CAMBRIAN SOURCE ROCK GEOCHEMISTRY, STANSBURY BASIN

3. THERMAL MATURITY OF EARLY CAMBRIAN MOUNT McDONNELL FORMATION IN INVESTIGATOR-2, NORTHERN KANGAROO ISLAND

Report for Canyon (Australia) Pty Limited

by

DAVID M. McKIRDY

Organic Geochemistry in Basin Analysis Group
Department of Geology and Geophysics
University of Adelaide

August 1994

INTRODUCTION

The first part of this study (McKirdy and Padley, 1993) involved the organic geochemical analysis of seventeen outcrop samples of the Mount McDonnell Formation from four coastal exposures in the vicinity of Hummocky Point. This preliminary work found that the mudstone lithofacies of the formation is organically lean (TOC <0.2%) and contains low concentrations of solvent-extractable organic matter (EOM <70 ppm). GC analysis of the saturated hydrocarbons showed them to be contaminated by non-indigenous waxy alkanes; whereas GC-MS analysis of the two-ring aromatic hydrocarbons revealed maturity-dependent isomer distributions consistent with the gas-condensate stage of petroleum generation (VR_{calc} = 1.10–1.24%). The last of these findings, if confirmed by additional studies, is of profound significance for the petroleum prospectivity of the southern Stansbury Basin. However, caution is necessary in accepting this result at face value. As pointed out by McKirdy and Padley (1993, p. 9), "the effects of weathering on such low concentrations of extractable organic matter are potentially great, involving both contamination by recent plant- and soil-derived hydrocarbons, and selective removal of indigenous aromatic hydrocarbons".

In an attempt to validate the aforementioned aromatic maturity measurements, five core samples from the Mount McDonnell Formation in a nearby stratigraphic well were analysed in the same manner. It was hoped that the previously encountered artefacts of weathering and contamination would be eliminated or, at least, minimised by using *subsurface* material. The samples selected for analysis come from 139–505 metres depth in the SADME drillhole Investigator-2 (Table 1).

Preliminary data from this investigation were forwarded to Earl Sebring, Canyon (Australia) Pty Ltd, in fax messages dated 21 April, 30 April and 30 June 1993.

SAMPLES AND ANALYTICAL METHODS

The rock samples from SADME Investigator-2 analysed in this study were lengths of quarter core (weight = 120–140 g)

The analytical procedures employed were the same as those described by McKirdy and Padley (1993) except that, in this case, GC-MS analysis of the aromatic hydrocarbons was undertaken by Geotechnical Services Pty Ltd.

The aromatic fraction of selected rock extracts were analysed by GC-MS in the selected ion monitoring (SIM) mode using the following analytical conditions:

Instrument	HP 5970 MSD
Column	60 m x 0.25 mm ID, 0.25 µm film thickness, 5% phenylmethylsilicone DB-5 (J&W) connected directly to the ion source
Injector	automatic on-column
Carrier gas	helium
Temperature program	70°C for 1 min, 70–300°C at 3°C/ min; data collection commenced at 10 min
Mass spectrometer settings	Em voltage 1500–1800 V; electron energy 70 eV

RESULTS

Analytical data are summarised and presented herein as follows:

	Table	Figure	Appendix
TOC, C_{15+} extract data	1	–	–
GC of saturated hydrocarbons	2	1	–
GC-MS of aromatic hydrocarbons	3 & 4	2	1, 2 & 3
Calculated vitrinite reflectance	4	–	–

DISCUSSION

Source Richness

The samples of mudstone from Investigator-2 selected for organic geochemical analysis contain low concentrations of total organic carbon (TOC = 0.08–0.12%) and extractable organic matter (EOM = 26–279 ppm; 32–253 mg/g TOC). These TOC contents fall within the relatively narrow range of values exhibited by surface samples from adjacent coastal outcrops (TOC = 0.06–0.18%: McKirdy and Padley, 1993), whereas three of the cores give extract yields significantly higher than the maximum recorded outcrop value (64 ppm; 80 mg/g TOC). Thus, quantitatively, EOM is better preserved in the core samples of Mount McDonnell mudstone, although weathering of the same rock type in outcrop appears to have had little discernable effect on whole-rock TOC values.

The hydrocarbon fractions of the three core samples with the highest extract yields (EOM = 120–279 ppm: Table 1) were analysed by GC (saturates) and GC-MS (aromatics) to obtain information on the type and thermal maturity of their organic matter.

Type of organic matter

Inspection of the FID chromatograms in Figure 1 reveals saturated hydrocarbon (alkane) distributions that differ markedly from those previously reported for outcrop samples of the Mount McDonnell Formation. The most notable difference is the absence of waxy C_{23+} *n*-alkanes with a marked predominance of odd-carbon-numbered homologues. Thus, as anticipated, *the core material is free of overt contamination by recent plant- or soil-derived organic matter.*

The indigenous alkanes (Fig. 1) are derived from *microbial (i.e. bacterial, cyanobacterial and algal) organic matter* that was exposed to *suboxic* conditions during deposition and early diagenesis, as indicated by the following parameters:

1) a high relative concentration of branched (iso, anteiso) alkanes;
2) a pristane/*n*-heptadecane ratio in the range 0.33–0.40;
3) a phytane/*n*-octadecane ratio in the range 0.18–0.24; and
4) a low pristane/phytane ratio (pr/ph = 1.13–1.37).

However, such molecular signatures are usually accompanied by a unimodal *n*-alkane profile with a maximum at C_{15}–C_{19}. The fact that these mudstone cores have *n*-alkane distributions which are not only skewed towards higher carbon numbers, but also superimposed on broad naphthene humps (Fig. 1), distinguishes them from the least contaminated outcrop sample (see McKirdy and Padley, 1993, fig. 2A). Their naphthene humps are centred about the *n*-C_{30} position and comprise unresolved complex mixtures (UCM) of high-molecular-weight branched and cyclic alkanes. The alkane chromatograms of the outcrop samples also have naphthene humps, but these are less prominent (in most cases) and centred on *n*-C_{22} or thereabouts.

The most likely explanation for the differences between the alkanes in the core samples and those indigenous to the outcrop samples is that the former sustained greater evaporative losses during the analytical work-up procedure. Similar depletion of the more volatile components of the aromatic hydrocarbon fractions is evident in their total ion chromatograms (Fig. 2). Given the small size of the saturated and aromatic hydrocarbon fractions isolated from the core samples (0.7–11.5 mg), such evaporative loss could not have been avoided. It occurred during the final stages of solvent removal following liquid chromatography of the EOM; and is likely to have been most severe in the four smallest fractions (< 4 mg).

Several other aspects of the alkane distributions require comment. In two samples (RS 1171 and RS 1252) the *n*-alkanes display a slight predominance of even carbon-numbered homologues over the range C_{16}–C_{22}. The same unusual feature (albeit more pronounced) was observed in many of the outcrop samples of Mount McDonnell Formation analysed by McKirdy and Padley (1993) who tentatively attributed it to bacterial or cyanobacterial precursors. In the remaining sample (RS 1201), the naphthene hump is somewhat more pronounced (relative to the normal and isoprenoid alkanes) and the saturates/aromatics ratio is considerably higher (S/A = 8: Table 1) than is the case for the other two cores. This may indicate *staining of the mudstone in question by migrated hydrocarbons.*

Some di- and tri-aromatic hydrocarbons (e.g. 1,2,5-trimethylnaphthalene, 1-methylphenanthrene, 1,7-dimethylphenanthrene and retene) have specific higher plant precursors and therefore can be used as molecular markers of a particular biota, depositional environment or geological age (Strachan *et al.*, 1988; Alexander *et al.*, 1988). The low values of all the source-sensitive aromatic parameters listed in Table 3 are consistent with the absence of land-plant terpenoid material in these Cambrian mudstones, and hence also their lack of contamination by recent plant-derived hydrocarbons. The presence of trace amounts of these particular aromatics in the Mount McDonnell Formation is probably due to the catagenetic aromatisation and degradation of algal steranes and bacteriohopanoid triterpanes.

Thermal maturity

GC-MS analysis of the aromatic hydrocarbons isolated from the three mudstone samples allowed determination of various ratios (Table 4), based on the isomer distributions of dimethylnaphthalenes, trimethylnaphthalenes and methylphenanthrenes (Appendices 1–3), that are known to respond systematically to increasing thermal maturity (Radke, 1987). Calibrations against measured vitrinite reflectance, the traditional maturity scale, are available for several of these isomer ratios (DNR-1, MPI-1, MPR and MPDF: Radke and Welte, 1983; Radke *et al.*, 1984; Kvalheim *et al.*, 1987; Boreham *et al.*, 1988). However, these calibrations are based on data from younger Phanerozoic sequences that contain humic coals or dispersed organic matter incorporating recognisable vitrinite phytoclasts. The Mount McDonnell Formation, like all pre-Devonian sediments, lacks both true vitrinite and land-plant precursors for polyaromatic hydrocarbons. Thus, for such rocks, calculated vitrinite reflectance (VR_{calc}) values derived from any of the aforementioned aromatic maturity parameters must be of uncertain validity. Notwithstanding this uncertainty, the "aromatic maturity" of the organic matter preserved in these Cambrian mudstones, and its expression in terms of equivalent or calculated vitrinite reflectance, is the best available guide to their level of thermal alteration.

As mentioned previously, the di- and tri-aromatic hydrocarbon fractions of the three mudstones analysed (Fig. 2) show signs of evaporative depletion. Susceptibilty to depletion increases with volatility as follows: dimethylphenanthrenes < methylphenanthrenes < phenanthrene < tetramethylnaphthalenes < trimethylnaphthalenes < dimethylnaphthalenes < methylnaphthalenes. All three samples are totally devoid of methylnaphthalenes (the most volatile components), thereby precluding determination of MNR (cf. McKirdy and Padley, 1993). In two samples (RS 1201 and RS 1252) evaporation has also significantly depleted the dimethylnaphthalenes, giving rise to low signal to noise ratios and poor peak shape in their respective m/z = 156 mass chromatograms. In the case of RS1201, the aromatic fraction most affected by evaporation, significant differential loss of individual aromatic compounds extends back along the series as far as phenanthrene, giving rise to an anomalously high value of MPI-1 in relation to the other two samples (Table 4).

The most reliable and internally consistent aromatic maturity data were obtained from sample RS 1171. Its DNR-1 and MPR values convert to equivalent vitrinite reflectances of 1.07% and 1.10%, respectively (Table 4). On the basis of its MPR value, sample RS 1252 appears to be of similar maturity (VR_{calc} = 1.05%). These maturities of core material from Investigator-2 are in excellent agreement with those derived from the measurement of MNR (VR_{calc} = 1.04 – 1.19%) and DNR-1 (VR_{calc} = 1.10 – 1.24%) in nearby outcrop samples of the Mount McDonnell Formation (McKirdy and Padley, 1993). The slightly higher maturity of the third core sample RS 1201 (MPR = 1.49; VR_{calc} = 1.34%) may be due to its staining by migrated, condensate-like hydrocarbons.

Although there is no published calibration of TNR-1 against vitrinite reflectance, the values obtained for this parameter (0.60–0.68: Table 4) are consistent with the above assessment of maturity. However, for reasons that are as yet unclear, measurements of both MPI-1 and MPDF (and their corresponding VR_{calc} values) in these core samples indicate a lower maturity than do the other aromatic parameters.

CONCLUSIONS

1. Core samples of mudstone from the Early Cambrian Mount McDonnell Formation in SADME Investigator-2, located near Hummocky Point on northern Kangaroo Island, are organically lean (TOC ~ 0.1%) and contain low concentrations of extractable organic matter (EOM < 280 ppm).

2. Although no more organic-rich than surface samples of the same formation and lithofacies from adjacent coastal outcrops, three of the five cores examined have extract yields appreciably greater than the maximum outcrop value (viz. 64 ppm). EOM is better preserved in the core samples, and its hydrocarbons (saturates and aromatics) display no evidence of contamination by younger, non-indigenous, organic matter.

3. The low hydrocarbon contents of these mudstones, and the limited amount of core made available for destructive analysis (maximum sample size ~150 g), together conspired to produce very small samples (in most cases < 4 mg) for GC and GC-MS analysis. Inevitably, the resulting saturated and aromatic hydrocarbon fractions sustained significant (but variable) evaporative loss of their more volatile components during the solvent-removal stages of the isolation procedure.

4. Notwithstanding the aforementioned analytical problems, reliable maturity data were obtained for three samples from 139–344 metres depth in Investigator-2. GC-MS analysis of the two-ring and three-ring aromatic hydrocarbons revealed maturity levels (VR_{calc} ~1.1%) equivalent to the wet gas-condensate phase of petroleum generation from a source rock containing Type II kerogen. Such source beds, now overmature, are present elsewhere in the Stansbury Basin (e.g. within the upper Heatherdale Shale on Fleurieu Peninsula).

5. The excellent agreement between these maturities and those previously obtained from nearby outcrop samples of the Mount McDonnell Formation reinforces the conclusion that the Early Cambrian sequence, immediately north of the Snelling Fault on the southern margin of the Stansbury Basin, is still within the oil preservation window.

6. The Mount McDonnell Formation at 244.3 metres depth in Investigator-2 shows signs of slight staining by migrated hydrocarbons.

ACKNOWLEDGEMENTS

Sample preparation, Soxhlet extraction, liquid chromatography of the EOM, and gas chromatography of the saturated hydrocarbons were undertaken in the Organic Geochemistry Laboraory, Department of Geology and Geophysics, University of Adelaide, by Elizabeth Fontaine-Geary.

Aliquots of powdered core were analysed for TOC at AMDEL Limited (Petroleum Services), Torrensville, SA.

GC-MS analysis of the aromatic hydrocarbons was performed by Geotechnical Services Pty Ltd, Victoria Park, WA.

REFERENCES CITED

Alexander, R., Larcher, A.V., Kagi, R.I. and Price, P.L., 1988. The use of plant-derived biomarkers for correlation of oils with source rocks in the Cooper/Eromanga Basin system, Australia. *APEA Journal,* 28(1): 310–324.

Boreham, C.J., Crick, I.H. and Powell, T.G., 1988. An alternative calibration of the Methylphenanthrene Index against vitrinite reflectance: Application to maturity measurements in oils and sediments. *Organic Geochemistry,* 12: 289–294.

Kvalheim, O.M., Christy, A.A., Telnaes, N. and Bjorseth, A., 1987. Maturity determination of organic matter in coals using the methylphenathrene distribution. *Geochimica et Cosmochimica Acta,* 51: 1833–1888.

McKirdy, D.M. and Padley, D., 1993. Cambrian source rock geochemistry, Stansbury Basin. 1. Preliminary evaluation of Mount McDonnell Formation in coastal exposures on northern Kangaroo Island. *Report for Canyon (Australia) Pty Ltd* (unpublished).

Radke, M., 1987. Organic geochemistry of aromatic hydrocarbons. In: *Advances in Petroleum Geochemistry, Vol. 2.* (J. Brooks and D. Welte, eds.), Academic Press, London, pp. 141–207.

Radke, M. and Welte, D.H., 1983. The methylphenanthrene index (MPI): a maturity parameter based on aromatic hydrocarbons. In: *Advances in Organic Geochemistry 1981* (M. Bjoroy *et al.*, eds.), Wiley, Chichester, pp. 504–512.

Radke, M., Leythaeuser, D. and Teichmuller, M., 1984. Relationship between rank and composition of aromatic hydrocarbons for coals of different origins. *Organic Geochemistry,* 6: 423–430.

Strachan, M.G., Alexander, R. and Kagi, R.I., 1988. Trimethylnaphthalenes in crude oils and sediments: Effects of source and maturity. *Geochimica et Cosmochimica Acta,* 52: 1255–1264.

Table 1 Total organic carbon and extract data on Mount McDonnell Formation, SADME Investigator-2

Sample	Depth	Weight sample	TOC	EOM Yield		EOM Composition			
	m	g	%	ppm	mg/g TOC	Sat %	Arom %	NSO %	S/A
RS 1171	138.9	119.26	0.11	279	253	10.4	26.1	63.5	0.40
RS 1190	222.2	–	0.08	nd	nd	nd	nd	nd	nd
RS 1201	244.3	133.42	0.12	187	155	46.3	5.8	47.9	8.00
RS 1252	343.5	127.60	0.08	120	96	18.3	4.3	77.4	4.21
RS 1302	429.0	135.72	0.12	37	44	27.0	6.5	66.5	4.18
RS 1342	505.3	133.79	0.12	26	32	33.9	12.3	53.8	2.75

S/A = saturated hydrocarbons/aromatic hydrocarbons nd = not determined

Table 2 Alkane parameters in selected mudstones from the Mount McDonnell Formation, SADME Investigator-2

Sample	Depth m	Pr/Ph	Pr/n-C_{17}	Ph/n-C_{18}	n-Alkane Profile Maximum	 EOP
RS 1171	138.9	1.37	0.40	0.18	30	+
RS 1201	244.3	1.13	0.33	0.21	20	–
RS 1252	343.5	1.25	0.38	0.24	22	+

EOP = even/odd predominance in C_{16}–C_{24} n-alkanes

nd = not determined + = present – = absent

Table 3 Source- and age-dependent aromatic hydrocarbon ratios in three mudstones from the Mount McDonnell Formation, SADME Investigator-2

Sample	Depth m	TNR-5 (*m/z* 170)	1-MP/9-MP (*m/z* 192)	1,7-DMP/X (*m/z* 206)	Retene/9-MP (*m/z* 219, 192)
RS 1171	138.9	0.50	0.92	0.58	1.18
RS 1201	244.3	0.46	0.71	0.48	1.49
RS 1252	343.5	0.44	0.85	0.44	1.12

These four ratios were defined by Alexander *et al.* (1988) and Strachan *et al.* (1988). The key to the abbreviations is as follows:

$$\text{TNR-5} = \frac{\text{1,2,5-TMN}}{\text{1,3,6-TMN}}$$

$$\text{1,7-DMP/X} = \frac{\text{1,7-DMP}}{\text{1,3-DMP} + \text{3,9-DMP} + \text{2,10-DMP} + \text{3,10-DMP}}$$

1,2,5-TMN = 1,2,5-trimethylnaphthalene
1,3,6-TMN = 1,3,6-trimethylnaphthalene
1-MP = 1-methylphenanthrene
9-MP = 9-methylphenanthrene
1,7-DMP = 1,7-dimethylphenanthrene
1,3-DMP = 1,7-dimethylphenanthrene
3,9-DMP = 3,9-dimethylphenanthrene
2,10-DMP = 2,10-dimethylphenanthrene
3,10-DMP = 3,10-dimethylphenanthrene

Table 4 Thermal maturity based on diaromatic and triaromatic hydrocarbons in three mudstones from the Mount McDonnell Formation, SADME Investigator-2

Sample	Depth m	DNR-1 (*m/z* 156)	TNR-1 (*m/z* 170)	MPI-1 (m/z 178, 192)	MPR (m/z 192)	MPDF (m/z 192)	VR$_{calc}$ %			
							(a)	(b)	(c)	(d)
RS 1171	138.9	3.82	0.68	0.48	1.18	0.494	1.07	0.70	~~1.10~~ 1·01	0.94
RS 1201	244.3	nd	0.65	[1.04]	1.49	0.510	nd	[1.01]	~~1.34~~ 1·11	0.98
RS 1252	343.5	nd	0.60	0.59	1.12	0.458	nd	0.76	~~1.05~~ ·99	0.86

McKirdy et al.

See next page for key to aromatic maturity indicators

nd = not determined [ ] = affected by evaporative depletion of phenanthrene

KEY TO AROMATIC MATURITY PARAMETERS

Dimethylnaphthalene ratio (DNR-1), trimethylnaphthalene ratio (TNR-1), methylphenanthrene index (MPI-1), methylphenanthrene ratio (MPR), methylphenanthrene distribution factor (MPDF), and VR_{calc} are defined by Radke and Welte (1983), Radke *et al.* (1984), Radke (1987) and Kvalheim *et al.* (1987) as follows:

$$\text{DNR-1} = \frac{\text{2,6-DMN} + \text{2,7-DMN}}{\text{1,5-DMN}}$$

$$\text{TNR-1} = \frac{\text{2,3,6-TMN}}{\text{1,3,5-TMN} + \text{1,4,6-TMN}}$$

$$\text{MPI-1} = \frac{1.5\,[\,\text{2-MP} + \text{3-MP}\,]}{\text{P} + \text{1-MP} + \text{9-MP}}$$

$$\text{MPR} = \frac{\text{2-MP}}{\text{1-MP}}$$

$$\text{MPDF} = \frac{\text{2-MP} + \text{3-MP}}{\text{2-MP} + \text{3-MP} + \text{1-MP} + \text{9-MP}}$$

VR_{calc} (a) = 0.046 DNR + 0.89 (for VR in the range 0.7–1.5%; r = 0.83)

VR_{calc} (b) = 0.55 MPI-1 + 0.44 (for VR in the range 0.65–1.35%; r = 0.94)

VR_{calc} (c) = 0.99 $\log_{10}$ MPR + 0.94 (for VR in the range 0.4–1.7%; r = 0.84)

VR_{calc} (d) = − 0.166 + 2.242 MPDF (for VR in the range 0.5–1.3%)

where 1,5-DMN = 1,5-dimethylnaphthalene
2,6-DMN = 2,6-dimethylnaphthalene
2,7-DMN = 2,7-dimethylnaphthalene
1,3,5-TMN = 1,3,5-trimethylnaphthalene
1,4,6-TMN = 1,4,6-trimethylnaphthalene
2,3,6-TMN = 2,3,6-trimethylnaphthalene
1-MP = 1-methylphenanthrene
2-MP = 2-methylphenanthrene
3-MP = 3-methylphenanthrene
9-MP = 9-methylphenanthrene

FIGURE 1

GC FID chromatograms of saturated hydrocarbons (total alkanes)
in core samples of mudstone from the Mount McDonnell Formation,
SADME Investigator-2

Figure	*Sample*	*Depth (metres)*
1A	RS 1171	138.9
1B	RS 1201	244.3
1C	RS 1252	343.5

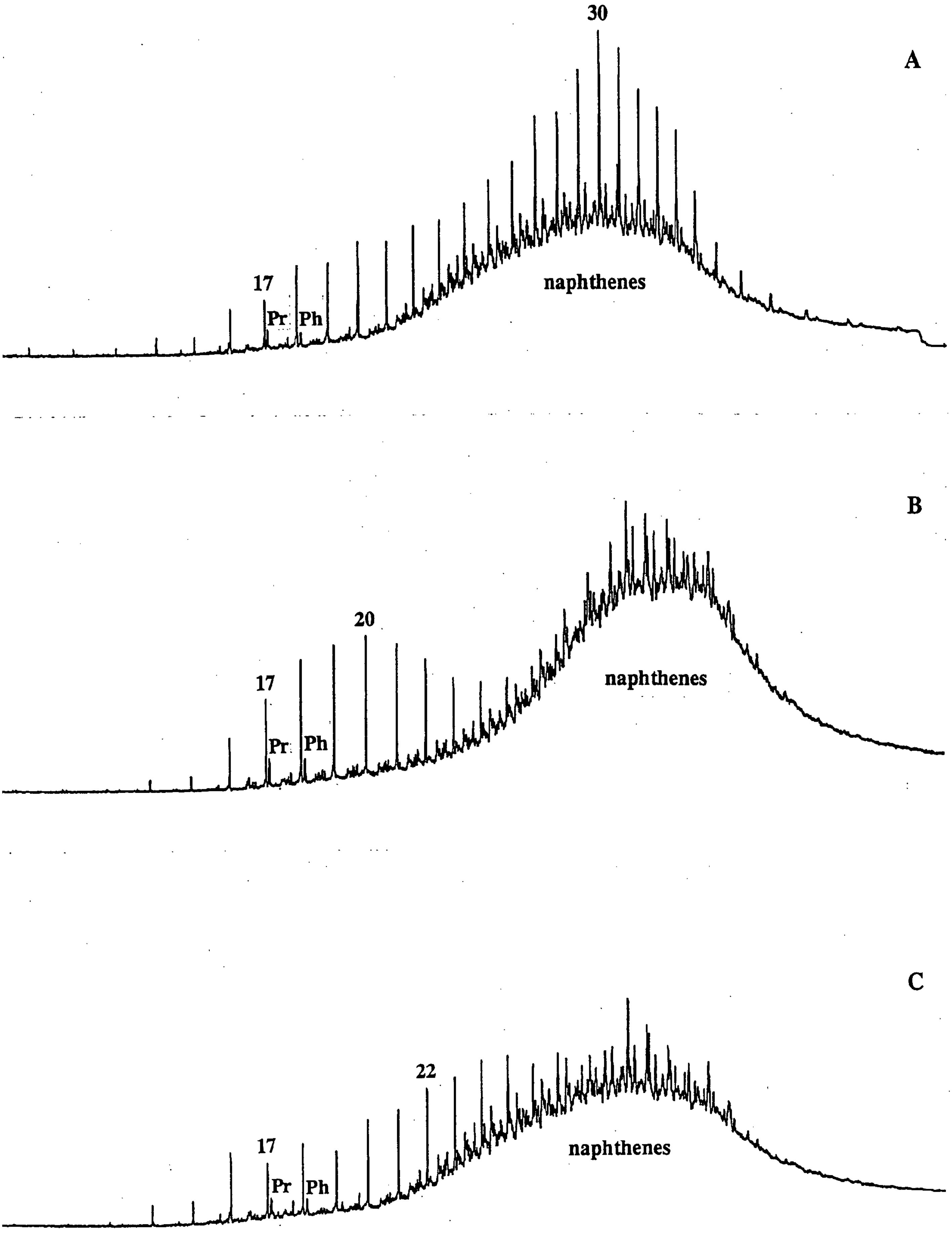

30
A
17
Pr
Ph
naphthenes
B
20
17
Pr
Ph
naphthenes
C
22
17
Pr
Ph
naphthenes

FIGURE 2

GC-MS TIC chromatograms of aromatic hydrocarbons
in core samples of mudstone from the Mount McDonnell Formation,
SADME Investigator-2

Figure	*Sample*	*Depth (metres)*
2A	RS 1171	138.9
2B	RS 1201	244.3
2C	RS 1252	343.5

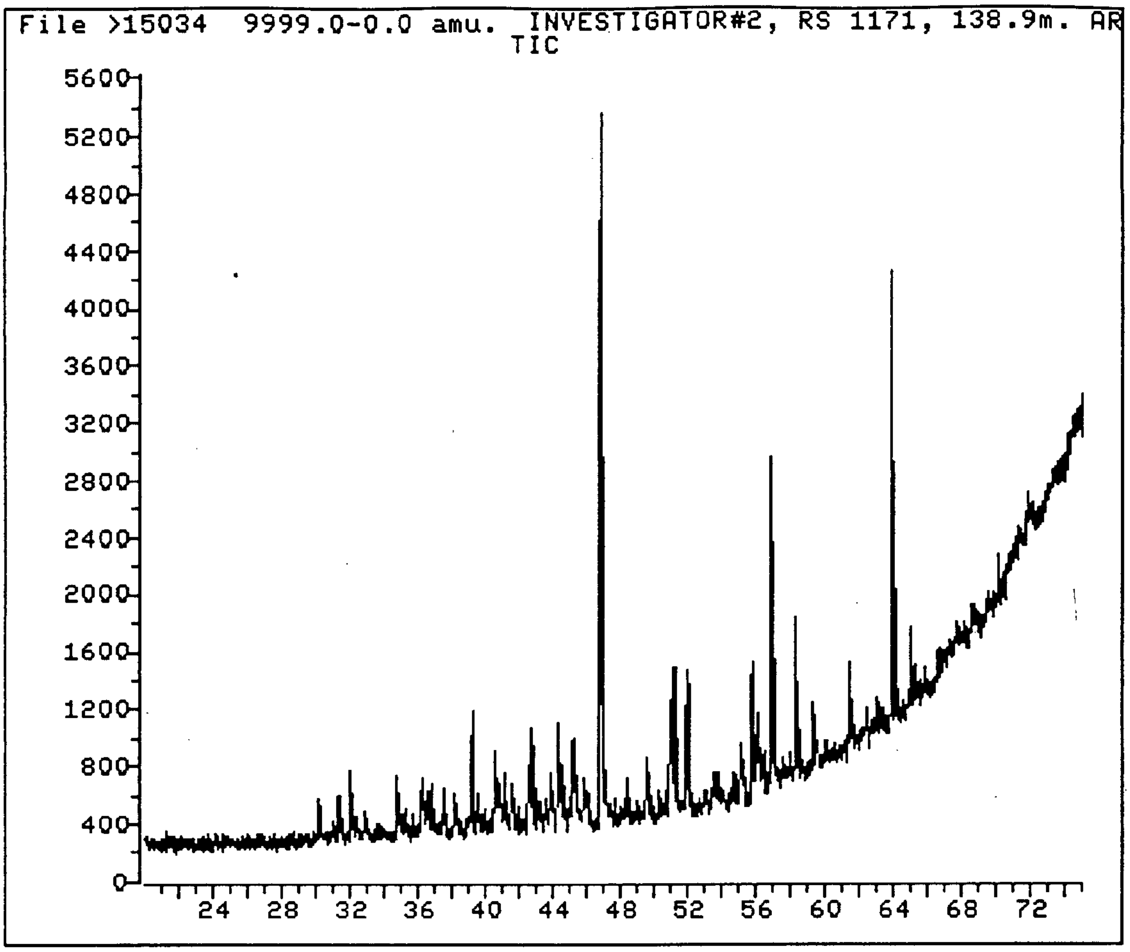

File >15034 9999.0-0.0 amu. INVESTIGATOR#2, RS 1171, 138.9m. AR
TIC
5600
5200
4800
4400
4000
3600
3200
2800
2400
2000
1600
1200
800
400
0
24
28
32
36
40
44
48
52
56
60
64
68
72

FIGURE 2A

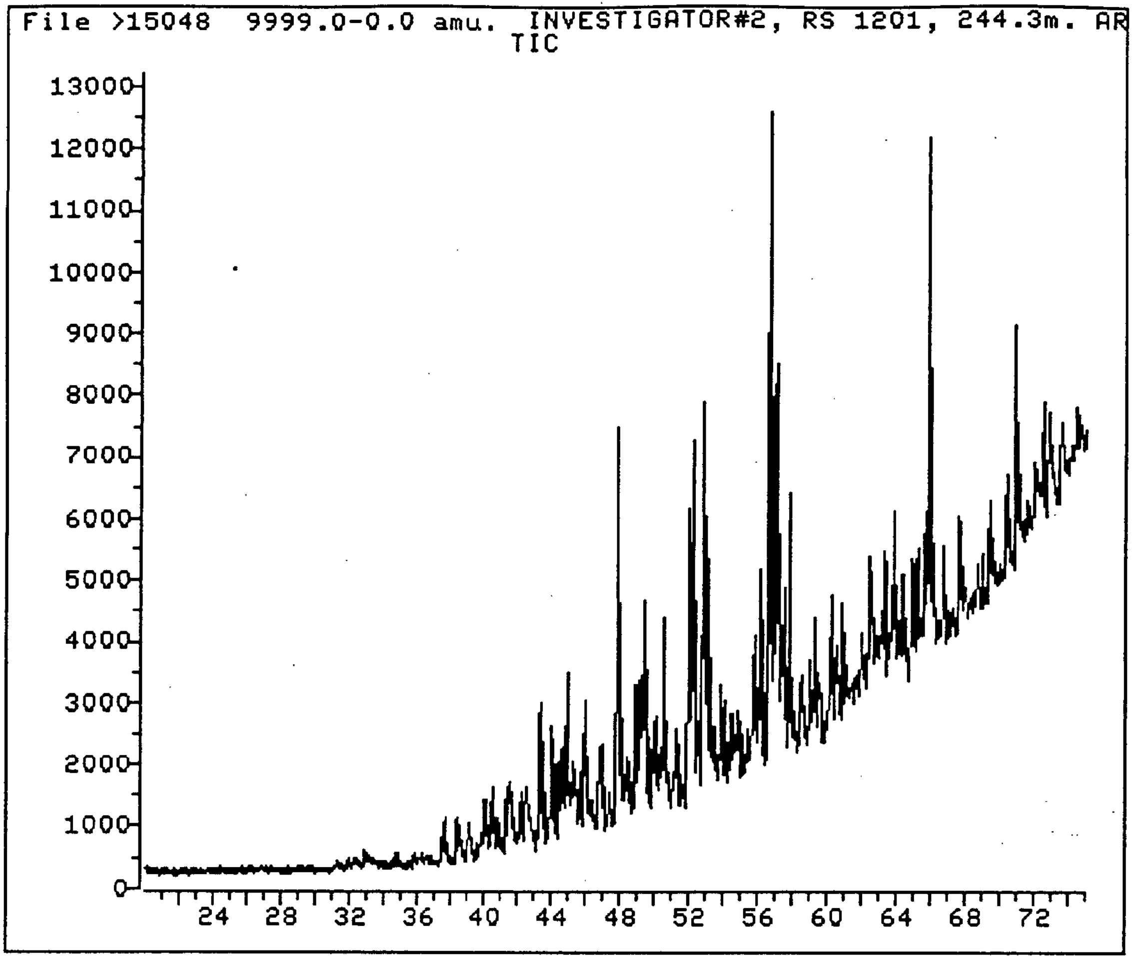

File >15048 9999.0-0.0 amu. INVESTIGATOR#2, RS 1201, 244.3m. AR
TIC
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
24
28
32
36
40
44
48
52
56
60
64
68
72

FIGURE 2B

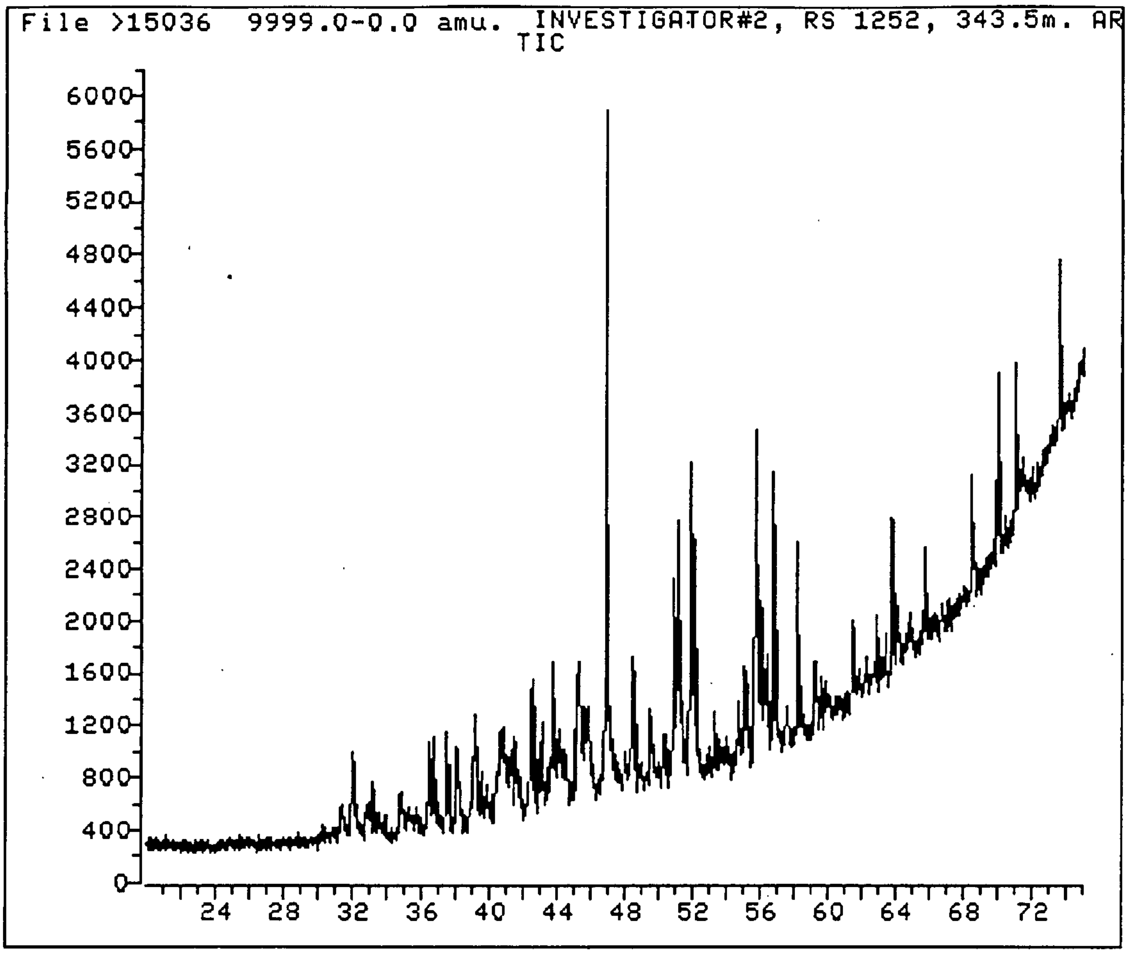
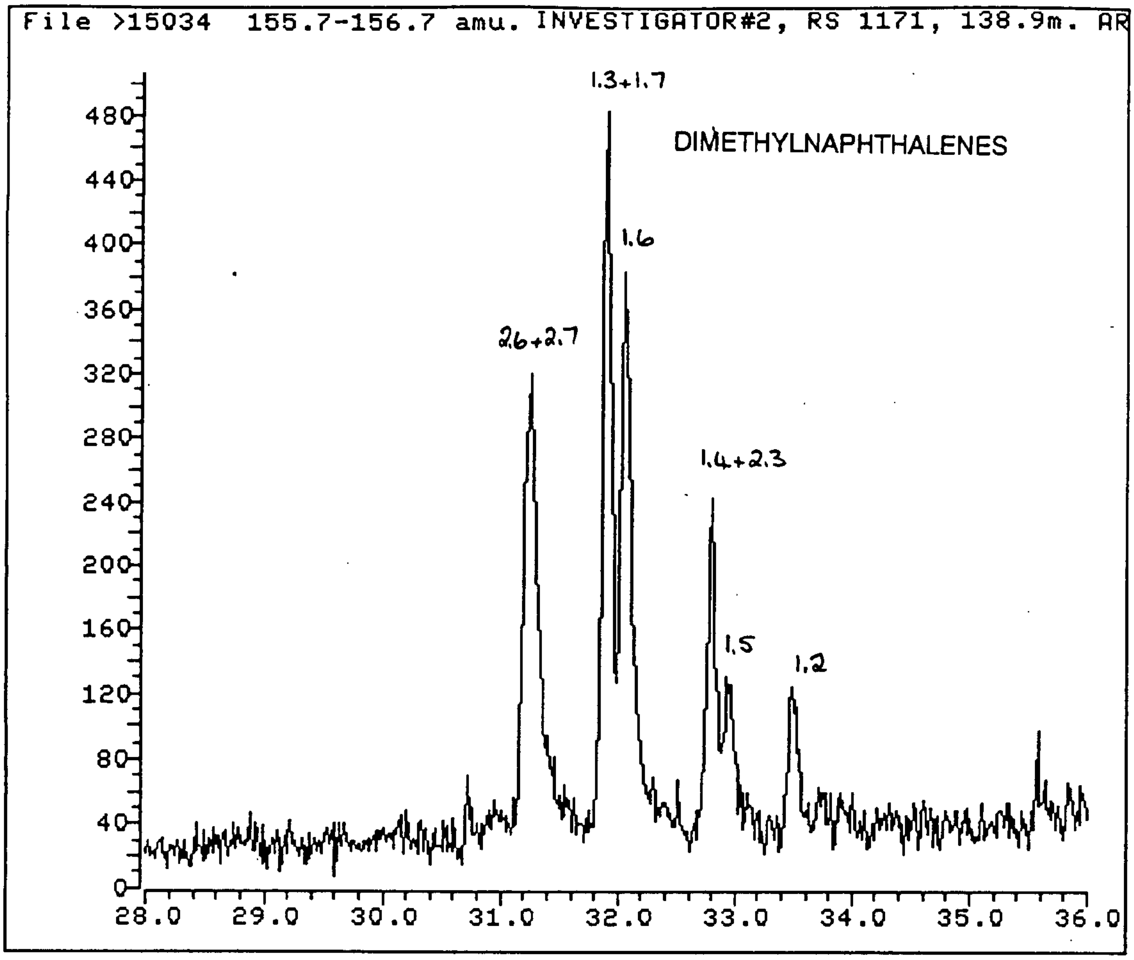

File >15036 9999.0-0.0 amu. INVESTIGATOR#2, RS 1252, 343.5m. AR
TIC
6000
5600
5200
4800
4400
4000
3600
3200
2800
2400
2000
1600
1200
800
400
0
24
28
32
36
40
44
48
52
56
60
64
68
72

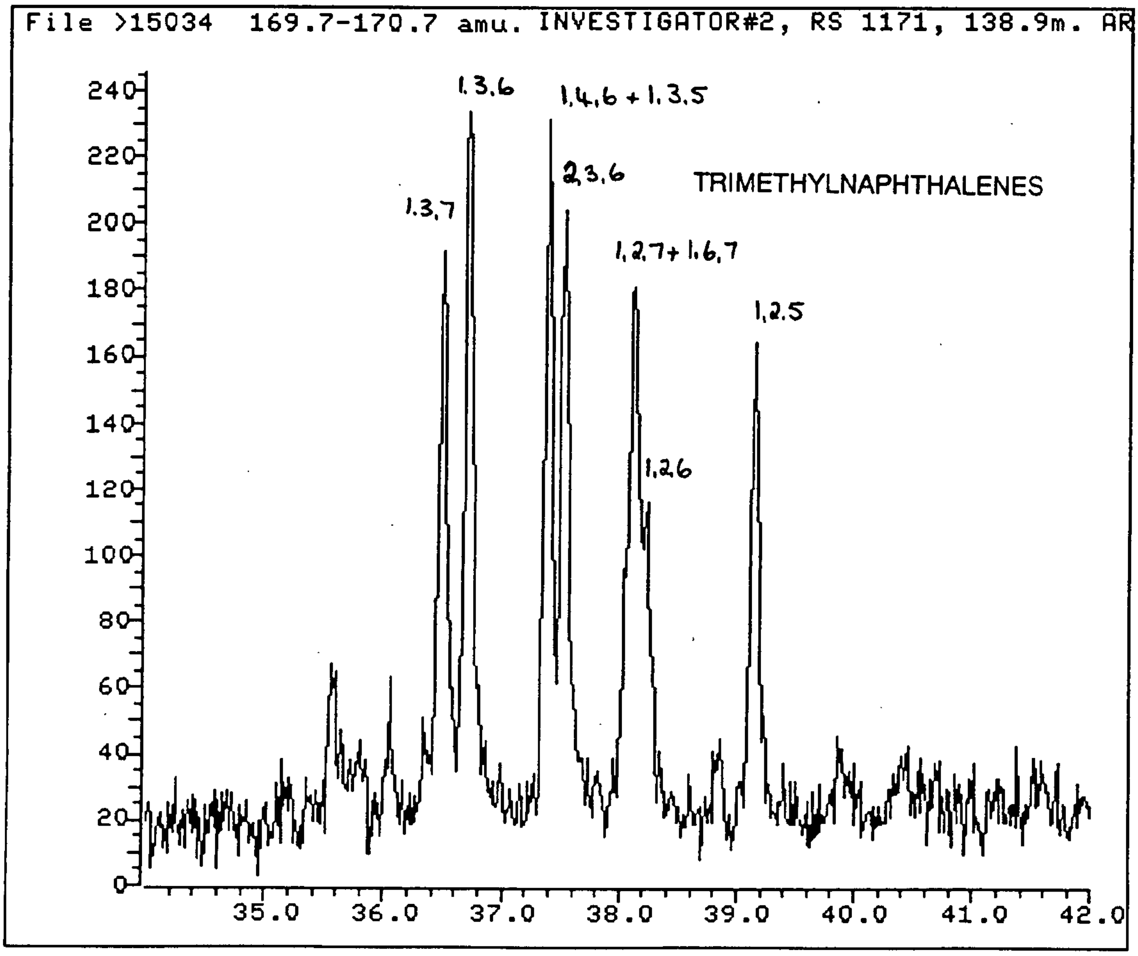
FIGURE 2C

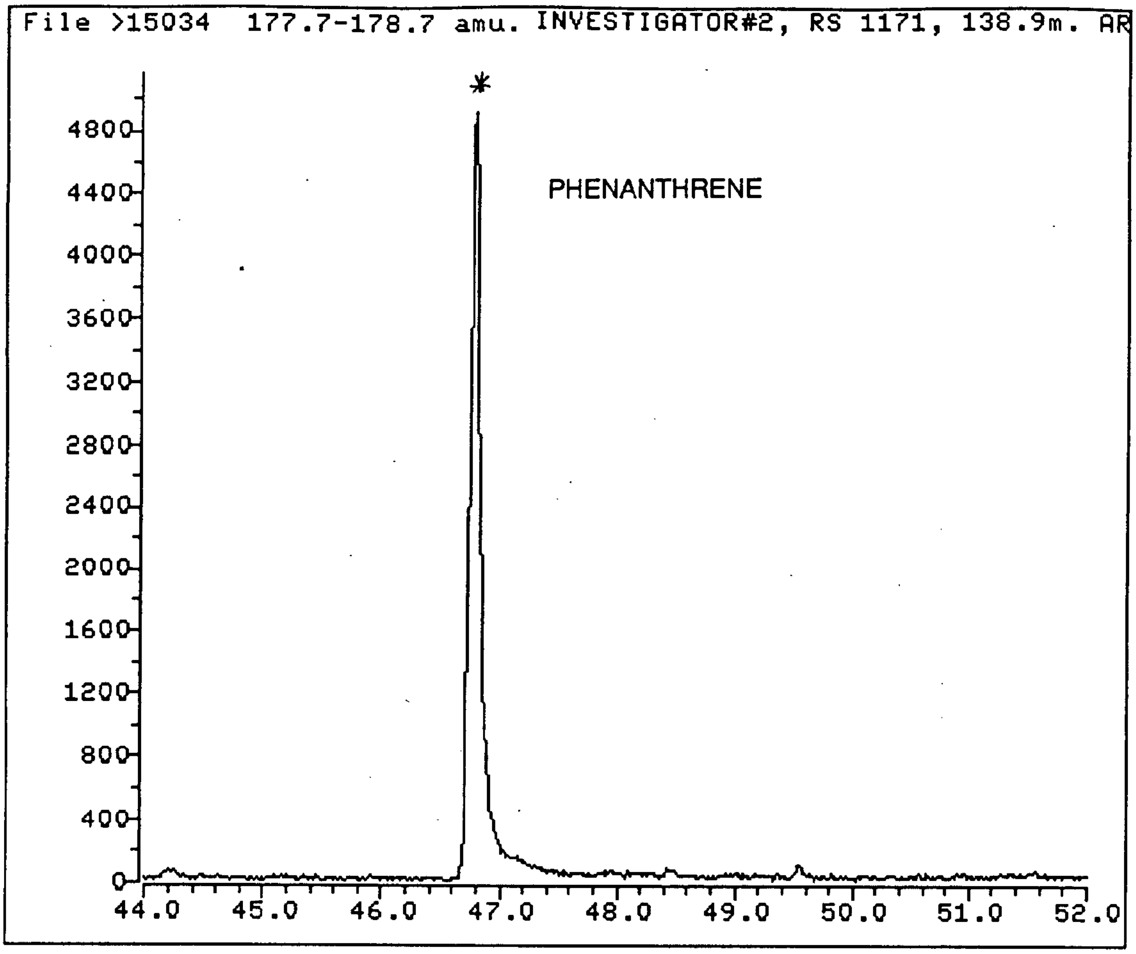
APPENDIX 1

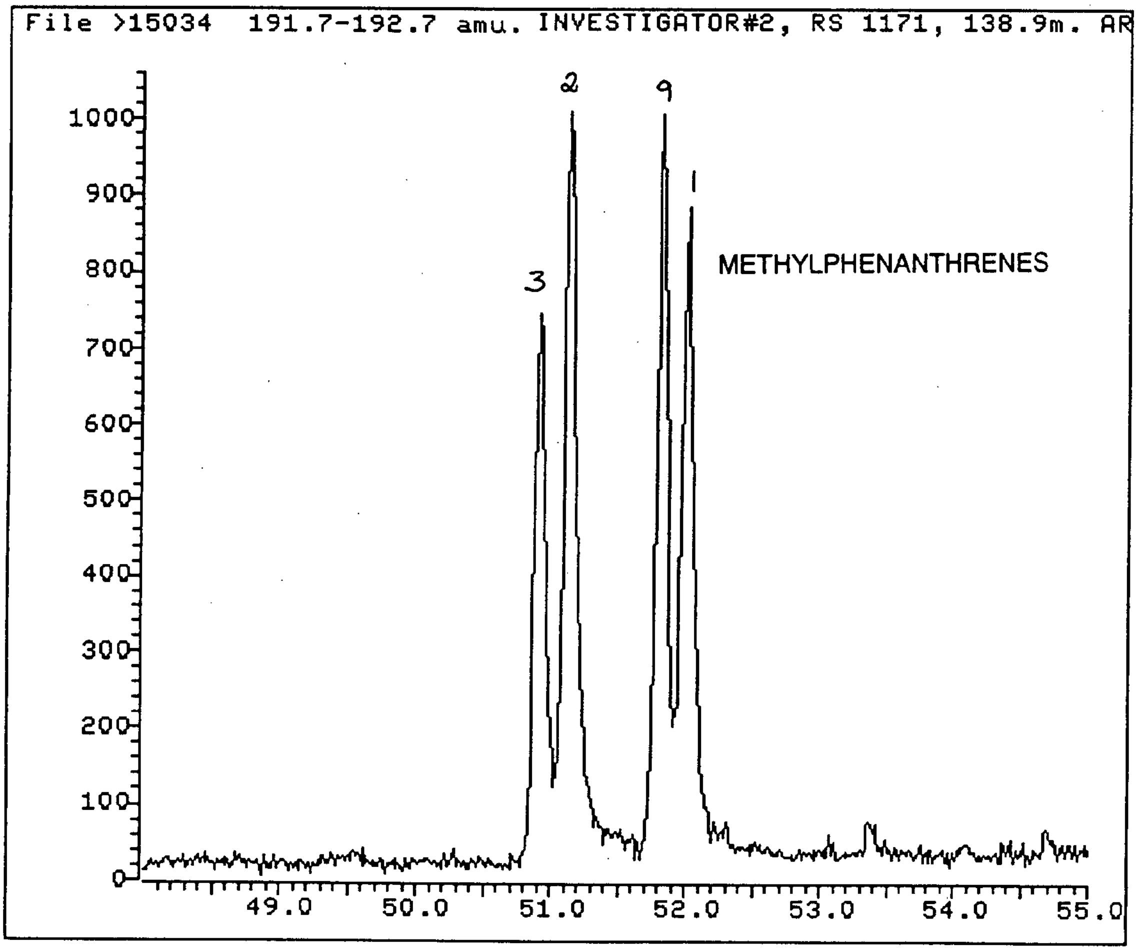
GC-MS SIM chromatograms of aromatic hydrocarbons
in core sample RS 1171 from the Mount McDonnell Formation,
SADME Investigator-2

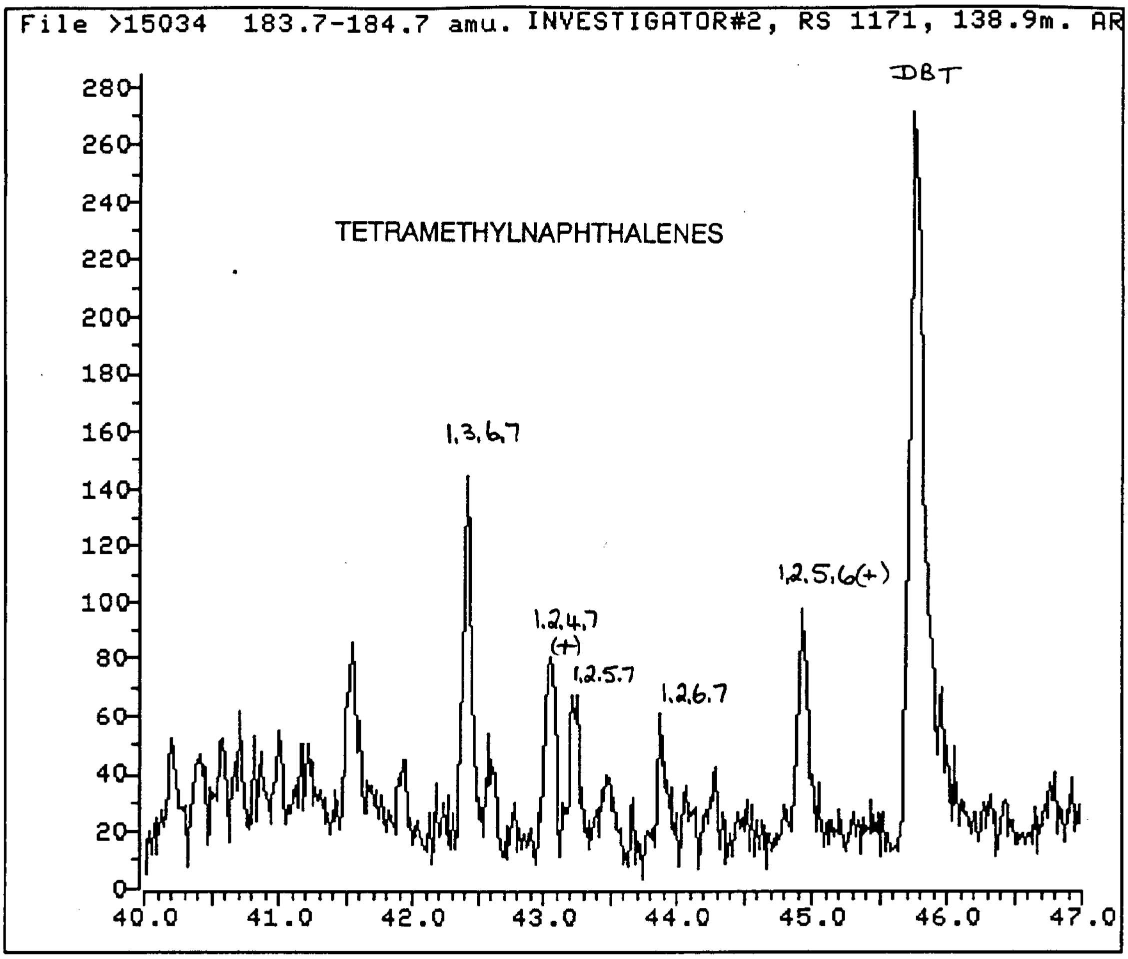
m/z	*Compounds*
156	dimethylnaphthalenes
170	trimethylnaphthalenes
184	tetramethylnaphthalenes
178	phenanthrene
192	methylphenanthrenes
206	dimethylphenanthrenes
219	retene

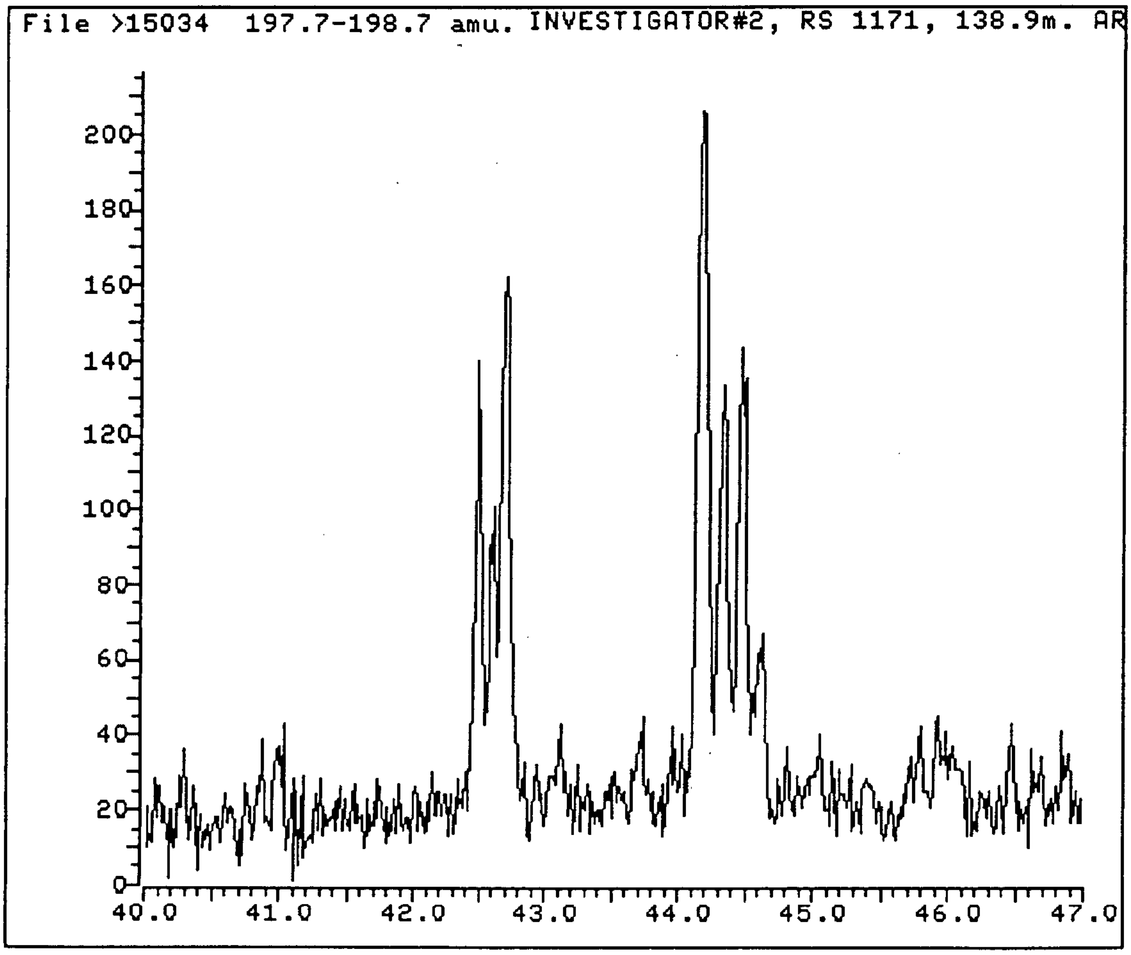

File >15034 155.7-156.7 amu. INVESTIGATOR#2, RS 1171, 138.9m. AR
DIMETHYLNAPHTHALENES
1.3+1.7
1.6
2.6+2.7
1.4+2.3
1.5
1.2
0
40
80
120
160
200
240
280
320
360
400
440
480
28.0
29.0
30.0
31.0
32.0
33.0
34.0
35.0
36.0

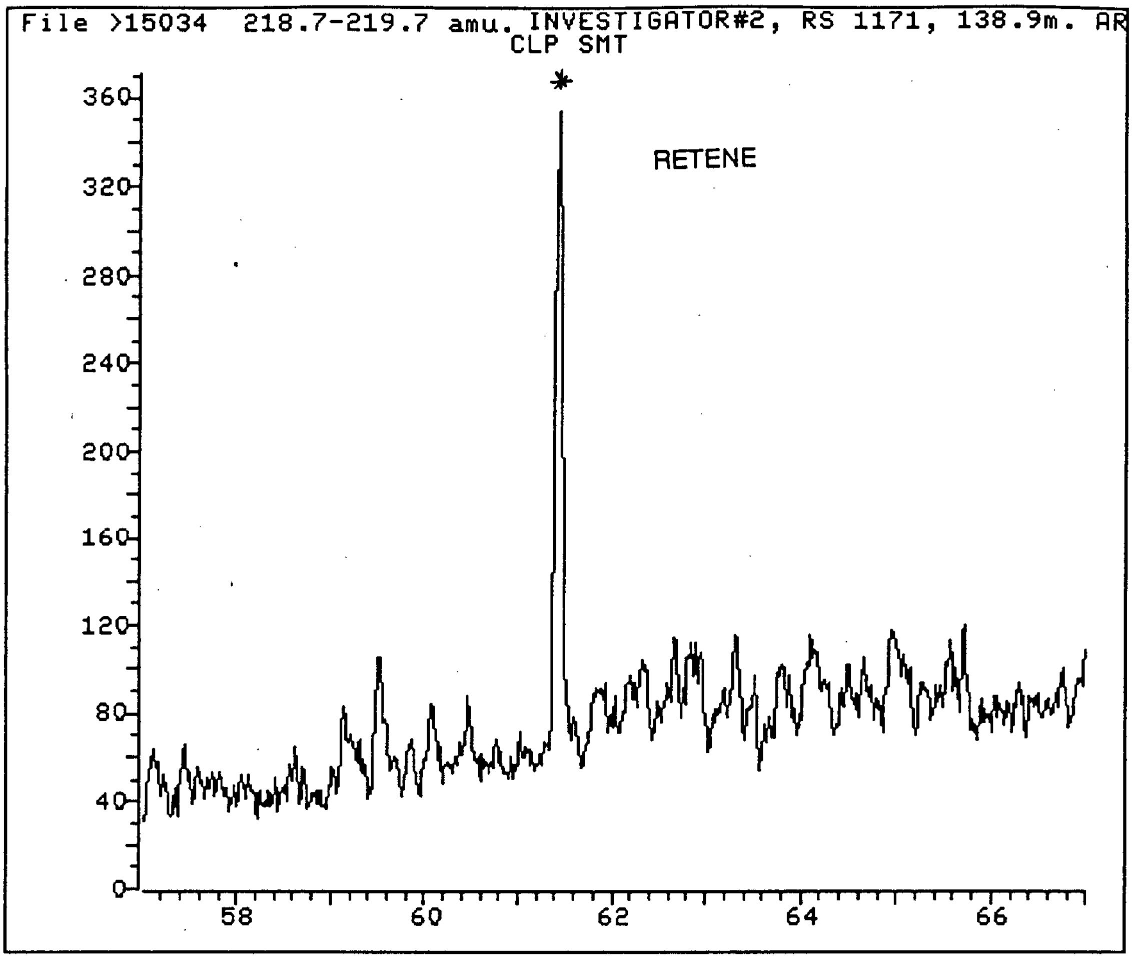

File >15034 169.7-170.7 amu. INVESTIGATOR#2, RS 1171, 138.9m. AR
TRIMETHYLNAPHTHALENES
1.3.7
1.3.6
1.4.6 + 1.3.5
2.3.6
1.2.7+ 1.6.7
1.2.6
1.2.5
0
20
40
60
80
100
120
140
160
180
200
220
240
35.0
36.0
37.0
38.0
39.0
40.0
41.0
42.0


File >15034 177.7-178.7 amu. INVESTIGATOR#2, RS 1171, 138.9m. AR
*
PHENANTHRENE
4800
4400
4000
3600
3200
2800
2400
2000
1600
1200
800
400
0
44.0
45.0
46.0
47.0
48.0
49.0
50.0
51.0
52.0

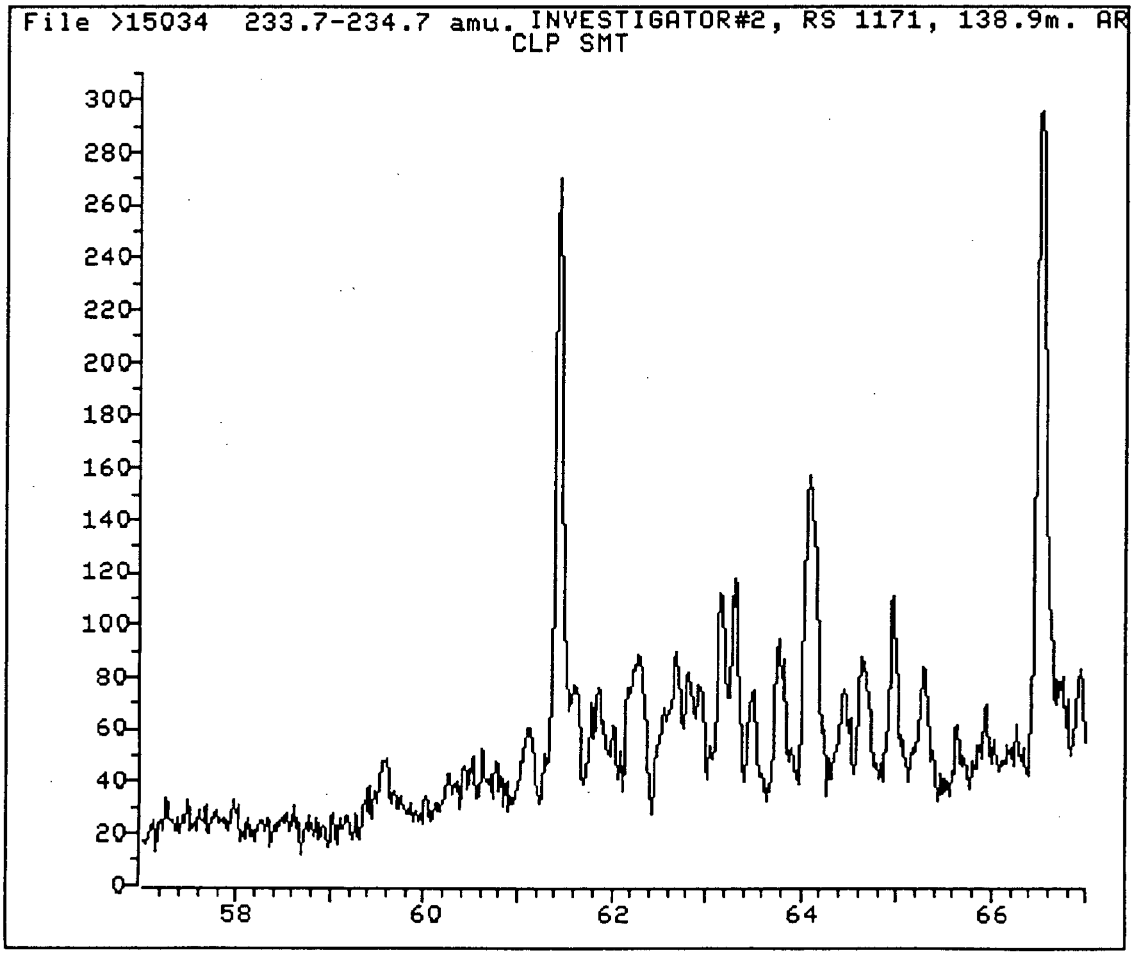

File >15034 191.7-192.7 amu. INVESTIGATOR#2, RS 1171, 138.9m. AR
3
2
9
1
METHYLPHENANTHRENES
1000
900
800
700
600
500
400
300
200
100
0
49.0
50.0
51.0
52.0
53.0
54.0
55.0


File >15034 183.7-184.7 amu. INVESTIGATOR#2, RS 1171, 138.9m. AR
TETRAMETHYLNAPHTHALENES
DBT
1,3,6,7
1,2,4,7
(+)
1,2,5,7
1,2,6,7
1,2,5,6(+)
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
40.0
41.0
42.0
43.0
44.0
45.0
46.0
47.0

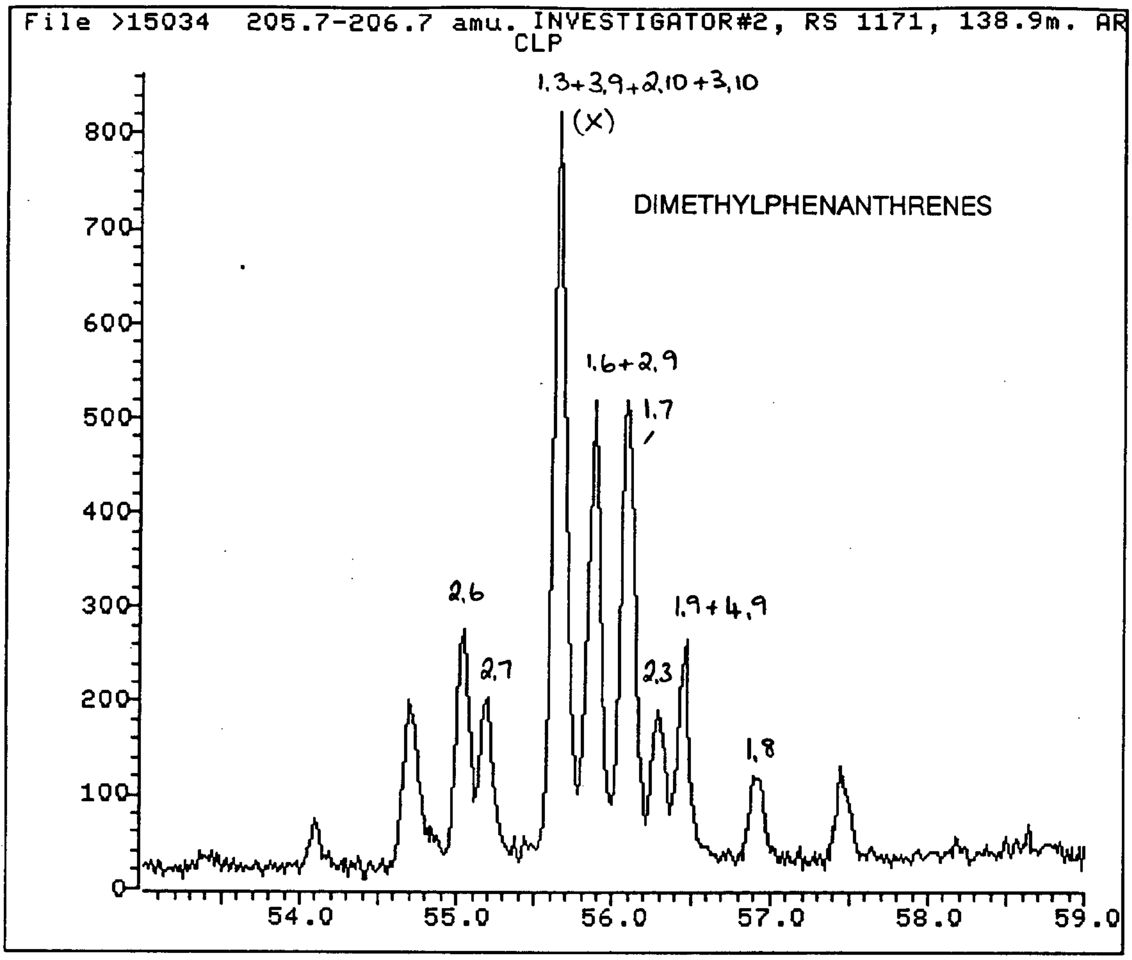

File >15034 197.7-198.7 amu. INVESTIGATOR#2, RS 1171, 138.9m. AR
0
20
40
60
80
100
120
140
160
180
200
40.0
41.0
42.0
43.0
44.0
45.0
46.0
47.0



File >15034 218.7-219.7 amu. INVESTIGATOR#2, RS 1171, 138.9m. AR
CLP SMT



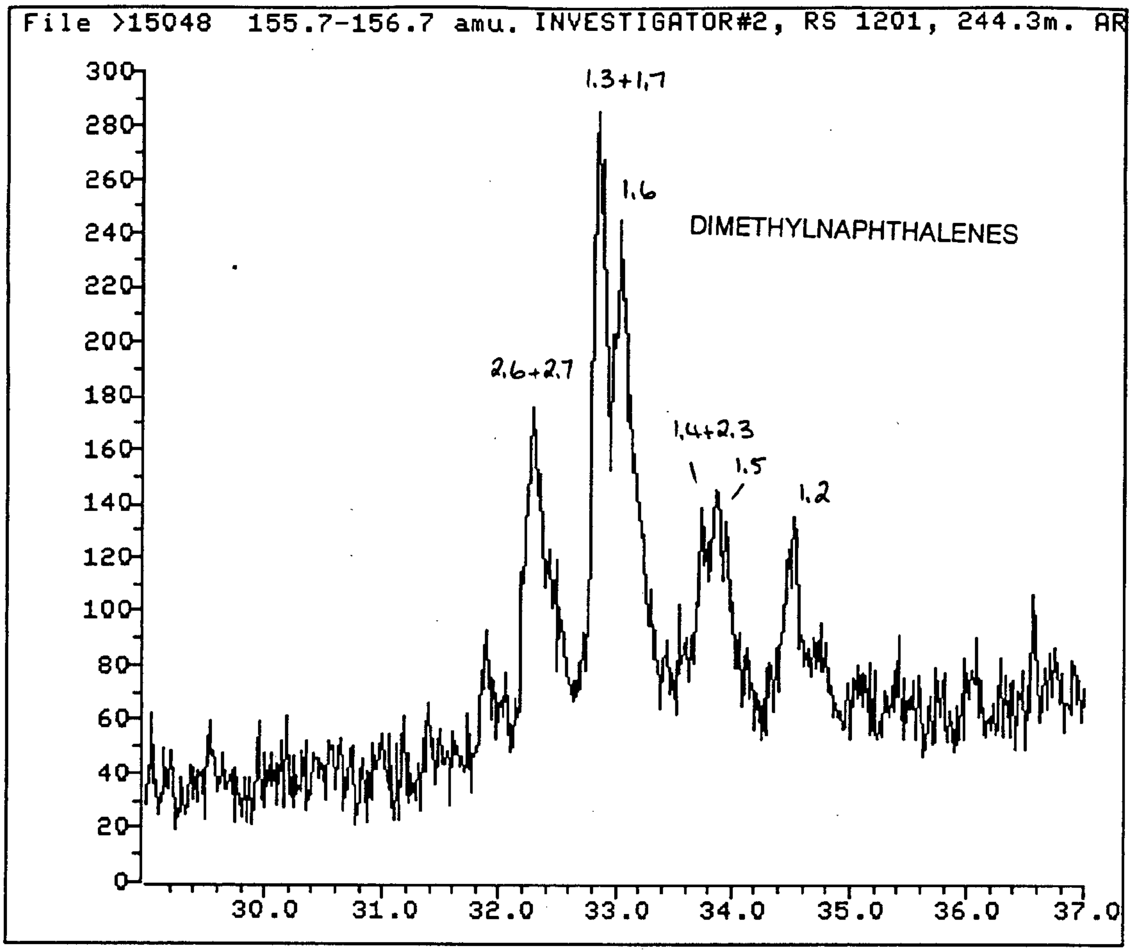
File >15034 233.7-234.7 amu. INVESTIGATOR#2, RS 1171, 138.9m. AR
CLP SMT

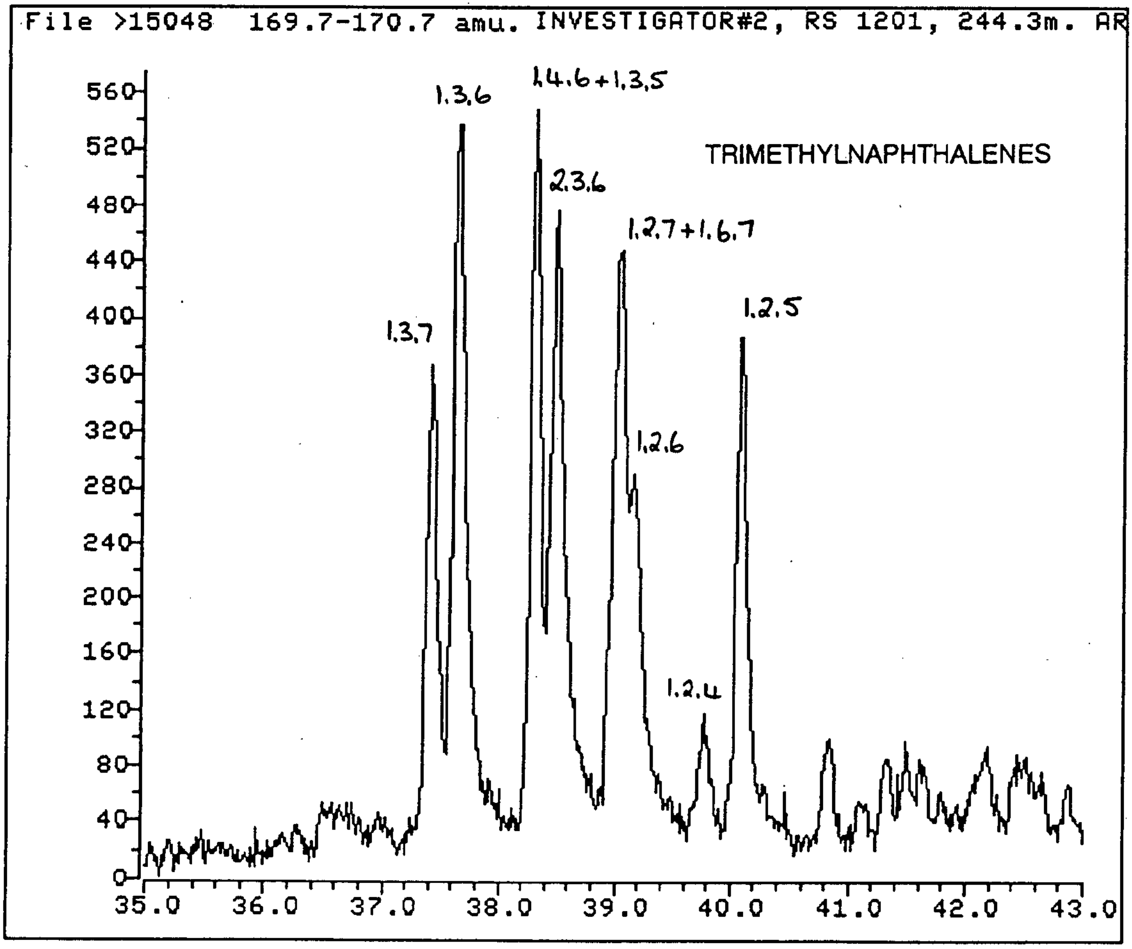

File >15034 205.7-206.7 amu. INVESTIGATOR#2, RS 1171, 138.9m. AR
CLP
1.3+3.9+2.10+3.10
(X)
DIMETHYLPHENANTHRENES
1.6+2.9
1.7
2.6
2.7
2.3
1.9+4.9
1.8
800
700
600
500
400
300
200
100
0
54.0
55.0
56.0
57.0
58.0
59.0

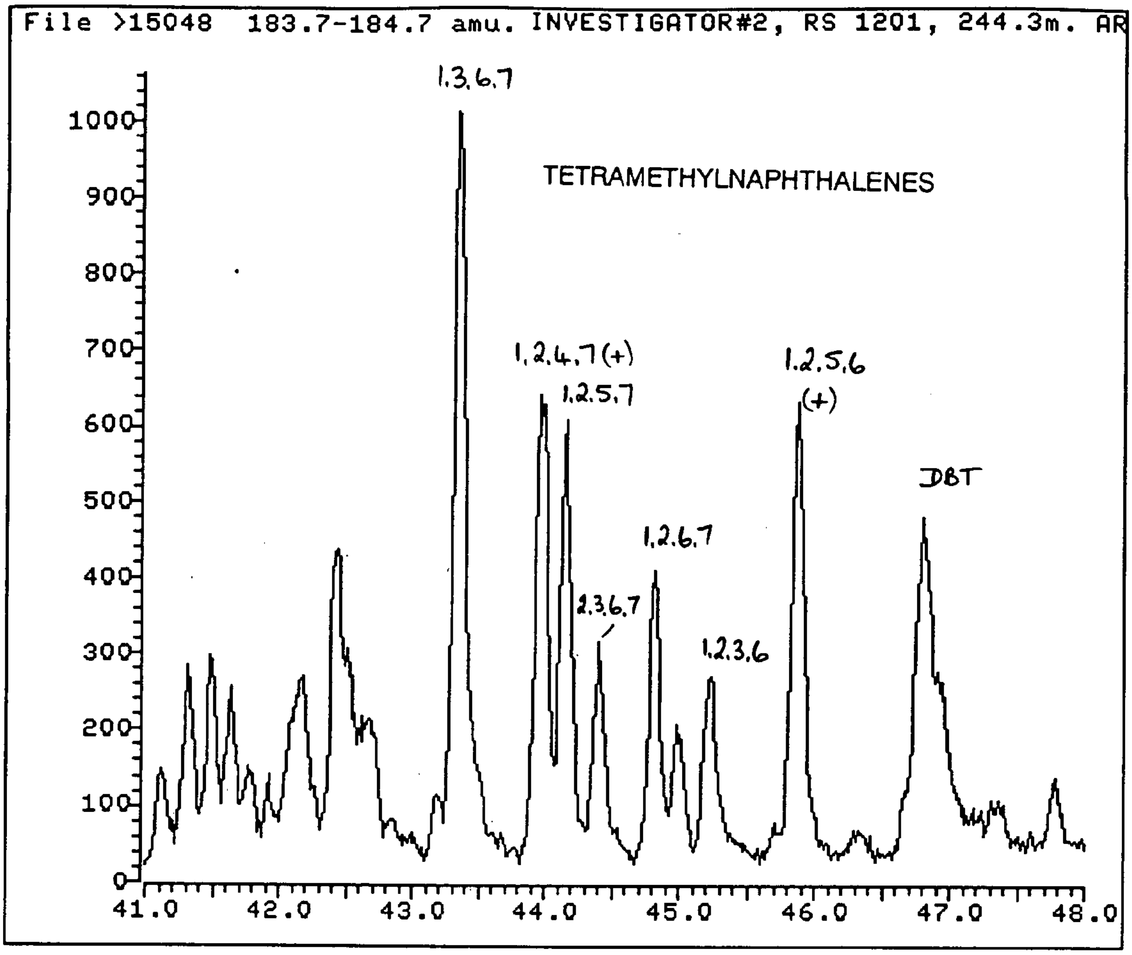
APPENDIX 2

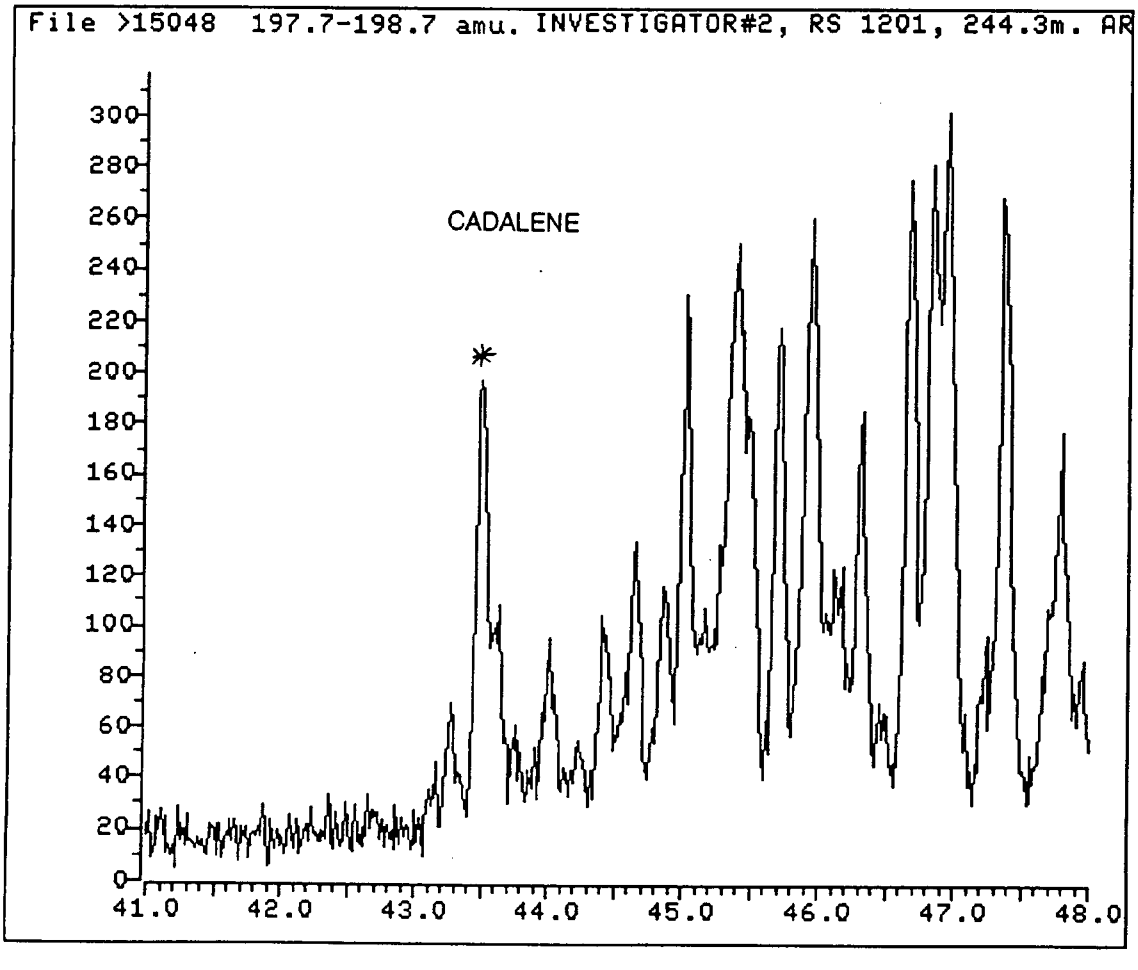
GC-MS SIM chromatograms of aromatic hydrocarbons in core sample RS 1201 from the Mount McDonnell Formation, SADME Investigator-2

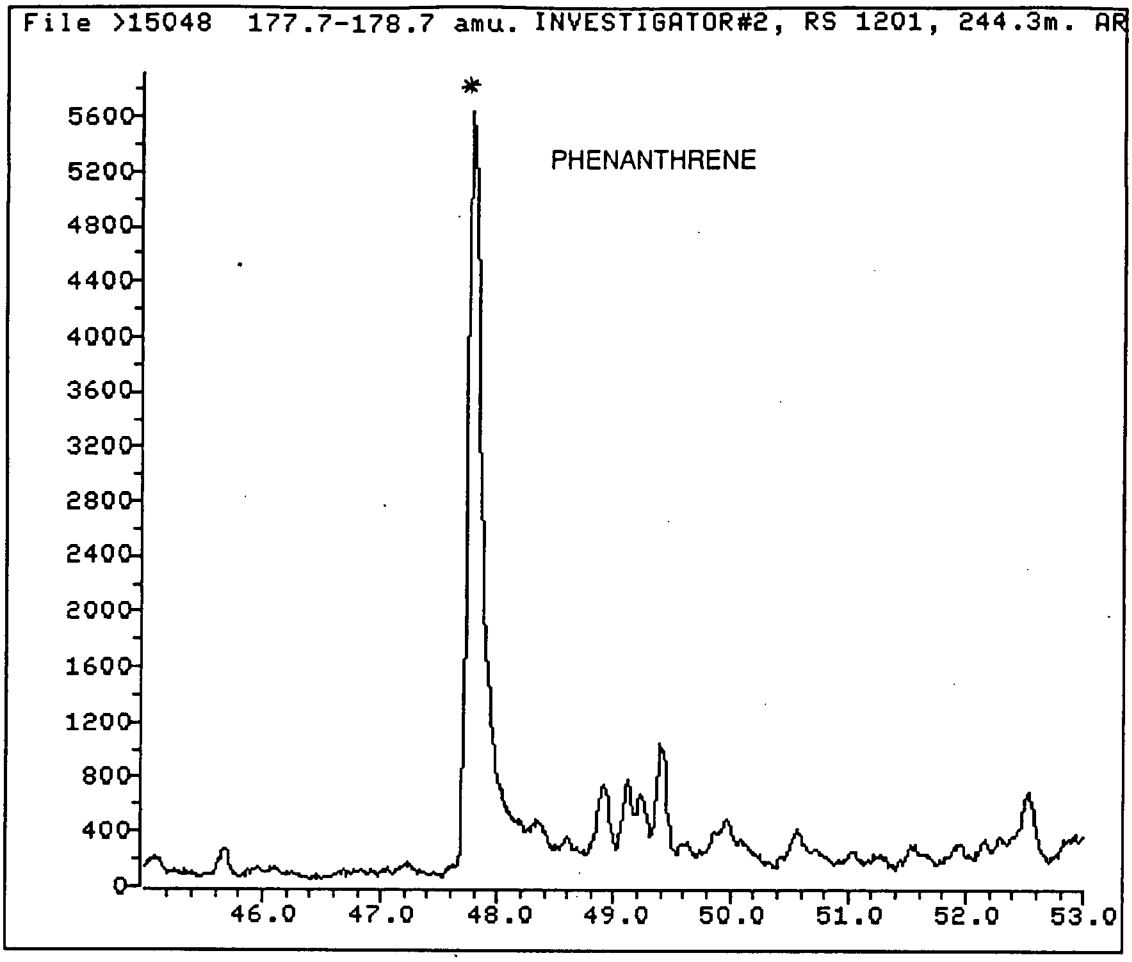
m/z	*Compounds*
156	dimethylnaphthalenes
170	trimethylnaphthalenes
184	tetramethylnaphthalenes
178	phenanthrene
192	methylphenanthrenes
206	dimethylphenanthrenes
219	retene

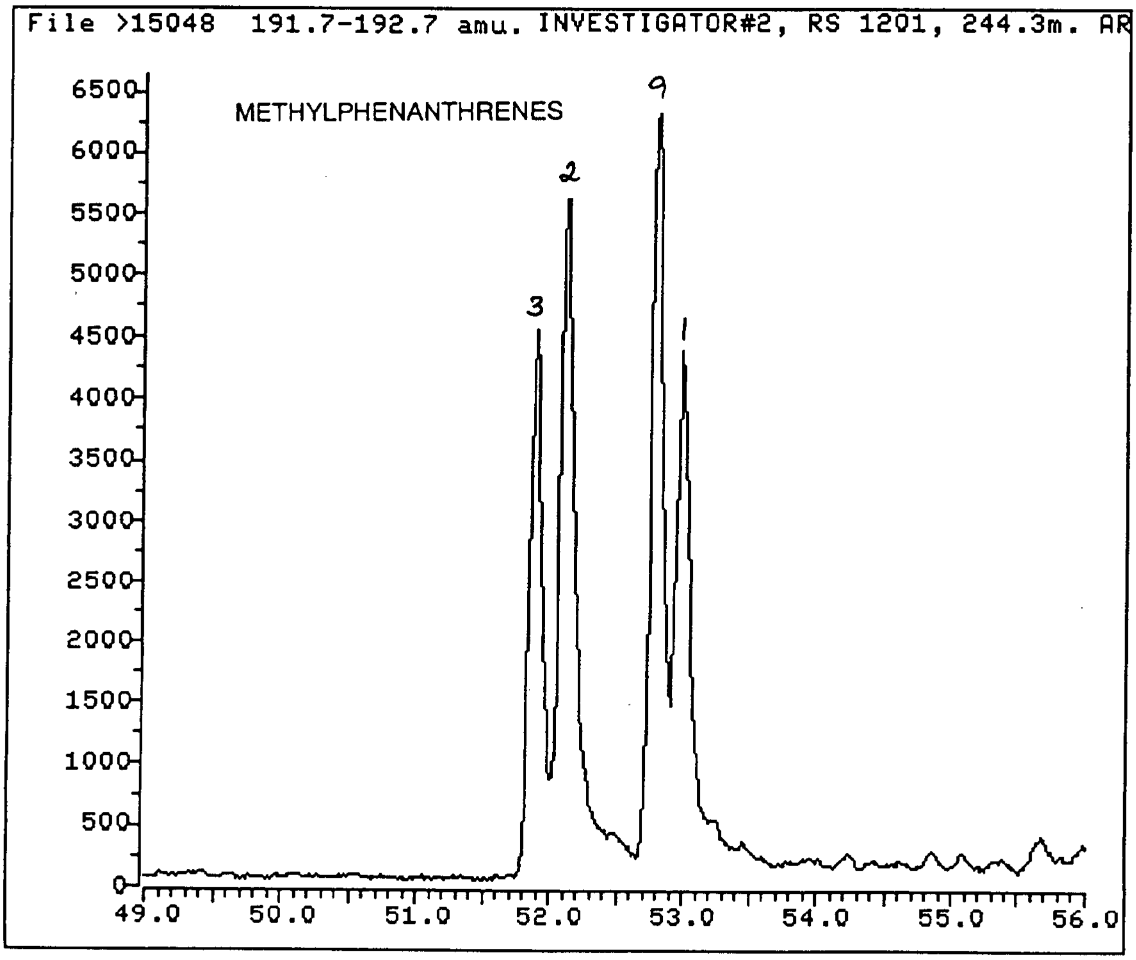

File >15048 155.7-156.7 amu. INVESTIGATOR#2, RS 1201, 244.3m. AR
DIMETHYLNAPHTHALENES
1.3+1.7
1.6
2.6+2.7
1.4+2.3
1.5
1.2
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
30.0
31.0
32.0
33.0
34.0
35.0
36.0
37.0

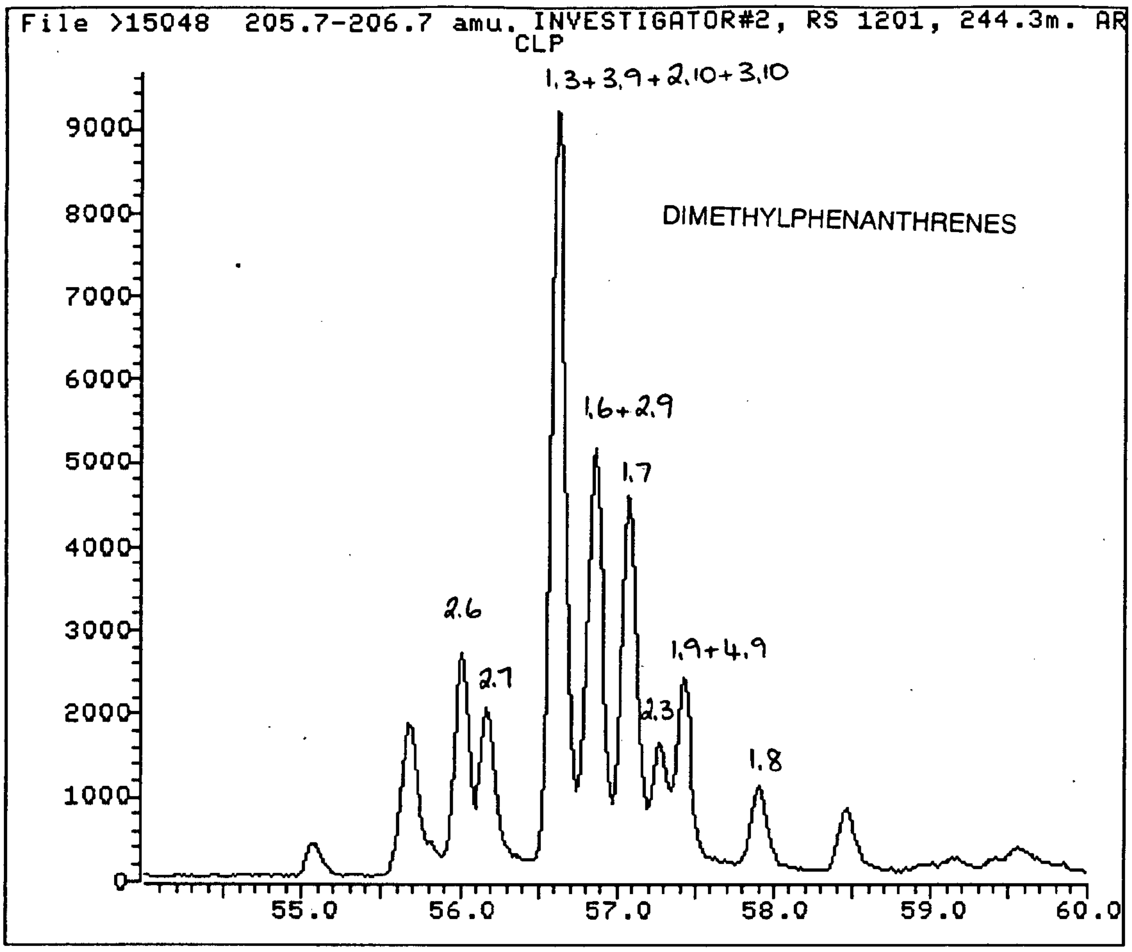

File >15048 169.7-170.7 amu. INVESTIGATOR#2, RS 1201, 244.3m. AR
TRIMETHYLNAPHTHALENES
1.3.6
1.4.6+1.3.5
2.3.6
1.2.7+1.6.7
1.3.7
1.2.5
1.2.6
1.2.4
560
520
480
440
400
360
320
280
240
200
160
120
80
40
0
35.0
36.0
37.0
38.0
39.0
40.0
41.0
42.0
43.0

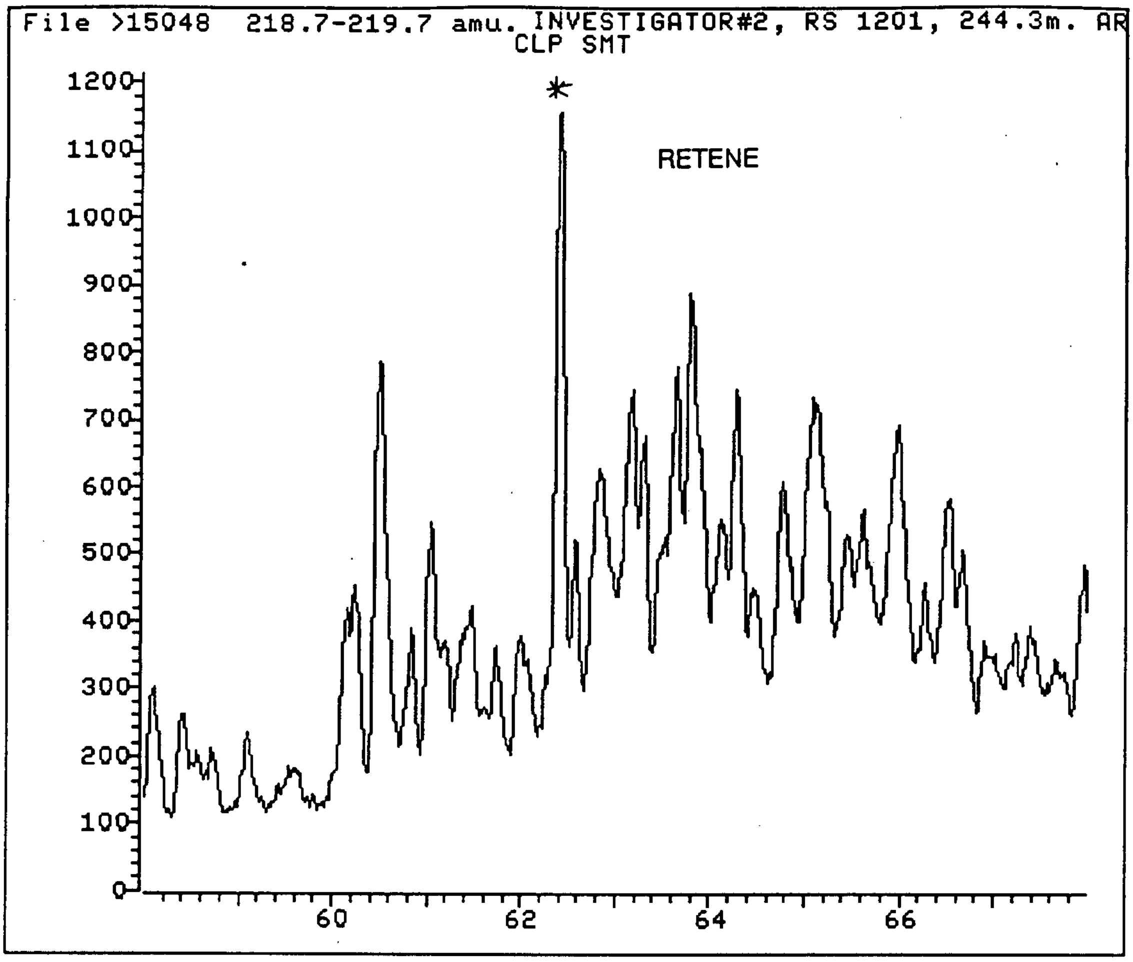

File >15048 183.7-184.7 amu. INVESTIGATOR#2, RS 1201, 244.3m. AR
TETRAMETHYLNAPHTHALENES
1,3,6,7
1,2,4,7 (+)
1,2,5,7
2,3,6,7
1,2,6,7
1,2,3,6
1,2,5,6 (+)
DBT
1000
900
800
700
600
500
400
300
200
100
0
41.0
42.0
43.0
44.0
45.0
46.0
47.0
48.0

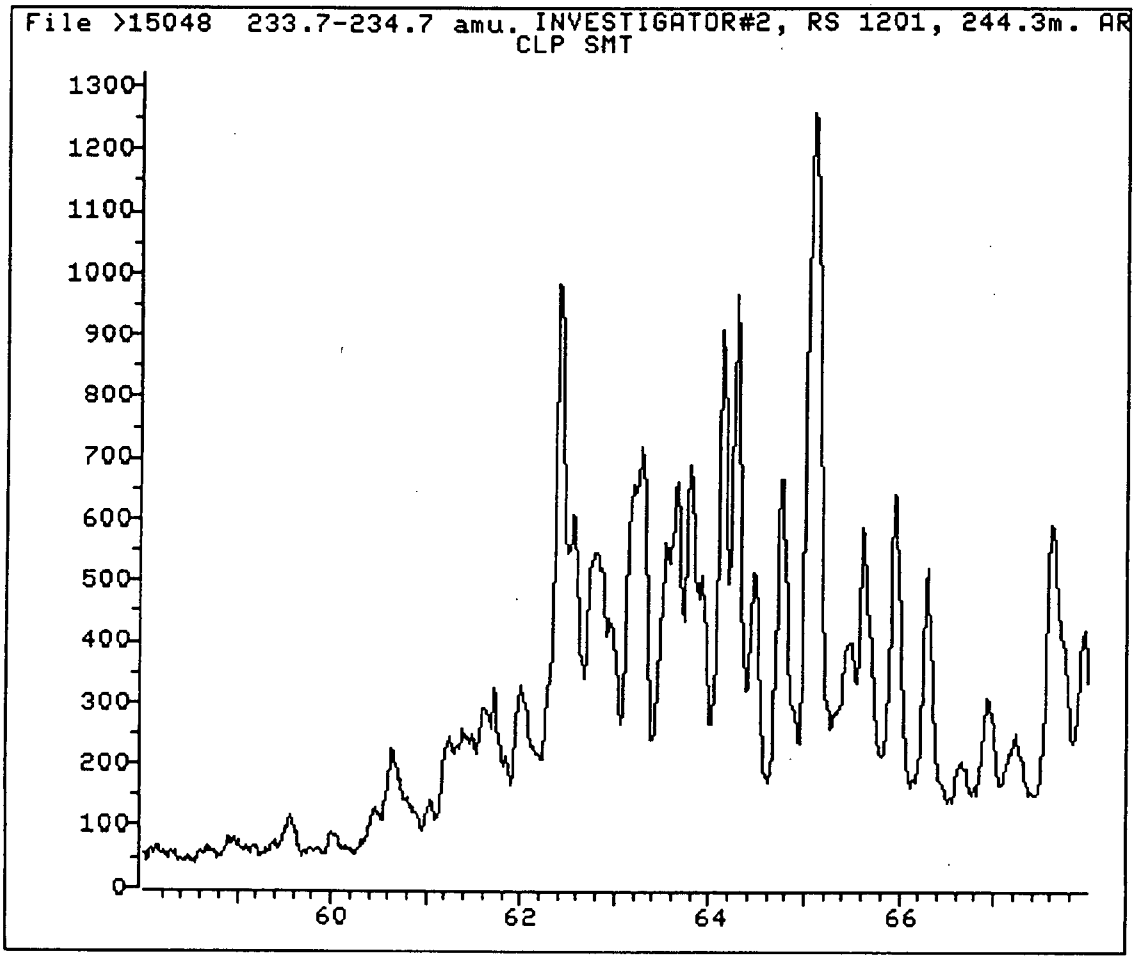

File >15048 197.7-198.7 amu. INVESTIGATOR#2, RS 1201, 244.3m. AR
CADALENE
*
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
41.0
42.0
43.0
44.0
45.0
46.0
47.0
48.0


File >15048 177.7-178.7 amu. INVESTIGATOR#2, RS 1201, 244.3m. AR
*
PHENANTHRENE
5600
5200
4800
4400
4000
3600
3200
2800
2400
2000
1600
1200
800
400
0
46.0
47.0
48.0
49.0
50.0
51.0
52.0
53.0


File >15048 191.7-192.7 amu. INVESTIGATOR#2, RS 1201, 244.3m. AR
METHYLPHENANTHRENES
3
2
9
1
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
49.0
50.0
51.0
52.0
53.0
54.0
55.0
56.0


File >15048 205.7-206.7 amu. INVESTIGATOR#2, RS 1201, 244.3m. AR
CLP
1,3+3,9+2,10+3,10
DIMETHYLPHENANTHRENES
1,6+2,9
1,7
2,6
2,7
2,3
1,9+4,9
1,8
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
55.0
56.0
57.0
58.0
59.0
60.0

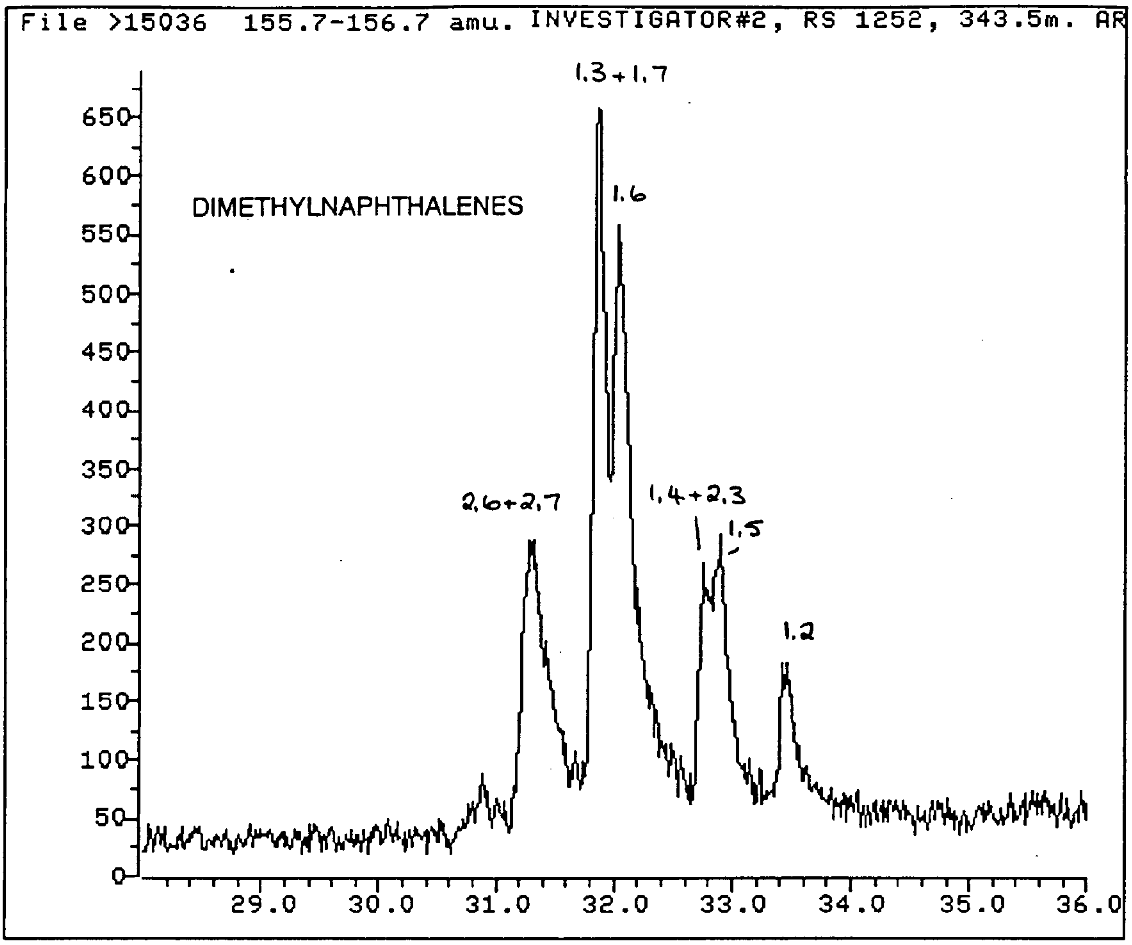

File >15048 218.7-219.7 amu. INVESTIGATOR#2, RS 1201, 244.3m. AR
CLP SMT
RETENE
*
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
60
62
64
66

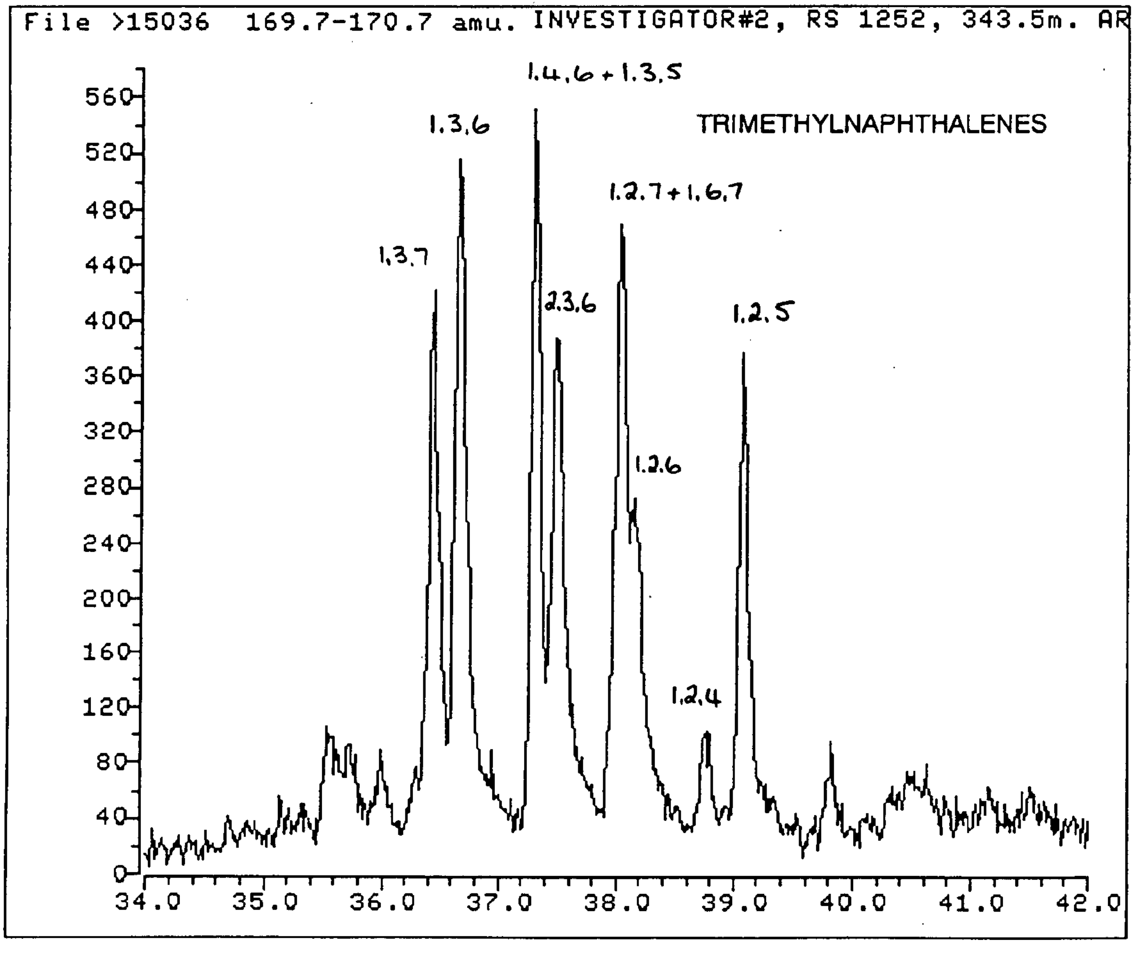

File >15048 233.7-234.7 amu. INVESTIGATOR#2, RS 1201, 244.3m. AR
CLP SMT
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
60
62
64
66

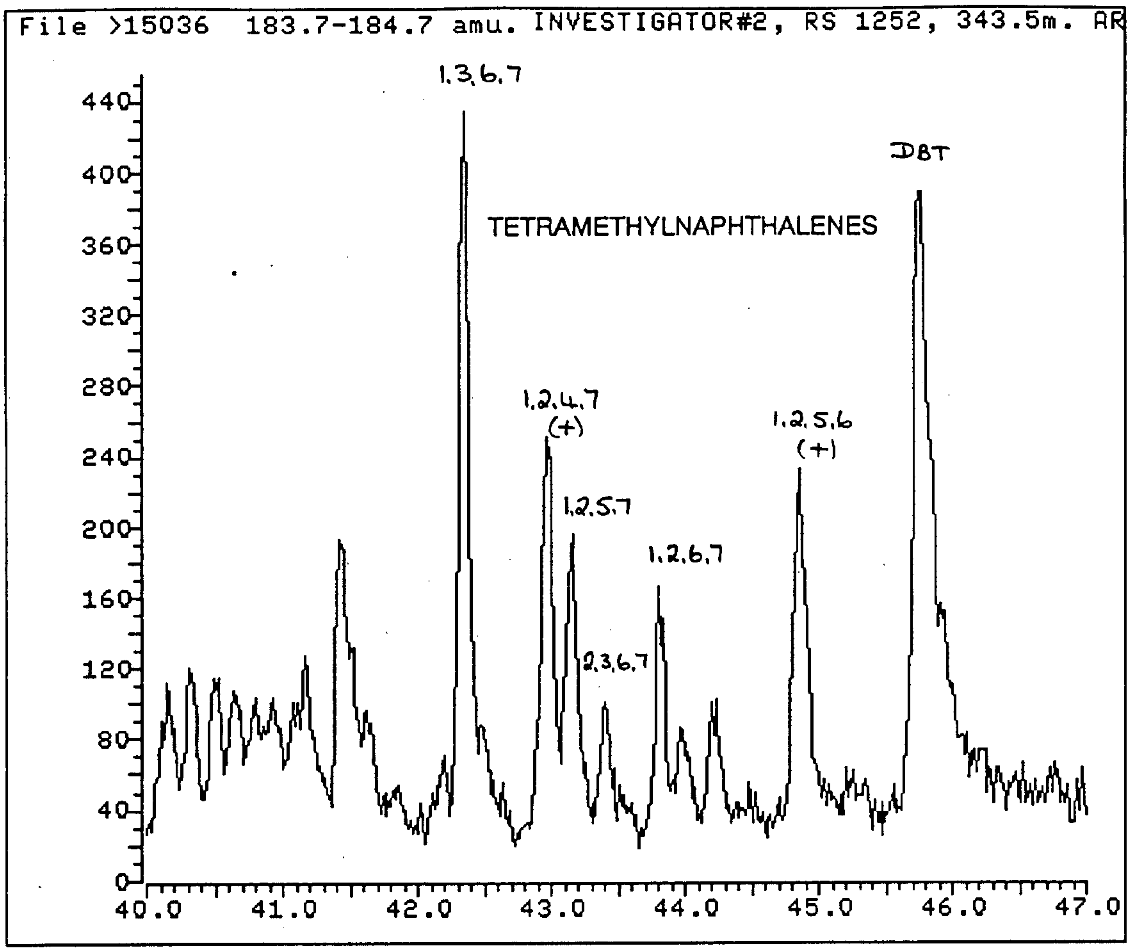
APPENDIX 3

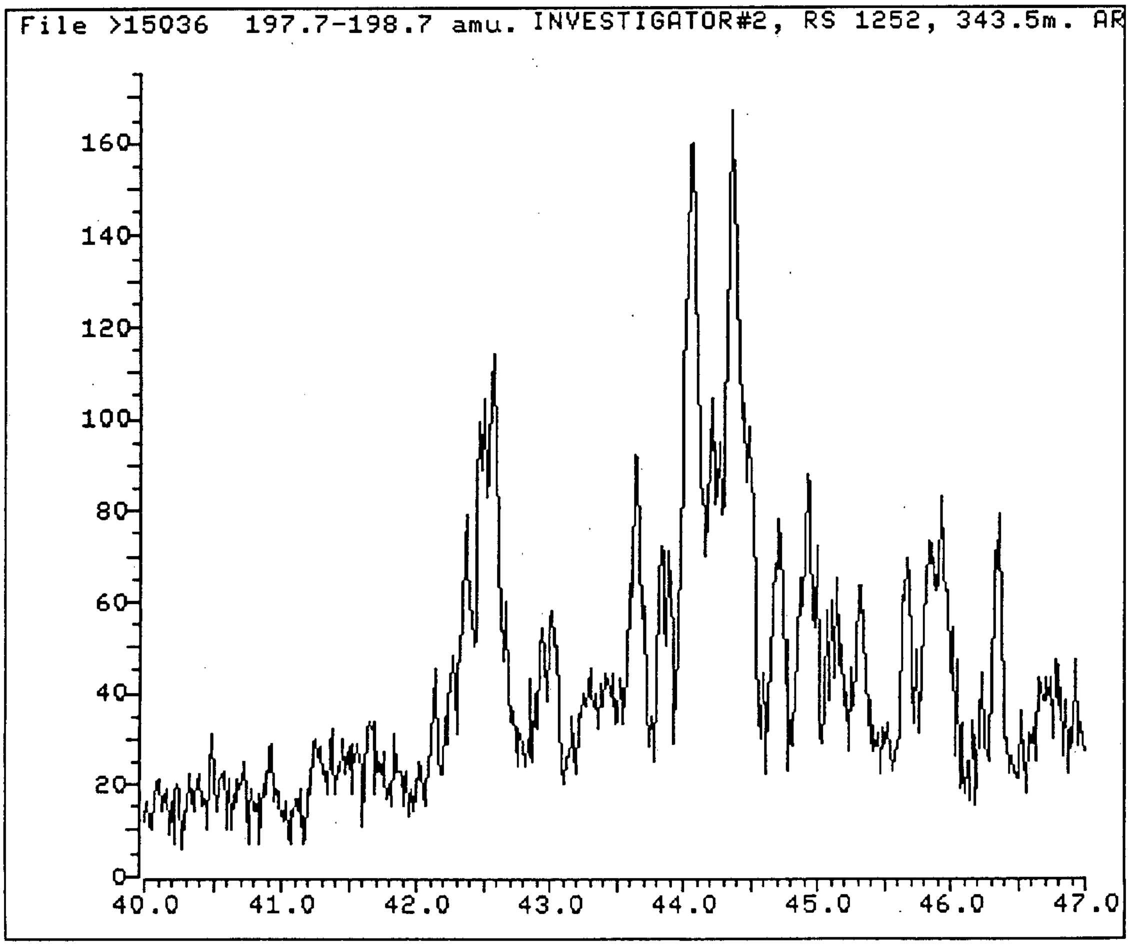
GC-MS SIM chromatograms of aromatic hydrocarbons in core sample RS 1252 from the Mount McDonnell Formation, SADME Investigator-2

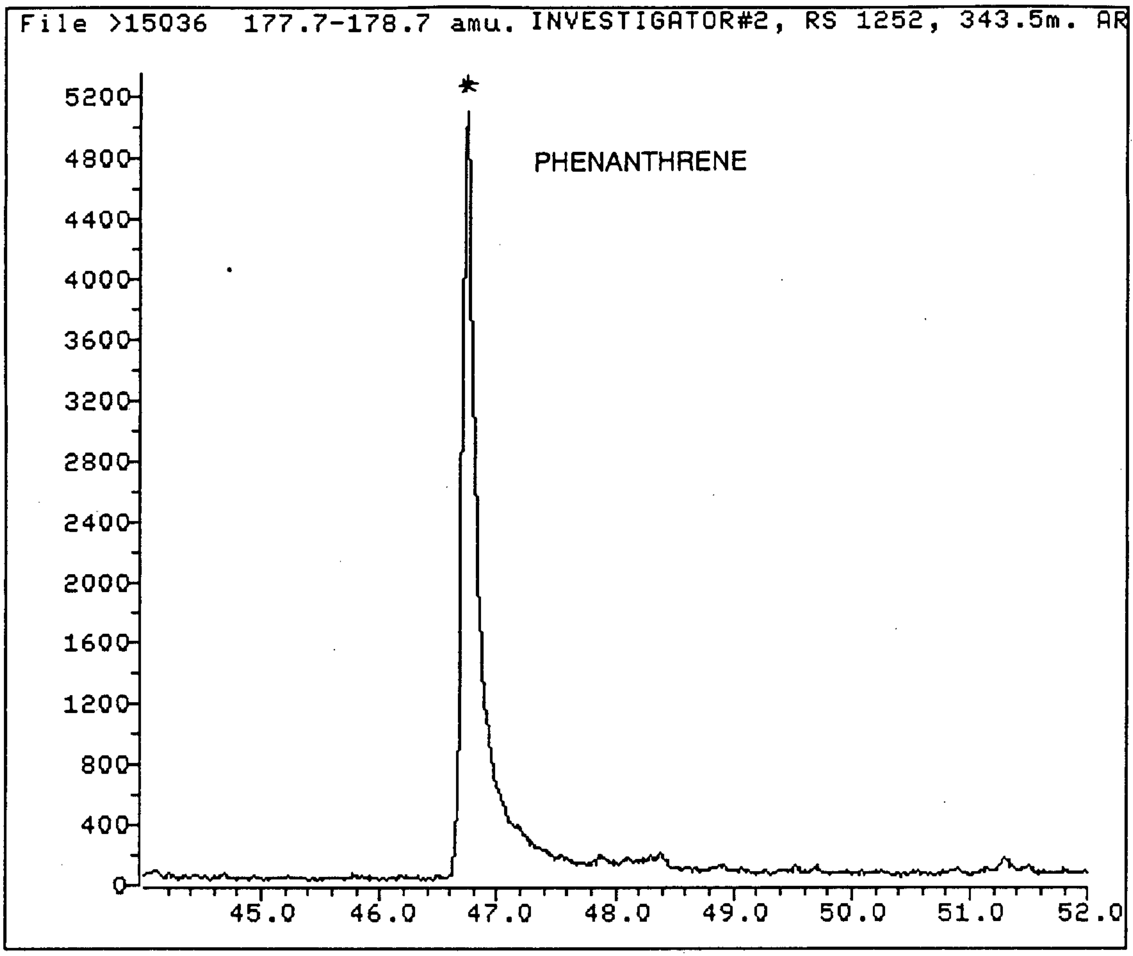
m/z	*Compounds*
156	dimethylnaphthalenes
170	trimethylnaphthalenes
184	tetramethylnaphthalenes
178	phenanthrene
192	methylphenanthrenes
206	dimethylphenanthrenes
219	retene

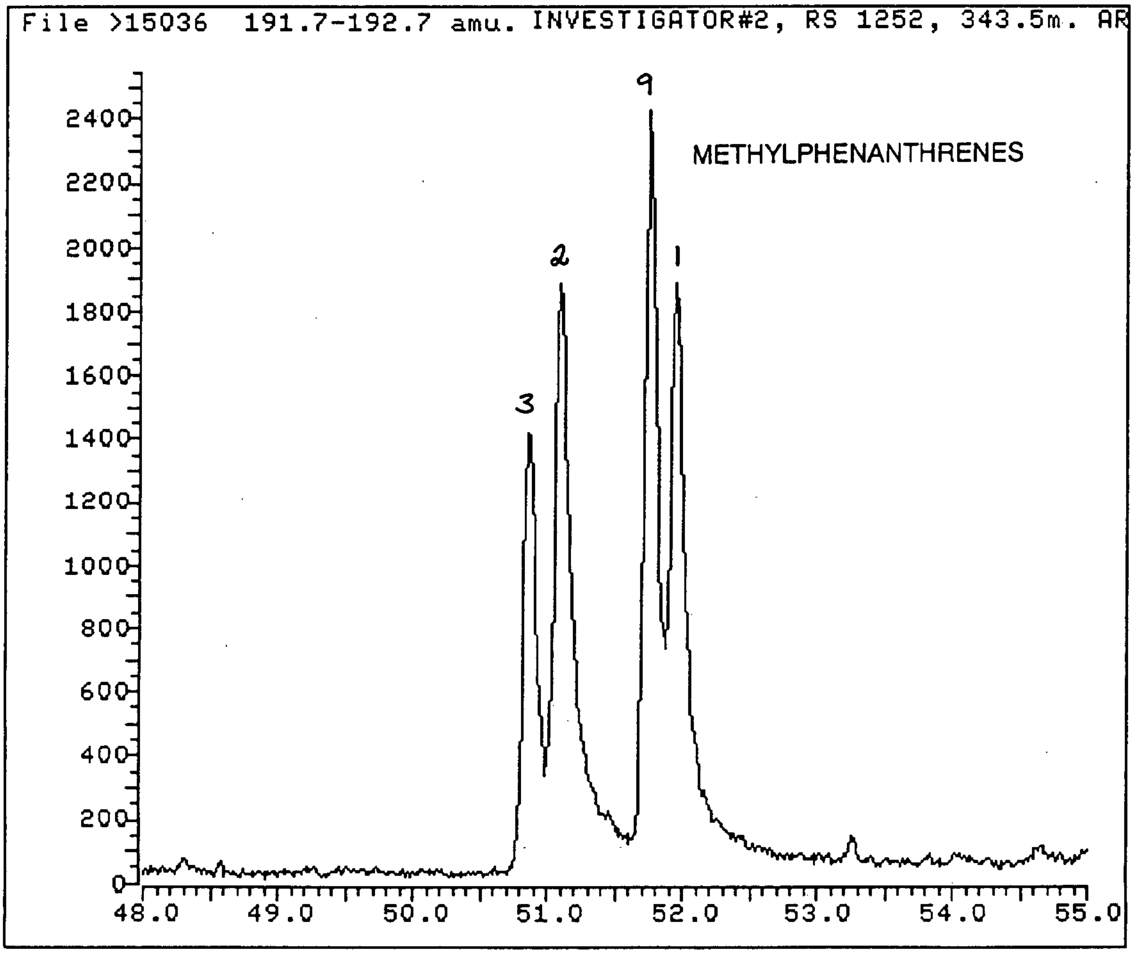

File >15036 155.7-156.7 amu. INVESTIGATOR#2, RS 1252, 343.5m. AR
DIMETHYLNAPHTHALENES
1.3+1.7
1.6
2.6+2.7
1.4+2.3
1.5
1.2
650
600
550
500
450
400
350
300
250
200
150
100
50
0
29.0
30.0
31.0
32.0
33.0
34.0
35.0
36.0

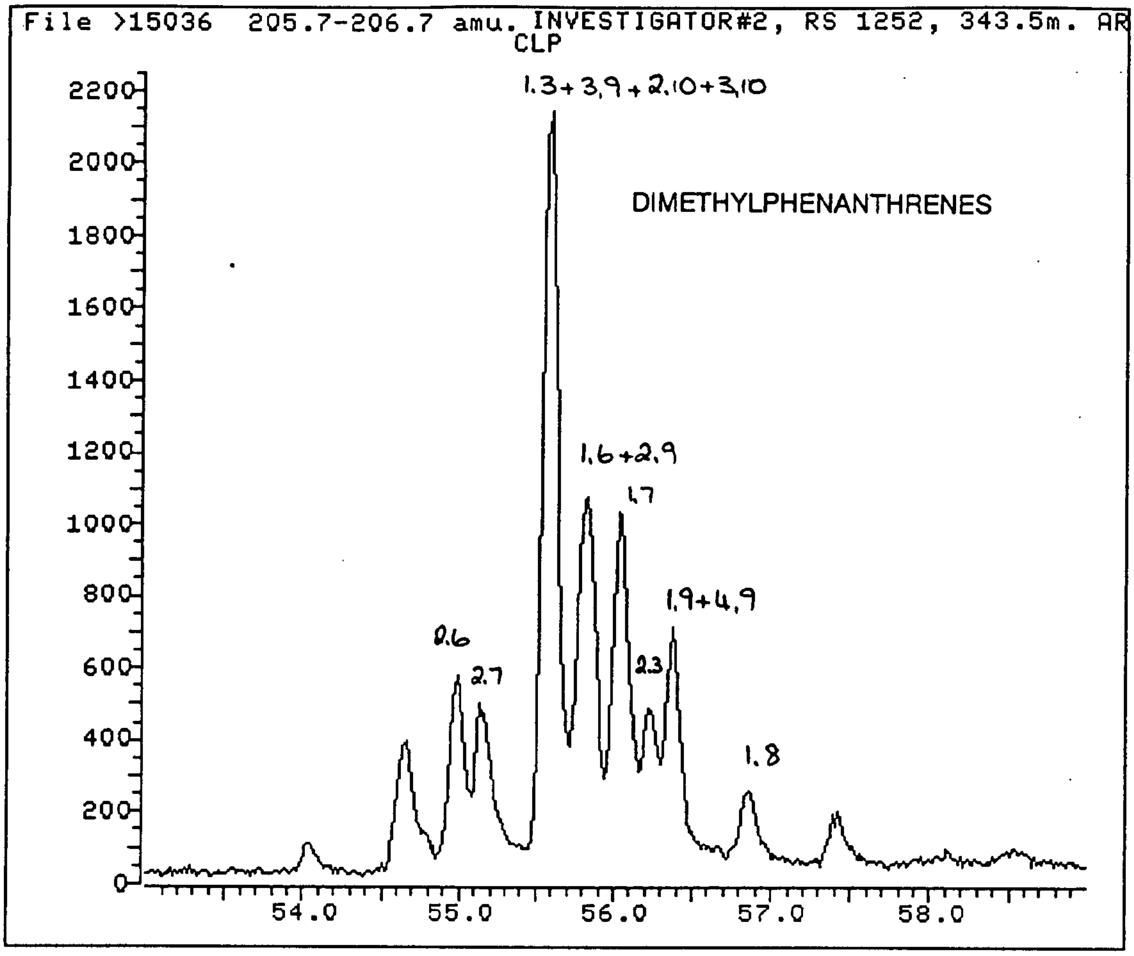

File >15036 169.7-170.7 amu. INVESTIGATOR#2, RS 1252, 343.5m. AR
TRIMETHYLNAPHTHALENES
1.4.6+1.3.5
1.3.6
1.3.7
2.3.6
1.2.7+1.6.7
1.2.6
1.2.5
1.2.4
560
520
480
440
400
360
320
280
240
200
160
120
80
40
0
34.0
35.0
36.0
37.0
38.0
39.0
40.0
41.0
42.0

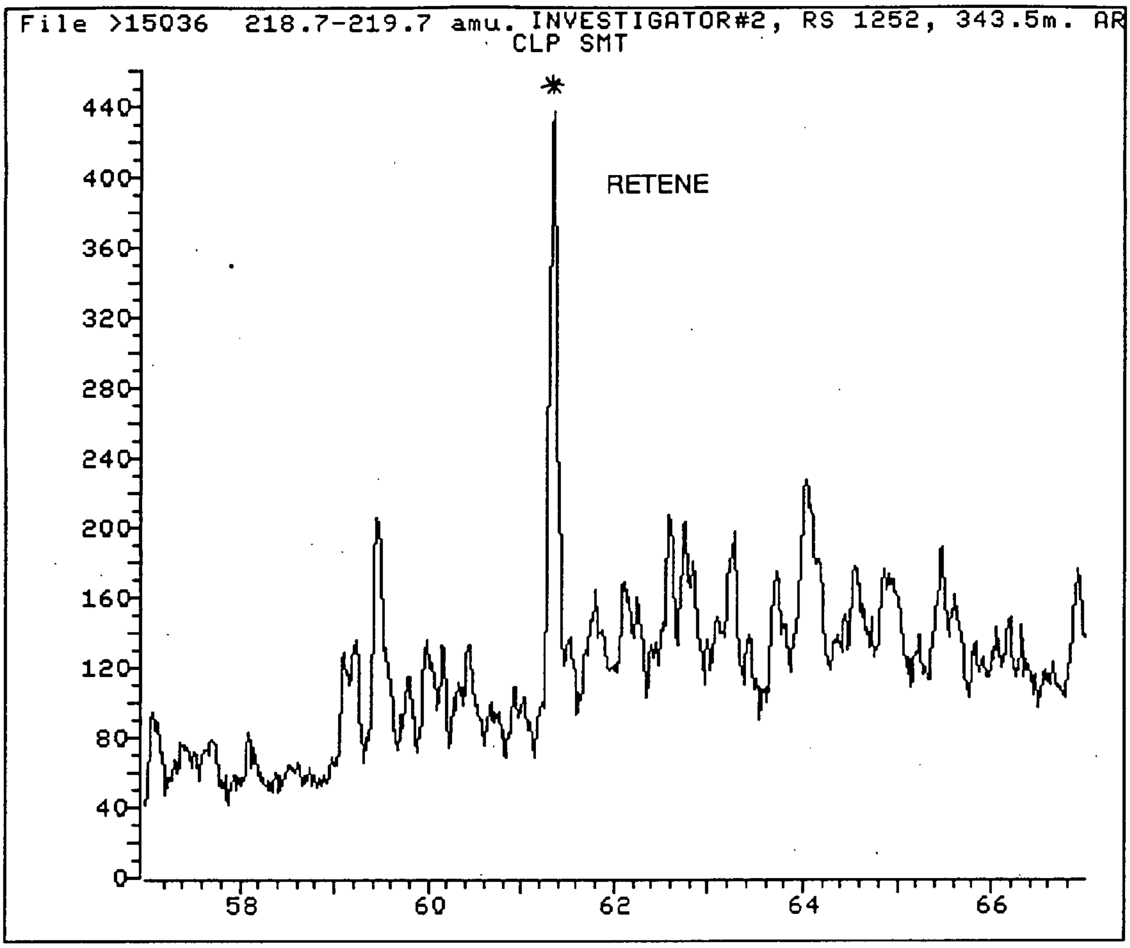

File >15036 183.7-184.7 amu. INVESTIGATOR#2, RS 1252, 343.5m. AR
TETRAMETHYLNAPHTHALENES
1,3,6,7
1,2,4,7
(+)
1,2,5,7
2,3,6,7
1,2,6,7
1,2,5,6
(+)
DBT
440
400
360
320
280
240
200
160
120
80
40
0
40.0
41.0
42.0
43.0
44.0
45.0
46.0
47.0

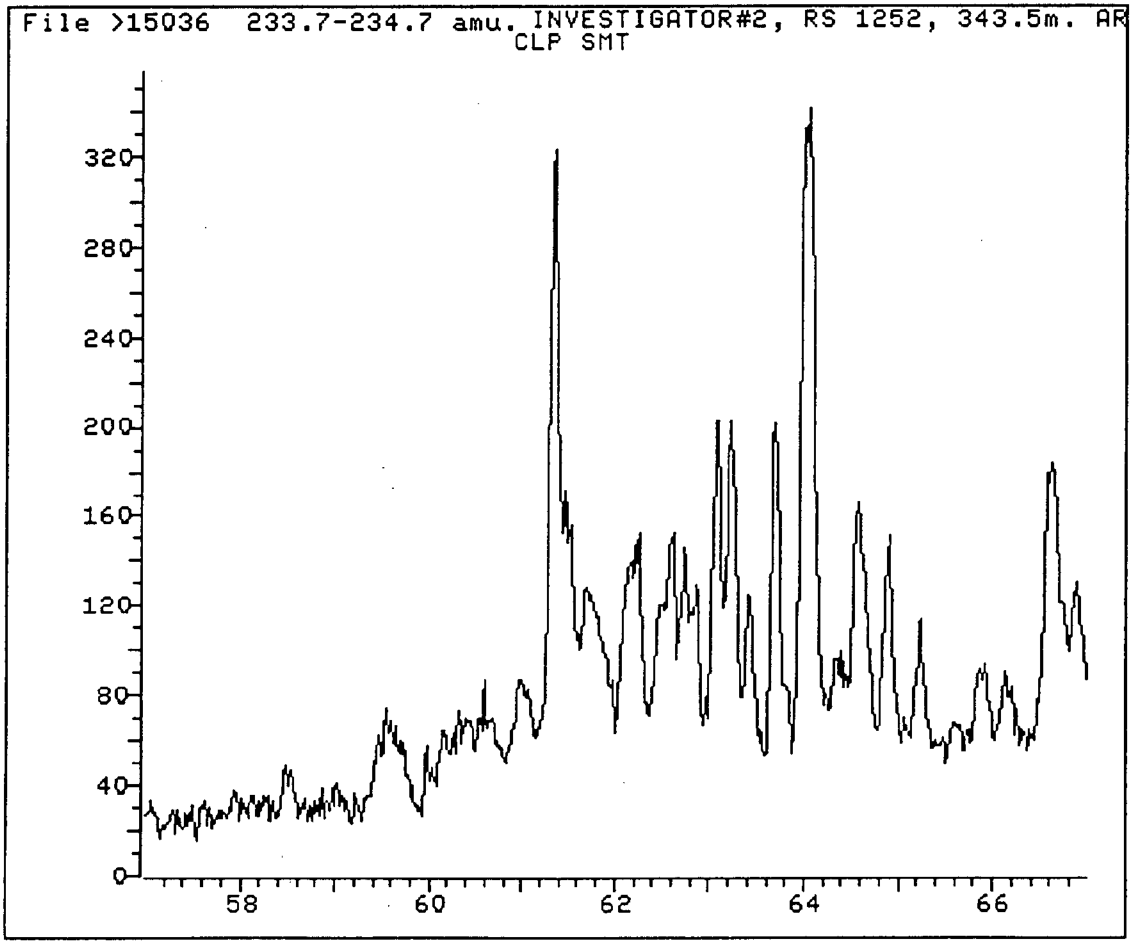

File >15036 197.7-198.7 amu. INVESTIGATOR#2, RS 1252, 343.5m. AR
160
140
120
100
80
60
40
20
0
40.0
41.0
42.0
43.0
44.0
45.0
46.0
47.0


File >15036 177.7-178.7 amu. INVESTIGATOR#2, RS 1252, 343.5m. AR
*
PHENANTHRENE
5200
4800
4400
4000
3600
3200
2800
2400
2000
1600
1200
800
400
0
45.0
46.0
47.0
48.0
49.0
50.0
51.0
52.0


File >15036 191.7-192.7 amu. INVESTIGATOR#2, RS 1252, 343.5m. AR
METHYLPHENANTHRENES
3
2
9
1
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
48.0
49.0
50.0
51.0
52.0
53.0
54.0
55.0


File >15036 205.7-206.7 amu. INVESTIGATOR#2, RS 1252, 343.5m. AR
CLP
1.3+3,9+2,10+3,10
DIMETHYLPHENANTHRENES
1,6+2,9
1,7
1,9+4,9
2.6
2.7
2.3
1.8
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
54.0
55.0
56.0
57.0
58.0


File >15036 218.7-219.7 amu. INVESTIGATOR#2, RS 1252, 343.5m. AR
CLP SMT


File >15036 233.7-234.7 amu. INVESTIGATOR#2, RS 1252, 343.5m. AR
CLP SMT