Supporting Information

Rottlerin Derivatives and Other Compounds from *Mallotus philippinensis* Fruits and Their Potential Antimycobacterial Activity

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Fig. S1 $^1$H NMR of compound 1 (Chloroform $d$).

Fig. S2 $^{13}$C NMR of compound 1 (Chloroform $d$).
Fig. S3 DEPT NMR of compound 1 (Chloroform d).

Fig. S4 The key COSY ( ), HMBC ( ), and NOESY ( ) correlations of 1.
**Fig. S5** Dose-response curve for compound 11 against *Mycobacterium tuberculosis* H37Ra.

Antitubercular activity of compound 11 against Dormant *M.tuberculosis* H37Ra

![](image1)

- **MIC**: 2.06 µg/mL
- **IC₅₀**: 0.89 µg/mL

**Fig. S6** Dose-response curve of compound 12 against *Mycobacterium tuberculosis* H37Ra.

Antitubercular activity of compound 12 against Dormant *M.tuberculosis* H37Ra

![](image2)

- **MIC**: 11.56 µg/mL
- **IC₅₀**: 7.59 µg/mL
Extraction and Isolation of Compounds 1-13

Whole fruits obtained after extraction with acetone were dried under airflow and pulverized. The pulverized fruit powder, 1.2 kg, was extracted by a cold maceration technique with methanol (3 L × 3 × 14 h) at room temperature. After solvent evaporation at a reduced pressure, a red-brown extract (31.0 g, 2.58%, based on dry weight) was yielded.

Methanol extract, 30 g, was separated by CC (Column dimensions: length: 50 cm, width: 8 cm) on silica gel, 100-200 mesh, and acetone-petroleum ether gradient as an elution system to collect 49 fractions of 100 mL volume each. Fractions exhibiting a similar TLC pattern were combined to get 10 fractions (M1-M10).

Fraction M2, 2.5 g, was subjected to CC (length: 35 cm, width: 2.5 cm) with a gradient of acetone from 5% to 20% in petroleum ether to collect 11 fractions (M2a-M2k) of 20 mL volume each. Fractions M2e to M2h (94 mg) were combined and subjected to CC (length: 20 cm, width: 1.2 cm) using 5% acetone in petroleum ether as an elution system to collect six fractions (M2eh-1-M2eh-6) of 5 mL volume each. Fractions M2i to M2j (64 mg) were subjected to CC (length: 20 cm, width: 1 cm) using 5% acetone in petroleum ether as an elution system to collect five fractions (M2ij1-M2ij5) of 5 mL volume each. Fractions M2eh-1, M2eh-2, and M2ij3 were combined (80 mg) and acetylated using anhydrous acetic anhydride and pyridine, 2 mL, at room temperature for 24 h. The acetate mixture was separated by preparative TLC using 5% acetone in petroleum ether as a developing system to isolate 1 (20 mg), and a mixture of compounds 2 and 3. Compound 1 was purified further by crystallization from ethanol (1 mL) while a mixture of compounds 2 and 3 was separated by preparative TLC using 10% ethyl acetate in petroleum ether as a developing system to isolate compounds 2 (18 mg) and 3 (15 mg). Fraction M3, 1.9 g, was subjected to CC (length: 40 cm, width: 2.5 cm) using gradient acetone from 5% to 20% in petroleum ether as an elution system to collect 13 fractions (M3a-M3m) of 10 mL volume each. Fractions M3a to M3c (100 mg) were combined and subjected to crystallization using cyclohexane:acetone (80:20) to obtain crystals of compound 4 (12 mg). Fractions M3i to M3j (70 mg) were subjected to CC (length: 40 cm, width: 1.2 cm) using 5% acetone in petroleum ether as an elution system to collect eight fractions (M3ij1- M3ij8) of 5 mL volume each. Compound 4 (10 mg) precipitated from fraction M3ij5. Fraction M5, 3.2 g and fraction M6, 1.2 g, were separately subjected to CC (length: 50 cm, width: 3 cm) using gradient methanol from...
2% to 20% in chloroform as an eluting system to collect 17 fractions each (M5a-M5q and M6a-M6q, respectively) of 15 mL volume each. Fractions M5a (120 mg) and M5d (95 mg) were separately subjected to preparative TLC using methanol:chloroform (9:91) as a developing system to obtain compound 5 (20 mg). Fractions M6a-M6c were combined (105 mg) and subjected to CC (length: 40 cm, width: 1.2 cm) using gradient acetone in petroleum ether from 15% to 30% as an elution system to collect five fractions (M6ac1-M6ac5) of 5 mL volume each. Compound 6 (17 mg) was precipitated from fraction M6ac3. Fraction M7, 1.2 g, was subjected to CC (length: 45 cm, width: 1.5 cm) using gradient methanol from 2% to 20% in chloroform as an eluting system to collect 12 fractions (M7a–M7l) of 10 mL volume each. Fractions M7d (75 mg) and M7g (60 mg) were separately subjected to preparative TLC using methanol:chloroform (5:95) as a developing system to isolate compounds 7 (22 mg) and 8 (12 mg). Fraction M7i contained a solid compound that was crystallized from ethanol to obtain crystals of compound 9 (10 mg). Mother liquor from fraction M7i and fraction M6e (120 mg) were combined and subjected to CC (length: 50 cm, width: 1.2 cm) with gradient methanol from 2% to 20% in chloroform as an eluting system to collect 10 fractions (M7i6e1-M7i6e10) of 10 mL volume each. Fractions M7i6e3 to M7i6e7 were combined and subjected to preparative TLC using methanol:chloroform (3:97) as a developing system to isolate compounds 10 (5 mg) and 11 (10 mg) and a mixture of compounds 11 and 12 (27 mg). This mixture was subjected to preparative TLC in methanol:chloroform (5:95) to isolate compounds 12 (13 mg) and 11 (6 mg) along with small amounts of compound 10 (6 mg). Fractions M8, 400 mg, contained a solid compound that was subjected to successive washing using acetone and then methanol followed by hexane to yield compound 13 (18 mg).

NMR and Other Characterization Data of Compounds 1–13

7,11-Diketo-lanost-3-ol, acetate (1)
Gum; IR (CHCl₃): 3419, 2953, 1737, 1716, 1703, 1124, 1253 cm⁻¹; ¹H NMR (CDCl₃, 400 MHz) δ_H 0.72 (3H, s, H₃-18), 0.85 (3H, d, 6.0 Hz, H₃-21), 0.92 (3H, s, H₃-30), 0.87 (6H, d, 6.7 Hz, H₃-26, H₃-27), 1.21 (3H, s, H₃-28), 0.91 (3H, s, H₃-29), 1.10 (1H, m, H-1), 1.13 (2H, m, H-24), 1.17 (1H, m, H-22), 1.26 (1H, m, H-5), 1.30 (3H, s, H-19), 1.35 (1H, m, H-20), 1.36 (1H, m, H-22) 1.38 (1H, m, H-16), 1.42(1H, m, H-15), 1.53 (1H, sp, 6.9 Hz, H-25), 1.60 (1H, m, H-17), 1.73
(2H, m, H₂-2), 2.07 (3H, s, acetate), 2.08 (1H, m, H-16), 2.15 (1H, m, H-15), 2.22 (1H, d, 12.9 Hz, H-9), 2.33-2.35 (2H, d 5.3 Hz, H₂-6), 2.40-2.59 (2H, m, H₂-12), 2.67 (1H, d, 12.7 Hz, H-8), 2.87 (1H, dt, 13.4, 3.4 Hz, H-1), 4.51(1H, dd, 7.6, 5.6 Hz, H-3); ^13^C NMR (CDCl₃, 100 MHz) δC 13.7 (C-19), 16.0 (C-29), 16.1 (C-18), 17.5 (C-30), 18.4 (C-27), 21.2 (acetate, Me), 22.5 (C-26), 22.8 (C-21), 23.6 (C-2), 23.9 (C-22), 27.6 (C-28), 27.9 (C-25), 28.6 (C-16), 33.0 (C-15), 35.6 (C-1), 35.8 (C-20), 36.2 (C-23), 36.6 (C-10), 38.1 (C-4), 39.1 (C-6), 39.3 (C-24), 46.4 (C-14), 48.5 (C-17), 49.0 (C-13), 52.3 (C-5), 52.4 (C-12), 53.0 (C-8), 60.3 (C-9), 79.9 (C-3), 170.8 (acetate), 209.0 (C-7), 209.5 (C-11); LC-ESI-MS at m/z 501.02 [M + 1]^+ 539.01 [M + K]^+ (calculated for C₃₂H₅₂O₄, 500.76).

*Lanosta-8-ene-3β-ol, acetate (2)*

Gum; 18 mg; ^1^H NMR (CDCl₃, 400 MHz) δH 0.67 (3H, s, H-18), 0.87(3H, s, H-30), 0.88 (3H, s, H-28), 0.88 (3H, s, H-29), 0.91 (3H, d, 6.6 Hz, H-21), 1.02 (3H, s, H-19), 1.61 (3H, s, H-27), 1.69 (3H, s, H-26), 2.06 (3H, s, acetate), 4.51 (1H, dd, 11.7, 4.7 Hz, H-3), 5.11 (1H, t, 6.9 Hz, H-24); ^13^C NMR (CDCl₃, 100 MHz) δC 15.7 (C-18), 16.5 (C-29), 17.6 (C-27), 18.1 (C-6), 18.6 (C-21), 19.1 (C-19), 21.0 (C-11), 21.3 (acetate Me), 24.1 (C-2), 24.2 (C-30), 24.9 (C-23), 25.7 (C-26), 26.3 (C-7), 27.9 (C-28), 28.2 (C-16), 30.8 (C-15), 30.9 (C-12), 35.2 (C-1), 36.8 (C-10), 37.8 (C-4), 44.4 (C-13), 49.8 (C-14), 50.3 (C-17), 50.4 (C-5), 80.9 (C-3), 125.2 (C-24), 130.9 (C-25), 134.2 (C-9), 134.4 (C-8), 171.0 (acetate); LC-ESI-MS at m/z 507.29 [M + K]^+ (calculated for C₃₂H₅₄O₂, 468.77).

*Pregnenolone acetate (3)*

White amorphous solid; 15 mg; ^1^H NMR (CDCl₃, 500 MHz) δH 0.65 (3H, s, H-18), 1.04 (3H, s, H-19), 2.05 (3H, s, acetate), 2.14 (3H, s, H-21), 4.62 (1H, m, H-3), 5.40 (1H, d, H-6); ^13^C NMR (CDCl₃, 125 MHz) δC 13.2 (C-18), 19.3 (C-19), 21.0 (C-11), 21.4 (acetate), 22.8 (C-15), 24.5 (C-16), 27.7 (C-2), 31.5 (C-21), 31.7 (C-7), 31.8 (C-8), 36.6 (C-10), 37.0 (C-1), 38.0 (C-4), 38.8 (C-12), 44.0 (C-13), 49.9 (C-9), 56.8 (C-14), 63.7 (C-17), 73.8 (C-3), 122.3 (C-6), 139.7.2 (C-5), 170.5 (acetate), 209.6 (C-20); LC-ESI-MS at m/z 359.50 [M + 1]^+ (calculated for C₂₃H₄₄O₃,358.52).
**Trans-Chalcone (4)**

Yellow amorphous; 10 mg; IR: 1664, 1606, 1577 cm\(^{-1}\); \(^1\)H NMR (CDCl\(_3\), 500 MHz) \(\delta_H\) 7.44 (4H), 7.48 (1H, d, 16 Hz, H-2), 7.65-7.37 (2H), 7.85 (1H, d 16 Hz, H-3), 8.03-8.08 (3H, m); \(^1\)H NMR (CDCl\(_3\), 500 MHz) \(\delta_H\) 7.44 (4H), 7.48 (1H, d, 16 Hz, H-2), 7.65-7.37 (2H), 7.85 (1H, d 16 Hz, H-3), 8.03-8.08 (3H, m); \(^13\)C NMR (CDCl\(_3\), 125 MHz) \(\delta_C\) 122.0 (C-2), 128.39 (C-5/9, C-6/8, C-2'/6', C-3'/5'), 128.44 (C-5/9, C-6/8, C-2'/6', C-3'/5'), 128.6 (C-5/9, C-6/8, C-2'/6', C-3'/5'), 130.5 (C-7), 132.7 (C-4'), 134.8 (C-4), 138.1 (C-1'), 144.8 (C-3), 190.5 (C-1); LC-ESI-MS at \(m/z\) 209.00 [M + 1]\(^+\) (calculated for C\(_{15}\)H\(_{12}\)O, 208.26).

**Kamalachalcone E (5)**

Orange amorphous solid, 20 mg; UV \(\lambda_{max}\) (log \(\varepsilon\)) 270 (8.02), 380 (8.11) nm. \(^1\)H NMR (DMSO \(d_6\), 500 MHz) \(\delta_H\) 1.29 (3H, s, H-19'), 1.45 (3H, s, H-19), 1.50 (3H, s, H-20), 1.58 (3H, s, H-20'), 1.77 (3H, s, H-9''/H-9'''), 1.90 (1H, bs, H-17), 1.88 (3H, s, H-9''/H-9'''), 2.05 (1H, d, 9.58Hz, H-17), 2.20 (3H, s, H-8''), 2.23 (1H, bs, H-17'), 2.41 (3H, s, H-8''), 2.58 (1H, d 10.32Hz, H-16), 3.73 (2H, m, H-21'), 3.87 (2H, m, H-21), 4.84 (1H, s, H-16'), 6.86 (4H, bt, 8.14 Hz, H-12 and 14 or 12' and 14'), 7.56 (4H, bd, 8.14 Hz, H-11 and 15 or 11' and 15'), 7.72 (2H, d, 15.37 Hz, H-9 and H-9'), 7.83 (1H, d, 15.37 Hz, H-8), 7.89 (1H, d, 15.37 Hz, H-8'); \(^13\)C-NMR (DMSO \(d_6\), 125 MHz) \(\delta_C\) 7.9 (C-9''/C-9'''), 8.4 (C-9''/C-9'''), 15.9 (C-21), 16.2 (C-21'), 20.2 (C-19'), 24.2 (C-16), 26.6 (C-20), 27.9 (C-20'), 29.9 (C-19), 32.2 (C-8'''), 32.3 (C8''), 40.5 (C-17), 45.6 (C-17'), 70.5 (C-16'), 78.9 (C-18), 79.1 (C-18'), 100.2 (C-3'), 102.7 (C-5''/C-5''''), 103.1 (C-5'''/C-5'''), 103.4 (C-3/C-1''), 103.6 (C-3/C-1''), 104.8 (C-1'''), 104.9 (C-3'''), 105.7 (C-3'''), 106.1 (C-1) 107.0 (C-1'), 107.7 (C-5'), 108.1 (C-5), 116.2 (C-12 and 14/12' and 14'), 116.3 (C-12 and 14/12' and 14'), 123.1 (C-8'), 123.2 (C-8), 126.0 (C-10), 126.1 (C-10'), 130.6 (C-11 and 15/11' and 15'), 130.7 (C-11 and 15/11' and 15'), 143.4 (C-9'), 144.1 (C-9), 155.1 (C-2 and C-2'), 155.4 (C-4), 157.2 (C-2''), 158.4 (C-2'''/C-6'''/C-4'), 159.5 (C-2'''/C-6'''/C-4'), 159.8 (C-4''/C-4'''), 160.20 (C-6/C-6''/C-13/C-13'), 160.22 (C-6/C-6'' and C-13/C-13'), 160.3 (C-2'''/C-6'''/C-4'), 160.5 (C-13/C-13'), 159.6 (C-4''/4'''), 164.3 (C-6'), 191.0 (C-7'), 192.9 (C-7), 203.3 (C-7') and 203.5(C7'''); LC-ESI-MS at \(m/z\) 1087.33 [M + Na]\(^+\) (calculated for C\(_{60}\)H\(_{59}\)O\(_{18}\)Na, 1087.33).
**Oleanolic acid (6)**

White amorphous solid; 17 mg; IR (ATR) 1688, cm\(^{-1}\); \(^1\)H NMR (pyridine \(d_5\), 500 MHz) \(\delta_H\) 0.91 (3H, s, H-25), 0.97 (3H, d, 6 Hz, H-30), 1.05 (3H, s, H-26), 1.08 (3H, s, H-24), 1.025 (3H, d, 6 Hz, H-29), 1.24 (3H, s, H-23), 1.27 (3H, s, H-27), 5.51 (1H, m, H-12); \(^{13}\)C NMR (pyridine \(d_5\), 125 MHz) \(\delta_C\) 15.7 (C-25), 16.6 (C-24), 17.5 (C-29), 17.6 (C-26), 18.8 (C-6), 21.5 (C-30), 23.7 (C-11), 24.0 (C-27), 25.0 (C-16), 28.2 (C-2), 28.8 (C-15), 28.84 (C-23), 31.1 (C-21), 33.6 (C-7), 37.47 (C-10), 37.48 (C-22), 39.1 (C-1), 39.4 (C-20), 39.5 (C-19), 40.0 (C-8), 42.5 (C-14), 48.1 (C-9), 48.1 (C-17), 53.6 (C-18), 55.8 (C-5), 78.2 (C-3), 125.7 (C-12), 139.3 (C-13), 39.51 (C-4), 179.9 (C-28); LC-ESI-MS at \(m/z\) 479.28 [M + Na]\(^+\), \(m/z\) 495.30 [M + K]\(^+\) (calculated for \(C_{30}H_{48}O_3\), 456.30).

**Gallic acid (7)**

White crystals; m. p. 258-260\(^\circ\)C; 22 mg; \(^1\)H NMR (CDCl\(_3\), 500 MHz) \(\delta_H\) 7.06 (2H, s, H-2, H-6); \(^{13}\)C NMR (CDCl\(_3\), 125 MHz) \(\delta_C\) 110.3 (C-6), 121.9 (C-1), 139.6 (C-4), 146.4 (C-3, C-5), 170.4 (C-7); LC-ESI-MS at \(m/z\) 170.98 [M + 1]\(^+\) (calculated for \(C_7H_6O_5\), 170.00).

**Kaempferol (8)**

Yellow amorphous solid; 12 mg; \(^1\)H NMR (methanol-\(d_4\), 400 MHz) \(\delta_H\) 6.17 (d, \(J = 1.83\) Hz, 1 H), 6.38 (d, \(J = 1.83\) Hz, 1 H), 6.90 (d, \(J = 9.16\) Hz, 2 H), 8.07 (d, \(J = 9.16\) Hz, 2 H); \(^{13}\)C NMR (methanol-\(d_4\), 100 MHz) \(\delta_C\) 94.4 (C-6), 99.2 (C-8), 104.5 (C-10), 116.3 (C-2’, C-6’), 123.7 (C-1’), 130.7 (C-3’, C-5’), 137.1 (C-4’), 148.0 (C-3), 158.2 (C-2), 160.5 (C-9), 162.5 (C-5), 165.4 (C-7), 177.3 (C-4); LC-ESI-MS at \(m/z\) 309.00 [M + Na]\(^+\) (calculated for \(C_{15}H_{10}O_6\), 286.05).

**Myricetin (9)**

Yellow amorphous solid; 10 mg; \(^1\)H NMR (methanol-\(d_4\), 400 MHz) \(\delta_H\) 6.18 (d, \(J = 1.83\) Hz, 1 H) 6.37 (d, \(J = 1.83\) Hz, 1 H) 7.34 (s, 2H); \(^{13}\)C NMR (methanol-\(d_4\), 100 MHz) \(\delta_C\) 94.3 (C-6), 99.2 (C-8), 104.5 (C-10), 108.5 (C-2’, C-6’), 123.1 (C-1’), 136.9 (C-4’), 137.4 (C-3), 146.7 (C-3’, C-5’), 148.0 (C-2), 158.2 (C-9), 162.5 (C-5), 165.6 (C-7), 177.3 (C-4); LC-ESI-MS at \(m/z\) 319.20 [M + 1]\(^+\) (calculated for \(C_{15}H_{10}O_8\), 318.24).
1-(5,7-Dihydroxy-2,2,6-trimethyl-2H-1-benzopyran-8-yl)-3-phenyl-2-propen-1-one (10)
Orange amorphous solid; 6 mg; UV $\lambda_{\text{max}}$ (log $\varepsilon$) 220 (5.63), 240 (6.54), 340 (6.58) nm; $^1$H NMR, (CDCl$_3$, 200 MHz) $\delta_H$ 1.56 (6H, s, H-21 and H-22), 2.10 (3H, s, H-20), 5.52 (1H, d, $J = 9.85$ Hz, H-3), 6.62 (1H, d, $J = 9.85$ Hz, H-4), 7.40-7.48 (3H, m, H-15, 17 and 19), 7.60-7.64 (2H, m, H-16 and 18), 7.78 (1H, d, $J = 15.51$ Hz, H-12), 8.15 (1H, d, $J = 15.51$ Hz, H-13), 14.40 (1H, s, OH). $^{13}$C NMR (CDCl$_3$, 50 MHz), $\delta_C$ 7.1 (C-20), 27.8 (C-21 and 22), 77.0 (C-2), 101.8 (C-21'), 102.4 (C-20'), 106.3 (C-16), 116.6 (C-4), 125.2 (C-3), 127.7 (C-13), 128.2 (C-15, C-19), 128.9 (C-16, C-18), 130.0 (C-17), 135.6 (C-14), 142.1 (C-13), 154.4 (C-9), 156.0 (C-5), 164.2 (C-7), 193.1 (C-11); LC-ESI-MS at $m/z$ 337.30 [M + 1]$^+$ (calculated for C$_{21}$H$_{20}$O$_4$, 336.39).

4'-Hydroxyisorottlerin (11)
Dark reddish powder; [$\alpha$]$^26_D$ -12.11 (c 0.66, Chloroform); $^1$H NMR (CDCl$_3$, 500 MHz) $\delta_H$ 1.59 (3H, s, H-21, H-14), 1.63 (3H, s, H-15, H-22), 2.01 (3H, s, H-9'''), 2.55 (3H, s, H-8''), 2.85 (1H, dd, $J = 17.2$, 2.7 Hz, H-3), 3.25 - 3.39 (1H, m, H-3), 3.64 (2H, s, H-16), 5.48 (1H, dd, $J = 13.0$, 2.3 Hz, H-2), 5.62 (1H, d, $J = 9.9$ Hz, H-12), 6.69 (1H, d, $J = 10.9$ Hz, H-11), 6.97 (2H, d, $J = 8.4$ Hz, H-3', H-5'), 7.42 (2H, d, $J = 8.4$ Hz, H-2', H-6''), 7.75 (1H, s, OH) 7.88 (1H, s, OH) 12.31 (1H, s, OH) 13.72 (1H, s, 5-OH); $^{13}$C NMR (CDCl$_3$, 125 MHz) $\delta_C$ 7.6 (C-9''), 16.6 (C-16), 27.8 (C-14), 27.9 (C-15), 33.1 (C-8''), 42.7 (C-3), 81.3 (C-2), 81.5 (C-13), 103.1 (C-6), 103.2 (C-5'''), 104.1 (C-10), 104.6 (C-1''), 105.5 (C-3'''), 106.1 (C-8), 115.6 (C-11), 116.0 (C-3', C-5'), 126.4 (C-12), 127.9 (C), 129.0 (C-2', C-6'), 156.2 (C-5), 157.4 (C-2'''), 157.5 (C-7), 158.0 (C-9), 159.7 (C-6''), 162.4 (C-4''), 196.2 (C-4), 204.0 (C-7'''); LC-ESI-MS at $m/z$ 533.40 [M + 1]$^+$ (calculated for C$_{30}$H$_{28}$O$_9$, 532.54).

Rottlerin (12)
Dark reddish powder; $^1$H NMR (CDCl$_3$, 500 MHz) $\delta_H$ 1.55 (6H, s, H-21, H-22), 2.10 (3H, s, H-9''), 2.73 (3H, s, H-8''), 3.83 (2H, s, H-20), 5.50 (1H, d, $J = 9.9$ Hz, H-4), 6.68 (1H, d, $J = 9.9$ Hz, H-3), 7.40 - 7.48 (3H, m, H-16, H-17, H-18), 7.63 (2H, dd, $J = 7.3$, 1.9 Hz, H-15, H-19), 7.85 (1H, d, $J = 16.0$ Hz, H-13), 8.21 (1H, d, $J = 16.0$ Hz, H-12), 16.53 (1H, s, 5-OH); $^{13}$C NMR (CDCl$_3$, 125 MHz) $\delta_C$ 7.5 (C-9''), 15.8 (C-20), 28.0 (C-21, C-22), 32.6 (C-8''), 78.2 (C-2), 101.9 (C-10/C-5''), 103.7 (C-10/C-5''), 105.3 (C-1'', C-3''), 106.0 (C-8), 106.5 (C-6), 117.2 (C-4), 125.1 (C-3), 126.8 (C-8), 128.4 (C-16, C-18/C-15, C-19), 129.0 (C-16, C-18/C-15, C-19), 130.4 (C-...
17), 135.4 (C-14), 143.3 (C-13), 155.4 (C-9), 158.8 (C-5, C-2’), 159.6 (C-4’, C-6’), 162.8 (C-7), 192.9 (C-11), 204.1 (C-7’); LC-ESI-MS at \( m/z \) 539.45 [M + Na]\(^+\) (calculated for \( \text{C}_{30}\text{H}_{28}\text{O}_8 \), 516.55).

**Shikimic acid (13)**

White amorphous solid, 18 mg; \(^1\)H NMR (CDCl\(_3\), 500 MHz) \( \delta_H \) 2.20 (1H, m), 2.70 (1H, m), 3.80 4.00 (1H, m), 4.40 (1H, m), 6.90 (1H, m); \(^{13}\)C NMR (CDCl\(_3\), 125 MHz) \( \delta_C \) 132.2 (C-1), 142.3 (C-2), 69.0 (C-3), 65.3 (C-4), 67.2 (C-5), 28.1 (C-6), 171.2 (C-7); LC-ESI-MS at \( m/z \) 197.10 [M + Na]\(^+\) (calculated for \( \text{C}_7\text{H}_{10}\text{O}_5 \), 174.15).