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Poster Session Day 3

Position-Specific Carbon Isotope Analyses of C_{16} *n*-alkane with Gas Chromatography-Orbitrap Mass Spectrometer

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Long chain *n*-alkanes (length $\geq$ 27), primarily derived from leaf wax of higher plants, can be well preserved in the geological records, which underpin reconstruction of past vegetation and climate. However, current studies on composition and compound-specific isotope signatures of long chain n-alkanes cannot distinguish their diverse origins clearly. Position-specific isotope analyses (PSIA) using chemical degradation and nuclear magnetic resonance (NMR) have identified distinct intra-molecular isotopic compositions in acetogenic lipids including fatty acids and *n*-alkanes across different organisms. To extend this proxy for geological applications, we develop PSIA of *n*-alkanes using fragmentation with an Orbitrap MS that has significantly lower sample size limit. In order to learn the fragmentation paths (as a prerequisite for reconstructing position-specific isotope signature), we examined fragmentation patterns of hexadecane (C_{16}) with 1,2-$^{13}C_2$-labeled. By optimizing source temperature (200°C) and C-trap offset (2V), we attained sufficient intensities of all C_4-C_{14} fragments. The isotopologue ratios of $^{13}C_2{}^{12}C_{n-2}H_{2n+1}/{}^{12}C_nH_{2n+1}$ and $^{13}C{}^{12}C_{n-1}H_{2n+1}/{}^{12}C_nH_{2n+1}$ ($4 \leq n \leq 14$) can be compared with corresponding theoretical values for different fragmentation patterns (single cleavage *vs.* second cleavage *vs.* random rearrangement). We found that $C_{\geq 10}$ fragments are primarily generated by single cleavage, providing their efficacy for PSIA of hexadecane. And as expected, the smaller fragments are generated partly by random rearrangement or second-cleavage from larger fragments. Our results of optimized fragmentation conditions and fragment selection can be generalized for PSIA of *n*-alkanes.