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Session 9) Metabolism & Medical Application of Isotopologue

Site-Specific $\delta^{13}C$, D and Clumped Isotope Analysis of Steroidal Compounds for Forensic and Geochemical Applications

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Steroidal compounds are crucial biomolecules in nature, governing diverse biological functions and serving as indicators of organic matter origin, depositional environmental history, and facilitating geological correlations in petroleum geochemistry (Moldowan et al., 1985; Volkman, 2003). Nevertheless, different organisms can generate identical steroidal compounds, so confident identifications of sources can be enhanced by stable isotope analysis. Prior studies have demonstrated the utility of molecular-average $\delta^{13}C$ to improve interpretations of the phylogenetic and environmental origins of steroidal compounds (Freeman et al., 1990). However, there are challenges and limitations associated with interpretation of $\delta^{13}C$ values of steroids in geochemical contexts, including post-depositional alteration and the influence of different abiotic and biotic processes. In addition, $\delta^{13}C$ values of steroidal compounds from different sources might overlap which in turn might challenge the interpretation of their origin based on their $\delta^{13}C$ (Piper and Thevis, 2022).

We will present results of a study that aims to develop a novel analytical method for measuring multiple stable-isotope properties of steroidal compounds, including the intramolecular distributions of ^{13}C and D, with the aim of providing more reliable constraint of sources, environments and alteration histories. Unlike traditional bulk carbon isotope analysis, site-specific carbon isotope analysis focuses on specific carbon positions within organic molecules, enabling detection of subtle variations in carbon cycling, metabolic pathways, and microbial processes that may not be evident from bulk measurements alone. A first proof of concept study focuses on forensic discrimination of isotopic structures of natural and synthetic steroids in human subjects for the purpose of sports doping applications. Preliminary results reveal differences in the measured site-specific ^{13}C, D and clumped isotope of various isotopologues derived from natural and synthetic steroids despite the similarity in their molecular isotope values.

References

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