



INTERTIDAL STUDY OF THE
SOUTHERN CALIFORNIA BIGHT

VOLUME 111

2.5 INTERTIDAL GC/MS

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TABLE OF CONTENTS

<u>Section</u>	<u>Page</u>
2.5 GC/MS STUDIES	1
2.5.1 Introduction	1
2.5.2 Methods and Results	1
2.5.2.1 Instrumentation and Operating Parameters. .	1
2.5.2.2 Data Processing and Interpretation.	2
2.5.2.3 Standard Mixtures	5
2.5.2.4 Intertidal Fauna-Samples	7
2.5.3 Discussion.	7

LIST OF TABLES

<u>Table</u>		<u>Page</u>
2.5-1	GC/MS Operating Parameters	3
2.5-2	Retention of Aliphatic Hydrocarbon Standards	6
2.5-3	Description of Southern California Bight Samples Analyzed.	9
2.5-4	Cross Reference List for GC/MS Run No. and PI Sample Identification. , . . .	13
2.5-5	Summary of Southern California Bight Samples According to Compound Class and Location	17
2.5-6	Occurrence of Chlorinated Organics and Plasticizers in Intertidal Organisms	23

LIST OF FIGURES

2.5-1	Location of Intertidal GC/MS Samples	11
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2.5 GC/MS STUDIES

2.5.1 Introduction

An important aspect of the OCS oil and gas development program is the recognition of changes in the chemical composition of intertidal organisms. The second year studies of Southern California Intertidal Bight samples are expected to produce information on the status of the biota, their fluctuations and the environmental impacts on them in areas believed to be critical in OCS oil and gas development. As set forth by the Bureau of Land Management contract (U.S. Dept. of Interior, BLM, 1977), these studies shall predominantly address the fate of oil-related hydrocarbons or, more specifically, the fate of high molecular weight aliphatic and aromatic hydrocarbons. This requirement inherently assumes knowledge of the chemical constitution of natural oils present in the Southern California Bight. It does not, however, fully acknowledge the chemical complexity and diversity of natural oils and the interference of chemical constituents normally present in organisms.

Analyses of aliphatic and aromatic hydrocarbons in intertidal organisms are mainly carried out using gas chromatography (GC), with gas chromatography/mass spectrometry being performed on a small fraction of samples already analyzed by GC. The primary objectives of GC/MS analyses are the confirmation and clarification of results obtained by GC analyses. The results of the GC/MS analyses reported here, therefore, serve as background for the interpretation profiles and may allow for the selection of specific compounds in the assessment of effects of natural oils and anthropogenic activities on the chemical constitution of intertidal organisms.

2.5.2 Methods and Results

2.5.2.1 Instrumentation and Operating Parameters

The GC/MS analyses of the second year intertidal fauna samples were performed with the same basic instrumentation used during the first year program (Burlingame, 1977); however, some significant improvements in both gas chromatographic separation and mass spectral data generation were achieved by the use of wall coated open tubular (WCOT) glass capillaries, the installation of a versatile and more accurate scan control unit, and the replacement of the separator between capillary outlet and mass spectrometer by a direct connection of the column to the mass spectrometer (Neumer-Jehle, 1973).

The now-installed scan control unit is a prerequisite for the use of WCOT glass capillaries since it allows for faster scan rates (1, 1.5, 2 sec/decade) and thus shorter scan cycle times necessary to cope with the short elution times (10-20 sees) of single component peaks.

The direct connection of the capillary to the mass spectrometer eliminates any loss of components during the transfer into the mass spectrometer.

The operating parameters for gas chromatography, interface, mass spectrometer and data system are summarized in Table 2.5-1.

2.5.2.2 Data Processing and Interpretation

The repetitive acquisition of mass spectra from a WCOT glass capillary effluent typically yields 800 to 1500 individual mass spectra. In order to reduce the number of spectra for data interpretation, each GC/MS run was subjected to the generation of a total ionization chromatogram (TIC) and mass chromatograms (MCs) of significant ions. These chromatograms, in conjunction with the respective flame ionization detector (FID) chromatogram and its corresponding description by the PI, were used for the selection of mass spectra for interpretation. The selected mass spectra were output on hard copy, inspected and interpreted. Selected spectra were subject to computer-assigned structure elucidation using a file search algorithm and the library containing representative members of compounds found during the first year benthic and intertidal program (Burlingame, 1977; Burlingame *et al.*, 1977). The results of the interpretation process were transferred to summary sheets for individual GC/MS runs. These summary sheets together with their corresponding total ionization chromatogram are presented in Appendix B. The information contained in the summary sheets consists of:

1. significant ions in cases where the unambiguous assignment of compound class was not possible;
2. compound class or identification of the compound (or compounds) by chemical name wherever possible.

The nomenclature used in these tables was kept as consistent as possible with the nomenclature used for the previous report (Burlingame, 1977). It is summarized as follows:

H/C Abbreviation for hydrocarbon

FAME : Fatty acid methylester

FAEE : Fatty acid ethylester

Cx:y: Shorthand for a compound with x carbon atoms and y double bond equivalents (e.g., alkadiene C_{19:2}: hydrocarbon with 19 carbon atoms and two double bonds; C_{18:1} FAME: methylated acid with 18 carbon atoms and one double bond in the carbon chain, note: elemental composition is C₁₉H₃₆O₂)

TABLE 1
GC/MS OPERATING PARAMETERS

		GC/MS Sample Numbers			
		1350-1397	1457-1475	1565-1589	1594-1616 1560, 1562
<u>Gas Chromatograph:</u>					
Injector type		All glass			
Injector temperature		270° - 240°			
Injection technique		Splitless			
Sample size		2 - 5 μ l			
Column					
type:	glass	SCOT	WCOT	WCOT	WCOT
phase		OV101	SE52	SE52	SE52
length		130 ft	28 m	31 m	31 m
i.d.		0.75mm	.38mm	.31mm	.31mm
carrier gas		He	He	He	He
carrier gas flow rate		4ml/min	2ml/min	.5ml/min	.5ml/min
temperature:					
ambient then heated to		90°	80°	80°	80°
program		90°-2800, 50/rein	80°-2400, 30 /rein	80°-2600, 30/rein	80°-2600, 3°/min
start program (min. after injection)		8	5	8.5	8.5
<u>Interface:</u>					
type		single-stage all-glass jet with make-up He		direct connection with glass transfer line	
temperature		280°	280°	270°	270°

TA13LE 1. (continued)

GC/MS Sample Numbers

1350-1397	1457-1475	1565-1589	1594-1616 1560, 1562
-----------	-----------	-----------	-------------------------

Mass Spectrometer:

Ion source

ionization voltage

70 eV

emission current

200 μ A

temperature

200° c

Mass range

m/e 20 - 600

Scan rate (see/decade)

1.5

1.5

1.5

1

Scan time (see)

2.0

2.0

2.0

1.64

Reset time (see)

1.3

1.25

1.25

1.3

Scan cycle time (see)

3.3

3.25

3.25

2.94

Data System:

ADC clock rate

12.2 kHz

15.5 kHz

15.5 kHz

15.5 kHz

min points/peak

8

8

8

8

min area

100

100

100

100

Commencement of
data acquisition

9

5

10

11

(min. after injection)

Si : Compounds with one or more silicon atoms. Samples which exhibit Si components found to originate from septum rubber particles are marked as such.

DDE : Unspecified isomer of 1, 1-dichloro-2, 2-bis (chlorophenyl) ethylene

PCB: Polychlorinated biphenyl

Phthalate: Unspecified isomer of phthalic acid esters

$C_n H_{2n+1}$ fragments

$C_n H_{2n-1}$ Series of ions saturated, mono and diunsaturated fragments.

$C_n H_{2n-3}$

2.5.2.3 Standard Mixtures

The performance of the instrumentation described in Section 2.5.2.1 was regularly checked with standard solutions of authentic compounds consisting of normal alkanes and isoprenoid hydrocarbons. One such standard contained the even numbered alkanes C_{10} to C_{24} , C_{28} , C_{30} , C_{36} , $n-C_{17}$ and pristane ($C_{19}H_{40}$), while a C_{12} to C_{32} standard used contained all normal alkanes from C_{12} to C_{32} , pristane ($C_{19}H_{40}$) and phytane ($C_{20}H_{42}$). Total ionization chromatograms of two authentic alkane mixtures are given in Appendix A, Figures 2.5.A-1 and 2.5.A-2.

The operating conditions of the GC/MS system were held constant for a finite set of sample runs. Retention indices (Kovats, 1958) for sample components may therefore be closely estimated by comparing scan numbers of sample peaks with scan numbers of authentic compounds in the corresponding standard analyses.

The scan numbers for authentic compounds for each of the four sample sets are given in Table 2.5-2 together with the maximum deviation observed in any sample set.

The deviations observed are due to human inaccuracy in the initial part of the analysis and fluctuation of instrumental parameters. They include initiation of data acquisition (e.g., a 10 sec delay would result in a deviation of 3 to 4 scans), variations in time from start of heating to initial isothermal temperature, and the instrumental history itself which can produce a higher temperature because of residual heat in the gas chromatography. The difference for a n -alkane in any given sample run, however, never exceeded more than six scans from the average deviation and was normally better than three scans.

TABLE 2

RETENTION OF ALIPHATIC HYDROCARBON STANDARDS
(Retention index vs scan number)

GC/MS Run No. (Standard)	1350	1402	1457	1565	2394
GC/MS Run No. (Samples)	1352-1397	1352-1397	1459-1475	1567-1589	1560, 1562 1576-1616
A Scan*	+3 to -5		+23 to +37	+1 to -10	-3 to -19
RI Scan number					
1000	34	11	1	--	--
1200	74	5s	50	10s	105
1300	--	--	--	164	166
1400	126	120	139	227	235
1500	--	--	--	293	306
1600	190	190	257	359	378
1700	223	225	317	424	449
1800	225	258	378	485	516
1900	--	--	--	545	582
2000	318	321	492	601	644
2100	--	--	--	657	703
2200	375	379	597	707	760
2300	--	--	--	757	816
2400	428	432	694	803	866
2500	--	--	--	848	916
2600	--	--	--	892	964
2700	--	--	--	933	1010
2800	524	527	867	974	1055
2900	--	--	--	1013	1098
3000		--	--	1056	1143
3100	--	--	--	1104	1195
3200	605	609	--	1160	1255
3400	--	718	--	--	--

* Δ Scan: differences between scan number of **n-alkanes** in intertidal samples and standard run. Numbers indicate the largest offset encountered in **any** sample set.
Deviations within a **single sample** are better than 6 scans.

A mixture containing n-decane, n-undecane, n-dodecane, 5-nonanone and octanol-1 was used for the evaluation of separation efficiency of the chromatographic system and the inertness of the GC/MS system. A typical TI chromatogram and selected mass chromatograms are given in Appendix A, Figure 2.5.A-3.

2.5.2.4 Intertidal Fauna Samples

The intertidal fauna samples analyzed by GC/MS are described in Table 2.5-3*. The samples consist of 16 hexane and 27 benzene fractions which were collected along the mainland and island shores. Sampling locations are given in Figure 2.5-1. The fractions were obtained from the following species:

	Total	Hexane	Benzene
<u>Mytilus californianus</u>	19	5	14
<u>Haliotis cracherodii</u>	8	3	5
<u>Macrocystis pyrifera</u>	7	3	4
<u>Emerita analoga</u>	7	4	3
<u>Pisaster ochraceus</u>	2	1	1

The samples were selected by the staff of the respective PI involved in the GC analysis and supposedly represent characteristic fractions perceived in those laboratories.

2.5.3 Discussion

The fractions of selected intertidal organisms as described in Section 2.5.2.4 are those of hexane and benzene eluates from a alumina/silica gel liquid chromatography system (U.S. Department of Interior, 1977), which, theoretically, should yield predominantly aliphatic and aromatic compounds in the respective fractions. The mass spectra obtained by GC/MS, however, indicate a much wider distribution of compound classes than anticipated. In general, the hexane fractions consist of alkanes, alkenes, isoprenoid hydrocarbons, polycyclic hydrocarbons and plasticizers while major constituents in the benzene fractions are various esters of long chain acids (fatty acids), polyunsaturated hydrocarbons, polycyclic hydrocarbons,

* A cross reference table (Table 2.5-4) allows for the correlation of GC/MS run number with sample identification used in the collaborating GC laboratories.

TABLE 3
DESCRIPTION OF SOUTHERN CALIFORNIA BIGHT SAMPLES ANALYZED
By GC/MS

Principal Investigator (PI)	PI Lab ID	Location	Station No.	Organism	Fraction	GC /MS Run No.
Risebrough	BLM 306	San Miguel Island	108	Macrocystis	Benzene	1364
Risebrough	BLM 317	Government Point	111	Mytilus Californians	Hexane	1356
Risebrough	BLM 317	Government Point	111	Mytilus Californianus	Benzene	1366
Risebrough	BLM 319	Government Point	111	Haliotis	Hexane	1362
Risebrough	BLM 319	Government Point	111	Haliotis	Benzene	1368 ⁺⁺ 1370
Risebrough	BLM 320	Government Point	111	Haliotis	Hexane	1354
Risebrough	BLM 320	Government Point	111	Haliotis	Benzene	1374
Risebrough	BLM 323	Santa Catalina Island	101	Mytilus Californianus	Benzene	1376
Risebrough	BLM 326	San Nicolas Island	110	Mytilus Californianus	Hexane	1358
Risebrough	BLM 326	San Nicolas Island	110	Mytilus Californianus	Benzene	1380
Risebrough	BLM 329	San Diego	106	Mytilus Californianus	Benzene	1386
Risebrough	BLM 331	San Clemente Island	104	Mytilus Californianus	Benzene	1393
Risebrough	BLM 341	Horseshoe Cove	---	Pisaster Ochraceus	Hexane	1 3 6 0
Risebrough	BLM 341	Horseshoe Cove	---	Pisaster Ochraceus	Benzene	1397
Risebrough	BLM 345	Corona del Mar	105	Haliotis	Benzene	1571
Risebrough	BLM 346	Santa Catalina Island	101	Mytilus Californianus	Hexane	1567

TABLE 3. (continued)

Principal Investigator (PI)	PI Lab ID	Location	Station No.	Organism	Fraction	GC /MS Run No.
Risebrough	BLM 346	Santa Catalina Island	101	Mytilus Californianus	Benz ene	1569
Risebrough	BLM 349	Santa Catalina Island	101	Haliotis	Hexane	1596
Risebrough	BLM 349	Santa Catalina Island	101	Haliotis	Benzene	1560 ^T
Risebrough	BLM 382	Government Point	111	Haliotis	Benzene	(1574) ^{††} 1576
Risebrough	BLM 418	San Clemente Island	104	Mytilus Californianus	Benzene	1589
Risebrough	BLM 422	San Nicolas Island	110	Macrocystis	Hexane	1585
Risebrough	BLM 422	San Nicolas Island	110	Macrocystis	Benzene	1587
Risebrough	BLM 433	San Nicolas Island	110	Mytilus Californianus	Hexane	1562 [†]
Risebrough	BLM 433	San Nicolas Island	110	Mytilus Californians	Benz ene	1601
Risebrough	BLM 437	San Nicolas Island	110	Mytilus Californianus	Benzene	1610
Risebrough	BLM 442	San Diego	106	Mytilus Californianus	Benzene	1616
Risebrough	BLM 445	San Nicolas Island	211	Emerita	Hexane	1583
Risebrough	BLM 445	San Nicolas Island	211	Emerita	Benzene	1578
Risebrough	BLM 469	Santa Cruz Island	109	Mytilus Californianus	Benzene	1614
Risebrough	BLM 470	San Miguel Island	108	Mytilus Californianus	Benzene	1608
Risebrough	BLM 482	Santa Cruz Island	109	Mytilus Californianus	Benzene	1612
Risebrough	BLM 483	San Miguel Island	108	Mytilus Californianus	Hexane	1603

TABLE 3. (continued)

Principal Investigator (PI)	PI Lab No.	Location	Station No.	Organism	Fraction	GC/MS Run No.
Risebrough	BLM 483	San Miguel Island	108	Mytilus Californianus	Benzene	1605
Benson	201-1076-04-1	Coal Oil Point	201	Emerita	Hexane	1465
Benson	201-1076-04-1	Coal Oil Point	201	Emerita	Benzene	1467
Benson	202-1076-01-1	Corona del Mar	202	Emerita	Hexane	1469
Benson	202-1076-01-1	Corona del Mar	202	Emerita	Benz ene	1471
Benson	211-1076-02-1	San Nicolas Island	211	Emerita	Hexane	1473
Benson	211-1076-02-1	San Nicolas Island	211	Emerita	Benz ene	1475
Benson	107-0177-01-6A	Coal Oil Point	107	Macrocystis	Hexane	1439 ^{††}
Benson	107-0177-01-6A	Coal Oil Point	107	Macrocystis	Benzene	1459 ^{††}
Benson	111-0177-01-6A	Government Point	111	Macrocystis	Hexane	1461
Benson	111-0177-01-6A	Government Point	111	Macrocystis	Benzene	1463
TOTAL : 46 runs						

† GC/MS run. no. out of sequence

†† low sample concentration for minor peaks

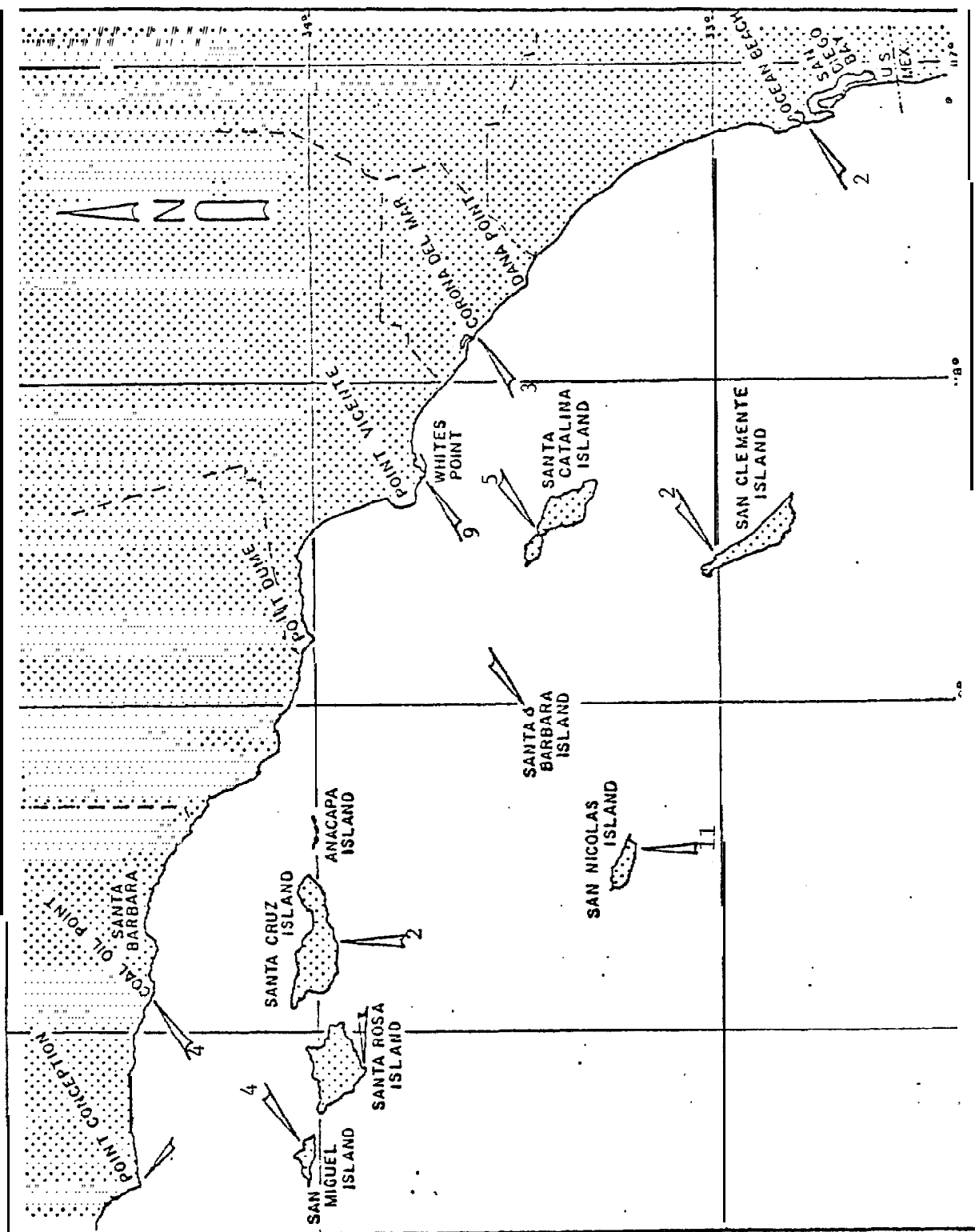


Figure 1. Location of Intertidal GC/MS Samples.

TABLE 4
CROSS REFERENCE LIST FOR GC/MS RUN NO.
AND PI SAMPLE IDENTIFICATION

<u>GC /MS Run No.</u>	<u>PI Sample Identification</u>	<u>Origin Lab</u>	<u>Comments</u>
1350	C ₁₀ - C ₃₆ Standard	SSL	
1352	BLM 319 (Hexane Fr)	Bodega	Sample concentration low, not reported
1354	BLM 320 (Hexane Fr)	Bodega	
1356	BLM 317 (Hexane Fr)	Bodega	
1358	BLM 326 (Hexane Fr)	Bodega	
1360	BLM 341 (Hexane Fr)	Bodega	
1362	BLM 319 (Hexane Fr)	Bodega	Rerun
1364	BLM 306 (Benzene Fr)	Bodega	
1366	BLM 317 (Benzene Fr)	Bodega	
1368	BLM 319 (Benzene Fr)	Bodega	Sample concentration high
1370	BLM 319 (Benzene Fr)	Bodega	Rerun
1374	BLM 320 (Benzene Fr)	Bodega	
1376	BLM 323 (Benzene Fr)	Bodega	
1380	BLM 326 (Benzene Fr)	Bodega	
1386	BLM 329 (Benzene Fr)	Bodega	
1393	BLM 331 (Benzene Fr)	Bodega	
1397	BLM 341 (Benzene Fr)	Bodega	
1402	C ₁₀ - C ₃₆ Standard	SSL	
1437	107-0177-01-6A-F1 (Hexane Fr)	Benson	Sample concentration low, not reported
1439	107-0177-01-6A-F1 (Hexane Fr)	Benson	Sample concentration low

TABLE 4. (continued)

<u>GC /MS Run No.</u>	<u>PI Sample Identification</u>	<u>Origin Lab</u>	<u>Comments</u>
1441	C ₁₀ - C ₃₆ Standard	S SL	
1449	C ₁₀ - C ₁₂ , ol, 'n' 10	SSL	
1457	C ₁₀ - C ₃₆ Standard	SSL	
1459	107-0177-01-6A-F2 (Benzene Fr)	Benson	
1461	111-0177-6A-F1 (Hexane Fr)	Benson	
1463	111-0177-6A-F2 (Benzene Fr)	Benson	
1465	201-1076-04-1-F1 (Hexane Fr)	Benson	
1467	201-1076-04-1-F2 (Benzene Fr)	Benson	
1469	202-1076-01-1-F1 (Hexane Fr)	Benson	
1471	202-1076-01-1-F2 (Benzene Fr)	Benson	
1473	211-1076-02-1-F1 (Hexane Fr)	Benson	
1475	211-1076-02-1-F2 (Benzene Fr)	Benson	
1560*	BLM 349 F2 (Benzene Fr)	Bodega	
1562*	BLM 433 F1 (Hexane Fr)	Bodega	
1564	C ₁₀ - C ₃₆ Standard	SSL	
1565	C ₁₂ - C ₂₂ , BLM Standard	Bodega	
1567	ELM 346 F1 (Hexane Fr)	Bodega	
1569	BLM 346 F2 (Benzene Fr)	Bodega	
1571	BLM 345 F2 (Benzene Fr)	Bodega	
1574	BLM 382 F2 (Benzene Fr)	Bodega	Sample concentration low
1576	BLM 382 F2 (Benzene Fr)	Bodega	Rerun

TABLE 4. (continued)

<u>GC /MS Run No.</u>	<u>PI Sample Identification</u>	<u>Origin Lab</u>	<u>Comment</u>
1578	ELM 445 F2 (Benzene Fr)	Bodega	
1583	BLM 445 F1 (Hexane Fr)	Bodega	
1585	BLM 422 F1 (Hexane Fr)	Bodega	
1587	BLM 422 F2 (Benzene Fr)	Bodega	
1589	BLM 418 F2 (Benzene Fr)	Bodega	
1594	C ₁₂ - ¹³ C ₂ , BLM Standard	Bodega	
1596	ELM 349 F1 (Hexane Fr)	Bodega	
1560*	BLM 349 F2 (Benzene Fr)	Bodega	
1562*	BLM 433 F1 (Hexane Fr)	Bodega	
1601	BLM 433 F2 (Benzene Fr)	Bodega	
1603	BLM 483 F1 (Hexane Fr)	Bodega	
1605	BLM 483 F2 (Benzene Fr)	Bodega	
1608	BLM 470 F2 (Benzene Fr)	Bodega	
1610	BLM 437 F2 (Benzene Fr)	Bodega	
1612	BLM 482 F2 (Benzene Fr)	Bodega	
1614	BLM 469 F2 (Benzene Fr)	Bodega	
1616	BLM 442 F2 (Benzene Fr)	Bodega	

* GC/MS Run No, sequence error. Sample Nos. 1560 and 1562 were chronologically run after sample No. 1596 and with the operating conditions used for sample Nos. 1594 to 1616.

aldehydes and ketones and plasticizers and artifacts. A summary of constituents found in the Southern California Bight samples according to compound classes and location is given in Table 2.5-5. This table is organized similarly to Table 3.5-8 in Southern California Baseline Study, Final Report, Vol. III, Report 3,5. 1977. The list of compound classes, however, contains an additional column J for aldehydes and ketones. Since hexane and benzene fractions analyzed did not always originate from the same sample, the fractions from each area are grouped according to their elution solvent (hexane or benzene).

The results reported here characterize the major constituents as well as selected minor constituents of fractions from intertidal organisms. The criteria for selection of gas chromatographic peaks for interpretation are necessarily subjective but reflect both the interest of the PIs of the contributing GC laboratories and the experience of this laboratory in the analyses of organic mixtures of high complexity. In the following sections the results of the GC/MS analyses are analyzed. For more specific information on the chemical constitution of single samples, the summary tables in Appendix B should be consulted.

The inspection of Table 2.5-5 for hydrocarbons shows that some compound classes may be present in both the hexane and the benzene fractions. This already holds true for alkanes (column A) which were frequently found in the hexane fraction but occasionally also in the benzene fraction. Though these alkanes in the benzene fraction normally consist of C_{28} , C_{34} alkanes, they sometimes include even C_{17} alkanes. The next compound class (alkenes, column B), with a few exceptions, is found in both fractions. The hexane fraction predominantly contains hydrocarbons with a degree of unsaturation of two double bond equivalents, while the alkenes found in the benzene fraction in general exhibit a higher degree of unsaturation with up to five double bond equivalents.

Aromatic hydrocarbons are neither present in high abundance nor in a large variety in any samples analyzed. The most frequently encountered mass spectrum with features for an aromatic compound indicates the structure of acenaphthen ($C_{12}H_{10}$, MW 154). A second aromatic compound present in some samples in low concentration is 1, 2 diphenylethane ($C_{14}H_{14}$, MW 182, m/e 91, 182).

The most abundant components in the majority of benzene fractions examined for this study are those of esters of fatty acids and ketones and aldehydes. Most of these esters were methylesters but some ethyl and butylesters were also encountered.

Because of the methodological uncertainties which are demonstrated by distribution of alkanes and the presence of esterified acids, ketones and aldehydes, it is difficult to assess the distribution of petroleum hydrocarbons in intertidal organisms. There are, however, some

TABLE 5
SUMMARY OF SOUTHERN CALIFORNIA BIGHT SAMPLES
ACCORDING TO COMPOUND CLASS AND LOCATION

BLM Station No.	Sample Type	Fraction	GC/MS Run No.	alkanes A	alkenes B	isoprenoid hydrocarbons C	polycyclic hydrocarbons D	aromatic hydrocarbons E	fatty acid esters F	chlorinated organics G	plasticizers and artifacts H	unresolved I	aldehydes ketones J
COAL OIL POINT													
201	E	H	1465	+	+	+	+					+	
107	Mc	H	1439	+	+							+	
III-25-16	201	E	1467										
	107	Mc	1459*										
SAN MIGUEL ISLAND													
108	M	H	1603		+						+		
108	M	B	1605		+		+		+		+		
108	M	B	1608		+		+	(+)	+				
108	Mc	B	1364		+	+			+		+		

TABLE 5. (continued)
SUMMARY OF SOUTHERN CALIFORNIA BIGHT SAMPLES
ACCORDING TO COMPOUND CLASS AND LOCATION

BIM Station No.	Sample Type	Fraction	GC/MS Run No.	A alkanes	B alkenes	C isoprenoid hydrocarbons	D polycyclic hydrocarbons	E aromatic hydrocarbons	F fatty acid esters	G chlorinated organics	H plasticizers and artifacts	I unresolved hump	J aldehydes ketones
ORSESHOE COVE													
	P	H	1360		+	+					+		
	P	B	1397		+	+	+		+	+	+		
OVERNMENT POINT													
111	H	H	1354	+	+						+		
111	H	H	1362	+	+	+	+		+		+		
111	M	H	1356	+	+	+	+					+	
111	Mc	H	1461	+	+	+	(+)					+	
111	H	B	1374			+			+		+		
111	H	B	1368/1370				(+)		+		+	+	

TABLE 5. (continued)
SUMMARY OF SOUTHERN CALIFORNIA BIGHT SAMPLES
ACCORDING TO COMPOUND CLASS AND LOCATION

BLM Station No.	Sample Type	Fraction	GC/MS Run No.	alkanes A	alkenes B	isoprenoid hydrocarbons C	polycyclic hydrocarbons D	aromatic hydrocarbons E	fatty acid esters F	chlorinated organics G	plasticizers and artifacts H	unresolved hump I	aldehydes ketones J
GOVERNMENT POINT (continued)													
111	H	B	1574*/1576	+	+	+	+	(+)			+		
111	M	B	1366		+		+		+	+		+	
111	Mc	B	1463	+	+					+			
SANTA CRUZ ISLAND													
I H-2.5-18	109	M	B		+				+		+		+
	109	M	B		+				+		+		+
CORONA DEL MAR													
202	E	H	1469	+	+	+	+					+	
202	E	B	1471	+	+					+			

TABLE 5. (continued)
SUMMARY OF SOUTHERN CALIFORNIA BIGHT SAMPLES
ACCORDING TO COMPOUND CLASS AND LOCATION

LM Station No.	Sample Type	Fraction	GC/MS Run No.	A alkanes	B alkenes	C isoprenoid hydrocarbons	D polycyclic hydrocarbons	E aromatic hydrocarbons	F fatty acid esters	G chlorinated organics	H plasticizers and artifacts	I unresolved hump	J aldehydes ketones
CRONA DEL MAR (continued)													
105	H	B	1571		+				+				
ANTA CATALINA ISLAND													
101	M	H	1567	+	+						+		
101	H	H	1596	+	+	+					+		
101	M	B	1569						+		+		
101	M	B	1376		+	+	+		+	(+)	+	+	+
101	H	B	1560	+	+		+		+		+		+
SAN CLEMENTE ISLAND													
104	M	B	1393		+		+	(+)	+		+		+

TABLE 5. (continued)
SUMMARY OF SOUTHERN CALIFORNIA BIGHT SAMPLES
ACCORDING TO COMPOUND CLASS AND LOCATION

BLM Station No.	Sample Type	Fraction	GC/MS Run No.	A alkanes	B alkenes	C isoprenoid hydrocarbons	D polycyclic hydrocarbons	E aromatic hydrocarbons	F fatty acid esters	G chlorinated organics	H plasticizers and artifacts	I unresolved hump	J aldehydes ketones
SAN CLEMENTE ISLAND (continued)													
104	M	B	1589		+		+	(+)	+				+
SAN DIEGO													
106	M	B	1386		+		+		+		+		+
106	M	B	1616		+		+		+	(+)	+		
SAN NICOLAS ISLAND													
110	M	H	1358	+	+	+	+		+			+	
110	M	H	1562	+	+	+	+						
110	Mc	H	1585	+	+	+			+		+		
211	E	H	1473	+	+	+	+						

TABLE 5. (continued)
SUMMARY OF SOUTHERN CALIFORNIA BIGHT SAMPLES
ACCORDING TO COMPOUND CLASS AND LOCATION

BLM Station No.	Sample Type	Fraction	GC/MS Run No.	alkanes A	alkenes B	isoprenoid hydrocarbons C	polycyclic hydrocarbons D	aromatic hydrocarbons E	fatty acid esters F	chlorinated organics G	plasticizers and artifacts H	unresolved hump I	aldehydes ketones J
SAN NICOLAS ISLAND (continued)													
211	E	H	1583	+	+	+	+		+				
110	M	B	1380		+		+		+	+			
110	M	B	1601		+		+	(+)	+	+	+		
110	M	B	1610	(+)	+	(+)	+		+				
110	Mc	B	1587		+			(+)	+		+		
211	E	B	1475	+	+				+	+			
211	E	B	1578		+		+		+	+			

* low sample concentration, no structure elucidation possible

Species:

Fraction:

M = *Mytilus Californians*

H = Hexane/Heptane

H = *Haliotis*

B = Benzene

Mc = *Macrocystis*

E = *Emerita*

P = *Pisaster ochraceus*

interesting findings related to other anthropogenic components such as chlorinated organics and plasticizers which were found in different areas. Though some of the plasticizers found in the samples analyzed may come from laboratory contamination, it is believed that most of these compounds are intrinsic constituents of the organisms since such compounds are even found in open ocean samples (Giam et al., 1975).

In the following sections the geographic distribution of these clearly anthropogenic components is discussed.

San Miguel Island (Bill Site 108)

Besides the esters of fatty acid which were detected in all benzene fractions, the samples predominantly consist of unsaturated hydrocarbons and, in the case of the hexane fraction examined (GC/MS Run No. 1601), many components with spectra of phthalic acid esters were detected.

Government Point (BLM Site 111)

The Haliotis cracherodii samples (hexane and benzene fraction) all contain plasticizers but no chlorinated organics. The benzene fractions of Mytilus californianus and Macrocystis pyrifera collected at this site both contain chlorinated organics (DDE, PCBs). Though the limited number of samples precludes a final judgment, it appears that chlorinated organics are not retained in H. cracherodii but are retained in all other species examined for their organic constituents (see Table 25-6) .

The two benzene fractions contain two plasticizers (dioctyladipate, and dioctylphthalate) besides the major components which exhibit mass spectral features of fatty acid esters and unsaturated hydrocarbons.

Corona del Mar (BLM Sites 202, 105)

In the benzene fraction of the Emerita analoga samples (Site 202) two chlorinated organic organics, namely trichlorodiphenylethylene and DDE, were positively identified. The benzene fraction of the H. cracherodi sample from a different location (Site 205) does not contain an indication of chlorinated organics. As mentioned above, this fact may be explained by the specific behavior of H. cracherodii towards contamination with halogenated organics.

Santa Catalina Island (BLM Site 101)

In the benzene fraction of one Mytilus californianus sample (GC/MS Run No. 1376) an indication for DDE was obtained by mass spectral data and chromatographic retention time. All samples were found to contain adipate and/or phthalate.

TABLE 6
OCCURRENCE OF CHLORINATED ORGANICS AND
PLASTICIZERS IN INTERTIDAL ORGANISMS

Species	Hexane Fraction	Benzene Fraction	Chlorinated Organics	Plastizers
Haliotis	3		0	3
Haliotis		5	0	4
Mytilus californianus	5		0	3
Mytilus californianus		13	4	9
Macrocystis	3		0	1
Macrocystis		4	2	2
Emerita	4		0	0
Emerita		4	3	
Piaster	1		0	1
Piaster		1	1	1
TOTAL	16		0	8
		27	9	16

San Nicolas Island (BLM Sites 110, 211)

The samples from these two stations do not indicate a consistent distribution of clearly anthropogenic components since chlorinated organics were found in samples from both locations irrespective of collected organisms but not in every sample of the same organism (GC/MS Run No. 1610). Also, the presence of plastic plasticizers in some samples and their absence in others provides a similar picture.

2. 5.4 References

- A. L. Burlingame, in Southern California Baseline Study, Final Report, Volume III, Report 3.5, 1977, 1-298.
- A. L. Burlingame and J. Meili, SAI/BLM Fourth Quarterly Report, April 1 - June 30, 1977.
- Committee to Evaluate Outer Continental Shelf Environmental Studies, Commission on Natural Resources, National Research Council, National Academy of Sciences, OCS Oil and Gas: An Assessment of the Department of the Interior Environmental Studies Program, A report to the Department of the Interior, Bureau of Land Management, Washington D.C., 1977, p. 45 ff.
- C. S. Giam, H. S. Chain and G. S. Neff, Anal. Chem., 47, 2225 (1975).
- E. Kovats, Helv. Chim. Acts, 41, 1915 (1958).
- N. Neuner-Jehle, F. Etzweiler and G. Zarshe, Chromatographia, 6, 211, (1973).
- U. S. Department of the Interior, Bureau of Land Management, Southern California Intertidal Study, Work Statement for Proposed Follow-On Efforts in FY 1977.

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Appendix A

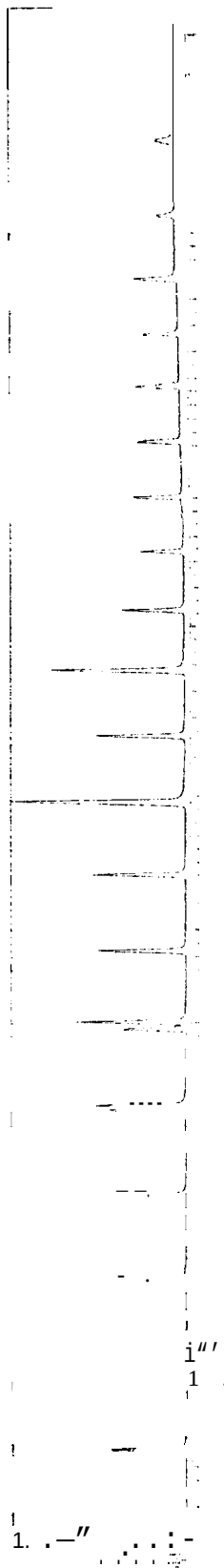


Figure 1. TIC trace for GC/MS 1565

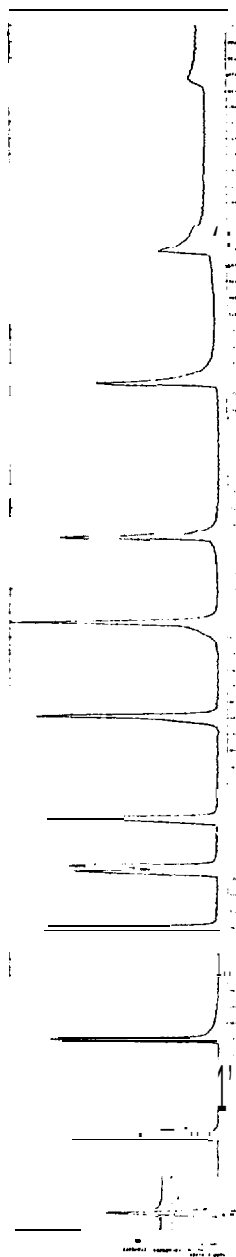


Figure 2. TIC trace for GC/MS 1402

Figure 3. To be included in final.

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Appendix B

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GC/MS RUN #: 1465

SAMPLE TYPE: INTERTIDAL, EMERITA, Hexane Fraction

SAMPLE ID: Benson 201-1076-04-1 /F1

OTHER ID:

LOCATION: 201/ Coal Oil point

COMMENTS/SUMMARY : Normal alkanes $C_{15:0}$, $C_{28:0}$, branched, isoprenoid, saturated and unsaturated hydrocarbons; sterane-type cyclic hydrocarbons

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS .
122	Perfluorokerosene			instrumental artifacts
150				
163	alkene			43, 57, 85, 97, 99, 113
200	isoprenoid alkane $C_{16:0}$	226	$C_{16}H_{34}$	113, 183; 141, 211, M^+ 226
211	branched alkene, $C_{16:1}?$	224 ?	$C_{16}H_{32}$	85; 97, 111, 127, M^+ 244 ?
224	n-alkane $C_{15:0}$	212	$C_{15}H_{32}$	
258	branched alkene, $C_{16:0}?$	224 ?	$C_{16}H_{32}$	85, 97, 111, 125, 155, 183, M^+ 224 ?
264	isoprenoid alkene, $C_{17:1}$	238	$C_{17}H_{34}$	85, 97, 111, 127 → 197, 141 + 211, M^+ 238
287	n-alkane $C_{16:0}$	226	$C_{16}H_{34}$	C_nH_{2n+1} fragments, M^+ 226
	branched alkene $C_{17:1}$	238	$C_{17}H_{34}$	97, 111, 125, 141, 155, 169, M^+ 238
319	isoprenoid alkane $C_{18:0}$	254	$C_{18}H_{38}$	C_nH_{2n+1} fragments, 99, 169, 113, 183
	branched alkene $C_{18:0}$	252	$C_{18}H_{36}$	83, 97, 111, 125, M^+ 252

Continued

GC/MS RUN #: 1465 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
327	branched C _{18:2}	250	C ₁₈ H ₅₄	41, 55, 69, 81, 83, 95, 97, 109, 111, 123, 111, $\left\{ \begin{array}{l} M^+ 250 \\ M^+ 252 \end{array} \right.$
	branched C _{18:1}	252	C ₁₈ H ₅₆ }	
355	n-alkane C _{17:0}	240	C ₁₇ H ₃₆	
357	isoprenoid alkane C _{19:0} , pristene	268	C ₁₉ H ₄₀	85, 97, 99, 113, 183, M ⁺ 268
366	branched alkene C _{19:1}	266	C ₁₉ H ₃₈	55, 69, 83, 97, 111, 125, M ⁺ 266
384	alkenes			M ⁺ : 250, 252, 262, 264, 266
395	branched alkene C _{19:1}	266	C ₁₉ H ₃₈ }	57, 69, 83, 97, 111, 123, 125, 137, 139, 151, $\left\{ \begin{array}{l} M^+ 266 \\ M^+ 264 \end{array} \right.$
	branched alkadiene C _{19:2}	264	C ₁₉ H ₃₆ }	
415	n-alkane C _{18:0}	254	C ₁₈ H ₅₈	
	phytenes	280	C ₂₀ H ₄₀	125, 280
	phytadienes	278	C ₂₀ H ₃₈	123, 278

Continued

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY :

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
420	isoprenoid alkane C _{20:0} , phytene	282	C ₂₀ H ₄₂	85, 97, 99, 113 → 183, 127 → 197, 253, M ⁺ 282
433	branched C _{20:1}	280	C ₂₀ H ₄₀	55, 69, 83, 97, 111, 125, M ⁺ 280
447	alkenes			M ⁺ : 264 (C _{19:2}), 278 (C _{20:2}), 280 (C _{20:1})
469	alkenes			M ⁺ : 264, 272, 274, 276> 278, 280, 292 (C _{21:2}), 294 (C _{21:1})
474	n-alkane C _{19:0}	268	C ₁₉ H ₄₀	
	alkenes			M ⁺ 264, 278, . 292
479	alkenes			M ⁺ 264, 278, 280, 292, 294
484	branched alkene C _{21:1}	294	C ₂₁ H ₄₂	43, 55, 69, 83, 97, 111, 125, M ⁺ 294
519	branched alkadiene C _{21:2}	292	C ₂₁ H ₄₀	41, 55, 69, 81, 83, 95, 97, 109, 111, 123, 125 137, 151, M ⁺ 292

Continued

HH-2.5-34

GC/MS RUN #: 1465 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION : _____

COMMENTS/SUMMARY:

III-2.5-35

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	M(IL) . FORMULA	SIGNIFICANT IONS
528	branched alkadiene C _{21:2}	292	C ₁₉ H ₄₀	C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} fragments, 151, 165, . 179 $\left\{ \begin{array}{l} M^+ 292 \\ M^+ 306 \end{array} \right.$
	branched alkadiene C _{22:2}	306	C ₂₂ H ₄₂	
531	n-alkane C _{20:0}	282	C ₂₀ H ₄₂	.
	(n-?) alkadiene C _{21:2}	"292	C ₂₁ H ₄₀	
539	branched alkene C _{22:1}	308	C ₂₂ H ₄₄	57, 69, 83, 97, 111, 125, 137, 139, M ⁺ 308
572	alkenes			M ⁺ : 286, 288, 290, 292, 302, 306, 308, 320, 322
585	n-alkane C _{21:0}	296	C ₂₁ H ₄₄	C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} , C _n H _{2n-5} fragments, 184
601				
625				C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} , C _n H _{2n-5} fragments, 218, 273, 288
637	n-alkane C _{22:0}	310	C ₂₂ H ₄₆	183 → 253, 197 → 267
654	isoprenoid C _{25:0} ?			

Continued

GC/MS RUN #: 1465 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER 15: _____

LOCATION: _____

COMMENTS/SUMMARY:

III-2.5-36

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
668				$C_n H_{2n+1}$, $C_n H_{2n-1}$, $C_n H_{2n-3}$ fragments, 191, M^+ 318 ?
687	n-alkane $C_{23:0}$	324	$C_{23} H_{48}$	
694				$C_n H_{2n+1}$, $C_n H_{2n-1}$, $C_n H_{2n-3}$ fragments
703				$C_n H_{2n+1}$, $C_n H_{2n-1}$, $C_n H_{2n-3}$ fragments
719		364 ?	$C_{26} H_{52}$?	$C_n H_{2n-1}$, $C_n H_{2n-3}$ fragments, 249, 253 809, M^+ 364 ?
735	n-alkane $C_{24:0}$			
742				$C_n H_{2n+1}$, $C_n H_{2n-1}$, $C_n H_{2n-3}$ fragments
767		378 ?	$C_{27} H_{54}$	$C_n H_{2n-1}$, $C_n H_{2n-3}$ fragments, 253, 263, 323 M^+ 378
780	n-alkane $C_{25:0}$	352	$C_{25} H_{52}$	
823	n-alkane $C_{26:0}$	366	$C_{26} H_{54}$	

Continued

GC/MS RUN #: 1465 continued

SAMPLE TYPE:

SAMPLE ID:

OTHER ID:

LOCATION :

COMMENTS/SUMMARY:

III-2.5-37

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
829	cholestane (5 β ?)	372	C ₂₇ H ₄₈	149, 165, 217, 218, 253, M ⁺ ; 372
844	steroid alkenes			C _n H _{2n-1} , C _n H _{2n-3} fragments, 165 179, 217, 253, 372, 386
865	n-alkane C _{27:0} + steroid alkenes	380	C ₂₇ H ₅₆	165, 179, 217, 218, 239, 253, '386, 600
875	steroid alkenes (ergostene type ?)			C _n H _{2n-1} , C _n H _{2n-3} fragmen s, 165, 179, 193, 253, 267> 386,388
894	5 α -cholestane	372	C ₂₇ H ₄₈	149, 217, 218, 372
906	n-alkane C _{28:0} + steroid alkenes	394	C ₂₈ H ₅₈	217, 218, 253, 267, 400
934	5 α -24-Methyl-cholestane	386	C ₂₈ H ₅₀	149, 217, 218, 259, M ⁺ 386
944	5 α -H-stigmastane	400	C ₂₉ H ₅₂	149, 217, 218, M ⁺ 400

Continued

GC/MS RUN #: 1465 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

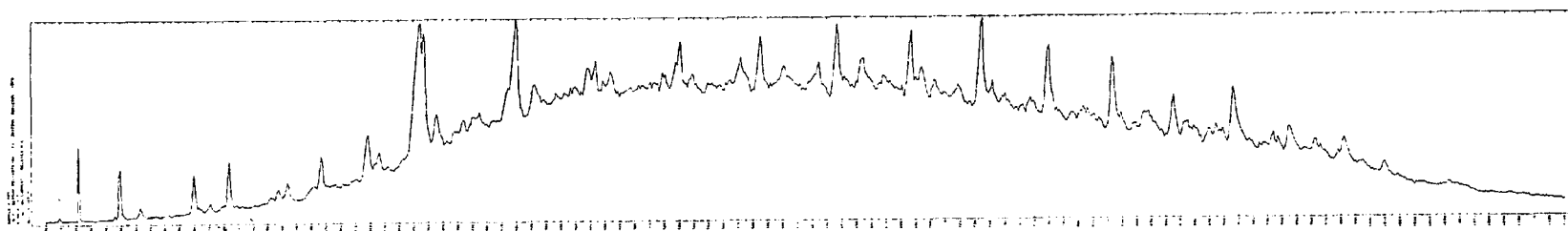
LOCATION : _____

COMMENTS/SUMMARY:

HH-2.5-38

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
962	^c 28 triterpane	384	^c 28H48	191, 348
	+ steroids	400	C ₂₉ H ₅₂	217, 218, 400
	+ 4-Methyl steranes	414	^c 30H54	232, 414
982	steroids			191
	+ methyl steranes			217, 218, 232
1010	hopane	412	C ₃₀ H ₅₂	191, 205, 219, 231 259, 397, M ⁺ 412

III-2 5-39



TIC trace for GC/MS 1465

GC/MS RUN #: 1439

SAMPLE TYPE: INTERTIDAL, MACROCYSTIS, Hexane Fraction

SAMPLE ID: BLM Benson 107-0177-01-6A-F1

OTHER ID:

LOCATION: 107/Coal Oil Point

COMMENTS/SUMMARY: Sample concentration low, saturated and unsaturated hydrocarbon, predominantly normal structure.

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
143	alkane n-C _{15:0}	212	C ₁₅ H ₃₂	
181				
211	unsaturated H/C			C _n H _{2n-1} fragments
217	unsaturated H/C			C _n H _{2n-1} fragments
22.0	alkane			C _n H _{2n+1} fragments
231	unsaturated H/C			C _n H _{2n-1} fragments
324	unsaturated H/C			C _n H _{2n+1} , C _n H _{2n-1} fragments
348	unsaturated H/C			C _n H _{2n-1} fragments
356	unsaturated H/C			C _n H _{2n-1} fragments
386	unsaturated H/C			C _n H _{2n+1} , C _n H _{2n-1} fragments
415	n-alkane			C _n H _{2n+1} fragments, 97, 111

Continued

II-2.5-40

GC/MS RUN #: 1439 continued

SAMPLE TYPE: _____

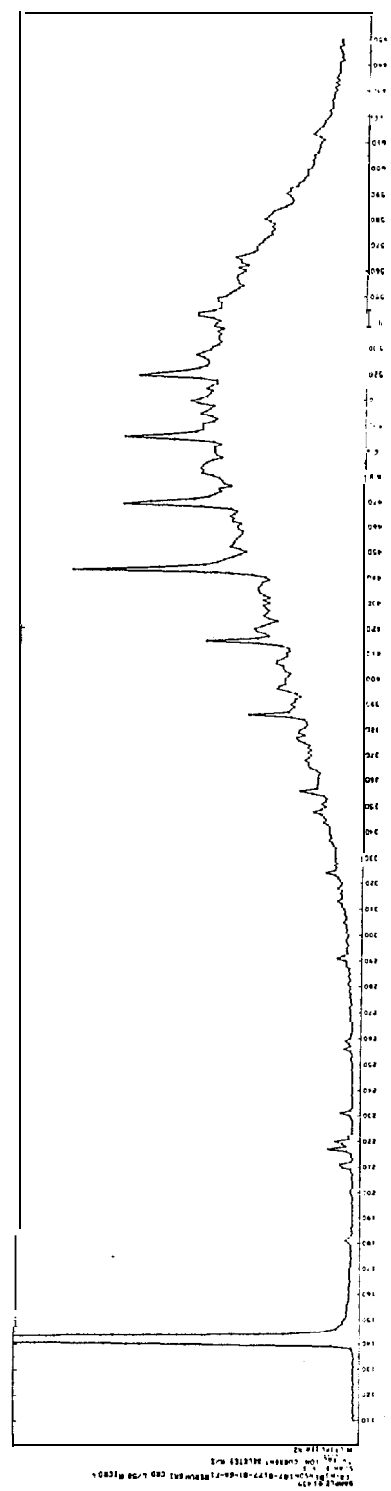
SAMPLE ID: _____

OTHER ID: _____

LOCATION : _____

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
420	unsaturated H/C			C_nH_{2n+1} , C_nH_{2n-1} fragments
443	alkane n-C ₂₄ :0	338	C ₂₄ H ₅₀	
452	unsaturated H/C			C_nH_{2n+1} , C_nH_{2n-1} , C_nH_{2n-3} fragments
469	alkane n-C ₂₅ :0	352	C ₂₅ H ₅₂	
481	unsaturated H/C			C_nH_{2n+1} , C_nH_{2n-1} , C_nH_{2n-3} fragments
495	alkane n-C ₂₆ :0 ?			C_nH_{2n+1} fragments
504	unsaturated H/C	372	C ₂₇ H ₄₈	C_nH_{2n+1} , C_nH_{2n-1} , C_nH_{2n-3} fragments, M ⁺ 272
509	unsaturated H/C	372	C ₂₇ H ₄₈	C_nH_{2n+1} , C_nH_{2n-1} , C_nH_{2n-3} fragments, 253, M ⁺ 272
590	alkane n-C ₂₇ :0	380	C ₂₇ H ₅₆	
527	unsaturated H/C			C_nH_{2n+1} , C_nH_{2n-1} , C_nH_{2n-3} fragments, 253



TIC trace for GC/MS 143

GC/MS RUN #: 1467

SAMPLE TYPE: INTERTIDAL, EMERITA, Benzene Fraction

SAMPLE ID: Benson 201-1076-04-1-F2

OTHER ID:

LOCATION: 201/Coal Oil Point

COMMENTS/SUMMARY:

Predominantly polyunsaturated hydrocarbons, most GC peaks exhibiting ions of several components.

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
788	branched ketone (see 1471, scan)	366		$C_n H_{2n-1}$ fragments to 111; 91, 91 + 14n, n=1,8; 131, 145; 290, 292, 294, 296; 304 306, 308, 310, 312, 314, 316; 320, 322, 324, 326 328, 330, 340, 342, 344
815				57, 69, 83, 97, 91, 91 + 14n, n=1,40; 131, 145; 290, 302, 304, 308, 310, 320, 322, 324, 326, 328, 330; 338, 340, 342, 344; 354, 356
832				$C_n H_{2n-1}$ fragments to 111; 91, 91 + 14n, n=1,11; 131, 145; 342, ,344; 354, 370
858				$C_n H_{2n-1}$ fragments to 111; 91, 91 + 14n, n=1,11; 131, 145; 352, 354, 356; 368, 370, 372
880				
901				$C_n H_{2n-1}$ fragments to 111; 89, 96; 91, 105, 119; 131, 145; 354, 370, 372; 386
905				$C_n H_{2n-1}$ fragments to 111; 91, 105, 119, 133; 131, 145; 181; 354, 370, 372, 386

Continued

GC/MS RUN #: 1467 continued

SAMPLE ID:

SAMPLE TYPE:

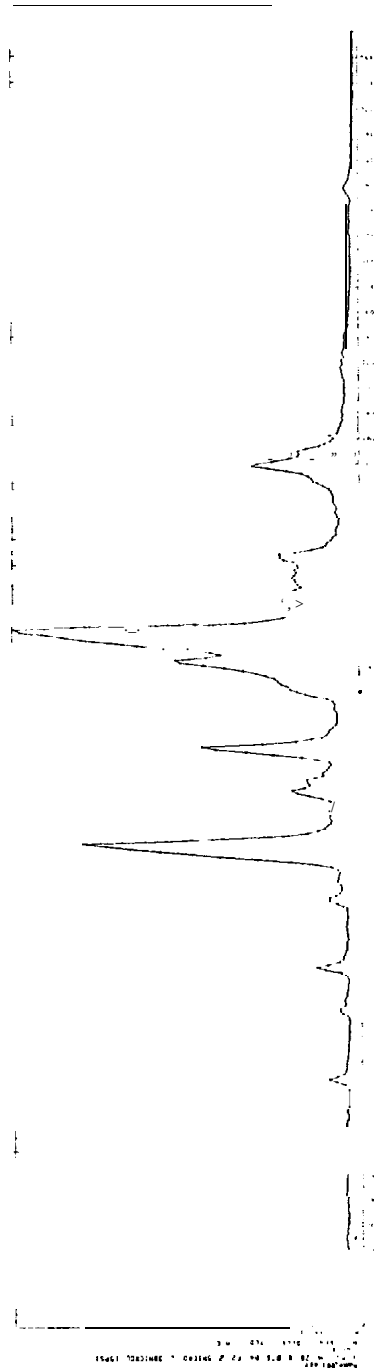
OTHER ID:

LOCATION:

COMMENTS/SUMMARY:

HHH-2.5-44

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
918	branched ketone (see 1471, scan)	394		C_nH_{2n-1} fragments to 125; 70, 82, 96, 110, 124, 138, 152; 236; 168, 210, 238; 251
952				C_nH_{2n-1} fragments to 125; 135, 137, 152, 247, 266, 380, 386, 394
964				
972				C_nH_{2n-1} fragments to 125; 91, 105, 119, 133, 161, 175, 189, 231; 152, 250; 384, 386, 394, 396, 398, 400, 414
978				C_nH_{2n-1} fragments to 111; 123, 189, 250, 362, 384, 386, 398, 400, 414
994				C_nH_{2n-1} fragments to 125; 91, 105, 119; 189
1029				C_nH_{2n-1} fragments to 125; 96, 110; 131, 231, 250
1035				C_nH_{2n-1} fragments to 125; 82, 96, 98, 110, 131; 231, 245, 250, 252, 376, 412



TIC trace for 1467

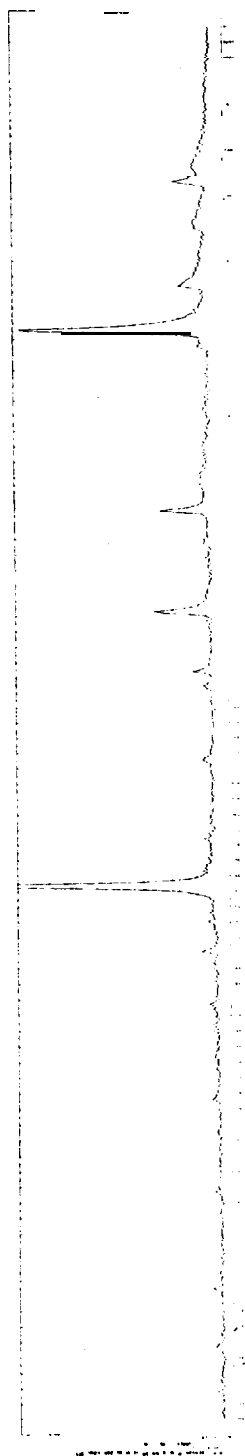
SAMPLE ID: 107-0177-01-6A-F2

OTHER ID:

LOCATION: 107, Coal Oil Point

COMMENTS/SUMMARY : Sample concentration weak, no structure elucidation possible.

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS



TIC trace for GC/MS 1459

GC/MS RUN #: 1603

SAMPLE TYPE: INTERTIDAL, MYTILUS, Hexane Fraction

SAMPLE ID: BLM 483 F1

OTHER ID:

LOCATION: 108/ San Miguel Island

COMMENTS/SUMMARY: All major components exhibit the mass spectral pattern of silicone oil components, sample also contains phthalates and adipate. Minor components are mainly unsaturated hydrocarbons,

HHH-2.5-48

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
292	*			
413	*			
432	alkane n-C _{17:0}	240	C ₁₇ H ₃₆	
435	isoprenoid alkane C _{19:0} (pristane)		C ₁₉ H ₄₀	113, 183, no M ⁺ (identification by MS data and GC retention time)
522	*			
619	*			
625	dibutylphthalate	278	C ₁₆ H ₂₂ O ₄	149, 205, 223, M ⁺ 278
652	unsaturated hydrocarbon		†	
667	unsaturated hydrocarbon		t	
679	alkatriene C _{25:3}	346	C ₂₅ H ₄₆	83, 95, 97, 109, 123, 135, 137, 139 149, 151, 165, 233, 291, M ⁺ 346
690	unsaturated hydrocarbon		†	
Continued				

GC/MS RUN #: 1603 continued

SAMPLE TYPE:

SAMPLE ID:

OTHER ID:

LOCATION :

COMMENTS/SUMMARY:

HH-2-576

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
708	*			
726	unsaturated hydrocarbon		†	
741			†	85, 97, 109, 111, 123, 125, 127, 135, 137, 141, 149, 207, 218
790	*			
796	unsaturated hydrocarbon		†	
848	unsaturated hydrocarbon		†	
855	dioctyladipate	370	C ₂₂ H ₄₂ O ₄	129, 147, 241, 259
865	*			
897	unsaturated hydrocarbon		†	
932	dioctylphthalate			149, 167, 279
936	*			

Continued

GC/MS RUN #: 1603 continued

SAMPLE ID: _____

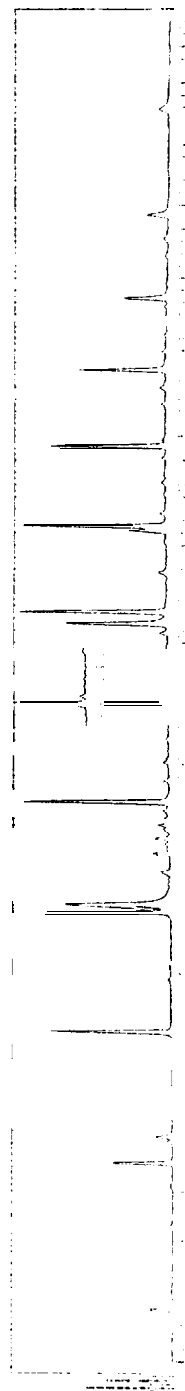
SAMPLE PE _____

OTHER ID _____

LOCATION _____

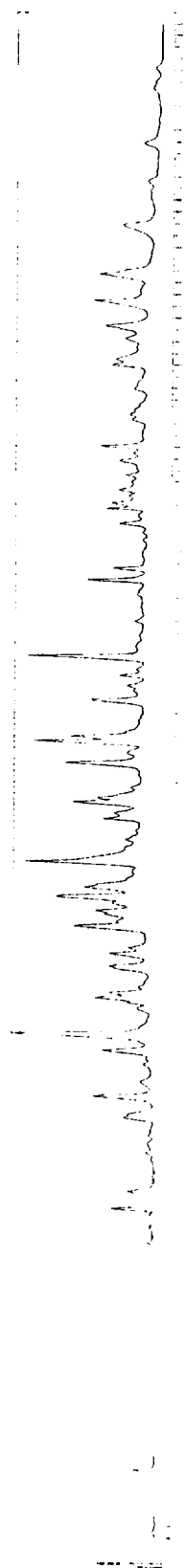
COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
1002	*			
1036	*			
1050	cholestene ?	370	+	
1064	*			
1124	*			
1192	*			
* mass spectral data indicate silicone oil for Si atoms, base peak 73, significant 355, 429, 503 + sample concentration is too weak for mass quality for further structural assignment				
			isotope pattern 207, 221, 281, sufficient	



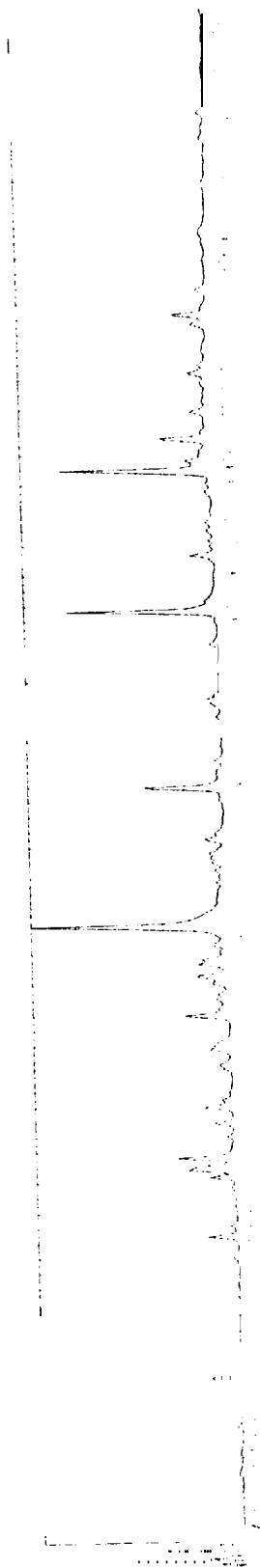
TIC trace for GC/MS 1603

GC/MS Run #1605
TO BE INCLUDED IN FINAL



TIC trace for GC/MS 1605

GC/MS Run #1608
TO BE INCLUDED IN FINAL



TIC trace for GC/MS 1608

GC/MS RUN #: 1364

SAMPLE TYPE: INTERTIDAL, MACROCYSTIS, Benzene Fraction

SAMPLE ID: BLM 306 Benzene Fr.

OTHER ID:

LOCATION: San Miguel Island

COMMENTS/SUMMARY: Polyunsaturated hydrocarbons, fatty acid esters, plasticizers

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
258	1 AEE C _{14:0}	(256)	C ₁₆ H ₃₂ O ₂	55, 57, 60, 69, 73, 85, 97, 102, 115, 129, 168, 185, 186 ?, 211, (M-45, 228 (M-28), no M ⁺
263	isoprenoid ketone C ₁₈	268	C ₁₈ H ₃₆ O ₁	55, 57, 58, 69, 71, 81, 82, 85, 95, 109, 123, 137, 151, 165, 179, 193, 207, 210, 235, 250, 253, M ⁺ 268
288	FAME C _{16:0}	270	C ₁₇ H ₃₄ O ₁	74, 87, 143, 227, M ⁺ 270
321	polyunsaturated hydrocarbon C _{21:6}	284	C ₂₁ H ₃₂	
324	polyunsaturated hydrocarbon C _{21:6}	284	C ₂₁ H ₃₂	
335	polyunsaturated hydrocarbon			55, 67, 79, 91, 93, 105, 108, 117, 119, 131, 133, 145, 147, 159, 162, 173, 175, 187, 201, 215, 243, no M ⁺
364	hexadecanoic-acid-n-butyl-ester	312	C ₂₀ H ₄₀ O ₂	56, 60, 69, 71, 73, 83, 95, 97, 101, 111, 116, 129, 239, 257, M ⁺ 312
Continued				

GC/MS RUN #: 1364 continued

SAMPLE TYPE:

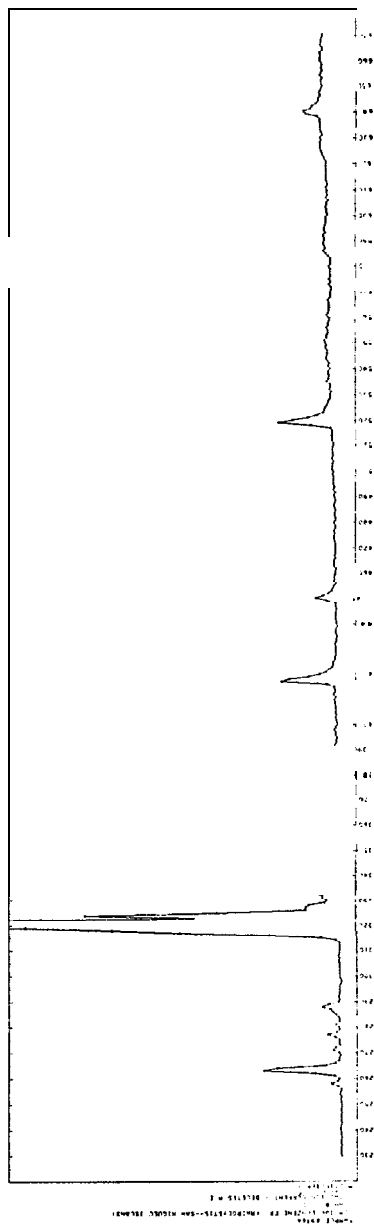
SAMPLE ID:

OTHER ID:

LOCATION :

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
417	octadecanoic-acid-n-butyl-ester	340	C ₂₂ H ₄₄ O ₂	60, 73, 116, 129, 267, 285, M ⁺ 340
440	octyldiphenyl phosphate	362	C ₂₀ H ₂₇ O ₄	55, 70, 94, 112, 140, 170, 249, 250, 251, 252, M ⁺ 362
450	dioctylphthalate			149, 167, 279
519	isoprenoid hydrocarbon C _{30:6}	410	C ₃₀ H ₅₀	
640		426	C ₃₀ H ₅₀ O ₁ ? C ₃₁ H ₅₄ ?	71, 73, 81, 95, 96, 109, 123, 125, 135, 147, 161, 163, 177, 179, 191, 205, 217, 231, 246, 273, 302, 411, M ⁺ 426



TIC trace for GC, 1364

GC/MS RUN #: 1360

SAMPLE ID: BLM 341 Hexane Fraction

SAMPLE TYPE: INTERTIDAL, PISASTER OCHRACEUS, Hexane Fraction

OTHER ID:

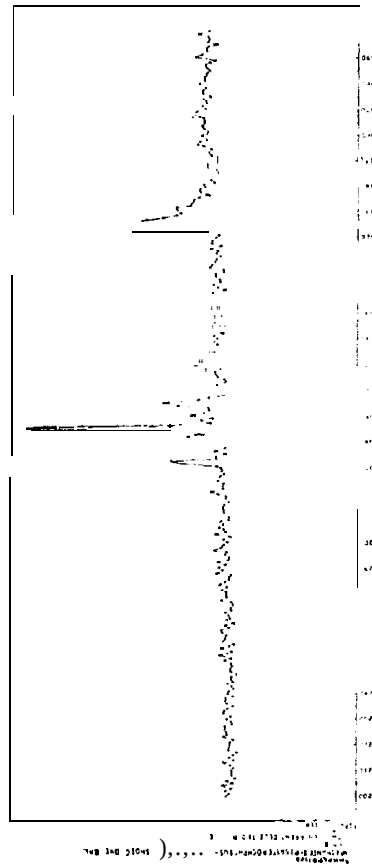
LOCATION: Horseshoe Cove

COMMENTS/SUMMARY: Sample concentration low, weak mass spectra
unsaturated hydrocarbons, isoprenoid unsaturated hydrocarbons.

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
332	isoprenoid alkene			55, 57, 83, 95; 97, 109, 139, 165
341	isoprenoid alkapolyene			55, 57, 69, 81, 83., 95, 97, 107, 109, 111, 121, 123, 135, 137, 149, 219, 289
345	isoprenoid alkatriene C _{25:3} ? *	346 ?	C ₂₅ H ₄₆	55, 57, 69, 71, 83, 95, 97, 109, 123, 137, 139, 151, 165, 167, 179, 233, 291
350	unsaturated hydrocarbon			55, 57, 69, 71, 81, 83, 95, 97, 105, 107, 109, 121, 123, 139, 141
355	unsaturated hydrocarbon			55, 57, 69, 71, 81, 83, 95, 97, 109, 123, 137
423	dioctyladipate			112, 129, 147, 241, 259

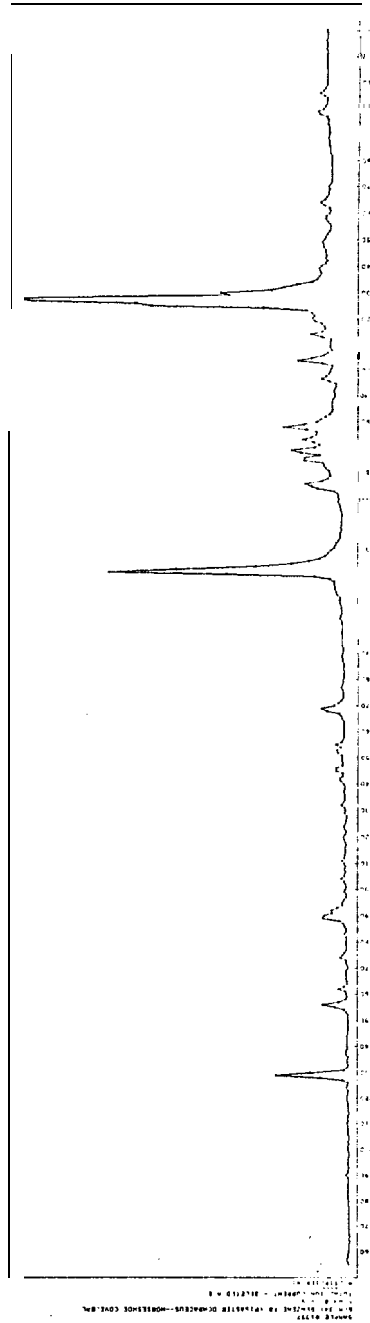
* assignment based on mass spectral data and
GC retention

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TIC trace for GC/MS 1360

GC/MS Run #1397
TO BE INCLUDED IN FINAL



TIC trace for GC/MS 1397

GC/MS RUN #: 1362

SAMPLE TYPE: INTERTIDAL, HALOTIS, Hexane Fraction

SAMPLE ID: BLM 319 Hexane Fraction

OTHER ID:

LOCATION: ill/Government point

COMMENTS/SUMMARY: Normal and branched saturated and unsaturated hydrocarbons, aldehydes, esters of fatty acids, polycyclic hydrocarbons.

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
157	branched alkene C _{15:0}	210	C ₁₅ H ₃₀	
161	alkene C _{15:0}	212	C ₁₅ H ₃₂	
193	alkane n-C _{16:0}	226	C ₁₆ H ₃₄	
214	alkadiene C _{17:2}	236	C ₁₇ H ₃₂	
217	alkene C _{17:1}	238	C ₁₇ H ₃₄	
222	alkene C _{17:1}	238	C ₁₇ H ₃₄	
225	alkane n-C _{17:0}	240	C ₁₇ H ₃₆	
257	alkane n-C _{18:0}	254	C ₁₈ H ₃₈	
	aldehyde C _{16:0}	(240)	C ₁₆ H ₃₂ O ₁	222 (M-18), 196 (M-44), 194 (M-18-28), no M ⁺
268	phthalate			149, 223

Continued

GC/MS RUN #: 1362 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

III-2.5-64

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
276				55, 57, 69, 83, 97, 111, 123, 135, 137, 151, 165, 194, 210, 220, 228
281	alkene C _{19:1}	266	C ₁₉ H ₃₈	
289	alkane n-C _{19:0}	268	C ₁₉ H ₄₀	
	aldehyde C _{17:0}	(254)	C ₁₇ H ₃₄ O ₁	236 (M-18), 210 (M-44), 208 (M-18-28), no M ⁺
293	FAME C _{16:0}	270	C ₁₇ H ₃₄ O ₂	
296	Phthalate			149, 205, 223
308				55, 57, 67, 69, 70, 71, 81, 83, 95, 97, 109, 111, 121, 123, 125, 135, 137, 139, 141, 149, 151, 164, 165
312				55, 57, 60, 67, 69, 73, 81, 83, 95, 97, 98, 109, 111, 121, 125, 129, 143, 149, 228, 248, 251, 256, 266, 270
320	alkane n-C _{20:0}	282	C ₂₀ H ₄₂	

Continued

GC/MS RUN #: 1362 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY :

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
337	aldehyde C _{18:1} ?	266	C ₁₈ H ₃₄ O	228, 256, 268, 274 . 55, 57, 67, 69, 70, 83, 96, 97, 109, 111, 121, 123, 125 135, 137, 149, 151, 152, 166, 180, 194, 196, 209, 211, 222 (M-64), 248 (M-18), M ⁺ 266
342	alkene			C _n H _{2n-1} fragments
349	alkene C _{21:0}	296	C ₂₁ H ₄₄	
351	alkatriene C _{25:3} (isoprenoid?)	346	C ₂₅ H ₄₆	233, 261, 289; M ⁺ 346
370	hexadecanoic acid n-butyl-ester	312	C ₂₀ H ₄₀ O ₂	73, 116, 129, 239, 257, M ⁺ 312
377	alkane n-C _{22:0}	310	C ₂₂ H ₄₆	
388				55, 57, 67, 69, 70, 71, 81, 83, 85, 95, 97, 109, 111, 121 123, 125, 135, 137, 149, 151, 152, 153, 155, 163, 165, 169, 175, 177, 189, 192, 217, 219, 221, 239, 256, 274, 292, 302, 305, 322
				Continued

GC/MS RUN #: 1362 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER Ill: _____

LOCATION: _____

COMMENTS/SUMMARY:

HH-2.5-66

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
404	alkane n-C _{23:0}	324	^c 23 ^H 48	
422	dioctyladipate ?	(370)	^c 22 ^H 42 ^O 4	71 83, 97, 101, 112, 129, 147, 241, 259, no M ⁺
	octadecanoic acid n-butyl-ester	340	^c 22 ^H 44 ^O 2	73 101, 116, 129, 267, 285, M ⁺ 340
429	alkane C _{24:0}	338	^c 24 ^H 50	
454	alkane C _{25:0}	352	C ₂₅ H ₅₂	
	dioctylphthalate	(390)	^c 24 ^H 38 ^O 4	113, 149, 167, 279, no M ⁺
479	sterane ?			149, 217, 219, 372
	alkane ^c 26:0	366	^c 26 ^H 54	253, 267, 281, 366
501	branched alkane	380	C ₂₇ H ₅₆	C _n H _{2n+1} fragments; 253, 267, M ⁺ 380

Continued

GC/MS RUN #: 1362 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

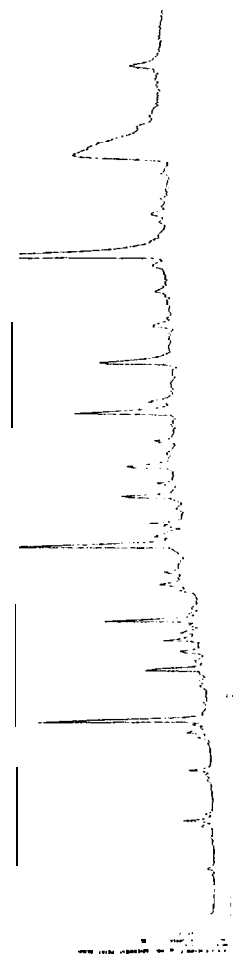
OTHER ID: _____

LOCATION : _____

COMMENTS/SUMMARY:

HM-2.5-67

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
524	isoprenoid alkahexaene	410	C ₃₀ H ₅₀	
551	bis-nor-hopane	384	C ₂₈ H ₄₈	163, 177, 191, 217, 369, M ⁺ 384
560	nor-hopane	398	C ₂₉ H ₅₀	163, 177, 191, 219, M ⁺ 398
577	triterpane (hopane ?)	412	C ₃₀ H ₅₂	191, 219, 397, M ⁺ 412
589	cholesterol	386	C ₂₇ H ₄₆ O	353, 368, 371, M ⁺ 386
	triterpane (hopane ?)	412	C ₃₀ H ₅₂	
	homohopane ?	426	C ₃₁ H ₅₄	
600				430, 473
644	homohopane	426	C ₃₁ H ₅₄	191, 217



TIC tr for GC/MS 1362

GC/MS RUN #: 1354SAMPLE TYPE: INTERTIDAL, HALIOTIS, Hexane FractionSAMPLE ID: BLM 320 Hexane Fraction

OTHER ID: _____

LOCATION: Ill/Government Point

COMMENTS/SUMMARY: Mainly phthalates and adipates, saturated and unsaturated hydrocarbons.

III-2.5-69

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
162	alkane C _{15:0}	212	C ₁₅ H ₃₂	
219	alkene C _{17:1}	238	C ₁₇ H ₃₂	
226	alkane n-C _{17:0}	240	C ₁₇ H ₃₄	
351	alkatriene C _{25:3}	346	C ₂₅ H ₄₆	
391	adipate			69, 70, 71, 112, 129, 147, 213, 231, 241, 259
415	dioctyladipate	370	C ₂₂ H ₄₂ O ₄	70, 71, 112, 129, 147, 241, 259, M ⁺ 370
422	dioctyladipate	370	C ₂₂ H ₄₂ O ₄	
444	dioctylphthalate			113, 129, 149, 167, 279
449	dioctylphthalate	390	C ₂₄ H ₃₈ O ₄	113, 129, 149, 167, 279, M ⁺ 390
457	dioctylphthalate	390	C ₂₄ H ₃₈ O ₄	113, 129, 149, 167, 261, 279, M ⁺ 390

Continued

GC/MS RUN #: 1354 continued

SAMPLE TYPE:

SAMPLE ID:

OTHER ID:

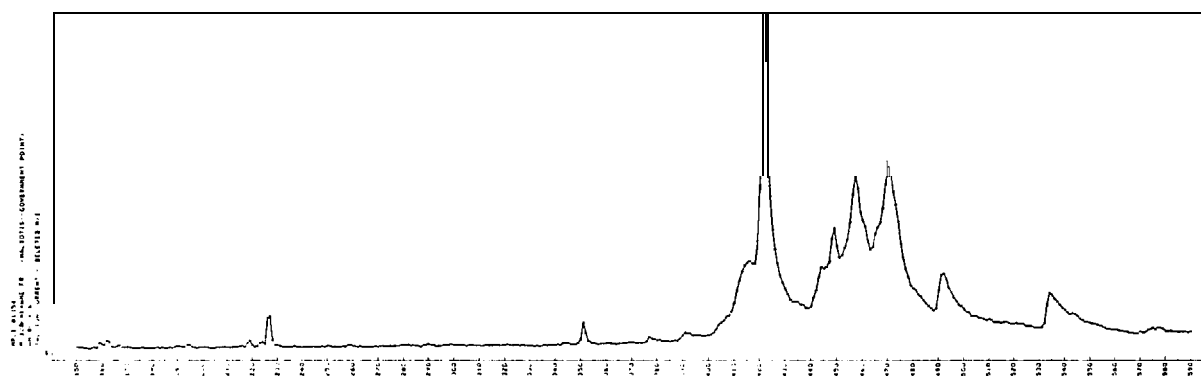
LOCATION:

COMMENTS/SUMMARY :

11-2.5-70

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
470	lioctylphthalate	390	$C_{24}H_{38}O_4$	113, 149, 167, 261, 279, 333, M ⁺ 390
491	lioctylphthalate	390	$C_{24}H_{38}O_4$	113, 149, 167, 253, 261, 279, M ⁺ 390
534	octyl,decyl phthalate	418	$C_{26}H_{42}O_4$	149, 167, 279, 307, M ⁺ 418

HHH-2.5-71



TIC trace for GC/MS 1354

GC/MS RUN #: 1356

SAMPLE TYPE: INTERTIDAL, MYTILUS CALIFORNIANUS, Hexane Fraction

SAMPLE ID: BLM 317 Hexane Fr.

OTHER ID: _____

LOCATION: ill/Government point

COMMENTS/SUMMARY: Large unresolved "hump" with 'Superimposed chromatographic peaks, unsaturated hydrocarbons, polycyclic hydrocarbons. Due to significant ion contribution of unresolved components to the mass spectra of distinct chromatographic peaks, the structure assignments to these peaks is either not possible or only tentative.

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
144				43, 57, 71, 85, 95, 91, 109, 111, 113, 123, 137, 141, 183, 208, 209, 220 -
156	alkane C _{15:0}	212	C ₁₅ H ₃₂	
189	C _{17:1} , C _{17:2} , C _{17:3} alkenes			C _n H _{2n-1} , C _n H _{2n-3} fragments, 234, 236, 238
209	alkene C _{18:1} branched	252	C ₁₈ H ₃₆	C _n H _{2n-1} , C _n H _{2n-3} fragments, M ⁺ 252
222	alkane C _{17:0}	240	C ₁₇ H ₃₄	C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} fragments M ⁺ 240
	alkenes C _{18:2} , C _{18:3} C _{18:4}			250, 248, 246
	C _{19:2} , C _{19:3} , C _{19:4} C _{19:5}			264, 262, 260, 258
225	isoprenoid alkane C _{19:0}	268	C ₁₉ H ₄₀	113, 183, M ⁺ 268
230	alkene C _{19:1}	266	C ₁₉ H ₃₈	C _n H _{2n+1} , C _n H _{2n-1} C _n H _{2n-3} fragments, M ⁺ 266
244	branched alkadiene C _{19:2}	264	C ₁₉ H ₃₆	109, 123, 179, M ⁺ 264

Continued

III-2.5-72

GC/MS RUN #: _____ SAMPLE _____

SAMPLE D _____ OTHER D _____

LOCATION: _____

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
254	H/C's C _{18:2} , C _{19:3} , C _{19:4} , C _{19:5}			264, 262, 260, 258
257	H/C's C _{19:2} , C _{19:3} , C _{19:4} , C _{19:5} , C _{19:6}			264, 262, 260, 258, 256
263	H/C's C _{19:2} , C _{19:3} , C _{19:4} , C _{19:5} , C _{19:6}			264, 262, 260, 258, 256
269	H/C's C _{19:2} , C _{19:3} , C _{19:4} , C _{19:5} , C _{19:6}			280, 278
274	C _{20:1} , C _{20:2}			264, 262, 260, 256
	C _{20:2} , C _{20:3} , C _{20:4}			278, 276, 274
	predominantly H/C C _{19:3}	262	C ₉ H ₃₄	M ⁺ 262

Continued

GC/MS RUN #: 1356 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

III-2.5-74

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
278	H/C's C _{20:2} , C _{20:3} , C _{20:4} , C _{20:5} , C _{20:6}			278, 276, 274, 272, 270
285	H/C's C _{20:2} , C _{20:3} , C _{20:4} , C _{20:5} , C _{20:6} , C _{20:7} or C _{19:0}			278, 276, 274, 272, 270, 268
295	C ₁₉ sterane (androstande ?)	260	C ₁₉ H ₃₂	203, 217, 245, M ⁺ 260
303	C ₁₉ sterane (androstande ?)	260	C ₁₉ H ₃₂	203, 217, 245, M ⁺ 260
327	H/C C _{21:0}	296	C ₂₁ H ₄₄	C _n H _{2n+1} fragments, M ⁺ 296
	H/C C _{25:3}	346	C ₂₅ H ₄₆	291, M ⁺ 346
332	unsaturated H/C's			
343	C ₂₁ sterane (pregnane ?)	288	C ₂₁ H ₃₆	217, 231, 259, M ⁺ 288
	alkane C _{21:0} branched	296	C ₂₁ H ₄₄	253, M ⁺ 296 "

Continued

GC/MS RUN #: 1356 continued

SAMPLE ID:

SAMPLE TYPE:

OTHER ID:

LOCATION:

COMMENTS/SUMMARY:

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SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
347	^c ₂₁ sterane	288	C ₂₁ H ₃₆	217, 218, 259, 273, M ⁺ 288
	unsaturated H/C ^c _{23:3}	320	^c ₂₃ H ₄₂	M ⁺ 320
355	unsaturated H/C 's			
362	C ₂₁ sterane (5α pregnane ?)	288	^c ₂₁ H ₃₆	217, 218, 273, M ⁺ 288
373	unsaturated H/C s			
383	H/C's (saturated & unsaturated)			
391	^c ₂₂ sterane	302	^c ₂₂ H ₄	217, 219, 287, M ⁺ 302
424	alkane C _{24:0}	338	^c ₂₄ H ₅₀	C _n H _{2n+1} fragments
450	alkane C _{25:0}	352	^c ₂₅ H ₅₂	239, 253, M ⁺ 352
474	H/C ^c _{27:4}	372	^c ₂₇ H ₄₈	253, M ⁺ 372
494	H/C ^c _{28:4}	386	^c ₂₈ H ₅₀	253, M ⁺ 386

Continued

GC/MS RUN #: 1356 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

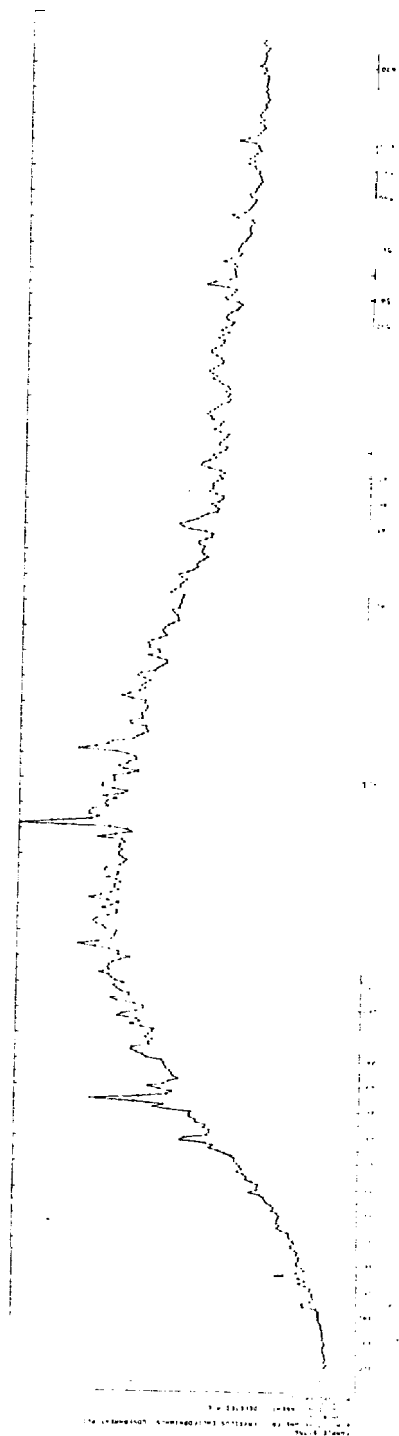
OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

III-2.5-76

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
511	H/C 'S			207, 218, 253, 259, 267, 281, 295, 372, 386, 400
545	triterpanes			191, 400, 414
	sterenes			217, 231, 328 355, 369, 384
554	triterpanes	398		191, 217, 232, 246, .383, 385, 398, 400
571	pentacyclic triterpane C ₃₀ (hopane ?)	412	C ₃₀ H ₅₂	191, 217, 355, 369, 397, M ⁺ 412
601	pentacyclic triterpane (hopene ?)	410	C ₃₀ H ₅₀	189, 191, M ⁺ 410



TIC trace for GC/MS 1356

SAMPLE ID: BENSON 111-0177-01-6A-F1

OTHER ID: _____

LOCATION: 111/GOVERNMENT POINT, SANTA BARBARA COUNTY

COMMENTS/SUMMARY :

Two groups of n-alkanes: n-C_{15:0} - n-C_{17:0} n-C_{21:0} - n-C_{28:0}

Isoprenoid components: saturated, mono- and di-unsaturated

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS .
219	n-pentadecane C _{15:0}	212	C ₁₅ H ₃₂	
277	11-C ₁₆ (MS + GC data)			57, 71, 85, 99, 113, 127, 141, 155: MS i- GC data, no M ⁺
325	heptadecene C _{17:1}	238	C ₁₇ H ₃₄	55, 57, 69, 83, 97, 111, 125, 139, M ⁺ 238
335	heptadecene C _{17:1}	238	C ₁₇ H ₃₄	43, 55, 57, 69, 83, 97, 111, 125, 139, M ⁺ 238
340	n-heptadecane C _{17:0}	240	C ₁₇ H ₃₆	C _n H _{2n+1} fragments M ⁺ 240
344	isoprenoid alkene, pristane	268	C ₁₉ H ₄₀	57, 71, 85, 99, 113, 127, 141, 155, 183, M ⁺ 268
358	isoprenoid alkene, pristene			C _n H _{2n-1} fragments, 126
406	alkene and phytane?			57, 71, 85, 97, 99, 113, 127, 183, 197
424	branched alkatriene	278	C ₂₀ H ₃₈	
440	isoprenoid C _{20:2} (phytadiene)	278	C ₂₀ H ₃₈	43, 57, 81, <u>82</u> , 95, 123, 137, M ⁺ 278
444	isoprenoid C _{20:2} (phytadiene)			41, <u>43</u> , 55, 57, 69, 81, 82, 95, 123, 137, M ⁺ 278
453	isoprenoid C _{20:2} (phytadiene)	278	C ₂₀ H ₃₈	41, 43, <u>55</u> , 57, 68, 69, 81, 82, 95, 123, 137, 179, M ⁺ 278
463	isoprenoid C _{20:2} (phytadiene)	278	C ₂₀ H ₃₈	<u>43</u> , 57, 69, 82, 95, " 123, M ⁺ 278

continued

HH-2.5-78

GC/MS RUN #: 1461 (continued)

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

11-2-5-79

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
813	n-C ₂₆ :0	366	C ₂₆ H ₅₄	n H _{2n+1} fragments, M ⁺ 366
854	n-C ₂₇ 0	380	C ₂₇ H ₅₆	" " M ⁺ 380
895	n-C ₂₈ 0	394	C ₂₈ H ₅₈	" " M ⁺ 394
933	n-C ₂₉ :0	408	C ₂₉ H ₆₀	n H _{2n+1} fragments, M ⁺ 408
	+ stigmastane ?	400	C ₂₉ H ₅₂	217, 218
	+ C ₂₈ sterane ?	386		
951	alkene ?			n H _{2n+1} , C _n H _{2n} fragments

GC/MS RUN #: 1461 (continued)

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

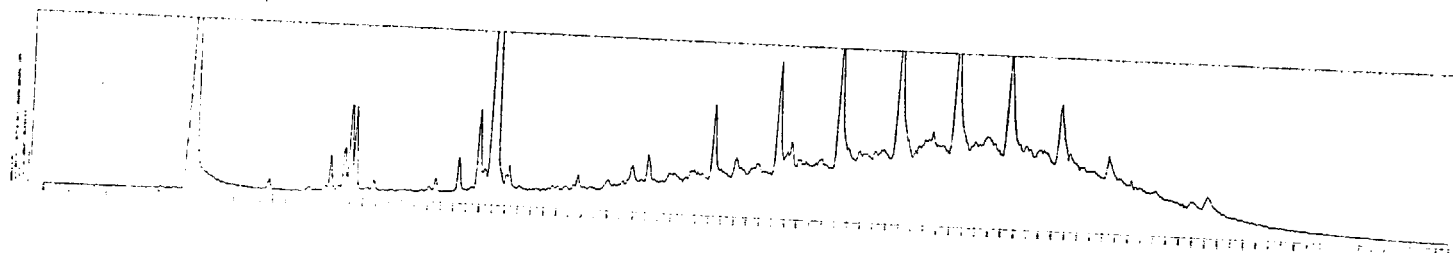
LOCATION: _____

COMMENTS/SUMMARY: .

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
517	n-alkane C _{20:0} ? + sterane?	282	C ₂₀ H ₄₂	C _n H _{2n+1} fragments
540	unsaturated HC, possibly branched	270		43, 57, 69, 83, 97, 111, 123, 141, 155, 211, 239, 291
559	n-alkene C _{21:1}	294	C ₂₁ H ₄₂	C _n H _{2n+1} fragments, C _n H _{2n} fragments: 97, 111, 125
571	n-C _{21:0}	296	C ₂₁ H ₄₄	C _n H _{2n+1} fragments M ⁺ 296
623	n-C _{22:0}	310	C ₂₂ H ₄₆	C _n H _{2n+1} fragments M ⁺ 310
641	alkene C _{23:1} (branched?)	322	C ₂₃ H ₄₆	C _n H _{2n+1} fragments, 97, 111, 125, 281, M ⁺ 322
658	alkene C _{23:1}	322	C ₂₃ H ₄₆	C _n H _{2n+1} fragments, 97, 111, 125, 295, M ⁺ 322
674	n-C _{23:0}	324	C ₂₃ H ₄₈	C _n H _{2n+1} fragments M ⁺ 324
684	branched C _{20:2} -cyclopentan	346	C ₂₅ H ₄₆	41, 43, 55, 57, 69, 71, 81, 83, 85, 95, 97, 109, 111, 123, 125
722	n-C _{24:0}	338	C ₂₄ H ₅₀	
769	n-C _{25:0}	352	C ₂₅ H ₅₂	C _n H _{2n+1} fragments, M ⁺ 352
795				C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} fragments

continued

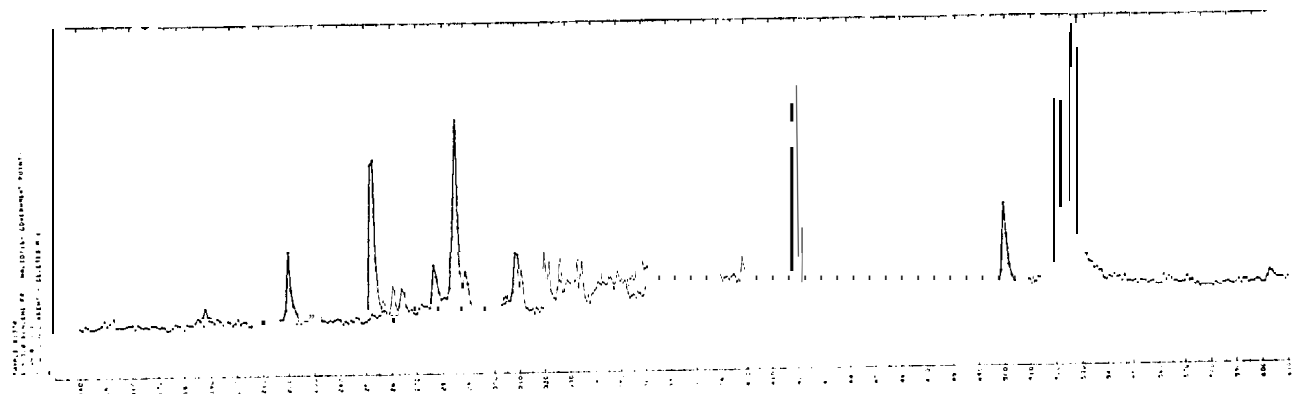
HHH-2.5-81



TIC trace for GC/MS 1461

GC/MS Run #1374
TO BE INCLUDED IN FINAL

HHH-2.5-8



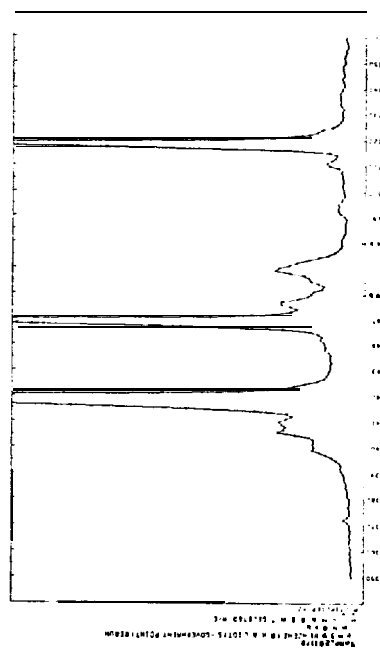
TIC trace for GC/MS 1374

GC/MS Run #1368
TO BE INCLUDED IN FINAL



TIC trace for GC/MS 1368

GC/MS Run #1370
TO BE INCLUDED IN FINAL



TIC = race for GC/MS 1370

GC/MS Run #1380
TO BE INCLUDED IN FINAL

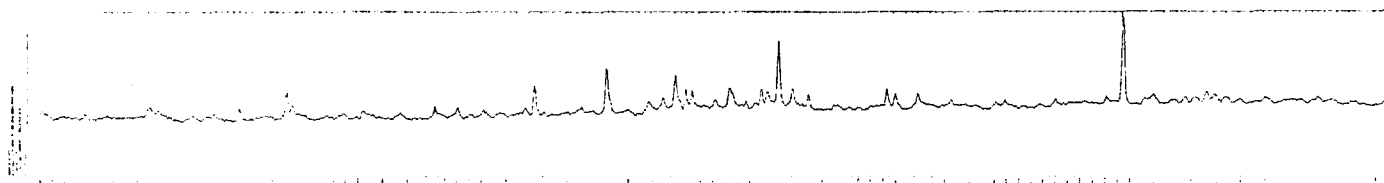
TIC trace for GC/MS #1380

TO BE INCLUDED IN FINAL

GC/MS Run #1386
TO_BE INCLUDED IN FINAL

GC/MS Run #1574
TO BE INCLUDED IN FINAL

II-2.5-82

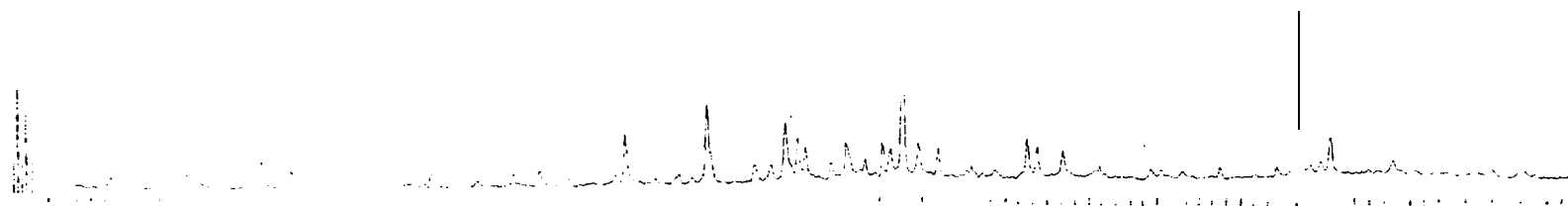


TIC trace for GC/MS 1574

GC/MS Run #1576

TO BE INCLUDED IN FINAL

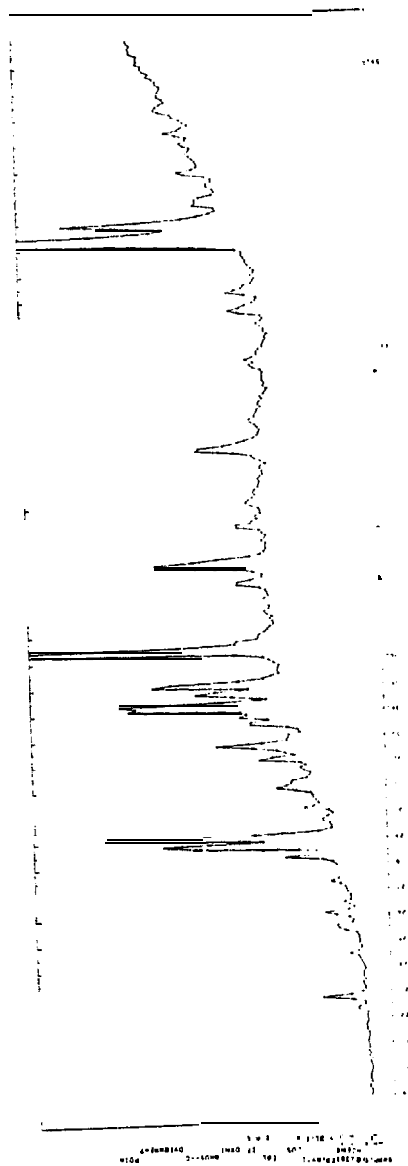
11-2.5-94



TIC trace for CC/MS 1576

GC/MS Run #1366
TO BE INCLUDED IN FINAL

e



TIC trace for GC/MS 1366

GC/MS RUN # 1463

SAMPLE TYPE: INTERTIDAL> MACROCYSTIS, Benzene Fraction

SAMPLE ID: 111-0177-01-6A F2

OTHER ID:

LOCATION: 111/ Government Point, Santa Barbara County

COMMENTS/SUMMARY:

Chlorinated HC; unsaturated hydrocarbons; n-alkanes C_{30:0}, C_{31:0}

SCAN	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
468		240 ?		41, 43, 55, 69, 70, 83, 85, 95, 97, 115, 119, 155, 165, 192, 209, 223, M ⁺ ? 240
473				41, 43, 55, 69, 81, 95, 107, 109, 123, 137, 150, 165, 209, 224, 263, 274, 278
547				41, 43, 55, 67, 79, 91, 93, 95, 105, 108, 117, 119, 129, 131, 133, 148, 202, 226, 282, 292
552				39, 41, 43, 55, 67, 78, 79, 91, 93, 95, 105, 108, 115, 117, 119, 128, 129, 131, 133, 135, 165, 222, 226, 252, 282, 291
573	trichlorodiphenylethylene	282	C ₁₄ H ₉ Cl ₃	175, 212*, 226, 247*, M ⁺ 282,
612	DDE	316	C ₁₄ H ₈ Cl ₄	105, 123, 176, 210*, 246*, 316*,
704	alkatetraene, branched C ₂₅ :	344	C ₂₅ H ₄₄ (4F)	41, 55, 69; 81, 95, 109, 123, 137; 149, 163, 177, 191, 205 219; 231, 273, 301, M ⁺ 344

Continued

GC/MS RUN #: 1463 continued

AM YPE:

SAMPLE ID:

OTHER ID:

LOCATION

COMMENTS/SUMMARY:

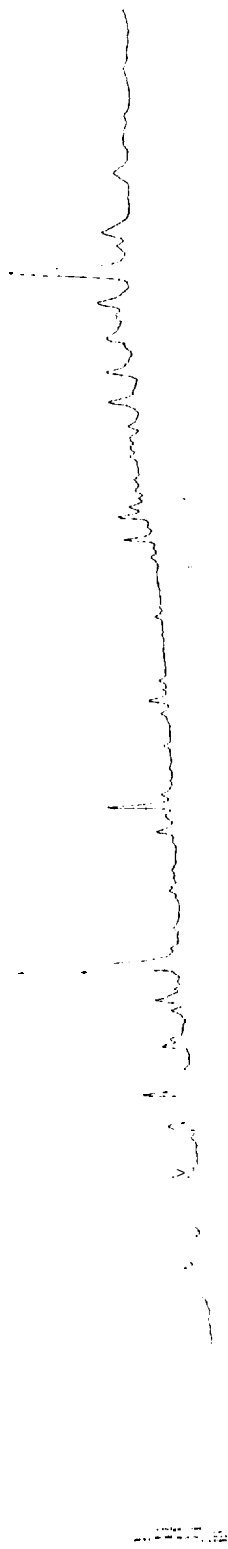
SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
914	alkahexaene, branched C ₃₀ :6 (squalene ?)	410	C ₃₀ H ₅₀	41, 55, 69; 81, 95, 109, 123, 137; 149, 163, 177, 191; 203 217, 231, 273; 299, 341; 367, M ⁺ 410
940	n-alkane C ₂₉ :5	408	C ₂₉ H ₆₀	C _n H _{2n+1} fragments, M ⁺ 408
979	n-alkane C ₃₀ :5	422	C ₃₀ H ₆₂	C _n H _{2n+1} fragments, M ⁺ 422
1006	unsaturated hydrocarbon	432	C ₃₁ H ₆₀	C _n H _{2n-1} fragments, M ⁺ 432
1021	unsaturated hydrocarbon	432	C ₃₁ H ₆₀	C _n H _{2n-1} fragments, M ⁺ 432

* isotope pattern for chlorine



TIC trace for GC/MS 1463

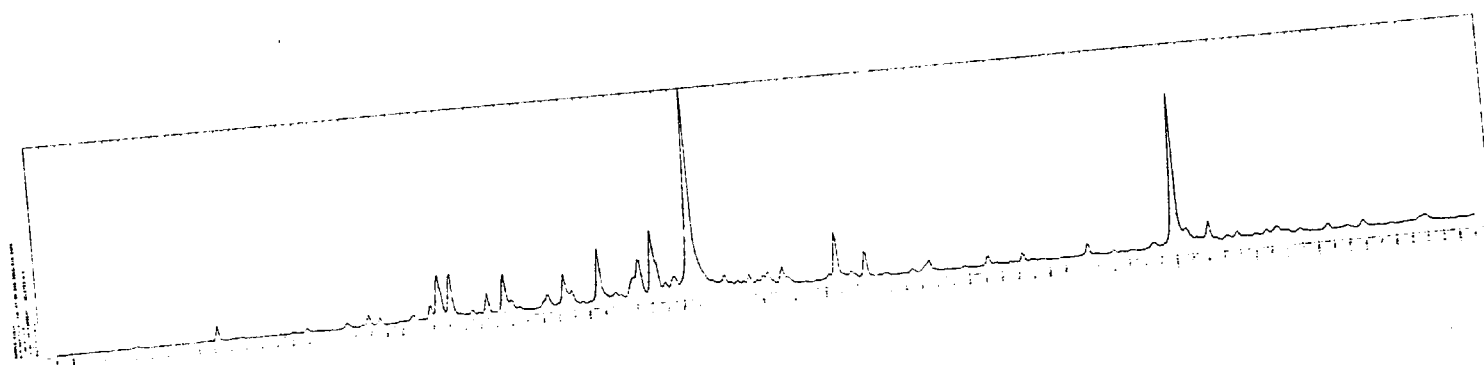
GC/MS Run #1612
TO BE INCLUDED IN FINAL



TIC trace for GC/MS 1612

GC/MS Run #1614
TO BE INCLUDED IN FINAL

111-2.5-103



TIC trace for GC/MS 1614

GC/MS RUN #: 1469

SAMPLE TYPE: INTERTIDAL, EMERITA, Hexane Fraction

SAMPLE ID: Benson 202-1076-01-F1

OTHER ID:

LOCATION: 202/Corona Del Mar

COMMENTS/SUMMARY: Normal hydrocarbons; isoprenoid and other branched hydrocarbons, saturated and unsaturated cyclic hydrocarbons, sterane type hydrocarbons.

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
215	n-C _{15:0}	212	C ₁₅ H ₃₂	C _n H _{2n+1} fragments; 99, 169; 113, 183
279	n-C _{16:0}	224	C ₁₆ H ₃₄	
310	isoprenoid C _{18:0}	?		
347	n-C _{17:0}	240	C ₁₇ H ₃₆	
350	isoprenoid C _{19:0} (pristane)	268	C ₁₉ H ₄₀	C _n H _{2n+1} , C _n H _{2n-1} fragments
371	isoprenoid alkene C _{19:1} (pristene)	266	C ₁₉ H ₃₈	
376	branched alkene			C _n H _{2n+1} , C _n H _{2n-1} fragments
383	branched alkene			C _n H _{2n+1} , C _n H _{2n-1} fragments
407	n-C _{18:0}	254	C ₁₈ H ₃₈	
412	isoprenoid alkane C _{20:0} (phytane)	282	C ₂₀ H ₄₂	
()	()		()	

III-2.5-104

GC/MS RUN #: 1469 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION : _____

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
444	isoprenoid alkadiene C _{20:2} (phytadiene)	278	C ₂₀ H ₃₈	C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} fragments
454	isoprenoid alkadiene C _{20:2} (phytadiene)	278	C ₂₀ H ₃₈	C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} fragments
461	branched alkene C _{20:1}	280	C ₂₀ H ₄₀	C _n H _{2n+1} , C _n H _{2n-1} fragments; 183
468	n-C _{19:0}	268	C ₁₉ H ₄₀	
477	alkadiene C _{20:2} + branched alkene C _{21:1}	278 294	C ₂₀ H ₃₈ C ₂₁ H ₄₂	C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} fragments
489	alkadiene C _{20:2}	278	C ₂₀ H ₄₂	C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} fragments
502	alkadiene C _{21:2}	292	C ₂₁ H ₄₂	C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} fragments
507	branched alkadiene C _{21:2}	292	C ₂₁ H ₄₂	

Continued

GC/MS RUN #: 1469 continued

SAMPLE TYPE: _____

SAMPLE 10: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

III-2.5-106

SCAN #	COMPOUND IDENTIFICATION'	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
514	branched alkadiene C _{21:2}	292	C ₂₁ H ₄₂	
526	n-C _{20:0}	282	C ₂₀ H ₄₂	
532	alkenes; alkadienes	308	C ₂₂ H ₄₄	
		292	C ₂₁ H ₄₂	
546	alkadiene C _{21:2}	292	C ₂₁ H ₄₂	
559	alkenes	*		C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} fragments
565	alkenes	*		C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} fragments
580	n-C _{21:0}	296	C ₂₁ H ₄₄	
595	alkenes; nest branched	*		C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} fragments
612	alkadiene C _{23:2}	320	C ₂₃ H ₄₄	C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} fragments

Continued

GC/MS RUN #: 1469 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
634	i-C ₂₂ :0	310	C ₂₂ H ₄₆	
649	branched alkenes	*		C _n H _{2n+1} , C _n H _{2n-1} , C _n H _{2n-3} fragments
664		318	C ₂₃ H ₄₂	191, 293, 318
683	n-C ₂₃ :0	324	C ₂₃ H ₄₈	
690	homologue to 664	332	C ₂₄ H ₄₄	191, 317, 332
	+ alkenes	*		
714	alkenes			C _n H _{2n+1} : to 323; C _n H _{2n-1} : to 237; C _n H _{2n-3} : to 319 249
733	i-C ₂₄ :0	338	C ₂₄ H ₅₀	
744	homologue to 690, 664	346	C ₂₅ H ₄₆	191, 331, 346
766	alkenes	*		C _n H _{2n+1} : to 337; C _n H _{2n-1} : to 251; C _n H _{2n-3} : to 361; 263

Continued

GC/MS RUN #: 1469 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOLE WT.	MOLE FORMULA	SIGNIFICANT IONS
777	n-C ₂₅ :0	352	C ₂₅ H ₅₂	191, 219, 360, 362, 364, 372, 374, 376
783				191, 193, 219, 356, 358, 360, 370, 372, 374, 376, 378, 384
786				C _n H _{2n+1} : to 351; C _n H _{2n-1} : to 209; C _n H _{2n-3} : to 347; 249
803	n-C ₂₆ :0	366	C ₂₆ H ₅₄	217, 259, 359, 372
822	cholestane	372	C ₂₇ H ₄₈	253
840	+ sterene			253, 372
844	ster ene (?)	372		
861	n-C ₂₇ :0	380	C ₂₇ H ₅₆	217, 218, 259, 372, 386
	+ Me-cholestane	386	C ₂₈ H ₅₂	217, 218, 259, 371, 386
876	Me-cholestane	386	C ₂₈ H ₅₂	
	stigmastane (?)			217, 218, 259, 371, 372, 386, 400
886	28 sterane or Et-cholestane	386/400		

Continued

GC/MS RUN #: 1469 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
893	stigmastane	400	C ₂₉ H ₅₄	217, 218, 259, 372
904	n-C ₂₈ :0	394	C ₂₈ H ₅₈	
908	steranes; sterenes	386/400		217, 259, 267, 371, 386, 394, 400
923	steranes	386/400/ 414		191, 217, 232, 371, 386, 394, 400, 414
942	n-C ₂₉ :0	408	C ₂₉ H ₆₀	
	sterene, sterane	400/414		
960	sterene, sterane, hopane ?			191, 217, 384, 400, 414, 428
975	nor-hopane	398	C ₂₉ H ₅₂	191, 383, 398
	+ sterene sterane			
979	n-C ₃₀ :0	422	C ₃₀ H ₆₂	
	+ nor-hopane type	398		191, 219, 398, 412
	+ steranes, sterenes			400, 414

Continued

GC/MS RUN #: 1469 continued

SAMPLE TYPE:

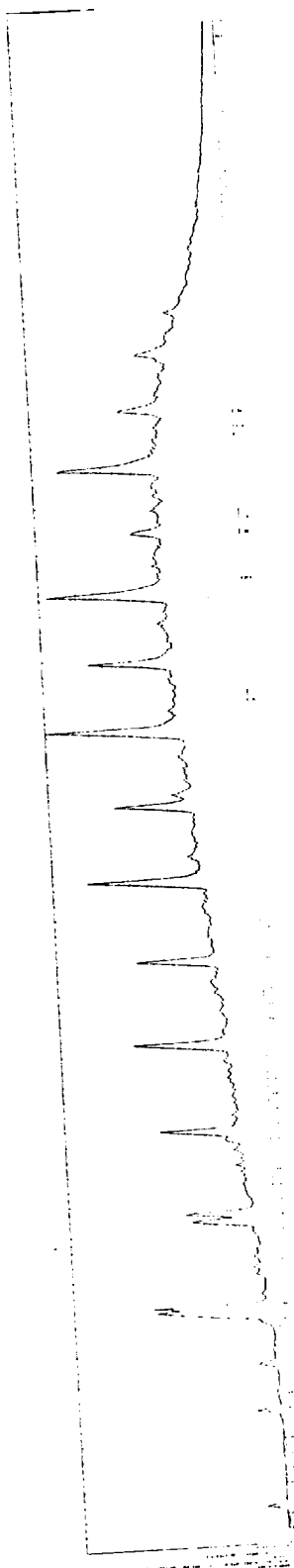
SAMPLE ID:

OTHER ID:

LOCATION:

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
1007	hopane	412	C ₃₀ H ₅₂	191, 205, 219, 397, 412
1022	hopane; sterane types			191, 217, 219, 412, 421, 428, 442
1050	homo-hopane ?	426	C ₃₁ H ₅₄	191, 219, 411, 426
1092	bis-homo-hopane ?	440	C ₃₂ H ₅₆	191, 219, 440
1212				
* several	compounds with different degrees of			
unsaturation;	M ⁺ not discernible			



T_{PC} trace for GC/MS 1469

GC/MS RUN #: 1471

SAMPLE TYPE: INTERTIDAL, EMERITA, Benzene Fraction

SAMPLE ID: BENSON 202-1076-01-1-F2

OTHER ID:

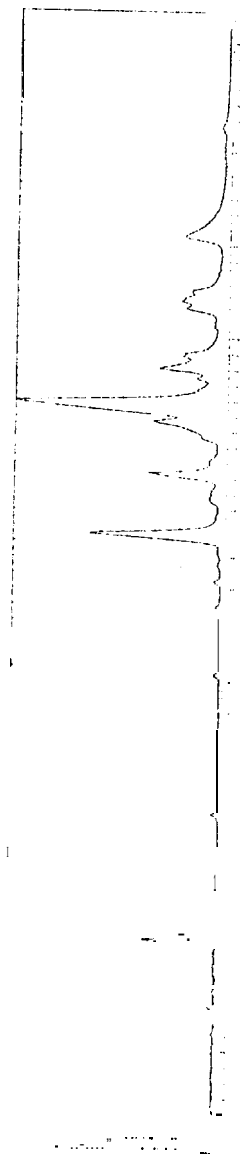
LOCATION: 202/CORONA DEL MAR

COMMENTS/SUMMARY:

HHH-2.5-112

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
572	trichloro diphenyl ethylene	282	$C_{14}H_9Cl_3$	176, 212*, 247*, M^+ 282*
613	DDE	316	$C_{14}H_8Cl_4$	176, 210*, 246*, 281*, M^+ 316*
643	pentachlorobiphenyl	324	$C_{12}H_5Cl_5$	184*, 218, 219, 254*, M^+ 324*
666	hexachlorobiphenyl ?	358	$C_{12}H_4Cl_6$	228, M^+ 358*
694	hexachlorobiphenyl	358	$C_{12}H_4Cl_6$	288*, M^+ 358*
875	branched ketone	366	$C_{25}H_{50}O_1$	150, 152, 166, 168, 194, 196, 222, 224, M^+ 366
914	unsaturated hydrocarbons			mainly C_nH_{2n-1} "fragments to m/e 123, 168, 210, 236, M^+ 364, 366, 394, 406
947	unsaturated hydrocarbons			mainly C_nH_{2n-1} fragments, 248, 250, M^+ 382, 394, 408
960	branched ketone	394	$C_{27}H_{54}O_1$	150, 152, 166, 168, 180, 182, 194, 196, 208, 222, 224, 240, 250, 252, 268, M^+ 394; homologue to compound in scan 875
975	unsaturated hydrocarbons			C_nH_{2n-1} , C_nH_{2n-3} fragments
981	n-C ₃₀ :0	422	$C_{30}H_{62}$	

continued



TIC = trace for GC/MS 1471

GC/MS RUN #: 1571

SAMPLE TYPE: INTERTIDAL, HALIOTIS, benzene fraction

SAMPLE ID: BLM 345 F2

OTHER ID:

LOCATION: 105/CORONA DEL MAR

COMMENTS/SUMMARY:

predominantly methyl esters of saturated and unsaturated branched fatty acids; minor components are unsaturated hydrocarbons

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
256	α -ionone	192	$C_{13}H_{20}O_1$	43, 58, 77, 91, 93, 121, 136, M^+ 192 (192→136 RDA)
295	β -ionone	192	$C_{13}H_{20}O_1$	43, 55, 58, 77, 91, 93, 95, 107, 121, 135, 149, 159, 177, 178, M^+ 192
436				43, 55, 57, 58, 69, 71, 82, 91, 96, 109, 111, 167, 168, 169
441	FAME $C_{14:0}$	242	$C_{15}H_{30}O_2$	74, 87, 143, 199, 211, M^+ 242
471	FAME			74, 87, 127, 157, 197, 213
499				43, 57, 69, 71, 82, 96, 109, 123
559		236	$C_{17}H_{32}$	43, 55, 57, 69, 71, 82, 83, 96, 109, 123, 137, 166, 180, M^+ 236
562	FAME $C_{16:0}$ branched	270	$C_{17}H_{34}O_2$	
593	FAME ($C_{16:1}$?)	268 ?	$C_{17}H_{32}O_2$?	55, 69, 74, 87, 97, 101, 113, 123, 127, 152, 194, 236, 237
615				43, 55, 57, 69, 71, 82, 83, 96, 109, 123, 137, 152, 250, 256

continued

GC/MS RUN #: 1571 continued

SAMPLE TYPE:

LOCATION:

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
628	FAME (C _{17:1} ?)	282 ?	C ₁₈ H ₃₄ O ₂	55, 57, 58, 69, 84, 81, 87, 95, 97, 109, 113, 123, 141, 165, 237, 239, 250, 251
648	FAME (C _{18:0} ?) branched	298 ?	C ₁₉ H ₃₈ O ₂ ?	55, 57, 69, 71, 74, 81, 83, 87, 97, 113, 141, 143, 166, 185, 208, 250, 251
658	FAME (C _{18:1} ?)	296 ?	C ₁₉ H ₃₆ O ₂ ?	55, 57, 69, 74, 81, 83, 87, 97, 101, 111, 115, 123, 141, 143, 152, 166, 180, 222, 264, 265
661	FAME C _{18:0}	296	C ₁₉ H ₃₆ O ₂	55, 69, 74, 81, 83, 87, 95, 96, 97, 109, 111, 129, 135, 180, 199, 220, 222, 264, 265, M 296
671	FAME C _{18:0}	298	C ₁₉ H ₃₈ O ₂	74, 87, 97, 111, 129, 143, 185, 199, 255, 267, 298
692				55, 69, 81, 83, 91, 95, 105, 109, 113, 123, 129, 135, 145, 159, 168, 185, 189, 215, 243, 258
703	FAME C _{18:1}	296	C ₁₉ H ₃₆ O ₂	55, 57, 67, 69, 71, 74, 81, 82, 84, 87, 95, 97, 100, 113, 123, 127, 141, 166, 185, 199, 213, 222, 265, M 296
742	polyunsaturated HC			55, 67, 79, 78, 91, 93, 95, 105, 106, 107, 119, 121, 133, 135, 147, 150, 161, 175, 180, 203, 207, 217, 220, 221

continued

III-2.5-116

GC/MS RUN #: 1571 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

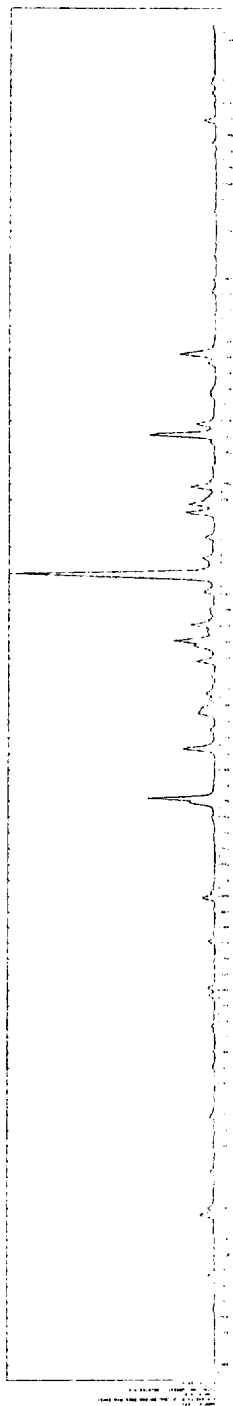
OTHER ID: _____

LOCATION : _____

COMMENTS/SUMMARY:

III-2.5-117

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
747	polyunsaturated HC			55, 67, 79, 91, 93, 95, 105, 109, 119, 131, 133, 147, 161 175, 180, 201, 215, 220
758	FAME (C _{20:1} ?) branched	324 ?	C ₂₁ H ₄₀ O ₂	55, 69, 74, 81, 83, 87, 96, 109, 123, 137, 141, 151, 165, 194, 208, 250, 292, 293
791	FAME C _{20:2}	322	C ₂₁ H ₃₈ O ₂	55, 67, 69, 81, 83, 87, 95, 109, 113, 123, 135, 137, 150, 167, 181, 240, 248, 262, 290, 291, 322
798	FAME C _{21:0} branched	340		56, 57, 69, 71, 73, 81, +83, 85, 87, 97, 101, 116, 129, 141, 185, 241, 267, 285, M 340
842	polyunsaturated HC			55, 67, 79, 81, 82, 91, 95, 96, 108, 109, 119, 123, 133, 150, 178, 194, 208, 223, 251, 350



TIC trace for GC/MS 1571

GC/MS RUN #: 1567SAMPLE TYPE: INTERTIDAL, MYTILUS, Heptane FractionSAMPLE ID: BLM 346 F1

OTHER ID: _____

LOCATION: 101/Santa Catalina Island

COMMENTS/SUMMARY: Low sample concentration, all spectra weak, predominantly unsaturated hydrocarbons.

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
628	unsaturated HC, isoprenoid ?			55, 57, 69_, 83, 95, 109, 165
649	unsaturated HC			55, 57, 69, 83, 95, 107, 109, 111, 121, 123, 135, 137, 163, 177
653	unsaturated HC			55, 57, 69, 83, 95, 109, 123, 165
658	alkane			57, 71, 85, 95
662	unsaturated branched HC			55, 57, 69, 81, 95, 109, 111, 123, 137, 151, 207
669	unsaturated or cyclic HC			55, 57, 69, 81, 82, 95, 109, 123, 137
674	unsaturated HC			55, 57, 69, 81, 95, 109, 123
684	unsaturated HC			55, 57, 69, 81, 95, 109
709	unsaturated HC			55, 56, 57, 69, 71, 83, 85, 97, 111
714	unsaturated HC			57, 69, 71, 81, 83, 85

Continued

GC/MS RUN #: 1567 continued

SAMPLE TYPE:

SAMPLE ID:

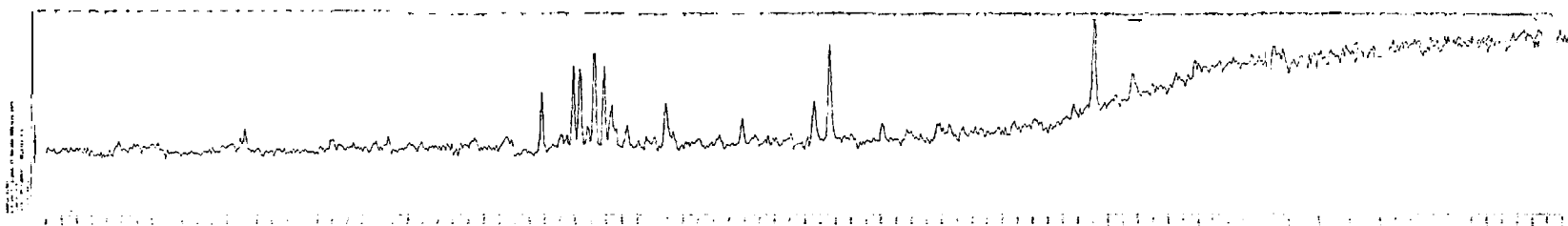
OTHER ID:

LOCATION:

COMMENTS/SUMMARY:

HHH-2.5-120

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
759	alkane ?			57, 71, 85, 97, 111
806	alkane ?			57, 71, 85, 97, 99, 111
816	adipate			70, 71, 83, 112, 129, 147
990	unsaturated HC			69, 81, 95, 107, 109, 123, 137, 149



TIC trace for GC/MS 1567

111-2.5-121

GC/MS RUN #: 1596 SAMPLE TYPE: INTERTIDAL, HALIOTIS, Hexane Fraction

SAMPLE ID: BLM 349 FI OTHER D: LOCATION: 349/Santa Catalina Island

COMMENTS/SUMMARY: Low sample concentration precludes compound assignment; components from septum rubber (silicone compounds) present.

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIF. CANT IONS
364	HC			
415	Si compound			*
435	alkane n-C ₁₇ :0	240	C ₁₇ H ₃₆	
439	isoprenoid C ₁₉ :0 pristane†			
503	alkene n-C ₁₈ :0†			
509	isoprenoid C ₂₀ :0, phytane†			
525	Si compound			*
569	alkane n-C ₁₉ :0†			
623	Si compound			*
632	alkane n-C ₂₀ :0†			
692	alkane n-C ₂₁ :0	294	C ₂₁ H ₄₄	

continued

GC/MS RUN #: 1596 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
714	Si compound			*
749	alkane n-C ₂₂ :0	310	C ₂₂ H ₄₆	
804	alkane n-C ₂₃ :0	324	C ₂₃ H ₄₈	
856	alkane n-C ₂₄ :0 [†]			
866	dioctyladipate			112, 129, 147, 241, 259
907	alkane n-C ₂₅ :0 [†]			
956	alkane n-C ₂₆ :0 [†]			
995	Si compound			*
1002	alkane n-C ₂₇ :0 [†]			
1042	unsaturated hydrocarbon			
1091	unsaturated hydrocarbon			

Continued

GC/MS RUN #: 1596 continued

SAMPLE TYPE:

SAMPLE ID:

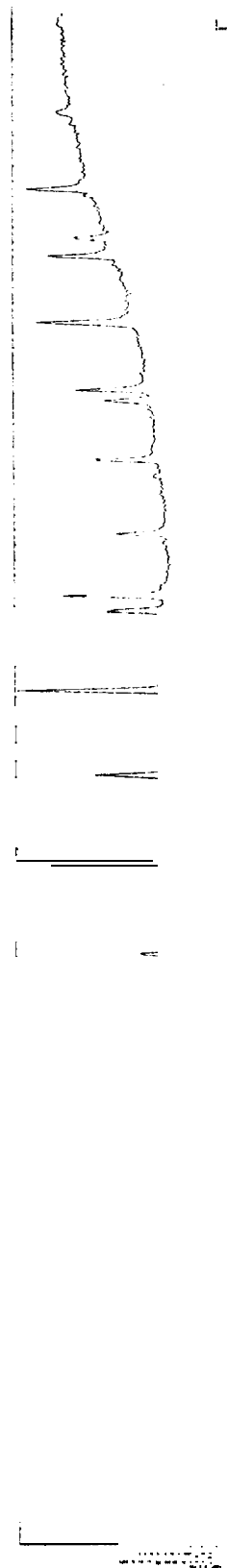
OTHER ID:

LOCATION:

COMMENTS/SUMMARY :

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
1103	Si compound			*
1135	unsaturated HC ?			
* comp	ents from silicone rubber seal	urn		
† C ₂ H ₅ N ₂	1 fragments predominantly, as	igment		
bas	on GC retention			

III-2.5-124



TIC trace for GC-MS 1596

GC/MS RUN #: 1569

SAMPLE TYPE: INTERTIDAL, MYTILUS, Benzene Fraction

SAMPLE ID: BLM 346 F2

OTHER ID: _____

LOCATION: 101, Santa Catalina island

COMMENTS/SUMMARY: Predominantly methylesters of saturated and unsaturated branched fatty acids;
minor components are unsaturated "hydrocarbons"

HI-2.5-126

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
452	FAME C _{14:0}	242	C ₁₅ H ₃₀ O ₂	74, 87, 143, 199, 211, M ⁺ 242
513	FAME C _{15:0}	256	C ₁₆ H ₃₂ O ₂	74, 87, 143, M ⁺ 256
531				55, <u>69</u> , 81, 95, 109, 121
561	FAME C _{16:1}	268	C ₁₇ H ₃₂ O ₂	74, 87, 96, 110, 111, 123, 137, 141, 152, 194, 236, 237, M ⁺ 268
565				55, <u>69</u> , 81, 93, 95, 107, 120, 121, 133, 161
573	FAME C _{16:0} (branched ?)	270	C ₁₇ H ₃₄ O ₂	74, 87, 101, 115, 129, 143, 157, 171, 185, 199, 213, 227, 239, M ⁺ 270
593				55, <u>69</u> , 85, 93, 105, 107, 119, 135, 191
604	FAME (C _{16:1} ?)	268 ?	C ₁₇ H ₃₂ O ₂	74, 87, 101, 113, 141, 155, 194, 236, 237
607	FAME C _{17:0} branched	284	C ₁₈ H ₃₆ O ₂	74, 87, 101, 129, 143, 241, M ⁺ 284

Continued

GC/MS RUN #: 1569 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

III-2.5-127

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
628	FAME C _{17:0} branched ?	284	C ₁₈ H ₃₆ O ₂	74, 87, 101, 115, 129, 143, 185, 199, 241, M ⁺ 284
"659	FAME C _{18:0} branched	298	C ₁₉ H ₃₈ O ₂	74, 87, 92, 113, 115, 141, 143, 166, 185, 208, " 250, ,251, M ⁺ 298 .
668	FAME (C _{18:1} ?)	296 ?	C ₁₉ H ₃₆ O ₂ ?	74, 87, 95, 96, 97, 109, 110, 111, 123, 152, 168, 180, 222, 264, 265
671/672	FAME (C _{18:1} ?)	296 ?	C ₁₉ H ₃₆ O ₂ ?	74, 87, 95, 96, 97, 109, 110, 111, 123, 166, 180, 222, 264, 265
674	FAME (C _{18:1} ?)	296 ?	C ₁₉ H ₃₆ O ₂ ?	69, 74, . 87, 95, 97, 109, 110, 111, 123, 180, 222, 264, 265
680	FAME C _{18:0} branched	298	C ₁₉ H ₃₈ O ₂	74, 87, 97, 101, 111, 115, 129, 143, 255, 267, M ⁺ 298
688	FAME C _{18:1}	296	C ₁₉ H ₃₆ O ₂	69, 74, 81, 84, 87, 97, 101, '109, 113, 123, 141, 151, 181, 199, 213, 264, 265, 296

Continued

GC/MS RUN #: 1569 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY: .

II-2.5-128

SCAN #	COMPOUND IDENTIFICATION	MOL. MT.	MOL. FORMULA	SIGNIFICANT IONS
697				55, 57, 69, 81, 95, 109, 123, 135, 137, 149
712	FAME C _{18:1}	296	C ₁₉ H ₃₆ O ₂	74, 87, 95, 96, 97, 100, 101, 113, 123, 127, 141, 152, 166, 180, 199, 213, 222, 264, 296
757	polyunsaturated HC			55, 67, 79, 91, 93, 105, 119, 133, 147, 161, 175, 180, 194, 201
768	F A M E (C _{20:1} ?)	324 ?	C ₂₁ H ₄₀ O ₂ ?	55, 69, 74, 83, 87, 95, 96, 97, 109, 110, 111, 123, 166, 208, 250, 292, 293
772	FAME (C _{20:1} ?)	324 ?	C ₂₁ H ₄₀ O ₂	74, 87, 152, 292, 293
800				55, 69, 81, 95, 100, 109, 113, 123, 135, 137, 150
806	FAME C _{21:0} branched	340	C ₂₂ H ₄₄ O ₂	56, 60, 73, 87, 97, 116, 129, 169, 185, 267, 284, 285, M ⁺ 340
817	adipate			83, 112, 129, 147, 241

Continued

GC/MS RUN #: 1569 continued

SAMPLE TYPE:

SAMPLE ID:

OTHER ID:

LOCATION :

COMMENTS/SUMMARY:

SCAN	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
846	polyunsaturated HC			55, 67, 79, 91, 93, 105, 109, 117, 119, 131, 133, 145, 147, 159, 161
853	unsaturated HC			55, 67, 81, 95, 96, 109, 123, 135
904	unsaturated HC			55, 69, 81, 95, 109, 121, 123, 135, 137, 149
992	unsaturated HC			55, 69, 81, 95, 107, 109, 121, 123, 137, 149

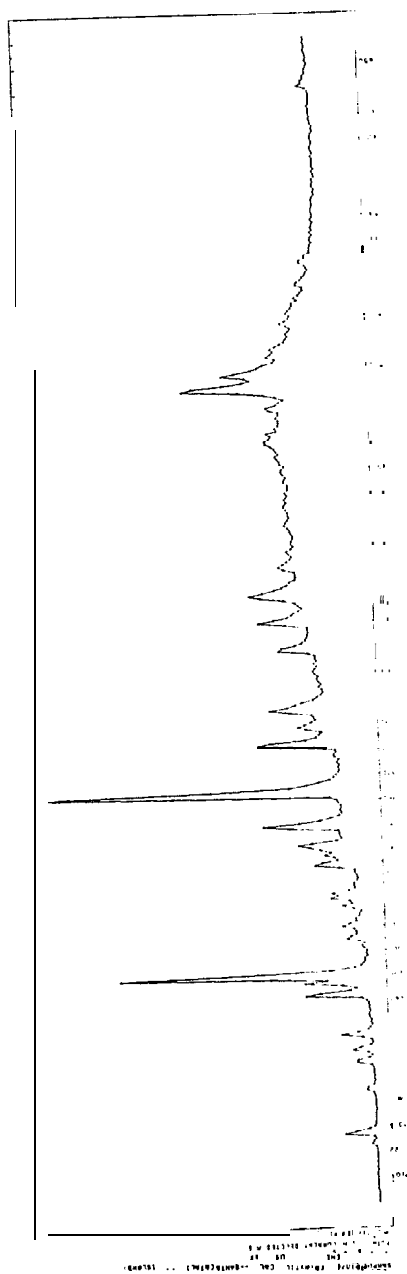
III-2.5-129



TIC trace for GC/MS 1569

GC/MS Run #1376

TO BE INCLUDED IN FINAL

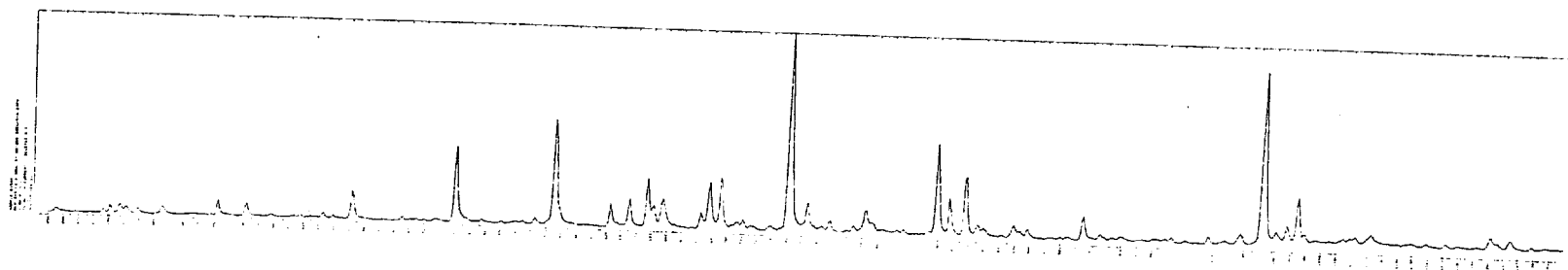


TIC trace for 1376

GC/MS Run #1560

TO BE INCLUDED IN FINAL

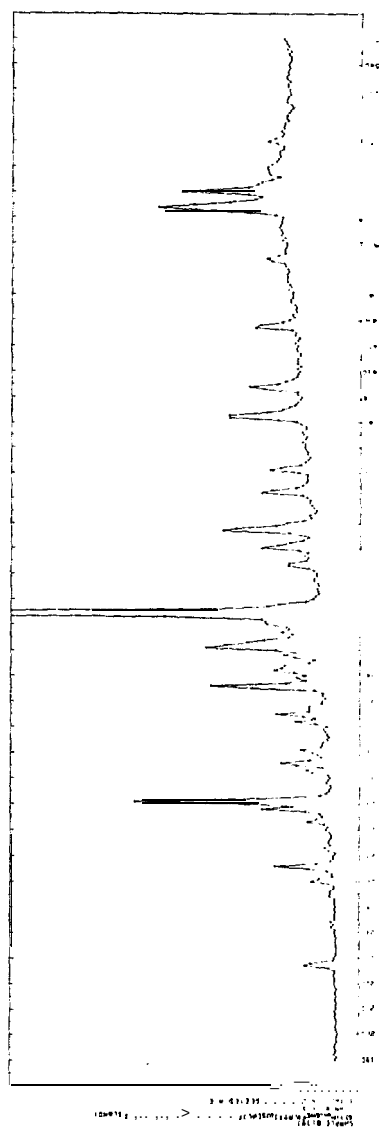
II_2.5-134



TIC trace for GC/MS 1560

GC/MS Run #1393

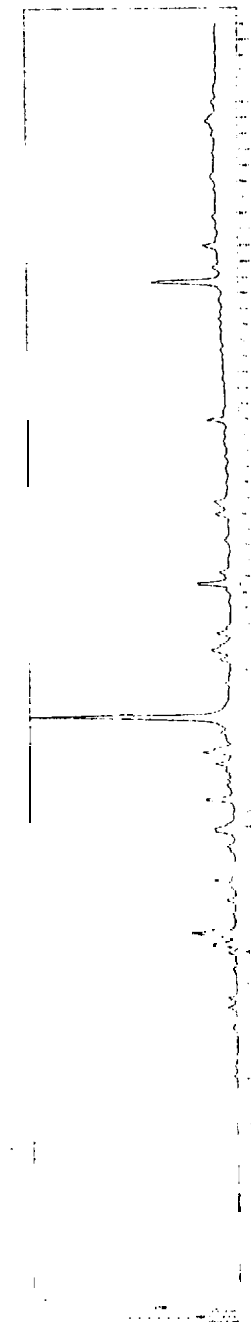
TO BE INCLUDED IN FINAL



TIC trace for GC/MS L393

GC/MS Run #1589

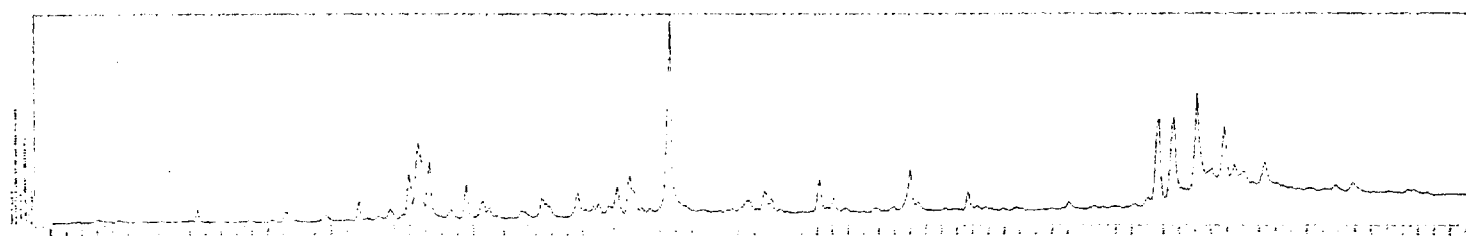
TO BE INCLUDED IN FINAL



TIC trace for GC/MS 1589

GC/MS Run #1616

TO BE INCLUDED IN FINAL



TIC trace for GC/MS 1616

GC/MS RUN #: 1358

SAMPLE TYPE: INTERTIDAL, MYTILUS CALIFORNIANUS, Hexane Fraction

SAMPLE ID: BLM 326 Hexane Fraction

OTHER ID:

LOCATION: 110/San Nicolas Island

COMMENTS/SUMMARY: Normal alkanes n-C_{15:0} to n-C_{29:0}, isoprenoid alkanes, branched and cyclic
C₂₅ components, steranes, triterpanes, aldehydes, butylesters of palmitic and stearic acid.

±II-2.5-141

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
152	alkane n-C _{15:0}	212	C ₁₅ H ₃₂	
"185	alkane n-C _{16:0}	226	C ₁₆ H ₃₄	
218	alkane n-C _{17:0}	240	C ₁₇ H ₃₆	
222	isoprenoid alkane C _{19:0} (pristene)	268	C ₁₉ H ₄₀	113, 183, M ⁺ 268
251	c ₁₆ aldehyde	(240)	C ₁₆ H ₃₂ O ₁	CnH2n_2 fragments to m/e 194, 196, 222, no M ⁺
262				
270	alkadiene C _{20:2}	278	C ₂₀ H ₃₈	55, 57, ,69, 71, 81, 82, 83, 95, 97, 109, 111, 123, 137, .151, 165, M ⁺ 278
275	alkadiene C _{20:2}	278	c ₂₀ H ₃₈	55, 57, ,69, 71, 81, 82, 83, 95, 97, 109, 111, 123, 137, 149, 151, M ⁺ 278
283	c ₁₇ aldehyde	(259)	C ₁₇ H ₃₄ O ₁	55, 57, 69, 71, 81, 82, 83, 85, 95, 96, 97, 109, 110, 111, 123, 124, 125, 137, 151, 165, 179, 194, 208, 210, 236, no M ⁺

Continued

GC/MS RUN #: 1358 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

I 11-2 5-142

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
313	branched C _{20:0} alkane	282	C ₂₀ H ₄₂	
325	branched C _{25:3} 'Hydrocarbon	346	C ₂₅ H ₄₆	165, 207, 233, 291, M ⁺ 346
330	unsaturated aldehyde C _{18:1}	266	C ₁₈ H ₃₄ O	166, 180, 194, 207, "222, 248, M ⁺ 266
336	branched C _{25:4} 'Hydrocarbon	344	C ₂₅ H ₄₄	149, 191, 205, 273, 288, 189, M ⁺ 344
339	branched C _{25:3} hydrocarbon	346	C ₂₅ H ₄₆	165, 179, 193, 207, 233, 291, M ⁺ 346
342	alkane n-C _{21:0}	296	C ₂₁ H ₄₄	
344	branched C _{25:3} 'Hydrocarbon	346	C ₂₅ H ₄₆	149, 151, 163, 165, 177, 179, 207, 210, 233, 261, 289, M ⁺ 346
346		342	C ₂₅ H ₄₂ ?	69, 81, 95, 109; 109 + 14n, n = 1 to 4; 149 + 14n, , n = 0 to 5, 218, 233, 235, 273, 277, M ⁺ 342
349	unsaturated C _{25:4} hydrocarbon	344	C ₂₅ H ₄₄	69, 81, 95, 97, 107, 109, 111, 123, 135, 137, 149> 163, 177, 191, 205, 219, 231, 2.75, 289, M ⁺ 344

Continued

GC/MS RUN #: 1358 continued

SAMPLE TYPE:

SAMPLE ID:

OTHER ID:

LOCATION:

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
353	unsaturated C _{25:4} hydrocarb	342	C ₂₅ H ₄₄	57, 69, 81, 83, 85, 93, 95, 97, 109, 111, 123, 135, 149, 205, 275, M ⁺ 344 "
359	polycyclic C ₂₅ hydrocarbon	342	C ₂₅ H ₄₂	69, 81, 83, 95, 97, 109, 123, 135, 149, 191, 217, 231, 273, M ⁺ 342
362	hexadecanoic acid-n-butyl-ester	340	C ₂₀ H ₄₀ O ₂	73, 116, 129, 239, 257, M ⁺ 312
370	alkane n-C _{22:0}	310	C ₂₂ H ₄₆	
381	isoprenoid alkane (C _{25:0} ?)	(352)	C ₂₅ H ₅₂	71, 85, 97, 99, 113, 127, 141, 155, 169, 183, 197, 239, 267, 337, no M ⁺
397	ant iso C _{25:0} alkane	(352)	C ₂₅ H ₅₂	C _n H _{2n+1} fragments to m/e 323, 323 is local maximum, no M ⁺
401	cyclic C ₂₅ hydrocarbon	346	C ₂₅ H ₄₆	69, 81, 83, 95, 97, 109, 111, 123, 125, 191, 193, 221, 261, M ⁺ 346

Continued

GC/MS RUN #: 1358 continued

SAMPLE TYPE:

SAMPLE ID:

OTHER ID:

LOCATION:

COMMENTS/SUMMARY:

HE-2.5-144

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
416	octadecanoic acid-n-butyl-ester	340	C ₂₂ H ₄₄ O ₂	73, 116, 129, 267 285, M ⁺ 340
423	alkane n-C _{24:0}	338	C ₂₄ H ₅₀	
447	alkane n-C _{25:0}	352	C ₂₅ H ₅₂	
471	alkane n-C _{26:0}	366	C ₂₆ H ₅₄	
486	various branched and/or cyclic hydrocarbons			possible molecular ions: 370, 372, 386, 392
494	alkane n-C _{27:0}	380	C ₂₇ H ₅₆	
505		368	C ₂₇ H ₄₄	55, 57, 69, 71, 81, 83, 95, 97 109, 111, 123, 125, 141, 149, 255, 257, 281, 284, 336 M ⁺ 368
513	Δ ² cholestene	370	C ₂₇ H ₄₆	161, 176, 203, 215, 230, 316, 355, M ⁺ 370
538	alkane n-C _{29:0}	408	C ₂₉ H ₆₀	
				Continued

GC/MS RUN #: 1358 continued

SAMPLE ID: _____

SAMPLE TYPE: _____

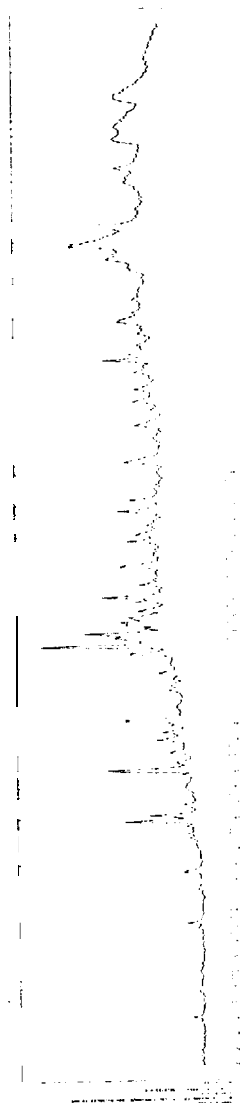
OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

TII-2.5-145

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
577 578	polycyclic hydrocarbons			191, 211, 217, 219, 221, 231, 263, 281, 355, 365, 371, 386, 393, 399, 407, 414, 421, 428, 432, 436
587	isoprenoid alkane C _{33:0}	464	C ₃₃ H ₆₈	57, 71, 85, 97, 99, 111, 113, 127, 141, 155, 211, 225, 281, 295, 365, M ⁺ 464
600	hop-22(29)-ene	410	C ₃₀ H ₅₀	189, 191, 204, 218, 231, 281, 299, 301, 341, 342, 354, 355, 367, 395, M ⁺ 410
638	triterpane	426	C ₃₁ H ₅₄	179, 191, 193, 219, 233, 273, 341, 355, 411, M ⁺ 426



TIC trace for GC/MS 1358

GC/MS RUN #: 1562

SAMPLE TYPE: INTERTIDAL, MYTILUS, Hexane Fraction

SAMPLE ID: BLM 433 F1

OTHER ID:

LOCATION: 110/San Nicolas Island

COMMENTS/SUMMARY: Predominantly higher alkanes $n\text{-C}_{17}$ - $n\text{-C}_{33}$; unsaturated and branched hydrocarbons;
(isoprenoid) unsaturated C_{25} hydrocarbons, branched and cyclic

PI-2 5-147

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
399	diethylphthalate ?			149, 177
433	alkane $n\text{-C}_{17:0}$	240	$\text{C}_{17}\text{H}_{36}$	
437	isoprenoid alkane (pristan)			71, 85, 99, 113, 183
501	hydrocarbon			$\text{C}_n\text{H}_{2n+1}$ fragments to m/e 127
507	hydrocarbon			$\text{C}_n\text{H}_{2n+1}$ fragments to m/e 127
545	branched alkadiene $\text{C}_{20:2}$	278	$\text{C}_{20}\text{H}_{18}$	69, 71, 81, 82, 95, 109, 123, 137, M^+ 278
556	branched alkadiene $\text{C}_{20:2}$	278	$\text{C}_{20}\text{H}_{18}$	69, 71, 81, 95, 109, 111, 123, 151, M^+ 278
566	alkane $n\text{-C}_{19:0}^*$	268	$\text{C}_{19}\text{H}_{40}$	$\text{C}_n\text{H}_{2n+1}$ fragments to m/e 155, M^+ 268
628	alkane $n\text{-C}_{20:0}^*$ + unsaturated hydrocarbon	282	$\text{C}_{20}\text{H}_{42}$	$\text{C}_n\text{H}_{2n+1}$ fragments: 97, 111, 125
654	isoprenoid alkatriene $\text{C}_{25:}$ or cycloalkadiene	346	$\text{C}_{25}\text{H}_{46}$	
668	isoprenoid alkene			$\text{C}_n\text{H}_{2n+1}$ fragments to m/e 195; 151, 165, 179, 193, 207

continued

GC/MS RUN #: 1562 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

III-2.5-148

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
673	unsaturated branched hydrocarbon			$C_n H_{2n-1}$, $C_n H_{2n-3}$ fragments; 152, 207, 235, 266, 267, no M^+
677	'unsaturated branched hydrocarbon			$C_n H_{2n-1}$, $C_n H_{2n-3}$, $C_n H_{2n-5}$ fragments; 163, 233, 289, no M^+
682	isoprenoid alkatriene $C_{25:3}$ or cyclic alkadiene	346	$C_{25}H_{46}$	83, 151; 95, 165, 233; 109, 179; 123, 193, 261; 291; M^+ 346
687	alkane n- $C_{21:0}$ + unsaturated hydrocarbon	296	$C_{21}H_{44}$	
694	isoprenoid alkatriene $C_{25:3}$	346	$C_{25}H_{46}$	83, 151; 95, 163, 165, 233; 109, 177, 179, 192, 261, M^+ 346
699	cyclic alkadiene $C_{25:2}$	346	$C_{25}H_{46}$	69, 81, 82, 95, 109, 123, 137, 151, 163, 165, 177, 179, 205, 222, 235, 250, 277, 290, M^+ 346
704	unsaturated branched hydrocarbon			$C_n H_{2n-1}$, $C_n H_{2n-3}$, $C_n H_{2n-5}$ fragments; 163, 231; 205, 273, 219; 289, no M^+
716	unsaturated hydrocarbon			$C_n H_{2n+1}$, $C_n H_{2n-1}$, $C_n H_{2n-3}$, $C_n H_{2n-5}$ fragments; 183, 253; 205, 275, no M^+

continued

GC/MS RUN #: 1562 continued

SAMPLE ID: _____

SAMPLE TYPE: {t} _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY: .

III-2.5-143

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
729	unsaturated hydrocarbon	342	$C_{25}H_{42}$	
730	alkadiene $C_{22:2}$	306	$C_{22}H_{42}$	
766	alkadiene ?			C_nH_{2n-1} , C_nH_{2n-3} fragments, 151, 165, 193, 297, 221, 263; 267, no M^+
745	alkane $n-C_{22:0}$ contains unsaturated hydrocarbon	310	$C_{22}H_{46}$	
763	branched alkane (isoprenoi ?)			C_nH_{2n+1} fragments, 155, 169, 183, 197, 239, 253, 267, no M^+
791	silicone compound			207, 281, 355, 429; 221, 295;
798	alkane $n-C_{23:0}$ contains unsaturated hydrocarbon	324	$C_{23}H_{48}$	
814	alkatriene $C_{25:3}$	346	$C_{25}H_{46}$	C_nH_{2n-1} , C_nH_{2n-3} , C_nH_{2n-5} fragments; 109, 151, 163, 177, 191, 205, $M^+ 346$

continued

GC/MS RUN #: 1562 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

HH-2.5-150

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
851	alkane n-C _{24:0}	338	C ₂₄ H ₅₀	112, 129, 241, 259
860	dioctyladipate			
866	silicone compound			
901	alkane n-C _{25:0}	352	C ₂₅ H ₅₂	71; 85, 155; 97, 99, 169, 239; 111, 113, 183 253; 123, 125, 127; 151, 266, 336, M ⁺ 368
938	silicone compound phthalate			
950	alkane n-C _{26:0}	366	C ₂₆ H ₅₄	
976	isoprenoid alcohol C _{25:0}	368	C ₂₅ H ₅₂ O	161, 176, 203 215, 230, 316 355 M ⁺ 370
996	alkane n-C _{27:0}	380	C ₂₇ H ₅₆	
1041	alkane n-C _{28:0}	394	C ₂₈ H ₅₈	
1053	A* cholestene	370	C ₂₇ H ₄₆	continued
1083	alkane n-C _{29:0}	408	C ₂₉ H ₆₀	

SAMPLE TYPE: 11

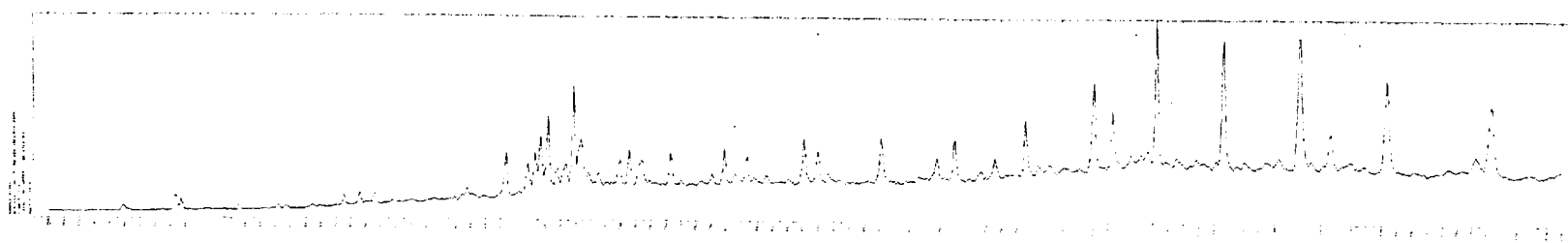
OTHER ID: _____

LOCATION:

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
1126	alkane n-C _{30:0}	422	C ₃₀ H ₆₂	85, 155, 295, 365, 435; 169, 183, 197; 211, 281; no M ⁺ 189, 191, 207, 218, 342, 355, 368, M ⁺ 410
1176	alkane	436	C ₃₁ H ₆₄	
1196	isoprenoid alkane			
1234	alkane n-C _{32:0}	450	C ₃₂ H ₆₆	
1293	diploptene	410	C ₃₀ H ₅₀	
1303	alkane n-C _{33:0}	464	C ₃₃ H ₆₈	
* GC	Identification based on mass spectral data			

III-2 5-152



TIC trace for GC/MS 1562

GC/MS RUN #: 1585

SAMPLE TYPE: INTERTIDAL, MACROCYSTIS, Hexane Fraction

SAMPLE ID: BLM 422 F2 (misabeled: is F1)

OTHER ID:

LOCATION: 110/San Nicolas Island

COMMENTS/SUMMARY : Predominantly n-alkanes C_{15} to C_{32} , isoprenoid alkanes C_{19} to C_{20} , unsaturated hydrocarbons C_{17} to C_{20} , C_{30} , butylesters of fatty acids (C_{16} , C_{18}).

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
294	alkane n- $C_{15:0}$	212	$C_{15}H_{32}$	
357	alkane n- $C_{16:0}$	226	$C_{16}H_{34}$	
394	diethylphthalate	222	$C_{12}H_{14}O_4$	149, 177, M^+ 222
403	alkadiene $C_{17:2}$	236	$C_{17}H_{32}$	
407	alkene $C_{17:1}$	238	$C_{17}H_{34}$	
418	alkene $C_{17:1}$	238	$C_{17}H_{34}$	
421	alkane n- $C_{17:0}$	240	$C_{17}H_{36}$	
425	isoprenoid alkane $C_{19:0}$	268	$C_{19}H_{40}$	43, 113, 183, M^+ 268
441	isoprenoid alkene $C_{19:1}$	266	$C_{19}H_{38}$	56, 126, 196, 266; 55, 57, 69, 83, 97, 111, 140, 153, 169, 181, M^+ 266

Continued

GC/MS RUN #: 1585 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY :

I 11-2.5-150

SCAN #	COMPOUND IDENTIFICATION	MOLE WT.	MOLE. FORMULA	SIGNIFICANT IONS
482	alkane n-C _{18:0}	254	C ₁₈ H ₃₈	
487	isoprenoid C _{20:0}	282	C ₂₀ H ₄₂	
506	alkadiene C _{20:2}	278	C ₂₀ H ₃₈	55, 57, 68, 69, 71, 81, 82, 83, 95, 97, 109, 111, 123, M ⁺ 278
540	alkane n-C _{19:0}	268	C ₁₉ H ₄₀	
594	alkene C _{20:1}	280	C ₂₀ H ₄₀	
596	alkane n-C _{20:0}	282	C ₂₀ H ₄₂	
650	alkane n-C _{21:0}	296	C ₂₁ H ₄₄	
701	hexadecanoic acid n-butyl-ester	312	C ₂₀ H ₄₀ O ₂	73, 116, 129, 239, 257, M ⁺ 312
702	alkane n-C _{22:0}	310	C ₂₂ H ₄₆	

Continued

a

GC/MS RUN #: 1585 continued

SAMPLE ID: _____

SAMPLE TYPE: _____

OTHER ID: _____

LOCATION : _____

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION,	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
750	alkane n-C _{23:0}			
797	alkane n-C _{24:0}	338	C ₂₄ H ₅₀	
	octadecanoic acid n-butyl-ester	340	C ₂₂ H ₄₄ O ₂	73, 116, 129, 267, 285, M ⁺ 340
841	alkane n-C _{25:0}	352	C ₂₅ H ₅₂	
885	alkane n-C _{26:0}	366	C ₂₆ H ₅₄	
927	alkane n-C _{27:0}	380	C ₂₇ H ₅₆	
967	alkane n-C _{28:0}	394	C ₂₈ H ₅₈	
980	alkapolyene C _{30:6} (isoprenoi	? 410	C ₃₀ H ₅₀	69, 81, 95, 97, 121, 123, 137, 191, 203, 205, 255, 341, M ⁺ 410
1006	alkane n-C _{29:0}	408	C ₂₉ H ₆₀	

Continued

GC/MS RUN #: 1585 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

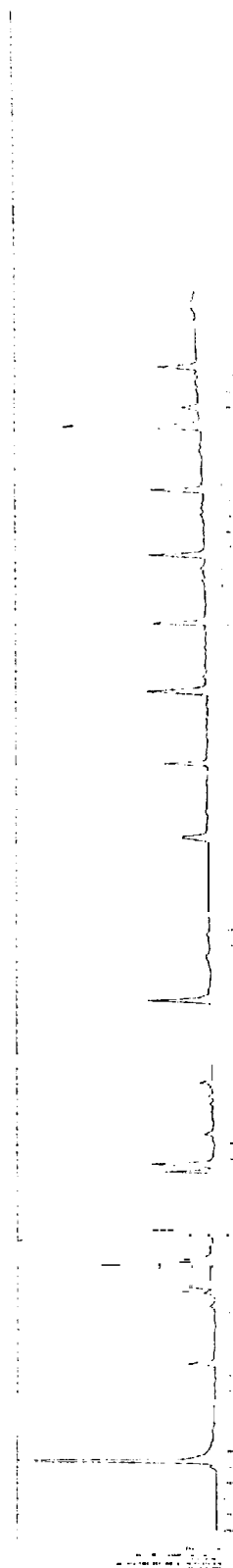
OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

11-2.5-156

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
1046	alkane n-C _{30:0} + additional compound	422	C ₃₀ H ₆₂	203, 220, 368
1094	alkane n-C _{31:0}	436	C ₃₁ H ₆₄	
1150	alkane n-C _{32:0}	450	C ₃₂ H ₆₆	



TIC trace for GC/MS 1585

GC/MS RUN #: 1473

SAMPLE TYPE: INTERTIDAL, EMERITA, Hexane Fraction

SAMPLE ID: BLM BENSON 211-1076-02-1-F1

OTHER ID:

LOCATION: 211/ SAN NICHOLAS

COMMENTS/SUMMARY:

n-alkanes, n-alkenes, isoprenoid components, saturated, mono- and di-unsaturated, steranes and sterenes

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
152	alkene C _{14:1}		C ₁₄ H ₂₈ ?	43, 57, 71, 82, 85, 97, 126
189	isoprenoid alkane C _{16:0}		C ₁₆ H ₃₄ ?	43, 57, 70, 85, 99, 113, 127, 141, 183
208	n-alkene C _{15:1}	210	C ₁₅ H ₃₀	43, 55, 69, 83, 97, 111, 125, 126, 140, 210
213	n-alkane C _{15:0}	212	C ₁₅ H ₃₂	C _n H _{2n+1} fragments, b.p.m/e 57
223	n-alkene C _{15:1} ?			43, 55, 69, 83, 97, 111, 125, 126, 140, 210 (C _n H _{2n} fragments)
276	n-alkane C _{16:0} ?			C _n H _{2n+1} fragments
325	alkene			C _n H _{2n} fragments
330	alkene C _{17:1}	238	C ₁₇ H ₃₂	C _n H _{2n} fragments, M ⁺ 238
335	alkene C _{17:1}	238	C ₁₇ H ₃₂	C _n H _{2n} fragments, M ⁺ 238
340	n-alkane C _{17:0}	240	C ₁₇ H ₃₄	C _n H _{2n+1} fragments, M ⁺ 240
344	isoprenoid alkane, pristane		C ₁₉ H ₄₀	57, 71, 85, 97, 99, 113, 183
358	isoprenoid alkene, pristene	266	C ₁₉ H ₃₈	43, 55, 56, 57, 69, 71, 83, 97, 111, 126, 141, 168, 182, 266

continued

HHH-2-5-158

GC/MS RUN #: 1473 (continued)

SAMPLE ID: _____

SAMPLE TYPE: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY: .

FID-2.5-159

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS .
401	alkene?			43, 57, 71, 85, 97, 111
406	alkene?			43, 57, 71, 85, 97, 111, 127, 168, 183, 219
421	isoprenoid alkene , phytene, C _{20:1}	280	C ₂₀ H ₄₀	43, 55, 57, 69, 70, 83, 97, 111, 125, 140, 154, 186, 280
424	alkene?			
429	isoprenoid alkene, phytene, C _{20:1}	280	C ₂₀ H ₄₀	43, 55, 70, 83, 97, 111, 125, 126, 140, 210, 280
439	isoprenoid alkadiene, phytadiene C _{20:2}	278	C ₂₀ H ₃₈	43, 57, 67, 69, 71, 82, 95, 109, 111, 123, 168, 186, 278
449	isoprenoid alkadiene, phytadiene C _{20:2}	278	C ₂₀ H ₃₈	43, 57, 69, 71, 82, 83, 95, 97, 109, 111, 123, 278
461	n-alkane C _{19:0}	268	C ₁₉ H ₄₀	C _n H _{2n+1} fragments, M ⁺ 268
541	alkatriene?	346	C ₂₅ H ₄₆ ?	43, 57, 69, 83, 95, 109, 123, 125, 165, 179, 193, 233, 291, 346

continued

GC/MS RUN #: 1473 (continued)

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
555				43, 57, 69, 83, 97, 111, 125
563		348	C ₂₅ H ₄₈	43, 55, 69, 83, 95, 109, 111, 123, 125, 137, 151, 165, 179, 193, 207, 348
567	alkatriene?	346	C ₂₅ H ₄₆	41, 43, 55, 57, 69, 71, 83, 95, 97, 109, 123, 137, 151, 165, 179, 191, 233, 291, 346
573	n-alkene C _{21:0}	296	C ₂₁ H ₄₂	C _n H _{2n+1} fragments M ⁺ 296
625	n-alkane C _{22:0}	310	C ₂₂ H ₄₆	C _n H _{2n+1} fragments M ⁺ 310
642	branched alkane (isoprenoid?)			C _n H _{2n+1} fragments, 113, 183, 267
660	n-alkene C _{23:1}	322	C ₂₃ H ₄₆	C _n H _{2n+1} fragments, M ⁺ 322
675	n-alkane C _{23:0}	324	C ₂₃ H ₄₈	C _n H _{2n+1} fragments, M ⁺ 324
723	n-alkane C _{24:0}	338	C ₂₄ H ₅₀	C _n H _{2n+1} fragments, M ⁺ 338
756	n-alkene C _{25:1}	350	C ₂₅ H ₅₀	C _n H _{2n+1} fragments, M ⁺ 350
769	n-alkane C _{25:0}	352	C ₂₅ H ₅₂	C _n H _{2n+1} fragments, M ⁺ 352
813	n-alkane C _{26:0}	366	C ₂₆ H ₅₄	C _n H _{2n+1} fragments

continued

GC/MS RUN #: 1473 (continued)

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY: ' _____

111-2.5-16

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
841	n-alkane C _{27:0}	380	C ₂₇ H ₅₆	C _n H _{2n+1} fragments, 337, 365, M ⁺ 380
857	n-alkane C _{27:0}	380	C ₂₇ H ₅₆	C _n H _{2n+1} fragments, M ⁺ 380
897	Δ ² -cholestane	370	C ₂₇ H ₄₆	370, 355, 316
	+n-alkane C _{28:0}	394	C ₂₈ H ₅₈	C _n H _{2n+1} fragments
923	n-alkane C _{29:0}	408	C ₂₉ H ₆₀	C _n H _{2n+1} fragments, 365, 393, M ⁺ 408
	+ C ₂₈ sterane?	386?	C ₂₈ H ₅₀ ?	
929	n-alkane C _{29:0}	408	C ₂₉ H ₆₀	C _n H _{2n+1} fragments, M ⁺ 408
	+ C ₂₈ sterene?	384	C ₂₈ H ₄₈	
	+ stigmastane	400	C ₂₉ H ₅₂	
999	branched alkene? C _{31:1}	434	C ₃₁ H ₆₂	C _n H _{2n+1} fragments, M ⁺ 434
1004	triterpane (hopane?)			191, 412, + additional fragments
1016	alkadiene C _{31:2}	432	C ₃₁ H ₆₀	C _n H _{2n} fragments, M ⁺ 432
1020	alkadiene C _{31:2}	432	C ₃₁ H ₆₀	
1034	n-alkane C _{31:0}	436	C ₃₁ H ₆₄	C _n H _{2n+1} fragments, M ⁺ 436
	+ isoprenoid alkane? C _{35:0}		C ₃₅ H ₇₂ ?	463, 407, 365, 295, 281, 211, 141

TIC trace for GC/MS #1473

TO BE INCLUDED IN FINAL

GC/MS RUN #: 1583

SAMPLE TYPE: INTERTIDAL, EMERITA, Hexane Fraction

SAMPLE ID: BLM 445 F1

OTHER ID:

LOCATION: 211/San Nicolas Island

COMMENTS/SUMMARY:

Normal alkanes n-C_{17:0} to n-C_{31:0}, isoprenoid alkanes, polyunsaturated and/or cyclic C₂₅ hydrocarbons, polycyclic hydrocarbons, fatty acid-n-butyl-esters.

11-2-5-163

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
425	alkane n-C _{17:0}	240	C ₁₇ H ₃₆	
428	isoprenoid alkane C _{19:0} (pristane)			85, 155; 113, 183
526	branched alkadiene C _{20:2} (phytadiene ?)	278	C ₂₀ H ₃₈	64, 69, 82, 95, 123, M ⁺ 278
536	branched alkadiene C _{20:2} (phytadiene ?)	278	C ₂₀ H ₃₈	64, 69, 81, 82, 95, 97, 123, 151, 165, 179, 207, M ⁺ 278
545	alkane n-C _{19:0}	268	C ₁₉ H ₄₀	
625	isoprenoid alkatriene C _{25:3}	346	C ₂₅ H ₄₆	55, 57, 69, 83, 95, 109, 123, 151, 165, 179, 193, 233, 261, 293, M ⁺ 346
638	C _{25:2}	348	C ₂₅ H ₄₈	55, 57, 69, 71, 83, 97, 111, 125, 139, 153, 167, 181, 195, 207, 222, 264, 266, M ⁺ 348
642	C ₂₅ cyclo alkenes C _{25:2}	348	C ₂₅ H ₄₈	55, 69, 81, 83, 95, 109, 111, 123, 126, 137, 151, 152, 165, 179, 193, 196, 207, 221, 235, 250, 263, 266, 280, 319, M ⁺ 348

GC/MS RUN #: 1583 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

III-2.5-164

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
650	isoprenoid alkatriene C _{25:3}	346	C ₂₅ H ₄₆	
655	alkane n-C _{21:0}	296	C ₂₁ H ₄₄	
660	isoprenoid alkatriene C _{25:3}	346	C ₂₅ H ₄₆	55, 69, 81, 83, 95, 109, 123, 137, 151, 165, 177, 179, 191, 193, 207, 233, 261, M ⁺ 346
665	branched alkatriene ? C _{25:3} C ₂₅ cycloalkene ?	346	C ₂₅ H ₄₆	55, 69, 81, 82, 83, 95, 97, 109, 123, 137, 151, 163, 165, 177, 179, 193, 205, 207, 221, 235, 250, 263, 277, 278, 303, M ⁺ 346
68	branched alkatetraene ? C _{25:4} isoprenoid	344	C ₂₅ H ₄₄	
693	alkapentaene C _{25:5}	342	C ₂₅ H ₄₂	69_, 81, 83, 95, 97, 109, 111, 123, 135, 137, 151, 161, 163, 165, 177, 191, 203, 205, 217, 219, 273, M ⁺ 342
Continued				

GC/MS RUN #: 1583 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION : _____

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
699	isoprenoid C _{15:0} - decahydro naphthalene	348	C ₂₅ H ₄₈	55, 57, 69, 83, 95, 97, 109, 111, 123, 137, 151, 165, 193, 207, 263, M ⁺ 348
705	hexadecanoic acid-n-butyl-ester	312	C ₂₀ H ₄₀ O ₂	73, 116, 239, 255, 256, M ⁺ 312
	alkane n-C _{22:0}	310	C ₂₂ H ₄₆	
723	branched alkene C _{24:1} ?	336 ?	C ₂₄ H ₄₈ ?	57, 71, 85, 97, 111, 113, 125, 127, 141, 155, 169, 183, 197, 211, 239, 267, no M ⁺
756	alkane n-C _{23:0}	324	C ₂₃ H ₄₈	
769	C ₂₅ cycloalkene C _{25:3}	346	C ₂₅ H ₄₆	55, 69, 81, 82, 83, 95, 109, 123, 137, 151, 163, 165, 177, 179, 191, 205, 207, 233, 261, 303, M ⁺ 346
782	C ₂₅ cycloalkene (C _{25:4})	344	C ₂₅ H ₄₄	55, 69, 81, 83, 95, 109, 123, 136, 151, 163, 177, 272, 301, M ⁺ 344
803	alkane n-C _{24:0}	338	C ₂₄ H ₅₀	

Continued

GC/MS RUN #: 1583 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION : _____

COMMENTS/SUMMARY:

11-2.5-166

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
848	octadecanoic acid-n-butyl- ester	340	$C_{22}H_{44}O_2$	73, 116, 267, 285, M ⁺ 340
879	alkane n-C _{25:0}	352	$C_{25}H_{52}$	43, 55, 57, 69, 81, 83, 85, 95, 97, 107, 109, 111, 121, 123, 125, 137, 151, 155, 163, 169, 175, 177, 183, 191, 207, 337, 357, 412
892	alkane n-C _{26:0}	366	$C_{26}H_{54}$	43, 55, 57, 69, 71, 81, 83, 85, 95, 97, 109, 111, 123, 125, 151, 153, 163, 165, 169, 191 207, 253, 268
934	alkane n-C _{27:0}	380	$C_{27}H_{56}$	
974	alkane n-C _{28:0} (predominantly)	394	$C_{28}H_{58}$	

Continued

GC/MS RUN #: 1583 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

SCAN i%	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
988	A ² cholestene	370	C ₂₇ H ₄₆	203, 215, 217, 316, M ⁺ 370
999	iso-alkane C _{29:0}	408	C ₂₉ H ₆₀	C _n H _{2n+1} fragments to 309; 365, 393, M ⁺ 408
1004	alkene C _{29:1} (predominantly;	406	C ₂₉ H ₅₈	additional ions:
1013	alkane n-C _{29:0}	408	C ₂₉ H ₆₀	
1025				C _n H _{2n+1} fragments to m/e 281; 168, 196, 224, 406
1055	contains alkane n-C _{30:0}	422	C ₃₀ H ₆₂	
1091		432	C ₃₁ H ₆₀ ?	55, 69, 83, 97, 111, 125, C _n H _{2n-2} fragments from m/e 82 to 390, M ⁺ 432
			C ₃₀ H ₅₆ O ₁ ?	
1103	alkane n-C _{31:0}	436	C ₃₁ H ₆₄	

Continued

GC/MS RUN #: 1583 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
1107	isoprenoid alkene C ₂₆ :1	432	C ₃₁ H ₆₀ ?	55, 69, 83, 97, 109, 111, 123, 155, C _n H _{2n-2} fragments from m/e 82 to 390, M ⁺ 432
1123		462	C ₃₀ H ₅₆ O ₁ ?	
1210			C ₂₆ H ₅₂	C _n H _{2n+1} fragments to m/e 295; 337, 365, 435, M ⁺ 462
				152, 163, 169, 171, 185, 196, 210, 228, 238, 254, 255, 280, 383, 367, M ⁺ 458 ?

11-2 5-169



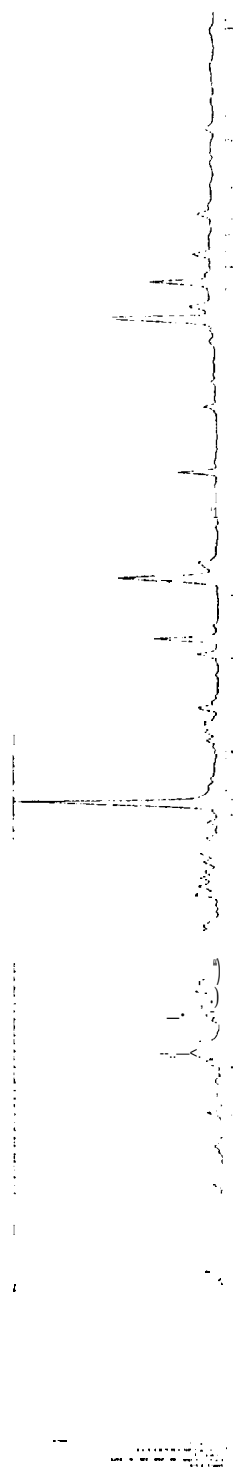
TIC trace for GC/MS 1583

GC/MS Run #1601

TO BE INCLUDED IN FINAL

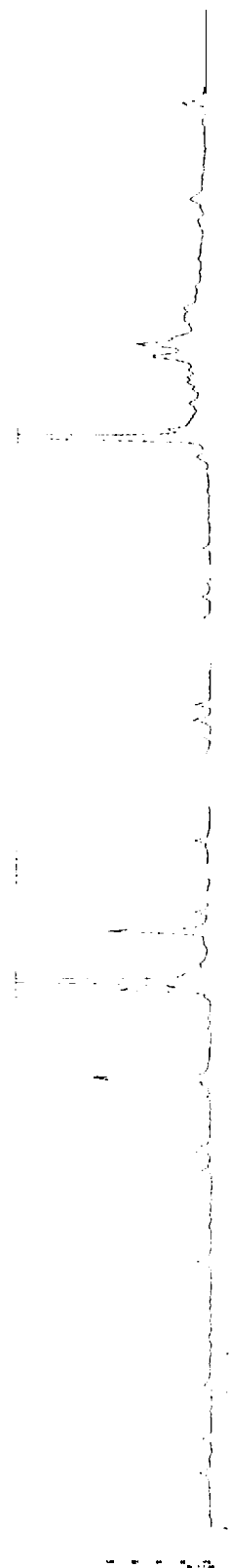
T[±]C trace for GC/MS 1601

GC/MS Run #1610
TO BE INCLUDED IN FINAL



TIC trace for GC/MS 1610

GC/MS Run #1587
TO BE INCLUDED IN FINAL



TIC trace for GC/MS 1587

GC/MS RUN #: 1475

SAMPLE TYPE: INTERTIDAL, EMERITA, Benzene Fraction

SAMPLE ID: Benson 211-1076-02-1-F2

OTHER ID:

LOCATION: 211/San Nicolas

COMMENTS/SUMMARY: Methyl esters; chlorinated HC; n-alkanes C_{29:0}, C_{31:0}; cyclic hydrocarbons, unsaturated hydrocarbons.

SCAN #	COMPOUND IDENTIFICATION	MOL. WT.	MOL. FORMULA	SIGNIFICANT IONS
214		190 ?		43, 55, 69, 77, 91, 105, 118, 123, 142, 157, 159, 172, 175, 177, M ⁺ ? 190 -
243		180 ?		43, 67, 69, 77, 79, 91, 93, 95, 105, 109, 111, 119, 121, 137, 147, 152, 162
353		186 ?		41, 43, 55, 56, 69, 83, 97, 140, 141, M ⁺ ? 186/165, M ⁺ ? 180
358				41, 43, 55, 56, 69, 83, 97, 140, 141, 186, 227
407				41, 43, 55, 56, 69, 83, 97, 101, 111, 140, 141, 181, 186, 227, 241
446				41, 43, 55, 57, 69, 70, 83, 95, 97, 109, 111, 140, 141, 168, 186, 260, 262
483	FAME n-C _{16:0}	270		74, 87, M ⁺ 270
503				43, 55, 57, 69, 71, 83, 97, 111, 112, 125, 154, 168, 185
520	Pristanic acid 'E' C _{19:0}	312	C ₂₀ H ₄₀ O ₂	88, 101, 126, 157, 222, M ⁺ 312

Continued

GC/MS RUN #: 1475 continued

SAMPLE TYPE: _____

SAMPLE ID: _____

OTHER ID: _____

LOCATION: _____

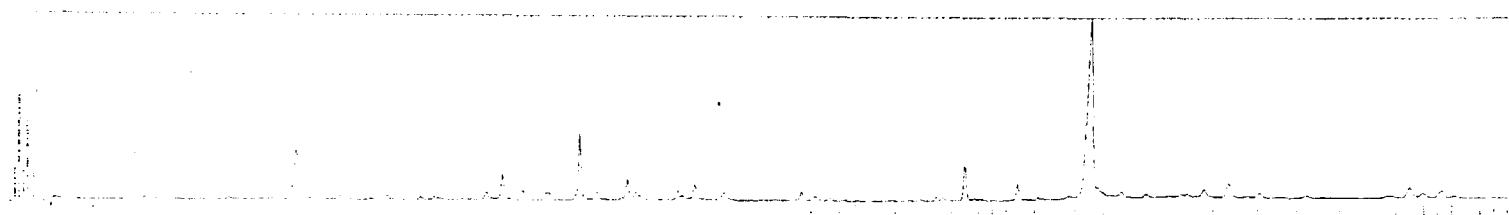
COMMENTS/SUMMARY:

SCAN #	COMPOUND IDENTIFICATION	MOL. WT	MOL. FORMULA	SIGNIFICANT IONS
547				41, <u>43</u> , 55, 57, 69, 70, 71, 83, 84, 87, 97, 99, 111, 125 126, 168, 185
576	Phytanic acid 'E C _{20:0}	326	C ₂₁ H ₄₂ O ₂	74, 101, 112, 140, 171, M ⁺ 326
608				
612	DDE	316	C ₁₄ H ₈ Cl ₄	176, 210 [*] , 246 [*] , M ⁺ 316 [*]
829	Perfluorokerosene fragment:			instrumental artifacts
911	Triterpene ?	410	C ₃₀ H ₅₀	<u>69</u> , 81, 93, 109, 121, 137, 231, 341, M ⁺ 410
920	*3,5 cholestadiene ?	368	C ₂₇ H ₄₄	255, M ⁺ 368
940	n-alkane C _{29:0}	408	C ₂₉ H ₆₀	C _n H _{2n+1} fragments, M ⁺ 408
1020	n-alkane C _{31:0}	436	C ₃₁ H ₆₄	C _n H _{2n+1} fragments, M ⁺ 436
* 35 cl.,	37 cl. isotope cluster			

TIC trace for GC/MS #1475
TO BE INCLUDED IN FINAL

GC/MS Run #1578

TO BE INCLUDED IN FINAL



TIC trace for GC/MS 1578