

## MATERIAL SUPLEMENTAR

### **Insecticidal activity of dienamides on cabbage caterpillar and beneficial insects**

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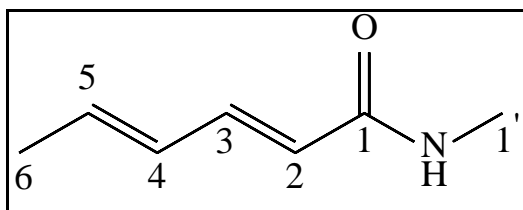
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**(2E,4E)-N-methylhexa-2,4-dienamide [1].**



[1]

**Molecular Formula:** C<sub>7</sub>H<sub>11</sub>NO

**Feature:** White solid.

**TLC:** R<sub>f</sub> = 0.43 (hexane/ethyl acetate 1:2 v/v)

**Yield:** 74% (423.3 mg)

**m.p.:** 80.6 – 81.3 °C

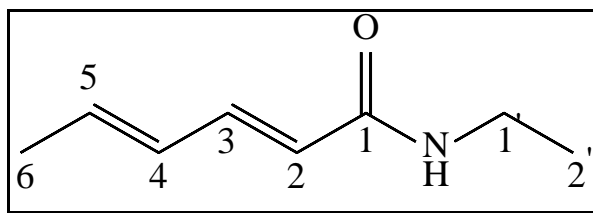
**IR (KBr pellet,  $\bar{\nu}/\text{cm}^{-1}$ ):** 3301; 2940; 2914; 1658; 1629; 1618; 992.

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  (J/Hz):** 1.80 (d, *J* = 5.7 Hz, 3H), 2.85 (d, *J* = 4.7 Hz, 3H), 5.78 (d, *J* = 15.3 Hz, 1H), 6.18 – 5.98 (m, 3H), 7.15 (dd, *J* = 15.0, 10.0 Hz, 1H),

**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$ :** 18.5 (C6), 26.2 (C1'), 121.3 (C2), 129.6 (C4), 137.5 (C5), 140.8 (C3), 167.2 (C1).

**MS, m/z (%):** 125 (M<sup>+</sup>, C<sub>7</sub>H<sub>11</sub>NO, 32); 110 (50); 95 (52); 81 (4); 67 (100); 43 (15); 41 (9)

**(2E,4E)-N-ethylhexa-2,4-dienamide [2].**



[2]

**Molecular Formula:** C<sub>8</sub>H<sub>13</sub>NO

**Feature:** White solid.

**TLC:** R<sub>f</sub> = 0.61 (hexane/ethyl acetate 1:2 v/v)

**Yield:** 69% (428.5 mg)

**m.p.:** 68.5 – 69.6 °C

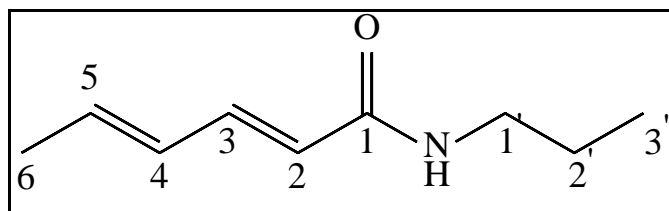
**IR (KBr pellet,  $\bar{\nu}/\text{cm}^{-1}$ ):** 3291; 2979; 2882; 1655; 1612; 1255; 995.

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  (J/Hz):** 1.13 (t, *J* = 7.2 Hz, 3H), 1.79 (t, *J* = 6.0 Hz, 3H), 3.33 (q, *J* = 7.1 Hz, 2H), 5.76 (d, *J* = 15.0 Hz, 1H), 6.18 – 5.96 (m, 3H), 7.14 (dd, *J* = 15.0, 10.0 Hz, 1H).

**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$ :** 14.7 (C2'), 18.4 (C6), 34.3 (C1'), 121.7 (C2), 129.6 (C4), 137.3 (C5), 140.7 (C3), 166.3 (C1).

**MS, m/z (%):** 139 (M<sup>+</sup>, C<sub>8</sub>H<sub>13</sub>NO, 33); 124 (43); 110 (7); 95 (94); 81 (11); 67 (100); 44 (48); 41 (94).

**(2E,4E)-N-propylhexa-2,4-dienamide [3].**



**[3]**

**Molecular Formula:** C<sub>9</sub>H<sub>15</sub>NO

**Feature:** White solid.

**TLC:** R<sub>f</sub> = 0.55 (hexane/ethyl acetate 1:2 v/v)

**Yield:** 86% (587.1 mg)

**m.p.:** 82.3 – 84.1 °C

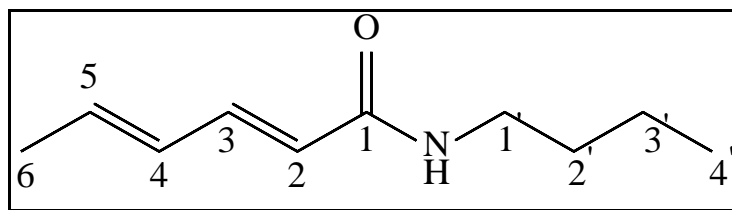
**IR (KBr pellet,  $\bar{\nu}/\text{cm}^{-1}$ ):** 3291; 2979; 2882; 1655; 1612

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  (J/Hz):** 0.91 (t,  $J$  = 7.4 Hz, 3H), 1.53 (sext,  $J$  = 7.3 Hz, 2H), 1.80 (d,  $J$  = 5.8 Hz, 3H), 3.27 (Ha, t,  $J$  = 7.1 Hz, 1H) e (Hb, t,  $J$  = 6.6 Hz, 1H), 5.77 (d,  $J$  = 15.1 Hz, 1H), 6.21 – 5.92 (m, 3H), 7.16 (dd,  $J$  = 15.0, 10.1 Hz, 1H).

**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$ :** 11.3 (C3'), 18.5 (C6), 22.8 (C2'), 41.2 (C1'), 121.6 (C2), 129.6 (C4), 137.4 (C5), 140.8 (C3), 166.4 (C1).

**MS, m/z (%):** 153 (M<sup>+</sup>, C<sub>9</sub>H<sub>15</sub>NO, 32); 138 (19); 124 (9); 110 (11); 95 (100); 81 (6); 67 (56); 65 (19); 41 (67); 39 (41).

**(2E,4E)-N-butylhexa-2,4-dienamide [4].**



**[4]**

**Molecular Formula:** C<sub>10</sub>H<sub>17</sub>NO

**Feature:** Yellow solid.

**TLC:** R<sub>f</sub> = 0.65 (hexane/ethyl acetate 2:1 v/v)

**Yield:** 68% (509.2 mg)

**m.p.:** 59.3 – 60.1 °C

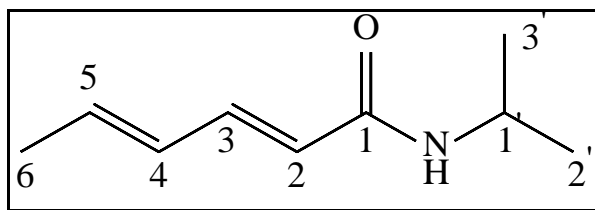
**IR (KBr pellet,  $\bar{\nu}/\text{cm}^{-1}$ ):** 3304; 2967; 2936; 1656; 1618; 1540, 996.

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  (J/Hz):** 0.90 (t, *J* = 7.2 Hz, 3H), 1.33 (dq, *J* = 14.1, 7.0 Hz, 2H), 1.49 (dq, *J* = 11.9, 7.0 Hz, 2H), 1.80 (d, *J* = 5.7 Hz, 3H), 3.30 (dd, *J* = 13.0, 7.0 Hz, 2H), 5.77 (d, *J* = 15.0 Hz, 1H), 6.19 – 5.95 (m, 3H), 7.15 (dd, *J* = 15.0, 10.0 Hz, 1H).

**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$ :** 13.7 (C4'), 18.4 (C6), 20.0 (C3'), 31.6 (C2'), 39.2 (C1'), 121.6 (C2), 129.6 (C4), 137.3 (C5), 140.7 (C3), 166.4 (C1).

**MS, m/z (%):** 167 (M<sup>+</sup>, C<sub>10</sub>H<sub>17</sub>NO, 32); 152 (16); 138 (7); 124 (12); 110 (16); 95 (100); 82 (5); 67 (100); 65 (16); 44 (32); 41 (84); 32 (76).

**(2E,4E)-N-isopropylhexa-2,4-dienamide [5].**



[5]

**Molecular Formula:** C<sub>9</sub>H<sub>15</sub>NO

**Feature:** White solid.

**TLC:** R<sub>f</sub> = 0.68 (hexane/ethyl acetate/dichloromethane 1:1:1 v/v)

**Yield:** 57% (309.9 mg)

**m.p.:** 108.1 – 109.7 °C

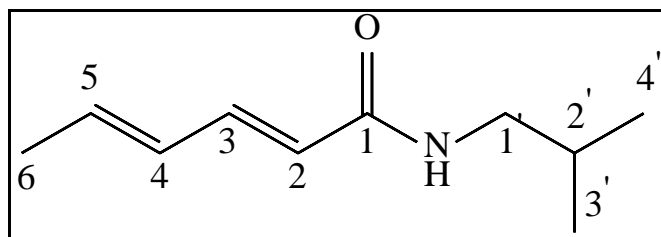
**IR (KBr pellet,  $\bar{\nu}$ /cm<sup>-1</sup>):** 3209; 2971; 2930; 2874; 1656; 1628; 1546; 908.

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  (J/Hz):** 1.15 (d, *J* = 6.3 Hz, 6H), 1.79 (d, *J* = 5.7 Hz, 3H), 4.13 (dhept, *J* = 19.8, 6.6 Hz, 1H), 5.77 (dd, *J* = 18.4, 10.3 Hz, 2H), 6.17 – 5.96 (m, 2H), 7.14 (dd, *J* = 15.0, 10.0 Hz, 1H).

**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$ :** 18.4 (C<sub>6</sub>), 22.6 (C<sub>2'</sub> e C<sub>3'</sub>), 41.2 (C<sub>1'</sub>), 121.9 (C<sub>2</sub>), 129.6 (C<sub>4</sub>), 137.2 (C<sub>5</sub>), 140.7 (C<sub>3</sub>), 165.5 (C<sub>1</sub>).

**MS, m/z (%):** 153 (M<sup>+</sup>, C<sub>9</sub>H<sub>15</sub>NO, 22); 138 (12); 112 (1); 110 (6); 95 (100); 81 (10); 67 (61); 44 (33); 41 (81).

**(2E,4E)-N-isobutylhexa-2,4-dienamide [6].**



**Molecular Formula:** C<sub>10</sub>H<sub>17</sub>NO

**Feature:** White solid.

**TLC:** R<sub>f</sub> = 0.40 (hexane/ethyl acetate 3:1 v/v)

**Yield:** 73% (554.1 mg)

**m.p.:** 87.9 – 88.7 °C

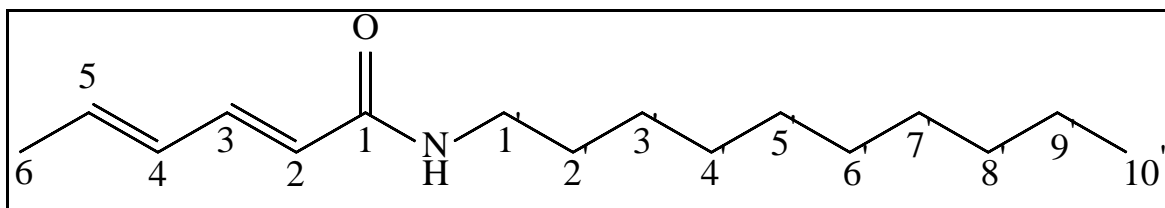
**IR (KBr pellet,  $\bar{\nu}/\text{cm}^{-1}$ ):** 3297; 2971; 2914; 2868; 1657; 1630; 1546; 908.

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  (J/Hz):** 0.90 (d, *J* = 6.7 Hz, 6H), 1.86 – 1.69 (m, 4H), 3.13 (t, *J* = 6.5 Hz, 2H), 5.79 (d, *J* = 15.0 Hz, 1H), 6.20 – 5.96 (m, 3H), 7.16 (dd, *J* = 15.0, 10.0 Hz, 1H).

**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$ :** 18.5 (C6), 20.0 (C3' e C4'), 28.5 (C2'), 46.8 (C1'), 121.6 (C2), 129.6 (C4), 137.4 (C5), 140.8 (C3), 166.5 (C1).

**MS, m/z (%):** 167 (M<sup>+</sup>, C<sub>10</sub>H<sub>17</sub>NO, 5); 152 (15); 124 (4); 110 (4); 95 (100); 77 (6); 67 (42); 52 (6); 41 (38).

(2E,4E)-N-decylohexa-2,4-dienamide [7].



[7]

**Molecular Formula:** C<sub>16</sub>H<sub>29</sub>NO

**Feature:** White solid.

**TLC:** R<sub>f</sub> = 0.58 (hexane/ethyl acetate/dichloromethane 3:1:1 v/v)

**Yield:** 77% (870.6 mg)

**m.p.:** 81.9 – 82.7 °C

**IR (KBr pellet,  $\bar{\nu}/\text{cm}^{-1}$ ):** 3295; 3021; 2952; 2925; 2851; 1657; 1540; 995.

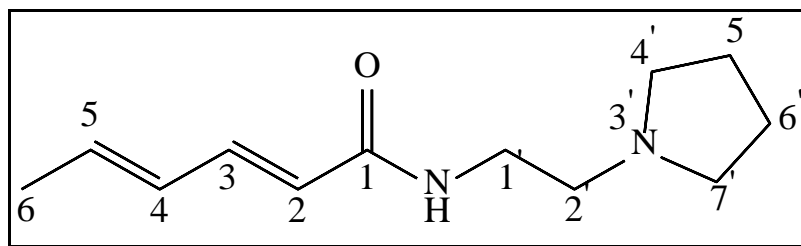
**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  (J/Hz):** 0.86 (t, *J* = 6.6 Hz, 3H), 1.24 (s, 16H), 1.57 – 1.43 (m, 2H), 1.81 (d, *J* = 5.7 Hz, 1H), 3.30 (dd, *J* = 12.9, 6.6 Hz, 2H), 5.75 (d, *J* = 15.0 Hz, 2H), 6.20 – 5.99 (m, 2H), 7.17 (dd, *J* = 14.9, 9.9 Hz, 1H).

**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$ :** 14.0 (C10'), 18.5 (C6), 22.6 (C9'), 26.9 (C3'), 29.2 (C7'), 29.2 (C4'), 29.5 (C5' e C6'), 29.6 (C8'), 31.8 (C2'), 39.6 (C1'), 121.6 (C2), 129.6 (C4), 137.4 (C5), 140.8 (C3), 166.3 (C1).

**MS, m/z (%):** 251 (M<sup>+</sup>, C<sub>16</sub>H<sub>29</sub>NO, 9); 236 (9); 222 (3); 208 (4); 194 (3); 180 (6); 166 (12); 152 (13); 138 (8), 125 (19); 110 (21), 95 (100); 83 (5), 67 (36); 55 (10), 41 (51); 39 (19).



(2*E*,4*E*)-*N*-(2-(pyrrolidin-1-yl)ethyl)hexa-2,4-dienamide [8].



[8]

**Molecular Formula:** C<sub>12</sub>H<sub>20</sub>N<sub>2</sub>O

**Feature:** Yellow solid.

**TLC:** R<sub>f</sub> = 0.16 (ethyl acetate/methanol 25%/dichloromethane 10%)

**Yield:** 41% (384.8 mg)

**m.p.:** 99.5 – 100.1 °C

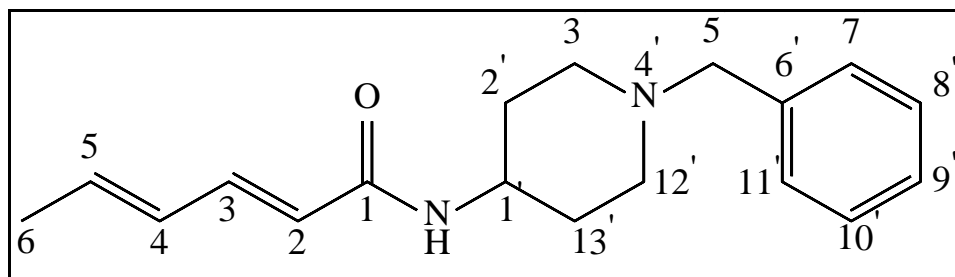
**IR (KBr pellet,  $\bar{\nu}$ /cm<sup>-1</sup>):** 3444; 3258; 2940; 2794; 2770; 1656; 1631; 1567; 1001.

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  (J/Hz):** 1.45 (d, *J* = 4.8 Hz, 2H), 1.64 – 1.57 (m, 3H), 1.81 (d, *J* = 6.0 Hz, 3H), 2.53 – 2.35 (m, 5H), 3.42 (dd, *J* = 11.1, 5.4 Hz, 2H), 5.79 (d, *J* = 15.0 Hz, 1H), 6.21 – 5.96 (m, 2H), 6.50 (s, 1H), 7.16 (dd, *J* = 15.0, 10.0 Hz, 1H).

**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$ :** 18.5 (C<sub>6</sub>), 25.5 (C<sub>5'</sub> e C<sub>6'</sub>), 35.8 (C<sub>1'</sub>), 54.2 (C<sub>4'</sub> e C<sub>7'</sub>), 57.2 (C<sub>2'</sub>), 121.6 (C<sub>2</sub>), 129.6 (C<sub>4</sub>), 137.4 (C<sub>5</sub>), 140.8 (C<sub>3</sub>), 166.3 (C<sub>1</sub>).

**MS, m/z (%):** 208 (M<sup>+</sup>, C<sub>12</sub>H<sub>20</sub>N<sub>2</sub>O, 2); 138 (3); 125 (0.1); 111 (18); 98 (100); 82 (3); 67 (9); 55 (11); 41 (38); 32 (13).

(2*E*,4*E*)-*N*-(1-benzylpiperidin-4-yl)hexa-2,4-dienamide [9].



[9]

**Molecular Formula:** C<sub>18</sub>H<sub>24</sub>N<sub>2</sub>O

**Feature:** White solid.

**TLC:** R<sub>f</sub> = 0.41 (ethyl acetate/methanol – 95:5 v/v)

**Yield:** 52% (663.3 mg)

**m.p.:** 153.3 – 154.7 °C

**IR (KBr pellet,  $\bar{\nu}/\text{cm}^{-1}$ ):** 3235; 3066; 2955; 2800; 2762; 1656; 1627; 1555; 995. Falta c

**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  (J/Hz):** 1.56 – 1.40 (m, *J* = 3.6 Hz, 1H), 1.82 (d, *J* = 5.4 Hz, 3H), 1.92 (d, *J* = 12.3 Hz, 2H), 2.13 (dt, *J* = 11.4 Hz, 2H), 2.27 (s, 1H), 2.82 (d, *J* = 12.0 Hz, 2H), 3.49 (s, 2H), 3.97 – 3.79 (m, 1H), 5.51 (d, *J* = 7.8 Hz, 1H), 5.71 (d, *J* = 15.0 Hz, 1H), 6.20 – 5.98 (m, 2H), 7.16 (dd, *J* = 15.0, 9.9 Hz, 1H), 7.30 (d, *J* = 3.9 Hz, 4H).

**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$ :** 18.5 (C<sub>6</sub>), 32.1 (C<sub>2'</sub> e C<sub>13'</sub>), 46.4 (C<sub>1'</sub>), 52.2 (C<sub>3'</sub> e C<sub>12'</sub>), 63.0 (C<sub>5'</sub>), 121.5 (C<sub>2</sub>), 127.0 (C<sub>9'</sub>), 128.1 (C<sub>7'</sub> e C<sub>11'</sub>), 129.1 (C<sub>8'</sub> e C<sub>10'</sub>), 129.5 (C<sub>4</sub>), 137.7 (C<sub>5</sub>), 138.0 (C<sub>6'</sub>), 141.1 (C<sub>3</sub>), 165.6 (C<sub>1</sub>)

**MS, m/z (%):** 284 (M<sup>+</sup>, C<sub>18</sub>H<sub>24</sub>N<sub>2</sub>O, 4); 269 (1); 253 (0.37); 207 (1); 193 (3); 172 (65); 159 (5); 146 (6); 132 (7); 118 (4); 91 (100); 82 (78); 65 (16); 56 (12); 41 (28).



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