## **One-Pot Synthesis of 4-Arylidene Imidazolin-5-ones**

## by Reaction of Amino Acid Esters with Isocyanates

## and a-Bromoketones

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#### **Characterization Data**

#### (S)-methyl 3-(3,4-dimethoxyphenyl)-2-(3-phenethylthioureido)propanoate (3b)

Yellow oil, (84%, 141 mg); <sup>1</sup>H NMR (600 MHz, acetone- $d_6$ )  $\delta$  7.35 - 7.30 (m, 1H), 7.29 - 7.24 (m, 2H), 7.23 - 7.18 (m, 2H), 6.94 (d, J = 3.7 Hz, 1H), 6.82 (d, J = 4.0 Hz, 1H), 6.74 (s, 1H), 6.66 (d, J = 5.3 Hz, 1H), 5.39 (s, 1H), 3.87 (t, J = 6.3 Hz, 1H), 3.77 (m, 2H), 3.78, 3.76 (s, 3H), 3.75 (s, 3H), 3.69 s, 3H), 3.18 (dd, J = 9.3 Hz, J = 3.8 Hz, 1H), 3.02 (dd, J = 9.3 Hz, J = 4.1 Hz, 1H), 2.88 (t, J = 4.9 Hz, 2H); <sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>)  $\delta$  183.3, 173.5, 149.0, 148.8, 137.7, 128.5, 128.4, 128.3, 126.5, 121.5, 112.4, 77.1, 76.9, 60.4, 58.8, 55.9, 55.7, 37.3, 36.8, 34.8, 33.2; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>21</sub>H<sub>26</sub>N<sub>2</sub>O<sub>4</sub>S 403.1692, Found 403.1686; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = + 146.62 (c = 0.09, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 10% *i*-PrOH / Hexane, 0.5 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 33.7 min; IR (cm<sup>-1</sup>, neat): 3342, 2924, 2834, 1512.

#### (S)-methyl 2-(3-cyclohexylureido)-3-(3,4-dimethoxyphenyl)propanoate (3k)

White solid, (88%, 134 mg); mp 149 – 151 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  6.73 (d, J = 8.0 Hz, 1H), 6.62 (s, 1H), 6.60 (d, J = 7.6 Hz, 1H), 5.08 (d, J = 8.0 Hz, 1H), 4.76 (d, J = 8.0 Hz, 1H), 4.68 (dd, J = 13.9 Hz, J = 6.0 Hz, 1H), 3.80 (s, 3H), 3.79 (s, 3H), 3.68 (s, 3H), 3.42 (m, 1H), 2.99 (dd, J = 13.9 Hz, J = 6.0 Hz, 1H), 2.93 (dd, J = 13.9 Hz, J = 6.0 Hz, 1H), 1.83 (m, 2H), 1.59 (m, 3H), 1.27 (m, 2H), 1.06 (m, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  173.6, 156.7, 148.7, 147.9, 128.8, 121.3, 112.5, 111.1, 55.8, 55.7, 54.1, 52.1, 49.1, 38.1, 33.8, 33.7, 25.5, 24.8; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>19</sub>H<sub>29</sub>N<sub>2</sub>O<sub>5</sub> 365.2076, Found 365.2071; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = + 51.28 (c = 0.019, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 13.4 min; IR (cm<sup>-1</sup>, neat): 3322, 2929, 2851, 1572.

#### (S)-methyl 3-(3,4-dimethoxyphenyl)-2-(3-phenylselenoureido) propanoate (3h)

Yellow oil, (85%, 150 mg); <sup>1</sup>H NMR (600 MHz, acetone- $d_6$ )  $\delta$  9.52 (s, 1H), 7.36 (t, J = 7.7 Hz, 2H), 7.26 - 7.21 (m, 3H), 6.84 (d, J = 8.1 Hz, 2H), 6.77 (s, 1H), 6.68 (d, J = 8.1 Hz, 2H), 5.54 (s, 1H), 3.77 (s, 3H), 3.73 (s, 3H), 3.72 (s, 3H), 3.30 (dd, J = 14.1 Hz, J = 5.7 Hz, 1H), 3.12 (dd, J = 14.1 Hz, J = 6.5 Hz, 1H); <sup>13</sup>C NMR (151 MHz, acetone- $d_6$ )  $\delta$  179.9, 171.5, 149.3, 148.5, 137.4, 129.5, 128.5, 126.3, 124.5, 124.5, 124.4, 121.3, 113.0, 111.9, 60.8, 55.2, 55.1, 51.7, 36.5; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>19</sub>H<sub>22</sub>N<sub>2</sub>O<sub>4</sub>Se 423.0823, Found 423.0858; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = + 60.35 (c = 0.10, CH<sub>2</sub>Cl<sub>2</sub>); HPLC

analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee:  $t_R = 13.6$  min.; IR (cm<sup>-1</sup>, neat): 3331, 2951, 1737, 1463.

#### 5-(benzo[d][1,3]dioxol-5-ylmethyl)-3-methyl-2-thioxoimidazolidin-4-one (6g)

Pale Yellow solid, (85%, 94 mg); mp 165 – 167 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.29 (s, 1H), 6.76 (d, *J* = 7.9 Hz, 1H), 6.69 – 6.62 (m, 2H), 5.95 (s, 2H), 4.24 (dd, *J* = 9.3 Hz, *J* = 3.9 Hz, 1H), 3.23 (dd, *J* = 14.1 Hz, *J* = 3.9 Hz, 1H), 3.20 (s, 3H), 2.76 (dd, *J* = 14.1 Hz, *J* = 9.3 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  184.1, 173.2, 148.2, 147.1, 128.4, 122.2, 109.2, 108.7, 101.2, 60.8, 37.3, 27.5; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>12</sub>H<sub>13</sub>N<sub>2</sub>O<sub>3</sub>S 265.0647, Found 265.0642; IR (cm<sup>-1</sup>, neat): 3202, 2915, 2849, 1500.

#### 5-(3,4-dimethoxybenzyl)-3-(3-phenylpropyl)-2-selenoxoimidazolidin-4-one (6c)

Yellow solid, (87%, 157 mg); mp 160 – 162 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.90 (s, 1H), 7.22 (m, 5H), 6.72 (m, 3H), 4.05 (dd, J = 8.6 Hz, J = 3.8 Hz, 1H), 3.86 (s, 3H), 3.85 (m, 2H), 3.77 (s, 3H), 3.20 (dd, J = 14.2 Hz, J = 3.9 Hz, 1H), 2.80 (dd, J = 14.1 Hz, J = 8.3 Hz, 1H), 2.57 (t, J = 6.8 Hz, 1H), 1.88 (m, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  184.5, 172.7, 149.0, 148.5, 140.8, 128.3, 128.2, 128.2, 128.1, 126.2, 125.9, 121.5, 112.4, 111.4, 111.3, 61.5, 56.0, 55.8, 42.4, 36.2, 32.8, 28.7; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>21</sub>H<sub>25</sub>N<sub>2</sub>O<sub>3</sub>Se 433.1030, Found 433.1018; IR (cm<sup>-1</sup>, neat): 3288, 2931, 2850, 1515.

#### 3-cyclohexyl-5-(3,4-dimethoxybenzyl)imidazolidine-2,4-dione (6k)

White solid, (78%, 108 mg); mp 155 – 157 °C; <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD)  $\delta$  6.83 (d, J = 8.4 Hz, 1H), 6.79 (s, 1H), 6.71 (d, J = 8.4 Hz, 1H), 4.23 (s, 1H), 3.79 (s, 3H), 3.77 (s, 3H), 3.58 (t, J = 11.1 Hz, 1H), 3.45 (t, J = 11.1 Hz, 1H), 3.30 (s, 1H), 1.86 (m, 2H), 1.71 (m, 2H), 1.59 (m, 1H), 1.31 (m, 3H), 1.17 (m, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  173.0, 149.1, 148.3, 127.5, 121.4, 112.2, 111.4, 57.6, 55.9, 55.8, 51.3, 37.6, 32.8, 32.2, 29.2, 29.0, 25.7, 25.1, 24.9, 24.7, 24.4; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>18</sub>H<sub>25</sub>N<sub>2</sub>O<sub>4</sub> 333.1814, Found 333.1814; IR (cm<sup>-1</sup>, neat): 3330, 2927, 2852, 1706.

#### (Z)-5-(3,4-dimethoxybenzylidene)-3-(3-phenylpropyl)-2-selenoxoimidazo-lidin-4one (8b)

Yellow solid, (80%, 144 mg); mp 130 – 132 °C; <sup>1</sup>H NMR (600 MHz, acetone- $d_6$ )  $\delta$  7.41 (d, J = 6.8 Hz, 1H), 7.32 (s, 1H), 7.28 - 7.25 (m, 3H), 7.19 - 7.14 (m, 1H), 7.06 -

6.96 (m, 2H), 6.73(s, 1H), 4.01 (t, J = 7.4Hz, 2H), 3.89 (s, 3H), 3.87 (s, 3H), 2.79 (s, 2H), 2.70 (d, J = 8.1 Hz, 1H); <sup>13</sup>C NMR (151 MHz, acetone- $d_6$ )  $\delta$  151.2, 149.6, 141.3, 128.2, 128.2, 126.2, 125.8, 125.7, 123.9, 113.4, 111.8, 111.2, 55.4, 55.2, 55.1, 42.2, 32.8, 32.7; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>21</sub>H<sub>23</sub>N<sub>2</sub>O<sub>3</sub>Se 431.0874, Found 431.0868; IR (cm<sup>-1</sup>, neat): 3272, 2927, 2850, 1516.

### ((*S*, *Z*)-methyl 3-(3,4-dimethoxyphenyl)-2-(2-(phenethylimino)-4-phenyl-thiazol-3(2H)-yl)propanoate (5b)

Yellow oil, (79%, 166 mg); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.31 (m, 3H), 7.14 (m, 3H), 6.98 (d, J = 6.7 Hz, 2H), 6.86 (d, J = 6.0 Hz, 1H), 6.80 (m, 2H), 6.73 (d, J = 8.6 Hz, 1H), 5.60 (s, 1H), 3.98 (m, 2H), 3.83 (s, 3H), 3.81 (m, 1H), 3.79 (s, 3H), 3.68 (s, 3H), 3.28 (dd, J = 13.6 Hz, J = 5.5 Hz, 1H), 3.11 (dd, J = 13.6 Hz, J = 5.5 Hz, 1H), 2.77 (t, J = 7.3 Hz, 2H); <sup>13</sup>C NMR (101 MHz, Chloroform-*d*)  $\delta$  173.3, 161.2, 148.6, 147.5, 140.7, 138.6, 131.6, 131.1, 128.9, 128.8, 128.7, 128.4, 128.4, 128.3, 126.2, 121.6, 112.6, 111.0, 94.8, 69.2, 55.8, 55.8, 52.0, 46.5, 39.9, 33.2, 29.7; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>29</sub>H<sub>30</sub>N<sub>2</sub>O<sub>4</sub>S 503.2005, Found 503.2003; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = -150.22 (c = 0.11, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 10% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 86% ee: t<sub>R</sub> = 34.0 min; IR (cm<sup>-1</sup>, neat): 3026, 2834, 1741, 1613.

### (S, Z)-methyl 3-(3,4-dimethoxyphenyl)-2-(4-phenyl-2-((3-phenylpropyl) imino)-1,3-selenazol-3(2H)-yl)propanoate (5c)

Yellow oil, (75%, 177 mg); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.36 (m, 3H), 7.26 (m, 2H), 7.19 (m, 2H), 7.12 (m, 1H), 6.97 (d, *J* = 6.8 Hz, 2H), 6.81 (d, *J* = 6.4 Hz, 2H), 6.69 (d, *J* = 8.8 Hz, 1H), 6.80 (m, 2H), 6.06 (s, 1H), 3.86 (m, 1H), 3.82 (s, 3H), 3.81 (m, 1H), 3.78 (s, 3H), 3.67 (m, 2H), 3.28 (dd, *J* = 13.6 Hz, *J* = 5.6 Hz, 1H), 3.10 (dd, *J* = 13.6 Hz, *J* = 5.6 Hz, 1H), 2.39 (m, 2H), 1.77 (m, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  172.9, 161.0, 148.6, 147.5, 141.8, 141.3, 133.4, 130.8, 128.8, 128.8, 128.5, 128.2, 128.1, 125.7, 121.6, 112.6, 111.0, 94.5, 72.7, 55.8, 51.9, 46.0, 39.8, 32.7, 29.0; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>30</sub>H<sub>33</sub>N<sub>2</sub>O<sub>4</sub>Se 565.1606, Found 565.1609; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = -160.04 (c = 0.16, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 30.9 min.; IR (cm<sup>-1</sup>, neat): 3025, 2949, 1741, 1613.

#### (*S*, *Z*)-methyl 3-(3,4-dimethoxyphenyl)-2-(2-((4-methoxyphenyl)imino)-4phenylthiazol-3(2H)-yl)propanoate (5d)

(85%, 178 mg), Yellow oil; <sup>1</sup>H NMR (400 MHz, Acetone-*d*<sub>6</sub>) δ 7.31 (m, 3H), 6.98 (d, J = 9.0 Hz, 2H), 6.86 (d, J = 9.0 Hz, 2H), 6.80 (m, 2H), 6.73 (d, J = 8.6 Hz, 1H), 5.60 (s, 1H), 3.98 (m, 2H), 3.83 (s, 3H), 3.81 (m, 1H), 3.79 (s, 3H), 3.68 (s, 3H), 3.28 (dd, J = 13.6 Hz, J = 5.5 Hz, 1H), 3.11 (dd, J = 13.6 Hz, J = 5.5 Hz, 1H), 2.77 (t, J = 7.3 Hz, 2H); <sup>13</sup>C NMR (101 MHz, Chloroform-*d*) δ 173.3, 161.2, 148.6, 147.5, 140.7, 138.6, 131.6, 131.1, 128.9, 128.8, 128.7, 128.4, 128.4, 128.3, 126.2, 121.6, 112.6, 111.0, 94.8, 69.2, 55.8, 55.8, 52.0, 46.5, 39.9, 33.2, 29.7; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>29</sub>H<sub>30</sub>N<sub>2</sub>O<sub>4</sub>S 505.1797, Found 505.1804; [α]<sup>27</sup><sub>D</sub> = - 57.52 (c = 0.001, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 32.3 min.; IR (cm<sup>-1</sup>, neat): 2996, 2833, 1613, 1503.

### ((*S*, *Z*)-methyl 3-(3,4-dimethoxyphenyl)-2-(2-(phenethylimino)-4-phenyl-thiazol-3(2H)-yl)propanoate (5e)

(89%, 193 mg), Yellow solid; mp 128 – 130 °C; <sup>1</sup>H NMR (400 MHz, acetone-*d*<sub>6</sub>) δ 7.93 (d, *J* = 9.0 Hz, 2H), 7.38 (m, 4H), 7.01 (dd, *J* = 8.4 Hz, *J* = 1.1 Hz, 2H), 6.85 (d, *J* = 9.0 Hz, 1H), 6.62 (dd, *J* = 8.0 Hz, *J* = 2.0 Hz, 1H), 6.54 (d, *J* = 2.0 Hz, 1H), 6.34 (s, 1H), 3.96 (dd, *J* = 10.2 Hz, *J* = 4.8 Hz, 1H), 3.87 (s, 3H), 3.85 (s, 3H), 3.77 (dd, *J* = 13.8 Hz, *J* = 10.2 Hz, 1H), 3.61 (s, 3H), 3.40 (d, *J* = 11.8 Hz, 2H), 3.21 (dd, *J* = 13.8 Hz, *J* = 4.7 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 174.6, 157.5, 150.3, 148.8, 148.1, 147.5, 147.1, 130.4, 129.6, 129.5, 129.1, 128.4, 123.9, 123.6, 123.1, 121.8, 121.3, 121.1, 112.8, 111.1, 93.0, 61.0, 56.0, 55.7, 53.5, 43.7, 34.0; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>26</sub>N<sub>3</sub>O<sub>6</sub>S 520.1542, Found 520.1542; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = - 380.22 (c = 0.005, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 34.0 min.; IR (cm<sup>-1</sup>, neat): 2919, 2851, 1707, 1590.

### (*S*, *Z*)-methyl 3-(3,4-dimethoxyphenyl)-2-(4-phenyl-2-(phenylimino)-1,3selenazol-3(2H)-yl)propanoate (5f)

Yellow oil, (80%, 174 mg); <sup>1</sup>H NMR (400 MHz, acetone- $d_6$ )  $\delta$  7.38 (m, 3H), 7.30 (t, J = 8.3 Hz, 2H), 7.08 (m, 3H), 6.79 (d, J = 8.0 Hz, 3H), 6.57 (d, J = 2.0 Hz, 1H), 6.53 (dd, J = 8.0 Hz, J = 2.0 Hz, 1H), 6.08 (s, 1H), 4.61 (dd, J = 11.0 Hz, J = 3.9 Hz, 1H), 3.82 (s, 3H), 3.80 (s, 3H), 3.79 (m, 1H), 3.66 (s, 3H), 3.14 (dd, J = 13.9 Hz, J = 3.9 Hz,

1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  170.6, 156.2, 152.0, 148.8, 147.7, 141.7, 132.7, 130.1, 129.6, 129.1, 128.8, 128.3, 123.6, 121.4, 120.6, 112.2, 111.2, 93.9, 61.2, 56.0, 55.6, 52.5, 32.5; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>27</sub>N<sub>2</sub>O<sub>4</sub>Se 523.1136, Found 522.1131; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = - 503.50 (c = 0.064, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 21.8 min.; IR (cm<sup>-1</sup>, neat): 3027, 2834, 1617, 1582.

# (S, Z)-methyl3-(3,4-dimethoxyphenyl)-2-(2-(phenylimino)-4-(ptolyl)thiazol-3(2H)-yl)propanoate (5g)

(75%, 153 mg), Yellow oil; <sup>1</sup>H NMR (400 MHz, acetone- $d_6$ )  $\delta$  7.35 (t, J = 8.0 Hz, 2H), 7.09 (m, 5H), 6.79 (d, J = 7.8 Hz, 1H), 6.69 (d, J = 7.8 Hz, 2H), 6.53 (d, J = 8.2 Hz, 2H), 5.77 (s, 1H), 4.69 (dd, J = 11.1 Hz, J = 4.0 Hz, 1H), 3.84 (dd, J = 11.1 Hz, J = 2.0Hz, 1H), 3.81 (s, 3H), 3.80 (s, 3H), 3.62 (s, 3H), 3.16 (dd, J = 13.9 Hz, J = 4.0 Hz, 1H), 2.34 (s, 3H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  170.5, 156.4, 150.5, 148.8, 147.7, 140.4, 139.0, 130.1, 129.3, 129.0, 122.9, 121.4, 121.3, 121.3, 112.1, 111.2, 94.6, 60.2, 56.0, 55.5, 52.6, 32.4, 21.3; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>28</sub>H<sub>29</sub>N<sub>2</sub>O<sub>4</sub>S 489.1848, Found 489.1847; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = - 335.87 (c = 0.023, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 31.6 min.; IR (cm<sup>-1</sup>, neat): 2998, 2870, 1617, 1582.

# (S, Z)-methyl3-(3,4-dimethoxyphenyl)-2-((4-nitrophenyl)-2-((3-phenyl-<br/>propyl)imino)-1,3-selenazol-3(2H)-yl)propanoate (5h)

Brown oil, (78%, 199 mg); <sup>1</sup>H NMR (400 MHz, acetone- $d_6$ )  $\delta$  8.22 (d, J = 8.9 Hz, 2H), 7.63 (d, J = 8.9 Hz, 1H), 7.16 (t, J = 6.8 Hz, 2H), 7.08 (t, J = 6.8 Hz, 1H), 7.02 (d, J = 7.6 Hz, 2H), 6.91 (m, 2H), 6.86 (d, J = 8.2 Hz, 1H), 6.79 (m, 3H), 6.52 (s, 1H), 4.75 (m, 1H), 3.78 (d, J = 5.7 Hz, 3H), 3.72 (d, J = 4.6 Hz, 3H), 3.67 (s, 3H), 3.24 (dd, J = 5.1 Hz, J = 2.6 Hz, 1H), 3.20 (dd, J = 5.1 Hz, J = 2.6 Hz, 1H), 3.03 (m, 2H), 2.41 (m, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  170.4, 149.1, 148.5, 129.3, 128.2, 128.1, 126.8, 125.8, 123.8, 121.6, 121.3, 112.6, 112.2, 111.4, 111.0, 55.8, 55.8, 55.7, 53.6, 52.8, 36.8, 29.7, 28.9; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>30</sub>H<sub>32</sub>N<sub>3</sub>O<sub>6</sub>Se 610.1456, Found 610.1456; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = - 93.14 (c = 0.015, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 1.5 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 42.3 min.; IR (cm<sup>-1</sup>, neat): 2952, 2850, 1723, 1516.

(S, Z)-methyl

3-(benzo[d][1,3]dioxol-5-yl)-2-(4-(4-bromophenyl)-2-

#### (phenylimino)thiazol-3(2H)-yl)propanoate (5i)

Yellow oil, (84%, 199 mg);<sup>1</sup>H NMR (400 MHz, acetone- $d_6$ )  $\delta$  7.55 (d, J = 8.6 Hz, 2H), 7.35 (t, J = 8.1 Hz, 2H), 7.06 (m, 3H), 6.85 (d, J = 8.1 Hz, 2H), 6.71 (d, J = 7.8 Hz, 1H), 6.51 (d, J = 7.5 Hz, 1H), 6.48 (s, 1H), 6.00 (d, J = 8.4 Hz, 2H), 5.89 (s, 1H), 4.72 (dd, J = 11.1 Hz, J = 4.0 Hz, 1H), 4.81 (dd, J = 14.0 Hz, J = 11.1 Hz, 1H), 3.80 (s, 3H), 3.17 (dd, J = 14.0 Hz, J = 4.0 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  190.3, 170.1, 156.2, 150.3, 147.6, 146.3, 139.0, 131.7, 130.5, 129.9, 123.5, 122.4, 121.2, 109.7, 108.4, 108.3, 102.1, 100.9, 95.9, 77.3, 77.0, 76.7, 60.3, 52.7, 32.6, 29.7; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>26</sub>H<sub>22</sub>BrN<sub>2</sub>O<sub>4</sub>S 537.0484, Found 537.0483; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = - 356.81 (c = 0.021, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 32.2 min.; IR (cm<sup>-1</sup>, neat): 2916, 2850, 1585, 1487.

### (S, Z)-methyl 2-(2-(allylimino)-4-phenylthiazol-3(2H)-yl)-3-(benzo[d][1,3]-dioxol-5-yl)propanoate (5j)

Yellow oil, <sup>(88%)</sup>, 155 mg); <sup>1</sup>H NMR (400 MHz, Acetone-*d*<sub>6</sub>) δ 7.46 – 7.37 (m, 5H), 6.82 (s, 1H), 6.76 – 6.70 (m, 2H), 5.96 (s, 3H), 5.83 – 5.72 (m, 1H), 5.03 (dd, J = 10.4 Hz, J = 1.5 Hz, 1H), 4.85 (dd, J = 17.3 Hz, J = 1.6 Hz, 1H), 4.40 (dd, J = 16.2 Hz, J = 5.1 Hz, 1H), 4.23 (dd, J = 16.2 Hz, J = 5.1 Hz, 1H), 3.82 (dd, J = 7.8 Hz, J = 5.6 Hz, 1H), 3.63 (s, 3H), 3.15 (dd, J = 13.4 Hz, J = 5.6 Hz, 1H), 2.96 (dd, J = 13.4 Hz, J = 5.6 Hz, 1H); <sup>13</sup>C NMR (101 MHz, Chloroform-*d*) δ 173.0, 161.3, 147.3, 146.0, 140.7, 132.9, 132.2, 131.6, 129.1, 128.8, 128.7, 128.5, 122.5, 116.4, 110.2, 107.9, 100.7, 95.3, 69.1, 53.5, 51.9, 47.4, 39.9; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>23</sub>H<sub>23</sub>N<sub>2</sub>O<sub>4</sub>S 423.1379, Found 423.1372; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = - 151.69 (c = 0.20, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 21.9 min.; IR (cm<sup>-1</sup>, neat): 2987, 2897, 1614, 1380.

## (*S*, *Z*)-methyl 3-(benzo[d][1,3]dioxol-5-yl)-2-(4-(4-nitrophenyl)-2-(phenyl-imino)-1,3-selenazol-3(2H)-yl)propanoate (5k)

Yellow oil, (74%, 171 mg); <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD)  $\delta$  7.36 (t, *J* = 7.9 Hz, 2H), 7.2 (t, *J* = 7.8 Hz, 1H), 7.12 - 7.07 (m, 2H), 7.02 (d, *J* = 7.8 Hz, 2H), 6.90 (d, *J* = 7.9 Hz, 1H), 6.70 (d, *J* = 19.6 Hz, 1H), 6.65 (d, *J* = 7.8 Hz, 1H), 6.42 (d, *J* = 7.9 Hz, 1H), 6.32 (s, 1H), 6.22 (s, 1H), 5.95 (s, 1H), 5.91 (s, 1H), 5.86 (d, *J* = 5.5 Hz, 1H), 4.62 (d, *J* = 7.7 Hz, 1H), 3.84 (s, 3H), 3.73 (dd, *J* = 23.5 Hz, *J* = 10.7 Hz, 1H); <sup>13</sup>C NMR (151 MHz, CD<sub>3</sub>OD)  $\delta$  170.5, 156.9, 152.0, 147.7, 139.7, 138.6, 130.9, 129.4, 128.8, 124.5, 123.4, 122.3, 122.0, 120.1, 109.3, 109.0, 107.7, 107.7, 100.9, 100.8, 96.9, 61.1, 60.5, 51.7, 39.1, 32.2; HRMS (ESI) m/z:  $[M + H]^+$  Calcd for C<sub>26</sub>H<sub>22</sub>N<sub>3</sub>O<sub>6</sub>Se 552.0674, Found 552.0675;  $[\alpha]^{27}_D = -236.46$  (c = 0.04, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 31.6 min.; IR (cm<sup>-1</sup>, neat): 2917, 2850, 1740, 1586.

# (*S*, *Z*)-methyl 3-(benzo[d][1,3]dioxol-5-yl)-2-(2-((3-phenylpropyl)imino)-4-(p-tolyl)-1,3-selenazol-3(2H)-yl)propanoate (5l)

Yellow oil, (82%, 192 mg); <sup>1</sup>H NMR (400 MHz, Acetone-*d*<sub>6</sub>)  $\delta$  7.24 – 7.20 (m, 4H), 7.18 (d, *J* = 7.4 Hz, 2H), 7.12 (t, *J* = 7.2 Hz, 1H), 7.02 (d, *J* = 8.2 Hz, 2H), 6.83 (s, 1H), 6.74 (d, *J* = 7.4 Hz, 1H), 6.68 (d, *J* = 8.2 Hz, 1H), 6.23 (s, 1H), 5.89 (s, 2H), 3.84 – 3.74 (m, 1H), 3.73 – 3.67 (m, 2H), 3.64 (s, 3H), 3.19 (dd, *J* = 13.4 Hz, *J* = 5.5 Hz, 1H), 3.02 (dd, *J* = 13.4 Hz, *J* = 5.5 Hz, 1H), 2.46 -2.39 (m, 2H), 2.37 (s, 3H), 1.86 – 1.73 (m, 2H); <sup>13</sup>C NMR (101 MHz, Chloroform-*d*)  $\delta$  172.8, 161.2, 147.3, 146.0, 142.0, 141.4, 138.7, 132.0, 129.4, 129.2, 128.9, 128.8, 128.2, 128.1, 125.6, 122.5, 110.0, 108.0, 100.7, 94.1, 72.4, 52.0, 45.9, 39.9, 32.7, 29.0, 21.3; HRMS (ESI) m/z: [M + H] <sup>+</sup> Calcd for C<sub>30</sub>H<sub>31</sub>N<sub>2</sub>O<sub>4</sub>Se 563.1449, Found 563.1454; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = - 186.41 (c = 0.06, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 21.4 min.; IR (cm<sup>-1</sup>, neat): 3024, 2918, 1600, 1486.

### (*S*, *Z*)-methyl 3-(3,4-dimethoxyphenyl)-2-(5-methyl-4-phenyl-2-(phenylimino)thiazol-3(2H)-yl)propanoate (5m)

Yellow oil, (82%, 192 mg); <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  7.42 - 7.28 (m, 4H), 7.27 - 7.20 (m, 1H), 7.18 - 7.04 (m, 4H), 6.75 (d, *J* = 8.2 Hz, 2H), 6.52 (d, *J* = 7.8 Hz, 1H), 6.48 (s, 1H), 5.99 (s, 1H), 4.28 (s, 1H), 3.90 (s, 3H), 3.87 - 3.83 (m, 1H), 3.81 (s, 3H), 3.77 (s, 3H), 3.13 (dd, *J* = 15.1 Hz, *J* = 3.7 Hz, 1H); <sup>13</sup>C NMR (101 MHz, Chloroform-*d*)  $\delta$  170.4, 148.7, 147.7, 130.8, 129.9, 129.3, 128.9, 128.4, 128.3, 121.4, 112.3, 111.1, 60.8, 56.0, 55.6, 52.6, 32.6, 31.8, 29.6, 29.0, 22.6, 14.1, 12.6; HRMS (ESI) m/z: [M + H] <sup>+</sup> Calcd for C<sub>28</sub>H<sub>28</sub>N<sub>2</sub>O<sub>4</sub>S 489.1848, Found 489.1845; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = - 20.76 (c = 0.01, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 28.8 min.; IR (cm<sup>-1</sup>, neat): 2949, 2834, 1745, 1489.

### (*S*, *Z*)-methyl 3-(3,4-dimethoxyphenyl)-2-(5-methyl-4-phenyl-2-(phenyl-imino)-1,3-selenazol-3(2H)-yl)propanoate (5n)

Yellow oil, (76%, 170 mg); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.42 - 7.28 (m, 4H), 7.27 - 7.20 (m, 1H), 7.18 - 7.04 (m, 4H), 6.75 (d, J = 8.2 Hz, 2H), 6.52 (d, J = 7.8 Hz, 1H), 6.48 (s, 1H), 5.99 (s, 1H), 4.28 (s, 1H), 3.90 (s, 3H), 3.87 - 3.83 (m, 1H), 3.81 (s, 3H), 3.77 (s, 3H), 3.13 (dd, J = 15.1 Hz, J = 3.7 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  170.6, 148.7, 147.6, 136.0, 131.0, 130.9, 130.4, 129.9, 129.5, 128.7, 128.4, 128.2, 123.5, 121.5, 120.8, 112.4, 111.1, 61.7, 56.0, 55.7, 52.5, 32.6, 31.8, 29.6, 29.0, 22.6, 14.9, 14.1; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>28</sub>H<sub>28</sub>N<sub>2</sub>O<sub>4</sub>Se 537.1293, Found 537.1295; [ $\alpha$ ]<sup>27</sup>D = - 520.00 (c = 0.017, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 33.8 min.; IR (cm<sup>-1</sup>, neat): 2948, 2834, 1743, 1514.

## (S, Z)-methyl 2-(2-(cyclohexylimino)-4-phenyloxazol-3(2H)-yl)-3-(3,4-dimethoxyphenyl)propanoate (50)

White solid, (68%, 130 mg); mp 155 – 157 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.51 – 7.46 (m, 4H), 7.32 - 7.25 (m, 3H), 7.07, 7.05 (t, *J* = 7.4 Hz, 1H), 6.89 - 6.83 (m, 1H), 6.80 (d, *J* = 8.1 Hz, 1H), 6.69 (s, 1H), 6.53 (d, *J* = 8.1 Hz, 1H), 6.05 (d, *J* = 8.1 Hz, 1H), 4.63 (dd, *J* = 12.8 Hz, *J* = 6.9 Hz, 1H), 3.78 (s, 3H), 3.76 (s, 3H), 3.71 (s, 3H), 3.06 (dd, *J* = 13.9 Hz, *J* = 5.2 Hz, 1H), 2.96 (dd, *J* = 14.0 Hz, *J* = 7.0 Hz, 1H); <sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>)  $\delta$  171.7, 155.8, 152.3, 148.9, 148.2, 137.7, 136.2, 130.0, 129.5, 129.4, 128.8, 127.5, 123.8, 120.9, 120.0, 111.9, 111.2, 55.8, 55.75, 54.4, 52.4, 37.0, 29.6; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = - 285.72 (c = 0.023, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH / Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee: t<sub>R</sub> = 13.7 min.; IR (cm<sup>-1</sup>, neat): 2916, 2849, 1734, 1346.

#### (S,Z)-methyl 3-(3,4-dimethoxyphenyl)-2-(4,5-diphenyl-2-(phenylimino) thiazol-3(2H)-yl)propanoate (5p)

White solid; 76% (170 mg); mp 105 – 107 °C; <sup>1</sup>H NMR (400 MHz, acetone- $d_6$ )  $\delta$  7.50 - 7.36 (m, 5H), 7.21 - 7.02 (m, 5H), 6.92 - 6.83 (m, 3H), 6.66 (d, J = 2.0 Hz, 1H), 6.62 (dd, J = 8.1 Hz, J = 7.0 Hz, 1H), 5.92 (s, 1H), 4.43 (dd, J = 11.0 Hz, J = 3.9 Hz, 1H), 3.91 (dd, J = 13.9 Hz, J = 11.0 Hz, 1H), 3.81 (s, 3H), 3.79 (s, 3H), 3.71 (s, 3H), 3.40 (q, J = 7.0 Hz, 1H), 3.17 (dd, J = 13.9 Hz, J = 4.0 Hz, 1H); <sup>13</sup>C NMR (151 MHz, acetone- $d_6$ )  $\delta$  169.5, 154.7, 151.0, 149.5, 148.4, 135.6, 132.1, 131.1, 130.2, 130.2, 129.3, 128.8, 128.6, 128.2, 127.5, 126.8, 123.0, 121.5, 121.23, 113.1, 112.1, 109.8, 65.2, 60.4, 55.4, 54.9, 51.8, 32.1, 14.7; HRMS (ESI) m/z: [M + H] + Calcd for C<sub>33</sub>H<sub>31</sub>N<sub>2</sub>O4S 551.2005, Found 551.2008; [ $\alpha$ ]<sup>27</sup><sub>D</sub> = - 699.63 (c = 0.068, CH<sub>2</sub>Cl<sub>2</sub>); HPLC analysis: 15% *i*-PrOH /

Hexane, 0.3 mL min<sup>-1</sup>, 254 nm); 99% ee:  $t_R = 16.5$  min.; IR (cm<sup>-1</sup>, neat): 2916, 2849, 1734, 1346.

#### 4-(3,4-dimethoxybenzyl)-2-((2-oxo-2-phenylethyl)thio)-1-phenethyl-1H-imidazol-5(4H)-one (7b)

Yellow oil, (56%, 114 mg); <sup>1</sup>H NMR (600 MHz, acetone-*d*<sub>6</sub>)  $\delta$  8.08 (d, *J* = 7.0 Hz, 1H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.27 (t, *J* = 7.6 Hz, 2H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.15 (d, *J* = 7.4 Hz, 2H), 6.80 (d, *J* = 2.0 Hz, 1H), 6.70 (d, *J* = 8.2 Hz, 1H), 6.65 (dd, *J* = 8.2 Hz, *J* = 4.3 Hz, 1H), 4.86 (s, 2H), 4.15 (dd, *J* = 7.3 Hz, *J* = 2.0 Hz, 1H), 3.70 (s, 6H), 3.65 15 (dd, *J* = 14.8 Hz, *J* = 7.1 Hz, 1H), 3.52 (dd, *J* = 14.8 Hz, *J* = 7.1 Hz, 1H), 3.01 (dd, *J* = 13.8 Hz, *J* = 4.3 Hz, 1H), 2.73 (dd, *J* = 13.8 Hz, *J* = 4.3 Hz, 1H, 2.68 (t, *J* = 7.7 Hz, 2H); <sup>13</sup>C NMR (151 MHz, acetone-*d*<sub>6</sub>)  $\delta$  192.3, 180.3, 160.5, 148.9, 148.2, 137.9, 136.0, 133.4, 129.3, 128.7, 128.7, 128.4, 128.3, 126.5, 121.8, 113.5, 111.5, 69.3, 55.2, 55.1, 41.5, 37.8, 36.6, 34.4; HRMS (ESI) m/z: [M + H] <sup>+</sup> Calcd for C<sub>28</sub>H<sub>29</sub>N<sub>2</sub>O<sub>4</sub>S 489.1848, Found 489.1807; IR (cm<sup>-1</sup>, neat): 3337, 2919, 2850, 1727.

## 4-(3,4-dimethoxybenzyl)-2-((2-oxo-2-phenylethyl)selanyl)-1-(3-phenyl-propyl)-1H-imidazol-5(4H)-one (7c)

Yellow oil, (65%, 149 mg); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.06 (d, *J* = 7.0 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 8.1 Hz, 2H), 7.25 (t, *J* = 7.1 Hz, 2H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 6.7 Hz, 2H), 6.74 (d, *J* = 2.0 Hz, 1H), 6.70 (dd, *J* = 8.2 Hz, *J* = 2.0 Hz, 1H), 6.61 (d, *J* = 8.2 Hz, 1H), 4.78 (s, 2H), 4.37 (dd, *J* = 6.3 Hz, *J* = 4.4 Hz, 1H), 3.85 (m, 1H), 3.76 (s, 3H)), 3.67 (s, 3H), 3.54 – 3.37 (m, 2H), 3.30 – 3.20 (m, 2H), 2.98 (dd, *J* = 13.9 Hz, *J* = 6.3 Hz, 1H), 2.44 – 2.35 (m, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  194.1, 148.3, 147.8, 140.4, 135.1, 133.9, 128.8, 128.7, 128.6, 128.4, 128.3, 128.2, 128.2, 126.0, 121.8, 112.9, 110.7, 77.4, 77.0, 76.7, 70.3, 65.8, 55.7, 55.6, 40.9, 36.5, 34.0, 32.6, 30.1, 15.2; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>29</sub>H<sub>31</sub>N<sub>2</sub>O4Se 551.1449, Found 551.1447; IR (cm<sup>-1</sup>, neat): 3336, 2931, 2835, 1724.

#### 4-(3,4-dimethoxybenzyl)-1-(4-methoxyphenyl)-2-((2-oxo-2-phenylethyl) thio)-1Himidazol-5(4H)-one (7d)

Yellow oil, (78%, 160 mg); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.98 (d, *J* = 7.2 Hz, 2H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.7 Hz, 2H), 6.83 (dd, *J* = 17.4 Hz, *J* = 9.0 Hz, 4H), 6.73 (s, 1H), 6.27 (s, 1H), 4.62 (d, J = 3.4 Hz, 1H), 4.41 (dd, J = 5.9 Hz, J = 4.6 Hz, 1H), 3.80 (s, 3H), 3.73 (s, 3H), 3.71 (s, 3H), 3.21 (dd, J = 13.8 Hz, J = 4.3 Hz, 1H), 3.03 (dd, J = 13.8 Hz, J = 4.3 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  192.6, 180.0, 160.2, 148.4, 147.9, 135.3, 133.9, 128.9, 128.8, 128.8, 128.7, 128.7, 128.6, 128.5, 128.5, 128.1, 127.6, 124.0, 122.0, 114.8, 113.0, 110.8, 69.5, 58.2, 56.0, 55.9, 55.8, 55.5, 55.4, 39.0, 36.9; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>27</sub>N<sub>2</sub>O<sub>5</sub>S 491.1641, Found 491.1644; IR (cm<sup>-1</sup>, neat): 3337, 2932, 2837, 1513.

#### 4-(3,4-dimethoxybenzyl)-2-((2-(4-nitrophenyl)-2-oxoethyl)thio)-1-phenyl -1Himidazol-5(4H)-one (7e)

Yellow solid, (72%, 165 mg); mp 162 – 164 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.59 (d, J = 8.4 Hz, 2H), 8.40 (d, J = 8.5 Hz, 2H), 7.55 (m, 3H), 7.26 (s, 1H), 7.16 (d, J = 2.0 Hz, 1H), 6.96 (d, J = 8.1 Hz, 1H), 6.83 (d, J = 8.1 Hz, 3H), 5.77 (d, J = 17.7 Hz, 1H), 5.56 (d, J = 17.7 Hz, 1H), 5.04 (s, 1H), 3.93 (dd, J = 15.2 Hz, J = 5.2 Hz, 1H), 3.88 (s, 3H), 3.82 (s, 3H), 3.46 (d, J = 16.2 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  189.5, 174.2, 170.8, 151.3, 149.0, 149.0, 137.6, 131.8, 130.7, 130.6, 130.1, 129.1, 128.5, 128.1, 127.3, 124.3, 124.0, 122.2, 113.7, 111.2, 63.7, 56.4, 56.1, 56.0, 46.3, 35.6, 30.1, 29.7; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>26</sub>H<sub>24</sub>N<sub>3</sub>O<sub>6</sub>S 506.1386, Found 506.1384; IR (cm<sup>-1</sup>, neat): 3102, 2916, 2849, 1558.

#### 4-(3,4-dimethoxybenzyl)-2-((2-oxo-2-(p-tolyl)ethyl)thio)-1-phenyl-1H-imidazol-5(4H)-one (7f)

Brown solid, (67%, 133 mg); mp 135 – 137 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.91 (d, J = 8.2 Hz, 2H), 7.38 (m, 3H), 7.28 (d, J = 8.0 Hz, 2H), 6.94 (m, 2H), 6.76 (s, 1H), 6.71 (s, 2H), 4.47 (dd, J = 6.2 Hz, J = 4.4 Hz, 1H), 3.84 (s, 3H), 3.74 (s, 3H), 3.27 (dd, J = 13.7 Hz, J = 4.3 Hz, 1H), 3.07 (dd, J = 13.7 Hz, J = 4.3 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  192.1, 179.8, 161.7, 148.4, 147.9, 144.9, 132.9, 131.7, 129.5, 129.5, 129.3, 128.6, 128.2, 127.3, 122.0, 113.0, 110.8, 69.6, 55.9, 55.8, 39.0, 36.9, 21.7; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>27</sub>N<sub>2</sub>O<sub>4</sub>S 475.1692, Found 475.1698; IR (cm<sup>-1</sup>, neat): 3326, 2917, 2834, 1741.

4-(benzo[d][1,3]dioxol-5-ylmethyl)-2-((2-(4-bromophenyl)-2-oxoethyl) thio)-1phenyl-1H-imidazol-5(4H)-one (7g) Orange solid; (78%, 193 mg); mp 100 – 102 °C; <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  7.94 (d, *J* = 8.5 Hz, 2H), 7.76 (d, *J* = 8.6 Hz, 2H), 7.48 (m, 3H), 7.06 (d, *J* = 6.6 Hz, 2H), 6.70 (d, *J* = 7.9 Hz, 1H), 6.65 (d, *J* = 1.6 Hz, 1H), 6.54 (dd, *J* = 7.9 Hz, *J* = 1.7 Hz, 1H), 5.94 (dd, *J* = 11.4 Hz, *J* = 1.0 Hz, 2H), 4.76 (q, *J* = 17.1 Hz, 1H), 4.50 (dd, *J* = 7.0 Hz, *J* = 4.3 Hz, 1H), 3.03 (dd, *J* = 13.8 Hz, *J* = 4.4 Hz, 1H), 2.81 (dd, *J* = 13.8 Hz, *J* = 7.2 Hz, 1H); <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  194.2, 179.7, 168.3, 162.9, 155.8, 149.4, 148.0, 146.2, 136.2, 135.2, 130.8, 129.8, 126.9, 124.1, 123.3, 110.7, 110.3, 108.6, 108.4, 102.0, 101.2, 69.3, 57.6, 55.3, 44.5; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>25</sub>H<sub>20</sub>BrN<sub>2</sub>O<sub>4</sub>S 523.0327, Found 523.0163; IR (cm<sup>-1</sup>, neat): 3102, 2916, 2849, 1517.

## 1-allyl-4-(benzo[d][1,3]dioxol-5-ylmethyl)-2-((2-oxo-2-phenylethyl)thio)-1Himidazol-5(4H)-one (7h)

Yellow oil, (82%, 140 mg); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.36 (d, J = 7.2 Hz, 2H), 7.68 (t, J = 8.5 Hz, 1H), 7.57 (t, J = 8.0 Hz, 2H), 6.89 (dd, J = 8.0 Hz, J = 1.7 Hz, 1H), 6.84 (d, J = 1.9 Hz, 1H), 6.69 (d, J = 7.9 Hz, 1H), 5.89 (s, 2H), 5.67 (dd, J = 47.2 Hz, J = 17.1 Hz, 2H), 5.40 (m, 1H), 5.19 (d, J = 10.3 Hz, 1H), 4.86 (m, 2H), 4.31 (dd, J = 16.4 Hz, J = 5.4 Hz, 1H), 4.02 (dd, J = 16.4 Hz, J = 5.8 Hz, 1H), 3.82 (dd, J = 14.4 Hz, J = 4.9 Hz, 1H), 3.32 (dd, J = 14.4 Hz, J = 4.9 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  190.7, 173.6, 171.2, 147.8, 147.4, 135.2, 134.0, 133.3, 130.4, 129.5, 129.2, 128.9, 128.8, 127.3, 125.4, 123.7, 122.6, 120.6, 118.0, 110.3, 109.7, 108.5, 108.5, 101.1, 101.1, 63.0, 46.72, 43.6, 35.1; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>22</sub>H<sub>21</sub>N<sub>2</sub>O<sub>4</sub>S 409.1222, Found 409.1213; IR (cm<sup>-1</sup>, neat): 2898, 1777, 1711, 1489.

### 4-(3,4-dimethoxybenzyl)-2-((1-oxo-1-phenylpropan-2-yl)thio)-1-phenyl-1Himidazol-5(4H)-one (7i)

Yellow solid, 80% (159 mg); mp 132 – 134 °C; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>)  $\delta$  8.04 (dd, J = 18.2 Hz, J = 7.7 Hz, 2H), 7.65.- 7.58 (m, 1H), 7.52 - 7.45 (m, 2H), 7.40 – 7.34 (m, 3H), 6.96 - 6.88 (m, 2H), 6.82 - 6.70 (m, 2H), 6.63 - 6.59 (m, 1H), 5.63 (s, 1H), 4.51 (s, 1H), 3.87, 3.81 (s, 3H), 3.77 (s, 3H), 3.29 (dd, *J* = 15.1Hz, *J* = 7.7 Hz, 1H), 3.12 (dd, *J* = 13.8 Hz, *J* = 5.7 Hz, 1H), 1.61 (t, *J* = 6.9 Hz, 3H); <sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>)  $\delta$  197.3, 148.5, 148.4, 148.0, 147.8, 133.7, 129.4, 129.3, 128.8, 128.7, 127.2, 127.2, 122.1, 121.9, 113.0, 112.7, 110.8, 110.7, 55.9, 55.8, 55.7, 37.0, 36.9, 18.5; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>26</sub>N<sub>2</sub>O4S 475.1692, Found 475.1685; IR (cm<sup>-1</sup>, neat): 3063, 2931, 2834, 1740.

### 1-cyclohexyl-4-(3,4-dimethoxybenzyl)-2-(2-oxo-2-phenylethoxy)-1H-imida-zol-5(4H)-one (7k)

Yellow solid, (48%, 90 mg); mp 145 – 147 °C; <sup>1</sup>H NMR (600 MHz, acetone- $d_6$ )  $\delta$  8.00 (d, J = 7.3 Hz, 2H), 7.68 (t, J = 7.5 Hz, 1H), 7.55 (t, J = 7.6 Hz, 2H), 6.85 (s, 1H), 6.78 (dd, J = 17.7 Hz, J = 8.2 Hz, 2H), 5.15 (d, J = 18.4 Hz, 1H), 4.78 (d, J = 18.4 Hz, 1H), 4.36 (t, J = 4.4 Hz, 1H), 3.75 (s, 3H), 3.73 (s, 3H), 3.48 (s, 1H), 3.24 (dd, J = 14.5 Hz, J = 4.4 Hz, 1H), 3.01 (dd, J = 14.5 Hz, J = 4.7 Hz, 1H), 2.99 (m, 1H), 2.99 (m, 1H), 1.99 (m, 1H), 1.83 (m, 2H), 1.77 (m, 1H), 1.41 (m, 1H), 1.14 (m, 3H); <sup>13</sup>C NMR (151 MHz, acetone  $d_6$ )  $\delta$  193.9, 172.2, 156.9, 149.2, 148.6, 134.9, 133.6, 128.7, 127.8, 127.8, 122.0, 113.8, 113.4, 111.9, 55.2, 55.2, 50.9, 47.4, 34.0, 33.6, 25.6, 25.5, 25.0; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>26</sub>H<sub>31</sub>N<sub>2</sub>O<sub>5</sub> 451.2233, Found 451.2230; IR (cm<sup>-1</sup>, neat): 2927, 2853, 1707, 1448.

### 4-(3,4-bis(allyloxy)benzyl)-2-((2-oxo-2-phenylethyl)selanyl)-1-phenyl-1Himidazol-5(4H)-one (7l)

Yellow solid, (73%, 164 mg); mp 76 – 78 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.03 (d, J = 7.0 Hz, 2H), 7.57 (q, J = 6.7 Hz, 1H), 7.46 (d, J = 8.0 Hz, 2H), 7.37 - 7.32 (m, 3H), 6.90 - 6.84 (m, 2H), 6.80 (d, J = 1.8 Hz, 1H), 6.76 - 6.70 (m, 2H), 6.09 - 5.91 (m, 2H), 5.33 (q, J = 17.3 Hz, 2H), 5.18 (q, J = 10.5 Hz, 2H), 4.70 (s, 2H), 4.55 (d, J = 5.3 Hz, 2H), 4.51 (dd, J = 5.6 Hz, J = 4.3 Hz, 2H), 4.47 – 4.44 (m, 2H), 3.28 (dd, J = 13.8 Hz, J = 4.4 Hz, 1H), 3.10 (dd, J = 13.8 Hz, J = 5.7 Hz, 1H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  191.7, 168.8, 161.7, 150.9, 148.7, 136.1, 135.4, 133.9, 132.3, 129.6, 129.2, 128.9, 128.3, 127.3, 127.2, 126.6, 125.4, 113.6, 110.7, 55.8, 55.4, 38.8; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>30</sub>H<sub>29</sub>N<sub>2</sub>O<sub>4</sub>S 561.1293, Found 561.1297; IR (cm<sup>-1</sup>, neat): 3059, 2919, 2851, 1420.

# (Z)-4-(3,4-dimethoxybenzylidene)-2-((2-(4-nitrophenyl)-2-oxoethyl)selanyl)-1-(3-phenylpropyl)-1H-imidazol-5(4H)-one (9b)

Red solid, (69%, 171 mg); mp 153 – 155 °C; <sup>1</sup>H NMR (400 MHz, acetone- $d_6$ )  $\delta$  8.33 (d, J = 8.5 Hz, 2H), 8.21 (d, J = 8.8 Hz, 2H), 7.31 - 7.28 (m, 5H), 7.24 (m, 1H), 7.16 (d, J = 8.3 Hz, 2H), 6.73 (s, 1H), 6.18 (s, 1H), 4.01 (s, 3H), 3.92 (s, 3H), 3.89 (d, J = 7.6 Hz, 2H), 2.85 - 2.73 (m, 2H), 2.14 - 2.09 (m, 2H); <sup>13</sup>C NMR (151 MHz, Chloroform-

*d*)  $\delta$  185.7, 163.5, 154.8, 150.4, 149.5, 149.3, 144.6, 140.3, 128.6, 128.4, 128.0, 126.3, 126.2, 123.9, 123.6, 123.0, 114.2, 111.7, 111.4, 56.0, 56.0, 39.1, 32.6, 29.1; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>29</sub>H<sub>28</sub>N<sub>3</sub>O<sub>6</sub>Se 594.1143, Found 594.1145; IR (cm<sup>-1</sup>, neat): 2917, 2849, 1594, 1414.

#### (Z)-4-(benzo[d][1,3]dioxol-5-ylmethylene)-2-((2-(4-nitrophenyl)-2-oxoethyl) selanyl)-1-phenyl-1H-imidazol-5(4H)-one (9c)

Yellow solid, (67%, 150 mg); mp 78 – 80 °C; <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ )  $\delta$  8.32 (m, 5H), 7.69 (s, 1H), 7.55 (m, 3H), 7.42 (d, J = 7.1 Hz, 2H), 7.23 (s, 1H), 7.00 (d, J = 8.2 Hz, 1H), 6.86 (s, 1H), 6.80 (d, J = 8.1 Hz, 1H), 6.09 (s, 1H), 5.97 (s, 1H), 4.94 (d, J = 12.2 Hz, 2H); <sup>13</sup>C NMR (101 MHz, Chloroform-d)  $\delta$  192.7, 168.4, 158.6, 150.7, 149.8, 148.0, 139.9, 136.4, 132.6, 130.1, 129.8, 129.6, 129.5, 129.3, 129.2, 128.8, 128.5, 126.9, 126.1, 126.0, 124.2, 124.0, 110.2, 108.6, 101.6, 33.0; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>25</sub>H<sub>18</sub>N<sub>3</sub>O<sub>6</sub>Se 536.0361, Found 536.0357; IR (cm<sup>-1</sup>, neat): 2923, 2854, 1717, 1489.

#### (Z)-4-(benzo[d][1,3]dioxol-5-ylmethylene)-2-((2-oxo-2-(p-tolyl)ethyl)selanyl) -1-(3-phenylpropyl)-1H-imidazol-5(4H)-one (9d)

Yellow solid, (73%, 167 mg); mp: 140 – 142 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.99 (t, J = 8.0 Hz, 2H), 7.40 (d, J = 8.4 Hz, 1H), 7.28 (t, J = 8.0 Hz, 3H), 7.19 (d, J = 7.3 Hz, 3H), 6.88 (s, 1H), 6.76 (d, J = 8.1 Hz, 1H), 6.01 (s, 2H), 4.91 (s, 2H), 3.62 (t, J = 7.4 Hz, 2H), 2.67 (t, J = 7.7 Hz, 2H), 2.43 (s, 3H), 2.01 (m, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  193.6, 169.5, 159.6, 149.4, 148.0, 145.0, 140.6, 137.2, 132.7, 129.6, 128.9, 128.8, 128.5, 128.3, 128.3, 128.2, 126.1, 124.9, 110.9, 108.5, 101.5, 41.4, 34.3, 33.0, 30.6, 29.7, 21.8; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>29</sub>H<sub>27</sub>N<sub>2</sub>O<sub>4</sub>Se 547.1136, Found 547.1138; IR (cm<sup>-1</sup>, neat): 2916, 2849, 1705, 1482.

# (Z)-4-(3,4-dimethoxybenzylidene)-2-((2-oxo-2-phenylethyl)selanyl)-1-(3-phenylpropyl)-1H-imidazol-5(4H)-one (9e)

Yellow solid, (68%, 156 mg); mp 145 – 147 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.07 (d, J = 7.1 Hz, 3H), 7.63 (t, J = 7.5 Hz, 1H), 7.54 – 7.41 (m, 3H), 7.31- 7.16 (m, 5H), 6.93 (s, 1H), 6.79 (d, J = 8.4 Hz, 1H), 4.93 (s, 2H), 3.91 (s, 3H), 3.83 (s, 3H), 3.64 (t, J = 7.5 Hz, 2H), 2.68 (t, J = 7.8 Hz, 2H), 2.08 – 1.97 (m, 2H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  193.6, 169.5, 159.1, 151.0, 148.8, 140.6, 137.0, 135.1, 134.0, 128.9, 128.6, 128.5, 128.3,

127.4, 126.8, 126.1, 125.3, 113.7, 110.8, 55.9, 55.6, 41.4, 34.0, 33.0, 30.6; HRMS (ESI) m/z:  $[M + H]^+$  Calcd for C<sub>29</sub>H<sub>29</sub>N<sub>2</sub>O<sub>4</sub>Se 549.1293, Found 549.1290; IR (cm<sup>-1</sup>, neat): 2921, 2850, 1704, 1511.

#### (Z)-4-(3,4-dimethoxybenzylidene)-2-((1-oxo-1-phenylpropan-2-yl)thio)-1-phenyl-1H-imidazol-5(4H)-one (9f)

Yellow solid, (74%, 146 mg); mp 150 – 152 °C; <sup>1</sup>H NMR (400 MHz, Chloroform-*d*)  $\delta$  8.09 (d, *J* = 7.1 Hz, 2H), 7.88 (d, *J* = 2.0 Hz, 3H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.57 - 7.40 (m, 7H), 7.32 (d, *J* = 6.9Hz, 2H), 7.03 (s, 1H), 6.68 (d, *J* = 8.4 Hz, 1H), 5.82 (q, *J* = 7.2 Hz, 1H), 3.94 (m, 1H), 3.92 (s, 6H), 1.78 (d, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (101 MHz, Chloroform-*d*)  $\delta$  196.4, 168.7, 161.5, 150.9, 148.7, 136.2, 134.5, 133.7, 132.2, 129.5, 129.1, 128.9, 128.7, 127.3, 127.2, 126.4, 125.4, 113.9, 110.9, 55.9, 55.7, 45.5, 18.3; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>24</sub>N<sub>2</sub>O<sub>4</sub>S 473.1535, Found 473.1534; IR (cm<sup>-1</sup>, neat): 3059, 2916, 2849, 1593.

#### (Z)-4-(3,4-dimethoxybenzylidene)-2-((1-oxo-1-phenylpropan-2-yl)selanyl)-1phenyl-1H-imidazol-5(4H)-one (9g)

Yellow solid, (79%, 172 mg); mp 86 – 88 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.20 (d, *J* = 1.8 Hz, 1H), 8.10 (d, *J* = 7.4 Hz, 2H), 7.62 - 7.57 (m, 2H), 7.50 - 7.43 (m, 5H), 7.30 (dd, *J* = 7.6 Hz, *J* = 1.5 Hz, 2H), 7.26 (d, *J* = 0.7 Hz, 1H), 7.08 (s, 1H), 6.90 (d, *J* = 8.4 Hz, 1H), 5.93 (q, *J* = 7.0 Hz, 1H), 4.00 (m, 1H), 3.96 (s, 3H), 3.92 (s, 3H), 1.96 (d, *J* = 7.0 Hz, 3H); <sup>13</sup>C NMR (151 MHz, CDCl<sub>3</sub>)  $\delta$  197.4, 168.5, 159.2, 151.2, 148.9, 136.5, 134.3, 133.8, 132.6, 129.6, 129.3, 128.9, 128.6, 127.4, 127.0, 126.9, 126.9, 125.9, 113.6, 110.9, 55.9, 55.6, 42.4, 19.1; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>27</sub>H<sub>25</sub>N<sub>2</sub>O<sub>4</sub>Se 521.0980, Found 521.0980; IR (cm<sup>-1</sup>, neat): 3059, 2919, 2851, 1420.

#### (Z)-4-(3,4-dimethoxybenzylidene)-2-((2-oxo-2-phenylethyl)selanyl)-1-phenyl -1Himidazol-5(4H)-one (9h)

Yellow solid, (72%, 152 mg); mp: 150 – 152 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.62 (s, 1H), 8.44 (s, 1H), 8.35 (d, *J* = 7.3 Hz, 2H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.65 (m, 4H), 7.54 (t, *J* = 7.6 Hz, 2H), 7.48 - 7.42 (m, 2H), 6.92 (d, *J* = 8.5 Hz, 1H), 5.85 (s, 2H), 3.98 (s, 3H), 3.91 (s, 3H); <sup>13</sup>C NMR (151 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  193.9, 168.1, 160.0, 151.2, 148.8, 136.5, 135.7, 134.2, 133.2, 130.1, 129.9, 129.4, 128.9, 127.8, 127.1, 127.0, 124.8, 114.2, 111.7, 55.9, 55.4, 35.5; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>26</sub>H<sub>22</sub>N<sub>2</sub>O<sub>4</sub>Se 507.0823, Found 507.0828; IR (cm<sup>-1</sup>, neat): 3065, 2927, 1718, 1449.

#### (Z)-4-(3,4-dimethoxybenzylidene)-2-((2-oxo-1,2-diphenylethyl)thio)-1-phenyl-1Himidazol-5(4H)-one (9i)

Yellow solid, (76%, 170 mg); mp 86 – 88 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.10 (d, *J* = 8.6 Hz, 1H), 7.91 (d, *J* = 8.7 Hz, 1H), 7.61 - 7.56, 7.56 (m, 2H), 7.51 – 7.45 (m, 6H), 7.43 (d, *J* = 7.4 Hz, 1H), 7.39 - 7.35 (m, 3H), 7.33 - 7.29 (m, 2H), 6.96 (q, *J* = 8.6 Hz, 2H), 6.29 (d, *J* = 8.6 Hz, 1H), 3.97 – 3.90 (m, 1H), 3.85 (s, 3H), 3.80 (s, 3H); <sup>13</sup>C NMR (151 MHz, acetone)  $\delta$  193.7, 193.4, 179.3, 160.3, 148.9, 148.9, 135.6, 134.6, 134.5, 133.4, 132.5, 132.5, 129.2, 129.2, 129.0, 129.0, 128.9, 128.87, 128.8, 128.7, 128.6, 128.5, 127.3, 122.1, 113.7, 113.4, 111.5, 69.8, 69.5, 55.3, 55.1, 36.8, 36.7, 14.7; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>32</sub>H<sub>27</sub>N<sub>2</sub>O<sub>4</sub>S 535.1692, Found 535.1693; IR (cm<sup>-1</sup>, neat): 3059, 2919, 2851, 1420.

#### (Z)-4-(3,4-bis(allyloxy)benzylidene)-2-(2-oxo-2-(p-tolyl)ethoxy)-1-phenyl-1Himidazol-5(4H)-one (9j)

Yellow solid, (64%, 130 mg); mp 94 – 96 °C; <sup>1</sup>H NMR (400 MHz, CDcl<sub>3</sub>)  $\delta$  7.55 – 7.45 (m, 5H), 7.38 (q, *J* = 7.2 Hz, 1H), 7.28 – 7.24 (m, 1H), 7.15 (d, *J* = 8.6 Hz, 2H), 6.98 (s, 1H), 6.73 – 6.68 (m, 2H), 6.63 (d, *J* = 8.6 Hz, 1H), 6.04 – 5.92 (m, 2H), 5.35 (d, *J* = 7.9 Hz, 2H), 5.25 (d, *J* = 10.4 Hz, 2H), 4.98 (s, 2H), 4.44 – 4.42 (m, 4H), 2.37 (s, 3H); <sup>13</sup>C NMR (101 MHz, cdcl3)  $\delta$  191.1, 162.5, 155.2, 148.6, 148.1, 144.8, 132.9, 131.7, 131.6, 129.2, 129.0, 128.9, 128.4, 128.2, 127.7, 126.0, 125.06, 122.21, 120.0, 117.8, 117.7, 114.5, 113.4, 113.3, 69.7, 69.6, 48.6, 29.6, 21.7; HRMS (ESI) m/z: [M + H]<sup>+</sup> Calcd for C<sub>31</sub>H<sub>28</sub>N<sub>2</sub>O<sub>5</sub>S 509.2076, Found 509.2071; IR (cm<sup>-1</sup>, neat): 3059 ,2919, 2851, 1420.



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **3b** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **3b** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **3b** in acetone- $d_6$ 



 $^{13}$ C NMR Spectrum (101 MHz) of compound **3b** in CDCl<sub>3</sub>



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## Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **3b** in CDCl<sub>3</sub>





Chiral HPLC of compound 3b



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FT-IR Spectrum of compound **3b** 





Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **3k** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **3k** in CDCl<sub>3</sub>



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **3k** in CDCl<sub>3</sub>



Expansion of  ${}^{13}$ C NMR Spectrum (101 MHz) of compound 3k in CDCl<sub>3</sub>

			Display	Report				
Analysis Info Analysis Name Method Sample Name Comment	D:\Data\NCTU Small molecul L140-d	SERVICI e.m	E\Data\2018\20180817	7-2\L140-d_BA	Acquisition A4_01_19488 Operator Instrumen	n Date 8/17/20 .d NCTU t impact HD	18 12:10:06 P 1819696.0	M 0164
Acquisition Pa Source Type Focus Scan Begin Scan End	ESI Active 50 m/z 1500 m/z		Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Bar 200 °C 6.0 I/min Waste 0 °C	
1015 105 5- 4	240.1230			_0		U140-d_BA4_01_19	488.d: +MS, 0.7r	nin #39
3-122.0	960	387.1896	75	1.3914	) ~	⊥ HN 3k	$\bigcirc$	
Intens.	200 36	400	600	800	1000	1200	1400 +MS, 0.7r	m/z nin #39
1.5								
0.5		366.2	2107		1010			
x10 <sup>5</sup>	36	1+ 5.2071	367.2150		1		C19H29N2O5, 36	5.2071
1.0								
0.5		366.2	* 2103 1+					
0.0 362	364	366	367.2127	370	372	374	376	m/z

HRMS of compound 3k

CSM: Linda Series: 0168	Report Name: modified System: Sys	1
-------------------------	-----------------------------------	---

#### **Chromaster System Manager Report**

Analyzed Date and Time: 2018/09/15 Reported Date and Time: 2018/09/17 10:33 上午 10:23:03 上午 Processed Date and Time: 2018/09/17 10:22 上午 Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0168\ Processing Method: L140-d ee System (acquisition): Sys 1 Series: 0168 Application(data): Linda Vial Number: 1 Sample Name: UNKNOWN001 Vial Type: UNK Injection from this vial: 1 of 1 Volume: 10.0 ul Sample Description:









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FT-IR Spectrum of compound 3k





Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **3h** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **3h** in acetone- $d_6$ 



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **3h** in acetone- $d_6$


Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **3h** in acetone- $d_6$ 

				Dis	play R	eport				
Analysis Analysis Method Sample I Commer	Name Name Name	D:\Data\NCT\ Small molecu L322-P	U SERVICE\D lle.m	)ata\2018\20	0180817-2	L322-P_BA	Acquisitio 5_01_1948 Operator Instrumer	n Date 8/17/20 9.d NCTU nt impact HD	18196	25 PM 96.00164
Acquisit Source Ty Focus Scan Beg Scan End	tion Para ype In	ESI Active 50 m/z 1500 m/z	loi Se Se Se	n Polarity et Capillary et End Plate C et Charging V et Corona	offset oltage	Positive 4500 V -500 V 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 B 200 ° 6.0 M Wast 0 °C	ar 'C min je
Intens.			391.0563					L322-P_BA5_01_1	19489.d: +MS,	0.6min #36
0.8-						_C			0	
0.6-						`⊂			,se	
0.4										]
0.2-	122.096	50						3h	~	
		h in house		548.2383	763.2	247				
0.0~		200	400	600		800	1000	1200	14	400 m/z
Intens. x10 <sup>5</sup>				423.	0822				+MS,	0.6min #36
2.0										
1.5			421	0826						
1.0			411	1						
0.5			420.0849		424.0850	I.				
×10 <sup>5</sup> 2.5	-t	417.0868	<u>h</u> I.	423.	0818		429.	0128	C <sub>18</sub> H <sub>28</sub> N <sub>2</sub> O <sub>8</sub> 5	e, 423.0818
2.0										
1.5			421	1+ .0830						
1.0			1+		1+					
0.5		1+	420.0857	1+ 422.0859	424.0849	1+				
0.0	41	417.0877	420	422	424	426,0855	428	430 4	132	434 m/z

HRMS of compound **3h** 

CSM: Linda Series: 0169 Report Name: modified System: Sys 1

## **Chromaster System Manager Report**

Reported Date and Time: 2018/09/17 Analyzed Date and Time: 2018/09/17 09:15 上午 10:21:16 上午 Processed Date and Time: 2018/09/17 10:20 上午 Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0169\ Processing Method: L322 ee System (acquisition): Sys 1 Series: 0169 Application(data): Linda Vial Number: 1 Sample Name: UNKNOWN001 Vial Type: UNK Injection from this vial: 1 of 1 Volume: 10.0 ul Sample Description:









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FT-IR Spectrum of compound **3h** 



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **6g** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **6g** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 6g in CDCl<sub>3</sub>



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **6g** in CDCl<sub>3</sub>



Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **6g** in CDCl<sub>3</sub>

				Display	Report			
Analysis Analysis I Method Sample N	Info Name	D:\Data\ Small m	\nctu service\a iolecule.m	data\2018\20180518\L15	6-p_GC6_01_	Acquisition 18329.d Operator	Date 5/18/20 NCTU	18 2:55:56 PM
Commen	t	L100-p				mstrument	Impact no	1013030.00104
Acquisiti	ion Para	meter						
Source Ty Focus Scan Begi Scan End	n in	ESI Active 50 m/ 1500	e /z m/z	Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	9 9 9 9 9 9	Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Bar 200 °C 6.0 I/min Waste 0 °C
Intens. x10 <sup>6</sup>							L156-p_GC6_01_18	3329.d: +MS, 0.7min #37
1.0-		265.	0642					
0.8-					0	H N	_	
0.6 -			421.3	293		O N	S	
0.4 -	135.04	25	338.3419			6g		
0.2	135.04			705.58 635.5045	819.6691			
0.0~		200	400	600	800	1000	1200	1400 m/z

HRMS of compound 6g



FT-IR Spectrum of compound 6g



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **6c** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 6c in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 6c in CDCl<sub>3</sub>



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **6c** in CDCl<sub>3</sub>



Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **6c** in CDCl<sub>3</sub>

		Displ	ay Repor	t		
Analysis Info Analysis Name Method Sample Name Comment	H:\20181-6\201805 Smail molecule.m L290-I-1	25iL290-1-1_GC7_01_	18407.d	Acquisition D Operator Instrument	ate 5/25/20 NCTU Impact HD	18 12:07:12 PM 1819696.0016
Acquisition Pa Jource Type Focus Josen Begin Josen End	ESI Active 50 m/z 1500 m/z	ion Polerity Set Capillary Set End Plate Offs Set Charging Volts Set Corons	Positive 4500 V et -500 V ge 2000 V 0 nA	2 e 2 e 2 e 2 e 2 e 2 e	Nebulizer Dry Heater Dry Gas Divert Valve APCI Heater	1.0 Ber 200 °C 8.0 Vmin Weste 0 °C
Intens.	421	2799		L29	0++1_GC7_01_18	407.d: +MS, 0.7min #
£10- 6-						H N Se N
2- 122.00	367.3649		799.2632	6	c Ph	
	240.1229 200 40	eóo		1000	1200	1400 m
x10 <sup>5</sup>		43	3.5018			+MS, 0.7min P
2		431.0957				
1	429.094	.	434.1050	437.3022		
	428.0912	432.0983		436.1052 4	38.3053	441.2968
×10 <sup>8</sup>	- i - i - i	A A. 40	1, 2036			C2:H21N20250, 433.30
		1.				
2		431.3038				
2	1*	431.3038 1+ 130.1064 1+ 432.1067	1* 434.1057	1+ 436.1062		

HRMS of compound 6c



FT-IR Spectrum of compound 6c



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **6k** in CD<sub>3</sub>OD



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **6k** in CD<sub>3</sub>OD





<sup>13</sup>C NMR Spectrum (101 MHz) of compound **6k** in CDCl<sub>3</sub>



Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **6k** in CDCl<sub>3</sub>

				Display	Report				
Analysis Analysis Method Sample I Commen	<b>s Info</b> Name Name It	D:\Data\nctu Small molect L298-I	service\data\2 ule.m	018\20180821\L29	8-I_GB6_01_1	Acquisition 19574.d Operator Instrument	Date 8/21/201 NCTU impact HD	8 2:31:27 PM 1819696.001	64
Acquisit Source Ty Focus Scan Beg Scan End	i <b>on Para</b> /pe in	ESI Active 50 m/z 1500 m/z	lor Se Se Se	n Polarity t Capillary t End Plate Offset t Charging Voltage t Corona	Positive 4500 ∨ -500 ∨ 2000 ∨ 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Bar 200 °C 6.0 l/min Waste 0 °C	
Intens x10 <sup>6</sup> 2.5		333	.1814				L298-I_GB6_01_19	574.d: +MS, 0.6min	#33
2.0		225.1959							
1.0			431.3753			6k			
0.5		200	400	687.3379 600	800	1000	1200	1400	m/z

HRMS of compound 6k



FT-IR Spectrum of compound 6k



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **5a** in CDCl<sub>3</sub>





Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5a** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5a** in CDCl<sub>3</sub>







HRMS of compound 5a

CSM: Linda Series: 0093 Report Name: modified System	n: Sy	3	1
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## **Chromaster System Manager Report**

Analyzed Date and Time: 2017/12/05 02:30 下午	Reported Date and Time: 2017/12/05 04:49:13 下午					
Processed Date and Time: 2017/12/05 04:48 下午						
Data Path: C:\WIN32APP\CHROMASTER\Linda	\DATA\0093\					
Processing Method: L170_ee						
System (acquisition): Sys 1	Series: 0093					
Application(data): Linda	Vial Number: 1					
Sample Name: UNKNOWN001	Vial Type: UNK					
Injection from this vial: 1 of 1	Volume: 20.0 ul					
Sample Description:						





## Chiral HPLC of compound 5a



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FT-IR Spectrum of compound 5a



 $^{1}$ H NMR Spectrum (400 MHz) of compound **5b** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5b** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5b** in CDCl<sub>3</sub>


<sup>13</sup>C NMR Spectrum (101 MHz) of compound **5b** in CDCl<sub>3</sub>



Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **5b** in CDCl<sub>3</sub>

			Display	Repor	t			
Analysis Info Analysis Name Method Sample Name Comment	H120181-6(20180 Smail molecule.m L121	4171L121_RA	2_D1_17989.d	I	Acquisitio Operator Instrumer	NCTU NCTU nt impact HD	018 12:46:44 P 1819696.0	M 0164
Acquisition Par Source Type Focus Scan Begin Scan End	Fameter ESI Active 50 m/z 1500 m/z	Ion Pole Set Cap Set End Set Cha Set Core	rity Elsry Piste Offset rging Voltage ma	Positive 4500 V -500 V 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Ber 200 °C 6.0 Vmin Weste 0 °C	
Intens. x10 <sup>5</sup>						L121_RA2_01_	17989.d: +MS, 0.8r	nin M7
		503.2003						
2.0	105				_0			
1.5	41	3.2658		~		N N		
0.5	279.1590			783.57	Pn	S—⁄		
0.0	200 4	100 Aug 100	800	800	1000	1200	1400	miz
intens.: x10 <sup>5</sup>		503,2003					+MS, 0.8r	nin #47
2.5		1						
2.0								
1.5		504	.2037					
0.5								
0.0			505.2026			511,4707		
x10+		503 1999					ColHaNyO45, 50	1999
20								
1.5								
1.0		504	1+					
0.5			1+ 505,2016					
0.0	500	viz ***	1 1		óa sie	512	514	mir

HRMS of compound **5b** 

Report Name: modified System: Sys 1 Series: 0033 CSM: Linda **Chromaster System Manager Report** Analyzed Date and Time: 2017/11/03 Reported Date and Time: 2017/11/03 01:39 下午 04:33:51 下午 Processed Date and Time: 2017/11/03 04:05 下午 Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0033\ Processing Method: L121\_ee System (acquisition): Sys 1 Series: 0033 Application(data): Linda Vial Number: 1 Vial Type: UNK Sample Name: UNKNOWN001 Injection from this vial: 1 of 1 Volume: 15.0 ul Sample Description:





1, Hex 10

Chiral HPLC of compound 5b



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FT-IR Spectrum of compound **5b** 



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **5c** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 5c in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 5c in CDCl<sub>3</sub>



 $^{13}$ C NMR Spectrum (101 MHz) of compound **5c** in CDCl<sub>3</sub>



149 148 147 146 145 144 143 142 141 140 139 138 137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 120 119 118 117 116 115 114 113 112 111 fl (ppm)

Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **5c** in CDCl<sub>3</sub>

		Display	Report			
<b>Analysis Info</b> Analysis Name Method Sample Name Comment	D:\Data\nctu servic Small molecule.m L165	e\data\2018\20180417\L16	5_RA3_01_17	Acquisition Date 7990.d Operator NCT Instrument impa	4/17/2018 12 U act HD 18	::51:03 PM 319696.00164
Acquisition Par Source Type Focus Scan Begin Scan End	ameter ESI Active 50 m/z 1500 m/z	lon Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	Set Neb Set Dry Set Dry Set Dive Set APC	ulizer Heater Gas rt Valve I Heater	1.0 Bar 200 °C 6.0 I/min Waste 0 °C
Intens. x107 2.0 1.5 1.5		565.1609	_O  Ph~∕	L165_	_RA3_01_17990.d	: +MS, 0.6min #33
0.0	200 40	00 600	800	1000	1200	1400 m/z

HRMS of compound 5c

		Ch	romostor Sv	stom M	Ionog	Papart		-1-	-	
CSM:	Linda	Series:	0119	Report	Name:	modified	System:	Svs	1	

enfoliaster syste	in manager report
Analyzed Date and Time: 2018/09/05 08:19 上午	Reported Date and Time: 2018/09/11 09:08:01 上午
Processed Date and Time: 2018/09/11 09:07 上午	
Data Path: C:\WIN32APP\CHROMASTER\Linda	\DATA\0119\
Processing Method: L165_ee	
System (acquisition): Sys 1	Series: 0119
Application(data): Linda	Vial Number: 1
Sample Name: UNKNOWN001	Vial Type: UNK
Injection from this vial: 1 of 1	Volume: 10.0 ul
Sample Description:	





## Chiral HPLC of compound **5**c



FT-IR Spectrum of compound **5**c



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **5d** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5d** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5d** in acetone- $d_6$ 



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **5d** in CDCl<sub>3</sub>



Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **5d** in CDCl<sub>3</sub>

		Display	y Report			
Analysis Info Analysis Name Method Sample Name Comment	D:\Data\nctu servi Small molecule.m L224	ce\data\2018\20180417\L2	24_RA5_01_179	Acquisition D 992.d Operator Instrument	ate 4/17/201 NCTU impact HD	8 12:59:43 PM 1819696.00164
Acquisition Par Source Type Focus Scan Begin Scan End	ameter ESI Active 50 m/z 1500 m/z	lon Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 ∨ -500 ∨ 2000 ∨ 0 nA	Se Se Se Se	t Nebulizer t Dry Heater t Dry Gas t Divert Valve t APCI Heater	1.0 Bar 200 °C 6.0 l/min Waste 0 °C
Intens, x10 <sup>7</sup> -					L224_RA5_01_179	992.d: +MS, 0.6min #33
1.5		505.1804				
1.0			S-			
0.5						
0.0	200 4	600 600	800	1000	1200	1400 m/z
		HRMS of	f compound 5d	l		

## 

```
Processing Method: 27d_ee

System (acquisition): Sys 1 Series: 0206

Application(data): Linda Vial Number: 1

Sample Name: UNKNOWN001 Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 10.0 ul

Sample Description:
```





Chiral HPLC of compound 5d





<sup>1</sup>H NMR Spectrum (400 MHz) of compound **5e** in acetone- $d_6$ 



Expending <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5e** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5e** in acetone- $d_6$ 



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **5e** in CDCl<sub>3</sub>



Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound 5e in CDCl<sub>3</sub>

		Display	Report		
Analysis Info	D:\Data\nctu.sonvico	\data\2018\20180417\  22	5 046 01 17	Acquisition Date 4/17/20	18 1:04:01 PM
Method Sample Name Comment	Small molecule.m L225	uala 2010/20100417/L22	<u>5_KA0_01_17</u>	Operator NCTU Instrument impact HD	1819696.00164
Acquisition Par Source Type Focus Scan Begin Scan End	ameter ESI Active 50 m/z 1500 m/z	Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Bar 200 °C 6.0 I/min Waste 0 °C
Intens. x107 2.0		538.1650		L225_RA6_01_1	7993.d: +MS, 0.6min #
1.5				NO <sub>2</sub>	
1.0			5e	1	
0.5					
0.01	200 400		800	1000 1200	1400 n
		HRMS of c	ompound 56	•	

## 



HRMS of compound 5e

```
Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0208\

Processing Method: 27e_ee

System (acquisition): Sys 1 Series: 0208

Application(data): Linda Vial Number: 1

Sample Name: UNKNOWN001 Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 10.0 ul

Sample Description:
```





Method Description: flow rate : 0.3 mL/min , Daicel Chiral OD, IPA 15, Hex 85

Chiral HPLC of compound 5e



FT-IR Spectrum of compound **5**e



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **5f** in  $d_6$ -Acetone



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5f** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5f** in acetone- $d_6$ 



 $^{13}\text{C}$  NMR Spectrum (101 MHz) of compound 5f in CDCl\_3



Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **27f** in CDCl<sub>3</sub>

## **Display Report** Analysis Info Acquisition Date 4/17/2018 1:08:21 PM Analysis Name D:\Data\nctu service\data\2018\20180417\L227\_RA7\_01\_17994.d Operator NCTU Method Small molecule.m L227 Sample Name Instrument impact HD 1819696.00164 Comment **Acquisition Parameter** Ion Polarity ESI Set Nebulizer Source Type Positive 1.0 Bar Set Capillary Focus Active 4500 V Set Dry Heater 200 °C Scan Begin Set Dry Gas 50 m/z Set End Plate Offset -500 V 6.0 l/min Set Divert Valve Scan End Set Charging Voltage 2000 V 1500 m/z Waste 0°C Set APCI Heater Set Corona 0 nA Intens. L227\_RA7\_01\_17994.d: +MS, 0.5min #31 x107 2.0 523.1131 1.5-Se-1.0 5f 0.5-0.0 800 200 400 600 1000 1200 1400 m/z HRMS of compound **5**f


```
Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0213\

Processing Method: 27f_ee

System (acquisition): Sys 1 Series: 0213

Application(data): Linda Vial Number: 1

Sample Name: UNKNOWN001 Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 10.0 ul

Sample Description:
```





Chiral HPLC of compound 5f



FT-IR Spectrum of compound **5f** 



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **5g** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5g** in acetone- $d_6$ 





<sup>13</sup>C NMR Spectrum (101 MHz) of compound **5g** in CDCl<sub>3</sub>



Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **5g** in CDCl<sub>3</sub>

			Display	Report			
Analysis Info Analysis Name Method Sample Name Comment	H120181-6\201 Smail molecule. L228	80417\L228_RA m	8_01_17995.d	I	Acquisition Operator Instrument	NCTU Impact HD	18 1:12:40 PM 1819696.0016
Acquisition Par Source Type Focus Scen Begin Scen End	ESI Active 50 m/z 1500 m/z	ion Pols Set Cap Set End Set Cha Set Con	rity Iliary Plate Offset rging Voltage ons	Positive 4500 V -500 V 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Ber 200 °C 6.0 l/min Weste 0 °C
Intens.						L228_RA8_01_17	995.d: +MS, 0.4min #
×10-		489.1847					
3			_0				
2.			<u>`</u> c				$\sum$
1					s-		
122.09	66				5g		
0, 10, 10,	200	400	600	800	1000	1200	1400 #
x10 <sup>6</sup>		489.3847					+MS, 0.4min #
2							
1			450.1877		491.1862	83 1070	
x10 <sup>8</sup>		1+	A		A	432,1833	C <sub>28</sub> H <sub>28</sub> N <sub>2</sub> O <sub>4</sub> S, 489.18
3		10.1073					
2		Announced in Announcement	490,1874				
					1+ 491_1858 2	1+ 492.1867	
0-		80	400			402	400 -

HRMS of compound 5g

```
Processing Method: 27k_ee

System (acquisition): Sys 1 Series: 0201

Application(data): Linda Vial Number: 1

Sample Name: UNKNOWN001 Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 10.0 ul

Sample Description:
```





Hex 85

Chiral HPLC of compound **5**g



FT-IR Spectrum of compound 5g



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **5h** in acetone- $d_6$ 







Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5h** in acetone- $d_6$ 



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **5h** in CDCl<sub>3</sub>



		Display	Report				
Analysis Info				Acquisition Date 4/17/20	18 1:17:02 PM		
Analysis Name Method Sample Name Comment	me D:\Data\nctu service\data\2018\20180417\L190_RB1_0 Small molecule.m ne L190			17996.d Operator NCTU Instrument impact HD 1819696.00164			
Acquisition Par Source Type Focus Scan Begin Scan End	ameter ESI Active 50 m/z 1500 m/z	lon Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Bar 200 °C 6.0 I/min Waste 0 °C		
Intens. x10 <sup>7</sup>				L190_RB1_01_1	7996.d: +MS, 0.6min #32		
1.5		610.1456					
1.0			Ph	N N NO2 Se			
0.5	250.027						
0.0	200 400	600	800	1000 1200	1400 m/z		
	-	HRMS of c	ompound 5	5h			

```
Processing Method: 27h_ee

System (acquisition): Sys 1 Series: 0214

Application(data): Linda Vial Number: 1

Sample Name: UNKNOWN001 Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 10.0 ul

Sample Description:
```





Chiral HPLC of compound **5h** 



FT-IR Spectrum of compound **5h** 



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **5i** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5i** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5i** in acetone- $d_6$ 



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **5i** in CDCl<sub>3</sub>



		Display	Report		
Analysis Info				Acquisition Date 4/17/2	018 1:21:21 PM
Analysis Name Method Sample Name Comment	D:\Data\nctu service Small molecule.m L230	\data\2018\20180417\L23	0_RB2_01_1799	97.d Operator NCTU Instrument impact HD	1819696.00164
Acquisition Par Source Type Focus Scan Begin Scan End	ameter ESI Active 50 m/z 1500 m/z	lon Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Bar 200 °C 6.0 l/min Waste 0 °C
Intens. x10 <sup>7</sup>		539.0466		L230_RB2_01_	17997.d: +MS, 0.7min #
1.5				Br	
1.0			5i		
0.5					
0.0	200 400	600	800	1000 1200	1400 n
		HRMS of co	ompound 5i		



HRMS of compound 5i

Processing Method: 27i_ee	
System (acquisition): Sys 1	Series: 0217
Application(data): Linda	Vial Number: 1
Sample Name: UNKNOWN001	Vial Type: UNK
Injection from this vial: 1 of 1	Volume: 10.0 ul
Sample Description:	





Chiral HPLC of compound 5i



FT-IR Spectrum of compound 5i





Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5**j in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5**j in acetone- $d_6$ 



 $^{13}C$  NMR Spectrum (101 MHz) of compound **5j** in CDCl<sub>3</sub>



Display Report								
Analysis Info Analysis Name Method Sample Name Comment	H:120181-6120 Smail molecul L232	1804171L e.m	232_RB3_01_17998.d		Acquisition Operator Instrument	NCTU NCTU t Impact HD	8 1:25:40 PM 1819696.00164	
Acquisition Pa Source Type Focus Scan Begin Scan End	Fameter ESI Active 50 m/z 1500 m/z		Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Ber 200 °C 8.0 Vmin Wests 0 °C	
118408 x10 <sup>6</sup> 4- 3- 2-		423.137	2			5j	HHLd: +MS, D.Amin #23	
0	200	400	539.0458 800	800	1000	1200	1400 m/z	
x10 <sup>8</sup> 3 2 1 x10 <sup>8</sup> 4 3 2 1		423.1	424,5400 425,1373 373 424,3406 425,1379 424,3406 425,1379				+NG, 0.4min #23 C <sub>11</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub> S, 423.1373	
418	420	422	424 426	428	430	432 434	436 m/z	

HRMS of compound 5j

Series: 0118 Report Name: modified System: Sys 1 CSM: Linda **Chromaster System Manager Report** Analyzed Date and Time: 2018/09/04 Reported Date and Time: 2018/09/18 08:53 下午 02:32:58 下午 Processed Date and Time: 2018/09/18 02:32 下午 Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0118\ Processing Method: L232\_ee System (acquisition): Sys 1 Series: 0118 Application(data): Linda Vial Number: 1 Sample Name: UNKNOWN001 Vial Type: UNK Injection from this vial: 1 of 1 Volume: 10.0 ul Sample Description:





Hex 85

Chiral HPLC of compound 5j



FT-IR Spectrum of compound 5j


<sup>1</sup>H NMR Spectrum (400 MHz) of compound **5k** in CD<sub>3</sub>OD



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5k** in CD<sub>3</sub>OD



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5k** in CD3OD



 $^{13}$ C NMR Spectrum (101 MHz) of compound **5k** in CDCl<sub>3</sub>



Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **5k** in CDCl<sub>3</sub>

Analysic Info Analysic Info Sample Name L233 Comment Sample Name L233 Comment Sample Name L233 Comment Sample Name L233 Sample Name Sample Name Sam			Displa	y Report			
Acquisition Parameter Bouns Type         ESI ESI ESI Sear Bight         Ion Polarity Sear Dight         Positive 450 V         Bet Netulizer 450 V         1.0 Ber Bet Netulizer         1.0 Ber 200 °C           Sear Bight         Store a Store Bight         Sear Dight Sear D	nalysis Info nalysis Name lethod ample Name komment	H120181-6/201804 Small molecule.m L233	1171L233_R84_01_1799	9.d	Acquisition Date Operator NC1 Instrument Imp	4/17/2018 1:2 TU act HD 18	29:59 PM 19696.00164
$\begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \end{array} \end{array} \end{array} \end{array} \\ \begin{array}{c} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	oquisition Par ource Type ocus can Begin can End	ESI Active 50 m/z 1500 m/z	Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	Set Net Set Dry Set Dry Set Div Set APC	ulizer Hexter Gas et Valve 21 Hexter	1.0 Ber 200 °C 8.0 Vmin Weste 0 °C
$ \begin{array}{c} 133 \\ 0 \\ 0 \\ 0 \\ 122,0967 \\ 1 \\ 200 \\ 1 \\ 200 \\ 1 \\ 200 \\ 1 \\ 200 \\ 1 \\ 200 \\ 1 \\ 200 \\ 1 \\ 200 \\ 1 \\ 200 \\ 1 \\ 1 \\ 200 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\$	Intens.				L233	_RB4_01_17999.d	+MS, 0.5min #23
1         200         400         800         800         1000         1200         1400           1         100         552.0675         +M6, 0.5         -	5 4 3 2 122.09	67 282-2789 738-3434	552,0675		Se 5k		10 <sub>2</sub>
1         200         400         600         800         1000         1200         1400           1         100         552.0675         +M6, 0.5         +M6, 0.5         +M6, 0.5           2         550.0887         553.0704         554.0677         555.0682         550.0887           3         554.0727         551.0712         553.0704         555.0682         550.0887           4         550.0887         552.0670         CauHu, WAG, 56, 5         550.0882         550.0882           4         550.0682         552.0670         CauHu, WAG, 56, 5         550.0882         550.0682           2         1         1         551.0712         553.0701         1+		البرية والمراجع		783.5789			
Interne x109 552.0675 4 3 550.0887 551.0712 553.0704 554.0677 553.0704 554.0677 553.0704 554.0677 555.0662 555.0662 555.0662 555.0662 555.0667 555.0677 555.0667 555.0677 555.0667 555.0677 555.0667 555.067 555.07 555.07 555.07 555.07 555	0	200 40	οίο ούο	800	1000	1200	1400 m/s
4 3 550,0887 551,0704 551,0704 551,0704 551,0704 555,0662 555,0662 555,0662 555,0662 555,0662 555,0662 555,0662 555,0662 555,0677 CaiHi1NG,056,59 550,0882 14 550,0882 14 551,0701 1*	x10 <sup>5</sup>		552.	0675			+MS, 0.5min #2
Z 1 546.0727 x10 <sup>9</sup> 546.0727 x10 <sup>9</sup> 546.0727 x10 <sup>9</sup> 546.0727 555.0662 555.0676 555.0662 555.0662 555.0662 555.0662 555.0662 555.0676 555.0676 555.0676 555.0662 555.0676 555.0676 555.0676 555.0677 555.0676 555.0677 555.0677 555.0677 555.0677 555.0677 555.0677 555.0677 555.0677 555.0677 555.0677 555.0677 555.0678 555.0678 550.0711 555.0678 550.0711 555.0678 550.0711 555.0678 550.0711 555.0678 550.0711 555.0678 550.0711 555.0678 550.0711 555.0678 550.0711 550.0711 555.0678 550.0711 550.07	4 3		550,0687				
1 546,0727 551,0712 551,0712 555,0682 556,0678 559,13 109 5 51,0770 5 555,0682 556,0678 559,13 510 510,0710 1* 550,0682 550,0682 550,0682 550,0682 550,0682 550,0682 550,0682 550,0682 550,0682 550,0682 550,0682 550,0682 550,0682 550,0701 1*	Z			553,0704	1477		
110 <sup>3 5469/C/7</sup> <u>A A I I A A S060/C/7</u> <u>Califul W/G/66, 5</u> 110 <sup>3</sup> 5 4 3 2 2 1 1 1 1 1 1 1 1 1 1 1 1 1	1	548,0696 549.0	551.0712	254	555.0682 pec acro		EE0 1336
5 4 3 5500682 2 1 1 1 1 5500682 1 5500701 1*	x10 <sup>8</sup>	h		1020	1 356/16/16	C <sub>36</sub> H <sub>11</sub>	NyO456, 552.0668
4 3 550,0682 2 1 1 550,0682 1 550,0682 1 550,0682 1 550,0701 1+	5						
	4 3 2	14 3	550.0682	1+ 551.0701 3			
1 1+ 548.0603 549.0709 1+ 551.0711 1+ 1+	1 1+	548,0605 549,0	709 1+ 551,0711	554.	1+		
0 <sup>1546,0728</sup>	546.0728	548			300.000		

HRMS of compound 5k

```
Processing Method: 27k_ee

System (acquisition): Sys 1 Series: 0201

Application(data): Linda Vial Number: 1

Sample Name: UNKNOWN001 Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 10.0 ul

Sample Description:
```





mL/min , Daicel Chiral OD, IPA 15, Hex 85

Chiral HPLC of compound **5**k



FT-IR Spectrum of compound **5**k



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **5**l in acetone- $d_6$ 



Expending <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5**l in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5**l in acetone- $d_6$ 



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **51** in CDCl<sub>3</sub>



Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **51** in CDCl<sub>3</sub>

		Display	Report				
Analysis Info Analysis Name Method Sample Name Comment	H:\20181-6\20180417 Smail molecule.m L235	L235_R85_01_18000.4	d	Acquisition Operator Instrument	NCTU Impact HD	18 1:34:19 PN 1819696.0	N 10164
Acquisition Pa	rameter						
Source Type Focus Scen Begin Scen End	ESI Active 50 m/z 1500 m/z	Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	8 8 8 8 8	et Nebulizer et Dry Heater et Dry Gas et Divert Valve et APCI Heater	1.0 Ber 200 °C 6.0 Vmin Wieste 0 °C	
intens. x10 <sup>7</sup>		561.1454			1735 805 01 10	nna aik na	nin #2
0.8-				$\sim$			
0.6-			Ph <sub>2</sub>	_N <sub>≥</sub>	N		
0.4				S	e_/		
0.2-				51			
0.0	200 400	600	800	1000	1200	1400	m
intens. x107		563.1	454			+MS, 0.4r	nin #2
0.8							
0.6		561.1468					
0.1-			564.1488				
0.2	557.1502	562.1499	565.1472	1499			
x107_		1 563.1	446			C <sub>10</sub> H <sub>at</sub> N <sub>2</sub> O <sub>4</sub> Se, 56	3.144
0.8		1.					
0.6-		561.1459	1+				
0.2-	1+	560.1485 1+ 562.1487	564.1477 1+	14			
0.01	557.1503		1 500	1404	570.0	8T0 6	

HRMS of compound **5**I

CSM: Linda Series: 0125 Report Name: modified System: Sys 1 **Chromaster System Manager Report** Analyzed Date and Time: 2018/09/06 Reported Date and Time: 2018/09/11 08:03 下午 12:05:13 下午 Processed Date and Time: 2018/09/11 12:04 下午 Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0125\ Processing Method: L235 ee System (acquisition): Sys 1 Series: 0125 Application(data): Linda Vial Number: 1 Sample Name: UNKNOWN001 Vial Type: UNK Volume: 10.0 ul Injection from this vial: 1 of 1 Sample Description:





Chiral OD, IH Hex 85

Chiral HPLC Spectrum of compound 51



FT-IR Spectrum of compound **5**l



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **5m** in CDCl<sub>3</sub>





Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5m** in CDCl<sub>3</sub>





Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **5m** in CDCl<sub>3</sub>

			Display	Report			
Analysis Info Analysis Name Method Sample Name Comment	D:\Data\nctu se Small molecule L323	rvice\data\2018 .m	3\20180824\L32	3_BB4_01_19	Acquisition 9657.d Operator Instrument	Date 8/24/201 NCTU impact HD	8 12:59:50 PM 1819696.00164
Acquisition Par Source Type Focus Scan Begin Scan End	ameter ESI Active 50 m/z 1500 m/z	lon Po Set Ca Set Er Set Cl Set Co	olarity apillary nd Plate Offset narging Voltage prona	Positive 4500 V -500 V 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Bar 200 °C 6.0 I/min Waste 0 °C
Intens. x10 <sup>7</sup> 1.50		489.1845				L323_BB4_01_19	657.d: +MS, 0.7min #39
1.25							
1.00					N S		
0.75					5m		
0.50							
0.25	202.275	421.3291					
0.00	282.2784	400	600	800	1000	1200	1400 m/z

HRMS of compound **5m** 

```
Processing Method: 27m_ee

System (acquisition): Sys 1 Series: 0221

Application(data): Linda Vial Number: 1

Sample Name: UNKNOWN001 Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 10.0 ul

Sample Description:
```

Chrom Type: Chromaster Channel : 1



Chiral HPLC of compound 5m

Hex 85



FT-IR Spectrum of compound 5m



<sup>1</sup>H NMR Spectrum (400 MHz) of compound 5n in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5n** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5n** in CDCl<sub>3</sub>



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **5n** in CDCl<sub>3</sub>



151 150 149 148 147 146 145 144 143 142 141 140 139 138 137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 120 119 118 117 116 115 114 113 112 111 110 fl (ppm)

Expansion of  ${}^{13}$ C NMR Spectrum (101 MHz) of compound **5n** in CDCl<sub>3</sub>

		Display	Report		
Analysis Info Analysis Name Method Sample Name Comment	D:\Data\nctu servi Small molecule.m L324	ce\data\2018\20180824\L32	4_BB5_01_19	Acquisition Date 8/24/20 658.d Operator NCTU Instrument impact HD	018 1:04:13 PM 1819696.00164
Acquisition Par Source Type Focus Scan Begin Scan End	ESI Active 50 m/z 1500 m/z	Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Bar 200 °C 6.0 l/min Waste 0 °C
Intens. x10 <sup>6</sup>	4		Se 5n	L324_BB5_01_1	19658.d: +MS, 0.7min #37
0	226.9512 8.9635 362.920 200 4	537.1295 63 100 600	819.6692	1000 1200	, 1400 m/z

HRMS of compound **5n** 



HRMS of compound **5n** 

Processing Method: 27n_ee	
System (acquisition): Sys 1	Series: 0218
Application(data): Linda	Vial Number: 1
Sample Name: UNKNOWN001	Vial Type: UNK
Injection from this vial: 1 of 1	Volume: 10.0 ul
Sample Description:	

Chrom Type: Chromaster Channel : 1



Chiral HPLC of compound **5n** 



FT-IR Spectrum of compound **5n** 



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **50** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **50** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **50** in acetone- $d_6$


<sup>13</sup>C NMR Spectrum (101 MHz) of compound **50** in CDCl<sub>3</sub>



CSM: Linda Serie:	s: 0163	Report Name: modified System: Sys 1					
Chromaster System Manager Report							
Analyzed Date and Time	: 2018/09/14 08:16 下午	Reported Date and Time: 2018/09/15 08:54:50 上午					
Processed Date and Time: 2018/09/15 08:54 上午							
Data Path: C:\WIN32APP\CHROMASTER\Linda\DATA\0163\							
Processing Method: L320_ee							
System (acquisition):	Sys 1	Series: 0163					
Application(data): Lin	da	Vial Number: 1					
Sample Name: UNKNOWN00	1	Vial Type: UNK					
Injection from this vi	al: 1 of 1	Volume: 10.0 ul					
Sample Description:							





thod Description: flow rate : 0.3 mL/min , Daicel Chiral OD, IFA15, Hex 85

Chiral HPLC of compound 50



FT-IR Spectrum of compound **50** 



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **5p** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5p** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **5p** in acetone- $d_6$ 



<sup>13</sup>C NMR Spectrum (151 MHz) of compound **5p** in acetone- $d_6$ 



Expansion of <sup>13</sup>C NMR Spectrum (151 MHz) of compound **5p** in acetone- $d_6$ 

				Display	Report				
Analysis Analysis Method Sample I Commer	s Info Name Name It	D:/Data/NCT Smail molecu L331	U SERVICE/Data( (ie.m	2018/20180921	11331_RA6_D	Acquisition 1_20109.d Operator Instrument	Date 9/21/20 NCTU Impact HD	18 12:09:17 PI 1819696.00	M 0164
Acquisit Source Ty Focus Scen Beg Scen End	ton Para pe in	ESI Active 50 m/z 1500 m/z	ion Poi Set Ca Set En Set Ch Set Ch	arity pillary I Plate Offset arging Voltage rona	Positive 4500 V -500 V 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Ber 200 °C 6.0 Vmin Weste 0 °C	
x10 <sup>6</sup>							L331_RA6_01_201	109.d: +MS, 1.7mi	n #100
0.8-			551.	008	_0. `0	N			
0,4-	124.086	•			,		s–( Ph	I	
0.2-		255.1947	399.3461	608, 1308	5 077 404	0	5p		
0.0		200	400	600	800	1000	1200	1400	m/z
x10 <sup>6</sup>			551,2008					+MS, 1.7min	n ¥100
0.8									
0.6									
0.4				552.2038					
0.2					553,2027				
×168			// 24 551 1000	j,	7	554,2031		C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub> S, 553	L 1999
0.8			1999						
0.6									
0.4				1+ 552,2031					
0.2					553,2022	1+			
0.0	549	550	551	552	553	554	555	506	miz

HRMS of compound 5p

```
Processing Method: 27r_ee

System (acquisition): Sys 1 Series: 0204

Application(data): Linda Vial Number: 1

Sample Name: UNKNOWN001 Vial Type: UNK

Injection from this vial: 1 of 1 Volume: 10.0 ul

Sample Description:
```





Chiral HPLC of compound **5**p



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **7a** in CDCl<sub>3</sub>



Expending <sup>1</sup>H NMR Spectrum (400 MHz) of compound 7a in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 7a in CDCl<sub>3</sub>



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **7a** in CDCl<sub>3</sub>



148 147 146 145 144 143 142 141 140 139 138 137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 120 119 118 117 116 115 114 113 112 111 fl (ppm)

Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **7a** in CDCl<sub>3</sub>

			Display	Report			
<b>Analysis In</b> Analysis Na	fo me D:\Data\nc	tu service\da	ta\2018\20180420\L17	5_RC5_01_18	Acquisition Da	ate 4/20/201	8 12:06:25 PM
Method Sample Nar Comment	Small mole me L175	ecule.m			Operator I Instrument i	NCTU impact HD	1819696.00164
Acquisition Source Type	n Parameter ESI		Ion Polarity	Positive	Set	Nebulizer	1.0 Bar
Scan Begin Scan End	50 m/z 1500 m/z	2	Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	-500 V 2000 V 0 nA	Set Set Set	Dry Gas Divert Valve APCI Heater	6.0 l/min Waste 0 °C
Intens. x10 <sup>6</sup> 8-		461.	1530			L175_RC5_01_18	028.d: +MS, 0.5min #31
6 -	253.0790				N S C		
4 -					7a		
2-	167.0695		555.0775 611.1682	010	2702		
0	200	400	600	800	1000	1200	1400 m/z

HRMS of compound 7a



FT-IR Spectrum of compound 7a



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **7b** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **7b** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 7b in acetone- $d_6$ 





Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **7b** in acetone- $d_6$ 



HRMS of compound 7b



FT-IR Spectrum of compound 7b



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **7c** in CDCl<sub>3</sub>





Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **7c** in CDCl<sub>3</sub>





 $^{13}$ C NMR Spectrum (101 MHz) of compound 7c in CDCl<sub>3</sub>



150 149 148 147 146 145 144 143 142 141 140 139 138 137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 120 119 118 117 116 115 114 113 112 111 110 fl (ppm)

Expansion of  ${}^{13}$ C NMR Spectrum (101 MHz) of compound 7c in CDCl<sub>3</sub>



HRMS of compound 7c



FT-IR Spectrum of compound 7c



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **7d** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 7d in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 7d in CDCl<sub>3</sub>



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **7d** in CDCl<sub>3</sub>
		Display	Report		
Analysis Info Analysis Name Method Sample Name Comment	D:\Data\nctu servio Small molecule.m L244	ce\data\2018\20180420\L24	4_RC6_01_1	Acquisition Date 4/20/ 8029.d Operator NCTU Instrument impact HD	2018 12:10:45 PM 1819696.00164
Acquisition Pa Source Type Focus Scan Begin Scan End	Arameter ESI Active 50 m/z 1500 m/z	lon Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heate	1.0 Bar 200 °C 6.0 I/min Waste er 0 °C
Intens. x107 2.0 1.5		491.1644	.0	L244_RC6_01	18029.d: +MS, 0.6min #32
1.0				7d	
0.0	283.0895 <sub>379.12</sub> 200 4	262 657.2256 00 600	800	1003.2969 1000 1200	

HRMS of compound 7d



FT-IR Spectrum of compound 7d



<sup>1</sup>H NMR Spectrum (400 MHz) of compound 7e in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 7e in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 7e in CDCl<sub>3</sub>



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **7e** in CDCl<sub>3</sub>

		Displa	ynepon			
Analysis Info Analysis Name Method Sample Name Comment	H:120181-6120180 Small molecule.m L245	420/L245_RC7_01_18030	1.d	Acquisition D Operator Instrument	Note 4/20/20 NCTU Impact HD	18 12:15:06 PM
Acquisition Par	rameter					
Source Type Focus Scan Begin Scan End	ESI Active 50 m/z 1500 m/z	Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	4500 V -500 V 2000 V 0 nA	Se Se Se	t Nebulizer t Dry Heater t Dry Gas t Divert Valve t APCI Heater	1.0 Ber 200 °C 6.0 Vmin Weste 0 °C
Intens.					L245_RC7_01_18	030.d: +NS, 1.0min (
e.]		505.1384				
				<u> </u>	- (	2
					-s_	
3			~0~ ~~	0 1		
	- 1			(	í 🐧 🤞	
2	19.3			7	=/	NO <sub>2</sub>
				7e		2
1	41	3.2653				
	338.3405					
السب ان	بليل والمراجعة و	hand han a second se	783.5785	1000	*200	
Intens, 1	200	60 600	000	1000	1200	+MS, 1.0min
×105		506.1384				
4						
3						
2		507.1413				
1			508.1356 509.1395			
x108		14 D 506.1380				CallaNuOuS, 506.1
5						
4						
3		1+				
2		507.1411	1+			
			508.1393 14 509.1406			
	504	506	506	510	512	514

HRMS of compound 7e



FT-IR Spectrum of compound 7e



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **7f** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **7f** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **7f** in CDCl<sub>3</sub>



 $^{13}\text{C}$  NMR Spectrum (101 MHz) of compound **7f** in CDCl\_3



149 148 147 146 145 144 143 142 141 140 139 138 137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 120 119 118 117 116 115 114 113 112 111 11 fl (ppm)

Expansion of  ${}^{13}$ C NMR Spectrum (101 MHz) of compound 7f in CDCl<sub>3</sub>

Display Report						
<b>Analysis Info</b> Analysis Name Method Sample Name Comment	D:\Data\nctu ser\ Small molecule.n L246	vice\data\2018\20180420\L2 1	46_RD5_01_18	Acquisition D 032.d Operator Instrument	ate 4/20/201 NCTU impact HD	8 12:23:47 PM 1819696.00164
Acquisition Par Source Type Focus Scan Begin Scan End	ameter ESI Active 50 m/z 1500 m/z	lon Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	Se Se Se Se Se	t Nebulizer t Dry Heater t Dry Gas t Divert Valve t APCI Heater	1.0 Bar 200 °C 6.0 I/min Waste 0 °C
Intens. x107 2.0 1.5 1.5		475.1698	T J N S S	47.3125	L246_RD5_01_18	032.d: +MS, 0.6min #35
0.0	200	400 600	800	1000	1200	1400 m/z

HRMS of compound 7f



FT-IR Spectrum of compound 7f



<sup>1</sup>H NMR Spectrum (400 MHz) of compound 7g in CDCl<sub>3</sub>





Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **7g** in CDCl<sub>3</sub>



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **7g** in DMSO- $d_6$ 



Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **7g** in DMSO- $d_6$ 



HRMS of compound 7g



FT-IR Spectrum of compound 7g







Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **7h** in CDCl<sub>3</sub>



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **7h** in CDCl<sub>3</sub>





HRMS of compound 7h



FT-IR Spectrum of compound 7h



<sup>1</sup>H NMR Spectrum (400 MHz) of compound 7i in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 7i in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 7i in CDCl<sub>3</sub>





Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound 7i in CDCl<sub>3</sub>

Display Report						
Analysis Info Analysis Name Method	D:\Data\nctu servio Small molecule.m	e\data\2018\20180831\L33	0-P_RB5_01_197	Acquisition Date 8/30/20 746.d Operator NCTU	18 6:26:26 PM	
Sample Name Comment	L330-P			Instrument impact HD	1819696.00164	
Acquisition Par	ameter		and statements and		No. Contraction	
Source Type Focus Scan Begin Scan End	ESI Active 50 m/z 1500 m/z	Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Bar 200 °C 6.0 l/min Waste 0 °C	
Intens.7				L330-P_RB5_01_1	9746.d: +MS, 0.4min #24	
1.0-		475.1685				
0.8-			_0	N o		
0.6-						
0.4-				7i		
0.2-		607 2267				
0.0	282.2785 200 4	00 600 714.21	851 815.2571 947. 800	3153 1000 1200	1400 m/z	

HRMS of compound 7i



FT-IR Spectrum of compound 7i


<sup>1</sup>H NMR Spectrum (400 MHz) of compound 7k in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 7k in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 7k in acetone- $d_6$ 



<sup>13</sup>C NMR Spectrum (101 MHz) of compound 7k in acetone- $d_6$ 

			Displa	ay Repo	ort			
Analysis Info Analysis Name Method Sample Name Comment	D:IData/NC1 Small molec L298-4-2	TU SERVICE\D ule.m	ata(2018),20180	1907/L298-4-1	Acquisi6 2_GB7_01_1988 Operato Instrume	on Date 9/7/2011 86.d r NCTU ent Impact HD	8 12:19:23 PM 1819696.0	1 0164
Acquisition Pa Source Type Focus Scan Begin Scan End	ESI Active 50 m/z 1500 m/z	neter ESI Ion Poi Active Set Ce 50 m/2 Set En 1500 m/2 Set Ch Set Ch		Positive 4500 V t -500 V je 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Ges Set Divert Valve Set APCI Heater	1.0 Bar 200 °C 6.0 l/min Wisste 0 °C	
Intens.						L298-4-2_G87_01_1	1895.ct +MS, 0.5n	nin #27
x10 <sup>7</sup>	225.1963							
1.0				~0~ `0`	$\bigcirc$	N O O		
0.8						$\langle \rangle \langle$		
0.6		451.2230			;	7k		
0.4								
0.2	241 129							
0.0	200	· U.	eòn		925,4227	*200		
Intens.1	200	400	600	000	1000	1200	+NS 0.5a	in gord
x10 <sup>6</sup>		451.22	30				1103 0.00	
6								
4.								
			452 1269					
2								
	440.3040 4	50.3877		453,2297			0.0.00.0	1 3 3 3 2
XIUS		451.22	27				Camandos, 40	
6								
4								
			1+					
2			404.2260	1+				
<u>ملبب</u>				451.2288				.,
	49 450	451	452	453	454 455	456	457	m/z

HRMS of compound 7k



FT-IR Spectrum of compound 7k



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **71** in  $CDCl_3$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **7l** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **7l** in CDCl<sub>3</sub>



 $^{13}C$  NMR Spectrum (101 MHz) of compound 71 in CDCl\_3



Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **71** in CDCl<sub>3</sub>

		Display	Report		
<b>alysis Info</b> alysis Name thod mple Name mment	D:\Data\nctu service Small molecule.m L340-3	\data\2018\20181102\L34	0-3_RD1_01_	Acquisition Date 11/2/20 20832.d Operator NCTU Instrument impact HD	18 11:45:18 AM 1819696.0016
<b>quisition Par</b> urce Type cus an Begin an End	rameter ESI Active 50 m/z 1500 m/z	Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Bar 200 °C 6.0 I/min Waste 0 °C
ntens.⊺ x10 <sup>6</sup>				L340-3_RD1_01_20	)832.d: +MS, 0.7min #
5-		561.1297			
4				N Se O	
3-				71	
2					
1-					
0	379.164 282.2785	6	<b>.</b> .,,		
	200 400	600	800	1000 1200	1400 r

HRMS of compound **7** 



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **9a** in DMSO- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **9a** in DMSO- $d_6$ 



High resolution mass (ESI)+ spectrum of compound 9a



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **9b** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **9b** in acetone- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **9b** in acetone- $d_6$ 





Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **9b** in CDCl<sub>3</sub>



FT-IR Spectrum of compound 9b



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **9c** in DMSO- $d_6$ 



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 9c in DMSO- $d_6$ 





Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **9c** in CDCl<sub>3</sub>

## **Display Report**

Analysis Info					Acquisition	Date 4/20/201	18 12:41:08 PM
Analysis Name Method Sample Name Comment	D:\Data\nctu sei Small molecule. L252	rvice∖data∖20 m	18\20180420\L25	2_RE1_01_180	36.d Operator Instrument	NCTU impact HD	1819696.00164
Acquisition Par Source Type Focus Scan Begin Scan End	ameter ESI Active 50 m/z 1500 m/z	lon Set Set Set	Polarity Capillary End Plate Offset Charging Voltage Corona	Positive 4500 V -500 V 2000 V 0 nA	ទ ទ ទ ទ ទ	et Nebulizer et Dry Heater et Dry Gas et Divert Valve et APCI Heater	1.0 Bar 200 °C 6.0 l/min Waste 0 °C
Intens. x106 2.0 85.0594 1.5 1.0 0.5	226.9509	409.1216	9c 0 <sub>2</sub> N			L252_RE1_01_18	036.d: +MS, 0.5min #31
0.0	200	400	600 ·	800	1000	1200	1400 m/z
			HRMS of c	ompound 9c			



High resolution mass (ESI)+ spectrum of compound **9c** 



FT-IR Spectrum of compound 9c



<sup>1</sup>H NMR Spectrum (400 MHz) of compound 9d in CDCl<sub>3</sub>



Expansion <sup>1</sup>H NMR Spectrum (400 MHz) of compound **9d** in CDCl<sub>3</sub>



Expending <sup>1</sup>H NMR Spectrum (400 MHz) of compound **9d** in CDCl<sub>3</sub>



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **9d** in CDCl<sub>3</sub>



		Displa	y Report				_
Analysis Info Analysis Name Method Sample Name Comment	H:120181-612018043 Small molecule.m L256	201.256_RE2_01_18037	Acquisition Date 4/20/2018 12:45:27 PM Operator NCTU Instrument Impact HD 1819695.0016/				
Acquisition Par Source Type Focus Scan Begin Scan End	ESI Active 50 m/z 1500 m/z	Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Bar 200 °C 6.0 I/min Weste 0 °C	
k10 <sup>5</sup> 3.0		547.1138			L256_RE2_01_18	037.d: +WS, 1.4mir	n 198
2.5			Ç	$\mathbf{D}^{*}$		Ph	
1.5	165		0	Ý	Se		
0.5	413.	2657		9d /			
0.0 <sup>1</sup>	200 40	600 E00	803.5479 500	1000	1200	1400	m
x10 <sup>5</sup>		547.313	8			+WS, 1.4min	n #8
2		545.1146					
1	541.1220	544.1176 546.1174	548.1164	185			
x10 <sup>8</sup>		547.113	2			CwHwNuOuSe, 547.:	113
2		1+ 545.1145	1+				
1	541.1190	544.1172 546.1174	\$49.1147 \$50,11	171			

HRMS of compound 9d



FT-IR Spectrum of compound 9d



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **9e** in CDCl<sub>3</sub>


Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **9e** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **9e** in CDCl<sub>3</sub>



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **9e** in CDCl<sub>3</sub>



Expansion of  ${}^{13}$ C NMR Spectrum (101 MHz) of compound **9e** in CDCl<sub>3</sub>

Analysis Info Analysis Name Method Sample Name Comment	H:120181-6120180- Small molecule.m L257	420/L267_RE3	01_18038.4	d	Acquisit Operato Instrume	ion Date 4/20/20 r NCTU ent Impact HD	18 12:49:46 F 1819696.0	9M 10164
Acquisition Par Source Type Socus Scan Begin Scan End	ESI Active 50 m/z 1500 m/z	Ion Polar Set Capil Set End I Set Cher Set Coro	ity lary Plate Offset ging Voltage na	Positive 4500 V -500 V 2000 V 0 nA		Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater	1.0 Ber 200 °C 6.0 Vmin Weste 0 °C	
x10 <sup>5</sup> 3.0		549.12	90				Ph	nin M
2.5					J	N= Se		
1.5	65				9e			
1.0		I						
0.5	41	3.2654						
0.5	413 338.3410	3.2654		783.5755				
0.5	413 338.3410 200 4	3.2654 00	600	783.5755 	1000	1200	1400	
0.5 0.0	413 338.3410 200 4	3.2654 100	600 549.	783.5755 19. 800 1290	1000	1200	1400 +NS, 3.0	m nin P
0.5 0.0 intens, 2	411 338.3410 200 40	3.2654 00 547	600 549. 1264	783.5755 800 1290	1000	1200	1400 +W5,1.0	min P
0.5 0.0 x10 <sup>9</sup> 2	411 3383.3410 200 4	52654 50 45.1258	600 549. 1264 548.1304	783.5755 500 1290 550.1323 551.1	1000	1200	1400 +W5, 1.0	min Ré
0.5 0.0 x10 <sup>9</sup> 2	411 3383.3410 200 40 5 544.116	45.1258 9	600 549. 1264 548.1304	783.5755 132 800 1290 550.1523 551.1	1000 1000	1200	5400 +W5, 1.0	m nin R
0.5 0.0 x10 <sup>3</sup> 2 1 x10 <sup>8</sup> 3	413 338.3410 200 40 5 544.116	32654 300 45.1258 9	1254 548,1304 548,1304	783.5755 193 500 1290 550.1323 553. 1289	1000 1304 552,1329	1200	1400 +NIS, 3.0/ CuHuMOUSE, 54	min #8
0.5 0.0 1 1 x109 2 1 x109 3 2	411 338.3410 200 40 5 544.116	82654 00 45.1258 9 9	549. 549. 548.1304 548.1304	783.5755 600 1250 557.1323 551.1323 1289 14	1000 1304 1552,11279 1	1200	1400 +NIS, 1.0 CuHuMOOSe, 54	m nin R
0.5 0.0 x109 2 1 x108 3 2 1	411 3383.3410 200 4 5 544.116	32654 50 45 1258 9 547 547 547 547	1264 548,1304 1302 14,1302 14,1302	783.5755 500 1290 550.1323 551.1323 1289 14 550.1320 1 551.1 55	1000 304 552.1329 304 1. 552.1327	1200	1400 +NIS, 1.0 CurturNAOSe, 54	m nin R

HRMS of compound 9e



FT-IR Spectrum of compound 9e



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **9f** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **9f** in CDCl<sub>3</sub>



 $^{13}$ C NMR Spectrum (101 MHz) of compound **9f** in CDCl<sub>3</sub>



137.0 136.5 136.0 135.5 135.0 134.5 134.0 133.5 133.0 132.5 132.0 131.5 131.0 130.5 130.0 129.5 129.0 128.5 128.0 127.5 127.0 126.5 126.0 125.5 125.0 124.5 124.0 123.5 12. fl (ppm)

## Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **9f** in CDCl<sub>3</sub>

		Displa	y Repor	t		
Analysis Info Analysis Nam Method Sample Name Comment	e D::Data/NCTU SEF Small molecule.m :: L328	WICE\Data\2018\20180	828/L328_BD6	Acquisition I _D1_19697.d Operator Instrument	Date 8/28/20 NCTU Impact HD	18 2:22:16 PM 1819696.00164
Acquisition F Source Type Focus Scan Begin Scan End	Parameter ESI Active 50 m/z 1500 m/z	Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	20 20 20 20 20 20 20 20 20 20 20 20 20 2	et Nebulizer et Dry Heater et Dry Gas et Divert Valve et APCI Heater	1.0 Ber 200 *C 6.0 Whin Wisste 0 *C
Interes x105 2.5 2.0 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5	.0955 42 255.1954 250 40 472.1451	473.1534 473.1534 473.1559 473.1534 474.1559 475.1425 475.1425 475.1425 475.1425	476.1677	945 2095 1000		697.d +N6, 0.4min 920
0.01	470 472	474	476	478	480	482 m/z

HRMS of compound 9f



FT-IR Spectrum of compound 9f



<sup>1</sup>H NMR Spectrum (400 MHz) of compound **9g** in CDCl<sub>3</sub>



Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **9g** in CDCl<sub>3</sub>



<sup>13</sup>C NMR Spectrum (101 MHz) of compound **9h** in CDCl<sub>3</sub>



Expansion of  ${}^{13}$ C NMR Spectrum (101 MHz) of compound **9h** in CDCl<sub>3</sub>

				Display	Report		
Analysis Analysis Method Sample I Commer	<b>s Info</b> Name Name nt	D:\Data\nctu s Small molecule L329	ervice\data\ ə.m	2018\20180828\L32§	9_BD7_01_19	Acquisition Date 8 0698.d Operator NCTU Instrument impact	/28/2018 2:26:38 PM HD 1819696.00164
Acquisit Source Ty Focus Scan Beg Scan End	t <b>ion Par</b> a ype jin I	ameter ESI Active 50 m/z 1500 m/z	k S S S S	on Polarity et Capillary et End Plate Offset et Charging Voltage et Corona	Positive 4500 V -500 V 2000 V 0 nA	Set Nebuliz Set Dry Hea Set Dry Ga Set Divert V Set APCI H	er 1.0 Bar ater 200 °C s 6.0 l/min /alve Waste leater 0 °C
Intens. x10 <sup>6</sup> 1.0 -			421.3290			L329_BD	7_01_19698.d: +MS, 0.5min #27
0.8-					_c `c	N Se	
0.6 -		282.2788	5	21.0980		9g	
0.2 -	122.09			656.1681	819.6696	941.4231	
		200	400	600	800	1000 12	200 1400 m/z

HRMS of compound 9g

![](_page_305_Figure_0.jpeg)

FT-IR Spectrum of compound 9g

![](_page_306_Figure_0.jpeg)

<sup>1</sup>H NMR Spectrum (400 MHz) of compound **9h** in  $CDCl_3$ 

![](_page_307_Figure_0.jpeg)

Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **9h** in CDCl<sub>3</sub>

![](_page_308_Figure_0.jpeg)

Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **9h** in CDCl<sub>3</sub>

![](_page_309_Figure_0.jpeg)

<sup>13</sup>C NMR Spectrum (101 MHz) of compound **9h** in DMSO- $d_6$ 

![](_page_310_Figure_0.jpeg)

Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **9h** in DMSO- $d_6$ 

		Display	Report			
Analysis Info	D:\Doto\potu.com/	ao\data\2019\20190420\1 24	7 0.0 01 10	Acquisition	Date 4/20/201	8 12:19:25 PM
Method Sample Name Comment	Small molecule.m L247	ce/data/2016/20160420/L24	7_KC0_U1_10	Operator Instrument	NCTU impact HD	1819696.00164
Acquisition Par	ameter					
Source Type Focus Scan Begin Scan End	ESI Active 50 m/z 1500 m/z	Ion Polarity Set Capillary Set End Plate Offset Set Charging Voltage Set Corona	Positive 4500 V -500 V 2000 V 0 nA	S S S S S	et Nebulizer et Dry Heater et Dry Gas et Divert Valve et APCI Heater	1.0 Bar 200 °C 6.0 l/min Waste 0 °C
1.25 1.00 0.75 0.50 85.0594	282.2791 226.9511	507.0828		9h	L247_RC8_01_18	031.d: +MS, 0.5min #31
اسلینا 1_0.00	ميغ <b>انا ا</b> دبارد الاحتسباد. بااد. 4	ւպ <b>մեմն և մեների Ամ</b> եսի ամերած առաջին դրարուց 100 600	800	1000	1200	1400 m/z
	200 2	100 000	800	1000	1200	1400 m/

HRMS of compound **9h** 

![](_page_312_Figure_0.jpeg)

Page 1/1

FT-IR Spectrum of compound 9h

![](_page_313_Figure_0.jpeg)

<sup>1</sup>H NMR Spectrum (400 MHz) of compound **9i** in CDCl<sub>3</sub>

![](_page_314_Figure_0.jpeg)

Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound 9i in CDCl<sub>3</sub>

![](_page_315_Figure_0.jpeg)

<sup>13</sup>C NMR Spectrum (101 MHz) of compound **9i** in acetone- $d_6$ 

![](_page_316_Figure_0.jpeg)

Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **9i** in acetone- $d_6$ 

![](_page_317_Figure_0.jpeg)

HRMS of compound 9i

![](_page_318_Figure_0.jpeg)

HRMS of compound 9i

![](_page_319_Figure_0.jpeg)

<sup>1</sup>H NMR Spectrum (400 MHz) of compound **9j** in CDCl<sub>3</sub>

![](_page_320_Figure_0.jpeg)

![](_page_320_Figure_1.jpeg)

Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **9j** in CDCl<sub>3</sub>

![](_page_321_Figure_0.jpeg)

Expansion of <sup>1</sup>H NMR Spectrum (400 MHz) of compound **9j** in CDCl<sub>3</sub>

![](_page_322_Figure_0.jpeg)

<sup>13</sup>C NMR Spectrum (101 MHz) of compound **9j** in CDCl<sub>3</sub>

![](_page_323_Figure_0.jpeg)

Expansion of <sup>13</sup>C NMR Spectrum (101 MHz) of compound **9j** in CDCl<sub>3</sub>


## X-ray crystallographic data of compound 7a



**ORTEP diagram of compound 7a.** Atomic displacement ellipsoids are drawn at the 50% probability level

## **CCDC No.:** 1884822

Table 1. Crystal data and structure refinement for 181208lt_0m_a.					
Identification code	181208lt_0m_a				
Empirical formula	C26 H24 N2 O4 S				
Formula weight	460.53				
Temperature	100(2) K				
Wavelength	0.71073 Å				
Crystal system	Monoclinic				
Space group	P 21/c				
Unit cell dimensions	a = 14.9997(15) Å	$\alpha = 90^{\circ}$ .			
	b = 8.0616(7)  Å	$\beta = 107.259(4)^{\circ}.$			
	c = 20.034(2)  Å	$\gamma = 90^{\circ}.$			
Volume	2313.4(4) Å <sup>3</sup>				
Z	4				
Density (calculated)	1.322 Mg/m <sup>3</sup>				
Absorption coefficient	0.176 mm <sup>-1</sup>				
F(000)	968				
Crystal size	0.20 x 0.12 x 0.04 mm <sup>3</sup>				
Theta range for data collection	1.422 to 26.506°.				

Index ranges	-18<=h<=18, -7<=k<=10, -25<=l<=24
Reflections collected	13728
Independent reflections	4756 [R(int) = 0.0835]
Completeness to theta = $25.242^{\circ}$	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.2965
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	4756 / 0 / 300
Goodness-of-fit on F <sup>2</sup>	1.010
Final R indices [I>2sigma(I)]	R1 = 0.0760, wR2 = 0.1852
R indices (all data)	R1 = 0.0986, wR2 = 0.2052
Extinction coefficient	n/a
Largest diff. peak and hole	1.150 and -0.791 e.Å <sup>-3</sup>

Table 2. Atomic coordinates  $(x \ 10^4)$  and equivalent isotropic displacement parameters (Å<sup>2</sup>x  $10^3$ ) for 181208lt\_0m\_a. U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

	X	у	Z	U(eq)
C(1)	4269(2)	3016(3)	5244(2)	24(1)
C(2)	4656(2)	5252(3)	5951(1)	22(1)
C(3)	5304(2)	3047(3)	5642(1)	23(1)
C(4)	2945(2)	4884(3)	5256(2)	23(1)
C(5)	2516(2)	5167(4)	4550(1)	26(1)
C(6)	1584(2)	5620(4)	4332(2)	33(1)
C(7)	1090(2)	5803(4)	4815(2)	38(1)
C(8)	1523(2)	5504(4)	5513(2)	37(1)
C(9)	2449(2)	5034(4)	5742(2)	30(1)
C(10)	5613(2)	7552(3)	6822(1)	22(1)
C(11)	5997(2)	6431(3)	7448(1)	22(1)
C(12)	7015(2)	6546(3)	7826(1)	22(1)
C(13)	7606(2)	7658(4)	7627(2)	27(1)
C(14)	8553(2)	7666(4)	7975(2)	30(1)
C(15)	8925(2)	6567(4)	8509(2)	31(1)
C(16)	8343(2)	5477(4)	8721(2)	30(1)
C(17)	7393(2)	5484(4)	8387(1)	26(1)
C(18)	5573(2)	1511(3)	6110(1)	24(1)

C(19)	6608(2)	1467(3)	6481(1)	23(1)
C(20)	6981(2)	2114(4)	7146(2)	28(1)
C(21)	7938(2)	2119(4)	7462(2)	28(1)
C(22)	8542(2)	1472(4)	7124(1)	24(1)
C(23)	8168(2)	804(3)	6455(1)	23(1)
C(24)	7219(2)	811(3)	6139(1)	23(1)
C(25)	9897(2)	2229(4)	8042(2)	36(1)
C(26)	8456(2)	-532(5)	5483(2)	37(1)
N(1)	3906(1)	4406(3)	5484(1)	23(1)
N(2)	5459(1)	4585(3)	6051(1)	22(1)
O(1)	3836(1)	2026(3)	4825(1)	34(1)
O(2)	5498(1)	5479(3)	7648(1)	30(1)
O(3)	9495(1)	1409(3)	7395(1)	30(1)
O(4)	8817(1)	182(2)	6157(1)	28(1)
S(1)	4430(1)	7100(1)	6323(1)	24(1)

C(1)-O(1)	1.201(3)
C(1)-N(1)	1.392(3)
C(1)-C(3)	1.519(4)
C(2)-N(2)	1.279(3)
C(2)-N(1)	1.408(3)
C(2)-S(1)	1.744(3)
C(3)-N(2)	1.466(3)
C(3)-C(18)	1.533(4)
C(3)-H(3)	1.0000
C(4)-C(5)	1.388(4)
C(4)-C(9)	1.394(4)
C(4)-N(1)	1.430(3)
C(5)-C(6)	1.384(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.390(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.379(5)
C(7)-H(7)	0.9500
C(8)-C(9)	1.380(4)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.515(4)
C(10)-S(1)	1.797(3)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-O(2)	1.220(3)
C(11)-C(12)	1.493(4)
C(12)-C(17)	1.393(4)
C(12)-C(13)	1.400(4)
C(13)-C(14)	1.384(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.374(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.389(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.383(4)

Table 3. Bond lengths [Å] and angles [°] for 181208lt\_0m\_a.

C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-C(19)	1.510(3)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.384(4)
C(19)-C(24)	1.400(4)
C(20)-C(21)	1.388(4)
C(20)-H(20)	0.9500
C(21)-C(22)	1.383(4)
C(21)-H(21)	0.9500
C(22)-O(3)	1.372(3)
C(22)-C(23)	1.399(4)
C(23)-C(24)	1.376(4)
C(23)-O(4)	1.378(3)
C(24)-H(24)	0.9500
C(25)-O(3)	1.420(3)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-O(4)	1.419(3)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
O(1)-C(1)-N(1)	126.2(3)
O(1)-C(1)-C(3)	129.4(2)
N(1)-C(1)-C(3)	104.4(2)
N(2)-C(2)-N(1)	115.4(2)
N(2)-C(2)-S(1)	125.9(2)
N(1)-C(2)-S(1)	118.62(18)
N(2)-C(3)-C(1)	106.0(2)
N(2)-C(3)-C(18)	111.9(2)
C(1)-C(3)-C(18)	110.5(2)
N(2)-C(3)-H(3)	109.5
C(1)-C(3)-H(3)	109.5
C(18)-C(3)-H(3)	109.5
C(5)-C(4)-C(9)	121.0(2)

C(5)-C(4)-N(1)	119.2(2)
C(9)-C(4)-N(1)	119.7(2)
C(6)-C(5)-C(4)	119.0(3)
C(6)-C(5)-H(5)	120.5
C(4)-C(5)-H(5)	120.5
C(5)-C(6)-C(7)	120.4(3)
C(5)-C(6)-H(6)	119.8
C(7)-C(6)-H(6)	119.8
C(8)-C(7)-C(6)	120.0(3)
C(8)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	120.0
C(7)-C(8)-C(9)	120.7(3)
C(7)-C(8)-H(8)	119.6
C(9)-C(8)-H(8)	119.6
C(8)-C(9)-C(4)	118.9(3)
C(8)-C(9)-H(9)	120.5
C(4)-C(9)-H(9)	120.5
C(11)-C(10)-S(1)	114.19(18)
C(11)-C(10)-H(10A)	108.7
S(1)-C(10)-H(10A)	108.7
C(11)-C(10)-H(10B)	108.7
S(1)-C(10)-H(10B)	108.7
H(10A)-C(10)-H(10B)	107.6
O(2)-C(11)-C(12)	120.5(2)
O(2)-C(11)-C(10)	121.9(2)
C(12)-C(11)-C(10)	117.6(2)
C(17)-C(12)-C(13)	118.9(3)
C(17)-C(12)-C(11)	118.8(2)
C(13)-C(12)-C(11)	122.3(2)
C(14)-C(13)-C(12)	120.1(3)
C(14)-C(13)-H(13)	119.9
C(12)-C(13)-H(13)	119.9
C(15)-C(14)-C(13)	120.5(3)
C(15)-C(14)-H(14)	119.7
C(13)-C(14)-H(14)	119.7
C(14)-C(15)-C(16)	119.9(3)
C(14)-C(15)-H(15)	120.0
C(16)-C(15)-H(15)	120.0

C(17)-C(16)-C(15)	120.0(3)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-C(12)	120.4(3)
C(16)-C(17)-H(17)	119.8
C(12)-C(17)-H(17)	119.8
C(19)-C(18)-C(3)	111.5(2)
C(19)-C(18)-H(18A)	109.3
C(3)-C(18)-H(18A)	109.3
C(19)-C(18)-H(18B)	109.3
C(3)-C(18)-H(18B)	109.3
H(18A)-C(18)-H(18B)	108.0
C(20)-C(19)-C(24)	118.5(2)
C(20)-C(19)-C(18)	121.9(2)
C(24)-C(19)-C(18)	119.6(2)
C(19)-C(20)-C(21)	120.5(2)
C(19)-C(20)-H(20)	119.7
C(21)-C(20)-H(20)	119.7
C(22)-C(21)-C(20)	120.9(3)
C(22)-C(21)-H(21)	119.5
C(20)-C(21)-H(21)	119.5
O(3)-C(22)-C(21)	125.2(2)
O(3)-C(22)-C(23)	116.1(2)
C(21)-C(22)-C(23)	118.7(2)
C(24)-C(23)-O(4)	124.7(2)
C(24)-C(23)-C(22)	120.3(2)
O(4)-C(23)-C(22)	115.0(2)
C(23)-C(24)-C(19)	120.9(3)
C(23)-C(24)-H(24)	119.5
C(19)-C(24)-H(24)	119.5
O(3)-C(25)-H(25A)	109.5
O(3)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
O(3)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
O(4)-C(26)-H(26A)	109.5
O(4)-C(26)-H(26B)	109.5

H(26A)-C(26)-H(26B)	109.5
O(4)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(1)-N(1)-C(2)	107.6(2)
C(1)-N(1)-C(4)	124.6(2)
C(2)-N(1)-C(4)	127.8(2)
C(2)-N(2)-C(3)	106.4(2)
C(22)-O(3)-C(25)	117.0(2)
C(23)-O(4)-C(26)	116.1(2)
C(2)-S(1)-C(10)	97.20(12)

Symmetry transformations used to generate equivalent atoms:

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
C(1)	26(1)	16(2)	31(2)	0(1)	10(1)	0(1)
C(2)	21(1)	18(2)	27(1)	-1(1)	8(1)	-1(1)
C(3)	25(1)	17(2)	28(1)	-2(1)	10(1)	-1(1)
C(4)	18(1)	16(1)	36(2)	2(1)	8(1)	1(1)
C(5)	22(1)	24(2)	32(2)	4(1)	6(1)	-4(1)
C(6)	28(2)	26(2)	42(2)	10(1)	4(1)	-4(1)
C(7)	18(1)	33(2)	60(2)	10(2)	8(1)	2(1)
C(8)	26(2)	40(2)	51(2)	-2(2)	19(1)	-2(1)
C(9)	26(2)	28(2)	37(2)	3(1)	12(1)	0(1)
C(10)	20(1)	16(1)	31(1)	-4(1)	9(1)	-2(1)
C(11)	27(1)	14(1)	31(1)	-5(1)	16(1)	-1(1)
C(12)	27(1)	16(1)	26(1)	-4(1)	13(1)	0(1)
C(13)	26(1)	20(2)	37(2)	1(1)	13(1)	-1(1)
C(14)	26(1)	24(2)	41(2)	-2(1)	14(1)	-3(1)
C(15)	26(1)	30(2)	36(2)	-6(1)	8(1)	3(1)
C(16)	38(2)	26(2)	26(1)	-1(1)	8(1)	4(1)
C(17)	35(2)	23(2)	24(1)	-3(1)	14(1)	-2(1)
C(18)	24(1)	17(1)	34(2)	0(1)	11(1)	-1(1)
C(19)	25(1)	12(1)	32(1)	2(1)	9(1)	1(1)
C(20)	32(2)	21(2)	33(2)	-3(1)	12(1)	2(1)
C(21)	35(2)	22(2)	26(1)	-3(1)	7(1)	1(1)
C(22)	27(1)	17(1)	27(1)	2(1)	5(1)	-2(1)
C(23)	26(1)	15(1)	31(1)	2(1)	12(1)	2(1)
C(24)	28(1)	14(1)	26(1)	0(1)	8(1)	-2(1)
C(25)	30(2)	42(2)	31(2)	-6(1)	2(1)	-9(1)
C(26)	31(2)	47(2)	37(2)	-12(2)	14(1)	2(1)
N(1)	20(1)	17(1)	32(1)	-3(1)	7(1)	0(1)
N(2)	21(1)	14(1)	30(1)	-1(1)	9(1)	0(1)
<b>O</b> (1)	30(1)	24(1)	44(1)	-11(1)	5(1)	-2(1)
O(2)	31(1)	27(1)	37(1)	2(1)	16(1)	-5(1)
O(3)	24(1)	29(1)	33(1)	-4(1)	5(1)	-3(1)
O(4)	26(1)	29(1)	31(1)	-5(1)	10(1)	0(1)
<b>S</b> (1)	20(1)	17(1)	35(1)	-4(1)	9(1)	2(1)

Table 4.Anisotropic displacement parameters $(Å^2x \ 10^3)$  for 181208lt\_0m\_a.The anisotropicdisplacement factor exponent takes the form: $-2\pi^2 [h^2 \ a^{*2} U^{11} + ... + 2 \ h \ k \ a^* \ b^* \ U^{12} ]$ 

	Х	у	Z	U(eq)
H(3)	5676	3073	5303	27
H(5)	2857	5052	4222	32
H(6)	1280	5806	3850	40
H(7)	453	6135	4663	45
H(8)	1181	5622	5841	45
H(9)	2745	4816	6223	36
H(10A)	6016	7456	6512	27
H(10B)	5646	8715	6986	27
H(13)	7357	8408	7253	32
H(14)	8949	8437	7843	36
H(15)	9579	6553	8734	37
H(16)	8599	4727	9094	36
H(17)	6996	4759	8542	32
H(18A)	5226	1516	6460	29
H(18B)	5393	500	5820	29
H(20)	6577	2559	7387	34
H(21)	8183	2572	7918	34
H(24)	6974	365	5682	27
H(25A)	9712	3399	7998	54
H(25B)	10579	2147	8169	54
H(25C)	9677	1706	8406	54
H(26A)	8042	-1458	5506	56
H(26B)	8972	-939	5322	56
H(26C)	8103	307	5156	56

Table 5. Hydrogen coordinates (  $x \ 10^4$ ) and isotropic displacement parameters (Å<sup>2</sup>x 10<sup>3</sup>) for 181208lt\_0m\_a.

## X-ray crystallographic data of compound 9h



**ORTEP diagram of compound 9h.** Atomic displacement ellipsoids are drawn at the 50% probability level

## CCDC No.: 1882293

5				
Identification code	mo_180912LT_0m_b			
Empirical formula	C26 H22 N2 O4 Se	C26 H22 N2 O4 Se		
Formula weight	505.41			
Temperature	100(2) K			
Wavelength	elength 0.71073 Å			
Crystal system	Monoclinic			
Space group	P 21			
Unit cell dimensions	a = 5.0331(3) Å	α= 90°.		
	b = 12.9922(8) Å	$\beta = 93.403(2)^{\circ}.$		
	c = 17.1983(11) Å	$\gamma = 90^{\circ}$ .		
Volume	1122.63(12) Å <sup>3</sup>			
Z	2			
Density (calculated)	1.495 Mg/m <sup>3</sup>			
Absorption coefficient	1.709 mm <sup>-1</sup>			
F(000)	516			
Crystal size	$0.20 \text{ x} 0.10 \text{ x} 0.09 \text{ mm}^3$			
Theta range for data collection	1.966 to 26.482°.			
Index ranges	-6<=h<=5, -16<=k<=16, -21<=l<=21			
Reflections collected	19872			
Independent reflections	4603 [R(int) = 0.0465]			

Table 1. Crystal data and structure refinement for mo\_180912lt\_0m\_b.

Completeness to theta = $25.242^{\circ}$	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6698
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	4603 / 217 / 355
Goodness-of-fit on F <sup>2</sup>	1.077
Final R indices [I>2sigma(I)]	R1 = 0.0335, wR2 = 0.0644
R indices (all data)	R1 = 0.0394, wR2 = 0.0658
Absolute structure parameter	0.031(8)
Extinction coefficient	n/a
Largest diff. peak and hole	0.349 and -0.628 e.Å <sup>-3</sup>

Table 2. Atomic coordinates  $(x \ 10^4)$  and equivalent isotropic displacement parameters (Å<sup>2</sup>x  $10^3$ ) for mo\_180912lt\_0m\_b. U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

	X	У	Z	U(eq)
Se(1)	2258(1)	2815(1)	7472(1)	28(1)
O(1)	5717(5)	7873(3)	6605(2)	44(1)
O(2)	9129(7)	9253(2)	7034(2)	47(1)
O(3)	9792(8)	3516(3)	9557(2)	47(1)
O(4)	-1765(5)	2774(4)	6264(2)	40(1)
N(1)	5893(7)	4427(2)	7911(2)	24(1)
N(2)	6314(6)	3014(3)	8683(2)	24(1)
C(1)	3753(9)	7127(4)	6358(3)	43(1)
C(2)	11139(13)	10020(4)	7223(3)	63(2)
C(3)	7445(9)	7592(3)	7203(3)	33(1)
C(4)	9313(11)	8357(3)	7453(3)	35(1)
C(5)	11113(12)	8159(3)	8064(3)	47(2)
C(6)	11145(12)	7203(4)	8434(3)	44(2)
C(7)	9370(9)	6435(3)	8191(3)	30(1)
C(8)	7524(8)	6639(3)	7577(3)	28(1)
C(9)	9474(9)	5456(3)	8602(3)	33(1)
C(10)	7949(10)	4604(3)	8484(3)	26(1)
C(11)	8293(10)	3685(3)	8995(3)	31(1)
C(13)	5027(8)	3504(3)	8053(3)	25(1)

C(14)	1362(9)	3979(3)	6791(3)	27(1)
C(15)	-877(8)	3649(4)	6234(3)	28(1)
C(16)	-1966(9)	4394(3)	5642(3)	30(1)
C(17)	-4112(9)	4125(4)	5137(3)	38(1)
C(18)	-5128(11)	4797(4)	4585(3)	47(1)
C(19)	-4033(10)	5769(4)	4509(3)	45(1)
C(20)	-1877(11)	6053(4)	4994(3)	46(1)
C(21)	-859(10)	5370(4)	5561(3)	37(1)
C(22)	5970(50)	1953(12)	9015(12)	19(3)
C(23)	3565(18)	1683(6)	9277(5)	22(2)
C(24)	3158(17)	663(6)	9513(5)	26(2)
C(25)	5220(40)	-27(12)	9524(10)	25(2)
C(26)	7681(17)	251(6)	9282(5)	26(2)
C(27)	8133(15)	1258(6)	9031(5)	20(2)
C(22')	5900(50)	2005(13)	8877(13)	20(3)
C(23')	5077(17)	1806(6)	9603(5)	21(2)
C(24')	4945(17)	781(6)	9855(6)	26(2)
C(25')	5510(40)	-19(12)	9355(11)	26(3)
C(26')	6217(16)	197(6)	8619(5)	27(2)
C(27')	6416(18)	1193(6)	8357(5)	23(2)

1.892(4)
1.949(4)
1.357(6)
1.431(6)
1.371(5)
1.443(6)
1.210(6)
1.224(7)
1.304(5)
1.405(6)
1.372(17)
1.383(6)
1.406(6)
1.506(16)
0.9800
0.9800
0.9800
0.9800
0.9800
0.9800
1.395(6)
1.416(6)
1.370(7)
1.395(6)
0.9500
1.388(6)
0.9500
1.389(6)
1.454(6)
0.9500
1.355(6)
0.9500
1.487(6)
1.498(6)
0.9900
0.9900

Table 3. Bond lengths [Å] and angles [°] for mo\_180912lt\_0m\_b.

C(15)-C(16)	1.485(7)
C(16)-C(17)	1.390(6)
C(16)-C(21)	1.395(6)
C(17)-C(18)	1.366(7)
C(17)-H(17)	0.9500
C(18)-C(19)	1.387(8)
C(18)-H(18)	0.9500
C(19)-C(20)	1.379(7)
C(19)-H(19)	0.9500
C(20)-C(21)	1.393(7)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(23)	1.36(2)
C(22)-C(27)	1.414(19)
C(23)-C(24)	1.404(10)
C(23)-H(23)	0.9500
C(24)-C(25)	1.371(17)
C(24)-H(24)	0.9500
C(25)-C(26)	1.378(18)
C(25)-H(25)	0.9500
C(26)-C(27)	1.400(10)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(22')-C(23')	1.363(17)
C(22')-C(27')	1.417(19)
C(23')-C(24')	1.403(10)
C(23')-H(23')	0.9500
C(24')-C(25')	1.389(17)
C(24')-H(24')	0.9500
C(25')-C(26')	1.363(16)
C(25')-H(25')	0.9500
C(26')-C(27')	1.376(11)
C(26')-H(26')	0.9500
C(27')-H(27')	0.9500
	0100/10
C(13)-Se(1)- $C(14)$	94.99(18)
C(3)-O(1)-C(1)	116.4(4)
C(4)-O(2)-C(2)	116.3(4)

C(13)-N(1)-C(10)	105.0(4)
C(22')-N(2)-C(13)	124.0(13)
C(22')-N(2)-C(11)	127.8(13)
C(13)-N(2)-C(11)	107.6(3)
C(13)-N(2)-C(22)	131.2(11)
C(11)-N(2)-C(22)	121.2(11)
O(1)-C(1)-H(1A)	109.5
O(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
O(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
O(2)-C(2)-H(2A)	109.5
O(2)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
O(2)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
O(1)-C(3)-C(8)	126.0(4)
O(1)-C(3)-C(4)	115.2(4)
C(8)-C(3)-C(4)	118.8(5)
C(5)-C(4)-O(2)	125.7(4)
C(5)-C(4)-C(3)	119.9(4)
O(2)-C(4)-C(3)	114.4(5)
C(4)-C(5)-C(6)	120.3(4)
C(4)-C(5)-H(5)	119.8
C(6)-C(5)-H(5)	119.8
C(7)-C(6)-C(5)	120.9(5)
C(7)-C(6)-H(6)	119.6
C(5)-C(6)-H(6)	119.6
C(6)-C(7)-C(8)	118.7(4)
C(6)-C(7)-C(9)	118.6(5)
C(8)-C(7)-C(9)	122.7(4)
C(7)-C(8)-C(3)	121.3(4)
C(7)-C(8)-H(8)	119.3
C(3)-C(8)-H(8)	119.3
C(10)-C(9)-C(7)	129.7(5)
C(10)-C(9)-H(9)	115.2

C(7)-C(9)-H(9)	115.2
C(9)-C(10)-N(1)	128.7(4)
C(9)-C(10)-C(11)	121.6(5)
N(1)-C(10)-C(11)	109.8(4)
O(3)-C(11)-N(2)	126.0(4)
O(3)-C(11)-C(10)	131.5(4)
N(2)-C(11)-C(10)	102.5(4)
N(1)-C(13)-N(2)	115.1(4)
N(1)-C(13)-Se(1)	125.4(4)
N(2)-C(13)-Se(1)	119.5(3)
C(15)-C(14)-Se(1)	107.5(3)
C(15)-C(14)-H(14A)	110.2
Se(1)-C(14)-H(14A)	110.2
C(15)-C(14)-H(14B)	110.2
Se(1)-C(14)-H(14B)	110.2
H(14A)-C(14)-H(14B)	108.5
O(4)-C(15)-C(16)	120.9(4)
O(4)-C(15)-C(14)	120.1(4)
C(16)-C(15)-C(14)	119.0(4)
C(17)-C(16)-C(21)	117.8(5)
C(17)-C(16)-C(15)	120.4(4)
C(21)-C(16)-C(15)	121.8(4)
C(18)-C(17)-C(16)	121.2(5)
C(18)-C(17)-H(17)	119.4
C(16)-C(17)-H(17)	119.4
C(17)-C(18)-C(19)	120.9(5)
C(17)-C(18)-H(18)	119.6
C(19)-C(18)-H(18)	119.6
C(20)-C(19)-C(18)	119.3(5)
C(20)-C(19)-H(19)	120.4
C(18)-C(19)-H(19)	120.4
C(19)-C(20)-C(21)	119.8(5)
C(19)-C(20)-H(20)	120.1
C(21)-C(20)-H(20)	120.1
C(20)-C(21)-C(16)	121.1(5)
C(20)-C(21)-H(21)	119.5
C(16)-C(21)-H(21)	119.5
C(23)-C(22)-C(27)	121.8(12)

C(23)-C(22)-N(2)	119.1(13)
C(27)-C(22)-N(2)	119.0(14)
C(22)-C(23)-C(24)	119.1(9)
C(22)-C(23)-H(23)	120.4
C(24)-C(23)-H(23)	120.4
C(25)-C(24)-C(23)	119.9(10)
C(25)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1
C(24)-C(25)-C(26)	121.2(12)
C(24)-C(25)-H(25)	119.4
C(26)-C(25)-H(25)	119.4
C(25)-C(26)-C(27)	120.2(9)
C(25)-C(26)-H(26)	119.9
C(27)-C(26)-H(26)	119.9
C(26)-C(27)-C(22)	117.6(10)
C(26)-C(27)-H(27)	121.2
C(22)-C(27)-H(27)	121.2
C(23')-C(22')-N(2)	117.6(14)
C(23')-C(22')-C(27')	120.9(13)
N(2)-C(22')-C(27')	121.4(12)
C(22')-C(23')-C(24')	119.1(10)
C(22')-C(23')-H(23')	120.4
C(24')-C(23')-H(23')	120.4
C(25')-C(24')-C(23')	120.2(10)
C(25')-C(24')-H(24')	119.9
C(23')-C(24')-H(24')	119.9
C(26')-C(25')-C(24')	119.7(12)
C(26')-C(25')-H(25')	120.1
C(24')-C(25')-H(25')	120.1
C(25')-C(26')-C(27')	121.7(10)
C(25')-C(26')-H(26')	119.2
C(27')-C(26')-H(26')	119.2
C(26')-C(27')-C(22')	118.3(10)
C(26')-C(27')-H(27')	120.9
C(22')-C(27')-H(27')	120.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters  $(Å^2 x \ 10^3)$  for mo\_180912lt\_0m\_b. The anisotropic

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Se(1)	20(1)	15(1)	50(1)	0(1)	5(1)	-5(1)
O(1)	34(2)	25(2)	73(2)	9(2)	4(2)	-7(2)
O(2)	76(3)	18(2)	49(2)	-3(2)	21(2)	-15(2)
O(3)	82(3)	33(2)	24(2)	-1(2)	-6(2)	-26(2)
O(4)	38(2)	30(2)	50(2)	-6(2)	0(1)	-12(2)
N(1)	23(2)	16(2)	34(2)	-5(2)	13(2)	-6(1)
N(2)	23(2)	14(2)	36(2)	-3(2)	11(2)	-4(1)
C(1)	29(3)	34(3)	66(4)	9(3)	8(3)	-4(2)
C(2)	129(6)	29(3)	34(3)	-10(2)	26(3)	-44(3)
C(3)	35(2)	19(3)	46(3)	-6(2)	20(2)	-4(2)
C(4)	59(3)	18(2)	30(3)	-10(2)	22(3)	-12(2)
C(5)	85(4)	30(2)	28(3)	-12(2)	11(3)	-36(3)
C(6)	75(4)	37(3)	20(3)	-7(2)	3(3)	-30(3)
C(7)	43(3)	22(2)	26(3)	-9(2)	16(2)	-15(2)
C(8)	31(3)	19(2)	37(3)	-9(2)	15(2)	-10(2)
C(9)	49(3)	29(2)	21(3)	-9(2)	10(2)	-20(2)
C(10)	36(3)	21(2)	23(3)	-7(2)	12(2)	-10(2)
C(11)	48(3)	22(2)	23(3)	-9(2)	13(2)	-11(2)
C(13)	17(2)	14(2)	45(3)	-5(2)	12(2)	0(2)
C(14)	30(2)	19(2)	31(3)	-1(2)	10(2)	-7(2)
C(15)	25(2)	28(2)	31(3)	-9(2)	12(2)	-3(2)
C(16)	28(2)	35(2)	27(3)	-11(2)	13(2)	-2(2)
C(17)	37(3)	38(3)	38(3)	-8(2)	7(2)	0(2)
C(18)	51(3)	51(3)	39(3)	-14(3)	1(3)	6(3)
C(19)	57(3)	50(3)	28(3)	-4(2)	9(3)	19(3)
C(20)	57(3)	37(3)	46(4)	1(2)	15(3)	0(3)
C(21)	39(3)	34(3)	39(3)	-1(2)	4(2)	-5(2)
C(22)	23(4)	10(4)	23(6)	-3(4)	2(5)	-1(4)
C(23)	21(4)	23(3)	23(4)	3(3)	1(4)	0(3)
C(24)	25(4)	26(4)	27(4)	6(3)	1(4)	-9(3)
C(25)	28(5)	18(4)	28(6)	6(4)	-4(4)	-8(4)
C(26)	29(4)	18(3)	31(4)	4(3)	0(4)	4(3)

displacement factor exponent takes the form:  $-2\pi^2$ [ h<sup>2</sup> a<sup>\*2</sup>U<sup>11</sup> + ... + 2 h k a<sup>\*</sup> b<sup>\*</sup> U<sup>12</sup> ]

C(27)	18(3)	19(3)	24(4)	1(3)	0(3)	-2(3)
C(22')	19(4)	17(4)	24(6)	1(4)	7(5)	0(4)
C(23')	16(4)	19(3)	28(4)	2(3)	5(4)	-2(3)
C(24')	17(4)	28(4)	33(4)	10(3)	3(4)	-6(3)
C(25')	23(5)	14(4)	40(6)	7(4)	-4(5)	-2(4)
C(26')	22(4)	18(3)	43(4)	-3(3)	-1(4)	3(3)
C(27')	19(4)	19(4)	30(5)	-3(3)	4(4)	-1(3)

	Х	У	Z	U(eq)
	1624	6516	6150	64
H(1A)	4034	0010	5044	64
H(1B)	2305	/421 6022	6800	04 64
H(1C)	11000	10205	7775	04
H(2R)	10787	10205	6902	95
H(2D)	12895	9742	7121	95
H(2C)	12393	8676	8236	57
H(6)	12399	7077	8858	53
H(8)	6291	6120	7409	34
H(9)	10810	5407	9014	39
H(14A)	812	4576	7102	32
H(14B)	2925	4183	6503	32
H(17)	-4885	3462	5176	45
H(18)	-6603	4597	4249	57
H(19)	-4761	6235	4128	54
H(20)	-1088	6712	4942	55
H(21)	613	5572	5898	45
H(23)	2182	2177	9300	27
H(24)	1457	452	9665	31
H(25)	4948	-709	9702	30
H(26)	9075	-242	9285	31
H(27)	9834	1467	8878	24
H(23')	4599	2353	9933	25
H(24')	4470	634	10370	31
H(25')	5397	-713	9524	31
H(26')	6584	-355	8280	33
H(27')	6887	1332	7841	27

Table 5. Hydrogen coordinates ( x  $10^4$ ) and isotropic displacement parameters (Å<sup>2</sup>x  $10^3$ ) for mo\_180912lt\_0m\_b.