

# Supplementary Materials: Characterization of Secondary Metabolites from Purple *Ipomoea batatas* Leaves and Their Effects on Glucose Uptake

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IBW 1H 500MHz/C5D5N 2015.03.13

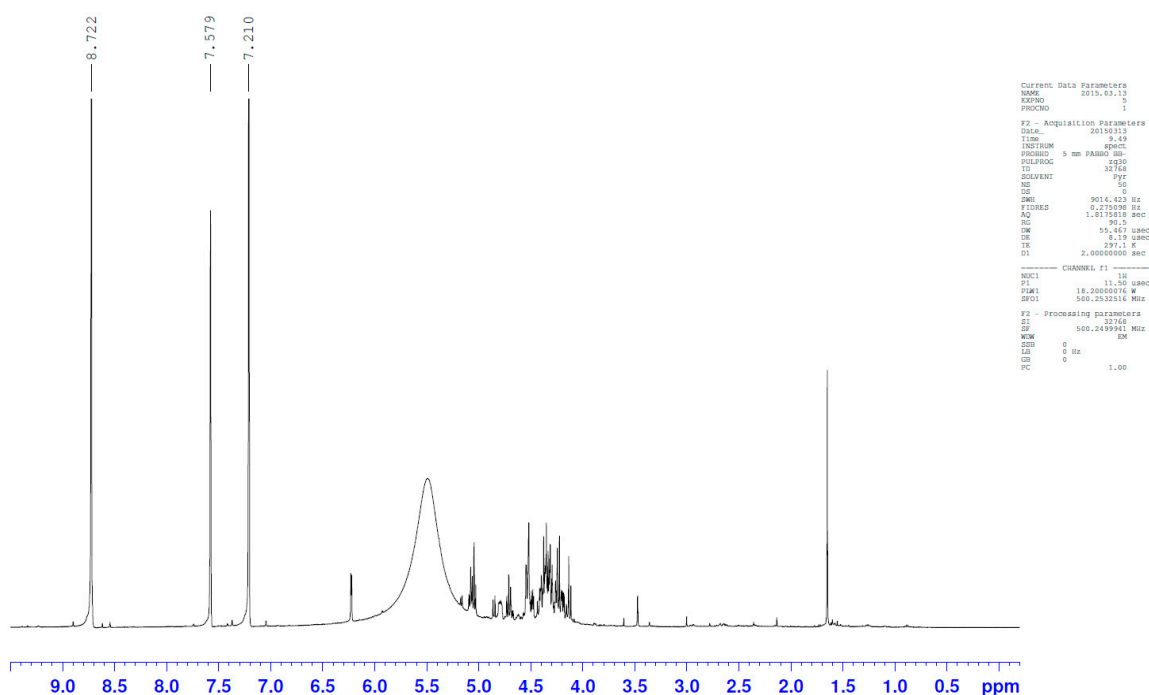


Figure S1. <sup>1</sup>H-NMR (500 MHz, C<sub>5</sub>D<sub>5</sub>N) of IBW.

IBW 13C 125MHz/C5D5N 2015.04.20

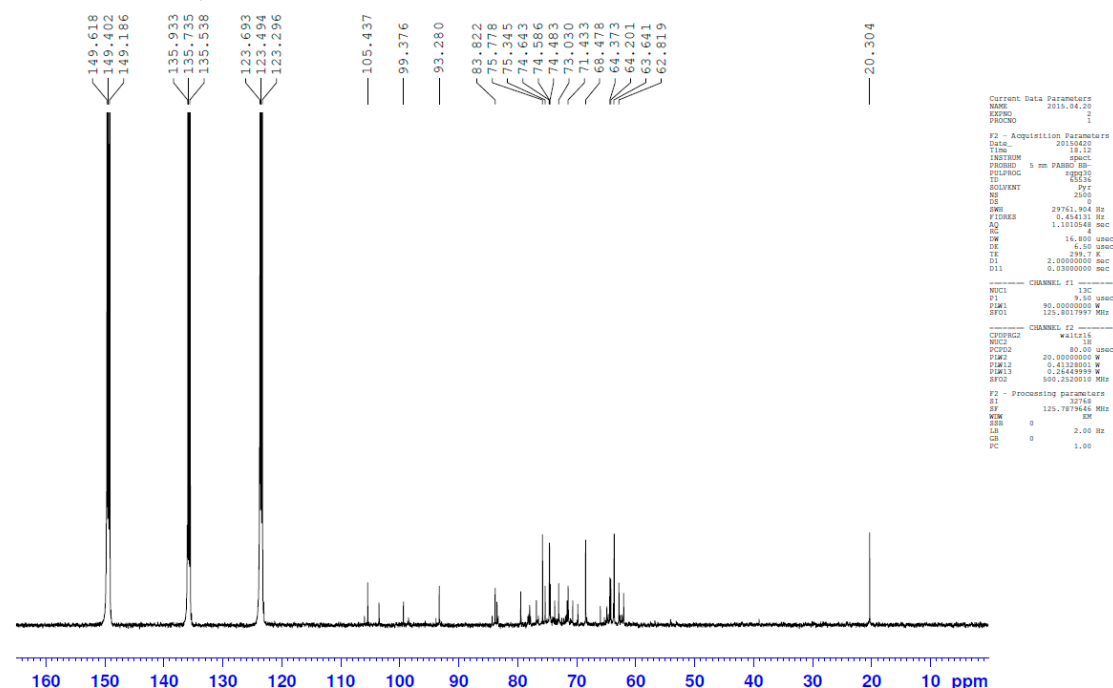


Figure S2. <sup>13</sup>C-NMR (125 MHz, C<sub>5</sub>D<sub>5</sub>N) of IBW.

IBW dept135 500MHz/C5D5N 2015.04.20

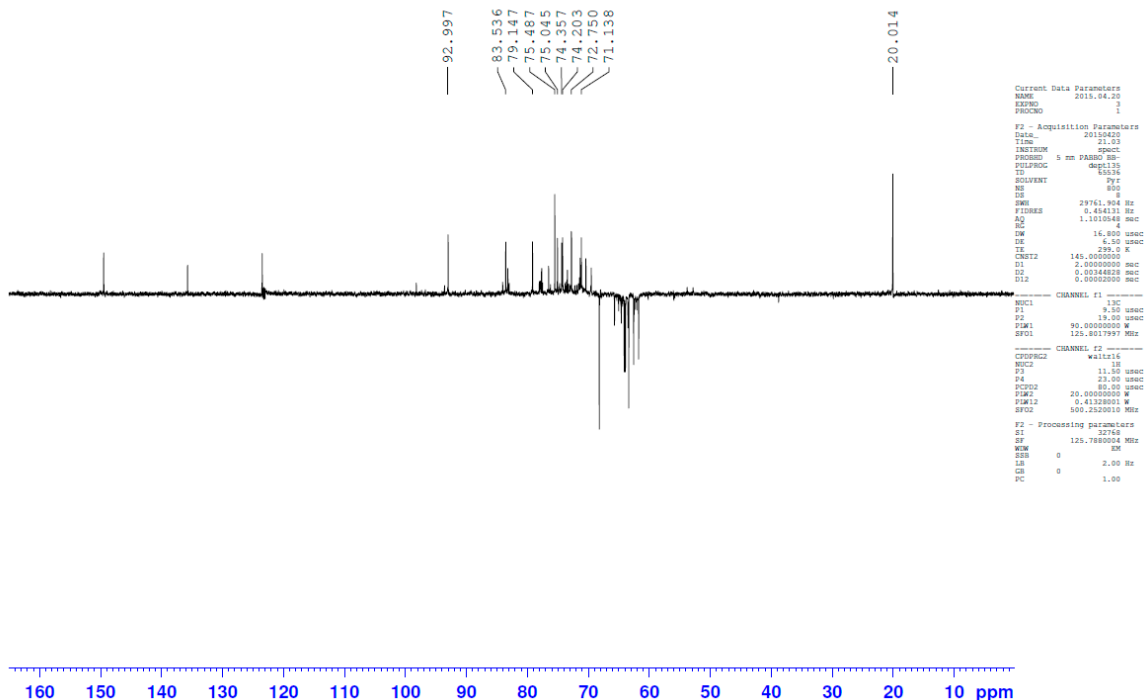


Figure S3. DEPT135 NMR (500 MHz, C<sub>5</sub>D<sub>5</sub>N) of IBW.

IBW COSY 500MHz/C5D5N 2015.04.20

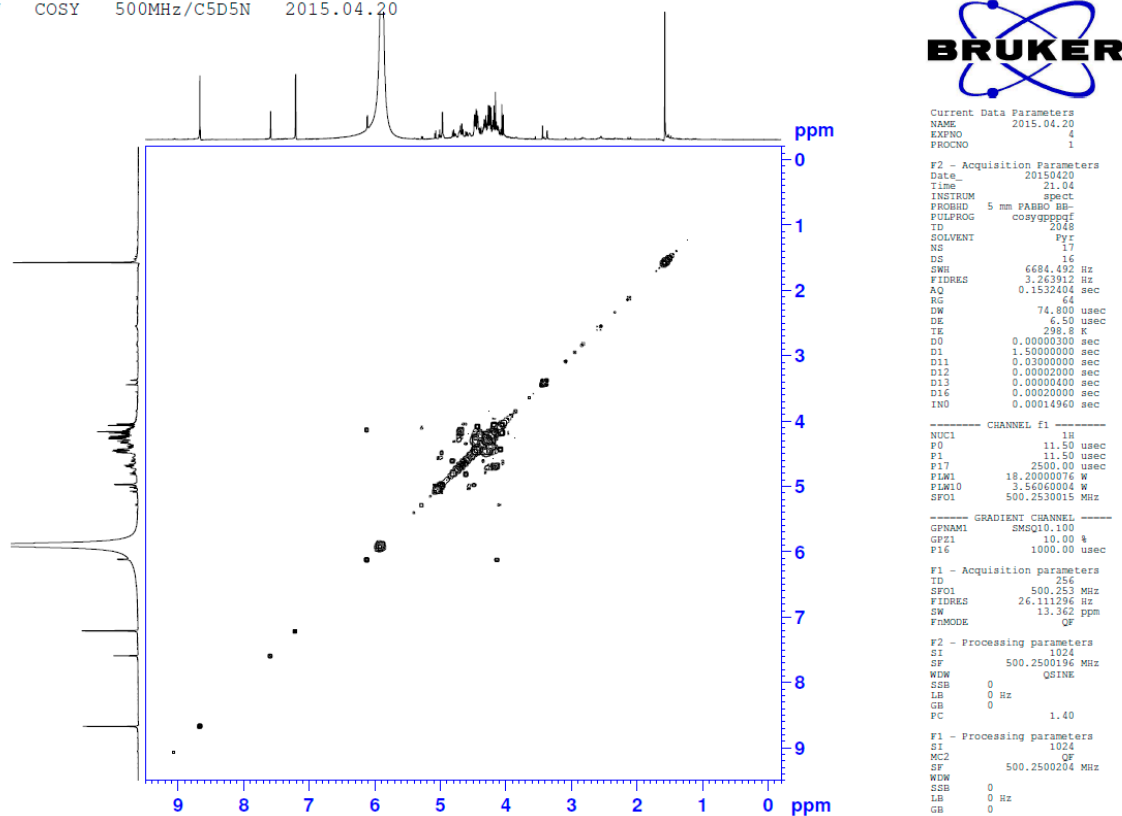
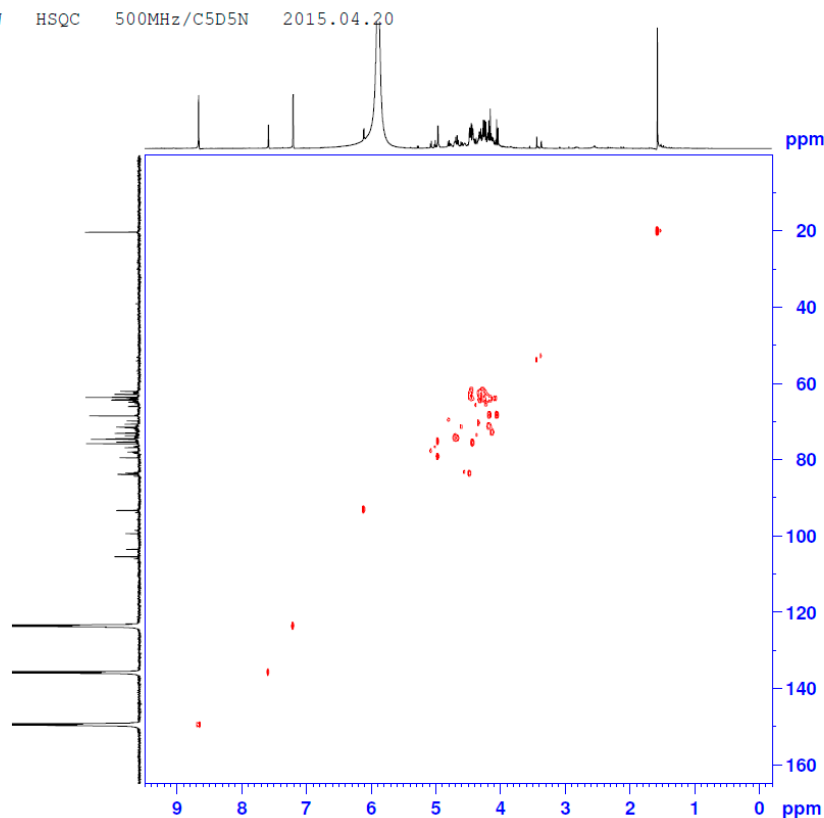


Figure S4. COSY NMR (500 MHz, C<sub>5</sub>D<sub>5</sub>N) of IBW.

IBW HSQC 500MHz/C5D5N 2015.04.20



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PROCNO   1

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D15       0.0300000 sec
D16       0.0002000 sec
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P16L4    1.9155904 W
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SFO3     Ccp40, 0.5, 0.1
SFO4     Ccp40, 0.5, 0.1
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SFO6     Ccp40, 0.5, 0.1
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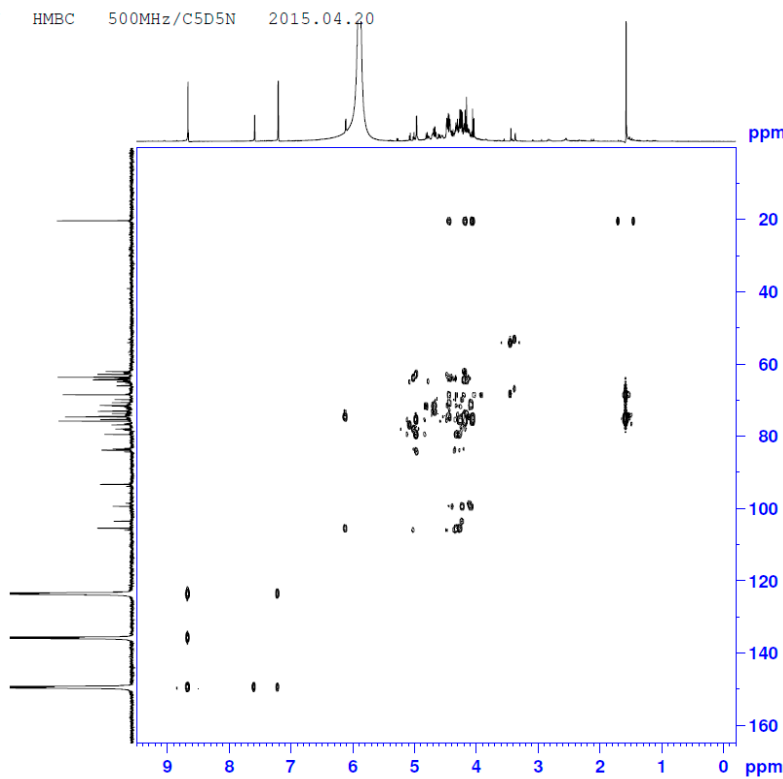
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CP19     300.00 usec

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F1 - Processing parameters
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WDW       SINC
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GB        0
    
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Figure S5. HSQC NMR (500 MHz, C<sub>5</sub>D<sub>5</sub>N) of IBW.

IBW HMBC 500MHz/C5D5N 2015.04.20



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PROCNO   1

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DS        4
SWH       6684.492 Hz
FIDRES   3.263912 Hz
AQ        0.1333048 sec
RG        203
DW        74.800 usec
DE        6.50 usec
TE        299.2 K
CNS12    145.000000
CNS13    8.0000000
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F1 - Processing parameters
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WDW       SINC
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Figure S6. HMBC NMR (500 MHz, C<sub>5</sub>D<sub>5</sub>N) of IBW.

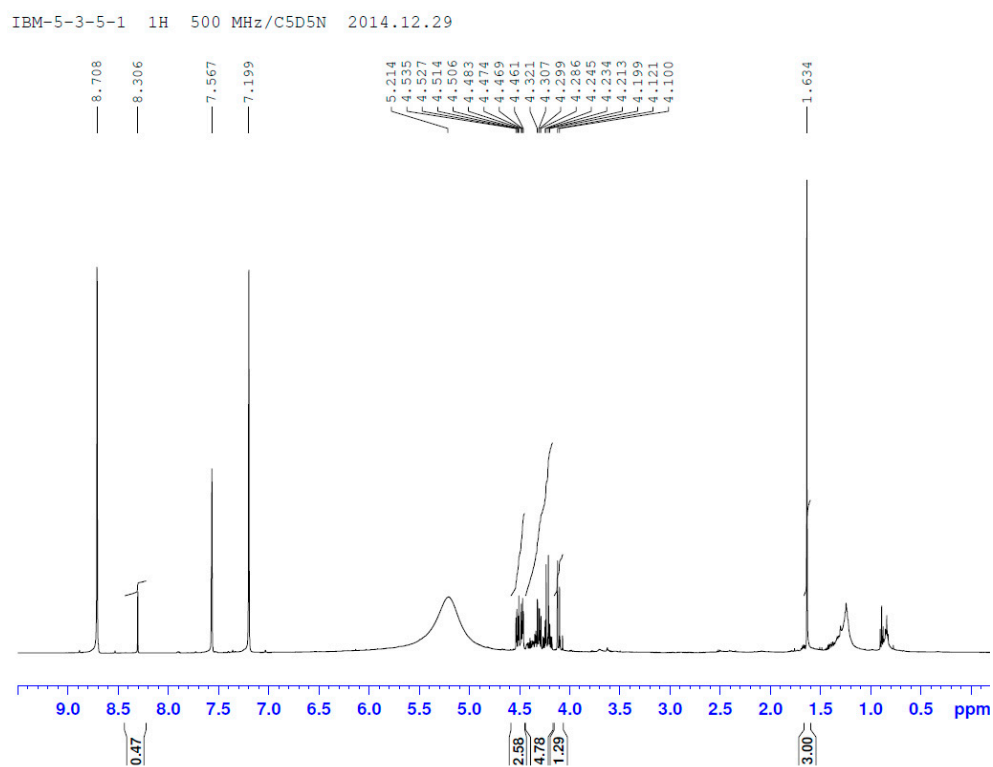


Figure S7.  $^1\text{H-NMR}$  (500 MHz,  $\text{C}_5\text{D}_5\text{N}$ ) of compound 19 isolated from IBM.

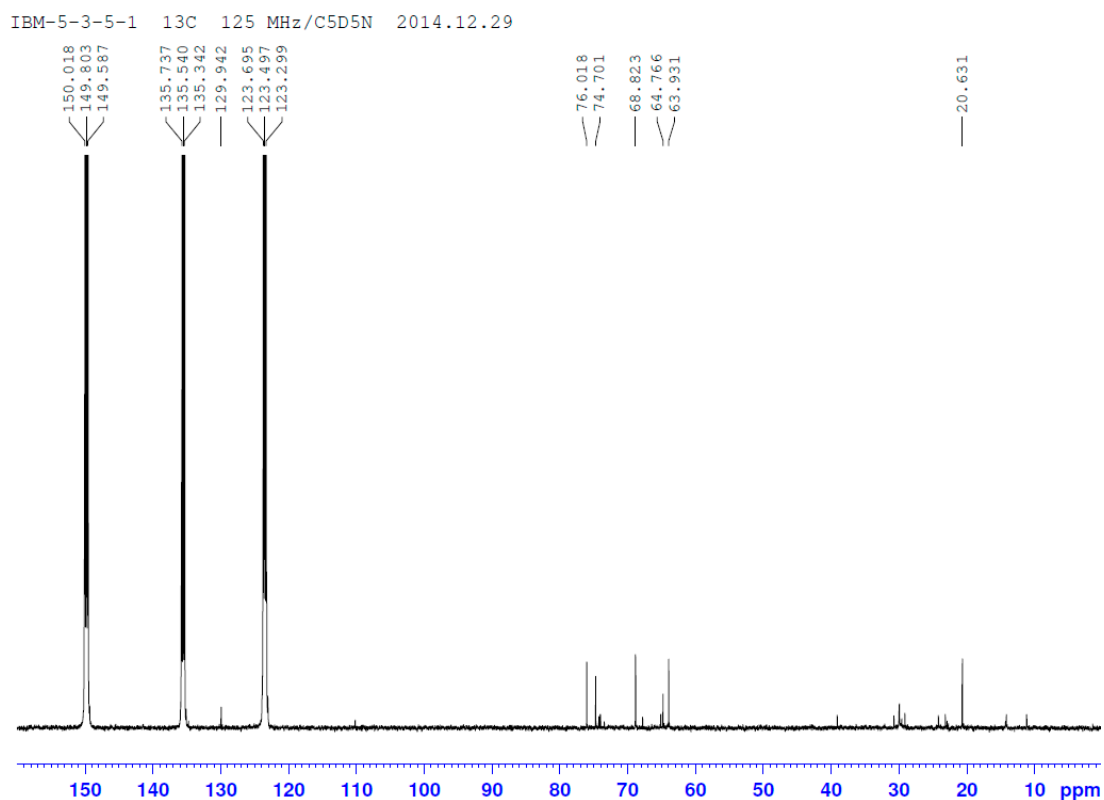


Figure S8.  $^{13}\text{C-NMR}$  (125 MHz,  $\text{C}_5\text{D}_5\text{N}$ ) of compound 19 isolated from IBM.

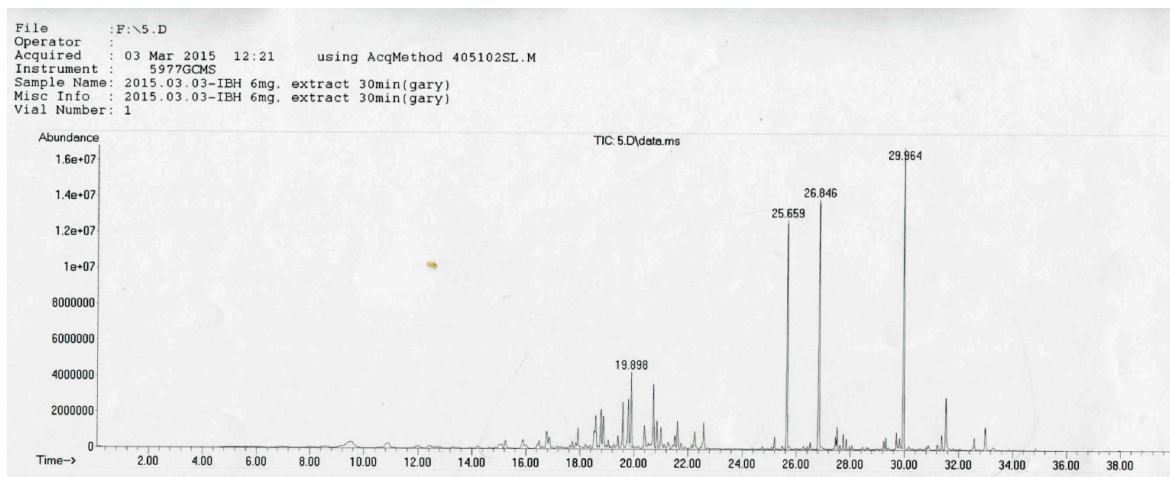


Figure S9. GC/MS analysis of *n*-hexane-soluble fraction (IBH).

### Three major compounds (39.44%)

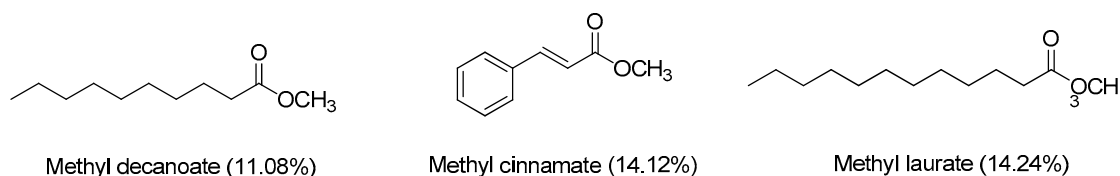


Figure S10. Three major compounds of IBH fraction.

### Sesquiterpenes (6.67%)

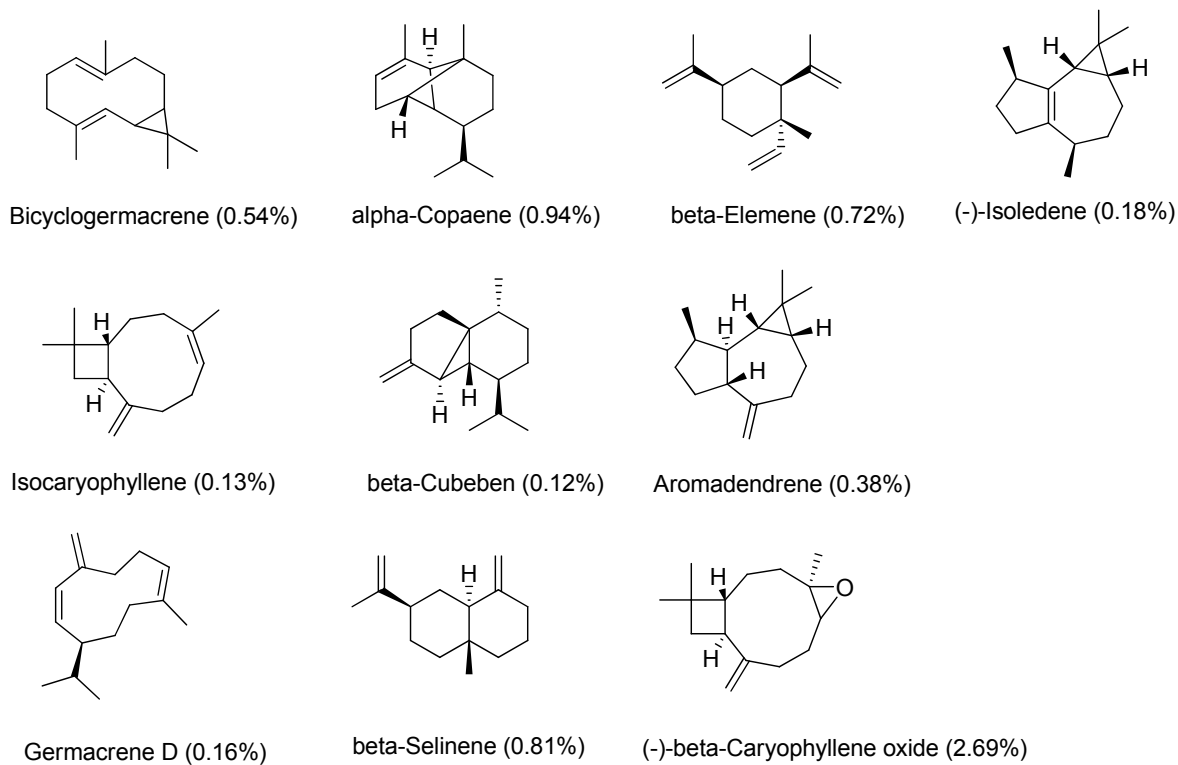
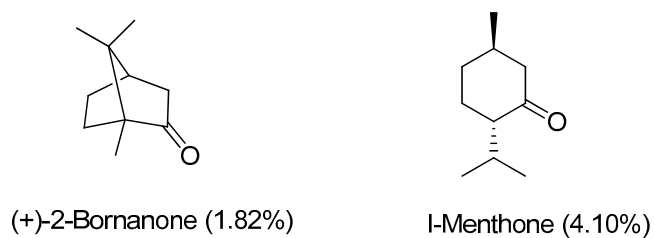
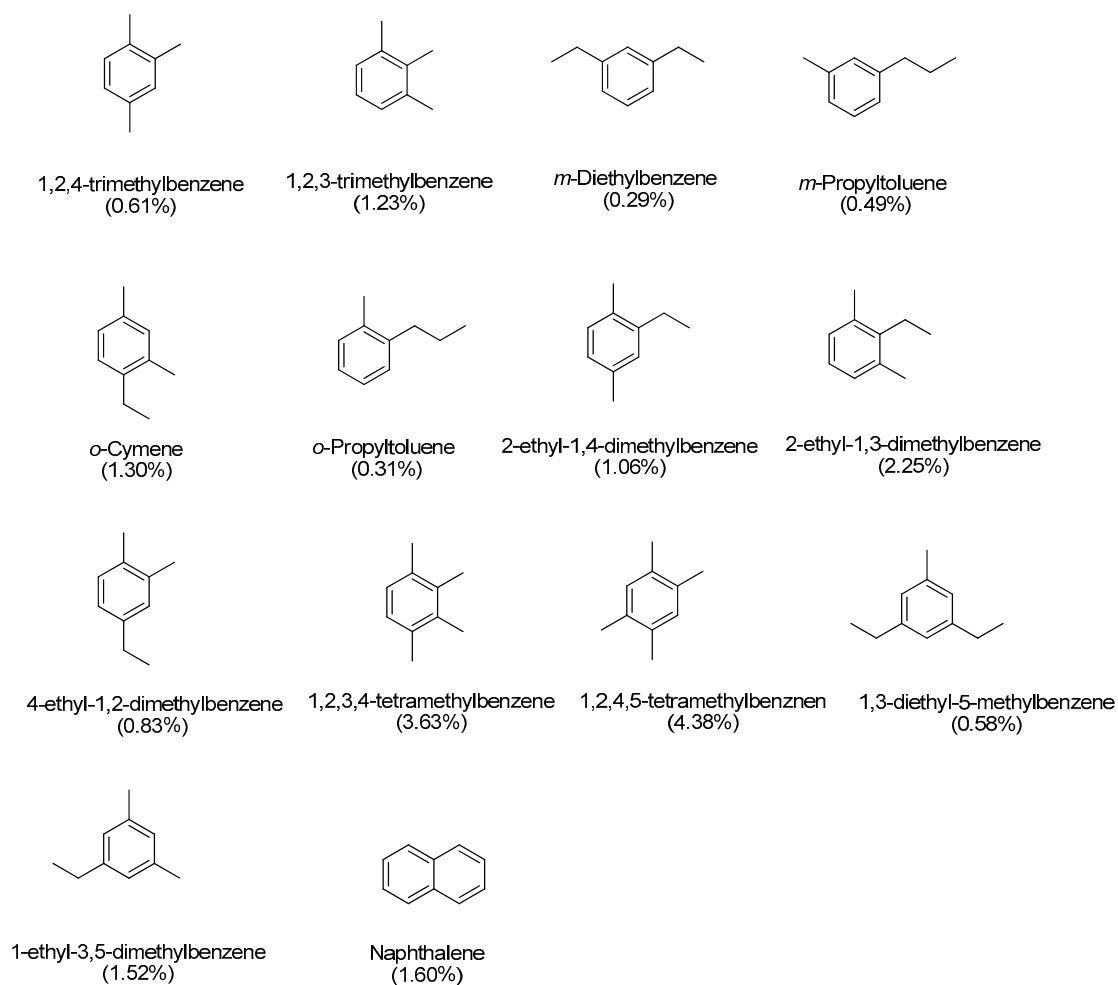
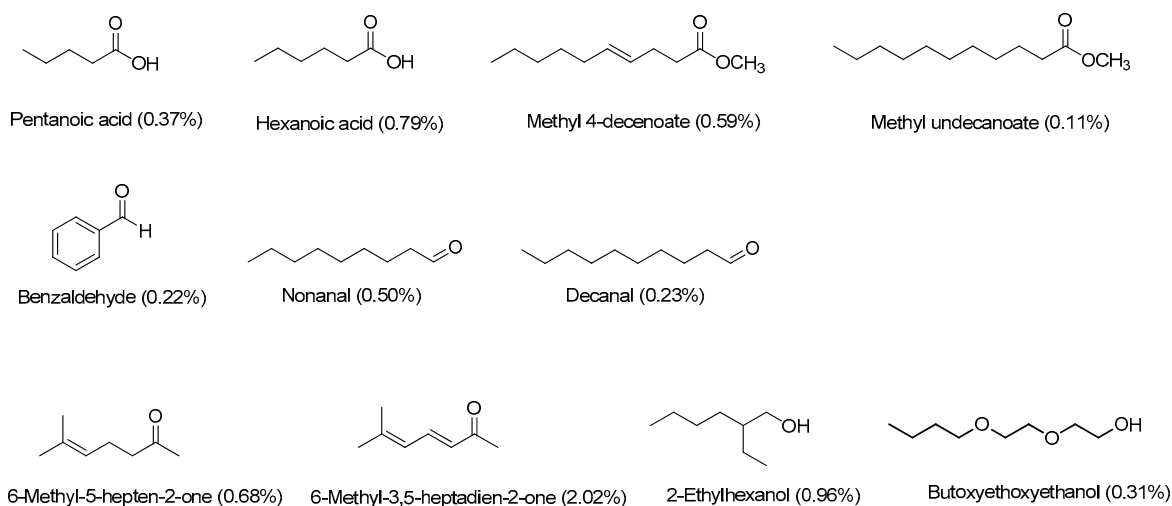
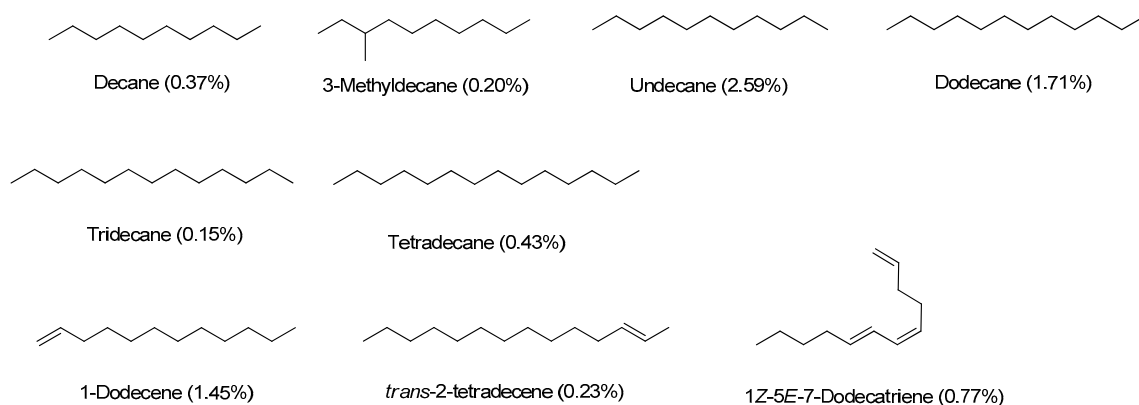
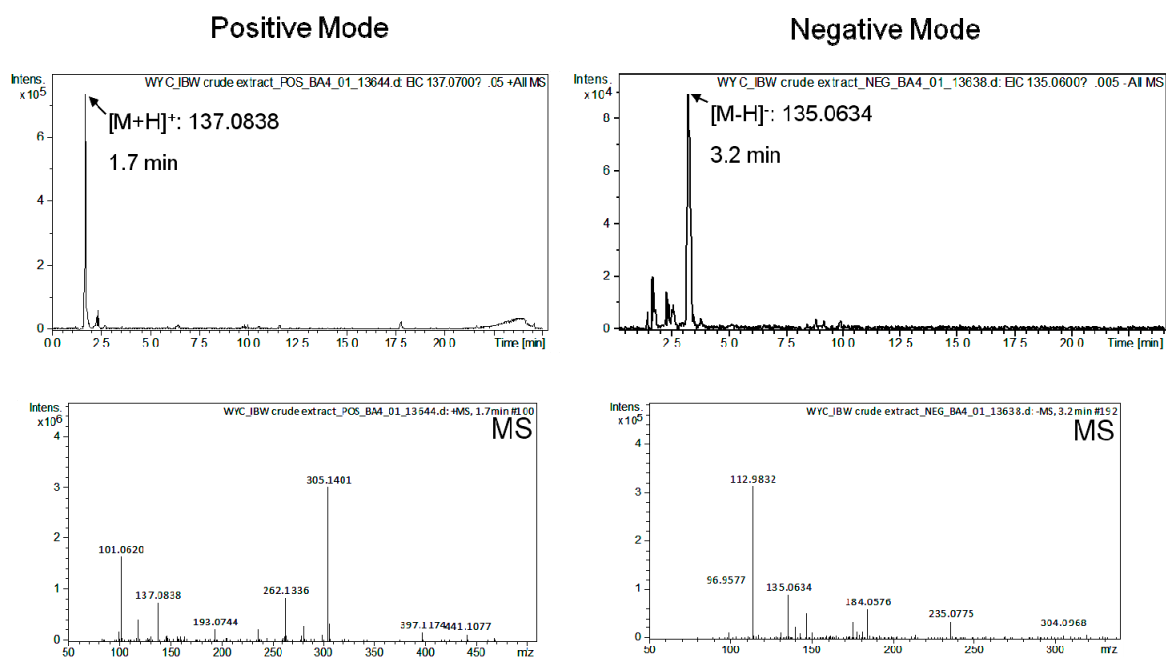


Figure S11. Sesquiterpenes of IBH fraction.

**Monoterpenes (5.92%)****Figure S12.** Monoterpenes of IBH fraction.**Aromatic compounds (20.08%)****Figure S13.** Aromatic compounds of IBH fraction.

**Acids (1.16%), esters (0.70%), aldehydes (0.95%), ketones (2.70%), alcohols (1.27%)****Figure S14.** Acids, esters, aldehydes, ketones, and alcohols of IBH fraction.**Alkanes (5.45%), alkenes (2.45%)****Figure S15.** Alkanes and alkenes of IBH fraction.**Figure S16.** LC/MS analysis of H<sub>2</sub>O-soluble fraction (IBW).

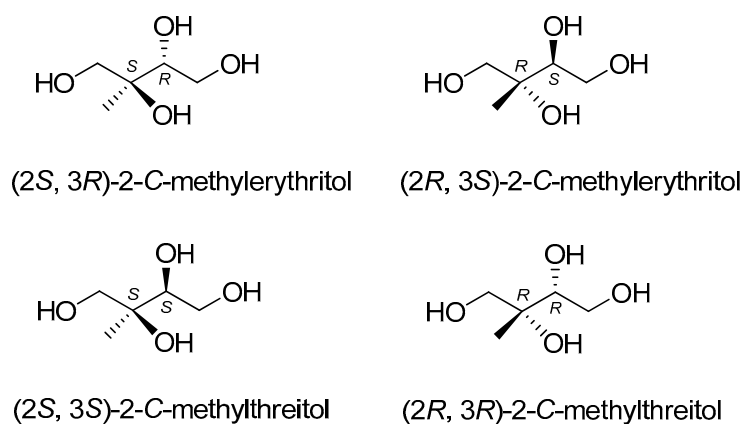


Figure S17. Four stereoisomers of 2-methyl-1,2,3,4-butanetrol.

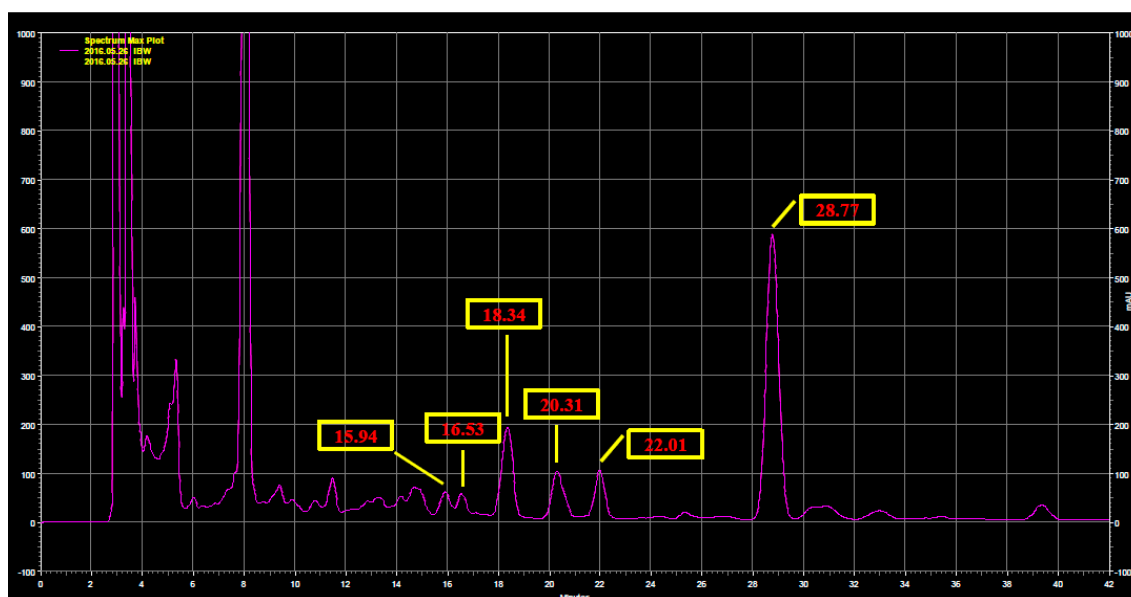


Figure S18. HPLC sugar derivatives analysis of IBM.

Table S1. Chemical composition of IBM and IBB crude fractions from purple *I. batatas* leaves.

| IBM Crude Fraction                       | IBB Crude Fraction                        |
|--|---|
| benzyl $\beta$ -D-glucoside (10)         | quercetin 3-O- $\beta$ -D-sophoroside (1) |
| eugenol (11)                             | quercetin 3 $\beta$ -O-glucoside (2)      |
| 4-hydroxy-3-methoxybenzaldehyde (12)     | quercetin (3)                             |
| methyl 4-hydroxy-3-methoxybenzoate (13)  | 3,4-di-O-caffeoyl isoquinic acid (4)      |
| caryolane-1,9 $\beta$ -diol (14)         | anosmoside A (5)                          |
| clovane-2 $\beta$ ,9 $\alpha$ -diol (15) | 8-O-acetyl-harpagide (6)                  |
| indole-3-aldehyde (16)                   | triol (7)                                 |
| 6-methoxy-7-hydroxycoumarin (17)         | eugenyl O- $\beta$ -D-glucopyranoside (8) |
| <i>trans</i> -N-feruloyltyramine (18)    | (+)-pinoselinol- $\beta$ -D-glucoside (9) |
| 2-methyl-1,2,3,4-butanetrol (19)         |   |
| andrographolide (20)                     |   |
| sitosterol-3- $\beta$ -D-glucose (21)    |   |



**Appendix S1:** Characterization of all compounds isolated from IBM and IBB fractions

**Compound 1:** <sup>1</sup>H-NMR (C<sub>5</sub>D<sub>5</sub>N, 500 MHz): 3.94 (m), 4.10–4.49 (7H), 4.57 (dd, *J* = 12.0, 2.5 Hz), 5.63 (d, *J* = 7.5 Hz), 6.54 (d, *J* = 2.0 Hz), 6.62 (d, *J* = 7.5 Hz), 6.67 (d, *J* = 2.0 Hz), 7.38 (d, *J* = 8.5 Hz), 8.03 (dd, *J* = 8.5, 2.0 Hz), 8.40 (d, *J* = 2.0 Hz), 13.49 (brs); <sup>13</sup>C-NMR (C<sub>5</sub>D<sub>5</sub>N, 125 MHz): 62.1, 62.3, 70.9, 71.2, 76.1, 78.3, 78.4 (2C), 78.8, 84.5, 94.2, 99.5, 99.9, 105.1, 106.3, 116.3, 117.8, 122.4, 122.6, 134.5, 146.5, 150.4, 156.6, 157.2, 162.8, 165.4, 178.8; ESIMS *m/z* 625.0 [M – H]<sup>–</sup>.

**Compound 2:** <sup>1</sup>H-NMR (C<sub>5</sub>D<sub>5</sub>N, 500 MHz): 4.19–4.44 (6H), 6.21 (d, *J* = 7.5 Hz), 6.64 (d, *J* = 2.0 Hz), 6.69 (d, *J* = 2.0 Hz), 7.27 (d, *J* = 8.5 Hz), 8.06 (dd, *J* = 8.5, 2.0 Hz), 8.46 (d, *J* = 2.0 Hz), 13.17 (brs); <sup>13</sup>C-NMR (C<sub>5</sub>D<sub>5</sub>N, 125 MHz): 62.6, 71.4, 76.1, 78.6, 78.9, 94.5, 99.8, 104.5, 105.2, 116.2, 117.9, 122.3, 122.6, 134.5, 146.7, 149.8, 157.6, 157.7, 162.7, 165.9, 178.7; ESIMS *m/z* 487.1 [M + Na]<sup>+</sup>, 462.9 [M – H]<sup>–</sup>.

**Compound 3:** <sup>1</sup>H-NMR (C<sub>5</sub>D<sub>5</sub>N, 500 MHz): 6.73 (d, *J* = 2.0 Hz), 6.77 (d, *J* = 2.0 Hz), 7.40 (d, *J* = 8.5 Hz), 8.12 (dd, *J* = 8.5, 2.0 Hz), 8.63 (d, *J* = 2.5 Hz), 13.34 (brs); ESIMS *m/z* 303.1 [M + H]<sup>+</sup>, 300.9 [M – H]<sup>–</sup>.

**Compound 4:** <sup>1</sup>H-NMR (C<sub>5</sub>D<sub>5</sub>N, 500 MHz): 2.61–2.75 (4H), 4.58 (brs), 6.09 (brs), 6.49 (d, *J* = 10.5 Hz), 6.57 (d, *J* = 16.0 Hz), 6.70 (d, *J* = 16.0 Hz), 7.03 (d, *J* = 8.0 Hz), 7.10 (d, *J* = 8.0 Hz), 7.14 (d, *J* = 8.5 Hz), 7.21 (overlap), 7.50 (brs), 7.60 (brs), 7.94 (d, *J* = 16.0 Hz), 8.01 (d, *J* = 16.0 Hz); <sup>13</sup>C-NMR (C<sub>5</sub>D<sub>5</sub>N, 125 MHz): 38.27 (2C), 67.83, 69.32, 73.59, 74.80, 114.97, 115.07, 115.67, 115.87, 116.59 (2C), 122.18, 122.24, 126.76 (2C), 146.10, 146.25, 147.47, 147.55, 150.33, 150.44, 166.99 (2C), 182.50; ESIMS *m/z* 517.4 [M + H]<sup>+</sup>, 539.1 [M + Na]<sup>+</sup>, 515.0 [M – H]<sup>–</sup>.

**Compound 5:** <sup>1</sup>H-NMR (C<sub>5</sub>D<sub>5</sub>N, 500 MHz): 0.99 (3H, d, *J* = 6.5 Hz), 1.23 (3H, s), 1.42 (3H, d, *J* = 6.0 Hz), 1.59, 1.73 (3H, s), 1.90 (2H), 1.97, 2.20, 2.33, 2.46, 3.66, 3.67, 3.94–4.37 (4H), 4.59 (brd, *J* = 11.0 Hz), 5.00 (overlap), 5.01; <sup>13</sup>C-NMR (C<sub>5</sub>D<sub>5</sub>N, 125 MHz): 14.5, 22.9, 23.2, 23.5, 24.4, 25.8, 29.1, 36.4, 40.8, 41.6, 42.3, 51.2, 63.0, 71.9, 72.3, 75.6, 78.4, 78.5, 78.8, 79.2, 100.3; ESIMS *m/z* 441.3 [M + Na]<sup>+</sup>.

**Compound 6:** <sup>1</sup>H-NMR (C<sub>5</sub>D<sub>5</sub>N, 500 MHz): 1.58 (3H, s), 1.83 (3H, s), 2.01 (dd, *J* = 15.0, 4.5 Hz), 2.53 (d, *J* = 15.0 Hz), 3.51 (s), 3.96, 4.04, 4.06, 4.21, 4.25, 4.31 (dd, *J* = 12.0, 5.5 Hz), 4.50 (dd, *J* = 11.5, 2.0 Hz), 5.15 (overlap), 5.30 (d, *J* = 7.5 Hz), 6.51 (d, *J* = 6.0 Hz), 6.68 (s); <sup>13</sup>C-NMR (C<sub>5</sub>D<sub>5</sub>N, 125 MHz): 21.9, 22.5, 45.7, 55.2, 62.7, 71.6, 72.9, 74.7, 76.8, 78.3, 78.6, 87.2, 94.5, 99.2, 107.9, 142.2, 170.9; ESIMS *m/z* 429.1 [M + Na]<sup>+</sup>, 405.0 [M – H]<sup>–</sup>.

**Compound 7:** <sup>1</sup>H-NMR (C<sub>5</sub>D<sub>5</sub>N, 500 MHz): 1.47 (3H, s), 1.49 (3H, s), 1.50 (3H, s), 1.92, 1.94, 2.20, 2.42, 3.77 (dd, *J* = 10.0, 1.5 Hz), 6.20 (dd, *J* = 17.0, 10.5 Hz), 5.14 (dd, *J* = 6.5, 2.0 Hz), 5.78 (dd, *J* = 17.5, 2.0 Hz); <sup>13</sup>C-NMR (C<sub>5</sub>D<sub>5</sub>N, 125 MHz): 25.9, 26.1, 26.9, 28.7, 41.1, 72.5, 72.7, 79.8, 111.1, 147.5; ESIMS *m/z* 211.2 [M + Na]<sup>+</sup>, 399.2 [2M + Na]<sup>+</sup>, 187.1 [M – H]<sup>–</sup>.

**Compound 8:** <sup>1</sup>H-NMR (C<sub>5</sub>D<sub>5</sub>N, 500 MHz): 3.32 (2H, d, *J* = 7.0 Hz), 3.73 (3H, s), 4.11, 4.34–4.40 (4H), 4.53 (brd, *J* = 11.0 Hz), 5.08 (2H), 5.66 (d, *J* = 7.0 Hz), 6.00, 6.77 (dd, *J* = 8.5, 2.0 Hz), 6.90 (d, *J* = 1.5 Hz), 7.53 (d, *J* = 8.5 Hz); <sup>13</sup>C-NMR (C<sub>5</sub>D<sub>5</sub>N, 125 MHz): 39.9, 55.9, 62.4, 71.3, 74.9, 78.6, 78.8, 102.4, 113.6, 115.6, 116.6, 121.3, 134.3, 138.3, 146.4, 149.9; ESIMS *m/z* 349.1 [M + Na]<sup>+</sup>, 325.0 [M – H]<sup>–</sup>.

**Compound 9:** <sup>1</sup>H-NMR (C<sub>5</sub>D<sub>5</sub>N, 500 MHz): 3.21, 3.76 (3H, s), 3.79 (3H, s), 4.34 (2H), 4.94 (2H), 5.71 (d, *J* = 6.5 Hz), 7.01 (dd, *J* = 8.0, 1.5 Hz), 7.09 (dd, *J* = 8.0, 1.5 Hz), 7.23 (d, *J* = 8.0 Hz), 7.23 (d, *J* = 2.0 Hz), 7.26 (d, *J* = 2.0 Hz), 7.60 (d, *J* = 8.0 Hz); <sup>13</sup>C-NMR (C<sub>5</sub>D<sub>5</sub>N, 125 MHz): 54.7, 54.8, 55.9, 56.0, 62.4, 71.3 (2C), 72.0, 74.9, 78.6, 78.9, 86.3, 86.4, 102.4, 110.9, 111.3, 116.3, 116.5, 119.0, 119.7, 133.0, 136.0, 147.0, 147.9, 148.8, 150.1; ESIMS *m/z* 543.2 [M + Na]<sup>+</sup>, 519.0 [M – H]<sup>–</sup>.

**Compound 10:** <sup>1</sup>H-NMR (C<sub>5</sub>D<sub>5</sub>N, 500 MHz): 3.98, 4.12, 4.28, 4.42 (dd, *J* = 12.0, 5.5 Hz), 4.59 (d, *J* = 11.0 Hz), 4.83 (d, *J* = 12.0 Hz), 4.99 (d, *J* = 7.5 Hz), 5.16 (d, *J* = 12.0 Hz), 7.28 (3H), 7.52 (2H, d, *J* = 7.0 Hz); <sup>13</sup>C-NMR (C<sub>5</sub>D<sub>5</sub>N, 125 MHz): 62.8, 70.8, 71.7, 75.2, 78.5, 78.6, 104.0, 127.7, 128.2 (2C), 128.6 (2C), 138.9; ESIMS *m/z* 293.1 [M + Na]<sup>+</sup>, 269.0 [M – H]<sup>–</sup>.

**Compound 11:**  $^1\text{H-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 500 MHz): 3.36 (2H, d,  $J = 6.5$  Hz), 3.75 (3H, s), 5.00 (2H, overlap), 6.05, 6.84 (d,  $J = 8.0$  Hz), 6.91 (s), 7.21 (overlap);  $^{13}\text{C-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 125 MHz): 40.0, 55.8, 113.1, 115.3, 116.5, 121.7, 131.2, 138.8, 146.6, 148.6.

**Compound 12:**  $^1\text{H-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 500 MHz): 3.73 (3H), 7.26 (d,  $J = 8.0$  Hz), 7.57 (overlap), 7.64 (brs), 10.01 (s);  $^{13}\text{C-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 125 MHz): 55.7, 110.9, 116.5, 127.1, 129.7, 149.2, 154.8, 190.7; ESIMS  $m/z$  153.3  $[\text{M} + \text{H}]^+$ , 175.3  $[\text{M} + \text{Na}]^+$ , 151.1  $[\text{M} - \text{H}]^-$ .

**Compound 13:**  $^1\text{H-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 500 MHz): 3.88 (3H, s), 3.94 (3H, s), 6.05 (s), 6.93 (d,  $J = 8.0$  Hz), 7.55 (d,  $J = 1.5$  Hz), 7.63 (dd,  $J = 1.5, 8.0$  Hz);  $^{13}\text{C-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 125 MHz): 51.9, 56.1, 111.7, 114.0, 122.3, 124.2, 146.1, 145.0, 166.9; ESIMS  $m/z$  183.3  $[\text{M} + \text{H}]^+$ , 181.1  $[\text{M} - \text{H}]^-$ .

**Compound 14:**  $^1\text{H-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 500 MHz): 1.05 (3H, s), 1.05 (3H, s), 1.19, 1.20 (3H, s), 1.46, 1.56, 1.62, 1.81, 1.97, 2.05, 2.20, 2.29, 2.46, 3.73;  $^{13}\text{C-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 125 MHz): 21.0, 21.2, 27.9, 29.4, 30.8, 34.7, 35.0, 35.1, 36.2, 39.3, 39.9, 43.9, 44.4, 70.1, 71.8; ESIMS  $m/z$  256.3  $[\text{M} + \text{NH}_4]^+$ , 221.3  $[\text{M} + \text{H} - \text{H}_2\text{O}]^+$ , 203.3  $[\text{M} + \text{H} - 2\text{H}_2\text{O}]^+$ .

**Compound 15:**  $^1\text{H-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 500 MHz): 0.92 (3H, s), 1.06 (d,  $J = 12.0$  Hz), 1.13 (3H, s), 1.22 (3H, s), 1.22 (overlap), 1.41 (2H), 1.43, 1.59 (dd,  $J = 11.5, 5.0$  Hz), 1.89 (d,  $J = 8.0$  Hz), 1.95 (bt,  $J = 15.8, 2.5$  Hz), 2.14 (tt,  $J = 14.0, 4.0$  Hz), 2.21 (d,  $J = 12.5$  Hz), 2.51 (td,  $J = 13.5, 5.0$  Hz), 3.59 (s), 4.16 (t,  $J = 8.0$  Hz);  $^{13}\text{C-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 125 MHz): 21.3, 25.8, 27.3, 27.9, 29.5, 31.8, 33.8, 35.4, 36.5, 37.3, 45.3, 48.4, 51.2, 74.6, 80.4; ESIMS  $m/z$  256.3  $[\text{M} + \text{NH}_4]^+$ .

**Compound 16:**  $^1\text{H-NMR}$  ( $\text{CD}_3\text{OD}$ , 500 MHz): 7.24 (td,  $J = 6.0, 1.0$  Hz), 7.28 (td,  $J = 6.0, 1.0$  Hz), 7.47 (d,  $J = 8.0$  Hz), 8.09 (s), 8.15 (d,  $J = 8.0$  Hz), 9.88 (s);  $^{13}\text{C-NMR}$  ( $\text{CD}_3\text{OD}$ , 125 MHz): 113.1, 120.2, 122.3, 123.7, 125.1, 125.7, 138.9, 139.5, 187.3; ESIMS  $m/z$  146.0  $[\text{M} + \text{H}]^+$ , 143.7  $[\text{M} - \text{H}]^-$ .

**Compound 17:**  $^1\text{H-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 500 MHz): 3.77 (3H, s), 6.30 (d,  $J = 9.5$  Hz), 7.04 (s), 7.13 (s), 7.69 (d,  $J = 9.5$  Hz);  $^{13}\text{C-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 125 MHz): 56.2, 104.1, 109.4, 111.0, 112.2, 144.1, 146.3, 151.2, 154.3, 161.5; ESIMS  $m/z$  214.9  $[\text{M} + \text{Na}]^+$ , 190.7  $[\text{M} - \text{H}]^-$ .

**Compound 18:**  $^1\text{H-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 500 MHz): 3.01 (2H, t,  $J = 7$  Hz), 3.88 (m), 6.88 (d,  $J = 15.5$  Hz), 7.12–1.26 (7H, m), 8.11 (d,  $J = 15.5$  Hz), 8.66 (NH);  $^{13}\text{C-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 125 MHz): 35.6, 41.9, 55.7, 111.2, 116.3 (2C), 116.8, 119.7, 122.4, 127.4, 130.4 (2C), 130.5, 140.3, 148.8, 149.9, 157.4, 166.7; ESIMS  $m/z$  311.9  $[\text{M} - \text{H}]^-$ .

**Compound 19:**  $^1\text{H-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 500 MHz): 1.63 (3H, s), 4.10–4.54 (5H);  $^{13}\text{C-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 125 MHz): 20.6, 63.9, 68.8, 74.7, 76.0; ESIMS  $m/z$  159.3  $[\text{M} + \text{Na}]^+$ , 135.3  $[\text{M} - \text{H}]^-$ .

**Compound 20:**  $^1\text{H-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 500 MHz): 0.67 (3H, s), 1.21, 1.22, 1.32 (td,  $J = 13.0, 4.0$  Hz), 1.51 (3H, s), 1.67 (dt,  $J = 13.0, 3.0$  Hz), 1.79 (dt,  $J = 13.0, 2.0$  Hz), 1.87 (dd,  $J = 9.5, 4.0$  Hz), 1.95, 1.97 (2H), 2.32 (brd,  $J = 10.0$  Hz), 2.72 (2H), 3.66, 4.87 (2H, d,  $J = 10.0$  Hz), 5.38 (d,  $J = 6.0$  Hz), 7.18 (t,  $J = 5.5$  Hz);  $^{13}\text{C-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 125 MHz): 15.2, 23.7, 24.3, 25.0, 29.0, 37.3, 38.2, 39.1, 43.2, 55.3, 56.3, 64.2, 66.0, 75.4, 79.8, 108.8, 130.2, 147.0, 147.9, 170.8; ESIMS  $m/z$  373.2  $[\text{M} + \text{Na}]^+$ , 349.1  $[\text{M} - \text{H}]^-$ .

**Compound 21:**  $^1\text{H-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 500 MHz): 3.97, 3.99, 4.07 (brt,  $J = 8.1$  Hz), 4.30 (2H, m), 4.42 (dd,  $J = 11.7, 5.3$  Hz), 4.58 (dd,  $J = 11.8, 2.5$  Hz), 5.07 (d,  $J = 7.7$  Hz), 5.36 (brs);  $^{13}\text{C-NMR}$  ( $\text{C}_5\text{D}_5\text{N}$ , 125 MHz): 12.0, 12.2, 19.0, 19.2, 19.4, 20.0, 21.3, 23.4, 24.5, 26.5, 28.6, 29.5, 30.3, 32.1, 32.2, 34.3, 36.4, 37.0, 37.5, 39.4, 40.0, 42.5, 46.1, 50.4, 56.3, 56.9, 62.9, 71.8, 75.4, 78.2, 78.5, 78.6, 102.6, 121.9, 141.0.