Supporting information

An Efficient Organocatalytic Enantioselective Synthesis of Spironitrocyclopropanes

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General methods: All reagents were used as purchased from commercial suppliers without further purification. IR spectra were recorded on a Perkin Elmer 500 spectrometer. NMR spectra were recorded on a Bruker Avance 400/500 NMR spectrometer. Chemical shifts are reported in δ ppm referenced to an internal TMS standard for ¹H NMR and chloroform-d (δ 77.0 ppm) for ¹³C NMR. Enantioselectivities were determined by high performance liquid chromatography (HPLC) analysis. HRMS spectra were recorded on JEOL SX-102A. The X-ray diffraction measurements were carried out at 298 K on a KAPPA APEX II CCD area detector system equipped with a graphite monochromator and a Mo-Kα fine-focus sealed tube (k = 0.71073 Å). Analytical thin layer chromatography (TLC) was performed using Merck 60 F254 precoated silica gel plate (0.2 mm thickness). Flash-chromatography was performed using Merck silica gel 60 (70–230 mesh).
Table 1. Optimization (amount of water) of enantioselective spironitrocyclopropanation reaction between 1a and 2a

<table>
<thead>
<tr>
<th>Entry</th>
<th>H₂O (mmol)</th>
<th>t (h)</th>
<th>Yield (%)&lt;sup&gt;b&lt;/sup&gt;</th>
<th>dr&lt;sup&gt;c&lt;/sup&gt;</th>
<th>ee (%)&lt;sup&gt;d&lt;/sup&gt;</th>
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<tbody>
<tr>
<td>1</td>
<td>-</td>
<td>24</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2&lt;sup&gt;e&lt;/sup&gt;</td>
<td>1.0</td>
<td>2</td>
<td>49</td>
<td>6.5:1</td>
<td>75</td>
</tr>
<tr>
<td>3</td>
<td>0.25</td>
<td>20</td>
<td>70</td>
<td>11:1</td>
<td>90</td>
</tr>
<tr>
<td>4</td>
<td>0.5</td>
<td>9</td>
<td>77</td>
<td>11:1</td>
<td>90</td>
</tr>
<tr>
<td>5</td>
<td>1.0</td>
<td>5</td>
<td>76</td>
<td>11:1</td>
<td>91</td>
</tr>
</tbody>
</table>

<sup>a</sup> Reaction condition: 1a (0.1 mmol), 2a (1.5 eq.), cat. (20 mol%), Na₂CO₃ (1 eq) in 0.5 mL solvent. <sup>b</sup> Isolated yield. <sup>c</sup> Diastereomeric ratio was determined by <sup>1</sup>H NMR spectroscopic analysis of the crude reaction mixture. <sup>d</sup> Enantiomeric excess was determined by HPLC analysis. <sup>e</sup> Reaction was performed at room temperature.
**Table 2.** Optimization (catalyst, temperature screening) of enantioselective spironitrocyclopropanation reaction between 1a and 2a

<table>
<thead>
<tr>
<th>Entry</th>
<th>Cat.</th>
<th>t (h)</th>
<th>Yield (%)</th>
<th>dr</th>
<th>ee (%)</th>
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<tr>
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<tr>
<td>2</td>
<td>II</td>
<td>5</td>
<td>69</td>
<td>11:1</td>
<td>91</td>
</tr>
<tr>
<td>3</td>
<td>III</td>
<td>5</td>
<td>65</td>
<td>10:1</td>
<td>-88</td>
</tr>
<tr>
<td>4</td>
<td>IV</td>
<td>6</td>
<td>79</td>
<td>12:1</td>
<td>-75</td>
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<tr>
<td>5&lt;sup&gt;e&lt;/sup&gt;</td>
<td>V</td>
<td>48</td>
<td>49</td>
<td>-</td>
<td>±</td>
</tr>
<tr>
<td>6&lt;sup&gt;e&lt;/sup&gt;</td>
<td>VI</td>
<td>48</td>
<td>49</td>
<td>-</td>
<td>±</td>
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<tr>
<td>7&lt;sup&gt;g&lt;/sup&gt;</td>
<td>I</td>
<td>6</td>
<td>79</td>
<td>19:1</td>
<td>94</td>
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<tr>
<td>8&lt;sup&gt;h&lt;/sup&gt;</td>
<td>I</td>
<td>24</td>
<td>81</td>
<td>19:1</td>
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<td>9&lt;sup&gt;h&lt;/sup&gt;</td>
<td>I</td>
<td>14</td>
<td>79</td>
<td>16:1</td>
<td>88</td>
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</tbody>
</table>

*Reaction condition: 1a (0.1 mmol), 2a (1.5 eq), cat. (20 mol%), H<sub>2</sub>O (1 eq), Na<sub>2</sub>CO<sub>3</sub> (1 eq.) in 0.5 mL toluene. Isolated yield. Diastereomeric ratio was determined by <sup>1</sup>H NMR spectroscopic analysis of the crude reaction mixture. Enantiomeric excess was determined by HPLC analysis. 60% conversion (determined by <sup>1</sup>H NMR analysis of the crude reaction mixture using CH<sub>2</sub>Br<sub>2</sub> as an internal standard). 66% conversion. Reaction was performed at -20°C in 0.2 mL toluene. Reaction was performed at -40°C in 0.2 mL toluene. Reaction was performed at -20°C in 0.2 mL toluene using 10 mol% I.*
Table 3. Optimization (solvent screening) of enantioselective spironitrocyclopropanation reaction between 1a and 2a

<table>
<thead>
<tr>
<th>Entry</th>
<th>Solvent</th>
<th>t (h)</th>
<th>Yield (%)</th>
<th>dr</th>
<th>ee (%)</th>
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<tbody>
<tr>
<td>1</td>
<td>toluene</td>
<td>5</td>
<td>76</td>
<td>11:1</td>
<td>91</td>
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<tr>
<td>2</td>
<td>CH₂Cl₂</td>
<td>6</td>
<td>78</td>
<td>6.5:1</td>
<td>87</td>
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<td>3</td>
<td>THF</td>
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<td>64</td>
<td>4.3:1</td>
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<td>4</td>
<td>CH₃CN</td>
<td>36</td>
<td>&lt;10</td>
<td>-</td>
<td>nd</td>
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</table>

*a* Reaction condition: 1a (0.1 mmol), 2a (1.5 eq), Na₂CO₃ (1 eq) in 0.2 mL solvent. *b* Isolated yield. *c* Diastereomeric ratio was determined by ¹H NMR spectroscopic analysis of the crude reaction mixture. *d* Enantiomeric excess was determined by HPLC analysis. *e* nd: not determined.

66% conversion (determined by ¹H NMR analysis of the crude reaction mixture using CH₂Br₂ as an internal standard).

Table 4. Optimization (base screening) of enantioselective spironitrocyclopropanation reaction between 1a and 2a

<table>
<thead>
<tr>
<th>Entry</th>
<th>Base</th>
<th>t (h)</th>
<th>Yield (%)</th>
<th>dr</th>
<th>ee (%)</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>Na₂CO₃</td>
<td>5</td>
<td>76</td>
<td>11:1</td>
<td>91</td>
</tr>
<tr>
<td>2</td>
<td>NaHCO₃</td>
<td>48</td>
<td>49</td>
<td>10:1</td>
<td>90</td>
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<tr>
<td>3</td>
<td>K₂CO₃</td>
<td>3</td>
<td>71</td>
<td>9:1</td>
<td>86</td>
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<tr>
<td>4</td>
<td>Cs₂CO₃</td>
<td>2</td>
<td>76</td>
<td>10:1</td>
<td>88</td>
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<td>5</td>
<td>DABCO</td>
<td>2</td>
<td>54</td>
<td>6:1</td>
<td>55</td>
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<td>6</td>
<td>2,6-lutidine</td>
<td>30</td>
<td>47</td>
<td>6:1</td>
<td>77</td>
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</table>

*a* Reaction condition: 1a (0.1 mmol), 2a (1.5 equiv.), Na₂CO₃ (1 eq), NaHCO₃ (1 eq), K₂CO₃ (1 eq), Cs₂CO₃ (1 eq), DABCO (1 eq). Toluene (0.1 mL) was added to the vial after cooling to –20 °C. Bromonitroalkane (2a-c) was added followed by H₂O (0.1 mL) and the resulting mixture was stirred at this condition until completion (monitored by TLC / ¹H NMR). *b* Isolated yield. *c* Diastereomeric ratio was determined by ¹H NMR spectroscopic analysis of the crude reaction mixture. *d* Enantiomeric excess was determined by HPLC analysis. *e* 60% conversion (determined by ¹H NMR analysis of the crude reaction mixture using CH₂Br₂ as an internal standard).

General procedure for the Organocatalytic Enantioselective Synthesis of Spironitrocyclopropanes (3a-o): All the reactions were performed in anhydrous solvents. In a capped glass vial equipped with a magnetic stirring bar was added 2-arylidene-1,3-indandiones 1a-l (0.1 mmol), Na₂CO₃ (0.1 mmol) and catalyst I (20 mol%). Toluene (0.2 mL) was added to the vial after cooling to –20 °C. Bromonitroalkane (2a-c) was added followed by H₂O (0.1 mmol) and the resulting mixture was stirred at this condition until completion (monitored by TLC / ¹H NMR). The reaction mixture was directly subjected to flash column chromatography using ethyl acetate and hexanes (4:1) as eluent.
3a: The compound was prepared following the general procedure and was obtained as a colorless solid.

![Chemical Structure of 3a](image)

$^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ/ppm: 8.09 - 8.01 (m, 1H), 7.95 - 7.83 (m, 3H), 7.47 (d, 2H, J = 8.4 Hz), 7.17 (d, 2H, J = 8.4 Hz), 5.48 (d, 1H, J = 6.8 Hz), 4.41 (d, 1H, J = 6.8 Hz). $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ/ppm: 191.10, 190.80, 142.11, 141.66, 136.02, 135.93, 131.94, 130.49, 128.16, 123.70, 123.40, 123.15, 69.65, 45.57, 41.06. IR (KBr) $\tilde{\nu}$ (cm$^{-1}$): 3010, 1708, 1546, 1365, 1347. HRMS (ESI) C$_{17}$H$_9$BrNO$_4$, [M-H] $^{-}$ (369.9715) found: 369.9718.

The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AD-H column, 254 nm, n-Hexane: IPA = 90:10, flow rate: 1.0 mL/min, t$_R$ (minor) = 35.12 min; t$_R$ (major) = 61.15 min] ee 96%.

Crystallographic data for 3a (CCDC 892806 contains the supplementary crystallographic data for 3a. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre): C$_{17}$H$_9$BrNO$_4$, M = 372.16, monoclinic, Space group $P 2_1$, T = 200 K, a = 9.2201(4) b = 5.4993(3) c = 14.8584(9) Å, alpha = 90 beta = 93.833(3) gamma = 90, V = 751.70(7) Å$^3$, $\lambda$(Mo-K$\alpha$) = 0.71073 Å, Z = 2, D = 1.644 g/cm$^3$, R = 0.0299, wR2 = 0.0825.

![ORTEP Diagram of 3a](image)

3b: The compound was prepared following the general procedure and was obtained as a colorless solid.
$^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ/ppm: 8.08 - 8.02 (m, 1H), 7.95 – 7.82 (m, 3H), 7.33 (d, 2H, $J = 8.8$ Hz), 7.24 (d, 2H, $J = 8.4$ Hz), 5.49 (d, 1H, $J = 7.2$ Hz), 4.44 (d, 1H, $J = 6.8$ Hz). $^{13}$C NMR (125 MHz, CDCl$_3$, 25 °C) δ/ppm: 191.15, 190.89, 142.07, 141.61, 136.04, 135.96, 134.99, 130.20, 128.98, 127.54, 123.70, 123.41, 69.65, 45.59, 40.98. IR (KBr) $\tilde{\nu}$ (cm$^{-1}$): 3022, 1741, 1705, 1587, 1546, 1491, 1351, 1074. HRMS (ESI) C$_{17}$H$_9$ClNO$_4$, [M-H] (326.0220) found: 326.0211.

The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AD-H column, 254 nm, n-Hexane: IPA = 90:10, flow rate: 1.0 mL/min, $t_R$ (minor) = 30.92 min; $t_R$ (major) = 53.22 min] ee 95%.

3c: The compound was prepared following the general procedure and was obtained as a colorless solid.

$^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ/ppm: 8.12 - 8.04 (m, 1H), 7.97 - 7.86 (m, 3H), 7.50 (d, 2H, $J = 8.8$ Hz), 5.54 (d, 1H, $J = 6.8$ Hz), 4.52 (d, 1H, $J = 7.2$ Hz). $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ/ppm: 190.95, 190.38, 148.00, 142.06, 141.51, 136.36, 136.31, 136.22, 130.99, 130.01, 123.85, 123.55, 69.26, 45.29, 39.90. IR (KBr) $\tilde{\nu}$ (cm$^{-1}$): 3025, 1745, 1712, 1590, 1550, 1505, 1347. HRMS (ESI) C$_{17}$H$_9$N$_2$O$_6$, [M-H] (337.0461) found: 337.0466.

The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AD-H column, 254 nm, n-Hexane: IPA = 85:15, flow rate: 1.0 mL/min, $t_R$ (minor) = 59.30 min; $t_R$ (major) = 131.05 min] ee 86%.

3d: The product was prepared following the general procedure and was obtained as a colorless solid.

$^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ/ppm: 8.12 - 8.04 (m, 1H), 7.99 – 7.86 (m, 3H), 7.66 (d, 2H, $J = 8.0$ Hz), 7.44 (d, 2H, $J = 8.0$ Hz), 5.51 (d, 1H, $J = 7.2$ Hz), 4.48 (d, 1H, $J = 7.2$ Hz). $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ/ppm: 190.95, 190.45, 142.01, 141.51, 136.36, 136.31, 136.22, 130.99, 130.01, 123.85, 123.55, 69.26, 45.29, 39.90. IR (KBr) $\tilde{\nu}$ (cm$^{-1}$): 3025, 1745, 1712, 1590, 1550, 1505, 1347. HRMS (ESI) C$_{18}$H$_{10}$N$_2$O$_6$, [M-H] (317.0562) found: 317.0554.

The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AD-H column, 254 nm, n-Hexane: IPA = 80:20, flow rate: 1.0 mL/min, $t_R$ (minor) = 40.73 min; $t_R$ (major) = 80.03 min] ee 92%.
3e: The compound was prepared following the general procedure and was obtained as a colorless solid.

![Structure of compound 3e]

$^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ/ppm: 8.10 - 8.03 (m, 1H), 7.94 – 7.83 (m, 3H), 7.51 (d, 1H, J = 8.0 Hz), 7.46 – 7.36 (m, 2H), 7.30 – 7.21 (m, 1H), 5.43 (d, 1H, J = 6.8 Hz), 4.42 (d, 1H, J = 6.8 Hz).

$^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ/ppm: 190.98, 190.96, 142.14, 141.47, 135.86, 135.81, 132.83, 130.43, 130.35, 129.62, 127.65, 125.64, 123.61, 123.28, 69.85, 44.82, 41.51. IR (KBr) $\tilde{\nu}$ (cm$^{-1}$): 3062, 1738, 1708, 1590, 1557, 1365, 1203.

HRMS (ESI) C$_{17}$H$_9$BrNO$_4$, [M-H] $^{-}$ (369.9715) found: 369.9708.

The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AD-H column, 254 nm, n-Hexane: IPA = 80:20, flow rate: 1.0 mL/min, t$_{R}$ (minor) = 16.55 min; t$_{R}$ (major) = 34.77 min] ee 96%.

3f: The compound was prepared following the general procedure and was obtained as a colorless solid.

![Structure of compound 3f]

$^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ/ppm: 8.10 - 8.03 (m, 1H), 7.94 – 7.83 (m, 3H), 7.51 (d, 1H, J = 8.0 Hz), 7.46 – 7.36 (m, 2H), 7.30 – 7.21 (m, 1H), 5.43 (d, 1H, J = 6.8 Hz), 4.42 (d, 1H, J = 6.8 Hz).

$^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) δ/ppm: 191.04, 190.87, 163.63, 161.66, 142.05, 141.65, 136.03 (d, J = 8.12 Hz), 131.41 (d, J = 7.87 Hz), 130.34 (d, J = 8.37 Hz), 124.63 (d, J = 3.0 Hz), 123.73, 123.46, 116.13 (d, J = 5.0 Hz), 115.95 (d, J = 3.25 Hz), 69.59, 45.51, 40.90 (d, J = 2.25 Hz). IR (KBr) $\tilde{\nu}$ (cm$^{-1}$): 3024, 1730, 1708, 1583, 1553, 1354, 1266. HRMS (ESI) C$_{17}$H$_9$FNO$_6$, [M-H] $^{-}$ (310.0516) found: 310.0513.

The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AD-H column, 254 nm, n-Hexane: IPA = 90:10, flow rate: 1.0 mL/min, t$_{R}$ (minor) = 20.65 min; t$_{R}$ (major) = 32.88 min] ee 86%.

3g: The compound was prepared following the general procedure and was obtained as a colorless solid.

![Structure of compound 3g]

$^1$H NMR (400 MHz, CDCl$_3$, 25 °C) δ/ppm: 8.07 - 8.02 (m, 1H), 7.93 – 7.81 (m, 3H), 7.38 – 7.32 (m, 3H), 7.32 – 7.24 (m, 2H), 5.54 (d, 1H, J = 5.6 Hz), 4.49 (d, 1H, J = 5.6 Hz).

$^{13}$C NMR (125 MHz, CDCl$_3$, 25 °C) δ/ppm: 191.20, 191.19, 142.04, 141.66, 135.87, 135.82, 129.01, 128.88, 128.86, 128.70, 123.60,
123.33, 69.80, 45.77, 42.00. IR (KBr) $\tilde{\nu}$ (cm$^{-1}$): 2915, 1738, 1705, 1587, 1546, 1358. HRMS (ESI) C17H11NO4, [M]$^-$ (293.0688) found: 293.0694.

The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AD-H column, 254 nm, n-Hexane: IPA = 90:10, flow rate: 1.0 mL/min, $t_R$ (minor) = 22.31 min; $t_R$ (major) = 37.60 min] ee 96%.

For ent-3g: The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AD-H column, 254 nm, n-Hexane: IPA = 90:10, flow rate: 1.0 mL/min, $t_R$ (major) = 22.38 min; $t_R$ (minor) = 37.37 min] ee 35%.

3h: The compound was prepared following the general procedure and was obtained as a colorless solid.

\begin{center}
\includegraphics[width=0.2\textwidth]{3h.png}
\end{center}

$^1$H NMR (400 MHz, CDCl$_3$, 25 °C) $\delta$/ppm: 8.03 (d, 1H, $J = 7.2$ Hz), 7.93 – 7.79 (m, 3H), 7.21 – 7.11 (m, 4H), 5.52 (d, 1H, $J = 6.8$ Hz), 4.46 (d, 1H, $J = 6.8$ Hz), 2.32 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) \(\delta\)/ppm: 191.29 (2C), 142.07, 141.66, 138.89, 135.81, 135.76, 129.41, 128.72, 125.90, 123.56, 123.29, 69.91, 45.93, 42.14, 21.19. IR (KBr) $\tilde{\nu}$ (cm$^{-1}$): 2915, 1705, 1601, 1561, 1351. HRMS (ESI) C18H13NO4, [M]$^-$ (307.0845) found: 307.0853.

The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AD-H column, 254 nm, n-Hexane: IPA = 88:12, flow rate: 1.0 mL/min, $t_R$ (minor) = 22.03 min; $t_R$ (major) = 34.01 min] ee 96%.

3i: The compound was prepared following the general procedure and was obtained as a colorless solid.

\begin{center}
\includegraphics[width=0.2\textwidth]{3i.png}
\end{center}

$^1$H NMR (400 MHz, CDCl$_3$, 25 °C) $\delta$/ppm: 8.12 – 8.03 (m, 1H), 7.94 – 7.83 (m, 3H), 7.33 – 7.21 (m, 3H), 7.18 – 7.11 (m, 1H), 5.50 (d, 1H, $J = 7.2$ Hz), 4.41 (d, 1H, $J = 6.8$ Hz), 2.02 (m, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$, 25 °C) \(\delta\)/ppm: 191.36, 191.02, 141.90, 141.28, 137.56, 135.92 (2C), 130.46, 129.05, 128.38, 127.69, 126.15, 123.65, 123.34, 69.95, 45.09, 40.50, 19.49. IR (KBr) $\tilde{\nu}$ (cm$^{-1}$): 2922, 1741, 1708, 1553, 1351, 1258. HRMS (ESI) C18H12NO4, [M-H]$^-$ (306.0766) found: 306.0758.

The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AD-H column, 254 nm, n-Hexane: IPA = 90:10, flow rate: 1.0 mL/min, $t_R$ (minor) = 23.77 min; $t_R$ (major) = 34.01 min] ee 96%.
3j: The compound was prepared following the general procedure and was obtained as a colorless solid.

\[ \text{H NMR (400 MHz, CDCl}_3, 25 ^\circ \text{C)} \delta/\text{ppm: 8.03 (d, 1H, J = 7.2 Hz), 7.95 – 7.79 (m, 3H), 7.36 (d, 2H, J = 8.4 Hz), 7.23 (d, 2H, J = 8.0 Hz), 5.54 (d, 1H, J = 7.2 Hz), 4.44 (d, 1H, J = 7.2 Hz), 1.29 (s, 9H).} \]

\[ \text{C NMR (100 MHz, CDCl}_3, 25 ^\circ \text{C)} \delta/\text{ppm: 191.31, 191.28, 152.04, 142.04, 141.72, 135.81, 135.76, 128.57, 125.97, 125.65, 123.57, 123.32, 70.02, 46.14, 42.26, 34.66, 31.17.} \]

\[ \text{IR (KBr) } \tilde{\nu} (\text{cm}^{-1}): 2959, 2863, 1708, 1601, 1553, 1358.} \]

\[ \text{HRMS (ESI) C21H18NO4, } [\text{M-H}]^- (349.1314) \text{ found: 349.1304.} \]

The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AD-H column, 254 nm, n-Hexane: IPA = 95:05, flow rate: 0.8 mL/min, t_R (minor) = 32.90 min; t_R (major) = 48.04 min] ee 98%.

3k: The compound was prepared following the general procedure and was obtained as a colorless solid.

\[ \text{H NMR (400 MHz, CDCl}_3, 25 ^\circ \text{C)} \delta/\text{ppm: 8.12 – 7.98 (m, 2H), 7.97 – 7.88 (m, 2H), 7.48 (d, 2H, J = 8.0 Hz), 7.02 (d, 2H, J = 8.0 Hz), 4.37 (s, 1H), 1.99 (s, 3H).} \]

\[ \text{C NMR (100 MHz, CDCl}_3, 25 ^\circ \text{C)} \delta/\text{ppm: 192.63, 191.95, 142.73, 141.12, 135.94, 135.89, 131.90, 131.15, 127.95, 123.67, 123.24, 122.63, 80.36, 45.27, 42.71, 13.83.} \]

\[ \text{IR (KBr) } \tilde{\nu} (\text{cm}^{-1}): 3125, 1738, 1705, 1590, 1546, 1347.} \]

\[ \text{HRMS (FAB+) C18H13NO4Br, } [\text{M+H}]^+ (386.0028) \text{ found: 386.0030.} \]

The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AD-H column, 254 nm, n-Hexane: IPA = 90:10, flow rate: 1.0 mL/min, t_R (minor) = 29.38 min; t_R (major) = 31.30 min] ee 96%.

Crystallographic data for 3k (CCDC 892808 contains the supplementary crystallographic data for 3k. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre): C18H12BrN2O4, M = 386.19, monoclinic, Space group P 21, T = 200 K, a = 8.8074(11) b = 9.7518(15) c = 9.7363(14) Å, alpha = 90 beta = 93.785(5) gamma = 90 Å³, \( \lambda(\text{Mo-K}\alpha) = 0.71073 \) Å, Z = 2, D = 1.537 g/cm³, R = 0.0350, wR2 = 0.0731.
3l: The compound was prepared following the general procedure and was obtained as a colorless solid.

\[ \text{ORTEP diagram of 3k} \]

\[^1\text{H NMR}\] (400 MHz, CDCl\textsubscript{3}, 25 °C) δ/ppm: 8.08 – 7.95 (m, 2H), 7.94 – 7.84 (m, 2H), 7.41 – 7.31 (m, 3H), 7.09 - 7.19 (m, 2H), 4.46 (s, 1H), 2.02 (s, 3H). \[^{13}\text{C NMR}\] (100 MHz, CDCl\textsubscript{3}, 25 °C) δ/ppm: 193.01, 192.06, 142.79, 141.08, 135.77 (2C), 129.98, 128.87, 128.45, 128.23, 125.85, 80.72, 45.42, 43.72, 13.96. \[^{\text{IR}}\] (KBr) \(\tilde{\nu}\) (cm\(^{-1}\)): 2988, 1738, 1701, 1590, 1542, 1351, 1247. HRMS (ESI) C\textsubscript{18}H\textsubscript{13}NO\textsubscript{4}Na, [M+Na]\(^+\) (330.0742) found: 330.0750.

The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK IA column, 254 nm, n-Hexane: EtOH = 90:10, flow rate: 1.0 mL/min, \(t_R\) (minor) = 12.67 min; \(t_R\) (major) = 14.36 min] ee 93%.

3m: The compound was prepared following the general procedure and was obtained as a colorless solid.

\[ \text{ORTEP diagram of 3m} \]

\[^1\text{H NMR}\] (400 MHz, CDCl\textsubscript{3}, 25 °C) δ/ppm: 8.07 – 7.96 (m, 2H), 7.94 – 7.85 (m, 2H), 7.15 (d, 2H, \(J = 7.6\) Hz), 7.20 (d, 2H, \(J = 8.0\) Hz), 4.42 (s, 1H), 2.35 (s, 3H), 2.02 (s, 3H). \[^{13}\text{C NMR}\] (100 MHz, CDCl\textsubscript{3}, 25 °C) δ/ppm: 193.12, 192.14, 142.79, 141.09, 138.17, 135.72 (2C), 129.35, 129.31, 125.79, 123.54, 123.12, 80.86, 45.49, 43.72, 21.17, 13.97. \[^{\text{IR}}\] (KBr) \(\tilde{\nu}\) (cm\(^{-1}\)): 2981, 2915, 1741, 1705, 1587, 1546, 1351, 1251. C\textsubscript{19}H\textsubscript{15}NO\textsubscript{4}Na, [M+Na]\(^+\) (344.0899) found: 344.0909.
The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AS-H column, 254 nm, n-Hexane: IPA = 98:02, flow rate: 0.9 mL/min, \( t_R \) (major) = 27.72 min; \( t_R \) (minor) = 108.83 min] ee 96%.

3n: The compound was prepared following the general procedure and was obtained as a colorless solid.

![Chemical structure of 3n](image)

\(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \( \delta \)/ppm: 8.07 – 7.98 (m, 2H), 7.95 – 7.86 (m, 2H), 7.48 (d, 2H, \( J = 8.4 \) Hz), 7.08 (d, 2H, \( J = 8.4 \) Hz), 4.33 (s, 1H), 2.51 – 2.38 (m, 1H), 2.38 – 2.25 (m, 1H), 0.99 (t, 3H, \( J = 7.6 \) Hz). \(^13\)C NMR (100 MHz, CDCl\(_3\), 25 °C) \( \delta \)/ppm: 192.80, 192.26, 142.63, 141.07, 135.97, 135.86, 131.84, 131.17, 128.07, 123.69, 123.23, 122.57, 85.26, 45.43, 43.76, 20.60, 9.84. IR (KBr) \( \nu \) (cm\(^{-1}\)): 2996, 1738, 1701, 1590, 1546, 1351. HRMS (FAB+): C\(_{19}\)H\(_{15}\)NO\(_4\)Br, [M+H]\(^+\) (400.0184) found: 400.0188.

The enantiomeric excess was determined by HPLC analysis. [CHIRALPAK AD-H column, 254 nm, n-Hexane: IPA = 90:10, flow rate: 1.0 mL/min, \( t_R \) (major) = 14.25 min; \( t_R \) (minor) = 17.06 min] ee 56%.

3o: The compound was prepared following the general procedure and was obtained as a colorless liquid. The available data (spectroscopy, hplc) suggest that compound 3o contains (other than diastereomer) an unknown compound. As it was obtained as an inseparable mixture, we are unable to identify the mixture composition, yield or diastereoselectivity.

The following data were obtained from the mixture (after flash column chromatography).

![Chemical structure of 3o](image)

\(^1\)H NMR (400 MHz, CDCl\(_3\), 25 °C) \( \delta \)/ppm: 8.05 – 7.94 (m, 6H), 7.92 – 7.82 (m, 6H), 4.97 - 4.89 (m, 3H), 3.11 – 3.01 (m, 2H), 2.50 – 2.36 (m, 1H), 2.28 – 2.11 (m, 3H), 1.97 – 1.71 (m, 7H), 1.70 – 1.51 (m, 9H), 1.45 – 1.10 (m, 18H), 1.10 – 0.93 (m, 4H). \(^13\)C NMR (100 MHz, CDCl\(_3\), 25 °C) \( \delta \)/ppm: 195.07, 193.53, 192.03, 191.53, 143.92, 141.77, 141.42, 140.43, 135.88, 135.82, 135.64, 135.55, 123.51, 123.43, 123.32, 123.16, 123.11, 71.22, 69.94, 44.83, 43.66, 43.43, 40.70, 33.45, 32.81, 32.30, 32.22, 31.97, 30.59, 25.92, 25.75, 25.53, 25.41, 25.23. IR (KBr) \( \nu \) (cm\(^{-1}\)): 3040, 2922, 2848, 1745, 1708, 1590, 1553, 1354. HRMS (ESI): C\(_{17}\)H\(_{18}\)NO\(_4\), [M+H]\(^+\) (300.1236) found: 300.1234.

The enantiomeric excess was determined by HPLC. [CHIRALPAK IA column, 254 nm, n-Hexane: EtOH = 95:05, flow rate: 0.8 mL/min. \( t_R \) (minor) = 8.95 min; \( t_R \) (major) = 10.45 min] ee 72%.
\( t_R \) (major) = 12.81 min; \( t_R \) (minor) = 16.67 min] ee 87%.
\( t_R \) (minor) = 15.23 min; \( t_R \) (major) = 27.97 min] ee 70%
Current Data Parameters
NAME            Das-371B
EXPNO                1
PROCNO                1

F2 - Acquisition Parameters
Date          20120317
Time              17.09
INSTRUM           spect
PROBHD  5 mm BBO BB-1H
PULPROG            zg30
TD               32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH              0.221142 Hz
FIDRES         2.2611110 sec
AQ                  128
DW               69.000 usec
DE                6.50 usec
TE                303.9 K
D1       2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                14.00 usec
PL1          0 dB
SF01        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF           400.1300087 MHz
WDW                  EM
SSB      0
LB       0 Hz
GB       0
PC                 1.00
Current Data Parameters
NAME             Das-371B
EXPNO            2
PROCNO           1

F2 - Acquisition Parameters
Date              20120317
Time              17.11
INSTRUM           spect
PROBHD            5 mm BBO BB-1H
PULPROG           zgpg30
TD                32768
SOLVENT           CDCl3
NS                1044
DS                24038.461 Hz
FIDRES           0.733596 Hz
AQ                0.6816452 sec
RG                8192
DW               20.800 usec
DE                6.50 usec
TE               303.9 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0              1

======== CHANNEL f1 ========
NUC1              13C
P1                10.50 usec
PL1               7.00 dB
SFO1          100.6233325 MHz

======== CHANNEL f2 ========
CPDPROG2         waltz16
NUC2              1H
PCPD2            90.00 usec
PL2               -0.60 dB
PL12              15.00 dB
PL13               18.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF               100.6127682 MHz
WDW              EM
SSB               0
LB                1.00 Hz
GB               1.00
Current Data Parameters
NAME      Das-425-1
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date       20120510
Time       22.01
INSTRUM    spect
PBH       5 mm PABBO BB-
PULPROG    zgpg30
TD        65536
SOLVENT   CDCl3
NS        3000
DS        0
SWR       30300.029 Hz
F1RES      0.458222 Hz
AQ         1.0912410 sec
RG         9195.2
DW        16.650 usec
DE         6.50 usec
TE        295.4 K
D1        2.0000000 sec
D11       0.2300000 sec
TOO       1

------- CHANNEL f1 -------
NUC1       13C
P1        10.50 usec
PL1       7.00 dB
SFO1      125.7709931 MHz

------- CHANNEL f2 -------
CPDPRG2    waltz16
NUC2       1H
P2        90.00 usec
PL2       -0.60 dB
PL12      15.00 dB
PL13      18.00 dB
SFO2      500.1320005 MHz

F2 - Processing parameters
SI       65536
SF       125.7577917 MHz
WOW      EM
SSB       0
LB       1.00 Hz
GB       0
PC       1.00
Current Data Parameters
NAME       Das-423
EXPNB      3
PROCNO      1

F2 - Acquisition Parameters
Date          20120509
Time           17.14
INSTRUM       spect
PROBHD     5 mm BBO BB-1H
PULPROG     zg30
TD            32768
SOLVENT      CDCl3
NS            16
DS            0
SWN       7246.377 Hz
FIDRES     0.221142 Hz
AQ            2.2611110 sec
RG            322.5
DW            69.000 us
DE            6.50 usec
TE             298.9 K
D1        2.00000000 sec
TDD            1

======== CHANNEL f1 ========
NUC1            1H
P1            11.70 usec
PL1            4.00 dB
SF01    400.1324008 MHz

F2 - Processing parameters
SI            16384
SF           400.1300073 MHz
WDM         EM
SSB            0
LB            0 Hz
GB            0
PC            1.00
Current Data Parameters
NAME              Das-423
EXPNO             6
PROCNO            1

F2 - Acquisition Parameters
Date_            20120512
Time             18.10
INSTRUM          spect
PROBHD            5 mm BBO BB-1H
PULPROG          zgpg30
TD               32768
SOLVENT          CDCl3
NS               1000
DS                0
SNMR            2038.461 Hz
FIDRES         0.733596 Hz
AQ               0.6816452 sec
RG               8192
DW              20.800 usec
DE              6.50  usec
TE               298.7 K
D1           2.00000000 sec
D11          0.00000000 sec
TD0              1

======== CHANNEL f1 ========
NUC1             13C
P1                9.00 usec
PL1               7.00 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2        waltz16
NUC2             1H
PCPD2           90.00 usec
PL2              3.80  dB
PL12            21.60  dB
PL13            24.60  dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI               32768
SF          100.6127723 MHz
WDW            EM
SSB             0
LB               1.00 Hz
GB              0
PC               1.00
Current Data Parameters

NAME            lynn330
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20120413
Time              11.33
PROBHM            spec
PROBHD 5 mm BBO BB-1H
POLPROG            zg30
TB                32768
SOLVENT           CDCl3
MS                16
SWH            7246.377 Hz
FIDRES         0.221142 Hz
AQ               2.2611110 sec
RG                256
DW               69.000 usec
DE                6.50 usec
TE                298.9 K
D1          2.00000000 sec
D20               1

======== CHANNEL f1 ========
NUC1               1H
P1                11.70 usec
PL1               4.00 dB
LP01        400.1334008 MHz

F2 - Processing parameters
SI                16384
SP        400.13340073 MHz
WDM            EM
ZRB                0
LB                 0 Hz
GB                0
PC                1.00
Current Data Parameters
NAME            Das-426
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20120509
Time              17.23
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
POLPROG          zpg30
TD                32768
SOLVENT           CDCl3
NS                  720
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.681452 sec
RG                 8192
DW               20.800 usec
TE                298.8 K
D0           2.00000000 sec
D11          0.00000000 sec
TDD                   1

======== CHANNEL f1 ========
NUC1                13C
P1                 8.90 usec
PL1                7.00 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.80 dB
PL12              21.60 dB
PL13              24.60 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127709 MHz
WDW                  EM
SSB      0
LB                 1.00 Hz
PC                 1.00
Current Data Parameters
NAME          lynn377-1
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20120614
Time              10.44
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
POLPROG            zg30
SOLVENT           CDCl3
NS                   16
SWH            7246.377 Hz
FIDRES         0.221142 Hz
AQ            2.2611110 sec
RG                  256
DW               69.000 usec
TE                298.4 K
D1           2.00000000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                11.70 usec
PL1                4.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
Zf        400.13000000 Hz
WDM        400.13240000 Hz
SUB                    0
LB                    0 Hz
GB                    0
PC                 1.00
**Current Data Parameters**

- **NAME**: lynn377
- **EXPNO**: 2
- **PROCNO**: 1

**F2 - Acquisition Parameters**

- **Date**: 20120627
- **Time**: 20.20
- **INSTRUM**: spect
- **PROBHD**: 5 mm PABBO BB-
- **PULPROG**: zgpg30
- **TD**: 65536
- **SOLVENT**: CDCl3
- **NS**: 15740
- **DS**: 0
- **SWH**: 30030.029 Hz
- **FIDRES**: 0.458222 Hz
- **AQ**: 1.0912410 sec
- **RG**: 9195.2
- **DW**: 16.650 usec
- **DE**: 6.50 usec
- **TE**: 295.7 K
- **D1**: 2.00000000 sec
- **D11**: 0.03000000 sec
- **TD0**: 1

**======== CHANNEL f1 ========**

- **NUC1**: 13C
- **P1**: 10.50 usec
- **PL1**: 7.00 dB
- **SFO1**: 125.7709931 MHz

**======== CHANNEL f2 ========**

- **CPDPRG2**: waltz16
- **NUC2**: 1H
- **PCPD2**: 90.00 usec
- **PL2**: -0.60 dB
- **PL12**: 15.00 dB
- **PL13**: 18.00 dB
- **SFO2**: 500.1320005 MHz

**F2 - Processing parameters**

- **SI**: 65536
- **SF**: 125.7577908 MHz
- **WDW**: EM
- **SSB**: 0
- **LB**: 1.00 Hz
- **GB**: 0
- **PC**: 1.00
Current Data Parameters
NAME          Das-436-1
EXPNO                 1
PROCNO                1
F2 - Acquisition Parameters
Date_          20120519
Time              11.18
INSTRUM           spect
PROBHD   5 mm PABBO BB-
POLPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    1
SMH         9057.971 Hz
F1 RES    0.276427 Hz
AQ            1.8089888 sec
RG                161.3
DW               55.200 usec
DE                 6.50 usec
TE                294.5 K
DS           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
PL1      0 dB
SFO1        500.1330008 MHz
F2 - Processing parameters
SI                16384
SF      500.1300134 MHz
WSWM           5.001300134 MHz
PC                 1.00
Current Data Parameters
NAME  Das-436
EXPN   2
PROCNO 1

F2 - Acquisition Parameters
Date_    20120519
Time     11.21
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD      65536
SOLVENT CDCl3
NS      1315
DS      0
DM68  30030.009 Hz
F1RES   0.458222 Hz
AQ       1.0912410 sec
RG      91.95.2
SM      16.650 usec
TE      295.1 K
D1    2.00000000 sec
D13  0.03000000 sec
TD0    1

======== CHANNEL f1 ========
NUC1    13C
P1     10.50 usec
PL1    7.00 dB
SFO1  125.7709931 MHz

======== CHANNEL f2 ========
CPERIOD walsh216
WAV1  1H
PCPD2  90.00 usec
PL2  -0.60 dB
PL12  15.00 dB
PL13  18.00 dB
SFO2  500.000005 MHz

F2 - Processing parameters
SI  65536
DF  125.7577945 MHz
WMR   EM
SUB    0
LB  1.00 Hz
DR   0
PC   1.00
Current Data Parameters
NAME        Das-443-1
EXPNO      1
PROCNO     1

F2 - Acquisition Parameters
Date_        20120527
Time        10.03
INSTRUM     spect
PROBHD   5 mm BBO BB-1H
PULPROG     zg30
TD        32768
SOLVENT    CDCl3
NS            16
DS            0
SMM       7244.377 Hz
TIMES       0.221142 Hz
AQ         2.2611110 sec
RG        128
SW          69.000 usec
SE         6.50 usec
TE        299.1 K
D1        2.00000000 sec
TDO      1

F2 - Processing parameters
SI        16384
SF    400.1324008 MHz
WDW         EM
SSB        0
LB          0 Hz
GB        0
PC        1.00
Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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Current Data Parameters
NAME          lynn367-1
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20120602
Time              11.26
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
T0                30768
SOLVENT           CDCl3
NS                    1
DS                    0
SNR                     7246.377 Hz
F1RES           0.221142 Hz
AQ                  2.261111 sec
RG                  256
DW               69.000 usec
DE                 6.50 usec
TE                298.7 K
D1           2.00000000 sec
T20                1

======== CHANNEL f1 ========
NUC1                 1H
P1               11.70 usec
PL1                4.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                16384
SF          400.1300079 MHz
WDW                  EM
SSB      0
LB       0 Hz
GB       0
PC                 1.00
Current Data Parameters
NAME          lynn367-1
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20120602
Time              11.27
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  851
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6814452 sec
RG               9195.2
DW               20.800 usec
DE                 6.50 usec
TE                298.7 K
S1           2.000000000 sec
D11          0.000000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                 8.90 usec
PL1                7.00 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.80 dB
PL12               21.60 dB
PL13               24.60 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127701 MHz
WDM               EM
SUB                  0
LB                 1.00 Hz
GR                  0
PC                 1.00
 Current Data Parameters
 NAME            Das-451
 EXNO                 3
 PROCNO                1

F2 - Acquisition Parameters
 Date_          20120528
 Time              18.04
 INSTRUM           spect
 PROBHD   5 mm BBO NR-1H
 PULPROG            zg30
 TD                32768
 SOLVENT           CDCl3
 NS                   16
 DS                    0
 DMS 7246.377 Hz
 FILESS 0.221142 Hz
 AQ                  128
 DM          69.000 usec
 DE          6.50 usec
 TE                298.4 K
 DI                2.00000000 sec
 TDO                   1

======== CHANNEL f1 ========
 NUC1                 1H
 P1                11.70 usec
 PL1                4.00 dB
 SFO1        400.1324008 MHz

F2 - Processing parameters
 SI                16384
 SF          400.1324008 MHz
 NFBM   0
 SSM 0
 LN          0 Hz
 GB          0 Hz
 PC                1.00
Current Data Parameters
NAME            Das-451
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20120528
Time              18.07
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 1327
DS                    0
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816452 sec
RG                 8192
DW               20.800 usec
DE                 6.50 usec
TE                298.5 K
D1           2.00000000 sec
D11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 8.90 usec
PL1                7.00 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDP RG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.80 dB
PL12                21.60 dB
PL13                24.60 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB      0
LB                 1.00 Hz
GR       0
PC                 1.00
Current Data Parameters
NAME          Das-458
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20120608
Time              16.23
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  480
DS                  0
SNW       24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6816452 sec
RG                 8192
DW               20.800 usec
DE                 6.50 usec
TE                298.1 K
D1          2.00000000 sec
D11         0.03000000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 8.90 usec
PL1                7.00 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                3.60 dB
PL12              21.60 dB
PL13              24.60 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127723 MHz
WDW                  EM
SSB                  0
LB                 1.00 Hz
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PC                 1.00
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### Current Data Parameters

**NAME**  | **Das-459**
---|---
**EXPNO** | 2
**PROCNO** | 1

### Acquisition Parameters

- **Date_** 20120609
- **Time** 12.01
- **INSTRUM** spect
- **PROBHD** 5 mm PABBO BB-
- **PULPROG** zgpg30
- **TD** 65536
- **SOLVENT** CDCl3
- **NS** 558
- **DS** 0
- **SWH** 30030.029 Hz
- **FIDRES** 0.458222 Hz
- **AQ** 1.0912410 sec
- **RG** 9195.2
- **DW** 16.650 usec
- **DE** 6.50 usec
- **TE** 294.7 K
- **D1** 2.00000000 sec
- **D11** 0.03000000 sec

### Processing Parameters

- **SI** 65536
- **SF** 125.7577936 MHz
- **WDW** EM
- **SSB** 0
- **LB** 1.00 Hz
- **GB** 0
- **PC** 1.00

### Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

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