

Mechanisms of Herb-Drug Interactions Involving Cinnamon and Cytochrome P450 2A6: Focus on Time-dependent Inhibition by Cinnamaldehyde and 2-Methoxycinnamaldehyde

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Drug Metabolism and Disposition-AR-2020-000087

Supplementary Material 6 LC-MS/MS traces and spectra for metabolites generated from CYP2A6-mediated MCA metabolism

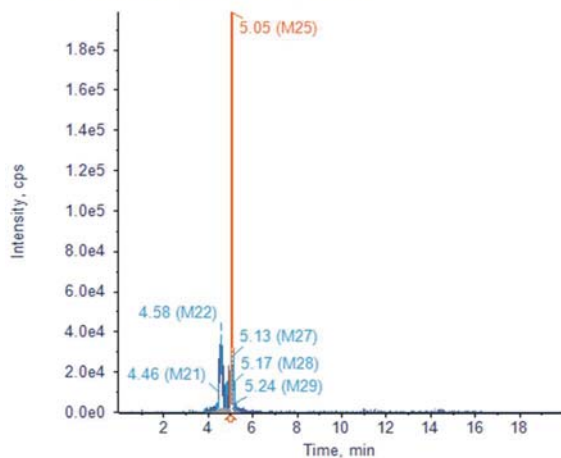
M25 - Loss of CH₂+Glutathione Conjugation [M+H]⁺

Formula: C₁₉H₂₅N₃O₈S

RT: 5.05 min

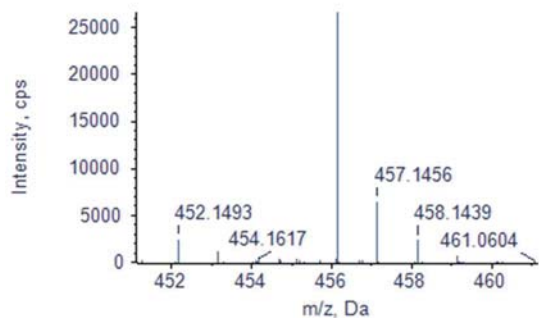
m/z: 456.1436

MS Sample, XIC from 456.1300 to 456.1604



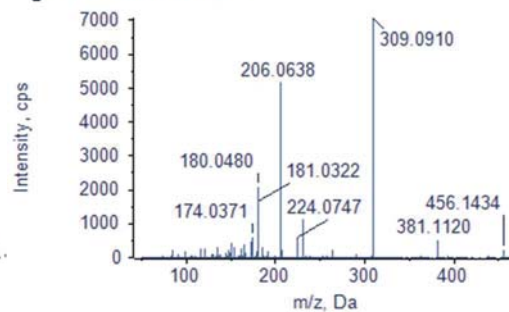
MS Spectrum

+TOF MS at 5.05 min



MS/MS Spectrum

+TOF MS/MS of 456.1



Common product ions (m/z): 51.0230, 55.0175, 65.0377, 77.0384, 79.0534, 91.0541, 103.0540, 105.0679, 107.0493, 115.0534, 119.0481, 120.0605, 131.0520, 135.0807, 145.0647

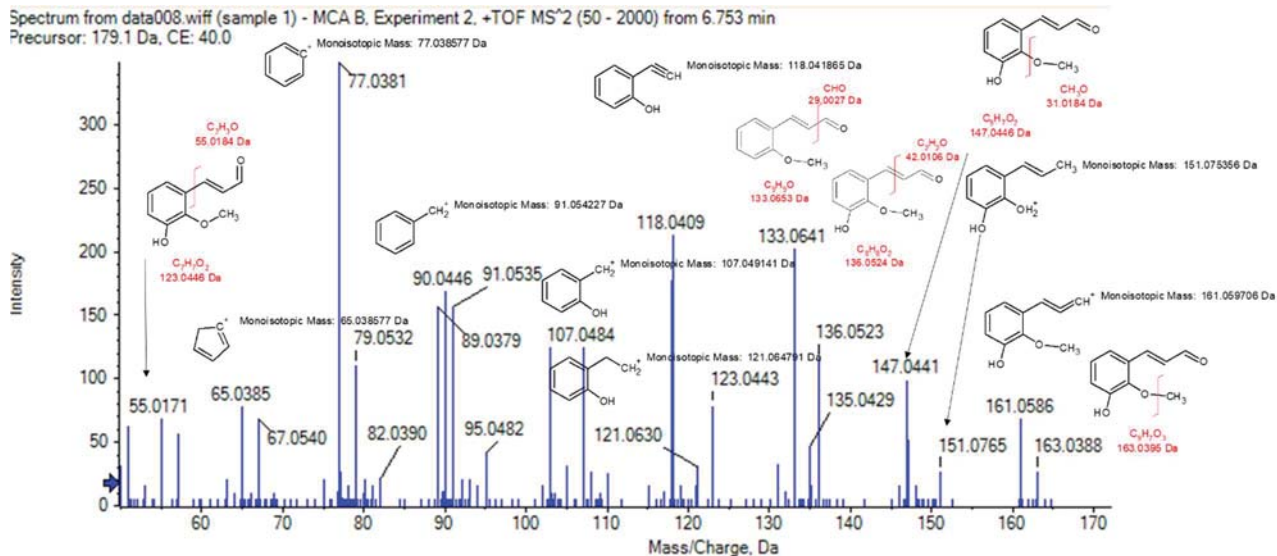
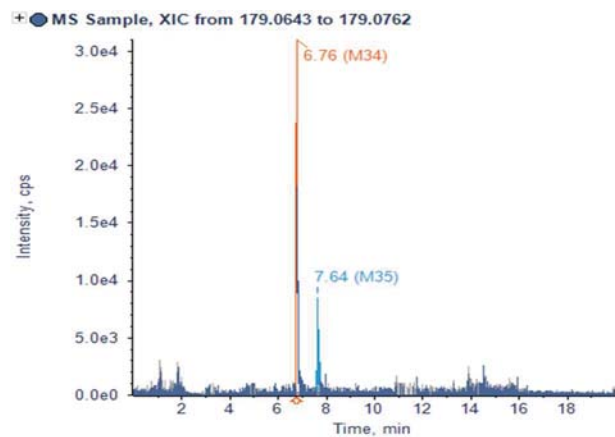
Peaks selected for assignment (m/z): 84.0442, 91.0541, 98.0056, 116.0160, 121.0647, 129.0661, 130.0496, 135.0437, 138.0139, 144.0112, 147.0676, 149.0297, 149.0601, 151.0760, 153.0373, 162.0221, 165.0242, 173.0832, 174.0371, 180.0480, 185.0381, 191.0408, 206.0638, 224.0747, 231.0440, 263.0856, 290.0861, 309.0910, 381.1120, 456.1434

M34 – Aromatic Oxidation

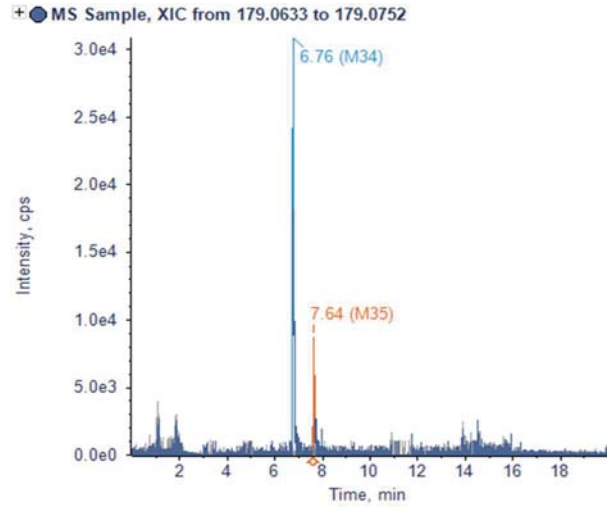
Formula: C₁₀H₁₀O₃

RT: 6.76 min

m/z: 178.0630



M35 – Epoxide [M+H]⁺
Formula: C₁₀H₁₀O₃
RT: 7.64 min
m/z: 179.0692



Spectrum from data008.wiff (sample 1) - MCA B, Experiment 2, +TOF MS² (50 - 2000) from 7.647 min
Precursor: 179.1 Da, CE: 40.0

