Nutrition&Metabolism

Electronic Supplementary Material

Disintegration of wheat aleurone structure has an impact on the bioavailability of phenolic compounds and other phytochemicals as evidenced by altered urinary metabolite profile of diet-induced obese mice

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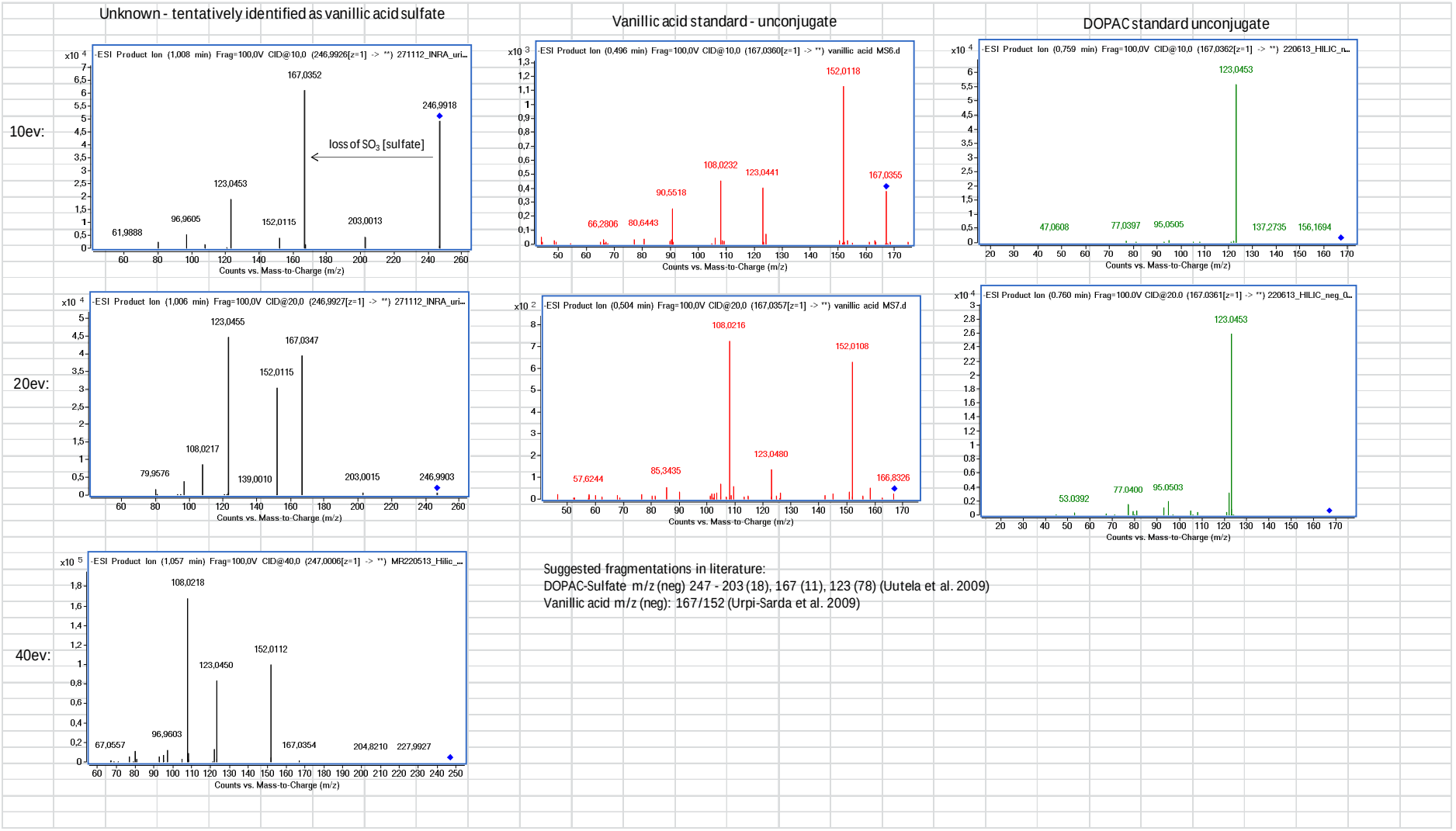
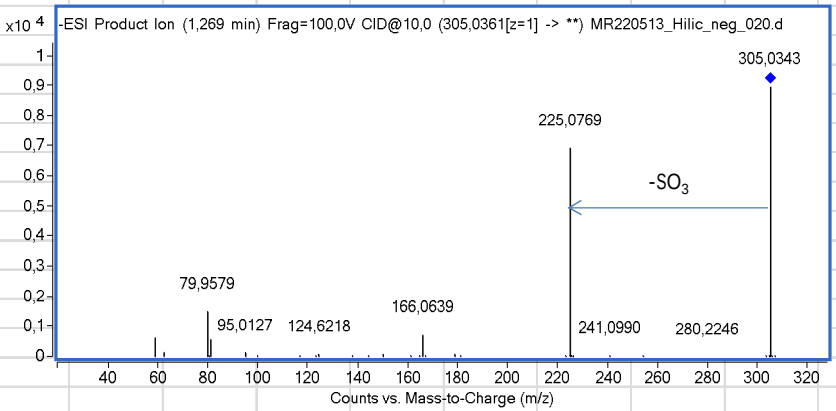
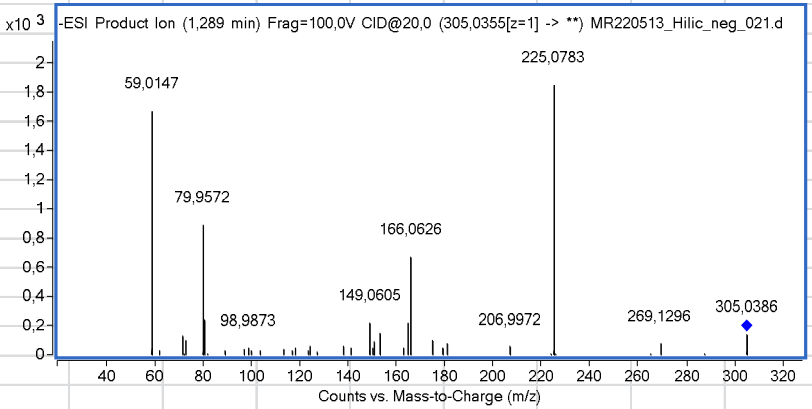


Suggested fragmentations in literature:
DOPAC-Sulfate m/z (neg) 247 - 203 (18), 167 (11), 123 (78) (Uutela et al. 2009)
Vanillic acid m/z (neg): 167/152 (Urpi-Sarda et al. 2009)

Figure S1. Shows the MS/MS spectra for tentatively identified vanillic acid sulfate m/z 246.9918 with retention time 0.99 min. The identification was based on comparing the MS/MS spectra with the MS/MS spectra of standard compounds vanillic acid and DOPAC (both unconjugated), and to the suggested fragments for DOPAC sulfate and vanillic acid found in the existing literature.





1) Molecular formula: $C_{11}H_{14}O_8S$, mfg-score 98.36, diff 0.63ppm)
2) the MS/MS fragmentation created fragments 225.0783 $[M\text{-}SO_3\text{-}H]^-$, 206.9972 $[M\text{-}SO_3\text{-}OH\text{-}H]^-$, and 166.0639 $[2H^+$ more than one of the suggested fragments of sinapic acid (MID 45738)]

The metabolite is tentatively dihydrosinapic acid sulfate.

Figure S2. The fragmentation pattern of tentatively identified sinapic acid sulfate with m/z 305.0386. The identification is based on matching molecular formula and the MS/MS fragmentation pattern.