Supporting Information for:

**Palladium-catalyzed carbonylation of allylamines via C–N bond activation leading to β,γ-unsaturated amides**

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1. General experiment details and materials

**Experimental:** All solvents before use were dried and degassed by standard methods and stored under argon atmosphere. NMR spectra were recorded on BRUKER DRX 400 spectrometers. Chemical shifts are reported in parts per million (ppm) down field from TMS with the solvent resonance as the internal standard. Coupling constants (J) are reported in Hz and refer to apparent peak multiplications. High resolution mass spectra (HRMS) were recorded on Bruker MicroTOF-QII mass (ESI). IR spectra were recorder on Nexus 870 FT-IR spectrometers. GC was performed on Agilent 7890 with a HP-5 column. All kinds of allylamines are known compounds and prepared according to the literature.¹
2. Optimization of the reaction conditions

A mixture of catalyst, ligand, and allylamine was added into a teflon tube which was placed in an autoclave. Then the autoclave was purged and charged with CO at the designed pressure. The reaction mixture was stirred at the designed temperature for 15 h, and then CO was carefully released. The yield was determined by GC analysis relative to the 1 with n-hexadecane as internal standard.

Table 1. Screening of the catalysts

<table>
<thead>
<tr>
<th>Entry</th>
<th>[Pd] (5 mol%)</th>
<th>Solvent</th>
<th>Yield (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>PdCl₂</td>
<td>NMP/THF(1/1)</td>
<td>43</td>
</tr>
<tr>
<td>2</td>
<td>Pd(PPh₃)₂Cl₂</td>
<td>NMP/THF(1/1)</td>
<td>38</td>
</tr>
<tr>
<td>3</td>
<td>Pd(DPPP)Cl₂</td>
<td>NMP/THF(1/1)</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>Pd(Xantphos)Cl₂</td>
<td>NMP/THF(1/1)</td>
<td>82</td>
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<tr>
<td>5</td>
<td>Pd(BINAP)Cl₂</td>
<td>NMP/THF(1/1)</td>
<td>0</td>
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<tr>
<td>6</td>
<td>Pd(DPE-phos)Cl₂</td>
<td>NMP/THF(1/1)</td>
<td>29</td>
</tr>
</tbody>
</table>

*Reaction conditions: 1a (0.5 mmol), CO (10 atm), [Pd] (0.025 mmol), solvent (2.0 mL), 120 °C, 15 h, yields determined by GC using n-hexadecane as an internal standard.

Table 2. Screening of the solvents

<table>
<thead>
<tr>
<th>Entry</th>
<th>[Pd]</th>
<th>Solvent</th>
<th>Yield (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Pd(Xantphos)Cl₂</td>
<td>NMP</td>
<td>77</td>
</tr>
<tr>
<td>2</td>
<td>Pd(Xantphos)Cl₂</td>
<td>THF</td>
<td>87(81)ᵇ</td>
</tr>
<tr>
<td>3</td>
<td>Pd(Xantphos)Cl₂</td>
<td>CH₃CN</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>Pd(Xantphos)Cl₂</td>
<td>toluene</td>
<td>99(91)ᵇ</td>
</tr>
<tr>
<td>5</td>
<td>Pd(Xantphos)Cl₂</td>
<td>xylene</td>
<td>99</td>
</tr>
<tr>
<td>6</td>
<td>Pd(Xantphos)Cl₂</td>
<td>mesitylene</td>
<td>22</td>
</tr>
</tbody>
</table>

*Reaction conditions: 1a (0.5 mmol), CO (10 atm), Pd(Xantphos)Cl₂ (0.025 mmol), solvent (2.0 mL), 120 °C, 15 h, yields determined by GC using n-hexadecane as an internal standard.ᵇ Isolated yields.
Table 3. Screening of pressure of CO

![Chemical Reaction](attachment:image.png)

<table>
<thead>
<tr>
<th>Entry</th>
<th>CO (atm)</th>
<th>Yield (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10</td>
<td>99(91)&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>2</td>
<td>6</td>
<td>90</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>44</td>
</tr>
</tbody>
</table>

<sup>a</sup> Reaction conditions: 1a (0.5mmol), Pd(Xantphos)Cl<sub>2</sub> (0.025 mmol), toluene (2.0 mL), 120 °C, 15 h, yield determined by GC using n-hexadecane as an internal standard. <sup>b</sup> Isolated yield.
3. General procedure for Pd-catalyzed carbonylation of allylamines

A mixture of allylamine (0.5 mmol), Pd(Xantphos)Cl₂ (18.8 mg, 5% mmol), toluene (2.0 mL) was added into a teflon tube which was placed in an autoclave. Then the autoclave was purged and charged with CO at 10 atm. The reaction mixture was stirred at 120 °C for 15 h, and then CO was carefully released. The E/Z ratio of the product was determined by checking the ¹H NMR of crude reaction mixture. The corresponding reaction mixture was purified by flash column chromatography on a silica gel to give the desired product.

4. Experimental characterization data for products 2

N,N-dibenzyl-4-phenylbut-3-enamide (2a) (E/Z=9:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 155.2 mg, 91% yield. ¹H NMR (400 MHz, CDCl₃) δ 3.39 (t, J = 2.4 Hz, 2H), 4.50 (s, 2H), 4.63 (s, 2H), 6.42 (t, J = 2.4 Hz, 2H), 7.17-7.39 (m, 15H); ¹³C NMR (100 MHz, CDCl₃) δ 38.0, 48.4, 50.2, 123.3, 126.4, 126.5, 127.6, 127.6, 127.8, 128.5, 128.6, 128.8, 129.1, 132.9, 136.5, 137.1, 137.4, 171.7; HRMS (ESI) calcd. for C₂₄H₂₃NO [M+Na]: 364.1672, found: 364.1689.

N,N-diethyl-4-phenylbut-3-enamide (2b) (E/Z=9:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to white solid, 100.9 mg, 93% yield. ¹H NMR (400 MHz, CDCl₃) δ 1.06 (t, J = 7.2 Hz, 6H), 2.56 (q, J =7.2 Hz, 4H), 3.24 (dd, J₁ =1.2 Hz, J₂ =6.8 Hz 2H), 6.26-6.33 (m, 1H), 6.49 (d, J = 16.0 Hz, 1H), 7.19-7.39 (m, 5H); ¹³C NMR (100 MHz, CDCl₃) δ 13.2, 14.6, 38.0, 40.3, 42.3, 124.0, 126.3, 127.4, 128.6, 132.4, 137.2, 170.2; HRMS (ESI) calcd. for C₁₄H₁₉NO [M+Na]: 240.1359, found: 240.1369.

4-phenyl-N,N-dipropylbut-3-enamide (2c) (E/Z=13:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 100.5 mg, 82% yield. ¹H NMR (400 MHz, CDCl₃) δ 0.88-0.95 (m, 6H), 1.53-1.66 (m, 4H), 3.23 (t, J = 8.0 Hz, 2H), 3.29 (dd, J₁ = 6.0 Hz, J₂ =
9.6 Hz, 4H), 6.35-6.48 (m, 2H), 7.19-7.38 (m, 5H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 11.4, 11.5, 21.0, 22.4, 38.0, 47.7, 49.9, 124.0, 126.3, 127.4, 128.6, 132.4, 137.2, 170.6; HRMS (ESI) calcd. for C$_{16}$H$_{23}$NO [M+Na]: 268.1672, found: 268.1678.

$\textit{N,N}$-diisopropyl-4-phenylbut-3-enamide (2d) (E/Z>20:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 95.6 mg, 78% yield. $^1$H NMR (400 MHz, CDCl$_3$) δ 1.19 (d, $J = 6.8$, 6H), 1.40 (d, $J = 6.8$, 6H), 3.25 (d, $J = 6.0$ Hz, 2H), 3.47 (s, 1H), 3.97-4.03 (m, 1H), 6.33-6.48 (m, 2H), 7.18-7.38 (m, 5H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 20.8, 21.1, 40.1, 45.9, 49.0, 124.1, 126.3, 127.4, 128.6, 132.3, 137.3, 169.9; HRMS (ESI) calcd. for C$_{16}$H$_{23}$NO [M+Na]: 268.1672, found: 268.1679.

$\textit{N,N}$-dibutyl-4-phenylbut-3-enamide (2e) (E/Z=11:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 102.4 mg, 75% yield. $^1$H NMR (400 MHz, CDCl$_3$) δ 0.91-0.97(m, 6H), 1.29-1.37 (m, 4H), 1.49-1.69 (m, 4H), 3.23-3.35 (m, 6H), 6.34-6.48 (m, 2H), 7.19-7.38 (m, 5H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 14.0, 14.0, 28.3, 28.4, 30.0, 31.4, 38.1, 45.9, 48.1, 124.1, 126.4, 127.4, 128.6, 132.4, 137.3, 170.5; HRMS (ESI) calcd. for C$_{18}$H$_{27}$NO [M+Na]: 296.1985, found: 296.1991.

$\textit{N,N}$-dioctyl-4-phenylbut-3-enamide (2f) (E/Z=7:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 138.6 mg, 72% yield. $^1$H NMR (400 MHz, CDCl$_3$) δ 0.79 (q, $J = 6.4$ Hz, 6H), 1.20 (d, $J = 3.6$ Hz, 20H), 1.48 (t, $J = 7.2$ Hz, 4H), 3.14-3.25 (m, 6H), 6.28-6.40 (m, 2H), 7.11-7.30 (m, 5H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 14.2, 22.7, 22.7, 27.0, 27.1, 27.8, 29.3, 29.3, 29.3, 29.4, 29.5, 31.8, 31.9, 38.0, 46.1, 48.2, 124.0, 126.3, 127.4, 128.5, 132.4, 137.2, 170.4; HRMS (ESI) calcd. for C$_{26}$H$_{43}$NO [M+Na]: 408.3237, found: 408.3232.
4-phenyl-1-(pyrrolidin-1-yl)but-3-en-1-one (2g) (E/Z=12:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 54.8 mg, 51% yield. $^1$H NMR (400 MHz, CDCl$_3$) δ 1.82-1.99 (m, 4H), 3.24-3.25 (m, 2H), 3.46-3.51 (m, 4H), 6.34-6.50 (m, 2H), 7.19-7.39 (m, 5H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 24.5, 26.3, 39.6, 45.9, 46.8, 123.3, 126.3, 127.5, 128.6, 132.8, 137.2, 169.5; HRMS (ESI) calcd. for C$_{14}$H$_{17}$NO [M+Na]: 238.1202, found: 238.1210.

4-phenyl-1-(piperidin-1-yl)but-3-en-1-one (2h) (E/Z=13:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 75.6 mg, 66% yield. $^1$H NMR (400 MHz, CDCl$_3$) δ 1.53-1.57 (m, 4H), 1.62-1.66 (m, 2H), 3.30 (dd, $J_1$ = 1.6 Hz, $J_2$ = 6.8 Hz, 2H), 3.44 (t, $J$ = 5.6 Hz, 2H), 3.58 (t, $J$ = 5.6 Hz, 2H), 6.30-6.38 (m, 1H), 6.45 (d, $J$ = 16.0 Hz, 1H), 7.20-7.38 (m, 5H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 24.6, 25.7, 26.7, 38.3, 43.0, 47.2, 123.6, 126.3, 127.5, 128.6, 132.6, 137.2, 169.3; HRMS (ESI) calcd. for C$_{15}$H$_{19}$NO [M+Na]: 252.1359, found: 252.1364.

1-morpholino-4-phenylbut-3-en-1-one (2i) (E/Z=19:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 95.9 mg, 83% yield. $^1$H NMR (400 MHz, CDCl$_3$) δ 3.30 (dd, $J_1$ = 1.6 Hz, $J_2$ = 6.8 Hz, 2H), 3.51 (t, $J$ = 5.2 Hz, 2H), 3.65-3.68 (m, 6H), 6.29-6.36 (m, 1H), 6.46 (d, $J$ = 16.0 Hz, 1H), 7.21-7.38 (m, 5H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 37.9, 42.2, 46.4, 66.8, 67.0, 122.8, 126.4, 127.7, 128.7, 133.1, 136.9, 169.7; HRMS (ESI) calcd. for C$_{14}$H$_{17}$NO$_2$ [M+Na]: 254.1151, found: 254.1155.

$N$-benzyl-4-phenyl-$N$-propylbut-3-enamide (2j) (E/Z=7:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 92.3 mg, 63% yield. $^1$H NMR (400 MHz, CDCl$_3$) δ 0.87-0.92
(m, 3H), 1.56-1.63 (m, 2H), 3.18-3.38 (m, 4H), 4.58 (s, 1H), 4.63 (s, 1H), 6.36-6.47 (m, 2H), 7.18-7.38 (m, 10H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 11.4, 11.5, 20.9, 22.0, 37.9, 38.2, 48.2, 48.4, 49.0, 51.4, 123.6, 123.7, 126.3, 126.4, 126.4, 127.4, 127.5, 127.5, 127.7, 128.2, 128.6, 128.6, 128.7, 129.1, 132.7, 137.1, 137.2, 137.9, 171.1, 171.4; HRMS (ESI) calcd. for C$_{20}$H$_{23}$NO [M+Na]: 316.1672, found: 316.1678

(E)-N,N-dibenzyl-4-p-tolylbut-3-enamide (2k) (E/Z=7:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 133.1 mg, 75 % yield. $^1$H NMR (400 MHz, CDCl$_3$) δ 2.30 (s, 0.43H), 2.32 (s, 2.32H), 3.37-3.38 (m, 1.69H), 3.45-3.46 (m, 0.23H), 4.45 (s, 0.25H), 4.49 (s, 1.75H), 4.62-4.64 (m, 2H), 6.22-6.42 (m, 2H), 6.99-7.31 (m, 14H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 21.3, 38.1, 48.4, 50.2, 122.2, 126.3, 126.6, 127.6, 127.8, 128.5, 128.8, 129.1, 129.3, 132.8, 134.3, 136.6, 137.3, 137.4, 171.9; HRMS (ESI) calcd. for C$_{25}$H$_{25}$NO [M+Na]: 378.1828, found: 378.1831

N,N-dibenzyl-4-m-tolylbut-3-enamide (2l) (E/Z>20:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 129.6 mg, 73% yield. $^1$H NMR (400 MHz, CDCl$_3$) δ 2.32 (s, 3H), 3.37 (d, $J$ = 4.8 Hz, 2H), 4.49 (s, 2H), 4.63 (s, 2H), 6.39-6.41 (m, 2H), 7.02-7.39 (m, 14H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 21.5, 38.0, 48.4, 50.2, 123.1, 123.6, 126.5, 127.1, 127.6, 127.8, 128.3, 128.5, 128.5, 128.8, 129.1, 133.0, 136.5, 137.0, 137.4, 138.1, 171.8; HRMS (ESI) calcd. for C$_{25}$H$_{25}$NO [M+Na]: 378.1828, found: 378.1839

N,N-dibenzyl-4-(4-tert-butylphenyl)but-3-enamide (2m) (E/Z=6:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 151.0 mg, 76% yield. $^1$H NMR (400 MHz, CDCl$_3$) δ 1.30 (s, 9H), 3.37 (d, $J$ = 4.8 Hz, 2H), 4.48 (s, 2H), 4.62 (s, 2H), 6.37 (d, $J$ = 7.2 Hz, 2H), 7.16-7.38 (m, 14H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 31.4, 34.7, 38.1, 48.4,
**N,N-dibenzyl-4-(4-methoxyphenyl)but-3-enamide (2n)** (E/Z=6:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 137.3 mg, 74% yield. $^{1}$H NMR (400 MHz, CDCl$_3$) $\delta$ 3.35-3.37 (m, 2H), 3.79 (s, 3H), 4.49 (s, 2H), 4.62 (s, 2H), 6.23-6.38 (m, 2H), 6.81-6.85 (m, 2H), 7.17-7.39 (m, 12H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 38.0, 48.4, 50.2, 55.4, 114.0, 120.8, 126.5, 127.5, 127.6, 127.8, 128.5, 129.1, 129.9, 132.3, 136.6, 137.4, 159.2, 171.9; HRMS (ESI) calcd. for C$_{25}$H$_{23}$NO$_2$ [M+Na]: 394.1778, found: 394.1781.

**N,N-dibenzyl-4-(4-ethoxyphenyl)but-3-enamide (2o)** (E/Z=14:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 142.5 mg, 74% yield. $^{1}$H NMR (400 MHz, CDCl$_3$) $\delta$ 1.40 (t, $J = 7.2$ Hz, 3H), 3.35 (d, $J = 6.4$ Hz, 2H), 4.00 (q, $J = 6.8$ Hz, 2H), 4.49 (s, 2H), 4.62 (s, 2H), 6.22-6.38 (m, 2H), 6.80 (d, $J = 8.4$ Hz, 2H), 7.16-7.38 (m, 12H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 14.9, 38.0, 48.4, 50.2, 63.5, 114.6, 120.8, 126.5, 127.5, 127.6, 128.5, 128.7, 129.1, 129.8, 132.4, 136.6, 137.4, 158.6, 171.9; HRMS (ESI) calcd. for C$_{26}$H$_{27}$NO$_2$ [M+Na]: 408.1934, found: 408.1931.

**N,N-dibenzyl-4-(4-fluorophenyl)but-3-enamide (2p)** (E/Z=8:1): The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 154.4 mg, 86% yield. $^{1}$H NMR (400 MHz, CDCl$_3$) $\delta$ 3.63 (d, $J = 4.8$ Hz, 2H), 4.49 (s, 2H), 4.63 (s, 2H), 6.33-6.35 (m, 2H), 6.98-6.99 (m, 2H), 7.17-7.39 (m, 14H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 37.8, 48.6, 50.3, 115.4, 115.6, 123.1, 123.1, 126.5, 127.7, 127.8, 127.9, 127.9, 128.6, 128.8, 129.2, 131.8, 133.3, 133.3, 136.5, 137.4, 171.7; HRMS (ESI) calcd. for
C_{24}H_{23}FNO [M+H]: 360.1758, found: 360.1762.

**N,N-dibenzyl-4-(4-chlorophenyl)but-3-enamide (2q) (E/Z=7:1):** The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 144.4 mg, 77% yield. **1H NMR** (400 MHz, CDCl₃) δ 3.37 (d, J = 5.6 Hz, 2H), 4.49 (s, 2H), 4.63 (s, 2H), 6.32-6.43 (m, 2H), 7.17-7.39 (m, 14H); **13C NMR** (100 MHz, CDCl₃) δ 37.8, 48.6, 50.2, 124.1, 126.5, 127.6, 127.7, 127.9, 128.6, 128.8, 129.2, 131.7, 133.2, 135.6, 136.5, 137.3, 171.6; **HRMS** (ESI) calcd. for C_{24}H_{22}ClNO [M+Na]: 398.1282, found: 398.1289.

**N,N-dibenzyl-4-(naphthalen-2-yl)but-3-enamide (2s) (E/Z=13:1):** The title compound was prepared according to the general procedure and purified by flash column chromatography to give white solid, 164.2 mg, 84% yield. **1H NMR** (400 MHz, CDCl₃) δ 3.43 (t, J = 2.4 Hz, 2H), 4.52 (s, 2H), 4.64 (s, 2H), 6.54-6.56 (m, 2H), 7.18-7.79 (m, 17H); **13C NMR** (100 MHz, CDCl₃) δ 38.1, 48.5, 50.3, 123.7, 125.9, 126.1, 126.3, 126.6, 127.6, 127.8, 128.1, 128.3, 128.6, 128.8, 129.2, 131.3, 133.1, 133.7, 134.6, 136.5, 137.4, 171.8; **HRMS** (ESI) calcd. for C_{28}H_{25}NO [M+Na]: 414.1828, found: 414.1841.

**N,N-dibenzyl-4-(naphthalen-2-yl)but-3-enamide (2t) (E/Z=3:1):** The title compound was prepared...
according to the general procedure and purified by flash column chromatography to give white solid, 93.5 mg, 67% yield. \textit{\textsuperscript{1}H NMR} (400 MHz, CDCl\textsubscript{3}) \(\delta\) 1.56-1.70 (m, 3H), 3.15-3.23 (m, 2H), 4.44 (s, 2H), 4.59 (d, \(J = 6.8\) Hz, 2H), 5.48-5.69 (m, 2H), 7.14-7.38 (m, 10H); \textit{\textsuperscript{13}C NMR} (100 MHz, CDCl\textsubscript{3}) \(\delta\) 13.2, 18.1, 32.5, 37.7, 48.2, 48.3, 50.0, 123.2, 124.1, 126.5, 126.5, 127.0, 127.5, 127.7, 128.4, 128.5, 128.7, 128.9, 129.0, 136.6, 137.5, 172.2, 172.3; \textbf{HRMS} (ESI) calcd. for C\textsubscript{23}H\textsubscript{24}N [M+1]: 302.1515, found: 302.1530.

**References:**

6 \textbf{Copies for \textsuperscript{1}H NMR and \textsuperscript{13}C NMR of the products}
$\text{N} (n-\text{Pr})_2$
S18

$N(i$-Pr)$_2$

2d

YH-160312-2-HNMR
S19

YH-140312-2-CNMR

[Chemical structure image]

2d

N-(i-Pr)_2
$\text{N}(n\text{-Bu})_2$
$\text{N}(1\text{-Octane})_2$ 

2f
\[ \text{N} \text{B} \text{n}_2 \text{O}_2 \\text{N} \text{B} \text{n}_2 \]

\[ 2k + 2k' \]

- \[ \text{ppm} \]
  - 8.0
  - 7.5
  - 7.0
  - 6.5
  - 6.0
  - 5.5
  - 5.0
  - 4.5
  - 4.0
  - 3.5
  - 3.0
  - 2.5
  - 2.0
  - 1.5
  - 1.0
  - 0.5

\[ 14.3\% \]

\[ 12.0\% \]

\[ 20.1\% \]

\[ 17.6\% \]

\[ 0.25\% \]

\[ 0.3\% \]

\[ 1.0\% \]

\[ 0.8\% \]

\[ 0.4\% \]
2p

YH-140414-5-HNMR
2s

N
B
n
2
O
2s
\[ \text{N} \text{Bn}_2 \text{O}_2 \text{t} + \text{N} \text{Bn}_2 \text{O}_2 \text{t}' \]