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Characteristics of Spilled Oils, Fuels, and Petroleum Products:

1. Composition and Properties of Selected Oils

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Notice

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Foreword

The National Exposure Research Laboratory’s Ecosystems Research Division (ERD) in Athens, Georgia, conducts research on organic and inorganic chemicals, greenhouse gas biogeochemical cycles, and land use perturbations that create direct and indirect, chemical and non-chemical stresses, exposures, and potential risks to humans and ecosystems. ERD develops, tests, applies and provides technical support for exposure and ecosystem response models used for assessing and managing risks to humans and ecosystems, within a watershed / regional context.

The Regulatory Support Branch (RSB) conducts problem-driven and applied research, develops technology tools, and provides technical support to customer Program and Regional Offices, States, Municipalities, and Tribes. Models are distributed and supported via the EPA Center for Exposure Assessment Modeling (CEAM) and through access to Internet tools (www.epa.gov/athens/onsite).

At the request of the US EPA Oil Program Center, ERD is developing an oil spill model that focusses on fate and transport of oil components under various response scenarios. Since crude oils and petroleum products are composed of many chemicals that have varying physical properties, data are required to characterize these fluids for use in models. The data presented in this report provide input to compositional models by characterizing oil composition by several approaches, but also by providing physical transport properties at corresponding levels of weathering and temperature. EPA expects these data to be useful both for modeling and to provide a resource for the oil spill response community as a whole.

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Abstract

Multicomponent composition and corresponding physical properties data of crude oils and petroleum products are needed as input to environmental fate simulations. Complete sets of such data, however, are not available in the literature due to the complexity and expense of making the measurements. Environment Canada has previously developed a database of various physical and chemical properties of crude oils and petroleum products. In this cooperative project, ten “typical” crude oils and refined products in common use or transport were identified for subsequent characterization. Measured oil physical properties include API gravity, density, sulphur content, water content, flash point, pour point, viscosity, surface and interfacial tension, adhesion, the equation for predicting evaporation, emulsion formation, and simulated boiling point distribution. The chemical composition of the oils are quantified for hydrocarbon groups, volatile organic compounds, n-alkane distribution, distribution of alkylated polyaromatic hydrocarbon (PAH) homologues and other EPA priority PAHs, and biomarker concentrations. This project will provide the most complete and comprehensive database for the selected oils to date. The new composition data will be integrated into the existing Environment Canada oil properties database. The results will be made available to the public both on the world wide web and as a database on disc.

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1. Introduction

During any oil spill incident, the properties of the spilled oil, including the oil phase composition and oil compositional changes due to weathering, ideally would be known immediately, so that models could be used to predict the environmental impacts of the spill or various treatment alternatives. Unfortunately, the properties routinely measured by oil producers and refiners are not the ones that on-scene commanders need to know most urgently. Oil producers and refiners typically do not know to what extent or at what rate their oils will evaporate; the detailed chemical composition of the oil and its differential compositional changes over time; how these changes affect its behavior and fate in the environment; the viscosity of the oil at ambient temperature as it evaporates; if the oil likely to sink or submerge; if the use of chemical dispersants can enhance its dispersion; if emulsions will form; the hazard to on-site personnel during cleanup; or the oil toxicity to marine or aquatic organisms.

Since 1984, the Emergencies Science and Technology Division (ESTD) of Environment Canada has continued to develop a database on various physical-chemical properties of crude oils and petroleum products. This database addresses the properties and behaviors listed in the previous paragraph and can be queried via the internet at www.etcentre.org/spills. Through many years endeavor, the oil properties database now contains information on over 400 oils from all over the world. Environment Canada is the largest single source of data in the oil properties database.

The U.S. EPA's immediate interest in developing a database of properties and compositions is for use in supporting the development of models for application to accidental spills and releases of petroleum hydrocarbons and other multicomponent oils. This multicomponent composition data is not typically available in the literature nor immediately available on an incident-specific basis due to the complexity and expense of making the measurements. Thus the creation of a database containing both physical property and composition data for various conditions of weathering would be useful for emergency response modeling. In this situation the data could be used for simulation of an example oil that would be chosen for its similarity to the spilled oil. This approach recognizes that performing detailed characterization of an oil during an emergency is more than unlikely. It would further be desirable to have access to similar data for planning purposes in advance of spills.

Ten representative oils and refined petroleum products with spill potential were chosen after discussion with the US EPA. These oils were collected from various sources. For each oil, the properties presented are those that determine its environmental behavior and effects. Whenever possible, ESTD has used standard test methods, such as those of the American Society for Testing and Materials (ASTM), to obtain oil property data. The physical property measurements include API gravity, density, sulphur, water content, flash point, pour point, viscosity, vapor pressure, surface tension, and adhesion. Many oil analytical methods have been developed by ESTD specifically to determine environmentally-significant individual components, oil hydrocarbon groups, and chemical properties. These include methods for determining evaporation equations, emulsion formation and characterization, measuring chemical dispersibility, measuring volatile organic compounds, important saturated and biomarker compounds, and environmentally hazardous PAH compounds. Because evaporative loss results in significant changes in physical properties and chemical composition of spilled oils, we measure most properties not only for fresh oils, but also for evaporated oils prepared in the lab to represent various degrees of evaporation. Upon the completion of the project, a complete set of physical properties and comprehensive multicomponent data on important chemical composition of the selected oils will be provided and integrated into the existing ESTD database. Finally, the unique information produced from this project is intended by EPA to advance the state-of-the-art of oil spill modeling. As such it will be available to the public through the Internet at www.etcentre.org/spills.

2. List of Definitions

Acyclic: A compound with straight or branched carbon-carbon linkages but without cyclic (ring) structures.

Adhesion: The degree to which an oil will coat a surface, expressed as the mass of oil adhering per unit area. A test has been developed for a standard surface that gives a semi-quantitative measure of this property.

Aliphatics: *Hydrocarbons* in petroleum that contain saturated and/or single unsaturated bonds and elute during chromatography using non-polar solvents such hexane. It includes *alkanes* and *alkenes*, but not *aromatics*.

Alkane (Paraffin): A group of *hydrocarbons* composed of only carbon and hydrogen with no double bonds or aromaticity. They are said to be "saturated" with hydrogen. They may by straight-chain (normal), branched or cyclic. The smallest alkane is methane (CH_4), the next, ethane (CH_3CH_3), then propane ($CH_3CH_2CH_3$), and so on.

Alkene (Olefin): An unsaturated *hydrocarbon*, containing only hydrogen and carbon with one or more double bonds, but having no aromaticity. *Alkenes* are not typically found in crude oils, but can occur as a result of heating.

Alkyl Groups: A *hydrocarbon* functional group (C_nH_{2n+1}) obtained by dropping one hydrogen from fully saturated compound; e.g., methyl ($-CH_3$), ethyl ($-CH_2CH_3$), propyl ($-CH_2CH_2CH_3$), or isopropyl [$(CH_3)_2CH-$].

API Gravity: An American Petroleum Institute measure of *density* for petroleum:

$$\text{API Gravity} = [141.5/(\text{specific gravity at } 15.6\ ^\circ\text{C}) - 131.5]$$

Fresh water has a gravity of 10 °API. The scale is commercially important for ranking oil quality. Heavy, inexpensive oils are < 25 °API; medium oils are 25 to 35 °API; light, commercially-valuable oils are 35 to 45 °API..

Aromatics: Cyclic, planar hydrocarbon compounds that are stabilized by a delocalized π-electron system. They include such compounds as the *BTEX* group (benzene, toluene, ethylbenze and the three xylene isomers), polycyclic aromatic hydrocarbons (*PAHs*, such as naphthalene), and some heterocyclic aromatics such as the di-benzothiophenes.

Asphaltenes: A complex mixture of heavy organic compounds precipitated from oils and *bitumens* by natural processes or in laboratory by addition of excess *n*-pentane, or *n*-hexane. After precipitation of *asphaltenes*, the remaining oil or *bitumen* consists of *saturates*, *aromatics*, and *resins*. Asphaltenes are so named because they make up the largest percentage of the asphalt used to pave roads.

Biological Marker (Biomarker): Complex organic compounds composed of carbon, hydrogen, and other elements which are found in oil, *bitumen*, rocks, and sediments and which have undergone little or no change in structure from their parent organic molecules in living organisms. Most, but not all, biomarkers are isoprenoids, composed of isoprene subunits. Biomarkers include pristane, phytane, *triterpanes*, steranes, porphyrins, and other compounds. These compounds are typically analyzed by GC/MS.

Bitumen: Mixture of *hydrocarbons* of natural or pyrogenous origin or a combination of both. Unlike oil, *bitumen* is indigenous to the fine-grained rock in which it is found.

Boiling Point: The temperature at which a liquid begins to boil. That is, it is the temperature at which the vapour pressure of a liquid is equal to the atmospheric or external pressure. It is measured at standard pressure. The boiling point distributions of crude oils and petroleum products may be in a range from 30 °C to 700 °C.

BTEX: The collective name given to benzene, toluene, ethylbenzene and the xylene isomers (*p*-, *m*-, and *o*-xylene).

Carbon Preference Index (CPI): The ratio of odd to even *n*-alkanes. Odd/even CPI *alkanes* are equally abundant in petroleum but not in biological material. A CPI near 1 is an indication of petroleum.

Check Standard: An analyte with a well-characterized property of interest, *e.g.*, concentration, density, etc... used to verify method, instrument and operator performance during regular operation. *Check standards* may be obtained from a certified supplier, may be a pure substance with properties obtained from the literature or may be developed in-house.

Chemical Dispersion: In relation to oil spills, this term refers to the creation of oil-in-water *emulsions* by the use of chemical dispersants made for this purpose.

Complex Modulus: The *complex modulus* is a measure of the overall resistance of a material to flow under an applied stress, in units of force per unit area. It combines *viscosity* and elasticity elements to provide a measure of "stiffness", or resistance to flow. The *complex modulus* is more useful than *viscosity* for assessing the physical behaviour of very non-Newtonian materials such as *emulsions*.

Cycloalkanes (Naphthene, Cycloparaffin): A saturated, cyclic compound containing only carbon and hydrogen. One of the simplest *cycloalkanes* is cyclohexane (C_6H_{12}). Steranes and triterpanes are branched naphthenes consisting of multiple condensed five- or six-carbon rings.

Density: The mass per unit volume of a substance. *Density* is temperature-dependent, generally decreasing with temperature. The density of oil relative to water, its specific gravity, governs whether a particular oil will float on water. Most fresh crude oils and fuels will float on water. Bitumen and certain residual fuel oils, however, may have densities greater than water at some temperature ranges and may submerge in water. The density of a spilled oil will also increase with time as components are lost due to weathering.

Dispersants or Chemical Dispersants: Chemicals that reduce the surface tension between water and a hydrophobic substance such as oil. In the case of an oil spill, dispersants facilitate the breakup and dispersal of an oil slick throughout the water column in the form of an oil-in-water emulsion. Chemical dispersants can only be used in areas where biological damage will not occur and must be approved for use by government regulatory agencies.

Emulsion: A stable mixture of two immiscible liquids, consisting of a continuous phase and a dispersed phase. Oil and water can form both oil-in-water and water-in-oil emulsions. The former is termed a dispersion, while *emulsion* implies the latter. Water-in-oil emulsions formed from petroleum and brine can be grouped into four stability classes: stable, a formal emulsion that will persist indefinitely; meso-stable, which gradually degrade over time due to a lack of one or more stabilizing factors; entrained water, a mechanical mixture characterized by high viscosity of the petroleum component which impedes separation of the two phases; and unstable, which are mixtures that rapidly separate into immiscible layers.

Emulsion stability is generally accompanied by a marked increase in *viscosity* and elasticity, over that of the parent oil which significantly changes behaviour. Coupled with the increased volume due to the introduction of brine, emulsion formation has a large effect on the choice of countermeasures employed to combat a spill.

Emulsification: The process of *emulsion* formation, typically by mechanical mixing. In the environment, *emulsions* are most often formed as a result of wave action. Chemical agents can be used to prevent the formation of *emulsions* or to “break” the *emulsions* to their component oil and water phases.

Equipment Blank: A sample of analyte-free media which has been used to rinse the sampling equipment. It is collected after completion of decontamination and prior to sampling. This blank is useful in documenting and controlling the preparation of the sampling and laboratory equipment.

“Fingerprint”: A chromatographic signature of relative intensities used in oil-oil or oil-source rock correlations. Mass chromatograms of *steranes* or *terpanes* are examples of *fingerprints* that can be used for qualitative or quantitative comparison of oils.

Flash Point: The temperature at which the vapour over a liquid will ignite when exposed to an ignition source. A liquid is considered to be flammable if its *flash point* is less than 60 °C.

Flash point is an extremely important factor in relation to the safety of spill cleanup operations. Gasoline and other light fuels can ignite under most ambient conditions and therefore are a serious hazard when spilled. Many freshly spilled crude oils also have low *flash points* until the lighter components have evaporated or dispersed.

GC-MS: Gas chromatography-mass spectrometry.

GC-TPH: GC detectable total petroleum hydrocarbons, that is the sum of all GC-resolved and unresolved hydrocarbons. The resolvable hydrocarbons appear as peaks and the unresolvable hydrocarbons appear as the area between the lower baseline and the curve defining the base of resolvable peaks.

Hydrocarbon: A hydrocarbon is an organic compound containing only hydrogen and carbon. Hydrocarbons are the principal constituents of crude oils and refined petroleum products. Oil hydrocarbons can be grouped into four major classes of compounds: *saturates* (including *waxes*), *aromatics*, *asphaltenes*, and *resins*.

Hopane: Pentacyclic *hydrocarbons* of the *triterpane* group believed to be derived primarily from bacteriohopanoids in bacterial membranes.

Interfacial Tension: The net energy per unit area at the interface of two substances, such as oil and water or oil and air. The air/liquid interfacial tension is often referred to as surface tension. The SI units for *interfacial tension* are milliNewtons per meter (mN/m). The higher the *interfacial tension*, the less attractive the two surfaces are to each other and the more size of the interface will be minimized. Low surface tensions can drive the spreading of one fluid on another. The surface tension of an oil, together its viscosity, affects the rate at which spilled oil will spread over a water surface or into the ground.

Internal Standard (IS): A pure analyte added to a sample extract in a known amount, which is used to measure the relative responses of other analytes and surrogates that are components of the same solution. The *internal standard* must be an analyte that is not a sample component.

PAHs: Polycyclic aromatic hydrocarbons. Alkylated *PAHs* are *alkyl group* derivatives of the parent *PAHs*. The five target alkylated *PAHs* referred to in this report are the alkylated naphthalene, phenanthrene, dibenzothiophene, fluorene, and chrysene series.

Polar Compounds: An organic compound with distinct regions of positive and negative charge. *Polar compounds* include alcohols, such as sterols, and some *aromatics*, such as monoaromatic-steroids. Because of their polarity, these compounds are more soluble in polar solvents, including water, compared to non-polar compounds of similar molecular structure.

Pour Point: The lowest temperature at which an oil will appear to flow under ambient pressure over a period of five seconds. The *pour point* of crude oils generally varies from -60 °C to 30 °C. Lighter oils with low *viscosities* generally have lower *pour points*.

Resins: This is the name given to a large group of *polar compounds* in oil. These include hetero-substituted *aromatics*, acids, ketones, alcohols and monoaromatic steroids. Because of their polarity, these compounds are more soluble in *polar* solvents, including water, than the non-polar compounds, such as *waxes* and *aromatics*, of similar molecular weight. They are largely responsible for oil *adhesion*.

RRF: Relative response factor.

Saturates (Saturated Fraction): Nonaromatic *hydrocarbons* in petroleum. This grouping includes both normal and branched *alkanes* (paraffins), and *cycloalkanes* (naphthenes).

SIM (Selecting Ion Monitoring): Mass spectrometric monitoring of a specific mass/charge (m/z) ratio. The *SIM* mode offers better sensitivity than can be obtained using the full scan mode.

Solubility: The amount of a substance (solute) that dissolves in a given amount of another substance (solvent). Particularly relevant to oil spill cleanup is the measure of how much and the composition of oil which will dissolve in the water column. This is important as the soluble fractions of the oil are often toxic to aquatic life, especially at high concentrations. The *solubility* of oil in water is very low, generally less than 1parts per million (ppm).

Steranes: A class of tetracyclic, saturated biomarkers constructed from six isoprene subunits (~C_{30}). *Steranes* are derived from sterols, which are important membrane and hormone components in eukaryotic organisms. Most commonly used *steranes* are in the range of C_{26} to C_{30} and are detected using m/z 217 mass chromatograms.

Surrogate Analyte: A pure analyte that is extremely unlikely to be found in any sample, which is added to a sample aliquot in a known amount and is measured with the same procedures used to measure other components. The purpose of a *surrogate analyte* is to monitor the method performance with each sample.

Terpanes: A broad class of complex branched, cyclic alkane biomarkers including *hopanes* and tricyclic compounds. They are commonly monitored using m/z 191 mass chromatograms.

Triterpanes: A class of cyclic saturated *biomarkers* constructed from six isoprene subunits. Cyclic *terpane* compounds containing two, four, and six isoprene subunits are called monoterpane (C_{10}), diterpane (C_{20}) and *triterpane* (C_{30}), respectively.

Total n-alkanes: The sum of all resolved *n-alkanes* (from C_8 to C_{40} plus pristane and phytane).

Total 5 Alkylated PAH Homologues: The sum of the 5 target PAHs (naphthalene, phenanthrene, dibenzothiophene, fluorene, chrysene) and their alkylated (C_1 to C_4) homologues, as determined by GC-MS. These 5 target alkylated PAH homologous series are oil-characteristic aromatic compounds.

Total Aromatics: The sum of all resolved and unresolved aromatic hydrocarbons including the total of BTEX and other alkyl benzene compounds, total 5 target alkylated PAH homologues, and other EPA priority PAHs.

Total Saturates: The sum of all resolved and unresolved aliphatic hydrocarbons including the total n-alkanes, branched alkanes, and cyclic saturates.

Vapour Pressure: A measure of how oil partitions between the liquid and gas phases, or the partial pressure of a vapour above a liquid oil at a fixed temperature.

Viscosity: *Viscosity* is the resistance of a fluid to shear, movement or flow. The viscosity of an oil is a function of its composition. In general, the greater the fraction of *saturates* and *aromatics* and the lower the amount of *asphaltenes* and *resins*, the lower the viscosity. As oil weathers, the evaporation of the lighter components leads to increased viscosity. Viscosity also increases with decreased temperature, and decreases with increased temperature.

The viscosity of an ideal, non-interacting fluid does not change with shear rate. Such fluids are called Newtonian. Most crude oils and oil products are Newtonian. The viscosity of non-Newtonian materials may vary with shear rate, as well as duration of shear. Oils with high *wax* content are often non-Newtonian, and stable water-in-oil *emulsions* are always non-Newtonian. A material that exhibits a decrease in viscosity with shear stress is termed pseudoplastic, while those that exhibit a decrease in viscosity with time of applied shear force are referred to as thixotropic. Both effects are caused by internal interactions of the molecules and larger structures in the fluid which change with the movement of the material under applied stress. Generally, non-Newtonian oils are pseudoplastic, while *emulsions* may be either thixotropic or pseudoplastic.

In terms of oil spill cleanup, viscous oils do not spread rapidly, do not penetrate soils as rapidly, and affect the ability of pumps and skimmers to handle the oil.

Volatile Organic Compounds (VOC): Organic compounds with high *vapour pressures* at normal temperatures. *VOCs* include light *saturates* and *aromatics*, such as pentane, hexane, *BTEX* and other lighter substituted benzene compounds, which can make up to a few percent of the total mass of some crude oils.

Waxes: Waxes are predominately straight-chain *saturates* with melting points above 20 °C (generally, the *n*-alkanes C_{18} and heavier).

Weathering: Processes related to the physical and chemical actions of air, water and organisms after oil spill. The major weathering processes include evaporation, dissolution, dispersion, photochemical oxidation, water-in-oil *emulsification*, microbial degradation, adsorption onto suspended particulate materials, interaction with mineral fines, sinking, sedimentation, and formation of tar balls.

UCM: GC unresolved complex mixture of hydrocarbons. The UCM appear as the “envelope” or hump area between the solvent baseline and the curve defining the base of resolvable peaks.

3. Methods for Measurement of Physical and Chemical Properties of Selected Oils

3.1 Selection and Collection of Oils

Ten oils and refined petroleum products with significant potential to be spilled in U.S. waters were chosen based on discussion with the US EPA. These oils were collected by ESTD from various oil companies and refineries in North America. The oils include: Alberta Sweet Mix Blend (Reference #5), Arabian Light, South Louisiana, West Texas Intermediate, Sockeye, Alaska North Slope, Fuel Oil No.2, Fuel Oil No.5 ("Bunker B"), Heavy Fuel Oil 6303 ("Bunker C"), and Orimulsion-400.

3.2 Instruments

The major instruments used to determine the oil physical properties and chemical composition are the following:

- Oil Weathering System (Wheaton Spin-Vap –10)
- GC-MS (HP)
- GC-FID (HP)
- XRF (Spectro Titan)
- Viscometer (ThermoHaake VT550)
- Rheometer (ThermoHaake RheoStress 300)
- Density meter (Anton Parr DMA 48)
- Flash point analyzer (Herzog HFP360/362)
- Vapor pressure tester (Herzog HVP970)
- Karl Fisher automatic titrator (Metrohm)
- Tensiometer (Krüss K10)

3.3 Evaporation (Weathering) of Oils

A laboratory oil-weathering technique by rotary evaporation is used by Emergencies Science and Technology Division to artificially weather oils with varying degrees of weight loss. The oil-weathering system consists of a Wheaton N-10 Spin Vap with a 10 L flask, an integral water bath (capacity 14 L), a Haake F3-CH circulating bath and a Millipore vacuum pump (Figure 1). The bath temperature can be set from 20 °C to 100 °C ± 0.5 °C. The rotation speed can be continuously varied from 10 to 135 rpm.

Figure 1 Rotary evaporator used for artificial weathering of oils.

The following evaporation procedure is used to evaporate oils:

(1) The water bath of distilled water is brought to a temperature of 80 °C.
(2) The empty rotary flask is weighed, approximately 2 L of oil added and the flask reweighed.
(3) The flask is mounted on the apparatus and the flask partially immersed in the water bath and spun at full speed, 135 rpm. A constant flow of air of 13 L/min through the flask is maintained by the vacuum pump;
(4) At set intervals, the sample flask is removed and weighed. Periodically, a sample of about 1 g is removed for chemical analysis.
(5) When evaporation is stopped (*i.e.* overnight and weekends), the flask is sealed and stored at 5 °C. After removal and prior to restarting, the flask is weighed to ensure that no evaporation has occurred during storage.

Typically, three weathered fractions are prepared for each oil sample. The initial weathering period is 48 hours, a duration chosen to simulate the eventual final state of an oil in the environment. In addition, intermediate fractions of approximately one- and two-thirds of the 48 hour loss by weight are prepared.

The exact time taken to prepare these intermediate fractions is determined by estimation from the measured fractional mass-loss as a function of time for the 48-hour sample. The fraction mass-loss is calculated as:

$$\%weathering = (m_i - m_f) / (m_i - m_e) \times 100\%,$$

where, *%weathering* is the percentage evaporative mass-loss over the 48 hour period, m_i is the initial mass of the flask and oil, m_f is the final mass of the flask and oil, and m_e is the mass of the empty flask. A graph of *%weathering* as a function of time is plotted using the interval weighing data.

The times for one-third ($t_{1/3}$) and two-thirds ($t_{2/3}$) of the final mass loss are interpolated from the time-weathering graph. Typical times for $t_{1/3}$ range from 30 minutes to 2 hours, for $t_{2/3}$, 8 to 12 hours.

This technique allows for precise control of the evaporative weight loss for a target oil, and can be directly correlated to compositional changes of the target weathered oil. By tracking weight loss as a function of time, an equation for predicting evaporation can be found. Also, from this same graph, it is possible to determine a point at which the evaporation rate is sufficiently slow that the oil may be considered to have achieved the maximum evaporative loss likely to be observed under the conditions of a marine spill.

3.4 Equation(s) for Predicting Evaporation

The evaporation kinetics, reported as percentage mass loss as a function of time, are determined for each oil by measuring the weight loss over time from a shallow dish (Fingas 97, Fingas 98a, Fingas 01). Approximately 20 g of oil is weighed into a 139mm petri dish. Measurements are conducted in a climate-controlled chamber at 15 °C. Temperatures are monitored by a digital thermometer. The oil weight is recorded by an electronic balance accurate to 0.01 g at geometrically increasing intervals and collected on a computer logging system. Near the anticipated end of the run, the measurement interval is reset such that the number of points near the beginning and end of the run are approximately equal. The evaporation period can last from a few days for light oils to weeks for heavier products.

The time *versus* weight loss data series are fitted to a set of simple equations. From long experience (Fingas 98a, Fingas 01), either a square-root or a natural logarithm function is chosen as the simplest, most representative equation for evaporative mass loss. The best-fit equations have the form:

$$\%Ev = (A + B\,T)\ln t$$
$$\%Ev = (A + B\,T)\,t^{1/2}$$

where: *%Ev* is weight-percent evaporated, *T* is the oil surface temperature (°C), *t* is time (in minutes), and *A* and *B* are constants fitted to the measured data.

The apparatus is periodically checked by conducting a run with a 15-g mass in place of the oil.

3.5 Method for Determining Sulphur Content

The mass fraction of atomic sulphur in oil is determined using X-ray fluorescence by closely following ASTM method D 4294.

The XRF spectrometer is calibrated using a duplicate series of six NIST sulphur-in-oil standards. A linear calibration chart is prepared from the twelve standard measurements. Single element standards are used to calibrate and remove chlorine interference in the sulphur signal. Instrument and operator performance is monitored by a triplicate measurement of a check standard consisting of a known crude oil. Check standard measurements are tracked on a quality control chart.

Approximately 3 g of oil is weighed out into 31mm HDPE XRF cells, sealed with 0.25 mm thick mylar film. The sealed cells are measured on a Spectro Titan XRF spectrometer. Each unknown is measured in triplicate and the mean reported as the final value.

3.6 Method for Determining Water Content

The mass fraction of water in oil or an emulsion, expressed as a percentage, is determined by Karl Fischer titration using a Metrohm 701 automatic titrator. The method used closely follows ASTM method D 4377. The Karl Fischer reaction is an amine-catalyzed reduction of water in a methanolic solution:

$$CH_3OH + SO_2 + RN \rightarrow [RNH]^+ [SO_3CH_3]^-$$
$$2RN + H_2O + I_2 + [RNH]SO_3CH_3 \rightarrow [RNH]^+ [SO_4CH_3]^- + 2\,[RNH]^+ I^-$$

The amine, RN, or mixture of amines is proprietary to each manufacturer.

A sample of oil or emulsion in the range of 50 to 100 mg is accurately weighed and introduced to the reaction vessel of the autotitrator. A solution of 1:1:2 (by volume) mixture of methanol:chloroform:toluene is used as a working fluid. The autotitrator is loaded with 5-mg/mL, pyridine-free Karl Fischer reagent from a certified supplier. Samples are repeated in triplicate and the mean reported as the water percentage. The instrument calibration is checked by a series of five replicate titrations of 25 µL of distilled, deionized water.

3.7 Method for Determining Flash Point

The flash point of an oil or product sample, in degrees Celcius, is determined by one of two methods, depending on the sample. Lower viscosity samples, including light fuel oils and most crudes, are measured using a Herzog HFP 362 TAG2 analyzer (Figure 2), following ASTM method D 1310. Heavier samples, such as intermediate and heavy fuel oils or highly weather crude oils, are measured using a Herzog 360 Pensky-Martens analyser, following ASTM D 93.

In both methods, 50 to 70 mL of sample is measured into the flash point cup (Figure 3), then the method program initiated. Pre-cooling of the instrument is necessary for subambient flash points. Samples are repeated in triplicate and the mean reported. Flash points below -10 °C or above 110 °C are confirmed in duplicate and reported as outside of the measurable temperature range.

Figure 2 Flashpoint tester.

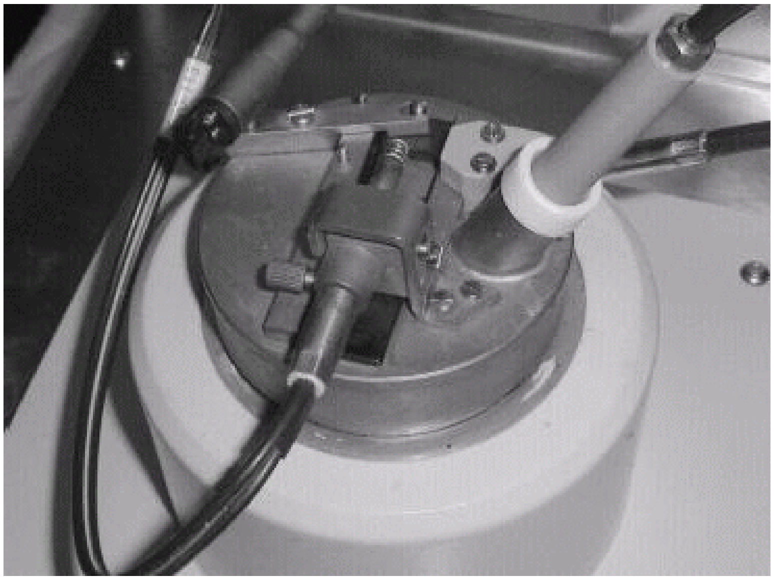


Figure 3 Flashpoint tester cup in TAG configuration.

Reagent-grade *p*-xylene is periodically measured by both the TAG2 and the Pensky-Martens methods as a check on instrument and operator performance. A control chart is kept of the results.

3.8 Method for Determining Pour Point

The pour point of an oil sample, in degrees Celsius, is determined by following ASTM method D 97. Two aliquots of sample are poured into test jars (as described by ASTM D 97), stopped and fixed with ASTM 5C or 6C thermometers, as appropriate.

Pour point is determined, as described in ASTM D97, by tilting the test jar to the horizontal and observing the flow of the sample past the fill mark on the jar. If no flow is visible after 5 seconds, the pour point is considered to have been reached. When the pour point is reached, 3 °C is added to the temperature recorded. The average of the two measurements is reported as the pour point.

If the samples are below their pour point at room temperature, then they are heated to 50 °C in a glycol-filled heat bath. The bath temperature is lowered until the pour point is reached. If samples are liquid at room temperature, they are cooled in the glycol bath to -5 °C, and measured at intervals as described by ASTM method D 97. Further cooling, if required, is done first to -20 °C and then -30 °C in a series of refrigerators and finally to -56 °C in an acetone/dry ice bath.

3.9 Method for Determining Density and API Gravity

The density of an oil sample, in g/mL, is measured using an Anton Parr DMA 48 digital density meter following ASTM method D 5002 (Figure 4). Measurements are performed at 0.0 °C and 15.0 °C. The instrument is calibrated using air and distilled, deionized water at each temperature. Method and operator performance is monitored by periodic measurement of a check standard fo *p*-xylene at 15.0 °C. A method control chart is kept of these measurements.

Figure 4 Digital densitometer taking a reading.

Densities are corrected for sample viscosity, as specified by the instrument manufacturer. Measurements are repeated in triplicate and the mean reported as the density.

API gravity (API 82) is calculated using the standard formula for the specific gravity of an oil at 60 °F (15.56 °C). The oil density at 15.56 °C is estimated by exponential extrapolation from the 15.0 °C and 0.0 °C data points. This is converted to specific gravity by division by the density of water at 15.5 °C, using the following equation:

$$s.g.^{15.56} = \rho^0 \;\exp\left[\left(\ln \rho^{15} - \ln \rho^0 \right)/15 \times 15.56 \right] / \rho\,(H_2O)^{15.56}$$

where: $s.g.^{15.56}$ is the specific gravity of the oil or product at 15.56 °C (60 °F), ρ^0 and ρ^{15} are the measured oil densities at 0 °C and 15 °C, respectively, and $\rho\,(H_2O)^{15.56}$ is the literature value for the density of water at 15.56 °C. The API Gravity is then determined using the formula (API 82):

$$API = 141.5 / (s.g.^{15.56}) - 131.5$$

3.10 *Method for Determining Dynamic Viscosity*

The dynamic viscosity of an oil sample, in mPa.s or cP, is measured using a Thermo-Haake VT550 viscometer using standard NV and SV1 cup-and-spindle sensors (Figure 5). Measurements are made at 0.0 °C and 15.0 °C. The instrument is calibrated with ASTM-traceable standards at 15.0 °C. Check standards of pure ethylene glycol and glycerine are used to validate the NV and SV1 methods respectively. Control charts are kept for each set of sensors, based on the ethylene glycol measurements at 15.0 °C for the NV sensors and glycerine measurements at 20.0 °C for the SV1 sensors.

Figure 5
Viscometer.

From a qualitative observation of the oil either the NV or the SV1 sensor is chosen to measure the sample. The NV sensor is used for oils with viscosities below 100 cP, the SV1 sensor, for oils above 70 cP. In both cases, the measurement cup is filled with 9.1 mL of sample. The sensor is mounted onto the instrument and the sample volume is adjusted to the proper level. The sample is allowed to equilibrate for 15 minutes for 15.0 °C measurements, or 30 minutes at 0.0 °C. Samples and sensors are kept chilled at the appropriate temperature prior to use.

For the NV sensor, the rotational shear rate is set at 1000/s, the SV1 sensor at 50/s. If the oil is observed to be non-Newtonian, single samples are run at shear rates of 1/s, 10/s and 50/s. In all cases, the sensors are ramped up to speed over a period of five minutes. The viscosity is measured for a subsequent five minutes, sampled once per second. The viscosity reported is that at time zero of the second, constant-shear rate interval. This may be obtained by the mean of the constant-shear rate interval data or by linear fit to the time-viscosity series if friction-heating has occurred during the measurement. For Newtonian samples, triplicate measurements are averaged and the mean reported as the absolute or dynamic viscosity. For non-Newtonian samples, viscosities are reported for each of the three shear rates.

3.11 Method for the Evaluation of the Stability of Emulsions Formed from Saline and Oils and Oil Products

Water-in-oil emulsions are formed in 2.2-litre fluorinated vessels on an end-over-end rotary mixer (Associated Design, VA) at a nominal rotational speed of 50 RPM (Jokuty 95, Fingas 98b).

(1) A 600-mL volume of salt water (3.3% w/v NaCl) is dispensed into a mixing vessel.
(2) A 30-mL aliquot of oil is added to each vessel for a 1:20 oil:water ratio.
(3) The vessels are sealed and placed in the rotary mixer such that the cap of each mixing vessel follows, rather than leads, the direction of rotation. The rotary mixer is kept in a temperature controlled cold room at 15 °C .
(4) The vessels and their contents are allowed to stand for approximately 4 hours before rotation begins, then mixed continuously for 12 hours.
(5) At the conclusion of the mixing time, the emulsions are collected from the vessels for measurement of water content, viscosity and the complex modulus. The emulsions are stored in the cold room at 15 °C for one week, then observed for changes in physical appearance.

Emulsions are classified into one of four stability classes: unstable, entrained water, meso-stable (Figure 6) and stable (Figure 7) . Water content for the emulsions is measured using method 5.6 Method for Determining Water Content. The complex modulus is measured on an RS300 RheoStress rheometer using a 35 mm plate-plate geometry. A stress sweep is performed in the range 100 to 10,000 mPa in the forced oscillation mode at a frequency of 1 Hz. The complex modulus value in the linear viscoelastic region is reported.

Figure 6 Meso-stable emulsion of Alberta Sweet Mix Blend #5 (ASMB#5) and 33‰ brine.

Figure 7 Stable emulsion of Sockeye (1991) and 33‰ brine.

3.12 Method for Determining the Chemical Dispersibility of an Oil or Oil Product

This method determines the relative ranking of effectiveness for the dispersibility of an oil sample by the surfactant Corexit 9500. This method follows closely ASTM F2059.

A pre-mix of 1:25.0 dispersant:oil is made up by adding oil to 100mg of dispersant (approximately 2.50mL of oil in total).

Six side-spout Erlenmeyer flasks, as described in ASTM F2059, containing 120 mL of 33‰ brine are placed into an incubator-shaker. An aliquot of 100 µL of premix is added to the surface of the liquid in each flask, care being taken to not disturb the bulk brine. The flasks are mechanically shaken at 20.0 °C with a rotation speed of 150 rpm for exactly 20 minutes (Figure 8). The solutions are allowed to settle for 10 minutes.

Figure 8 Shaker flasks for dispersant effectiveness testing in shaker/incubator.

Using the side spout, 30 mL of the oil-in-water phase is transferred to a 250 mL separatory funnel, first clearing the spout by draining 3 mL of liquid. The 30 mL aliquot is extracted with 3×5 mL of 70:30 (v:v) dichloromethane:pentane, collected into a 25-mL graduated cylinder (Figure 9).

Sample analysis done using a GC/FID to determine the oil concentration in the solvent. A 900 µL aliquot of the 15-mL solvent extract is combined with 100 µL of internal standard (200 ppm of 5-α-androstane in hexane) in a crimp-top injection vial and shaken well. Total petroleum hydrocarbon content of the sample is quantified by the internal standard method using the total resolved peak area (RPA) and the average hydrocarbon response factor over the entire analytical range:

$$RPH = A_{TOTAL}/A_{I.S.}\ /RRF \times 20 \times 15 \times 120\ /30\ /0.9$$

Where RPH is the resolved petroleum hydrocarbon (mg/mL), A_{TOTAL} is the total resolved peak area, $A_{I.S.}$ is the internal standard peak area and RRF is the average relative response factor for a series of alkane standards covering the analytical range.

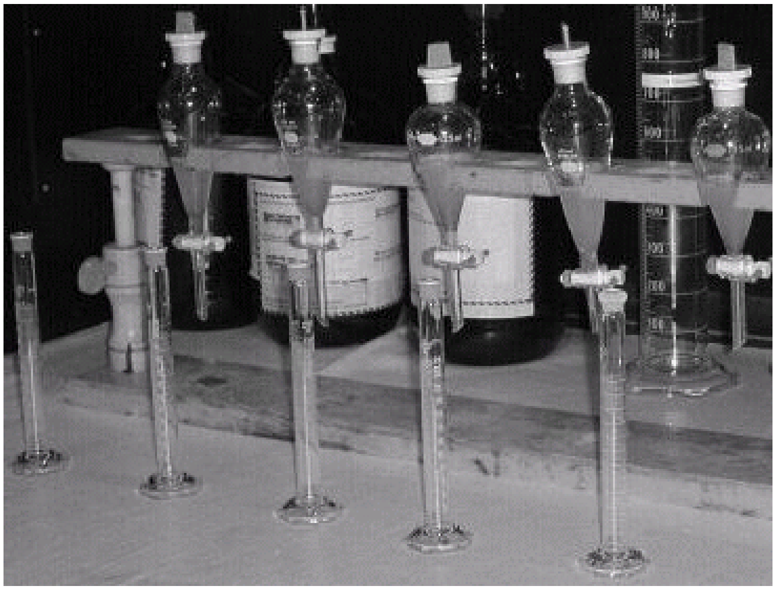


Figure 9 Aqueous to methylene chloride extraction for dispersant effectiveness testing.

The method is calibrated using a series of six oil-in-solvent mixtures prepared from the premix for each oil. The volume of premix dispersant/oil solution for each standard is selected to represent a percentage efficiency of the dispersed oil. The volume of the premix is then carefully applied to the surface of the brine in a shaker flask and shaken exactly as one of the samples, as described previously. Upon removal from the shaker however, the entire contents of the flask is transferred to the separatory funnel. This is extracted with 3×20 mL of 70:30 (v:v) dichloromethane:pentane and made up to 60 mL. Chromatographic quantitation is then performed using the formula:

$$RPH = A_{TOTAL}/A_{I.S.}\ /RRF \times 20 \times 60 \times 120\ /120\ /0.9$$

The RPH values as a function of %effectiveness for the calibration standards are plotted. The sample RPH values are then used to determine the %effectiveness of the dispersant.

The results of this test provide a means of ranking effectiveness of dispersant/oil combinations relative to each other, but do not directly imply the effectiveness for any other specific conditions. This is due to the broad range of parameters affecting dispersant effectiveness: turbulent energy, time of mixing, dosage rate, brine salinity, temperature, evaporative loss, dilution, settling time and thoroughness of the mixing between dispersant and oil.

3.13 *Method for the Determination of the Hydrocarbon Group Constituents*

The asphaltene and resin mass fractions (Speight 91) of an oil or oil product are determined gravimetrically. The asphaltene precipitation is a minor variation on the procedure given in ASTM method D 2007. The saturate fraction (F1) and aromatic fraction (F2) are calculated by mass-balance from the total petroleum hydrocarbon measurement, method 3.17, following. Wax content is determined by summing the individual areas for the *n*-alkanes *n*-C_{18} upto *n*-C_{120} in the simulated boiling point chromatograms, obtained in method 3.16.

A 60 mL quantity of *n*-pentane is added to a pre-weighed sample of approximately 5g of oil. The flask is shaken well and allowed to stand for 30 minutes. The sample is filtered through a 0.45-μm membrane using a minimum of rinsings of *n*-pentane. The precipitate is allowed to dry then weighed. The weight of the precipitate as a fraction of the initial oil sample weight is reported as the percentage asphaltenes (Figure 10).

The filtrate from the precipitation, the "maltene" fraction, is recovered and made up to 100 mL with *n*-pentane. A 15-g, 1-cm diameter column of activated silica gel is prepared. The top of the column is protected by a 1-cm layer of sodium sulphate. A 5-mL aliquot of the maltene fraction is loaded onto the column. A 60-mL volume of 1:1 (v:v) benzene:hexane is eluted through the column and discarded. A 60-mL volume of methanol, followed by a 60-mL volume of dichloromethane are eluted through the column and combined. The methanol/dichloromethane fractions are reduced by rotary evaporation and blown down to dryness under nitrogen. The mass fraction of this dried eluent, compensating for the volume fraction used, is reported as the percentage of resins in the sample (Figure 11).

Measurements are repeated three times for each sample and the means are reported as the final values.

Figure 10 Asphaltenes after filtering and drying.

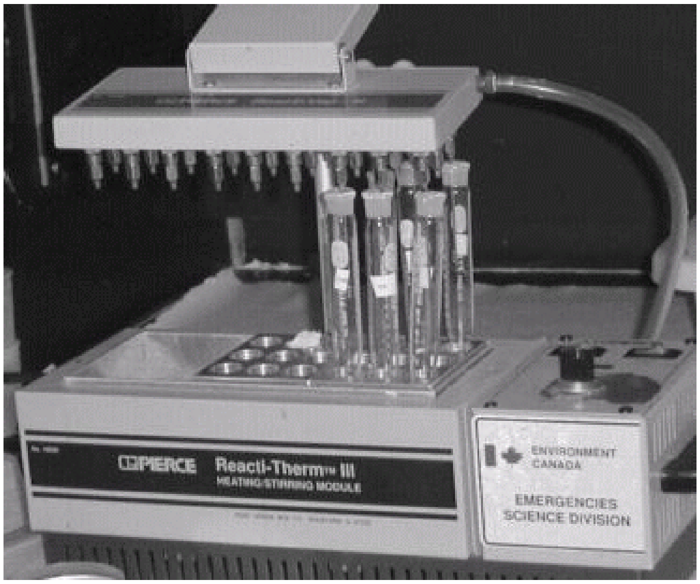


Figure 11 Resin samples being reduced under dry nitrogen.

3.14 Method of Determining Adhesion

An analytical balance is prepared by hanging an ASTM method D 6 standard penetrometer needle from the balance hook and allowing the apparatus to stabilize and tare. Approximately 80 mL of oil sample is poured into a 100-mL beaker. The beaker is elevated until the oil reaches the top of the stainless steel needle, but not touching the brass support shaft. The needle is kept immersed in oil for 30 seconds. The beaker is then lowered until the needle is clear of the oil. The system is left undisturbed, closed inside a draft shield. After 30 minutes the weight of the oil adhering to the needle is recorded. The mass of the oil divided by the surface area of the needle is the adhesion of the oil in g/cm^2. Four measurements are taken for each oil sample and the mean reported as the final value (Jokuty 96).

3.15 Method of Determining Surface and Interfacial Tensions

Surface and interfacial tensions, in mN/m, are measured using a Krüss K10 Tensiometer by the de Noüy ring method (Figures 12 and 13). The experimental method used follows closely ASTM method D 971. The instrument calibration is checked using a vendor-supplied weight. Method and operator performance is monitored by periodic measurement of the surface tension of *p*-xylene at 15 °C. A control chart is kept of the history of check standard measurements.

Figure 12 Digital tensiometer.

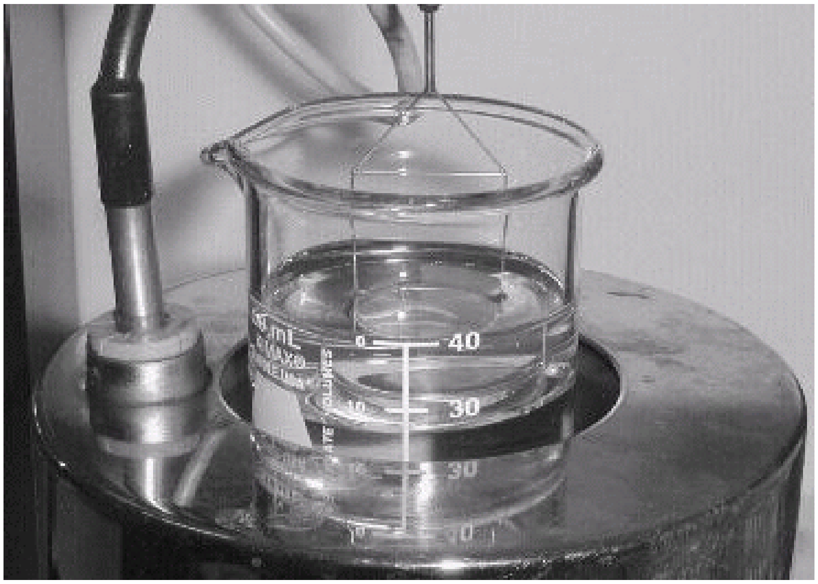


Figure 13 Close-up of du Nöuy ring interfacial tension measurement of 33‰ brine and diesel

For sample/air surface tensions, the measurement ring is first zeroed in air. A small amount of sample, approximately 15 mL, is poured into a 43-mm diameter vessel. The ring is dipped into the sample to a depth of no more than 5 mm, then pulled up such that it is just visible on the surface of the liquid. The system is allowed to rest for 30 seconds. The measurement is initiated, automatically terminating when the upward pulling force on the ring just balances the downward force exerted by the liquid. The apparent surface tension, σ_{APP}, is recorded.

For sample/water and sample/brine (3.3% w/v NaCl) interfacial tensions, the ring is zeroed in the sample at a depth of not more than 5 mm. The ring is removed and cleaned. A 25-mL volume of water or brine is dispensed into a 43-mm diameter vessel. The ring is dipped 5 mm into the aqueous phase. A 10-mL to 15-mL volume of sample is carefully poured down the side of the vessel wall, with great care taken so as to disturb the aqueous/oil interface as little as possible. The ring is then raised to the bottom on the interface and the system is allowed to rest for exactly 30 seconds. The measurement is started and the apparent interfacial tension is recorded, σ_{APP}, when the force balance is reached.

The apparent surface tension is corrected for mass of the upper phase lifted by the ring during measurement using the Zuidema and Waters correction:

$$\sigma=\sigma_{APP}\left(0.7250+\sqrt{\frac{1.452\sigma_{APP}}{C^2(D-d)}+0.04534-\frac{1.679}{R/r}}\right)$$

where: σ is the interfacial tension, σ_{APP} is the instrument scale reading, C is the ring diameter, D is the density of the lower phase, d is the density of the upper phase, R is the radius of the du Noüy ring, and r is the radius of the ring wire. Measurements are made at 0.0 °C and 15.0 °C and repeated in triplicate. Samples, aqueous phases and glassware are all kept at temperature for a minimum of 30 minutes before measurement. The mean of at least three corrected interfacial tensions is reported as the measured value.

3.16 Method for Determining the Simulated Boiling Point Distribution

This analysis is performed on an Analytical Controls SIMDIS analyser, a modified Hewlett-Packard 5890 series II gas chromatograph. The system has a custom cryogenically-cooled inlet and a high-temperature column. Reference and calibration mixtures are run according to Analytical Controls specifications.

Oil samples are made up as 2% (m/m) solutions in carbon disulphide. An aliquot of 0.5 µL is injected into the inlet. The inlet temperature program runs from 40 °C to 430 °C a 70 °C per minute. The oven temperature program runs from -20 °C for 1 min, ramp at 10 ^{0}C/min to 430 ^{0}C, and hold for 3 minutes at this final temperature. The flame ionization detector operates at 430 °C.

The Analytical Controls Software outputs a series of simulated boiling point ranges as a function of temperature and has the option of producing a “wax report” for the relative abundances of all *n*-alkanes in the oil sample.

3.17 Method for the Determination of Individual (n–Alkanes and Isoprenoids) and Total Petroleum Hydrocarbons (TPH), Polycyclic Aromatic Hydrocarbons (PAHs) and Biomarker Triterpanes and Steranes in Oil and Oil-spill-related Environmental Samples (Water, Particulates and Soils/Sediments)

A chromatographic column with a PTFE-stopcock (10.5 mm I.D. x 200 mm length) is plugged with borosilicate glass wool at the bottom, and serially rinsed with methanol, hexane and dichloromethane, and allowed to dry. The column is dry-packed with 3 grams of activated silica gel with tapping to settle the silica gel, and topped with about 0.5 cm anhydrous sodium sulphate. The column is conditioned with 20 mL of hexane, and the eluent is discarded. Just prior to exposure of the sodium sulphate layer to air, a 200 µL of crude oil solution containing approximately 16 mg of oil (~80 mg/mL in hexane) is quantitatively transferred onto the column using an additional 3 mL of hexane to complete the transfer. All eluent up to this point is discarded. Twelve mL of hexane is used to elute aliphatic hydrocarbons, and 15 mL of 50% benzene in hexane (v/v) is used to elute aromatic hydrocarbons.

Half of the hexane fraction (labelled "F1") is used for analysis of aliphatics, triterpanes and steranes; half of the 50% benzene fraction is labelled "F2" and used for analysis of target PAHs and alkylated PAH homologues. The remaining half of F1 and F2 is combined into a fraction (labelled as "F3") and used for the determination of total petroleum hydrocarbons (TPH). These three fractions are concentrated under a stream of nitrogen to appropriate volumes, spiked with internal standards (5-α-androstane for GC-TPH and n-alkane determination, d_{14}-terphenyl for PAH analysis, and C_{30}-$\beta\beta$-hopane for biomarker analysis), and then adjusted to accurate preinjection volume of 0.5 mL for GC-MS and GC-FID analysis (see Figure 1 for oil analysis protocol).

The concentrations of individual n-alkanes, selected isoprenoids such as pristane and phytane, and total petroleum hydrocarbons are determined by high resolution capillary GC/FID using the following equation:

$$Concentration\ (\mu g / g) = 2 \times \frac{A_S\, W_{IS}\ D}{A_{IS}\ RRF\ W_S}$$

where:

A_S = Response for the analyte in the sample, units may be in area counts or peak height.

A_{IS} = Response for the internal standard in the sample, units same as A_s.

W_{IS} = Amount (µg) of internal standard added to the sample.

D = Dilution factor. If dilution was made on the sample prior to analysis. If no dilution was made, D = 1, dimensionless.

W_S = Weight of sample extracted, g. Either a dry or wet weight may be used, depending upon the specific application of the data.

Note that F1 and F2 are split in half for analyses, so the final concentration of individual analytes must be multiplied by 2 in the Equation.

Prior to sample analysis, the instrument is calibrated using a standard solution, which is composed of C_8 through C_{34} n-alkanes, and 5-α-androstane as the internal standard. A 5-point calibration is established demonstrating the linear range of the analysis. The relative response factor (RRF) for each hydrocarbon component is calculated relative to the internal standard. Total GC detectable petroleum hydrocarbons (TPH), defined as the sum of resolved plus unresolved aliphatic and aromatic hydrocarbons, is quantified by the internal standard method using the baseline corrected total area of the chromatogram. The RRF used for the determination of TPH is the average of the n-alkane relative response factors over the entire analytical range.

Quantitation of target PAHs, alkylated PAH, and dibenzothiophene homologues is performed on GC/MS in SIM mode with RRFs for each compound determined during instrument calibration. The ions monitored are 128, 142, 156, 170, and 184 for alkyl homologues of naphthalene; 178, 192, 206, 220, and 234 for phenanthrene alkyl series; 184, 198, 212, and 226 for dibenzothiophene alkyl series; and 166, 180, 194 and 208 for fluorene alkyl series. The RRF for target PAH compounds are calculated from authentic standards. PAH alkyl homologues are quantified by using the straight baseline integration of each level of alkylation. Although the alkylated homologue groups can be quantified using the RRF of the respective unsubstituted parent PAH compounds, it is preferable to obtain the RRFs directly from alkylated PAH standards, if they are commercially available. In this project, the RRFs obtained from 1-methyl-naphthalene, 2-methyl-naphthalene, 2,6-dimethyl-naphthalene, 2,3,5-trimethyl-naphthalene, and 1-methyl-phenanthrene are used for quantitation of 1-methyl-naphthalene, 2-methyl-naphthalene, C_2-naphthalene, C_3-naphthalene, and C_1-phenanthrene in oil, respectively. The RRFs of 2,3,5-trimethyl-naphthalene and 1-methyl-phenanthrene are used for quantification of C_4-naphthalene, and C_2-, C_3-, and C_4-phenanthrenes respectively. The selection criteria for the integration and reporting of each alkylated homologue are based primarily on pattern recognition and the presence of selected confirmation ions.

The average RRF for the biomaker compound C_{30} 17β(H) 21α(H)-hopane is determined relative to the internal standard C_{30} 17β(H) 21β(H)-hopane. The average RRF for C_{30} 17β(H) 21 α(H)-hopane (m/z 191) is used for quantitation of C_{30} 17α(H) 21β(H)-hopane and other triterpanes in the oil sample. For quantitation of steranes, the RRF of C_{29} 20R ααα-ethylcholestane monitored at m/z 217 is determined relative to C_{30} 17β(H) 21β(H)-hopane monitored at m/z 191, and then the average RRF of C_{29} 20R ααα-ethylcholestane is used for estimation of sterane compounds in the oil.

3.18 Analytical Method for Identification of BTEX Compounds and Alkyl Benzenes and Direct Determination of BTEX and (BTEX + C_3-benzenes) in Oils and Refined Products by Gas Chromatography / Mass Spectrometry

The identification of BTEX and other alkyl substituted benzene components in oils are accomplished based on mass spectral data, comparison of GC retention data with reference standards, and calculation of retention index values and comparison with those reported in the literature.

Quantitation of BTEX and (BTEX + C_3-benzenes) is accomplished by GC/MS using an internal standard method. The strict quality control measures are used in order to guarantee the precision and accuracy of analytical data. The GC/MS is carefully maintained and tuned daily to achieve the required sensitivity. Prior to sample analysis, the instrument is calibrated using a standard solution that is composed of 5 BTEX compounds, 6 C_3-benzene compounds, 2 C_4-, 2 C_5-, 1 C_6- and 1 C_7-benzene compounds. The internal standard used is d_{10}-ethylbenzene. A 5-point calibration curve that demonstrates the linear range (0.01 ppm to 200 ppm) of the analysis is established for each target compound. The RRFs for each compounds are calculated relative to the internal standard.

Oil samples are directly weighed and dissolved in n-pentane (without using any solvent evaporation and concentration step, which may result in the loss of BTEX compounds) to an approximately concentration of 2 mg/mL for GC/MS analysis. To achieve improved precision and accuracy of analytical data, the following refinements are implemented in addition to the routine quality control measures: (1) The oil solutions in vials are tightly capped to avoid any possible loss of volatile BTEX compounds, and are then put in a refrigerator for 30 minutes to precipitate the asphaltenes to the bottom of the vials in order to void performance deterioration of the column due to introduction of asphaltenes; (2) Blanks and calibration check standards are analyzed before and after each sample batch (about 7-10 samples) to monitor analysis precision; (3) C_3-benzenes in oil are quantified using the RRF directly obtained from the respective individual C_3-benzene standards instead of using the RRF obtained from benzene or C_1/C_2 substituted benzenes.

The concentration of the analyte of interest in the sample is determined using the following equation:

$$Concentration\ (\mu g\ /\ g) = \frac{A_S\ W_{IS}\ \ D}{A_{IS}\ \ RRF\ W_S}$$

where:

A_S = Response for the analyte in the sample, units may be in area counts or peak height.

A_{IS} = Response for the internal standard in the sample, units same as A_s.

W_{IS} = Amount (μg) of internal standard added to the sample.

D = Dilution factor, if dilution was made on the sample prior to analysis. If no dilution is made, D = 1. Dimensionless.

W_S = Weight of sample, in g.

The extensive qualitative and quantitative information obtained pertaining to alkylbenzenes is useful for evaluating weathering behaviour, potential toxicity, composition and concentration changes of oil in the short term following a spill. The data can be also used to evaluate the fate and transport of alkylated benzene compounds and other petroleum hydrocarbons in the environment and to assess the possible biological effects and damage of the spill to the environment and natural resources.

3.19 Method for the Determination of Trace Metals in Oil Samples

The metal content of an oil or oil product is determined by oxidation of the oil in hot acid, dissolution in aqueous solution then measurement by inductively-coupled plasma atomic emission spectroscopy (ICP-AES).

The oil sample is warmed in a water bath and mixed thoroughly. Approximately 1g of sample is weighed into a 150 mL teflon beaker. To the oil is added 0.5 mL of concentrated nitric acid and 1.5 mL of concentrated hydrochloric acid. The beaker is covered and heated on a 120 °C hotplate. The beaker is swirled gently until the mixture begins to fume. A further amount of 0.5 mL of concentrated nitric acid and 1.5 mL of concentrated hydrochloric acid is added to the beaker. The beaker is recovered and heated until approximately 0.5 mL of the mixture remains.

The acid-mixture is quantitatively filtered into a glass test tube through a Number 4 Whatman filter with a deionized water rinse. The solution is made up to 10.00 mL. The solution is mixed thoroughly by vortex and submitted to the ICP-AES for analysis.

The ICP-AES is calibrated with commercial multi-element aqueous standards and verified using a certified aqueous reference standard. The 29 metal analytes are determined from each respective calibration chart and corrected for the 10:1 dilution in sample preparation. Duplicate measurements are made for each sample. Method blanks, matrix blanks, and blind standards were included with the analyte samples to ensure method performance.

The ICP-AES analysis was performed under contract to Environment Canada by Caduceon Environmental Laboratories of Ottawa, Canada.

3.20 Method for the Sample Handling, Storage and Disposal of Oil and Oil Products

This method describes the procedures for the safe and non-destructive manipulation and sampling of hydrocarbon unknowns. Procedures are outlined for the reception and disbursal of samples to and from the laboratory, the handling of oil to avoid damaging the sample, the techniques necessary to obtain a representative sample and the safe storage and disposal of oil.

4. Summary of Quality Assurance and Quality Control (QA/QC) Plan

4.1 Quality Assurance Statement

As a federal government science and technology institute it has been one of our fundamental operating principles that the Oil Research Laboratory of the Emergencies Science and Technology Division (ESTD) of Environment Canada should set an example by adopting the most stringent standards possible for our work. A critical part of our official Mission Statement is to provide "specialized sampling and analytical expertise and services of the highest standards". Quality management has always been a fundamental element of our programs. We continue to refine our quality procedures and protocols whenever new information and processes become available. Our quality program is certified through SCC-CAEAL, the Standards Council of Canada/Canadian Association for Environmental Analytical Laboratories. Participation in the SCC-CAEAL accreditation program provides us a systematic, internationally recognized quality system. A quality web site has been created which provides staff with easy and fast access to all current and approved quality system documentation. The Emergencies Science and Technology Division QA/QC system includes the following:

-Laboratory profile, mission and organization;
-Quality system;
-Personnel;
-Methodology;
-Service, equipment and supplies;
-Facilities;
-Sample management;
-Data management;
-Work load management.

4.2 Quality Assurance in Chemical Composition Methods

The Oil Research Laboratory at Emergencies Science and Technology Division presently performs the following chemical measurements for crude oils, oil products, and oil-spill-related environmental samples: total petroleum hydrocarbons (TPH), total saturates, total aromatics, *n*-alkane distribution, oil-characteristic alkylated PAH homologous series, and other EPA priority PAHs, BTEX and alkyl-benzene compounds, biomarker triterpanes and steranes. The methods of *"Analytical Method for Identification of BTEX Compounds and Alkyl Benzenes and Direct Determination of BTEX and (BTEX + C3-benzenes) in Oils and Refined Products by Gas Chromatography/Mass Spectrometry" and "Analytical Method for the Determination of Individual n-Alkanes and Isoprenoids and Total Petroleum Hydrocarbons (TPH), Polycyclic Aromatic Hydrocarbons (PAHs), and Biomarker Triterpanes and Steranes in Oils, Petroleum Products, and Oil-spill-related Environmental Samples"* have been approved by SCC and CAEAL and have become official ETC methods.

Chromatographic techniques are used for analyses of oil chemical compositions. In addition to a formal quality control program, a number of specific measures have been added to the processing of oil samples to monitor quality control and to aid in assessment of the data quality with respect to the project objectives. An important part of this is the evaluation of specific QC samples for accuracy, precision, and potential contamination. Before sample analysis, a five point initial calibration composed of the target oil components (for example, n-alkanes and EPA priority PAHs) are established, demonstrating the linear range of the analyses. Check standards at the mid-point of the established calibration curves are run before and after each analytical batch of samples (7-10 samples) to validate the integrity of the initial calibration. The method of internal standards (such as EPA Method 8000 for PAH analysis) using the average relative response factors (RRF) generated from the linear initial calibration is used to quantify the target oil compounds. The RRF stability is a key factor in maintaining the quality of the analysis. Mass discrimination, that is the reduced response of high molecular weight components, must be carefully monitored. If there is a problem with mass discrimination, it can be minimized by trimming the capillary column and by replacing the quartz liner in the injection port. All samples and quality control samples are spiked with appropriate surrogate compounds to measure individual sample matrix effects associated with sample preparation and analysis. Method detection limits (MDL) studies of target compounds are performed according to the procedure described in the EPA protocol titled "Definition and Procedure for the Determination of the Method Detection Limit" (Code of Federal Regulations 40 CFR Part 136). Control charts of standards are prepared and monitored. Validations of analytes in the control chart should be no more than 25% from historical average.

Trace metal analysis was performed under contract by Caduceon Environmental Laboratories, a CAEAL-certfied laboratory in Ottawa, Canada. Each batch of samples contained reagent blanks, method duplicates and matrix-matched reference materials. Blind standards were also submitted with the oils for analysis. The ICP-AES was calibrated using commercial standards and verified against a certified reference standard.

4.3 Quality Assurance in Physical Property Methods

The ESTD Oil Research Laboratory performs the following physical property measurements on crude oils and oil products: adhesion, boiling point distribution, density/API gravity, dispersibility, evaporation equation, flash point, hydrocarbon group analysis, sulphur content, surface and interfacial tensions, viscosity, and water content. Many of these procedures are ASTM standard methods, and must meet the reproducibility and repeatability of the appropriate method. Others, however, are methods developed in-house and control systems are defined for them in the standard operating procedures (SOP) for those methods. The following table details the measurement procedures:

Adhesion	In-house Method
Boiling Point Distribution	Commercial Package
Density/API Gravity	ASTM D5002
Dispersibility	ASTM F2059
Evaporation Equation	In-house Method
Flash Point	ASTM D93 and ASTM D56

Hydrocarbon Group Analysis	In-house Method
Pour Point	ASTM D97
Sulphur Content	ASTM D4294
Surface and Interfacial Tensions	ASTM D971
Viscosity	In-house Method
Water Content	ASTM D4377

Two physical property methods are considered semi-quantitative: adhesion and pour point. For these methods, although the range of variability in the results is closely monitored, no calibrations, blanks or check standards are preformed. Note that while pour point is measured according to ASTM D97, no calibration or check standard is specified by that method. While the ASTM D97 reproducibility requirements are achieved, no further controls for pour point are used in the Emergencies Science and Technology Division Oil Research Laboratory.

Several physical property methods rely on a single instrument and involve a simple measurement with little sample manipulation. These measurements include: density/API gravity, the development of the evaporation equation, flash point, sulphur content, surface and interfacial tensions, viscosity and water content. For all of these methods, the instruments are calibrated as directed by the manufacturer or the appropriate ASTM method with chemical and/or gravimetric standards as appropriate. In addition, instrumental and operator performance is monitored by periodic measurement of check standards. A log is kept for each instrument, in which calibration and check standard measurements are recorded. The check standard measurements are monitored closely. Failure of the check standard measurement to fall within the smaller of either a historical 95% confidence limit or the appropriate ASTM required repeatability results in an investigation of the procedure. This investigation includes recalibration and measurement of the check standard until the desired precision and accuracy is reached.

Finally, the last class of physical property methods involve significant sample preparation, followed by a measurement by gas chromatography or gravimetry. These methods include: boiling point distribution, dispersibility, and hydrocarbon group analysis. The boiling point distribution is measured using a commercial package provided by Analytical Controls. The quality control for this procedure involves the minimization of the variance of a check sample chromatogram. The dispersibility test is defined by ASTM F2059 and uses the calibration and standard procedure defined by that method. The hydrocarbon group analysis is carried out under the same protocols as described for the other chromatographic techniques previously.

4.4 Example Method Quality Control Procedures

As examples, the QA/QC procedures follow taken from a typical physical property method, for Surface and Interfacial Tension (see method 5.15), and from the chemical composition method for determination of the oil characteristic alkylated PAH homologues and other EPA priority unsubstituted PAH compounds (see method 5.17):

From the Standard Operating Procedure for the determination of the oil characteristic alkylated PAH homologues and other EPA priority unsubstituted PAH compounds:

14. QUALITY CONTROL

14.1 Each laboratory that uses this method is required to operate a formal quality control program. The minimum requirements of this program consist of an initial demonstration of laboratory capability and the analysis of spiked samples as a continuing check on performance.

The laboratory is required to maintain performance records to define the quality of data that is generated. Ongoing performance checks must be compared with established performance criteria to determine if the results of analyses are within accuracy and precision limits expected of the method.

14.2 The reliability of this method is dependent on the quality control procedures followed with each analytical batch (approximately 7-10 samples), one procedure blank, one check standard, and one standard oil are analyzed.

14.3 Initial Calibration and Continuing Calibration Check

14.3.1 Prior to the use of this method, a five-point response factor calibration curve must be established showing the linear range of the analysis. Each calibration standard is analyzed and the response factor (RRF) for each compound at each concentration level is calculated.

14.3.2 A check standard at about the mid-point of the established calibration curve must be analyzed before and after each set of up to 7 samples or once per working day, whichever is more frequent, in order to determine the response factors for the analytes of interest relative to the initial calibration. The PAH calibration standard (NIST SRM 1491) contains 24 PAH compounds plus dibenzothiophene and 4 deuderated PAH surrogate compounds. d_{14}-terphenyl is added to purified sample extract prior to GC/MS analysis as an internal standard.

14.3.3 The percent difference between the response factors in the check standard and those of the initial calibration is calculated using Equation 9:

$$Difference(\%) = \frac{(RRF_I - RRF_C)}{RRF_I} \times 100\% \tag{9}$$

where:
RRF_I *= Average response factor from the initial calibration*
RRF_C *= Response factor from continuing calibration*

If the difference of response factors is within 20%, analyses may proceed. If not, a five-point calibration curve must be repeated for that compound prior to analysis of the sample.

14.3.4 RRF stability is a key factor in maintaining the quality of the analysis. Mass discrimination, that is the reduced response of high molecular weight compounds, must be carefully monitored. The ratio of RRF of n-C_{32} to n-C_{21} should not be allowed to fall below 80% in the check standard. If there is a problem with mass discrimination, it can be reduced by trimming the first 20 cm of the capillary column and by replacing the quartz *liner in the injection port.*

14.4 Procedural Blank Analysis

14.5 Surrogate Compounds Analysis

14.5.1 All samples and quality control samples are required to be spiked with surrogate o-terphenyl (OTP). OTP is spiked into sample prior to extraction. This will measure individual sample matrix effects associated with sample preparation and analysis. Recovery of surrogate OTP should be within 60% to 120%. If the recovery for any surrogate standard does not fall within the control limits for method performance, the following corrective actions can be taken:

(1) Check calculations to ensure there are no errors.
(2) Check instrument performance and initial standard and surrogate solutions for degradation, contamination or other possible problems.
(3) reanalyze the sample or extract if the steps above fail to reveal a problem. If reanalysis yields surrogate recoveries within the stated limits, the reanalysis data will be used.

14.5.2 If the surrogate could not be measured because the sample diluted prior to analysis, or surrogate co-elutes with a compound, no corrective action needs be taken.

14.6 A control chart of the standard should be prepared and monitored. Variations of analytes in the control chart should be no more than 25% from historical average.

14.7 Detection Limit
Under optimum conditions an instrumental detection limit of 8 pg/μL per PAH target analyte (mean value) can be achieved.

14.8 GC Resolution
The target compounds, surrogate and internal standards must be resolved from one another and from interfering compounds. Potential problems may arise from the lack of baseline resolution of these compounds. Corrective action must be taken to correct resolution problem, i.e. rerun samples with a different temperature program.

From the Standard Operating Procedure for the determination of surface and interfacial tensions:

10 QUALITY CONTROL

10.1 Each laboratory that uses this method is required to operate a formal quality control program. The minimum requirements of this program consist of an initial demonstration of laboratory capability and the analysis of reference standards as a continuing check on performance.

10.2 The laboratory is required to maintain performance records to define the quality of data that is generated. Ongoing performance checks must be compared with established performance criteria to determine if the results of analyses are within accuracy and precision limits expected of the method.

10.3 Before performing any analysis, the analyst must demonstrate the ability to generate acceptable accuracy and precision with this method.

10.4 A method log book is maintained, containing all instrumental maintenance and calibration and check standard measurements.

10.5 The instrument is calibrated using a standard weight provided by the manufacturer. The instrument calibration is checked before each batch of samples and recorded in the log book. If the instrument calibration is outside the manufacturer’s parameters, the cause must be investigated and the fault corrected.

10.6 A check standard of p-xylene is used to define the operating characteristics of the instrument. Before each batch of samples is measured, a sample of reagent grade p-xylene is measured in triplicate at 15 °C. These measurements are noted in the instrument log book and tracked to ensure instrument and operator performance.

10.7 If the check standard falls outside the historical 95% confidence limit, as tracked by a control plot, the instrument function and/or operator technique is corrected as necessary. ASTM method D971 requires a repeatability of 4%, approximately ±1.2 mN/m. Measurements are not to be taken until the check standard measurements fall within the acceptable range for accuracy and precision.

5. Physical Properties and Chemical Composition of Alaska North Slope Crude Oil (2002)

5.1 Origin:

Origin: Alaska, U.S.A (the oil was drawn as a line sample off the TAPS pipeline where it spurs off to the Petrostar Refinery in Valdez on March 19, 2002)

Synonyms: ANS

Appearance: Brown-black, light, little odour, fine black particulates dispersed through-out liquid.

Values are reported for the **fresh oil** and for artificially weathered fractions of **10.0%**, **22.5%** and **30.5%** loss by weight.

5.2 API Gravity

30.89 *(calc)*

5.3 Equation for Predicting Evaporation

$$\%Ev = (2.86 + 0.045\ T) \ln t$$

Where: %Ev = weight percent evaporated; T = surface temperature (°C); t = time (minutes)

5.4 Sulphur Content

Weathering (weight %)	Sulphur (weight %)	
0	1.11	*(n=3)*
10.0	1.20	*(n=3)*
22.5	1.38	*(n=3)*
30.5	1.50	*(n=3)*

5.5 Water Content

Weathering (weight %)	Water (volume %)	
0	< 0.1	*(n=3)*
10.0	< 0.1	*(n=3)*
22.5	< 0.1	*(n=3)*
30.5	< 0.1	*(n=3)*

5.6 Flash Point

Weathering (weight %)	Flash Point (°C)	
0	<-8	*(n=3)*
10.0	19	*(n=3)*
22.5	75	*(n=3)*
30.5	115	*(n=3)*

5.7 Density

Weathering (weight %)	Temperature (°C)	Density (g/mL)	
0	0	0.8777	*(n=3)*
	15	0.8663	*(n=3)*
10.0	0	0.9054	*(n=3)*
	15	0.8940	*(n=3)*
22.5	0	0.9303	*(n=3)*
	15	0.9189	*(n=3)*
30.5	0	0.9457	*(n=3)*
	15	0.9340	*(n=3)*

5.8 Pour Point

Weathering (weight %)	Pour Point (°C)	
0	-32	*(n=2)*
10.0	-20	*(n=2)*
22.5	-9	*(n=2)*
30.5	-6	*(n=2)*

5.9 Dynamic Viscosity

Weathering (weight %)	Temperature (°C)	Viscosity (cP)	
0	0	23.2	*(n=3)*
	15	11.5	*(n=3)*
10.0	0	76.7	*(n=3)*
	15	31.8	*(n=3)*
22.5	0	614	*(n=2)*
	15	152	*(n=3)*
30.5	0	4230	*(n=2)*
	15	624.7	*(n=2)*

5.10 Chemical Dispersibility

Weathering (weight %)	Chemical Dispersibility using Corexit 9500 (%)	
0	47	*(n=6)*
10.0	45	*(n=6)*
22.5	34	*(n=6)*
30.5	15	*(n=6)*

5.11 Adhesion

Weathering (weight %)	Adhesion (g/m^2)	
0	20	*(n=4)*
10.0	35	*(n=4)*
22.5	38	*(n=4)*
30.5	40	*(n=4)*

5.12 Surface and Interfacial Tensions

5.12.1 Surface Tension (Oil/Air Interfacial Tension)

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	27.3	*(n=3)*
	15	26.4	*(n=3)*
10.0	0	29.8	*(n=3)*
	15	28.4	*(n=3)*
22.5	0	31.2	*(n=3)*
	15	30.4	*(n=3)*
30.5	0	33.1	*(n=3)*
	15	31.8	*(n=3)*

5.12.2 Oil/Brine (33‰) Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	22.5	*(n=3)*
	15	20.2	*(n=3)*
10.0	0	25.3	*(n=3)*
	15	23.1	*(n=3)*
22.5	0	26.8	*(n=3)*
	15	24.2	*(n=3)*
30.5	0	30.1	*(n=3)*
	15	25.6	*(n=3)*

5.12.3 Oil/Fresh Water Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	26.7	*(n=3)*
	15	23.6	*(n=3)*
10.0	0	28.1	*(n=3)*
	15	25.5	*(n=3)*
22.5	0	30.8	*(n=3)*
	15	27.7	*(n=3)*
30.5	0	33.2	*(n=3)*
	15	30.2	*(n=3)*

5.13 Emulsion Formation

Weathering (weight %)	Visual Stability	Complex Modulus (Pa)	Emulsion Water Content (%)
0	Unstable		
10.0	Unstable		
22.5	Unstable		
30.5	Mesostable	155	72.9

5.14 Boiling Point Distribution

	Cumulative Weight Fraction (%)			
Boiling Point (°C)	0% weathered	10.0% weathered	22.5% weathered	30.5% weathered
40	2.5	0.1		
60	3.9	0.5		
80	6.5	1.4		
100	10.0	3.6		
120	13.4	6.6	0.1	
140	16.6	9.8	0.6	
160	19.8	13.1	2.0	
180	22.6	16.3	4.4	
200	25.2	19.2	7.3	0.5
250	32.6	27.4	16.6	7.5
300	40.7	36.4	27.0	18.7
350	49.5	46.1	38.2	31.1
400	57.7	55.3	48.7	42.8
450	66.0	64.5	59.3	54.5
500	72.8	72.1	68.2	64.2
550	79.0	79.0	76.0	72.8
600	84.1	84.7	82.6	79.9
650	88.4	89.5	88.0	85.8

5.15 Hydrocarbon Groups

Component	Concentration (weight %) 0% weathered	10.0% weathered	22.5% weathered	30.5% weathered
Saturates	75.0	72.1	69.2	64.8
Aromatics	15.0	16.0	16.5	18.5
Resins	6.1	7.4	8.9	10.3
Asphaltenes	4.0	4.4	5.4	6.4
Waxes	2.6	2.9	3.3	3.6

5.16 Volatile Organic Compounds

Component	Concentration (µg/g oil) 0% weathered	30.5% weathered
Benzene	2866	0
Toluene	5928	0
Ethylbenzene	1319	0
Xylenes†	6187	0
C_3-Benzenes‡	5620	30
Total BTEX	16300	0
Total BTEX and C_3-Benzenes‡	21920	30

†“Xylenes” include *o*-, *m*-, and *p*-xylene isomers.
‡“C_3-Benzenes” include eight isomers.

5.17 *n*-Alkane Distribution

***n*-Alkane Component**	**Concentration (mg/g oil)** **0% weathered**	 **30.5% weathered**
n-C8	5.55	
n-C9	4.29	
n-C10	4.13	
n-C11	3.98	0.73
n-C12	3.71	2.51
n-C13	3.57	3.80
n-C14	3.42	4.58
n-C15	3.28	4.34
n-C16	3.15	4.05
n-C17	3.06	4.00
Pristane	1.89	2.41
n-C18	2.68	3.46
Phytane	1.41	1.80
n-C19	2.32	2.93
n-C20	2.11	2.71
n-C21	1.96	2.50
n-C22	1.90	2.45
n-C23	1.79	2.34
n-C24	1.65	2.16
n-C25	1.47	1.94
n-C26	1.27	1.73
n-C27	0.97	1.28
n-C28	0.78	1.03
n-C29	0.70	0.98
n-C30	0.56	0.69
n-C31	0.44	0.60
n-C32	0.31	0.43
n-C33	0.27	0.33
n-C34	0.24	0.31
n-C35	0.22	0.25
n-C36	0.11	0.14
n-C37	0.09	0.13
n-C38	0.07	0.10
n-C39	0.05	0.07
n-C40	0.03	0.06
n-C41	0.02	0.04
TOTAL	**63.4**	**56.9**
C17/PRISTANE	1.62	1.66
C18/PHYTANE	1.9	1.92
PRISTANE/PHYTANE	1.35	1.34
CPI	0.9	1.0

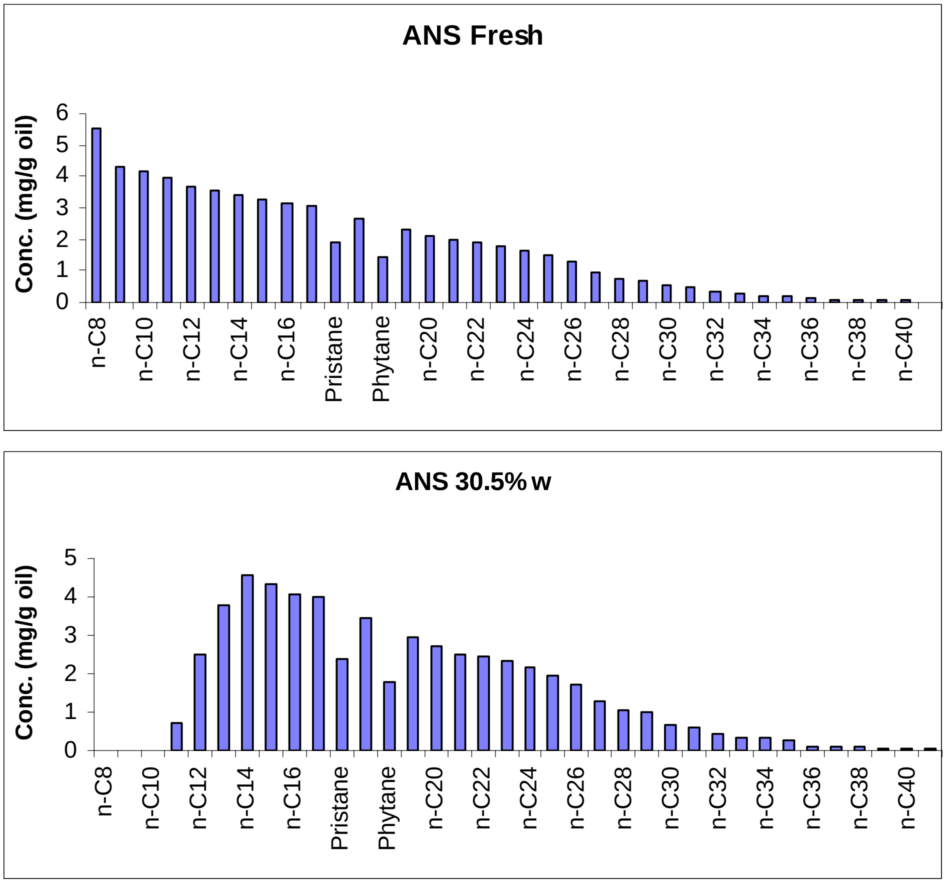


Figure 5.1 *n*–Alkane Distribution for Alaska North Slope crude oil (mg/g oil)

5.18 PAH Distribution

	Concentration (µg/g oil)	
Alkylated PAH	**0% weathered**	**30.5% weathered**
Naphthalene		
C0-N	261	167
C1-N	1015	1288
C2-N	1800	2716
C3-N	1702	2575
C4-N	815	1174
Sum	5594	7919
Phenanthrene		
C0-P	209	295
C1-P	666	932
C2-P	710	988
C3-P	486	707
C4-P	296	432
Sum	2368	3354
Dibenzothiophene		
C0-D	122	174
C1-D	225	319
C2-D	318	456
C3-D	265	362
Sum	931	1312
Fluorene		
C0-F	142	197
C1-F	328	449
C2-F	447	647
C3-F	379	525
Sum	1295	1819
Chrysene		
C0-C	48	68
C1-C	74	107
C2-C	99	141
C3-C	84	115
Sum	306	430
TOTAL	**10493**	**14834**
2-m-N/1-m-N	1.49	1.41
(3+2-m/phen)/(4-/9-+1m-phen)	0.76	0.76
4-m:2/3m:1-m-DBT	1 : 0.65 : 0.34	1 : 0.65 : 0.34
Other PAHs		
Biphenyl	134.71	176.9
Acenaphthylene	12.03	18.43
Acenaphthene	13.03	20.02
Anthracene	2.88	4.55
Fluoranthene	2.88	3.81
Pyrene	8.40	11.92
Benz(a)anthracene	4.64	8.11
Benzo(b)fluoranthene	5.14	7.49
Benzo(k)fluoranthene	0.50	0.70
Benzo(e)pyrene	10.28	14.74
Benzo(a)pyrene	2.26	3.69
Perylene	3.01	4.42
Indeno(1,2,3cd)pyrene	0.13	0.25
Dibenz(a,h)anthracene	0.63	1.02
Benzo(ghi)perylene	3.13	4.91
TOTAL	**204**	**281**

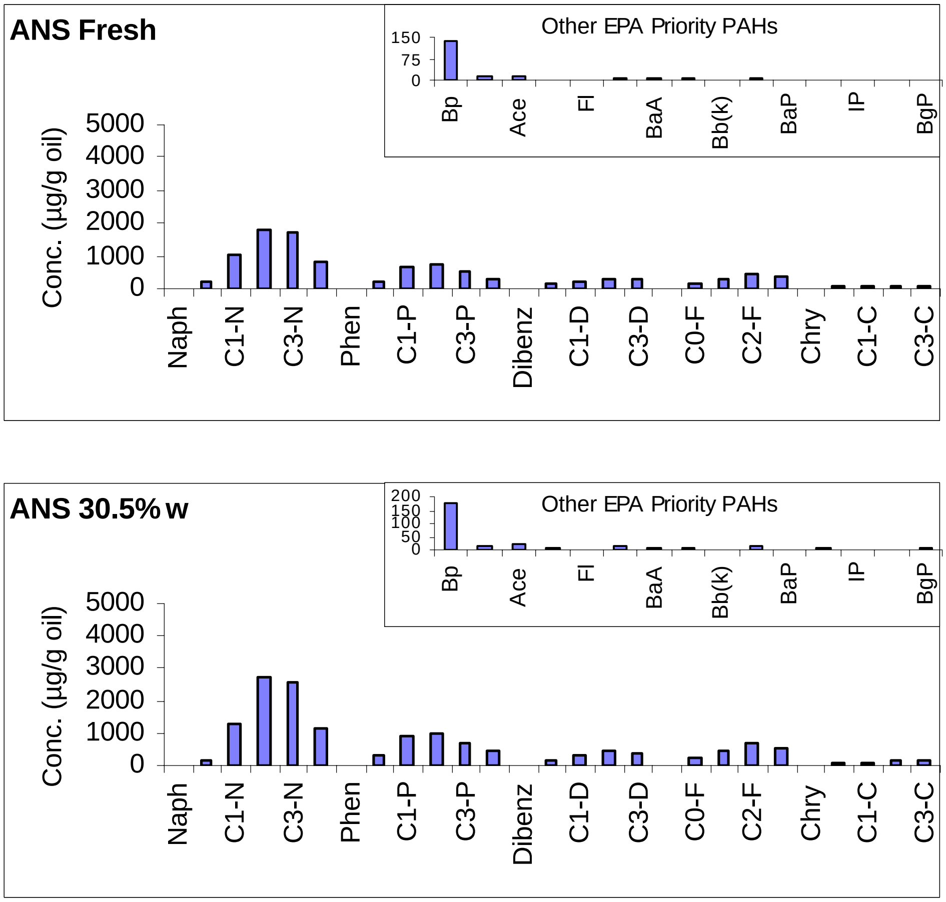


Figure 5.2 PAH Distribution for Alaska North Slope crude oil (µg/g oil)

5.19 Biomarker Concentrations

	Concentration (μg/g oil)	
Biomarker	**0% weathered**	**30.5% weathered**
C23	65.6	91.8
C24	40.8	57.8
C29	77.6	104.6
C30	116.6	161.1
C31(S)	46.9	64.1
C31(R)	33.0	46.1
C32(S)	34.2	46.5
C32(R)	21.6	30.9
C33(S)	21.6	31.0
C33(R)	13.3	19.3
C34(S)	15.1	21.0
C34(R)	8.6	12.4
Ts	20.9	31.8
Tm	28.5	43.0
C27αββ steranes	73.6	103.2
C29αββ steranes	84.2	113.8
TOTAL	**702**	**978**
Diagnostic Ratios		
C23/C24	1.61	1.59
C23/C30	0.56	0.57
C24/C30	0.35	0.36
C29/C30	0.67	0.65
C31(S)/C31(R)	1.42	1.39
C32(S)/C32(R)	1.58	1.51
C33(S)/C33(R)	1.62	1.60
C34(S)/C34(R)	1.76	1.70
Ts/Tm	0.73	0.74
C27αββ/C29αββ	0.87	0.91

6. Physical Properties and Chemical Composition of Alberta Sweet Mixed Blend (ASMB, Reference #5)

6.1 Origin:

Origin: Alberta, Canada (ESTD storage, originally from ESSO, Alberta, Canada)
Synonyms: ASMB #5

Values are reported for the **fresh oil** and for artificially weathered fractions of **12.6%**, **24.3%** and **36.8%** loss by weight.

6.2 API Gravity

35.72 *(calc)*

6.3 Equation for Predicting Evaporation

$$\%Ev = (3.35 + 0.045\,T) \ln t$$

Where: %Ev = weight percent evaporated; T = surface temperature (°C); t = time (minutes)

6.4 Sulphur Content

Weathering (weight %)	Sulphur (weight %)	
0	0.63	*(n=3)*
12.6	0.70	*(n=3)*
24.3	0.78	*(n=3)*
36.8	0.89	*(n=3)*

6.5 Water Content

Weathering (weight %)	Water (volume%)	
0	<0.1	*(n=3)*
12.6	<0.1	*(n=3)*
24.3	<0.1	*(n=3)*
36.8	<0.1	*(n=3)*

6.6 Flash Point

Weathering (weight %)	Flash Point (°C)	
0	-4.3	*(n=2)*
12.6	27.8	*(n=3)*
24.3	67.8	*(n=3)*
36.8	>110	*(n=2)*

6.7 Density

Weathering (weight %)	Temperature (°C)	Density (g/mL)	
0	0	0.8536	*(n=3)*
	15	0.8404	*(n=3)*
12.6	0	0.8805	*(n=3)*
	15	0.8676	*(n=3)*
24.3	0	0.8987	*(n=3)*
	15	0.8852	*(n=3)*
36.8	0	0.9151	*(n=3)*
	15	0.9017	*(n=3)*

6.8 Pour Point

Weathering (weight %)	Pour Point (°C)	
0	-18	*(n=2)*
12.6	-12	*(n=2)*
24.3	-12	*(n=2)*
36.8	9	*(n=2)*

6.9 Dynamic Viscosity

Weathering (weight %)	Temperature (°C)	Viscosity (cP)	
0	0	23.6	*(n=3)*
	15	6.1	*(n=3)*
12.6	0	45.3	*(n=3)*
	15	13.8	*(n=3)*
24.3	0	D = 1 14170	
		D = 10 1802	
		D = 100 310	
	15	31.5	*(n=3)*
36.8	0	D = 1 41690	
		D = 10 6097	
		D = 100 897	
	15	123.2	*(n=3)*

6.10 Chemical Dispersibility

Weathering (weight %)	Chemical Dispersibility using Corexit 9500 (%)	
0	28.1	*(n=6)*
12.6	26.6	*(n=6)*
24.3	17.2	*(n=6)*
36.8	10.9	*(n=6)*

6.11 Adhesion

Weathering (weight %)	Adhesion (g/m²)	
0	4.8	*(n=3)*
12.6	25.0	*(n=4)*
24.3	33.6	*(n=4)*
36.8	43.7	*(n=3)*

6.12 Surface and Interfacial Tensions

6.12.1 Surface Tension (Oil/Air Interfacial Tension)

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	28.3	*(n=3)*
	15	25.5	*(n=3)*
12.6	0	29.1	*(n=3)*
	15	27.2	*(n=3)*
24.3	0	30.1	*(n=3)*
	15	28.0	*(n=3)*
36.8	0	31.1	*(n=3)*
	15	29.9	*(n=3)*

6.12.2 Oil/Brine (33‰) Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	19.2	*(n=3)*
	15	23.1	*(n=3)*
12.6	0	29.0	*(n=3)*
	15	23.1	*(n=3)*
24.3	0	21.1	*(n=3)*
	15	24.1	*(n=3)*
36.8	0	20.1	*(n=3)*
	15	23.2	*(n=3)*

6.12.3 Oil/Fresh Water Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	30.7	*(n=3)*
	15	14.3	*(n=3)*
12.6	0	33.9	*(n=3)*
	15	16.0	*(n=3)*
24.3	0	31.1	*(n=3)*
	15	15.3	*(n=3)*
36.8	0	32.7	*(n=3)*
	15	14.3	*(n=3)*

6.13 Emulsion Formation

Weathering (weight %)	Visual Stability	Complex Modulus (Pa)	Emulsion Water Content (%)
0	Meso	133	89.6
12.6	Meso	409	92.9
24.3	Stable	630	87.7
36.8	Stable	1025	86.0

6.14 Boiling Point Distribution

	Cumulative Weight Fraction (%)			
Boiling Point (°C)	0% weathered	12.6% weathered	24.3% weathered	36.8% weathered
40	2.4	0.2		
60	3.8	0.8	0.1	
80	6.5	1.6	0.1	
100	10.2	3.4	0.1	
120	13.6	6.1	0.2	
140	17.4	9.5	1.1	
160	21.5	13.8	3.4	
180	25.9	18.2	7.2	0.1
200	29.7	22.4	11.4	1.1
250	39.4	32.8	23.1	10.4
300	49.5	43.5	35.5	24.5
350	59.5	54.5	48.1	39.3
400	68.0	63.5	58.6	51.6
450	76.0	72.1	68.7	63.4
500	82.2	78.9	76.5	72.7
550	86.6	84.0	82.4	79.7
600	90.4	87.7	86.6	84.7
650	93.1	90.4	89.7	88.3

6.15 Hydrocarbon Groups

Component	Concentration (weight %) 0% weathered	12.6% weathered	24.3% weathered	36.8% weathered
Saturates	77.3	77.0	76.5	72.4
Aromatics	16.8	15.7	15.4	18.0
Resins	4.2	5.4	5.7	6.5
Asphaltenes	1.7	2.0	2.4	3.1
Waxes	3.2	3.5	4.0	4.4

6.16 Volatile Organic Compounds

Component	Concentration (µg/g oil) 0% weathered	36.8% weathered
Benzene	2261	0
Toluene	5308	10
Ethylbenzene	1646	0
Xylenes†	8954	0
C_3-Benzenes‡	1240	110
Total BTEX	18170	10
Total BTEX and C_3-Benzenes‡	30570	120

†“Xylenes” include *o*-, *m*-, and *p*-xylene isomers.
‡“C_3-Benzenes” include eight isomers.

6.17 *n*-Alkane Distribution

	Concentration (mg/g oil)	
n-Alkane Component	**0% weathered**	**36.8% weathered**
n-C8		
n-C9	5.52	
n-C10	5.09	
n-C11	5.02	1.39
n-C12	4.45	4.12
n-C13	4.43	5.93
n-C14	4.37	5.92
n-C15	4.57	6.98
n-C16	4.18	6.69
n-C17	3.85	6.16
Pristane	2.45	4.05
n-C18	3.14	5.19
Phytane	1.96	3.28
n-C19	3.01	4.85
n-C20	2.80	4.33
n-C21	2.56	4.13
n-C22	2.29	3.72
n-C23	2.02	3.34
n-C24	1.86	2.96
n-C25	1.75	2.83
n-C26	1.56	2.44
n-C27	1.30	2.07
n-C28	1.14	1.83
n-C29	1.03	1.66
n-C30	0.76	1.28
n-C31	0.66	1.06
n-C32	0.44	0.74
n-C33	0.35	0.52
n-C34	0.29	0.49
n-C35	0.24	0.43
n-C36	0.10	0.18
n-C37	0.08	0.12
n-C38	0.05	0.09
n-C39	0.04	0.06
n-C40	0.03	0.05
n-C41		
TOTAL	**78.8**	**88.9**
C17/PRISTANE	1.58	1.52
C18/PHYTANE	1.61	1.58
PRISTANE/PHYTANE	1.25	1.23
CPI	0.96	1.04

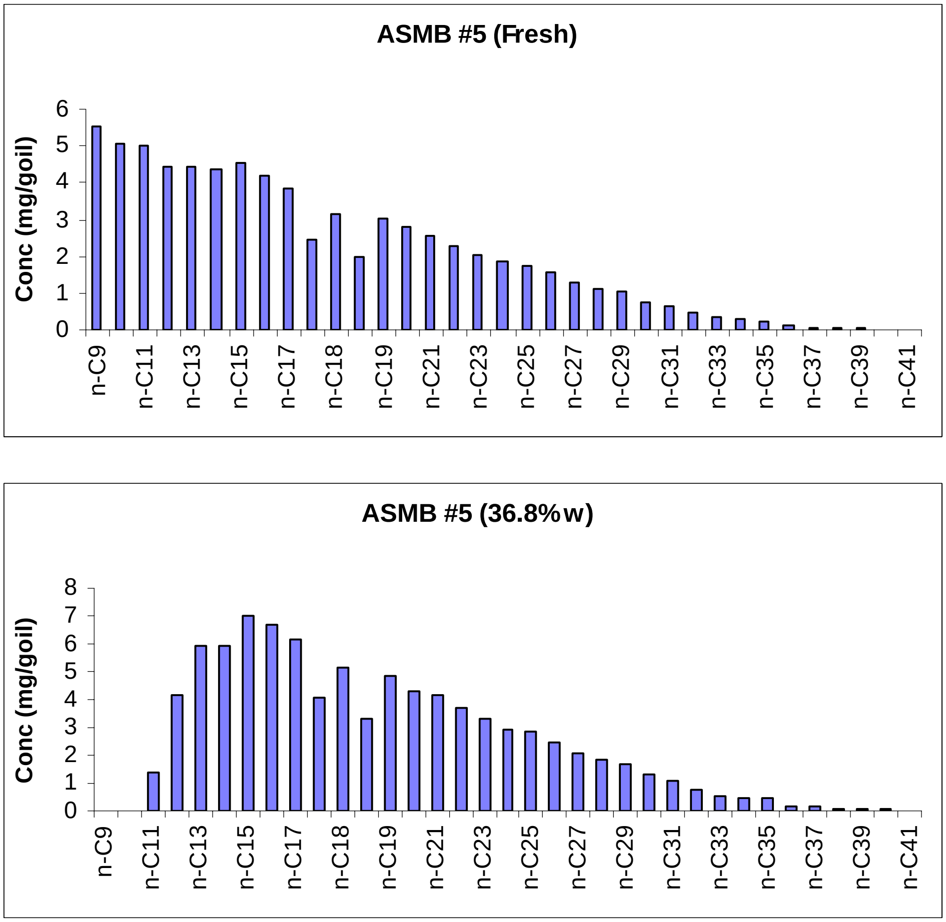


Figure 6.1 *n*-Alkane Distribution for Alberta Sweet Mixed Blend #5 crude oil (mg/g oil)

6.18 PAH Distribution

	Concentration (μg/g oil)	
Alkylated PAH	**0% weathered**	**36.8% weathered**
Naphthalene		
C0-N	245	153
C1-N	987	1209
C2-N	1769	2662
C3-N	1734	2830
C4-N	763	1311
Sum	**5498**	**8165**
Phenanthrene		
C0-P	141	235
C1-P	559	924
C2-P	642	1052
C3-P	456	748
C4-P	294	487
Sum	**2092**	**3446**
Dibenzothiophene		
C0-D	121	201
C1-D	219	360
C2-D	298	501
C3-D	201	333
Sum	**839**	**1395**
Fluorene		
C0-F	81	133
C1-F	189	317
C2-F	289	475
C3-F	295	481
Sum	**854**	**1405**
Chrysene		
C0-C	29	49
C1-C	62	107
C2-C	100	169
C3-C	92	159
Sum	**282**	**483**
TOTAL	**9565**	**14895**
2-m-N/1-m-N	1.75	1.65
(3+2-m/phen)/(4-/9-+1m-phen)	0.95	0.95
4-m:2/3m:1-m-DBT	1:0.74:0.28	1:0.76:0.28
Other PAHs		
Biphenyl	70.8	99.5
Acenaphthylene	7.61	11.97
Acenaphthene	15.95	26.31
Anthracene	2.09	3.87
Fluoranthene	2.45	4.24
Pyrene	18.28	21.57
Benz(a)anthracene	2.94	5.36
Benzo(b)fluoranthene	2.94	4.61
Benzo(k)fluoranthene	0.49	0.62
Benzo(e)pyrene	8.71	15.21
Benzo(a)pyrene	0.86	1.25
Perylene	1.72	2.62
Indeno(1,2,3cd)pyrene	0.74	0.75
Dibenz(a,h)anthracene	1.25	1.8
Benzo(ghi)perylene	2.94	4.36
TOTAL	**140**	**203**

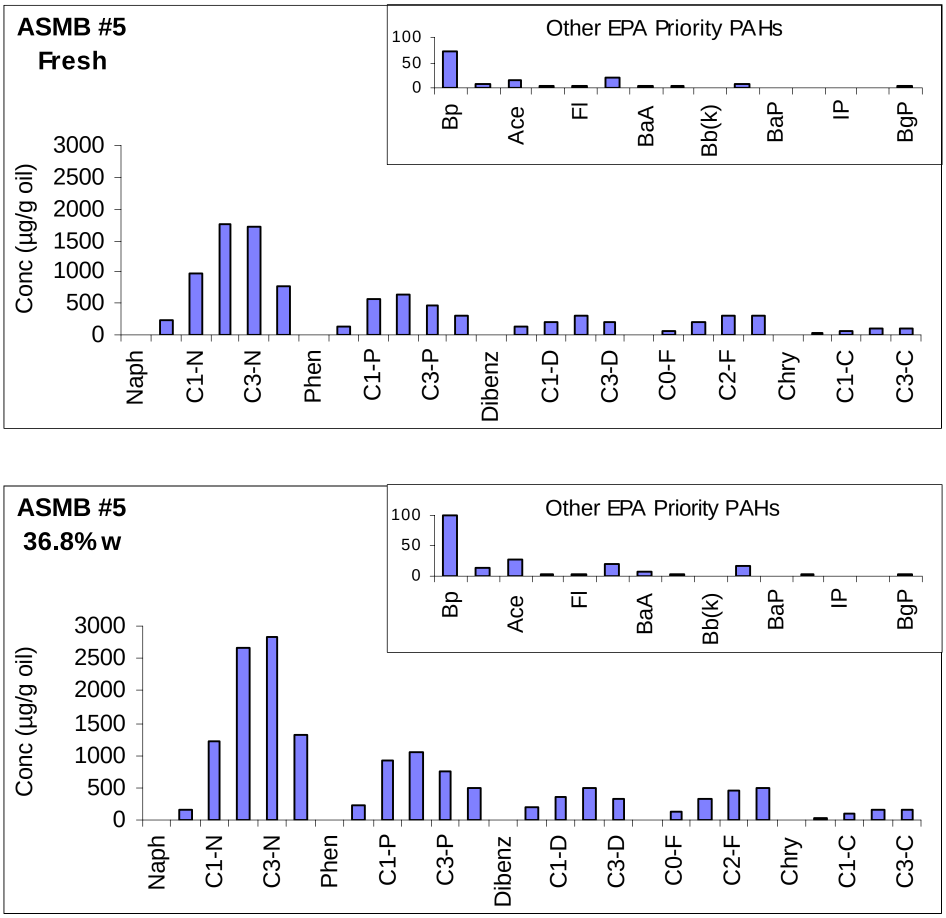


Figure 6.2 PAH Distribution for Alberta Sweet Mixed Blend #5 crude oil (µg/g oil)

6.19 Biomarker Concentrations

	Concentration (μg/g oil)	
Biomarker	**0% weathered**	**36.8% weathered**
C23	48.4	83.0
C24	25.5	43.1
C29	57.0	103.6
C30	87.7	155.9
C31(S)	33.4	58.5
C31(R)	31.7	54.6
C32(S)	24.9	40.4
C32(R)	17.4	28.8
C33(S)	15.2	25.6
C33(R)	10.7	17.7
C34(S)	10.1	17.7
C34(R)	6.3	10.4
Ts	26.1	46.1
Tm	23.8	42.2
C27αββ steranes	51.5	87.3
C29αββ steranes	60.2	107.5
TOTAL	**530**	**922**
Diagnostic Ratios		
C23/C24	1.90	1.93
C29/C30	0.55	0.53
C31(S)/C31(R)	0.29	0.28
C32(S)/C32(R)	0.65	0.66
C33(S)/C33(R)	1.05	1.07
C34(S)/C34(R)	1.44	1.40
Ts/Tm	1.43	1.45
C27αββ/C29αββ	1.60	1.69

7. Physical Properties and Chemical Composition of Arabian Light (2000)

7.1 **Origin:** Saudi Arabia (Sampled from Irving Oil Refinery, St. John, NB, 2000)

Synonyms: None

Values are reported for the **fresh oil** and for artificially weathered fractions of **9.2%**, **17.6%** and **26.0%** loss by weight.

7.2 API Gravity

31.30 *(calc)*

7.3 Equation for Predicting Evaporation

$$\%Ev = (2.4 + 0.045\, T) \ln t$$

Where: %Ev = weight percent evaporated; T = surface temperature (°C); t = time (minutes)

7.4 Sulphur Content

Weathering (weight %)	Sulphur (weight %)	
0	1.93	*(n=3)*
9.2	2.17	*(n=3)*
17.6	2.36	*(n=3)*
26.0	2.60	*(n=3)*

7.5 Water Content

Weathering (weight %)	Water (volume %)	
0	<0.1	*(n=3)*
9.2	<0.1	*(n=3)*
17.6	<0.1	*(n=3)*
26.0	<0.1	*(n=3)*

7.6 Flash Point

Weathering (weight %)	Flash Point (°C)	
0	<-10	*(n=2)*
9.2	36.5	*(n=3)*
17.6	71.7	*(n=3)*
26.0	>110	*(n=2)*

7.7 Density

Weathering (weight %)	Temperature (°C)	Density (g/mL)	
0	0	0.8776	*(n=3)*
	15	0.8641	*(n=3)*
9.2	0	0.8994	*(n=3)*
	15	0.8660	*(n=3)*
17.6	0	0.9154	*(n=3)*
	15	0.9028	*(n=3)*
26.0	0	0.9321	*(n=3)*
	15	0.9193	*(n=3)*

7.8 Pour Point

Weathering (weight %)	Pour Point (°C)	
0	-21	*(n=2)*
9.2	-15	*(n=2)*
17.6	-8	*(n=1)*
26.0	-9	*(n=2)*

7.9 Dynamic Viscosity

Weathering (weight %)	Temperature (°C)	Viscosity (cP)	
0	0	32.6	*(n=3)*
	15	13.0	*(n=3)*
9.2	0	77.6	*(n=3)*
	15	27.4	*(n=3)*
17.6	0	D = 1 3546	
		D = 10 1073	
		D = 100 368	
	15	59.9	*(n=3)*
26.0	0	D = 1 17190	
		D = 10 3869	
		D = 100 1096	
	15	173.7	*(n=3)*

7.10 Chemical Dispersibility

Weathering (weight %)	Chemical Dispersibility using Corexit 9500 (%)	
0	19.0	*(n=6)*
9.2	13.8	*(n=6)*
17.6	10.0	*(n=6)*
26.0	7.9	*(n=6)*

7.11 Adhesion

Weathering (weight %)	Adhesion (g/m^2)	
0	17	*(n=3)*
9.2	28	*(n=3)*
17.6	30	*(n=4)*
26.0	35	*(n=3)*

7.12 Surface and Interfacial Tensions

7.12.1 Surface Tension (Oil/Air Interfacial Tension)

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	27.2	*(n=3)*
	15	26.0	*(n=3)*
9.2	0	29.2	*(n=3)*
	15	27.9	*(n=3)*
17.6	0	30.6	*(n=3)*
	15	28.4	*(n=3)*
26.0	0	30.9	*(n=3)*
	15	30.2	*(n=3)*

7.12.2 Oil/Brine (33‰) Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	21.3	*(n=3)*
	15	21.6	*(n=3)*
9.2	0	22.2	*(n=3)*
	15	22.8	*(n=3)*
17.6	0	16.4	*(n=3)*
	15	24.6	*(n=3)*
26.0	0	26.8	*(n=3)*
	15	20.4	*(n=3)*

7.12.3 Oil/Fresh Water Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	23.5	*(n=3)*
	15	23.8	*(n=3)*
9.2	0	22.4	*(n=3)*
	15	22.0	*(n=3)*
17.6	0	28.3	*(n=3)*
	15	25.7	*(n=3)*
26.0	0	30.1	*(n=3)*
	15	22.4	*(n=3)*

7.13 Emulsion Formation

Weathering (weight %)	Visual Stability	Complex Modulus (Pa)	Emulsion Water Content (%)
0	Meso	92.7	91.1
9.2	Meso	212	88.6
17.6	Stable	274	83.8
26.0	Stable	503	83.8

7.14 Boiling Point Distribution

	Cumulative Weight Fraction (%)			
Boiling Point (°C)	0% weathered	9.2% weathered	17.6% weathered	26.0% weathered
40	1.1			
60	1.3			
80	1.7			
100	4.7	1.2		
120	6.8	2.9	0.1	
140	9.6	5.3	0.6	
160	12.6	8.2	2.0	
180	15.9	11.7	4.7	0.2
200	19.1	15.0	8.0	1.2
250	26.8	23.5	17.3	8.6
300	35.1	32.4	27.3	19.4
350	43.7	41.7	37.7	30.9
400	51.4	50.1	47.0	41.4
450	58.9	58.2	56.1	51.5
500	65.5	65.4	64.0	60.5
550	71.4	71.8	71.1	68.5
600	76.2	77.0	76.8	75.0
650	80.1	81.2	81.4	80.2

7.15 Hydrocarbon Groups

Component	Concentration (weight %) 0% weathered	9.2% weathered	17.6% weathered	26.0% weathered
Saturates	75.5	73.3	72.4	70.1
Aromatics	15.2	16.9	16.7	16.3
Resins	5.7	6.0	6.6	8.8
Asphaltenes	3.6	3.8	4.3	4.8
Waxes	2.7	2.9	3.2	3.6

7.16 Volatile Organic Compounds

Component	Concentration (µg/g oil) 0% weathered	26.0% weathered
Benzene	979	11
Toluene	3050	74
Ethylbenzene	1995	434
Xylenes†	4927	1508
C_3-Benzenes‡	8620	6520
Total BTEX	10950	2030
Total BTEX and C_3-Benzenes‡	19570	8550

†“Xylenes” include *o*-, *m*-, and *p*-xylene isomers.
‡“C_3-Benzenes” include eight isomers.

7.17 *n*-Alkane Distribution

n-Alkane Component	**Concentration (mg/g oil)** **0% weathered**	**26.0% weathered**
n-C8	6.87	
n-C9	7.61	
n-C10	7.25	0.29
n-C11	7.00	2.47
n-C12	6.41	5.41
n-C13	5.93	6.56
n-C14	5.62	7.13
n-C15	5.30	7.14
n-C16	4.76	6.46
n-C17	3.99	5.51
Pristane	0.57	0.79
n-C18	3.42	4.55
Phytane	1.13	1.51
n-C19	2.79	3.88
n-C20	2.57	3.43
n-C21	2.24	3.17
n-C22	1.98	2.62
n-C23	1.57	2.19
n-C24	1.43	2.01
n-C25	1.12	1.54
n-C26	1.00	1.38
n-C27	0.80	1.16
n-C28	0.71	1.02
n-C29	0.58	0.92
n-C30	0.48	0.69
n-C31	0.40	0.61
n-C32	0.29	0.42
n-C33	0.21	0.29
n-C34	0.18	0.24
n-C35	0.15	0.19
n-C36	0.08	0.11
n-C37	0.06	0.06
n-C38	0.05	0.05
n-C39	0.03	0.04
n-C40	0.02	0.03
n-C41		
TOTAL	**84.6**	**73.9**
C17/PRISTANE	6.95	6.99
C18/PHYTANE	3.03	3.02
PRISTANE/PHYTANE	0.51	0.52
CPI	0.93	1.00

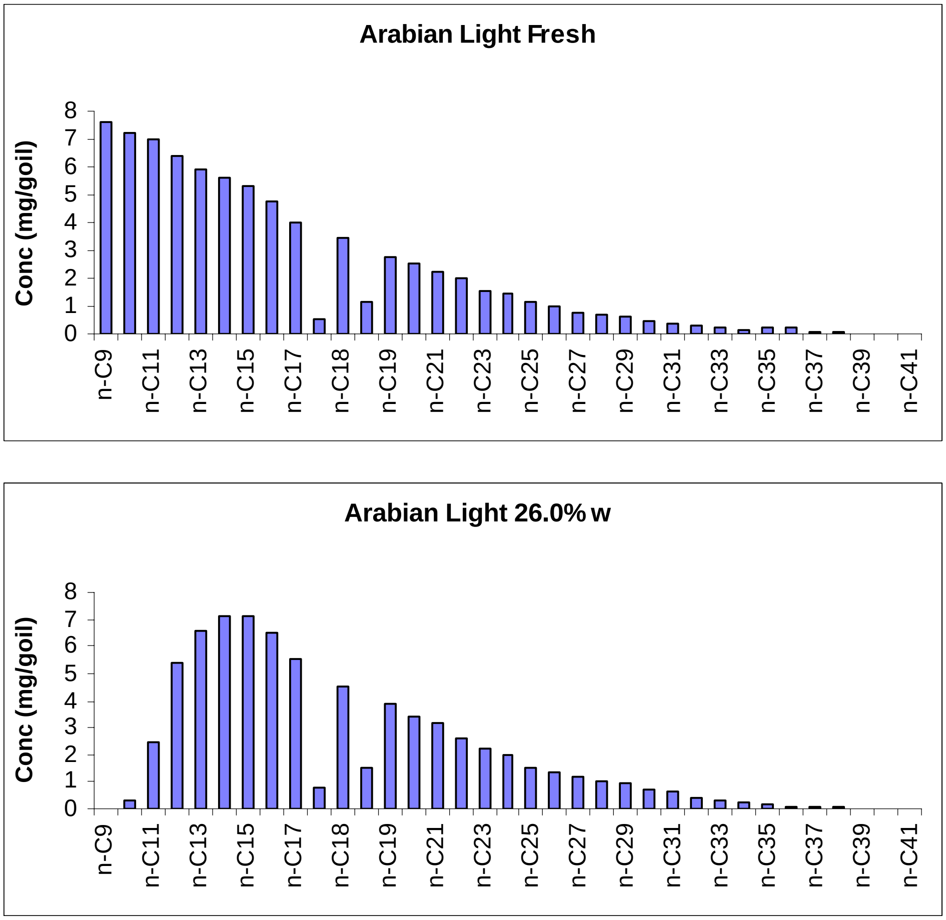


Figure 7.1 *n*-Alkane Distribution for Arabian Light crude oil (mg/g oil)

7.18 PAH Distribution

	Concentration (µg/g oil)	
Alkylated PAH	**0% weathered**	**26.0% weathered**
Naphthalene		
C0-N	50.3	25.7
C1-N	391.7	332.5
C2-N	1123.3	903.8
C3-N	1542.2	1739.9
C4-N	831.2	1000.2
Sum	3939	4002
Phenanthrene		
C0-P	51.2	64.1
C1-P	293.0	367.5
C2-P	384.5	488.0
C3-P	310.2	393.1
C4-P	257.1	328.2
Sum	1296	1641
Dibenzothiophene		
C0-D	147.7	181.2
C1-D	438.8	544.4
C2-D	770.3	980.6
C3-D	675.9	856.6
Sum	2033	2563
Fluorene		
C0-F	35.2	40.4
C1-F	94.6	117.7
C2-F	183.9	222.1
C3-F	199.0	251.9
Sum	513	632
Chrysene		
C0-C	13.0	16.8
C1-C	29.5	37.9
C2-C	54.4	72.7
C3-C	69.8	90.1
Sum	167	217
TOTAL	**7947**	**9055**
2-m-N/1-m-N	0.98	0.97
(3+2-m/phen)/(4-/9-+1m-phen)	0.55	0.55
4-m:2/3m:1-m-DBT	1 : 0.87 : 0.57	1 : 0.88 : 0.57
Other PAHs		
Biphenyl	7.83	8.79
Acenaphthylene	7.83	8.66
Acenaphthene	2.86	3.22
Anthracene	0.99	1.73
Fluoranthene	0.27	0.37
Pyrene	4.10	5.07
Benz(a)anthracene	0.50	1.98
Benzo(b)fluoranthene	1.61	2.48
Benzo(k)fluoranthene	0.99	1.11
Benzo(e)pyrene	4.22	5.69
Benzo(a)pyrene	1.24	1.99
Perylene	0.00	0.00
Indeno(1,2,3cd)pyrene	0.52	0.74
Dibenz(a,h)anthracene	0.49	1.12
Benzo(ghi)perylene	1.86	2.23
TOTAL	**37**	**43**

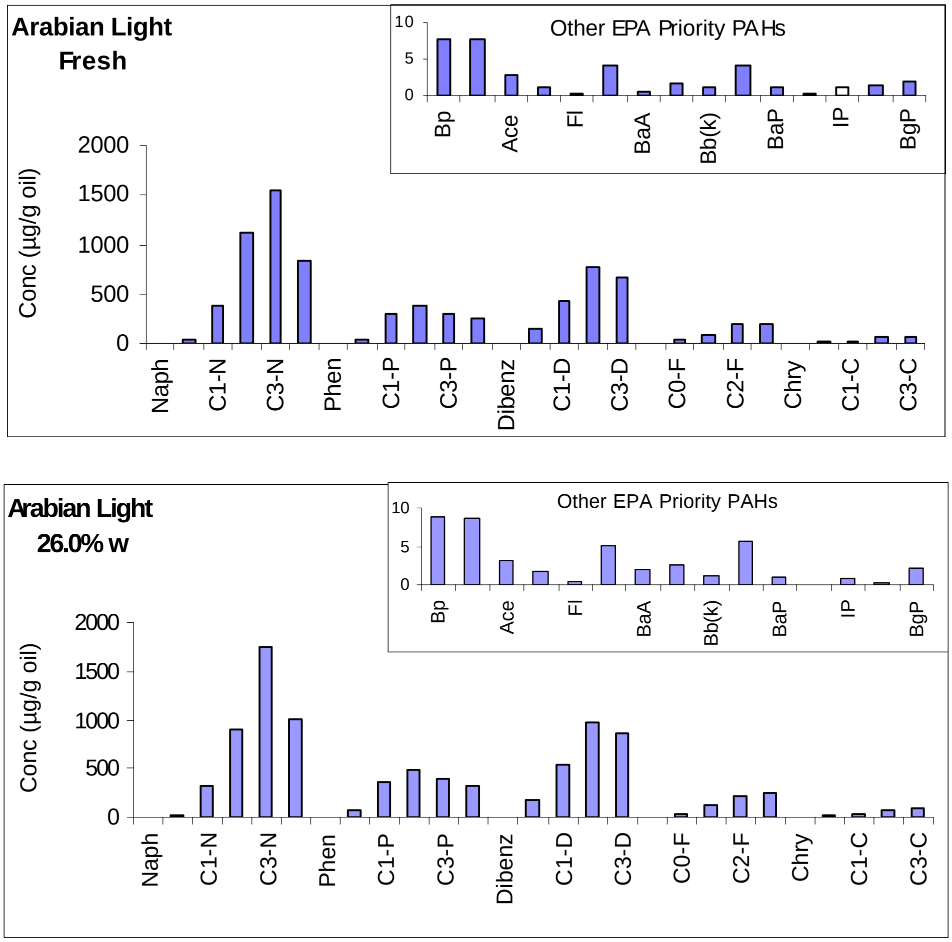


Figure 7.2 PAH Distribution for Arabian Light crude oil (µg/g oil)

7.19 Biomarker Concentrations

	Concentration (µg/g oil)	
Biomarker	**0% weathered**	**26.0% weathered**
C23	17.7	21.6
C24	6.6	7.9
C29	152.2	184.2
C30	124.6	148.9
C31(S)	79.9	96.5
C31(R)	65.7	77.3
C32(S)	48.1	57.2
C32(R)	29.8	36.7
C33(S)	27.0	32.5
C33(R)	17.8	21.9
C34(S)	14.4	17.5
C34(R)	8.8	11.1
Ts	42.6	51.3
Tm	36.5	43.8
C27αββ steranes	35.1	40.4
C29αββ steranes	55.1	67.6
TOTAL	**762**	**917**
Diagnostic Ratios		
C23/C24	2.70	2.72
C29/C30	0.14	0.14
C31(S)/C31(R)	0.05	0.05
C32(S)/C32(R)	1.22	1.24
C33(S)/C33(R)	1.22	1.25
C34(S)/C34(R)	1.62	1.56
Ts/Tm	1.51	1.49
C27αββ/C29αββ	1.63	1.58

8. Physical Properties and Chemical Composition of Sockeye (2000)

8.1 Origin:

Origin: California, U.S.A. (Via U.S. Dept. Int., M.M.S., OHMSETT, NJ)
Synonyms: Sockeye Sour
Appearance: Black, heavy, sticky, sour odour.

Values are reported for the **fresh oil** and for artificially weathered fractions of **6.9%**, **13.0%** and **19.8%** loss by weight.

8.2 API Gravity

19.32 *(calc)*

8.3 Equation for Predicting Evaporation

$$\%Ev = (1.52 + 0.045\,T) \ln t$$

Where: %Ev = weight percent evaporated; T = surface temperature (°C); t = time (minutes)

8.4 Sulphur Content

Weathering (weight %)	Sulphur (weight %)	
0	4.51	*(n=3)*
6.9	4.95	*(n=3)*
13.0	5.19	*(n=3)*
19.8	5.47	*(n=3)*

8.5 Water Content

Weathering (weight %)	Water (volume%)	
0	0.8	*(n=3)*
6.9	0.1	*(n=3)*
13.0	0.1	*(n=3)*
19.8	<0.1	*(n=3)*

8.6 Flash Point

Weathering (weight %)	Flash Point (°C)	
0	-4	*(n=4)*
6.9	35	*(n=3)*
13.0	72	*(n=3)*
19.8	>110	*(n=2)*

8.7 Density

Weathering (weight %)	Temperature (°C)	Density (g/mL)	
0	0	0.9465	*(n=3)*
	15	0.9354	*(n=3)*
6.9	0	0.9642	*(n=3)*
	15	0.9537	*(n=3)*
13.0	0	0.9798	*(n=3)*
	15	0.9692	*(n=3)*
19.8	0	0.9951	*(n=3)*
	15	0.9839	*(n=3)*

8.8 Pour Point

Weathering (weight %)	Pour Point (°C)	
0	-25	*(n=2)*
6.9	-18	*(n=2)*
13.0	2	*(n=2)*
19.8	13	*(n=2)*

8.9 Dynamic Viscosity

Weathering (weight %)	Temperature (°C)	Viscosity (cP)	
0	0	3220	*(n=3)*
	15	761	*(n=3)*
6.9	0	13600	*(n=3)*
	15	2720	*(n=3)*
13.0	0	143000*	*(n=3)*
	15	15100	*(n=3)*
19.8	0	5300000*	*(n=3)*
	15	274000**	*(n=3)*

* Measured at a shear rate of 1 s^{-1} with a 60mm a cone and plate sensor.

** Measured under static conditions with a 60mm cone and plate sensor, applied shear stress of 100 Pa .

8.10 Chemical Dispersibility

Weathering (weight %)	Chemical Dispersibility using Corexit 9500 (%)	
0	11.8	*(n=6)*
6.9	9.6	*(n=6)*
13.0	10.1	*(n=6)*
19.8	8.9	*(n=6)*

8.11 Adhesion

Weathering (weight %)	Adhesion (g/m^2)	
0	70	*(n=4)*
6.9	70	*(n=4)*
13.0	90	*(n=4)*
19.8	350	*(n=4)*

8.12 Surface and Interfacial Tensions

8.12.1 Surface Tension (Oil/Air Interfacial Tension)

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	30.1	*(n=4)*
	15	28.8	*(n=4)*
6.9	0	NM	
	15	31.3	*(n=3)*
13.0	0	NM	
	15	32.2	*(n=3)*
19.8	0	NM	
	15	NM	

8.12.2 Oil/Brine (33‰) Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	23.0	*(n=3)*
	15	21.9	*(n=3)*
6.9	0	NM	
	15	23.1	*(n=3)*
13.0	0	NM	
	15	NM	
19.8	0	NM	
	15	NM	

8.12.3 Oil/Fresh Water Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	23.7	*(n=3)*
	15	21.4	*(n=3)*
6.9	0	NM	
	15	24.9	*(n=3)*
13.0	0	NM	
	15	NM	
19.8	0	NM	
	15	NM	

8.13 Emulsion Formation

Weathering (weight %)	Visual Stability	Complex Modulus (Pa)	Emulsion Water Content (%)
0	Meso-stable	183	75.6
6.9	Meso-stable	251	73.3
13.0	Entrained Water	391	53.4
19.8	Entrained Water	1298	17.7

8.14 Boiling Point Distribution

	Cumulative Weight Fraction (%)			
Boiling Point (°C)	0% weathered	6.9% weathered	13.0% weathered	19.8% weathered
40	0.4			
60	0.4			
80	1.5	0.1		
100	3.3	0.7		
120	5.1	1.6		
140	7.1	3.1	0.2	
160	9.2	5.0	0.9	
180	11.3	7.1	2.3	
200	13.2	9.2	4.1	0.4
250	18.9	15.4	10.5	4.6
300	24.7	21.6	17.1	11.3
350	30.9	28.3	24.2	19.0
400	36.8	34.6	30.9	26.3
450	43.3	41.7	28.5	34.6
500	50.1	49.0	46.4	43.4
550	57.3	56.6	54.9	52.9
600	63.5	63.2	62.1	60.9
650	69.2	69.1	68.5	68.0

8.15 Hydrocarbon Groups

Component	Concentration (weight %) 0% weathered	6.9% weathered	13.0% weathered	19.8% weathered
Saturates	49.2	46.2	44.4	40.3
Aromatics	17.2	17.6	18.0	18.0
Resins	15.1	16.4	17.1	17.2
Asphaltenes	18.5	19.8	20.5	24.5
Waxes	1.6	1.7	1.8	2.1

8.16 Volatile Organic Compounds

Component	Concentration (µg/g oil) 0% weathered	19.8% weathered
Benzene	1343	9
Toluene	2031	12
Ethylbenzene	974	0
Xylenes†	3880	1
C_3-Benzenes‡	5810	70
Total BTEX	8230	20
Total BTEX and C_3-Benzenes‡	14040	90

†“Xylenes” include *o*-, *m*-, and *p*-xylene isomers.
††“C_3-Benzenes” include eight isomers.

8.17 *n*-Alkane Distribution

	Concentration (mg/g oil)	
***n*-Alkane Component**	**0% weathered**	**19.8% weathered**
n-C8	1.27	
n-C9	0.95	
n-C10	0.85	
n-C11	1.02	0.13
n-C12	1.14	0.63
n-C13	1.37	1.08
n-C14	1.43	1.52
n-C15	1.54	1.73
n-C16	1.52	1.76
n-C17	1.32	1.55
Pristane	1.68	1.90
n-C18	1.19	1.41
Phytane	1.79	2.11
n-C19	1.08	1.25
n-C20	1.02	1.20
n-C21	0.91	1.09
n-C22	0.81	0.97
n-C23	0.71	0.85
n-C24	0.65	0.75
n-C25	0.59	0.71
n-C26	0.51	0.60
n-C27	0.30	0.37
n-C28	0.30	0.36
n-C29	0.30	0.36
n-C30	0.28	0.29
n-C31	0.23	0.28
n-C32	0.15	0.17
n-C33	0.14	0.17
n-C34	0.23	0.24
n-C35	0.33	0.39
n-C36	0.07	0.10
n-C37	0.08	0.10
n-C38	0.07	0.08
n-C39	0.03	0.04
n-C40	0.02	0.02
n-C41		
TOTAL	25.9	24.2
C17/PRISTANE	0.78	0.82
C18/PHYTANE	0.66	0.67
PRISTANE/PHYTANE	0.94	0.90
CPI	0.95	1.00

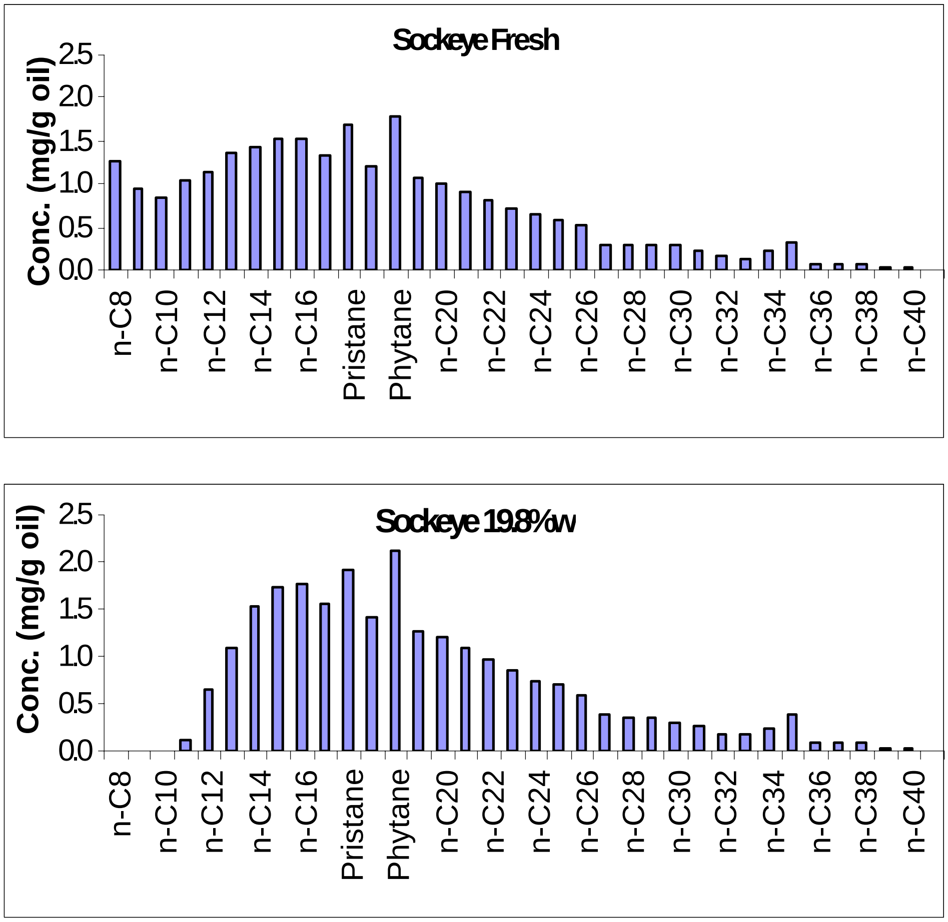


Figure 8.1 *n*-Alkane Distribution for Sockeye Crude Oil (mg/g oil)

8.18 PAH Distribution

Alkylated PAH		Concentration (µg/g oil) 0% weathered	19.8% weathered
Naphthalene			
	C0-N	111	72
	C1-N	511	560
	C2-N	1057	1272
	C3-N	1144	1541
	C4-N	599	824
	Sum	3424	4269
Phenanthrene			
	C0-P	60	76
	C1-P	237	314
	C2-P	319	424
	C3-P	283	362
	C4-P	179	241
	Sum	1078	1417
Dibenzothiophene			
	C0-D	34	45
	C1-D	86	117
	C2-D	155	216
	C3-D	128	171
	Sum	404	550
Fluorene			
	C0-F	13	17
	C1-F	39	50
	C2-F	68	89
	C3-F	64	84
	Sum	183	239
Chrysene			
	C0-C	5	7
	C1-C	11	15
	C2-C	22	29
	C3-C	22	29
	Sum	61	81
TOTAL		5149	6556
2-m-N/1-m-N		1.35	1.33
(3+2-m/phen)/(4-/9-+1m-phen)		1.09	1.10
4-m:2/3m:1-m-DBT		1 : 0.89 :0.36	1 : 0.89 :0.35
Other PAHs			
Biphenyl		34.23	38.98
Acenaphthylene		6.72	8.99
Acenaphthene		7.70	10.37
Anthracene		2.20	3.12
Fluoranthene		1.22	1.62
Pyrene		5.01	6.75
Benz(a)anthracene		3.18	4.25
Benzo(b)fluoranthene		0.98	1.12
Benzo(k)fluoranthene		0.40	0.50
Benzo(e)pyrene		1.59	2.50
Benzo(a)pyrene		0.49	0.50
Perylene		19.32	25.98
Indeno(1,2,3cd)pyrene		0.00	0.00
Dibenz(a,h)anthracene		0.12	0.20
Benzo(ghi)perylene		0.86	1.00
TOTAL		84	106

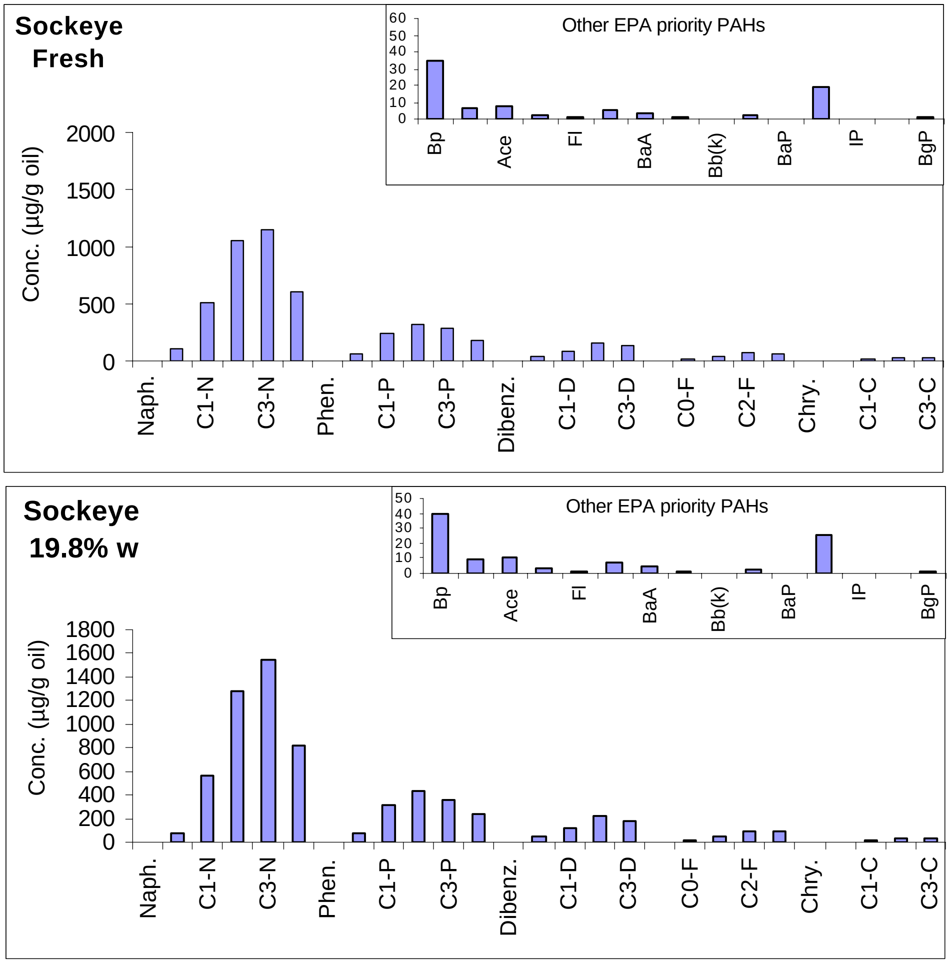


Figure 8.2 PAH Distribution for Sockeye crude oil (µg/g oil)

8.19 Biomarker Concentrations

Biomarker	**Concentration (μg/g oil)** **0% weathered**	 **19.8% weathered**
C23	46.2	57.7
C24	31.3	38.9
C29	61.2	78.2
C30	99.5	126.5
C31(S)	38.7	52.3
C31(R)	40.6	54.4
C32(S)	27.5	36.9
C32(R)	18.9	25.3
C33(S)	18.8	26.3
C33(R)	12.8	18.1
C34(S)	8.4	11.9
C34(R)	5.7	8.0
Ts	6.9	8.7
Tm	35.4	42.9
C27αββ steranes	207.8	262.1
C29αββ steranes	151.7	191.4
TOTAL	811	1039
Diagnostic Ratios		
C23/C24	1.48	1.48
C23/C30	0.46	0.46
C24/C30	0.31	0.31
C29/C30	0.62	0.62
C31(S)/C31(R)	0.95	0.96
C32(S)/C32(R)	1.45	1.46
C33(S)/C33(R)	1.47	1.46
C34(S)/C34(R)	1.47	1.48
Ts/Tm	0.19	0.20
C27αββ/C29αββ	1.37	1.37

9. Physical Properties and Chemical Composition of South Louisiana (2001)

9.1 Origin:

Origin: Baton Rouge, Louisiana, U.S.A. (Exxon-Mobil)
Synonyms: Louisiana

Values are reported for the **fresh oil** and for artificially weathered fractions of **10.9%**, **19.7%** and **27.7%** loss by weight.

9.2 API Gravity

32.72 *(calc)*

9.3 Equation for Predicting Evaporation

$$\%Ev = (2.74 + 0.045\,T)\ \ln t$$

Where: %Ev = weight percent evaporated; T = surface temperature (°C); t = time (minutes)

9.4 Sulphur Content

Weathering (weight %)	Sulphur (weight %)	
0	0.49	*(n=3)*
10.9	0.71	*(n=3)*
19.7	0.79	*(n=3)*
27.7	0.88	*(n=3)*

9.5 Water Content

Weathering (weight %)	Water (volume %)	
0	<0.1	*(n=3)*
10.9	<0.1	*(n=3)*
19.7	<0.1	*(n=3)*
27.7	<0.1	*(n=3)*

9.6 Flash Point

Weathering (weight %)	Flash Point (°C)	
0	<-10	*(n=2)*
10.9	42.3	*(n=3)*
19.7	80.7	*(n=3)*
27.7	>110	*(n=2)*

9.7 Density

Weathering (weight %)	Temperature (°C)	Density (g/mL)	
0	0	0.8668	*(n=3)*
	15	0.8562	*(n=3)*
10.9	0	0.8888	*(n=3)*
	15	0.8770	*(n=3)*
19.7	0	0.9025	*(n=3)*
	15	0.8906	*(n=3)*
27.7	0	0.9135	*(n=3)*
	15	0.9018	*(n=3)*

9.8 Pour Point

Weathering (weight %)	Pour Point (°C)	
0	-41	*(n=2)*
10.9	-19	*(n=2)*
19.7	-14	*(n=1)*
27.7	-11	*(n=2)*

9.9 Dynamic Viscosity

Weathering (weight %)	Temperature (°C)	Viscosity (cP)	
0	0	18.5	*(n=3)*
	15	10.1	*(n=3)*
10.9	0	54.8	*(n=3)*
	15	23.7	*(n=3)*
19.7	0	217.3	*(n=3)*
	15	48.9	*(n=2)*
27.7	0	515.9	*(n=3)*
	15	141.0	*(n=3)*

9.10 Chemical Dispersibility

Weathering (weight %)	Chemical Dispersibility using Corexit 9500 (%)	
0	26.5	*(n=6)*
10.9	23.5	*(n=6)*
19.7	15.8	*(n=6)*
27.7	10.3	*(n=6)*

9.11 Adhesion

Weathering (weight %)	Adhesion (g/m^2)	
0	24	*(n=4)*
10.9	34	*(n=4)*
19.7	50	*(n=5)*
27.7	28	*(n=4)*

9.12 Surface and Interfacial Tensions

9.12.1 Surface Tension (Oil/Air Interfacial Tension)

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	28.3	*(n=3)*
	15	26.1	*(n=3)*
10.9	0	29.3	*(n=3)*
	15	28.1	*(n=3)*
19.7	0	30.4	*(n=3)*
	15	29.4	*(n=3)*
27.7	0	31.1	*(n=3)*
	15	29.8	*(n=3)*

9.12.2 Oil/Brine (33‰) Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	20.9	*(n=2)*
	15	16.8	*(n=3)*
10.9	0	22.0	*(n=3)*
	15	19.4	*(n=2)*
19.7	0	22.0	*(n=3)*
	15	22.2	*(n=2)*
27.7	0	20.6	*(n=4)*
	15	18.4	*(n=3)*

9.12.3 Oil/Fresh Water Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	20.8	*(n=3)*
	15	15.5	*(n=2)*
10.9	0	25.2	*(n=3)*
	15	15.8	*(n=3)*
19.7	0	25.3	*(n=3)*
	15	22.3	*(n=3)*
27.7	0	24.7	*(n=3)*
	15	21.9	*(n=3)*

9.13 Emulsion Formation

Weathering (weight %)	Visual Stability	Complex Modulus (Pa)	Emulsion Water Content (%)
0	Unstable		
10.9	Unstable		
19.7	Unstable		
27.7	Unstable		

9.14 Boiling Point Distribution

	Cumulative Weight Fraction (%)			
Boiling Point (°C)	0% weathered	10.9% weathered	19.7% weathered	27.7% weathered
40	1.2			
60	1.6			
80	2.1			
100	5.6	0.9		
120	8.2	2.4	0.1	
140	11.1	4.8	0.4	
160	14.1	7.8	1.6	0.1
180	17.5	11.4	4.0	0.3
200	20.6	14.9	7.2	1.4
250	29.8	25.2	18.1	10.6
300	39.9	36.6	30.6	24.1
350	49.7	47.7	42.8	37.5
400	58.1	57.0	53.1	49.0
450	65.8	65.7	62.7	59.6
500	72.0	72.7	70.4	68.2
550	77.1	78.5	76.7	75.2
600	80.9	82.8	81.5	80.5
650	83.8	86.0	85.0	84.5

9.15 Hydrocarbon Groups

	Concentration (%)			
Component	0% weathered	10.9% weathered	19.7% weathered	27.7% weathered
Saturates	80.8	80.4	78.4	77.3
Aromatics	12.6	12.3	12.5	13.3
Resins	5.9	6.4	8.0	8.0
Asphaltenes	0.8	0.9	1.1	1.5
Waxes	1.7	1.8	2.0	2.2

9.16 Volatile Organic Compounds

	Concentration (µg/g oil)	
Component	0% weathered	27.7% weathered
Benzene	1598	0
Toluene	3552	10
Ethylbenzene	891	0
Xylenes†	6164	2
C_3-Benzenes‡	6680	190
Total BTEX	12210	12
Total BTEX and C_3-Benzenes‡	18890	202

†"Xylenes" include *o*-, *m*-, and *p*-xylene isomers.
‡"C_3-Benzenes" include eight isomers.

9.17 *n*-Alkane Distribution

	Concentration (mg/g oil)	
***n*-Alkane Component**	**0% weathered**	**27.7% weathered**
n-C8	4.33	
n-C9	4.12	
n-C10	4.12	0.21
n-C11	4.56	1.81
n-C12	4.25	3.81
n-C13	4.14	4.94
n-C14	3.81	5.19
n-C15	3.88	5.29
n-C16	3.48	4.75
n-C17	3.05	4.13
Pristane	2.10	2.76
n-C18	2.24	3.11
Phytane	1.35	1.84
n-C19	2.00	2.61
n-C20	1.70	2.27
n-C21	1.55	2.11
n-C22	1.33	1.81
n-C23	1.13	1.58
n-C24	1.03	1.44
n-C25	0.92	1.28
n-C26	0.72	1.08
n-C27	0.54	0.78
n-C28	0.49	0.70
n-C29	0.42	0.62
n-C30	0.38	0.54
n-C31	0.31	0.46
n-C32	0.23	0.34
n-C33	0.18	0.27
n-C34	0.16	0.24
n-C35	0.15	0.20
n-C36	0.08	0.12
n-C37	0.07	0.10
n-C38	0.05	0.08
n-C39	0.04	0.07
n-C40	0.03	0.05
n-C41	0.02	0.04
TOTAL	**59.0**	**56.7**
C17/PRISTANE	1.45	1.50
C18/PHYTANE	1.65	1.68
PRISTANE/PHYTANE	1.55	1.49
CPI	0.95	1.02

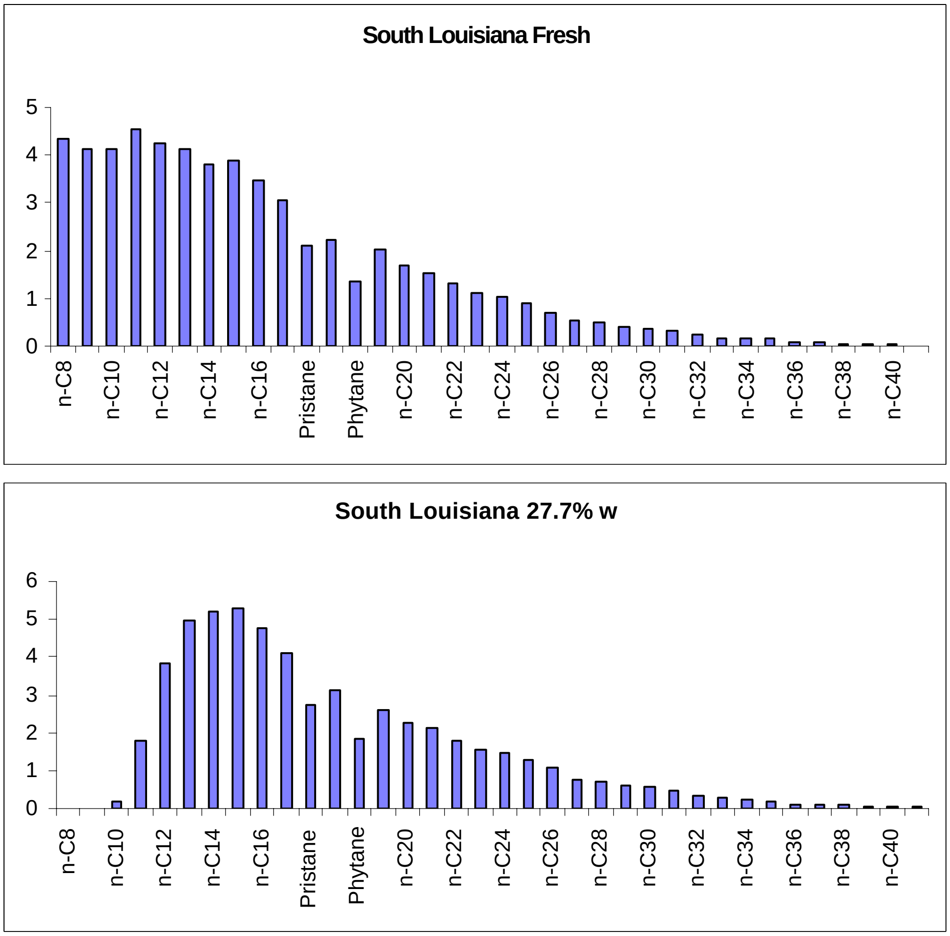
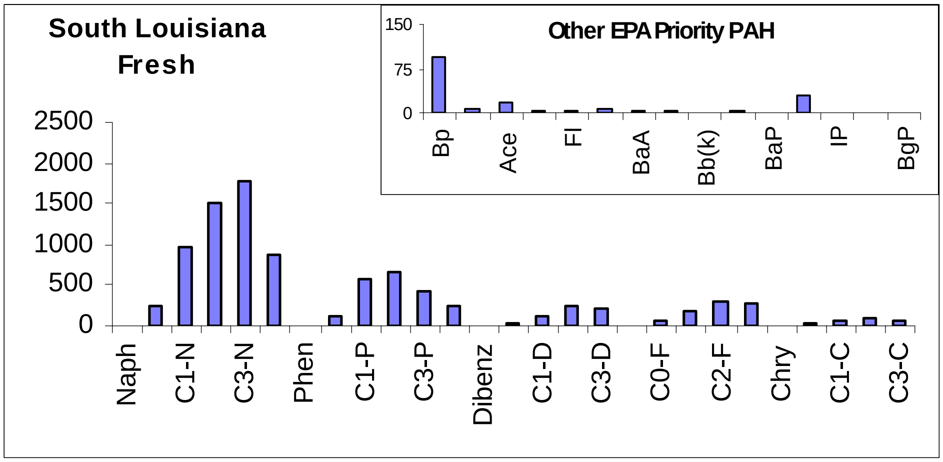


Figure 9.1 *n*-Alkane Distribution for South Louisiana Crude Oil (mg/g oil)

9.18 PAH Distribution

	Concentration (µg/g oil)	
Alkylated PAH	**0% weathered**	**27.7% weathered**
Naphthalene		
C0-N	248.6	164.1
C1-N	952.7	1058.9
C2-N	1500.1	1965.6
C3-N	1765.7	2403.6
C4-N	886.3	1222.3
Sum	**5353**	**6815**
Phenanthrene		
C0-P	134.4	188.3
C1-P	569.8	777.8
C2-P	654.6	887.1
C3-P	427.4	574.6
C4-P	251.8	349.6
Sum	**2038**	**2777**
Dibenzothiophene		
C0-D	40.0	55.4
C1-D	125.7	172.4
C2-D	237.4	323.1
C3-D	205.5	272.6
Sum	**609**	**823**
Fluorene		
C0-F	67.3	94.8
C1-F	181.7	253.2
C2-F	291.4	396.4
C3-F	246.0	354.1
Sum	**804**	**1098**
Chrysene		
C0-C	23.0	30.4
C1-C	58.8	80.1
C2-C	81.6	108.4
C3-C	69.1	90.7
Sum	**233**	**310**
TOTAL	**9037**	**11823**
2-m-N/1-m-N	1.63	1.59
(3+2-m/phen)/(4-/9-+1m-phen)	1.00	1.01
4-m:2/3m:1-m-DBT	1:0.62:0.31	1:0.61:0.31
Other PAHs		
Biphenyl	94.32	120.60
Acenaphthylene	8.15	10.70
Acenaphthene	17.90	24.27
Anthracene	2.47	3.61
Fluoranthene	3.70	5.10
Pyrene	8.64	11.33
Benz(a)anthracene	5.19	6.35
Benzo(b)fluoranthene	2.10	3.73
Benzo(k)fluoranthene	0.37	1.24
Benzo(e)pyrene	4.07	5.97
Benzo(a)pyrene	0.49	0.62
Perylene	30.37	38.95
Indeno(1,2,3cd)pyrene	0.50	1.12
Dibenz(a,h)anthracene	0.86	1.12
Benzo(ghi)perylene	1.23	1.99
TOTAL	**180**	**237**



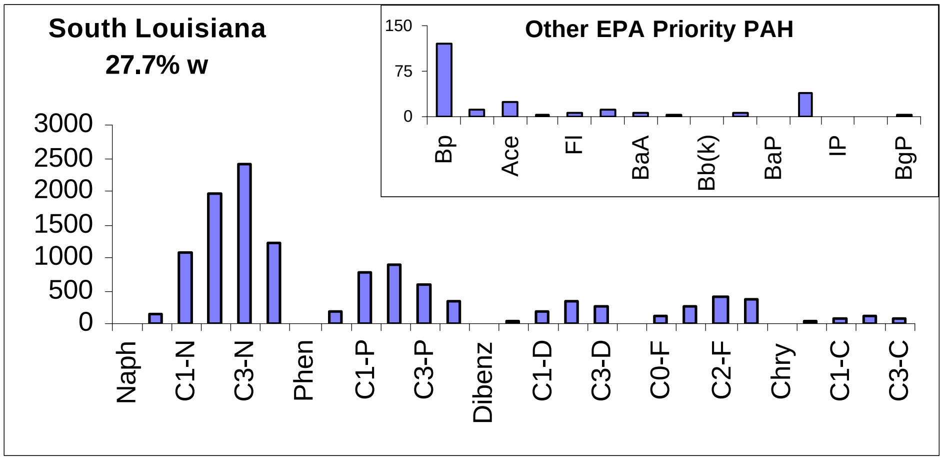


Figure 9.2 PAH Distribution for South Louisiana crude oil (μg/g oil)

9.19 Biomarker Concentrations

Biomarker	Concentration (µg/g oil) 0% weathered	 27.7% weathered
C23	16.9	22.7
C24	11.2	14.7
C29	59.9	75.9
C30	81.5	105.6
C31(S)	31.0	40.2
C31(R)	27.5	35.7
C32(S)	20.1	25.1
C32(R)	13.6	17.4
C33(S)	12.2	15.4
C33(R)	8.8	10.5
C34(S)	6.1	7.3
C34(R)	4.4	5.2
Ts	19.0	24.3
Tm	23.1	30.3
C27αββ steranes	65.0	85.8
C29αββ steranes	72.8	94.3
TOTAL	**473**	**610**
Diagnostic Ratios		
C23/C24	1.50	1.54
C23/C30	0.21	0.21
C24/C30	0.14	0.14
C29/C30	0.73	0.72
C31(S)/C31(R)	1.13	1.13
C32(S)/C32(R)	1.48	1.44
C33(S)/C33(R)	1.39	1.46
C34(S)/C34(R)	1.37	1.41
Ts/Tm	0.82	0.80
C27αββ/C29αββ	0.89	0.91

10. Physical Properties and Chemical Composition of West Texas Intermediate (2002)

10.1 Origin:

Origin: Galveston, Texas, U.S.A. (Via Texas A & M)
Synonyms: None

Values are reported for the **fresh oil** and for artificially weathered fractions of **10.1%**, **21.0%** and **31.7%** loss by weight.

10.2 API Gravity

34.38 *(calc)*

10.3 Equation for Predicting Evaporation

$$\%Ev = (3.08 + 0.045\,T)\ln t$$

Where: %Ev = weight percent evaporated; T = surface temperature (°C); t = time (minutes)

10.4 Sulphur Content

Weathering (weight %)	Sulphur (weight %)	
0	0.86	*(n=3)*
10.1	1.01	*(n=3)*
21.0	1.11	*(n=3)*
31.7	1.24	*(n=3)*

10.5 Water Content

Weathering (weight %)	Water (volume%)	
0	<0.1	*(n=3)*
10.1	<0.1	*(n=3)*
21.0	<0.1	*(n=3)*
31.7	<0.1	*(n=3)*

10.6 Flash Point

Weathering (weight %)	Flash Point (°C)	
0	<-10	*(n=2)*
10.1	32.8	*(n=3)*
21.0	66.0	*(n=3)*
31.7	>110	*(n=2)*

10.7 Density

Weathering (weight %)	Temperature (°C)	Density (g/mL)	
0	0	0.8594	*(n=3)*
	15	0.8474	*(n=3)*
10.1	0	0.8792	*(n=3)*
	15	0.8665	*(n=3)*
21.0	0	0.8956	*(n=3)*
	15	0.8827	*(n=3)*
31.7	0	0.9103	*(n=3)*
	15	0.8973	*(n=3)*

10.8 Pour Point

Weathering (weight %)	Pour Point (°C)	
0	-22	*(n=2)*
10.1	-12	*(n=2)*
21.0	1	*(n=2)*
31.7	7	*(n=2)*

10.9 Dynamic Viscosity

Weathering (weight %)	Temperature (°C)	Viscosity (cP)	
0	0	19.2	*(n=3)*
	15	8.6	*(n=3)*
10.1	0	42.1	*(n=3)*
	15	16.4	*(n=3)*
21.0	0	253.6	*(n=3)*
	15	37.5	*(n=3)*
31.7	0	853.6	*(n=3)*
	15	112.3	*(n=3)*

10.10 Chemical Dispersibility

Weathering (weight %)	Chemical Dispersibility using Corexit 9500 (%)	
0	27.7	*(n=6)*
10.1	23.6	*(n=6)*
21.0	13.3	*(n=6)*
31.7	12.8	*(n=6)*

10.11 Adhesion

Weathering (weight %)	Adhesion (g/m^2)	
0	12.4	*(n=3)*
10.1	16.8	*(n=4)*
21.0	27.6	*(n=4)*
31.7	33.2	*(n=3)*

10.12 Surface and Interfacial Tensions

10.12.1 Surface Tension (Oil/Air Interfacial Tension)

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	27.4	*(n=3)*
	15	26.0	*(n=3)*
10.1	0	28.7	*(n=3)*
	15	27.6	*(n=3)*
21.0	0	29.7	*(n=3)*
	15	28.7	*(n=3)*
31.7	0	31.4	*(n=3)*
	15	29.2	*(n=3)*

10.12.2 Oil/Brine (33‰) Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	18.8	*(n=3)*
	15	15.6	*(n=3)*
10.1	0	19.4	*(n=3)*
	15	14.6	*(n=3)*
21.0	0	19.2	*(n=3)*
	15	12.6	*(n=3)*
31.7	0	19.9	*(n=3)*
	15	17.3	*(n=3)*

10.12.3 Oil/Fresh Water Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	19.3	*(n=3)*
	15	15.8	*(n=3)*
10.1	0	19.9	*(n=3)*
	15	18.1	*(n=3)*
21.0	0	21.0	*(n=3)*
	15	17.2	*(n=3)*
31.7	0	22.7	*(n=3)*
	15	17.1	*(n=3)*

10.13 Emulsion Formation

Weathering (weight %)	Visual Stability	Complex Modulus (Pa)	Emulsion Water Content (%)
0	Unstable		
10.1	Unstable		
21.0	Mesostable	19.1	82.7
31.7	Mesostable	81.9	83.6

10.14 Boiling Point Distribution

	Cumulative Weight Fraction (%)			
Boiling Point (°C)	0% weathered	10.1% weathered	21.0% weathered	31.7% weathered
40	0.7			
60	0.7			
80	1.0			
100	5.5	1.8		
120	8.9	4.2	0.1	
140	12.6	7.5	0.9	
160	16.2	11.2	2.8	
180	20.0	15.3	6.2	0.4
200	23.5	19.2	10.1	1.9
250	32.4	29.0	21.1	11.4
300	41.2	38.9	32.3	23.7
350	50.0	48.7	43.4	36.2
400	57.5	57.0	52.9	47.0
450	64.6	64.9	61.9	57.2
500	70.7	71.7	69.6	66.0
550	75.8	77.4	76.2	73.4
600	79.8	81.8	81.2	79.1
650	82.8	85.2	85.0	83.3

10.15 Hydrocarbon Groups

Component	Concentration (weight %) 0% weathered	10.1% weathered	21.0% weathered	31.7% weathered
Saturates	78.5	78.6	76.3	74.8
Aromatics	14.8	13.7	14.6	13.8
Resins	6.0	6.9	8.0	9.9
Asphaltenes	0.7	0.8	1.1	1.6
Waxes	2.8	3.1	3.4	4.0

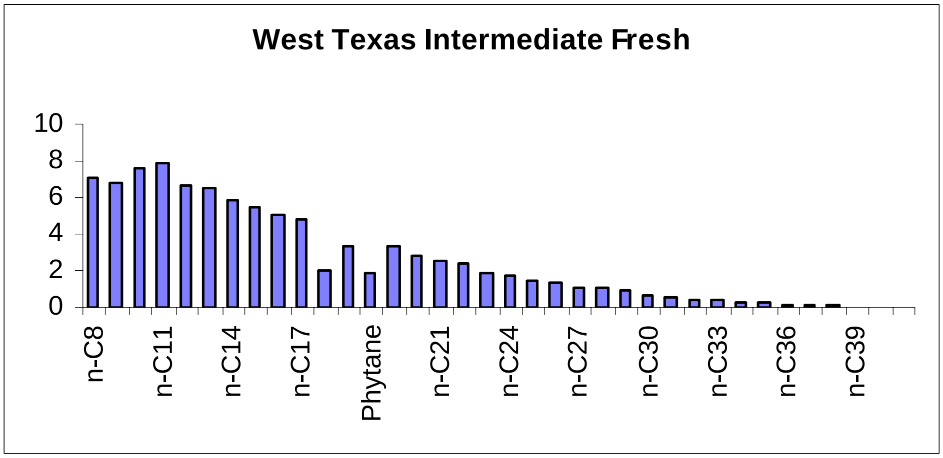
10.16 Volatile Organic Compounds

Component	Concentration (μg/g oil) 0% weathered	31.7% weathered
Benzene	4026	0
Toluene	7395	13
Ethylbenzene	4845	0
Xylenes†	7105	1
C_3-Benzenes‡	10190	310
Total BTEX	23370	14
Total BTEX and C_3-Benzenes‡	33560	324

†“Xylenes” include *o*-, *m*-, and *p*-xylene isomers.
‡“C_3-Benzenes” include eight isomers.

10.17 *n*-Alkane Distribution

	Concentration (mg/g oil)	
***n*-Alkane Component**	**0% weathered**	**31.7% weathered**
n-C8	7.08	
n-C9	6.80	
n-C10	7.59	0.43
n-C11	7.84	3.31
n-C12	6.72	6.21
n-C13	6.57	8.20
n-C14	5.93	8.10
n-C15	5.53	7.94
n-C16	5.02	7.19
n-C17	4.76	6.77
Pristane	1.99	2.79
n-C18	3.39	4.76
Phytane	1.85	2.56
n-C19	3.38	4.74
n-C20	2.78	3.87
n-C21	2.51	3.56
n-C22	2.35	3.37
n-C23	1.92	2.78
n-C24	1.73	2.52
n-C25	1.52	2.28
n-C26	1.33	1.93
n-C27	1.07	1.57
n-C28	1.02	1.54
n-C29	0.88	1.33
n-C30	0.71	1.04
n-C31	0.57	0.86
n-C32	0.45	0.67
n-C33	0.34	0.52
n-C34	0.31	0.51
n-C35	0.28	0.45
n-C36	0.14	0.22
n-C37	0.10	0.16
n-C38	0.08	0.13
n-C39	0.06	0.10
n-C40	0.04	0.08
n-C41	0.02	0.05
TOTAL	**94.7**	**92.5**
C17/PRISTANE	2.40	2.43
C18/PHYTANE	1.83	1.86
PRISTANE/PHYTANE	1.07	1.09
CPI	0.95	1.05



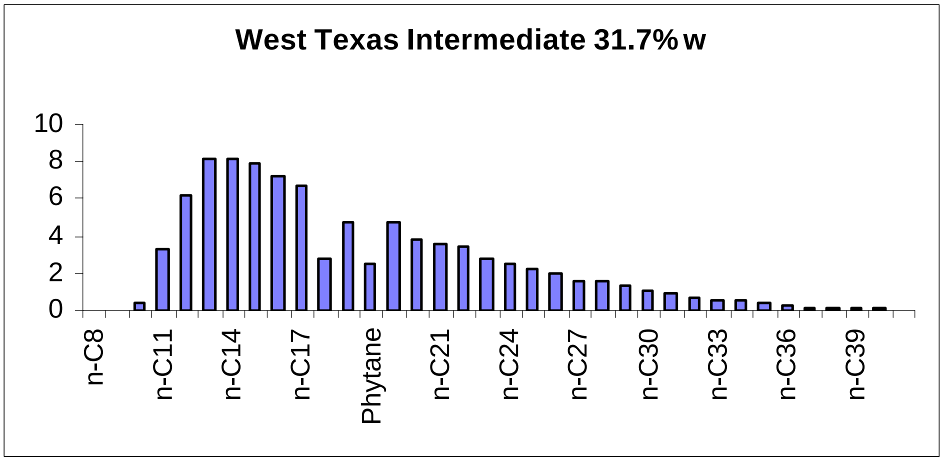


Figure 10.1 *n*-Alkane Distribution for West Texas Intermediate crude oil (mg/g oil)

10.18 PAH Distribution

	Concentration (µg/g oil)	
Alkylated PAH	**0% weathered**	**31.7% weathered**
Naphthalene		
C0-N	292.6	212.8
C1-N	951.6	1056.6
C2-N	1451.7	1517.0
C3-N	1546.3	2025.8
C4-N	929.5	1257.2
Sum	**5172**	**6069**
Phenanthrene		
C0-P	125.2	176.6
C1-P	358.9	505.3
C2-P	350.6	510.9
C3-P	264.5	372.6
C4-P	196.2	278.7
Sum	**1295**	**1844**
Dibenzothiophene		
C0-D	139.0	194.6
C1-D	207.1	293.1
C2-D	268.4	377.6
C3-D	201.2	279.8
Sum	**826**	**1145**
Fluorene		
C0-F	48.9	63.0
C1-F	108.6	141.3
C2-F	160.7	208.8
C3-F	140.2	186.5
Sum	**458**	**600**
Chrysene		
C0-C	13.5	19.3
C1-C	22.5	31.8
C2-C	32.7	47.5
C3-C	31.4	47.0
Sum	**100**	**146**
TOTAL	**7841**	**9804**
2-m-N/1-m-N	1.27	1.22
(3+2-m/phen)/(4-/9-+1m-phen)	0.72	0.71
4-m:2/3m:1-m-DBT	1:0.94:0.46	1:0.95:0.46

Other PAHs		
Biphenyl	68.45	82.79
Acenaphthylene	11.08	14.09
Acenaphthene	8.84	11.47
Anthracene	1.00	1.87
Fluoranthene	2.12	3.12
Pyrene	6.72	10.22
Benz(a)anthracene	1.24	1.50
Benzo(b)fluoranthene	1.37	1.75
Benzo(k)fluoranthene	0.37	0.37
Benzo(e)pyrene	3.48	5.24
Benzo(a)pyrene	0.25	0.33
Perylene	0.12	0.20
Indeno(1,2,3cd)pyrene	0.18	0.25
Dibenz(a,h)anthracene	0.18	0.25
Benzo(ghi)perylene	0.50	0.69
TOTAL	**106**	**135**

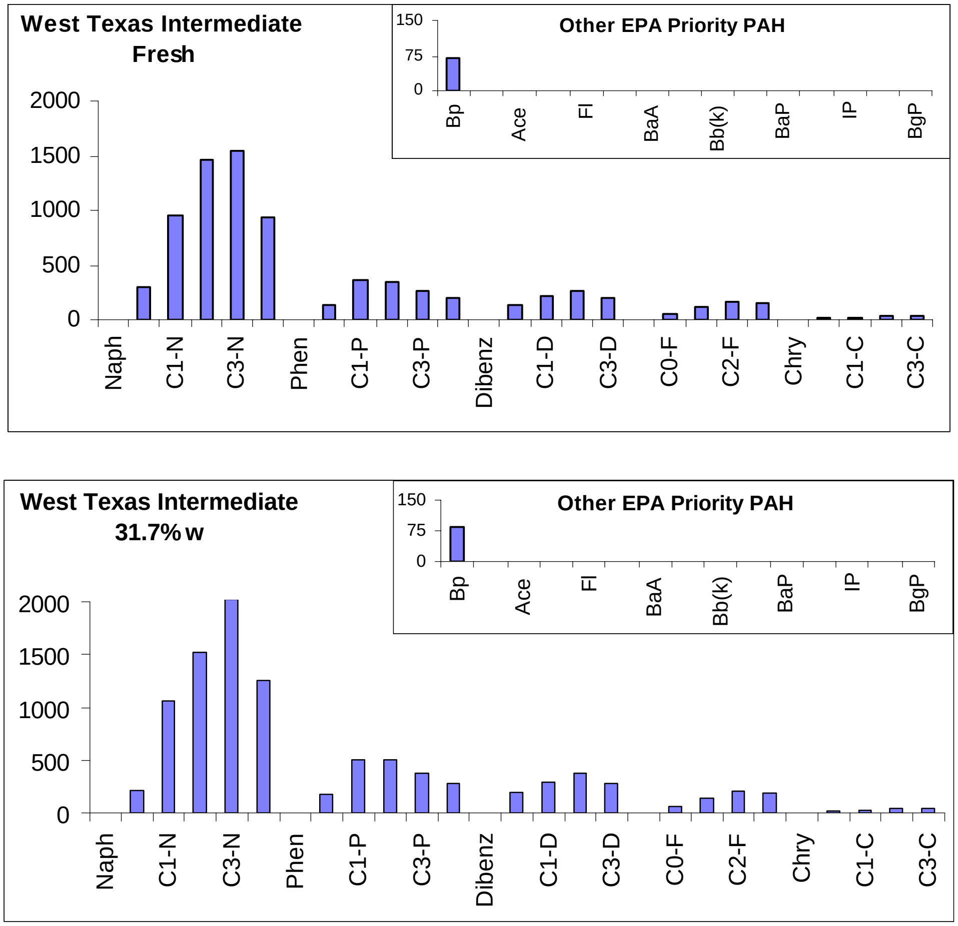


Figure 10.2 PAH Distribution for West Texas Intermediate crude oil (μg/g oil)

10.19 Biomarker Concentrations

Biomarker	**Concentration (μg/g oil)** **0% weathered**	**31.7% weathered**
C23	42.5	62.6
C24	23.7	34.5
C29	53.5	75.7
C30	74.7	104.4
C31(S)	33.2	47.6
C31(R)	31.2	45.1
C32(S)	26.5	38.3
C32(R)	17.9	26.0
C33(S)	14.9	21.7
C33(R)	9.8	14.3
C34(S)	9.2	13.8
C34(R)	5.8	8.9
Ts	16.5	23.9
Tm	21.8	30.7
C27αββ steranes	63.3	92.7
C29αββ steranes	79.0	114.1
TOTAL	**524**	**755**
Diagnostic Ratios		
C23/C24	1.80	1.81
C23/C30	0.57	0.60
C24/C30	0.32	0.33
C29/C30	0.72	0.73
C31(S)/C31(R)	1.06	1.06
C32(S)/C32(R)	1.48	1.47
C33(S)/C33(R)	1.52	1.52
C34(S)/C34(R)	1.57	1.55
Ts/Tm	0.76	0.78
C27αββ/C29αββ	0.80	0.81

11. Physical Properties and Chemical Composition of Fuel Oil No. 2/Diesel (2002)

11.1 Origin:

Origin: Local Retailer, Ontario, Canada (Stinsons' Gas)
Synonyms: "Summer" Diesel, Fuel Oil No. 2
Appearance: Golden-coloured, light, characteristic "fuel" odour.

Values are reported for the **fresh oil** and for artificially weathered fractions of **7.2%**, **14.2%** and **22.0%** loss by weight.

11.2 API Gravity

37.52 *(calc)*

11.3 Equation for Predicting Evaporation

$$\%Ev = (0.02 + 0.013\,T)\,\mathrm{sqrt}(t)$$

Where: %Ev = weight percent evaporated; T = surface temperature (°C); t = time (minutes)

11.4 Sulphur Content

Weathering (weight %)	Sulphur (weight %)	
0	0.09	*(n=3)*
7.2	0.10	*(n=3)*
14.2	0.10	*(n=3)*
22.0	0.10	*(n=3)*

11.5 Water Content

Weathering (weight %)	Water (volume %)	
0	<0.1	*(n=3)*
7.2	<0.1	*(n=3)*
14.2	<0.1	*(n=3)*
22.0	<0.1	*(n=3)*

11.6 Flash Point

Weathering (weight %)	Flash Point (°C)	
0	54	*(n=2)*
7.2	65	*(n=2)*
14.2	76	*(n=2)*
22.0	85	*(n=2)*

11.7 Density

Weathering (weight %)	Temperature (°C)	Density (g/mL)	
0	0	0.8423	*(n=3)*
	15	0.8310	*(n=3)*
7.2	0	0.8468	*(n=3)*
	15	0.8350	*(n=3)*
14.2	0	0.8493	*(n=3)*
	15	0.8383	*(n=3)*
22.0	0	0.8524	*(n=3)*
	15	0.8416	*(n=3)*

11.8 Pour Point

Weathering (weight %)	Pour Point (°C)	
0	-50	*(n=2)*
7.2	-49	*(n=2)*
14.2	-43	*(n=2)*
22.0	-41	*(n=2)*

11.9 Dynamic Viscosity

Weathering (weight %)	Temperature (°C)	Viscosity (cP)	
0	0	4.08	*(n=3)*
	15	2.76	*(n=3)*
7.2	0	4.55	*(n=3)*
	15	3.27	*(n=3)*
14.2	0	5.16	*(n=3)*
	15	3.42	*(n=2)*
22.0	0	5.59	*(n=3)*
	15	4.18	*(n=2)*

11.10 Chemical Dispersibility

Weathering (weight %)	Chemical Dispersibility using Corexit 9500 (%)	
0	72	*(n=6)*
7.2	71	*(n=6)*
14.2	64	*(n=6)*
22.0	66	*(n=6)*

11.11 Adhesion

Weathering (weight %)	Adhesion (g/m^2)	
0	2	*(n=4)*
7.2	12	*(n=4)*
14.2	13	*(n=3)*
22.0	8	*(n=4)*

11.12 Surface and Interfacial Tensions

11.12.1 Surface Tension (Oil/Air Interfacial Tension)

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	28.7	*(n=3)*
	15	27.5	*(n=3)*
7.2	0	28.8	*(n=3)*
	15	27.7	*(n=3)*
14.2	0	28.6	*(n=3)*
	15	28.1	*(n=3)*
22.0	0	29.3	*(n=3)*
	15	28.3	*(n=3)*

11.12.2 Oil/Brine (33‰) Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	21.5	*(n=3)*
	15	18.1	*(n=8)*
7.2	0	24.8	*(n=3)*
	15	19.5	*(n=3)*
14.2	0	26.6	*(n=2)*
	15	20.7	*(n=3)*
22.0	0	28.5	*(n=3)*
	15	21.9	*(n=3)*

11.12.3 *Oil/Fresh Water Interfacial Tension*

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	25.0	*(n=3)*
	15	21.6	*(n=3)*
7.2	0	28.1	*(n=3)*
	15	23.9	*(n=3)*
14.2	0	28.5	*(n=3)*
	15	24.3	*(n=3)*
22.0	0	29.1	*(n=3)*
	15	25.7	*(n=2)*

11.13 Emulsion Formation

Weathering (weight %)	Visual Stability	Complex Modulus (Pa)	Emulsion Water Content (%)
0	Unstable		
7.2	Unstable		
14.2	Unstable		
22.0	Unstable		

11.14 Boiling Point Distribution

	Cumulative Weight Fraction (%)			
Boiling Point (°C)	0% weathered	7.2% weathered	14.2% weathered	22.0% weathered
40				
60				
80	0.2	0.1		
100	0.5	0.1		
120	1.2	0.1		
140	2.8	0.7	0.1	
160	7.8	4.0	1.4	0.3
180	16.4	11.8	7.1	3.2
200	26.8	22.4	17.0	11.2
250	57.4	55.4	51.7	46.7
300	84.1	84.5	83.3	81.4
350	96.4	98.1	98.1	97.8
400	97.9	99.7	99.8	99.7
450	98.1	99.9		
500	98.2			
550	98.3			
600	98.4			
650	98.6			

11.15 Hydrocarbon Groups

	Concentration (weight %)			
Component	0% weathered	7.2% weathered	14.2% weathered	22.0% weathered
Saturates	88.2	86.1	86.1	85.6
Aromatics	10.2	11.9	11.7	11.4
Resins	1.7	2.0	2.2	3.0
Asphaltenes	0.0	0.0	0.0	0.0
Waxes	1.7	1.8	2.0	1.8

11.16 Volatile Organic Compounds

	Concentration (µg/g oil)	
Component	0% weathered	22.0% weathered
Benzene	136	0
Toluene	1024	0
Ethylbenzene	619	0
Xylenes†	3774	7
C_3-Benzenes‡†	13780	2260
Total BTEX	5550	7
Total BTEX and C_3-Benzenes‡	19330	2267

†Note that the “Xylenes” include *o*-, *m*-, and *p*-xylene isomers.
††Note that the “C_3-Benzenes” include eight isomers.

11.17 *n*-Alkane Distribution

n-Alkane Component	Concentration (mg/g oil) 0% weathered	 22.0% weathered
n-C8	1.15	
n-C9	4.24	
n-C10	10.93	3.96
n-C11	13.43	11.79
n-C12	13.23	15.25
n-C13	13.02	16.51
n-C14	12.33	15.77
n-C15	11.98	15.58
n-C16	10.96	13.70
n-C17	9.22	11.37
Pristane	3.81	4.82
n-C18	6.72	8.20
Phytane	2.52	3.10
n-C19	4.72	5.88
n-C20	3.01	3.74
n-C21	1.70	2.11
n-C22	0.85	1.06
n-C23	0.41	0.52
n-C24	0.19	0.24
n-C25	0.09	0.11
n-C26	0.04	0.05
n-C27	0.02	0.03
n-C28	0.02	0.02
n-C29	0.01	0.01
n-C30	0.01	0.01
n-C31	0.01	0.01
n-C32		
n-C33		
n-C34		
n-C35		
n-C36		
n-C37		
n-C38		
n-C39		
n-C40		
n-C41		
TOTAL	124.6	133.8
C17/PRISTANE	1.58	1.52
C18/PHYTANE	1.61	1.58
PRISTANE/PHYTANE	1.25	1.23
CPI	0.99	1.03

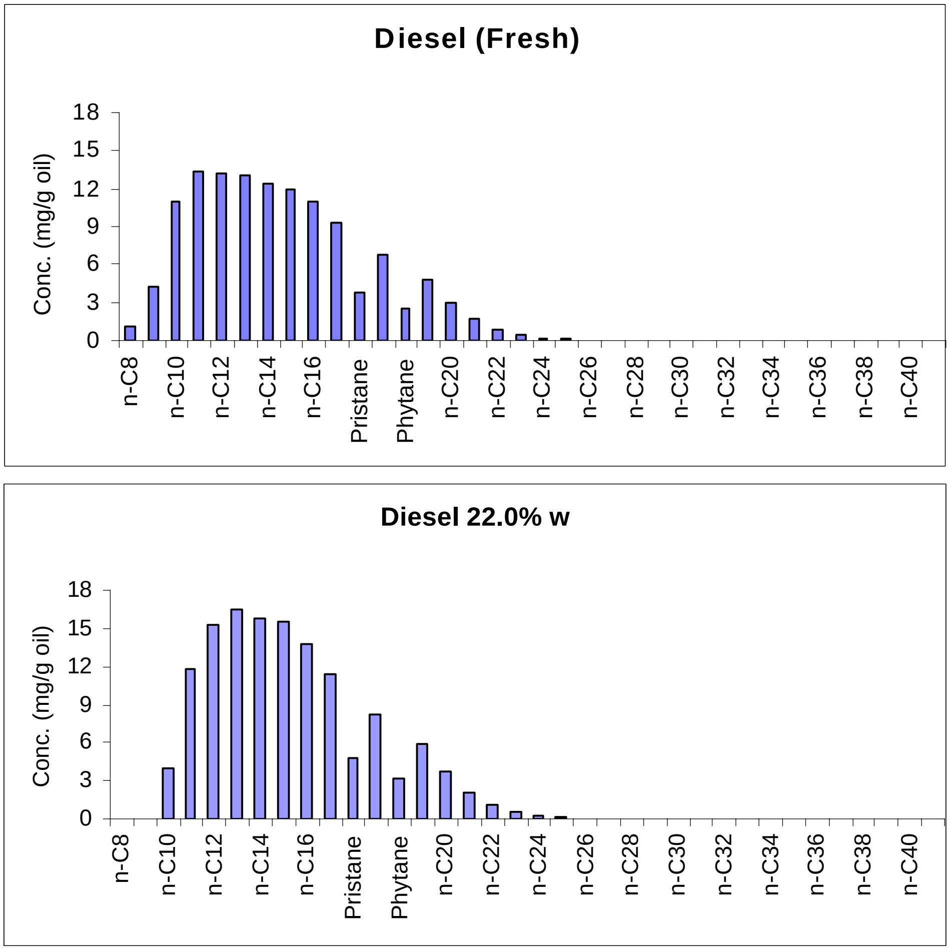


Figure 11.1 Alkane Distribution for Fuel Oil No. 2 (Diesel) (mg/g oil)

11.18 PAH Distribution

	Concentration (µg/g oil)	
Alkylated PAH	**0% weathered**	**22.0% weathered**
Naphthalene		
C0-N	820	677
C1-N	3664	3968
C2-N	6927	8101
C3-N	6636	8163
C4-N	2805	3427
Sum	**20852**	**24337**
Phenanthrene		
C0-P	437	557
C1-P	1000	1262
C2-P	617	769
C3-P	185	237
C4-P	53	65
Sum	**2293**	**2890**
Dibenzothiophene		
C0-D	65	82
C1-D	110	137
C2-D	99	123
C3-D	38	50
Sum	**312**	**392**
Fluorene		
C0-F	567	713
C1-F	799	1025
C2-F	756	961
C3-F	360	458
Sum	**2481**	**3157**
Chrysene		
C0-C	0.02	0.03
C1-C	0.03	0.04
C2-C	0.04	0.04
C3-C	0.00	0.00
Sum	0.09	0.12
TOTAL	**25938**	**30776**
2-m-N/1-m-N	1.56	1.53
(3+2-m/phen)/(4-/9-+1m-phen)	1.50	1.52
4-m:2/3m:1-m-DBT	1 : 0.35 : 0.16	1 : 0.36 : 0.17
Other PAHs		
Biphenyl	839.73	1072.40
Acenaphthylene	34.87	42.29
Acenaphthene	153.55	187.34
Anthracene	13.08	14.09
Fluoranthene	6.60	8.48
Pyrene	30.88	38.84
Benz(a)anthracene	0.25	0.28
Benzo(b)fluoranthene	0.00	0.00
Benzo(k)fluoranthene	0.00	0.00
Benzo(e)pyrene	0.00	0.00
Benzo(a)pyrene	0.00	0.00
Perylene	0.00	0.00
Indeno(1,2,3cd)pyrene	0.00	0.00
Dibenz(a,h)anthracene	0.00	0.00
Benzo(ghi)perylene	0.00	0.00
TOTAL	**1080**	**1364**

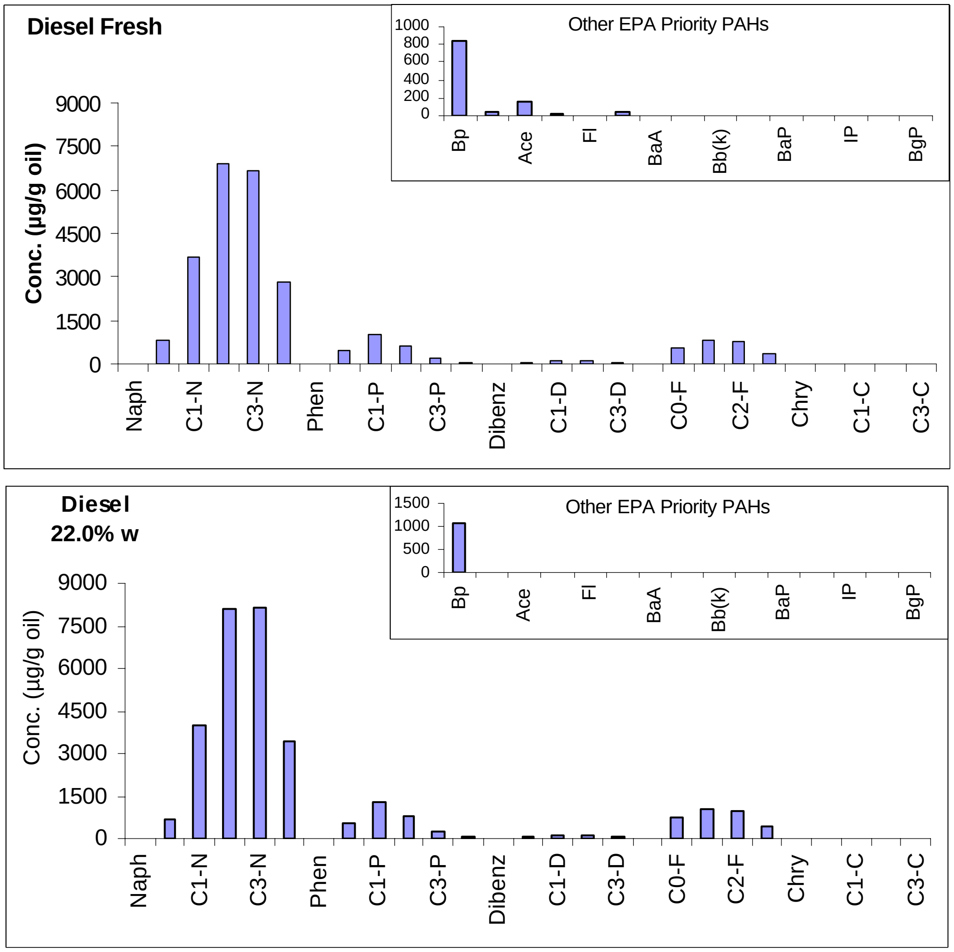


Figure 11.1 PAH Distribution for Fuel Oil No. 2 (Diesel) (µg/g oil)

11.19 Biomarker Concentrations

	Concentration (μg/g oil)	
Biomarker	**0% weathered**	**22.0% weathered**
C23	4.0	5.3
C24	1.4	1.8
C29		
C30		
C31(S)		
C31(R)		
C32(S)		
C32(R)		
C33(S)		
C33(R)		
C34(S)		
C34(R)		
Ts		
Tm		
C27αββ steranes		
C29αββ steranes		
TOTAL	**5**	**7**
Diagnostic Ratios		
C23/C24	3.0	2.9
C23/C30		
C24/C30		
C29/C30		
C31(S)/C31(R)		
C32(S)/C32(R)		
C33(S)/C33(R)		
C34(S)/C34(R)		
Ts/Tm		
C27αββ/C29αββ		

Note: except for the C23 and C24 terpanes, no other biomarkers were detected.

12. Physical Properties and Chemical Composition of Fuel Oil No. 5 (2000)

12.1 Origin:

Origin: New Jersey, U.S.A, (Via U.S. Dept. Int., M.M.S., OHMSETT, NJ, 2000)
Synonyms: Bunker B
Appearance: Black, heavy, sticky, little odour.

Values are reported for the **fresh oil** and for an artificially weathered fraction of **7.2%** loss by weight.

12.2 API Gravity

11.55 *(calc)*

12.3 Equation for Predicting Evaporation

$$\%Ev = (-0.14 + 0.013\,T)\,t^{1/2}$$

Where: %Ev = weight percent evaporated; T = surface temperature (°C); t = time (minutes)

12.4 Sulphur Content

Weathering (weight %)	Sulphur (weight %)	
0	1.00	*(n=3)*
7.2	1.08	*(n=3)*

12.5 Water Content

Weathering (weight %)	Water (volume%)	
0	3.1	*(n=3)*
7.2	<0.1	*(n=3)*

12.6 Flash Point

Weathering (weight %)	Flash Point (°C)	
0	94	*(n=3)*
7.2	136	*(n=3)*

12.7 Density

Weathering (weight %)	Temperature (°C)	Density (g/mL)	
0	0	1.0034	*(n=3)*
	15	0.9883	*(n=3)*
7.2	0	1.0160	*(n=3)*
	15	1.0032	*(n=3)*

12.8 Pour Point

Weathering (weight %)	Pour Point (°C)	
0	-19	*(n=2)*
7.2	-3	*(n=2)*

12.9 Dynamic Viscosity

Weathering (weight %)	Temperature (°C)	Viscosity (cP)	
0	0	18600	*(n=3)*
	15	1410	*(n=3)*
7.2	0	72000	*(n=3)*
	15	4530	*(n=3)*

12.10 Chemical Dispersibility

Weathering (weight %)	Chemical Dispersibility using Corexit 9500 (%)	
0	15	*(n=6)*
7.2	7	*(n=6)*

12.11 Adhesion

Weathering (weight %)	Adhesion (g/m^2)	
0	34	*(n=4)*
7.2	47	*(n=4)*

12.12 Surface and Interfacial Tensions

12.12.1 Surface Tension (Oil/Air Interfacial Tension)

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)
0	0	NM
	15	NM
7.2	0	NM
	15	NM

12.12.2 Oil/Brine (33‰) Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)
0	0	NM
	15	NM
7.2	0	NM
	15	NM

†NM: not measurable

12.12.3 Oil/Fresh Water Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)
0	0	NM
	15	NM
7.2	0	NM
	15	NM

12.13 Emulsion Formation

Weathering (weight %)	Visual Stability	Complex Modulus (Pa)	Emulsion Water Content (%)
0	Stable	1590	78.3
7.2	Stable	2490	72.8

12.14 Boiling Point Distribution

	Cumulative Weight Fraction (%)	
Boiling Point (°C)	0% weathered	7.2% weathered
40		
60		
80		
100		
120	0.1	
140	0.2	
160	0.6	
180	1.3	
200	2.3	0.2
250	7.2	3.8
300	14.6	11.3
350	24.4	21.7
400	39.9	38.0
450	55.8	55.0
500	66.2	66.2
550	74.0	74.5
600	80.4	81.5
650	85.6	86.9

12.15 Hydrocarbon Groups

Component	Concentration (weight %) 0% weathered	7.2% weathered
Saturates	44.2	39.9
Aromatics	39.5	39.1
Resins	8.0	8.3
Asphaltenes	8.4	12.8
Waxes	2.3	2.5

12.16 Volatile Organic Compounds

Component	Concentration (µg/g oil) 0% weathered	7.2% weathered
Benzene	0	0
Toluene	149	0
Ethylbenzene	124	1
Xylenes†	612	2
C_3-Benzenes‡	1750	30
Total BTEX	890	0
Total BTEX and C_3-Benzenes‡	2640	30

†“Xylenes” include *o*-, *m*-, and *p*-xylene isomers.
‡“C_3-Benzenes” include eight isomers.

12.17 *n*-Alkane Distribution

	Concentration (mg/g oil)	
***n*-Alkane Component**	**0% weathered**	**7.2% weathered**
n-C8		
n-C9	0.34	
n-C10	0.54	
n-C11	0.74	0.1
n-C12	1.01	0.49
n-C13	1.35	1.08
n-C14	1.71	1.60
n-C15	1.89	2.11
n-C16	2.22	2.53
n-C17	2.03	2.38
Pristane	1.11	1.27
n-C18	1.79	2.10
Phytane	0.76	0.88
n-C19	1.70	1.90
n-C20	1.55	1.90
n-C21	1.70	2.00
n-C22	1.85	2.23
n-C23	2.25	2.73
n-C24	2.46	2.98
n-C25	2.47	3.03
n-C26	2.08	2.55
n-C27	1.77	2.20
n-C28	1.34	1.66
n-C29	1.01	1.26
n-C30	0.58	0.70
n-C31	0.37	0.48
n-C32	0.21	0.26
n-C33	0.14	0.17
n-C34	0.11	0.12
n-C35	0.07	0.09
n-C36	0.06	0.07
n-C37	0.04	0.06
n-C38	0.02	0.03
n-C39	0.01	0.02
n-C40		0.02
n-C41		
TOTAL	**37.3**	**41**
C17/PRISTANE	1.83	1.87
C18/PHYTANE	2.35	2.39
PRISTANE/PHYTANE	1.45	1.45
CPI	1.02	1.02

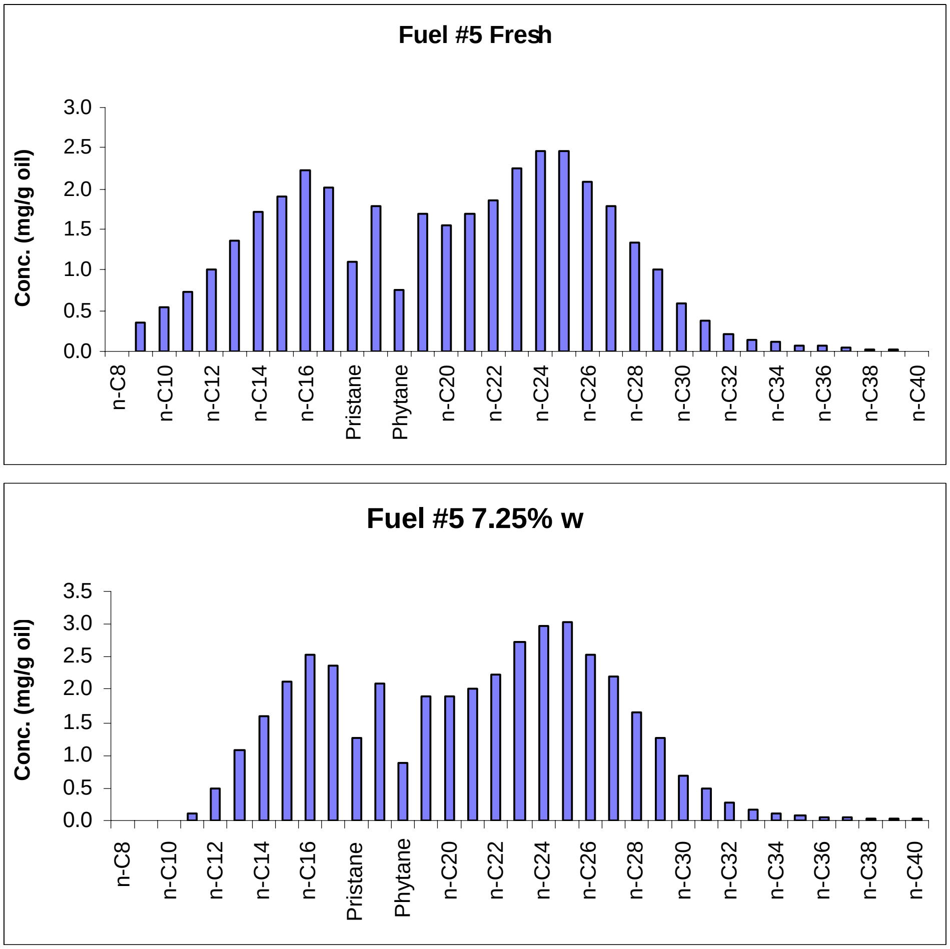


Figure 12.1 *n*-Alkane Distribution for Fuel Oil No. 5 (mg/g oil)

12.18 PAH Distribution

	Concentration (µg/g oil)	
Alkylated PAH	**0% weathered**	**7.2% weathered**
Naphthalene		
C0-N	236	128
C1-N	2048	1722
C2-N	4790	4708
C3-N	5001	5288
C4-N	2385	2736
Sum	**14460**	**14582**
Phenanthrene		
C0-P	848	895
C1-P	4274	4533
C2-P	6974	7362
C3-P	6610	6971
C4-P	4074	4369
Sum	**22779**	**24130**
Dibenzothiophene		
C0-D	92	99
C1-D	295	315
C2-D	610	661
C3-D	582	638
Sum	**1579**	**1713**
Fluorene		
C0-F	357	370
C1-F	1021	1075
C2-F	1809	1936
C3-F	1799	1888
Sum	**4986**	**5269**
Chrysene		
C0-C	920	965
C1-C	2808	3195
C2-C	4676	4923
C3-C	3482	3598
Sum	**11887**	**12681**
TOTAL	**55692**	**58375**
2-m-N/1-m-N	1.88	1.81
(3+2-m/phen)/(4-/9-+1m-phen)	1.63	1.59
4-m:2/3m:1-m-DBT	1 : 1.00 : 0.27	1 : 0.99 : 0.26
Other PAHs		
Biphenyl	132.98	123.02
Acenaphthylene	33.69	34.29
Acenaphthene	167.50	168.82
Anthracene	217.67	224.82
Fluoranthene	80.43	84.89
Pyrene	552.67	563.19
Benz(a)anthracene	551.51	530.94
Benzo(b)fluoranthene	125.74	132.61
Benzo(k)fluoranthene	34.08	39.74
Benzo(e)pyrene	221.23	224.46
Benzo(a)pyrene	449.35	459.47
Perylene	159.07	180.00
Indeno(1,2,3cd)pyrene	25.15	27.70
Dibenz(a,h)anthracene	68.56	74.10
Benzo(ghi)perylene	83.87	87.05
TOTAL	**2863**	**2975**

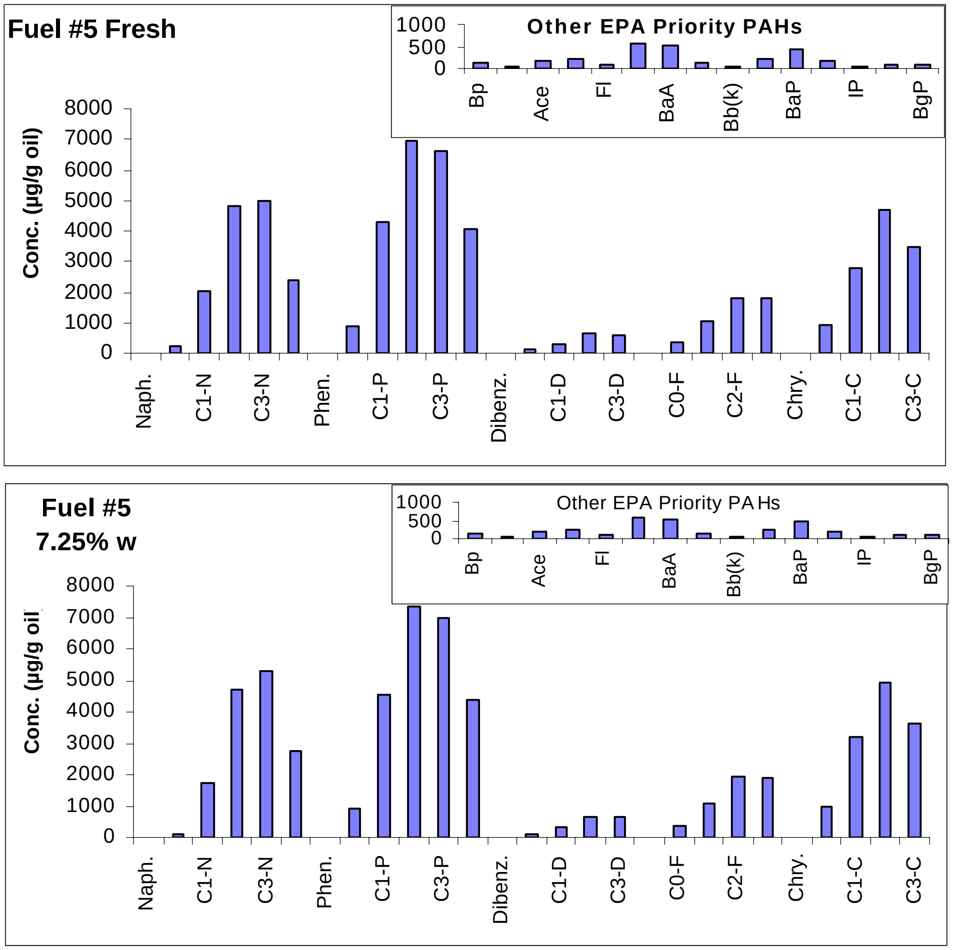


Figure 12.2 PAH Distribution for Fuel Oil No. 5 (µg/g oil)

12.19 Biomarker Concentrations

Biomarker	Concentration (μg/g oil) 0% weathered	 7.2% weathered
C23	49.7	53.6
C24	20.1	22.7
C29	71.0	74.8
C30	67.6	71.8
C31(S)	17.6	19.4
C31(R)	16.9	19.2
C32(S)	11.5	12.6
C32(R)	10.2	11.4
C33(S)	7.0	7.3
C33(R)	4.4	4.7
C34(S)	4.0	4.7
C34(R)	2.3	2.7
Ts	21.7	22.6
Tm	16.2	16.3
C27αββ steranes	17.2	18.6
C29αββ steranes	18.0	19.2
TOTAL	**355**	**381**
Diagnostic Ratios		
C23/C24	2.47	2.36
C23/C30	0.74	0.75
C24/C30	0.30	0.32
C29/C30	1.05	1.04
C31(S)/C31(R)	1.04	1.01
C32(S)/C32(R)	1.12	1.11
C33(S)/C33(R)	1.58	1.55
C34(S)/C34(R)	1.78	1.76
Ts/Tm	1.34	1.39
C27αββ/C29αββ	0.96	0.97

13. Physical Properties and Chemical Composition of Heavy Fuel Oil 6303 (2002)

13.1 Origin:

Origin: Imperial Oil Ltd., Nova Scotia, Canada (2002)
Synonyms: Bunker C, Land Bunker
Appearance: Black, heavy, sticky, little odour.

Values are reported for the **fresh oil** and for an artificially weathered fraction of **2.5%** loss by weight.

13.2 API Gravity

11.47 *(calc)*

13.3 Equation for Predicting Evaporation

$$\%Ev = (-0.16 + 0.013\ T)\ t^{1/2}$$

Where: %Ev = weight percent evaporated; *T* = surface temperature (°C); *t* = time (minutes)

13.4 Sulphur Content

Weathering (weight %)	Sulphur (weight %)	
0	1.48	*(n=3)*
2.5	1.50	*(n=3)*

13.5 Water Content

Weathering (weight %)	Water (volume%)	
0	0.1	*(n=3)*
2.5	<0.1	*(n=3)*

13.6 Flash Point

Weathering (weight %)	Flash Point (°C)	
0	111	*(n=3)*
2.5	133	*(n=3)*

13.7 Density

Weathering (weight %)	Temperature (°C)	Density (g/mL)	
0	0	1.0015	*(n=3)*
	15	0.9888	*(n=3)*
2.5	0	1.0101	*(n=3)*
	15	0.9988	*(n=3)*

13.8 Pour Point

Weathering (weight %)	Pour Point (°C)	
0	-1	*(n=2)*
2.5	11	*(n=2)*

13.9 Dynamic Viscosity

Weathering (weight %)	Temperature (°C)	Viscosity (cP)	
0	0	241000	*(n=3)*
	15	22800	*(n=3)*
2.5	0	3600000	*(n=3)*
	15	149000	*(n=3)*

13.10 Chemical Dispersibility

Weathering (weight %)	Chemical Dispersibility using Corexit 9500 (%)	
0	9	*(n=6)*
2.5	6	*(n=6)*

13.11 Adhesion

Weathering (weight %)	Adhesion (g/m^2)	
0	100	*(n=4)*
2.5	240	*(n=4)*

13.12 Surface and Interfacial Tensions

13.12.1 Surface Tension (Oil/Air Interfacial Tension)

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)
0	0	NM
	15	NM
2.5	0	NM
	15	NM

13.12.2 Oil/Brine (33‰) Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)
0	0	NM
	15	NM
2.5	0	NM
	15	NM

†NM: not measurable

13.12.3 Oil/Fresh Water Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)
0	0	NM
	15	NM
2.5	0	NM
	15	NM

13.13 Emulsion Formation

Weathering (weight %)	Visual Stability	Complex Modulus (Pa)	Emulsion Water Content (%)
0	Entrained	752	57.7
2.5	Entrained	984	24.1

13.14 Boiling Point Distribution

	Cumulative Weight Fraction (%)	
Boiling Point (°C)	0% weathered	2.5% weathered
40		
60		
80		
100		
120	0.1	
140	0.2	
160	0.3	
180	0.6	
200	1.2	0.2
250	5.5	3.5
300	12.5	10.2
350	23.3	21.2
400	33.5	31.5
450	38.8	37.0
500	41.2	39.7
550	45.3	44.1
600	55.7	54.8
650	70.1	69.6

13.15 Hydrocarbon Groups

Component	Concentration (weight %) 0% weathered	2.5% weathered
Saturates	42.5	38.8
Aromatics	29.0	26.9
Resins	15.5	16.6
Asphaltenes	13.0	17.7
Waxes	2.5	2.7

13.16 Volatile Organic Compounds

Component	Concentration (µg/g oil) 0% weathered	2.5% weathered
Benzene	40	0
Toluene	136	0
Ethylbenzene	58	0
Xylenes†	396	0
C_3-Benzenes‡	940	50
Total BTEX	630	0
Total BTEX and C_3-Benzenes‡	1570	50

†“Xylenes” include *o*-, *m*-, and *p*-xylene isomers.
‡“C_3-Benzenes” include eight isomers.

13.17 *n*-Alkane Distribution

n-Alkane Component	Concentration (mg/g oil) 0% weathered	 2.5% weathered
n-C8		
n-C9	0.09	
n-C10	0.19	
n-C11	0.41	0.10
n-C12	0.68	0.42
n-C13	0.99	0.71
n-C14	1.21	1.23
n-C15	1.43	1.59
n-C16	1.78	2.07
n-C17	2.00	2.33
Pristane	2.20	2.55
n-C18	2.17	2.62
Phytane	1.85	2.24
n-C19	2.26	2.66
n-C20	2.14	2.48
n-C21	1.85	2.18
n-C22	1.49	1.78
n-C23	1.36	1.63
n-C24	1.23	1.51
n-C25	1.00	1.23
n-C26	0.67	0.84
n-C27	0.44	0.57
n-C28	0.31	0.38
n-C29	0.20	0.25
n-C30	0.11	0.13
n-C31	0.07	0.09
n-C32	0.04	0.04
n-C33	0.02	0.02
n-C34	0.02	0.02
n-C35		
n-C36		
n-C37		
n-C38		
n-C39		
n-C40		
n-C41		
TOTAL	**28.2**	**31.7**
C17/PRISTANE	0.91	0.91
C18/PHYTANE	1.17	1.17
PRISTANE/PHYTANE	1.19	1.14
CPI	1.00	0.99

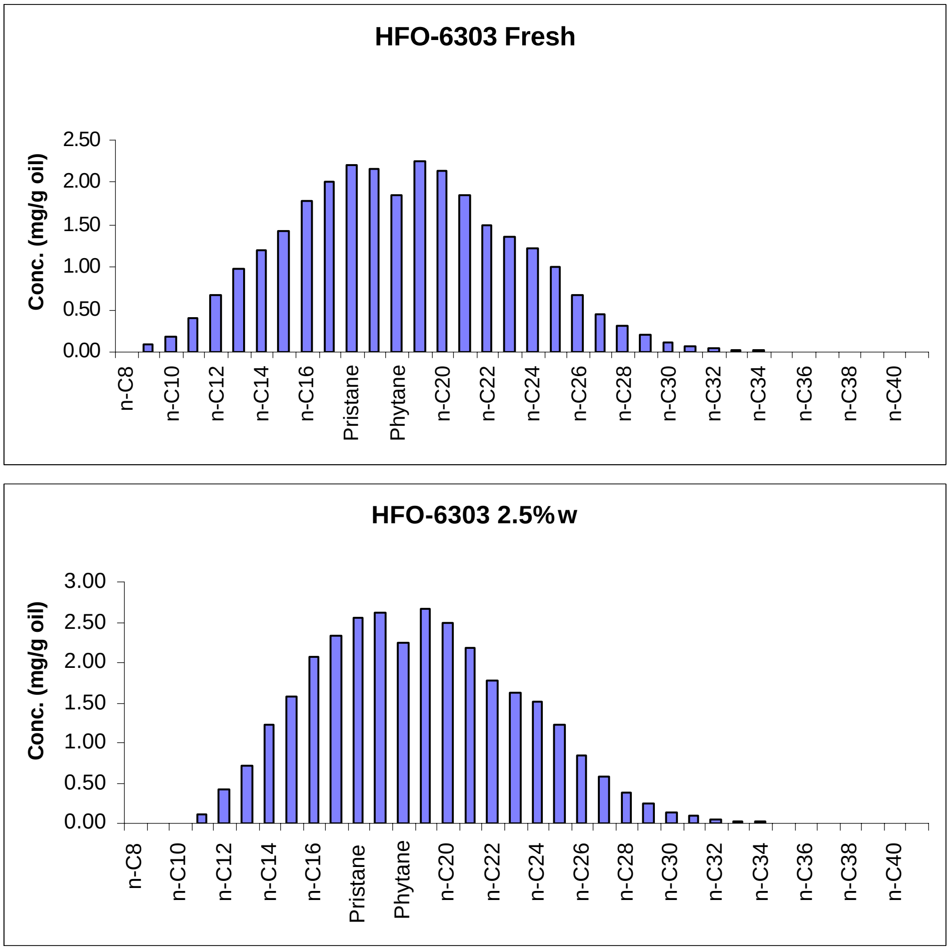


Figure 13.1 *n*-Alkane Distribution for HFO 6303 (Bunker C) (mg/g oil)

13.18 PAH Distribution

Alkylated PAH		Concentration (µg/g oil) 0% weathered	2.5% weathered
Naphthalene			
	C0-N	140	89
	C1-N	1250	1091
	C2-N	2861	2806
	C3-N	2886	2956
	C4-N	1422	1509
	Sum	8558	8450
Phenanthrene			
	C0-P	422	458
	C1-P	1870	2029
	C2-P	2910	3171
	C3-P	3107	3376
	C4-P	2211	2459
	Sum	10520	11492
Dibenzothiophene			
	C0-D	108	115
	C1-D	315	335
	C2-D	620	665
	C3-D	701	766
	Sum	1744	1881
Fluorene			
	C0-F	224	233
	C1-F	565	600
	C2-F	978	1015
	C3-F	936	963
	Sum	2703	2811
Chrysene			
	C0-C	376	415
	C1-C	1173	1274
	C2-C	1806	1961
	C3-C	1379	1397
	Sum	4733	5047
TOTAL		**28258**	**29682**
2-m-N/1-m-N		1.86	1.83
(3+2-m/phen)/(4-/9-+1m-phen)		1.39	1.4
4-m:2/3m:1-m-DBT		1 : 1.01 : 0.37	1 : 1.03 : 0.37

Other PAHs		
Biphenyl	69.22	66.79
Acenaphthylene	19.74	19.87
Acenaphthene	92.54	93.24
Anthracene	95.99	99.34
Fluoranthene	41.09	44.52
Pyrene	226.28	247.88
Benz(a)anthracene	198.27	210.88
Benzo(b)fluoranthene	53.42	57.21
Benzo(k)fluoranthene	11.84	13.29
Benzo(e)pyrene	93.03	99.94
Benzo(a)pyrene	151.14	164.81
Perylene	48.37	57.33
Indeno(1,2,3cd)pyrene	9.50	10.10
Dibenz(a,h)anthracene	21.84	24.30
Benzo(ghi)perylene	28.62	29.92
TOTAL	**1161**	**1239**

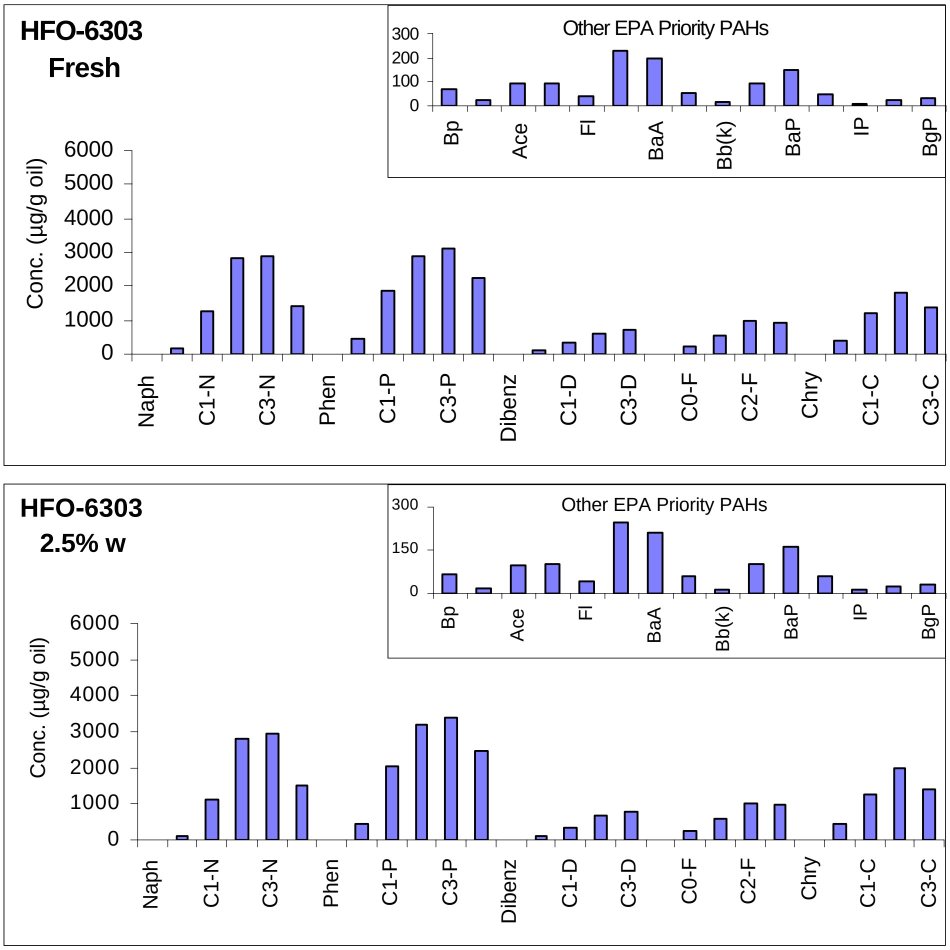


Figure 13.2 PAH Distribution for HFO 6303 (Bunker C) (µg/g oil)

13.19 Biomarker Concentrations

Biomarker	Concentration (µg/g oil) 0% weathered	 2.5% weathered
C23	92.3	106.4
C24	45.9	51.8
C29	14.4	15.1
C30	11.5	12.7
C31(S)	3.7	4.0
C31(R)	3.3	3.7
C32(S)	3.2	3.6
C32(R)	2.0	2.3
C33(S)	1.5	1.6
C33(R)	1.2	1.3
C34(S)	1.1	1.2
C34(R)	0.9	1.0
Ts	5.7	6.5
Tm	1.6	1.9
C27αββ steranes	10.7	12.6
C29αββ steranes	5.5	6.2
TOTAL	**204**	**232**
Diagnostic Ratios		
C23/C24	2.01	2.10
C23/C30	8.01	8.40
C24/C30	3.99	4.10
C29/C30	1.25	1.20
C31(S)/C31(R)	1.11	1.10
C32(S)/C32(R)	1.58	1.60
C33(S)/C33(R)	1.21	1.23
C34(S)/C34(R)	1.28	1.27
Ts/Tm	3.69	3.39
C27αββ/C29αββ	1.94	2.04

14. Physical Properties and Chemical Composition of Orimulsion-400 (2001)

14.1 Origin: Bitor America Corporation, Venezuela (2001)

Synonyms: None
Appearance: Black, easily-poured, very sticky, no odour.

Values are reported for the **fresh product** only. Note that some of the composition results are reported both as bitumen only, *i.e.* dried product, and as Orimulsion-400, as calculated using the measured water mass fraction of section 15.5 below.

14.2 API Gravity

8.63 *(calc)*

14.3 Equation for Predicting Evaporation

Not Measured

14.4 Sulphur Content

Weathering (weight %)	Sulphur (weight %)	
0	2.00*	*(n=3)*

*Note: Including water. Dried bitumen is 2.8%.

14.5 Water Content

Weathering (weight %)	Water (volume%)	
0	28	*(n=5)*

14.6 Flash Point

Weathering (weight %)	Flash Point (°C)	
0	>320*	*(n=2)*

*Note: After water had completely boiled-off sample was cooled and re-tested. The residual bitumen flashed between 130 and 140°C.

14.7 Density

Weathering (weight %)	Temperature (°C)	Density (g/mL)	
0	0	1.0155	*(n=3)*
	15	1.0093	*(n=3)*

14.8 Pour Point

Weathering (weight %)	Pour Point (°C)	
0	1	

14.9 Dynamic Viscosity

Weathering (weight %)	Temperature (°C)	Viscosity (cP)	
0	0	330	*(n=3)*
	15	256	*(n=3)*

14.10 Chemical Dispersibility

Weathering (weight %)	Chemical Dispersibility using Corexit 9500 (%)	
0	100*	*(n=6)*

*Note: Orimulsion-400 is an oil-in-water dispersion.

14.11 Adhesion

Weathering (weight %)	Adhesion (g/m^2)	
0	90	*(n=6)*

14.12 Surface and Interfacial Tensions

14.12.1 Surface Tension (Oil/Air Interfacial Tension)

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	NM	
	15	36.3	*(n=3)*

14.12.2 Oil/Brine (33‰) Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	NM	
	15	NM	

†NM: not measurable

14.12.3 Oil/Fresh Water Interfacial Tension

Weathering (weight %)	Temperature (°C)	Surface Tension (mN/m)	
0	0	NM	
	15	NM	

14.13 Emulsion Formation

Weathering (weight %)	Visual Stability	Complex Modulus (Pa)	Emulsion Water Content (%)
0	Unstable*		

*Note: Dispersion in water; bitumen settled-out on vessel walls.

14.14 Boiling Point Distribution

The boiling point distribution of Orimulsion was not measured.

14.15 Hydrocarbon Groups

	Concentration (weight %)	
Component	Orimulsion-400	Orimulsion-400 (after water content correction)
Saturates	32.1	44.6
Aromatics	19.7	27.3
Resins	9.6	13.3
Asphaltenes	10.6	14.8
Waxes	NM	NM

14.16 Volatile Organic Compounds

Component	Concentration (µg/g oil) Orimulsion-400	Orimulsion-400* (after water content correction)
Benzene	16	22
Toluene	29	41
Ethylbenzene	22	31
Xylenes†	29	40
C_3-Benzenes‡	80	120
Total BTEX	100	130
Total BTEX and C_3-Benzenes‡	180	250

†"Xylenes" include *o*-, *m*-, and *p*-xylene isomers.
‡"C_3-Benzenes" include eight isomers.
*Data for Bitumen were obtained by correction for the water content (28%) from the data for the original Orimulsion-400.

14.17 *n*-Alkane Distribution

No *n*-Alkanes were detected.

14.18 PAH Distribution

	Concentration (µg/g oil)	
Alkylated PAH	**Orimulsion-400**	**Orimulsion-400***
Naphthalene		
C0-N	5	8
C1-N	31	43
C2-N	90	125
C3-N	143	199
C4-N	212	295
Sum	482	670
Phenanthrene		
C0-P	28	39
C1-P	86	119
C2-P	231	320
C3-P	286	397
C4-P	183	255
Sum	814	1131
Dibenzothiophene		
C0-D	10	14
C1-D	39	55
C2-D	140	194
C3-D	264	367
Sum	454	630
Fluorene		
C0-F	12	16
C1-F	41	57
C2-F	145	202
C3-F	212	294
Sum	410	569
Chrysene		
C0-C	10	14
C1-C	24	33
C2-C	45	63
C3-C	52	72
Sum	131	182
TOTAL	**2291**	**3182**
2-m-N/1-m-N	1.51	1.51
(3+2-m/phen)/(4-/9-+1m-phen)	1.02	1.02
4-m:2/3m:1-m-DBT	1 : 0.83 : 1.20	1 : 0.83 : 1.20
Other PAHs		
Biphenyl	2.38	3.30
Acenaphthylene	0.71	0.99
Acenaphthene	6.90	9.58
Anthracene	2.97	4.13
Fluoranthene	1.78	2.48
Pyrene	4.40	6.11
Benz(a)anthracene	2.14	2.97
Benzo(b)fluoranthene	1.31	1.82
Benzo(k)fluoranthene	0.12	0.17
Benzo(e)pyrene	2.14	2.97
Benzo(a)pyrene	2.50	3.47
Perylene	6.07	8.43
Indeno(1,2,3cd)pyrene	0.00	0.00
Dibenz(a,h)anthracene	0.24	0.33
Benzo(ghi)perylene	1.55	2.15
TOTAL	**35**	**49**

[*] Data for Bitumen were obtained by correction for the water content (28%) from the data for the original Orimulsion-400.

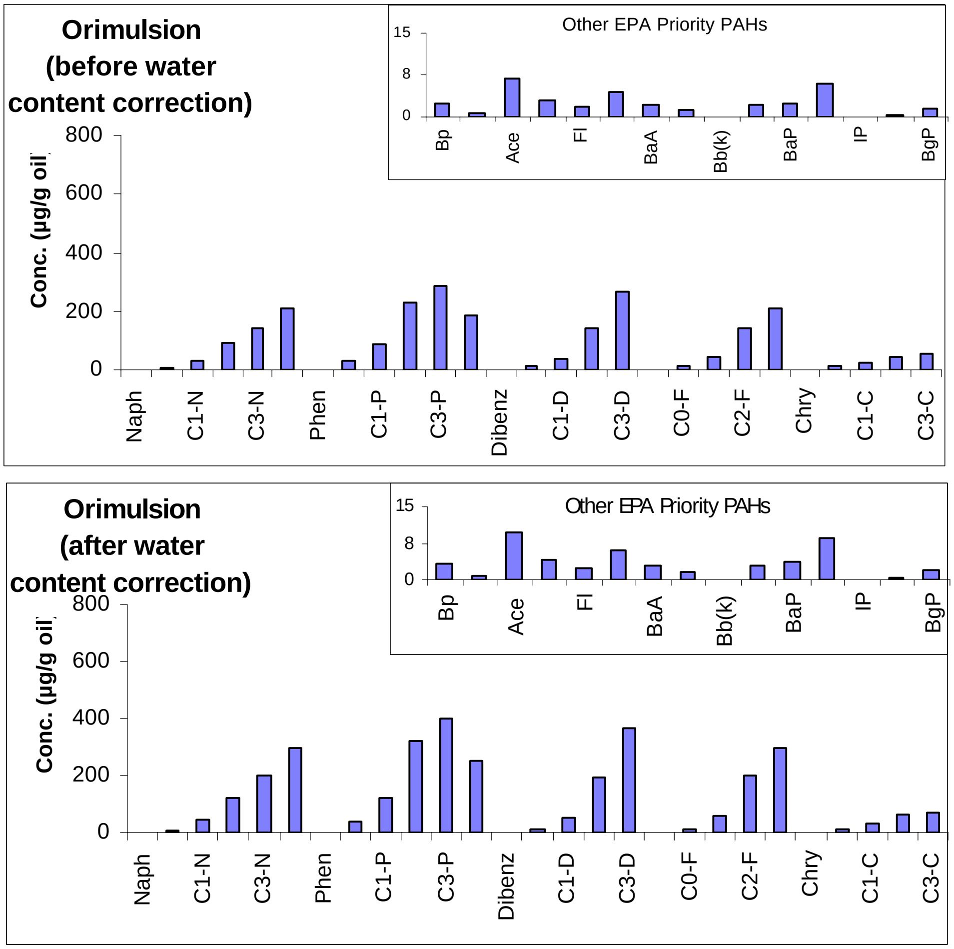


Figure 14.1 PAH Distribution for Orimulsion-400 (µg/g oil)

14.19 Biomarker Concentrations

	Concentration (µg/g oil)	
Biomarker	**Orimulsion-400**	**Orimulsion-400* (after water content correction)**
C23	97.9	135.9
C24	45.4	63.0
C29	85.9	119.3
C30	87.1	121.0
C31(S)	48.5	67.4
C31(R)	34.4	47.8
C32(S)	30.8	42.8
C32(R)	19.3	26.8
C33(S)	19.3	26.8
C33(R)	11.4	15.9
C34(S)	11.9	16.6
C34(R)	7.4	10.3
Ts	11.7	16.3
Tm	45.3	62.9
C27αββ steranes	79.9	111.0
C29αββ steranes	82	113.8
TOTAL	**718**	**998**
Diagnostic Ratios		
C23/C24	2.16	
C23/C30	1.12	
C24/C30	0.52	
C29/C30	0.99	
C31(S)/C31(R)	1.41	
C32(S)/C32(R)	1.60	
C33(S)/C33(R)	1.69	
C34(S)/C34(R)	1.61	
Ts/Tm	0.26	
C27αββ/C29αββ	0.98	

[*] Data for Bitumen were obtained by correction for the water content (28%) from the data for the original Orimulsion-400.

15. Trace Metals

Metal	Alaska North	ASMB #5	Arabian Light	Soceye	South Louisiana	West Texas	Fuel Oil No. 2	Fuel Oil No. 5	HFO 6303	Orimulsion -400
Ba				0.05	0.51			0.05	0.10	
Be	0.015									
Bi		0.7		0.5	0.7					
Ca		10.6	20.9	75.3	37.4	18.6	15.0	34.4	145.0	60.3
Cu	0.3	0.2			0.1	6.7				
Fe	2.9	9.6	1.0		2.0	39.6	0.3		0.3	
Li	1.03	0.05				0.08				
Mg			2.7	0.5	1.5	1.9	0.2	1.4	1.2	2.6
Mn						0.5				
Mo				0.4						
Na		78	31	58	139	88	93	97	94	73
Ni	1.24	0.4	0.5	1.9	1.2	0.8		1.0	0.3	1.0
Sr				0.12	0.27	0.14			0.10	0.17
Ti				0.1						0.2
V	0.1	7.5	4.0	9.7	3.3	2.1		4.7	2.3	10.1
Zn			1.2	1.0	4.2	0.5		3.4	3.2	0.4

All metal content results reported as g/L oil.

Not detected in any samples: Ag, Al, As, Co, Cr, K, Pb, Y

16. References

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17. Appendices

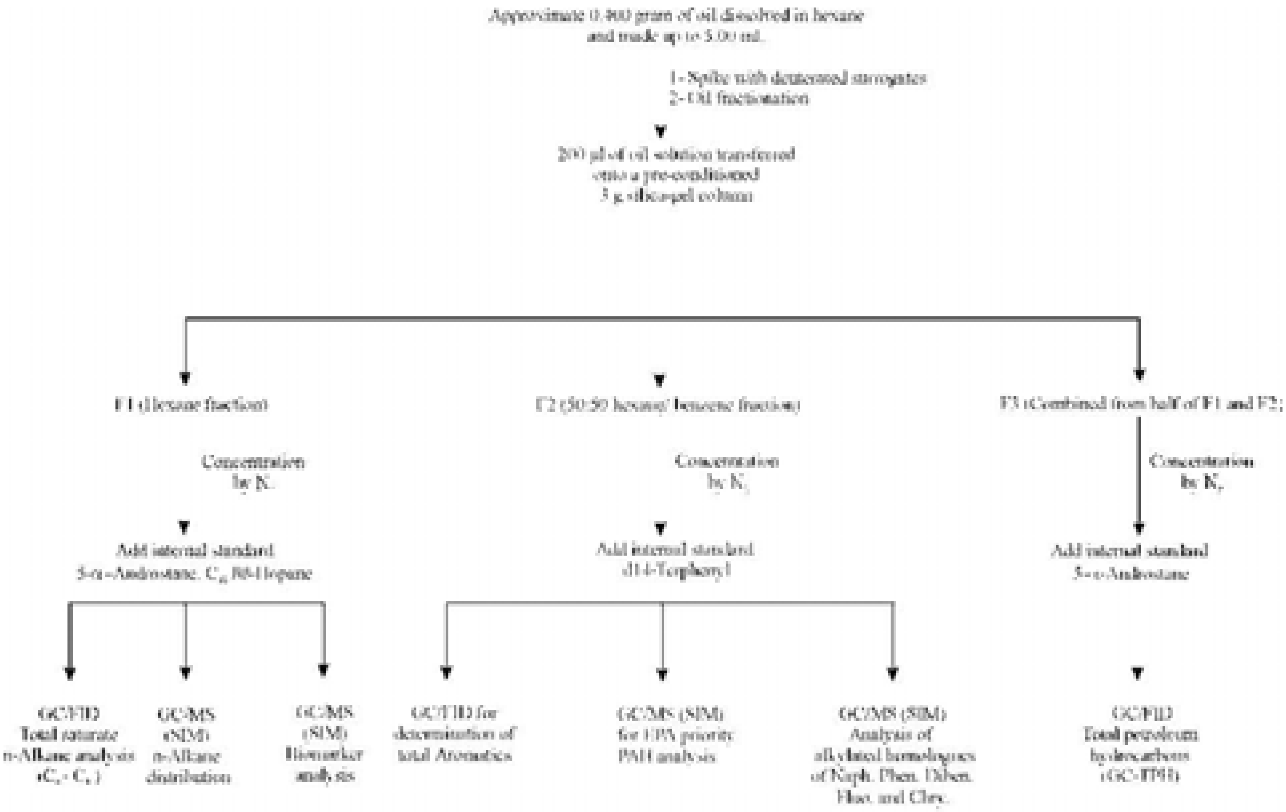
1 Chemical Abstract Service (CAS) Registry Numbers for Selected Analytes

Compound	**CAS Number**
Benzene	71-43-2
Toluene	108-88-3
Ethylbenzene	100-41-4
m-Xylene	108-38-3
p-Xylene	106-42-3
o-Xylene	95-47-6
Isopropylbenzene	98-82-8
Propylbenzene	103-65-1
2-ethyltoluene	611-14-3
3-ethyltoluene	620-14-4
4-ethyltoluene	622-96-8
1,2,4-trimethylbenzene	95-63-6
1,2,3-trimethylbenzene	526-73-8
1,3,5-trimethylbenzene	108-67-8
Isoproplybenzne	98-82-8
1-Methylethylbenzene	98-82-8
1-Ethyl-2-methylbenzene	611-14-3
1-Ethyl-3-methylbenzene	620-14-4
1-Ethyl-4-methylbenzene	622-96-8
n-butylbenzene	104-51-8
Isobutylbenzene	538-93-2
tert-Butylbenzene	98-06-6
sec-Butylbenzene	135-98-8
1-Methyl-2-propylbenzne	1074-17-5
1-Methyl-3-propylbenzne	1074-43-7
1-Methyl-4-propylbenzne	1074-55-1
1-Methyl-2-isopropylbenzene	527-84-4
1-Methyl-3-isopropylbenzene	535-77-3
1-Methyl-4-isopropylbenzene	99-87-6
1,2-Diethylbenezne	135-01-3
1,3-Diethylbenzene	141-93-5
1,4-Diethylbenzene	105-05-5
1-Ethyl-2,3-dimethylbenzene	933-98-2
1-Ethyl-2,4-dimethylbenzene	874-41-9
2-Ethyl-1,4-dimethylbenzene	1758-88-9
2-Ethyl-1,3-dimethylbenzene	354380
4-Ethyl-1,2-dimethylbenzene	934-80-5
1-Ethyl-3,5-dimethylbenzene	934-74-7
1,2,3,4-Tetramethylbenzene	488-43-3
1,2,3,5-Tetramethylbenzene	527-53-7
1,2,4,5-Tetramethylbenzene	95-93-2
ar,ar-Diethylmethylbenzene	8638347
1-Ethyl-2,4,5-trimethylbenzene	17851-27-3
ar-Ethyl-1,2,4-trimethylbenzene	54120-62-6
Pentamethylbenzne	700-12-9
1-Isopropyl-2,5-dimethylbenzene	4132-72-3
1-Isopropyl-3,5-dimethylbenzene	4706-90-5
1,3-Diethyl-5-methylbenzene	2050-24-0
tert-Butyltoluene	37307
1-Ethyl-3-isopropyl-benzene	4920-99-4
1-Ethyl-4-isopropyl-benzene	4218-48-8
2,4-Dimethyl-1-isopropylbenzene	4706-89-2
1-Methyl-4-isobutylbenzene	1191151
1-Methyl-3-*tert*-butylbenzene	1075-38-3
1-Methyl-4-*tert*-butylbenzene	98-51-1
(1-Ethylpropyl)-benzene	1196-58-3
(1,1-Dimethylpropyl)-benzene	2049-95-8
(1,2-Dimethylpropyl)-benzene	4481-30-5
(2,2-Dimethylpropyl)-benzene	1007-26-7
n-Pentylbenzene	538-68-1
(1-methylbutyl)-benzene	2719-52-0
(2-methylbutyl)-benzene	3968-85-2
(3-methylbutyl)-benzene	2049-94-7
n-Hexylbenzene	1077-16-3
(1-Methylpentyl)-benzene	1508850
(2-Methylpentyl)-benzene	39916-61-5
(3-Methylpentyl)-benzene	54410-69-4
(1-Ethylbutyl)-benzene	4468-42-2
(2-Ethylbutyl)-benzene	19219-85-3
(1,1-Dimethylbutyl)-benzene	1985-57-5
(1,3-Dimethylbutyl)-benzene	19219-84-2
(2,2-Dimethylbutyl)-benzene	28080-86-6
(3,3-Dimethylbutyl)-benzene	17314-92-0
(1-Ethyl-1-methylpropyl)-benzene	1985-97-3
(1,1,2-trimethylpropyl)-benzene	8932673
(1,2,2-trimethylpropyl)-benzene	19262-20-5
1-Methyl-2-(1-ethylpropyl)-benzene	54410-74-1
1-(1-Ethylpropyl)-4-methylbenzene	22975-58-2
sec-Butylethylbenzene	28654-79-7
1,3-Dimethyl-4-*sec*-butylbenzene	1483-60-9
1,4-Dimethyl-2-isobutylbenzene	55669-88-0
1,2-Dimethyl-4-*tert*-butylbenzene	2007889
1,4-Dipropylbenzene	4815-57-0
1,2-Diisopropylbenzene	577-55-9
1,3-Dimethyl-5-*tert*-butylbenzene	98-19-1
1,2,4-Trimethyl-5-isopropylbenzene	10222-95-4
1,2,4-Triethylbenzene	877-44-1
1,3,5-Triethylbenzene	102-25-0
1,2-Dimethyl-3,4-diethylbenzene	54410-75-2

Compound	**CAS Number**
1,2-Diethyl-4,5-dimethylbenzene	6596821
1,2,4,5-Tetramethyl-3-ethylbenzene	31365-98-7
Hexamethylbenzene	87-85-4
1,3-Diisopropylbenzene	99-62-7
1,4-Diisopropylbenzene	100-18-5
Biphenyl	92-52-4
Acenaphthylene	208-96-8
Acenaphthene	83-32-9
Anthracene	120-12-7
Fluoranthene	206-44-0
Pyrene	129-00-0
Benzo(a)anthracene	56-55-3
Benzo(b)fluoranthrene	205-99-2
Benzo(j)fluoranthrene	205-82-3
Benzo(k)fluoranthrene	207-08-9
Benzo(j,k)fluorene	206-44-0
Benzo(r,s,t)pentaphene	189-55-9
Benzo(a)phenanthrene	218-01-9
Benzo(a)pyrene	50-32-8
Benzo(e)pyrene	192-97-2
Perylene	198-55-0
Indeno(1,2,3-cd)pyrene	193-39-5
Dibenz(a,h)anthracene	53-70-3
Benzo(g,h,i)perylene	191-24-2
n-C_{8} (*n*-Octane)	111-65-9
n-C_{9} (*n*-Nonane)	111-84-2
n-C_{10} (*n*-Decane)	124-18-5
n-C_{11} (*n*-Undecane)	1120-21-4
n-C_{12} (*n*-Dodecane)	112-40-3
n-C_{13} (*n*-Tridecane)	629-50-5
n-C_{14} (*n*-Tetradecane)	629-59-4
n-C_{15} (*n*-Pentadecane)	629-62-9
n-C_{16} (*n*-Hexadecane)	544-76-3
n-C_{17} (*n*-Heptadecane)	629-78-7
Pristane	1921-70-6
n-C_{18} (*n*-Octadecane)	593-45-3
Phythane	638-36-8
n-C_{19} (*n*-Nonadecane)	629-92-5
n-C_{20} (*n*-Eicosane)	112-95-8
n-C_{21} (Heneicosane)	629-94-7
n-C_{22} (Docosane)	629-97-0
n-C_{23} (Tricosane)	638-67-5
n-C_{24} (Tetracosane)	646-31-1
n-C_{25} (Pentacosane)	629-99-2
n-C_{26} (Hexacosane)	630-01-3
n-C_{27} (Heptacosane)	593-49-7
n-C_{28} (Octacosane)	630-02-4
n-C_{29} (Nonacosane)	630-03-5
n-C_{30} (Triacontane)	638-68-6
n-C_{31} (Hentriacontane)	630-04-6
n-C_{32} (Dotriacontane)	544-85-4
n-C_{33} (Tritriacontane)	630-05-7
n-C_{34} (Tetratriacontane)	14167-59-0
n-C_{35} (Pentatriacontane)	630-07-9
n-C_{36} (Hexatriacontane)	630-06-8
n-C_{37} (Heptatriacontane)	7194-84-5
n-C_{38} (Octatriacontane)	7194-85-6
n-C_{39} (Nonatriacontane)	7194-86-7
n-C_{40} (Tetracontane)	4181-95-7
n-C_{41} (Hentetracontane)	7194-87-8
n-C_{42} (Dotetracontane)	7098-20-6
n-C_{44} (Tetratetracontane)	7098-22-8
n-C_{46} (Hexatetracontane)	7098-24-0
n-C_{48} (Octatetracontane)	7098-26-2
n-C_{50} (Pentacontane)	6596-40-3
Naphthalene	90-20-3
1-methylnaphthalene	90-12-0
2-methylnaphthalene	91-57-6
1-ethylnaphthalene	1127-76-0
2-ethylnaphthalene	939-27-5
2-isoproplynaphthalene	2027-17-0
1,2-dimethylnaphthalene	573-98-8
1,3-dimethylnaphthalene	575-41-7
1,4-dimethylnaphthalene	571-58-4
1,5-dimethylnaphthalene	571-61-9
1,6-dimethylnaphthalene	575-43-9
1,7-dimethylnaphthalene	575-37-1
1,8-dimethylnaphthalene	569-41-5
2,3-dimethylnaphthalene	581-40-8
2,6-dimethylnaphthalene	581-42-0
2,7-dimethylnaphthalene	582-16-11
1,2,3-trimethylnaphthalene	879-12-9
1,2,4-trimethylnaphthalene	2717-42-2
1,2,5-trimethylnaphthalene	641-91-8
1,2,6-trimethylnaphthalene	413217
1,4,5-trimethylnaphthalene	2131-41-1
1,4,6-trimethylnaphthalene	2131-42-2
2,3,5-trimethylnaphthalene	2245-38-7
Eudalene	490-65-3
Cadalene	483-78-3
2,6-diisopropylnaphthalene	24157-81-11
Fluorene	86-73-7
1-methylfluorene	1730-37-6
2-methylfluorene	1430-97-3

Compound	**CAS Number**
4-methylfluorene	1556-99-6
9-methylfluorene	2523-37-7
1,7-dimethylfluorene	442-66-0
9-ethylfluorene	2294-82-8
Phenanthrene	85-01-8
1-methylphenanthrene	832-69-9
2-methylphenanthrene	2531-84-2
3-methylphenanthrene	832-71-3
4-methylphenanthrene	832-64-4
9-methylphenanthrene	883-20-5
1,2-dimethylphenanthrene	20291-72-9
1,3-dimethylphenanthrene	16664-45-2
1,4-dimethylphenanthrene	22349-59-3
1,6-dimethylphenanthrene	483-87-4
1,7-dimethylphenanthrene	20291-74-1
1,8-dimethylphenanthrene	7372-87-4
1,9-dimethylphenanthrene	20291-73-0
2,3-dimethylphenanthrene	3674-65-5
2,4-dimethylphenanthrene	15254-64-5
2,5-dimethylphenanthrene	3674-66-6
2,6-dimethylphenanthrene	17980-16-4
2,7-dimethylphenanthrene	1576-69-8
2,9-dimethylphenanthrene	17980-09-5
3,5-dimethylphenanthrene	33954-06-2
3,6-dimethylphenanthrene	1576-67-6
3,9-dimethylphenanthrene	66291-32-5
3,10-dimethylphenanthrene	66291-33-6
4,5-dimethylphenanthrene	3674-69-9
9,10-dimethylphenanthrene	604-83-11
1,2,6-trimethylphenanthrene	30436-55-6
1,2,8-trimethylphenanthrene	20291-75-2
Retene	483-65-8
3-ethylphenanthrene	1576-68-7
9-ethylphenanthrene	3674-75-7
Anthracene	120-12-7
1-methylanthracene	610-48-0
2-methylanthracene	613-12-7
9-methylanthracene	779-02-2
2-ethylanthracene	52251-71-5
2-(Tert-butyl)anthracene	18801-00-8
1,2-dimethylanthracene	53666-94-7
1,3-dimethylanthracene	610-46-8
1,4-dimethylanthracene	781-92-0
1,5-dimethylanthracene	15815-48-2
2,3-dimethylanthracene	613-06-9
2,7-dimethylanthracene	782-23-0
9,10-dimethylanthracene	178-43-1
1,2,4-trimethylanthracene	20153-28-0
1,2,3,4-tetramethylanthracene	66553-01-3
Fluoranthene	206-44-0
1-methylfluoranthene	25889-60-5
2-methylfluoranthene	33543-31-6
3-methylfluoranthene	1706-01-0
Pyrene	129-00-0
1-methylpyrene	2381-21-7
4-methylpyrene	531037
Chrysene	218-01-9
1-methylchrysene	3351-28-8
2-methylchrysene	3351-32-4
3-methylchrysene	3351-31-3
4-methylchrysene	3351-30-2
5-methylchrysene	3697-24-3
6-methylchrysene	1705-85-7

2 Oil Chemical Analysis Protocol



Chemical Oil Analysis Protocol

3 GC Chromatograms for Alaska North Slope Crude Oil

Figure A3-1	GC-FID chromatograms of fraction 1 (F1) for saturates of Alaska North Slope crude oil
Figure A3-2	GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of Alaska North Slope crude oil
Figure A3-3	GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of Alaska North Slope crude oil
Figure A3-4	Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of Alaska North Slope crude oil
Figure A3-5	Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184, 178, 192, 206, 220, 234, 198, 212, 226, 166, 180, 194, 208, 228, 242, 256, and 270) of Alaska North Slope crude oil
Figure A3-6	GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of Alaska North Slope crude oil
Figure A3-7	GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218) of Alaska North Slope crude oil

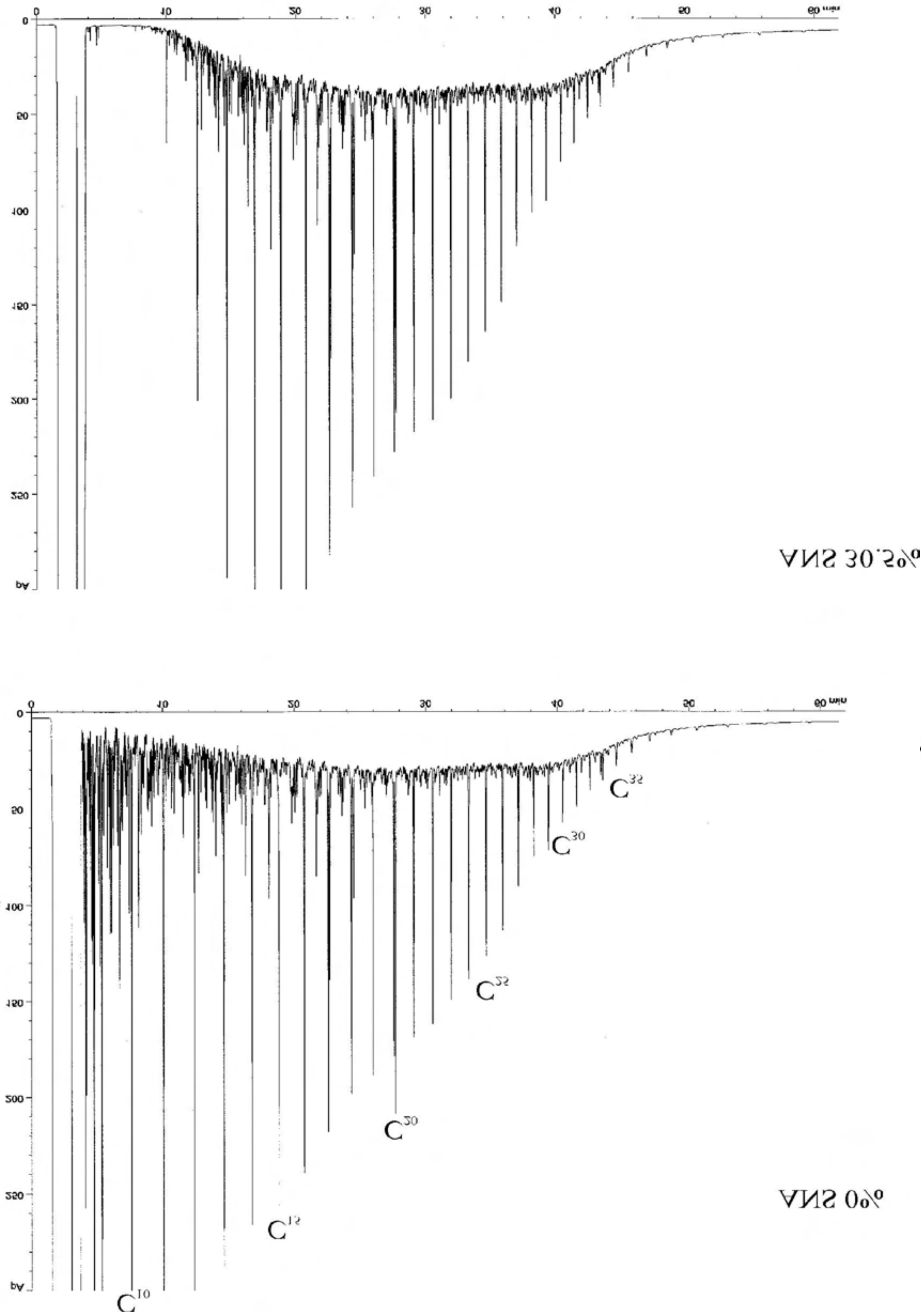


Figure A3-1 GC-FID chromatograms of fraction 1 (F1) for saturates of Alaska North Slope crude oil

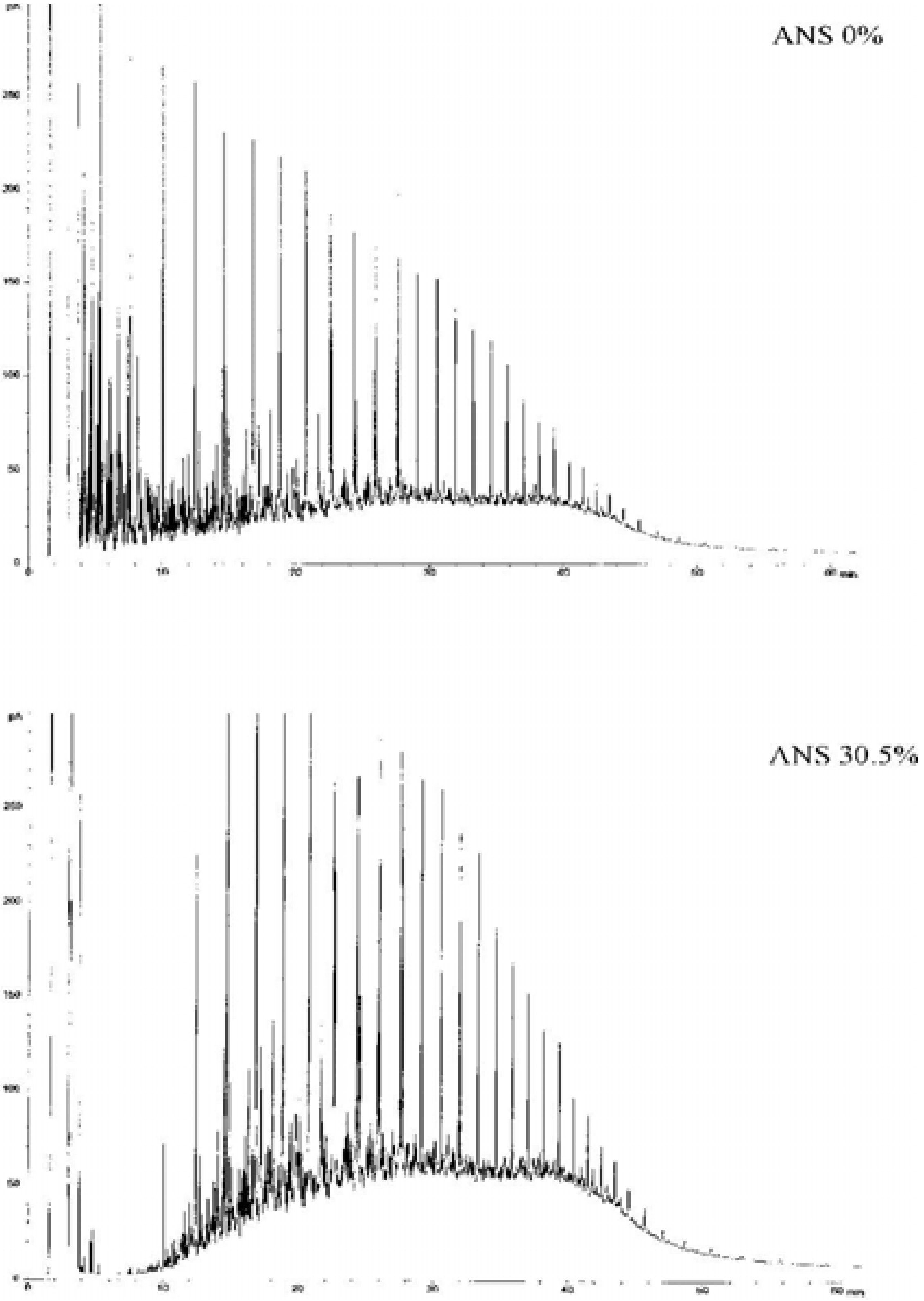


Figure A3-2 GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of Alaska North Slope crude oil

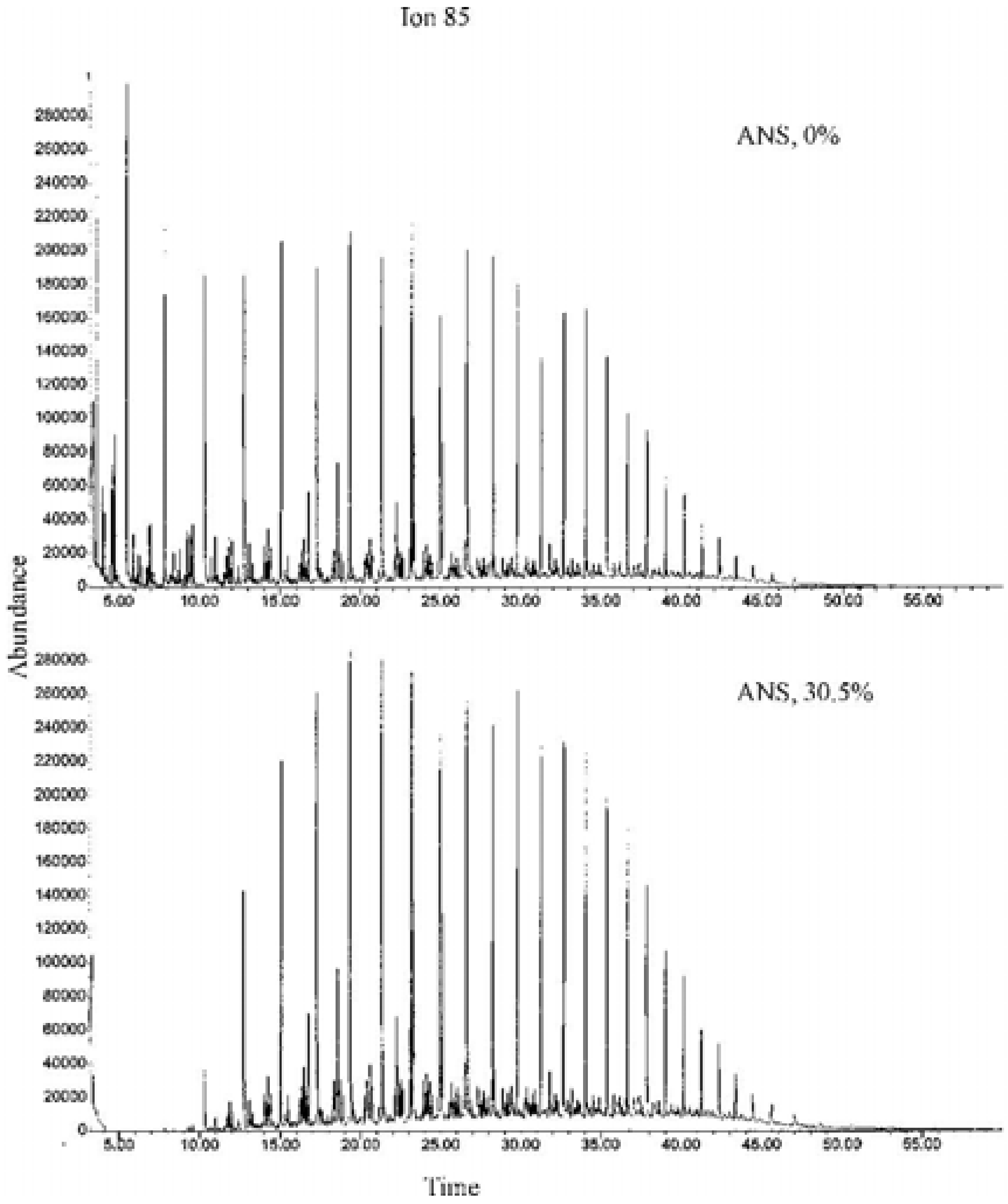


Figure A3-3 GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of Alaska North Slope crude oil

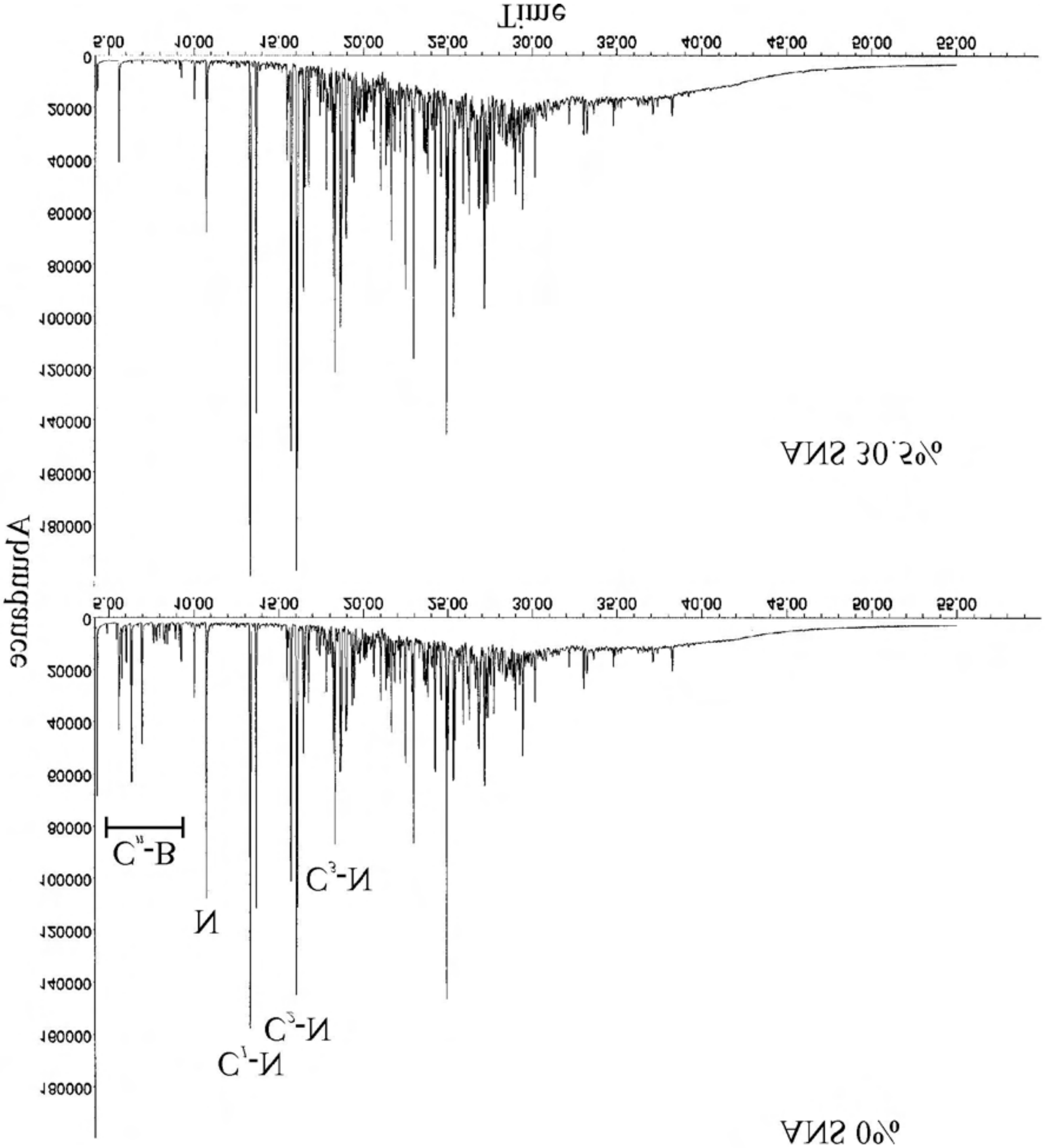


Figure A3-4 Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of Alaska North Slope crude oil (Peaks are labelled for the alkylated benzenes, C_n-B, naphthalene, N, and the alkylated naphthalenes, C_1-N, C_2-N, and C_3-N).

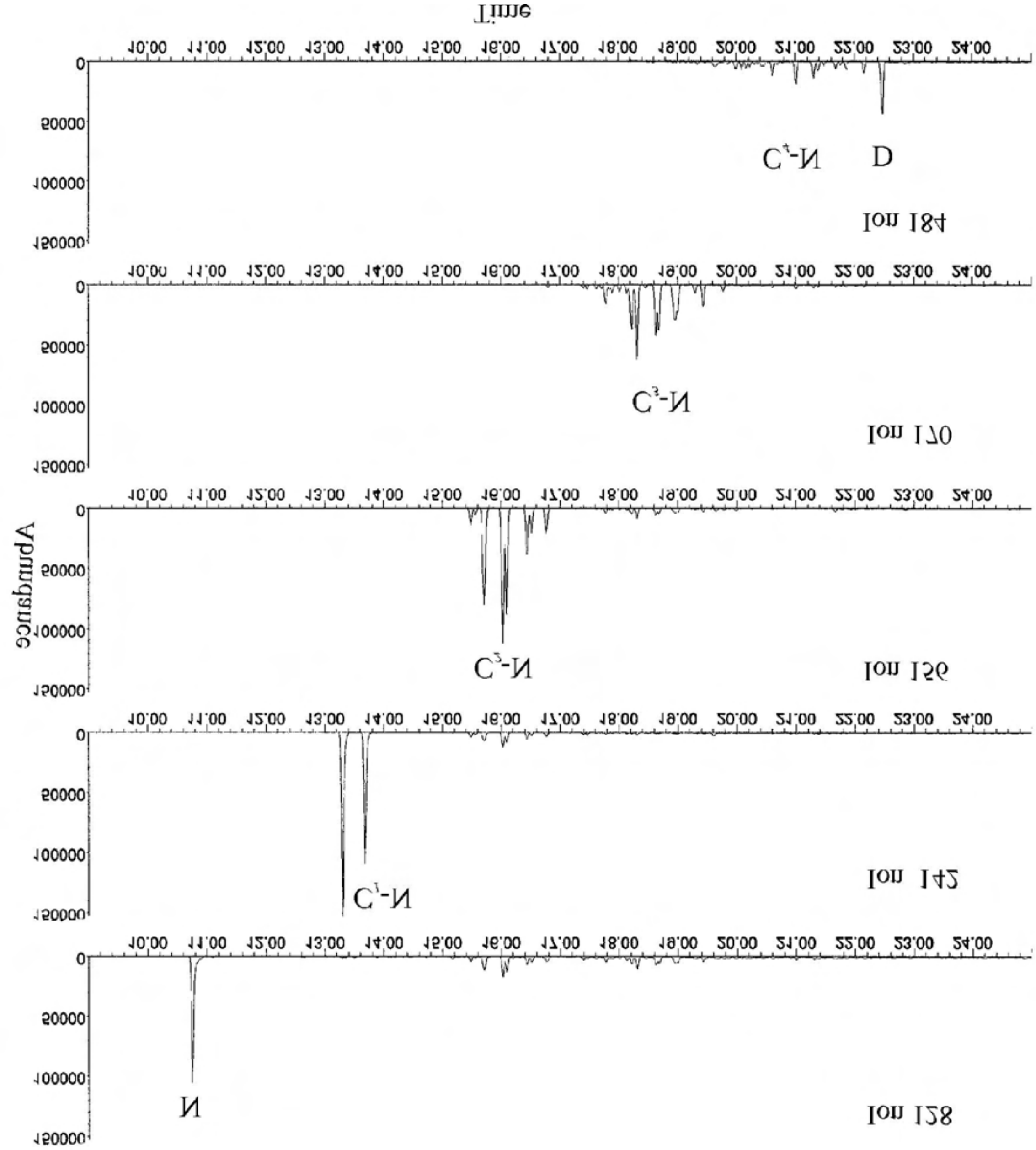


Figure A3-5a Extracted ion GC-MS chromatograms offraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184) of Alaska North Slope crude oil (Peaks are labelled for naphthalene, N, the alkylted naphthalenes, C_1-N, C_2-N, C_3-N, C_4-N, and dibenzothiophene, D).

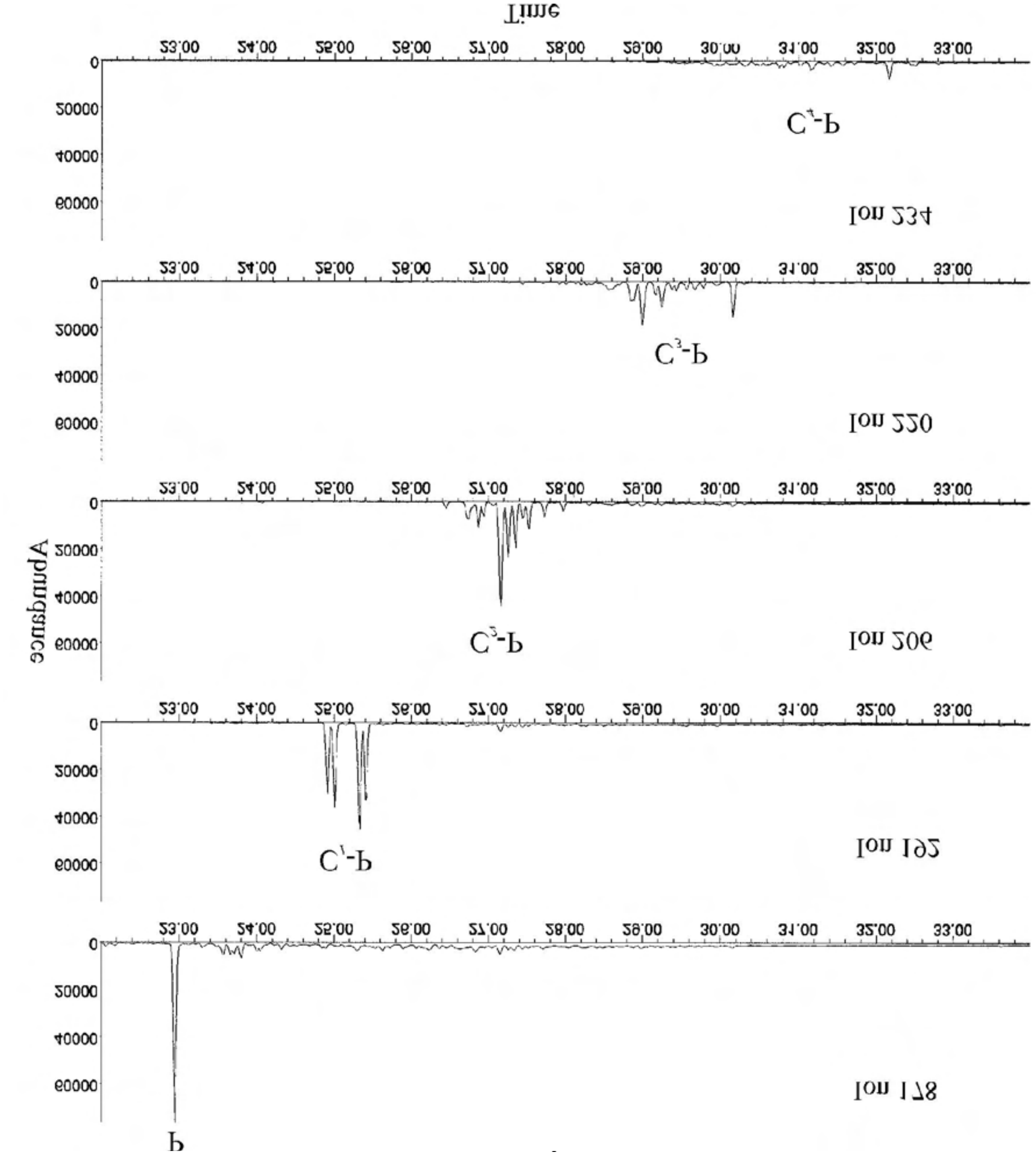


Figure A3-5b Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 178, 192, 206, 220, 234) of Alaska North Slope crude oil (Peaks are labelled for phenanthrene, P, and its alkylated homologues, C_1-P, C_2-P, C_3-P, and C_4-P).

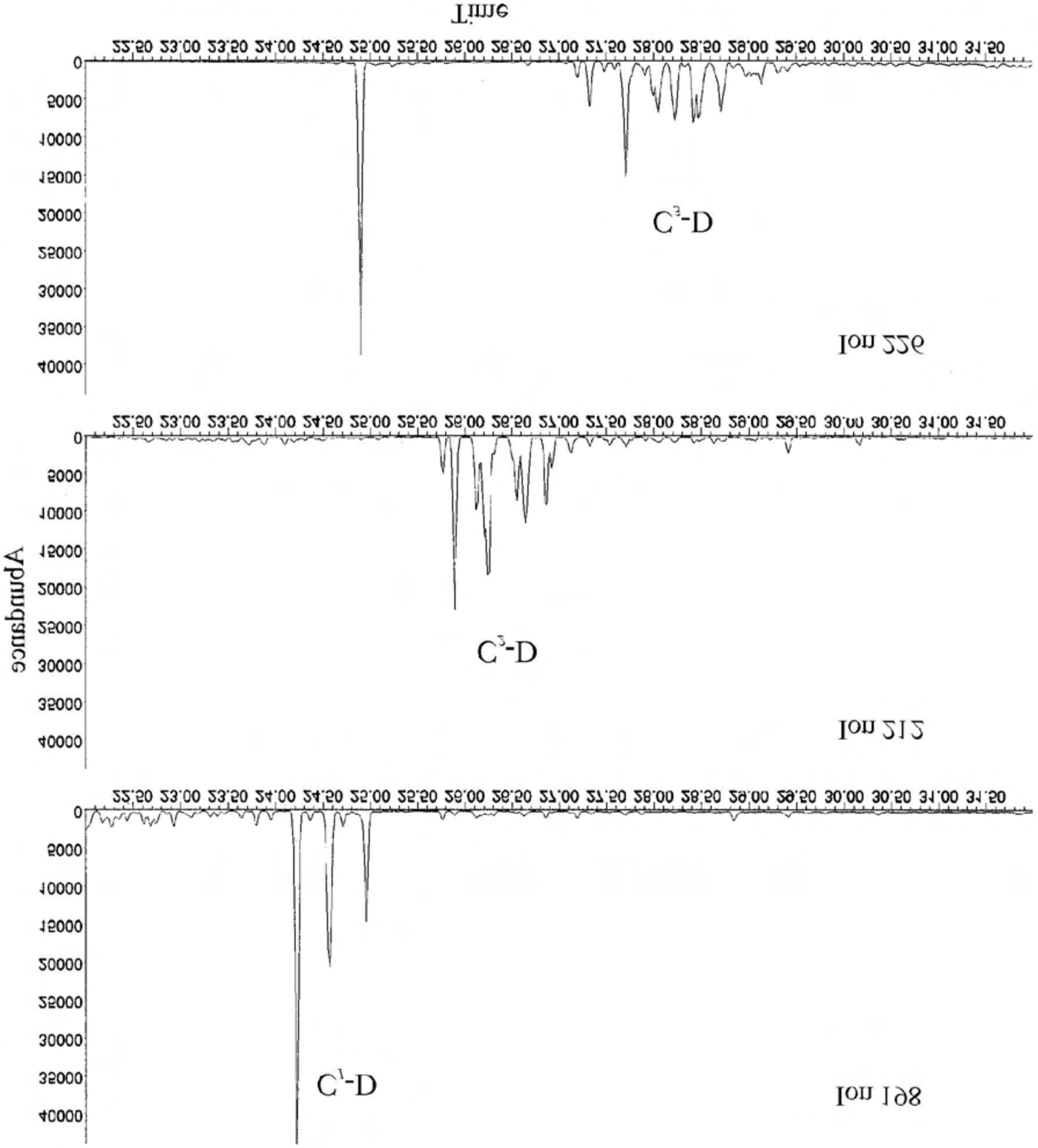


Figure A3-5c Extracted ion GC-MS chromatograms offraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 198, 212, 226) of Alaska North Slope crude oil (Peaks are labelled for the alkylated homologues of dibenzothiophene, C_1-D, C_2-D, and C_3-D).

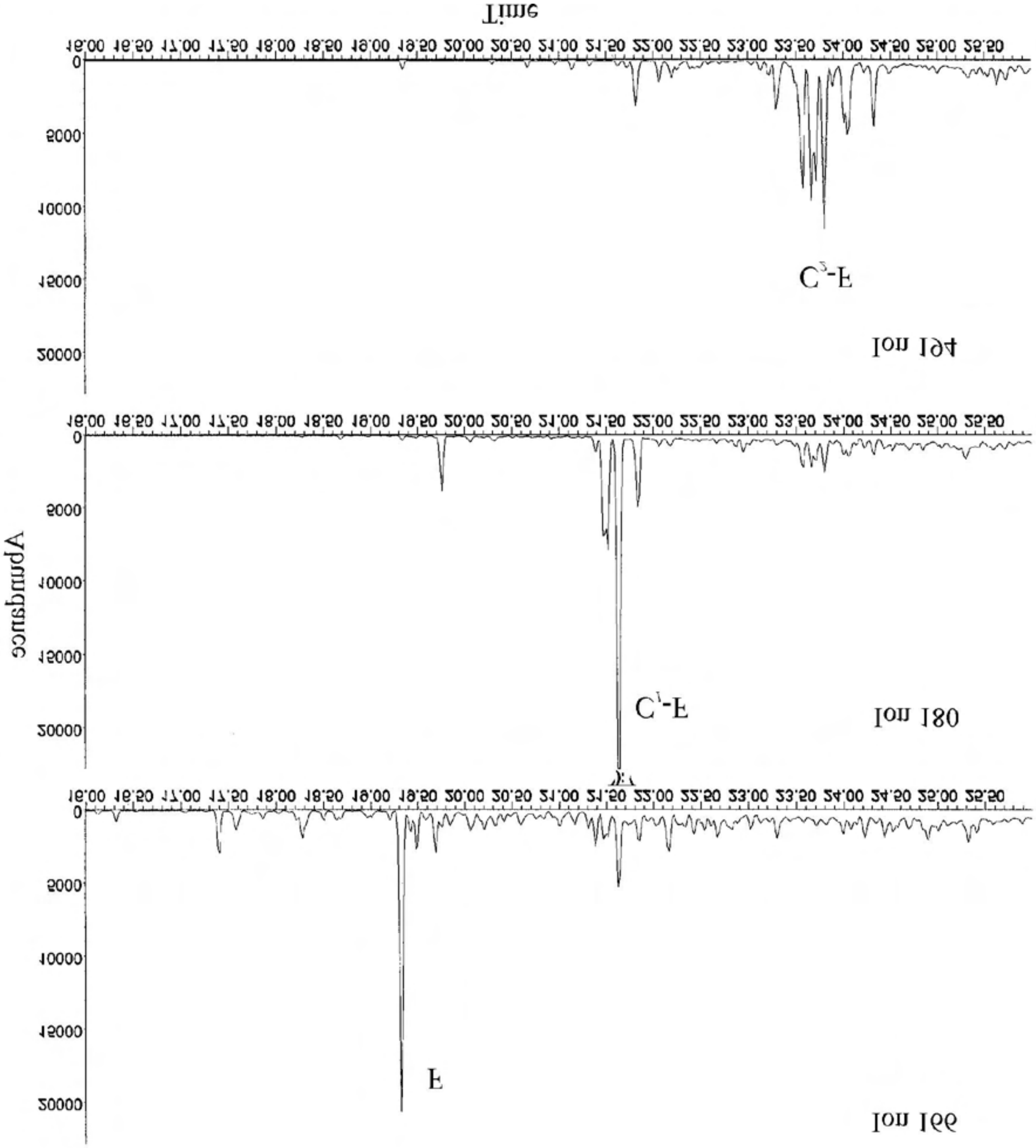


Figure A3-5d Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 166, 180, 194) of Alaska North Slope crude oil (Peaks are labelled for fluorene, F, and its alkylated homologues, C_1-F, and C_2-F).

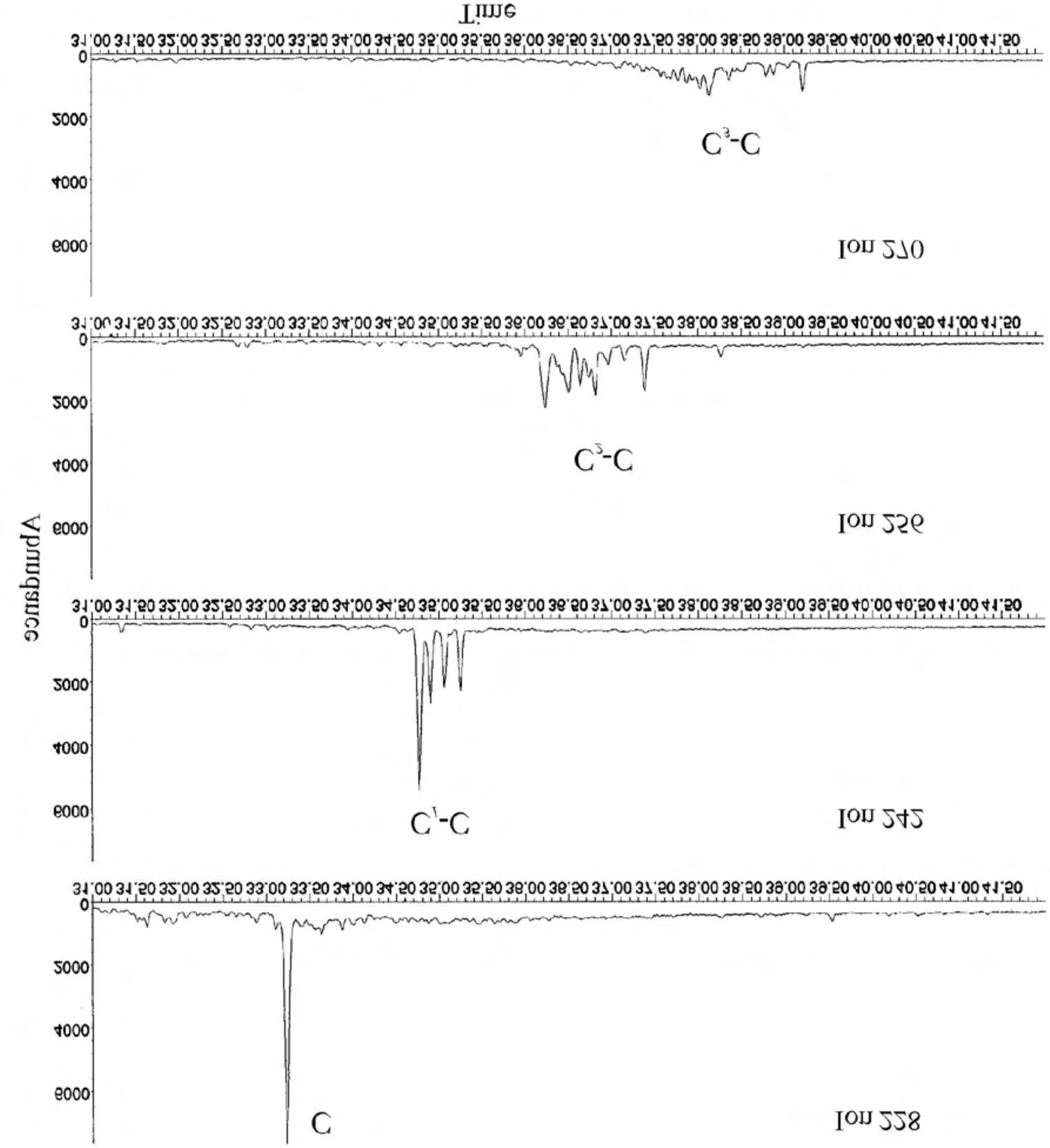


Figure A3-5e Extracted ion GC-MS chromatograms offraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 228, 242, 256, 270) of Alaska North Slope crude oil (Peaks are labelled for chrysene, C, and its alkylated homologues, C_1-C, C_2-C, and C_3-C).

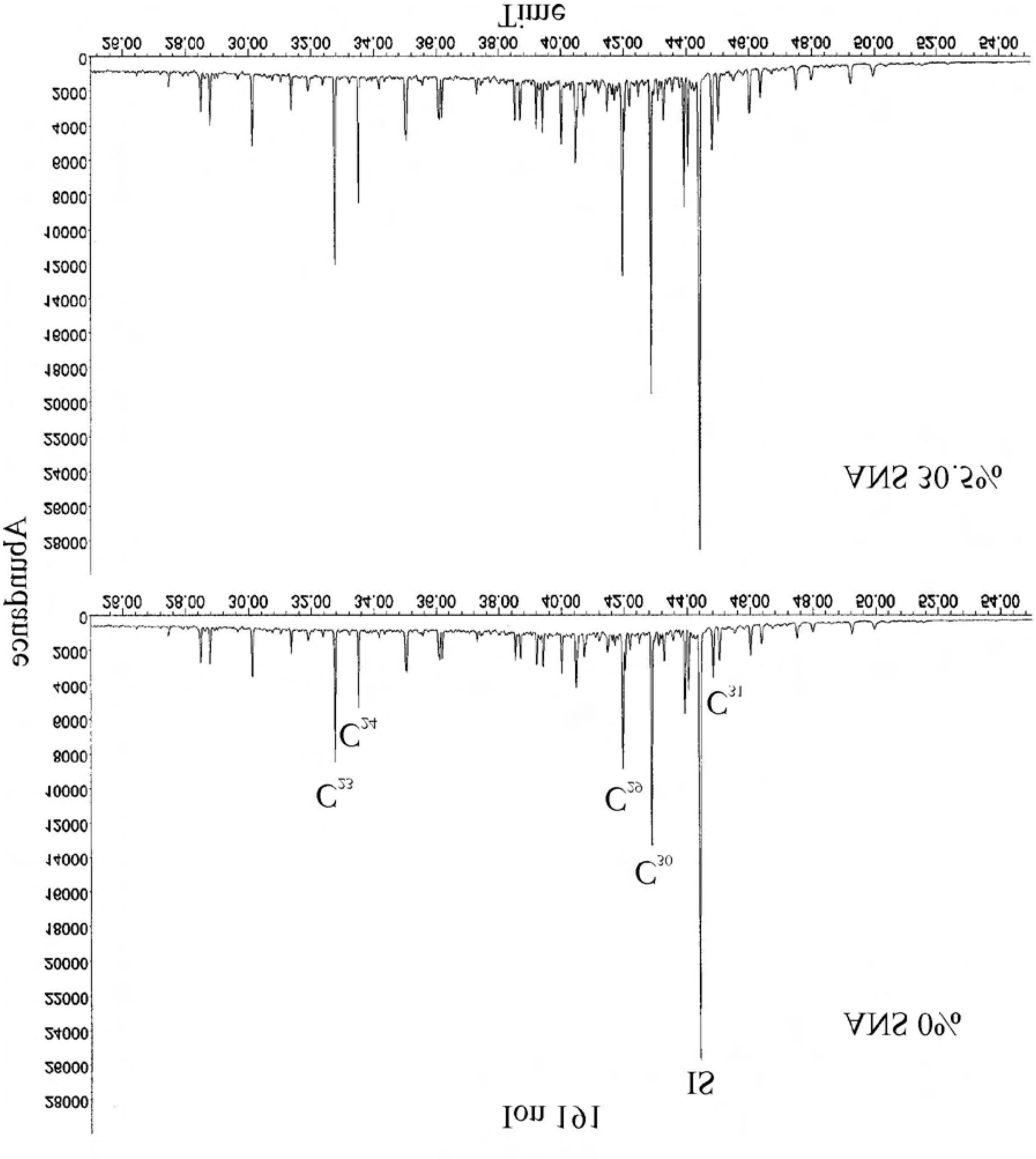


Figure A3-6 GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of Alaska North Slope crude oil

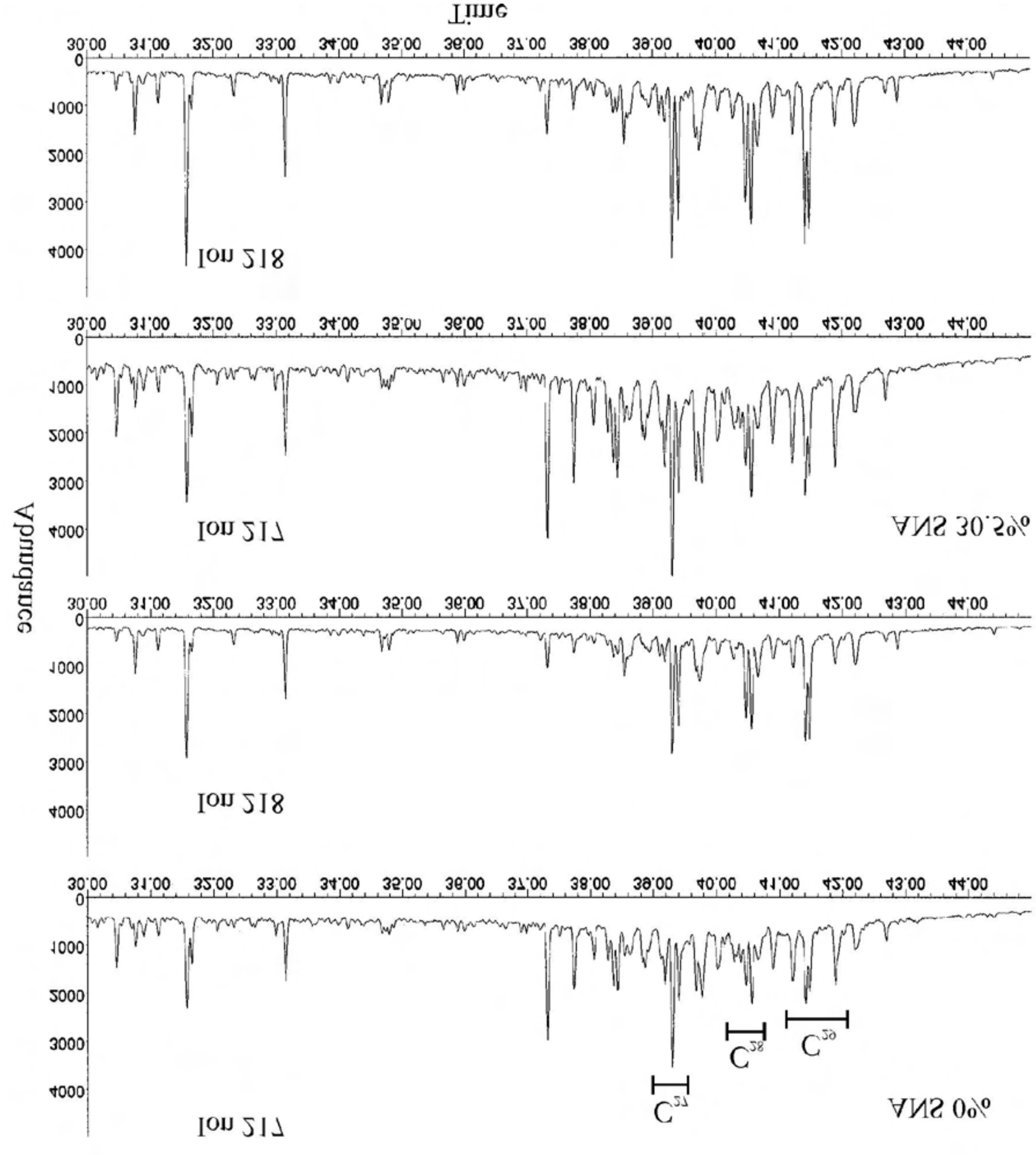


Figure A3-7 GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218) of Alaska North Slope crude oil

4 GC Chromatograms for Alberta Sweet Mixed Blend #5 Crude Oil

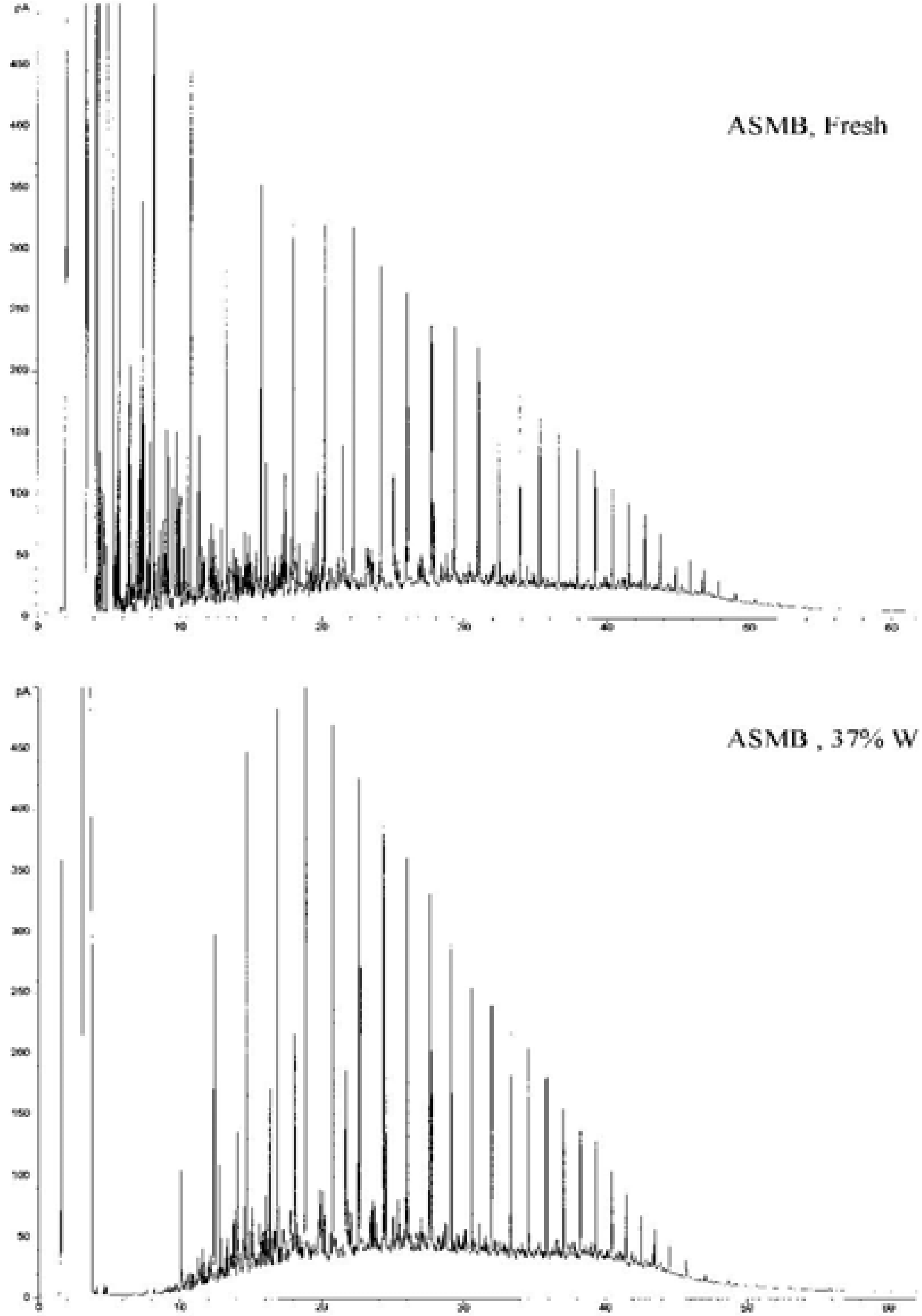


Figure A4-1 GC-FID chromatograms of fraction 1 (F1) for saturates of ASMB #5 crude oil

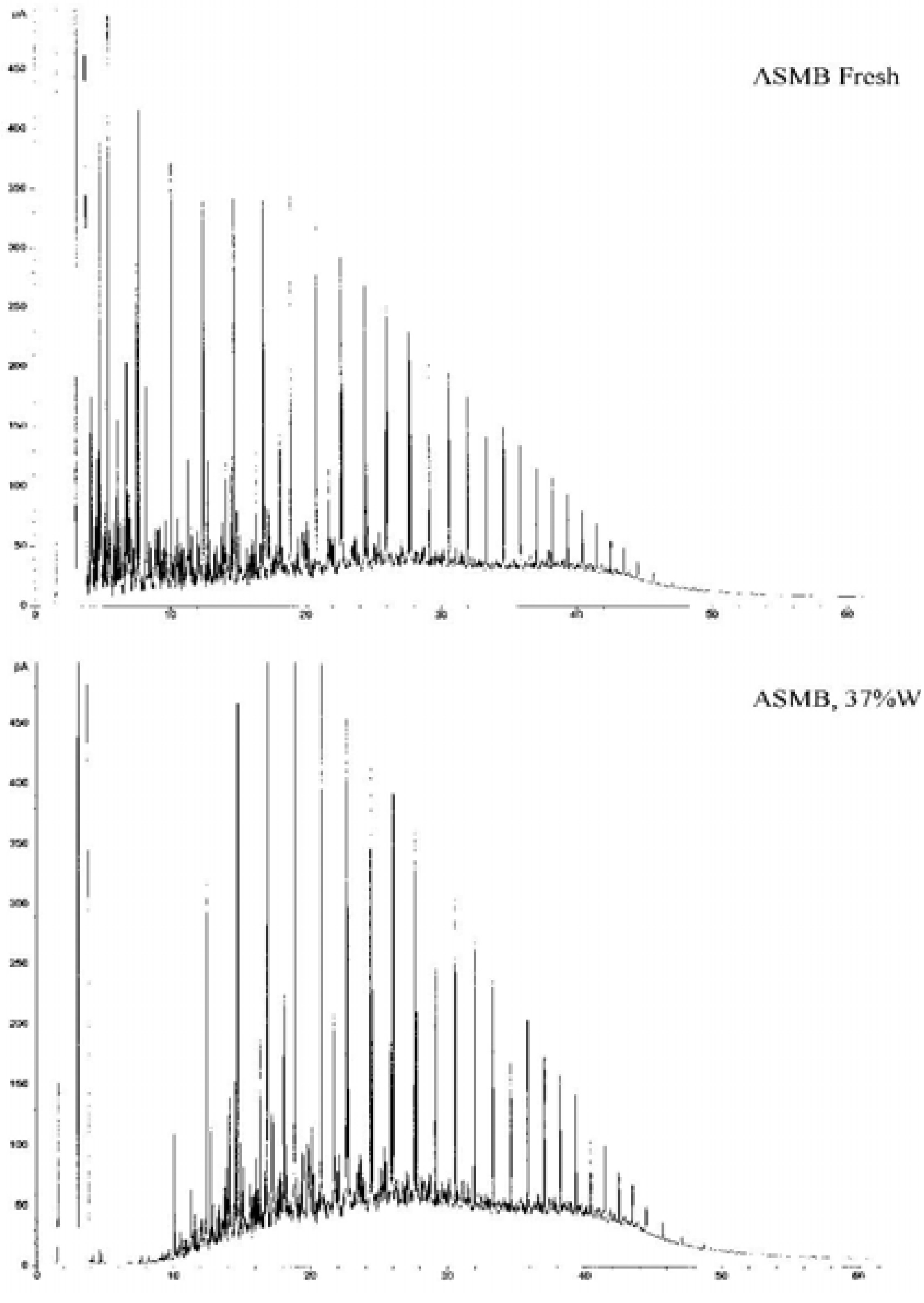


Figure A4-2 GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of ASMB #5 crude oil

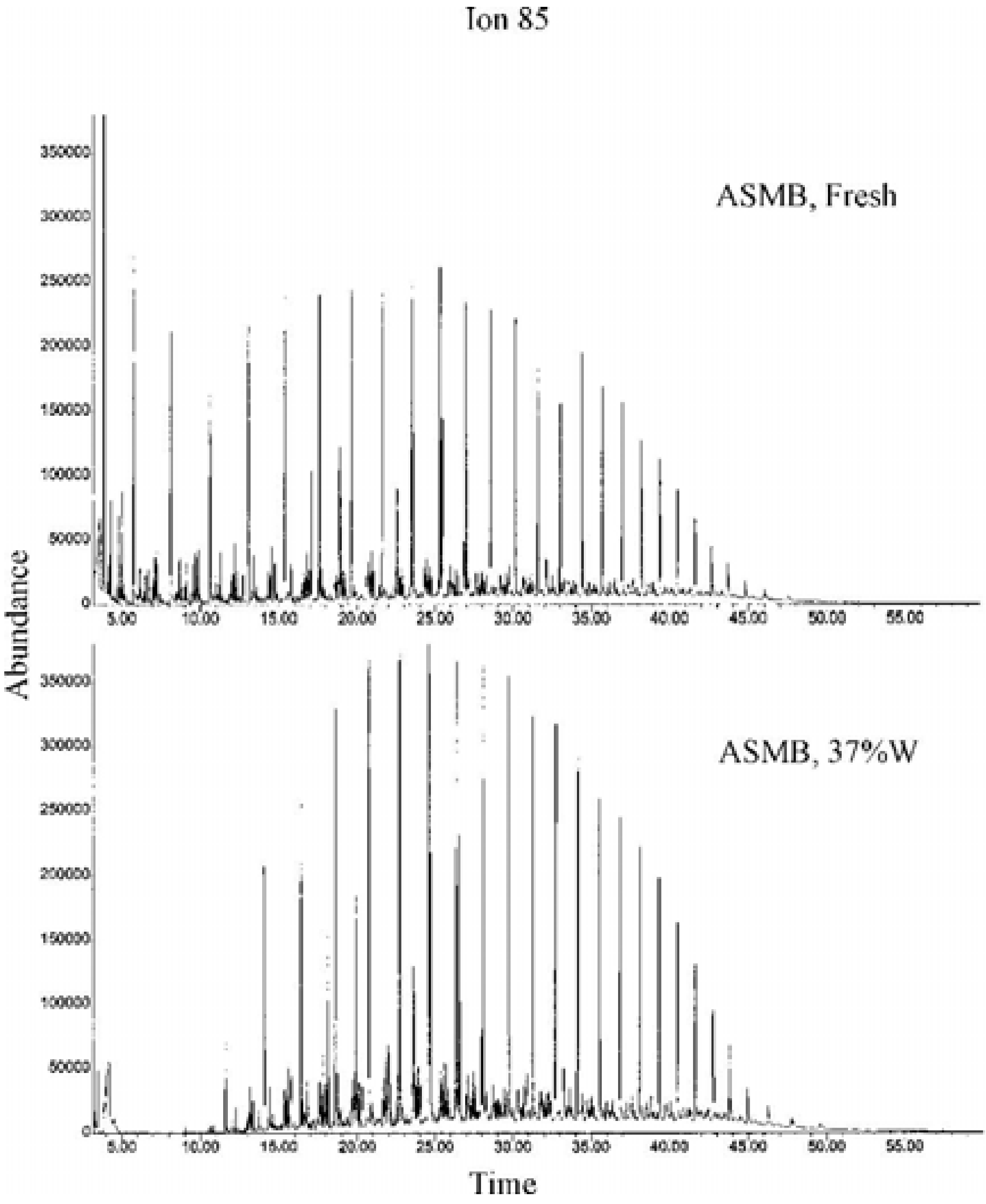


Figure A4-3 GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of ASMB #5 crude oil

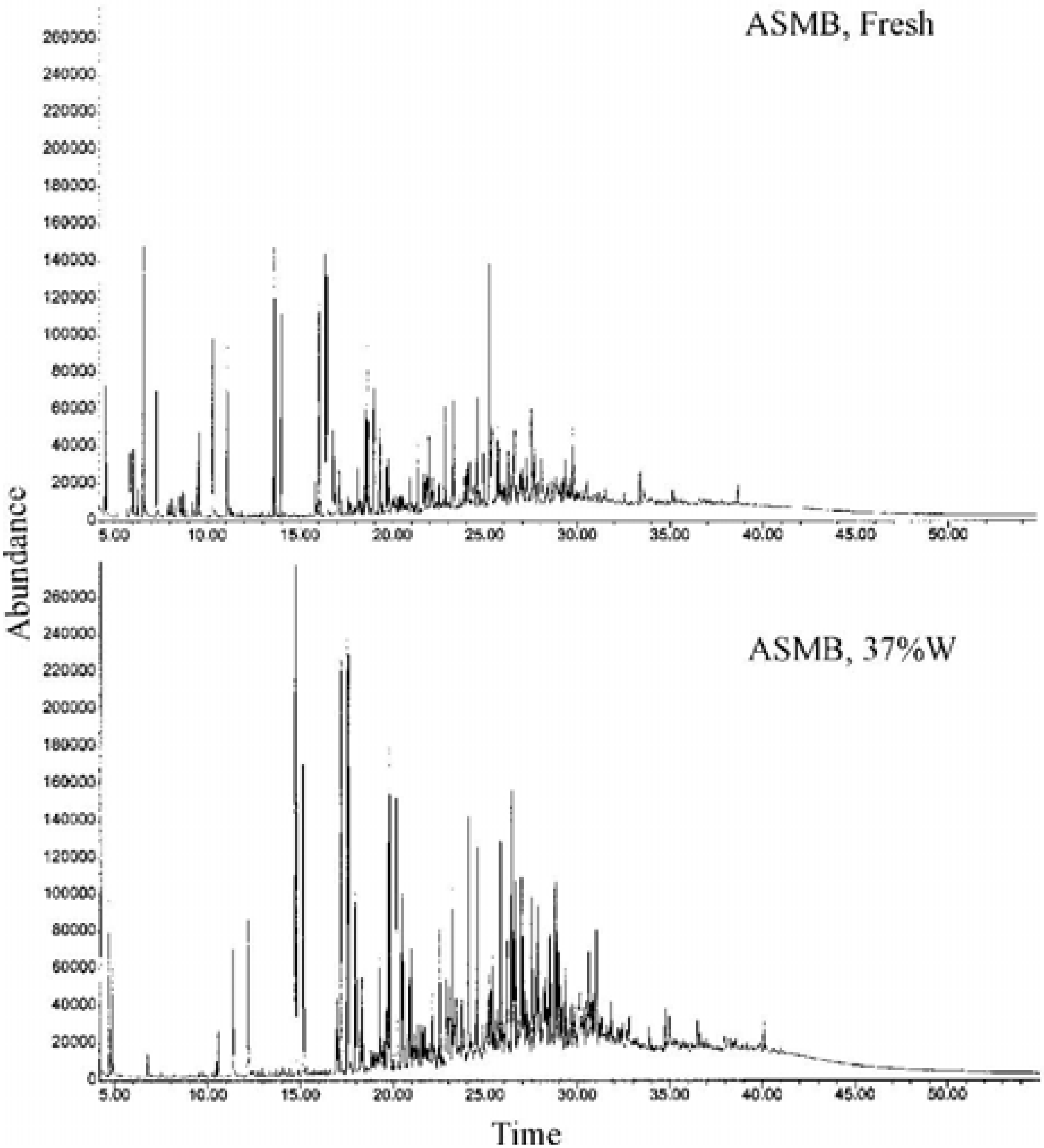


Figure A4-4 Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of ASMB #5 crude oil

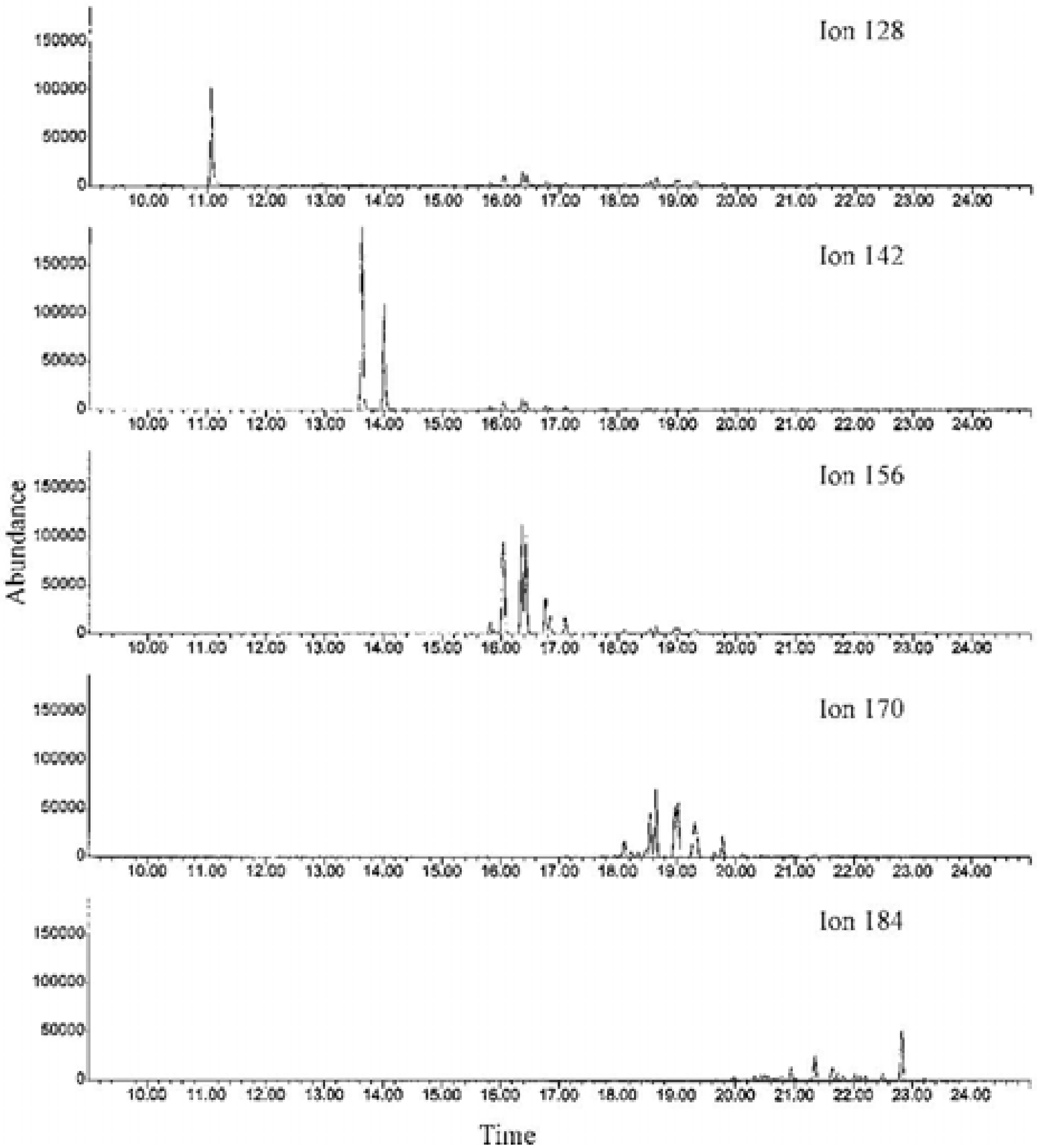


Figure A4-5a Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184) of ASMB #5 crude oil

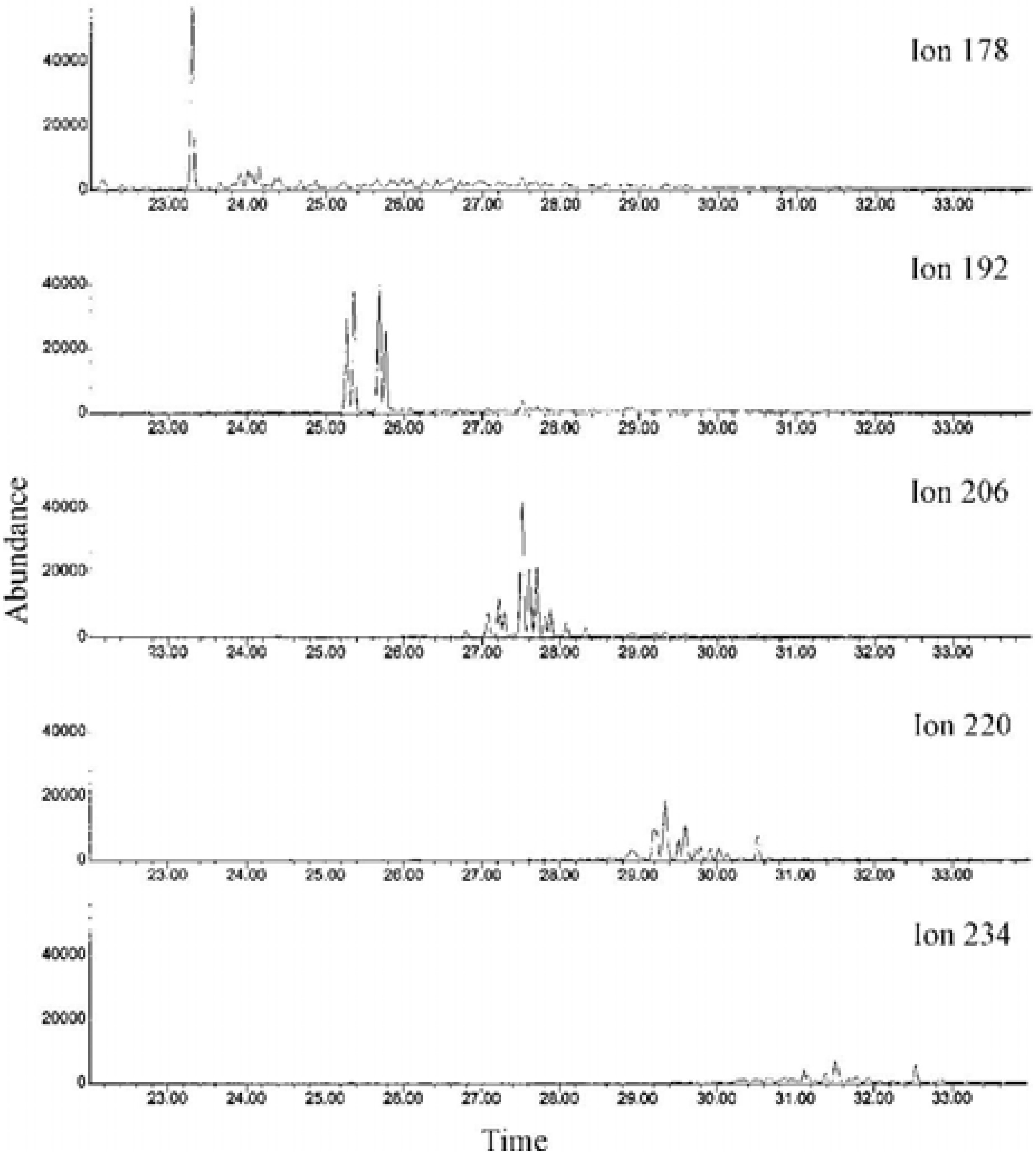


Figure A4-5b Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 178, 192, 206, 220, 234) of ASMB #5 crude oil

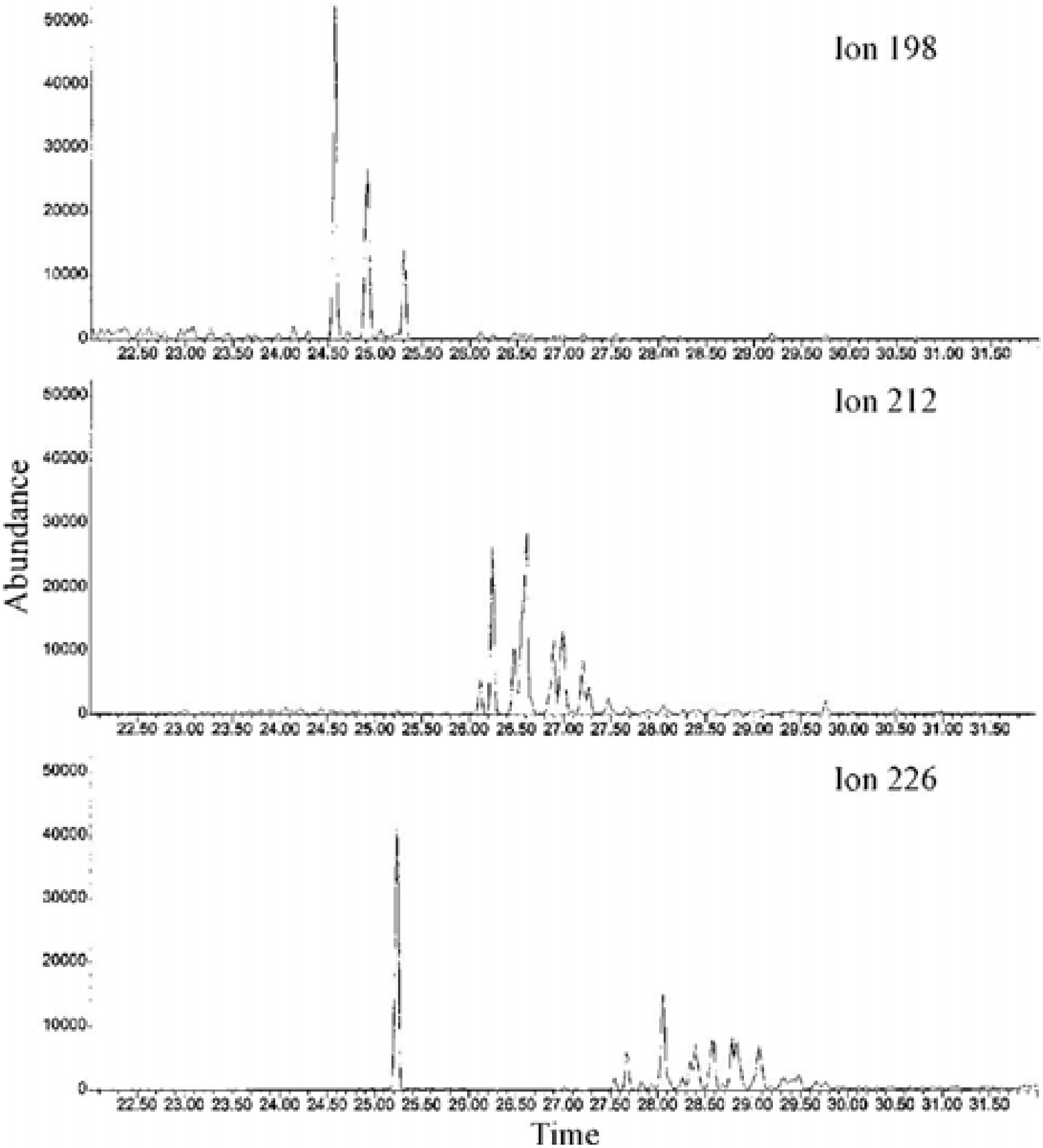


Figure A4-5c Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 198, 212, 226) of ASMB #5 crude oil

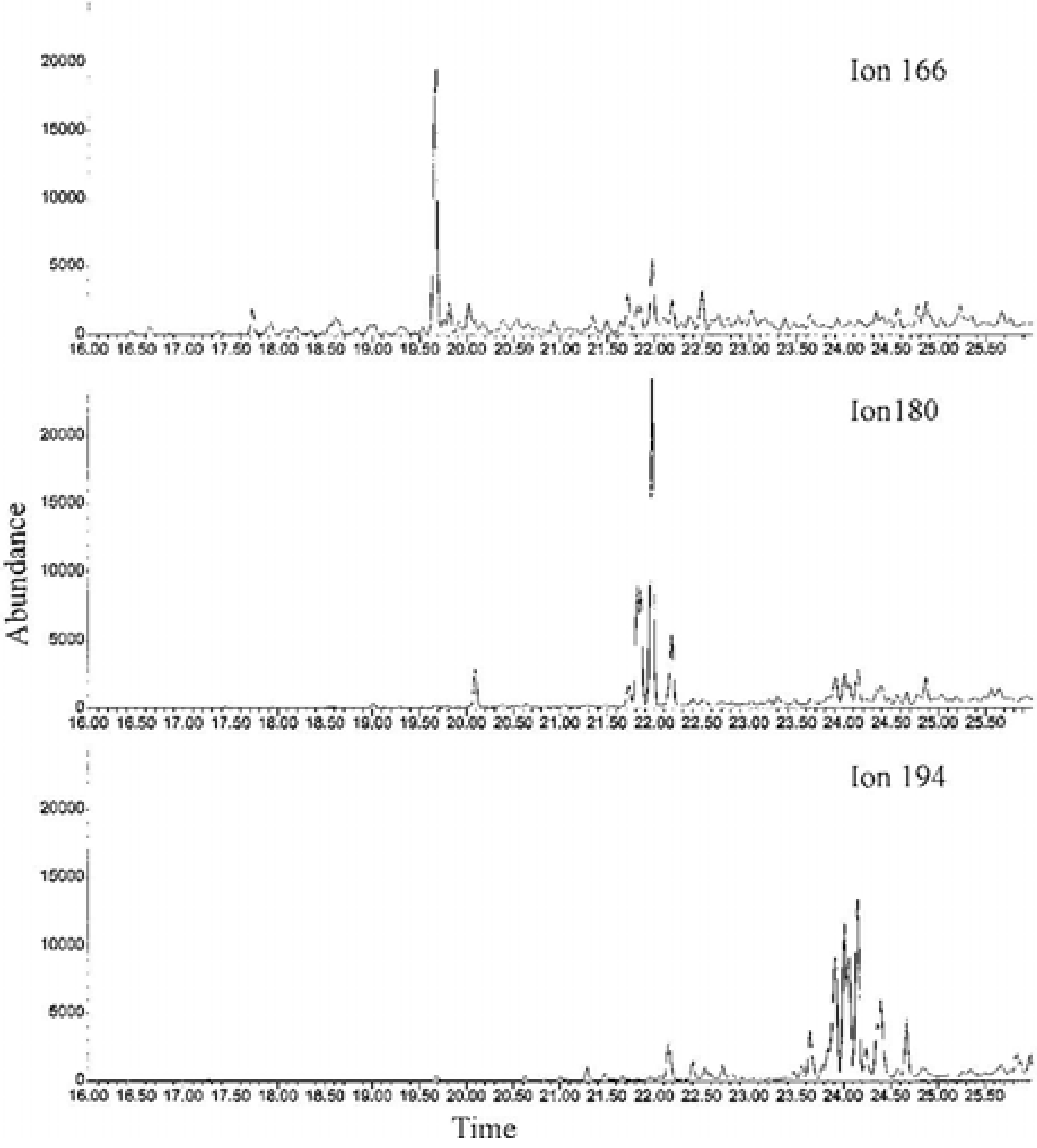


Figure A4-5d Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 166, 180, 194) of ASMB #5 crude oil

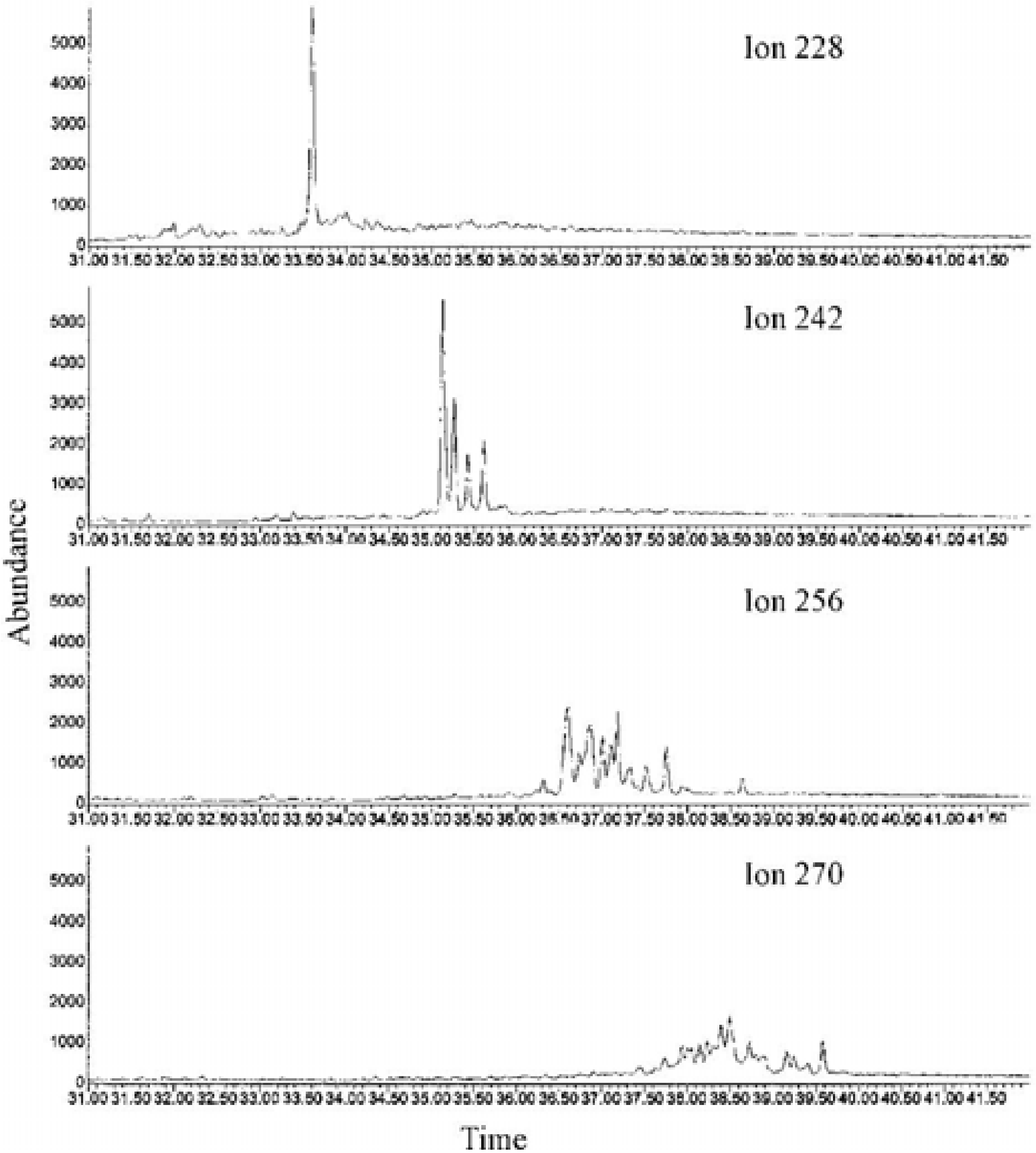


Figure A4-5 Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 228, 242, 256, 270) of ASMB #5 crude oil

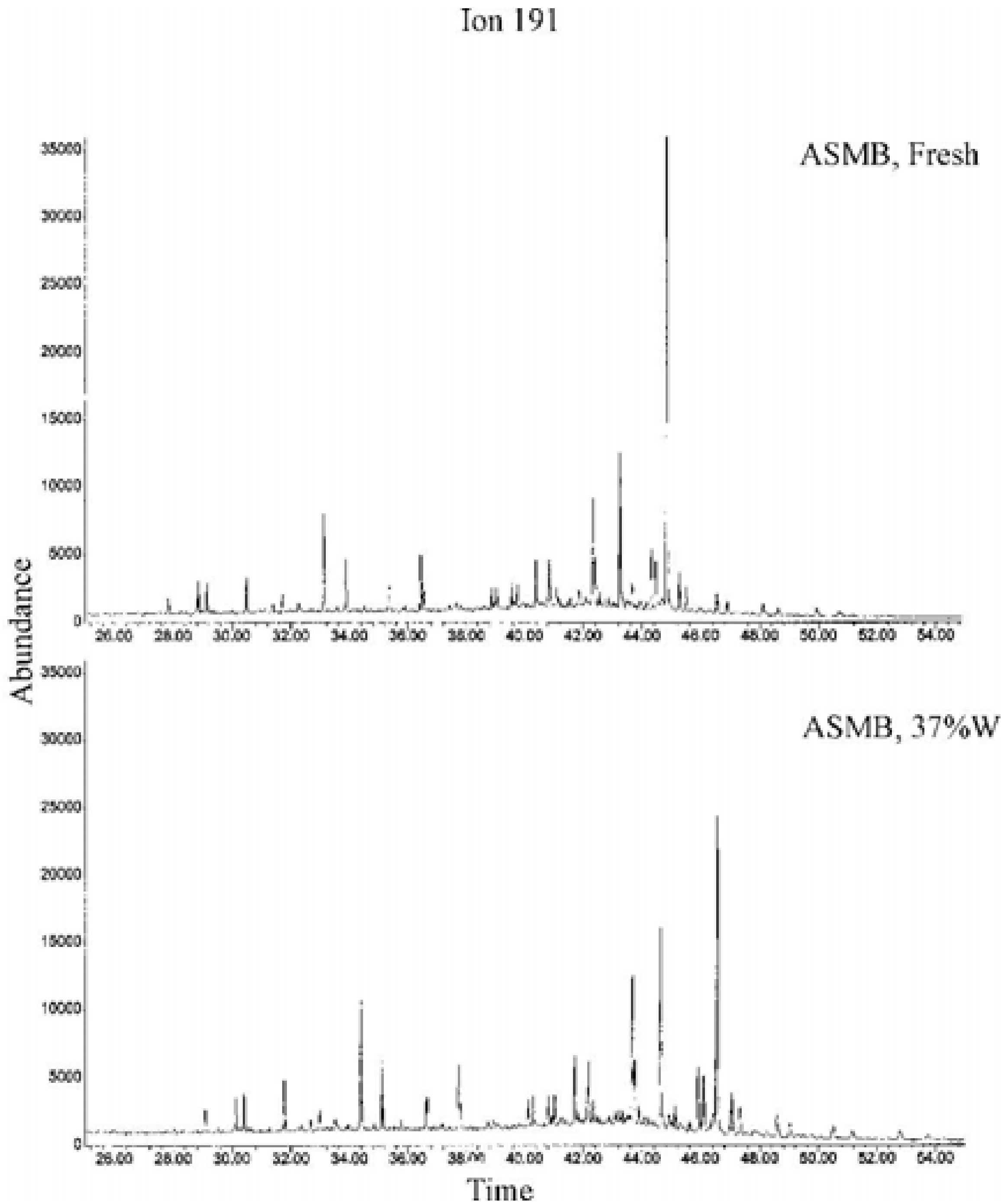


Figure A4-6 GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of ASMB #5 crude oil

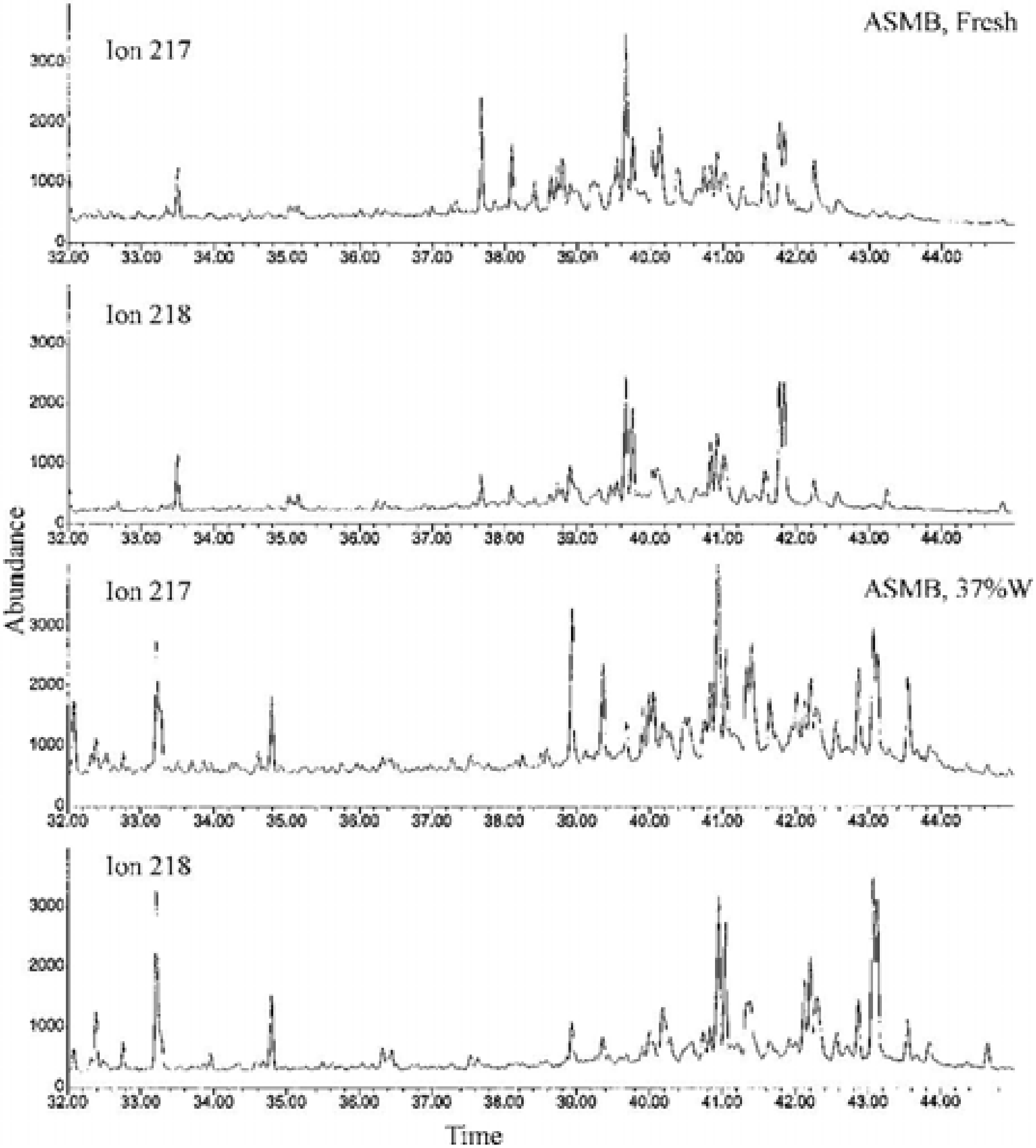


Figure A4-7 GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218)

5 GC Chromatograms for Arabian Light Crude Oil

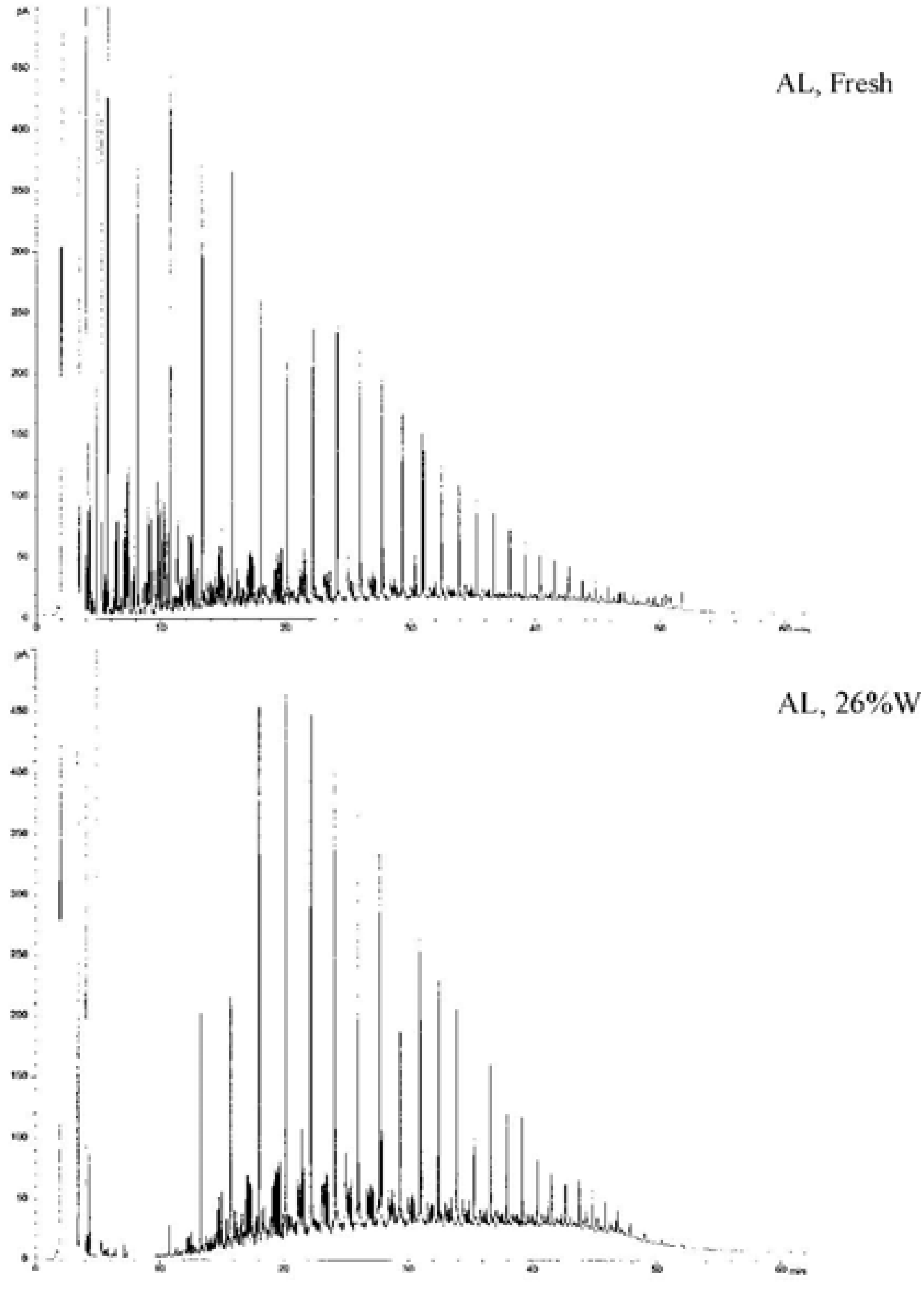


Figure A5-1 GC-FID chromatograms of fraction 1 (F1) for saturates of Arabian Light crude oil

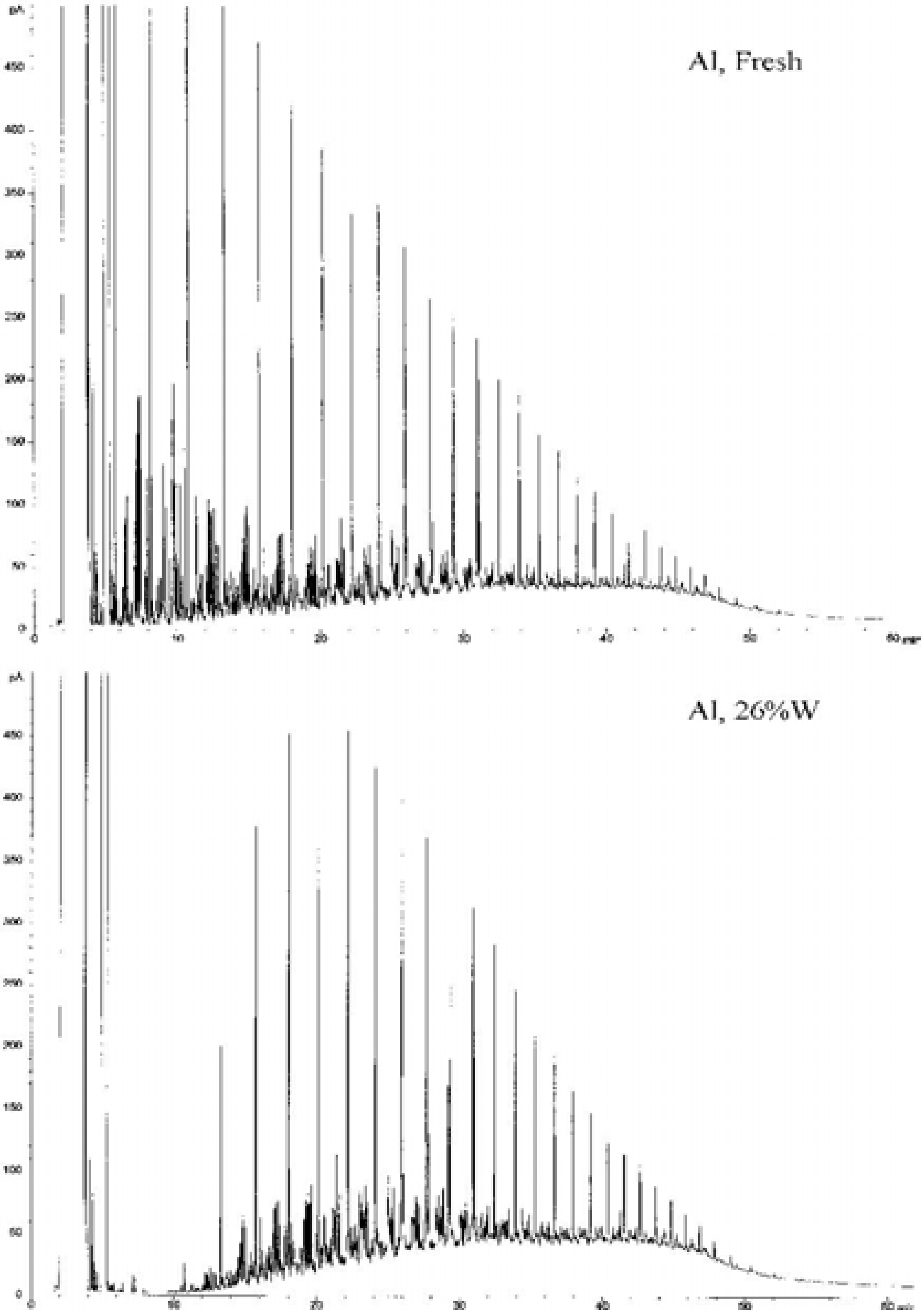


Figure A5-2 GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH of Arabian Light crude oil

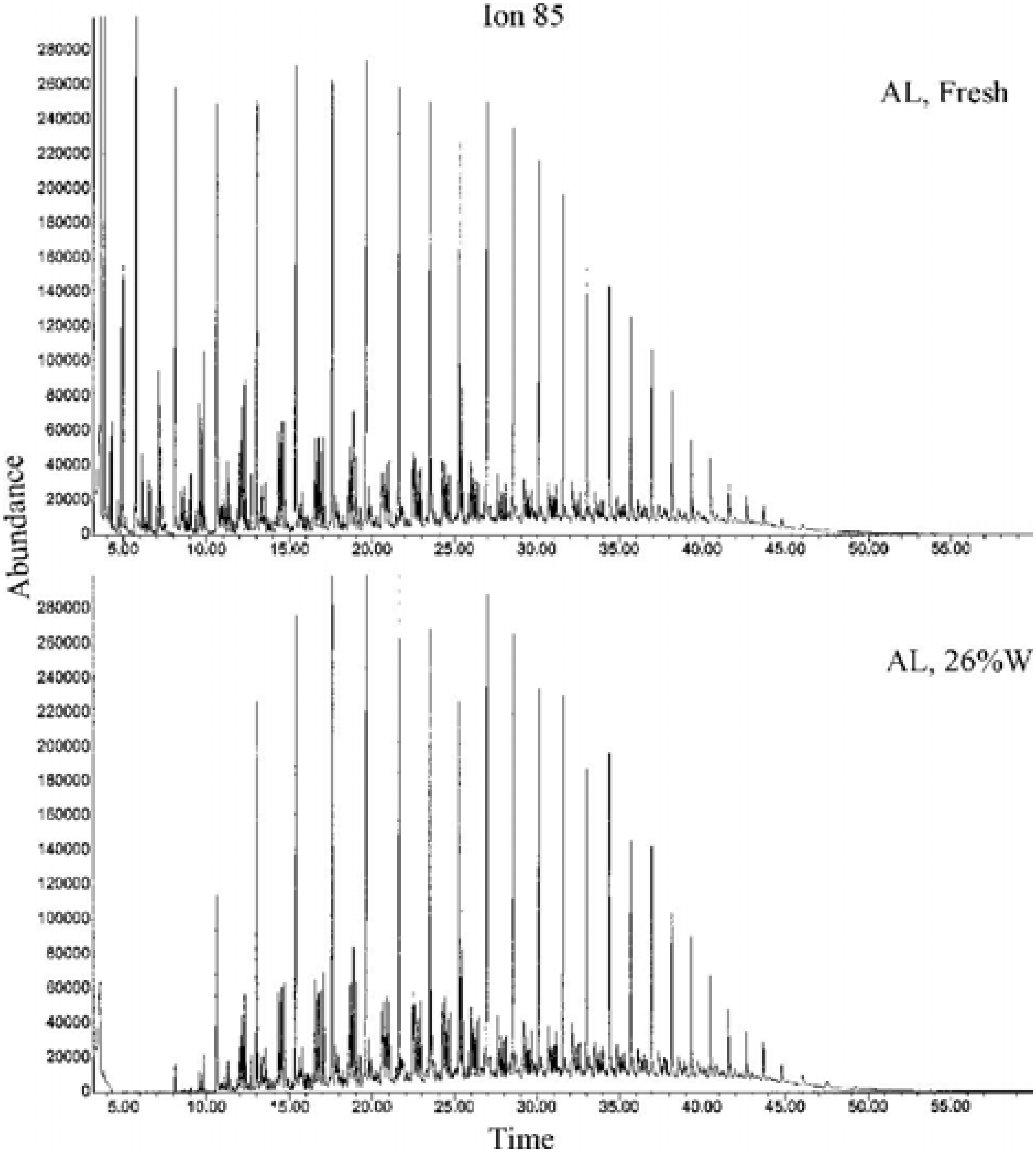


Figure A5-3 GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of Arabian Light crude oil

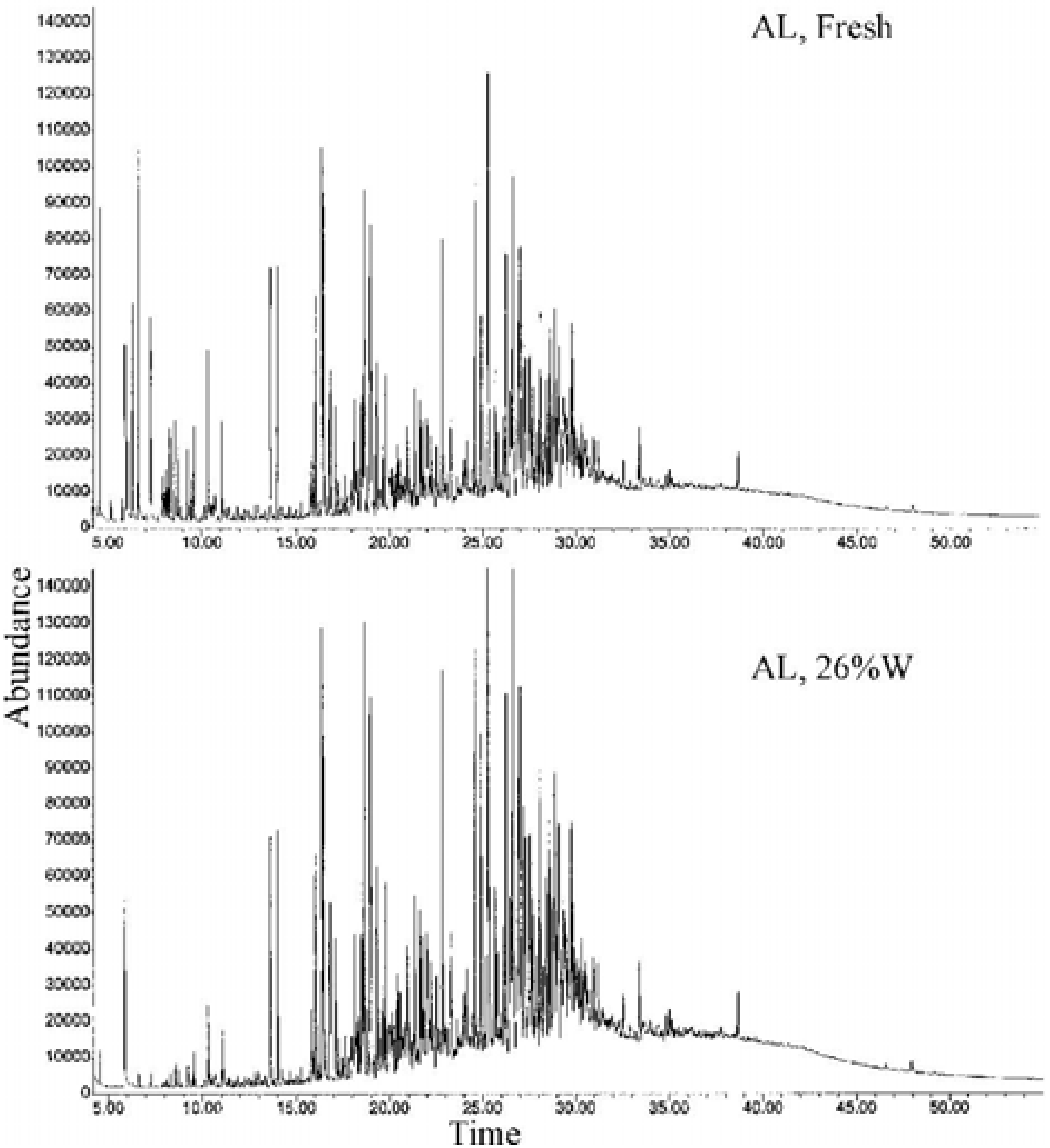


Figure A5-4 Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of Arabian Light crude oil

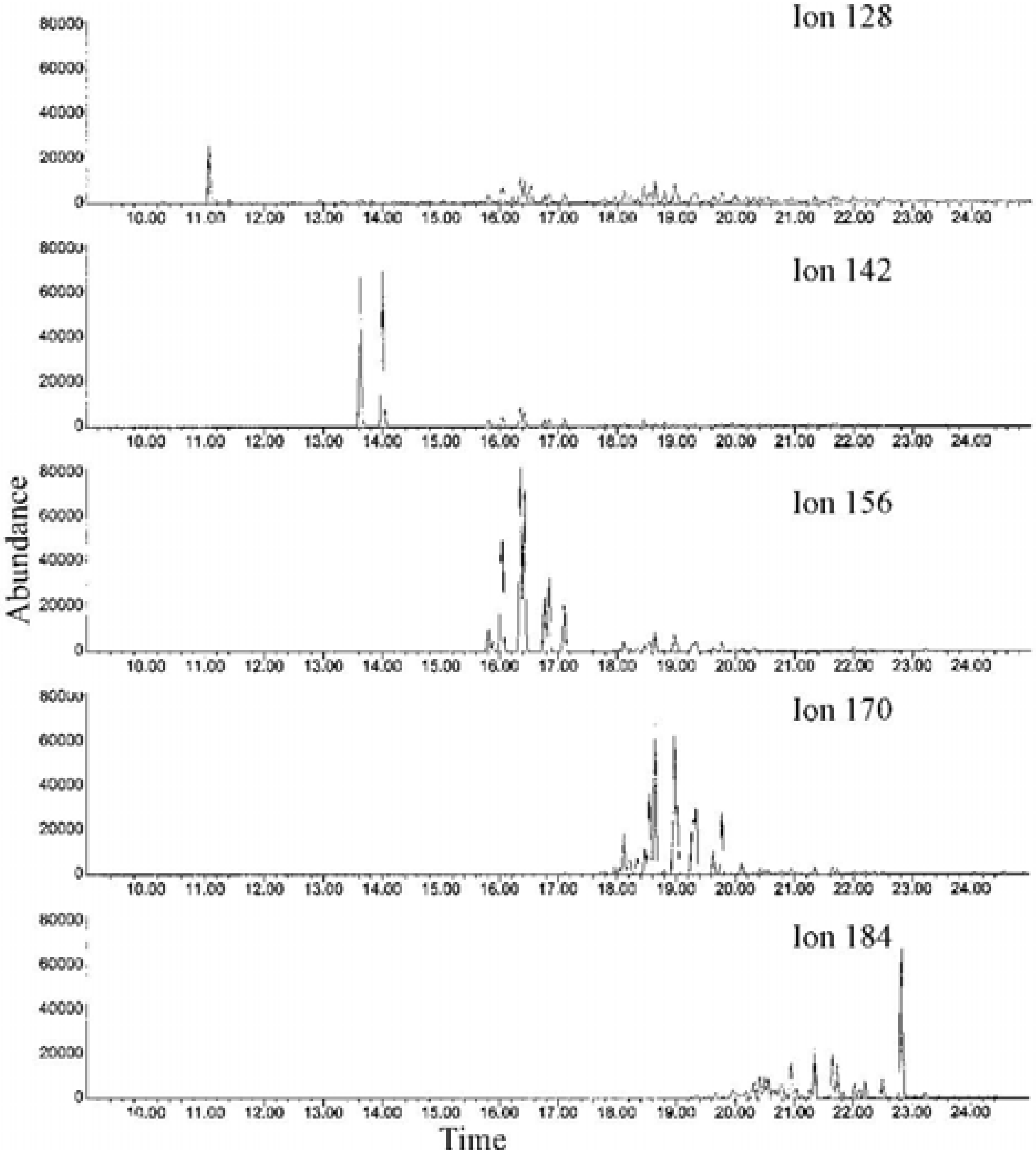


Figure A5-5a Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184) of Arabian Light crude oil

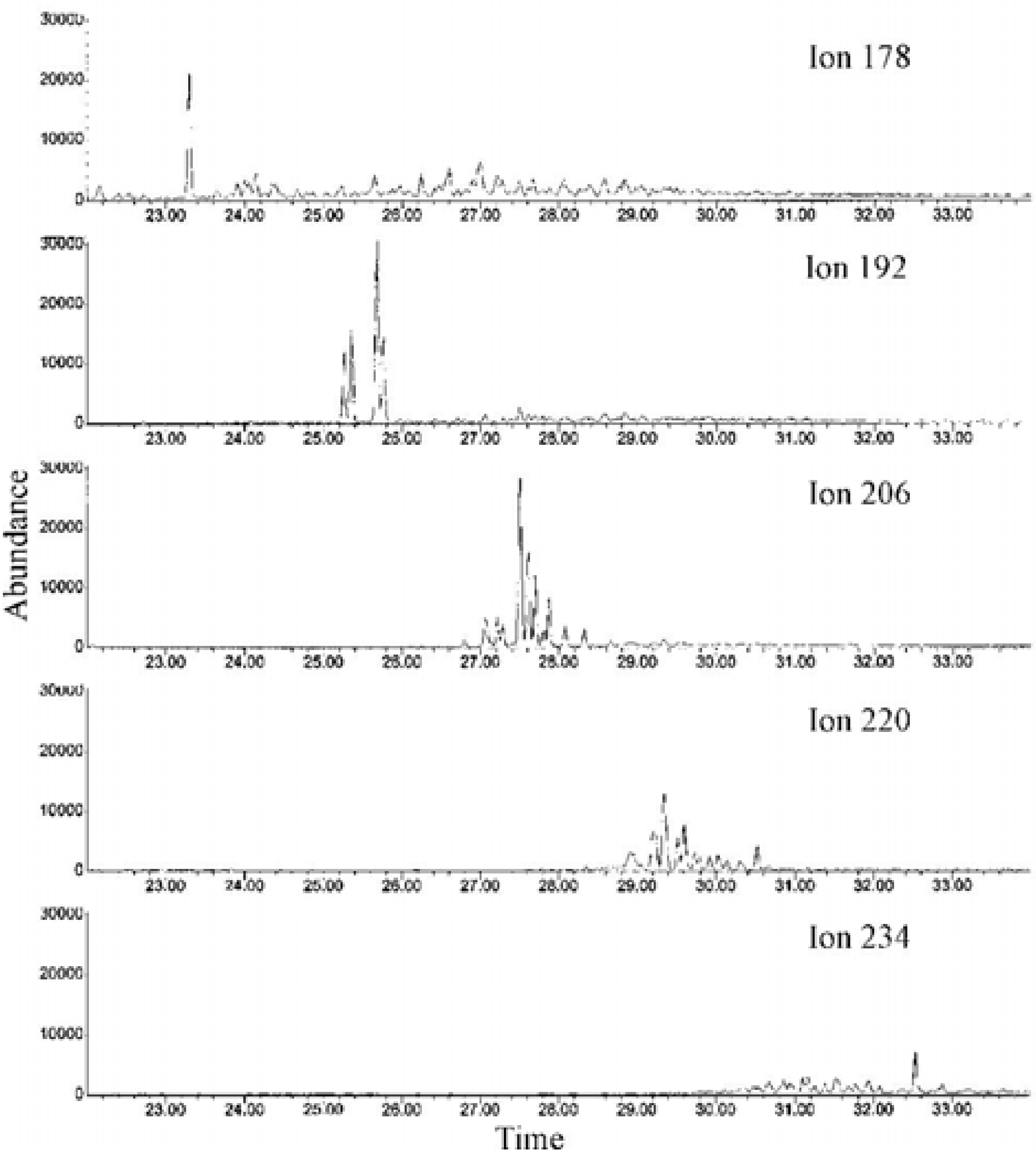


Figure A5-5b Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 178, 192, 206, 220, 234) of Arabian Light crude oil

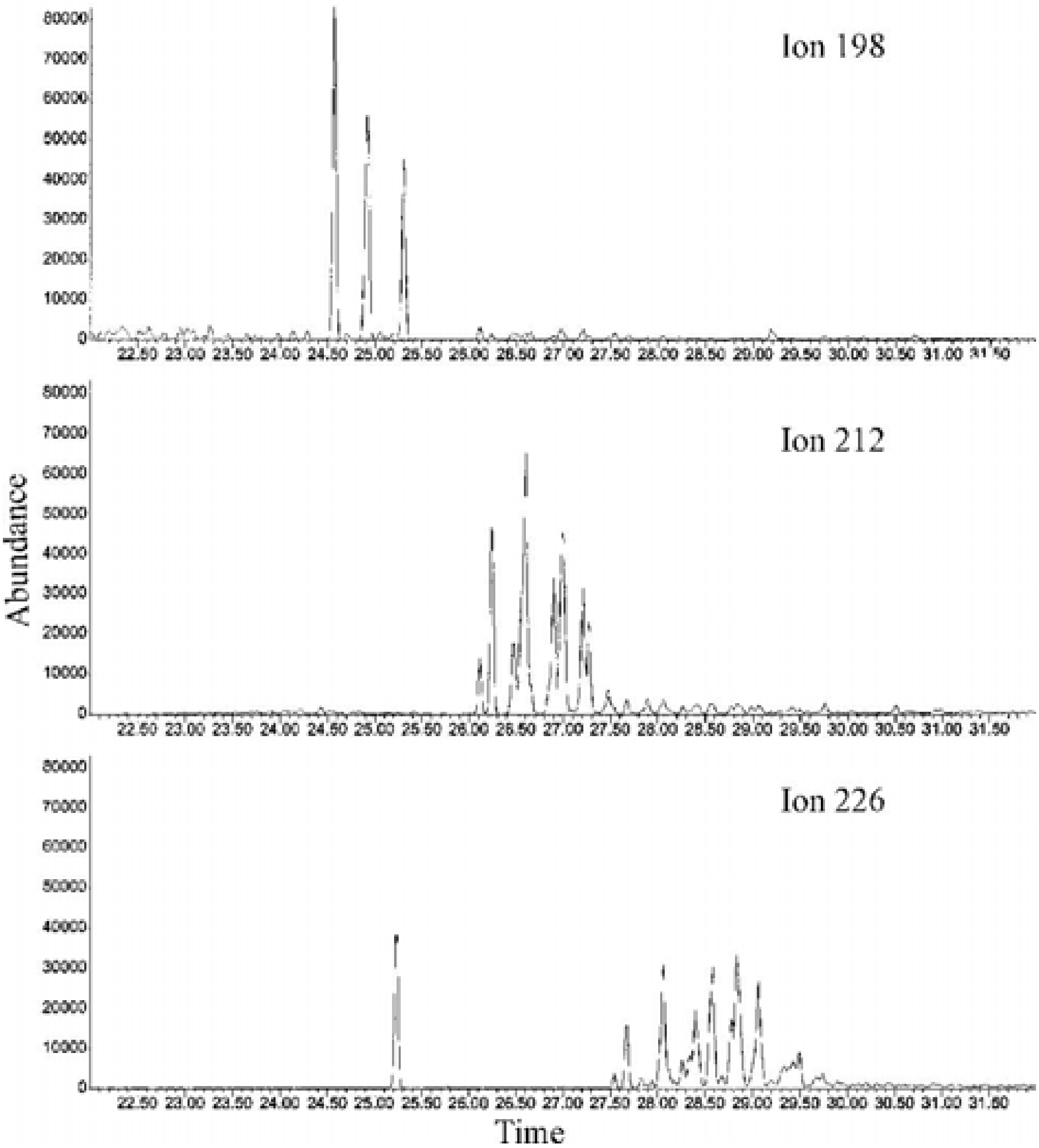


Figure A5-5c Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 198, 212, 226) of Arabian Light crude oil

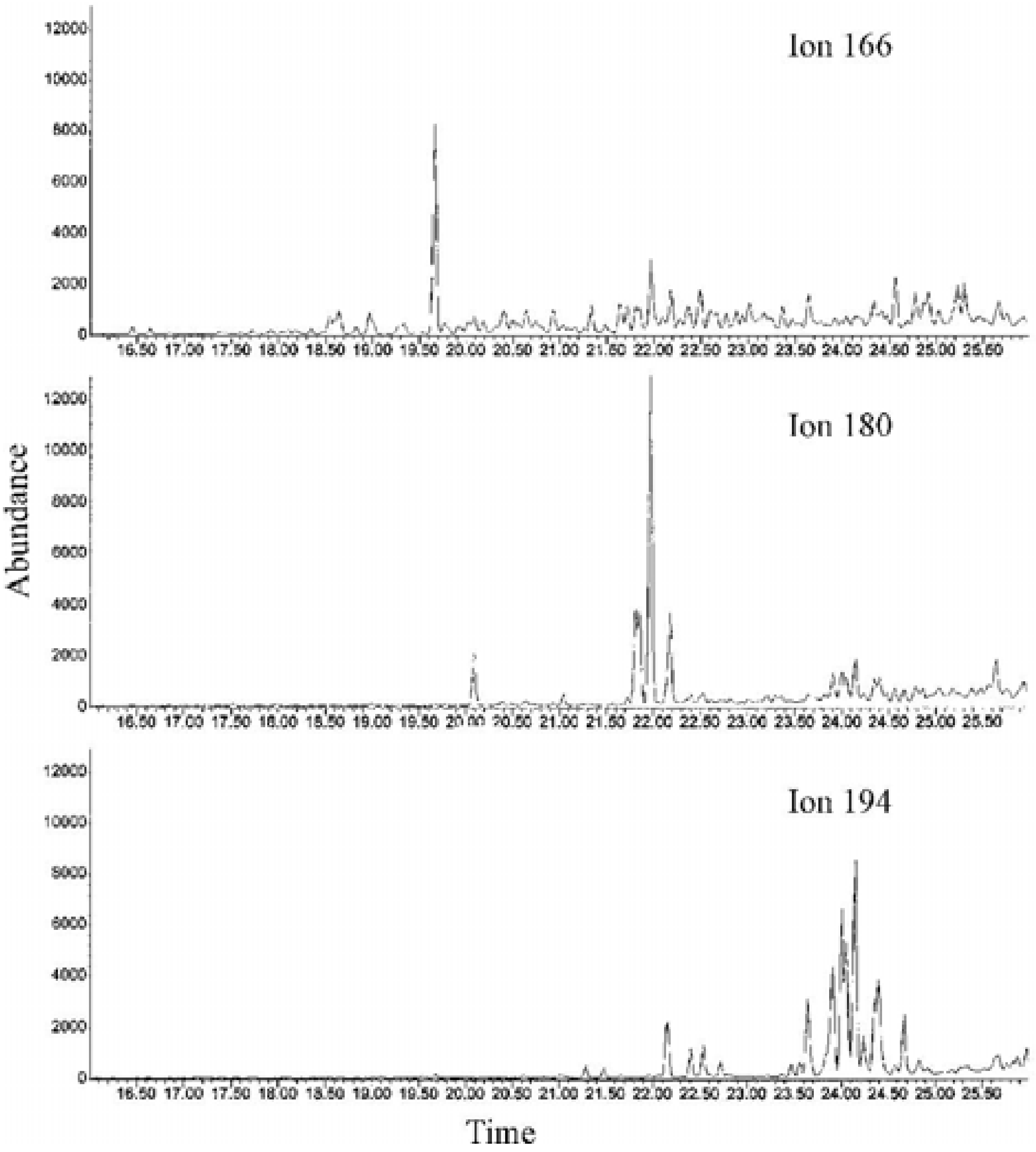


Figure A5-5d Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 166, 180, 194) of Arabian Light crude oil

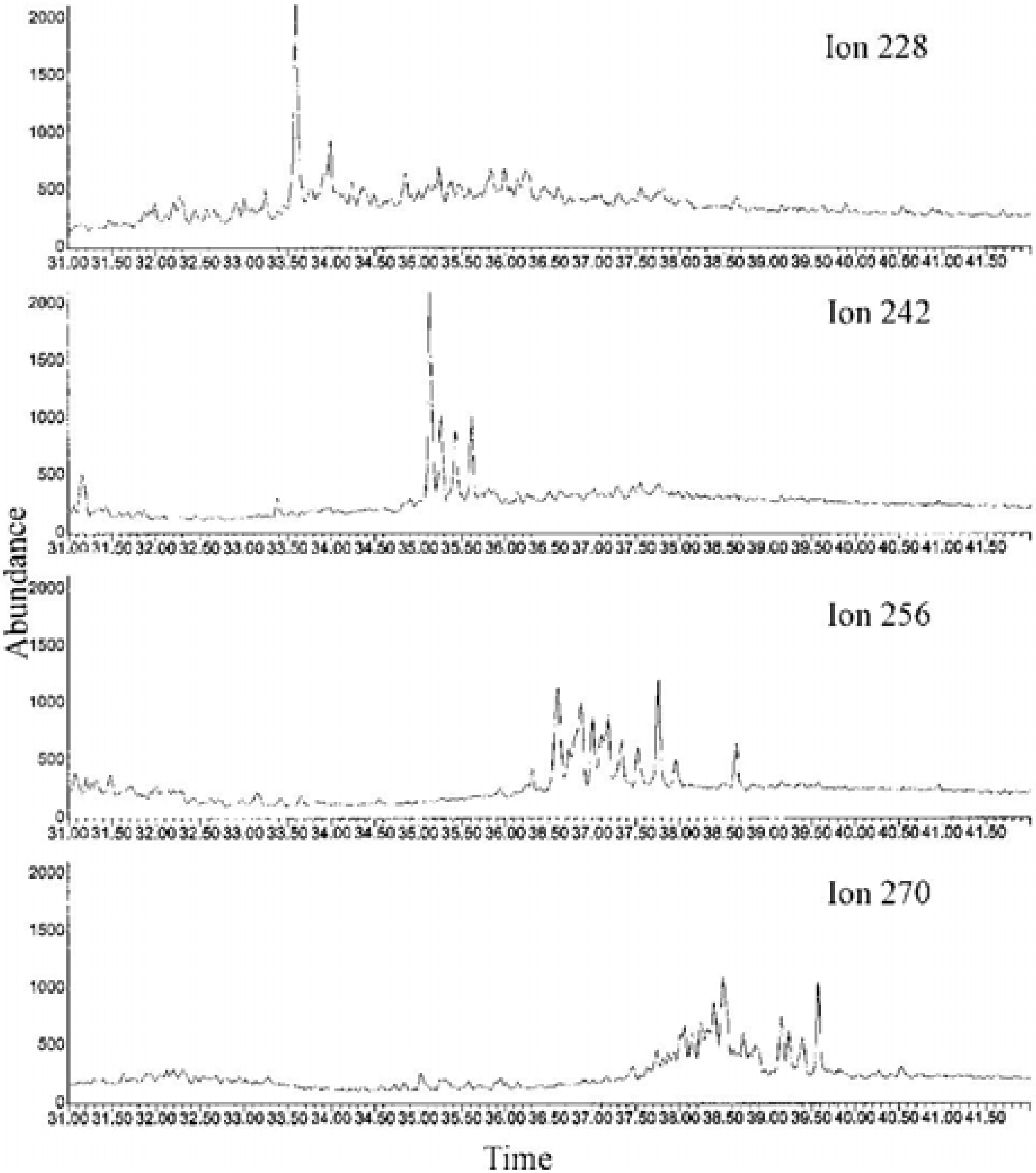


Figure A5-5e Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 228, 242, 256, 270) of Arabian Light crude oil

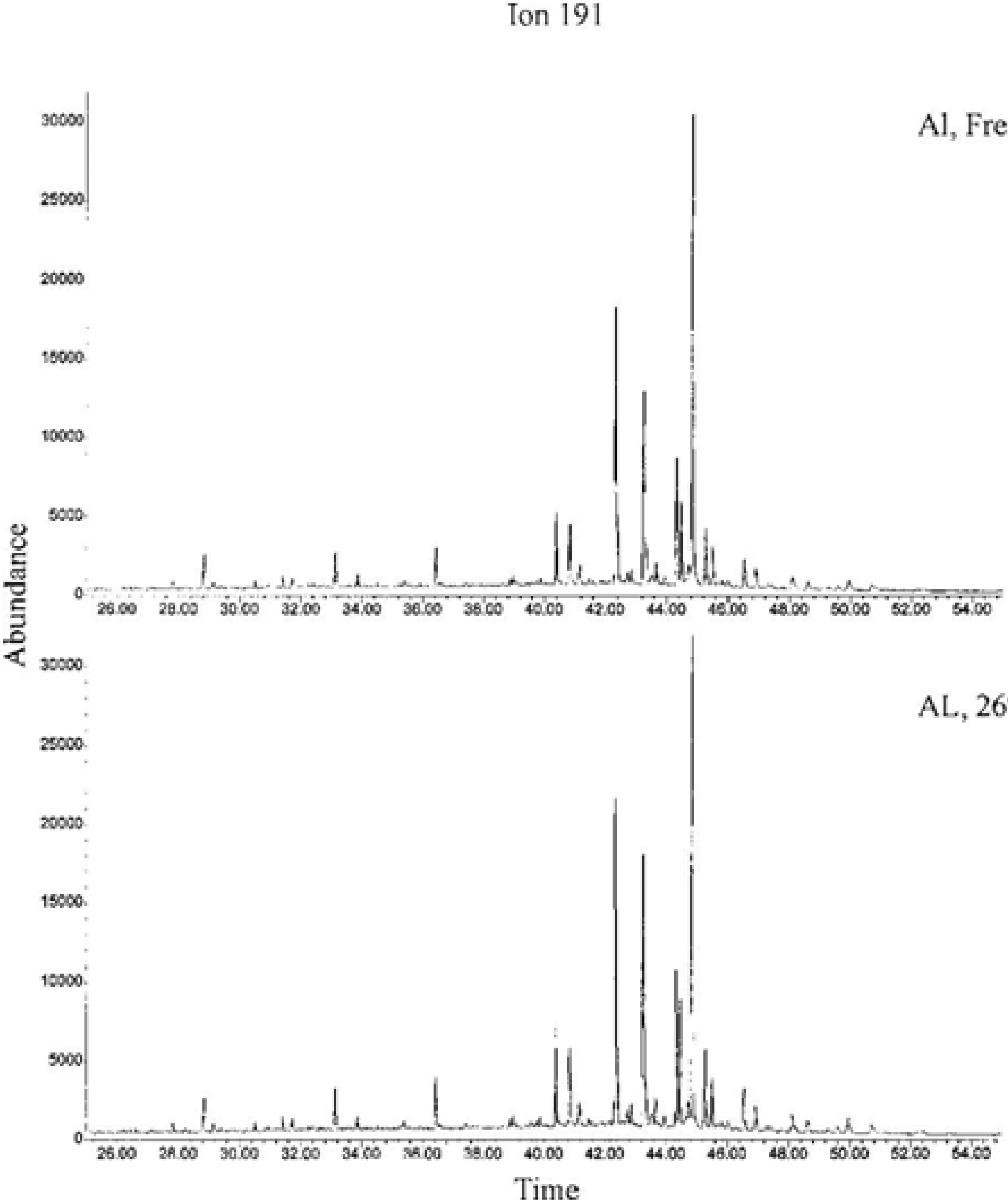


Figure A5-6 GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of Arabian Light crude oil

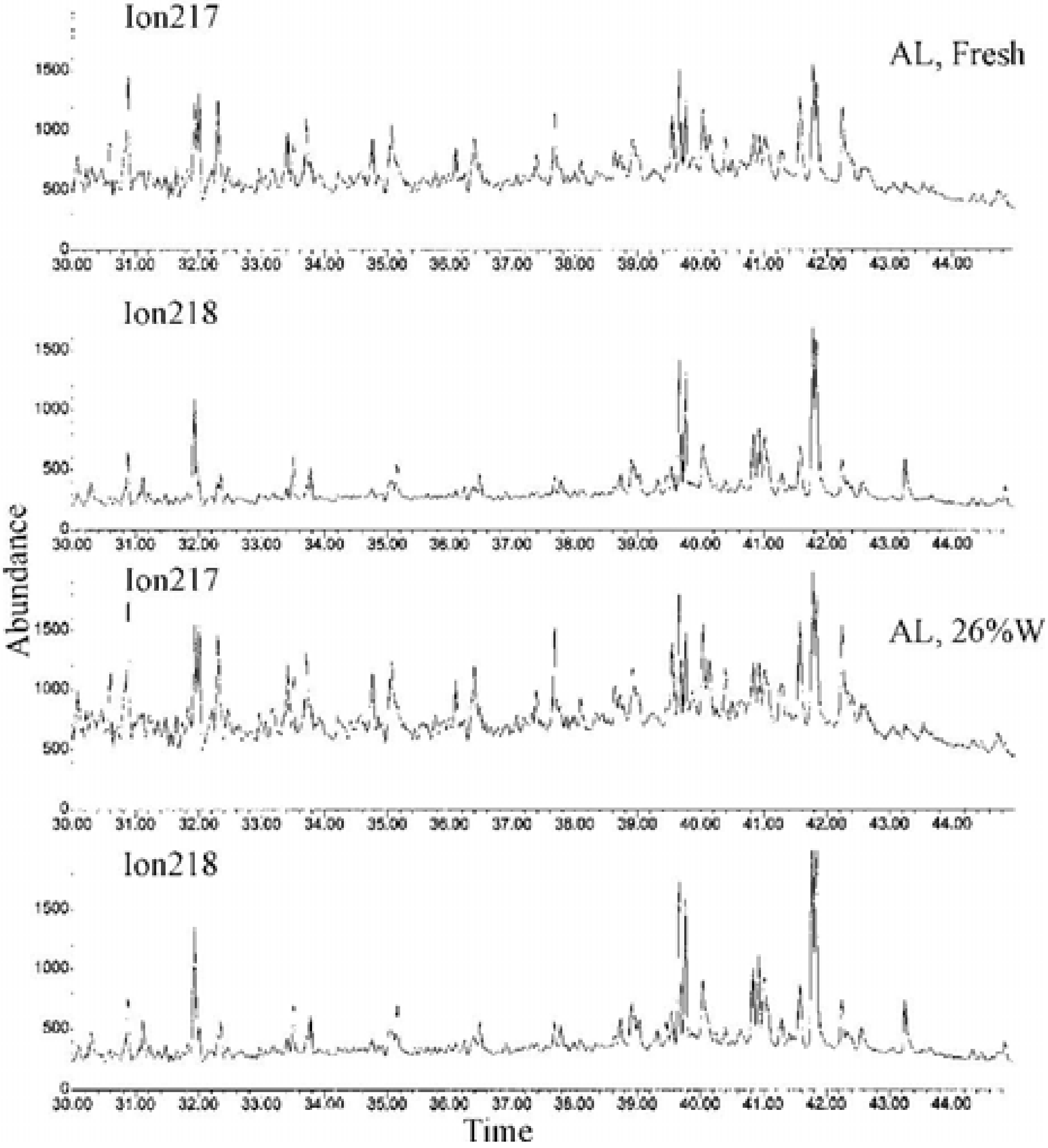


Figure A5-7 GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218) of Arabian Light crude oil

6 GC Chromatograms for Sockeye Crude Oil

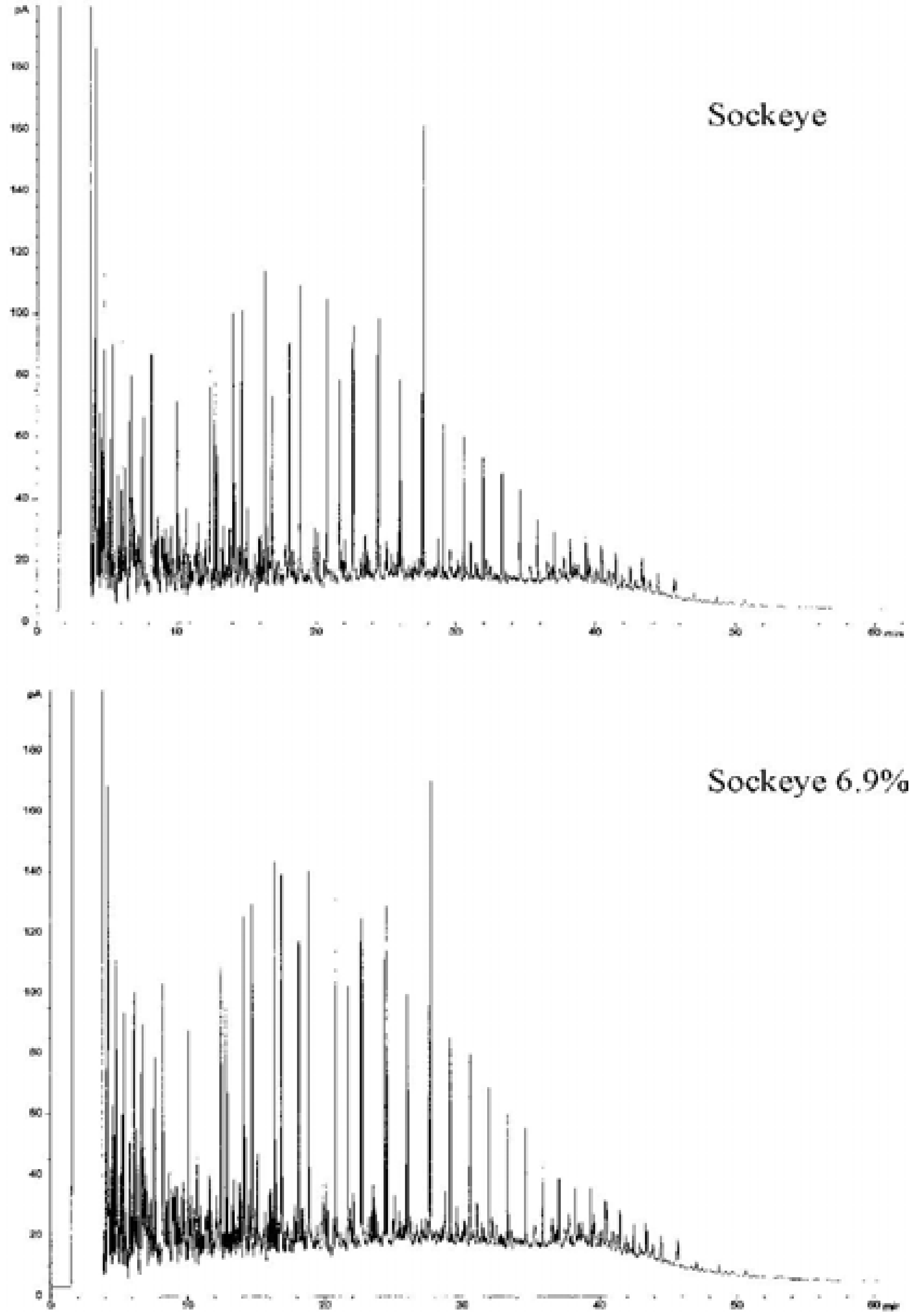


Figure A6-1a GC-FID chromatograms of fraction 1 (F1) for saturates of Sockeye crude oil

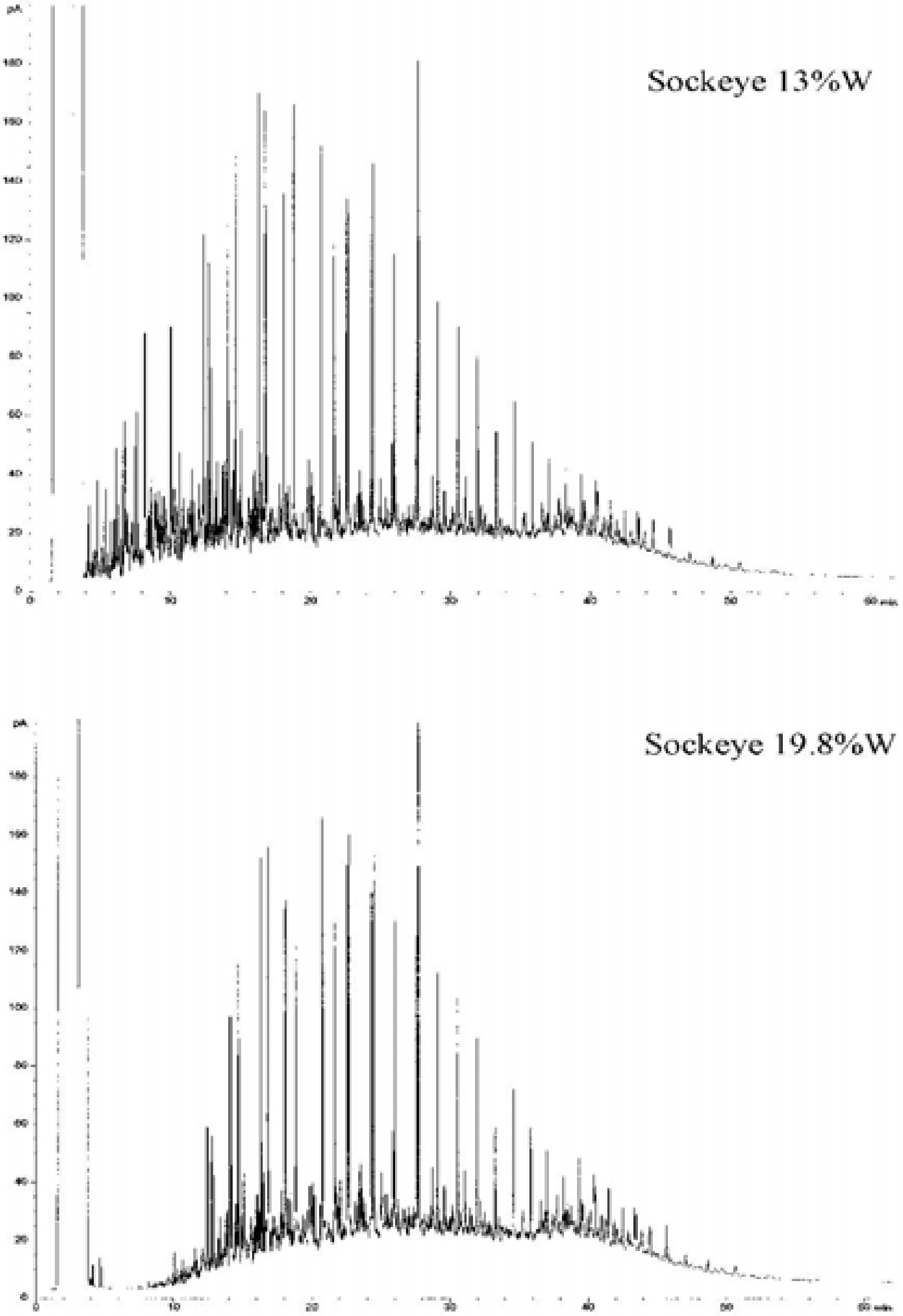


Figure A6-1b GC-FID chromatograms of fraction 1 (F1) for saturates of Sockeye crude oil

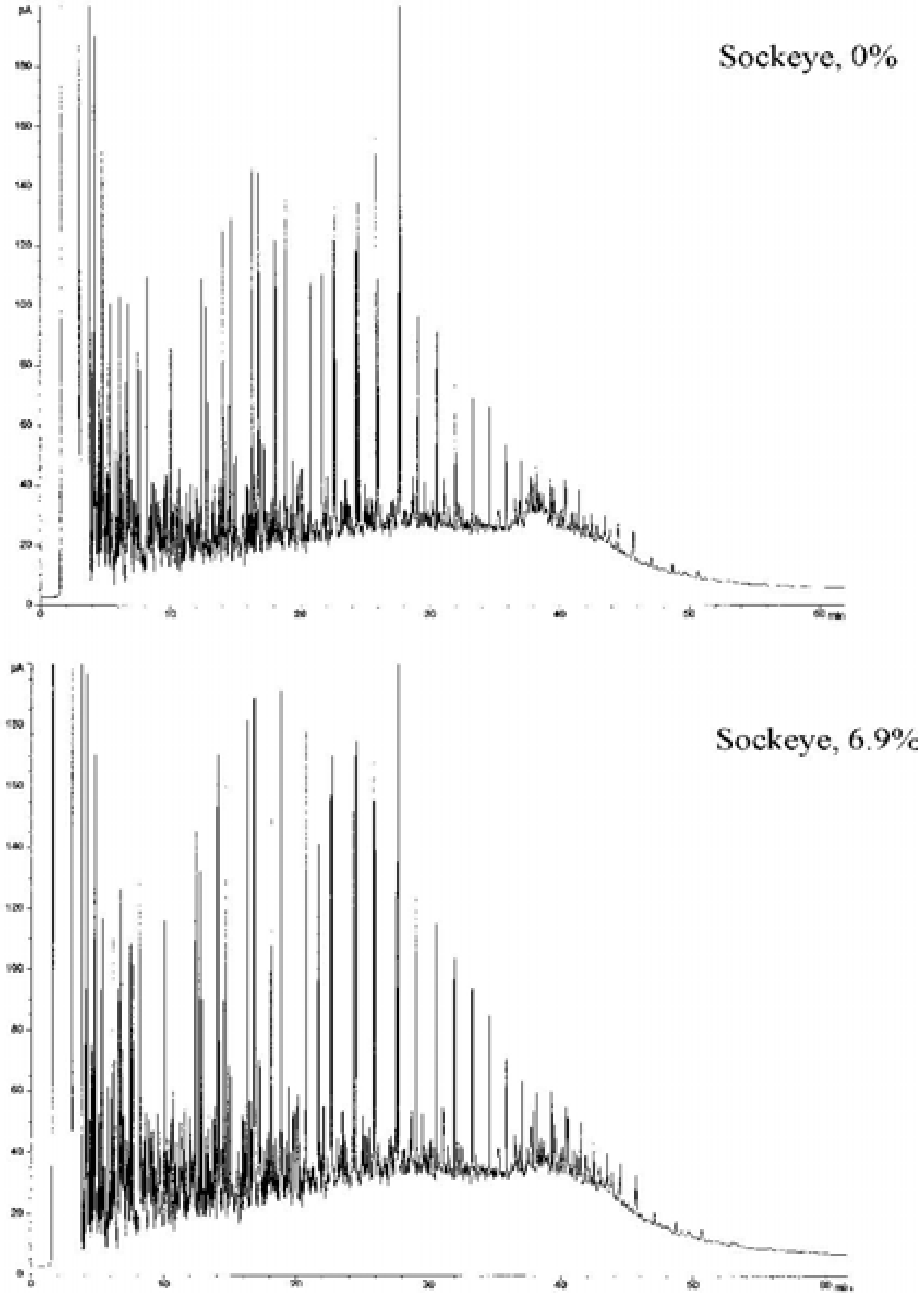


Figure A6-2a GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of Sockeye crude oil

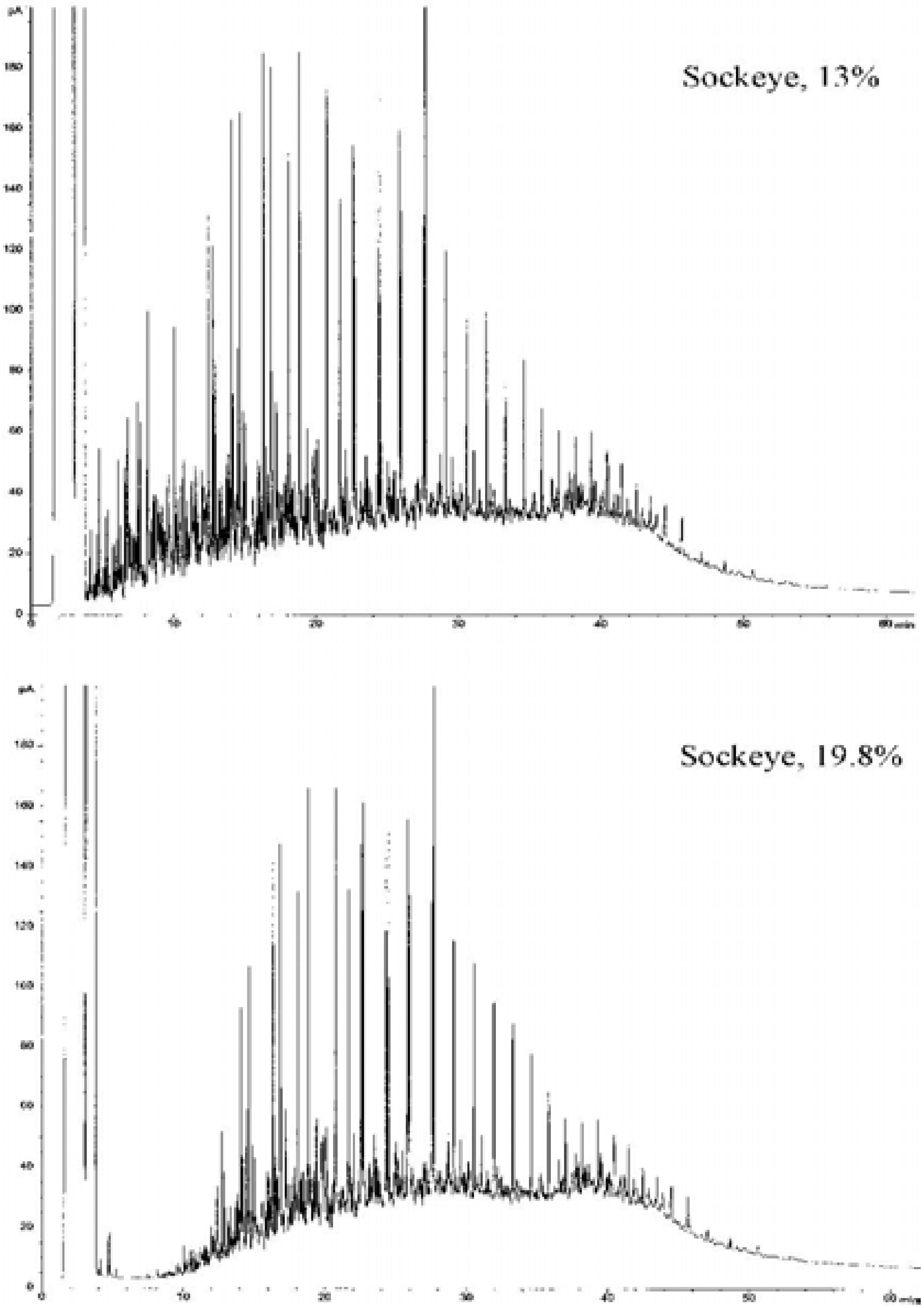


Figure A6-2b GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of Sockeye crude oil

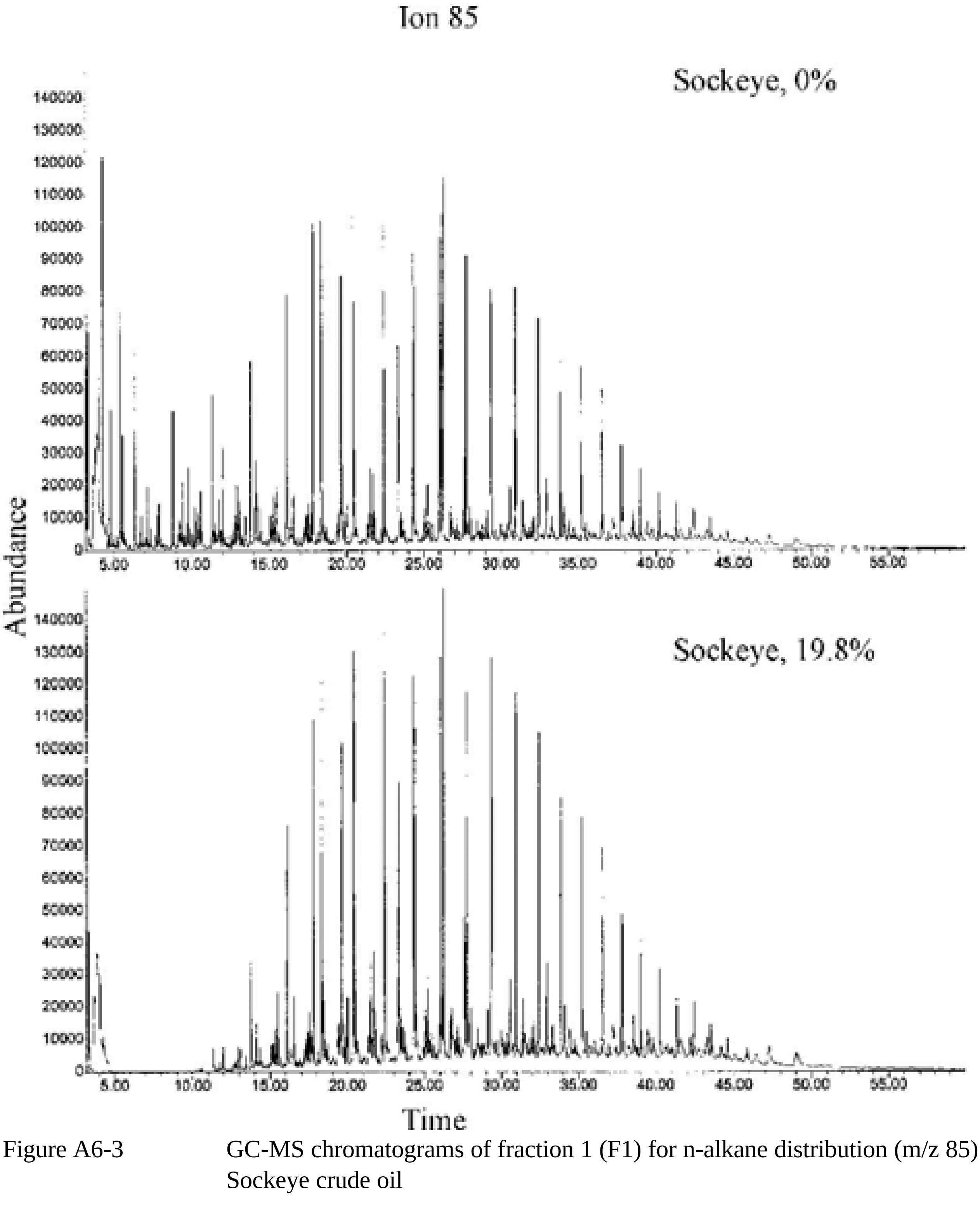


Figure A6-3 GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of Sockeye crude oil

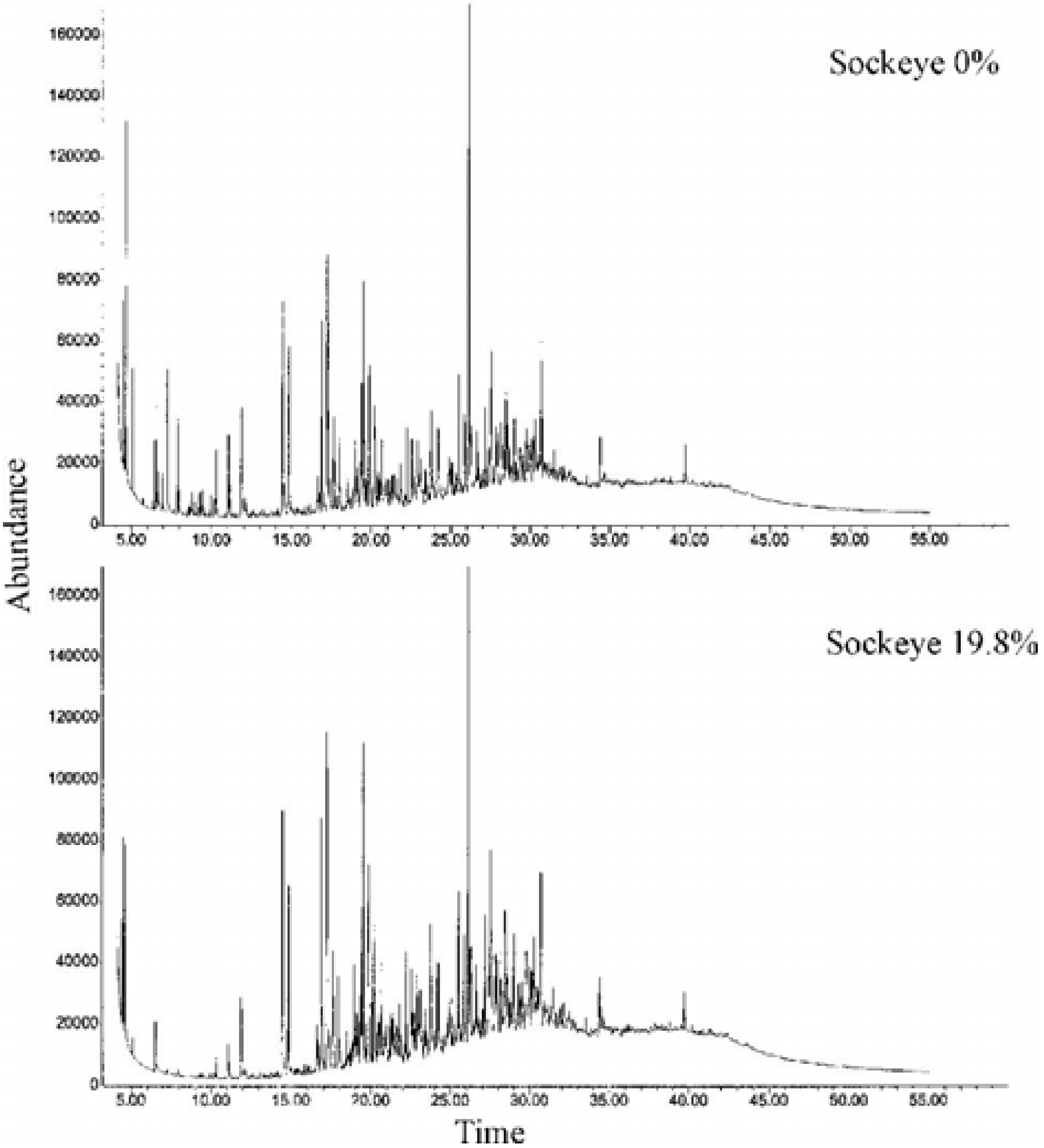


Figure A6-4 Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of Sockeye crude oil

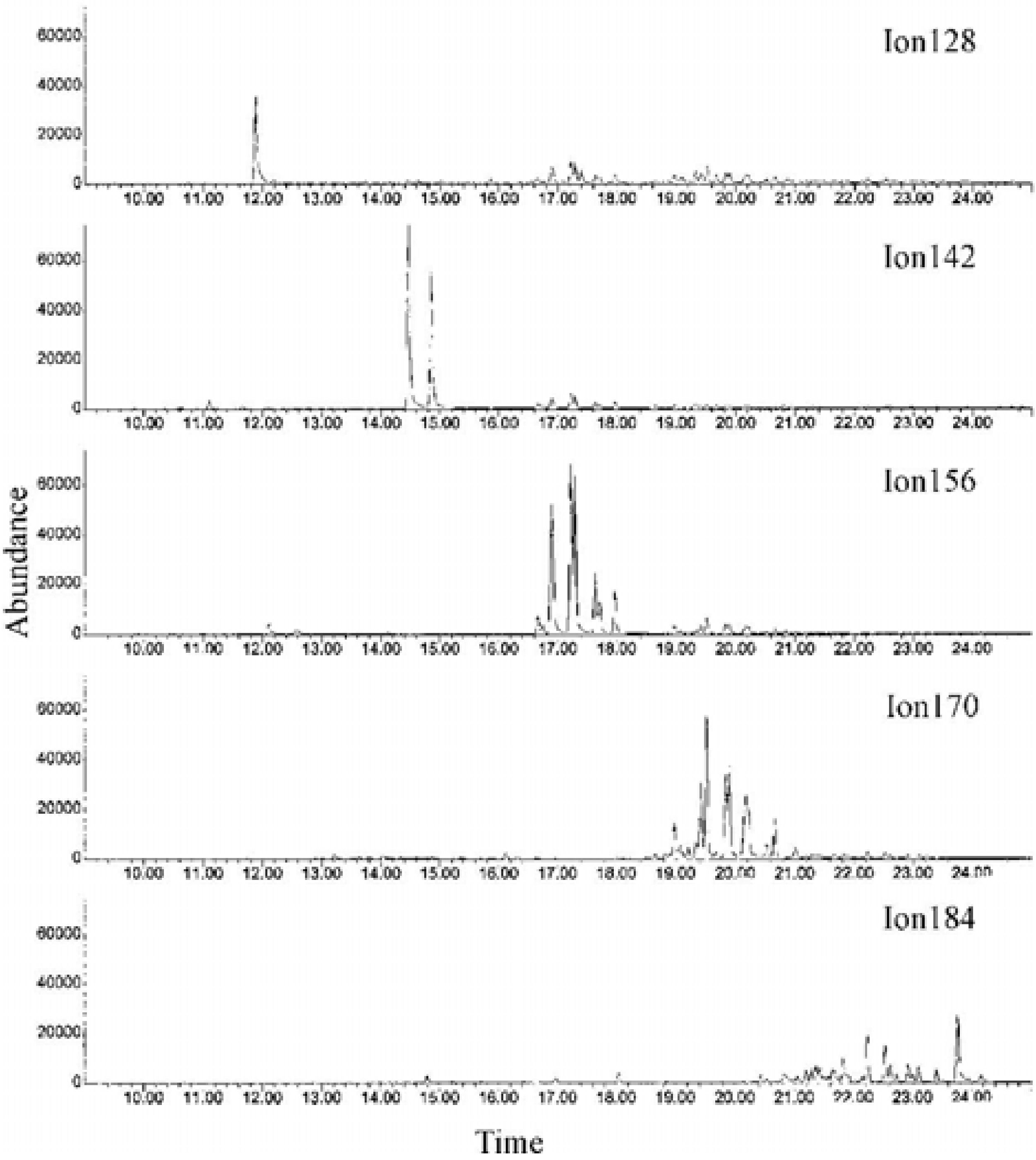


Figure A6-5a Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184) of Sockeye crude oil

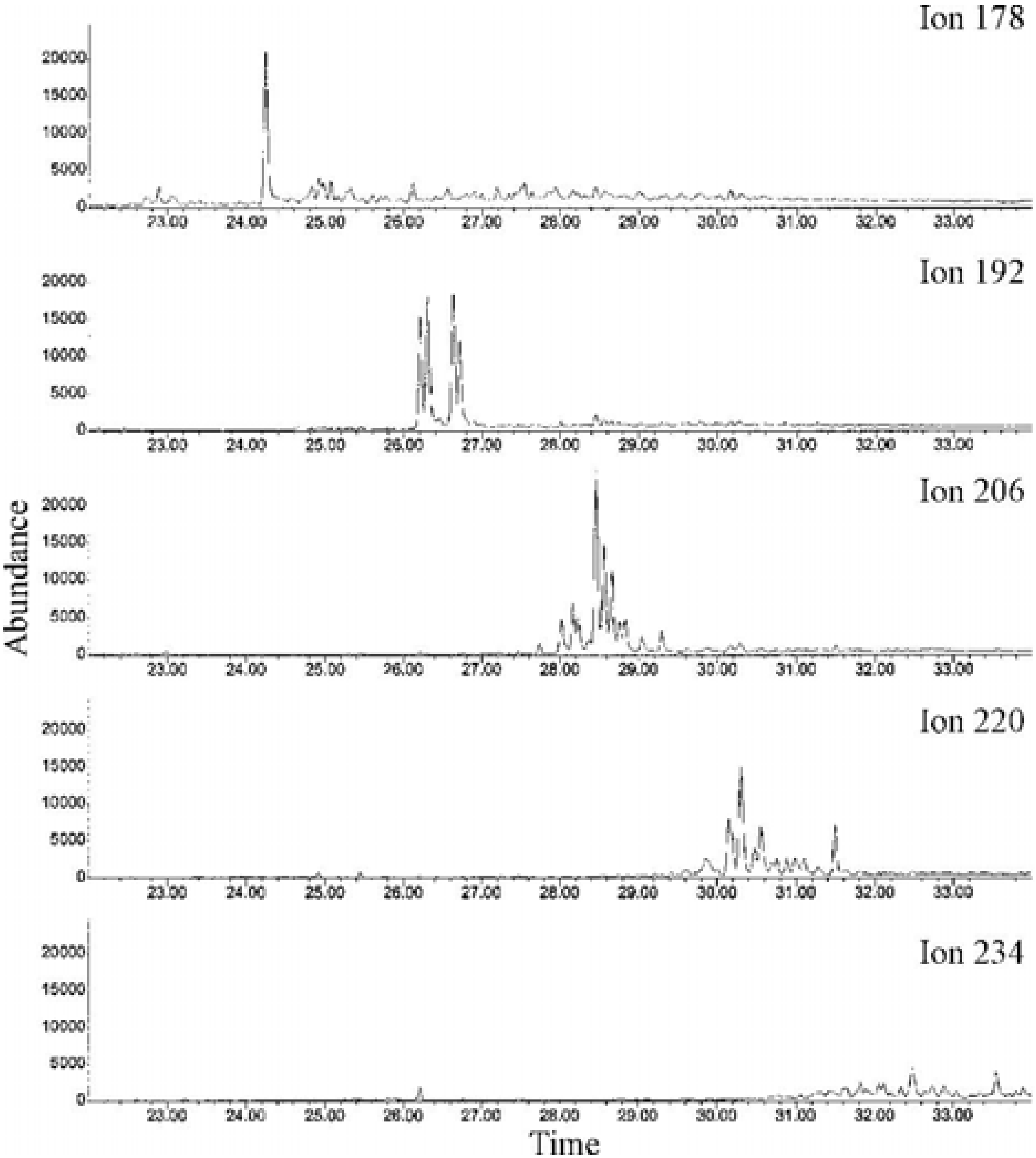


Figure A6-5b Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 178, 192, 206, 220, 234) of Sockeye crude oil

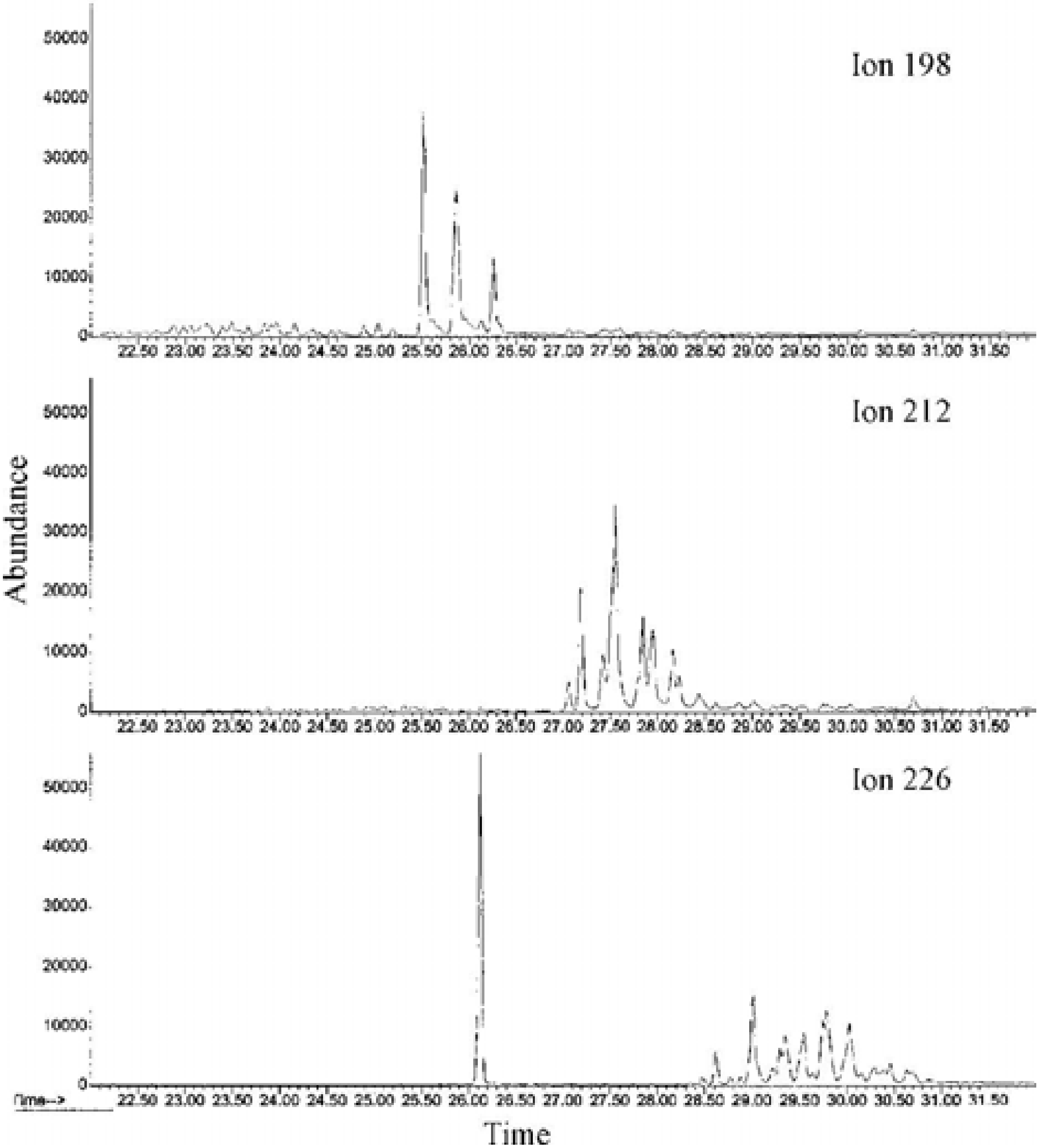


Figure A6-5c Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 198, 212, 226) of Sockeye crude oil

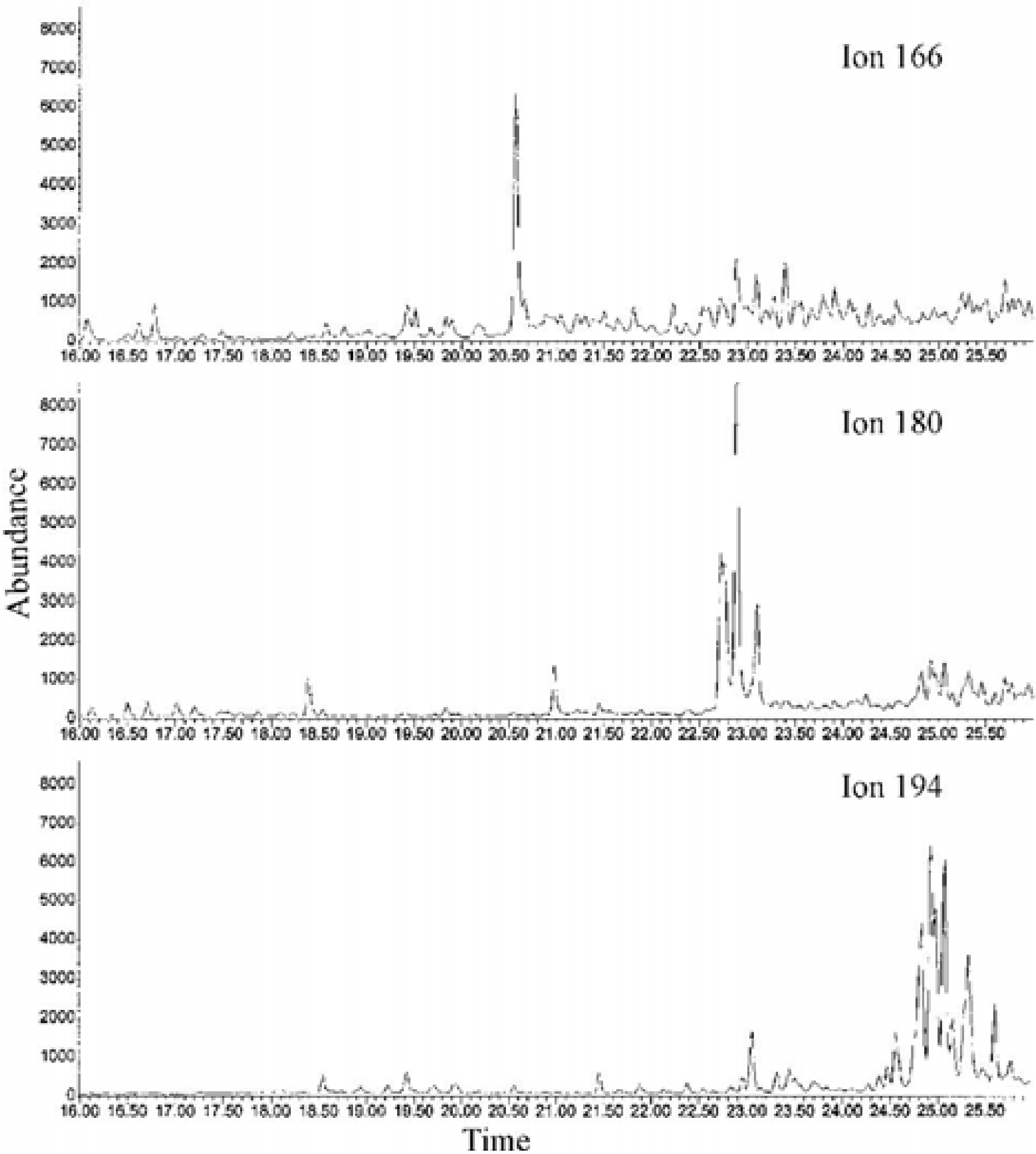


Figure A6-5d Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 166, 180, 194) of Sockeye crude oil

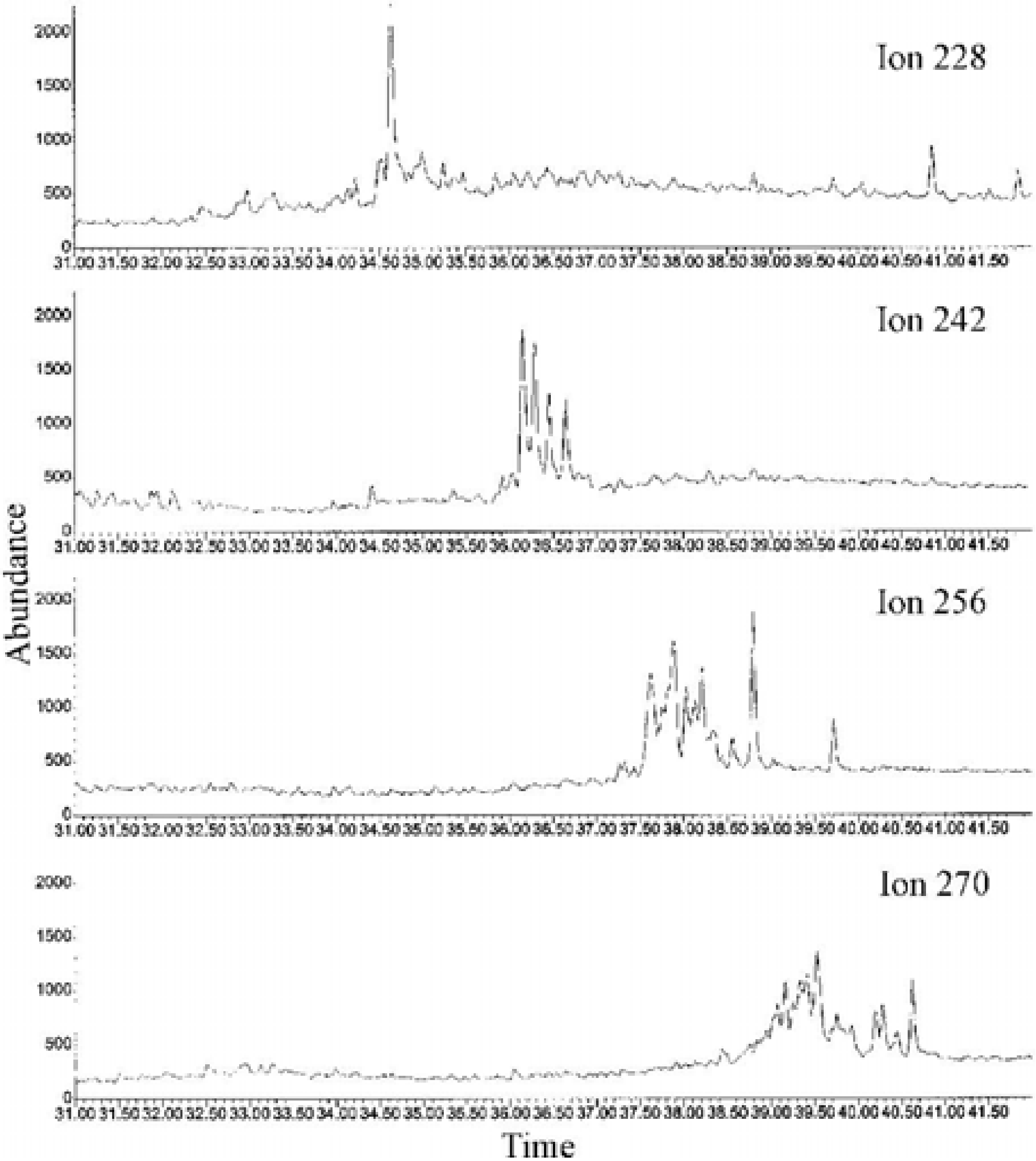


Figure A6-5e Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 228, 242, 256, 270) of Sockeye crude oil

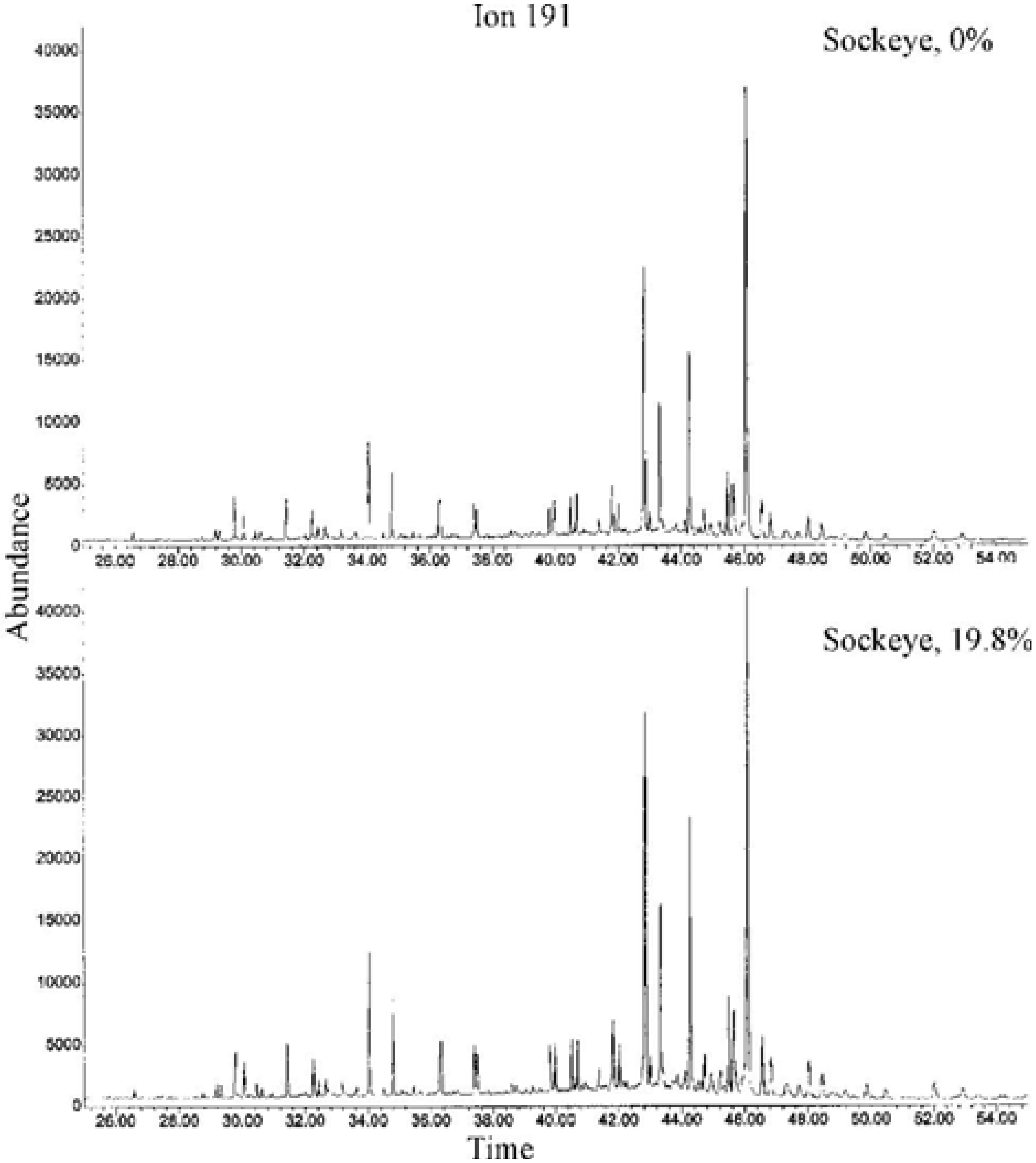


Figure A6-6 GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of Sockeye crude oil

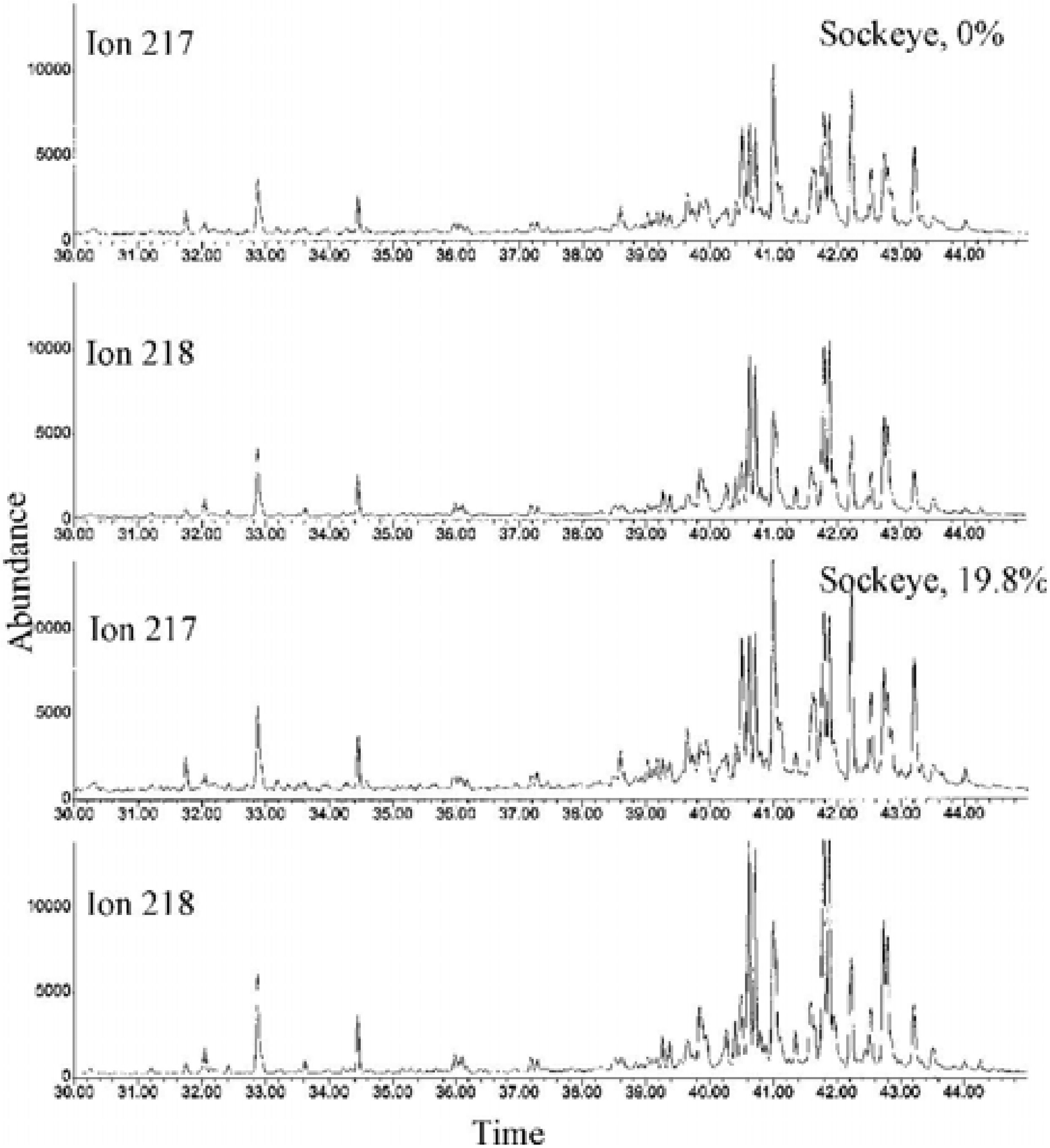


Figure A6-7 GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218) of Sockeye crude oil

7 GC Chromatograms for South Louisiana Crude Oil

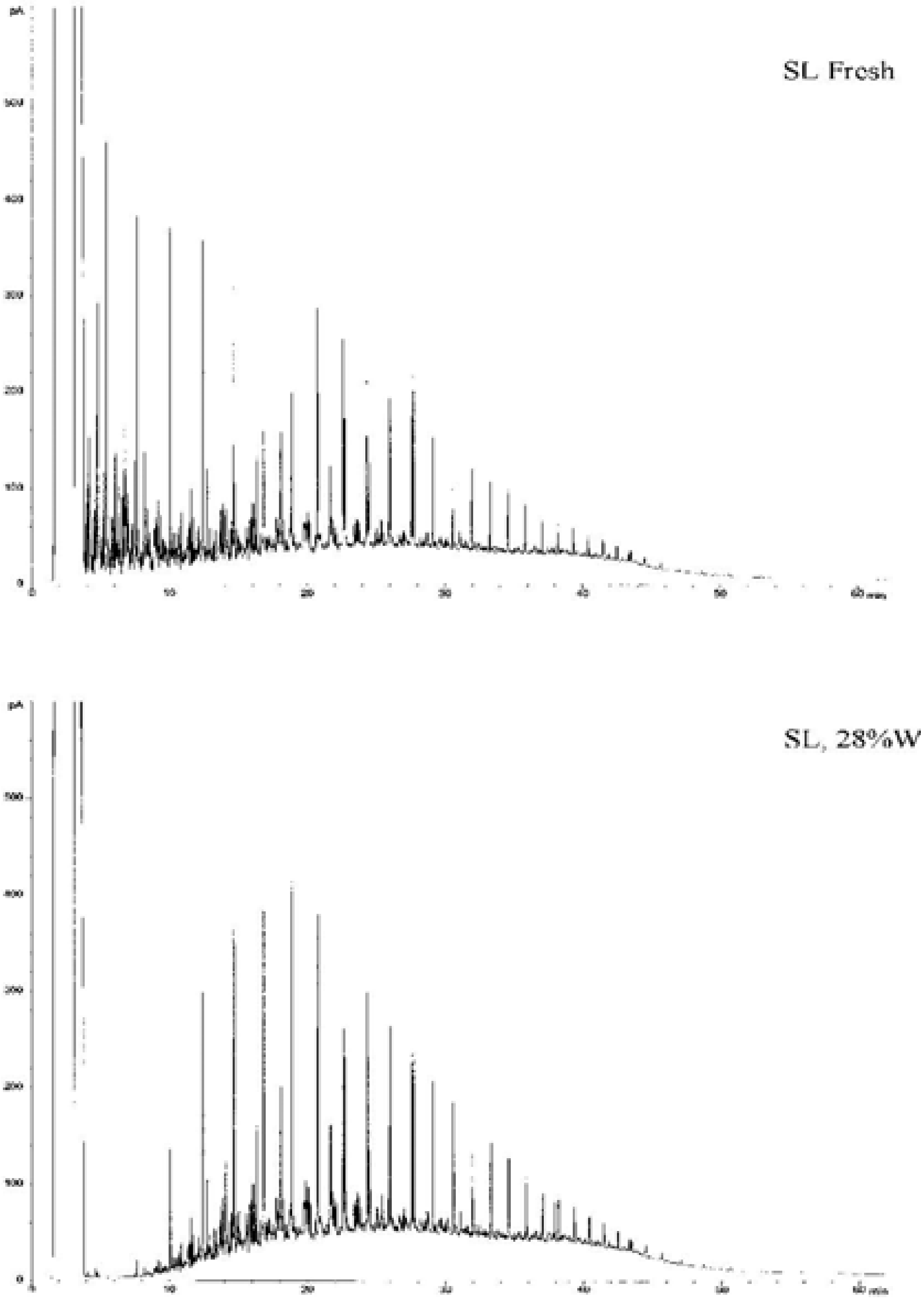


Figure A7-1 GC-FID chromatograms of fraction 1 (F1) for saturates of South Louisiana crude oil

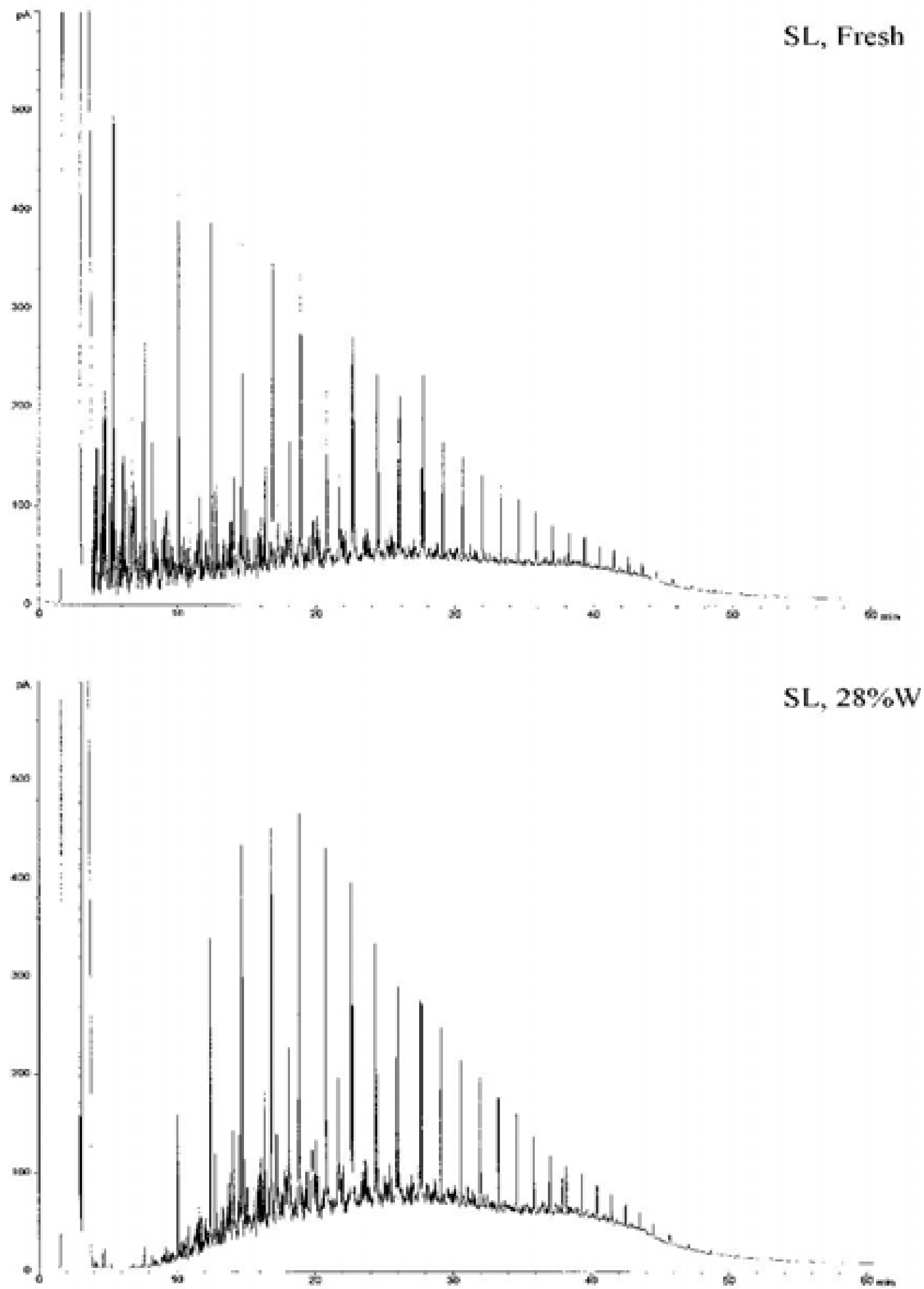


Figure A7-2 GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of South Louisiana crude oil

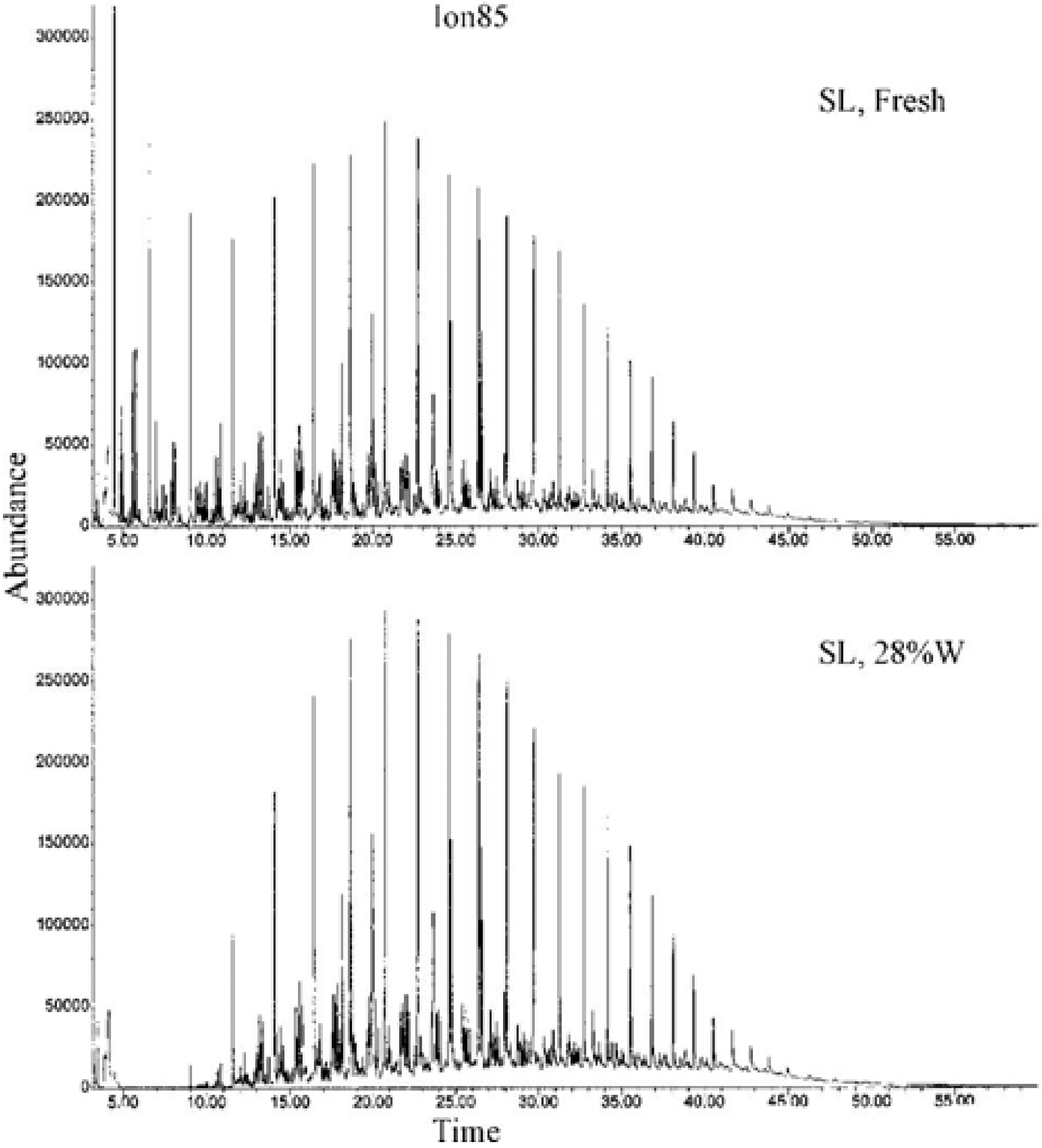


Figure A7-3 GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of South Louisiana crude oil

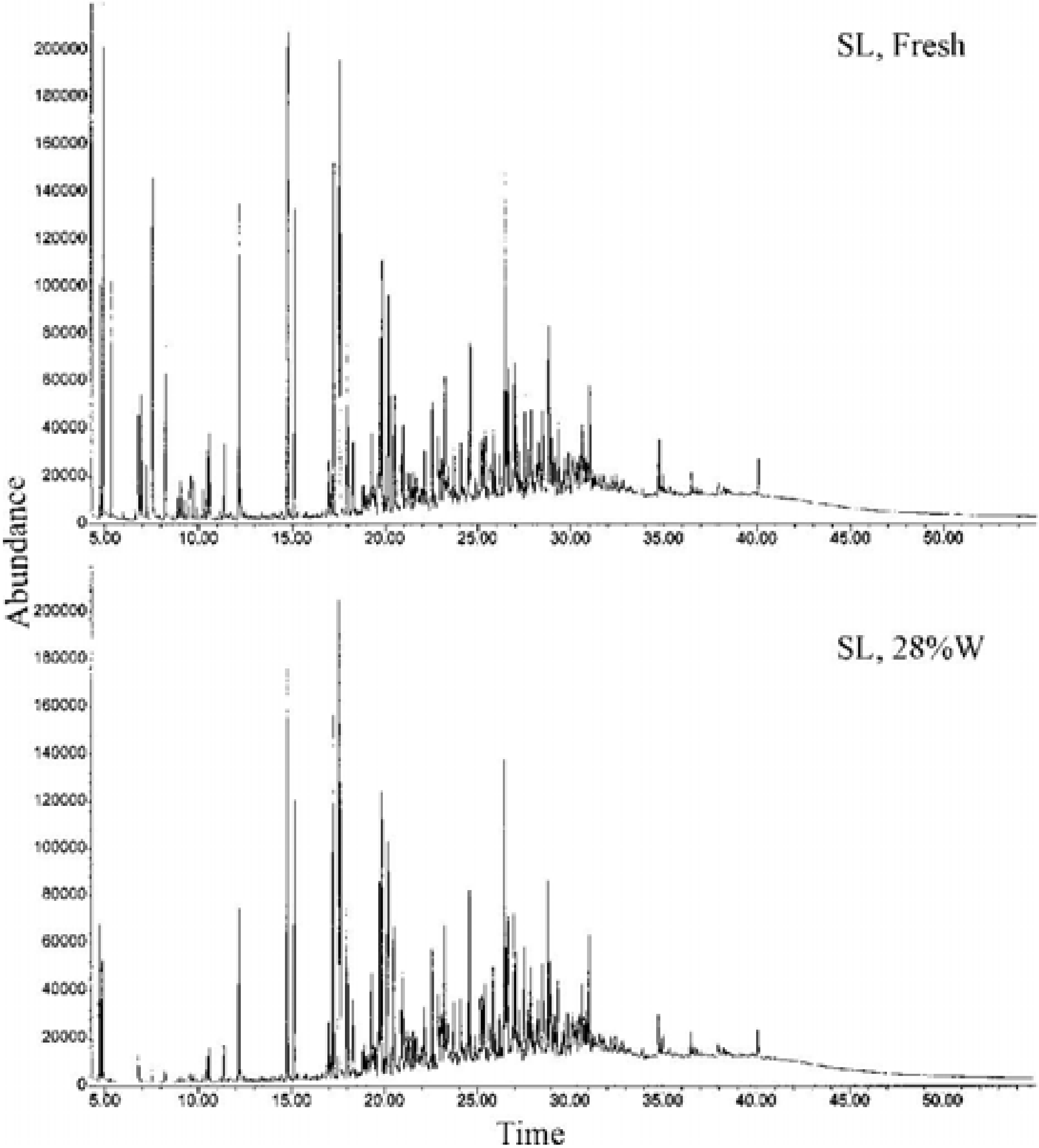


Figure A7-4 Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of South Louisiana crude oil

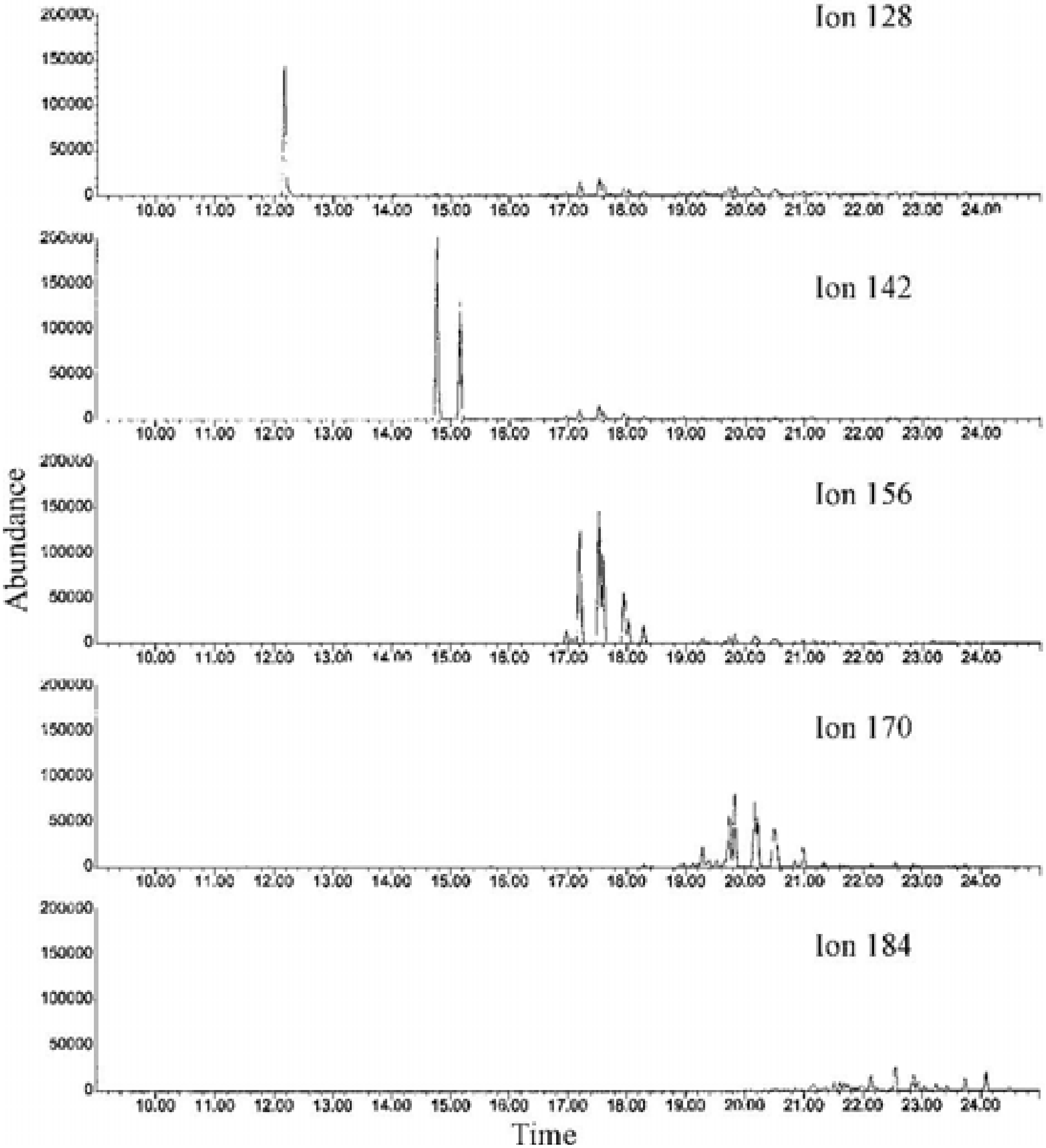


Figure A7-5a Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184) of South Louisiana crude oil

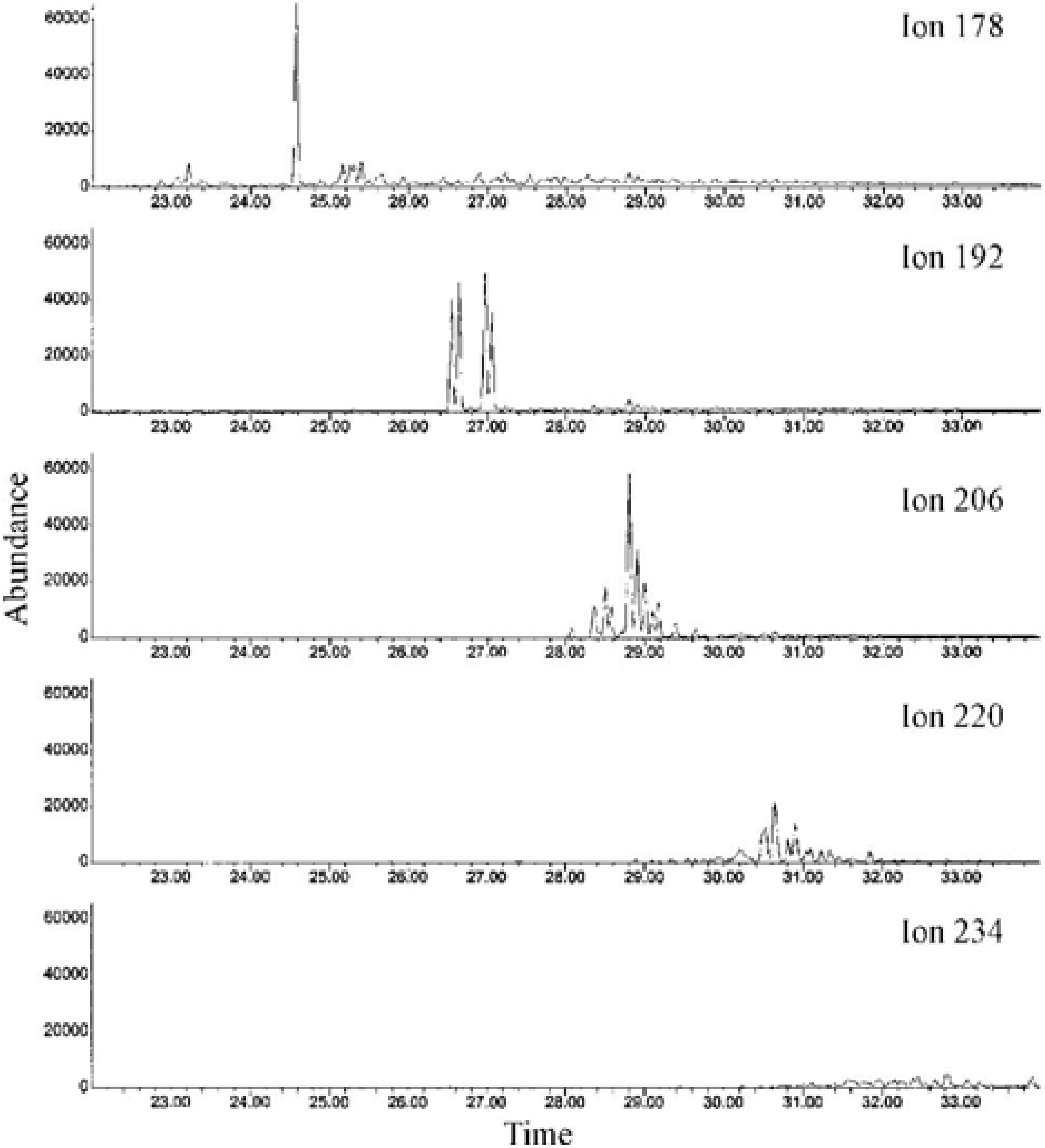


Figure A7-5b Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 178, 192, 206, 220, 234) of South Louisiana crude oil

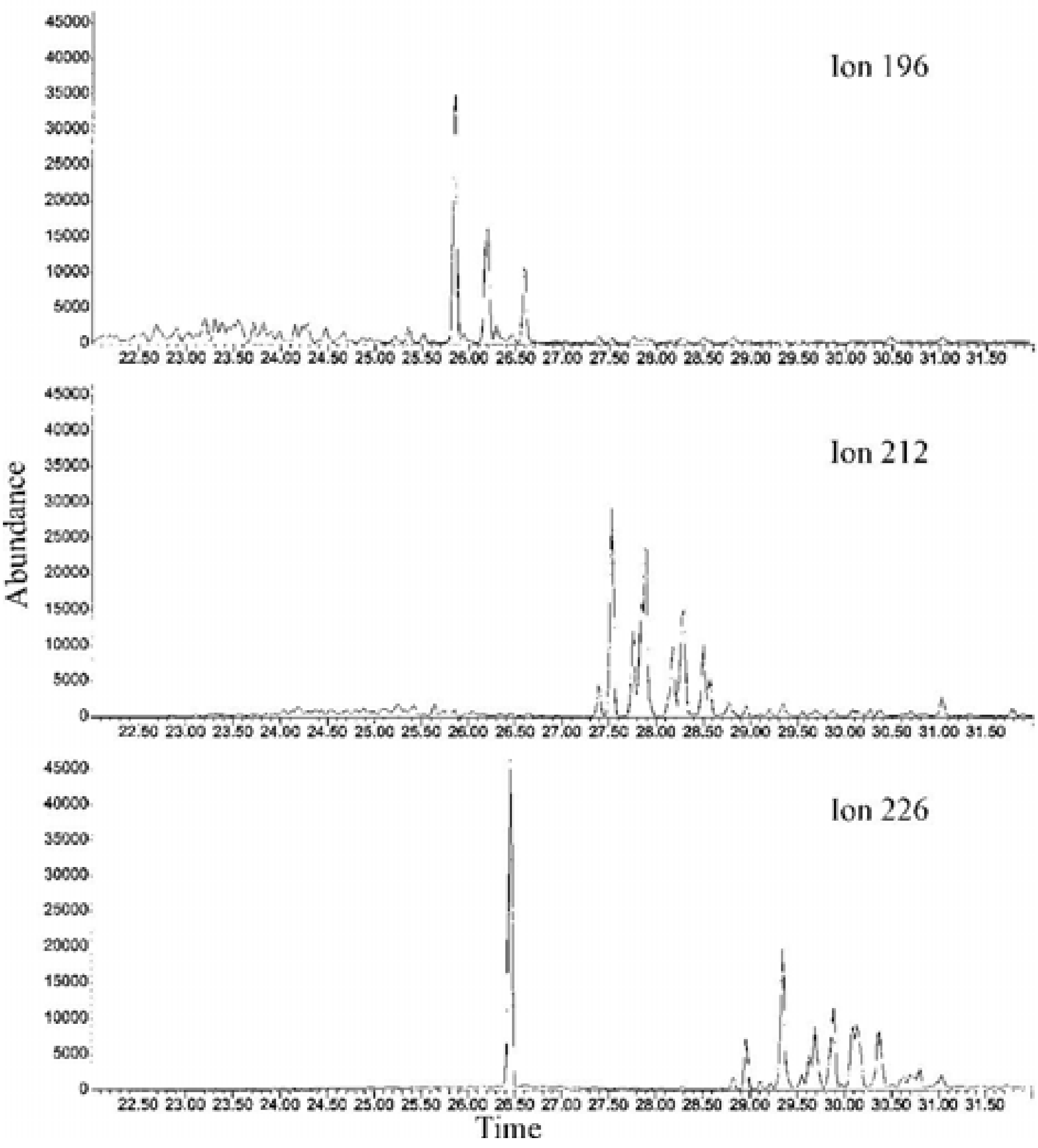


Figure A7-5c Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 198, 212, 226) of South Louisiana crude oil

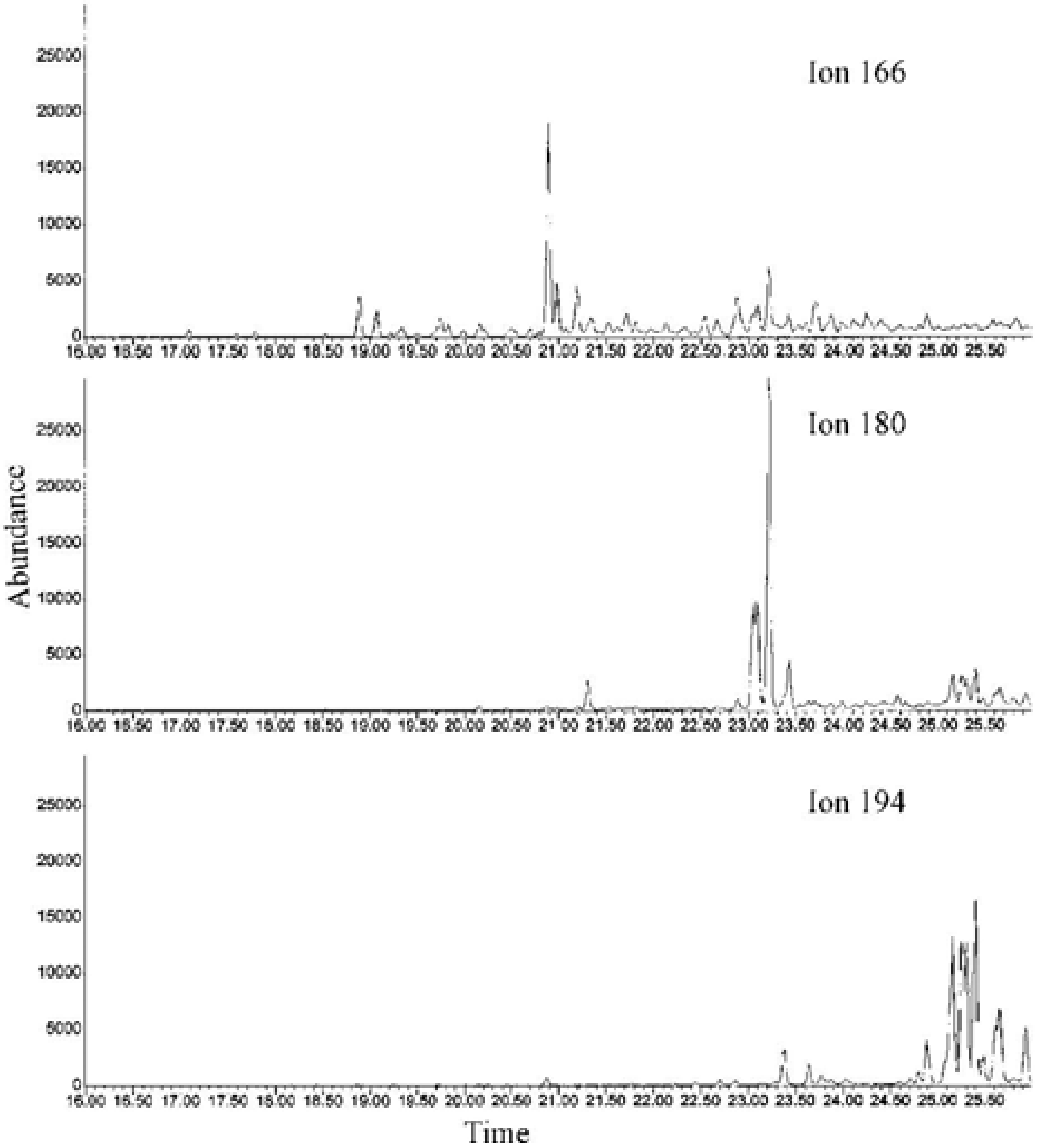


Figure A7-5d Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 166, 180, 194) of South Louisiana crude oil

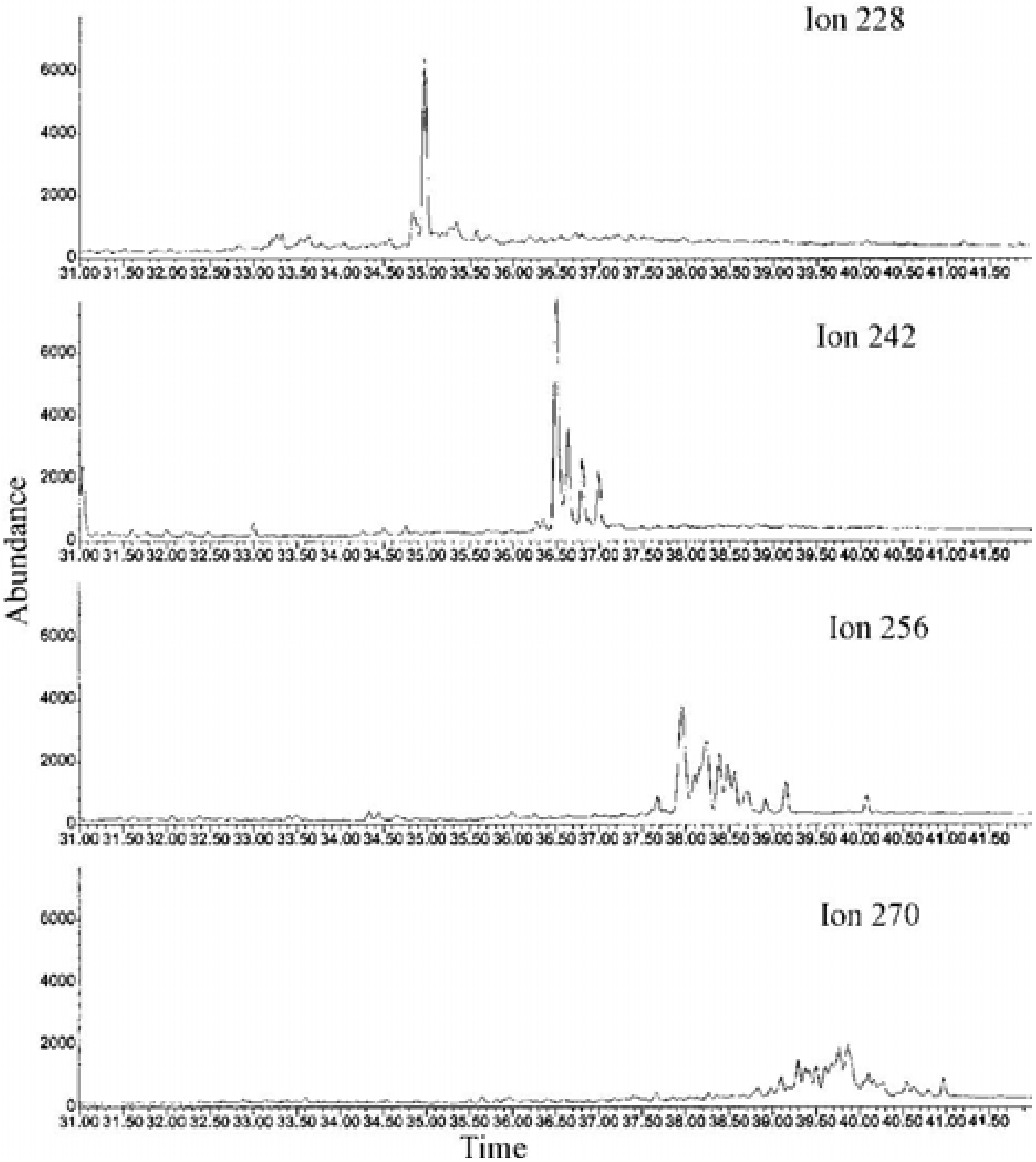


Figure A7-5e Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 228, 242, 256, 270) of South Louisiana crude oil

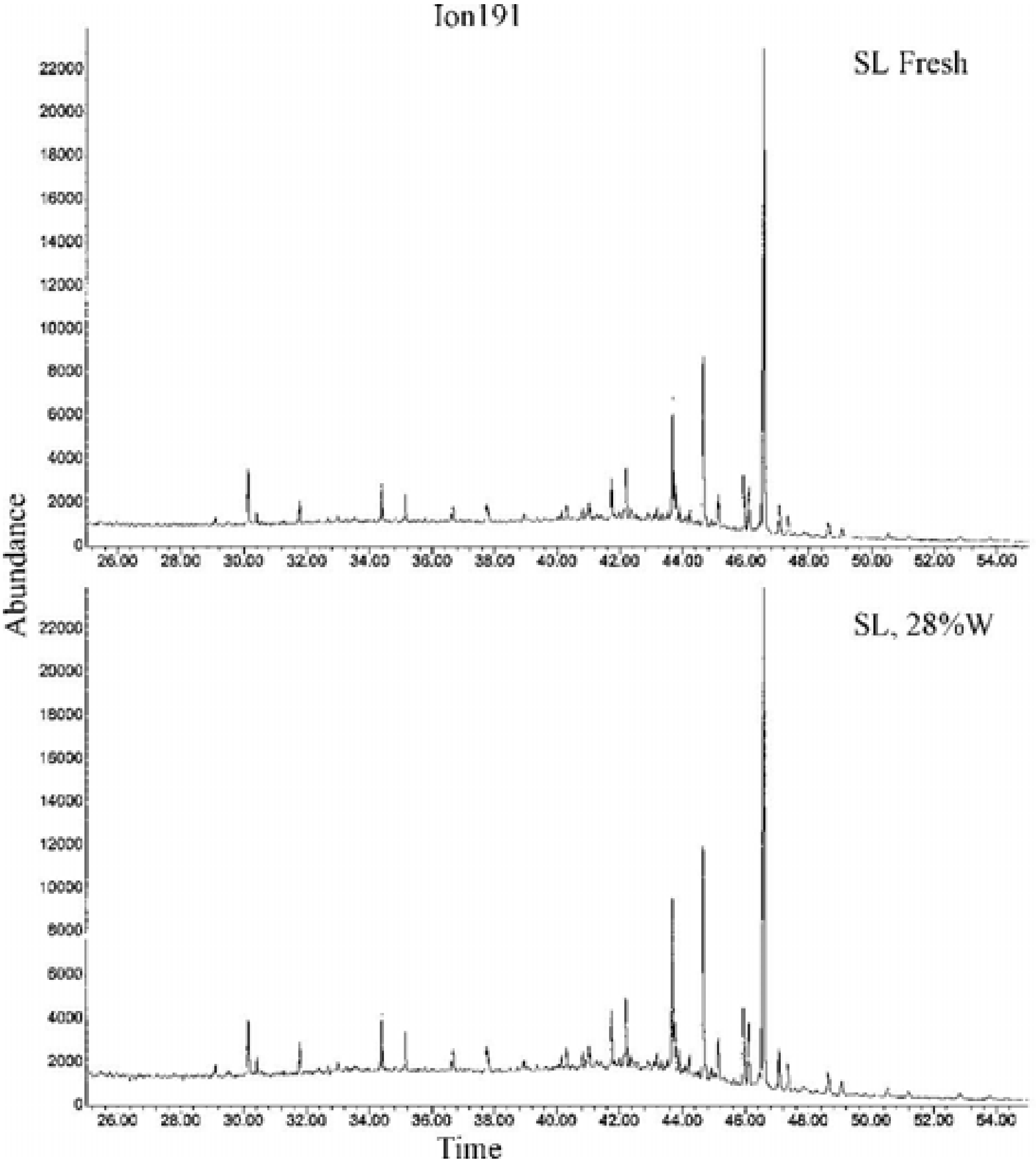


Figure A7-6 GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of South Louisiana crude oil

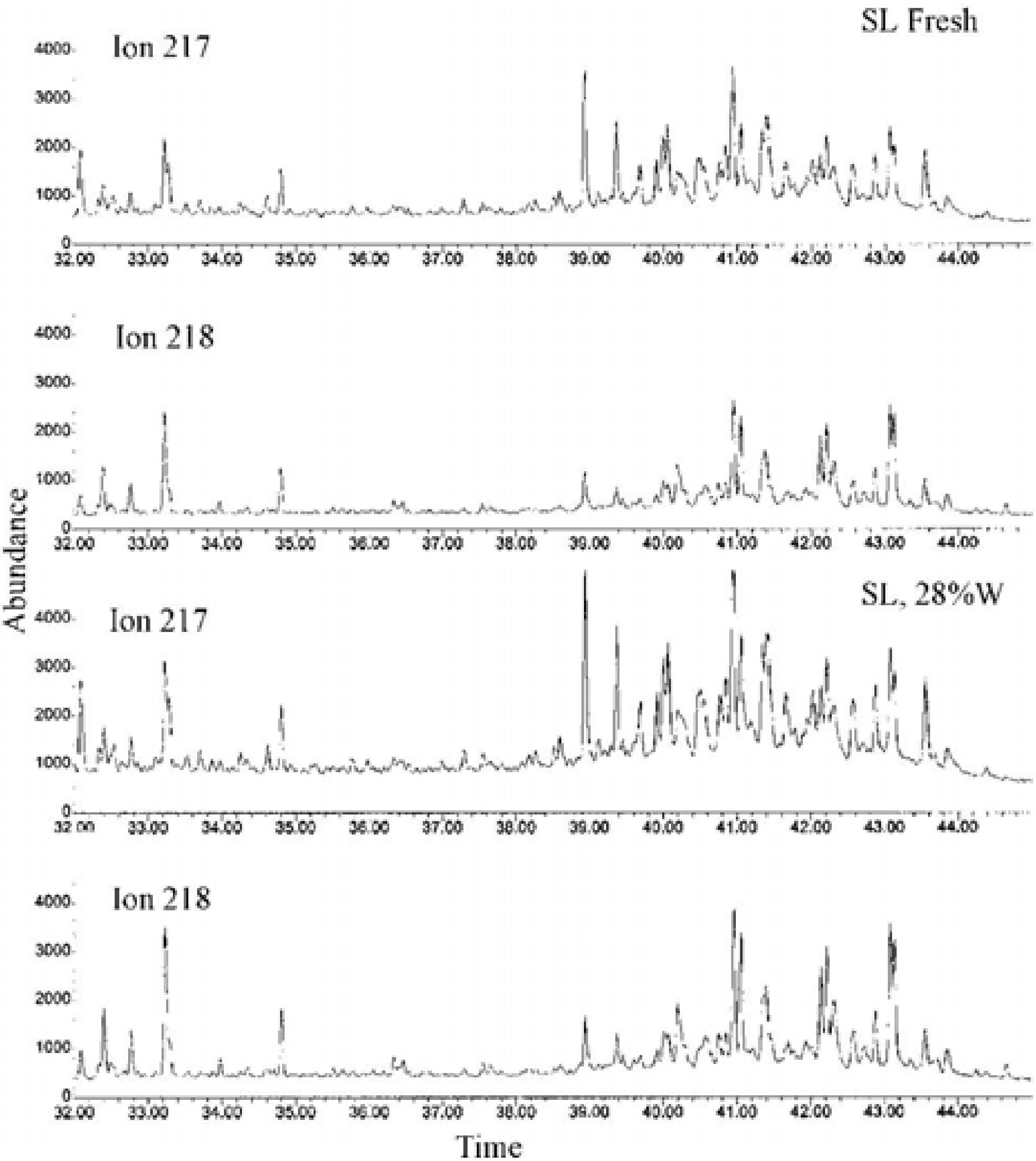


Figure A7-7 GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218) of South Louisiana crude oil

8 GC Chromatograms for West Texas Intermediate Crude Oil

Figure A8-1	GC-FID chromatograms of fraction 1 (F1) for saturates of WestTexas Intermediate crude oil
Figure A8-2	GC-FID chromatograms of fraction 3 (F3) fortotal petroleum hydrocarbons (TPH) of West Texas Intermediate crude oil
Figure A8-3	GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of West Texas Intermediate crude oil
Figure A8-4	Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of West Texas Intermediate crude oil
Figure A8-5	Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184, 178, 192, 206, 220, 234, 198, 212, 226, 166, 180, 194, 228, 242, 256, and 270) of West Texas Intermediate crude oil
Figure A8-6	GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of West Texas Intermediate crude oil
Figure A8-7	GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218) of West Texas Intermediate crude oil

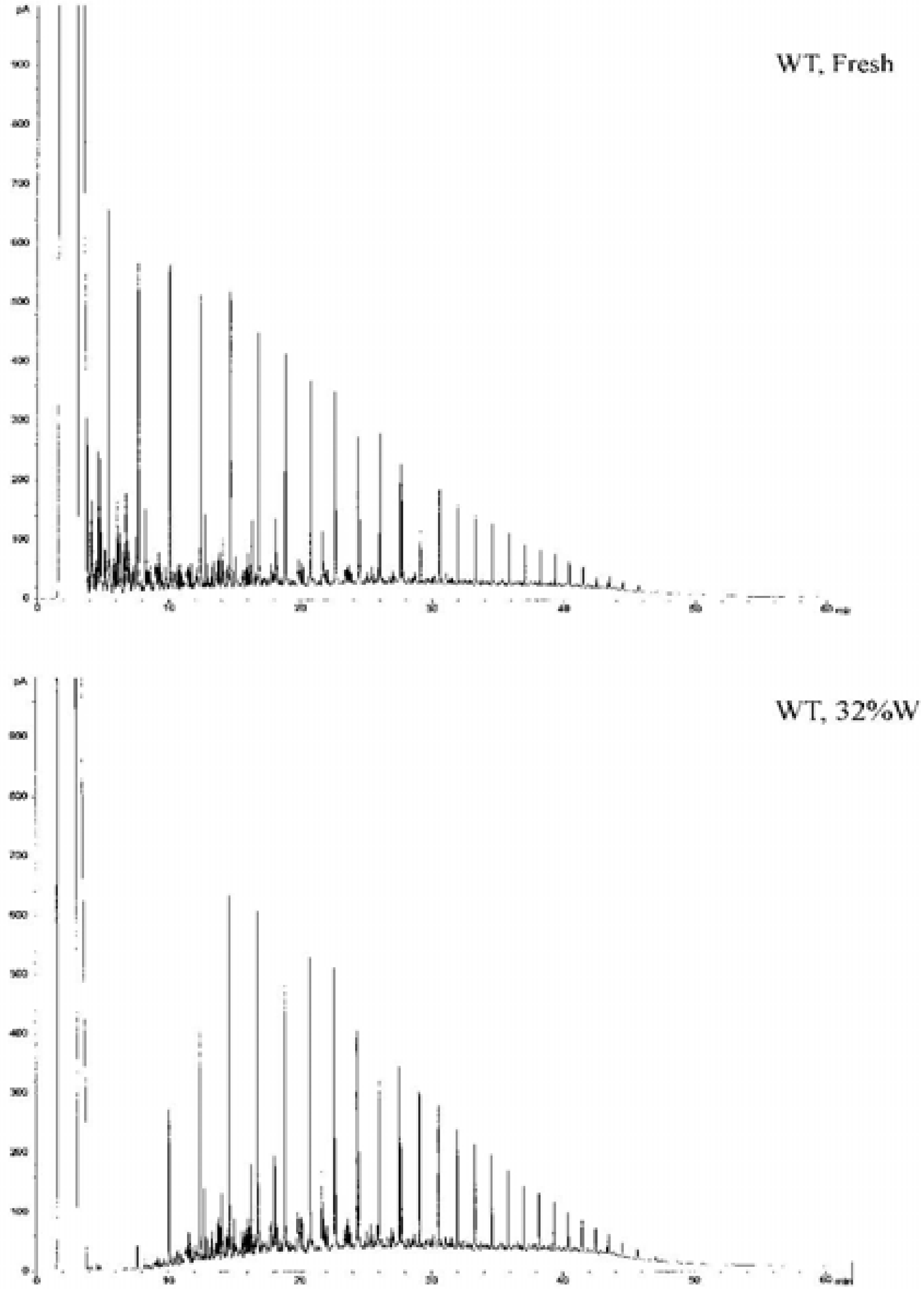


Figure A8-1 GC-FID chromatograms of fraction 1 (F1) for saturates of West Texas Intermediate crude oil

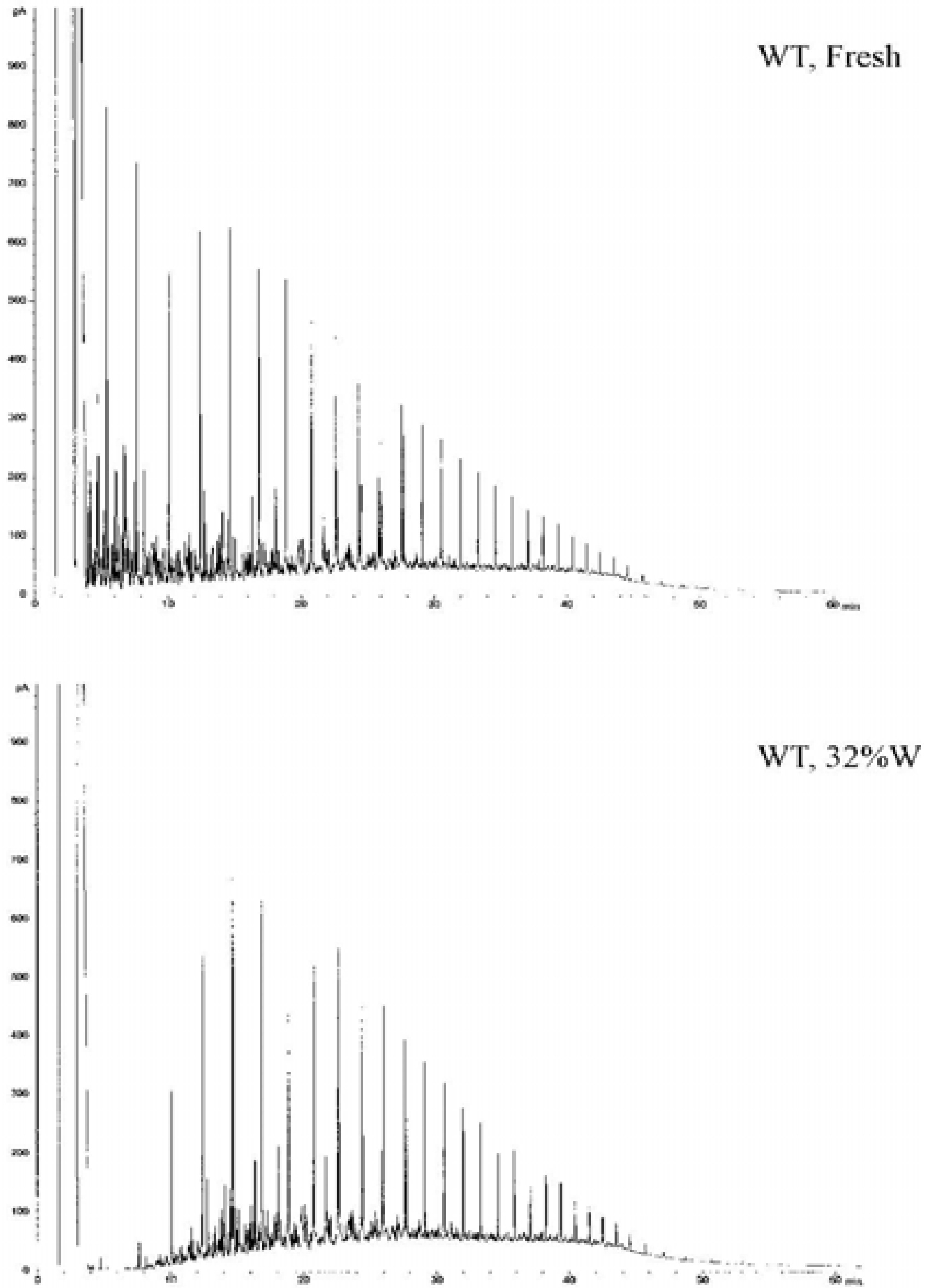


Figure A8-2 GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of West Texas Intermediate crude oil

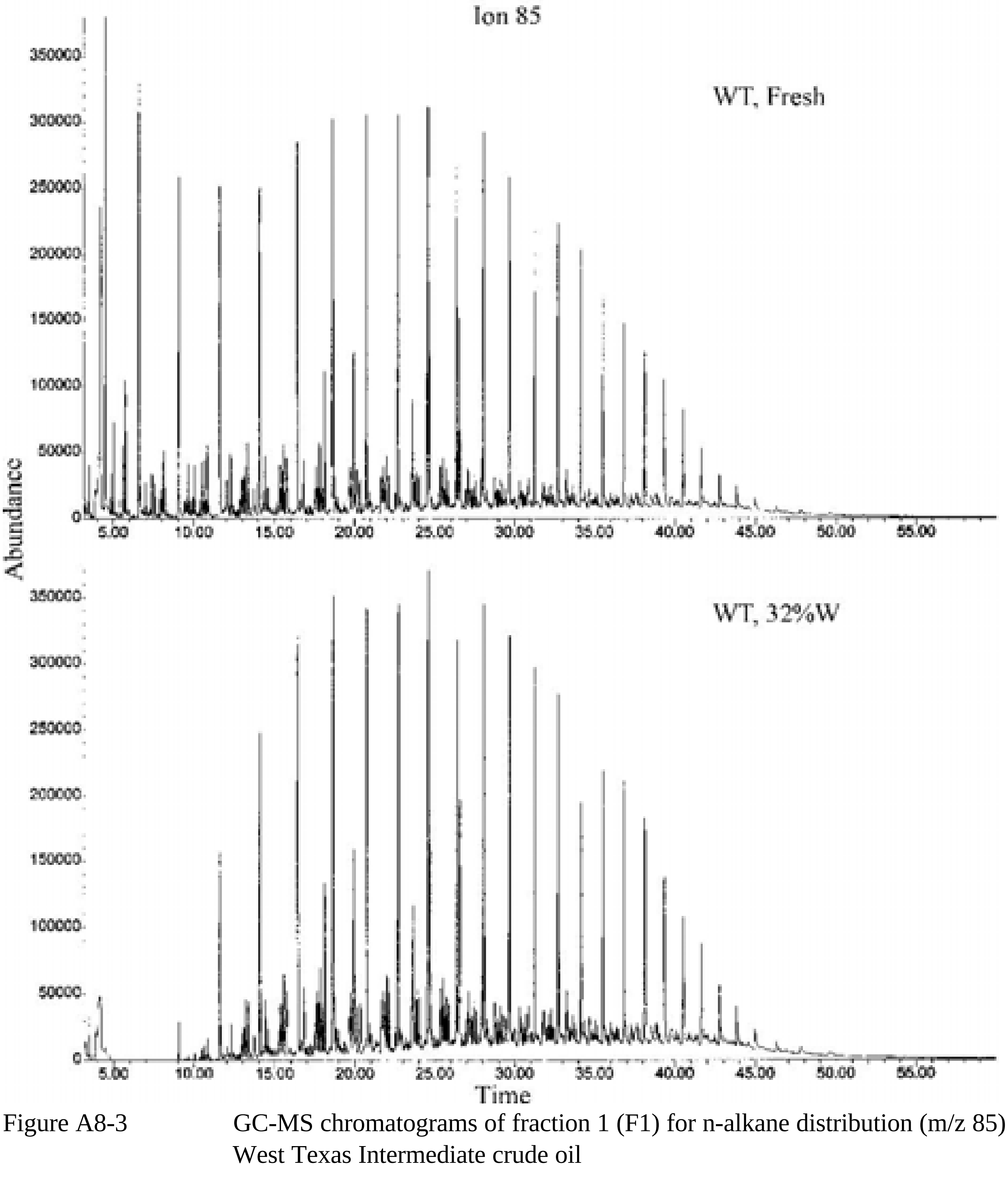


Figure A8-3 GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of West Texas Intermediate crude oil

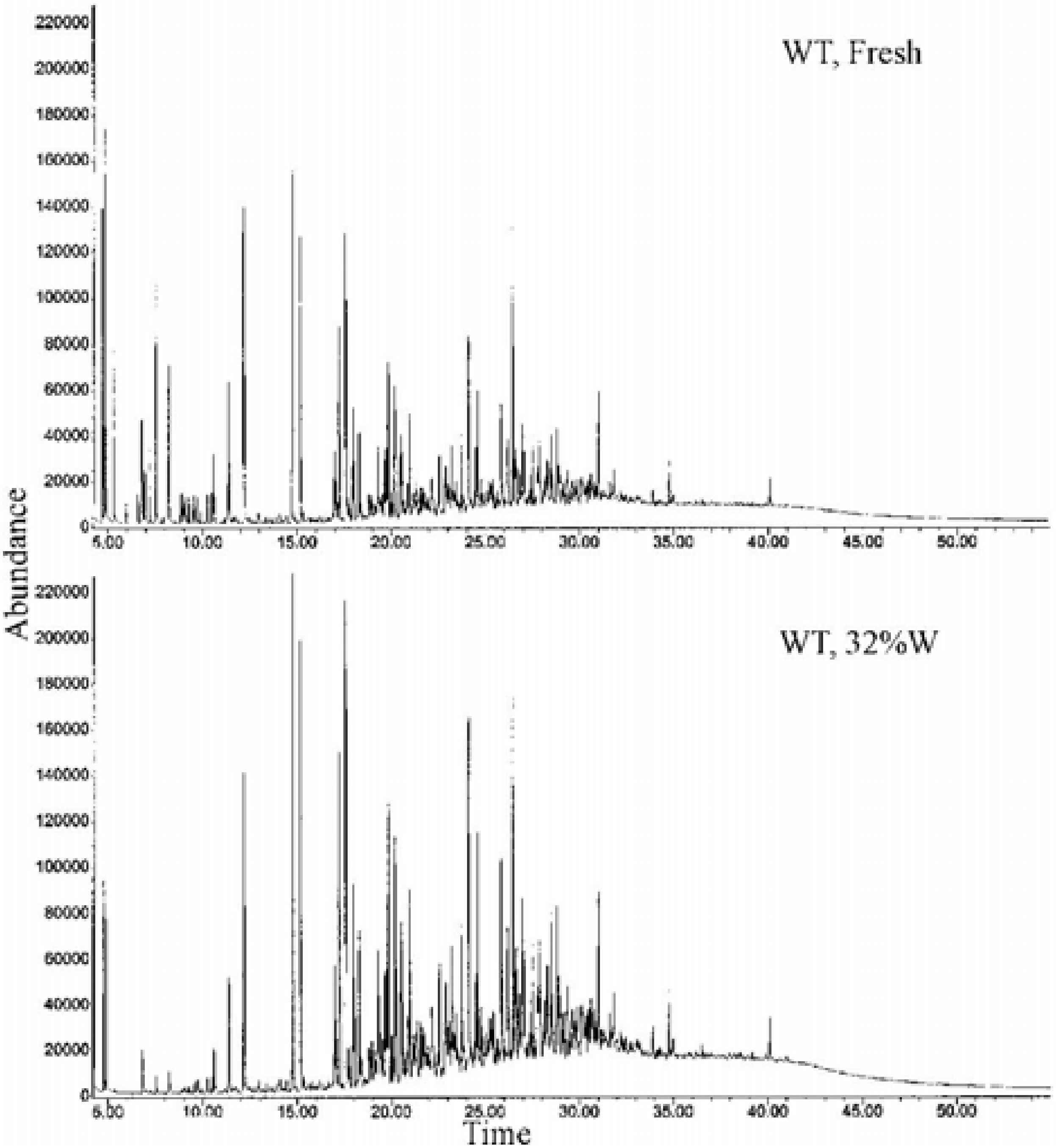


Figure A8-4 Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of West Texas Intermediate crude oil

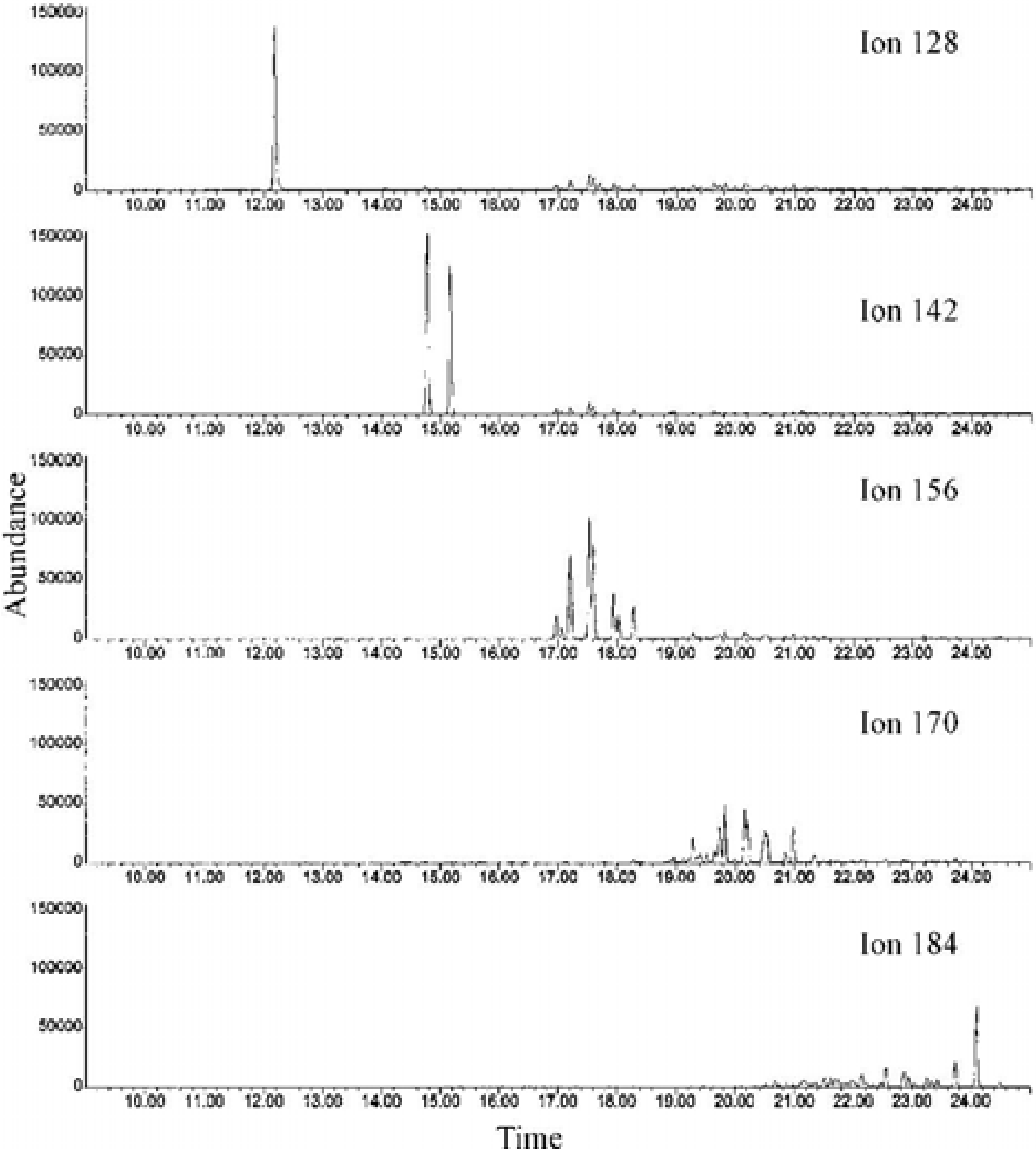


Figure A8-5a Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184) of West Texas Intermediate crude oil

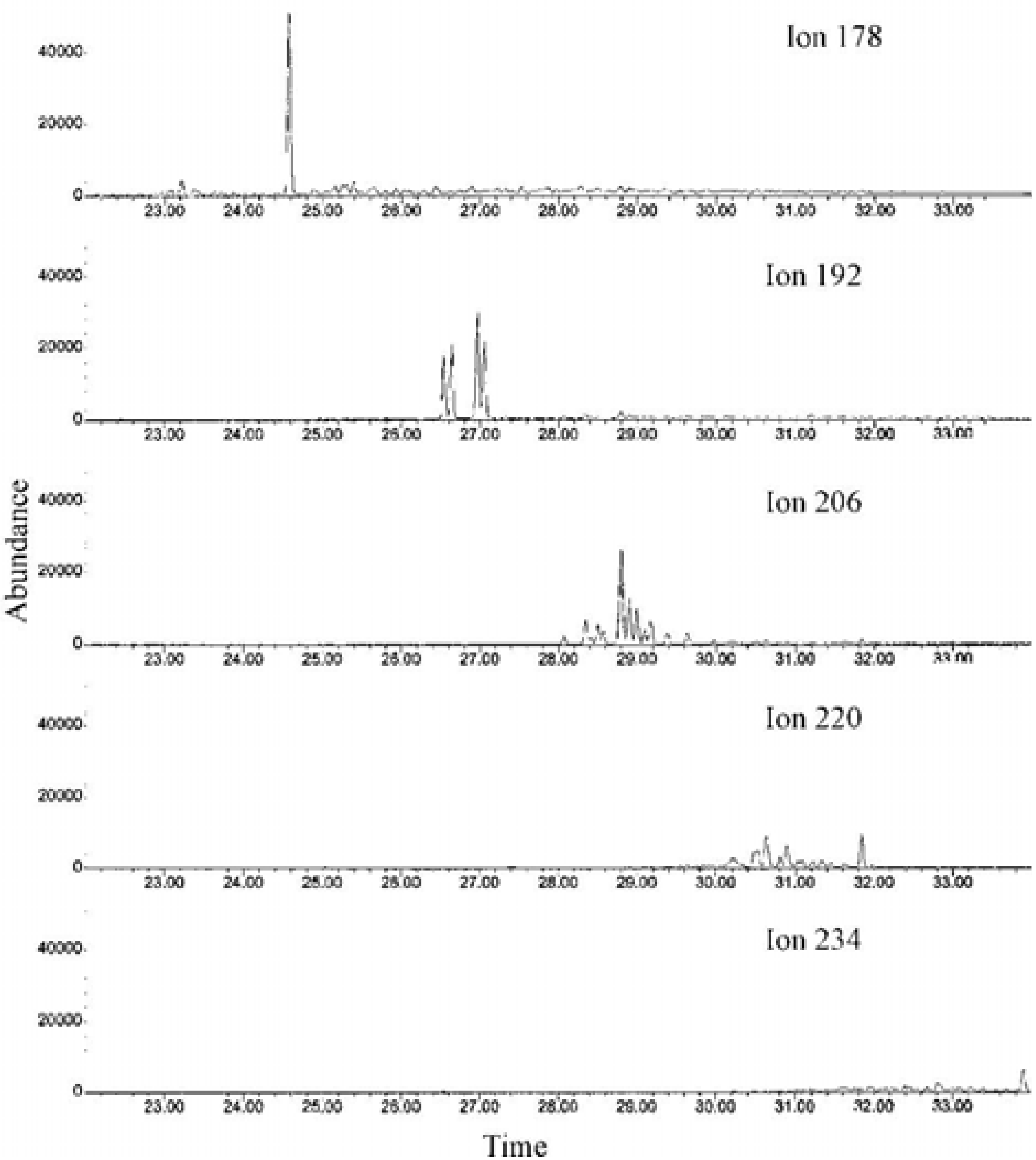


Figure A8-5b Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 178, 192, 206, 220, 234) of West Texas Intermediate crude oil

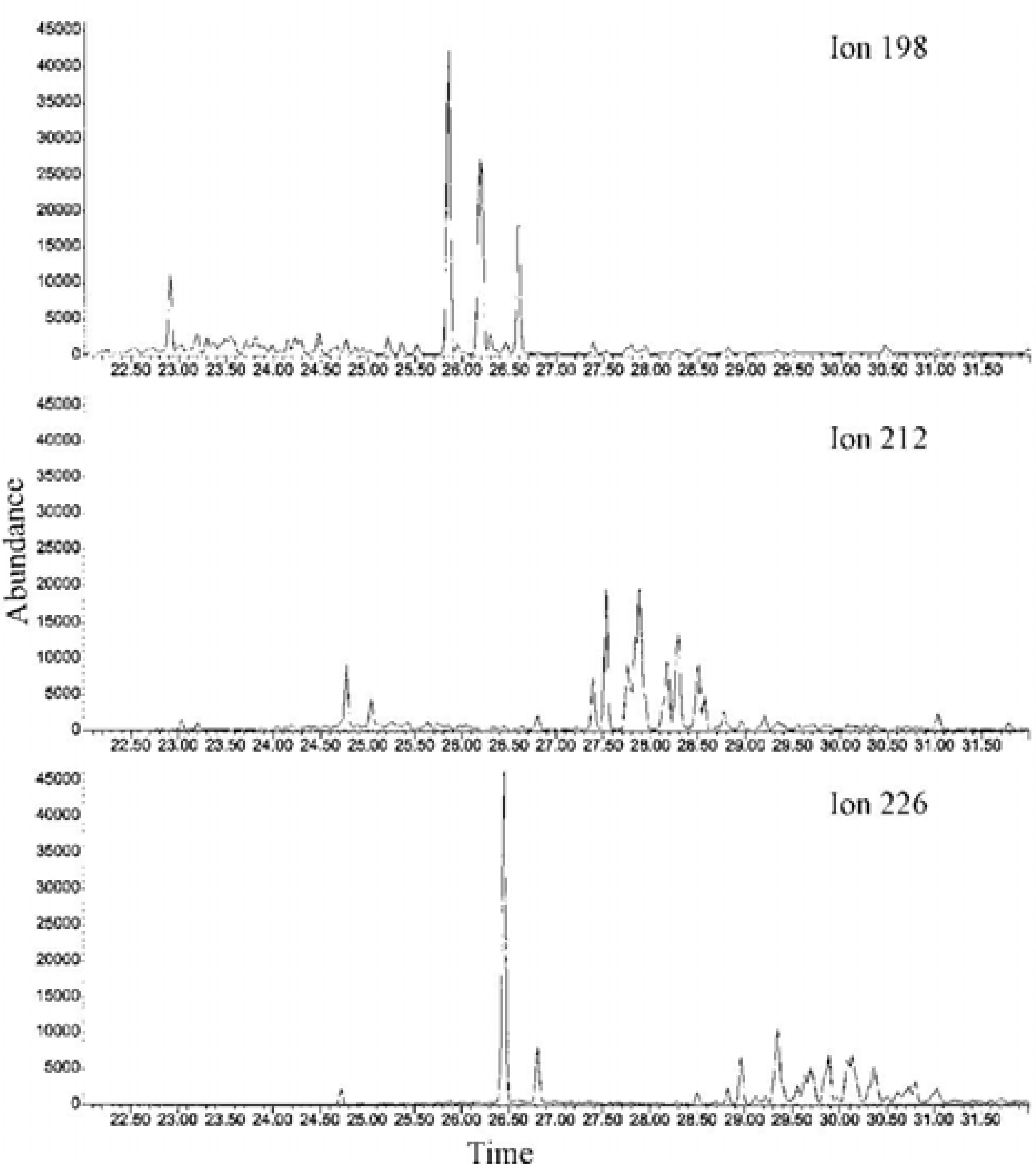


Figure A8-5c Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z 198, 212, 226) of West Texas Intermediate crude oil

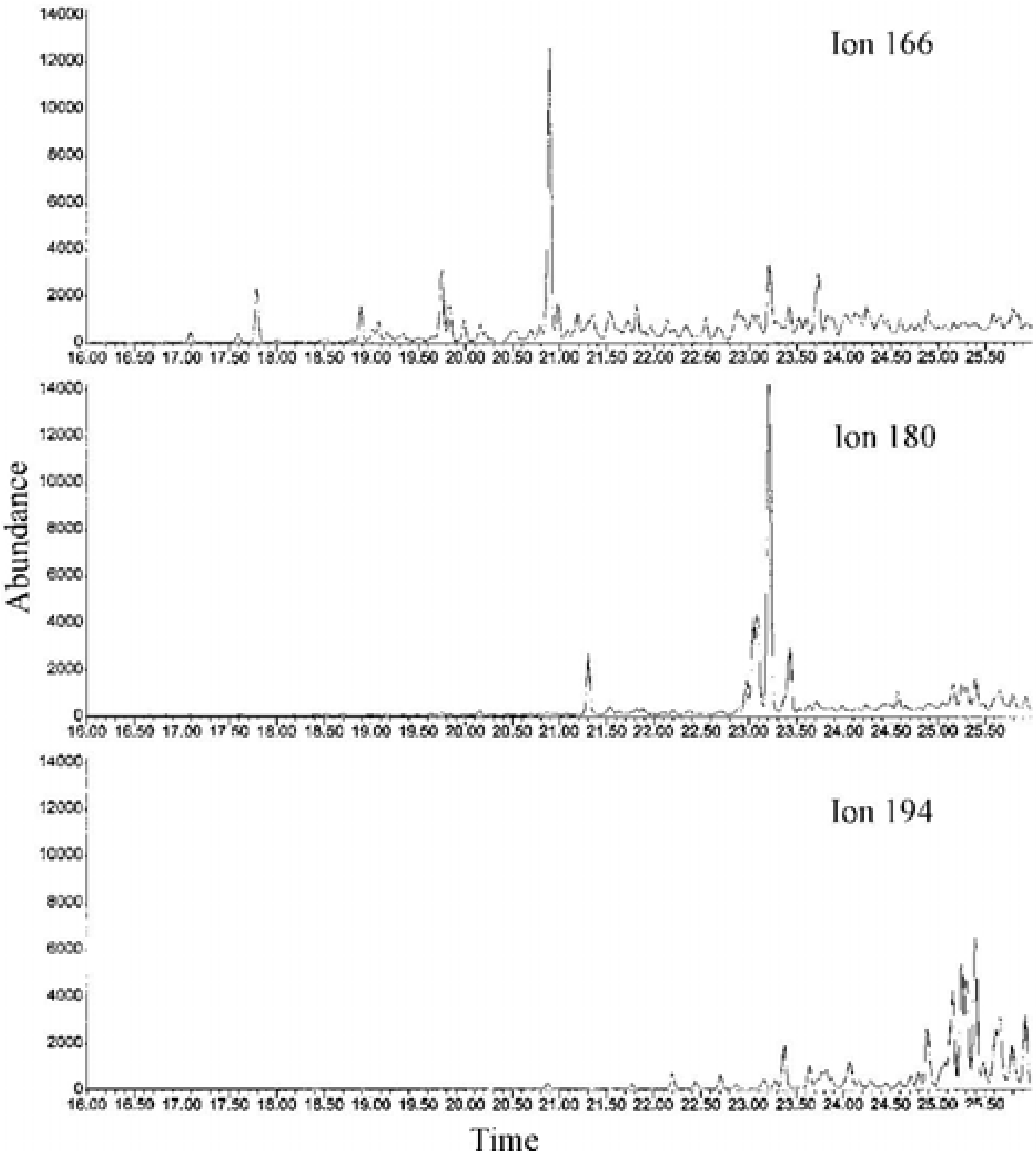


Figure A8-5d Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 166, 180, 194) of West Texas Intermediate crude oil

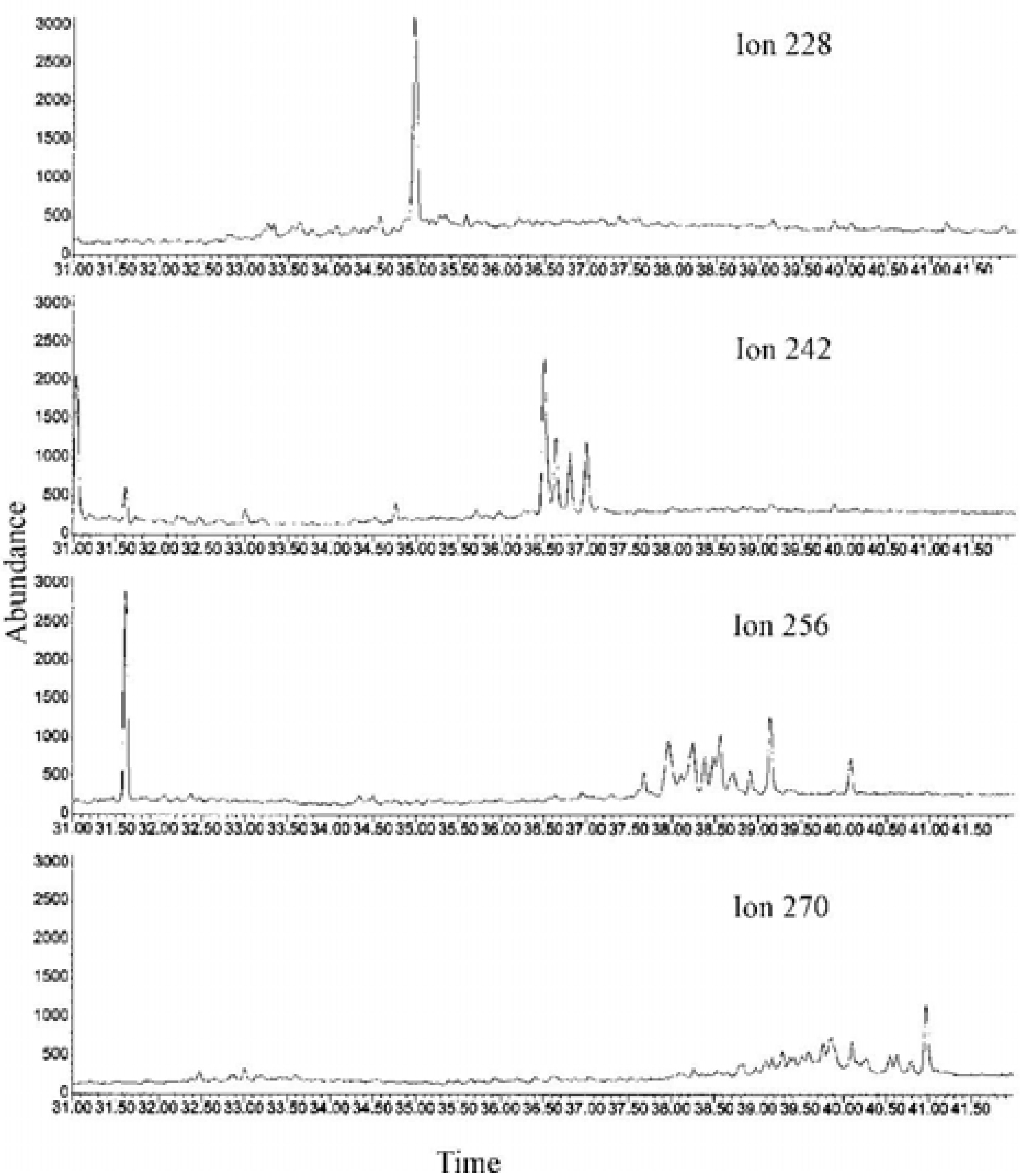


Figure A8-5e Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 228, 242, 256, 270) of West Texas Intermediate crude oil

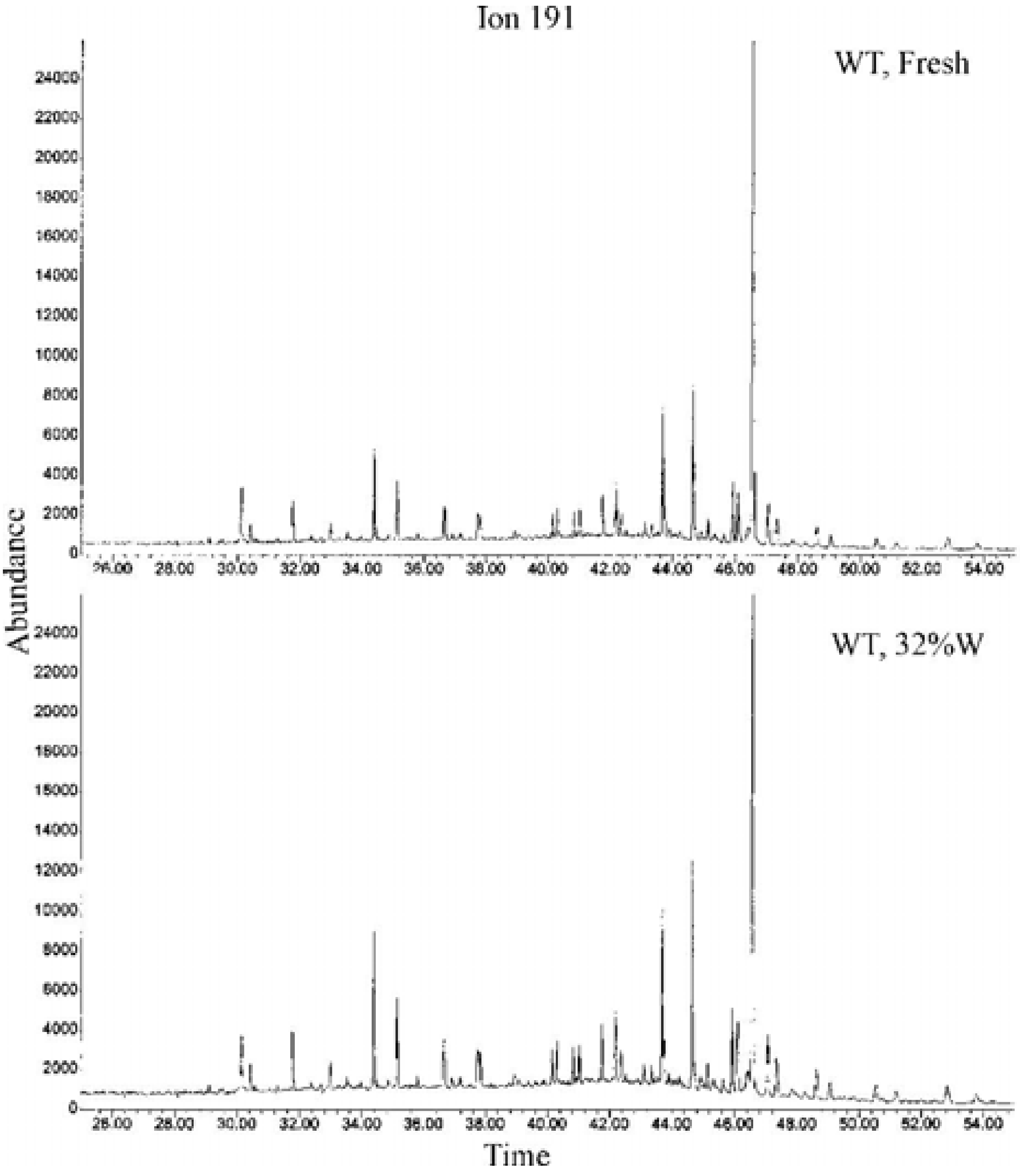


Figure A8-6 GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of West Texas Intermediate crude oil

9 GC Chromatograms for Fuel Oil Number 2

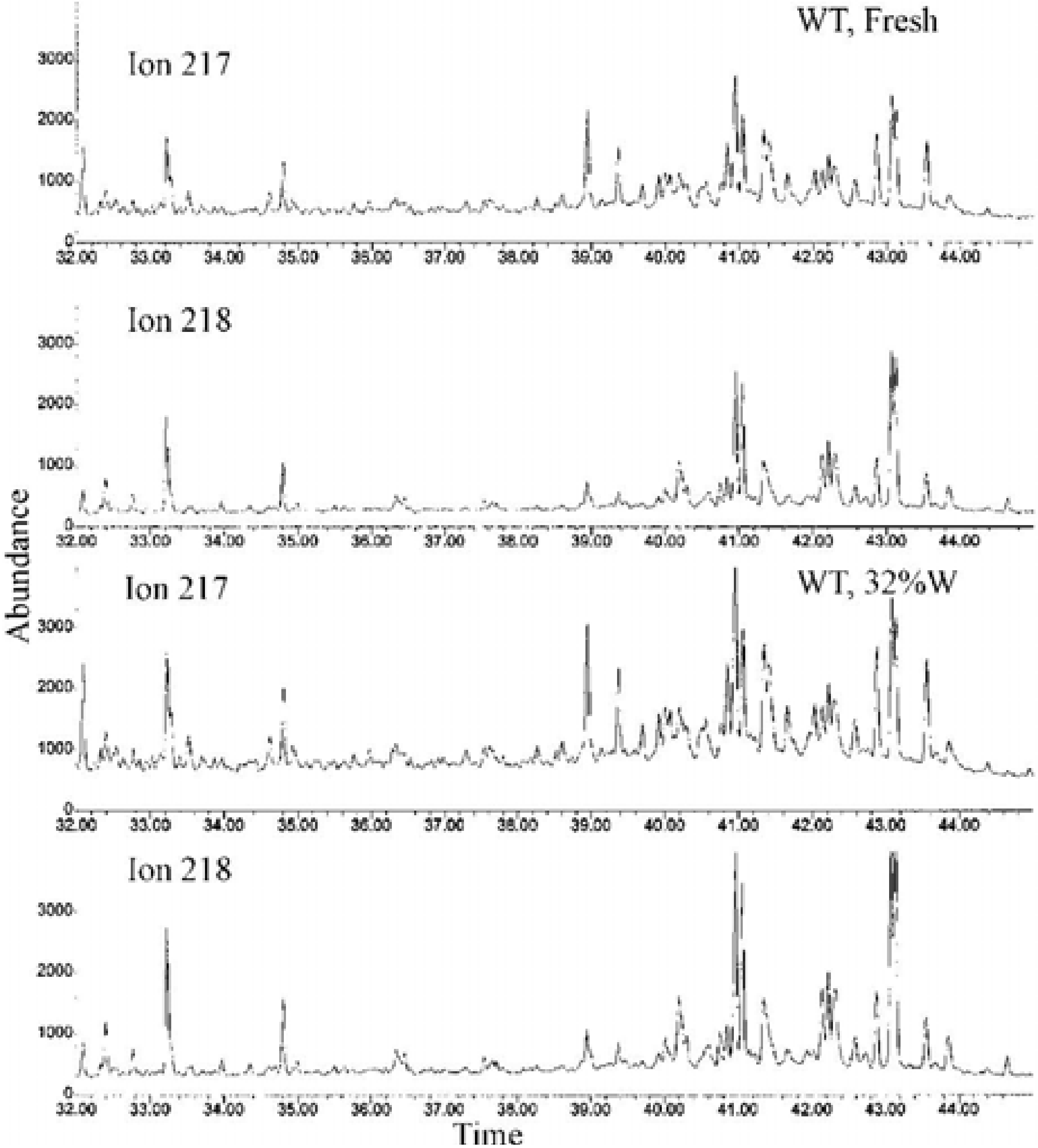


Figure A8-7 GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218) of West Texas Intermediate crude oil

Figure A9-1 GC-FID chromatograms of fraction 1 (F1) for saturates of Fuel Oil No. 2

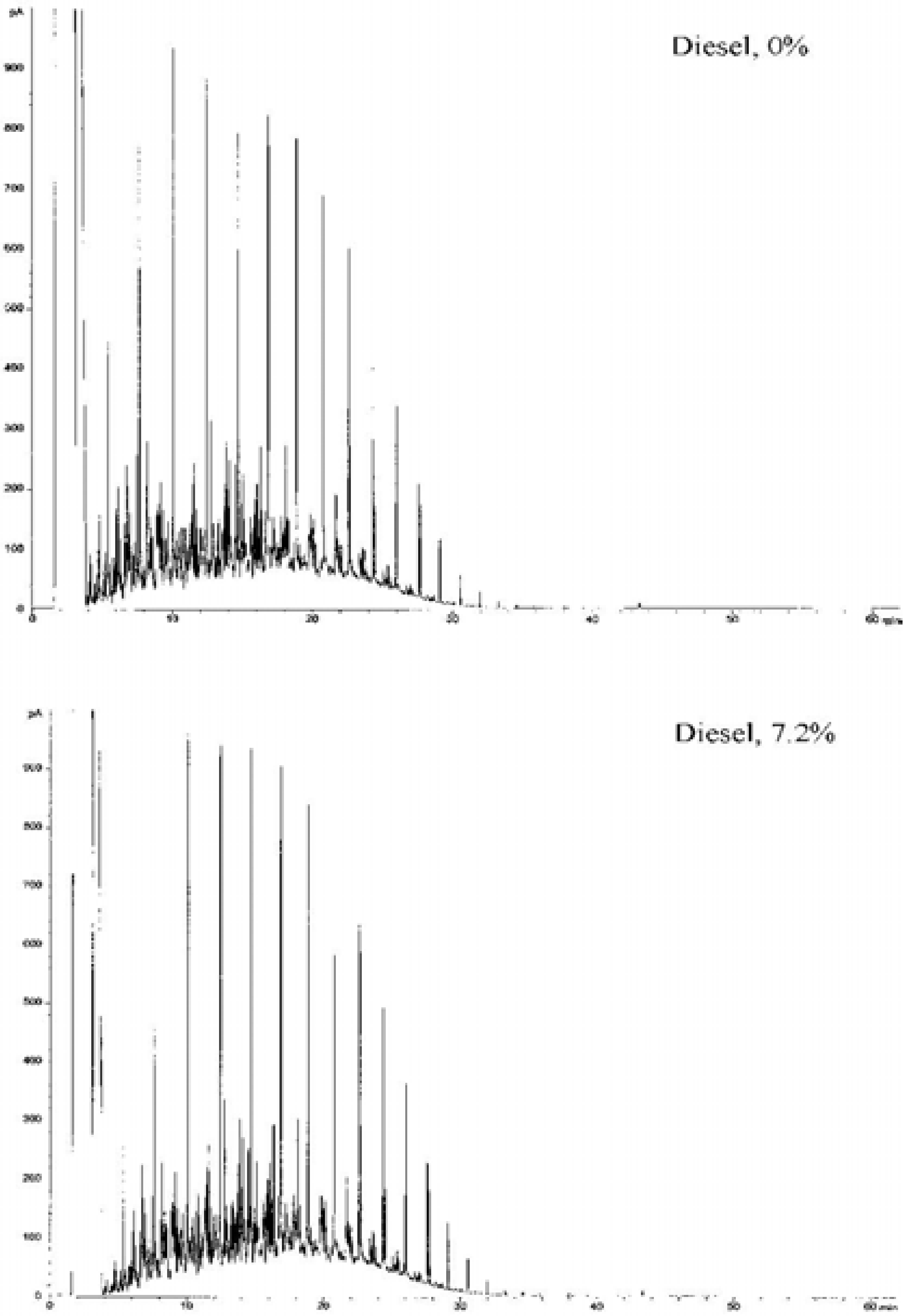


Figure A9-1a GC-FID chromatograms of fraction 1 (F1) for saturates of Fuel Oil No. 2

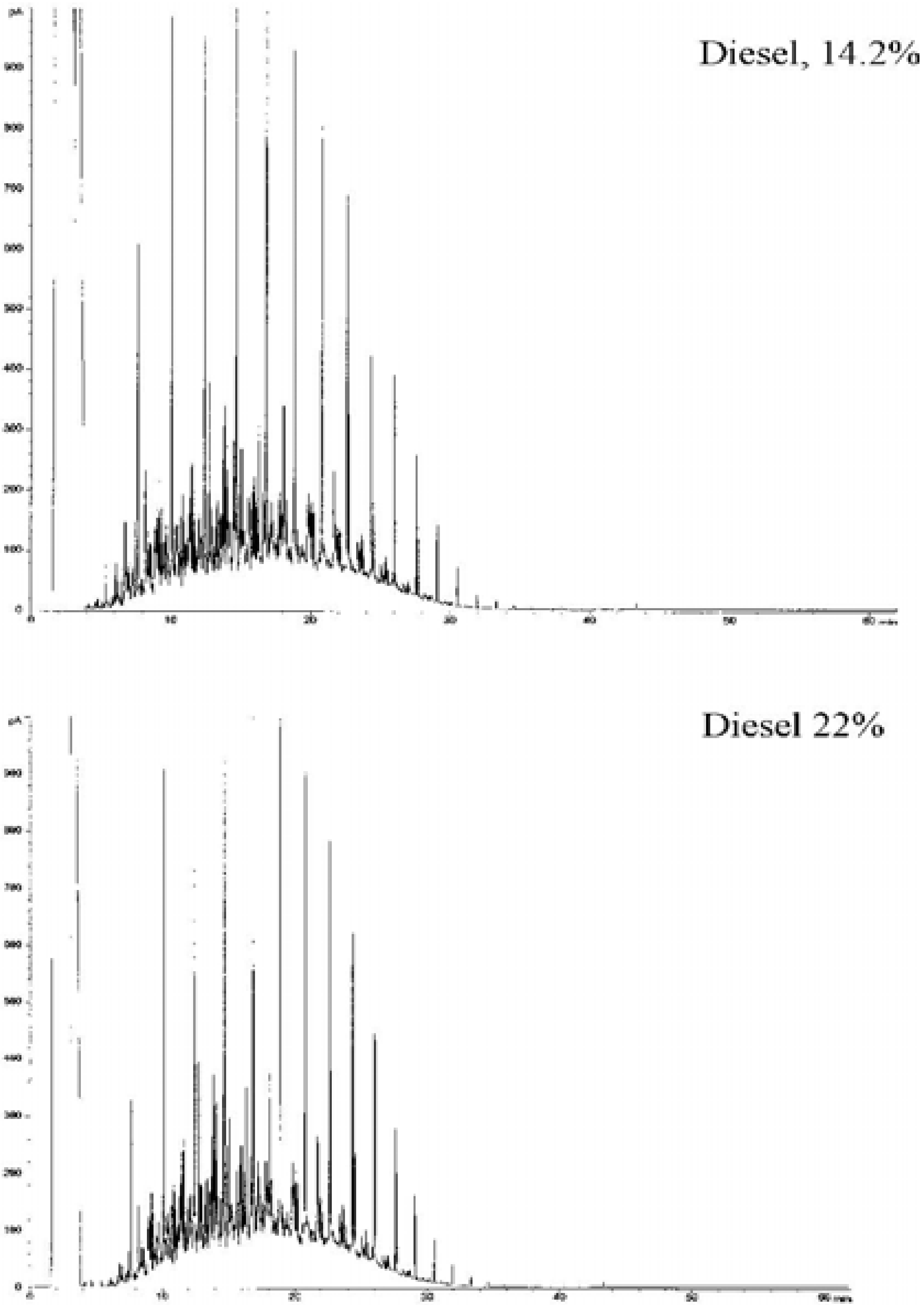


Figure A9-1b GC-FID chromatograms of fraction 1 (F1) for saturates of Fuel Oil No. 2

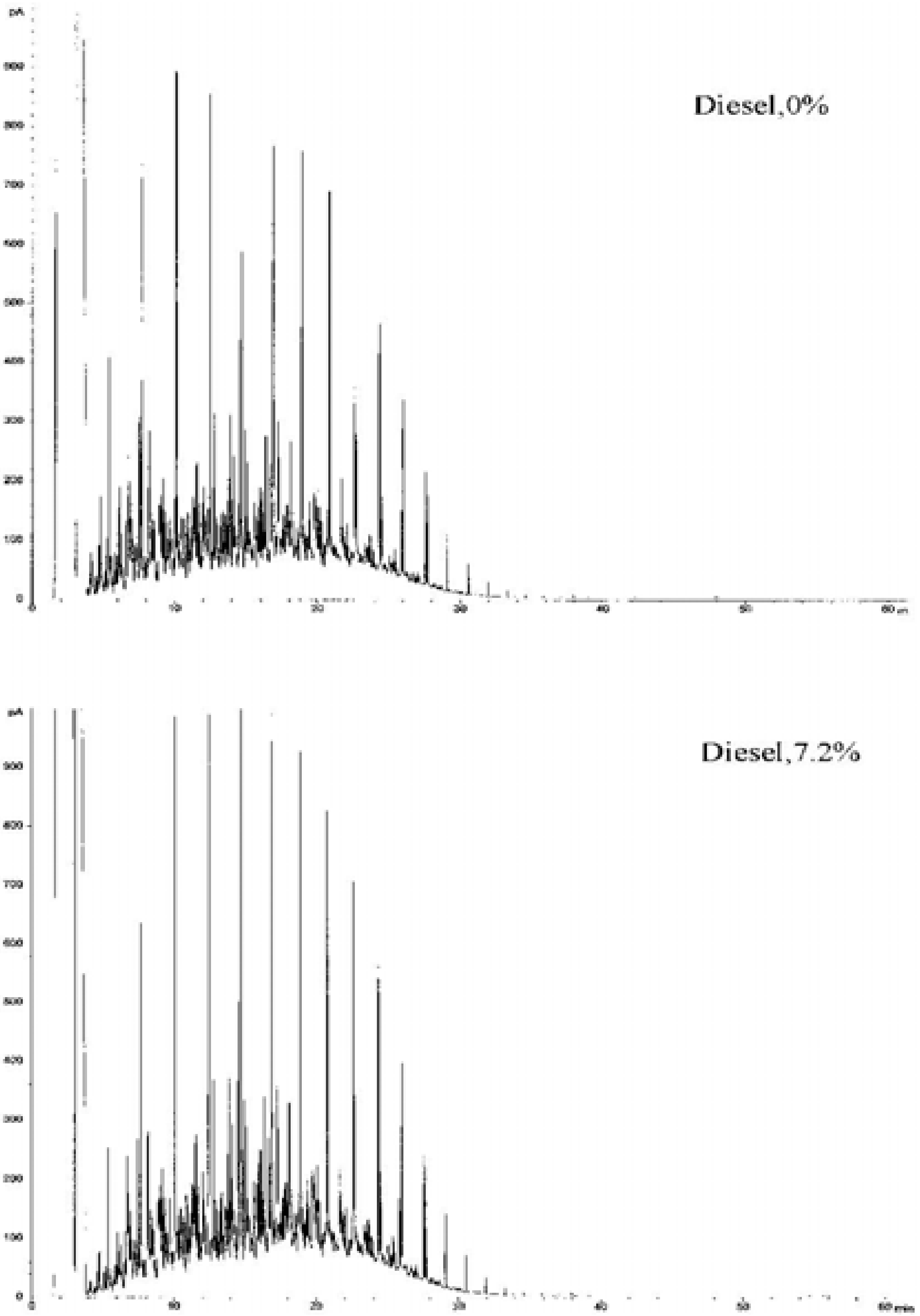


Figure A9-2a GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of of Fuel Oil No. 2

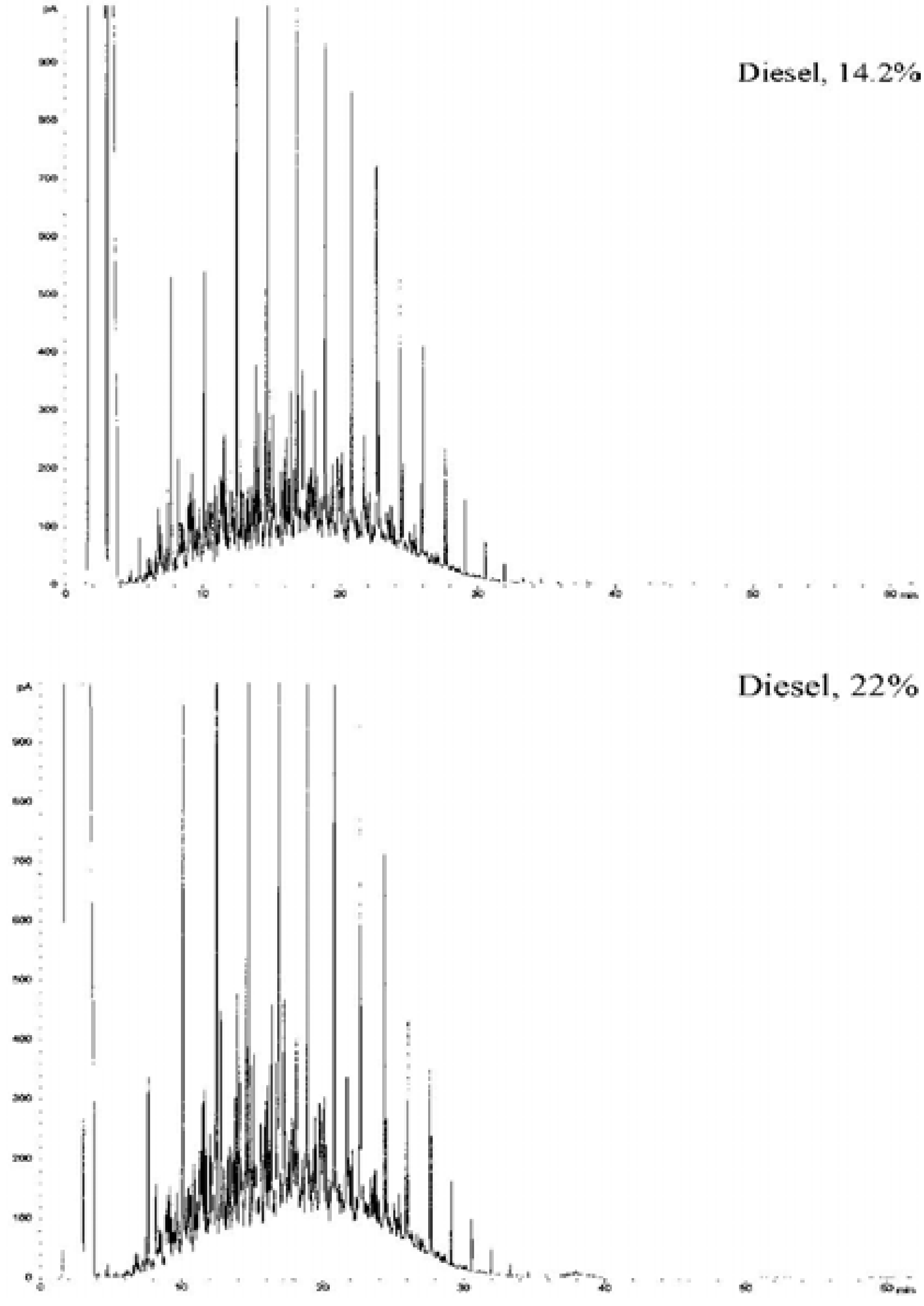


Figure A9-2b GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of of Fuel Oil No. 2

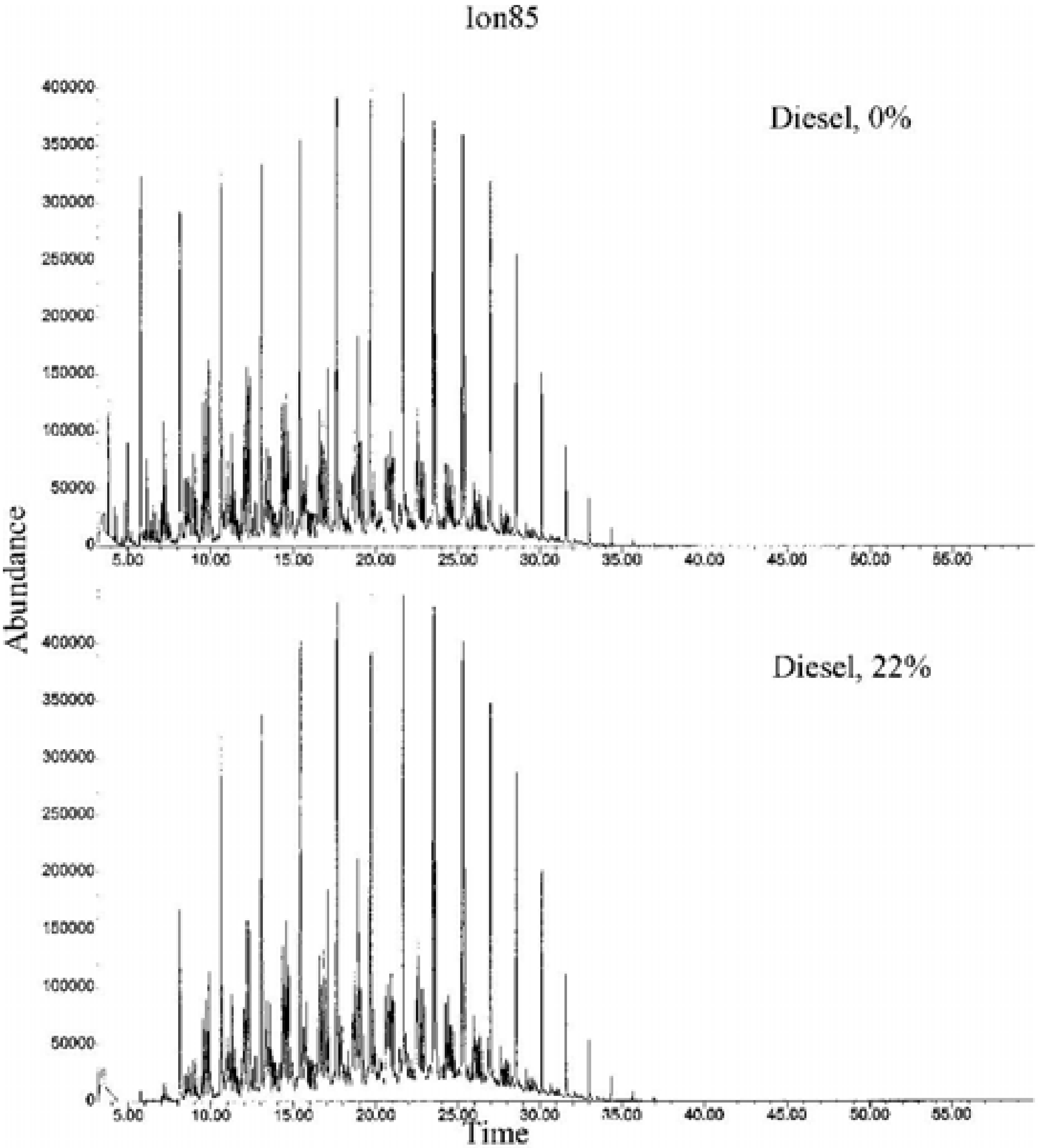


Figure A9-3 GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of Fuel Oil No. 2

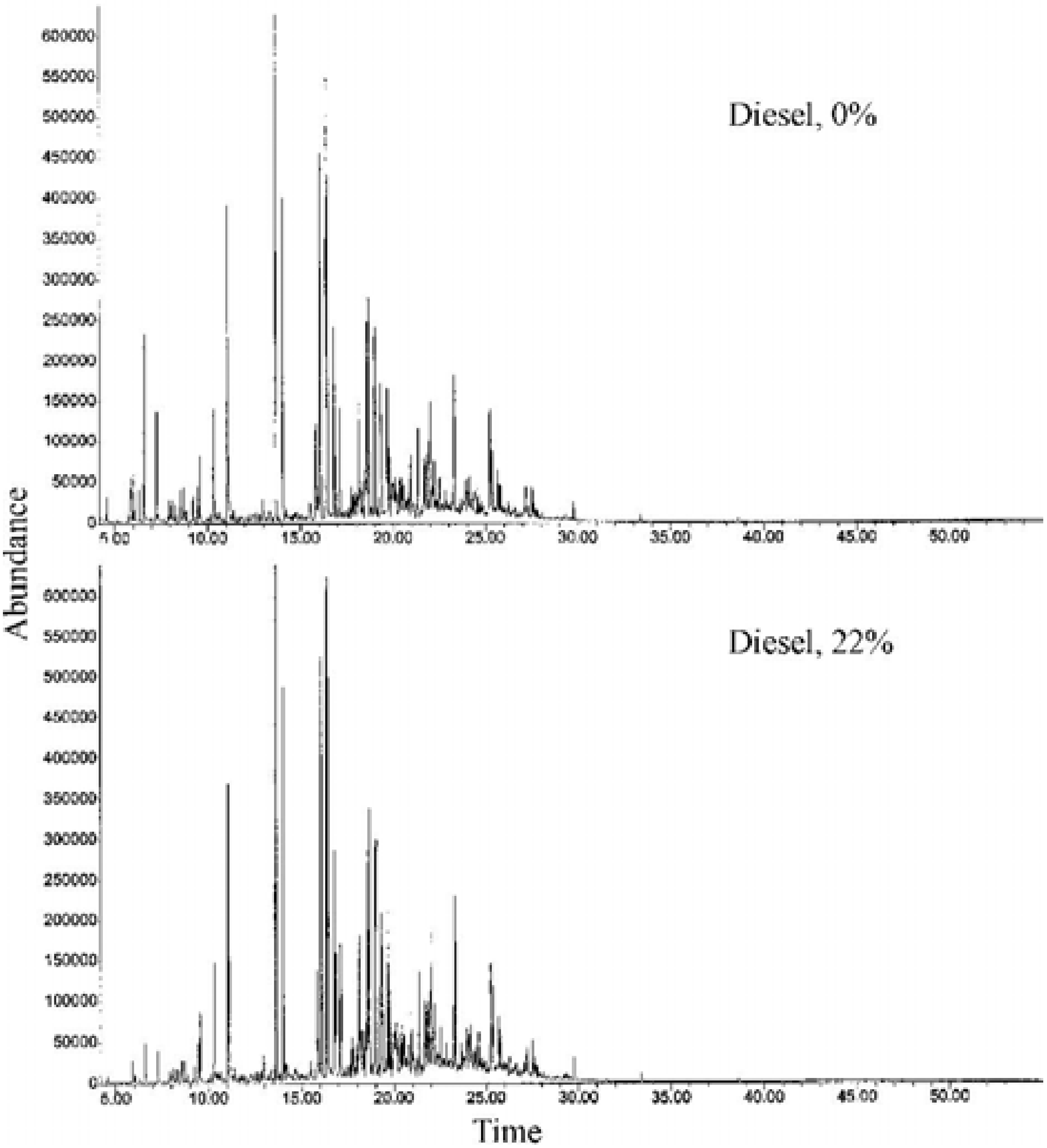


Figure A9-4 Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of Fuel Oil No. 2

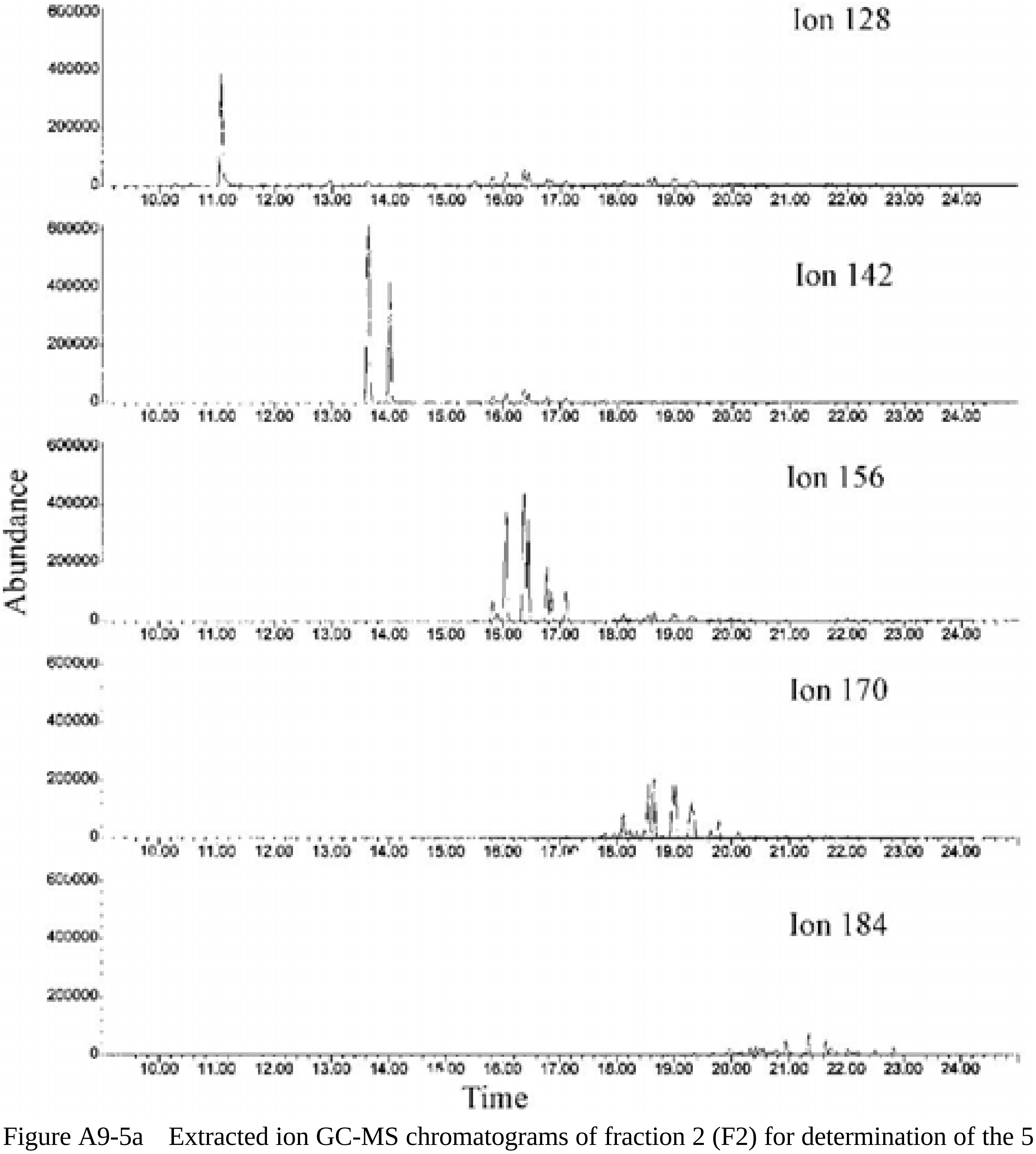


Figure A9-5a Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184) of Fuel Oil No. 2

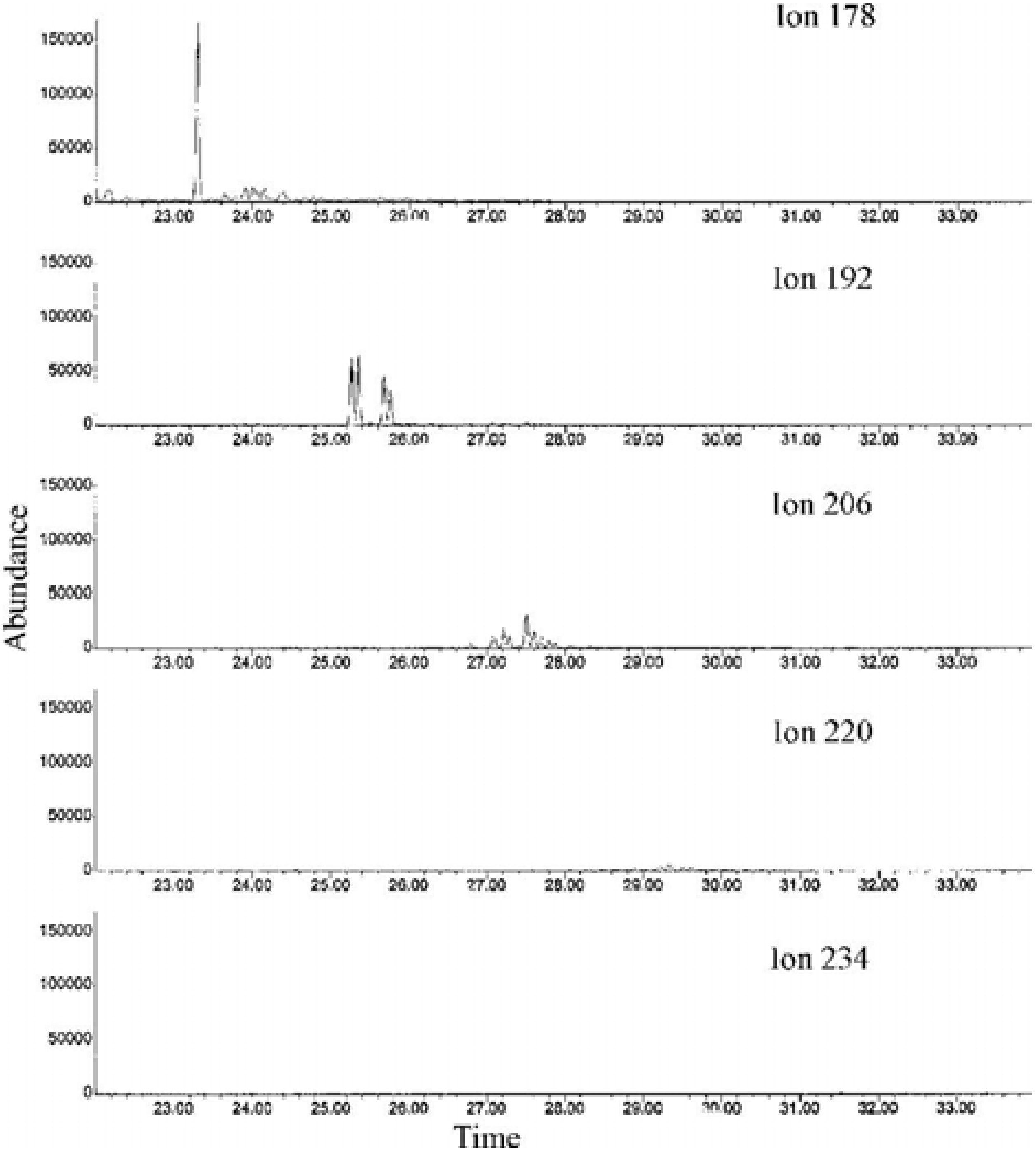


Figure A9-5b Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 178, 192, 206, 220, 234) of Fuel Oil No. 2

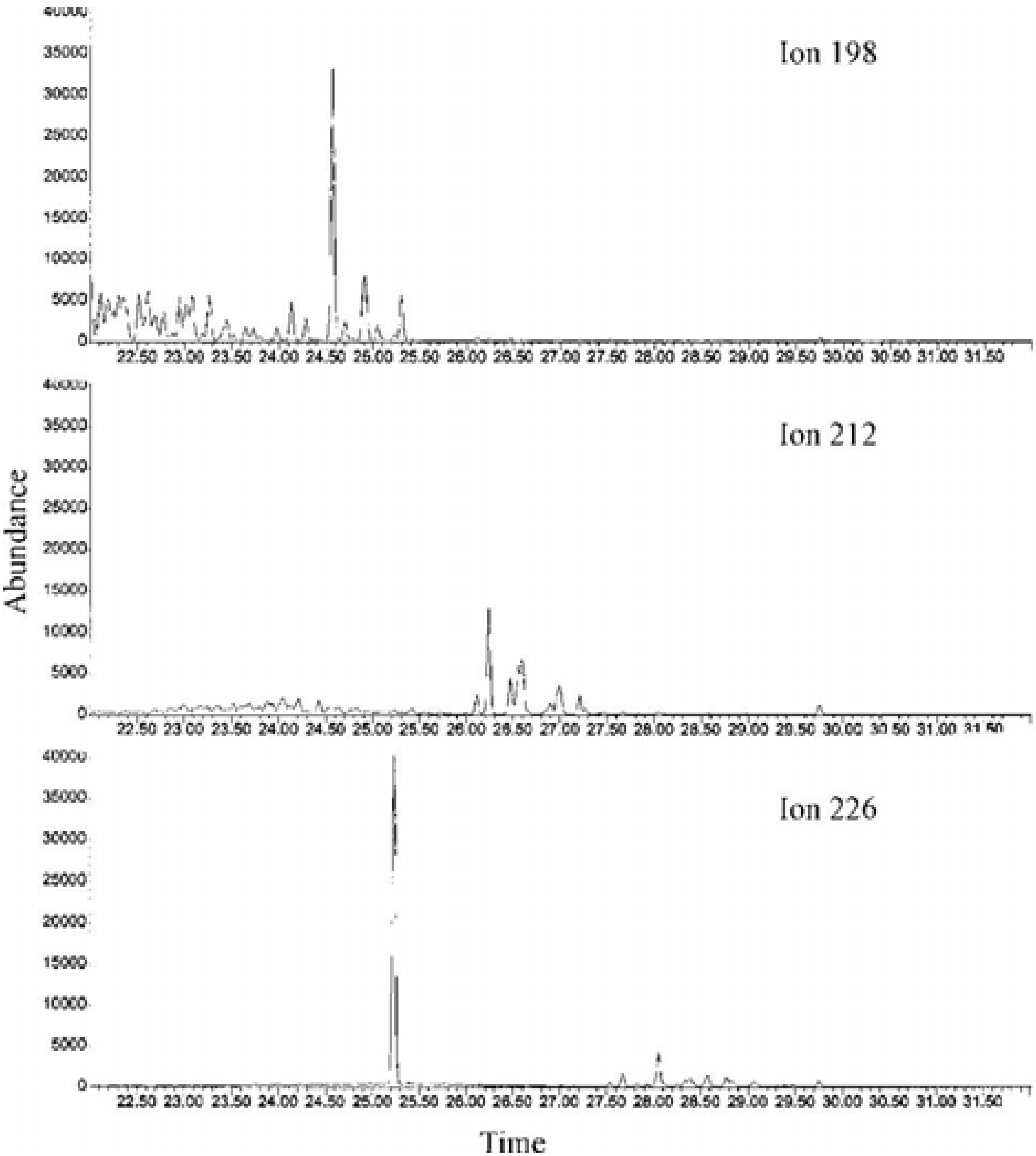


Figure A9-5c Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 198, 212, 226) of Fuel Oil No. 2

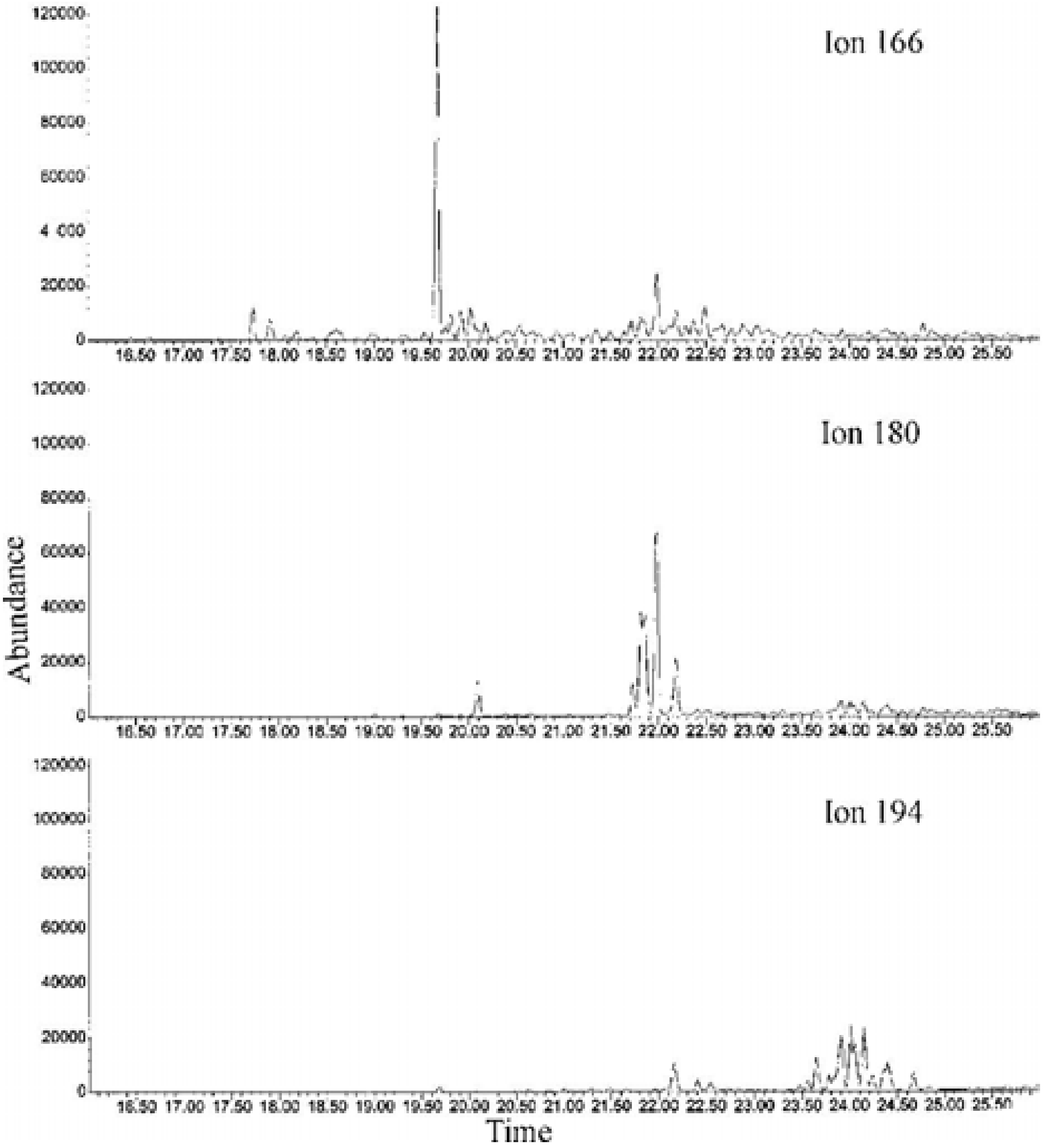


Figure A9-5d Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 166, 180, 194) of Fuel Oil No. 2

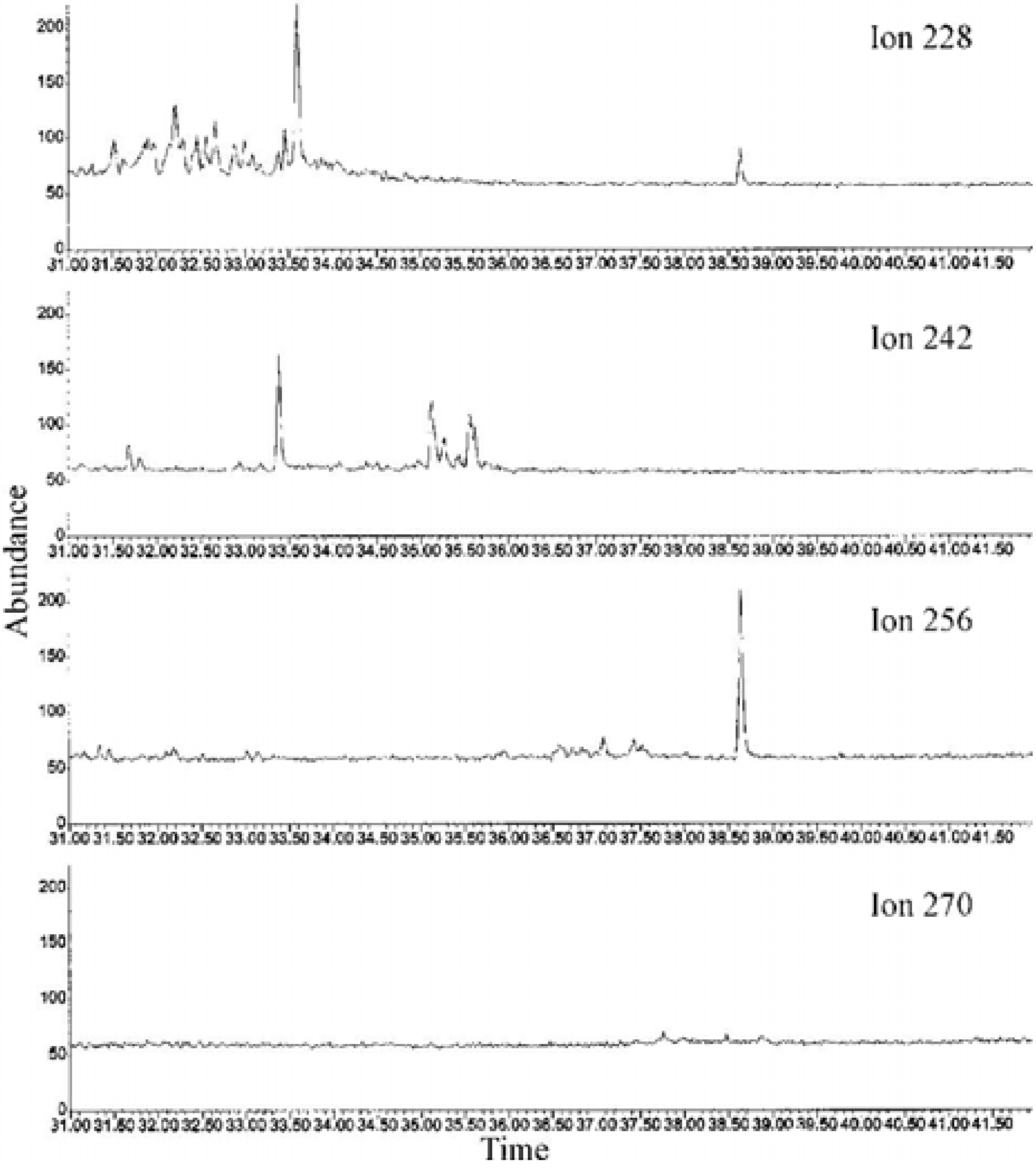


Figure A9-5e Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 228, 242, 256, 270) of Fuel Oil No. 2

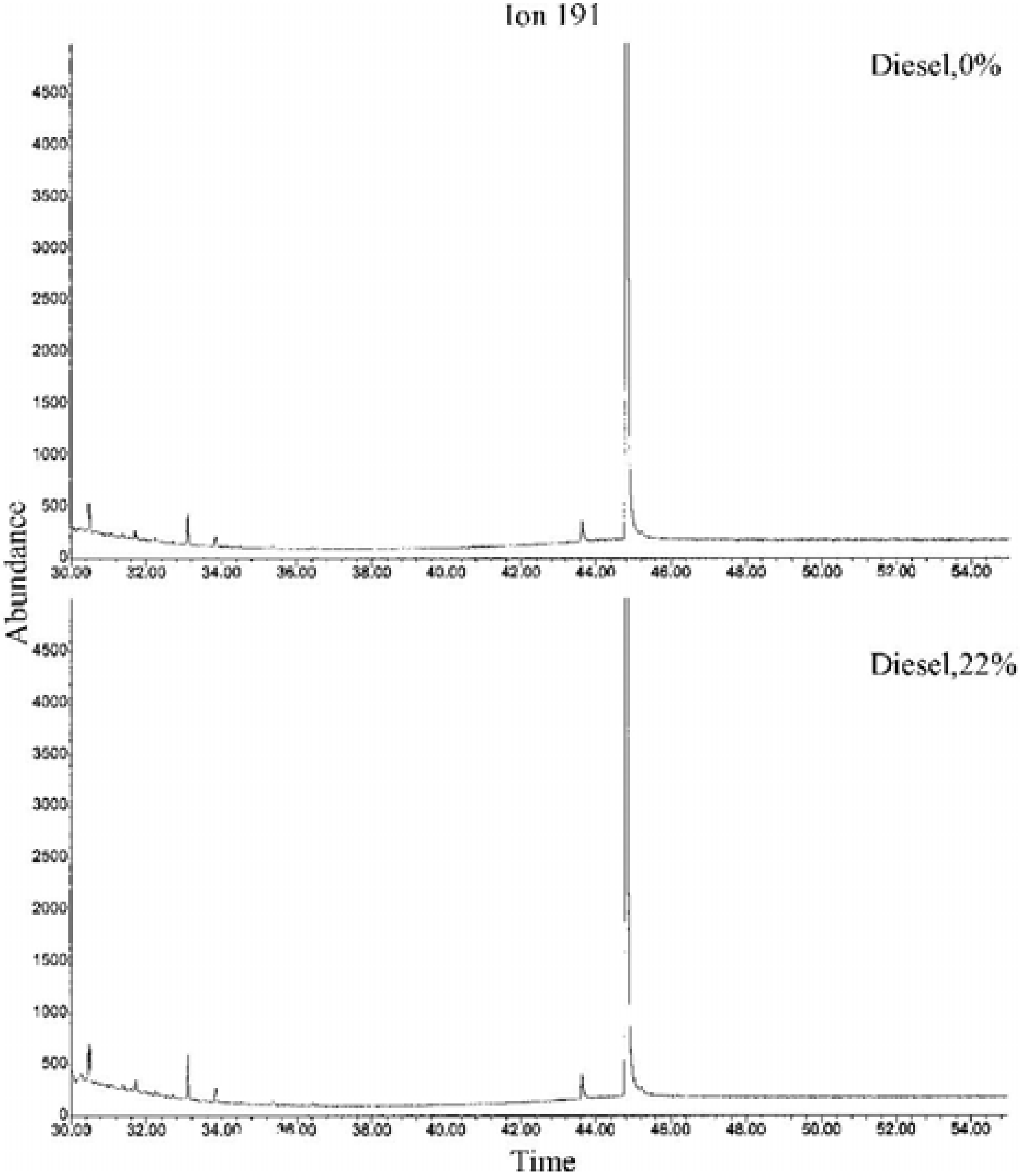


Figure A9-6 GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of Fuel Oil No. 2

10 GC Chromatograms for Fuel Oil Number 5

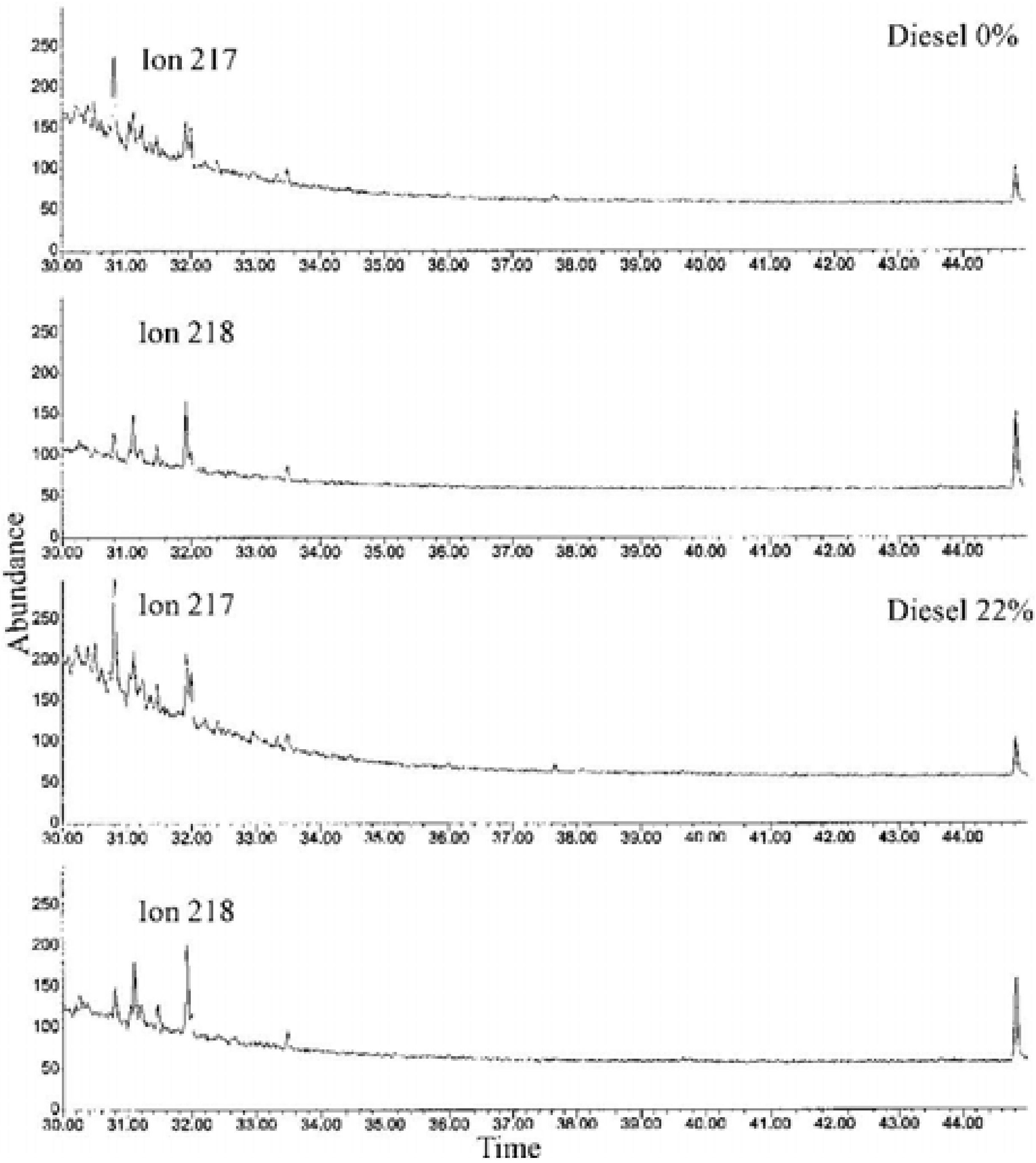


Figure A9-7 GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218) of Fuel Oil No. 2

Figure A10-1 GC-FID chromatograms of fraction 1 (F1) for saturates of Fuel Oil No.5

Figure A10-2	GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of Fuel Oil No.5
Figure A10-3	GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of Fuel Oil No. 5
Figure A10-4	Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of Fuel Oil No. 5
Figure A10-5	Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184, 178, 192, 206, 220, 234, 198, 212, 226, 166, 180, 194, 228, 242, 256, and 270) of Fuel Oil No. 5
Figure A10-6	GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of Fuel Oil No. 5
Figure A10-7	GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218) of Fuel Oil No. 5

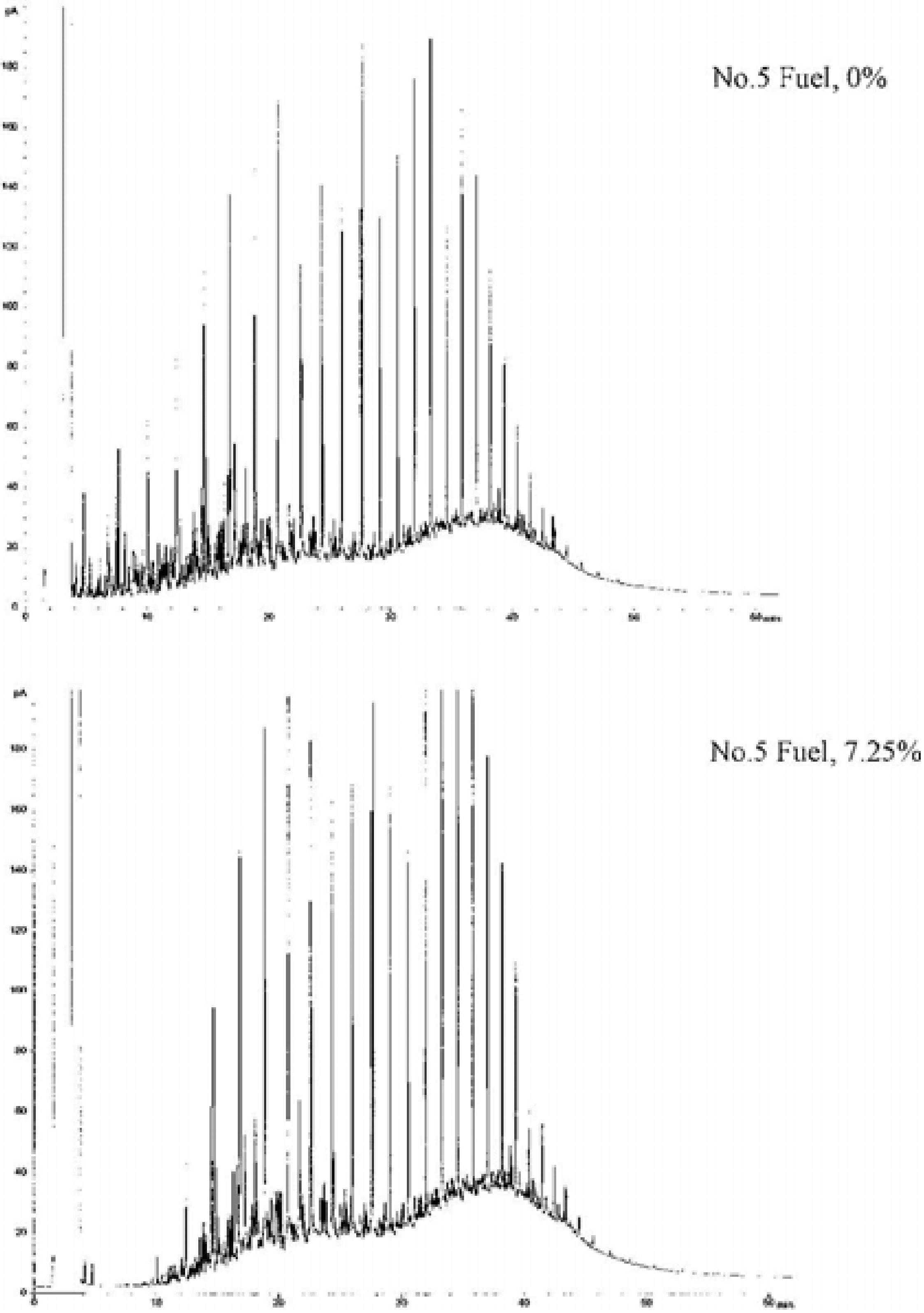
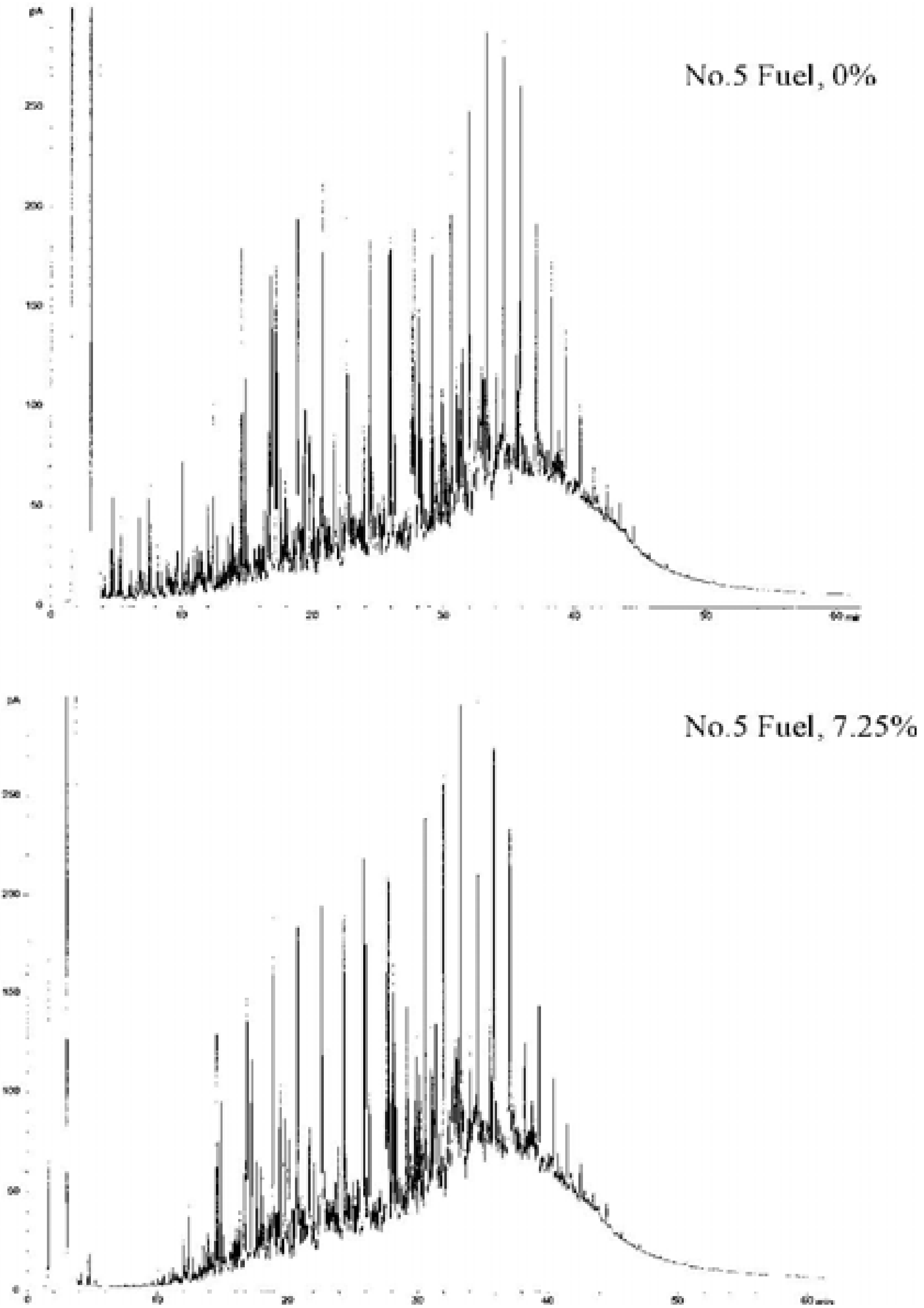


Figure A10-1 GC-FID chromatograms of fraction 1 (F1) for saturates of Fuel Oil No.5


No.5 Fuel, 0%

No.5 Fuel, 7.25%

Figure A10-2 GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of Fuel Oil No.5

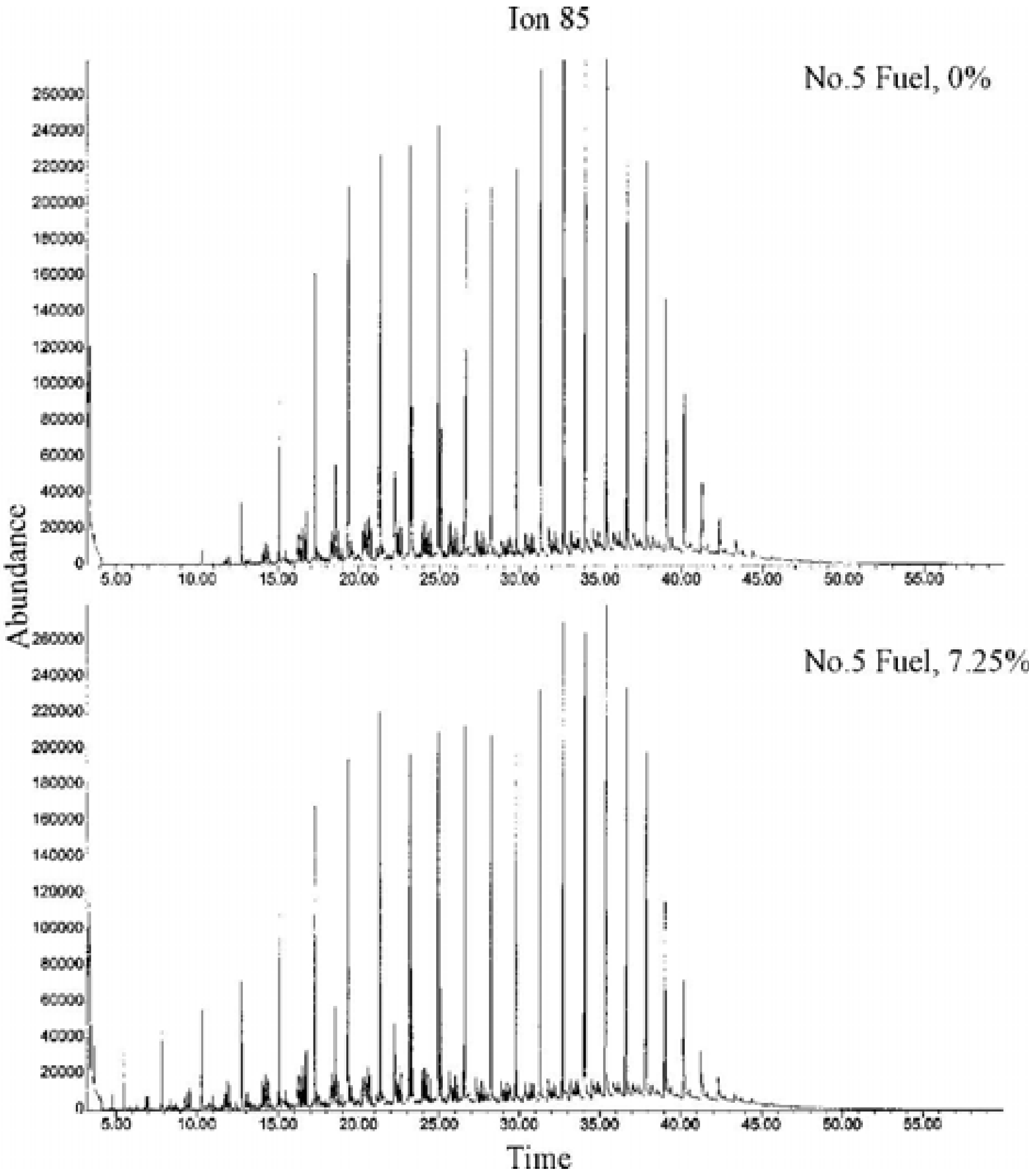


Figure A10-3 GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of Fuel Oil No. 5

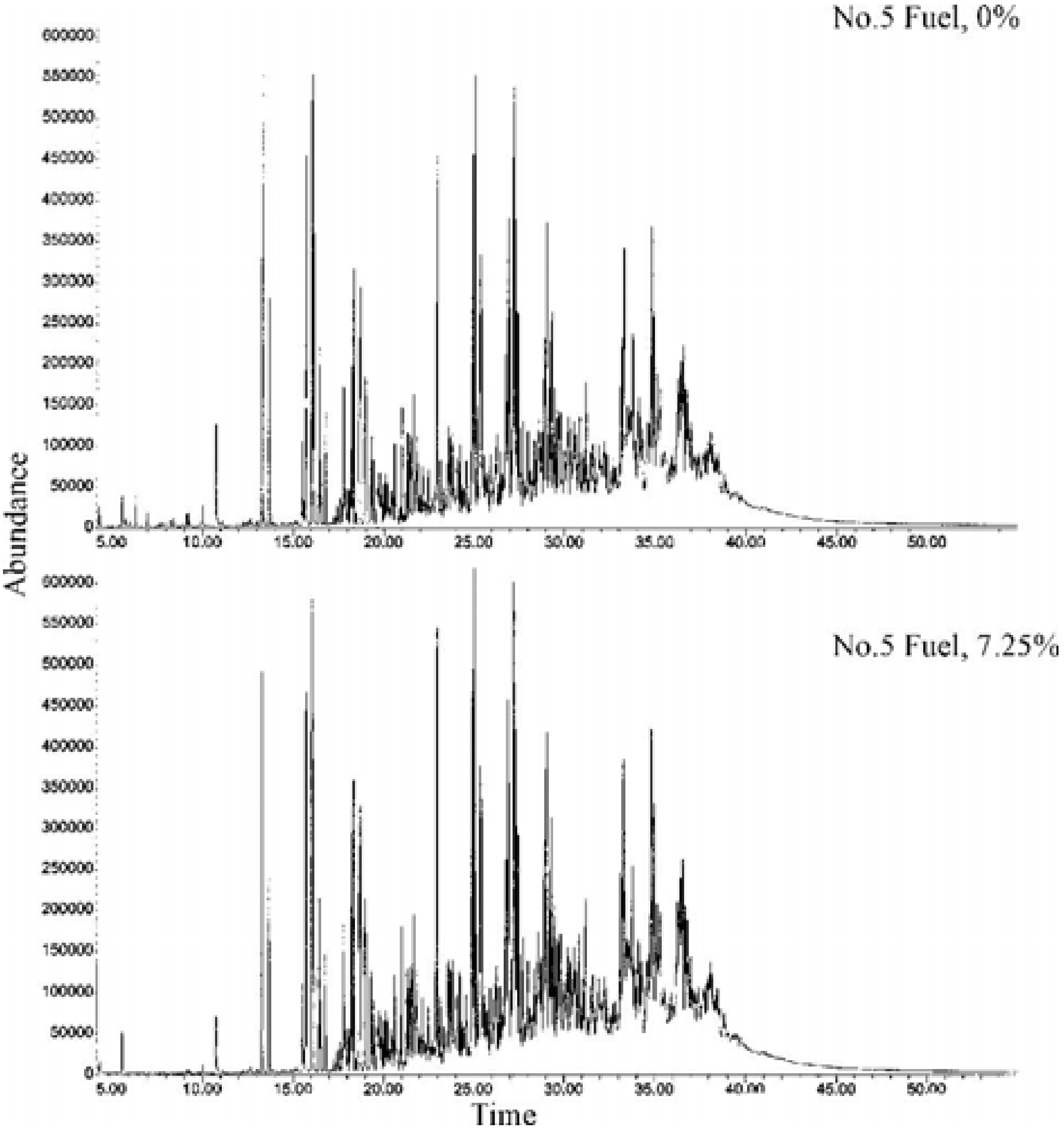


Figure A10-4 Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of Fuel Oil No. 5

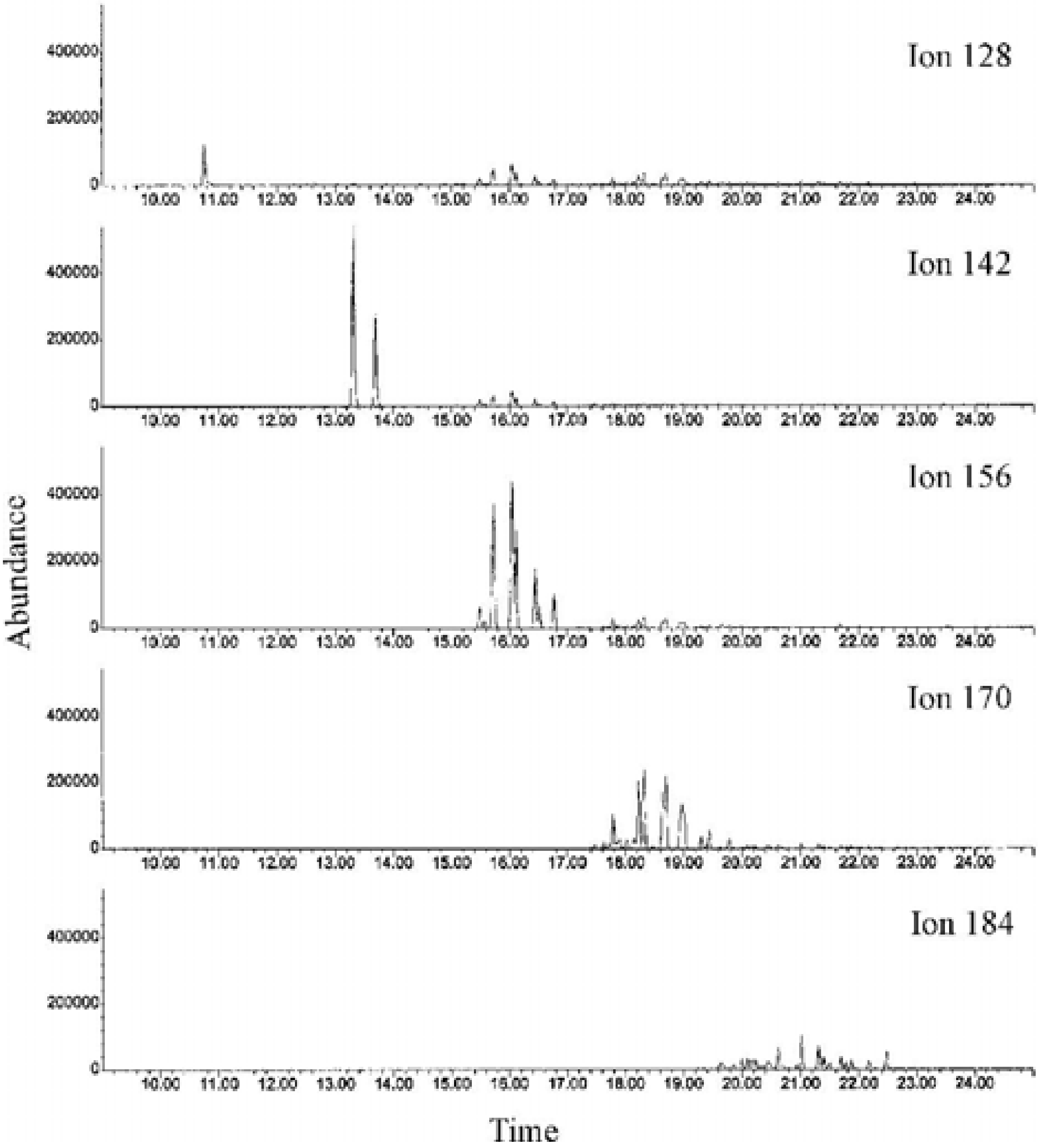


Figure A10-5a Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184) of Fuel Oil No. 5

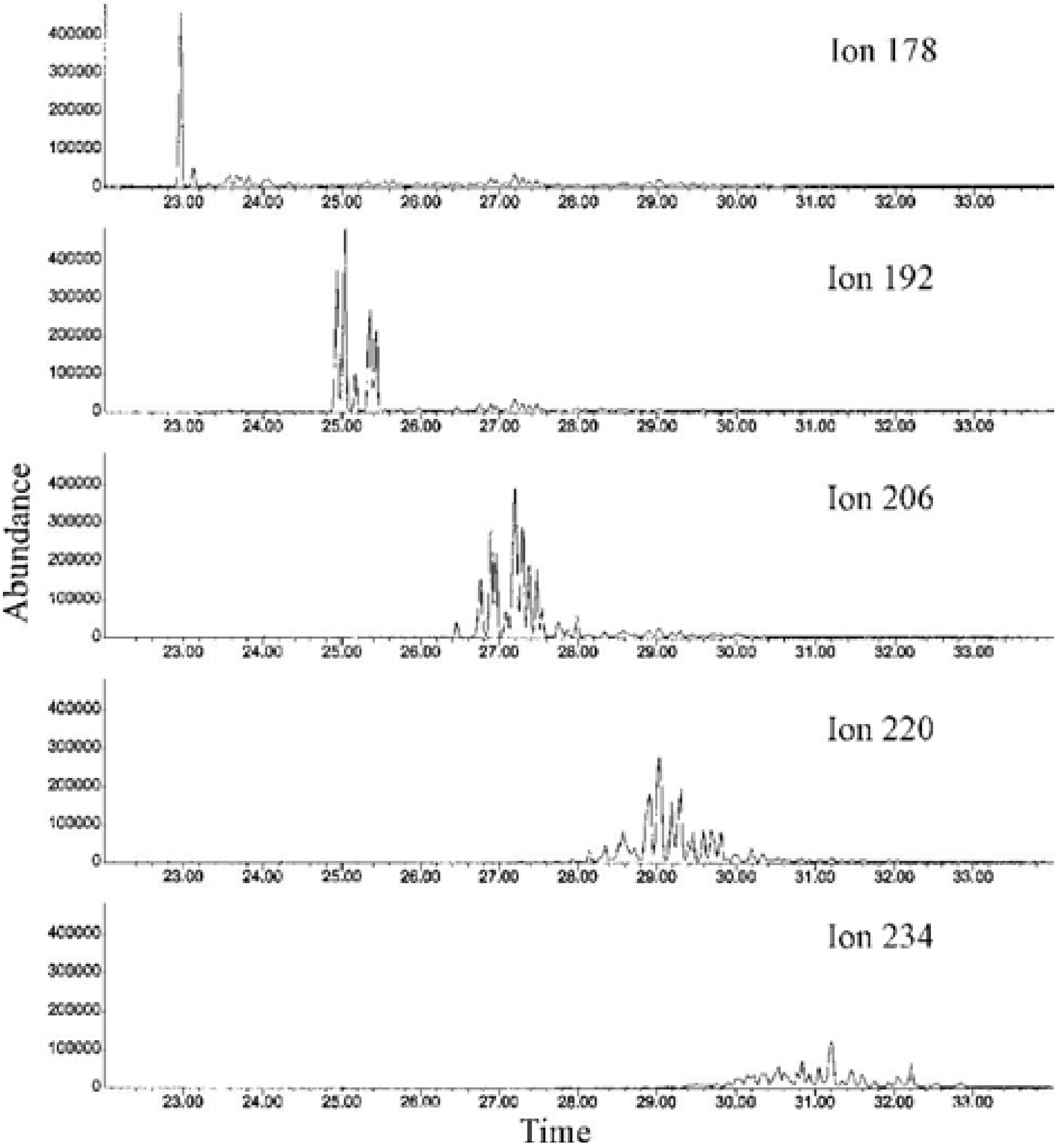


Figure A10-5b Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 178, 192, 206, 220, 234) of Fuel Oil No. 5

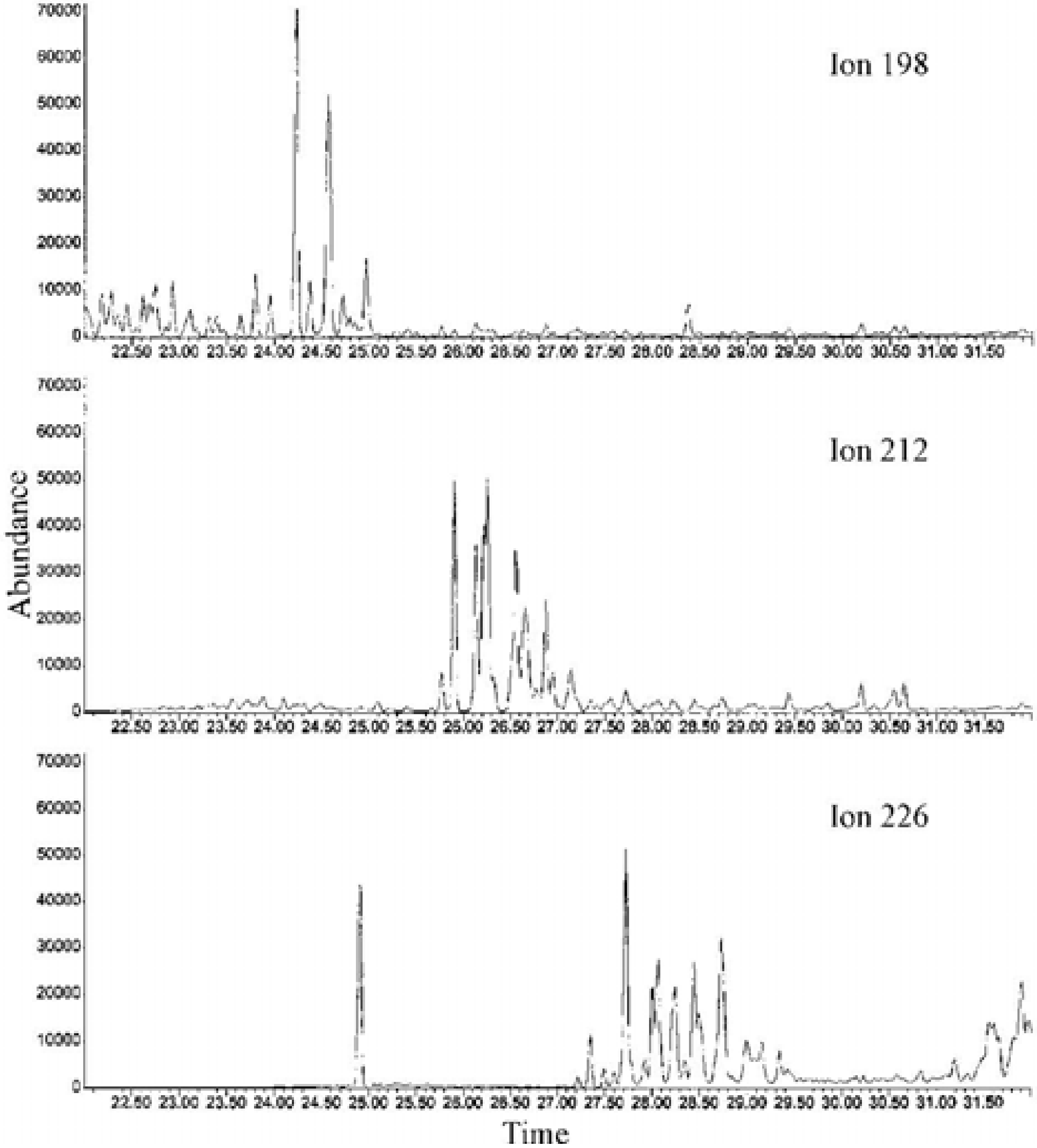


Figure A10-5c Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 166, 180, 194) of Fuel Oil No. 5

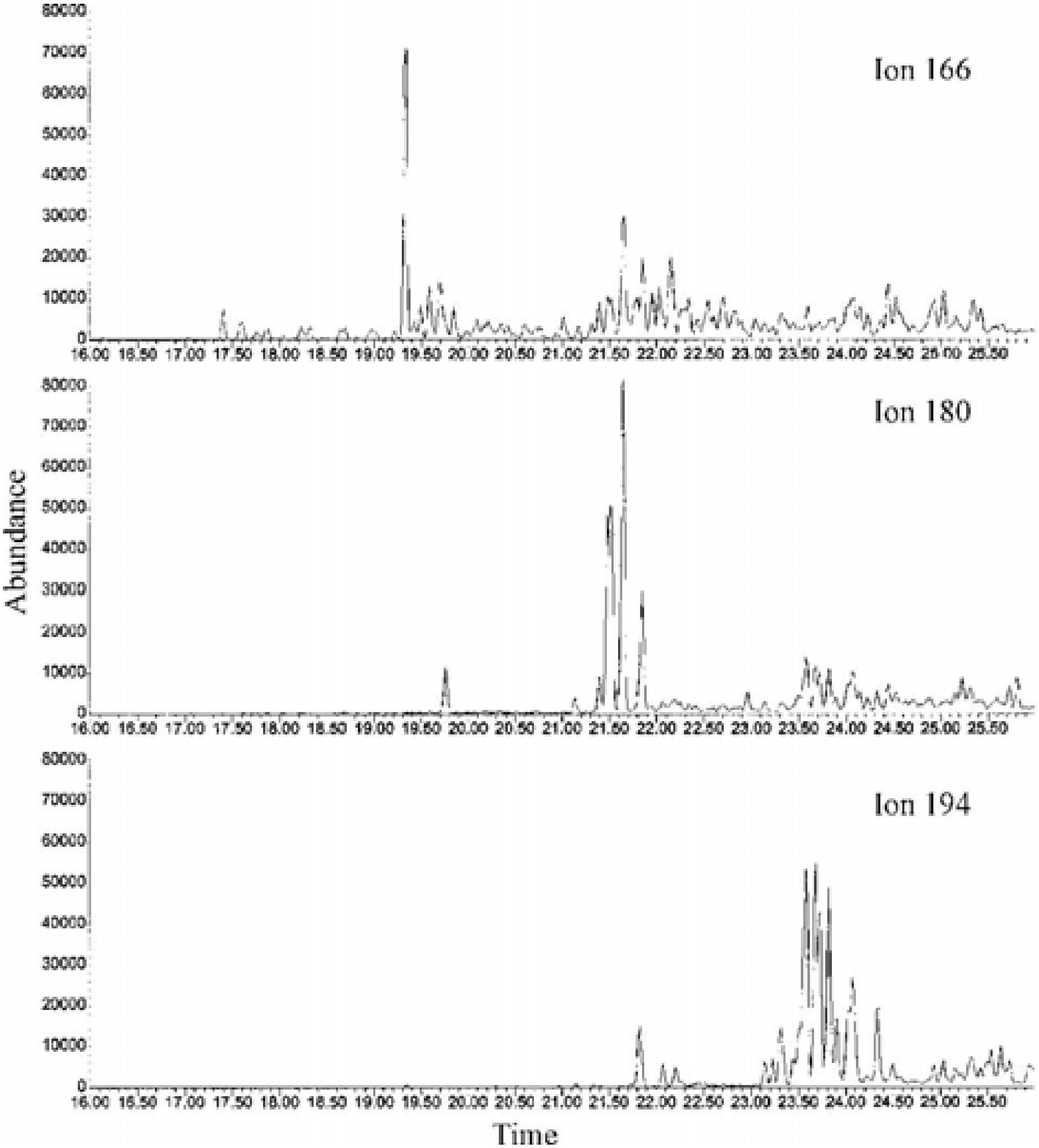


Figure A10-5d Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 166, 180, 194) of Fuel Oil No. 5

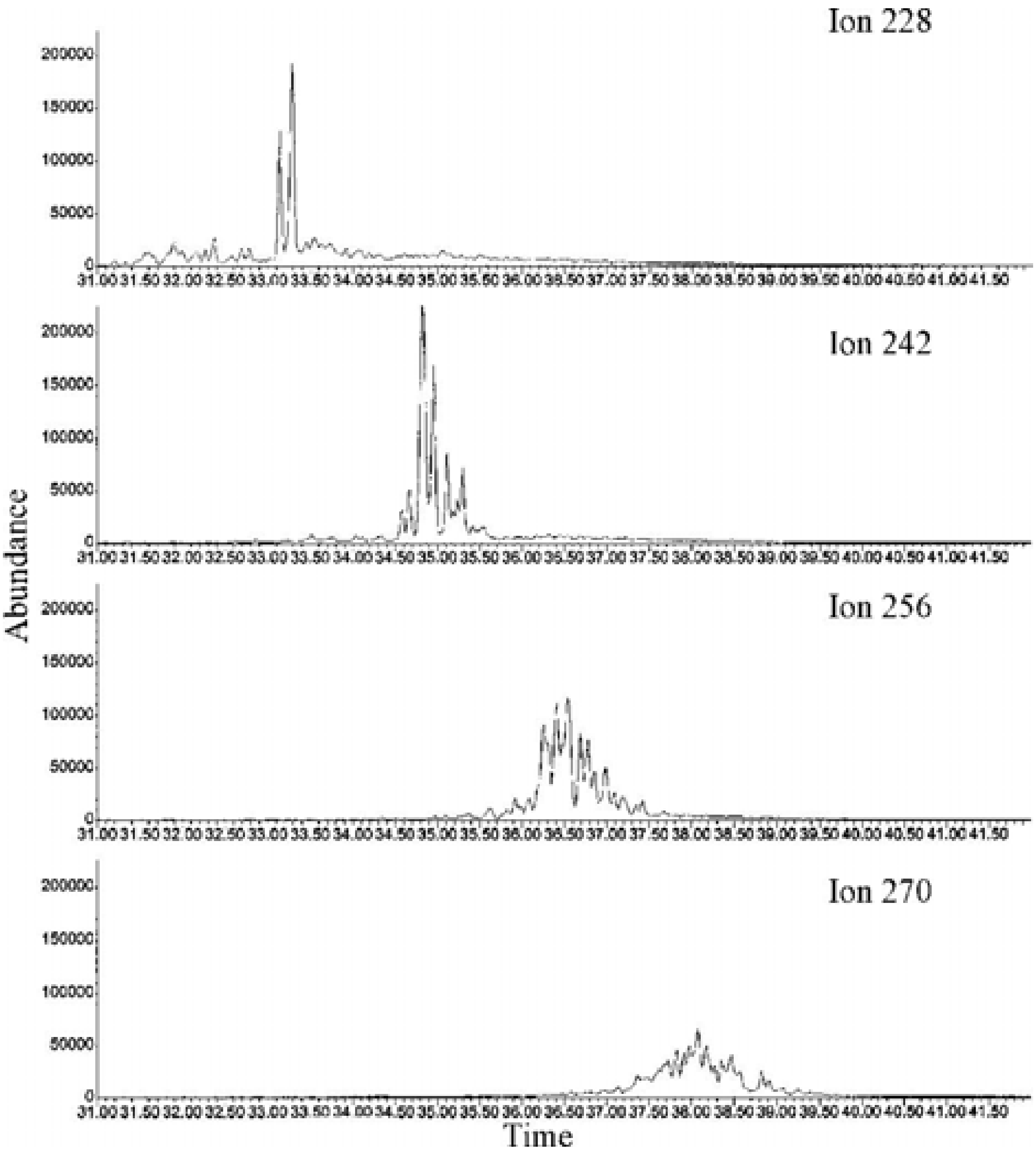


Figure A10-5e Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 228, 242, 256, 270) of Fuel Oil No. 5

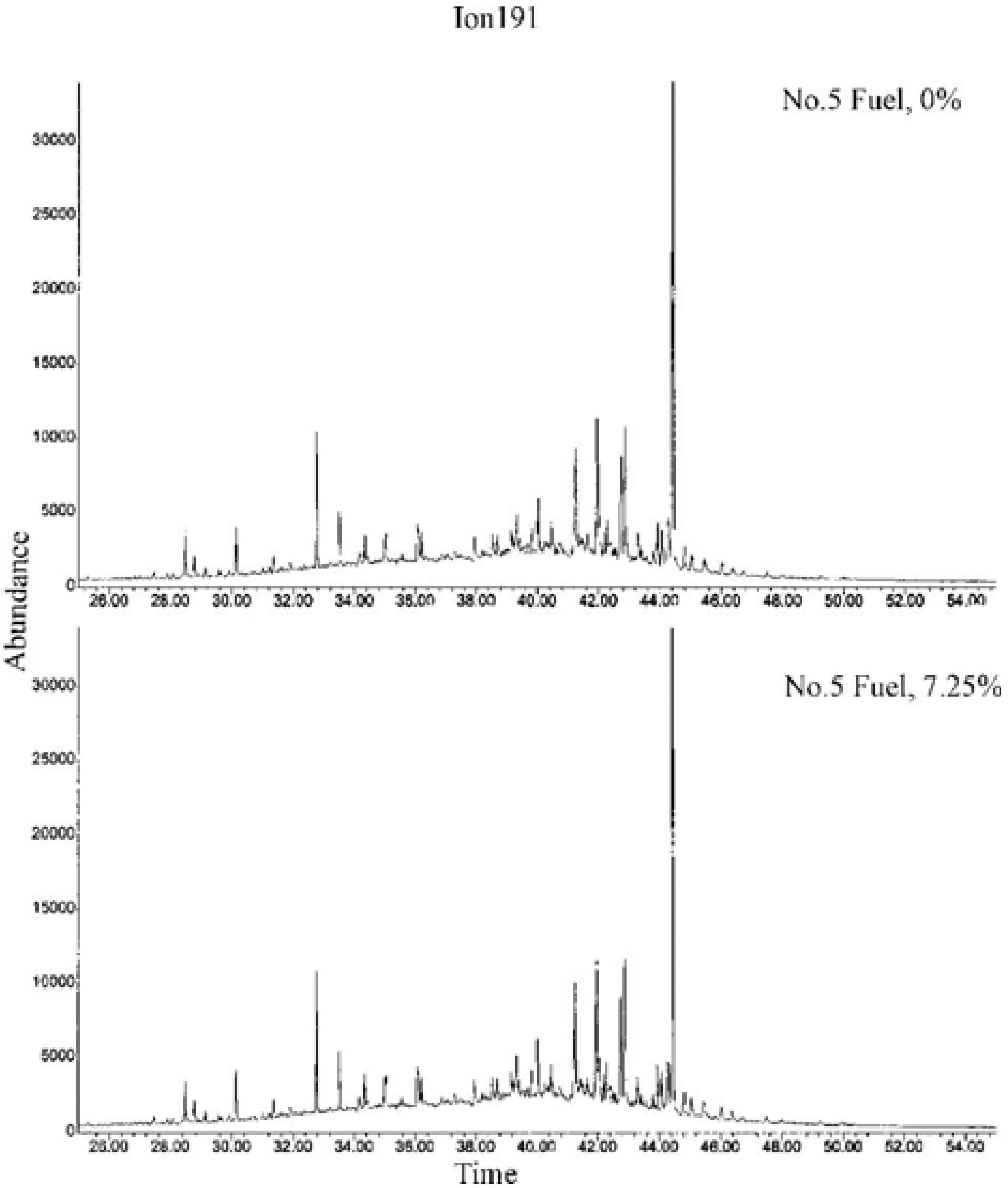


Figure A10-6 GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of Fuel Oil No. 5

11 GC Chromatograms for HFO 6303

Figure A11-1 GC-FID chromatograms of fraction 1(F1) for saturates of HFO 6303

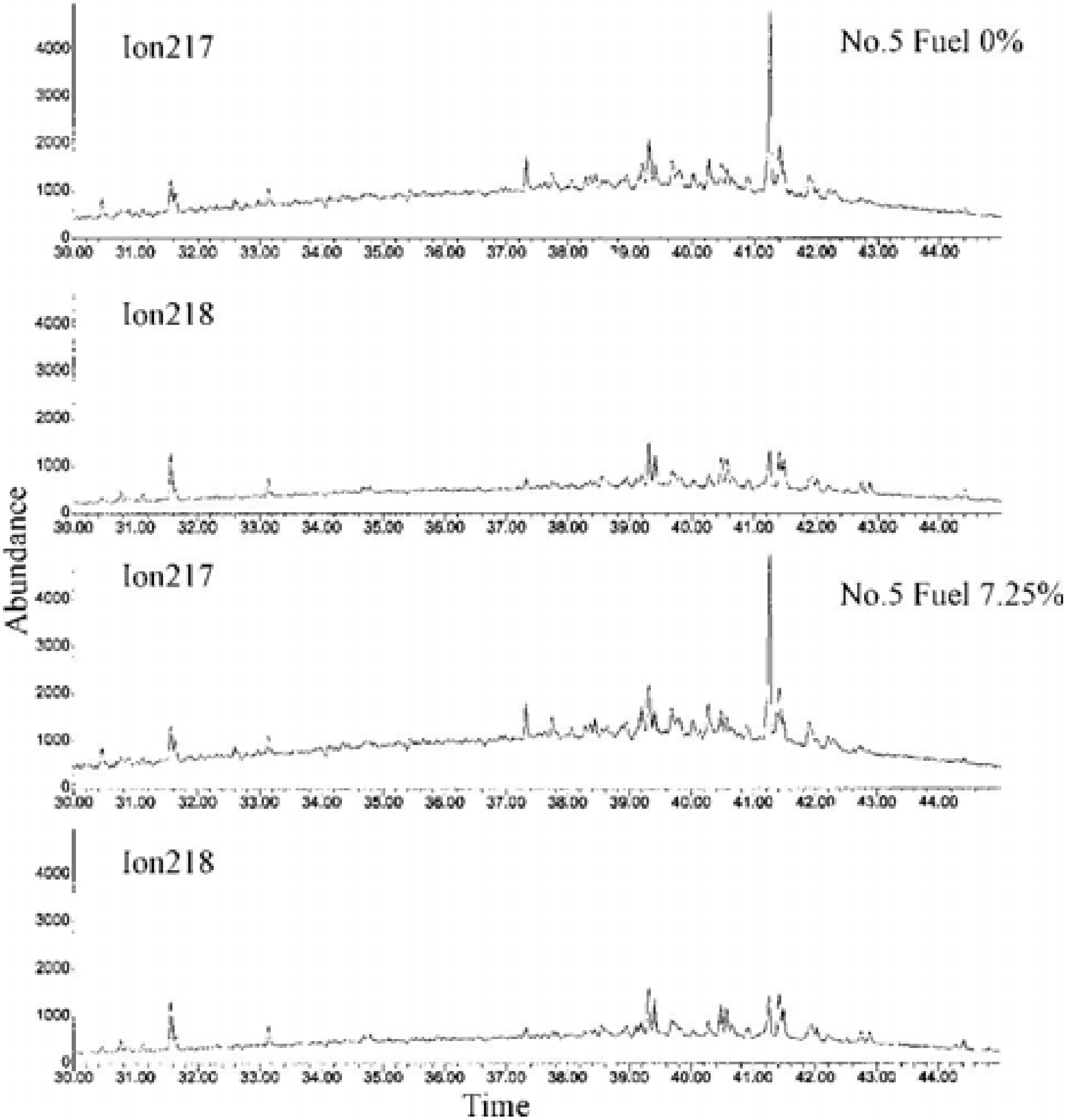


Figure A10-7 GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218) of Fuel Oil No. 5

Figure A11-2 GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of

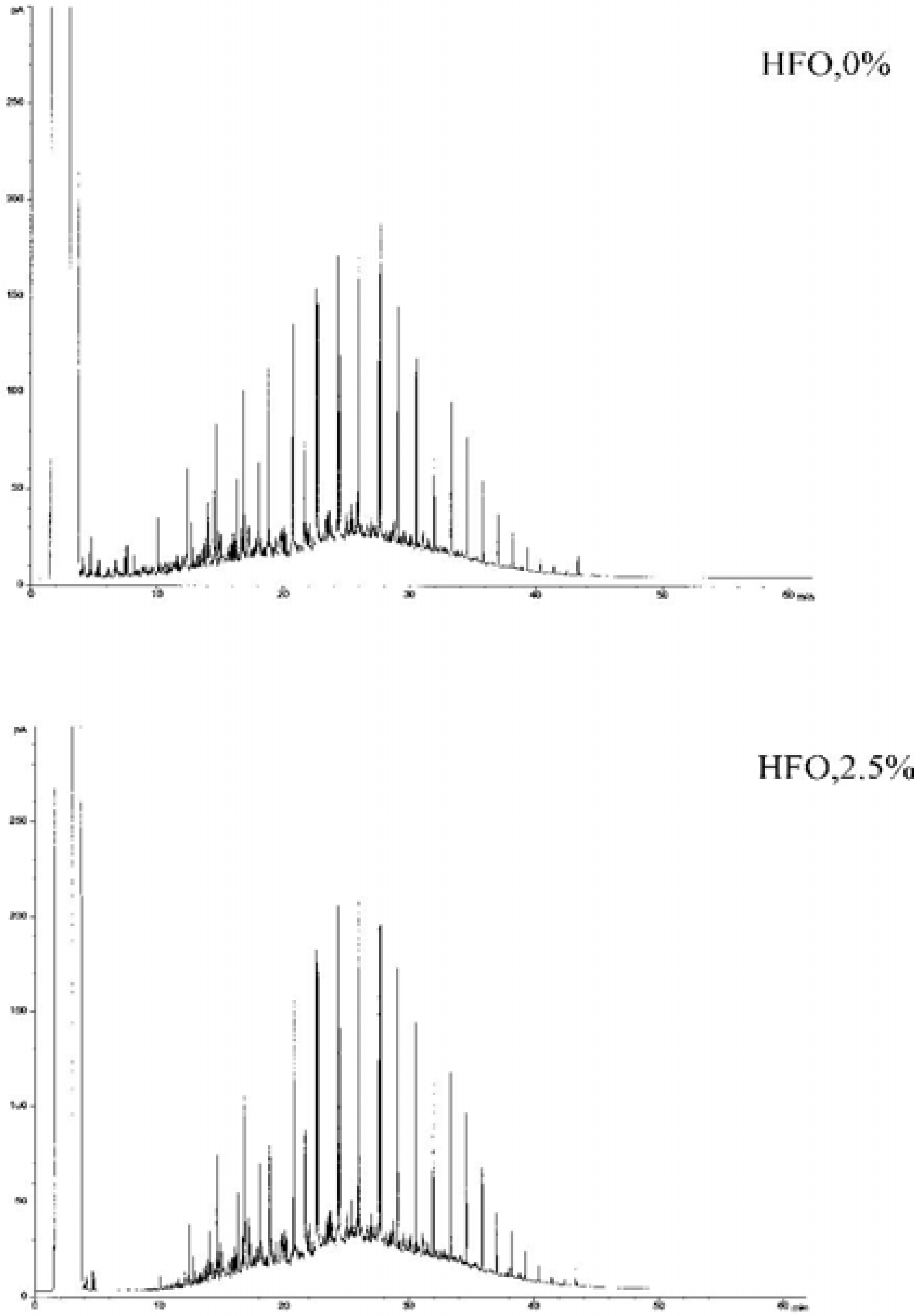


Figure A11-1 GC-FID chromatograms of fraction 1 (F1) for saturates of HFO 6303

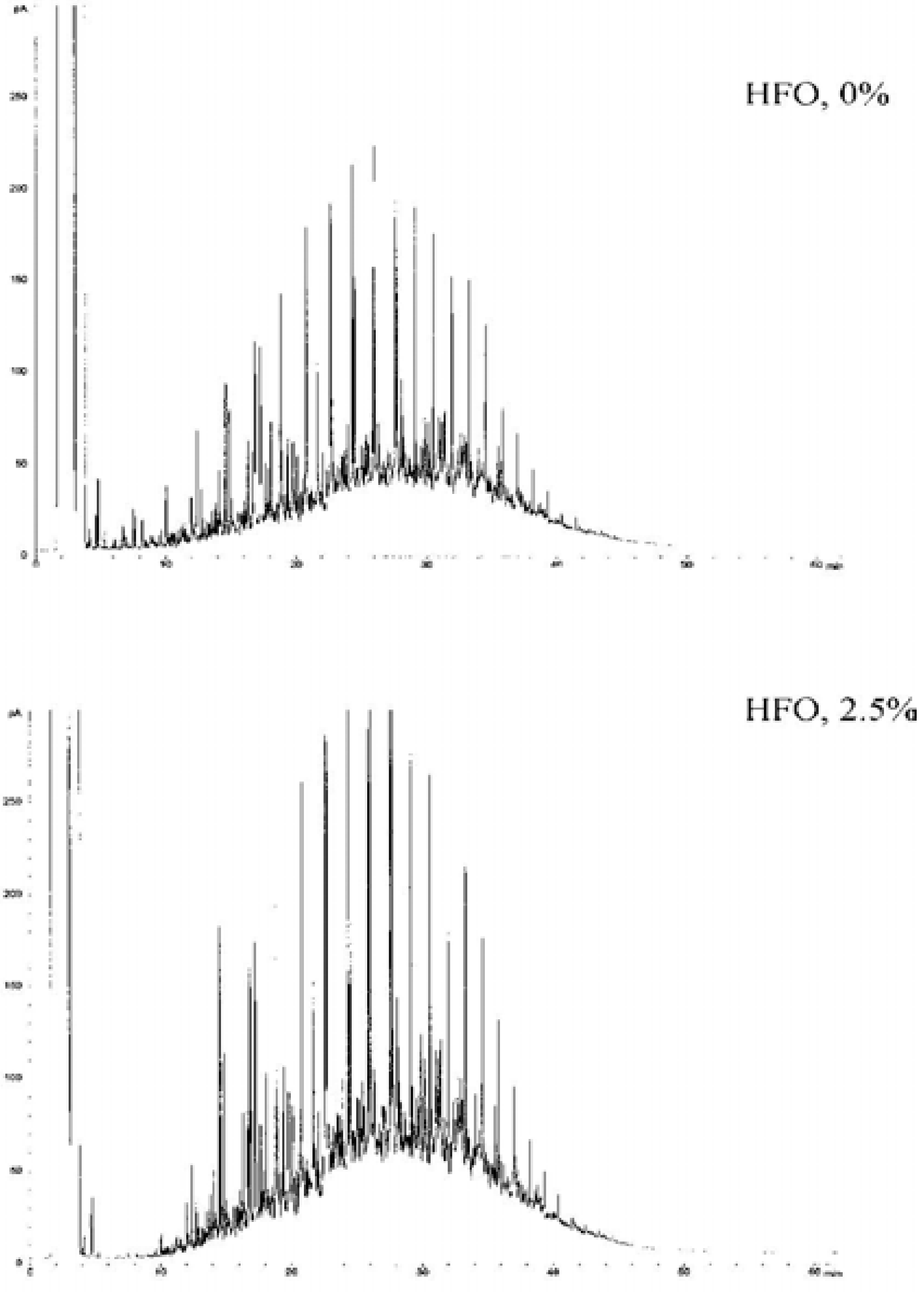


Figure A11-2 GC-FID chromatograms of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of HFO 6303

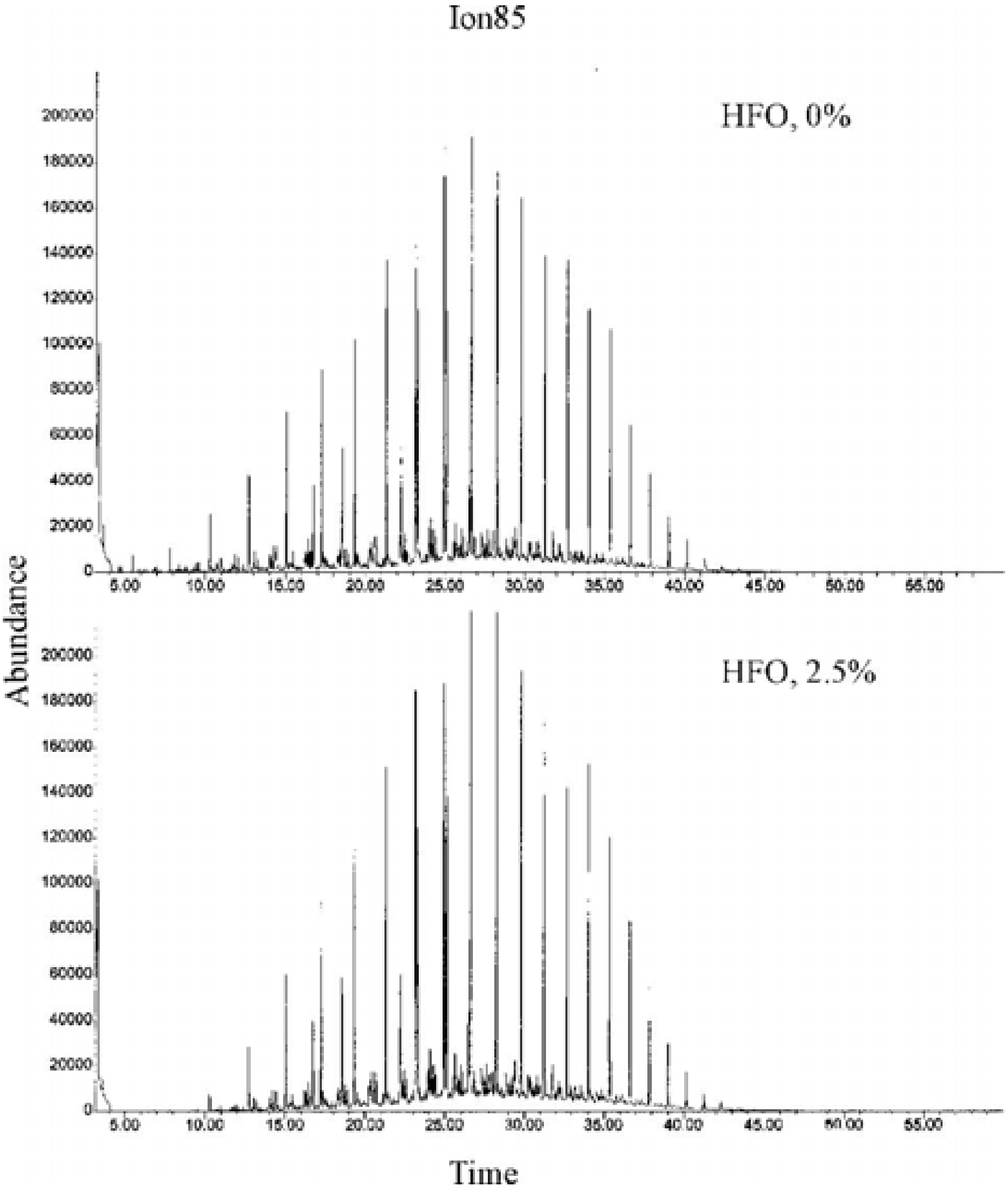


Figure A11-3 GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of HFO 6303

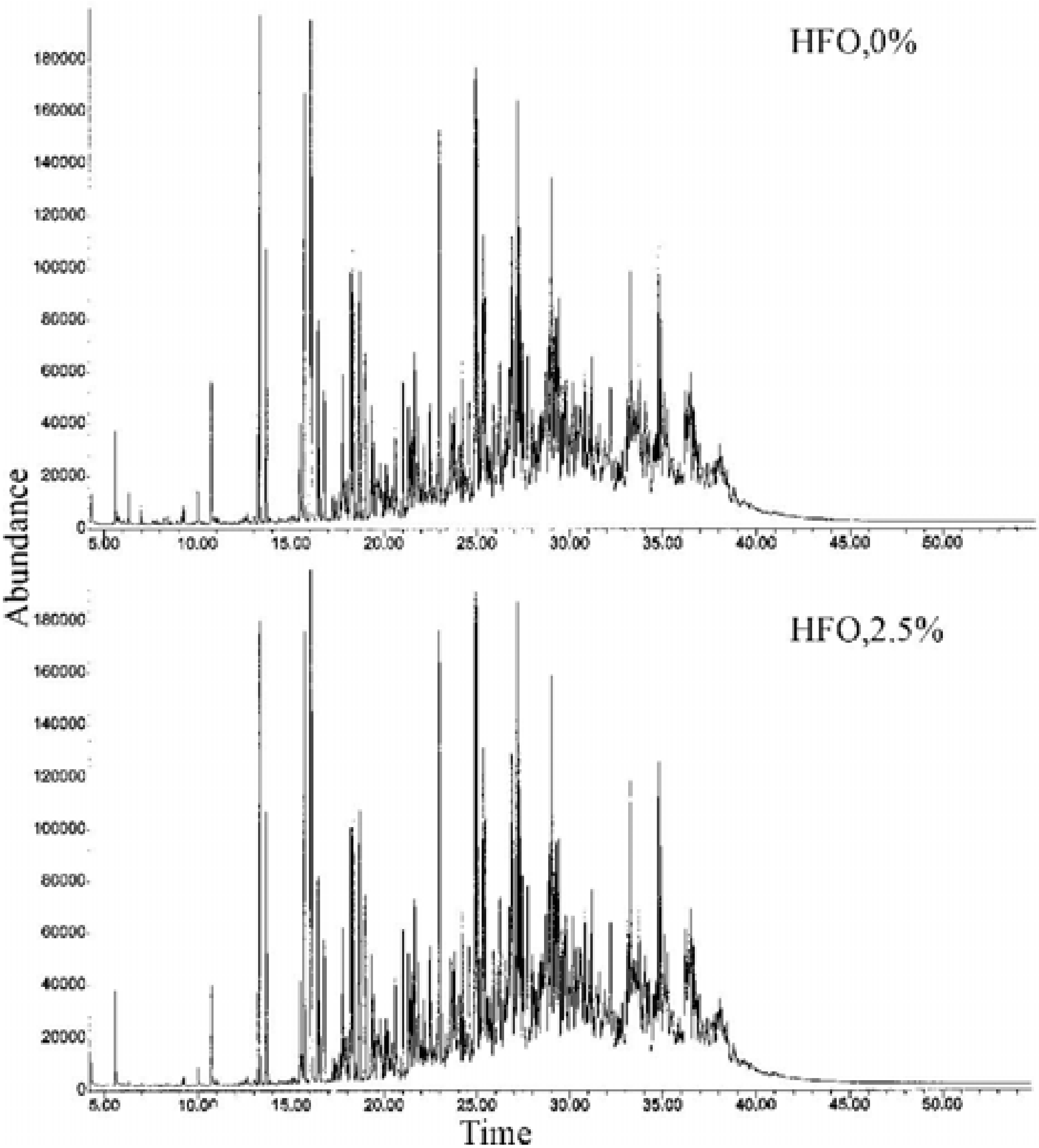


Figure A11-4 Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of HFO 6303

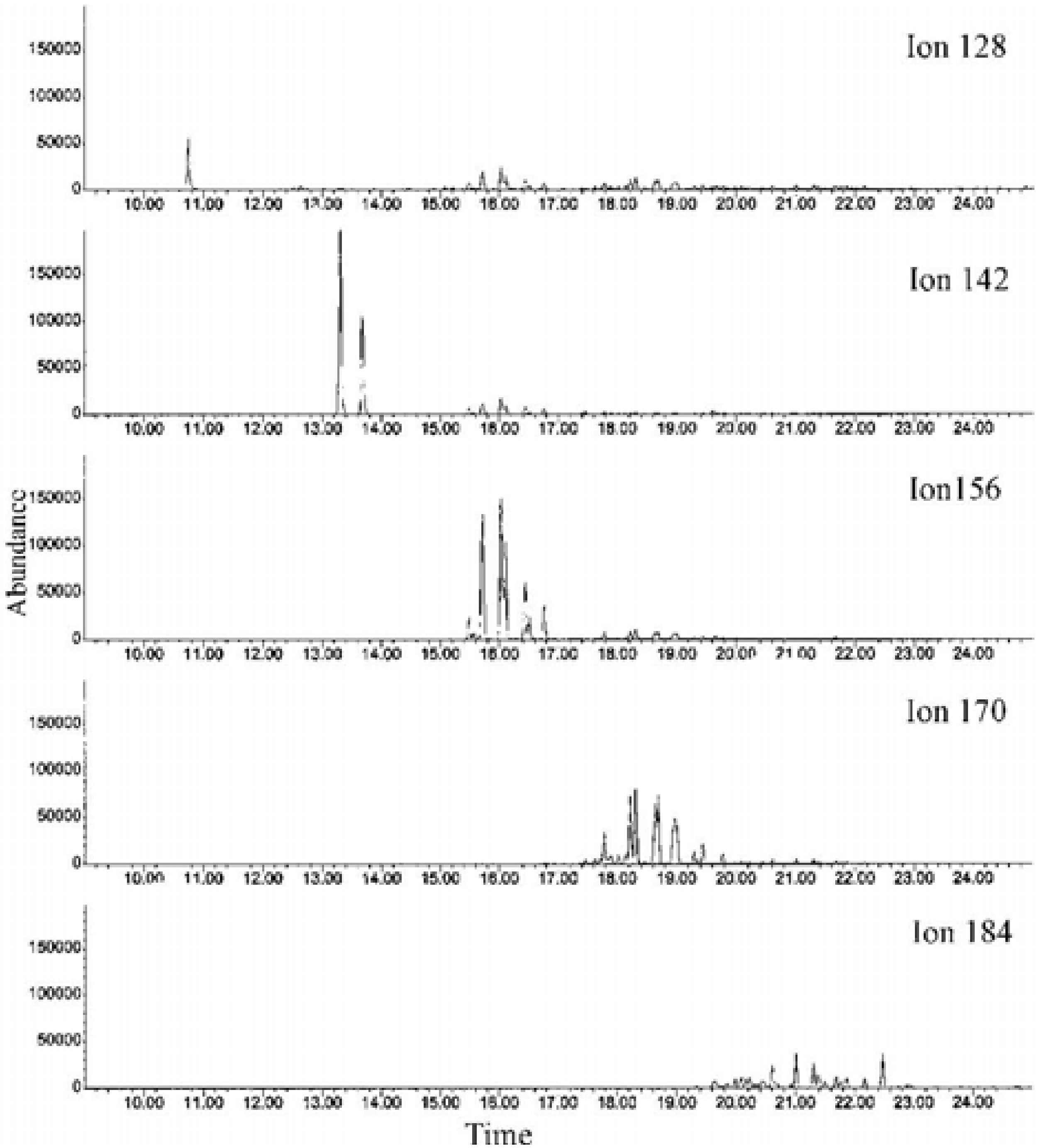


Figure A11-5a Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184) of HFO 6303

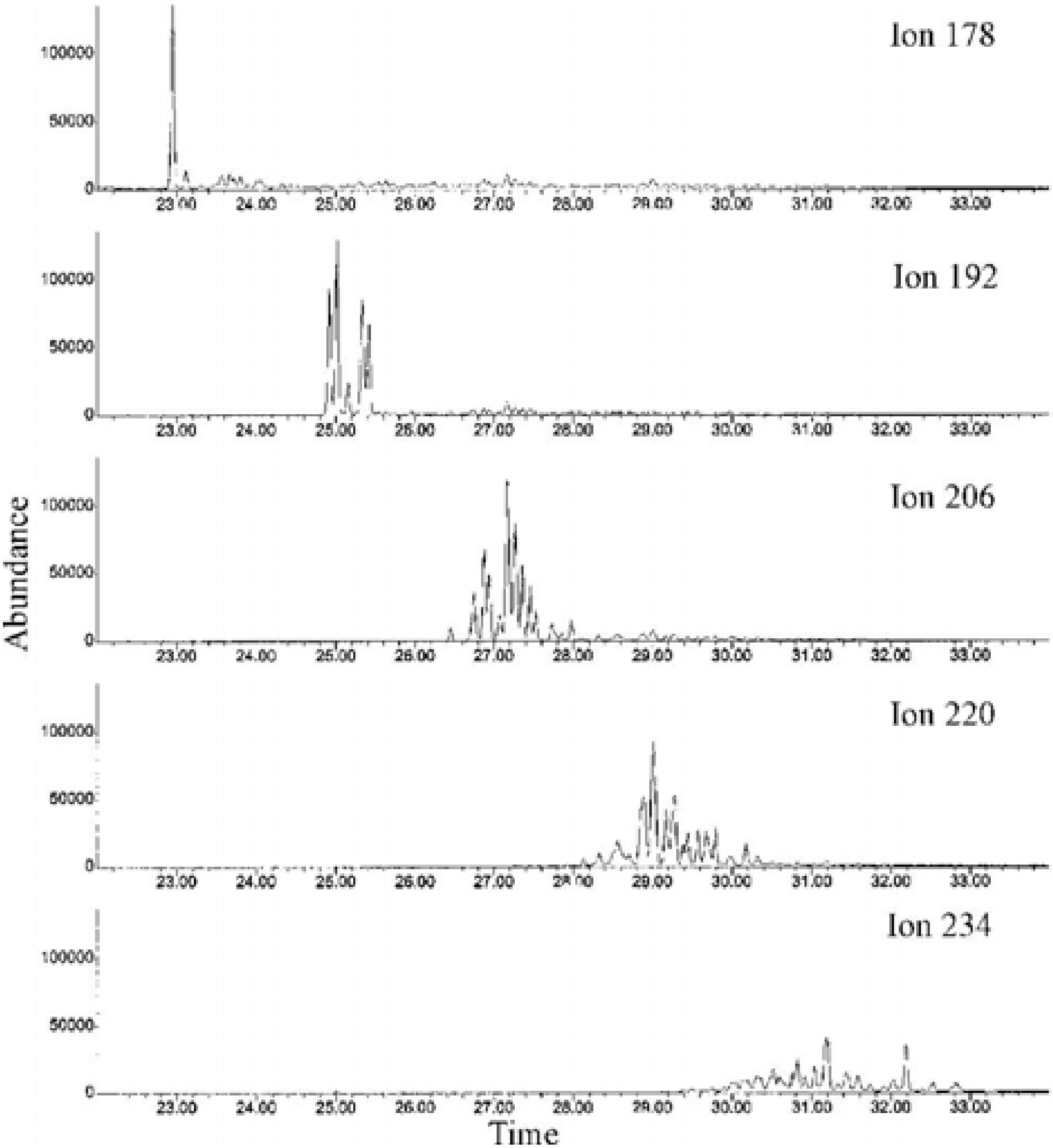


Figure A11-5b Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 178, 192, 206, 220, 234) of HFO 6303

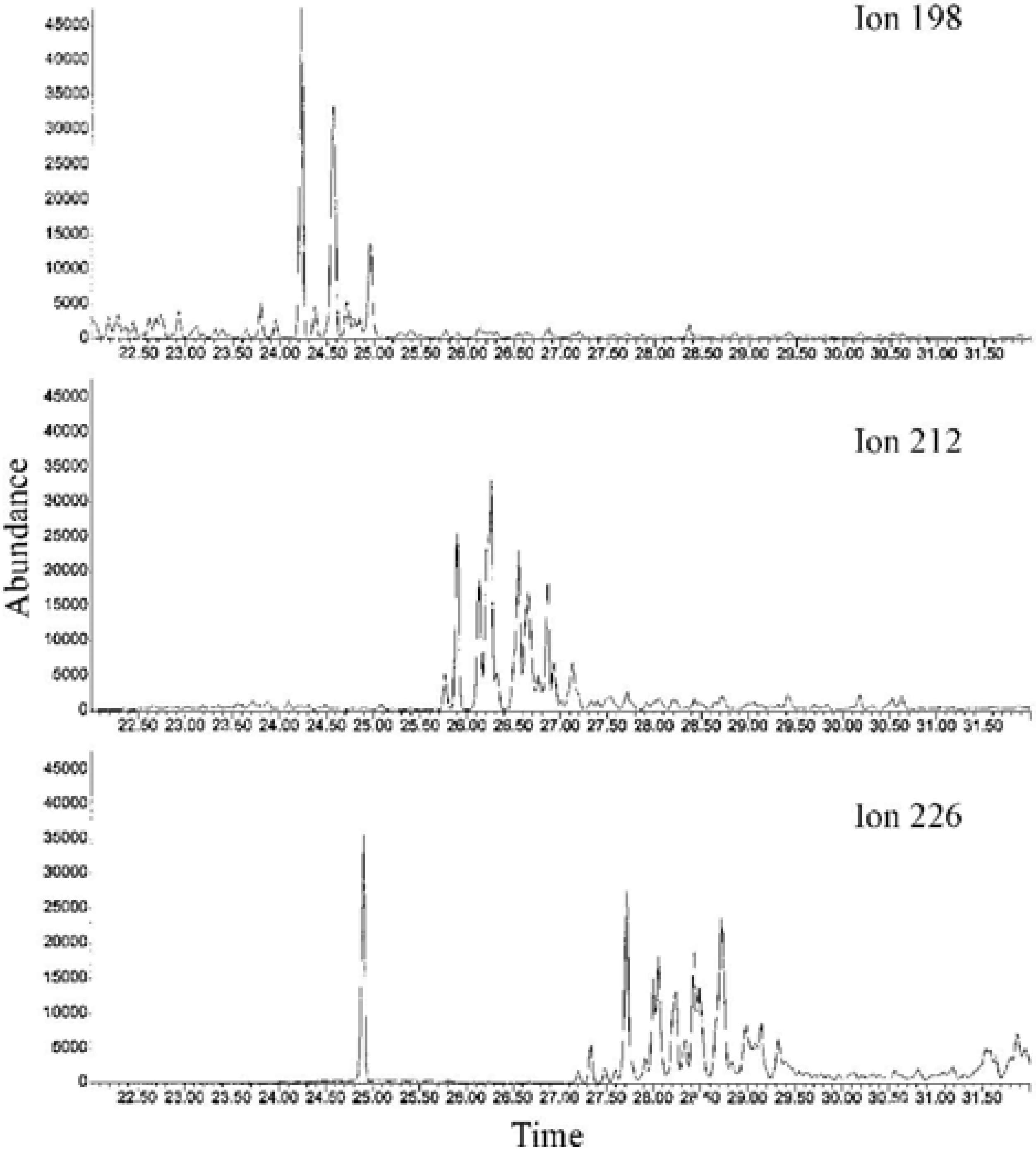


Figure A11-5c Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 198, 212, 226) of HFO 6303

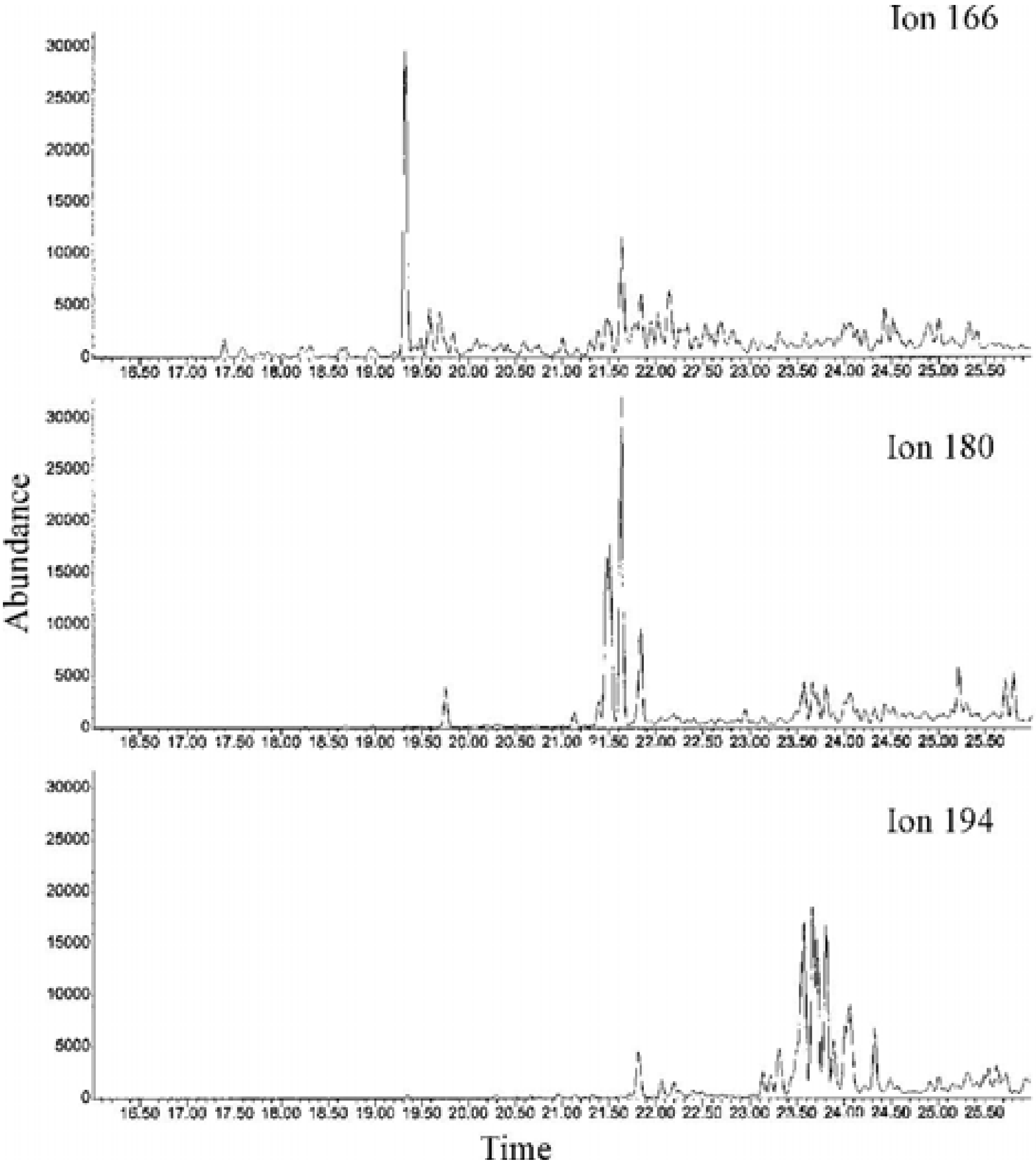


Figure A11-5d Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 166, 180, 194) of HFO 6303

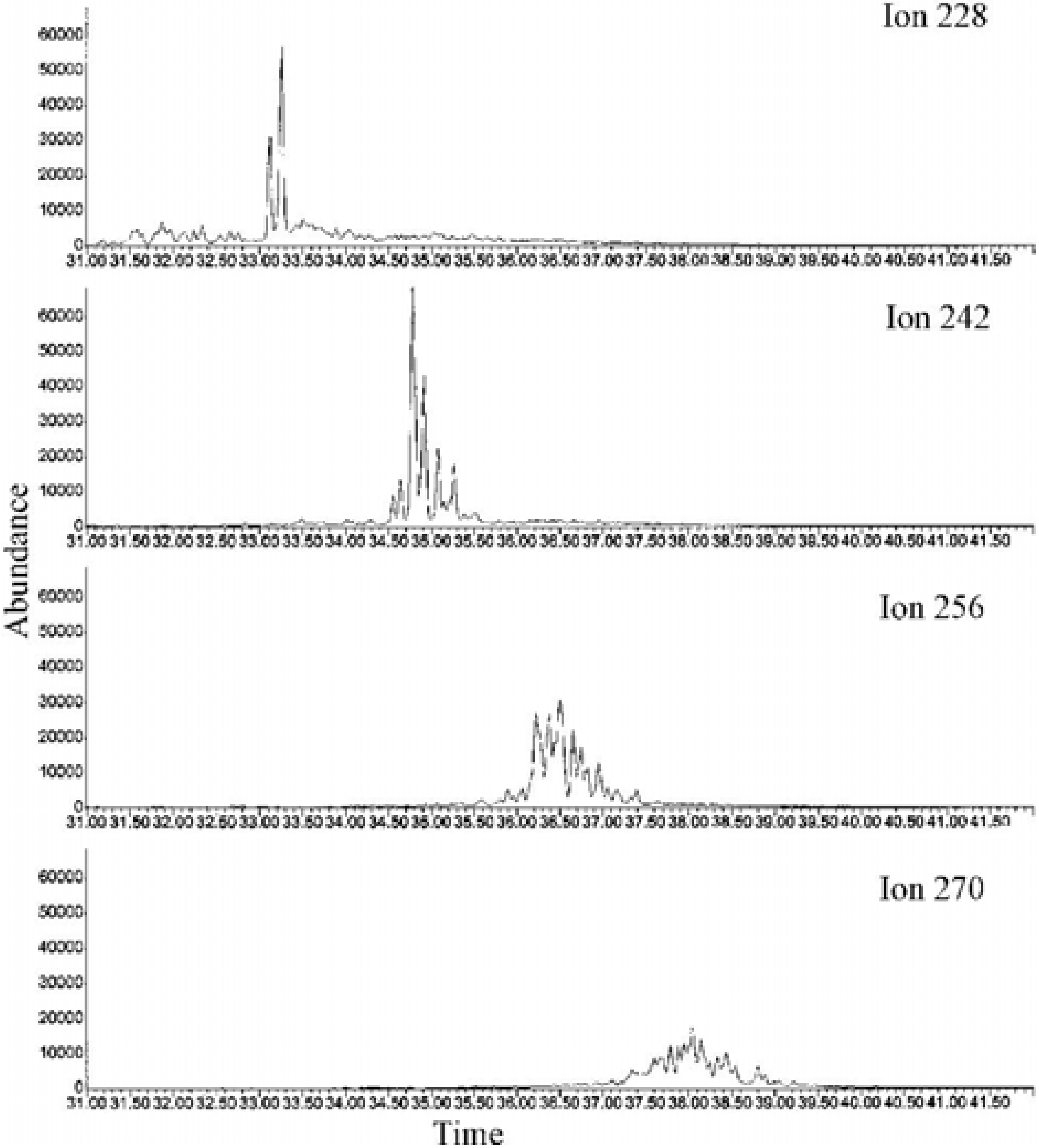


Figure A11-5e Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 228, 242, 256, 270) of HFO 6303

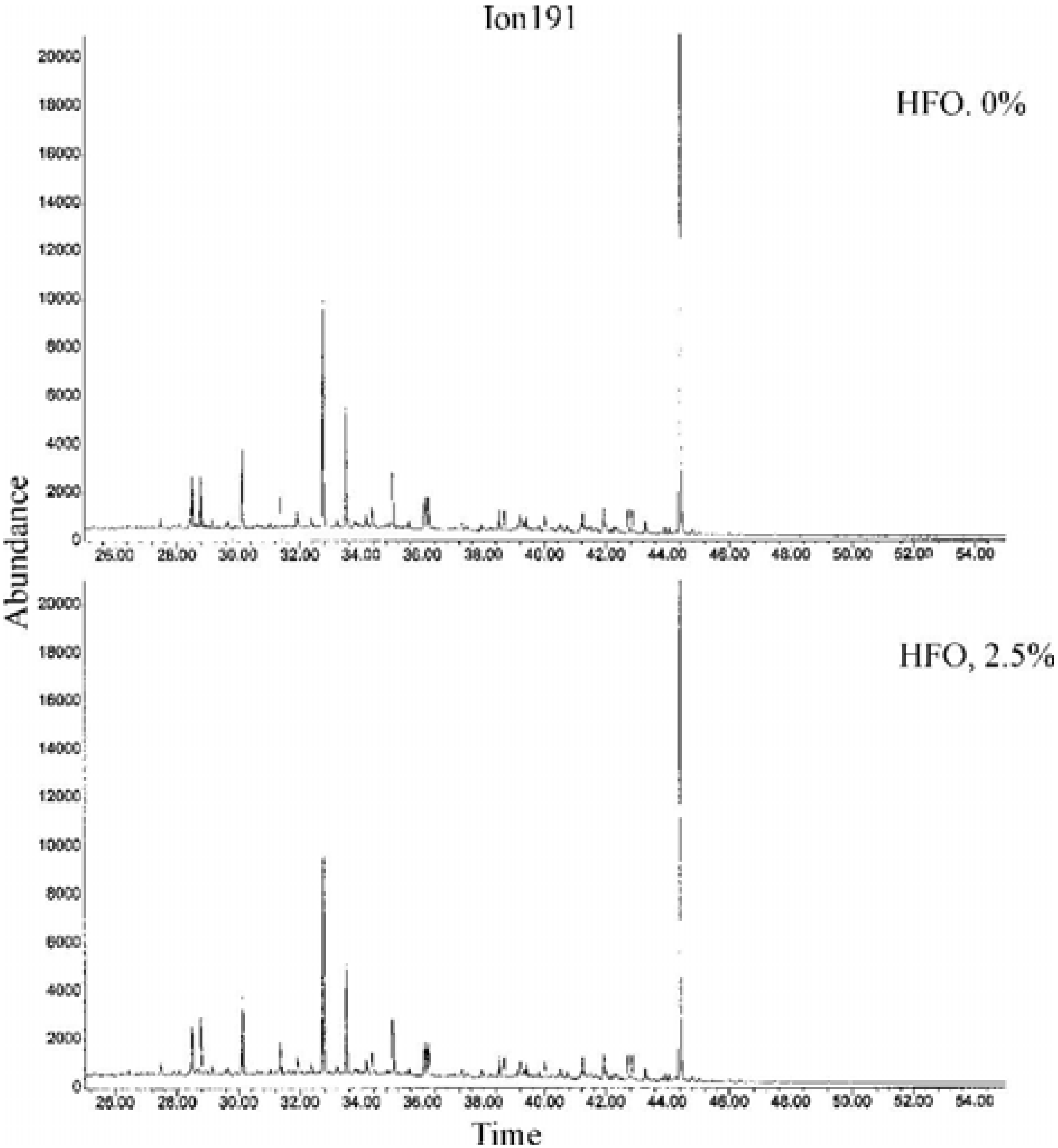


Figure A11-6 GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of HFO 6303

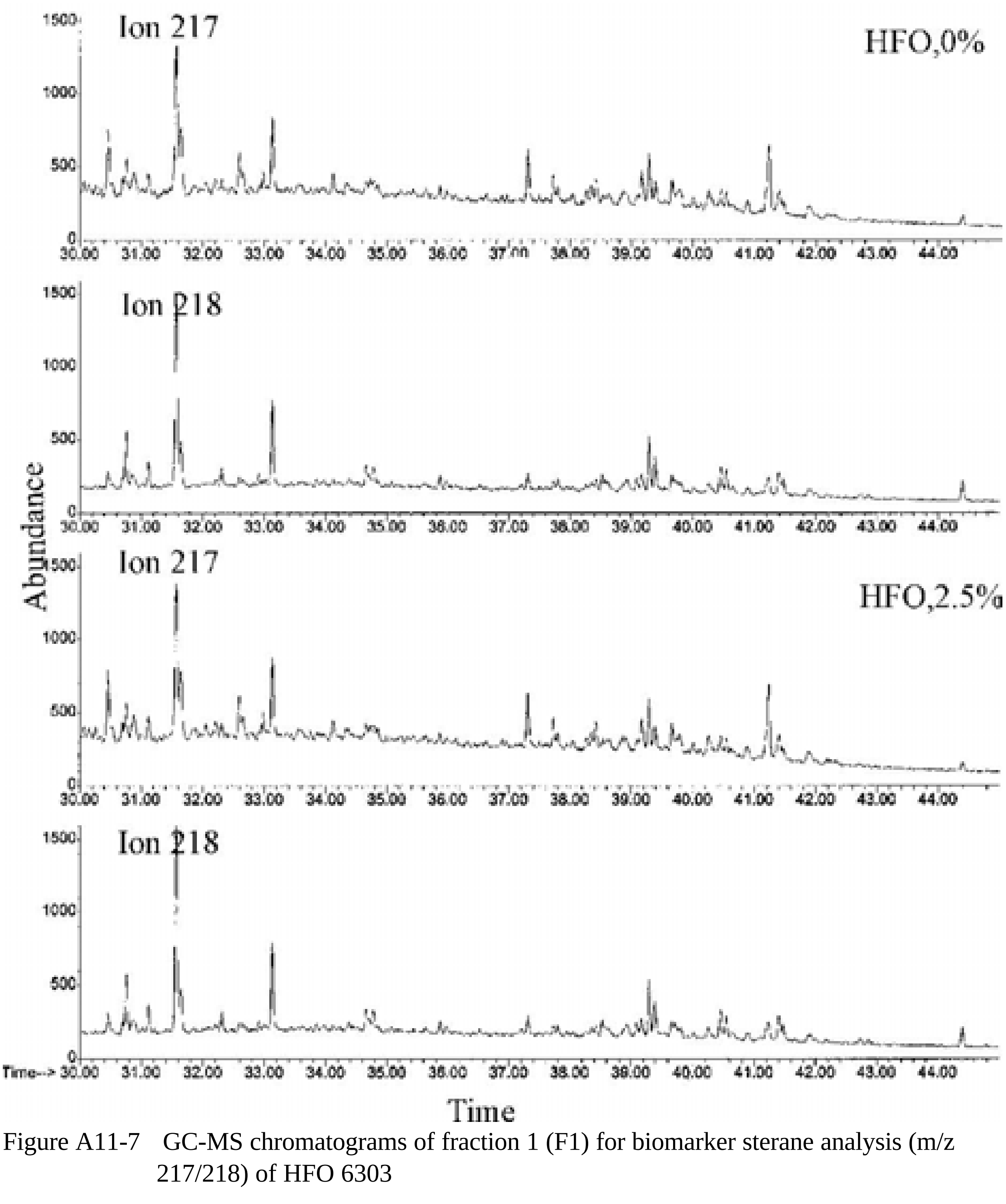


Figure A11-7 GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218) of HFO 6303

12 GC Chromatograms for Orimulsion-400

Figure A12-1 GC-FID chromatograms of fraction 1 (F1) for saturates and of fraction 3 (F3) for total petroleum hydrocarbons (TPH) of Orimulsion-400

Figure A12-2 GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of Orimulsion-400

Figure A12-3 Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of Orimulsion-400

Figure A12-4 Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184, 178, 192, 206, 220, 234, 198, 212, 226, 166, 180, 194, 228, 242, 256, and 270) of Orimulsion-400

Figure A12-5 GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of Orimulsion-400

Figure A12-6 GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218) of Orimulsion-400

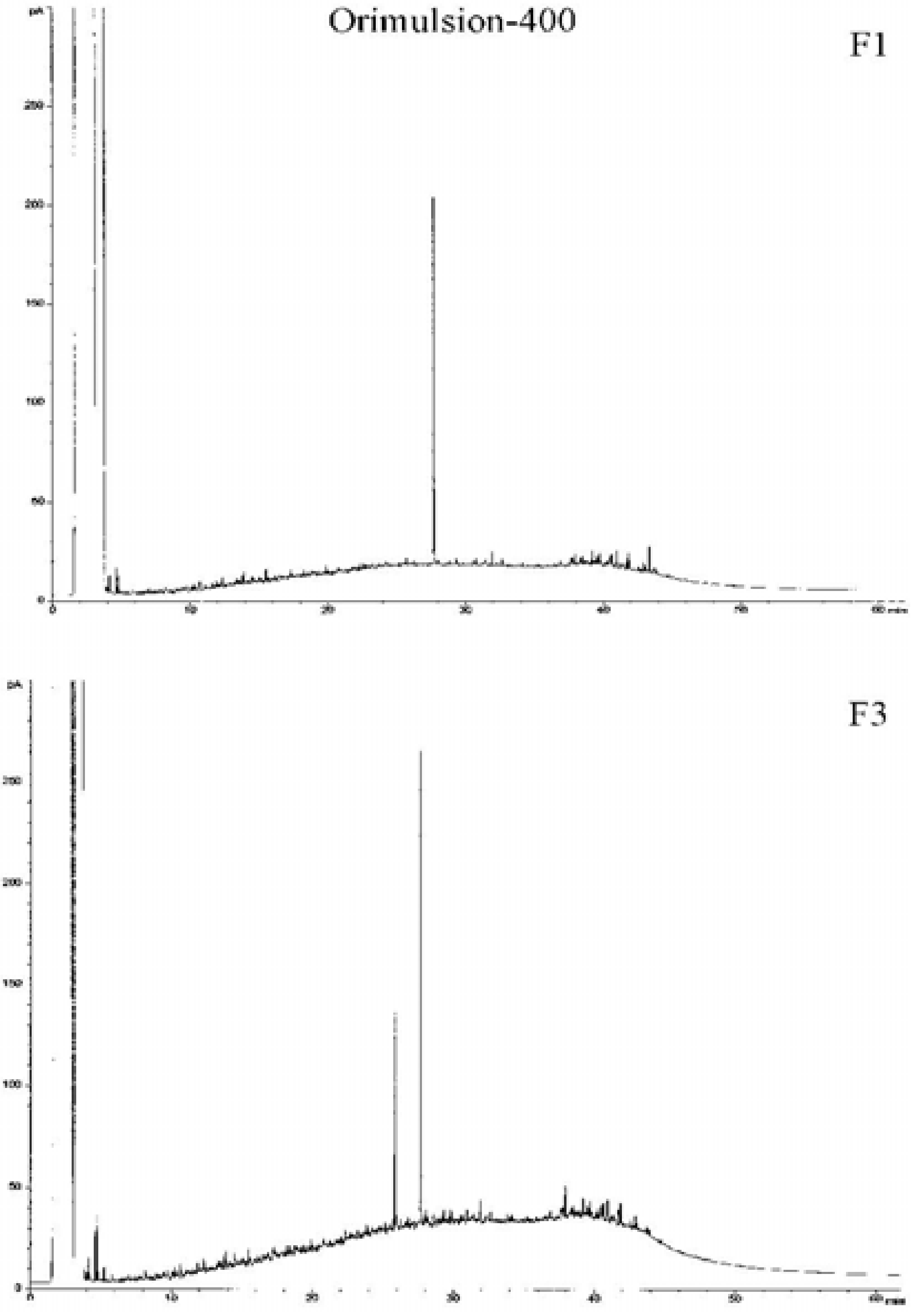


Figure A12-1 GC-FID chromatograms of fraction 1 (F1) for saturates and of fraction 3 (F3) for total petroleum hydrocarbons (TPH) Orimulsion-400

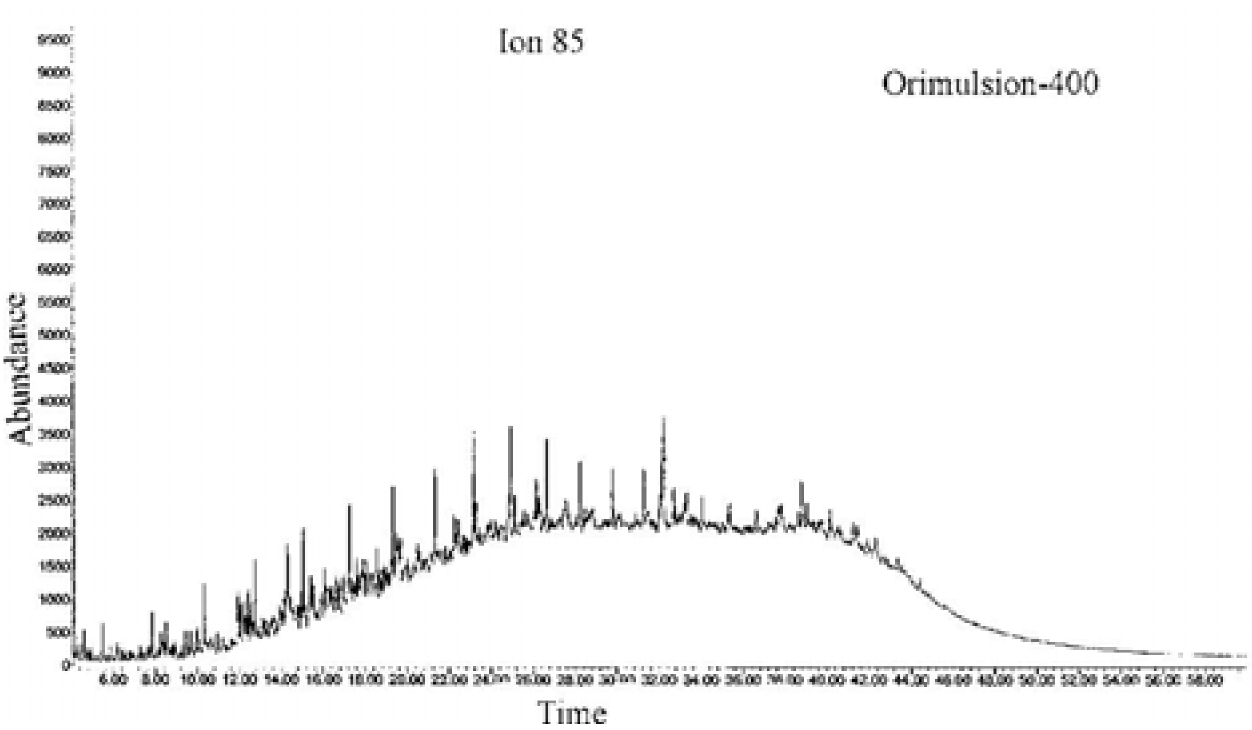


Figure A12-2 GC-MS chromatograms of fraction 1 (F1) for n-alkane distribution (m/z 85) of Orimulsion-400

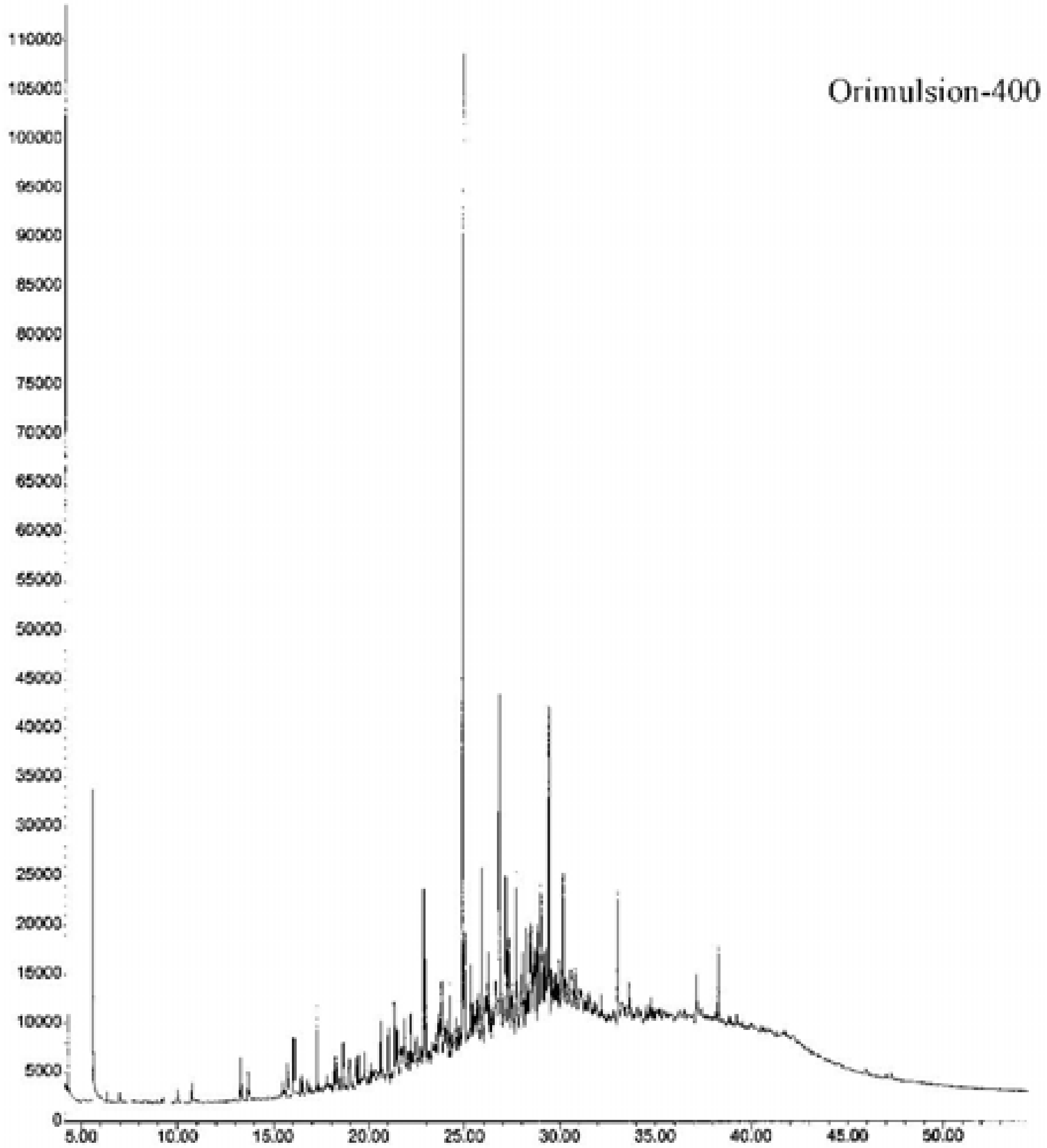


Figure A12-3 Total ion GC-MS chromatograms of fraction 2 (F2) for determination of PAHs of Orimulsion-400

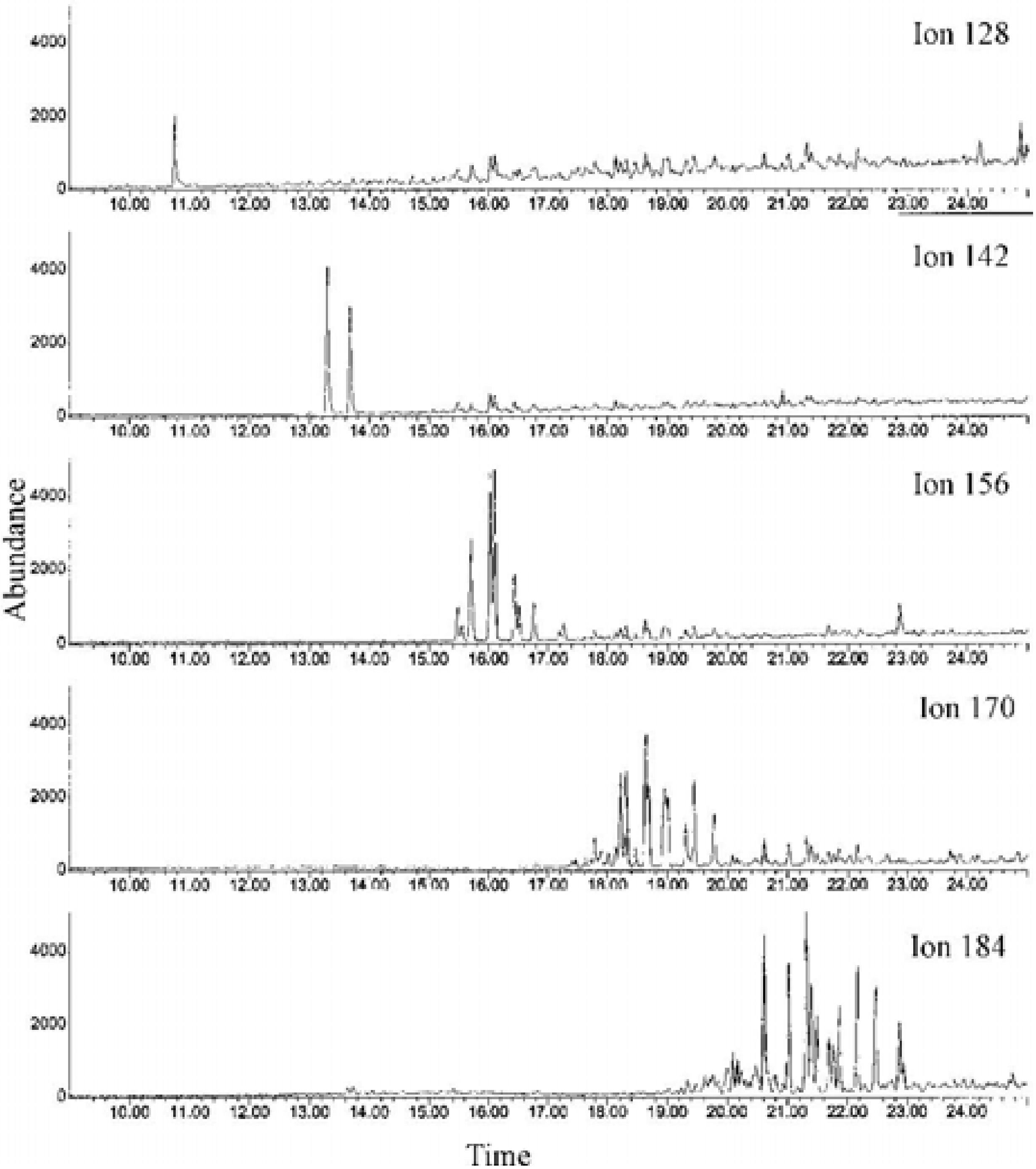


Figure A12-4a Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 128, 142, 156, 170, 184) of Orimulsion-400

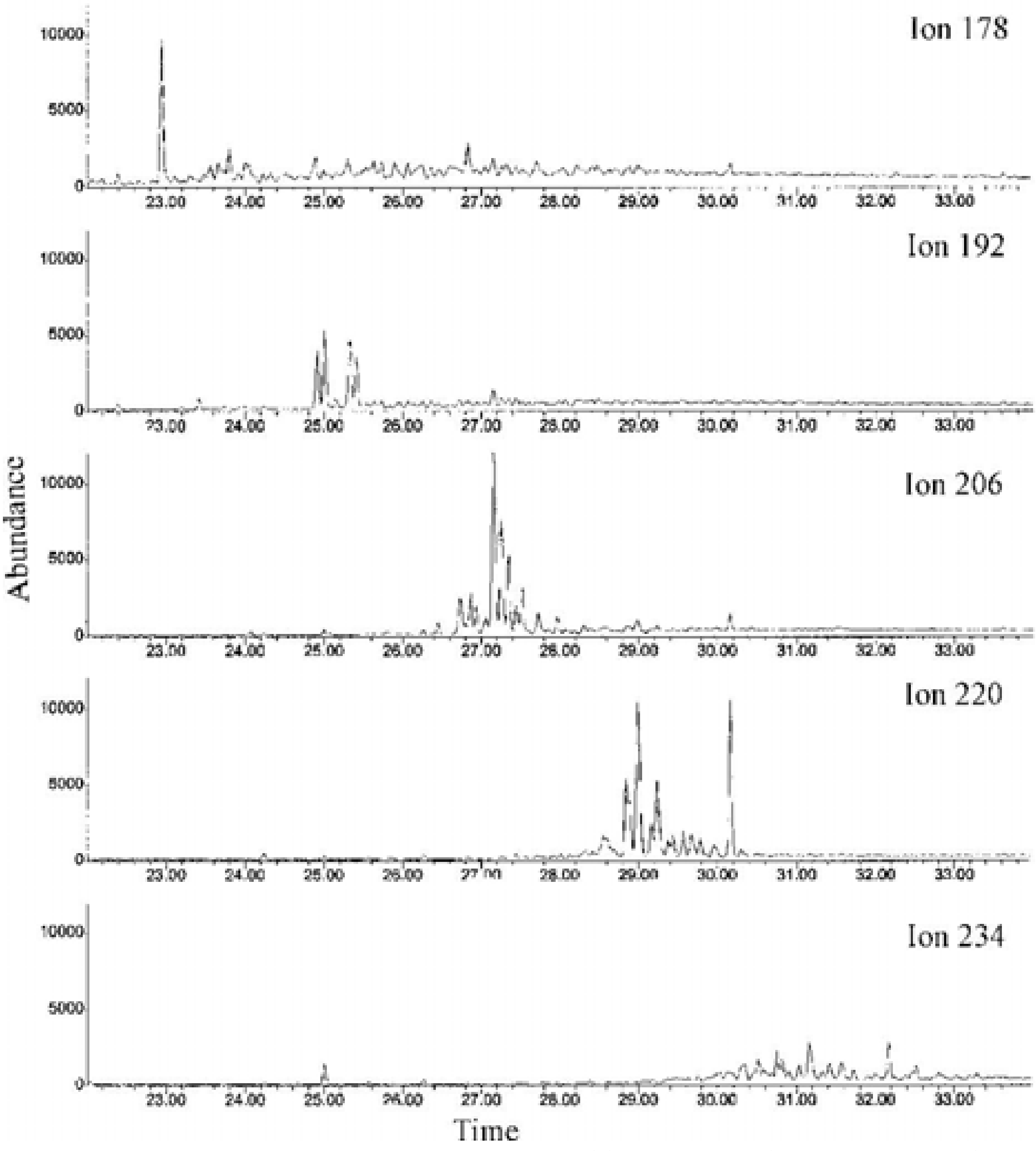


Figure A12-4b Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 178, 192, 206, 220, 234) of Orimulsion-400

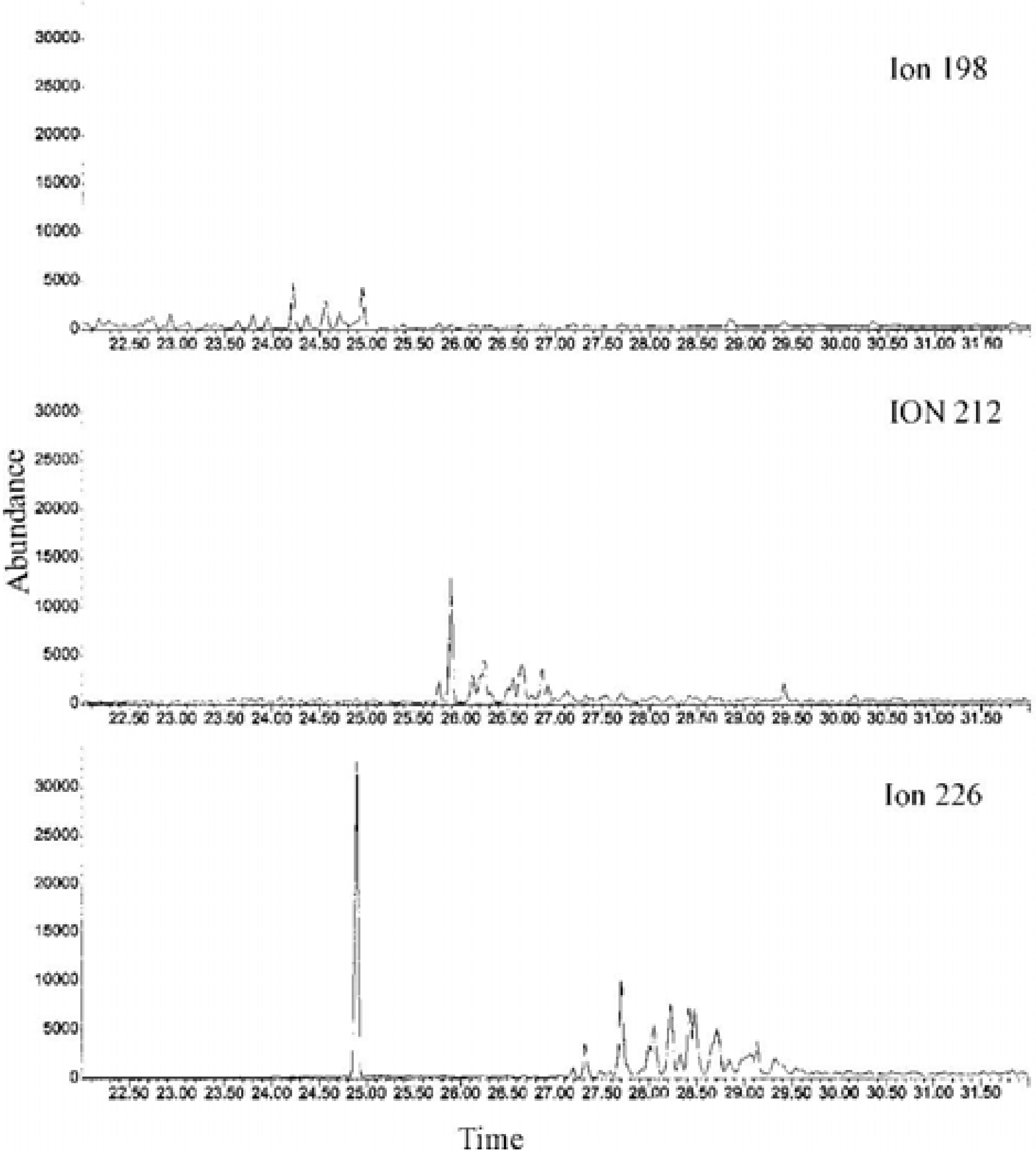


Figure A12-4c Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 198, 212, 226) of Orimulsion-400

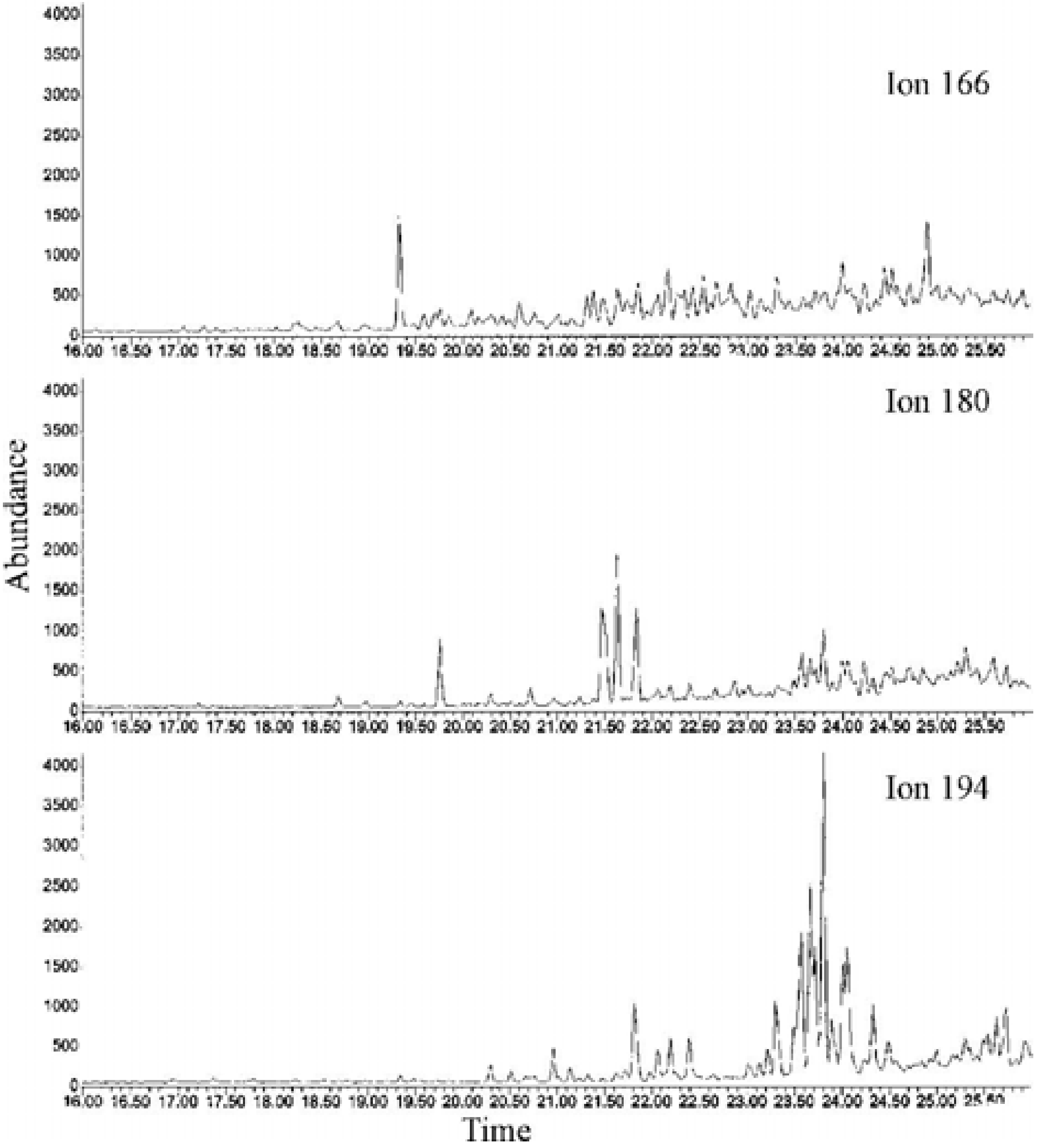


Figure A12-4d Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 166, 180, 194) of Orimulsion-400

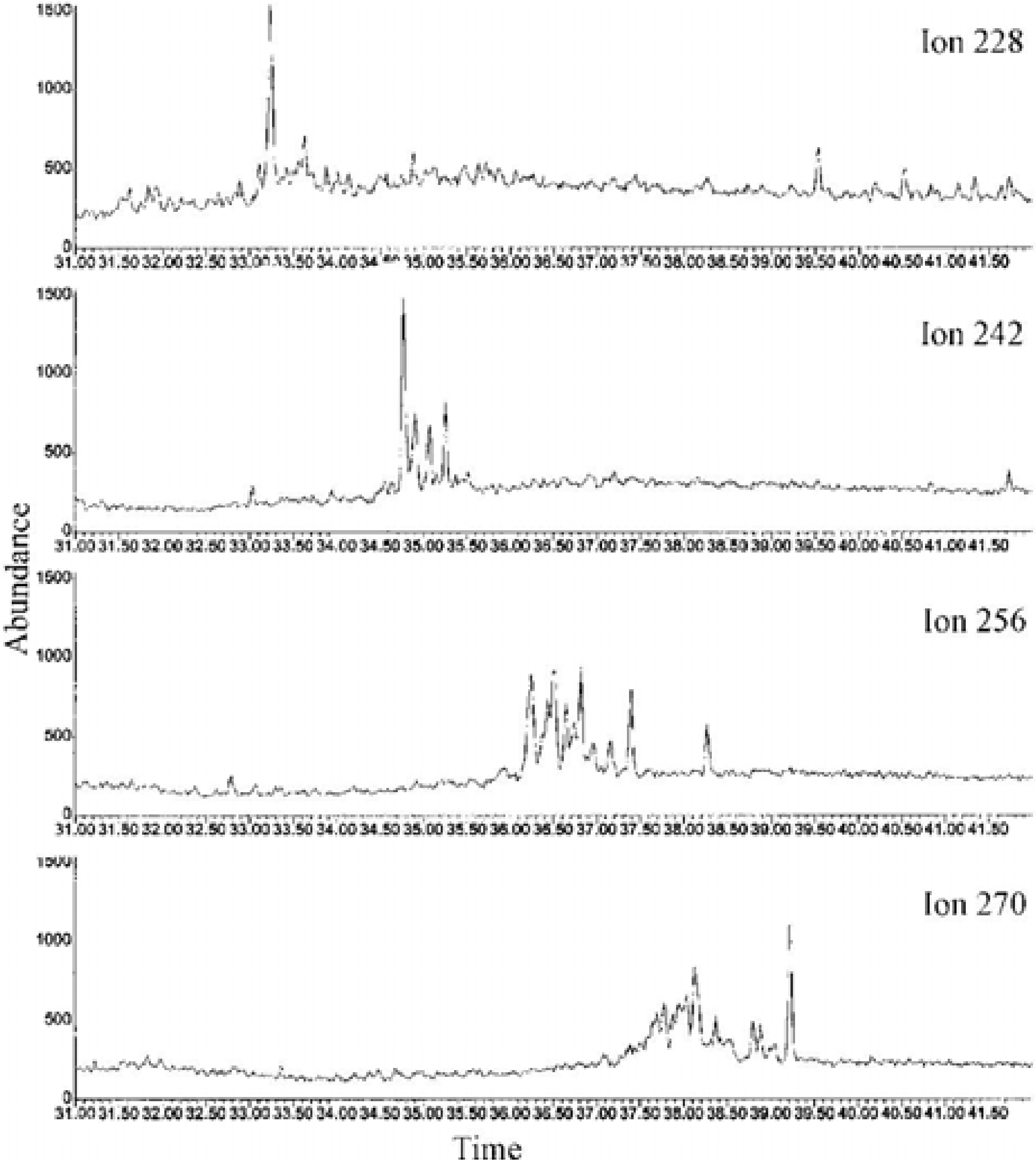


Figure A12-4e Extracted ion GC-MS chromatograms of fraction 2 (F2) for determination of the 5 target alkylated PAH homologues (m/z: 228, 242, 256, 270) of Orimulsion-400

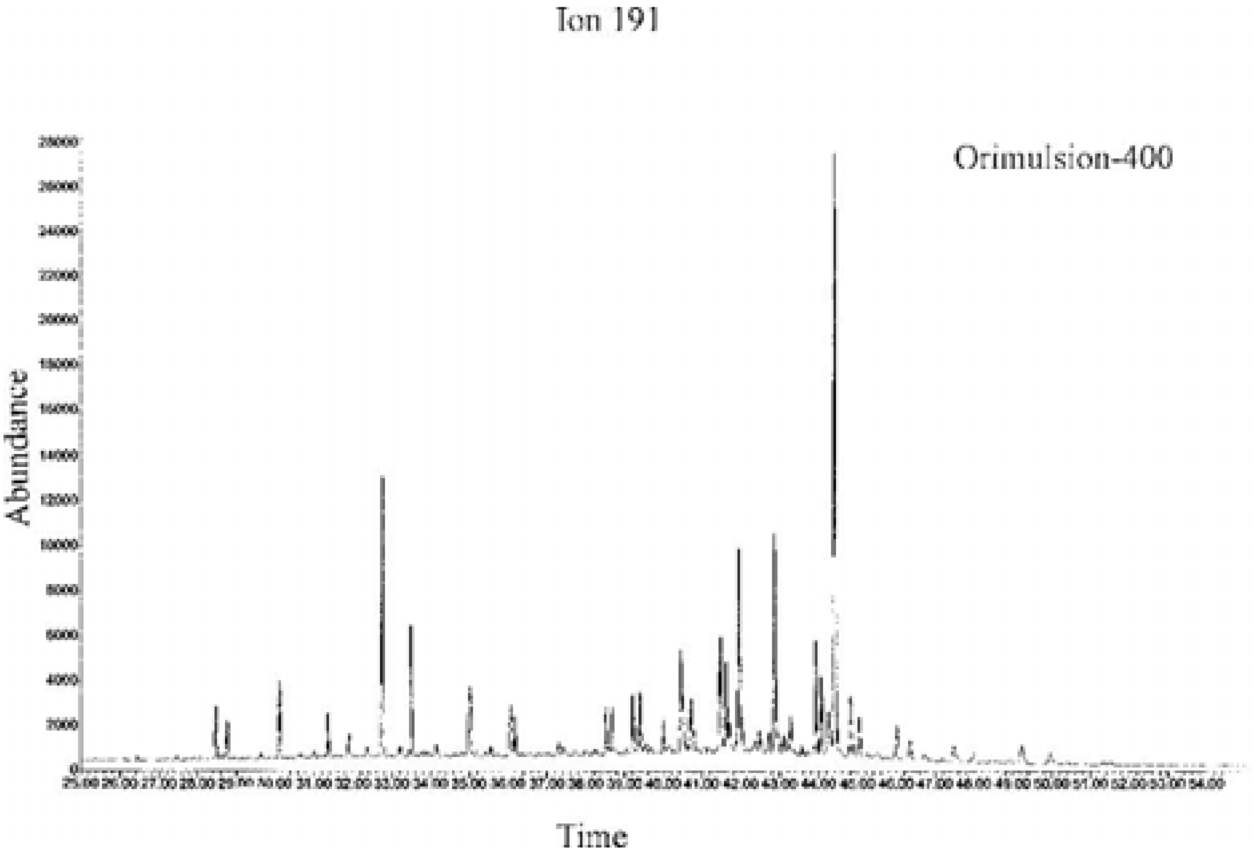


Figure A12-5 GC-MS chromatograms of fraction 1 (F1) for biomarker terpane analysis (m/z 191) of Orimulsion-400

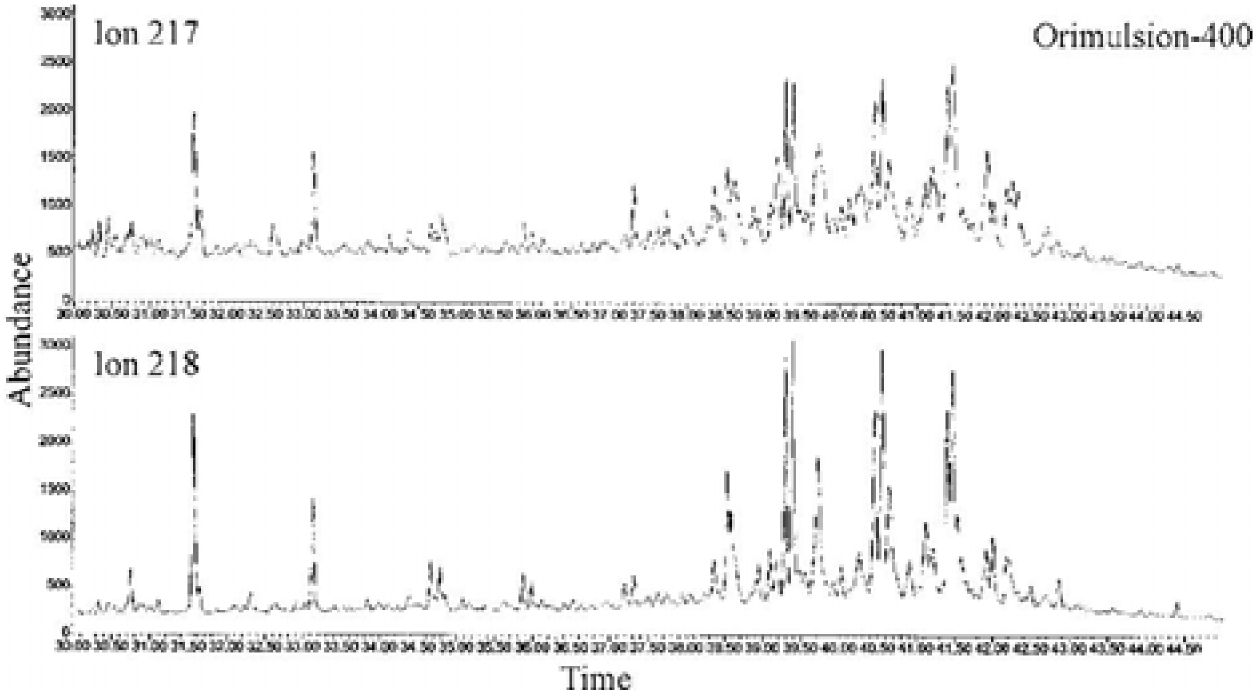


Figure A12-6 GC-MS chromatograms of fraction 1 (F1) for biomarker sterane analysis (m/z 217/218) of Orimulsion-400