

Supplementary Materials

Study on the polar extracts of *Dendrobium nobile*, *D. officinale*, *D. loddigesii* and *Flickingeria fimbriata*: metabolite identification, content evaluation and bioactivity assay

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Figure Legends:

Figure S1. Structures of **1–8** and their target protons (a–g) for content determination

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Figure S3 ^{13}C NMR for flifimdioside A (**1**) from *F. fimbriata*

Figure S4 ^1H - ^1H COSY for flifimdioside A (**1**) from *F. fimbriata*

Figure S5 HSQC for flifimdioside A (**1**) from *F. fimbriata*

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Figure S11 ^1H NMR for anosmine (**4**) from *D. nobile*

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Figure S16 ^1H NMR for mixture of three fructose isomer (**7**) from *D. officinale*

Figure S17 ^{13}C NMR the mixture of three fructose isomer (**7**) from *D. officinale*

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Figure S19 ^1H NMR of polar-extract-f for content determination

Figure S20 ^1H NMR of polar-extract-n for content determination

Figure S21 ^1H NMR of polar-extract-o for content determination

Figure S22 ^{13}C NMR of polar-extract-o for content determination

Figure S23 ^1H NMR of polar-extract-l for content determination

Figure S24 ^1H NMR of salicylic acid for an external standard

All NMR data were recorded in CD_3OD .

Figure S25 The inhibitory activities of the polar extracts on α -glucosidase

Figure S26 The inhibitory activities of isolated metabolites on α -glucosidase

Table S1 The chemical shifts and splitting patterns of diagnostic signals of isolated metabolites

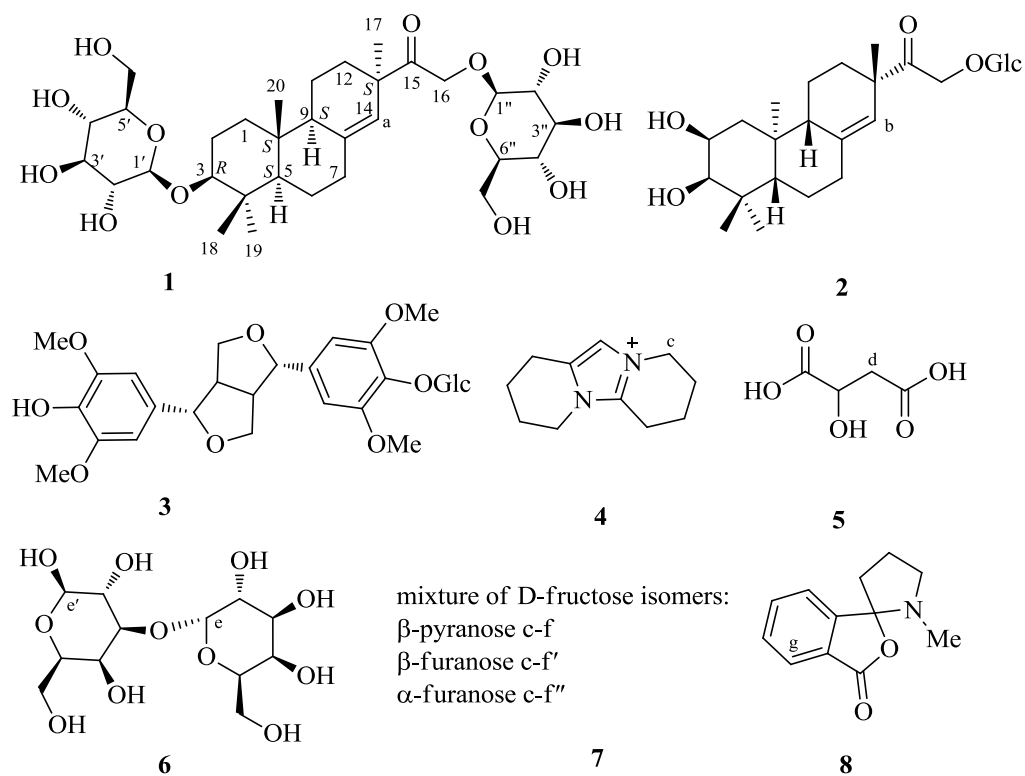


Figure S1. Structures of **1–8** and their target protons (a–g) for content determination.

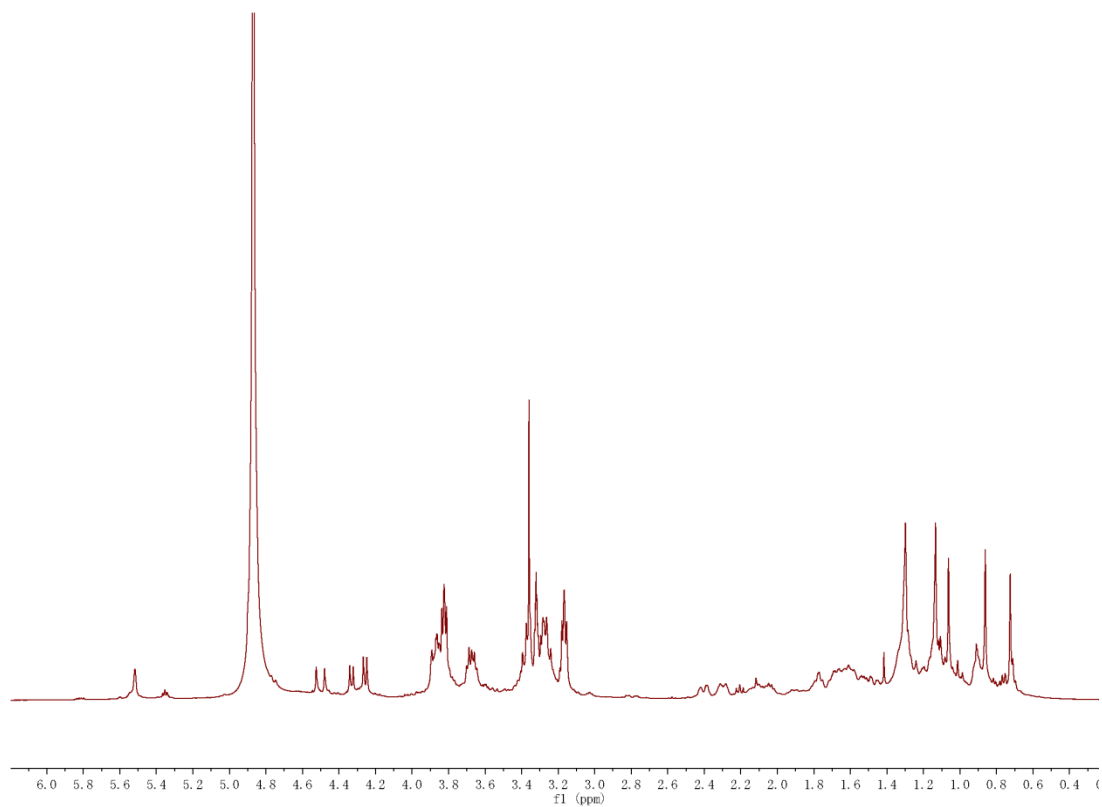


Figure S2 ^1H NMR for flifimdioside A (**1**) from *F. fimbriata*

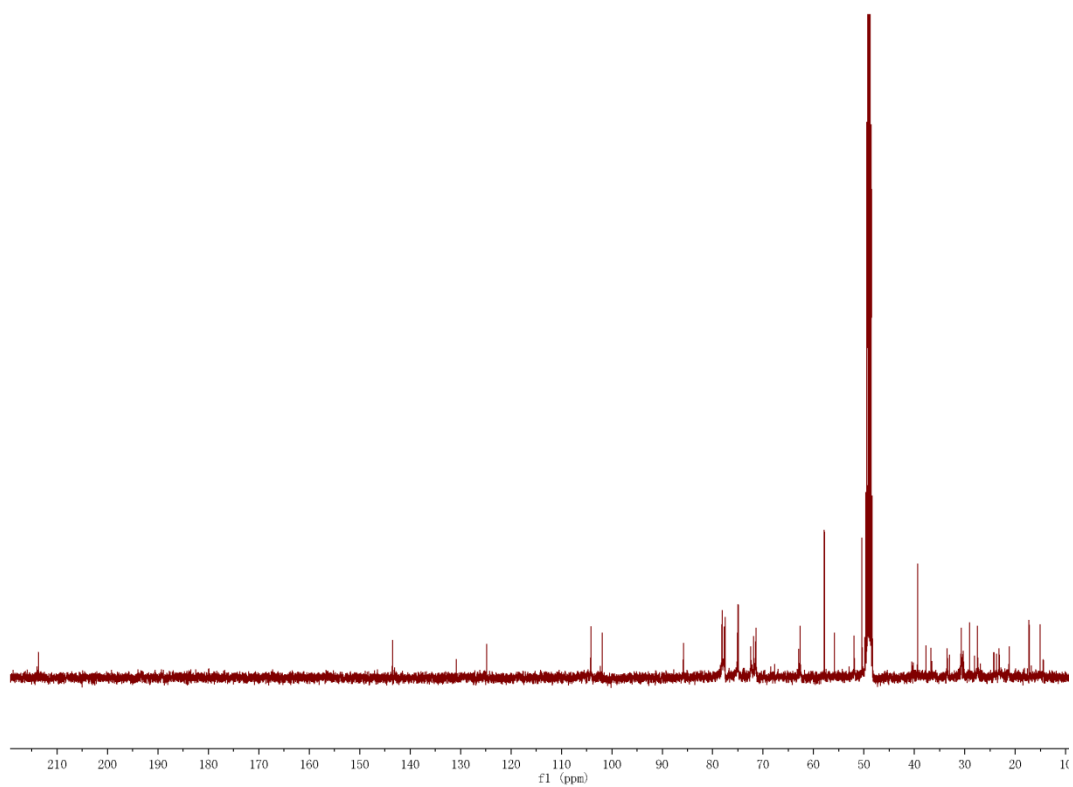


Figure S3 ^{13}C NMR for flifimdioside A (**1**) from *F. fimbriata*

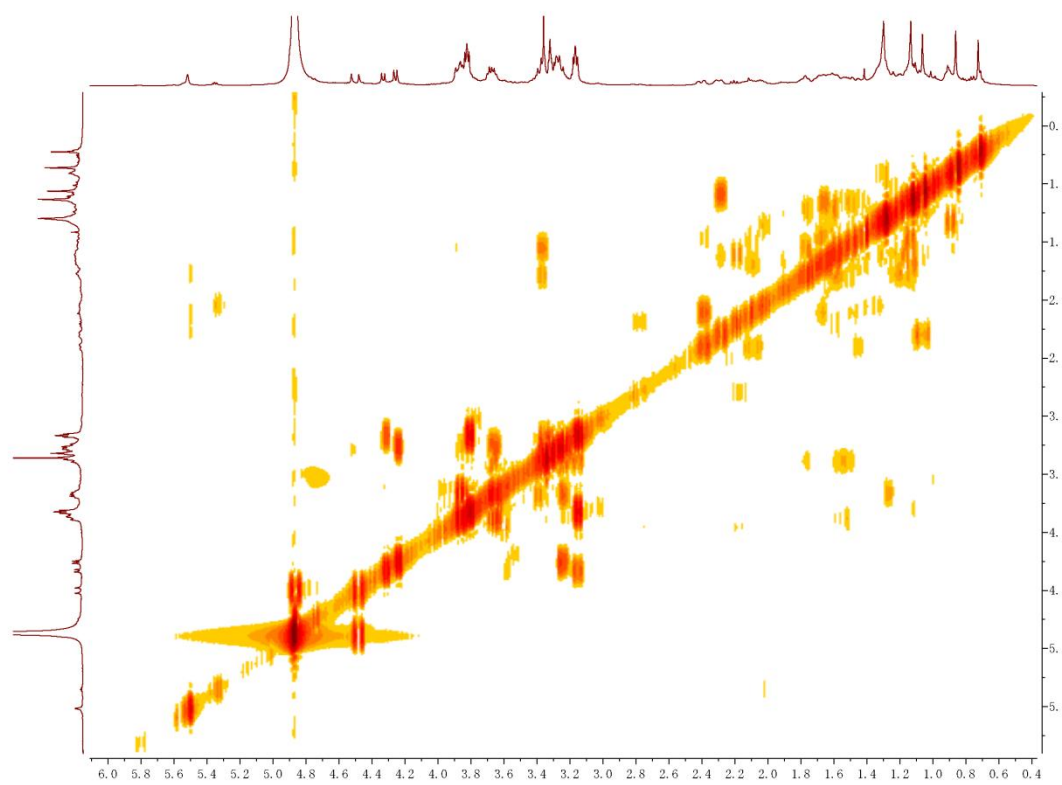


Figure S4 ^1H - ^1H COSY for flifimdioside A (**1**) from *F. fimbriata*

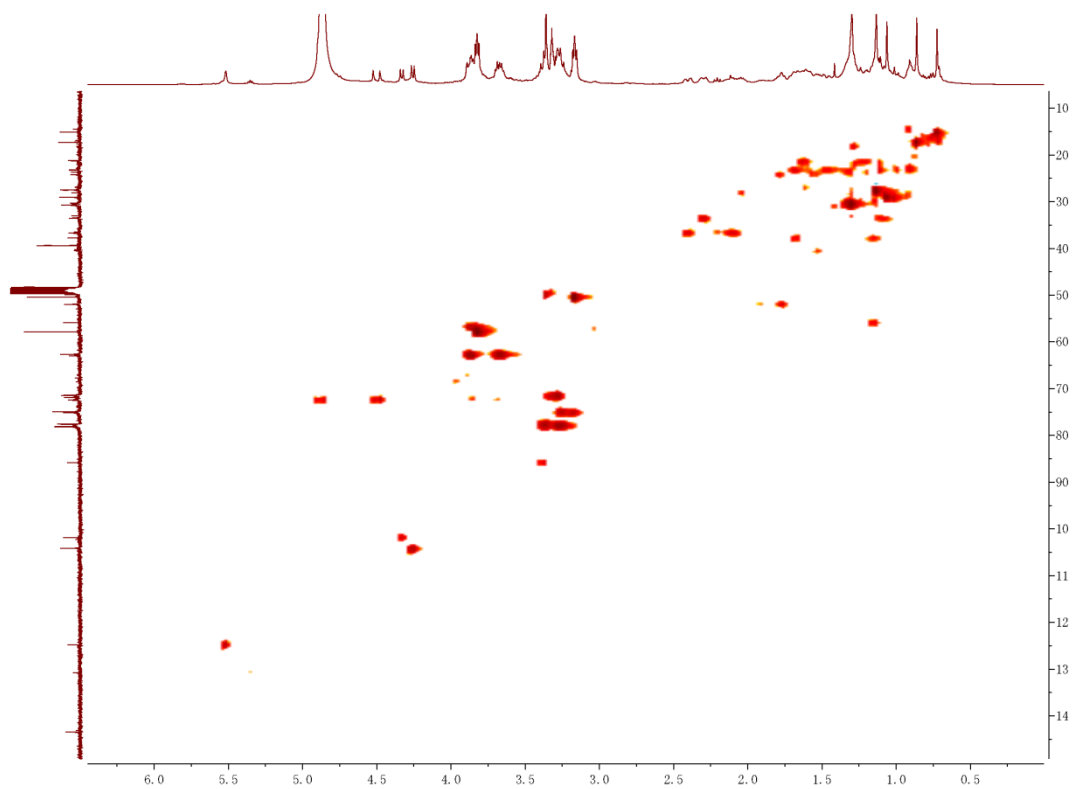


Figure S5 HSQC for flifimdioside A (**1**) from *F. fimbriata*

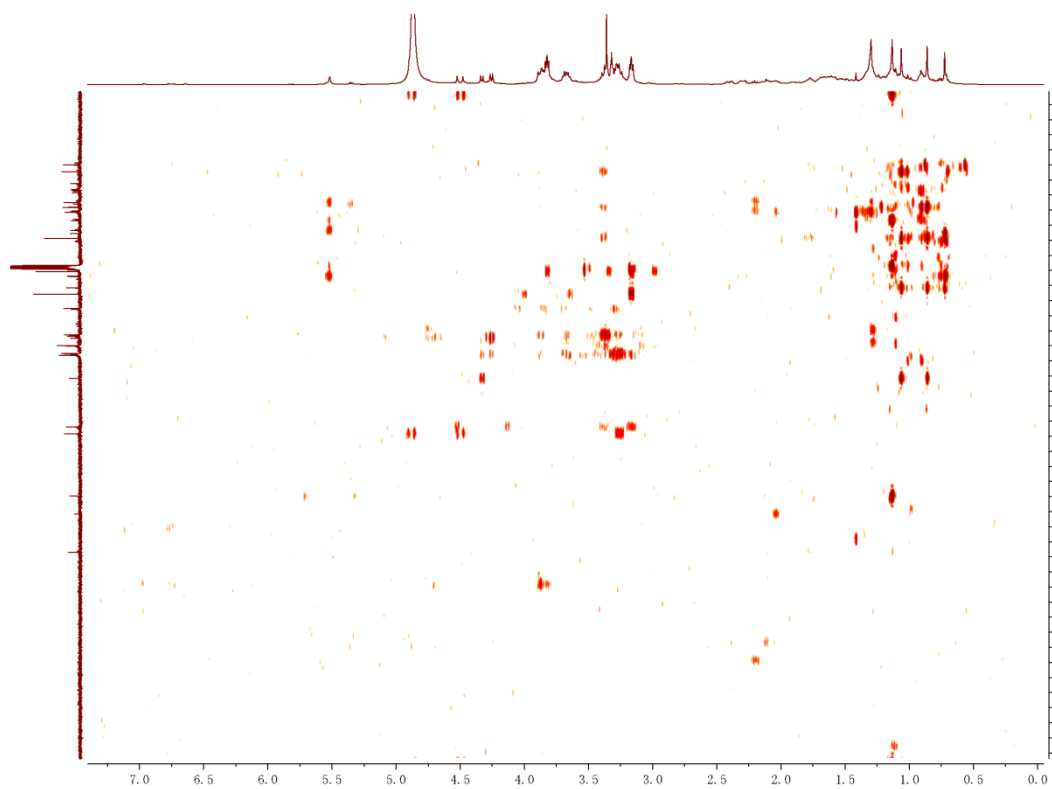
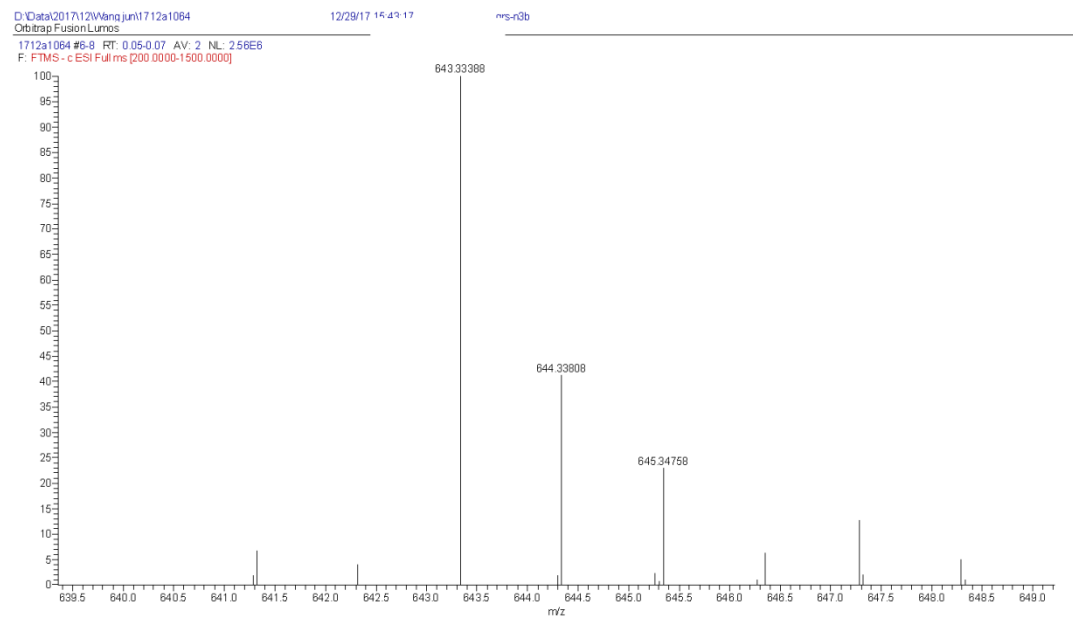


Figure S6 HMBC for flifimdioside A (**1**) from *F. fimbriata*



SPECTRUM - simulation :

| m/z | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|-----------|------------|-------------|------------|-------------|
| 643.33388 | 643.33351 | 0.57 | 7.5 | C32 H51 O13 |

Limits:

- 1) Charge: -1
- 2) Nitrogen-role: Do not use
- 3) Mass tolerance: 5 ppm
- 4) Element in use: ^{12}C (0~35), ^1H (0~60), ^{16}O (0~15)

Figure S7 HRMS spectrometry for flifimdioside A (**1**) from *F. fimbriata*

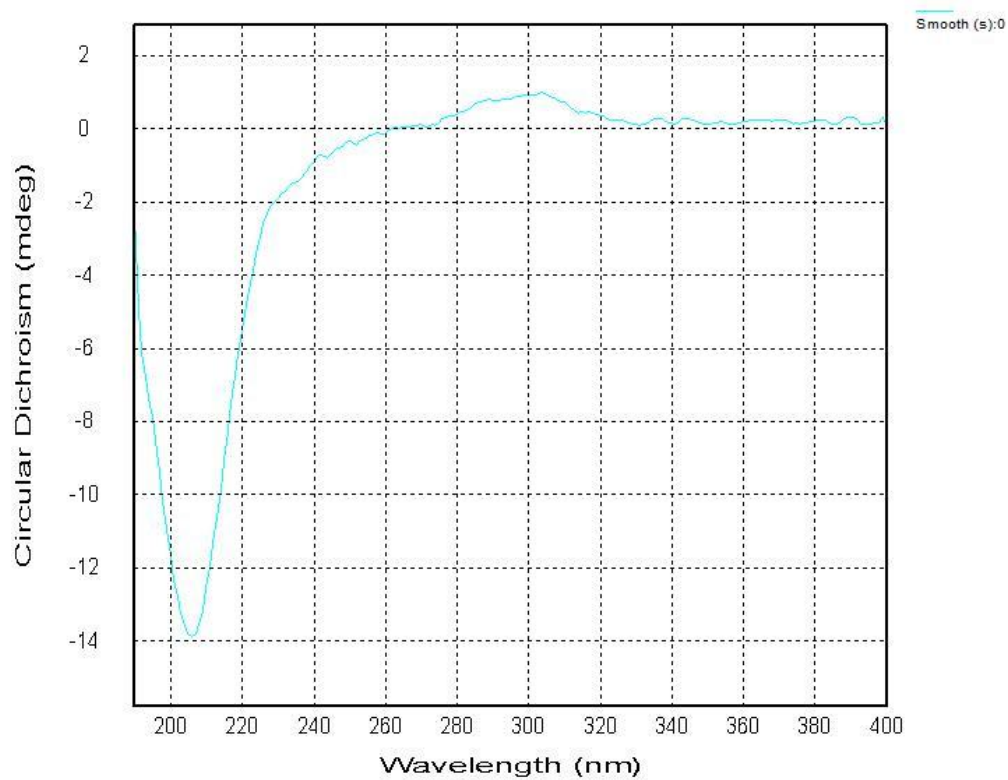


Figure S8 ECD spectra for flifimdioside A (**1**) from *F. fimbriata*

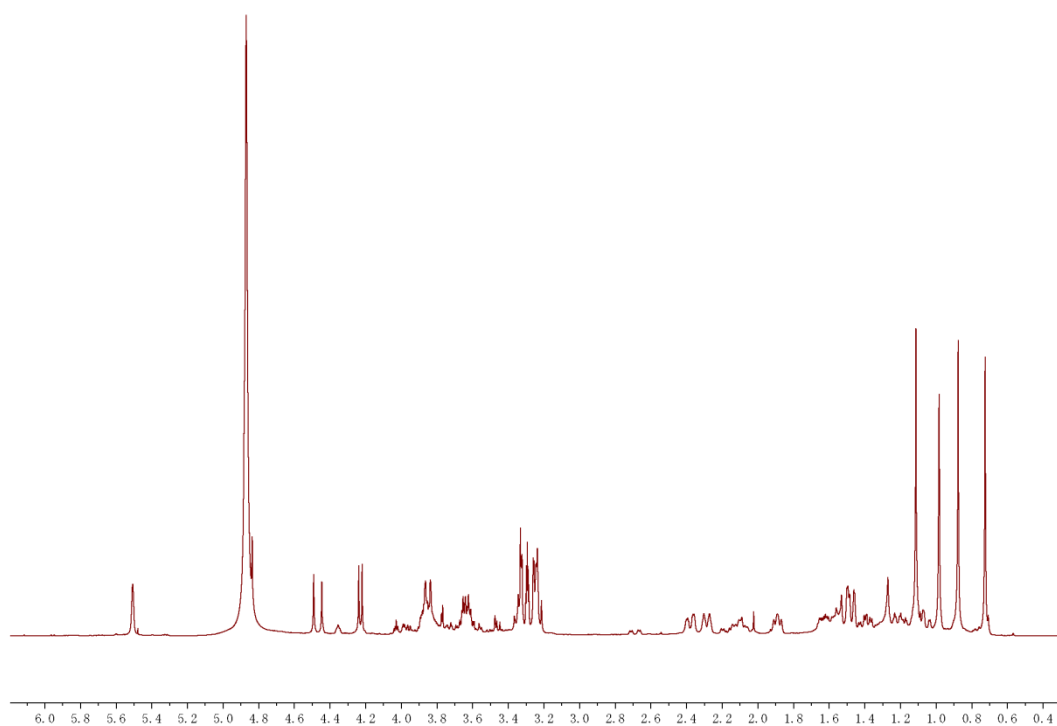


Figure S9 ^1H NMR for flickinflimoside B (**2**) from *F. fimbriata*

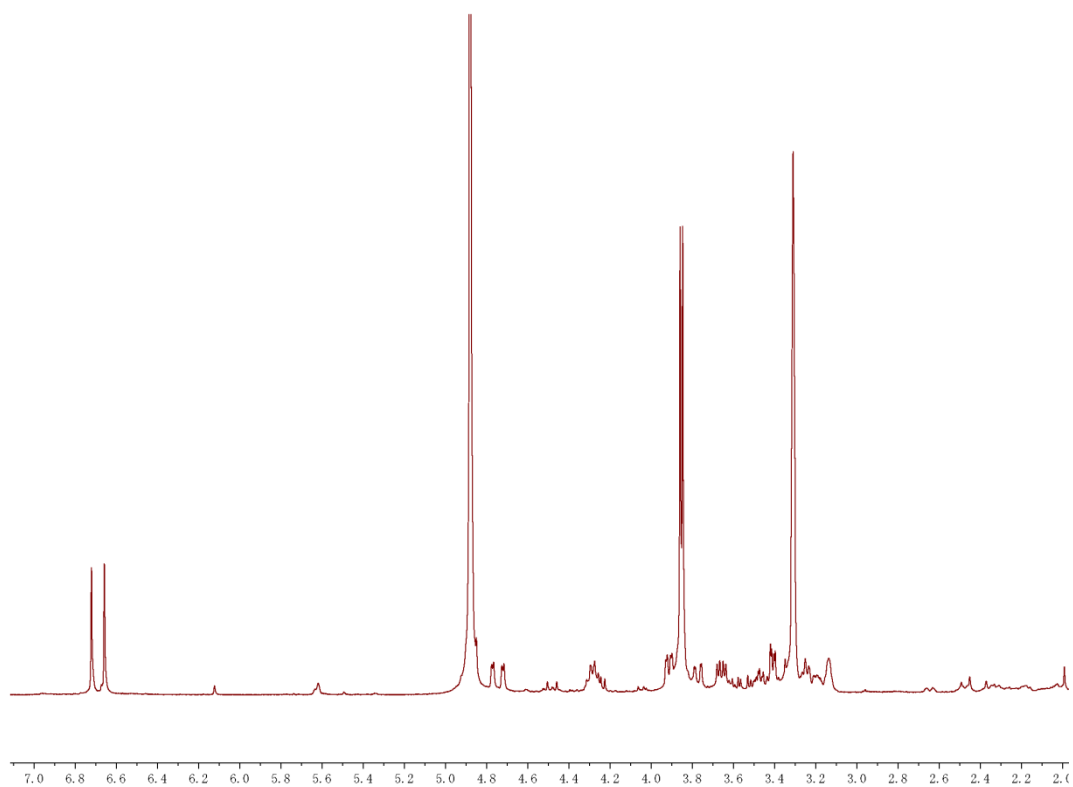


Figure S10 ^1H NMR for syringaresinol-4'-O-D-glucopyranoside (**3**) from *F. fimbriata*

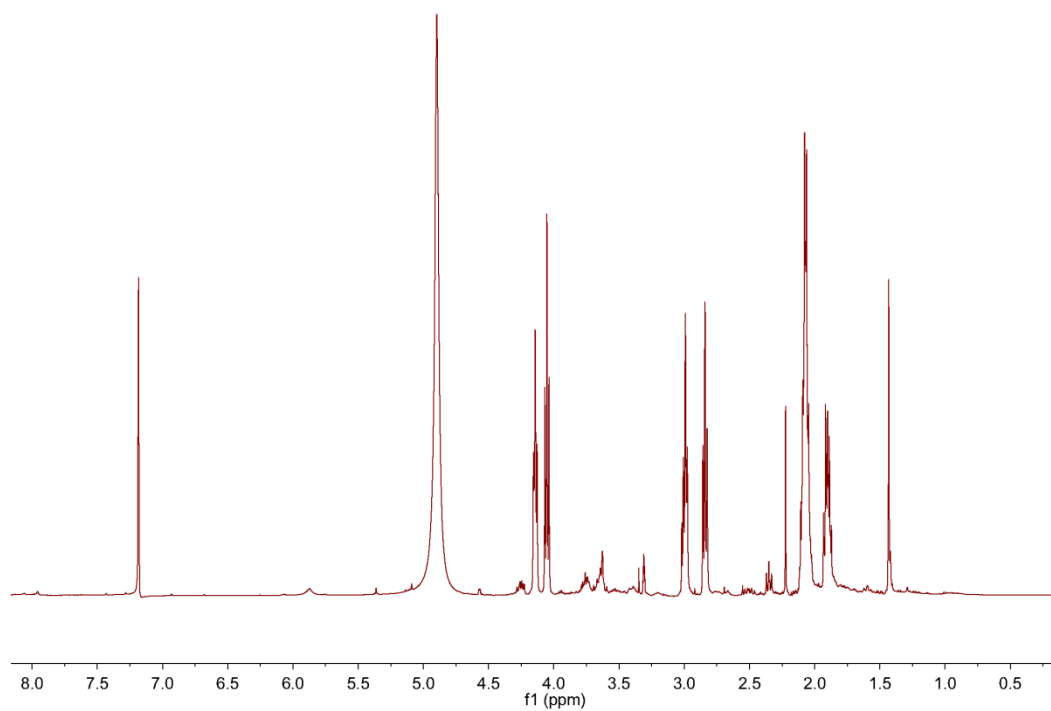


Figure S11 ^1H NMR for anosmine (**4**) from *D. nobile*

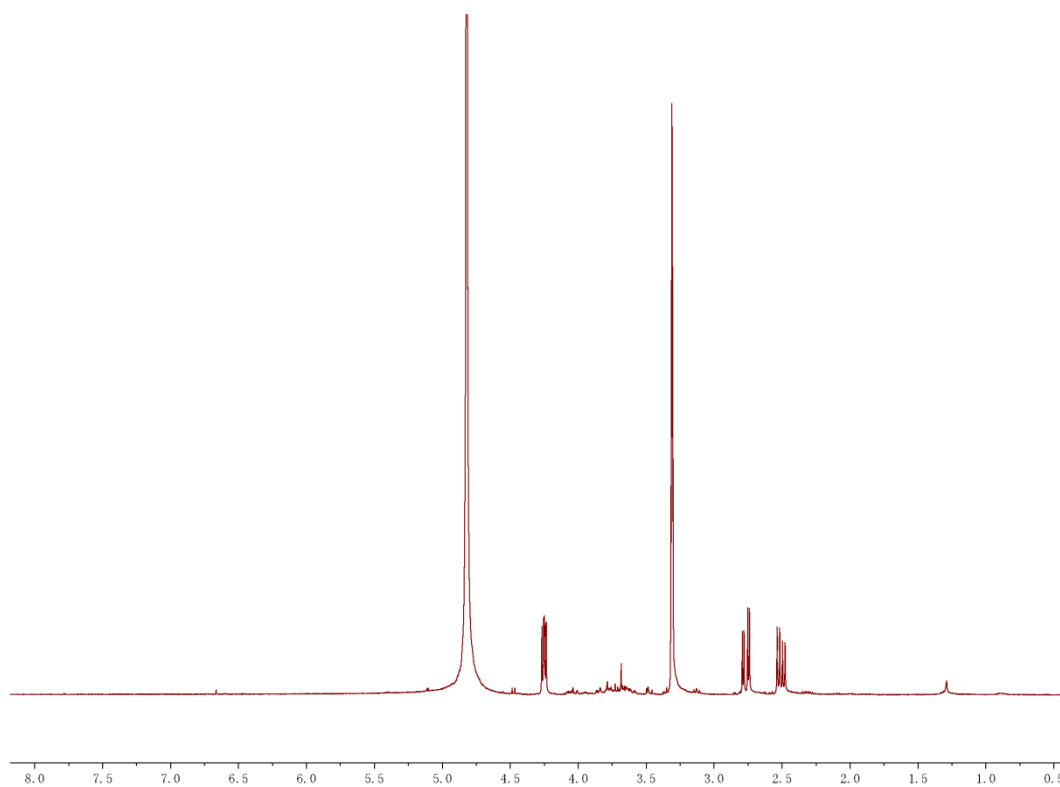


Figure S12 ^1H NMR for malic acid (5) from *D. officinale*

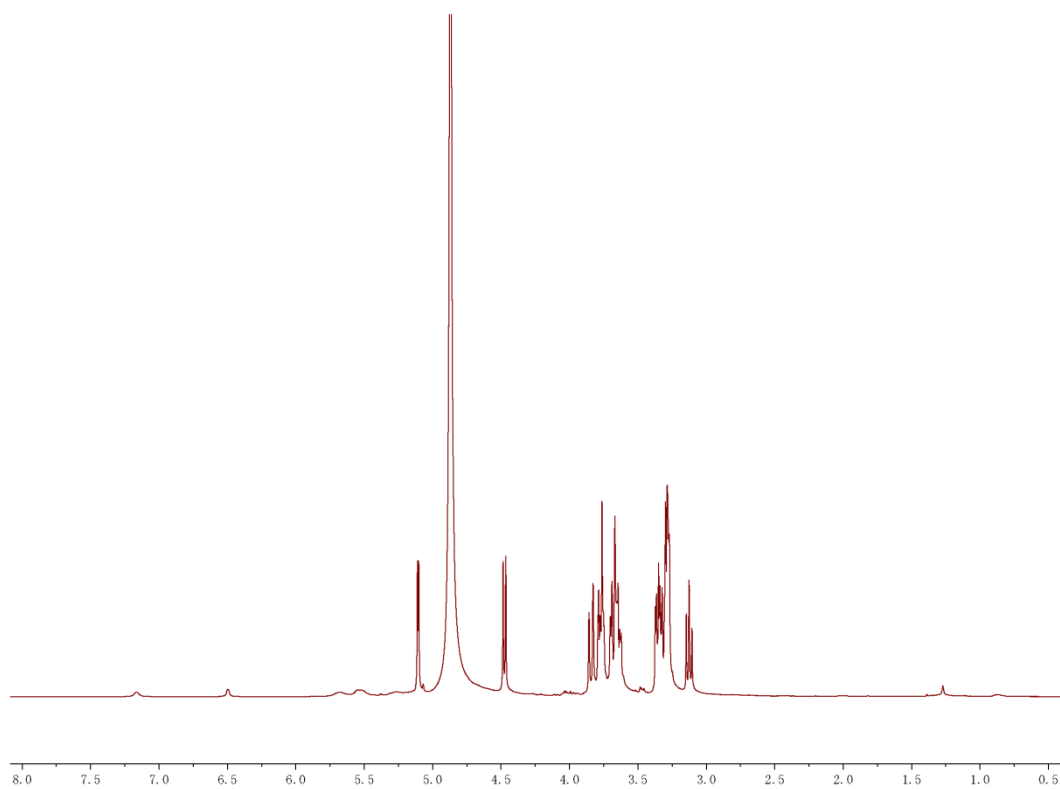


Figure S13 ^1H NMR for compound (6) from *D. officinale*

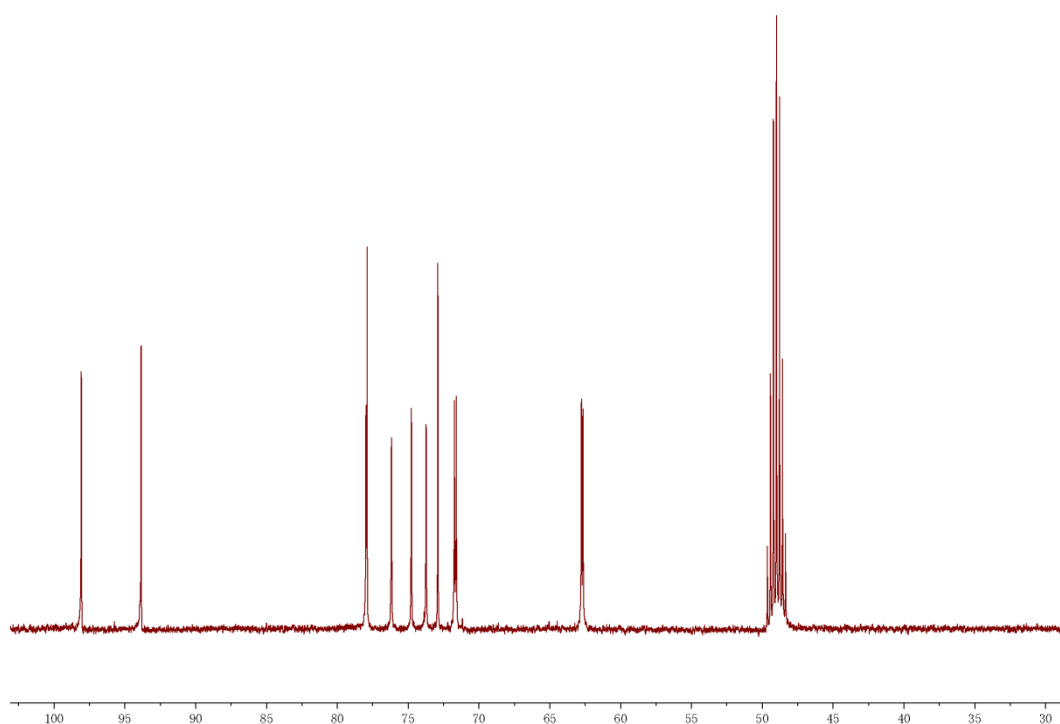


Figure S14 ^{13}C -NMR for compound (6) from *D. officinale*

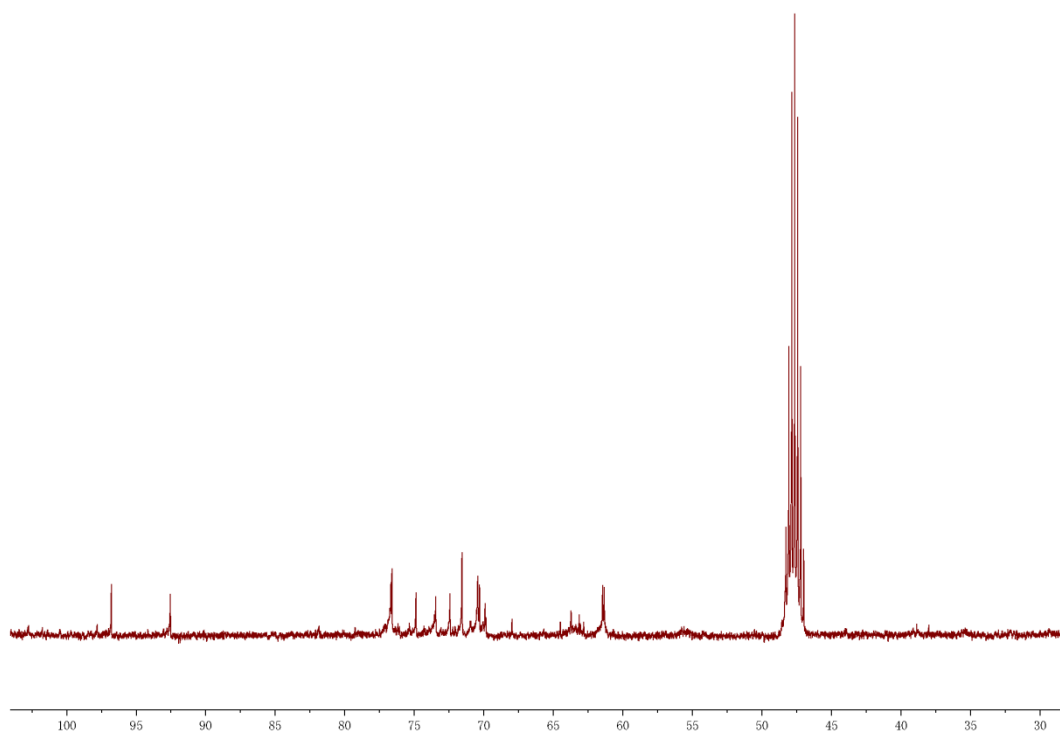


Figure S15 ^{13}C -NMR for compound (6) from *F. fimbriata*

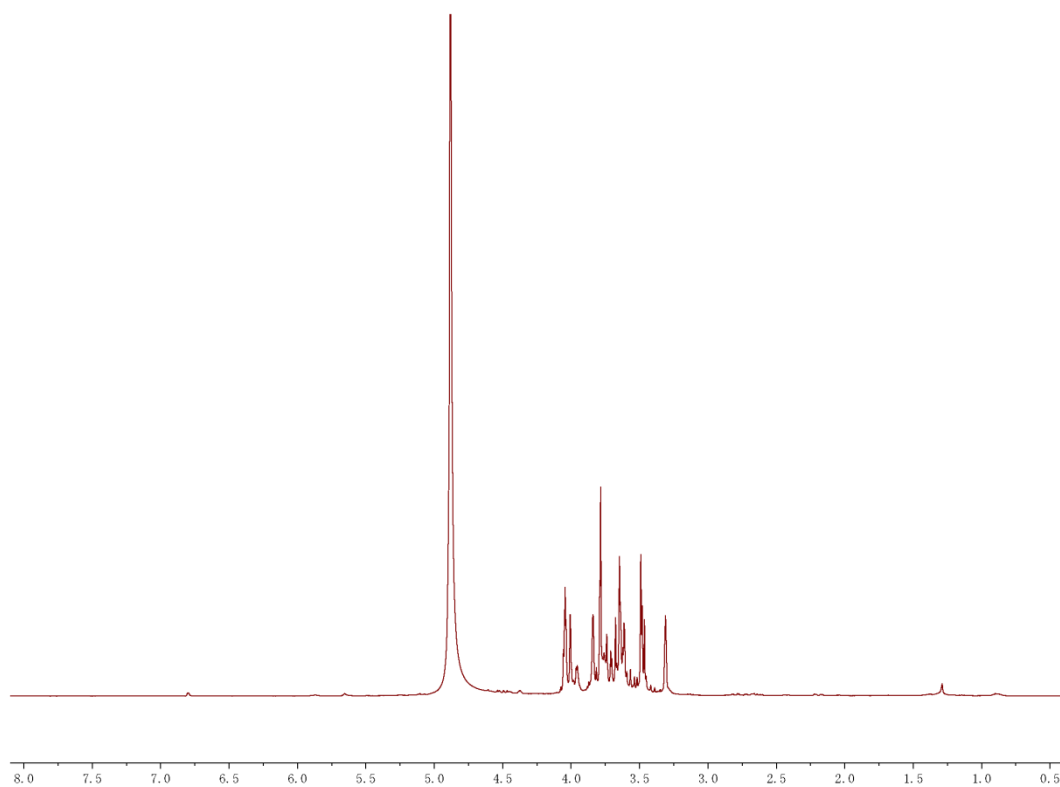


Figure S16 ^1H NMR for mixture of three fructose isomer (7) from *D. officinale*

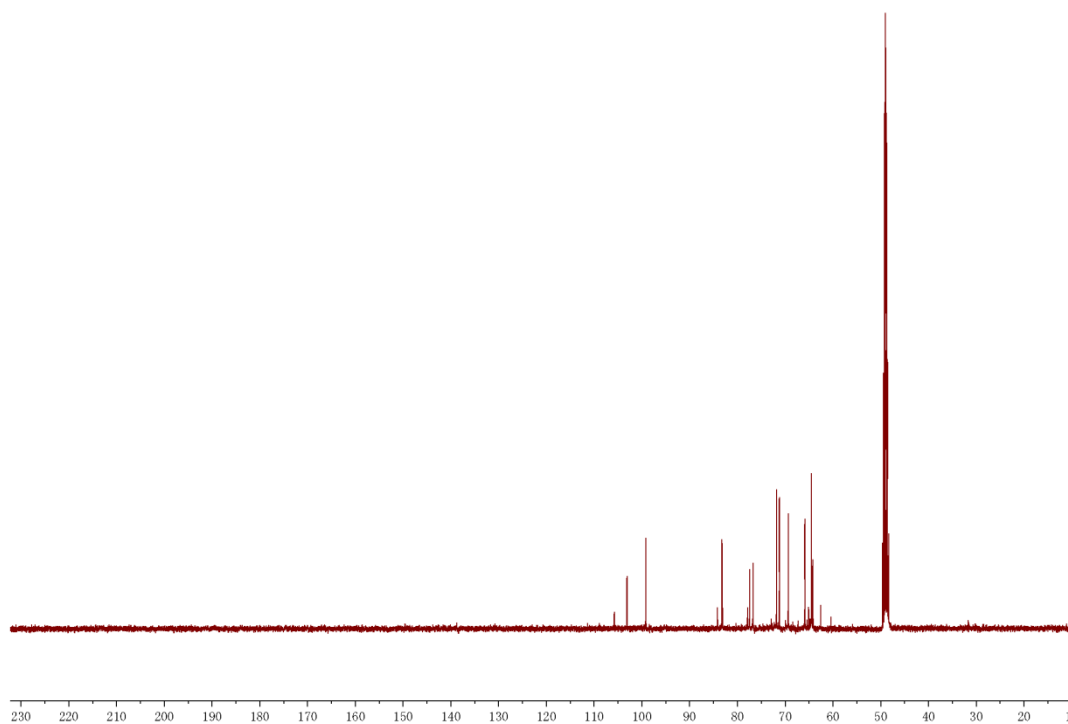


Figure S17 ^{13}C -NMR for mixture of three fructose isomer (7) from *D. officinale*

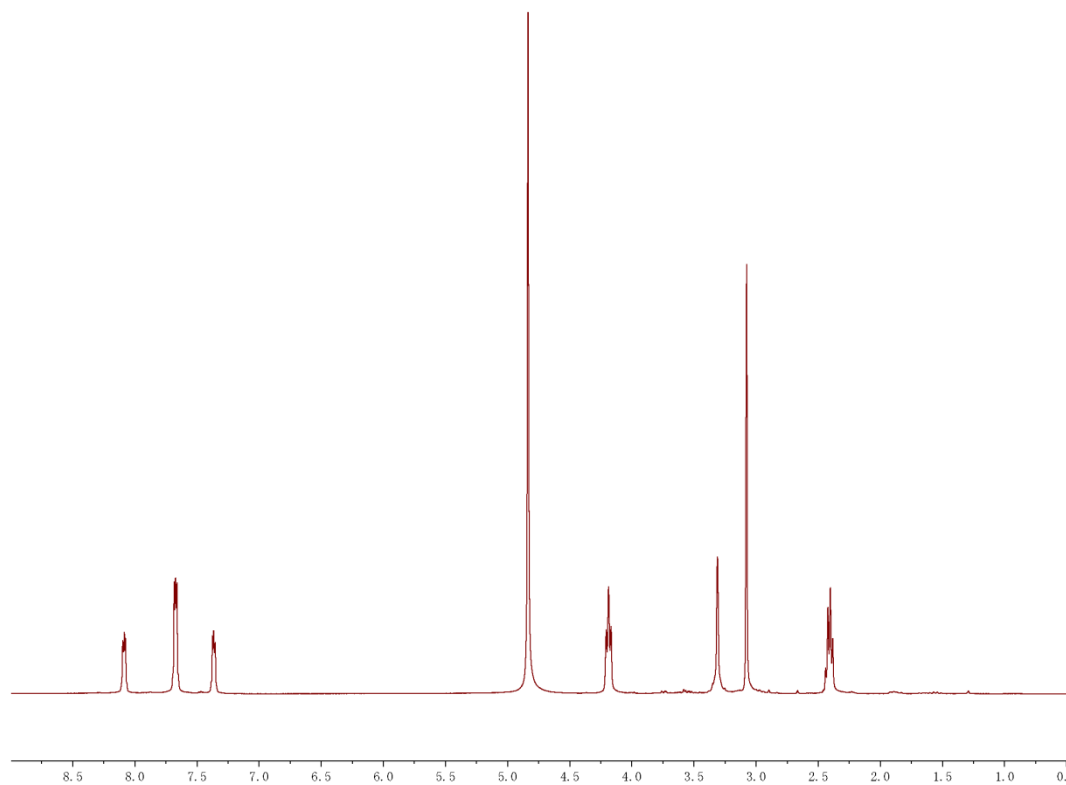


Figure S18 ^1H NMR for shihunine (8) from *D. loddigesii*

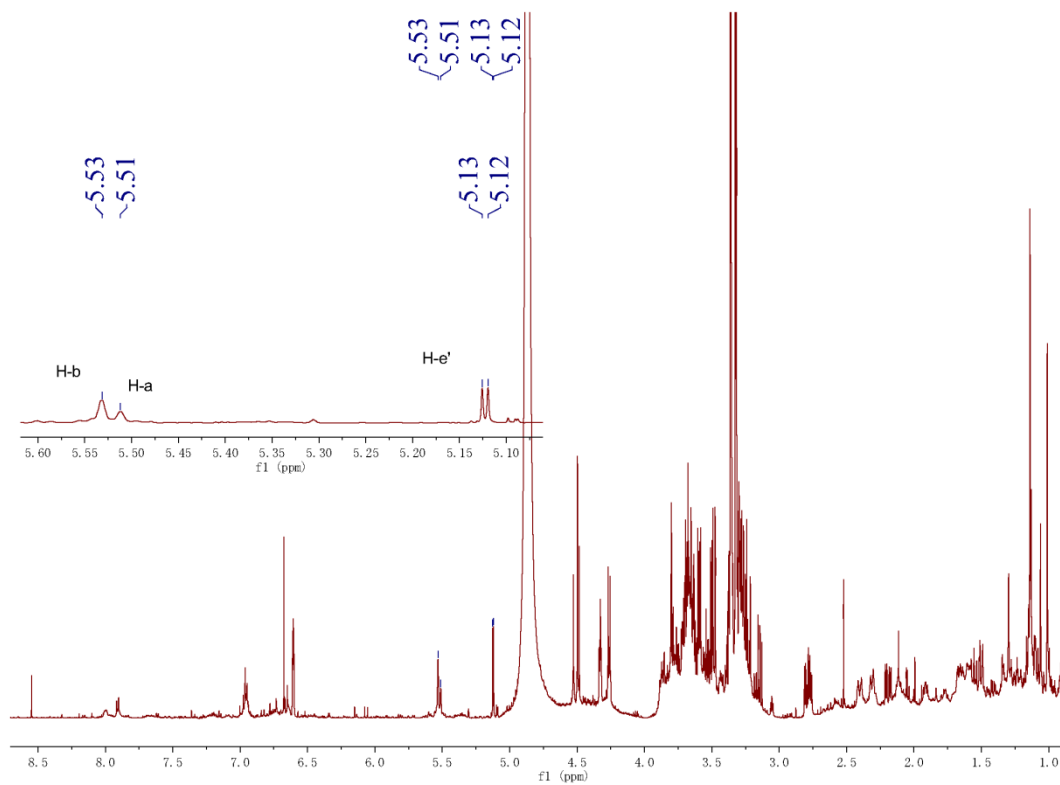


Figure S19 ^1H NMR of polar-extract-f for content determination

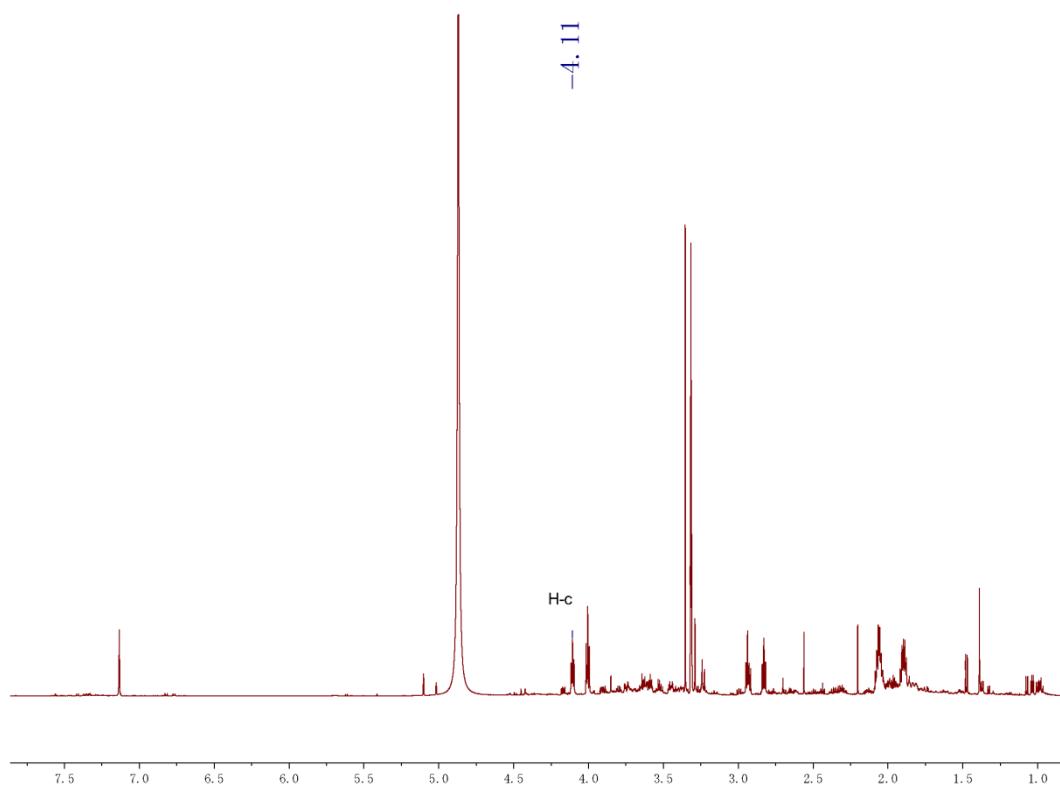


Figure S20 ^1H NMR of polar-extract-n for content determination

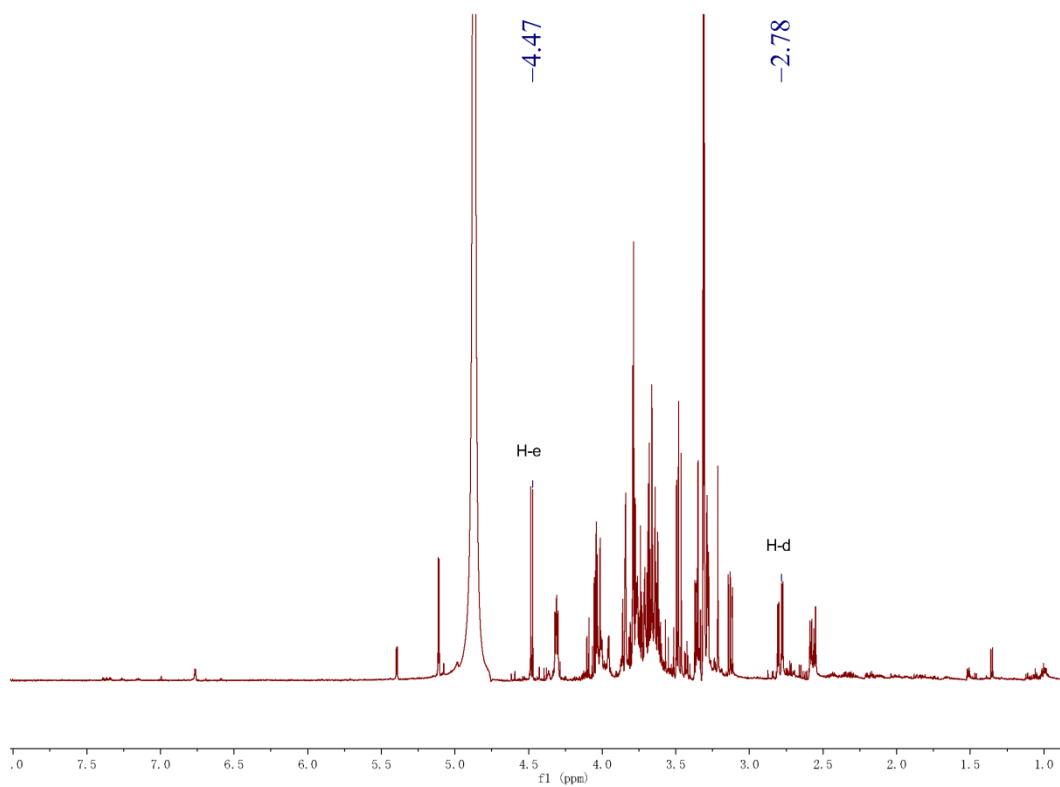


Figure S21 ^1H NMR of polar-extract-o for content determination

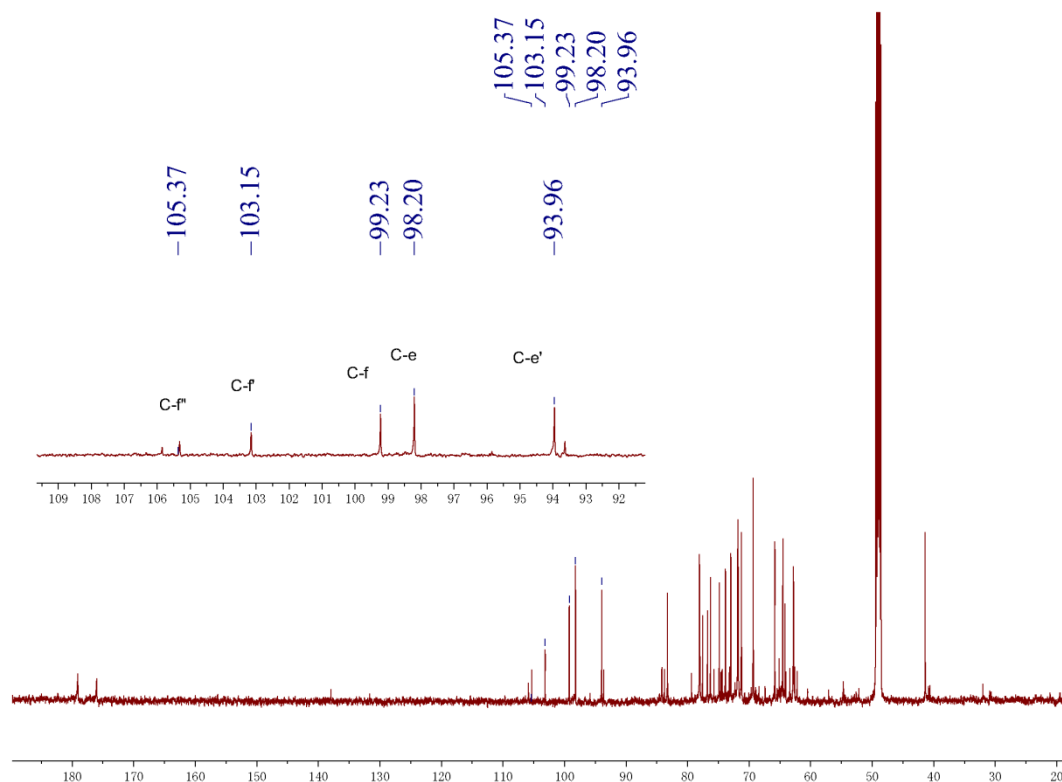


Figure S22 ^{13}C -NMR of polar-extract-o for content determination

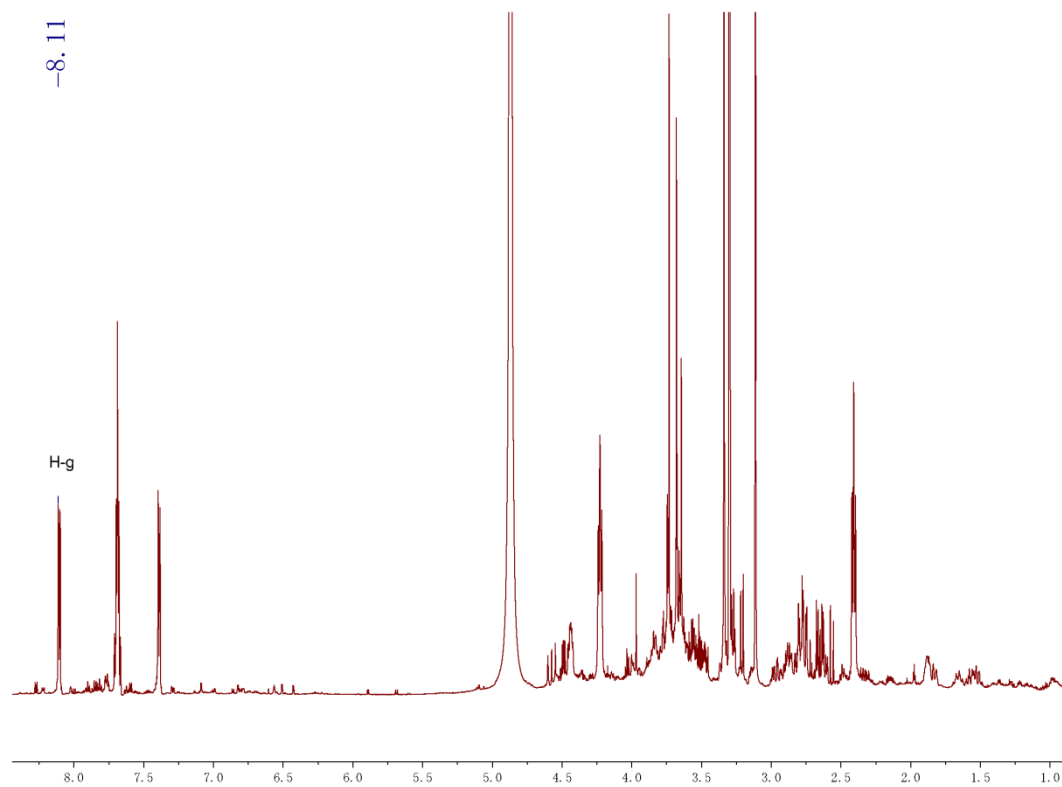


Figure S23 ^1H NMR of polar-extract-l for content determination

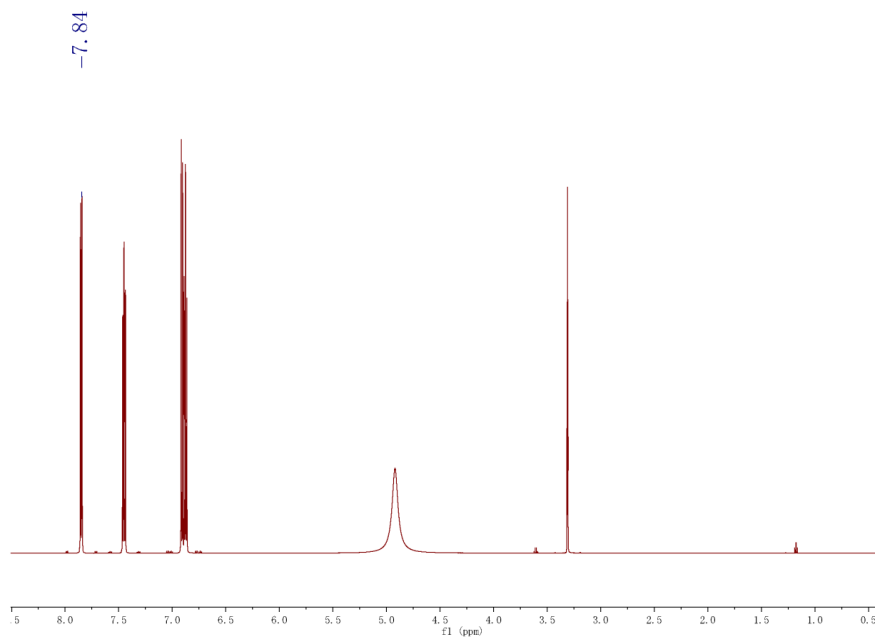


Figure S24 ^1H NMR of salicylic acid for an external standard

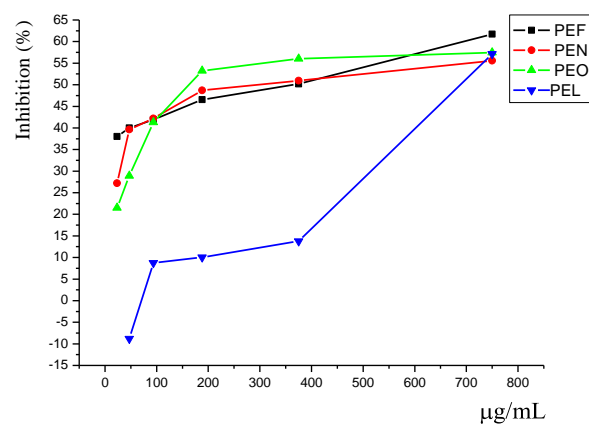


Figure S25 The inhibitory activities of the polar extracts on α -glucosidase

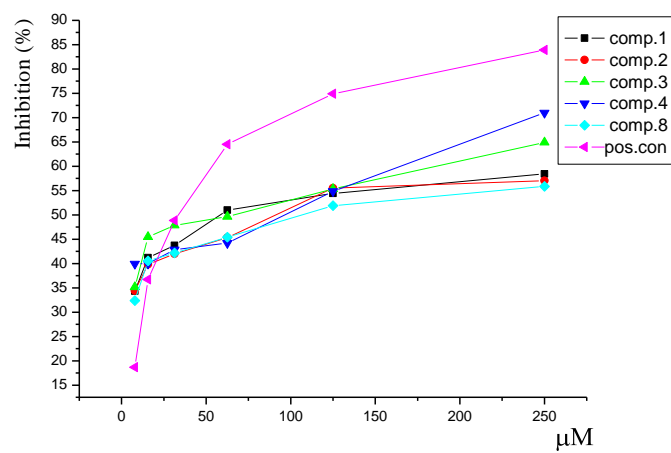


Figure S26 The inhibitory activities of isolated metabolites on α -glucosidase

Table S1.The chemical shifts and splitting patterns of diagnostic signals of isolated metabolites

| Plant | Compound | Diagnostic signals |
|----------------------|---|--|
| | | δ (ppm, J, Hz) |
| <i>F. fimbriata</i> | flifimdioside A (1) | 5.51 (s, 1H-a), 1.13 (s, 3H), 1.06 (s, 3H), 0.86 (s, 3H), 0.72 (s, 3H). |
| | flickinflimoside B (2) | 5.54 (s, 1H-b), 1.14 (s, 3H), 1.01 (s, 3H), 0.90 (s, 3H), 0.76 (s, 3H). |
| | syringaresinol-4'-O-D-glucopyranoside (3) | / |
| | 3-O- β -D-galactopyranosyl- β -D-galactopyranose (6) | 5.12 (d, 2.4, 1H-e'). |
| <i>D. nobile</i> | anosmine (4) | 7.14 (s, 1H), 4.11 (t, 3.6, 2H-c), 4.01 (t, 4.4, 2H), 2.94 (t, 4.4, 2H), 2.83 (t, 4.4, 2H), 2.07 (m 4H), 1.89 (m 4H) |
| <i>D. officinale</i> | malic acid (5) | 4.31 (m 1H), 2.78 (dd, 10.8, 3.6, 2H-d), 2.57 (dd, 10.8, 4.8) |
| | 3-O- β -D-galactopyranosyl- β -D-galactopyranose (6) | 5.11 (d, 2.4, 1H-e'), 4.48 (d, 5.2, 1H-e) |
| | β -pyranose (7) | C-f/99.2 (s) |
| | β -furanose (7) | C-f'/103.1 (s) |
| | α -furanose (7) | C-f''/105.3 (s) |
| <i>D. loddigesii</i> | shihunine (8) | 8.11 (dd, 4.4, 1.2, 1H-g/), 7.69 (m, 2H), 7.39 (dd, 4.4, 1.2, 1H), 4.23 (t, 5.2, 2H), 2.41 (dd, 5.2, 2H) |