

Poster

Biomarker characterization in bitumen from Irati Formation by two-dimensional gas chromatography with time of flight mass spectrometry (GC x GC-TOFMS)

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Irati Formation is a geological formation of the Paraná basin in Brazil with reserve of oil shale estimated at 700 million barrels [1]. Correct biomarker characterization is essential to determinate important geochemical parameters such as origin, thermal maturity and depositional environment. GCxGC-TOFMS has been recently employed in biomarker characterization allowing better separation of class of molecules, individual identification of compounds and discovery of new molecules [2].

GCxGC-TOFMS was employed to the analysis of biomarkers in bitumen from an outcrop of Irati Formation suitable for bitumen extraction. Steranes and hopanes were detected and unambiguously identified, besides six unknown compounds were found, **Figure 1** shows the mass spectrum of one of them with a structure proposed based on relative retention time and the $M^{+•}$ m/z 316, coherent with a tetracyclic terpane C23, since tricyclic terpanes C23 have $M^{+•}$ m/z 318.

17 α (H)-Diahopane (DH30) was identified by relative retention time in both dimensions and comparison of its mass spectrum (**Figure 2**) with mass spectrum described in the literature [3]. DH30 is differentiated from other isomeric hopanes like Hopane 30 or Lupane by the diagnostic fragment m/z 274. DH30 is reported in bitumen from Irati Formation for the first time.

The same sample was studied by GC-qMS which was unable to identify DH30 and detect the six unknown compounds [4]. The TOF mass analyzer furnishes cleaner spectra and present less spectral distortion. Thus, this work shows that GCxGC-TOFMS can uncover unexplored geochemical information.

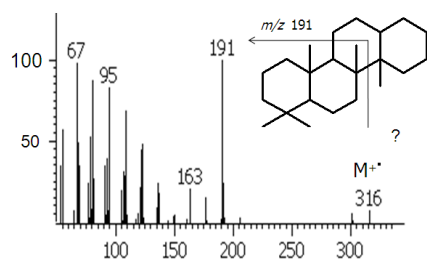


Figure 1: Unknown compound mass spectrum and proposed structure.

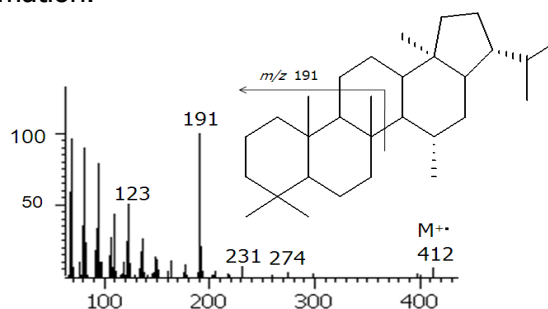


Figure 2: DH30 mass spectrum.

- [1] Afonso, J. C.; Schmal, M.; Cardoso, J. N. *Fuel*, **1994**, 73, 363-366.
- [2] Ventura, G. T.; Kenig, F.; Reddy, C. M.; Frysinger, G. S.; Nelson, R. K.; Mooy, B. V.; Gaines, R. B., *Org. Geochem.*, **2008**, 39, 846-867.
- [3] Farrimond, P.; Telnes, N. *Org. Geochem.*, **1996**, 25, 167-177.
- [4] Lisboa, A. C., *MSc Dissertation*, Universidade Federal do Rio de Janeiro, Brazil, **2006**.