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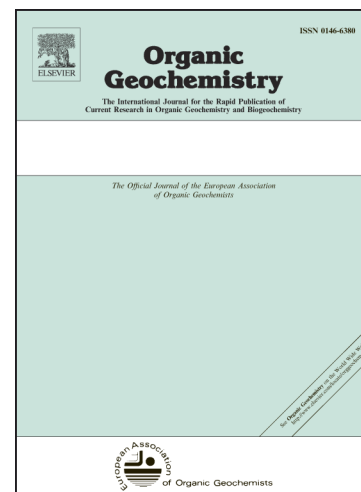
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Universal Biomarker Analysis: Aromatic hydrocarbons

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Highlights

- GC×GC with dual FID and ToF-MS (EI/FI) detection provides superior biomarker analyses
- Non-targeted, pseudo parent-daughter mass spectra are available for all components
- Application for aromatized biomarker discovery is demonstrated
- A/B-ring C₂₆-C₂₉ diaromatic steroidal hydrocarbons identified in a crude oil

Abstract

Universal Biomarker Analysis is a GC×GC-ToFMS method that provides absolute quantification and non-targeted pseudo MS-MS for all resolved hydrocarbon components in petroleum and rock extracts. This is achieved by merging two chromatographic datasets obtained under field ionization (FI), which provides molecular ions, and electron impact (EI), which provides diagnostic fragment ions. We recently demonstrated this technique for the analysis of saturated biomarkers (Walters et al., 2018. *Org. Geochem.* 115, 57). Here, we show its application to aromatic biomarkers. Universal Biomarker Analysis is compared to conventional GC-MS for frequently analyzed aromatic hydrocarbons, such as the alkylated naphthalenes and biphenyls, mono- and tri-aromatic steroidal hydrocarbons to illustrate where this new method provides demonstrated advantages. The technique is well suited for the analysis of rare species not commonly analyzed in targeted GC-MS/MS analyses. This is illustrated by the tentative identification of A/B-ring C₂₆-C₂₉ diaromatic steroidal hydrocarbons in a crude oil, compounds that have been previously identified as minor components of immature rock extracts, and indications of previously unknown C₂₆ methyl-triaromatic steroidal hydrocarbons.

1. Introduction

Petroleum and rock extracts are some of the most complex mixtures in nature and the quest to understand their composition has pushed organic geochemists to become early adaptors of new technologies in molecular analysis. Much of our current knowledge of the hydrocarbon content of source rock and petroleum can be traced to advances in gas chromatography and mass spectrometry - from the early hybrid GC-MS systems introduced in the 1960s, the capillary columns with bonded phases of the 1970s, to spectrometers capable of MS-MS in the 1980s. Through this instrumentation, the identification and quantification of all major and minor hydrocarbon species in geologic samples, as well

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