

## Pentacyclic Triterpenoid Esters from the Fruits of *Bruguiera cylindrica*

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Six new pentacyclic triterpenoid esters (**1–6**) together with 3 $\alpha$ - and 3 $\beta$ -taraxerol were isolated from the fruits of *Bruguiera cylindrica*. The structures of the new compounds were characterized as 3 $\alpha$ -*E*-feruloyltaraxerol (**1**), 3 $\alpha$ -*Z*-feruloyltaraxerol (**2**), 3 $\beta$ -*E*-feruloyltaraxerol (**3**), 3 $\beta$ -*Z*-feruloyltaraxerol (**4**), 3 $\alpha$ -*E*-coumaroyltaraxerol (**5**), and 3 $\alpha$ -*Z*-coumaroyltaraxerol (**6**), respectively. Compounds **2** and **6** exhibited weak cytotoxicity against the NCI-H187 cell line.

*Bruguiera cylindrica* Blume (Rhizophoraceae), a mangrove plant, is distributed in Southeast Asia. This plant has been used by the local Thai people in folk medicine for the treatment of diarrhea and the healing of wounds.<sup>1</sup> An ethanolic extract of the leaves has shown antiviral activity.<sup>2</sup> In a previous report, Kato et al. isolated several sulfur-containing compounds from the CHCl<sub>3</sub> extract of the stem bark.<sup>3</sup> As part of our continuing chemical studies on Thai medicinal mangrove plants,<sup>4–6</sup> we report herein the isolation and structural elucidation of six new triterpene esters along with two known compounds, 3 $\alpha$ - and 3 $\beta$ -taraxerol,<sup>7</sup> from the hexane extract as well as the evaluation of the cytotoxicity of the new compounds.

Compound **1** was obtained as a white solid with a molecular formula of C<sub>40</sub>H<sub>58</sub>O<sub>4</sub>, on the basis of the [M – H]<sup>–</sup> ion at *m/z* 601.4242 in the ESITOFMS (calcd *m/z* 601.4256). The IR spectrum exhibited absorption bands at 3438 (hydroxy), 1705, 1684 (carbonyl), and 1635, 1605 (aromatic ring) cm<sup>–1</sup>, which together with the UV spectrum ( $\lambda_{\text{max}}$  228, 300, and 326 nm) was consistent with the presence of a substituted cinnamoyl chromophore. The <sup>13</sup>C NMR spectrum of **1** (Table 2) showed 40 signals, attributable to eight methyls, one methoxy group, 10 methylenes, 10 methines, and 11 quaternary carbons, as determined by a DEPT experiment. It was deduced to be a triterpenoid through a purple vanillin-sulfuric acid test and the appearance of seven three-proton singlets of eight methyl groups at  $\delta$  0.83, 0.89, 0.91, 0.95, 0.95, 0.96, 0.98, and 1.12 in the <sup>1</sup>H NMR spectrum (Table 1). The signal of one olefinic proton at  $\delta$  5.57 (dd, *J* = 3, 8 Hz) together with <sup>13</sup>C NMR signals of C-14 ( $\delta$  158.5) and C-15 ( $\delta$  116.2) suggested a taraxerane moiety.<sup>7,8</sup> The <sup>1</sup>H NMR spectrum also exhibited two olefinic signals that were characteristic of a *trans* double bond at  $\delta$  6.32 (1H, d, *J* = 16 Hz, H-2') and 7.59 (1H, d, *J* = 16 Hz, H-3') and three aromatic protons (a typical pattern of 1,2,4-trisubstituted benzene) at  $\delta$  7.08 (1H, dd, *J* = 1.5, 8 Hz, H-9'), 7.06 (1H, d, *J* = 1.5 Hz, H-5'), and 6.91 (1H, d, *J* = 8 Hz, H-8'). <sup>13</sup>C NMR signals from the HMQC spectrum confirmed the assignments at  $\delta$  116.8

(C-2'), 144.4 (C-3'), 123.2 (C-9'), 109.1 (C-5'), and 114.6 (C-8'). This ester substituent, characterized as a feruloyloxy group,<sup>9,10</sup> was placed at C-3 in the axial position because of the downfield effect observed on H-3 with a small coupling constant at  $\delta$  4.76 (t, *J* = 2.5 Hz)<sup>7</sup> and an observed HMBC cross-peak between H-3 and C-1' at  $\delta$  167.0. Thus, compound **1** was identified as 3 $\alpha$ -*E*-feruloyltaraxerol. Additional HMBC spectral data are summarized in Table S1 (Supporting Information).

Compound **2**, a white solid, showed a molecular ion peak at *m/z* 601.4247 [M – H]<sup>–</sup> in the ESITOFMS (calcd *m/z* 601.4256), corresponding to a molecular formula of C<sub>40</sub>H<sub>58</sub>O<sub>4</sub>. The UV and IR spectra of **2** exhibited the same patterns as those of **1**. The <sup>1</sup>H NMR spectrum of **2** (Table 1) was similar to that of **1**, but differed in the downfield shift of H-5', which was at  $\delta$  7.76 instead of  $\delta$  7.06 because of an anisotropic effect of the carbonyl group. The presence of two olefinic protons at  $\delta$  5.86 (H-2') and 6.76 (H-3') with a mutual coupling (*J* = 13 Hz) was consistent with a *cis* configuration of the ester group.<sup>11–14</sup> Thus, compound **2**, a geometric isomer of **1**, was assigned as 3 $\alpha$ -*Z*-feruloyltaraxerol. Its absolute configuration has been confirmed by X-ray crystallography.<sup>15</sup>

Compound **3** was obtained as a white solid, for which the molecular formula of C<sub>40</sub>H<sub>58</sub>O<sub>4</sub> was inferred by ESITOFMS (*m/z* 601.4269 [M – H]<sup>–</sup>, calcd 601.4256). The <sup>1</sup>H and <sup>13</sup>C NMR spectra of **3** (Tables 1 and 2) were similar to those of **1**, except that the splitting pattern of H-3 at  $\delta$  4.60 was a doublet of doublets (*J* = 5.5, 11 Hz) instead of a triplet at  $\delta$  4.76 (*J* = 2.5 Hz).<sup>7</sup> The difference in the multiplicity with a larger coupling constant of H-3 in **3** was in agreement with the respective coupling pattern (axial–equatorial and axial–axial) of H-3 and H<sub>2</sub>-2, indicating that H-3 is situated in an axial position. The HMBC spectrum of **3** (Table S1, Supporting Information) showed a long-range correlation between C-1' at  $\delta$  167.1 and H-3 ( $\delta$  4.60) and both vinyl protons, H-2' ( $\delta$  6.28) and H-3' ( $\delta$  7.58). Thus, **3** was determined as 3 $\beta$ -*E*-feruloyltaraxerol, an epimer of **1**.

Compound **4**, detected as a minor component in the <sup>1</sup>H NMR spectrum of **3**, was postulated as 3 $\beta$ -*Z*-feruloyltaraxerol by comparison of the multiplicity and coupling con-

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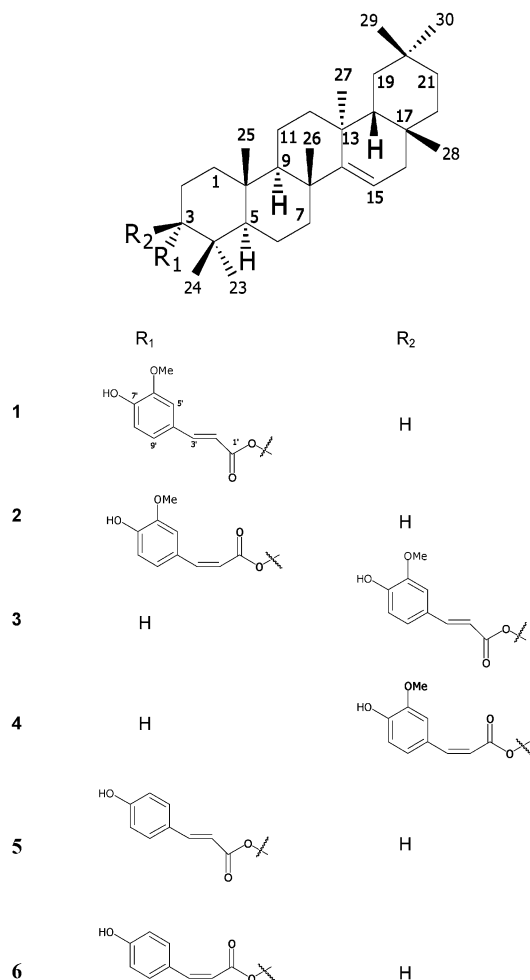
<sup>‡</sup> Walailak University.

**Table 1.**  $^1\text{H}$  NMR Data of Compounds 1–6

| position | 1                | 2                | 3                 | 4 <sup>a</sup>    | 5              | 6                  |
|----------|------------------|------------------|-------------------|-------------------|----------------|--------------------|
| 1        | 0.98 m, 1.30 m   | 0.98 m, 1.32 m   | 0.94 m, 1.30 m    |                   | 0.98 m, 1.32 m | 0.98 m, 1.32 m     |
| 2        | 1.62 m, 1.90 m   | 1.60 m, 1.88 m   | 1.68 m            |                   | 1.60 m, 1.86 m | 1.64 m, 1.92 m     |
| 3        | 4.76 t (2.5)     | 4.70 t (2.5)     | 4.60 dd (5.5, 11) | 4.53 dd (5.5, 11) | 4.75 t (3)     | 4.71 dd (2.5, 5.5) |
| 5        | 1.36 m           | 1.28 m           | 0.92 m            |                   | 1.20 m         | 1.36 m             |
| 6        | 1.42 m, 1.54 m   | 1.42 m, 1.50 m   | 1.48 m, 1.62 m    |                   | 1.48 m, 1.68 m | 1.66 m             |
| 7        | 1.50 m, 1.62 m   | 1.54 m, 1.62 m   | 1.50 m, 1.62 m    |                   | 1.62 m         | 1.62 m             |
| 9        | 0.98 m           | 0.96 m           | 0.94 m            |                   | 0.94 m         | 0.96 m             |
| 11       | 1.48 m, 1.64 m   | 1.46 m, 1.62 m   | 1.42 m, 1.62 m    |                   | 1.34 m         | 1.48 m             |
| 12       | 1.02 m, 1.38 m   | 1.00 m, 1.38 m   | 1.03 m, 1.34 m    |                   | 1.02 m, 1.34 m | 1.03 m, 1.34 m     |
| 15       | 5.57 dd (3, 8)   | 5.55 dd (3.5, 8) | 5.54 dd (2, 9)    | 5.53 dd (2, 9)    | 5.56 dd (3, 8) | 5.56 dd (3, 8)     |
| 16       | 1.64 m, 1.92 m   | 1.64 m, 1.92 m   | 1.62 m, 1.90 m    |                   | 1.68 m, 1.92 m | 1.64 m, 1.94 m     |
| 18       | 1.58 m           | 1.50 m           | 1.46 m            |                   | 1.46 m         | 1.55 m             |
| 19       | 1.44 m, 2.04 m   | 1.38 m, 2.02 m   | 1.34 m, 2.02 m    |                   | 1.40 m, 2.00 m | 1.44 m, 2.04 m     |
| 21       | 1.24 m           | 1.24 m           | 1.24 m            |                   | 1.24 m         | 1.22 m             |
| 22       | 1.36 m           | 1.34 m           | 1.34 m            |                   | 1.36 m         | 1.38 m             |
| 23       | 0.89 s           | 0.85 s           | 0.91 s            |                   | 0.88 s         | 0.83 s             |
| 24       | 0.95 s           | 0.94 s           | 0.96 s            |                   | 0.96 s         | 0.96 s             |
| 25       | 0.98 s           | 0.94 s           | 0.98 s            |                   | 0.97 s         | 0.94 s             |
| 26       | 1.12 s           | 1.09 s           | 1.10 s            |                   | 1.11 s         | 1.09 s             |
| 27       | 0.95 s           | 0.95 s           | 0.91 s            |                   | 0.94 s         | 0.91 s             |
| 28       | 0.83 s           | 0.82 s           | 0.82 s            |                   | 0.83 s         | 0.83 s             |
| 29       | 0.96 s           | 0.92 s           | 0.95 s            |                   | 0.96 s         | 0.96 s             |
| 30       | 0.91 s           | 0.91 s           | 0.91 s            |                   | 0.91 s         | 0.91 s             |
| 2'       | 6.32 d (16)      | 5.86 d (13)      | 6.28 d (16)       | 5.82 d (13)       | 6.35 d (16)    | 5.81 d (13)        |
| 3'       | 7.59 d (16)      | 6.76 d (13)      | 7.58 d (16)       | 6.77 d (13)       | 7.60 d (16)    | 6.85 d (13)        |
| 5'       | 7.06 d (1.5)     | 7.76 d (1.5)     | 7.03 d (2)        | 7.78 d (2)        | 7.45 d (8.5)   | 7.60 d (8.5)       |
| 6'       |                  |                  |                   |                   | 6.83 d (8.5)   | 6.79 d (8.5)       |
| 8'       | 6.91 d (8)       | 6.86 d (8)       | 6.91 d (8.5)      | 6.87 d (8)        | 6.83 d (8.5)   | 6.79 d (8.5)       |
| 9'       | 7.08 dd (1.5, 8) | 7.10 dd (1.5, 8) | 7.07 dd (2, 8.5)  | 7.11 dd (8, 2)    | 7.45 d (8.5)   | 7.60 d (8.5)       |
| -OMe     | 3.95 s           | 3.91 s           | 3.93 s            | 3.92 s            |                |                    |

<sup>a</sup> Only partial  $^1\text{H}$  NMR data of compound 4 are reported.

stants to those of 1–3. Efforts to separate compounds 3 and 4 were unsuccessful.



Compounds 5 and 6 were both obtained as viscous colorless oils. Their  $^1\text{H}$  NMR spectra (Table 1) showed

**Table 2.**  $^{13}\text{C}$  NMR Spectral Data of Compounds 1–3, 5, and 6

| position | 1     | 2     | 3     | 5     | 6     | DEPT <sup>a</sup> |
|----------|-------|-------|-------|-------|-------|-------------------|
| 1        | 36.6  | 36.6  | 37.4  | 36.6  | 36.7  | CH <sub>2</sub>   |
| 2        | 22.7  | 22.6  | 23.6  | 22.7  | 22.6  | CH <sub>2</sub>   |
| 3        | 78.2  | 78.0  | 80.8  | 78.3  | 78.3  | CH                |
| 4        | 36.7  | 36.6  | 37.5  | 36.7  | 36.6  | C                 |
| 5        | 50.5  | 50.3  | 55.6  | 50.6  | 50.2  | CH                |
| 6        | 18.6  | 18.5  | 18.7  | 18.6  | 18.5  | CH <sub>2</sub>   |
| 7        | 33.6  | 33.7  | 36.6  | 33.7  | 33.7  | CH <sub>2</sub>   |
| 8        | 39.2  | 39.1  | 39.0  | 39.2  | 39.1  | C                 |
| 9        | 48.6  | 48.7  | 48.7  | 48.7  | 48.7  | CH                |
| 10       | 37.6  | 37.6  | 37.9  | 37.6  | 37.6  | C                 |
| 11       | 17.4  | 17.4  | 17.5  | 17.4  | 17.4  | CH <sub>2</sub>   |
| 12       | 35.1  | 35.1  | 35.1  | 35.1  | 35.1  | CH <sub>2</sub>   |
| 13       | 38.0  | 37.9  | 37.9  | 38.0  | 37.9  | C                 |
| 14       | 158.5 | 158.2 | 158.0 | 158.3 | 158.5 | C                 |
| 15       | 116.2 | 116.8 | 116.9 | 116.8 | 116.8 | CH                |
| 16       | 37.7  | 37.7  | 37.7  | 37.7  | 37.7  | CH <sub>2</sub>   |
| 17       | 35.8  | 35.8  | 35.8  | 35.8  | 35.8  | C                 |
| 18       | 49.2  | 48.9  | 49.2  | 49.1  | 48.9  | CH                |
| 19       | 41.2  | 41.0  | 41.2  | 41.2  | 41.0  | CH <sub>2</sub>   |
| 20       | 28.8  | 28.8  | 28.8  | 28.8  | 28.8  | C                 |
| 21       | 33.0  | 33.1  | 33.7  | 33.1  | 33.1  | CH <sub>2</sub>   |
| 22       | 33.0  | 32.9  | 33.1  | 33.0  | 32.9  | CH <sub>2</sub>   |
| 23       | 27.9  | 27.8  | 28.0  | 27.9  | 27.8  | CH <sub>3</sub>   |
| 24       | 21.4  | 21.3  | 16.8  | 21.4  | 21.4  | CH <sub>3</sub>   |
| 25       | 15.2  | 15.2  | 15.5  | 15.2  | 15.2  | CH <sub>3</sub>   |
| 26       | 26.0  | 26.0  | 25.9  | 26.0  | 26.0  | CH <sub>3</sub>   |
| 27       | 29.8  | 29.8  | 29.8  | 29.8  | 29.8  | CH <sub>3</sub>   |
| 28       | 29.9  | 29.9  | 29.9  | 29.9  | 29.9  | CH <sub>3</sub>   |
| 29       | 33.3  | 33.4  | 33.3  | 33.4  | 33.4  | CH <sub>3</sub>   |
| 30       | 21.8  | 21.8  | 21.3  | 21.8  | 21.8  | CH <sub>3</sub>   |
| 1'       | 167.0 | 166.2 | 167.1 | 167.2 | 166.3 | C                 |
| 2'       | 116.8 | 117.7 | 116.2 | 116.2 | 118.3 | CH                |
| 3'       | 144.4 | 143.1 | 144.3 | 144.1 | 142.8 | CH                |
| 4'       | 127.1 | 127.4 | 127.1 | 127.3 | 127.8 | C                 |
| 5'       | 109.1 | 112.7 | 109.2 | 129.9 | 132.1 | CH                |
| 6'       | 146.7 | 145.9 | 146.7 | 115.8 | 115.0 | C                 |
| 7'       | 147.8 | 146.8 | 147.8 | 157.6 | 156.4 | C                 |
| 8'       | 114.6 | 113.8 | 114.6 | 115.8 | 115.0 | CH                |
| 9'       | 123.2 | 125.4 | 123.0 | 129.9 | 132.1 | CH                |
| -OMe     | 56.0  | 56.0  | 55.9  |       |       | CH <sub>3</sub>   |

<sup>a</sup> The data were analyzed by DEPT 90° and 135°.

characteristics similar to those of 1–3, except for the disappearance of a methoxy signal at ca.  $\delta$  3.9. Therefore, compounds 5 and 6 were determined as 3 $\alpha$ -*E*-coumaroyltaraxerol and 3 $\alpha$ -*Z*-coumaroyltaraxerol, respectively. Their

HMBC spectral data are summarized in Table S1 (Supporting Information).

The other two known compounds were identified as 3 $\alpha$ -taraxerol<sup>7</sup> and 3 $\beta$ -taraxerol<sup>7</sup> by analysis of 1D and 2D NMR information and comparison of their physical and spectral data with reported values.

Compounds **2** and **6** exhibited weak cytotoxicity against the NCI-H187 (human small cell lung cancer) cell line with IC<sub>50</sub> values of 12.2 and 20.0  $\mu$ g/mL, respectively. No activity was observed in both the BC (human breast cancer cells) and KB (oral human epidermoid carcinoma) cell lines, while compounds **1**, **3**, and **5** showed no cytotoxicity. It is interesting to note that the 3 $\alpha$ -*cis*-taraxeryl esters (**2**, **6**) were somewhat active, while their *trans* isomers were inactive.

## Experimental Section

**General Experimental Procedures.** Melting points were determined on an Electrothermal melting point apparatus and are uncorrected. Optical rotation values were determined with an Autopol II automatic polarimeter. UV spectra were measured with a UV 160A spectrophotometer (Shimadzu). The IR spectra were measured with a Perkin-Elmer FTS FT-IR spectrophotometer. The <sup>1</sup>H and <sup>13</sup>C spectral data were recorded using a 500 MHz Varian UNITY INOVA spectrometer in CDCl<sub>3</sub>. Chemical shifts are recorded in parts per million ( $\delta$ ) in CDCl<sub>3</sub>. The ESITOFMS were obtained from a Micromass LCT mass spectrometer. Quick column chromatography and column chromatography were carried out on silica gel 60 F<sub>254</sub> (Merck) and silica gel 100, respectively. Precoated thin-layer plates of silica gel 60 GF<sub>254</sub> were used for analytical purposes.

**Plant Material.** The fruits of *Bruguiera cylindrica* were collected in March 2002 at the Mangrove Research Station in Nakhon Si Thammarat Province, Thailand. The plant was identified by Prof. Puangpen Siriruga, and a voucher specimen (No. 0012531) has been deposited at the Department of Biology, Faculty of Science, Prince of Songkla University, Songkhla, Thailand.

**Extraction and Isolation.** Air-dried fruits of *B. cylindrica* (6 kg) were extracted with hexane, methylene chloride, and methanol, successively. The hexane extract (35 g) was subjected to quick column chromatography (QCC) over silica gel and eluted with a gradient of hexane–acetone to afford 15 fractions (A1–A15). Fraction A6 (2.50 g) was crystallized from acetone–hexane to give 3 $\alpha$ -taraxerol (1.50 g). Fraction A8 (1.25 g), upon washing with hexane, gave a white solid (121 mg), which was further subjected to column chromatography using acetone–hexane (1:9) as eluent to give two subfractions (A8/1 and A8/2). Of these, subfraction A8/2 (20 mg) was further purified by preparative TLC (acetone–hexane, 1:9) to afford 3 $\beta$ -taraxerol (5.2 mg). Fraction A9 (2.80 g) was crystallized from acetone–hexane to give compound **2** (1.50 g). Fraction A12 (4 g) was crystallized from acetone–hexane to give a mixture of compounds **3** and **4** (10 mg, detected from the <sup>1</sup>H NMR spectrum to be in the ratio 8:2). The mixture was further purified by preparative TLC (acetone–hexane, 1:9) to yield compound **3** (5.2 mg). The mother liquor of fraction A12 (3.70 g) was recrystallized from acetone–hexane to give compound **1** (2.50 g). Fraction A13 (100 mg) was subjected to column chromatography using 100% methylene chloride as eluent to give two subfractions (A13/1 and A13/2). Subfraction A13/2 (30 mg) was further purified by preparative TLC (diethyl ether–hexane, 2.5:7.5) to afford compounds **5** (10 mg) and **6** (7 mg), respectively.

**3 $\alpha$ -E-Feruloyltaraxerol (1):** white solid, mp 125–126 °C; [ $\alpha$ ]<sub>D</sub><sup>27</sup> –37.5° (c 0.08, CHCl<sub>3</sub>); UV (MeOH)  $\lambda$ <sub>max</sub> (log  $\epsilon$ ) 326 (4.31), 300 (4.24), 228 (4.08); IR (KBr)  $\nu$ <sub>max</sub> 3438, 1705, 1684, 1635, 1605, 1515 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz), see Table 1; <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz), see Table 2; EIMS *m/z* 602 (3) [M]<sup>+</sup>, 408 (18), 194 (24), 177 (100); ESITOFMS (negative mode) *m/z* [M – H]<sup>-</sup> 601.4242 (calcd for C<sub>40</sub>H<sub>57</sub>O<sub>4</sub>, 601.4256).

**3 $\alpha$ -Z-Feruloyltaraxerol (2):** white solid, mp 185–186 °C; [ $\alpha$ ]<sub>D</sub><sup>27</sup> –104.4° (c 0.067, CHCl<sub>3</sub>); UV (MeOH)  $\lambda$ <sub>max</sub> (log  $\epsilon$ ) 323 (4.29), 300 (4.17), 237 (4.16); IR (KBr)  $\nu$ <sub>max</sub> 3463, 1708, 1697, 1623, 1594, 1513 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz), see Table 1; <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz), see Table 2; EIMS *m/z* 602 (3) [M]<sup>+</sup>, 408 (12), 194 (28), 177 (100); ESITOFMS (negative mode) *m/z* [M – H]<sup>-</sup> 601.4247 (calcd for C<sub>40</sub>H<sub>57</sub>O<sub>4</sub>, 601.4256).

**3 $\beta$ -E-Feruloyltaraxerol (3):** white solid, mp 132–133 °C; [ $\alpha$ ]<sub>D</sub><sup>27</sup> –62.5° (c 0.016, CHCl<sub>3</sub>); UV (MeOH)  $\lambda$ <sub>max</sub> (log  $\epsilon$ ) 327 (4.25), 300 (4.08), 237 (4.03); IR (KBr)  $\nu$ <sub>max</sub> 3449, 1704, 1682, 1635, 1509 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz), see Table 1; <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz), see Table 2; EIMS *m/z* 602 (2) [M]<sup>+</sup>, 408 (8), 194 (48), 177 (100); ESITOFMS (negative mode) *m/z* [M – H]<sup>-</sup> 601.4269 (calcd for C<sub>40</sub>H<sub>57</sub>O<sub>4</sub>, 601.4256).

**3 $\alpha$ -E-Coumaroyltaraxerol (5):** colorless, viscous oil, [ $\alpha$ ]<sub>D</sub><sup>27</sup> +136.36° (c 0.022, CHCl<sub>3</sub>); UV (MeOH)  $\lambda$ <sub>max</sub> (log  $\epsilon$ ) 311 (4.23), 300 (4.18), 237 (4.10); IR (neat)  $\nu$ <sub>max</sub> 3449, 1767, 1712, 1638, 1603, 1505 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz), see Table 1; <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz), see Table 2; ESITOFMS (negative mode) *m/z* [M – H]<sup>-</sup> 571.4144 (calcd for C<sub>39</sub>H<sub>55</sub>O<sub>3</sub>, 571.4151).

**3 $\alpha$ -Z-Coumaroyltaraxerol (6):** colorless, viscous oil, [ $\alpha$ ]<sub>D</sub><sup>27</sup> +26.31° (c 0.038, CHCl<sub>3</sub>); UV (MeOH)  $\lambda$ <sub>max</sub> (log  $\epsilon$ ) 311 (4.27), 300 (4.22); IR (neat)  $\nu$ <sub>max</sub> 3372, 1704, 1675, 1635, 1600, 1509 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz), see Table 1; <sup>13</sup>C NMR (CDCl<sub>3</sub>, 125 MHz), see Table 2; ESITOFMS (negative mode) *m/z* [M – H]<sup>-</sup> 571.4131 (calcd for C<sub>39</sub>H<sub>55</sub>O<sub>3</sub>, 571.4151).

**Cytotoxicity Assay.** The cytotoxicity assay employed the colorimetric method.<sup>16</sup> Ellipticine, the reference substance, exhibited activity toward BC, KB, and NCI-H187 cell lines, with the IC<sub>50</sub> range of 0.3–0.6  $\mu$ g/mL.

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**Supporting Information Available:** Table S1, summarizing the HMBC correlation of compounds **1–3**, **5**, and **6**. This material is available free of charge via the Internet at <http://pubs.acs.org>.

## References and Notes

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