

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 exist.

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<sup>2</sup>):** 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 ( $^{\circ}/_{\infty}$  PDB):** These are the results of carbon isotope analysis on four fractions of the sample extract. Results are expressed in parts per thousand ( $^{\circ}/_{\infty}$ ) 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 co-injected 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. B-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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- 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

$5\beta(\text{H})14\alpha(\text{H})17\alpha(\text{H})$  and  $5\alpha(\text{H})14\alpha(\text{H})17\alpha(\text{H})$   $\text{C}_{27}$ ,  $\text{C}_{28}$  and  $\text{C}_{29}$  regular (normal) steranes and  $5\alpha(\text{H})14\beta(\text{H})17\beta(\text{H})$   $\text{C}_{27}$ ,  $\text{C}_{28}$  and  $\text{C}_{29}$  isosteranes

Peak	Assignment	NPD Codes
S27a	$\text{C}_{27}$ $5\beta(\text{H})14\alpha(\text{H})17\alpha(\text{H})$ 20R cholestane	
S27c	$\text{C}_{27}$ $5\alpha(\text{H})14\alpha(\text{H})17\alpha(\text{H})$ 20S cholestane	27 $\alpha\alpha$ S
S27d	$\text{C}_{27}$ $5\alpha(\text{H})14\beta(\text{H})17\beta(\text{H})$ 20R isocholestane	27BBR
S27e	$\text{C}_{27}$ $5\alpha(\text{H})14\beta(\text{H})17\beta(\text{H})$ 20S isocholestane	27BBS
S27b	$\text{C}_{27}$ $5\alpha(\text{H})14\alpha(\text{H})17\alpha(\text{H})$ 20R cholestane	27 $\alpha\alpha$ R
S28a	$\text{C}_{28}$ 24-methyl- $5\beta(\text{H})14\alpha(\text{H})17\alpha(\text{H})$ 20R cholestane	
S28c	$\text{C}_{28}$ 24-methyl- $5\alpha(\text{H})14\alpha(\text{H})17\alpha(\text{H})$ 20S cholestane	28 $\alpha\alpha$ S
S28d	$\text{C}_{28}$ 24-methyl- $5\alpha(\text{H})14\beta(\text{H})17\beta(\text{H})$ 20R isocholestane	28BBR
S28e	$\text{C}_{28}$ 24-methyl- $5\alpha(\text{H})14\beta(\text{H})17\beta(\text{H})$ 20S isocholestane	28BBS
S28b	$\text{C}_{28}$ 24-methyl- $5\alpha(\text{H})14\alpha(\text{H})17\alpha(\text{H})$ 20R cholestane	28 $\alpha\alpha$ R
S29a	$\text{C}_{29}$ 24-ethyl- $5\beta(\text{H})14\alpha(\text{H})17\alpha(\text{H})$ 20R cholestane	
S29c	$\text{C}_{29}$ 24-ethyl- $5\alpha(\text{H})14\alpha(\text{H})17\alpha(\text{H})$ 20S cholestane	29 $\alpha\alpha$ S
S29d	$\text{C}_{29}$ 24-ethyl- $5\alpha(\text{H})14\beta(\text{H})17\beta(\text{H})$ 20R isocholestane	29BBR
S29e	$\text{C}_{29}$ 24-ethyl- $5\alpha(\text{H})14\beta(\text{H})17\beta(\text{H})$ 20S isocholestane	29BBS
S29b	$\text{C}_{29}$ 24-ethyl- $5\alpha(\text{H})14\alpha(\text{H})17\alpha(\text{H})$ 20R cholestane	20 $\alpha\alpha$ R

#### Configurations:

- a  $5\beta(\text{H})14\alpha(\text{H})17\alpha(\text{H})$  20R (immature or biological configuration)
- b  $5\alpha(\text{H})14\alpha(\text{H})17\alpha(\text{H})$  20R (regular or normal sterane)
- c  $5\alpha(\text{H})14\alpha(\text{H})17\alpha(\text{H})$  20S (regular or normal sterane)
- d  $5\alpha(\text{H})14\beta(\text{H})17\beta(\text{H})$  20R (isosterane)
- e  $5\alpha(\text{H})14\beta(\text{H})17\beta(\text{H})$  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  $\text{C}_{27}$ ,  $\text{C}_{28}$  and  $\text{C}_{29}$  groups is as shown in the above listing:  $5\alpha(\text{H})14\alpha(\text{H})17\alpha(\text{H})$  20S,  $5\alpha(\text{H})14\beta(\text{H})17\beta(\text{H})$  20R,  $5\alpha(\text{H})14\beta(\text{H})17\beta(\text{H})$  20S,  $5\alpha(\text{H})14\alpha(\text{H})17\alpha(\text{H})$  20R. The  $\text{C}_{27}$ ,  $\text{C}_{28}$  and  $\text{C}_{29}$

5 $\beta$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R steranes approximately coelute with the respective C<sub>27</sub>, C<sub>28</sub> and C<sub>29</sub> 5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) 20R isosteranes. The order of thermal stability of the steranes is 5 $\alpha$ (H) > 5 $\beta$ (H), 5 $\alpha$ (H) 20S > 5 $\alpha$ (H) 20R and 14 $\beta$ (H)17 $\beta$ (H) > 14 $\alpha$ (H)17 $\alpha$ (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<sub>30</sub> 4-methylsteranes without metastable ion monitoring (GC-MS-MS). C<sub>30</sub> 4-desmethylsteranes occur with 5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R and 20S and 5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) 20R and 20S (isosterane) configurations. C<sub>26</sub> steranes have also been identified (Shi Ji-Yang *et al.*, 1982) but are rare.

**METHYLSTERANES**

4 $\alpha$ (H) and 4 $\beta$ (H) C<sub>28</sub>, C<sub>29</sub> and C<sub>30</sub> methylsteranes

Peak	Assignment
ms28d	C <sub>28</sub> 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20S cholestane
ms28b	C <sub>28</sub> 4 $\alpha$ (H)-methyl-5 $\beta$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R cholestane
ms28e	C <sub>28</sub> 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) 20R cholestane
ms28f	C <sub>28</sub> 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) 20S cholestane
ms28c	C <sub>28</sub> 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R cholestane
ms28a	C <sub>28</sub> 4 $\beta$ (H)-methyl-5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R cholestane
ms29d	C <sub>29</sub> 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20S methylcholestane
ms29b	C <sub>29</sub> 4 $\alpha$ (H)-methyl-5 $\beta$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R methylcholestane
ms29e	C <sub>29</sub> 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) 20R methylcholestane
ms29f	C <sub>29</sub> 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) 20S methylcholestane
ms29c	C <sub>29</sub> 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R methylcholestane
ms29a	C <sub>29</sub> 4 $\beta$ (H)-methyl-5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R methylcholestane
ms30d	C <sub>30</sub> 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20S ethylcholestane
ms30b	C <sub>30</sub> 4 $\alpha$ (H)-methyl-5 $\beta$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R ethylcholestane
ms30e	C <sub>30</sub> 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) 20R ethylcholestane
ms30f	C <sub>30</sub> 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) 20S ethylcholestane
ms30c	C <sub>30</sub> 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R ethylcholestane
ms30a	C <sub>30</sub> 4 $\beta$ (H)-methyl-5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R ethylcholestane

**Configurations:**

- a 4 $\beta$ (H)5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R (immature)
- b 4 $\alpha$ (H)5 $\beta$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R (immature)
- c 4 $\alpha$ (H)5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20R (regular or normal methylsterane)
- d 4 $\alpha$ (H)5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20S (regular or normal methylsterane)
- e 4 $\alpha$ (H)5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) 20R (isomethylsterane)
- f 4 $\alpha$ (H)5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (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<sub>28</sub>, C<sub>29</sub> and C<sub>30</sub> 4-methyl-14 $\alpha$ (H)17 $\alpha$ (H) 20R steranes is 4 $\alpha$ (H)5 $\beta$ (H), 4 $\alpha$ (H)5 $\alpha$ (H) and 4 $\beta$ (H)5 $\alpha$ (H). In synthetic mixtures of 4-methylsteranes, the 4 $\beta$ (H)5 $\beta$ (H) isomer elutes between the 4 $\alpha$ (H)5 $\beta$ (H) and 4 $\alpha$ (H)5 $\alpha$ (H) (Goodwin *et al.*, 1988), but does not appear to occur naturally.

The order of thermal stability of the naturally occurring 4-methylsteranes is 4 $\alpha$ (H) > 4 $\beta$ (H) and 4 $\alpha$ (H)5 $\alpha$ (H) > 4 $\alpha$ (H)5 $\beta$ (H) (Wolff *et al.*, 1986). The elution sequence of 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) and 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) steranes for each of the C<sub>27</sub>, C<sub>28</sub> and C<sub>29</sub> groups is similar to the desmethyl steranes and is as shown in the above listing: 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (H) 20S, 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) 20R,

4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) 20S, 4 $\alpha$ (H)-methyl-5 $\alpha$ (H)14 $\alpha$ (H)17 $\alpha$ (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)**

13 $\beta$ (H)17 $\alpha$ (H) and 13 $\alpha$ (H)17 $\beta$ (H) C<sub>27</sub>, C<sub>28</sub> and C<sub>29</sub> rearranged steranes

Peak	Assignment	NPD Codes
r27d	C <sub>27</sub> 13 $\beta$ (H)17 $\alpha$ (H) 20S diacholestane	27dBS
r27c	C <sub>27</sub> 13 $\beta$ (H)17 $\alpha$ (H) 20R diacholestane	27dB <sub>R</sub>
r27b	C <sub>27</sub> 13 $\alpha$ (H)17 $\beta$ (H) 20S diacholestane	27d $\alpha$ S
r27a	C <sub>27</sub> 13 $\alpha$ (H)17 $\beta$ (H) 20R diacholestane	27d $\alpha$ R
r28d	C <sub>28</sub> 24-methyl-13 $\beta$ (H)17 $\alpha$ (H) 20S diacholestane	28dBS
r28c	C <sub>28</sub> 24-methyl-13 $\beta$ (H)17 $\alpha$ (H) 20R diacholestane	28dB <sub>R</sub>
r28b	C <sub>28</sub> 24-methyl-13 $\alpha$ (H)17 $\beta$ (H) 20S diacholestane	28d $\alpha$ S
r28a	C <sub>28</sub> 24-methyl-13 $\alpha$ (H)17 $\beta$ (H) 20R diacholestane	28d $\alpha$ R
r29d	C <sub>29</sub> 24-ethyl-13 $\beta$ (H)17 $\alpha$ (H) 20S diacholestane	29dBS
r29c	C <sub>29</sub> 24-ethyl-13 $\beta$ (H)17 $\alpha$ (H) 20R diacholestane	29dB <sub>R</sub>
r29b	C <sub>29</sub> 24-ethyl-13 $\alpha$ (H)17 $\beta$ (H) 20S diacholestane	29d $\alpha$ S
r29a	C <sub>29</sub> 24-ethyl-13 $\alpha$ (H)17 $\beta$ (H) 20R diacholestane	29d $\alpha$ R

**Configurations:**

- a 13 $\alpha$ (H)17 $\beta$ (H) 20R
- b 13 $\alpha$ (H)17 $\beta$ (H) 20S
- c 13 $\beta$ (H)17 $\alpha$ (H) 20R
- d 13 $\beta$ (H)17 $\alpha$ (H) 20S

**Notes:**

All rearranged steranes listed are likely to be 24R and 24S epimers which, with the exception of C<sub>28</sub> 24-methyl-13 $\beta$ (H)17 $\alpha$ (H) diacholestanes, cannot normally be separated with the chromatography conditions used.

The C<sub>29</sub> 24-ethyl-13 $\beta$ (H)17 $\alpha$ (H) 20S diacholestane co-elutes with the C<sub>27</sub> 5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) 20R isocholestane and the C<sub>29</sub> 24-ethyl-13 $\alpha$ (H)17 $\beta$ (H) 20R diacholestane co-elutes with the C<sub>28</sub> 24-methyl-5 $\alpha$ (H)14 $\beta$ (H)17 $\beta$ (H) 20R isocholestane under normal chromatography conditions. The 13 $\alpha$ (H)17 $\beta$ (H) configuration is less thermally stable than 13 $\beta$ (H)17 $\alpha$ (H).

C<sub>30</sub> rearranged steranes also occur, with 13 $\beta$ (H)17 $\alpha$ (H) 20R and 20S and 13 $\alpha$ (H)17 $\beta$ (H) 20R and 20S configurations.

**BICYCLIC SESQUITERPANES**

Peak	Assignment
DM	8 $\beta$ (H)-drimane
HD	8 $\beta$ (H)-homodrimane
ED	4 $\beta$ (H)-eudesmane

**TRICYCLIC TERPANES**

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

**Notes:**

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

**TETRACYCLIC TERPANES**

Seco-17,21-hopanes

Peak	Assignment	NPD Code
T24	C <sub>24</sub> tetracyclic terpane	24/4
T26	C <sub>26</sub> 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  $C_{35}$   $17\alpha(H)21\beta(H)$  and  $17\beta(H)21\beta(H)$  hopane and  $17\beta(H)21\alpha(H)$  moretane series.

$C_{27}$  and  $C_{29}$  to  $C_{35}$   $17\alpha(H)21\beta(H)$  hopane series:

Peak	Assignment	NPD Codes
h27s	$C_{27}$ $18\alpha(H)$ -22,29,30-trisnorneohopane (Ts)	27Ts
h27m	$C_{27}$ $17\alpha(H)$ -trisorhopane (Tm)	27Tm
h29	$C_{29}$ $17\alpha(H)21\beta(H)$ -30-norhopane	29 $\alpha\beta$
h30	$C_{30}$ $17\alpha(H)21\beta(H)$ -30-hopane	30 $\alpha\beta$
h31S	$C_{31}$ $17\alpha(H)21\beta(H)$ -30,31-homohopane 22S	31 $\alpha\beta$ S
h31R	$C_{31}$ $17\alpha(H)21\beta(H)$ -30,31-homohopane 22R	31 $\alpha\beta$ R
h32S	$C_{32}$ $17\alpha(H)21\beta(H)$ -30,31-bishomohopane 22S	32 $\alpha\beta$ S
h32R	$C_{32}$ $17\alpha(H)21\beta(H)$ -30,31-bishomohopane 22R	32 $\alpha\beta$ R
h33S	$C_{33}$ $17\alpha(H)21\beta(H)$ -30,31-trishomohopane 22S	33 $\alpha\beta$ S
h33R	$C_{33}$ $17\alpha(H)21\beta(H)$ -30,31-trishomohopane 22R	33 $\alpha\beta$ R
h34S	$C_{34}$ $17\alpha(H)21\beta(H)$ -30,31-tetrakishomohopane 22S	34 $\alpha\beta$ S
h34R	$C_{34}$ $17\alpha(H)21\beta(H)$ -30,31-tetrakishomohopane 22R	34 $\alpha\beta$ R
h35S	$C_{35}$ $17\alpha(H)21\beta(H)$ -30,31-pentakishomohopane 22S	35 $\alpha\beta$ S
h35R	$C_{35}$ $17\alpha(H)21\beta(H)$ -30,31-pentakishomohopane 22R	35 $\alpha\beta$ R

$C_{27}$  and  $C_{29}$  to  $C_{35}$   $17\beta(H)21\alpha(H)$  moretane series

Peak	Assignment	NPD Codes
m29	$C_{29}$ $17\beta(H)21\alpha(H)$ -30-normoretane	29 $\beta\alpha$
m30	$C_{30}$ $17\beta(H)21\alpha(H)$ -30-moretane	30 $\beta\alpha$
m31	$C_{31}$ $17\beta(H)21\alpha(H)$ -homomoretane	
m32	$C_{32}$ $17\beta(H)21\alpha(H)$ -bishomomoretane	

$C_{27}$   $17\beta(H)$  and  $C_{29}$  to  $C_{35}$   $17\beta(H)21\beta(H)$  hopane series

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

Notes:

The C<sub>29</sub> to C<sub>35</sub> pentacyclic triterpane (hopane) series of compounds have been identified with 17 $\alpha$ (H)21 $\beta$ (H) (hopane), 17 $\beta$ (H)21 $\alpha$ (H) (moretane) and 17 $\beta$ (H)21 $\beta$ (H) (hopane) configurations. C<sub>27</sub> trisnorhopanes have no side-chain at C-21 and have either the 17 $\alpha$ (H) or 17 $\beta$ (H) configuration, the former being the more thermally stable and the latter form generally present in immature samples only. The C<sub>27</sub> 18 $\alpha$ (H)-trisnor $\alpha$ hopane (T<sub>s</sub>) is more thermally stable than C<sub>27</sub> 17 $\alpha$ (H)-trisnorhopane (T<sub>m</sub>). 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 <sub>27</sub> 22,29,30-trisnorneohop-13(18)-ene
uh2	C <sub>27</sub> trisnorhop-17-ene
uh3	C <sub>29</sub> norhop-17(21)-ene
uh4	C <sub>29</sub> 30-neonor-13(18)-ene
uh5	C <sub>30</sub> hop-17(21)-ene
uh6	C <sub>30</sub> neohop-13(18)-ene
uh7	C <sub>31</sub> 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 <sub>27</sub> 17 $\alpha$ (H)18 $\alpha$ (H)21 $\beta$ (H)-25,28,30-trisnorhopane	25 nor 28 $\alpha\beta$
Tm	C <sub>27</sub> 17 $\beta$ (H)18 $\alpha$ (H)21 $\alpha$ (H)-25,28,30-trisnormoretane	
B	C <sub>28</sub> 17 $\alpha$ (H)18 $\alpha$ (H)21 $\beta$ (H)-28,30-bisnorhopane	28 $\alpha\beta$
Bnm	C <sub>28</sub> 17 $\beta$ (H)18 $\alpha$ (H)21 $\alpha$ (H)-28,30-bisnormoretane	
G	C <sub>30</sub> gammacerane	30G
O	C <sub>30</sub> 18 $\alpha$ (H) oleanane	30O
J	C <sub>30</sub> 18 $\beta$ (H) oleanane ('compound J')	
L	C <sub>30</sub> lupane	
BL	C <sub>28</sub> bisnorlupane	
d28	C <sub>28</sub> diahopane	
X	C <sub>30</sub> diahopane	30d

**Notes:**

The C<sub>30</sub> 18 $\alpha$ (H) oleanane and 18 $\beta$ (H) oleanane (formerly 'compound J' of Grantham *et al.*, 1983) coelute on standard GC columns. The 18 $\beta$ (H) oleanane is less thermally stable than 18 $\alpha$ (H) oleanane (Riva *et al.*, 1988).

The C<sub>30</sub> and C<sub>28</sub> 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<sub>26</sub> and C<sub>28</sub> to C<sub>34</sub> 17 $\alpha$ (H)21 $\beta$ (H)-25-norhopanes and 17 $\beta$ (H)21 $\alpha$ (H)-25-normoretanes

Peak	Assignment	NPD Codes
dh26s	C <sub>26</sub> 18 $\alpha$ (H)-22,25,29,30-tetrakisnorhopane	
dh26m	C <sub>26</sub> 17 $\alpha$ (H)-22,25,28,30-tetrakisnorhopane	
dh28	C <sub>28</sub> 17 $\alpha$ (H)21 $\beta$ (H)-25,30-bisnorhopane	
dm28	C <sub>28</sub> 17 $\beta$ (H)21 $\alpha$ (H)-25,30-bisnormoretane	
dh29	C <sub>29</sub> 17 $\alpha$ (H)21 $\beta$ (H)-25-norhopane	25nor30 $\alpha\beta$
dm29	C <sub>29</sub> 17 $\beta$ (H)21 $\alpha$ (H)-25-normoretane	
dh30s	C <sub>30</sub> 17 $\alpha$ (H)21 $\beta$ (H)-25-norhomohopane 22S	
dh30R	C <sub>30</sub> 17 $\alpha$ (H)21 $\beta$ (H)-25-norhomohopane 22R	
dh31s	C <sub>31</sub> 17 $\alpha$ (H)21 $\beta$ (H)-25-norbishomohopane 22S	
dh31R	C <sub>31</sub> 17 $\beta$ (H)21 $\beta$ (H)-25-norbishomohopane 22R	
dh32s	C <sub>32</sub> 17 $\alpha$ (H)21 $\beta$ (H)-25-nortrishomohopane 22S	
dh32R	C <sub>32</sub> 17 $\alpha$ (H)21 $\beta$ (H)-25-nortrishomohopane 22R	
dh33s	C <sub>33</sub> 17 $\alpha$ (H)21 $\beta$ (H)-25-nortetrakishomohopane 22S	
dh33R	C <sub>33</sub> 17 $\alpha$ (H)21 $\beta$ (H)-25-nortetrakishomohopane 22R	
dh34s	C <sub>34</sub> 17 $\alpha$ (H)21 $\beta$ (H)-25-norpentakishomohopane 22S	
dh34R	C <sub>34</sub> 17 $\alpha$ (H)21 $\beta$ (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 <sub>18</sub> tricyclic terpane
dt19	C <sub>19</sub> tricyclic terpane
dt20	C <sub>20</sub> tricyclic terpane
dt21	C <sub>21</sub> tricyclic terpane
dt22	C <sub>22</sub> tricyclic terpane
dt23	C <sub>23</sub> tricyclic terpane
dt24	C <sub>24</sub> tricyclic terpane
dt25	C <sub>25</sub> tricyclic terpanes
dt26	C <sub>26</sub> tricyclic terpanes
dt27	C <sub>27</sub> tricyclic terpanes
dt28	C <sub>28</sub> tricyclic terpanes
dt29	C <sub>29</sub> tricyclic terpanes

**Notes:**

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

**SECOHOPANES**

## Seco-8,14-hopanes

Peak	Assignment
sh1	C <sub>27</sub> seco-8,14-hopane
sh2	C <sub>29</sub> seco-8,14-hopane
sh3	C <sub>30</sub> 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 <sub>34</sub> botryococcane
S	C <sub>30</sub> 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**

<b>Peak</b>	<b>Assignment</b>
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**

<b>Peak</b>	<b>Assignment</b>
P	phenanthrene
3MP	3-methylphenanthrene
2MP	2-methylphenanthrene
9MP	9-methylphenanthrene
1MP	1-methylphenanthrene
DMP	dimethylphenanthrene trimethylphenanthrene
TMP	

**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 <sub>21</sub> monoaromatic steroid	A1
MAS22	C <sub>22</sub> monoaromatic steroid	B1
MAS27	C <sub>27</sub> monoaromatic steroid	D1
MAS29B28 $\alpha$	5B(H)C <sub>29</sub> + 5 $\alpha$ (H)C <sub>28</sub> monoaromatic steroid (20R)	H1 I1
MAS29 $\alpha$	5 $\alpha$ (H)C <sub>29</sub> monoaromatic steroid (20R)	

**TRIAMOMATIC STEROIDS**

Peak	Assignment	NPD Codes
TAS20	C <sub>20</sub> triaromatic steroid	a1
TAS21	C <sub>21</sub> triaromatic steroid	b1
TAS26S	C <sub>26</sub> triaromatic steroid 20S	c1
TAS26R	C <sub>26</sub> triaromatic steroid 20R	d1
TAS27S	C <sub>27</sub> triaromatic steroid 20S	
TAS27R	C <sub>27</sub> triaromatic steroid 20R	f1
TAS28S	C <sub>28</sub> triaromatic steroid 20S	e1
TAS28R	C <sub>28</sub> 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**

<b>Peak</b>	<b>Assignment</b>
2BT	C <sub>2</sub> -benzothiophene
3BT	C <sub>3</sub> -benzothiophene
4BT	C <sub>4</sub> -benzothiophene
DBT	dibenzothiophene
4MDBT	4-methyldibenzothiophene
3MDBT	3-methyldibenzothiophene
2MDBT	2-methyldibenzothiophene
1MDBT	1-methyldibenzothiophene
DMDBT	dimethyldibenzothiophenes
TMDBT	trimethyldibenzothiophenes
BNT	benzonaphthothiophenes

**Notes:**

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

**OTHER AROMATIC COMPOUNDS**

<b>Peak</b>	<b>Assignment</b>
A	Anthracene
MA	Methylantracene
F	Fluorene
MF	Methylfluorene
C	Chrysene
MC	Methylchrysene
PY	Pyrene
MPY	Methylpyrene
Ca	Cadalene (1,6-dimethyl-4-isopropyl-naphthalene)
Eu	Eudalene (1-methyl-7-isopropyl-naphthalene)
BH	Benzohopanes
MBH	Methylbenzohopanes

**Notes:**

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

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

## Appendix 6

### Gas Chromatogram Peak Assignments

#### ALKANE GAS CHROMATOGRAMS

##### *n*-alkanes

*n*-C<sub>10-36</sub> homologous series of normal alkanes, identified within the carbon number range 10 to 36

##### isoprenoids

*i*-C<sub>15</sub> Farnesane  
*i*-C<sub>16</sub>  
*i*-C<sub>18</sub> 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 Methyl dibenzothiophene  
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-)