HOPANOID COMPOSITION FROM MIOCENE SEDIMENT SAMPLES (LOWER TAGUS BASIN, PORTUGAL) BY GCMS

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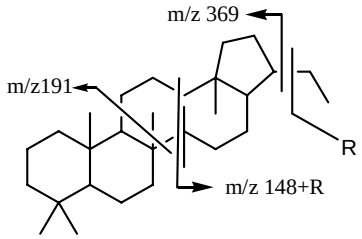
Geohopanoids constitute an important class of natural compounds of bacterial origin, which are near ubiquitous in the geosphere. In the last few years there has been an increasing interest in the characterization of hopanoids from sediments, since these molecular fossils play a role of geochemical markers to preserve information regarding the inputs of bacterial biomass to sediments, and the paleoenvironmental conditions prevailing at the time of sediment deposition.[1]

In this communication we report the GCMS characterization of hopanoids extracted from Miocene sediment samples (Lower Tagus Basin, BEL and PP - Belverde borehole, CAP – Costa de Caparica). Following cleavage of hopanoid polyhydroxylated side chains with periodic acid, and sodium borohydride reduction, the structures were determined from characteristic mass fragmentation displayed in the corresponding "hopanograms" of acetylayed derivatives, using single ion monitoring (SIM) at *m/z* 191 (Figs.1 and 2). Nine geohopanoids could be identified, whose molecular masses were confirmed by GCMS with field ionization (FI) (Table 1).



R = H, CH_3, C_2H_5, etc.
R = $CH(CH_3)_2$: Hopane ($C_{30}H_{52}$)

Fig.1. Characteristic mass fragments of hopanoid spectra.

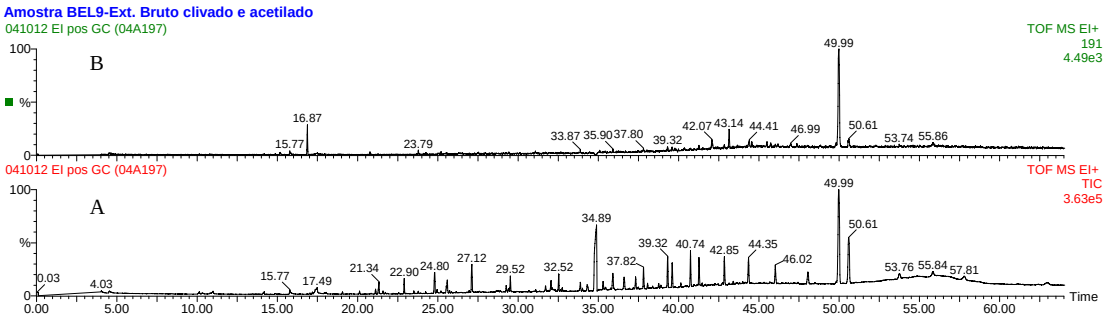
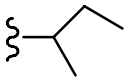
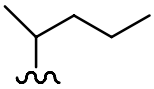
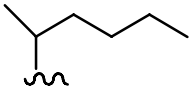
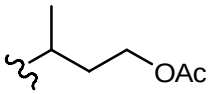
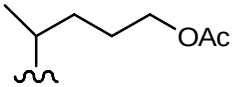


Fig.2. GCMS chromatograms from BEL extract after cleavage and acetylation;- A-Total ion chromatogram (TIC); B-SIM at *m/z* 191.

Table 1. Identification of geohopanoids from SIM spectra at *m/z* 191

Retention time (EI)	Side chain fragment (R)	M^+
42.04		398
43.15		412
44.55		426
45.72		440
47.42		454
57.56		484
62.12		498

References

1. Ourisson, G., Albrecht, P., *Accounts of Chemical Research*, **25**, 398 (1992).

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