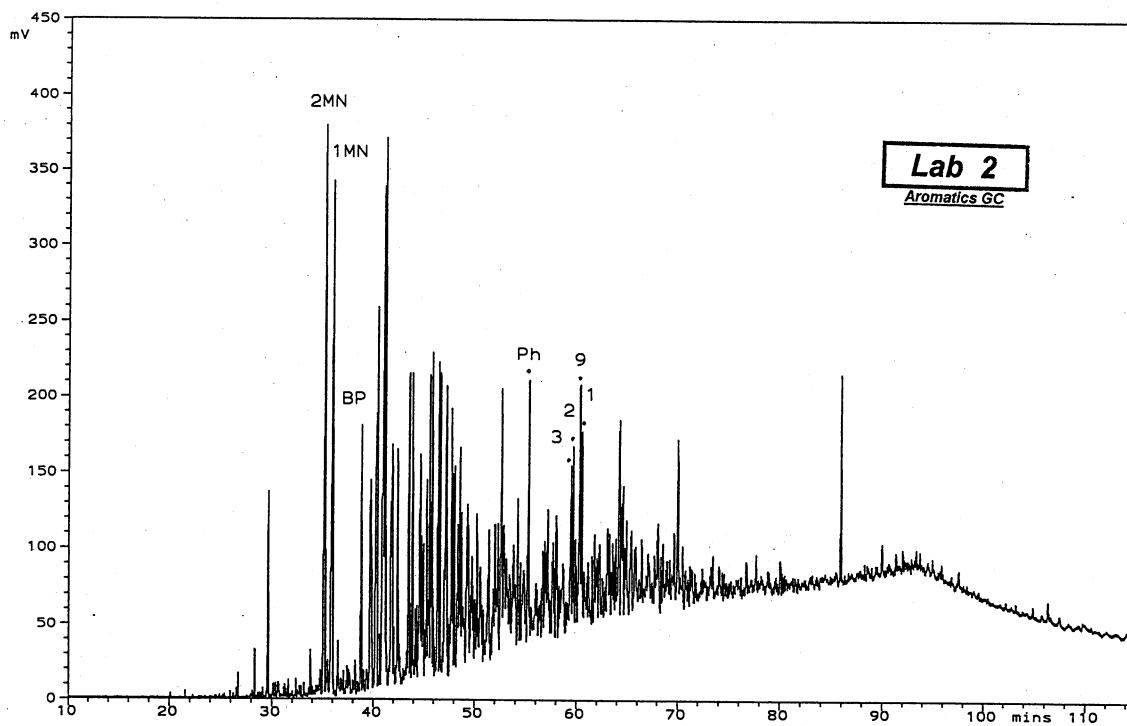


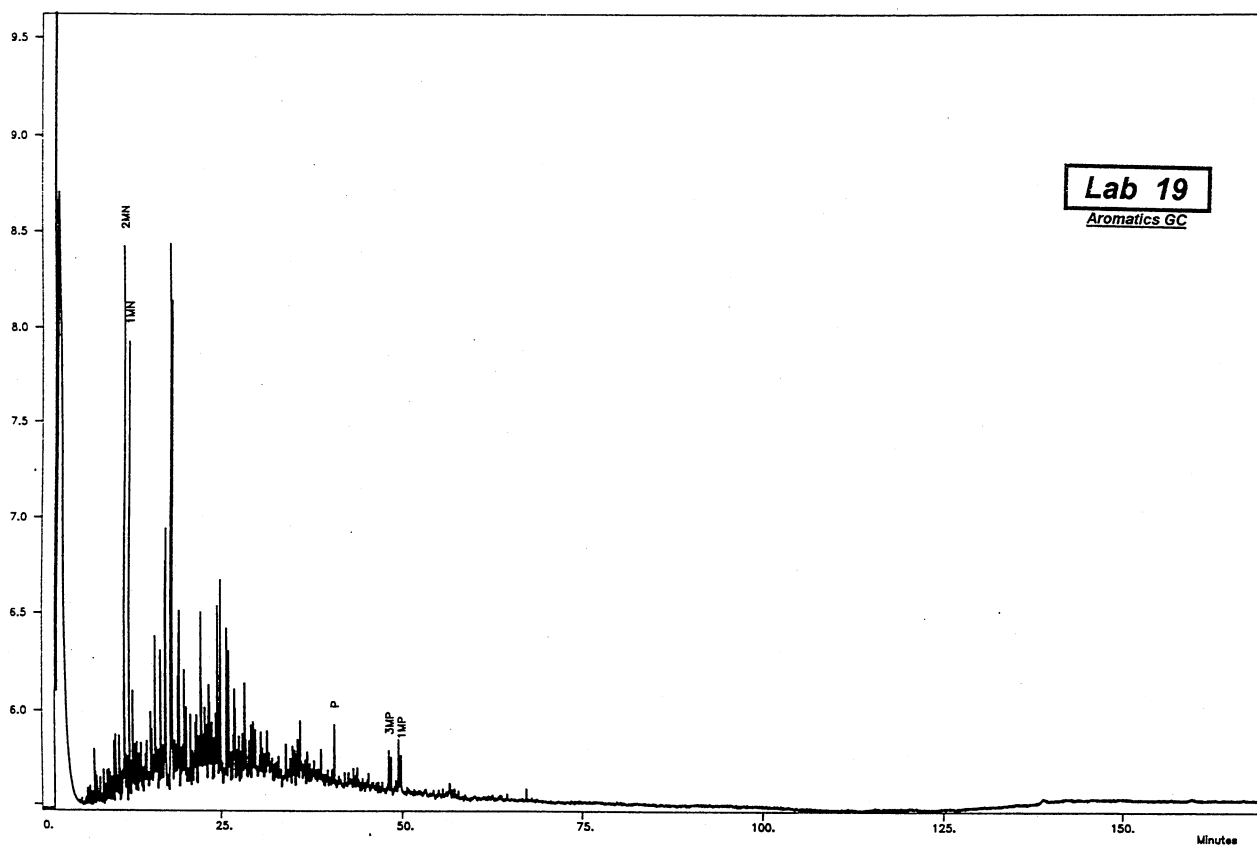
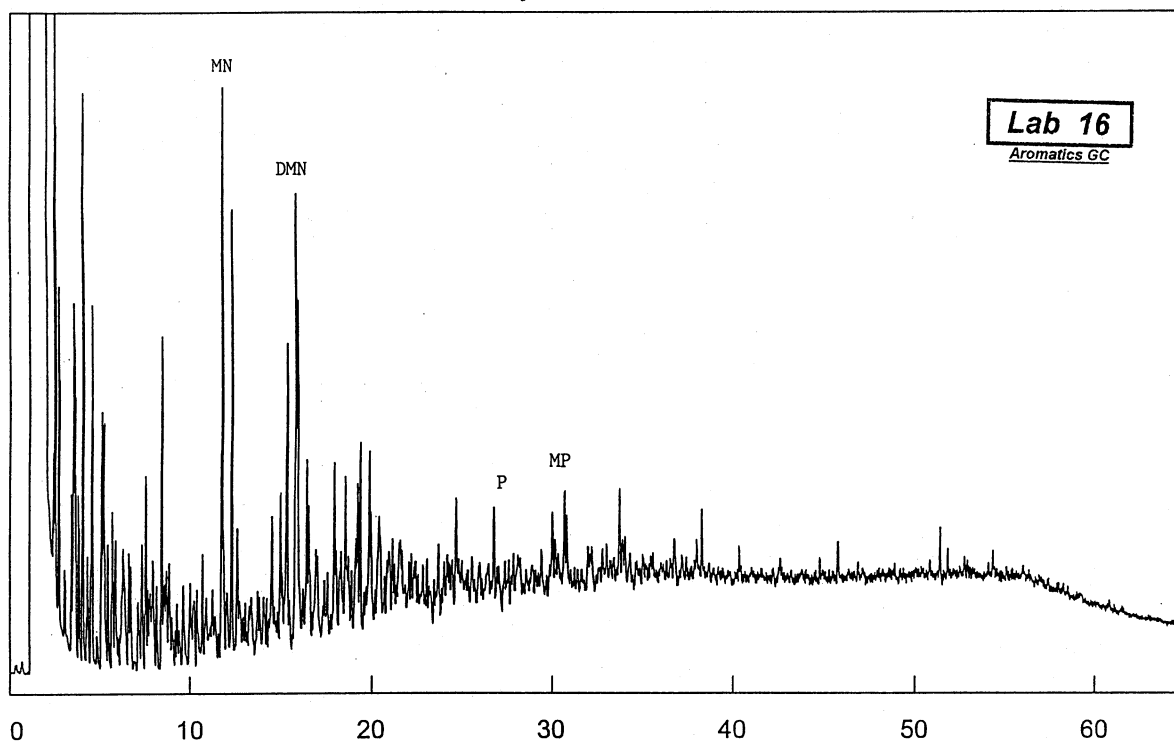


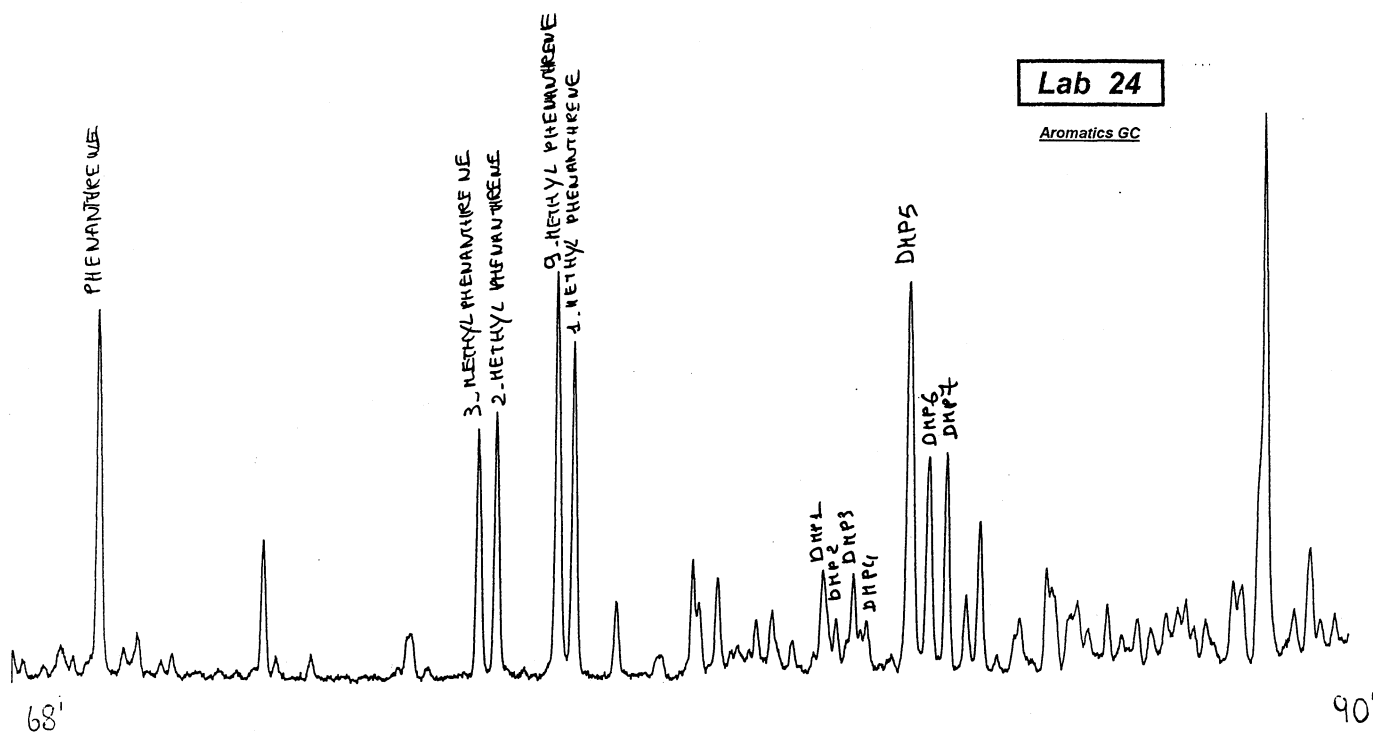
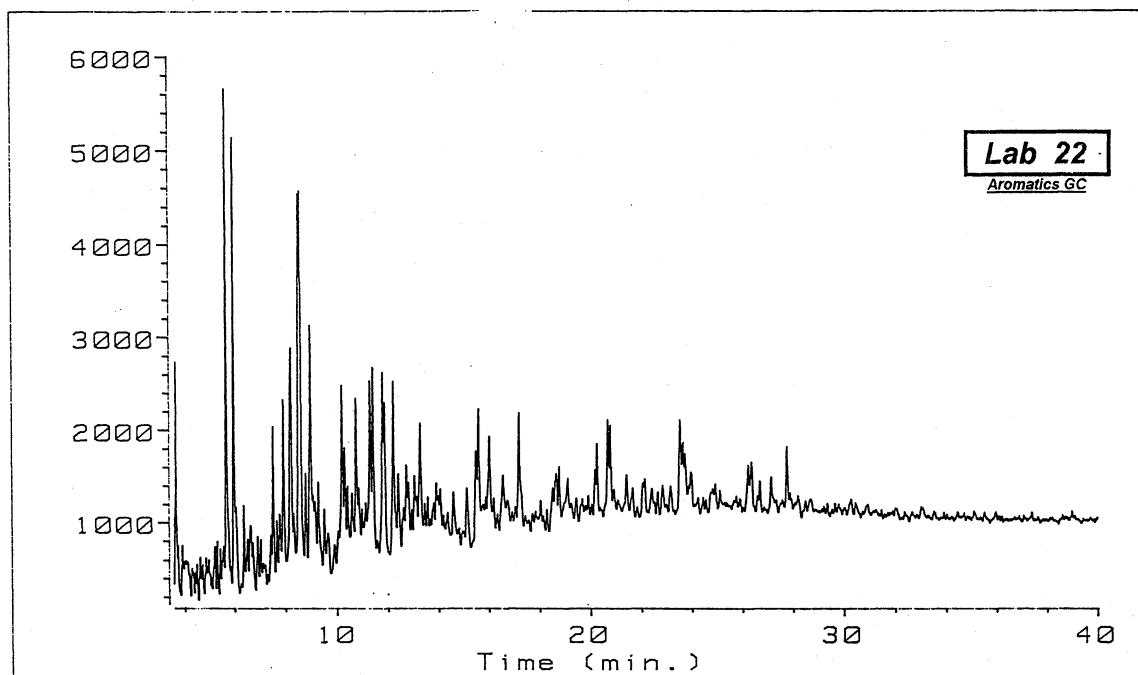
NGS NSO-1

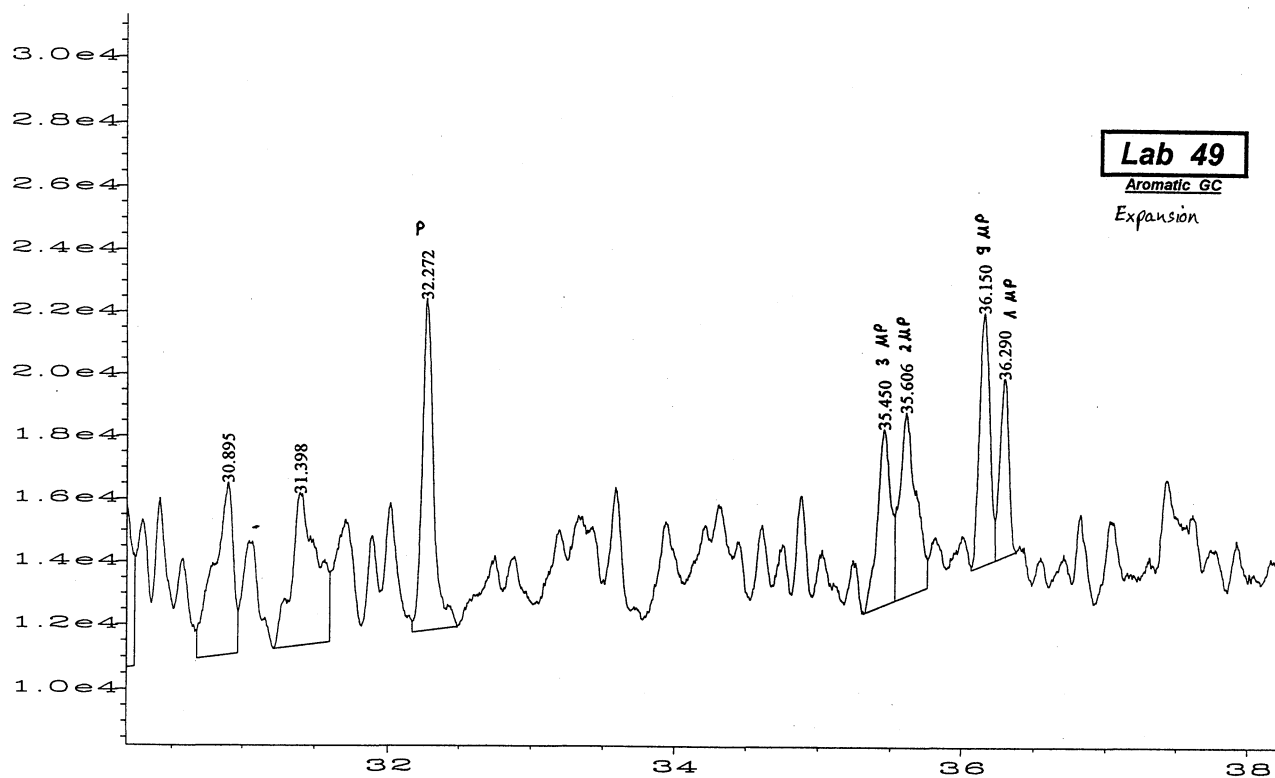
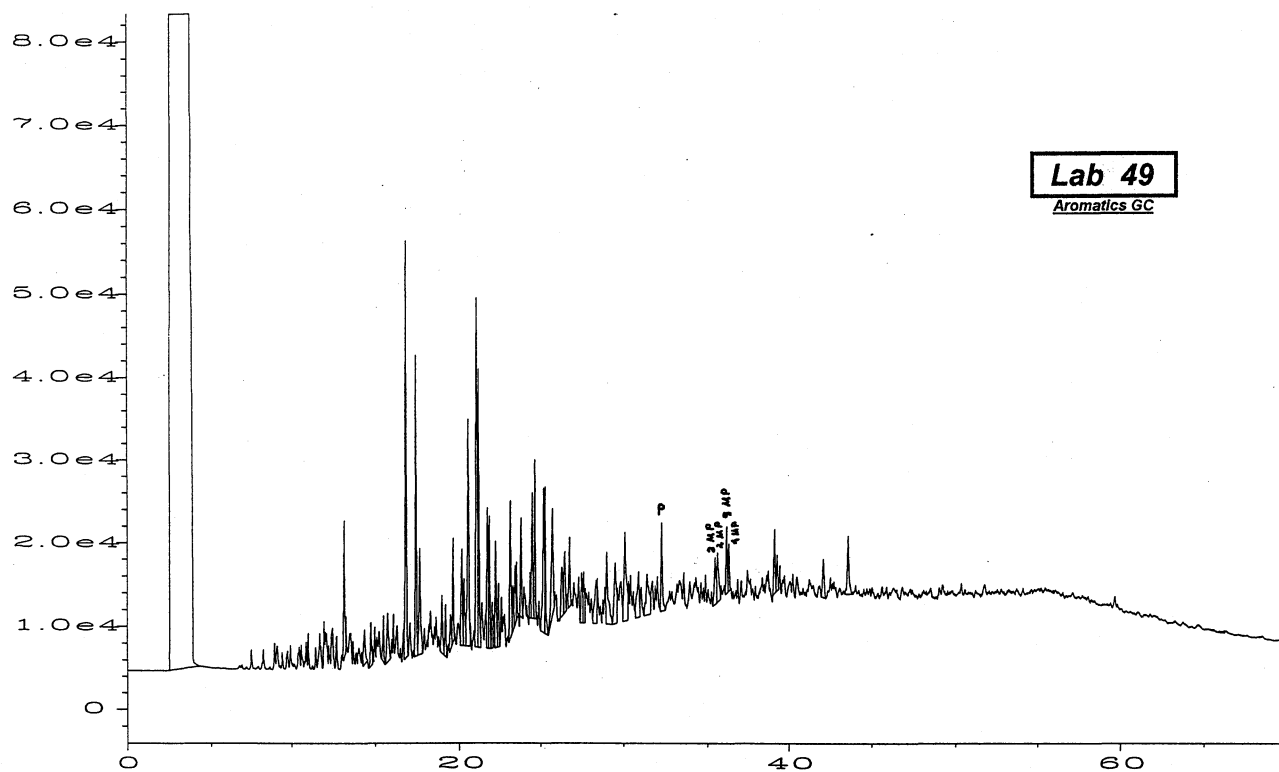
Appendix A3.3c

Aromatic fraction GC chromatograms



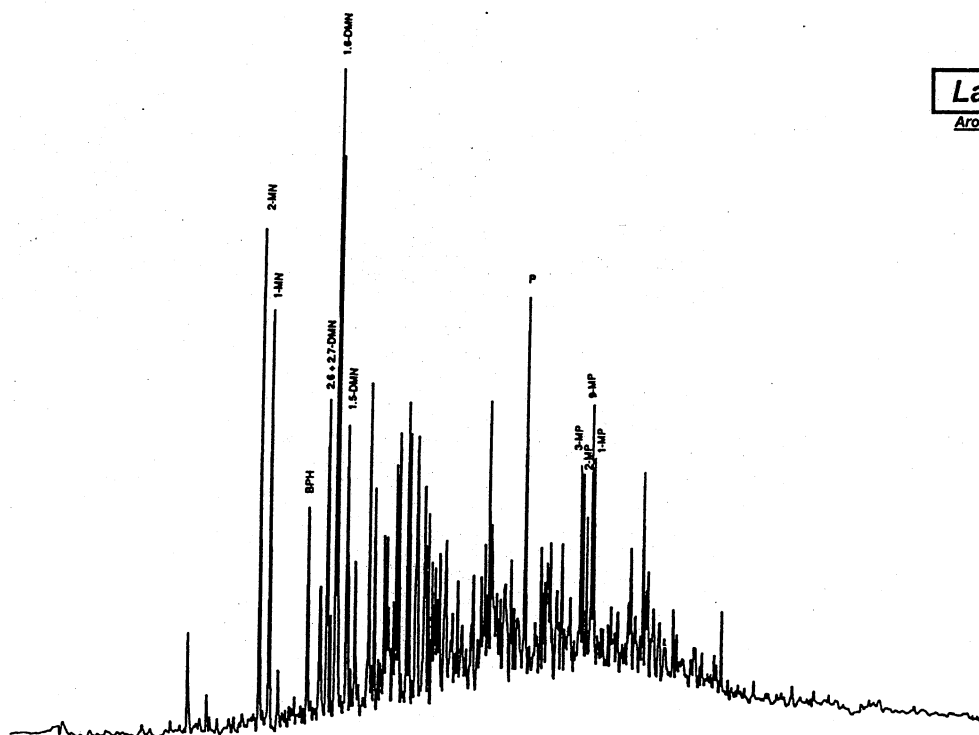


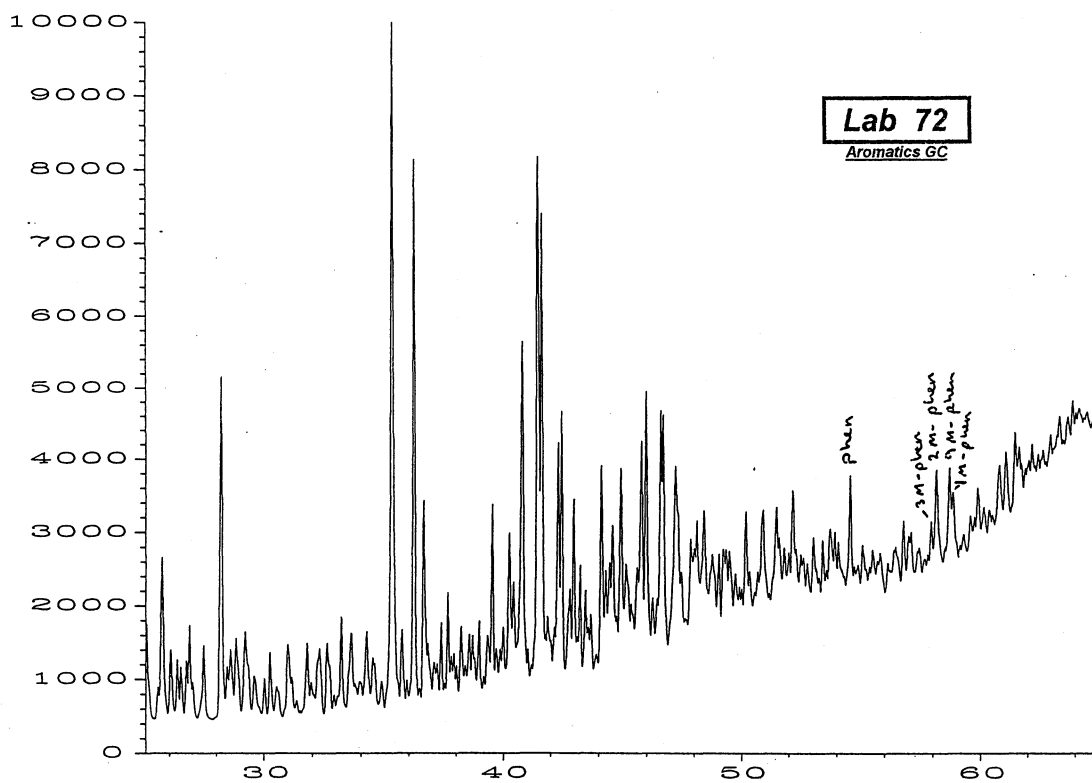
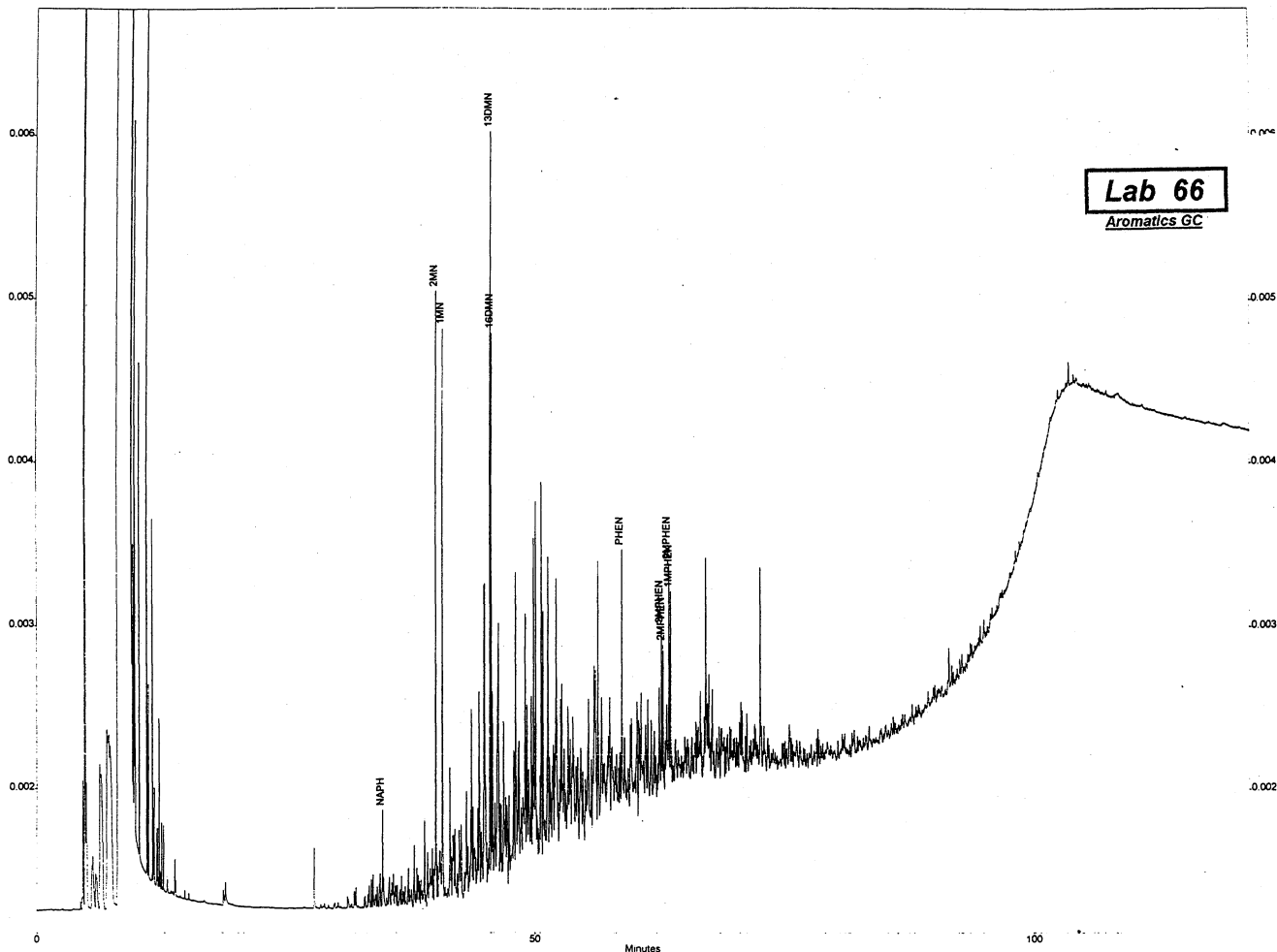


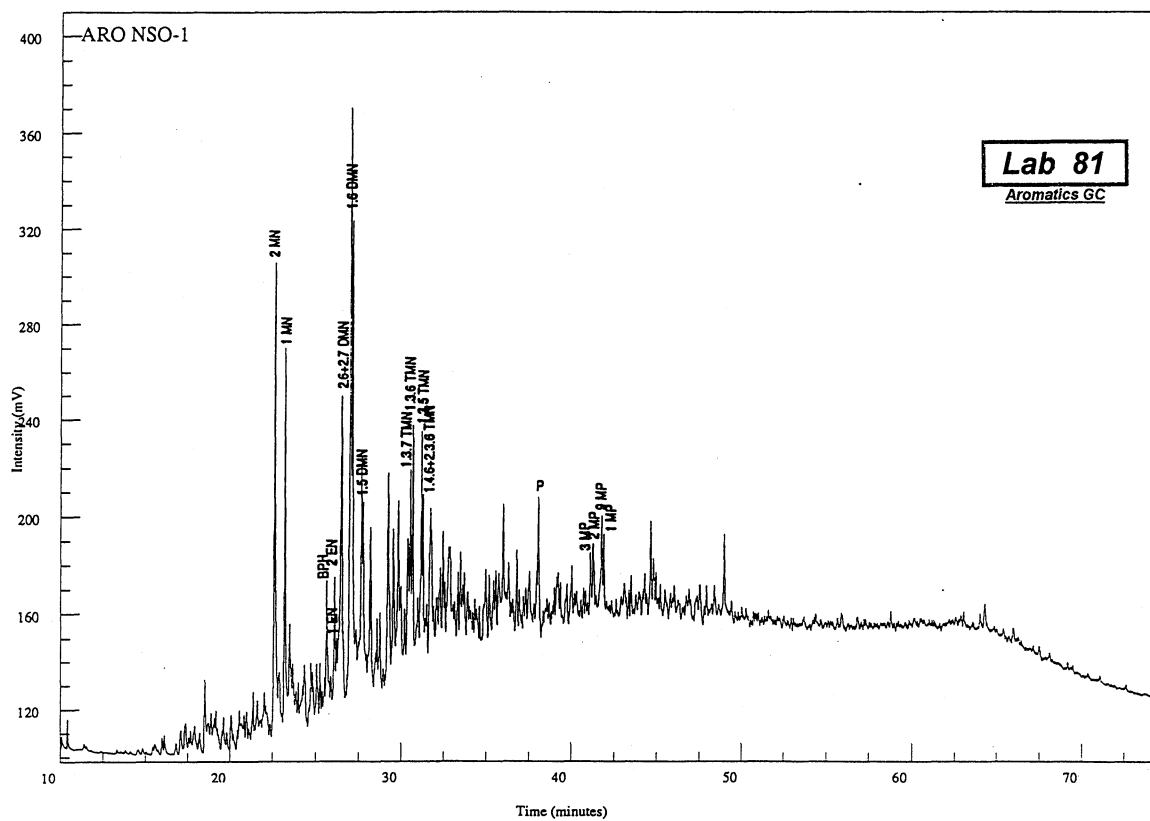
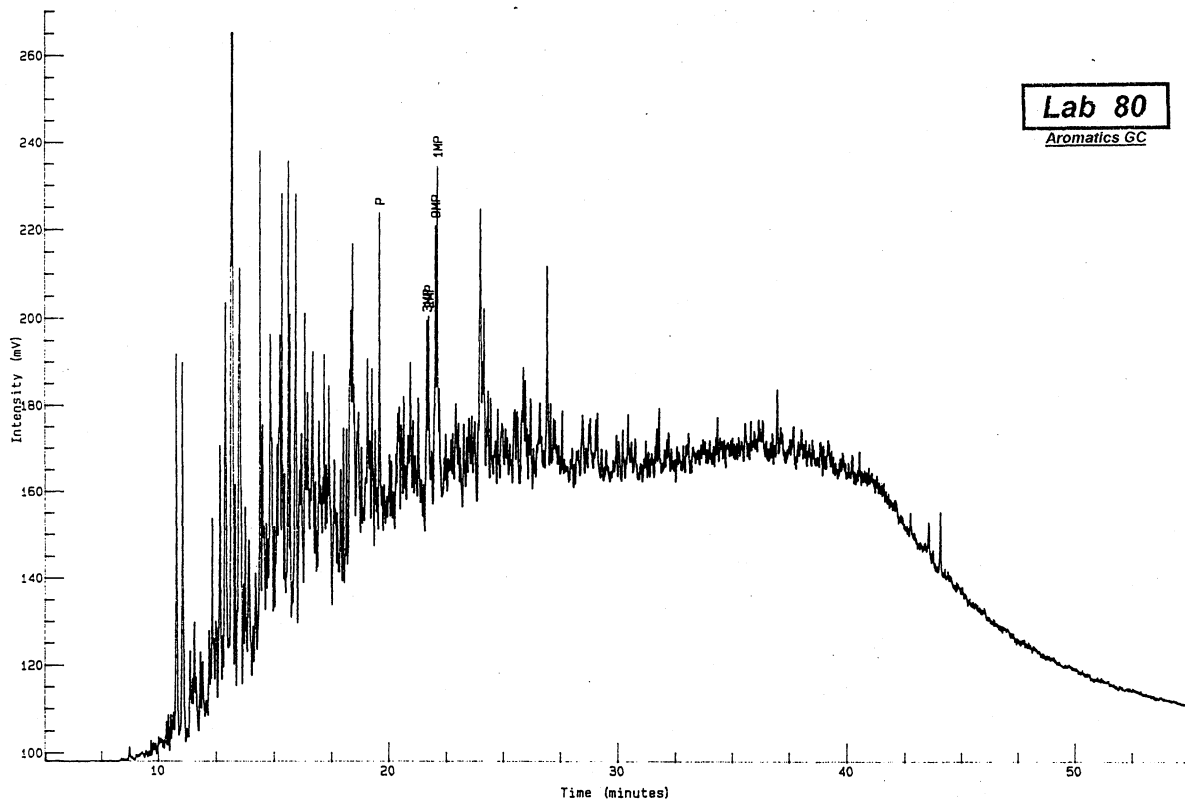


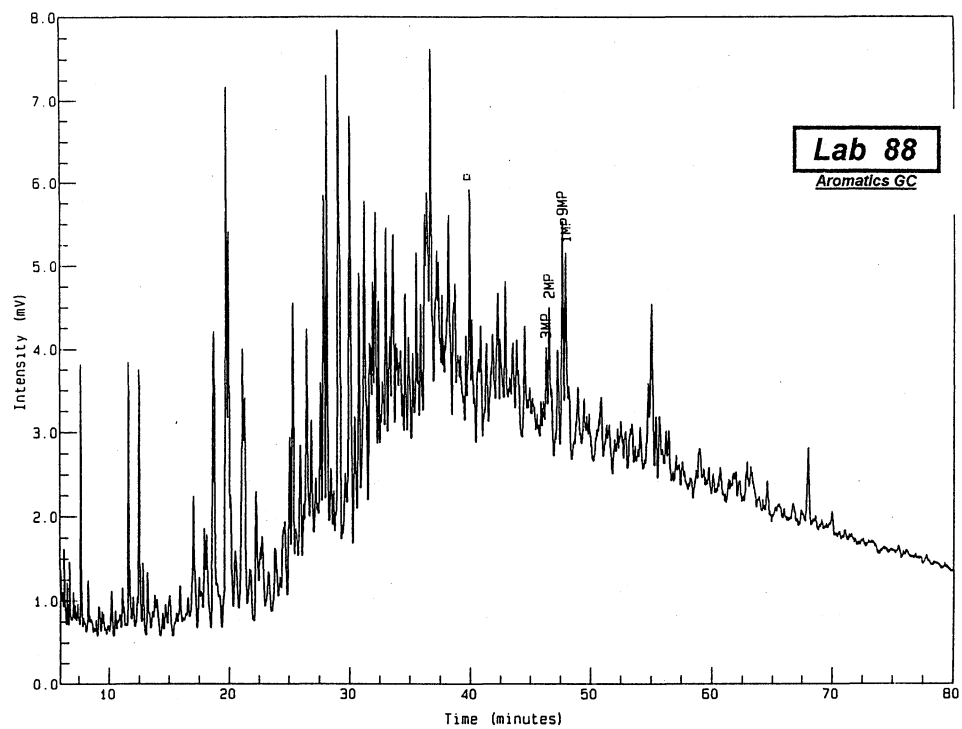
Lab 58

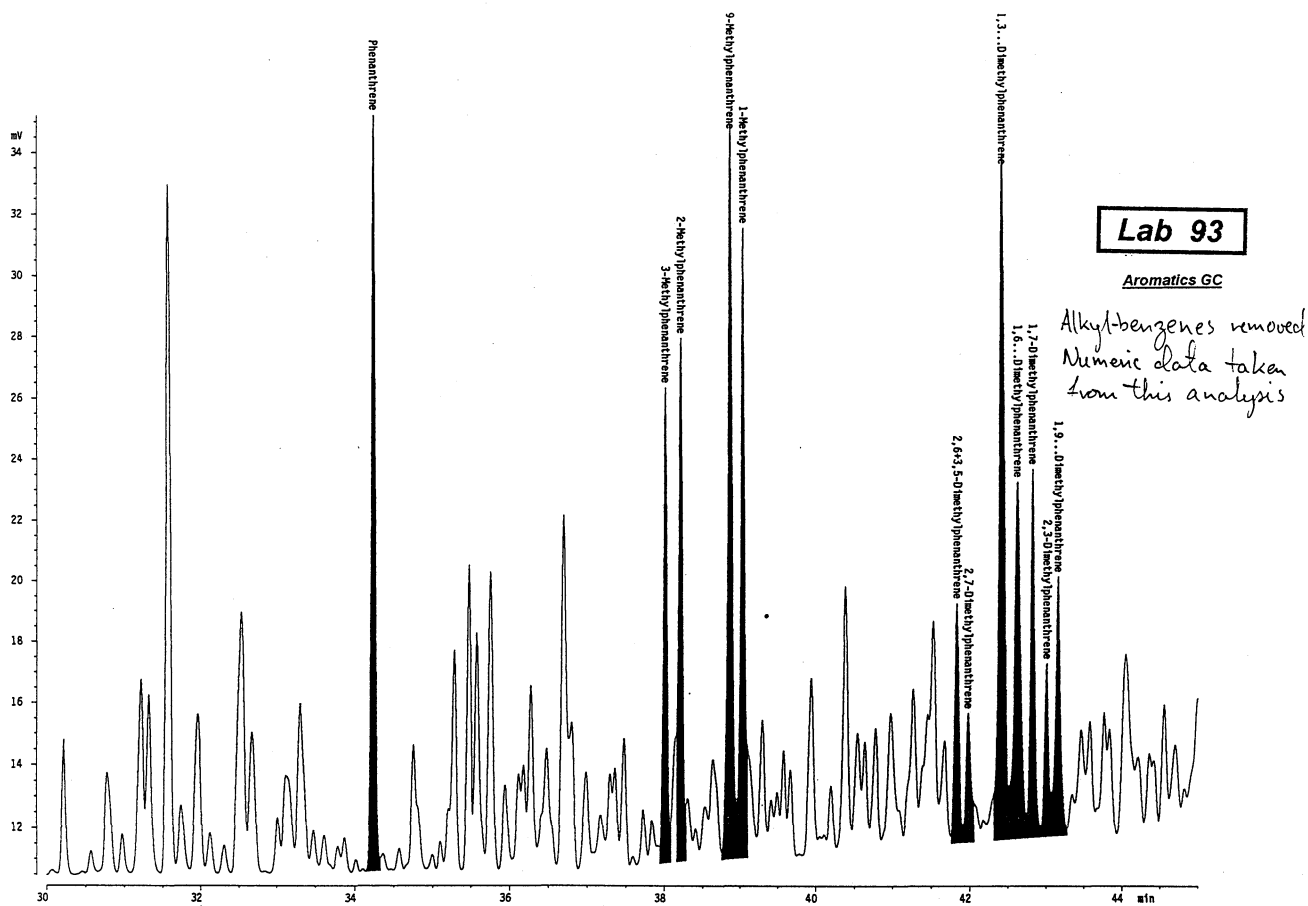
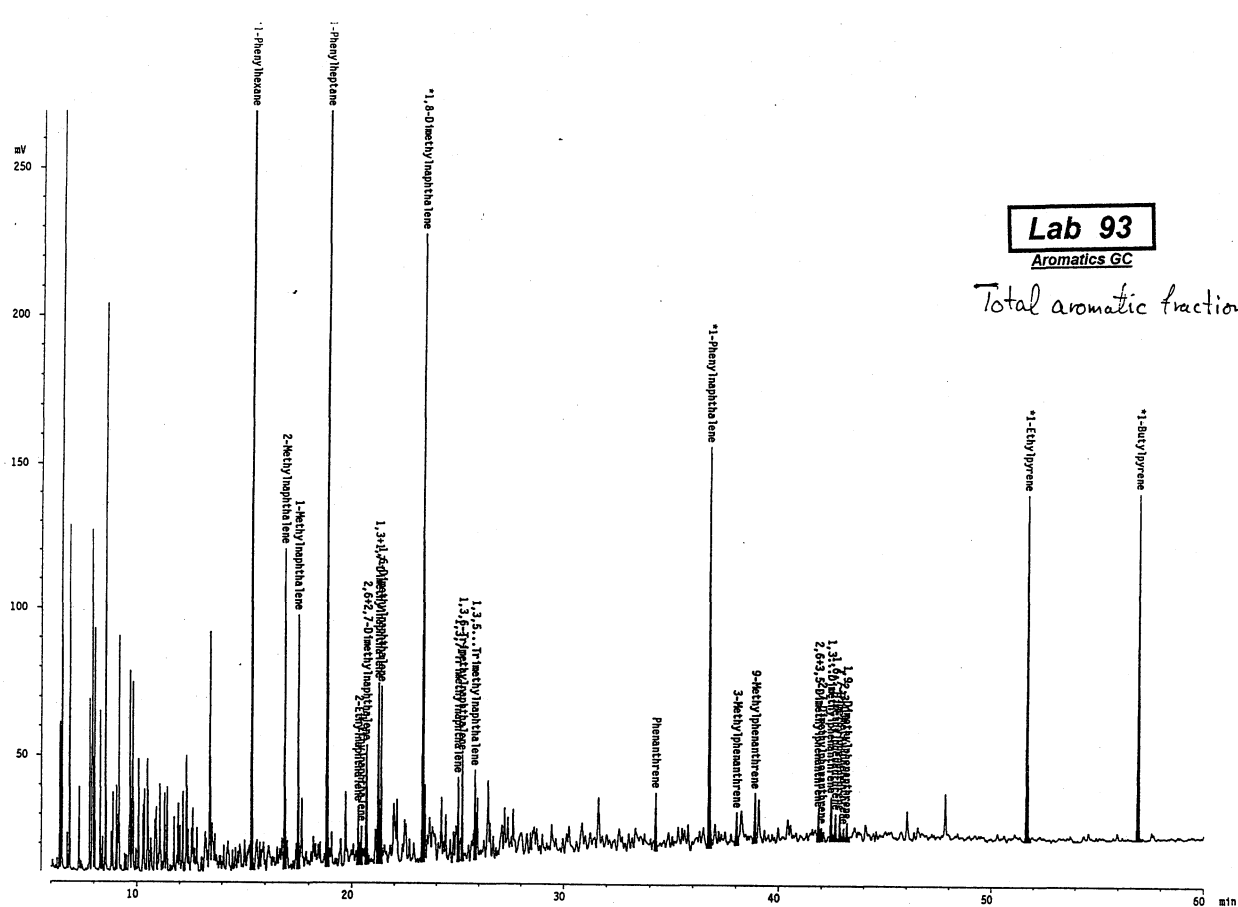
Aromatics GC

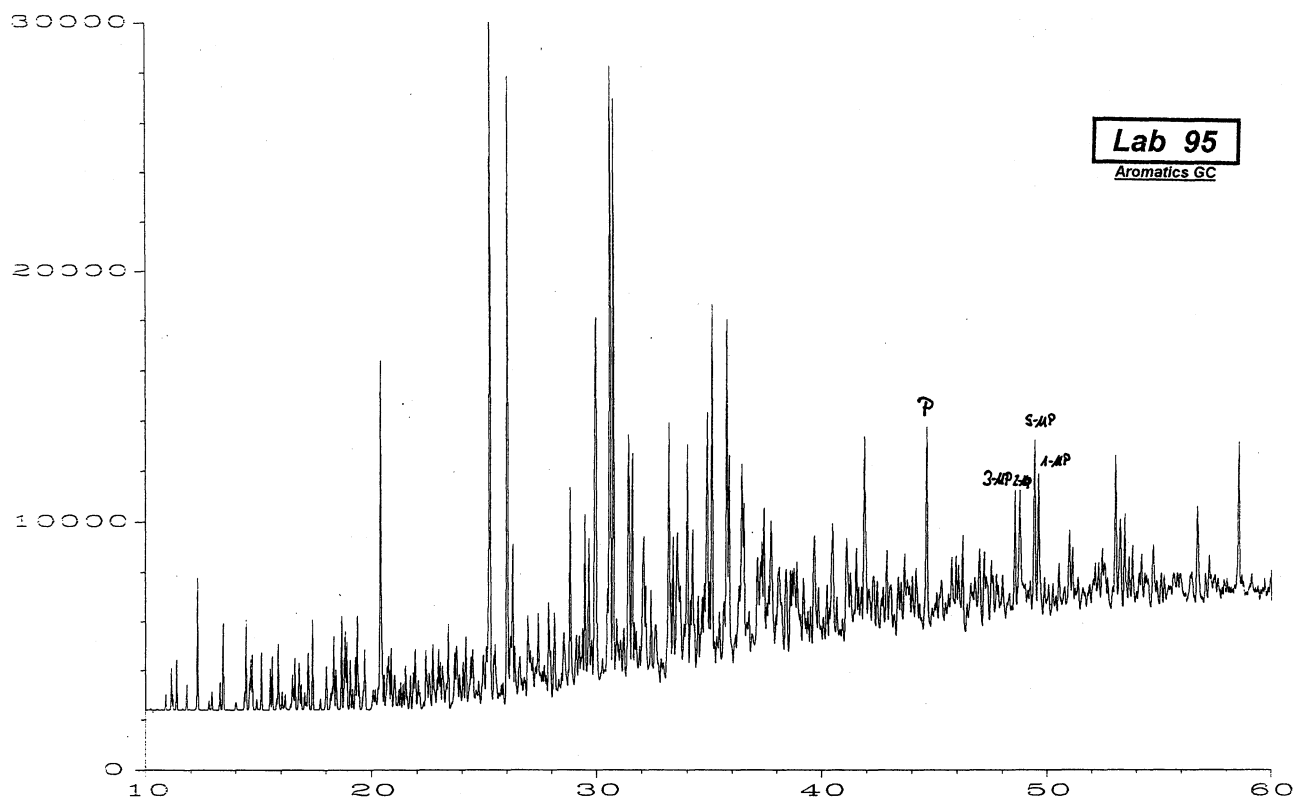








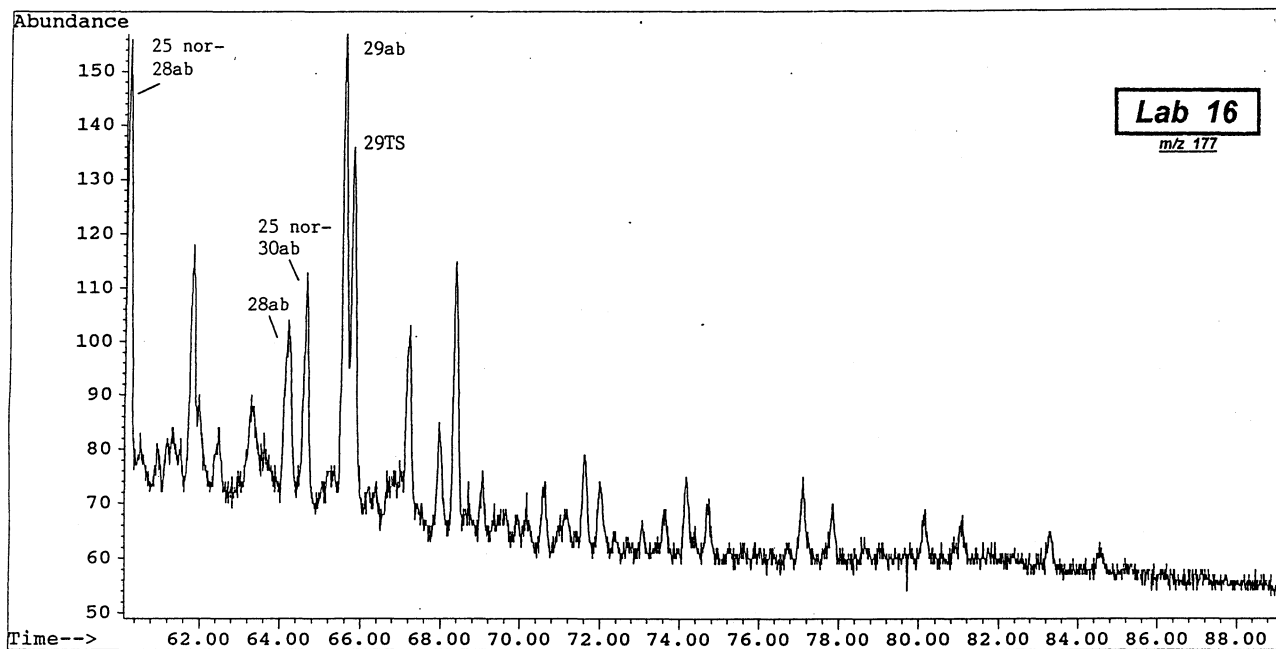
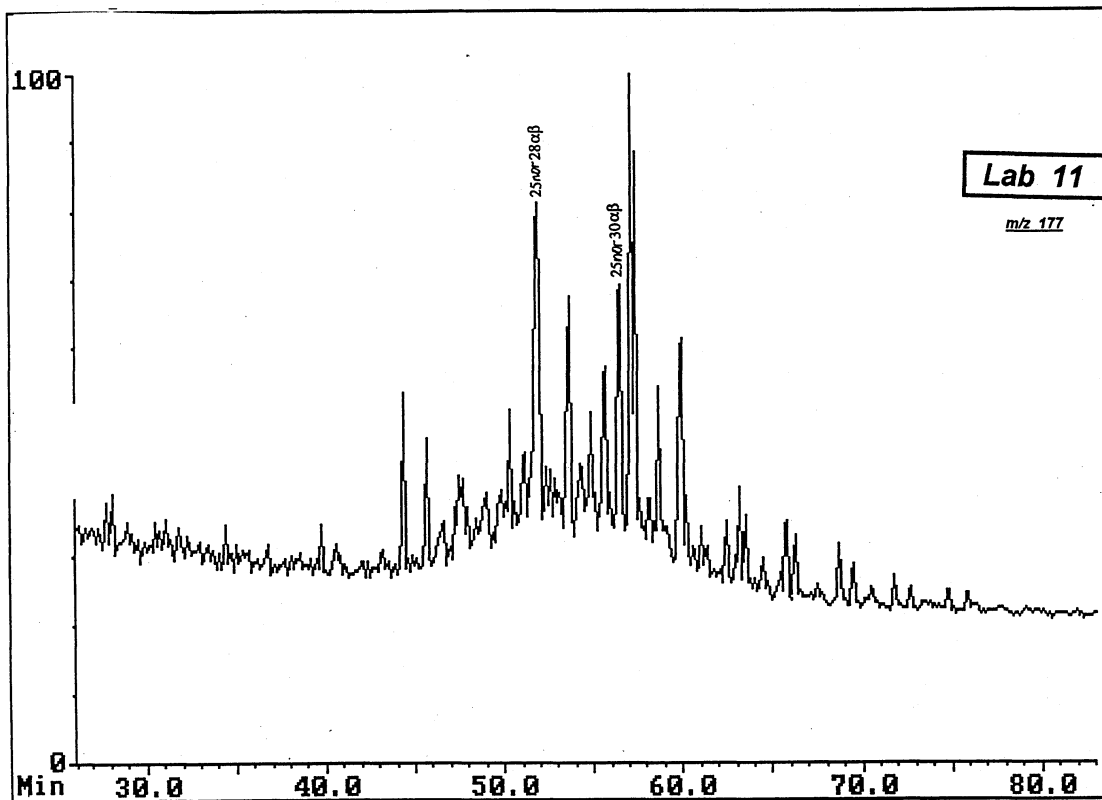


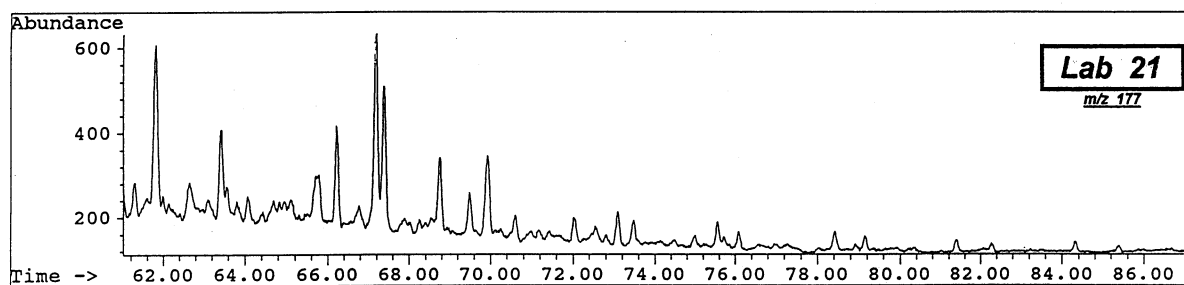
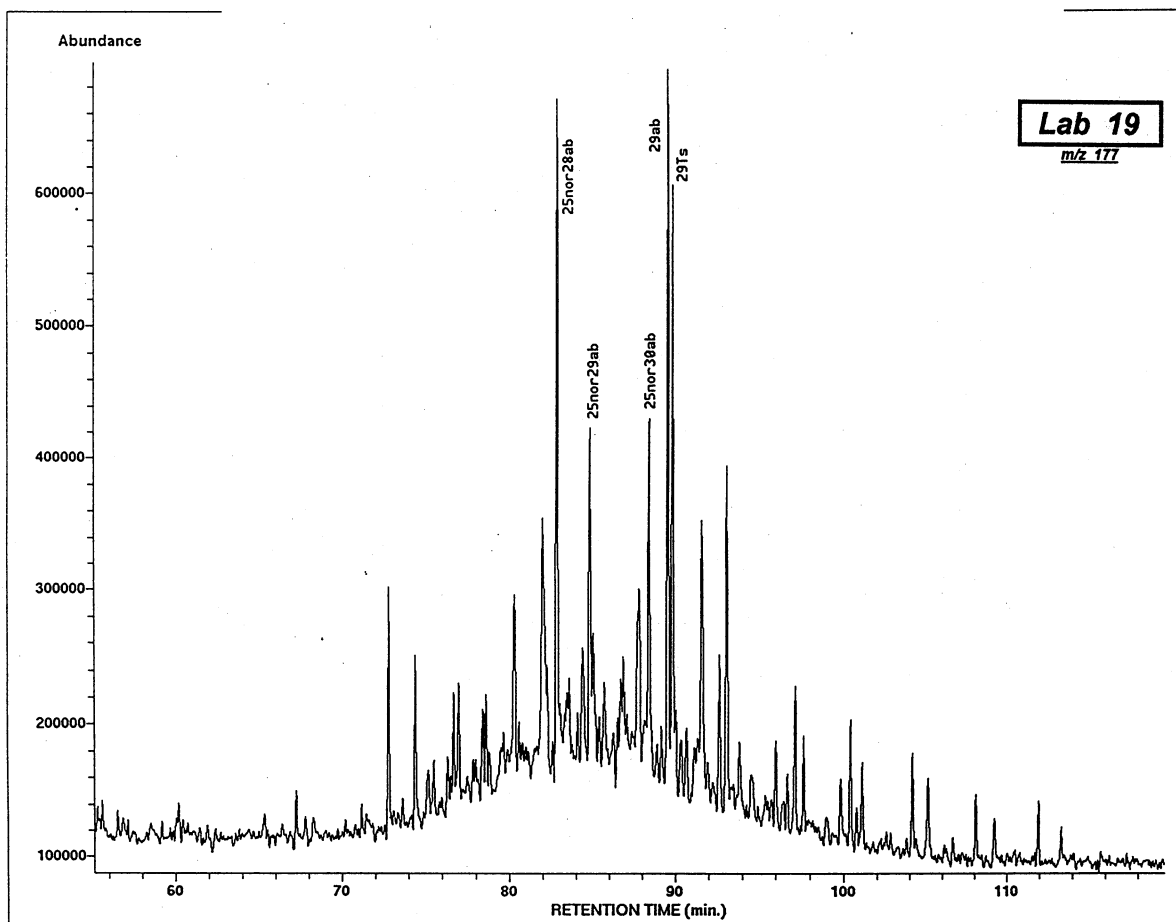


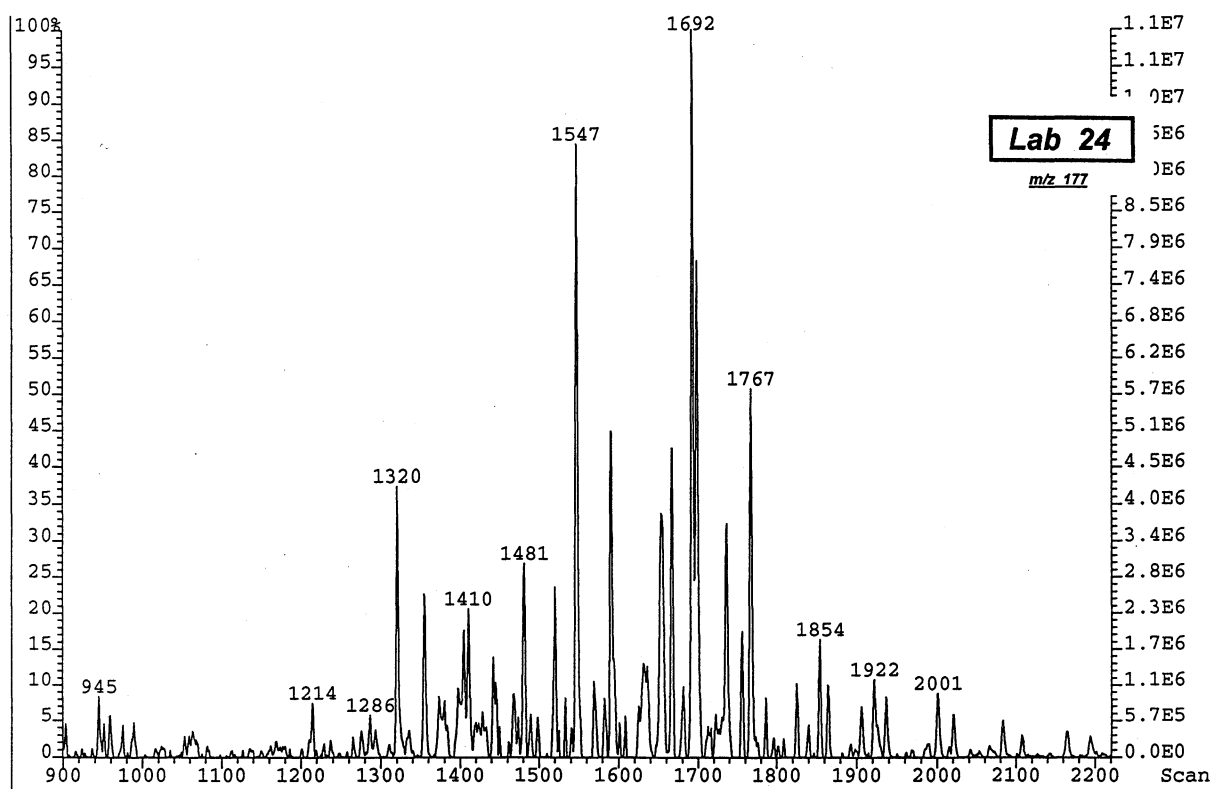
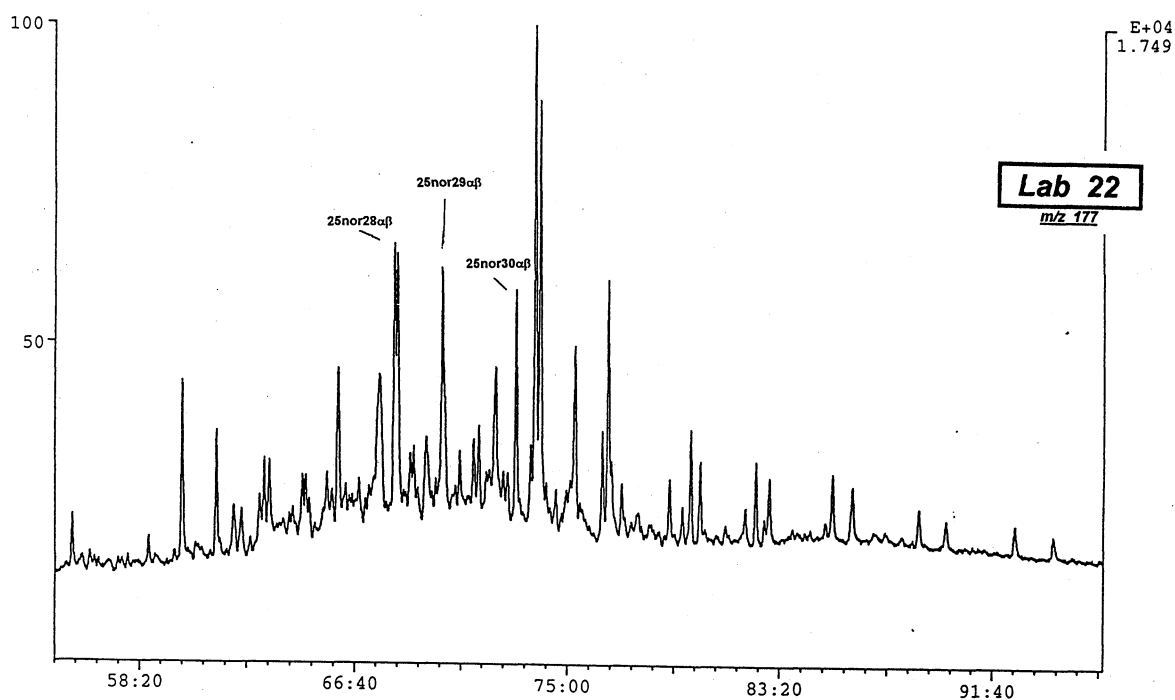
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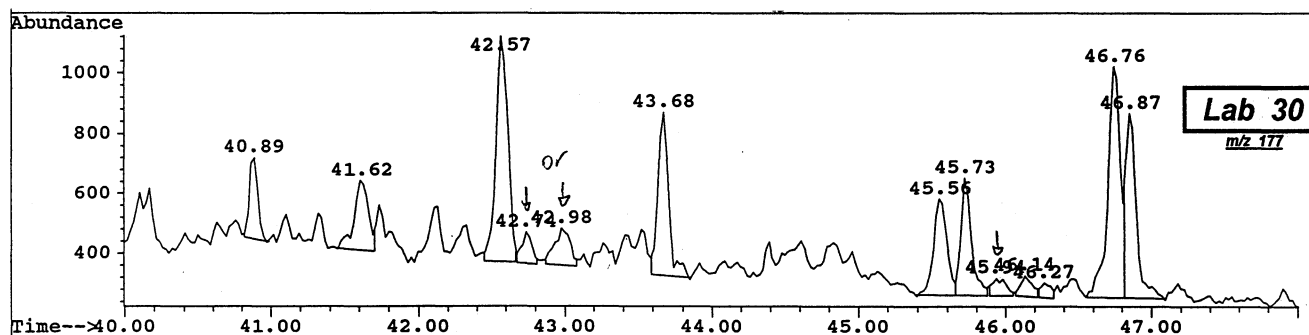
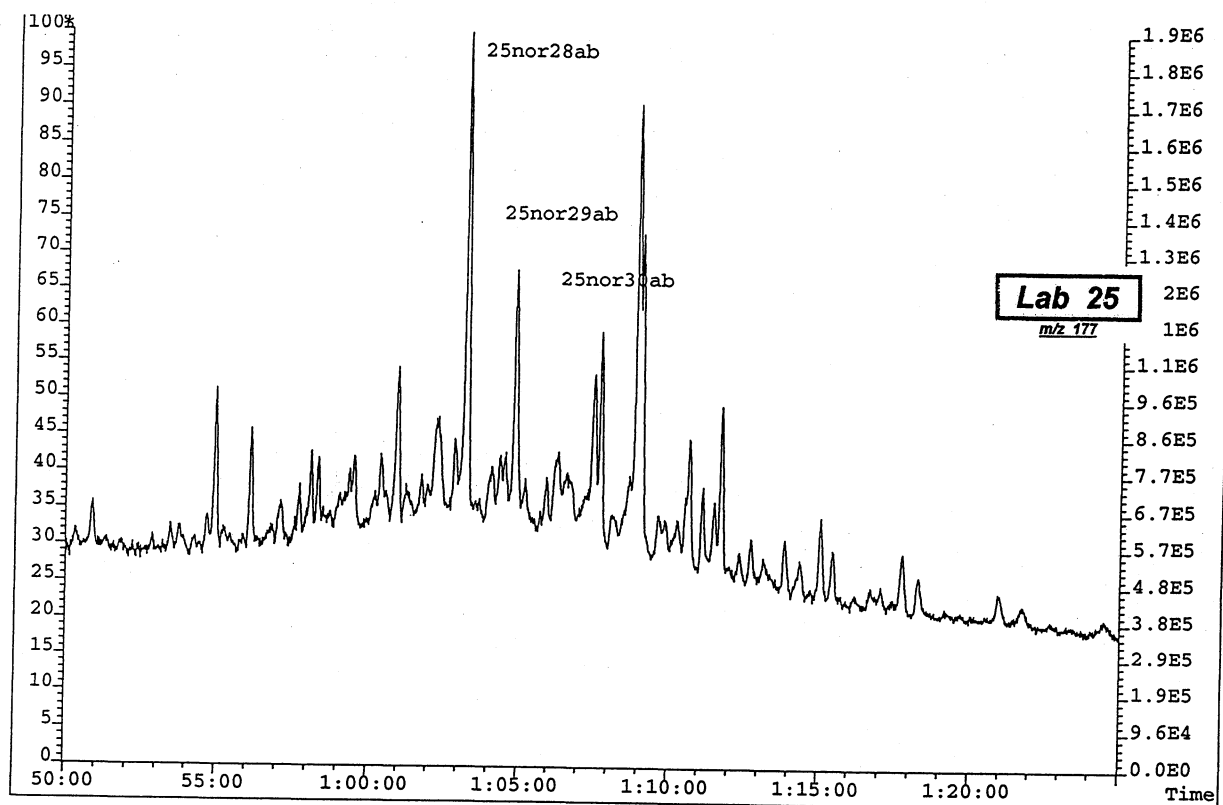
Appendix A3.4a-1

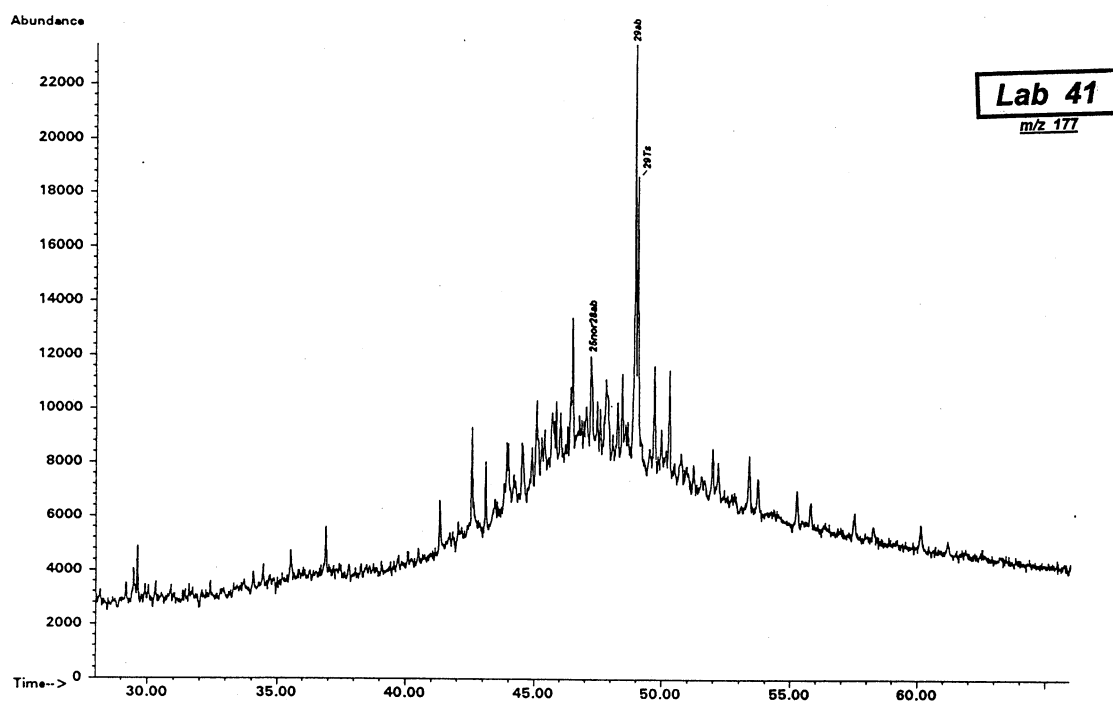
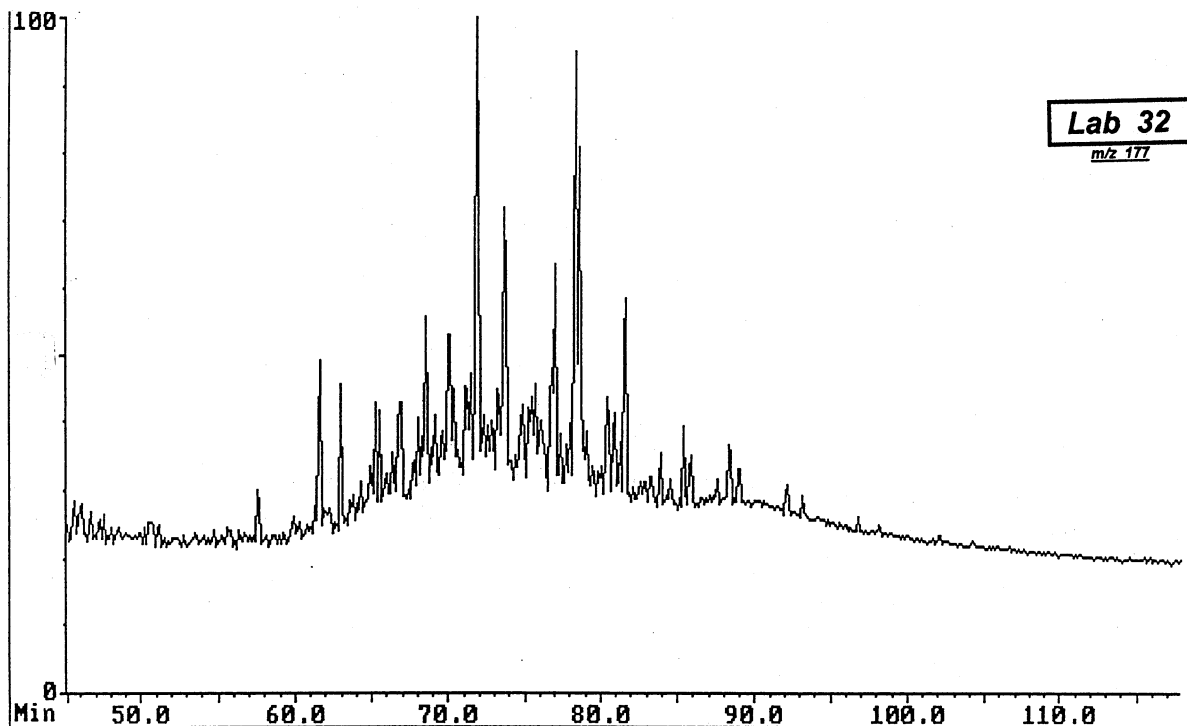
Saturates fraction m/z 177 GC-MS fragmentograms

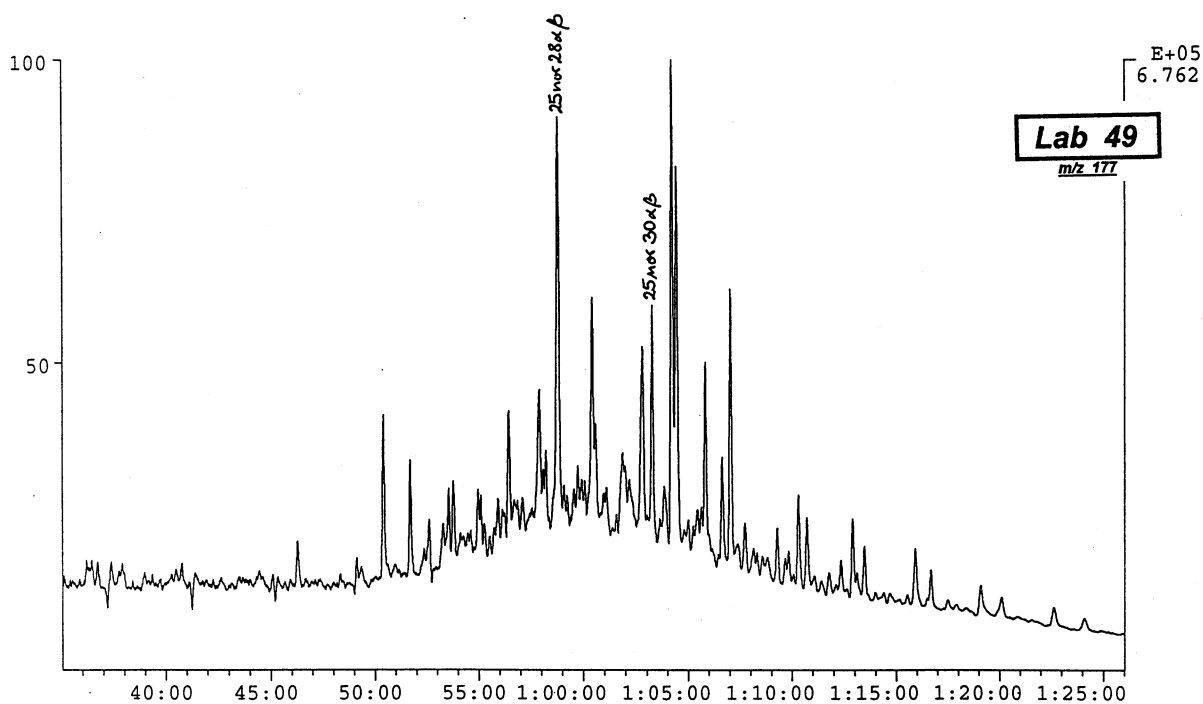
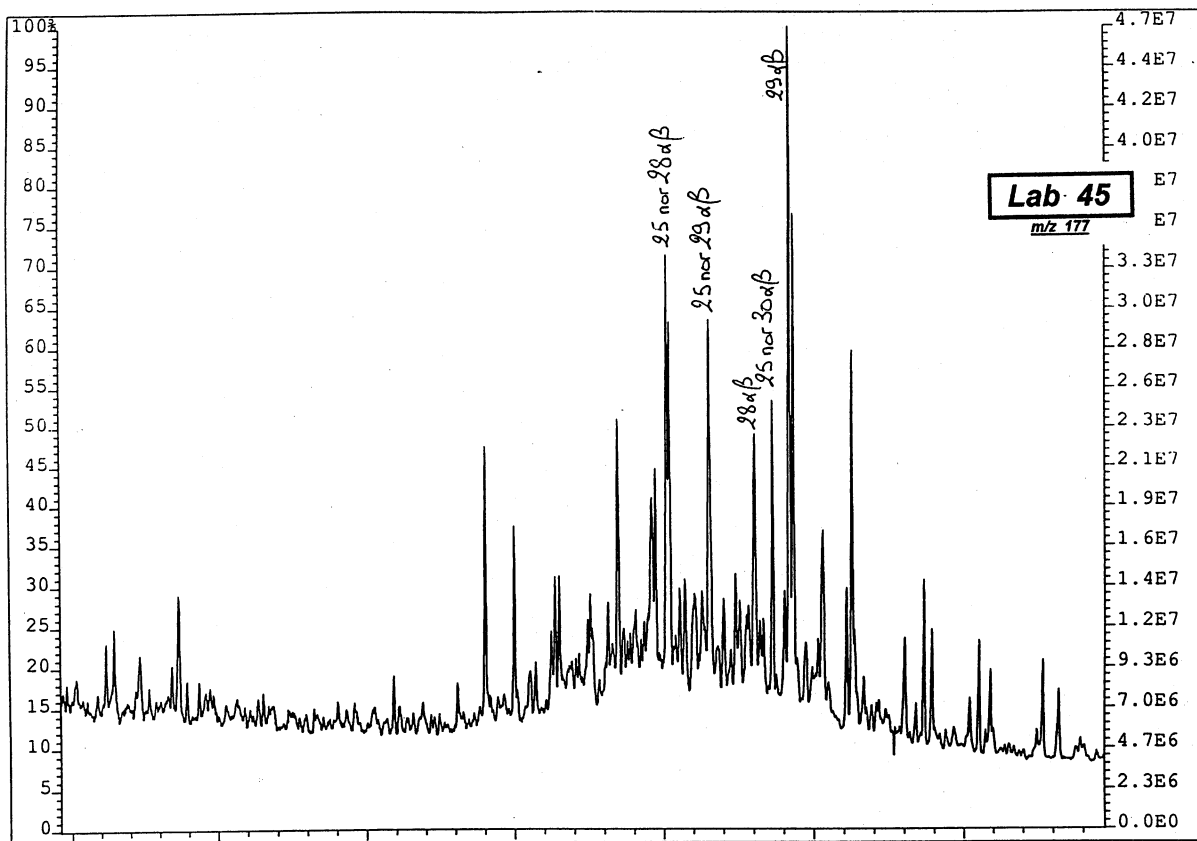


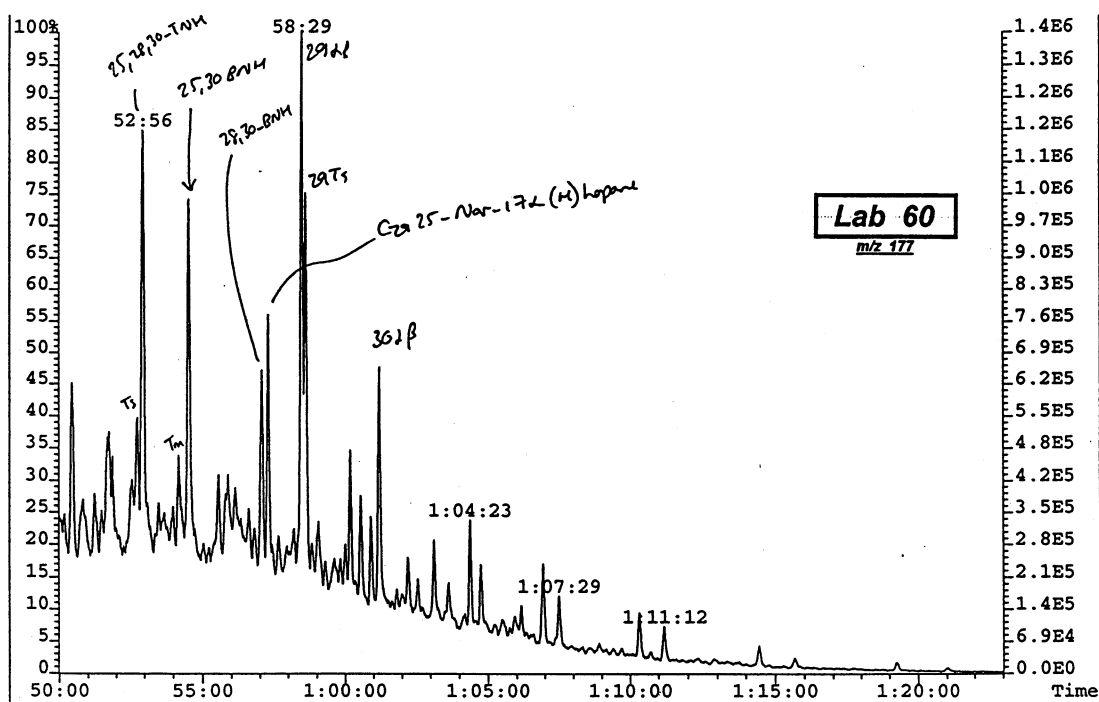
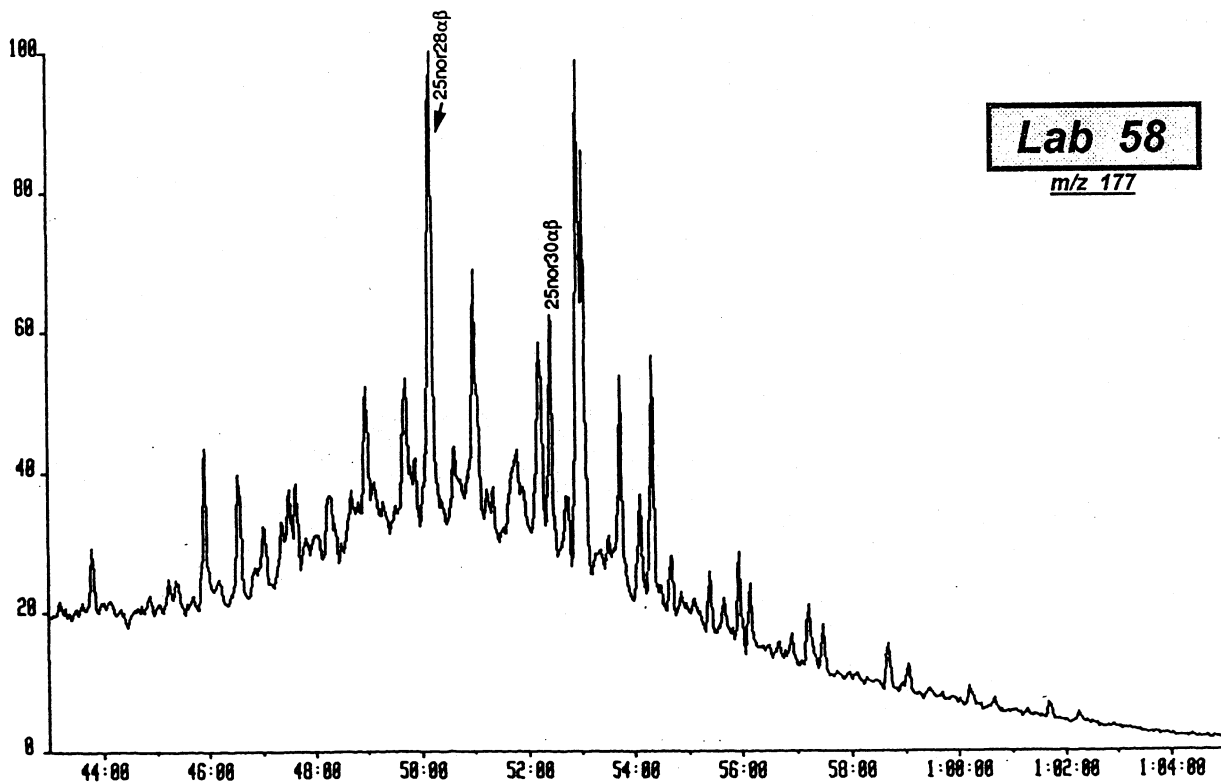


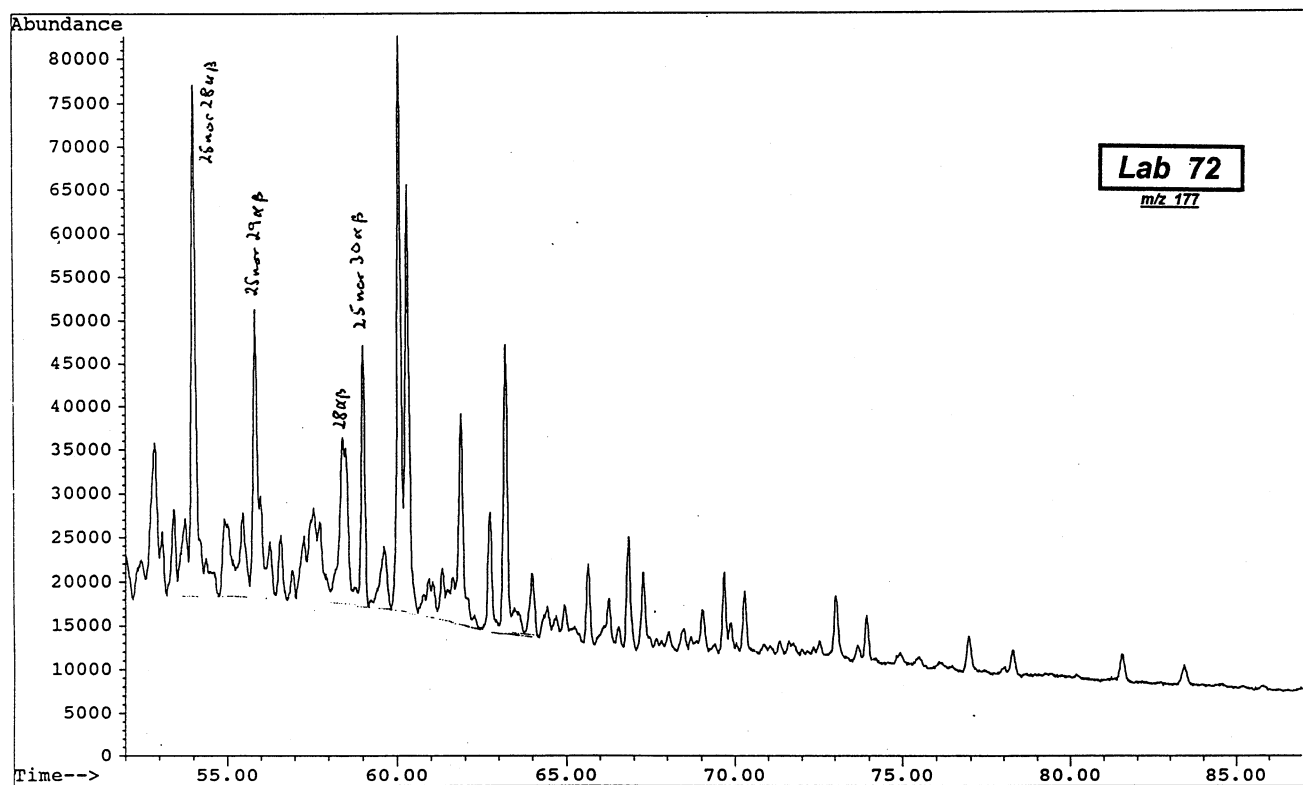
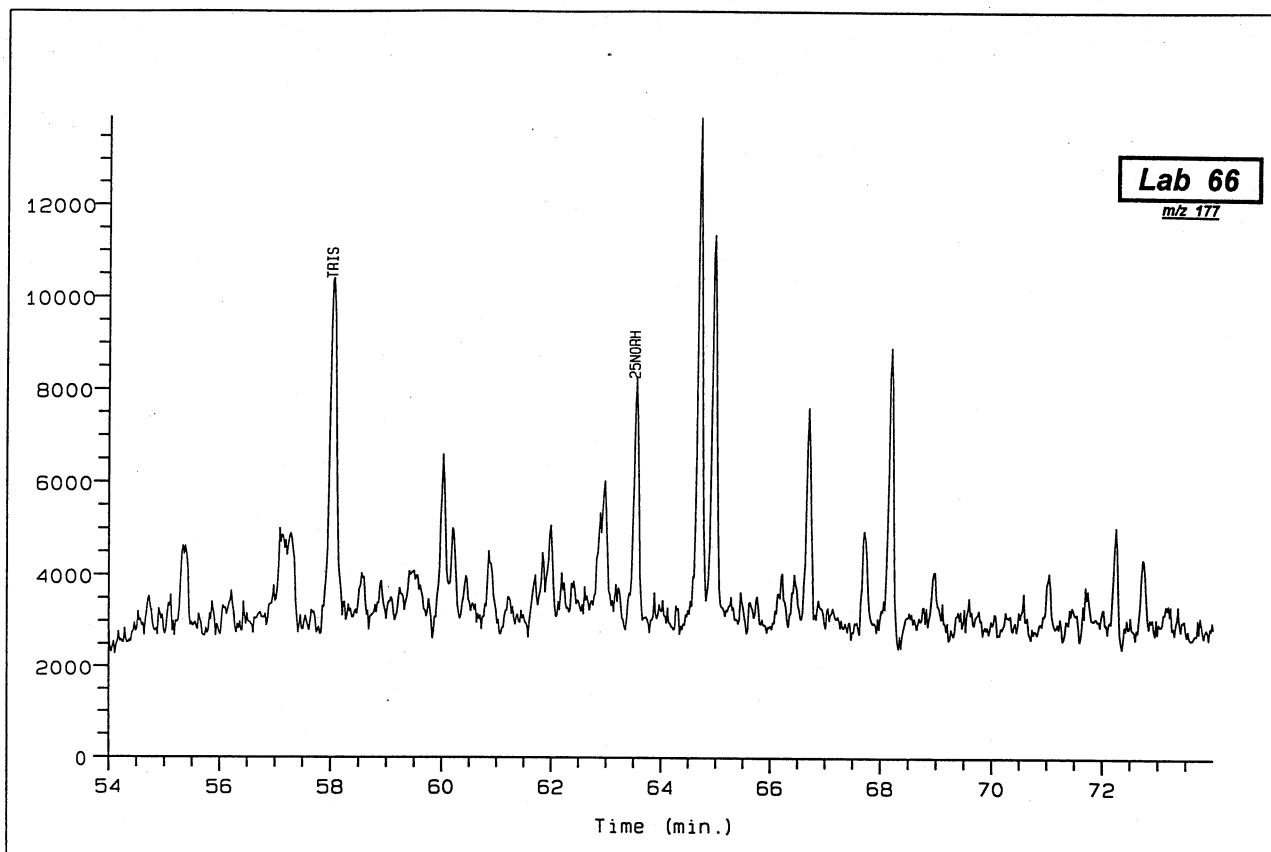


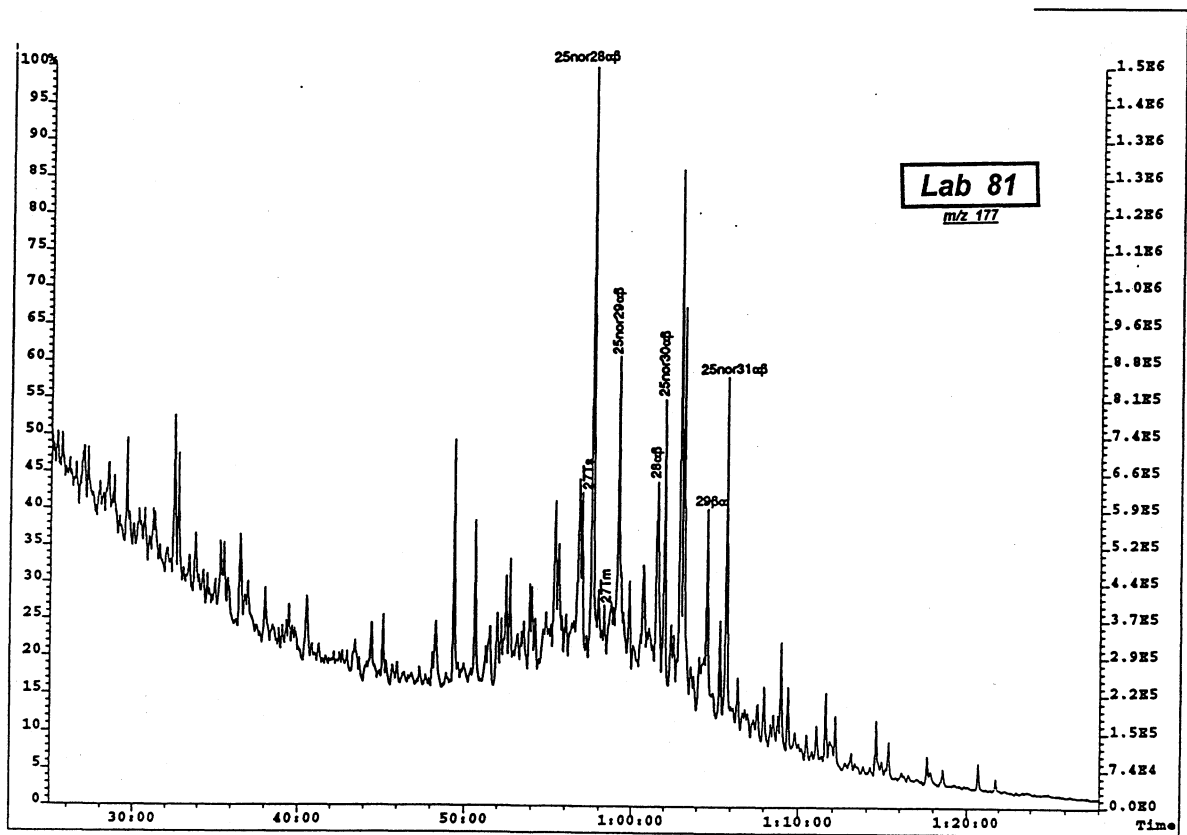
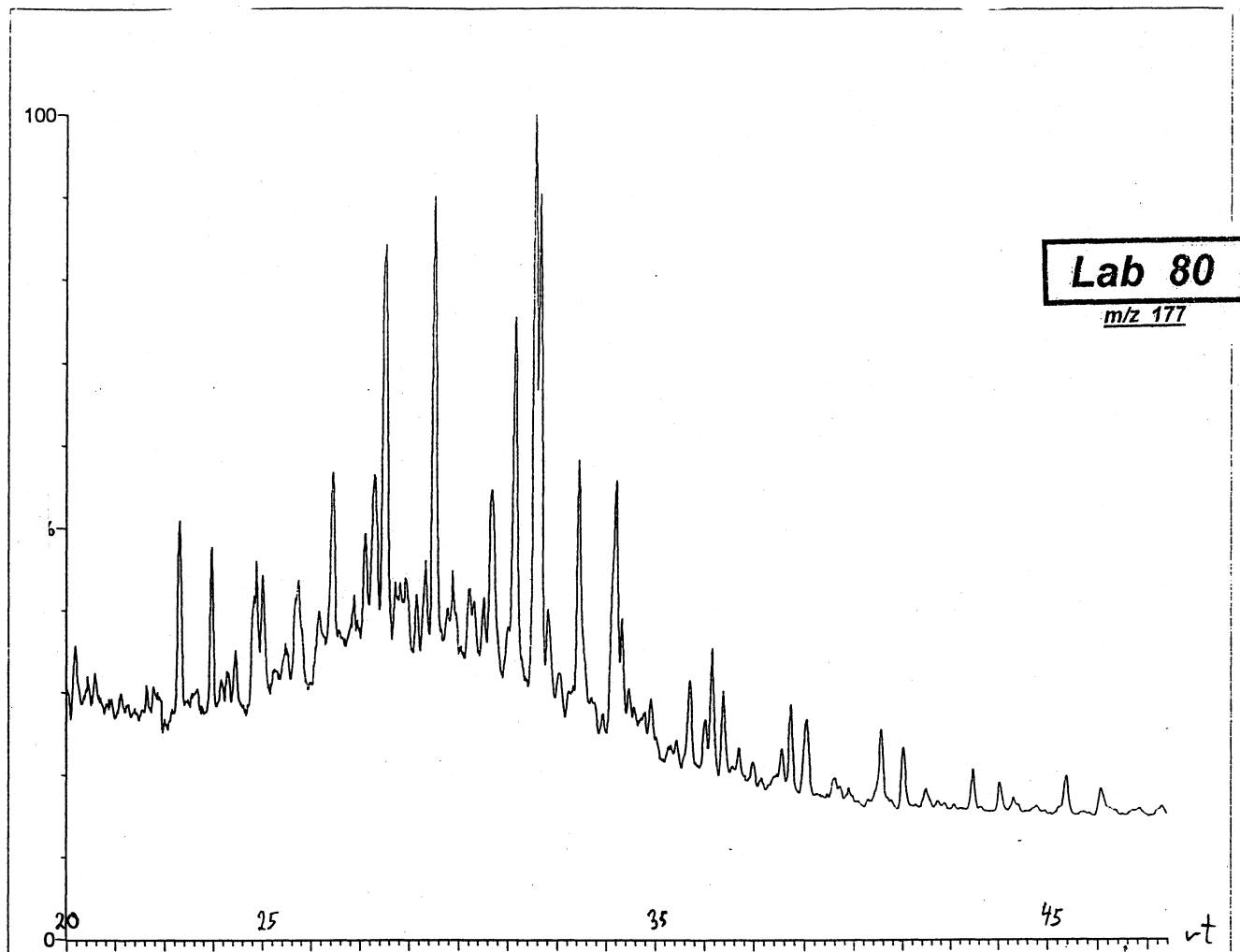


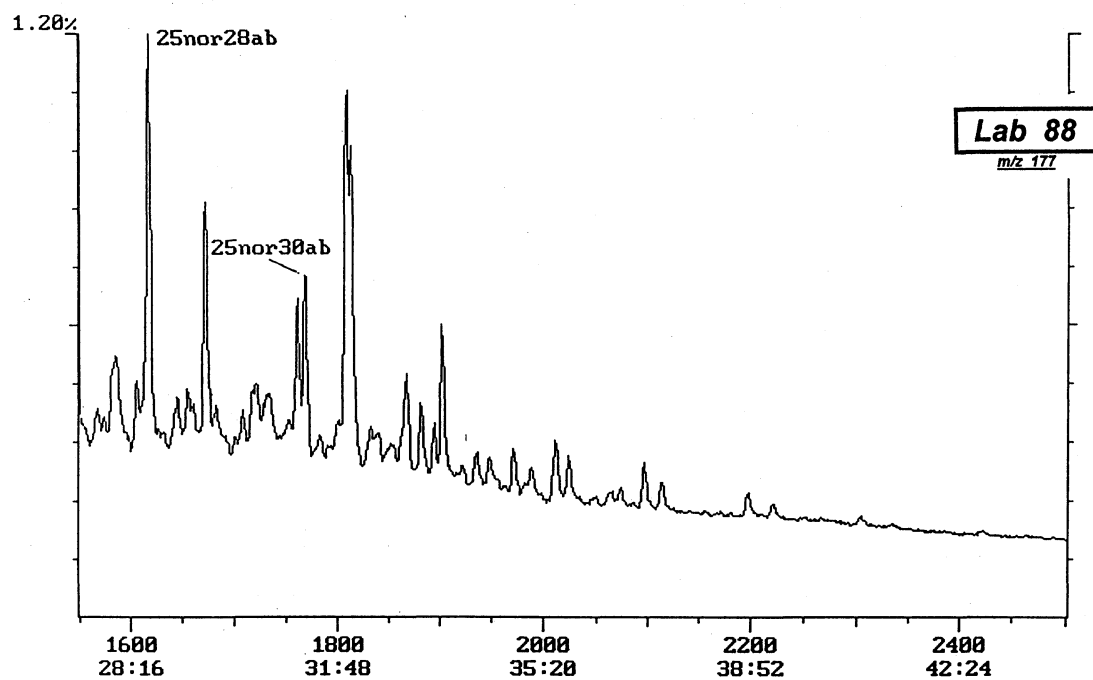


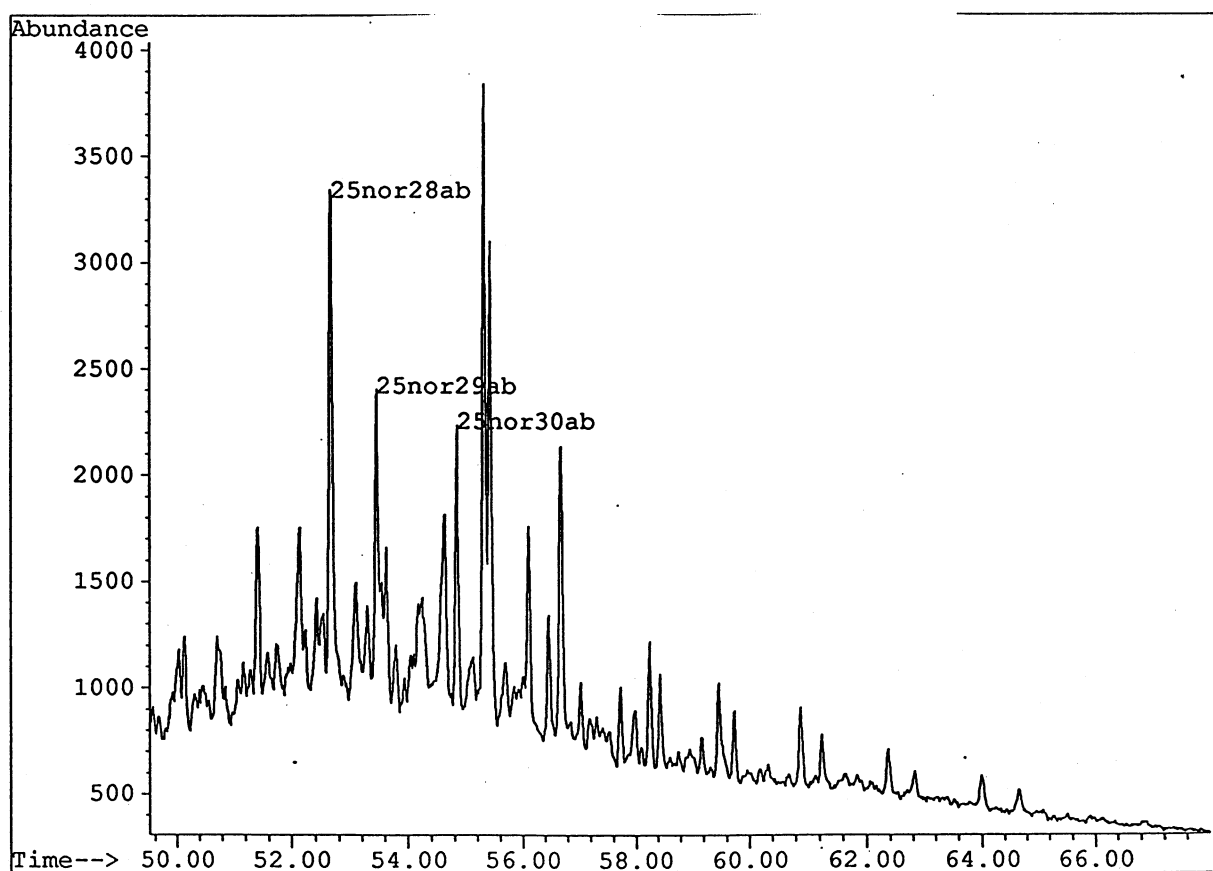
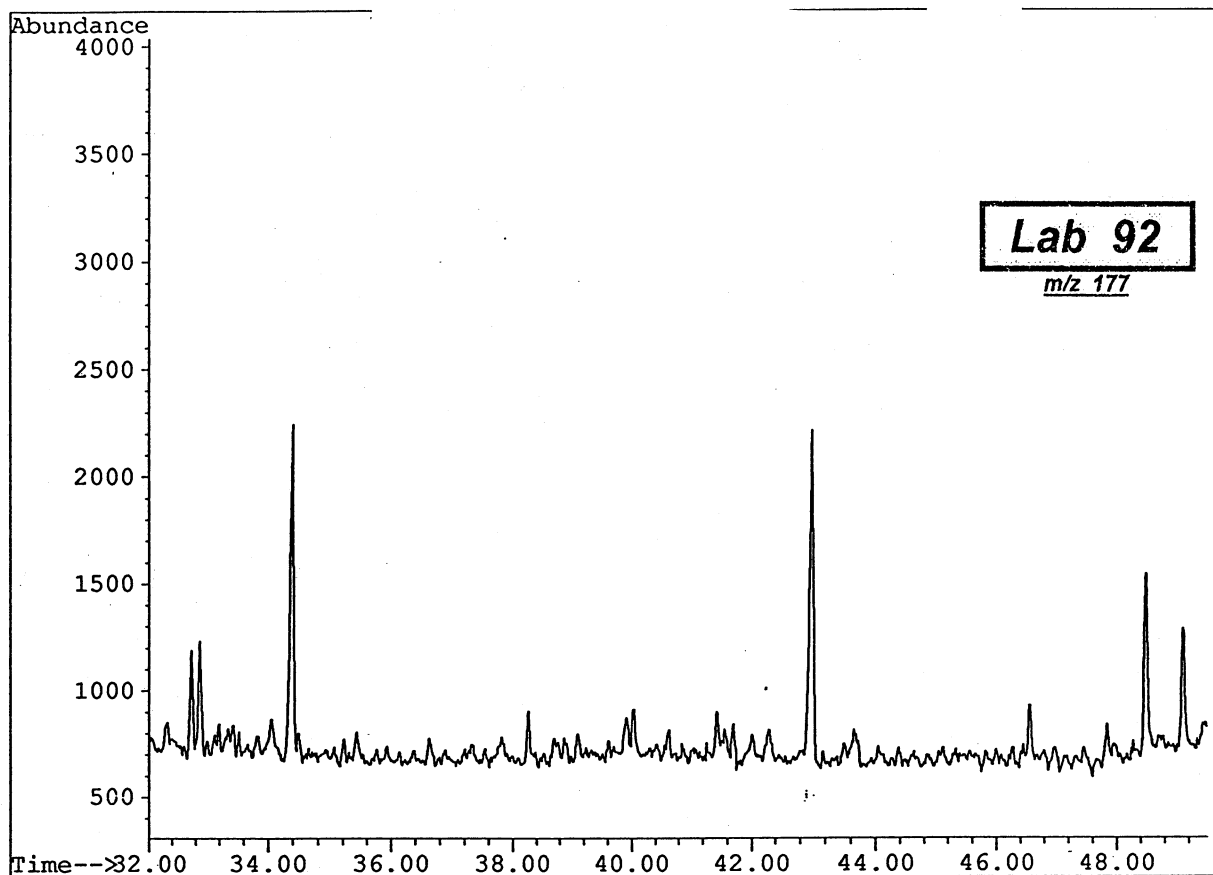


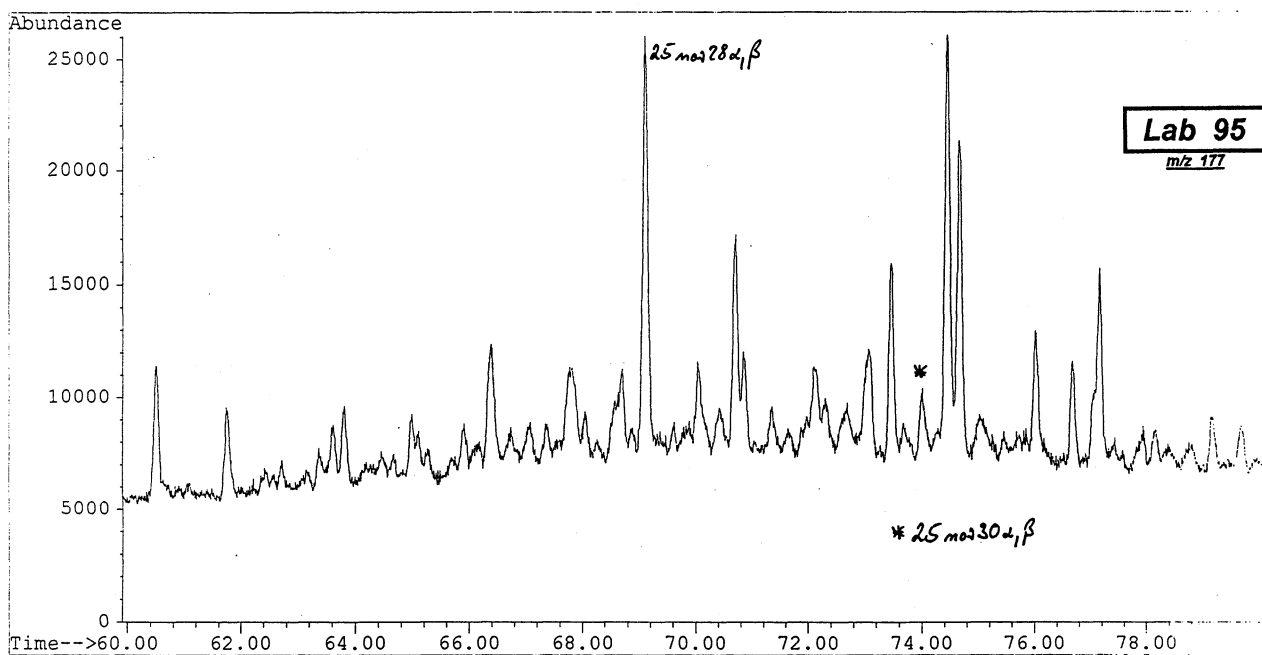








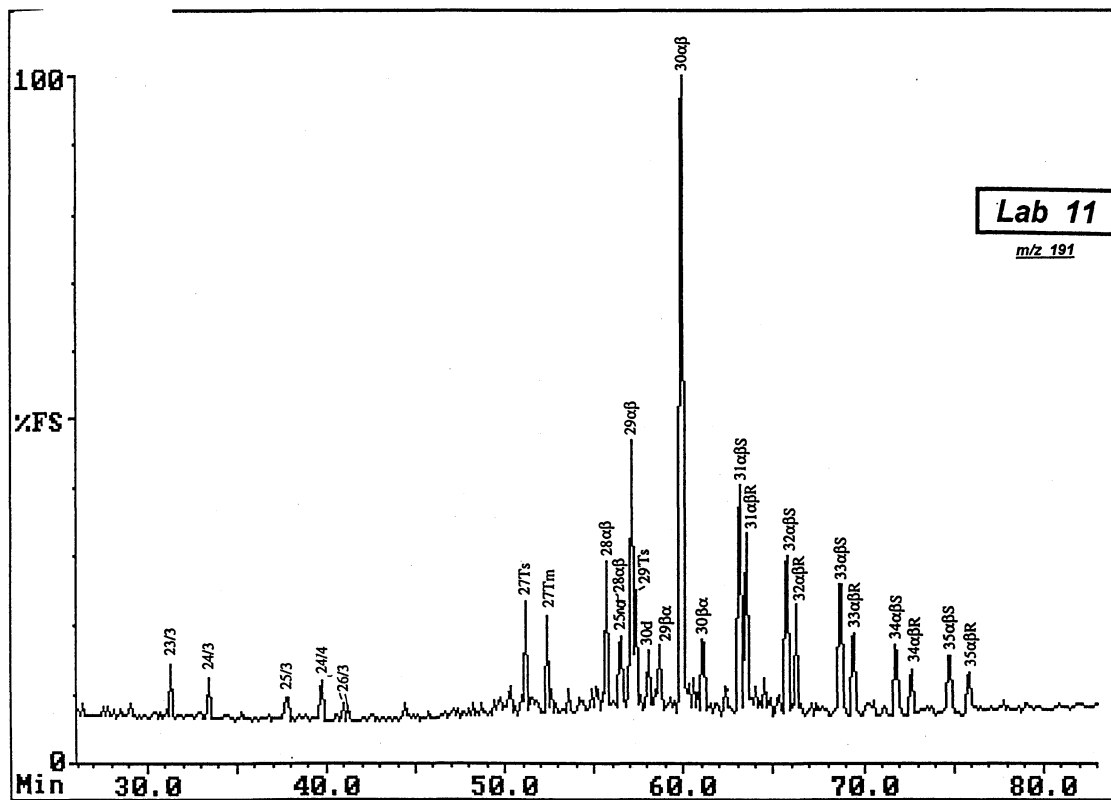
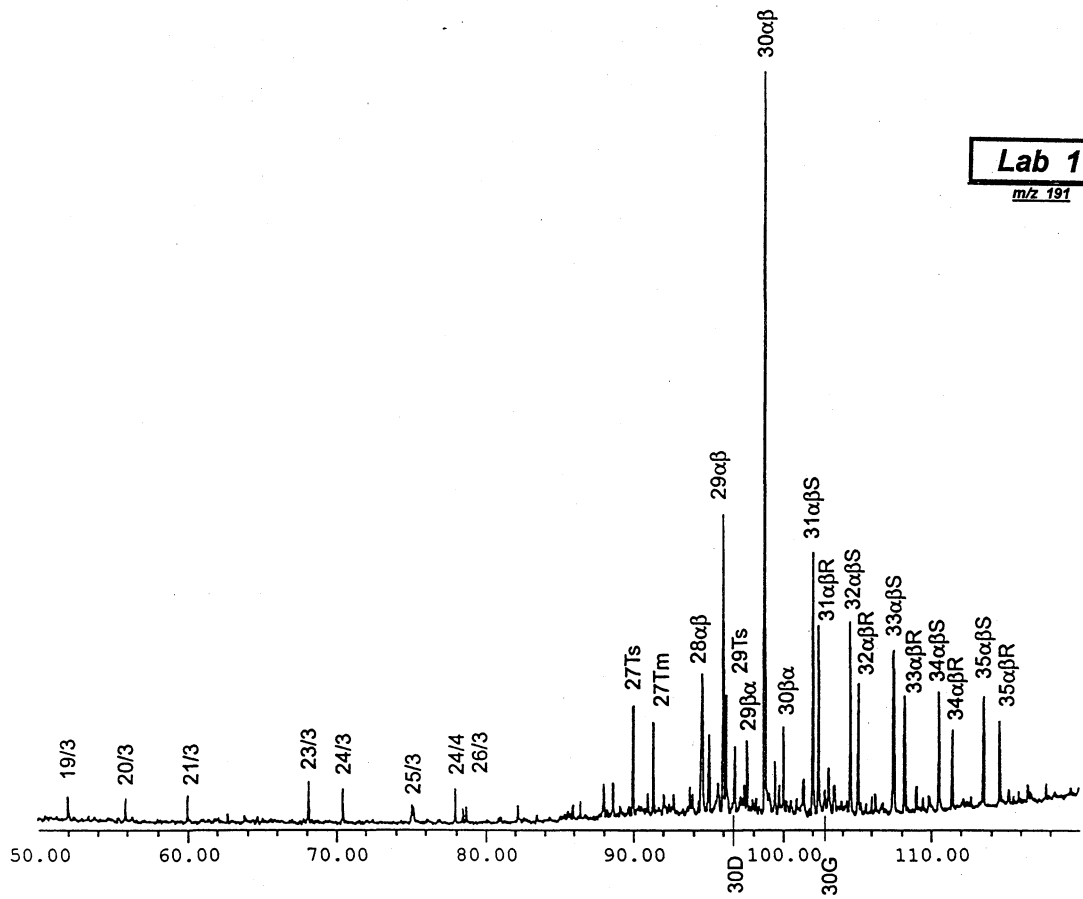


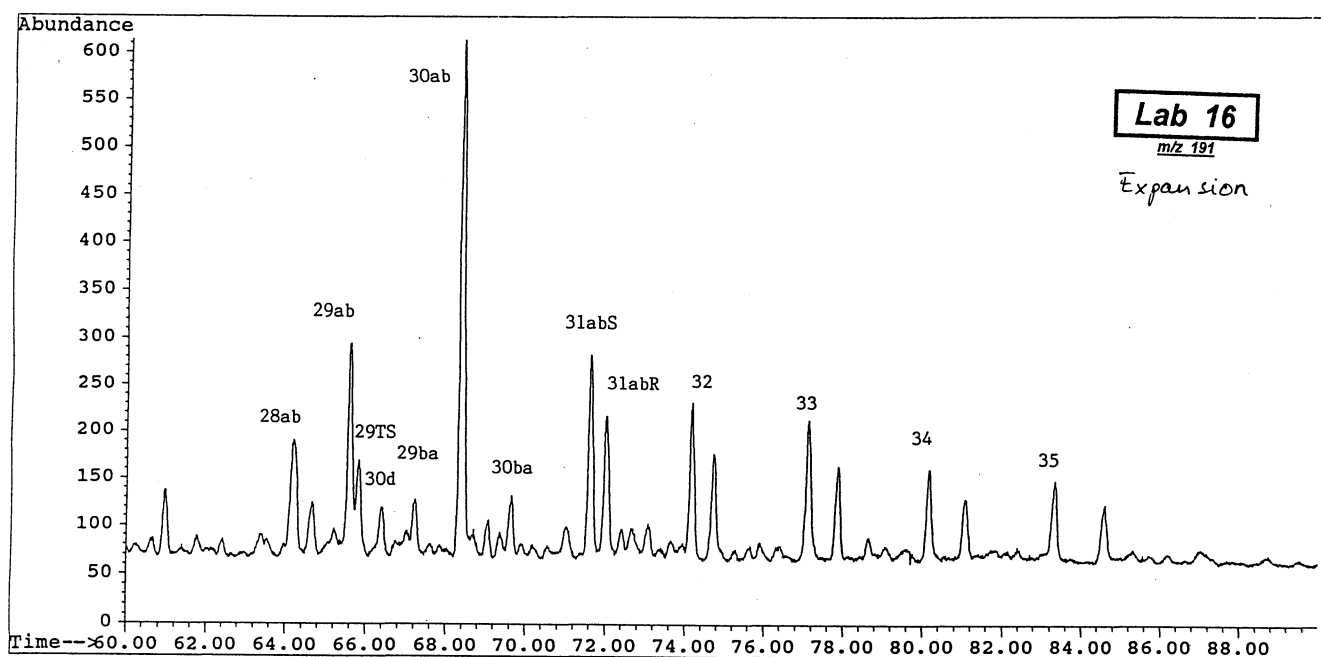
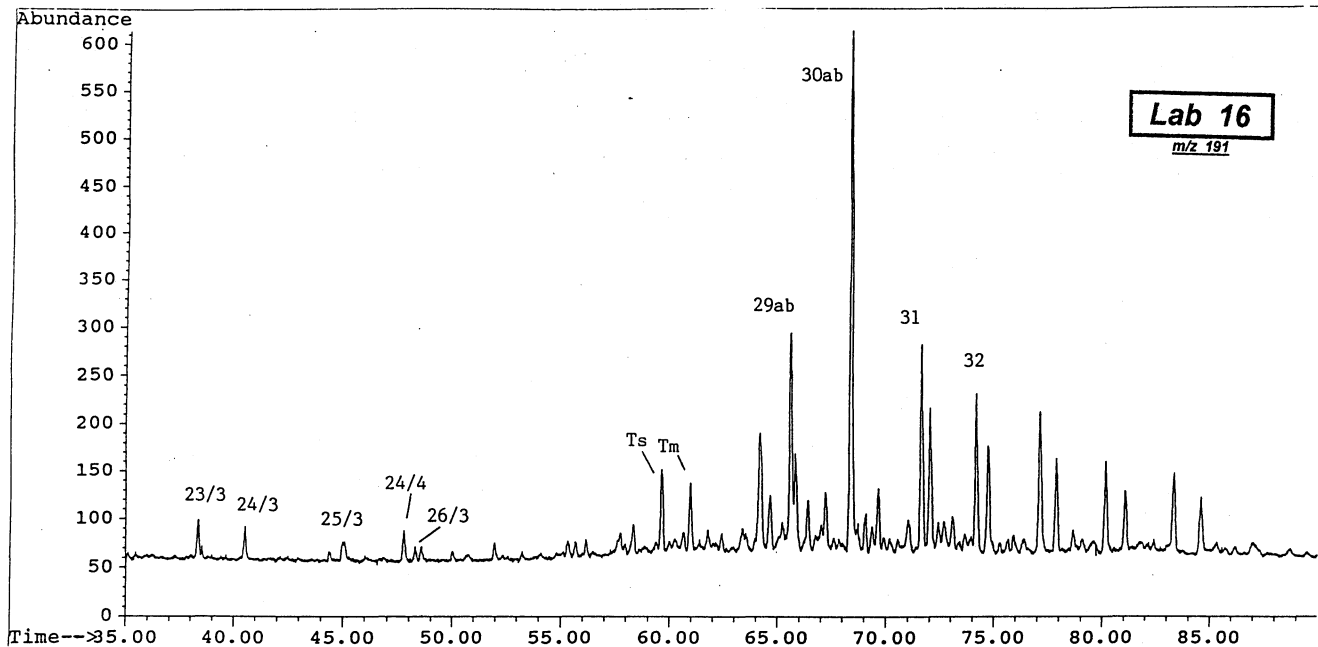


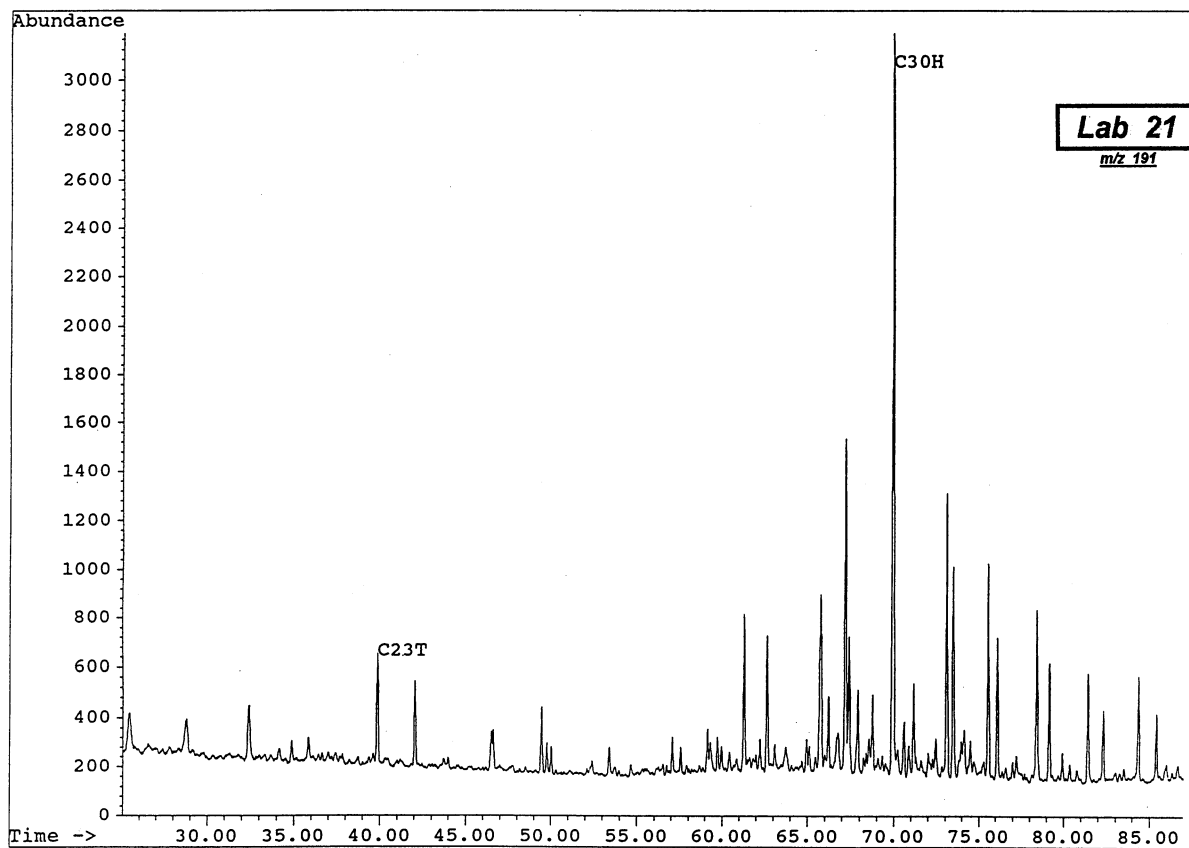
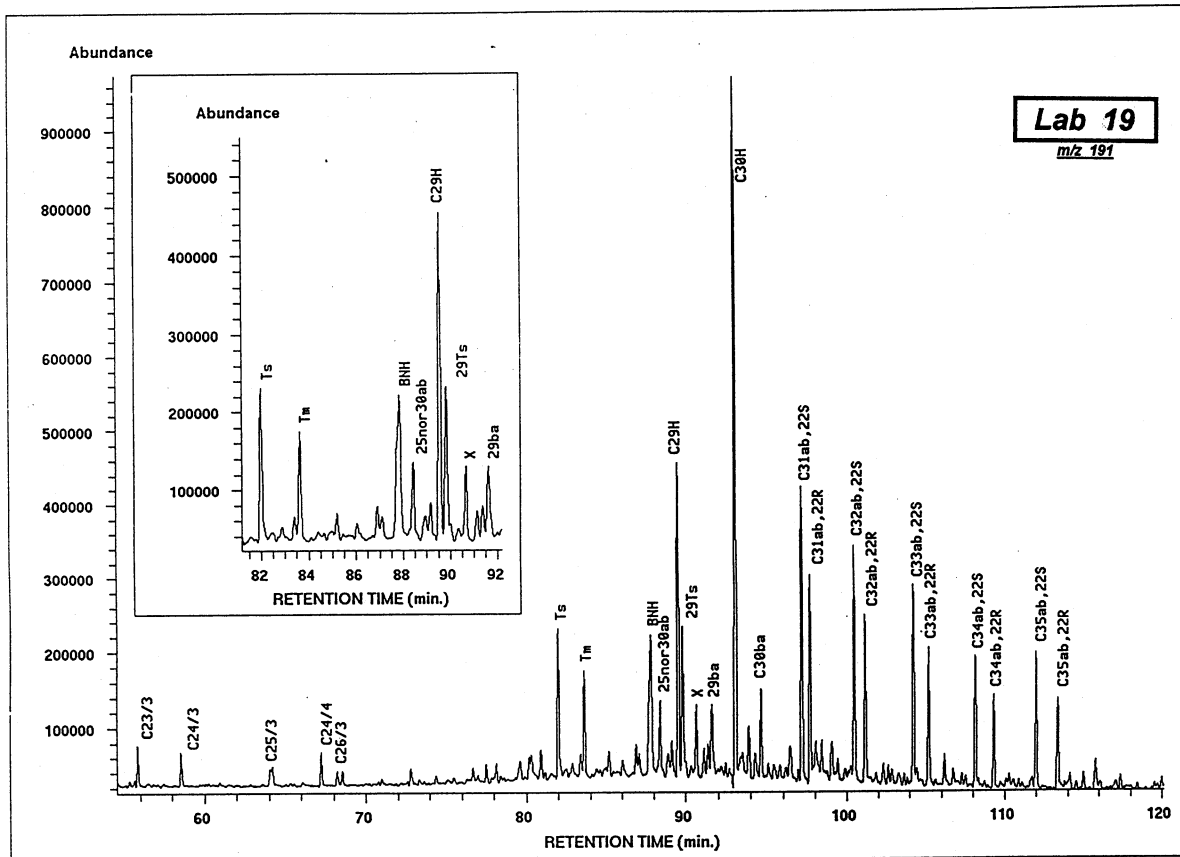
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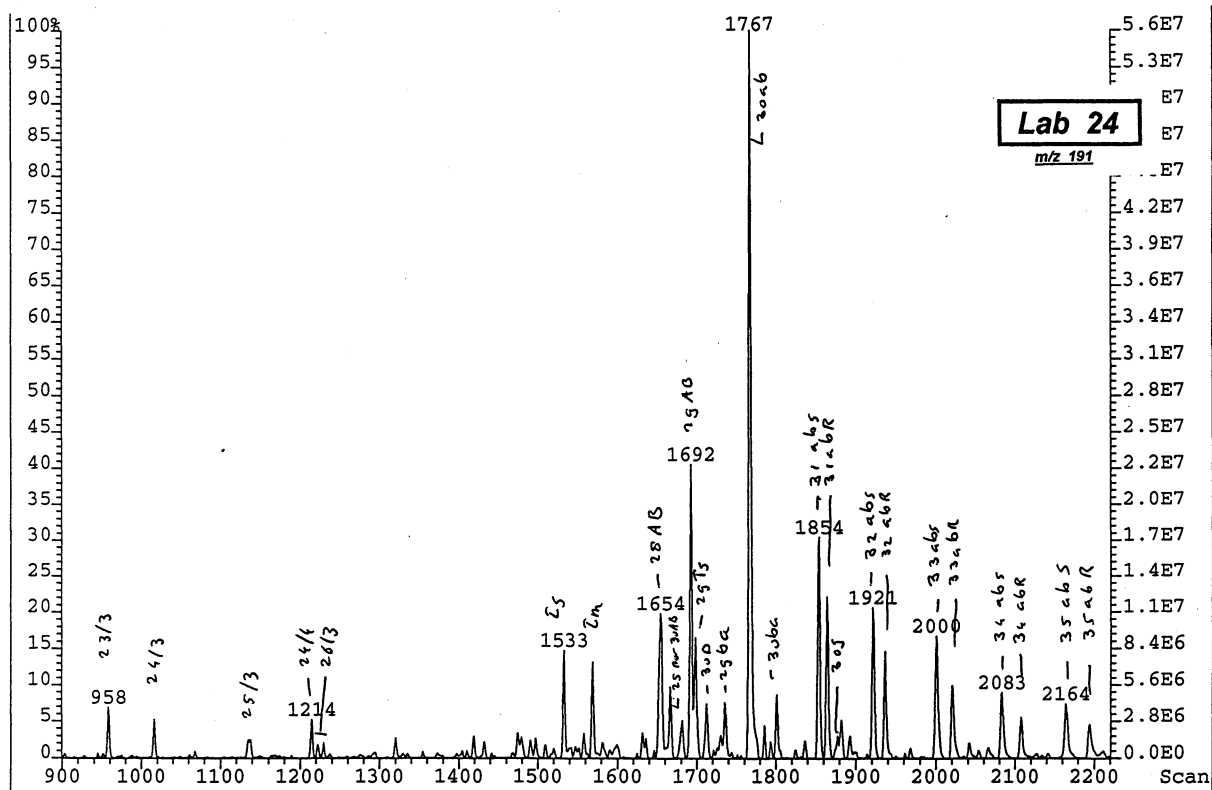
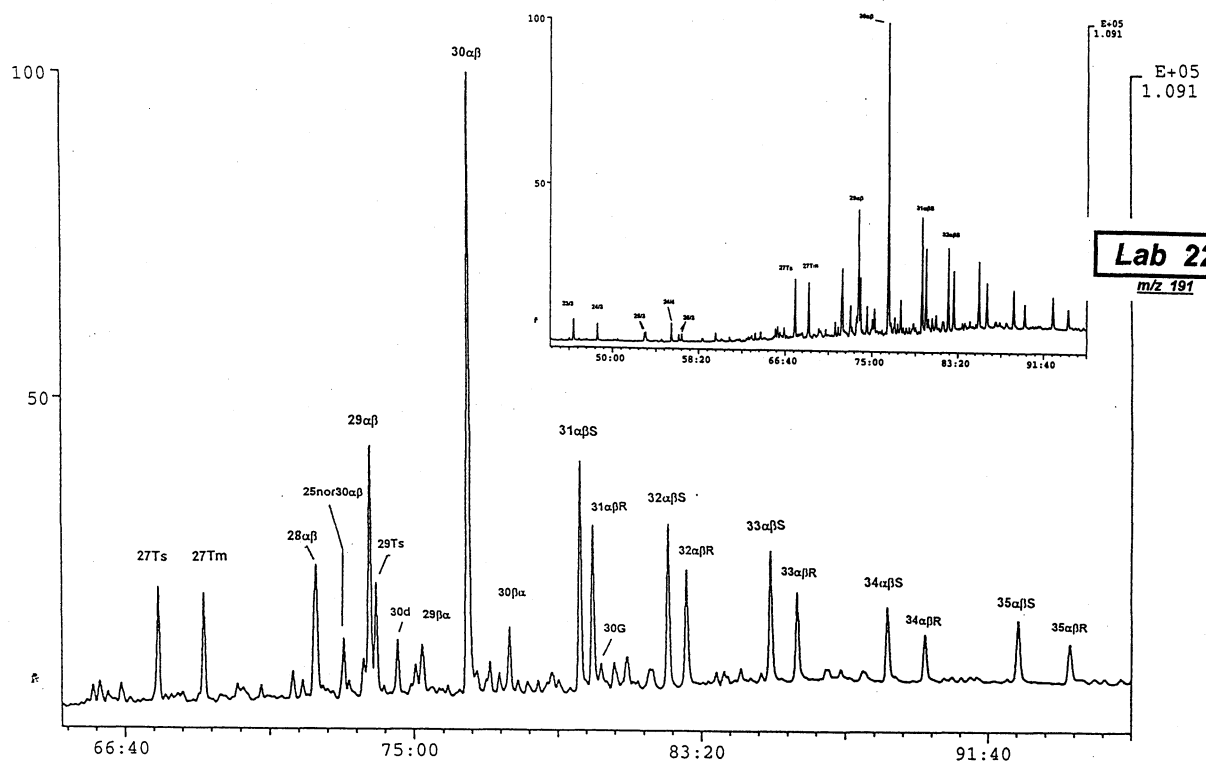
Appendix A3.4a-2

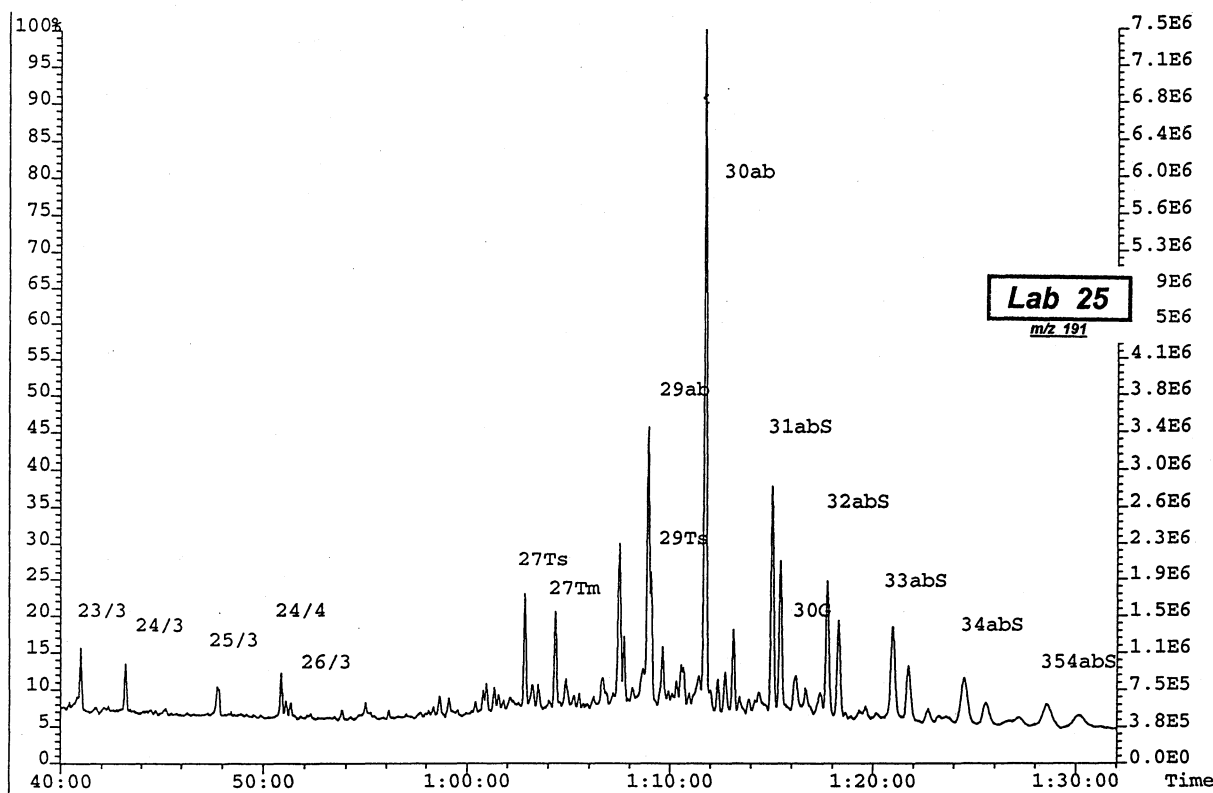
Saturates fraction m/z 191 GC-MS fragmentograms

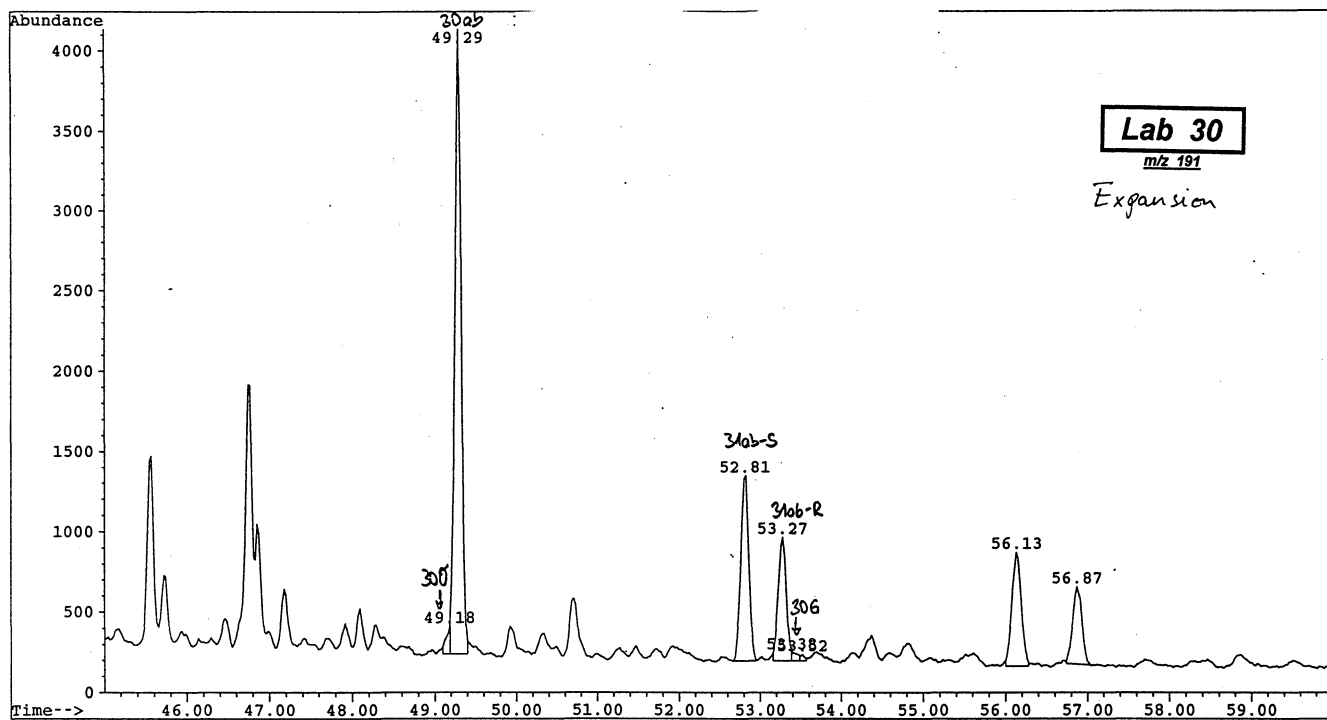
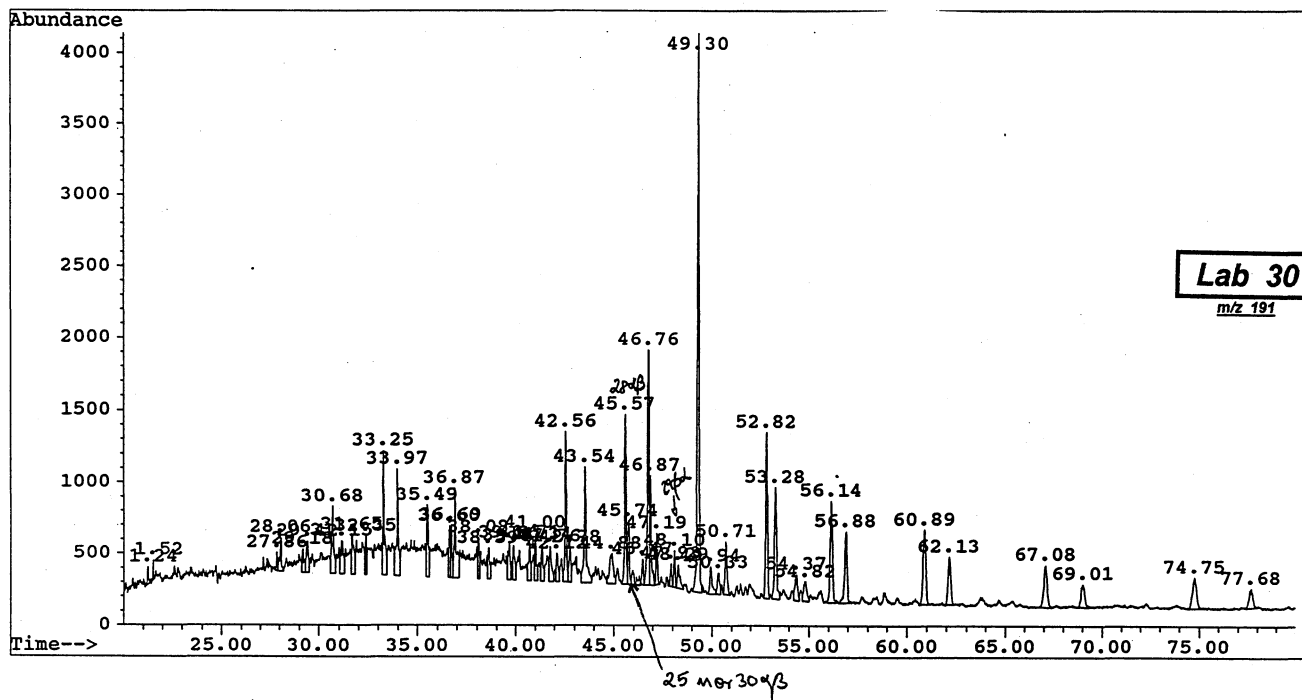


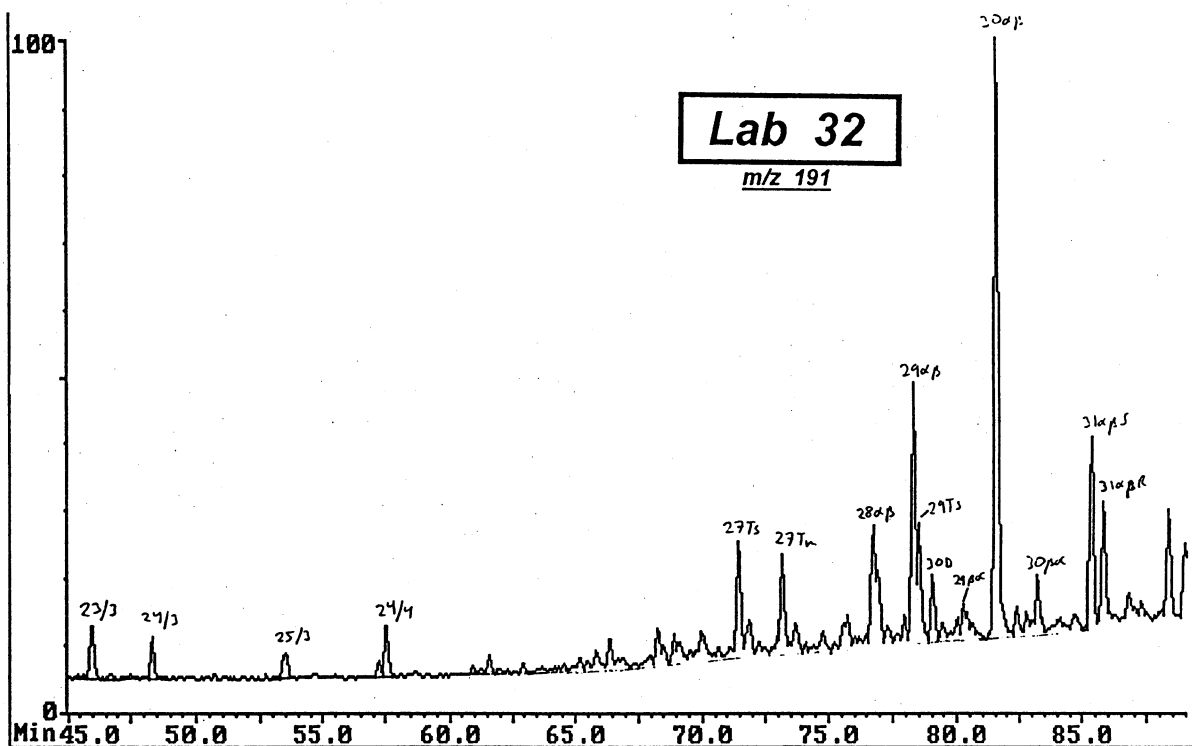
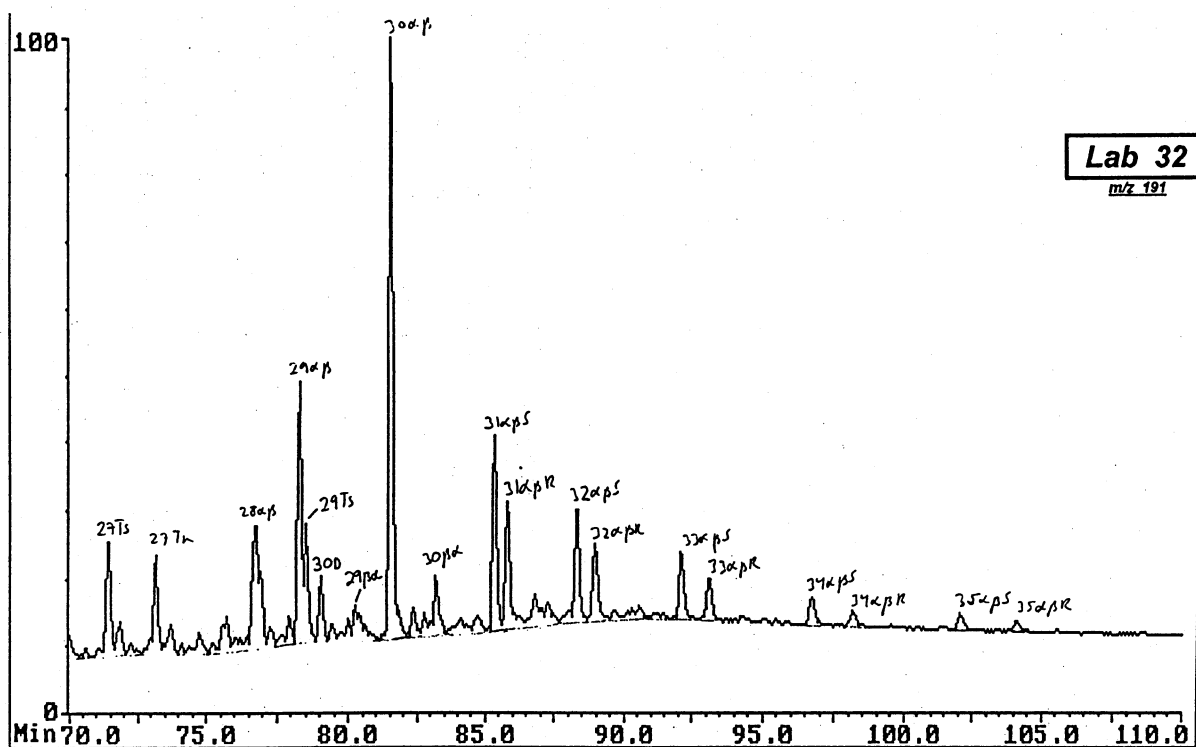


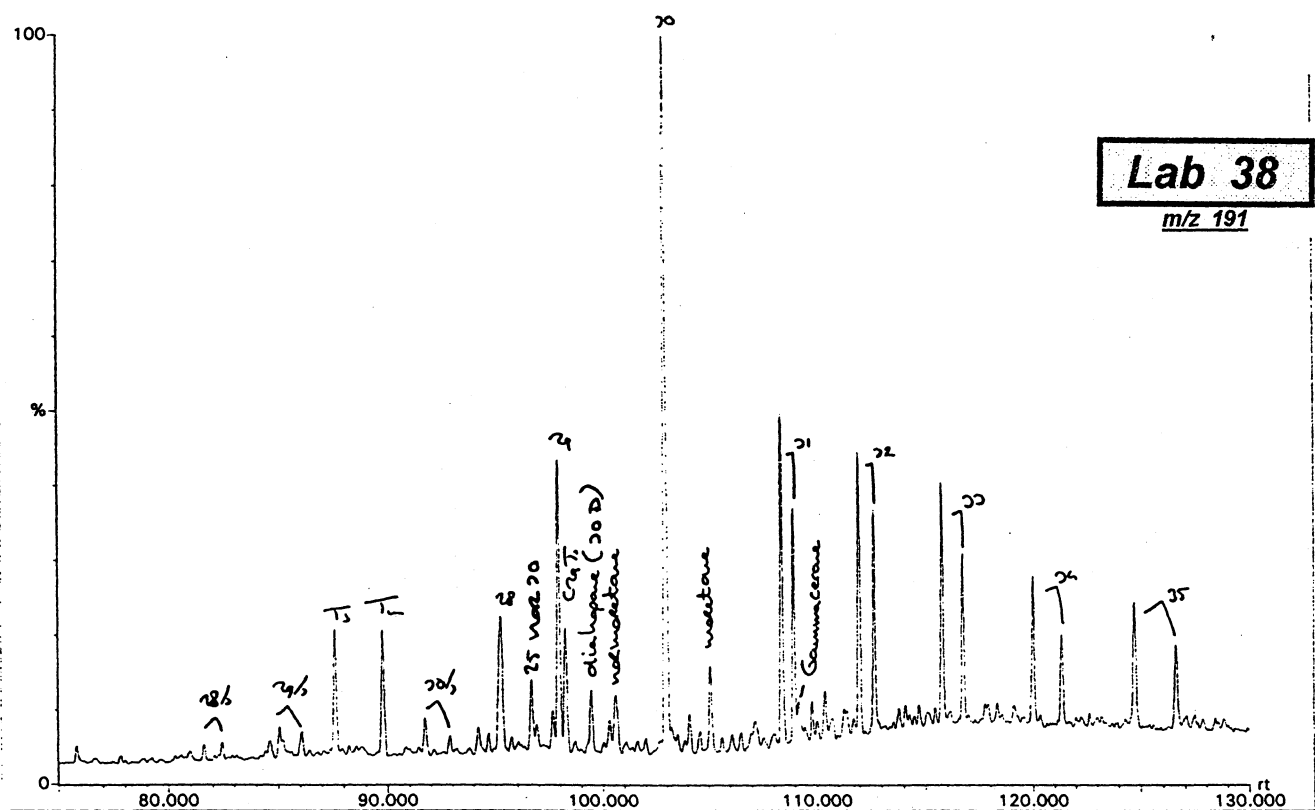
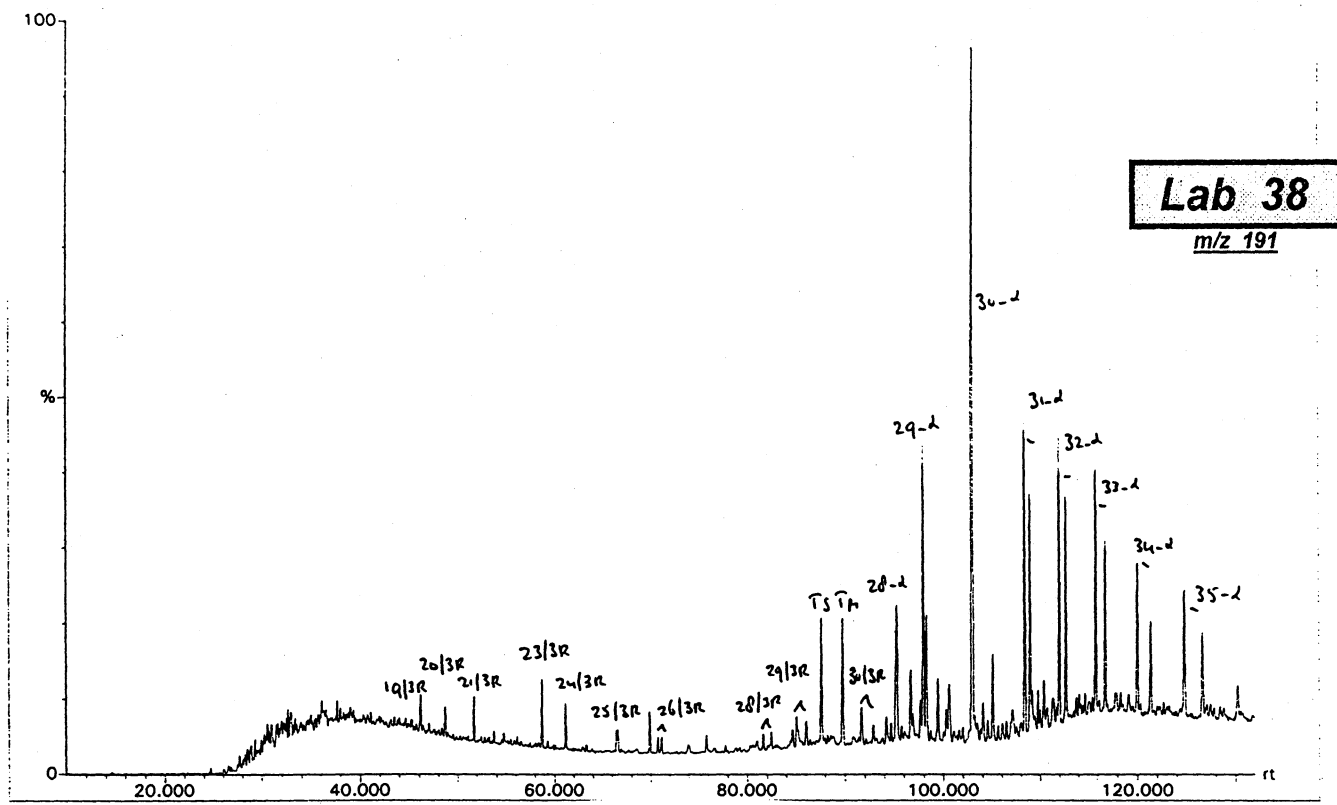


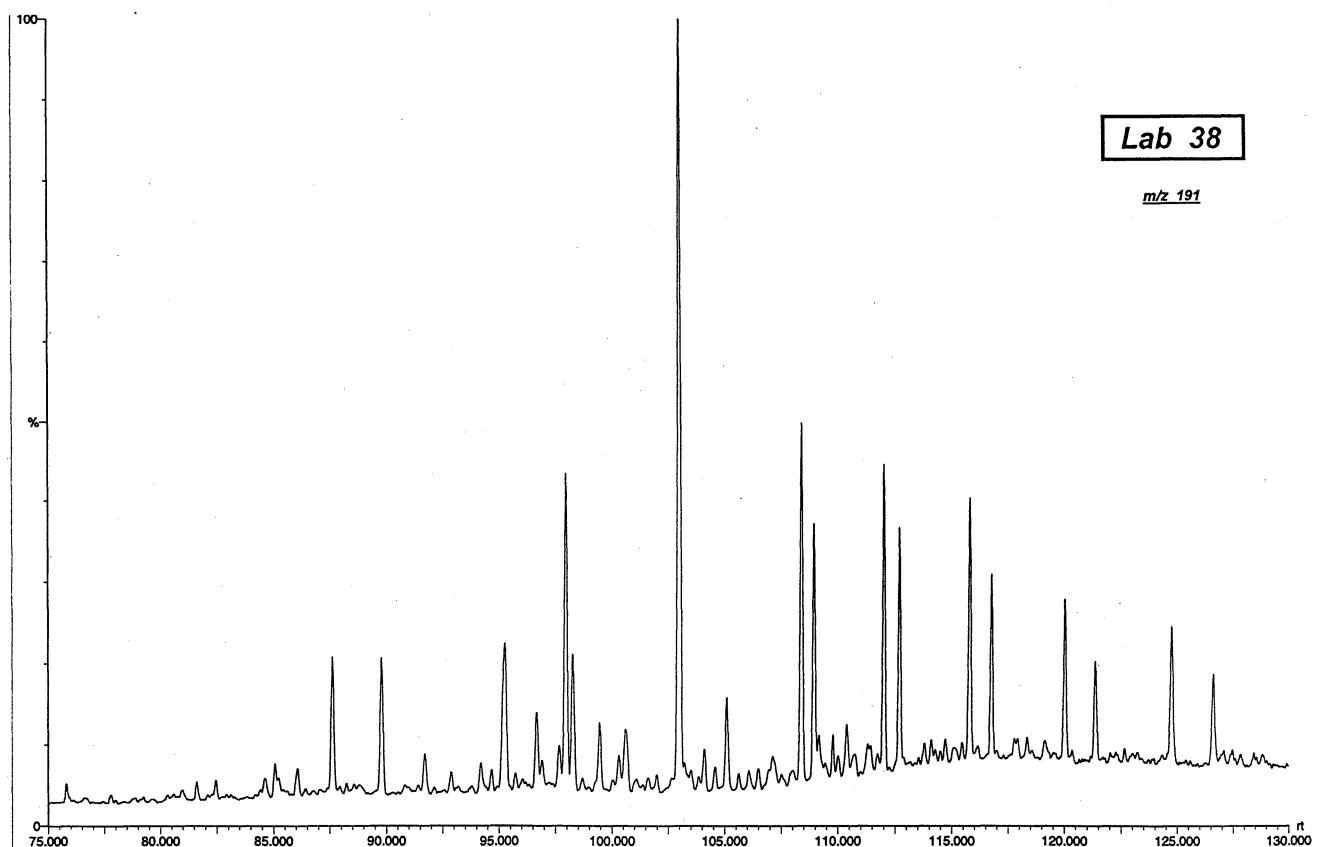
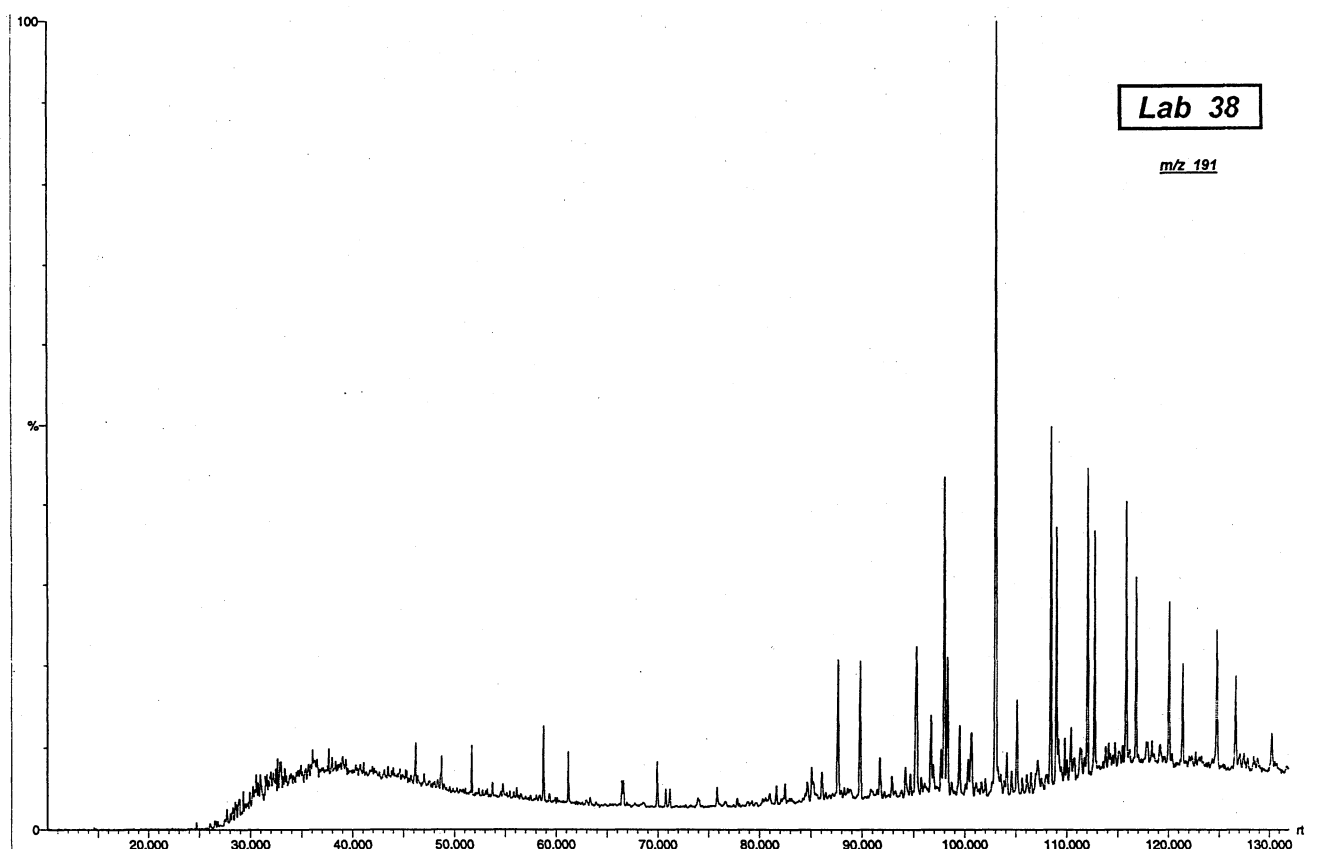


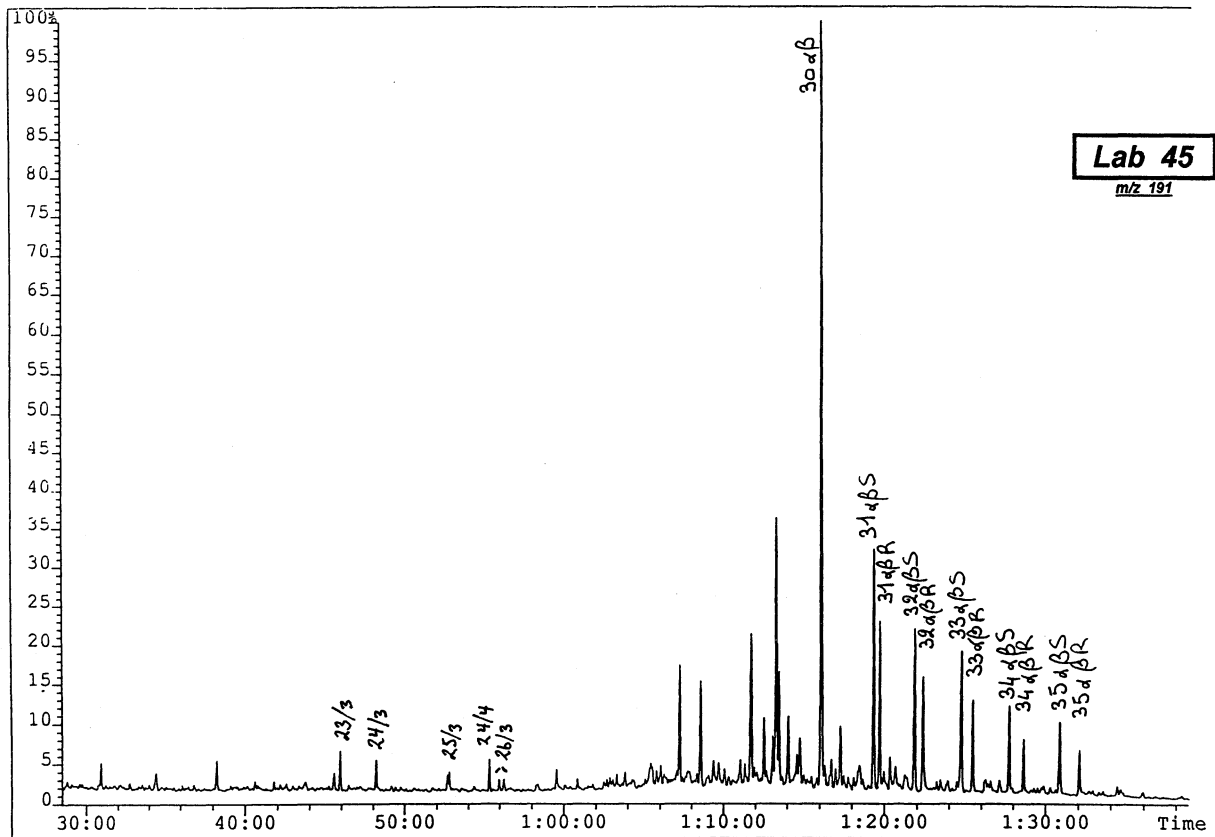
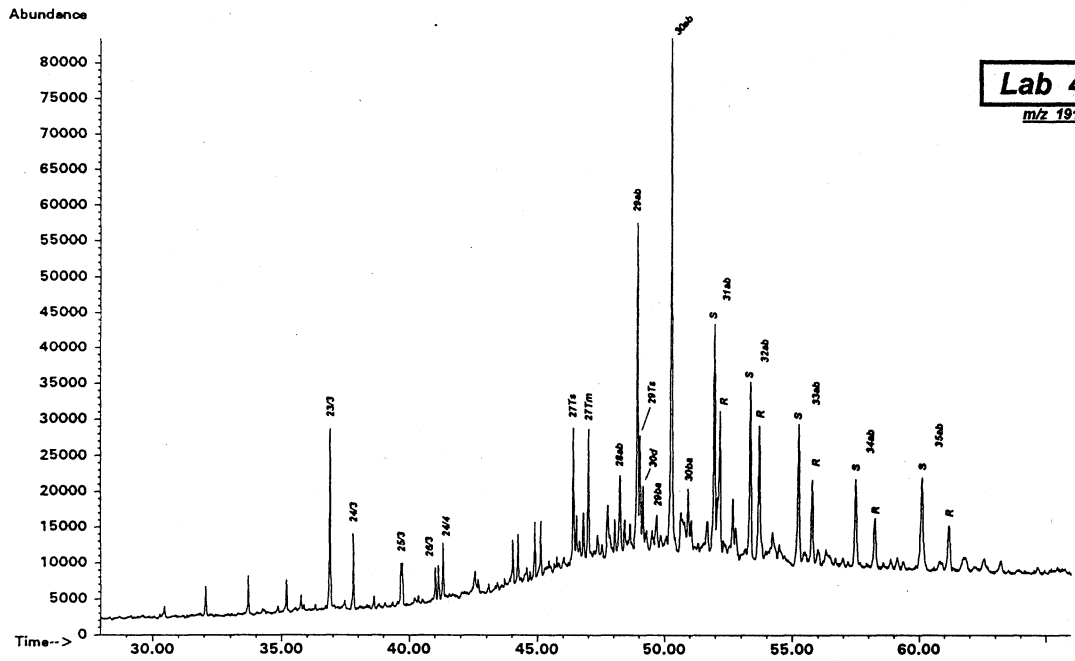


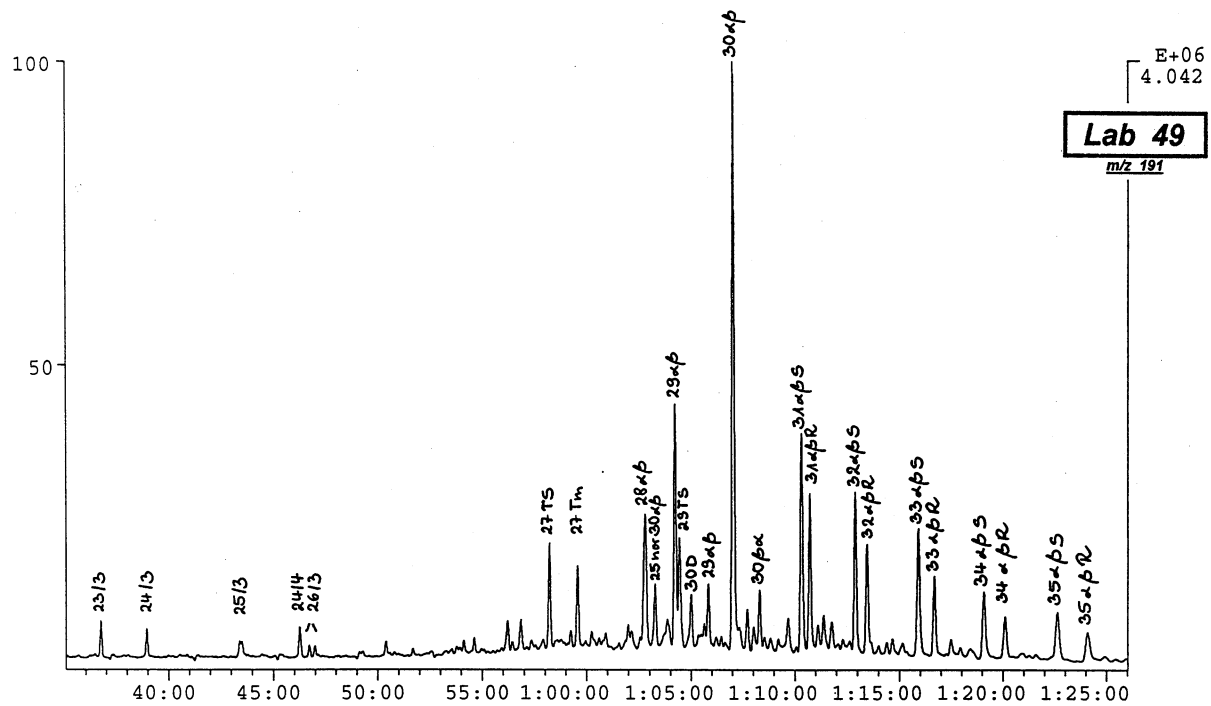


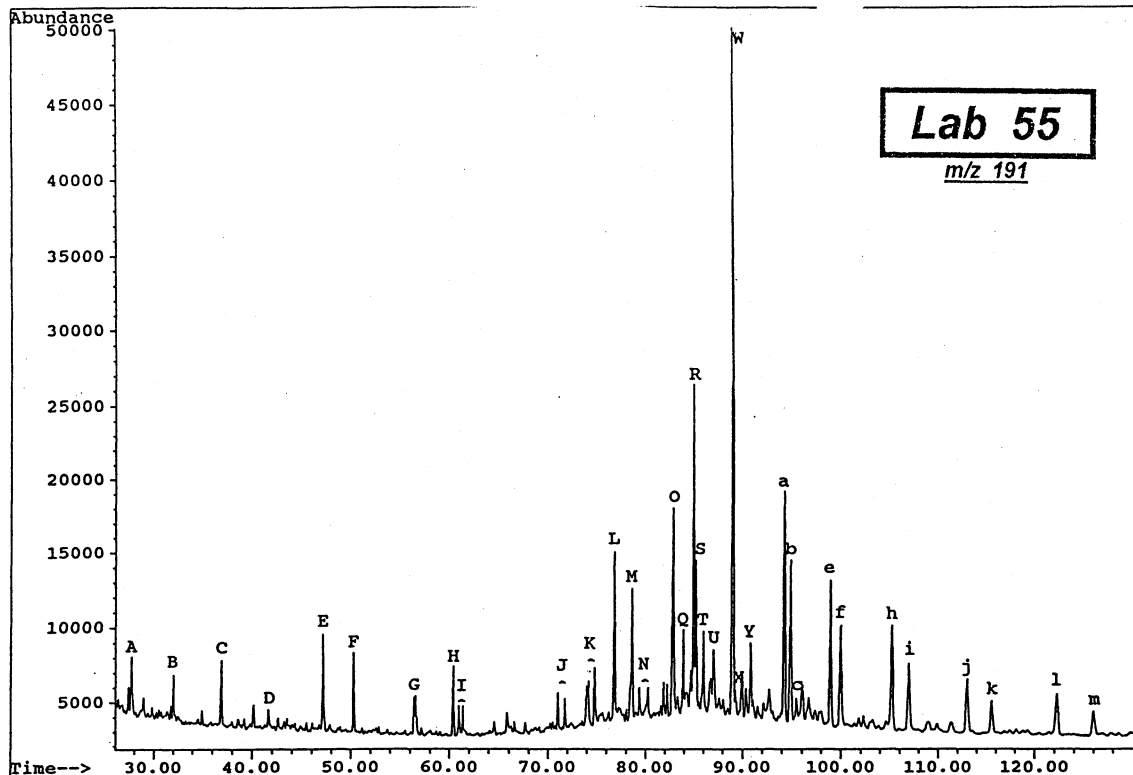




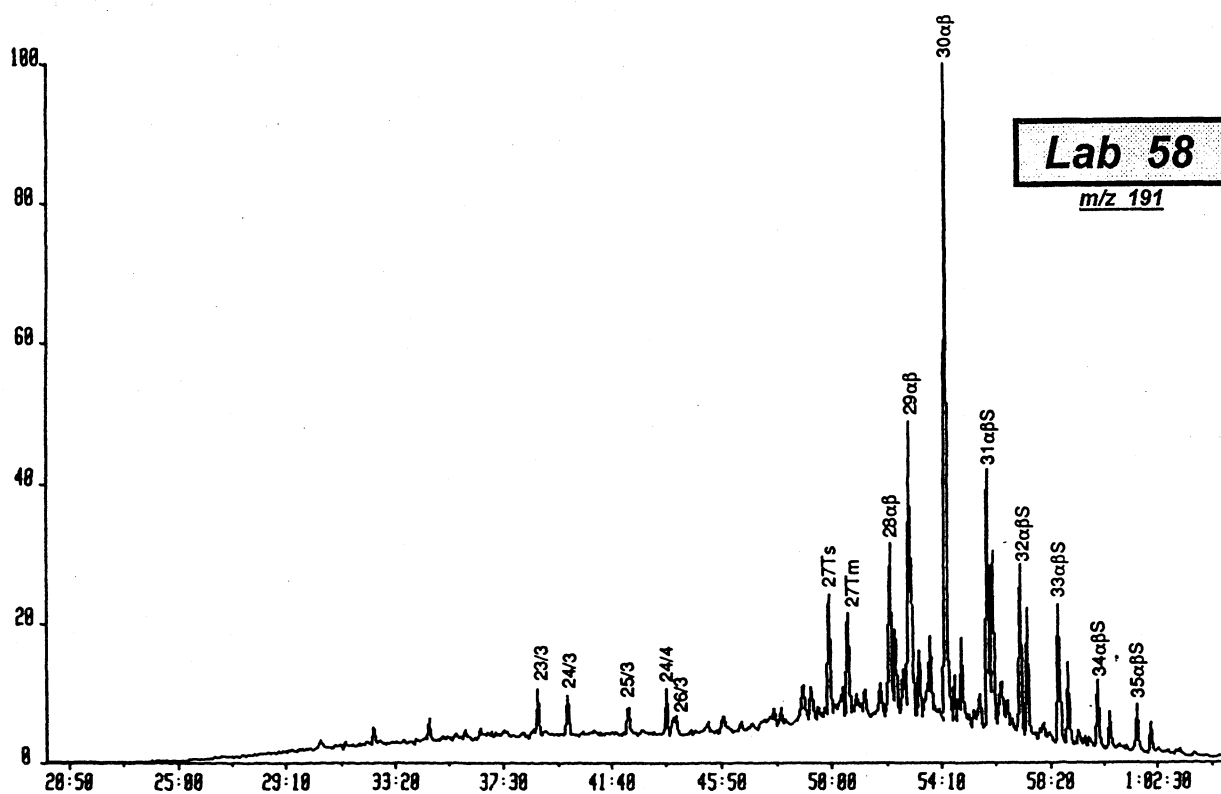


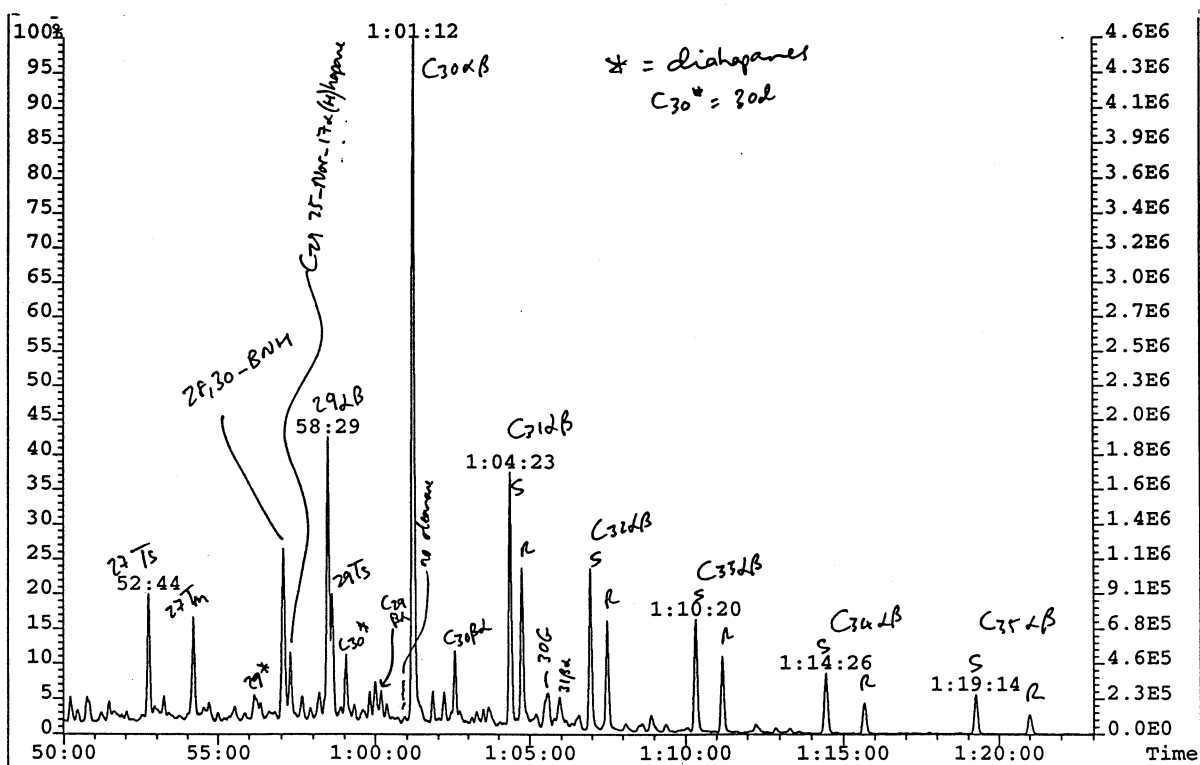
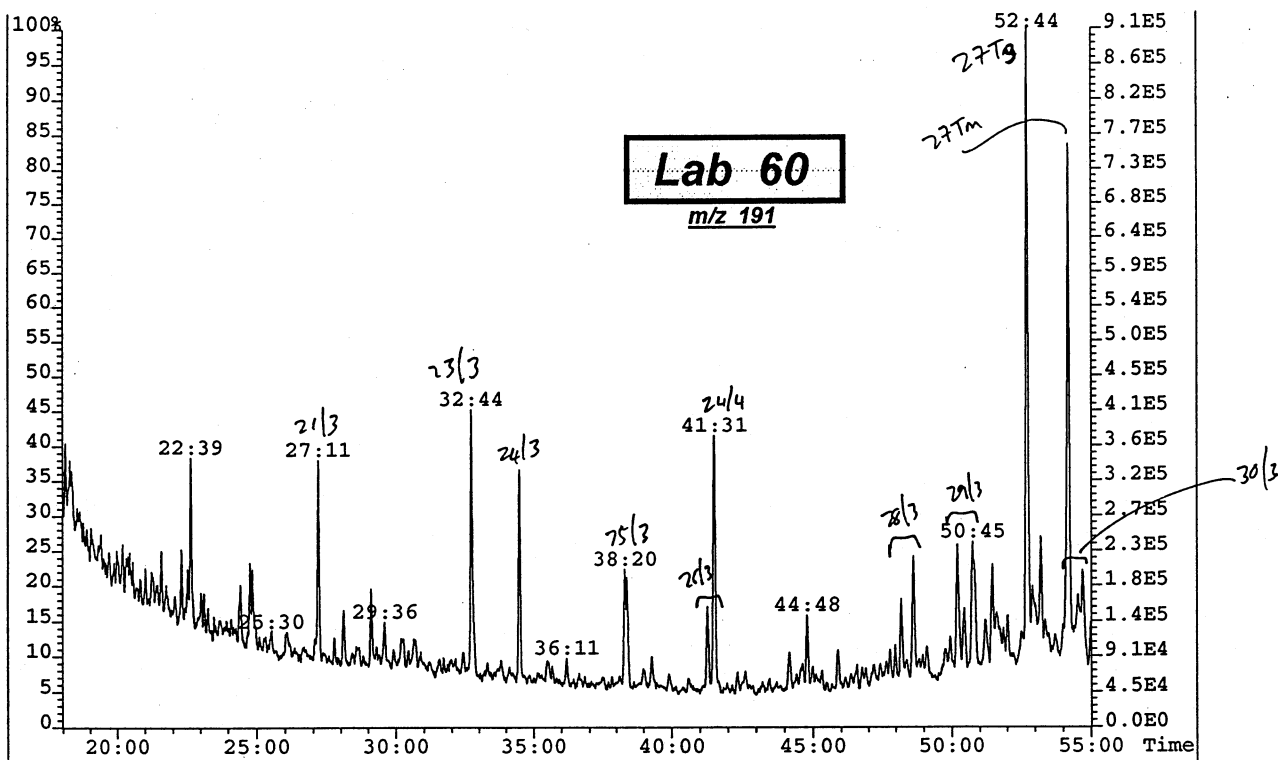


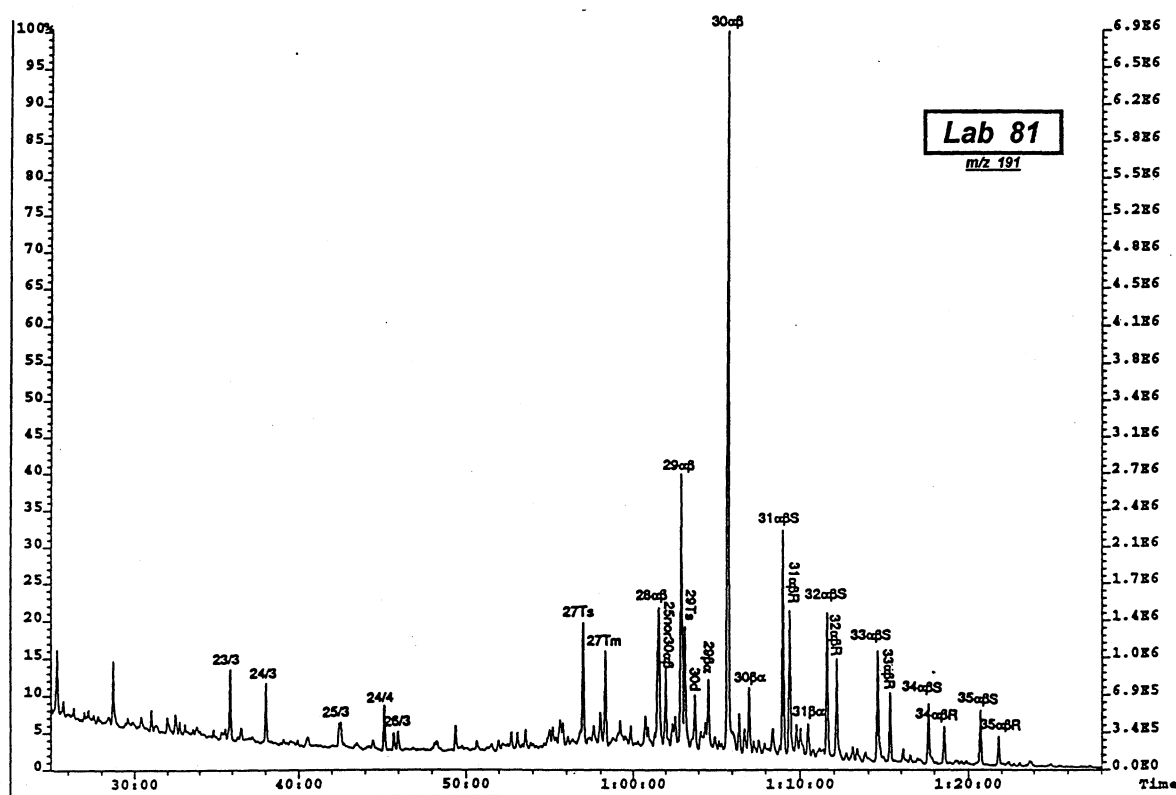
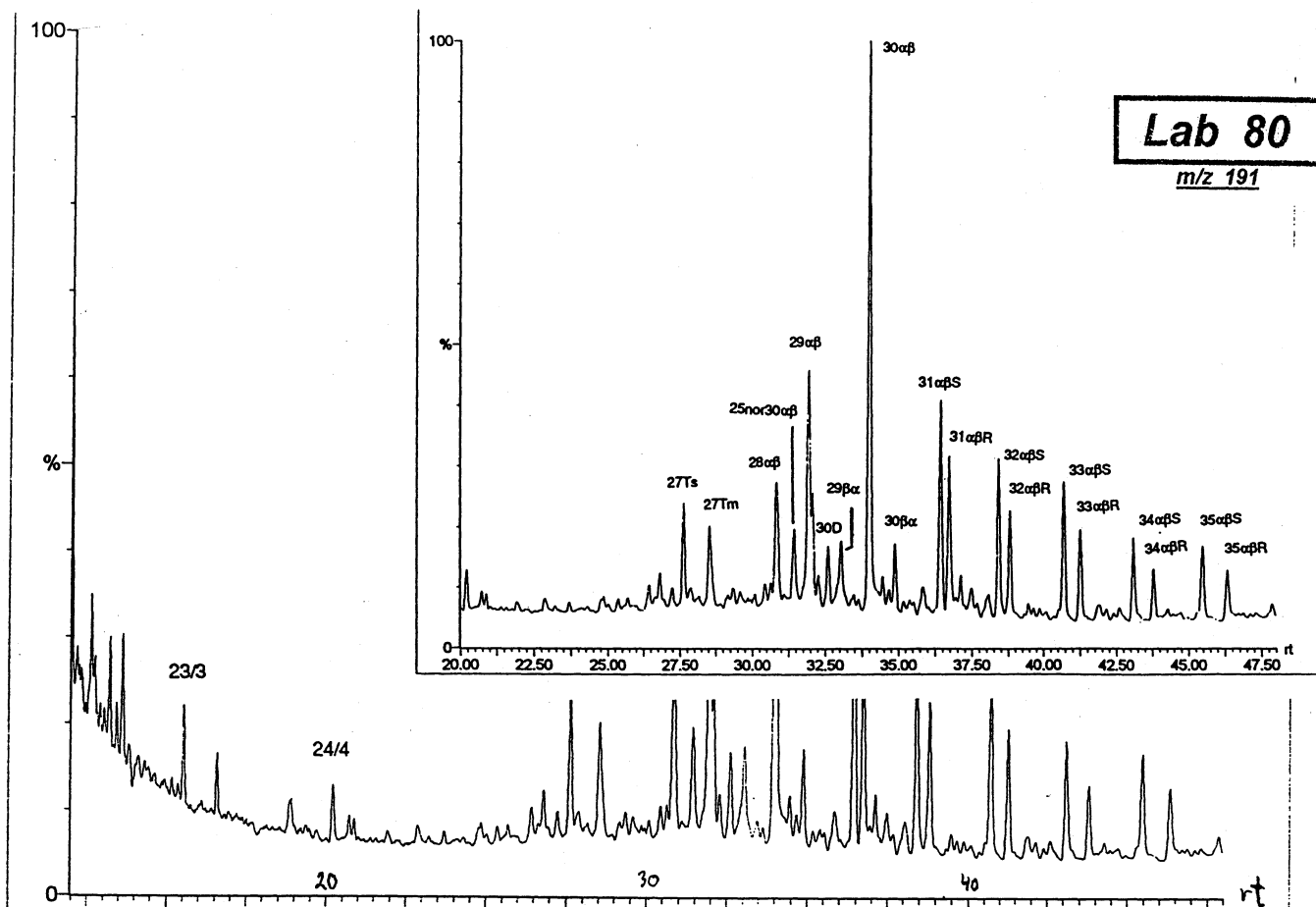


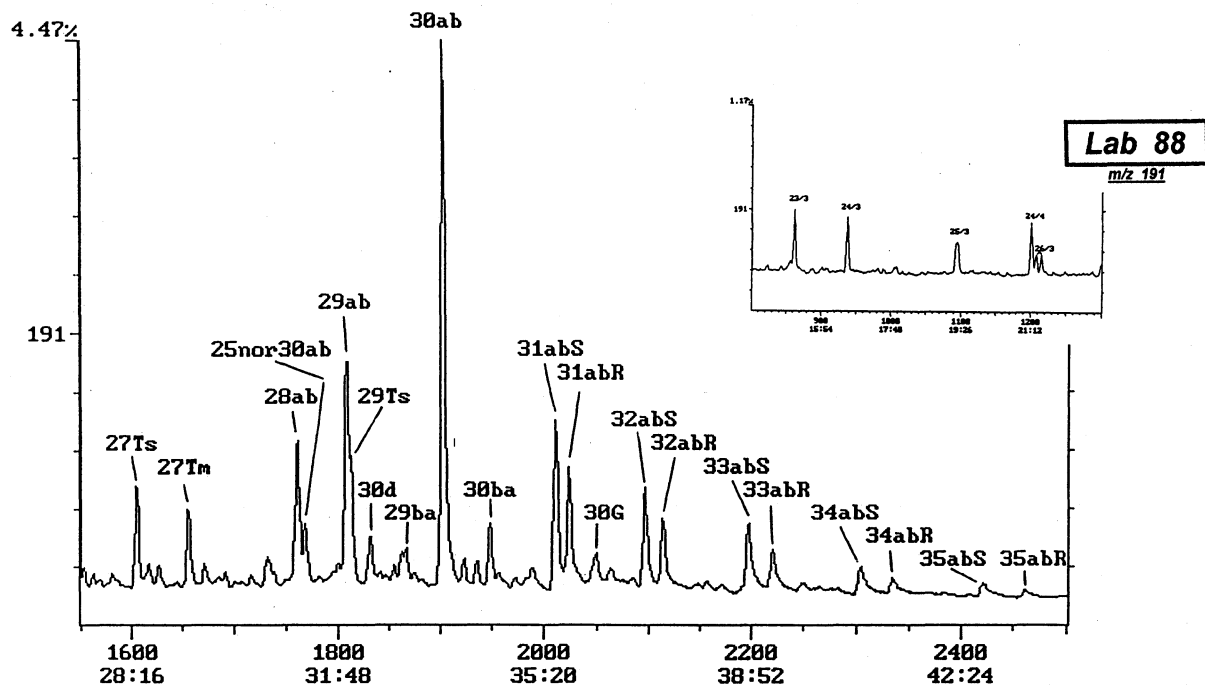


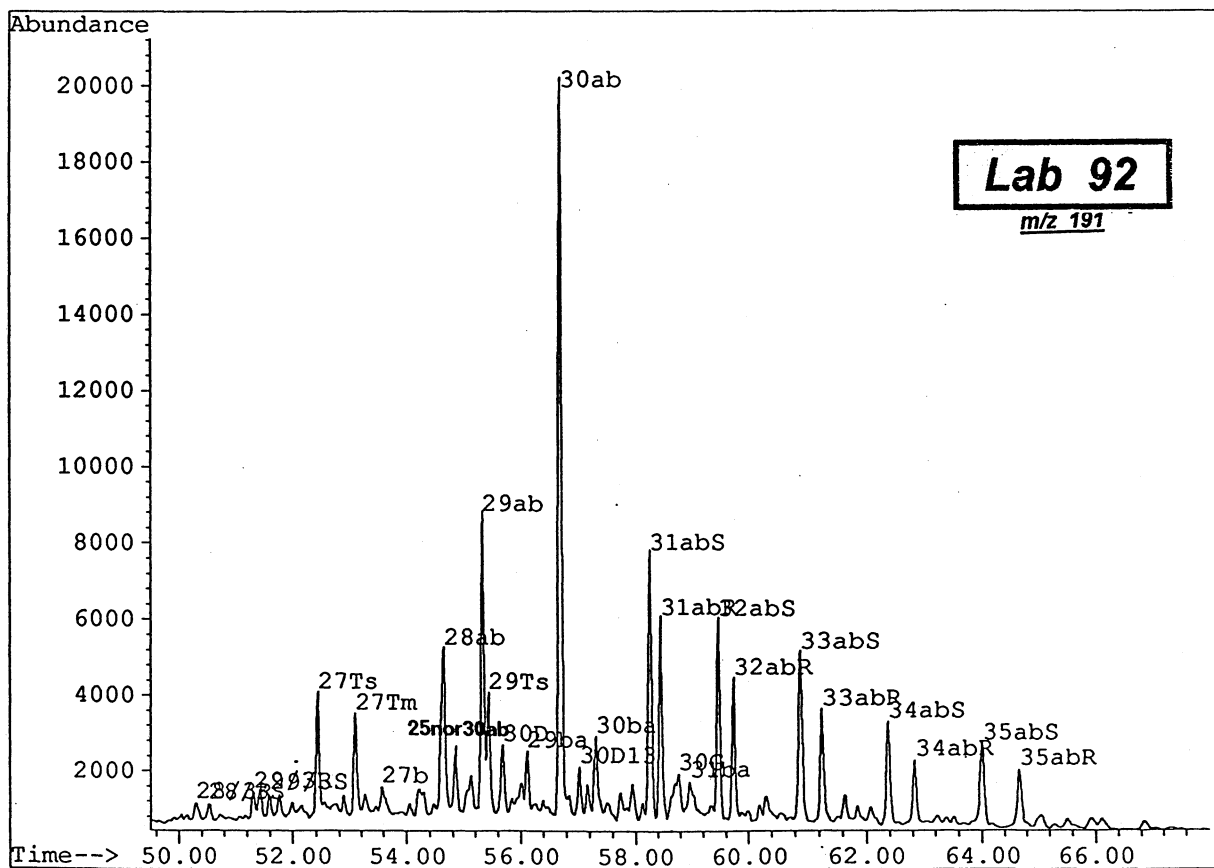
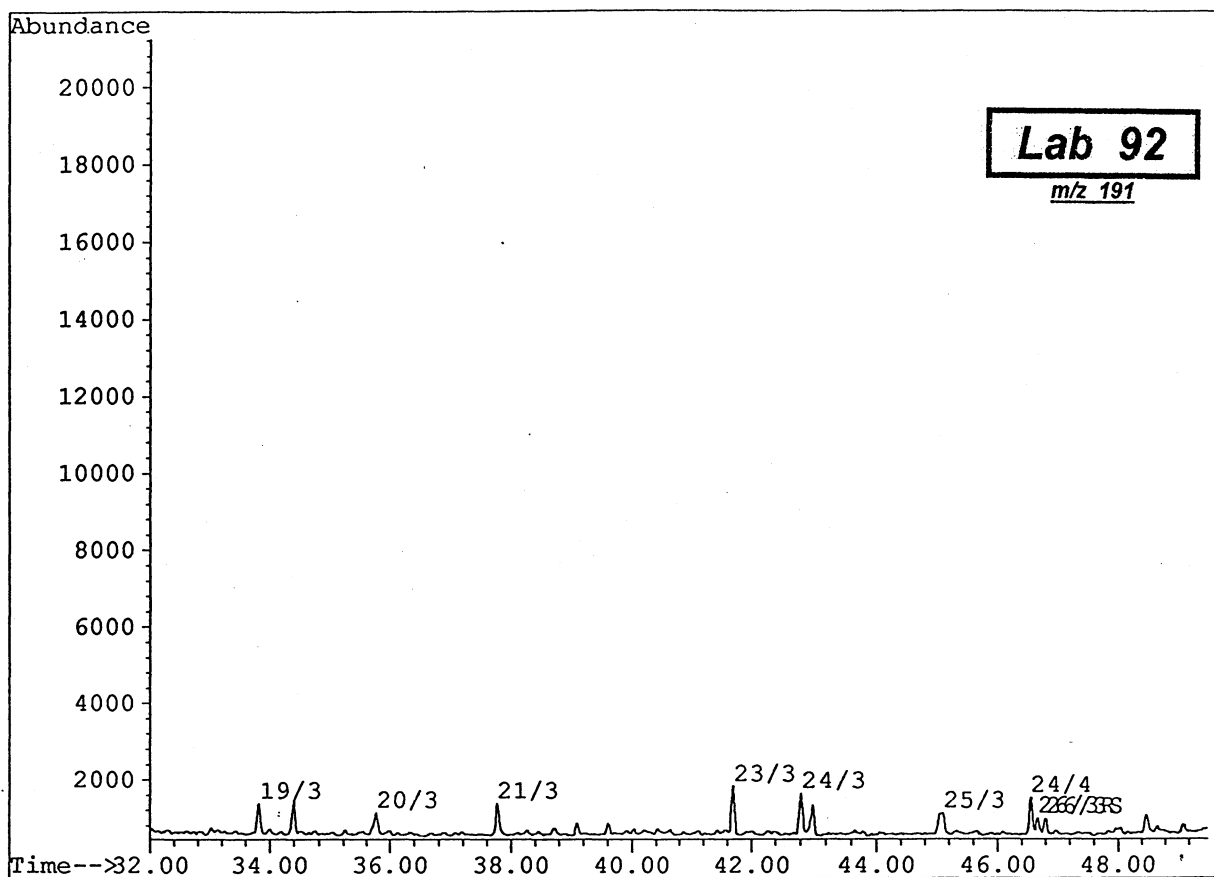
Peak ID	Triterpane Name		Ret Time	Area	Area%	ppm	
1	A	C ₁₉ Tricyclic Terpane	27.655	465989	1.67	31	
2	B	C ₂₀ Tricyclic Terpane	32.011	307583	1.10	20	
3	C	C ₂₁ Tricyclic Terpane	36.891	383561	1.37	25	
4	D	C ₂₂ Tricyclic Terpane	41.595	148911	0.53	10	
5	E	C ₂₃ Tricyclic Terpane	23/3	47.149	603303	2.16	40
6	F	C ₂₄ Tricyclic Terpane	24/3	50.261	468507	1.68	31
7	G	C ₂₅ Tricyclic Terpane (22R)	25/3	56.410	181354	0.65	12
8	G	C ₂₅ Tricyclic Terpane (22S)	25/3	56.590	255622	0.91	17
9	H	C ₂₄ Tetracyclic Terpane	24/4	60.357	400613	1.43	27
10	I	C ₂₆ Tricyclic Terpane (22R)	26/3	60.933	195907	0.70	13
11	I	C ₂₆ Tricyclic Terpane (22S)	26/3	61.346	193627	0.69	13
12	J	C ₂₈ Tricyclic Terpane (22R)		71.023	214423	0.77	14
13	J	C ₂₈ Tricyclic Terpane (22S)		71.744	170159	0.61	11
14	K	C ₂₉ Tricyclic Terpane (22R)		73.967	263846	0.94	18
15	K	C ₂₉ Tricyclic Terpane (22S)		74.782	374490	1.34	25
16	L	C ₂₇ 18 α H-Trisnorhopane (Ts)	27Ts	76.768	1061913	3.80	70
17	M	C ₂₇ 17 α H-Trisnorhopane (Tm)	27Tm	78.573	836242	2.99	56
18	N	C ₃₀ Tricyclic Terpane (22R)		79.339	212586	0.76	14
19	N	C ₃₀ Tricyclic Terpane (22S)		80.246	207269	0.74	14
20	O	C ₂₈ 17 α H,18 α H,21 β H-28,30-Bisnorhopane	28 $\alpha\beta$	82.820	1671122	5.98	111
21	P	C ₃₁ Tricyclic Terpane (22R)			0	0.00	0
22	Q	C ₂₉ 17 α H, 21 β H 25-Norhopane	25nor30 $\alpha\beta$	83.890	556450	1.99	37
23	P	C ₃₁ Tricyclic Terpane (22S)			0	0.00	0
24	R	C ₂₉ 17 α H,21 β H-Norhopane	29 $\alpha\beta$	84.940	2047112	7.33	136
25	S	C ₂₉ 18 α H-Norneohopane (29Ts)	29Ts	85.195	925916	3.31	61
26	T	C ₃₀ 17 α H Diahopane	30d	85.966	565339	2.02	38
27	U	C ₂₉ 17 β H,21 α H-Normoretane	29 $\beta\alpha$	86.998	630053	2.26	42
28	V	C ₃₀ 18 α H + 18 β H-Oleanane	300		0	0.00	0
29	W	C ₃₀ 17 α H,21 β H-Hopane	30 $\alpha\beta$	88.968	4635841	16.59	308
30	X	C ₃₀ 30-Nor-29-homo-17 α H-Hopane		89.292	191461	0.69	13
31	Y	C ₃₀ 17 β H,21 α H-Moretane	30 $\beta\alpha$	90.818	530037	1.90	35
32	Z	C ₃₃ Tricyclic Terpane (22R)			0	0.00	0
33	Z	C ₃₃ Tricyclic Terpane (22S)			0	0.00	0
34	a	C ₃₁ 17 α H,21 β H-Homohopane (22S)	31 $\alpha\beta$ S	94.201	1766114	6.32	117
35	b	C ₃₁ 17 α H,21 β H-Homohopane (22R)	31 $\alpha\beta$ R	94.859	1270776	4.55	84
36	c	C ₃₀ Gammacerane	30G	95.459	185813	0.67	12
37	d	C ₃₄ Tricyclic Terpane (22R)			0	0.00	0
38	d	C ₃₄ Tricyclic Terpane (22S)			0	0.00	0
39	e	C ₃₂ 17 α H,21 β H-Bishomohopane (22S)	32 $\alpha\beta$ S	98.902	1250256	4.48	83
40	f	C ₃₂ 17 α H,21 β H-Bishomohopane (22R)	32 $\alpha\beta$ R	99.960	910883	3.26	60
41	g	C ₃₅ Tricyclic Terpane (22R)			0	0.00	0
42	g	C ₃₅ Tricyclic Terpane (22S)			0	0.00	0
43	h	C ₃₃ 17 α H,21 β H-Trishomohopane (22S)	33 $\alpha\beta$ S	105.222	1141338	4.09	76
44	i	C ₃₃ 17 α H,21 β H-Trishomohopane (22R)	33 $\alpha\beta$ R	106.940	707259	2.53	47
45	j	C ₃₄ 17 α H,21 β H-Tetrahomohopane (22S)	34 $\alpha\beta$ S	112.994	651445	2.33	43
46	k	C ₃₄ 17 α H,21 β H-Tetrahomohopane (22R)	34 $\alpha\beta$ R	115.564	410269	1.47	27
47	l	C ₃₅ 17 α H,21 β H-Pentahomohopane (22S)	35 $\alpha\beta$ S	122.253	577034	2.07	38
48	m	C ₃₅ 17 α H,21 β H-Pentahomohopane (22R)	35 $\alpha\beta$ R	126.009	367364	1.31	24

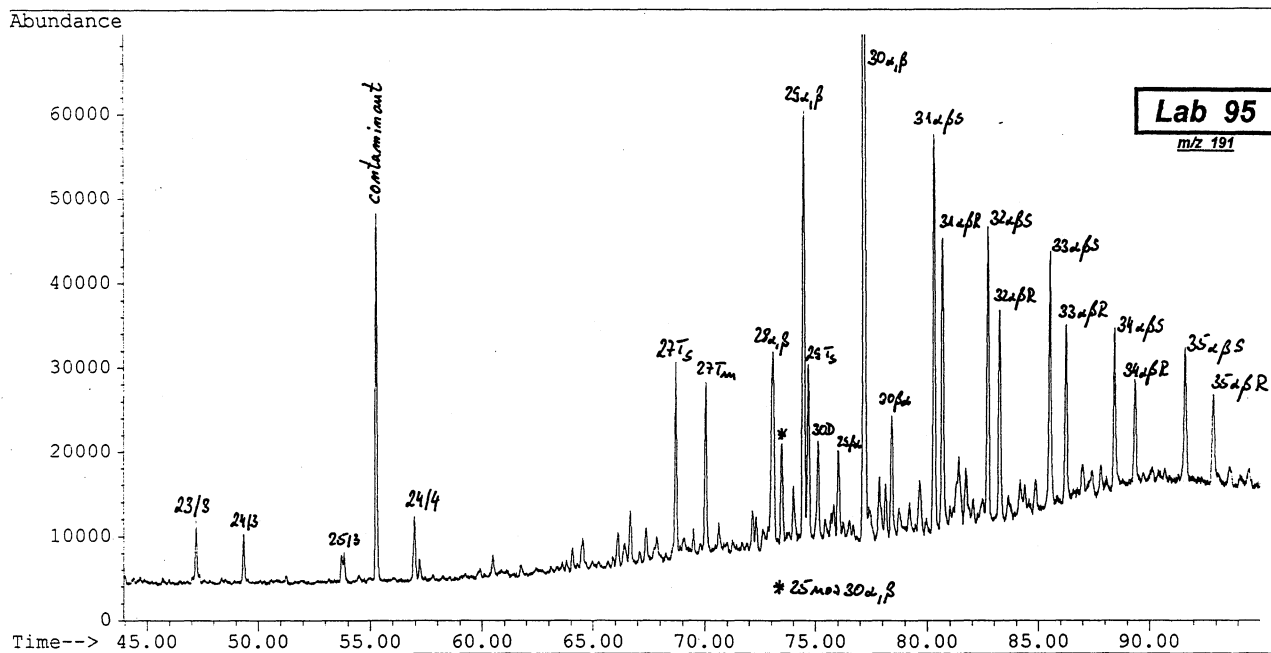








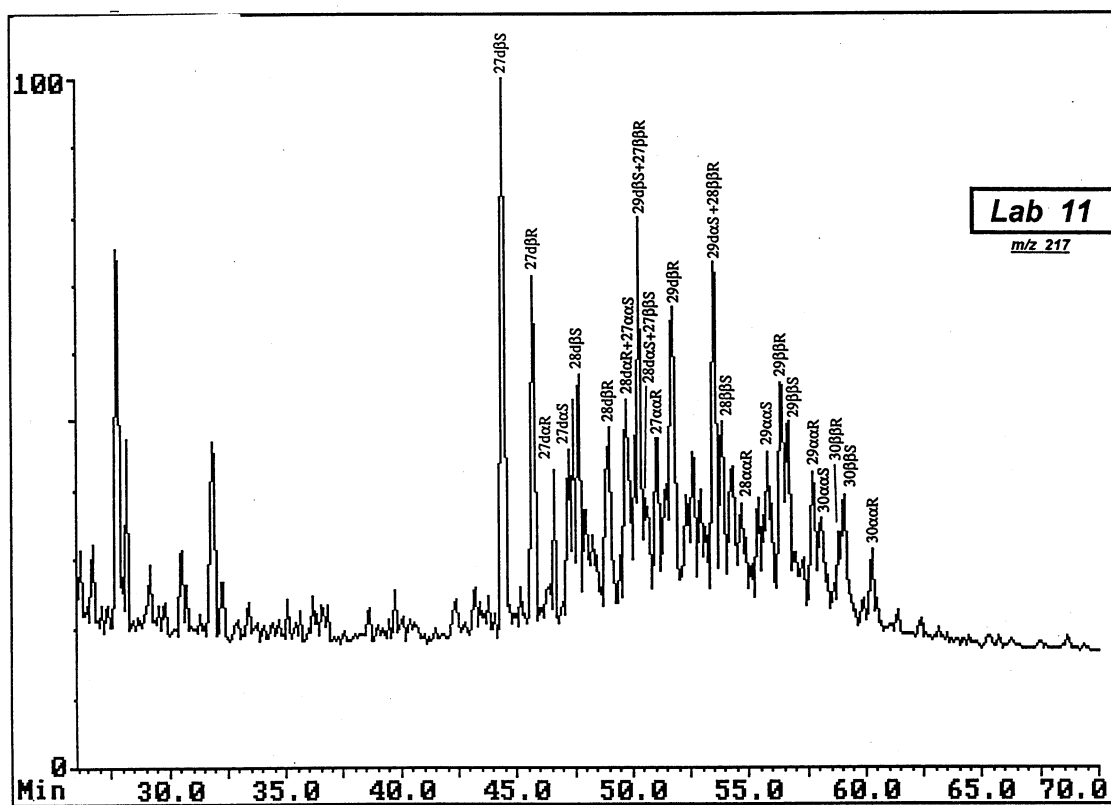
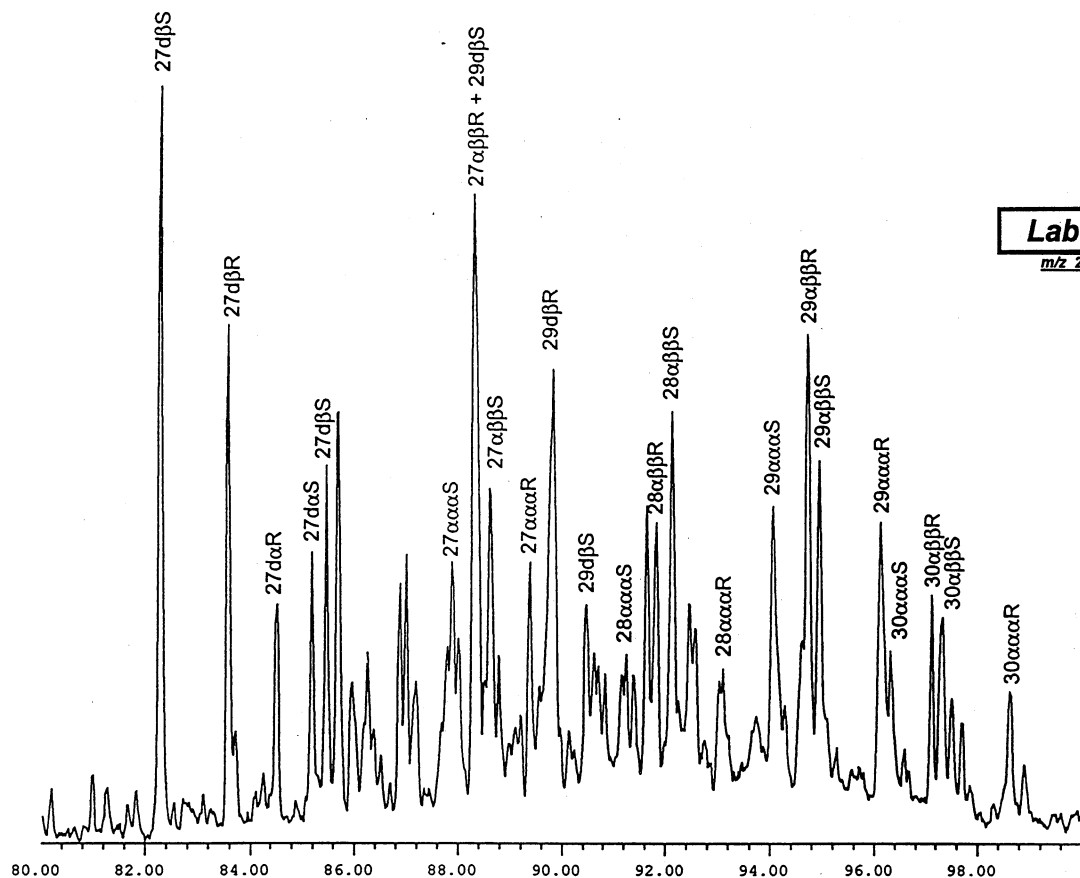


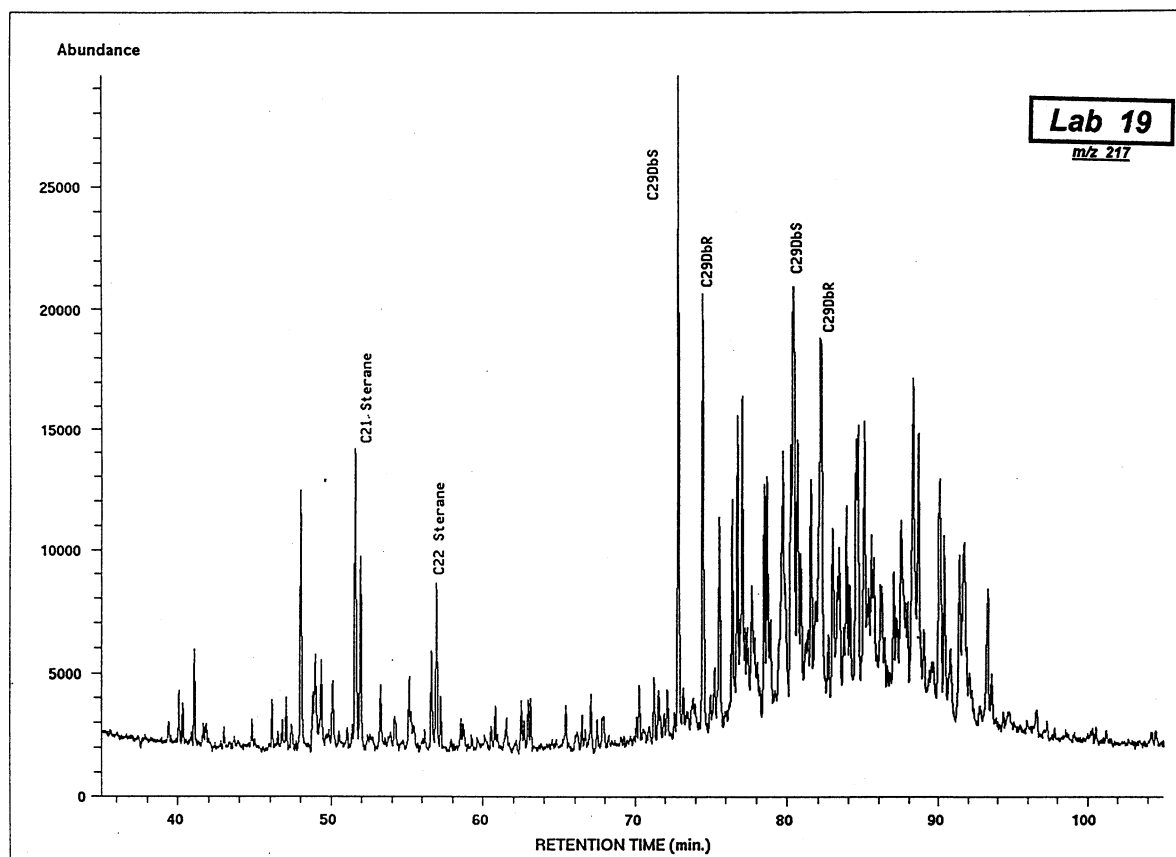
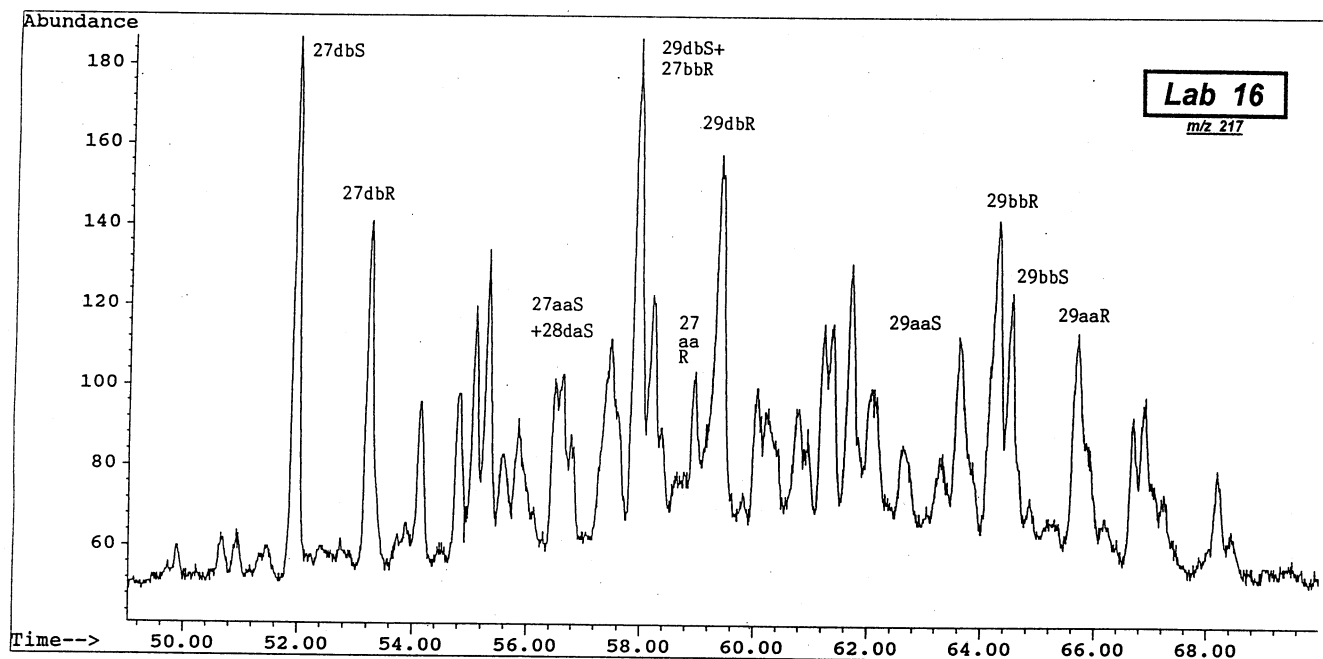


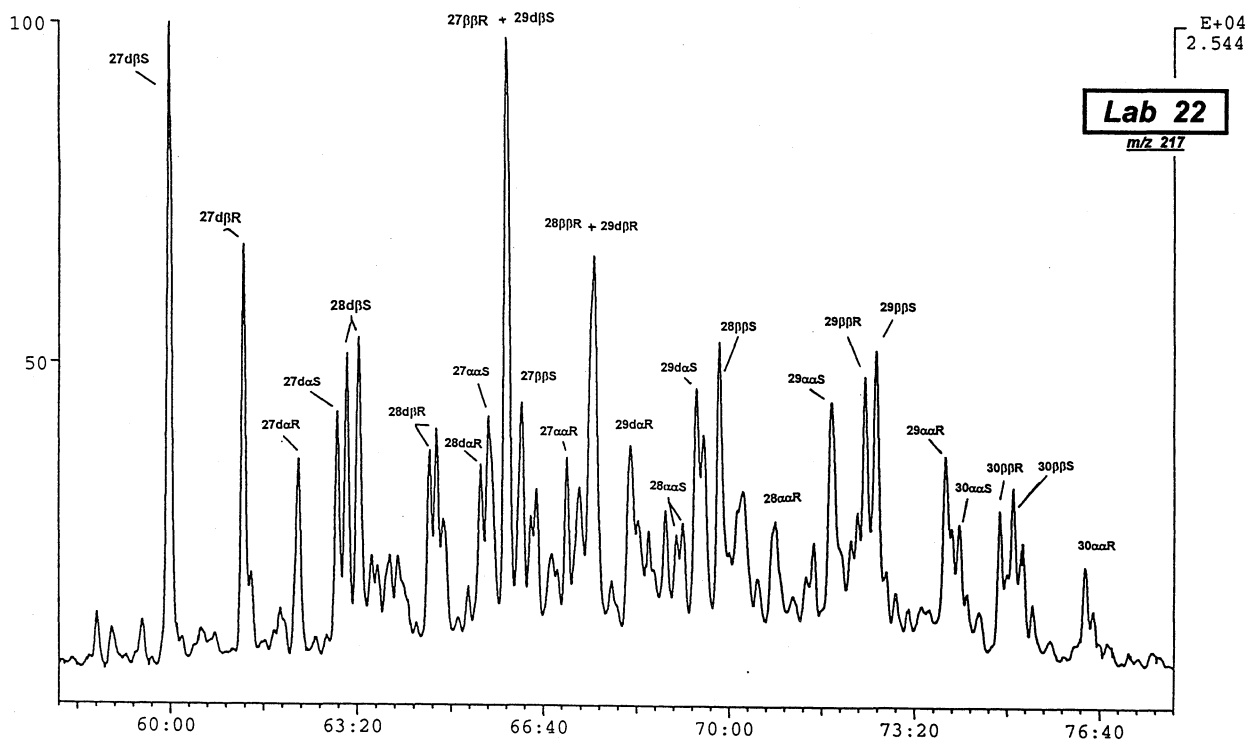
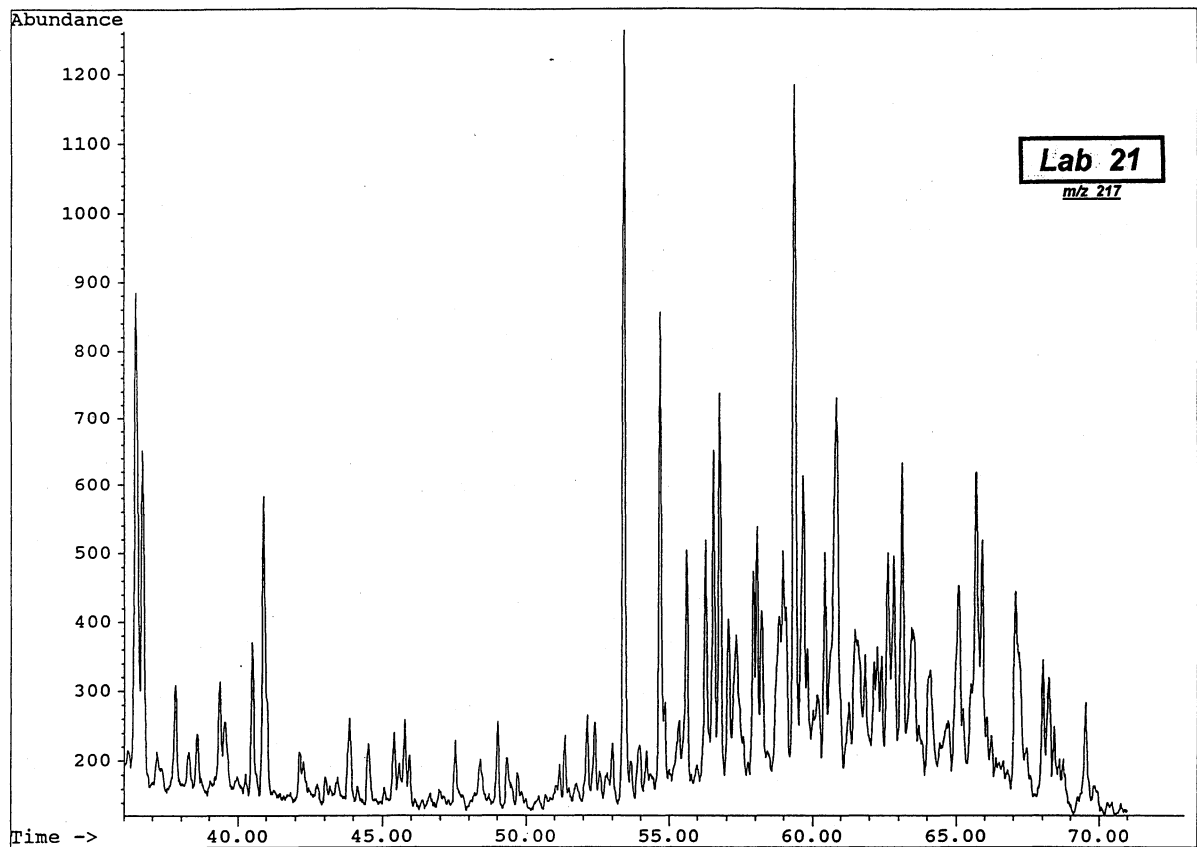
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Appendix A3.4a-3

Saturates fraction m/z 217 GC-MS fragmentograms

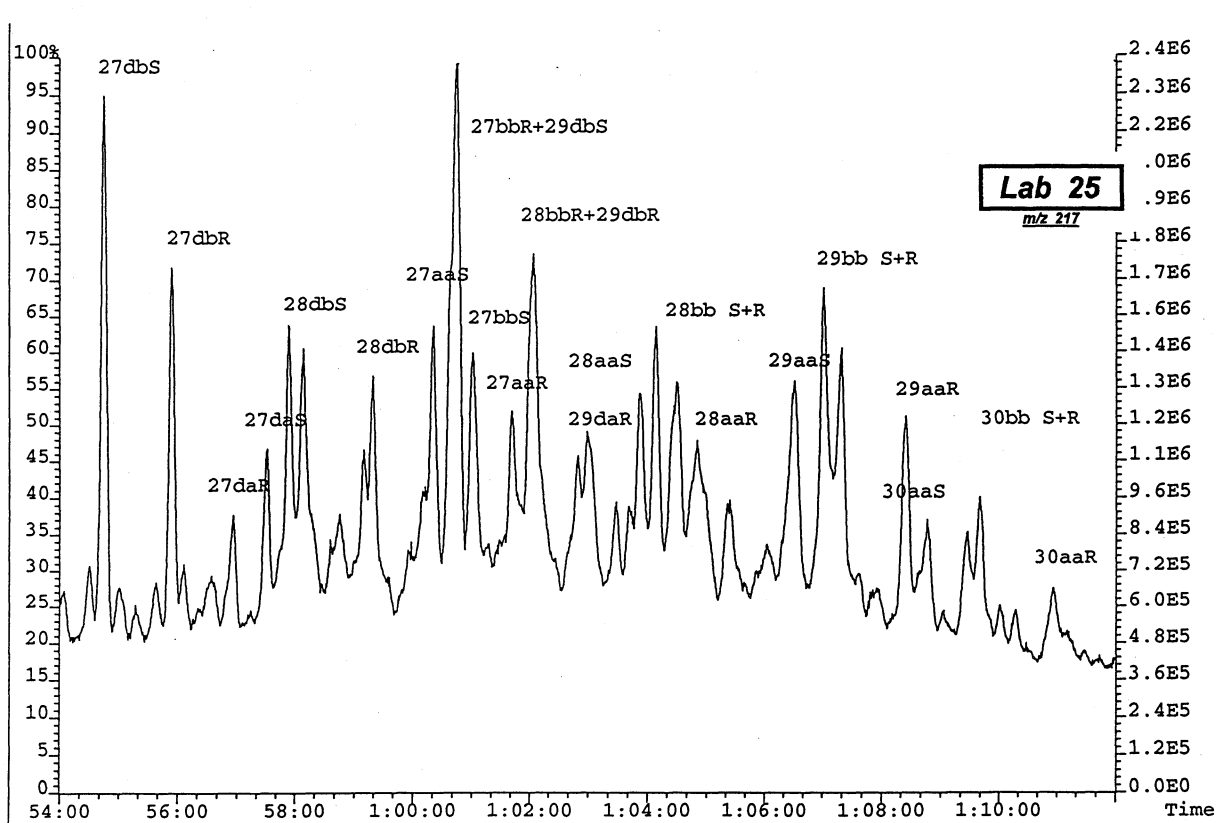
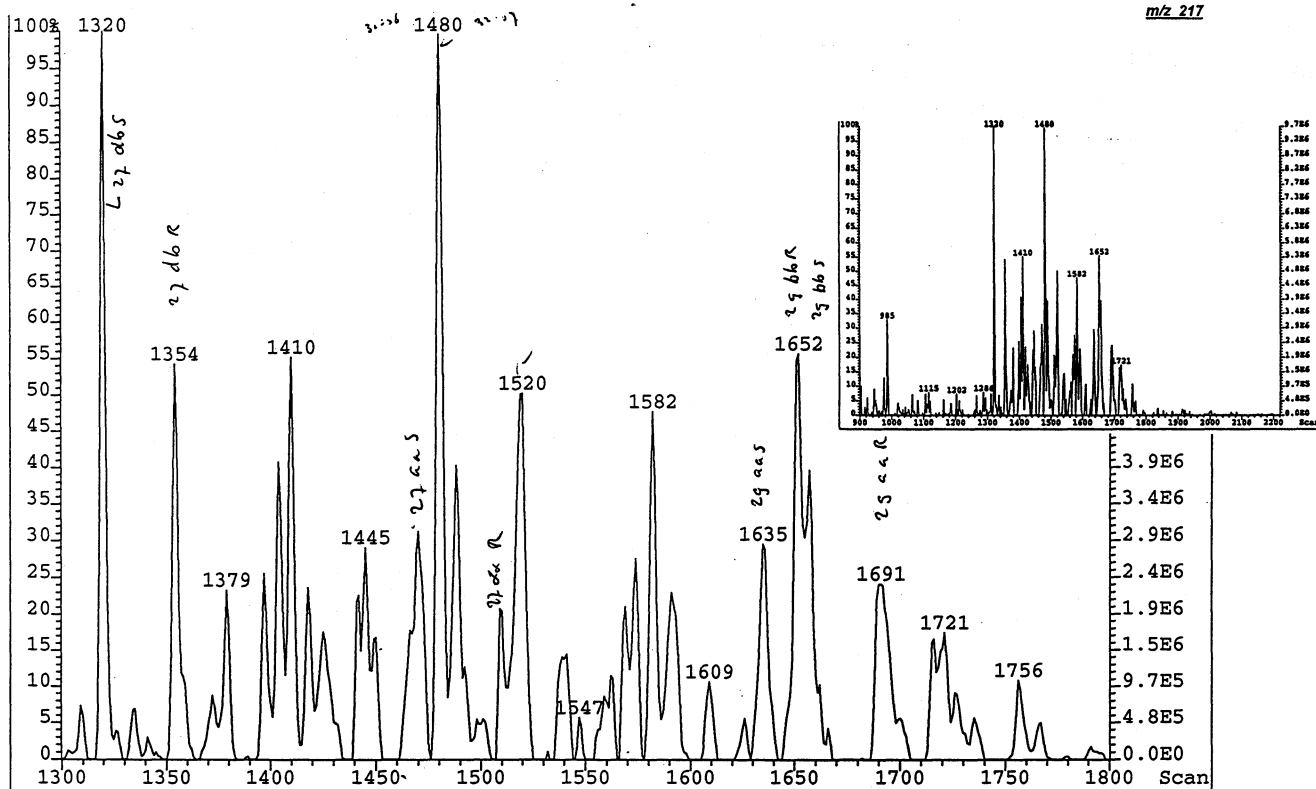


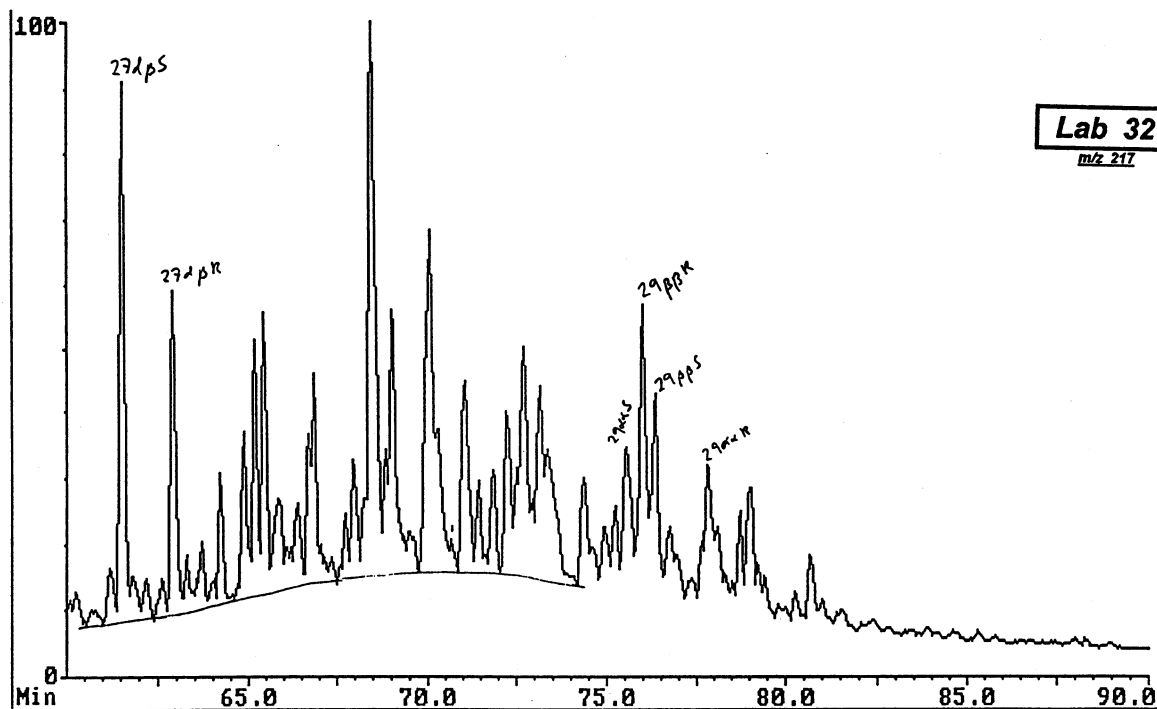
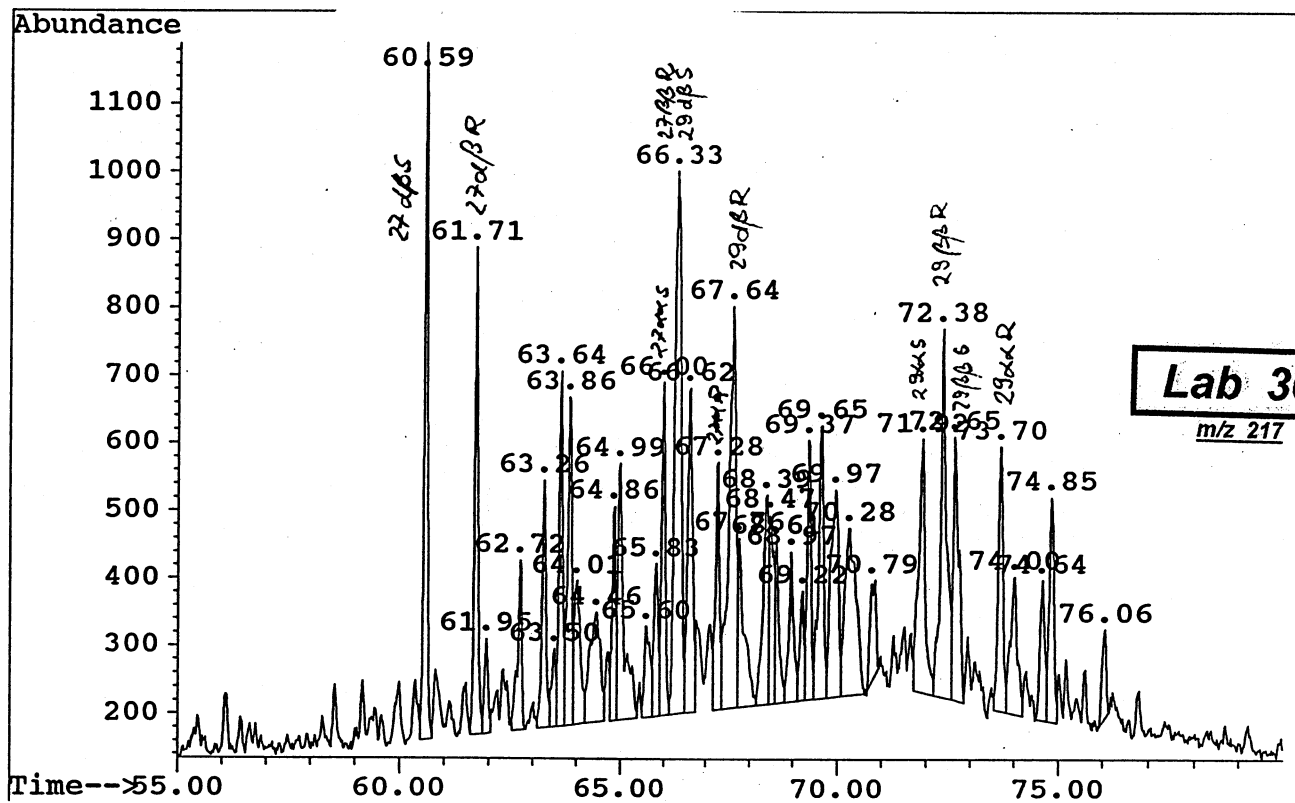


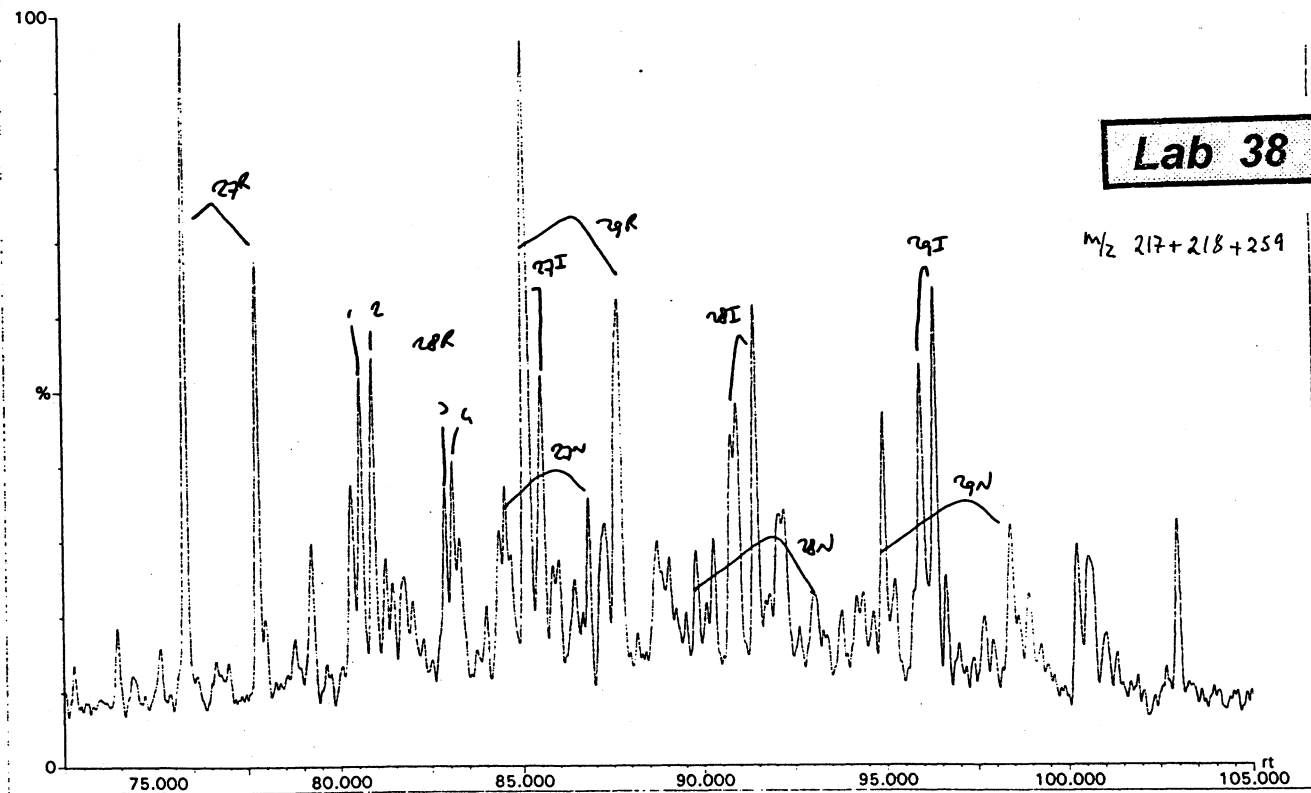
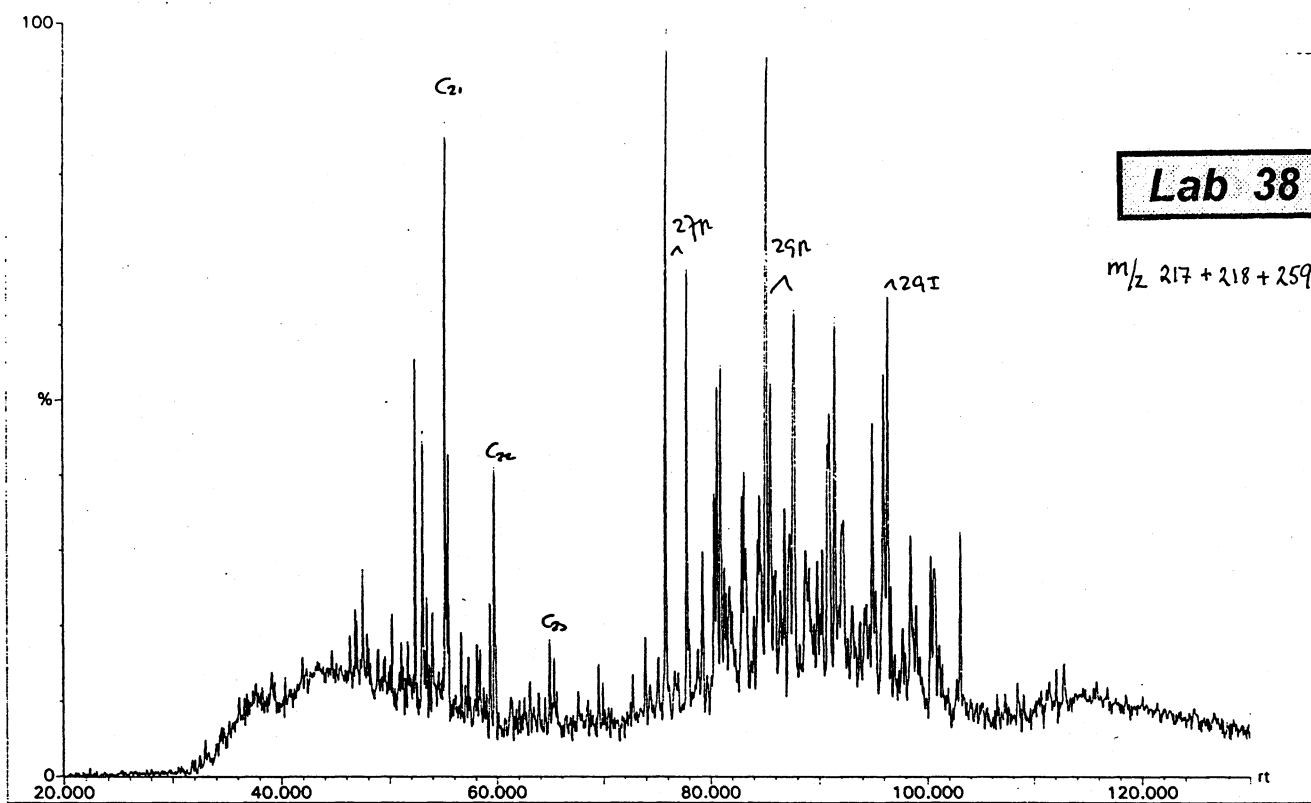


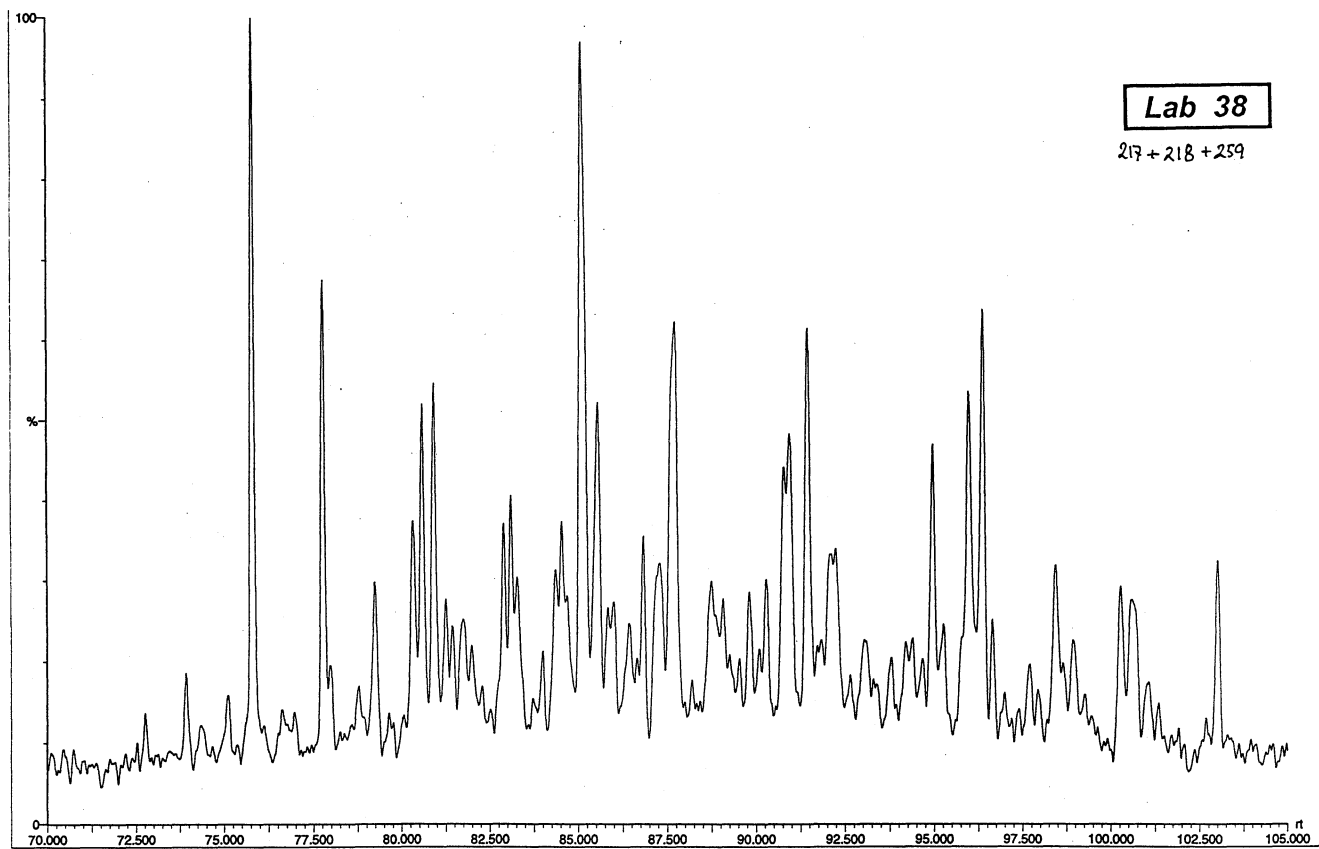
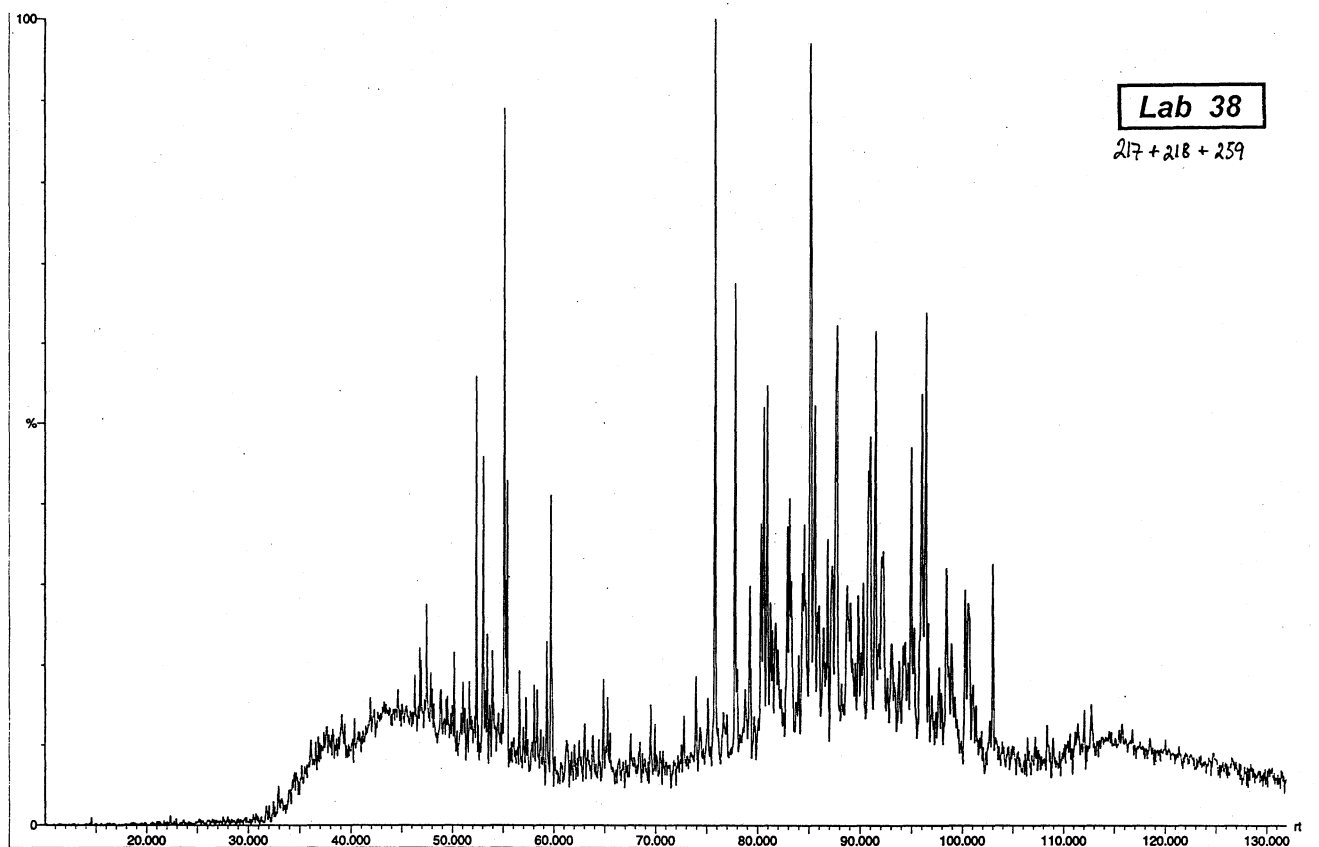
Lab 24

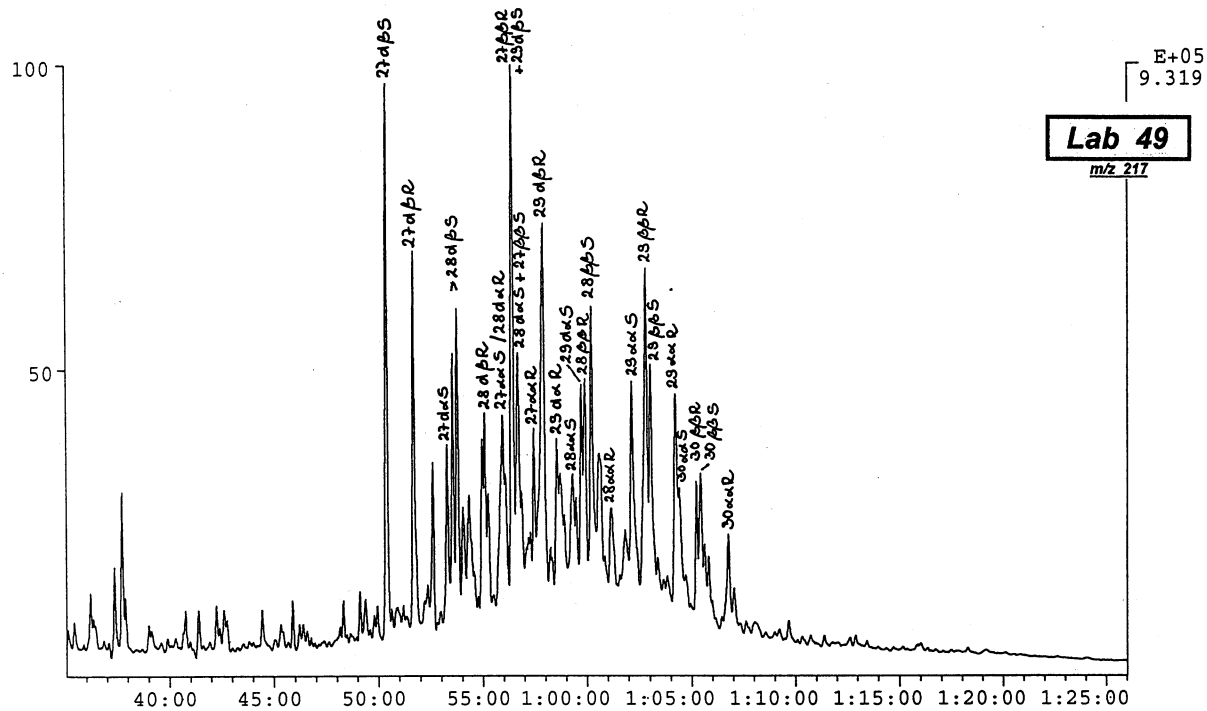
m/z 217

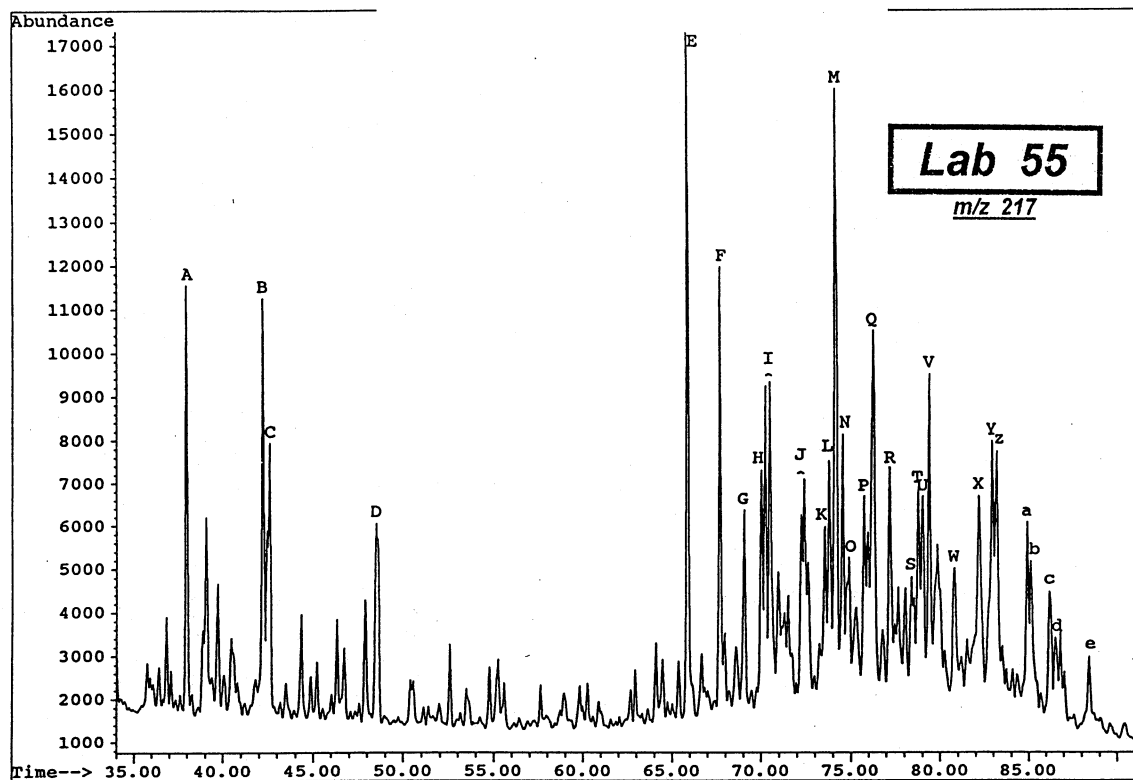




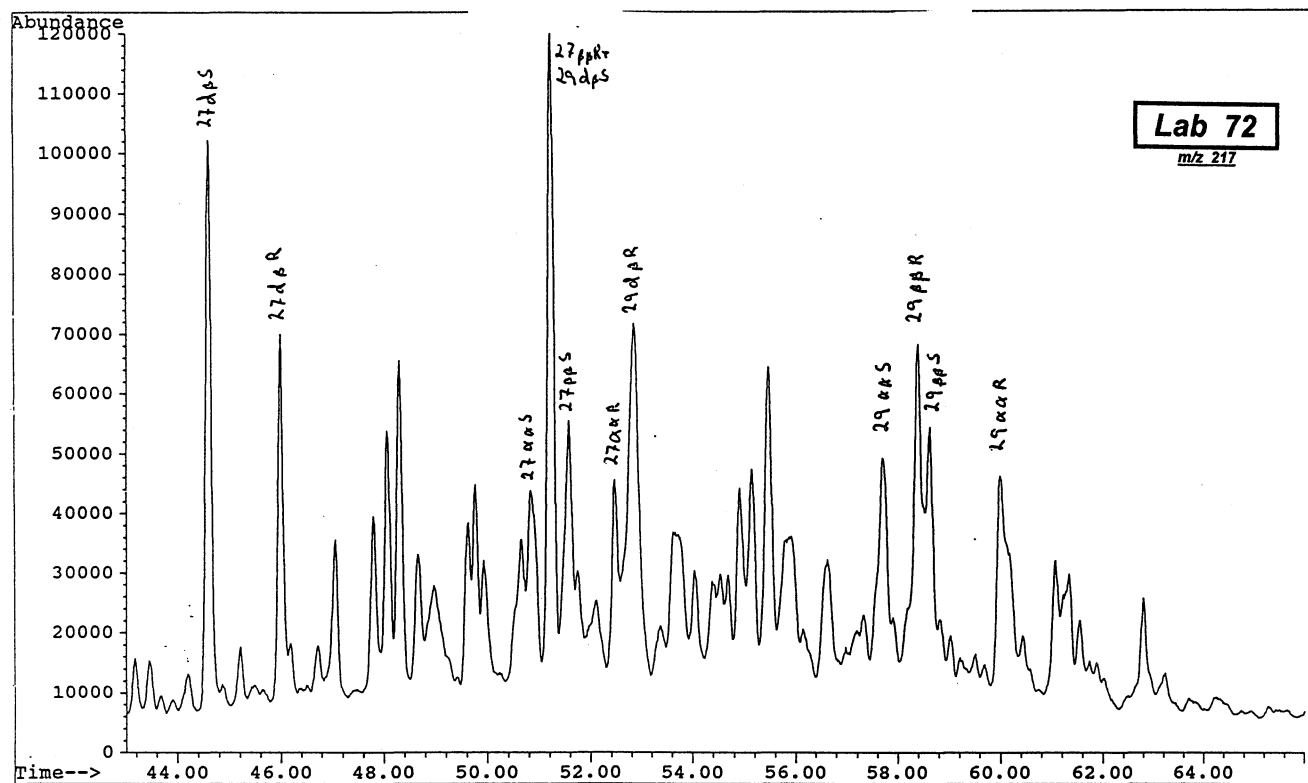
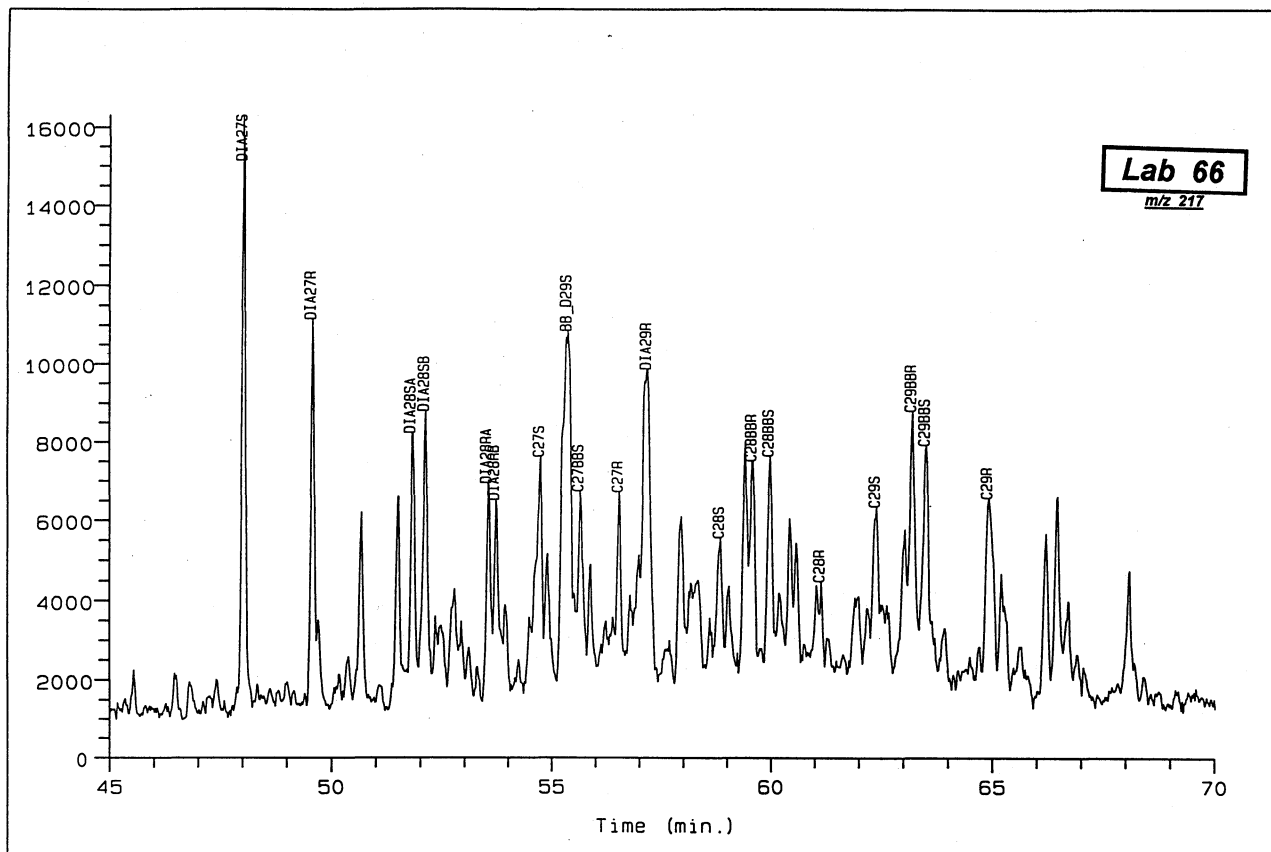


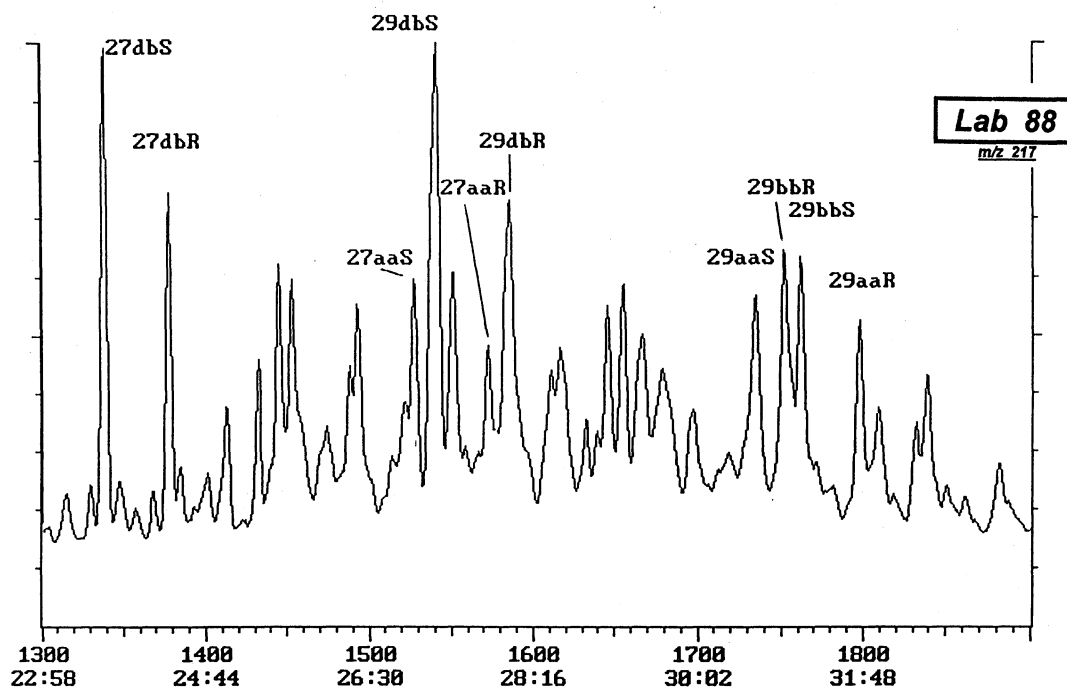


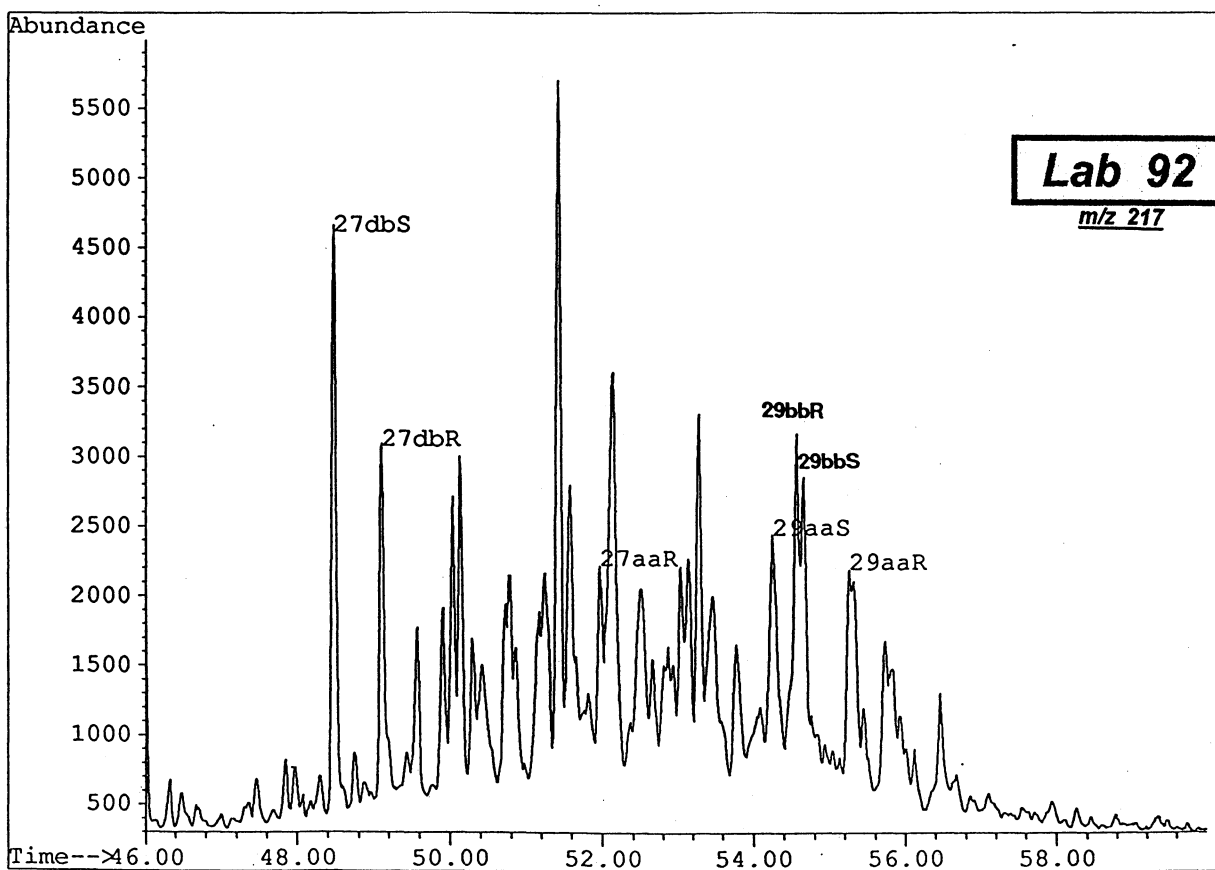
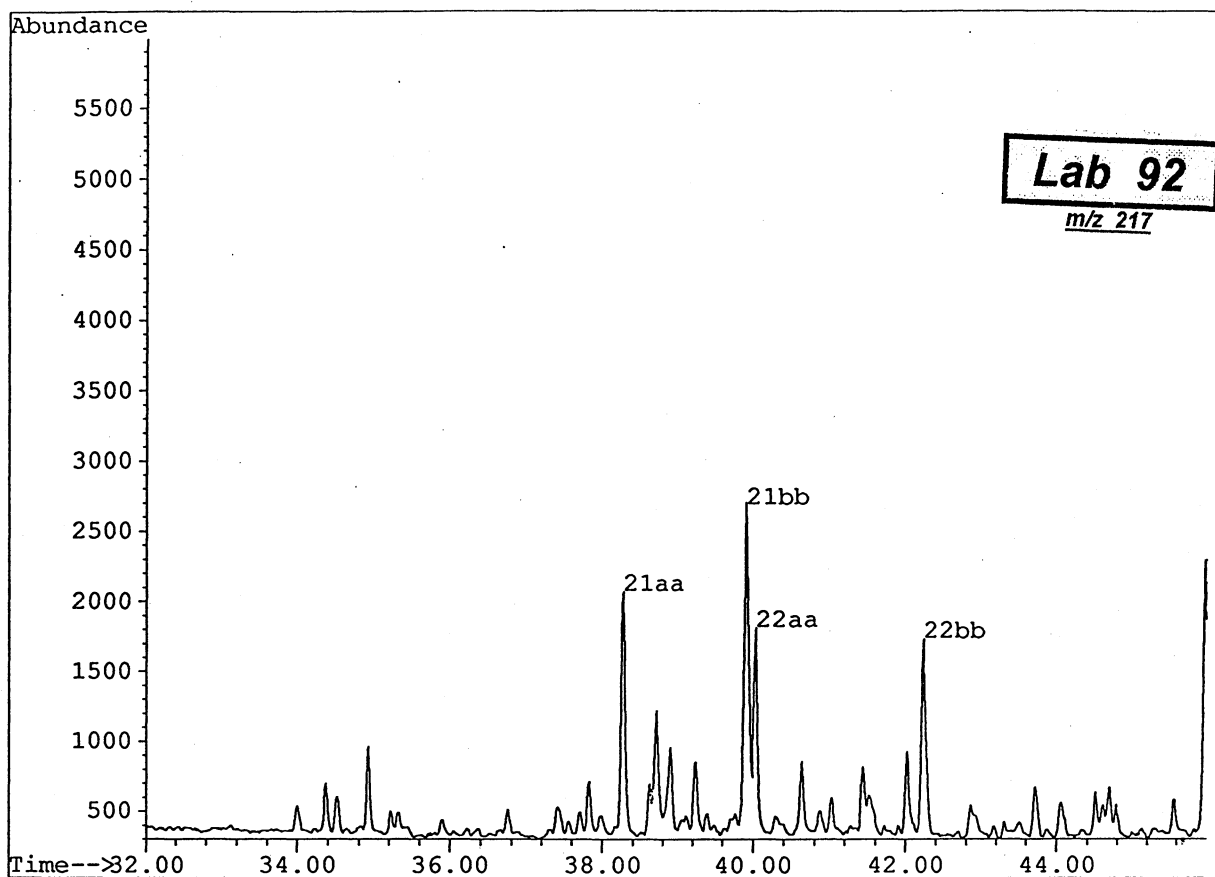


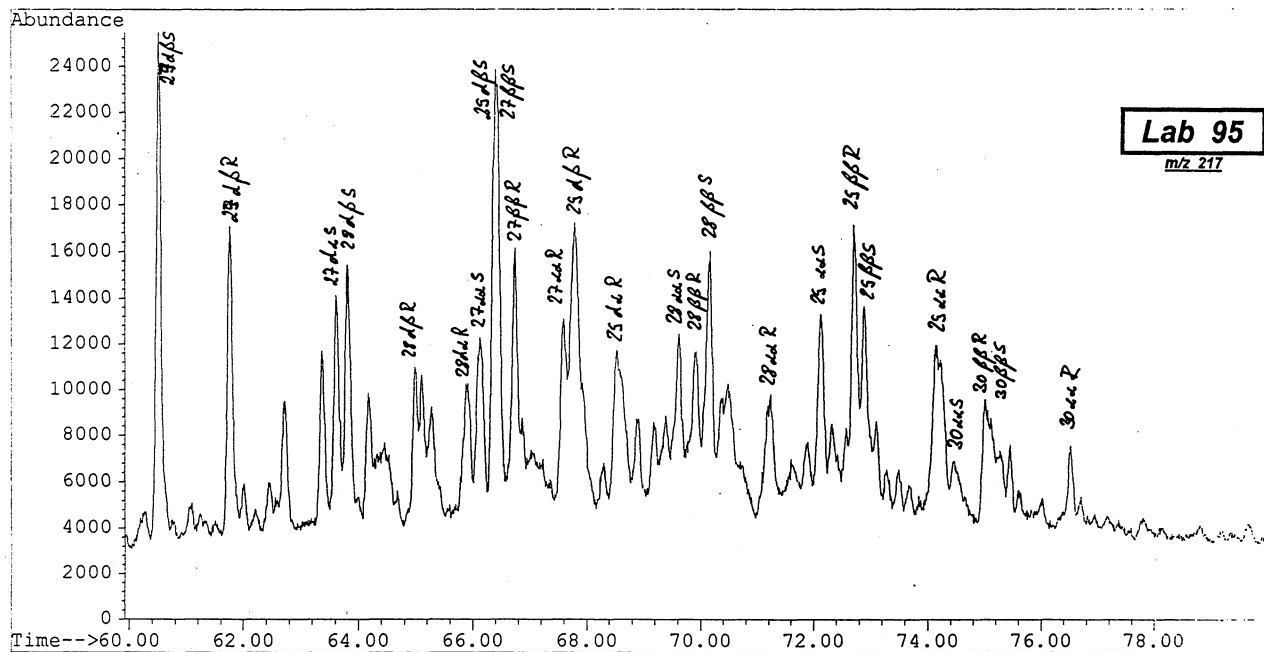


Peak ID	Sterane Name	Ret Time	Area	Area%	ppm
1 A	C ₂₁ diasterane	37.971	838287	4.03	56
2 B	C ₂₁ αβ sterane	42.207	911581	4.39	61
3 C	C ₂₂ diasterane	42.582	849856	4.09	56
4 D	C ₂₂ αβ sterane	48.522	673639	3.24	45
5 E	C ₂₇ βα diasterane (20S)	27δβS ✓ 65.853	1383584	6.66	92
6 F	C ₂₇ βα diasterane (20R)	27δβR ✓ 67.675	914157	4.40	61
7 G	C ₂₇ αβ diasterane (20S)	27δαR 69.072	478343	2.30	32
8 H	C ₂₇ αβ diasterane (20R)	27δαS 70.003	484453	2.33	32
9 I	C ₂₈ βα diasterane (20S)	28δβS 70.221	1322584	6.37	88
10 J	C ₂₈ βα diasterane (20R)	28δβR 72.377	876826	4.22	58
11 K	C ₂₈ αβ diasterane (20S)	28δαR 73.518	370224	1.78	25
12 L	C ₂₇ ααα sterane (20S)	27ααS ✓ 73.769	624974	3.01	41
13 M	C ₂₇ αβ ster- (20R) + C ₂₈ βα dia- (20S)	27ββR + 29δβS ✓ 74.133	1551949	7.47	103
14 N	C ₂₇ αβ sterane (20S)	27ββS 74.519	621195	2.99	41
15 O	C ₂₈ αβ diasterane (20R)	28δαS 74.875	436031	2.10	29
16 P	C ₂₇ ααα sterane (20R)	27ααR ✓ 75.717	400188	1.93	27
17 Q	C ₂₈ βα diasterane (20R)	29δβR ✓ 76.223	1246337	6.00	83
18 R	C ₂₈ αβ diasterane (20S)	29δαR 77.157	652824	3.14	43
19 S	C ₂₈ ααα sterane (20S)	28ααS 78.360	177094	0.85	12
20 T	C ₂₈ αβ diasterane (20R)	29δαS 78.748	496809	2.39	33
21 U	C ₂₈ αβ sterane (20R)	28ββR 79.001	550972	2.65	37
22 V	C ₂₈ αβ sterane (20S)	28ββS 79.365	785487	3.78	52
23 W	C ₂₈ ααα sterane (20R)	28ααR 80.789	386299	1.86	26
24 X	C ₂₈ ααα sterane (20S)	29ααS ✓ 82.147	659830	3.18	44
25 Y	C ₂₈ αβ sterane (20R)	29ββR ✓ 82.902	769753	3.70	51
26 Z	C ₂₈ αβ sterane (20S)	29ββS ✓ 83.145	659764	3.18	44
27 a	C ₂₉ ααα sterane (20R)	29ααR ✓ 84.892	412346	1.98	27
28 b	C ₃₀ ααα sterane (20S)	30ααS 85.114	407879	1.96	27
29 c	C ₃₀ αβ sterane (20R)	30ββR 86.180	364414	1.75	24
30 d	C ₃₀ αβ sterane (20S)	30ββS 86.505	281464	1.35	19
31 e	C ₃₀ ααα sterane (20R)	30ααR 88.407	188657	0.91	13





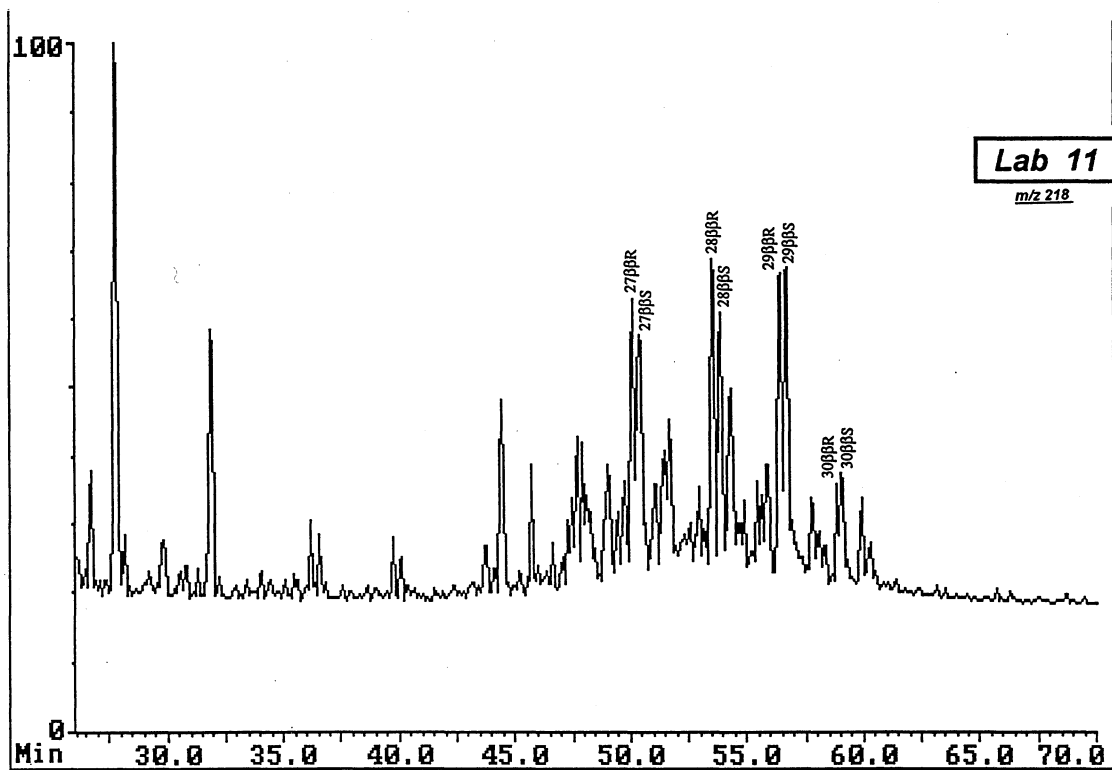
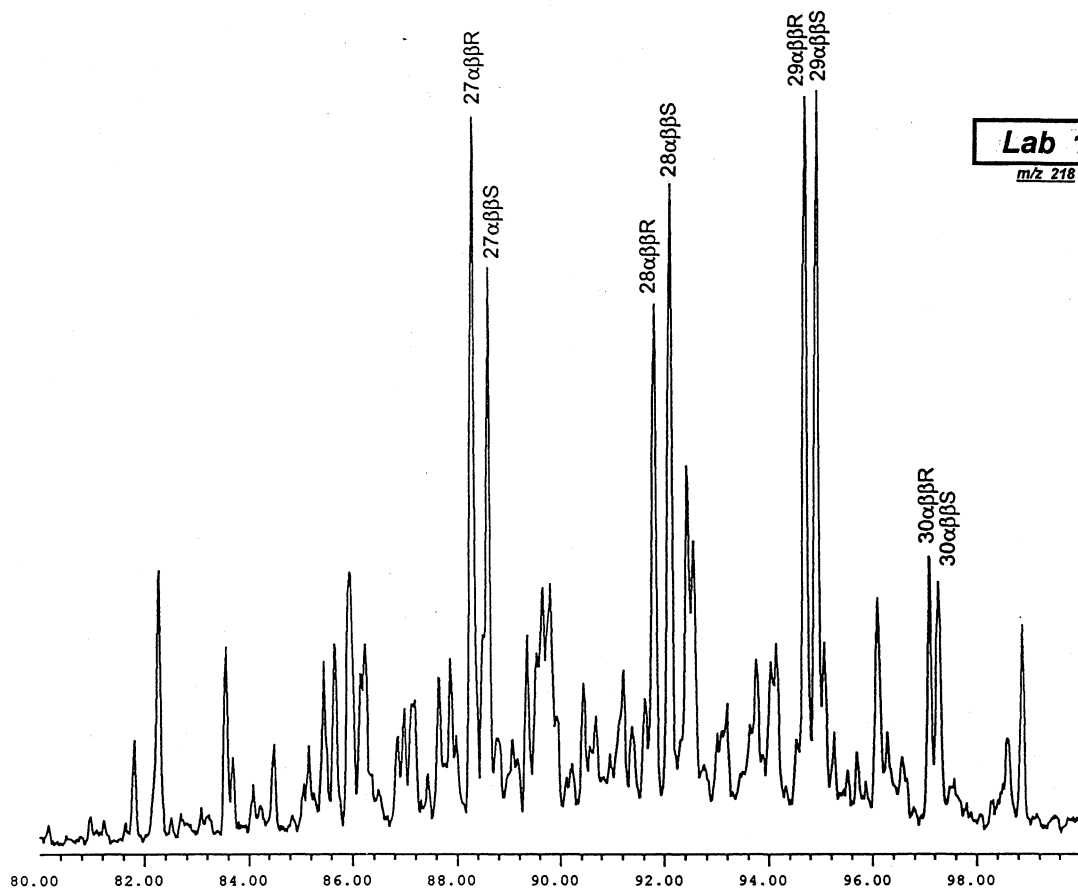


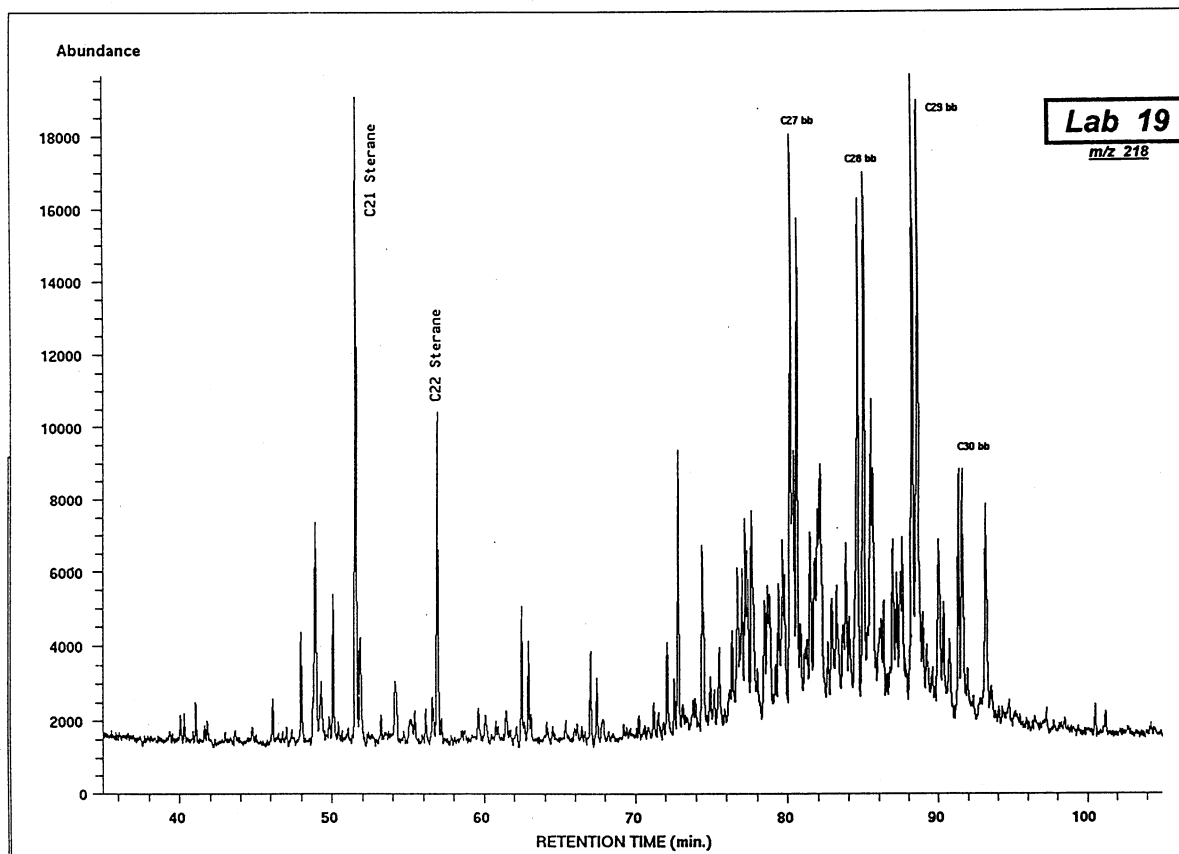
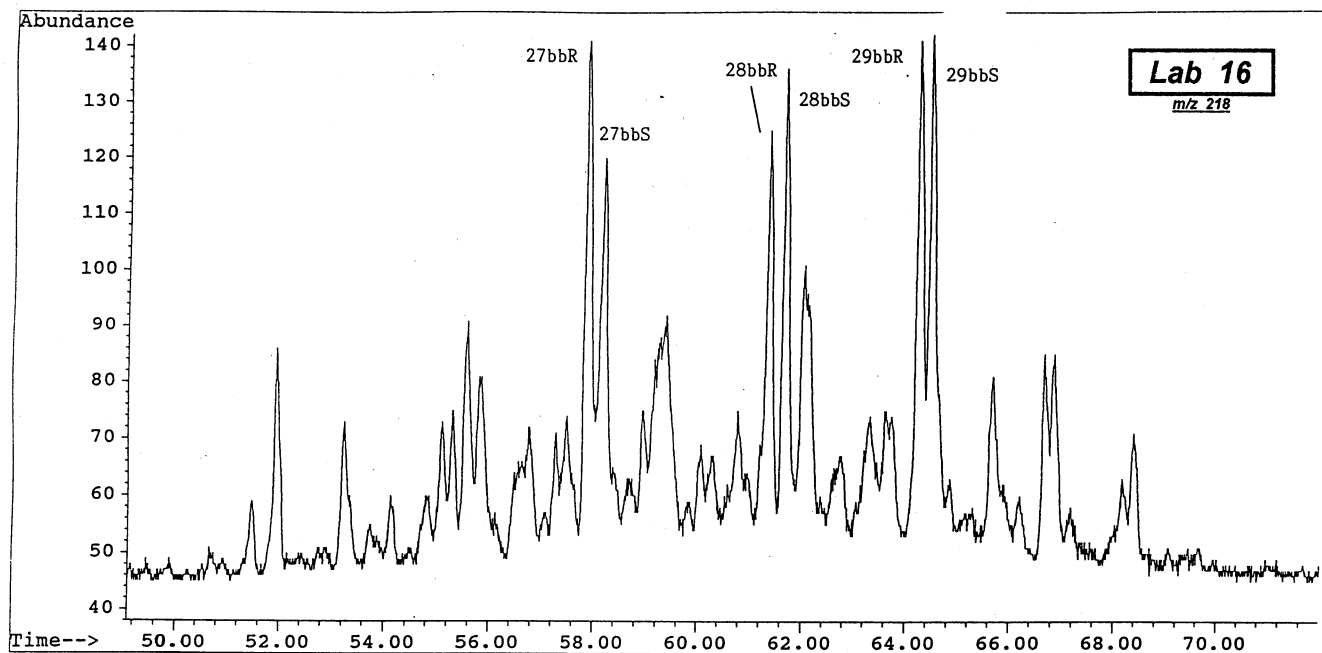


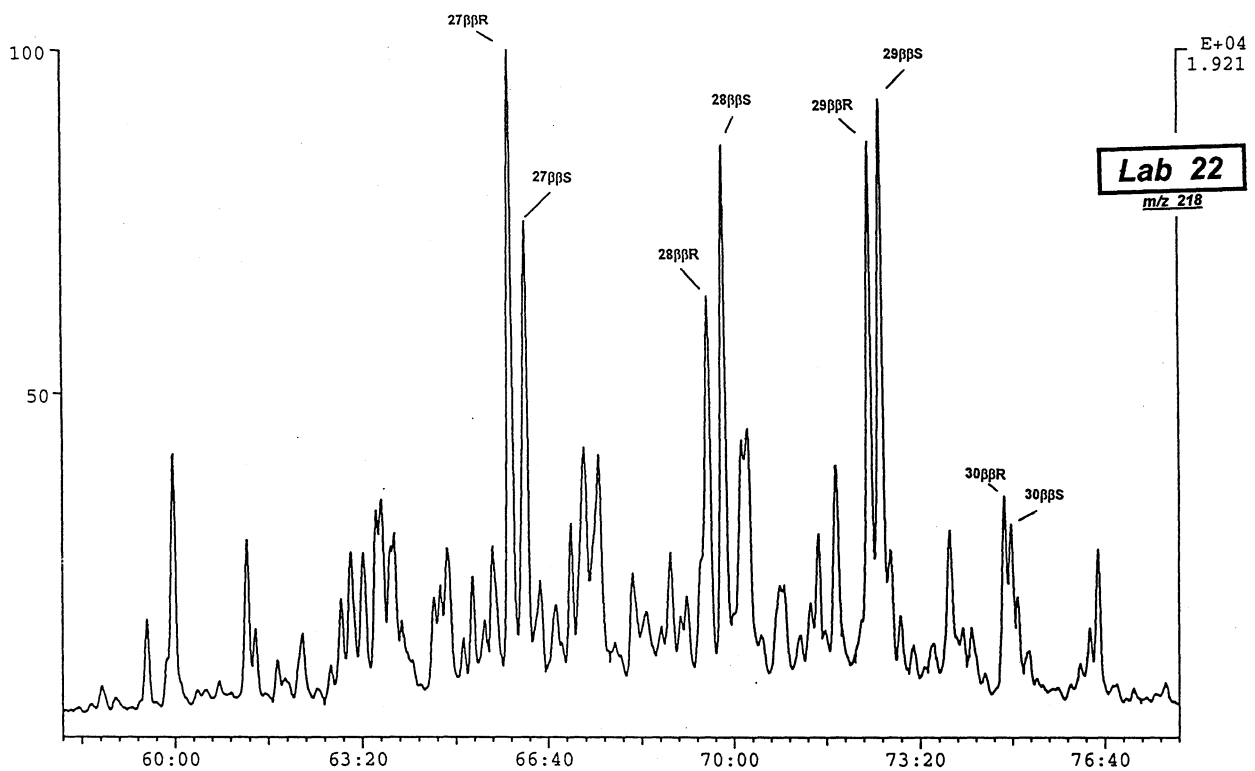
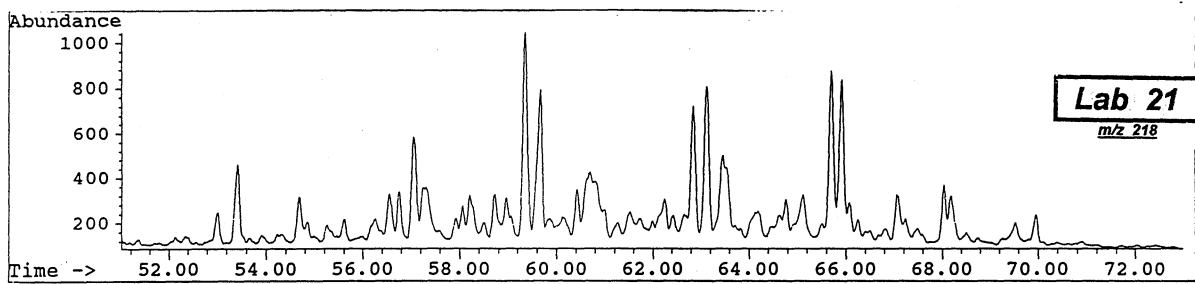
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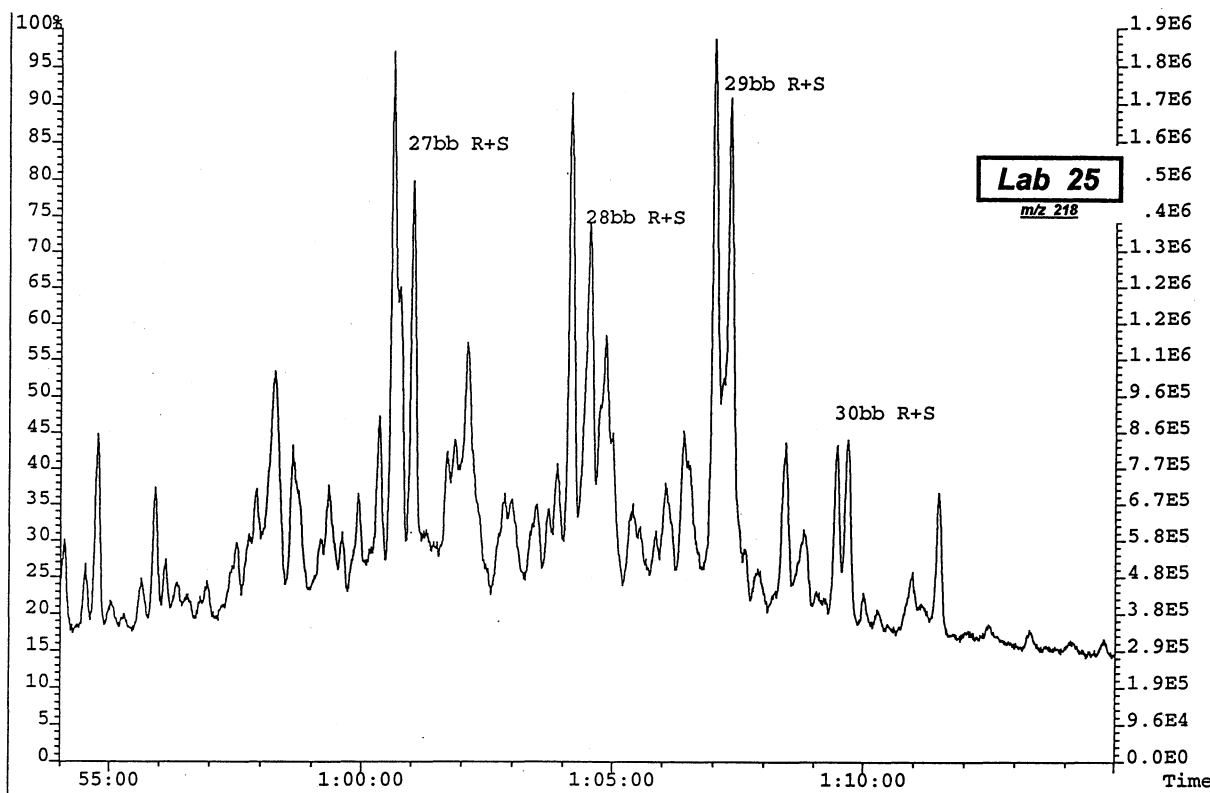
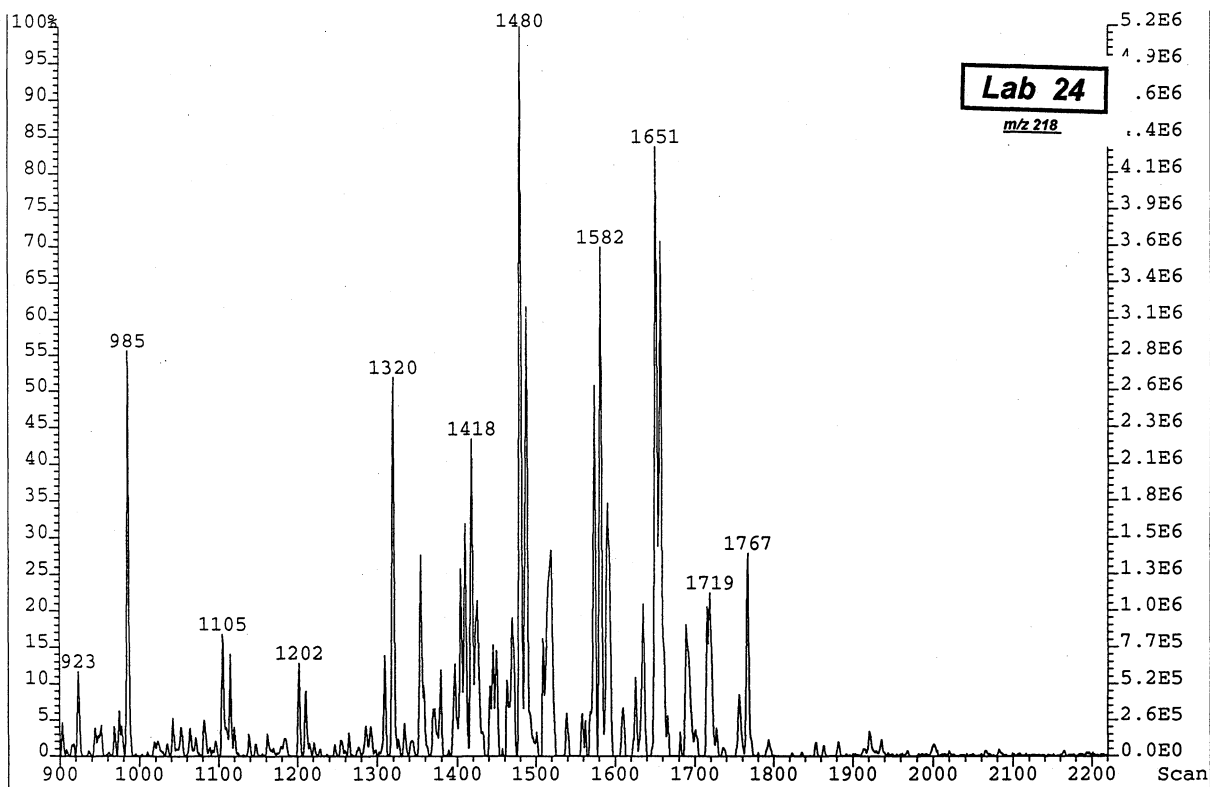
Appendix A3.4a-4

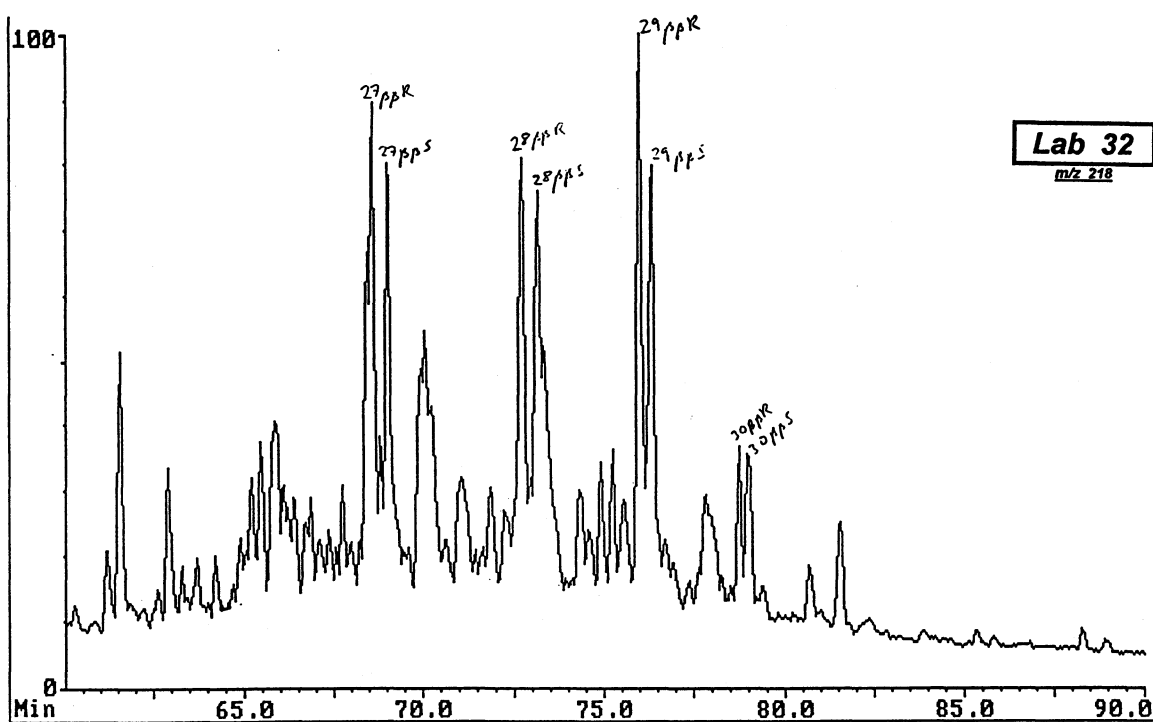
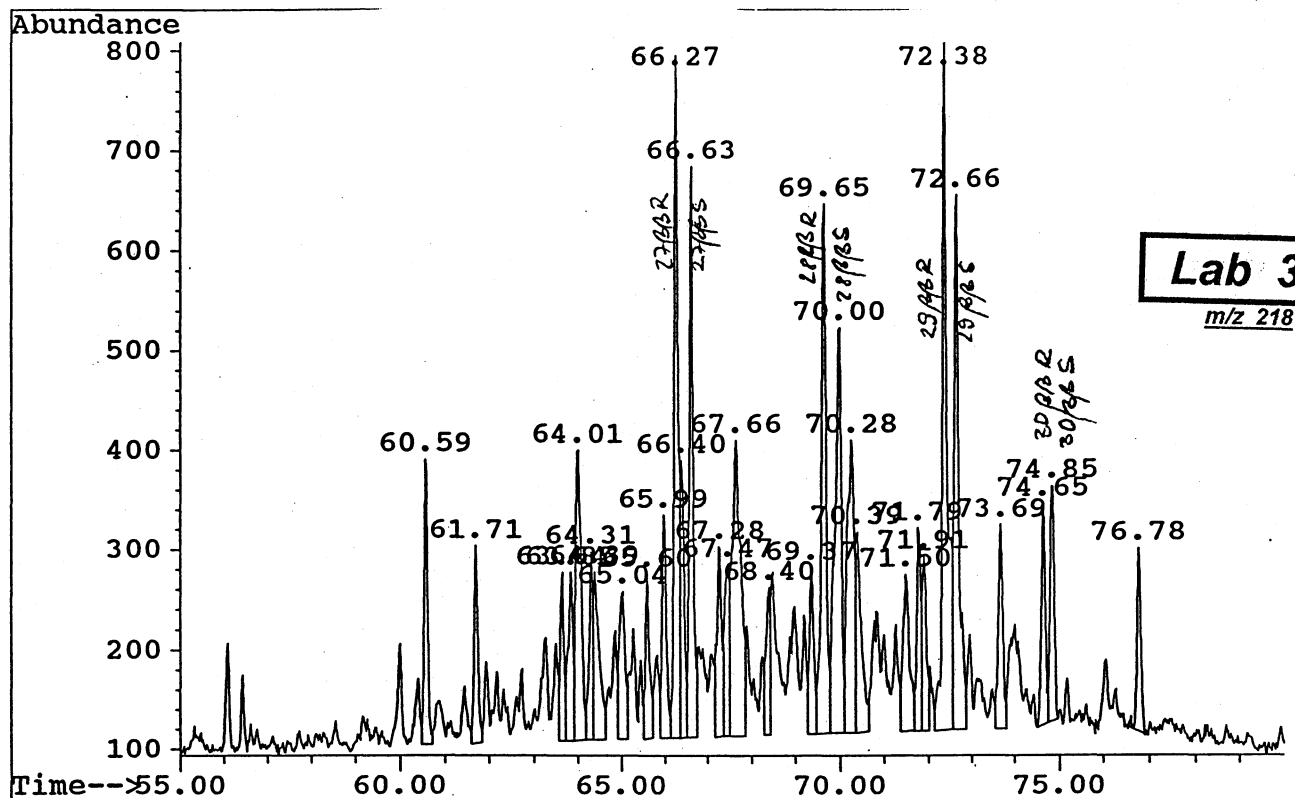
Saturates fraction m/z 218 GC-MS fragmentograms

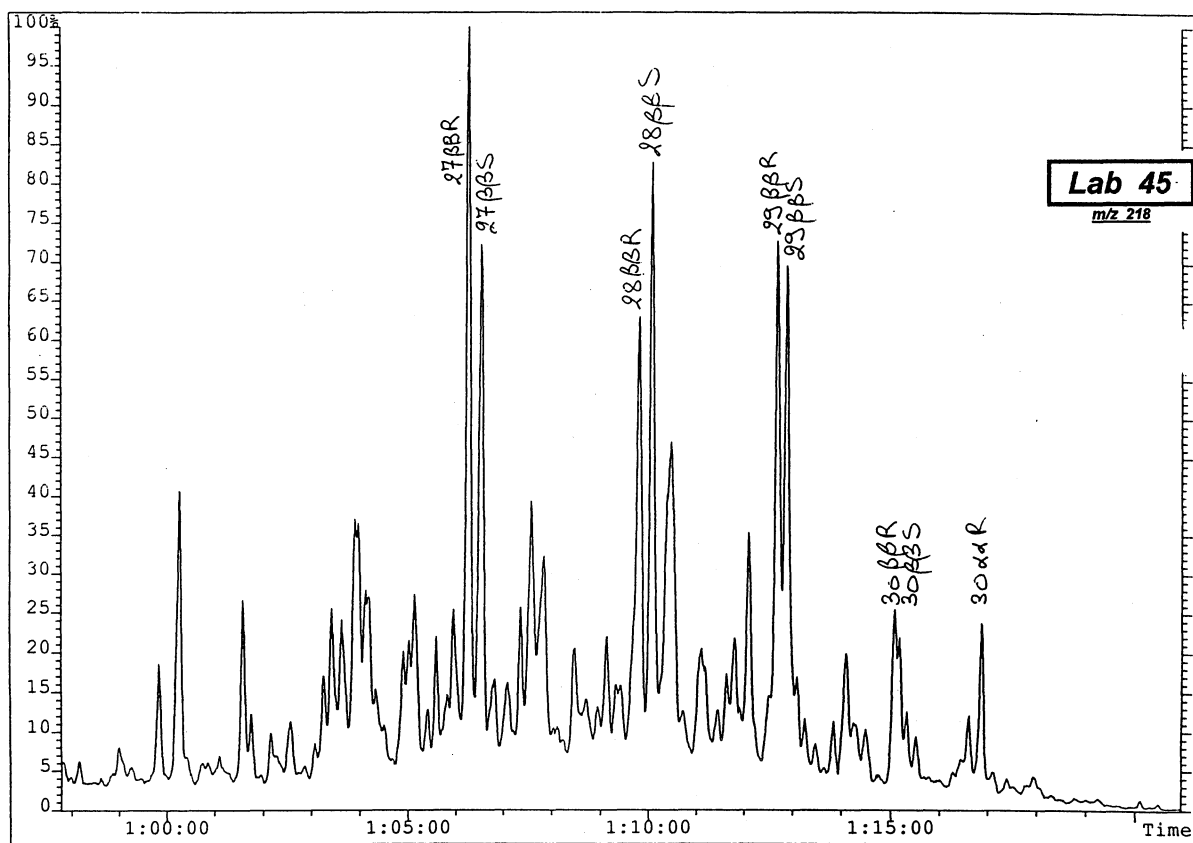
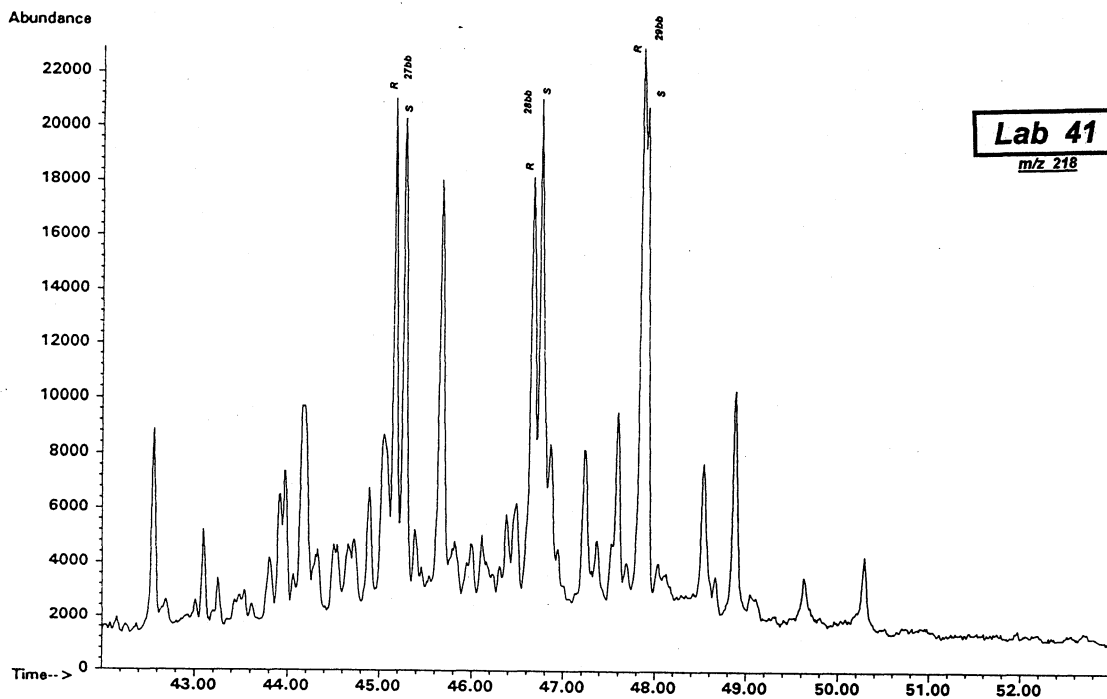


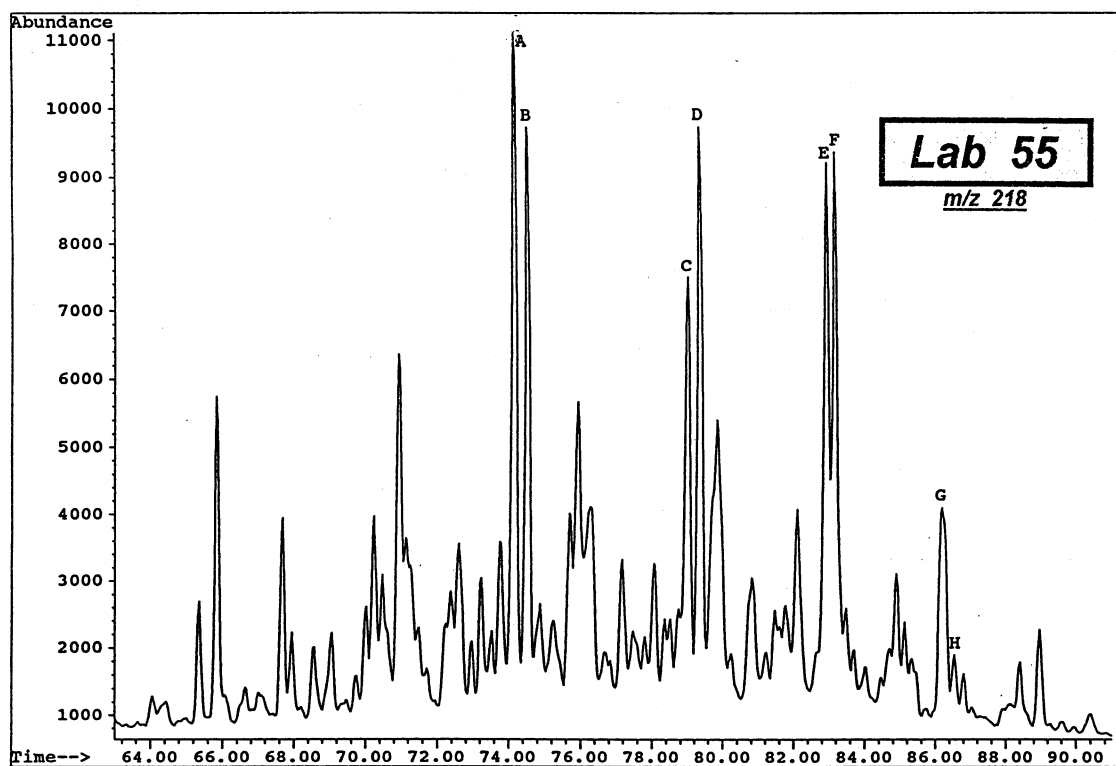
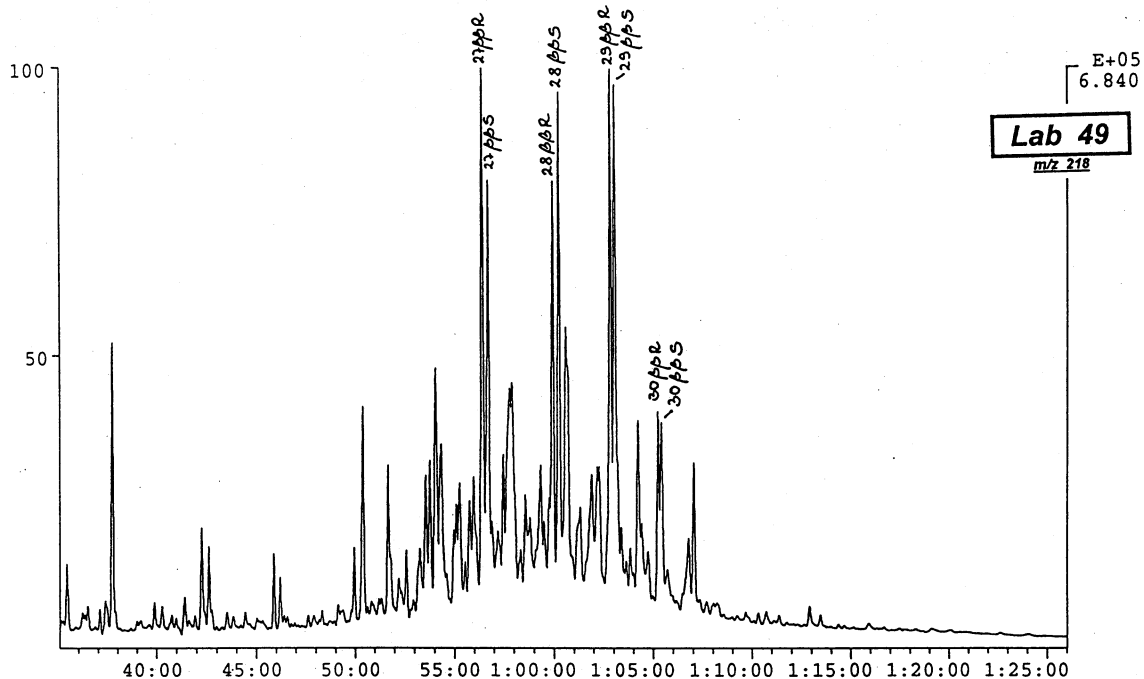




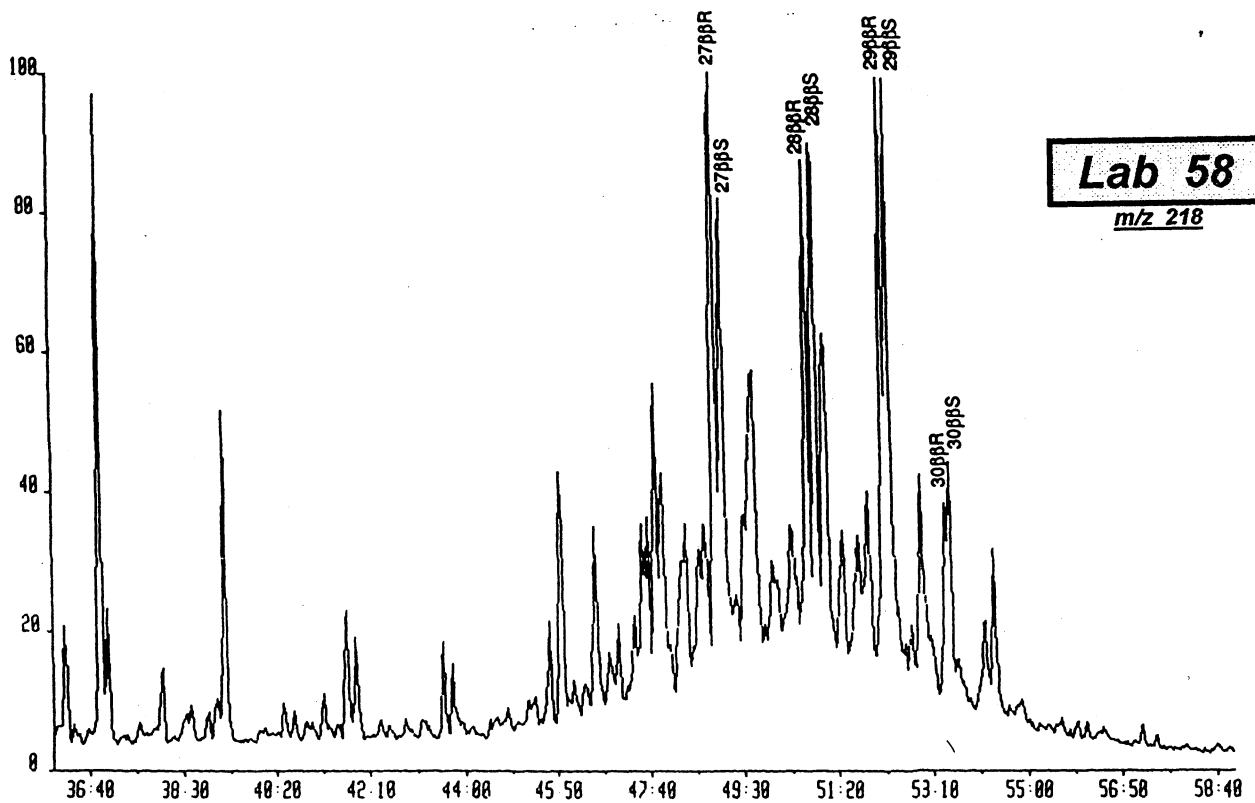
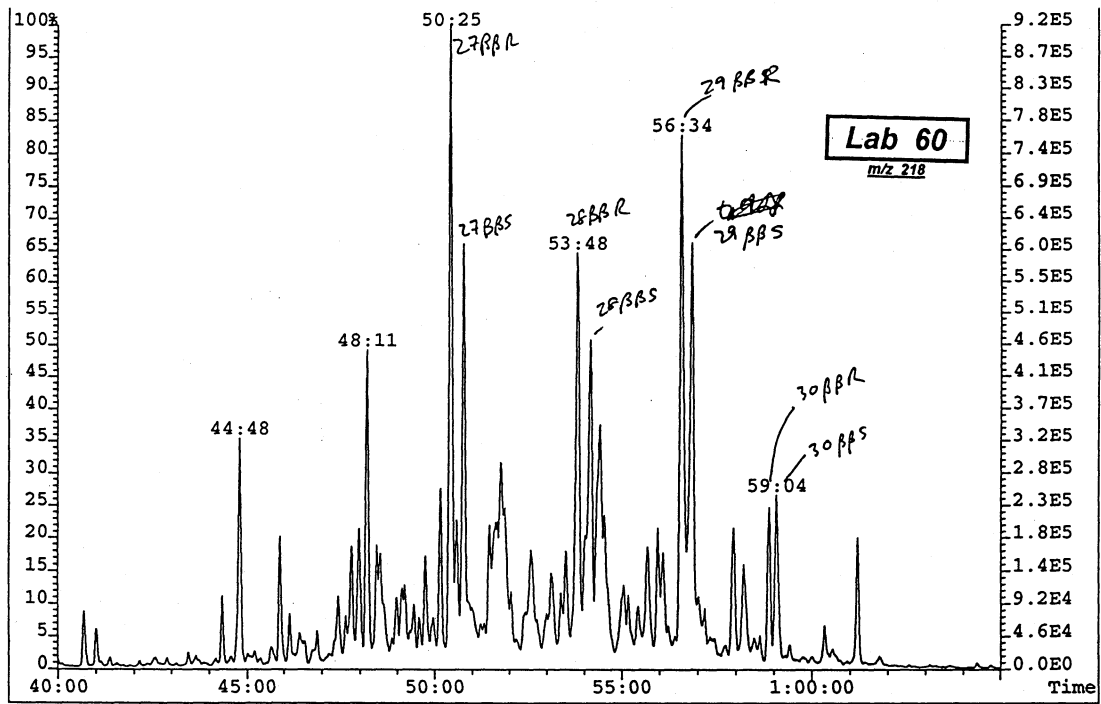


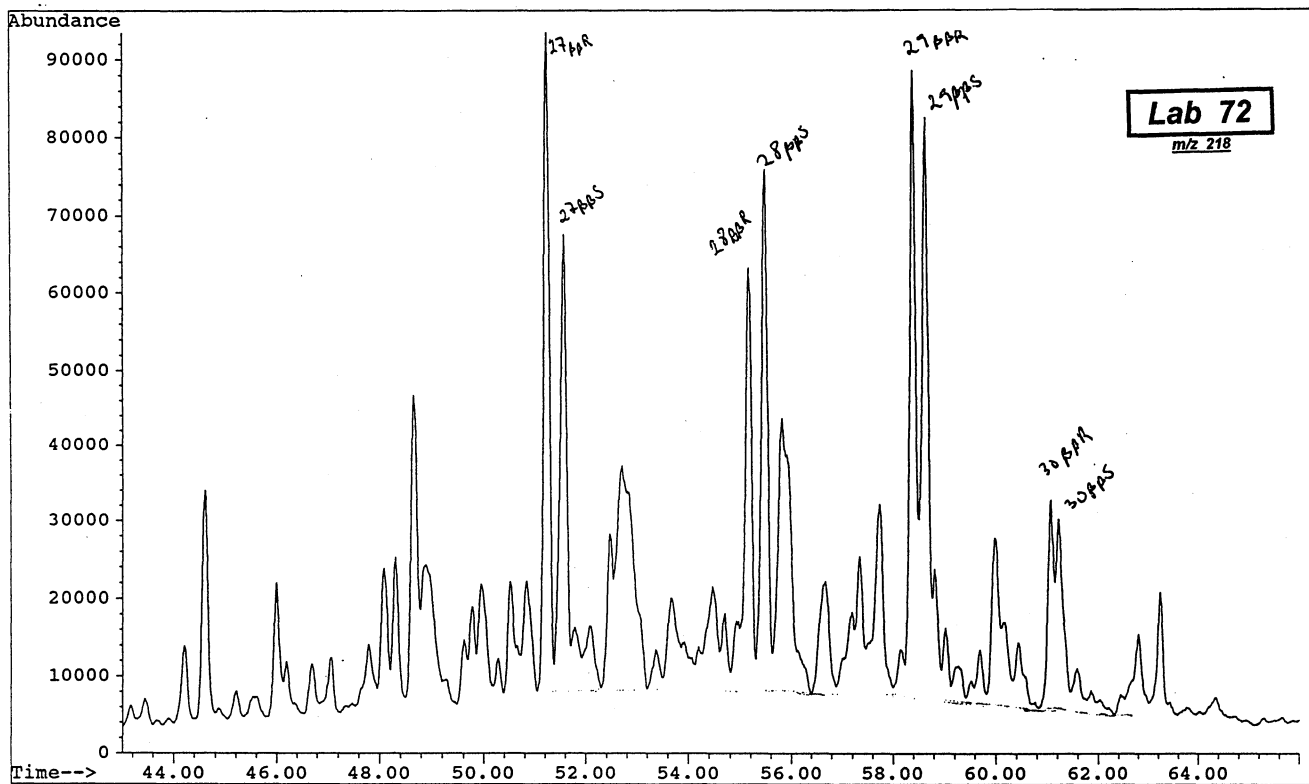
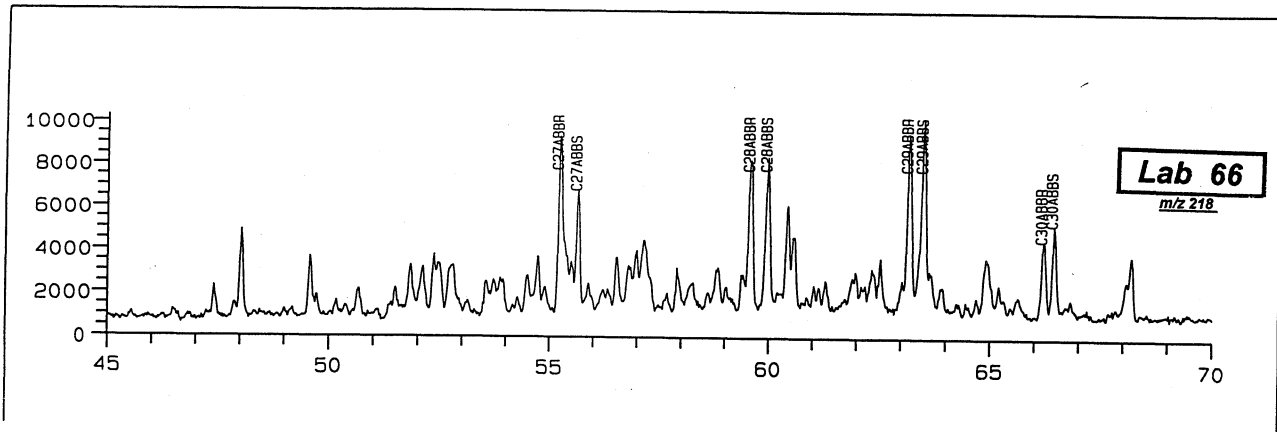


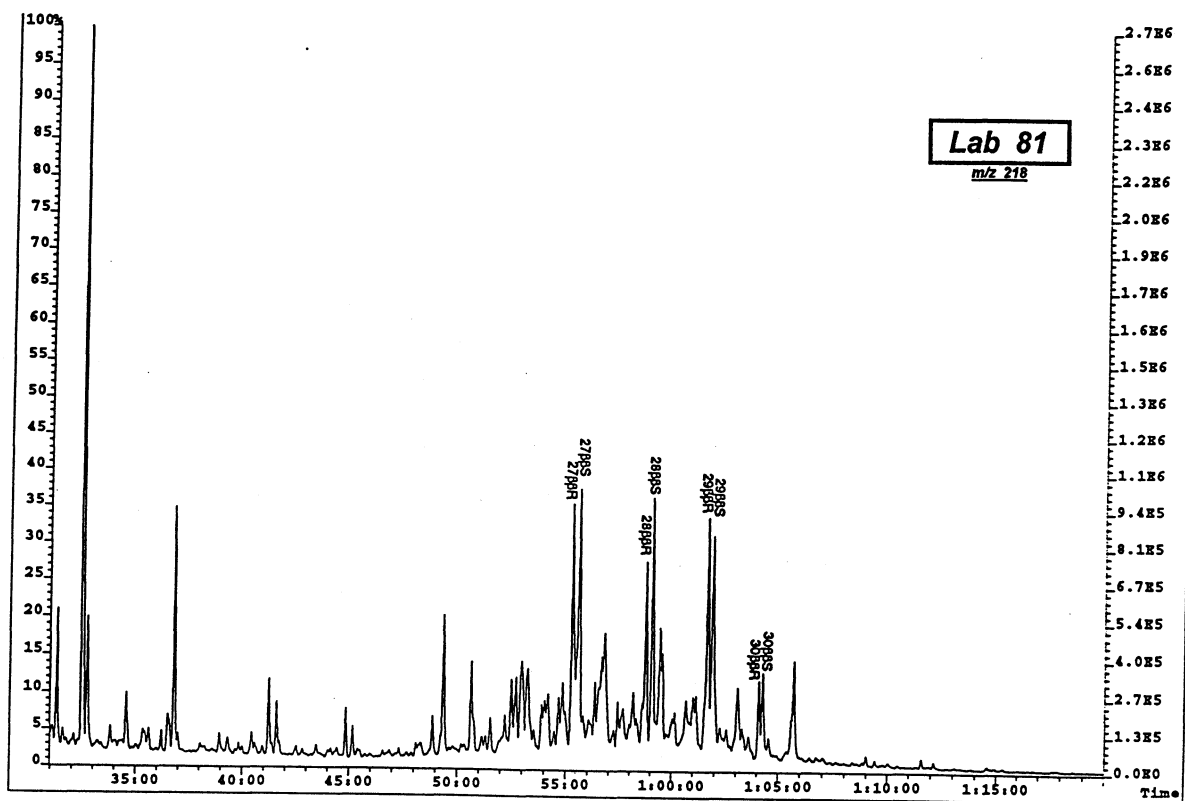
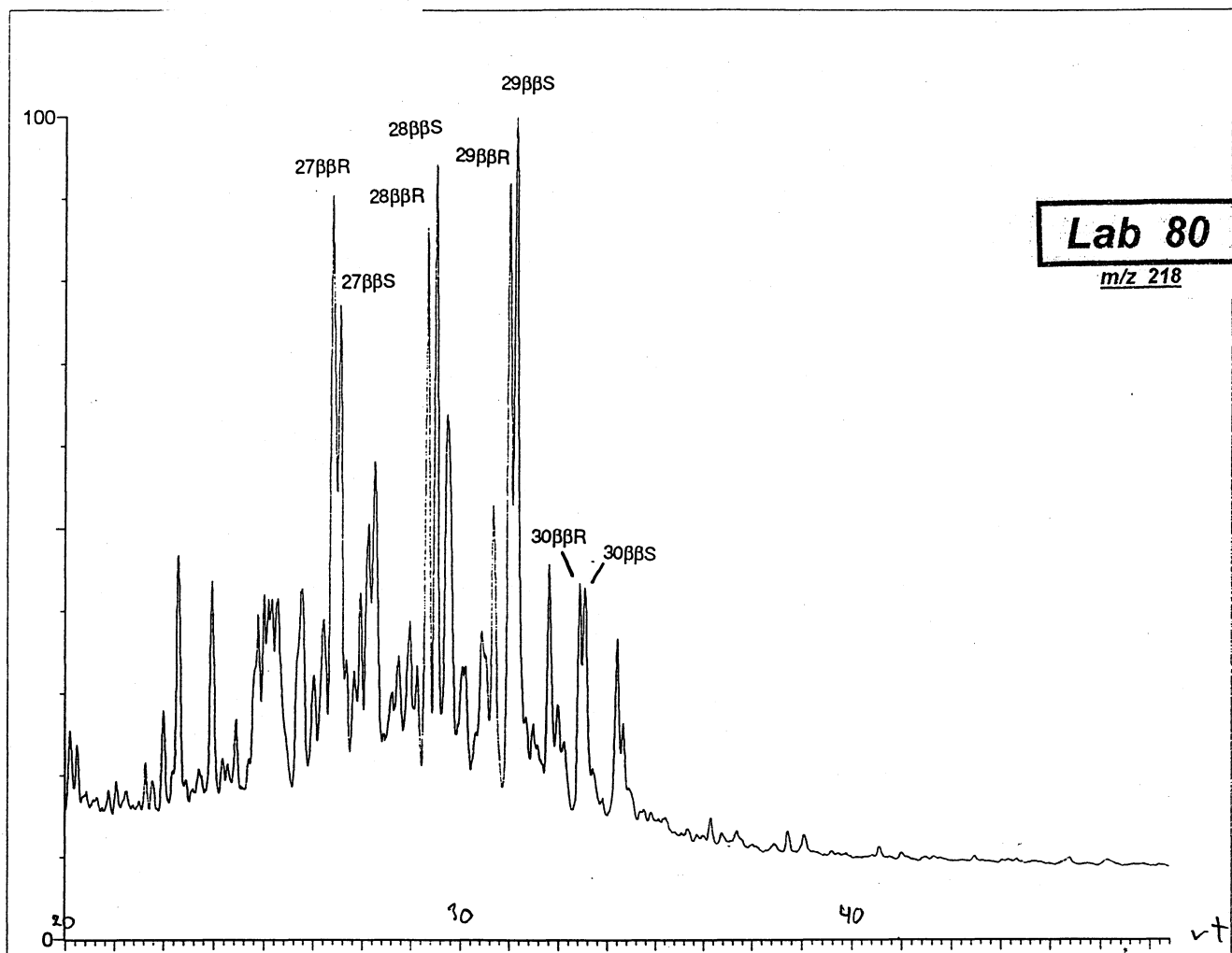


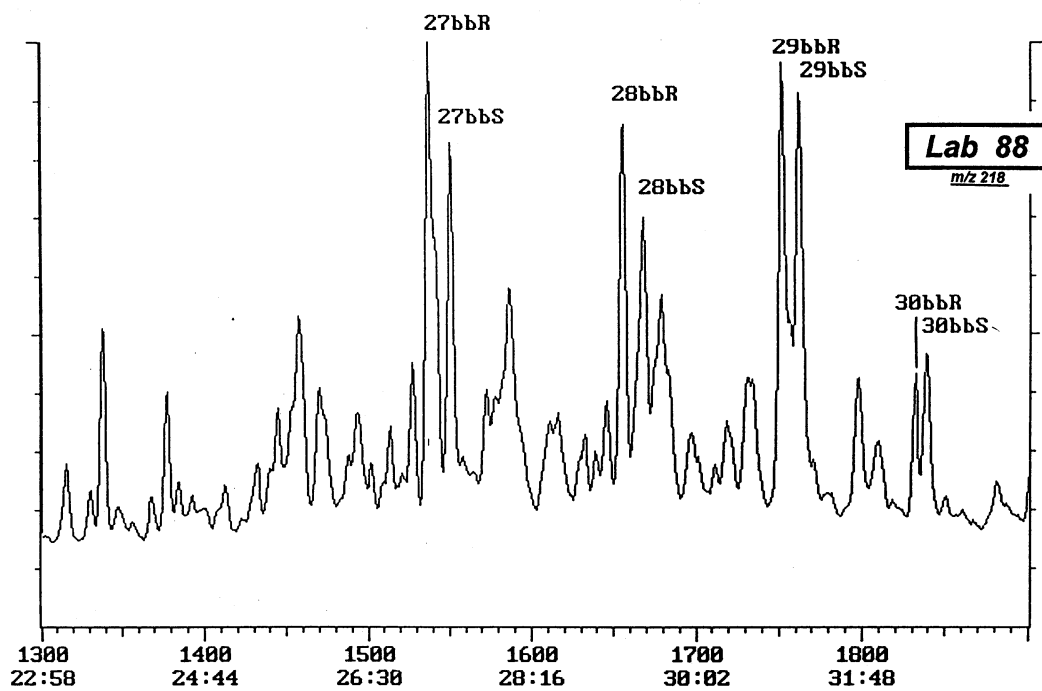


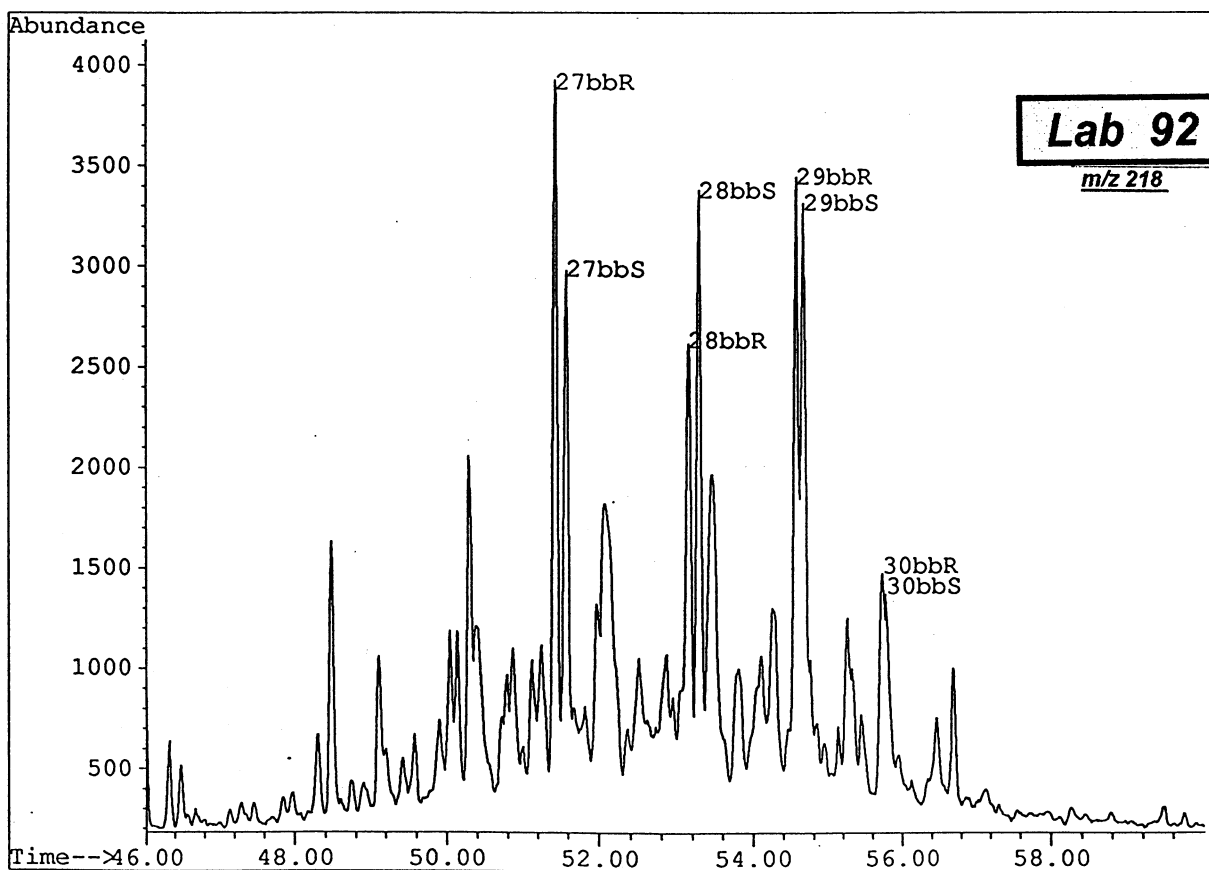
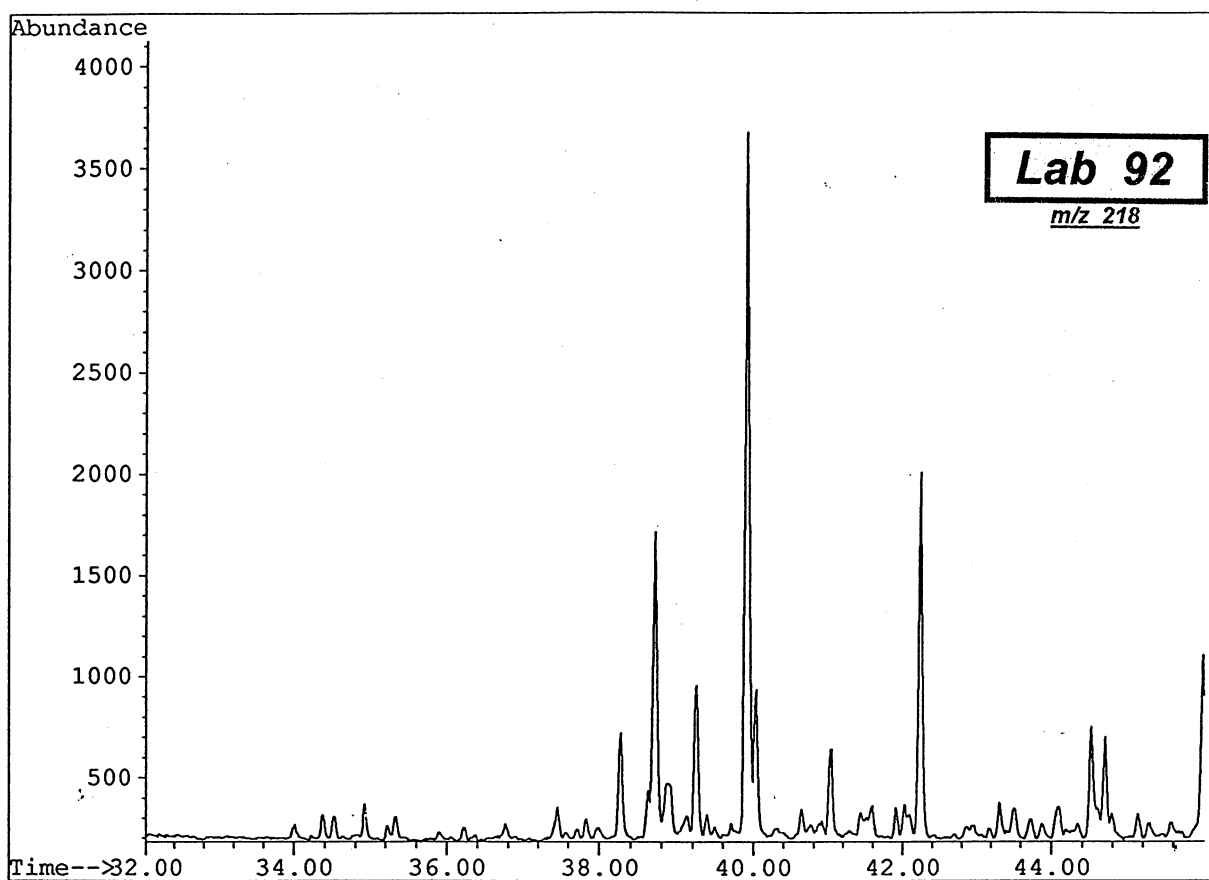
Sterane Report (m/z 218)						
Peak ID	Sterane Name	Ret Time	Area	Area%	ppm	
A	27 28ppR	74.176	1041729	18.00	69	
B	27 28ppS	74.540	830418	14.35	55	
C	28ppR	79.009	710078	12.27	47	
D	28ppS	79.351	852539	14.73	57	
E	29ppR	82.916	861358	14.88	57	
F	29ppS	83.153	898526	15.53	60	
G	30ppR	86.171	482112	8.33	32	
H	30ppS	86.533	110461	1.91	7	

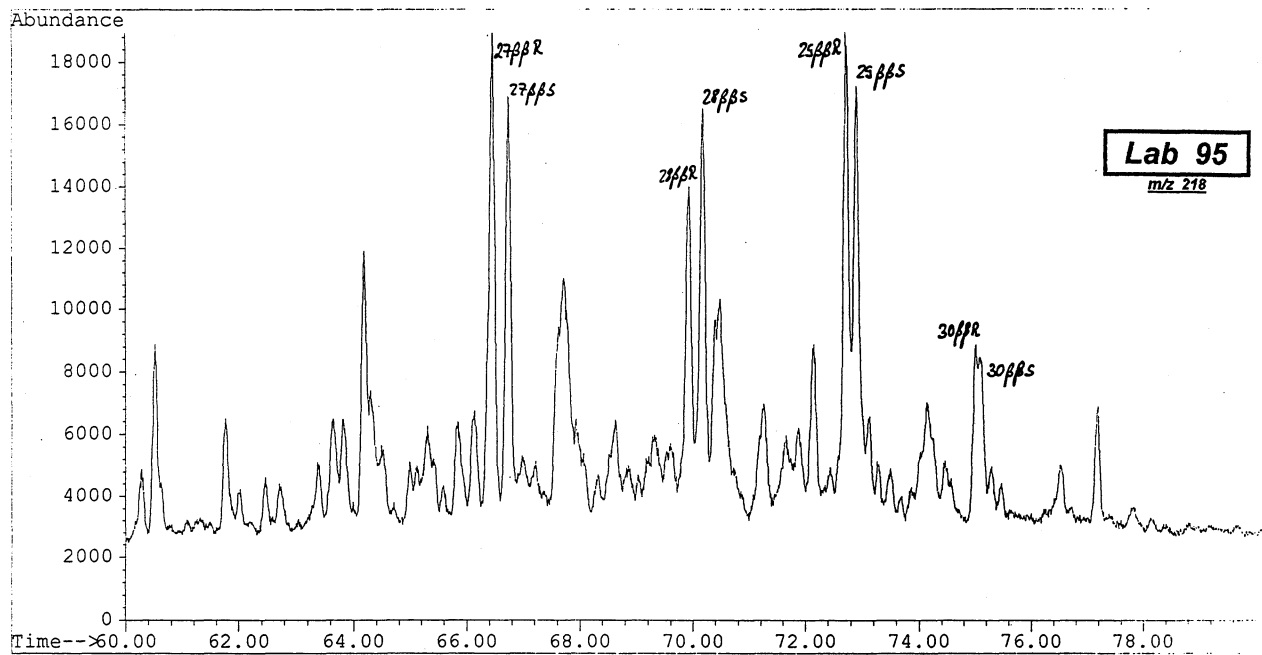








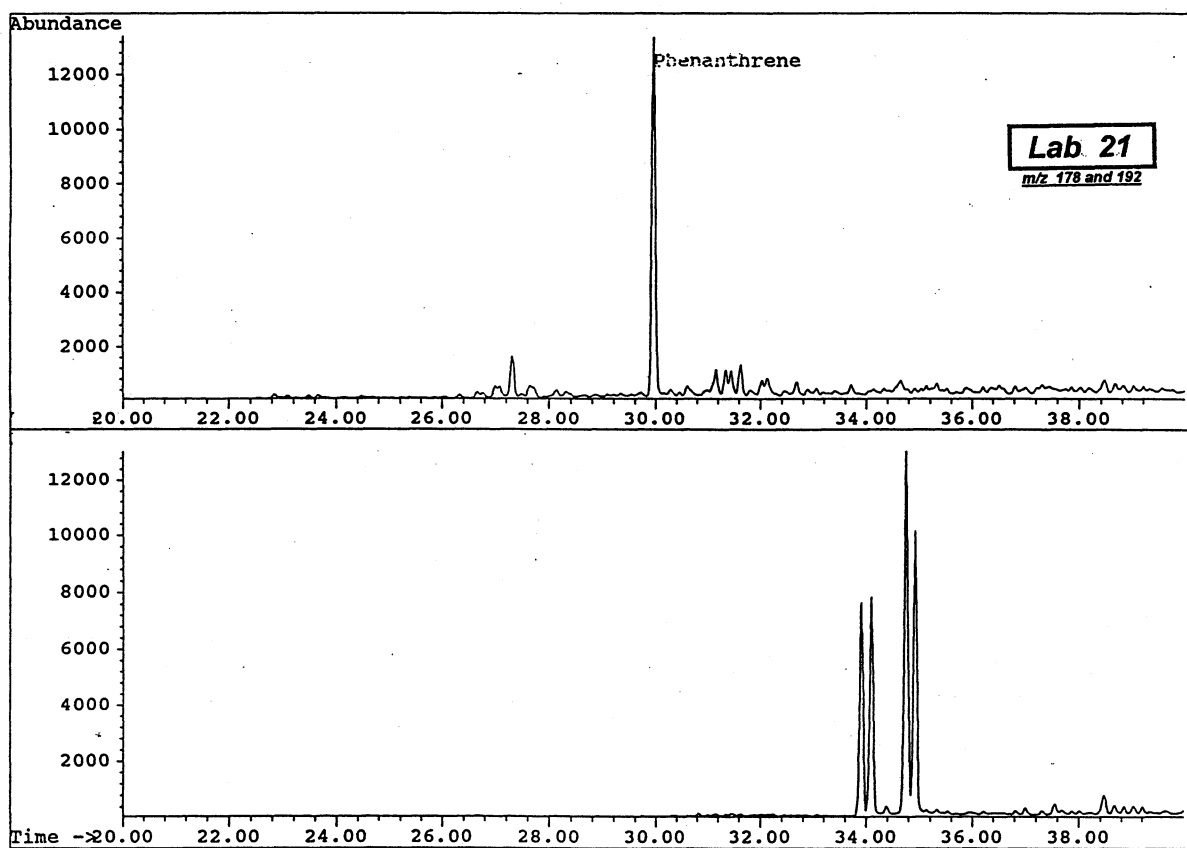
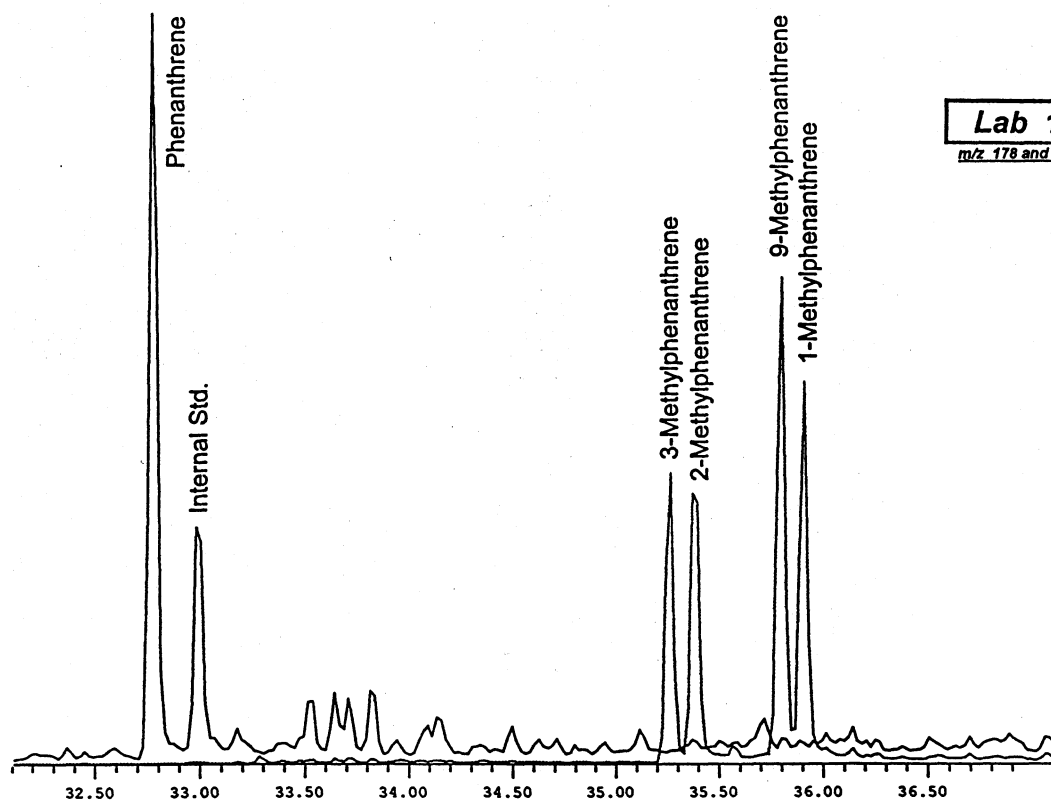


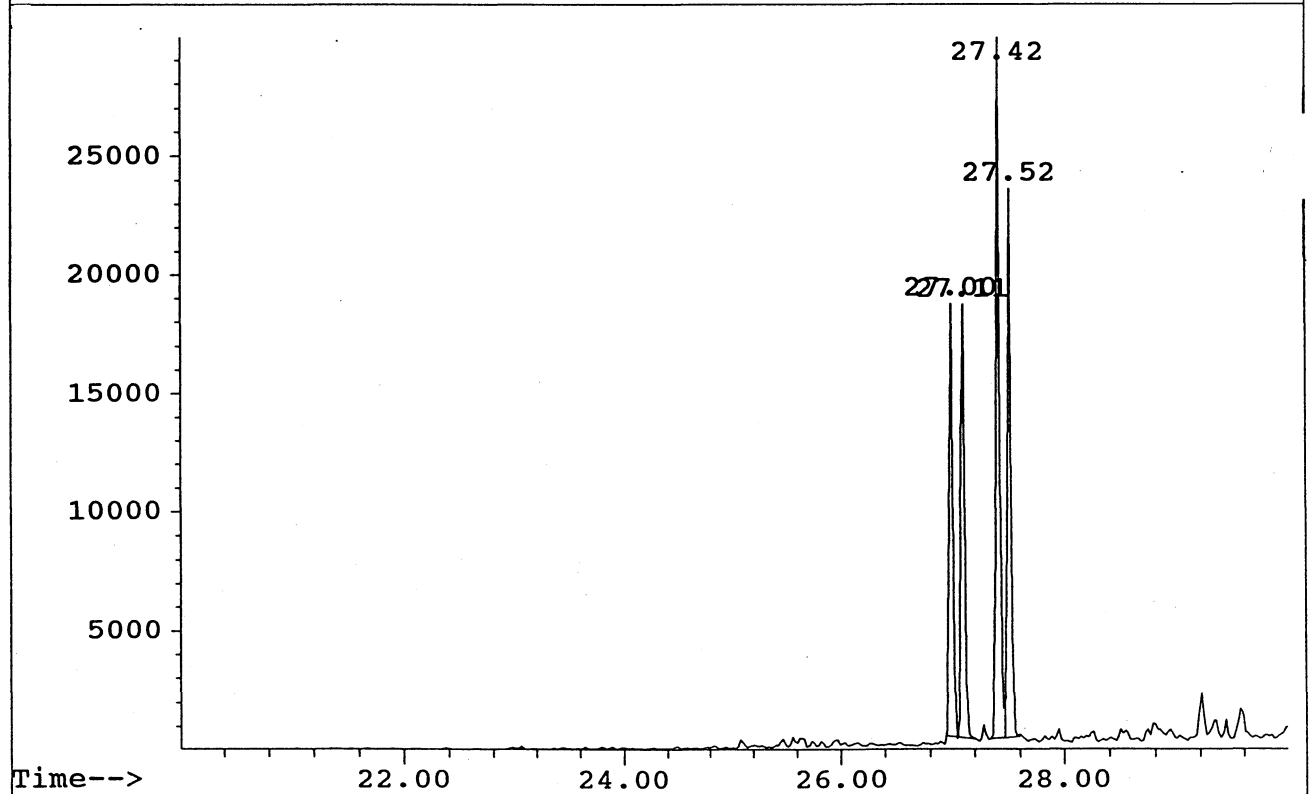
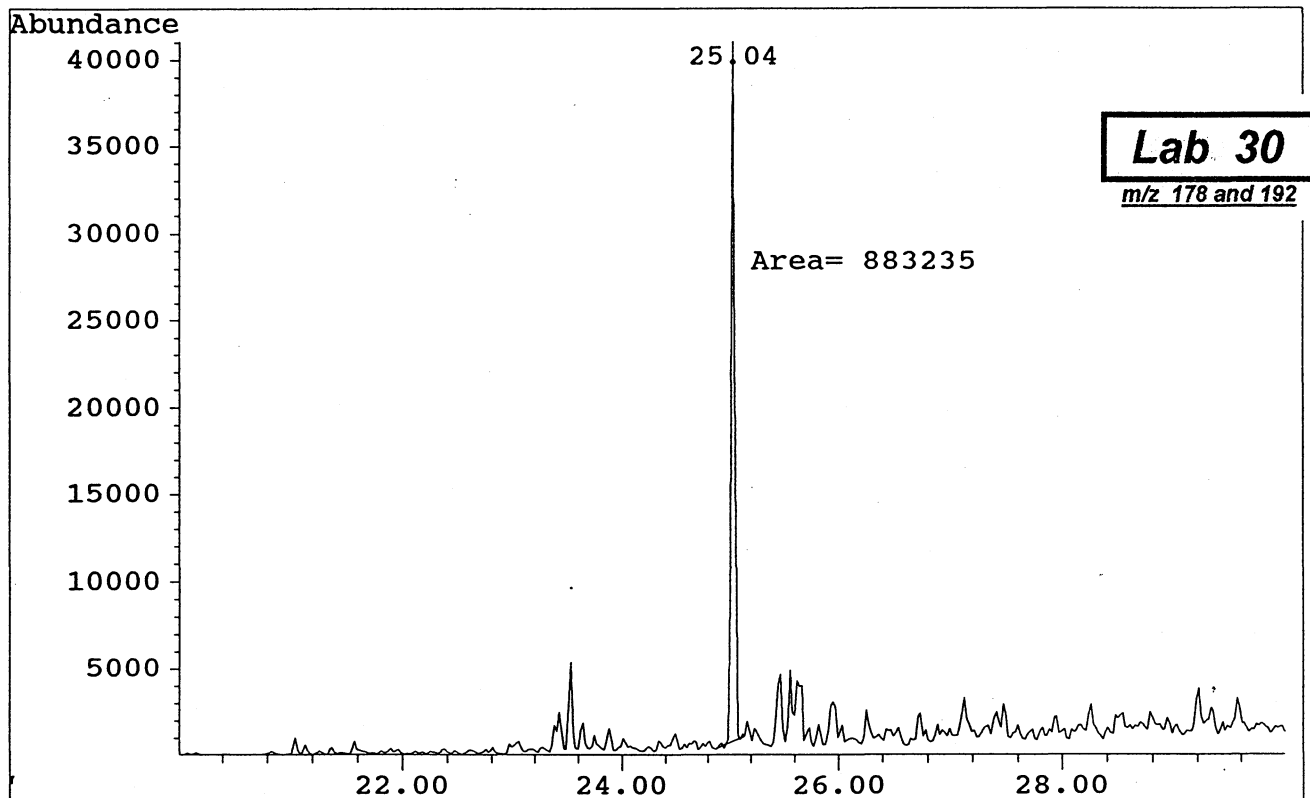


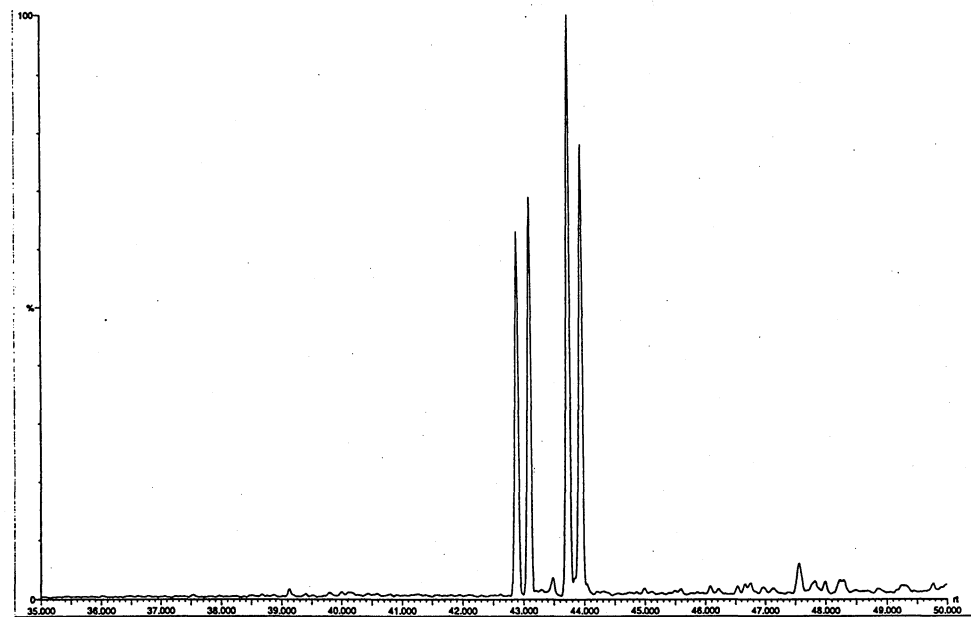
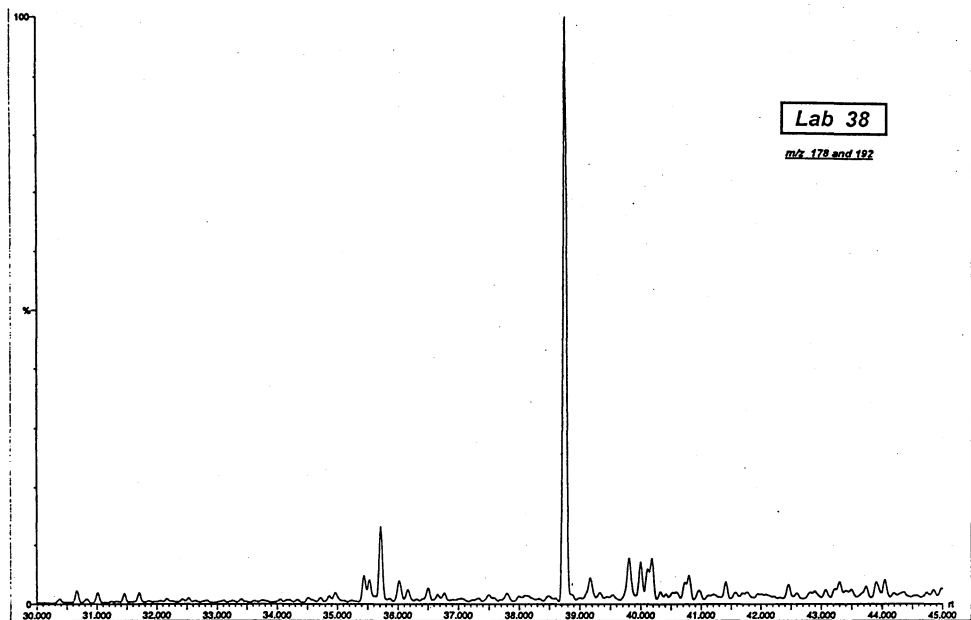
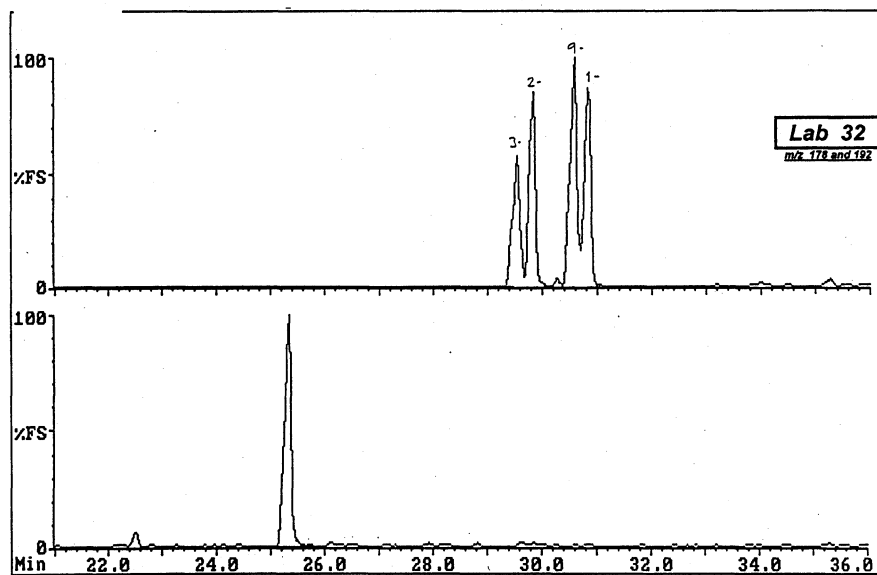
NGS NSO-1

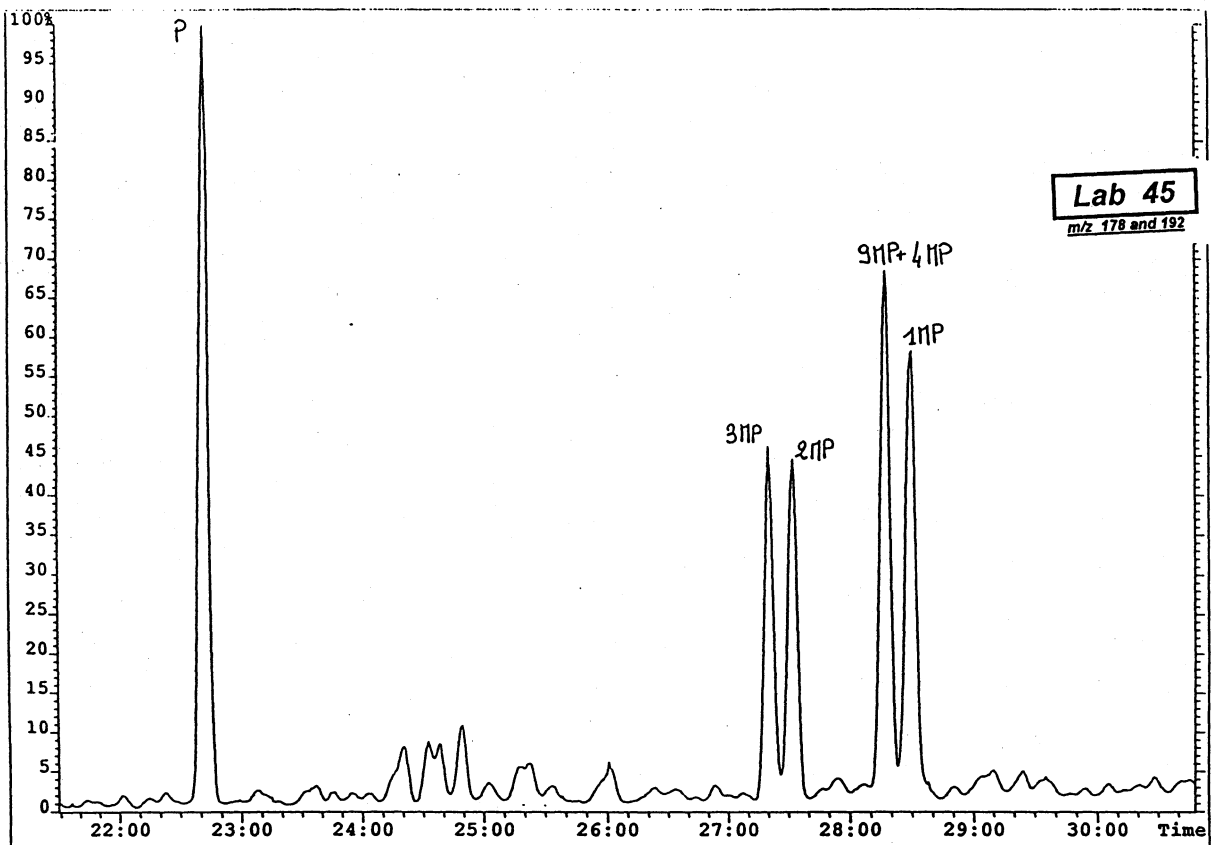
Appendix A3.4b-1

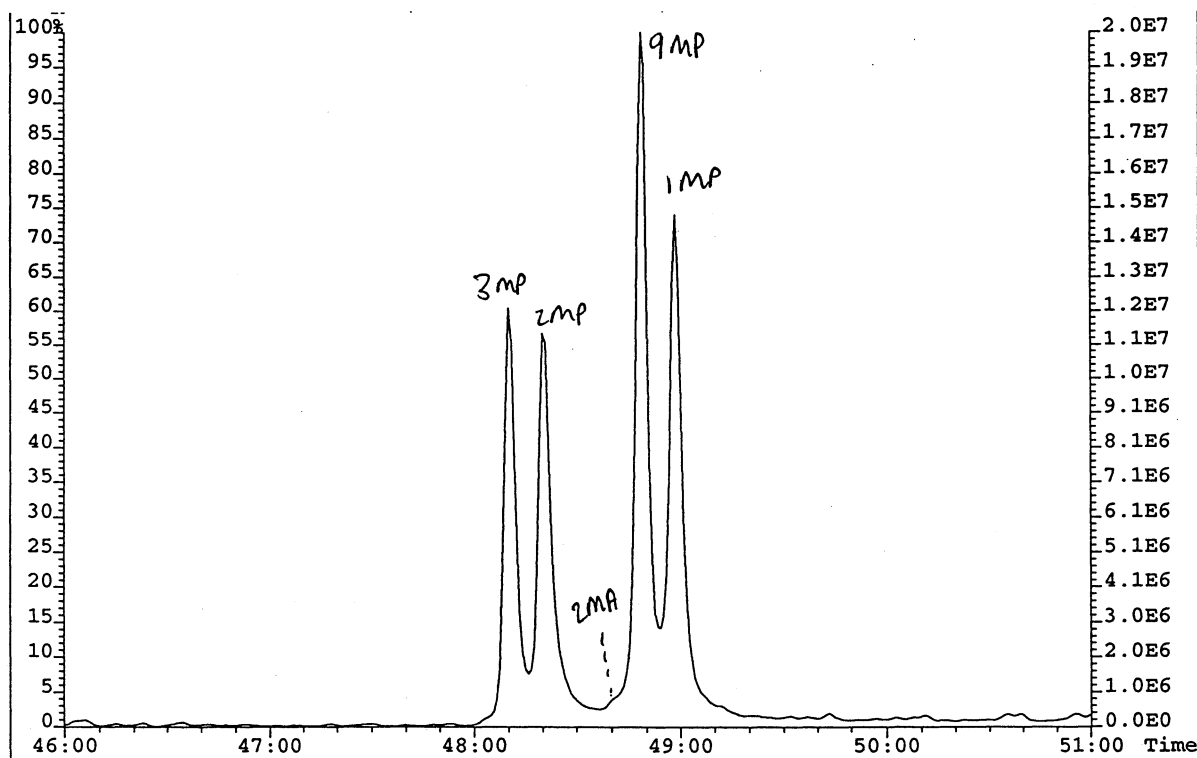
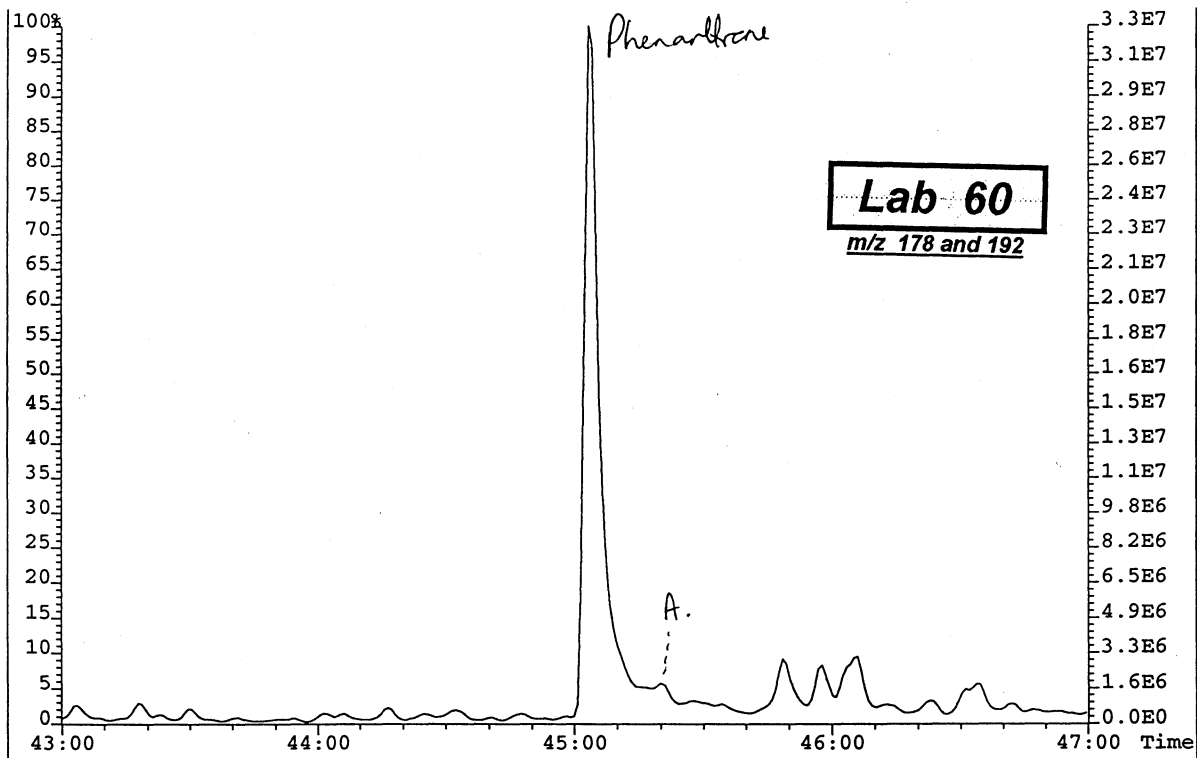
Aromatic fraction m/z 178 and 192 GC-MS fragmentograms

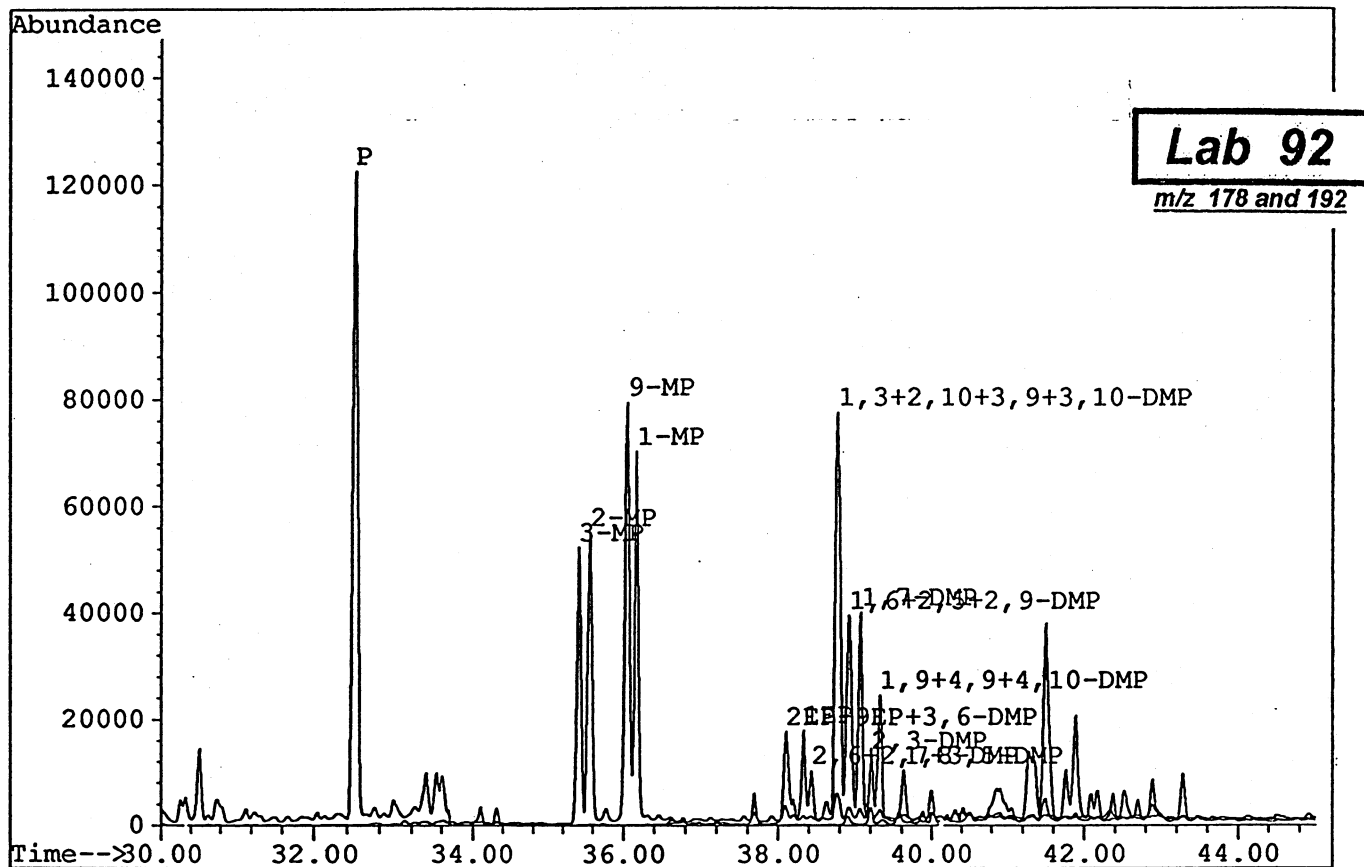








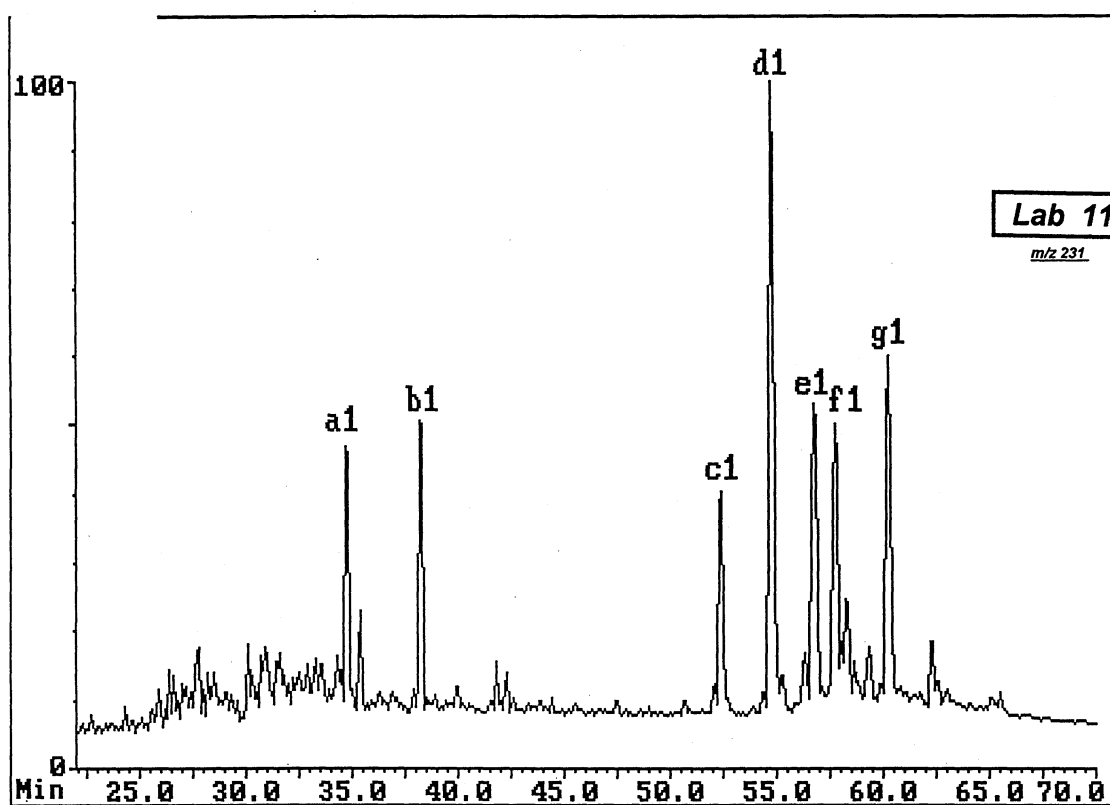
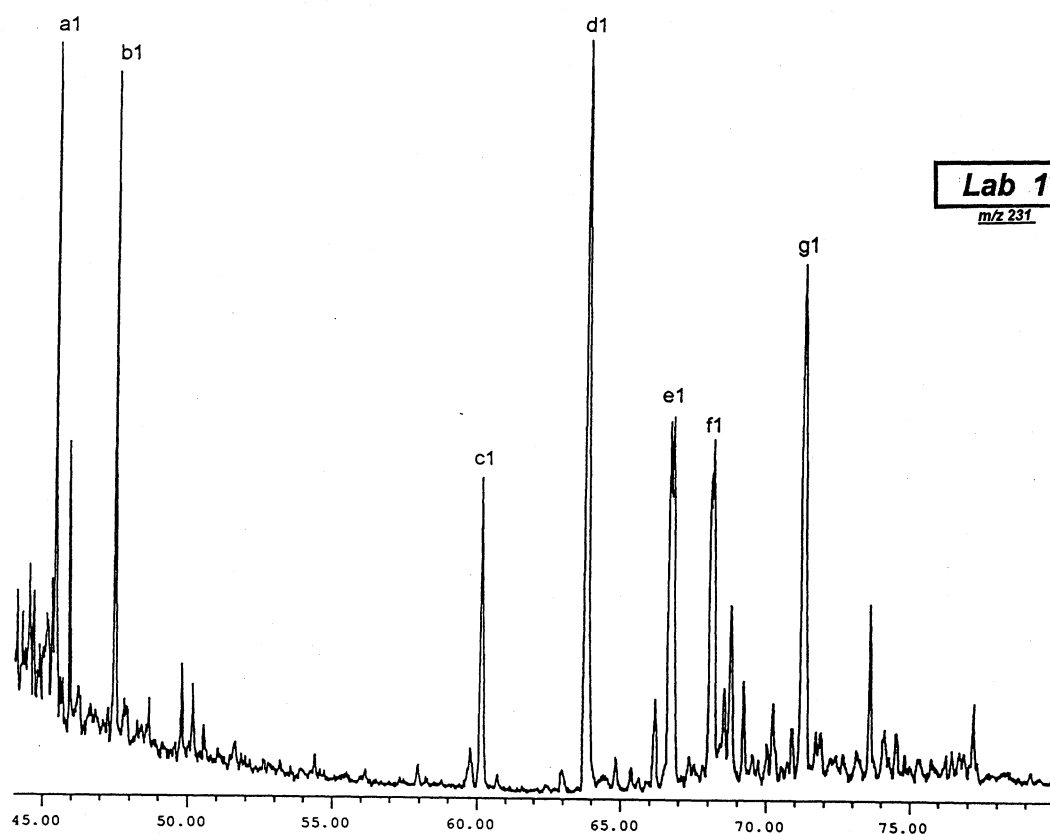


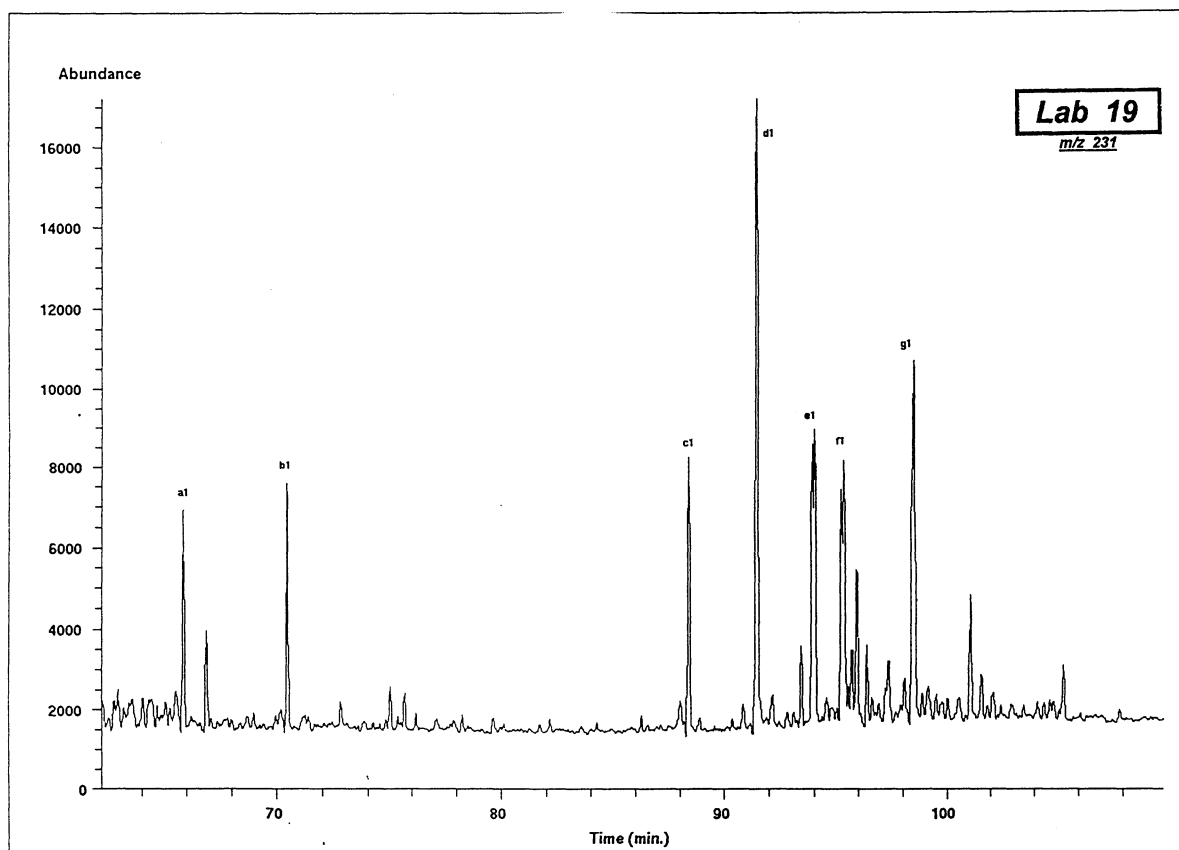
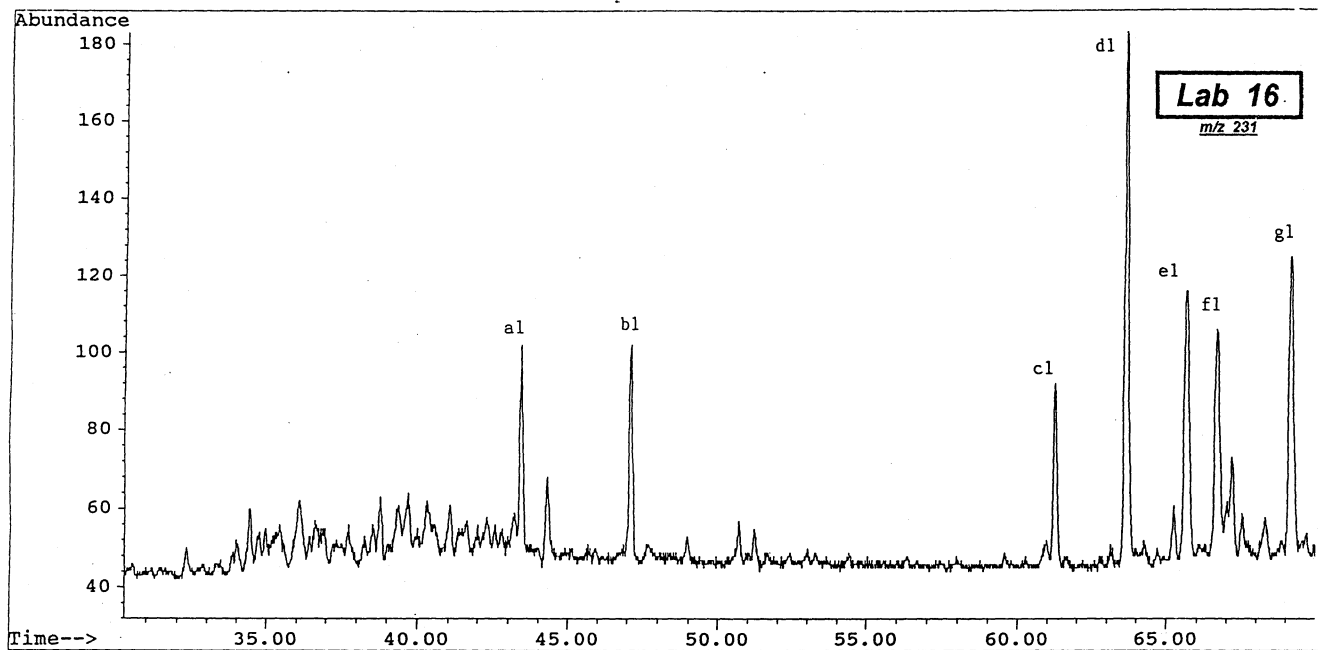


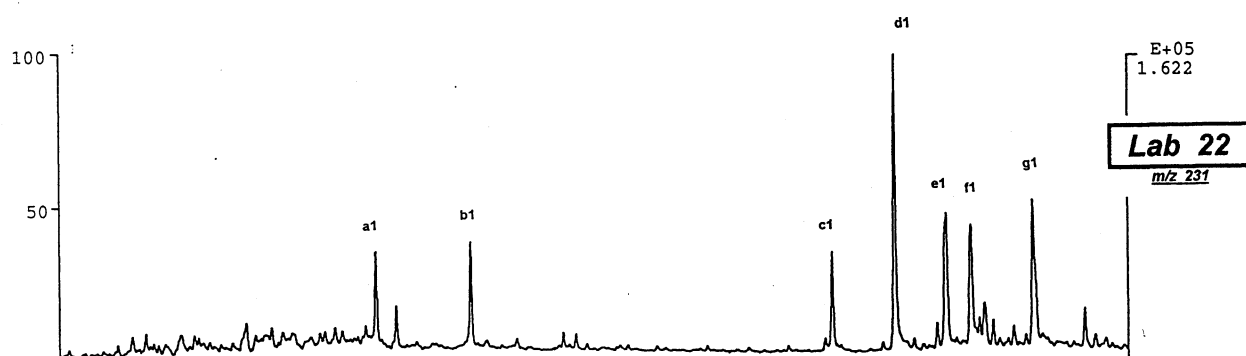
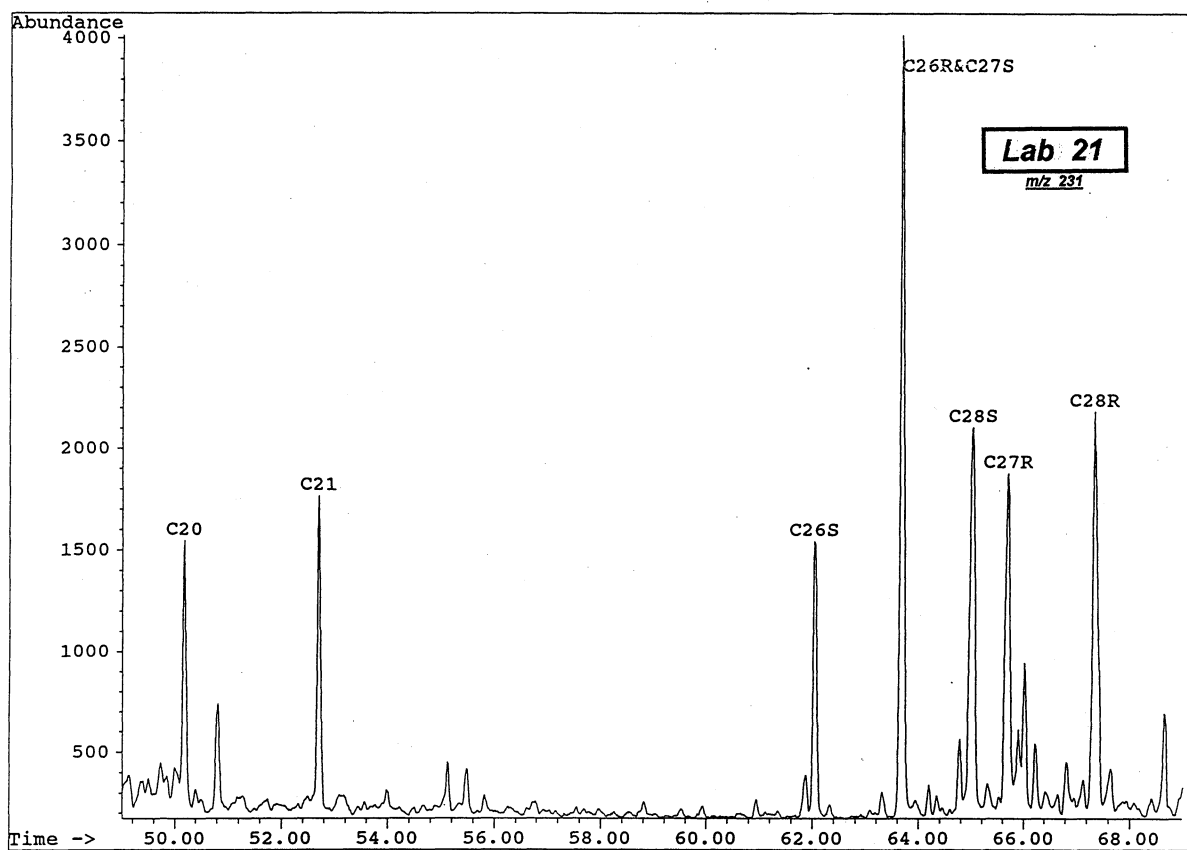
NGS NSO-1

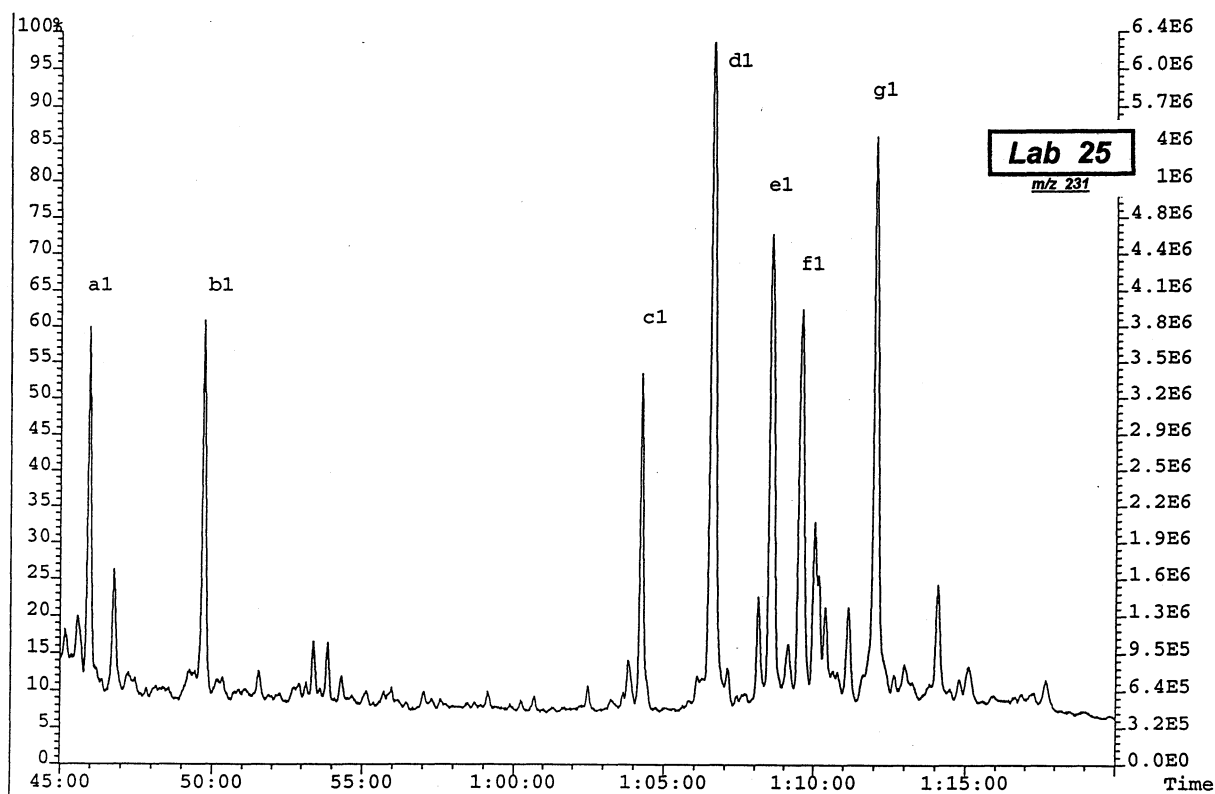
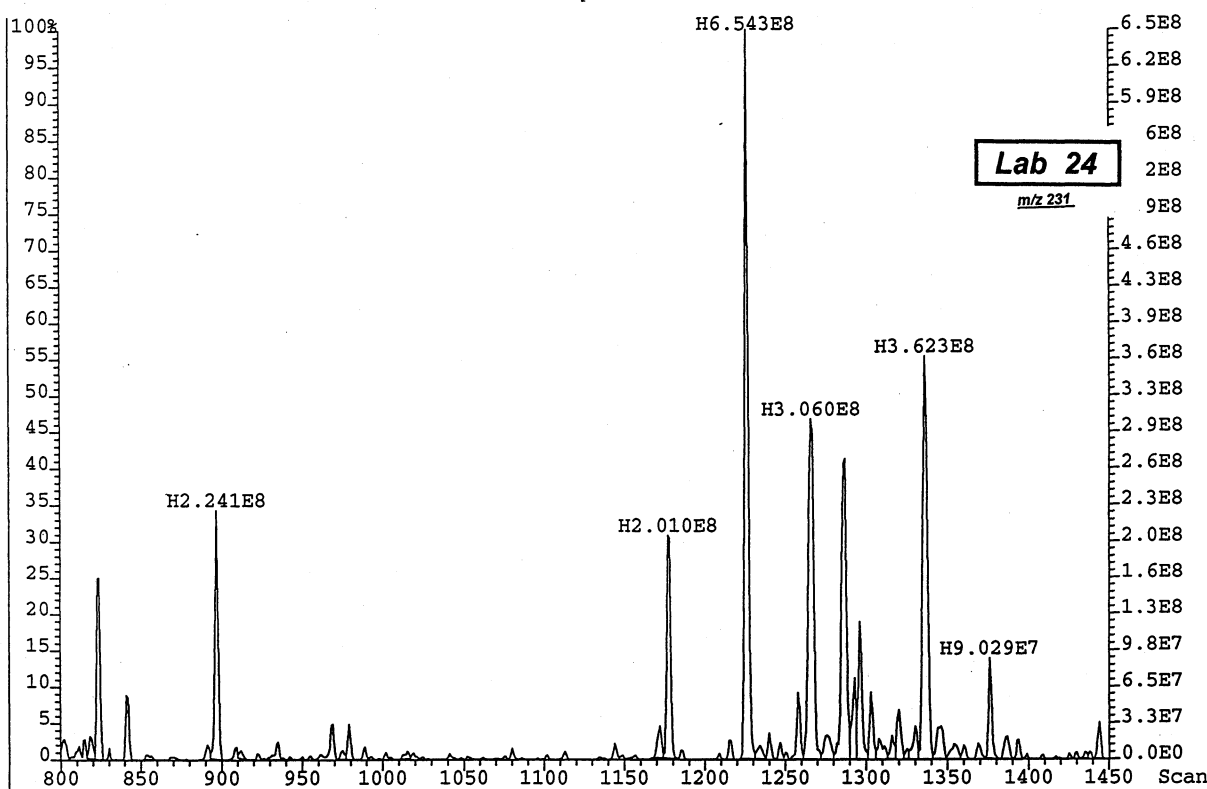
Appendix A3.4b-2

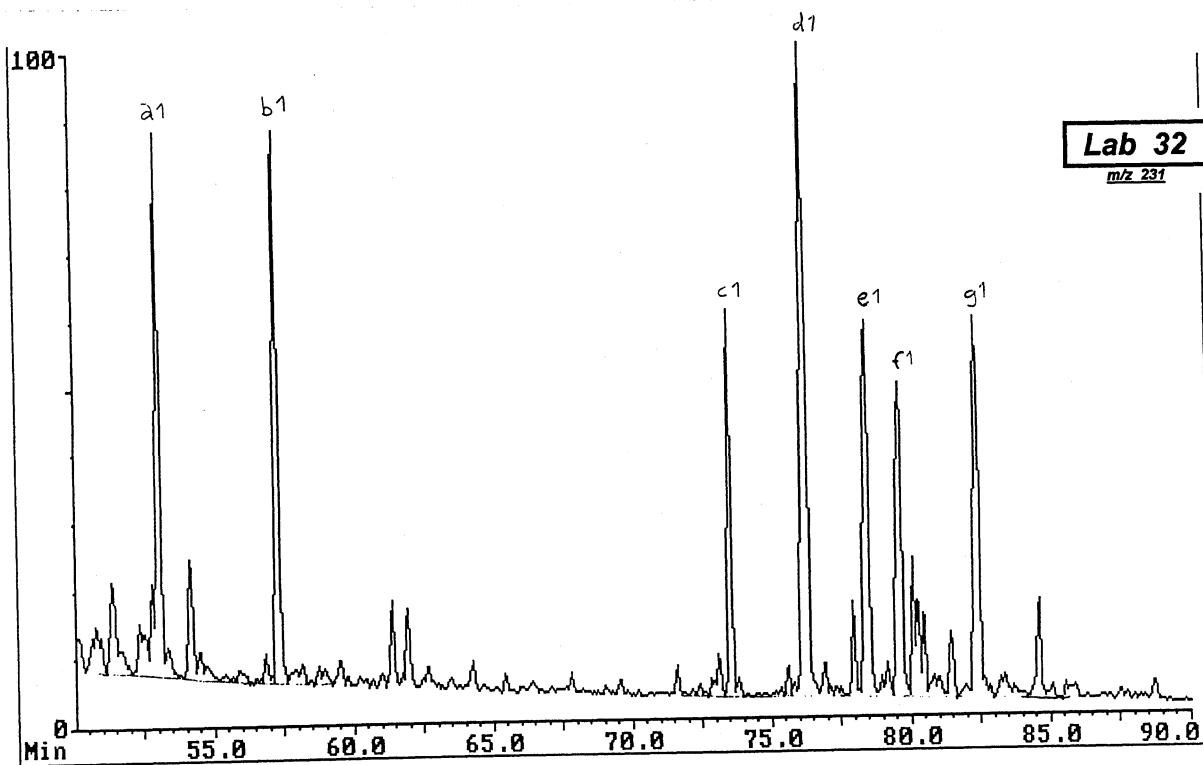
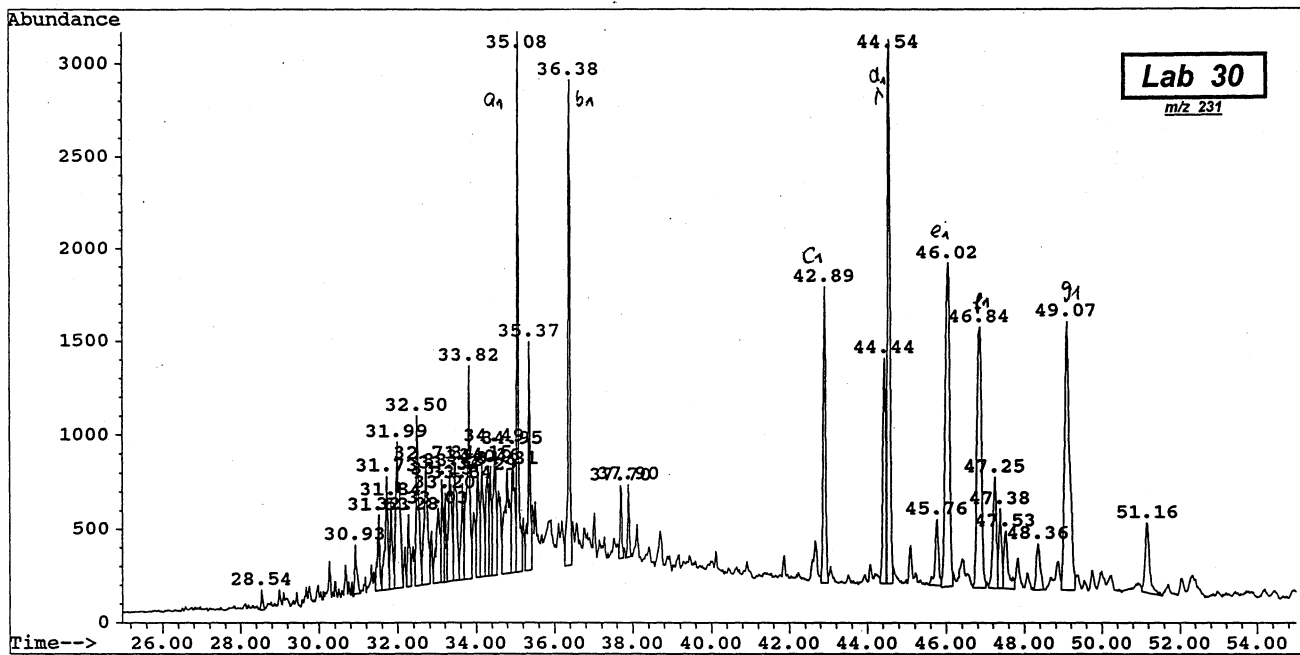
Aromatic fraction m/z 231 GC-MS fragmentograms



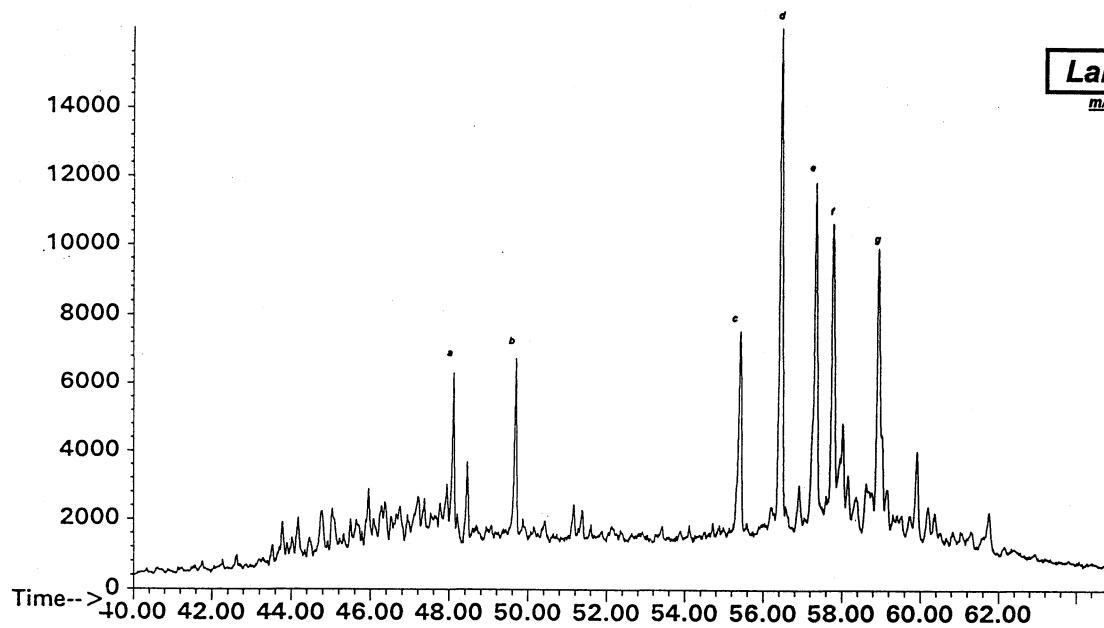






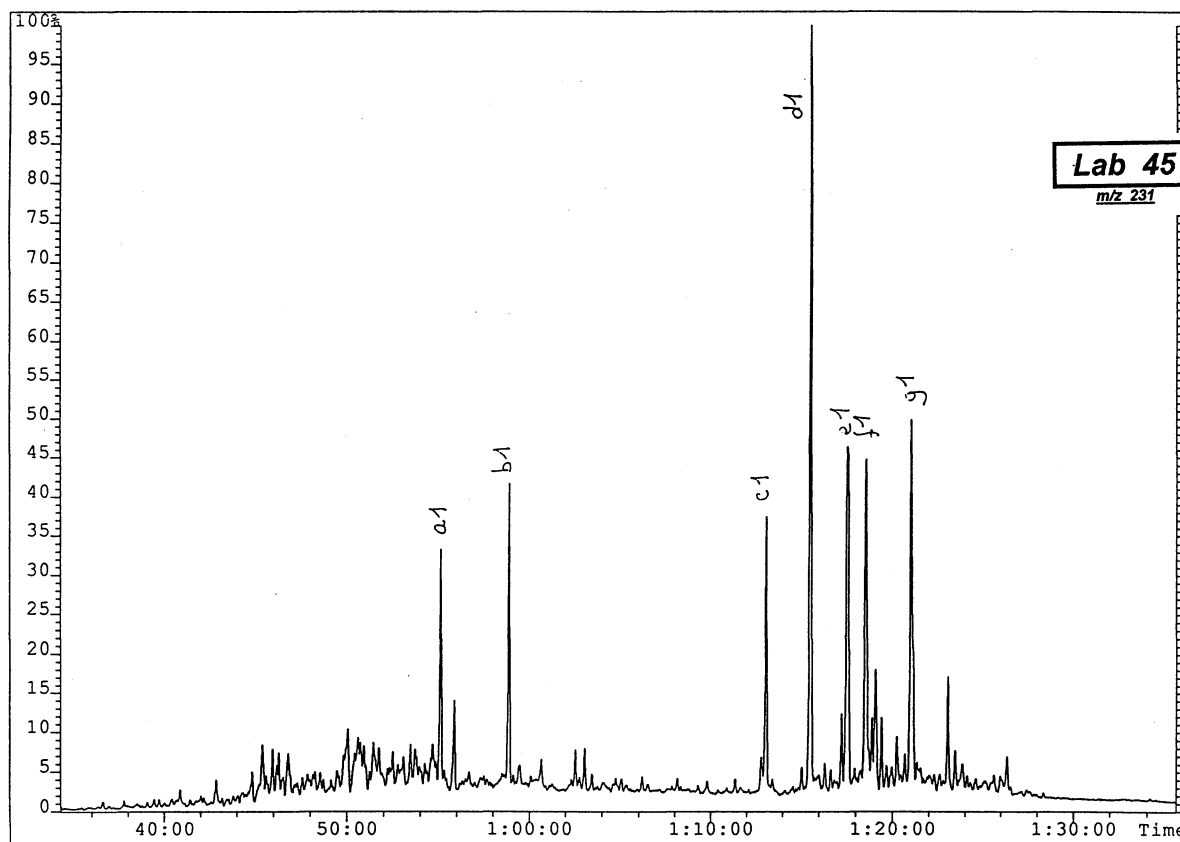


Abundance



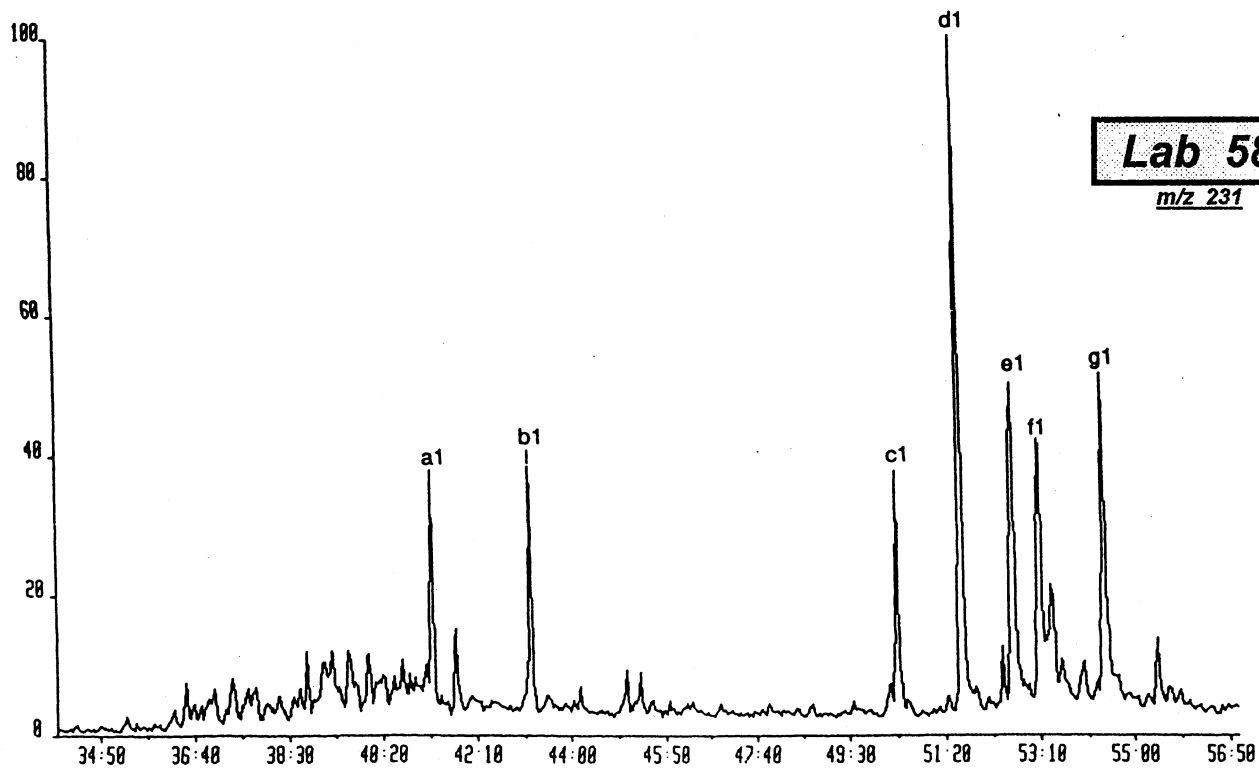
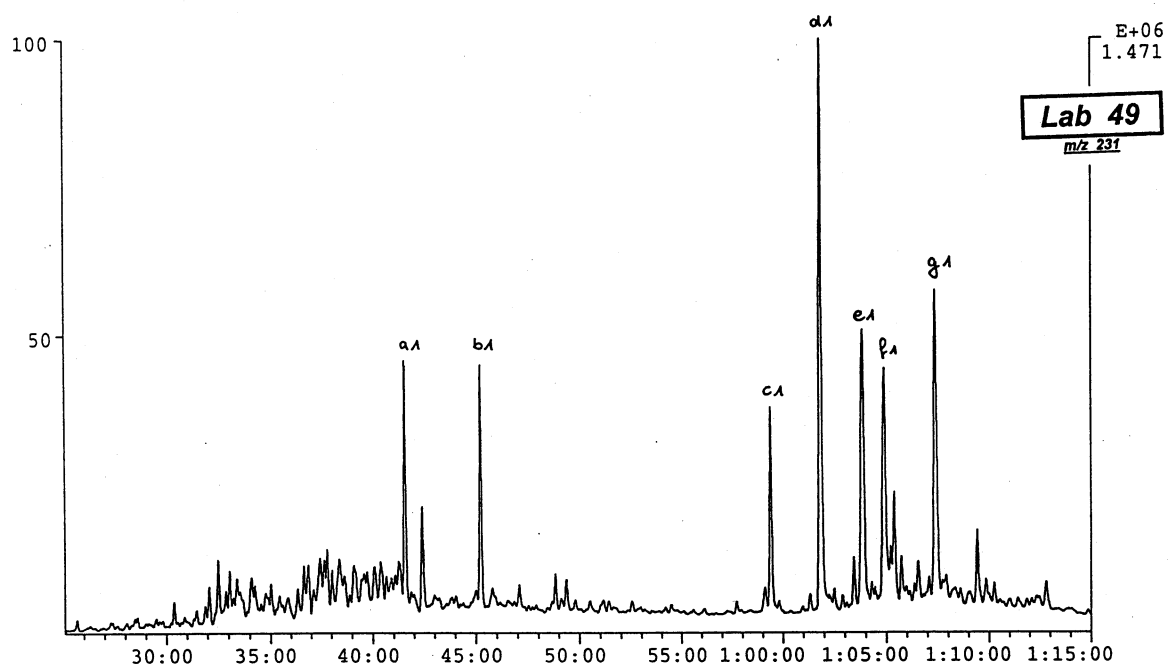
Lab 41

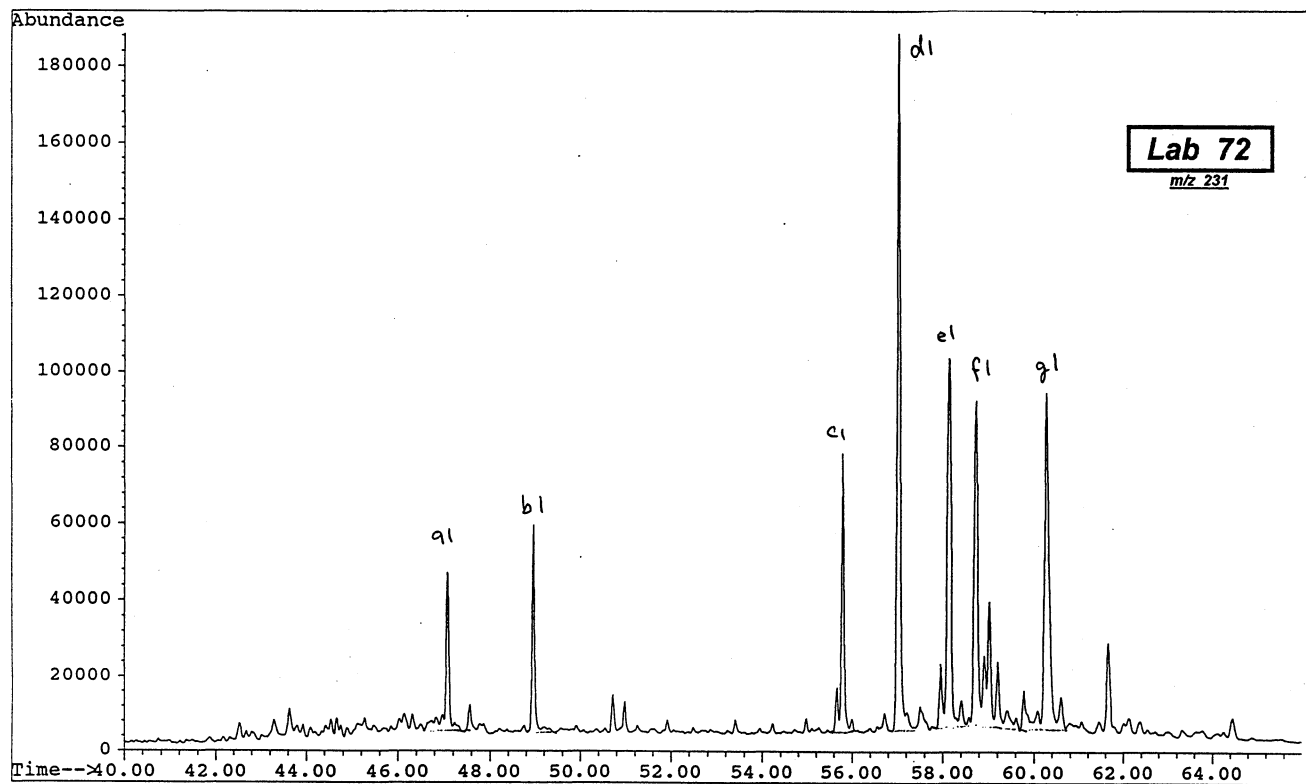
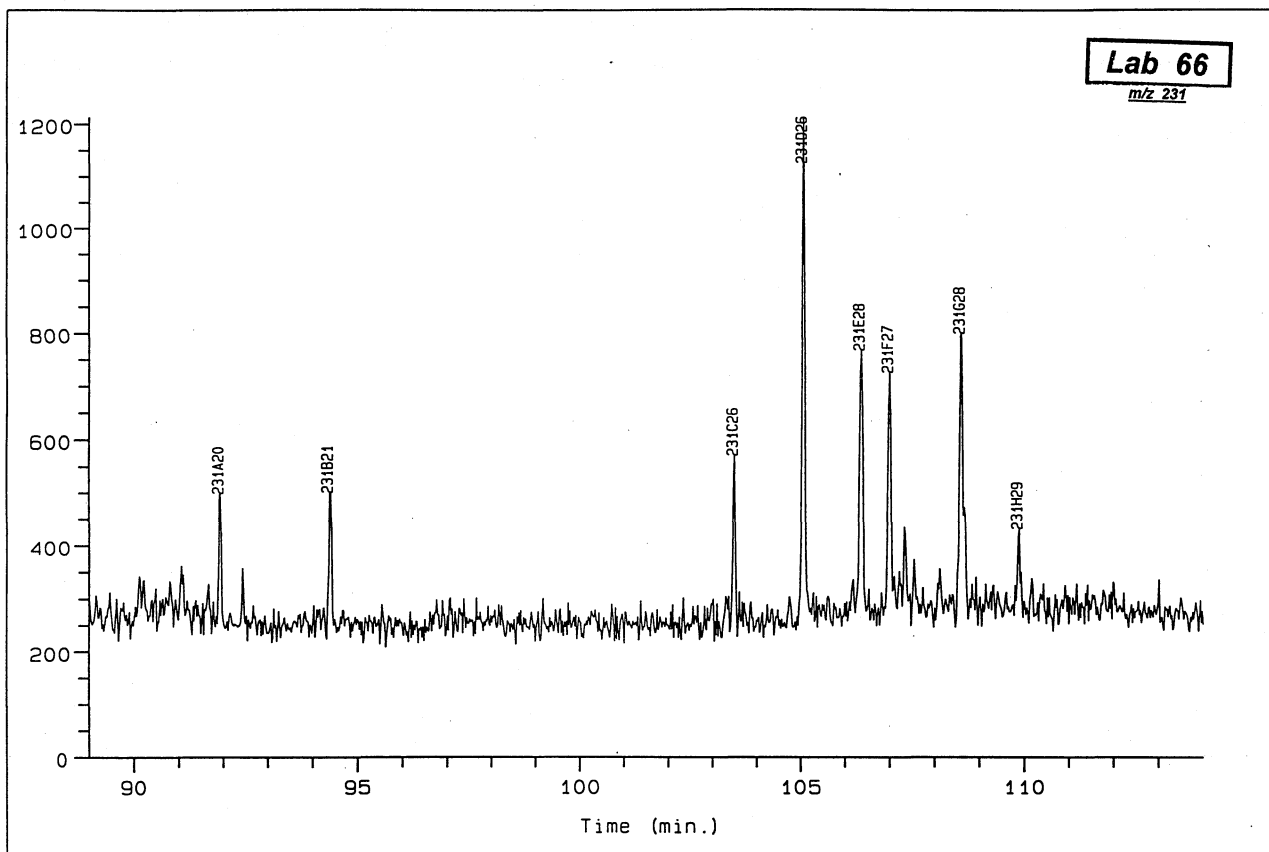
m/z 231

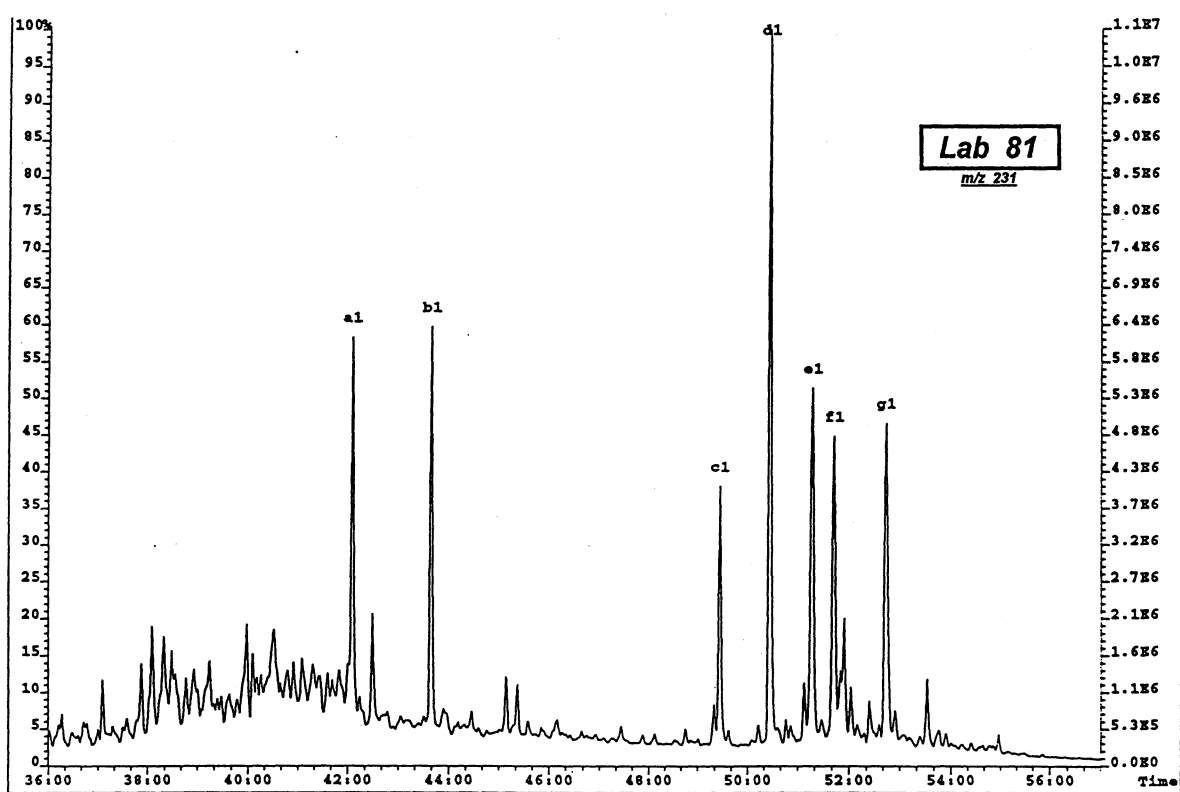
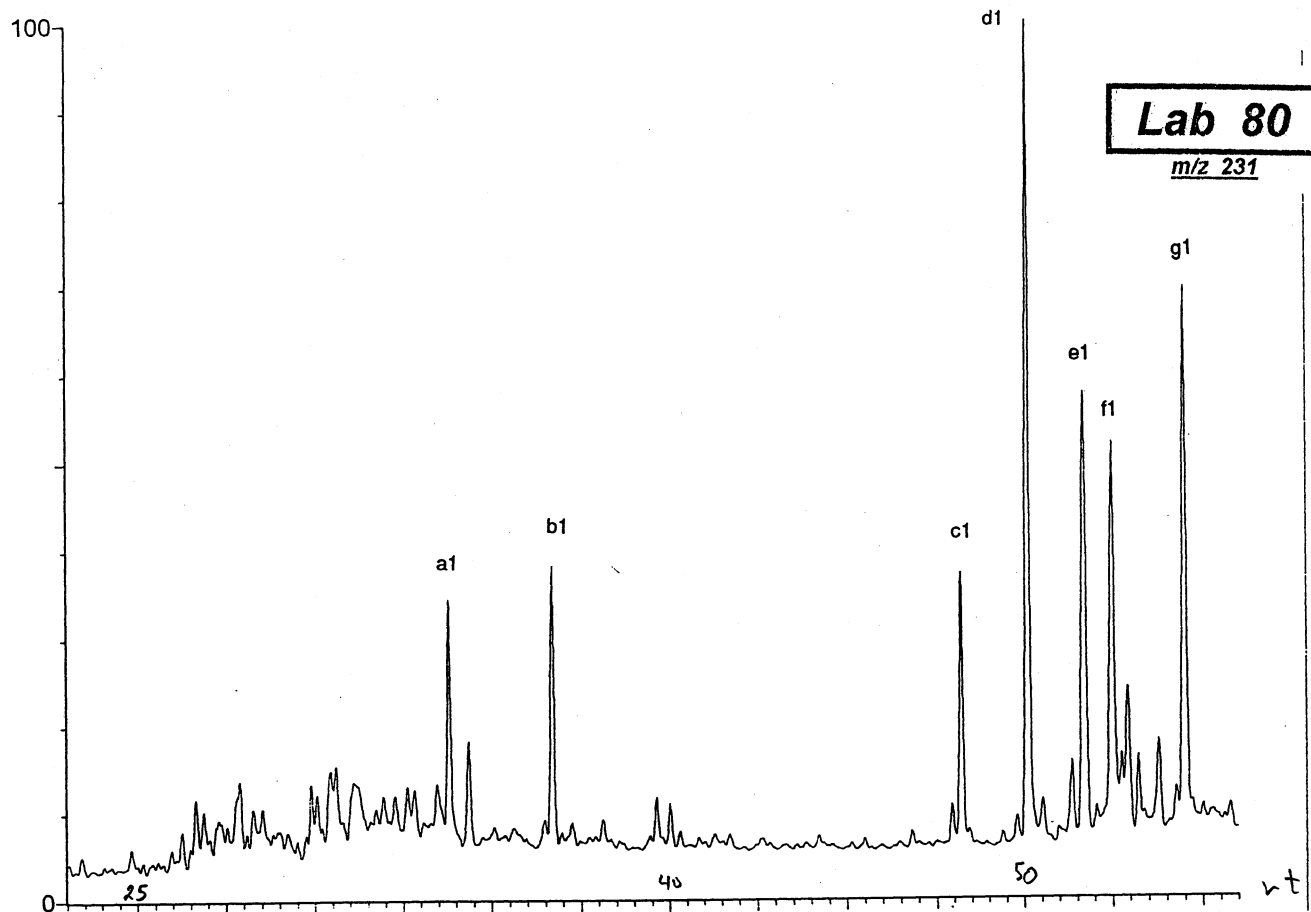


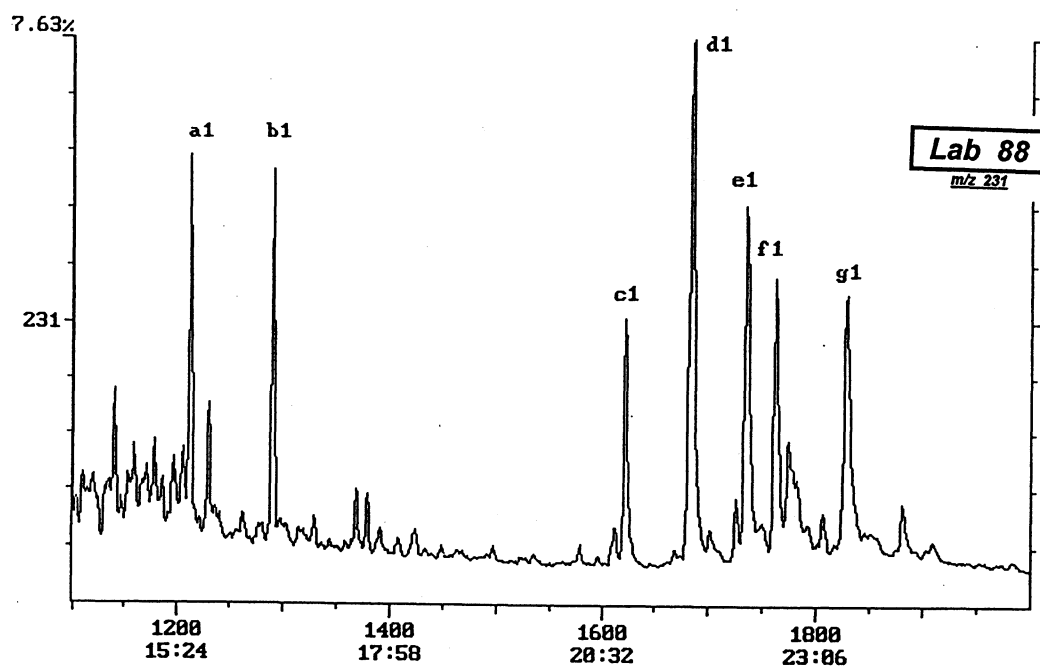
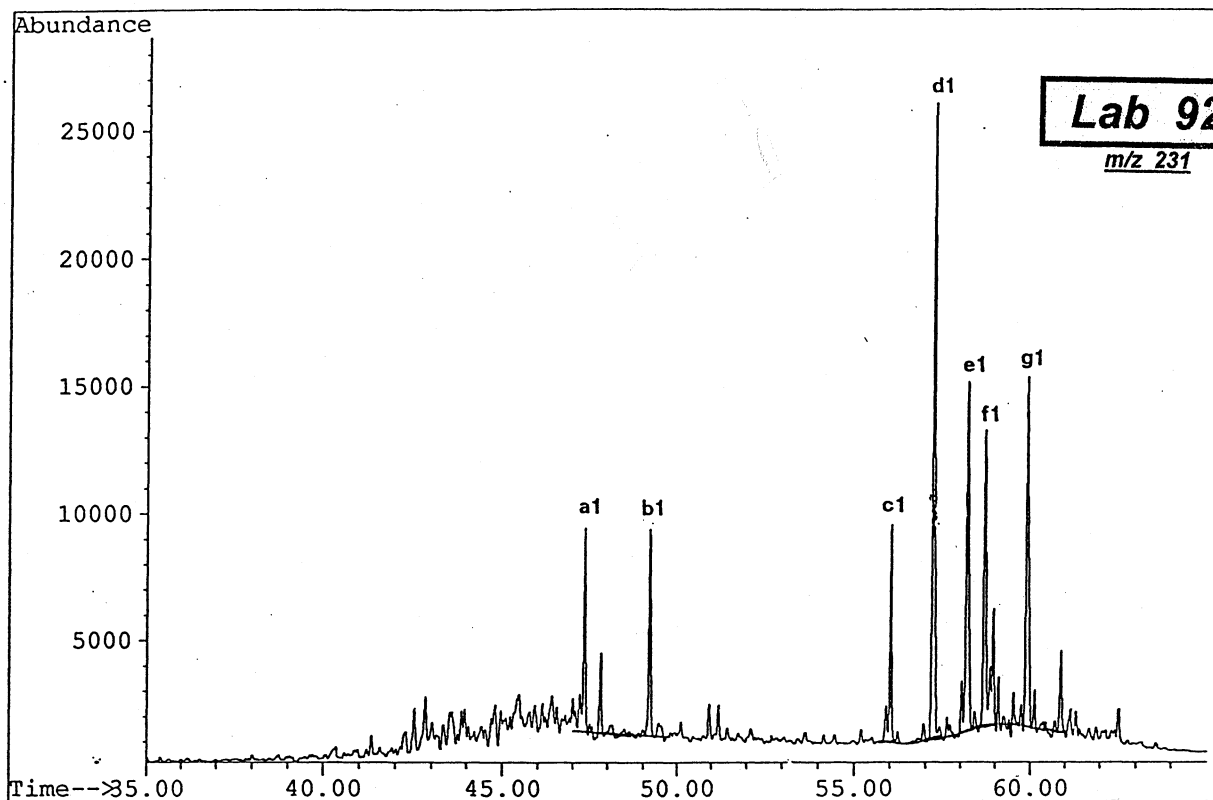
Lab 45

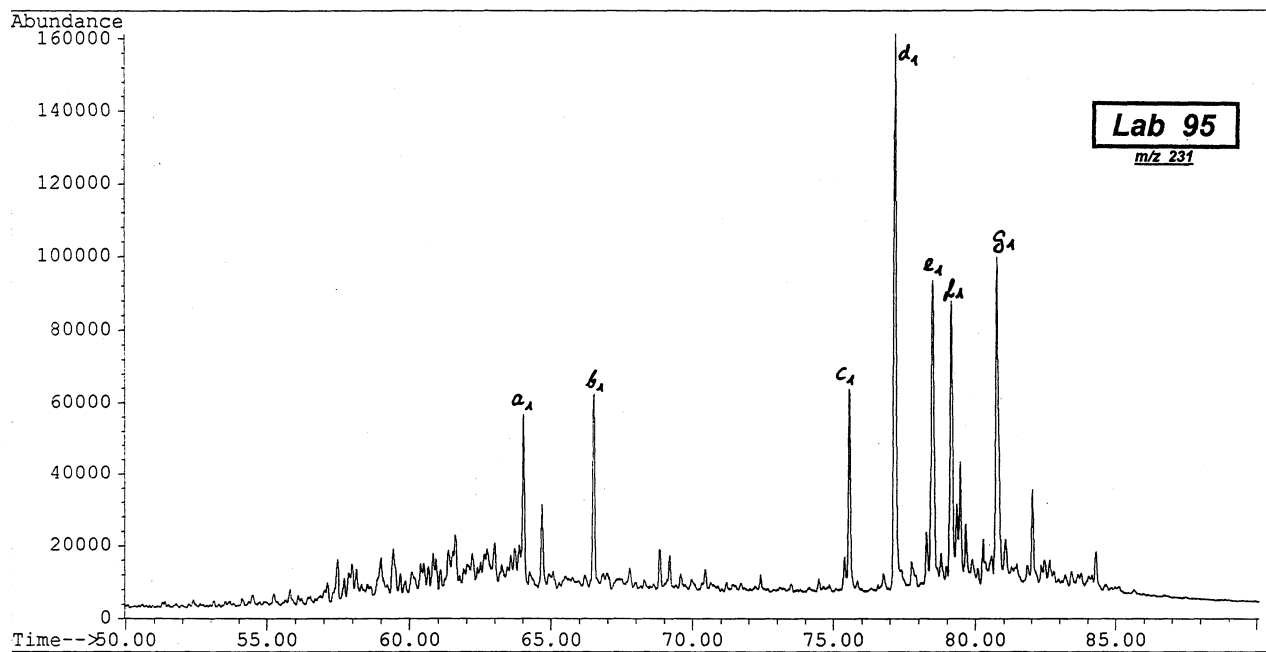
m/z 231







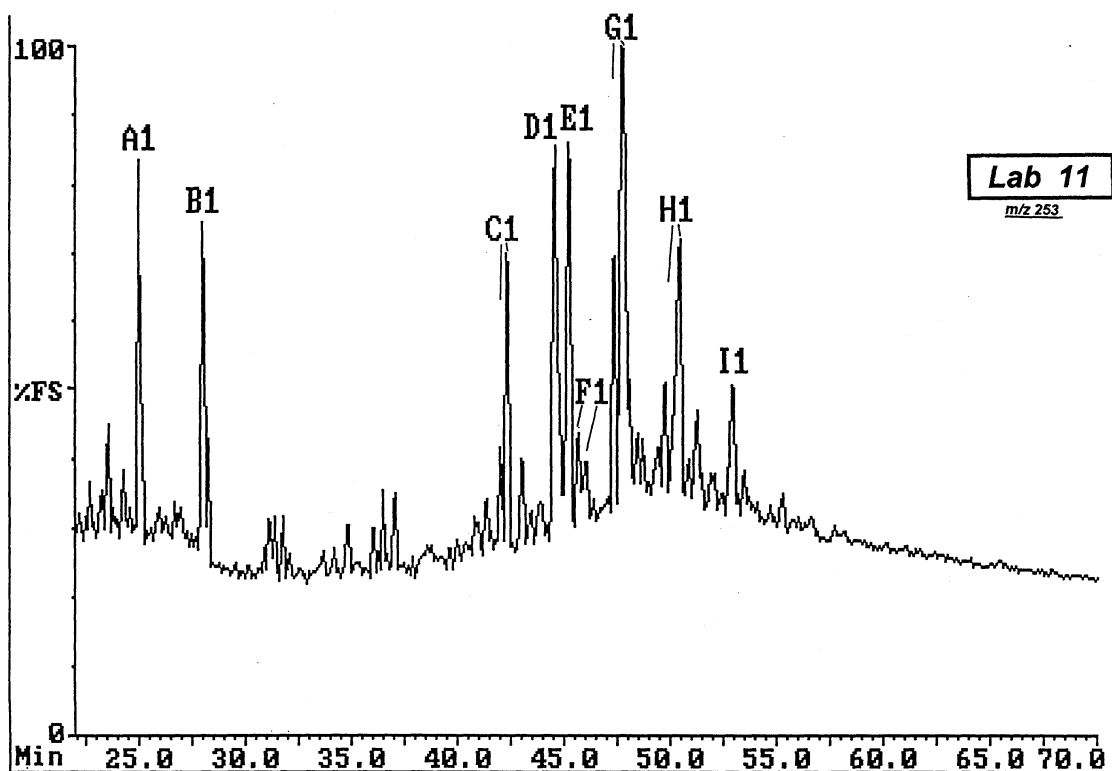
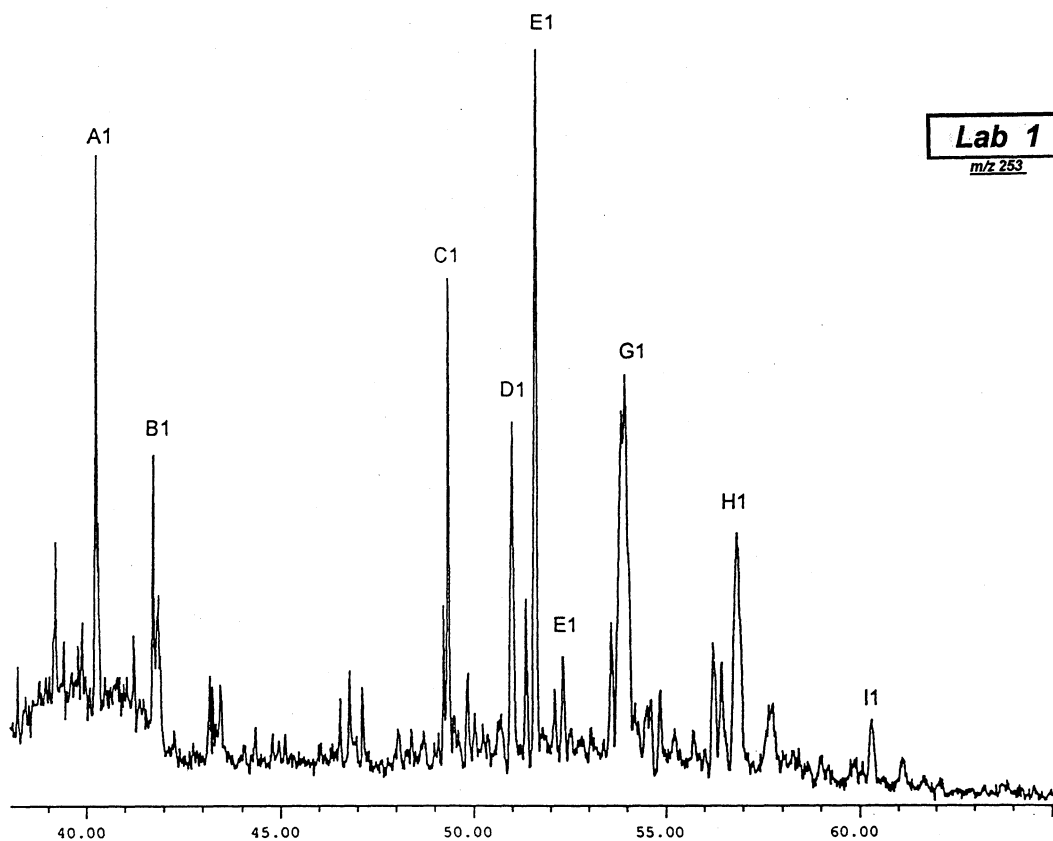


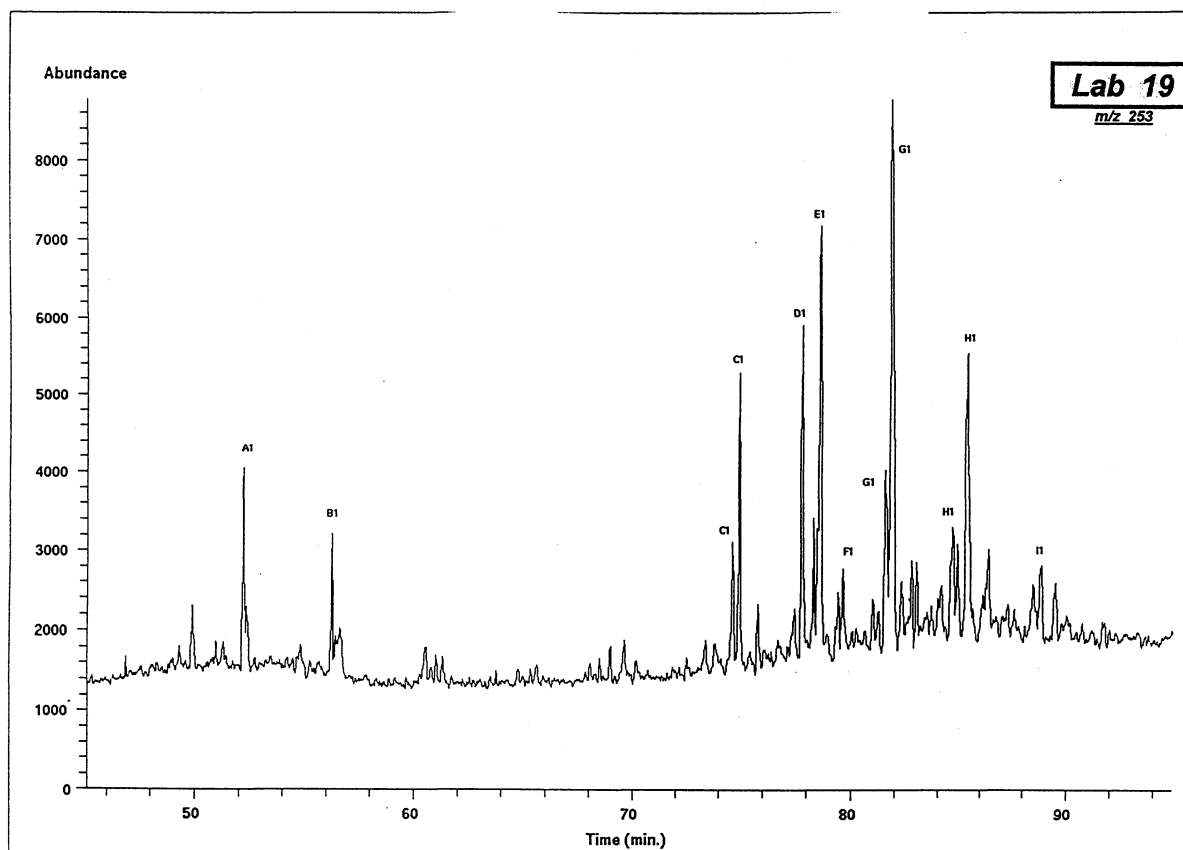
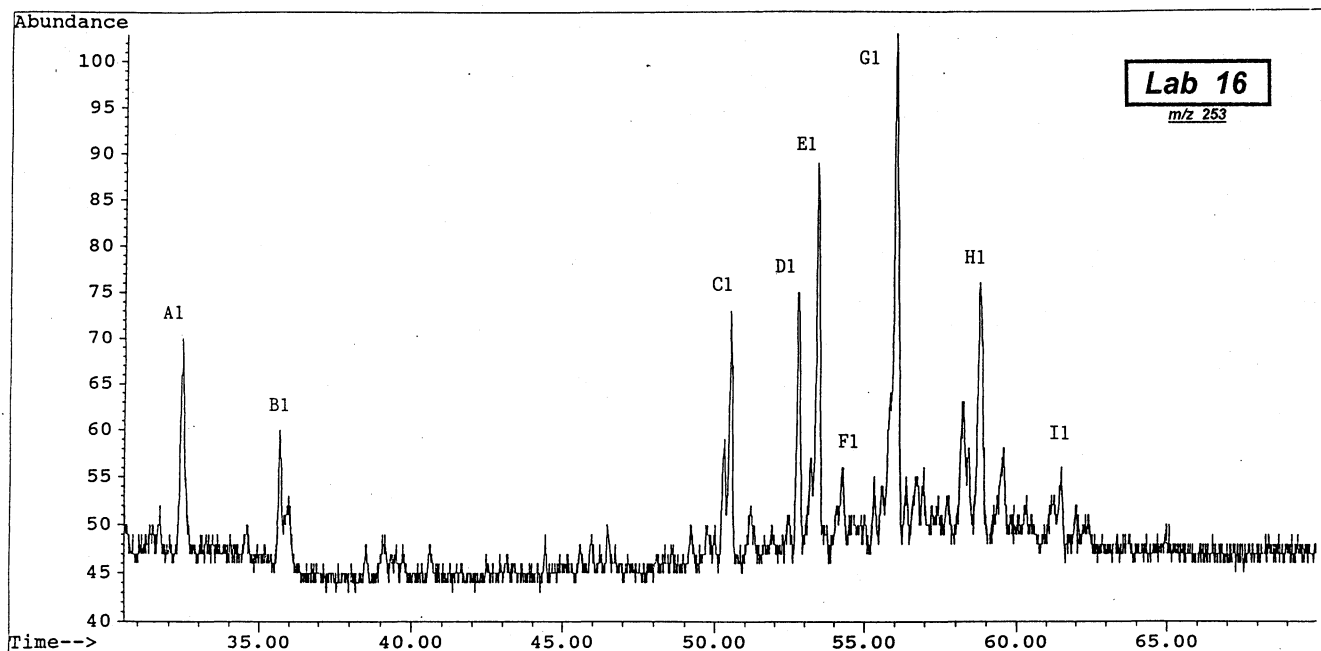


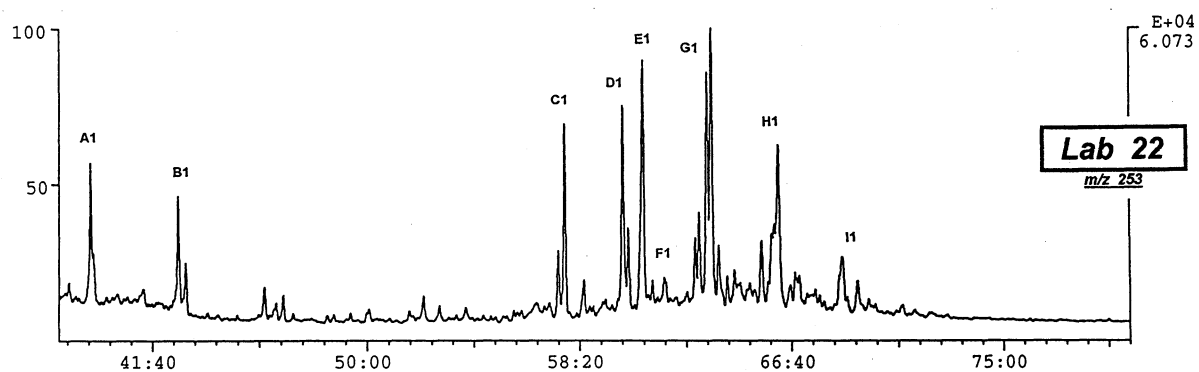
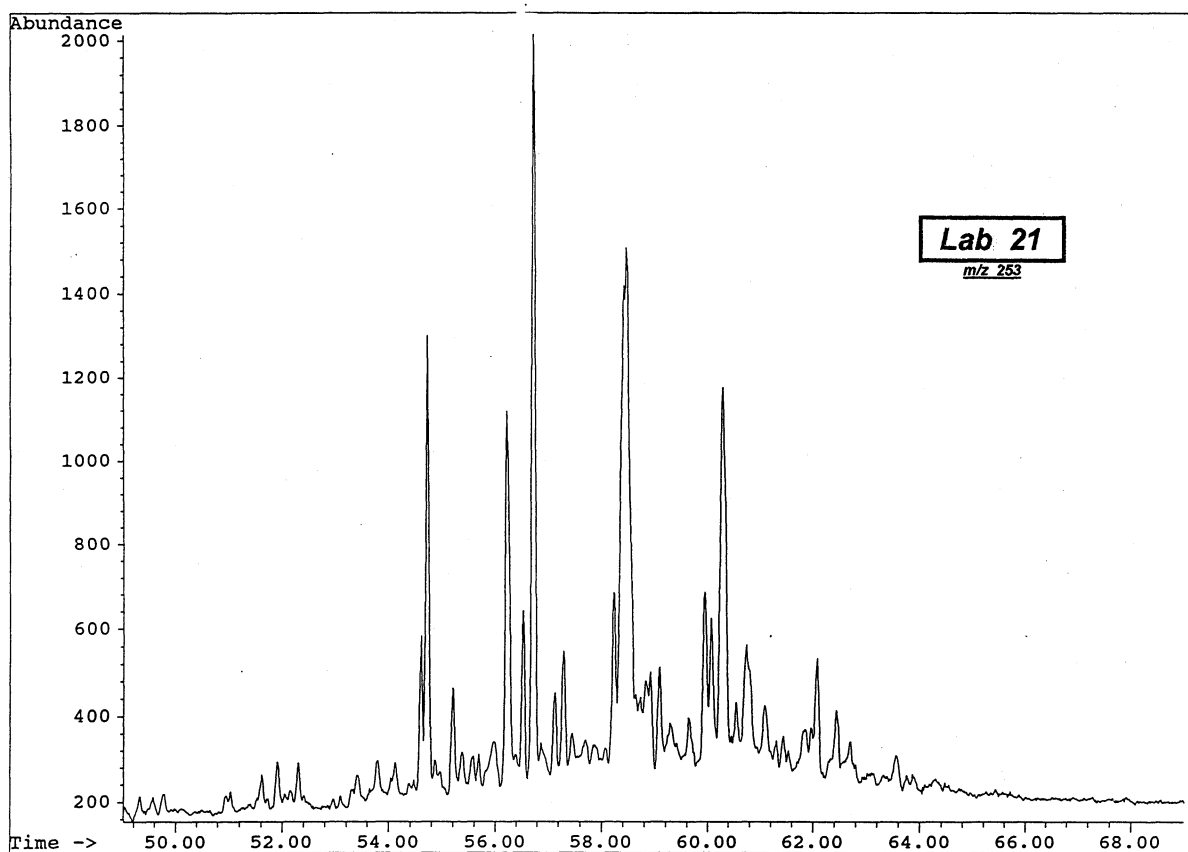
NGS NSO-1

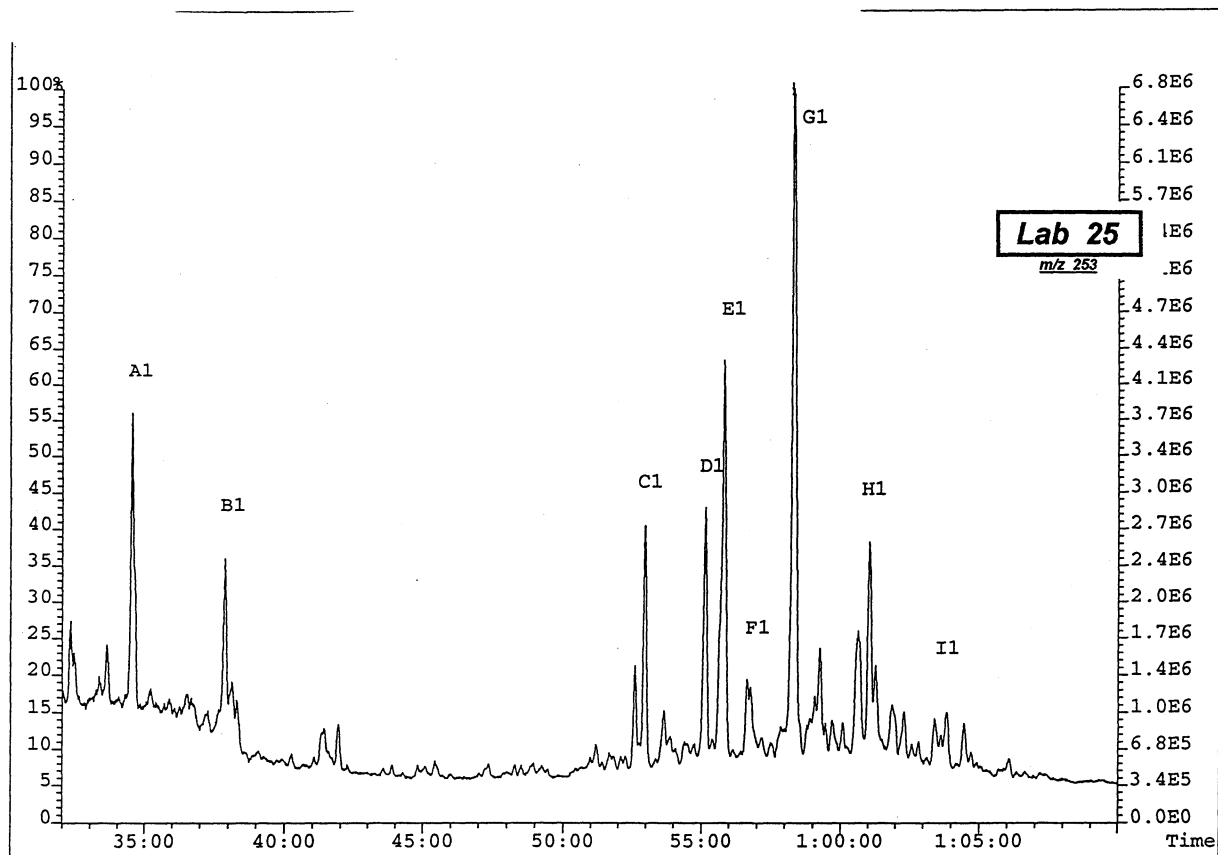
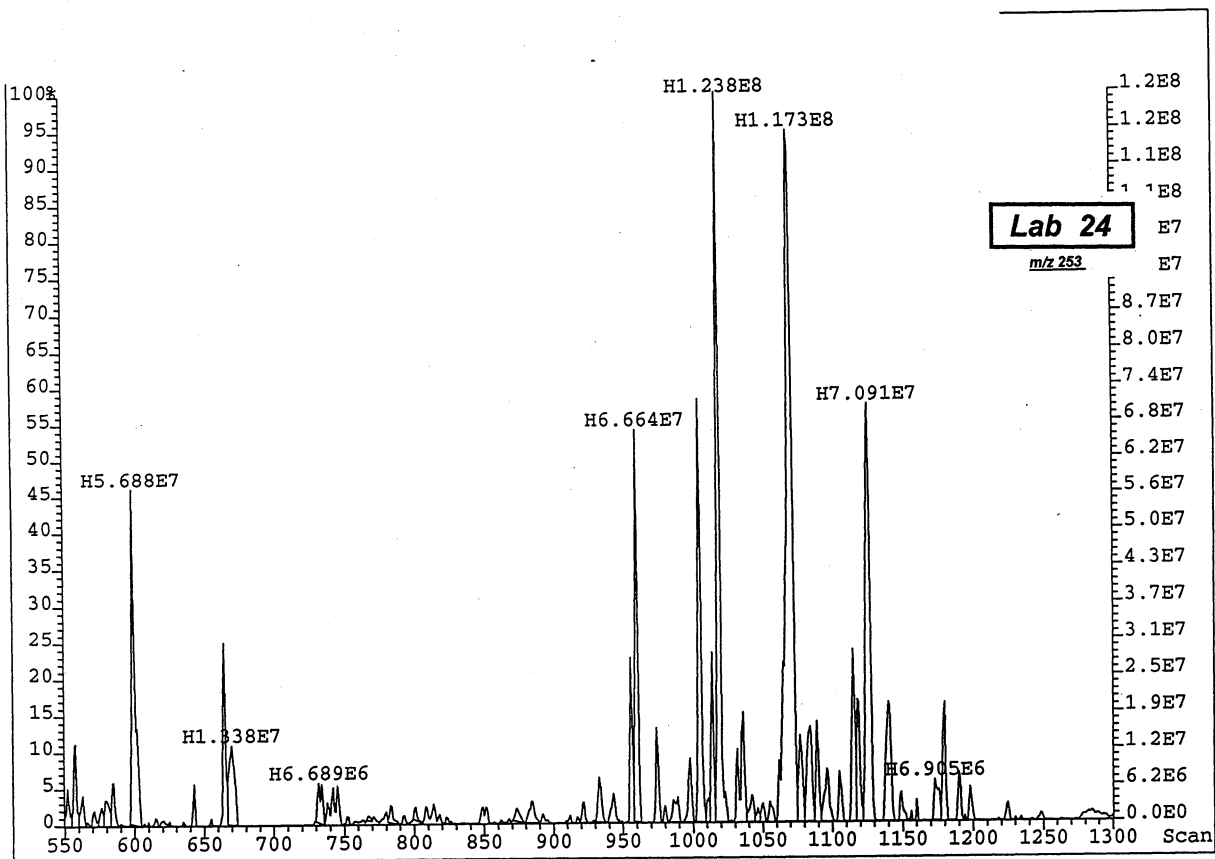
Appendix A3.4b-3

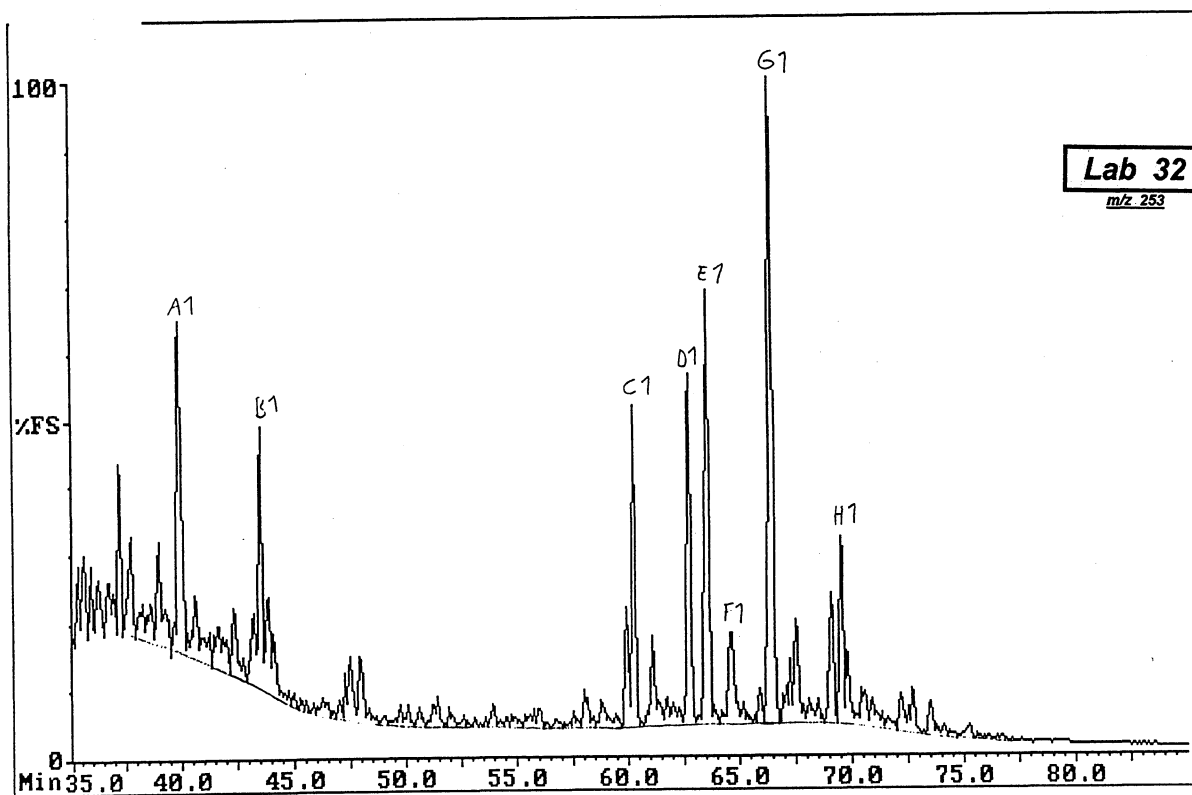
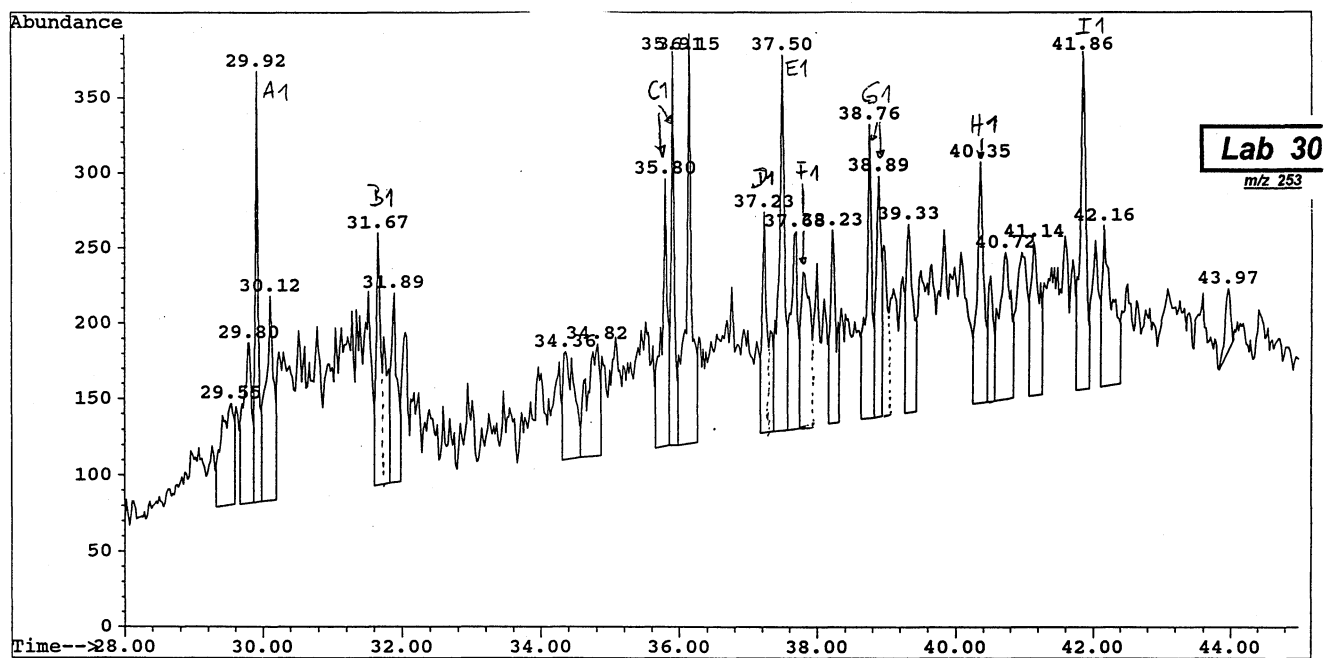
Aromatic fraction m/z 253 GC-MS fragmentograms

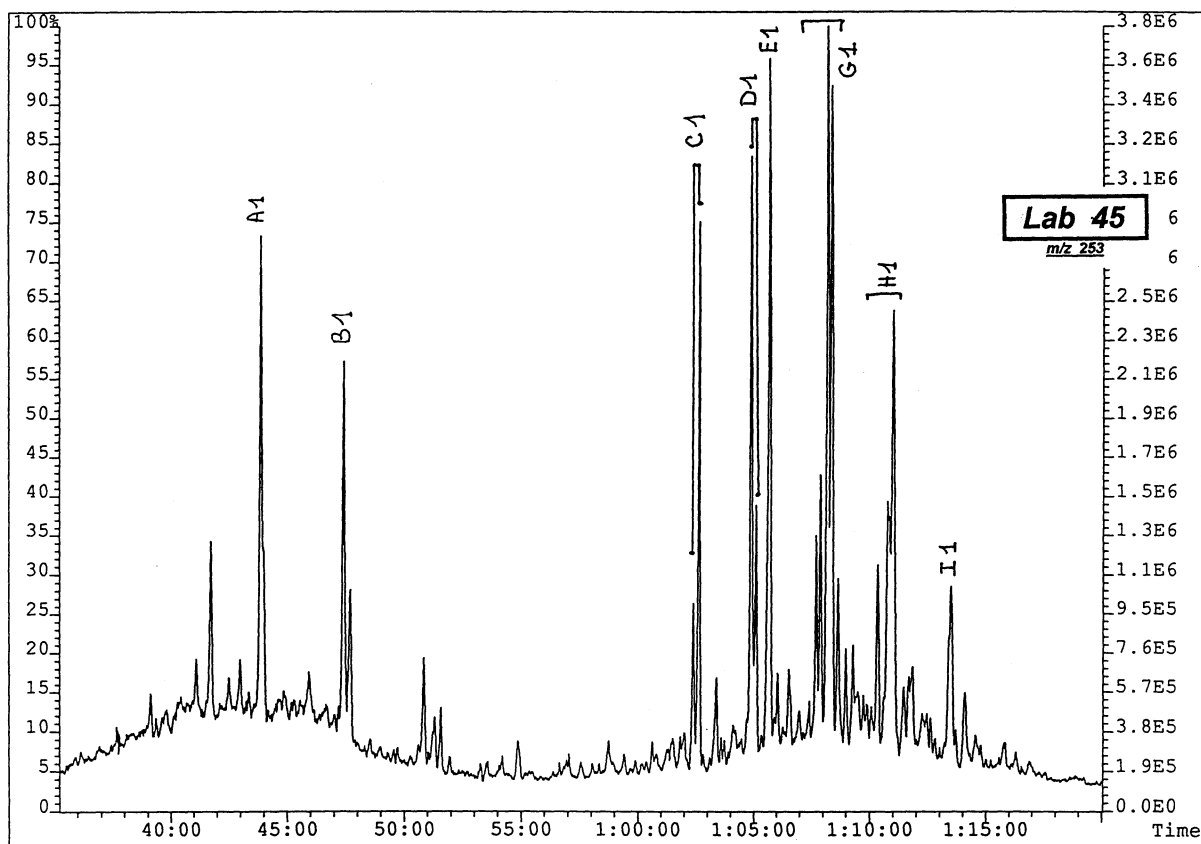
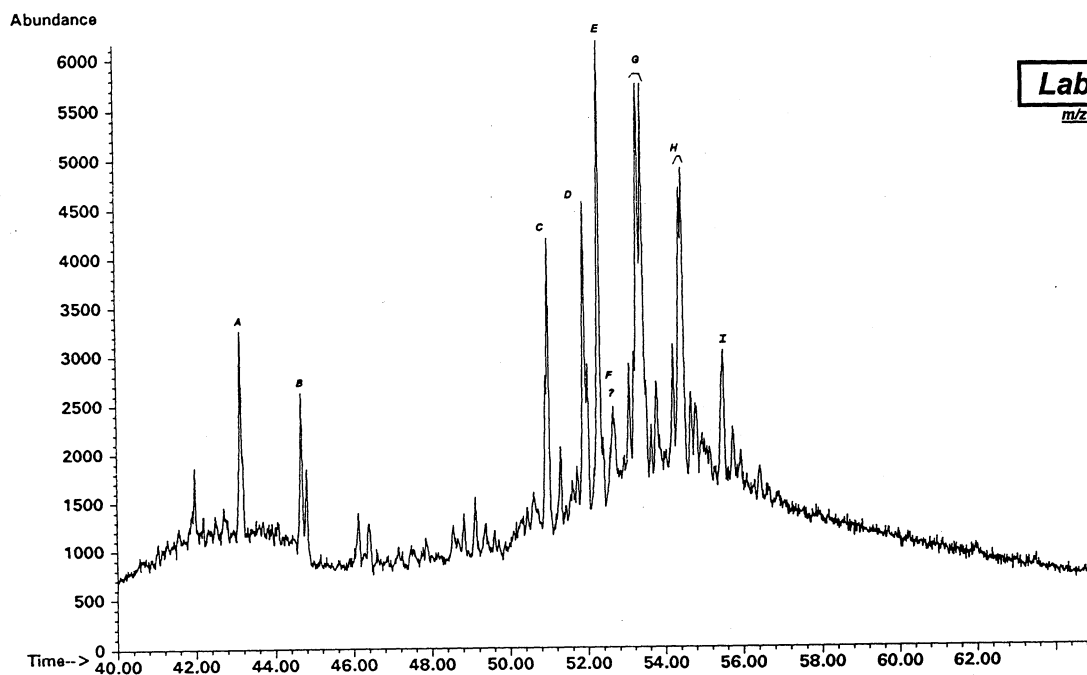


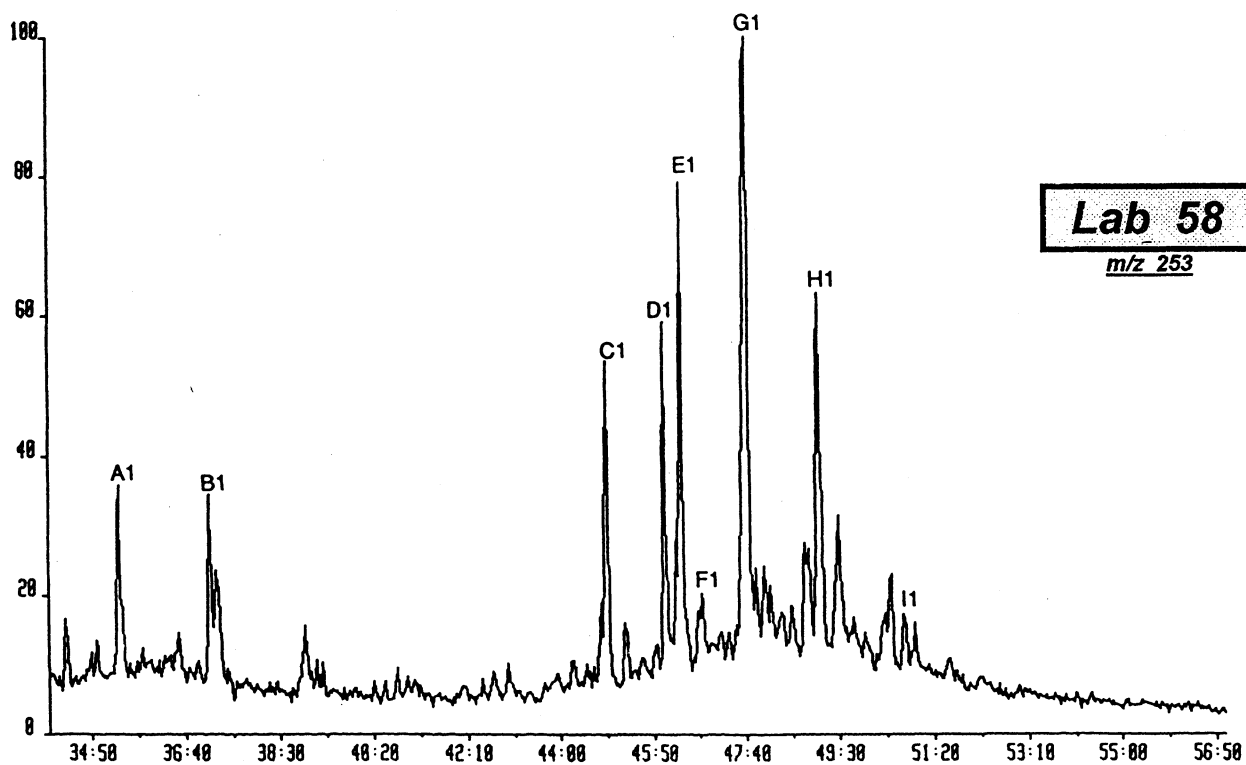
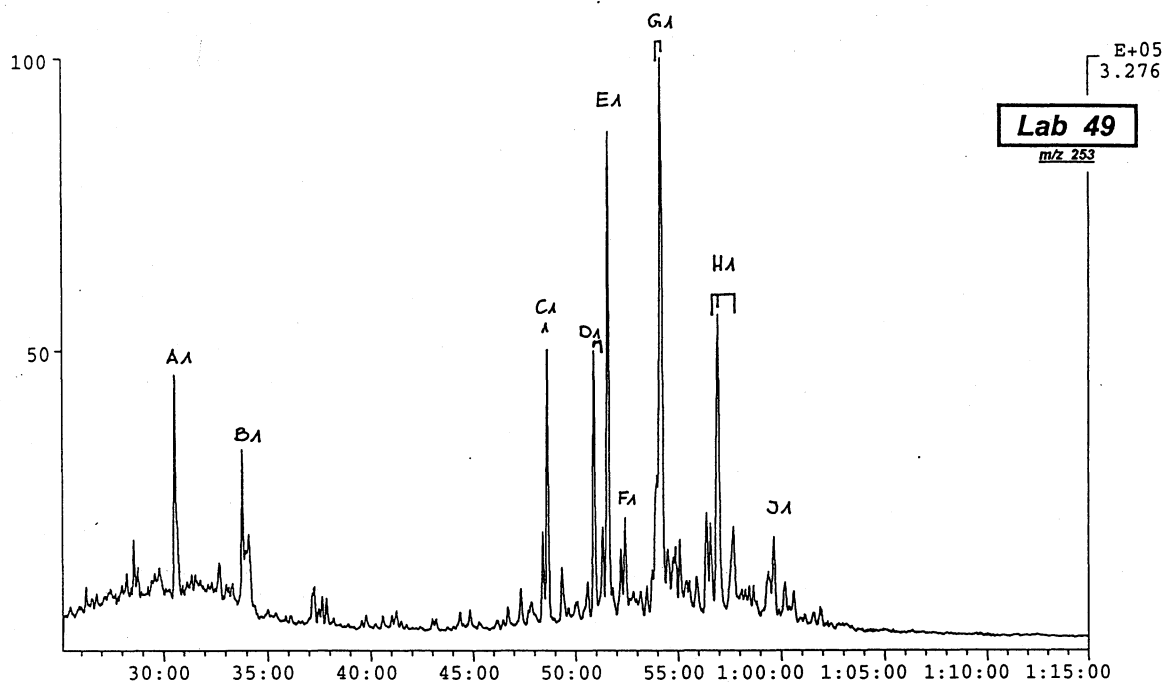


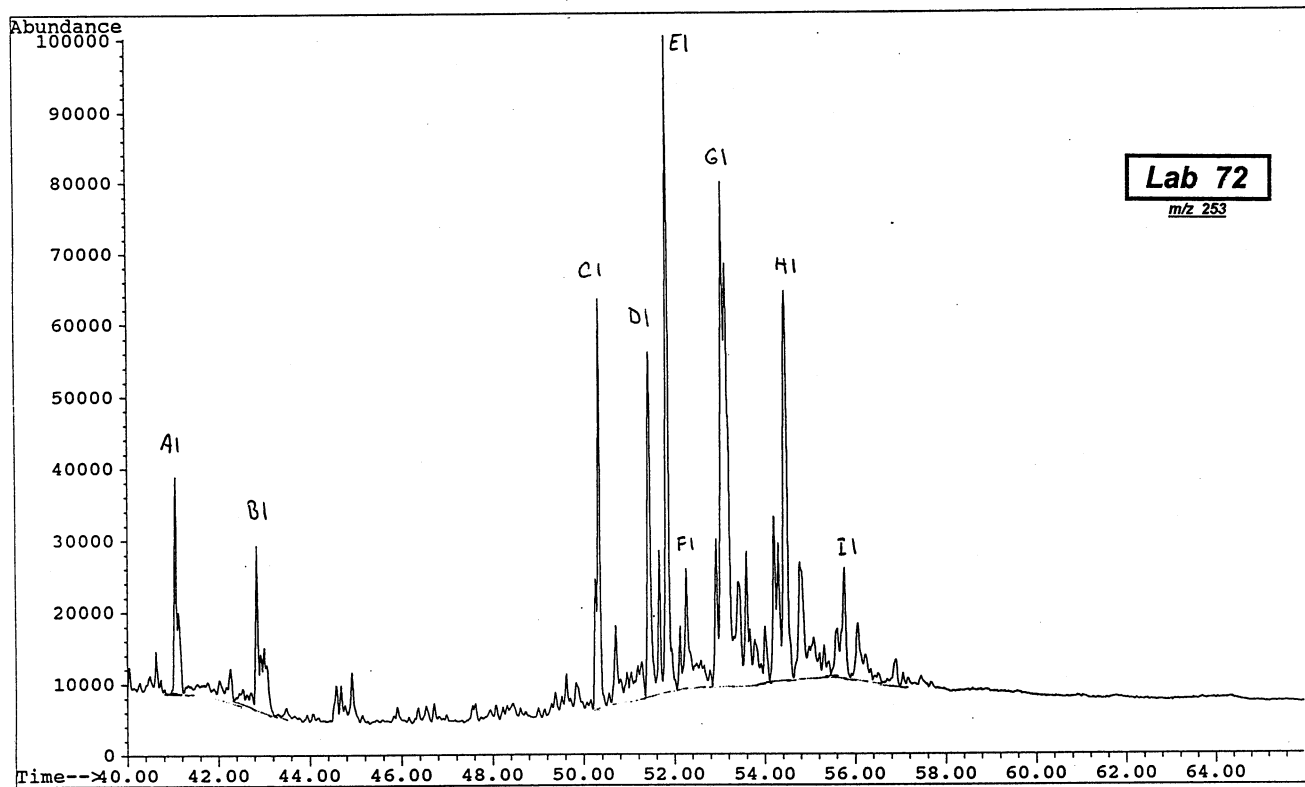
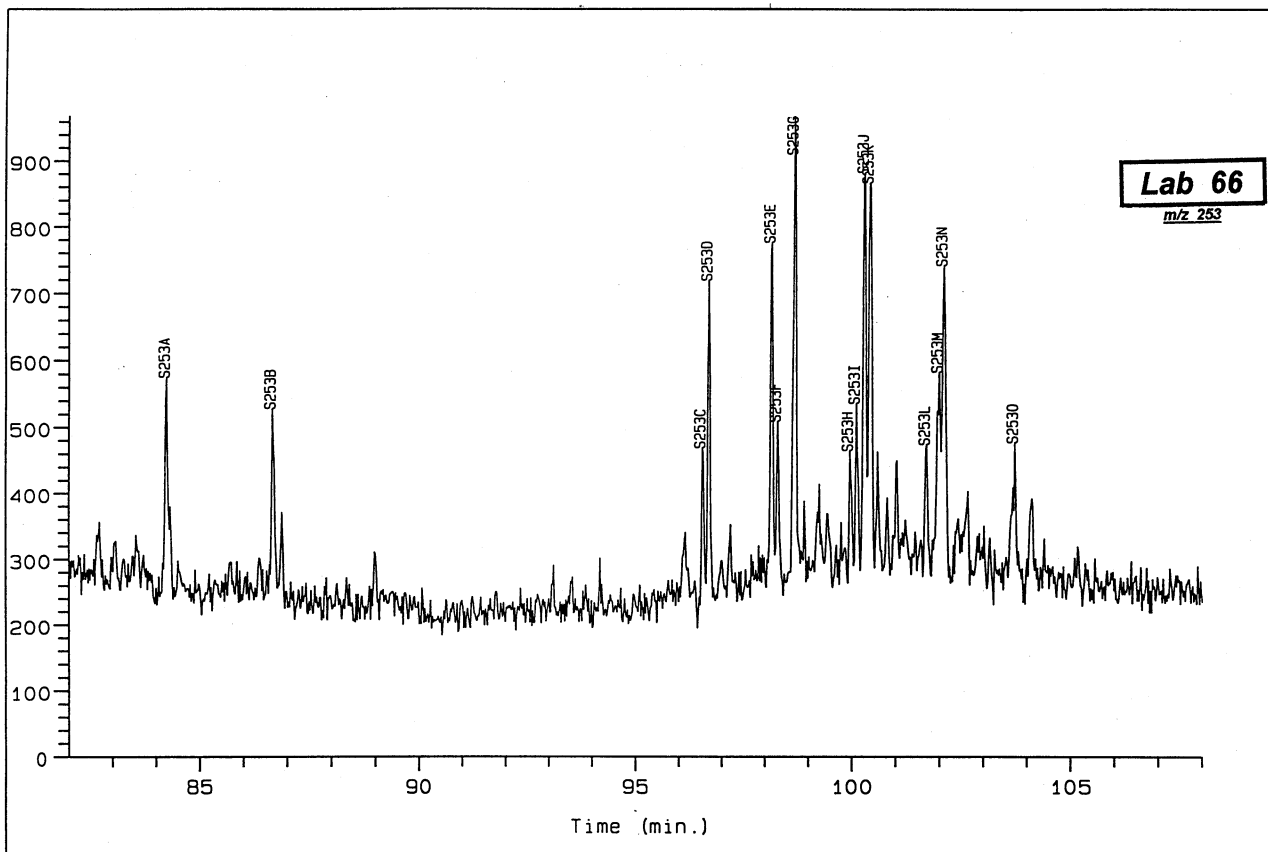


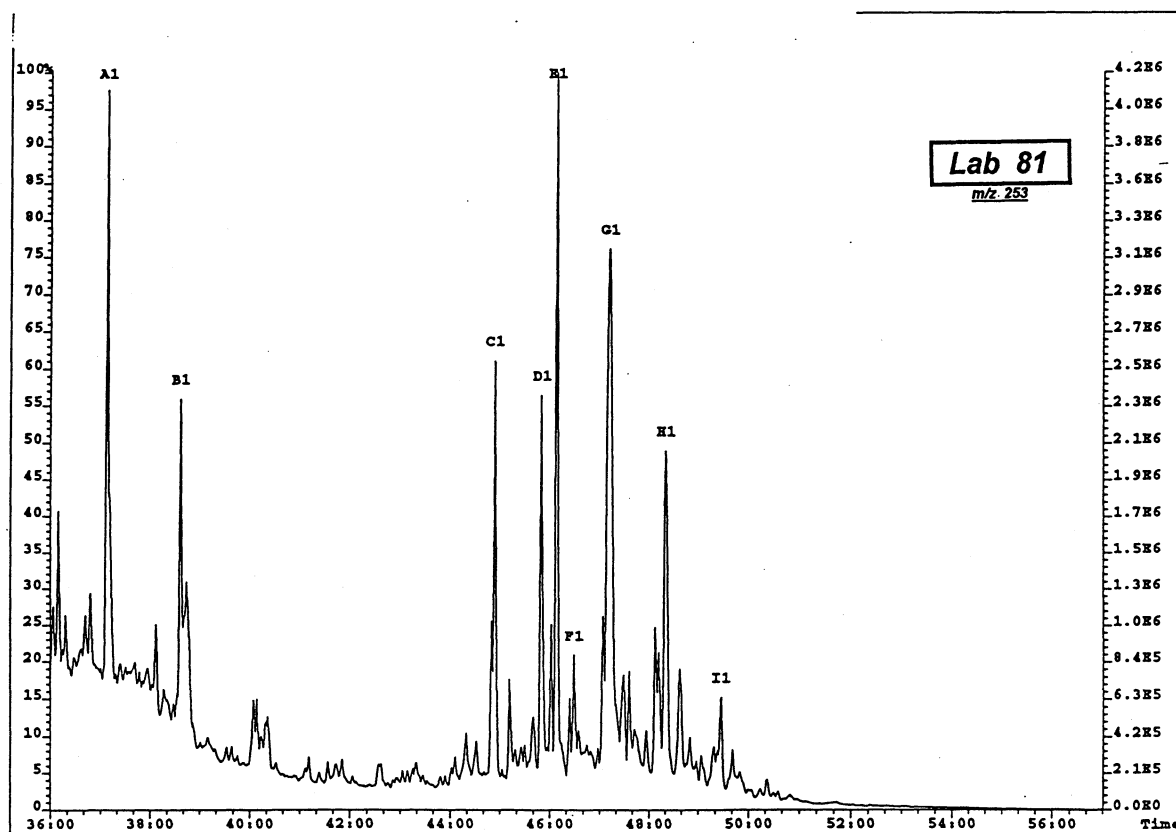
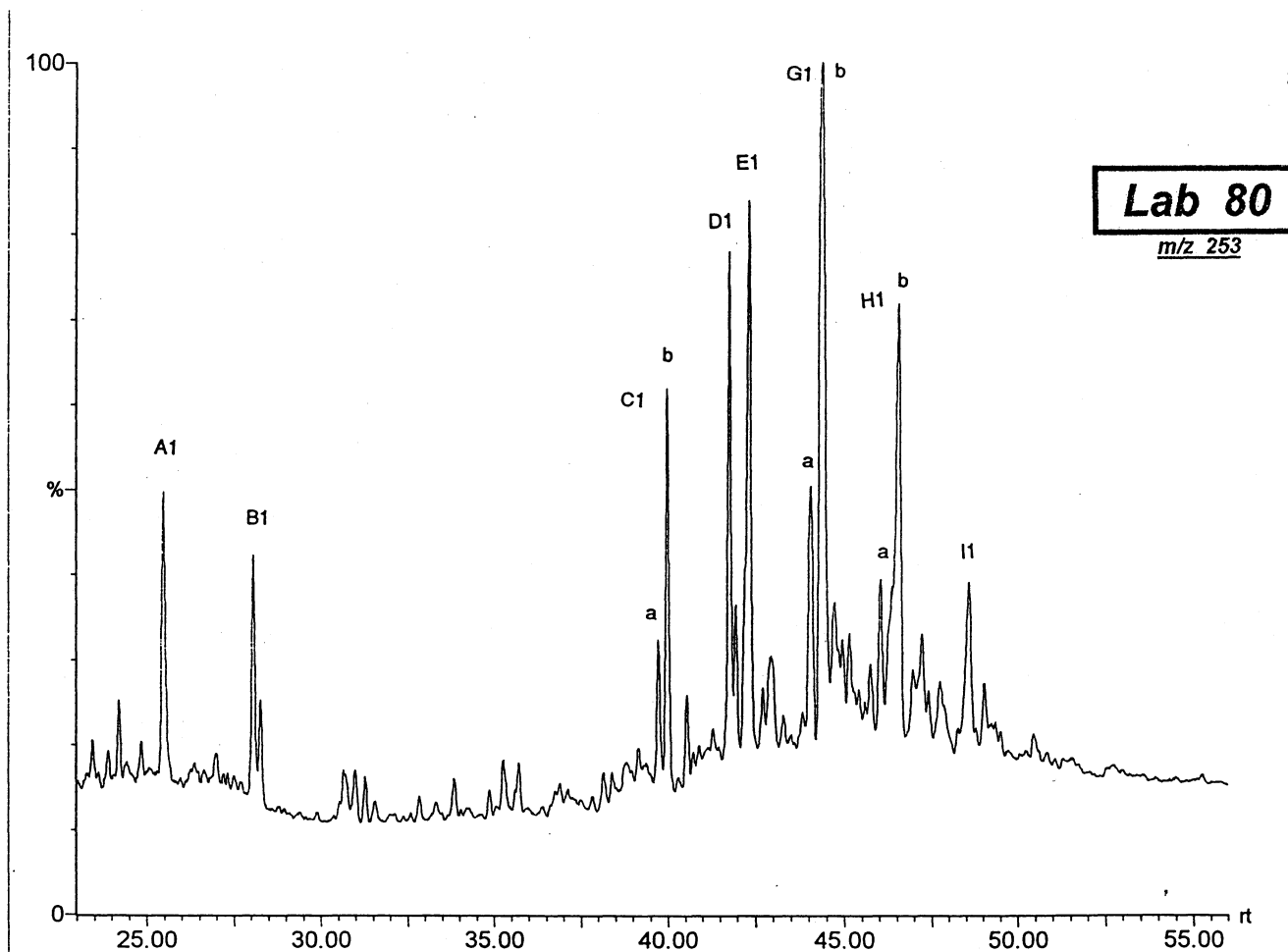


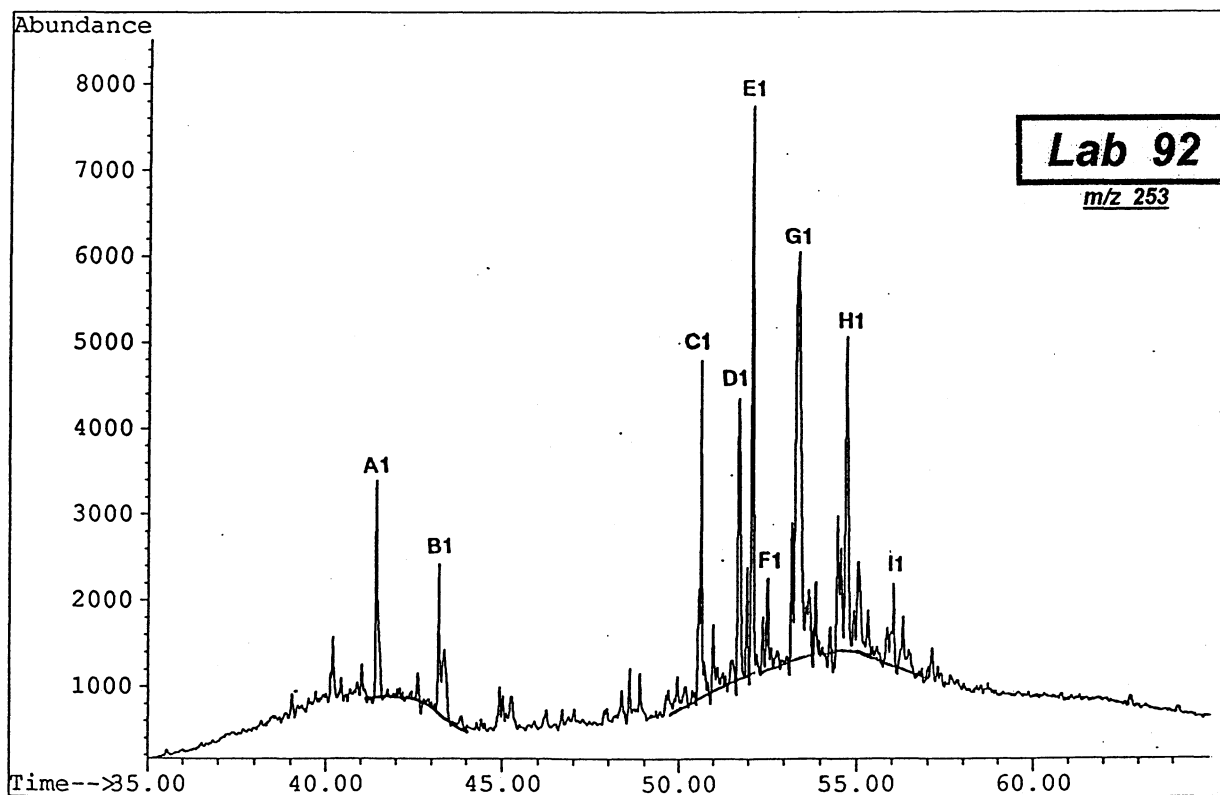
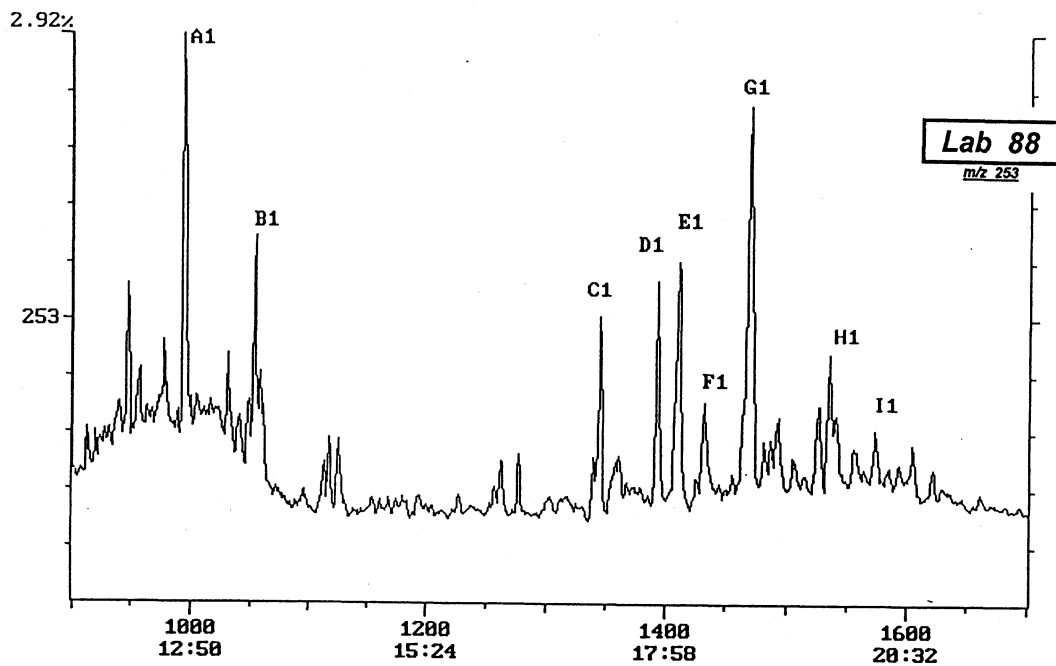


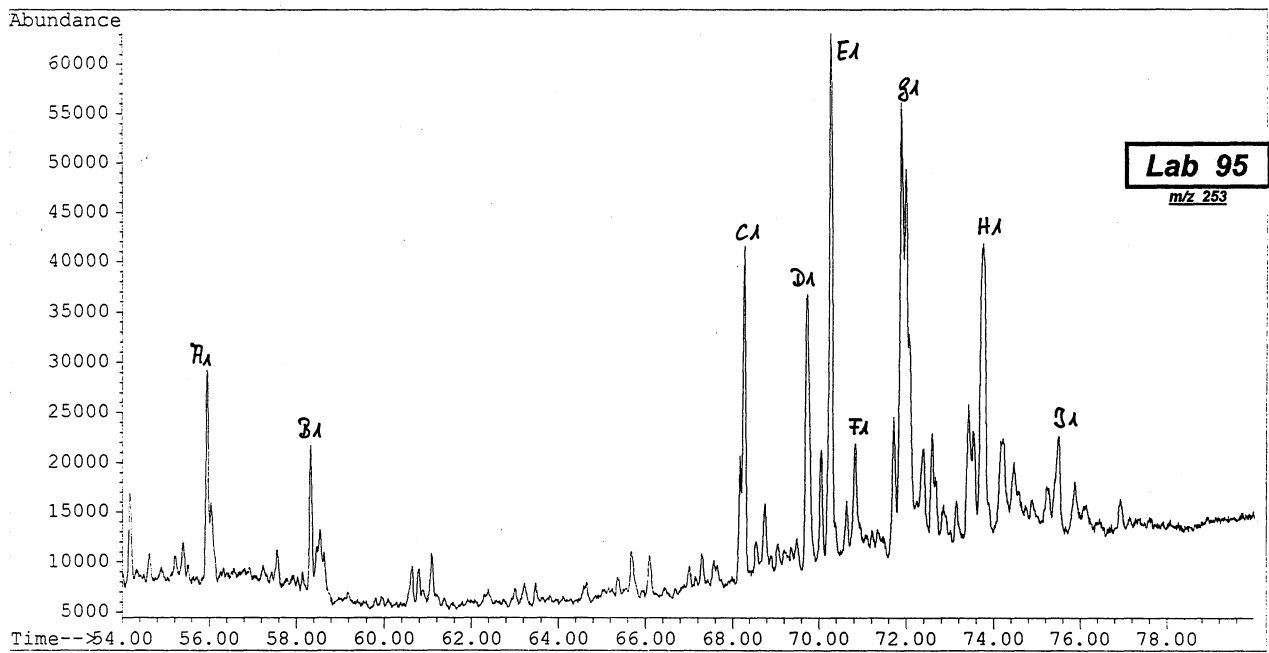












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Appendix A3.5

latroscan chromatograms

IATROSCAN : 3 replicates

Lab 32

