

In vitro biotransformations of isocupressic acid by cow rumen preparations: formation of agathic and dihydroagathic acids.

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Abstract

Isocupressic acid [15-hydroxy λ -8(17),13E-dien-19-oic acid] (1) was incubated under anaerobic conditions for 48 h in an in vitro ruminal fluid mixture and was transformed into two metabolites. The two metabolites were identified by GC/MS as agathic acid [λ -8(17),13(E)-diene-15,19-dioic acid] (4E) and dihydroagathic acid [λ -8(17)-ene-15,19-dioic acid] (6). Metabolite identities were confirmed by chemical conversions of isocupressic acid (1) and imbricatolonic acid (5) into 4E and 6, respectively. Structures of synthetic metabolites were confirmed by ¹H and ¹³C NMR, specific rotation, GC/MS, and high-resolution mass spectrometry. Plasma obtained from cows that were fed Ponderosa pine needles contained (13R,S)-dihydroagathic acid (6) but not isocupressic acid (1) or 4E. The results suggest that isocupressic acid (1) is metabolically oxidized to agathic acid (4E), subsequently reduced to (13R,S)-dihydroagathic acid (6) in the rumen, and then absorbed into the bloodstream of cattle.