Supplementary material

Article

Antimicrobial and immunomodulating activities of two endemic *Nepeta* species and their major iridoids isolated from natural sources

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Supplementary Figure captions

Figure S1. Structural characterization of *trans*,*cis*-NL (a) using NMR techniques: 1D (^{1}H and ^{13}C) (b and c) and 2D (COSY, NOESY and HSQC) (d to f).

Figure S2. Structural characterization of *cis*,*trans*-NL (a) using NMR techniques: 1D (^{1}H and ^{13}C) (b and c) and 2D (COSY and HSQC, respectively) (d and e);.

Figure S3. Structural characterization of 1,5,9-epideoxyloganic acid (a), using NMR techniques: 1D (^{1}H and ^{13}C) (b and c) and 2D (NOESY) (d).

Figure S4. Proposed structural formula and detailed fragmentation pathway of trihydroxycinnamoylquinic acid (a), boschnaloside (b), deoxyloganetic acid pentoside (c), 3,4-dihydroxyphenethyl alcohol 4-*O*-hexoside (d).

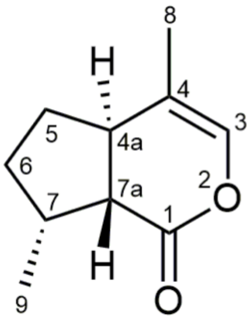

Figure S1a. Chemical structure of *trans, cis* nepetalactone.

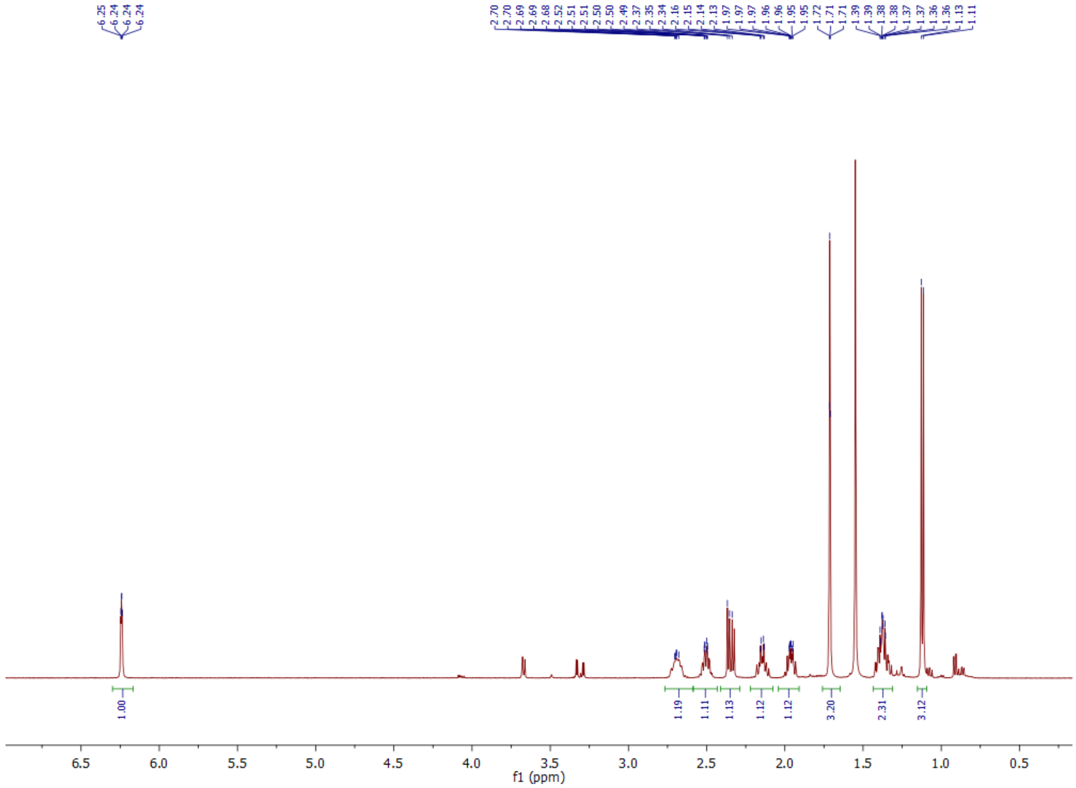

Figure S1b. ^{1}H-NMR spectrum (500 MHz) of *trans, cis* nepetalactone in chloroform –*d*.

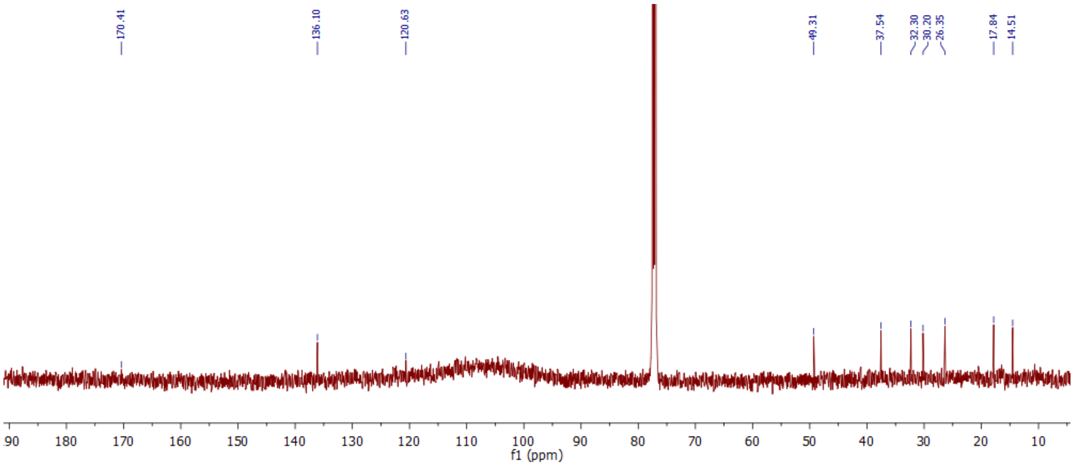

Figure S1c. ^{13}C-NMR spectrum (125 MHz) of *trans, cis* nepetalactone in chloroform –*d*.

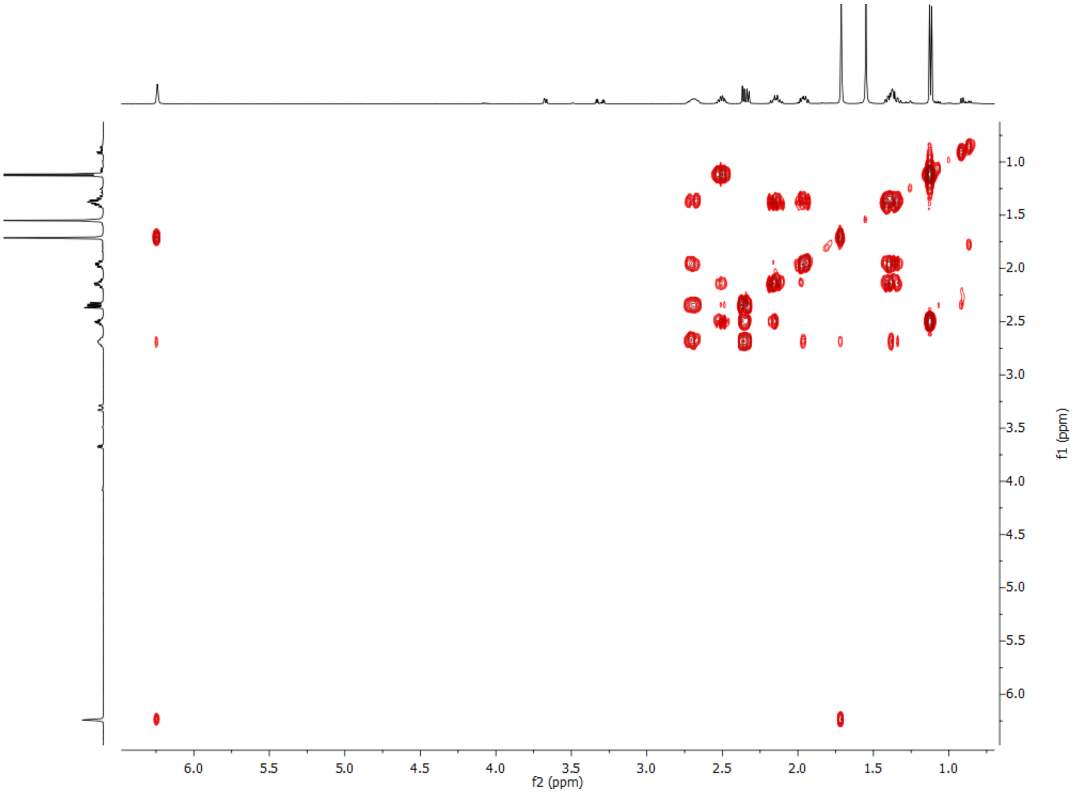

Figure S1d. COSY spectrum of *trans, cis* nepetalactone in chloroform –*d*.

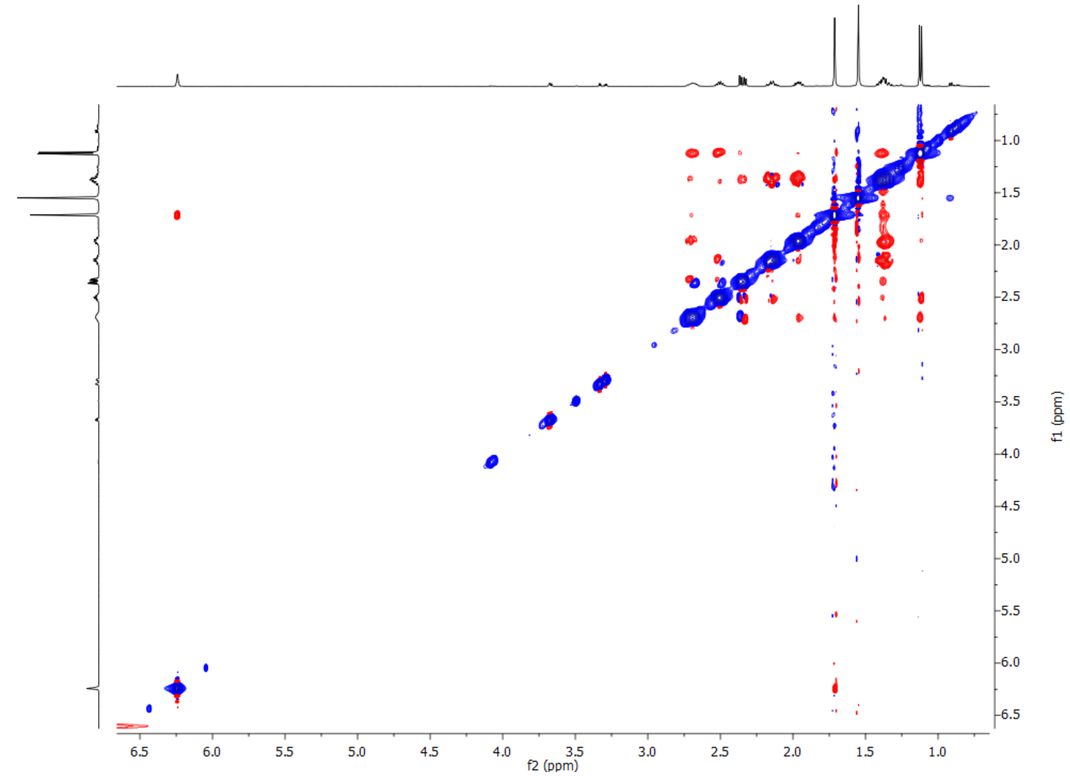

Figure S1e. NOESY spectrum of *trans, cis* nepetalactone in chloroform –*d*.

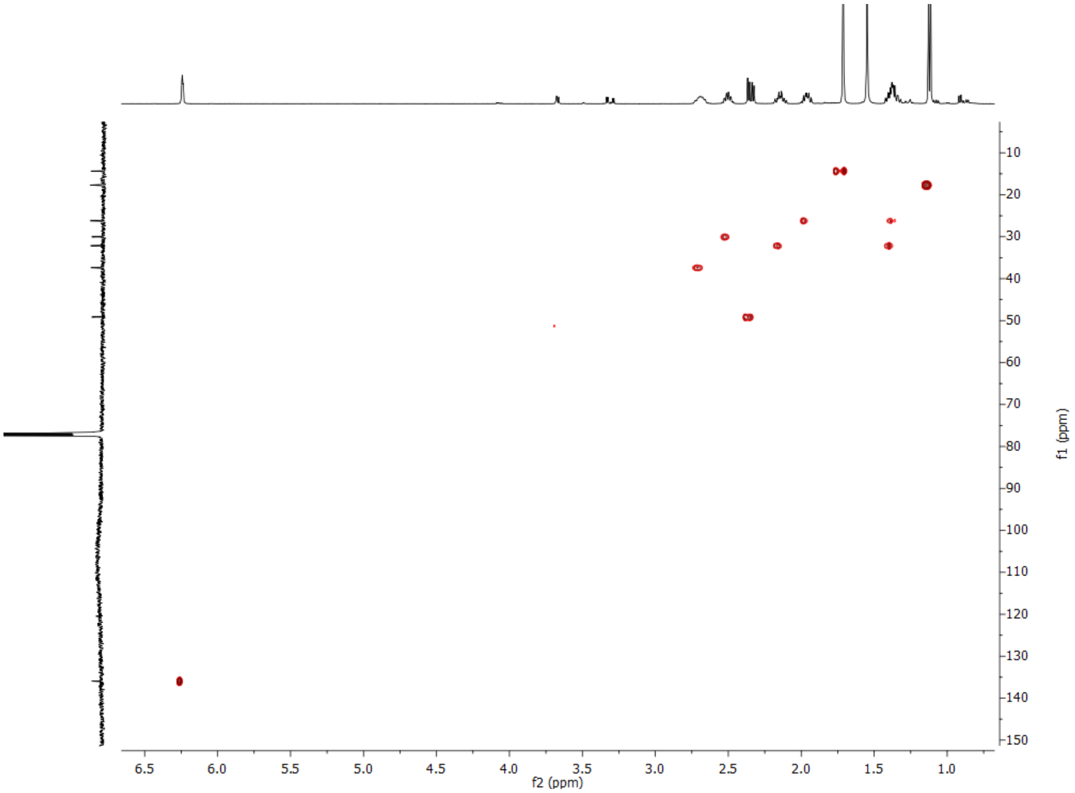

Figure S1f. HSQC spectrum of *trans, cis* nepetalactone in chloroform –*d*.

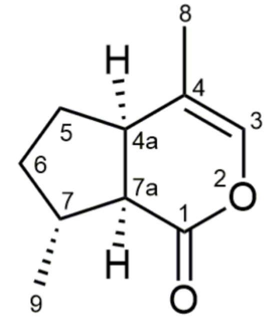

Figure S2a. Chemical structure of *cis,trans* nepetalactone.

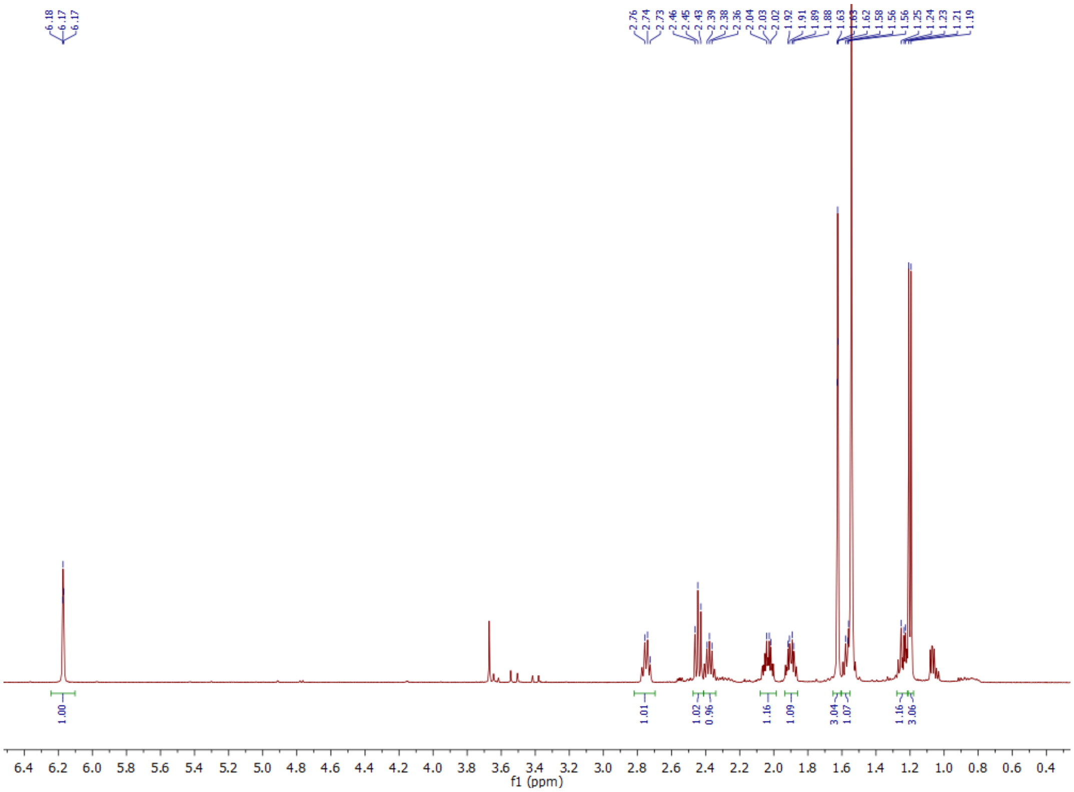

Figure S2b. ^{1}H-NMR spectrum (500 MHz) of *cis, trans* nepetalactone in chloroform –*d*.

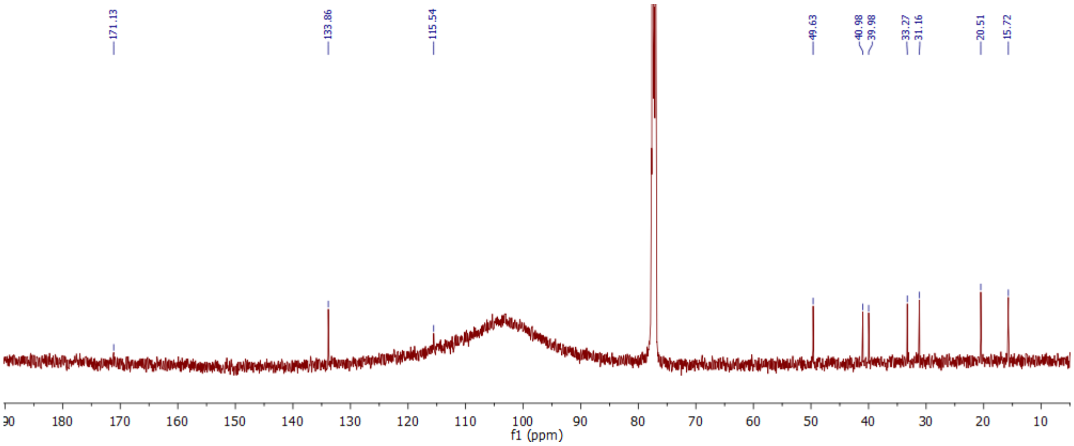

Figure S2c. ^{13}C-NMR spectrum (125 MHz) of *cis, trans* nepetalactone in chloroform –*d*.

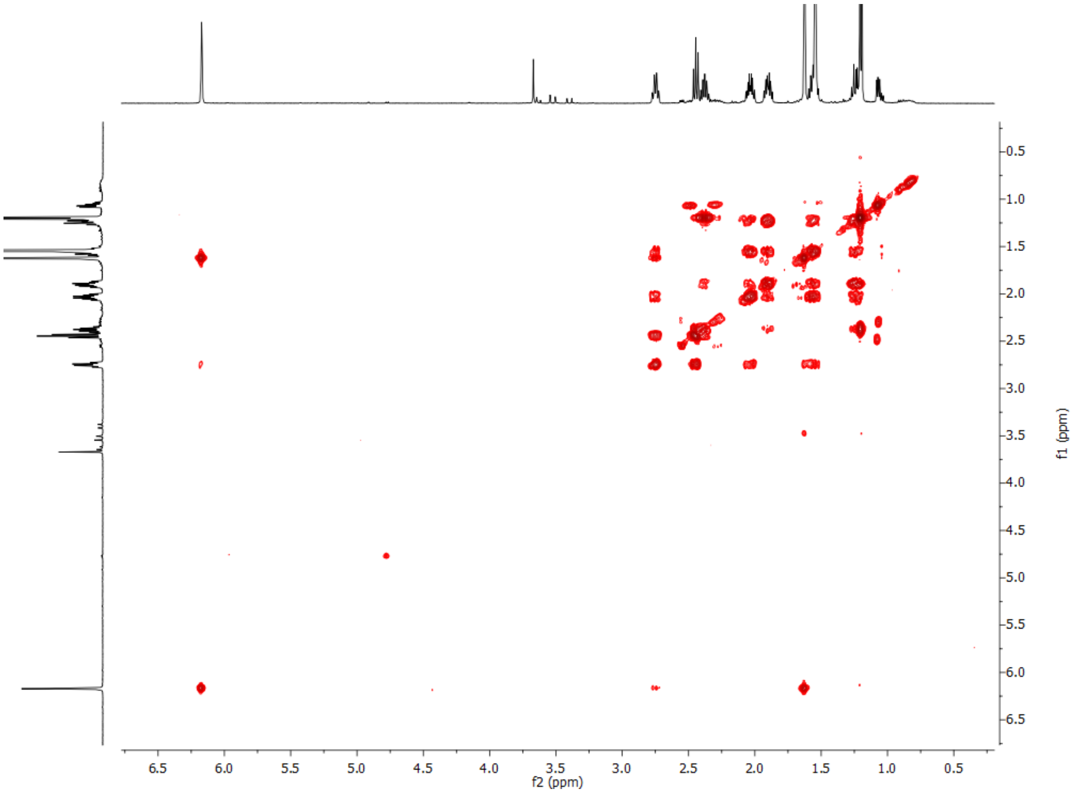

Figure S2d. H-H COSY spectrum of *cis, trans* nepetalactone in chloroform –*d*.

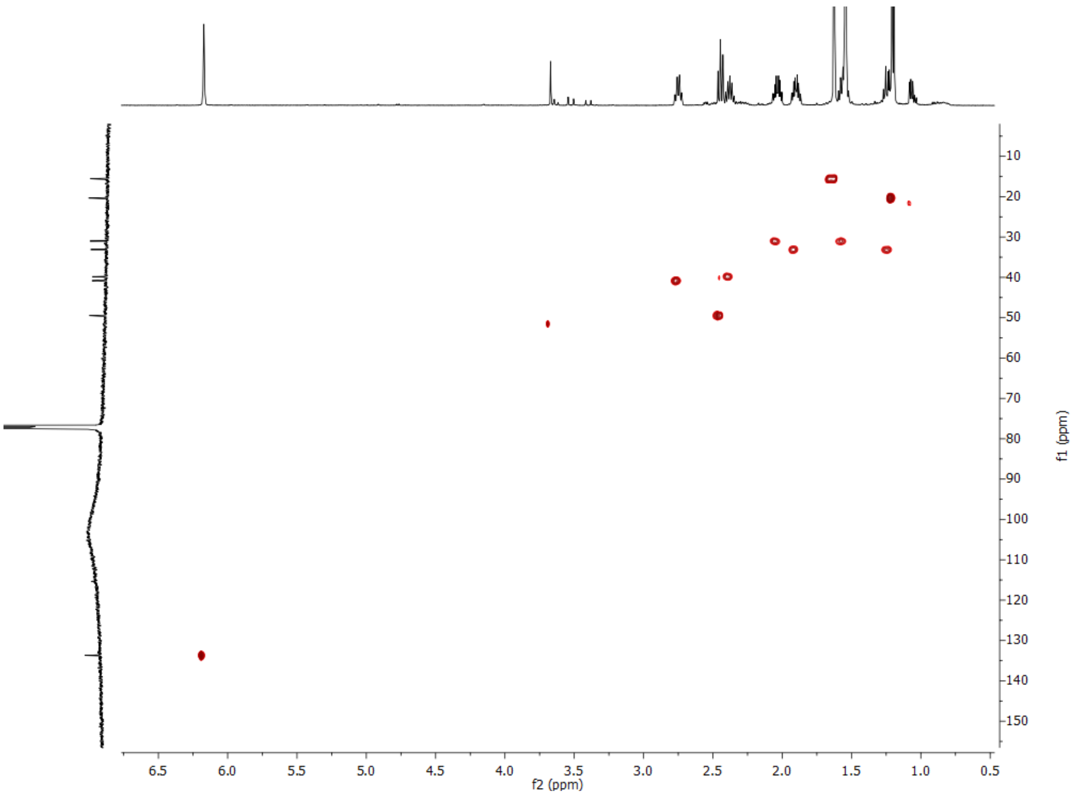

Figure S2e. HSQC spectrum of *cis, trans* nepetalactone in chloroform –*d*.

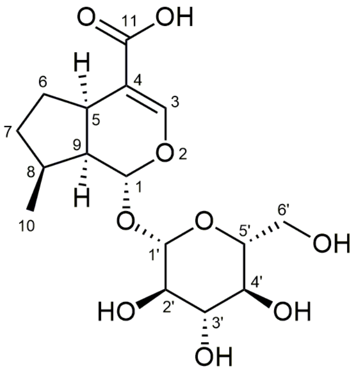

Figure S3a. Chemical structure of 1,5,9-epideoxyloganic acid.

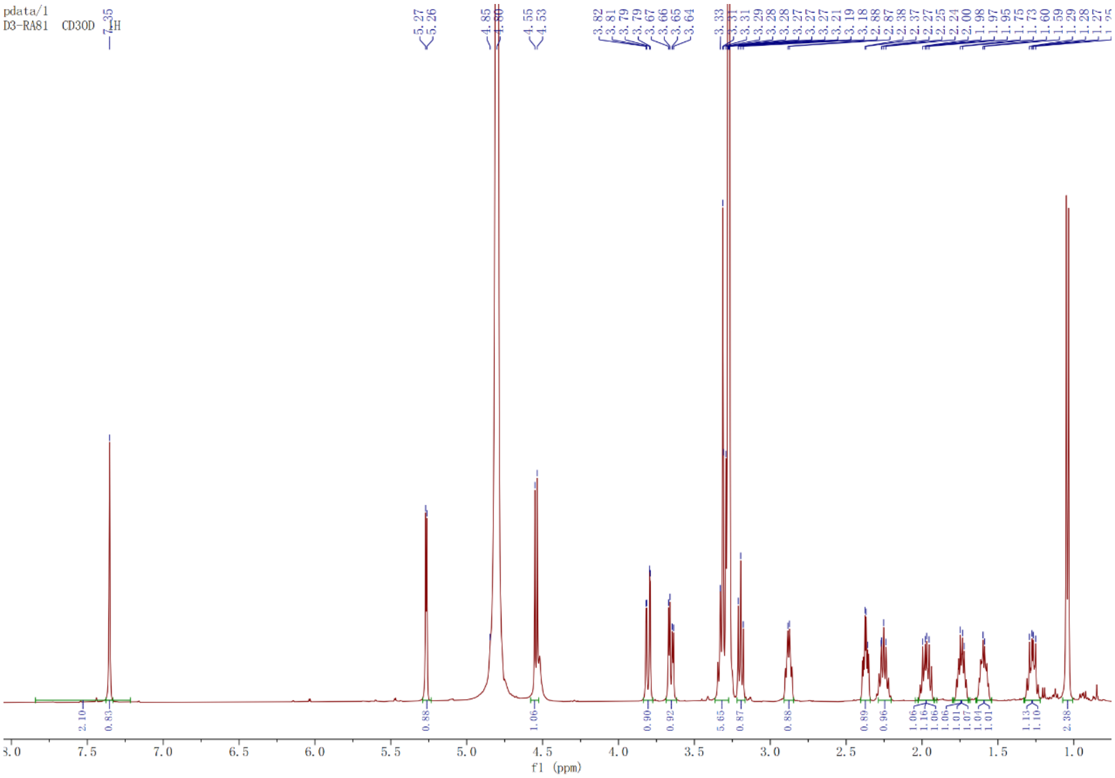

Figure S3b. ^{1}H-NMR spectrum (500 MHz) of 1,5,9-epideoxyloganic acid in methanol-*d*$_4$

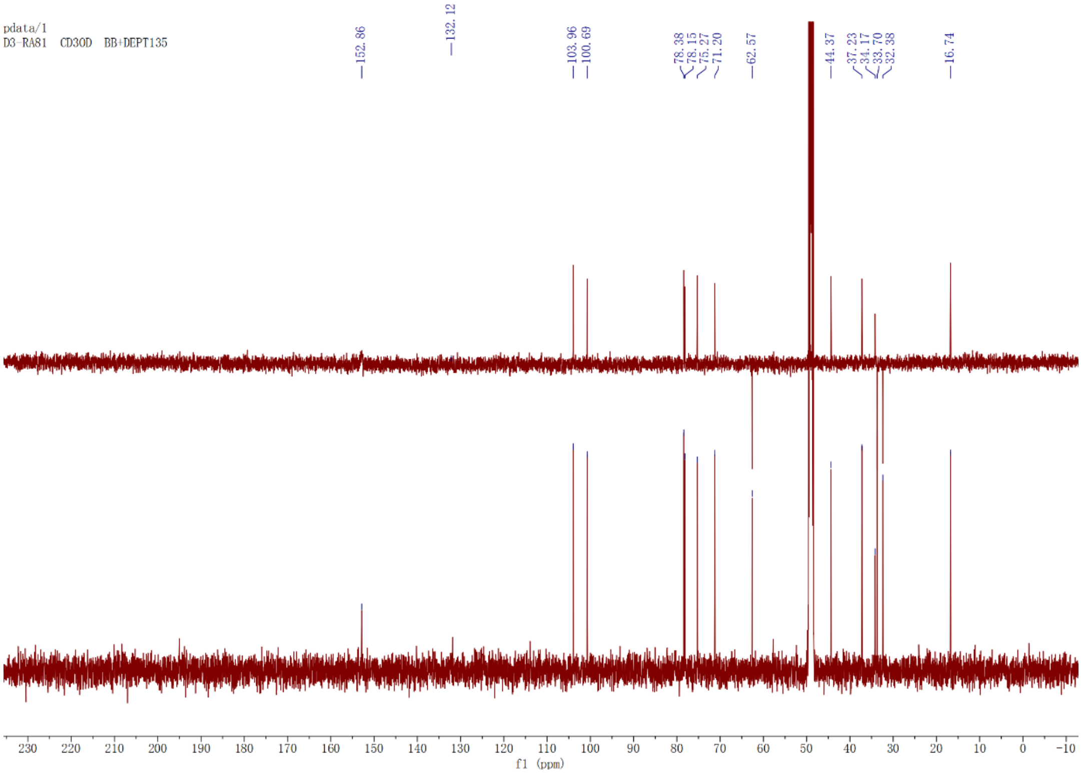

Figure S3c. ^{13}C-NMR spectrum (125 MHz) of 1,5,9-epideoxyloganic acid in methanol-*d*$_4$

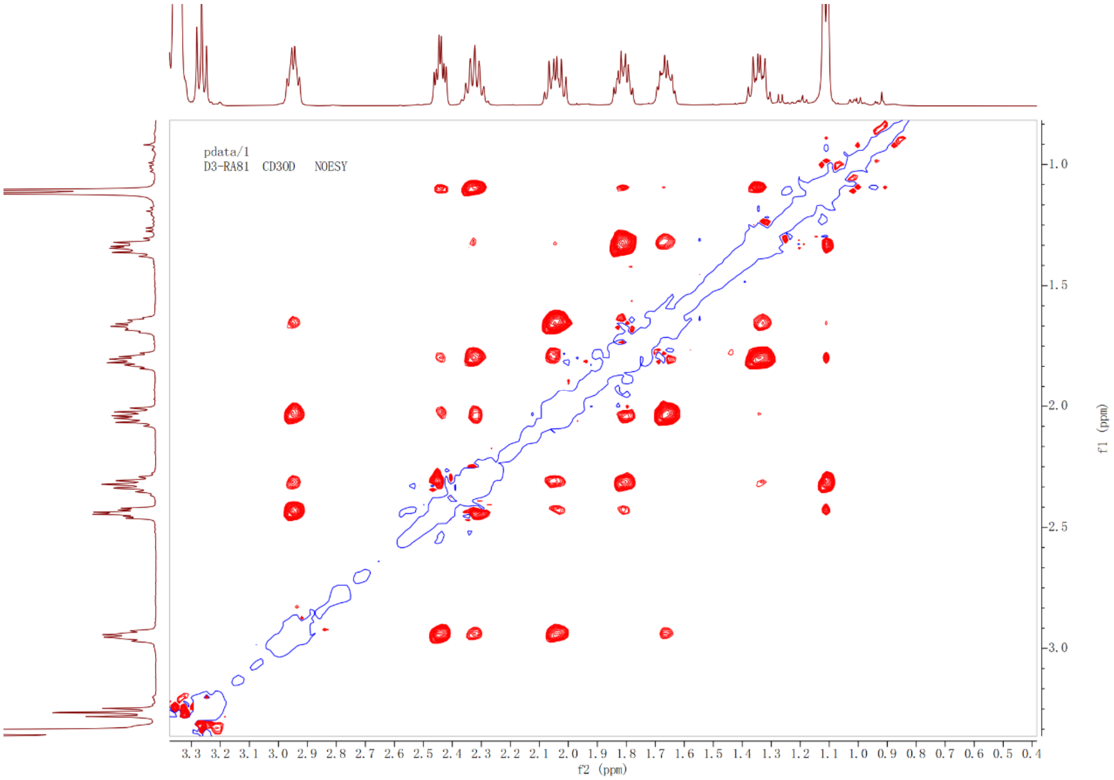

Figure S3d. NORSY spectrum (500 MHz) of 1,5,9-epideoxyloganic acid in methanol-*d*$_4$

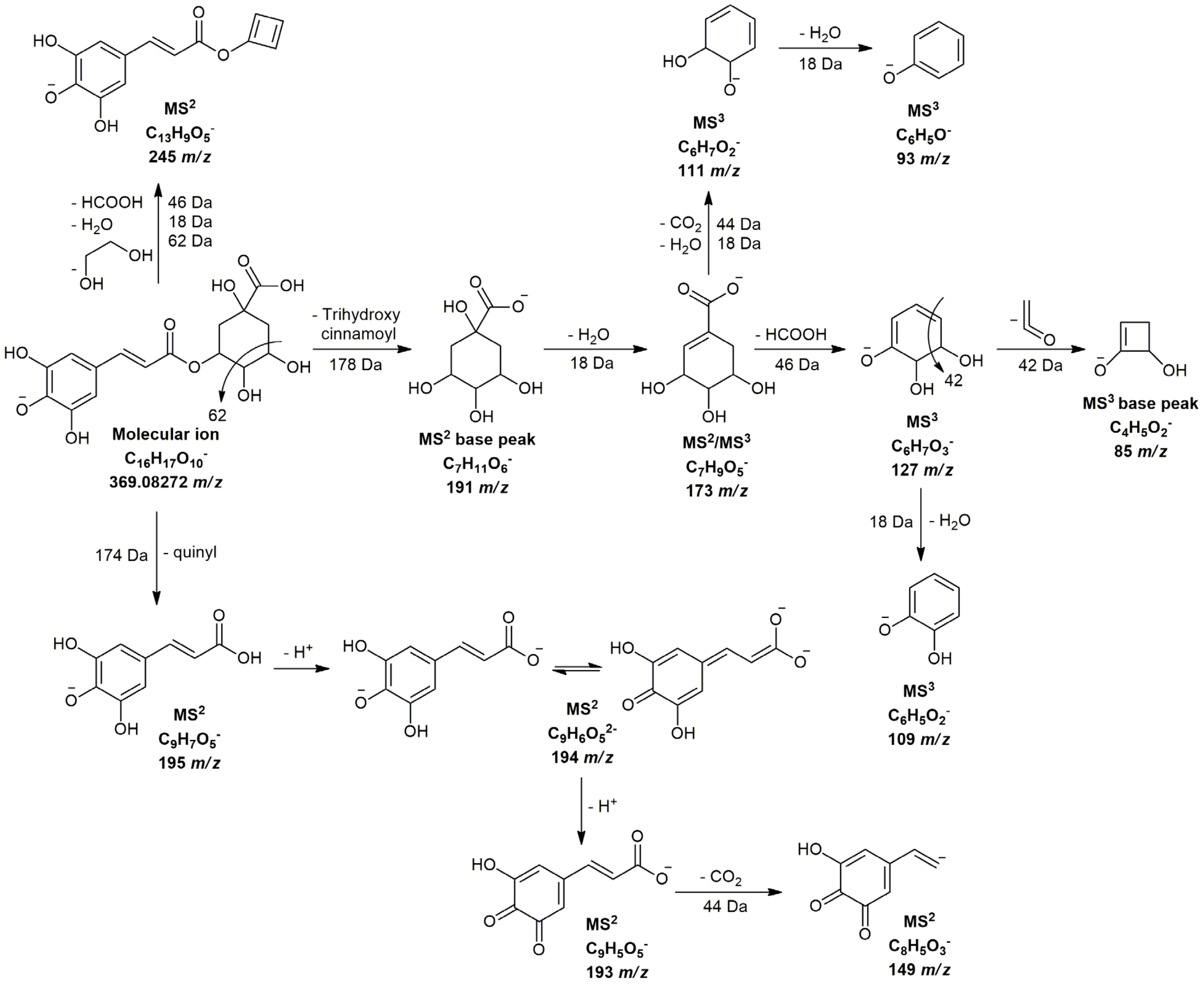

Figure S4a. Proposed structural formula of trihydroxycinnamoylquinic acid (compound **8**), as well as its detailed fragmentation pathway.

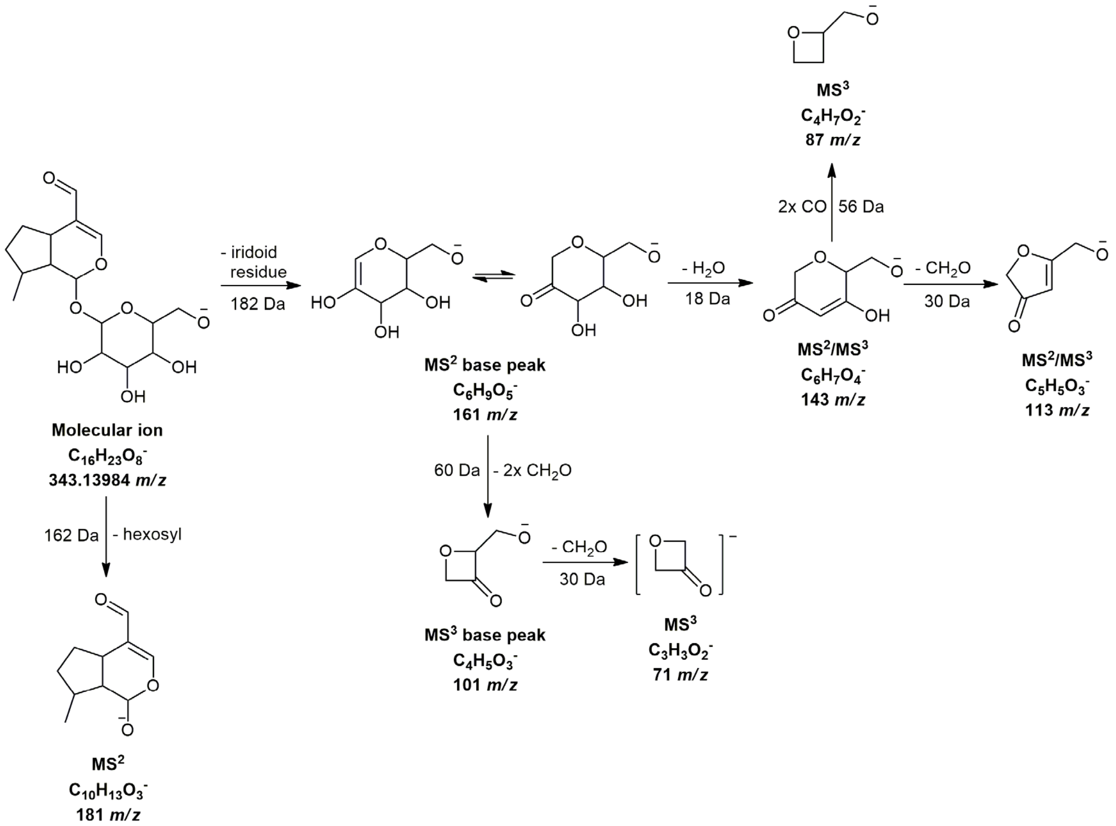

Figure S4b. Proposed fragmentation pathway of boschnaloside (compound **42**).

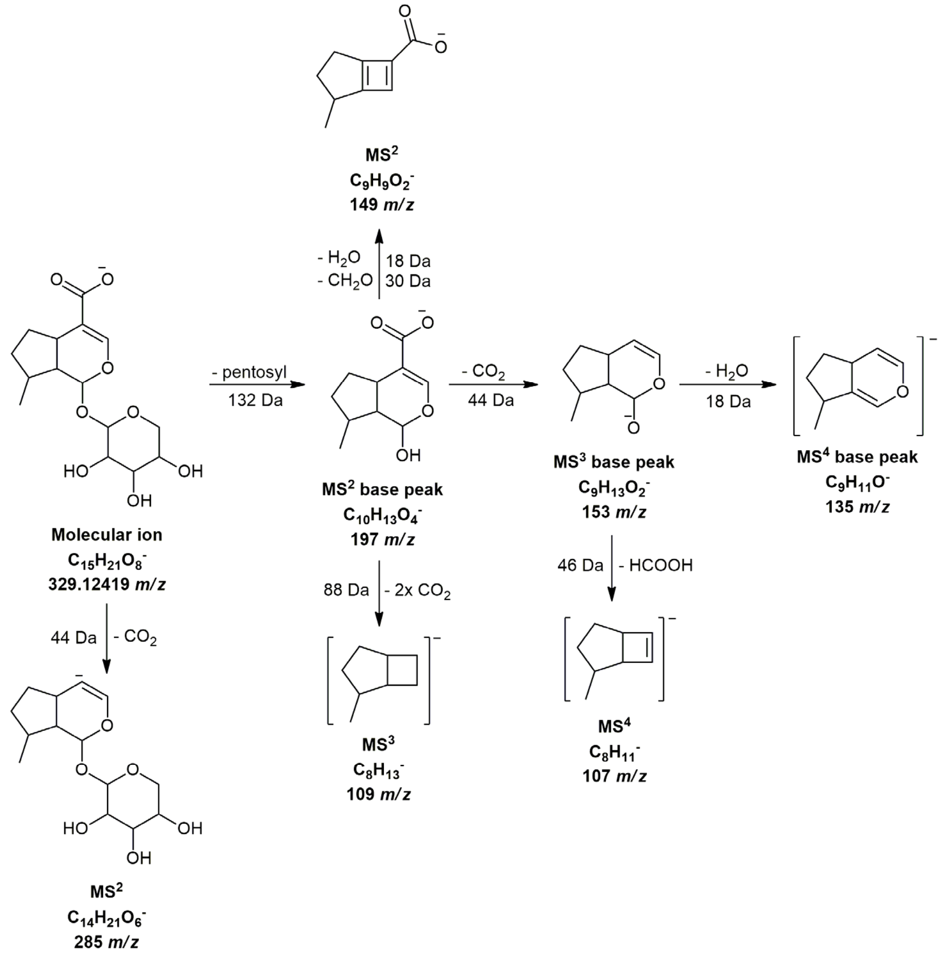

Figure S4c. Proposed structure and detailed fragmentation pathway deoxyloganetic acid pentoside (compound **43**).

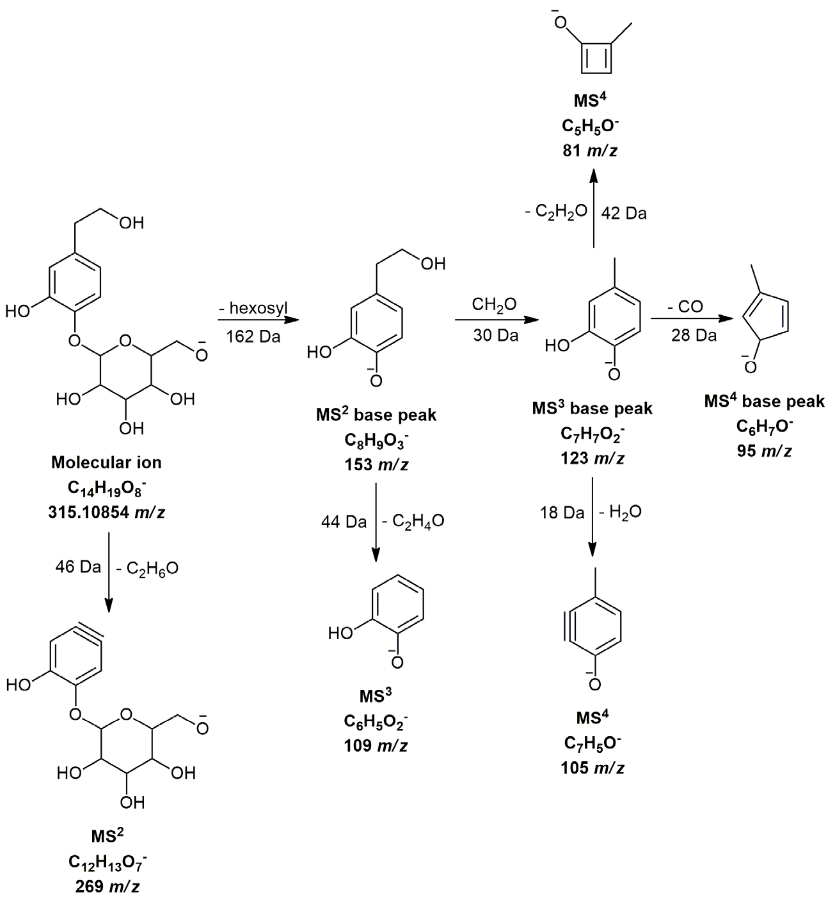

Figure S4d. Fragmentation pathway of 3,4-dihydroxyphenethyl alcohol 4-*O*-hexoside (compound **47**).