Supplementary materials

Chemical and Pharmacological Potential of *Coccoloba cowellii*, an Endemic Endangered Plant from Cuba

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Keywords: *Coccoloba cowellii*; endemic plant; UHPLC-ESI-QTOF-MS; flavonoids; antifungal; antibacterial; COX-1/2 inhibition.

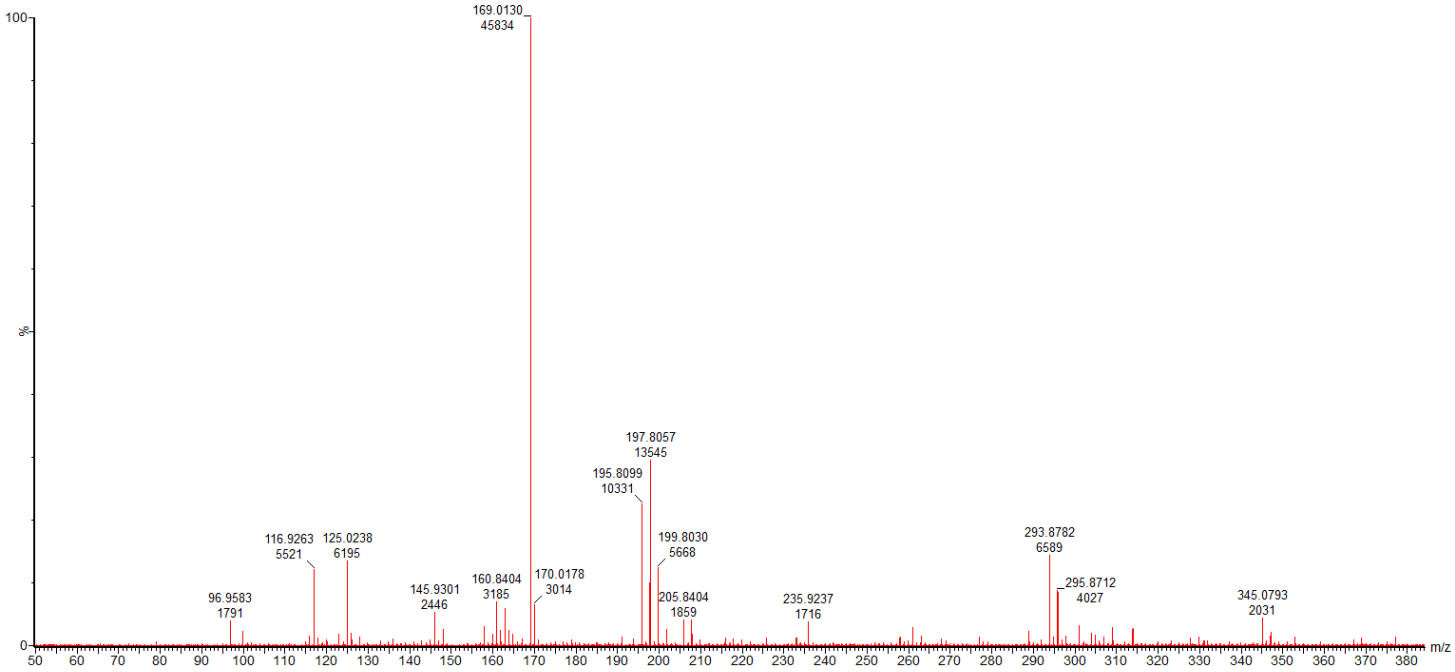
Table S1. Library hits found in the spectra of the methanolic extract of *C. cowellii* against the GNPS database.

Compound name	Library class	Cosine	Shared peaks	MZErrorPPM	LibMZ
Quercetin-3-*O*-rhamnoside (Quercitrin)	Bronze	0.85	8	1	447.093
Quercetin-3-*O*-galactoside (Hyperoside)	Bronze	0.80	7	0	463.088
Quercetin-3-*O*-arabinoside (Avicularin)	Bronze	0.72	6	0	433.078
Quercetin-3-*O*-glucuronide (Miquelianin)	Bronze	0.84	6	1	477.067
Quercetin 3-(2-galloylglucoside)	Bronze	0.73	6	37	615.099
Myricetin-3-*O*-pentoside	Bronze	0.85	6	10	449.067
Myricetin-3-*O*-galactoside	Bronze	0.93	9	2	479.083
4′-*O*-Methylmyricetin-3-*O*-rhamnoside (Mearnsitrin)	Gold	0.83	8	93	477.104
Procyanidin B1	Bronze	0.81	11	1	577.136
Procyanidin B2	Bronze	0.71	9	14	575.108
Catechin-3-*O*-gallate	Bronze	0.81	8	2	441.083
Epicatechin-3-*O*-gallate	Bronze	0.71	8	10	487.088

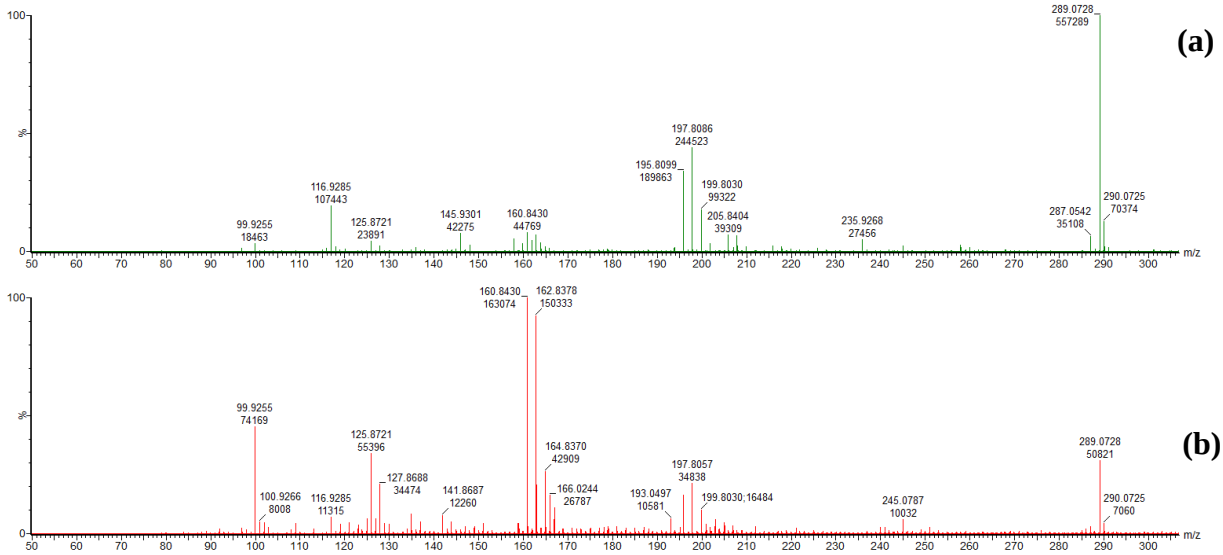
MZErrorPPM: ppm error with the spectral library match, LibMZ: *m*/*z* value of the spectral library match.

Figure S1. Molecular network of the total extract of *Coccoloba cowellii*, created with the Feature-Based Molecular Networking (FBMN) workflow on the Global Natural Products Social (GNPS) molecular networking web-platform (The molecular networking job can be publicly accessed at https://gnps.ucsd.edu/ProteoSAFe/status.jsp?task=a2f9e6e25ca64043a36a3d2fb09270c5)

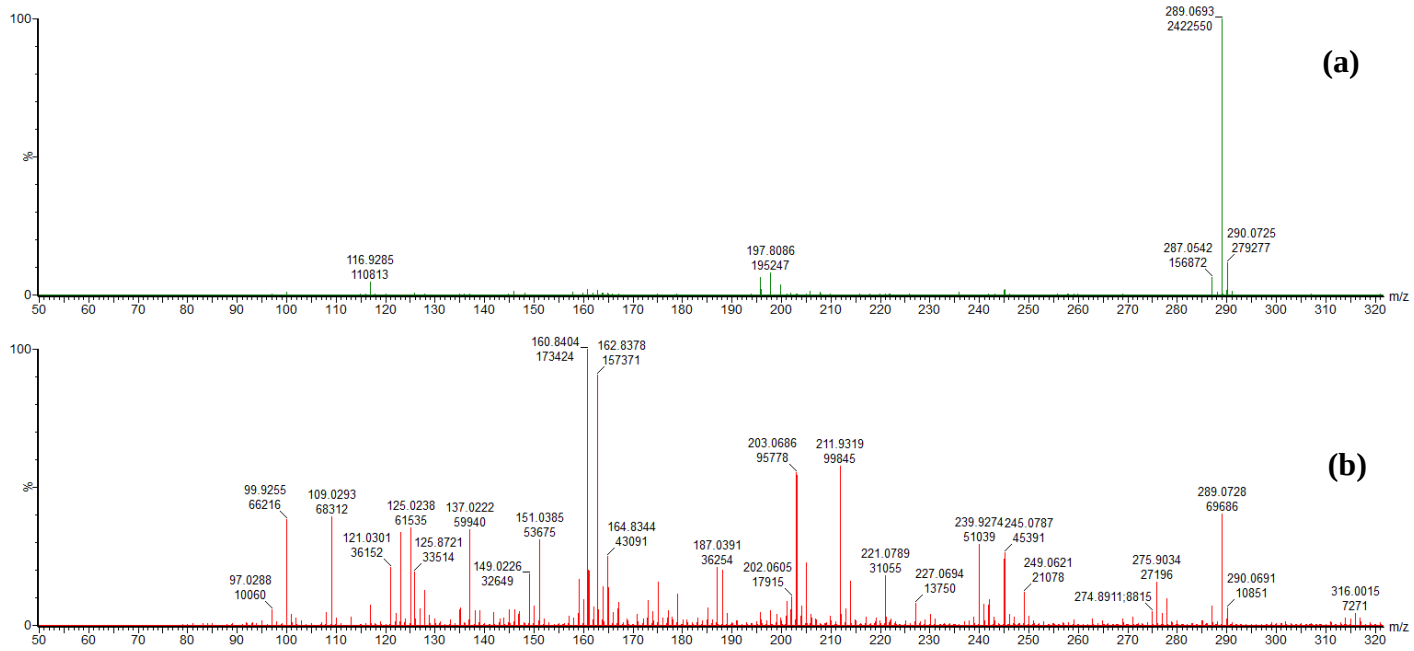
Figure S2. Full MS and MS/MS spectra of compounds 1-15.



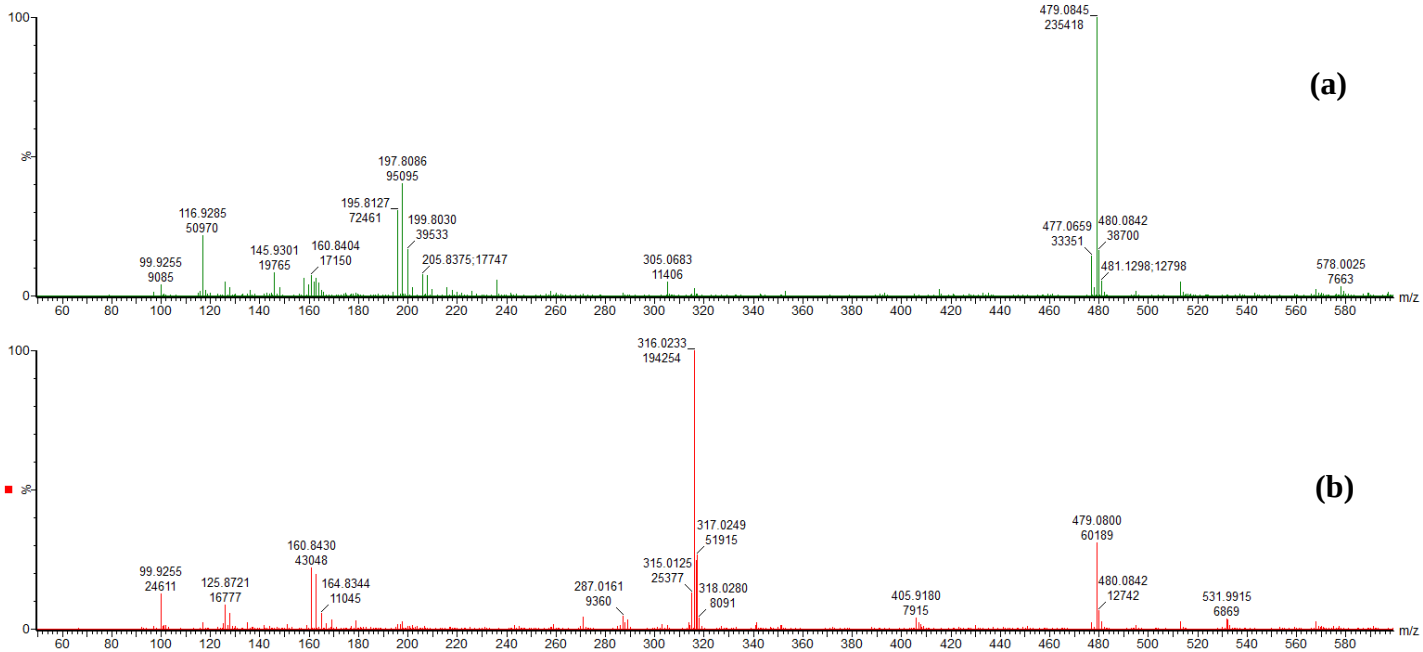
a) Peak 1 MS spectrum, Rt 2.03 min



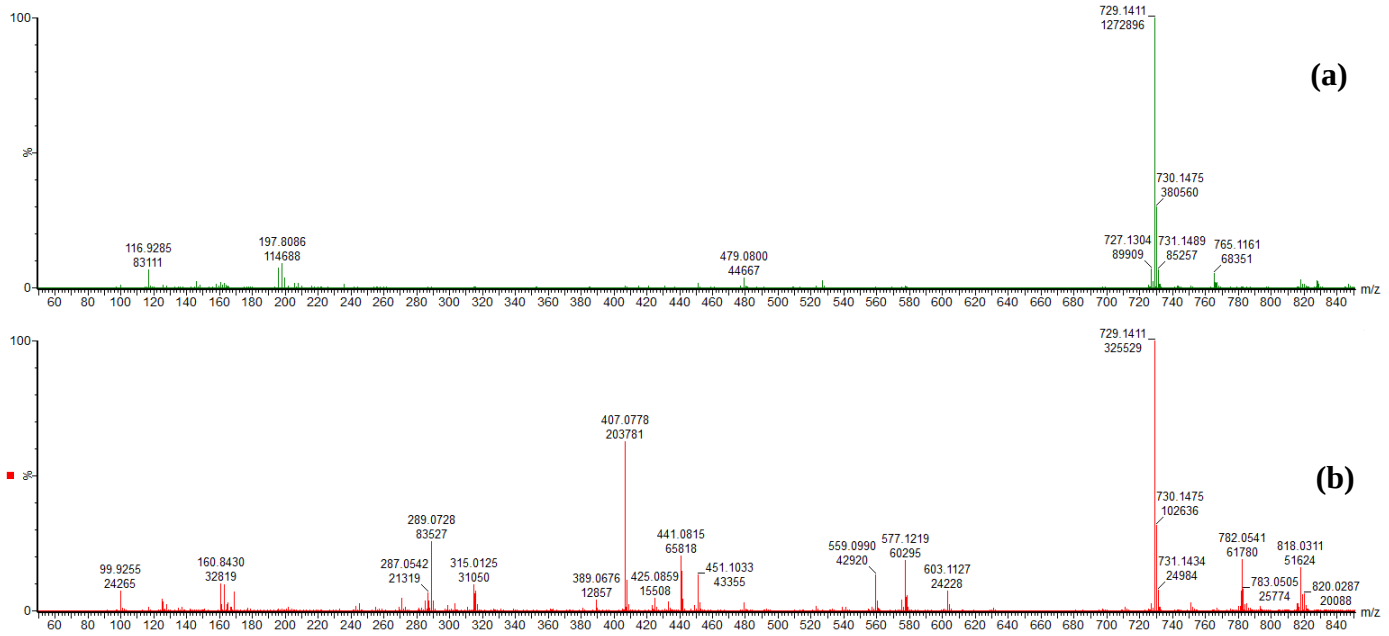
b) Peak 2 [(a) MS spectrum and (b) MS/MS spectrum], Rt 6.04 min



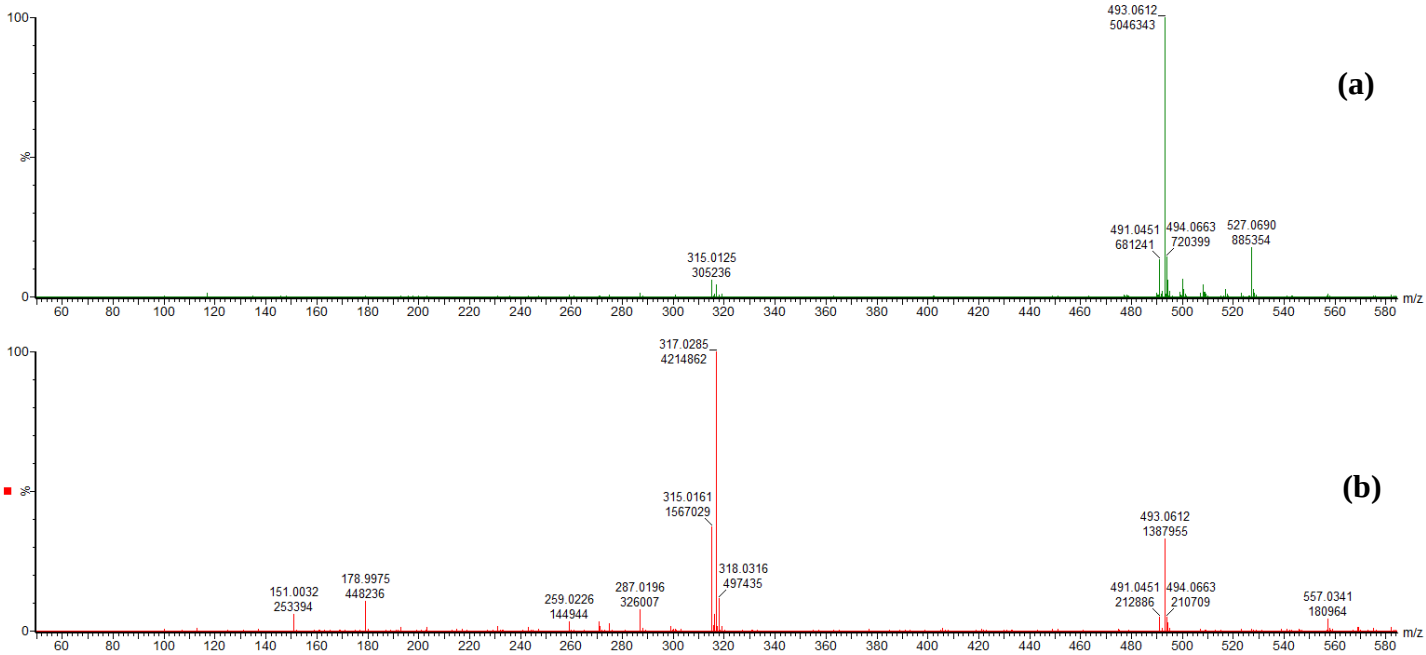
c) Peak 3 [(a) MS spectrum and (b) MS/MS spectrum], Rt 7.22 min



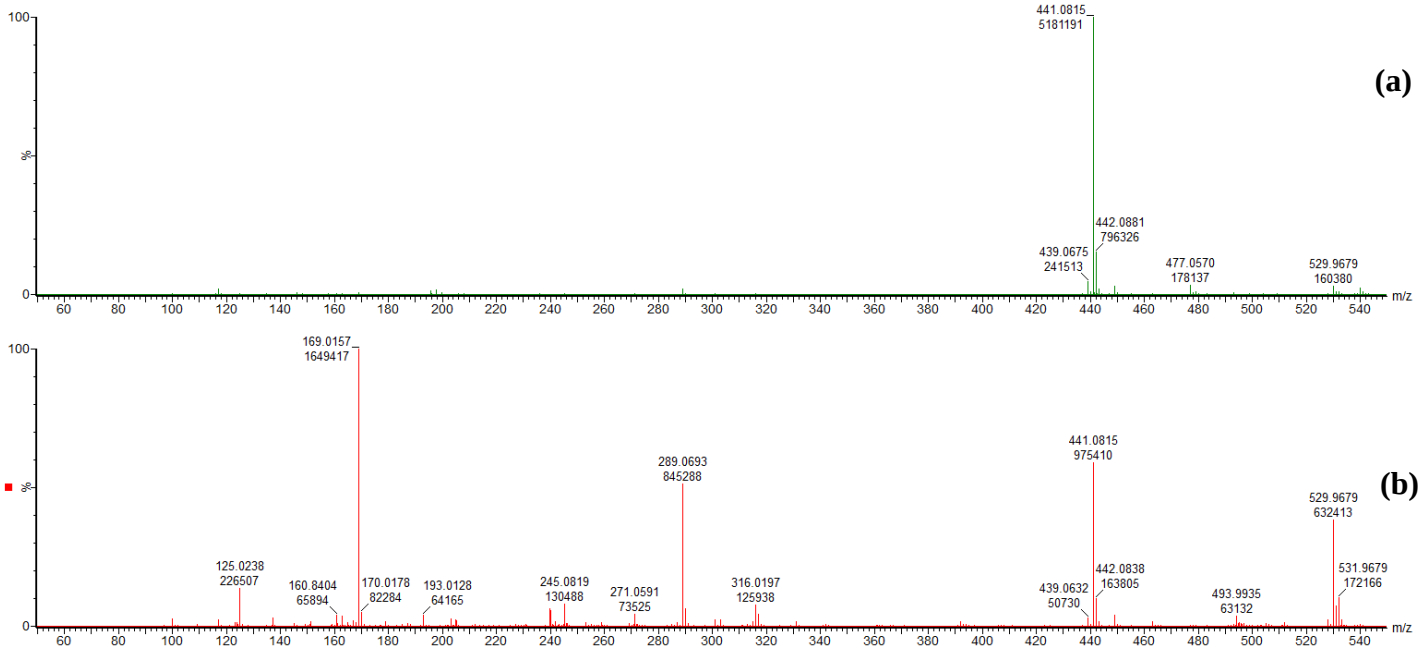
d) Peak 4 [(a) MS spectrum and (b) MS/MS spectrum], Rt 9.98 min



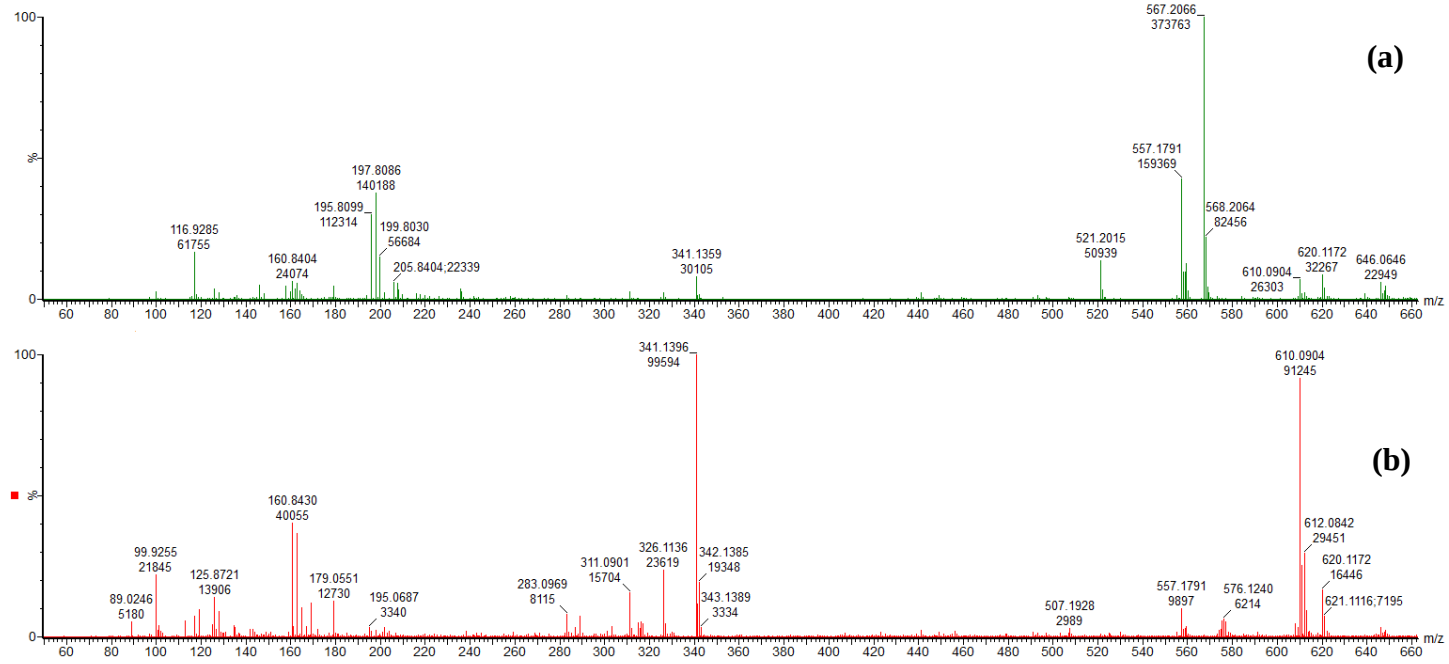
e) Peak 5 [(a) MS spectrum and (b) MS/MS spectrum], Rt 10.21 min



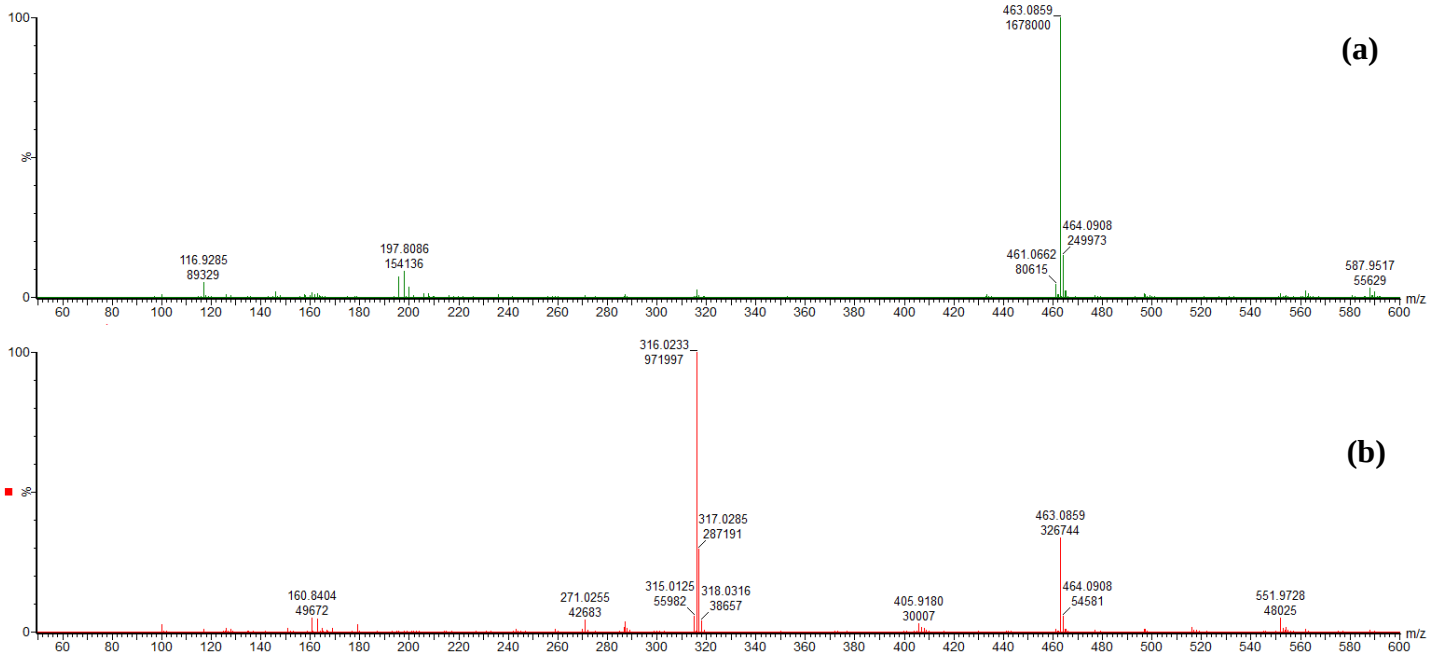
f) Peak 6 [(a) MS spectrum and (b) MS/MS spectrum], Rt 10.60 min



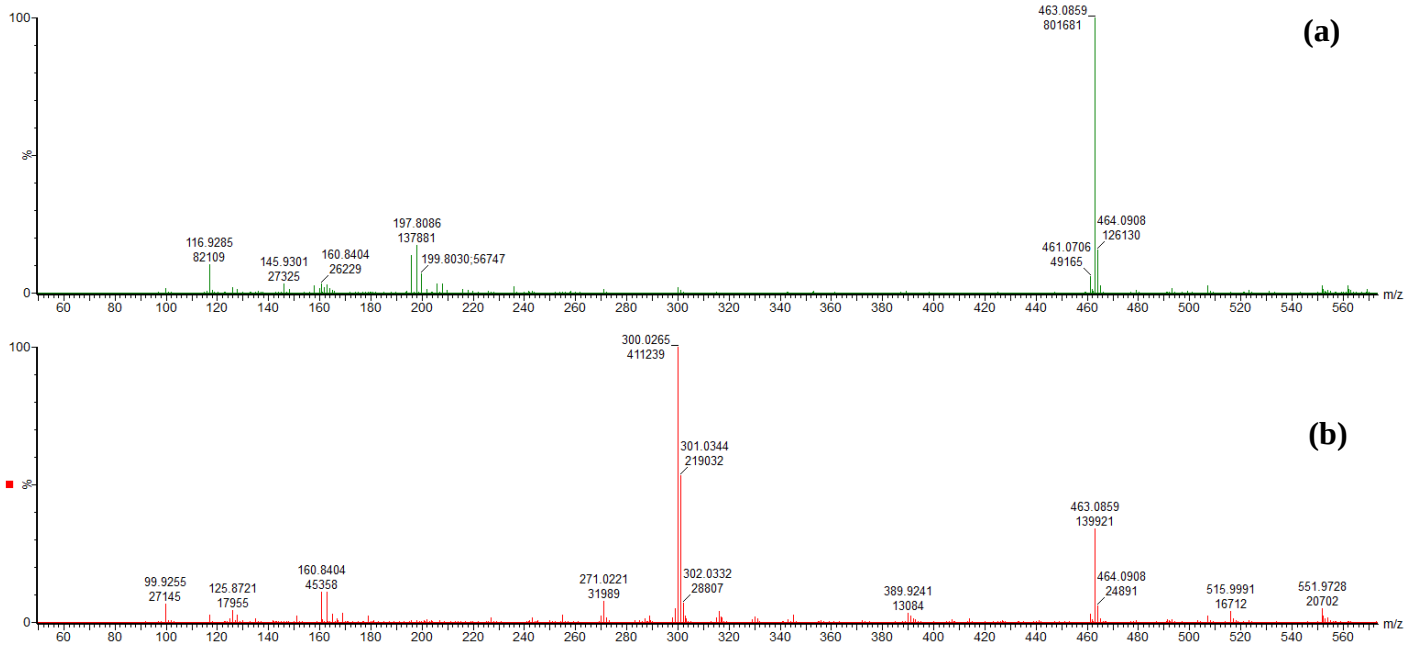
g) Peak 7 [(a) MS spectrum and (b) MS/MS spectrum], Rt 10.87 min



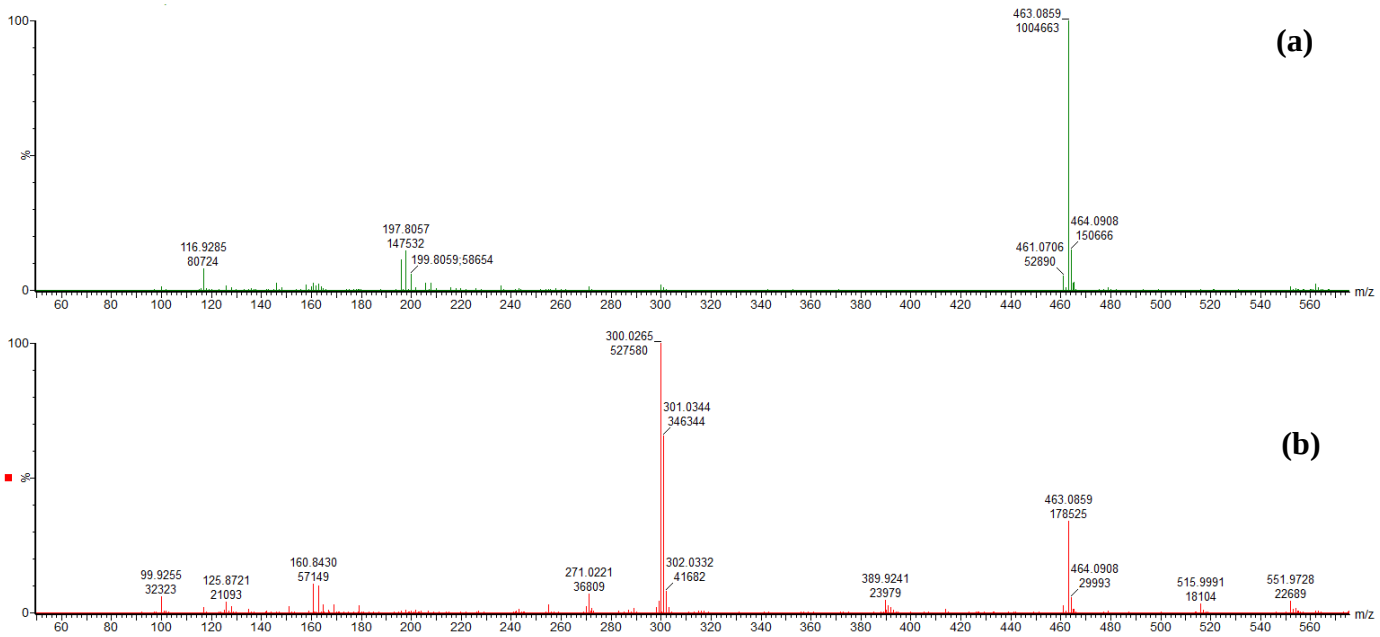
h) Peak 8 [(a) MS spectrum and (b) MS/MS spectrum], Rt 11.11 min



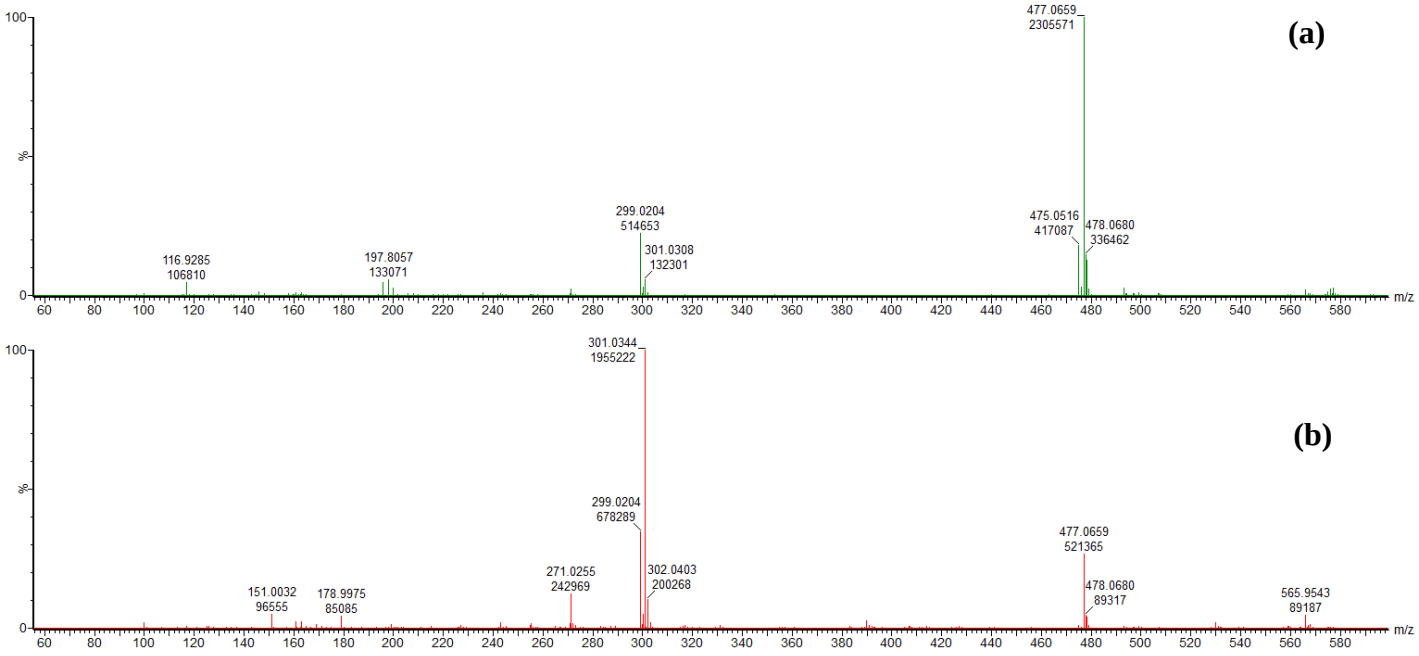
i) Peak 9 [(a) MS spectrum and (b) MS/MS spectrum], Rt 11.29 min



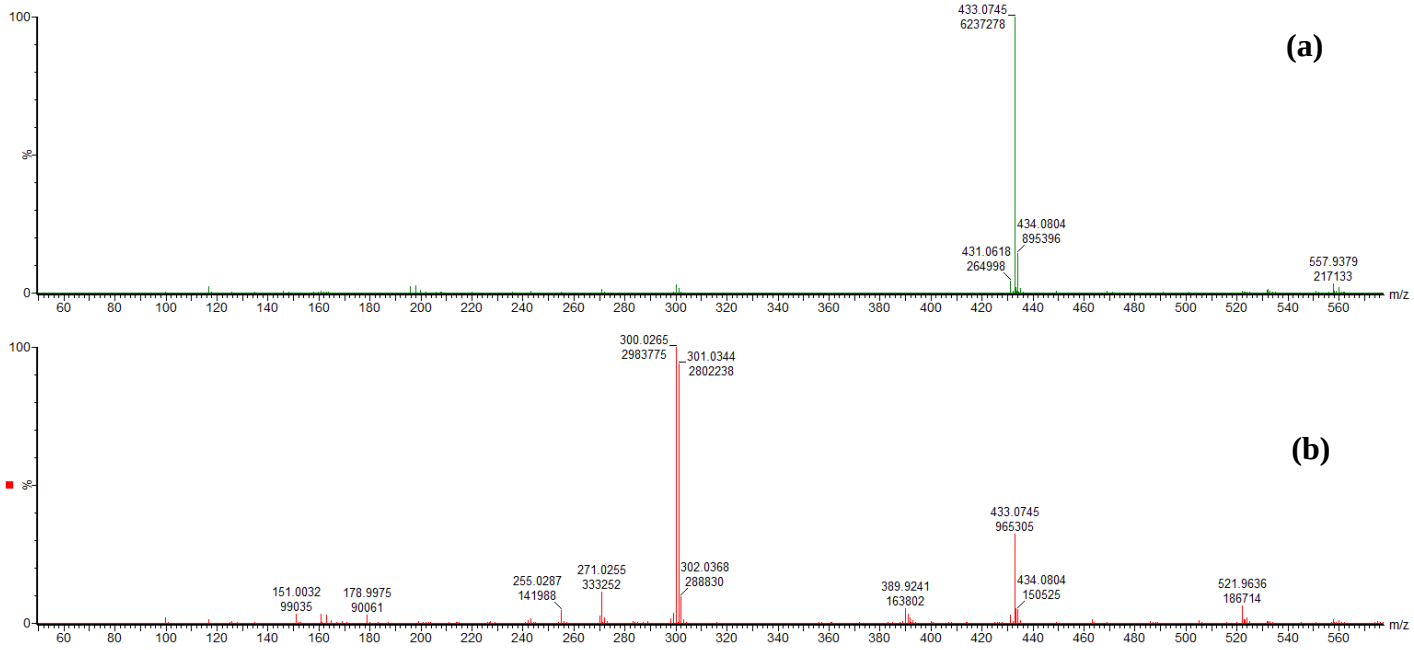
j) Peak 10 [(a) MS spectrum and (b) MS/MS spectrum], Rt 11.43 min



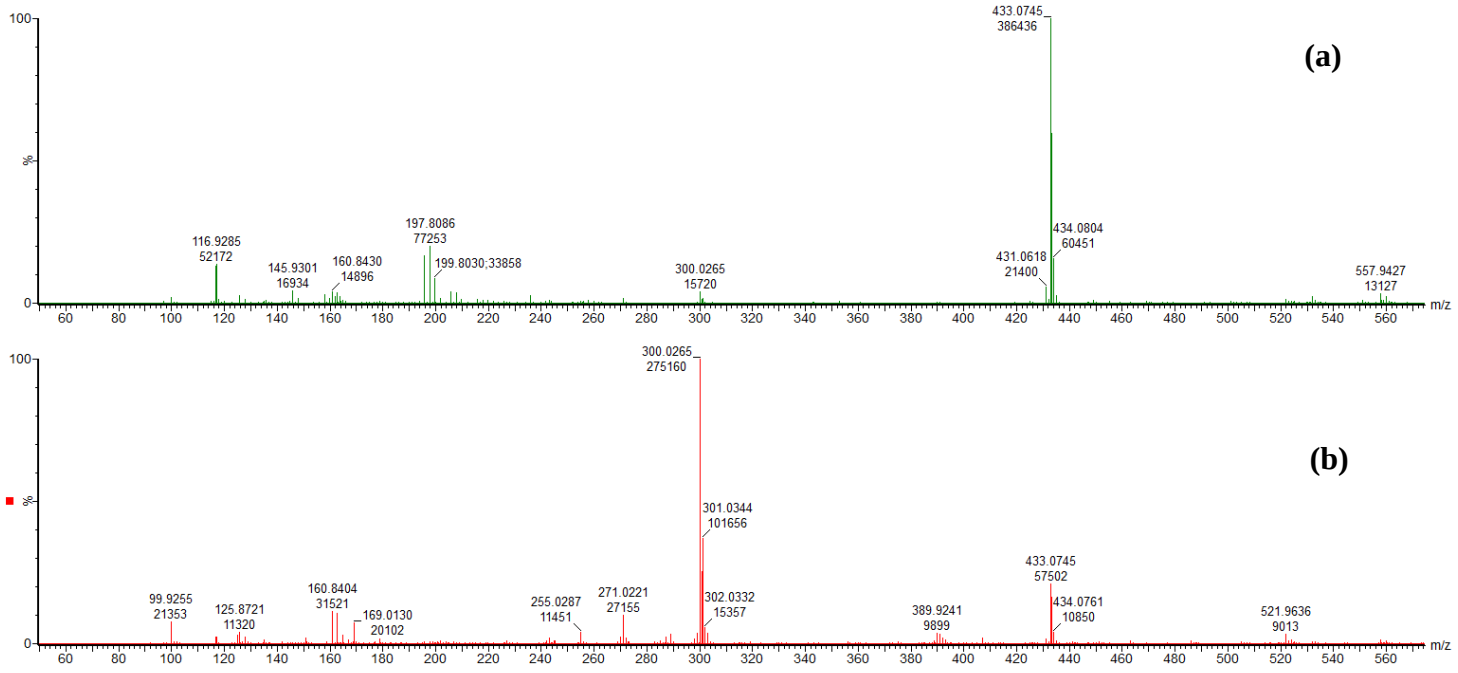
k) Peak 11 [(a) MS spectrum and (b) MS/MS spectrum], Rt 11.58 min



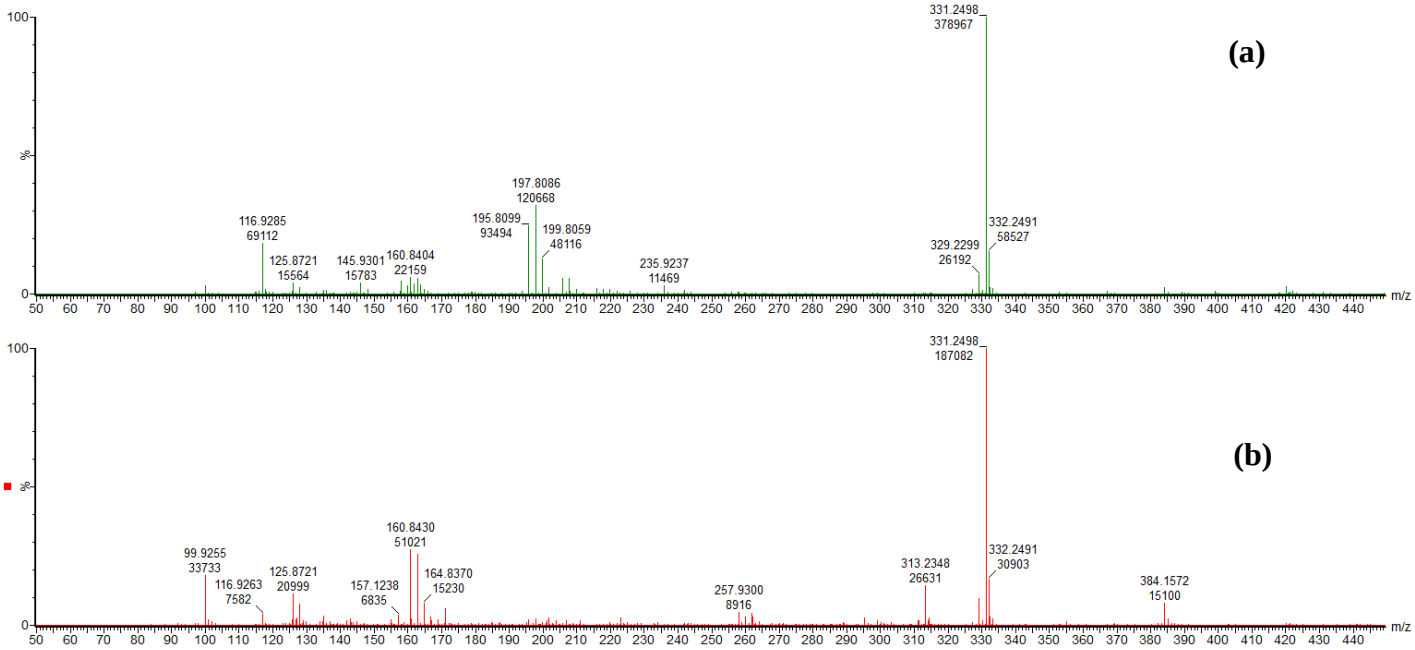
l) Peak 12 [(a) MS spectrum and (b) MS/MS spectrum], Rt 12.02 min



m) Peak 13 [(a) MS spectrum and (b) MS/MS spectrum], Rt 12.38 min

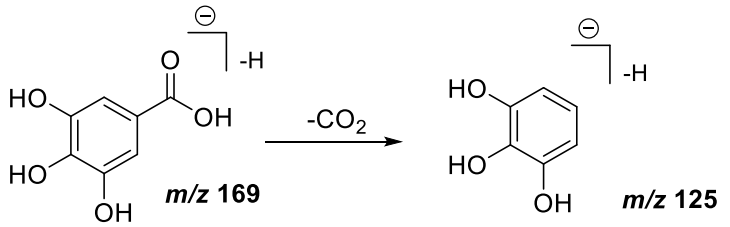


n) Peak 14 [(a) MS spectrum and (b) MS/MS spectrum], Rt 12.51 min

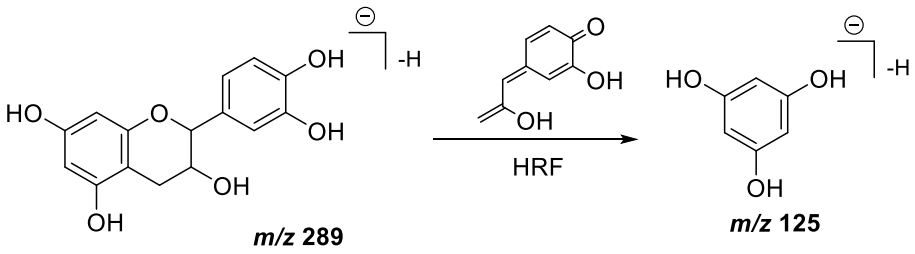


o) Peak 15 [(a) MS spectrum and (b) MS/MS spectrum], Rt 17.12 min

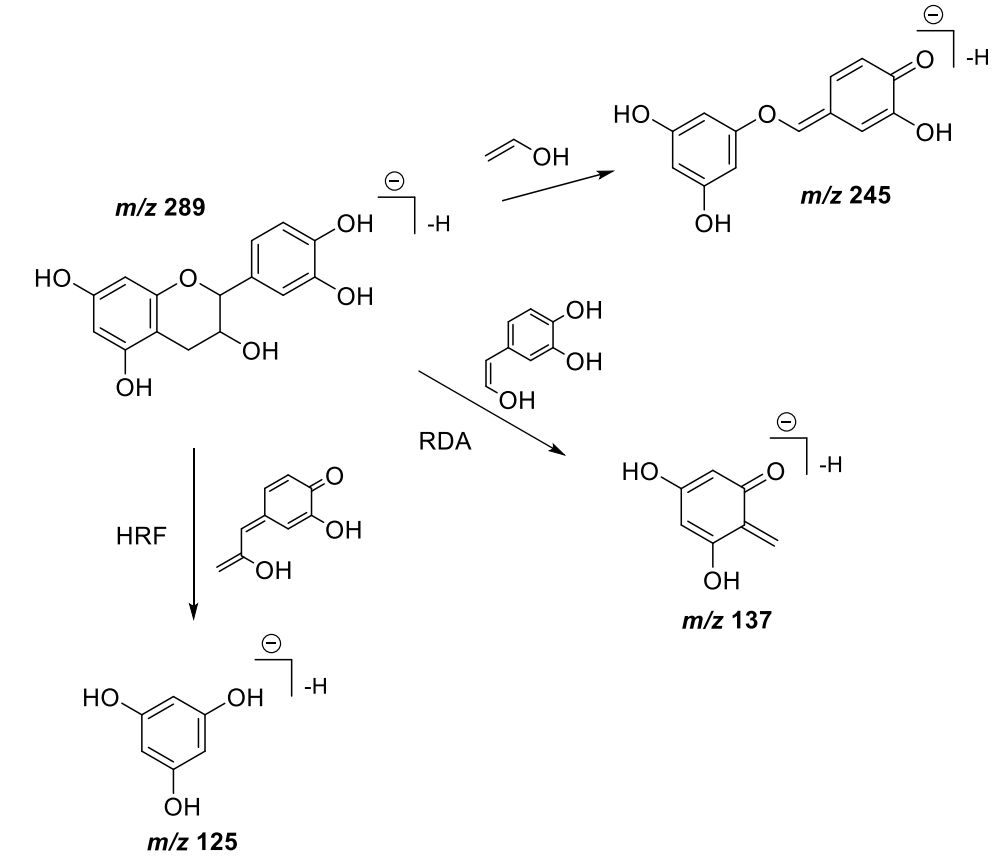
Figure S3. Tentative fragmentation pathways of some compounds present in the total extract of *C. cowellii*.



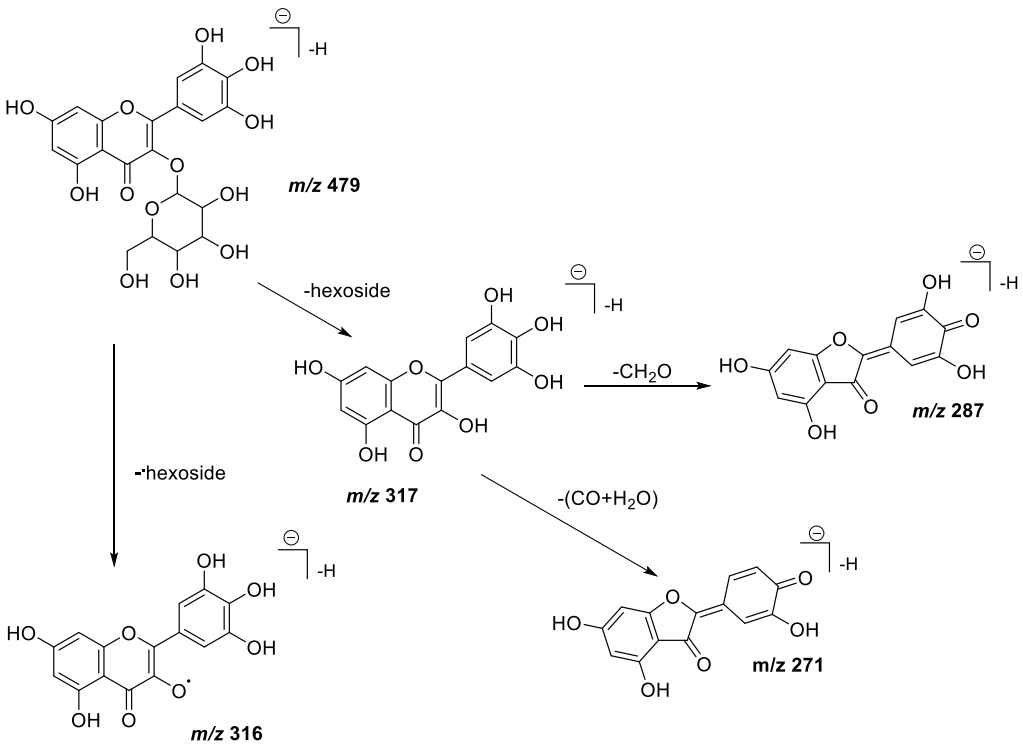
a) Peak 1, Rt 2.03 min, tentative identification: Gallic acid



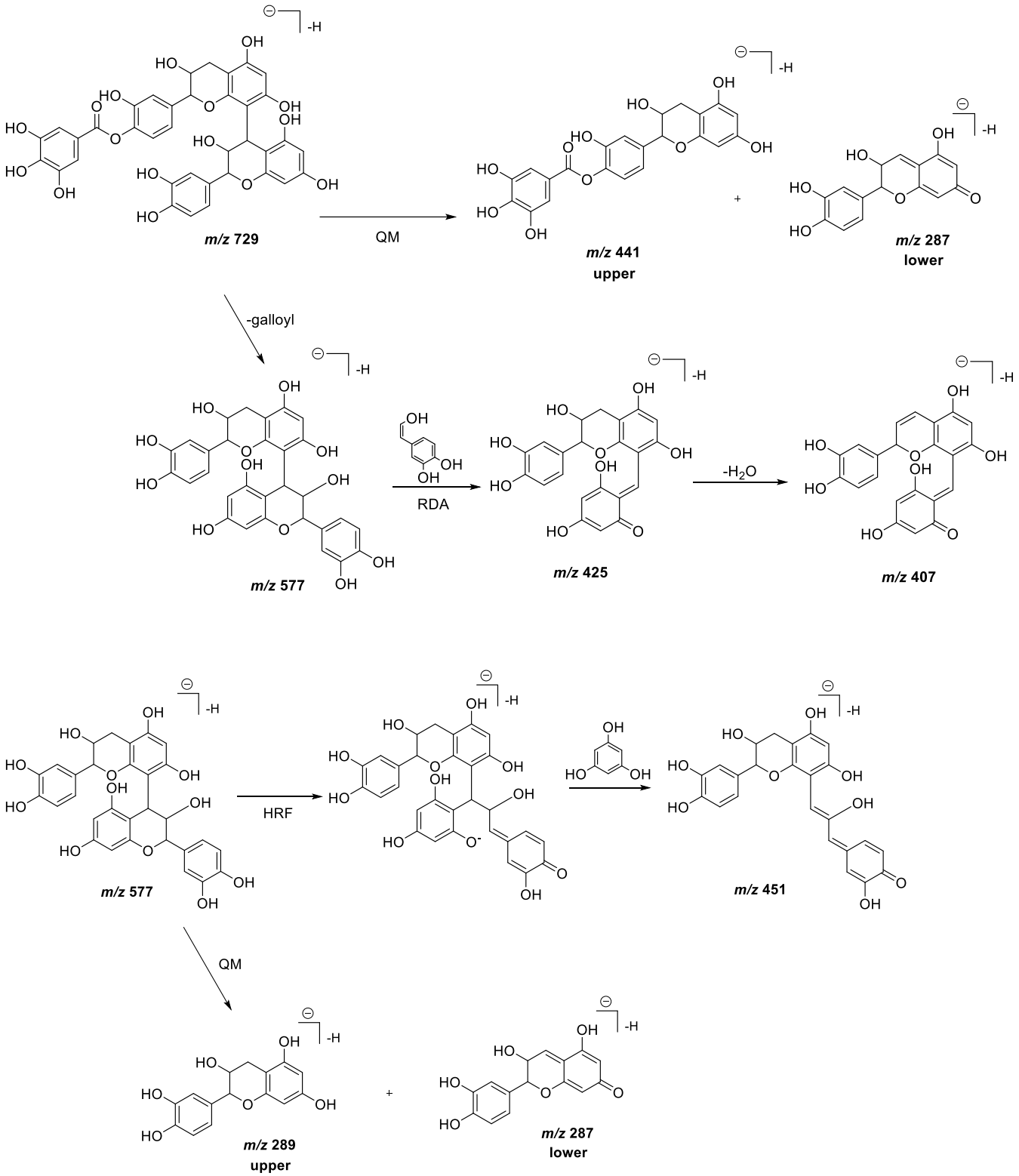
b) Peak 2, Rt 6.04 min, tentative identification: Catechin. Hypothetical fragmentation pattern taken from Callemien and Collin, 2008 [1].



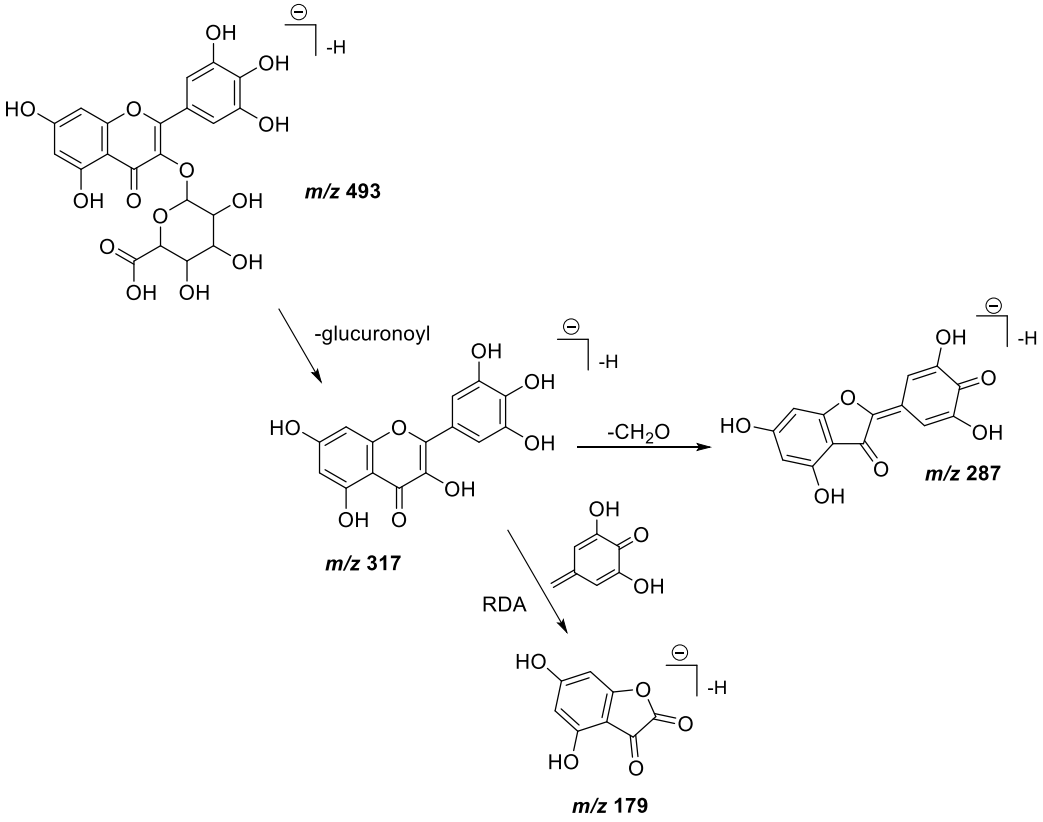
c) Peak 3, Rt 7.22 min, tentative identification: Epicatechin. Hypothetical fragmentation pattern taken from Callemien and Collin, 2008 [1].



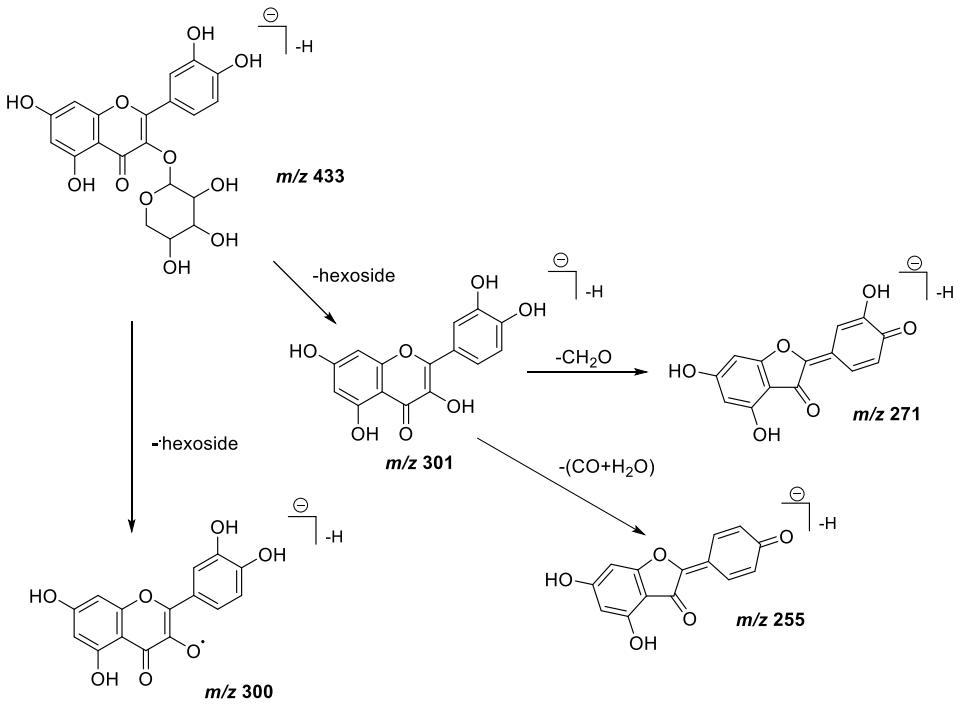
d) Peak 4, Rt 9.98 min, tentative identification: Myricetin-3-O-galactoside. Hypothetical fragmentation pattern taken and adapted from Li et al., 2016 [2].



e) Peak 5, Rt 10.21 min, tentative identification: Procyanidin B1 monogallate (position of the galloyl substituent is arbitrary). Hypothetical fragmentation pattern taken from Callemien and Collin, 2008 [1].



f) Peak 6, Rt 10.60 min, tentative identification: Myricetin-3-O-glucuronide. Hypothetical fragmentation pattern taken and adapted from Li et al., 2016 [2].



g) Peak 13, Rt 12.38 min, tentative identification: Quercetin-O-pentoside 1. (position of hexoside substituent is arbitrary). Hypothetical fragmentation pattern taken from Li et al., 2016 [2].

1. Callemien, D.; Collin, S. Use of RP-HPLC-ESI(-)-MS/MS to differentiate various proanthocyanidin isomers in lager beer extracts. *J. Am. Soc. Brew. Chem.* **2008**, *66*, 109–115, doi:10.1094/ASBCJ-2008-0215-01.
2. Li, Z.H.; Guo, H.; Xu, W. Bin; Ge, J.; Li, X.; Alimu, M.; He, D.J. Rapid Identification of Flavonoid Constituents Directly from PTP1B Inhibitive Extract of Raspberry (Rubus idaeus L.) Leaves by HPLC-ESI-QTOF-MS-MS. *J. Chromatogr. Sci.* **2016**, *54*, 805–810, doi:10.1093/chromsci/bmw016.