

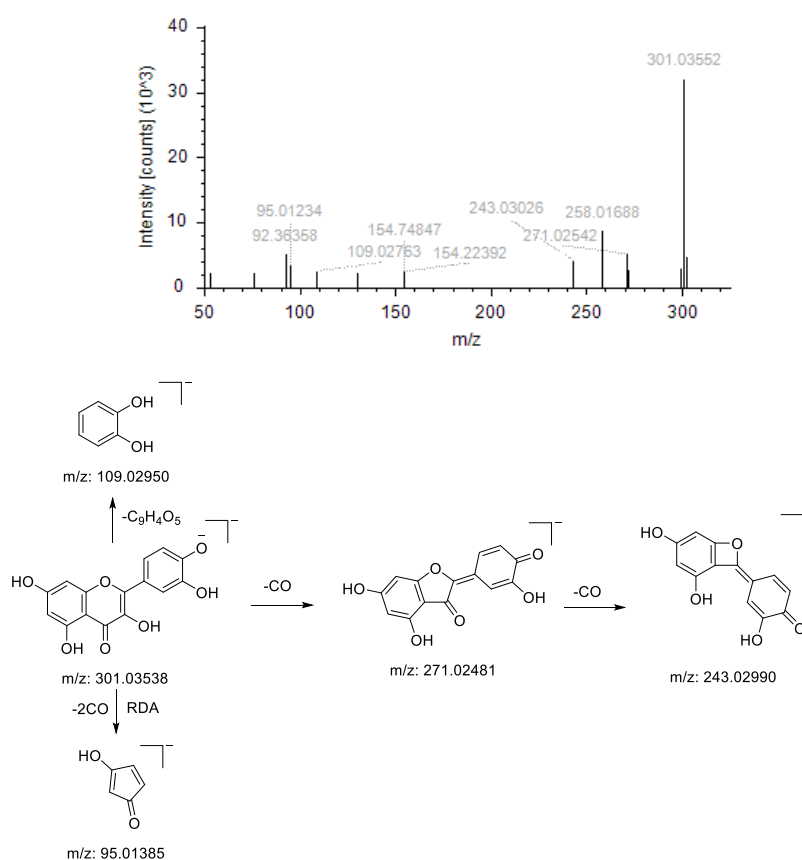
# **Optimisation of Extraction Process and Analysis of Biological Activity from Leaves of Cultivation 'Qi-Nan' Agarwood**

**Qingle Li, Penglian Wei, Yingjian Li and Yunlin Fu \***

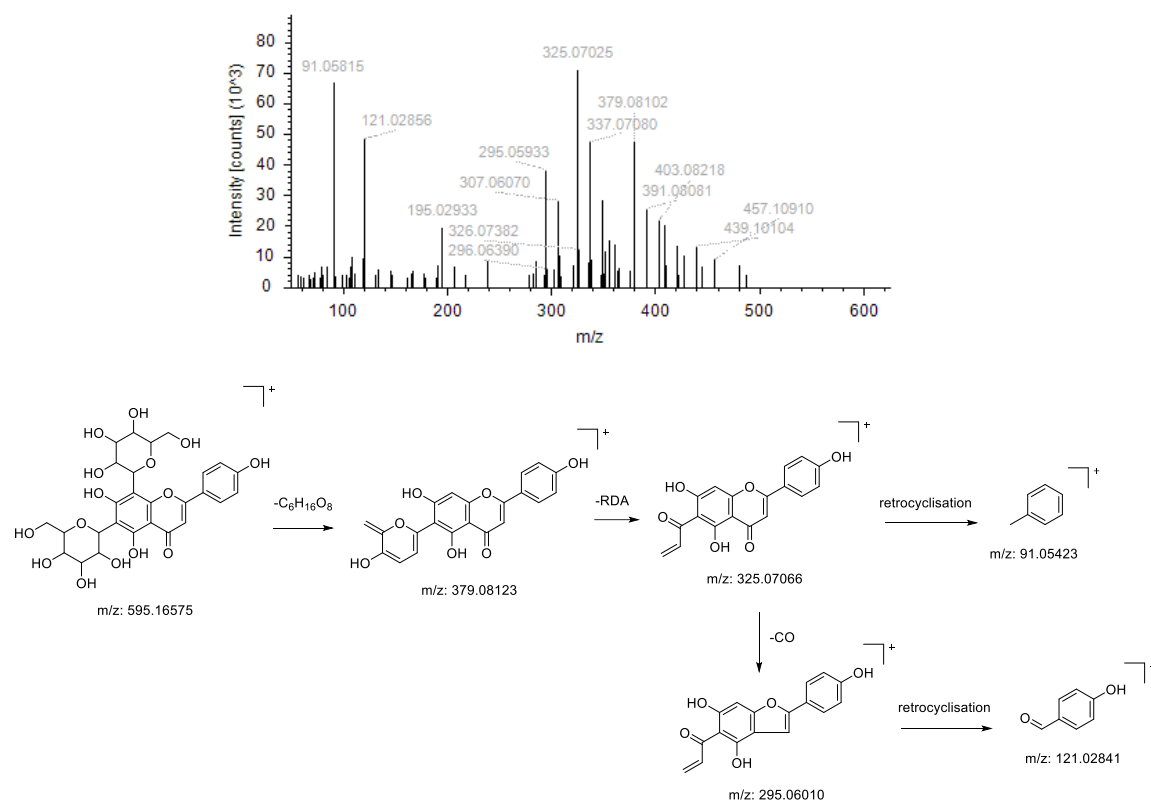
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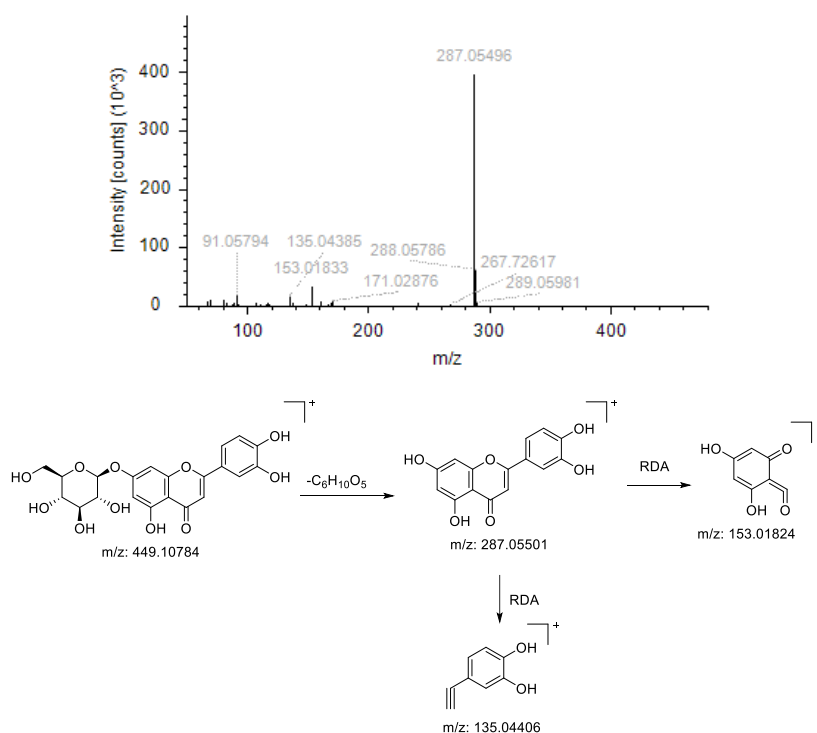
Compound NO.1, its quasimolecular ion peak  $m/z$  301.03552[M-H]<sup>-</sup> has the chemical formula C<sub>15</sub>H<sub>10</sub>O<sub>7</sub>; this parent ion ( $m/z$ 301.03552) first loses one molecule of CO to produce the fragmentation ion  $m/z$  271.02542 fragmentation ions, followed by the loss of another molecule of CO to produce the fragmentation ion  $m/z$ 243.03026; this parent ion ( $m/z$  301.03552) undergoes RDA cleavage and loses two molecules of CO to produce the fragmentation ion  $m/z$ 95.01234; this parent ion ( $m/z$  301.03552) undergoes The parent ion ( $m/z$  301.03552) undergoes RDA cleavage and loses two molecules of CO to generate the fragment ion  $m/z$ 95.01234; the parent ion ( $m/z$  301.03552) undergoes a simple rupture to generate the fragment ion  $m/z$ 109.02763. Combined with literature and mass spectrometry library, the compound is presumed to be Quercetin.



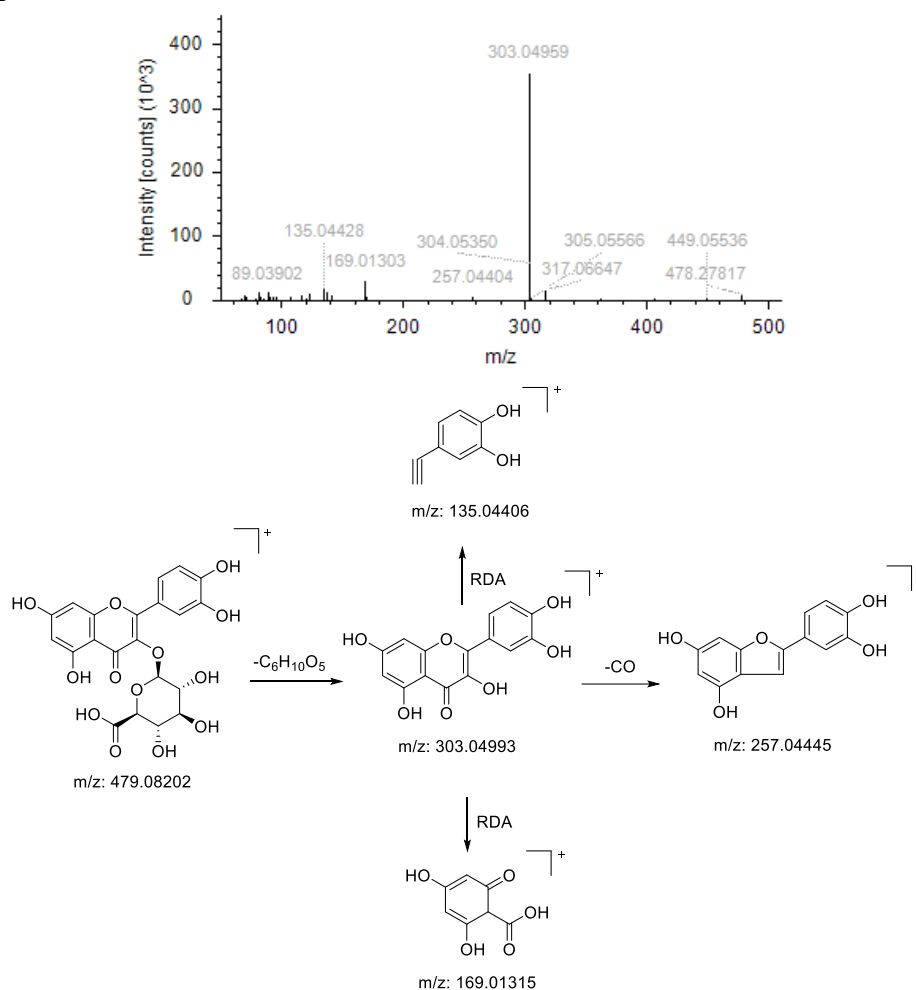
Compound NO.2, Its quasimolecular ion peak  $m/z$ 595.16575[M+H]<sup>+</sup> has the chemical formula C<sub>27</sub>H<sub>30</sub>O<sub>15</sub>, and this parent ion ( $m/z$ 595.16575) firstly dehydrogenates one molecule of sugar and three molecules of water to produce the fragmentation ion  $m/z$ 379.08102 fragmentation ion, then undergoes RDA cleavage to produce the fragmentation ion  $m/z$ 325.07025, and finally undergoes retrocyclisation and dehydration to produce the fragment ion  $m/z$ 91.05815; this parent ion ( $m/z$ 325.07025) lost one molecule of CO to produce the fragment ion  $m/z$ 295.05933, followed by reverse cyclisation to produce the fragment ion  $m/z$ 121.02856, Combined with literature and mass spectrometry library, the compound is presumed to be Vicenin-2.



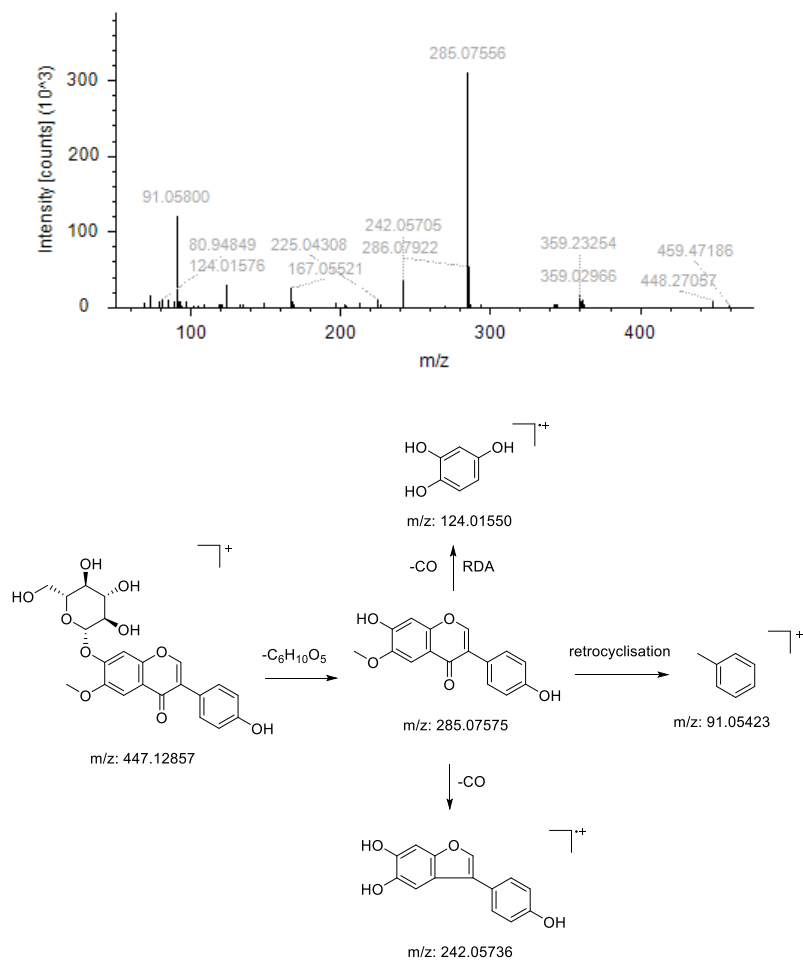
Compound NO.3, Its quasimolecular ion peak  $m/z 449.10784[M+H]^+$  chemical formula is  $C_{21}H_{20}O_{11}$ , and the parent ion ( $m/z 449.10784$ ) first loses a molecule of sugar to produce the fragment ion  $m/z 287.05496$ . The parent ion ( $m/z 287.05496$ ) underwent RDA cleavage to form fragment ions  $m/z 153.01833$  and  $m/z 135.04385$ , respectively. Combined with literature and mass spectrometry library, the compound is presumed to be Cynaroside.



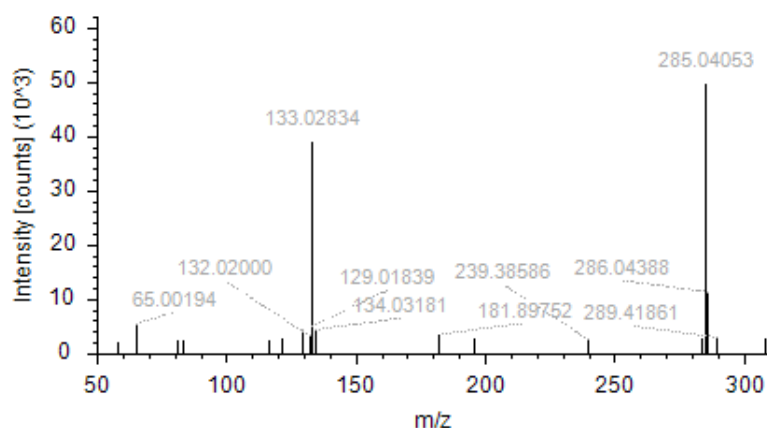
Compound NO.4, Its quasimolecular ion peak  $m/z$  479.08202 $[M+H]^+$  chemical formula is  $C_{21}H_{18}O_{13}$ . The parent ion ( $m/z$  479.08202) first loses a molecule of sugar to produce the fragment ion  $m/z$  303.04959 and then loses a molecule of CO to produce the fragment ion  $m/z$  257.04404. The parent ion ( $m/z$  303.04959) underwent RDA cleavage to form fragment ions  $m/z$  169.01303 and  $m/z$  135.04428 respectively. Combined with literature and mass spectrometry library, the compound is presumed to be Miquelianin.

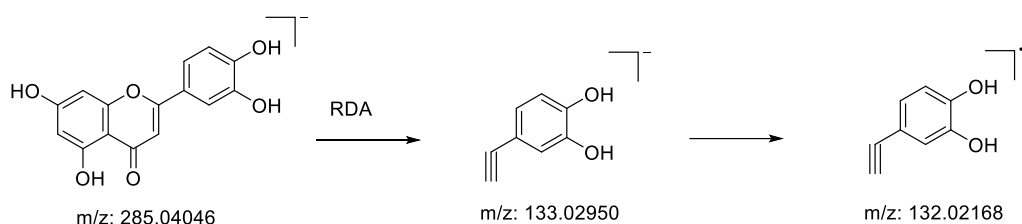


Compound NO.5, Its quasimolecular ion peak  $m/z$  447.12857 $[M+H]^+$  has the chemical formula  $C_{22}H_{22}O_{10}$ ; this parent ion ( $m/z$  447.12857) first loses a molecule of sugar to produce the fragment ion  $m/z$  285.07556 fragment ion, followed by the loss of a molecule of CO to produce the fragment ion  $m/z$  242.05705; this parent ion ( $m/z$  285.07556) undergoes RDA cleavage and loses a methyl radical and a molecule of CO to produce the fragment ion  $m/z$  124.01576; the parent ion ( $m/z$  285.07556) undergoes a reverse cycloaddition reaction and dehydrates to produce the fragment ion  $m/z$  91.05800. Combined with literature and mass spectrometry library, the compound is presumed to be Glycitin.

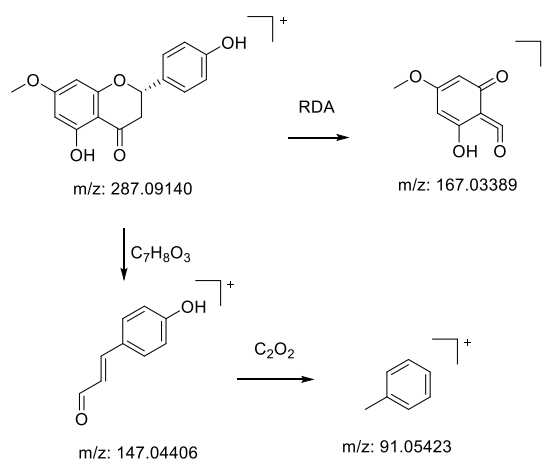
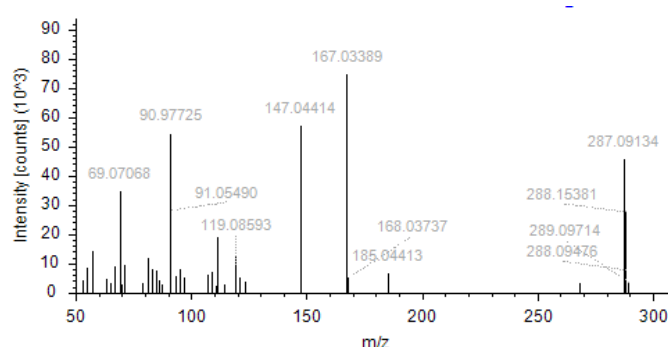


Compound NO.6, Its quasimolecular ion peak  $m/z$  285.04046 [M-H]<sup>-</sup> the chemical formula is  $C_{15}H_{10}O_6$ . The parent ion ( $m/z$  285.04046) first underwent RDA cleavage to form fragment ion  $m/z$  133.02834 and then lost hydrogen radical to form fragment ion  $m/z$  132.02000. Combined with literature and mass spectrometry library, the compound is presumed to be Luteolin.

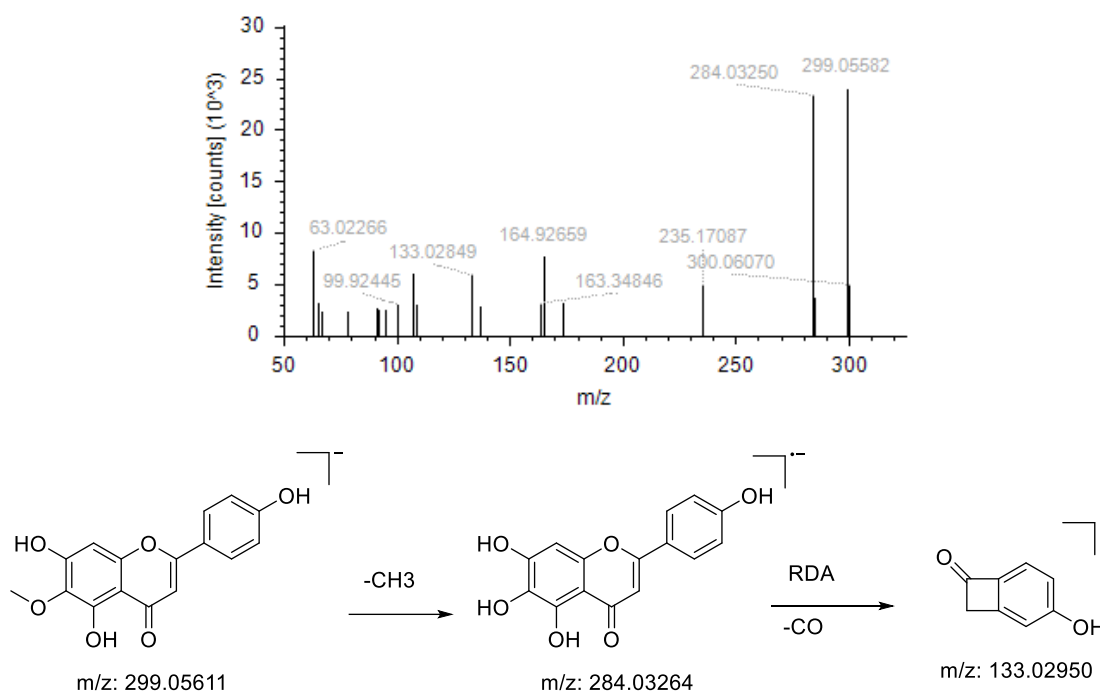




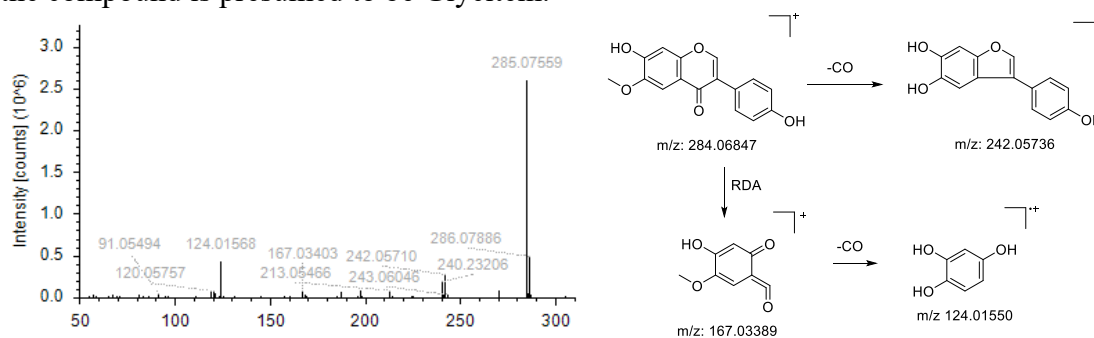
Compound NO.7, Its quasimolecular ion peak  $m/z 287.09140 [M+H]^+$  has the chemical formula  $C_{16}H_{14}O_5$ , and this parent ion ( $m/z 287.09140$ ) undergoes first a reverse cycloaddition reaction to produce the fragmentation ion  $m/z 147.04414$  fragmentation ion, and then a simple fracture to produce the fragmentation ion  $m/z 91.05490$ ; the parent ion ( $m/z 287.09140$ ) undergoes RDA cleavage to produce the fragment ion  $m/z 167.03389$  Combined with literature and mass spectrometry library, the compound is presumed to be Sakuranetin.



Compound NO.8, Its quasimolecular ion peak  $m/z 299.05611 [M-H]^-$  has the chemical formula  $C_{16}H_{12}O_6$ , and the parent ion ( $m/z 299.05611$ ) first loses methyl radicals to produce the fragment ion  $m/z 284.03250$  fragment ions, and then undergoes RDA cleavage and loses a molecule of CO to produce the fragment ion  $m/z 133.02849$ . Combined with literature and mass spectrometry library, the compound is presumed to be Hispidulin.



Compound NO.9, Its quasimolecular ion peak  $m/z 284.06847[M+H]^+$  has the chemical formula  $C_{16}H_{12}O_5$ , and this parent ion ( $m/z 284.06847$ ) first loses a molecule of CO to produce the fragment ion  $m/z 242.05710$  of the fragment ion; the parent ion ( $m/z 284.06847$ ) undergoes RDA cleavage to generate a fragment ion of fragment ion  $m/z 167.03403$ , which then loses CO and methyl radicals to generate a fragment ion of fragment ion  $m/z 124.01568$ . Combined with literature and mass spectrometry library, the compound is presumed to be Glycitein.



Compound NO.10, Its quasimolecular ion peak  $m/z 315.08631[M+H]^+$  has the chemical formula  $C_{17}H_{14}O_6$ , and this parent ion ( $m/z 315.08631$ ) first loses oxymethylene groups to produce the fragmentation ion  $m/z 300.06281$  fragmentation ions, then loses a molecule of CO to produce the fragmentation ion  $m/z 272.06754$ , and loses oxymethyl groups to produce the fragmentation ions  $m/z 257.04379$ ; This parent ion ( $m/z 300.06281$ ) undergoes RDA cleavage and dehydrates to produce the fragment ion  $m/z 167.03355$ ; The parent ion ( $m/z 300.06281$ ) demethoxylates and loses a molecule of CO to form the fragment ion  $m/z 243.06512$ . Combined with literature and mass spectrometry library, the compound is presumed to be Scrophulein.

