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LGC Geochemistry

Geochemical Analysis of Shallow
Core Samples from 83/20-sb01
and 83/20-sb02, Rockall, IRLCS

October, 2000

LGC/2000 LFX/228/203

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Contact Point:

Petroleum Geochemistry Team, LGC

Tel: (UK)-0208-943-7527

(Direct Line and Voicemail)

FAX: (UK)-0208-943-2767

Email: geochem@lgc.co.uk

Report Prepared by:

N Goodwin

Checked by:

M Dee

Date: October, 2000

LGC/2000 LFX/228/203

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1. Summary

Five samples from two cores taken in the Irish Rockall area have been analysed by organic geochemical methods. All samples examined have negligible potential for hydrocarbon generation ($\text{TOC} \leq 2\%$, $\text{S}_2 < 5\text{Kg/Tonne}$). GC analysis of the two “richest” samples indicates both samples are very immature. No indications of migrated mature hydrocarbons (oil seepage) were found. The depositional environment of the samples is difficult to assess completely due to their low maturity. However strong bias of steranes to C29 (only C29's), suggests organic input dominated by landplant material, probably a deltaic environment. There are limited indications that of the two solvent-extracted samples (SB01 176.26 and 176.57), the deeper sample is slightly more marine in nature.

2. Introduction

This report contains geochemical data for shallow core samples from the Irish Rockall area (Table 1).

Five samples have been screened for organic richness by Total Organic Carbon content ($\text{TOC}\%$ wt) and for their hydrocarbon yield on pyrolysis. Hydrocarbon yield was determined by bulk flow pyrolysis as, i) free hydrocarbons - the “S1 component” and ii) their hydrocarbon potential - the “S2 component” (cf. “Rock Eval” type analysis in $\text{Kg}_{\text{oil}}/\text{Tonne}_{\text{rock}}$; Espitalie, 1977). The two samples with the greatest hydrocarbon potential were solvent extracted and the extract obtained fractionated by HPLC into saturate-alkanes, aromatic and residue material. Samples were further characterised by gas chromatography of the saturate fractions and by GCMS analysis of the whole oil for biological markers. The latter techniques are used to characterise the thermal maturity and source organo-facies of hydrocarbon materials.

3. Results

The organic screening data are presented in Table 2 with their derived geochemical parameters. Appendix-A contains the GC chromatograms from the saturate alkanes, Appendix-B the GCMS mass chromatograms for the biological markers, Appendix-C the GCMS molecular parameter data and Appendix-D the peak identification codes in the GCMS chromatograms. Numerical data derived from HPLC fractionation, GC and GCMS analysis are summarised in Tables 3 to 4.

4. Discussion

4.1 Organic Richness

All the samples have negligible potential for hydrocarbon generation as they have TOC contents of 2%wt or less (cf. Kimmeridge N Sea 5 to 12%wt when immature). This conclusion is supported by the low yield on pyrolysis ($\text{S}_2 \text{ Kg/T}$, Table 2) where all samples are well below the 5Kg/T threshold for effective source rocks (Tissot & Welte, 1984). Where organic carbon is present the Hydrogen Indices ($100 \times \text{S}_2/\text{TOC}$) are low indicating predominantly inert material. Two samples SB02 71.47m and SB01 177.13m show slightly higher HI typical of gas prone coals, however, their carbon content is negligible. Due to the low hydrocarbon potential of the samples none were selected for Pyrolysis GC analysis to characterise their products.

The two “richest” samples were selected for solvent extraction (SB01 176.26 and 176.57) and further analysis.

4.2 Saturate Fraction GC

Examination of the saturate GC chromatograms (Appendix-A) indicates that one sample 176.26 has an n-alkane distribution characteristic of a highly immature extract with a bimodal distribution maximising at n-C16 and C27. The shorter chain material originates from marine algal input, while the long chain n-alkanes with the strong odd/even predominance (CPI of 2) are typical of terrestrial land plant derived waxes. Land plant waxes give rise to odd carbon chain length alkanes, particularly in the C25 to C33 range; thus, the odd/even predominance (CPI) tends to be high in deltaic environments, but will diminish with maturity.

In the more organic “rich” siltstone 176.57m there is a more complete suite of n-alkanes, maximising at n-C16 and ranging to C40+. This suggests a sample with a larger marine algal content, but the strong odd/even predominance and amount of longer chain material still suggests a significant terrestrial land plant contribution.

In both these samples the saturate alkanes represent a minor part of the extractable material, typical of a very immature sample (Tissot and Welte, 1984).

4.3 Biological Markers (GCM S data)

4.3.1 Source Facies

Examination of the Sterane and Triterpane mass chromatograms (m/z 217 and 191 Appendix-B1.1 and 2.1), indicate both samples organic matter is mostly derived from terrestrial land plant material. This is shown by the singular dominance of C29 steranes over all other types (Peters and Moldowan, 1993). Much of the pentacyclic triterpane components are unsaturated hopenes, due to the sample immaturity, making a more comprehensive assessment difficult.

4.3.2 Maturity

Examination of molecular parameters, used to assess the maturity of hydrocarbon extracts and oils, indicate that both the samples contain very immature hydrocarbons. This is shown by the absence of the 20S $\alpha\alpha\alpha$ sterane isomers and the presence of 20R 5 β steranes. Methylbiphenyl maturity parameters (Cumbers et al., 1987) of 8.2 and 9.9 (MBP, Appendix-C) are typical of immature extract (for terrestrial kerogens, as MBP is a facies dependent parameter). Methyldibenzothiophene data MDR 1.4 and 1.72 are again typical of immature values for landplant derived materials (Schou and Myhr, 1987). It was possible to measure the ratio of triaromatic to monoaromatic sterane hydrocarbons (parameters A1 and A2 ca 0.05, Appendix-C; after Mackenzie, 1980) in the 176.27 sample, which confirmed the immaturity of the sample

5. Conclusions

- All samples examined have negligible potential for hydrocarbon generation (TOC \leq 2%, P2 <5Kg/Tonne)
- GC analysis of 2 “richest” samples indicate both samples are very immature (high Odd/Even preference of n-alkanes and molecular parameters from biomarkers)
- There are no indications of migrated mature hydrocarbons (oil seepage)
- The depositional environment difficult to assess completely due to immaturity, however the strong bias of steranes to C29 (only C29’s) suggests organic input is dominated by landplant material, probably in a deltaic environment.
- There are limited indications that of the two samples extracted (SB01 176.26 and 176.57), the deeper sample is slightly more marine in nature.

6. References

- Cumbers K.M., Alexander R and Kagi R.I. (1987). Methylbiphenyl, ethylbiphenyl and dimethyl biphenyl isomer distributions in some sediments and crude oils. *Geochim et Cosmochim ACTA* 51, 3105-3111
- Espitalie J., Laporte J.L., Madec M., Marquis F., Leplat P., Paulet J. and Boutefeu A. (1977) Methode rapide de caracterisation des roches meres , de le potentiel petrolier et de leur degre d'evolution. *Rev Inst. Fr. Pet.* 32, p23-42.
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- Schou L. and Myhr M. (1987). Sulphur aromatic compounds as maturity parameters. *Adv. Org. Geochem 1987 Pt1*, 61-66. Pergamon Press, Oxford.
- Tissot B.P. and Welte D.H. (1984) *Petroleum formation and Occurrence*. Springer-Verlag, Berlin. 697pp.
- Peters K.E. and Moldowan (1993) *The Biomarker Guide. Interpreting molecular fossils in petroleum and ancient sediments*. Prentice Hall, NJ 07632. 363pp.

Table 1 - Samples

Sample code	Well name	Max sample depth	Sample type
0007SED010S004	83/20-sb01	177.13	COR
0007SED010S001	83/20-sb01	169.76	COR
0007SED010S002	83/20-sb01	176.26	COR
0007SED010S003	83/20-sb01	176.57	COR
0007SED011S001	83/20-sb02	71.47	COR

Table 2

SOURCE ROCK QUALITY INDICATORS

COUNTRY: UKCS
WELL: 83/20-sb01

DEPTH (M)	DEPTHRANGE (M)	FORMATION	PICKED LITHOLOGY	S1 (kg/t)	S1 (mg/gC)	S2 (kg/t)	TOC (%)	TMAX deg C	HI	GOGI	CARBT (%)	S (%)
169.76			Limestone	0.47	782.5	0.50	0.06	473	835		77.2	0.03
176.26			Mudstone	0.73	40.7	1.11	1.79	411	62		3.6	2.76
176.57			Siltstone	0.50	23.3	1.54	2.15	435	72		27.4	1.36
177.13			Limestone	0.56	69.7	1.14	0.81	405	140		61.1	0.61

SOURCE ROCK QUALITY INDICATORS

COUNTRY: UKCS
WELL: 83/20-sb02

DEPTH (M)	DEPTHRANGE (M)	FORMATION	PICKED LITHOLOGY	S1 (kg/t)	S1 (mg/gC)	S2 (kg/t)	TOC (%)	TMAX deg C	HI	GOGI	CARBT (%)	S (%)
71.47			Mudstone	0.65	154.7	0.68	0.42	556	162		6.0	0.19

Table 3

Sediment/Extract Analysis

```
Well name : 83/20-sb01
Suite name : Rockall
Country Of Origin : United Kingdom
Depth (m) : 176.26
Sample name :
Lab Number: 0007SED010S002
```

HPLC

Saturates	%wt :	22.87
Aromatics	%wt :	24.41
Residues	%wt :	52.72

Asphaltenes (Micro Method) %wt :

Extraction

Sediment Weight (g) :
Total Soluble Extract Weight (g) :

TSE %wt : 0.017

Saturates GC

Pristane/Phytane	:	0.47
Pristane/nC17	:	0.04
Phytane/nC18	:	0.90
CPI	:	2.00
ALKIND	:	68.58
R22	:	0.67

Biomarker Ratios

H1 :	S1 :	M2 :0.15
H2 :	S2 :	M3 :0.18
H3 :	S3 : ::	M4 :
H4 :		
	S4 : ::	M5 :
H5 : :::::	S5 :	A1 :0.05
H6 :		A2 :0.05
H7 :	S6 :	A3 :
	S7 :	
H8 :	S8 :	A4 :
H9 :		A5 :
H10 :	S9 :	A6 :
	S10 :	MDR : 1.40
H11 :		
H12 :		MBP :8.24
H13 :		
H14 :		
H15 :		
H16 :		
H17 :	N.B.	ALL
H18 :		

Light Hydrocarbons

MCH	%	:
HER	%	:
HXR	%	:

Stable Carbon Isotopes

```

Saturates :
      TSE :
Aromatics :
      Residue :
Asphaltenes :

```

Kerogen :

STANDARD:

N.B.

ALKIND -
R22 -

MCH% - Methylcyclohexane as Percentage of nC7's

Sediment/Extract Analysis

HPLC

Asphaltenes (Micro Method) %wt :

Saturates GC

Pristane/Phytane	:	1.91
Pristane/nC17	:	1.09
Phytane/nC18	:	0.67
CPI	:	1.35
ALKIND	:	56.94
R22	:	1.08

Light Hydrocarbons

MCH $\frac{\circ}{\circ}$:

HER :

HXR :

```
Saturates :
      TSE :
Aromatics :
      Residue :
Asphaltenes :
```

Kerogen :

STANDARD:

N.B. ALKIND -
R22 -

MCH% - Methylcyclohexane as Percentage of sum nC7's

Appendix A

Saturate GC Chromatograms

Saturate GC's – Double click to view



Chromatograms.ppt

Software Version: 4.1<2F12>

Date: 29/08/2000 08:44

Sample Name: 0007SED010S002 83/20-sb01 176.26m

Data File: C:_DATA\B0007010\SAC002.RAW Date: ##### 13:26

Sequence File: C:_DATA\B0007010\SAC_GC.SEQ Cycle: 2 Channel: A

Instrument: SAC_GC Rack/Vial: 0 0 Operator:

Sample Amount: 1 Dilution Fa 1

Saturates Fraction GC Analysis

Component Name	Time [min]	Area [μV·s]	Amount [%]
N-C12	8.203	1356	0.04
N-C13	9.696	5605	0.15
N-C14	11.115	104088	2.84
N-C15	12.482	716671	19.52
N-C16	13.755	934211	25.45
N-C17	14.94	456440	12.43
PRISTANE	15.042	17031	0
N-C18	16.056	40559	1.1
PHYTANE	16.213	36563	0
N-C19	17.143	57440	1.56
N-C20	18.174	27471	0.75
N-C21	19.166	35715	0.97
N-C22	20.114	33294	0.91
N-C23	21.025	63278	1.72
N-C24	21.897	41257	1.12
N-C25	22.744	140622	3.83
N-C26	23.547	47106	1.28
N-C27	24.341	209143	5.7
N-C28	25.084	57389	1.56
N-C29	25.823	199207	5.43
N-C30	26.718	145263	3.96
N-C31	27.204	121433	3.31
N-C32	27.783	146221	3.98
N-C33	28.675	43634	1.19
N-C34	29.51	8417	0.23
N-C35	30.45	26451	0.72
N-C36	31.504	8610	0.23
		3724475	100

→ Batch Code 0007SED010S002
Data File C:_DATA\B0007010\SAC002.RAW
CPI (24 to 32) 2.00
Pr/Ph Ratio 0.47
Pr/n-C17 0.04
Ph/n-C18 0.90
Alkane Index (C17/(C17+C27))% 68.58
R22 Index 2*C22/(C21+C23) 0.67
Note: -1 denotes not calculated

Software Version: 4.1<2F12>

Date: 29/08/2000 08:44

Sample Name: 0007SED010S003 83/20-sb01 176.57m

Data File: C:_DATA\B0007010\SAC003.RAW Date: ##### 16:05

Sequence File: C:_DATA\B0007010\SAC_GC.SEQ Cycle: 3 Channel: A

Instrument: SAC_GC Rack/Vial: 0 0 Operator:

Sample Amount: 1 Dilution Fa 1

Saturates Fraction GC Analysis

Component Name	Time [min]	Area [μV·s]	Amount [%]
N-C12	8.24	0	0
N-C13	9.698	35640	1.14
N-C14	11.123	175159	5.62
N-C15	12.466	242787	7.79
N-C16	13.734	241497	7.75
N-C17	14.932	181101	5.81
PRISTANE	15.054	197129	0
N-C18	16.07	154154	4.95
PHYTANE	16.222	103422	0
N-C19	17.154	152994	4.91
N-C20	18.19	146907	4.72
N-C21	19.179	157206	5.05
N-C22	20.128	166296	5.34
N-C23	21.036	149368	4.8
N-C24	21.909	124373	3.99
N-C25	22.748	148567	4.77
N-C26	23.557	118795	3.81
N-C27	24.339	136972	4.4
N-C28	25.09	101518	3.26
N-C29	25.822	136688	4.39
N-C30	26.52	83885	2.69
N-C31	27.208	119003	3.82
N-C32	27.914	70902	2.28
N-C33	28.682	87325	2.8
N-C34	29.52	54763	1.76
N-C35	30.467	76050	2.44
N-C36	31.525	52885	1.7
		3415387	100

→ Batch Code 0007SED010S003
Data File C:_DATA\B0007010\SAC003.RAW
CPI (24 to 32) 1.35
Pr/Ph Ratio 1.91
Pr/n-C17 1.09
Ph/n-C18 0.67
Alkane Index (C17/(C17+C27))% 56.94
R22 Index 2*C22/(C21+C23) 1.08
Note: -1 denotes not calculated

Appendix B

GCM S Chromatograms

GCM S Chromatograms – click to view



Chromatograms.ppt

Appendix C

Molecular Parameters

* CONFIRMED *

BP METH - BIOMARKER PARAMETERS 29-AUG-00 09:58:44 (V 3.20)

Sample#6 Text:83/20-sb01 176.26m \$0007SED010S002\$ File Text:6000RP GCMS
ANALYSIS: MPDMIO00926061.LIS EQUATION FILE: sacaro.EQN
HSRUN = MPDMIO00926061

H1	C32 HOPANES 22S/(22S+22R)	=
H2	C31 HOPANES 22S/(22S+22R) M/Z205	=
H3	C30: HOPANE/(HOPANE+MORETANE)	=
H4	C30: BB HOPANE / C30 HOPANE AS %	=
H5_0	C29 HOPANE AS % OF C30	=
H5_1	HOPANE DISTRIBUTION RELATIVE TO C30	=
H5_2	C31 HOPANES AS % OF C30 (M/Z205 CORRECTED)	=
H5_3	C32 HOPANES	=
H5_4	C33 HOPANES	=
H5_5	C34 HOPANES	=
H5_6	C35 HOPANES	=
H6	C27 HOPANES TS/(TS+TM)	=
H7	C33 HOPANES 22S/(22S+22R)	=
H11	C23 TRICYCLIC/C30 HOPANE AS %	=
H12	C24 TETRACYCLIC/C30 HOPANE AS %	=
H13	28,30 BISNORHOPANE/HOPANE AS %	=
H14	C30 DIAHOPANE PI/HOPANE AS %	=
H15	OLEANANE/HOPANE AS %	=
H16	GAMMACERANE/HOPANE AS % (205 BACK CALCULATED)	=
H17	HOPANE INDEX C35/(C35+C34) %	=
H18	25-NORHOPANE(Y)/HOPANE AS % G	=
H19	C29 18A-NORHOPANE D2/C30 HOPANE AS %	=
S1	C29 STERANES 20S/(20S+20R)	=
S2	C29 STERANES m/z218 ABB/(ABB+AAA)	=
S3_1	STERANE DISTRIBUTION AAA C27 %	=
S3_2	C28 %	=
S3_3	C29 %	=
S4_1	STERANE DISTRIBUTION ABB C27 %	=
S4_2	C28 %	=
S4_3	C29 %	=
S5	BA DIASTERANES/(BA DIASTERANES+AAA+ABB STERANES) %	=
S7	STERANE INDEX C27/(C27+C29) % FROM S3	=
S8	C30 4-ME STERANE AS % OF C29 20R AAA	=
M4	SUM C27 TO C35 HOPANES/(SAME+C27 TO C29 STERANES)	=
PR/PH	PRISTANE/PHYTANE RATIO ESTIMATE	=

* CONFIRMED *

BP METH - BIOMARKER PARAMETERS 29-AUG-00 09:58:44 (V 3.20)

-- -----
Sample#6 Text:83/20-sb01 176.26m \$0007SED010S002\$ File Text:6000RP GCMS
ANALYSIS: MPDMIO00926061.LIS EQUATION FILE: sacaro.EQN
continued...

T19	C19	TRICYCLIC/C23	TRICYCLIC	%	=
T20	C20	TRICYCLIC/C23	TRICYCLIC	%	=
T21	C21	TRICYCLIC/C23	TRICYCLIC	%	=
T22	C22	TRICYCLIC/C23	TRICYCLIC	%	=
T23	C23	TRICYCLIC/C23	TRICYCLIC	%	=
T24	C24	TRICYCLIC/C23	TRICYCLIC	%	=
T25	C25	TRICYCLIC/C23	TRICYCLIC	%	=
T26	C26	TRICYCLICS/C23	TRICYCLIC	%	=
T28	C28	TRICYCLICS/C23	TRICYCLIC	%	=
T29	C29	TRICYCLICS/C23	TRICYCLIC	%	=
T30	C30	TRICYCLICS/C23	TRICYCLIC	%	=
19/23	C19	TRICYCLIC/C23	TRICYCLIC	AS %	=
20/21	C20	TRICYCLIC/C21	TRICYCLIC	AS %	=
22/21	C22	TRICYCLIC/C21	TRICYCLIC	AS %	=
24/23	C24	TRICYCLIC/C23	TRICYCLIC	AS %	=
26/25	C26	TRICYCLICS/C25	TRICYCLIC	AS %	=
244_24	C24	TETRACYCLIC/C24	TRICYCLIC	AS %	=
TET_23	C24	TETRACYCLIC/C23	TRICYCLIC	AS %	=

* CONFIRMED *

BP METH - BIOMARKER PARAMETERS 29-AUG-00 09:58:44 (V 3.20)

-- -----
Sample#6 Text:83/20-sb01 176.26m \$0007SED010S002\$ File Text:6000RP GCMS
ANALYSIS: MPDMIO00926061.LIS EQUATION FILE: sacaro.EQN
continued...

M2	PHENANTHRENES (3ME+2ME) / (9ME+1ME)	=	0.15
M3	MPI1 PHENANTHRENES (3ME+2ME) / (9ME+1ME+PHEN) * 1.5	=	0.18
A1	ARO STERANES: C28 20R TRI/(SAME+C29 20R 5A&B MONO 12	=	0.05
A2	ARO STERANES: SUM TRI/(SAME+SUM MONO) (F9&F12split)	=	0.05
A3	TRI ARO STERANES: C20/(C20+C28 20R)	=	
A4	TRI ARO STERANES: (C20+C21)/(SAME+SUM C26 TO C28)	=	
A5	TRI ARO STERANES: C26 20S / C28 20S	=	
A6	TRI ARO STERANES: C27 20R / C28 20R	=	
MDR	4-ME DIBENZOTHIOPHENE / 1-ME DIBENZOTHIOPHENE	=	1.40
MBP	3-METHYLBIPHENYL / 2-METHYLBIPHENYL	=	8.24
MNR	2-ME NAPHTHALENE/1-ME NAPHTHALENE	=	0.91
SMN	(2-ME NAPTH+1-ME NAPTH)/C23 TRICYCLIC	=	
DBTP	DIBENZOTHOIOPHENE (MZ184) / PHENANTHRENE (MZ178)	=	0.11

SAC% 0 ARO% 0 OIL/TSE (MG) 0
SAC STD (UG) 0 ARO STD (UG) 0 ROCK (G) 0 TOC% 0

* CONFIRMED *

BP METH - BIOMARKER PARAMETERS 29-AUG-00 09:54:43 _ (V 3.20)

Sample#4 Text:83/20-sb01 176.57m \$0007SED010S003\$ File Text:6000RP GCMS
ANALYSIS: MPDMIO00926041.LIS EQUATION FILE: sacaro.EQN
HSRUN = MPDMIO00926041

H1	C32 HOPANES 22S/(22S+22R)	=	
H2	C31 HOPANES 22S/(22S+22R) M/Z205	=	
H3	C30: HOPANE/(HOPANE+MORETANE)	=	
H4	C30: BB HOPANE / C30 HOPANE AS %	=	
H5_0	C29 HOPANE AS % OF C30	=	
H5_1	HOPANE DISTRIBUTION RELATIVE TO C30	=	
H5_2	C31 HOPANES AS % OF C30 (M/Z205 CORRECTED)	=	
H5_3	C32 HOPANES	=	
H5_4	C33 HOPANES	=	
H5_5	C34 HOPANES	=	
H5_6	C35 HOPANES	=	
H6	C27 HOPANES TS/(TS+TM)	=	
H7	C33 HOPANES 22S/(22S+22R)	=	
H11	C23 TRICYCLIC/C30 HOPANE AS %	=	
H12	C24 TETRACYCLIC/C30 HOPANE AS %	=	
H13	28,30 BISNORHOPANE/HOPANE AS %	=	
H14	C30 DIAHOPANE PI/HOPANE AS %	=	
H15	OLEANANE/HOPANE AS %	=	
H16	GAMMACERANE/HOPANE AS % (205 BACK CALCULATED)	=	
H17	HOPANE INDEX C35/(C35+C34) %	=	
H18	25-NORHOPANE(Y)/HOPANE AS % G	=	
H19	C29 18A-NORHOPANE D2/C30 HOPANE AS %	=	
S1	C29 STERANES 20S/(20S+20R)	=	
S2	C29 STERANES m/z218 ABB/(ABB+AAA)	=	
S3_1	STERANE DISTRIBUTION AAA C27 %	=	
S3_2	C28 %	=	
S3_3	C29 %	=	
S4_1	STERANE DISTRIBUTION ABB C27 %	=	
S4_2	C28 %	=	
S4_3	C29 %	=	
S5	BA DIASTERANES/(BA DIASTERANES+AAA+ABB STERANES) %	=	
S7	STERANE INDEX C27/(C27+C29) % FROM S3	=	
S8	C30 4-ME STERANE AS % OF C29 20R AAA	=	
M4	SUM C27 TO C35 HOPANES/(SAME+C27 TO C29 STERANES)	=	
PR/PH	PRISTANE/PHYTANE RATIO ESTIMATE	=	2.42

* CONFIRMED *

BP METH - BIOMARKER PARAMETERS 29-AUG-00 09:54:43 _ (V 3.20)

-- -----
Sample#4 Text:83/20-sb01 176.57m \$0007SED010S003\$ File Text:6000RP GCMS
ANALYSIS: MPDMIO00926041.LIS EQUATION FILE: sacaro.EQN
continued...

T19	C19	TRICYCLIC/C23	TRICYCLIC	%	=
T20	C20	TRICYCLIC/C23	TRICYCLIC	%	=
T21	C21	TRICYCLIC/C23	TRICYCLIC	%	=
T22	C22	TRICYCLIC/C23	TRICYCLIC	%	=
T23	C23	TRICYCLIC/C23	TRICYCLIC	%	=
T24	C24	TRICYCLIC/C23	TRICYCLIC	%	=
T25	C25	TRICYCLIC/C23	TRICYCLIC	%	=
T26	C26	TRICYCLICS/C23	TRICYCLIC	%	=
T28	C28	TRICYCLICS/C23	TRICYCLIC	%	=
T29	C29	TRICYCLICS/C23	TRICYCLIC	%	=
T30	C30	TRICYCLICS/C23	TRICYCLIC	%	=
19/23	C19	TRICYCLIC/C23	TRICYCLIC	AS %	=
20/21	C20	TRICYCLIC/C21	TRICYCLIC	AS %	=
22/21	C22	TRICYCLIC/C21	TRICYCLIC	AS %	=
24/23	C24	TRICYCLIC/C23	TRICYCLIC	AS %	=
26/25	C26	TRICYCLICS/C25	TRICYCLIC	AS %	=
244_24	C24	TETRACYCLIC/C24	TRICYCLIC	AS %	=
TET_23	C24	TETRACYCLIC/C23	TRICYCLIC	AS %	=

* CONFIRMED *

BP METH - BIOMARKER PARAMETERS 29-AUG-00 09:54:43 _ (V 3.20)

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Sample#4 Text:83/20-sb01 176.57m \$0007SED010S003\$ File Text:6000RP GCMS
ANALYSIS: MPDMIO00926041.LIS EQUATION FILE: sacaro.EQN
continued...

M2	PHENANTHRENES (3ME+2ME) / (9ME+1ME)	=	0.31
M3	MPI1 PHENANTHRENES (3ME+2ME) / (9ME+1ME+PHEN) * 1.5	=	0.35
A1	ARO STERANES: C28 20R TRI/(SAME+C29 20R 5A&B MONO 12	=	
A2	ARO STERANES: SUM TRI/(SAME+SUM MONO) (F9&F12split)	=	
A3	TRI ARO STERANES: C20/(C20+C28 20R)	=	
A4	TRI ARO STERANES: (C20+C21)/(SAME+SUM C26 TO C28)	=	
A5	TRI ARO STERANES: C26 20S / C28 20S	=	
A6	TRI ARO STERANES: C27 20R / C28 20R	=	
MDR	4-ME DIBENZOTHIOPHENE / 1-ME DIBENZOTHIOPHENE	=	1.72
MBP	3-METHYLBIPHENYL / 2-METHYLBIPHENYL	=	9.96
MNR	2-ME NAPHTHALENE/1-ME NAPHTHALENE	=	1.04
SMN	(2-ME NAPTH+1-ME NAPTH)/C23 TRICYCLIC	=	18.23
DBTP	DIBENZOTHOIOPHENE (MZ184) / PHENANTHRENE (MZ178)	=	0.04

SAC% 0 ARO% 0 OIL/TSE (MG) 0
SAC STD (UG) 0 ARO STD (UG) 0 ROCK (G) 0 TOC% 0

Appendix D

GCM S Peak Identification Codes

BIOMARKER IDENTIFICATION - PENTACYCLIC HYDROCARBONS

LGC

CODE ASSIGNMENT BASED ON MASS SPECTROMETRY (m/e 191)

I	9-DODECYLPERHYDROANTHRACENE [INTERNAL STANDARD]
Ts	18 α (H)-22,29,30-TRISNORNEOHOPANE
Tm	17 α (H)-22,29,30-TRISNORHOPANE
Q	17 β (H)-22,29,30-TRISNORHOPANE
W	17 α (H)-25,30-BISNORHOPANE
X	17 α (H),18 α (H),21 β (H)-28,30-BISNORHOPANE
Y	17 α (H)-25-NORHOPANE
D	17 α (H),21 β (H)-30-NORHOPANE
D2	18 α (H)-30-NORNEOHOPANE
π	17 α (H),15 α (Me)-27-NORHOPANE ("DIAHOPANE")
A	17 β (H),21 α (H)-30-NORMORETANE
B	18 α (H)-OLEANANE
G	17 α (H),21 β (H)-HOPANE
H	17 β (H),21 β (H)-30-NORHOPANE
K	17 β (H),21 α (H)-MORETANE
N	(22S)-17 α (H),21 β (H)-30-METHYLBOPANE
O	(22R)-17 α (H),21 β (H)-30-METHYLBOPANE
S	GAMMACERANE
P	17 β (H),21 β (H)-HOPANE
R	17 β (H),21 α (H)-30-METHYLMORETANE
U	(22S)-17 α (H),21 β (H)-30-ETHYLBOPANE
V	(22R)-17 α (H),21 β (H)-30-ETHYLBOPANE
J	17 β (H),21 β (H)-METHYLBOPANE
α	(22S)-17 α (H),21 β (H)-30-n-PROPYLBOPANE
β	(22R)-17 α (H),21 β (H)-30-n-PROPYLBOPANE
L	17 β (H),21 β (H)-ETHYLBOPANE
γ	(22S)-17 α (H),21 β (H)-30-n-BUTYLBOPANE
δ	(22R)-17 α (H),21 β (H)-30-n-BUTYLBOPANE
ϵ	(22S)-17 α (H),21 β (H)-30-n-PENTYLBOPANE
ζ	(22R)-17 α (H),21 β (H)-30-n-PENTYLBOPANE

BIOMARKER IDENTIFICATION - AROMATIC STEROIDAL
HYDROCARBONS

(AROMATIC STERANES)

LGC

CODE TENTATIVE ASSIGNMENT BASED ON MASS SPECTROMETRY
(m/e 253 mass fragmentogram)

F22	C ₂₁ DIMETHYL MONOAROMATIC STEROID
F23	C ₂₂ DIMETHYL MONOAROMATIC STEROID
F2	C ₂₇ (20S)5 β (H)DIMETHYL MONOAROMATIC STEROID
F3	C ₂₇ (20R)5 β (H)DIMETHYL MONOAROMATIC STEROID
F4	C ₂₇ (20S)5 α (H)DIMETHYL MONOAROMATIC STEROID
F5	C ₂₈ (20S)5 β (H)DIMETHYL MONOAROMATIC STEROID
F6	C ₂₇ (20R)5 α (H)DIMETHYL MONOAROMATIC STEROID
F7	C ₂₈ (20S)5 α (H)DIMETHYL MONOAROMATIC STEROID
F8	C ₂₈ (20R)5 β (H)DIMETHYL MONOAROMATIC STEROID
F9	C ₂₉ (20S)5 β (H)DIMETHYL MONOAROMATIC STEROID
F10	C ₂₉ (20S)5 α (H)DIMETHYL MONOAROMATIC STEROID
F11	C ₂₈ (20R)5 α (H)DIMETHYL MONOAROMATIC STEROID
F12	C ₂₉ (20R)5 β (H)DIMETHYL MONOAROMATIC STEROID
F13	C ₂₉ (20R)5 α (H)DIMETHYL MONOAROMATIC STEROID

(m/e 231 mass fragmentogram)

F14	C ₂₀ METHYL TRIAROMATIC STEROID
F15	C ₂₁ METHYL TRIAROMATIC STEROID
F16	C ₂₆ (20S)METHYL TRIAROMATIC STEROID
F17	C ₂₆ (20R)METHYL TRIAROMATIC STEROID
F18	C ₂₇ (20S)METHYL TRIAROMATIC STEROID
F19	C ₂₈ (20S)METHYL TRIAROMATIC STEROID
F20	C ₂₇ (20R)METHYL TRIAROMATIC STEROID
F21	C ₂₈ (20R)METHYL TRIAROMATIC STEROID

BIOMARKER IDENTIFICATION - STERANES

LGC

CODE ASSIGNMENT BASED ON MASS SPECTROMETRY (m/e 217)

10	(20S)-13 β (H),17 α (H)-DIACHOLESTANE
11	(20R)-13 β (H),17 α (H)-DIACHOLESTANE
13	(20R)-13 α (H),17 β (H)-DIACHOLESTANE
14	(20S)-13 α (H),17 β (H)-DIACHOLESTANE
15	(24S/R)-(20S)-13 β (H),17 α (H)-24-METHYLDIACHOLESTANE
16	(24S/R)-(20S)-13 β (H),17 α (H)-24-METHYLDIACHOLESTANE
18	(24S/R)-(20R)-13 β (H),17 α (H)-24-METHYLDIACHOLESTANE
19	(24R/S)-(20R)-13 β (H),17 α (H)-24-METHYLDIACHOLESTANE
20A	(24S/R)-(20S)-13 α (H),17 β (H)-24-METHYLDIACHOLESTANE
20B	(20S)-5 α (H),14 α (H),17 α (H)-CHOLESTANE
21A	(24R+S)-(20S)-13 β (H),17 α (H)-24-ETHYLDIACHOLESTANE
21B	(20R)-5 α (H),14 β (H),17 β (H)-ISOCHOLESTANE
22	(20S)-5 α (H),14 β (H),17 β (H)-ISOCHOLESTANE
25	(20R)-5 α (H),14 α (H),17 α (H)-CHOLESTANE
27	(24S+R)-(20R)-13 β (H),17 α (H)-24-ETHYLDIACHOLESTANE
29	(24S+R)-(20S)-13 α (H),17 β (H)-24-ETHYLDIACHOLESTANE
33A	(24S+R)-(20R)-5 α (H),14 β (H),17 β (H)-24-METHYLISOCHOLESTANE
33B	(24S+R)-(20R)-13 α (H),17 β (H)-24-ETHYLDIACHOLESTANE
34	(24S+R)-(20S)-5 α (H),14 β (H),17 β (H)-24-METHYLISOCHOLESTANE
36	(24S+R)-(20R)-5 α (H),14 α (H),17 α (H)-24-METHYLCHOLESTANE
39	(24S+R)-(20S)-5 α (H),14 α (H),17 α (H)-24-ETHYLCHOLESTANE
40	(24S+R)-(20R)-5 α (H),14 β (H),17 β (H)-24-ETHYLISOCHOLESTANE
41	(24S+R)-(20S)-5 α (H),14 β (H),17 β (H)-24-ETHYLISOCHOLESTANE
42	(24S+R)-(20R)-5 α (H),14 α (H),17 α (H)-24-ETHYLCHOLESTANE
43	(24S+R)-(20S)-5 α (H),14 α (H),17 α (H)-24-PROPYLCHOLESTANE
44	(24S+R)-(20R)-5 α (H),14 β (H),17 β (H)-24-PROPYLCHOLESTANE
45	(24S+R)-(20S)-5 α (H),14 β (H),17 β (H)-24-PROPYLCHOLESTANE
46	(24S+R)-(20R)-5 α (H),14 α (H),17 α (H)-24-PROPYLCHOLESTANE
47	C30 4 α -ME-24-ETHYLCHOLESTANE
48	C30 4 β -ME-24-ETHYLCHOLESTANE
49	C30 4 α ,23,24-TRIMETHYLCHOLESTANE