Isolation, Identification and Bioactivities of Abietane Diterpenoids from Premna szemaoensis

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Figure 3S. HSQC spectrum of (1) recorded in CD$_3$OD

Figure 4S. HMBC spectrum of (1) recorded in CD$_3$OD
Figure 5S. $^1$H-$^1$H COSY spectrum of (1) recorded in CD$_3$OD

Figure 6S. ROESY spectrum of (1) recorded in CD$_3$OD
Figure 7S. HRESIMS spectrum of (1)
Figure 8S. UV spectrum of (1)

Figure 9S. IR spectrum of (1)
Figure 10S-18S. NMR, MS, UV, and IR spectra of compound 2

Figure 10S. $^1$H NMR spectrum of (2) recorded in CD$_3$OD at 600 MHz

Figure 11S. $^{13}$C NMR spectrum of (2) recorded in CD$_3$OD at 150 MHz
Figure 12S. HSQC spectrum of (2) recorded in CD$_3$OD

Figure 13S. HMBC spectrum of (2) recorded in CD$_3$OD
Figure 14S. $^1$H-$^1$H COSY spectrum of (2) recorded in CD$_3$OD

Figure 15S. ROESY spectrum of (2) recorded in CD$_3$OD
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Figure 17S. UV spectrum of (2)

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Figure 29S. $^{13}$C NMR spectrum of (4) recorded in CD$_3$OD at 150 MHz
Figure 30S. HSQC spectrum of (4) recorded in CD$_3$OD

Figure 31S. HMBC spectrum of (4) recorded in CD$_3$OD
Figure 32S. $^1$H-$^1$H COSY spectrum of (4) recorded in CD$_3$OD

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Figure 47S. $^{13}$C NMR spectrum of (6) recorded in CD$_3$OD at 150 MHz
Figure 48S. HSQC spectrum of (6) recorded in CD$_3$OD

Figure 49S. HMBC spectrum of (6) recorded in CD$_3$OD
Figure 50S. $^1$H-$^1$H COSY spectrum of (6) recorded in CD$_3$OD

Figure 51S. ROESY spectrum of (6) recorded in CD$_3$OD
Figure 52S. HRESIMS spectrum of (6)
Figure 53S. UV spectrum of (6)

Figure 54S. IR spectrum of (6)
Figure 55S-63S. NMR, MS, UV, and IR spectra of compound 7

Figure 55S. $^1$H NMR spectrum of (7) recorded in CD$_3$OD at 600 MHz

Figure 56S. $^{13}$C NMR spectrum of (7) recorded in CD$_3$OD at 150 MHz
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Figure 58s. HMBC spectrum of (7) recorded in CD$_3$OD
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Figure 63S. IR spectrum of (7)
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Figure 64S. $^1$H NMR spectrum of (8) recorded in CD$_3$OD at 600 MHz

Figure 65S. $^{13}$C NMR spectrum of (8) recorded in CD$_3$OD at 150 MHz
Figure 66S. HSQC spectrum of (8) recorded in CD$_3$OD

Figure 67S. HMBC spectrum of (8) recorded in CD$_3$OD
Figure 68S. $^1$H-$^1$H COESY spectrum of (8) recorded in CD$_3$OD

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Figure 74S. $^{13}$C NMR spectrum of (9) recorded in CD$_3$OD at 150 MHz
Figure 75S. HSQC spectrum of (9) recorded in CD$_3$OD

Figure 76S. HMBC spectrum of (9) recorded in CD$_3$OD
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Figure 78S. ROESY spectrum of (9) recorded in CD$_3$OD
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Figure 85S. HMBC spectrum of (10) recorded in acetone-$d_6$
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Figure 92S. $^{13}$C NMR spectrum of (11) recorded in acetone-$d_6$ at 150 MHz
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Figure 101S. $^{13}$C NMR spectrum of (12) recorded in acetone-$d_6$ at 150MHz
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Figure 103S. HMBC spectrum of (12) recorded in acetone-$d_6$
Figure 104S. $^1$H-$^1$H COSY spectrum of (12) recorded in acetone-$d_6$

Figure 105S. ROESY spectrum of (12) recorded in acetone-$d_6$
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Figure 107S. UV spectrum of (12)

Figure 108S. IR spectrum of (12)
Figure 109S. The pack drawing of compound 1

Figure 109S. View of the Pack drawing motif of 1

(Hydrogen-bonds are shown as dashed lines)
Figure 110S. The pack drawing of compound 3

Figure 110S. View of the pack drawing of 3.

(Hydrogen-bonds are shown as dashed lines)
Figure 111S. The pack drawing compound 10

Figure 111S. View of the pack drawing of 10

(Hydrogen-bonds are shown as dashed lines)
### Table 1S. Crystal data and structure refinement for 1

| Property                                      | Value                                           |
|-----------------------------------------------|-------------------------------------------------|
| Identification code                           | cu_xpp40_0m                                     |
| Empirical formula                             | C26 H38 O11                                     |
| Formula weight                                | 526.56                                          |
| Temperature                                   | 100(2) K                                        |
| Wavelength                                    | 1.54178 Å                                       |
| Crystal system, space group                   | Monoclinic, P 21                                |
| Unit cell dimensions                          | a = 5.70480(10) Å, b = 23.8602(5) Å, c = 9.3419(2) Å |
| Volume                                        | 1271.53(4) Å³                                  |
| Z, Calculated density                         | 2, 1.375 Mg/m³                                  |
| Absorption coefficient                       | 0.898 mm⁻¹                                      |
| F(000)                                        | 564                                             |
| Crystal size                                  | 0.67 x 0.62 x 0.38 mm                           |
| Theta range for data collection               | 3.70 to 69.31 deg.                             |
| Limiting indices                              | h: -6 to 6, k: -26 to 24, l: -11 to 11          |
| Reflections collected / unique                | 10232 / 3499 [R(int) = 0.0328]                  |
| Completeness to theta                         | 93.3 %                                          |
| Absorption correction                         | Semi-empirical from equivalents                 |
| Max. and min. transmission                    | 0.7267 and 0.5846                               |
| Refinement method                             | Full-matrix least-squares on F²                |
| Data / restraints / parameters                | 3499 / 1 / 344                                  |
| Goodness-of-fit on F²                         | 1.113                                           |
| Final R indices [I>2σ(I)]                    | R1 = 0.0300, wR2 = 0.0884                       |
| R indices (all data)                          | R1 = 0.0300, wR2 = 0.0885                       |
| Absolute structure parameter                  | 0.17(14)                                        |
### Table 2S. Crystal data and structure refinement for 3

| Parameter                              | Value                                  |
|----------------------------------------|----------------------------------------|
| Identification code                    | cu_xpp57_0m-sr                         |
| Empirical formula                      | C104 H146 O45                          |
| Formula weight                         | 2116.20                                |
| Temperature                            | 100(2) K                               |
| Wavelength                             | 1.54178 Å                              |
| Crystal system                         | Orthorhombic                           |
| Space group                            | P2\(_1\)2\(_1\)2\(_1\)                 |
| Unit cell dimensions                   | a = 17.5477(6) Å, b = 21.7199(7) Å, c = 33.3592(12) Å, \(\alpha = 90^\circ\), \(\beta = 90^\circ\), \(\gamma = 90^\circ\) |
| Volume                                 | 12714.3(8) Å\(^3\)                    |
| Z                                      | 4                                      |
| Density (calculated)                   | 1.106 Mg/m\(^3\)                      |
| Absorption coefficient                 | 0.728 mm\(^{-1}\)                     |
| F(000)                                 | 4520                                   |
| Crystal size                           | 0.980 x 0.660 x 0.470 mm\(^3\)         |
| Theta range for data collection        | 2.427 to 69.708°.                      |
| Index ranges                           | -21 <= h <= 21, -26 <= k <= 25, -37 <= l <= 40 |
| Reflections collected                  | 112641                                 |
| Independent reflections                | 23429 [R(int) = 0.0484]                |
| Completeness to theta = 67.679°        | 99.7%                                  |
| Absorption correction                  | Semi-empirical from equivalents        |
| Refinement method                      | Full-matrix least-squares on F\(^2\)  |
Table 3S. Crystal data and structure refinement for 10

| Identification code        | cu_xpp14_0m |
|----------------------------|-------------|
| Empirical formula          | C20 H26 O5  |
| Formula weight             | 346.41      |
| Temperature                | 100(2) K    |
| Wavelength                 | 1.54178 Å   |
| Crystal system, space group| Monoclinic, P21 |
| Unit cell dimensions       | a = 11.5843(7) Å  |
|                           | b = 9.5501(6) Å  |
|                           | c = 15.2093(10) Å |
| Volume                     | 1680.53(18) Å³ |
| Z, Calculated density      | 4, 1.369 Mg/m³ |
| Absorption coefficient     | 0.794 mm⁻¹ |
| F(000)                     | 744         |
| Crystal size               | 0.40 x 0.28 x 0.02 mm |
| Theta range for data collection | 2.91 to 69.25 deg. |
| Limiting indices           | -14 ≤ h ≤ 13, -11 ≤ k ≤ 11, -18 ≤ l ≤ 17 |
| Reflections collected / unique | 10384 / 4801 [R(int) = 0.0536] |
| Description                                      | Value                                |
|-------------------------------------------------|--------------------------------------|
| Completeness to theta = 69.25                    | 92.0 %                               |
| Absorption correction                           | Semi-empirical from equivalents      |
| Max. and min. transmission                       | 0.9843 and 0.7419                    |
| Refinement method                               | Full-matrix least-squares on F^2     |
| Data / restraints / parameters                   | 4801 / 1 / 464                       |
| Goodness-of-fit on F^2                          | 1.058                                |
| Final R indices [I>2sigma(I)]                    | R1 = 0.0627, wR2 = 0.1682            |
| R indices (all data)                             | R1 = 0.0701, wR2 = 0.1743            |
| Absolute structure parameter                    | 0.0(2)                               |
| Largest diff. peak and hole                      | 0.444 and -0.561 e.A^{-3}            |