

SUPPORTING INFORMATION: Mass Spectrometric Analysis of Isotope-enriched Compounds Used in the Study of OMP Decarboxylase

A Substantial Oxygen Isotope Effect at O2 in the OMP Decarboxylase Reaction: Mechanistic
Implications

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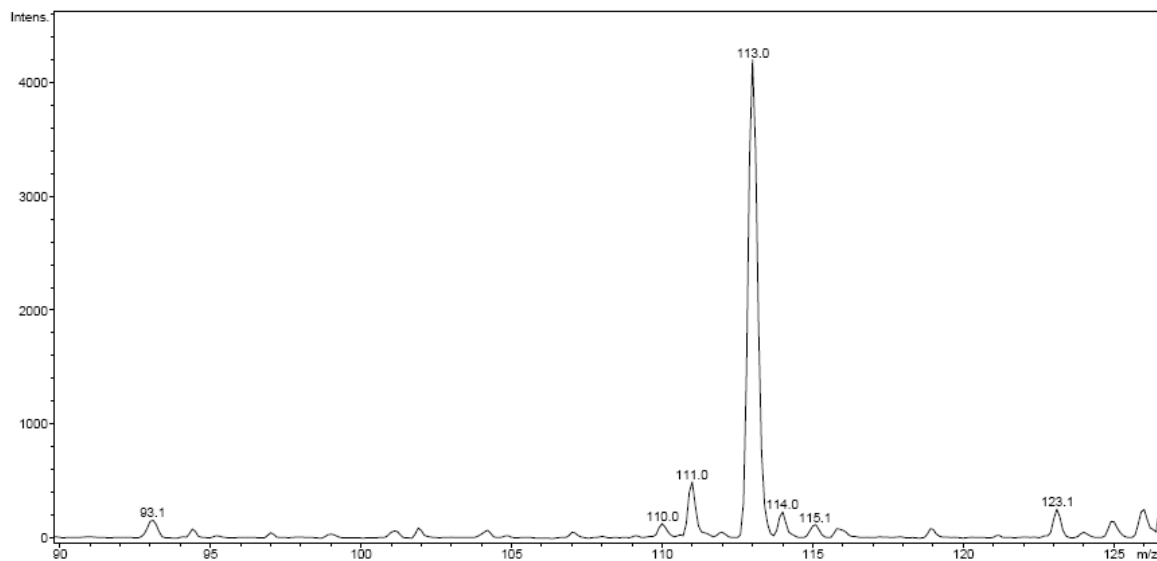


Figure 1: Mass spectrometric analysis of [$^{18}\text{O}_2$] uracil following synthesis by hydrolysis of 2-ethylthiouracil in acidified H_2^{18}O . Data is for anion detection within the MS. Desired compound with single ^{18}O incorporation has monoanion mass of 113.

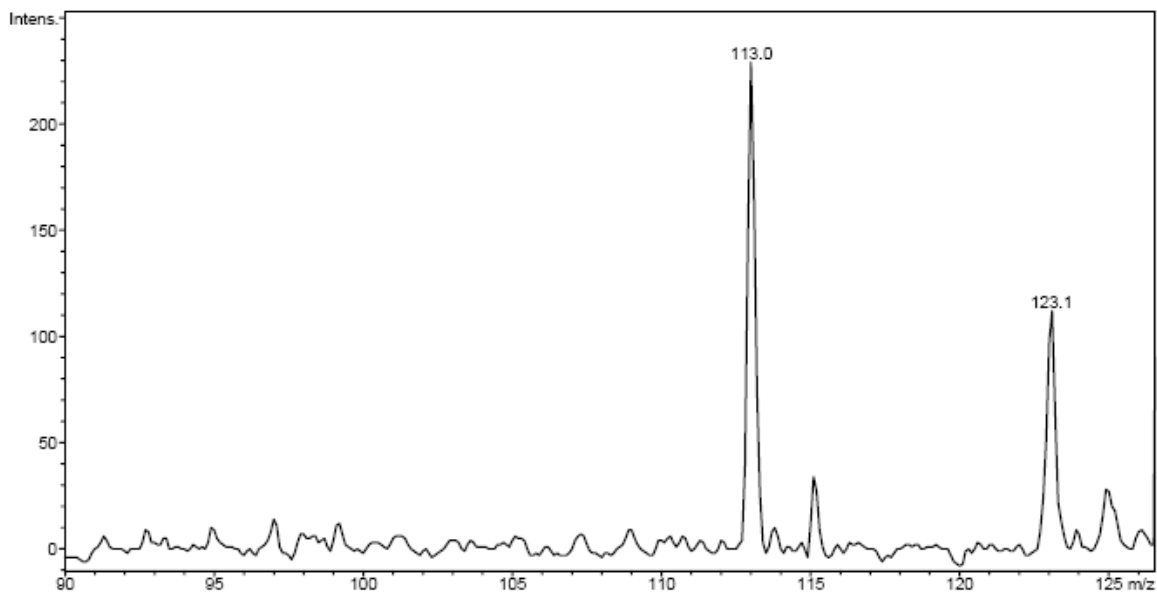


Figure 2: Mass spectrometric analysis of [$^{18}\text{O}_2$] uracil following exposure to 0.5 M NaOH at room temperature for 8 days. Data is for anion detection within the MS. Desired compound with single ^{18}O incorporation has monoanion mass of 113.

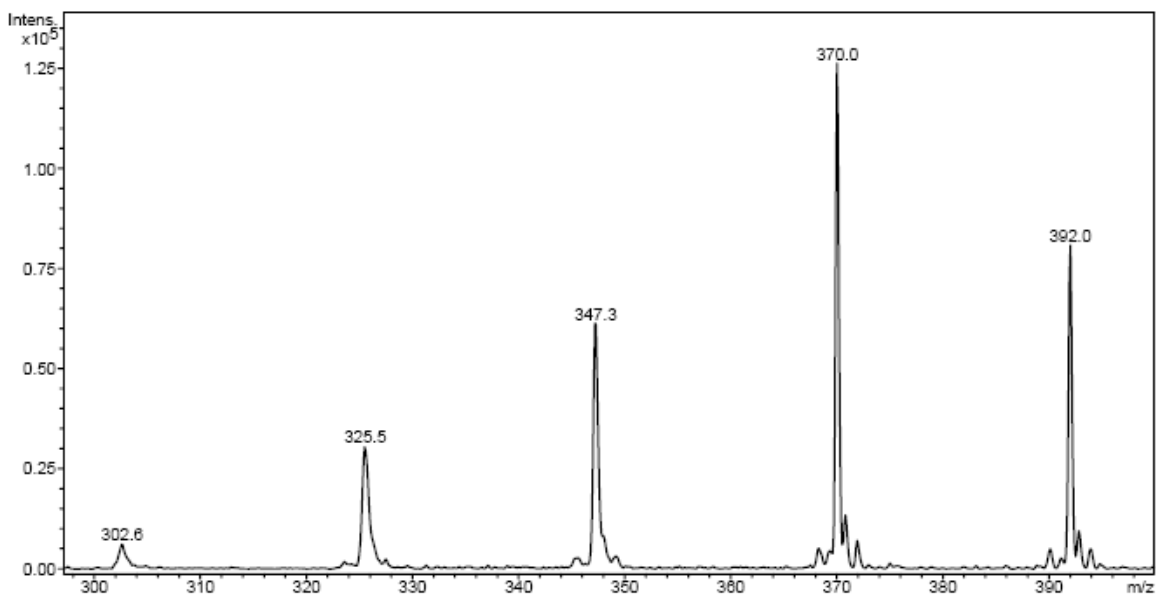


Figure 3: MS data on [¹⁸O₂, ¹³C-carboxyl]-OMP. The target monoanion mass is 370. Decarboxylation and presence of sodium produces peaks at 392, 347, and 325. Mass of 325 is consistent with decarboxylation within the MS to lose ¹³CO₂.