

## 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 (<sup>1</sup>H and <sup>13</sup>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 (<sup>1</sup>H and <sup>13</sup>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 (<sup>1</sup>H and <sup>13</sup>C) (b and c) and 2D (NOESY) (d).

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

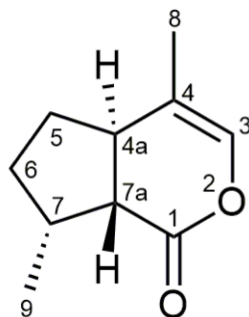


Figure S1a. Chemical structure of *trans, cis* nepetalactone.

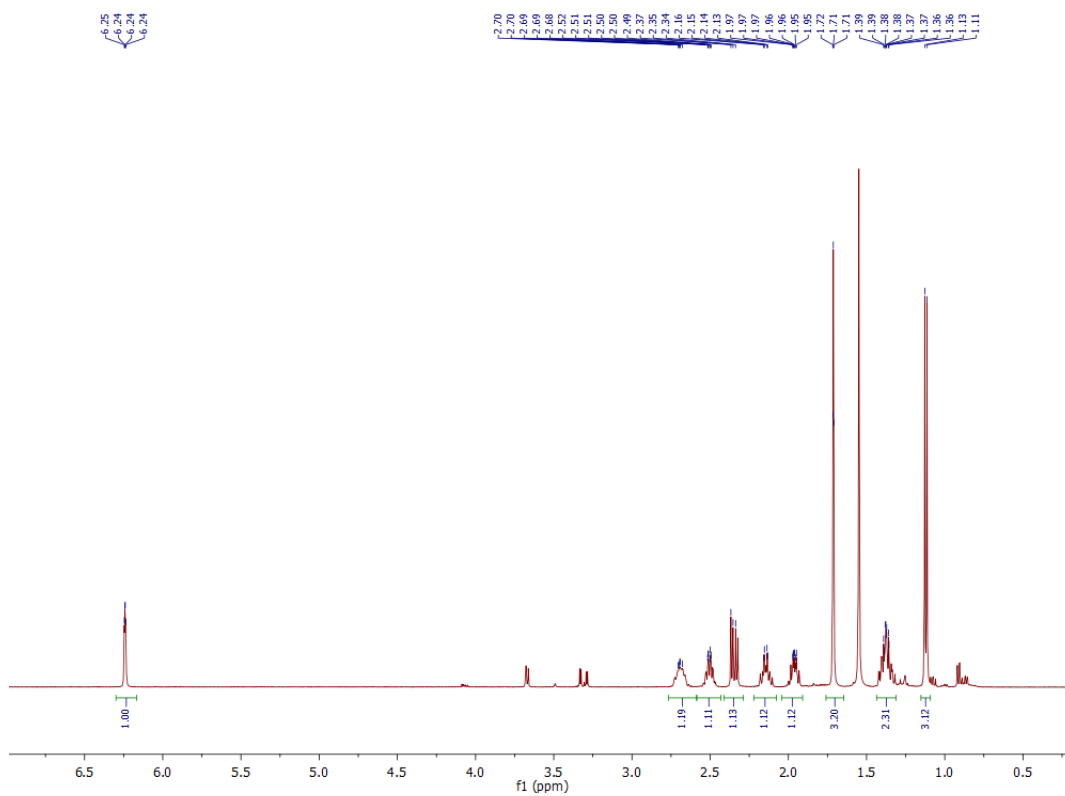
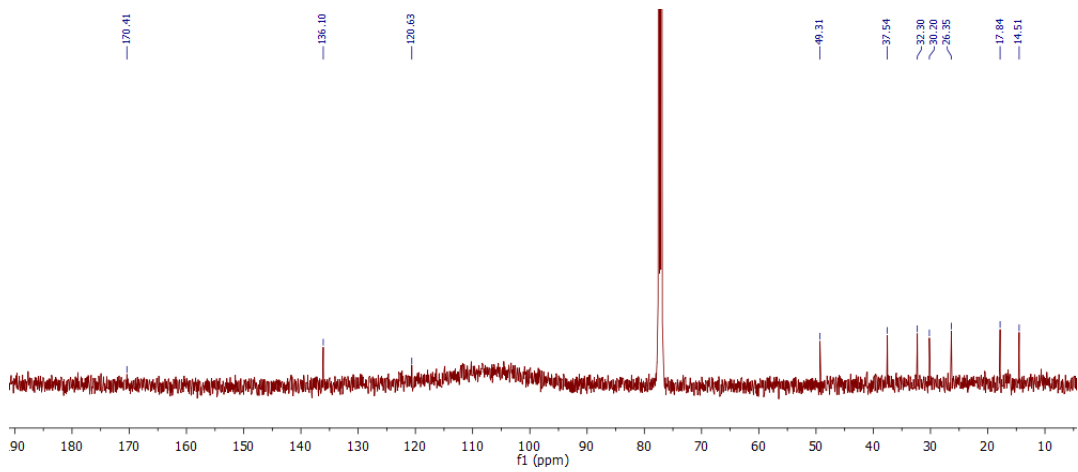
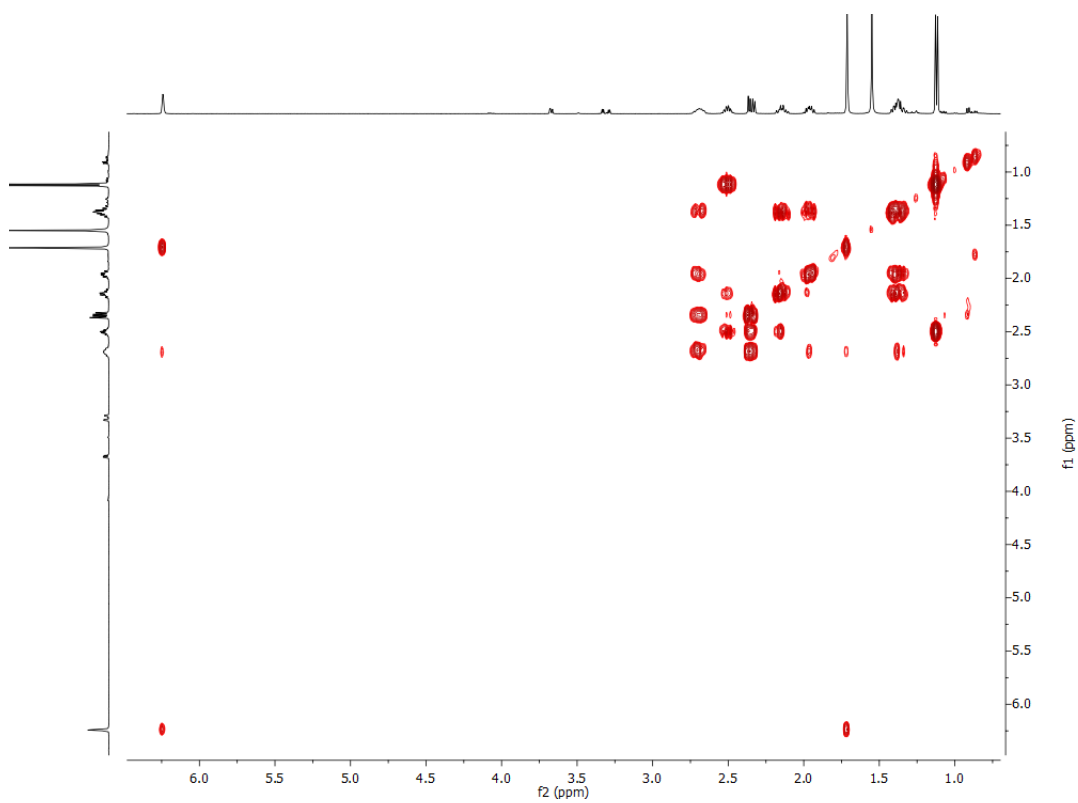


Figure S1b.  $^1\text{H-NMR}$  spectrum (500 MHz) of *trans, cis* nepetalactone in chloroform  $-d$ .



**Figure S1c.** <sup>13</sup>C-NMR spectrum (125 MHz) of *trans, cis* nepetalactone in chloroform-*d*.



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

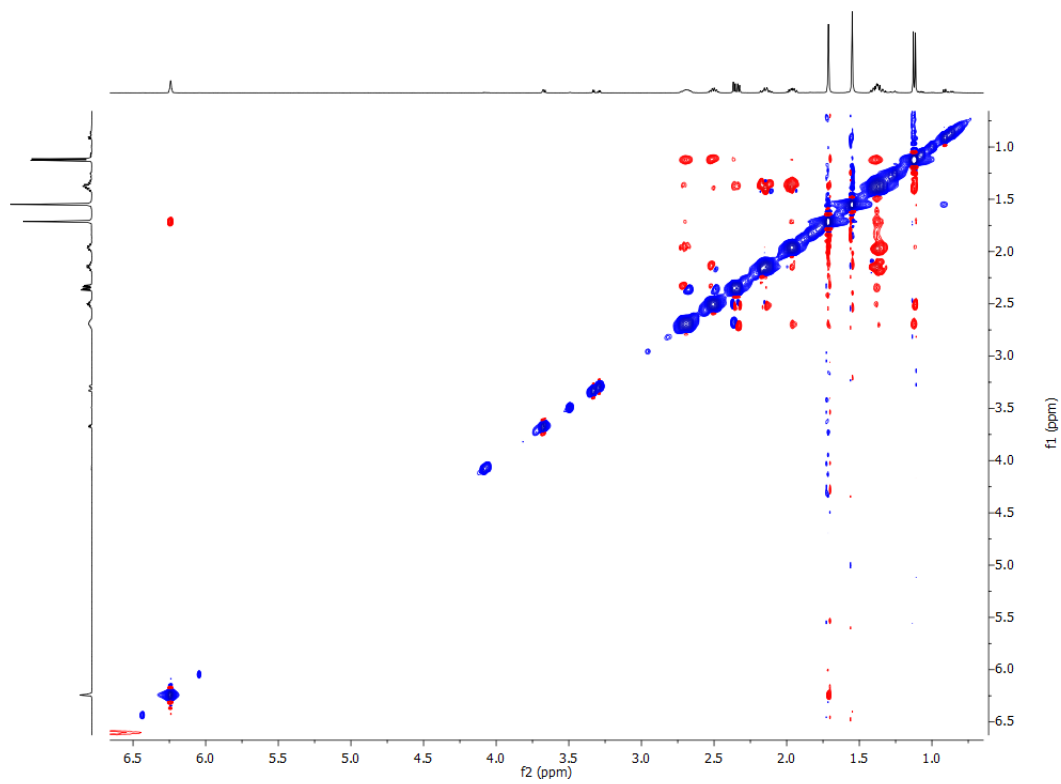


Figure S1e. NOESY spectrum of *trans, cis* nepetalactone in chloroform *-d*.

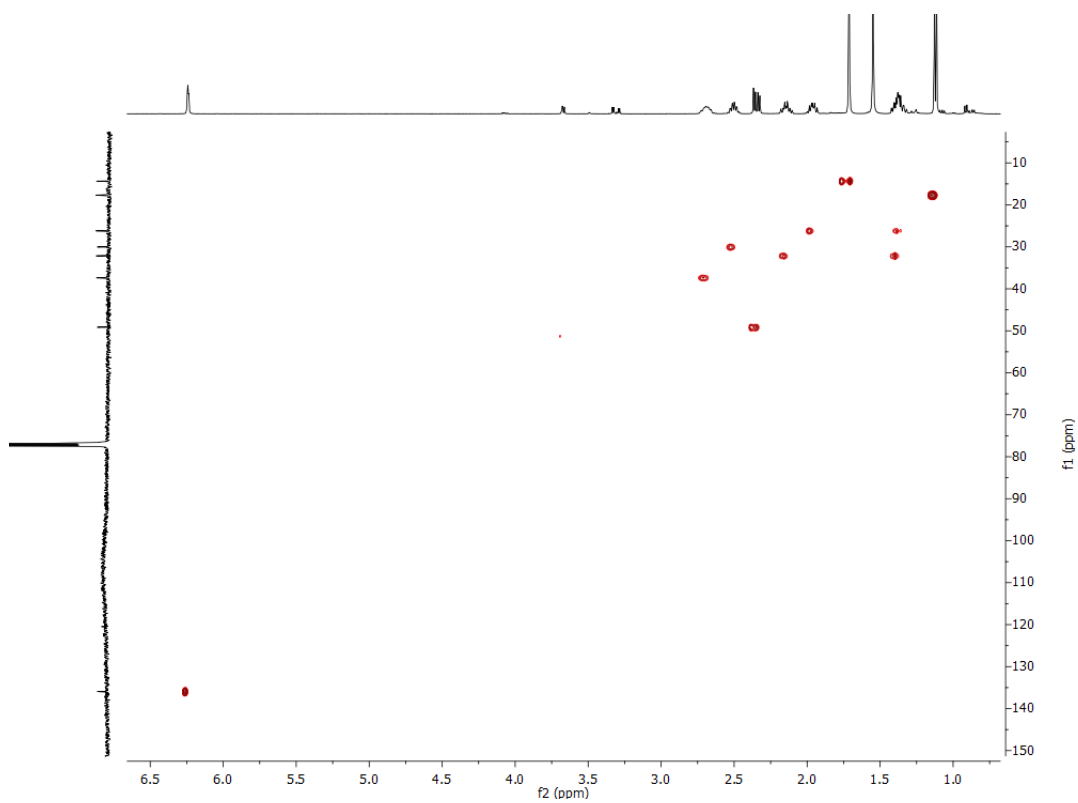
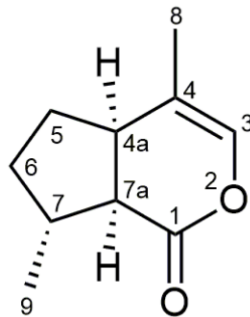
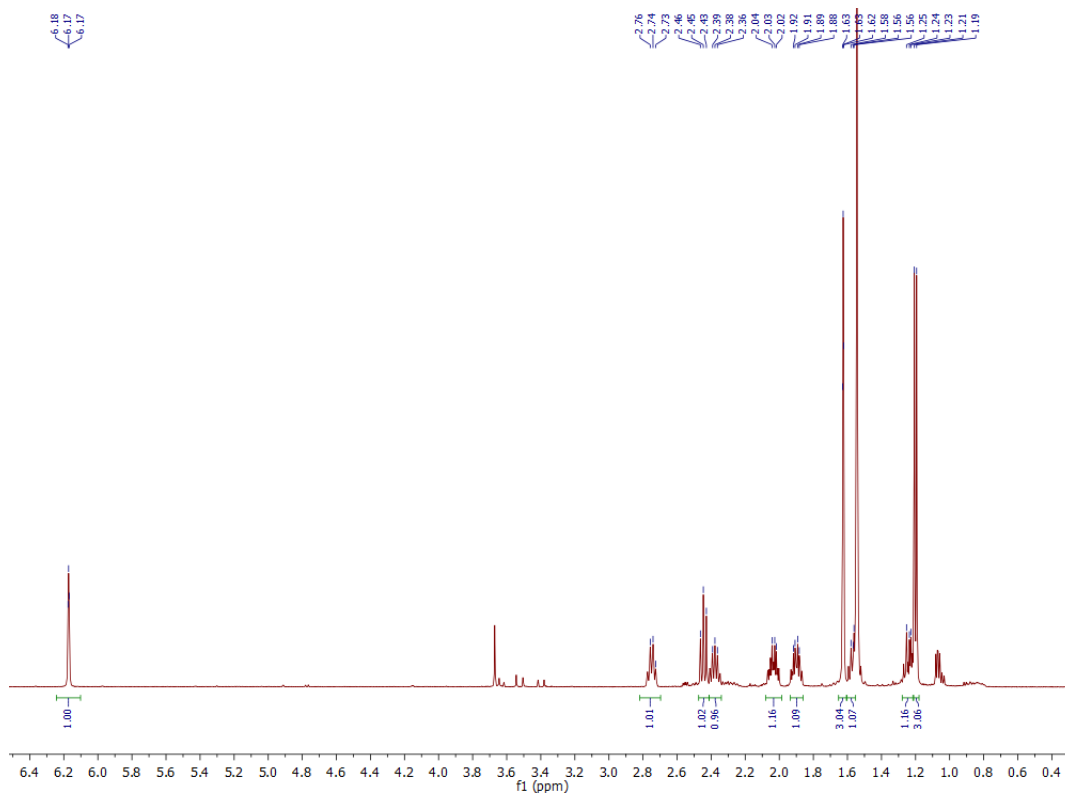


Figure S1f. HSQC spectrum of *trans, cis* nepetalactone in chloroform *-d*.



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



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

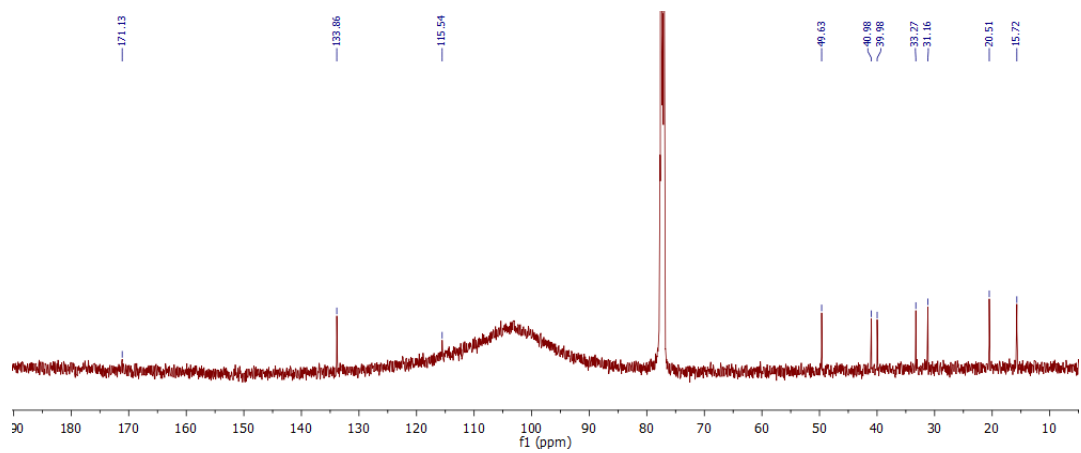


Figure S2c. <sup>13</sup>C-NMR spectrum (125 MHz) of *cis, trans* nepetalactone in chloroform *-d*.

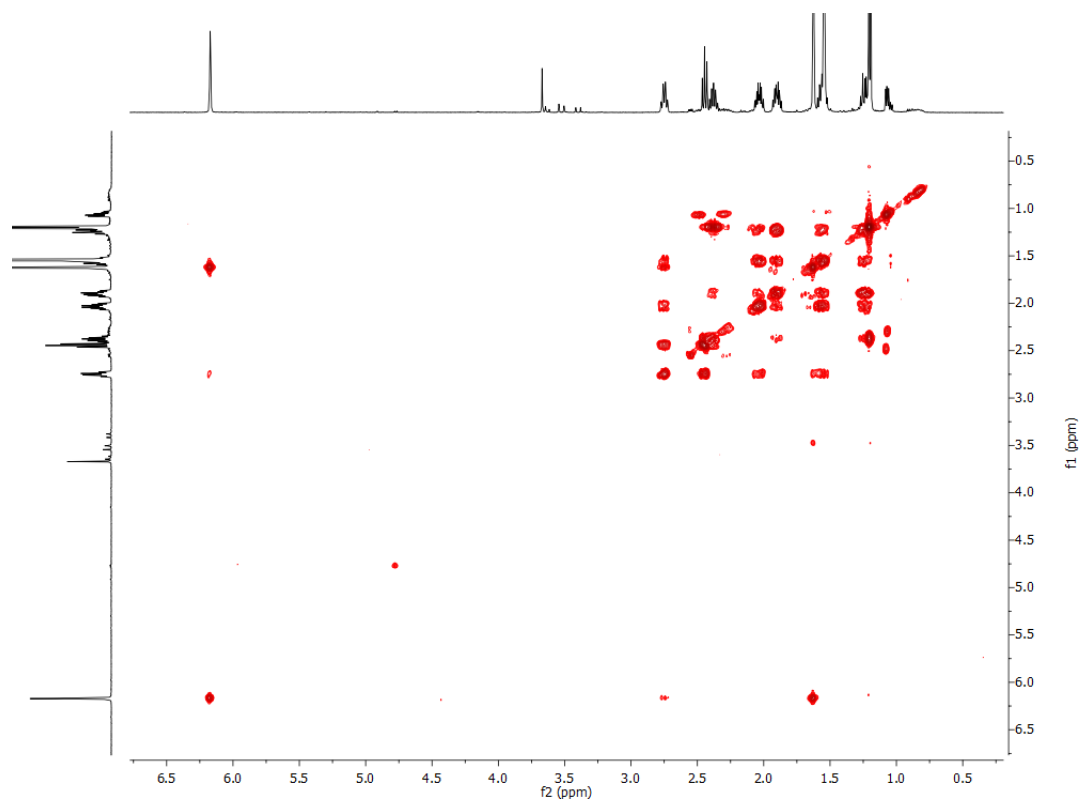


Figure S2d. H-H COSY spectrum of *cis, trans* nepetalactone in chloroform *-d*.

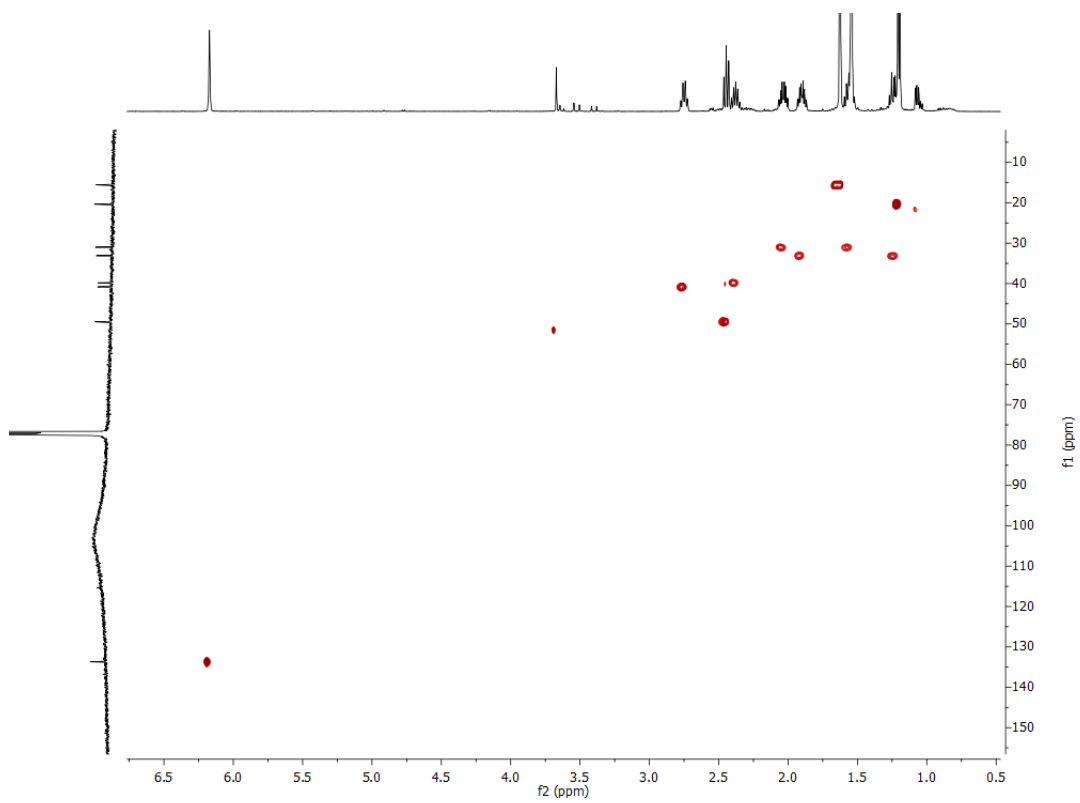
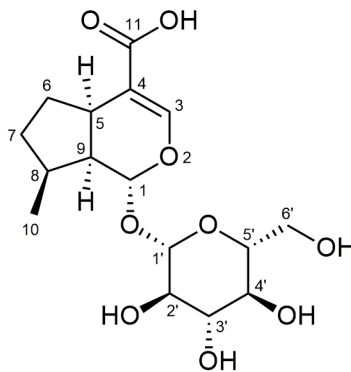
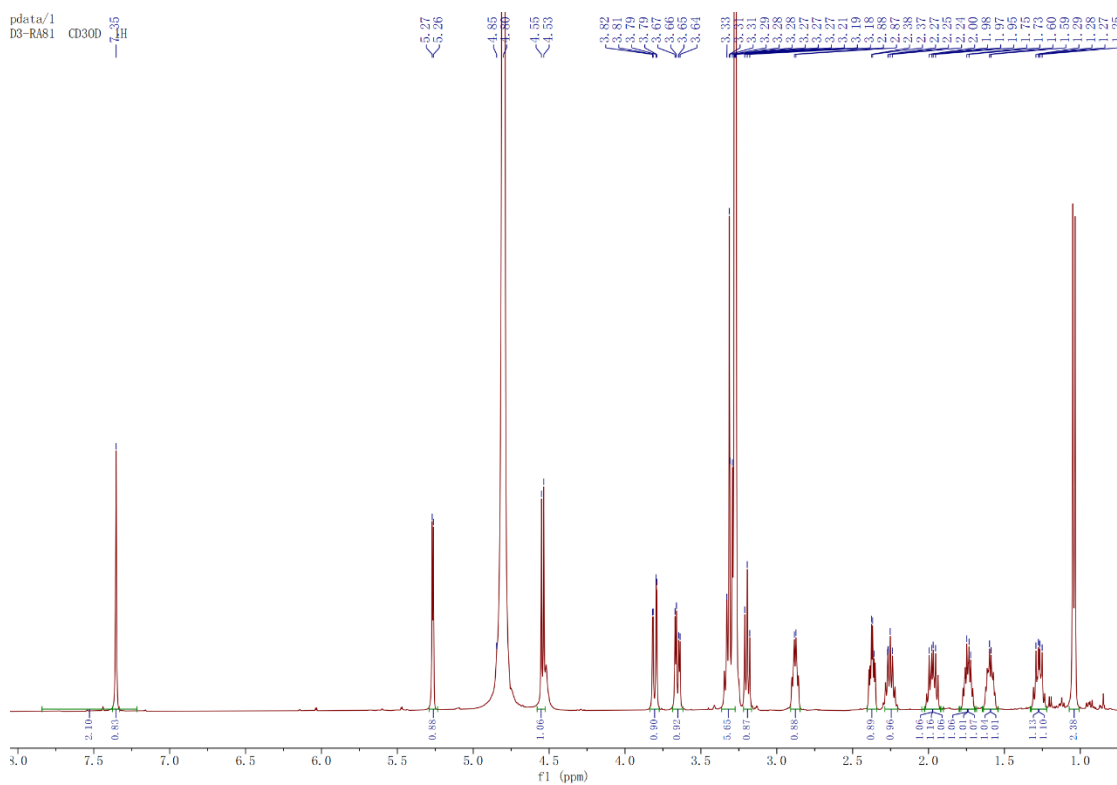


Figure S2e. HSQC spectrum of *cis, trans* nepetalactone in chloroform *-d*.



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



**Figure S3b.**  $^1\text{H-NMR}$  spectrum (500 MHz) of 1,5,9-epideoxyloganic acid in methanol- $d_4$



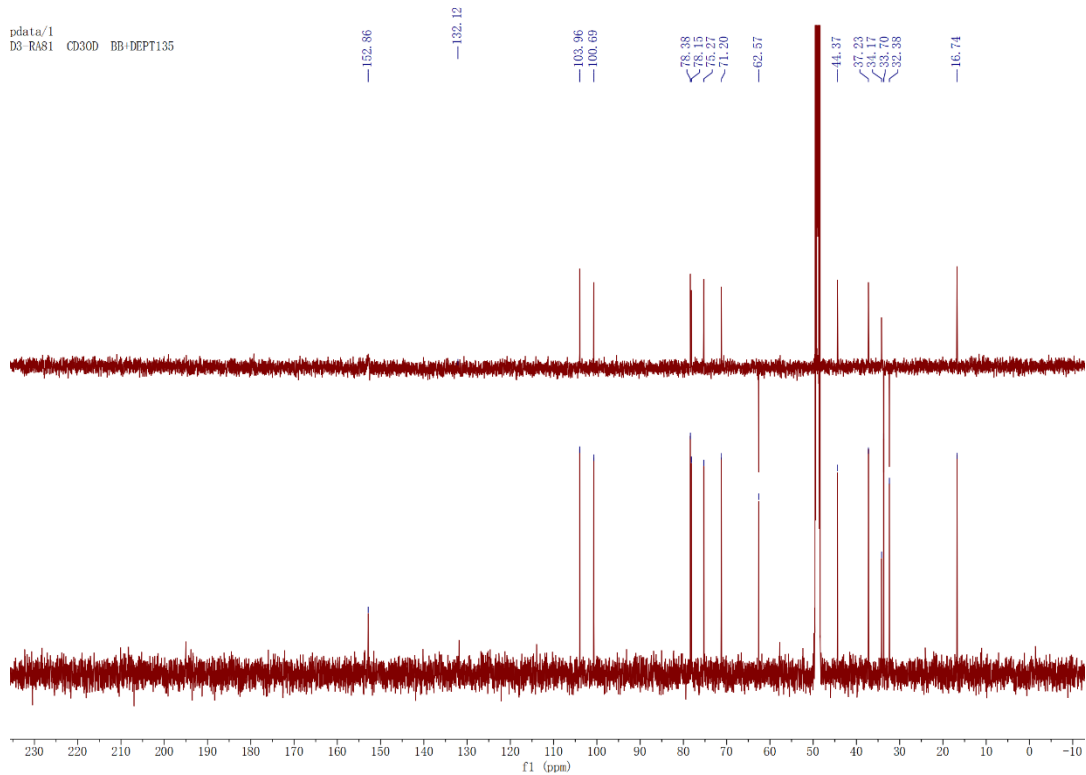


Figure S3c.  $^{13}\text{C}$ -NMR spectrum (125 MHz) of 1,5,9-epideoxyloganic acid in methanol- $d_4$

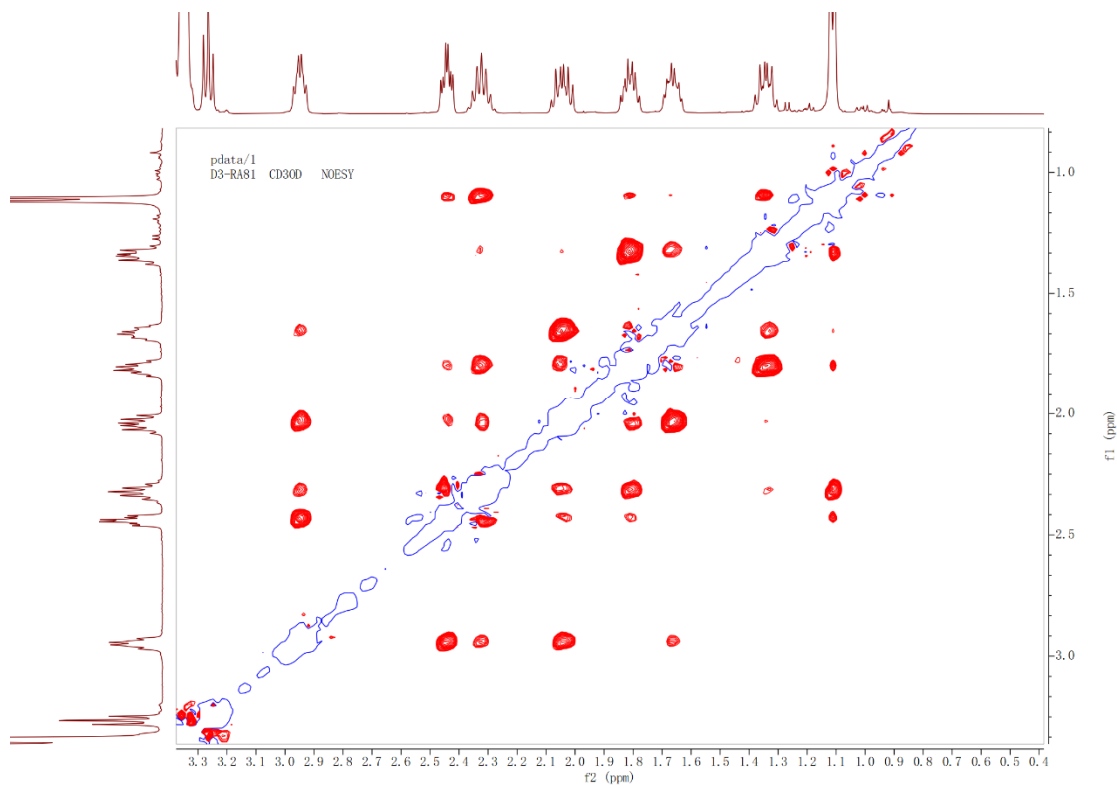
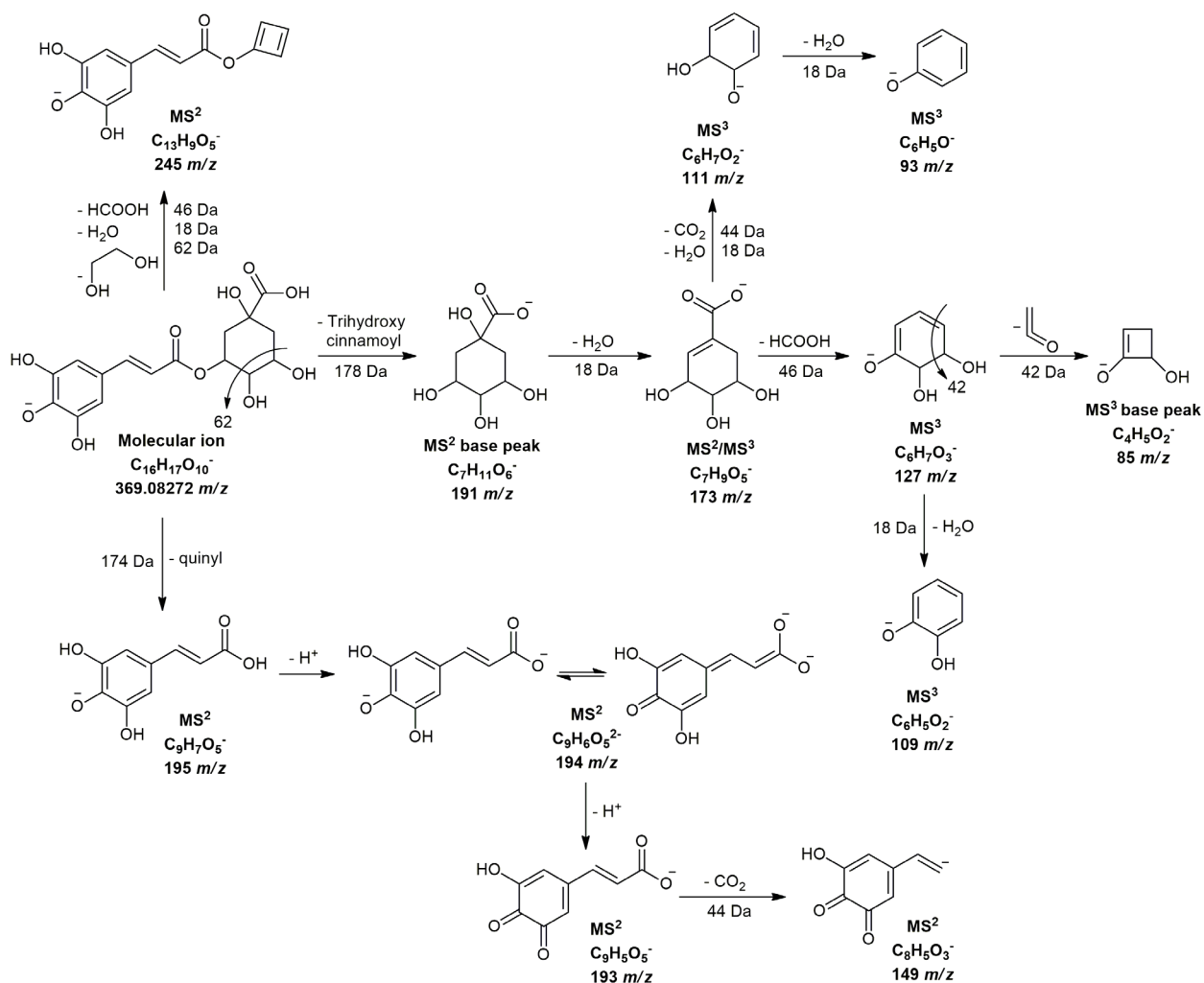
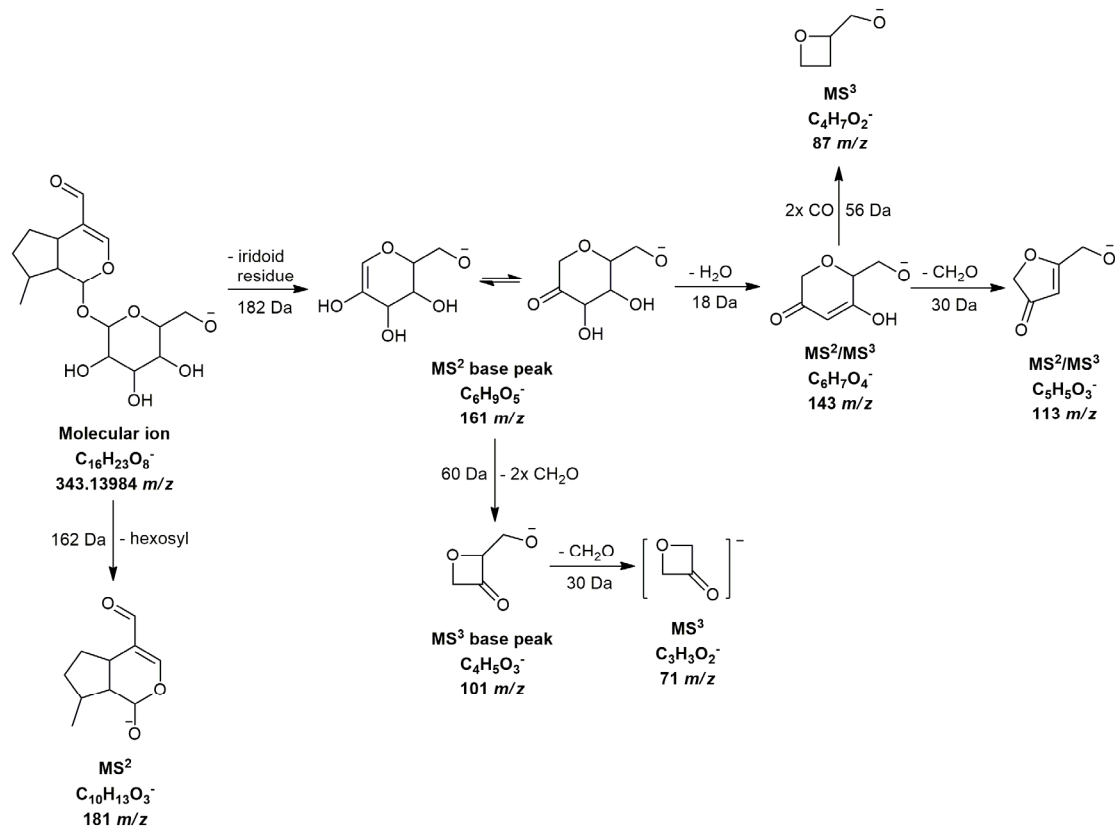


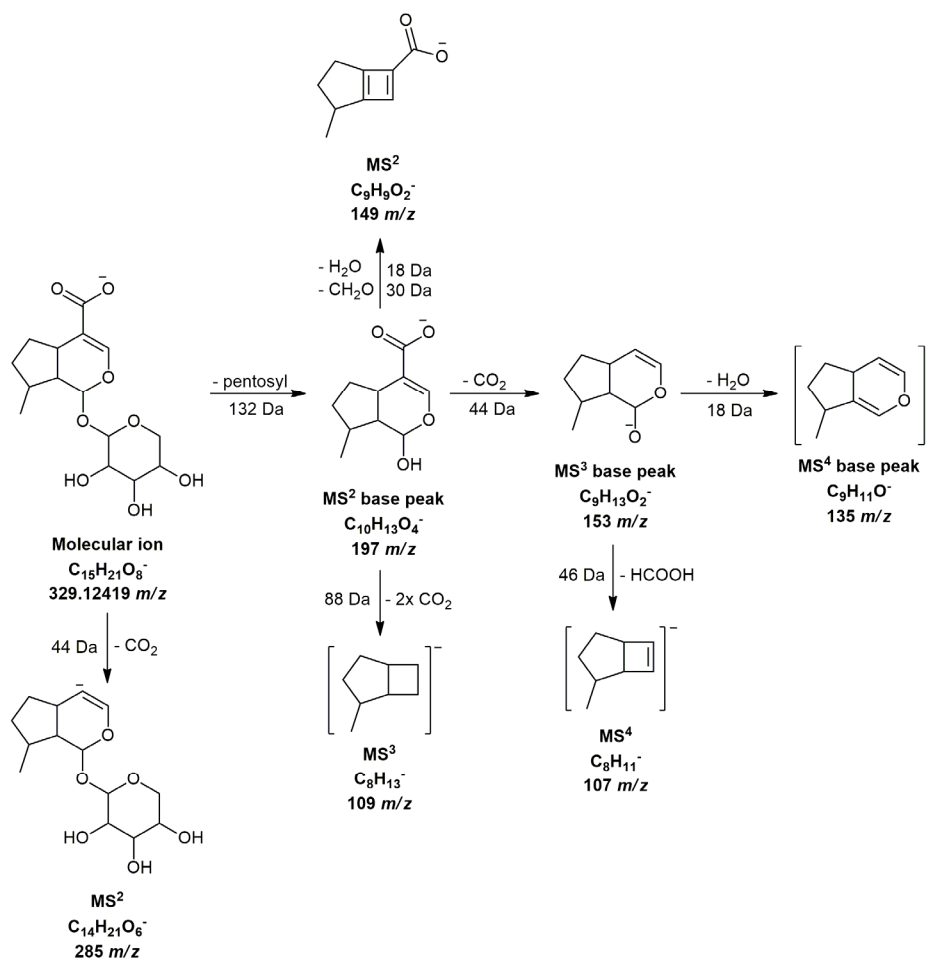
Figure S3d. NOESY spectrum (500 MHz) of 1,5,9-epideoxyloganic acid in methanol- $d_4$



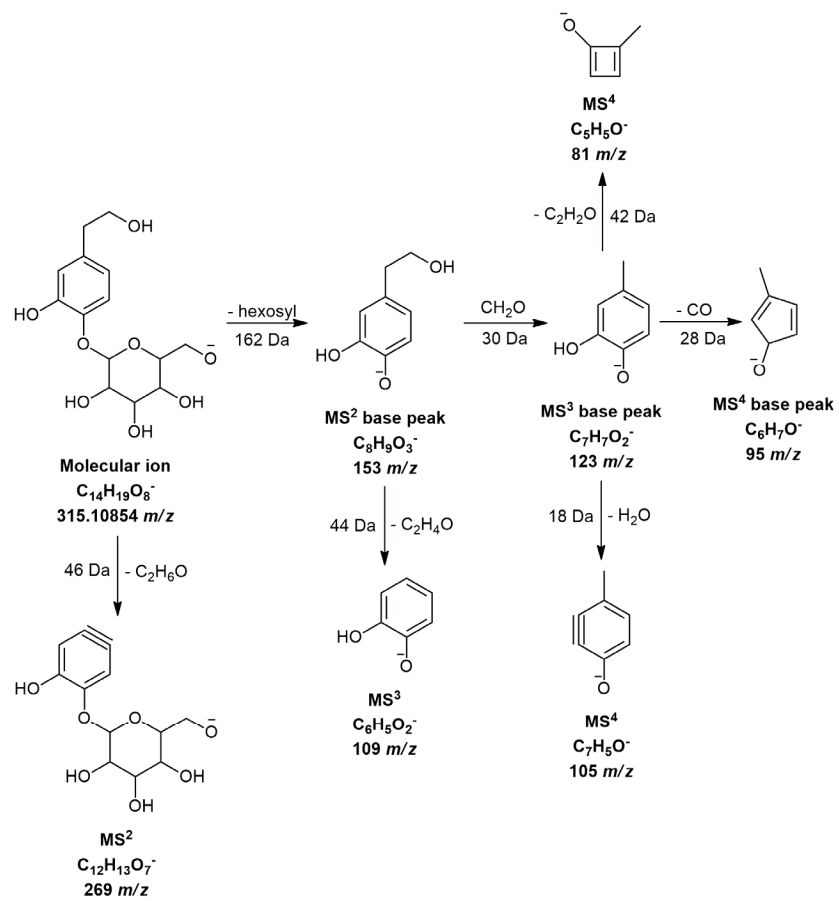
**Figure S4a.** Proposed structural formula of trihydroxycinnamoylquinic acid (compound 8), as well as its detailed fragmentation pathway.



**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).