

Supplementary Materials: Phytochemical Profiles and Antimicrobial Activities of *Allium cepa* Red cv. and *A. sativum* Subjected to Different Drying Methods: A Comparative MS-Based Metabolomics

Mohamed A. Farag, Sara E. Ali, Rashad H. Hodaya, Hesham R. El-Seedi, Haider N. Sultani, Annegret Laub, Tarek F. Eissa, Fouad O. F. Abou-Zaid and Ludger A. Wessjohann

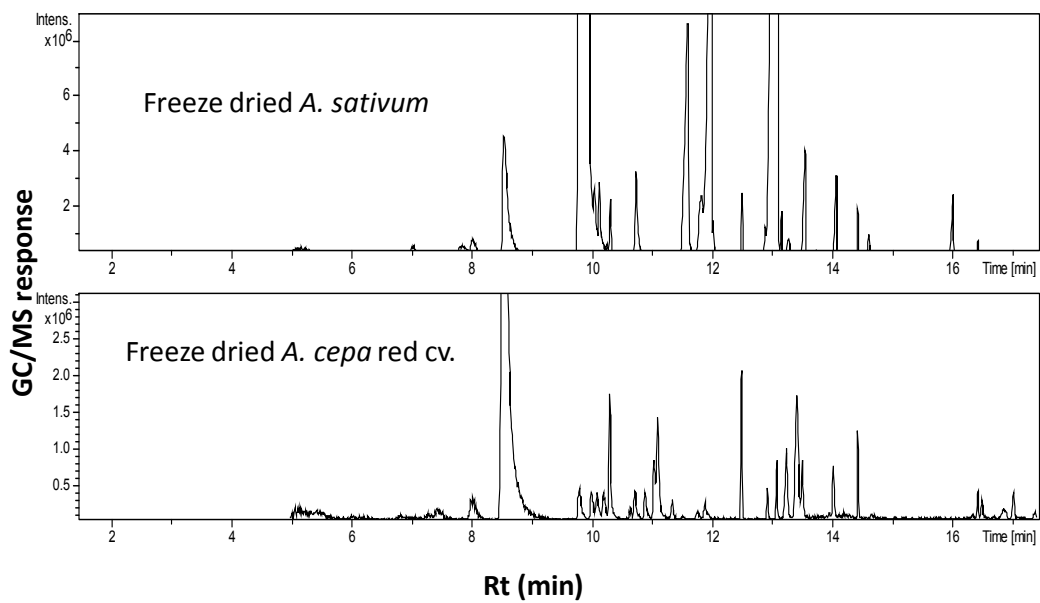


Fig. S1 Representative SPME–GC/MS chromatograms of volatiles collected from freeze dried *A. sativum* and *A. cepa* red cv.

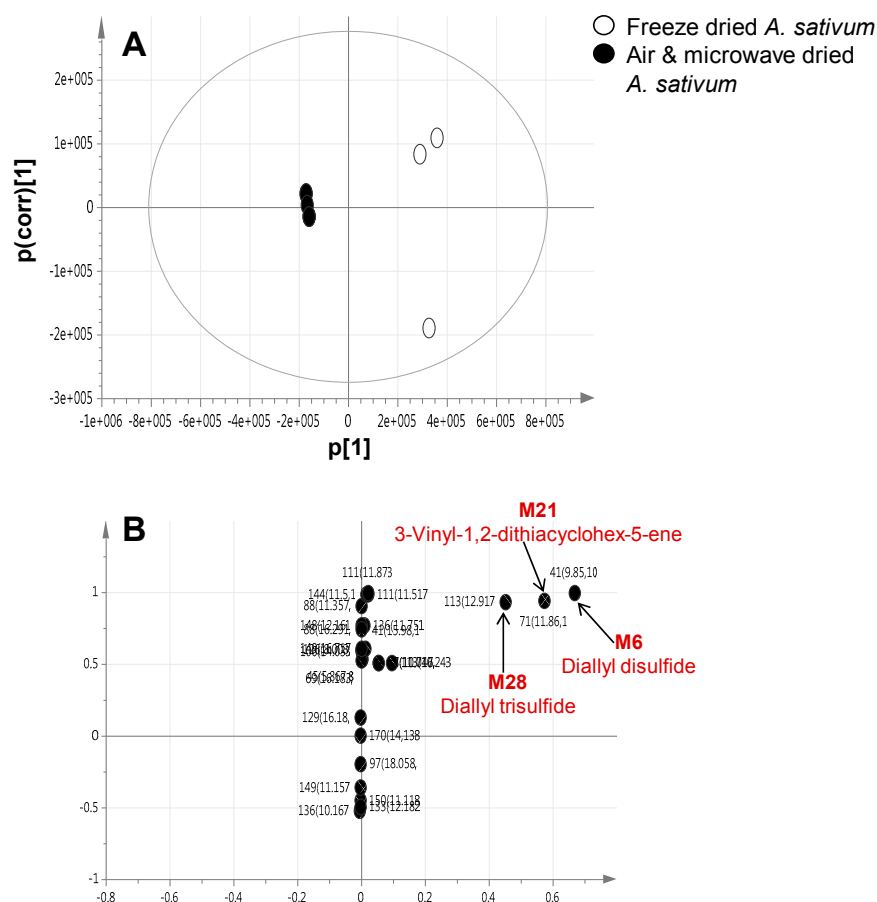


Fig. S2 SPME-GC/MS based orthogonal projection to latent structures-discriminant analysis (OPLS-DA) of freeze dried *A. sativum* (○) versus air and microwave dried garlic (●). (A) OPLS-DA score plot (B) loading plot derived from samples modeled against each other. The loading plot shows the covariance $p[1]$ against the correlation $p(\text{corr})[1]$ of the variables of the discriminating component of the OPLS-DA model. Selected variables are highlighted in the loading plot with each metabolite denoted by its mass/rt (min) value: M6; diallyl disulfide, M21; 3-Vinyl-1,2-dithiacyclohex-5-ene and M28; diallyl trisulfide. Peaks numbering follow those listed in (Table 1) for volatiles identification using SPME-GC/MS.

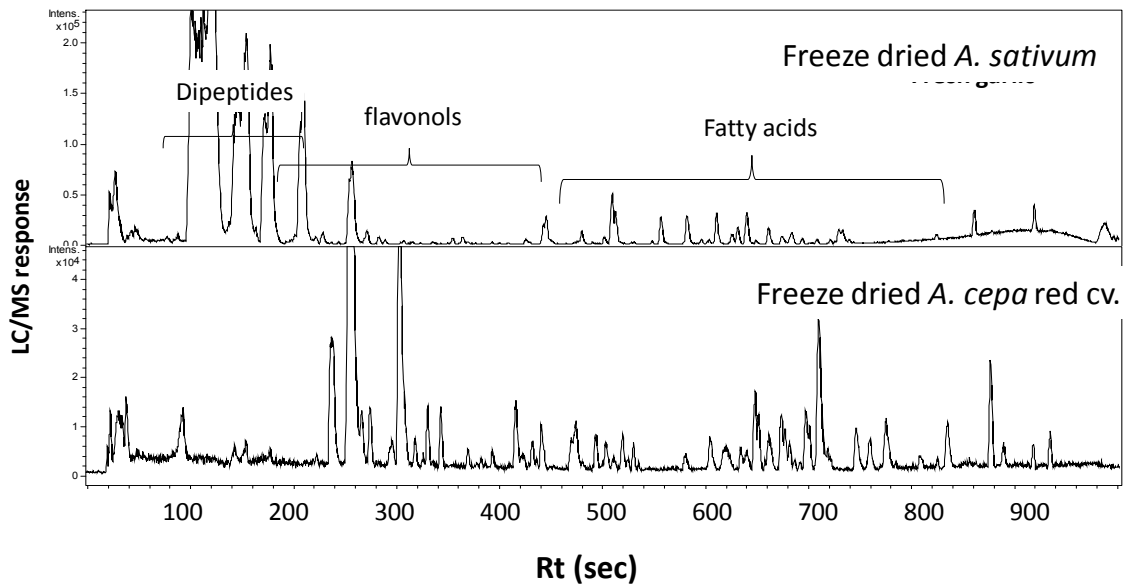
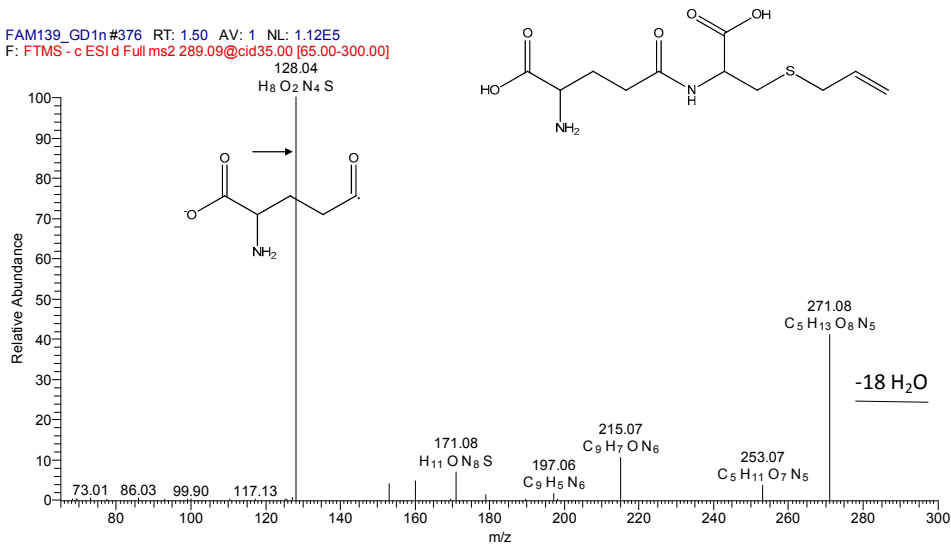


Fig. S3 Representative UPLC-QTOF-MS fingerprinting analyses of freeze dried garlic *A. sativum* and red onion cv. *A. cepa* extracts analysed using negative ionization mode.

Peak L6, N-γ-Glutamyl-S-allylcysteine, 289.0873 (M-H)⁻

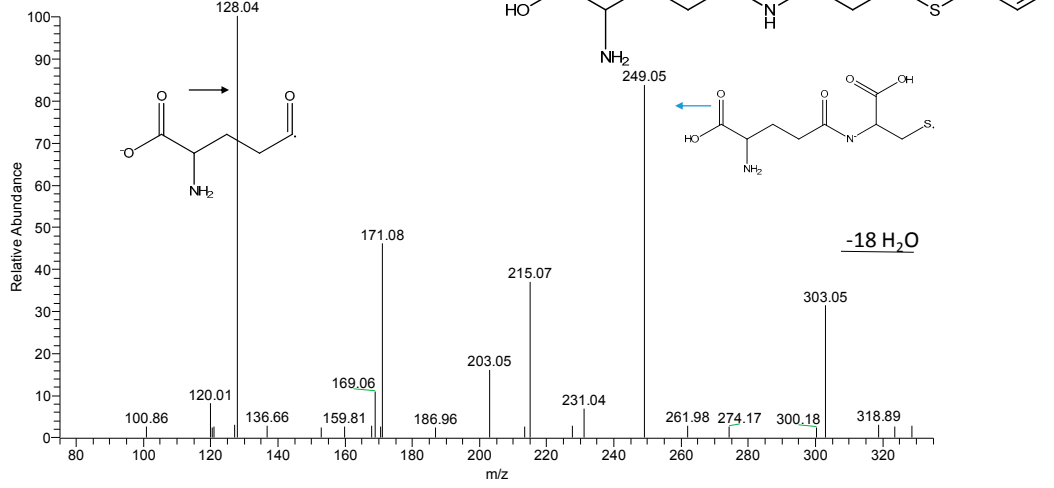
FAM139_GD1n#376 RT: 1.50 AV: 1 NL: 1.12E5
 F: FTMS - c ESI d Full ms2 289.09@cid35.00 [65.00-300.00]



(A)

Peak L8, γ -Glutamyl-S-allylthiocysteine, 321.061 (M-H)⁻

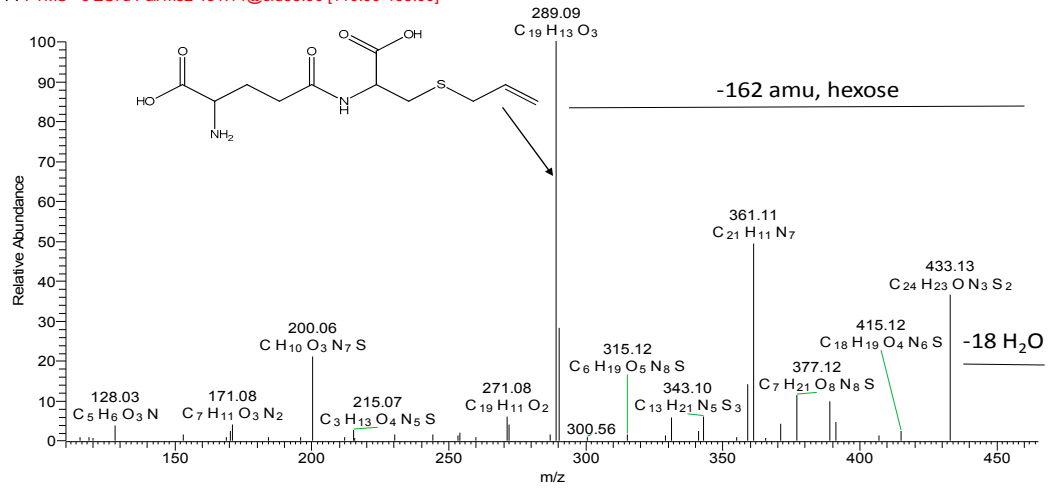
FAM139_GD1n#1396 RT: 5.59 AV: 1 NL: 3.23E3
F: FTMS - c ESI d Full ms2 321.06@cid35.00 [75.00-335.00]



(B)

Peak L5, N- γ -Glutamyl-S-allylcysteine, 451.1401 (M-H)⁻

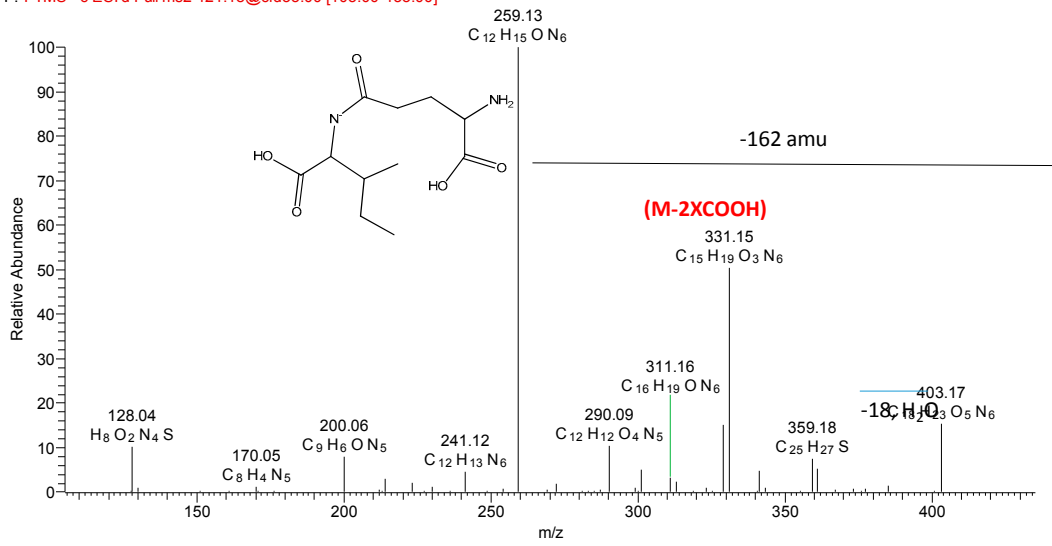
FAM139_GD1n#556 RT: 2.22 AV: 1 NL: 1.14E4
F: FTMS - c ESI d Full ms2 451.14@cid35.00 [110.00-465.00]



(C)

Peak L9, N-(β-hexosyl)-γ-Glutamylisoleucine, 421.182 (M-H)⁻

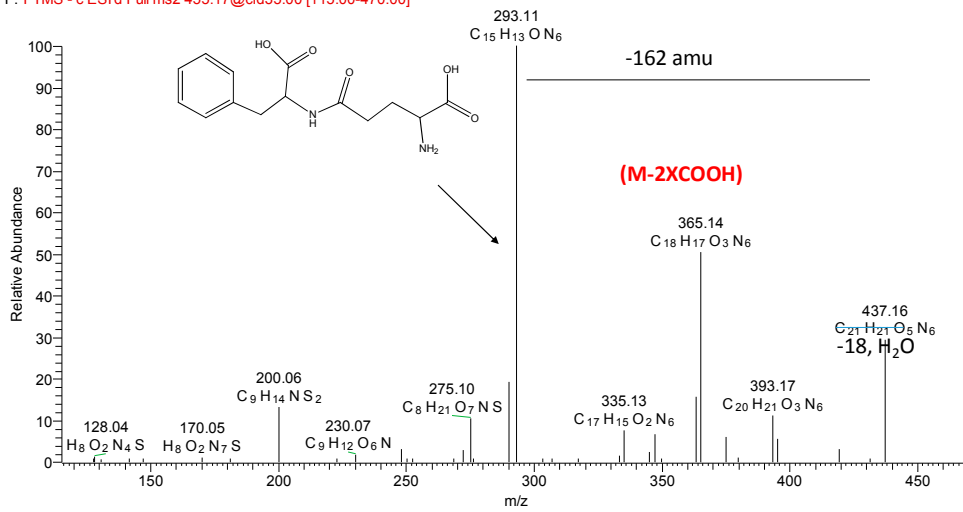
FAM139_OD1n#464 RT: 1.83 AV: 1 NL: 8.99E4
F: FTMS - c ESI d Full ms2 421.18@cid35.00 [105.00-435.00]



(D)

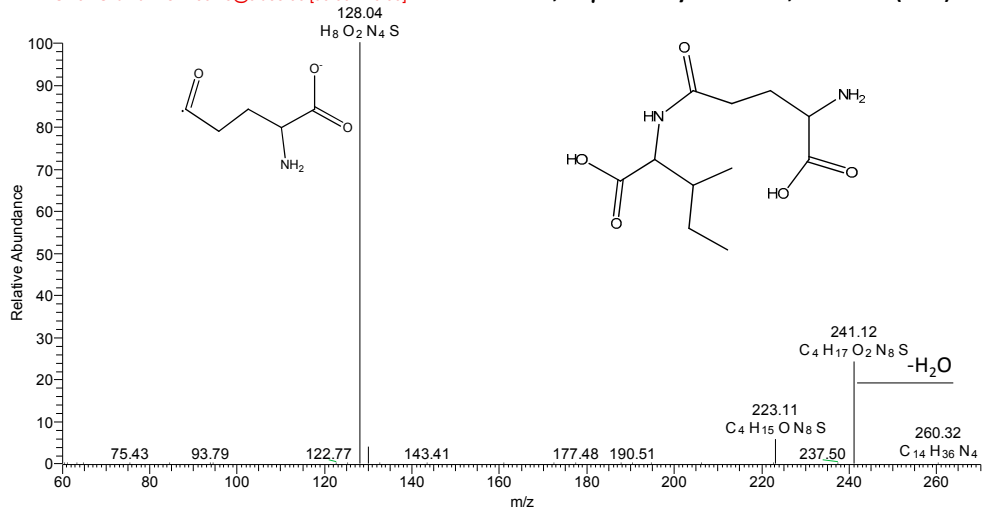
Peak L12, N-(β-hexosyl)-Glutamylphenylalanine, 455.166 (M-H)⁻

FAM139_GD1n#812 RT: 3.23 AV: 1 NL: 1.02E4
F: FTMS - c ESI d Full ms2 455.17@cid35.00 [115.00-470.00]



(E)

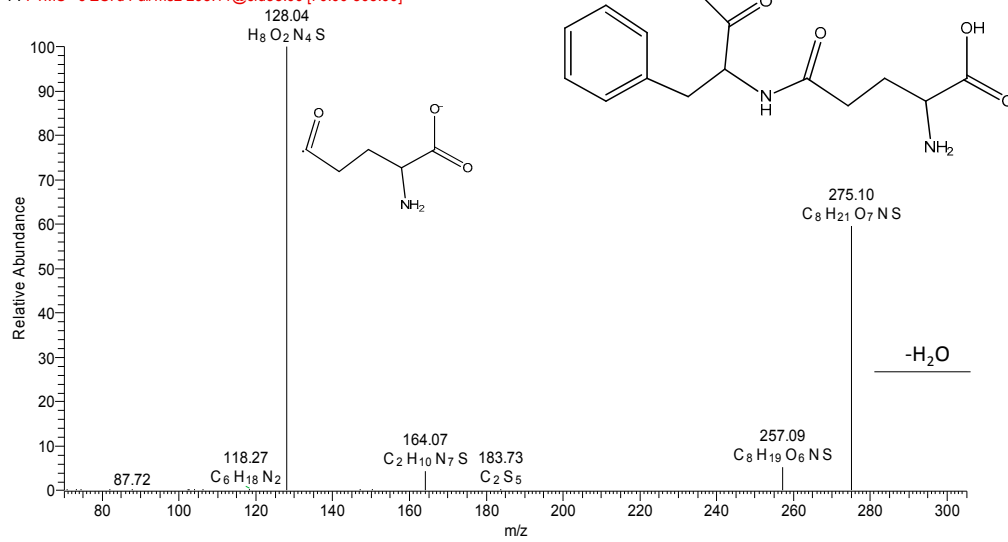
FAM139_OD1n#410 RT: 1.61 AV: 1 NL: 6.82E4
F: FTMS - c ESI d Full ms2 259.13@cid35.00 [60.00-270.00]



(F)

Peak L11, *N*- γ -Glutamylphenylalanine, 293.1135 (M-H)

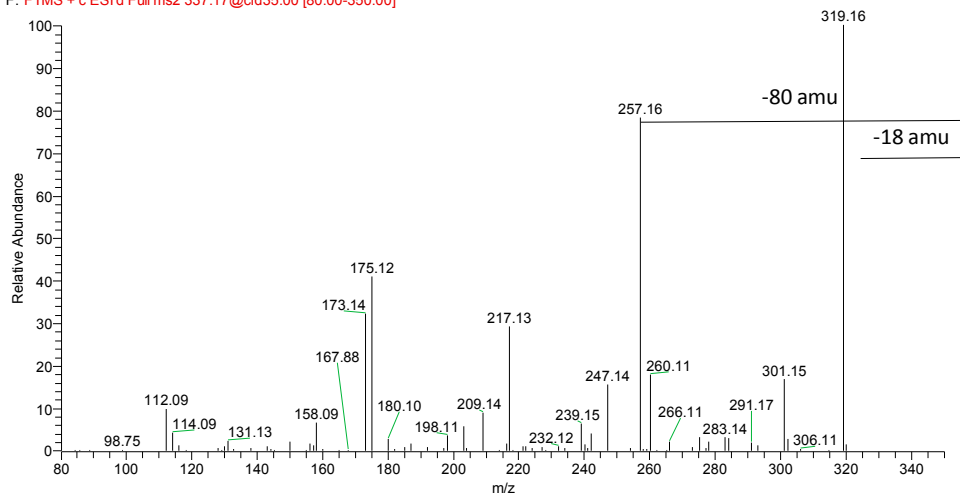
FAM139_OD1n#718 RT: 2.84 AV: 1 NL: 9.02E4
F: FTMS - c ESI d Full ms2 293.11@cid35.00 [70.00-305.00]



(G)

Peak 3, 337.1711 (M+H)⁺

FAM139_GD1 #112 RT: 0.59 AV: 1 NL: 2.94E5
F: FTMS + c ESI d Full ms2 337.17@cid35.00 [80.00-350.00]

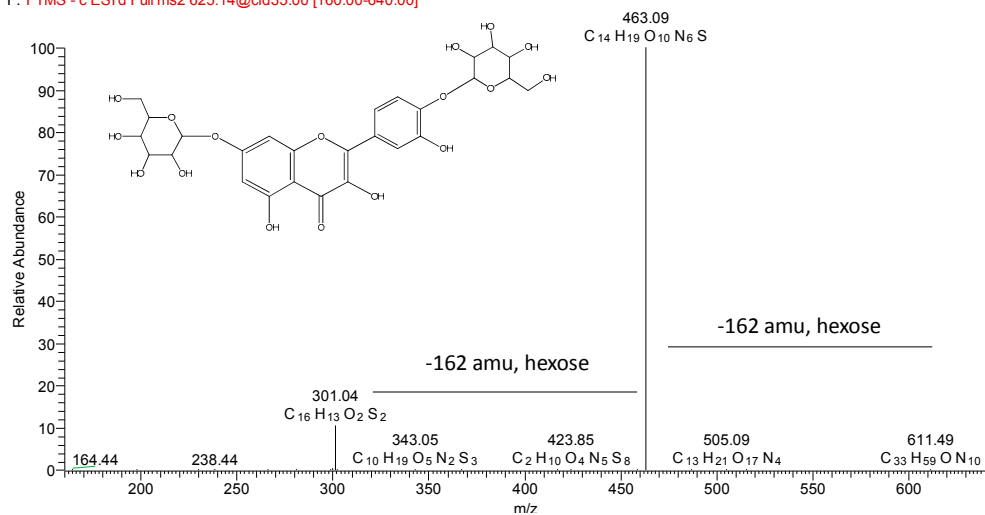


(H)

Fig. S4. (A) ESI-MS/MS spectrum of peak (L6) in the negative ion mode. (B) ESI-MS/MS spectrum of peak (8) in the negative ion mode. (C) ESI-MS/MS spectrum of peak (L5) in the negative ion mode. (D) ESI-MS/MS spectrum of peak (L9) in the negative ion mode. (E) ESI-MS/MS spectrum of peak (L12) in the negative ion mode. (F) ESI-MS/MS spectrum of peak (L7) in the negative ion mode. (G) ESI-MS/MS spectrum of peak (L11) in the negative ion mode. (H) ESI-MS/MS spectrum of peak (L3) in the negative ion mode.

Peak L16, Quercetin-O-diglucoside, 625.1405 (M-H)⁻

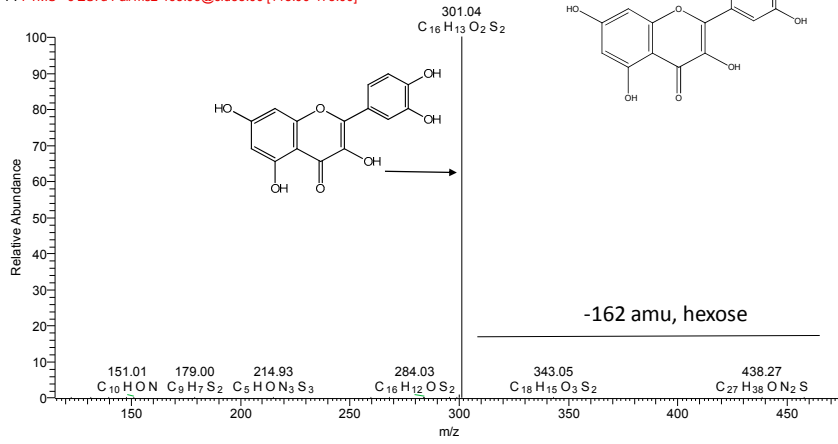
FAM139_OD1n#2340 RT: 9.31 AV: 1 NL: 5.19E5
F: FTMS - c ESI d Full ms2 625.14@cid35.00 [160.00-640.00]



(A)

Peak L21 Quercetin hexoside m/z 463.0883 [M-H]⁻

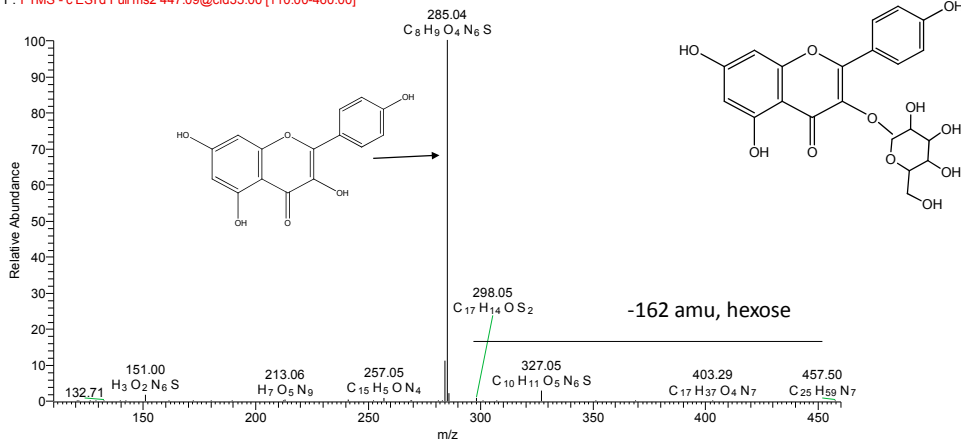
FAM139_OD1n#2596 RT: 10.35 AV: 1 NL: 7.26E5
F: FTMS - c ESI d Full ms2 463.09@cid35.00 [115.00-475.00]



(B)

Peak L22, Kaempferol-O-hexoside (astragalol) m/z 447.0933 [M-H]⁻

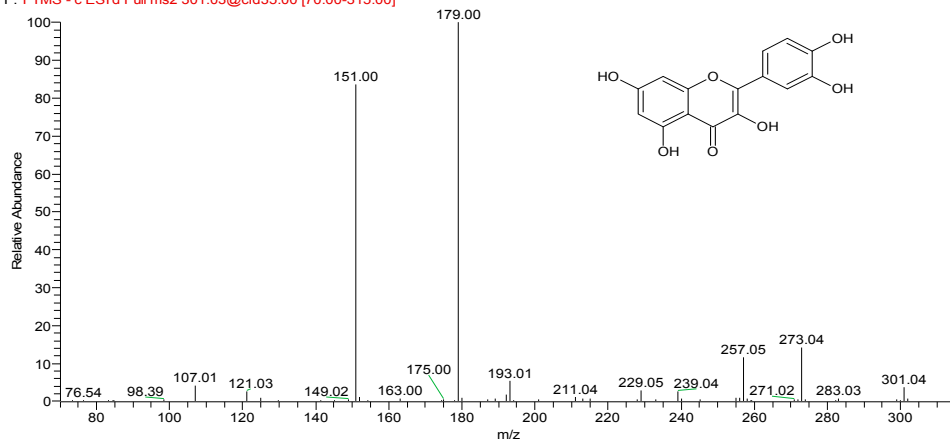
FAM139_OD1n#2628 RT: 10.46 AV: 1 NL: 1.18E5
F: FTMS - c ESI d Full ms2 447.09@cid35.00 [110.00-460.00]



(C)

Peak L33, quercetin m/z 301.0357 [M-H]⁻

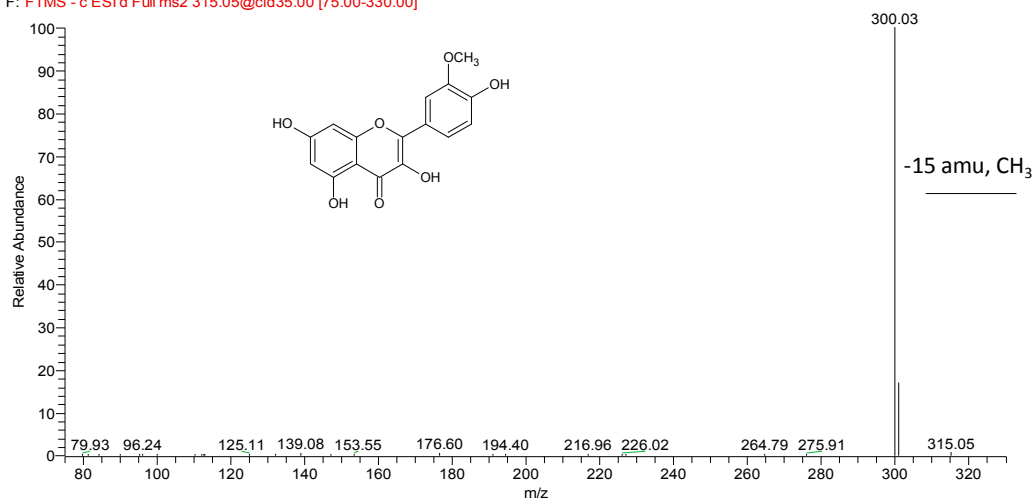
FAM139_OD1n#2812 RT: 11.21 AV: 1 NL: 5.12E4
F: FTMS - c ESI d Full ms2 301.03@cid35.00 [70.00-315.00]



(D)

FAM139_OD1n#2992 RT: 11.92 AV: 1 NL: 2.10E4
F: FTMS - c ESI d Full ms2 315.05@cid35.00 [75.00-330.00]

Peak L38, isorhamnetin m/z 315.051 [M-H]⁻



(F)

Fig. S5. (A) ESI-MS/MS spectrum of peak (L16) in the negative ion mode. (B) ESI-MS/MS spectrum of peak (L21) in the negative ion mode. (C) ESI-MS/MS spectrum of peak (L22) in the negative ion mode. (D) ESI-MS/MS spectrum of peak (L33) in the negative ion mode. (E) ESI-MS/MS spectrum of peak (L38) in the negative ion mode.

Peak L39, 9,12,13-trihydroxy octadeca-7-enoic acid m/z 329.2337 [M-H]⁻

FAM139_OD1n#3046 RT: 12.12 AV: 1 NL: 1.68E4
F: FTMS - c ESI d Full ms2 329.23@cid35.00 [80.00-340.00]

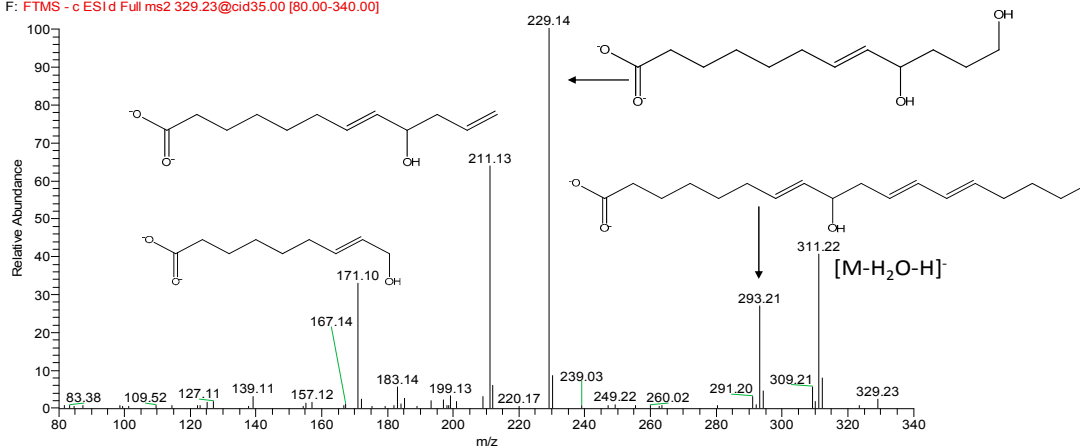


Fig. S6. ESI-MS/MS spectrum of peak (L39) in the negative ion mode.