For each source rock there are four data sheets:

Sheet 1: Presents general, geological and analytical data for the source rock including a location map, and a stratigraphic section. Also included on Sheet 1 is a summary of the geochemical data for the sample that was selected for detailed analyses.

Sheet 2: Presents screening and detailed analytical data generated by SPT that is both typical and representative of the source rock.

Sheet 3: Presents numerical data from gas chromatography and gas chromatography-mass spectrometry analyses.

Sheet 4: Presents GC-MS fragmentograms of biomarker compounds in the alkane and aromatic fractions of the source rock extract.

As well as the data sheets, illustrative photomicrographs of the kerogens are given in Appendix 1 and detailed kerogen typing is given in Appendix 2.

2.4.2 Detailed Explanation of Data Sheets

2.4.2.1 Sheet 1

Sheet 1 presents the non-analytical and analytical data for the source rock. The sheet is divided into six sections:

a. basin setting of source rock;
b. location map;
c. generalised basin stratigraphy and geochemical log;
d. geological setting of source rock;
e. analysed sample information;
f. summary.

In order to provide a rational and consistent approach in defining the general characteristics of the basins we have utilised two recently completed SPT studies. These are the 'Global tectonics, basin configurations and reserves statistics' (SPT, 1992a) and the 'Phanerozoic palaeogeographic reconstructions, palaeoenvironments and major source rocks of the world' (1992b). These were used to provide consistency firstly in basin names, areas, reserves and tectonic classification (SPT, 1992a) and secondly in the source rock's depositional environment, palaeolatitude, palaeoclimate and basin morphology (SPT, 1992b). Both these 1992 reports and this report are available in hard copy and digital format and the datasets are intended to be mutually compatible.

It is also to be noted that considerable effort has been put into establishing this report in digital format. In sheet 1, in particular, the emphasis is on numeric information with where necessary alphanumeric text.

Where possible all data types listed have been entered into the database for each source rock. However, in some instances no data are available in which case the following convention has been applied:

Symbol	Explanation
-	No data available because the data type required does not exist for good geological reasons e.g. no reserves because there are no reserves in the basin or attributed to the source.
?	No data located in the data sources available to us although data for the particular property in question clearly must exit.

It is also to be noted that in some instances the data were either difficult to find or of questionable quality. We have not in general indicated the level of confidence in the data presented.

a. Basin setting of source rock

The first section gives geographical and geological details of the occurrence of the source rock. It also gives details of the petroleum generated from the source rock.

Basin name and **Sub-basin name**: This refers to the sedimentary basin from which the analysed source rock samples came. All basin names and sub-basin names are as defined in the SPT global basins study (SPT, 1992a).

Occurrence in other basins/sub-basins: This gives the names of other sedimentary basins in which the source rock or its lateral equivalents are known to occur. All basin names and sub-basin names are as defined in the SPT global basins study (SPT, 1992a).

Tectonic regime at present and **Basin area (km^2)**: The data are taken from the SPT global basins study (SPT, 1992a) and refer to the basin/sub-basin from which the samples come and its area. Figure 2.2 taken from the global basins study defines the tectonic regime code numbers. In some instances the area of the basin at the time of source rock deposition has been preferred.

Country(ies): This gives the political boundaries of the basin from which the samples come.

Formation/member name: This is the common name of the source rock horizon.

Formation/member age (Ma): This is the chronological age, in millions of years before present, of the source rock horizon and stratigraphic age name. All ages quoted throughout the database follow the scheme of Harland *et al.* (1990). It is recognised that there are considerable differences in chronostratigraphy between Harland *et al.* (1990) and other published schemes (e.g. Haq *et al.*, 1987) particularly for the pre-Permian stages and for the Tethyan basins in the Cretaceous/Jurassic. Where any doubt arises, the named stages should be referred to and the preferred chronostratigraphic calibration used.

Hydrocarbon reserves of basin (MMBOE): This gives estimated oil and gas reserves in millions of barrels oil equivalent. Unless indicated otherwise, these figures refer to the basin from which the samples were taken. These reserves are taken from the SPT (1992a) global basins study.

Hydrocarbon reserves attributable to source: This gives oil and gas reserves in millions of barrels of oil equivalent attributable to the source rock being studied. The data are taken from the SPT global source rock time slice study (SPT, 1992b).

Oil type (Tissot and Welte): This classifies the oil generated by the source rock as either paraffinic, paraffinic-naphthenic, naphthenic or aromatic after the classification of Tissot and Welte (1978). These data are taken from literature, the SPT database or information received from contributors.

Oil gravity (range; average) (°API) and **Sulphur content (range; average) (%)**: These data relate to the characteristics of the petroleum generated from the source rock. These data are taken from literature, the SPT database or information received from contributors.

Timing of hydrocarbon generation (Ma): This is an estimate of when the main phase or phases of oil generation took place. This information is taken from the literature or estimated from a knowledge of the subsidence history of the basin.

Bibliographic references: This lists a selection of the pertinent references used in the compilation of data for the source rock. The references are presented here in numerical form from the SPT literature references database and the full references are listed in Section II after the data sheets. This reference list is given twice, firstly sorted by geographic area (as are the source rocks) and ordered numerically within those geographic areas, secondly in alphabetical order.

b. Location map

The location map shows the geographic area in which the source rock is present and pin-points the location of the samples analysed for this study. The map also shows the limit of sedimentary basins or source rock outcrop. Basins not containing the source rock are also shown to help users of the manual see the relative positions of well known basins in the area. For a more definitive list of sedimentary basins containing a given source rock see the section 'Basin Setting of Source Rock'.

c. Generalised basin stratigraphy and geochemical log

This section shows the relative stratigraphic position of the source rock and attempts to relate gamma ray response, geochemical characteristics and lithology to each other. The stratigraphic section has a linear time scale (except where noted) using the scheme of Harland *et al.* (1990). The stratigraphic information is taken from The Robertson Group 'Stratigraphic database of major sedimentary basins of the World' (1990) or from other SPT data sources such as the various regional non-proprietary reports. The geochemical log is compiled from data taken from this report, other SPT data sources such as the various regional non-proprietary reports and the literature.

d. Geological setting of source rock

This section describes the depositional setting and some sedimentological and geochemical characteristics of the source rock. In general the properties reported here are considered on a basin wide scale.

Lithology: This is the main lithotype (e.g. shale, mudstone, siltstone, limestone, coal) of the source rock followed by any relevant qualifiers (e.g. laminated, bituminous, carbonaceous, calcareous, argillaceous).

Depositional environment: This classifies the source rock into one of three categories, marine, deltaic (organic matter is terrestrially sourced) or lacustrine. It is to be noted that in several instances (e.g. Tertiary Etolonskiy Horizon of West Kamchatka) the source rock may be dominated by terrestrial material but be deposited in proximal marine or lacustrine settings. In these instances it is the setting that is utilised.

Tectonic regime: This describes the tectonic regime at the time of deposition. The classification is taken from the SPT global source rock time slice study (SPT, 1992b) and classifications are defined in Figure 2.2 of this report.

Palaeolatitude: This is the latitude of the sedimentary basin at time of deposition of the source rock. These data are taken from the SPT global source rock time slice study (SPT, 1992b) which was assisted by SPT's subscription to the PALEOMAP project (Scotese, 1992).

Relative global sea level (m) or salinity: This gives the sea level at time of deposition for marine source rocks. These data are taken from Harland *et al.* (1990) which utilises the curves devised by Haq *et al.* (1987) and are quoted to the nearest 10m. For lacustrine source rocks this heading gives broadly classified salinity levels of the water body in the lake at the time of source rock deposition.

Basin morphology: This classifies the sedimentary basin at time of deposition as silled, continental shelf or inland drainage system. This information is taken from the SPT global source rock time slice study (SPT, 1992b).

Palaeoclimate: This classifies the atmospheric temperature at time of deposition as being hot, warm or cool and the moisture levels as being arid, seasonally wet or everwet. These data are derived from the SPT global source rock time slice study (1992b) which was assisted by the PALEOMAP data.

Carbonate/clastic dominance: This defines whether the dominant depositional system in the basin at time of source rock deposition was carbonate or clastic.

Mineral association: This gives secondary mineralogical information about the source rock sequence, e.g. carbonate, evaporite, phosphate, chert, stromatolite.

Lithologically homogeneous (Y/N): This indicates whether the source rock sequence is lithologically homogeneous or heterogeneous (e.g. generally continuous shale or interbedded sand/shale/siltstone).

Thickness (range; average) (m): This gives a range and average of the typical thickness of the source rock sequence in metres.

Radioactivity: This gives typical values for the total electric log gamma-ray response in the source rock unit. The units are usually gamma API units but, occasionally for source rocks from some of the Asian and East European countries and older wells (e.g. Canadian source rocks), other units, i.e. micro-roentgens per second, are reported.

TOC (range; average) (%) and **Pyrolysis hydrogen index (range; average)**: This gives typical values from these geochemical analyses for source rocks analysed throughout the basin.

Kerogen types: This defines the kerogen type of the source rock within the geochemical classification (e.g. I, II or III) followed by an organic petrographical classification reflecting the origin or characteristics of the organic matter), e.g. A (= algal), S (= amorphous sapropel), W (= waxy), V (= vitrinitic).

Maturity: This gives the thermal maturity reached by the source rock within the sedimentary basin as a range and average of the SCI and %VR.

Hydrocarbon generation: This estimates the residual potential to generate hydrocarbons and the amount of hydrocarbons already generated by the source rock in the basin and is frequently based upon the analysed sample. Residual potential is based upon average pyrolysis S2 yields (i.e. the ultimate yield of the source rock when it reaches post maturity). The amount of hydrocarbons generated to date is based upon pyrolysis data of sediments at their currently observed level of maturity. The model used to estimate these data is shown in Figure 2.3.

e. Analysed sample information

This section gives location details and analytical results for the sample that was chosen for detailed analysis. Certain information in this section, in particular basin name, sub-basin name and age (Ma) are taken from the 'Basin Setting of Source Rock' section.

Well/field sample name/number: This gives the name of the well or field section from which the sample was taken. In some cases this information is proprietary and the sample location is indicated as being confidential.

Location: This gives the co-ordinates of the sample in conventional latitude and longitude. The precision of these co-ordinates is variable from very high to rather low. In some instances co-ordinates were converted from other co-ordinate systems (e.g. domestic USA and Canadian or UTM) while in others they have been estimated from maps. The accuracy of location can be gauged from the apparent precision quoted. In some instances the equivalent co-ordinate system is quoted after the latitude and longitude in brackets.

Basin name and **Sub-basin name**: This gives the sedimentary basin from which the sample came. All basin and sub-basin names are defined by the SPT global basins study (SPT, 1992a).

Age (Ma): This gives the chronological age of the sample in millions of years before present and a stratigraphic age name. All ages follow the scheme of Harland *et al.* (1990).

Depth (m)/sample number: This specifies the depths or sample number for the sample selected for detailed analysis. Where the sample depth was originally measured in metres, the depth is quoted in metres. Where originally measured in feet it has been converted to metres and the original depths quoted after the converted depth in brackets.

TOC (%), Pyrolysis potential yield (kg/tonne) and **Pyrolysis hydrogen index**: These are the analytical results for the sample.

Kerogen (%) and type: This is the main component of the kerogen as a percentage, derived from transmitted light microscopy. The letter following the percentage is one of the following, A = algal origin, S = amorphous sapropel, W = waxy, V = vitrinitic.

Maturity: This is the level of thermal maturity of the sample based upon transmitted light microscopy (SCI) and reflected light microscopy (%VR).

Carbon isotope data (°/oo PDB): These are the results of carbon isotope analysis on four fractions of the sample extract. Results are expressed in parts per thousand (°/oo) relative to the PDB standard and are all negative values.

Pyrolysis-gas chromatography data: These are the measured results of pyrolysis-gas chromatography carried out on the extracted rock sample. The **% Area** column gives the area under the peaks following the NPD guidelines.

Summary

This section briefly expands on some of the data presented about the source rock and comments on the results from the analysed sample.

2.4.2.2 Sheet 2

Sheet 2 presents the analytical data generated by SPT from the source rock. The top data table 'Summary of Chemical Analysis' presents data from screening and maturity analyses. Some of the data on this table have originated from the previous SPT database (e.g. non-proprietary regional reports etc.), but at least one of the samples will have been analysed or re-analysed specifically for this project. The smaller data table 'Kerogen Type' shows a six component kerogen type derived from transmitted light microscopy analysis for this project. Underneath this table is a brief description of the environment of deposition derived from the transmitted light microscopy analysis. A detailed classification of the kerogen composition into 30 components is shown in Appendix 2. The chromatograms and fragmentograms presented on Sheet 2 are all for the sample that was selected for detailed analysis and the data are original to this manual. Explanations of the abbreviations used for peak identification are given in Appendices 5, 6 and 7.

2.4.2.3 Sheet 3

Sheet 3 presents numerical data related to individual compound peak size and calculated ratios from GC and GC-MS analyses.

The topmost data-table set lists GC-MS data and is divided into five columns.

- The first column, 'Ion fragment', gives the fragment ion from which the compound peak measurement was taken.
- The second column, 'Peak No.', assigns each quantified peak a number which is merely used as a reference for the definitions in the ratio tables below. These peak numbers are not used for labelling of peaks on the fragmentograms.
- The third column, 'Peak name', shows the abbreviated peak identifications that are used to label the fragmentograms and these are explained in Appendices 6 and 7.
- The fourth column, 'Peak height, counts', shows the peak heights which were measured as per NPD guidelines. Compounds that were not quantified but identified as present are marked with a 'P'.
- Column five, 'Relative compound abundance', shows the relative concentrations of the peak, which have been calculated using a coinjected deuterated cholestane internal standard. A suitable internal standard was not used in the aromatic fraction and therefore there are no data in column five for the aromatic compounds.

The middle set of three tables shows GC-MS biomarker ratios generated from the data above. Each ratio is defined using the abbreviated compound peak name and the definition is repeated using the peak number for ease of reference.

The bottom set of data tables show data derived from alkane and aromatic fraction gas chromatography using an FID detector. The definitions of the alkane GC ratios are given in Appendix 4. Methylphenanthrene data were abstracted from the aromatic GC rather than the GC-MS data.

2.4.2.4 Sheet 4

Sheet 4 presents the GC-MS fragmentograms from the alkane and aromatic fractions. Peak labels are explained in Appendices 6 and 7. The selection of fragmentograms is intended to provide traces for the most commonly used ions and where necessary to illustrate the presence of diagnostic or particular individual biomarkers e.g. ß-carotane.

2.5 ACKNOWLEDGEMENTS

Although the majority of samples and analytical data used in this study come from SPT's own sample collection and non-proprietary database, some samples and information were also provided by our contacts and associates. SPT would like to express its gratitude to the following individuals and organisations who made contributions of sample material, analytical data or geological information.

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- Dr R Parmely, Gas Research Institute, Chicago, USA
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- Repsol Exploracion, Madrid, Spain
- United States Geological Survey, Denver, USA

We should also like to thank the many colleagues outside and within SPT who have given their time to provide useful information and helpful discussion which have enhanced this study.

2.6 PERSONNEL INVOLVED IN STUDY

The following SPT personnel were involved in the production of this report:

Colin Darlington	-	Project manager
Patrick Barnard	-	Database co-ordinator
Sandra Martin and Andrew Home	-	Data compilation
Rick Harding	-	Microscopy
Jim Fenton	-	Co-ordinator of biostratigraphy
Martin Wadsworth	-	Co-ordinator of analysis

Appendix 3

Index of Alkane Molecular Biomarker

Gas Chromatography-Mass Spectrometry Peak Assignments

STERANES

5β(H)14α(H)17α(H) and 5α(H)14α(H)17α(H) C_{27}, C_{28} and C_{29} regular (normal) steranes and 5α(H)14β(H)17β(H) C_{27}, C_{28} and C_{29} isosteranes

Peak	Assignment	NPD Codes
S27a	C_{27} 5β(H)14α(H)17α(H) 20R cholestane	
S27c	C_{27} 5α(H)14α(H)17α(H) 20S cholestane	27ααS
S27d	C_{27} 5α(H)14β(H)17β(H) 20R isocholestane	27ββR
S27e	C_{27} 5α(H)14β(H)17β(H) 20S isocholestane	27ββS
S27b	C_{27} 5α(H)14α(H)17α(H) 20R cholestane	27ααR
S28a	C_{28} 24-methyl-5β(H)14α(H)17α(H) 20R cholestane	
S28c	C_{28} 24-methyl-5α(H)14α(H)17α(H) 20S cholestane	28ααS
S28d	C_{28} 24-methyl-5α(H)14β(H)17β(H) 20R isocholestane	28ββR
S28e	C_{28} 24-methyl-5α(H)14β(H)17β(H) 20S isocholestane	28ββS
S28b	C_{28} 24-methyl-5α(H)14α(H)17α(H) 20R cholestane	28ααR
S29a	C_{29} 24-ethyl-5β(H)14α(H)17α(H) 20R cholestane	
S29c	C_{29} 24-ethyl-5α(H)14α(H)17α(H) 20S cholestane	29ααS
S29d	C_{29} 24-ethyl-5α(H)14β(H)17β(H) 20R isocholestane	29ββR
S29e	C_{29} 24-ethyl-5α(H)14β(H)17β(H) 20S isocholestane	29ββS
S29b	C_{29} 24-ethyl-5α(H)14α(H)17α(H) 20R cholestane	20ααR

Configurations:

a 5β(H)14α(H)17α(H) 20R (immature or biological configuration)
b 5α(H)14α(H)17α(H) 20R (regular or normal sterane)
c 5α(H)14α(H)17α(H) 20S (regular or normal sterane)
d 5α(H)14β(H)17β(H) 20R (isosterane)
e 5α(H)14β(H)17β(H) 20S (isosterane)

Notes:

All steranes listed are likely to be 24R and 24S epimers which cannot be separated with the chromatography conditions used.

The elution sequence of normal and isosteranes for each of the C_{27}, C_{28} and C_{29} groups is as shown in the above listing: 5α(H)14α(H)17α(H) 20S, 5α(H)14β(H)17β(H) 20R, 5α(H)14β(H)17β(H) 20S, 5α(H)14α(H)17α(H) 20R. The C_{27}, C_{28} and C_{29}

5β(H)14α(H)17α(H) 20R steranes approximately coelute with the respective C_{27}, C_{28} and C_{29} 5α(H)14β(H)17β(H) 20R isosteranes. The order of thermal stability of the steranes is 5α(H) > 5β(H), 5α(H) 20S > 5α(H) 20R and 14β(H)17β(H) > 14α(H)17α(H).

4-desmethylsteranes have been identified and are considered to be biological markers for marine organic material; however, these compounds cannot be differentiated from C_{30} 4-methylsteranes without metastable ion monitoring (GC-MS-MS). C_{30} 4-desmethylsteranes occur with 5α(H)14α(H)17α(H) 20R and 20S and 5α(H)14β(H)17β(H) 20R and 20S (isosterane) configurations. C_{26} steranes have also been identified (Shi Ji-Yang *et al.*, 1982) but are rare.

METHYLSTERANES

4α(H) and 4β(H) C_{28}, C_{29} and C_{30} methylsteranes

Peak	Assignment
ms28d	C_{28} 4α(H)-methyl-5α(H)14α(H)17α(H) 20S cholestane
ms28b	C_{28} 4α(H)-methyl-5β(H)14α(H)17α(H) 20R cholestane
ms28e	C_{28} 4α(H)-methyl-5α(H)14β(H)17β(H) 20R cholestane
ms28f	C_{28} 4α(H)-methyl-5α(H)14β(H)17β(H) 20S cholestane
ms28c	C_{28} 4α(H)-methyl-5α(H)14α(H)17α(H) 20R cholestane
ms28a	C_{28} 4β(H)-methyl-5α(H)14α(H)17α(H) 20R cholestane
ms29d	C_{29} 4α(H)-methyl-5α(H)14α(H)17α(H) 20S methylcholestane
ms29b	C_{29} 4α(H)-methyl-5β(H)14α(H)17α(H) 20R methylcholestane
ms29e	C_{29} 4α(H)-methyl-5α(H)14β(H)17β(H) 20R methylcholestane
ms29f	C_{29} 4α(H)-methyl-5α(H)14β(H)17β(H) 20S methylcholestane
ms29c	C_{29} 4α(H)-methyl-5α(H)14α(H)17α(H) 20R methylcholestane
ms29a	C_{29} 4β(H)-methyl-5α(H)14α(H)17α(H) 20R methylcholestane
ms30d	C_{30} 4α(H)-methyl-5α(H)14α(H)17α(H) 20S ethylcholestane
ms30b	C_{30} 4α(H)-methyl-5β(H)14α(H)17α(H) 20R ethylcholestane
ms30e	C_{30} 4α(H)-methyl-5α(H)14β(H)17β(H) 20R ethylcholestane
ms30f	C_{30} 4α(H)-methyl-5α(H)14β(H)17β(H) 20S ethylcholestane
ms30c	C_{30} 4α(H)-methyl-5α(H)14α(H)17α(H) 20R ethylcholestane
ms30a	C_{30} 4β(H)-methyl-5α(H)14α(H)17α(H) 20R ethylcholestane

Configurations:

a 4β(H)5α(H)14α(H)17α(H) 20R (immature)
b 4α(H)5β(H)14α(H)17α(H) 20R (immature)
c 4α(H)5α(H)14α(H)17α(H) 20R (regular or normal methylsterane)
d 4α(H)5α(H)14α(H)17α(H) 20S (regular or normal methylsterane)
e 4α(H)5α(H)14β(H)17β(H) 20R (isomethylsterane)
f 4α(H)5α(H)14β(H)17β(H) 20S (isomethylsterane)

Notes:

The full stereochemistry of the methylsteranes, that is, either the 23,24-dimethyl (dinosterane) or the 24-ethyl configuration, cannot be determined without full scan GC-MS analysis and examination of mass spectra. Mass spectra of 23,24-dimethylsteranes (dinosteranes) show a significant ion at m/e 198 (Goodwin *et al.*, 1988). The elution sequence of the C_{28}, C_{29} and C_{30} 4-methyl-14α(H)17α(H) 20R steranes is 4α(H)5β(H), 4α(H)5α(H) and 4β(H)5α(H). In synthetic mixtures of 4-methylsteranes, the 4β(H)5β(H) isomer elutes between the 4α(H)5β(H) and 4α(H)5α(H) (Goodwin *et al.*, 1988), but does not appear to occur naturally.

The order of thermal stability of the naturally occurring 4-methylsteranes is 4α(H) > 4β(H) and 4α(H)5α(H) > 4α(H)5β(H) (Wolff *et al.*, 1986). The elution sequence of 4α(H)-methyl-5α(H)14α(H)17α(H) and 4α(H)-methyl-5α(H)14β(H)17β(H) steranes for each of the C_{27}, C_{28} and C_{29} groups is similar to the desmethyl steranes and is as shown in the above listing: 4α(H)-methyl-5α(H)14α(H)17α(H) 20S, 4α(H)-methyl-5α(H)14β(H)17β(H) 20R,

4α(H)-methyl-5α(H)14β(H)17β(H) 20S, 4α(H)-methyl-5α(H)14α(H)17α(H) 20R. The order of thermal stability is presumed to be comparable to the desmethyl steranes.

Compounds identified as methylsteranes, but substituted at a position other than at C-4 on the A-ring, have been reported (Fowler and Douglas, 1987; Summons and Powell, 1987; Summons *et al.*, 1987) but appear to be rare.

REARRANGED STERANES (DIASTERANES)

13β(H)17α(H) and 13α(H)17β(H) C_{27}, C_{28} and C_{29} rearranged steranes

Peak	Assignment	NPD Codes
r27d	C_{27} 13β(H)17α(H) 20S diacholestane	27dβS
r27c	C_{27} 13β(H)17α(H) 20R diacholestane	27dβR
r27b	C_{27} 13α(H)17β(H) 20S diacholestane	27dαS
r27a	C_{27} 13α(H)17β(H) 20R diacholestane	27dαR
r28d	C_{28} 24-methyl-13β(H)17α(H) 20S diacholestane	28dβS
r28c	C_{28} 24-methyl-13β(H)17α(H) 20R diacholestane	28dβR
r28b	C_{28} 24-methyl-13α(H)17β(H) 20S diacholestane	28dαS
r28a	C_{28} 24-methyl-13α(H)17β(H) 20R diacholestane	28dαR
r29d	C_{29} 24-ethyl-13β(H)17α(H) 20S diacholestane	29dβS
r29c	C_{29} 24-ethyl-13β(H)17α(H) 20R diacholestane	29dβR
r29b	C_{29} 24-ethyl-13α(H)17β(H) 20S diacholestane	29dαS
r29a	C_{29} 24-ethyl-13α(H)17β(H) 20R diacholestane	29dαR

Configurations:

a 13α(H)17β(H) 20R
b 13α(H)17β(H) 20S
c 13β(H)17α(H) 20R
d 13β(H)17α(H) 20S

Notes:

All rearranged steranes listed are likely to be 24R and 24S epimers which, with the exception of C_{28} 24-methyl-13β(H)17α(H) diacholestanes, cannot normally be separated with the chromatography conditions used.

The C_{29} 24-ethyl-13β(H)17α(H) 20S diacholestane co-elutes with the C_{27} 5α(H)14β(H)17β(H) 20R isocholestane and the C_{29} 24-ethyl-13α(H)17β(H) 20R diacholestane co-elutes with the C_{28} 24-methyl-5α(H)14β(H)17β(H) 20R isocholestane under normal chromatography conditions. The 13α(H)17β(H) configuration is less thermally stable than 13β(H)17α(H).

C_{30} rearranged steranes also occur, with 13β(H)17α(H) 20R and 20S and 13α(H)17β(H) 20R and 20S configurations.

BICYCLIC SESQUITERPANES

Peak	Assignment
DM	8β(H)-drimane
HD	8β(H)-homodrimane
ED	4β(H)-eudesmane

TRICYCLIC TERPANES

Peak	Assignment	NPD Codes
t19	C_{19} tricyclic terpane	
t20	C_{20} tricyclic terpane	
t21	C_{21} tricyclic terpane	
t22	C_{22} tricyclic terpane	
t23	C_{23} tricyclic terpane	23/3
t24	C_{24} tricyclic terpane	24/3
t25	C_{25} tricyclic terpane	25/3
t26	C_{26} tricyclic terpanes	26/3
t27	C_{27} tricyclic terpanes	
t28	C_{28} tricyclic terpanes	
t29	C_{29} tricyclic terpanes	
t30	C_{30} tricyclic terpanes	

Notes:

C_{26}, C_{28}, C_{29} and C_{30} tricyclic terpanes occur as isomeric (at C-22) C_{22} and C_{27} tricyclic terpanes are generally less abundant, suggesting branching at these positions. Tricyclic terpanes of higher molecular weight, up to C_{40} and higher, have been identified (Moldowan *et al.*, 1983), but are unusual. Mello *et al.* (1988) identified C_{31}, C_{33}, C_{34} and C_{35} tricyclic terpanes in Brazilian oils.

TETRACYCLIC TERPANES

Seco-17,21-hopanes

Peak	Assignment	NPD Code
T24	C_{24} tetracyclic terpane	24/4
T26	C_{26} tetracyclic terpane	

Notes:

The tetracyclic terpanes are hopane related compounds and have the structure seco-17,21-hopane.

PENTACYCLIC TRITERPANES

C_{27} and C_{29} to C_{35} 17α(H)21β(H) and 17β(H)21β(H) hopane and 17β(H)21α(H) moretane series.

C_{27} and C_{29} to C_{35} 17α(H)21β(H) hopane series:

Peak	Assignment	NPD Codes
h27s	C_{27} 18α(H)-22,29,30-trisnorneohopane (T_s)	27Ts
h27m	C_{27} 17α(H)-trisnorhopane (T_m)	27Tm
h29	C_{29} 17α(H)21β(H)-30-norhopane	29αβ
h30	C_{30} 17α(H)21β(H)-30-hopane	30αβ
h31S	C_{31} 17α(H)21β(H)-30,31-homohopane 22S	31αβS
h31R	C_{31} 17α(H)21β(H)-30,31-homohopane 22R	31αβR
h32S	C_{32} 17α(H)21β(H)-30,31-bishomohopane 22S	32αβS
h32R	C_{32} 17α(H)21β(H)-30,31-bishomohopane 22R	32αβR
h33S	C_{33} 17α(H)21β(H)-30,31-trishomohopane 22S	33αβS
h33R	C_{33} 17α(H)21β(H)-30,31-trishomohopane 22R	33αβR
h34S	C_{34} 17α(H)21β(H)-30,31-tetrakishomohopane 22S	34αβS
h34R	C_{34} 17α(H)21β(H)-30,31-tetrakishomohopane 22R	34αβR
h35S	C_{35} 17α(H)21β(H)-30,31-pentakishomohopane 22S	35αβS
h35R	C_{35} 17α(H)21β(H)-30,31-pentakishomohopane 22R	35αβR

C_{27} and C_{29} to C_{35} 17β(H)21α(H) moretane series

Peak	Assignment	NPD Codes
m29	C_{29} 17β(H)21α(H)-30-normoretane	29βα
m30	C_{30} 17β(H)21α(H)-30-moretane	30βα
m31	C_{31} 17β(H)21α(H)-homomoretane	
m32	C_{32} 17β(H)21α(H)-bishomomoretane	

C_{27} 17β(H) and C_{29} to C_{35} 17β(H)21β(H) hopane series

Peak	Assignment
b27	C_{27} 17β(H) trisnorhopane
b29	C_{29} 17β(H)21β(H) norhopane 22R
b30	C_{30} 17β(H)21β(H) hopane 22R
b31	C_{31} 17β(H)21β(H) homohopane 22R
b32	C_{32} 17β(H)21β(H)-30,31-bishomohopane 22R
b33	C_{33} 17β(H)21β(H)-30,31-trishomohopane 22R
b34	C_{34} 17β(H)21β(H)-30,31-tetrakishomohopane 22R
b35	C_{35} 17β(H)21β(H)-30,31-pentakishomohopane 22R

Notes:

The C_{29} to C_{35} pentacyclic triterpane (hopane) series of compounds have been identified with 17α(H)21β(H) (hopane), 17β(H)21α(H) (moretane) and 17β(H)21β(H) (hopane) configurations. C_{27} trisnorhopanes have no side-chain at C-21 and have either the 17α(H) or 17β(H) configuration, the former being the more thermally stable and the latter form generally present in immature samples only. The C_{27} 18α(H)-trisnorneohopane (T_s) is more thermally stable than C_{27} 17α(H)-trisnorhopane (T_m). 3-methylhopanes are rarely present and may be detected by use of m/e 205 mass chromatograms (McEvoy and Giger, 1986).

UNSATURATED PENTACYCLIC TRITERPENOIDS

Peak	Assignment
uh1	C_{27} 22,29,30-trisnorneohop-13(18)-ene
uh2	C_{27} trisnorhop-17-ene
uh3	C_{29} norhop-17(21)-ene
uh4	C_{29} 30-neonor-13(18)-ene
uh5	C_{30} hop-17(21)-ene
uh6	C_{30} neohop-13(18)-ene
uh7	C_{31} homohop-17(21)-ene (22R and 22S)

Notes:

Unsaturated pentacyclic compounds usually occur only in thermally immature samples.

OTHER PENTACYCLIC TRITERPENOIDS

Peak	Assignment	NPD Codes
T	C_{27} 17α(H)18α(H)21β(H)-25,28,30-trisnorhopane	25 nor 28αβ
Tm	C_{27} 17β(H)18α(H)21α(H)-25,28,30-trisnormoretane	
B	C_{28} 17α(H)18α(H)21β(H)-28,30-bisnorhopane	28αβ
Bnm	C_{28} 17β(H)18α(H)21α(H)-28,30-bisnormoretane	
G	C_{30} gammacerane	30G
O	C_{30} 18α(H) oleanane	30O
J	C_{30} 18β(H) oleanane ('compound J')	
L	C_{30} lupane	
BL	C_{28} bisnorlupane	
d28	C_{28} diahopane	
X	C_{30} diahopane	30d

Notes:

The C_{30} 18α(H) oleanane and 18β(H) oleanane (formerly 'compound J' of Grantham *et al.*, 1983) coelute on standard GC columns. The 18β(H) oleanane is less thermally stable than 18α(H) oleanane (Riva *et al.*, 1988).

The C_{30} and C_{28} diahopanes were formerly identified as the structurally elucidated pentacyclic triterpanes X and Y, respectively, of Philp and Gilbert (1986).

DEMETHYLATED HOPANES AND DEMETHYLATED MORETANES

C_{26} and C_{28} to C_{34} 17α(H)21β(H)-25-norhopanes and 17β(H)21α(H)-25-normoretanes

Peak	Assignment	NPD Codes
dh26S	C_{26} 18α(H)-22,25,29,30-tetrakisnorneohopane	
dh26m	C_{26} 17α(H)-22,25,28,30-tetrakisnorhopane	
dh28	C_{28} 17α(H)21β(H)-25,30-bisnorhopane	
dm28	C_{28} 17β(H)21α(H)-25,30-bisnormoretane	
dh29	C_{29} 17α(H)21β(H)-25-norhopane	25nor30αβ
dm29	C_{29} 17β(H)21α(H)-25-normoretane	
dh30S	C_{30} 17α(H)21β(H)-25-norhomohopane 22S	
dh30R	C_{30} 17α(H)21β(H)-25-norhomohopane 22R	
dh31S	C_{31} 17α(H)21β(H)-25-norbishomohopane 22S	
dh31R	C_{31} 17β(H)21β(H)-25-norbishomohopane 22R	
dh32S	C_{32} 17α(H)21β(H)-25-nortrishomohopane 22S	
dh32R	C_{32} 17α(H)21β(H)-25-nortrishomohopane 22R	
dh33S	C_{33} 17α(H)21β(H)-25-nortetrakishomohopane 22S	
dh33R	C_{33} 17α(H)21β(H)-25-nortetrakishomohopane 22R	
dh34S	C_{34} 17α(H)21β(H)-25-norpentakishomohopane 22S	
dh34R	C_{34} 17α(H)21β(H)-25-norpentakishomohopane 22R	

Notes:

Nuclear demethylated hopanes are biological markers for severe bacterial degradation (Volkman *et al.*, 1983a and b). Demethylation involves the loss of the C-25 methyl group from the C-10 position on the A-ring (Rullkotter and Wendisch, 1982).

DEMETHYLATED TRICYCLIC TERPANES

Peak	Assignment
dt18	C_{18} tricyclic terpane
dt19	C_{19} tricyclic terpane
dt20	C_{20} tricyclic terpane
dt21	C_{21} tricyclic terpane
dt22	C_{22} tricyclic terpane
dt23	C_{23} tricyclic terpane
dt24	C_{24} tricyclic terpane
dt25	C_{25} tricyclic terpanes
dt26	C_{26} tricyclic terpanes
dt27	C_{27} tricyclic terpanes
dt28	C_{28} tricyclic terpanes
dt29	C_{29} tricyclic terpanes

Notes:

These compounds are relatively unusual and are indicative of the severest levels of biodegradation (Howell *et al.*, 1984). C_{25}, C_{27}, C_{28} and C_{29} demethylated tricyclic terpanes occur as isomeric (at C-22) pairs.

SECOHOPANES

Seco-8,14-hopanes

Peak	Assignment
sh1	C_{27} seco-8,14-hopane
sh2	C_{29} seco-8,14-hopane
sh3	C_{30} seco-8,14-hopane

Notes:

Tetracyclic terpanes in degraded oil stains from the Morondava Basin of Madagascar have been identified as Ring-C opened seco-8,14-hopanes by Rullkotter and Wendisch (1982). Stereochemistry at C-8 and C-14 gives rise to several isomers and higher and lower carbon numbers may also be present. Minor amounts of secohopanes were detected in Brazilian oils by Mello *et al.* (1988).

OTHER COMPOUNDS

Peak	Assignment
BC	C_{34} botryococcane
S	C_{30} squalane
βC	β-carotane
γC	γ-carotane

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Appendix 4

Index of Aromatic Molecular Biomarker

Gas Chromatography-Mass Spectrometry Peak Assignments

SUBSTITUTED NAPHTHALENES

Methylnaphthalenes

Peak	**Assignment**
2MN	2-methylnaphthalene
1MN	1-methylnaphthalene

Ethylnaphthalenes

Peak	**Assignment**
2EN	2-ethylnaphthalene
1EN	1-ethylnaphthalene

Dimethylnaphthalenes

Peak	**Assignment**
26DMN	2,6-dimethylnaphthalene
27DMN	2,7-dimethylnaphthalene
13DMN	1,3-dimethylnaphthalene
17DMN	1,7-dimethylnaphthalene
16DMN	1,6-dimethylnaphthalene
23DMN	2,3-dimethylnaphthalene
14DMN	1,4-dimethylnaphthalene
15DMN	1,5-dimethylnaphthalene
12DMN	1,2-dimethylnaphthalene

Notes:

Methylnaphthalene and ethylnaphthalene isomers identified after Volkman *et al.* (1984). Dimethylnaphthalene isomers identified after Volkman *et al.* (1984), Hall *et al.* (1985), Radke *et al.* (1986) and Rowland *et al.* (1986).

Trimethylnaphthalenes

Peak	**Assignment**
137TMN	1,3,7-trimethylnaphthalene
136TMN	1,3,6-trimethylnaphthalene
146TMN	1,4,6-trimethylnaphthalene
135TMN	1,3,5-trimethylnaphthalene
236TMN	2,3,6-trimethylnaphthalene
127TMN	1,2,7-trimethylnaphthalene
167TMN	1,6,7-trimethylnaphthalene
126TMN	1,2,6-trimethylnaphthalene
124TMN	1,2,4-trimethylnaphthalene
125TMN	1,2,5-trimethylnaphthalene

Notes:

Trimethylnaphthalene isomers identified after Rowland *et al.* (1986) and Strachan *et al.* (1988). Heating rate effects on dimethylnaphthalene and trimethylnaphthalene maturity parameters are discussed in Alexander *et al.* (1986).

PHENANTHRENE AND SUBSTITUTED PHENANTHRENES

Peak	Assignment
P	phenanthrene
3MP	3-methylphenanthrene
2MP	2-methylphenanthrene
9MP	9-methylphenanthrene
1MP	1-methylphenanthrene
DMP	dimethylphenanthrene
TMP	trimethylphenanthrene

Notes:

Methylphenanthrene maturation parameters, and empirical correlations with vitrinite reflectance, are discussed by Radke and Welte (1983), Radke *et al.* (1984, 1986), Kvalheim *et al.* (1987), Boreham *et al.* (1988) and Radke (1988). Ethylphenanthrene and dimethylphenanthrene isomers are identified by Radke *et al.* (1986).

MONOAROMATIC STEROIDS (C-ring)

Peak	Assignment	NPD Codes
MAS21	C_{21} monoaromatic steroid	A1
MAS22	C_{22} monoaromatic steroid	B1
MAS27	C_{27} monoaromatic steroid	D1
MAS29β28α	$5\beta(H)C_{29}$ + $5\alpha(H)C_{28}$ monoaromatic steroid (20R)	H1 I1
MAS29α	$5\alpha(H)C_{29}$ monoaromatic steroid (20R)	

TRIAROMATIC STEROIDS

Peak	Assignment	NPD Codes
TAS20	C_{20} triaromatic steroid	a1
TAS21	C_{21} triaromatic steroid	b1
TAS26S	C_{26} triaromatic steroid 20S	c1
TAS26R	C_{26} triaromatic steroid 20R	d1
TAS27S	C_{27} triaromatic steroid 20S	
TAS27R	C_{27} triaromatic steroid 20R	f1
TAS28S	C_{28} triaromatic steroid 20S	e1
TAS28R	C_{28} triaromatic steroid 20R	g1

Notes:

Identification of monoaromatic and triaromatic steroids from Mackenzie *et al.* (1981), Seifert *et al.* (1983), Wardroper *et al.* (1984), Killops and Readman (1985), Riolo *et al.* (1986) and Williams *et al.* (1986).

THIOPHENIC-SULPHUR COMPOUNDS

Peak	Assignment
2BT	C_2-benzothiophene
3BT	C_3-benzothiophene
4BT	C_4-benzothiophene
DBT	dibenzothiophene
4MDBT	4-methyldibenzothiophene
3MDBT	3-methyldibenzothiophene
2MDBT	2-methyldibenzothiophene
1MDBT	1-methyldibenzothiophene
DMDBT	dimethyldibenzothiopenes
TMDBT	trimethyldibenzothiophenes
BNT	benzonaphthothiophenes

Notes:

2-methyldibenzothiophene and 3-methyldibenzothiophene coelute. See Hughes (1983), Leythauser *et al.* (1988) and Schou and Myhr (1988) for identification and significance of benzothiophenes, dibenzothiophene and substituted dibenzothiophenes.

OTHER AROMATIC COMPOUNDS

Peak	Assignment
A	Anthracene
MA	Methylanthracene
F	Fluorene
MF	Methylfluorene
C	Chrysene
MC	Methylchrysene
PY	Pyrene
MPY	Methylpyrene
Ca	Cadalene (1,6-dimethyl-4-isopropylnaphthalene)
Eu	Eudalene (1-methyl-7-isopropylnaphthalene)
BH	Benzohopanes
MBH	Methylbenzohopanes

Notes:

For benzohopane identification see Belayouni and Trichet (1984) and Hussler *et al.* (1984).

Methylanthracene identified in Williams *et al.* (1986).

Appendix 6

Gas Chromatogram Peak Assignments

ALKANE GAS CHROMATOGRAMS

n-alkanes

n-C_{10-36} homologous series of normal alkanes, identified within the carbon number range 10 to 36

isoprenoids

i-C_{15}	Farnesane
i-C_{16}	
i-C_{18}	Norpristane
Pr	Pristane
Ph	Phytane

AROMATIC GAS CHROMATOGRAMS (AND AROMATIC GC-MS RIC)

MN	Methylnaphthalenes
Bip	Biphenyl
EN	Ethyl naphthalenes
DMN	Dimethylnaphthalenes
TMN	Trimethylnaphthalenes
DBT	Dibenzothophene
P	Phenanthrene
MDBT	Methyldibenzothiophene
IS	Internal standard
MP	Methylphenanthrenes
DMP	Dimethylphenanthrenes
MAS	Monoaromatic steroids
TAS	Triaromatic steroids

PYROLYSIS GAS CHROMATOGRAMS

6,7,8,9,10,15,20,25: Homologous series of the n-alkane/n-alkane doublets, where the number refers to the number of carbon atoms in the molecule.

B	Benzene
T	Toluene
X	Xylenes (ortho-, meta- and para-)