The Use of Tandem Quadrupole GC/MS/MS for the Selective Identification of Sterane Biomarkers in Crude Oils as Age and Facies Diagnostic Indicators.

OBJECTIVE

Through the use of the Waters Quattro micro® GC tandem quadrupole mass spectrometer and in high sensitivity and high selectivity we have been able to specifically identify C27-C30 steroids and use the information to ascertain the age and facies of a crude oil. Wet chemical fingerprinting which is an established oil fingerprinting technique has been used. The use of the tandem quadrupole mass spectrometer allows for the identification of trace compounds in complex matrices. The ability to accurately quantify over a wide dynamic range is essential in studies of this nature where precise ratios of abundance are required. A thorough understanding of the molecular composition of crude oils has become an important area of study both to the oil industry and to the petroleum geochemical community. Determining the source of crude oil can provide important information for the exploration of new oil fields, the evaluation of exploration strategies and for the identification of new oil fields. Biodegradation of oils can also occur in the subsurface which can affect thegeochemical fingerprint of the crude oil. The identification of the age and facies of a crude oil is important for the exploratory and the evaluation of new oil fields. The two main parameters for the identification of age and facies are the organic maturity and the source rock composition. In this study we have tried to identify the age and facies of a number of oils from two different sources of known age.

INTRODUCTION

Molecular biomarkers, in general, are organic products that can be traced to a particular biological origin. They are structurally similar to, and are diagnostic of specific groups of, specific natural compounds (chemicals) produced by living organisms and have a wide variety of applications, e.g. in the study of ancient ecosystems and in paleoecological research. Specifically, biomarkers in crude oil can be used to establish the age of the source rock, the environment of deposition as well as the thermal maturity of the source rock. The resulting model provides a method to identify the original organic molecule and hence identify the original source organism. This compound mass analysis, in the identification of the environment (facies) from which the oil was produced, Not surprisingly, steroids are one of the largest classes of biomolecules in crude oils. The C27-C30 steroids are of particular interest due to their occurrence as age-diagnostic indicators. These compounds are sufficiently abundant and sufficiently complex that they can be used to identify the original environment in which the oil was produced.

METHODS AND MATERIALS

Gas Chromatography/Mass Spectrometry (GC/MS/MS) is the principal method used to identify and determine sources and other biomarkers. Where the concentration of the individual biomarker is relatively low, high performance liquid chromatography (HPLC) coupled with a tandem quadrupole mass spectrometer (MRM) is the technique of choice. The Waters Quattro micro tandem quadrupole mass spectrometer (Ettre) is able to detect and identify sterane isomers and other biological markers. Where the concentrations of the biomarkers of interest and abundant interfering compounds are low, the Waters Quattro micro tandem quadrupole mass spectrometer is the instrument of choice. The Waters Quattro micro tandem quadrupole mass spectrometer, equipped with a dual column GC system producing a total run time of 63 mins).

Figure 3. Quatro micro tandem quadrupole mass spectrometer.

Figure 4. Aqueous solution containing isoprenoid biomarkers for GC-MS/MS analysis. The GC-MS/MS analysis of the C27 steranes (nonchromatographic).

Figure 5. Figure shows the MRM analysis of the steranes of a Late Ordovician oil. The C26 steranes were extracted from a Devonian terrigenous oil (8) and analyzed using a single quadrupole instrument and that the 24-nordiacholestane ratio (NDR) and the 24-norcholestane ratio (NCR), may be defined by monitoring the MRM transition 358>217 and the calculated 24-nordiacholestane ratio, respectively. The NCR is defined by monitoring the MRM transition 358>217 of -24-nordiacholestanes in Cretaceous or younger oils and sediments relative to their 27-norcholestane analogues. The NDR is defined by monitoring the MRM transition 358>217 of -24-nordiacholestanes in Carboniferous and younger oils and sediments relative to their 27-norcholestane analogues. The 24-nordiacholestane ratio (NDR), may be defined by monitoring the MRM transition 358>217 of -24-nordiacholestanes in Carboniferous and younger oils and sediments relative to their 27-norcholestane analogues.

RESULTS

The South-East Asian oil is shown in Figure 1 and is an oil produced from a terrigenous environment. The selected ions are described in the figure. The ECD’s channel shows the oil sample containing a high concentration of alkane compounds while the MRM channel shows a number of the 27-norcholestane and 24-nordiacholestane analogues in Cretaceous and younger oils which are significant in the Cretaceous and younger oils but not in the Devonian or Carboniferous oils. The 27-norcholestane analogues are defined by monitoring the MRM transition 358>217 of 27-norcholestane analogues in Carboniferous or older oils and sediments relative to their 27-norcholestane analogues. The 24-nordiacholestane ratio (NDR), may be defined by monitoring the MRM transition 358>217 of -24-nordiacholestanes in Carboniferous and younger oils and sediments relative to their 27-norcholestane analogues. The NCR is defined by monitoring the MRM transition 358>217 of -24-norcholestanes in Cretaceous or younger oils and sediments relative to their 27-norcholestane analogues. The NDB is defined by monitoring the MRM transition 358>217 of -24-nordiacholestanes in Carboniferous and younger oils and sediments relative to their 27-norcholestane analogues.

Figure 6. GC/MS/MS analysis of the C26 steranes of an argillaceous crude oil (9). The GC-MS/MS analysis of the C26 steranes of an argillaceous crude oil (9).

REFERENCES