Electronic Supplementary Material (ESI) for ChemComm.


# Mn(II)-Catalysed Alkylation of Methylene Ketones with Alcohols: Direct Access to Functionalised Branched Products

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**1.1 General Experimental Details:** All solvents and reagents were used, as received from the suppliers. TLC was performed on Merck Kiesel gel 60, $F_{254}$ plates with the layer thickness of 0.25 mm. Column chromatography was performed on silica gel (100-200 mesh) using a gradient of ethyl acetate and hexane as mobile phase. $^{1}H$ NMR spectral data were collected at, 400 MHz (JEOL), and $^{13}C$ NMR were recorded at 100 MHz. $^{1}H$ NMR spectral data are given as chemical shifts in ppm followed by multiplicity (s- singlet; d- doublet; t- triplet; q- quartet; m- multiplet), number of protons and coupling constants. $^{13}C$ NMR chemical shifts are expressed in ppm. GC-MS were recorded using Agilent Gas Chromatography Mass Spectrometry. Elemental analysis data were recorded using Vario Micro Cube elemental analyser. All the reactions were performed in a closed system using Schlenk tube. All manganese salts were purchased from Alfa Aesar. $Mn(acac)_2$ (Assay $\geq$94.0 to $\leq$106.0% by Mn EA; CAS Number 14024-58-9; MDL number: MFCD00000022; Pack Size- No A18762-100G). Potassium tert-butoxide was purchased from Avra Synthesis Pvt. Ltd., India. (Purity-98%, CAS No: 865-47-4, Catalog No- ASP2012).

**[1.2] General Procedure for Manganese-catalyzed alkylation with Ketones:**

**Procedure A:**

In a 15 mL oven dried Schlenk tube, ketone (0.25 mmol), *t*-BuOK (0.25 mmol), $Mn(acac)_2$ (0.00625 mmol), Phen (0.0075 mmol), and alcohols (0.3125 mmol, 1.25 equiv.) were added followed by toluene 2.0 mL under an atmosphere of $N_2$ and the reaction mixture was refluxed at 140 $^{o}$C for 36 h in a closed system. The reaction mixture was cooled to room temperature and 3.0 mL of ethyl acetate was added and concentrated *in vacuo.* The residue was purified by column chromatography using a gradient of hexane and ethyl acetate (eluent system) to afford the pure product.

**Procedure B:**

In a 15 mL oven dried Schlenk tube, ketone (0.25 mmol), *t*-BuOK (0.375 mmol), $Mn(acac)_2$ (0.00625 mmol), Phen (0.0075 mmol), and alcohols (0.3125 mmol, 1.25 equiv.) were added followed by toluene 2.0 mL under an atmosphere of $N_2$ and the reaction mixture was refluxed at 140 $^{o}$C for 36 h in a closed system. The reaction mixture was cooled to room temperature and 3.0 mL of ethyl acetate was added and concentrated *in vacuo.* The residue was purified by column chromatography using a gradient of hexane and ethyl acetate (eluent system) to afford the pure product.

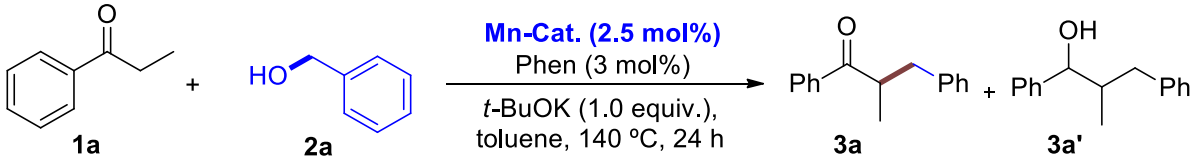
**Procedure C:**

In a 15 mL oven dried Schlenk tube, ketone (0.25 mmol), *t*-BuOK (0.25 mmol), $Mn(acac)_2$ (0.00625 mmol), Phen (0.0075 mmol), and alcohols (0.3125 mmol, 1.25 equiv.) were added followed by toluene 2.0 mL under an atmosphere of $N_2$ and the reaction mixture was refluxed at 140 $^{o}$C for 24 h

in a closed system. The reaction mixture was cooled to room temperature and 3.0 mL of ethyl acetate was added and concentrated *in vacuo*. The residue was purified by column chromatography using a gradient of hexane and ethyl acetate (eluent system) to afford the pure product.

### [1.3] Alkylation of propiophenone with alcohol:

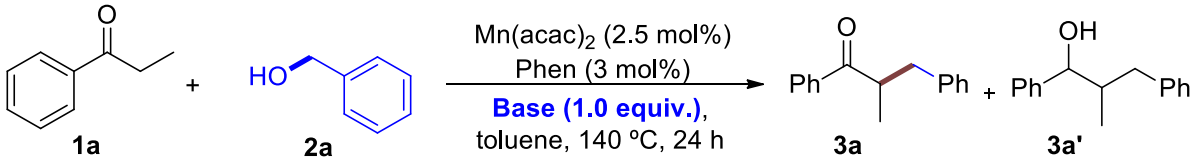
**Table S1**: Screening of catalysts[a]




| Entry | **Mn-Catalyst** | GC-MS Conversion **3a** (%) | GC-MS Conversion **3a'** (%) |
|---|---|---|---|
| 1 | $Mn(CO)_5Br$ | 45 | 50 |
| **2** | **$Mn(acac)_2$** | **72(67)** [b] | **18** |
| 3 | No Catalyst, No Ligand | <15 | <25 |

*Reaction condition:*[a] Propiophenone (0.25 mmol), Benzyl alcohol (0.3125 mmol), **Mn-catalyst (2.5 mol%)**, Phen (3 mol%), *t*-BuOK (0.25 mmol), toluene (2.0 mL), Schlenk tube under nitrogen atmosphere, 140 °C oil bath, 24 h reaction time. [b] Isolated yield (average of two run).

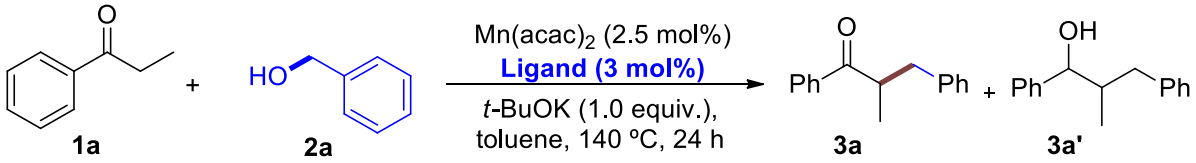
**Table S2**: Screening of base [a]

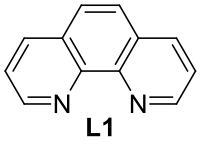
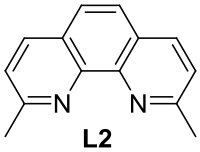
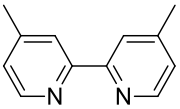
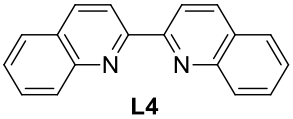
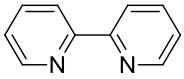
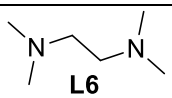



| Entry | **Base** | GC-MS Conversion **3a** (%) | GC-MS Conversion **3a'** (%) |
|---|---|---|---|
| **1** | ***t*-BuOK** | **72(67)**[b] | **18** |
| 2 | *t*-BuONa | 37 | 47 |
| 3 | $K_2CO_3$ | 14 | 33 |
| 4 | $K_3PO_4$ | 4 | 0 |
| 5 | $Cs_2CO_3$ | 0 | 0 |
| 6 | No Base | 0 | 0 |

*Reaction condition:*[a] Propiophenone (0.25 mmol), Benzyl alcohol (0.3125 mmol), $Mn(acac)_2$ (2.5 mol%), Phen (3 mol%), **Base (0.25 mmol)**, toluene (2.0 mL), Schlenk tube under nitrogen atmosphere, 140 °C oil bath, 24 h reaction time. [b] Isolated yield (average of two run).

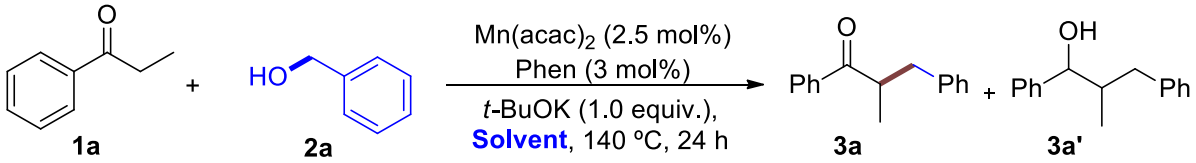
**Table S3**: Screening of ligands[a]




| Entry | **Ligand** | GC-MS Conversion **3a** (%) | GC-MS Conversion **3a'** (%) |
|---|---|---|---|
| **1** |  **L1** | **72(67)[b]** | **18** |
| 2 |  **L2** | 42 | 58 |
| 3 |  **L3** | 27 | 68 |
| 4 |  **L4** | 22 | 30 |
| 5 |  **L5** | 15 | 42 |
| 6 |  **L6** | 57 | 24 |

*Reaction condition:*[a] Propiophenone (0.25 mmol), Benzyl alcohol (0.3125 mmol), $Mn(acac)_2$ (2.5 mol%), **Ligand (3 mol%)**, *t*-BuOK (O.25 mmol), toluene (2.0 mL), Schlenk tube under nitrogen atmosphere, 140 ºC oil bath, 24 h reaction time. [b] Isolated yield (average of two run).

**Table S4**: Screening of solvents [a]




| Entry | **Solvent** | GC-MS Conversion **3a** (%) | GC-MS Conversion **3a'** (%) |
|---|---|---|---|
| **1** | **toluene** | **72(67)[b]** | **18** |
| 2 | P-Xylene | 5 | 0 |
| 3 | t-amyl alcohol | 60 | 38 |
| 4 | DMA | <1 | 0 |
| 5 | DMF | 5 | <1 |

*Reaction condition:* [a] Propiophenone (0.25 mmol), Benzyl alcohol (0.3125 mmol), $Mn(acac)_2$ (2.5 mol%), Phen (3 mol%), *t*-BuOK (O.25 mmol), **Solvent (2.0 mL)**, Schlenk tube under nitrogen atmosphere, 140 °C oil bath, 24 h reaction time. [b] Isolated yield (average of two run).

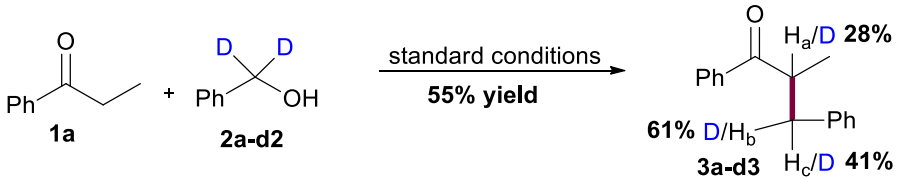
**Table S5**: Screening of alcohol equivalents [a]

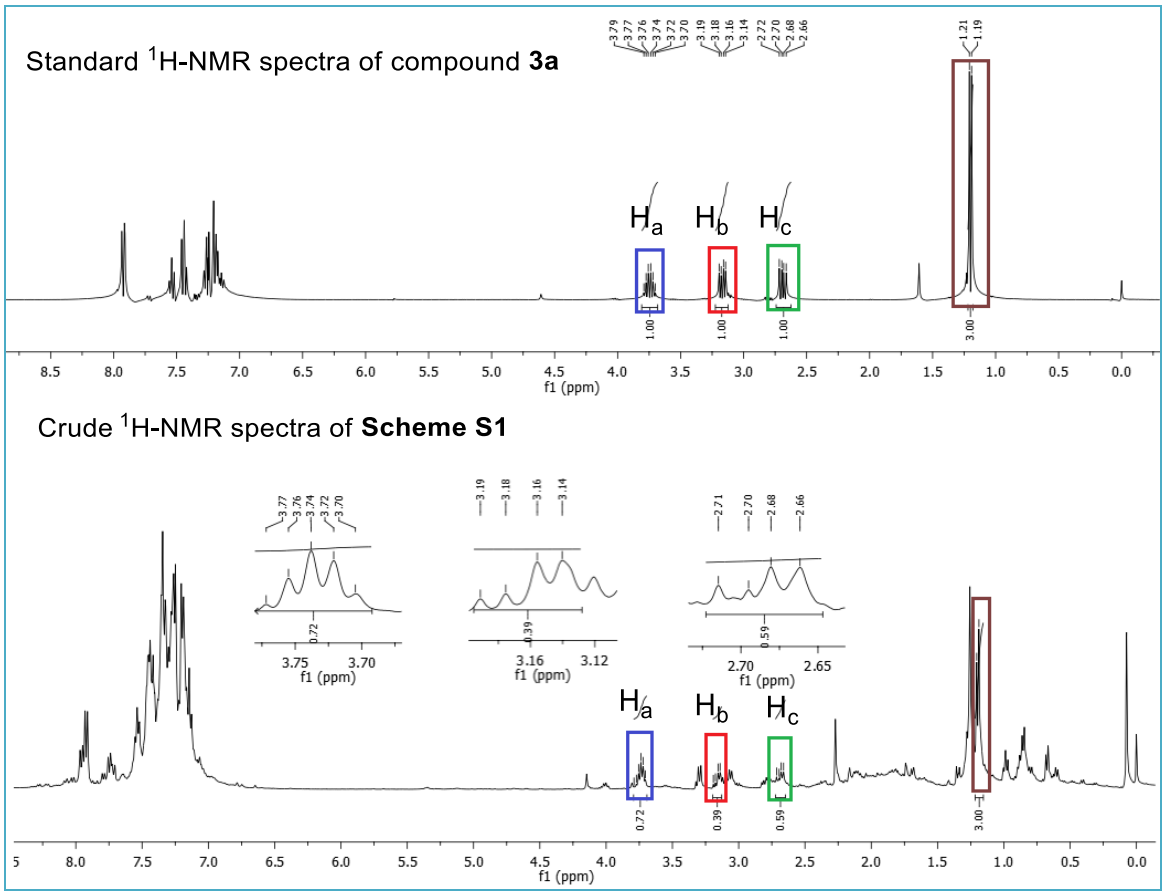
| Entry | **Benzyl alcohol (X equiv.)** | GC-MS Conversion **3a** (%) | GC-MS Conversion **3a'** (%) |
|---|---|---|---|
| 1 | 1.5 | 33 | 67 |
| 2 | 1.25 | 72(67)[b] | 18 |
| **3[c]** | **1.25** | **80(72)[b]** | **20** |
| 4 | 1.1 | 38 | 30 |

*Reaction condition:*[a] Propiophenone (0.25 mmol), **Benzyl alcohol (0.375, 0.3125, 0.275 mmol)**, $Mn(acac)_2$ (2.5 mol%), Phen (3 mol%), *t*-BuOK (O.25 mmol), toluene (2.0 mL), Schlenk tube under nitrogen atmosphere, 140 °C oil bath, 24 h reaction time. [b] Isolated yield (average of two run). [c] 36 h reaction time.

**Deuterium Incorporation Experiments:**

**Scheme S1:**

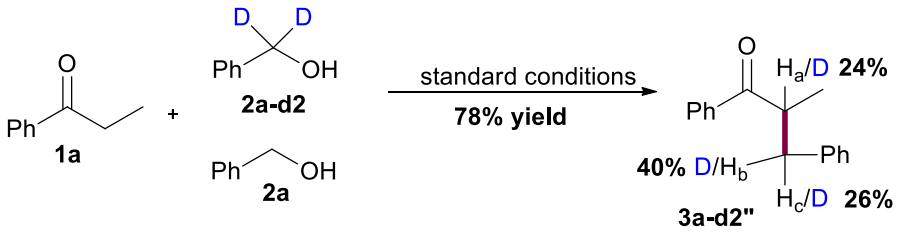


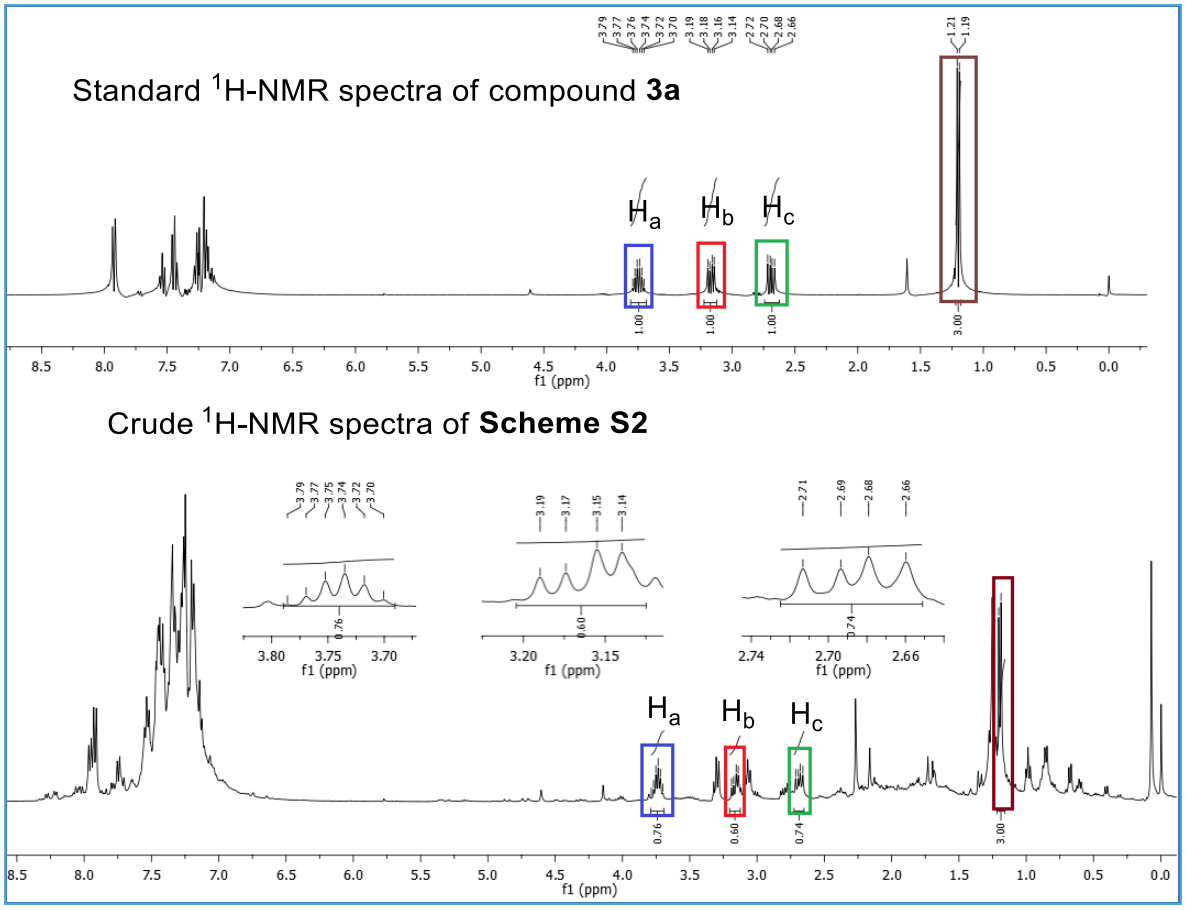




Conversion was calculated by $^{1}$H-NMR integration value

| | | Deuterium incorporation in **$H_a$** Position | Deuterium incorporation in **$H_b$** Position | Deuterium incorporation in **$H_c$** Position |
|---|---|---|---|---|
| Signal $\delta$ ppm | 1.2 [d, $CH_3$, (3H)] | 3.75 (1H) | 3.17 (1H) | 2.69 (1H) |
| Integral Value | 3.0 | 0.72 | 0.39 | 0.59 |
| **Calculated ratio** | | (1-0.72)×100 = **28%** | (1-0.39)×100 = **61%** | (1-0.59)×100 = **41%** |

**Scheme S2:**

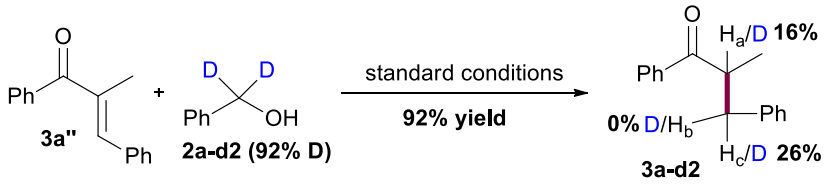


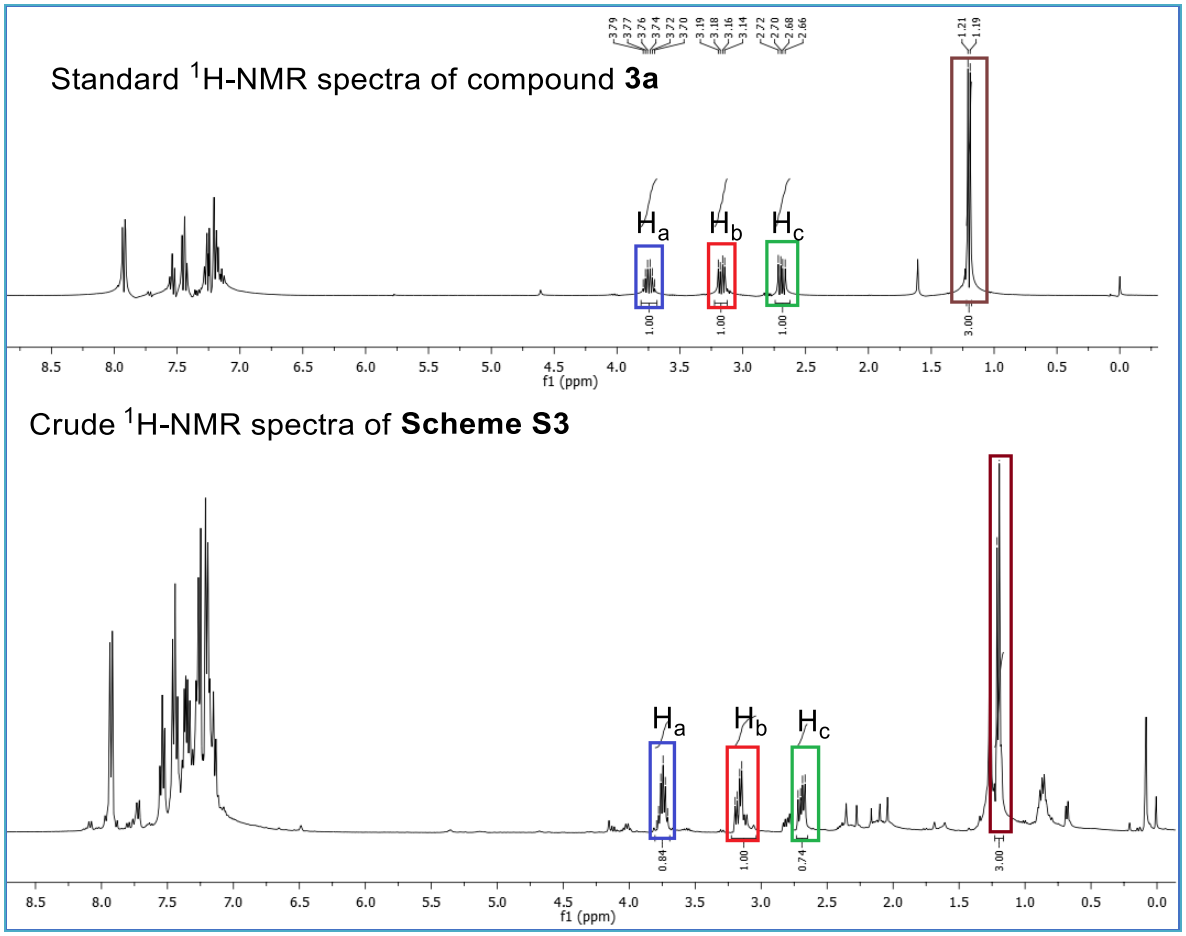




Conversion was calculated by $^{1}$H-NMR integration value

| | | Deuterium incorporation in **$H_a$** Position | Deuterium incorporation in **$H_b$** Position | Deuterium incorporation in **$H_c$** Position |
|---|---|---|---|---|
| Signal δ | 1.2 [d, $CH_3$, (3H)] | 3.75 (1H) | 3.17 (1H) | 2.69 (1H) |
| Integral Value | 3.0 | 0.76 | 0.60 | 0.74 |
| **Calculated ratio** | | (1-0.76)×100 = **24%** | (1-0.60)×100 = **40%** | (1-0.74)×100 = **26%** |

**Scheme S3:**

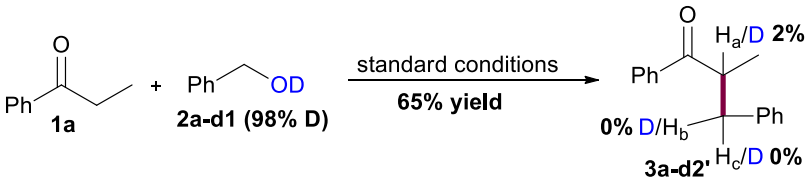


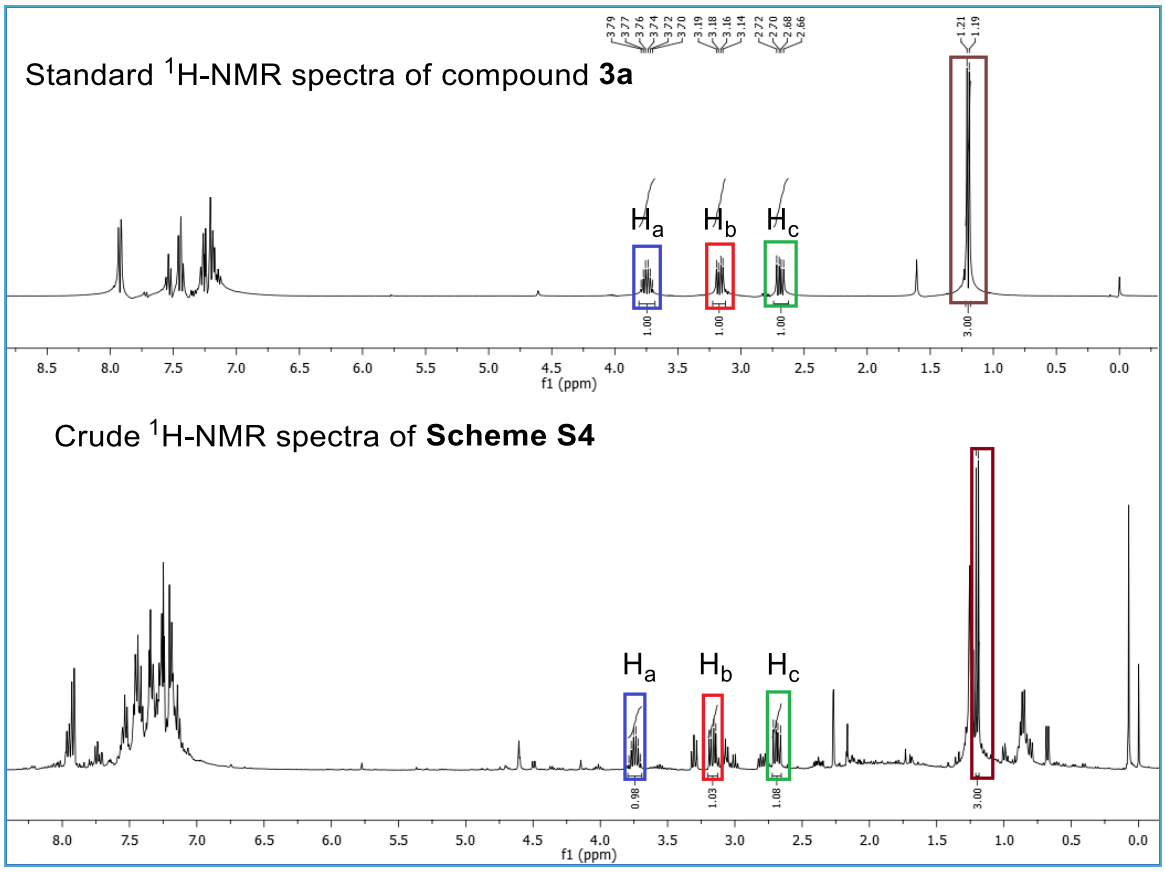




Conversion was calculated by $^{1}$H-NMR integration value

| | | Deuterium incorporation in **$H_a$** Position | Deuterium incorporation in **$H_b$** Position | Deuterium incorporation in **$H_c$** Position |
|---|---|---|---|---|
| Signal $\delta$ ppm | 1.2 [d, $CH_3$, (3H)] | 3.75 (1H) | 3.17 (1H) | 2.69 (1H) |
| Integral Value | 3.0 | 0.84 | 1.0 | 0.74 |
| **Calculated ratio** | | (1-0.84)×100 = **16%** | (1-1)×100 = **0%** | (1-0.74)×100 = **26%** |

**Scheme S4:**

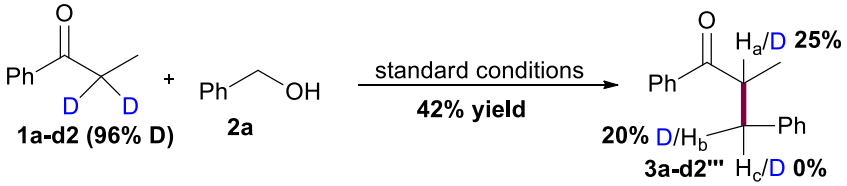


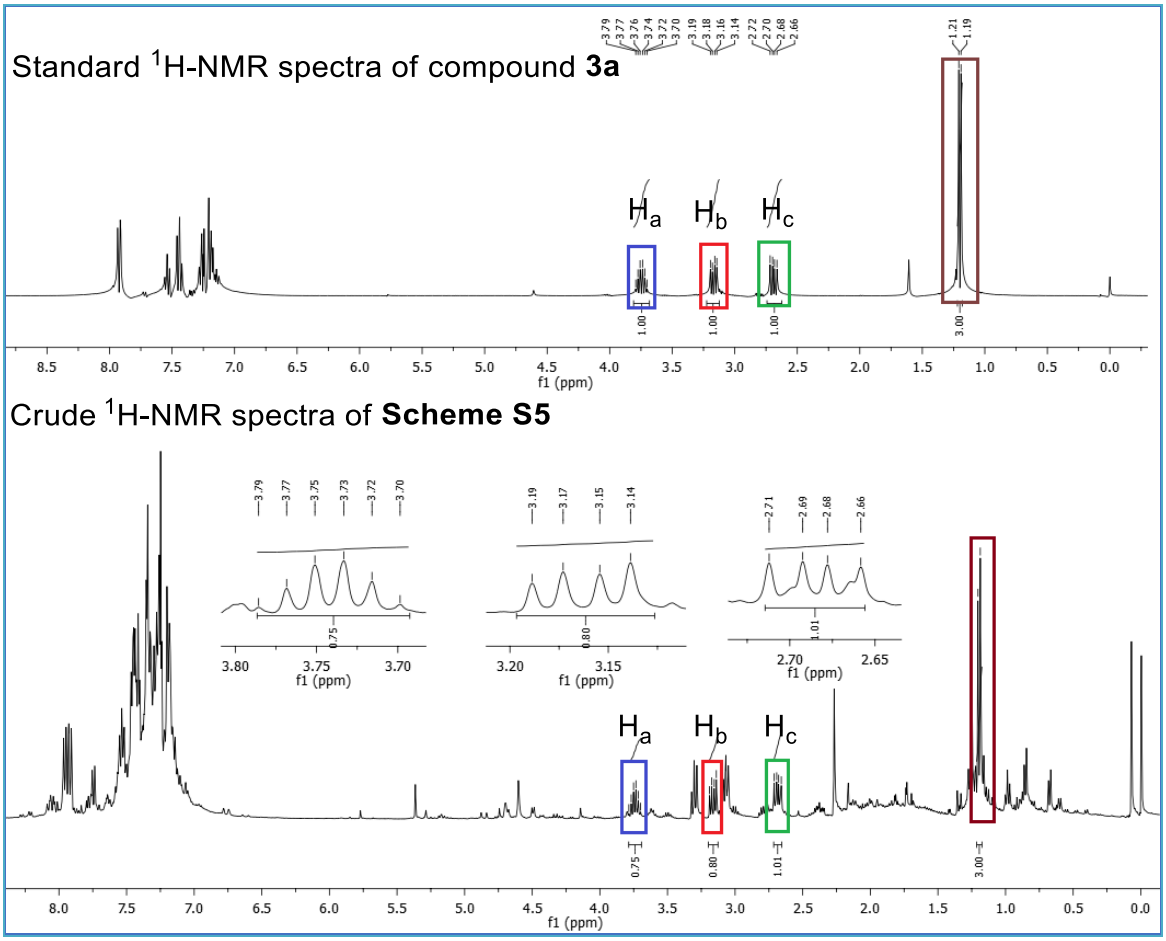




Conversion was calculated by $^{1}$H-NMR integration value

| | | Deuterium incorporation in **$H_a$** Position | Deuterium incorporation in **$H_b$** Position | Deuterium incorporation in **$H_c$** Position |
|---|---|---|---|---|
| Signal $\delta$ ppm | 1.2 [d, $CH_3$, (3H)] | 3.75 (1H) | 3.17 (1H) | 2.69 (1H) |
| Integral Value | 3.0 | 0.98 | 0.99 | 1.0 |
| **Calculated ratio** | | (1-0.98)×100 = **2%** | (1-1)×100 = **0%** | (1-1)×100 = **0%** |

**Scheme S5:**



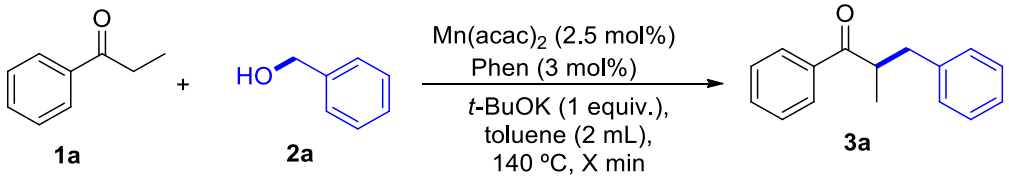

Conversion was calculated by $^1$H-NMR integration value

| | | Deuterium incorporation in **$H_a$** Position | Deuterium incorporation in **$H_b$** Position | Deuterium incorporation in **$H_c$** Position |
|---|---|---|---|---|
| Signal $\delta$ ppm | 1.2 [d, $CH_3$, (3H)] | 3.75 (1H) | 3.17 (1H) | 2.69 (1H) |
| Integral Value | 3.0 | 0.75 | 0.80 | 1.0 |
| **Calculated ratio** | | (1-0.75)×100 = **25%** | (1-0.80)×100 = **20%** | (1-1.0)×100 = **0%** |

**Reaction condition**: Unless otherwise specified, Propiophenone **1a** (0.1 mmol), Benzyl Alcohol **2a** (0.125 mmol), $Mn(acac)_2$ (2.5 mol%), Phen (3 mol%), *t*-BuOK (0.1 mmol), toluene (1.0 mL), Schlenk tube under nitrogen atmosphere, 140 °C oil bath, 36 h reaction time.

**Scheme S6: Determination of rate and order of reaction**

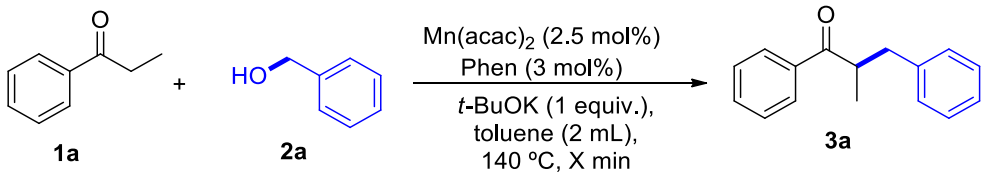
Run 1: Reaction was carried out in 2 mL of toluene and yield was calculated by GC




| No. | **1a** (mmol) | **2a** (mmol) | $Mn(acac)_2$ (mmol) | Phen (mmol) | *t*-BuOK (mmol) | toluene (mL) |
|---|---|---|---|---|---|---|
| Run 1 | 0.2 | 0.25 | 0.005 | 0.006 | 0.2 | 2.0 |

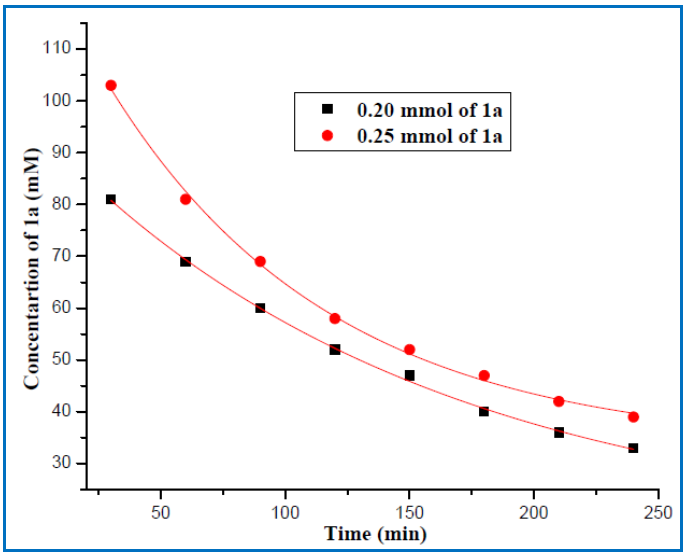
| Sl. No. | Time (min) | Concentration of **1a** (mM) |
|---|---|---|
| 1 | 30 | 81 |
| 2 | 60 | 69 |
| 3 | 90 | 60 |
| 4 | 120 | 52 |
| 5 | 150 | 47 |
| 6 | 180 | 40 |
| 7 | 210 | 36 |
| 8 | 240 | 33 |

Run 2: Reaction was carried out in 2 mL of toluene and yield was calculated by GC




| No. | **1a** (mmol) | **2a** (mmol) | $Mn(acac)_2$ (mmol) | Phen (mmol) | t-BuOK (mmol) | toluene (mL) |
|---|---|---|---|---|---|---|
| Run 2 | 0.25 | 0.3125 | 0.00625 | 0.0075 | 0.25 | 2.0 |

| Sl. No. | Time (min) | Concentration of **1a** (mM) |
|---|---|---|
| 1 | 30 | 103 |
| 2 | 60 | 81 |
| 3 | 90 | 69 |
| 4 | 120 | 58 |
| 5 | 150 | 52 |
| 6 | 180 | 47 |
| 7 | 210 | 42 |
| 8 | 240 | 39 |




Graphical representation for determination of rate and order of reaction

**Considering steady state approximation for benzyl alcohol**

From Run 1: Slope = k [1a] $^{x}$

$- 0.224 = k [0.20]^{x}$

From Run 2: Slope = k [1a] $^{x}$

$-0.284 = k [0.25]^{x}$

$-0.284 /- 0.224 = [0.25]^{x} / [0.2]^{x}$

$1.267 = [1.25]^{x}$

Log (1.267) = x. Log (1.25)

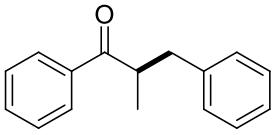
x = 0.103 / 0.0969

= 1.06 ≈ 1

Rate = k [1a] $^{1}$

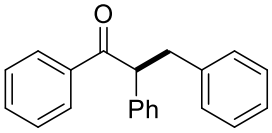
**[1.4] Analytical data:**

**2-Methyl-1,3-diphenylpropan-1-one (3a)**:[1] Following the general procedure A, the title product was



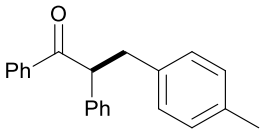
obtained as a colourless oil (40 mg, 72% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.92 (dd, $J$ = 8.7, 1.4 Hz, 2H), 7.56 – 7.52 (m, 1H), 7.44 (t, $J$ = 7.8 Hz, 2H), 7.28 – 7.21 (m, 2H), 7.19 – 7.13 (m, 3H), 3.75 (dq, $J$ = 13.9, 7.0 Hz, 1H), 3.17 (dd, $J$ = 14.0, 6.5 Hz, 1H), 2.69 (dd, $J$ = 14.0, 8.0 Hz, 1H), 1.20 (d, $J$ = 7.1 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 203.85, 140.04, 136.52, 133.02, 129.18, 128.73, 128.47, 128.37, 126.29, 42.84, 39.44, 17.49.

**1,2,3-Triphenylpropan-1-one (3b):**[1] Following the general procedure A, the title product was



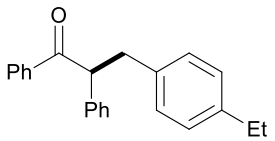
obtained as a colourless solid (59 mg, 82% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.89 (dd, $J$ = 8.3, 1.2 Hz, 2H), 7.44 – 7.42 (m, 1H), 7.33 (dd, $J$ = 8.0, 7.3 Hz, 2H), 7.25 – 7.21 (m, 4H), 7.20 – 7.17 (m, 3H), 7.14 – 7.12 (m, 1H), 7.08 – 7.06 (m, 2H), 4.80 (t, $J$ = 7.3 Hz, 1H), 3.56 (dd, $J$ = 13.7, 7.5 Hz, 1H), 3.06 (dd, $J$ = 13.7, 7.0 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 199.32, 139.86, 139.17, 136.84, 132.91, 129.21, 128.97, 128.81, 128.54, 128.37, 128.30, 127.22, 126.19, 55.96, 40.20.

**1,2-diphenyl-3-(p-tolyl)propan-1-one (3c):**[2] Following the general procedure A, the title product



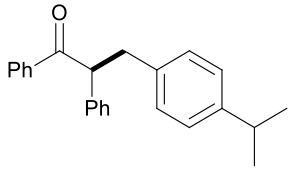
was obtained as a colourless solid (63 mg, 84% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.83 (d, $J$ = 8.6 Hz, 2H), 7.38 (t, $J$ = 7.4 Hz, 1H), 7.27 (t, $J$ = 7.6 Hz, 2H), 7.20 – 7.16 (m, 5H), 6.95 – 6.88 (m, 4H), 4.72 (t, $J$ = 7.2 Hz, 1H), 3.46 (dd, $J$ = 13.8, 7.6 Hz, 1H), 2.95 (dd, $J$ = 13.8, 6.9 Hz, 1H), 2.19 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 199.41, 139.27, 136.82, 136.75, 135.64, 132.91, 129.06, 129.00, 128.96, 128.77, 128.55, 128.38, 127.18, 56.04, 39.76, 21.10.

**3-(4-ethylphenyl)-1,2-diphenylpropan-1-one (3d):** Following the general procedure A, the title



product was obtained as a colourless solid (54 mg, 69% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.83 (d, $J$ = 8.0 Hz, 2H), 7.38 (t, $J$ = 7.4 Hz, 1H), 7.27 (t, $J$ = 7.6 Hz, 2H), 7.21 – 7.16 (m, 5H), 6.98 – 6.92 (m, 4H), 4.76 – 4.72 (m, 1H), 3.47 (dd, $J$ = 13.8, 7.7 Hz, 1H), 2.95 (dd, $J$ = 13.8, 6.7 Hz, 1H), 2.50 (q, $J$ = 7.6 Hz, 2H), 1.11 (t, $J$ = 7.6 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 199.42, 142.05, 139.35, 137.04, 136.92, 132.85, 129.09, 128.93, 128.75, 128.51, 128.38, 127.78, 127.16, 56.14, 39.63, 28.22, 15.49; Aanl. Calcd. For $C_{23}H_{22}O$: C, 87.86; H, 7.05; Found C, 87.54; H, 7.21.

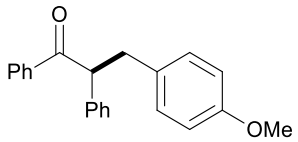
**3-(4-isopropylphenyl)-1,2-diphenylpropan-1-one (3e):** Following the general procedure A, the title



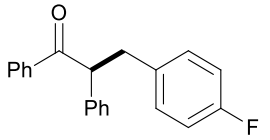
product was obtained as a colourless solid (59 mg, 72% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.83 (d, $J$ = 7.1 Hz, 2H), 7.38 (t, $J$ = 7.3 Hz, 1H), 7.27

(t, *J* = 7.6 Hz, 2H), 7.21 – 7.17 (m, 5H), 6.97 (q, *J* = 8.2 Hz, 4H), 4.75 (t, *J* = 7.2 Hz, 1H), 3.49 (dd, *J* = 13.9, 7.9 Hz, 1H), 2.95 (dd, *J* = 13.8, 6.5 Hz, 1H), 2.81 – 2.71 (m, 1H), 1.12 (d, *J* = 7.1 Hz, 6H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 199.40, 146.70, 139.40, 137.20, 136.85, 132.89, 129.06, 128.98, 128.79, 128.54, 128.37, 127.18, 126.36, 55.94, 39.78, 33.73, 24.09; Aanl. Calcd. for $C_{24}H_{24}O$: C, 87.76; H, 7.37; Found C, 87.85; H, 7.28.

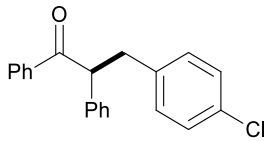
**3-(4-methoxyphenyl)-1,2-diphenylpropan-1-one (3f):**[3] Following the general procedure A, the title product was obtained as a colourless solid (46 mg, 58% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.82 (d, *J* = 7.2 Hz, 2H), 7.37 (t, *J* = 7.4 Hz, 1H), 7.27 (t, *J* = 7.6 Hz, 2H), 7.21 – 7.14 (m, 5H), 6.92 (d, *J* = 8.6 Hz, 2H), 6.66 (d, *J* = 8.7 Hz, 2H), 4.70 (t, *J* = 7.3 Hz, 1H), 3.67 (s, 3H), 3.43 (dd, *J* = 13.8, 7.5 Hz, 1H), 2.93 (dd, *J* = 13.8, 7.0 Hz, 1H);$^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 199.51, 158.04, 139.25, 136.93, 132.85, 131.94, 130.11, 128.94, 128.73, 128.53, 128.39, 127.16, 113.33, 56.26, 55.25, 39.36.



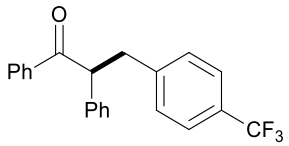

**3-(4-fluorophenyl)-1,2-diphenylpropan-1-one (3g):**[4] Following the general procedure B, the title product was obtained as a colourless solid (39 mg, 51% yield); $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 7.83 (d, *J* = 7.5 Hz, 2H), 7.39 (t, *J* = 7.3 Hz, 1H), 7.29 (t, *J* = 7.7 Hz, 2H), 7.19 – 7.10 (m, 5H), 6.97 – 6.94 (m, 2H), 6.81 (t, *J* = 8.7 Hz, 2H), 4.69 (t, *J* = 7.3 Hz, 1H), 3.45 (dd, *J* = 13.8, 7.4 Hz, 1H), 2.97 (dd, *J* = 13.8, 7.2 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 198.89, 161.5 (d, $J_{C\text{-}F}$ = 242 Hz), 138.90, 136.69, 135.45 (d, $J_{C\text{-}F}$ = 3 Hz), 133.03, 130.65 (d, $J_{C\text{-}F}$ = 8 Hz), 129.05, 128.76, 128.60, 128.35, 127.33, 115.05 (d, $J_{C\text{-}F}$ = 21 Hz), 56.10, 39.36.




**3-(4-chlorophenyl)-1,2-diphenylpropan-1-one (3h):**[3] Following the general procedure A, the title product was obtained as a colourless solid (62.5 mg, 78% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.89 (d, *J* = 7.1 Hz, 2H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 2H), 7.26 (t, *J* = 7.3 Hz, 3H), 7.21 (d, *J* = 7.3 Hz, 2H), 7.15 (d, *J* = 8.4 Hz, 2H), 7.02 – 6.98 (m, 2H), 4.75 (t, *J* = 7.3 Hz, 1H), 3.50 (dd, *J* = 13.8, 7.4 Hz, 1H), 3.03 (dd, *J* = 13.7, 7.2 Hz, 1H);$^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 199.00, 138.80, 138.30, 136.67, 133.03, 132.02, 130.58, 129.07, 128.74, 128.59, 128.41, 128.33, 127.36, 55.82, 39.36.

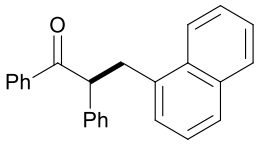



**1,2-diphenyl-3-(4-(trifluoromethyl)phenyl)propan-1-one (3i):** Following the general procedure B, the title product was obtained as a colourless solid (71 mg, 80% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.89 (d, *J* = 7.4 Hz, 2H), 7.45 (t, *J* = 8.9 Hz, 3H), 7.34 (t, *J* = 7.7 Hz, 2H), 7.29 – 7.24 (m, 2H), 7.19 (dd, *J* = 12.8, 7.6 Hz, 5H), 4.78 (t, *J* = 7.3 Hz, 1H), 3.59 (dd, *J* = 13.7, 7.5 Hz, 1H), 3.11 (dd, *J* = 13.8, 7.1 Hz, 1H); $^{13}$C



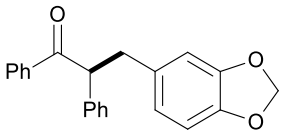
NMR (100 MHz, $CDCl_3$) $\delta$ 198.70, 143.99, 143.97, 138.64, 136.45, 133.15, 129.56, 129.17, 128.79, 128.64, 128.30, 127.49, 125.25, 125.21, 55.71, 39.93; Aanl. Calcd. for $C_{22}H_{17}F_3O$: C, 74.57; H, 4.84; Found C, 74.90; H, 4.72.

**3-(naphthalen-1-yl)-1,2-diphenylpropan-1-one (3j):** Following the general procedure A, the title



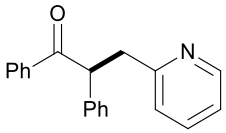

product was obtained as a colourless solid (62 mg, 73% yield); $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 8.04 (d, $J$ = 8.3 Hz, 1H), 7.84 (d, $J$ = 7.8 Hz, 3H), 7.66 (d, $J$ = 8.2 Hz, 1H), 7.54 – 7.46 (m, 2H), 7.41 (t, $J$ = 7.4 Hz, 1H), 7.29 (t, $J$ = 7.7 Hz, 2H), 7.25 – 7.17 (m, 6H), 7.10 (d, $J$ = 7.0 Hz, 1H), 4.99 (t, $J$ = 7.0 Hz, 1H), 4.09 (dd, $J$ = 13.4, 6.7 Hz, 1H), 3.48 (dd, $J$ = 14.1, 6.7 Hz, 1H);$^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 199.37, 139.52, 136.75, 135.59, 133.97, 132.96, 131.90, 129.08, 129.06, 128.81, 128.55, 128.39, 128.26, 127.70, 127.29, 127.08, 126.12, 125.48, 123.54, 54.66, 37.03; Aanl. Calcd. for $C_{25}H_{20}O$: C, 89.25; H, 5.99; Found C, 89.39; H, 5.87.

**3-(1,3-dihydroisobenzofuran-5-yl)-1,2-diphenylpropan-1-one (3k):** Following the general



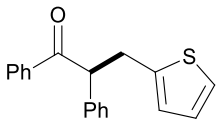

procedure A, the title product was obtained as a colourless solid (45 mg, 55% yield); $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 7.83 (d, $J$ = 7.4 Hz, 2H), 7.39 (t, $J$ = 7.3 Hz, 1H), 7.29 (t, $J$ = 7.7 Hz, 2H), 7.20 – 7.11 (m, 5H), 6.58 – 6.46 (m, 3H), 5.81 (s, 2H), 4.69 (t, $J$ = 7.2 Hz, 1H), 3.41 (dd, $J$ = 13.8, 7.6 Hz, 1H), 2.91 (dd, $J$ = 13.8, 6.9 Hz, 1H);$^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 199.30, 147.44, 145.89, 139.07, 136.78, 133.64, 132.97, 129.01, 128.77, 128.58, 128.34, 127.27, 122.17, 109.64, 108.13, 100.82, 56.21, 39.91; Aanl. Calcd. for $C_{22}H_{18}O_3$: C, 79.98; H, 5.49; Found C, 79.91; H, 5.58.

**1,2-diphenyl-3-(pyridin-2-yl)propan-1-one (3l):**[5] Following the general procedure B, the title




product was obtained as a yellow oil (54.5 mg, 76% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.46 – 8.42 (m, 1H), 7.92 (dt, $J$ = 8.6, 1.7 Hz, 2H), 7.43 (ddd, $J$ = 13.1, 9.4, 4.6 Hz, 2H), 7.31 (t, $J$ = 7.6 Hz, 2H), 7.27 – 7.19 (m, 4H), 7.13 (ddd, $J$ = 6.1, 4.6, 2.4 Hz, 1H), 7.01 (t, $J$ = 6.2 Hz, 2H), 5.30 (dd, $J$ = 8.5, 6.3 Hz, 1H), 3.69 (dd, $J$ = 14.1, 8.5 Hz, 1H), 3.18 (dd, $J$ = 14.1, 6.3 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 199.51, 159.48, 149.17, 139.25, 136.79, 136.21, 132.83, 129.00, 128.90, 128.48, 128.37, 127.17, 124.19, 121.31, 53.27, 42.30.

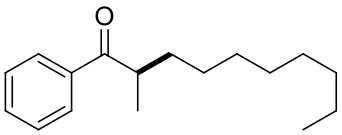
**(S)-1,2-diphenyl-3-(thiophen-2-yl)propan-1-one (3m):** Following the general procedure A, the title




product was obtained as a pale yellow solid (31 mg, 42% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.92 (d, $J$ = 8.6 Hz, 2H), 7.48 – 7.43 (m, 1H), 7.36 (t, $J$ = 7.6 Hz, 2H), 7.27 (dd, $J$ = 3.8, 3.3 Hz, 4H), 7.23 – 7.19 (m, 1H), 7.05 (d, $J$ = 5.1 Hz, 1H), 6.82 (dd, $J$ = 5.1, 3.4 Hz, 1H), 6.68 (d, $J$ = 3.4 Hz, 1H), 4.84 (dd, $J$ = 7.9, 6.6 Hz, 1H), 3.78 (dd, $J$ = 14.5, 7.5 Hz, 1H), 3.27 (dd, $J$ = 14.8, 6.6 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 198.92, 142.16,

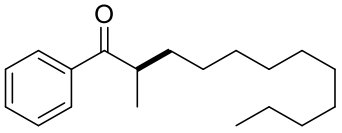
138.73, 133.07, 133.06, 129.08, 128.82, 128.61, 128.32, 127.45, 126.75, 125.78, 123.71, 56.37, 34.21; Aanl. Calcd. for $C_{19}H_{16}OS$: C, 78.05; H, 5.52; S, 10.97; Found C, 78.19; H, 5.69; S, 11.08.

**2-methyl-1-phenyldecan-1-one (3n):**[1] Following the general procedure C, the title product was



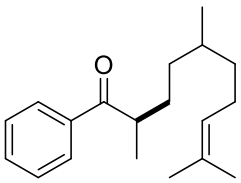
obtained as a colourless oil (20 mg, 33% yield); $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 7.98 (d, $J$ = 7.3 Hz, 2H), 7.59-7.57 (m, 1H), 7.50 (t, $J$ = 7.4 Hz, 2H), 3.51-3.45 (m, 1H), 1.85 – 1.78 (m, 1H), 1.48 – 1.42 (m, 1H),1.29 – 1.26 (m, 12H), 1.22 (d, $J$ = 6.7 Hz, 3H), 0.89 (t, $J$ = 6.4 Hz, 3H); GC-MS (EI) m/z = 246.2.

**2-Methyl-1-phenyldodecan-1-one (3o):**[1] Following the general procedure C, the title product was



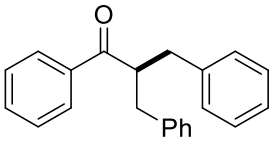
obtained as a colourless oil (21 mg, 30% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.88 (d, $J$ = 7.3 Hz, 2H), 7.51 – 7.45 (m, 1H), 7.39 (t, $J$ = 7.6 Hz, 2H), 3.43 – 3.35 (m, 1H), 1.82 – 1.62 (m, 1H), 1.42 – 1.27 (m, 1H), 1.21 – 1.17 (m, 16H), 1.12 (d, $J$ = 6.8 Hz, 3H), 0.80 (t, $J$ = 7.0 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 204.68, 136.90, 132.83, 128.66, 128.35, 40.67, 33.83, 31.96, 30.03, 29.80, 29.65, 29.55, 29.37, 27.48, 22.74, 17.27, 14.17.

**2,5,9-Trimethyl-1-phenyldec-8-en-1-one (3p):**[1] Following the general procedure C, the title product



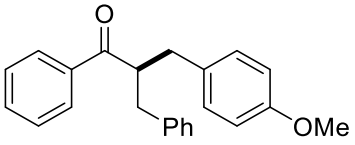
was obtained as a pale yellow oil (34 mg, 50% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.94 (d, $J$ = 7.9 Hz, 2H), 7.54 (dd, $J$ = 8.2, 6.5 Hz, 1H), 7.45 (t, $J$ = 7.6 Hz, 2H), 5.05 (ddd, $J$ = 12.8, 5.8, 1.3 Hz, 1H), 3.41 (ddd, $J$ = 13.5, 6.7, 2.2 Hz, 1H), 1.97 – 1.74 (m, 3H), 1.65 (d, $J$ = 4.2 Hz, 3H), 1.57 (d, $J$ = 5.0 Hz, 2H), 1.47 – 1.24 (m, 5H), 1.18 (d, $J$ = 6.9 Hz, 3H), 1.15 – 1.08 (m, 2H), 0.84 (t, $J$ = 6.5 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 204.66, 133.34, 132.84, 131.16, 129.03, 128.66, 128.28, 40.93, 37.03, 36.85, 34.63, 32.57, 31.22, 25.51, 19.47, 17.24.

**2-benzyl-1,3-diphenylpropan-1-one (3q):**[1] Following the general procedure A, the title product was



obtained as a colourless oil (34 mg, 45% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.72 (d, $J$ = 8.2 Hz, 2H), 7.45 (t, $J$ = 7.5 Hz, 1H), 7.34 – 7.30 (m, 2H), 7.22 (dd, $J$ = 15.4, 7.1 Hz, 4H), 7.19 – 7.11 (m, 6H), 4.05 – 3.98 (m, 1H), 3.13 (dd, $J$ = 14.2, 8.1 Hz, 2H), 2.80 (dd, $J$ = 14.1, 6.5 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 203.46, 139.59, 137.45, 132.88, 129.11, 128.53, 128.50, 128.19, 126.36, 50.57, 38.30.

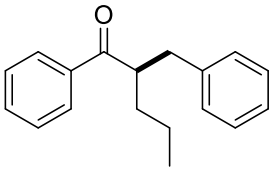
**2-Benzyl-3-(4-methoxyphenyl)-1-phenylpropan-1-one (3r):**[1] Following the general procedure A,



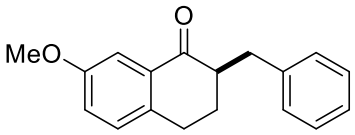
the title product was obtained as a colourless oil (33 mg, 40% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.71 (d, $J$ = 7.5 Hz, 2H), 7.45 (t, $J$ = 7.4 Hz, 1H), 7.32 (t, $J$ = 7.7 Hz, 2H), 7.21 – 7.18 (m, 2H), 7.13 – 7.10 (m, 3H), 7.04 (d, $J$ = 8.6 Hz, 2H), 6.74 (d, $J$ = 8.6 Hz, 2H), 4.00 – 3.93 (m, 1H), 3.73 (s, 3H), 3.12 – 3.03

(m, 2H), 2.80 – 2.71 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 203.60, 158.11, 139.68, 137.50, 132.82, 131.60, 130.05, 129.08, 128.51, 128.46, 128.18, 126.29, 113.89, 55.29, 50.80, 38.21, 37.45.

**2-benzyl-1-phenylpentan-1-one (3s):**[1] Following the general procedure A, the title product was obtained as a colourless oil (22 mg, 35% yield);$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.86 – 7.84 (m, 2H), 7.52 – 7.49 (m, 1H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.24 – 7.14 (m, 5H), 3.76 – 3.70 (m, 1H), 3.10 (dd, *J* = 13.5, 7.7 Hz, 1H), 2.77 (dd, *J* = 13.6, 6.5 Hz, 1H), 1.76 (m, 1H), 1.52 (m, 1H), 1.31 – 1.25 (m, 2H), 0.85 (t, *J* = 7.3 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 204.14, 140.12, 137.62, 132.90, 129.09, 128.63, 128.43, 128.21, 126.20, 48.24, 38.32, 34.68, 20.69, 14.29.



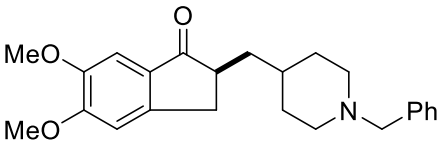
**2-Benzyl-7-methoxy-3,4-dihydronaphthalen-1(2*H*)-one (3t):**[1] Following the general procedure A, the title product was obtained as a pale yellow oil (33 mg, 50% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.54 (d, *J* = 2.8 Hz, 1H), 7.32 – 7.28 (m, 2H), 7.25 – 7.19 (m, 3H), 7.12 (d, *J* = 8.4 Hz, 1H), 7.04 (dd, *J* = 8.4, 2.8 Hz, 1H), 3.83 (s, 3H), 3.47 (dd, *J* = 13.4, 3.8 Hz, 1H), 2.88 – 2.86 (m, 2H), 2.69 – 2.61 (m, 2H), 2.10 – 2.06 (m, 1H), 1.81 – 1.72 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 199.49, 158.40, 140.13, 136.74, 133.30, 130.02, 129.35, 128.48, 126.22, 121.77, 109.52, 55.57, 49.37, 35.80, 27.98, 27.85.



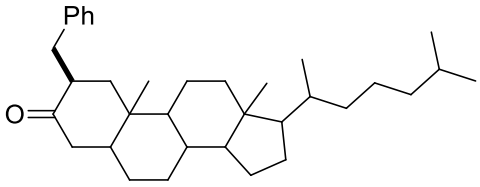
**2-Benzyl-3,4-dihydronaphthalen-1(2*H*)-one (3u):**[1] Following the general procedure A, the title product was obtained as a colourless oil (45 mg, 76% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.07 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.45 (td, *J* = 7.5, 1.4 Hz, 1H), 7.33 – 7.28 (m, 3H), 7.25 – 7.19 (m, 4H), 3.49 (dd, *J* = 13.6, 3.9 Hz, 1H), 2.95 – 2.92 (m, 2H), 2.79 – 2.69 (m, 1H), 2.64 (dd, *J* = 13.6, 9.6 Hz, 1H), 2.13 – 2.07 (m, 1H), 1.83 – 1.73 (m, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 199.52, 144.13, 140.14, 133.37, 132.55, 129.36, 128.81, 128.50, 127.64, 126.72, 126.23, 49.55, 35.75, 28.71, 27.74.



**2-((1-Benzylpiperidin-4-yl)methyl)-5,6-dimethoxy-2,3-dihydro-1*H*-inden-1-one (3v):**[1] Following the general procedure A, the title product was obtained as a yellow oil (38 mg, 40% yield); $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 7.55 (d, *J* = 7.2 Hz, 2H), 7.43-7.36 (m, 3H), 7.12 (s, 1H), 6.84 (s, 1H), 3.95 (s, 3H), 3.88 (s, 3H), 3.64 (s, 2H), 3.34-3.25 (m, 1H), 2.71 – 2.51 (m, 4H), 1.97 – 1.85 (m, 5H), 1.50 – 1.27 (m, 4H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 207.14, 155.67, 149.54, 148.69, 137.53, 131.05, 129.38, 129.01, 127.11, 107.37, 104.31, 70.54, 56.25, 56.07, 52.23, 44.58, 33.73, 31.89, 29.66, 22.66, 14.10.

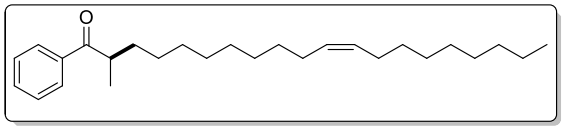


**2-Benzyl-10,13-dimethyl-17-(6-methylheptan-2-yl)-6,7,8,9,10,11,12,13,14,15,16,17-dodecahydro-3*H*-cyclopenta[*a*]phenanthren-3-one (3w):**[6]

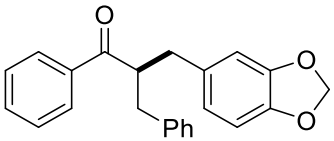



Following the general procedure A, the title product was obtained as a yellow oil (89.3 mg, 75% yield); $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 7.29 – 7.26 (m, 3H), 7.11 (t, $J$ = 8.8 Hz, 2H), 3.23 – 3.02 (m, 2H), 2.73 – 2.67 (m, 1H), 2.37 (dt, $J$ = 14.4, 4.7 Hz, 1H), 1.98 – 1.75 (m, 5H), 1.58 – 1.44 (m, 4H), 1.40 – 1.09 (m, 18H), 0.95 (s, 3H), 0.91 – 0.86 (m, 10H), 0.63 (s, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 213.56, 142.01, 129.38, 128.87, 128.23, 128.16, 125.91, 56.44, 56.25, 54.17, 48.27, 47.16, 46.83, 44.49, 42.66, 39.89, 39.51, 37.03, 36.57, 36.14, 35.76, 35.12, 32.01, 29.71, 28.31, 28.02, 24.16, 23.80, 23.19, 22.82, 21.51, 18.68, 13.85, 11.96.

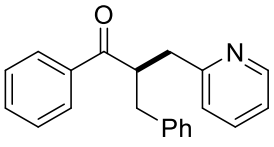
**2-methyl-1-phenylicos-11-en-1-one (3x):**[1] Following the general procedure C, the title product was obtained as a pale yellow oil (48 mg, 50% yield); $^1$H NMR (500 MHz, $CDCl_3$) $\delta$ 7.38 – 7.29 (m, 5H), 5.38 (t, $J$ = 3.7 Hz, 2H), 3.59 – 3.52 (m, 1H), 2.09-2.04 (m, 4H), 1.89– 1.70 (m, 2H), 1.35-1.30 (m, 24H), 0.95 – 0.77 (m, 6H);$^{13}$C NMR (125 MHz, $CDCl_3$) $\delta$ 206.05, 142.78, 128.84, 127.07, 126.32, 125.61, 125.27, 113.91, 39.10, 32.07, 31.15, 30.82, 29.88, 28.88, 28.70, 28.56, 28.44, 28.23, 26.14, 25.93, 21.60, 14.59, 13.02.



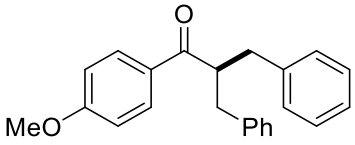

**3-(Benzo[*d*][1,3]dioxol-5-yl)-2-benzyl-1-phenylpropan-1-one (3y):**[1] Following the general procedure A, the title product was obtained as a colourless liquid (40 mg, 46% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.72 (d, $J$ = 8.0 Hz, 2H), 7.46 (dd, $J$ = 11.9, 4.4 Hz, 1H), 7.34 (t, $J$ = 7.9 Hz, 2H), 7.25 – 7.18 (m, 2H), 7.14 – 7.10 (m, 3H), 6.65 – 6.57 (m, 3H), 5.86 (dd, $J$ = 3.3, 1.5 Hz, 2H), 3.98 – 3.91 (m, 1H), 3.12 – 3.01 (m, 2H), 2.80 – 2.68 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 203.40, 147.61, 145.99, 139.54, 137.44, 133.34, 132.89, 129.08, 128.55, 128.50, 128.18, 126.36, 122.09, 109.46, 108.24, 100.85, 50.79, 38.27, 37.95.



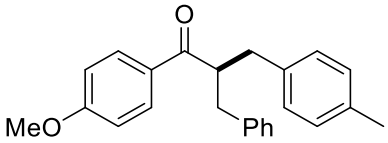

**2-Benzyl-1-phenyl-3-(pyridin-2-yl)propan-1-one (3z):**[1] Following the general procedure A, the title product was obtained as a pale yellow oil (27 mg, 36% yield);$^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.37 (d, $J$ = 4.0 Hz, 1H), 7.77 (dd, $J$ = 8.1, 0.9 Hz, 2H), 7.40 – 7.36 (m, 2H), 7.27 (t, $J$ = 7.6 Hz, 2H), 7.14 – 6.96 (m, 6H), 6.94 (dd, $J$ = 6.9, 5.2 Hz, 1H), 4.43 – 4.36 (m, 1H), 3.23 (dd, $J$ = 14.1, 8.5 Hz, 1H), 3.08 (dd, $J$ = 13.6, 7.6 Hz, 1H), 2.90 (dd, $J$ = 14.1, 5.8 Hz, 1H), 2.74 (dd, $J$ = 13.6, 6.6 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 203.58, 159.38, 149.34, 139.31, 137.36, 136.25, 136.23, 132.76, 129.18, 128.45, 128.42, 126.34, 123.99, 121.32, 47.98, 40.20, 38.53.



**2-Benzyl-1-(4-methoxyphenyl)-3-phenylpropan-1-one (3ab):**[1] Following the general procedure A, the title product was obtained as a colourless oil (66 mg, 80% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.73 (d, $J$ = 9.2 Hz, 2H), 7.43 – 7.37 (m, 1H), 7.23 – 7.19 (m, 4H), 7.13 (d, $J$ = 7.7 Hz, 5H), 6.80 (d, $J$ = 9.1 Hz, 2H), 3.98 – 3.94 (m, 1H), 3.80 (s, 3H), 3.12 (dd, $J$ = 14.2, 8.1 Hz, 2H), 2.79 (dd, $J$ = 14.1, 6.5 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 201.76, 163.37, 139.79, 130.53, 130.45, 129.09, 128.46, 126.29, 113.70, 55.49, 50.06, 38.43.




**2-Benzyl-1-(4-methoxyphenyl)-3-(*p*-tolyl)propan-1-one (3ac):**[1] Following the general procedure A, the title product was obtained as a colourless liquid (47 mg, 55% yield); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.73 (d, $J$ = 8.9 Hz, 2H), 7.26 – 7.17 (m, 3H), 7.13 – 7.10 (m, 3H), 7.01 (d, $J$ = 3.0 Hz, 3H), 6.80 (d, $J$ = 8.9 Hz, 2H), 3.98 – 3.89 (m, 1H), 3.80 (s, 3H), 3.10 – 3.04 (m, 2H), 2.79 – 2.72 (m, 2H), 2.25 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 201.79, 163.33, 139.88, 136.63, 135.71, 130.53, 130.45, 129.08, 128.95, 128.41, 127.69, 126.21, 113.69, 55.50, 50.09, 38.26, 37.95, 21.13.




**[1.5] References:**

1. J. Das, K. Singh, M. Vellakkaran and D. Banerjee, *Org. Lett*., 2018, **20**, 5587−5591.

2. A. S. S. Sido, S. Chassaing, M. Kumarraja, P. Paleb and J. Sommera, *Tetrahedron Letters*, 2007, **48**, 5911–5914.

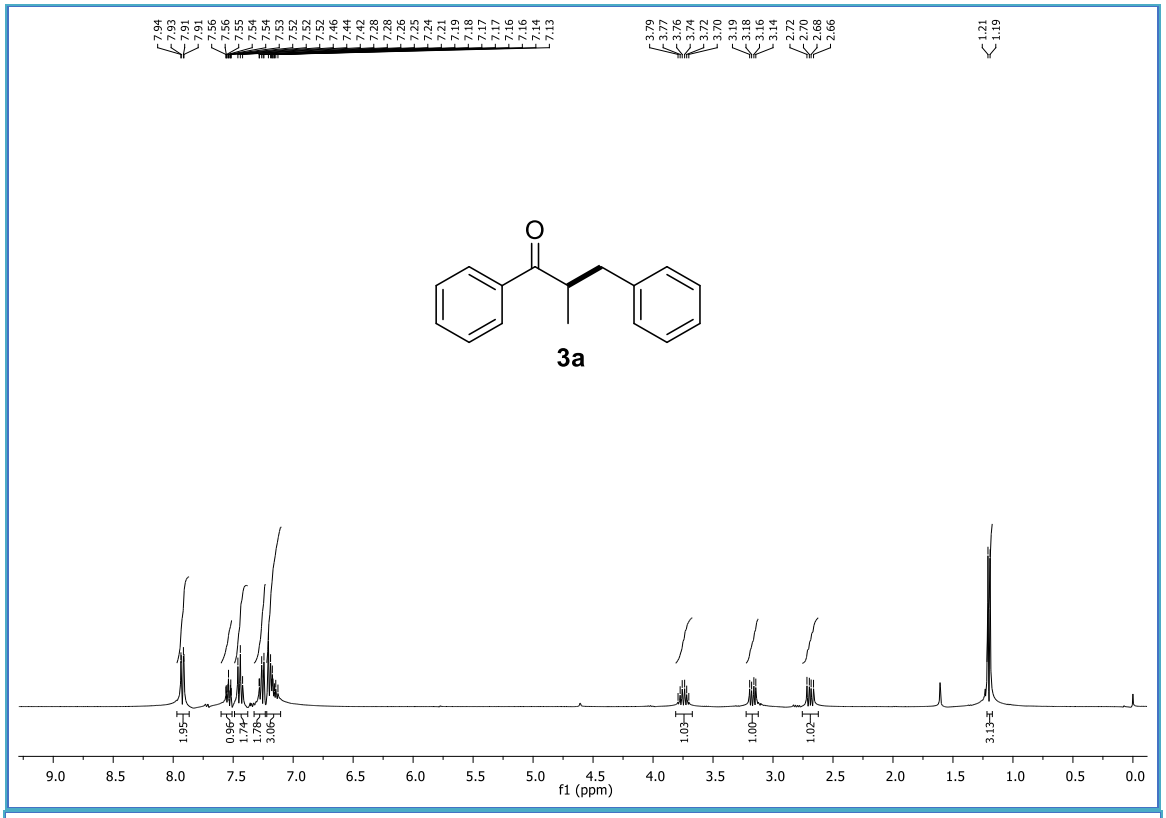
3. X. Cao, X. Wan, F. Yang, K. Li, X. Hao, T. Shao, X. Zhu and M. Song, *J. Org. Chem*., 2018, **83**, 3657−3668.

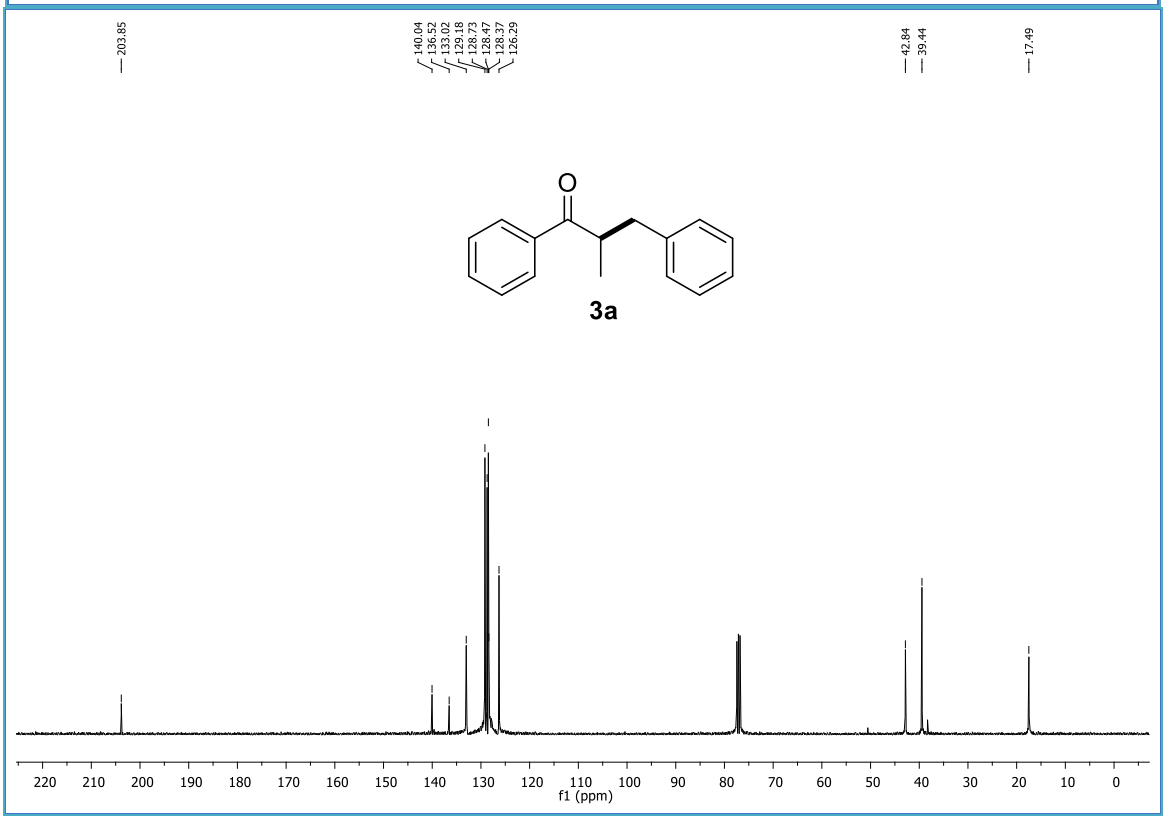
4. D. Kaiser, L. F. Veiros and N. Maulidea, *Adv. Synth. Catal*., 2017, **359**, 64 – 77.

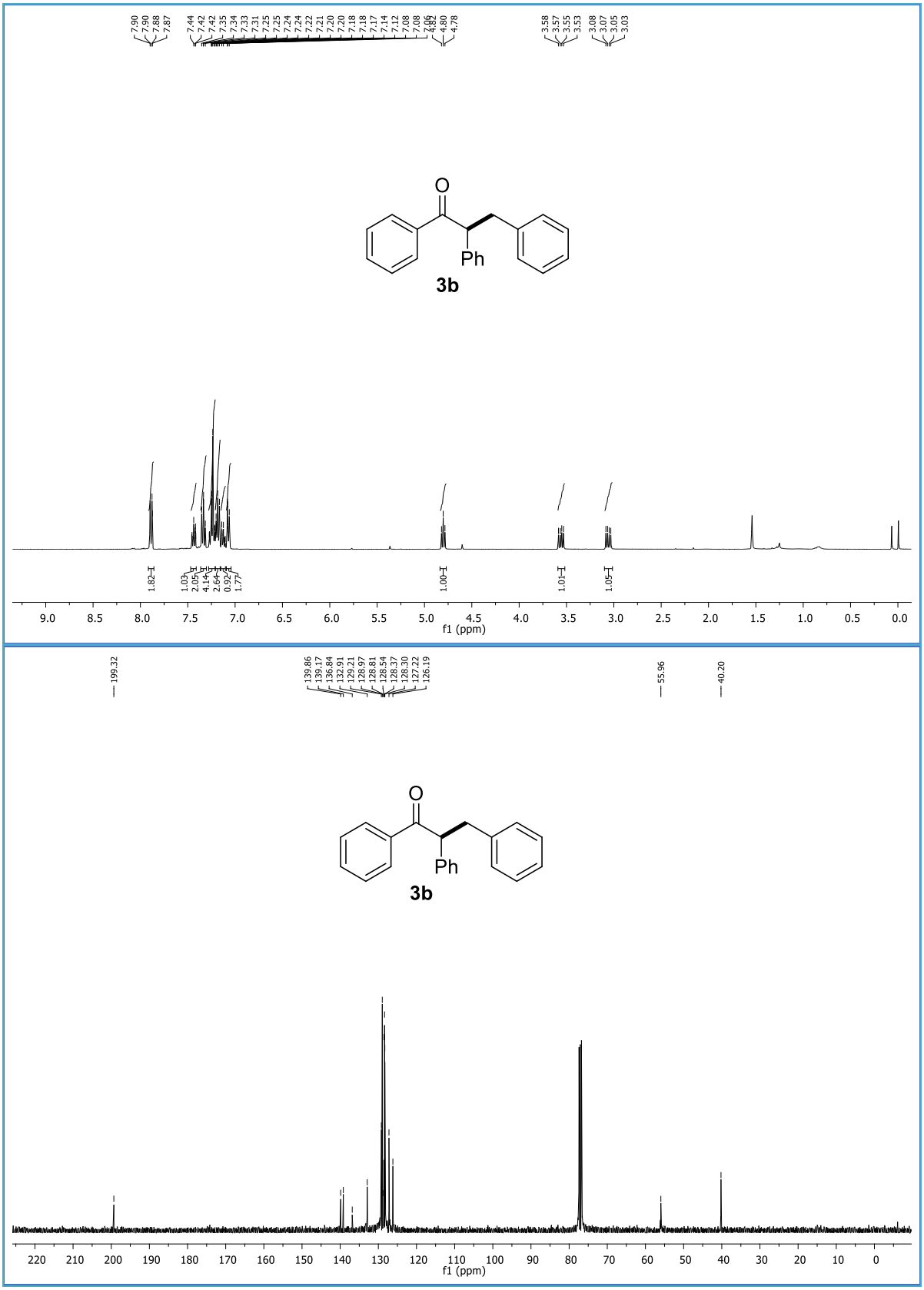
5. F.Yan , M. Zhang, X. Wang, F. Xie, M. Chen and H. Jiang, *Tetrahedron*, 2014, **70**, 1193–1198.

6. C. Schlepphorst, B. Maji and F. Glorius, *ACS Catal*. 2016, **6**, 4184−4188.

## [1.6] Copies of $^{1}$H NMR and $^{13}$C NMR for selected compounds

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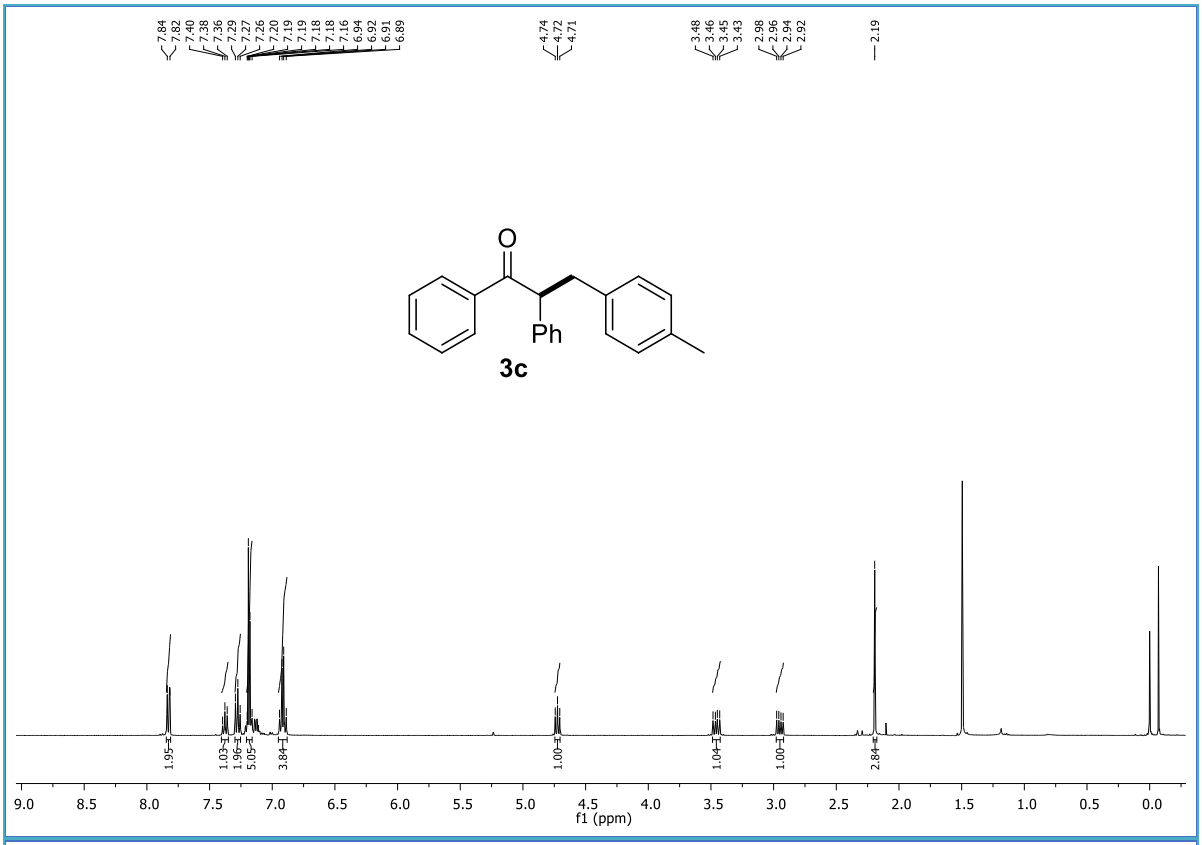
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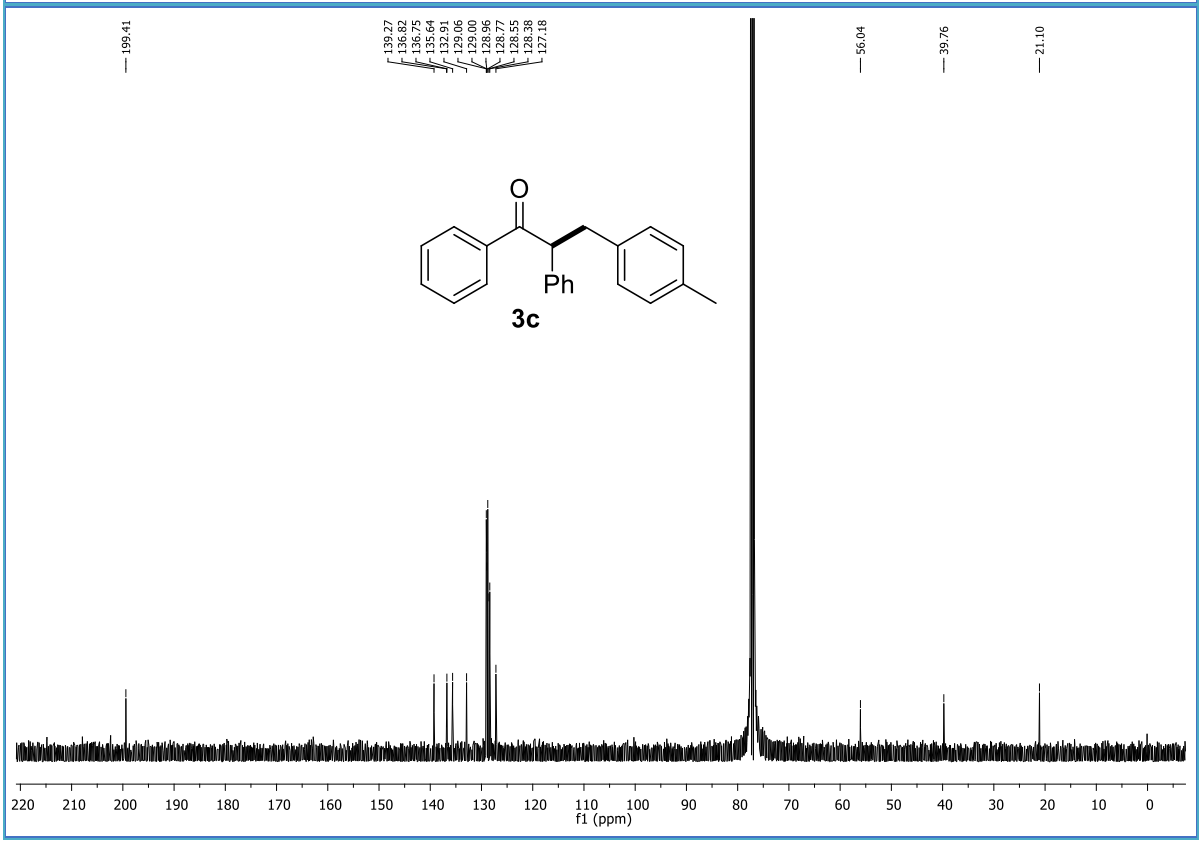
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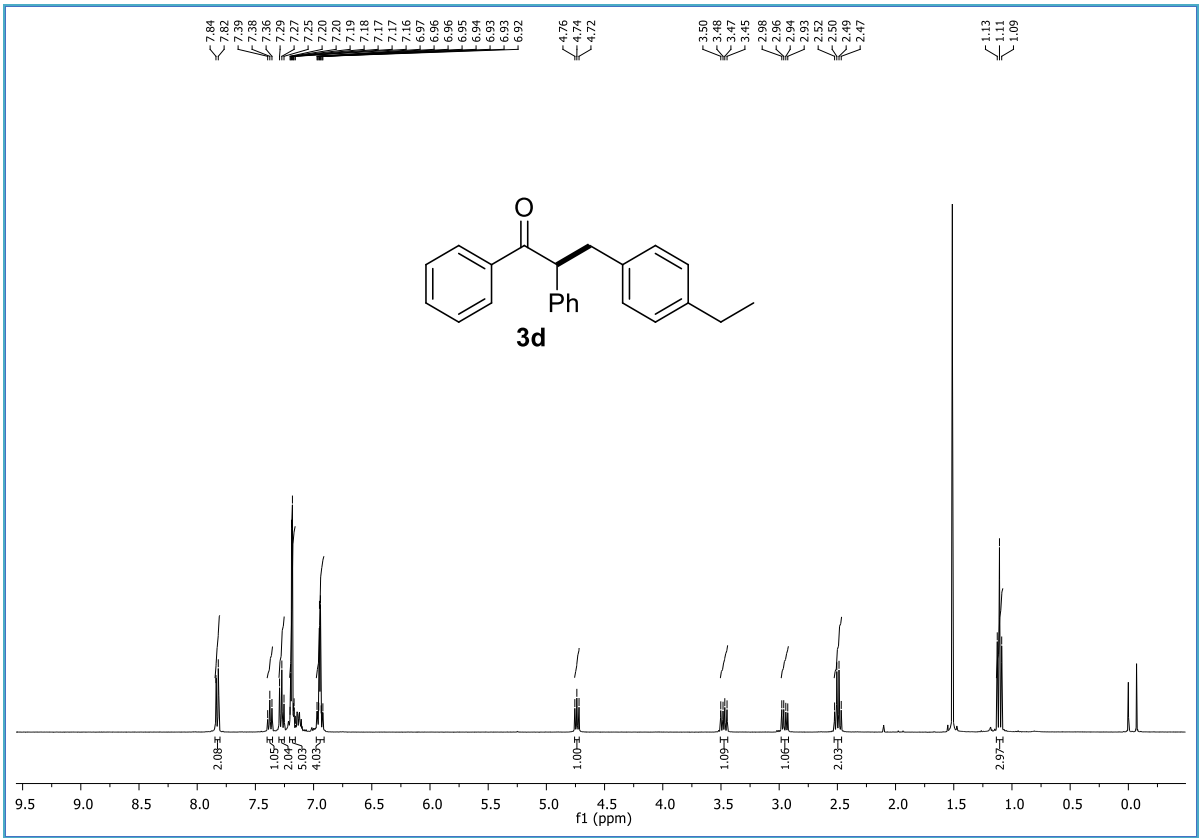
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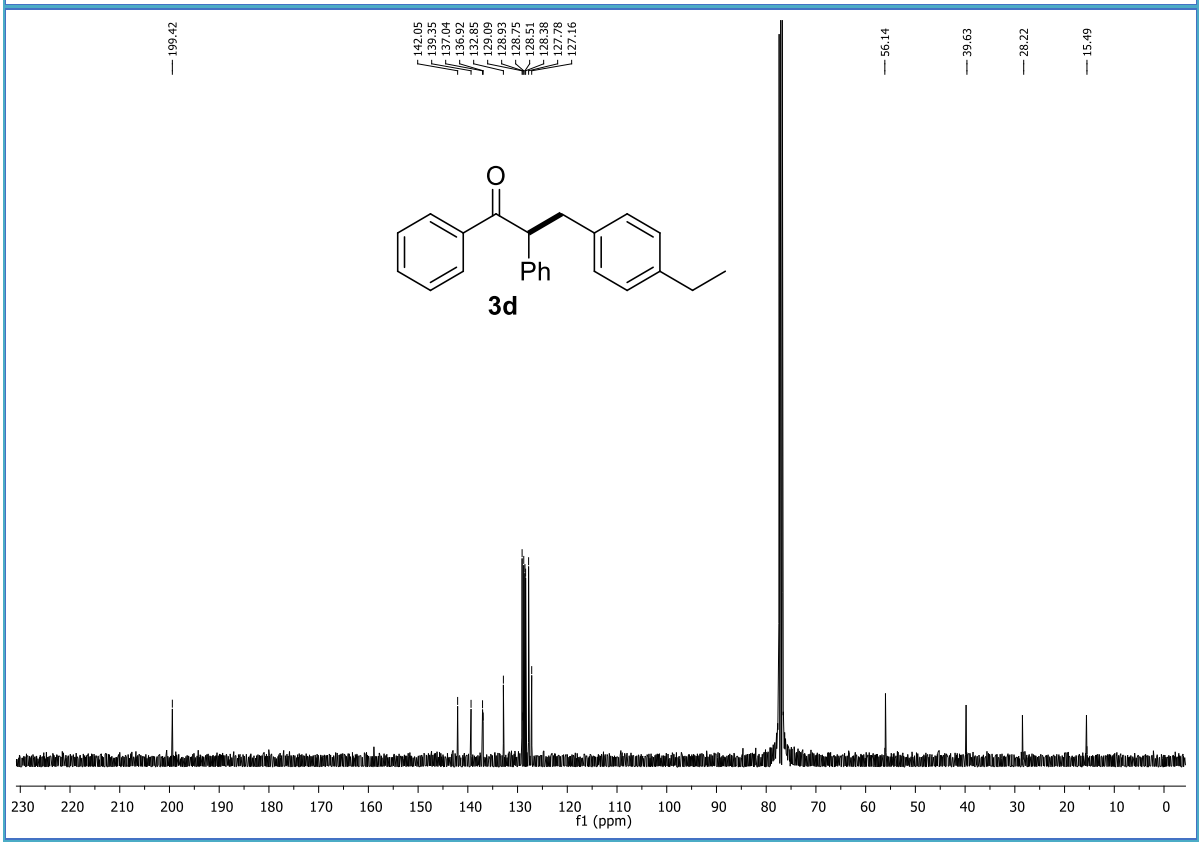
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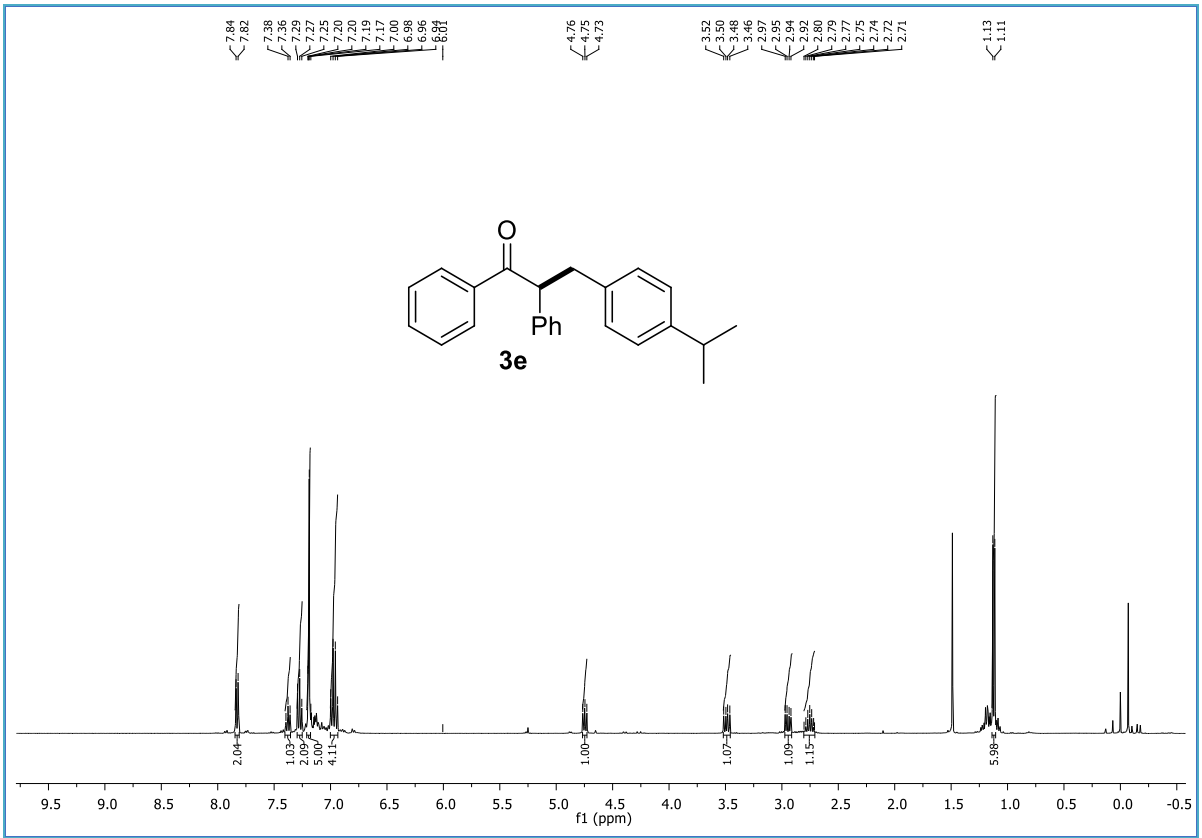
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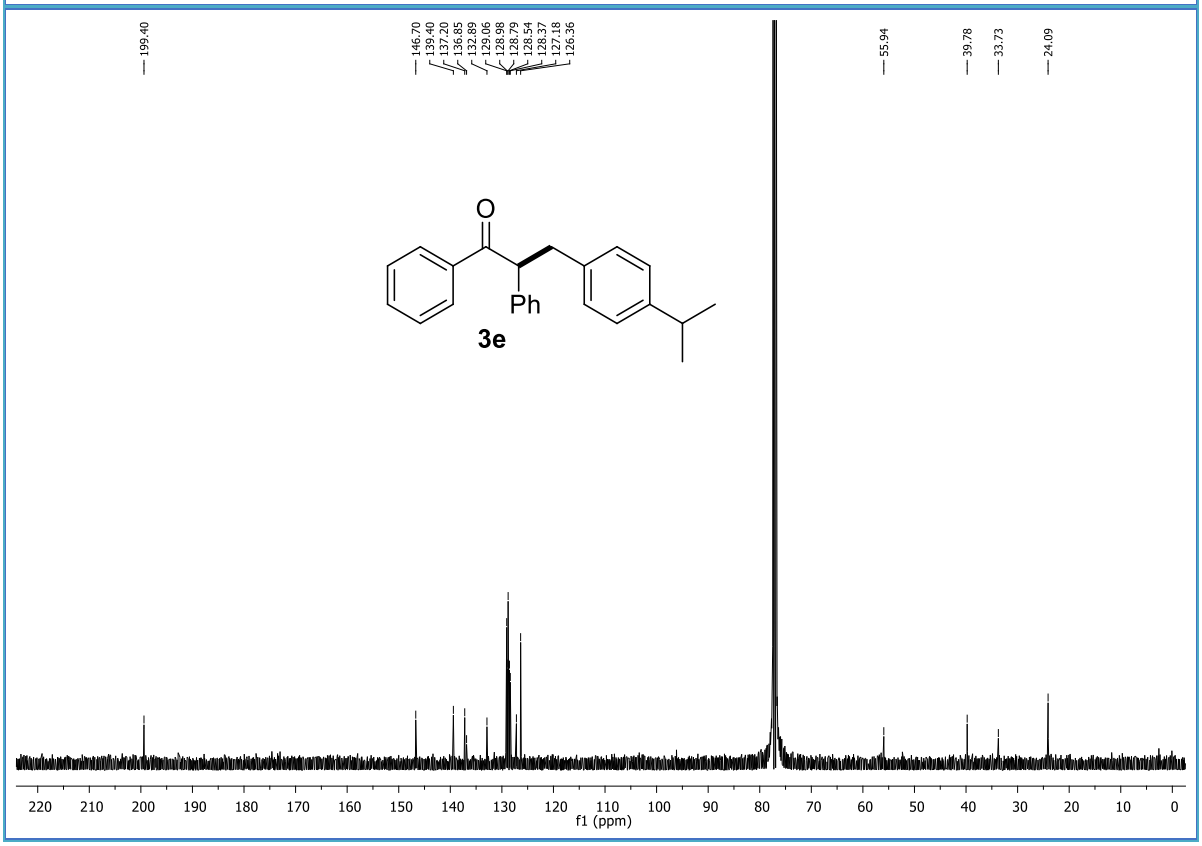
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Ph
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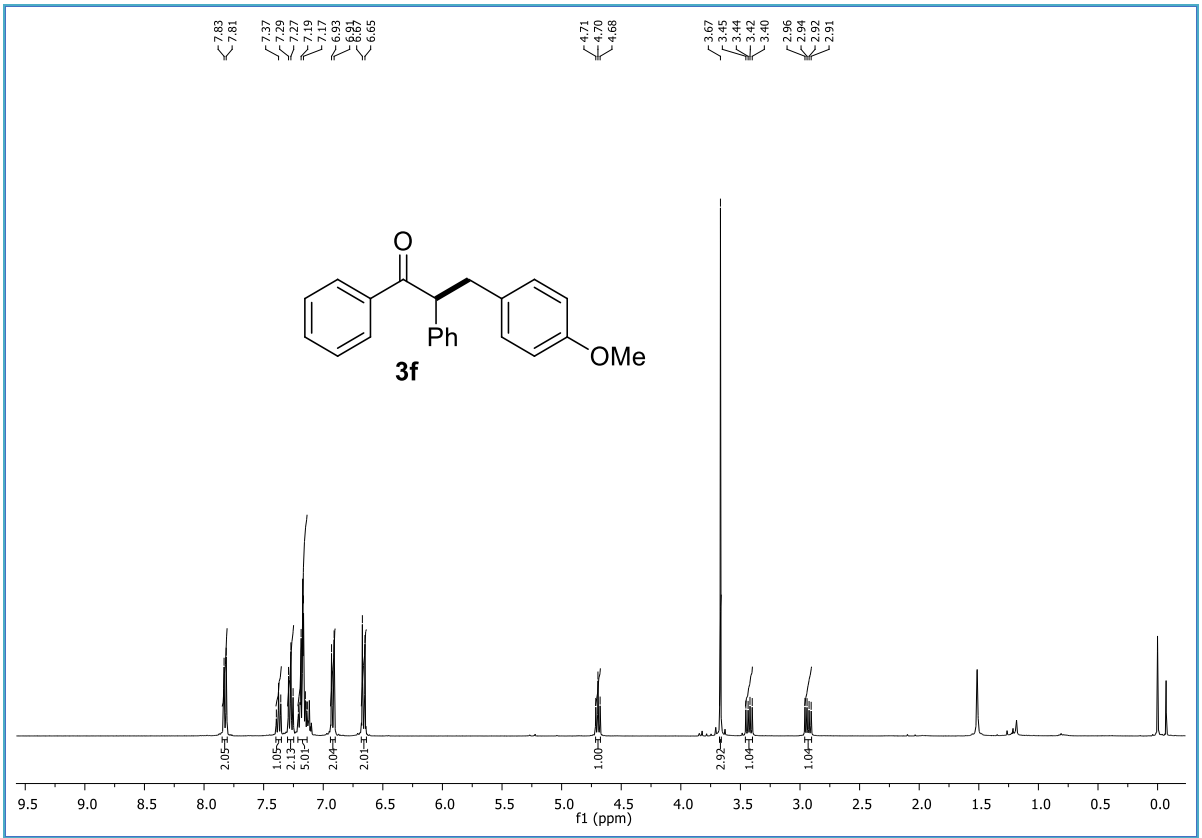
f1 (ppm)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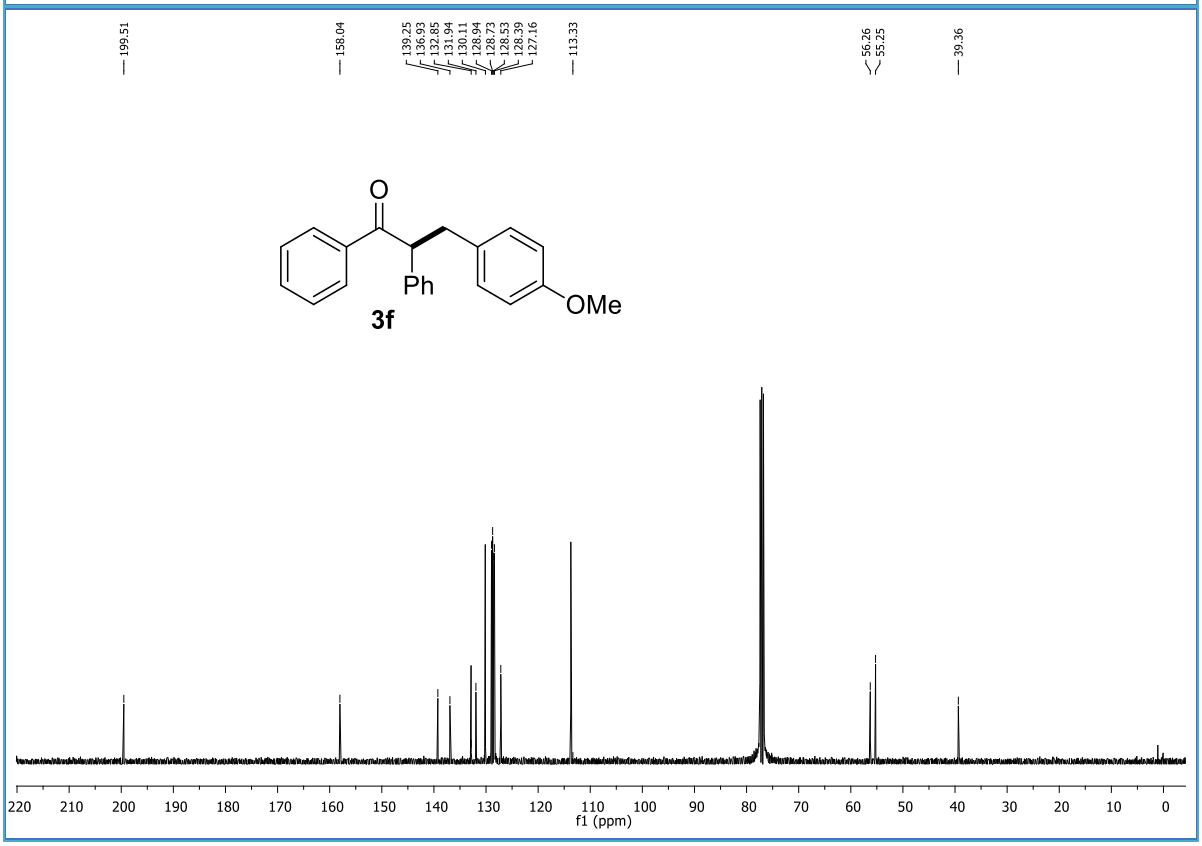
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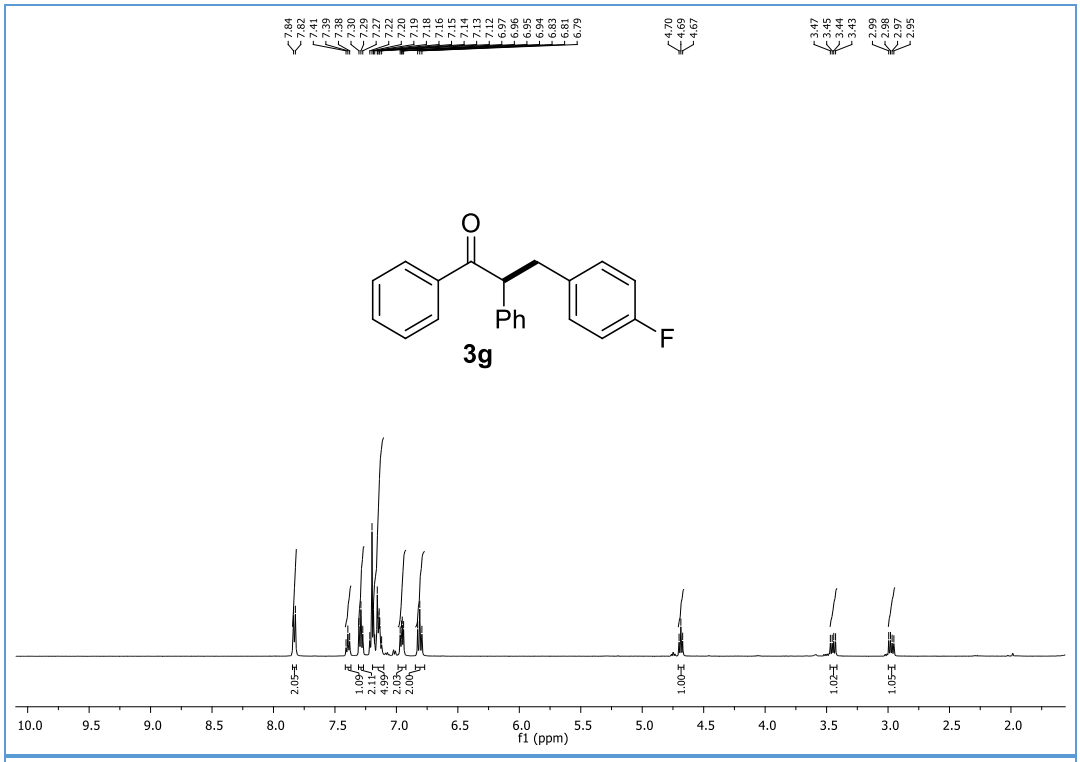
f1 (ppm)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7.14
7.13
7.12
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6.96
6.95
6.94
6.83
6.81
6.79
4.70
4.69
4.67
3.47
3.45
3.44
3.43
2.99
2.98
2.97
2.95
O
Ph
F
3g
2.05
1.09
2.13
4.93
2.03
2.00
1.00
1.02
1.05
10.0
9.5
9.0
8.5
8.0
7.5
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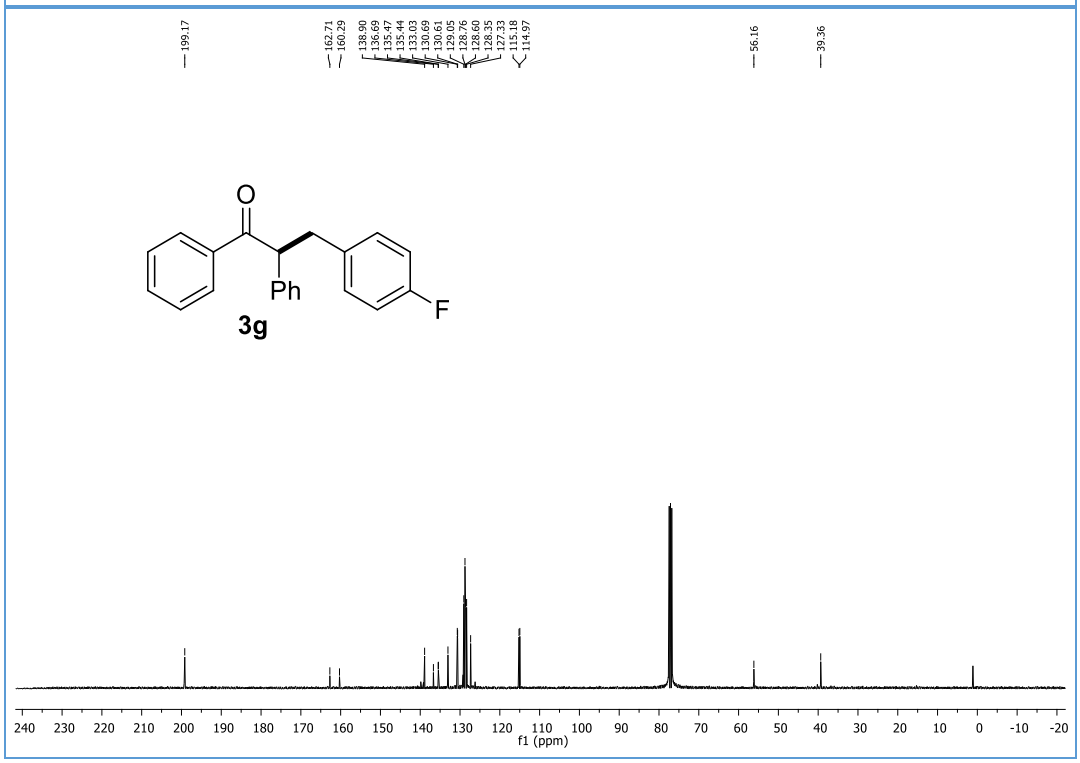
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)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129.05
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128.60
128.35
127.33
115.18
114.97
56.16
39.36
O
Ph
F
3g
240
230
220
210
200
190
180
170
160
150
140
130
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100
90
80
70
60
50
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30
20
10
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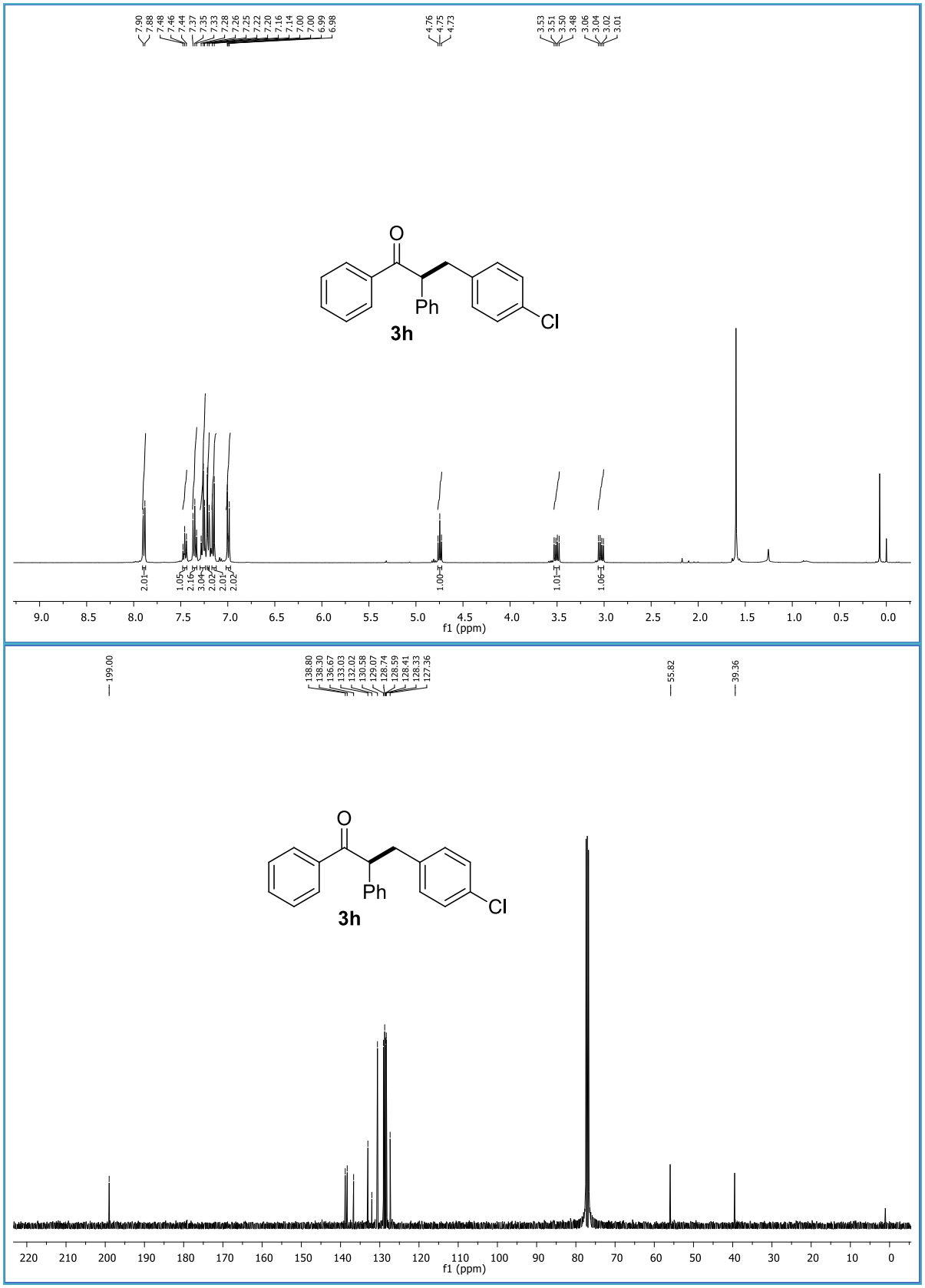
-10
-20
f1 (ppm)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7.20
7.16
7.14
7.00
7.00
6.99
6.98
4.76
4.75
4.73
3.53
3.51
3.50
3.48
3.06
3.04
3.02
3.01
O
Ph
Cl
3h
2.01
1.05
2.16
3.04
2.02
2.01
2.02
1.00
1.01
1.06
f1 (ppm)
199.00
138.80
138.30
136.67
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132.02
130.58
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128.41
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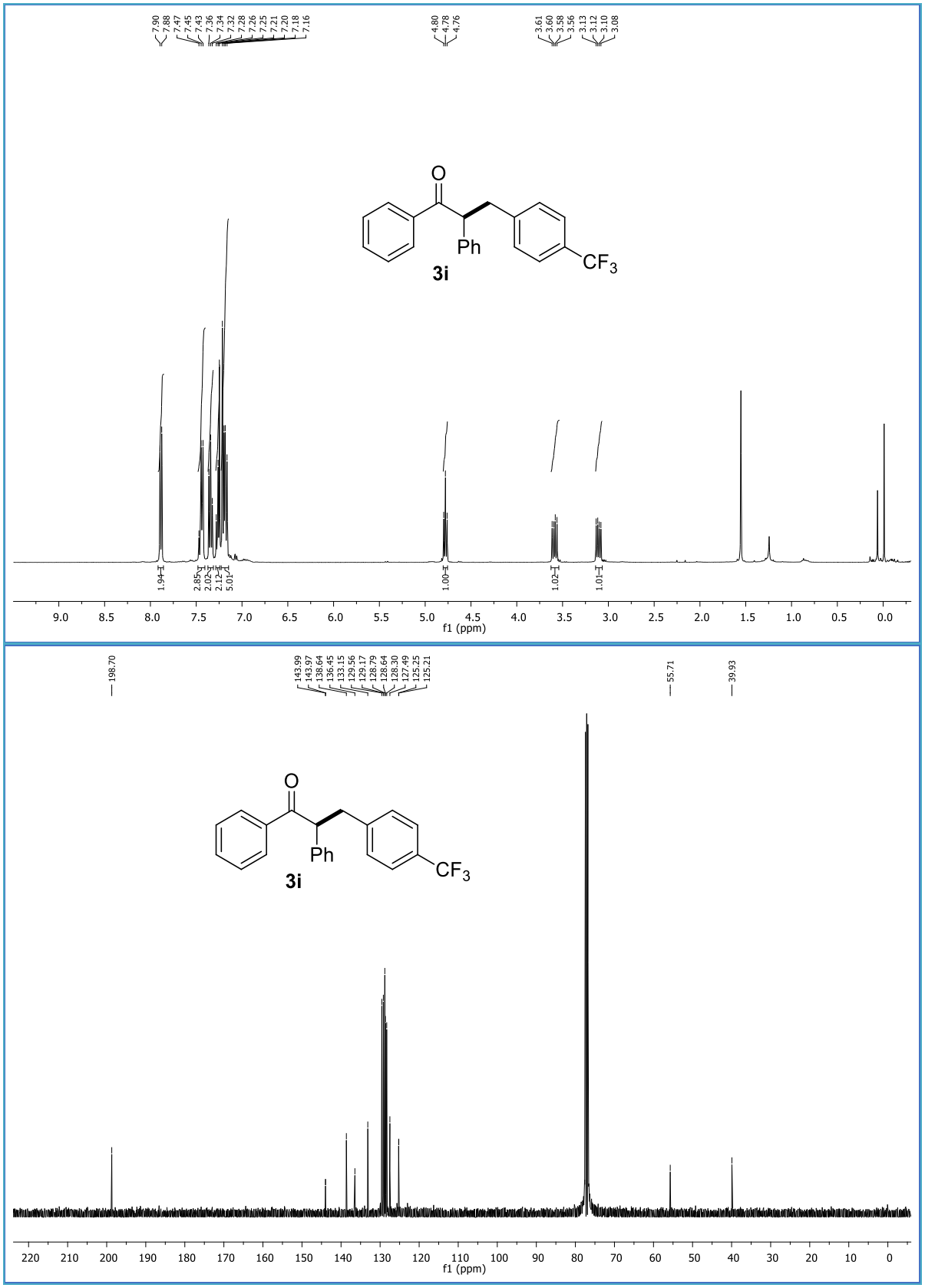
127.36
55.82
39.36
O
Ph
Cl
3h
f1 (ppm)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7.18
7.16
4.80
4.78
4.76
3.61
3.60
3.58
3.56
3.13
3.12
3.10
3.08
O
Ph
CF3
3i
1.94
2.85
2.02
2.12
5.01
1.00
1.02
1.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
198.70
143.99
143.97
138.64
136.45
133.15
129.56
129.17
128.79
128.64
128.30
127.49
125.25
125.21
55.71
39.93
O
Ph
CF3
3i
220
210
200
190
180
170
160
150
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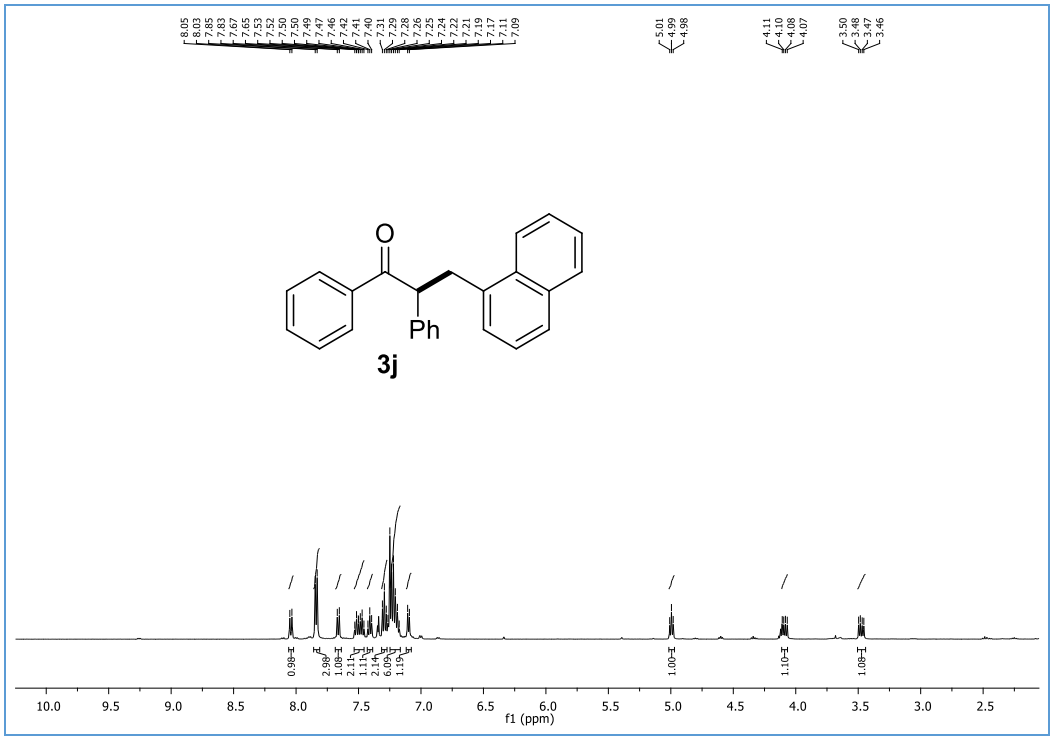
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.47
7.46
7.42
7.41
7.40
7.31
7.29
7.28
7.26
7.25
7.24
7.22
7.21
7.19
7.17
7.11
7.09
5.01
4.99
4.98
4.11
4.10
4.08
4.07
3.50
3.48
3.47
3.46
O
Ph
3j
0.98
2.99
1.08
2.11
1.11
2.14
6.09
1.19
1.00
1.10
1.08
10.0
9.5
9.0
8.5
8.0
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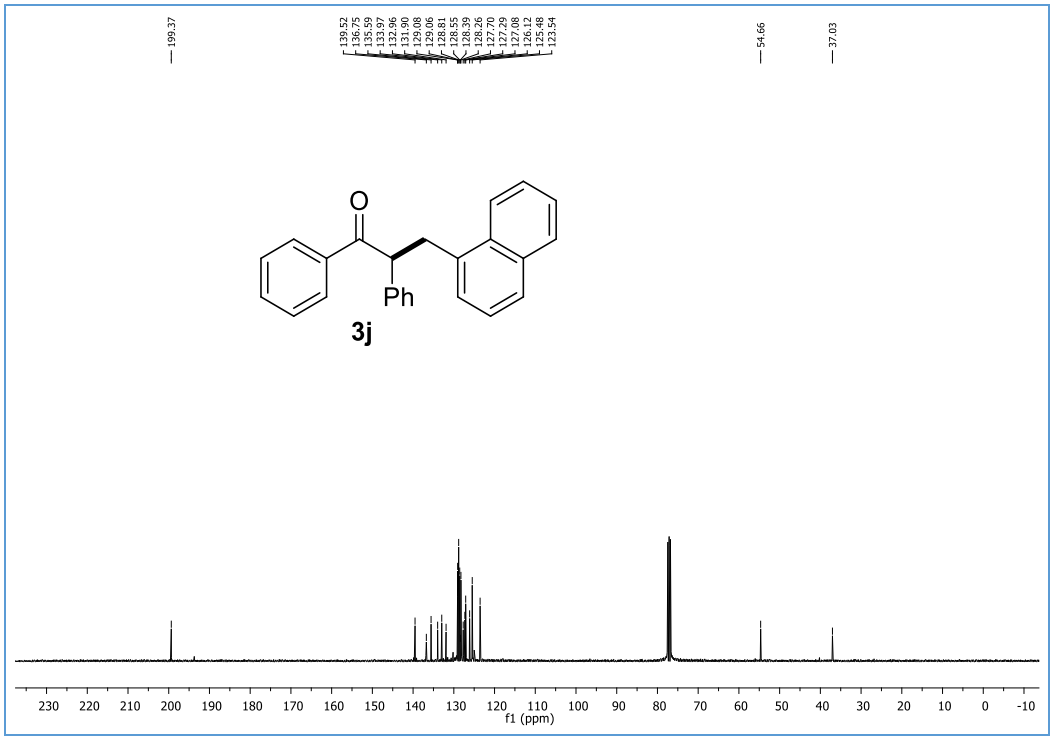
4.0
3.5
3.0
2.5
f1 (ppm)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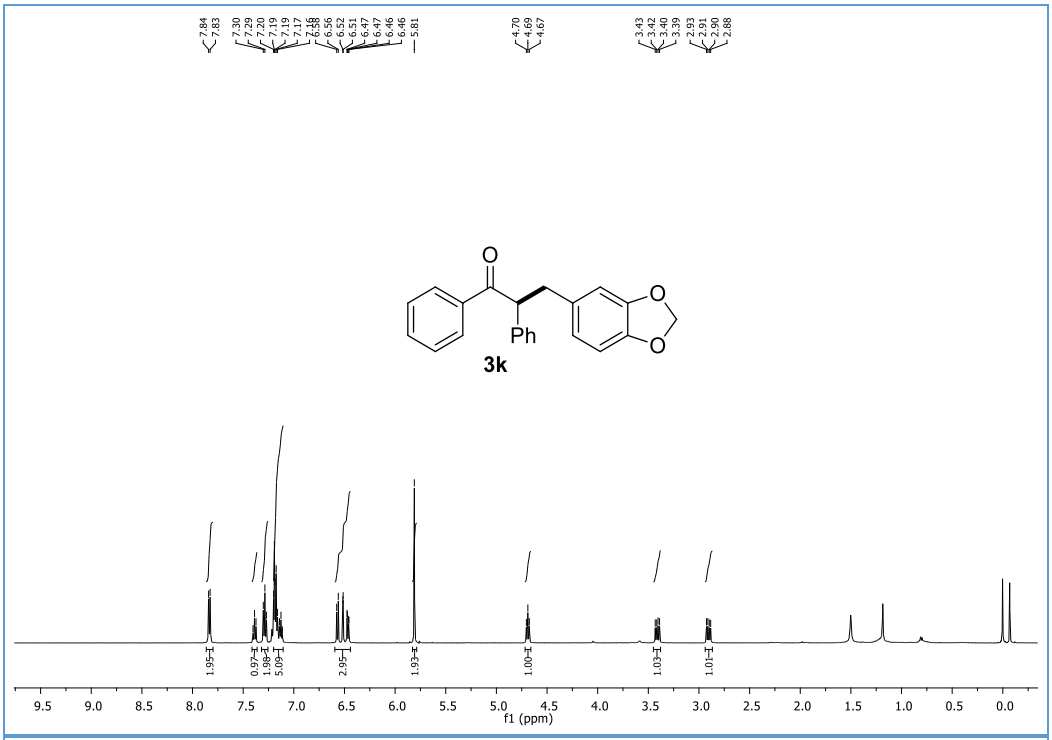
129.08
129.06
128.81
128.55
128.39
128.26
127.70
127.29
127.08
126.12
125.48
123.54
54.66
37.03
O
Ph
3j
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.83
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7.17
7.16
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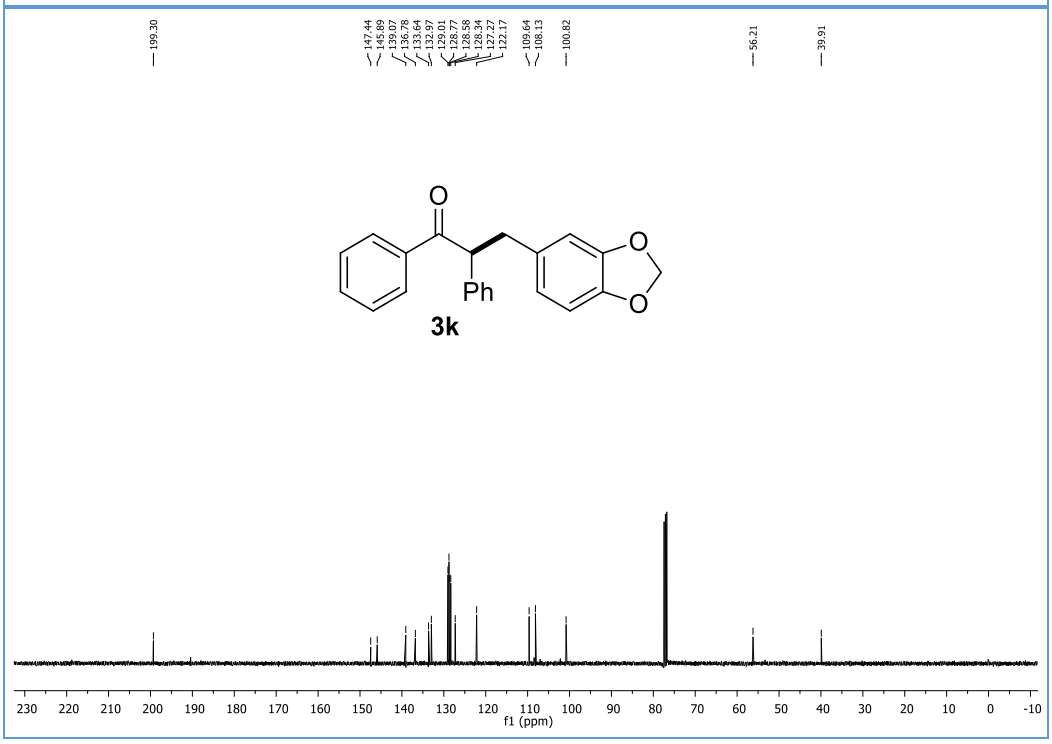
6.53
6.51
6.47
6.47
6.46
6.46
5.81
4.70
4.69
4.67
3.43
3.42
3.40
3.39
2.93
2.91
2.90
2.88
O
O
O
Ph
3k
1.95
0.97
1.98
5.09
2.95
1.93
1.00
1.03
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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147.44
145.89
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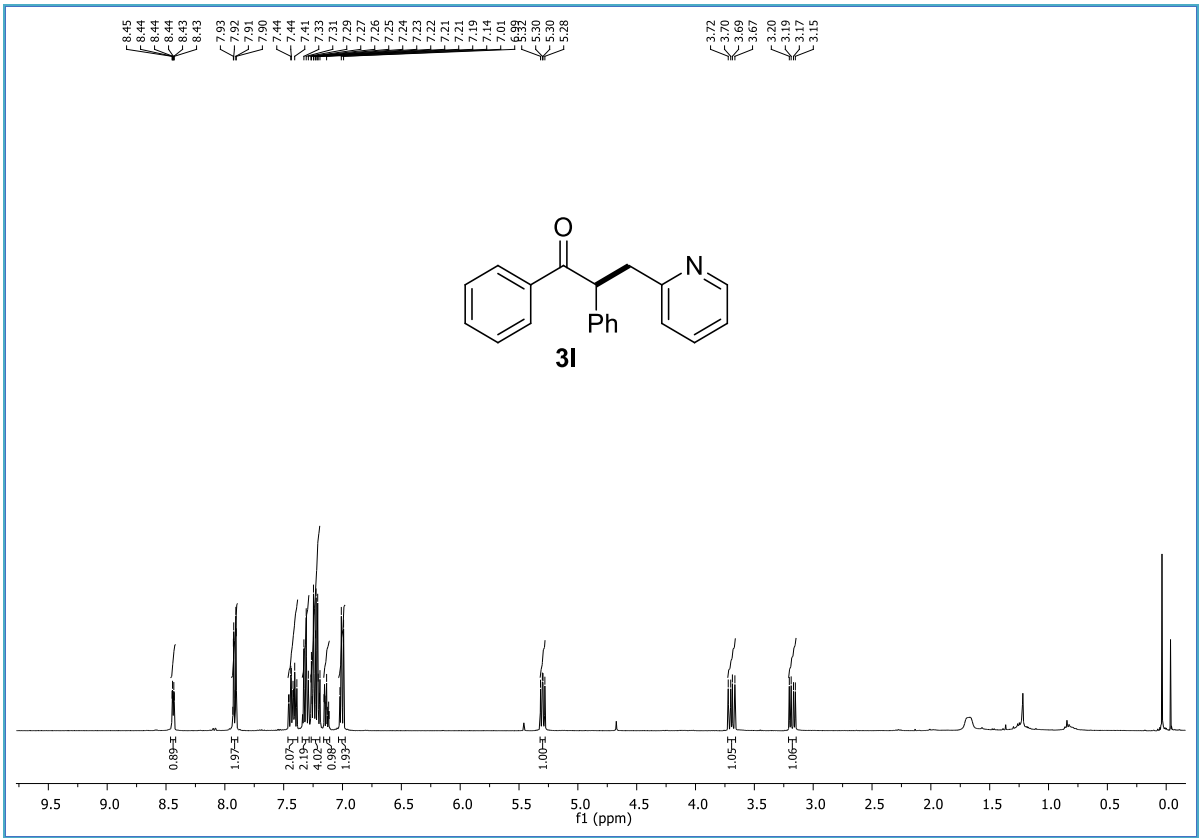
129.01
128.77
128.58
128.34
127.27
122.17
109.64
108.13
100.82
56.21
39.91
O
O
O
Ph
3k
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.92
7.91
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7.44
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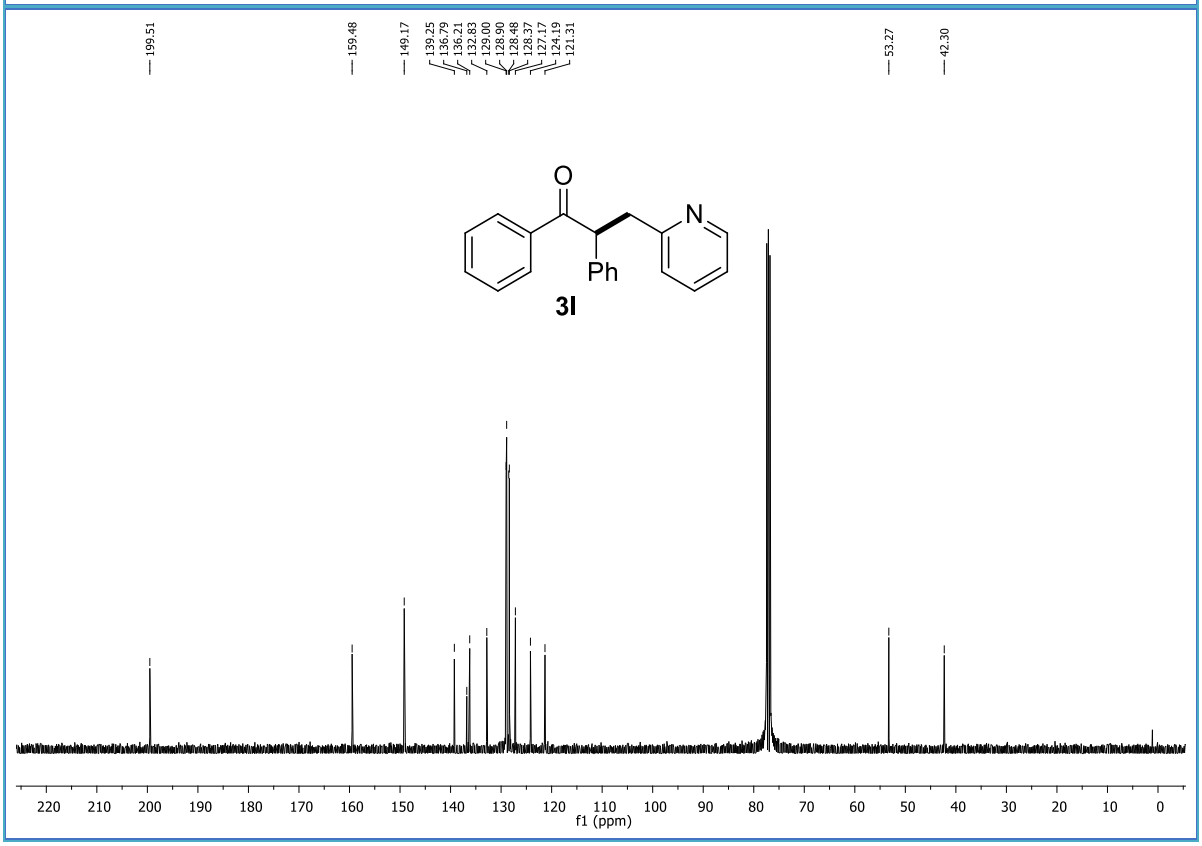
7.33
7.31
7.29
7.27
7.26
7.25
7.24
7.23
7.22
7.21
7.21
7.19
7.14
7.01
6.99
5.30
5.30
5.28
3.72
3.70
3.69
3.67
3.20
3.19
3.17
3.15
O
N
Ph
3l
0.89
1.97
2.07
2.15
4.02
0.98
1.93
1.00
1.05
1.06
f1 (ppm)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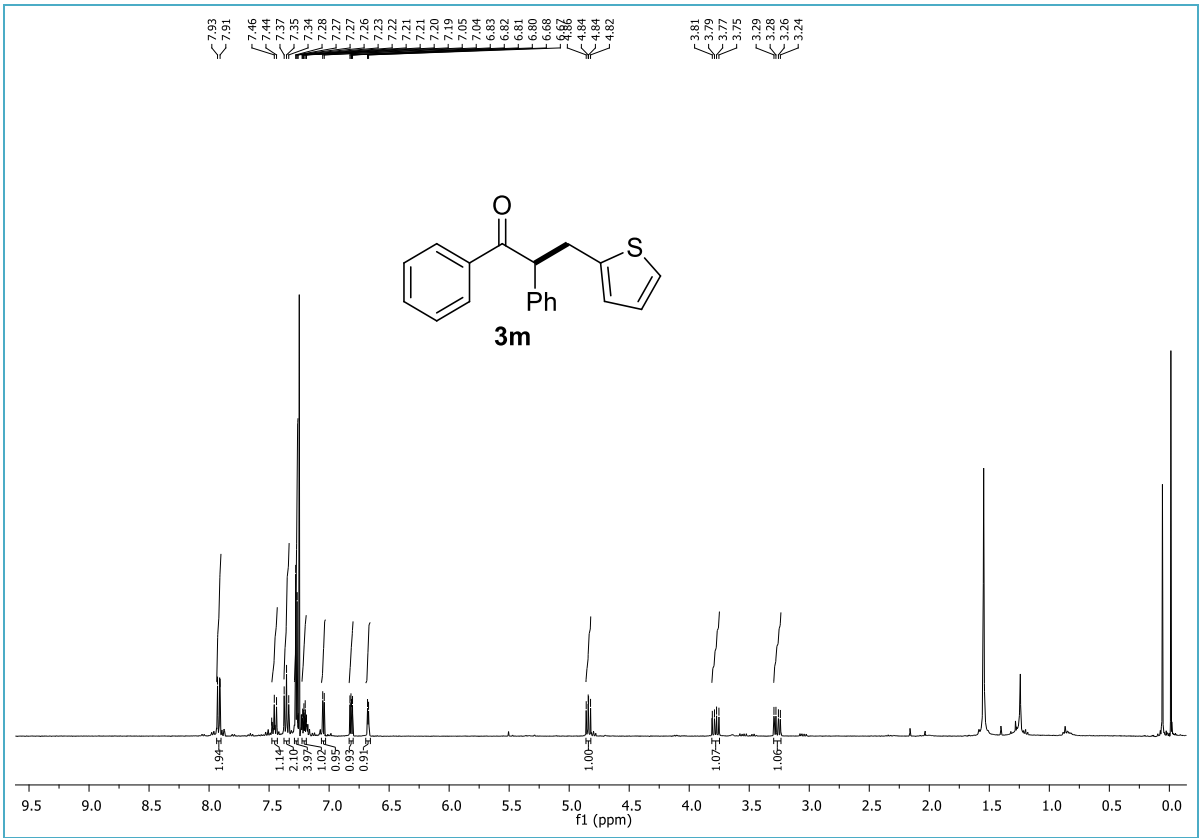
124.17
124.19
121.31
53.27
42.30
O
N
Ph
3l
f1 (ppm)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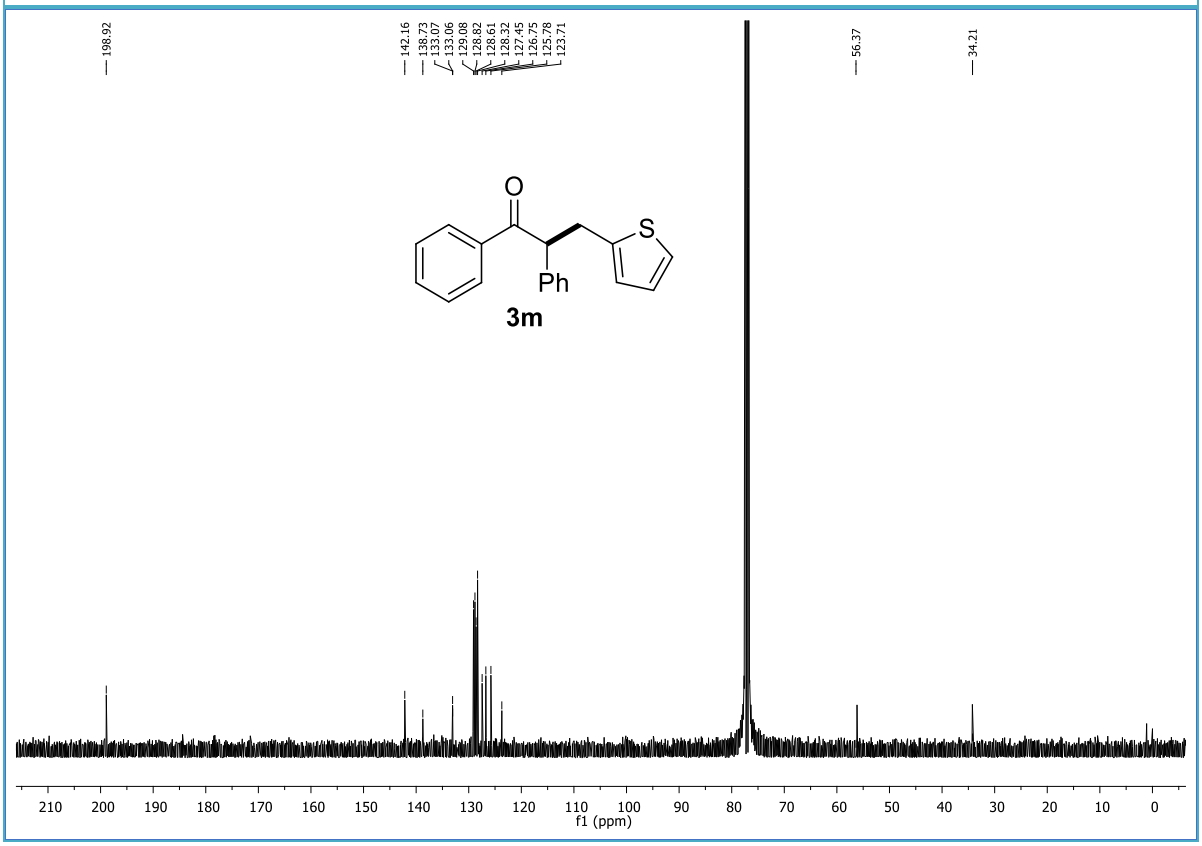
7.23
7.22
7.21
7.21
7.20
7.19
7.05
7.04
6.83
6.82
6.81
6.80
6.68
4.86
4.84
4.84
4.82
3.81
3.79
3.77
3.75
3.29
3.28
3.26
3.24
O
S
Ph
3m
1.94
1.14
2.10
3.97
1.02
0.95
0.93
0.91
1.00
1.07
1.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.08
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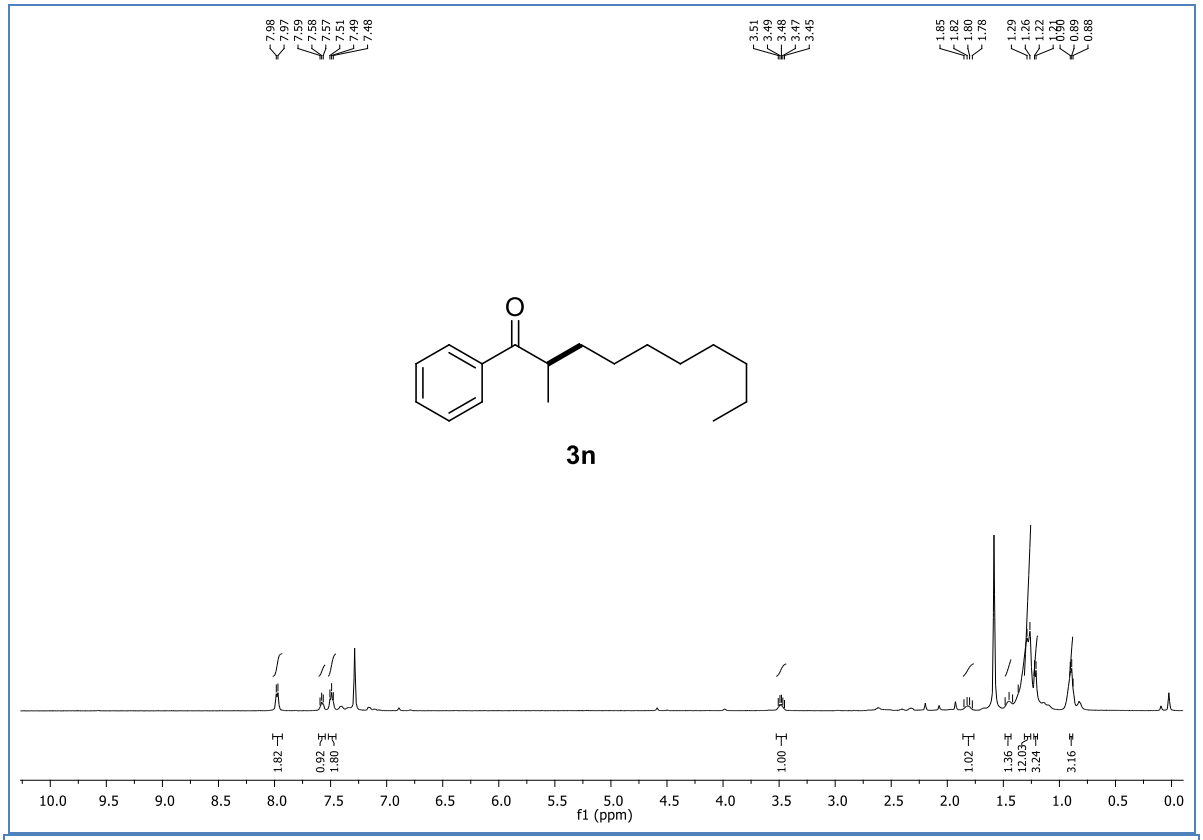
128.61
128.32
127.45
126.75
125.78
123.71
56.37
34.21
O
S
Ph
3m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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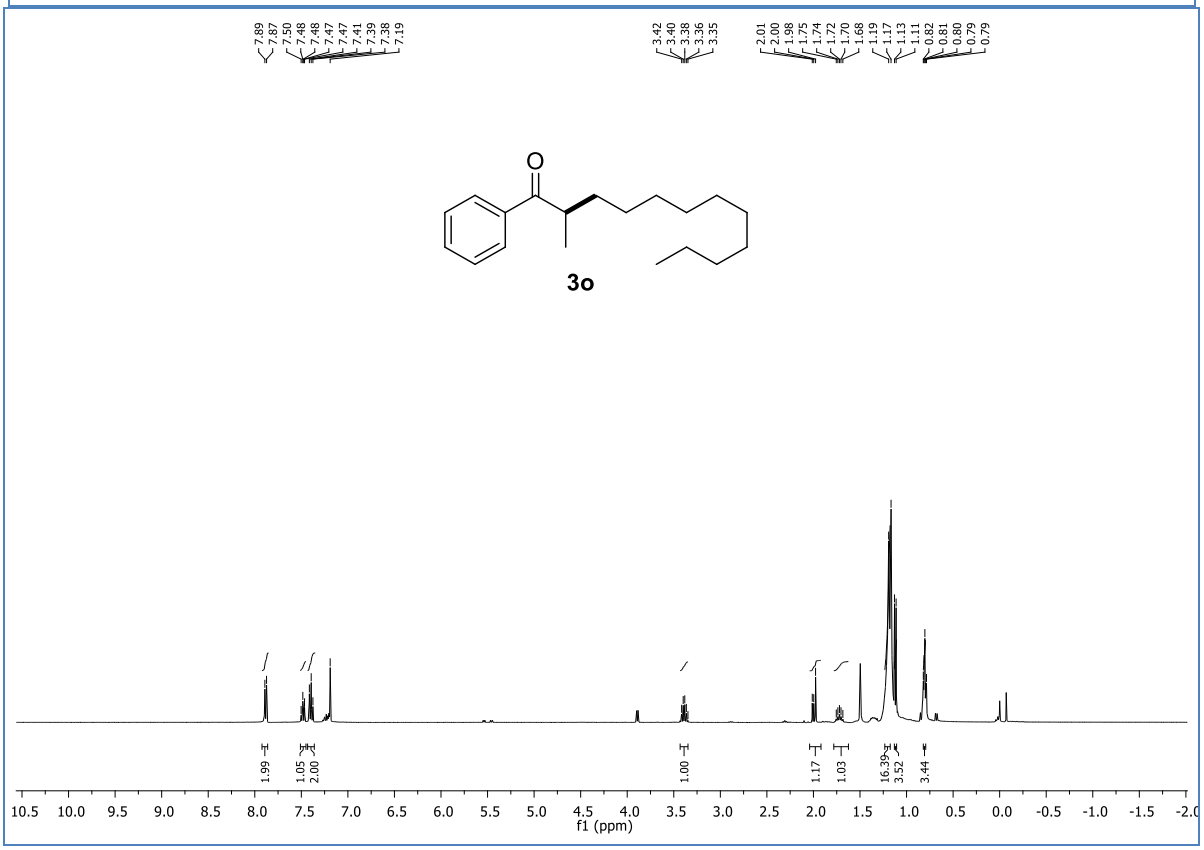
3.49
3.48
3.47
3.45
1.85
1.82
1.80
1.78
1.29
1.26
1.22
1.21
0.90
0.89
0.88
O
3n
1.82
0.92
1.80
1.00
1.02
1.36
12.03
3.24
3.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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7.19
3.42
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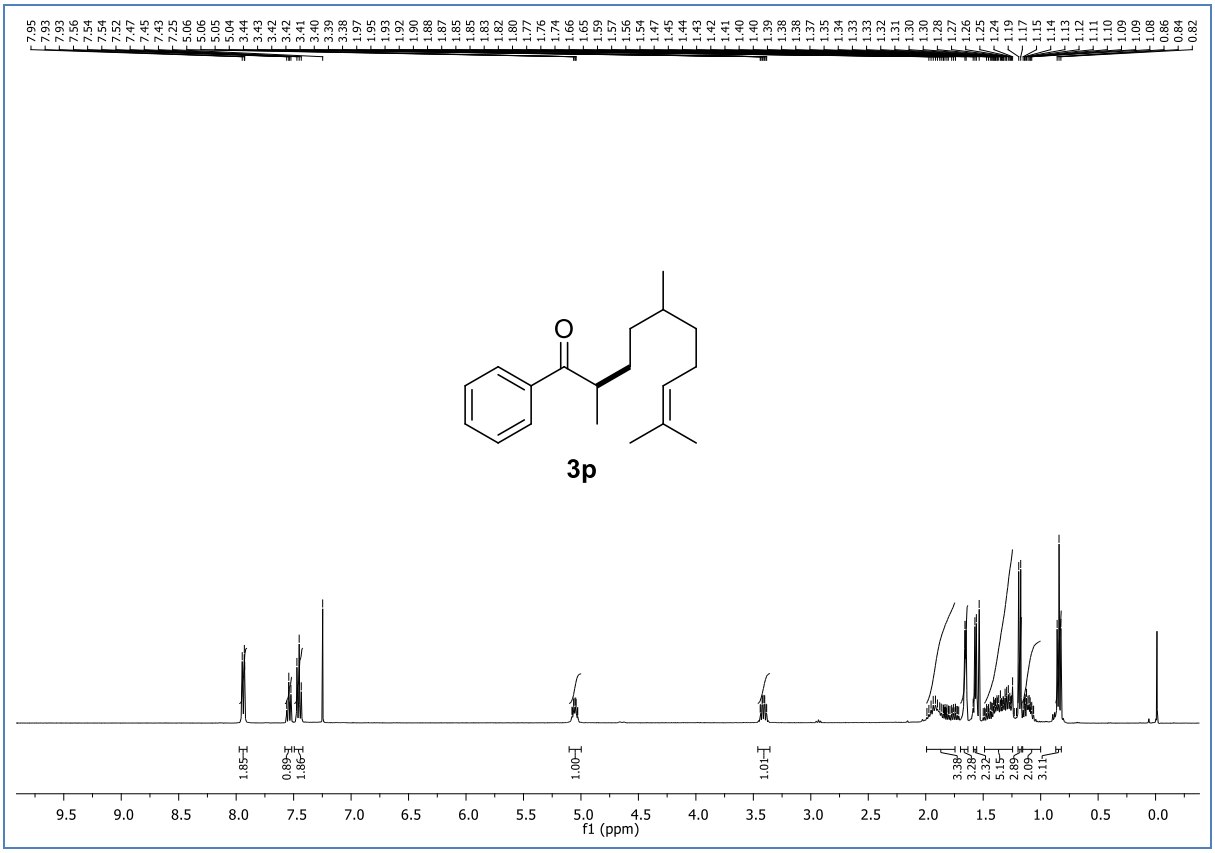
1.98
1.75
1.74
1.72
1.70
1.68
1.19
1.17
1.13
1.11
0.82
0.81
0.80
0.79
0.79
O
3o
1.99
1.05
2.00
1.00
1.17
1.03
16.39
3.52
3.44
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)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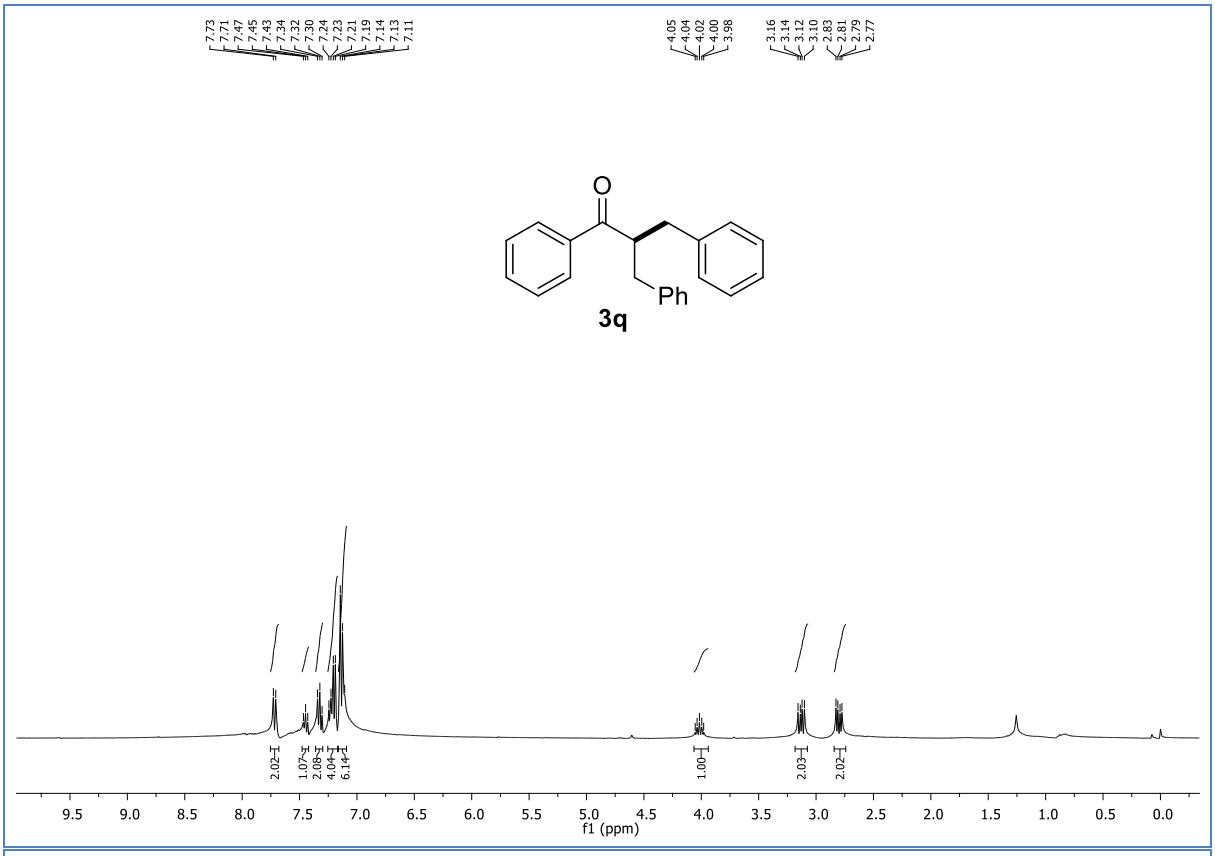
O
3p
1.85 0.89 1.86 1.00 1.01 3.38 3.28 2.32 5.15 2.89 2.09 3.11
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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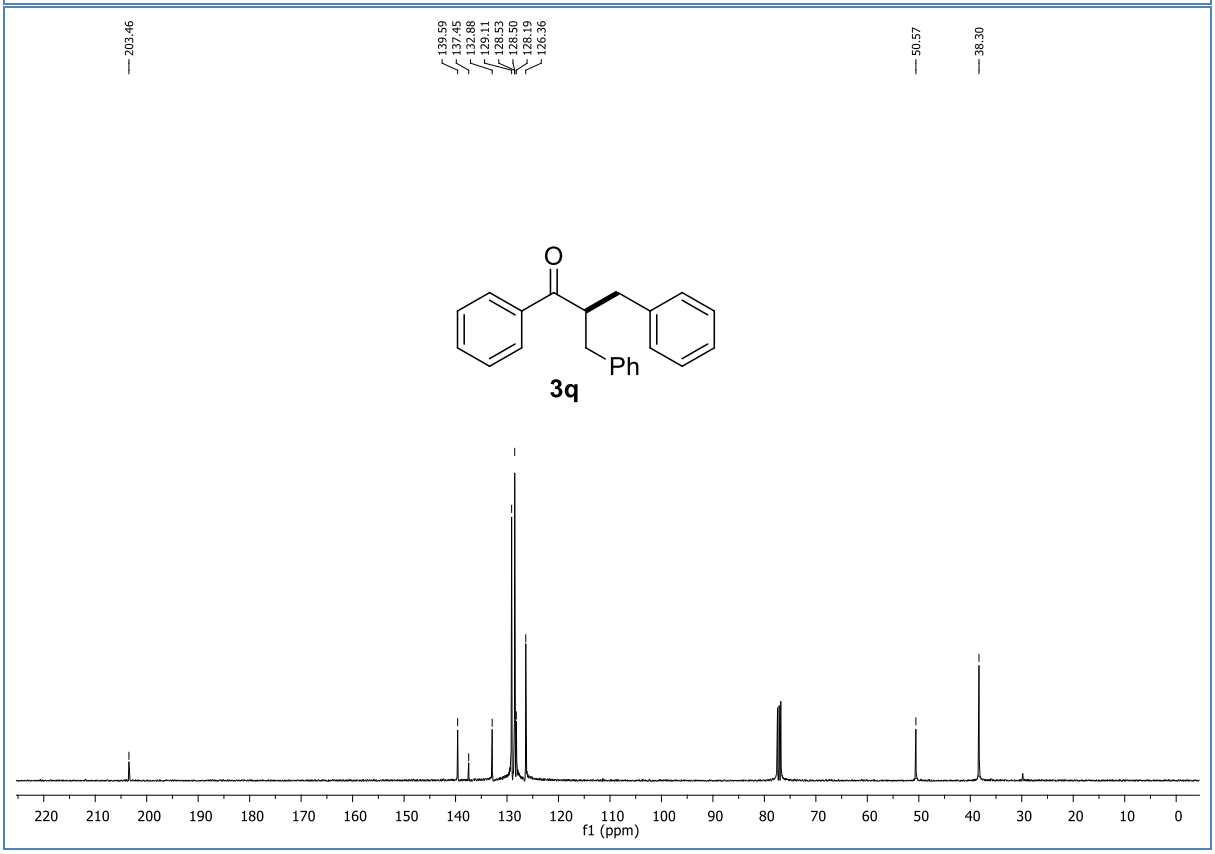
7.21
7.19
7.14
7.13
7.11
4.05
4.04
4.02
4.00
3.98
3.16
3.14
3.12
3.10
2.83
2.81
2.79
2.77
O
Ph
3q
2.02
1.07
2.08
4.04
6.14
1.00
2.03
2.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.19
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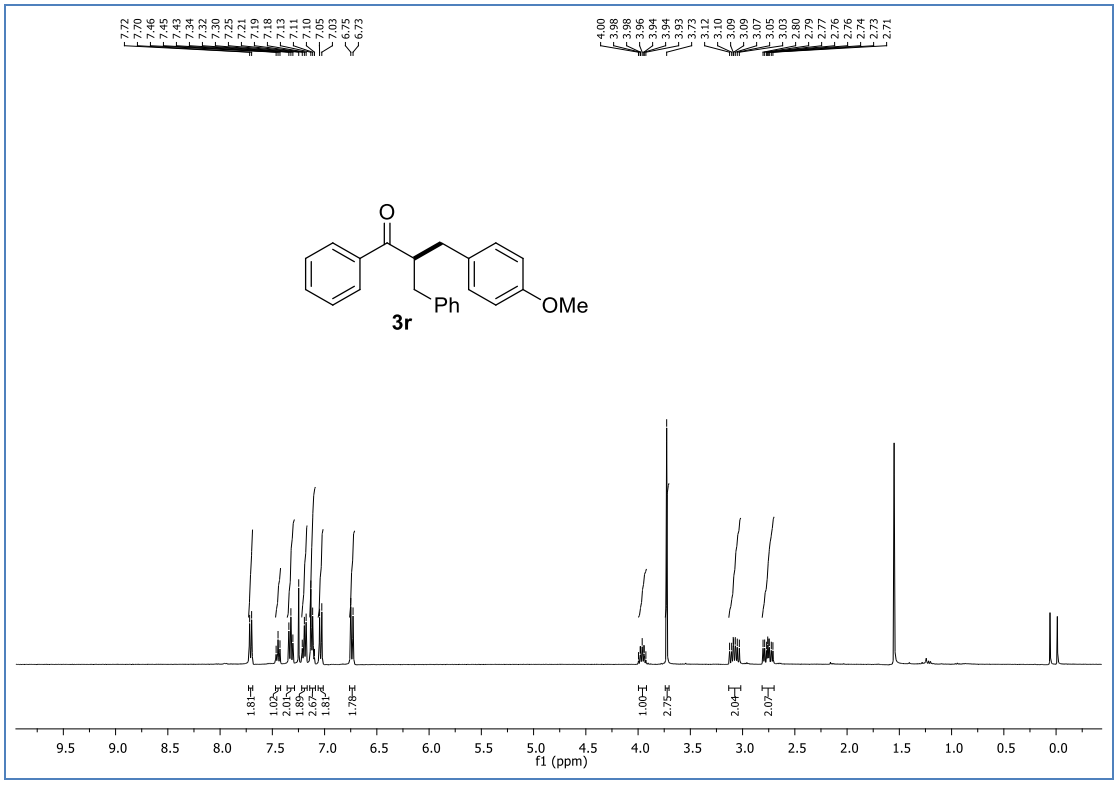
38.30
O
Ph
3q
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.05
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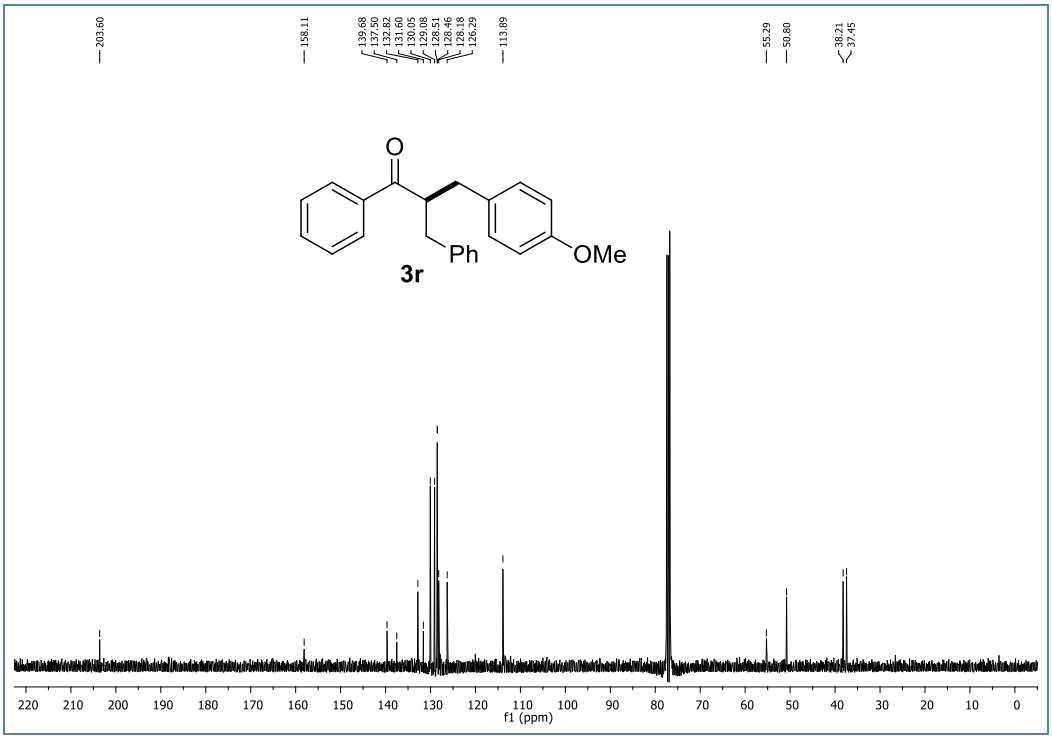
3.09
3.07
3.05
3.03
2.80
2.79
2.77
2.77
2.76
2.74
2.73
2.71
O
Ph
OMe
3r
1.81
1.02
2.01
1.89
2.67
1.81
1.78
1.00
2.75
2.04
2.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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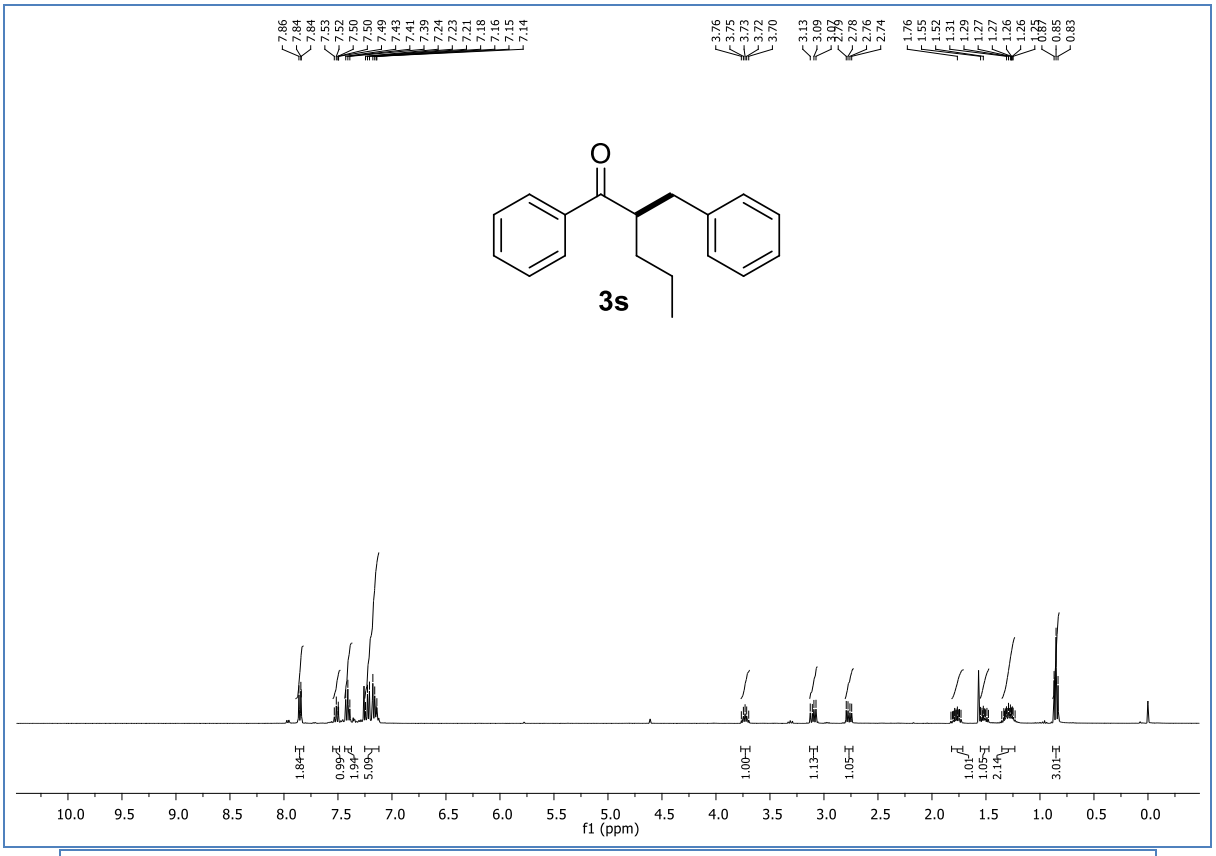
128.46
128.18
126.29
113.89
55.29
50.80
38.21
37.45
O
Ph
OMe
3r
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.21
7.18
7.16
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7.14
3.76
3.75
3.73
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3.70
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3.07
3.05
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2.76
2.74
1.76
1.55
1.52
1.31
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1.27
1.27
1.26
1.26
0.87
0.85
0.83
O
3s
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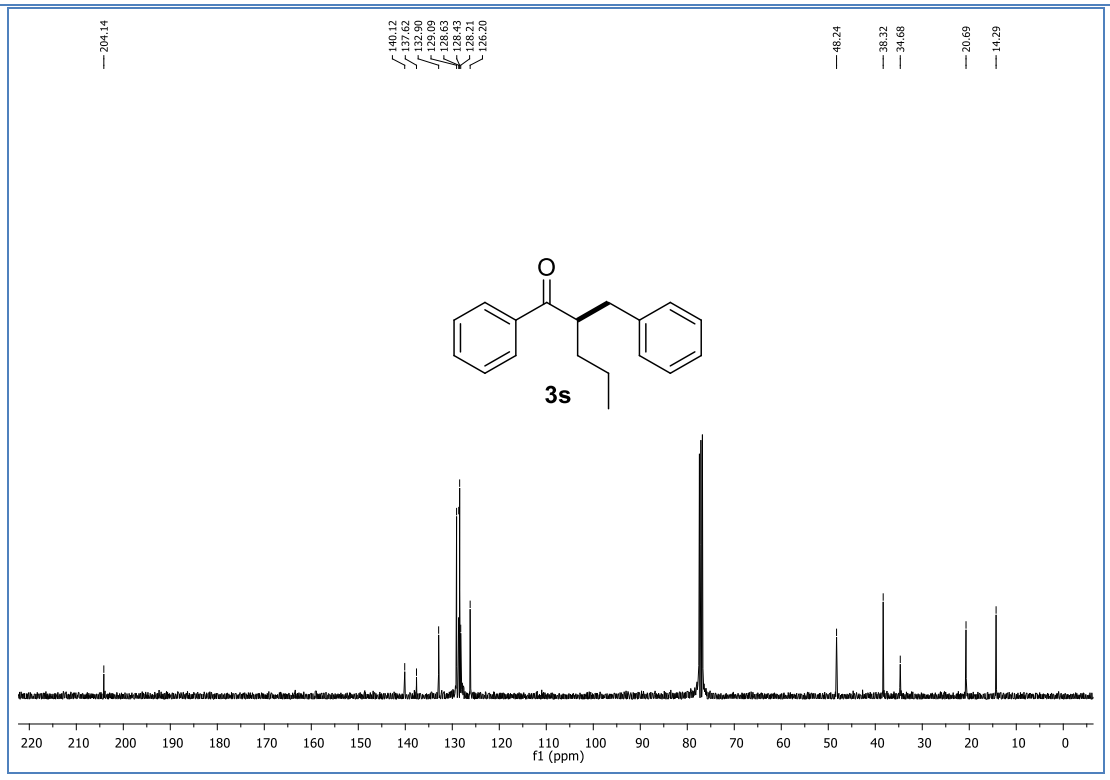
0.99
1.94
5.09
1.00
1.13
1.05
1.01
1.05
2.14
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.43
128.21
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48.24
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20.69
14.29
O
3s
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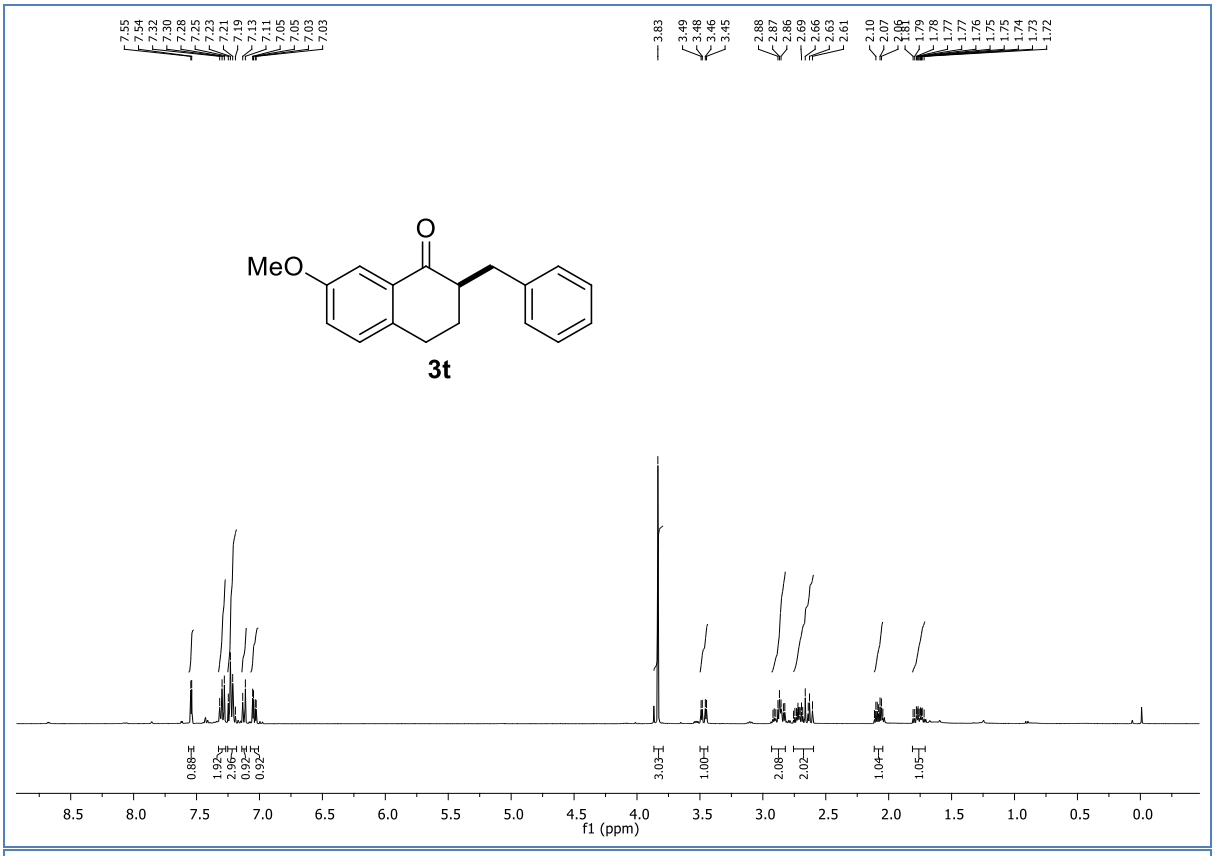
f1 (ppm)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7.54
7.32
7.30
7.28
7.25
7.23
7.21
7.19
7.13
7.11
7.05
7.05
7.03
7.03
3.83
3.49
3.48
3.46
3.45
2.88
2.87
2.86
2.69
2.66
2.63
2.61
2.10
2.07
2.06
1.81
1.79
1.78
1.77
1.77
1.76
1.75
1.75
1.74
1.73
1.72
O
MeO
3t
0.88
1.92
2.96
0.92
0.92
3.03
1.00
2.08
2.02
1.04
1.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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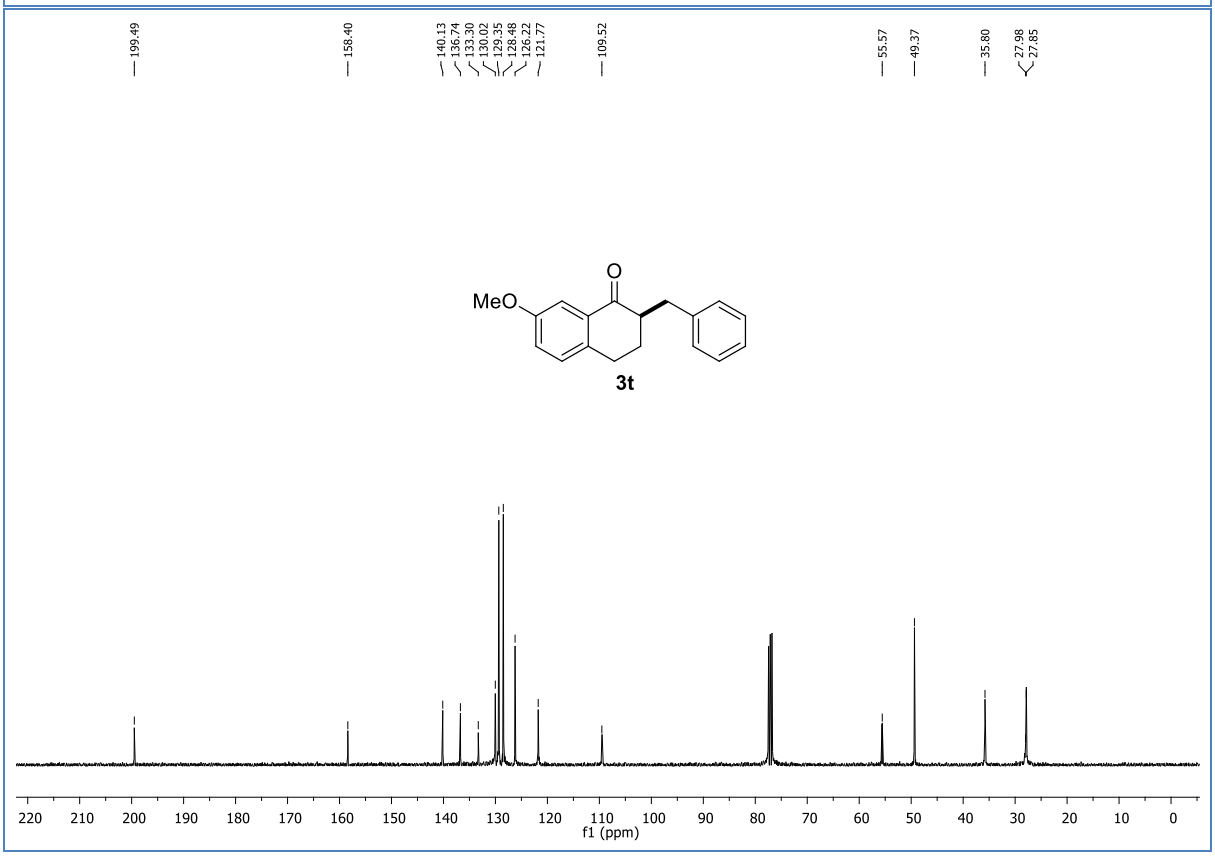
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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158.40
140.13
136.74
133.30
130.02
129.35
128.48
126.22
121.77
109.52
55.57
49.37
35.80
27.98
27.85
O
MeO
3t
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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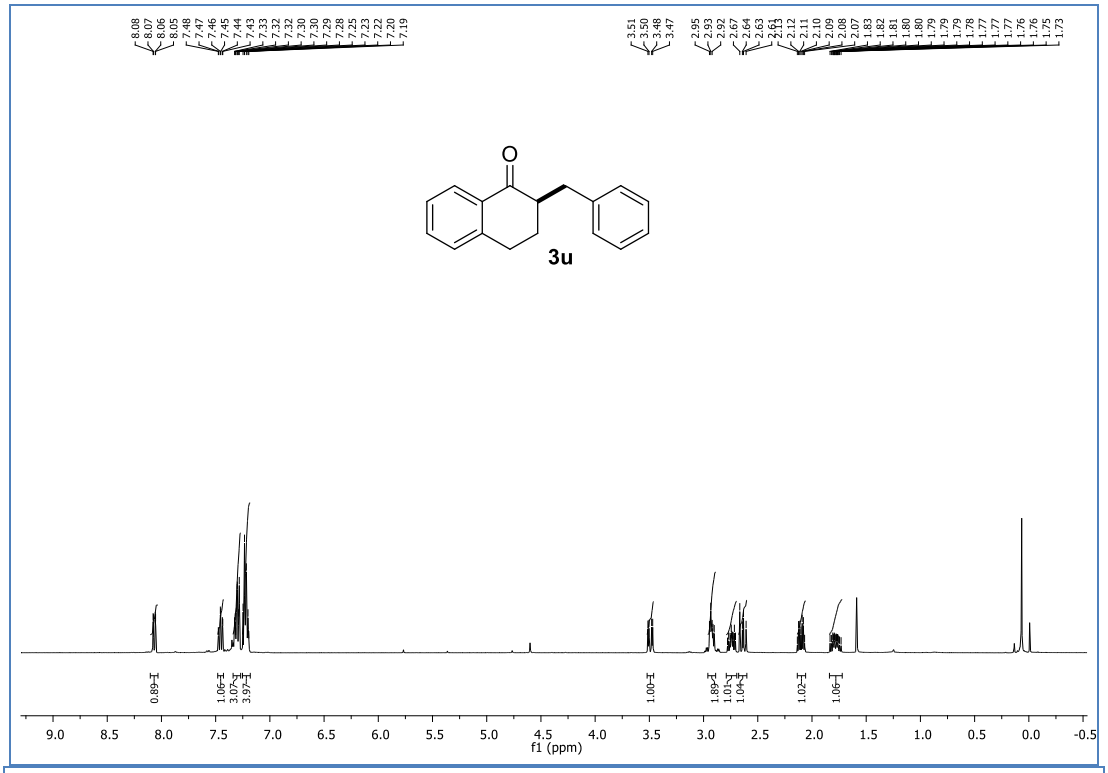
f1 (ppm)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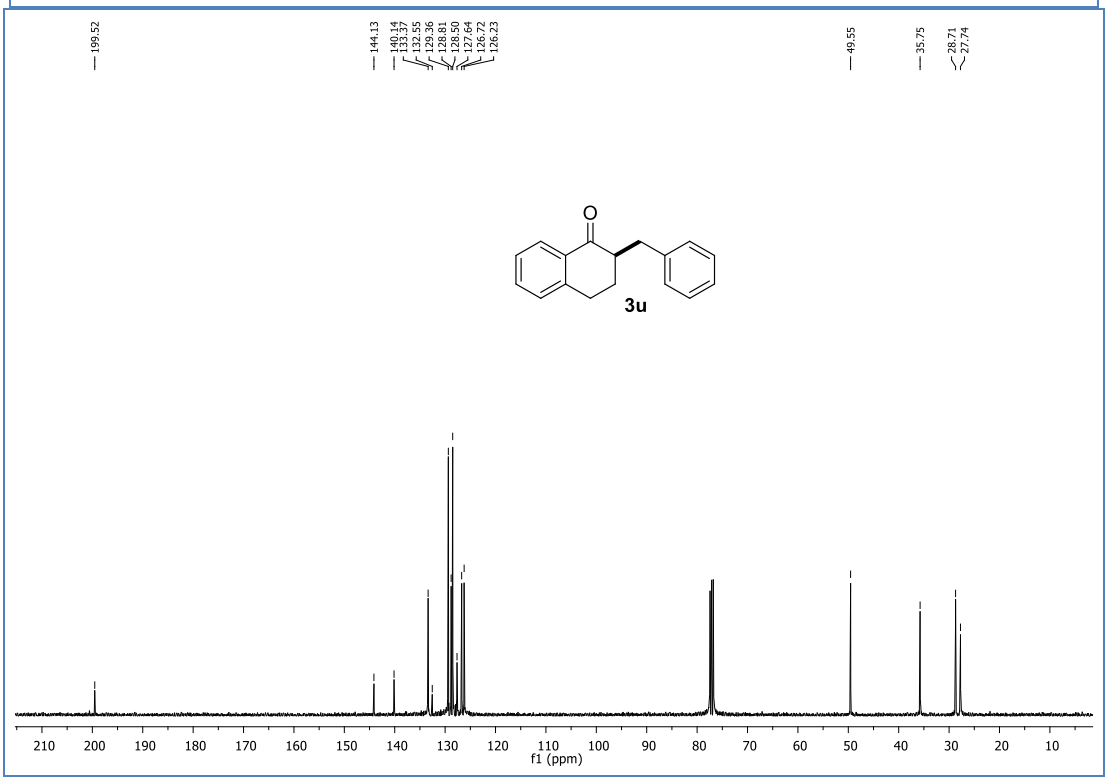
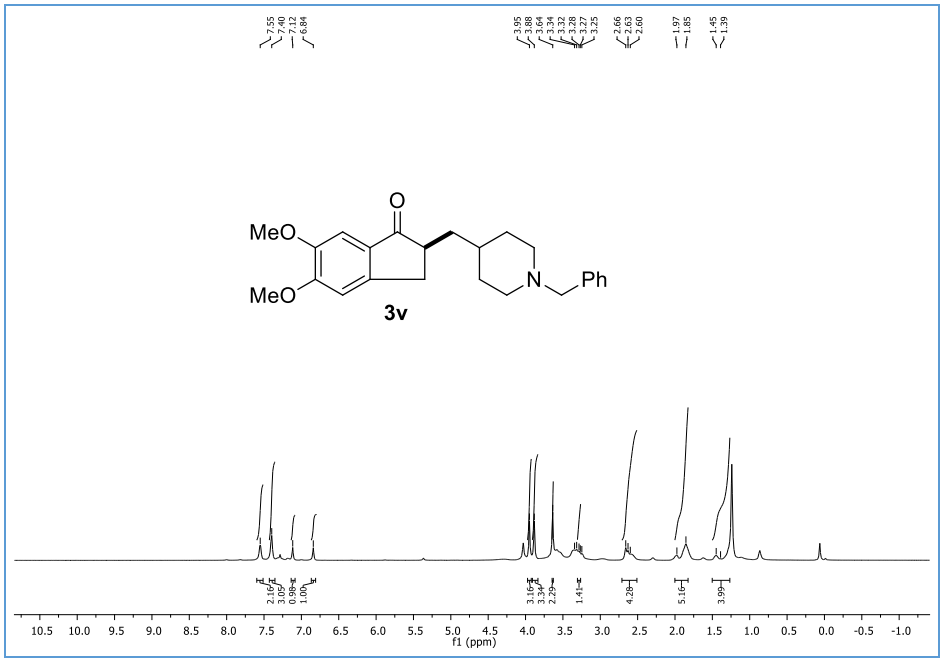
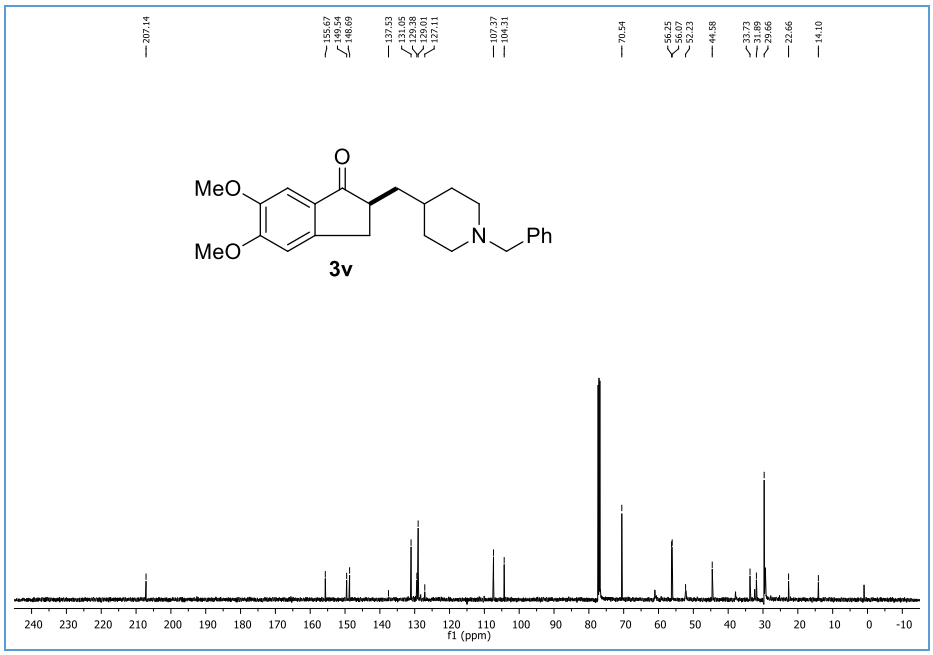
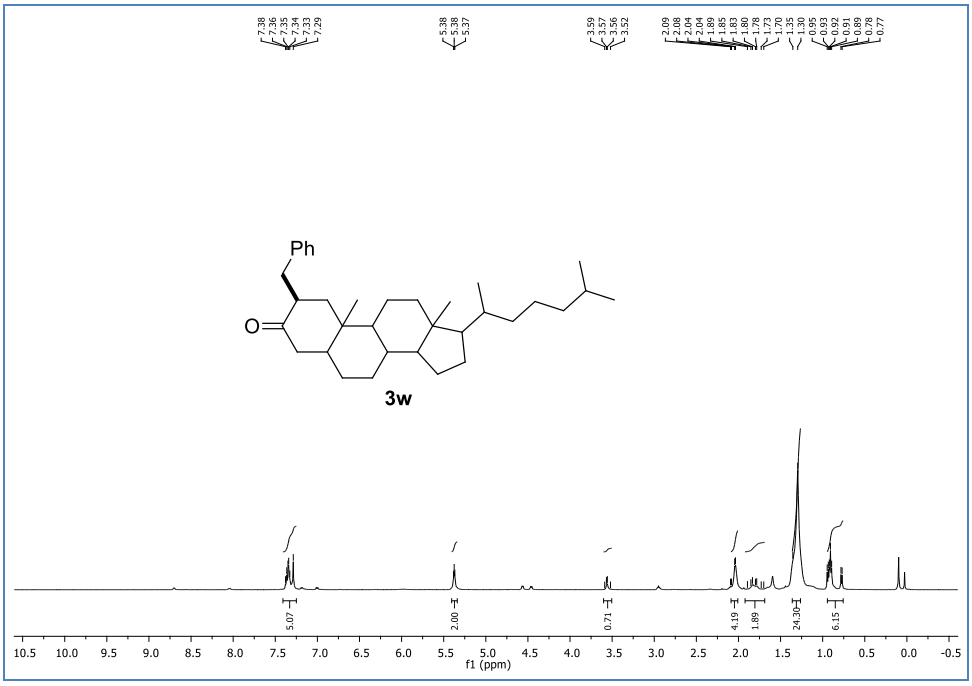
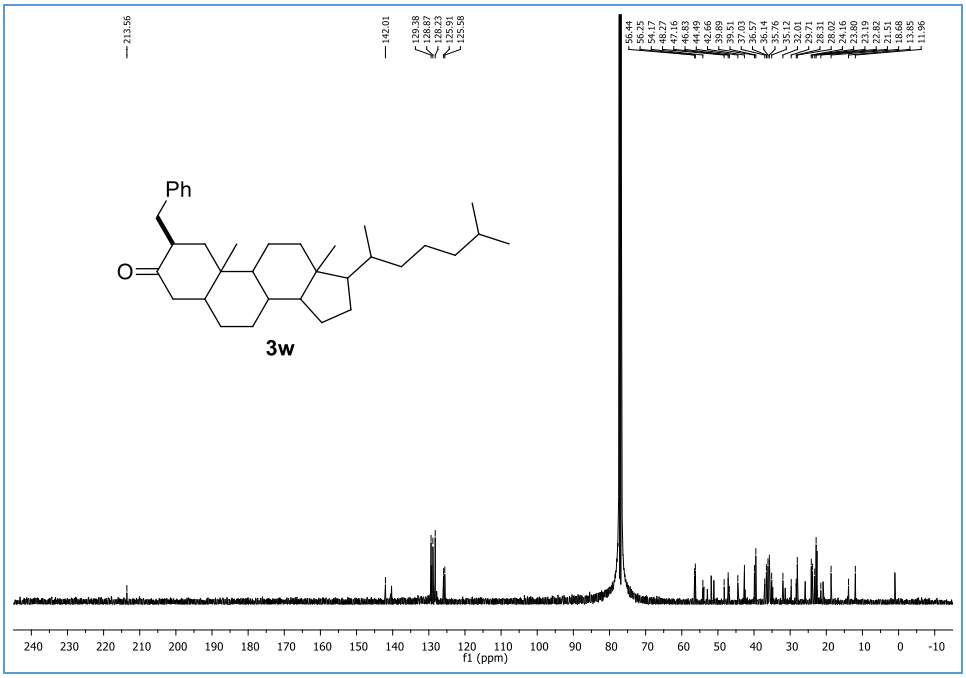
8.07
8.06
8.05
7.48
7.47
7.46
7.45
7.44
7.43
7.33
7.32
7.32
7.30
7.30
7.29
7.28
7.25
7.23
7.22
7.20
7.19
3.51
3.50
3.48
3.47
2.95
2.93
2.92
2.67
2.64
2.63
2.61
2.13
2.12
2.11
2.10
2.09
2.08
2.07
1.83
1.82
1.81
1.80
1.79
1.79
1.79
1.78
1.77
1.77
1.77
1.76
1.76
1.75
1.73
O
3u
0.89
1.06
3.07
3.97
1.00
1.89
1.01
1.04
1.02
1.06
9.0
8.5
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
0.0
-0.5
f1 (ppm)

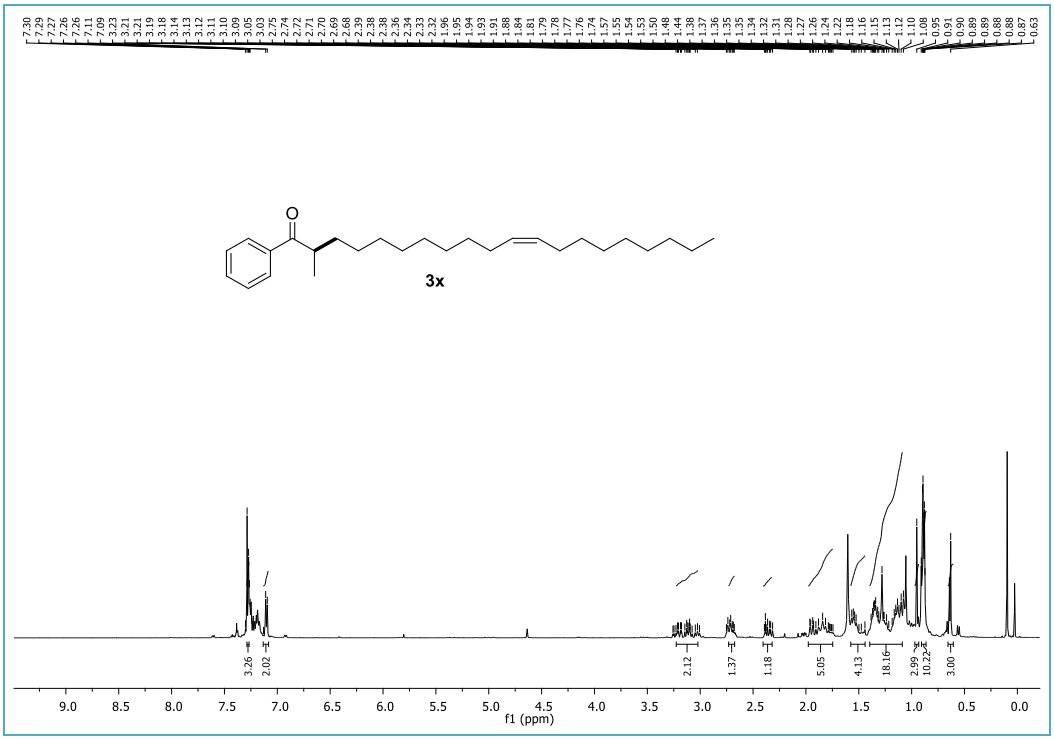

199.52
144.13
140.14
133.37
132.55
129.36
128.81
128.50
127.64
126.72
126.23
49.55
35.75
28.71
27.74
O
3u
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

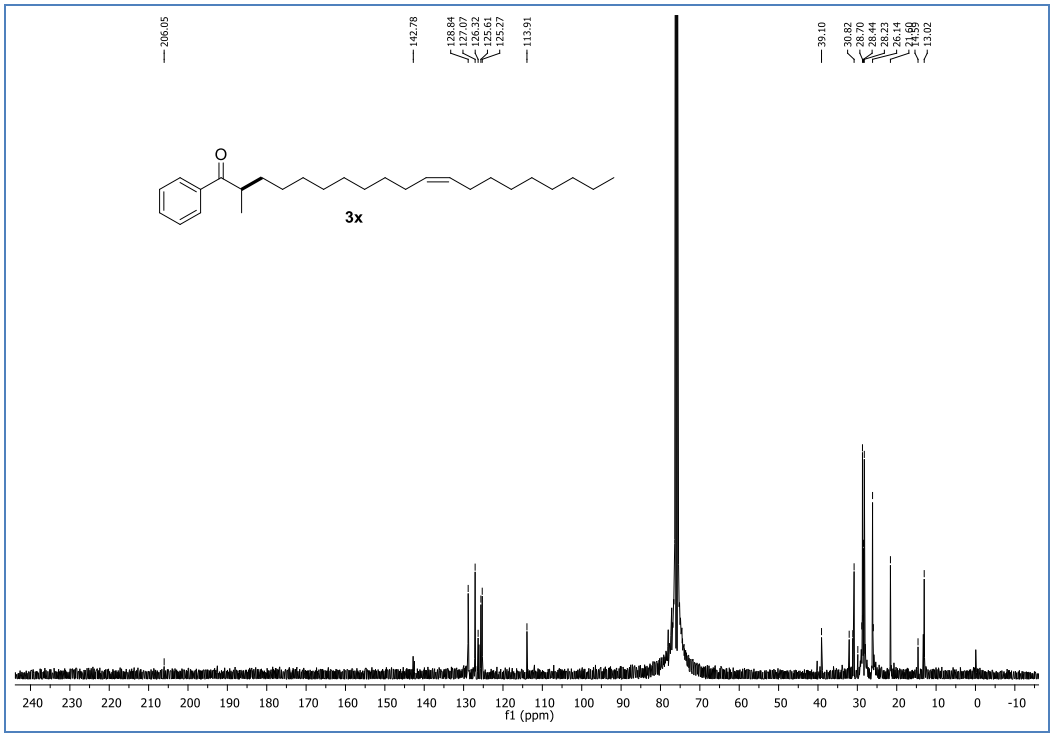

7.55
7.40
7.12
6.84
3.95
3.88
3.64
3.34
3.32
3.28
3.27
3.25
2.66
2.63
2.60
1.97
1.85
1.45
1.39
O
MeO
MeO
N
Ph
3v
2.16
3.05
0.98
1.00
3.16
3.34
2.29
1.41
4.28
5.16
3.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

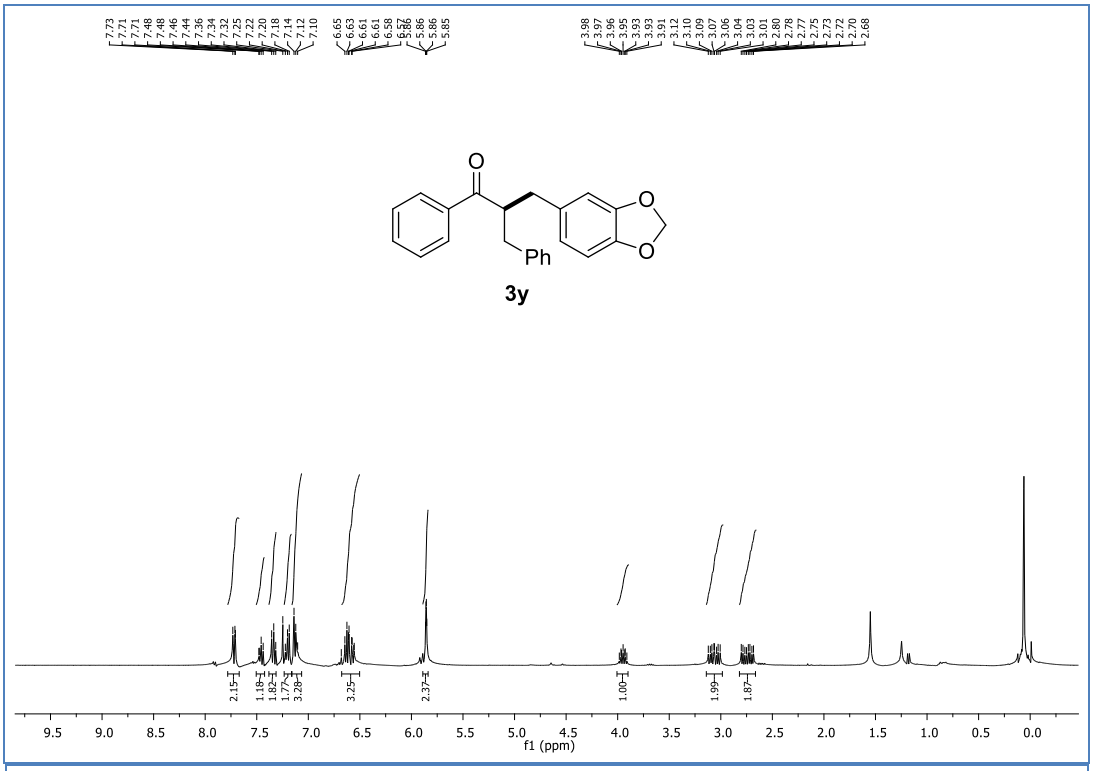

207.14
155.67
149.64
148.69
137.53
131.05
129.38
129.01
127.11
107.37
104.31
70.54
56.25
56.07
52.23
44.58
33.73
31.88
29.66
22.66
14.10
O
MeO
MeO
N
Ph
3v
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

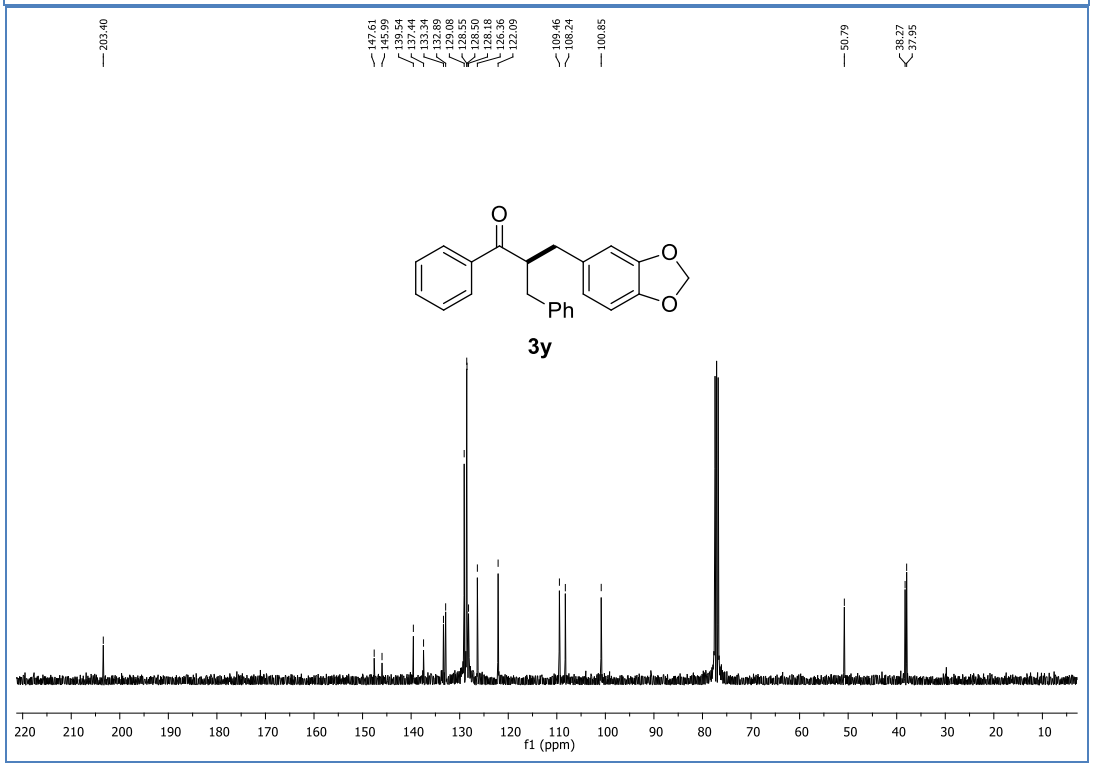

Ph
O
3w
f1 (ppm)

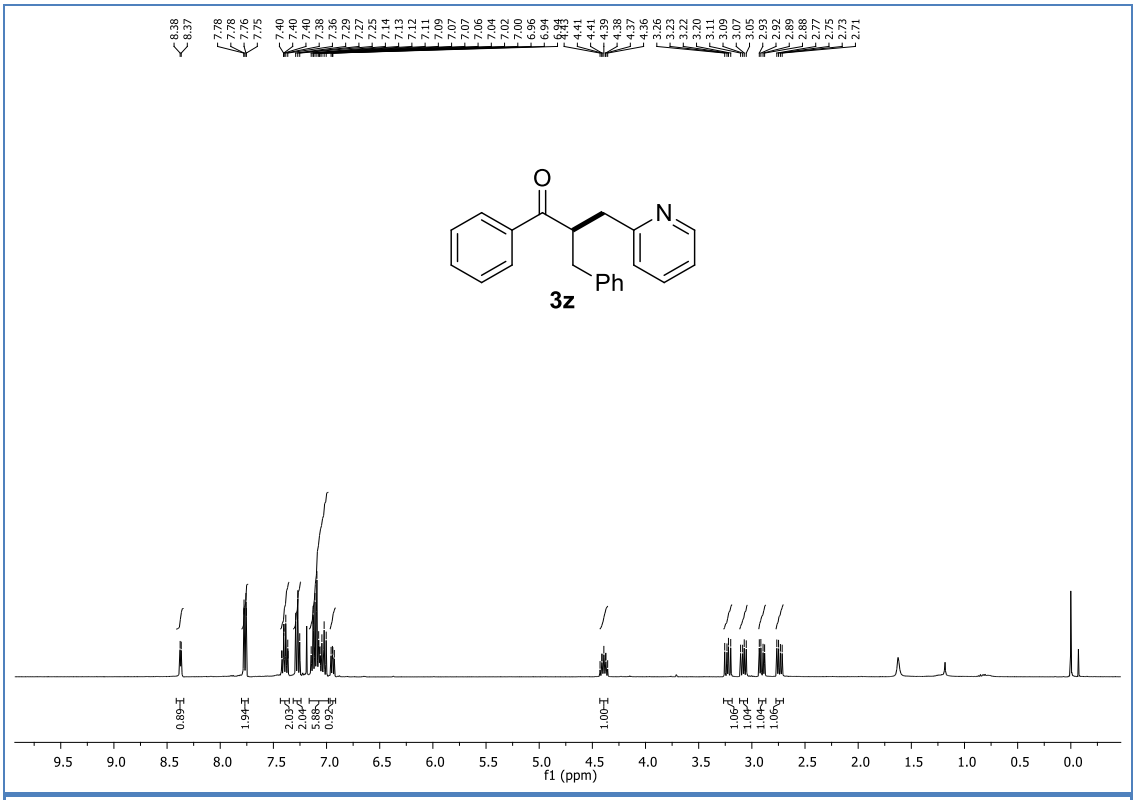

Ph
O
3w
f1 (ppm)

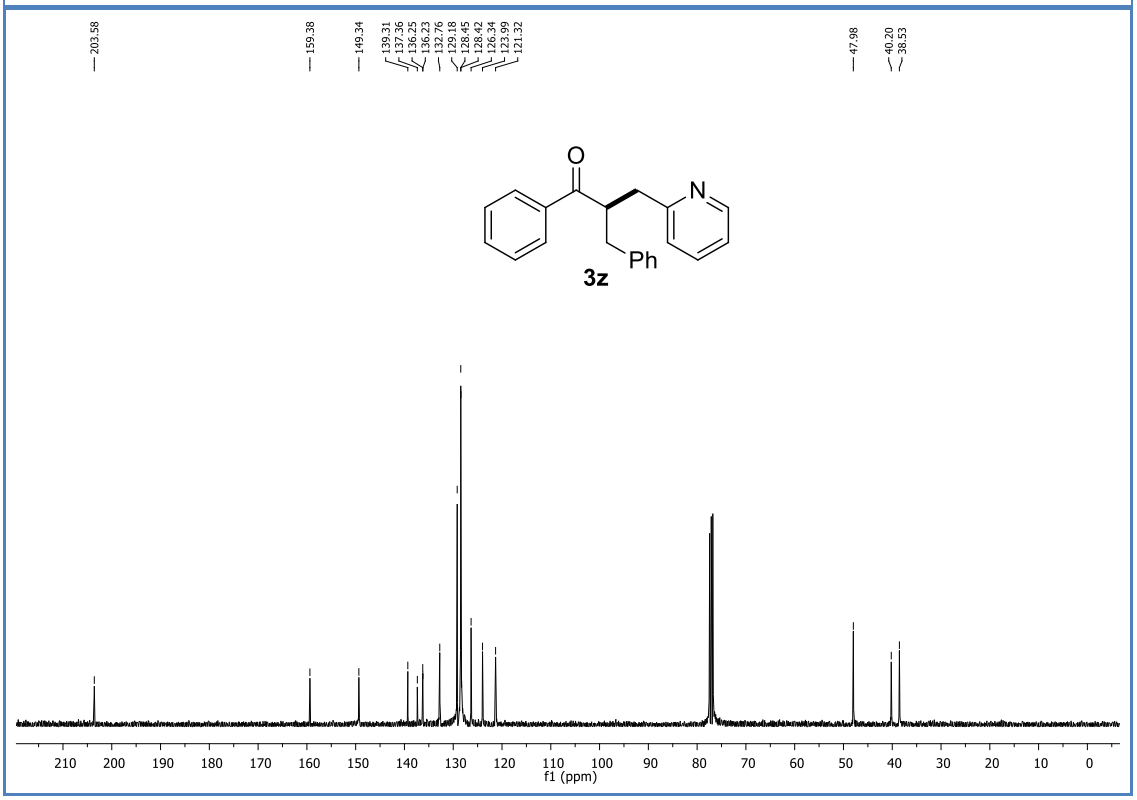

3x
3.26
2.02
2.12
1.37
1.18
5.05
4.13
18.16
2.99
10.22
3.00
f1 (ppm)


206.05
142.78
128.84
127.07
126.32
125.61
125.27
113.91
39.10
30.82
28.44
28.23
26.14
13.02
3x
f1 (ppm)


7.73 7.71 7.71 7.48 7.46 7.44 7.36 7.34 7.32 7.25 7.22 7.20 7.18 7.14 7.12 7.10
6.65 6.63 6.61 6.61 6.58 6.57 5.86 5.86 5.85
3.98 3.97 3.96 3.95 3.93 3.93 3.91 3.12 3.10 3.09 3.07 3.06 3.04 3.03 3.01 2.80 2.78 2.77 2.75 2.73 2.72 2.70 2.68
O
O
O
Ph
3y
2.15 1.18 1.82 1.77 3.28 3.25 2.37 1.00 1.99 1.87
9.5 9.0 8.5 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 0.0
f1 (ppm)


203.40
147.61 145.99 139.54 137.44 133.34 132.89 129.08 128.55 128.50 128.18 126.36 122.09
109.46 108.24
100.85
50.79
38.27 37.95
O
O
O
Ph
3y
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


8.38
8.37
7.78
7.78
7.76
7.75
7.40
7.40
7.40
7.38
7.36
7.29
7.27
7.25
7.14
7.13
7.12
7.11
7.09
7.07
7.07
7.06
7.04
7.02
7.00
6.96
6.94
6.93
4.41
4.41
4.39
4.38
4.37
4.36
3.26
3.23
3.22
3.20
3.11
3.09
3.07
3.05
2.93
2.92
2.89
2.88
2.77
2.75
2.73
2.71
O
N
Ph
3z
0.89
1.94
2.03
2.04
5.88
0.92
1.00
1.06
1.04
1.04
1.06
9.5
9.0
8.5
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
0.0
f1 (ppm)


203.58
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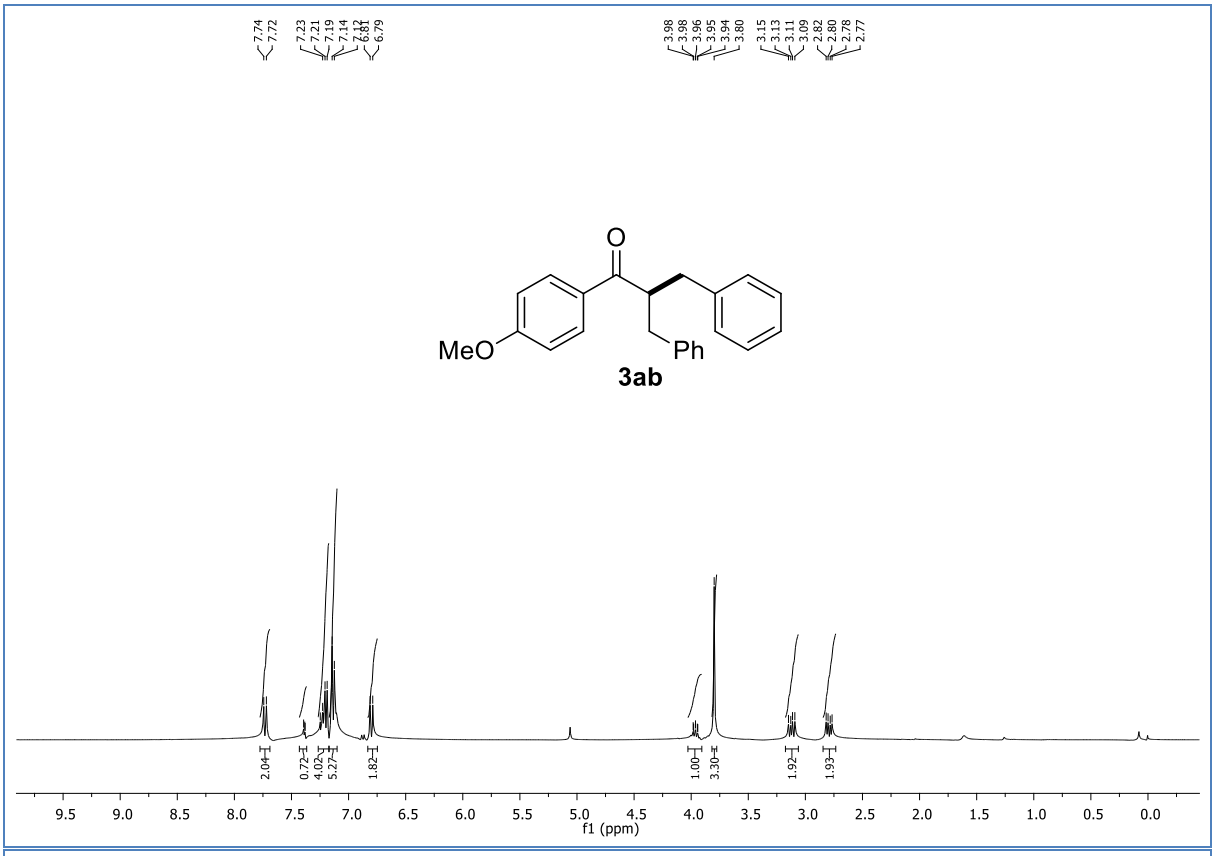
139.31
137.36
136.25
136.23
132.76
129.18
128.45
128.42
126.34
123.99
121.32
47.98
40.20
38.53
O
N
Ph
3z
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.74
7.72
7.23
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7.14
6.81
6.79
3.98
3.98
3.96
3.95
3.94
3.80
3.15
3.13
3.11
3.09
2.82
2.80
2.78
2.77
O
MeO
Ph
3ab
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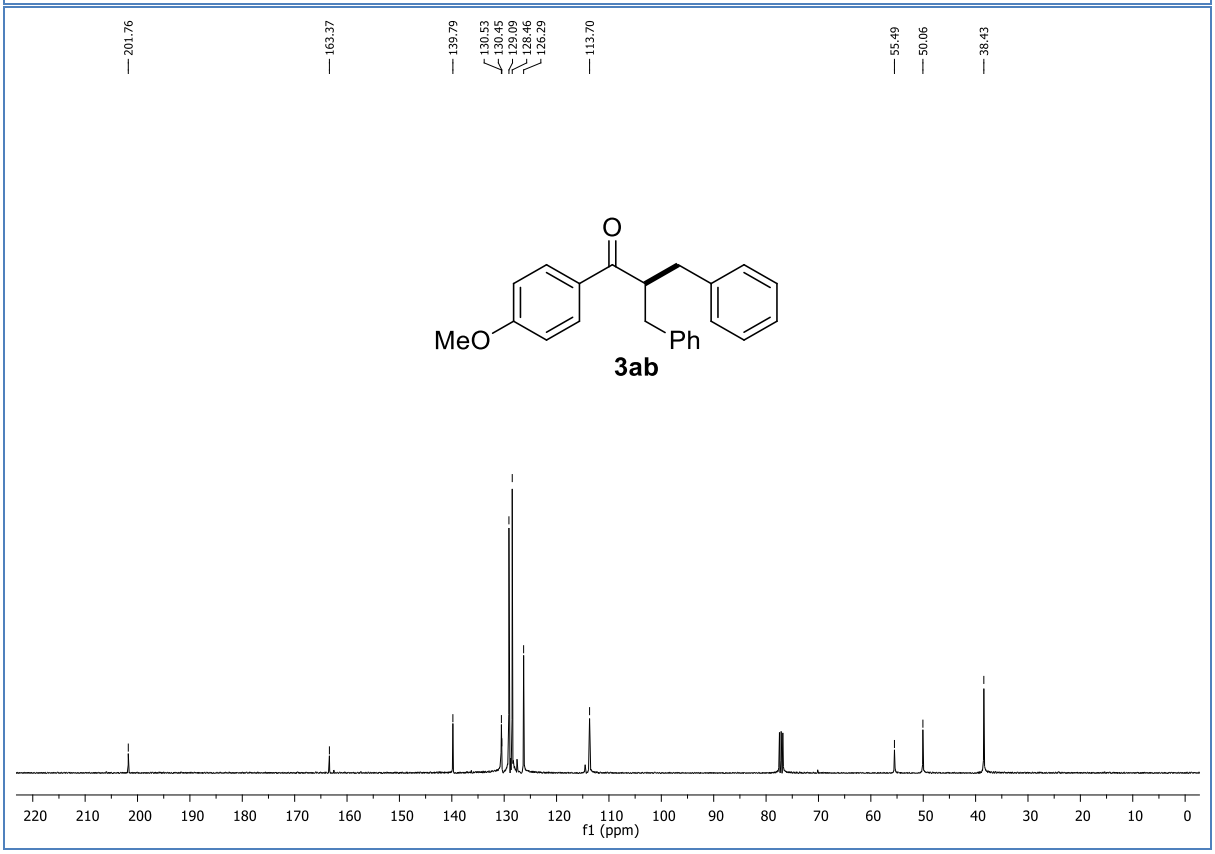
0.72
4.02
5.27
1.82
1.00
3.30
1.92
1.93
f1 (ppm)


201.76
163.37
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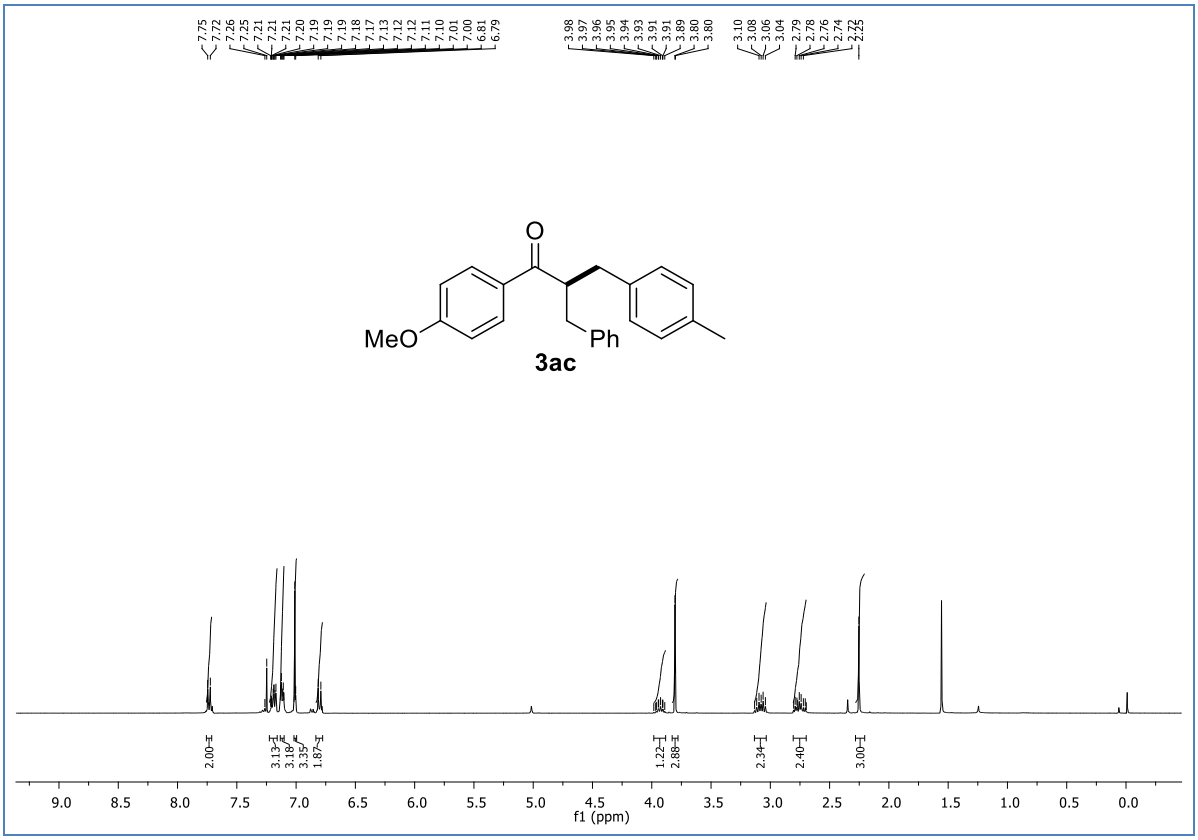
130.53
130.45
129.09
128.46
126.29
113.70
55.49
50.06
38.43
O
MeO
Ph
3ab
f1 (ppm)


7.75
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7.19
7.18
7.17
7.13
7.12
7.12
7.11
7.10
7.01
7.00
6.81
6.79
3.98
3.97
3.96
3.95
3.94
3.93
3.91
3.91
3.89
3.80
3.80
3.10
3.08
3.06
3.04
2.79
2.78
2.76
2.74
2.25
O
MeO
Ph
3ac
2.00
3.13
3.18
3.39
1.87
1.22
2.88
2.34
2.40
3.00
9.0
8.5
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
0.0
f1 (ppm)