Supplementary Materials

Rare Chromone Derivatives from the Marine-Derived Penicillium citrinum with Anti-Cancer and Anti-Inflammatory Activities

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| Mass       | Intensity | Calc. Mass | Mass Difference [mDa] | Mass Difference [ppm] | Possible Formula          |
|------------|-----------|------------|-----------------------|-----------------------|--------------------------|
| 599.11558  | 16867.59  | 599.11654  | -0.96                 | -1.60                 | \(^{12}\text{C}_{30}{^{1}\text{H}}_{53}{^{25}\text{Na}}_{1}{^{16}\text{O}}_{12}\) |

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Figure S34. CD spectrum of 4.
Figure S35. HRESIMS spectrum of 5.

| Mass      | Intensity | Calc. Mass | Mass Difference [mDa] | Mass Difference [ppm] | Possible Formula |
|-----------|-----------|------------|------------------------|------------------------|------------------|
| 381.17094 | 17911.35  | 381.17020  | 0.74                   | 1.94                   | $^{12}$C$_{25}$H$_{55}$O$_{5}$ |

Figure S36. $^1$H NMR spectrum (CDCl$_3$, 600 MHz) of 5.
Figure S37. HRESIMS spectrum of 6.

Figure S38. $^1$H NMR spectrum (CDCl$_3$, 600 MHz) of 6.
Figure S39. HRESIMS spectrum of 7.

| Mass    | Intensity | Calc. Mass | Mass Difference [mDa] | Mass Difference [ppm] | Possible Formula |
|---------|-----------|------------|------------------------|------------------------|------------------|
| 247.09688 | 2701.97   | 247.09703  | -0.16                  | -0.64                  | $^{12}$C$_4$H$_8$O$_4$ |

Figure S40. $^1$H NMR spectrum (CDCl$_3$, 600 MHz) of 7.
Figure S41. CD and ECD spectra of epiremisporine B.

Table S1. $^1$H NMR spectrum of 4 and epiremisporine B.

| Position | 4 (2'S) | 4 (2'R) | epiremisporine B (2'S) | epiremisporine B (2'R) |
|----------|---------|---------|------------------------|------------------------|
|          | δH (J in Hz) |         | δH (J in Hz) |         | δH (J in Hz) |         | δH (J in Hz) |         |
| 3        | 3.92 (t, 9.0) | 3.88 (dd, 9.0, 8.3) | 3.78 (dd, 9.2, 9.0) | 3.88 (dd, 9.0, 8.4) |
| 4        | 5.19 (d, 9.0) | 5.21 (d, 9.0) | 4.98 (d, 9.0) | 5.02 (d, 9.0) |
| 8        | 6.68 (br s) | 6.69 (br s) | 6.79 (s) | 6.77 (s) |
| 10       | 6.60 (br s) | 6.61 (br s) | 6.64 (s) | 6.64 (s) |
| 15       | 2.33 (s) | 2.33 (s) | 2.30 (s) | 2.28 (s) |
| 16       | 3.79 (s) | 3.83 (s) | 3.69 (s) | 3.70 (s) |
| 3'       | 3.02 (ddd, 11.7, 9.0, 5.9) | 2.92 (ddd, 12.7, 8.3, 5.4) | 3.10 (ddd, 10.1, 9.2, 6.4) | 2.79 (ddddd, 12.5, 8.4, 5.9) |
| 4'α      | 2.87 (dd, 16.8, 5.9) | 2.82 (dd, 16.0, 5.4) | 2.70 (dd, 17.0, 6.4) | 2.48 (dd, 15.9, 5.9) |
| 4'β      | 2.62 (dd, 16.8, 11.7) | 2.46 (dd, 16.0, 12.7) | 2.64 (dd, 17.0, 10.1) | 2.43 (dd, 15.9, 12.4) |
| 8'       | 6.71 (br s) | 6.70 (br s) | 6.90 (s) | 6.88 (s) |
| 10'      | 6.70 (br s) | 6.70 (br s) | 6.71 (s) | 6.71 (s) |
| 15'      | 2.42 (s) | 2.42 (s) | 2.38 (s) | 2.38 (s) |
| 16'      | 3.88 (s) | 3.86 (s) | 3.74 (s) | 3.75 (s) |
| 11-OH    | 12.04 (s) | 12.00 (s) | 12.15 (s) | 12.12 (s) |
| 2'-OH    | 4.65 (br s) | 4.41 (br s) | 7.80 (s) | 7.53 (s) |
| 11'-OH   | 12.34 (s) | 12.29 (s) | 12.49 (s) | 12.47 (s) |

* Recorded in CDCl$_3$ at 500 MHz.

* Recorded in DMSO-$d_6$ at 600 MHz.
Table S2. $^{13}$C NMR spectrum of 4 and epiremisporine B.

| Position | 4 (2'S) $^a$ | 4 (2'R) $^a$ | epiremisporine B (2'S) $^b$ | epiremisporine B (2'R) $^b$ |
|----------|-------------|-------------|----------------------------|----------------------------|
| δ, Type  | C           | C           | C                          | C                          |
| 1        | 171.0, C    | 172.3, C    | 170.8, C                   | 171.3, C                   |
| 2        | 88.7, C     | 90.7, C     | 88.2, C                    | 89.5, C                    |
| 3        | 48.3, CH    | 48.2, CH    | 47.0, CH                   | 46.6, CH                   |
| 4        | 37.1, CH    | 36.4, CH    | 36.9, CH                   | 36.2, CH                   |
| 5        | 168.8, C    | 168.6, C    | 169.3, C                   | 168.9, C                   |
| 6        | 157.3, C    | 157.2, C    | 156.8, C                   | 156.8, C                   |
| 7        | 108.3, CH   | 108.3, CH   | 108.3, CH                  | 108.3, CH                  |
| 8        | 147.3, C    | 147.5, C    | 147.5, C                   | 147.5, C                   |
| 9        | 113.1, CH   | 113.2, CH   | 112.3, CH                  | 112.3, CH                  |
| 10       | 160.4, C    | 160.8, C    | 159.9, C                   | 159.9, C                   |
| 11       | 108.9, C    | 108.9, C    | 108.4, C                   | 108.4, C                   |
| 12       | 179.1, C    | 179.0, C    | 178.9, C                   | 178.9, C                   |
| 13       | 119.2, C    | 118.5, C    | 119.2, C                   | 118.7, C                   |
| 14       | 22.2, CH₃   | 22.2, CH₃   | 21.5, CH₃                  | 21.4, CH₃                  |
| 15       | 53.2, CH₃   | 53.6, CH₃   | 52.8, CH₃                  | 52.6, CH₃                  |
| 16       | 169.4, C    | 167.3, C    | 169.4, C                   | 167.7, C                   |
| 17       | 104.8, C    | 105.9, C    | 105.7, C                   | 106.2, C                   |
| 18       | 43.4, CH    | 47.1, CH    | 42.7, CH                   | 47.3, CH                   |
| 19       | 26.3, CH₂   | 27.5, CH₂   | 26.3, CH₂                  | 26.9, CH₂                  |
| 20       | 166.7, C    | 166.0, C    | 168.0, C                   | 167.4, C                   |
| 21       | 156.1, C    | 156.1, C    | 155.5, C                   | 155.6, C                   |
| 22       | 107.6, CH   | 107.6, CH   | 107.6, CH                  | 107.6, CH                  |
| 23       | 147.5, C    | 147.7, C    | 147.4, C                   | 147.4, C                   |
| 24       | 112.6, CH   | 112.6, CH   | 112.0, CH                  | 112.0, CH                  |
| 25       | 160.4, C    | 160.8, C    | 159.5, C                   | 159.6, C                   |
| 26       | 108.4, C    | 108.5, C    | 107.7, C                   | 107.8, C                   |
| 27       | 179.8, C    | 179.7, C    | 179.4, C                   | 179.3, C                   |
| 28       | 112.6, C    | 112.4, C    | 111.9, C                   | 111.7, C                   |
| 29       | 22.4, CH₃   | 22.4, CH₃   | 21.8, CH₃                  | 21.8, CH₃                  |
| 30       | 53.3, CH₃   | 53.1, CH₃   | 52.3, CH₃                  | 52.3, CH₃                  |

$^a$ Recorded in CDCl₃ at 125 MHz. $^b$ Recorded in DMSO-d₆ at 150 MHz.
Table S3. The ROESY correlations for compounds 1–3.

| Position | 1<sup>a</sup> | 2<sup>a</sup> | 3<sup>a</sup> |
|----------|--------------|--------------|--------------|
| 3        | 4, 16, 3', 4'α | 4, 16, 3', 4'α | 4, 16, 3', 4'α |
| 4        | 3            | 3            | 3            |
| 8        | 15           | 15           | 15           |
| 10       | 15           | 15, 11-OMe   | 15, 11-OMe   |
| 15       | 8, 10        | 8, 10        | 8, 10        |
| 16       | 3            | 3            | 3            |
| 3'       | 3, 4'α, 4'β, 2'-OMe | 3, 4'α, 4'β, 2'-OMe | 3, 4'α, 4'β   |
| 4'α      | 3, 3', 4'β   | 3, 3', 4'β   | 3, 3', 4'β   |
| 4'β      | 3', 4'α      | 3', 4'α      | 3', 4'α, 2'-OMe |
| 8'       | 15'          | 15'          | 15'          |
| 10'      | 15'          | 15'          | 11'-OH, 15'  |
| 15'      | 8', 10'      | 8', 10'      | 8', 10'      |
| 11-OMe   |              | 10           | 10           |
| 2'-OMe   | 3'           | 3'           | 4'β          |
| 11'-OH   |              |              | 10'          |

<sup>a</sup> Recorded in CDCl<sub>3</sub> at 500 MHz.