

Supplementary Information

Chemical constituents from *Coleus strobilifer* and their xanthine oxidase inhibitory activity

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Coleus strobilifer, the dried rhizome and root of *Coleus strobilifer* (Roxb.) A. J. Paton, is widely used for dampness-detoxification and detumescence in Chinese folklore. This study marks the first comprehensive investigation into the chemical composition of the whole herb of *C. strobilifer*, leading to the isolation and identification of two new abietane diterpenes, 10*R*-carnosuain (**1**) and 10*R*-coleon U-3-one (**2**), along with 34 known compounds (**3-36**). Their structures were unambiguously elucidated by analyses of NMR, HRESIMS, UV, IR and single-crystal X-ray diffraction data, and comparison with literature. All the isolated compounds were screened for their xanthine oxidase (XO) inhibitory activity. Among them, apigenin (**8**), luteolin (**9**) and esculetin (**29**) showed moderate XO inhibitory activity with IC₅₀ values of 0.034 ± 0.004 , 0.067 ± 0.005 and 0.284 ± 0.01 mM, respectively.

Keywords: *Coleus strobilifer*; abietane diterpenes; xanthine oxidaseinhibitory activity

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Isolation of all compounds

The EtOH extracts (1974.9 g) of *Coleus strobilifer* were separated by silica gel column chromatography and eluted successively with CH₂Cl₂-MeOH (100:0-5:1) to give Fr-A- Fr-E according to TLC analysis. Fr-A (80.2 g) was separated by repeated silica gel CC and eluted successively with PE-EtOAc (1:0-0:1) to obtain Fr-A1- Fr-A3. Fr-A1 (12.6 g) was separated by repeated silica gel CC and eluted successively with PE- CH₂Cl₂ (1:0-0:1) to obtain Fr-A1a- Fr-A1c; Fr-A1a (2.1 g) was purified by Sephadex LH-20 (MeOH: CH₂Cl₂, 1:1) and was then purified by preparative TLC (PTLC) to obtain compound **26** (11 mg) and **27** (7 mg); Fr-A1b (1.7 g) was purified by Sephadex LH-20 (MeOH: CH₂Cl₂, 1:1) and was then purified by re-crystallization to obtain compound **28** (11 mg) and **35** (23 mg); Fr-A1c (2.8 g) was purified by Sephadex LH-20 (MeOH: CH₂Cl₂, 1:1) to obtain compound **33** (17 mg). Fr-A2 (16.7 g) was separated by repeated silica gel CC and eluted successively with PE- EtOAc (100:0-10:1) to afford Fr-A2a- Fr-A2c, and was then by Sephadex LH-20 (MeOH: CH₂Cl₂, 1:1) and recrystallization to obtain compounds **6** (283 mg), **18** (31 mg), **19** (26 mg), **20** (32 mg) and **21** (21 mg), respectively. Fr-A3 (15.3 g) was separated by repeated silica gel CC and eluted successively with PE- EtOAc (1:0-5:1) to afford Fr-A3a- Fr-A3d; Fr-A3a (4.5 g) was purified by Sephadex LH-20 (MeOH: CH₂Cl₂,

1:1) and recrystallization to obtain compound **4** (2.2 g); Fr-A3b (1.8 g) was purified by semi-preparative HPLC (30% ACN-70% H₂O) to give compound **2** (28 mg); Fr-A3c (3.1 g) was purified by semi-preparative HPLC (77% ACN-23% H₂O) to give compound **3** (230 mg); Fr-A3d (0.9 g) was purified by LH-20 (MeOH: CH₂Cl₂, 1:1) to give compound **7** (3 mg). Fr-B (19 g) was purified by ODS CC (MeOH: H₂O, 30%-90%) to afford compounds **16** (45 mg), **22** (7 mg), **23** (28 mg) and **27** (29 mg). Fr-C (12 g) was separated by repeated silica gel CC and eluted successively with CH₂Cl₂-MeOH (80:0-10:1, in 0.1% HCOOH) to obtain Fr-C1- Fr-C3; Fr-C1 (1.9 g) was purified by ODS CC (MeOH: H₂O, 50%- 30%, in 0.1% HCOOH) to afford compounds **23** (28 mg) and **24** (37 mg); Fr-C2 (1.8 g) was purified by LH-20 (MeOH: CH₂Cl₂, 1:1) to give compound **29** (17 mg). Fr-D (10 g) was separated by ODS CC (MeOH: H₂O, 30%- 90%) and was then purified by LH-20 (MeOH) to obtain compounds **9** (37 mg), **10** (24 mg), **15** (17 mg), and **34** (25 mg). Fr-E (75 g) was separated by repeated silica gel CC and eluted successively with CH₂Cl₂-MeOH (50:0-5:1) to obtain Fr-E1- Fr-E3; Fr-E1 (3.5 g) was purified by recrystallization to obtain compound **1** (450 mg), and was then purified by PTLC to obtain compound **5** (48 mg). Fr-E2 (5.3 g) was separated by ODS CC (MeOH: H₂O, 30%- 90%) to produce Fr-E2a- Fr-E2d; Fr-E2a (2.1 g) purified by LH-20 (MeOH) to obtain compounds **8** (47 mg) and **32** (18 mg); Fr-E2b (0.9 g) was purified by LH-20 (MeOH) to obtain compounds **11** (18 mg) and **12** (35 mg); Fr-E2c (1.1 g) was purified by ODS CC (MeOH: H₂O, 50%- 80%) to obtain compounds **31** (47 mg) and **36** (6 mg); Fr-E3

(4.7 g) was separated by LH-20 (MeOH) to produce Fr-E3a and Fr-E3b; Fr-E3a (1.8 g) was purified by ODS CC (MeOH: H₂O, 30%- 70%) to obtain compounds **13** (28 mg) and **14** (39 mg); Fr-E3b (1.1 g) was purified by repeated silica gel CC and eluted successively with CH₂Cl₂-MeOH (30:1) to obtain compound **30** (18 mg).

Xanthine oxidase inhibition assay

The reaction mixture included 50 µL of the sample and 50 µL of 0.02 U/mL, XO solution that was properly shaken for 30 s and incubated at 37 °C for 5 min. Then, 150 µL of 0.48 mM xanthine solution was added, and again, the mixture was carefully shaken for 30 s and incubated at 37 °C for 30 min. Finally, the absorbance at 290 nm was measured, and the inhibitory activity was calculated using the following equation:

$$\text{Inhibition percentage (\%)} = [1 - (A_1 - A_2) / (A_3 - A_4)] \times 100$$

where A₁ is the absorbance of the production with the sample and XOD, A₂ is the absorbance of the production with the sample, A₃ is the absorbance of the production with the buffer solution and XOD, and A₄ is the absorbance of the production with the buffer solution. Each experiment was repeated three times. Allopurinol was used as a positive control. The extent of inhibition and IC₅₀ values were calculated by GraphPad Prism 6.0 software.

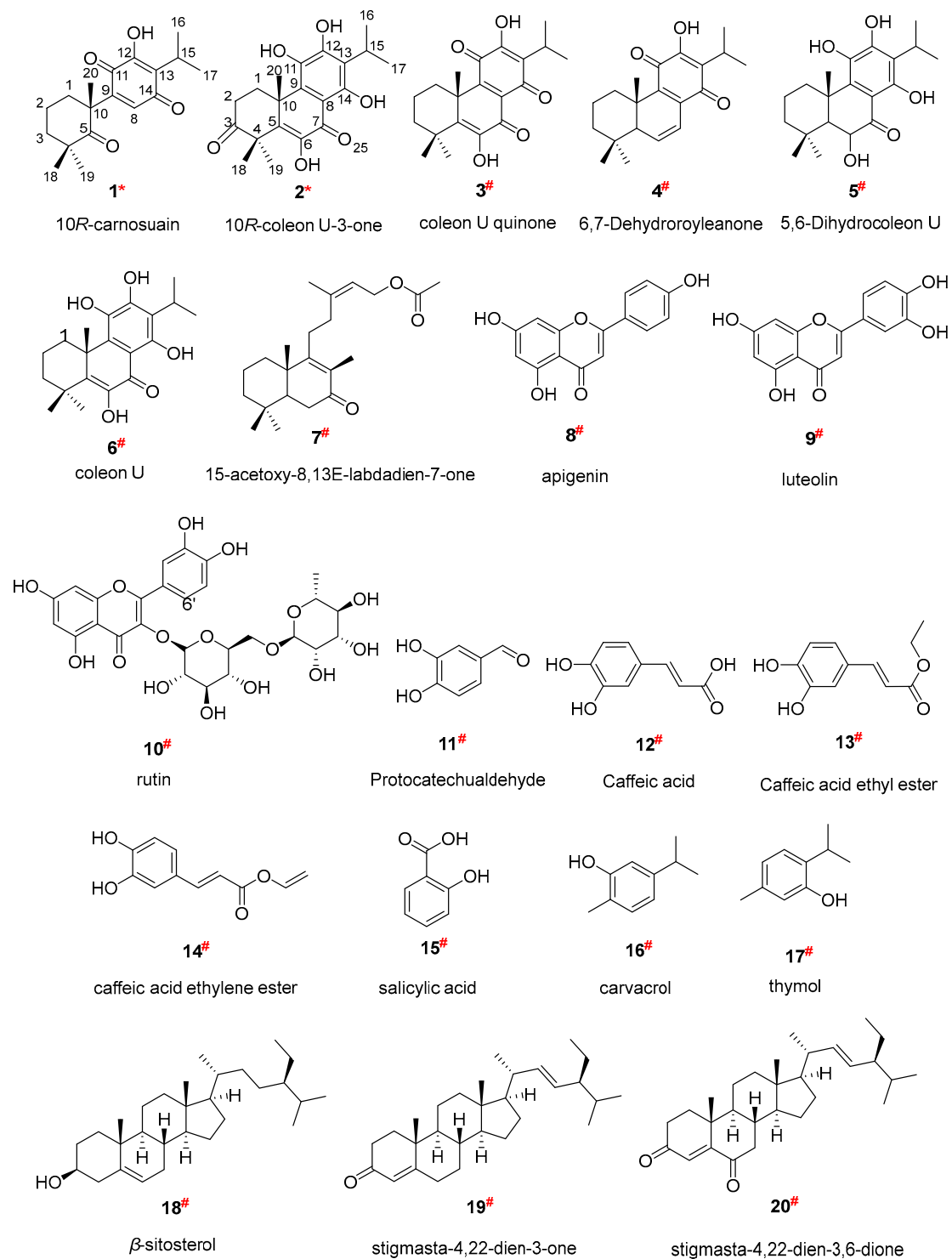


Figure S1 Chemical structures of compounds **1-20**.

* New compounds were isolated from *Coleus strobilifer*. # Compounds have not been reported in *Coleus strobilifer*.

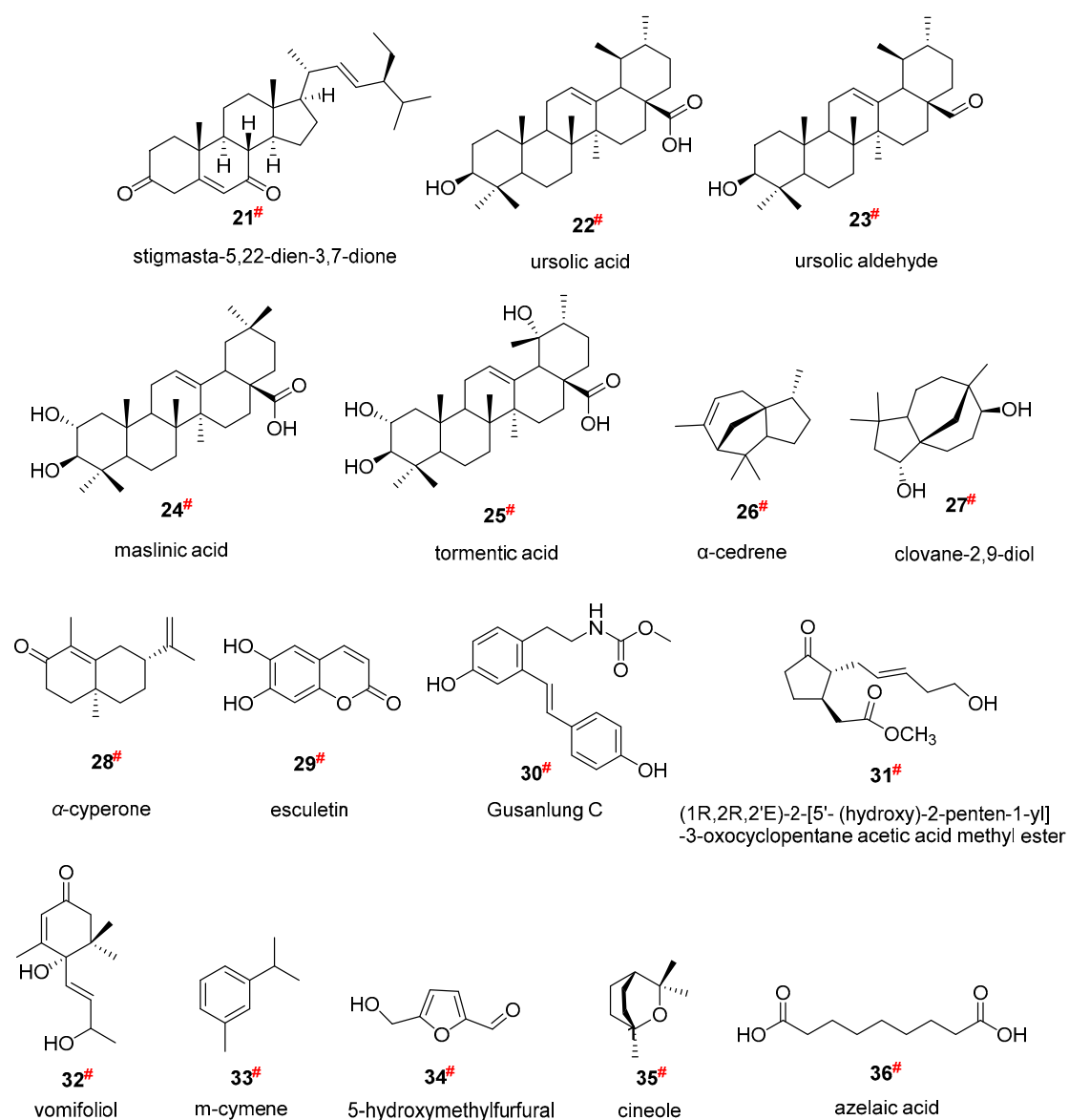


Figure S2 Chemical structures of compounds **21-36**.

[#] Compounds have not been reported in *Coleus strobilifer*.

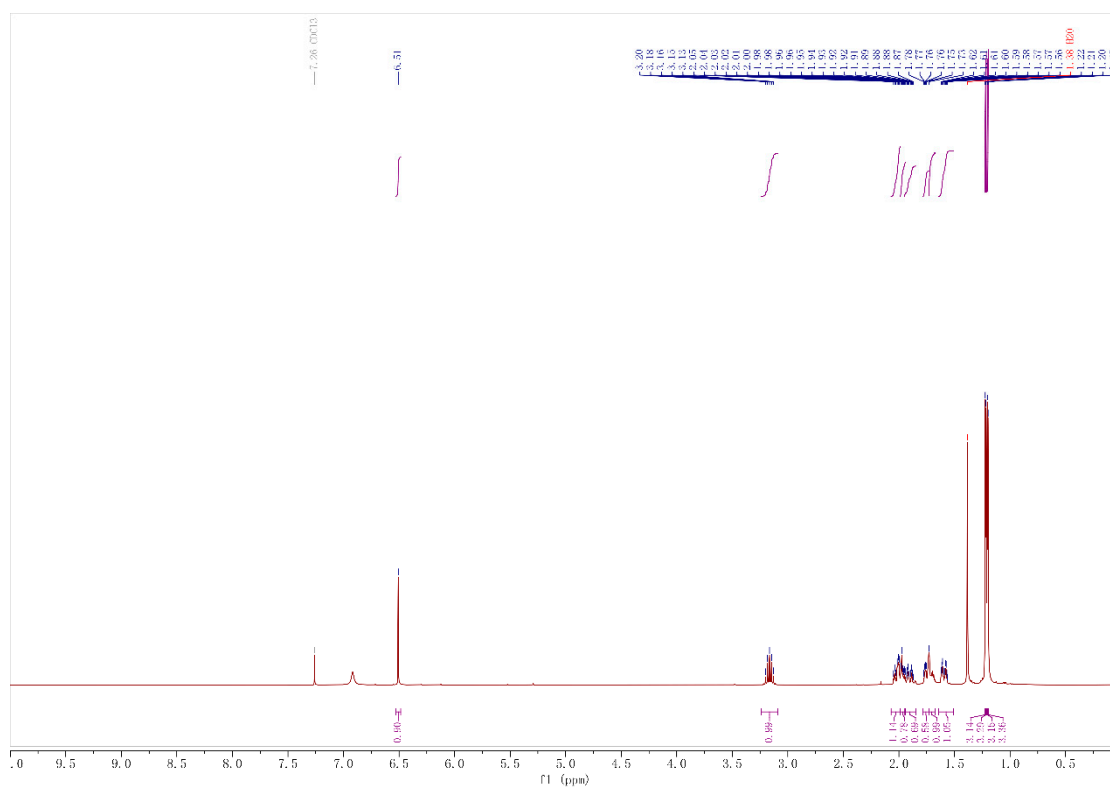


Figure S3 ¹H NMR (400 MHz, CDCl₃) spectrum of compound **1**.

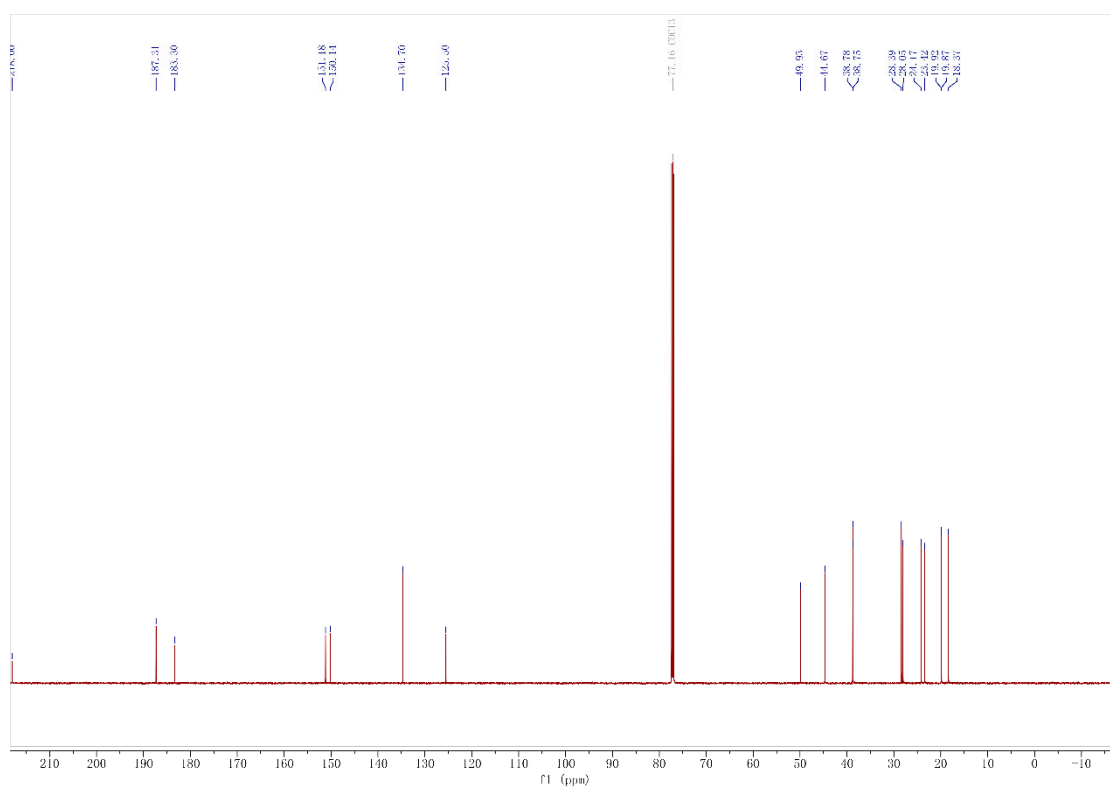
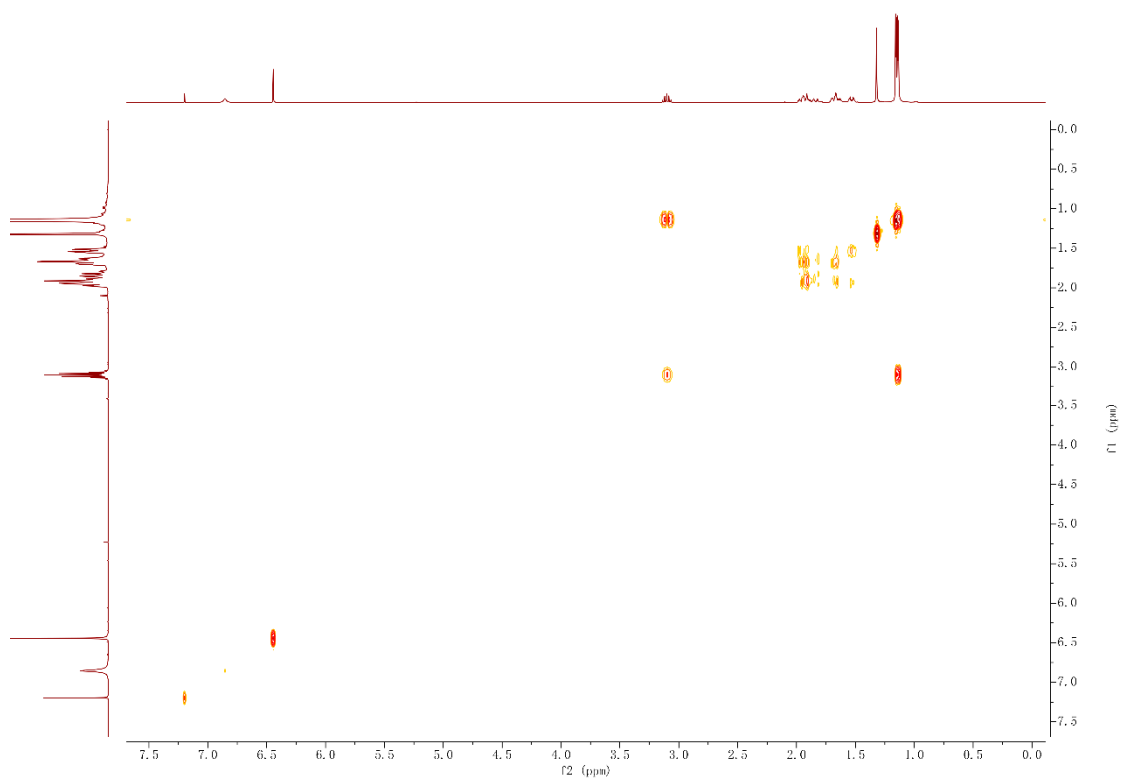


Figure S4 ¹³C NMR (101 MHz, CDCl₃) spectrum of compound **1**.



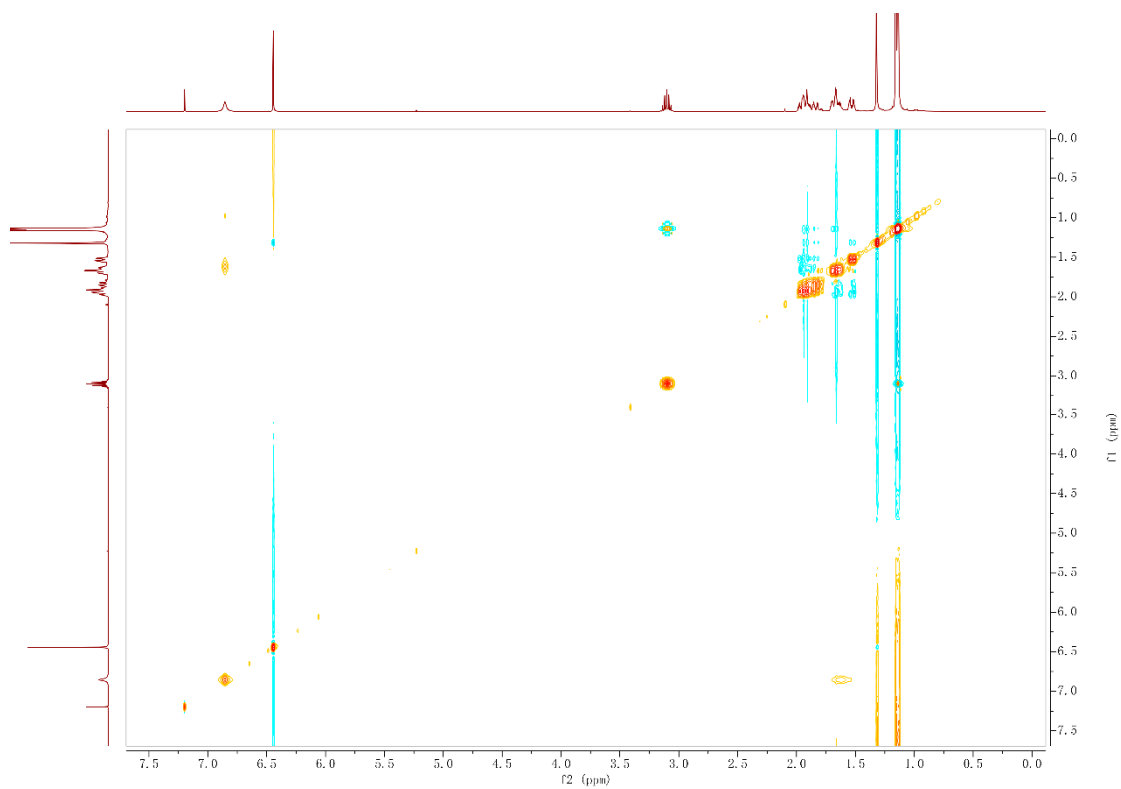


Figure S7 NOESY spectrum of compound **1** in CDCl_3 .

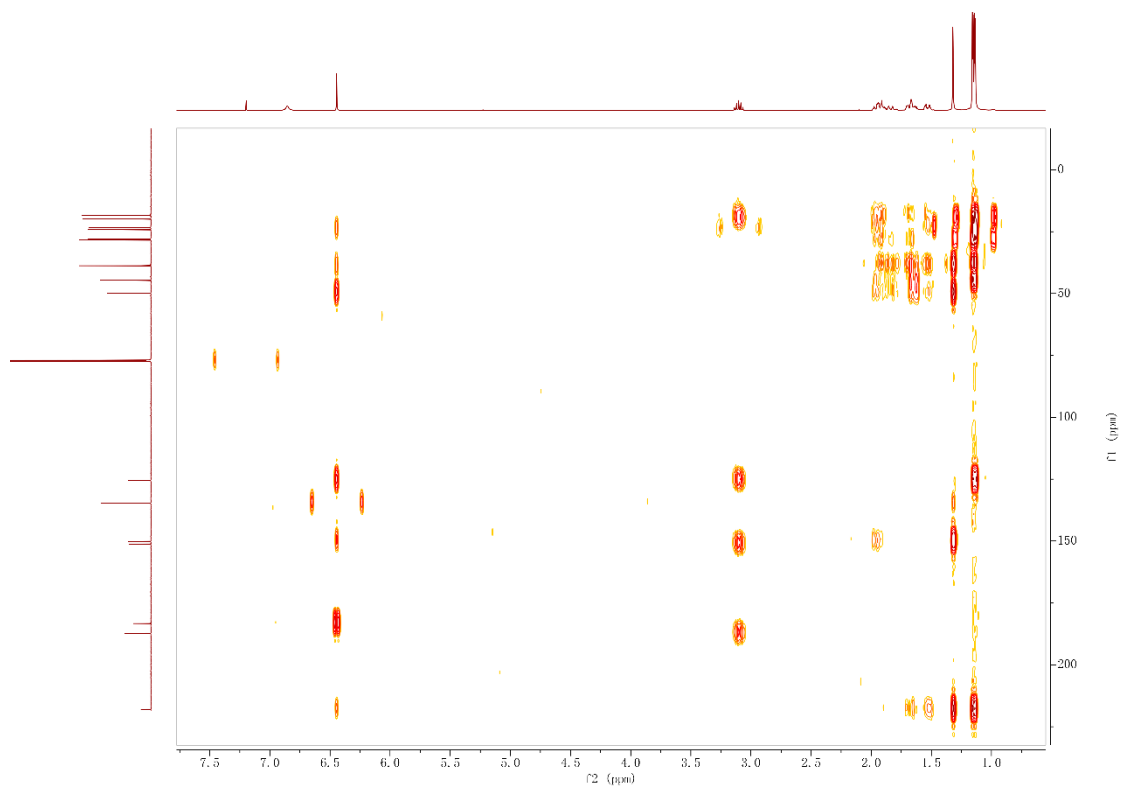


Figure S8 HMBC spectrum of compound **1** in CDCl_3 .

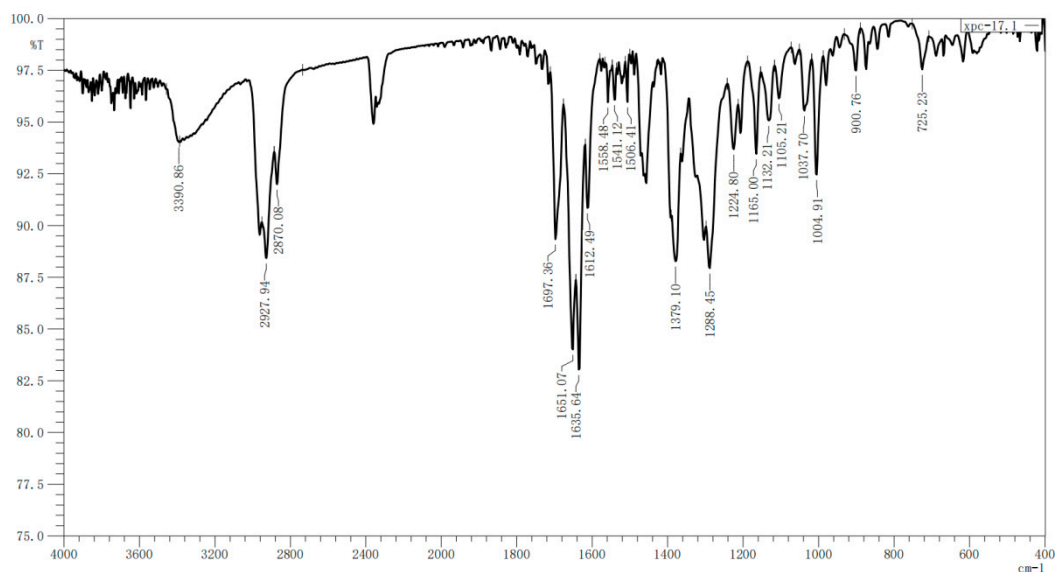


Figure S9 IR (KBr) spectrum of compound 1.

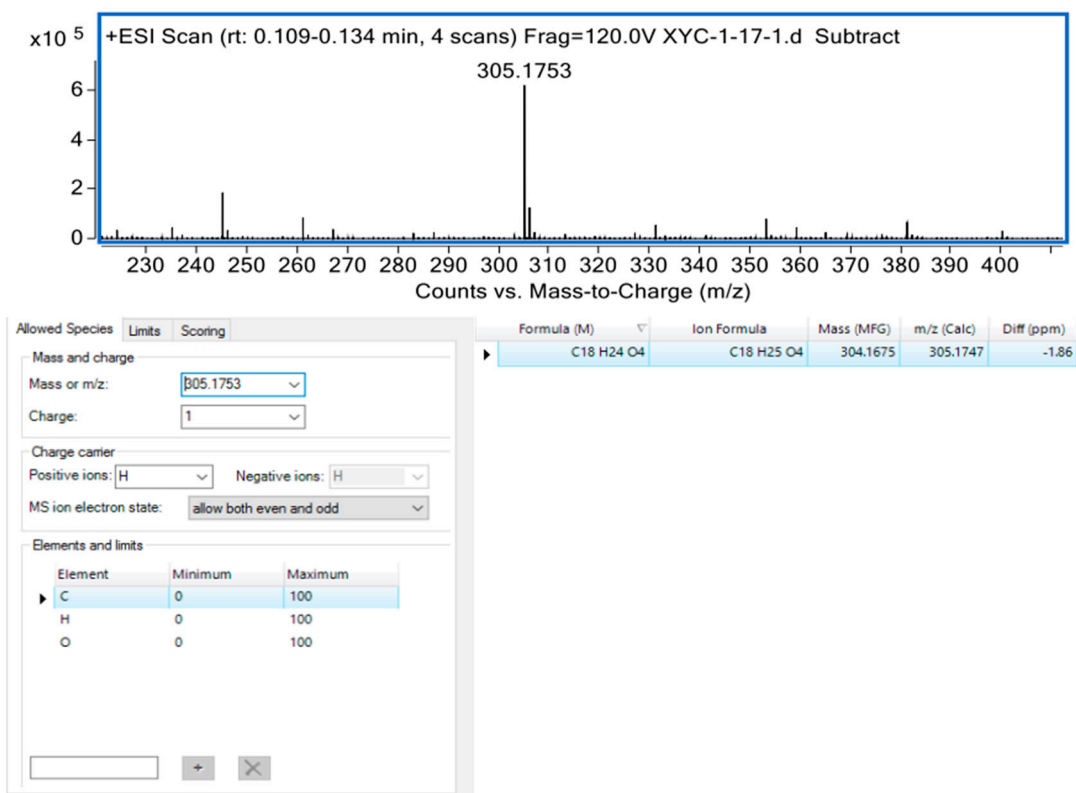
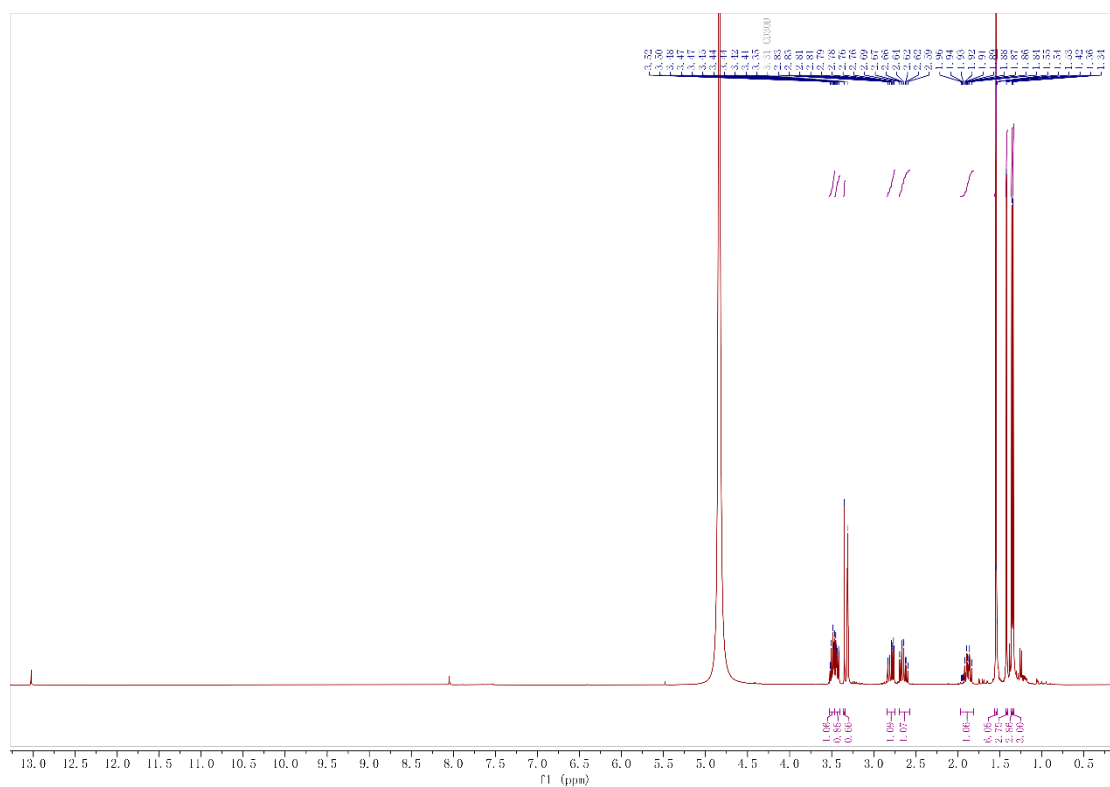


Figure S10 HR-ESI-MS spectrum of compound 1.



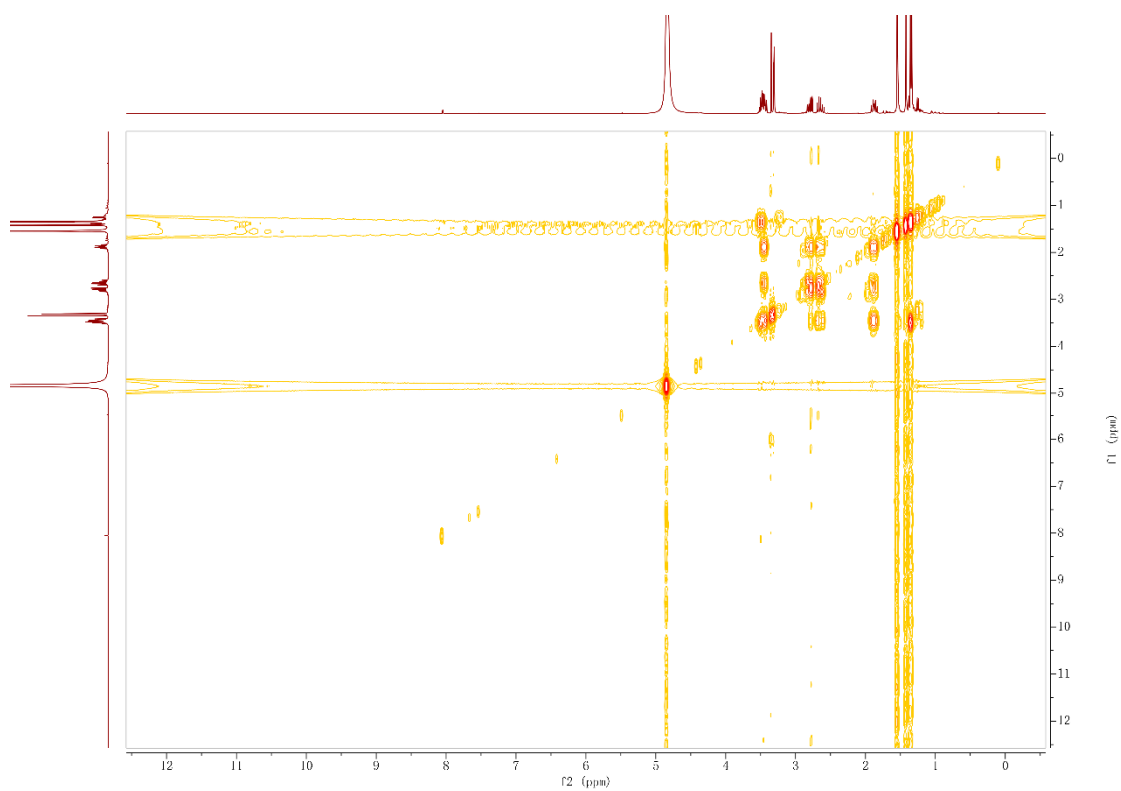


Figure S13 ^1H - ^1H COSY spectrum of compound **2** in CD_3OD .

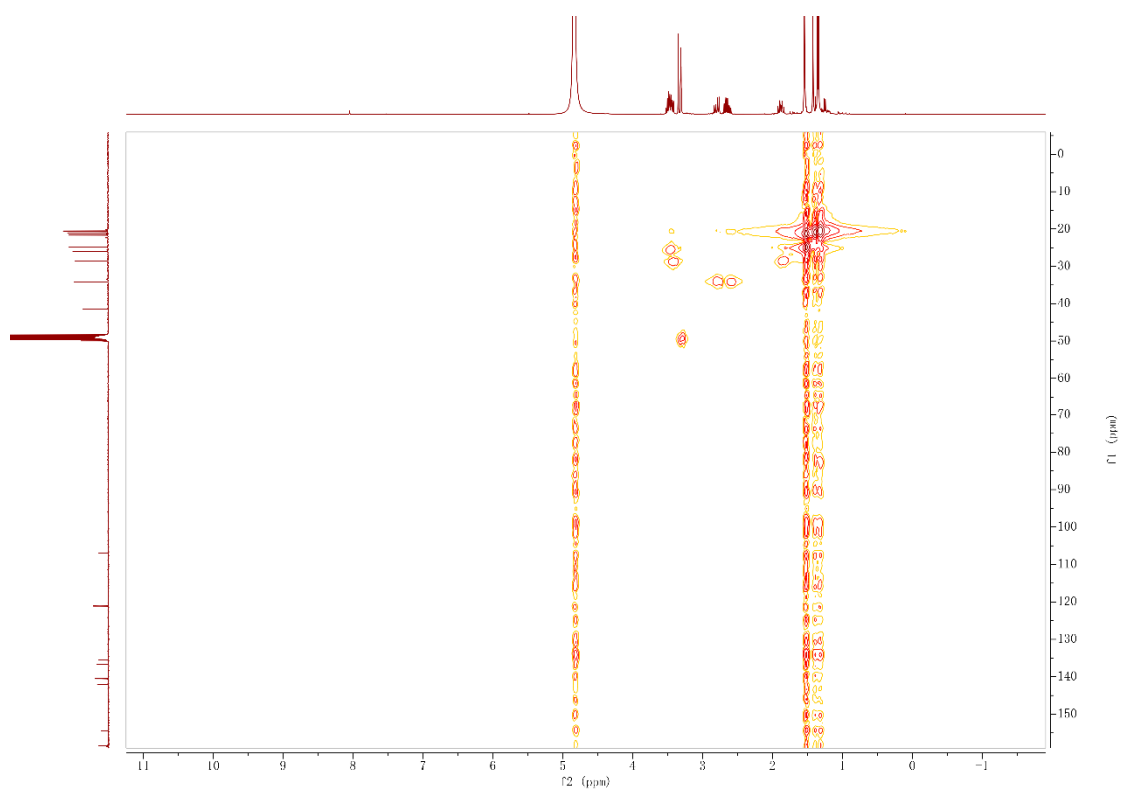


Figure S14 HMQC spectrum of compound **2** in CD_3OD .

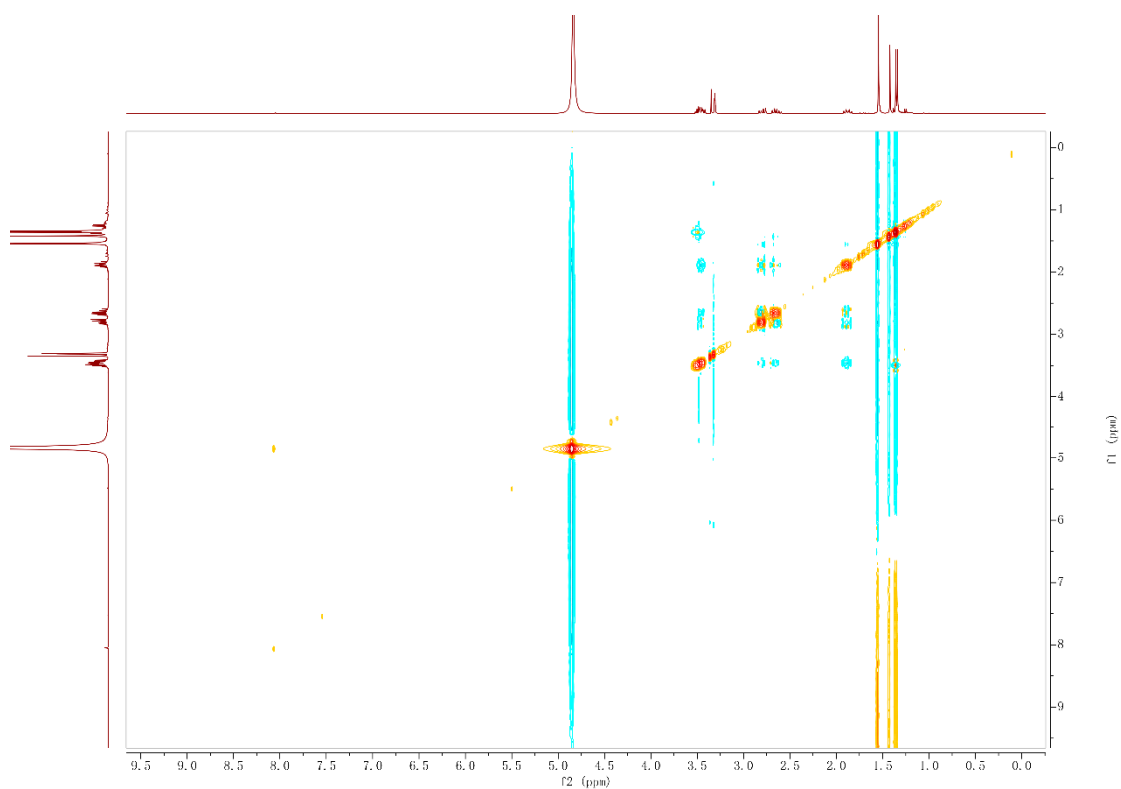


Figure S15 NOESY spectrum of compound **2** in CD₃OD.

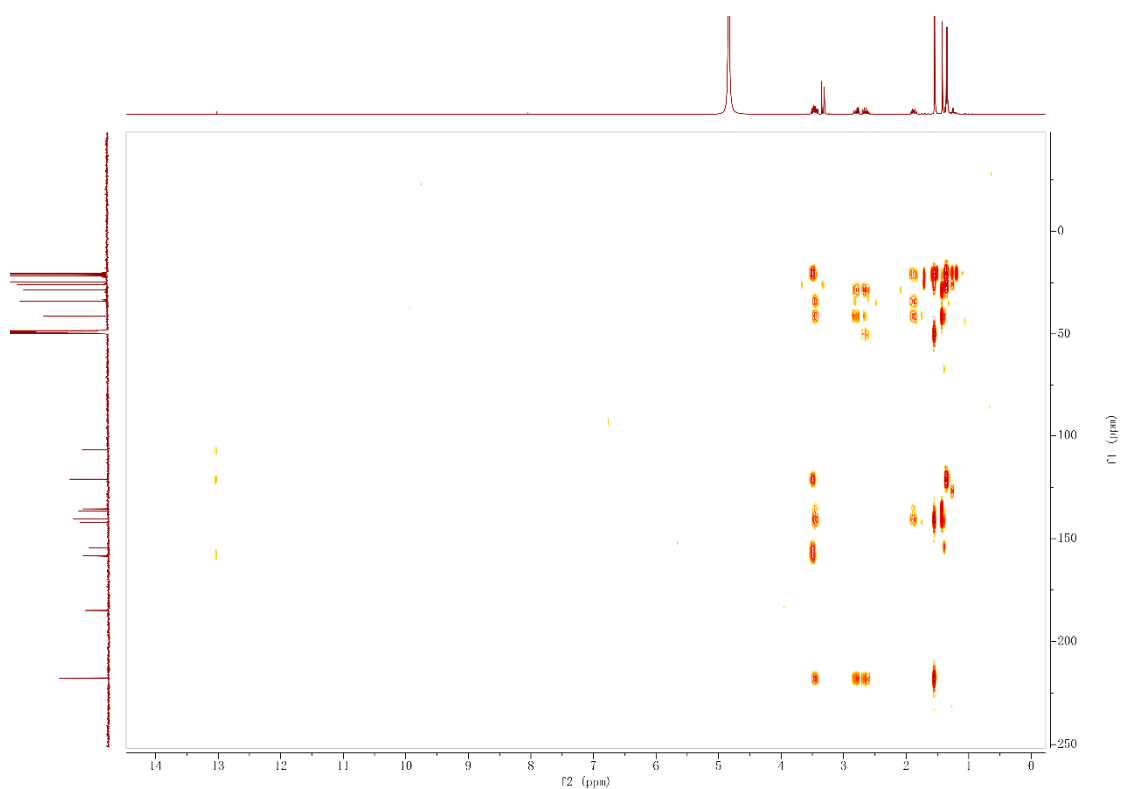


Figure S16 HMBC spectrum of compound **2** in CD₃OD.

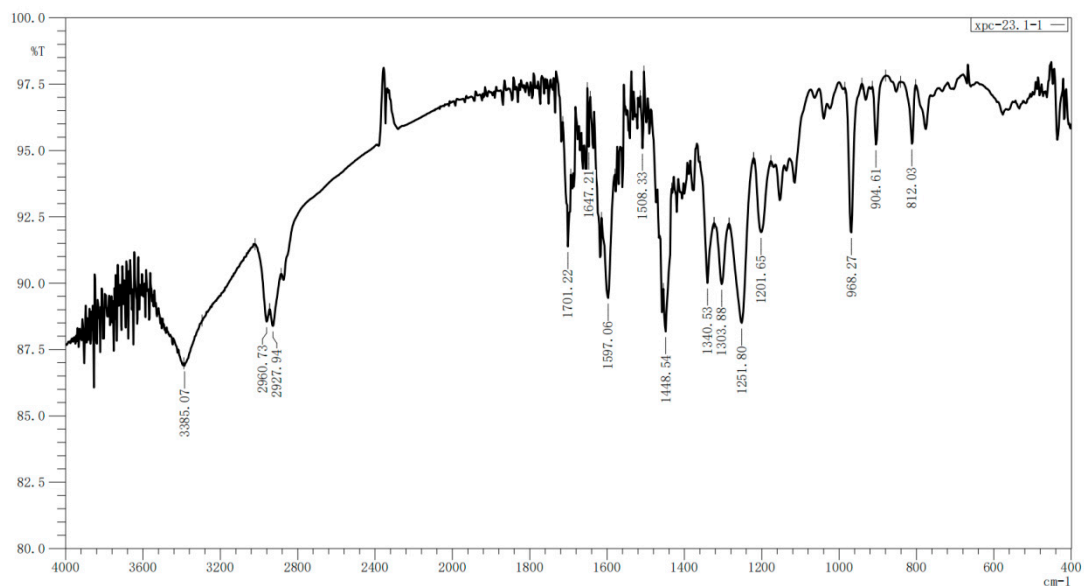


Figure S17 IR (KBr) spectrum of compound **2**.

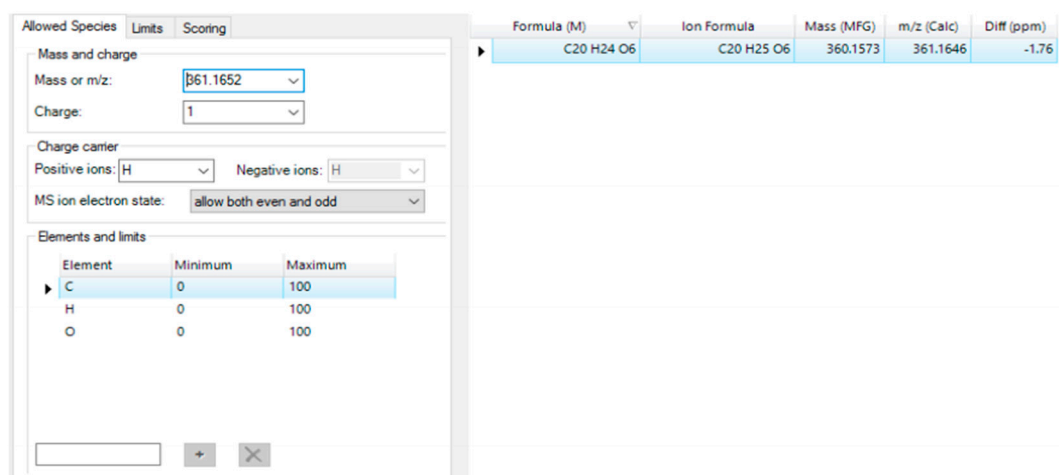
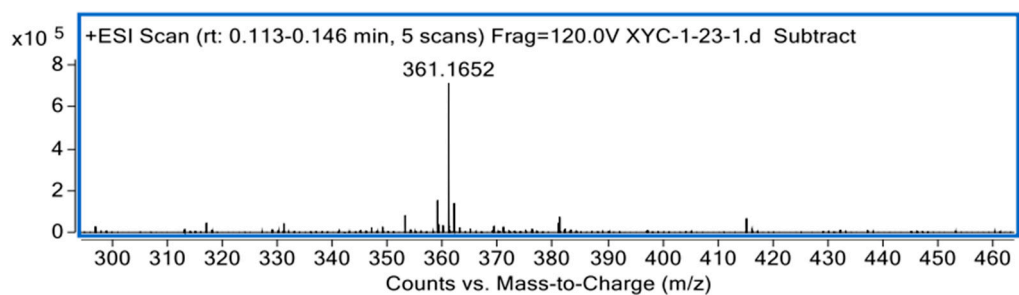


Figure S18 HR-ESI-MS spectrum of compound **2**.

Spectral data of compounds 3-36

oleon U quinone (**3**): Yellow powder; m/z 345.1692 $[M + H]^+$ (calcd for $C_{20}H_{27}O_3$, 345.1692). ^1H NMR (600 MHz, $CDCl_3$): δ_H 3.24 (1H, hept, $J = 7.0$ Hz, H-15), 1.26 (6H, d, $J = 7.1, 1.1$ Hz, H-16/17), 1.44 (6H, d, $J = 6.1$ Hz, H-18/19), 1.64 (3H, s, H-20); ^{13}C NMR (151 MHz, $CDCl_3$): δ_C 30.9 (C-1), 17.8 (C-2), 36.4 (C-3), 36.4 (C-4), 143.5 (C-5), 146.9 (C-6), 177.7 (C-7), 126.9 (C-8), 155.2 (C-9), 41.5 (C-10), 183.7 (C-11), 150.8 (C-12), 126.1 (C-13), 184.5 (C-14), 24.5 (C-15), 19.9 (C-16), 19.9 (C-17), 27.3 (C-18), 29.2 (C-19), 27.6 (C-20).

6,7-Dehydroroleanone (**4**): Red needle-like crystals; m/z 315.1592 $[M + H]^+$ (calcd for $C_{20}H_{25}O_5$, 315.1592). ^1H NMR (600 MHz, $CDCl_3$): δ_H 2.92 (2H, d, $J = 13.5$ Hz, H-1), 1.57 (2H, m, H-2), 1.45 (2H, dd, $J = 34.6, 13.2$ Hz, H-3), 2.14 (1H, d, $J = 3.4$ Hz, H-5), 6.48 (1H, d, $J = 9.7$ Hz, H-6), 6.74 (1H, d, $J = 9.6$ Hz, H-7), 3.15 (1H, m, H-15), 1.18 (3H, d, $J = 4.0$ Hz, H-16), 1.20 (3H, d, $J = 3.2$ Hz, H-17), 0.98 (3H, d, $J = 2.9$ Hz, H-18), 1.03 (3H, s, H-19), 1.04 (3H, s, H-20); ^{13}C NMR (151 MHz, $CDCl_3$): δ_C 36.3 (C-1), 19.7 (C-2), 41.7 (C-3), 34.2 (C-4), 53.4 (C-5), 139.6 (C-6), 121.9 (C-7), 138.3 (C-8), 142.6 (C-9), 40.6 (C-10), 184.6 (C-11), 123.8 (C-13), 187.6 (C-14), 25.2 (C-15), 20.2 (C-16), 20.4 (C-17), 33.1 (C-18), 23.2 (C-19), 15.4 (C-20).

5,6-Dihydrooleon U (**5**): Yellow powder; m/z 349.2007 $[M + H]^+$ (calcd for $C_{20}H_{29}O_5$, 349.2010). ^1H NMR (400 MHz, $CDCl_3$): δ_H 1.63 (1H, m, H-5), 4.52 (1H, d, $J = 2.5$ Hz, H-6), 3.44 (1H, d, $J = 8.6$ Hz, H-15), 1.33 (6H, s, H-16/17), 1.05 (3H, s, H-18), 1.34 (3H, s, H-19), 1.72 (3H, s, H-20); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 38.9 (C-1), 19.4 (C-2), 42.9 (C-3), 33.42 (C-4), 52.7 (C-5), 71.8 (C-6), 201.0 (C-7), 106.6 (C-8), 139.0 (C-9), 39.9 (C-10), 133.3 (C-11), 153.6 (C-12), 118.8 (C-13), 161.3 (C-14), 24.5 (C-15), 20.3 (C-16), 20.4 (C-17), 24.3 (C-18), 35.9 (C-19), 22.6 (C-20).

oleon U (**6**): Yellow needle-like crystals; m/z 347.1860 $[M + H]^+$ (calcd for $C_{20}H_{27}O_5$, 347.1853). ^1H NMR (400 MHz, CD_3OD): δ_H 2.91 (1H, ddd, $J = 14.3, 12.4, 6.3$ Hz, H-15), 1.44 (3H, s, H-20), 1.22 (6H, d, $J = 11.0$ Hz, H-18, 19), 1.18 (6H, dd, $J = 7.1, 1.9$ Hz, H-16/17); ^{13}C NMR (101 MHz, CD_3OD): δ_C 18.7 (C-2), 20.5 (C-17), 20.6 (C-16), 25.6 (C-15), 27.4 (C-18), 28.4 (C-20), 28.6 (C-1), 31.5 (C-19), 37.2 (C-3), 37.3 (C-4), 42.2 (C-10), 106.1 (C-8), 120.0 (C-13), 135.3 (C-11), 140.1 (C-9), 142.9 (C-5), 144.1 (C-6), 154.2 (C-12), 157.9 (C-14), 184.1 (C-7).

15-acetoxy-8,13E-labdadien-7-one (**7**): White powder; m/z 369.2411 $[M + Na]^+$ (calcd for $C_{20}H_{34}NaO_3$, 369.2400). ^1H NMR (400 MHz, $CDCl_3$): δ_H 5.40 (1H, tq, $J = 7.1, 1.3$

Hz, H-14), 4.60 (2H, d, $J = 7.0$ Hz, H-15), 2.07 (s, 3H, -COCH₃), 1.76 (6H, d, $J = 2.0$ Hz, H-16, 17), 1.08 (3H, s, H-20), 0.92 (3H, s, H-19), 0.89 (3H, s, H-18); ¹³C NMR (101 MHz, CDCl₃): δ_c 36.0 (C-1), 18.8 (C-2), 41.5 (C-3), 33.3 (C-4), 50.4 (C-5), 38.4 (C-6), 200.4 (C-7), 130.4 (C-8), 167.5 (C-9), 41.1 (C-10), 28.3 (C-11), 35.4 (C-12), 141.6 (C-13), 118.9 (C-14), 61.4 (C-15), 16.7 (C-16), 18.3 (C-17), 32.7 (C-18), 21.5 (C-19), 11.6 (C-20), 21.2 (-COCH₃), 171.2 (-COCH₃).

apigenin (**8**): Green powder; m/z 271.0599 [M + H]⁺ (calcd for C₁₅H₁₁O₅, 271.0601).

¹H NMR (400 MHz, DMSO-*d*₆) δ_H 6.77 (1H, s, H-3), 6.19 (1H, d, $J = 2.0$ Hz, H-6), 6.48 (1H, d, $J = 2.0$ Hz, H-8), 7.92 (2H, d, $J = 8.5$ Hz, H-2', 6'), 6.92 (2H, d, $J = 8.5$ Hz, H-3', 5'); ¹³C NMR (101 MHz, DMSO): δ_c 164.0 (C-2), 102.8 (C-3), 181.7 (C-4), 161.2 (C-5), 98.8 (C-6), 163.7 (C-7), 94.0 (C-8), 157.3 (C-9), 103.7 (C-10), 121.2 (C-1'), 128.5 (C-2'), 116.0 (C-3'), 161.5 (C-4'), 116.0 (C-5'), 128.5 (C-6').

luteolin (**9**): Yellow powder; m/z 287.0558 [M + H]⁺ (calcd for C₁₅H₁₁O₆, 287.0550).

¹H NMR (400 MHz, CD₃OD): δ_H 7.41-7.35 (2H, m, H-2', H-6'), 6.90 (1H, d, $J = 9.0$ Hz, H-5'), 6.53 (1H, s, H-3), 6.44 (1H, d, $J = 2.1$ Hz, H-8), 6.21 (1H, d, $J = 2.1$ Hz, H-6); ¹³C NMR (101 MHz, CD₃OD): δ_c 95.0 (C-8), 100.1 (C-6), 103.9 (C-3), 105.3 (C-10), 114.2 (C-2'), 116.8 (C-5'), 120.3 (C-1'), 123.7 (C-6'), 147.0 (C-3'), 151.0 (C-4'), 159.4 (C-9), 163.2 (C-5), 166.0 (C-2), 166.4 (C-7), 183.9 (C-4).

rutin (**10**): Yellow powder; m/z 633.1434 [M + Na]⁺ (calcd for C₂₇H₃₁O₁₆, 633.1461).

¹H NMR (400 MHz, CD₃OD): δ_H 7.69 (1H, d, $J = 2.1$ Hz, H-2'), 7.65 (1H, dd, $J = 8.5$, 2.2 Hz, H-6'), 6.89 (1H, d, $J = 8.4$ Hz, H-5'), 6.41 (1H, d, $J = 2.1$ Hz, H-8), 6.22 (1H, d, $J = 2.1$ Hz, H-6), 5.13 (1H, d, $J = 7.5$ Hz, H-1''), 4.54 (1H, d, $J = 1.7$ Hz, H-1'''), 3.83 (1H, d, $J = 10.8$ Hz, H-6''), 3.66 (1H, dd, $J = 3.5$, 1.6 Hz, H-2'''), 3.56 (1H, dd, $J = 9.5$, 3.4 Hz, H-3'''), 1.14 (3H, d, $J = 6.2$ Hz, H-6'''); ¹³C NMR (101 MHz, CD₃OD): δ_c 17.9 (C-6'''), 68.5 (C-6''), 69.7 (C-5'''), 71.4 (C-4''), 72.1 (C-2'''), 72.2 (C-3'''), 73.9 (C-4'''), 75.7 (C-2''), 77.2 (C-5''), 78.2 (C-3''), 94.9 (C-8), 99.9 (C-6), 102.4 (C-1'''), 104.7 (C-1''), 105.6 (C-10), 116.0 (C-5'), 117.7 (C-2'), 123.1 (C-1''), 123.6 (C-6'), 135.6 (C-3), 145.8 (C-3'), 149.8 (C-4'), 158.5 (C-9), 159.3 (C-2), 162.9 (C-5), 166.0 (C-7), 179.4 (C-4).

protocatechualdehyde (**11**): Yellow powder; m/z 139.0388 [M + H]⁺ (calcd for C₇H₇O₃, 139.0390). ¹H NMR (400 MHz, CD₃OD): δ_H 7.30 (2H, dd, $J = 4.3$, 2.4 Hz, H-2, 6), 6.91 (1H, d, $J = 8.6$ Hz, H-5), 9.68 (1H, s, -CHO); ¹³C NMR (101 MHz, CD₃OD): δ_c 130.8 (C-1), 115.3 (C-2), 147.1 (C-3), 153.7 (C-4), 116.2 (C-5), 126.4 (C-6), 193.1 (C-7).

caffeic acid (**12**): Yellow powder; m/z 181.0493 $[M + H]^+$ (calcd for $C_9H_9O_4$, 181.0495). ^1H NMR (400 MHz, CD_3OD) δ_H 7.04 (1H, d, $J = 2.1$ Hz, H-2), 6.78 (1H, d, $J = 8.2$ Hz, H-5), 6.93 (1H, dd, $J = 8.2, 2.1$ Hz, H-6), 7.53 (1H, d, $J = 15.8$ Hz, H-7), 6.22 (1H, d, $J = 15.9$ Hz, H-8); ^{13}C NMR (101 MHz, CD_3OD): δ_C 127.7 (C-1), 115.0 (C-2), 146.7 (C-3), 149.4 (C-4), 116.5 (C-5), 122.9 (C-6), 147.0 (C-7), 115.5 (C-8), 171.1 (C-9).

caffeic acid ethyl ester (**13**): Yellow powder; m/z 209.0812 $[M + H]^+$ (calcd for $C_{11}H_{13}O_4$, 209.0808). ^1H NMR (400 MHz, $CDCl_3$) δ_H 7.03 (1H, d, $J = 2.0$ Hz, H-2), 6.78 (1H, d, $J = 8.2$ Hz, H-5), 6.92 (1H, dd, $J = 8.1, 2.0$ Hz, H-6), 7.52 (1H, d, $J = 15.8$ Hz, H-7), 6.25 (1H, d, $J = 15.9$ Hz, H-8), 4.20 (2H, q, $J = 7.1$ Hz, H-10), 4.60 (3H, t, $J = 7.1$ Hz, H-11); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 127.7 (C-1), 115.3 (C-2), 146.7 (C-3), 149.5 (C-4), 116.5 (C-5), 122.9 (C-6), 146.7 (C-7), 115.1 (C-8), 169.3 (C-9), 61.5 (C-10), 14.6 (C-11).

caffeic acid ethylene ester (**14**): Yellow powder; m/z 205.0504 $[M + H]^+$ (calcd for $C_{11}H_9O_4$, 205.0506). ^1H NMR (400 MHz, $CDCl_3$) δ_H 7.07 (1H, d, $J = 2.0$ Hz, H-2), 6.78 (1H, d, $J = 8.3$ Hz, H-5), 6.97 (1H, dd, $J = 8.3, 2.0$ Hz, H-6), 7.64 (1H, d, $J = 15.9$ Hz, H-7), 6.25 (1H, d, $J = 15.9$ Hz, H-8), 7.38 (1H, dd, $J = 14.0, 6.3$ Hz, H-10), 4.93 (1H, dd, $J = 14.0, 1.4$ Hz, H-11 α), 4.60 (1H, dd, $J = 6.3, 1.5$ Hz, H-11 β); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 127.5 (C-1), 115.3 (C-2), 146.8 (C-3), 150.0 (C-4), 116.6 (C-5), 123.4 (C-6), 148.7 (C-7), 113.5 (C-8), 165.5 (C-9), 142.5 (C-10), 97.7 (C-11).

salicylic acid (**15**): Colorless crystal; m/z 137.0247 $[M - H]^-$ (calcd for $C_7H_5O_3$, 137.0244). ^1H NMR (400 MHz, CD_3OD) : δ_H 7.85 (1H, dd, $J = 7.9, 1.8$ Hz, H-2), 7.39 (1H, ddd, $J = 8.5, 7.2, 1.5$ Hz, H-3), 6.92-6.81 (2H, m, H-4/5); ^{13}C NMR (101 MHz, CD_3OD) : δ_C 112.9 (C-4), 117.8 (C-5), 119.7 (C-6), 131.6 (C-3), 135.7 (C-1), 163.0 (C-2), 174.4 (C-7)

carvacrol (**16**): Yellow oil; ^1H NMR (400 MHz, $CDCl_3$): δ_H 7.04 (1H, d, $J = 7.6$ Hz, H-3), 6.73 (1H, dd, $J = 7.6, 1.7$ Hz, H-6), 6.66 (1H, d, $J = 1.8$ Hz, H-4), 2.82 (1H, tq, $J = 13.5, 6.6$ Hz, H-7), 2.22 (3H, s, H-10), 1.22 (6H, d, $J = 6.9$ Hz, H-8/9); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 15.4 (C-10), 24.1 (C-8, 9), 33.8 (C-7), 113.1 (C-6), 118.9 (C-4), 120.9 (C-2), 130.9 (C-3), 148.6 (C-5), 153.8 (C-1).

thymol (**17**): White powder; ^1H NMR (400 MHz, $CDCl_3$) : δ_H 7.17 (1H, d, $J = 7.7$ Hz, H-5), 6.82 (1H, d, $J = 7.8$ Hz, H-6), 6.62 (1H, d, $J = 1.8$ Hz, H-2), 3.25 (1H, hept, $J = 6.8$ Hz, H-8), 2.34 (3H, s, H-7), 1.32 (6H, dd, $J = 7.0, 1.5$ Hz, H-9/10); ^{13}C NMR (101

MHz, CDCl₃): δ_C 20.9 (C-7), 22.8 (C-9, 10), 26.8 (C-8), 116.2 (C-2), 121.8 (C-6), 126.3 (C-5), 131.6 (C-4), 136.7 (C-1), 152.6 (C-3).

β -sitosterol (**18**): White crystals; ¹H NMR (400 MHz, CDCl₃): δ_H 5.34 (1H, dd, J = 5.3, 2.5 Hz, H-6), 3.60-3.43 (1H, m, H-3), 2.33-2.17 (2H, m, H-4); ¹³C NMR (101 MHz, CDCl₃): δ_C 36.3 (C-1), 71.9 (C-3), 42.4 (C-4), 140.9 (C-5), 32.0 (C-6), 32.0 (C-7), 50.3 (C-8), 37.4 (C-9), 23.2 (C-10), 40.6 (C-11), 42.5 (C-12), 57.0 (C-13), 25.5 (C-14), 56.2 (C-15), 36.6 (C-17), 29.3 (C-18), 46.0 (C-21), 29.1 (C-22), 20.0 (C-23), 19.2 (C-24), 12.0 (C-25), 19.5 (C-26), 24.5 (C-27), 12.1 (C-28), 21.2 (C-29).

stigmasta-4,22-dien-3-one (**19**): White crystals; m/z 411.3629 [$M + H$]⁺ (calcd for C₂₉H₄₇O, 411.3621). ¹H NMR (400 MHz, CDCl₃): δ_H 5.67 (1H, d, J = 1.8 Hz, H-4), 5.10 (1H, dd, J = 15.2, 8.5 Hz, H-23), 4.97 (1H, dd, J = 15.2, 8.6 Hz, H-22), 1.13 (3H, s, H-19), 0.97 (3H, d, J = 6.6 Hz, H-21), 0.87-0.84 (3H, m, H-26), 0.79 (3H, d, J = 2.4 Hz, H-27), 0.77 (3H, d, J = 1.8 Hz, H-29), 0.76 (3H, d, J = 2.3 Hz, H-18); ¹³C NMR (151 MHz, CDCl₃): δ_C 199.9 (C-3), 171.9 (C-5), 138.3 (C-22), 129.5 (C-23), 123.9 (C-4), 56.1 (C-14), 56.0 (C-17), 53.9 (C-9), 51.3 (C-24), 42.4 (C-13), 40.6 (C-20), 39.6 (C-12), 38.7 (C-10), 35.8 (C-8), 35.7 (C-1), 34.1 (C-2), 33.1 (C-6), 32.1 (C-7), 32.0 (C-25), 29.0 (C-16), 25.5 (C-28), 24.4 (C-15), 21.3 (C-26), 21.2 (C-21), 21.1 (C-11), 19.1 (C-27), 17.5 (C-19), 12.4 (C-29), 12.3 (C-18).

stigmasta-4,22-dien-3,6-dione (**20**): White crystals; m/z 425.3418 [$M + H$]⁺ (calcd for C₂₉H₄₅O₂, 425.3414). ¹H NMR (400 MHz, CDCl₃): δ_H 6.15 (1H, d, J = 0.9 Hz, H-4), 5.14 (1H, dd, J = 15.2, 8.5 Hz, H-23), 5.03 (1H, dd, J = 15.2, 8.6 Hz, H-22), 1.15 (3H, s, H-19), 1.02 (3H, d, J = 6.6 Hz, H-21), 0.73 (3H, s, H-18); ¹³C NMR (101 MHz, CDCl₃): δ_C 202.4 (C-3), 199.5 (C-6), 161.1 (C-5), 137.9 (C-22), 129.9 (C-23), 125.6 (C-4), 56.8 (C-14), 56.0 (C-17), 51.3 (C-24), 46.9 (C-7), 42.5 (C-13), 39.9 (C-20), 39.2 (C-10), 36.1 (C-1), 34.3 (C-8), 32.5 (C-25), 28.8 (C-16), 25.5 (C-28), 24.1 (C-15), 21.3 (C-27), 21.0 (C-21), 19.1 (C-26), 19.1 (C-11), 17.6 (C-19), 12.1 (C-29), 12.0 (C-18).

stigmasta-5,22-dien-3,7-dione (**21**): White crystals; m/z 425.3418 [$M + H$]⁺ (calcd for C₂₉H₄₅O₂, 425.3414). ¹H NMR (400 MHz, CDCl₃): δ_H 6.15 (1H, d, J = 0.9 Hz, H-6), 5.14 (1H, dd, J = 15.2, 8.5 Hz, H-22), 5.03 (1H, dd, J = 15.2, 8.6 Hz, H-23); ¹³C NMR (101 MHz, CDCl₃): δ_C 202.4 (C-7), 199.6 (C-3), 161.2 (C-5), 137.9 (C-22), 129.9 (C-23), 125.5 (C-6), 56.7 (C-17), 55.9 (C-14), 51.1 (C-9), 51.1 (C-24), 46.9 (C-8), 45.9 (C-4), 42.6 (C-13), 39.9 (C-20), 39.2 (C-10), 39.1 (C-1), 35.6 (C-12), 34.1 (C-2),

32.0 (C-25), 29.3 (C-16), 26.2 (C-15), 24.1 (C-11), 23.2 (C-28), 21.2 (C-21), 21.0 (C-26), 19.9 (C-27), 17.6 (C-19), 12.4 (C-29), 12.2 (C-18).

ursolic acid (**22**): White powder; m/z 457.3672 $[M + H]^+$ (calcd for $C_{30}H_{49}O_3$, 457.3676). ^1H NMR (400 MHz, $CDCl_3$): δ_H 5.05 (1H, t, $J = 3.4$ Hz, H-12), 3.16 (1H, dd, $J = 11.1, 5.2$ Hz, H-3), 1.00 (3H, s, H-26), 0.93 (6H, d, $J = 4.5$ Hz, H-23/30), 0.88 (3H, s, H-29), 0.80 (3H, d, $J = 7.5$ Hz, H-27), 0.72 (6H, d, $J = 2.8$ Hz, H-24/25); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 14.3 (C-25), 15.8 (C-24), 17.0 (C-29), 17.6 (C-26), 18.5 (C-6), 21.5 (C-30), 22.8 (C-27), 23.4 (C-11), 24.9 (C-16), 26.8 (C-2), 27.4 (C-15), 28.3 (C-23), 31.4 (C-21), 33.1 (C-7), 37.0 (C-10), 38.9 (C-1, 4), 39.8 (C-8, 19), 41.7 (C-14), 47.9 (C-17), 55.3 (C-5), 59.2 (C-18), 79.3 (C-3), 124.6 (C-12), 139.7 (C-13), 178.8 (C-28).

ursolic aldehyde (**23**): White powder; m/z 463.3555 $[M + Na]^+$ (calcd for $C_{30}H_{48}NaO_2$, 463.3547). ^1H NMR (400 MHz, $CDCl_3$): δ_H 9.30 (1H, d, $J = 1.3$ Hz, H-28), 5.29 (1H, t, $J = 3.8$ Hz, H-12), 3.19 (1H, dd, $J = 10.7, 5.1$ Hz, H-3), 1.07 (3H, s, H-27), 0.96 (3H, s, H-23), 0.94 (3H, d, $J = 2.5$ Hz, H-30), 0.90 (3H, s, H-25), 0.85 (3H, d, $J = 6.5$ Hz, H-29), 0.76 (3H, s, H-24), 0.74 (3H, s, H-26); ^{13}C NMR (101 MHz, $CDCl_3$): δ_C 15.6 (C-25), 15.7 (C-24), 16.8 (C-29), 17.3 (C-26), 18.4 (C-6), 21.2 (C-30), 23.3 (C-11), 23.4 (C-16), 27.0 (C-15), 27.3 (C-2), 28.3 (C-23), 30.3 (C-21), 32.0 (C-7), 33.2 (C-22), 37.0 (C-10), 38.8 (C-1, 4), 38.9 (C-20), 39.1 (C-19), 39.9 (C-8), 42.3 (C-14), 47.7 (C-9), 50.2 (C-17), 52.7 (C-18), 55.3 (C-5), 79.1 (C-3), 126.3 (C-12), 137.9 (C-13), 207.6 (C-28).

maslinic acid (**24**): Yellow powder; m/z 495.3450 $[M + Na]^+$ (calcd for $C_{30}H_{48}NaO_4$, 495.3445). ^1H NMR (400 MHz, $DMSO-d_6$): δ_H 12.01 (1H, s, -COOH), 5.17 (1H, d, $J = 3.6$ Hz, H-12), 4.32 (1H, d, H-2), 2.74 (1H, d, $J = 8.9$ Hz, H-3), 1.09 (3H, s, H-27), 0.92 (3H, s, H-25), 0.90 (3H, s, H-26), 0.87 (6H, s, H-29/30), 0.70 (6H, d, $J = 2.2$ Hz, H-23/24); ^{13}C NMR (101 MHz, $DMSO-d_6$): δ_C 16.3 (C-26), 16.9 (C-25), 17.1 (C-24), 18.1 (C-6), 22.6 (C-11), 23.0 (C-16), 23.4 (C-30), 25.7 (C-27), 27.2 (C-15), 28.8 (C-23), 30.4 (C-20), 32.1 (C-22), 32.3 (C-7), 32.9 (C-29), 33.3 (C-21), 37.7 (C-10), 38.9 (C-4), 38.9 (C-8), 40.8 (C-18), 41.3 (C-14), 45.4 (C-17), 45.7 (C-19), 46.8 (C-1), 47.1 (C-9), 54.8 (C-5), 67.1 (C-2), 82.2 (C-3), 121.5 (C-12), 143.9 (C-13), 178.6 (C-28).

tormentic acid (**25**): Yellowish-brown powder; m/z 487.3426 $[M - H]^-$ (calcd for $C_{30}H_{47}O_5$, 487.3429). ^1H NMR (400 MHz, $DMSO-d_6$): δ_H 5.17 (1H, s, H-12), 3.75 (1H, d, $J = 5.7$ Hz, 19-OH), 2.74 (1H, d, $J = 9.4$ Hz, H-3), 2.37 (1H, s, H-18), 1.28

(3H, d, $J = 4.0$ Hz, H-27), 1.08 (3H, s, H-29), 0.92 (6H, d, $J = 7.1$ Hz, H-25/26), 0.85 (3H, d, $J = 5.3$ Hz, H-30), 0.70 (6H, d, $J = 4.6$ Hz, H-23/24); ^{13}C NMR (101 MHz, DMSO- d_6): δ_{C} 16.3 (C-15, 30), 16.6 (C-26), 17.2 (C-24), 18.2 (C-6), 23.2 (C-11), 24.0 (C-27), 25.2 (C-16), 26.0 (C-21), 26.4 (C-29), 28.1 (C-15), 28.8 (C-23), 32.6 (C-7), 37.3 (C-10), 37.6 (C-22), 39.0 (C-4), 39.4 (C-8), 41.2 (C-14), 41.4 (C-20), 46.7 (C-9), 46.9 (C-1), 47.0 (C-17), 53.2 (C-18), 54.9 (C-5), 67.2 (C-2), 71.7 (C-19), 82.3 (C-3), 126.8 (C-12), 138.7 (C-13), 179.0 (C-28).

α -cedrene (**26**): Light yellow liquid; ^1H NMR (400 MHz, CDCl_3): δ_{H} 5.23 (1H, dq, $J = 3.9, 1.8$ Hz, H-4), 2.18 (1H, dp, $J = 16.7, 2.5$ Hz, H-5), 1.68 (3H, q, $J = 2.0$ Hz, H-15), 1.03 (3H, s, H-13), 0.96 (3H, s, H-12), 0.85 (3H, d, $J = 7.2$ Hz, H-14); ^{13}C NMR (101 MHz, CDCl_3): δ_{C} 15.6 (C-14), 24.9 (C-15), 25.0 (C-9), 25.8 (C-12), 27.8 (C-13), 36.3 (C-8), 39.0 (C-5), 40.8 (C-1), 41.6 (C-7), 48.3 (C-11), 54.0 (C-6), 55.0 (C-2), 59.2 (C-10), 119.4 (C-4), 140.7 (C-3).

clovane-2,9-diol (**27**): Yellow oil; m/z 256.2270 $[\text{M} + \text{NH}_4]^+$ (calcd for $\text{C}_{15}\text{H}_{30}\text{NO}_2$, 256.2271). ^1H NMR (400 MHz, CD_3OD): δ_{H} 3.73 (1H, dd, $J = 10.6, 5.9$ Hz, H-11), 3.23 (1H, d, $J = 3.0$ Hz, H-4), 1.99 (1H, tdd, $J = 14.2, 5.0, 3.2$ Hz, H-7), 1.71 (1H, dd, $J = 13.4, 4.7$ Hz, H-3), 1.03 (3H, s, H-14), 0.93 (3H, s, H-12), 0.86 (3H, s, H-15); ^{13}C NMR (101 MHz, CD_3OD): δ_{C} 21.7 (C-13), 25.8 (C-15), 26.9 (C-7), 27.8 (C-3), 29.1 (C-12), 31.8 (C-14), 34.5 (C-6), 35.8 (C-5), 36.7 (C-2), 37.7 (C-9), 45.4 (C-1), 48.2 (C-10), 52.0 (C-8), 75.9 (C-4), 81.4 (C-11).

α -cyperone (**28**): Yellow oil; m/z 219.1750 $[\text{M} + \text{H}]^+$ (calcd for $\text{C}_{15}\text{H}_{23}\text{O}$, 219.1743). ^1H NMR (400 MHz, CDCl_3): δ_{H} 4.77 (2H, d, $J = 1.3$ Hz, H-12), 2.79-2.67 (1H, m, H-8a), 2.52 (1H, ddd, $J = 16.9, 13.4, 6.1$ Hz, H-3 α), 2.41 (1H, t, $J = 4.1$ Hz, H-3 β), 2.10-1.98 (1H, m, H-8 β), 1.77 (3H, q, $J = 1.1$ Hz, H-13), 1.22 (3H, s, H-9); ^{13}C NMR (101 MHz, CDCl_3): δ_{C} 11.1 (C-10), 20.8 (C-13), 22.7 (C-9), 27.0 (C-6), 33.1 (C-8), 34.0 (C-3), 36.0 (C-15), 37.6 (C-4), 42.1 (C-5), 46.1 (C-7), 109.3 (C-12), 129.0 (C-1), 149.3 (C-11), 162.3 (C-14), 199.3 (C-2).

esculetin (**29**): Yellow powder; m/z 177.0915 $[\text{M} - \text{H}]^-$ (calcd for $\text{C}_9\text{H}_5\text{O}_4$, 177.0193). ^1H NMR (400 MHz, DMSO- d_6): δ_{H} 7.84 (1H, d, $J = 9.4$ Hz, H-4), 6.97 (s, 1H, H-5), 6.74 (1H, s, H-8), 6.15 (1H, d, $J = 9.4$ Hz, H-3); ^{13}C NMR (101 MHz, DMSO- d_6): δ_{C} 102.7 (C-5), 110.8 (C-8), 111.6 (C-3), 112.4 (C-9), 142.9 (C-7), 144.5 (C-4), 148.6 (C-6), 150.5 (C-10), 160.9 (C-2).

gusanlung C (**30**): Yellow powder; m/z 314.1396 $[\text{M} + \text{H}]^+$ (calcd for $\text{C}_{18}\text{H}_{20}\text{NO}_4$, 314.1387). ^1H NMR (400 MHz, Acetone- d_6): δ_{H} 7.15 (1H, d, $J = 1.9$ Hz, H-1), 7.03

(1H, d, $J = 1.9$ Hz, H-3), 6.83 (1H, d, $J = 8.1$ Hz, H-4), 2.75 (2H, t, $J = 7.3$ Hz, H-5), 3.49 (2H, t, $J = 7.4$ Hz, H-6), 7.06 (1H, d, $J = 8.4$ Hz, H-9), 6.76 (1H, d, $J = 8.4$ Hz, H-10), 6.76 (1H, d, $J = 8.4$ Hz, H-12), 7.06 (1H, d, $J = 8.4$ Hz, H-13), 7.46 (1H, dd, $J = 15.6, 2.8$ Hz, H-15), 6.51 (1H, d, $J = 15.6$ Hz, H-16), 3.87 (3H, s, -OCH₃); ¹³C NMR (101 MHz, Acetone-*d*₆): δ_c 120.0 (C-1), 156.6 (C-2), 122.6 (C-3), 116.0 (C-4), 131.1 (C-4a), 35.7 (C-5), 41.8 (C-6), 166.5 (C-8), 116.0 (C-9), 130.5 (C-10), 149.2 (C-11), 130.5 (C-12), 116.0 (C-13), 148.6 (C-14), 140.4 (C-15), 111.3 (C-16), 128.3 (C-16a), 56.2 (-OCH₃).

(1*R*,2*R*,2'*E*)-2-[5'-(hydroxy)-2-penten-1-yl]-3-oxocyclopentane acetic acid methyl ester (**31**): White powder; m/z 241.1434 [$M + H$]⁺ (calcd for C₁₃H₂₁O₄, 241.1434). ¹H NMR (400 MHz, CD₃OD): δ_H 2.38 (1H, m, H-1), 1.99 (1H, m, H-2), 2.10 (1H, m, H-4), 2.20 (1H, m, H-5 α), 1.53 (1H, m, H-5 β), 2.35 (1H, m, H-1'), 5.42 (1H, m, H-2'), 5.49 (1H, m, H-3'), 2.25 (1H, m, H-4'), 3.55 (1H, t, $J = 6.8$ Hz, H-5'), 2.72 (1H, t, $J = 14.8, 4.0$ Hz, H-1'' α), 2.36 (1H, m, H-1'' β), 3.68 (3H, s, H-3''); ¹³C NMR (101 MHz, CD₃OD): δ_c 39.1 (C-1), 55.0 (C-2), 38.5 (C-4), 28.0 (C-5), 26.4 (C-1'), 129.0 (C-2'), 129.1 (C-3'), 31.8 (C-4'), 62.5 (C-5'), 39.5 (C-1''), 174.4 (C-2''), 52.1 (C-3'')

vomifoliol (**32**): Yellow powder; m/z 314.1396 [$M + H$]⁺ (calcd for C₁₈H₂₀NO₄, 314.1387). ¹H NMR (400 MHz, CDCl₃): δ_H 2.43 (1H, d, $J = 17.1$ Hz, H-2 α), 2.22 (1H, d, $J = 17.1$ Hz, H-2 β), 5.88 (1H, s, H-4), 5.76 (1H, d, $J = 15.7$ Hz, H-7), 5.82 (1H, d, $J = 5.1$ Hz, H-8), 4.38 (1H, p, $J = 6.2$ Hz, H-9), 1.28 (3H, d, $J = 6.4$ Hz, H-10), 0.99 (3H, d, $J = 4.5$ Hz, H-11), 1.07 (3H, d, $J = 6.7$ Hz, H-12), 1.89 (3H, s, H-13); ¹³C NMR (101 MHz, CDCl₃): δ_c 41.3 (C-1), 49.8 (C-2), 198.5 (C-3), 129.0 (C-4), 163.4 (C-5), 79.1 (C-6), 126.9 (C-7), 135.9 (C-8), 68.0 (C-9), 23.0 (C-10), 24.2 (C-11), 23.0 (C-12), 19.1 (C-13)

m-cymene (**33**): Colorless crystals; ¹H NMR (400 MHz, CD₃OD): δ_H 7.11 (1H, t, $J = 7.6$ Hz, H-5), 7.01 (1H, s, H-2), 6.97 (1H, d, $J = 7.8$ Hz, H-6), 6.94 (1H, d, $J = 7.6$ Hz, H-4), 2.81 (1H, hept, $J = 6.9$ Hz, H-7), 2.28 (3H, s, H-8), 1.21 (6H, d, $J = 7.0$ Hz, H-9, 10); ¹³C NMR (101 MHz, CD₃OD): δ_c 21.6 (C-8), 24.5 (C-9, 10), 35.3 (C-7), 124.3 (C-6), 127.4 (C-4), 128.0 (C-2), 129.2 (C-5), 138.7 (C-3), 149.9 (C-1).

5-hydroxymethylfurfural (**34**): Light yellow crystals; m/z 127.0393 [$M + H$]⁺ (calcd for C₆H₇O₃, 127.0390). ¹H NMR (400 MHz, CDCl₃): δ_H 9.55 (1H, s, -CHO), 7.20 (1H, d, $J = 3.6$ Hz, H-3), 6.50 (1H, d, $J = 3.6$ Hz, H-4), 4.69 (2H, s, -CH₂OH); ¹³C NMR (101 MHz, CDCl₃): δ_c 152.4 (C-2), 123.1 (C-3), 110.1 (C-4), 160.9 (C-5), 177.8 (-CHO), 57.6 (-CH₂OH)

cineole (**35**): Colorless liquid; ^1H NMR (400 MHz, CDCl_3): δ_{H} 2.06-1.96 (2H, m, H-2), 1.49 (4H, dd, $J = 8.8, 1.3$ Hz, H-3, 5), 1.23 (s, 6H, H-9, 10), 1.04 (s, 3H, H-7); ^{13}C NMR (101 MHz, CDCl_3): δ_{C} 23.0 (C-9, 10), 27.7 (C-7), 29.0 (C-2, 6), 31.6 (C-3, 5), 33.1 (C-4), 70.0 (C-1), 73.8 (C-8)

azelaic acid (**36**): White powder; m/z 189.1124 $[\text{M} + \text{H}]^+$ (calcd for $\text{C}_9\text{H}_{17}\text{O}_4$, 189.1121). ^1H NMR (400 MHz, CD_3OD): δ_{H} 2.28 (4H, t, $J = 7.3$ Hz, H-2, 8), 1.60 (4H, t, $J = 8.5$ Hz, H-3, 7), 1.34 (6H, m, H-4, 5, 6), ^{13}C NMR (101 MHz, CD_3OD): δ_{C} 177.6 (C-2), 34.9 (C-3), 26.0 (C-4), 30.0 (C-5), 30.0 (C-6), 30.0 (C-7), 34.9 (C-8), 177.6 (C-9).

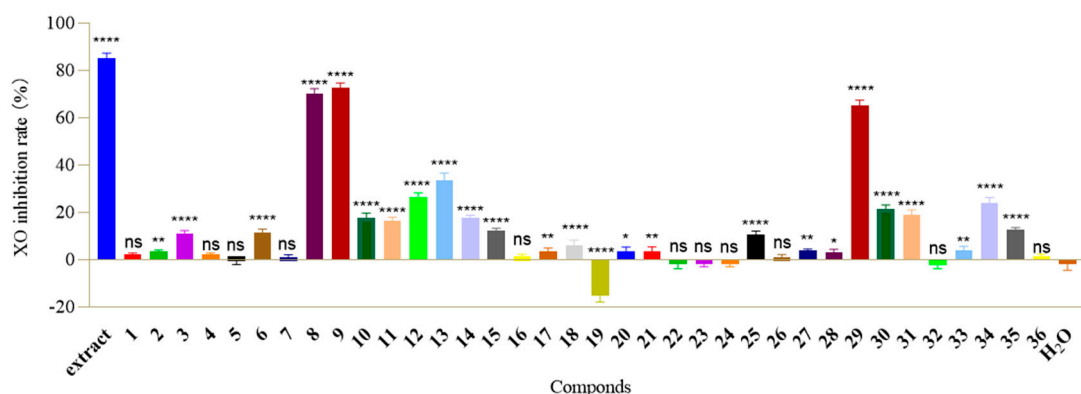


Figure S19 XO inhibitory activity of compounds compounds **1-36** and *C. strobilifer* extract at 0.2 mM. (n = 3, ns = nonsignificance, * $p < 0.01$, ** $p < 0.001$, **** $p < 0.00001$ compared to H_2O).

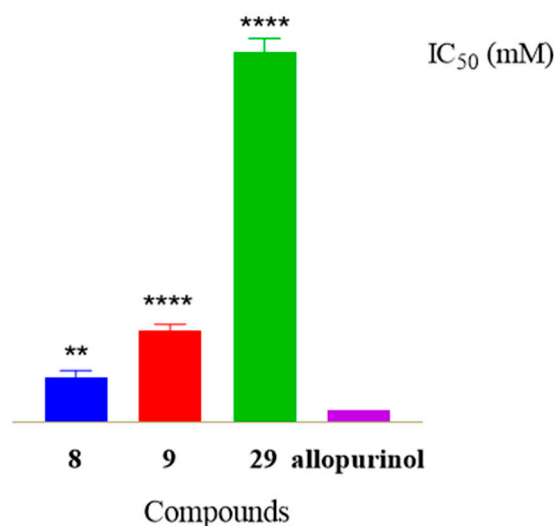


Figure S20 XO inhibitory activity of compounds **8**, **9**, **29** and allopurinol (n = 3; allopurinol was used as a positive control). (** $p < 0.001$, **** $p < 0.00001$ compared to allopurinol)

Table S1 XO inhibitory activity of compounds **1-36** and allopurinol

Compound	IC ₅₀ (mM) ^a
8	0.034 ± 0.004
9	0.067 ± 0.005
29	0.284 ± 0.01
others	> 0.3
Allopurinol ^b	0.009 ± 0.000117

^a IC₅₀ values were presented as means ± SD (n = 3). ^b Allopurinol was used as a positive control.

Determination of the content of compounds **8**, **9**, and **29** in *Coleus strobilifer*

Preparation of Samples

Coleus strobilifer (50 g) underwent dual reflux extractions with water and 70% ethanol (8× and 6× solvent volumes for 2 h and 1 h, respectively). Combined filtrates were concentrated *via* rotary evaporation and lyophilized to yield aqueous/ethanolic extracts. For analysis, 200 mg of extract was dissolved in methanol (10 mL volumetric flask), sonicated (30 min), adjusted to volume, filtered (0.22 µm), and the filtrate retained.

Preparation of Standard Solutions

An appropriate amount of apigenin (**8**), luteolin (**9**), and esculetin (**29**) reference standards was precisely weighed and dissolved in methanol to prepare a mixed standard solution containing 1 mg/mL of each compound.

High-performance liquid chromatography

This research was carried on a Waters UPLC system comprising a PDA detector. The chromatographic analysis was performed using an ACQUITY UPLC® HSS T3 column (2.1 mm × 100 mm, 1.8 µm) maintained at 30°C. The mobile phase comprised two components: (A) aqueous solution containing 0.2% acetic acid and (B) acetonitrile. Separation was achieved at a flow rate of 0.4 mL/min with UV detection

monitored at 340 nm. Samples were injected at a volume of 1 μ L using the following optimized gradient elution protocol: an elution ratio of 0-2 min, acetonitrile (10%~10%); 2-9 min, acetonitrile (10%~20%); 9-28 min, acetonitrile (20%~30%); 28-38 min, acetonitrile (30%~90%); 38-40 min, acetonitrile (90%~10%).

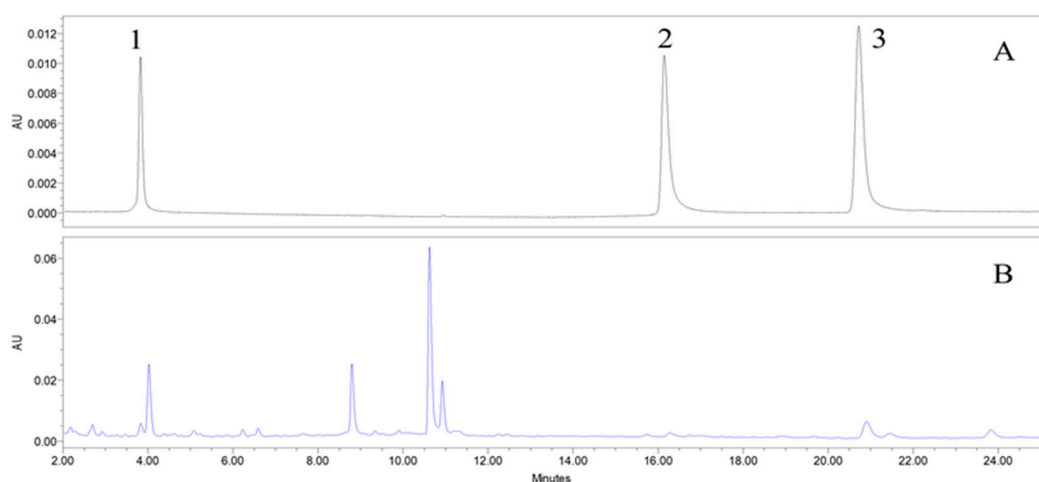
Establishment of the standard curve

The standard stock solution prepared above was serially diluted with methanol to obtain working solutions at concentrations of 0.625, 1.25, 2.5, 5, 10, and 20 μ g/mL. A linear calibration curve was constructed by plotting the peak areas against the corresponding concentrations of the injected solutions, and the regression equation was subsequently derived through statistical analysis.

Table S2 Analytical figures of merit by UPLC.

Analyte	Calibration relationship	Correlation coefficient	Linear dynamic range (μ g/mL)
8	$Y=8884X-3832.8$	0.9996	0.625~20
9	$Y=7040.1X-4366.6$	0.9985	0.625~20
29	$Y=3424X-1137.4$	0.9998	0.625~20

Result



Figure

Figure S21 UPLC of standards and samples (A- standard solution, B- sample solution, 1- esculetin (**29**), 2- luteolin (**9**), 3- apigenin (**8**)).

Table S3 The contents of **8**, **9**, and **29** in *C. strobilifer* extract (n = 2).

Samples	Content (8)	Content (9)	Content (29)
Water extract of <i>C. strobilifer</i> -1	/	/	0.0385%
Ethanol extract of <i>C. strobilifer</i> -1	0.0065%	0.0207%	0.0645%
Water extract of <i>C. strobilifer</i> -2	0.0098%	0.0048%	0.0276%
Ethanol extract of <i>C. strobilifer</i> -2	0.0397%	0.0121%	0.0272%

Table S4 XOD inhibitory activity of compounds **8**, **9**, **29**, and *C. strobilifer* extract.

Samples	Content (µg/mL)	XO inhibition rate
<i>C. strobilifer</i> extract	1000	90.1%
8	0.397	8.4%
9	0.207	5.3%
29	0.645	3.2%
Mixed solutions of 8 , 9 and 29	0.645+0.207+0.397	10.8%