

# Geochemical Data Report Well 7131/4-1 (Guovca)



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## REPORT

TITLE

Analysis of headspace and occluded gas (C1-C9) from well 7131/4-1

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SUMMARY

This report contains tables and figures with data from gas chromatographic analysis of headspace and occluded gas from 5 canned cuttings samples from well 7131/4-1. The yields (in  $\mu\text{l}/\text{kg}$  dry rock) and relative proportions (in volume %) of 68 hydrocarbon compounds ranging from C1 to C9 are tabulated. Some geochemically relevant peak ratios are also listed and plotted.

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## **1. Introduction**

Five canned cutting samples from the well 7131/4-1 were received from Statoil for gas chromatographic analysis of the C1 to C9 hydrocarbons contained in the headspace and occluded gas.

This report contains the results of the analyses. The hydrocarbon concentrations are expressed as  $\mu\text{l}$  gas per kg of dried cuttings. The hydrocarbon composition is expressed in volume percent of all recorded hydrocarbons.

Aliquots of the headspace and occluded gas were sampled in vacuum tubes and sent to Applied Petroleum Technology AS, Norway (APT) for isotope analyses.

## **2. Experimental**

### **2.1 Headspace gas**

A septum was attached to the can and a sample of headspace gas was taken and injected into a gas chromatograph for analysis of C1 to C9 hydrocarbons.

The can was opened and the volume of the headspace was determined. The cuttings were washed with water (ca. 30 °C) on 4.0, 1.0 and 0.125 mm sieves in order to remove the drilling mud, and were then weighed and dried.

### **2.2 Occluded gas**

Prior to drying, an aliquot of the 1-4 mm fraction was crushed in water for 10 minutes using a gas-tight ball mill. An aliquot of the evolved gas was injected into a gas chromatograph for analysis of C1 to C9 hydrocarbons.

### **2.3 Samples for isotope analysis**

10 ml of each gas fraction (headspace and occluded gas) were extracted from all samples and injected to vacuum-based test tubes provided by Applied Petroleum Technology AS, Norway (APT). The tubes were sent to APT for analyses.

### **2.4 Gas chromatographic analysis**

The gas was analysed on a gas chromatograph fitted with an gas injector. The GC temperature program started at 35 °C, since separation of alkenes from alkanes was of no interest in this project. The instrument was fitted with a capillary column connected to an FID for hydrocarbon detection. Details of the instrumentation are listed in Table 2.1.

*Table 2.1 Analytical equipment*

Gas chromatograph	Agilent 6890
Injector	Gas injector connected to a 1.0 ml loop
Columns	HP-PONA column: 50 m x 0.20 mm i.d, 0.5 µm film thickness.
Carrier gas	Helium
Detector	FID (250 °C)
Temperature program	35 °C (5 min.) - 8 °C/min. - 180 °C (10 min.)
Chromatographic data system	HP ChemStation Rev. A.10.01

## 2.5 Identification

Peaks were identified based on three Supelco Reference Standards, guidelines in “The Norwegian Industry Guide to Organic Geochemical Analyses” (Edition 4.0) and internal procedures. Figure 2.1 shows a gas chromatogram with the annotation used in this project. Identified compounds, retention indices and comments are listed in Table 2.2.

*Table 2.2 Identified compounds with retention indices (RI) and comments. For peak labels see explanation below the table.*

Peak label	RI (Kováts)	Comments
C1	100	
C2	158 + 200	Includes ethane and ethene
C3	300	Includes propane and propene
iC4	354	
C4ene	385	
nC4	400	
2,2-DMC3	410	
iC5	467	
nC5	500	
2,2-DMC4	531	
CyC5 + 2,3-DMC4	561	Separated in some analyses, but summed up in the tables
2-MC5	565	
3-MC5	581	
nC6	600	
MCyC5	627	
2,4-DMC5	630	
Benzene	651	
CyC6	661	
2-MC6	668	
2,3-DMC5	670	
1,1-DMCyC5	674	
3-MC6	676	
c-1,3-DMCyC5	684	
t-1,3-DMCyC5	687	
t-1,2-DMCyC5 + 3-EC5 + 2,2,4-TMC5	690	
nC7	700	
MCyC6 + c-1,2-DMCyC5	725	
2,2-DMC6 + 1,1,3-TMCyC5	727	
2,5-DMC6 + 2,2,3-TMC5	734	May include E-CyC5
2,4-DMC6	736	
3,3-DMC6 + t-1,c-2,4-TMCyC5	744	May include c-1,t-2,4-TMCyC5

t-1,c-2,3-TMCyC5	751	
2,3,4-TMC5	754	
Toluene + 2,3,3-TMC5	759	
2,3-DMC6	763	May include 1,1,2-TMCyC5
2-M, 3-EC5	765	
2-MC7	768	
4-MC7 + 3-M,3-EC5	769	May also include an isomer of 3,4-DMC6
3,4-DMC6	773	Isomer
3-MC7 + c-1,t-2,3-TMCyC5	775	May also include c-1,3-DMCyC6
RI=781 (DMCyC6)	781	Possibly a DMCyC6 isomer
RI=783 (DMCyC6)	783	Possibly a DMCyC6 isomer
RI=790	790	Possibly a DMCyC6 isomer, minimum 2 compounds
RI=794	794	Possibly a DMCyC6 isomer, minimum 2 compounds
RI=796	797	Possibly CyC7 or a DMCyC6 isomer
nC8	800	Minimum 2 compounds
RI=805	805	Unknown
RI=807	807	Unknown
RI=815	815	Unknown
RI=821	821	Unknown
RI=825	825	Possibly 2,2-DMC7 or 2,4-DMC7
RI=831	831	Possibly 2,4-DMC7 or ECyC6
RI=834	834	Unknown, minimum 2 compounds
RI=838	838	Possibly ECyC6 and/or 2,6-DMC7, minimum 2 compounds
RI=843	843	Unknown
RI=847	847	Unknown
RI=848	848	Unknown
E-Benzene	855	
RI=859	860	Unknown, minimum 2 compounds
m+p-Xylene	863	
RI=867	867	Unknown
4-MC8 + 2-MC8	874	
RI=883	883	Possibly 3-MC8
o-Xylene	886	
RI=890	890	Unknown
RI=893	893	Unknown
RI=896	896	Unknown
nC9	900	

*Explanations:*

Structural groups	Parent structures	Numbers of functional groups	Names of functional groups	Steric configurations
n = normal	C1 = methane	D = di	M = methyl	c = cis
i = iso	C2 = ethane	T = tri	E = ethyl	t = trans
Cy = cyclo	etc.		P = propyl	o = ortho
				m = meta
				p = para

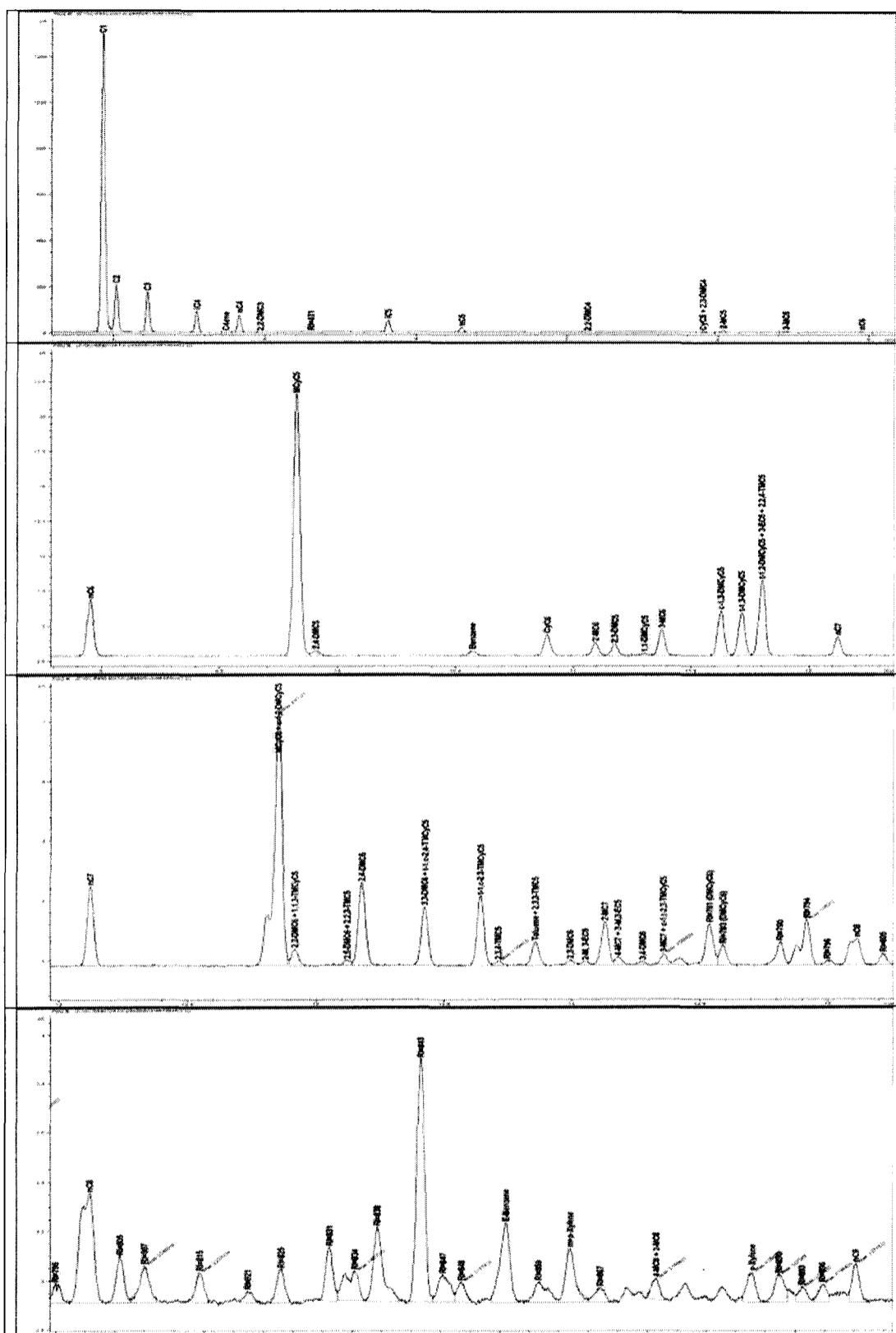


Figure 2.1 Gas chromatogram with annotation. Expanded views of C1 to n-C6, n-C6 to n-C7, n-C7 to n-C8 and n-C8 to n-C9 ranges.



## 2.6 Quantification

A 1000 ppm ( $\mu\text{l/l}$ ) standard gas sample containing methane, ethane, propane, i-butane, n-butane, n-pentane and n-hexane was used for quantification. The variation between all standard analysed over a period was small (Table 2.3), and the average response factors were used for quantification of all samples. The response factor for n-C5 was used for all compounds eluting between n-C4 and n-C5 and so on. For the C6-C7, C7-C8 and C8-C9 component groups the response factors were extrapolated based on molecular mass.

A 100 ppm ( $\mu\text{l/l}$ ) standard gas sample containing methane, ethane, propane, n-butane, n-pentane and n-hexane was used for control of linearity.

Rock-related concentrations (in  $\mu\text{l/kg}$ ) for compounds having a concentration of less than 0.2 ppm ( $\mu\text{l/l}$ ) in the analysed gas are not reported, as this corresponds to an area of about 0.08, which is the lowest reliable area in the gas chromatograms.

Table 2.3 Results from analyses of 1000 ppm standard (based on peak area)

	C1	C2	C3	iC4	nC4	nC5	nC6
Average peak area	70.6	137.8	199.9	279.9	286.0	327.2	371.6
Stdev.	0.7	0.9	1.4	2.1	2.4	3.7	7.7
Stdev. (% of average)	0.9	0.7	0.8	0.7	0.8	1.1	2.1
n	30	30	30	30	30	30	30

## 2.7 Concentrations and ratios

The yields of hydrocarbons ( $\mu\text{l/kg}$  dry rock) in headspace (H) and occluded (O) gas and the sum of H + O are given in Table 4.3, and the hydrocarbon composition (volume %) is given in Table 4.4. Selected summary data and peak ratios are calculated and reported in Table 4.5. Abbreviations used in Table 4.5 are explained in Table 2.4.

As coelution of 3-EC5 and 2,2,4-TMC5 with t-1,2-DMCyC5 and of c-1,2-DMCyC5 with MCyC6 cannot be avoided at the chosen experimental conditions, only some of the Mango ratios can be calculated (see tables).

Table 2.4 Explanations of the variables listed in Table 4.5.

Abbreviation	Explanation
<b>Hydrocarbon yields for selected C-number ranges</b>	
CncC1	Concentration of C1 ( $\mu\text{l/kg}$ dry rock)
CncC2C4	Concentration of C2 through n-C4 ( $\mu\text{l/kg}$ dry rock)
CncC5C9	Concentration of C5 through n-C9, i.e. all peaks eluting after n-C4 ( $\mu\text{l/kg}$ dry rock)
CncC1C9	Sum of these concentrations
<b>Hydrocarbon composition for selected C-number ranges</b>	
PctC1	Fraction of C1 (% volume of all C1-C9 HC)
PctC2C4	Fraction of C2 through n-C4 (% volume of all C1-C9 HC)
PctC5C9	Fraction of C5 through n-C9, i.e. all peaks eluting after n-C4 (% volume of all C1-C9 HC).
PctC1C9	Sum of these fractions (= 100 vol %)

Table 2.4 Continued

Abbreviation	Explanation
<b>Wetness and i-C4/n-C4 ratio</b>	
Wetness	100* (Sum C2 to n-C4) / (Sum C1 to n-C4) (volume %)
Ratic4nc4	Volume ratio i-C4 / n-C4
<b>Composition of C7 hydrocarbons by compound class</b>	
PctnC7	Fraction of n-alkanes in n-C7 range (volume % of all C7 compounds)
PctIsoC7	Fraction of iso-alkanes in n-C7 range (volume % of all C7 compounds)
PctCycC7	Fraction of cycloalkanes in n-C7 range (volume % of all C7 compounds)
PctAroC7	Fraction of aromatics in n-C7 range (volume % of all C7 compounds)
PctSumC7	Sum of these fractions (= 100 vol %)
<b>Thompson ratios (mass ratios), assessed property in brackets</b>	
Thompson_A	A = Benzene / n-Hexane [Aromaticity (fractionation)]
Thompson_B	B = Toluene / n-Heptane [Aromaticity (fractionation)]
Thompson_X	X = Xylene (m & p) / n-Octane [Aromaticity (fractionation)]
Thompson_C	C = (n-Hexane + n-Heptane) / (Cyclohexane + Methylcyclohexane) [Paraffinicity (maturity)]
Thompson_I	I = Isoheptane value = (Methylhexanes (2- & 3-)) / (Dimethylcyclopentanes (c1,3-, t1,3-, & t1,2-)) [Paraffinicity (maturity)]
Thompson_F	F = n-Heptane / Methylcyclohexane [Paraffinicity (maturity)]
Thompson_H	H = Heptane Value = 100 * n-Heptane / (Sum Cyclohexane through Methylcyclohexane, excluding cis-1,2-Dimethylcyclopentane) [Paraffinicity (maturity)]
Thompson_R	R = n-Heptane / 2-Methylhexane [Normality (branching)]
Thompson_U	U = Cyclohexane / 2-Methylhexane [Normality (branching)]
<b>Mango ratios (mass ratios)</b>	
Mango_P1	P1 = n-C7 (mass% of sum C7 HC) [first parents in SS kinetic scheme], Mango 1994
Mango_P2	P2 = 2-MC6 + 3-MC6 (mass% of sum C7 HC) [second parent in SS kinetic scheme], Mango 1994
Mango_P3	P3 = 3-EC5 + 3,3-DMC5 + 2,3-DMC5 + 2,4-DMC5 + 2,2-DMC5 + 2,2,3-TMC4 (mass% of sum C7 HC) [daughter isoalkane product of P2], Mango 1994 [Remark 1]
Mango_N15	N15 = ECyC5 + c-1,2-DMCyC5 + t-1,2-DMCyC5 (mass% of sum C7 HC) [Daughter cyclopentane products of P2], Mango 1994 [Remark 2]
Mango_N16	N16 = MCyC6 + TOLUENE (mass% of sum C7 HC) [Daughter cyclohexane products of P1], Mango 1994
Mango_N2	N2 = 1,1-DMCyC5 + c-1,3-DMCyC5 + t-1,3-DMCyC5 (mass% of sum C7 HC) [Daughter cyclopentane products of P2], Mango 1994 [Remark 3]
Mango_K1	K1 = (2-MC6 + 2,3-DMC5) / (3-MC6 + 2,4-DMC5), Mango 1987 in Mango 1994
Mango_K2	K2 = P3 / (P2 + N2) = (3-EC5 + 2,3-DMC5 + 2,4-DMC5 + 2,2-DMC5 + 2,2,3-TMC4) / (2-MC6 + 3-MC6 + 1,1-DMCyC5 + c-1,3-DMCyC5 + t-1,3-DMCyC5) (Mango 1990 in Mango 1994)
Mango_N15N16	N15/N16 = k15/k16 [a ratio of P1 daughters], Mango 1994
Mango_P3N2	P3/N2 = k23/k25 [a ratio of P2 daughters], Mango 1994

**Remarks on Mango ratios**

- Remark 1 The 2,2,3-TMC4 peak is consistently called "2,3,3-TMC4" in the Mango papers, but this is probably a mistyping, as 2,3,3-TMC4 is normally not identified.
- Remark 2 Actually  $N_1^5$ , where 1 means the first daughter generation and 5 stands for the parent cyclopentane.
- Remark 3 Analog to N15.

**Coelution of compounds**

'CyC5' contains coeluting 2,3-DMC4.

't-1,2-DMCyC5' contains coeluting 3-EC5 and 2,2,4-TMC5. The Mango ratios P3 and N15 can therefore not be calculated. The Thompson ratios H and I may be slightly affected.

'MCyC6' contains coeluting c-1,2-DMCyC5. The Mango ratios N15 and N16 can therefore not be calculated. The Thompson ratios C, F and H may be slightly affected.

Toluene coelutes with 2,3,3-TMC5 and 'n-C8' contains an unknown coeluting compound. The Thompson ratios B, H and X may be slightly affected.

**References**

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## 2.8 Water content

The water content of the cuttings was determined by weighing the fractions before and after drying at 35 °C for at least 24 hours. The dry weight of the rock used for occluded gas analysis was determined using the wet weight of this rock and the water content of the remaining 1-4 mm fraction. Water contents for the three individual grain size fractions are listed in Table 4.2.

## 3. Comments on samples and analytical data

The wet cutting samples were received in pressure-lid cans of 1 l volume at ambient temperature. Secondary modification of the gas composition by microbial activity cannot be completely ruled out.

Sample descriptions are listed in Table 4.1.

One of the samples, H6167 at 931 m depth, contained no fraction above 4 mm, and a very small fraction between 1 and 4 mm. The whole of this fraction was used in the occluded gas analyses, and the water content was estimated and set to 30 %.

Some of the peak ratios show erratic values for the shallowest sample. This is typically due to low concentration or absence of the respective compounds. Care should, therefore, be taken in the interpretation of these ratios. Also note the remarks in Table 2.4 on the possible effects of coelution on the various peak ratios.

## **4. Results**

**Table 4.1**  
**Sample description**

Table 4.1 Sample description. Lithologies in order of decreasing abundance.

Sample ID	Btm Depth (m RKB)	Lithology (numbers represent roughly estimated percentages)	Gas volume headspace (ml)	Gas volume occluded (ml)	Rock weight total sample dry (g)	Rock weight occluded sample dry (g)
H6163	811	55 SLST-SST(vfgr), calc cmt., wt-ltgy 45 CLYST, red tr SH, blk	284	20.0	154.9	9.7
H6164	841	60 CLYST, red 20 CLYST, gn-gy 20 LST, wt, with PY crystals tr CLYST, blk	244	30.4	221.5	16.5
H6165	871	100 CLYST, blk-vdkgy tr CLYST, red tr LST, wt, with PY crystals	288	18.5	383.4	16.0
H6166	901	>45 CLYST/SH, dkgy-blk 20 SH-SLST (calc), mgy 20 CLYST, red <10 SST, mgr-cgr, wt, glauc. few % QTZ grains few % LST with PY crystals	225	20.8	391.3	15.3
H6167	931	Only 125 µm - 1 mm fraction available: 99 QTZ grains 1 PY crystals	282	30.7	406.7	2.7

Key: SH = shale, SLST = siltstone, SST = sandstone, DOL = dolomite, LST = limestone, ADD = mud additive, PY = pyrite, cc = calcite, cmtd = cemented, tr = trace, vfgr = very fine grained, gy = grey, dk = dark, m = medium, lt = light, wt = white.

**Table 4.2**  
**Water contents of different grain size fractions**

*Table 4.2 Water contents of different grain size fractions.*

<b>Sample ID</b>	<b>Btm Depth</b>	<b>Water content &gt;4 mm fraction (wt% of wet fraction)</b>	<b>Water content 4-1 mm fraction (wt% of wet fraction)</b>	<b>Water content 1-0.125 mm fraction (wt% of wet fraction)</b>	<b>Water content &gt;0.125 mm (wt% of wet fraction)</b>
H6163	811	50.0	47.1	39.8	40.8
H6164	841	18.0	22.8	27.1	23.3
H6165	871	25.2	28.1	37.8	29.2
H6166	901	27.8	24.5	20.5	22.7
H6167	931	-1 <sup>1</sup>	30.0 <sup>2</sup>	20.1	20.0

*Comments:*

- 1) No fraction
- 2) Estimated value due to a very small sample amount



**Table 4.3**  
**Yield of hydrocarbons in headspace and occluded gas**  
**( $\mu\text{l}/\text{kg}$  dry rock)**

Table 4.3 Yield of hydrocarbons in headspace and occluded gas ( $\mu\text{l}/\text{kg}$  dry rock).

Sample-ID Gas fraction Depth (m) Compound	H6163	H6163	H6163	H6164	H6164	H6164	H6165	H6165	H6165
	H 811	O 811	H+O 811	H 841	O 841	H+O 841	H 871	O 871	H+O 871
C1	234	44	277	2940	423	3363	167685	1792	169477
C2	22	5	27	200	56	256	6560	944	7505
C3	39	2	41	212	24	236	2858	1361	4219
iC4	16	1	17	89	10	99	882	504	1386
C4ene	4	0	4	1	2	4	1	1	2
nC4	19	1	20	101	19	119	683	651	1334
2,2-DMC3	0	0	0	1	0	1	1	0	1
iC5	12	1	13	73	19	92	399	413	811
nC5	11	1	13	31	14	44	146	210	356
2,2-DMC4	0	0	0	0	0	0	0	0	1
CyC5 + 2,3-DMC4	1	1	2	6	2	9	24	26	50
2-MC5	3	3	6	13	7	20	59	86	144
3-MC5	2	2	3	8	5	13	36	50	86
nC6	3	3	7	6	6	12	21	36	57
MCyC5	4	1	5	25	10	35	100	107	208
2,4-DMC5	0	1	1	1	0	1	2	3	5
Benzene	1	0	1	1	1	2	2	3	5
CyC6	1	0	1	2	1	3	6	6	12
2-MC6	0	3	4	1	2	3	4	6	10
2,3-DMC5	0	1	2	1	1	2	4	5	9
1,1-DMCyC5	0	1	1	0	0	0	0	0	1
3-MC6	1	6	6	2	2	4	9	13	22
c-1,3-DMCyC5	1	2	2	3	2	6	16	19	34
t-1,3-DMCyC5	1	2	3	3	2	6	16	19	34
t-1,2-DMCyC5 + 3-EC5 + 2,2,4-TMC5	1	3	4	5	3	8	26	29	55
nC7	2	4	5	2	3	5	6	10	16
MCyC6 + c-1,2-DMCyC5	2	7	9	6	4	10	20	21	40
2,2-DMC6 + 1,1,3-TMCyC5	0	2	2	0	0	0	1	1	2
2,5-DMC6 + 2,2,3-TMC5	0	1	1	0	0	0	0	0	1
2,4-DMC6	0	2	2	1	1	3	6	7	14
3,3-DMC6 + t-1,c-2,4-TMCyC5	0	2	2	1	1	1	4	5	9
t-1,c-2,3-TMCyC5	0	2	2	1	1	1	5	6	11
2,3,4-TMC5	0	0	0	0	0	0	0	0	1
Toluene + 2,3,3-TMC5	1	0	1	1	1	2	2	3	5
2,3-DMC6	0	1	1	0	0	0	0	0	1
2-M, 3-EC5	0	0	0	0	0	0	0	0	1
2-MC7	0	2	2	1	1	2	3	5	8
4-MC7 + 3-M,3-EC5	0	2	2	0	0	0	0	1	1
3,4-DMC6	0	0	0	0	0	0	0	0	0
3-MC7 + c-1,t-2,3-TMCyC5	0	3	3	0	1	1	1	1	3
RI=781 (DMCyC6)	0	5	5	1	1	1	3	3	6
RI=783 (DMCyC6)	0	2	2	0	0	0	1	1	3
RI=790	0	1	1	0	0	1	2	2	4
RI=794	0	2	2	1	1	1	5	5	10
RI=796	0	0	0	0	0	0	0	0	1
nC8	1	4	5	1	1	2	3	4	7
RI=805	0	1	1	0	0	0	1	1	1
RI=807	0	1	1	0	0	0	1	1	1
RI=815	0	0	0	0	0	0	0	0	1
RI=821	0	0	0	0	0	0	0	0	0
RI=825	0	1	1	0	0	0	1	1	1
RI=831	0	1	1	0	0	0	1	1	2
RI=834	0	1	1	0	0	0	1	1	2
RI=838	0	4	4	0	0	1	1	1	3
RI=843	0	4	4	1	1	2	4	4	9
RI=847	0	1	1	0	0	0	1	1	1
RI=848	0	1	1	0	0	0	0	0	1
E-Benzene	0	1	1	0	0	1	2	2	3
RI=859	0	3	3	0	0	0	0	0	1
m+p-Xylene	1	1	2	1	0	1	1	1	2
RI=867	0	1	1	0	0	0	0	0	1
4-MC8 + 2-MC8	0	1	1	0	0	0	0	0	1
RI=883	0	1	1	0	0	0	0	0	0
o-Xylene	0	0	0	0	0	0	1	1	1
RI=890	0	1	1	0	0	0	1	1	1
RI=893	0	2	2	0	0	0	0	0	0
RI=896	0	1	1	0	0	0	0	0	1
nC9	0	1	1	1	0	1	1	1	1
Sum FID	382	152	534	3743	628	4371	179621	6380	186002

Table 4.3 Continued

Sample-ID	H6166	H6166	H6166	H6167	H6167	H6167
Gas fraction	H	O	H+O	H	O	H+O
Depth (m)	901	901	901	931	931	931
Compound						
C1	18769	687	19455	605	756	1361
C2	1468	444	1911	71	182	253
C3	794	926	1720	54	111	165
iC4	307	488	795	40	51	91
C4ene	1	1	2	1	21	23
nC4	256	720	977	35	105	140
2,2-DMC3	1	2	3	0	0	0
iC5	170	552	722	37	126	163
nC5	68	344	412	16	120	137
2,2-DMC4	0	1	1	0	0	0
CyC5 + 2,3-DMC4	12	45	57	3	19	22
2-MC5	30	166	196	10	78	88
3-MC5	19	93	112	6	44	50
nC6	12	82	93	4	60	65
MCyC5	52	208	261	16	125	141
2,4-DMC5	1	6	7	0	5	5
Benzene	1	4	5	0	3	4
CyC6	4	14	18	1	10	11
2-MC6	2	16	19	1	14	15
2,3-DMC5	2	12	14	1	9	10
1,1-DMCyC5	0	1	2	0	0	0
3-MC6	5	32	37	2	29	31
c-1,3-DMCyC5	8	41	50	4	36	40
t-1,3-DMCyC5	8	41	50	4	37	41
t-1,2-DMCyC5 + 3-EC5 + 2,2,4-TMC5	15	69	84	6	56	62
nC7	3	26	29	2	35	37
MCyC6 + c-1,2-DMCyC5	12	53	66	6	55	60
2,2-DMC6 + 1,1,3-TMCyC5	1	4	4	0	3	4
2,5-DMC6 + 2,2,3-TMC5	0	1	2	0	0	0
2,4-DMC6	3	17	21	2	24	26
3,3-DMC6 + t-1,c-2,4-TMCyC5	2	13	16	1	16	18
t-1,c-2,3-TMCyC5	3	16	19	2	19	20
2,3,4-TMC5	0	1	1	0	0	0
Toluene + 2,3,3-TMC5	1	4	5	0	7	7
2,3-DMC6	0	1	2	0	0	0
2-M, 3-EC5	0	1	1	0	0	0
2-MC7	2	13	14	1	19	20
4-MC7 + 3-M,3-EC5	0	2	3	0	3	3
3,4-DMC6	0	1	1	0	0	0
3-MC7 + c-1,t-2,3-TMCyC5	1	5	5	0	6	7
RI=781 (DMCyC6)	2	9	11	1	14	15
RI=783 (DMCyC6)	1	4	5	1	6	7
RI=790	1	5	6	1	10	10
RI=794	2	13	16	1	23	24
RI=796	0	1	1	0	0	0
nC8	2	10	12	1	21	23
RI=805	0	3	3	0	5	5
RI=807	0	2	2	0	3	3
RI=815	0	1	2	0	3	3
RI=821	0	1	1	0	0	0
RI=825	0	2	2	0	3	3
RI=831	0	3	4	0	7	7
RI=834	0	2	3	0	5	6
RI=838	1	4	5	1	8	9
RI=843	2	11	13	1	22	24
RI=847	0	2	2	0	5	5
RI=848	0	1	1	0	2	3
E-Benzene	1	4	5	1	11	11
RI=859	0	1	2	0	5	5
m+p-Xylene	1	2	3	0	7	8
RI=867	0	1	1	0	4	4
4-MC8 + 2-MC8	0	1	1	0	4	4
RI=883	0	0	0	0	0	0
o-Xylene	0	1	2	0	0	0
RI=890	0	2	2	0	6	6
RI=893	0	1	1	0	0	0
RI=896	0	1	1	0	3	3
nC9	0	2	2	0	6	6
Sum FID	22054	5245	27300	947	2368	3314

**Table 4.4**  
**Composition of hydrocarbons in headspace and occluded gas**  
**(volume %)**

Table 4.4 Composition of hydrocarbons in headspace and occluded gas (volume %).

Sample-ID	H6163	H6163	H6163	H6164	H6164	H6164	H6165	H6165	H6165
Gas fraction	H	O	H+O	H	O	H+O	H	O	H+O
Depth (m)	811.0	811.0	811.0	841.0	841.0	841.0	871.0	871.0	871.0
<b>Compound</b>									
C1	61.1	28.8	51.9	78.5	67.3	76.9	93.4	28.1	91.1
C2	5.8	3.4	5.1	5.3	8.8	5.8	3.7	14.8	4.0
C3	10.3	1.3	7.7	5.7	3.8	5.4	1.6	21.3	2.3
iC4	4.2	0.4	3.1	2.4	1.6	2.3	0.5	7.9	0.7
C4ene	1.0	0.0	0.7	0.0	0.3	0.1	0.0	0.0	0.0
nC4	5.1	0.7	3.8	2.7	3.0	2.7	0.4	10.2	0.7
2,2-DMC3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
iC5	3.3	0.6	2.5	2.0	3.0	2.1	0.2	6.5	0.4
nC5	2.9	0.9	2.4	0.8	2.2	1.0	0.1	3.3	0.2
2,2-DMC4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CyC5 + 2,3-DMC4	0.4	0.4	0.4	0.2	0.4	0.2	0.0	0.4	0.0
2-MC5	0.8	2.0	1.1	0.3	1.2	0.5	0.0	1.3	0.1
3-MC5	0.4	1.0	0.6	0.2	0.8	0.3	0.0	0.8	0.0
nC6	0.8	2.3	1.2	0.2	0.9	0.3	0.0	0.6	0.0
MCyC5	1.0	0.8	0.9	0.7	1.6	0.8	0.1	1.7	0.1
2,4-DMC5	0.0	0.5	0.1	0.0	0.1	0.0	0.0	0.0	0.0
Benzene	0.1	0.0	0.1	0.0	0.1	0.0	0.0	0.0	0.0
CyC6	0.3	0.0	0.2	0.1	0.2	0.1	0.0	0.1	0.0
2-MC6	0.1	2.1	0.7	0.0	0.2	0.1	0.0	0.1	0.0
2,3-DMC5	0.1	0.9	0.3	0.0	0.1	0.0	0.0	0.1	0.0
1,1-DMCyC5	0.0	0.5	0.1	0.0	0.0	0.0	0.0	0.0	0.0
3-MC6	0.1	3.7	1.1	0.0	0.3	0.1	0.0	0.2	0.0
c-1,3-DMCyC5	0.1	1.2	0.4	0.1	0.3	0.1	0.0	0.3	0.0
t-1,3-DMCyC5	0.2	1.5	0.5	0.1	0.4	0.1	0.0	0.3	0.0
t-1,2-DMCyC5 + 3-EC5 + 2,2,4-TMC5	0.2	1.9	0.7	0.1	0.5	0.2	0.0	0.5	0.0
nC7	0.4	2.4	1.0	0.1	0.5	0.1	0.0	0.2	0.0
MCyC6 + c-1,2-DMCyC5	0.5	4.6	1.6	0.2	0.6	0.2	0.0	0.3	0.0
2,2-DMC6 + 1,1,3-TMCyC5	0.0	1.4	0.4	0.0	0.0	0.0	0.0	0.0	0.0
2,5-DMC6 + 2,2,3-TMC5	0.0	0.6	0.2	0.0	0.0	0.0	0.0	0.0	0.0
2,4-DMC6	0.0	1.2	0.3	0.0	0.2	0.1	0.0	0.1	0.0
3,3-DMC6 + t-1,c-2,4-TMCyC5	0.0	1.6	0.5	0.0	0.1	0.0	0.0	0.1	0.0
t-1,c-2,3-TMCyC5	0.0	1.6	0.5	0.0	0.1	0.0	0.0	0.1	0.0
2,3,4-TMC5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Toluene + 2,3,3-TMC5	0.1	0.0	0.1	0.0	0.1	0.1	0.0	0.0	0.0
2,3-DMC6	0.0	0.5	0.1	0.0	0.0	0.0	0.0	0.0	0.0
2-M, 3-EC5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2-MC7	0.0	1.6	0.5	0.0	0.2	0.0	0.0	0.1	0.0
4-MC7 + 3-M,3-EC5	0.0	1.1	0.3	0.0	0.0	0.0	0.0	0.0	0.0
3,4-DMC6	0.0	0.3	0.1	0.0	0.0	0.0	0.0	0.0	0.0
3-MC7 + c-1,t-2,3-TMCyC5	0.0	1.9	0.5	0.0	0.1	0.0	0.0	0.0	0.0
RI=781 (DMCyC6)	0.0	3.4	1.0	0.0	0.1	0.0	0.0	0.0	0.0
RI=783 (DMCyC6)	0.0	1.2	0.3	0.0	0.0	0.0	0.0	0.0	0.0
RI=790	0.0	0.8	0.2	0.0	0.1	0.0	0.0	0.0	0.0
RI=794	0.0	1.1	0.3	0.0	0.1	0.0	0.0	0.1	0.0
RI=796	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
nC8	0.2	2.8	1.0	0.0	0.2	0.1	0.0	0.1	0.0
RI=805	0.0	0.5	0.1	0.0	0.0	0.0	0.0	0.0	0.0
RI=807	0.0	0.6	0.2	0.0	0.0	0.0	0.0	0.0	0.0
RI=815	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
RI=821	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
RI=825	0.0	0.5	0.1	0.0	0.0	0.0	0.0	0.0	0.0
RI=831	0.0	0.8	0.2	0.0	0.0	0.0	0.0	0.0	0.0
RI=834	0.0	0.5	0.1	0.0	0.0	0.0	0.0	0.0	0.0
RI=838	0.0	2.9	0.8	0.0	0.1	0.0	0.0	0.0	0.0
RI=843	0.0	2.7	0.8	0.0	0.1	0.0	0.0	0.1	0.0
RI=847	0.0	0.6	0.2	0.0	0.0	0.0	0.0	0.0	0.0
RI=848	0.0	0.3	0.1	0.0	0.0	0.0	0.0	0.0	0.0
E-Benzene	0.0	0.5	0.1	0.0	0.1	0.0	0.0	0.0	0.0
RI=859	0.0	1.7	0.5	0.0	0.0	0.0	0.0	0.0	0.0
m+p-Xylene	0.2	0.6	0.3	0.0	0.0	0.0	0.0	0.0	0.0
RI=867	0.0	0.7	0.2	0.0	0.0	0.0	0.0	0.0	0.0
4-MC8 + 2-MC8	0.0	0.6	0.2	0.0	0.0	0.0	0.0	0.0	0.0
RI=883	0.0	0.5	0.2	0.0	0.0	0.0	0.0	0.0	0.0
o-Xylene	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
RI=890	0.0	0.9	0.2	0.0	0.0	0.0	0.0	0.0	0.0
RI=893	0.0	1.0	0.3	0.0	0.0	0.0	0.0	0.0	0.0
RI=896	0.0	0.5	0.1	0.0	0.0	0.0	0.0	0.0	0.0
nC9	0.1	0.6	0.3	0.0	0.1	0.0	0.0	0.0	0.0
Sum FID	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0

Table 4.4 Continued

Sample-ID Gas fraction Depth (m) Compound	H6166 H 901.0	H6166 O 901.0	H6166 H+O 901.0	H6167 H 931.0	H6167 O 931.0	H6167 H+O 931.0
	C1	85.1	13.1	71.3	63.9	31.9
C2	6.7	8.5	7.0	7.5	7.7	7.6
C3	3.6	17.6	6.3	5.7	4.7	5.0
iC4	1.4	9.3	2.9	4.2	2.2	2.8
C4ene	0.0	0.0	0.0	0.1	0.9	0.7
nC4	1.2	13.7	3.6	3.7	4.4	4.2
2,2-DMC3	0.0	0.0	0.0	0.0	0.0	0.0
iC5	0.8	10.5	2.6	3.9	5.3	4.9
nC5	0.3	6.6	1.5	1.7	5.1	4.1
2,2-DMC4	0.0	0.0	0.0	0.0	0.0	0.0
CyC5 + 2,3-DMC4	0.1	0.9	0.2	0.3	0.8	0.7
2-MC5	0.1	3.2	0.7	1.1	3.3	2.7
3-MC5	0.1	1.8	0.4	0.6	1.9	1.5
nC6	0.1	1.6	0.3	0.5	2.5	1.9
MCyC5	0.2	4.0	1.0	1.6	5.3	4.3
2,4-DMC5	0.0	0.1	0.0	0.0	0.2	0.2
Benzene	0.0	0.1	0.0	0.0	0.1	0.1
CyC6	0.0	0.3	0.1	0.1	0.4	0.3
2-MC6	0.0	0.3	0.1	0.1	0.6	0.5
2,3-DMC5	0.0	0.2	0.1	0.1	0.4	0.3
1,1-DMCyC5	0.0	0.0	0.0	0.0	0.0	0.0
3-MC6	0.0	0.6	0.1	0.3	1.2	0.9
c-1,3-DMCyC5	0.0	0.8	0.2	0.4	1.5	1.2
t-1,3-DMCyC5	0.0	0.8	0.2	0.4	1.6	1.2
t-1,2-DMCyC5 + 3-EC5 + 2,2,4-TMC5	0.1	1.3	0.3	0.6	2.4	1.9
nC7	0.0	0.5	0.1	0.2	1.5	1.1
MCyC6 + c-1,2-DMCyC5	0.1	1.0	0.2	0.6	2.3	1.8
2,2-DMC6 + 1,1,3-TMCyC5	0.0	0.1	0.0	0.0	0.1	0.1
2,5-DMC6 + 2,2,3-TMC5	0.0	0.0	0.0	0.0	0.0	0.0
2,4-DMC6	0.0	0.3	0.1	0.2	1.0	0.8
3,3-DMC6 + t-1,c-2,4-TMCyC5	0.0	0.3	0.1	0.1	0.7	0.5
t-1,c-2,3-TMCyC5	0.0	0.3	0.1	0.2	0.8	0.6
2,3,4-TMC5	0.0	0.0	0.0	0.0	0.0	0.0
Toluene + 2,3,3-TMC5	0.0	0.1	0.0	0.0	0.3	0.2
2,3-DMC6	0.0	0.0	0.0	0.0	0.0	0.0
2-M, 3-EC5	0.0	0.0	0.0	0.0	0.0	0.0
2-MC7	0.0	0.2	0.1	0.1	0.8	0.6
4-MC7 + 3-M,3-EC5	0.0	0.0	0.0	0.0	0.1	0.1
3,4-DMC6	0.0	0.0	0.0	0.0	0.0	0.0
3-MC7 + c-1,t-2,3-TMCyC5	0.0	0.1	0.0	0.1	0.3	0.2
RI=781 (DMCyC6)	0.0	0.2	0.0	0.1	0.6	0.4
RI=783 (DMCyC6)	0.0	0.1	0.0	0.1	0.3	0.2
RI=790	0.0	0.1	0.0	0.1	0.4	0.3
RI=794	0.0	0.3	0.1	0.1	1.0	0.7
RI=796	0.0	0.0	0.0	0.0	0.0	0.0
nC8	0.0	0.2	0.0	0.2	0.9	0.7
RI=805	0.0	0.0	0.0	0.0	0.2	0.2
RI=807	0.0	0.0	0.0	0.0	0.1	0.1
RI=815	0.0	0.0	0.0	0.0	0.1	0.1
RI=821	0.0	0.0	0.0	0.0	0.0	0.0
RI=825	0.0	0.0	0.0	0.0	0.1	0.1
RI=831	0.0	0.1	0.0	0.0	0.3	0.2
RI=834	0.0	0.0	0.0	0.0	0.2	0.2
RI=838	0.0	0.1	0.0	0.1	0.3	0.3
RI=843	0.0	0.2	0.0	0.2	0.9	0.7
RI=847	0.0	0.0	0.0	0.0	0.2	0.2
RI=848	0.0	0.0	0.0	0.0	0.1	0.1
E-Benzene	0.0	0.1	0.0	0.1	0.5	0.3
RI=859	0.0	0.0	0.0	0.0	0.2	0.1
m+p-Xylene	0.0	0.0	0.0	0.0	0.3	0.2
RI=867	0.0	0.0	0.0	0.0	0.2	0.1
4-MC8 + 2-MC8	0.0	0.0	0.0	0.0	0.2	0.1
RI=883	0.0	0.0	0.0	0.0	0.0	0.0
o-Xylene	0.0	0.0	0.0	0.0	0.0	0.0
RI=890	0.0	0.0	0.0	0.0	0.2	0.2
RI=893	0.0	0.0	0.0	0.0	0.0	0.0
RI=896	0.0	0.0	0.0	0.0	0.1	0.1
nC9	0.0	0.0	0.0	0.1	0.2	0.2
Sum FID	100.0	100.0	100.0	100.0	100.0	100.0

**Table 4.5**  
**Ratios and summary data**

(See Table 2.4 for explanations and comments;  
-1 = ratio cannot be calculated)

Table 4.5 Ratios and summary data. (See Table 2.4 for explanation and comments;  
-I = ratio cannot be calculated

Sample-ID	H6163	H6163	H6163	H6164	H6164	H6164	H6165	H6165	H6165
Gas fraction	H	O	H+O	H	O	H+O	H	O	H+O
Depth (m)	811	811	811	841	841	841	871	871	871
<b>Compound</b>									
CncC1	234	44	277	2940	423	3363	167685	1792	169477
CncC2C4	101	9	110	603	111	713	10984	3462	14446
CncC5C9	47	100	147	201	94	295	952	1127	2079
CncC1C9	382	152	534	3743	628	4371	179621	6380	186002
PctC1	61.1	28.8	51.9	78.5	67.3	76.9	93.4	28.1	91.1
PctC2C4	26.4	5.7	20.5	16.1	17.6	16.3	6.1	54.3	7.8
PctC5C9	12.4	65.5	27.6	5.4	15.0	6.8	0.5	17.7	1.1
PctC1C9	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
Wetness	30.2	16.6	28.3	17.0	20.7	17.5	6.1	65.9	7.9
RatiC4nC4	0.8	0.6	0.8	0.9	0.5	0.8	1.3	0.8	1.0
PctnC7	22.6	12.5	14.5	8.6	14.5	11.2	6.0	7.9	7.1
PctIsoC7	18.0	37.1	33.3	16.2	24.7	19.9	17.5	21.3	19.6
PctCycC7	52.0	50.4	50.7	69.6	56.7	63.9	74.5	68.7	71.3
PctAroC7	7.4	0.0	1.5	5.6	4.0	4.9	2.0	2.1	2.0
PctSumC7	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
Thompson_A	0.2	0.0	0.1	0.3	0.2	0.2	0.1	0.1	0.1
Thompson_B	0.4	0.0	0.1	0.7	0.3	0.5	0.4	0.3	0.3
Thompson_X	1.0	0.2	0.4	0.6	0.0	0.3	0.4	0.4	0.4
Thompson_C	1.5	0.9	1.1	0.9	1.6	1.2	0.9	1.6	1.3
Thompson_I	0.5	1.3	1.1	0.2	0.5	0.3	0.2	0.3	0.3
Thompson_F	0.8	0.5	0.5	0.3	0.7	0.5	0.3	0.4	0.4
Thompson_H	20.3	12.4	14.1	8.3	14.3	10.9	5.7	7.7	6.8
Thompson_R	4.3	1.1	1.5	2.1	1.9	2.0	1.6	1.6	1.6
Thompson_U	2.9	0.0	0.3	2.0	0.7	1.2	1.6	0.9	1.2
Mango_P1	22.63	12.48	14.51	8.63	14.54	11.24	5.98	7.92	7.05
Mango_P2	12.62	30.18	26.68	10.51	18.12	13.87	12.05	15.14	13.76
Mango_N2	16.06	16.31	16.26	26.37	22.10	24.49	30.51	29.65	30.04
Mango_K1	1.43	0.72	0.78	0.89	0.95	0.93	0.74	0.73	0.74

Sample-ID	H6166	H6166	H6166	H6167	H6167	H6167
Gas fraction	H	O	H+O	H	O	H+O
Depth (m)	901	901	901	931	931	931
<b>Compound</b>						
CncC1	18769	687	19455	605	756	1361
CncC2C4	2826	2579	5405	201	471	672
CncC5C9	460	1979	2439	141	1141	1281
CncC1C9	22054	5245	27300	947	2368	3314
PctC1	85.1	13.1	71.3	63.9	31.9	41.1
PctC2C4	12.8	49.2	19.8	21.2	19.9	20.3
PctC5C9	2.1	37.7	8.9	14.9	48.2	38.7
PctC1C9	100.0	100.0	100.0	100.0	100.0	100.0
Wetness	13.1	79.0	21.7	24.9	38.4	33.0
RatiC4nC4	1.2	0.7	0.8	1.2	0.5	0.7
PctnC7	5.7	8.5	8.1	7.9	12.3	11.9
PctIsoC7	17.5	22.1	21.4	19.0	19.9	19.9
PctCycC7	75.1	68.1	69.2	71.6	65.3	65.8
PctAroC7	1.7	1.3	1.4	1.6	2.5	2.4
PctSumC7	100.0	100.0	100.0	100.0	100.0	100.0
Thompson_A	0.1	0.1	0.1	0.1	0.1	0.1
Thompson_B	0.3	0.2	0.2	0.2	0.2	0.2
Thompson_X	0.4	0.3	0.3	0.4	0.4	0.4
Thompson_C	0.8	1.4	1.3	0.9	1.3	1.3
Thompson_I	0.2	0.3	0.3	0.3	0.3	0.3
Thompson_F	0.2	0.4	0.4	0.3	0.6	0.5
Thompson_H	5.3	8.2	7.7	7.5	12.1	11.7
Thompson_R	1.4	1.6	1.6	1.7	2.4	2.4
Thompson_U	1.8	0.9	1.0	1.0	0.7	0.7
Mango_P1	5.68	8.54	8.07	7.85	12.32	11.94
Mango_P2	12.14	16.06	15.42	13.69	15.26	15.13
Mango_N2	29.21	27.72	27.96	27.67	25.90	26.05
Mango_K1	0.76	0.74	0.74	0.78	0.68	0.69