

## Supporting Information

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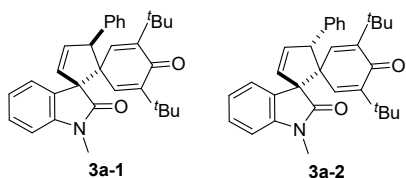
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## 1. General methods

Unless otherwise mentioned, all reagents were purchased from commercial suppliers without further purification. Solvent purification was conducted according to Purification of Laboratory Chemicals (Peerrin, D. D.; Armarego, W. L. and Perrins, D. R., Pergamon Press: Oxford, 1980). Reactions were monitored using Merck Kieselgel 60F<sub>254</sub> aluminium plates. TLC was visualized by UV fluorescence (254 nm) then one of the following: KMnO<sub>4</sub>, phosphomolybdic acid, ninhydrin, *p*-anisaldehyde, vanillin. The Displacement ellipsoids are scaled to the 30% probability level. If not specially mentioned, flash column chromatography was performed using Yantai xinnuo Chemicals (China) (particle size 0.040–0.063 mm). NMR spectra were recorded on JEOL 400 instruments and calibrated by using residual undeuterated chloroform-d ( $\delta$  <sup>1</sup>H = 7.26 ppm,  $\delta$  <sup>13</sup>C = 77.0 ppm) as internal references. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, b = broad, td = triple doublet, dt = double triplet, dq = double quartet, m = multiplet. Infrared (IR) spectra were recorded on a BFL WQF-530 FT-IR spectrometer. High-resolution mass spectra (HRMS) were recorded on a Thermo Fisher Q Exactive Orbitrap mass spectrometer using ESI (electrospray ionization) as ionization method.

## 2. Experimental procedures and characterization data

Typical Procedure: To a stirred solution of (*E*)-2,6-di-*tert*-butyl-4-(3-phenylallylidene)cyclohexa-2,5-dien-1-ones (0.10 mmol, 1.0 equiv) and 3-chlorooxindoles (0.12 mmol, 1.2 equiv) in CHCl<sub>3</sub> (1.0 mL) was added DBU (0.12 mmol, 1.2 equiv) at room temperature. The reaction was then heated at 50 °C until completion of the reaction as monitored by TLC analysis. The reaction mixture was directly charged to column chromatography on silica gel to give the cycloadduct.



Yellow foam, isolated yield 95% (44 mg);

dr = 1:1;

**3a-1:** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.23–7.16 (m, 4H), 7.06–7.04 (m, 2H), 7.01 (d, *J* = 7.6 Hz, 1H), 6.94–6.90 (m, 2H), 6.73 (d, *J* = 7.6 Hz, 1H), 6.69–6.63 (m, 2H), 5.92 (dd, *J* = 5.6, 2.8 Hz, 1H), 5.02 (s, 1H), 3.20 (s, 3H), 1.09 (s, 9H), 0.82 (s, 9H);

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  185.5, 176.1, 150.6, 146.4, 143.6, 140.4, 139.1, 138.7, 138.2, 132.5, 129.1, 127.9, 127.3, 127.2, 127.0, 126.5, 121.7, 107.7, 68.8, 60.6, 57.4, 34.9, 34.6, 29.5, 28.7, 26.2;

IR (neat):  $\nu$  3640, 2917, 1717, 1632, 1530, 1344, 1251, 1079, 881, 737 cm<sup>-1</sup>;

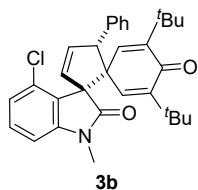
HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd. for C<sub>32</sub>H<sub>36</sub>NO<sub>2</sub>: 466.2741; found: 466.2756;

**3a-2:** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.33–7.27 (m, 2H), 7.21–7.18 (m, 3H), 7.13–7.09 (m, 1H), 7.04–7.02 (m, 2H), 6.87 (d, *J* = 2.8 Hz, 1H), 6.77 (d, *J* = 7.6 Hz, 1H), 6.54 (dd, *J* = 5.6 Hz, 1.6 Hz, 1H), 6.32 (d, *J* = 2.8 Hz, 1H), 6.06 (dd, *J* = 5.6, 2.8 Hz, 1H), 4.56 (s, 1H), 3.02 (s, 3H), 0.94 (s, 9H), 0.88 (s, 9H);

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>):  $\delta$  185.7, 175.8, 148.5, 144.8, 143.3, 142.2, 139.7, 137.6, 136.3, 132.8, 129.0, 128.8, 128.0, 127.4, 127.3, 124.1, 122.0, 108.3, 69.6, 58.7, 57.7, 34.7, 34.5, 29.1, 28.7, 26.1;

IR (neat):  $\nu$  3641, 2221, 1721 1635, 1521, 1314, 1220, 1048, 879, 745 cm<sup>-1</sup>;

HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd. for C<sub>32</sub>H<sub>36</sub>NO<sub>2</sub>: 466.2741; found: 466.2745;



Yellow solid, isolated yield: 93% (47 mg);

dr > 19:1;

mp: 182.5–183.1 °C;



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.25-7.12 (m, 3H), 7.03 (d,  $J$  = 6.4 Hz, 2H), 6.94 (d,  $J$  = 2.8 Hz, 1H), 6.76-6.67 (m, 1H), 6.70-6.62 (m, 2H), 6.63-6.57 (m, 2H), 5.90 (dd,  $J$  = 5.6, 2.8 Hz, 1H), 5.01 (s, 1H), 3.71 (s, 3H), 3.17 (s, 3H), 1.09 (s, 9H), 0.82 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.5, 175.8, 155.1, 150.5, 146.5, 140.3, 139.3, 138.7, 138.1, 137.1, 132.5, 128.7, 127.9, 127.2, 127.0, 114.6, 112.7, 107.8, 69.1, 60.6, 57.5, 55.7, 35.0, 34.6, 29.5, 28.7, 26.3;

IR (neat):  $\nu$  3642, 2312, 1723, 1643, 1519, 1394, 1247, 1046, 831, 748  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{33}\text{H}_{38}\text{NO}_3$ : 496.2846; found: 496.2853;

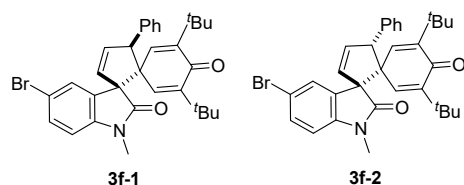
**3e-2**: mp: 177.3-178.2  $^\circ\text{C}$ ;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.27-7.15 (m, 3H), 7.08-7.00 (m, 2H), 6.90 (d,  $J$  = 2.4 Hz, 1H), 6.89-6.79 (m, 2H), 6.67 (d,  $J$  = 8.4 Hz, 1H), 6.53 (dd,  $J$  = 5.6, 1.6 Hz, 1H), 6.35 (d,  $J$  = 2.8 Hz, 1H), 6.05 (dd,  $J$  = 5.6, 2.8 Hz, 1H), 4.53 (s, 1H), 3.84 (s, 3H), 2.99 (s, 3H), 0.97 (s, 9H), 0.88 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.7, 175.4, 155.7, 148.5, 144.8, 142.2, 139.7, 137.6, 137.0, 136.4, 132.8, 130.2, 128.0, 127.4, 127.3, 112.5, 112.4, 108.4, 70.0, 58.6, 57.7, 56.1, 34.7, 34.5, 29.2, 28.7, 26.2;

IR (neat):  $\nu$  3645, 2278, 1765, 1645, 1547, 1365, 1241, 1045, 837, 796  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{33}\text{H}_{38}\text{NO}_3$ : 496.2846; found: 496.2851;



Yellow solid, isolated yield: 92% (50 mg);

dr = 1:1;

**3f-1**: mp: 191.1-191.9  $^\circ\text{C}$ ;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.34 (dd,  $J$  = 8.4, 2.0 Hz, 1H), 7.24-7.16 (m, 3H), 7.14 (d,  $J$  = 2.0 Hz, 1H), 7.08-6.99 (m, 2H), 6.90 (d,  $J$  = 2.8 Hz, 1H), 6.69 (dd,  $J$  = 5.6, 1.6 Hz, 1H), 6.67-6.56 (m, 2H), 5.90 (dd,  $J$  = 5.6, 2.8 Hz, 1H), 5.00 (s, 1H), 3.18 (s, 3H), 1.10 (s, 9H), 0.86 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.4, 175.6, 150.9, 146.9, 142.6, 139.8, 139.2, 138.7, 137.8, 131.84, 131.79, 129.6, 129.3, 128.0, 127.2, 127.1, 114.4, 109.1, 68.7, 60.5, 57.5, 35.0, 34.8, 29.5, 28.8, 26.3;

IR (neat):  $\nu$  3644, 2254, 1735, 1672, 1524, 1347, 1285, 1061, 821, 763  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{32}\text{H}_{35}\text{BrNO}_2$ : 544.1846; found: 544.1849;

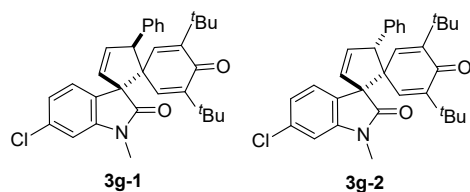
**3f-2**: mp: 190.5-191.2  $^\circ\text{C}$ ;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.44 (dd,  $J$  = 8.0, 2.0 Hz, 1H), 7.37 (d,  $J$  = 2.0 Hz, 1H), 7.29-7.15 (m, 3H), 7.11 - 6.97 (m, 2H), 6.77 (d,  $J$  = 2.8 Hz, 1H), 6.64 (d,  $J$  = 8.4 Hz, 1H), 6.56 (dd,  $J$  = 5.6, 1.6 Hz, 1H), 6.35 (d,  $J$  = 2.8 Hz, 1H), 6.01 (dd,  $J$  = 5.8, 2.8 Hz, 1H), 4.51 (s, 1H), 3.00 (s, 3H), 0.99 (s, 9H), 0.87 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.6, 175.3, 148.6, 145.2, 142.4, 141.7, 139.4, 137.4, 137.2, 132.1, 131.7, 131.0, 128.0, 127.5, 127.4, 127.3, 114.6, 109.6, 69.7, 58.8, 57.5, 34.7, 34.6, 29.2, 28.7, 26.2;

IR (neat):  $\nu$  3672, 2241, 1865, 1682, 1591, 1545, 1252, 1171, 862, 774  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{32}\text{H}_{35}\text{BrNO}_2$ : 544.1846; found: 544.1847;



Yellow foam, isolated yield: 93% (47 mg);

dr = 1:1;

**3g-1:** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.27-7.14 (m, 3H), 7.03-7.02(m, 2H), 6.93-9.91 (m, 3H), 6.73 (s, 1H), 6.69-6.74 (m, 1H), 6.63 (1H, *J* = 2.8 Hz, 1H), 5.87 (dd, *J* = 5.6, 2.8 Hz, 1H), 5.00 (s, 1H), 3.19 (s, 3H), 1.11 (s, 9H), 0.82 (s, 9H);

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 185.3, 176.1, 150.9, 146.7, 144.8, 139.9, 139.0, 138.7, 137.9, 134.8, 132.1, 128.0, 127.3, 127.2, 125.7, 121.6, 108.5, 68.3, 60.5, 57.5, 35.0, 34.7, 29.7, 29.5, 28.8, 26.3;

IR (neat): ν 3686, 2347, 1742, 1615, 1571, 1334, 1272, 1165, 887, 712 cm<sup>-1</sup>;

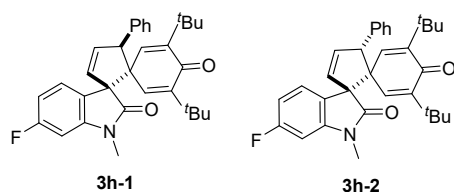
HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd. for C<sub>32</sub>H<sub>35</sub>ClNO<sub>2</sub>: 500.2351; found: 500.2354;

**3g-2:** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.27-7.15 (m, 4H), 7.11-6.94 (m, 3H), 6.83 (d, *J* = 2.8 Hz, 1H), 6.77 (d, *J* = 1.6 Hz, 1H), 6.58-6.49 (m, 1H), 6.32 (d, *J* = 2.8 Hz, 1H), 6.02 (dd, *J* = 5.6, 2.8 Hz, 1H), 4.52 (s, 1H), 3.01 (s, 3H), 0.98 (s, 9H), 0.87 (s, 9H);

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 185.6, 175.7, 148.8, 145.1, 144.4, 141.7, 139.2, 137.3, 136.7, 134.8, 132.4, 128.1, 127.42, 127.38, 127.2, 125.1, 121.8, 108.9, 69.2, 58.8, 57.8, 34.8, 34.6, 29.2, 28.7, 26.2;

IR (neat): ν 3672, 2241, 1765, 1682, 1591, 1345, 1252, 1071, 862, 774 cm<sup>-1</sup>;

HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd. for C<sub>32</sub>H<sub>35</sub>ClNO<sub>2</sub>: 500.2351; found: 500.2356;



Brown foam, isolated yield: 91% (44 mg);

dr = 1:1;

**3h-1:** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.21-7.17 (m, 3H), 7.05-7.02 (m, 2H), 6.96-6.93 (m, 1H), 6.91 (d, *J* = 2.8 Hz, 1H), 6.69-6.67 (m, 1H), 6.64 (d, *J* = 2.8 Hz, 1H), 6.60-6.57 (m, 1H), 6.48-6.46 (m, 1H), 5.88 (dd, *J* = 5.6, 2.8 Hz, 1H), 5.00 (s, 1H), 3.18 (s, 3H), 1.10 (s, 9H), 0.82 (s, 9H);

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 185.4, 176.5, 163.4 (d, *J*<sub>C-F</sub> = 246.6 Hz), 150.8, 146.7, 145.2 (d, *J*<sub>C-F</sub> = 11.6 Hz), 140.0, 138.9, 138.8, 138.0, 132.3, 128.0, 127.5 (d, *J*<sub>C-F</sub> = 9.7 Hz), 127.14, 127.11, 122.6 (d, *J*<sub>C-F</sub> = 2.9 Hz), 107.8 (d, *J*<sub>C-F</sub> = 22.2 Hz), 96.6 (d, *J*<sub>C-F</sub> = 27.5 Hz), 68.3, 60.6, 57.3, 35.0, 34.7, 29.5, 28.7, 26.3;

IR (neat): ν 3741, 2347, 1742, 1615, 1571, 1334, 1272, 1165, 887, 712 cm<sup>-1</sup>;

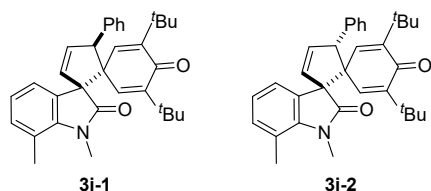
HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd. for C<sub>32</sub>H<sub>35</sub>FNO<sub>2</sub>: 484.2646; found: 484.2648;

**3h-2:** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.24-7.17 (m, 4H), 7.08-6.98 (m, 2H), 6.83 (d, *J* = 2.8 Hz, 1H), 6.82-6.74 (m, 1H), 6.58-6.47 (m, 2H), 6.32 (d, *J* = 2.8 Hz, 1H), 6.03 (dd, *J* = 5.6, 2.8 Hz, 1H), 4.52 (s, 1H), 3.01 (s, 3H), 0.98 (s, 9H), 0.87 (s, 9H);

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 185.7, 176.0, 163.5 (d, *J*<sub>C-F</sub> = 246.5 Hz), 148.7, 145.0, 144.8 (d, *J*<sub>C-F</sub> = 11.3 Hz), 141.9, 139.3, 137.4, 136.5, 132.6, 128.0, 127.4, 127.3, 125.2 (d, *J*<sub>C-F</sub> = 9.6 Hz), 124.1 (d, *J*<sub>C-F</sub> = 3.4 Hz), 108.0 (d, *J*<sub>C-F</sub> = 22.4 Hz), 97.1 (d, *J*<sub>C-F</sub> = 27.8 Hz), 69.1, 58.7, 57.7, 34.7, 34.6, 29.2, 28.7, 26.2;

IR (neat): ν 3686, 2210, 1814, 1689, 1533, 1310, 1221, 1054, 911, 698 cm<sup>-1</sup>;

HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd. for C<sub>32</sub>H<sub>35</sub>FNO<sub>2</sub>: 484.2646; found: 484.2652;



Yellow foam, isolated yield: 94% (45 mg);

dr = 1:1;

**3i-1:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.23-7.11 (m, 3H), 7.08-6.99 (m, 2H), 6.95-6.87 (m, 2H), 6.85-6.74 (m, 2H), 6.66 (dd,  $J = 5.6, 1.6$  Hz, 1H), 6.62 (d,  $J = 2.8$  Hz, 1H), 5.90 (dd,  $J = 5.6, 2.8$  Hz, 1H), 4.99 (s, 1H), 3.47 (s, 3H), 2.47 (s, 3H), 1.11 (s, 9H), 0.79 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.6, 176.9, 150.5, 146.2, 141.2, 140.5, 139.3, 138.6, 138.2, 132.8, 132.7, 127.9, 127.8, 127.2, 127.0, 124.5, 121.5, 119.2, 68.4, 60.8, 57.3, 35.0, 34.6, 29.7, 29.6, 28.7, 19.0;

IR (neat):  $\nu$  3765, 2311, 1713, 1654, 1524, 1312, 1278, 1056, 887, 779  $\text{cm}^{-1}$ ;

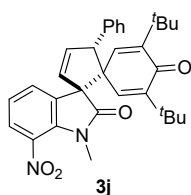
HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{33}\text{H}_{38}\text{NO}_2$ : 480.2897; found: 480.2902;

**3i-2:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.24-7.16 (m, 3H), 7.14-7.05 (m, 1H), 7.08-6.98 (m, 3H), 6.99 (d,  $J = 7.2$  Hz, 1H), 6.84 (d,  $J = 3.2$  Hz, 1H), 6.52 (dd,  $J = 5.6, 1.6$  Hz, 1H), 6.22 (d,  $J = 3.2$  Hz, 1H), 6.05 (dd,  $J = 5.6, 2.8$  Hz, 1H), 4.52 (s, 1H), 3.28 (s, 3H), 2.49 (s, 3H), 0.95 (s, 9H), 0.88 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.8, 176.6, 148.4, 144.6, 142.5, 141.1, 140.0, 137.7, 136.3, 132.8, 132.6, 129.4, 128.0, 127.3, 127.2, 121.9, 121.8, 120.0, 69.5, 58.4, 57.9, 34.7, 34.5, 29.4, 29.2, 28.7, 18.9;

IR (neat):  $\nu$  3748, 2318, 1792, 1578, 1513, 1378, 1258, 1057, 814, 768  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{33}\text{H}_{38}\text{NO}_2$ : 480.2897; found: 480.2901;



Yellow foam, isolated yield: 85% (43 mg);

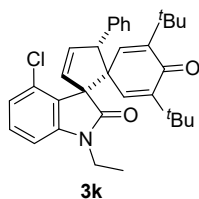
dr = 1:1;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.72 (d,  $J = 8.4$  Hz, 1H), 7.62 (d,  $J = 8.4$  Hz, 1H), 7.44 (d,  $J = 7.2$  Hz, 1H), 7.26-7.12 (m, 8H), 7.08-6.93 (m, 5H), 6.86-6.85 (m, 1H), 6.78 (s, 2H), 6.64-6.63 (m, 1H), 6.59-6.58 (m, 1H), 6.14 (d,  $J = 2.4$  Hz, 1H), 6.06 (dd,  $J = 5.6, 2.8$  Hz, 1H), 5.93-5.91 (m, 1H), 4.98 (s, 1H), 4.50 (s, 1H), 3.23 (s, 3H), 3.05 (s, 3H), 1.13 (s, 9H), 0.96 (s, 9H), 0.88 (s, 9H), 0.79 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.2, 185.1, 176.7, 176.5, 151.6, 149.6, 147.2, 145.6, 140.9, 140.2, 139.2, 138.01, 137.96, 137.8, 137.4, 137.3, 137.1, 136.9, 135.4, 135.1, 132.8, 131.5, 131.1, 131.0, 129.9, 128.13, 128.08, 127.5, 127.4, 127.31, 127.30, 127.1, 125.0, 124.7, 121.4, 121.0, 68.4, 67.6, 61.0, 58.6, 58.2, 57.1, 35.1, 34.8, 34.7, 34.6, 29.8, 29.41, 29.37, 29.1, 28.7, 28.6;

IR (neat):  $\nu$  3789, 2348, 1767, 1665, 1521, 1498, 1318, 1051, 798, 754  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{32}\text{H}_{35}\text{N}_2\text{O}_4$ : 511.2591; found: 511.2598;



Yellow solid, isolated yield: 91% (47 mg);

dr > 19:1;

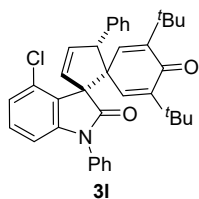
mp: 186.5-187.2  $^{\circ}\text{C}$ ;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.32-7.26 (m, 2H), 7.21 (d,  $J = 5.6$  Hz, 1H), 7.17-7.06 (m, 2H), 6.86 (d,  $J = 8.0$  Hz, 1H), 6.66 (s, 1H), 6.62 (d,  $J = 7.6$  Hz, 1H), 6.53-6.38 (m, 2H), 6.06 (s, 1H), 5.99 (dd,  $J = 15.6, 7.6$  Hz, 1H), 4.40 (d,  $J = 6.4$  Hz, 1H), 3.92-3.71 (m, 1H), 3.67-3.36 (m, 1H), 1.23 (t,  $J = 7.2$  Hz, 3H), 1.10 (s, 9H), 1.08 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.6, 175.1, 151.3, 146.6, 144.5, 139.1, 138.5, 137.6, 136.9, 132.2, 131.6, 130.1, 129.7, 128.5, 127.4, 126.3, 126.0, 124.4, 123.6, 106.5, 70.1, 62.3, 54.6, 35.3, 34.93, 34.89, 29.5, 28.9, 12.7;

IR (neat):  $\nu$  3747, 2364, 1785, 1634, 1598, 1357, 1265, 1067, 882, 771  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{33}\text{H}_{37}\text{ClNO}_2$ : 514.2507; found: 514.2511;



Yellow solid, isolated yield: 86% (48 mg);

dr > 19:1;

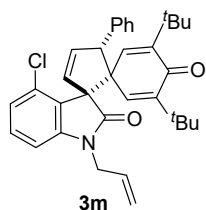
mp: 192.5-193.1 °C;

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.54 (t, *J* = 7.6 Hz, 2H), 7.46-7.36 (m, 3H), 7.21 (t, *J* = 7.6 Hz, 3H), 7.09 (d, *J* = 7.2 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 1H), 6.99 (d, *J* = 2.8 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 1H), 6.89 (d, *J* = 2.8 Hz, 1H), 6.74 (d, *J* = 5.6 Hz, 1H), 6.64 (d, *J* = 7.6 Hz, 1H), 6.27 (dd, *J* = 5.6, 2.8 Hz, 1H), 4.90 (s, 1H), 1.16 (s, 9H), 0.82 (s, 9H);

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 186.7, 174.8, 151.1, 146.0, 145.1, 139.5, 138.3, 137.94, 137.86, 133.8, 132.1, 130.6, 130.0, 129.6, 128.3, 127.9, 127.3, 127.1, 126.1, 124.5, 124.3, 107.9, 70.1, 63.1, 57.3, 35.1, 34.7, 29.6, 28.5;

IR (neat): ν 3811, 2331, 1774, 1621, 1534, 1345, 1215, 1068, 821, 789 cm<sup>-1</sup>;

HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd. for C<sub>37</sub>H<sub>37</sub>ClNO<sub>2</sub>: 562.2507; found: 562.2514;



Yellow foam, isolated yield: 91% (48 mg);

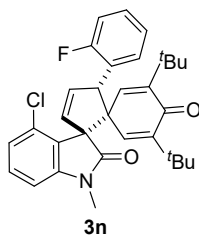
dr > 19:1;

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.23-7.17 (m, 3H), 7.09 (d, *J* = 7.2 Hz, 3H), 6.92-6.88 (m, 1H), 6.85 (d, *J* = 8.0 Hz, 1H), 6.82 (s, 1H), 6.70 (d, *J* = 5.6 Hz, 1H), 6.65-6.58 (m, 1H), 6.19-6.10 (m, 1H), 5.91-5.68 (m, 1H), 5.27 (d, *J* = 8.4 Hz, 1H), 5.23 (s, 1H), 4.90 (s, 1H), 4.38 (dd, *J* = 15.6, 4.4 Hz, 1H), 4.26-4.08 (m, 1H), 1.14 (s, 9H), 0.78 (s, 9H);

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 186.4, 175.4, 150.7, 145.8, 144.5, 139.3, 138.7, 138.1, 137.7, 132.0, 130.8, 130.5, 130.0, 127.9, 127.2, 127.1, 124.6, 123.8, 118.8, 107.3, 70.2, 62.5, 57.0, 43.0, 35.0, 34.6, 29.5, 28.5;

IR (neat): ν 3741, 2289, 1731, 1694, 1523, 1345, 1262, 1021, 841, 736 cm<sup>-1</sup>;

HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd. for C<sub>34</sub>H<sub>37</sub>ClNO<sub>2</sub>: 526.2507; found: 526.2514;



Yellow foam, isolated yield: 86% (45 mg);

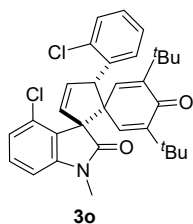
dr > 19:1;

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.30-7.27 (m, 1H), 7.22-7.02 (m, 3H), 6.96-6.85 (m, 2H), 6.89-6.79 (m, 2H), 6.60 (t, *J* = 6.4 Hz, 2H), 6.15 (dd, *J* = 5.6, 2.8 Hz, 1H), 5.15 (s, 1H), 3.15 (s, 3H), 1.09 (s, 9H), 0.80 (s, 9H);

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 186.1, 175.6, 161.0 (d, *J*<sub>C-F</sub> = 247.5 Hz), 149.6, 146.4, 145.3, 139.6, 138.5, 137.3, 132.0, 130.22, 130.19, 129.8 (d, *J*<sub>C-F</sub> = 4.4 Hz), 128.7 (d, *J*<sub>C-F</sub> = 8.2 Hz), 125.5 (d, *J*<sub>C-F</sub> = 14.9 Hz), 124.3, 123.7, 123.6 (d, *J*<sub>C-F</sub> = 3.4 Hz), 115.4 (d, *J*<sub>C-F</sub> = 22.6 Hz), 106.3, 70.6, 62.0, 51.1, 34.8, 34.6, 29.4, 28.5, 26.4;

IR (neat):  $\nu$  3721, 2265, 1712, 1652, 1531, 1495, 1245, 1014, 898, 714  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[M + H]^+$  calcd. for  $\text{C}_{32}\text{H}_{34}\text{ClFNO}_2$ : 518.2257; found: 518.2261;



Yellow solid, isolated yield: 89% (48 mg);

dr > 19:1;

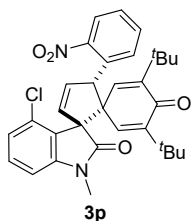
mp: 168.2-169.1  $^{\circ}\text{C}$ ;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.42 (d,  $J$  = 7.6 Hz, 1H), 7.25-7.22 (m, 2H), 7.17-7.07 (m, 2H), 6.97 (d,  $J$  = 2.4 Hz, 1H), 6.89 (d,  $J$  = 2.4 Hz, 1H), 6.85 (d,  $J$  = 8.4 Hz, 1H), 6.59 (d,  $J$  = 7.6 Hz, 1H), 6.51 (d,  $J$  = 5.6 Hz, 1H), 6.14 (dd,  $J$  = 5.6, 2.8 Hz, 1H), 5.35 (s, 1H), 3.14 (s, 3H), 1.09 (s, 9H), 0.81 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.8, 175.9, 148.0, 146.1, 145.3, 141.0, 138.4, 136.5, 134.2, 132.0, 130.42, 130.41, 130.3, 130.2, 129.9, 128.3, 126.3, 124.3, 123.7, 106.4, 71.2, 61.6, 54.3, 34.8, 34.7, 29.2, 28.6, 26.5;

IR (neat):  $\nu$  3686, 2347, 1742, 1615, 1571, 1334, 1272, 1165, 887, 712  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[M + H]^+$  calcd. for  $\text{C}_{32}\text{H}_{34}\text{Cl}_2\text{NO}_2$ : 534.1961; found: 534.1962;



Yellow solid, isolated yield: 86% (47 mg);

dr > 19:1;

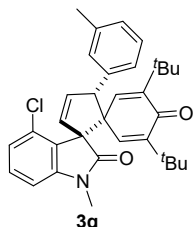
mp: 196.8-197.5  $^{\circ}\text{C}$ ;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.67 (d,  $J$  = 8.0 Hz, 1H), 7.64-7.53 (m, 2H), 7.35 (t,  $J$  = 7.5 Hz, 1H), 7.11 (t,  $J$  = 8.0 Hz, 1H), 6.82 (d,  $J$  = 8.2 Hz, 1H), 6.73-6.51 (m, 4H), 6.19-6.11 (m, 1H), 5.94 (s, 1H), 3.13 (s, 3H), 1.07 (s, 9H), 0.74 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.3, 175.3, 149.8, 149.3, 146.5, 145.3, 139.1, 137.5, 136.5, 133.3, 132.2, 131.9, 130.9, 130.4, 130.2, 127.9, 125.1, 123.9, 123.6, 106.4, 99.9, 71.1, 61.7, 34.8, 34.6, 29.0, 28.5, 26.5;

IR (neat):  $\nu$  3656, 2314, 1765, 1610, 1521, 1356, 1214, 1132, 898, 725  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[M + H]^+$  calcd. for  $\text{C}_{32}\text{H}_{34}\text{ClN}_2\text{O}_4$ : 545.2202; found: 545.2204;



Yellow foam, isolated yield: 80% (42 mg);

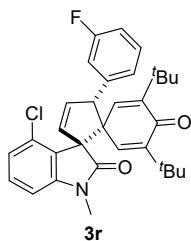
dr > 19:1;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.16-7.05 (m, 2H), 6.99 (d,  $J$  = 7.2 Hz, 1H), 6.93-6.77 (m, 5H), 6.70 (d,  $J$  = 5.2 Hz, 1H), 6.59 (d,  $J$  = 7.6 Hz, 1H), 6.14 (s, 1H), 4.85 (s, 1H), 3.16 (s, 3H), 2.26 (s, 3H), 1.12 (s, 9H), 0.77 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.3, 175.7, 150.7, 145.7, 145.2, 139.4, 139.0, 138.1, 137.8, 137.5, 131.9, 130.11, 130.08, 127.89, 127.87, 127.7, 124.5, 124.2, 123.7, 106.3, 70.5, 62.5, 56.5, 34.9, 34.6, 29.6, 28.4, 26.4, 21.3;

IR (neat):  $\nu$  3678, 2332, 1785, 1642 1568, 1314 1252, 1181, 839, 768  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{33}\text{H}_{37}\text{ClNO}_2$ : 514.2507; found: 514.2509;



Yellow solid, isolated yield: 93% (48 mg);

dr > 19:1;

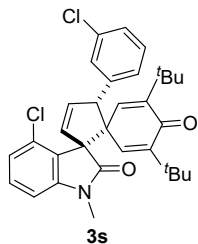
mp: 187.3-188.2  $^{\circ}\text{C}$ ;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.23-7.15 (m, 1H), 7.13 (t,  $J$  = 8.0 Hz, 1H), 6.93-6.84 (m, 3H), 6.84-6.75 (m, 3H), 6.65 (d,  $J$  = 5.8 Hz, 1H), 6.60 (d,  $J$  = 7.6 Hz, 1H), 6.17 (dd,  $J$  = 5.6, 2.8 Hz, 1H), 4.87 (s, 1H), 3.15 (s, 3H), 1.12 (s, 9H), 0.79 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.0, 175.5, 162.6 (d,  $J_{\text{C-F}}$  = 246.1 Hz), 151.2, 146.2, 145.2, 141.0 (d,  $J_{\text{C-F}}$  = 7.1 Hz), 138.7, 138.5, 136.9, 132.0, 130.8, 130.3, 129.4 (d,  $J_{\text{C-F}}$  = 8.2 Hz), 124.2, 123.8, 122.8 (d,  $J_{\text{C-F}}$  = 2.9 Hz), 114.1 (d,  $J_{\text{C-F}}$  = 21.7 Hz), 113.8 (d,  $J_{\text{C-F}}$  = 21.0 Hz), 106.4, 70.5, 62.3, 56.2, 35.0, 34.6, 29.5, 28.5, 26.5;

IR (neat):  $\nu$  3645, 2287, 1698, 1612, 1565, 1385, 1296, 1124, 847, 796  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{32}\text{H}_{34}\text{ClFNO}_2$ : 518.2257; found: 518.2258;



Yellow solid, isolated yield: 93% (50 mg);

dr > 19:1;

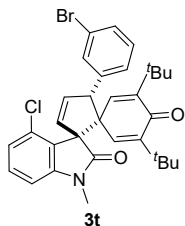
mp: 198.2-199.1  $^{\circ}\text{C}$ ;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.19-7.07 (m, 4H), 6.96 (d,  $J$  = 6.4 Hz, 1H), 6.86 (d,  $J$  = 8.0 Hz, 1H), 6.78 (d,  $J$  = 9.6 Hz, 2H), 6.66 (d,  $J$  = 5.6 Hz, 1H), 6.60 (d,  $J$  = 8.0 Hz, 1H), 6.23-6.14 (m, 1H), 4.85 (s, 1H), 3.16 (s, 3H), 1.12 (s, 9H), 0.80 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.2, 175.6, 151.4, 146.4, 145.3, 140.6, 138.8, 138.5, 136.9, 134.1, 132.1, 131.1, 130.4, 129.3, 127.4, 127.2, 125.4, 124.3, 123.9, 106.5, 70.5, 62.5, 56.3, 35.1, 34.8, 29.7, 28.6, 26.6;

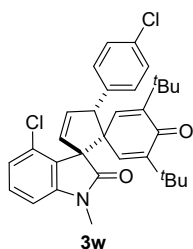
IR (neat):  $\nu$  3645, 2298, 1725, 1665, 1545, 1368, 1241, 1174, 898, 771  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{32}\text{H}_{34}\text{Cl}_2\text{NO}_2$ : 534.1961; found: 534.1964;



Yellow solid, isolated yield: 88% (51 mg);





Yellow solid, isolated yield: 93% (50 mg);

dr > 19:1;

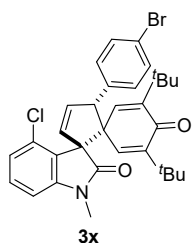
mp: 197.5-198.3 °C;

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.20 (d, *J* = 8.0 Hz, 2H), 7.12 (t, *J* = 8.0 Hz, 1H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.85 (d, *J* = 8.0 Hz, 1H), 6.78 (d, *J* = 8.0 Hz, 2H), 6.63 (d, *J* = 5.2 Hz, 1H), 6.59 (d, *J* = 7.6 Hz, 1H), 6.16 (dd, *J* = 5.6, 2.8 Hz, 1H), 4.85 (s, 1H), 3.15 (s, 3H), 1.11 (s, 9H), 0.80 (s, 9H);

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 186.0, 175.5, 151.2, 146.3, 145.2, 138.7, 138.5, 137.1, 136.9, 132.8, 131.9, 130.8, 130.3, 128.5, 128.1, 124.2, 123.8, 106.4, 70.6, 62.3, 56.0, 35.0, 34.7, 29.6, 28.5, 26.5;

IR (neat): ν 3658, 2268, 1796, 1614, 1526, 1341, 1295, 1147, 858, 698 cm<sup>-1</sup>;

HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd. for C<sub>32</sub>H<sub>34</sub>Cl<sub>2</sub>NO<sub>2</sub>: 534.1961; found: 534.1965;



Yellow solid, isolated yield: 87% (50 mg);

dr > 19:1;

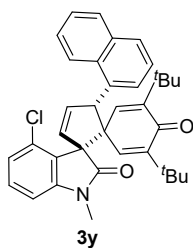
mp: 199.5-200.4°C;

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.20-7.08 (m, 4H), 6.96 (d, *J* = 6.8 Hz, 1H), 6.86 (d, *J* = 8.4 Hz, 1H), 6.78 (d, *J* = 9.6 Hz, 2H), 6.66 (d, *J* = 5.6 Hz, 1H), 6.60 (d, *J* = 7.6 Hz, 1H), 6.18 (dd, *J* = 5.6, 2.8 Hz, 1H), 4.85 (s, 1H), 3.16 (s, 3H), 1.12 (s, 9H), 0.80 (s, 9H);

<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>): δ 186.0, 175.5, 151.2, 146.3, 145.2, 138.6, 138.5, 137.4, 137.0, 131.9, 131.0, 130.8, 130.3, 128.8, 124.2, 123.8, 120.9, 106.4, 70.5, 62.3, 56.0, 35.0, 34.7, 29.6, 28.5, 26.5;

IR (neat): ν 3688, 2258, 1769, 1685, 1574, 1314, 1269, 1171, 834, 765 cm<sup>-1</sup>;

HRMS (ESI): *m/z* [M + H]<sup>+</sup> calcd. for C<sub>32</sub>H<sub>34</sub>BrClNO<sub>2</sub>: 578.1456; found: 578.1458;



Yellow foam, isolated yield: 87% (48 mg);

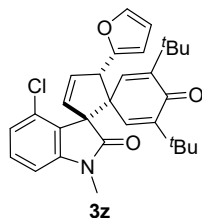
dr > 19:1;

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.94 (d, *J* = 8.0 Hz, 1H), 7.80-7.66 (m, 2H), 7.56 (d, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.40-7.30 (m, 2H), 7.17-7.04 (m, 2H), 6.85 (d, *J* = 8.4 Hz, 1H), 6.81 (d, *J* = 2.4 Hz, 1H), 6.74 (d, *J* = 5.6 Hz, 1H), 6.59 (d, *J* = 7.6 Hz, 1H), 6.23-6.14 (m, 1H), 5.67 (s, 1H), 3.17 (s, 3H), 1.06 (s, 9H), 0.56 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.4, 176.3, 148.4, 145.2, 145.0, 140.6, 139.8, 139.3, 135.2, 133.7, 132.0, 131.9, 130.1, 129.7, 128.4, 127.7, 126.0, 125.4, 125.1, 124.8, 124.74, 124.73, 123.7, 106.4, 71.6, 60.4, 53.7, 34.8, 34.4, 29.1, 28.3, 26.5;

IR (neat):  $\nu$  3626, 2297, 1769, 1641, 1562, 1352, 1214, 1118, 841, 763  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{36}\text{H}_{37}\text{ClNO}_2$ : 550.2507; found: 550.2511;



Yellow foam, isolated yield: 91% (45 mg);

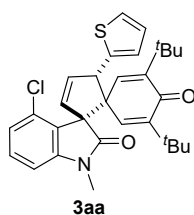
dr > 19:1;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.23 (s, 1H), 7.12 (t,  $J$  = 8.0 Hz, 1H), 6.95 (s, 1H), 6.85 (d,  $J$  = 8.0 Hz, 1H), 6.69 (s, 1H), 6.58 (t,  $J$  = 6.4 Hz, 2H), 6.23 (s, 1H), 6.12-6.09 (m, 1H), 6.04 (s, 1H), 4.89 (s, 1H), 3.13 (s, 3H), 1.09 (s, 9H), 0.92 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.2, 175.4, 152.4, 150.8, 146.5, 145.3, 141.4, 138.5, 138.3, 135.7, 132.1, 130.2(2C), 124.0, 123.8, 110.1, 106.33, 106.27, 70.4, 62.0, 51.0, 34.9, 34.6, 29.5, 28.6, 26.4;

IR (neat):  $\nu$  3668, 2297, 1699, 1614, 1514, 1294, 1215, 1165, 817, 764  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{30}\text{H}_{33}\text{ClNO}_3$ : 490.2143; found: 490.2147;



Yellow foam, isolated yield: 93% (47 mg);

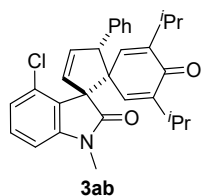
dr > 19:1;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.13 (t,  $J$  = 8.0 Hz, 1H), 7.07 (d,  $J$  = 5.2 Hz, 1H), 6.92-6.87 (m, 1H), 6.90-6.80 (m, 3H), 6.71 (d,  $J$  = 2.4 Hz, 1H), 6.67 (d,  $J$  = 5.6 Hz, 1H), 6.59 (d,  $J$  = 7.6 Hz, 1H), 6.15 (dd,  $J$  = 5.6, 2.8 Hz, 1H), 5.07 (s, 1H), 3.15 (s, 3H), 1.12 (s, 9H), 0.85 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.3, 175.3, 151.7, 146.5, 145.2, 141.3, 138.6, 137.9, 137.3, 132.0, 130.3, 130.2, 126.3, 124.2, 124.1, 123.8, 123.7, 106.3, 70.5, 62.3, 52.2, 35.0, 34.6, 29.5, 28.5, 26.4;

IR (neat):  $\nu$  3681, 2317, 1769, 1652, 1515, 1374, 1234, 1192, 865, 747  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{30}\text{H}_{33}\text{ClNO}_2\text{S}$ : 506.1915; found: 506.1919;



Yellow foam, isolated yield: 87% (41 mg);

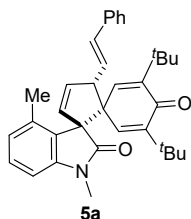
dr > 19:1;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.24-7.12 (m, 3H), 7.10 (d,  $J$  = 8.0 Hz, 2H), 7.05 (d,  $J$  = 6.8 Hz, 2H), 6.86 (d,  $J$  = 8.0 Hz, 1H), 6.82 (d,  $J$  = 2.4 Hz, 1H), 6.67 (d,  $J$  = 5.2 Hz, 1H), 6.60 (d,  $J$  = 7.6 Hz, 1H), 6.15 (dd,  $J$  = 5.6, 2.8 Hz, 1H), 4.86 (s, 1H), 3.16 (s, 3H), 2.98-2.84 (m, 1H), 2.53-2.38 (m, 1H), 1.03 (d,  $J$  = 6.8 Hz, 3H), 0.94 (d,  $J$  = 6.8 Hz, 3H), 0.72 (d,  $J$  = 6.8 Hz, 3H), 0.52 (d,  $J$  = 6.8 Hz, 3H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  184.6, 175.9, 148.8, 145.3, 143.6, 140.2, 139.5, 138.1, 137.9, 131.8, 130.2, 130.1, 128.0, 127.4, 127.1, 124.8, 124.0, 106.5, 70.4, 62.8, 56.9, 26.7, 26.5, 25.8, 22.31, 22.29, 20.8, 20.3;

IR (neat):  $\nu$  3664, 2357, 1739, 1641, 1552, 1364, 1214, 1173, 819, 697  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{30}\text{H}_{31}\text{ClNO}_2$ : 472.2038; found: 472.2038;



Yellow foam, isolated yield: 87% (44 mg);

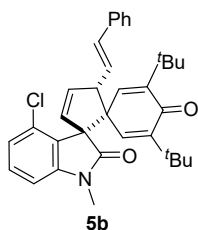
dr > 19:1;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.30-7.26 (m, 4H), 7.22 (d,  $J$  = 7.6 Hz, 1H), 7.09 (t,  $J$  = 7.6 Hz, 1H), 6.84-6.61 (m, 3H), 6.60-6.42 (m, 3H), 6.12-5.92 (m, 2H), 4.43 (s, 1H), 3.13 (s, 3H), 2.33 (s, 3H), 1.09 (s, 9H), 1.04 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.2, 176.2, 151.0, 147.0, 143.9, 139.6, 138.5, 137.9, 136.9, 135.7, 131.4, 130.6, 128.8, 128.6, 127.4, 126.6, 126.0, 124.9, 124.6, 105.3, 70.3, 61.7, 54.3, 34.9, 34.8, 29.5, 29.0, 26.3, 19.8;

IR (neat):  $\nu$  3621, 2297, 1743, 1654, 1525, 1362, 1217, 1127, 798, 714  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{35}\text{H}_{40}\text{NO}_2$ : 506.3054; found: 506.3056;



Yellow foam, isolated yield: 92% (48 mg);

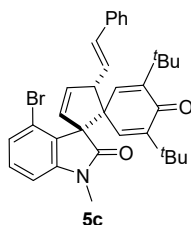
dr > 19:1;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.30-7.27 (m, 3H), 7.25-7.24 (m, 1H), 7.20 (s, 1H), 7.13 (t,  $J$  = 8.0 Hz, 1H), 7.09 (d,  $J$  = 2.4 Hz, 1H), 6.86 (d,  $J$  = 8.0 Hz, 1H), 6.64 (d,  $J$  = 2.4 Hz, 1H), 6.59 (d,  $J$  = 7.6 Hz, 1H), 6.51-6.45 (m, 2H), 6.12-5.91 (m, 2H), 4.39 (d,  $J$  = 6.4 Hz, 1H), 3.13 (s, 3H), 1.09 (s, 9H), 1.07 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.3, 175.5, 151.5, 146.8, 145.3, 138.9, 138.7, 137.8, 136.9, 132.0, 131.6, 130.2, 129.5, 128.5, 127.4, 126.3, 126.0, 124.1, 123.8, 106.3, 70.5, 62.3, 54.4, 34.92, 34.89, 29.6, 28.8, 26.4;

IR (neat):  $\nu$  3679, 2265, 1747, 1623, 1517, 1318, 1269, 1137, 854, 764  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{34}\text{H}_{37}\text{ClNO}_2$ : 526.2507; found: 526.2512;



Yellow solid, isolated yield: 95% (54 mg);

dr > 19:1;

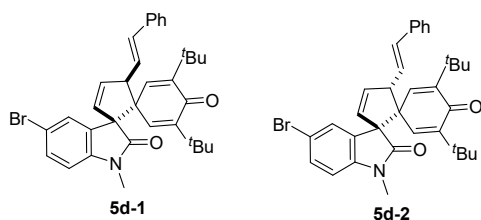
mp: 175.2-176.1  $^{\circ}\text{C}$ ;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.30-7.27 (m, 3H), 7.25-7.24 (m, 1H), 7.22-7.18 (m, 1H), 7.17-7.13 (m, 1H), 7.04 (d,  $J$  = 6.4 Hz, 2H), 6.67-6.58 (m, 2H), 6.56-6.37 (m, 2H), 6.08 (dd,  $J$  = 5.6, 2.8 Hz, 1H), 6.01 (dd,  $J$  = 15.6, 7.6 Hz, 1H), 4.36 (d,  $J$  = 6.4 Hz, 1H), 3.12 (s, 3H), 1.09 (s, 18H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.5, 175.4, 151.4, 146.9, 145.4, 138.7, 138.6, 137.6, 136.9, 131.6, 130.3, 129.5, 128.5, 127.4, 126.8, 126.3, 126.0, 125.9, 120.9, 106.9, 71.4, 62.3, 54.4, 34.94, 34.92, 29.6, 28.9, 26.4;

IR (neat):  $\nu$  3712, 2267, 1789, 1632, 1554, 1318, 1225, 1114, 834, 754  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{34}\text{H}_{37}\text{BrNO}_2$ : 570.2002; found: 570.2008;



Yellow foam, isolated yield: 91% (52 mg);

dr = 1:1;

**5d-1:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.41-7.33 (m, 3H), 7.30 (t,  $J$  = 7.6 Hz, 2H), 7.25-7.19 (m, 2H), 6.90 (d,  $J$  = 2.8 Hz, 1H), 6.61 (d,  $J$  = 8.4 Hz, 1H), 6.56-6.45 (m, 2H), 6.44-6.31 (m, 2H), 5.78 (dd,  $J$  = 5.6, 1.6 Hz, 1H), 3.80 (d,  $J$  = 8.8 Hz, 1H), 3.08 (s, 3H), 1.10 (s, 9H), 1.06 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.6, 175.8, 147.8, 147.3, 142.5, 141.1, 139.7, 138.7, 136.8, 132.3, 131.8, 130.6, 130.0, 128.5(2C), 128.2, 127.5, 126.3, 114.5, 109.3, 69.4, 58.6, 56.5, 35.0, 34.7, 29.3, 29.3, 26.3;

IR (neat):  $\nu$  3659, 2312, 1758, 1636, 1541, 1392, 1254, 1147, 862, 785  $\text{cm}^{-1}$ ;

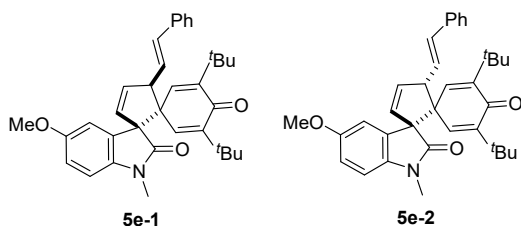
HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{34}\text{H}_{37}\text{BrNO}_2$ : 570.2002; found: 570.2006;

**5d-2:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.35 (dd,  $J$  = 8.4, 2.0 Hz, 1H), 7.33-7.21 (m, 1H), 7.26-7.14 (m, 4H), 7.12 (d,  $J$  = 2.0 Hz, 1H), 6.87 (d,  $J$  = 2.8 Hz, 1H), 6.77 (d,  $J$  = 2.8 Hz, 1H), 6.61 (d,  $J$  = 8.4 Hz, 1H), 6.50 (dd,  $J$  = 5.6, 1.6 Hz, 1H), 6.42 (d,  $J$  = 15.6 Hz, 1H), 5.91 (dd,  $J$  = 15.6, 7.6 Hz, 1H), 5.79 (dd,  $J$  = 5.6, 2.8 Hz, 1H), 4.51 (d,  $J$  = 7.6 Hz, 1H), 3.16 (s, 3H), 1.15 (s, 9H), 1.07 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.6, 175.4, 151.3, 148.1, 142.7, 139.6, 139.3, 138.7, 136.7, 131.82, 131.79, 131.0, 129.5, 129.0, 128.5, 127.5, 126.0, 125.8, 114.4, 109.1, 68.6, 60.3, 55.2, 35.1, 35.0, 29.6, 29.3, 26.3;

IR (neat):  $\nu$  3654, 2374, 1769, 1641, 1552, 1384, 1236, 1185, 841, 687  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{34}\text{H}_{37}\text{BrNO}_2$ : 570.2002; found: 570.2007;



Yellow foam, isolated yield: 93% (48 mg);

dr = 1:1;

**5e-1:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.37-7.27 (m, 4H), 7.24-7.20 (m, 1H), 6.97 (d,  $J$  = 2.8 Hz, 1H), 6.82-6.71 (m, 2H), 6.63 (d,  $J$  = 8.4 Hz, 1H), 6.48 (d,  $J$  = 2.8 Hz, 1H), 6.44-6.38 (m, 2H), 6.33 (dd,  $J$  = 5.6, 2.0 Hz, 1H), 5.83 (dd,  $J$  = 5.6, 2.0 Hz, 1H), 3.86-3.82 (m, 1H), 3.79 (s, 3H), 3.06 (s, 3H), 1.08 (s, 9H), 1.05 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.8, 175.8, 155.3, 147.3, 147.2, 141.3, 140.5, 137.8, 137.0, 136.9, 132.0, 131.4, 129.3, 128.5, 128.2, 127.4, 126.3, 113.6, 112.3, 108.1, 69.8, 58.1, 56.7, 55.8, 34.9, 34.6, 29.3, 29.2, 26.3;

IR (neat):  $\nu$  3736, 2249, 1742, 1665, 1565, 1331, 1214, 1132, 858, 763  $\text{cm}^{-1}$ ;

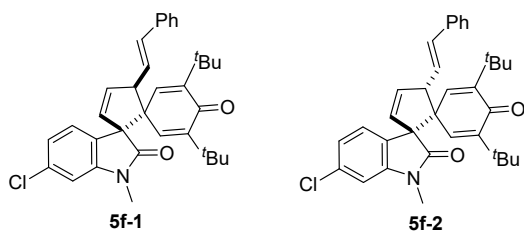
HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{35}\text{H}_{40}\text{NO}_3$ : 522.3003; found: 522.3006;

**5e-2:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.28-7.27 (m, 1H), 7.25-7.24 (m, 3H), 7.21-7.17 (m, 1H), 6.89 (d,  $J$  = 2.8 Hz, 1H), 6.82 (d,  $J$  = 2.8 Hz, 1H), 6.76-6.70 (m, 1H), 6.66-6.59 (m, 2H), 6.48 (dd,  $J$  = 5.6, 1.6 Hz, 1H), 6.45-6.37 (m, 1H), 5.92 (dd,  $J$  = 16.0, 7.6 Hz, 1H), 5.80 (dd,  $J$  = 5.6, 2.8 Hz, 1H), 4.57-4.47 (m, 1H), 3.73 (s, 3H), 3.15 (s, 3H), 1.12 (s, 9H), 1.08 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.7, 175.6, 155.0, 150.9, 147.6, 140.1, 139.3, 138.7, 137.1, 136.8, 131.6, 131.5, 128.5, 128.3, 127.4, 126.2, 126.0, 114.8, 112.4, 107.8, 69.0, 60.2, 55.7, 55.2, 35.0, 34.9, 29.6, 29.3, 26.3;

IR (neat):  $\nu$  3621, 2363, 1745, 1658, 1562, 1354, 1258, 1196, 825, 714  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{35}\text{H}_{40}\text{NO}_3$ : 522.3003; found: 522.3007;



Yellow solid, isolated yield: 95% (50 mg);

dr = 1:1;

mp: 176.5-176.9  $^{\circ}\text{C}$ ;

**5f-1**:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.36-7.27 (m, 4H), 7.24-7.19 (m, 1H), 7.03 (d,  $J$  = 8.0 Hz, 1H), 6.99 (dd,  $J$  = 8.0, 1.6 Hz, 1H), 6.94 (d,  $J$  = 2.8 Hz, 1H), 6.74 (d,  $J$  = 1.6 Hz, 1H), 6.46 (d,  $J$  = 2.8 Hz, 1H), 6.40 (d,  $J$  = 6.8 Hz, 2H), 6.34 (dd,  $J$  = 5.6, 2.4 Hz, 1H), 5.79 (dd,  $J$  = 5.6, 2.0 Hz, 1H), 3.86-3.79 (m, 1H), 3.08 (s, 3H), 1.08 (s, 9H), 1.06 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.6, 176.1, 147.55, 147.53, 144.6, 140.8, 140.0, 138.1, 136.8, 134.7, 132.2, 131.0, 128.5, 127.8, 127.5, 126.31, 126.26, 126.2, 121.6, 108.7, 69.0, 58.3, 56.7, 35.0, 34.7, 29.33, 29.27, 26.3;

IR (neat):  $\nu$  3716, 2246, 1774, 1632, 1564, 1396, 1231, 1195, 847, 736  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{34}\text{H}_{37}\text{ClNO}_2$ : 526.2507; found: 526.2512;

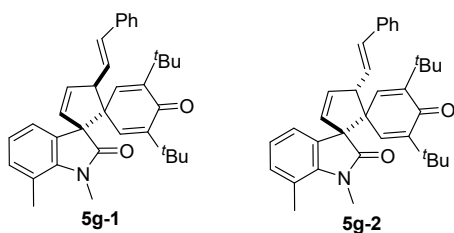
**5f-2**: mp: 178.6-179.1  $^{\circ}\text{C}$ ;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.38-7.32 (m, 1H), 7.30-7.27 (m, 1H), 7.25-7.17 (m, 4H), 7.12 (d,  $J$  = 2.0 Hz, 1H), 6.87 (d,  $J$  = 2.8 Hz, 1H), 6.77 (d,  $J$  = 2.8 Hz, 1H), 6.61 (d,  $J$  = 8.4 Hz, 1H), 6.50 (dd,  $J$  = 5.6, 1.6 Hz, 1H), 6.42 (d,  $J$  = 16.0 Hz, 1H), 5.91 (dd,  $J$  = 16.0, 7.6 Hz, 1H), 5.79 (dd,  $J$  = 5.6, 2.8 Hz, 1H), 4.55-4.47 (m, 1H), 3.16 (s, 3H), 1.15 (s, 9H), 1.07 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.6, 175.4, 151.3, 148.1, 142.7, 139.6, 139.3, 138.7, 136.7, 131.83, 131.80, 131.0, 129.5, 129.0, 128.5, 127.5, 126.0, 125.8, 114.4, 109.1, 68.6, 60.3, 55.2, 35.1, 35.0, 29.6, 29.4, 26.3;

IR (neat):  $\nu$  3656, 2284, 1714, 1662, 1575, 1369, 1287, 1136, 814, 687  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{34}\text{H}_{37}\text{ClNO}_2$ : 526.2507; found: 526.2512;



Yellow foam, isolated yield: 91% (46 mg);

dr = 1:1;

**5g-1**:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.35-7.28 (m, 4H), 7.24-7.18 (m, 1H), 7.01-6.93 (m, 3H), 6.90 (t,  $J$  = 7.6 Hz, 1H), 6.39-6.28 (m, 4H), 5.85 (dd,  $J$  = 5.6, 2.4 Hz, 1H), 3.88-3.85 (m, 1H), 3.35 (s, 3H), 2.48 (s, 3H), 1.11 (s, 9H), 1.01 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.8, 176.9, 147.4, 146.8, 141.2, 141.1, 141.0, 137.3, 136.8, 132.6, 131.9, 131.6, 128.6, 128.5, 127.7, 127.4, 126.2, 122.9, 121.7, 119.6, 69.3, 57.6, 57.0, 34.9, 34.6, 29.5, 29.3, 29.2, 18.9;

IR (neat):  $\nu$  3695, 2245, 1768, 1652, 1531, 1365, 1276, 1173, 795, 687  $\text{cm}^{-1}$ ;

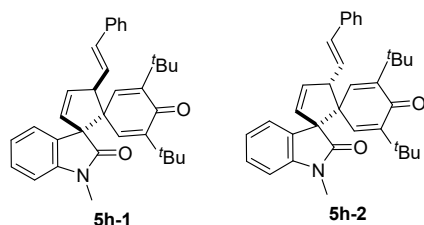
HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{35}\text{H}_{40}\text{NO}_2$ : 506.3054; found: 506.3056;

**5g-2:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.30-7.27 (m, 1H), 7.26-7.21 (m, 4H), 6.96-6.91 (m, 1H), 6.85 (d,  $J = 2.8$  Hz, 1H), 6.84-6.79 (m, 1H), 6.77 (d,  $J = 2.8$  Hz, 2H), 6.47 (dd,  $J = 5.6, 1.6$  Hz, 1H), 6.48-6.37 (m, 1H), 5.93 (dd,  $J = 15.6, 7.6$  Hz, 1H), 5.80 (dd,  $J = 5.6, 2.8$  Hz, 1H), 4.56-4.44 (m, 1H), 3.46 (s, 3H), 2.48 (s, 3H), 1.10 (s, 9H), 1.09 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.7, 176.7, 150.9, 147.4, 141.3, 140.3, 139.3, 138.6, 136.8, 132.8, 131.8, 131.5, 128.5 (2C), 127.4, 126.4, 126.0, 124.6, 121.5, 119.2, 68.4, 60.4, 55.0, 35.0, 34.9, 29.65, 29.59, 29.3, 19.0;

IR (neat):  $\nu$  3632, 2274, 1698, 1614, 1512, 1331, 1274, 1121, 884, 714  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{35}\text{H}_{40}\text{NO}_2$ : 506.3054; found: 506.3057;



Yellow foam, isolated yield: 92% (45 mg);

dr = 1:1;

**5h-1:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.37-7.27 (m, 5H), 7.25-7.18 (m, 1H), 7.13 (d,  $J = 7.2$  Hz, 1H), 7.05-6.93 (m, 2H), 6.73 (d,  $J = 7.6$  Hz, 1H), 6.45 (d,  $J = 2.8$  Hz, 1H), 6.40 (d,  $J = 5.6$  Hz, 2H), 6.36-6.29 (m, 1H), 5.92-5.78 (m, 1H), 3.95-3.78 (m, 1H), 3.09 (s, 3H), 1.09 (s, 9H), 1.03 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.8, 176.2, 147.4, 147.2, 143.5, 141.2, 140.6, 137.6, 136.9, 132.0, 131.5, 129.0, 128.5, 128.03, 128.01, 127.4, 126.3, 125.2, 121.8, 108.0, 69.5, 58.1, 56.8, 34.9, 34.7, 29.3, 29.2, 26.2;

IR (neat):  $\nu$  3696, 2271, 1754, 1635, 1554, 1357, 1236, 1158, 896, 787  $\text{cm}^{-1}$ ;

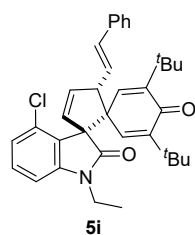
HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{34}\text{H}_{38}\text{NO}_2$ : 492.2897; found: 492.2899;

**5h-2:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.33-7.14 (m, 6H), 7.00 (d,  $J = 7.2$  Hz, 1H), 6.97-6.87 (m, 2H), 6.81 (d,  $J = 2.8$  Hz, 1H), 6.72 (d,  $J = 7.6$  Hz, 1H), 6.49 (dd,  $J = 5.6, 1.6$  Hz, 1H), 6.43 (d,  $J = 15.6$  Hz, 1H), 5.93 (dd,  $J = 15.6, 7.6$  Hz, 1H), 5.81 (dd,  $J = 5.6, 2.8$  Hz, 1H), 4.58-4.49 (m, 1H), 3.18 (s, 3H), 1.11 (s, 9H), 1.07 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.7, 176.0, 151.0, 147.5, 143.7, 140.2, 139.2, 138.7, 136.8, 131.7, 131.6, 129.1, 128.5, 127.4, 126.9, 126.6, 126.3, 126.0, 121.7, 107.7, 68.7, 60.3, 55.1, 35.0, 34.9, 29.5, 29.3, 26.2;

IR (neat):  $\nu$  3625, 2375, 1785, 1665, 1514, 1374, 1263, 1147, 868, 774  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{34}\text{H}_{38}\text{NO}_2$ : 492.2897; found: 492.2902;



Yellow solid, isolated yield: 91% (49 mg);

dr > 19:1;

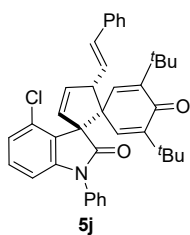
mp: 183.5-184.1  $^{\circ}\text{C}$ ;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.31-7.26 (m, 4H), 7.21 (d,  $J = 5.6$  Hz, 1H), 7.17-7.06 (m, 2H), 6.86 (d,  $J = 8.0$  Hz, 1H), 6.71-6.58 (m, 2H), 6.54-6.41 (m, 2H), 6.06 (s, 1H), 5.99 (dd,  $J = 15.6, 7.6$  Hz, 1H), 4.40 (d,  $J = 6.4$  Hz, 1H), 3.93-3.73 (m, 1H), 3.68-3.46 (m, 1H), 1.23 (t,  $J = 7.2$  Hz, 3H), 1.10 (s, 9H), 1.08 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.6, 175.1, 151.3, 146.7, 144.5, 139.1, 138.5, 137.6, 136.9, 132.2, 131.6, 130.1, 129.7, 128.5, 127.4, 126.3, 126.0, 124.4, 123.6, 106.5, 70.1, 62.3, 54.6, 35.3, 34.94, 34.89, 29.5, 28.9, 12.7;

IR (neat):  $\nu$  3654, 2296, 1687, 1601, 1563, 1347, 1269, 1135, 874, 764  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{35}\text{H}_{39}\text{ClNO}_2$ : 540.2664; found: 540.2668;



Yellow solid, isolated yield: 91% (54 mg);

dr > 19:1;

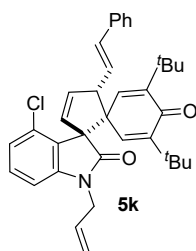
mp: 190.5-191.2 °C;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.53 (t,  $J$  = 7.6 Hz, 2H), 7.39 (t,  $J$  = 8.4 Hz, 3H), 7.29-7.27 (m, 3H), 7.25-7.18 (m, 3H), 7.07 (t,  $J$  = 8.0 Hz, 1H), 6.93 (d,  $J$  = 8.0 Hz, 1H), 6.75 (s, 1H), 6.64 (d,  $J$  = 8.0 Hz, 1H), 6.55 (d,  $J$  = 5.6 Hz, 1H), 6.43 (d,  $J$  = 15.6 Hz, 1H), 6.20-6.11 (m, 1H), 5.99 (dd,  $J$  = 15.6, 7.6 Hz, 1H), 4.41 (d,  $J$  = 7.6 Hz, 1H), 1.13 (s, 9H), 1.11 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.9, 174.6, 151.8, 147.0, 145.3, 139.3, 138.0, 137.9, 136.8, 133.8, 132.2, 131.7, 130.0, 129.8, 129.6, 128.5, 128.2, 127.5, 126.1, 126.02, 125.99, 124.33, 124.28, 107.9, 69.9, 62.9, 55.1, 35.1, 35.0, 29.6, 29.0;

IR (neat):  $\nu$  3667, 2296, 1754, 1665, 1547, 1368, 1274, 1136, 845, 769  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{39}\text{H}_{39}\text{ClNO}_2$ : 588.2664; found: 588.2667;



Yellow solid, isolated yield: 85% (47 mg);

dr > 19:1;

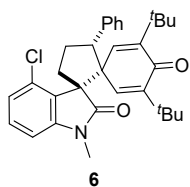
mp: 197.6-198.4 °C;

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.29-7.26 (m, 4H), 7.20 (t,  $J$  = 6.0 Hz, 1H), 7.16-7.04 (m, 2H), 6.86 (d,  $J$  = 8.0 Hz, 1H), 6.70-6.64 (m, 1H), 6.61 (d,  $J$  = 8.0 Hz, 1H), 6.50 (d,  $J$  = 5.6 Hz, 1H), 6.49-6.40 (m, 1H), 6.05 (dd,  $J$  = 5.6, 2.8 Hz, 1H), 5.99 (dd,  $J$  = 15.6, 7.6 Hz, 1H), 5.86-5.65 (m, 1H), 5.28-5.13 (m, 2H), 4.44-4.28 (m, 2H), 4.13 (dd,  $J$  = 16.0, 5.6 Hz, 1H), 1.11 (s, 9H), 1.07 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.6, 175.2, 151.3, 146.8, 144.6, 139.1, 138.5, 137.8, 136.8, 132.1, 131.7, 130.8, 130.1, 129.6, 128.5, 127.4, 126.2, 126.0, 124.3, 123.8, 118.8, 107.3, 70.0, 62.3, 54.8, 43.0, 35.0, 34.9, 29.5, 28.9 ;

IR (neat):  $\nu$  3696, 2285, 1675, 1636, 1547, 1352, 1247, 1154, 867, 727  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{36}\text{H}_{39}\text{ClNO}_2$ : 552.2664; found: 552.2664;



Compound **3b** (30 mg, 0.06 mmol, 1.0 equiv) was suspended in ethanol (0.4 mL) and treated with 5% palladium on charcoal (6 mg, 5%wt). The reaction mixture was stirred under an atmosphere of hydrogen at room temperature for 8 h. The solvent was removed under reduced pressure, and the residue was purified by column chromatography on silica gel using petroleum ether and ethyl acetate to give the final product.

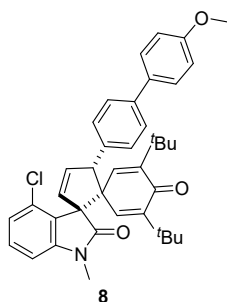
Yellow foam, isolated yield: 68% (21 mg);

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.16-7.07 (m, 6H), 6.93 (d,  $J$  = 2.8 Hz, 1H), 6.87 (d,  $J$  = 8.0 Hz, 1H), 6.58 (d,  $J$  = 7.2 Hz, 2H), 4.22-4.17 (m, 1H), 3.13 (s, 3H), 3.10-2.95 (m, 2H), 2.59-2.43 (m, 2H), 1.05 (s, 9H), 0.90 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.6, 179.8, 149.7, 146.5, 145.2, 140.6, 138.0, 137.7, 131.2, 129.6, 127.6, 127.5, 126.9, 126.1, 124.1, 106.3, 64.9, 60.1, 51.9, 34.80, 34.78, 29.4, 28.7, 28.5, 27.2, 26.3 ;

IR (neat):  $\nu$  3865, 2933, 1722, 1658, 1532, 1511, 1461, 1264, 1097, 802  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for:  $\text{C}_{32}\text{H}_{37}\text{ClNO}_2$ : 502.2507; found: 502.2502;



An oven-dried tube was charged with compound **3x** (15 mg, 0.026 mmol, 1.0 equiv), S-Phos (1 mg, 0.0026 mmol, 0.1 equiv), 4-methoxy-phenylboronic acid **7** (7.9 mg, 0.052 mmol, 2.0 equiv), anhydrous  $\text{K}_3\text{PO}_4$  (11 mg, 0.052 mmol, 2.0 equiv), and  $\text{Pd}(\text{OAc})_2$  (0.29 mg, 0.0013 mmol, 0.5 mol%). Anhydrous toluene (0.4 mL) was then added. The reaction mixture was stirred under nitrogen and heated at 60  $^\circ\text{C}$  during 4 h. The solvent was removed under reduced pressure, and the residue was purified by column chromatography on silica gel using petroleum ether and ethyl acetate to give the final product.

Yellow solid, isolated yield: 75% (12 mg);

mp: 215.2-215.9;

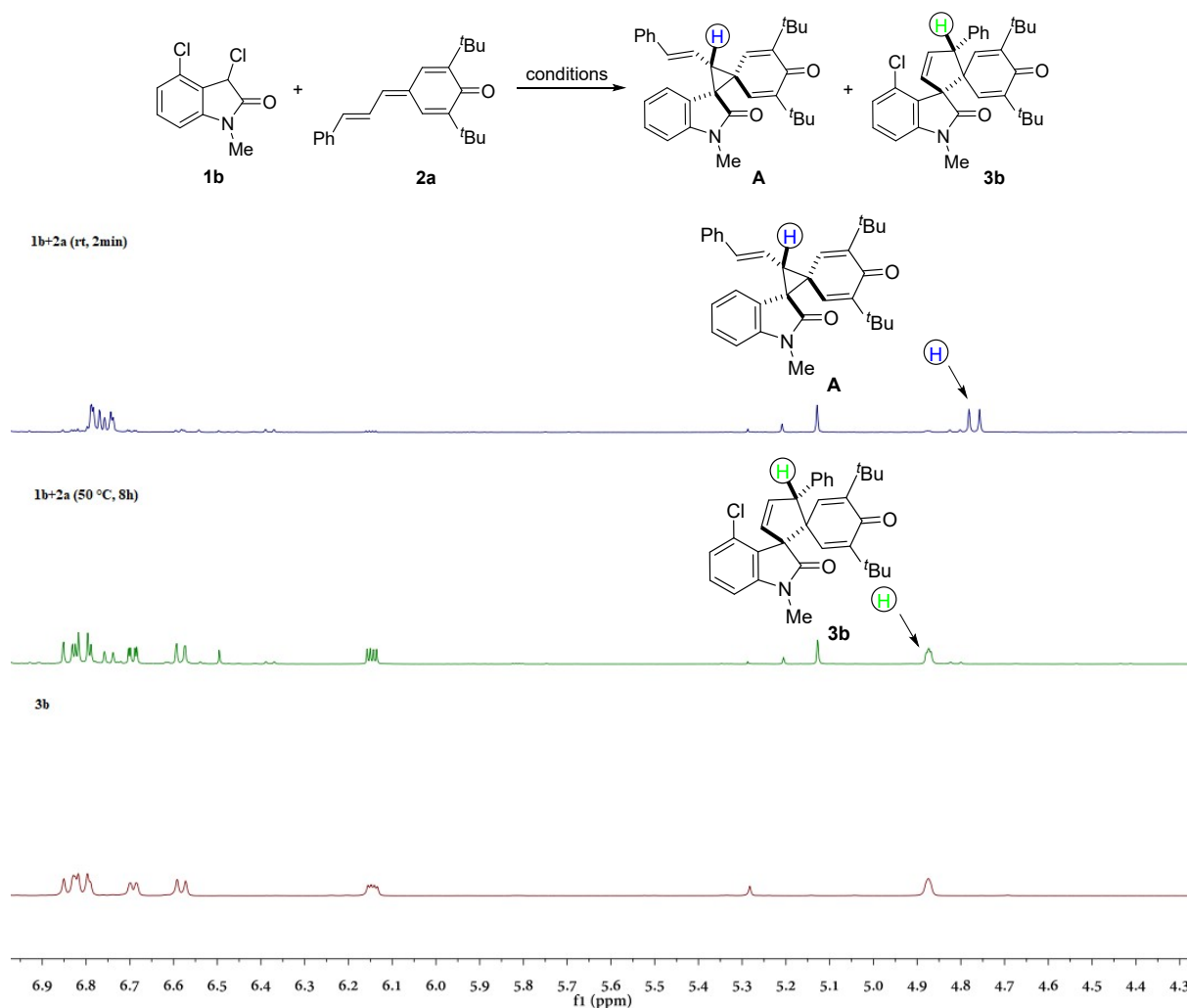
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.45-39 (m, 4H), 7.15-7.10 (m, 3H), 6.95 (d,  $J$  = 8.8 Hz, 2H), 6.87-6.83 (m, 3H), 6.78-6.72 (m, 1H), 6.60 (d,  $J$  = 7.6 Hz, 1H), 6.17 (dd,  $J$  = 5.8, 2.8 Hz, 1H), 4.91 (s, 1H), 3.83 (s, 3H), 3.17 (s, 3H), 1.14 (s, 9H), 0.77 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  186.2, 175.7, 159.1, 150.9, 145.9, 145.3, 139.8, 139.2, 139.0, 137.7, 136.8, 133.5, 132.0, 130.3, 130.2, 128.0, 127.5, 126.3, 124.5, 123.8, 114.2, 106.3, 70.6, 62.5, 56.4, 55.3, 35.0, 34.7, 29.6, 28.5, 26.5;

IR (neat):  $\nu$  3907, 3631, 2932, 1696, 1517, 1511, 1467, 1270, 1095, 757  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for:  $\text{C}_{39}\text{H}_{41}\text{ClNO}_3$ : 606.2769; found: 606.2764;

### 3. *in situ* $^1\text{H}$ NMR analysis



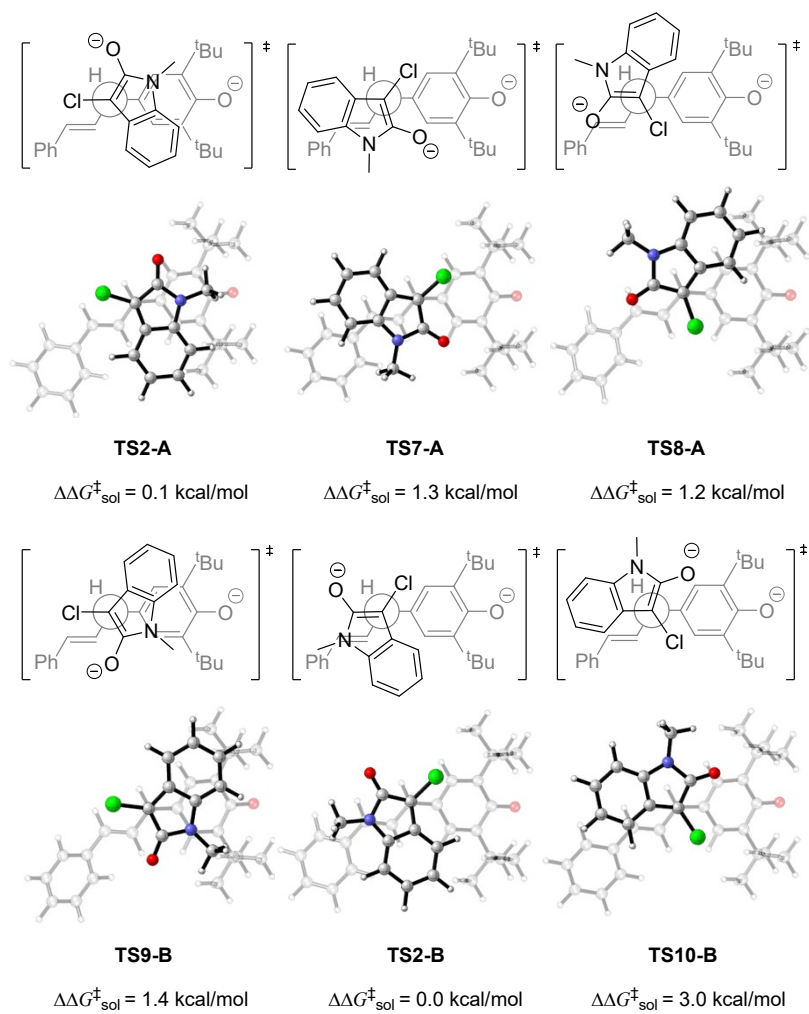
**Figure S1.** Monitoring the reaction pathway by  $^1\text{H}$  NMR.

### 4. DFT computational calculation studies

#### Computational details

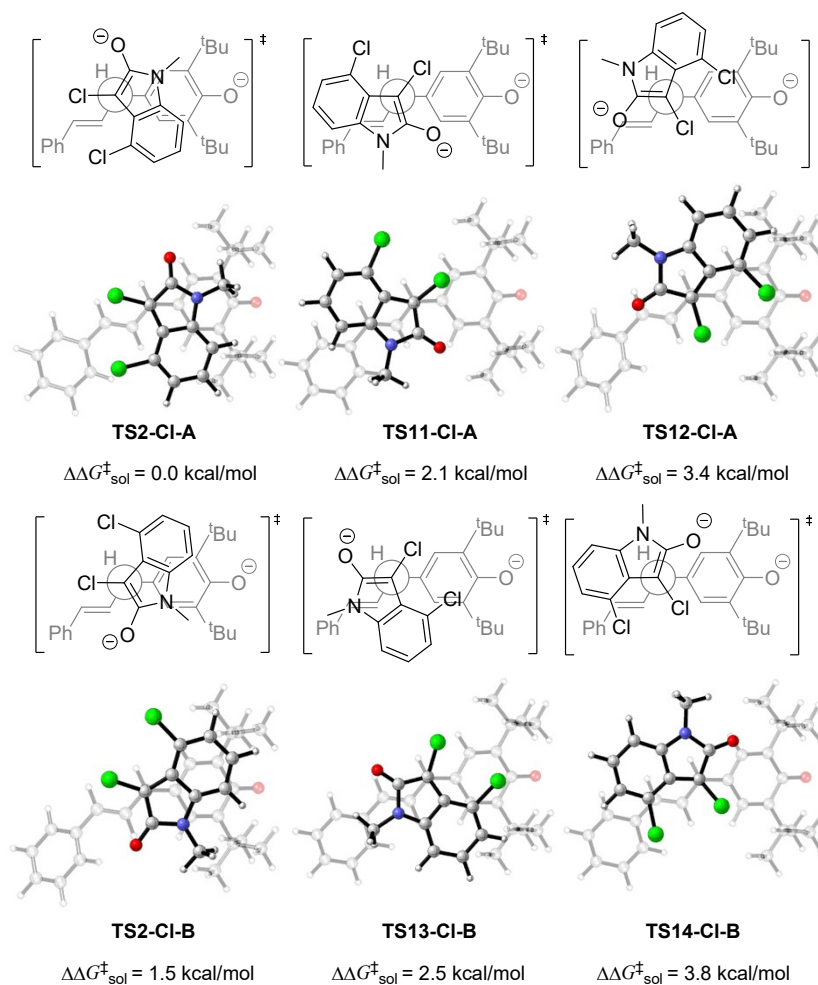
All the calculations were carried out with the Gaussian 16 package.[1] Geometry optimization and energy calculations were performed with (U)M06-2X. The 6-31G\* basis set was used for all the atoms. Frequency analysis was conducted at the same level of theory to verify the stationary points to be real minima or saddle points and to obtain the thermodynamic energy corrections. The single-point solvation energies were calculated at the (U)M06-2X/6-311+G\*\* level using SMD solvation model (solvent = chloroform). Computed structures are illustrated using CYLview.[2]

#### Structures and energies of 1,6-addition transition state for 1a



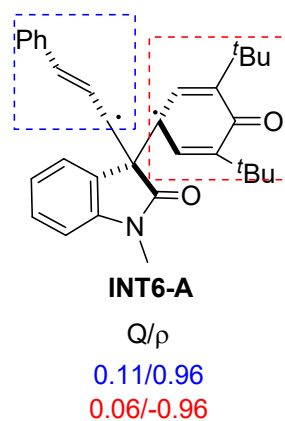
**Figure S2.** Structures and energies of 1,6-addition transition state for **1a**.

**Structures and energies of 1,6-addition transition state for 1b**



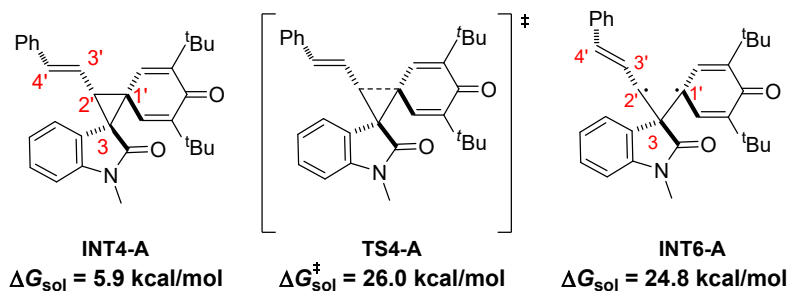
**Figure S3.** Structures and energies of 1,6-addition transition state for **1b**.

#### The diradical character of intermediate INT6-A



**Figure S4.** The Mulliken charges (Q) and spin densities ( $\rho$ ) on the diradical fragments (in blue and red) of intermediate **INT6-A**.

C1'-C2' bond cleavage:



C3-C2' bond cleavage:

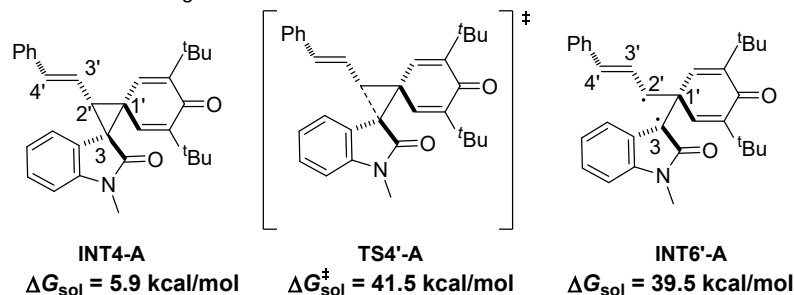


Figure S5. C1'-C2' and C3-C2' bond cleavages.

## Gibbs free energies of calculated structures

Table S1. Energies in Figure 1 and Figure 2. Zero-point correction (ZPE), thermal correction to energy (TCE), thermal correction to enthalpy (TCH), thermal correction to Gibbs free energy (TCG), and energies in solvation model ( $E_{\text{sol}}$ ), (in Hartree) of the structures calculated at the (U)M06-2X/6-311+G\*\*.-SMD(Chloroform)/(U)M06-2X/6-31G\* level of theory.

| Structures       | ZPVE     | TCE      | TCH      | TCG      | $E_{\text{sol}}$ | $G_{\text{sol}} (E_{\text{sol}} + \text{TCG})$ | Imaginary Frequency | $\Delta G_{\text{sol}}$ (kcal/mol) |
|------------------|----------|----------|----------|----------|------------------|------------------------------------------------|---------------------|------------------------------------|
| <b>1a</b>        | 0.155296 | 0.165329 | 0.166273 | 0.119047 | -937.9157701     | -937.7967231                                   | —                   | —                                  |
| <b>1b</b>        | 0.145538 | 0.156836 | 0.15778  | 0.107318 | -1397.516479     | -1397.409161                                   | —                   | —                                  |
| <b>2a</b>        | 0.455942 | 0.479863 | 0.480807 | 0.401884 | -968.3589718     | -967.9570878                                   | —                   | —                                  |
| <b>DBU</b>       | 0.250018 | 0.259671 | 0.260615 | 0.214899 | -462.0202553     | -461.8053563                                   | —                   | —                                  |
| <b>INT1</b>      | 0.406201 | 0.428015 | 0.428959 | 0.351575 | -1399.943058     | -1399.591483                                   | —                   | 6.6                                |
| <b>TS1</b>       | 0.402714 | 0.423688 | 0.424632 | 0.352008 | -1399.930323     | -1399.578315                                   | -630.92i            | 14.9                               |
| <b>INT2</b>      | 0.406064 | 0.42704  | 0.427984 | 0.356404 | -1399.946238     | -1399.589834                                   | —                   | 7.7                                |
| <b>TS2-A</b>     | 0.598586 | 0.632629 | 0.633574 | 0.534742 | -1905.789287     | -1905.254545                                   | -180.10i            | 27.7                               |
| <b>INT3-A</b>    | 0.600206 | 0.634398 | 0.635342 | 0.534544 | -1905.817432     | -1905.282888                                   | —                   | 9.9                                |
| <b>TS3-A</b>     | 0.599513 | 0.633602 | 0.634546 | 0.534184 | -1905.793263     | -1905.259079                                   | -280.65i            | 24.9                               |
| <b>INT4-A</b>    | 0.600814 | 0.633729 | 0.634673 | 0.535836 | -1445.467782     | -1444.931946                                   | —                   | 5.9                                |
| <b>INT5-A</b>    | 0.600728 | 0.633558 | 0.634503 | 0.536344 | -1445.467839     | -1444.931495                                   | —                   | 6.1                                |
| <b>TS4-A</b>     | 0.597251 | 0.630096 | 0.63104  | 0.532261 | -1445.432078     | -1444.899817                                   | -172.96i            | 26.0                               |
| <b>INT6-A</b>    | 0.597222 | 0.630678 | 0.631622 | 0.53115  | -1445.432949     | -1444.901799                                   | —                   | 24.8                               |
| <b>INT7-A</b>    | 0.597089 | 0.630412 | 0.631356 | 0.531573 | -1445.432579     | -1444.901006                                   | —                   | 25.3                               |
| <b>TS5-A</b>     | 0.597178 | 0.629446 | 0.630391 | 0.535791 | -1445.429037     | -1444.893246                                   | -41.20i             | 30.1                               |
| <b>3a</b>        | 0.601477 | 0.633577 | 0.634522 | 0.539228 | -1445.487094     | -1444.947866                                   | —                   | -4.1                               |
| <b>TS6-A</b>     | 0.597541 | 0.629890 | 0.630834 | 0.535453 | -1445.394095     | -1444.858642                                   | -220.18i            | 51.9                               |
| <b>TS7-A</b>     | 0.598181 | 0.632502 | 0.633446 | 0.532511 | -1905.785029     | -1905.252518                                   | -165.28i            | 29.0                               |
| <b>TS8-A</b>     | 0.597749 | 0.632285 | 0.633229 | 0.530543 | -1905.783127     | -1905.252584                                   | -217.70i            | 29.0                               |
| <b>TS9-B</b>     | 0.598748 | 0.632698 | 0.633642 | 0.535082 | -1905.787324     | -1905.252242                                   | -186.44i            | 29.2                               |
| <b>TS2-B</b>     | 0.598217 | 0.63258  | 0.633524 | 0.532076 | -1905.786764     | -1905.254688                                   | -222.17i            | 27.6                               |
| <b>TS10-B</b>    | 0.598218 | 0.632674 | 0.633618 | 0.531703 | -1905.781458     | -1905.249755                                   | -178.41i            | 30.7                               |
| <b>TS2-Cl-A</b>  | 0.588722 | 0.624148 | 0.625092 | 0.522069 | -2365.39224      | -2364.870171                                   | -187.43i            | 25.7                               |
| <b>TS11-Cl-A</b> | 0.588647 | 0.624187 | 0.625131 | 0.521056 | -2365.387932     | -2364.866876                                   | -290.15i            | 27.8                               |
| <b>TS12-Cl-A</b> | 0.588309 | 0.623923 | 0.624867 | 0.520709 | -2365.385426     | -2364.864717                                   | -292.79i            | 29.2                               |
| <b>TS2-Cl-B</b>  | 0.589075 | 0.624301 | 0.625246 | 0.523607 | -2365.391428     | -2364.867821                                   | -230.16i            | 27.2                               |
| <b>TS13-Cl-B</b> | 0.588739 | 0.624165 | 0.625109 | 0.522415 | -2365.388588     | -2364.866173                                   | -214.54i            | 28.2                               |
| <b>TS14-Cl-B</b> | 0.588703 | 0.624249 | 0.625193 | 0.521185 | -2365.385251     | -2364.864066                                   | -315.75i            | 29.6                               |
| <b>TS4'-A</b>    | 0.597127 | 0.629757 | 0.630701 | 0.533737 | -1445.408895     | -1444.875158                                   | -10.93i             | 41.5                               |
| <b>INT6'-A</b>   | 0.596963 | 0.630504 | 0.631448 | 0.530451 | -1445.408803     | -1444.878352                                   | —                   | 39.5                               |

## Cartesian Coordinates for Calculated Species

### 1a

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.77671400  | 0.68215300  | 0.01818000  |
| C  | 0.48285200  | -0.65474900 | 0.31368800  |
| C  | 1.48887400  | -1.60016800 | 0.35170500  |
| C  | 2.80317100  | -1.19359700 | 0.09718900  |
| C  | 3.08351600  | 0.13992200  | -0.18836700 |
| C  | 2.07245700  | 1.10469700  | -0.23360400 |
| C  | -1.50425700 | 0.67422000  | 0.30391700  |
| C  | -0.99279300 | -0.76335200 | 0.55253100  |
| H  | 1.25742100  | -2.64012000 | 0.56258500  |
| H  | 3.60693700  | -1.92139000 | 0.12006700  |
| H  | 4.10780000  | 0.44151200  | -0.38371800 |
| H  | 2.29534400  | 2.14200000  | -0.46103600 |
| O  | -2.64582800 | 1.05971900  | 0.35678700  |
| N  | -0.39525600 | 1.44568400  | 0.02486300  |
| C  | -0.46898800 | 2.85528800  | -0.27676700 |
| H  | 0.11618700  | 3.43469800  | 0.44429900  |
| H  | -0.09434600 | 3.05239100  | -1.28639200 |
| H  | -1.51834500 | 3.14541600  | -0.21344800 |
| Cl | -1.82575500 | -1.92106100 | -0.53020500 |
| H  | -1.24901700 | -1.06049300 | 1.57197900  |

**1b**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.53226700  | 1.17666000  | 0.02587200  |
| C  | -0.36139400 | 0.11513900  | -0.17409800 |
| C  | -1.71911000 | 0.35736400  | -0.12922100 |
| C  | -2.19285100 | 1.64602900  | 0.13334700  |
| C  | -1.28392800 | 2.67758300  | 0.34024500  |
| C  | 0.09702800  | 2.46625000  | 0.28534500  |
| C  | 1.88945000  | -0.62878000 | -0.39848200 |
| C  | 0.42720000  | -1.12970600 | -0.42844100 |
| H  | -3.26094500 | 1.82516000  | 0.17053200  |
| H  | -1.65866300 | 3.67550500  | 0.54373800  |
| H  | 0.79686700  | 3.28049700  | 0.43790900  |
| O  | 2.88435900  | -1.28101100 | -0.58961300 |
| N  | 1.84463500  | 0.71950900  | -0.10085600 |
| C  | 3.02608800  | 1.53760300  | 0.04039000  |
| H  | 3.03236700  | 2.33873200  | -0.70547400 |
| H  | 3.07162600  | 1.97528400  | 1.04243600  |
| H  | 3.88828600  | 0.88807200  | -0.11435500 |
| Cl | 0.21760300  | -2.38152000 | 0.83912300  |
| H  | 0.20686400  | -1.61134700 | -1.38287700 |
| Cl | -2.83832200 | -0.94019900 | -0.41199100 |

**2a**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.25625800 | -0.70391000 | -0.00011000 |
| C | -1.41544100 | -1.57531000 | -0.00004700 |
| C | -2.68640400 | -1.12142200 | -0.00012200 |
| C | -2.91372700 | 0.35484900  | -0.00054500 |
| C | -1.72770900 | 1.26766200  | -0.00019000 |
| C | -0.49083100 | 0.72701600  | -0.00010700 |
| H | -1.21050900 | -2.64206600 | 0.00011700  |
| H | 0.37738200  | 1.37517800  | 0.00000600  |
| O | -4.05251000 | 0.81289900  | -0.00006100 |
| C | -1.97057000 | 2.77699400  | -0.00009300 |
| C | -2.75582300 | 3.18463700  | -1.26100200 |
| C | -2.75554000 | 3.18453700  | 1.26102500  |
| C | -0.65044500 | 3.55713500  | -0.00020500 |
| H | -2.20177900 | 2.90736000  | -2.16466000 |
| H | -3.73627600 | 2.70935500  | -1.28841500 |
| H | -2.89335000 | 4.27190400  | -1.26883300 |
| H | -2.20133800 | 2.90710200  | 2.16453800  |
| H | -2.89297500 | 4.27181400  | 1.26902200  |
| H | -3.73602900 | 2.70933900  | 1.28857800  |
| H | -0.86863800 | 4.62955800  | 0.00001100  |
| H | -0.04907800 | 3.34038700  | 0.88977400  |
| H | -0.04940000 | 3.34069200  | -0.89047400 |
| C | -3.90153900 | -2.04822500 | 0.00005400  |
| C | -4.75110100 | -1.80189500 | 1.26099500  |
| C | -4.75155200 | -1.80175300 | -1.26055300 |
| C | -3.47958500 | -3.52213100 | -0.00009700 |
| H | -4.15895800 | -1.98529300 | 2.16441200  |
| H | -5.13096700 | -0.78043400 | 1.28945100  |
| H | -5.60214700 | -2.49243500 | 1.26829800  |
| H | -4.15976400 | -1.98515100 | -2.16420200 |
| H | -5.60266600 | -2.49221300 | -1.26757600 |
| H | -5.13133000 | -0.78025200 | -1.28880700 |
| H | -4.37509900 | -4.15134000 | 0.00024400  |
| H | -2.89379800 | -3.77782900 | -0.88999900 |
| H | -2.89311600 | -3.77780800 | 0.88936200  |
| C | 0.99000900  | -1.25970000 | -0.00005000 |
| C | 2.25617200  | -0.57457600 | -0.00002500 |
| H | 1.04729500  | -2.34862700 | -0.00001300 |
| H | 2.25714500  | 0.51156000  | -0.00006800 |
| C | 3.42653800  | -1.24625600 | 0.00004900  |
| H | 3.38552100  | -2.33591700 | 0.00007800  |
| C | 4.77324400  | -0.67531100 | 0.00009300  |
| C | 5.87318700  | -1.54465300 | 0.00008600  |
| C | 5.01837900  | 0.70719900  | 0.00015100  |
| C | 7.17447200  | -1.05562200 | 0.00012700  |
| H | 5.69811400  | -2.61749700 | 0.00004400  |
| C | 6.31686400  | 1.19596500  | 0.00019300  |
| H | 4.18849300  | 1.40694500  | 0.00017100  |
| C | 7.40097000  | 0.31763300  | 0.00018100  |
| H | 8.01124900  | -1.74700000 | 0.00011900  |

|   |            |            |            |
|---|------------|------------|------------|
| H | 6.48707200 | 2.26806100 | 0.00024000 |
| H | 8.41516400 | 0.70422000 | 0.00021600 |

## DBU

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.15053500 | 1.15983800  | 0.31376900  |
| C | -0.97697000 | 1.57420500  | -0.61997600 |
| C | -1.91949300 | -0.11997500 | 1.12631600  |
| C | -1.86122400 | -1.39089900 | 0.27361100  |
| C | -0.97063500 | -1.20032600 | -0.96227000 |
| H | -2.33595100 | 1.97656900  | 1.01757000  |
| H | -1.26906100 | 1.46446900  | -1.67041200 |
| H | -0.98243600 | -0.01519200 | 1.68704300  |
| H | -1.48866200 | -2.22299600 | 0.88355400  |
| H | -1.50696900 | -0.62095200 | -1.71885800 |
| H | -0.73751700 | -2.16480800 | -1.42592800 |
| C | 2.56827600  | 0.73117100  | 0.19362600  |
| C | 2.29234900  | -0.66200100 | 0.75472900  |
| C | 1.37659300  | -1.40361700 | -0.20878300 |
| C | 0.31833100  | 0.82173000  | -0.39386700 |
| H | 3.10371400  | 0.63969800  | -0.76385000 |
| H | 3.21465200  | -1.23086500 | 0.90537200  |
| H | 0.94359200  | -2.28556100 | 0.28063800  |
| N | 0.28804600  | -0.53825500 | -0.66003900 |
| N | 1.34194300  | 1.48676300  | -0.00244500 |
| H | -2.86711700 | -1.67170400 | -0.06289200 |
| H | -2.71410200 | -0.22221300 | 1.87320200  |
| H | -3.06855200 | 1.04942600  | -0.27660800 |
| H | -0.72590600 | 2.62468000  | -0.47141300 |
| H | 3.21918100  | 1.29730900  | 0.86684900  |
| H | 1.79839400  | -0.55682900 | 1.72771100  |
| H | 1.94666800  | -1.76134700 | -1.07752900 |

# INT1

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.27788000  | -2.33045300 | 0.09184300  |
| C  | 2.16634300  | -1.52031900 | -1.22960000 |
| C  | 3.04338900  | -1.64169800 | 1.22816200  |
| C  | 4.51329800  | -1.34064900 | 0.92721100  |
| C  | 4.68868800  | -0.63135200 | -0.42612700 |
| H  | 1.26615400  | -2.52848500 | 0.46078500  |
| H  | 2.86938900  | -1.90460400 | -1.97586900 |
| H  | 2.52916600  | -0.70396400 | 1.47036700  |
| H  | 4.92062900  | -0.71873800 | 1.73345900  |
| H  | 4.69605900  | -1.36653400 | -1.23450400 |
| H  | 5.65605600  | -0.12040700 | -0.47291700 |
| C  | 1.59502200  | 2.17048400  | -0.97749500 |
| C  | 2.57772800  | 2.38851300  | 0.16915100  |
| C  | 3.89418400  | 1.70367000  | -0.16819900 |
| C  | 2.38309900  | -0.03333600 | -1.05134200 |
| H  | 1.96889900  | 2.65933700  | -1.88968400 |
| H  | 2.74733300  | 3.45272400  | 0.35594800  |
| H  | 4.52110700  | 1.61836600  | 0.72850500  |
| N  | 3.65742000  | 0.35905200  | -0.69493100 |
| N  | 1.38418500  | 0.75215900  | -1.23497000 |
| H  | 5.10382500  | -2.26513600 | 0.91471700  |
| H  | 2.97909300  | -2.26520700 | 2.12651900  |
| H  | 2.73071000  | -3.30664600 | -0.12006000 |
| H  | 1.16768500  | -1.62915900 | -1.65690400 |
| H  | 0.62708300  | 2.62063900  | -0.73594700 |
| H  | 2.14951400  | 1.95056900  | 1.07815200  |
| H  | 4.45681700  | 2.29277700  | -0.90562400 |
| C  | -3.59931600 | -0.08023800 | -0.15081900 |
| C  | -2.37722400 | -0.75677300 | -0.04519800 |
| C  | -2.33046900 | -2.13125800 | -0.17044100 |
| C  | -3.52102100 | -2.82825500 | -0.40587800 |
| C  | -4.72759600 | -2.14249500 | -0.51410900 |
| C  | -4.78836600 | -0.75093100 | -0.38864000 |
| C  | -2.07240600 | 1.58943900  | 0.24955500  |
| C  | -1.30048200 | 0.26015900  | 0.17133700  |
| H  | -1.38517000 | -2.65822500 | -0.07498400 |
| H  | -3.50370900 | -3.90844000 | -0.50356800 |
| H  | -5.64347200 | -2.69547900 | -0.69795500 |
| H  | -5.73128100 | -0.22007600 | -0.47097400 |
| O  | -1.61968400 | 2.69273600  | 0.45085600  |
| N  | -3.40014500 | 1.29434700  | 0.01663500  |
| C  | -4.44329000 | 2.29062200  | 0.00288600  |
| H  | -4.95081400 | 2.30418600  | -0.96697200 |
| H  | -5.17756100 | 2.09046700  | 0.79014000  |
| H  | -3.97018100 | 3.25683300  | 0.18171400  |
| Cl | -0.34647800 | 0.00349700  | 1.67105200  |
| H  | -0.54672200 | 0.31420000  | -0.62998500 |

# TS1

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.95624300 | 2.27844200  | 0.30691800  |
| C  | -1.40410100 | 1.44685500  | -0.88652300 |
| C  | -3.07282100 | 1.61597000  | 1.12219200  |
| C  | -4.37997900 | 1.40436600  | 0.35204500  |
| C  | -4.13369300 | 0.80238900  | -1.03664000 |
| H  | -1.12504400 | 2.47456200  | 0.98905100  |
| H  | -1.70911300 | 1.88737200  | -1.84176600 |
| H  | -2.70392200 | 0.65436800  | 1.49896200  |
| H  | -5.04296500 | 0.75154800  | 0.93202400  |
| H  | -3.78221800 | 1.57259700  | -1.72742800 |
| H  | -5.05379900 | 0.39595700  | -1.46585200 |
| C  | -1.26802200 | -2.32786900 | -0.61892900 |
| C  | -2.63875600 | -2.44890400 | 0.03333700  |
| C  | -3.64985200 | -1.63985800 | -0.76779900 |
| C  | -1.83816900 | 0.00153300  | -0.88686600 |
| H  | -1.25981500 | -2.81473600 | -1.60180800 |
| H  | -2.95578500 | -3.49335900 | 0.08398900  |
| H  | -4.59646900 | -1.55516800 | -0.22416500 |
| N  | -3.15192200 | -0.27935700 | -1.00248000 |
| N  | -0.92268800 | -0.91691000 | -0.77827400 |
| H  | -4.90874500 | 2.35587400  | 0.22070800  |
| H  | -3.27334000 | 2.22796300  | 2.00711800  |
| H  | -2.29884700 | 3.25062500  | -0.06573000 |
| H  | -0.31103700 | 1.45823400  | -0.87891200 |
| H  | -0.48299000 | -2.77774400 | -0.00446600 |
| H  | -2.57883200 | -2.06061100 | 1.05617600  |
| H  | -3.85912300 | -2.12035600 | -1.73169700 |
| C  | 3.20601600  | 0.14200200  | -0.33944100 |
| C  | 2.09561200  | 0.75801600  | 0.28624700  |
| C  | 2.02627500  | 2.14458600  | 0.32732800  |
| C  | 3.03844800  | 2.89800300  | -0.27837700 |
| C  | 4.10530900  | 2.27410500  | -0.91984600 |
| C  | 4.20434900  | 0.87824600  | -0.95589700 |
| C  | 1.95964700  | -1.57171900 | 0.55555600  |
| C  | 1.21242300  | -0.31777900 | 0.70997800  |
| H  | 1.20801700  | 2.63503900  | 0.84958200  |
| H  | 2.99304100  | 3.98211900  | -0.24184300 |
| H  | 4.87911400  | 2.87415300  | -1.38831300 |
| H  | 5.04607900  | 0.38846700  | -1.43669500 |
| O  | 1.67046700  | -2.71929100 | 0.87785700  |
| N  | 3.09271100  | -1.23449900 | -0.19577800 |
| C  | 4.05241500  | -2.20562900 | -0.65086700 |
| H  | 4.14384700  | -2.18750900 | -1.74265400 |
| H  | 5.03806400  | -2.01708900 | -0.21040300 |
| H  | 3.69242900  | -3.18419500 | -0.32918600 |
| Cl | 0.17572100  | -0.12525500 | 2.13269900  |
| H  | 0.11060700  | -0.59561200 | -0.30420700 |

## INT2

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.18147700  | -1.52435900 | -1.31080900 |
| C  | 1.08817200  | -0.39581200 | -1.88184500 |
| C  | 0.60475200  | -2.05750300 | 0.06235800  |
| C  | 1.91190900  | -2.85833400 | 0.02429500  |
| C  | 2.97581100  | -2.16583000 | -0.83635300 |
| H  | -0.83998900 | -1.14362300 | -1.22668000 |
| H  | 1.61260000  | -0.73922800 | -2.78065700 |
| H  | 0.70710400  | -1.21096300 | 0.75304900  |
| H  | 2.28966800  | -2.99882400 | 1.04440400  |
| H  | 2.73349500  | -2.28145100 | -1.89634700 |
| H  | 3.95958100  | -2.62293500 | -0.69461500 |
| C  | 3.02166700  | 1.87439800  | 0.42208700  |
| C  | 3.53535100  | 0.77766500  | 1.34765800  |
| C  | 4.06800100  | -0.37298800 | 0.50722500  |
| C  | 2.12783000  | 0.12993600  | -0.91363300 |
| H  | 3.85847000  | 2.33222400  | -0.12366300 |
| H  | 4.32243200  | 1.15482800  | 2.00670600  |
| H  | 4.24917400  | -1.25228800 | 1.13450300  |
| N  | 3.10275500  | -0.74532800 | -0.52765700 |
| N  | 2.04860500  | 1.36268800  | -0.53242000 |
| H  | 1.73670600  | -3.85872100 | -0.39068600 |
| H  | -0.19904500 | -2.67944800 | 0.46922400  |
| H  | 0.14600800  | -2.35597700 | -2.02565200 |
| H  | 0.48679300  | 0.46217900  | -2.18704600 |
| H  | 2.53594300  | 2.66804900  | 0.99700300  |
| H  | 2.70705500  | 0.42204900  | 1.96922300  |
| H  | 5.02203500  | -0.10032700 | 0.03662700  |
| C  | -2.85955400 | 0.18867800  | -0.34024300 |
| C  | -2.20152800 | 0.06154800  | 0.90941100  |
| C  | -2.70202300 | -0.83710000 | 1.85760900  |
| C  | -3.83154200 | -1.57939700 | 1.54281600  |
| C  | -4.47195700 | -1.44082400 | 0.30022400  |
| C  | -3.99530100 | -0.55439300 | -0.65726400 |
| C  | -1.08661300 | 1.57711000  | -0.36926700 |
| C  | -1.09105700 | 0.95856300  | 0.86068600  |
| H  | -2.20967500 | -0.94295500 | 2.81985600  |
| H  | -4.23068100 | -2.27971800 | 2.26993300  |
| H  | -5.35347700 | -2.03565300 | 0.08344500  |
| H  | -4.48787900 | -0.44459400 | -1.61904100 |
| O  | -0.26040200 | 2.45313000  | -0.91723300 |
| N  | -2.16507700 | 1.10817800  | -1.10009600 |
| C  | -2.47274600 | 1.49020600  | -2.45745000 |
| H  | -2.44397300 | 0.61706700  | -3.11895900 |
| H  | -3.46552700 | 1.94752400  | -2.51470900 |
| H  | -1.72375400 | 2.21460500  | -2.77795700 |
| Cl | 0.01355900  | 1.27519100  | 2.15211500  |
| H  | 0.71977100  | 2.11673800  | -0.75986000 |

## TS2-A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.59310600 | -0.36019300 | -0.83855700 |
| C | -1.76195900 | -1.14326100 | -1.08371300 |
| C | -3.02142000 | -0.61620800 | -1.12242300 |
| C | -3.20495300 | 0.83001000  | -0.92052400 |
| C | -2.01267000 | 1.62597000  | -0.58216800 |
| C | -0.78318000 | 1.02590200  | -0.55613500 |
| H | -1.60588200 | -2.20792100 | -1.22764300 |
| H | 0.08864500  | 1.61510600  | -0.29033800 |
| O | -4.33338800 | 1.36115100  | -1.01839200 |
| C | -2.19633000 | 3.11269000  | -0.26518300 |
| C | -0.87100200 | 3.79272300  | 0.09743500  |
| C | -2.78267000 | 3.84483100  | -1.48637400 |
| C | -3.14597900 | 3.27245400  | 0.93602600  |
| H | -0.40094800 | 3.32830100  | 0.97223600  |
| H | -0.15785400 | 3.75802200  | -0.73435900 |
| H | -1.05918800 | 4.84724700  | 0.33147200  |
| H | -3.74443300 | 3.41205800  | -1.76373400 |
| H | -2.91689300 | 4.91024300  | -1.25685900 |
| H | -2.09812600 | 3.76469200  | -2.33891100 |
| H | -4.11065200 | 2.80921700  | 0.72418000  |
| H | -2.70947200 | 2.80044200  | 1.82465800  |
| H | -3.29926600 | 4.33665100  | 1.15834400  |
| C | -4.25469300 | -1.48662600 | -1.37597300 |
| C | -5.25359800 | -1.34126500 | -0.21277900 |
| C | -4.93638700 | -1.06032400 | -2.68817100 |
| C | -3.88424600 | -2.97067200 | -1.48325700 |
| H | -4.80670500 | -1.70176500 | 0.72071800  |
| H | -5.54782000 | -0.29873400 | -0.08739200 |
| H | -6.14808000 | -1.94577200 | -0.41222000 |
| H | -4.24751600 | -1.18762900 | -3.53137300 |
| H | -5.82126800 | -1.68353600 | -2.87380500 |
| H | -5.23942000 | -0.01356000 | -2.63472000 |
| H | -4.79743000 | -3.56425200 | -1.60925600 |
| H | -3.23895700 | -3.16440200 | -2.34778200 |
| H | -3.36375500 | -3.32162500 | -0.58466700 |
| C | 0.66257000  | -0.99455900 | -0.82537000 |
| C | 1.91390900  | -0.26837400 | -0.94116500 |
| H | 1.91148800  | 0.77559900  | -0.63822800 |
| C | 3.05890800  | -0.81600200 | -1.38660300 |
| H | 3.04722400  | -1.85054500 | -1.72581700 |
| C | 4.34987600  | -0.12357300 | -1.47472600 |
| C | 5.36648900  | -0.65703100 | -2.27928000 |
| C | 4.62077400  | 1.06090700  | -0.76967500 |
| C | 6.59887700  | -0.02390800 | -2.39901900 |
| H | 5.17607300  | -1.58044100 | -2.82065100 |
| C | 5.85069600  | 1.69477200  | -0.89149100 |
| H | 3.86810100  | 1.46861600  | -0.10024900 |
| C | 6.84622400  | 1.15936300  | -1.70839000 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 7.36817400  | -0.45666300 | -3.03241300 |
| H  | 6.03892700  | 2.60808100  | -0.33428100 |
| H  | 7.80835400  | 1.65527000  | -1.79637800 |
| H  | 0.68616100  | -2.03801300 | -1.13981700 |
| C  | 0.09368700  | -0.09921700 | 2.37146900  |
| C  | 1.36709700  | -0.57834300 | 1.97006200  |
| C  | 2.49327700  | 0.21631700  | 2.16266100  |
| C  | 2.33696600  | 1.48282600  | 2.73497300  |
| C  | 1.07582900  | 1.94946200  | 3.10971200  |
| C  | -0.06614400 | 1.15665300  | 2.93524100  |
| C  | -0.27008800 | -2.19334600 | 1.49600900  |
| C  | 1.11983400  | -1.82087300 | 1.30103500  |
| H  | 3.47172500  | -0.14826700 | 1.85907500  |
| H  | 3.21009600  | 2.11097400  | 2.89026700  |
| H  | 0.97259400  | 2.93995000  | 3.54338000  |
| H  | -1.04931200 | 1.51648300  | 3.22520900  |
| O  | -0.89262100 | -3.18790100 | 1.13418200  |
| N  | -0.85340400 | -1.07462500 | 2.10568400  |
| C  | -2.27386600 | -0.91330800 | 2.26747300  |
| H  | -2.63356800 | -0.05258600 | 1.69011100  |
| H  | -2.74056100 | -1.82251200 | 1.88374200  |
| H  | -2.53506400 | -0.78125200 | 3.32457100  |
| Cl | 2.33824600  | -3.01458100 | 0.99530000  |

## INT3-A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.34082000 | -0.63440200 | -0.48599800 |
| C | -1.39927000 | -1.51844400 | -0.73401300 |
| C | -2.65074000 | -1.10053200 | -1.15860100 |
| C | -2.90999000 | 0.31290200  | -1.38134700 |
| C | -1.80017800 | 1.22080600  | -1.13731800 |
| C | -0.57883300 | 0.72983300  | -0.69959400 |
| H | -1.21936200 | -2.57480900 | -0.54893900 |
| H | 0.22004400  | 1.43673700  | -0.48545800 |
| O | -4.04702500 | 0.73306500  | -1.76600600 |
| C | -2.02365000 | 2.71957100  | -1.36401000 |
| C | -0.76570300 | 3.55204200  | -1.09112800 |
| C | -2.44394500 | 2.97048900  | -2.82375500 |
| C | -3.13148200 | 3.22088400  | -0.41987100 |
| H | -0.42840900 | 3.45292800  | -0.05266900 |
| H | 0.06154300  | 3.26002500  | -1.74921700 |
| H | -0.98415300 | 4.61121100  | -1.27612000 |
| H | -3.33973800 | 2.39128900  | -3.05217200 |
| H | -2.64362800 | 4.03909000  | -2.98509900 |
| H | -1.63880500 | 2.66772000  | -3.50394800 |
| H | -4.04045700 | 2.63926200  | -0.58286300 |
| H | -2.80981600 | 3.10832200  | 0.62363300  |
| H | -3.33930900 | 4.28512500  | -0.59888800 |
| C | -3.78567000 | -2.09994200 | -1.40398600 |
| C | -4.98571800 | -1.76304800 | -0.49958300 |
| C | -4.22757800 | -2.02793000 | -2.87649500 |
| C | -3.36821300 | -3.54307000 | -1.09971700 |
| H | -4.71456300 | -1.89768400 | 0.55492700  |
| H | -5.29129500 | -0.72871900 | -0.66456200 |
| H | -5.82780900 | -2.43448200 | -0.71751400 |
| H | -3.39801500 | -2.31545400 | -3.53336700 |
| H | -5.06434300 | -2.71625000 | -3.06027200 |
| H | -4.53420400 | -1.00826700 | -3.11582400 |
| H | -4.22065000 | -4.21252200 | -1.26897900 |
| H | -2.54839300 | -3.87322800 | -1.74827200 |
| H | -3.04575400 | -3.65788900 | -0.05792900 |
| C | 0.92804100  | -1.15023100 | 0.16903600  |
| C | 2.18084800  | -0.54080100 | -0.39210500 |
| H | 2.12770900  | 0.52064000  | -0.62666800 |
| C | 3.30838400  | -1.22035600 | -0.62323600 |
| H | 3.32532900  | -2.28802500 | -0.40414400 |
| C | 4.56131700  | -0.66799200 | -1.16520900 |
| C | 5.57773600  | -1.54450400 | -1.56583700 |
| C | 4.79614000  | 0.70956900  | -1.29034800 |
| C | 6.77766600  | -1.07072700 | -2.08664600 |
| H | 5.41483400  | -2.61500200 | -1.46838800 |
| C | 5.99220800  | 1.18505400  | -1.81205200 |
| H | 4.03682100  | 1.41541500  | -0.96687700 |
| C | 6.99051600  | 0.29848900  | -2.21495600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 7.54735900  | -1.77368400 | -2.39254700 |
| H  | 6.14970500  | 2.25625600  | -1.89988200 |
| H  | 7.92568800  | 0.67357800  | -2.61989200 |
| H  | 0.96998000  | -2.24099500 | 0.05393300  |
| C  | -0.53959200 | 0.80177400  | 2.45846100  |
| C  | 0.78849600  | 0.50952400  | 2.12325500  |
| C  | 1.74366200  | 1.50614500  | 2.10263400  |
| C  | 1.35502800  | 2.81674500  | 2.40803000  |
| C  | 0.02659800  | 3.10003200  | 2.71524500  |
| C  | -0.94519900 | 2.09510300  | 2.74911100  |
| C  | -0.53762300 | -1.46665200 | 2.15665600  |
| C  | 0.84859800  | -0.93600200 | 1.72948100  |
| H  | 2.77413200  | 1.26753100  | 1.85155300  |
| H  | 2.08934000  | 3.61569200  | 2.39517700  |
| H  | -0.26763100 | 4.12347600  | 2.92910500  |
| H  | -1.98069900 | 2.32120700  | 2.98139600  |
| O  | -0.90313500 | -2.61810700 | 2.15465000  |
| N  | -1.30623400 | -0.36296800 | 2.46325400  |
| C  | -2.75159800 | -0.39163800 | 2.46194600  |
| H  | -3.12804900 | 0.19899700  | 1.61832800  |
| H  | -3.05084200 | -1.43249200 | 2.33190300  |
| H  | -3.15229700 | -0.00784400 | 3.40640600  |
| Cl | 2.15494300  | -1.84248200 | 2.57611200  |

## TS3-A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.38401800  | -0.05780600 | -0.99328900 |
| C | 1.65561100  | 0.09703500  | -1.59187000 |
| C | 2.74659600  | -0.66419000 | -1.24308100 |
| C | 2.60899300  | -1.71716100 | -0.23716100 |
| C | 1.27044400  | -1.93096700 | 0.31912900  |
| C | 0.23380400  | -1.12154100 | -0.07350400 |
| H | 1.75850000  | 0.87699600  | -2.33851700 |
| H | -0.75551200 | -1.27997600 | 0.34670200  |
| O | 3.59239200  | -2.41080900 | 0.13141800  |
| C | 1.07656800  | -3.03239500 | 1.36407400  |
| C | -0.38073500 | -3.14226800 | 1.82739800  |
| C | 1.49140600  | -4.39654500 | 0.78479500  |
| C | 1.93535600  | -2.71099800 | 2.60131500  |
| H | -0.72454700 | -2.21421100 | 2.29936500  |
| H | -1.05531400 | -3.37665200 | 0.99502200  |
| H | -0.46642200 | -3.94815900 | 2.56602800  |
| H | 2.52977800  | -4.36273700 | 0.45303400  |
| H | 1.37707400  | -5.18092300 | 1.54505200  |
| H | 0.85335700  | -4.65497700 | -0.06886400 |
| H | 2.98637600  | -2.63796100 | 2.31762000  |
| H | 1.61510100  | -1.75795100 | 3.03976400  |
| H | 1.81779300  | -3.49666300 | 3.36013000  |
| C | 4.12239600  | -0.41976600 | -1.86853400 |
| C | 5.12510300  | -0.02402300 | -0.76869200 |
| C | 4.61723900  | -1.69393100 | -2.57554700 |
| C | 4.09344500  | 0.71434600  | -2.89977200 |
| H | 4.81305100  | 0.91609700  | -0.29762900 |
| H | 5.17560200  | -0.80401600 | -0.00791200 |
| H | 6.12306100  | 0.12799200  | -1.20166900 |
| H | 3.93371600  | -1.96414300 | -3.38907200 |
| H | 5.61276300  | -1.52608100 | -3.00818600 |
| H | 4.66661500  | -2.52057400 | -1.86559800 |
| H | 5.10297400  | 0.86736400  | -3.29975500 |
| H | 3.43167000  | 0.47851500  | -3.74121500 |
| H | 3.75395600  | 1.65819600  | -2.45727100 |
| C | -0.78205400 | 0.82445100  | -1.35632300 |
| C | -2.10105500 | 0.11600900  | -1.40456000 |
| H | -2.07560300 | -0.77978300 | -2.02682900 |
| C | -3.23824900 | 0.46132700  | -0.79403800 |
| H | -3.27372200 | 1.38889700  | -0.22635100 |
| C | -4.48950700 | -0.31401200 | -0.87231600 |
| C | -5.71636700 | 0.33649300  | -0.68676900 |
| C | -4.50253300 | -1.69533400 | -1.11194800 |
| C | -6.91744400 | -0.36001200 | -0.76974200 |
| H | -5.71725700 | 1.40473200  | -0.48586900 |
| C | -5.70218300 | -2.39241400 | -1.19649100 |
| H | -3.55972200 | -2.22699900 | -1.20686200 |
| C | -6.91625200 | -1.72824400 | -1.02982900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -7.85701200 | 0.16700700  | -0.62939200 |
| H  | -5.68898400 | -3.46320300 | -1.37900900 |
| H  | -7.85235300 | -2.27555300 | -1.09047600 |
| H  | -0.58518700 | 1.34709900  | -2.30061200 |
| C  | 0.71996900  | 1.98755900  | 1.76293700  |
| C  | -0.43161100 | 1.40316100  | 1.20869500  |
| C  | -1.30521600 | 0.71106500  | 2.03162100  |
| C  | -1.00732300 | 0.58679800  | 3.39190900  |
| C  | 0.14751400  | 1.15761100  | 3.92073900  |
| C  | 1.03013500  | 1.87404100  | 3.10926100  |
| C  | 0.83882100  | 2.55592200  | -0.45413300 |
| C  | -0.43447000 | 1.72706200  | -0.24541900 |
| H  | -2.20166400 | 0.25642400  | 1.62335500  |
| H  | -1.68297600 | 0.03523700  | 4.03800900  |
| H  | 0.36883300  | 1.04690000  | 4.97815800  |
| H  | 1.93175500  | 2.32123200  | 3.51563400  |
| O  | 1.24736100  | 3.04561300  | -1.48378500 |
| N  | 1.44594200  | 2.65382400  | 0.78040600  |
| C  | 2.70406000  | 3.32023400  | 0.98653700  |
| H  | 3.44585300  | 2.62010400  | 1.38550600  |
| H  | 3.03522300  | 3.68734800  | 0.01400700  |
| H  | 2.59227900  | 4.16329800  | 1.67776200  |
| Cl | -1.73691300 | 3.44840500  | -0.27001800 |

**INT4-A**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.01209500 | 3.54211300  | 0.69123900  |
| C | -0.48758300 | 2.22274200  | 0.81547800  |
| C | -1.20295900 | 1.88230800  | 1.95543500  |
| C | -1.40989100 | 2.84004100  | 2.95413600  |
| C | -0.91161000 | 4.13031800  | 2.81540400  |
| C | -0.20506100 | 4.50296300  | 1.67005500  |
| C | 0.57888800  | 2.56118700  | -1.28904400 |
| C | -0.07368900 | 1.50441000  | -0.42325700 |
| H | -1.62079400 | 0.89123100  | 2.09287300  |
| H | -1.96892300 | 2.56790900  | 3.84287600  |
| H | -1.07828900 | 4.86142600  | 3.59987400  |
| H | 0.17547900  | 5.51171300  | 1.54690000  |
| O | 0.96913600  | 2.45160200  | -2.43547200 |
| N | 0.62930000  | 3.71155500  | -0.53726100 |
| C | 1.16202400  | 4.95943500  | -1.02955900 |
| H | 0.37854700  | 5.72322500  | -1.07078100 |
| H | 1.97384900  | 5.31072800  | -0.38534500 |
| H | 1.54498000  | 4.77462800  | -2.03362300 |
| C | 0.54509900  | 0.06769000  | -0.44990900 |
| C | 1.71198900  | -0.16974400 | -1.31156800 |
| C | 2.72236000  | -0.99262500 | -0.97951200 |
| C | 2.67972800  | -1.70624500 | 0.33202500  |
| C | 1.49196300  | -1.49945900 | 1.21997700  |
| C | 0.51701900  | -0.66765800 | 0.81857600  |
| H | 1.71672800  | 0.36370600  | -2.25370500 |
| H | -0.34343300 | -0.51576800 | 1.45425000  |
| O | 3.59059100  | -2.44996000 | 0.67569700  |
| C | 1.43408600  | -2.24378100 | 2.55487900  |
| C | 0.15192600  | -1.90738400 | 3.32633800  |
| C | 1.45582400  | -3.76385300 | 2.31150700  |
| C | 2.63079600  | -1.83519100 | 3.43414400  |
| H | 0.08624500  | -0.83774500 | 3.55855400  |
| H | -0.74664000 | -2.20187300 | 2.77085900  |
| H | 0.14893200  | -2.45466900 | 4.27398600  |
| H | 2.37570200  | -4.07135500 | 1.81350900  |
| H | 1.38507100  | -4.28890500 | 3.27084900  |
| H | 0.60161000  | -4.06679000 | 1.69585200  |
| H | 3.57701400  | -2.10278800 | 2.96368200  |
| H | 2.61957700  | -0.75543400 | 3.61954200  |
| H | 2.56370000  | -2.34582500 | 4.40151400  |
| C | 3.92382400  | -1.22108900 | -1.89875600 |
| C | 5.21442300  | -0.76489800 | -1.19315100 |
| C | 4.02958900  | -2.71110200 | -2.27164400 |
| C | 3.78909800  | -0.41791700 | -3.19783900 |
| H | 5.15518400  | 0.29860200  | -0.93648800 |
| H | 5.39433800  | -1.33849000 | -0.28348400 |
| H | 6.06722300  | -0.90276800 | -1.86757000 |
| H | 3.11746700  | -3.04529100 | -2.77848200 |
| H | 4.87040400  | -2.85661300 | -2.95934900 |
| H | 4.19061700  | -3.33183300 | -1.38973000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.67150800  | -0.59462100 | -3.82091600 |
| H | 2.90821600  | -0.72237500 | -3.77365400 |
| H | 3.72041900  | 0.65904600  | -3.00901600 |
| C | -0.77919600 | 0.39196600  | -1.14654900 |
| C | -2.07021100 | -0.16449600 | -0.70148600 |
| H | -2.24480700 | -0.26399200 | 0.36618600  |
| C | -3.02330300 | -0.53487500 | -1.56385100 |
| H | -2.84632600 | -0.38697200 | -2.62924700 |
| C | -4.32961300 | -1.11131300 | -1.21042500 |
| C | -5.36521800 | -1.07934800 | -2.15190300 |
| C | -4.58055100 | -1.70025500 | 0.03643300  |
| C | -6.62157900 | -1.59470300 | -1.85169800 |
| H | -5.18016400 | -0.63601000 | -3.12703300 |
| C | -5.83480300 | -2.21509500 | 0.33791100  |
| H | -3.78009800 | -1.77784700 | 0.76678800  |
| C | -6.86201400 | -2.16144400 | -0.60333400 |
| H | -7.41244100 | -1.55527600 | -2.59432200 |
| H | -6.00981400 | -2.67148100 | 1.30734700  |
| H | -7.83996700 | -2.56882100 | -0.36717800 |
| H | -0.66958800 | 0.48113200  | -2.22680300 |

**INT5-A**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.52231500  | 3.60909100  | 0.72267600  |
| C | -0.25832800 | 2.45935700  | 0.50529500  |
| C | -1.39989700 | 2.26488800  | 1.27013500  |
| C | -1.72004500 | 3.19292300  | 2.26753300  |
| C | -0.91437900 | 4.30504700  | 2.48808500  |
| C | 0.22116500  | 4.53578000  | 1.70708300  |
| C | 1.49877300  | 2.61272300  | -1.09346500 |
| C | 0.37703000  | 1.71900200  | -0.61715000 |
| H | -2.05895700 | 1.42090100  | 1.09071200  |
| H | -2.60967600 | 3.04161600  | 2.86938500  |
| H | -1.17476800 | 5.01329700  | 3.26814400  |
| H | 0.84021400  | 5.41382400  | 1.86031900  |
| O | 2.20973100  | 2.46748400  | -2.06906200 |
| N | 1.56608200  | 3.66338800  | -0.20518800 |
| C | 2.50681800  | 4.75049100  | -0.33170600 |
| H | 1.98315900  | 5.69556700  | -0.51017200 |
| H | 3.11277600  | 4.84087600  | 0.57496300  |
| H | 3.15121400  | 4.52439000  | -1.18186700 |
| C | 0.64433500  | 0.16756400  | -0.60268200 |
| C | 1.93295600  | -0.31519300 | -1.12241300 |
| C | 2.58748000  | -1.37254800 | -0.61134000 |
| C | 1.99154300  | -2.11053400 | 0.54418600  |
| C | 0.68911100  | -1.62968100 | 1.10284700  |
| C | 0.09743900  | -0.55912900 | 0.54850000  |
| H | 2.33602500  | 0.23444800  | -1.96396900 |
| H | -0.83934600 | -0.19891900 | 0.94703800  |
| O | 2.55226800  | -3.08785200 | 1.02541700  |
| C | 0.06789300  | -2.38008400 | 2.28176500  |
| C | -1.25707100 | -1.73900400 | 2.71370400  |
| C | -0.22269200 | -3.83612200 | 1.87390900  |
| C | 1.02217500  | -2.35356200 | 3.48956500  |
| H | -1.11994200 | -0.70189800 | 3.04139400  |
| H | -2.00040800 | -1.75187400 | 1.90663900  |
| H | -1.67151100 | -2.30309800 | 3.55502200  |
| H | 0.69342600  | -4.36286500 | 1.60527400  |
| H | -0.69883800 | -4.36327300 | 2.70837400  |
| H | -0.90992700 | -3.86496100 | 1.01979700  |
| H | 1.96587600  | -2.84849400 | 3.25924700  |
| H | 1.22791400  | -1.32100700 | 3.79239200  |
| H | 0.55448300  | -2.86793100 | 4.33677700  |
| C | 3.92638500  | -1.85276500 | -1.17488700 |
| C | 5.00811400  | -1.77715000 | -0.08136500 |
| C | 3.79926500  | -3.29927100 | -1.68633200 |
| C | 4.38121100  | -0.97548100 | -2.34733100 |
| H | 5.11761300  | -0.74816100 | 0.27863700  |
| H | 4.76630100  | -2.42315200 | 0.76317400  |
| H | 5.97102400  | -2.09348400 | -0.49825400 |
| H | 3.03532400  | -3.36337400 | -2.46920800 |
| H | 4.75386200  | -3.61864200 | -2.11976800 |
| H | 3.53665300  | -3.98486300 | -0.88019900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 5.35108800  | -1.33339700 | -2.70700500 |
| H | 3.67770900  | -1.02188100 | -3.18585400 |
| H | 4.49619500  | 0.07368900  | -2.05363200 |
| C | -0.30211800 | 0.81844900  | -1.59859600 |
| C | -1.77752300 | 0.62202000  | -1.55181000 |
| H | -2.37531100 | 1.51787000  | -1.71736900 |
| C | -2.36265800 | -0.56050800 | -1.33648600 |
| H | -1.72190600 | -1.42293400 | -1.14908300 |
| C | -3.80894700 | -0.82691400 | -1.27622300 |
| C | -4.24509500 | -2.04779600 | -0.74767500 |
| C | -4.77112300 | 0.09186500  | -1.71726900 |
| C | -5.60138200 | -2.33931700 | -0.64379000 |
| H | -3.50713200 | -2.77292500 | -0.41229900 |
| C | -6.12527300 | -0.19835300 | -1.61522600 |
| H | -4.45763100 | 1.03346500  | -2.15811100 |
| C | -6.54637800 | -1.41354900 | -1.07556700 |
| H | -5.91886500 | -3.29038900 | -0.22787800 |
| H | -6.85739300 | 0.52310000  | -1.96471500 |
| H | -7.60558800 | -1.63823200 | -0.99979400 |
| H | 0.13119800  | 0.90850400  | -2.59645800 |

**TS4-A**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.19987300 | 3.72724400  | 0.35125200  |
| C | -0.58767600 | 2.40112900  | 0.60220100  |
| C | -1.33231200 | 2.13534100  | 1.74291600  |
| C | -1.66466200 | 3.17941000  | 2.61422800  |
| C | -1.25579700 | 4.48033700  | 2.34727600  |
| C | -0.51434100 | 4.77515500  | 1.20136600  |
| C | 0.56093800  | 2.59047900  | -1.47917400 |
| C | -0.05298900 | 1.54240800  | -0.52646200 |
| H | -1.66763600 | 1.13121900  | 1.98112000  |
| H | -2.24582700 | 2.96527100  | 3.50456300  |
| H | -1.51739100 | 5.28044400  | 3.03228000  |
| H | -0.19870700 | 5.78969000  | 0.98123700  |
| O | 0.99805400  | 2.39385700  | -2.59385500 |
| N | 0.49909400  | 3.81037800  | -0.85475700 |
| C | 0.95929600  | 5.03742800  | -1.46151500 |
| H | 0.12188200  | 5.72425000  | -1.62249600 |
| H | 1.70606400  | 5.52198000  | -0.82540400 |
| H | 1.40752500  | 4.77696900  | -2.42067300 |
| C | 0.92974200  | 0.42821200  | -0.15606500 |
| C | 1.90337400  | -0.01626500 | -1.08743600 |
| C | 2.76839600  | -1.03962600 | -0.80117100 |
| C | 2.66514900  | -1.72316800 | 0.50153600  |
| C | 1.62550100  | -1.27391500 | 1.44822300  |
| C | 0.80505700  | -0.24155100 | 1.08543600  |
| H | 1.96007500  | 0.49596800  | -2.03909300 |
| H | 0.05583400  | 0.10720100  | 1.78024400  |
| O | 3.43301400  | -2.65530200 | 0.79831700  |
| C | 1.50409400  | -1.96380500 | 2.80537200  |
| C | 0.36849500  | -1.36490300 | 3.64505700  |
| C | 1.20083900  | -3.46105300 | 2.60346100  |
| C | 2.81554700  | -1.79856400 | 3.59636500  |
| H | 0.53080600  | -0.30141300 | 3.85489200  |
| H | -0.60426800 | -1.47960700 | 3.15232700  |
| H | 0.31747200  | -1.88924300 | 4.60441800  |
| H | 2.00578600  | -3.95355100 | 2.05778500  |
| H | 1.08736200  | -3.94521900 | 3.58022000  |
| H | 0.26466100  | -3.59180300 | 2.04944100  |
| H | 3.65224500  | -2.25337600 | 3.06562300  |
| H | 3.03371400  | -0.73751200 | 3.76072500  |
| H | 2.71496400  | -2.27991300 | 4.57592000  |
| C | 3.84134600  | -1.48851200 | -1.79148000 |
| C | 5.23778200  | -1.30892500 | -1.16569700 |
| C | 3.62392400  | -2.96776400 | -2.16406600 |
| C | 3.79586800  | -0.66653200 | -3.08532900 |
| H | 5.41078300  | -0.25769700 | -0.90983400 |
| H | 5.34645000  | -1.91462600 | -0.26569500 |
| H | 6.00338300  | -1.61128300 | -1.88943000 |
| H | 2.63643500  | -3.10795500 | -2.61768400 |
| H | 4.37915300  | -3.27349400 | -2.89722200 |
| H | 3.70454200  | -3.61060200 | -1.28738500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.58243300  | -1.01941500 | -3.75988300 |
| H | 2.83769300  | -0.77530500 | -3.60499700 |
| H | 3.96694600  | 0.39942800  | -2.90034700 |
| C | -0.97878900 | 0.63637700  | -1.27914200 |
| C | -2.14736600 | 0.06434900  | -0.79787700 |
| H | -2.50027400 | 0.36183000  | 0.18513400  |
| C | -2.89060300 | -0.83547300 | -1.53736100 |
| H | -2.49939100 | -1.12687700 | -2.51095000 |
| C | -4.15001900 | -1.43637000 | -1.15488400 |
| C | -4.74085900 | -2.38106100 | -2.01473000 |
| C | -4.82150800 | -1.12466400 | 0.04368400  |
| C | -5.94347400 | -2.99377400 | -1.69173500 |
| H | -4.23709100 | -2.63184500 | -2.94461900 |
| C | -6.02300900 | -1.73779100 | 0.36385000  |
| H | -4.40291100 | -0.39148000 | 0.72607100  |
| C | -6.59102900 | -2.67597200 | -0.49953100 |
| H | -6.37765800 | -3.72094100 | -2.37073600 |
| H | -6.52466100 | -1.48263100 | 1.29222600  |
| H | -7.53192500 | -3.15272700 | -0.24420100 |
| H | -0.62689000 | 0.38409700  | -2.27737700 |

**INT6-A**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.95402900 | 2.84918400  | -1.31256800 |
| C | -0.87513400 | 1.88584800  | -0.30014300 |
| C | -1.28631300 | 2.20915900  | 0.98269000  |
| C | -1.75960400 | 3.49988700  | 1.24529400  |
| C | -1.82117700 | 4.44584200  | 0.22608400  |
| C | -1.42028600 | 4.13368200  | -1.07540300 |
| C | -0.16858000 | 0.98618600  | -2.38935800 |
| C | -0.34054300 | 0.60021600  | -0.88916100 |
| H | -1.24155000 | 1.46716400  | 1.77630200  |
| H | -2.07945200 | 3.76223900  | 2.24797500  |
| H | -2.18940600 | 5.44404900  | 0.44083600  |
| H | -1.47489400 | 4.86941500  | -1.87118300 |
| O | 0.18867200  | 0.25750100  | -3.28848700 |
| N | -0.52110900 | 2.30890900  | -2.52515700 |
| C | -0.51850200 | 3.00543100  | -3.79013900 |
| H | -1.53007100 | 3.33284000  | -4.05135000 |
| H | 0.14266000  | 3.87649400  | -3.74718400 |
| H | -0.15469900 | 2.30652800  | -4.54391500 |
| C | 1.00550800  | 0.12686400  | -0.32557800 |
| C | 1.66977700  | -0.93720100 | -0.97595000 |
| C | 2.86288500  | -1.44151300 | -0.51830200 |
| C | 3.45061100  | -0.86361600 | 0.70038700  |
| C | 2.75619200  | 0.25099700  | 1.36188900  |
| C | 1.56942000  | 0.70231500  | 0.82558900  |
| H | 1.22669600  | -1.32666200 | -1.88368800 |
| H | 1.05934900  | 1.53635300  | 1.28629100  |
| O | 4.52383400  | -1.30513100 | 1.16215300  |
| C | 3.36561600  | 0.87787600  | 2.61305400  |
| C | 2.50006700  | 2.02436500  | 3.15142700  |
| C | 3.48421500  | -0.18479600 | 3.72332200  |
| C | 4.75892300  | 1.45021400  | 2.28723000  |
| H | 2.39697600  | 2.83693900  | 2.42395700  |
| H | 1.49789100  | 1.68189000  | 3.43330300  |
| H | 2.97347300  | 2.43798800  | 4.04729800  |
| H | 4.14172600  | -0.99934600 | 3.41944900  |
| H | 3.89174300  | 0.27991600  | 4.62827600  |
| H | 2.49894500  | -0.59645700 | 3.96855000  |
| H | 5.43893000  | 0.66482600  | 1.95676700  |
| H | 4.68802300  | 2.21193700  | 1.50298500  |
| H | 5.17565100  | 1.92436300  | 3.18303100  |
| C | 3.59338500  | -2.57123800 | -1.23950500 |
| C | 4.98774800  | -2.08920500 | -1.68484700 |
| C | 3.73551500  | -3.78622800 | -0.30234800 |
| C | 2.83085000  | -3.02574400 | -2.49021600 |
| H | 4.89976800  | -1.23051500 | -2.35938100 |
| H | 5.59948400  | -1.80555800 | -0.82804500 |
| H | 5.49411100  | -2.89523700 | -2.22779800 |
| H | 2.75014100  | -4.13983300 | 0.02078100  |
| H | 4.22812800  | -4.60388900 | -0.84064800 |
| H | 4.32804400  | -3.53813500 | 0.57846100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.39542500  | -3.82475700 | -2.98090500 |
| H | 1.84106000  | -3.42372500 | -2.24074800 |
| H | 2.70396200  | -2.21168900 | -3.21191500 |
| C | -1.30047200 | -0.56990400 | -0.82082000 |
| C | -2.52586300 | -0.57975100 | -0.21633400 |
| H | -2.87802600 | 0.33336900  | 0.25536500  |
| C | -3.35405300 | -1.71366300 | -0.19327600 |
| H | -2.97790100 | -2.61720900 | -0.66939700 |
| C | -4.66259700 | -1.80054400 | 0.39874900  |
| C | -5.36101600 | -3.02498500 | 0.33969100  |
| C | -5.29468100 | -0.71610400 | 1.04493600  |
| C | -6.62294000 | -3.16197200 | 0.89734700  |
| H | -4.89137100 | -3.87174700 | -0.15418600 |
| C | -6.55631600 | -0.85778100 | 1.60082900  |
| H | -4.79316300 | 0.24432400  | 1.10963200  |
| C | -7.22964300 | -2.07876300 | 1.53238700  |
| H | -7.13750500 | -4.11608800 | 0.83774600  |
| H | -7.02283300 | -0.00947400 | 2.09246500  |
| H | -8.21741000 | -2.18334400 | 1.96949100  |
| H | -0.94998400 | -1.46864200 | -1.32359000 |

**INT7-A**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.43899100 | -1.98452600 | 0.17357000  |
| C | -2.48672600 | -1.45474500 | 1.04969600  |
| C | -2.84911200 | -1.07690400 | 2.32762400  |
| C | -4.18131900 | -1.23931200 | 2.72617200  |
| C | -5.11865300 | -1.77120000 | 1.84522500  |
| C | -4.76268500 | -2.15457000 | 0.54810900  |
| C | -1.50522500 | -1.94012200 | -1.06601900 |
| C | -1.13520600 | -1.41692600 | 0.35589500  |
| H | -2.11058900 | -0.65515600 | 3.00461600  |
| H | -4.48495900 | -0.94622800 | 3.72543700  |
| H | -6.14860700 | -1.89084000 | 2.16629700  |
| H | -5.49619400 | -2.56793900 | -0.13663500 |
| O | -0.76721300 | -2.03290300 | -2.02007000 |
| N | -2.84125500 | -2.28091700 | -1.05496800 |
| C | -3.52969600 | -2.82454300 | -2.20159900 |
| H | -3.95505700 | -3.80493100 | -1.96488000 |
| H | -4.33253800 | -2.15296000 | -2.52318800 |
| H | -2.79605500 | -2.92665500 | -3.00194500 |
| C | -0.63768900 | 0.02233900  | 0.27101600  |
| C | -1.23700300 | 0.89674700  | -0.65816900 |
| C | -0.86124500 | 2.21404800  | -0.77040600 |
| C | 0.20904600  | 2.71346000  | 0.10934500  |
| C | 0.82035100  | 1.79295800  | 1.07985500  |
| C | 0.35733200  | 0.49776700  | 1.14148000  |
| H | -2.01476600 | 0.50019700  | -1.30290200 |
| H | 0.78925300  | -0.20386100 | 1.84332300  |
| O | 0.59313700  | 3.89928300  | 0.03009400  |
| C | 1.97142000  | 2.27863500  | 1.95576000  |
| C | 2.48653100  | 1.16487900  | 2.87631000  |
| C | 3.14321600  | 2.71932600  | 1.05560400  |
| C | 1.51274800  | 3.45529900  | 2.83760500  |
| H | 1.71199000  | 0.81652400  | 3.56864500  |
| H | 2.85787800  | 0.30564300  | 2.30588500  |
| H | 3.31662000  | 1.55275400  | 3.47490300  |
| H | 2.85609600  | 3.55337600  | 0.41464600  |
| H | 3.98569100  | 3.03076000  | 1.68339200  |
| H | 3.47837000  | 1.88517100  | 0.42868300  |
| H | 1.19109700  | 4.30099900  | 2.22960600  |
| H | 0.68456500  | 3.14957300  | 3.48660300  |
| H | 2.34300300  | 3.77518600  | 3.47734200  |
| C | -1.50516400 | 3.16186900  | -1.77860100 |
| C | -2.15821400 | 4.34599000  | -1.03960000 |
| C | -0.43808500 | 3.68216200  | -2.76141300 |
| C | -2.59506700 | 2.45912700  | -2.59763700 |
| H | -2.92404500 | 3.98892700  | -0.34224000 |
| H | -1.41658500 | 4.92191000  | -0.48580000 |
| H | -2.64447700 | 5.00461100  | -1.76807800 |
| H | 0.03072900  | 2.84856600  | -3.29571200 |
| H | -0.91442600 | 4.33414100  | -3.50234200 |
| H | 0.33442300  | 4.24811700  | -2.24053300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.02833100 | 3.17541200  | -3.30261200 |
| H | -2.19275300 | 1.62187500  | -3.17843200 |
| H | -3.40581100 | 2.08639300  | -1.96181600 |
| C | -0.17800900 | -2.40479300 | 0.99329400  |
| C | 1.14080800  | -2.58446700 | 0.66599200  |
| H | 1.67292000  | -3.32766200 | 1.25649100  |
| C | 1.85888800  | -1.89097900 | -0.32254800 |
| H | 1.30792400  | -1.22949900 | -0.98349100 |
| C | 3.27755500  | -1.98800700 | -0.55631700 |
| C | 3.83975900  | -1.23923800 | -1.61164200 |
| C | 4.14833000  | -2.77842500 | 0.22378100  |
| C | 5.19983200  | -1.28092800 | -1.87890900 |
| H | 3.18332200  | -0.62412200 | -2.22137700 |
| C | 5.50701400  | -2.81906800 | -0.04838300 |
| H | 3.75801800  | -3.36106000 | 1.05205800  |
| C | 6.04256200  | -2.07267900 | -1.09940400 |
| H | 5.60629200  | -0.69515700 | -2.69760100 |
| H | 6.15790800  | -3.43485900 | 0.56492200  |
| H | 7.10740900  | -2.10710600 | -1.30624100 |
| H | -0.61073900 | -3.03575800 | 1.76343900  |

**TS5-A**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.10866300 | -0.28103200 | 0.02261300  |
| C | -2.95270600 | -0.95737000 | 0.42780600  |
| C | -2.94636500 | -1.65706900 | 1.61973000  |
| C | -4.10657000 | -1.67168800 | 2.40295500  |
| C | -5.24712600 | -0.99206700 | 1.98607000  |
| C | -5.26794600 | -0.28199100 | 0.78194000  |
| C | -2.60189800 | 0.14337200  | -1.65357300 |
| C | -1.87553600 | -0.77020400 | -0.62878900 |
| H | -2.05324000 | -2.18065700 | 1.94909600  |
| H | -4.11457600 | -2.21433100 | 3.34214900  |
| H | -6.13907800 | -1.00994200 | 2.60431900  |
| H | -6.15781000 | 0.24751600  | 0.45704000  |
| O | -2.13328700 | 0.60102100  | -2.67501100 |
| N | -3.88625900 | 0.34624900  | -1.20784700 |
| C | -4.85715000 | 1.14492500  | -1.91764400 |
| H | -5.73840300 | 0.54533700  | -2.16648100 |
| H | -5.16591200 | 2.00293400  | -1.31182400 |
| H | -4.38151800 | 1.49565200  | -2.83409400 |
| C | -0.63686300 | -0.08533100 | -0.04363900 |
| C | -0.41484900 | 1.30091600  | -0.18890300 |
| C | 0.64680300  | 1.93614800  | 0.41108300  |
| C | 1.53914300  | 1.15700800  | 1.28978600  |
| C | 1.29773300  | -0.29021000 | 1.43418100  |
| C | 0.22765200  | -0.84373300 | 0.78327000  |
| H | -1.08030400 | 1.86237600  | -0.83331700 |
| H | 0.04474700  | -1.91100400 | 0.84478000  |
| O | 2.47513800  | 1.71158200  | 1.89502800  |
| C | 2.24038900  | -1.11766100 | 2.30404500  |
| C | 1.86824400  | -2.60466300 | 2.27792600  |
| C | 3.68319600  | -0.99134700 | 1.78180200  |
| C | 2.16147700  | -0.62751000 | 3.76214400  |
| H | 0.86156000  | -2.78413500 | 2.67307800  |
| H | 1.92516800  | -3.01331700 | 1.26205400  |
| H | 2.57292900  | -3.16151400 | 2.90352400  |
| H | 4.03391000  | 0.03940900  | 1.83423400  |
| H | 4.34534400  | -1.62152500 | 2.38732500  |
| H | 3.74042100  | -1.33258700 | 0.74309900  |
| H | 2.46570900  | 0.41690900  | 3.83973200  |
| H | 1.14112300  | -0.72939800 | 4.14859300  |
| H | 2.82416500  | -1.23552300 | 4.38874900  |
| C | 0.91682700  | 3.42600000  | 0.21271400  |
| C | 0.81385700  | 4.16024600  | 1.56403500  |
| C | 2.32367500  | 3.62909100  | -0.38315400 |
| C | -0.09469900 | 4.06292200  | -0.74798800 |
| H | -0.18083900 | 4.01976600  | 2.00125500  |
| H | 1.56317200  | 3.79625500  | 2.26695100  |
| H | 0.96616700  | 5.23420800  | 1.40693900  |
| H | 2.39240800  | 3.16593800  | -1.37434900 |
| H | 2.51732100  | 4.70124600  | -0.50213300 |
| H | 3.09124200  | 3.20235300  | 0.26300400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.15394800  | 5.12085900  | -0.87846900 |
| H | -0.07503300 | 3.58981300  | -1.73609700 |
| H | -1.11702900 | 4.00821200  | -0.35810600 |
| C | -1.52906600 | -2.08050400 | -1.32270300 |
| C | -0.37856200 | -2.22906600 | -2.00308300 |
| H | -0.11982200 | -3.21542100 | -2.38671400 |
| C | 0.54613300  | -1.13239600 | -2.18644800 |
| H | 0.12200100  | -0.16786600 | -2.44207300 |
| C | 1.96549500  | -1.21888300 | -2.06451200 |
| C | 2.72222500  | -0.02631300 | -2.10414200 |
| C | 2.65186300  | -2.43556100 | -1.84822400 |
| C | 4.10198700  | -0.05104800 | -1.96758000 |
| H | 2.19887700  | 0.91623400  | -2.24351700 |
| C | 4.03347300  | -2.45582100 | -1.74068200 |
| H | 2.09162600  | -3.36365300 | -1.78013700 |
| C | 4.76627200  | -1.26694100 | -1.80225700 |
| H | 4.66281500  | 0.87819500  | -1.99198700 |
| H | 4.54789100  | -3.40073900 | -1.59412900 |
| H | 5.84694000  | -1.28899000 | -1.70484700 |
| H | -2.24756800 | -2.89048200 | -1.23551500 |

**3a**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.38451500  | 0.63188200  | 0.31249600  |
| C | 2.20661100  | 1.24323900  | 0.76161800  |
| C | 2.00079100  | 1.40700300  | 2.12031000  |
| C | 2.96440400  | 0.93507800  | 3.01903700  |
| C | 4.11672400  | 0.30985600  | 2.55243800  |
| C | 4.34977300  | 0.15193300  | 1.18330000  |
| C | 2.30704000  | 1.24754500  | -1.61203700 |
| C | 1.36610300  | 1.61063900  | -0.43414000 |
| H | 1.10297900  | 1.89556900  | 2.48745800  |
| H | 2.80898900  | 1.05597500  | 4.08592700  |
| H | 4.85327500  | -0.05717800 | 3.26022500  |
| H | 5.25474000  | -0.32312000 | 0.81846800  |
| O | 2.09226500  | 1.42798700  | -2.79244900 |
| N | 3.41368100  | 0.62378000  | -1.08663300 |
| C | 4.48656800  | 0.09102300  | -1.89141200 |
| H | 5.42818700  | 0.60376700  | -1.66931900 |
| H | 4.60912300  | -0.98081500 | -1.70479100 |
| H | 4.21975000  | 0.25390000  | -2.93633600 |
| C | 0.02186100  | 0.77030400  | -0.60023800 |
| C | 0.25859300  | -0.57940900 | -1.18736300 |
| C | -0.04251700 | -1.74296500 | -0.59347900 |
| C | -0.68713000 | -1.71894700 | 0.76054100  |
| C | -1.04902900 | -0.39554100 | 1.35786200  |
| C | -0.67989800 | 0.71989500  | 0.71684600  |
| H | 0.70774200  | -0.57086500 | -2.17681800 |
| H | -0.91772200 | 1.69380100  | 1.13597700  |
| O | -0.91918100 | -2.76074500 | 1.35788200  |
| C | -1.82969500 | -0.37570400 | 2.67223000  |
| C | -2.16636600 | 1.05844100  | 3.09688400  |
| C | -3.16090700 | -1.12772400 | 2.48800200  |
| C | -0.99695400 | -1.02264000 | 3.79332700  |
| H | -1.26511600 | 1.65165100  | 3.29152300  |
| H | -2.76675300 | 1.57209700  | 2.33716500  |
| H | -2.74744700 | 1.03048500  | 4.02405100  |
| H | -2.99498700 | -2.17855000 | 2.24844900  |
| H | -3.74550700 | -1.07024400 | 3.41330600  |
| H | -3.74745700 | -0.66829000 | 1.68353200  |
| H | -0.79326200 | -2.07229000 | 3.58076300  |
| H | -0.04181200 | -0.49699400 | 3.91080600  |
| H | -1.54213000 | -0.95569800 | 4.74191000  |
| C | 0.24487800  | -3.09821600 | -1.24045600 |
| C | 1.24219000  | -3.88723500 | -0.37171500 |
| C | -1.06338400 | -3.89407400 | -1.40044300 |
| C | 0.86578900  | -2.93010200 | -2.63200300 |
| H | 2.17446900  | -3.32273800 | -0.25397100 |
| H | 0.83085100  | -4.09484300 | 0.61624600  |
| H | 1.48030300  | -4.83905000 | -0.86016900 |
| H | -1.78166900 | -3.33146700 | -2.00815400 |
| H | -0.85630900 | -4.84107400 | -1.91144900 |
| H | -1.51749600 | -4.11252700 | -0.43366300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.05830300  | -3.91846300 | -3.06086900 |
| H | 0.19730400  | -2.39398100 | -3.31505700 |
| H | 1.81972400  | -2.39189200 | -2.59057100 |
| C | 0.86559200  | 3.02927700  | -0.58203400 |
| C | -0.30231500 | 3.07292200  | -1.21815200 |
| H | -0.82177200 | 3.97987600  | -1.51205500 |
| C | -0.81421100 | 1.69594800  | -1.57276100 |
| H | -0.49794700 | 1.46648800  | -2.59899200 |
| C | -2.30051400 | 1.45471600  | -1.45125000 |
| C | -2.87196400 | 0.35783500  | -2.10110600 |
| C | -3.11082400 | 2.24700200  | -0.63482800 |
| C | -4.21801200 | 0.05027600  | -1.92873800 |
| H | -2.24942200 | -0.26482400 | -2.73994900 |
| C | -4.46024700 | 1.94713400  | -0.46547800 |
| H | -2.67938300 | 3.10142100  | -0.11774800 |
| C | -5.01675200 | 0.84438600  | -1.10864400 |
| H | -4.64472700 | -0.80895700 | -2.43714500 |
| H | -5.07612900 | 2.57438000  | 0.17217500  |
| H | -6.06750200 | 0.60705600  | -0.97476600 |
| H | 1.46411300  | 3.88033600  | -0.27486900 |

**TS6-A**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 4.03940200  | -0.26759200 | 0.44876100  |
| C | 3.13792800  | 0.56759600  | -0.22030900 |
| C | 3.47874700  | 1.88686700  | -0.45801500 |
| C | 4.72089800  | 2.35957000  | -0.01706500 |
| C | 5.60053800  | 1.51516400  | 0.65183900  |
| C | 5.27238900  | 0.17861600  | 0.89617700  |
| C | 2.26812600  | -1.64703400 | -0.03375200 |
| C | 1.89662500  | -0.23370800 | -0.55558900 |
| H | 2.79941800  | 2.55887300  | -0.97413300 |
| H | 4.99539700  | 3.39336700  | -0.19710400 |
| H | 6.55914200  | 1.89544900  | 0.99019400  |
| H | 5.95866000  | -0.48330400 | 1.41434600  |
| O | 1.61732800  | -2.66467600 | -0.12719800 |
| N | 3.50446700  | -1.55399600 | 0.56013500  |
| C | 4.18167600  | -2.68024000 | 1.15786900  |
| H | 5.12099900  | -2.88637700 | 0.63440300  |
| H | 4.39424700  | -2.48197500 | 2.21296000  |
| H | 3.51856200  | -3.54145200 | 1.07280500  |
| C | 0.59780300  | 0.29666800  | 0.00342100  |
| C | -0.16501400 | -0.43903200 | 0.92668600  |
| C | -1.38130200 | 0.00633000  | 1.38480200  |
| C | -1.97496700 | 1.22586900  | 0.79148300  |
| C | -1.13656500 | 2.01743500  | -0.12484000 |
| C | 0.09876100  | 1.53927500  | -0.47183000 |
| H | 0.23759200  | -1.36942800 | 1.30489900  |
| H | 0.71619100  | 2.10501900  | -1.16152600 |
| O | -3.13381400 | 1.57493100  | 1.07905100  |
| C | -1.67839300 | 3.34318300  | -0.65929900 |
| C | -0.66276900 | 4.04901500  | -1.56548700 |
| C | -2.95125400 | 3.08623900  | -1.48806500 |
| C | -2.00531100 | 4.28992500  | 0.50980800  |
| H | 0.26968900  | 4.27181000  | -1.03346300 |
| H | -0.42400800 | 3.45232100  | -2.45367700 |
| H | -1.08434300 | 4.99914900  | -1.90897300 |
| H | -3.73301500 | 2.64952900  | -0.86511300 |
| H | -3.31987400 | 4.02958800  | -1.90838800 |
| H | -2.73678700 | 2.40709000  | -2.32287900 |
| H | -2.74820200 | 3.84500700  | 1.17265300  |
| H | -1.10068200 | 4.50945700  | 1.08773100  |
| H | -2.39922200 | 5.23675600  | 0.12182700  |
| C | -2.09379600 | -0.66924800 | 2.55691400  |
| C | -2.27374300 | 0.36484500  | 3.68561700  |
| C | -3.46731400 | -1.21787600 | 2.13674400  |
| C | -1.28028500 | -1.84279300 | 3.11583900  |
| H | -1.30298000 | 0.76351400  | 4.00114300  |
| H | -2.90613800 | 1.19128700  | 3.35877000  |
| H | -2.74127400 | -0.11741500 | 4.55192400  |
| H | -3.34603300 | -2.03440700 | 1.41821000  |
| H | -3.98162100 | -1.61571300 | 3.02004500  |
| H | -4.08328700 | -0.43670100 | 1.68932100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.82290800 | -2.28422700 | 3.95821000  |
| H | -1.13297700 | -2.62780500 | 2.36551700  |
| H | -0.29855800 | -1.52140900 | 3.48111500  |
| C | 1.58276900  | -0.27277900 | -2.02232400 |
| C | 0.93490000  | -1.24275100 | -2.76313300 |
| H | 1.32305000  | -1.29604900 | -3.78515800 |
| C | -0.02534900 | -2.21907400 | -2.49268300 |
| H | 0.09900600  | -3.13337400 | -3.07468100 |
| C | -1.29695100 | -2.14080200 | -1.83136400 |
| C | -2.02711300 | -3.33621300 | -1.63118900 |
| C | -1.96453700 | -0.91060500 | -1.63157400 |
| C | -3.36108500 | -3.30104700 | -1.27163800 |
| H | -1.52462600 | -4.28865500 | -1.77664400 |
| C | -3.31420700 | -0.88402300 | -1.30036100 |
| H | -1.43397900 | 0.01657500  | -1.81989100 |
| C | -4.01580400 | -2.07230700 | -1.12447900 |
| H | -3.90482200 | -4.22817500 | -1.11954100 |
| H | -3.80691500 | 0.07279000  | -1.15314600 |
| H | -5.06674800 | -2.04602700 | -0.85353300 |
| H | 2.09883900  | 0.49399900  | -2.60179400 |

## TS7-A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.15751200 | -0.12457100 | -0.58766100 |
| C | -2.19899400 | -1.01079800 | -0.99129400 |
| C | -3.52504500 | -0.69397100 | -0.90978200 |
| C | -3.92030400 | 0.60970300  | -0.35330100 |
| C | -2.85007300 | 1.49600400  | 0.13272400  |
| C | -1.54577000 | 1.12137000  | -0.01116000 |
| H | -1.88774400 | -1.97023700 | -1.39648900 |
| H | -0.76052400 | 1.76106400  | 0.37330400  |
| O | -5.12272200 | 0.94889100  | -0.28891900 |
| C | -3.23919700 | 2.80884900  | 0.81668400  |
| C | -2.00772600 | 3.57859300  | 1.30992200  |
| C | -4.00789100 | 3.71308400  | -0.16302300 |
| C | -4.11957500 | 2.50989500  | 2.04406900  |
| H | -1.41711900 | 2.98278800  | 2.01466800  |
| H | -1.35733900 | 3.87467500  | 0.47798900  |
| H | -2.33344200 | 4.49333500  | 1.81926800  |
| H | -4.90750500 | 3.20870400  | -0.51783500 |
| H | -4.29080600 | 4.65130000  | 0.33282800  |
| H | -3.37695400 | 3.96112600  | -1.02489200 |
| H | -5.02492000 | 1.98082800  | 1.74404100  |
| H | -3.56610500 | 1.89279700  | 2.76035600  |
| H | -4.39984100 | 3.44774600  | 2.54192900  |
| C | -4.62335200 | -1.65770200 | -1.36512300 |
| C | -5.54465500 | -1.99512400 | -0.17854600 |
| C | -5.45217000 | -1.02074700 | -2.49520100 |
| C | -4.04525300 | -2.97597100 | -1.89255200 |
| H | -4.96998500 | -2.47923900 | 0.61934900  |
| H | -6.00105000 | -1.08710800 | 0.21695800  |
| H | -6.33540700 | -2.68617800 | -0.49977600 |
| H | -4.81378500 | -0.81206500 | -3.36182100 |
| H | -6.24654300 | -1.70857300 | -2.81453000 |
| H | -5.90077300 | -0.08707500 | -2.15397900 |
| H | -4.86603900 | -3.63699100 | -2.19471300 |
| H | -3.40376400 | -2.81654800 | -2.76689300 |
| H | -3.45843100 | -3.49445500 | -1.12580000 |
| C | 0.18528300  | -0.51791300 | -0.72408700 |
| C | 1.28083500  | 0.42495100  | -0.84559900 |
| H | 1.10195300  | 1.43915000  | -0.49354100 |
| C | 2.48411500  | 0.09527900  | -1.35393200 |
| H | 2.65439200  | -0.93828600 | -1.65750800 |
| C | 3.63233100  | 0.99523600  | -1.50544800 |
| C | 4.89022900  | 0.44951500  | -1.80333300 |
| C | 3.53868700  | 2.38945500  | -1.36352300 |
| C | 6.01365000  | 1.25831400  | -1.93425000 |
| H | 4.97692500  | -0.62918400 | -1.90655600 |
| C | 4.66170300  | 3.19745100  | -1.49184300 |
| H | 2.57428600  | 2.84509800  | -1.15919500 |
| C | 5.90694100  | 2.63793300  | -1.77662800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 6.97702600  | 0.80871900  | -2.15840900 |
| H  | 4.56306700  | 4.27313700  | -1.37619800 |
| H  | 6.78227100  | 3.27240700  | -1.87950000 |
| H  | 0.36131000  | -1.48685700 | -1.19302500 |
| C  | 3.01384800  | -1.13006700 | 1.29913100  |
| C  | 2.04441600  | -2.10309700 | 0.93478600  |
| C  | 2.45936000  | -3.26891900 | 0.29203800  |
| C  | 3.81707900  | -3.44827200 | 0.01927600  |
| C  | 4.75693500  | -2.47854300 | 0.37928100  |
| C  | 4.36285200  | -1.30373100 | 1.02894800  |
| C  | 0.97867400  | -0.29585600 | 1.97654600  |
| C  | 0.76772000  | -1.53991000 | 1.24743600  |
| H  | 1.72732500  | -4.02177200 | 0.01228400  |
| H  | 4.14726200  | -4.35564700 | -0.47864700 |
| H  | 5.80820900  | -2.63461400 | 0.15372100  |
| H  | 5.08756400  | -0.53858300 | 1.29324200  |
| O  | 0.18715300  | 0.48729400  | 2.48495400  |
| N  | 2.37142100  | -0.07506200 | 1.91632000  |
| C  | 2.98030000  | 1.17078100  | 2.29372200  |
| H  | 3.46870000  | 1.64441000  | 1.43238700  |
| H  | 2.17838200  | 1.81297800  | 2.66415400  |
| H  | 3.72378000  | 1.02660300  | 3.08691300  |
| Cl | -0.65614300 | -2.48852000 | 1.49786600  |

## TS8-A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.61616500  | -0.40732700 | -0.54255200 |
| C | 1.72760400  | 0.35099200  | -1.01447900 |
| C | 3.01841700  | -0.09964300 | -0.96511500 |
| C | 3.30275400  | -1.40362400 | -0.35278500 |
| C | 2.16151100  | -2.17452000 | 0.16761500  |
| C | 0.89498900  | -1.67298200 | 0.04952400  |
| H | 1.50338300  | 1.32646900  | -1.44100800 |
| H | 0.05637200  | -2.24483500 | 0.43113400  |
| O | 4.47212000  | -1.84625700 | -0.27503200 |
| C | 2.43786300  | -3.52448100 | 0.83549300  |
| C | 1.15172700  | -4.19166100 | 1.33711000  |
| C | 3.10504400  | -4.48420800 | -0.16622000 |
| C | 3.36185900  | -3.32417600 | 2.05087700  |
| H | 0.63418600  | -3.56864200 | 2.07544800  |
| H | 0.45620800  | -4.40150300 | 0.51644500  |
| H | 1.40188200  | -5.14547900 | 1.81610200  |
| H | 4.03908700  | -4.05803200 | -0.53351300 |
| H | 3.31242500  | -5.44846100 | 0.31661600  |
| H | 2.43844000  | -4.66641100 | -1.01733100 |
| H | 4.30451900  | -2.87275700 | 1.73994900  |
| H | 2.87996700  | -2.67040800 | 2.78704600  |
| H | 3.56510000  | -4.28987400 | 2.53249300  |
| C | 4.18893300  | 0.72497200  | -1.50663200 |
| C | 5.16348600  | 1.05318500  | -0.36122900 |
| C | 4.92895500  | -0.06266400 | -2.60287100 |
| C | 3.72326800  | 2.05098000  | -2.11947100 |
| H | 4.64921500  | 1.63747100  | 0.41091800  |
| H | 5.54562300  | 0.13468700  | 0.08609000  |
| H | 6.00489100  | 1.64978800  | -0.73820200 |
| H | 4.25397200  | -0.26684300 | -3.44243600 |
| H | 5.77535800  | 0.52537000  | -2.98222600 |
| H | 5.29776500  | -1.00961900 | -2.20775400 |
| H | 4.59484700  | 2.60076400  | -2.49456700 |
| H | 3.04235600  | 1.88682400  | -2.96285400 |
| H | 3.21306800  | 2.68344000  | -1.38426200 |
| C | -0.68440700 | 0.12322700  | -0.65438500 |
| C | -1.89971700 | -0.66801300 | -0.59887100 |
| H | -1.88374500 | -1.59217200 | -0.02541700 |
| C | -3.04614500 | -0.28556100 | -1.18646700 |
| H | -3.05269100 | 0.61526800  | -1.80089800 |
| C | -4.31739300 | -1.00952700 | -1.06161800 |
| C | -5.21761600 | -1.06808400 | -2.13258500 |
| C | -4.66326400 | -1.64485100 | 0.13923000  |
| C | -6.41128100 | -1.77393200 | -2.02426400 |
| H | -4.96624900 | -0.56328800 | -3.06231000 |
| C | -5.85435300 | -2.35319100 | 0.24594500  |
| H | -4.00554500 | -1.52825300 | 0.99565100  |
| C | -6.73098700 | -2.42636100 | -0.83577100 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -7.09341800 | -1.81519300 | -2.86901300 |
| H  | -6.11047200 | -2.83458300 | 1.18550300  |
| H  | -7.66420900 | -2.97519900 | -0.74749000 |
| H  | -0.77080200 | 1.05488700  | -1.21698500 |
| C  | -0.61428200 | 3.32583200  | 0.51459300  |
| C  | -0.02812600 | 2.21550500  | 1.17734700  |
| C  | 1.33409800  | 2.22217200  | 1.45572600  |
| C  | 2.08829600  | 3.34482100  | 1.09860000  |
| C  | 1.50040100  | 4.42771400  | 0.44539000  |
| C  | 0.13335300  | 4.42902400  | 0.13753300  |
| C  | -2.32700100 | 1.85094500  | 0.95207100  |
| C  | -1.06214600 | 1.23001100  | 1.30596700  |
| H  | 1.79539400  | 1.36339100  | 1.93515400  |
| H  | 3.15125200  | 3.36733700  | 1.32057400  |
| H  | 2.10874700  | 5.28333200  | 0.16677700  |
| H  | -0.32710000 | 5.27066300  | -0.37261700 |
| O  | -3.48139600 | 1.44932900  | 1.03394700  |
| N  | -1.96732200 | 3.07659500  | 0.34721200  |
| C  | -2.93364900 | 3.99032700  | -0.19380000 |
| H  | -2.71752200 | 4.22046900  | -1.24392700 |
| H  | -3.90645400 | 3.49979100  | -0.12008100 |
| H  | -2.95608200 | 4.93011000  | 0.37239800  |
| Cl | -1.00085000 | -0.06168600 | 2.46525600  |

## TS9-B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.37931500 | 0.15243100  | -0.73700800 |
| C | -1.56218400 | -0.43781100 | -1.26875100 |
| C | -2.79610000 | 0.14774400  | -1.18831700 |
| C | -2.93370300 | 1.44455800  | -0.51156500 |
| C | -1.72344700 | 2.03517900  | 0.08636000  |
| C | -0.52384000 | 1.38982800  | -0.04435600 |
| H | -1.44405300 | -1.39841000 | -1.76505700 |
| H | 0.36793500  | 1.82551000  | 0.39737100  |
| O | -4.03621700 | 2.03460000  | -0.45030000 |
| C | -1.84520900 | 3.39561100  | 0.78219600  |
| C | -0.50932300 | 3.86404600  | 1.37101500  |
| C | -2.30116300 | 4.45254400  | -0.24148300 |
| C | -2.86735000 | 3.33528200  | 1.93245200  |
| H | -0.12052000 | 3.15807800  | 2.11402700  |
| H | 0.25317500  | 3.99676700  | 0.59553800  |
| H | -0.65240000 | 4.83034000  | 1.86851100  |
| H | -3.26692100 | 4.17550900  | -0.66568200 |
| H | -2.38761800 | 5.43419500  | 0.24289400  |
| H | -1.56736300 | 4.53509100  | -1.05146000 |
| H | -3.83624100 | 2.99897600  | 1.56298200  |
| H | -2.52736300 | 2.64984700  | 2.71786500  |
| H | -2.97841400 | 4.32971200  | 2.38446200  |
| C | -4.04289600 | -0.47922900 | -1.81816100 |
| C | -5.12350600 | -0.70751700 | -0.74583900 |
| C | -4.59737600 | 0.45159300  | -2.91251200 |
| C | -3.73648300 | -1.83481000 | -2.46434400 |
| H | -4.74635900 | -1.39160500 | 0.02194700  |
| H | -5.39912500 | 0.23716900  | -0.27611300 |
| H | -6.01553700 | -1.15791300 | -1.20153700 |
| H | -3.85175600 | 0.59204300  | -3.70393600 |
| H | -5.49481200 | 0.00847100  | -3.36453400 |
| H | -4.85238700 | 1.42447800  | -2.49028600 |
| H | -4.65880200 | -2.25097700 | -2.88702700 |
| H | -3.00914500 | -1.73969100 | -3.27904100 |
| H | -3.34259100 | -2.54720200 | -1.73085700 |
| C | 0.86913300  | -0.48027700 | -0.92586500 |
| C | 2.14911900  | 0.19015900  | -0.78040100 |
| H | 2.23165300  | 0.96057400  | -0.01808800 |
| C | 3.25110000  | -0.15086300 | -1.46960600 |
| H | 3.17904500  | -0.88814600 | -2.26872000 |
| C | 4.58130900  | 0.40423400  | -1.18775400 |
| C | 5.53015500  | 0.55869100  | -2.20660700 |
| C | 4.93432400  | 0.76344100  | 0.12303900  |
| C | 6.78476100  | 1.09513700  | -1.93742100 |
| H | 5.26968600  | 0.26482500  | -3.22077200 |
| C | 6.18837500  | 1.30294800  | 0.38728400  |
| H | 4.22698400  | 0.56940400  | 0.92757400  |
| C | 7.11624200  | 1.47646100  | -0.63897600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 7.50537500  | 1.21590100  | -2.74173700 |
| H  | 6.45035900  | 1.57251000  | 1.40657700  |
| H  | 8.09688900  | 1.89251300  | -0.42583900 |
| H  | 0.87260300  | -1.33845200 | -1.59941100 |
| C  | -0.82097700 | -1.74776800 | 1.65663000  |
| C  | -0.04346000 | -2.56782800 | 0.80309200  |
| C  | -0.64641500 | -3.62976000 | 0.13686000  |
| C  | -2.00778200 | -3.86727700 | 0.33814600  |
| C  | -2.76358900 | -3.03980600 | 1.17169200  |
| C  | -2.17730400 | -1.96214300 | 1.84244200  |
| C  | 1.32567800  | -0.93904100 | 1.79010400  |
| C  | 1.25966500  | -1.96978200 | 0.76169500  |
| H  | -0.05626100 | -4.26549500 | -0.51792200 |
| H  | -2.48812200 | -4.70009700 | -0.16785200 |
| H  | -3.82408900 | -3.23388300 | 1.30274500  |
| H  | -2.76743600 | -1.30780500 | 2.47734500  |
| O  | 2.25974700  | -0.23714300 | 2.17661300  |
| N  | 0.00686400  | -0.79482800 | 2.23123300  |
| C  | -0.42118600 | 0.24723300  | 3.12386300  |
| H  | -0.82371100 | -0.17096700 | 4.05452500  |
| H  | 0.45811000  | 0.85447200  | 3.34920000  |
| H  | -1.18539900 | 0.86766000  | 2.64203000  |
| Cl | 2.67910500  | -2.83403000 | 0.26551300  |

## TS2-B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.06863000 | -0.36351600 | -0.72642100 |
| C | -2.21041300 | -1.20180000 | -0.88853600 |
| C | -3.49622000 | -0.74846000 | -0.79278900 |
| C | -3.74037100 | 0.66757200  | -0.48456200 |
| C | -2.56593800 | 1.53705400  | -0.30856900 |
| C | -1.30978100 | 1.01187900  | -0.43324300 |
| H | -2.01226500 | -2.24794800 | -1.10443600 |
| H | -0.45063000 | 1.65597900  | -0.28226300 |
| O | -4.90278100 | 1.11951200  | -0.37621600 |
| C | -2.79370000 | 3.01225300  | 0.03311800  |
| C | -1.47374900 | 3.77932800  | 0.17675200  |
| C | -3.61340400 | 3.69405700  | -1.07753200 |
| C | -3.54653200 | 3.12381400  | 1.37143000  |
| H | -0.84209100 | 3.36097100  | 0.96899000  |
| H | -0.89899000 | 3.77304900  | -0.75667900 |
| H | -1.68827700 | 4.82388500  | 0.43132400  |
| H | -4.57634500 | 3.19678400  | -1.19797000 |
| H | -3.77964200 | 4.75038300  | -0.82781200 |
| H | -3.07005600 | 3.65114000  | -2.02878400 |
| H | -4.50270500 | 2.60255100  | 1.31322300  |
| H | -2.94945900 | 2.68273300  | 2.17876100  |
| H | -3.72516400 | 4.17895100  | 1.61745900  |
| C | -4.70035100 | -1.67692000 | -0.96863200 |
| C | -5.52722500 | -1.70594600 | 0.32994600  |
| C | -5.58264200 | -1.18692600 | -2.13081400 |
| C | -4.27283500 | -3.11614100 | -1.27853000 |
| H | -4.91515900 | -2.08298000 | 1.15743900  |
| H | -5.87889500 | -0.70401300 | 0.57841800  |
| H | -6.39147000 | -2.37296900 | 0.21140600  |
| H | -5.01574200 | -1.20173100 | -3.06912400 |
| H | -6.45239900 | -1.84695100 | -2.24802200 |
| H | -5.92724700 | -0.16958800 | -1.94217600 |
| H | -5.16526700 | -3.74257000 | -1.39255000 |
| H | -3.69880300 | -3.17677200 | -2.21021200 |
| H | -3.66375400 | -3.53995500 | -0.47219400 |
| C | 0.22382500  | -0.91940300 | -0.80145900 |
| C | 1.40815100  | -0.11611000 | -1.05929500 |
| H | 1.34931400  | 0.94910200  | -0.84822900 |
| C | 2.55610600  | -0.63300500 | -1.53099600 |
| H | 2.59389700  | -1.70193000 | -1.74634400 |
| C | 3.79945600  | 0.11294500  | -1.75032300 |
| C | 4.81712200  | -0.45792000 | -2.52844100 |
| C | 4.03886000  | 1.36977700  | -1.16937500 |
| C | 6.01963300  | 0.20680500  | -2.74310100 |
| H | 4.65236200  | -1.43900100 | -2.96713800 |
| C | 5.24021000  | 2.03355800  | -1.38498500 |
| H | 3.29186600  | 1.80929400  | -0.51487700 |
| C | 6.23614800  | 1.45961900  | -2.17502800 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 6.79058300  | -0.25638000 | -3.35245600 |
| H  | 5.40588700  | 3.00182900  | -0.92111500 |
| H  | 7.17571200  | 1.97992400  | -2.33593400 |
| H  | 0.29658500  | -1.96638400 | -1.09948000 |
| C  | 2.50926700  | -0.28987200 | 1.84996000  |
| C  | 1.09370100  | -0.36238600 | 1.92489800  |
| C  | 0.37411500  | 0.72998100  | 2.39670900  |
| C  | 1.07190100  | 1.88331100  | 2.77713700  |
| C  | 2.46137100  | 1.94673000  | 2.68297500  |
| C  | 3.20308800  | 0.85003700  | 2.21885900  |
| C  | 1.93565700  | -2.35702900 | 1.02210700  |
| C  | 0.71911900  | -1.61111000 | 1.31873500  |
| H  | -0.71007600 | 0.68421600  | 2.45175100  |
| H  | 0.51885500  | 2.74175900  | 3.14822600  |
| H  | 2.98149600  | 2.85350700  | 2.97806300  |
| H  | 4.28628000  | 0.89459300  | 2.14231400  |
| O  | 2.09500800  | -3.45823300 | 0.50392700  |
| N  | 2.99006100  | -1.48948700 | 1.34830300  |
| C  | 4.36877100  | -1.79424300 | 1.07940900  |
| H  | 4.94192200  | -1.89130900 | 2.00985600  |
| H  | 4.38269800  | -2.74739300 | 0.54621800  |
| H  | 4.82964300  | -1.01820200 | 0.45732900  |
| Cl | -0.74701000 | -2.44800100 | 1.70416400  |

## TS10-B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.98086400 | 0.22798400  | -0.44594700 |
| C | -1.95241800 | -0.73441900 | -0.85137900 |
| C | -3.29758900 | -0.51045700 | -0.80771700 |
| C | -3.79462800 | 0.79013100  | -0.34233400 |
| C | -2.79887000 | 1.77453300  | 0.11995600  |
| C | -1.46897500 | 1.46986300  | 0.05953700  |
| H | -1.56796200 | -1.68824600 | -1.20068700 |
| H | -0.74254300 | 2.19366700  | 0.41203100  |
| O | -5.01740700 | 1.05503500  | -0.33280300 |
| C | -3.30028700 | 3.11495600  | 0.66432100  |
| C | -2.14862900 | 4.01472800  | 1.12803100  |
| C | -4.07508300 | 3.87204500  | -0.42971000 |
| C | -4.22032200 | 2.87649600  | 1.87565900  |
| H | -1.56565800 | 3.54498100  | 1.92828000  |
| H | -1.46830300 | 4.25997900  | 0.30413500  |
| H | -2.55729700 | 4.95523200  | 1.51558500  |
| H | -4.92137200 | 3.27684200  | -0.77392900 |
| H | -4.44190700 | 4.82995500  | -0.03736600 |
| H | -3.41860000 | 4.08246200  | -1.28231300 |
| H | -5.07374600 | 2.26179800  | 1.58795400  |
| H | -3.66912700 | 2.36637900  | 2.67370300  |
| H | -4.58237300 | 3.83634100  | 2.26761100  |
| C | -4.30921400 | -1.59509300 | -1.18256100 |
| C | -5.19904300 | -1.90027400 | 0.03663700  |
| C | -5.18262400 | -1.13562800 | -2.36241800 |
| C | -3.61330000 | -2.90300200 | -1.57826100 |
| H | -4.57943400 | -2.25027500 | 0.86973900  |
| H | -5.73971900 | -1.00530000 | 0.34710100  |
| H | -5.92207500 | -2.68840200 | -0.21310200 |
| H | -4.56071300 | -0.95313700 | -3.24698100 |
| H | -5.91529000 | -1.91356000 | -2.61604400 |
| H | -5.70985900 | -0.21569500 | -2.10616500 |
| H | -4.37043300 | -3.66397200 | -1.80194600 |
| H | -2.99133800 | -2.77732800 | -2.47271700 |
| H | -2.98047600 | -3.27179000 | -0.76303600 |
| C | 0.38562200  | -0.09166300 | -0.53981400 |
| C | 1.44034500  | 0.90588600  | -0.49499600 |
| H | 1.22048900  | 1.85254800  | -0.00807900 |
| C | 2.66558300  | 0.68641000  | -1.00668500 |
| H | 2.87554900  | -0.29122700 | -1.44193000 |
| C | 3.78914600  | 1.63020700  | -1.01251900 |
| C | 5.07206600  | 1.15600100  | -1.32354600 |
| C | 3.64323000  | 2.99584500  | -0.72496100 |
| C | 6.17128300  | 2.00747900  | -1.32998700 |
| H | 5.19625300  | 0.09787000  | -1.54034400 |
| C | 4.74135600  | 3.84684800  | -0.73110800 |
| H | 2.65733300  | 3.39619900  | -0.50868500 |
| C | 6.01232200  | 3.35858200  | -1.03178200 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 7.15575700  | 1.61424500  | -1.56787400 |
| H  | 4.60364800  | 4.90071500  | -0.50626100 |
| H  | 6.86834500  | 4.02690900  | -1.03833100 |
| H  | 0.63792000  | -0.98824400 | -1.10753400 |
| C  | 2.25167300  | -2.79765100 | 0.33778400  |
| C  | 2.32455200  | -1.58878400 | 1.08492900  |
| C  | 3.56681100  | -0.99548600 | 1.29592900  |
| C  | 4.71018000  | -1.60015100 | 0.76504100  |
| C  | 4.61873100  | -2.76907300 | 0.00921900  |
| C  | 3.37891200  | -3.38535600 | -0.21304200 |
| C  | 0.11204100  | -2.33273700 | 1.04556900  |
| C  | 0.97565500  | -1.20633400 | 1.36501400  |
| H  | 3.63574800  | -0.07187900 | 1.86354600  |
| H  | 5.68047900  | -1.13972900 | 0.92930700  |
| H  | 5.51716700  | -3.21736900 | -0.40529600 |
| H  | 3.30412500  | -4.30275100 | -0.79055400 |
| O  | -1.07672800 | -2.52628600 | 1.25064800  |
| N  | 0.93189700  | -3.20957800 | 0.29443000  |
| C  | 0.44567700  | -4.43152400 | -0.28268100 |
| H  | 0.95590000  | -5.30339100 | 0.14566200  |
| H  | -0.62055200 | -4.48758300 | -0.05363200 |
| H  | 0.58437700  | -4.44242600 | -1.37041000 |
| Cl | 0.52679100  | -0.06405600 | 2.58986700  |

## TS2-CI-A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.73773400 | -0.41690300 | -0.83413800 |
| C | -1.88353900 | -1.24191800 | -1.04164300 |
| C | -3.15235200 | -0.74668500 | -1.14830500 |
| C | -3.37163700 | 0.70543600  | -1.03784800 |
| C | -2.19981500 | 1.55196500  | -0.75557000 |
| C | -0.95882400 | 0.98228000  | -0.66965700 |
| H | -1.70107200 | -2.31066700 | -1.10836900 |
| H | -0.09964900 | 1.60690700  | -0.44317400 |
| O | -4.51328800 | 1.19986300  | -1.16941200 |
| C | -2.41473500 | 3.05659700  | -0.57071500 |
| C | -1.10392000 | 3.79251400  | -0.26985700 |
| C | -3.01018800 | 3.66591200  | -1.85334100 |
| C | -3.36961900 | 3.30537800  | 0.61069000  |
| H | -0.63037800 | 3.42036100  | 0.64602600  |
| H | -0.38697400 | 3.69405200  | -1.09329800 |
| H | -1.31284500 | 4.86039200  | -0.13520300 |
| H | -3.96375400 | 3.19474800  | -2.09246500 |
| H | -3.16316100 | 4.74504100  | -1.72007100 |
| H | -2.32223800 | 3.52162200  | -2.69460000 |
| H | -4.32407600 | 2.80480800  | 0.44227500  |
| H | -2.92259800 | 2.92597700  | 1.53725700  |
| H | -3.54538600 | 4.38214400  | 0.73408600  |
| C | -4.35873800 | -1.65706500 | -1.39336800 |
| C | -5.39400100 | -1.49045300 | -0.26543300 |
| C | -5.01371000 | -1.30002200 | -2.73993300 |
| C | -3.95339500 | -3.13524300 | -1.43683800 |
| H | -4.97397100 | -1.82039700 | 0.69165000  |
| H | -5.70225200 | -0.44780200 | -0.17987100 |
| H | -6.27604600 | -2.10972000 | -0.47467500 |
| H | -4.29809700 | -1.44159900 | -3.55810900 |
| H | -5.87667300 | -1.95337400 | -2.92461100 |
| H | -5.34487600 | -0.26059900 | -2.73637900 |
| H | -4.84899100 | -3.75284500 | -1.57242000 |
| H | -3.27424800 | -3.34315200 | -2.27139700 |
| H | -3.45726200 | -3.44916400 | -0.51100900 |
| C | 0.53114700  | -1.02116600 | -0.76652300 |
| C | 1.77310900  | -0.30609200 | -0.99774600 |
| H | 1.78776000  | 0.76019000  | -0.78266100 |
| C | 2.87404300  | -0.91349400 | -1.47729500 |
| H | 2.81515200  | -1.97920800 | -1.69358400 |
| C | 4.16800600  | -0.28675800 | -1.75965700 |
| C | 5.17755800  | -1.05469700 | -2.35765600 |
| C | 4.45374800  | 1.05552300  | -1.46204900 |
| C | 6.42115000  | -0.50900100 | -2.65578600 |
| H | 4.97436900  | -2.09768600 | -2.58769500 |
| C | 5.69497000  | 1.60190600  | -1.76021700 |
| H | 3.70201300  | 1.67172700  | -0.97990700 |
| C | 6.68605100  | 0.82519200  | -2.35984700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 7.18485300  | -1.12773200 | -3.11846800 |
| H  | 5.89325100  | 2.64185600  | -1.51724300 |
| H  | 7.65610200  | 1.25630700  | -2.58913200 |
| H  | 0.56465300  | -2.09240600 | -0.96999700 |
| C  | -0.35908600 | -0.01713200 | 2.35802900  |
| C  | 1.00005000  | -0.28857700 | 2.02973900  |
| C  | 1.91382700  | 0.74253500  | 2.23451400  |
| C  | 1.50686500  | 1.97849400  | 2.74089300  |
| C  | 0.16701800  | 2.20500000  | 3.04606300  |
| C  | -0.78677300 | 1.20127500  | 2.85830000  |
| C  | -0.32521700 | -2.17276100 | 1.57665500  |
| C  | 1.00256900  | -1.59383500 | 1.42944500  |
| H  | 2.25063900  | 2.75356200  | 2.89041700  |
| H  | -0.13856100 | 3.17420400  | 3.42826800  |
| H  | -1.83430100 | 1.36760200  | 3.08827400  |
| O  | -0.75844100 | -3.26764200 | 1.23235000  |
| N  | -1.11274200 | -1.14574400 | 2.10488900  |
| C  | -2.54554000 | -1.21385600 | 2.21674200  |
| H  | -3.01414200 | -0.41994200 | 1.62313300  |
| H  | -2.84873300 | -2.18487900 | 1.82020000  |
| H  | -2.86186000 | -1.12768700 | 3.26345500  |
| Cl | 2.36755200  | -2.64823500 | 1.27757300  |
| Cl | 3.61295800  | 0.52315900  | 1.86511400  |

# TS11-Cl-A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.22932300 | 0.03890300  | -0.51163000 |
| C | -2.22429600 | -0.89580500 | -0.90524100 |
| C | -3.56564700 | -0.62490500 | -0.86280300 |
| C | -4.02129800 | 0.67872900  | -0.36436200 |
| C | -2.99524500 | 1.61716100  | 0.11184000  |
| C | -1.67218300 | 1.28354700  | 0.01379700  |
| H | -1.87005200 | -1.85925300 | -1.26477600 |
| H | -0.92067600 | 1.96878200  | 0.38929700  |
| O | -5.23917200 | 0.97743500  | -0.33808400 |
| C | -3.44562100 | 2.94535900  | 0.72582700  |
| C | -2.25624000 | 3.78071100  | 1.21538500  |
| C | -4.21565100 | 3.77714200  | -0.31522200 |
| C | -4.35195500 | 2.67384100  | 1.94058700  |
| H | -1.66513100 | 3.24105800  | 1.96368600  |
| H | -1.59227100 | 4.06068200  | 0.38863200  |
| H | -2.62754800 | 4.70597300  | 1.67199500  |
| H | -5.08432900 | 3.22269800  | -0.67222800 |
| H | -4.54760900 | 4.72527700  | 0.12900400  |
| H | -3.56765600 | 4.00987200  | -1.16870400 |
| H | -5.22623000 | 2.09584800  | 1.63895300  |
| H | -3.79951900 | 2.11371700  | 2.70321800  |
| H | -4.68210200 | 3.62325100  | 2.38322600  |
| C | -4.61568800 | -1.64574100 | -1.30808600 |
| C | -5.55609700 | -1.97235500 | -0.13359700 |
| C | -5.43644200 | -1.08148700 | -2.48172600 |
| C | -3.97803500 | -2.96068100 | -1.77139100 |
| H | -4.98667200 | -2.40944700 | 0.69473800  |
| H | -6.05027100 | -1.06570000 | 0.21727600  |
| H | -6.31590900 | -2.70007700 | -0.44897500 |
| H | -4.78341300 | -0.88555900 | -3.34043100 |
| H | -6.20050100 | -1.80675800 | -2.79266600 |
| H | -5.92217000 | -0.15053400 | -2.18737700 |
| H | -4.76697700 | -3.66165800 | -2.06871000 |
| H | -3.32022800 | -2.81005300 | -2.63507100 |
| H | -3.39255500 | -3.42961800 | -0.97243100 |
| C | 0.14145900  | -0.31763700 | -0.60413000 |
| C | 1.18453800  | 0.68390100  | -0.80708800 |
| H | 0.97346300  | 1.69063700  | -0.45031100 |
| C | 2.37796500  | 0.40850100  | -1.36161700 |
| H | 2.58583400  | -0.61688100 | -1.67070900 |
| C | 3.48248300  | 1.35987800  | -1.53731600 |
| C | 4.76873600  | 0.86956400  | -1.80671500 |
| C | 3.31759600  | 2.75043000  | -1.43246000 |
| C | 5.85326200  | 1.72939400  | -1.94355300 |
| H | 4.90930400  | -0.20562500 | -1.88651400 |
| C | 4.40144000  | 3.60949500  | -1.56665200 |
| H | 2.32812100  | 3.16126300  | -1.25491400 |
| C | 5.67664600  | 3.10521000  | -1.82059100 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 6.84031100  | 1.32294500  | -2.14601000 |
| H  | 4.24844900  | 4.68155500  | -1.48088400 |
| H  | 6.52101400  | 3.77951100  | -1.92827400 |
| H  | 0.34180400  | -1.27238700 | -1.09372700 |
| C  | 3.01755500  | -0.81207200 | 1.31351100  |
| C  | 2.01313400  | -1.75983800 | 0.97559400  |
| C  | 2.42289200  | -2.90614400 | 0.30251600  |
| C  | 3.76960400  | -3.12655500 | 0.00778600  |
| C  | 4.72577800  | -2.17829100 | 0.36453600  |
| C  | 4.35908900  | -1.00016500 | 1.02047100  |
| C  | 1.02892900  | 0.10111500  | 2.00826100  |
| C  | 0.74011700  | -1.14696500 | 1.28102800  |
| H  | 4.05317000  | -4.03790800 | -0.50702200 |
| H  | 5.76904000  | -2.35615700 | 0.12150400  |
| H  | 5.09518800  | -0.24291100 | 1.27185000  |
| O  | 0.27318700  | 0.90891500  | 2.52067700  |
| N  | 2.42061000  | 0.27027600  | 1.92712300  |
| C  | 3.08321500  | 1.49946000  | 2.27358600  |
| H  | 3.56134800  | 1.94464400  | 1.39190300  |
| H  | 2.31470700  | 2.17299800  | 2.65765600  |
| H  | 3.84166700  | 1.33525300  | 3.04772600  |
| Cl | -0.66629900 | -2.03776600 | 1.76564700  |
| Cl | 1.24969400  | -4.09343100 | -0.22298800 |

## TS12-Cl-A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.41090700 | -0.48068100 | 0.66393100  |
| C | -1.52199600 | 0.20403200  | 1.23005700  |
| C | -2.79453500 | -0.30083600 | 1.22585300  |
| C | -3.05490700 | -1.59070600 | 0.57559700  |
| C | -1.91270300 | -2.28320500 | -0.03941300 |
| C | -0.66338700 | -1.73019500 | 0.03559000  |
| H | -1.31792200 | 1.17098400  | 1.68700800  |
| H | 0.17483300  | -2.24238200 | -0.42444300 |
| O | -4.20594300 | -2.08740900 | 0.54915400  |
| C | -2.16899700 | -3.60639000 | -0.76540300 |
| C | -0.88648300 | -4.18874100 | -1.37079800 |
| C | -2.74304200 | -4.64762700 | 0.21234800  |
| C | -3.16372300 | -3.37625700 | -1.91805400 |
| H | -0.43711700 | -3.50416600 | -2.09922700 |
| H | -0.13872200 | -4.41136600 | -0.60079200 |
| H | -1.12330900 | -5.12567600 | -1.88855800 |
| H | -3.67118000 | -4.28039400 | 0.65152600  |
| H | -2.93895000 | -5.59162300 | -0.31368900 |
| H | -2.02448000 | -4.84882400 | 1.01570800  |
| H | -4.10255600 | -2.97673900 | -1.53306200 |
| H | -2.74407500 | -2.66581900 | -2.63992000 |
| H | -3.36007700 | -4.32140400 | -2.44193100 |
| C | -3.96938300 | 0.44640500  | 1.86129300  |
| C | -5.02382200 | 0.76150000  | 0.78512900  |
| C | -4.60501500 | -0.41287100 | 2.96932600  |
| C | -3.53451500 | 1.77398300  | 2.49271600  |
| H | -4.58326500 | 1.39154900  | 0.00380300  |
| H | -5.38507900 | -0.16073000 | 0.32863100  |
| H | -5.86952400 | 1.30339600  | 1.22979700  |
| H | -3.87450100 | -0.60672100 | 3.76373900  |
| H | -5.45903700 | 0.11595800  | 3.41356800  |
| H | -4.94456900 | -1.36521600 | 2.56093200  |
| H | -4.40863700 | 2.26748700  | 2.93447100  |
| H | -2.79825300 | 1.61928000  | 3.29017300  |
| H | -3.09980000 | 2.45337300  | 1.75059400  |
| C | 0.87056500  | 0.12416900  | 0.69354500  |
| C | 2.10924600  | -0.63629400 | 0.59993700  |
| H | 2.09334100  | -1.56577200 | 0.03611500  |
| C | 3.26193100  | -0.22572000 | 1.15247000  |
| H | 3.26704100  | 0.68121500  | 1.75726400  |
| C | 4.54563800  | -0.92351200 | 1.00737200  |
| C | 5.49738300  | -0.88476000 | 2.03401900  |
| C | 4.85612200  | -1.62961600 | -0.16330200 |
| C | 6.70682200  | -1.56092900 | 1.91426600  |
| H | 5.27421600  | -0.32533800 | 2.93926700  |
| C | 6.06328400  | -2.30793300 | -0.28218400 |
| H | 4.15383000  | -1.60255400 | -0.99148800 |
| C | 6.99210800  | -2.28190600 | 0.75714600  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 7.42851000  | -1.52507000 | 2.72564700  |
| H  | 6.28910600  | -2.84550600 | -1.19871200 |
| H  | 7.93740400  | -2.80785300 | 0.65947300  |
| H  | 0.94417700  | 1.02663800  | 1.30462100  |
| C  | 0.42569700  | 3.29589200  | -0.33227600 |
| C  | -0.04693800 | 2.14974300  | -1.03142800 |
| C  | -1.41126700 | 2.08054600  | -1.30193200 |
| C  | -2.26196400 | 3.12072700  | -0.91317100 |
| C  | -1.76595600 | 4.22023300  | -0.22181100 |
| C  | -0.40510600 | 4.32198300  | 0.08397100  |
| C  | 2.27896600  | 2.02509700  | -0.80404900 |
| C  | 1.08301700  | 1.25950400  | -1.15654100 |
| H  | -3.31714800 | 3.04764900  | -1.15235900 |
| H  | -2.44746200 | 5.00805100  | 0.08402000  |
| H  | -0.00916100 | 5.17801800  | 0.62170000  |
| O  | 3.46502200  | 1.75750500  | -0.91716200 |
| N  | 1.79538700  | 3.18381500  | -0.16627600 |
| C  | 2.65958600  | 4.19273900  | 0.38089000  |
| H  | 2.43511200  | 4.37500300  | 1.43817300  |
| H  | 3.68059300  | 3.81890500  | 0.28261800  |
| H  | 2.56351300  | 5.13839200  | -0.16694700 |
| Cl | 1.23493400  | 0.03765600  | -2.38768700 |
| Cl | -2.10914000 | 0.73172700  | -2.15174100 |

## TS2-CI-B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.31728000 | 0.27171300  | -0.73216200 |
| C | -1.48183800 | -0.35706400 | -1.25431900 |
| C | -2.72438200 | 0.21657100  | -1.23436600 |
| C | -2.89435600 | 1.53411800  | -0.61089600 |
| C | -1.68989200 | 2.19917900  | -0.08305400 |
| C | -0.47877500 | 1.56229700  | -0.15186900 |
| H | -1.34001000 | -1.33464000 | -1.70987400 |
| H | 0.40669200  | 2.05252300  | 0.24525200  |
| O | -4.01681600 | 2.08838700  | -0.55290400 |
| C | -1.83608800 | 3.61797000  | 0.47873100  |
| C | -0.49642800 | 4.20327000  | 0.94220200  |
| C | -2.38416400 | 4.55225600  | -0.61742800 |
| C | -2.80172800 | 3.62665700  | 1.67782700  |
| H | -0.04205200 | 3.61758500  | 1.74906700  |
| H | 0.22400800  | 4.26230600  | 0.11876800  |
| H | -0.65838800 | 5.21934500  | 1.32043600  |
| H | -3.35502800 | 4.19977700  | -0.96609400 |
| H | -2.48937900 | 5.57198100  | -0.22405900 |
| H | -1.69137100 | 4.58431900  | -1.46623500 |
| H | -3.77194600 | 3.22706200  | 1.38101200  |
| H | -2.40483000 | 3.01801900  | 2.49976200  |
| H | -2.93011700 | 4.65115300  | 2.05156300  |
| C | -3.93352300 | -0.43797200 | -1.90994200 |
| C | -5.07519100 | -0.66819000 | -0.90421300 |
| C | -4.43565800 | 0.47678300  | -3.04294500 |
| C | -3.57758400 | -1.79648100 | -2.52500800 |
| H | -4.76925300 | -1.40326800 | -0.15328600 |
| H | -5.33763700 | 0.26586400  | -0.40631800 |
| H | -5.95861000 | -1.06017200 | -1.42605900 |
| H | -3.64498100 | 0.62800900  | -3.78700400 |
| H | -5.29597700 | 0.01644400  | -3.54668300 |
| H | -4.73347600 | 1.44673900  | -2.64184300 |
| H | -4.47472500 | -2.23655900 | -2.97647800 |
| H | -2.81928800 | -1.70113600 | -3.31048600 |
| H | -3.20045200 | -2.49453900 | -1.76835200 |
| C | 0.92357000  | -0.40675200 | -0.80953900 |
| C | 2.21770300  | 0.25449700  | -0.74203900 |
| H | 2.30693400  | 1.13906600  | -0.11575000 |
| C | 3.31341300  | -0.20638600 | -1.36773700 |
| H | 3.22467100  | -1.06315600 | -2.03498600 |
| C | 4.65048100  | 0.38057400  | -1.20786600 |
| C | 5.57168300  | 0.36099200  | -2.26300700 |
| C | 5.03676900  | 0.95425800  | 0.01347700  |
| C | 6.83061700  | 0.93467600  | -2.12169100 |
| H | 5.28559800  | -0.09888600 | -3.20598600 |
| C | 6.29527000  | 1.52975000  | 0.15011700  |
| H | 4.35276300  | 0.89470000  | 0.85716500  |
| C | 7.19474000  | 1.52867700  | -0.91515300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 7.52893400  | 0.91850500  | -2.95401500 |
| H  | 6.58364300  | 1.96591200  | 1.10243100  |
| H  | 8.17880700  | 1.97443200  | -0.80101200 |
| H  | 0.91884500  | -1.32380000 | -1.40089800 |
| C  | -0.74680000 | -0.98992400 | 2.00799600  |
| C  | -0.20523200 | -2.03201400 | 1.20775600  |
| C  | -1.10505200 | -2.95817600 | 0.69260700  |
| C  | -2.46155900 | -2.90117600 | 1.01088000  |
| C  | -2.94826200 | -1.86511100 | 1.80521000  |
| C  | -2.09445800 | -0.88216100 | 2.30501200  |
| C  | 1.50829800  | -0.59295300 | 1.90852400  |
| C  | 1.17676200  | -1.68756100 | 0.99441100  |
| H  | -3.13082400 | -3.65353500 | 0.60712900  |
| H  | -4.00960000 | -1.81674400 | 2.02551300  |
| H  | -2.47249100 | -0.05281800 | 2.89422600  |
| O  | 2.58310500  | -0.06075400 | 2.16699800  |
| N  | 0.28149000  | -0.15590700 | 2.40696500  |
| C  | 0.12169800  | 1.02452500  | 3.21023200  |
| H  | -0.21623500 | 0.77434600  | 4.22320100  |
| H  | 1.09799500  | 1.51069700  | 3.26285100  |
| H  | -0.60583200 | 1.69714400  | 2.74292000  |
| Cl | 2.43400800  | -2.80223900 | 0.55916900  |
| Cl | -0.56187000 | -4.20996400 | -0.40728000 |

## TS13-CI-B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.71799900 | -0.31902100 | -0.96286900 |
| C | -1.84534600 | -1.14247200 | -1.25297400 |
| C | -3.12967600 | -0.68130000 | -1.24518300 |
| C | -3.38507600 | 0.73437200  | -0.93223900 |
| C | -2.22618200 | 1.58203700  | -0.60305600 |
| C | -0.97053400 | 1.04599000  | -0.62804400 |
| H | -1.63524100 | -2.18220900 | -1.48632800 |
| H | -0.12216600 | 1.66477300  | -0.35223700 |
| O | -4.54452600 | 1.20143000  | -0.94768100 |
| C | -2.47902400 | 3.04057300  | -0.21370600 |
| C | -1.17941100 | 3.77678100  | 0.13285300  |
| C | -3.14794100 | 3.79084400  | -1.37977700 |
| C | -3.38971600 | 3.09428600  | 1.02630200  |
| H | -0.66338600 | 3.31115400  | 0.98069800  |
| H | -0.48997800 | 3.80344400  | -0.71935100 |
| H | -1.41353200 | 4.81275100  | 0.40515900  |
| H | -4.09064200 | 3.31272800  | -1.64760400 |
| H | -3.33998300 | 4.83387100  | -1.09498600 |
| H | -2.48926100 | 3.79361100  | -2.25637900 |
| H | -4.34727500 | 2.61620600  | 0.81746900  |
| H | -2.91228800 | 2.57239900  | 1.86335100  |
| H | -3.56239200 | 4.13767100  | 1.32218300  |
| C | -4.32356700 | -1.59384000 | -1.53218100 |
| C | -5.25418800 | -1.62058000 | -0.30570800 |
| C | -5.10042900 | -1.08905200 | -2.76127800 |
| C | -3.88472500 | -3.03580100 | -1.81204600 |
| H | -4.71751800 | -2.01664800 | 0.56418500  |
| H | -5.60881300 | -0.61542400 | -0.07485600 |
| H | -6.11699700 | -2.27109800 | -0.50153400 |
| H | -4.45542500 | -1.10009800 | -3.64785300 |
| H | -5.96026400 | -1.74320900 | -2.95786500 |
| H | -5.45444900 | -0.07119200 | -2.59491100 |
| H | -4.77066200 | -3.65546700 | -1.99369400 |
| H | -3.24339000 | -3.09974800 | -2.69859000 |
| H | -3.34025200 | -3.46308000 | -0.96250300 |
| C | 0.56714300  | -0.88827900 | -0.95534000 |
| C | 1.78326700  | -0.10496200 | -1.10943700 |
| H | 1.76696000  | 0.93568000  | -0.79007500 |
| C | 2.91626200  | -0.63182100 | -1.60970800 |
| H | 2.92905100  | -1.69255500 | -1.85142100 |
| C | 4.18703600  | 0.08074400  | -1.77234900 |
| C | 5.37882700  | -0.65736300 | -1.82277600 |
| C | 4.27056200  | 1.47914200  | -1.85410200 |
| C | 6.61152600  | -0.02270400 | -1.92529200 |
| H | 5.32224000  | -1.74066300 | -1.74874900 |
| C | 5.50302100  | 2.11339700  | -1.95527900 |
| H | 3.35849200  | 2.06887500  | -1.85214200 |
| C | 6.68052500  | 1.36736000  | -1.98884400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 7.52189600  | -0.61490500 | -1.95155900 |
| H  | 5.54488900  | 3.19716000  | -2.01731100 |
| H  | 7.64192100  | 1.86573800  | -2.07035800 |
| H  | 0.64809300  | -1.91889700 | -1.30135700 |
| C  | 1.84509100  | 0.00750800  | 2.18583200  |
| C  | 0.57647800  | -0.60183400 | 1.95588200  |
| C  | -0.54902500 | 0.07422200  | 2.42181000  |
| C  | -0.41751100 | 1.30267700  | 3.08015600  |
| C  | 0.83410700  | 1.87924700  | 3.26009500  |
| C  | 1.99199400  | 1.23239500  | 2.81122900  |
| C  | 2.27268300  | -1.94989900 | 1.06521700  |
| C  | 0.83378200  | -1.75653800 | 1.14085300  |
| H  | -1.31212100 | 1.79774900  | 3.44208100  |
| H  | 0.91176100  | 2.83999900  | 3.75969300  |
| H  | 2.97522900  | 1.66998500  | 2.95473400  |
| O  | 2.93743000  | -2.81996300 | 0.51166500  |
| N  | 2.83071100  | -0.81471900 | 1.67393300  |
| C  | 4.22949900  | -0.49247100 | 1.60294400  |
| H  | 4.66456600  | -0.40199700 | 2.60556500  |
| H  | 4.71557400  | -1.30940600 | 1.06610000  |
| H  | 4.39353900  | 0.44348000  | 1.05437000  |
| Cl | -0.21040200 | -3.13816500 | 1.00867100  |
| Cl | -2.15401700 | -0.58014200 | 2.23490300  |

## TS14-CI-B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.21426900 | 0.15925400  | -0.46188200 |
| C | -2.21158500 | -0.76775700 | -0.86537700 |
| C | -3.55316400 | -0.50504200 | -0.80506100 |
| C | -4.01037500 | 0.79864700  | -0.31624800 |
| C | -2.98299800 | 1.74736300  | 0.13494500  |
| C | -1.65860200 | 1.40621700  | 0.05340800  |
| H | -1.86153600 | -1.72779300 | -1.23492900 |
| H | -0.90824100 | 2.10931600  | 0.39922000  |
| O | -5.23013600 | 1.09396700  | -0.28279700 |
| C | -3.43648200 | 3.09927700  | 0.69359800  |
| C | -2.25373700 | 3.96527200  | 1.14306400  |
| C | -4.20802700 | 3.88254800  | -0.38402800 |
| C | -4.34387600 | 2.88023700  | 1.91804900  |
| H | -1.67087400 | 3.47608300  | 1.93179500  |
| H | -1.57968500 | 4.19578700  | 0.30970600  |
| H | -2.63024200 | 4.91489200  | 1.54129800  |
| H | -5.07144700 | 3.30728100  | -0.71973900 |
| H | -4.54789000 | 4.84617900  | 0.01902000  |
| H | -3.55816300 | 4.08326100  | -1.24409600 |
| H | -5.21366900 | 2.28421200  | 1.63978300  |
| H | -3.79228400 | 2.35642300  | 2.70712100  |
| H | -4.67932300 | 3.84692600  | 2.31736900  |
| C | -4.59751800 | -1.54945000 | -1.20534200 |
| C | -5.49987800 | -1.85861100 | 0.00340400  |
| C | -5.45541300 | -1.02935900 | -2.37168400 |
| C | -3.94686900 | -2.86789200 | -1.64160300 |
| H | -4.89710900 | -2.26076600 | 0.82541000  |
| H | -6.00135300 | -0.95103700 | 0.34167400  |
| H | -6.25482000 | -2.60800000 | -0.27086200 |
| H | -4.82765600 | -0.84647600 | -3.25206800 |
| H | -6.21653000 | -1.77308900 | -2.64429600 |
| H | -5.94697300 | -0.09763400 | -2.08892500 |
| H | -4.72994300 | -3.59550200 | -1.88660400 |
| H | -3.32279900 | -2.73566300 | -2.53362300 |
| H | -3.32465800 | -3.28672500 | -0.84237500 |
| C | 0.15844600  | -0.20245800 | -0.57128000 |
| C | 1.21600800  | 0.80528300  | -0.64738700 |
| H | 1.06370000  | 1.73779200  | -0.10951400 |
| C | 2.36565700  | 0.58888100  | -1.30754600 |
| H | 2.51035800  | -0.38048300 | -1.78747000 |
| C | 3.50446700  | 1.50926900  | -1.39826500 |
| C | 4.74448800  | 1.01553800  | -1.82653300 |
| C | 3.41691100  | 2.86694000  | -1.05648900 |
| C | 5.86196600  | 1.84073200  | -1.89653800 |
| H | 4.82518800  | -0.03744400 | -2.08593200 |
| C | 4.53179400  | 3.69188100  | -1.12738200 |
| H | 2.46313800  | 3.27943700  | -0.74180100 |
| C | 5.76141800  | 3.18425200  | -1.54594400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 6.81385400  | 1.43293900  | -2.22527500 |
| H  | 4.44074000  | 4.74017200  | -0.85761600 |
| H  | 6.63110900  | 3.83237100  | -1.60095700 |
| H  | 0.35821600  | -1.07412100 | -1.19878300 |
| C  | 2.13671300  | -2.78256300 | 0.24834200  |
| C  | 2.13670500  | -1.54713200 | 0.95521900  |
| C  | 3.36216700  | -0.90805200 | 1.11619000  |
| C  | 4.53477500  | -1.45990400 | 0.59335200  |
| C  | 4.49069900  | -2.65645800 | -0.11478900 |
| C  | 3.28308300  | -3.33943900 | -0.29460100 |
| C  | -0.02819600 | -2.43497100 | 0.92479500  |
| C  | 0.74813700  | -1.20999900 | 1.19020200  |
| H  | 5.46969800  | -0.92870600 | 0.73479900  |
| H  | 5.40792000  | -3.06787000 | -0.52488300 |
| H  | 3.24229100  | -4.27950400 | -0.83615700 |
| O  | -1.19305100 | -2.69663000 | 1.15319300  |
| N  | 0.84568700  | -3.27768900 | 0.21325300  |
| C  | 0.44367000  | -4.54717800 | -0.32825100 |
| H  | 0.98498100  | -5.37207900 | 0.15078700  |
| H  | -0.62487500 | -4.65061900 | -0.12984900 |
| H  | 0.61955800  | -4.58854900 | -1.40918800 |
| Cl | 0.19197500  | -0.19391200 | 2.48612300  |
| Cl | 3.48557400  | 0.60168700  | 1.98452300  |

# TS4'-A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.74565200  | 3.55873400  | 0.45585400  |
| C | 1.34351300  | 2.25462600  | 0.88806200  |
| C | 1.44743200  | 1.95034300  | 2.26226300  |
| C | 1.89679100  | 2.91843500  | 3.14378300  |
| C | 2.25979700  | 4.19636200  | 2.69025900  |
| C | 2.19557200  | 4.52943600  | 1.33936800  |
| C | 1.17233500  | 2.43005600  | -1.42723000 |
| C | 0.96516300  | 1.53344200  | -0.27149800 |
| H | 1.20025000  | 0.96037200  | 2.62616300  |
| H | 1.97688300  | 2.68419600  | 4.19985100  |
| H | 2.60806200  | 4.93678600  | 3.40334200  |
| H | 2.49282900  | 5.51181300  | 0.98699800  |
| O | 1.00391800  | 2.21197600  | -2.62172200 |
| N | 1.62886200  | 3.64345900  | -0.91230000 |
| C | 1.96930500  | 4.78209500  | -1.72940300 |
| H | 1.35426300  | 5.64785800  | -1.46439900 |
| H | 3.02642600  | 5.04209200  | -1.61325000 |
| H | 1.77598000  | 4.50233800  | -2.76575400 |
| C | 0.40063400  | 0.13717500  | -0.46227400 |
| C | 1.25146000  | -0.62904100 | -1.43863400 |
| C | 1.86769400  | -1.78876500 | -1.16940500 |
| C | 1.72101100  | -2.38799300 | 0.19389900  |
| C | 0.79515800  | -1.73064800 | 1.17749500  |
| C | 0.22860400  | -0.56371900 | 0.84672100  |
| H | 1.34456700  | -0.15152900 | -2.40857100 |
| H | -0.42779500 | -0.05536800 | 1.54728100  |
| O | 2.33725200  | -3.39650500 | 0.50708900  |
| C | 0.55646000  | -2.41649800 | 2.52450700  |
| C | -0.47519200 | -1.65487600 | 3.36578700  |
| C | 0.01092000  | -3.83935200 | 2.30132900  |
| C | 1.87175200  | -2.47553700 | 3.32272900  |
| H | -0.13986500 | -0.64383600 | 3.62364100  |
| H | -1.44123900 | -1.57837200 | 2.85293100  |
| H | -0.63870600 | -2.19301200 | 4.30454900  |
| H | 0.72790700  | -4.46315200 | 1.76789800  |
| H | -0.20150200 | -4.30369200 | 3.27079200  |
| H | -0.92381600 | -3.80728400 | 1.73028700  |
| H | 2.62728700  | -3.05944400 | 2.79659400  |
| H | 2.26359500  | -1.46631300 | 3.49541800  |
| H | 1.68760900  | -2.93813600 | 4.29899900  |
| C | 2.73343800  | -2.52164900 | -2.19728900 |
| C | 4.18944200  | -2.59490800 | -1.70105500 |
| C | 2.18604600  | -3.94157200 | -2.43087300 |
| C | 2.73156700  | -1.78972900 | -3.54429100 |
| H | 4.58949800  | -1.58803100 | -1.53840100 |
| H | 4.26649800  | -3.15962100 | -0.77157000 |
| H | 4.80864900  | -3.08581700 | -2.46047200 |
| H | 1.15120200  | -3.90041900 | -2.78841400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.78799000  | -4.44250900 | -3.19734500 |
| H | 2.22103800  | -4.53905400 | -1.51928100 |
| H | 3.35060000  | -2.34685100 | -4.25451100 |
| H | 1.72287600  | -1.71596600 | -3.96488700 |
| H | 3.14571700  | -0.77923200 | -3.46126400 |
| C | -0.95304200 | 0.44461600  | -1.09090000 |
| C | -2.18589700 | 0.15645900  | -0.55442100 |
| H | -2.23807000 | -0.38808400 | 0.38483100  |
| C | -3.37780400 | 0.50694800  | -1.19125200 |
| H | -3.29863100 | 1.06032000  | -2.12541800 |
| C | -4.71389400 | 0.20296400  | -0.74292000 |
| C | -5.80893200 | 0.65467400  | -1.50711700 |
| C | -4.99000500 | -0.52704200 | 0.43220900  |
| C | -7.11452300 | 0.39527100  | -1.11762100 |
| H | -5.61578600 | 1.21742000  | -2.41676200 |
| C | -6.29613800 | -0.78439000 | 0.81824400  |
| H | -4.17461200 | -0.89848100 | 1.04496700  |
| C | -7.36664100 | -0.32596000 | 0.04849700  |
| H | -7.93959400 | 0.75542000  | -1.72438500 |
| H | -6.48487000 | -1.34914000 | 1.72611100  |
| H | -8.38714500 | -0.53128800 | 0.35532100  |
| H | -0.89556200 | 0.95827100  | -2.04706200 |

## INT6'-A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.94201100  | 2.91844300  | 0.39931700  |
| C | 2.17113300  | 1.79232500  | 0.83901600  |
| C | 2.32851200  | 1.36075400  | 2.17605800  |
| C | 3.18716400  | 2.04541700  | 3.01579300  |
| C | 3.91141700  | 3.16007100  | 2.55858700  |
| C | 3.80208600  | 3.60613600  | 1.24440500  |
| C | 1.78352000  | 2.20560900  | -1.41351200 |
| C | 1.42163900  | 1.34475800  | -0.27095400 |
| H | 1.79809700  | 0.48720900  | 2.53549700  |
| H | 3.31011600  | 1.71438900  | 4.04136100  |
| H | 4.57744400  | 3.67871400  | 3.24081400  |
| H | 4.37307100  | 4.45782500  | 0.88935400  |
| O | 1.40832200  | 2.14709600  | -2.57874100 |
| N | 2.69164600  | 3.15045700  | -0.93138700 |
| C | 3.30036800  | 4.16857000  | -1.75226300 |
| H | 3.05699100  | 5.16727900  | -1.37648300 |
| H | 4.38811900  | 4.04796200  | -1.77787200 |
| H | 2.89841300  | 4.05127400  | -2.75942600 |
| C | 0.41318700  | 0.22052000  | -0.42869500 |
| C | 0.93146500  | -0.74927600 | -1.46016400 |
| C | 1.14193400  | -2.05599300 | -1.24553800 |
| C | 0.86059300  | -2.62212300 | 0.11102000  |
| C | 0.28749400  | -1.72224400 | 1.16899500  |
| C | 0.12120400  | -0.42376900 | 0.88902000  |
| H | 1.12757400  | -0.29498500 | -2.42644700 |
| H | -0.28453500 | 0.25444100  | 1.63570800  |
| O | 1.08739200  | -3.79757800 | 0.35993600  |
| C | -0.07357700 | -2.33008600 | 2.52633800  |
| C | -0.69309600 | -1.28427800 | 3.46163500  |
| C | -1.11011500 | -3.45329700 | 2.33729200  |
| C | 1.19005200  | -2.88694600 | 3.20723400  |
| H | -0.00155300 | -0.46448000 | 3.68750500  |
| H | -1.61081500 | -0.85498200 | 3.04295000  |
| H | -0.95345300 | -1.76316400 | 4.41057800  |
| H | -0.71058500 | -4.26876400 | 1.73459500  |
| H | -1.39875300 | -3.85177600 | 3.31635800  |
| H | -2.01257600 | -3.06418500 | 1.85171000  |
| H | 1.64142600  | -3.68255100 | 2.61425200  |
| H | 1.93174200  | -2.09278800 | 3.35347000  |
| H | 0.92842200  | -3.28893600 | 4.19255400  |
| C | 1.66662500  | -2.99749700 | -2.33271000 |
| C | 3.02397100  | -3.58758500 | -1.90745400 |
| C | 0.65499600  | -4.13148100 | -2.58069200 |
| C | 1.87185600  | -2.25357500 | -3.65728800 |
| H | 3.75254700  | -2.78764600 | -1.73518000 |
| H | 2.93335600  | -4.18406500 | -0.99929600 |
| H | 3.40931200  | -4.22833900 | -2.70871700 |
| H | -0.31327000 | -3.72150800 | -2.88839200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.02084400  | -4.77553500 | -3.38828300 |
| H | 0.51237700  | -4.74255900 | -1.68892500 |
| H | 2.24139800  | -2.95798100 | -4.40908600 |
| H | 0.93639000  | -1.82439900 | -4.03194600 |
| H | 2.60855500  | -1.44850600 | -3.56340400 |
| C | -0.85227800 | 0.87622500  | -0.97790200 |
| C | -2.11139000 | 0.72942700  | -0.46032000 |
| H | -2.24808500 | 0.09038500  | 0.40909900  |
| C | -3.23789600 | 1.34930800  | -1.01969900 |
| H | -3.07540100 | 1.98779700  | -1.88612400 |
| C | -4.59812900 | 1.22222600  | -0.56585700 |
| C | -5.61359900 | 1.93065400  | -1.24172600 |
| C | -4.97866600 | 0.42000100  | 0.53149700  |
| C | -6.93890300 | 1.84642300  | -0.84283900 |
| H | -5.34103900 | 2.55251400  | -2.09054900 |
| C | -6.30460000 | 0.33876200  | 0.92695200  |
| H | -4.22931500 | -0.14640400 | 1.07569100  |
| C | -7.29375200 | 1.04984000  | 0.24524100  |
| H | -7.69995100 | 2.40275800  | -1.38141400 |
| H | -6.57317400 | -0.28558600 | 1.77370400  |
| H | -8.33033000 | 0.98149800  | 0.55919000  |
| H | -0.70195800 | 1.48184700  | -1.86740500 |

## References

[1] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian 16, Revision C.01; Gaussian, Inc.: Wallingford, CT, 2019.

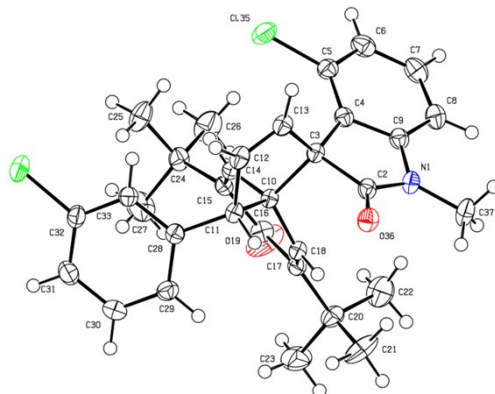
[2] Legault, C. Y. CYLview, 1.0b; Université de Sherbrooke, Canada, 2009; <http://www.cylview.org>.

## 5. Antiproliferative activity of representative compounds

The MM1S cells (20,000 per well) in the 96-well clear plates were incubated in a 37 °C, 5% CO<sub>2</sub> incubator for 12 hours, and then serially diluted compounds 3e, 3ab and 5i were added. After 48 hours of incubation, resazurin sodium salt was added to reach a final concentration of 0.091 mg/mL. Finally, let the mixture incubated for 2-4 hours. SpectraMAX®i3 spectrophotometer was used to measure the resorufin fluorescence intensity at 550 nm/590 nm (excitation/emission), the background was removed. IC<sub>50</sub>=100%\*average fluorescence intensity of treatment group/average fluorescence intensity of control group.

## 6. Crystallographic data

Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication nos. CCDC 2073136, CCDC 2052887, and CCDC 2052888. Copies of these data can be obtained free of charge from the Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).



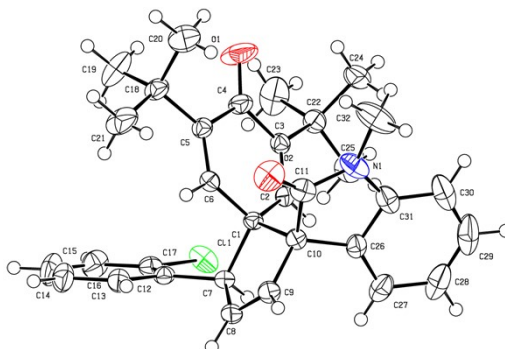
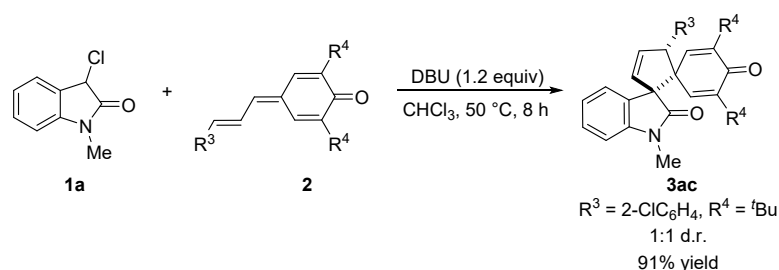
CCDC-2073136

Table S2. Crystal data and structure refinement for **3s**.

|                         |                                                                               |
|-------------------------|-------------------------------------------------------------------------------|
| Identification code     | <b>3s</b>                                                                     |
| Empirical formula       | C <sub>32</sub> H <sub>33</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub> |
| Formula weight          | 534.49                                                                        |
| Temperature/K           | 180.00(10)                                                                    |
| Crystal system          | monoclinic                                                                    |
| Space group             | P2 <sub>1</sub> /n                                                            |
| a/Å                     | 10.3762(2)                                                                    |
| b/Å                     | 14.8979(3)                                                                    |
| c/Å                     | 18.8221(5)                                                                    |
| α /°                    | 90                                                                            |
| β /°                    | 103.007(2)                                                                    |
| γ /°                    | 90                                                                            |
| Volume/Å <sup>3</sup>   | 2834.93(11)                                                                   |
| Z                       | 4                                                                             |
| ρ calcg/cm <sup>3</sup> | 1.252                                                                         |

|                                                  |                                                                        |
|--------------------------------------------------|------------------------------------------------------------------------|
| $\mu$ /mm <sup>-1</sup>                          | 0.258                                                                  |
| F(000)                                           | 1128.0                                                                 |
| Crystal size/mm <sup>3</sup>                     | 0.2 × 0.1 × 0.1                                                        |
| Radiation                                        | Mo K $\alpha$ ( $\lambda$ = 0.71073)                                   |
| 2 $\theta$ range for data collection/ $^{\circ}$ | 4.87 to 54.962                                                         |
| Index ranges                                     | -13 $\leq$ h $\leq$ 13, -19 $\leq$ k $\leq$ 19, -24 $\leq$ l $\leq$ 23 |
| Reflections collected                            | 53262                                                                  |
| Independent reflections                          | 6503 [Rint = 0.0292, Rsigma = 0.0146]                                  |
| Data/restraints/parameters                       | 6503/0/341                                                             |
| Goodness-of-fit on F <sup>2</sup>                | 1.100                                                                  |
| Final R indexes [ $I \geq 2\sigma(I)$ ]          | R1 = 0.0353, wR2 = 0.0973                                              |
| Final R indexes [all data]                       | R1 = 0.0394, wR2 = 0.1047                                              |
| Largest diff. peak/hole / e $\text{\AA}^{-3}$    | 0.30/-0.34                                                             |

The reaction of 3-chlorooxindole **1a** with *p*-VQM **2** ( $R^3$  = 2-ClC<sub>6</sub>H<sub>4</sub>,  $R^4$  = <sup>t</sup>Bu) was conducted, and the product exhibits 1:1 dr. The two diastereomers were isolated, and the relative configurations of the two diastereomers were determined by the X-ray analysis results. Therefore, the relative configurations of other products (1:1 dr) were assigned accordingly compared with the <sup>1</sup>H-NMR spectrum.

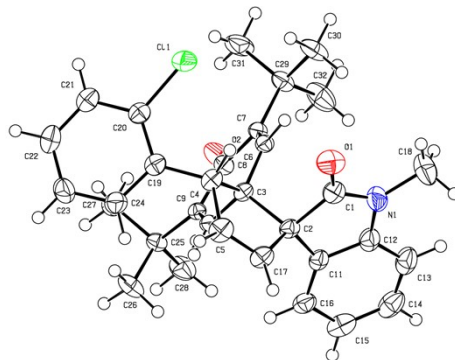


CCDC 2052887

Table S3 Crystal data and structure refinement for **3ac-1**

|                                       |                                                   |
|---------------------------------------|---------------------------------------------------|
| Identification code                   | <b>3ac-1</b>                                      |
| Empirical formula                     | C <sub>32</sub> H <sub>34</sub> ClNO <sub>2</sub> |
| Formula weight                        | 500.05                                            |
| Temperature/K                         | 180.00(10)                                        |
| Crystal system                        | monoclinic                                        |
| Space group                           | P2 <sub>1</sub> /n                                |
| a/ $\text{\AA}$                       | 16.0914(5)                                        |
| b/ $\text{\AA}$                       | 9.8835(3)                                         |
| c/ $\text{\AA}$                       | 18.7907(7)                                        |
| $\alpha$ / $^{\circ}$                 | 90                                                |
| $\beta$ / $^{\circ}$                  | 110.529(4)                                        |
| $\gamma$ / $^{\circ}$                 | 90                                                |
| Volume/ $\text{\AA}^3$                | 2798.68(17)                                       |
| Z                                     | 4                                                 |
| $\rho_{\text{calc}}/\text{g cm}^{-3}$ | 1.187                                             |
| $\mu/\text{mm}^{-1}$                  | 0.165                                             |

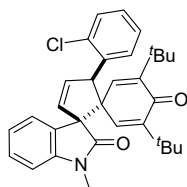
|                                             |                                                               |
|---------------------------------------------|---------------------------------------------------------------|
| F(000)                                      | 1064.0                                                        |
| Crystal size/mm <sup>3</sup>                | 0.2 × 0.2 × 0.2                                               |
| Radiation                                   | Mo Kα (λ = 0.71073)                                           |
| 2θ range for data collection/°              | 4.726 to 52.03                                                |
| Index ranges                                | -19 ≤ h ≤ 19, -12 ≤ k ≤ 12, -23 ≤ l ≤ 23                      |
| Reflections collected                       | 26608                                                         |
| Independent reflections                     | 5508 [R <sub>int</sub> = 0.0242, R <sub>sigma</sub> = 0.0185] |
| Data/restraints/parameters                  | 5508/0/332                                                    |
| Goodness-of-fit on F <sup>2</sup>           | 1.094                                                         |
| Final R indexes [I ≥ 2σ (I)]                | R <sub>1</sub> = 0.0389, wR <sub>2</sub> = 0.1224             |
| Final R indexes [all data]                  | R <sub>1</sub> = 0.0452, wR <sub>2</sub> = 0.1304             |
| Largest diff. peak/hole / e Å <sup>-3</sup> | 0.30/-0.33                                                    |



CCDC 2052888

Table S4 Crystal data and structure refinement for **3ac-2**

|                                             |                                                               |
|---------------------------------------------|---------------------------------------------------------------|
| Identification code                         | <b>3ac-2</b>                                                  |
| Empirical formula                           | C <sub>32</sub> H <sub>34</sub> ClNO <sub>2</sub>             |
| Formula weight                              | 500.05                                                        |
| Temperature/K                               | 179.99(10)                                                    |
| Crystal system                              | monoclinic                                                    |
| Space group                                 | Pn                                                            |
| a/Å                                         | 10.1923(3)                                                    |
| b/Å                                         | 9.7537(3)                                                     |
| c/Å                                         | 13.7328(4)                                                    |
| α/°                                         | 90                                                            |
| β/°                                         | 91.786(2)                                                     |
| γ/°                                         | 90                                                            |
| Volume/Å <sup>3</sup>                       | 1364.55(7)                                                    |
| Z                                           | 2                                                             |
| ρ <sub>calc</sub> /g/cm <sup>3</sup>        | 1.217                                                         |
| μ/mm <sup>-1</sup>                          | 0.169                                                         |
| F(000)                                      | 532.0                                                         |
| Crystal size/mm <sup>3</sup>                | 0.16 × 0.12 × 0.08                                            |
| Radiation                                   | Mo Kα (λ = 0.71073)                                           |
| 2θ range for data collection/°              | 5.782 to 52.044                                               |
| Index ranges                                | -12 ≤ h ≤ 12, -12 ≤ k ≤ 12, -16 ≤ l ≤ 16                      |
| Reflections collected                       | 33145                                                         |
| Independent reflections                     | 5337 [R <sub>int</sub> = 0.0361, R <sub>sigma</sub> = 0.0236] |
| Data/restraints/parameters                  | 5337/2/332                                                    |
| Goodness-of-fit on F <sup>2</sup>           | 1.035                                                         |
| Final R indexes [I ≥ 2σ (I)]                | R <sub>1</sub> = 0.0373, wR <sub>2</sub> = 0.1004             |
| Final R indexes [all data]                  | R <sub>1</sub> = 0.0387, wR <sub>2</sub> = 0.1015             |
| Largest diff. peak/hole / e Å <sup>-3</sup> | 1.18/-0.17                                                    |
| Flack parameter                             | 0.023(17)                                                     |



Yellow foam, isolated yield: 93% (47 mg);

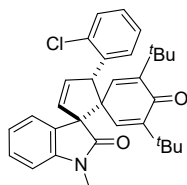
dr = 1:1;

**3ac-1:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.34-7.31 (m, 1H), 7.24-7.18 (m, 3H), 7.15-7.08 (m, 1H), 7.06 (d,  $J = 3.2$  Hz, 1H), 7.03-6.98 (m, 1H), 6.98-6.87 (m, 1H), 6.75 (d,  $J = 3.2$  Hz, 1H), 6.71 (d,  $J = 7.8$  Hz, 1H), 6.52 (dd,  $J = 5.6, 1.6$  Hz, 1H), 5.94 (dd,  $J = 5.6, 2.8$  Hz, 1H), 5.60-5.52 (m, 1H), 3.20 (s, 3H), 1.05 (s, 9H), 0.89 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.1, 176.1, 148.2, 146.6, 143.7, 140.7, 139.8, 139.4, 136.4, 134.2, 132.5, 130.2, 130.0, 129.2, 128.4, 126.9, 126.6, 126.1, 121.6, 107.7, 69.3, 60.5, 54.5, 34.84, 34.79, 29.1, 28.8, 26.2;

IR (neat):  $\nu$  3665, 2235, 1714, 1651, 1514, 1323, 1220, 1050, 873, 694  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{32}\text{H}_{34}\text{ClNO}_2$ : 500.2351; found: 500.2359;



**3ac-2:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.56 (d,  $J = 7.6$  Hz, 1H), 7.32-7.24 (m, 4H), 7.17-7.13 (m, 1H), 7.10-7.04 (m, 1H), 6.73 (d,  $J = 8.0$  Hz, 1H), 6.69 (d,  $J = 2.8$  Hz, 1H), 6.56 (d,  $J = 2.8$  Hz, 1H), 6.39-6.33 (m, 1H), 6.05-5.98 (m, 1H), 5.01 (s, 1H), 3.01 (s, 3H), 0.96 (s, 9H), 0.91 (s, 9H);

$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ):  $\delta$  185.6, 176.0, 145.7, 145.5, 143.4, 142.1, 140.7, 137.0, 136.4, 134.3, 132.9, 130.8, 129.4, 129.0, 128.53, 128.49, 126.3, 124.9, 122.0, 108.1, 70.1, 56.0, 55.8, 34.7, 34.5, 28.9, 28.8, 26.0;

IR (neat):  $\nu$  3715, 2201, 1765, 1674, 1534, 1371, 1204, 1073, 819, 671  $\text{cm}^{-1}$ ;

HRMS (ESI):  $m/z$   $[\text{M} + \text{H}]^+$  calcd. for  $\text{C}_{32}\text{H}_{34}\text{ClNO}_2$ : 500.2351; found: 500.2346;

## 7. Copies of NMR spectra

