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Supplemental information

Direct insertion into the C–C bond of unactivated ketones with NaH-mediated aryne chemistry

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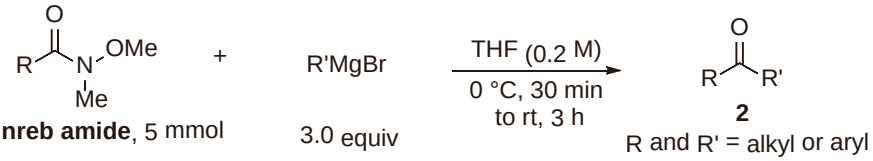
1. General information

Unless otherwise indicated, all glassware was oven dried by a heat gun before use and all reactions were performed under an atmosphere of nitrogen. All solvents were distilled from appropriate drying agents prior to use. All reagents were used as received from commercial suppliers unless otherwise stated. Reaction progress was monitored by thin layer chromatography (TLC) performed on glass plates coated with silica gel GF254 with 0.2 mm thickness. Chromatograms were visualized by fluorescence quenching with UV light at 254 nm or by staining using potassium permanganate. Flash column chromatography was performed using silica gel 60 (200-300 mesh). Mass spectra were obtained using a TOF MS instrument EI or ESI source. All ^{1}H NMR, ^{13}C NMR, ^{19}F NMR spectra were recorded on Bruker AV-400 or AV-500 or AV-600. Chemical shifts were given in parts per million (ppm, δ), referenced to the solvent peak of $CDCl_3$, defined at δ = 7.26 (^{1}H NMR), δ = 77.16 (^{13}C NMR). Coupling constants were quoted in Hz (*J*). ^{1}H NMR Spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t) and quadruplet (q). Splitting patterns that could not be interpreted or easily visualized were designated as multiplet (m).

2. General procedure for the synthesis of starting materials

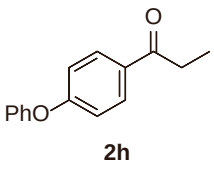
Ketones **2a–2g, 2m, 2q–2t, 2w, 2y, 2aa, 2ac, 2ad, 2ae, 2af–2aq, 2as, 2ay, 2bi–2bm, 2bo, 2bp, 2bs, 2cd–2cf, 2ck, 2cl, 2cm, 2co** and aryne precursors **1a, 1a1, 1a2, 1a3, 1m', 1m'', 1n, 1r, 1s** are commercially available. Ketones **2i**[S1], **2j**[S2], **2o**[S3], **2p**[S4], **2u**[S5], **2x**[S6], **2au**[S7], **2av**[S8], **2aw**[S9], **2be**[S10], **2bf**[S11], **2bg**[S12], **2bh**[S13], **2by**[S14], **2cg**[S15], **2ch**[S16], **2ci**[S17], **2cn**[S18], aryne precursors **1b**[S19], **1c**[S20], **1d**[S21], **1e**[S22], **1f**[S23], **1m**[S24], **1p**[S25] and 2-iodophenyl benzoate **15**[S26] are known compounds and synthesized according to reported literatures. The other ketones and aryne precursors were synthesized as detailed below.

General procedure for the synthesis of ketone 2



Weinreb amide, 5 mmol — 3.0 equiv — **2**, R and R' = alkyl or aryl

To the solution of Weinreb amide (5 mmol) in anhydrous THF (25 mL) was added Grignard reagent (15 mmol) slowly at 0 °C. After stirring for 30 min, the mixture was warmed to room temperature for another 3 h. Then the mixture was quenched with saturated aqueous NH_4Cl (30 mL) solution and the resulting mixture was extracted with EtOAc (30 mL × 3). The combined extracts were dried over Na_2SO_4, concentrated under vacuum and purified by silica gel chromatography eluting with an eluent (PE/EtOAc) to afford corresponding ketone **2**.



2h

1-(4-phenoxyphenyl)propan-1-one (2h):

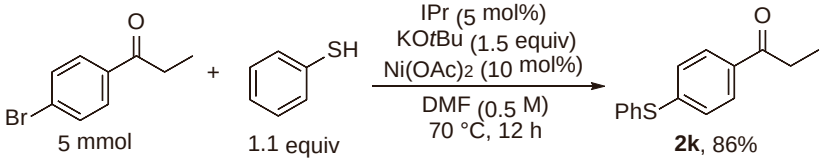
Following the general procedure, the title compound was prepared from *N*-methoxy-*N*-methyl-4-phenoxybenzamide (1.44 g, 5.6 mmol) and EtMgBr (1 M in THF, 16.8 mL, 16.8 mmol), and it was obtained as white solid, 1.23 g, 97% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 – 7.90 (m, 2H), 7.45 – 7.34 (m, 2H), 7.23 – 7.14 (m, 1H), 7.11 – 7.04 (m, 2H), 7.03 – 6.96 (m, 2H), 2.96 (q, *J* = 7.3 Hz, 2H), 1.22 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.6, 161.9, 155.7, 131.8, 130.4, 130.2, 124.7, 120.3, 117.4, 31.7, 8.5.

The ^{1}H NMR and ^{13}C NMR of **2h** are consistent with the reported spectra[S27].

1-(4-(phenylthio)phenyl)propan-1-one (2k):

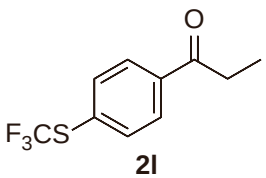


To a mixture of 1-(4-bromophenyl)propan-1-one (1.07 g, 5 mmol), benzenethiol (606.5 mg, 1 mmol), $Ni(OAc)_2$ (88.5 mg, 0.5 mmol), IPr (97.3 mg, 0.25 mmol) and KO*t*Bu (1.68 g,15 mmol) was added anhydrous DMF (10 mL) under nitrogen atmosphere. The resulting mixture was stirred at 70 °C for 12 h. After cooling to room temperature, the reaction was diluted with EtOAc (20 mL) and the organic layer was washed with water (20 mL) for three times. After that, the organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The obtained residue was purified by silica gel chromatography to give the title compound **2k** was obtained as white solid, 1.04 g, 86% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (d, *J* = 8.4 Hz, 2H), 7.53 – 7.45 (m, 2H), 7.44 – 7.35 (m, 3H), 7.21 (d, *J* = 8.4 Hz, 2H), 2.94 (q, *J* = 7.2 Hz, 2H), 1.20 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 200.0, 144.6, 134.4, 133.9, 132.4, 129.8, 128.9, 128.7, 127.7, 31.8, 8.4.

The ^{1}H NMR and ^{13}C NMR of **2k** are consistent with the reported spectra[S28].



2l

1-(4-((trifluoromethyl)thio)phenyl)propan-1-one (2l):

Following the general procedure, the title compound was prepared from *N*-methoxy-*N*-methyl-4-((trifluoromethyl)thio)benzamide (1.41 g, 5.3 mmol) and EtMgBr (1 M in THF, 15.9 mL, 15.9 mmol), and it was obtained as white solid, 1.23 g, 97% yield.

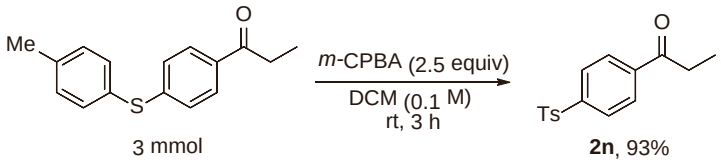
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.05 – 7.92 (m, 2H), 7.78 – 7.68 (m, 2H), 3.01 (q, *J* = 7.2 Hz, 2H), 1.23 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.9, 138.5, 135.9, 129.9, 129.4 (q, 308.1 Hz), 128.9, 32.2, 8.2.

^{19}F NMR (565 MHz, $CDCl_3$): δ -41.82.

HRMS (EI-TOF): calculated for $[C_{10}H_9F_3OS\ (M)]^+$: 234.0326, found: 234.0329.

1-(4-tosylphenyl)propan-1-one (2n):



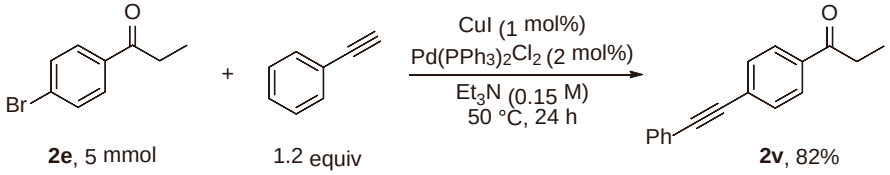
To a solution of 1-(4-(*p*-tolylthio)phenyl)propan-1-one (769.1 mg, 3 mmol) in DCM (15 mL) was added a solution of *m*-CPBA (85% purity, 1.52 g, 7.5 mmol) in DCM (15 mL) dropwise at room temperature. The resulting solution was stirred at room temperature for 3 h. After that, saturated aqueous $NaHCO_3$ (30 mL) was added to the reaction mixture and the resulting solution was extracted with DCM (30 mL×3). The combined extracts were dried over Na_2SO_4 and concentrated under reduced pressure. The obtained residue was purified by silica gel chromatography to give the title compound **2n** was obtained as white solid, 804.7 mg, 93% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 – 7.97 (m, 4H), 7.82 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 2.98 (q, *J* = 7.2 Hz, 2H), 2.39 (s, 3H), 1.20 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 199.6, 145.7, 144.9, 140.2, 137.9, 130.2, 128.8, 128.0, 127.9, 32.4, 21.7, 8.1.

HRMS (EI-TOF): calculated for $[C_{16}H_{16}O_3S\ (M)]^+$: 288.0820, found: 288.0817.

1-(4-(phenylethynyl)phenyl)propan-1-one (2v):

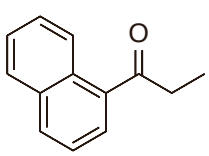


To a stirring mixture of **2e** (1.07 g, 5 mmol), Pd $(PPh_3)_2Cl_2$ (21.0 mg, 0.1 mmol) and CuI (2.9 mg, 0.05 mmol) in Et_3N (33.5 mL) was added phenylacetylene (0.67 mL, 6 mmol) via syringe under nitrogen atmosphere. The resulting mixture was stirred at 50 °C for 24 h. After cooling down to room temperature, the reaction mixture was quenched by water (40 mL), filtered through a short pad of celite and rinsed with EtOAc (40 mL). The filtrate was concentrated under reduced pressure to remove the organic solvent, and the remaining aqueous phase was extracted with EtOAc (40 mL × 2). The combined organic layers were washed with brine (40 mL × 2), dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel to afford the title compound **2v** as white solid, 960.4 mg, 82% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 – 7.90 (m, 2H), 7.63 – 7.58 (m, 2H), 7.58 – 7.52 (m, 1H), 7.41 – 7.33 (m, 3H), 3.00 (q, *J* = 7.2 Hz, 2H), 1.23 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.1, 136.1, 131.84, 131.79, 128.9, 128.6, 128.1, 122.8, 92.6, 88.8, 31.9, 8.3. One aromatic carbon peak is overlapped.

The ^{1}H NMR and ^{13}C NMR of **2v** are consistent with the reported spectra[S29].

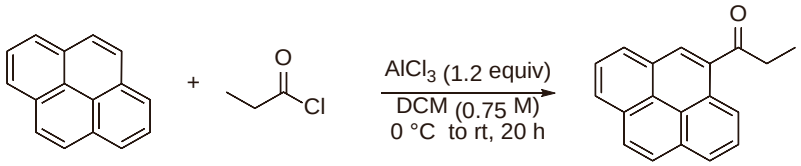


2z

1-(naphthalen-1-yl)propan-1-one (2z):
Following the general procedure, the title compound was prepared from *N*-methoxy-*N*-methyl-1-naphthamide (1.08 g, 5 mmol) and EtMgBr (1 M in THF, 15 mL, 15 mmol), and it was obtained as colorless oil, 903.2 mg, 98% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.58 (d, *J* = 8.7 Hz, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.90 – 7.83 (m, 2H), 7.63 – 7.45 (m, 3H), 3.08 (q, *J* = 7.3 Hz, 2H), 1.29 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 205.4, 136.3, 134.1, 132.4, 130.2, 128.5, 127.9, 127.2, 126.5, 125.9, 124.5, 35.5, 8.7.
The ^{1}H NMR and ^{13}C NMR of **2z** are consistent with the reported spectra[S30].

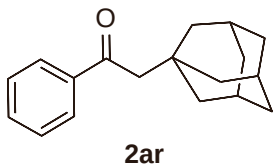
1-(pyren-4-yl)propan-1-one (2ab):



15 mmol 1.1 equiv **2ab**, 76%

To a solution of pyrene (3.03 g, 15 mmol) in DCM (20 mL) was added propionyl chloride (1.53 g, 16.5 mmol) at 0 °C stirring for 10 min. Then anhydrous $AlCl_3$ (2.40 g, 18 mmol) was slowly added into the reaction mixture at 0 °C. The resulting mixture was warmed to room temperature and stirred for 20 h. After that, the mixture was filtered through a short pad of celite and rinsed with DCM (20 mL). The filtrate was washed with saturated aqueous $NaHCO_3$ (40 mL × 3) solution, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel to afford the title compound **2ab** as yellow solid, 2.93 g, 76% yield.

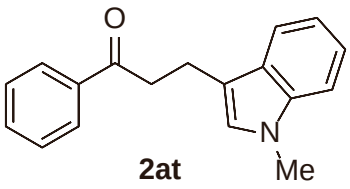
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.93 – 8.85 (m, 1H), 8.29 – 8.24 (m, 1H), 8.23 – 8.15 (m, 3H), 8.13 – 8.07 (m, 2H), 8.05 – 7.98 (m, 2H), 3.22 (q, *J* = 7.3 Hz, 2H), 1.37 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 205.6, 133.6, 132.6, 131.1, 130.6, 129.5, 129.4, 129.3, 127.1, 126.4, 126.2, 126.1, 126.0, 125.0, 124.9, 124.4, 124.1, 35.8, 9.0.
HRMS (EI-TOF): calculated for $[C_{19}H_{14}O\ (M)]^+$: 258.1045, found: 258.1043.



2ar

2-((*3r,5r,7r*)-adamantan-1-yl)-1-phenylethan-1-one (2ar):
Following the general procedure, the title compound was prepared from 2-((*3r,5r,7r*)-adamantan-1-yl)-*N*-methoxy-*N*-methylacetamide (2.46 g, 5 mmol) and PhMgBr (1 M in THF, 15 mL, 15 mmol), and it was obtained as colorless oil, 1.21 g, 95% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 – 7.90 (m, 2H), 7.57 – 7.50 (m, 1H), 7.48 – 7.41 (m, 2H), 2.72 (s, 2H), 1.98 – 1.90 (m, 3H), 1.72 – 1.58 (m, 12H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 200.5, 138.9, 132.8, 128.54, 128.48, 51.3, 43.1, 36.8, 34.1, 28.8.
The ^{1}H NMR and ^{13}C NMR of **2ar** are consistent with the reported spectra[S31].



2at

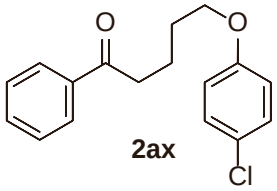
3-(1-methyl-1*H*-indol-3-yl)-1-phenylpropan-1-one (2at):

Following the general procedure, the title compound was prepared from *N*-methoxy-*N*-methyl-3-(1-methyl-1*H*-indol-3-yl)propanamide (2.21 g, 9 mmol) and PhMgBr (1 M in THF, 27 mL, 27 mmol), and it was obtained as colorless oil, 2.29 g, 97% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.67 (dd, *J* = 7.9, 0.7 Hz, 1H), 7.61 – 7.54 (m, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.39 – 7.31 (m, 1H), 7.30 – 7.25 (m, 1H), 7.20 – 7.13 (m, 1H), 6.94 (s, 1H), 3.76 (s, 3H), 3.45 – 3.38 (m, 2H), 3.26 (t, *J* = 7.5 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 200.1, 137.2, 133.1, 128.7, 128.2, 127.8, 126.6, 126.0, 121.7, 118.94, 118.87, 114.1, 109.4, 39.7, 32.7, 19.7.

The ^{1}H NMR and ^{13}C NMR of **2at** are consistent with the reported spectra[S32].



2ax

5-(4-chlorophenoxy)-1-phenylpentan-1-one (2ax):

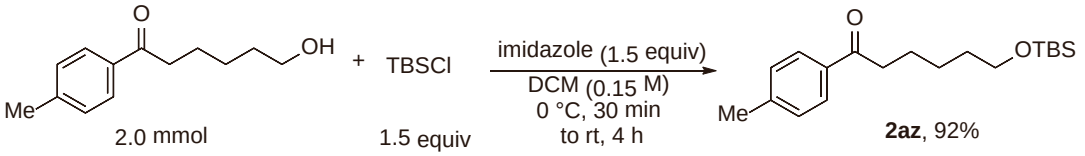
Following the general procedure, the title compound was prepared from 5-(4-chlorophenoxy)-*N*-methoxy-*N*-methylpentanamide (1.89 g, 6.9 mmol) and PhMgBr (1 M in THF, 20.7 mL, 20.7 mmol), and it was obtained as white solid, 1.65 g, 83 % yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, *J* = 7.7 Hz, 2H), 7.60 – 7.53 (m, 1H), 7.51 – 7.42 (m, 2H), 7.21 (d, *J* = 8.7 Hz, 2H), 6.80 (d, *J* = 8.7 Hz, 2H), 3.98 (t, *J* = 5.8 Hz, 2H), 3.06 (t, *J* = 6.8 Hz, 2H), 2.01 – 1.80 (m, 4H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.1, 157.7, 137.1, 133.2, 129.4, 128.8, 128.2, 125.6, 115.9, 68.06, 38.2, 28.9, 21.0.

HRMS (EI-TOF): calculated for $[C_{17}H_{17}ClO_2\ (M)]^+$: 288.0917, found: 288.0914.

6-((*tert*-butyldimethylsilyl)oxy)-1-(*p*-tolyl)hexan-1-one (2az):

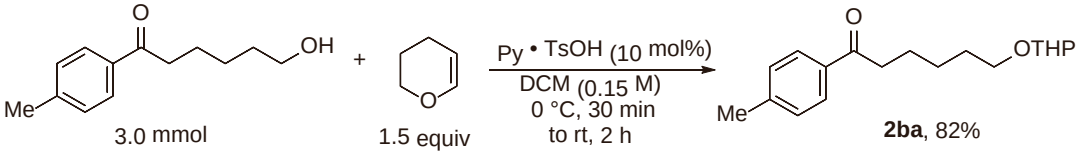


To a solution of 6-hydroxy-1-(*p*-tolyl)hexan-1-one (412.6 mg, 2 mmol) and imidazole (204.2 mg, 3 mmol) in DCM (13 mL) was added TBSCl (452.2 mg, 3 mmol) at 0 °C stirring for 30 min. The reaction mixture was stirred at room temperature for 4 h. The reaction mixture was diluted with DCM (20 mL) and washed with water (50 mL) and brine (50 mL). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel to afford the title compound **2az** as colorless oil, 590.2 mg, 92% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (d, *J* = 8.2 Hz, 2H), 7.27 – 7.23 (m, 2H), 3.61 (t, *J* = 6.5 Hz, 2H), 2.97 – 2.86 (m, 2H), 2.41 (s, 3H), 1.80 – 1.68 (m, 2H), 1.61 – 1.51 (m, 2H), 1.47 – 1.37 (m, 2H), 0.89 (s, 9H), 0.04 (s, 6H).

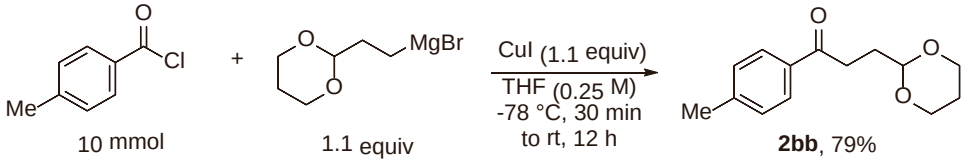
^{13}C NMR (151 MHz, $CDCl_3$): δ 200.3, 143.7, 134.7, 129.4, 128.3, 63.2, 38.6, 32.8, 26.1, 25.8, 24.4, 21.8, 18.5, -5.1.
HRMS (EI-TOF): calculated for $[C_{18}H_{29}O_2Si$ (M – $CH_3)]^+$: 305.1937, found: 305.1940.

6-((tetrahydro-2*H*-pyran-2-yl)oxy)-1-(*p*-tolyl)hexan-1-one (2ba):



To a solution of 6-hydroxy-1-(*p*-tolyl)hexan-1-one (619.0 mg, 3 mmol) and 3,4-dihydro-2*H*-pyran (252.4 mg, 3 mmol) in DCM (20 mL) was added pyridinium *p*-toluenesulfonate (75.4 mg, 0.3 mmol) at 0 °C stirring for 30 min. Then the reaction mixture was warmed to room temperature and stirred for 2 h. The reaction mixture was diluted with DCM (20 mL) and washed with saturated aqueous $NaHCO_3$ (50 mL) and brine (50 mL). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel to afford the title compound **2ba** as colorless oil, 714.2 mg, 82% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 7.9 Hz, 2H), 4.56 (dd, *J* = 4.4, 2.8 Hz, 1H), 3.90 – 3.81 (m, 1H), 3.79 – 3.70 (m, 1H), 3.52 – 3.45 (m, 1H), 3.44 – 3.34 (m, 1H), 2.97 – 2.92 (t, *J* = 7.4 Hz, 2H), 2.40 (s, 3H) 1.86 – 1.62 (m, 6H), 1.60 – 1.40 (m, 6H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 200.2, 143.7, 134.7, 129.3, 128.3, 99.0, 67.5, 62.5, 38.5, 30.9, 29.7, 26.2, 25.6, 24.4, 21.7, 19.8.
HRMS (ESI-TOF): calculated for $[C_{18}H_{26}O_3Na$ (M + Na)]$^+$: 313.1780, found: 313.1781.

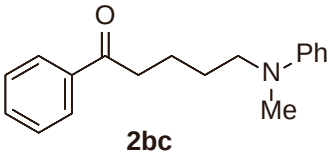
3-(1,3-dioxan-2-yl)-1-(*p*-tolyl)propan-1-one (2bb):



To the solution of 4-methylbenzoyl chloride (1.32 mL, 10 mmol) and CuI (2.09 g, 11 mmol) in THF (40 mL) was added (2-(1,3-dioxan-2-yl)ethyl)magnesium bromide (1 M in THF, 11 mL, 11 mmol) slowly at –78 °C. After stirring for 30 min, the mixture was warmed to room temperature for another 12 h. The solvent was removed under vacuum, and the residue was diluted in petroleum ether (60 mL), filtered, concentrated, and purified by silica gel chromatography to afford the title compound **2bb** as white solid, 1.86 g, 79% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 4.66 (t, *J* = 5.0 Hz, 1H), 4.09 (dd, *J* = 10.6, 5.0 Hz, 2H), 3.81 – 3.71 (m, 2H), 3.08 (t, *J* = 7.3 Hz, 2H), 2.40 (s, 3H), 2.14 – 1.99 (m, 3H), 1.37 – 1.29 (m, 1H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.4, 143.8, 134.6, 129.3, 128.3, 101.2, 67.0, 32.6, 29.5, 25.9, 21.8.

HRMS (EI-TOF): calculated for $[C_{14}H_{18}O_3$ (M)$]^+$: 234.1256, found: 234.1255.



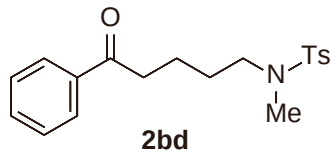
2bc

5-(methyl(phenyl)amino)-1-phenylpentan-1-one (2bc): Following the general procedure, the title compound was prepared from *N*-methoxy-*N*-methyl-5-(methyl(phenyl)amino)pentanamide (651.2 mg, 2.6 mmol) and PhMgBr (1 M in THF, 7.8 mL, 7.8 mmol), and it was obtained as white solid, 653.3 mg, 94 % yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (dd, *J* = 5.2, 3.3 Hz, 2H), 7.60 – 7.54 (m, 1H), 7.51 – 7.44 (m, 2H), 7.27 – 7.21 (m, 2H), 6.76 – 6.67 (m, 3H), 3.43 – 3.33 (t, *J* = 7.2 Hz, 2H), 3.01 (t, *J* = 7.1 Hz, 2H), 2.94 (s, 3H), 1.84 – 1.75 (m, 2H), 1.72 – 1.65 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 200.2, 149.4, 137.1, 133.1, 129.3, 128.7, 128.1, 116.1, 112.3, 52.7, 38.5, 38.4, 26.6, 22.0.

HRMS (EI-TOF): calculated for $[C_{18}H_{21}NO$ (M)$]^+$: 267.1623, found: 267.1620.



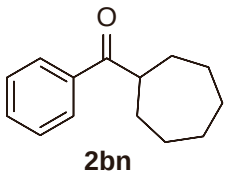
2bd

***N*,4-dimethyl-*N*-(5-oxo-5-phenylpentyl)benzenesulfonamide (2bd):** Following the general procedure, the title compound was prepared from 5-((*N*,4-dimethylphenyl)sulfonamido)-*N*-methoxy-*N*-methyl pentanamide (1.25 g, 3.8 mmol) and PhMgBr (1 M in THF, 11.4 mL, 11.4 mmol), and it was obtained as white solid, 1.19 g, 91 % yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 – 7.92 (m, 2H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.59 – 7.52 (m, 1H), 7.50 – 7.42 (m, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 3.02 (t, *J* = 7.0 Hz, 4H), 2.70 (s, 3H), 2.41 (s, 3H), 1.83 – 1.74 (m, 2H), 1.67 – 1.58 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 200.1, 143.4 137.0, 134.5, 133.2, 129.8, 128.7, 128.2, 127.5, 49.7, 37.7, 34.7, 27.0, 21.6, 21.1.

HRMS (ESI-TOF): calculated for $[C_{19}H_{23}NO_3SNa$ (M + Na)$]^+$: 313.1780, found: 313.1781.



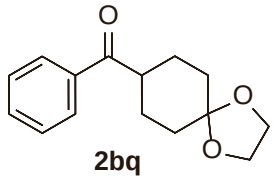
2bn

cycloheptyl(phenyl)methanone (2bn): Following the general procedure, the title compound was prepared from *N*-methoxy-*N*-methylcycloheptanecarboxamide (3.19 g, 17.2 mmol) and PhMgBr (1 M in THF, 51.6 mL, 51.6 mmol), and it was obtained as colorless oil, 2.98 g, 86 % yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (dd, *J* = 5.2, 3.3 Hz, 2H), 7.57 – 7.50 (m, 1H), 7.48 – 7.42 (m, 2H), 3.48 – 3.37 (m, 1H), 1.97 – 1.88 (m, 2H), 1.84 – 1.50 (m, 10H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 204.4, 136.5, 132.8, 128.7, 128.4, 46.7, 30.9, 28.4, 26.9.

The ^{1}H NMR and ^{13}C NMR of **2bn** are consistent with the reported spectra[S33].



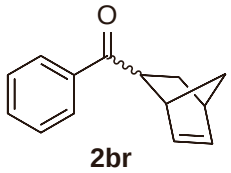
2bq

phenyl(1,4-dioxaspiro[4.5]decan-8-yl)methanone (2bq): Following the general procedure, the title compound was prepared from *N*-methoxy-*N*-methyl-1,4-dioxaspiro[4.5]decane-8-carboxamide (1.15 g, 5 mmol) and PhMgBr (1 M in THF, 15 mL, 15 mmol), and it was obtained as colorless oil, 1.16 g, 94% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 – 7.91 (m, 2H), 7.57 – 7.51 (m, 1H), 7.48 – 7.43 (m, 2H), 3.99 – 3.92 (m, 4H), 3.32 – 3.24 (m, 1H), 1.95 – 1.80 (m, 6H), 1.71 – 1.61 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 203.0, 136.3, 133.0, 128.8, 128.3, 108.3, 64.47, 64.45, 44.1, 34.2, 26.9.

HRMS (EI-TOF): calculated for $[C_{15}H_{18}O_3$ (M)$]^+$: 246.1256, found: 246.1253.



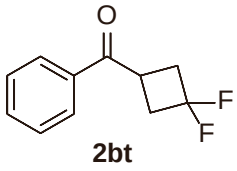
2br

((1S,4S)-bicyclo[2.2.1]hept-5-en-2-yl)(phenyl)methanone (2br): Following the general procedure, the title compound was prepared from (1*S*,4*S*)-*N*-methoxy-*N*-methylbicyclo[2.2.1]hept-5-ene-2-carboxamide (3.70 g, 20.4 mmol) and PhMgBr (1 M in THF, 61.2 mL, 61.2 mmol), and it was obtained as colorless oil, 3.84 g, 95% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 – 7.93 (m, 2H), 7.58 – 7.51 (m, 1H), 7.50 – 7.43 (m, 2H), 6.18 (dd, *J* = 5.6, 3.1 Hz, 1H), 5.82 (dd, *J* = 5.6, 2.8 Hz, 1H), 3.88 – 3.82 (m, 1H), 3.26 (s, 1H), 2.97 (s, 1H), 2.01 – 1.90 (m, 1H), 1.69 – 1.58 (m, 1H), 1.51 – 1.45 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 201.0, 137.5, 137.3, 132.7, 131.9, 128.6, 128.3, 50.1, 47.5, 47.3, 43.1, 29.1.

The ^{1}H NMR and ^{13}C NMR of **2br** are consistent with the reported spectra[S34].



2bt

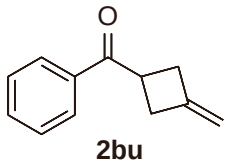
(3,3-difluorocyclobutyl)(phenyl)methanone (2bt): Following the general procedure, the title compound was prepared from 3,3-difluoro-*N*-methoxy-*N*-methylcyclobutane-1-carboxamide (1.06 g, 5.9 mmol) and PhMgBr (1 M in THF, 17.7 mL, 17.7 mmol), and it was obtained as colorless oil, 1.08 g, 93% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 – 7.85 (m, 2H), 7.65– 7.54 (m, 1H), 7.53– 7.44 (m, 2H), 3.84 – 3.74 (m, 1H), 3.04 – 2.79 (m, 4H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.9, 135.1, 133.8, 129.0, 128.5, 118.9 (dd, *J* = 285.4, 270.0 Hz), 38.4 (t, *J* = 24.3 Hz), 29.9 (dd, *J* = 13.8, 5.4 Hz).

^{19}F NMR (565 MHz, $CDCl_3$): δ -82.40 – -82.52 (m), -82.76 – -82.85 (m), -96.25 – -96.38 (m), -96.58 – -96.82 (m).

HRMS (EI-TOF): calculated for $[C_{11}H_{10}F_2O$ (M)$]^+$: 196.0700, found: 196.0702.



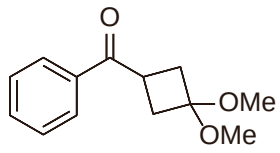
2bu

(3-methylenecyclobutyl)(phenyl)methanone (2bu):
Following the general procedure, the title compound was prepared from *N*-methoxy-*N*-methyl-3-methylenecyclobutane-1-carboxamide (1.51 g, 9.7 mmol) and PhMgBr (1 M in THF, 29.1 mL, 29.1 mmol), and it was obtained as colorless oil, 1.49 g, 91% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 – 7.87 (m, 2H), 7.60 – 7.50 (m, 1H), 7.50 – 7.42 (m, 2H), 4.87 – 4.81 (m, 2H), 4.01 – 3.92 (m, 1H), 3.17 – 3.09 (m, 2H), 3.03 – 2.94 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.1, 144.4, 135.6, 133.2, 128.8, 128.5, 107.0, 37.0, 35.1.

HRMS (EI-TOF): calculated for $[C_{12}H_{12}O\ (M)]^+$: 172.0888, found: 172.0890.



2bv

(3,3-dimethoxycyclobutyl)(phenyl)methanone (2bv):
Following the general procedure, the title compound was prepared from *N*,3,3-trimethoxy-*N*-methylcyclobutane-1-carboxamide (955.4 mg, 4.7 mmol) and PhMgBr (1 M in THF, 14.1 mL, 14.1 mmol), and it was obtained as colorless oil, 890.2 mg, 86% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 – 7.86 (m, 2H), 7.58 – 7.51 (m, 1H), 7.48 – 7.41 (m, 2H), 3.76 – 3.65 (m, 1H), 3.22 (s, 3H), 3.14 (s, 3H), 2.50 (d, *J* = 8.8 Hz, 4H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 199.9, 135.6, 133.2, 128.8, 128.5, 99.8, 48.9, 48.6, 35.2, 32.6.

HRMS (EI-TOF): calculated for $[C_{13}H_{16}O_3\ (M)]^+$: 220.1099, found: 220.1103.

(4-fluorophenyl)(1-tosylpiperidin-4-yl)methanone (2bw):

10 mmol 1.2 equiv **2bw**, 86%

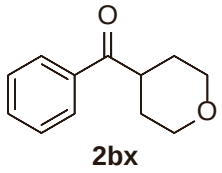
To the solution of (4-fluorophenyl)(piperidin-4-yl)methanone hydrochloride (2.43 g, 10 mmol) and Et_3N (2.43 g, 24 mmol) in DCM (50 mL) was added tosyl chloride (2.34 g, 12 mmol) slowly at 0 °C. The mixture was warmed to room temperature and stirred for 12 h, after which the mixture was treated with saturated aqueous $NaHCO_3$ (30 mL) and extracted by DCM (30 mL × 3). The combined extracts were dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel chromatography to afford the title compound as white solid, 3.11 g, 86% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 – 7.83 (m, 2H), 7.66 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.17 – 7.04 (m, 2H), 3.81 – 3.73 (m, 2H), 3.19 – 3.10 (m, 1H), 2.56 – 2.47 (m, 2H), 2.45 (s, 3H), 1.96 – 1.81 (m, 4H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.9, 165.9 (d, *J* = 255.4 Hz), 143.8, 133.2, 132.1 (d, *J* = 2.6 Hz), 131.0 (d, *J* = 9.6 Hz), 129.8, 127.9, 116.0 (d, *J* = 21.8 Hz), 45.7, 42.4, 28.0, 21.7.

^{19}F NMR (565 MHz, $CDCl_3$): δ -104.69 – -104.75 (m).

The ^{1}H NMR, ^{13}C NMR and ^{19}F NMR of **2bw** are consistent with the reported spectra[S35].



2bx

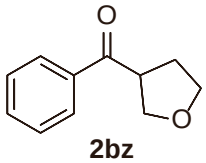
phenyl(tetrahydro-2*H*-pyran-4-yl)methanone (2bx):

Following the general procedure, the title compound was prepared from *N*-methoxy-*N*-methyltetrahydro-2*H*-pyran-4-carboxamide (848.6 mg, 4.9 mmol) and PhMgBr (1 M in THF, 14.7 mL, 14.7 mmol), and it was obtained as colorless oil, 895.3 mg, 96% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 – 7.90 (m, 2H), 7.60 – 7.52 (m, 1H), 7.50 – 7.43 (m, 2H), 4.08 – 4.01 (m, 2H), 3.60 – 3.45 (m, 3H), 1.93 – 1.73 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 201.9, 135.9, 133.2, 128.9, 128.4, 67.4, 42.7, 29.2.

The ^{1}H NMR and ^{13}C NMR of **2bx** are consistent with the reported spectra[S31].



2bz

phenyl(tetrahydrofuran-3-yl)methanone (2bz):

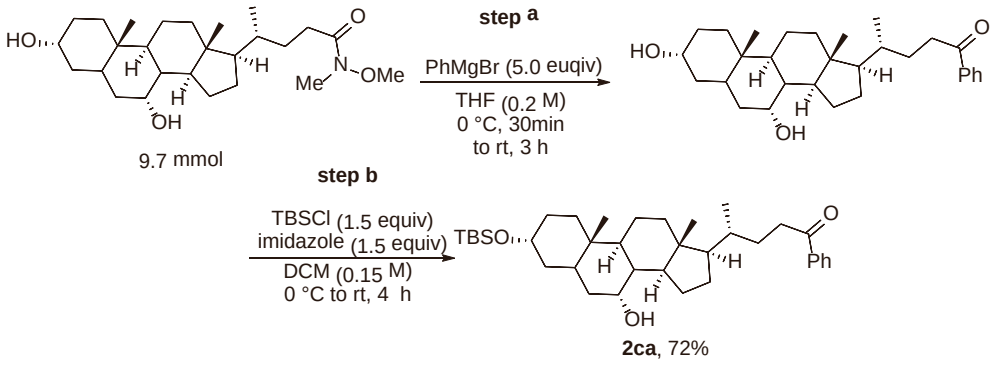
Following the general procedure, the title compound was prepared from *N*-methoxy-*N*-methyltetrahydrofuran-3-carboxamide (1.38 g, 8.7 mmol) and PhMgBr (1 M in THF, 26.1 mL, 26.1 mmol), and it was obtained as colorless oil, 1.41 g, 92% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 – 7.92 (m, 2H), 7.60 – 7.54 (m, 1H), 7.51 – 7.43 (m, 2H), 4.13 – 4.05 (m, 1H), 4.04 – 3.94 (m, 2H), 3.94 – 3.85 (m, 2H), 2.35 – 2.25 (m, 1H), 2.24 – 2.13 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 199.5, 136.4, 133.4, 128.8, 128.5, 70.3, 68.6, 46.4, 29.8.

HRMS (EI-TOF): calculated for $[C_{11}H_{12}O_2$ (M)$]^+$: 176.0837, found: 176.0840.

(4*R*)-4-((3*R*,7*R*,9S,10*S*,13*R*,14*S*,17*R*)-3-((*tert*-butyldimethylsilyl)oxy)-7-hydroxy-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)-1-phenylpentan-1-one (2ca):



2ca, 72%

Step a: Following the general procedure, (4*R*)-4-((3*R*,7*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-3,7-dihydroxy-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)-1-phenylpen tan-1-one was prepared from corresponding Weinreb amide (4.23 g, 9.7 mmol) and PhMgBr (1 M in THF, 48.5 mL, 48.5 mmol), and it was used without further purification for the next step.

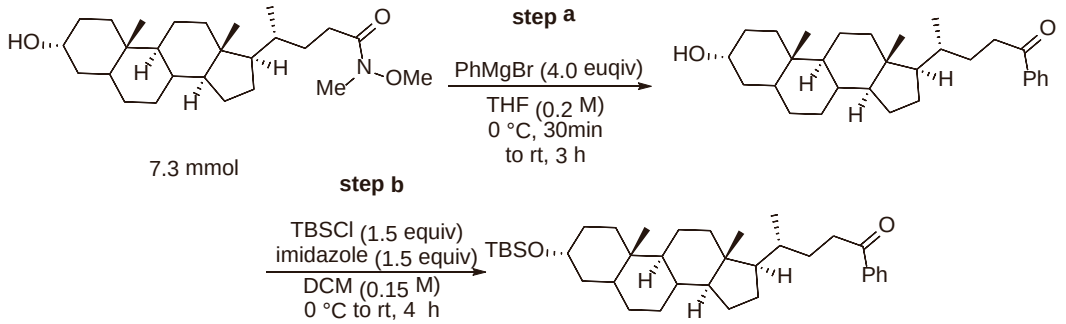
Step b: Following a similar procedure for the synthesis of **2az**, the title compound was obtained as white solid, 3.98 g, 72% yield.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.95 (d, *J* = 7.4 Hz, 2H), 7.57 – 7.51 (m, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 3.84 – 3.81 (m, 1H), 3.46 – 3.40 (m, 1H), 3.03 – 2.96 (m, 1H), 2.91 – 2.84 (m, 1H), 2.24 – 2.17 (m, 1H), 1.98 – 1.83 (m, 5H), 1.80 – 1.76 (m, 1H), 1.64 – 1.44 (m, 8H), 1.41 – 1.32 (m, 4H), 1.27 – 1.10 (m, 5H), 0.98 (d, *J* = 6.5 Hz, 3H), 0.97 – 0.91 (m, 1H), 0.88 (s, 3H), 0.88 (s, 9H), 0.66 (s, 3H), 0.04 (s, 6H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 201.1, 137.2, 133.0, 128.7, 128.2, 73.0, 68.7, 56.0, 50.6, 42.8, 41.7, 40.2, 39.8, 39.6, 35.7, 35.6, 35.5, 35.2, 34.8, 32.9, 31.2, 30.5, 28.3, 26.1, 23.9, 22.9, 20.7, 18.7, 18.4, 11.9, -4.4, -4.5.

HRMS (ESI-TOF): calculated for [$C_{36}H_{58}O_3SiNa$ (M + Na)]$^+$: 589.4053, found: 589.4055.

(4*R*)-4-((3*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-3-((*tert*-butyldimethylsilyl)oxy)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)-1-phenylpentan-1-one (2cb):



2cb, 78%

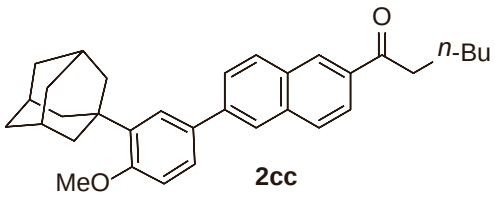
Step a: Following the general procedure, (4*R*)-4-((3*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-3-hydroxy-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)-1-phenylpentan-1-one was prepared from corresponding Weinreb amide (3.06 g, 7.3 mmol) and PhMgBr (1 M in THF, 29.2 mL, 29.2 mmol), and it was used without further purification for the next step.

Step b: Following a similar procedure for the synthesis of **2az**, the title compound was obtained as white solid, 3.13 g, 78% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, *J* = 7.3 Hz, 2H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 3.65 – 3.50 (m, 1H), 3.04 – 2.93 (m, 1H), 2.92 – 2.81 (m, 1H), 1.97 – 1.72 (m, 6H), 1.58 – 1.02 (m, 20H), 0.97 (d, *J* = 6.2 Hz, 3H), 0.93 – 0.85 (m, 12H), 0.64 (s, 3H), 0.06 (d, *J* = 8.0 Hz, 6H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.9, 137.2, 132.9, 128.6, 128.1, 72.8, 56.5, 56.1, 42.8, 42.3, 40.3, 40.2, 37.0, 35.9, 35.64, 35.56, 35.5, 34.6, 31.1, 30.5, 28.3, 27.4, 26.5, 26.1, 24.3, 23.5, 20.9, 18.7, 18.4, 12.1, -4.5.

HRMS (ESI-TOF): calculated for [$C_{36}H_{58}O_2SiK$ (M + Na)]$^+$: 589.3843, found: 589.3842.



2cc

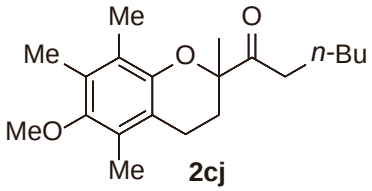
1-(6-(3-(adamantan-1-yl)-4-methoxyphenyl)naphthalen-2-yl)hexan-1-one (2cc):

Following the general procedure, the title compound was prepared from 6-(3-(adamantan-1-yl)-4-methoxyphenyl)-*N*-methoxy-*N*-methyl-2-naphthamide (2.60 g, 5.7 mmol) and *n*-pentylmagnesium bromide (1 M in THF, 17.1 mL, 17.1 mmol), and it was obtained as white solid, 2.61 g, 98% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.48 (s, 1H), 8.08 – 7.97 (m, 3H), 7.93 (d, *J* = 8.7 Hz, 1H), 7.81 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.63 (d, *J* = 2.2 Hz, 1H), 7.55 (dd, *J* = 8.4, 2.2 Hz, 1H), 7.00 (d, *J* = 8.5 Hz, 1H), 3.91 (s, 3H), 3.11 (t, *J* = 7.4 Hz, 2H), 2.23 – 2.18 (m, 6H), 2.15 – 2.10 (m, 3H), 1.87 – 1.78 (m, 8H), 1.48 – 1.37 (m, 4H), 0.96 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 200.6, 159.1, 141.6, 139.1, 136.1, 134.1, 132.6, 131.4, 130.0, 129.5, 128.6, 126.6, 126.1, 125.8, 124.8, 124.5, 112.2, 55.3, 40.7, 38.8, 37.33, 37.25, 31.8, 29.2, 24.4, 22.7, 14.1.

HRMS (ESI-TOF): calculated for $[C_{33}H_{39}O_2$ (M + H)$]^+$: 467.2950, found: 467.2948.



2cj

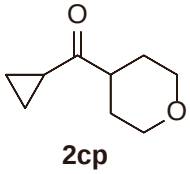
1-(6-methoxy-2,5,7,8-tetramethylchroman-2-yl)hexan-1-one (2cj):

Following the general procedure, the title compound was prepared from *N*,6-dimethoxy-*N*,2,5,7,8-pentamethylchromane-2-carboxamide (1.08 g, 3.5 mmol) and *n*-$C_5H_{11}MgBr$ (1 M in THF, 10.5 mL, 10.5 mmol), and it was obtained as colorless oil, 1.04 g, 93% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.63 (s, 3H), 2.78 – 2.68 (m, 1H), 2.60 – 2.43 (m, 2H), 2.41 – 2.32 (m, 1H), 2.22 (s, 3H), 2.20 (s, 3H), 2.11 (s, 3H), 1.83 – 1.73 (m, 1H), 1.57 – 1.39 (m, 5H), 1.30 – 1.12 (m, 4H), 0.85 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 214.9, 150.3, 147.5, 128.2, 126.3, 122.7, 117.8, 82.1, 60.4, 36.5, 31.4, 28.9, 24.1 23.0, 22.2, 20.6, 14.0, 12.6, 11.9, 11.7.

HRMS (ESI-TOF): calculated for $[C_{20}H_{30}O_3Na$ (M + Na)$]^+$: 341.2093, found: 341.2094.



2cp

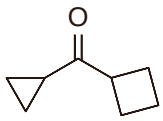
cyclopropyl(tetrahydro-2*H*-pyran-4-yl)methanone (2cp):

Following the general procedure, the title compound was prepared from *N*-methoxy-*N*-methyltetrahydro-2*H*-pyran-4-carboxamide (779.4 mg, 4.5 mmol) and cyclopropylmagnesium bromide (1 M in THF, 13.5 mL, 13.5 mmol), and it was obtained as colorless oil, 673.4 mg, 97% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.01 – 3.95 (m, 2H), 3.49 – 3.40 (m, 2H), 2.77 – 2.66 (m, 1H), 2.01 – 1.92 (m, 1H), 1.85 – 1.65 (m, 4H), 1.03 – 0.94 (m, 2H), 0.90 – 0.81 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 212.0, 67.4, 48.3, 28.3, 18.7, 11.0.

HRMS (EI-TOF): calculated for $[C_9H_{14}O_2$ (M)$]^+$: 150.0994, found: 150.0996.

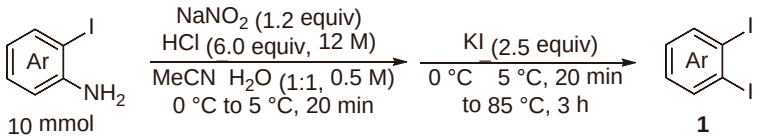


2cq

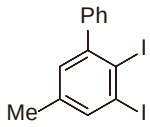
cyclobutyl(cyclopropyl)methanone (2cq):
Following the general procedure, the title compound was prepared from *N*-methoxy-*N*-methylcyclobutanecarboxamide (687.3 mg, 4.8 mmol) and cyclopropylmagnesium bromide (1 M in THF, 14.4 mL, 14.4 mmol), and it was obtained as colorless oil, 405.1 mg, 68% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.42 – 3.31 (m, 1H), 2.32 – 2.11 (m, 4H), 2.02 – 1.89 (m, 1H), 1.86 – 1.75 (m, 2H), 1.00 – 0.94 (m, 2H), 0.85 – 0.79 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 212.3, 46.0, 24.5, 18.3, 17.9, 10.6.
The ^{1}H NMR and ^{13}C NMR of **2cq** are consistent with the reported spectra[S36].

General procedure for the synthesis of *o*-diiodoarene 1



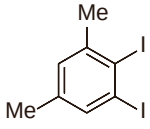
To a solution of 2-iodoaniline (10 mmol) in MeCN-H_2O (1:1, 20 ml) was added dropwise aqueous HCl (conc., 5 ml) at 0 °C. Keeping the temperature below 5 °C, to the resulting mixture was dropwise added solution of $NaNO_2$ (0.83 g, 12 mmol) in water (15 ml). After stirring for 20 min at that temperature, to the mixture was added a solution of KI (4.15 g, 25 mmol) in water (8 ml) and stirred for another 20 min. The resulting mixture was warmed to 85 °C for 3 h. After cooling to room temperature, the mixture was extracted with EtOAc (20 ml × 3). The combined extracts were successively washed with water (50 mL), saturated aqueous $NaHCO_3$ (50 mL) solution, saturated aqueous $Na_2S_2O_3$ (50 mL) solution and brine (50 mL). The organic layer was dried over the Na_2SO_4, concentrated under reduced pressure. The resulting residue was purified by silica gel chromatography affording the corresponding *o*-diiodoarene **1**.



1g

2,3-diiodo-5-methyl-1,1'-biphenyl (1g):
Following the general procedure, the title compound was prepared from 3-iodo-5-methyl-[1,1'-biphenyl]-2-amine (2.10 g, 6.8 mmol) and it was obtained as colorless oil, 2.06 g, 72% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 1.5 Hz, 1H), 7.47 – 7.36 (m, 3H), 7.30 – 7.23 (m, 2H), 7.06 (d, *J* = 1.5 Hz, 1H), 2.29 (s, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 149.3, 146.7, 139.6, 139.3, 129.9, 129.0, 128.0, 127.9, 110.1, 108.5, 20.5.
The ^{1}H NMR and ^{13}C NMR of **1g** are consistent with the reported spectra[S37].

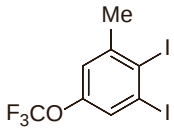


1h

1,2-diiodo-3,5-dimethylbenzene (1h):
Following the general procedure, the title compound was prepared from 2-iodo-4,6-dimethylaniline (2.47 g, 10 mmol) and it was obtained as colorless oil, 3.01 g, 84% yield.

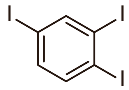
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.56 (s, 1H), 6.99 (s, 1H), 2.55 (s, 3H), 2.20 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 144.1, 139.6, 137.8, 129.8, 110.3, 109.8, 32.6, 20.5.
HRMS (EI-TOF): calculated for $[C_8H_8I_2$ (M)$]^+$: 357.8715, found: 357.8712.



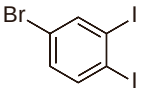
1i

1,2-diiodo-3-methyl-5-(trifluoromethoxy)benzene (1i):
Following the general procedure, the title compound was prepared from 2-iodo-6-methyl-4-(trifluoromethoxy)aniline (1.59 g, 5 mmol) and it was obtained as white solid, 1.73 g, 81% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (s, 1H), 7.07 (s, 1H), 2.61 (s, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 149.0, 146.0, 129.3, 121.2, 120.3 (q, *J* = 258.9 Hz), 112.3, 109.9, 33.1.
^{19}F NMR (565 MHz, $CDCl_3$): δ -57.89.
HRMS (EI-TOF): calculated for $[C_8H_5F_3I_2O$ (M)$]^+$: 427.8382, found: 427.8388.



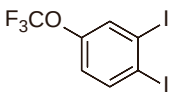
1j

1,2,4-triiodobenzene (1j):
Following the general procedure, the title compound was prepared from 2,4-diiodoaniline (2.0 g, 5.8 mmol) and it was obtained as white solid, 2.38 g, 90% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, *J* = 1.7 Hz, 1H), 7.55 (d, *J* = 8.3 Hz, 1H), 7.32 (dd, *J* = 8.3, 1.7 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 147.0, 140.7, 138.4, 109.6, 107.5, 93. 9.
The ^{1}H NMR and ^{13}C NMR of **1j** are consistent with the reported spectra[S38].



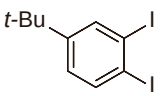
1k

4-bromo-1,2-diiodobenzene (1k):
Following the general procedure, the title compound was prepared from 4-bromo-2-iodoaniline (2.98 g, 10 mmol) and it was obtained as white solid, 3.39 g, 83% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 2.1 Hz, 1H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.15 (dd, *J* = 8.4, 2.1 Hz, 1H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 141.5, 140.3, 132.6, 122.5, 109.0, 106.3.
HRMS (EI-TOF): calculated for $[C_6H_3BrI_2$ (M)$]^+$: 407.7507, found: 407.7505.



1l

1,2-diiodo-4-(trifluoromethoxy)benzene (1l):
Following the general procedure, the title compound was prepared from 2-iodo-4-(trifluoromethoxy)aniline (2.40 g, 7.9 mmol) and it was obtained as white solid, 2.84 g, 87% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (d, *J* = 8.7 Hz, 1H), 7.72 (s, 1H), 6.93 (d, *J* = 8.6 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 148.8, 140.1, 132.0, 122.1, 120.3 (q, *J* = 258.9 Hz), 108.3, 105.6.
^{19}F NMR (565 MHz, $CDCl_3$): δ -57.99.
HRMS (EI-TOF): calculated for $[C_7H_3F_3I_2O$ (M)$]^+$: 413.8225, found: 413.8229.



1o

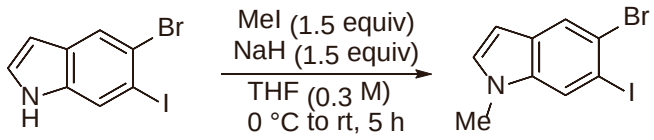
4-(*tert*-butyl)-1,2-diiodobenzene (1o):
Following the general procedure, the title compound was prepared from 4-(*tert*-butyl)-2-iodoaniline (2.75 g, 10 mmol) and it was obtained as colorless oil, 3.59 g, 93% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, *J* = 2.2 Hz, 1H), 7.76 (d, *J* = 8.3 Hz, 1H), 7.06 (dd, *J* = 8.3, 2.2 Hz, 1H), 1.28 (s, 9H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 153.1, 139.0, 136.9, 126.9, 108.1, 104.0, 34.6, 31.1.

The ^{1}H NMR and ^{13}C NMR of **1o** are consistent with the reported spectra[S39].

5-bromo-6-iodo-1-methyl-1*H*-indole (1q):



1.2 mmol **1q**, 94%

To a solution of 5-bromo-6-iodo-1*H*-indole (386 mg, 1.2 mmol) in dry THF (3.6 mL) was added NaH (60% in mineral oil, 72 mg, 1.8 mmol) at 0 °C. After stirring for 30 min, MeI (0.11 mL, 1.8 mmol) was added dropwise, then the mixture was allowed to stir at room temperature. After being stirred for 5 h, the mixture was quenched with cold water (3 mL), and extracted with EtOAc (5 mL × 3). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4 and concentrated under reduced pressure, the residue was purified by silica gel chromatography to afford **1q** as a light-yellow solid (379 mg, 94% yield).

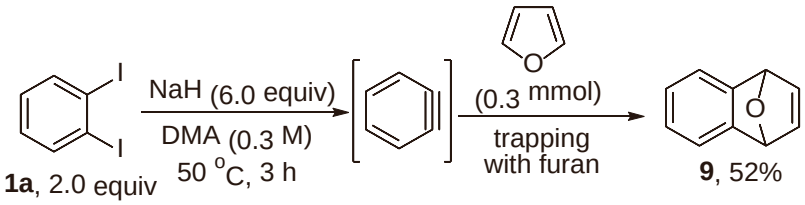
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (s, 1H), 7.85 (s, 1H), 7.00 (d, *J* = 3.1 Hz, 1H), 6.39 (dd, *J* = 3.1, 0.9 Hz, 1H), 3.74 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 137.0, 130.8, 130.3, 124.2, 120.8, 119.1, 100.8, 91.4, 33.2.

HRMS (EI-TOF): calculated for $[C_9H_7BrIN\ (M)]^+$: 334.8807, found: 334.8808.

3. Cyclization reactions of the formed benzyne from *o*-diiodoebenzene

Trapping benzyne by furan and benzyl azide



1a, 2.0 equiv **9**, 52%

To a suspension of NaH (60% dispersion in mineral oil, 72.5 mg, 1.8 mmol) in anhydrous DMA (1 mL) was added furan (20.4 mg, 0.3 mmol) and *o*-diiodoarene **1a** (198.0 mg, 0.6 mmol) respectively at 0 °C stirring for 5 min. The mixture was warmed to 50 °C for 3 h. After that, the reaction was quenched with saturated aqueous NH_4Cl (3 mL) solution at 0 °C. The mixture was then extracted with EtOAc (3 mL × 4). The combined extracts were dried over Na_2SO_4, concentrated under vacuum. The obtained

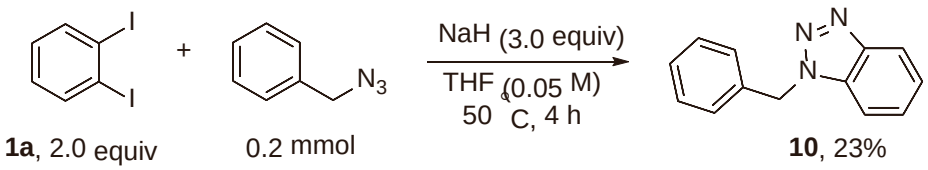
residue was purified by silica gel chromatography to afford the Diels-Alder adduct **9** as colorless oil, 22.4 mg, 52% yield.

1,4-dihydro-1,4-epoxynaphthalene (9):

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28 (dd, *J* = 5.0, 3.1 Hz, 2H), 7.05 (s, 2H), 7.00 (dd, *J* = 5.1, 3.0 Hz, 2H), 5.74 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 149.1, 143.1, 125.0, 120.3, 82.3.

The ^{1}H NMR and ^{13}C NMR of **9** are consistent with the reported spectra[S40].



1a, 2.0 equiv 0.2 mmol **10**, 23%

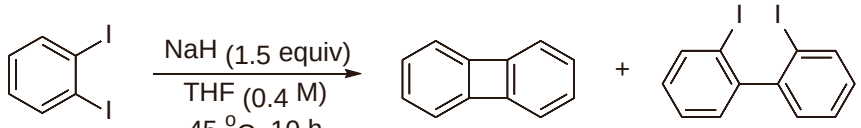
To an oven-dried 10 mL round flask equipped with a stir bar, was added benzyl azide (27 mg, 0.2 mmol), and anhydrous THF (4 mL) was added. Subsequently, the *o*-diiodoarene **1a** (134 mg, 0.4 mmol) and NaH (60% dispersion in mineral oil, 24 mg, 0.6 mmol) were added at room temperature. The resulted solution was stirred at 50 °C for 4 h. After that, the reaction was quenched with saturated aqueous NH_4Cl (2 mL) solution at 0 °C. The mixture was then extracted with EtOAc (5 mL × 3). The combined extracts were dried over Na_2SO_4, concentrated under vacuum. The obtained residue was purified by silica gel chromatography to afford the desired product **10** as light-yellow solid, 9.5 mg, 23% yield.

1-benzyl-1*H*-benzo[*d*][1,2,3]triazole (10):

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.07 (d, *J* = 8.1 Hz, 1H), 7.45 – 7.38 (m, 1H), 7.38 – 7.26 (m, 7H), 5.85 (s, 2H).

The ^{1}H NMR of **10** is consistent with the reported spectra[S41].

Benzyne dimerization



1a, 5 mmol **11**, 57% **12**, 4%

To a suspension of NaH (60% dispersion in mineral oil, 300 mg, 7.5 mmol) in anhydrous THF (10 mL) was added a solution of *o*-diiodoarene **1a** (1.65 g, 5 mmol) in anhydrous THF (2.5 mL) at room temperature. The mixture was warmed to 45 °C for 10 h. After that, the reaction was quenched with water (15 mL) at 0 °C. The mixture was then extracted with EtOAc (15 mL × 4). The combined extracts were dried over Na_2SO_4, concentrated under vacuum. The obtained residue was purified by silica gel chromatography to afford biphenylene **11**, 216.8 mg, 57% yield, and a little 2,2'-diiodo-1,1'-biphenyl **12**, 40.3 mg, 4% yield.

biphenylene (11):

^{1}H NMR (400 MHz, $CDCl_3$): δ 6.76 – 6.70 (m, 4H), 6.66 – 6.60 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 151.5, 128.3, 117.5.

HRMS (EI-TOF): calculated for $[C_{12}H_8\ (M)]^+$: 152.0626, found: 152.0624.

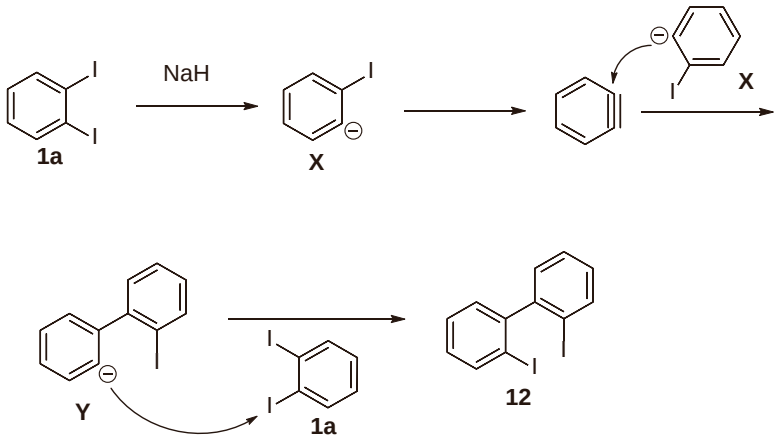
2,2'-diiodo-1,1'-biphenyl (12):

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, *J* = 7.9 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.20 (dd, *J* = 7.6, 1.3 Hz, 2H), 7.14 – 7.06 (m, 2H).

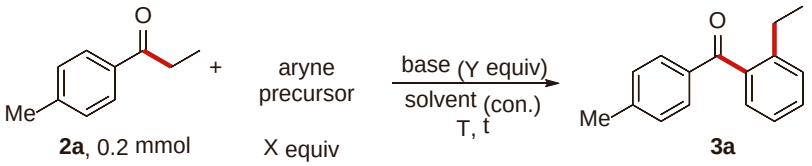
^{13}C NMR (101 MHz, $CDCl_3$): δ 149.1, 139.0, 130.0, 129.5, 128.2, 99.8.

HRMS (EI-TOF): calculated for $[C_{12}H_8I_2\ (M)]^+$: 405.8715, found: 405.8712.

The proposed mechanism for the generation of product **12**. (Ref: Angew. Chem. Int. Ed. 2002, 41, 4272-4274; Adv. Synth. Catal. 2007, 349, 2705-2713.)



4. Optimization of reaction conditions (Table S1)



2a, 0.2 mmol — **3a**

entry	aryne precursor (X equiv)	base (Y equiv)	temp (°C)	solvent	con.	time	yield (%)[a]
1	**1a**(2.0)	NaH(3.0)	rt(25)	THF	0.05 M	24 h	68
2	**1a1**(2.0)	NaH(3.0)	rt	THF	0.05 M	24 h	55
3	**1a2**(2.0)	NaH(3.0)	rt	THF	0.05 M	24 h	17
4	**1a3**(2.0)	NaH(3.0)	rt	THF	0.05 M	24 h	NR
5	**1a**(2.0)	NaH(3.0)	45	THF	0.05 M	12 h	78
6	**1a**(2.0)	NaH(3.0)	50	THF	0.05 M	12 h	92
7	**1a**(2.0)	NaH(3.0)	55	THF	0.05 M	12 h	90
8	**1a**(2.0)	NaH(3.0)	60	THF	0.05 M	12 h	85
9	**1a**(2.0)	KH(3.0)	50	THF	0.05 M	12 h	22
10	**1a**(2.0)	CaH_2(1.5)	50	THF	0.05 M	12 h	NR
11	**1a**(2.0)	LiH(3.0)	50	THF	0.05 M	12 h	NR
12	**1a**(2.0)	LDA(3.0)	0 - rt	THF	0.05 M	12 h	25[b]
13	**1a**(2.0)	BuLi(3.0)	0 - rt	THF	0.05 M	12 h	13[b]
14	**1a**(2.0)	*i*-PrMgCl(3.0)	0 - rt	THF	0.05 M	12 h	0[b]
15	**1a**(2.0)	LDA(3.0)	-78 - rt	THF	0.05 M	12 h	0[c]
16	**1a**(2.0)	BuLi(3.0)	-78 - rt	THF	0.05 M	12 h	0[c]
17	**1a**(2.0)	*i*-PrMgCl(3.0)	-78 - rt	THF	0.05 M	12 h	0[c]
18	**1a**(2.0)	NaH(3.0)	50	THF	0.05 M	6 h	92
19	**1a**(2.0)	NaH(3.0)	50	THF	0.05 M	4 h	92 (83)
20	**1a**(2.0)	NaH(3.0)	50	THF	0.05 M	3 h	88
21	**1a**(2.0)	NaH(3.0)	50	THF	0.05 M	2 h	85
22	**1a**(2.0)	NaH(3.0)	50	THF	0.05 M	1 h	83
23	**1a**(1.5)	NaH(2.5)	50	THF	0.05 M	4 h	80
24	**1a**(2.0)	NaH(3.0)	50	DMA	0.05 M	4 h	88
25	**1a**(2.0)	NaH(3.0)	50	DME	0.05 M	4 h	NR
26	**1a**(2.0)	NaH(3.0)	50	THF	0.1 M	4 h	87
27	**1a**(2.0)	NaH(3.0)	50	THF	0.02 M	4 h	97

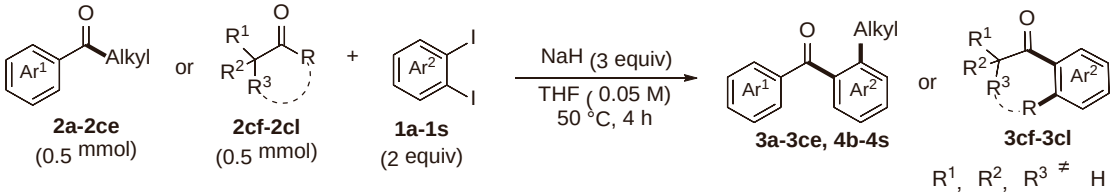
1a **1a1** **1a2** **1a3**

[a] NMR yield with mesitylene as internal standard, isolated yield from 0.5 mmol scale of **3a** in parentheses. [b] These reactions were performed at 0 °C for 1 h and warmed to rt for another 12 h. [c] These reactions were performed at -78 °C for 1 h and slowly warmed to rt for another 12 h. LDA= Lithium diisopropylamide, DMA = *N*,*N*-Dimethylacetamide, DME = 1,2-Dimethoxyethane.

General procedure for optimization of reaction conditions: To a solution of the indicated base in anhydrous solvent was added 4'-methylpropiophenone **2a** (0.2 mmol) and aryne precursor respectively at 0 °C stirring for 5 min. After that, the mixture was

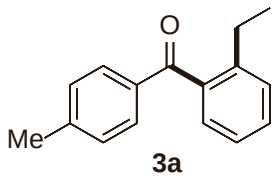
warmed to indicated temperature. After stirring for the indicated time, the reaction was quenched with saturated aqueous NH_4Cl (3 mL) solution at 0 °C. The mixture was then extracted with EtOAc (5 mL × 4). The combined extracts were dried over Na_2SO_4, concentrated under vacuum and prepared for NMR analysis with mesitylene as internal standard.

5. General procedure for the synthesis of *o*-alkylaryl ketones



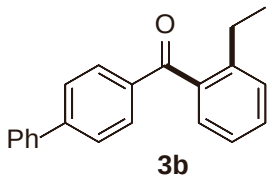
2a-2ce (0.5 mmol) **2cf-2cl** (0.5 mmol) **1a-1s** (2 equiv)

General procedure: To a suspension of NaH (60% dispersion in mineral oil, 60.5 mg, 1.5 mmol) in anhydrous THF (10 mL) was added ketone **2** (0.5 mmol) and *o*-diiodoarene **1** (2.0 equiv) respectively at 0 °C stirring for 5 min. The mixture was warmed to 50 °C for 4 h. After that, the reaction was quenched with saturated aqueous NH_4Cl (6 mL) solution at 0 °C. The mixture was then extracted with EtOAc (8 mL × 4). The combined extracts were dried over Na_2SO_4, concentrated under vacuum. The resulting residue was purified by silica gel chromatography affording *o*-alkylaryl ketone **3**.



3a

(2-ethylphenyl)(*p*-tolyl)methanone (3a):
Following the general procedure, the title compound was obtained as colorless oil, 93.2 mg, 83% yield.
Round 1: Following the general procedure, when **2a** (1.48 g, 10 mmol) and THF (100 mL) were used in this reaction, **3a** was obtained 1.78 g, 79% yield.
Round 2: Following the general procedure, when **2a** (1.48 g, 10 mmol) and THF (100 mL) were used in this reaction, **3a** was obtained 1.82 g, 81% yield.
Round 3: Following the general procedure, when **2a** (2.96 g, 20 mmol) and THF (200 mL) were used in this reaction, **3a** was obtained 3.68 g, 82% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67 – 7.60 (m, 2H), 7.36 – 7.30 (m, 1H), 7.27 – 7.23 (m, 1H), 7.19 – 7.13 (m, 4H), 2.58 (q, *J* = 7.5 Hz, 2H), 2.34 (s, 3H), 1.07 (t, *J* = 7.6 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.6, 144.3, 142. 9, 138.9, 135.4, 130.5, 130.2 129.4, 129.3, 128.2, 125.3, 26.5, 21.8, 16.0.
HRMS (EI-TOF): calculated for $[C_{16}H_{16}O (M)]^+$: 224.1201, found: 224.1199.

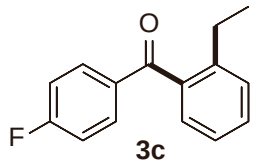


3b

[1,1'-biphenyl]-4-yl(2-ethylphenyl)methanone (3b):
Following the general procedure, the title compound was obtained as colorless oil, 109.1 mg, 76% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 – 7.75 (m, 2H), 7.59 – 7.49 (m, 4H), 7.39 – 7.23 (m, 5H), 7.22 – 7.12 (m, 2H), 2.60 (q, *J* = 7.5 Hz, 2H), 1.08 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.4, 146.0, 143.0, 134.0, 138.6, 136.6, 130.9, 130.3, 129.5, 129.1, 128.4, 128.3, 127.4, 127.2, 125.3, 26.5, 16.1.

HRMS (EI-TOF): calculated for $[C_{21}H_{18}O\ (M)]^+$: 286.1358, found: 286.1360.



3c

(2-ethylphenyl)(4-fluorophenyl)methanone (3c):

Following the general procedure, the title compound was obtained as colorless oil, 86.4 mg, 76% yield.

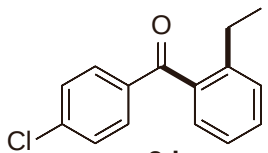
Following the general procedure, when **2c** (1.52 g, 10 mmol) and THF (50 mL) were used in this reaction, **3c** was obtained 1.48 g, 65% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 – 7.71 (m, 2H), 7.37 – 7.30 (m, 1H), 7.27 – 7.23 (m, 1H), 7.18 – 7.14 (m, 2H), 7.06 – 6.99 (m, 2H), 2.57 (q, *J* = 7.5 Hz, 2H), 1.07 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 197.2, 166.0 (d, *J* = 255.2 Hz), 143.0, 138.2, 134.3 (d, *J* = 2.9 Hz), 132.9 (d, *J* = 9.3 Hz), 130.5, 129.6, 128.2, 125.4, 115.7 (d, *J* = 21.9 Hz), 26.5, 16.0.

^{19}F NMR (377 MHz, $CDCl_3$): δ -104.77 – -104.89 (m).

HRMS (EI-TOF): calculated for $[C_{15}H_{13}FO\ (M)]^+$: 228.0950, found: 228.0947.



3d

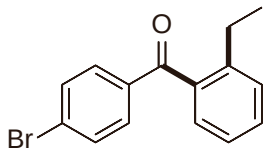
(4-chlorophenyl)(2-ethylphenyl)methanone (3d):

Following the general procedure, the title compound was obtained as colorless oil, 78.2 mg, 64% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 – 7.63 (m, 2H), 7.37 – 7.30 (m, 3H), 7.27 – 7.23 (m, 1H), 7.17 – 7.13 (m, 2H), 2.57 (q, *J* = 7.5 Hz, 2H), 1.06 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.5, 143.2, 139.8, 138.0, 136.3, 131.7, 130.6, 129.7, 128.9, 128.3, 125.4, 26.5, 16.1.

HRMS (EI-TOF): calculated for $[C_{15}H_{13}ClO\ (M)]^+$: 244.0655, found: 244.0650.



3e

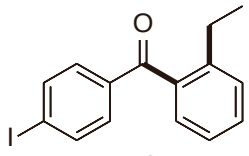
(4-bromophenyl)(2-ethylphenyl)methanone (3e):

Following the general procedure, the title compound was obtained as colorless oil, 82.6 mg, 57% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 – 7.55 (m, 2H), 7.53 – 7.46 (m, 2H), 7.37 – 7.31 (m, 1H), 7.27 – 7.23 (m, 1H), 7.17 – 7.13 (m, 2H), 2.57 (q, *J* = 7.5 Hz, 2H), 1.06 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.7, 143.2, 137.9, 136.7, 131.9, 131.7, 130.7, 129.7, 128.6, 128.3, 125.4, 26.5, 16.1.

HRMS (EI-TOF): calculated for $[C_{15}H_{13}BrO\ (M)]^+$: 288.0150, found: 288.0147.



3f

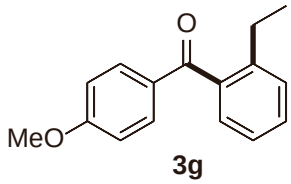
(2-ethylphenyl)(4-iodophenyl)methanone (3f):

Following the general procedure, the title compound was obtained as colorless oil, 108.8 mg, 65% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, *J* = 8.3 Hz, 2H), 7.42 (d, *J* = 8.3 Hz, 2H), 7.38 – 7.30 (m, 1H), 7.25 (d, *J* = 7.7 Hz, 1H), 7.18 – 7.14 (m, 2H), 2.57 (q, *J* = 7.5 Hz, 2H), 1.06 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.0, 143.2, 137.9, 137.8, 137.2, 131.6, 130.7, 129.7, 128.3, 125.4, 101.5, 26.5, 16.1.

HRMS (EI-TOF): calculated for $[C_{15}H_{13}IO\ (M)]^+$: 336.0011, found: 336.0014.



3g

(2-ethylphenyl)(4-methoxyphenyl)methanone (3g):

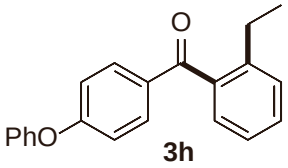
Following the general procedure, the title compound was obtained as colorless oil, 96.2 mg, 80% yield.

Following the general procedure, when **2g** (1.64 g, 10 mmol) and THF (50 mL) were used in this reaction, **3g** was obtained 1.73 g, 72% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 – 7.65 (m, 2H), 7.31 – 7.25 (m, 1H), 7.23 – 7.18 (m, 1H), 7.15 – 7.09 (m, 2H), 6.83 – 6.77 (m, 2H), 3.74 (s, 3H), 2.53 (q, *J* = 7.6 Hz, 2H), 1.03 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.5, 163.8, 142.6, 139.0, 132.6, 130.7, 129.9, 129.3, 127.8, 125.2, 113.7, 55.6, 26.4, 16.0.

HRMS (EI-TOF): calculated for $[C_{16}H_{16}O_2\ (M)]^+$: 240.1150, found: 240.1148.



3h

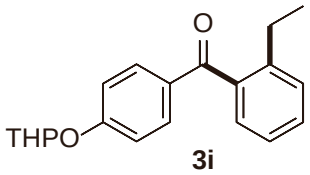
(2-ethylphenyl)(4-phenoxyphenyl)methanone (3h):

Following the general procedure, the title compound was obtained as colorless oil, 115.3 mg, 76% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 – 7.63 (m, 2H), 7.31 – 7.23 (m, 3H), 7.22 – 7.18 (m, 1H), 7.16 – 7.03 (m, 3H), 7.00 – 6.92 (m, 2H), 6.89 – 6.82 (m, 2H), 2.54 (q, *J* = 7.5 Hz, 2H), 1.04 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.4, 162.3, 155.4, 142.8, 138.7, 132.6, 132.3, 130.2, 130.1, 129.4, 128.0, 125.2, 124.8, 120.4, 117.2, 26.5, 16.0.

HRMS (EI-TOF): calculated for $[C_{21}H_{18}O_2\ (M)]^+$: 302.1307, found: 302.1302.



3i

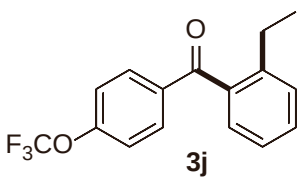
(2-ethylphenyl)(4-((tetrahydro-2*H*-pyran-2-yl)oxy)phenyl)methanone (3i):

Following the general procedure, the title compound was obtained as colorless oil, 92.4 mg, 62% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 – 7.68 (m, 2H), 7.36 – 7.30 (m, 1H), 7.25 (d, *J* = 7.6 Hz, 1H), 7.21 – 7.13 (m, 2H), 7.03 – 6.98 (m, 2H), 5.45 (t, *J* = 3.1 Hz, 1H), 3.84 – 3.73 (m, 1H), 3.61 – 3.48 (m, 1H), 2.58 (q, *J* = 7.5 Hz, 2H), 2.00 – 1.87 (m, 1H), 1.85 – 1.76 (m, 2H), 1.69 – 1.58 (m, 2H), 1.57 – 1.49 (m, 1H), 1.08 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.6, 161.4, 142.6, 139.0, 132.5, 131.3, 130.0, 129.3, 127.9, 125.2, 115.9, 96.1, 62.2, 30.2, 26.4, 25.1, 18.6, 16.0.

HRMS (EI-TOF): calculated for $[C_{20}H_{22}O_3\ (M)]^+$: 310.1569, found: 310.1575.



3j

(2-ethylphenyl)(4-(trifluoromethoxy)phenyl)methanone (3j):

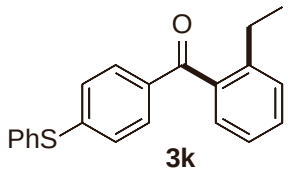
Following the general procedure, the title compound was obtained as colorless oil, 97.3 mg, 66% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 – 7.73 (m, 2H), 7.36 – 7.31 (m, 1H), 7.25 (d, *J* = 7.7 Hz, 1H), 7.20 – 7.12 (m, 4H), 2.57 (q, *J* = 7.5 Hz, 2H), 1.07 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.1, 152.8, 143.3, 137.9, 136.2, 132.3, 130.7, 129.7, 128.4, 125.3, 120.4 (q, *J* = 259.1 Hz), 120.3, 26.5, 16.0.

^{19}F NMR (565 MHz, $CDCl_3$): δ -57.61.

HRMS (EI-TOF): calculated for $[C_{16}H_{13}F_3O_2\ (M)]^+$: 294.0868, found: 294.0865.



3k

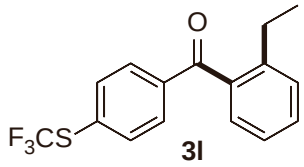
(2-ethylphenyl)(4-(phenylthio)phenyl)methanone (3k):

Following the general procedure, the title compound was obtained as colorless oil, 118.5 mg, 72% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 – 7.65 (m, 2H), 7.55 – 7.49 (m, 2H), 7.45 – 7.36 (m, 4H), 7.32 (d, *J* = 7.8 Hz, 1H), 7.26 – 7.21 (m, 2H), 7.21 – 7.16 (m, 2H), 2.66 (q, *J* = 7.5 Hz, 2H), 1.16 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.8, 145.6, 142.9, 138.4, 135.0, 134.3, 131.8, 130.8, 130.3, 129.8, 129.5, 129.0, 128.1, 127.0, 125.2, 26.5, 16.0.

HRMS (EI-TOF): calculated for $[C_{21}H_{18}OS\ (M)]^+$: 318.1078, found: 318.1081.



3l

(2-ethylphenyl)(4-((trifluoromethyl)thio)phenyl)methanone (3l):

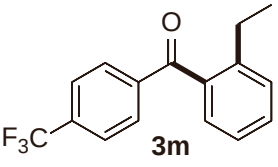
Following the general procedure, the title compound was obtained as colorless oil, 108.7 mg, 70% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 – 7.69 (m, 2H), 7.66 – 7.57 (m, 2H), 7.38 – 7.30 (m, 1H), 7.28 – 7.22 (m, 1H), 7.18 – 7.12 (m, 2H), 2.58 (q, *J* = 7.5 Hz, 2H), 1.06 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.6, 143.6, 139.6, 137.5, 135.6, 131.0, 130.12, 129.8, 129.4 (q, *J* = 308.8 Hz), 128.6, 125.4, 26.6, 16.1. One aromatic carbon peak is overlapped.

^{19}F NMR (565 MHz, $CDCl_3$): δ -41.65.

HRMS (EI-TOF): calculated for $[C_{16}H_{13}F_3OS\ (M)]^+$: 310.0639, found: 310.0644.



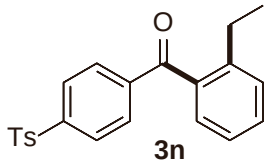
3m

(2-ethylphenyl)(4-(trifluoromethyl)phenyl)methanone (3m):

Following the general procedure, the title compound was obtained as colorless oil, 81.2 mg, 58% yield.

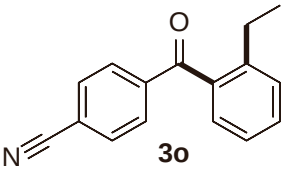
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 – 7.76 (m, 2H), 7.63 – 7.57 (m, 2H), 7.38 – 7.30 (m, 1H), 7.28 – 7.22 (m, 1H), 7.17 – 7.12 (m, 2H), 2.57 (q, *J* = 7.5 Hz, 2H), 1.05 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.6, 143.7, 140.9, 137.5, 134.5 (q, *J* = 32.2 Hz), 131.1, 130.5, 129.9, 128.7, 125.7 – 125.6 (m), 125.5, 123.8 (q, *J* = 272.4 Hz), 26.6, 16.1.
^{19}F NMR (565 MHz, $CDCl_3$): δ -63.07.



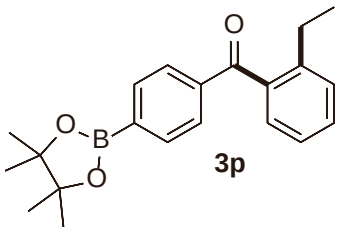
3n

HRMS (EI-TOF): calculated for $[C_{16}H_{13}F_3O\ (M)]^+$: 278.0918, found: 278.0915.**(2-ethylphenyl)(4-tosylphenyl)methanone (3n):**
Following the general procedure, the title compound was obtained as light-yellow oil, 64.1 mg, 35% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 – 7.98 m, 2H), 7.92 – 7.83 (m, 4H), 7.49 – 7.42 (m, 1H), 7.38 – 7.30 (m, 3H), 7.28 – 7.18 (m, 2H), 2.67 (q, *J* = 7.5 Hz, 2H), 2.41 (s, 3H), 1.15 (t, *J* = 7.5 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 197.2, 145.8, 144.9, 143.8, 141.5, 137.8, 137.1, 131.2, 130.8, 130.2, 129.9, 128.8, 128.0, 127.6, 125.4, 26.5, 21.7, 16.1.
HRMS (EI-TOF): calculated for $[C_{22}H_{20}O_3\ (M)]^+$: 364.1133, found: 364.1129.



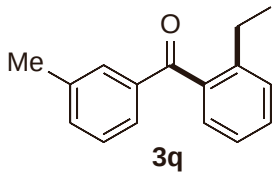
3o

4-(2-ethylbenzoyl)benzonitrile (3o):
Following the general procedure, the title compound was obtained as colorless oil, 53.4 mg, 45% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 – 7.84 (m, 2H), 7.80 – 7.71 (m, 2H), 7.50 – 7.44 (m, 1H), 7.41 – 7.33 (m, 1H), 7.30 – 7.22 (m, 2H), 2.68 (q, *J* = 7.5 Hz, 2H), 1.16 (t, *J* = 7.5 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 197.1, 143.8, 141.3, 137.0 132.4, 131.3, 130.5, 130.0, 128.7, 125.5, 118.1, 116.4, 26.6, 16.1.
HRMS (EI-TOF): calculated for $[C_{16}H_{13}NO\ (M)]^+$: 235.0997, found: 235.0994.



3p

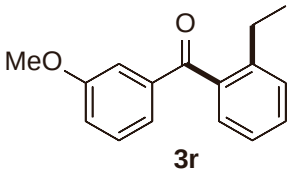
(2-ethylphenyl)(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanone (3p):
Following the general procedure, the title compound was obtained as colorless oil, 72.4 mg, 43% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 – 7.78 (m, 2H), 7.72 – 7.67 (m, 2H), 7.37 – 7.31 (m, 1H), 7.27 – 7.23 (m, 1H), 7.19 – 7.13 (m, 2H), 2.58 (q, *J* = 7.5 Hz, 2H), 1.27 (s, 12H), 1.06 (t, *J* = 7.5 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 199.1, 143.3, 139.9, 138.4, 134.8, 130.5, 129.6, 129.2, 128.5, 125.3, 84.3, 26.6, 25.0, 16.0. One aromatic carbon peak is overlapped.
HRMS (EI-TOF): calculated for $[C_{21}H_{25}BO_3\ (M + Na)]^+$:336.1897, found: 336.1894.



3q

(2-ethylphenyl)(*m*-tolyl)methanone (3q):
Following the general procedure, the title compound was obtained as colorless oil, 76.2 mg, 68% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (s, 1H), 7.48 – 7.43 (m, 1H), 7.33 – 7.25 (m, 2H), 7.23 – 7.17 (m, 2H), 7.17 – 7.09 (m, 2H), 2.56 (q, *J* = 7.5 Hz, 2H), 2.27 (s, 3H), 1.05 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.0, 143.0, 138.7, 138.4, 137.9, 134.1, 130.5, 130.3, 129.5, 128.4, 128.3, 127.7, 125.2, 26.5, 21.4, 16.0.



3r

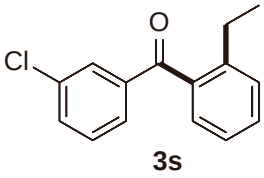
HRMS (EI-TOF): calculated for $[C_{16}H_{16}O\ (M)]^+$: 224.1201, found: 224.1204.**(2-ethylphenyl)(3-methoxyphenyl)methanone (3r):**

Following the general procedure, the title compound was obtained as colorless oil, 86.5 mg, 72% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 – 7.30 (m, 2H), 7.27 – 7.12 (m, 5H), 7.06 – 7.01 (m, 1H), 3.75 (s, 3H), 2.59 (q, *J* = 7.5 Hz, 2H), 1.08 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.6, 159.8, 143.0, 139.2, 138.4, 130.3, 129.5, 129.4, 128.3, 125.2, 123.5, 119.9, 113.8, 55.5, 26.5, 16.0.

HRMS (EI-TOF): calculated for $[C_{16}H_{16}O\ (M)]^+$: 240.1150, found: 240.1147.



3s

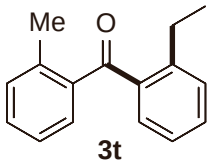
(3-chlorophenyl)(2-ethylphenyl)methanone (3s):

Following the general procedure, the title compound was obtained as colorless oil, 55.2 mg, 45% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (t, *J* = 1.6 Hz, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.46 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.39 – 7.34 (m, 1H), 7.33 – 7.25 (m, 2H), 7.18 (d, *J* = 4.1 Hz, 2H), 2.59 (q, *J* = 7.5 Hz, 2H), 1.09 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 197.3, 143.4, 139.6, 137.7, 134.9, 133.2, 130.8, 130.1, 129.9, 129.7, 128.5, 128.4, 125.4, 26.5, 16.1.

HRMS (EI-TOF): calculated for $[C_{15}H_{13}ClO\ (M)]^+$: 244.0655, found: 244.0652.



3t

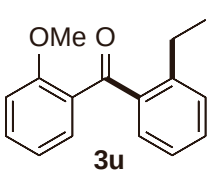
(2-ethylphenyl)(*o*-tolyl)methanone (3t):

Following the general procedure, the title compound was obtained as colorless oil, 61.9 mg, 55% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43 – 7.34 (m, 2H), 7.33 – 7.23 (m, 4H), 7.20 – 7.14 (m, 2H), 2.79 (q, *J* = 7.5 Hz, 2H), 2.48 (s, 3H), 1.20 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 200.9, 144.3, 139.1, 138.8, 138.7, 131.6, 131.4, 131.1, 131.0, 130.1, 129.9, 125.5, 125.4, 26.7, 21.0, 16.03.

The ^{1}H NMR and ^{13}C NMR of **3t** are consistent with the reported spectra[S42].



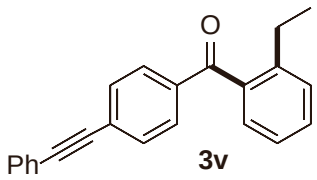
3u

(2-ethylphenyl)(2-methoxyphenyl)methanone (3u):

Following the general procedure, the title compound was obtained as colorless oil, 70.2 mg, 58% yield.

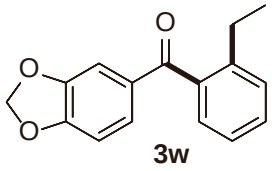
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 – 7.32 (m, 2H), 7.29 – 7.23 (m, 1H), 7.21 – 7.14 (m, 2H), 7.07 – 7.00 (m, 1H), 6.91 – 6.82 (m, 2H), 3.56 (s, 3H), 2.75 (q, *J* = 7.5 Hz, 2H), 1.11 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.5, 158.5, 144.0, 139.5, 133.1, 131.1, 130.8, 129.7, 129.7, 129.5, 125.2, 120.4, 111.9, 55.7, 26.7, 16.0.



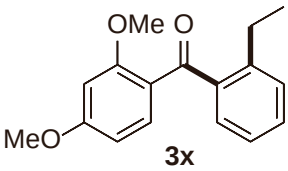
3v

HRMS (EI-TOF): calculated for $[C_{16}H_{16}O_2\ (M)]^+$: 240.1150, found: 240.1145. **(2-ethylphenyl)(4-(phenylethynyl)phenyl)methanone (3v):**
Following the general procedure, the title compound was obtained as light-yellow oil, 78.8 mg, 51% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, *J* = 8.2 Hz, 2H), 7.49 (d, *J* = 8.2 Hz, 2H), 7.47 – 7.42 (m, 2H), 7.36 – 7.30 (m, 1H), 7.28 – 7.22 (m, 4H), 7.19 – 7.12 (m, 2H), 2.57 (q, *J* = 7.5 Hz, 2H), 1.07 (t, *J* = 7.5 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.0, 143.1, 138.2, 137.0, 131.9, 131.7, 130.5, 130.2, 129.6, 128.9, 128.6, 128.4, 128.3, 125.3, 122.7, 93.0, 88.8, 26.5, 16.0.
HRMS (EI-TOF): calculated for $[C_{23}H_{18}O\ (M)]^+$: 310.1358, found: 310.1360.



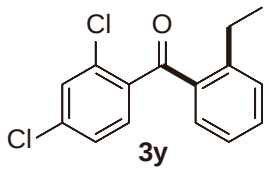
3w

benzo[*d*][1,3]dioxol-5-yl(2-ethylphenyl)methanone (3w):
Following the general procedure, the title compound was obtained as colorless oil, 91.5 mg, 72% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31 – 7.25 (m, 2H), 7.22 – 7.16 (m, 2H), 7.11 (d, *J* = 4.1 Hz, 2H), 6.68 (d, *J* = 8.1 Hz, 1H), 5.93 (s, 2H), 2.52 (q, *J* = 7.5 Hz, 2H), 1.03 (t, *J* = 7.6 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 197.1, 152.2, 148.2, 142.6, 138.8, 132.6, 130.0, 129.3, 127.8, 127.5, 125.2, 109.3, 107.8, 102.0, 26.4, 15.9.
HRMS (EI-TOF): calculated for $[C_{16}H_{14}O_2\ (M)]^+$: 254.0943, found: 254.0947.



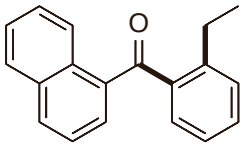
3x

(2,4-dimethoxyphenyl)(2-ethylphenyl)methanone (3x):
Following the general procedure, the title compound was obtained as colorless oil, 94.7 mg, 70% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 (d, *J* = 8.5 Hz, 1H), 7.28 – 7.21 (m, 1H), 7.19 – 7.15 (m, 1H), 7.12 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.09 – 7.02 (m, 1H), 6.42 – 6.34 (m, 2H), 3.75 (s, 3H), 3.58 (s, 3H), 2.65 (q, *J* = 7.5 Hz, 2H), 1.09 (t, *J* = 7.5 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 197.2, 164.4, 161.2, 142.8, 140.9, 134.3, 129.9, 129.3, 128.4, 125.1, 121.8, 104.7, 98.9, 55.7, 55.6, 26.4, 15.9.
HRMS (EI-TOF): calculated for $[C_{17}H_{18}O_3\ (M)]^+$: 270.1256, found: 270.1251.



3y

(2,4-dichlorophenyl)(2-ethylphenyl)methanone (3y):
Following the general procedure, the title compound was obtained as white solid, 56.2 mg, 40% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41 – 7.34 (m, 2H), 7.33 – 7.22 (m, 3H), 7.20 – 7.17 (m, 1H), 7.14 – 7.08 (m, 1H), 2.85 (q, *J* = 7.5 Hz, 2H), 1.18 (t, *J* = 7.5 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 196.3, 145.7, 137.9, 137.3, 136.7, 133.3, 132.4, 131.5, 131.1, 130.6, 130.5, 127.2, 125.7, 27.0, 15.9.



3z

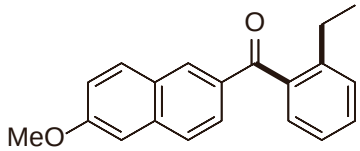
HRMS (EI-TOF): calculated for $[C_{15}H_{12}Cl_2O\ (M)]^+$: 278.0265, found: 278.0262.**(2-ethylphenyl)(naphthalen-1-yl)methanone (3z):**

Following the general procedure, the title compound was obtained as colorless oil, 81.2 mg, 62% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.69 (d, *J* = 8.5 Hz, 1H), 8.02 (d, *J* = 8.2 Hz, 1H), 7.96 – 7.90 (m, 1H), 7.66 – 7.54 (m, 3H), 7.49 – 7.41 (m, 2H), 7.40 – 7.32 (m, 2H), 7.25 – 7.19 (m, 1H), 2.85 (q, *J* = 7.5 Hz, 2H), 1.25 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 200.5, 144.4, 139.7, 136.3, 134.0, 132.9, 131.2, 131.14, 131.08, 130.2, 129.9, 128.6, 128.1, 126.6, 126.0, 125.4, 124.3, 26.8, 16.1.

HRMS (EI-TOF): calculated for $[C_{19}H_{16}O\ (M)]^+$: 260.1201, found: 260.1203.



3aa

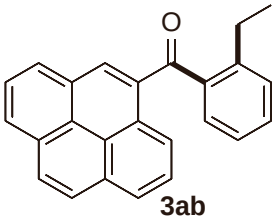
(2-ethylphenyl)(6-methoxynaphthalen-2-yl)methanone (3aa):

Following the general procedure, the title compound was obtained as colorless oil, 113.2 mg, 78% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (s, 1H), 7.88 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.69 – 7.60 (m, 2H), 7.36 – 7.30 (m, 1H), 7.28 – 7.18 (m, 2H), 7.18 – 7.12 (m, 1H), 7.08 – 7.02 (m, 2H), 3.81 (s, 3H), 2.58 (q, *J* = 7.5 Hz, 2H), 1.06 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.6, 160.0, 142.9, 138.9, 137.5, 133.2, 132.8, 131.3, 130.2, 129.5, 128.2, 127.8, 127.2, 125.9, 125.3, 119.8, 105.9, 55.5, 26.5, 16.0.

HRMS (EI-TOF): calculated for $[C_{20}H_{18}O_2\ (M)]^+$: 290.1307, found: 290.1305.



3ab

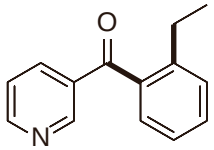
(2-ethylphenyl)(pyren-4-yl)methanone (3ab):

Following the general procedure, the title compound was obtained as yellow solid, 88.7 mg, 53% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.92 (d, *J* = 9.3 Hz, 1H), 8.30 – 8.15 (m, 4H), 8.12 – 8.01 (m, 4H), 7.51 – 7.46 (m, 1H), 7.45 – 7.34 (m, 2H), 7.25 – 7.20 (m, 1H), 2.87 (q, *J* = 7.5 Hz, 2H), 1.27 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 201.0, 144.4, 140.2, 134.0, 133.0, 131.22, 131.20, 130.7, 130.5, 130.4, 130.0, 129.8, 129.7, 129.2, 127.3, 126.54, 126.46, 126.3, 125.5, 125.1, 125.0, 124.5, 123.9, 26.9, 16.2.

HRMS (EI-TOF): calculated for $[C_{25}H_{18}O\ (M)]^+$: 334.1358, found: 334.1356.



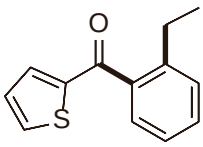
3ac

(2-ethylphenyl)(pyridin-3-yl)methanone (3ac):

Following the general procedure, the title compound was obtained as yellow oil, 27.6 mg, 26% yield.

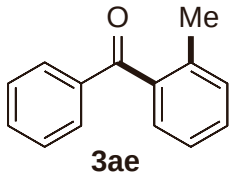
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76 (d, *J* = 2.0 Hz, 1H), 8.61 (dd, *J* = 4.8, 1.7 Hz, 1H), 7.98 – 7.93 (m, 1H), 7.31 – 7.22 (m, 2H), 7.19 (d, *J* = 7.7 Hz, 1H), 7.11 – 7.06 (m, 2H), 2.52 (q, *J* = 7.5 Hz, 2H), 0.99 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 197.2, 153.5, 151.7, 143.7, 137.2, 137.2, 133.4, 131.2, 130.0, 128.7, 125.5, 123.6, 26.6, 16.1.
HRMS (EI-TOF): calculated for $[C_{14}H_{13}NO\ (M)]^+$: 211.0997, found: 211.0993.



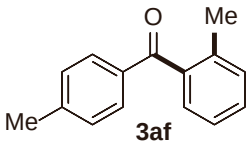
3ad

(2-ethylphenyl)(thiophen-2-yl)methanone (3ad):
Following the general procedure, the title compound was obtained as colorless oil, 43.6 mg, 40% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63 (dd, *J* = 4.9, 0.8 Hz, 1H), 7.37 – 7.30 (m, 3H), 7.25 (d, *J* = 7.5 Hz, 1H), 7.20 – 7.14 (m, 1H), 7.02 (dd, *J* = 4.7, 4.0 Hz, 1H), 2.64 (q, *J* = 7.5 Hz, 2H), 1.10 (t, *J* = 7.5 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 190.7, 145.3, 142.9, 138.3, 135.6, 135.0, 130.5, 129.6, 128.2, 128.1, 125.2, 26.4, 16.1.
HRMS (EI-TOF): calculated for $[C_{13}H_{12}OS\ (M)]^+$: 216.0609, found: 216.0605.



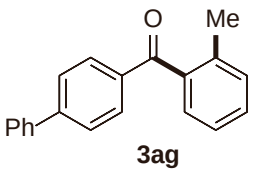
3ae

phenyl(*o*-tolyl)methanone (3ae):
Following the general procedure, the title compound was obtained as colorless oil, 52.2 mg, 53% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 – 7.78 (m, 2H), 7.61 – 7.55 (m, 1H), 7.48 – 7.43 (m, 2H), 7.42 – 7.37 (m, 1H), 7.34 – 7.28 (m, 2H), 7.27 – 7.22 (m, 1H), 2.34 (s, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 198.7, 138.7, 137.8, 136.8, 133.2, 131.1, 130.3, 130.2, 128.6, 128.5, 125.3, 20.1.
The ^{1}H NMR and ^{13}C NMR of **3ae** are consistent with the reported spectra[S43].



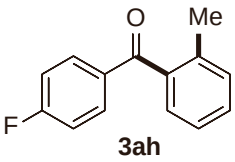
3af

***o*-tolyl(*p*-tolyl)methanone (3af):**
Following the general procedure, the title compound was obtained as colorless oil, 63.2 mg, 60% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (d, *J* = 8.2 Hz, 2H), 7.31 – 7.25 (m, 1H), 7.22 – 7.12 (m, 5H), 2.32 (s, 3H), 2.22 (s, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 198.5, 144.2, 139.1, 136.5, 135.2, 131.0, 130.4, 130.1, 129.3, 128.3, 125.3, 21.8, 20.0.
The ^{1}H NMR and ^{13}C NMR of **3af** are consistent with the reported spectra[S44].



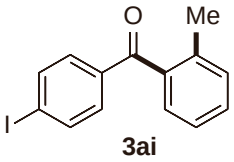
3ag

[1,1'-biphenyl]-4-yl(*o*-tolyl)methanone (3ag):
Following the general procedure, the title compound was obtained as colorless oil, 81.5 mg, 60% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 – 7.86 (m, 2H), 7.70 – 7.66 (m, 2H), 7.66 – 7.62 (m, 2H), 7.51 – 7.45 (m, 2H), 7.44 – 7.38 (m, 2H), 7.38 – 7.34 (m, 1H), 7.33 – 7.27 (m, 2H), 2.37 (s, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 198.4, 146.0, 140.0, 138.9, 136.8, 136.5, 131.2, 130.9, 130.4, 129.1, 128.6, 128.4, 127.5, 127.3, 125.4, 20.12.
The ^{1}H NMR and ^{13}C NMR of **3ag** are consistent with the reported spectra[S45].



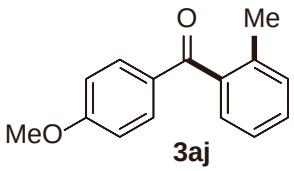
3ah

(4-fluorophenyl)(*o*-tolyl)methanone (3ah):
Following the general procedure, the title compound was obtained as colorless oil, 57.8 mg, 54% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.90 – 7.77 (m, 2H), 7.43 – 7.36 (m, 1H), 7.32 – 7.22 (m, 3H), 7.15 – 7.09 (m, 2H), 2.32 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 197.2, 165.95 (d, *J* = 255.5 Hz), 138.5, 136.7, 134.2 (d, *J* = 2.9 Hz), 132.9 (d, *J* = 9.4 Hz), 131.2, 130.5, 128.4, 125.4, 115.8 (d, *J* = 22.0 Hz), 20.0.
^{19}F NMR (565 MHz, $CDCl_3$): δ -104.86 – -104.99 (m).
The ^{1}H NMR, ^{13}C NMR and ^{19}F NMR of **3ah** are consistent with the reported spectra[S46].



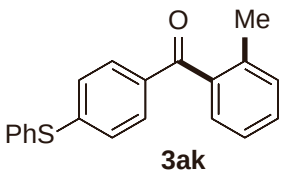
3ai

(4-iodophenyl)(*o*-tolyl)methanone (3ai):
Following the general procedure, the title compound was obtained as colorless oil, 54.7 mg, 34% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 – 7.77 (m, 2H), 7.54 – 7.47 (m, 2H), 7.43 – 7.36 (m, 1H), 7.31 – 7.21 (m, 3H), 2.33 (s, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 197.9, 138.0, 137.9, 137.2, 137.0, 131.6, 131.3, 130.6, 128.6, 125.4, 101.4, 20.1.
HRMS (EI-TOF): calculated for $[C_{14}H_{11}IO\ (M)]^+$: 321.9855, found: 321.9859.



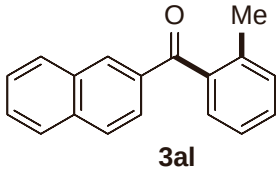
3aj

(4-methoxyphenyl)(*o*-tolyl)methanone (3aj):
Following the general procedure, the title compound was obtained as colorless oil, 58.2 mg, 51% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 – 7.67 (m, 2H), 7.31 – 7.25 (m, 1H), 7.22 – 7.12 (m, 3H), 6.87 – 6.82 (m, 2H), 3.78 (s, 3H), 2.22 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 197.5, 163.8, 139.3, 136.2, 132.6, 130.9, 130.6, 129.9, 128.0, 125.3, 113.8, 55.6, 19.9.
The ^{1}H NMR and ^{13}C NMR of **3aj** are consistent with the reported spectra[S47].



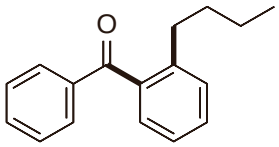
3ak

(4-(phenylthio)phenyl)(*o*-tolyl)methanone (3ak):
Following the general procedure, the title compound was obtained as colorless oil, 92.7 mg, 61% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 – 7.64 (m, 2H), 7.57 – 7.48 (m, 2H), 7.44 – 7.33 (m, 4H), 7.29 – 7.22 (m, 3H), 7.21 – 7.17 (m, 2H), 2.31 (s, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 197.7, 145.5, 138.7, 136.6, 135.0, 134.2, 131.9, 131.1, 130.8, 130.2, 129.8, 129.0, 128.3, 127.2, 125.3, 20.0.
HRMS (EI-TOF): calculated for $[C_{20}H_{16}OS\ (M)]^+$: 304.0922, found: 304.0919.



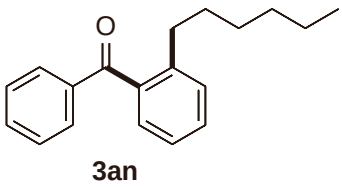
3al

naphthalen-2-yl(*o*-tolyl)methanone (3al):
Following the general procedure, the title compound was obtained as colorless oil, 51.8 mg, 42% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.20 (s, 1H), 8.03 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.96 – 7.85 (m, 3H), 7.64 – 7.58 (m, 1H), 7.56 – 7.51 (m, 1H), 7.47 – 7.37 (m, 2H), 7.37 – 7.27 (m, 2H), 2.38 (s, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 198.7, 139.0, 136.9, 135.7, 135.2, 132.8, 132.5, 131.1, 130.3, 129.7, 128.7, 128.63, 128.58, 127.9, 126.9, 125.4, 125.2, 20.1.
The ^{1}H NMR and ^{13}C NMR of **3al** are consistent with the reported spectra[S48].



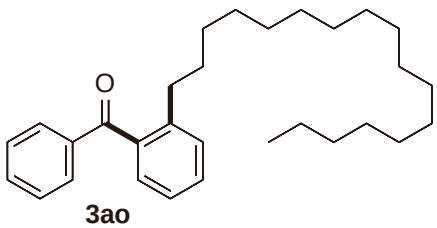
3am

(2-butylphenyl)(phenyl)methanone (3am):
Following the general procedure, the title compound was obtained as colorless oil, 99.1 mg, 83% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 – 7.64 (m, 2H), 7.47 – 7.41 (m, 1H), 7.35 – 7.25 (m, 3H), 7.21 – 7.17 (m, 1H), 7.16 – 7.08 (m, 2H), 2.53 (t, *J* = 7.8 Hz, 2H), 1.45 – 1.35 (m, 2H), 1.19 – 1.08 (m, 2H), 0.70 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.9, 141.8, 138.6, 138.0, 133.2, 130.22, 130.20, 128.5, 125.2, 33.9, 33.1, 22.6, 13.9. Two aromatic carbon peaks are overlapped.
HRMS (EI-TOF): calculated for $[C_{17}H_{18}O\ (M)]^+$: 238.1358, found: 238.1354.



3an

(2-hexylphenyl)(phenyl)methanone (3an):
Following the general procedure, the title compound was obtained as colorless oil, 101.4 mg, 76% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 – 7.66 (m, 2H), 7.47 – 7.41 (m, 1H), 7.35 – 7.24 (m, 3H), 7.21 – 7.17 (m, 1H), 7.16 – 7.07 (m, 2H), 2.56 – 2.48 (m, 2H), 1.46 – 1.35 (m, 2H), 1.16 – 1.03 (m, 6H), 0.69 (t, *J* = 6.6 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): 198.8, 141.9, 138.6, 138.0, 133.2, 130.23, 130.19, 128.47, 128.45, 125.2, 33.4, 31.7, 31.6, 29.2, 22.6, 14.1. One aromatic carbon peak is overlapped.
The ^{1}H NMR and ^{13}C NMR of **3an** are consistent with the reported spectra[S49].

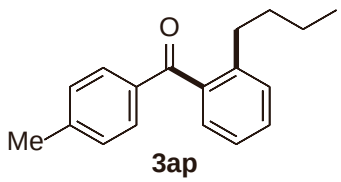


3ao

(2-heptadecylphenyl)(phenyl)methanone (3ao):
Following the general procedure, the title compound was obtained as colorless oil, 149.2 mg, 71% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 – 7.74 (m, 2H), 7.61 – 7.54 (m, 1H), 7.49 – 7.38 (m, 3H), 7.32 (d, *J* = 7.5 Hz, 1H), 7.29 – 7.21 (m, 2H), 2.64 (t, *J* = 7.8 Hz, 2H), 1.57 – 1.48 (m, 2H), 1.33 – 1.17 (m, 28H), 0.88 (t, *J* = 6.8 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.9, 142.0, 138.7, 138.1, 133.3, 130.3, 130.2, 128.52, 128.50, 125.2, 33.4, 32.1, 31.8, 29.84, 29.81, 29.79, 29.76, 29.64, 29.59, 29.51,

29.46, 22.8, 14.3. One aromatic carbon peak and four aliphatic carbon peaks are overlapped.

HRMS (ESI-TOF): calculated for $[C_{30}H_{45}O\ (M + H)]^+$: 421.3470, found: 421.3471.



3ap

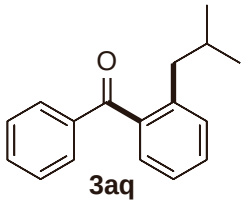
(2-butylphenyl)(*p*-tolyl)methanone (3ap):

Following the general procedure, the title compound was obtained as colorless oil, 111.3 mg, 88% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 – 7.60 (m, 2H), 7.36 – 7.31 (m, 1H), 7.27 – 7.23 (m, 1H), 7.22 – 7.14 (m, 4H), 2.61 – 2.55 (m, 2H), 2.36 (s, 3H), 1.51 – 1.39 (m, 2H), 1.25 – 1.14 (m, 2H), 0.76 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.6, 144.2, 141.7, 139.0, 135.5, 130.4, 130.1, 130.0, 129.2, 128.3, 125.2, 33.9, 33.1, 22.6, 21.8, 13.9.

HRMS (EI-TOF): calculated for $[C_{18}H_{20}O\ (M)]^+$: 252.1514, found: 252.1516.



3aq

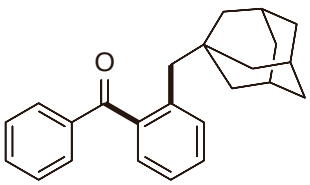
(2-isobutylphenyl)(phenyl)methanone (3aq):

Following the general procedure, the title compound was obtained as colorless oil, 108.6 mg, 91% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 – 7.64 (m, 2H), 7.45 (t, *J* = 7.4 Hz, 1H), 7.35 – 7.25 (m, 3H), 7.18 – 7.09 (m, 3H), 2.45 (d, *J* = 7.3 Hz, 2H), 1.73 – 1.61 (m, 1H), 0.69 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.9, 140.8, 138.9, 138.0, 133.2, 131.0, 130.2, 130.0, 128.7, 128.5, 125.3, 42.4, 30.3, 22.5.

The ^{1}H NMR and ^{13}C NMR of **3aq** are consistent with the reported spectra[S50].



3ar

(2-(((3*r*,5*r*,7*r*)-adamantan-1-yl)methyl)phenyl)(phenyl) methanone (3ar):

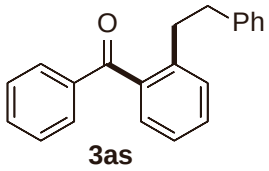
Following the general procedure, the title compound was obtained as colorless oil, 94.2 mg, 57% yield.

Following the general procedure, when *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained 104.3 mg, 63% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 – 7.78 (m, 2H), 7.59 – 7.54 (m, 1H), 7.47 – 7.37 (m, 3H), 7.34 – 7.30 (m, 1H), 7.29 – 7.21 (m, 2H), 2.57 (s, 2H), 1.87 – 1.80 (m, 3H), 1.61 – 1.55 (m, 3H), 1.51 – 1.45 (m, 3H), 1.39 – 1.35 (m, 6H).

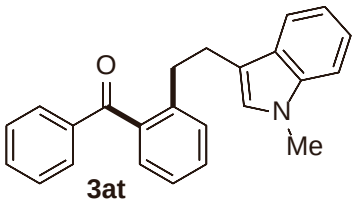
^{13}C NMR (151 MHz, $CDCl_3$): δ 199.2, 139.9, 138.2, 137.5, 133.1, 132.9, 130.4, 129.5, 129.0, 128.5, 125.5, 46.9, 42.7, 36.9, 34.6, 28.8.

HRMS (ESI-TOF): calculated for $[C_{24}H_{27}O\ (M + H)]^+$: 331.2062, found: 331.2063.



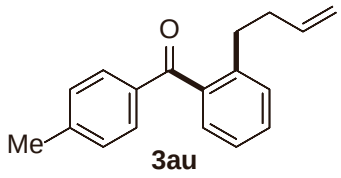
3as

(2-phenethylphenyl)(phenyl)methanone (3as):
Following the general procedure, the title compound was obtained as colorless oil, 103.3 mg, 72% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (d, *J* = 8.0 Hz, 2H), 7.65 – 7.59 (m, 1H), 7.53 – 7.43 (m, 3H), 7.38 – 7.22 (m, 5H), 7.21 – 7.10 (m, 3H), 3.04 (dd, *J* = 9.8, 6.0 Hz, 2H), 2.92 (dd, *J* = 10.1, 5.9 Hz, 2H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 198.6, 141.6, 140.9, 138.6, 138.0, 133.3, 130.5, 130.4, 130.3, 128.8, 128.54, 128.51, 128.4, 126.0, 125.5, 38.2, 35.6.
The ^{1}H NMR and ^{13}C NMR of **3as** are consistent with the reported spectra[S51].



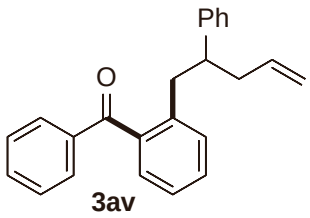
3at

(2-(2-(1-methyl-1*H*-indol-3-yl)ethyl)phenyl)(phenyl)methan one (3at):
Following the general procedure, the title compound was obtained as colorless oil, 111.7 mg, 66% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 – 7.72 (m, 2H), 7.59 – 7.53 (m, 1H), 7.48 – 7.38 (m, 5H), 7.31 – 7.24 (m, 2H), 7.23 – 7.16 (m, 2H), 7.08 – 7.03 (m, 1H), 6.71 (s, 1H), 3.60 (s, 3H), 3.13 – 3.07 (m, 2H), 3.06 – 3.00 (m, 2H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 198.6, 141.4, 138.7, 137.8, 136.9, 133.2, 130.5 130.30, 130.25, 128.6, 128.4, 127.8, 126.4, 125.4, 121.4, 119.0, 118.6, 114.3, 109.1, 34.5, 32.5, 27.6.
HRMS (ESI-TOF): calculated for $[C_{24}H_{22}NO\ (M + H)]^+$: 340.1701, found: 340.1703.



3au

(2-(but-3-en-1-yl)phenyl)(*p*-tolyl)methanone (3au):
Following the general procedure, the title compound was obtained as colorless oil, 92.8 mg, 74% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 – 7.56 (m, 2H), 7.31 – 7.25 (m, 1H), 7.21 – 7.17 (m, 1H), 7.16 – 7.09 (m, 4H), 5.68 – 5.56 (m, 1H), 4.85 – 4.74 (m, 2H), 2.63 (dd, *J* = 8.8, 6.9 Hz, 2H), 2.30 (s, 3H), 2.22 – 2.14 (m, 2H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 198.4, 144.2, 140.7, 138.9, 137.9, 135.4, 130.5, 130.3, 130.1, 129.2, 128.5, 125.4, 115.1, 35.7, 32.8, 21.8.
HRMS (EI-TOF): calculated for $[C_{18}H_{18}O\ (M)]^+$: 250.1358, found: 250.1360.



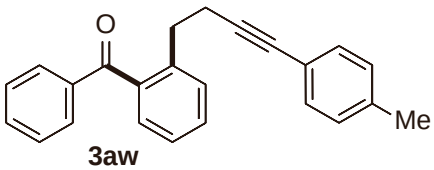
3av

phenyl(2-(2-phenylpent-4-en-1-yl)phenyl)methanone (3av):
Following the general procedure, the title compound was obtained as colorless oil, 167.1 mg, 90% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (d, *J* = 7.5 Hz, 1H), 7.64 (d, *J* = 7.5 Hz, 1H), 7.54 – 7.44 (m, 1H), 7.40 – 7.33 (m, 2H), 7.32 – 6.98 (m, 7H), 6.93 (d, *J* = 7.2 Hz, 1H), 5.71 – 5.59 (m, 0.48H), 5.57 – 5.45 (m, 0.52H), 5.01 – 4.89 (m, 1H), 4.88 – 4.78 (m, 1H), 3.50 – 3.41 (m, 0.48H), 3.32 –

3.19 (m, 1H), 3.12 – 3.04 (m, 0.52H), 2.98 – 2.91 (m, 0.48H), 2.89 – 2.81 (m, 0.52H), 2.49 – 2.37 (m, 1H), 2.31 (t, *J* = 7.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 199.0, 198.6, 144.4, 144.0, 139.78, 138.75, 137.9, 137.3, 136.7, 136.3, 133.1, 133.0, 131.2, 130.3, 129.9, 128.8, 128.6, 128.5, 128.4, 128.2, 128.1, 127.8, 127.6, 126.4, 126.2, 125.2, 116.9, 116.2, 47.7, 44.6, 40.79, 40.76, 40.4, 39.8.

HRMS (EI-TOF): calculated for $[C_{24}H_{22}O\ (M)]^+$: 326.1671, found: 326.1673.



3aw

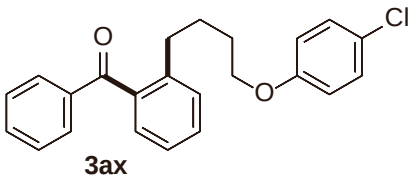
phenyl(2-(4-(*p*-tolyl)but-3-yn-1-yl)phenyl)methanone (3aw):

Following the general procedure, the title compound was obtained as colorless oil, 118.6 mg, 73% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (d, *J* = 7.5 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.51 – 7.41 (m, 4H), 7.35 – 7.28 (m, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 3.03 (t, *J* = 7.4 Hz, 2H), 2.72 (t, *J* = 7.4 Hz, 2H), 2.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.4, 139.9, 138.5, 137.8, 137.6, 133.3, 131.4, 130.9, 130.4, 129.0, 128.9, 128.5, 125.8, 120.8, 88.6, 81.7, 32.6, 21.7, 21.5. One aromatic carbon peak is overlapped.

HRMS (ESI-TOF): calculated for $[C_{24}H_{20}ONa\ (M + Na)]^+$: 347.1412, found: 347.1411.



3ax

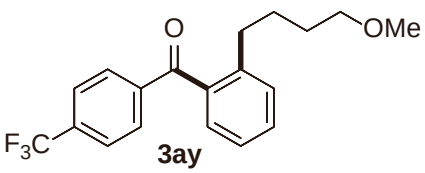
(2-(4-(4-chlorophenoxy)butyl)phenyl)(phenyl)methanone (3ax):

Following the general procedure, the title compound was obtained as colorless oil, 129.7 mg, 71% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 – 7.76 (m, 2H), 7.61 – 7.55 (m, 1H), 7.48 – 7.40 (m, 3H), 7.35 (d, *J* = 7.3 Hz, 1H), 7.32 – 7.24 (m, 2H), 7.22 – 7.14 (m, 2H), 6.77 – 6.70 (m, 2H), 3.84 (t, *J* = 5.9 Hz, 2H), 2.74 (t, *J* = 7.2 Hz, 2H), 1.79 – 1.69 (m, 4H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.7, 157.7, 141.2, 138.6, 137.9, 133.3, 130.4, 130.3, 130.2, 129.3, 128.7, 128.5, 125.5, 125.3, 115.8, 67.9, 33.0, 29.0, 28.1.

HRMS (EI-TOF): calculated for $[C_{23}H_{21}ClO_2\ (M)]^+$: 364.1230, found: 364.1233.



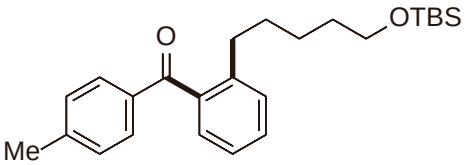
3ay

(2-(4-methoxybutyl)phenyl)(4-(trifluoromethyl)phenyl) methanone (3ay):

Following the general procedure, the title compound was obtained as white solid, 104.6 mg, 62% yield.

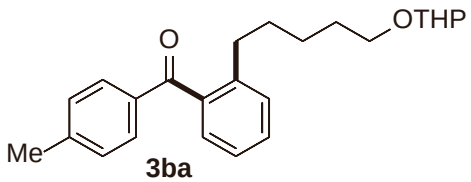
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, *J* = 8.1 Hz, 2H), 7.63 (d, *J* = 8.2 Hz, 2H), 7.38 – 7.32 (m, 1H), 7.27 (d, *J* = 7.6 Hz, 1H), 7.19 – 7.15 (m, 2H), 3.21 (t, *J* = 6.3 Hz, 2H), 3.16 (s, 3H), 2.62 (t, *J* = 7.7 Hz, 2H), 1.58 – 1.49 (m, 2H), 1.49 – 1.41 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.5, 142.1, 140.9, 137.6, 134.4 (q, *J* = 32.6 Hz), 131.0, 130.6, 130.5, 128.9, 125.7 – 125.5 (m), 125.50, 123.7 (q, *J* = 273.1 Hz), 72.5, 58.6, 33.2, 29.5, 28.4.
^{19}F NMR (376 MHz, $CDCl_3$): δ -63.06.
HRMS (EI-TOF): calculated for $[C_{19}H_{19}F_3O_2$ (M)$]^+$: 336.1337, found: 336.1333.



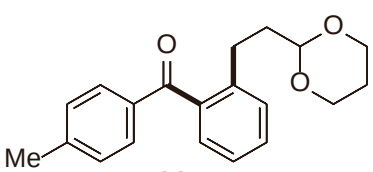
3az

(2-(5-((*tert*-butyldimethylsilyl)oxy)pentyl)phenyl)(*p*-tolyl)methanone (3az):
Following the general procedure, the title compound was obtained as colorless oil, 127.4 mg, 64% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.42 – 7.37 (m, 1H), 7.30 (d, *J* = 7.5 Hz, 1H), 7.27 – 7.20 (m, 4H), 3.52 (t, *J* = 6.6 Hz, 2H), 2.67 – 2.61 (m, 2H), 2.42 (s, 3H), 1.58 – 1.49 (m, 2H), 1.48 – 1.40 (m, 2H), 1.31 – 1.23 (m, 2H), 0.87 (s, 9H), 0.01 (s, 6H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 198.6, 144.2, 141.5, 139.0, 135.5, 130.5, 130.2, 130.0, 129.3, 128.3, 125.2, 63.2, 33.4, 32.7, 31.6, 26.1, 25.8, 21.8, 18.5, -5.2.
HRMS (EI-TOF): calculated for $[C_{25}H_{36}O_2Si$ (M)$]^+$: 396.2485, found: 396.2490.



3ba

(2-(5-((tetrahydro-2*H*-pyran-2-yl)oxy)pentyl)phenyl)(*p*-tolyl)methanone (3ba):
Following the general procedure, the title compound was obtained as colorless oil, 115.7 mg, 63% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, *J* = 8.2 Hz, 2H), 7.41 – 7.35 (m, 1H), 7.30 (d, *J* = 7.5 Hz, 1H), 7.26 – 7.19 (m, 4H), 4.51 (t, *J* = 3.5 Hz, 1H), 3.85 – 3.78 (m, 1H), 3.69 – 3.61 (m, 1H), 3.49 – 3.42 (m, 1H), 3.33 – 3.26 (m, 1H), 2.68 – 2.61 (m, 2H), 2.41 (s, 3H), 1.84 – 1.74 (m, 1H), 1.71 – 1.62 (m, 1H), 1.60 – 1.47 (m, 8H), 1.36 – 1.27 (m, 2H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 198.5, 144.2, 141.4, 138.9, 135.4, 130.4, 130.1, 130.0, 129.2, 128.3, 125.2, 98.9, 67.5, 62.4, 33.3, 31.6, 30.8, 29.5, 26.2, 25.6, 21.8, 19.7.
HRMS (EI-TOF): calculated for $[C_{24}H_{30}O_3$ (M)$]^+$: 366.2195, found: 366.2197.

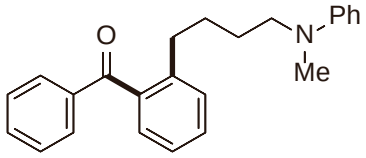


3bb

(2-(2-(1,3-dioxan-2-yl)ethyl)phenyl)(*p*-tolyl)methanone (3bb):
Following the general procedure, the title compound was obtained as colorless oil, 124.5 mg, 66% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (d, *J* = 8.2 Hz, 2H), 7.36 – 7.29 (m, 1H), 7.25 (d, *J* = 7.5 Hz, 1H), 7.21 – 7.12 (m, 4H), 4.33 (t, *J* = 5.3 Hz, 1H), 3.94 (dd, *J* = 10.9, 4.9 Hz, 2H), 3.64 – 3.54 (m, 2H), 2.74 – 2.62 (m, 2H), 2.33 (s, 3H), 2.01 – 1.86 (m, 1H), 1.82 – 1.72 (m, 2H), 1.19 (d, *J* = 13.1 Hz, 1H).

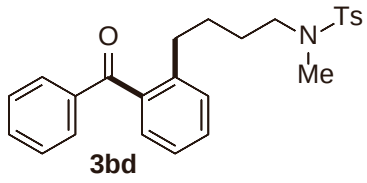
^{13}C NMR (151 MHz, $CDCl_3$): δ 198.2, 144.1, 140.7, 139.0, 135.4, 130.5, 130.22, 130.19, 129.2, 128.5, 125.4, 101.5, 66.8, 36.8, 27.7, 25.9, 21.8.
HRMS (EI-TOF): calculated for $[C_{20}H_{22}O_3$ (M)$]^+$: 310.1569, found: 310.1567.

(2-(4-(methyl(phenyl)amino)butyl)phenyl)(phenyl)methanone (3bc):



3bc

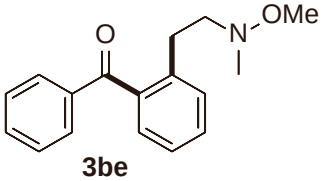
Following the general procedure, the title compound was obtained as colorless oil, 90.7 mg, 53% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 – 7.79 (m, 2H), 7.63 – 7.58 (m, 1H), 7.49 – 7.41 (m, 3H), 7.35 – 7.26 (m, 3H), 7.25 – 7.18 (m, 2H), 6.71 – 6.63 (m, 3H), 3.28 – 3.22 (m, 2H), 2.86 (s, 3H), 2.74 – 2.69 (m, 2H), 1.65 – 1.51 (m, 4H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.8, 149.3, 141.4, 138.5, 137.9, 133.3, 130.4, 130.28, 130.26, 129.2, 128.7 128.6, 125.4, 115.9, 112.2, 52.5, 38.3, 33.3, 29.3, 26.7
HRMS (EI-TOF): calculated for $[C_{24}H_{25}NO$ (M)$]^+$: 343.1936, found: 343.1939.



3bd

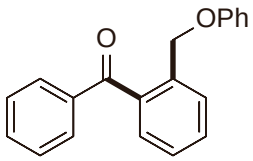
***N*-(4-(2-benzoylphenyl)butyl)-*N*,4-dimethylbenzenesulfon amide (3bd):**
Following the general procedure, the title compound was obtained as colorless oil, 130.6 mg, 62% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 – 7.75 (m, 2H), 7.63 – 7.55 (m, 3H), 7.47 – 7.39 (m, 3H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.29 – 7.22 (m, 4H), 2.90 (t, *J* = 7.1 Hz, 2H), 2.66 (t, *J* = 7.8 Hz, 2H), 2.61 (s, 3H), 2.40 (s, 3H), 1.64 – 1.54 (m, 2H), 1.51 – 1.42 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.7, 143.2, 141.1, 138.5, 137.9, 134.5, 133.3, 130.4, 130.3, 130.2, 129.7, 128.6, 128.5, 127.4, 125.4, 49.8, 34.6, 32.7, 28.5, 27.3, 21.6.
HRMS (ESI-TOF): calculated for $[C_{25}H_{27}NO_3SNa$ (M + Na)$]^+$: 444.1609, found: 444.1611.

(2-(2-(methoxy(methyl)amino)ethyl)phenyl)(phenyl)methanone (3be):



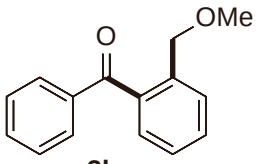
3be

Following the general procedure, the title compound was obtained as colorless oil, 82.2 mg, 61% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 – 7.76 (m, 2H), 7.61 – 7. 54 (m, 1H), 7.48 – 7.36 (m, 4H), 7.31 – 7.24 (m, 2H), 3.44 (s, 3H), 2.96 – 2.89 (m, 2H), 2.87 – 2.80 (m, 2H), 2.50 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.5, 139.2, 138.9, 137.9, 133.3, 130.8, 130.37, 130.35, 128.7, 128.5, 125.6, 62.1, 60.0, 45.0, 31.3.
HRMS (ESI-TOF): calculated for $[C_{17}H_{19}NO_2Na$ (M + Na)$]^+$: 292.1313, found: 292.1316.



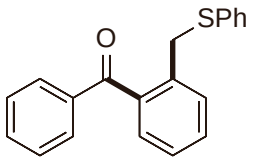
3bf

(2-(phenoxymethyl)phenyl)(phenyl)methanone (3bf):
Following the general procedure, the title compound was obtained as colorless oil, 57.9 mg, 40% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, *J* = 7.4 Hz, 2H), 7.73 (d, *J* = 7.7 Hz, 1H), 7.64 – 7.51 (m, 2H), 7.51 – 7.36 (m, 4H), 7.22 (t, *J* = 7.9 Hz, 2H), 6.92 (t, *J* = 7.3 Hz, 1H), 6.81 (d, *J* = 8.2 Hz, 2H), 5.23 (s, 2H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 197.9, 158.5, 137.7, 137.5, 137.2, 133.3, 130.9, 130.3, 129.5, 129.3, 128.50, 128.48, 127.2, 121.1, 114.8, 67.6.
HRMS (EI-TOF): calculated for $[C_{20}H_{16}O_2$ (M)$]^+$: 288.1150, found: 288.1146.



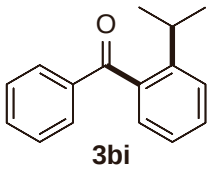
3bg

(2-(methoxymethyl)phenyl)(phenyl)methanone (3bg):
Following the general procedure, the title compound was obtained as colorless oil, 47.7 mg, 42% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, *J* = 7.7 Hz, 2H), 7.61 – 7.54 (m, 2H), 7.53 – 7.43 (m, 3H), 7.39 – 7.33 (m, 2H), 4.54 (s, 2H), 3.25 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.0, 138.1, 137.8, 133.1, 130.6, 130.1, 129.0, 128.5, 128.4, 127.1, 72.3, 58.5. One aromatic carbon peak is overlapped.
The ^{1}H NMR and ^{13}C NMR of **3bg** are consistent with the reported spectra[S52].



3bh

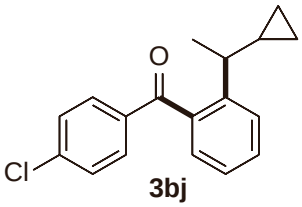
phenyl(2-((phenylthio)methyl)phenyl)methanone (3bh):
Following the general procedure, the title compound was obtained as colorless oil, 38.4 mg, 25% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 – 7.64 (m, 2H), 7.50 – 7.43 (m, 1H), 7.36 – 7.31 (m, 2H), 7.31 – 7.24 (m, 2H), 7.22 – 7.13 (m, 2H), 7.12 – 6.98 (m, 5H), 4.19 (s, 2H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 198.0, 138.4, 137.8, 137.7, 135.9, 133.2, 130.9, 130.5, 130.44, 130.42, 129.6, 128.9, 128.4, 126.64, 126.58, 36.5.
The ^{1}H NMR and ^{13}C NMR of **3bh** are consistent with the reported spectra[S53].



3bi

(2-isopropylphenyl)(phenyl)methanone (3bi):
Following the general procedure, the title compound was obtained as colorless oil, 79.8 mg, 71% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 – 7.81 (m, 2H), 7.62 – 7.57 (m, 1H), 7.51 – 7.43 (m, 4H), 7.29 – 7.21 (m, 2H), 3.13 – 3.00 (m, 1H), 1.22 (s, 3H), 1.20 (s, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 199.2, 147.3, 138.5, 137.9, 133.4, 130.3, 128.6, 127.6, 126.1, 125.3, 30.4, 24.2. One aromatic carbon peak is overlapped.
The ^{1}H NMR and ^{13}C NMR of **3bi** are consistent with the reported spectra[S54].

(4-chlorophenyl)(2-(1-cyclopropylethyl)phenyl)methanone (3bj):

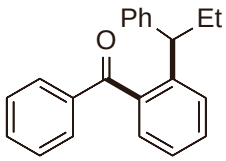


3bj

Following the general procedure, the title compound was obtained as colorless oil, 91.4 mg, 64% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 – 7.72 (m, 2H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.51 – 7.46 (m, 1H), 7.45 – 7.39 (m, 2H), 7.28 – 7.22 (m, 1H), 7.19 (dd, *J* = 7.6, 1.2 Hz, 1H), 2.19 – 2.10 (m, 1H), 1.26 (d, *J* = 6.9 Hz, 3H), 1.03 – 0.93 (m, 1H), 0.55 – 0.46 (m, 1H), 0.36 – 0.26 (m, 1H), 0.14 – 0.06 (td, *J* = 9.5, 4.8 Hz, 1H), 0.00 – -0.07 (m, 1H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 197.8, 146.6, 140.0, 138.0, 136.4, 131.7, 130.5, 128.9, 127.6, 127.4, 125.3, 40.8, 22.3, 18.5, 5.1, 4.4.



3bk

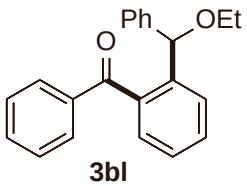
HRMS (EI-TOF): calculated for $[C_{18}H_{17}ClO\ (M)]^+$: 284.0968, found: 284.0964. **phenyl(2-(1-phenylpropyl)phenyl)methanone (3bk):**

Following the general procedure, the title compound was obtained as colorless oil, 58.4 mg, 39% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 – 7.67 (m, 2H), 7.58 – 7.52 (m, 1H), 7.51 – 7.42 (m, 2H), 7.42– 7.36 (m, 2H), 7.27 – 7.21 (m, 2H), 7.20 – 7.13 (m, 4H), 7.11 – 7.05 (m, 1H), 4.18 (t, *J* = 7.7 Hz, 1H), 2.15 – 2.01 (m, 2H), 0.85 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.1, 144.3, 144.1, 139.5, 138.0, 133.3, 130.33, 130.27, 128.4, 128.3, 128.1, 127.8, 126.1, 125.3, 48.1, 29.0, 12.8. One aromatic carbon peak is overlapped.

HRMS (EI-TOF): calculated for $[C_{22}H_{20}O\ (M)]^+$: 300.1514, found: 300.1511.



3bl

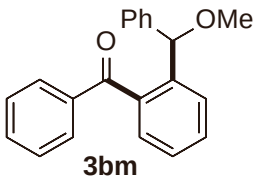
(2-(ethoxy(phenyl)methyl)phenyl)(phenyl)methanone (3bl):

Following the general procedure, the title compound was obtained as colorless oil, 57.2 mg, 36% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 – 7.68 (m, 2H), 7.51 – 7.45 (m, 1H), 7.37 – 7.28 (m, 3H), 7.27 – 7.17 (m, 7H), 7.17 – 7.12 (m, 1H), 5.61 (s, 1H), 3.31 – 3.22 (m, 1H), 3.21 – 3.12 (m, 1H), 0.84 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.3, 141.9, 141.1, 138.8, 137.8, 133.2, 130.3, 130.0, 128.4, 128.4, 127.9, 127.83, 127.75, 127.6, 126.7, 79.7, 64.9, 15.0.

HRMS (EI-TOF): calculated for $[C_{22}H_{20}O_2\ (M)]^+$: 316.1463, found: 316.1466.



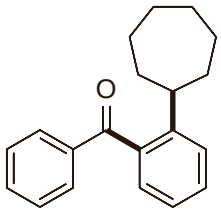
3bm

(2-(methoxy(phenyl)methyl)phenyl)(phenyl)methanone (3bm):

Following the general procedure, the title compound was obtained as colorless oil, 42.5 mg, 28% yield.

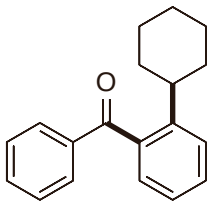
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67 – 7.62 (m, 2H), 7.47 – 7.41 (m, 1H), 7.33 – 7.23 (m, 4H), 7.22 – 7.12 (m, 6H), 7.12 – 7.06 (m, 1H), 5.46 (s, 1H), 3.04 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.3, 141.5, 140.8, 138.6, 137.8, 133.2, 130.21, 130.16, 128.4, 128.4, 128.1, 127.8, 127.7, 127.5, 126.8, 81.4, 57.0.
HRMS (EI-TOF): calculated for $[C_{21}H_{18}O_2$ (M)$]^+$: 302.1307, found: 302.1305.



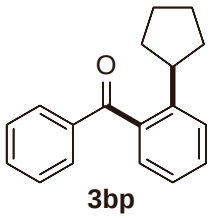
3bn

(2-cycloheptylphenyl)(phenyl)methanone (3bn):
Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 97.7 mg, 70% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 – 7.77 (m, 2H), 7.61 – 7.55 (m, 1H), 7.48 – 7.38 (m, 4H), 7.24 – 7.19 (m, 2H), 2.82 – 2.73 (m, 1H), 1.90 – 1.81 (m, 2H), 1.72 – 1.60 (m, 4H), 1.58 – 1.46 (m, 4H), 1.37 – 1.26 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 199.3, 148.5, 138.2, 137.7, 133.3, 130.4, 130.2, 128.5, 127.7, 127.0, 125.0, 42.6, 36.8, 27.8, 27.4.
HRMS (EI-TOF): calculated for $[C_{20}H_{22}O$ (M)$]^+$: 278.1671, found: 278.1673.



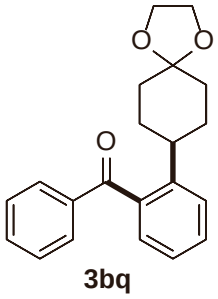
3bo

(2-cyclohexylphenyl)(phenyl)methanone (3bo):
Following the general procedure, the title compound was obtained as colorless oil, 45.8 mg, 36% yield.
Following the general procedure, when *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained 79.2 mg, 60% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 – 7.78 (m, 2H), 7.61 – 7.55 (m, 1H), 7.48 – 7.40 (m, 4H), 7.26 – 7.19 (m, 2H), 2.71 – 2.61 (m, 1H), 1.84 – 1.64 (m, 5H), 1.49 – 1.37 (m, 2H), 1.27 – 1.13 (m, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 199.2, 146.5, 138.6, 138.2, 133.4 130.3, 130.2, 128.5, 127.9, 126.9, 125.2, 40.8, 34.5, 26.8, 26.2.
HRMS (EI-TOF): calculated for $[C_{19}H_{20}O$ (M)$]^+$: 264.1514, found: 264.1511.



3bp

(2-cyclopentylphenyl)(phenyl)methanone (3bp):
Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 77.9 mg, 62% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 – 7.62 (m, 2H), 7.45 – 7.38 (m, 1H), 7.34 – 7.25 (m, 4H), 7.11 – 7.04 (m, 2H), 2.97 – 2.85 (m, 1H), 1.86 – 1.72 (m, 2H), 1.65 – 1.55 (m, 2H), 1.51 – 1.33 (m, 4H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 199.3, 145.2, 139.3, 137.9, 133.4, 130.3, 130.2, 128.5, 127.5, 126.7, 125.2, 42.4, 35.4, 25.9.
HRMS (EI-TOF): calculated for $[C_{18}H_{18}O$ (M)$]^+$: 250.1358, found: 250.1360.



3bq

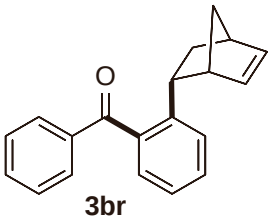
(2-(1,4-dioxaspiro[4.5]decan-8-yl)phenyl)(phenyl)methanone (3bq):

Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 101.7 mg, 63% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 – 7.73 (m, 2H), 7.61 – 7.54 (m, 1H), 7.53 – 7.37 (m, 4H), 7.27 – 7.20 (m, 2H), 4.01 – 3.85 (m, 4H), 2.80 – 2.65 (m, 1H), 1.87 – 1.70 (m, 6H), 1.56 – 1.42 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 199.0, 145.2, 138.6, 138.0, 133.4, 130.3, 130.2, 128.6, 128.1, 126.8, 125.4, 108.4, 64.34, 64.33, 39.4, 35.0, 31.6.

HRMS (EI-TOF): calculated for $[C_{21}H_{22}O_3$ (M)$]^+$: 322.1569, found: 322.1567.



3br

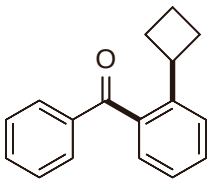
(2-((1*R*,4*R*)-bicyclo[2.2.1]hept-5-en-2-yl)phenyl)(phenyl)methanone (3br):

Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 99.2 mg, 72% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 – 7.83 (m, 2H), 7.62 – 7.56 (m, 1H), 7.49 – 7.44 (m, 2H), 7.36 – 7.30 (m, 1H), 7.23 – 7.16 (m, 3H), 6.29 (dd, *J* = 5.6, 3.1 Hz, 1H), 5.84 (dd, *J* = 5.6, 2.8 Hz, 1H), 3.53 – 3.48 (m, 1H), 3.01 (s, 1H), 2.88 (s, 1H), 2.10 – 2.02 (m, 1H), 1.43 – 1.38 (m, 1H), 1.33 – 1.29 (m, 1H), 1.28 – 1.22 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 199.5, 143.5, 139.9, 137.9, 137.4, 133.5, 133.0, 130.4, 129.3, 128.6, 127.8, 127.4, 125.1, 50.7, 49.0, 43.4, 40.3, 34.0.

HRMS (EI-TOF): calculated for $[C_{20}H_{18}O$ (M)$]^+$: 274.1358, found: 274.1361.



3bs

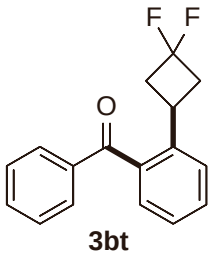
(2-cyclobutylphenyl)(phenyl)methanone (3bs):

Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 83.1 mg, 70% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 – 7.76 (m, 2H), 7.61 – 7.55 (m, 1H), 7.50 – 7.41 (m, 4H), 7.26 – 7.21 (m, 2H), 3.76 – 3.63 (m, 1H), 2.20 – 2.03 (m, 4H), 1.93 – 1.81 (m, 1H), 1.78 – 1.69 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): 199.0, 144.8, 138.0, 137.7, 133.3, 130.3, 130.2, 128.5, 127.9, 126.8, 125.3, 38.1, 29.9, 18.3.

HRMS (EI-TOF): calculated for $[C_{17}H_{16}O$ (M)$]^+$: 236.1201, found: 236.1203.



3bt

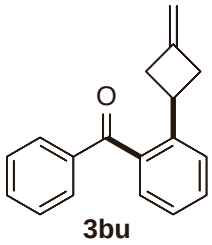
(2-(3,3-difluorocyclobutyl)phenyl)(phenyl)methanone (3bt):
Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 85.6 mg, 63% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 – 7.75 (m, 2H), 7.64 – 7.57 (m, 1H), 7.56 – 7.42 (m, 4H), 7.36 – 7.29 (m, 2H), 3.65 – 3.52 (m, 1H), 2.94 – 2.78 (m, 2H), 2.70 – 2.53 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.3, 141.9, 138.5, 137.5, 133.7, 130.9, 130.3, 128.8, 128.7, 126.5, 126.2, δ 119.5 (dd, *J* = 283.8, 271.0 Hz), 42.8 – 41.9 (m), 25.9 (d, *J* = 4.4 Hz), 25.8 (d, *J* = 4.1 Hz).

^{19}F NMR (376 MHz, $CDCl_3$): δ -82.08 – -82.20 (m), -82.56 – -82.75 (m), -98.99 – -99.23 (m), -99.50 – -99.74 (m).

HRMS (EI-TOF): calculated for $[C_{17}H_{14}F_2O\ (M)]^+$: 272.1013, found: 272.1009.



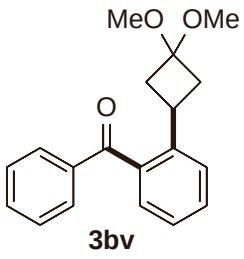
3bu

(2-(3-methylenecyclobutyl)phenyl)(phenyl)methanone (3bu):
Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 79.4 mg, 64% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 – 7.77 (m, 2H), 7.61 – 7.56 (m, 1H), 7.54 – 7.43 (m, 4H), 7.30 – 7.26 (m, 2H), 4.78 – 4.73 (m, 2H), 3.73 – 3.62 (m, 1H), 2.97 – 2.88 (m, 2H), 2.85 – 2.76 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.8, 145.5, 144.2, 138.4, 137.7, 133.4, 130.5, 130.2, 128.6, 128.1, 126.6, 125.6, 105.8, 39.7, 32.7.

HRMS (EI-TOF): calculated for $[C_{18}H_{16}O\ (M)]^+$: 248.1201, found: 248.1205.



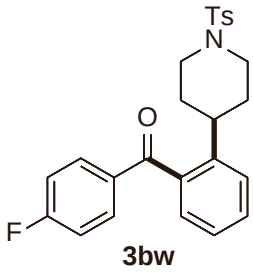
3bv

(2-(3,3-dimethoxycyclobutyl)phenyl)(phenyl)methanone (3bv):
Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 110.3 mg, 74% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 – 7.77 (m, 2H), 7.60 – 7.55 (m, 1H), 7.50 – 7.42 (m, 4H), 7.27 – 7.25 (m, 2H), 3.49 – 3.39 (m, 1H), 3.13 (s, 3H), 3.12 (s, 3H), 2.56 – 2.46 (m, 2H), 2.20 – 2.11 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.7, 143.8, 138.5, 137.6, 133.4, 130.5, 130.2, 128.5, 128.1, 126.8, 125.6, 99.8, 48.8, 48.4, 39.5, 27.8.

HRMS (EI-TOF): calculated for $[C_{19}H_{20}O_3\ (M)]^+$: 296.1412, found: 296.1414.



3bw

(4-fluorophenyl)(2-(1-tosylpiperidin-4-yl)phenyl)methanone (3bw):

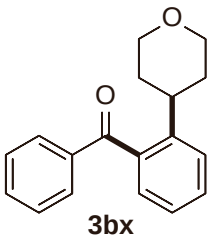
Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as light-yellow oil, 111.8 mg, 51% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 – 7.71 (m, 2H), 7.61 (d, *J* = 8.2 Hz, 2H), 7.51 – 7.44 (m, 1H), 7.40 (d, *J* = 7.6 Hz, 1H), 7.31 – 7.24 (m, 3H), 7.20 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.13 – 7.06 (m, 2H), 3.89 – 3.81 (m, 2H), 2.70 – 2.59 (m, 1H), 2.42 (s, 3H), 2.23 – 2.13 (m, 2H), 1.93 – 1.80 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 197.0, 166.0 (d, *J* = 256.1 Hz), 143.9 (d, *J* = 40.9 Hz), 137.8, 134.2 (d, *J* = 2.8 Hz), 133.1, 133.0, 132.9, 130.9, 129.7, 128.5, 127.8, 127.0, 125.8, 115.8 (d, *J* = 21.9 Hz), 46.9, 37.9, 32.7, 21.6.

^{19}F NMR (376 MHz, $CDCl_3$): δ -104.02 – -104.18 (m).

HRMS (EI-TOF): calculated for $[C_{25}H_{24}FNO_3S\ (M)]^+$: 437.1461, found: 437.1458.



3bx

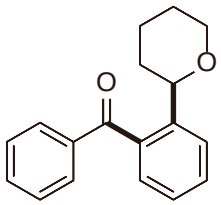
phenyl(2-(tetrahydro-2*H*-pyran-4-yl)phenyl)methanone (3bx):

Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 85.3 mg, 64% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65 – 7.56 (m, 2H), 7.41 – 7.35 (m, 1H), 7.29 – 7.22 (m, 4H), 7.07 – 7.03 (m, 2H), 3.80 – 3.72 (m, 2H), 3.19 – 3.10 (m, 2H), 2.81 – 2.72 (m, 1H), 1.69 – 1.57 (m, 2H), 1.52 – 1.44 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.8, 144.6, 138.5, 137.9, 133.5, 130.6, 130.3, 128.6, 128.3, 127.0, 125.6, 68.4, 37.9, 34.0.

HRMS (EI-TOF): calculated for $[C_{18}H_{18}O_2\ (M)]^+$: 266.1307, found: 266.1310.



3by

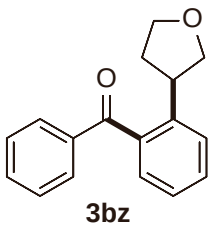
phenyl(2-(tetrahydro-2*H*-pyran-2-yl)phenyl)methanone (3by):

Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 53.6 mg, 40% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 – 7.78 (m, 2H), 7.68 – 7.63 (m, 1H), 7.60 – 7.54 m, 1H), 7.53 – 7.48 (m, 1H), 7.47 – 7.42 (m, 2H), 7.34 – 7.27 (m, 2H), 4.53 – 4.46 (m, 1H), 3.98 – 3.89 (m, 1H), 3.38 – 3.30 (m, 1H), 2.02 – 1.94 (m, 1H), 1.90 – 1.81 (m, 1H), 1.65 – 1.52 (m, 3H), 1.52 – 1.45 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.2, 142.7, 137.9, 137.1, 133.1, 130.6, 130.3, 128.43, 128.39, 126.60, 126.55, 68.9, 33.7, 25.8, 23.9. One aliphatic carbon peak is overlapped.

HRMS (EI-TOF): calculated for $[C_{18}H_{18}O_2\ (M)]^+$: 266.1307, found: 266.1305.



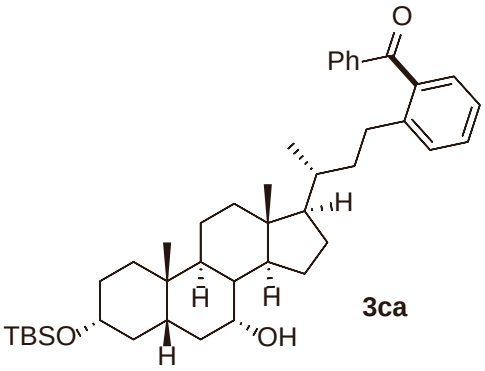
3bz

phenyl(2-(tetrahydrofuran-3-yl)phenyl)methanone (3bz): Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 65.8 mg, 52% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 – 7.76 (m, 2H), 7.62 – 7.55 (m, 1H), 7.52 – 7.42 (m, 4H), 7.30 – 7.24 (m, 2H), 4.07 – 4.00 (m, 1H), 3.97 (dd, *J* = 8.5, 7.7 Hz, 1H), 3.82 – 3.73 (m, 2H), 3.53 – 3.44 (m, 1H), 2.30 – 2.21 (m, 1H), 2.05 – 1.94 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.7, 142.2, 139.1, 137.7, 133.6, 130.8, 130.3, 128.6, 128.0, 126.9, 125.9, 75.1, 68.6, 41.4, 35.5.

HRMS (EI-TOF): calculated for $[C_{17}H_{16}O_2$ (M)$]^+$: 252.1150, found: 252.1152.



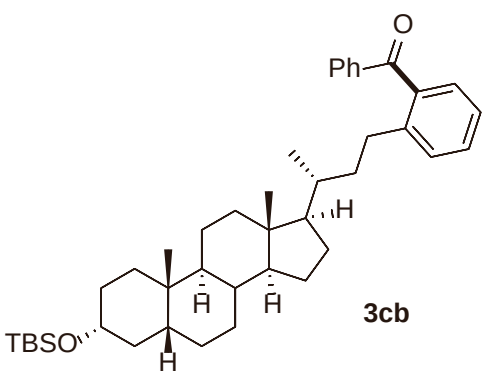
3ca

(2-((3*R*)-3-((3*R*,5*R*,7*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-3-((*tert*-butyldimethylsilyl)oxy)-7-hydroxy-10,13-dimethyl-hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)butyl)phenyl)(phenyl)methanone (3ca): Following the general procedure, *o*-diiodoarene **1a** (495.0 mg, 1.5 mmol) and NaH (60% dispersion in mineral oil, 80.5 mg, 2.0 mmol) were used, the title compound was obtained as colorless oil, 138.6 mg, 43% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 – 7.73 (m, 2H), 7.56 – 7.50 (m, 1H), 7.43 – 7.33 (m, 3H), 7.26 – 7.15 (m, 3H), 3.75 (s, 1H), 3.43 – 3.33 (m, 1H), 2.70 – 2.60 (m, 1H), 2.50 – 2.40 (m, 1H), 2.22 – 2.08 (m, 1H), 1.93 – 1.83 (m, 2H), 1.81 – 1.65 (m, 3H), 1.58 – 1.44 (m, 5H), 1.43 – 1.19 (m, 9H), 1.09 – 0.96 (m, 4H), 0.89 – 0.79 (m, 16H), 0.53 (s, 3H), 0.00 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.8, 142.3, 138.7, 138.0, 133.2, 130.3, 130.2, 128.5, 128.4, 125.1, 73.0, 68.6, 55.7, 50.5, 42.7, 41.7, 40.1, 39.6, 39.5, 38.4, 36.0, 35.6, 35.1, 34.7, 32.8, 31.2, 30.1, 28.1, 26.1, 23.8, 22.9, 20.6, 18.6, 18.4, 11.8, -4.4, -4.5. One aromatic carbon peak is overlapped.

HRMS (ESI-TOF): calculated for $[C_{42}H_{62}O_3SiNa$ (M + Na)$]^+$: 665.4366, found: 665.4364.



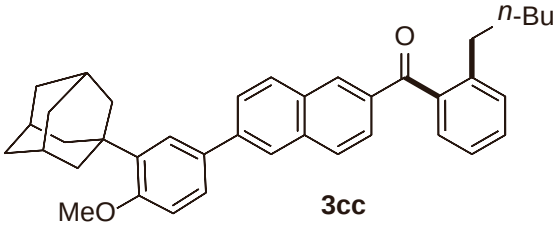
3cb

(2-((3*R*)-3-((3*R*,5*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-3-((*tert*-butyl-dimethylsilyl)oxy)-10,13-dimethylhexade cahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl) butyl)phenyl)(phenyl)-methanone (3cb): Following the general procedure, the title compound was obtained as colorless oil, 203.7 mg, 65% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (dd, *J* = 5.1, 3.3 Hz, 2H), 7.56 – 7.50 (m, 1H), 7.42 – 7.33 (m, 3H), 7.27 – 7.16 (m, 3H), 3.58 – 3.48 (m, 1H), 2.71 – 2.60 (m, 1H), 2.50 – 2.39 (m, 1H), 1.87 – 1.66 (m, 4H), 1.64 – 1.40 (m, 4H), 1.38 – 1.10 (m, 11H), 1.09 – 0.83 (m, 19H), 0.79 (d, *J* = 6.3 Hz, 3H), 0.52 (s, 3H), 0.01 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 198.7, 142.4, 138.8, 138.1, 133.2, 130.3, 130.21, 130.19, 128.5, 128.4, 125.1, 72.9, 56.5, 56.0, 42.8, 42.4, 40.4, 40.2, 38.5, 37.1, 36.01, 35.97, 35.7, 34.7, 31.2, 30.2, 28.2, 27.4, 26.5, 26.1, 24.3, 23.5, 20.9, 18.6, 18.4, 12.1, -4.5.

HRMS (ESI-TOF): calculated for $[C_{42}H_{62}O_2SiK\ (M + K)]^+$: 665.4156, found: 665.4155.



3cc

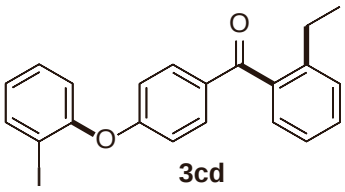
(6-(3-((3*r*,5*r*,7*r*)-adamantan-1-yl)-4-methoxy phenyl)naphthalen-2-yl)(2-pentylphenyl)met hanone (3cc):

Following the general procedure, the title compound was obtained as white solid, 181.6 mg, 67% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (s, 1H), 8.10 – 8.01 (m, 2H), 7.94 (dd, *J* = 19.5, 8.6 Hz, 2H), 7.80 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.63 (d, *J* = 2.3 Hz, 1H), 7.56 (dd, *J* = 8.4, 2.3 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.42 – 7.35 (m, 2H), 7.33 – 7.28 (m, 1H), 3.92 (s, 3H), 2.75 – 2.65 (m, 2H), 2.25 – 2.17 (m, 6H), 2.16 – 2.1 (m, 3H), 1.88 – 1.78 (m, 6H), 1.64 – 1.55 (m, 2H), 1.29 – 1.19 (m, 4H), 0.81 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 198.8, 159.1, 141.9, 139.1, 139.0, 136.2, 134.9, 132.7, 132.5, 131.2, 130.22, 130.15, 130.1, 128.6, 128.5, 126.6, 126.1, 125.9, 125.6, 125.3, 124.9, 112.2, 55.3, 40.7, 37.3, 37.2, 33.4, 31.8, 31.5, 29.2, 22.5, 14.1. One aromatic carbon peak is overlapped.

HRMS (ESI-TOF): calculated for $[C_{39}H_{43}O_2\ (M + H)]^+$: 543.3263, found: 543.3262.



3cd

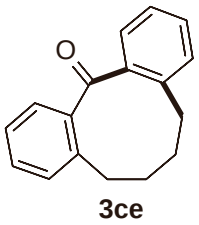
(2-ethylphenyl)(4-(2-iodophenoxy)phenyl)methanone (3cd):

Following the general procedure, *o*-diiodoarene **1a** (495.0 mg, 1.5 mmol) and NaH (60% dispersion in mineral oil, 80.5 mg, 2.0 mmol) were used, the title compound was obtained as colorless oil, 122.4 mg, 57% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.75 – 7.69 (m, 2H), 7.36 – 7.22 (m, 3H), 7.20 – 7.12 (m, 2H), 6.97 (dd, *J* = 8.1, 1.4 Hz, 1H), 6.92 – 6.82 (m, 3H), 2.58 (q, *J* = 7.5 Hz, 2H), 1.08 (t, *J* = 7.6 Hz, 3H).

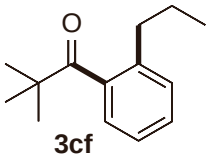
^{13}C NMR (151 MHz, $CDCl_3$): δ 197.4, 161.5, 155.0, 142.9, 140.3, 138.6, 132.7, 132.7, 130.2, 130.1, 129.5, 128.1, 126.9, 125.3, 121.5, 116.8, 90.1, 26.5, 16.1.

HRMS (EI-TOF): calculated for $[C_{21}H_{17}IO_2\ (M)]^+$: 428.0273, found: 428.0278.



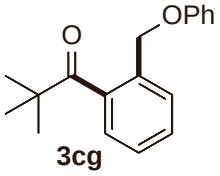
3ce

5,6,7,8-tetrahydro-13*H*-dibenzo[*a*,*d*][*9*]annulen-13-one (3ce):
Following the general procedure, the title compound was obtained as colorless oil, 35.2 mg, 30% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47 (dd, *J* = 7.6, 1.2 Hz, 2H), 7.41 – 7.34 (m, 2H), 7.30 – 7.25 (m, 2H), 7.17 (d, *J* = 7.5 Hz, 2H), 2.72 – 2.62 (m, 4H), 1.76 – 1.66 (m, 4H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 203.5, 141.5, 141.2, 131.0, 130.7, 126.7, 126.2, 33.0, 27.1.
HRMS (EI-TOF): calculated for $[C_{17}H_{16}O\ (M)]^+$: 236.1201, found: 236.1199.



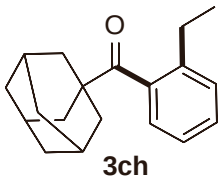
3cf

2,2-dimethyl-1-(2-propylphenyl)propan-1-one (3cf):
Following the general procedure, the title compound was obtained as colorless oil, 61.4 mg, 60% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31 – 7.23 (m, 2H), 7.20 – 7.10 (m, 2H), 2.47 – 2.40 (m, 2H), 1.68 – 1.56 (m, 2H), 1.25 (s, 9H), 0.94 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 215.2, 140.8, 138.8, 129.6, 128.7, 125.0, 124.6, 45.0, 35.9, 27.6, 24.7, 14.3.
HRMS (EI-TOF): calculated for $[C_{14}H_{20}O\ (M)]^+$: 204.1514, found: 204.1512.



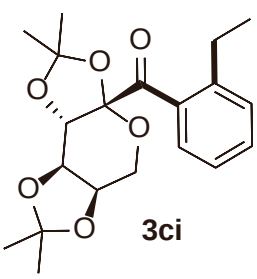
3cg

2,2-dimethyl-1-(2-(phenoxymethyl)phenyl)propan-1-one (3cg):
Following the general procedure, the title compound was obtained as colorless oil, 52.5 mg, 39% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31 – 7.23 (m, 2H), 7.20 – 7.10 (m, 2H), 2.47 – 2.40 (m, 2H), 1.68 – 1.56 (m, 2H), 1.25 (s, 9H), 0.94 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 213.9, 158.6, 140.2, 134.1, 129.6, 129.32, 129.26, 127.3, 125.1, 121.2, 114.8, 67.7, 44.9, 27.8.
HRMS (EI-TOF): calculated for $[C_{18}H_{20}O_2\ (M)]^+$: 268.1463, found: 268.1460.



3ch

adamantan-1-yl(2-ethylphenyl)methanone (3ch):
Following the general procedure, the title compound was obtained as colorless oil, 75.3 mg, 56% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.33 – 7.25 (m, 2H), 7.20 – 7.13 (m, 1H), 7.11 – 7.06 (m, 1H), 2.48 (q, *J* = 7.5 Hz, 2H), 2.07 – 2.00 (m, 3H), 1.92 (d, *J* = 2.7 Hz, 6H), 1.77 – 1.64 (m, 6H), 1.21 (t, *J* = 7.5 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 214.5, 140.31, 140.29, 128.9, 128.7, 124.8, 124.7, 47.2, 38.8, 36.6, 28.1, 26.8, 15.8.
HRMS (EI-TOF): calculated for $[C_{19}H_{24}O\ (M)]^+$: 268.1827, found: 268.1830.



3ci

(2-ethylphenyl)((3a*S*,5a*R*,8a*R*,8b*S*)-2,2,7,7-tetramethyltetrahydro-3a*H*-bis([1,3]dioxolo)[4,5-*b*:4',5'-*d*]pyran-3a-yl)methanone (3ci):

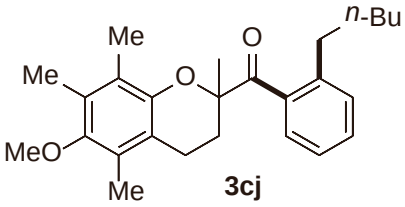
Following the general procedure, the title compound was obtained as colorless oil, 58.1 mg, 32% yield.

Following the general procedure, when *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 99.4 mg, 55% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, *J* = 7.7 Hz, 1H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.27 (d, *J* = 6.8 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 5.23 (d, *J* = 2.6 Hz, 1H), 4.69 (dd, *J* = 7.9, 2.6 Hz, 1H), 4.23 (dd, *J* = 7.9, 1.5 Hz, 1H), 3.95 (dd, *J* = 12.9, 1.9 Hz, 1H), 3.76 (d, *J* = 12.9 Hz, 1H), 2.80 – 2.65 (m, 2H), 1.59 (s, 3H), 1.41 (s, 3H), 1.32 (d, *J* = 8.5 Hz, 6H), 1.24 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 197.2, 144.8, 135.0, 131.1, 129.71, 129.66, 124.7, 110.0, 109.2, 102.6, 70.5, 70.42, 70.36, 61.7, 26.9, 26.3, 26.0, 24.9, 24.3, 16.2.

HRMS (ESI-TOF): calculated for $[C_{20}H_{26}O_6Na\ (M + Na)]^+$: 385.1627, found: 385.1625.



3cj

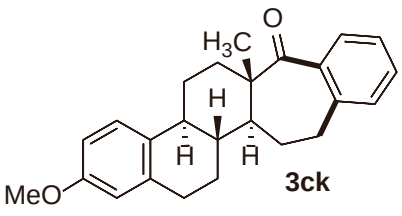
(6-methoxy-2,5,7,8-tetramethylchroman-2-yl)(2-pentylph enyl)-methanone (3cj):

Following the general procedure, the title compound was obtained as colorless oil, 160.3 mg, 81% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 (d, *J* = 7.6 Hz, 1H), 7.26 (t, *J* = 7.5 Hz, 1H), 7.16 – 7.09 (m, 2H), 3.58 (s, 3H), 2.65 (t, *J* = 6.7 Hz, 2H), 2.55 – 2.46 (m, 1H), 2.46 – 2.35 (m, 2H), 2.11 (s, 3H), 2.07 (s, 3H), 2.05 – 1.96 (m, 1H), 1.81 (s, 3H), 1.70 (s, 3H), 1.59 – 1.49 (m, 1H), 1.46 – 1.36 (m, 1H), 1.33 – 1.22 (m, 4H), 0.88 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 210.6, 150.2, 147.3, 141.4, 137.7, 129.8, 129.7, 128.1, 127.2, 125.9, 124.4, 123.3, 117.6, 82.7, 60.5, 33.4, 32.1, 31.6, 30.5, 25.0, 22.6, 20.7, 14.2, 12.5, 11.9, 11.7.

HRMS (ESI-TOF): calculated for $[C_{26}H_{34}O_3Na\ (M + Na)]^+$: 417.2406, found: 417.2408.



3ck

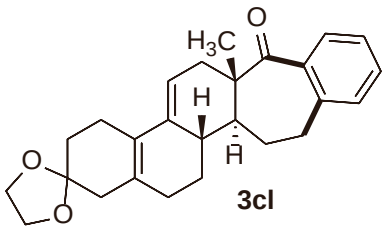
(6b*S*,8a*S*,15a*S*,15b*R*)-4-methoxy-8a-methyl-1,2,6b,7,8,8a, 14,15, 15a,15b-decahydro-9*H*-benzo[4,5]cyclohepta[1,2*a*] phenanthren-9-one (3ck):

Following the general procedure, the title compound was obtained as white solid, 102.9 mg, 57% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 – 7.37 (m, 1H), 7.35 – 7.28 (m, 2H), 7.21 – 7.12 (m, 2H), 6.72 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.63 (d, *J* = 2.5 Hz, 1H), 3.78 (s, 3H), 2.88 – 2.69 (m, 4H), 2.38 – 2.29 (m, 1H), 2.24 – 2.08 (m, 3H), 2.01 – 1.92 (m, 1H), 1.68 – 1.49 (m, 4H), 1.46 – 1.34 (m, 1H), 1.29 (s, 3H), 1.26 – 1.13 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 216.1, 157.7, 140.7, 137.8, 137.4, 132.4, 131.1, 127.6, 126.8, 126.4, 126.3, 113.5, 111.8, 55.3, 49.1, 43.2, 42.8, 40.7, 38.0, 30.6, 30.2, 28.1, 26.6, 26.2, 14.3.

HRMS (ESI-TOF): calculated for $[C_{25}H_{29}O_2\ (M + H)]^+$: 361.2168, found: 361.2167.



3cl

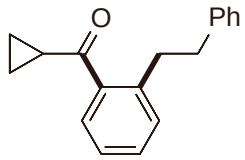
(8a*S*,15a*S*,15b*S*)-8a-methyl-1,3,5,6,8,8a,14,15,15a,15b-decahydrospiro[benzo[4,5]cyclohepta[1,2-*a*]phenanth rene-4,2'-[1,3]dioxolan]-9(2*H*)-one (3cl):

Following the general procedure, the title compound was obtained as colorless oil, 105.7 mg, 54% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38 – 7.30 (m, 1H), 7.26 – 7.21 (m, 2H), 7.12 – 7.07 (m, 1H), 5.55 – 5.47 (m, 1H), 4.00 – 3.93 (m, 4H), 2.85 – 2.64 (m, 2H), 2.52 – 2.42 (m, 1H), 2.32 – 2.05 (m, 7H), 2.03 – 1.88 (m, 3H), 1.83 – 1.69 (m, 2H), 1.65 – 1.49 (m, 2H), 1.18 (s, 3H), 1.16 – 1.04 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 215.1, 140.5, 137.4, 136.5, 130.8, 130.2, 127.6, 126.6, 126.4, 126.3, 115.4, 108.2, 64.6, 64.4, 47.8, 41.13, 41.07, 39.4, 37.7, 31.7, 31.3, 30.9, 28.8, 27.2, 24.5, 14.4.

HRMS (ESI-TOF): calculated for $[C_{26}H_{31}O_3\ (M + H)]^+$: 391.2273, found: 391.2275.



3cn

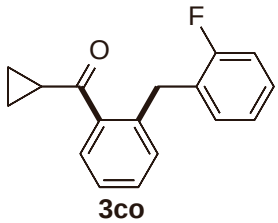
cyclopropyl(2-phenethylphenyl)methanone (3cn):

Following the general procedure, the title compound was obtained as colorless oil, 77.6 mg, 62% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.41 – 7.36 (m, 1H), 7.34 – 7.25 (m, 4H), 7.24 – 7.18 (m, 3H), 3.15 – 3.08 (m, 2H), 2.95 – 2.87 (m, 2H), 2.45 – 2.34 (m, 1H), 1.31 – 1.26 (m, 2H), 1.10 – 1.02 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 205.4, 142.0, 140.6, 140.1, 130.9, 130.8, 128.7, 128.4, 128.4, 126.0, 126.0, 38.5, 36.0, 21.1, 12.3.

HRMS (EI-TOF): calculated for $[C_{18}H_{18}O\ (M)]^+$: 250.1358, found: 250.1361.



3co

cyclopropyl(2-(2-fluorobenzyl)phenyl)methanone (3co):

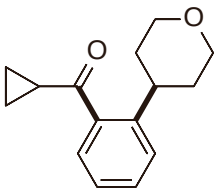
Following the general procedure, the title compound was obtained as colorless oil, 56.2 mg, 44% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 – 7.70 (m, 1H), 7.42 – 7.29 (m, 2H), 7.24 – 7.14 (m, 2H), 7.11 – 6.97 (m, 3H), 4.24 (s, 2H), 2.44 – 2.31 (m, 1H), 1.24 – 1.16 (m, 2H), 1.04 – 0.96 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 205.4, 161.1 (d, *J* = 245.4 Hz), 139.2 (d, *J* = 311.2 Hz), 131.3 (d, *J* = 4.2 Hz), 131.2, 131.0, 128.4, 128.1, 128.0 (d, *J* = 8.1 Hz), 126.4, 124.1 (d, *J* = 3.4 Hz), 115.3 (d, *J* = 22.1 Hz), 32.0 (d, *J* = 2.7 Hz), 21.1, 12.3. One aromatic carbon peak is overlapped.

^{19}F NMR (565 MHz, $CDCl_3$): δ -117.23 – -117.31 (m).

HRMS (EI-TOF): calculated for $[C_{17}H_{15}FO\ (M)]^+$: 254.1107, found: 254.1104.



3cp

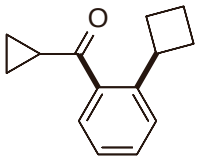
cyclopropyl(2-(tetrahydro-2*H*-pyran-4-yl)phenyl)methanone (3cp):

Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 80.7 mg, 70% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.46 – 7.35 (m, 2H), 7.30 – 7.24 (m, 1H), 4.03 (dd, *J* = 11.3, 3.9 Hz, 2H), 3.55 – 3.46 (m, 2H), 3.31 – 3.20 (m, 1H), 2.43 – 2.33 (m, 1H), 1.91 – 1.70 (m, 4H), 1.30 – 1.22 (m, 2H), 1.10 – 1.02 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 206.1, 144.0, 140.2, 130.9, 127.9, 127.0, 126.0, 68.5, 37.4, 34.2, 21.6, 12.4.

HRMS (EI-TOF): calculated for $[C_{15}H_{18}O_2\ (M)]^+$: 230.1307, found: 230.1309.



3cq

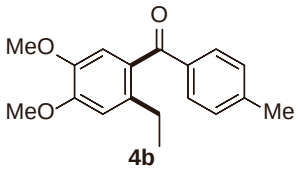
(2-cyclobutylphenyl)(cyclopropyl)methanone (3cq):

Following the general procedure, *o*-diiodoarene **1a** (824.8 mg, 2.5 mmol) and NaH (60% dispersion in mineral oil, 120.5 mg, 3.0 mmol) were used, the title compound was obtained as colorless oil, 41.2 mg, 41% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 – 7.52 (m, 1H), 7.45 – 7.39 (m, 2H), 7.28 – 7.22 (m, 1H), 4.02 – 3.89 (m, 1H), 2.41 – 2.27 (m, 3H), 2.17 – 1.91 (m, 3H), 1.85 – 1.75 (m, 1H), 1.28 – 1.21 (m, 2H), 1.08 – 1.01 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 206.4, 144.3, 139.8, 130.6, 127.5, 127.1, 125.6, 38.0, 29.9, 21.3, 18.3, 12.4.

HRMS (EI-TOF): calculated for $[C_{14}H_{16}O\ (M)]^+$: 200.1201, found: 200.1199.



4b

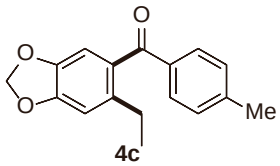
(2-ethyl-4,5-dimethoxyphenyl)(*p*-tolyl)methanone (4b):

Following the general procedure, the title compound was obtained as colorless oil, 105.5 mg, 74% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, *J* = 8.1 Hz, 2H), 7.27 – 7.22 (m, 2H), 6.81 (d, *J* = 3.7 Hz, 2H), 3.94 (s, 3H), 3.79 (s, 3H), 2.62 (q, *J* = 7.5 Hz, 2H), 2.42 (s, 3H), 1.15 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 197.8, 150.6, 146.2, 143.9, 137.3, 135.9, 130.5, 130.4, 129.2, 112.33, 112.31, 56.2, 56.0, 26.4, 21.8, 16.4.

HRMS (ESI-TOF): calculated for $[C_{18}H_{21}O_3\ (M + H)]^+$: 285.1491, found: 285.1490.

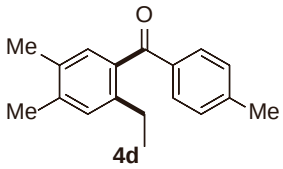


4c

(6-ethylbenzo[*d*][1,3]dioxol-5-yl)(*p*-tolyl)methanone (4c):

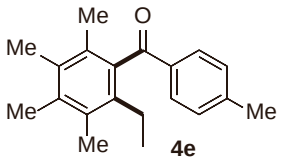
Following the general procedure, THF (5 mL) was used, the title compound was obtained as colorless oil, 102.3 mg, 76% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, *J* = 8.1 Hz, 2H), 7.24 (d, *J* = 7.9 Hz, 2H), 6.79 (s, 1H), 6.75 (s, 1H), 5.98 (s, 2H), 2.59 (q, *J* = 7.5 Hz, 2H), 2.41 (s, 3H), 1.13 (t, *J* = 7.5 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 197.5, 149.2, 145.0, 144.0, 138.8, 135.6, 131.7, 130.4, 129.2, 109.7, 109.0, 101.5, 26.5, 21.8, 16.3.
HRMS (EI-TOF): calculated for $[C_{17}H_{16}O_3$ (M)$]^+$: 268.1099, found: 268.1096.



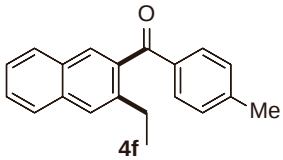
4d

(2-ethyl-4,5-dimethylphenyl)(*p*-tolyl)methanone (4d):
Following the general procedure, THF (5 mL) was used, the title compound was obtained as colorless oil, 81.7 mg, 65% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, *J* = 8.1 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.10 (s, 1H), 7.05 (s, 1H), 2.62 (q, *J* = 7.5 Hz, 2H), 2.43 (s, 3H), 2.31 (s, 3H), 2.24 (s, 3H), 1.14 (t, *J* = 7.5 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 198.7, 143.9, 140.7, 139.0, 136.2, 135.8, 133.4, 130.9, 130.4, 129.8, 129.2, 26.1, 21.8, 19.9, 19.3, 16.3.
HRMS (ESI-TOF): calculated for $[C_{18}H_{21}O$ (M + H)$]^+$: 253.1593, found: 253.1592.



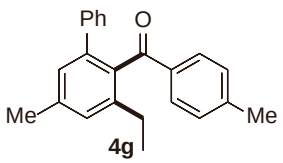
4e

(2-ethyl-3,4,5,6-tetramethylphenyl)(*p*-tolyl)methanone (4e):
Following the general procedure, the title compound was obtained as colorless oil, 70.4 mg, 50% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, *J* = 7.6 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 2.60 – 2.50 (m, 1H), 2.42 (s, 3H), 2.36 – 2.28 (m, 4H), 2.27 (s, 3H), 2.22 (s, 3H), 2.02 (s, 3H), 1.01 (t, *J* = 7.5 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 201.3, 144.4, 137.6, 136.1, 135.6, 135.4, 133.1, 132.4, 129.8, 129.4, 129.1, 24.7, 21.8, 17.7, 16.8, 16.0, 15.6, 15.1.
HRMS (ESI-TOF): calculated for $[C_{20}H_{25}O$ (M + H)$]^+$: 281.1905, found: 281.1907.



4f

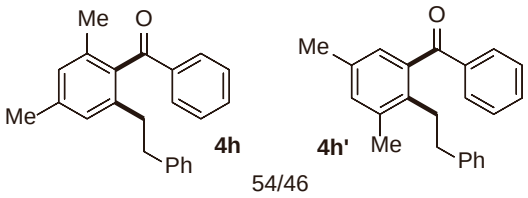
(3-ethylnaphthalen-2-yl)(*p*-tolyl)methanone (4f):
Following the general procedure, the title compound was obtained as yellow oil, 57.6 mg, 42% yield.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87– 7.83 (m, 1H), 7.82 – 7.76 (m, 5H), 7.57 – 7. 52 (m, 1H), 7.50 – 7.45 (m, 1H), 7.31 – 7.24 (m, 2H), 2.89 (q, *J* = 7.5 Hz, 2H), 2.45 (s, 3H), 1.25 (t, *J* = 7.5 Hz, 3H).
^{13}C NMR (151 MHz, $CDCl_3$): δ 198.3, 144.3, 140.1, 137.5, 135.5, 134.3, 130.8, 130.6, 129.3, 128.6, 128.3, 127.6, 127.41, 127.39, 126.1, 26.6, 21.9, 15.8.
HRMS (ESI-TOF): calculated for $[C_{20}H_{19}O$ (M + H)$]^+$: 275.1436, found: 275.1435.



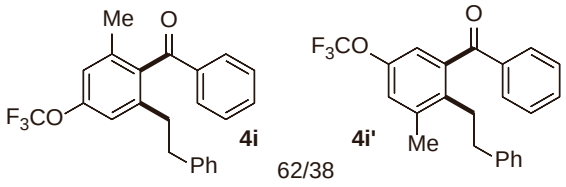
4g

(3-ethyl-5-methyl-[1,1'-biphenyl]-2-yl)(*p*-tolyl)methanone (4g):
Following the general procedure, THF (5 mL) was used, the title compound was obtained as colorless oil, 97.8 mg, 62% yield.

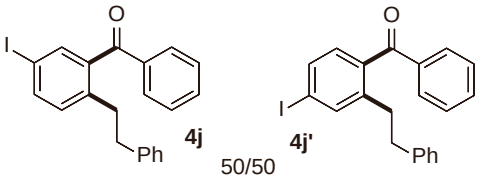
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 (d, *J* = 8.0 Hz, 2H), 7.30– 7.24 (m, 2H), 7.21–7.10 (m, 5H), 7.06 (d, *J* = 8.0 Hz, 2H), 2.57 (q, *J* = 7.4 Hz, 2H), 2.47 (s, 3H), 2.31 (s, 3H), 1.18 (t, *J* = 7.5 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 199.7, 143.8, 141.7, 140.7, 140.0, 138.9, 135.8, 135.7, 129.6, 129.3, 129.0, 128.5, 128.2, 128.0, 127.1, 26.5, 21.7, 21.5, 15.9.
HRMS (EI-TOF): calculated for $[C_{23}H_{22}O\ (M)]^+$: 314.1671, found: 314.1669.



(2,4-dimethyl-6-phenethylphenyl)(phenyl)meth-anone (4h) and (3,5-dimethyl-2-phenethylphenyl)(phenyl)methanone (4h'):
Following the general procedure, THF (5 mL) was used, the title compound was obtained as colorless oil, 75.6 mg, 48% yield.
^{1}H NMR (400 MHz, $CDCl_3$), mixture of **4h** and **4h':** δ 7.89 – 7.79 (m, 2H), 7.62 – 7.56 (m, 1H), 7.50 – 7.43 (m, 2H), 7.25 – 7.11 (m, 4.32H), 7.05 – 7.00 (m, 1.14H), 6.99 – 6.93 (m, 1.54H), 2.91 – 2.84 (m, 0.92H), 2.82 – 2.74 (m, 2H), 2.69 – 2.63 (m, 1.08H), 2.40 (s, 1.38H), 2.37 (s, 1.62H), 2.33 (s, 1.38H), 2.12 (s, 1.62H).
^{13}C NMR (101 MHz, $CDCl_3$), mixture of **4h** and **4h':** δ 200.8, 199.5, 142.1, 141.8, 139.5, 138.7, 138.5, 138.1, 137.7, 137.3, 136.7, 135.5, 135.0, 134.4, 133.7, 133.3, 133.1, 130.4, 129.6, 128.90, 128.89, 128.5, 128.43, 128.38, 127.6, 126.6, 125.99, 125.97, 38.1, 37.1, 35.9, 32.6, 21.4, 21.0, 19.6, 19.5. Two aromatic carbon peaks are overlapped.
HRMS (ESI-TOF): calculated for $[C_{23}H_{22}ONa\ (M + Na)]^+$: 337.1568, found: 337.1567.



(2-methyl-6-phenethyl-4-(trifluoromethoxy) phenyl)(phenyl)methanone (4i) and (3-meth yl-2-phenethyl-5-(trifluoromethoxy) phenyl) (phenyl)methanone (4i'):
Following the general procedure, THF (5 mL) was used, the title compound was obtained as colorless oil, 99.6 mg, 52% yield.
^{1}H NMR (400 MHz, $CDCl_3$), mixture of **4i** and **4i':** δ 7.85 – 7.79 (m, 2H), 7.65 – 7.59 (m, 1H), 7.51 – 7.46 (m, 2H), 7.25 – 7.10 (m, 4H), 7.04 – 6.95 (m, 3H), 2.94 – 2.87 (m, 0.76H), 2.83 – 2.76 (m, 2H), 2.74 – 2.69 (m, 1.24H), 2.45 (s, 1.14H), 2.17 (s, 1.86H).
^{13}C NMR (151 MHz, $CDCl_3$), mixture of **4i** and **4i':** δ 199.3, 197.4, 149.4, 146.5, 141.6, 140.94, 140.87, 140.8, 140.0, 138.1, 137.4, 137.2, 137.1, 137.0, 134.2, 133.9, 130.4, 129.6, 129.1, 128.8, 128.6, 128.50, 128.45, 128.4, 126.2, 124.4, 132.7 – 124.3 (m), 120.6 (q, *J* = 256.7 Hz), 120.3, 119.2, 118.5, 37.4, 36.8, 35.6, 32.4, 19.8, 19.7. One aromatic carbon peak is overlapped.
^{19}F NMR (565 MHz, $CDCl_3$), mixture of **4i** and **4i':** δ -57.49, -57.81.
HRMS (ESI-TOF): calculated for $[C_{23}H_{20}F_3O_2\ (M + H)]^+$: 385.1415, found: 385.1417.

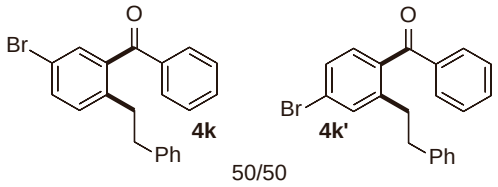


(5-iodo-2-phenethylphenyl)(phenyl)methanone (4j) and (4-iodo-2-phenethylphenyl)(phenyl)methanone (4j'): Following the general procedure, THF (5 mL) was used, the title compound was obtained as colorless oil, 127.9 mg, 61% yield.

^{1}H NMR (400 MHz, $CDCl_3$), mixture of **4j** and **4j':** δ 7.80 – 7.74 (m, 2H), 7.72 (dd, *J* = 8.1, 1.8 Hz, 0.5H), 7.69 (d, *J* = 1.4 Hz, 0.5H), 7.64 – 7.58 (m, 2H), 7.50 – 7.43 (m, 2H), 7.25 – 7.19 (m, 2H), 7.17 – 7.12 (m, 1H), 7.09 – 7.02 (m, 3H), 2.95 – 2.80 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$), mixture of **4j** and **4j':** δ 197.7, 196.8, 143.1, 141.1, 140.9, 140.3, 139.5, 139.2, 138.0, 137.6, 137.3, 136.9, 134.7, 133.7, 133.6, 132.4, 130.32, 130.30, 130.2, 128.8, 128.7, 128.53, 128.48, 128.46, 126.2, 126.2, 97.1, 90.4, 38.0, 37.8, 35.3, 35.1. Two aromatic carbon peaks are overlapped.

HRMS (ESI-TOF): calculated for $[C_{21}H_{17}IONa\ (M + Na)]^+$: 435.0222, found: 435.0221.

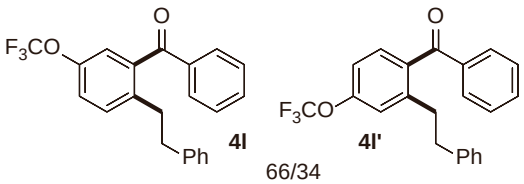


(5-bromo-2-phenethylphenyl)(phenyl)methanone (4k) and (4-bromo-2-phenethylphenyl)(phenyl)me thanone (4k'): Following the general procedure, THF (5 mL) was used, the title compound was obtained as colorless oil, 98.6 mg, 54% yield.

^{1}H NMR (400 MHz, $CDCl_3$), mixture of **4k** and **4k':** δ 7.80 – 7.73 (m, 2H), 7.64 – 7.57 (m, 1H), 7.52 (dd, *J* = 8.2, 2.1 Hz, 0.5H), 7.50 – 7.39 (m, 3.5H), 7.24 – 7.13 (m, 4H), 7.10 – 7.03 (m, 2H), 2.97 – 2.81 (m, 4H).

^{13}C NMR (151 MHz, $CDCl_3$), mixture of **4k** and **4k':** δ 197.6, 197.0, 143.3, 141.13, 141.11, 140.6, 139.7, 137.6, 137.4, 137.3, 133.7, 133.6, 133.5, 133.3, 132.2, 131.2, 130.5, 130.31, 130.25, 128.8, 128.7, 128.6, 128.54, 128.50, 128.47, 126.22, 126.18, 124.8, 119.3, 38.0, 37.9, 35.4, 35.0. One aromatic carbon peak is overlapped.

HRMS (ESI-TOF): calculated for $[C_{21}H_{18}BrO\ (M + H)]^+$: 356.0541, found: 356.0540.



(2-phenethyl-5-(trifluoromethoxy)phenyl)(phenyl)methanone (4l) and (2-phenethyl-4-(trifluoromethoxy)phenyl)(phenyl)methanone (4l'): Following the general procedure, THF (5 mL) was used, the title compound was obtained as colorless oil, 85.4 mg, 46% yield.

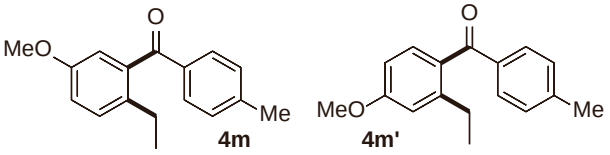
^{1}H NMR (400 MHz, $CDCl_3$), mixture of **4l** and **4l':** δ 7.94 – 7.84 (m, 2H), 7.76 – 7.70 (m, 1H), 7.63 – 7.56 (m, 2H), 7.48 – 7.44 (m, 0.66H), 7.43 (s, 0.34H), 7.41 – 7.36 (m,

1H), 7.36 – 7.30 (m, 2H), 7.29 – 7.22 (m, 2H), 7.20 – 7.16 (m, 2H), 3.15 – 3.05 (m, 2H), 3.02 – 2.94 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$), mixture of **4l** and **4l':** δ 197.4, 196.9, 150.4, 146.8, 143.8, 141.1, 140.9, 140.1, 139.5, 137.6, 137.12, 137.08, 133.8, 133.6, 132.0, 130.6, 130.30, 130.29, 128.8, 128.7, 128.6, 128.51, 128.49, 126.3, 126.2, 122.7, 122.6, 121.2, 120.6 (q, *J* = 257.5 Hz), 120.5 (q, *J* = 258.0 Hz), 117.7, 38.0, 37.8, 35.5, 35.0. One aromatic carbon peak is overlapped.

^{19}F NMR (565 MHz, $CDCl_3$), mixture of **4l** and **4l':** δ -57.53, -57.97.

HRMS (ESI-TOF): calculated for $[C_{22}H_{18}F_3O_2$ (M + H)$]^+$: 371.1259, found: 371.1261.



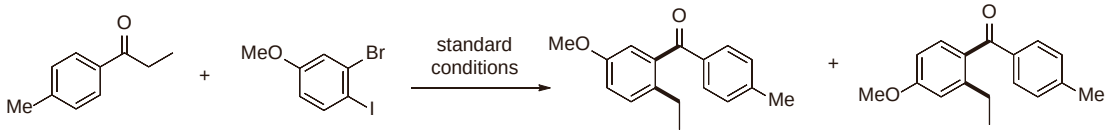
(2-ethyl-5-methoxyphenyl)(*p*-tolyl)meth-anone (4m) and (2-ethyl-4-methoxy-phen yl)(*p*-tolyl)methanone (4m'):

Following the general procedure, THF (5 mL) was used, the title compound was obtained as colorless oil, 98.8 mg, 78% yield. And a mixture of two isomers **4m/4m'** was obtained in 62:38 ratio.

^{1}H NMR (400 MHz, $CDCl_3$), mixture of **4m** and **4m':** δ 7.74 – 7.65 (m, 2H), 7.26 – 7.19 (m, 3H), 6.94 (dd, *J* = 8.5, 2.7 Hz, 0.38H), 6.85 (d, *J* = 2.4 Hz, 0.62H), 6.77 (d, *J* = 2.7 Hz, 0.38H), 6.72 (dd, *J* = 8.5, 2.5 Hz, 0.62H), 3.83 (s, 1.87H), 3.75 (s, 1.13H), 2.72 (q, *J* = 7.5 Hz, 1.25H), 2.54 (q, *J* = 7.5 Hz, 0.75H), 2.39 (s, 3H), 1.17 (t, *J* = 7.5 Hz, 1.87H), 1.09 (t, *J* = 7.5 Hz, 1.13H).

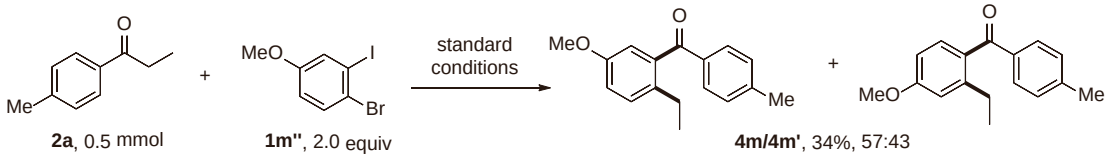
^{13}C NMR (101 MHz, $CDCl_3$), mixture of **4m** and **4m':** δ 198.2, 197.8, 161.2, 157.0, 146.4, 144.3, 143.6, 139.7, 136.2, 135.0, 134.6, 131.4, 130.9, 130.4, 130.3, 129.2, 129.1, 115.9, 115.3, 113.1, 110.0, 55.4, 55.3, 26.8, 25.6, 21.8, 21.7, 16.1, 16.0. One aromatic carbon peak is overlapped.

HRMS (ESI-TOF): calculated for $[C_{17}H_{19}O_2$ (M + H)$]^+$: 255.1385, found: 255.1384.



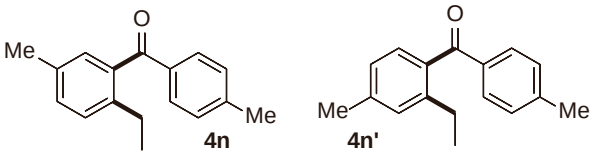
Following the general procedure, THF (5 mL) was used, when 2-bromo-1-iodo-4-methoxybenzene **1m'** instead of **1m** was used as the aryne precursor, the title compound was obtained in 39.2 mg, 31% yield. And a mixture of two isomers **4m/4m'** was obtained in 56:44 ratio.

^{1}H NMR (400 MHz, $CDCl_3$), mixture of **4m** and **4m':** δ 7.74 – 7.65 (m, 2H), 7.26 – 7.19 (m, 3H), 6.94 (dd, *J* = 8.5, 2.7 Hz, 0.44H), 6.85 (d, *J* = 2.4 Hz, 0.56H), 6.77 (d, *J* = 2.7 Hz, 0.44H), 6.72 (dd, *J* = 8.5, 2.5 Hz, 0.56H), 3.85 (s, 1.70H), 3.76 (s, 1.30H), 2.72 (q, *J* = 7.5 Hz, 1.12H), 2.54 (q, *J* = 7.5 Hz, 0.88H), 2.40 (s, 3H), 1.16 (t, *J* = 7.5 Hz, 1.70H), 1.10 (t, *J* = 7.5 Hz, 1.30H).



Following the general procedure, THF (5 mL) was used, when 1-bromo-2-iodo-4-methoxybenzene **1m''** instead of **1m** was used as the aryne precursor, the title compound was obtained in 42.8 mg, 34% yield. And a mixture of two isomers **4m/4m'** was obtained in 57:43 ratio.

^{1}H NMR (400 MHz, $CDCl_3$), mixture of **4m** and **4m':** δ 7.74 – 7.65 (m, 2H), 7.26 – 7.19 (m, 3H), 6.94 (dd, *J* = 8.5, 2.7 Hz, 0.43H), 6.85 (d, *J* = 2.4 Hz, 0.57H), 6.77 (d, *J* = 2.7 Hz, 0.43H), 6.72 (dd, *J* = 8.5, 2.5 Hz, 0.57H), 3.84 (s, 1.71H), 3.76 (s, 1.29H), 2.72 (q, *J* = 7.5 Hz, 1.14H), 2.54 (q, *J* = 7.5 Hz, 0.86H), 2.41 (s, 3H), 1.16 (t, *J* = 7.5 Hz, 1.71H), 1.09 (t, *J* = 7.5 Hz, 1.29H).



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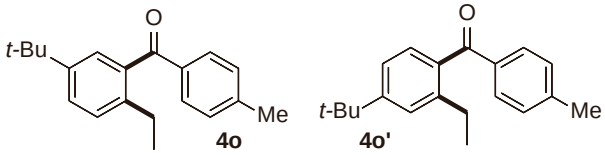
(2-ethyl-5-methylphenyl)(*p*-tolyl)methan-one (4n) and (2-ethyl-4-methylphenyl)(*p*-tolyl)methanone (4n'):

Following the general procedure, THF (5 mL) was used, the title compound was obtained as colorless oil, 95.7 mg, 80% yield.

^{1}H NMR (400 MHz, $CDCl_3$), mixture of **4n** and **4n':** δ 7.85– 7.74 (m, 2H), 7.35 – 7.28 (m, 3H), 7.25– 7.20 (m, 1H), 7.16 – 7.10 (m, 1H), 2.77 – 2.65 (m, 2H), 2.49 (s, 3H), 2.47 (s, 1.74H), 2.40 (s, 1.26H), 1.26– 1.18 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$), mixture of **4n** and **4n':** δ 198.8, 198.6, 144.2, 143.9, 143.3, 140.4, 139.8, 138.8, 135.9, 135.7, 135.4, 134.8, 130.9, 130.4, 130.3, 129.3, 129.23, 129.15, 128.8, 128.6, 128.2, 125.8, 26.5, 26.1, 21.80, 21.78, 21.6, 21.0, 16.13, 16.09.

HRMS (EI-TOF): calculated for $[C_{17}H_{18}O\ (M)]^+$: 238.1358, found: 238.1355.



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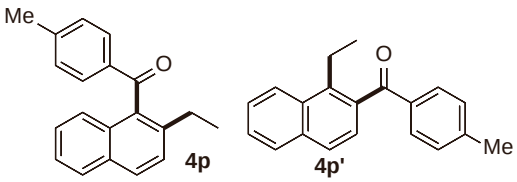
(5-(*tert*-butyl)-2-ethylphenyl)(*p*-tolyl)-meth anone (4o) and (4-(*tert*-butyl)-2-ethylphen yl)(*p*-tolyl)methanone (4o'):

Following the general procedure, THF (5 mL) was used, the title compound was obtained as colorless oil, 94.2 mg, 67% yield.

^{1}H NMR (400 MHz, $CDCl_3$), mixture of **4o** and **4o':** δ 7.79 (d, *J* = 8.0 Hz, 2H), 7.50 (dd, *J* = 8.1, 1.6 Hz, 0.4H), 7.40 (s, 0.6H), 7.34 – 7.27 (m, 4H), 2.76 (q, *J* = 7.5 Hz, 1.2H), 2.68 (q, *J* = 7.5 Hz, 0.8H), 2.47 (s, 3H), 1.42 (s, 5.4H), 1.35 (s, 3.6H), 1.26 – 1.16 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$), mixture of **4o** and **4o':** δ 199.0, 198.6, 153.5, 148.0, 144.1, 143.9, 143.0, 139.7, 138.3, 135.8, 135.6, 135.4, 130.5, 129.2, 129.13, 129.05, 128.6, 127.1, 126.6, 125.1, 122.1, 34.9, 34.5, 31.3, 26.9, 26.0, 21.8, 16.4, 16.0. One aromatic carbon peak and two aliphatic carbon peaks are overlapped.

HRMS (EI-TOF): calculated for $[C_{20}H_{24}O\ (M)]^+$: 280.1827, found: 280.1825.



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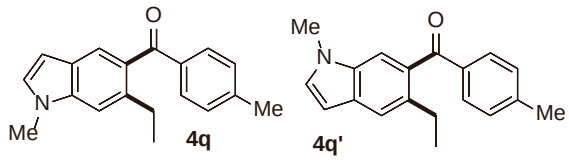
(2-ethylnaphthalen-1-yl)(*p*-tolyl)methanone (4p) and (1-ethylnaphthalen-2-yl)(*p*-tolyl)methanone (4p'):

Following the general procedure, THF (5 mL) was used, the title compound was obtained as colorless oil, 88.6 mg, 65% yield.

^{1}H NMR (400 MHz, $CDCl_3$), mixture of **4p** and **4p':** δ 7.94 (d, *J* = 8.2 Hz, 0.3H), 7.70 – 7.61 (m, 1.7H), 7.57 – 7.46 (m, 2.3H), 7.40 – 7.30 (m, 0.6H), 7.27 (d, *J* = 8.4 Hz, 0.7H), 7.24 – 7.17 (m, 1.4H), 7.15 – 7.09 (m, 1H), 7.04 – 6.98 (m, 2H), 2.86 (q, *J* = 7.5 Hz, 0.6H), 2.40 (q, *J* = 7.5 Hz, 1.4H), 2.20 (s, 0.9H), 2.18 (s, 2.1H), 1.08 (t, *J* = 7.5 Hz, 0.9H), 0.97 (t, *J* = 7.6 Hz, 2.1H).

^{13}C NMR (151 MHz, $CDCl_3$), mixture of **4p** and **4p':** δ 199.9, 199.1, 144.9, 144.5, 138.9, 138.5, 136.4, 135.7, 135.6, 135.3, 134.3, 131.80, 131.79, 130.7, 130.6, 130.1, 129.6, 129.3, 129.2, 129.0, 128.1, 127.0, 126.72, 126.69, 126.6, 126.1, 125.5, 125.3, 124.7, 124.6, 26.9, 23.1, 21.9, 21.8, 16.1, 15.8.

HRMS (ESI-TOF): calculated for $[C_{20}H_{19}O\ (M + H)]^+$: 275.1436, found: 275.1433.



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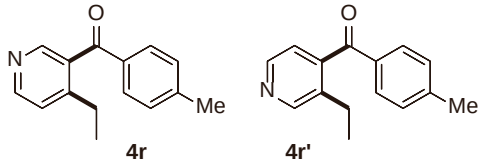
(6-ethyl-1-methyl-1*H*-indol-5-yl)(*p*-tolyl)methanone (4q) and (5-ethyl-1-methyl-1*H*-indol-6-yl)(*p*-tolyl)methanone (4q'):

Following the general procedure, THF (5 mL) was used, when 5-bromo-6-iodo-1-methyl-1*H*-indole **1q** (168.0 mg, 0.5 mmol) was used as the aryne precursor, and the reaction was performed at 100 °C for 8 h. The title compound was obtained as light-yellow oil, 55.4 mg, 40% yield.

^{1}H NMR (400 MHz, $CDCl_3$), mixture of **4q** and **4q':** δ 7.75 (t, J = 7.8 Hz, 2H), 7.59 (s, 0.58H), 7.55 (s, 0.42H), 7.29 – 7.22 (m, 3H), 7.13 (d, *J* = 3.1 Hz, 0.42H), 7.06 (d, *J* = 3.1 Hz, 0.58H), 6.48 (dd, *J* = 3.0, 0.7 Hz, 0.42H), 6.45 (dd, *J* = 3.1, 0.7 Hz, 0.58H), 3.83 (s, 1.74H), 3.74 (s, 1.26H), 2.91 (q, *J* = 7.5 Hz, 1.16H), 2.78 (q, *J* = 7.5 Hz, 0.84H), 2.45 – 2.41 (m, 3H), 1.23 (t, *J* = 7.5 Hz, 1.74H), 1.18 (t, *J* = 7.5 Hz, 1.26H).

^{13}C NMR (151 MHz, $CDCl_3$), mixture of **4q** and **4q':** δ 199.3, 199.2, 143.7, 143.4, 138.1, 138.0, 136.8, 136.5, 134.5, 134.3, 132.8, 131.1, 130.7, 130.3, 129.7, 129.1, 129.0, 125.4, 123.4, 121.2, 110.6, 109.8, 101.8, 100.8, 33.1, 33.0, 27.2, 26.7, 21.82, 21.79, 16.81, 16.76. Two aromatic carbon peaks are overlapped.

HRMS (ESI-TOF): calculated for $[C_{19}H_{19}NONa\ (M + Na)]^+$: 300.1364, found: 300.1365.



59/41

(4-ethylpyridin-3-yl)(*p*-tolyl)methanone (4r) and (3-ethylpyridin-4-yl)(*p*-tolyl)methanone (4r'):

Following the general procedure, THF (5 mL) was used, when 3-bromo-4-iodopyridine **1r**

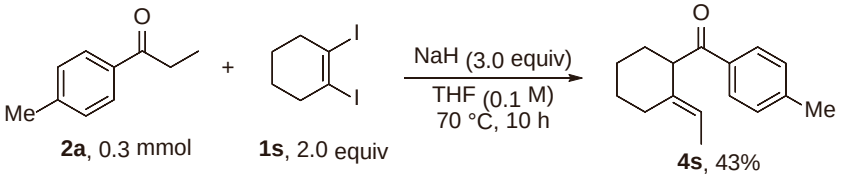
(142.0 mg, 0.5 mmol) was used as the aryne precursor, the title compound was obtained as light-yellow oil, 15.9 mg, 14% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.66 – 8.41 (m, 2H), 7.67 (t, *J* = 8.7 Hz, 2H), 7.25 (d, *J* = 7.8 Hz, 2.59H), 7.11 (d, *J* = 4.2 Hz, 0.41H), 2.70 – 2.57 (m, 2H), 2.41 (s, 3H), 1.18 – 1.10 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 196.14, 196.12, 152.3, 151.1, 151.0, 148.8, 147.1, 146.0, 145.4, 145.0, 136.5, 134.9, 134.8, 133.8, 130.4, 130.3, 129.6, 129.5, 124.2, 121.2, 26.0, 23.9, 21.89, 21.86, 15.7, 14.8.

HRMS (ESI-TOF): calculated for $[C_{15}H_{15}NONa\ (M + Na)]^+$: 248.1051, found: 248.1052.

(*E*)-(2-ethylidenecyclohexyl)(*p*-tolyl)methanone (4s):



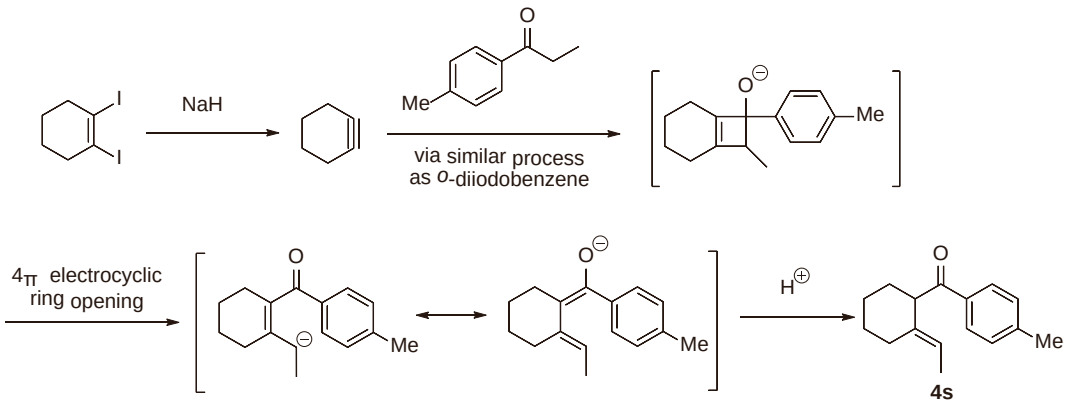
To a suspension of NaH (60% dispersion in mineral oil, 36 mg, 0.9 mmol) in anhydrous THF (3 mL) was added **2a** (44.5 mg, 0.3 mmol) and 1,2-diiodocyclohex-1-ene **1s** (200.4 mg, 0.6 mmol) respectively at 0 °C stirring for 5 min. The mixture was warmed to 70 °C for 10 h. After that, the reaction was quenched with saturated aqueous NH_4Cl (5 mL) solution at 0 °C. The mixture was then extracted with EtOAc (6 mL × 4). The combined extracts were dried over Na_2SO_4, concentrated under vacuum. The resulting residue was purified by silica gel chromatography to afford the title compound **4s** as colorless oil, 29.7 mg, 43% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.24 (t, *J* = 6.7 Hz, 2H), 5.45 – 5.28 (m, 1H), 4.52 – 4.35 (m, 1H), 2.48 – 2.32 (m, 4H), 2.22 – 2.06 (m, 2H), 1.84 – 1.74 (m, 1H), 1.71 – 1.50 (m, 6H), 1.38 – 1.27 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 202.0, 143.2, 138.3, 134.9, 129.2, 128.4, 118.9, 44.6, 34.9, 29.8, 28.3, 22.7, 21.7, 13.3.

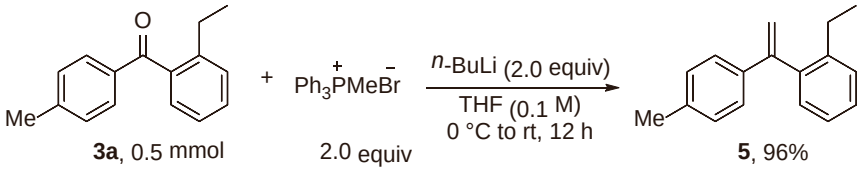
HRMS (ESI-TOF): calculated for $[C_{16}H_{20}ONa\ (M + Na)]^+$: 251.1412, found: 251.1409.

Proposed mechanism for the generation of **4s**:



6. Synthetic application

1-ethyl-2-(1-(*p*-tolyl)vinyl)benzene (5):



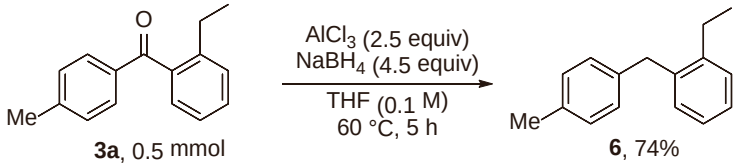
To a suspension of $[Ph_3PMe]^+[Br]^-$(357.2 mg, 1.0 mmol) in anhydrous THF (4 mL) was added *n*-BuLi (0.4 mL, 2.5 M in hexane) slowly at 0 ºC. After stirring for 30 min, a solution of ketone **3a** (112.5 mg, 0.5 mL) in THF (1 mL) was added to the mixture at 0ºC. Then the resulting mixture was warmed to room temperature for 12 h. After that, the mixture was treated with saturated aqueous NH_4Cl solution (5 mL) and extracted with EtOAc (5 mL × 3). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The obtained residue was purified by silica gel chromatography to afford the title compound as colorless oil, 106.8 mg, 96% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 – 7.30 (m, 1H), 7.29 – 7.25 (m, 1H), 7.25 – 7.18 (m, 4H), 7.14 – 7.09 (m, 2H), 5.78 (d, *J* = 1.2 Hz, 1H), 5.18 (d, *J* = 1.2 Hz, 1H), 2.46 (q, *J* = 7.6 Hz, 2H), 2.36 (s, 3H), 1.11 – 1.05 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 149.1, 142.3, 141.4, 138.2, 137.5, 130.3, 129.1, 128.5, 127.7, 126.5, 125.7, 114.1, 26.4, 21.3, 15.4.

HRMS (EI-TOF): calculated for $[C_{17}H_{18}O\ (M)]^+$: 222.1409, found: 222.1411.

1-ethyl-2-(4-methylbenzyl)benzene (6):



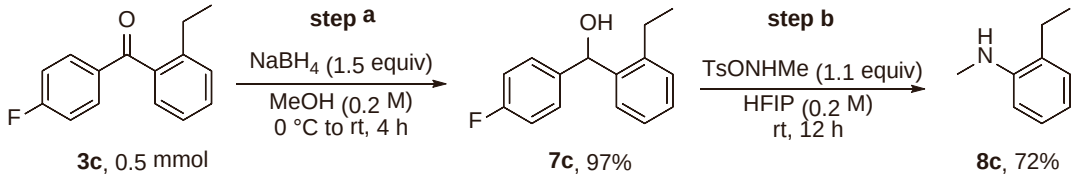
To a suspension of anhydrous $AlCl_3$(166.7 mg, 1.25 mmol) and $NaBH_4$ (85.1 mg, 2.25 mmol) in anhydrous THF (4 mL) was added a solution of ketone **3a** (112.5 mg, 0.5 mmol) in THF (1 mL) at 0ºC. Then the resulting mixture was warmed to 60 ºC for 5 h. After that, the mixture was treated with saturated aqueous Rochelle Salt solution (5 mL) and extracted with EtOAc (5 mL × 3). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The obtained residue was purified by silica gel chromatography to afford the title compound as colorless oil, 78.2 mg, 74% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28 – 7.22 (m, 2H), 7.22 – 7.17 (m, 1H), 7.16 – 7.11 (m, 3H), 7.09 – 7.05 (m, 2H), 4.04 (s, 2H), 2.68 (q, *J* = 7.6 Hz, 2H), 2.37 (s, 3H), 1.22 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 142.5, 138.6, 138.0, 135.5, 130.4, 129.2, 128.7, 128.5, 126.7, 126.0, 38.4, 25.9, 21.1, 15.0.

HRMS (EI-TOF): calculated for $[C_{16}H_{18}O\ (M)]^+$: 210.1409, found: 210.1412.

2-ethyl-*N*-methylaniline (8c):



3c, 0.5 mmol **7c**, 97% **8c**, 72%

Step a: To a solution of ketone **3c** (114.1 mg, 0.5 mmol) in MeOH (2.5 mL) was added $NaBH_4$ (28.4 mg, 0.75 mmol) at 0 ºC. After stirring for 10 min, the mixture was warmed to room temperature for 4 h. Then the mixture was treated with saturated aqueous NH_4Cl solution (4 mL) and extracted with DCM (5 mL × 3). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The obtained residue was purified by silica gel chromatography to afford **7c** as colorless oil, 111.6 mg, 97% yield.

(2-ethylphenyl)(4-fluorophenyl)methanol (7c):

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49 – 7.40 (m, 1H), 7.35 – 7.18 (m, 5H), 7.08 – 6.95 (m, 2H), 6.06 (s, 1H), 2.75 – 2.54 (m, 2H), 2.20 (s, 1H), 1.15 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 162.2 (d, *J* = 245.6 Hz), 141.5, 140.7, 139.23 (d, *J* = 2.7 Hz), 128.9 (d, *J* = 5.7 Hz), 128.8, 128.1, 126.7, 126.3, 115.4 (d, *J* = 21.1 Hz), 72.1, 25.3, 15.4.

^{19}F NMR (565 MHz, $CDCl_3$): δ -115.02 – -115.10 (m).

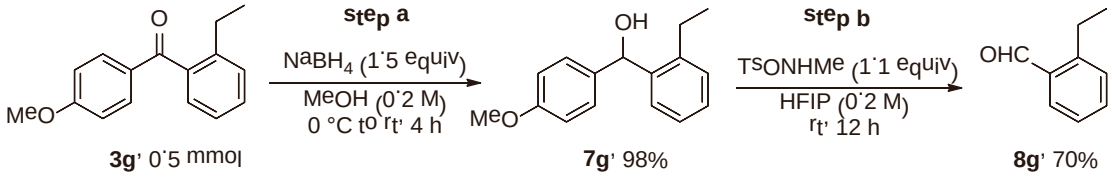
Step b: To a solution of **7c** (111.6 mg, 0.49 mmol) in HFIP (2.5 mL) was added TsONHMe (106.7 mg, 0.53 mmol) at room temperature under ambient atmosphere. The resulting mixture was stirred at room temperature for 12 h. Then the reaction was diluted with DCM (3 mL) and basified with saturated aqueous $NaHCO_3$ (3 mL) solution. The aqueous layer was extracted with DCM (5 mL × 3), and the combined organic layers were washed with brine (5 mL), dried over Na_2SO_4 and concentrated under reduced pressure. The obtained residue was purified by silica gel chromatography to afford the title compound as colorless oil, 47.3 mg, 72% yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.18 (t, *J* = 7.7 Hz, 1H), 7.09 (d, *J* = 7.4 Hz, 1H), 6.74 (t, *J* = 7.4 Hz, 1H), 6.65 (d, *J* = 8.0 Hz, 1H), 3.73 (brs, 1H), 2.91 (s, 3H), 2.50 (q, *J* = 7.5 Hz, 2H), 1.27 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$): δ 146.7, 127.74, 127.68, 127.2, 117.2, 109.6, 31.0, 23.8, 12.9.

The ^{1}H NMR and ^{13}C NMR of **8c** are consistent with the reported spectra[S55].

2-ethylbenzaldehyde (8g):



3g, 0.5 mmol **7g**, 98% **8g**, 70%

Step a: Following a similar procedure for the synthesis of **7c**, **7g** was prepared from ketone **3g** (120.2 mg, 0.5 mmol) and it was obtained as colorless oil, 118.7 mg, 98% yield.

(2-ethylphenyl)(4-methoxyphenyl)methanol (7g):

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 – 7.49 (m, 1H), 7.30 – 7.18 (m, 5H), 6.89 – 6.82 (m, 2H), 6.03 (s, 1H), 3.79 (s, 3H), 2.72 – 2.51 (m, 2H), 1.14 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 159.1, 141.4, 141.1, 135.8, 128.7, 128.5, 127.8, 126.5, 126.2, 113.9, 72.4, 55.4, 25.3, 15.2.

Step b: To a solution of **7g** (115.4 mg, 0.48 mmol) in HFIP (2.5 mL) was added TsONHMe (104.6 mg, 0.52 mmol) at room temperature under ambient atmosphere. The resulting mixture was stirred at room temperature for 12 h. Then the reaction was diluted with DCM (3 mL) and basified with saturated aqueous $NaHCO_3$ (3 mL) solution. The aqueous layer was extracted with DCM (5 mL × 3), and the combined organic layers were washed with brine (5 mL), dried over Na_2SO_4 and concentrated under reduced pressure. The obtained residue was purified by silica gel chromatography to afford the title compound as colorless oil, 44.8 mg, 70% yield.

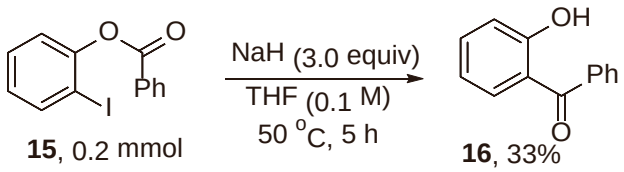
^{1}H NMR (400 MHz, $CDCl_3$): δ 10.29 (s, 1H), 7.82 (d, *J* = 7.6 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.30 (d, *J* = 7.6 Hz, 1H), 3.07 (q, *J* = 7.5 Hz, 2H), 1.27 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 192.5, 147.2, 134.1, 133.7, 131.9, 130.3, 126.5, 25.8, 16.4.

The ^{1}H NMR and ^{13}C NMR of **8g** are consistent with the reported spectra[S56].

7. Mechanism study

Fries rearrangement via an aryl anion



15, 0.2 mmol — **16**, 33%

To a solution of 2-iodophenyl benzoate **15** (64.8 mg, 0.2 mmol) in anhydrous THF (2 mL) was added NaH (60% dispersion in mineral oil, 24.0 mg, 0.6 mmol) at 50 °C stirring for 5 h. After that, the reaction was quenched with saturated aqueous NH_4Cl (2 mL) solution at 0 °C. The mixture was then extracted with EtOAc (3 mL × 4). The combined extracts were dried over Na_2SO_4, concentrated under vacuum. The resulting residue was purified by silica gel chromatography affording ketone **16** as yellow oil, 13.1 mg, 33% yield.

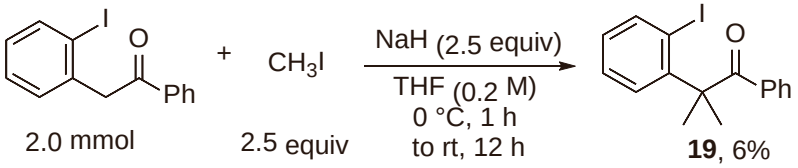
(2-hydroxyphenyl)(phenyl)methanone (16):

^{1}H NMR (400 MHz, $CDCl_3$): δ 12.04 (s, 1H), 7.68 (d, *J* = 7.4 Hz, 2H), 7.64 – 7.56 (m, 2H), 7.53 – 7.49 (m, 3H), 7.08 (d, *J* = 8.4 Hz, 1H), 6.88 (t, *J* = 7.5 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 201.8, 163.4, 138.0, 136.5, 133.7, 132.1, 129.3, 128.5, 119.3, 118.8, 118.5.

The ^{1}H NMR and ^{13}C NMR of **16** are consistent with the reported spectra[S57].

Preformed iodo ketone precursor for aryl anion engaged rearrangement



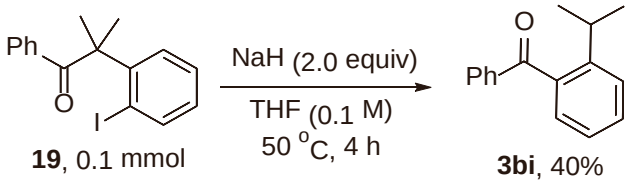
To a suspension of NaH (60% dispersion in mineral oil, 200 mg, 5 mmol) in anhydrous THF (5 mL) was added a solution of 2-(2-iodophenyl)-1-phenylethan-1-one (644.3 mg, 2 mmol) in THF (5 mL) at 0 °C stirring for 30 min. Then to the mixture was added CH_3I (311 μL, 5 mmol) at 0 °C for another 30 min. The resulting mixture was warmed to room temperature for 12 h. After that, the reaction was quenched with saturated aqueous NH_4Cl (10 mL) solution at 0 °C. The mixture was then extracted with EtOAc (10 mL × 3). The combined extracts were dried over Na_2SO_4, concentrated under vacuum. The resulting residue was purified by silica gel chromatography affording the desired product **19** as white solid, 41.7 mg, 6% yield.

2-(2-iodophenyl)-2-methyl-1-phenylpropan-1-one (19):

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.65 – 7.59 (m, 3H), 7.48 – 7.43 (m, 1H), 7.38 – 7.33 (m, 1H), 7.21 – 7.15 (m, 2H), 6.95 – 6.89 (m, 1H), 1.75 (s, 6H).

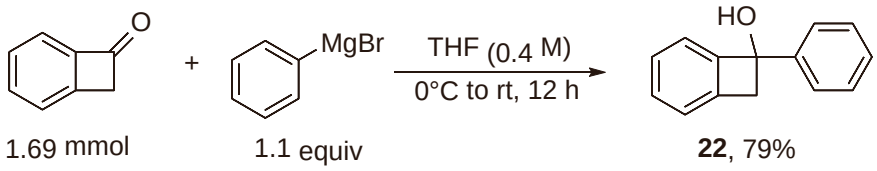
^{13}C NMR (101 MHz, $CDCl_3$): δ 202.9, 148.2, 142.6, 136.5, 132.1, 129.7, 129.0, 128.7, 128.0, 126.8, 98.5, 54.6, 28.1.

HRMS (ESI-TOF): calculated for $[C_{16}H_{16}IO\ (M + H)]^+$: 351.0246, found: 351.0247.



To a suspension of NaH (60% dispersion in mineral oil, 18 mg, 0.45 mmol) in anhydrous THF (1 mL) was added ketone **19** (35.0 mg, 0.1 mmol) respectively at 0 °C stirring for 5 min. The mixture was warmed to 50 °C for 4 h. After that, the reaction was quenched with saturated aqueous NH_4Cl (2 mL) solution at 0 °C. The mixture was then extracted with EtOAc (3 mL × 4). The combined extracts were dried over Na_2SO_4, concentrated under vacuum. The resulting residue was purified by silica gel chromatography affording *o*-alkylaryl ketone **3bi**, 8.9 mg, 40% yield.

Preformed benzocyclobutenol undergoes a NaH mediated ring opening



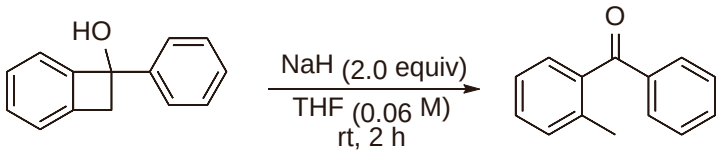
To a solution of bicyclo[4.2.0]octa-1,3,5-trien-7-one (200 mg, 1.69 mmol) in anhydrous THF (4 mL) was added PhMgBr (1 M in THF, 1.9 mL, 1.9 mmol) at 0 °C stirring for 30 min. The mixture was warmed to room temperature for 12 h. After that, the reaction was quenched with saturated aqueous NH_4Cl (5 mL) solution at 0 °C. The mixture was then extracted with EtOAc (5 mL × 3). The combined extracts were dried over Na_2SO_4, concentrated under vacuum. The resulting residue was purified by silica gel chromatography affording the desired product **22** as colorless oil, 262.1 mg, 79% yield.

7-phenylbicyclo[4.2.0]octa-1,3,5-trien-7-ol (22):

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52 (t, *J* = 1.8 Hz, 1H), 7.50 (dd, *J* = 1.9, 1.0 Hz, 1H), 7.43 – 7.25 (m, 7H), 3.77 – 3.63 (m, 1H), 3.63 – 3.54 (m, 1H), 3.00 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$): δ 149.3, 143.7, 142.3, 129.8, 128.4, 127.8, 127.5, 125.8, 124.2, 121.8, 81.5, 49.9.

HRMS (EI-TOF): calculated for $[C_{14}H_{12}O\ (M)]^+$: 196.0888, found: 196.0897.



22, 1.2 mmol **3ae**, 83%

To a solution of 7-phenylbicyclo[4.2.0]octa-1,3,5-trien-7-ol (50 mg, 0.25 mmol) in anhydrous THF (4 mL) was added NaH (60% dispersion in mineral oil, 20 mg, 0.5 mmol) at 0 °C stirring for 5 min. The mixture was warmed to room temperature for 2 h. After that, the reaction was quenched with saturated aqueous NH_4Cl (5 mL) solution at 0 °C. The mixture was then extracted with EtOAc (5 mL × 3). The combined extracts were dried over Na_2SO_4, concentrated under vacuum. The resulting residue was purified by silica gel chromatography affording *o*-alkylaryl ketone **3ae**, 41.5 mg, 83% yield.

8. Density functional theory (DFT) mechanistic study

8.1. Computational methods

All calculations were performed with the Gaussian 09 program.[S58] Geometry optimizations of all minima and transition structures were carried out using the hybrid B3LYP functional[S59] with the LANL2DZ[S60] basis set and pseudopotential for I and the 6-31+G(d)[S61] basis set for the other atoms in THF (ε = 7.4257) solvent with SMD[S62] model. The key word "5D" was used to specify that five d-type orbitals were used for all elements in the calculations. Frequency calculations at the same level were performed to confirm that each stationary point was either a minimum or a transition structure and to evaluate its zero-point energy and the thermal corrections at 298 K. Unless specified, transition-state structures were confirmed to connect their corresponding reactants and products by intrinsic reaction coordinate (IRC) calculations.[S63] A standard state of 298 K and 1 mol/L was used for calculating thermal corrections.[S64] The energy profile was drawn according to Gibbs free energies in solution (ΔG_{sol}). The computed structures were illustrated using CYLView.[S65] In order

to accelerate calculations, the ether coordinating to sodium (Na) center was simplified to dimethyl ether, mimicking tetrahydrofuran solvent.

8.2. Benzyne formation

Although, IRC for **TS1** (Scheme 6a) cannot be run here, we still locate both reactant and product in this step by geometry optimizations of structures with slightly changing C-I distances that are shorter or greater than 2.41 Å.

In addition to the benzyne formation pathway with $Na^+(ether)_2$ cation in Scheme 6a, possible processes with Na^+ cation and $Na^+(ether)$ cation were also taken into considerations in Figures S1 and S2, in which similar transition states could be located. The computed activation free energies for **TS1'** (with $Na^+(ether)$ cation) and **TS1"** (with Na^+ cation) are 9.0 and 9.6 kcal/mol, respectively.

For the nucleophilic attack of hydride to the electrophilic iodine (**TS1**, **TS1'** and **TS1"**), these two new pathways have similar results, compared to that in Scheme 6a. We found that the process with the adjacent iodine working as a directing group is quite easy, regardless of the ligand number on Na^+ cation. However, there are differences in the extrusion of the second iodide from **Int2**, **Int2'** and **Int2"** to benzyne. With the number of ether decreasing, this extrusion alters from an exergonic step of 3.5 kcal/mol (**Int2** to benzyne), to an exergonic step of 1.3 kcal/mol (**Int2'** to benzyne) and an endergonic step of 1.3 kcal/mol (**Int2"** to benzyne), which can be attributed to the destabilizing products Na(ether)I and NaI compared to $Na(ether)_2I$.

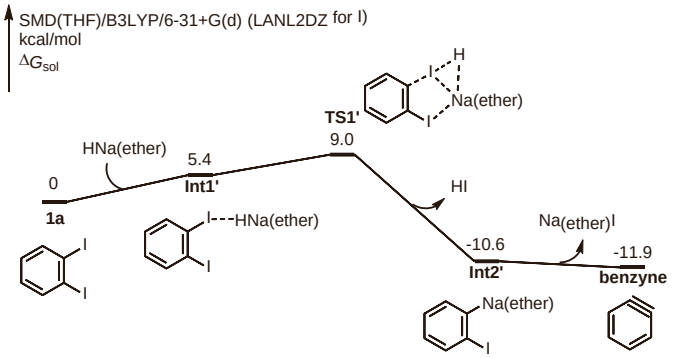


Figure S1. Benzyne formation with $Na^+(ether)$ cation.

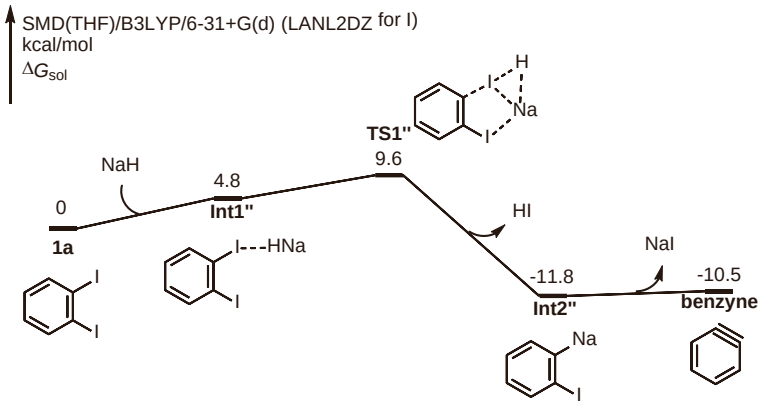


Figure S2. Benzyne formation with Na^+ cation.

For the extrusion of the second iodide in **Int2** that yields the key benzyne species, its corresponding transition state cannot be found. This extrusion is then demonstrated to be feasible by a flexible scan of the C-I bond in **Int2** (Figure S3). With the C-I bond of **Int2** increasing, single-point energies rise up steadily. However, the single-point energy increment is estimated to be 4.7 kcal/mol, which indicates that the extrusion of the second iodide in **Int2** is quite facile. This is also consistent with the exergonic process by 3.5 kcal/mol from **Int2** to benzyne in terms of the Gibbs free energy.

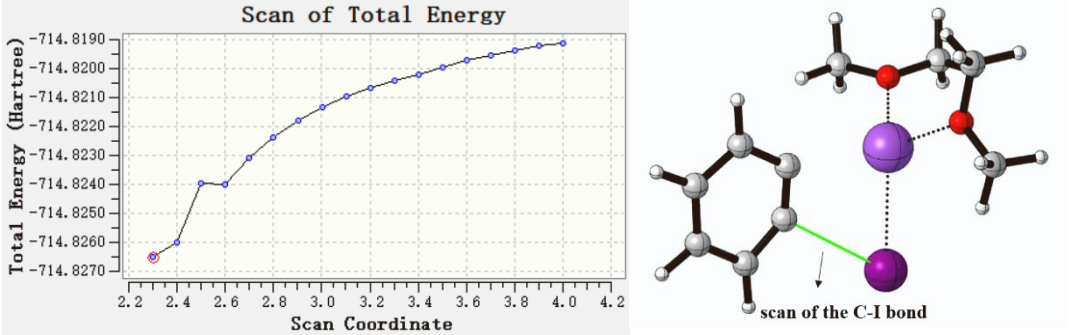


Figure S3. The scan of the C-I bond in **Int2.**

The reaction of mono-iodobenzene to form benzyne in the same conditions was also taken into considerations. As shown in Figure S4, we tried to explore the C-I cleavage of iodobenzene by using NaH. Because the result of benzyne formation with Na^+ cation is similar to that with $Na^+(ether)_2$ or $Na^+(ether)$ cation, no dimethyl ether is employed here to accelerate calculations. By a flexible scan of the C-I bond in Figure S5, it is found that single-point energies monotonously increase with the C-I bond being elongated. When the C-I bond is changed from 2.18 Å to 3.78 Å, it brings about a barrier of circa 32.9 kcal/mol in terms of the single-point energy. The single-point energy of the final point decreases, which can be attributed to the generation of stable phenyl sodium and hydrogen iodide (HI).

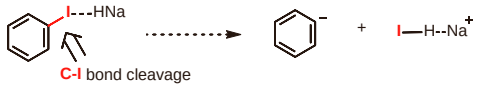


Figure S4. The reaction of mono-iodobenzene and NaH.

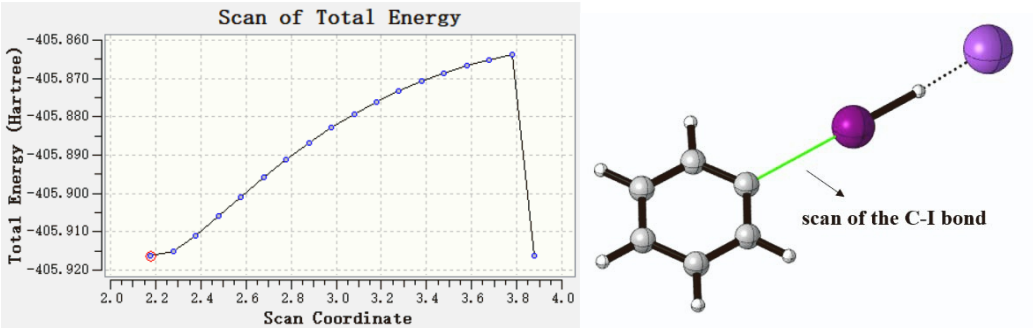


Figure S5. The scan of the C-I bond of iodobenzene with NaH.

8.3. The reaction of 2-iodophenyl benzoate 15 and NaH

The nucleophilic attack of hydride to the electrophilic iodine in 2-iodophenyl benzoate **15** was also investigated, in which the ester group acts as a directing group. As shown in Figure S6, a complexation between **15** and solvated NaH ($HNa(ether)_2$) to afford the complex **Int6** is firstly required, which is endergonic by 4.1 kcal/mol. Then, **Int6** can be converted to the phenyl sodium intermediate **Int7** and HI via NaH-mediated C-I bond dissociation transition state **TS4** by using ester as the directing group. This step is exergonic by 13.8 kcal/mol (from **Int6**), which has an activation free energy of 2.6 kcal/mol (from **Int6**). Overall, the reaction of **15** and NaH to give **Int7** has only a barrier of 6.7 kcal/mol. This feasible transformation and previous calculations demonstrate that both ester and iodide can directly facilitate the NaH-mediated dissociation of the C-I bond.

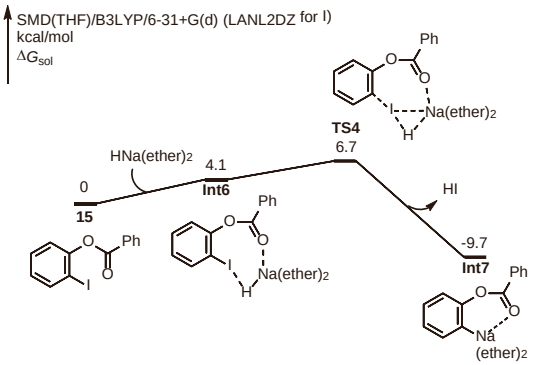


Figure S6. The energy profile for the reaction of **15** and NaH.

8.4. Regioselectivity of 2a and 1g

In fact, the regioselectivity of this reaction is determined at the nucleophilic attack of the formed enolate intermediate to aryne. The formed enolate intermediate is proposed to be a tetrameric aggregate according to Collum's work.[S66] However, we can only find it as a barrierless process through a flexible scan of the C-C bond in enolate tetramer **ET** and benzyne in Figure S7. As shown below, with the C-C bond in **ET** and benzyne shortening, single-point energies decrease steadily.

Although the barrierless nucleophilic attack is disclosed, the reaction of **2a** and **1g** still possesses high regioselectivity due to steric repulsions between large phenyl group (R^L) in **1g** and the tetrahydrofuran (L) and enolate (R) in **B**, which prevents the formation of its **D**. Hence, only single isomer product **1g** can be obtained because a small hydrogen group (R^S) in **1g** is oriented toward **ET** in **A** that leads to **C**.

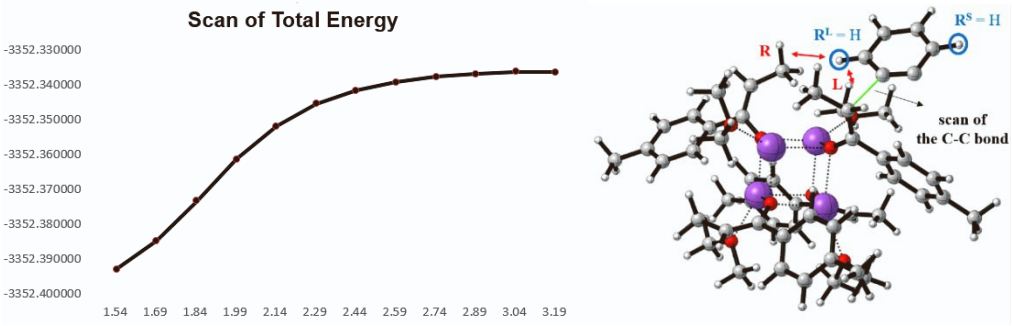


Figure S7. The scan of the C-C bond in **ET** and benzyne.

The reaction model of enolate monomer **EM** from **2a** and aryne from **1g** is also found to be a barrierless step, in which no regiochemistry can be observed (Figures S8-S10). In Figures S9 and S10, we conducted flexible scans of the C-C bond in enolate monomer **EM** from **2a** and aryne from **1g** to generate **Int8** and **Int8'**, respectively. During our calculations, Na^{+}(ether) cation coordinates with carbonyl group in **EM** and carbon anion in aryne at the same time. Both results display that single-point energies increase monotonously as the C-C bond is elongated from 1.80 Å to 3.20 Å, which indicates that generations of **Int8** and **Int8'** are barrierless and no regiochemistry can be observed between **4g** and **4g'**. Therefore, this possibility can be ruled out.

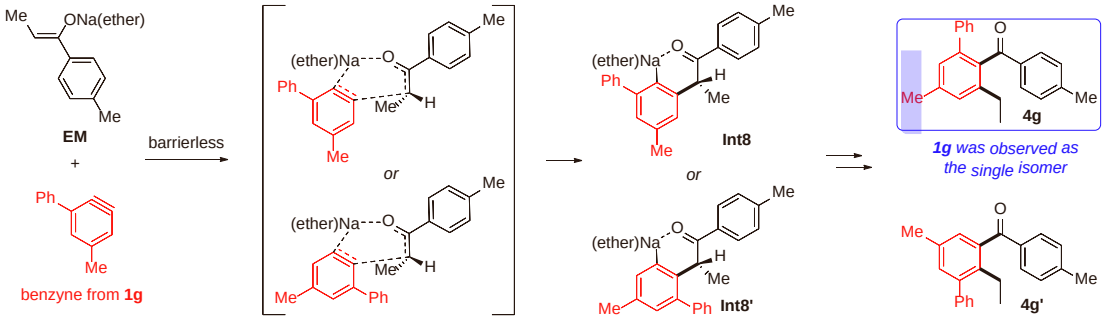


Figure S8. The reaction model of **EM** and aryne

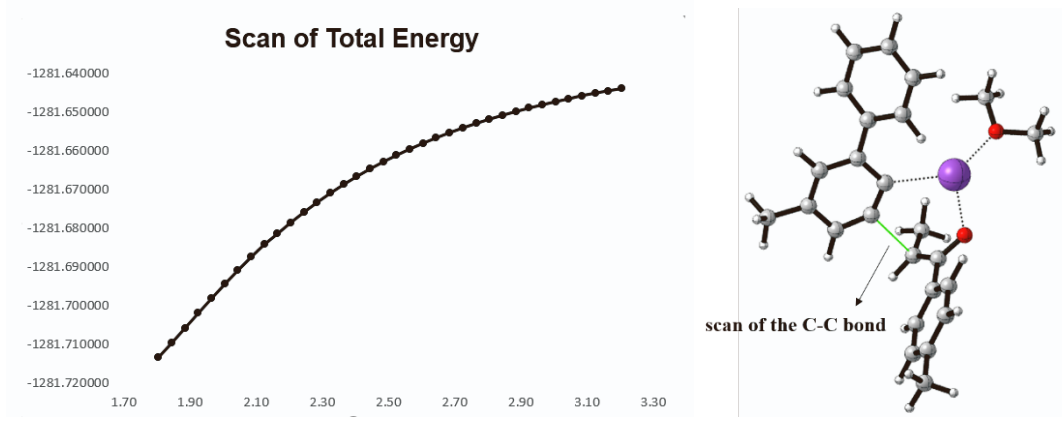


Figure S9. The flexible scans of the C-C bond to **Int8.**

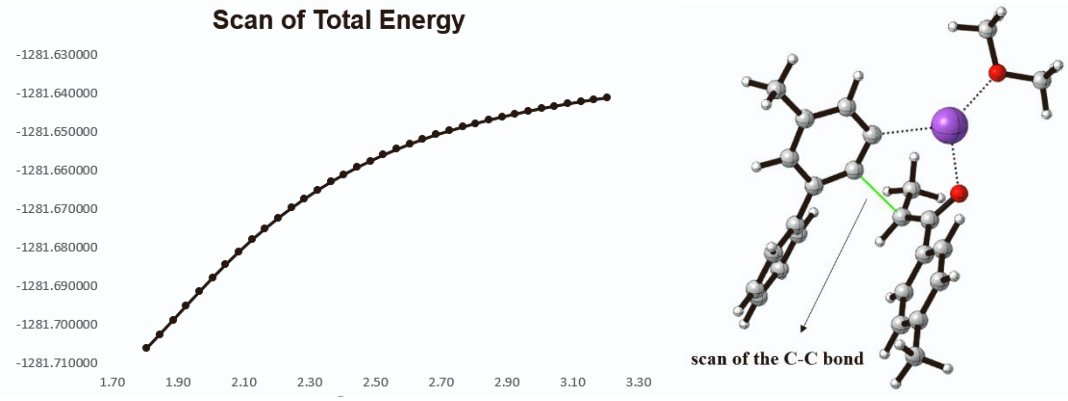


Figure S10. The flexible scans of the C-C bond to **Int8'.**

8.5. The formation of 3a with Na^+ cation

For the formation of product **3a**, another possible pathway starting from monomer **Int3'** with Na^+ cation has also been calculated (Figure S11). This energy profile indicates that ring opening via **TS3'** remains to be the rate-determining step in the Fries-type rearrangement of **Int3'** rather than intramolecular nucleophilic attack of the carbonyl group by aryl nucleophile via **TS2'**, which is similar to that in Scheme 6c. Overall, the energy barrier of the Fries-type rearrangement of **Int3'** is 14.5 kcal/mol, which is a facile process.

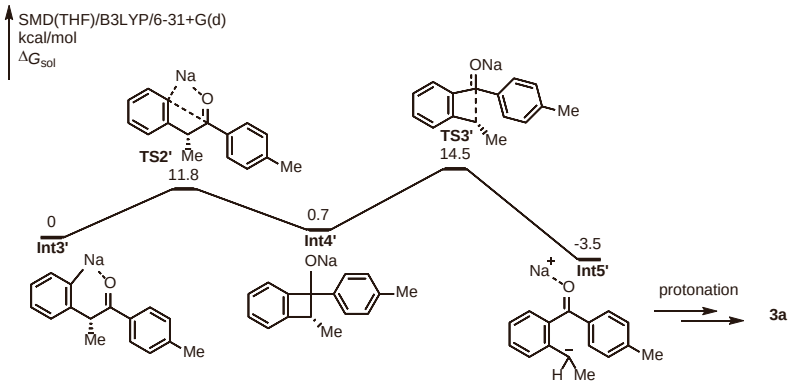


Figure S11. The formation of **3a** with Na^+ cation.

8.6. Anion-accelerated 4-membered ring opening

As shown in Scheme7c, the stable benzocyclobutenol **22** could be isolated, which was smoothly transformed to ketone product **3ae** in the alkaline condition. This is also supported by our calculations. In Figure S12, the ring opening of benzocyclobutenol **Int4"** is quite difficult with a quite high barrier of 32.1 kcal/mol compared to the Na^+(ether)-cation-bonded **Int4** (13.8 kcal/mol in Scheme 6c). It indicates that **22** is stable enough to be obtained but reactive after removing proton of the hydroxyl group. This ring opening step is endergonic by 10.9 kca/mol, which can be attributed to the formation of dearomative product **Int5"** (Figure S12).

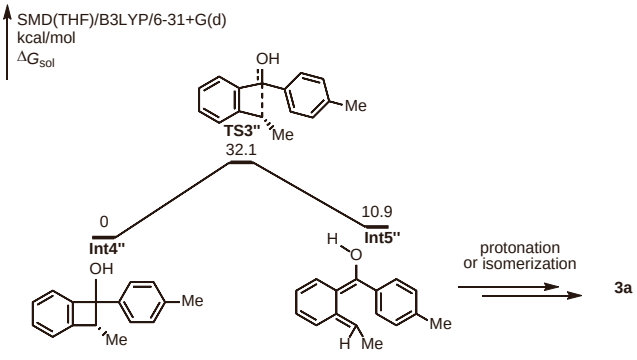


Figure S12. Ring opening of **Int4"**

As shown in Scheme 4 of the main text, 1,2-diiodocyclohex-1-ene **1s** and **2a** could also take place the same reaction to afford product **4s** that might undergo a 4π-electrocyclic ring opening process. The possible 4π-electrocyclic ring openings were also taken into considerations in Figures S13-S15 (the ether in them is dimethyl ether). In the presence

of NaH, ring openings of **Int9** and **Int9'** are very feasible. The subsequent protonation gives final products, which could be conjugated or non-conjugated, depending on the substituents and reaction conditions. The activation free energies are 13.5 kcal/mol for **Int9** with Na^+(ether) cation and 13.4 kcal/mol for **Int9'** with Na^+ cation, respectively. However, for the protonate intermediate **Int9''**, it has a higher computed activation free energy of 28.2 kcal/mol, which is similar to the result of **Int4''**. This is similar to oxy-Cope and anionic oxy-Cope rearrangements, where anion helps the C-C cleavage due to weakening the C-C bond connected to anion, as suggested by Houk and co-workers.[S67-S69]

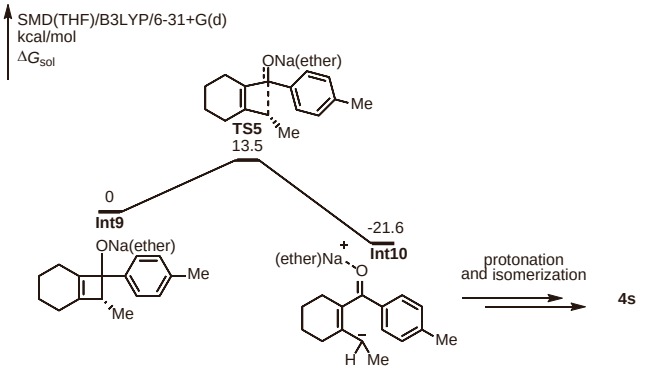


Figure S13. 4π-Electrocyclic ring opening of **Int9**

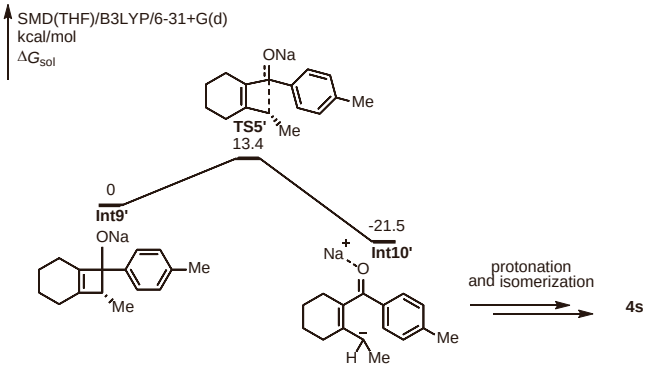


Figure S14. 4π-Electrocyclic ring opening of **Int9'**

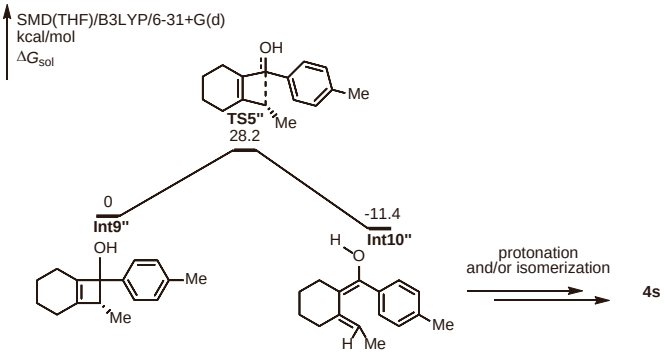


Figure S15. 4π-Electrocyclic ring opening of **Int9''**

8.7. Energy data

	G_{sol} [a]		G_{sol} [a]
1a	-253.765824	**15**	-662.515600
HNa(ether)$_2$	-472.854973	**Int6**	-1135.361070

Int1	-726.611123	**TS4**	-1135.356984
TS1	-726.604838	**Int7**	-1123.392587
Int2	-714.644198	**Int8**	-1281.342438
HI	-11.993484	**Int8'**	-1281.335066
Na(ether)$_2$I	-483.775616	**Int3'**	-856.076498
benzyne	-230.877184	**TS2'**	-856.057645
ET	-3120.488344	**Int4'**	-856.075342
Int3	-1011.057054	**TS3'**	-856.053380
TS2	-1011.040327	**Int5'**	-856.082094
Int4	-1011.059511	**Int4"**	-694.327550
TS3	-1011.037548	**TS3"**	-694.276436
Int5	-1011.064985	**Int5"**	-694.310220
HNa(ether)	-317.877466	**Int9**	-1013.411418
Int1'	-571.631594	**TS5**	-1013.389838
TS1'	-571.625855	**Int10**	-1013.445804
Int2'	-559.666651	**Int9'**	-858.428728
Na(ether)I	-328.794548	**TS5'**	-858.407439
NaH	-162.892609	**Int10'**	-858.463132
Int1"	-416.647694	**Int9"**	-696.685257
TS1"	-416.639978	**TS5"**	-696.640379
Int2"	-404.683593	**Int10"**	-696.703409
NaI	-173.807394		

[a] Computed at SMD(THF)/B3LYP/6-31+G(d) (LANL2DZ for I) level

8.8. Cartesian coordinates of all stationary points

1a

C	0.70043500	0.92828800	-0.00000800
C	1.39376100	2.14748000	-0.00000800
C	0.69834700	3.35748500	0.00000800
C	-1.39377900	2.14760300	-0.00000400
C	-0.70037000	0.92845300	-0.00000200
H	2.47922200	2.14859300	-0.00001400
H	1.25193200	4.29264800	0.00001500
H	-2.47925400	2.14878900	-0.00000400
I	1.89013700	-0.84985400	0.00000100
I	-1.89015400	-0.84985200	0.00000000
C	-0.69828100	3.35760700	0.00000200
H	-1.25168600	4.29286000	0.00001500

HNa(ether)$_2$

Na	-0.01964500	-1.35665900	-0.08760700
C	3.00804500	-0.34541500	0.63982700
H	2.79086200	-1.22580500	1.25056700
H	3.35729700	0.47046100	1.28786100
H	3.79216800	-0.59326600	-0.08879900
O	1.79957500	0.02586600	-0.02600000
C	1.96312700	1.17560100	-0.85619900
H	2.71726500	0.98961900	-1.63367800
H	0.99940900	1.38064300	-1.33014200
H	2.26739300	2.04551800	-0.25749500
C	-3.10873500	-0.37854400	-0.32098300
H	-3.00500400	-1.38306500	-0.73943600
H	-3.53424100	0.29212400	-1.08048200
H	-3.77895100	-0.41529800	0.54902600
O	-1.80585200	0.06349200	0.06561800
C	-1.81948800	1.37004100	0.63902100
H	-2.45069100	1.39247900	1.53850400
H	-0.79174700	1.62100400	0.91332500
H	-2.19459000	2.10722200	-0.08481200
H	-0.16056100	-3.40335400	-0.28770200

Int1

C	-2.51677100	1.13390400	-0.28911800
C	-2.95696200	2.45312400	-0.48772600
C	-4.30432700	2.79813700	-0.36054600
C	-4.82624400	0.49997600	0.17309500
C	-3.47074300	0.16865500	0.04009400

H	-2.23210900	3.22083700	-0.74587400
H	-4.61631700	3.82747200	-0.52047500
H	-5.55265300	-0.26410700	0.43125600
I	-0.35365400	0.76830300	-0.52184000
I	-2.97198100	-1.90356200	0.37003900
Na	3.99884000	0.11183700	-0.16982700
H	2.05386900	0.41287600	-0.81119500
O	4.84231300	0.52417400	1.90734600
O	5.73305800	-0.59816700	-1.45733800
C	5.37653800	-0.47279100	2.77930400
H	5.55668100	-1.37172300	2.18353000
H	6.32381000	-0.13245200	3.22017700
H	4.66527700	-0.70666000	3.58351500
C	4.55702800	1.74859000	2.58782400
H	5.47204400	2.16395800	3.03216800
H	4.16158900	2.45199600	1.85012700
H	3.80827100	1.58929000	3.37569100
C	7.11655400	-0.51494100	-1.11510400
H	7.64155800	0.17690300	-1.78841700
H	7.17971100	-0.14096700	-0.08985800
H	7.58965900	-1.50518200	-1.17194000
C	5.52387200	-1.07657700	-2.78800100
H	5.93774900	-2.08776400	-2.90402000
H	4.44509700	-1.10365200	-2.96214900
H	5.99373600	-0.40416100	-3.51894300
C	-5.24295300	1.81767200	-0.02754100
H	-6.29546800	2.06934800	0.07623100

TS1

C	-2.42797400	0.66661900	0.02489200
C	-3.67647000	1.31477300	0.07487500
C	-4.88055000	0.60381000	0.01837500
C	-3.63688800	-1.46761500	-0.14308400
C	-2.46409200	-0.70702700	-0.08334800
H	-3.70970000	2.40118500	0.16024000
H	-5.83057300	1.13331900	0.05899600
H	-3.61075200	-2.55028800	-0.22762400
I	-0.44109600	2.02616500	0.14552500
I	-0.59891300	-1.90921400	-0.18320700
Na	1.96234700	0.22688200	0.05440200
H	1.26924300	3.02630500	0.23948300
O	3.15001000	-0.38691100	1.87911800
O	3.29489200	0.12244900	-1.76605800
C	4.56861500	-0.23417600	1.95738200
H	4.93595600	-0.04733300	0.94487800
H	4.83264900	0.61394800	2.60382400
H	5.03297900	-1.14958400	2.34935000
C	2.55708100	-0.65377600	3.15277100
H	2.74805000	0.17375800	3.84941900
H	1.48023400	-0.75919400	2.99945100
H	2.95760800	-1.58592200	3.57421900
C	3.42292500	1.20981700	-2.68668600
H	2.93845900	0.96559500	-3.64182900
H	2.93174900	2.07839100	-2.24069900
H	4.48263200	1.44002400	-2.86260200
C	3.91352700	-1.07378200	-2.24260500
H	4.98731300	-0.91214400	-2.40977700
H	3.77845300	-1.84412200	-1.47838300
H	3.44557300	-1.40535100	-3.17971600
C	-4.86059900	-0.79175600	-0.09084900
H	-5.78787300	-1.35832100	-0.13536700

Int2

C	1.09103200	1.37902700	0.38108400
C	1.76647000	2.57749000	0.74621300
C	3.16320000	2.68889000	0.79633000
C	3.36272600	0.37551400	0.10899200
C	1.96704500	0.36651500	0.08913900
H	1.18002300	3.46279100	1.00271600
H	3.62853000	3.63145400	1.08234000
H	3.96387600	-0.49295800	-0.14288100
I	1.09108500	-1.66632900	-0.53884600
Na	-1.22819900	0.61151800	0.16924300
C	3.96582500	1.58524200	0.47790600
H	5.05108100	1.65620200	0.51259600
C	-4.04962000	1.44985200	-1.37890600
H	-4.32655700	1.24727900	-0.34099300
H	-4.70779500	0.87948100	-2.04937300
H	-4.16704300	2.52331000	-1.58392700
O	-2.69049600	1.04877800	-1.54787200
C	-2.21021700	1.28588100	-2.87254600
H	-2.25420200	2.35668200	-3.11567500
H	-1.17182500	0.94710400	-2.91145500
H	-2.80461200	0.72193700	-3.60486200
C	-3.42720400	-1.32405500	1.70152300
H	-3.63222600	-1.43260800	0.63317000
H	-4.37176000	-1.15585000	2.23771700
H	-2.95643800	-2.24369700	2.07609100

O	-2.55355700	-0.20650800	1.86146100
C	-2.20637000	0.02606900	3.22766700
H	-1.68921500	-0.84562400	3.65199700
H	-1.53876700	0.89126100	3.25438100
H	-3.10527500	0.24127400	3.82216400

HI

I	0.00000000	0.00000000	0.03026200
H	0.00000000	0.00000000	-1.60387500

Na(ether)$_2$I

I	2.31748600	-0.06551100	0.00290000
Na	-0.63717000	0.01276900	-0.05721900
C	-1.99370000	-2.82930900	-0.92770600
H	-1.44603600	-2.46986800	-1.80294800
H	-3.00879600	-3.12194800	-1.22890900
H	-1.47328200	-3.69892100	-0.50427400
O	-2.04394900	-1.75935000	0.02000000
C	-2.75463400	-2.11495400	1.20820100
H	-2.26440900	-2.95624100	1.71686800
H	-2.75435500	-1.24192000	1.86657900
H	-3.79136500	-2.38767200	0.96822800
C	-1.33609700	3.16817300	0.36871300
H	-0.33408000	2.98868600	0.76650000
H	-1.96504700	3.61714100	1.14954100
H	-1.27085000	3.85376700	-0.48705000
O	-1.87096200	1.90563500	-0.03903100
C	-3.18534700	2.01993200	-0.58725900
H	-3.17832200	2.66231100	-1.47860800
H	-3.51517100	1.01571100	-0.86597200
H	-3.87824200	2.43725400	0.15629900

benzyne

C	-1.46723200	-0.13346600	0.00001700
C	-0.62634000	-1.23789700	-0.00001200
C	0.62649400	-1.23790800	-0.00000900
C	1.46722600	-0.13332700	0.00001800
C	0.70476900	1.05877500	-0.00000600
C	-0.70488200	1.05871100	-0.00000200
H	-2.55208600	-0.13579700	0.00000100
H	2.55208200	-0.13553200	0.00000200
H	1.23159100	2.01105900	-0.00001900
H	-1.23179800	2.01094300	-0.00002200

ET

C	-6.40625700	-1.11168000	1.53645100
C	-5.31185300	-0.38754200	2.01038500
C	-3.99002100	-0.81435700	1.76886000
C	-3.82463900	-1.98559800	1.01192300
C	-4.92333800	-2.71181100	0.53957800
C	-6.23659500	-2.29313900	0.79301700
H	-7.41267100	-0.74655800	1.73692900
H	-5.48706900	0.53239600	2.56218100
H	-2.82203200	-2.34916000	0.80892700
H	-4.75266700	-3.62085200	-0.03463000
C	-2.78771400	-0.06567600	2.28018700
C	-2.87005600	0.59214000	3.47622500
H	-3.80604500	0.55167000	4.02683900
O	-1.69267600	-0.11548400	1.52678800
C	-1.74114600	1.37101700	4.09937300
H	-1.88828900	1.47856700	5.18151000
H	-0.76877000	0.87735900	3.95975600
H	-1.64721400	2.39464800	3.69878600
C	-7.42916100	-3.06903300	0.28305600
H	-7.11712300	-3.95904300	-0.27452200
H	-8.07469000	-3.39911700	1.10798300
H	-8.05133400	-2.45672700	-0.38350400
O	-0.59258800	-3.61063800	2.45067100
C	-0.03081200	-4.87683800	2.11024300
H	-0.82180300	-5.62968500	1.98335800
H	0.50630700	-4.75753500	1.16639500
H	0.66657900	-5.21677400	2.88984400
C	-1.35586400	-3.66053100	3.65485500
H	-1.75208400	-2.65925700	3.83953100
H	-2.19245900	-4.36604000	3.55199300
H	-0.72784800	-3.96816900	4.50348800
Na	0.07262500	-1.58640000	1.48791000
C	-3.93996800	3.87475200	-2.99172000
C	-2.57279500	3.65468500	-2.81863300
C	-2.07082500	3.02705000	-1.66066300
C	-3.01049800	2.60519000	-0.70441800
C	-4.38050600	2.83266500	-0.87700800
C	-4.87435900	3.47530300	-2.02040400
H	-4.28986300	4.35954400	-3.90228500
H	-1.88320500	3.96545000	-3.59935600
H	-2.67077000	2.11238500	0.20332000
H	-5.07422000	2.50533000	-0.10480400
C	-0.59429000	2.82761200	-1.42673100

C	0.25509100	3.82779600	-1.81053000
H	-0.18410400	4.72272900	-2.24578400
O	-0.23604800	1.70082700	-0.81352900
C	1.74539200	3.84342200	-1.60830700
H	2.03817400	4.35831000	-0.67768100
H	2.16973100	2.83573700	-1.56608900
H	2.24918900	4.37719800	-2.42687800
C	-6.35259500	3.72367800	-2.21437500
H	-6.93344800	3.36052100	-1.35933000
H	-6.56624300	4.79410900	-2.33513800
H	-6.72976900	3.21922400	-3.11419800
Na	-1.56784300	-0.21473200	-0.82099700
O	-2.84548200	-0.62029800	-2.74171800
C	-2.20562300	-0.95840100	-3.96978200
H	-2.38441500	-0.18067000	-4.72631700
H	-1.13345300	-1.03584900	-3.77443500
H	-2.57234900	-1.92251100	-4.34986900
C	-4.26394500	-0.56006400	-2.86576300
H	-4.66896700	-1.53989200	-3.15759900
H	-4.66930200	-0.27630500	-1.89262500
H	-4.55704300	0.18904200	-3.61470300
C	3.94026800	-3.87494700	-2.99102800
C	2.57304600	-3.65538900	-2.81767600
C	2.07109500	-3.02769800	-1.65973400
C	3.01080800	-2.60530300	-0.70376700
C	4.38086600	-2.83226600	-0.87661900
C	4.87471900	-3.47492100	-2.02000700
H	4.29015100	-4.35978300	-3.90157500
H	1.88339600	-3.96657800	-3.59817800
H	2.67108700	-2.11244000	0.20394400
H	5.07462400	-2.50451200	-0.10463000
C	0.59454100	-2.82861600	-1.42561600
C	-0.25459600	-3.82924200	-1.80879400
H	0.18481300	-4.72422600	-2.24373500
O	0.23610000	-1.70163500	-0.81288100
C	-1.74485400	-3.84528100	-1.60633900
H	-2.03738400	-4.36107100	-0.67613200
H	-2.16930100	-2.83769400	-1.56312500
H	-2.24875400	-4.37838400	-2.42529500
C	6.35300700	-3.72276500	-2.21425500
H	6.93394500	-3.35887800	-1.35957700
H	6.56708100	-4.79317500	-2.33446400
H	6.72971100	-3.21866500	-3.11447100
Na	1.56789100	0.21389200	-0.82102800
O	2.84538000	0.61835900	-2.74213200
C	4.26403300	0.56085100	-2.86525300
H	4.66928200	0.27751100	-1.89194600
H	4.55905900	-0.18743500	-3.61426000
H	4.66740400	1.54154400	-3.15647200
C	2.20568200	0.95563000	-3.97050600
H	2.38597800	0.17819500	-4.72698500
H	1.13330100	1.03153700	-3.77570900
H	2.57122000	1.92028600	-4.35035000
C	6.40604100	1.11322900	1.53740900
C	5.31177200	0.38871400	2.01107000
C	3.98984500	0.81501600	1.76913900
C	3.82424700	1.98612600	1.01204700
C	4.92281400	2.71272100	0.53998000
C	6.23615400	2.29457300	0.79384100
H	7.41253400	0.74850700	1.73822400
H	5.48718000	-0.53110500	2.56300200
H	2.82156800	2.34930200	0.80872400
H	4.75197100	3.62165900	-0.03434100
C	2.78767900	0.06599500	2.28030300
C	2.87006400	-0.59179500	3.47635200
H	3.80597300	-0.55106000	4.02708000
O	1.69270100	0.11547500	1.52679400
C	1.74129600	-1.37097600	4.09938000
H	0.76884300	-0.87738900	3.96001900
H	1.64743200	-2.39450500	3.69851800
H	1.88856400	-1.47881700	5.18146900
C	7.42857200	3.07086000	0.28413300
H	7.11636400	3.96111300	-0.27295900
H	8.07417600	3.40058500	1.10914100
H	8.05072200	2.45896200	-0.38282900
O	0.59211500	3.61101700	2.44976500
C	0.03063100	4.87707600	2.10833000
H	0.82177000	5.62972600	1.98120200
H	-0.50619900	4.75722900	1.16438700
H	-0.66696200	5.21761700	2.88748500
C	1.35515400	3.66161100	3.65406600
H	1.75118200	2.66040100	3.83950000
H	2.19187800	4.36692100	3.55089200
H	0.72701600	3.96992000	4.50236400
Na	-0.07262000	1.58638500	1.48741400

Int3

C	4.15978200	-0.04238900	-0.14089400

C	2.90024100	0.30434700	0.35249200
C	1.87042400	-0.64989200	0.42470800
C	2.14864200	-1.96171400	-0.01138100
C	3.40716300	-2.30318500	-0.49312200
C	4.43921100	-1.34825700	-0.56900900
H	4.93721900	0.71628700	-0.19477200
H	2.72882500	1.32821800	0.66535300
H	1.36283700	-2.70901500	0.03851300
H	3.59857800	-3.32395600	-0.81835000
C	0.50233500	-0.33999700	0.93585200
C	0.18402400	1.02940600	1.52336700
H	1.10899000	1.44692300	1.93174200
O	-0.38050800	-1.20844500	0.86258400
C	-0.82015200	0.92198900	2.68487800
H	-0.94864600	1.90854100	3.14540200
H	-1.80475200	0.58611300	2.34444300
H	-0.46736800	0.22581200	3.45675100
C	5.80043200	-1.72898300	-1.09514200
H	6.25607700	-2.51441600	-0.47780000
H	5.73138800	-2.12485100	-2.11675200
H	6.48022500	-0.87081600	-1.10821800
C	0.38232700	3.20287500	0.26451000
C	-0.31745600	1.98957200	0.41024900
C	-1.45647600	1.66033400	-0.37050800
C	-1.83314800	2.66319900	-1.29771700
C	-1.15506300	3.88298700	-1.46101300
C	-0.03426900	4.15674400	-0.67100600
H	1.25113700	3.41500700	0.88942300
H	-2.70301000	2.49616400	-1.94007900
H	-1.49639900	4.61226300	-2.19627200
H	0.50709500	5.09535500	-0.77584200
C	-3.99941200	-3.45453200	-0.17566200
H	-2.99857600	-3.66229800	0.21226300
H	-4.13269500	-3.97196800	-1.13590000
H	-4.74939400	-3.81810300	0.54037400
O	-4.11029100	-2.04053700	-0.34561500
C	-5.39073800	-1.64581100	-0.84183100
H	-6.18428600	-1.94214200	-0.14203400
H	-5.38405600	-0.55700100	-0.94150900
H	-5.58288500	-2.10013900	-1.82364000
Na	-2.39191900	-0.56948100	-0.04558900

TS2

C	3.81045600	0.01066300	-0.59397400
C	2.62252500	0.50295600	-0.05400800
C	1.67469600	-0.36121300	0.52635200
C	1.97272500	-1.73105200	0.54322200
C	3.16301000	-2.22357900	-0.00342900
C	4.10587000	-1.36456100	-0.58376400
H	4.52231200	0.70694400	-1.03496300
H	2.43329400	1.57135500	-0.10216600
H	1.26236400	-2.41089600	1.00447900
H	3.36307900	-3.29345800	0.02888900
C	0.37182100	0.11136100	1.16259600
C	0.32300300	1.60991500	1.64588700
H	1.33747800	1.96847100	1.87418300
O	-0.32161100	-0.77136300	1.77753400
C	-1.04742500	1.33690600	-1.72962200
C	-0.56221900	1.08926700	-0.43307900
C	-0.23065500	2.19444500	0.37191900
C	-0.37807500	3.51615000	-0.05909800
C	-0.88859900	3.74127600	-1.34780100
C	-1.21916500	2.66101900	-2.17782400
H	-1.29375800	0.52151300	-2.41374800
H	-0.10154500	4.35976500	0.57291800
H	-1.01908500	4.75945900	-1.70935400
H	-1.60474000	2.85166700	-3.17887900
C	5.39387900	-1.88577000	-1.17743500
H	6.26937400	-1.41814600	-0.70772700
H	5.45477300	-1.67016400	-2.25273700
H	5.48238700	-2.97018600	-1.04816500
Na	-1.91986300	-0.93180200	0.30148000
O	-3.78439100	-2.03754600	-0.32937300
C	-4.97025200	-1.38391000	-0.78982800
H	-5.24912200	-1.74952200	-1.78743700
H	-4.75715300	-0.31286800	-0.84331700
H	-5.80119400	-1.55636400	-0.09240200
C	-3.94299800	-3.45501600	-0.22658300
H	-2.99585800	-3.86832800	0.13051400
H	-4.18201000	-3.88768500	-1.20754300
H	-4.74095500	-3.70357000	0.48616400
C	-0.54915300	1.82520200	2.88758100
H	-0.14143900	1.29588300	3.75703100
H	-0.59585200	2.89465200	3.13067300
H	-1.57249500	1.46821300	2.72533600

Int4

C	4.15472500	0.29752300	-0.64579800

C	2.84375800	0.63165000	-0.29969300
C	1.94257900	-0.34017800	0.17362300
C	2.40973500	-1.65535400	0.27995300
C	3.72596200	-1.99103900	-0.06475800
C	4.62440700	-1.02357400	-0.53455200
H	4.82530900	1.07412100	-1.01223700
H	2.52049400	1.66544400	-0.40578300
H	1.71692700	-2.41179000	0.63696600
H	4.05731000	-3.02437000	0.03135200
C	0.49696900	-0.00826300	0.58502300
C	0.44193500	1.18337500	1.73508300
H	1.43707700	1.58377300	1.97374700
O	-0.25659300	-1.10646300	0.84103500
C	-0.75256800	1.25856900	-1.58222500
C	-0.20099900	1.05719000	-0.31768500
C	-0.29106300	2.01663300	0.69353700
C	-0.92548000	3.24014800	0.49261500
C	-1.49043400	3.45711500	-0.78010600
C	-1.40844300	2.48846200	-1.79416700
H	-0.67861200	0.52537900	-2.38491900
H	-1.00002100	4.00315800	1.26561700
H	-2.00136600	4.39544100	-0.98656200
H	-1.85372200	2.70021400	-2.76447800
C	6.04476100	-1.37728300	-0.91449700
H	6.77341700	-0.81151600	-0.31838900
H	6.24803000	-1.14778000	-1.96925200
H	6.24416800	-2.44390800	-0.76105200
Na	-2.25257300	-1.03684000	0.10733000
O	-4.36472900	-1.68777500	-0.33774400
C	-5.32036100	-0.91179900	-1.06568500
H	-5.64985000	-1.45101500	-1.96410200
H	-4.83223700	0.02099800	-1.36066900
H	-6.19142000	-0.68400100	-0.43647100
C	-4.89588600	-2.94093300	0.10248300
H	-4.10295800	-3.46390800	0.64431200
H	-5.21173500	-3.54818300	-0.75644600
H	-5.75177500	-2.78222300	0.77234400
C	-0.29339500	0.83796700	3.02294800
H	0.28293700	0.11598000	3.61589700
H	-0.44894000	1.73300800	3.64162500
H	-1.27138200	0.38907600	2.81494700

C	2.75369100	0.66438900	-0.38037600
C	1.97255700	-0.48723400	-0.14450900
C	2.64270200	-1.72187400	-0.06727000
C	4.03384200	-1.79650200	-0.17968500
C	4.81407600	-0.65017100	-0.39049300
H	4.71232200	1.49023800	-0.67351800
H	2.27222700	1.63425900	-0.47105000
H	2.06019300	-2.62460200	0.09119900
H	4.52159000	-2.76724500	-0.10473700
C	0.48299400	-0.45808600	-0.05135300
C	0.20304800	0.58394100	2.08591200
H	0.86114100	1.02193300	2.84683500
O	-0.17268500	-1.54741700	-0.20387300
C	-0.79950700	1.41526100	-1.35822100
C	-0.24711100	0.84666700	-0.20263600
C	-0.26007100	1.50321100	1.04074700
C	-0.65359100	2.85822100	1.08298300
C	-1.15292600	3.45770800	-0.07897900
C	-1.26093900	2.73831400	-1.28435800
H	-0.79372300	0.88460000	-2.31003400
H	-0.60274100	3.42291100	2.01305200
H	-1.48106300	4.49509700	-0.04945300
H	-1.65693600	3.22738800	-2.17140700
C	6.31837300	-0.72554100	-0.51255700
H	6.81591400	-0.15648100	0.28477300
H	6.66655800	-0.30776800	-1.46692300
H	6.67112500	-1.76122600	-0.45200300
Na	-2.32329100	-1.03846400	-0.17944600
O	-4.54878900	-1.21430300	-0.42689700
C	-5.35266400	-0.21469800	-1.06127900
H	-5.86122600	-0.63150000	-1.94092000
H	-4.68719900	0.59379200	-1.37565600
H	-6.09928400	0.18057800	-0.35972700
C	-5.31817500	-2.33185100	0.02771500
H	-4.62838600	-3.03966500	0.49535800
H	-5.82381500	-2.81965200	-0.81641800
H	-6.06513100	-2.00973700	0.76547000
C	-0.74540200	-0.44568800	2.66745900
H	-0.29168300	-0.91635900	3.54992800
H	-1.71635500	-0.03022600	2.99942300
H	-0.96890200	-1.27394500	1.96839400

TS3

C	4.13966200	0.58134600	-0.49352000

Int5

C	4.07667800	0.27454900	-0.34390800

C	2.71480900	0.53699400	-0.47979400
C	1.76716300	-0.49940900	-0.39224000
C	2.23843700	-1.80385800	-0.17282500
C	3.60439800	-2.06265200	-0.02841200
C	4.54996000	-1.03029400	-0.11124900
H	4.78868100	1.09398200	-0.42754200
H	2.38279600	1.55295500	-0.67189100
H	1.52297600	-2.61942000	-0.11741700
H	3.94004600	-3.08295800	0.14791500
C	0.30816300	-0.27130800	-0.64161400
C	0.48984100	1.61138600	1.93553200
H	0.65665300	2.44406500	2.62079700
O	-0.34045100	-1.23933200	-1.17590600
C	-1.29812300	1.42129400	-1.37972100
C	-0.31991900	1.00803300	-0.41192500
C	-0.00875400	1.94205100	0.69568700
C	-0.40336700	3.33129900	0.45509900
C	-1.27520400	3.68770700	-0.53396500
C	-1.79062600	2.70596900	-1.44705700
H	-1.55303500	0.71917900	-2.17453100
H	-0.03625700	4.08476700	1.15112100
H	-1.57838400	4.72816400	-0.63925700
H	-2.46575500	2.99938500	-2.24698400
C	6.02853200	-1.30025700	0.03696100
H	6.45456400	-0.73423600	0.87604900
H	6.58068900	-1.00019500	-0.86362400
H	6.22544800	-2.36329300	0.21365600
Na	-2.37817400	-0.89111200	-0.35313400
O	-4.42004900	-1.60659700	0.22858200
C	-5.35645900	-0.82817000	0.98051400
H	-6.25025000	-0.61539300	0.37881300
H	-4.86599000	0.11180800	1.24714600
H	-5.64913700	-1.35953800	1.89589800
C	-4.95289400	-2.87335100	-0.16970400
H	-4.17645700	-3.39521200	-0.73595100
H	-5.83794600	-2.73571000	-0.80520700
H	-5.22429700	-3.46994800	0.71139600
C	0.76491300	0.24815800	2.49704800
H	0.55650800	0.23306300	3.57644000
H	0.14046100	-0.52229000	2.02138000
H	1.80732600	-0.08836900	2.37429700

HNa(ether)

Na	1.88955200	-0.00090100	0.00016500
C	-1.14736900	1.18988800	0.00051400
H	-0.46310400	2.04272800	-0.00133800
H	-1.77761800	1.23025400	0.89903500
H	-1.78266800	1.23043800	-0.89441300
O	-0.35414100	-0.00044300	-0.00195800
C	-1.15092600	-1.18838300	0.00053000
H	-1.78788300	-1.22601900	-0.89335900
H	-0.46926000	-2.04323400	-0.00355300
H	-1.77971400	-1.22788100	0.90010100
H	3.89806600	-0.00185100	0.00111200

Int1'

C	1.92741200	1.17528900	0.00001300
C	2.35915200	2.51180800	-0.00003500
C	3.71742600	2.83549300	-0.00013900
C	4.26314000	0.48195200	-0.00015900
C	2.89691600	0.16821900	-0.00004400
H	1.62004900	3.30823100	0.00002100
H	4.02341800	3.87877500	-0.00017300
H	5.00371100	-0.31150100	-0.00019700
I	-0.23250200	0.84261100	0.00011400
I	2.40983300	-1.92872100	0.00000800
Na	-4.73584600	0.13268000	0.00010000
H	-2.75223200	0.51425900	0.00023200
O	-6.94850000	-0.19176700	-0.00005100
C	-7.73463900	-0.30923900	1.18959600
H	-7.05950000	-0.20519900	2.04333600
H	-8.49456000	0.48268700	1.22763200
H	-8.22563500	-1.29069200	1.23071700
C	-7.73426500	-0.30933900	-1.18994100
H	-8.49411000	0.48264500	-1.22834200
H	-7.05883400	-0.20547500	-2.04347100
H	-8.22533000	-1.29075500	-1.23109000
C	4.67350300	1.81652800	-0.00021900
H	5.73491700	2.05127100	-0.00029500

TS1'

C	-2.09399700	0.65549600	0.00004000
C	-3.34851300	1.29396200	-0.00005700
C	-4.54523100	0.56848700	-0.00020500
C	-3.28139000	-1.49727600	-0.00018000
C	-2.11746700	-0.72153500	-0.00003800
H	-3.39240600	2.38329600	-0.00001900
H	-5.50046100	1.09001900	-0.00027800

H	-3.24469200	-2.58295900	-0.00022800
I	-0.11074900	2.02502600	0.00015700
I	-0.24042900	-1.92130500	0.00008900
Na	2.21524100	0.21578200	-0.00094600
H	1.61657900	3.00149300	0.00012200
O	4.39325200	-0.20972400	-0.00009900
C	5.18309000	-0.29720400	-1.19049400
H	4.50427500	-0.21815700	-2.04388300
H	5.91276200	0.52235000	-1.22848600
H	5.70940700	-1.26008800	-1.23101000
C	5.18224600	-0.29787800	1.19080800
H	5.91181100	0.52172100	1.22983700
H	4.50281800	-0.21944800	2.04376900
H	5.70863300	-1.26073700	1.23107500
C	-4.51154900	-0.83104600	-0.00026700
H	-5.43310400	-1.40852100	-0.00038300

Int2'

C	-0.79914300	1.47046200	-0.11310300
C	-1.52105900	2.69549900	-0.15178400
C	-2.92008300	2.76469400	-0.09545800
C	-3.02619700	0.34945300	0.04396700
C	-1.63209200	0.38251700	-0.01739700
H	-0.97049400	3.63557200	-0.22835100
H	-3.42294400	3.73034100	-0.12836200
H	-3.59218800	-0.57394600	0.11971400
I	-0.66551300	-1.69088200	0.06126200
Na	1.50297200	0.73880400	-0.15078300
C	-3.67672100	1.58963100	0.00255500
H	-4.76320600	1.62813100	0.04658600
C	4.59849300	0.03721500	-0.96831700
H	3.95943400	-0.37873900	-1.75186500
H	5.14980600	-0.77643300	-0.47786800
H	5.31059400	0.74341900	-1.41608000
O	3.75206000	0.70706400	-0.03011000
C	4.48627000	1.29178400	1.04913400
H	5.19945000	2.03632200	0.67060900
H	3.76748700	1.78292900	1.71077500
H	5.02829100	0.51829400	1.60984800

Na(ether)I

I	-2.00035100	-0.00002500	0.01905200
Na	0.89398300	0.00039300	-0.17537000
C	3.89847800	1.19047600	0.05612200
H	3.21917700	2.04438000	-0.01262500
H	4.61858300	1.22965100	-0.77177400
H	4.43600200	1.22819700	1.01277200
O	3.10746100	-0.00000700	-0.02625900
C	3.89805300	-1.19078000	0.05604100
H	4.43551200	-1.22878300	1.01271500
H	3.21844300	-2.04442700	-0.01282400
H	4.61818500	-1.23011500	-0.77182300

NaH

Na	0.00000000	0.00000000	0.16402100
H	0.00000000	0.00000000	-1.80422800

Int1''

C	-0.50121700	1.21546400	-0.00004900
C	-0.71504400	2.60329000	-0.00003600
C	-2.00582900	3.13592100	0.00004100
C	-2.91604900	0.89763200	0.00013600
C	-1.61673500	0.37180600	0.00002700
H	0.14051300	3.27299700	-0.00008400
H	-2.14387900	4.21430900	0.00003700
H	-3.77259900	0.23049600	0.00024200
I	1.57010700	0.54070700	-0.00006600
I	-1.46407400	-1.77352100	-0.00000600
Na	5.94843500	-0.71588700	0.00023300
H	4.03722800	-0.21004500	-0.00070700
C	-3.11050900	2.28030400	0.00013800
H	-4.12151000	2.67963100	0.00022400

TS1''

C	0.36192000	1.36969000	-0.00100000
C	0.69359200	2.73845500	-0.01318100
C	2.02284800	3.17631300	-0.02429900
C	2.77172500	0.87310400	-0.01181400
C	1.42482300	0.49857100	-0.00189000
H	-0.10478100	3.48107800	-0.01422400
H	2.24789800	4.24113500	-0.03385300
H	3.57224600	0.13913000	-0.01100200
I	-1.98979600	0.74423700	0.01384600
I	1.12709700	-1.72369600	0.01394600
Na	-2.02812600	-2.17921400	-0.08622500
H	-3.82409500	0.07152400	0.01726300
C	3.06483300	2.24116600	-0.02308300
H	4.10270000	2.56598700	-0.03110100

H	4.55392000	0.20483900	-2.38030700

Int2''

C	-1.27921800	1.07318100	-0.00057400
C	-2.70079100	1.06001000	-0.00048200
C	-3.45727600	-0.12013400	0.00002500
C	-1.41498200	-1.42104400	0.00034500
C	-0.74699400	-0.19538100	-0.00021100
H	-3.24166100	2.00851500	-0.00083000
H	-4.54538400	-0.07338400	0.00011100
H	-0.89616600	-2.37452800	0.00064800
I	1.52821100	-0.38912600	-0.00006800
Na	0.50551200	2.65103900	0.00055200
C	-2.81466500	-1.36487700	0.00037100
H	-3.38903000	-2.28890100	0.00076900

NaI

I	0.00000000	0.00000000	0.49444400
Na	0.00000000	0.00000000	-2.38232200

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C	-1.35288400	0.65501200	-0.18329900
C	-1.98552600	1.48150300	-1.11886900
C	-1.90097200	2.87094900	-1.00374000
C	-0.54614200	2.62352600	0.98120200
C	-0.60564400	1.23270300	0.85060700
H	-2.55754600	1.03789100	-1.92750300
H	-2.40267600	3.49958500	-1.73436200
H	0.01161700	3.04557500	1.81253400
I	-1.62086800	-1.45330100	-0.33044000
C	-1.18972400	3.44338300	0.05548600
H	-1.13449900	4.52311600	0.16271500
O	-0.01475400	0.47304700	1.85608600
C	1.06511600	-0.36294100	1.67512800
O	1.24363000	-1.21880100	2.51489900
C	1.98355700	-0.15293100	0.51603400
C	2.42047200	1.11989500	0.11514900
C	2.49566000	-1.29628800	-0.12047900
C	3.35170200	1.24290500	-0.91922900
H	2.06442000	2.01129900	0.61928500
C	3.40788900	-1.16627900	-1.16740600
H	2.16840700	-2.27968200	0.20264600
C	3.83775900	0.10403800	-1.56871100
H	3.69659300	2.23007000	-1.21524200
H	3.78719700	-2.05456900	-1.66554800

Int6

C	-2.16048500	-1.37442000	-0.32515000
C	-3.31189700	-1.96007300	-0.86272200
C	-4.48857300	-2.05186500	-0.11109100
C	-3.38370000	-0.96634300	1.74680000
C	-2.22813700	-0.85670400	0.97168800
H	-3.28531200	-2.36344000	-1.87183700
H	-5.37169700	-2.51505800	-0.54427400
H	-3.38594700	-0.58466400	2.76418200
I	-0.23955200	-1.35979100	-1.41518800
Na	2.43206600	-0.17577200	-0.13756300
H	2.07563400	-1.13437700	-2.19994100
O	3.77287600	1.67150900	-0.49645800
O	3.52580400	-1.66442500	1.23721200
C	4.68794300	1.68525300	-1.59240300
H	4.38862400	0.88830900	-2.27787000
H	4.64675000	2.65038400	-2.11689000
H	5.71538800	1.50519200	-1.24479700
C	4.05251500	2.68870400	0.46279300
H	4.00847700	3.68344500	-0.00309600
H	3.28997700	2.62323700	1.24291800
H	5.04741800	2.54375900	0.90832300
C	3.74399800	-3.02172300	0.85259600
H	3.08555700	-3.69622100	1.41800400
H	3.51538300	-3.10025800	-0.21318500
H	4.79136900	-3.30813500	1.02485500
C	3.78580500	-1.43873100	2.62070000
H	4.83218600	-1.67492300	2.86207300
H	3.59894200	-0.38092300	2.82406800
H	3.12247600	-2.05114300	3.24799500
C	-4.52071500	-1.56456000	1.19991500
H	-5.42492600	-1.64802000	1.79694800
O	-1.07819000	-0.32821900	1.59532900
C	-0.43623600	0.78998300	1.15553300
O	0.77689000	0.84196000	1.30295900
C	-1.22699400	1.92165100	0.59739000
C	-2.47139500	2.29282800	1.13286600
C	-0.65606700	2.68644700	-0.43420100
C	-3.13719800	3.41439100	0.63454300
H	-2.90728400	1.73165900	1.95172400
C	-1.33679700	3.79139300	-0.94416000
H	0.30918800	2.40358900	-0.84249100

C	-2.57739000	4.15821700	-0.40931500
H	-4.09268000	3.70579400	1.06232800
H	-0.89904600	4.36694400	-1.75526600
H	-3.10406200	5.02398000	-0.80263000

TS4

C	-1.90293800	-1.48540300	-0.42998000
C	-2.93665200	-2.26556100	-0.96684700
C	-4.03577500	-2.66438500	-0.19448100
C	-3.10396900	-1.50489000	1.71179600
C	-2.04068500	-1.10182500	0.90207500
H	-2.87835000	-2.58757100	-2.00598900
H	-4.82085700	-3.27426700	-0.63672600
H	-3.14133300	-1.20521100	2.75628200
I	0.08303400	-1.06629500	-1.63366500
Na	2.30453800	0.16380600	0.15367700
H	1.91609100	-0.67737500	-2.51493300
O	4.00736400	1.65573500	-0.17416000
O	3.40317000	-1.45770600	1.33082900
C	5.24192900	1.20739500	-0.73669000
H	5.32446900	0.13572000	-0.53892700
H	5.26068400	1.37969300	-1.82154400
H	6.08840100	1.72992500	-0.26972200
C	3.79948400	3.05589100	-0.36490400
H	3.75631500	3.30148700	-1.43521600
H	2.84865800	3.31482000	0.10781600
H	4.60691300	3.63242900	0.10760200
C	3.05460800	-2.84256700	1.28823300
H	2.53548100	-3.14025300	2.20997900
H	2.38897700	-2.98704500	0.43384400
H	3.95331300	-3.46188100	1.16034900
C	4.27837600	-1.14665000	2.41431600
H	5.21713100	-1.71168100	2.32778900
H	4.49486400	-0.07619000	2.36696400
H	3.80319000	-1.37987700	3.37760400
C	-4.11358500	-2.29291100	1.15296600
H	-4.95211200	-2.61194700	1.76692900
O	-0.99561300	-0.37228300	1.53876900
C	-0.63724700	0.87546600	1.16242900
O	0.54175900	1.19341600	1.28862100
C	-1.66812900	1.83864600	0.68518400
C	-2.94804000	1.90253700	1.25999600
C	-1.30344400	2.76393600	-0.30747000
C	-3.85206000	2.88005900	0.83962200
H	-3.23231100	1.21189000	2.04585200
C	-2.21873500	3.72280600	-0.74077100
H	-0.31152900	2.71703500	-0.74580600
C	-3.49372900	3.78363900	-0.16629700
H	-4.83630900	2.93378100	1.29703400
H	-1.93756200	4.42266400	-1.52308200
H	-4.20475100	4.53520800	-0.49981600

Int7

C	-0.03181000	1.31766900	0.98834300
C	-0.06467300	2.23849900	2.06615600
C	-0.78916700	3.44270000	2.04940500
C	-1.57292100	2.91016800	-0.17233000
C	-0.83550500	1.72787100	-0.07693900
H	0.51735500	2.02398900	2.96658200
H	-0.76311300	4.11394800	2.90734900
H	-2.15275200	3.14325400	-1.06327600
Na	1.66143000	-0.28679900	0.07115500
O	2.90230700	-1.97025700	1.08312300
O	3.42139100	0.62255900	-1.14925900
C	4.14062500	-1.64565400	1.71434900
H	4.52203600	-0.73749000	1.24068300
H	3.99659400	-1.46472500	2.78915400
H	4.86790800	-2.45887400	1.57948600
C	2.31060600	-3.15299200	1.61935600
H	2.07915900	-3.02606400	2.68638600
H	1.38601800	-3.33724400	1.06629700
H	2.98439000	-4.01246200	1.49434100
C	3.41328000	2.00524900	-1.50460600
H	2.96437600	2.15150100	-2.49726000
H	2.81669600	2.53196900	-0.75554900
H	4.43586600	2.40866100	-1.50625200
C	4.17737400	-0.17227200	-2.06081900
H	5.22515700	0.15959700	-2.08793100
H	4.13555200	-1.20617000	-1.70826100
H	3.75475600	-0.11528600	-3.07417200
C	-1.54097200	3.78632200	0.91871500
H	-2.10069800	4.71864000	0.88426100
O	-0.86465400	0.89878900	-1.26483300
C	-1.00297200	-0.44062800	-1.08345700
O	-0.06831800	-1.18923500	-1.35190900
C	-2.33590700	-0.94299200	-0.65525600
C	-3.48255000	-0.13427300	-0.72610200
C	-2.45166500	-2.27355200	-0.21580900

C	-4.72615800	-0.65006800	-0.35732200
H	-3.40331800	0.88869000	-1.07611900
C	-3.69362000	-2.78241100	0.16125300
H	-1.56436000	-2.89677000	-0.16752400
C	-4.83323500	-1.97130700	0.09005900
H	-5.61037700	-0.02121000	-0.41888300
H	-3.77513800	-3.80882100	0.50927500
H	-5.80202100	-2.36916500	0.38176500

Int8

C	-4.88891200	-0.78003800	-0.67010000
C	-3.75093500	-0.61365000	0.12202800
C	-3.05337300	0.60687100	0.12803400
C	-3.53792200	1.65302100	-0.68363900
C	-4.67712700	1.48465800	-1.46257200
C	-5.37606500	0.26241800	-1.47182300
H	-5.40624300	-1.73671300	-0.66400200
H	-3.40735800	-1.45059000	0.71983800
H	-3.00844800	2.60066700	-0.68962800
H	-5.03478400	2.30941900	-2.07597100
C	-1.82750200	0.84441800	0.94727500
C	-1.33624200	-0.20944300	1.93058200
H	-2.20064000	-0.78955700	2.26701400
O	-1.20235300	1.90596400	0.80482100
C	-0.70560300	0.43449200	3.17819300
H	-0.44665000	-0.34955300	3.89939100
H	0.21301200	0.97883200	2.93756000
H	-1.40023500	1.13204000	3.66396600
C	-6.61290900	0.09097900	-2.31795600
H	-7.40354800	0.78565700	-2.00454100
H	-6.40167700	0.30234300	-3.37417100
H	-7.00959600	-0.92708600	-2.24702900
C	-0.63540000	-2.55997800	1.36366000
C	-0.35780000	-1.18627200	1.22270300
C	0.77132900	-0.69403500	0.52976700
C	1.62047300	-1.70070100	-0.00918300
C	1.35063300	-3.07825400	0.12950300
C	0.21577900	-3.52843200	0.81660600
H	-1.51964000	-2.88818400	1.91319000
H	2.01692400	-3.81534000	-0.32030900
C	1.79059900	4.94712400	0.45421700
H	0.72049200	4.85523900	0.25003100
H	2.26287900	5.54033100	-0.34110800
H	1.93484000	5.45301700	1.41902800
O	2.33747100	3.62825700	0.48857000
C	3.74299600	3.62309700	0.74632100
H	3.95917800	4.07377600	1.72499200
H	4.07449300	2.58153800	0.74429000
H	4.28061300	4.17660600	-0.03579700
Na	1.07449900	1.72383700	0.45771300
C	2.85877400	-1.30716300	-0.75367800
C	4.08692900	-1.96391600	-0.54026900
C	2.83686800	-0.26389000	-1.70063400
C	5.24247000	-1.59162500	-1.23537300
H	4.14248300	-2.76397300	0.19437300
C	3.98752300	0.10842100	-2.40206200
H	1.89435700	0.23762100	-1.90772300
C	5.20025800	-0.55170500	-2.17049400
H	6.17838500	-2.11095900	-1.03980900
H	3.93475200	0.90881900	-3.13748200
H	6.09717400	-0.26245000	-2.71329300
C	-0.08860900	-5.00619600	0.93802500
H	-0.40938000	-5.43259900	-0.02317000
H	0.79211400	-5.57626900	1.26145900
H	-0.89130100	-5.18982000	1.66213400

Int8'

C	2.25235400	3.11451700	0.56613900
C	1.54492900	2.06877100	-0.03087900
C	0.15274800	2.15010600	-0.20275600
C	-0.50321400	3.31657000	0.24244600
C	0.20609400	4.35473900	0.83539000
C	1.60112200	4.27427200	1.00946800
H	3.32945000	3.02526900	0.68804000
H	2.09366400	1.19181500	-0.35411700
H	-1.57846500	3.39425500	0.11587600
H	-0.32404900	5.24401200	1.17095200
C	-0.66135900	1.07200300	-0.84136400
C	-0.01831100	-0.24351500	-1.27310200
H	1.00887600	-0.02484800	-1.57150700
O	-1.87670100	1.25753100	-1.00493800
C	-0.73806400	-0.83049900	-2.50038300
H	-0.20350800	-1.71920100	-2.85270300
H	-1.76189500	-1.13812600	-2.26501700
H	-0.77932600	-0.10646600	-3.32442200
C	2.36191000	5.40381900	1.65803800
H	2.19367500	6.35023600	1.12802200
H	2.03298500	5.55502500	2.69481900

H	3.43890300	5.20666600	1.67045100
C	1.24475600	-1.83088200	0.31029800
C	0.01147900	-1.23230600	-0.07321300
C	-1.20486600	-1.51138300	0.60304400
C	-1.10619500	-2.40893100	1.68916800
C	0.09342400	-2.99226900	2.13439100
C	1.26003100	-2.69353500	1.42218600
C	-6.09617400	0.95272100	-1.07059100
H	-5.29607000	1.62910900	-1.38282100
H	-6.79175700	1.49121200	-0.41215700
H	-6.63796900	0.59528000	-1.95725700
O	-5.49097500	-0.13952200	-0.37628800
C	-6.44804700	-1.09770300	0.07882200
H	-6.99797000	-1.52893000	-0.76914500
H	-5.90085100	-1.89038500	0.59610100
H	-7.15958200	-0.63275500	0.77511200
Na	-3.23153500	-0.38333300	-0.15001000
C	0.13664300	-3.90762500	3.33890700
H	0.57190500	-3.40296800	4.21361000
H	-0.86971400	-4.23964900	3.62136600
H	0.74618700	-4.80094700	3.14986100
H	-2.01160700	-2.67816000	2.24340500
H	2.20179700	-3.15659000	1.71469200
C	2.55112700	-1.63288000	-0.39648800
C	3.66429200	-1.12134300	0.29799600
C	2.73168000	-2.00461800	-1.74201300
C	4.90599200	-0.97548100	-0.32927100
H	3.55047200	-0.82773800	1.33894100
C	3.97161300	-1.86071900	-2.37241100
H	1.89779200	-2.42889100	-2.29467200
C	5.06497300	-1.34194900	-1.66993200
H	5.74787500	-0.57369000	0.23041200
H	4.08451000	-2.16216700	-3.41152500
H	6.02935000	-1.23004900	-2.15974800

Int3'

C	2.97154200	1.35703800	0.41281800
C	1.71615600	0.79581200	0.65451900
C	1.41951900	-0.50971900	0.22525600
C	2.42521000	-1.23270300	-0.44923100
C	3.67657100	-0.67217100	-0.67742300
C	3.97458100	0.63654500	-0.25184600
H	3.17360000	2.37244600	0.74602800
H	0.96969900	1.39366700	1.16522700
H	2.21033000	-2.24201600	-0.78603400
H	4.43867000	-1.25226300	-1.19411200
C	0.09549800	-1.15961600	0.44458800
C	-0.97445900	-0.48221100	1.29241700
H	-0.47309800	0.16689300	2.01569600
O	-0.13287000	-2.25958100	-0.08496100
C	-1.78998400	-1.51284500	2.09390100
H	-2.47588400	-0.98648600	2.76777600
H	-2.39542900	-2.15244700	1.44369100
H	-1.13915600	-2.15643400	2.69945300
C	5.33452400	1.23606400	-0.50763400
H	6.12332400	0.64406200	-0.02507300
H	5.56085200	1.25504500	-1.58170500
H	5.39894500	2.26109200	-0.12837700
C	-1.99741300	1.76376800	0.79010700
C	-1.88261600	0.41370800	0.40668300
C	-2.59098300	-0.13117700	-0.69603700
C	-3.42869000	0.79230400	-1.36746400
C	-3.56213300	2.14237500	-1.00257900
C	-2.83907600	2.63399400	0.08849400
H	-1.43776100	2.14152000	1.64686500
H	-4.01336600	0.45511800	-2.22805800
H	-4.22254300	2.80423700	-1.56323100
H	-2.92770100	3.67526500	0.39310000
Na	-2.09245500	-2.43000500	-1.22099800

TS2'

C	2.68737200	-1.33087200	-0.66846400
C	1.40866500	-0.77963900	-0.74609700
C	1.12724400	0.48359800	-0.19207100
C	2.17932700	1.16389400	0.43718300
C	3.46056600	0.60694500	0.51799000
C	3.74156700	-0.65068400	-0.03232100
H	2.87110700	-2.31069000	-1.10681900
H	0.62462800	-1.35308900	-1.23199900
H	1.98539300	2.14766400	0.85430800
H	4.25490900	1.16407500	1.01217600
C	-0.23660600	1.15995000	-0.27038700
C	-1.19080700	0.70141800	-1.43778600
H	-0.60172900	0.29754100	-2.27396200
O	-0.30516800	2.36686600	0.15870300
C	-1.94094100	-1.14957200	1.61936000
C	-1.47989000	-0.22502900	0.66497400
C	-1.91752500	-0.36842800	-0.66441600

C	-2.79981500	-1.37557700	-1.06508500
C	-3.27187100	-2.27003000	-0.09071600
C	-2.84479500	-2.16072400	1.23987900
H	-1.60964900	-1.11299000	2.65971100
H	-3.11608600	-1.48193000	-2.10236700
H	-3.96439500	-3.06119200	-0.37135100
H	-3.21161300	-2.86975400	1.98118400
C	5.12315200	-1.25795700	0.04209500
H	5.80986200	-0.61916800	0.60846100
H	5.54996000	-1.40332300	-0.95951100
H	5.10235300	-2.24309100	0.52658600
Na	-1.46417500	1.94173300	1.93236100
C	-2.08137000	1.82451600	-1.97987000
H	-1.48328400	2.61784200	-2.44367100
H	-2.76583300	1.42537500	-2.73952700
H	-2.68398800	2.27787200	-1.18441200

Int4'

C	2.92627400	-1.38166100	-0.36771100
C	1.58069400	-1.00873400	-0.39051800
C	1.17285100	0.27990400	0.00057900
C	2.16704500	1.17375100	0.41540500
C	3.51773500	0.80125400	0.43486000
C	3.92507100	-0.48199800	0.04571200
H	3.20689400	-2.38901100	-0.67338000
H	0.83997900	-1.73740500	-0.71441000
H	1.85934000	2.16780500	0.72648400
H	4.26644800	1.52194700	0.76145000
C	-0.29551700	0.73355900	-0.03466100
C	-0.95808600	0.58110500	-1.54474000
H	-0.26848400	0.10860700	-2.25775900
O	-0.50731700	1.92874800	0.57725500
C	-1.82253900	-1.10882500	1.42803800
C	-1.32856600	-0.37180300	0.35171900
C	-1.91806100	-0.41801300	-0.91420600
C	-3.02520500	-1.21944300	-1.18067700
C	-3.53707000	-1.96867600	-0.10222900
C	-2.95192200	-1.91413200	1.17339000
H	-1.36411300	-1.09550600	2.41670400
H	-3.49365300	-1.27558600	-2.16167400
H	-4.40488200	-2.60629200	-0.25773900
H	-3.37615200	-2.51424000	1.97596600
C	5.37959100	-0.89438700	0.07373700
H	6.02409500	-0.05890400	0.36952800
H	5.71706500	-1.24653600	-0.91014600
H	5.55107700	-1.71553100	0.78313300
Na	-2.29301700	1.90555900	1.71497900
C	-1.53738700	1.84985100	-2.15515500
H	-0.73503900	2.54044200	-2.44534300
H	-2.12708800	1.62296200	-3.05438300
H	-2.18321900	2.37562000	-1.44248100

TS3'

C	-2.87550300	-1.37150900	0.07285500
C	-1.53565600	-1.01347600	-0.05878900
C	-1.15825600	0.33309400	-0.24730800
C	-2.18532300	1.29045200	-0.33540000
C	-3.52706400	0.92320800	-0.20082000
C	-3.90314400	-0.41144500	0.01091700
H	-3.13239100	-2.41965000	0.22019400
H	-0.77348000	-1.78628100	-0.00909600
H	-1.91974400	2.33027100	-0.50134600
H	-4.29706600	1.69063000	-0.26397700
C	0.25903200	0.76376400	-0.42549100
C	1.09160700	0.51111300	1.80887600
H	0.70291000	0.14504600	2.76674700
O	0.50352200	1.90826600	-0.94774900
C	1.95102600	-0.94769800	-1.46222000
C	1.35978900	-0.25937100	-0.39317000
C	1.71510400	-0.49826600	0.94661600
C	2.53583300	-1.60961100	1.23730200
C	3.08430500	-2.34431800	0.18022400
C	2.82775300	-2.00042600	-1.16103600
H	1.67506000	-0.73632200	-2.49495000
H	2.76906100	-1.87347900	2.26798900
H	3.73720400	-3.18815300	0.39532600
H	3.27278400	-2.58479400	-1.96293800
C	-5.35195500	-0.81410800	0.15871500
H	-6.01831000	0.04951100	0.05448300
H	-5.54465700	-1.26800700	1.14044700
H	-5.64280300	-1.55545100	-0.59784700
Na	2.69138900	2.03705800	-1.06145500
C	1.70572200	1.89335700	1.92397900
H	1.28466500	2.42037600	2.79003400
H	2.80356100	1.89067900	2.06895600
H	1.49013100	2.54328900	1.05247900

Int5'

C	2.74971000	1.17350700	-0.80577700
C	1.41611200	0.77475400	-0.74245100
C	1.06497600	-0.49661900	-0.25221500
C	2.10032100	-1.35082500	0.16094900
C	3.43646100	-0.94498100	0.10296100
C	3.78790300	0.32322900	-0.38155600
H	2.99353300	2.15857100	-1.20019200
H	0.64028900	1.44883300	-1.09292500
H	1.85005200	-2.34211800	0.52783100
H	4.21749500	-1.62582300	0.43621000
C	-0.34429200	-0.99815500	-0.27240300
C	-0.91669700	1.42633000	1.72859200
H	-1.12249900	2.40429600	2.16651600
O	-0.50378000	-2.26162400	-0.43410800
C	-2.59076700	-0.45594100	-1.08081500
C	-1.48057800	-0.10888600	-0.23499900
C	-1.58224900	1.13872000	0.55853800
C	-2.59788000	2.08309100	0.08946300
C	-3.59082000	1.72612400	-0.77720800
C	-3.63340100	0.40552500	-1.34095400
H	-2.52775700	-1.38767200	-1.64484900
H	-2.58936200	3.08353000	0.52054800
H	-4.35453800	2.45101600	-1.05383200
H	-4.41024900	0.13590500	-2.05188500
C	5.22881600	0.76931200	-0.45370700
H	5.90861500	-0.01619400	-0.10621200
H	5.40072300	1.66142000	0.16331200
H	5.51328800	1.03201400	-1.48122300
Na	-2.40903200	-2.53283400	0.64623700
C	-0.00180900	0.54310700	2.52371300
H	-0.11664500	0.74760300	3.59775500
H	-0.21582700	-0.52319300	2.35831600
H	1.06764800	0.67622700	2.29210900

Int4''

C	2.58309900	-1.20394000	-0.82629000
C	1.27212500	-0.78229700	-0.60590700
C	0.99420100	0.32043100	0.22114500
C	2.07567200	0.97900900	0.82018900
C	3.39052500	0.55089600	0.59648600
C	3.67174200	-0.54550700	-0.22814000
H	2.76429900	-2.06268600	-1.47056000
H	0.45763400	-1.32254200	-1.08241300
H	1.89319200	1.83005100	1.46728700
H	4.20943900	1.08305200	1.07706200
C	-0.43585600	0.79401400	0.41986400
C	-1.19922200	1.25503900	-0.93423500
H	-0.57942600	1.06991200	-1.82026800
O	-0.43094600	1.75650500	1.47021000
C	-1.96526600	-1.34159500	1.31275100
C	-1.52578400	-0.27858200	0.52972000
C	-2.17707000	0.12264100	-0.63537100
C	-3.31923300	-0.52474700	-1.09932200
C	-3.78341200	-1.59727800	-0.31637300
C	-3.12489100	-1.99577500	0.86139600
H	-1.45808600	-1.66128000	2.22016000
H	-3.84131500	-0.23316500	-2.00795500
H	-4.67604400	-2.13636100	-0.62616600
H	-3.52455000	-2.83172200	1.43097900
C	5.08795800	-1.01707400	-0.46343200
H	5.81458400	-0.35078800	0.01431700
H	5.32265700	-1.06016500	-1.53495400
H	5.24422800	-2.02681500	-0.06035600
C	-1.74111900	2.68054800	-0.98494600
H	-0.92242900	3.41037400	-0.98495300
H	-2.32285900	2.82774500	-1.90384100
H	-2.40402000	2.90715100	-0.14044500
H	-1.35055200	2.01050400	1.65521500

TS3''

C	-2.43589200	-1.47803000	0.19127200
C	-1.15124700	-1.01009800	-0.06118800
C	-0.92367100	0.34742000	-0.38602700
C	-2.04828500	1.19083400	-0.48967200
C	-3.33511000	0.70556100	-0.24006600
C	-3.55957200	-0.63195700	0.11241800
H	-2.57559400	-2.52904900	0.43916400
H	-0.31338500	-1.69906600	-0.00999000
H	-1.91447400	2.23500000	-0.75429400
H	-4.18050400	1.38648200	-0.32045800
C	0.41892900	0.86194400	-0.69197300
C	1.19243700	0.91616000	1.62440300
H	0.77645100	0.60636300	2.58945900
O	0.38138800	1.91089800	-1.56625000
C	2.48565400	-0.46868700	-1.50590900
C	1.65147000	0.11723700	-0.52991900
C	1.88479900	-0.07499700	0.85326000
C	2.72114000	-1.14233200	1.26535900

C	3.48055900	-1.78776500	0.29677000
C	3.40156500	-1.42240900	-1.07292900
H	2.35907900	-0.26068800	-2.56630800
H	2.82977700	-1.39331200	2.31890100
H	4.17566400	-2.57057400	0.59237500
H	4.02523100	-1.94050300	-1.79736000
C	-4.94863900	-1.16100000	0.37901500
H	-5.69930200	-0.36684600	0.30098000
H	-5.02522300	-1.59922800	1.38310500
H	-5.22044700	-1.95044300	-0.33499300
C	1.46518500	2.39720800	1.54700200
H	0.54171200	2.99326700	1.60004500
H	2.08570900	2.71481700	2.40328400
H	2.00310700	2.68251400	0.63679400
H	1.28515700	2.24954200	-1.70159300

Int5’’

C	-2.46115900	-0.84488500	-1.15333300
C	-1.16244600	-0.39268400	-0.94093700
C	-0.90011200	0.64898700	-0.02845100
C	-1.99279500	1.22618500	0.64290600
C	-3.29463300	0.76649800	0.42432800
C	-3.55599800	-0.27640600	-0.47443200
H	-2.63445500	-1.64426400	-1.87150000
H	-0.34401700	-0.83673000	-1.49922700
H	-1.82223600	2.03702100	1.34478300
H	-4.11922400	1.22967200	0.96232100
C	0.45869200	1.19424000	0.14744000
C	1.14010500	-1.69821900	1.19895500
H	1.38627200	-2.76096600	1.21474800
O	0.41204400	2.56240500	0.27274000
C	2.87940900	1.23566900	-0.29898200
C	1.66338900	0.51930900	0.06682500
C	1.81693500	-0.94566400	0.27972600
C	2.92056800	-1.58206800	-0.44267300
C	3.95911800	-0.85698100	-0.93474400
C	3.97047500	0.58105300	-0.78814900
H	2.89625100	2.32308100	-0.29898100
H	2.93342800	-2.66943600	-0.49040300
H	4.80061800	-1.35119300	-1.41450300
H	4.83572700	1.14630000	-1.12542500
C	-4.95996400	-0.77190300	-0.72400300
H	-5.68777500	-0.24200500	-0.10024400
H	-5.04799900	-1.84519300	-0.50985500
H	-5.24971000	-0.63078000	-1.77389900
C	0.15594400	-1.25608600	2.23358500
H	0.28428700	-1.84934300	3.14845000
H	0.26757500	-0.19426200	2.48430500
H	-0.88698600	-1.39622600	1.90885200
H	1.26672100	2.90281200	0.59029100

Int9

C	1.21123400	2.44014600	-1.12671800
C	0.23236400	1.44610500	-0.99995500
C	-0.01471100	0.80957400	0.22910700
C	0.77676700	1.20897900	1.32479400
C	1.75627900	2.20020600	1.19802900
C	1.99067100	2.84039500	-0.03089100
H	1.36901700	2.91296600	-2.09505600
H	-0.34594500	1.16167300	-1.87575800
H	0.62222300	0.73899300	2.29425700
H	2.34182700	2.48727000	2.07070200
C	-0.96986000	-0.39114100	0.34232900
C	-1.94107400	-0.30943300	1.65637900
H	-1.79859200	0.59920400	2.26487700
C	-2.29843500	-0.26128000	-0.44590200
C	-3.07238300	-0.20023300	0.64833600
C	-2.79635100	-0.31274400	-1.86145500
H	-2.26111400	-1.07716900	-2.44402800
H	-2.62001100	0.64335200	-2.38075200
C	-4.31294600	-0.62284900	-1.83613800
H	-4.45225500	-1.69346600	-1.62515700
H	-4.75328100	-0.43473400	-2.82472000
C	-5.06445100	0.19943700	-0.76673000
H	-6.14338900	0.00803100	-0.83975300
H	-4.91860300	1.26942300	-0.97758300
C	-4.56833900	-0.09799100	0.66933200
H	-4.91145900	0.68774500	1.36013600
H	-5.01375800	-1.03617200	1.03986200
C	-1.92729500	-1.53384300	2.56709100
H	-1.00256300	-1.57901300	3.15907100
H	-2.77048700	-1.51373600	3.27296300
H	-1.98807400	-2.45825500	1.98171300
C	3.02360800	3.93726800	-0.15547800
H	2.65096400	4.88385900	0.26067700
H	3.94409500	3.68872600	0.38719600
H	3.28652600	4.12136400	-1.20332000
O	-0.25453600	-1.54432800	0.16117900

Na	1.85098200	-1.26746600	-0.05584700
C	4.35412400	-2.97955900	-1.24980700
H	3.44895800	-3.28547800	-1.78180300
H	5.10792600	-2.64718100	-1.97623900
H	4.74740000	-3.83186300	-0.67924500
O	3.99842900	-1.90782000	-0.37190100
C	5.11479700	-1.41434800	0.37229700
H	5.88926600	-1.02949800	-0.30492700
H	4.75402700	-0.60129100	1.00792800
H	5.54136100	-2.20758900	1.00133000

TS5

C	-0.01241700	2.99904400	-0.98827100
C	-0.61318900	1.75920200	-0.77896800
C	-0.13664400	0.86482400	0.20772700
C	0.99919400	1.28102300	0.93853200
C	1.59485300	2.53043200	0.72514300
C	1.10633900	3.41848300	-0.24238300
H	-0.41373700	3.65598800	-1.75946400
H	-1.46878000	1.47502800	-1.38504400
H	1.36907800	0.65030500	1.74622200
H	2.45018800	2.82059700	1.33410800
C	-0.68561700	-0.51900700	0.41192800
C	-2.37907500	0.21500000	1.73853100
H	-2.67356500	1.22979000	2.05075000
C	-1.97605300	-0.90095700	-0.20710500
C	-2.96268200	-0.29571000	0.50137800
C	-2.19231800	-1.82083700	-1.38358200
H	-1.69549200	-2.79032100	-1.22906400
H	-1.73581000	-1.39344900	-2.29353700
C	-3.70544000	-2.03113700	-1.61012600
H	-4.08097000	-2.76764300	-0.88386800
H	-3.88038000	-2.45373900	-2.60861400
C	-4.49657600	-0.72014700	-1.43926700
H	-5.55103100	-0.87581300	-1.70413700
H	-4.10140000	0.02926600	-2.14160400
C	-4.38492600	-0.18156300	0.00287500
H	-4.72296000	0.86622500	0.05604100
H	-5.06372100	-0.74416600	0.66462600
C	-2.10782800	-0.69165600	2.91903400
H	-1.35551400	-0.25238000	3.59416000
H	-3.00771300	-0.87238700	3.53821400
H	-1.73091600	-1.67140100	2.60062800
C	1.74873400	4.76442500	-0.48788600
H	2.58589900	4.93635600	0.19825100
H	2.13568900	4.84745000	-1.51310900
H	1.03164800	5.58513800	-0.35119700
O	0.16820900	-1.42745700	0.76982000
Na	2.23618000	-1.15976300	0.17117400
C	4.87065300	-3.07167800	0.18679800
H	4.07764700	-3.59302100	0.72997400
H	5.72110600	-2.89834100	0.85982400
H	5.19571900	-3.68728300	-0.66254300
O	4.33391300	-1.82744400	-0.27292400
C	5.28758500	-1.05711900	-1.01033700
H	5.62192200	-1.60844300	-1.89936200
H	4.79507800	-0.13178500	-1.32121600
H	6.15551000	-0.81510000	-0.38225600

Int10

C	0.32957600	2.62582600	-1.31166500
C	-0.34595900	1.43058400	-1.05573000
C	-0.07541400	0.67034600	0.09702800
C	0.90677400	1.16469300	0.97564800
C	1.57900100	2.36676700	0.72157700
C	1.30478900	3.12110100	-0.42839800
H	0.09909500	3.18345300	-2.21852600
H	-1.08802100	1.07433700	-1.76550300
H	1.12521200	0.61629000	1.89154800
H	2.31930100	2.72664200	1.43431700
C	-0.68612200	-0.69292600	0.33606200
C	-3.27838000	1.19590100	0.92618900
H	-4.10768400	1.86454500	0.68185300
C	-2.04787200	-0.91780300	0.26010900
C	-3.10021700	0.11537000	0.12720400
C	-2.56601100	-2.34913000	0.28960400
H	-3.07629100	-2.55512100	1.24891700
H	-1.71706100	-3.03864300	0.23490000
C	-3.56539900	-2.63384800	-0.84807300
H	-3.98613200	-3.64418600	-0.73764200
H	-3.03176100	-2.61473200	-1.81103800
C	-4.69101700	-1.59158300	-0.87639300
H	-5.29012100	-1.67815000	0.04326600
H	-5.37224000	-1.78061700	-1.71828600
C	-4.12139600	-0.16369200	-0.97316200
H	-3.63461300	-0.05532000	-1.95660000
H	-4.93647700	0.57128800	-0.93418300
C	-2.48203800	1.59187900	2.13844000

H	-1.80535900	2.43661700	1.93824700
H	-3.15328000	1.91519000	2.94769200
H	-1.86824200	0.76392300	2.50997100
C	2.02598000	4.41813900	-0.71486900
H	2.74163200	4.66061500	0.07858300
H	2.57918000	4.36920900	-1.66242400
H	1.32180600	5.25641900	-0.79903100
O	0.20694900	-1.63493600	0.54601600
Na	2.28528100	-1.24946000	0.16355100
C	5.16216200	-1.69786900	-1.31957400
H	4.46065900	-1.33545000	-2.07603200
H	5.51482100	-2.69952200	-1.59986100
H	6.01803600	-1.01233100	-1.25942800
O	4.46695800	-1.74234500	-0.07001400
C	5.29516400	-2.20371700	1.00140000
H	6.15464600	-1.53389100	1.13858500
H	4.68835100	-2.20621300	1.91083800
H	5.65346700	-3.22225500	0.80037900

Int9'

C	2.71966400	-1.56689600	0.22738100
C	1.41477100	-1.10990600	0.45698600
C	0.95672100	0.10734800	-0.07893500
C	1.87568400	0.85368700	-0.84447500
C	3.17827800	0.39774000	-1.07287600
C	3.62626000	-0.82565300	-0.54506500
H	3.03410700	-2.51853700	0.65317900
H	0.74384100	-1.71425100	1.06298600
H	1.56630100	1.80615300	-1.26965600
H	3.85608500	0.99929800	-1.67723700
C	-0.41198500	0.69427400	0.30942700
C	-1.21305600	1.34137300	-0.95819200
H	-0.67922100	1.25759400	-1.91927600
C	-1.58431300	-0.32031300	0.32628000
C	-2.22119400	0.23099300	-0.71776900
C	-2.10086500	-1.45946500	1.15710400
H	-1.96818300	-1.26215300	2.23120900
H	-1.54523800	-2.38813400	0.94813900
C	-3.60112600	-1.66175300	0.83236700
H	-4.18247900	-0.87884000	1.34144200
H	-3.94698800	-2.62414400	1.23328100
C	-3.89257200	-1.59494400	-0.68273100
H	-4.95105600	-1.82108600	-0.86823200
H	-3.30895500	-2.37778500	-1.18979000
C	-3.52691000	-0.22217600	-1.29853700
H	-3.47820300	-0.29851400	-2.39578200
H	-4.31946600	0.51414700	-1.08553200
C	-1.69503700	2.77728700	-0.77265600
H	-0.85873500	3.48764900	-0.82781200
H	-2.41855100	3.05676900	-1.55226100
H	-2.17295000	2.90619800	0.20496000
C	5.02413900	-1.32928200	-0.82281500
H	5.11948700	-1.68543000	-1.85803200
H	5.77279600	-0.53888800	-0.68595100
H	5.28667300	-2.16357000	-0.16276400
O	-0.25599800	1.48324000	1.42098200
Na	1.74617900	1.50033700	2.12330100

TS5'

C	-2.31716800	-1.78673400	-0.46733700
C	-1.07791000	-1.15050200	-0.46506100
C	-0.92916700	0.17406800	0.00996500
C	-2.10853000	0.82342400	0.44339800
C	-3.35026600	0.17428900	0.44159500
C	-3.48613300	-1.14258700	-0.01568300
H	-2.38467400	-2.80778600	-0.84157100
H	-0.20551500	-1.68396000	-0.83139500
H	-2.03392300	1.81885000	0.88101100
H	-4.22544500	0.70378600	0.81594800
C	0.35877700	0.94258200	-0.05868100
C	1.11271500	0.05804400	1.88864100
H	0.67296600	-0.69264500	2.56433500
C	1.63232200	0.23613700	-0.32167000
C	1.96440600	-0.43465200	0.81067200
C	2.45548500	0.26594700	-1.58515600
H	2.67829400	1.29868700	-1.89186700
H	1.88968800	-0.17939200	-2.42209800
C	3.76886400	-0.51767300	-1.36932100
H	4.47976300	0.11372500	-0.81548600
H	4.23457100	-0.74330900	-2.33797300
C	3.53709600	-1.81647000	-0.57355300
H	4.46571300	-2.40054800	-0.52169600
H	2.80279000	-2.43750000	-1.10856600
C	3.01817100	-1.51729800	0.84929400
H	2.61010000	-2.42858800	1.31604200
H	3.85596600	-1.20541300	1.49408500
C	1.39368600	1.36785600	2.59070600
H	0.48717700	1.75844500	3.08091100

H	2.15666300	1.27208200	3.38693800
H	1.74678200	2.13587100	1.89199000
C	-4.82333800	-1.84645400	-0.03609700
H	-5.60970800	-1.21850200	0.39806200
H	-5.12974200	-2.10319300	-1.05986500
H	-4.79424800	-2.78582700	0.53211900
O	0.25378200	2.21787200	-0.28533300
Na	-1.51104700	2.80567100	-1.37259400

Int10'

C	-2.40048700	-1.03016500	-1.32534700
C	-1.13540300	-0.49072500	-1.08224000
C	-0.89117400	0.32241100	0.03959900
C	-1.97695400	0.57019400	0.90201200
C	-3.24444900	0.02550800	0.65881100
C	-3.48196500	-0.78418500	-0.46136900
H	-2.55357900	-1.65040100	-2.20744500
H	-0.32492300	-0.69412900	-1.77728300
H	-1.81880100	1.17065900	1.79785800
H	-4.05455300	0.22334700	1.35881300
C	0.42269200	1.04148500	0.25288500
C	1.30200800	-1.99907000	1.04812100
H	1.54991000	-3.04789100	0.86628000
C	1.63665000	0.38416100	0.24911600
C	1.83595700	-1.08348500	0.20358100
C	2.92308600	1.19823200	0.25304600
H	3.43992400	1.09695900	1.22522700
H	2.67646000	2.25903100	0.13990300
C	3.89975400	0.75045900	-0.85120400
H	4.85012400	1.29663600	-0.75978500
H	3.47682200	1.00965300	-1.83421200
C	4.15088700	-0.76199900	-0.79381100
H	4.66969500	-1.00906200	0.14528700
H	4.81268200	-1.07535700	-1.61377200
C	2.82772300	-1.54804400	-0.86010000
H	2.38742200	-1.39359800	-1.85925700
H	3.02292500	-2.62386700	-0.75755200
C	0.41488100	-1.75553300	2.23716400
H	-0.63392400	-2.02473600	2.03985800
H	0.73945500	-2.37199900	3.08834900
H	0.42982100	-0.70508000	2.54750200
C	-4.84586200	-1.37379400	-0.73632100
H	-5.55356300	-1.13229200	0.06435400
H	-5.26400600	-0.99547200	-1.67900700
H	-4.79764500	-2.46691300	-0.82454300
O	0.28668400	2.34699300	0.36736900
Na	-1.63379800	3.14235200	-0.11847100

Int9''

C	2.65123900	-1.40271700	-0.56783000
C	1.34760800	-0.94810300	-0.34464100
C	1.10614000	0.30808400	0.23273400
C	2.22001400	1.09253300	0.57710000
C	3.52113200	0.63537700	0.35277200
C	3.76432500	-0.62081800	-0.22540900
H	2.80332000	-2.38514000	-1.01115700
H	0.51081900	-1.58353900	-0.62299300
H	2.06684500	2.07086800	1.02341400
H	4.36248100	1.26738100	0.63283100
C	-0.31222800	0.82699600	0.43424800
C	-1.03474400	1.37685300	-0.88595700
H	-0.41573200	1.20960000	-1.77939100
C	-1.44994600	-0.19117300	0.48292200
C	-2.04615500	0.26610300	-0.62755000
C	-1.92099300	-1.32009600	1.34609800
H	-1.88042200	-1.05891200	2.41361000
H	-1.27368800	-2.20317300	1.22556000
C	-3.37635800	-1.65488000	0.93330100
H	-4.04929800	-0.90552200	1.37471300
H	-3.66777800	-2.62703200	1.35108700
C	-3.57878400	-1.66695400	-0.59865100
H	-4.60460400	-1.97916000	-0.83237200
H	-2.91062800	-2.42144900	-1.03897000
C	-3.28183600	-0.29602900	-1.25636400
H	-3.16452400	-0.40894700	-2.34404700
H	-4.13046100	0.39184300	-1.11397800
C	-1.52579400	2.82237500	-0.87599100
H	-0.68312800	3.52541300	-0.87172900
H	-2.12074100	3.02202000	-1.77749800
H	-2.14927500	3.03356200	-0.00092600
C	5.17420100	-1.10023600	-0.48268000
H	5.61755900	-0.58367300	-1.34541800
H	5.82717600	-0.90719800	0.37735300
H	5.19905200	-2.17506800	-0.69375500
O	-0.35360900	1.81897900	1.47131800
H	-0.05503400	1.40239900	2.29851300

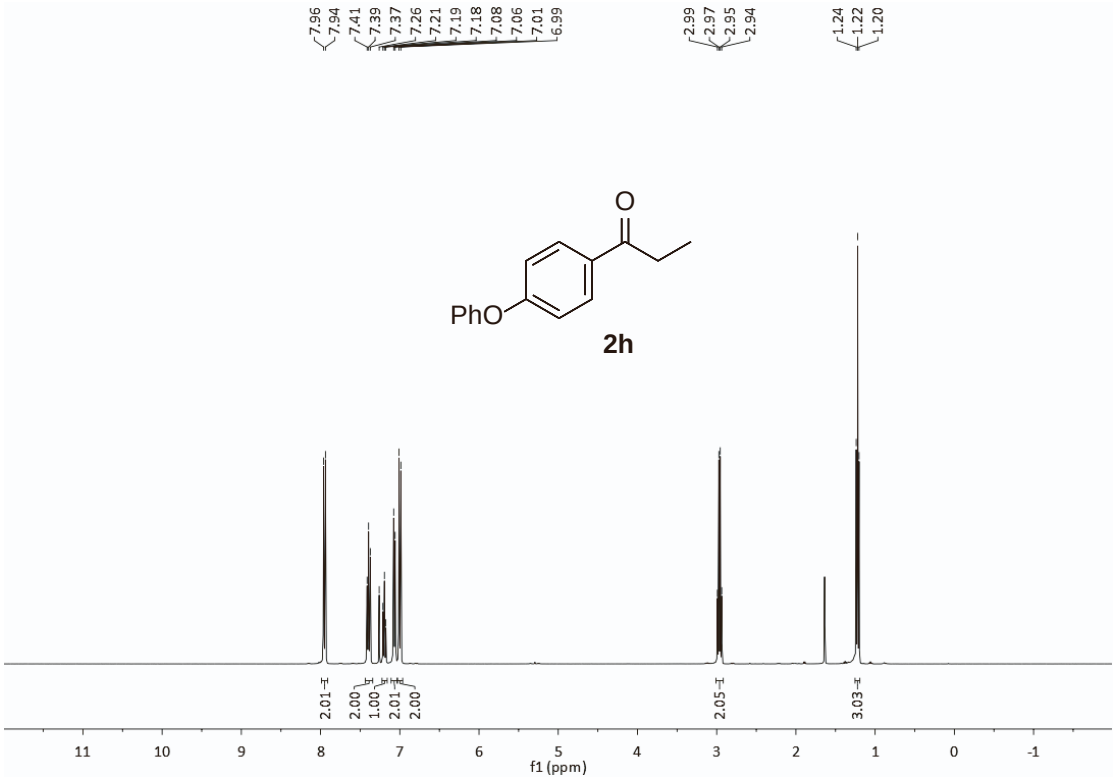
TS5''

C	-2.50139000	-1.51982700	0.08016900	C	-2.59595100	-0.80448100	-1.18654200
C	-1.22393000	-1.01545700	-0.14304400	C	-1.29412400	-0.33903700	-1.01206700
C	-1.01053600	0.36445300	-0.36020900	C	-1.00653100	0.66809300	-0.07173400
C	-2.14841800	1.19687200	-0.37485400	C	-2.07665600	1.19820500	0.67111100
C	-3.42980700	0.67765200	-0.15707300	C	-3.38119200	0.72786800	0.49016600
C	-3.63670100	-0.68670900	0.07878800	C	-3.66675800	-0.28178500	-0.43889000
H	-2.62514200	-2.58948600	0.24285300	H	-2.78871100	-1.58016600	-1.92559200
H	-0.37579400	-1.69352000	-0.15299600	H	-0.49241400	-0.74865700	-1.61935700
H	-2.04544400	2.27250200	-0.50678400	H	-1.89029100	1.97083900	1.41366400
H	-4.28102600	1.35596500	-0.16175600	H	-4.18694900	1.15154500	1.08617500
C	0.33674600	0.91525100	-0.64976500	C	0.36431500	1.21781400	0.08800300
C	0.96955500	1.01261600	1.53664900	C	1.07439900	-1.70841400	1.24453500
H	0.45594500	0.68441700	2.45207900	H	1.26680300	-2.78274500	1.20183200
C	1.58111600	0.20275400	-0.50176800	C	1.52732300	0.52982300	0.17276100
C	1.77605300	0.04326100	0.84701600	C	1.62728600	-0.95231300	0.27319200
C	2.49524100	-0.34059400	-1.57264100	C	2.87399700	1.23764100	0.14419600
H	2.88761600	0.45994600	-2.21546000	H	3.35567000	1.13889900	1.13060700
H	1.93427300	-1.01566900	-2.23868000	H	2.74114700	2.30713600	-0.03997000
C	3.66102500	-1.10601600	-0.90573100	C	3.80799600	0.62506300	-0.91980400
H	4.41741700	-0.38669800	-0.55833700	H	4.79546200	1.10223500	-0.85729500
H	4.15216500	-1.74716200	-1.64862100	H	3.40835700	0.84946400	-1.92004800
C	3.18638700	-1.94676400	0.29499100	C	3.93814900	-0.89441000	-0.75463700
H	4.01032000	-2.56441400	0.67449900	H	4.44433100	-1.11703400	0.19652600
H	2.39940100	-2.63878300	-0.03980700	H	4.56262400	-1.31393800	-1.55508000
C	2.63846400	-1.05038300	1.42608200	C	2.55491400	-1.57412400	-0.76043800
H	2.06576100	-1.64225900	2.15758000	H	2.11559200	-1.45633300	-1.76427100
H	3.47459800	-0.60834400	1.98963600	H	2.65703900	-2.65094400	-0.57668700
C	1.23174500	2.50019000	1.53233100	C	0.22558000	-1.26210600	2.40098200
H	0.29691700	3.07824900	1.58538000	H	-0.82645800	-1.55435700	2.26541300
H	1.82289500	2.78880200	2.41908100	H	0.56494300	-1.74301600	3.32922300
H	1.78477100	2.82310800	0.64468900	H	0.25238100	-0.17770600	2.54618400
C	-5.01738800	-1.25374900	0.31141600	C	-5.07362400	-0.79120700	-0.64470500
H	-5.07920800	-1.77785000	1.27442200	H	-5.78271000	-0.28624200	0.02002400
H	-5.77745900	-0.46466800	0.30967100	H	-5.40748500	-0.63056500	-1.67841400
H	-5.28830700	-1.98104100	-0.46603300	H	-5.13887900	-1.87001700	-0.45137700
O	0.35714300	1.94647800	-1.56209100	O	0.41905900	2.60479600	0.15559500
H	-0.53581900	2.11377100	-1.91883800	H	-0.39766300	2.97345200	-0.22309500

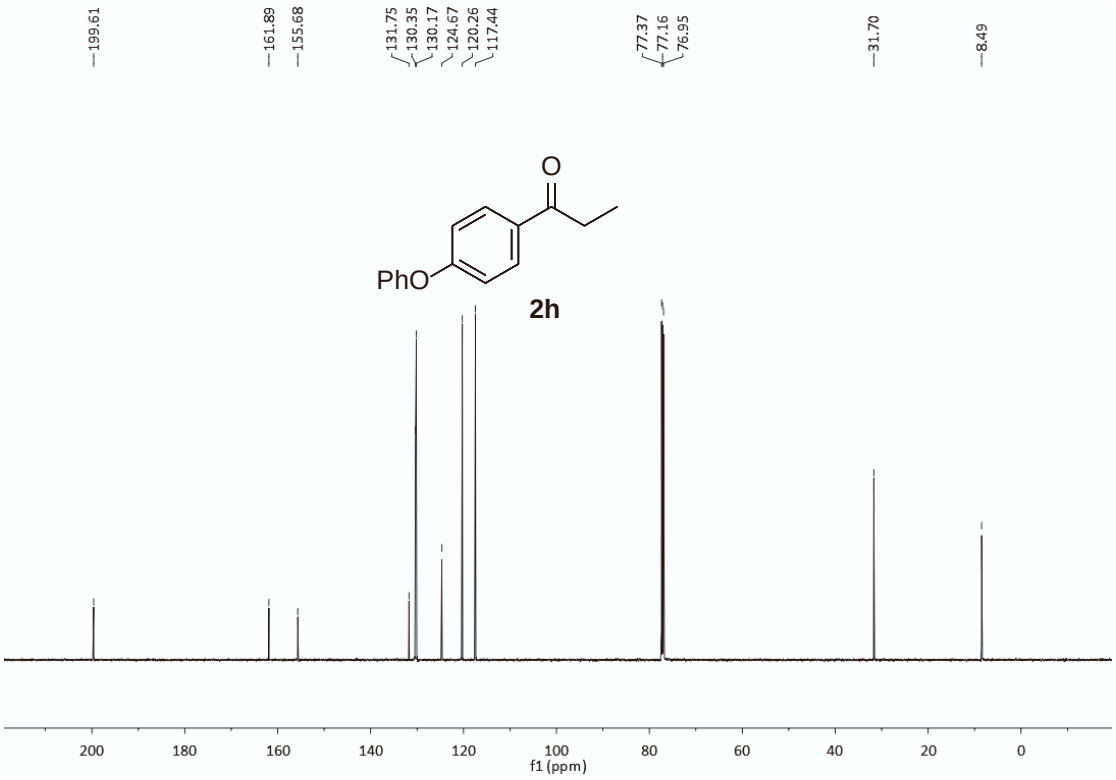
Int10' '

9. NMR spectra

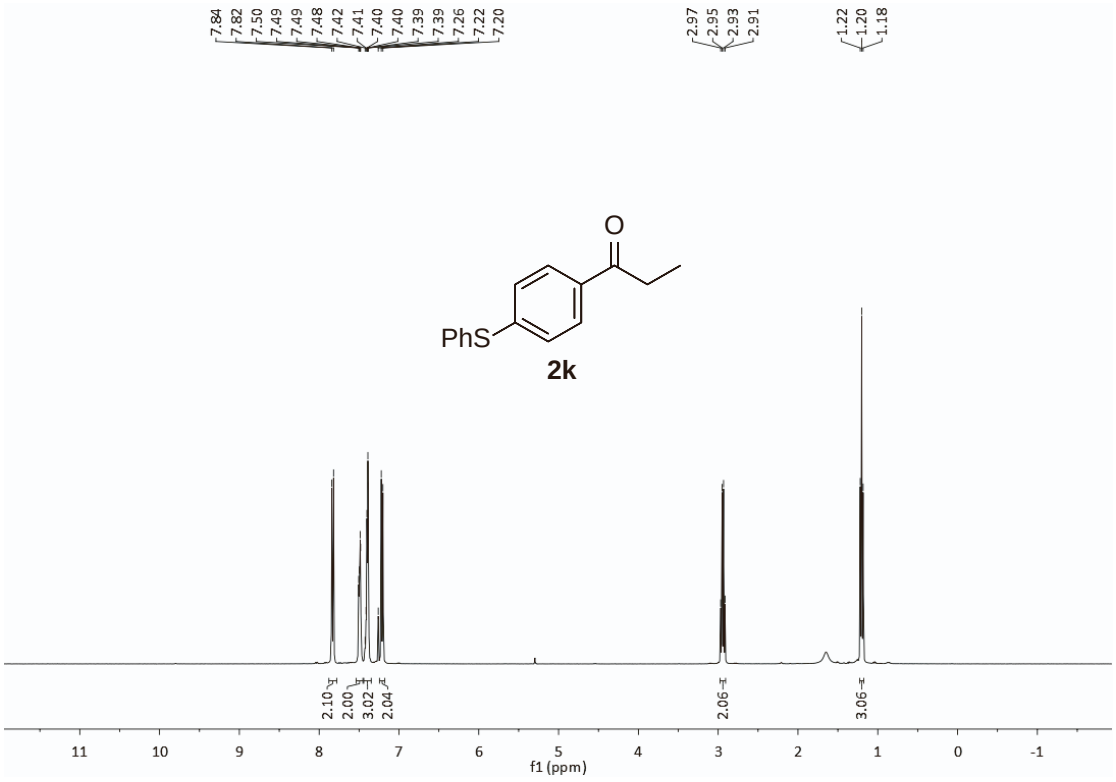
^{1}H NMR (400 MHz, $CDCl_3$)



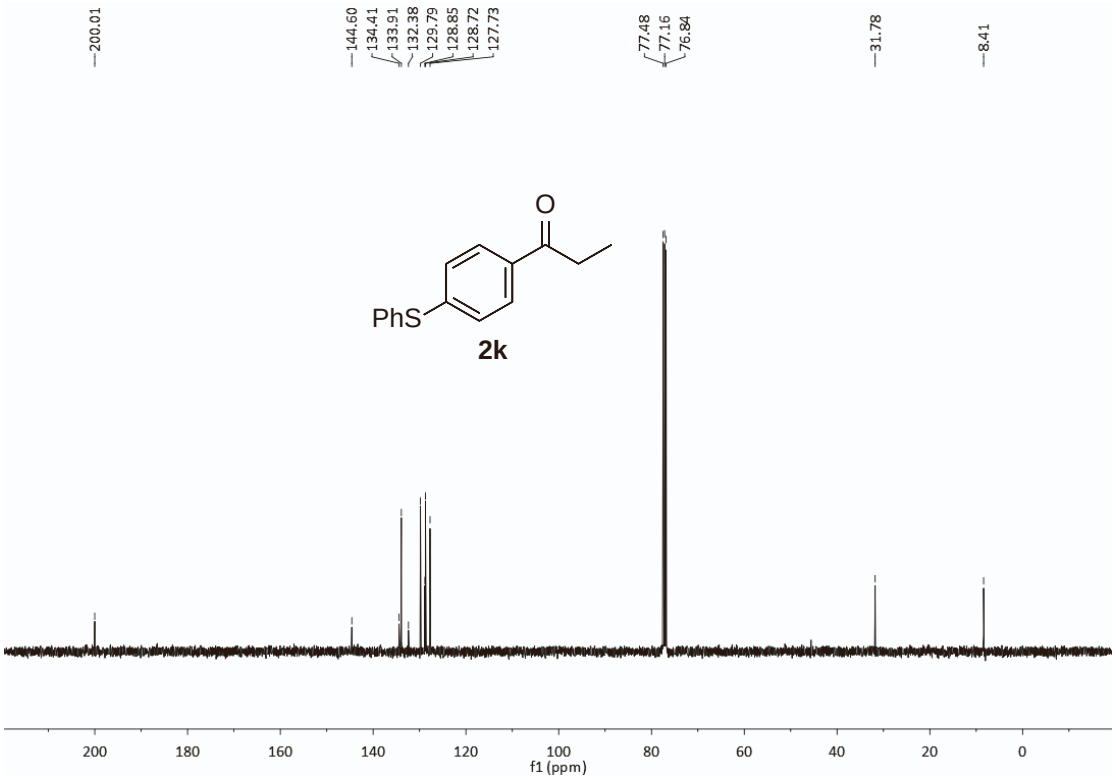
^{13}C NMR (151 MHz, $CDCl_3$)



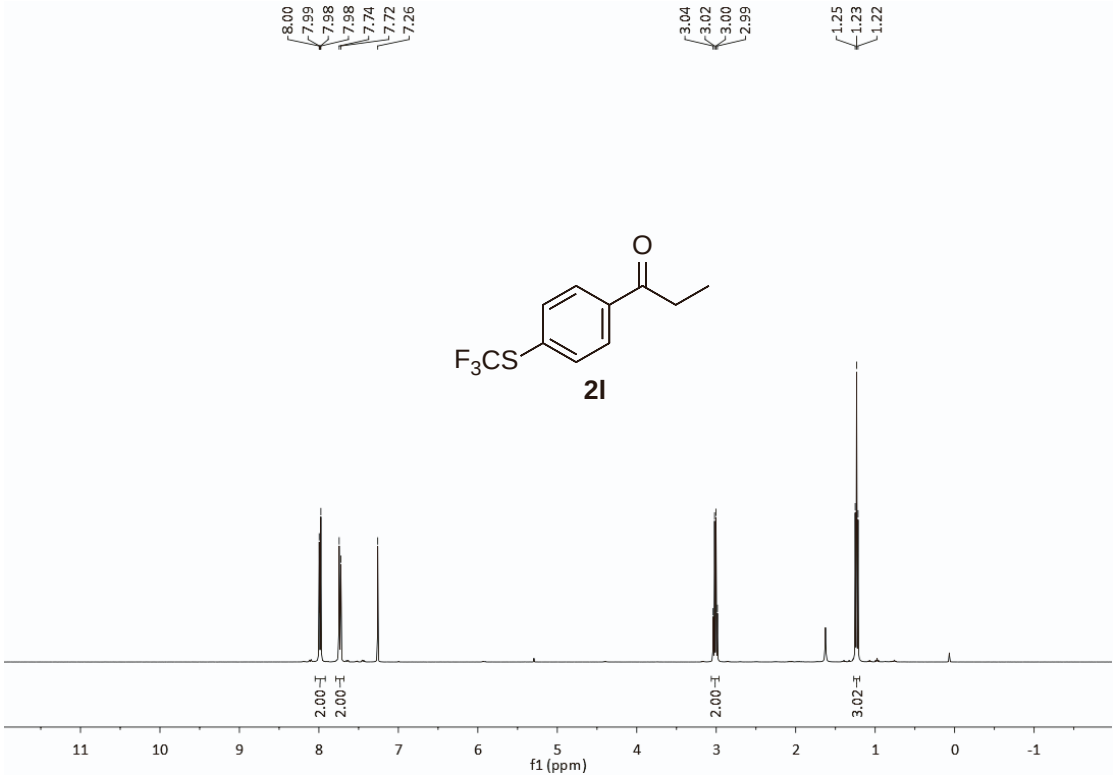
^{1}H NMR (400 MHz, $CDCl_3$)



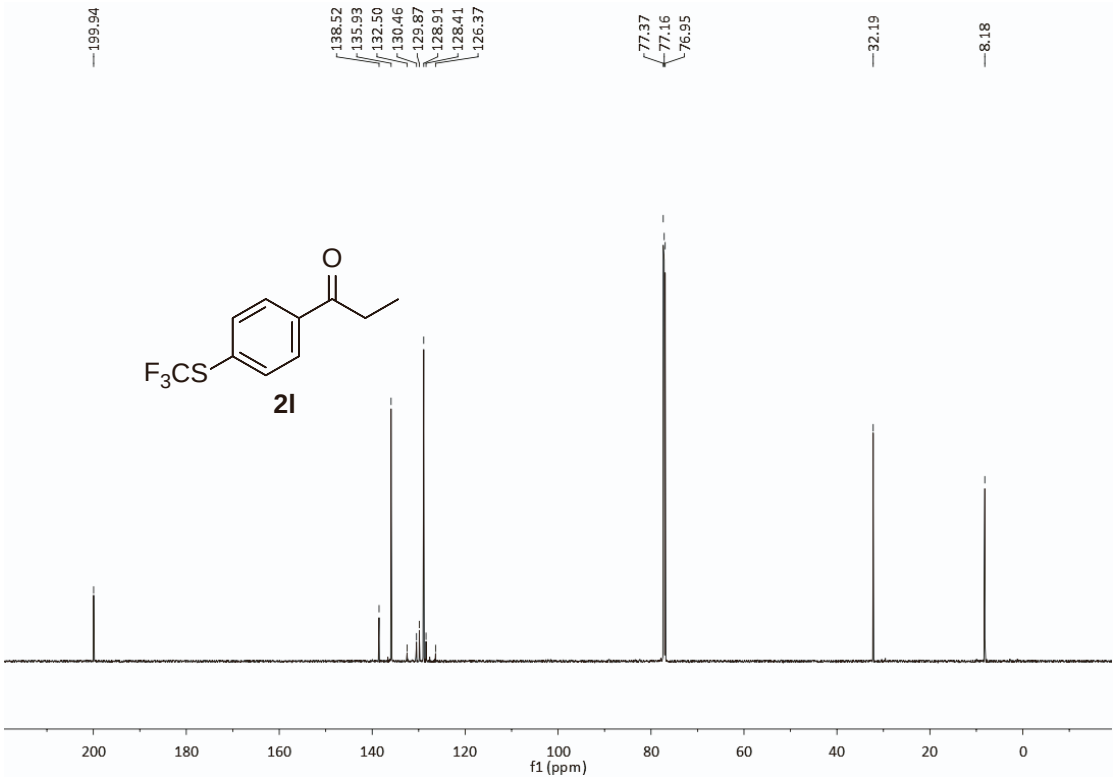
^{13}C NMR (101 MHz, $CDCl_3$)



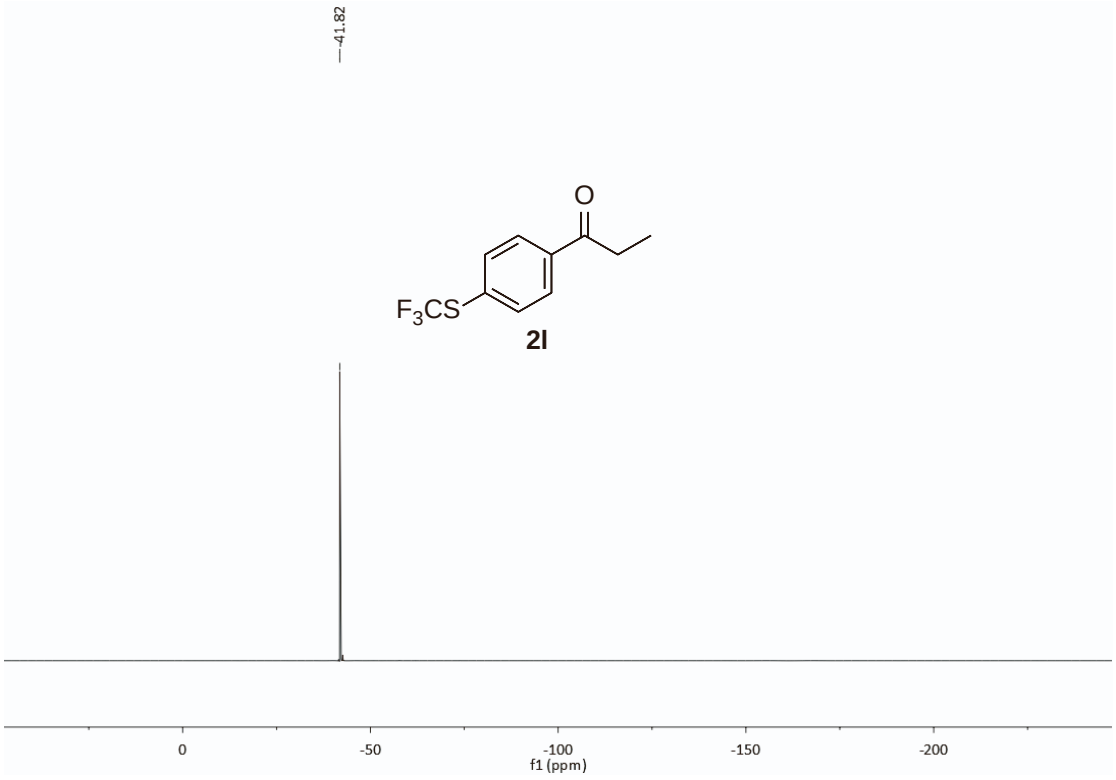
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (151 MHz, $CDCl_3$)

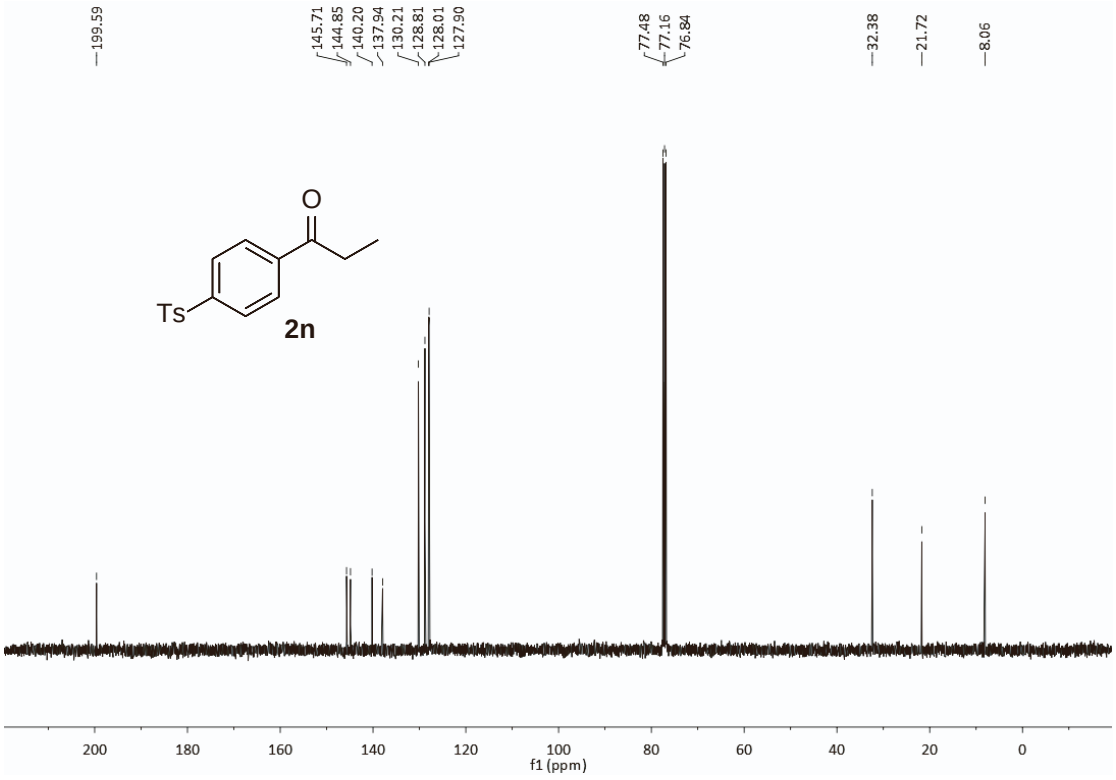


^{19}F NMR (565 MHz, $CDCl_3$)

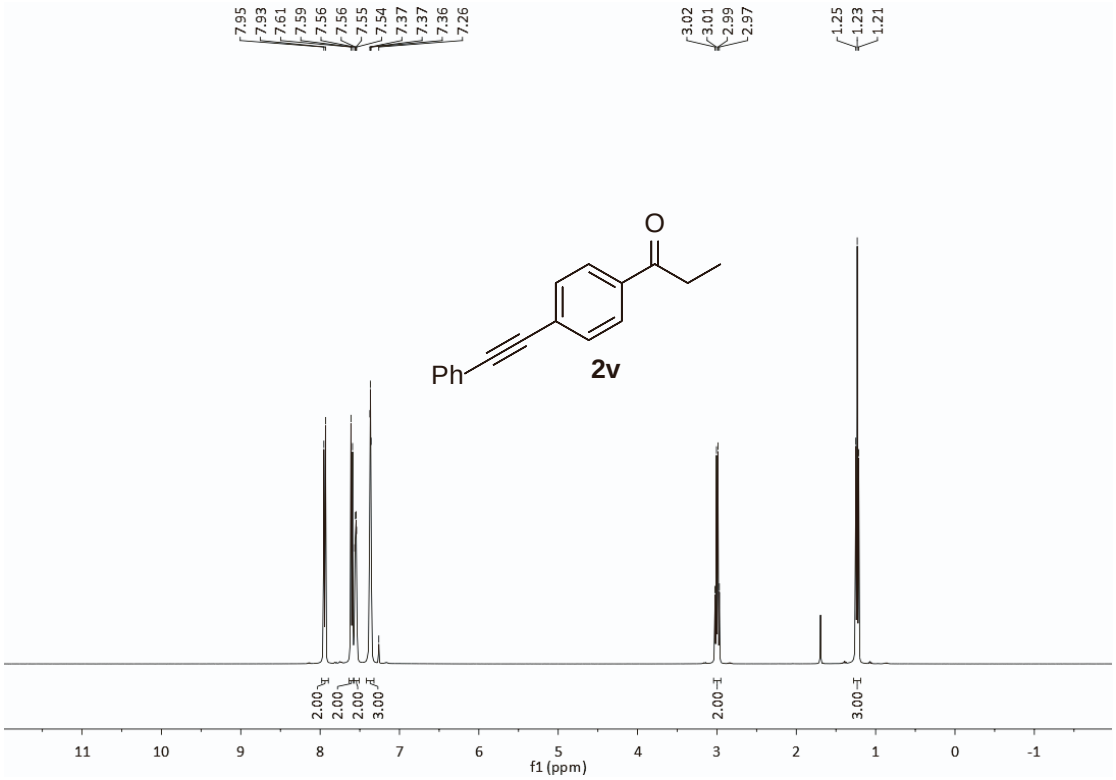


^{1}H NMR (400 MHz, $CDCl_3$)

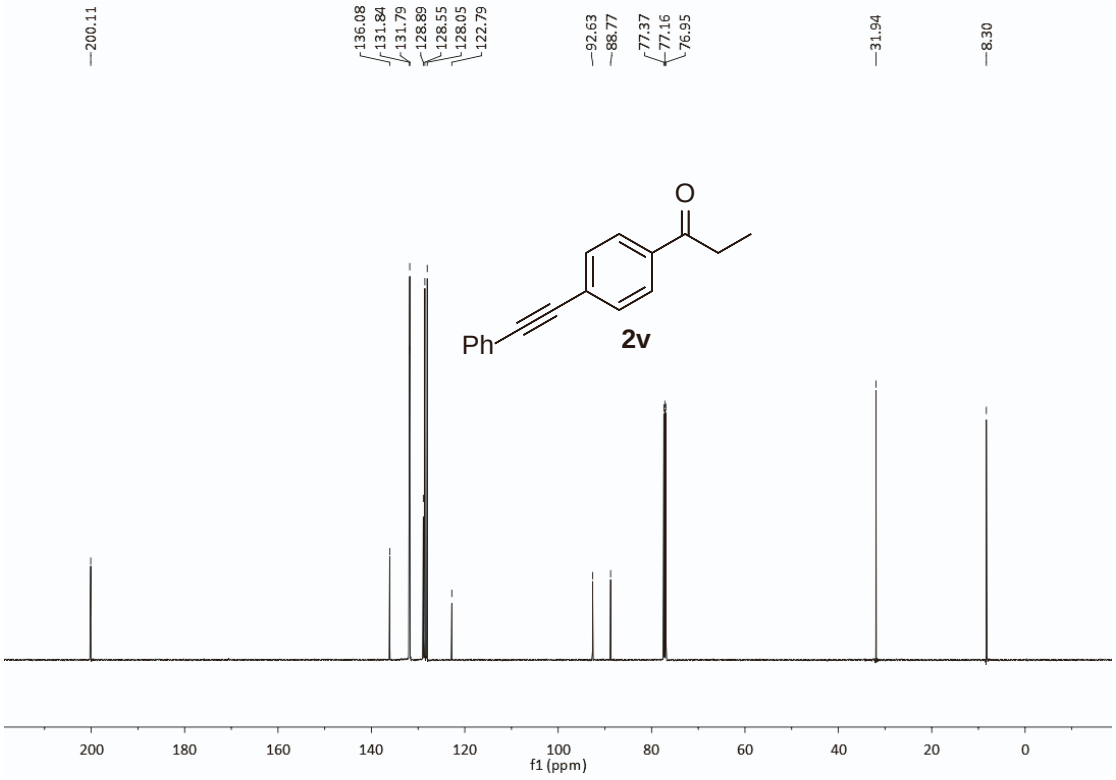
^{13}C NMR (101 MHz, $CDCl_3$)



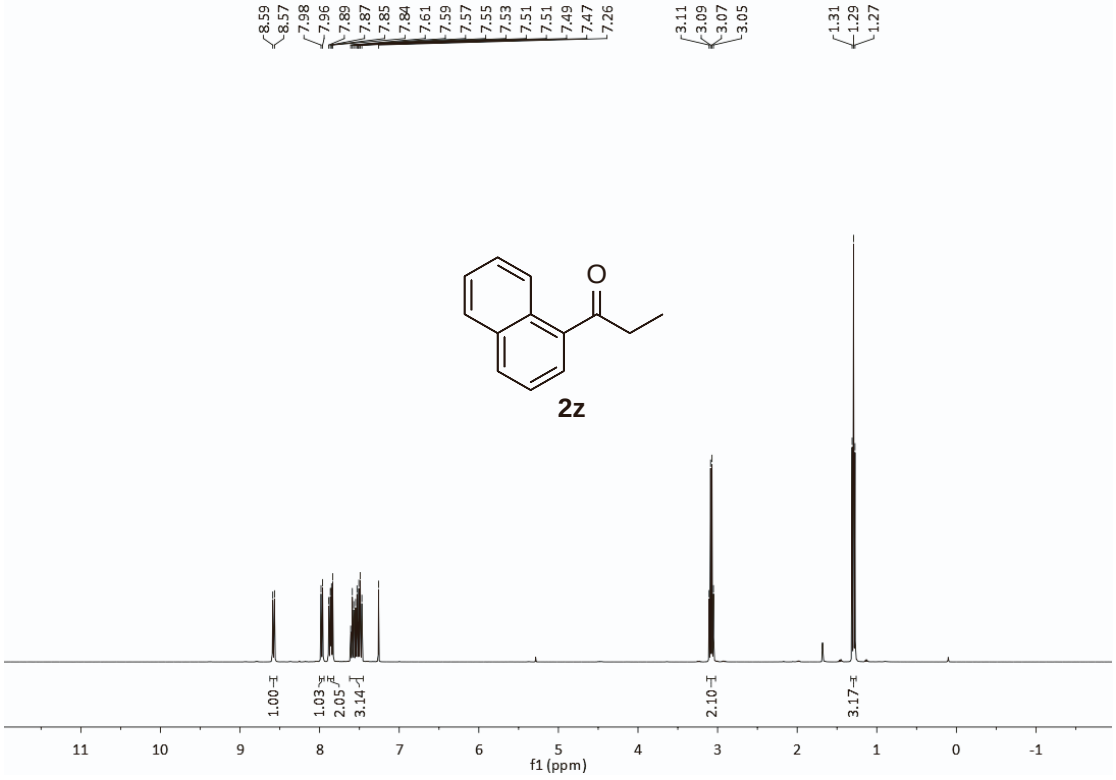
^{1}H NMR (400 MHz, $CDCl_3$)



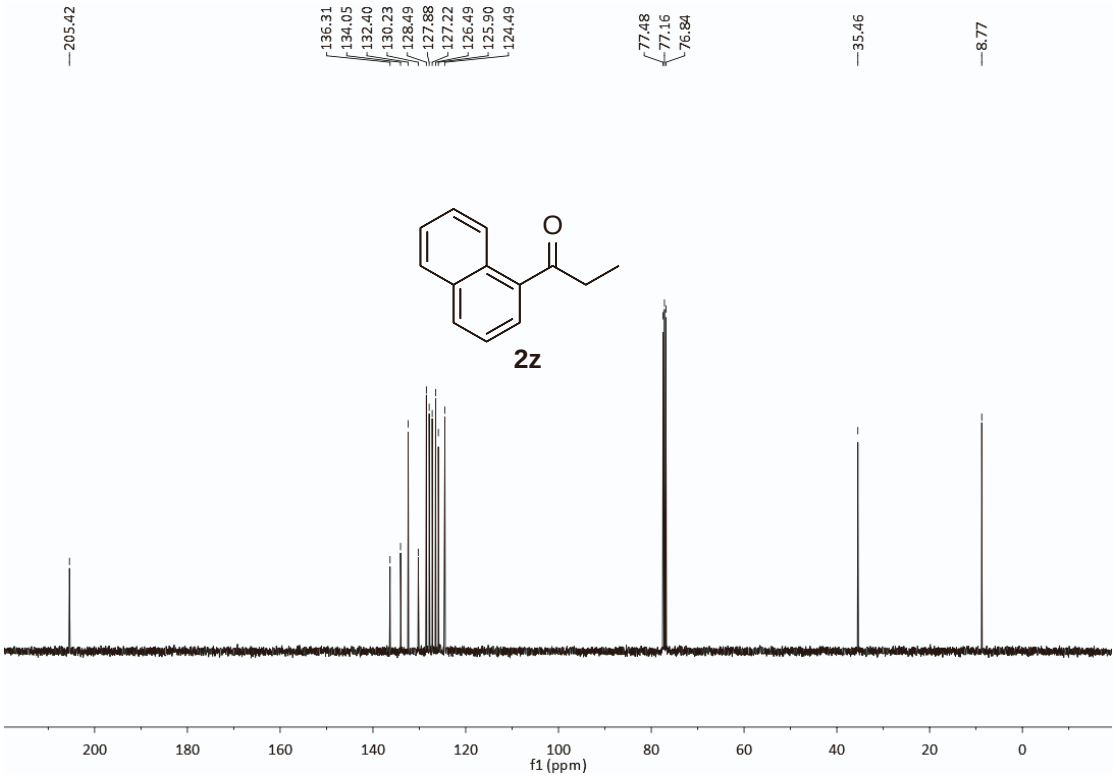
^{13}C NMR (151 MHz, $CDCl_3$)



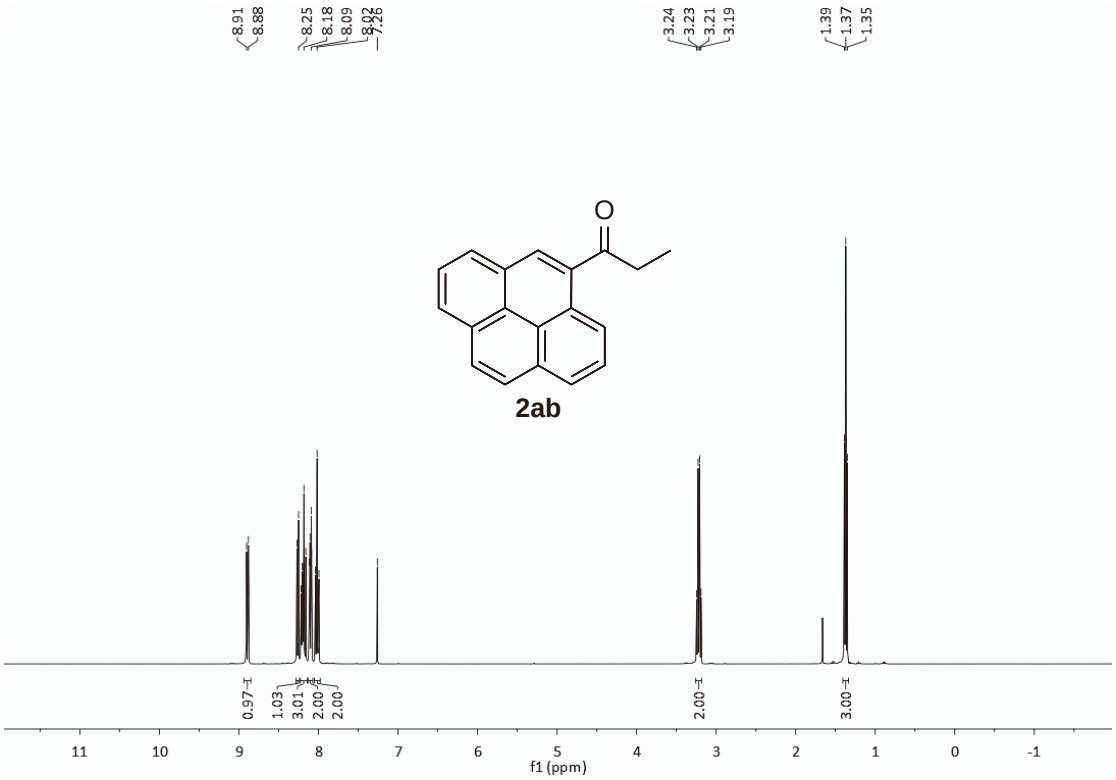
^{1}H NMR (400 MHz, $CDCl_3$)



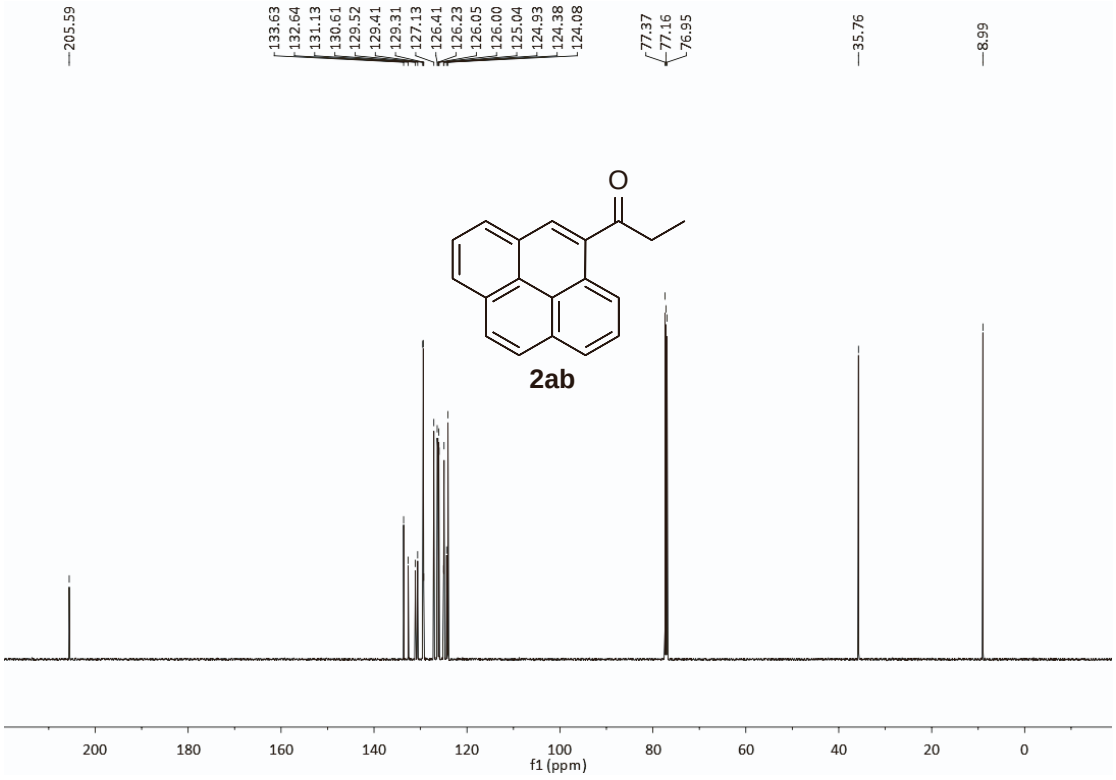
^{13}C NMR (101 MHz, $CDCl_3$)



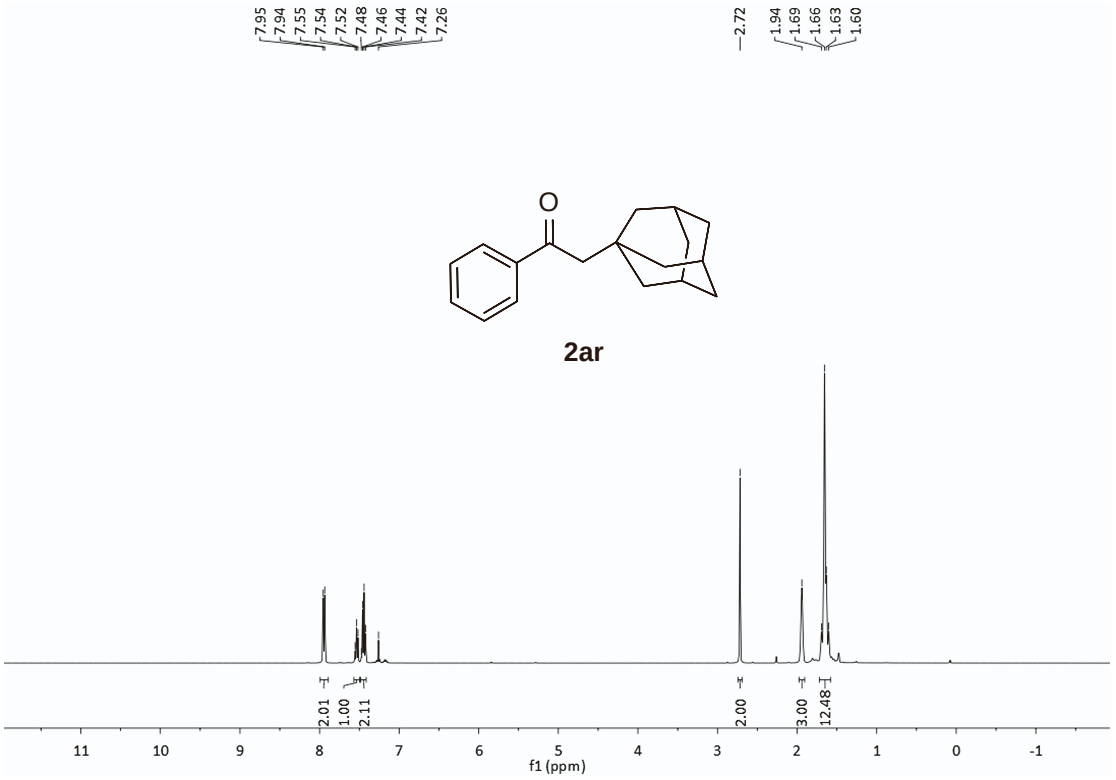
^{1}H NMR (400 MHz, $CDCl_3$)



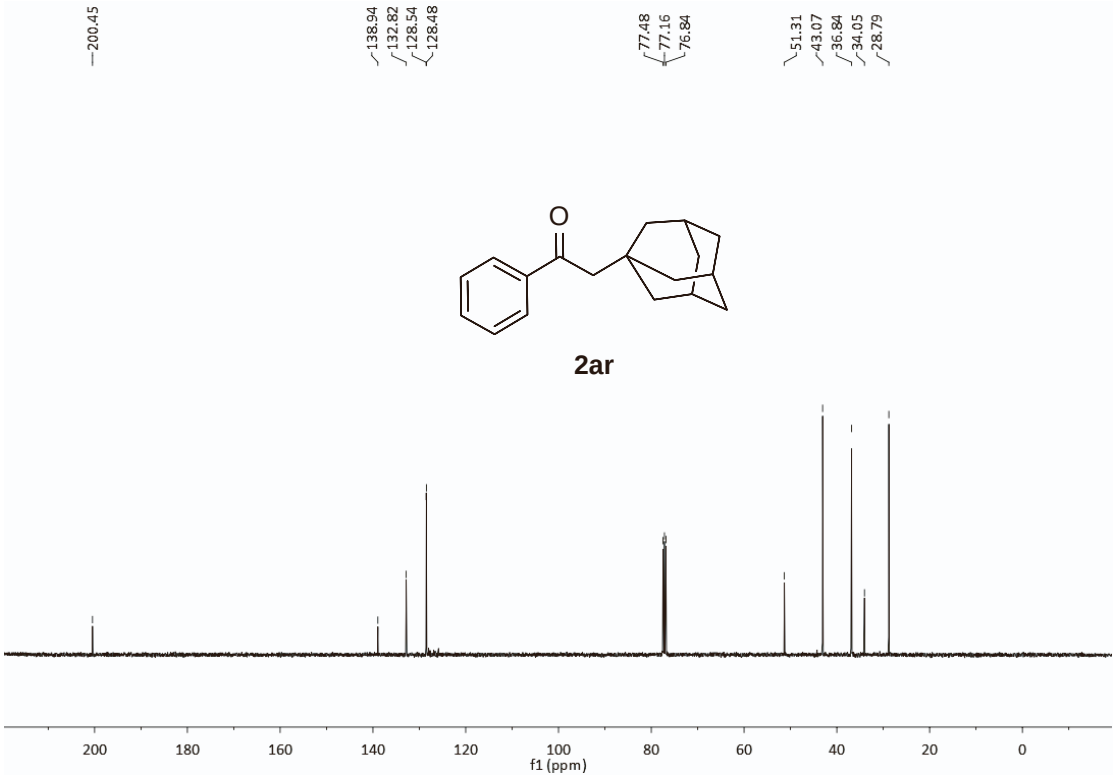
^{13}C NMR (151 MHz, $CDCl_3$)



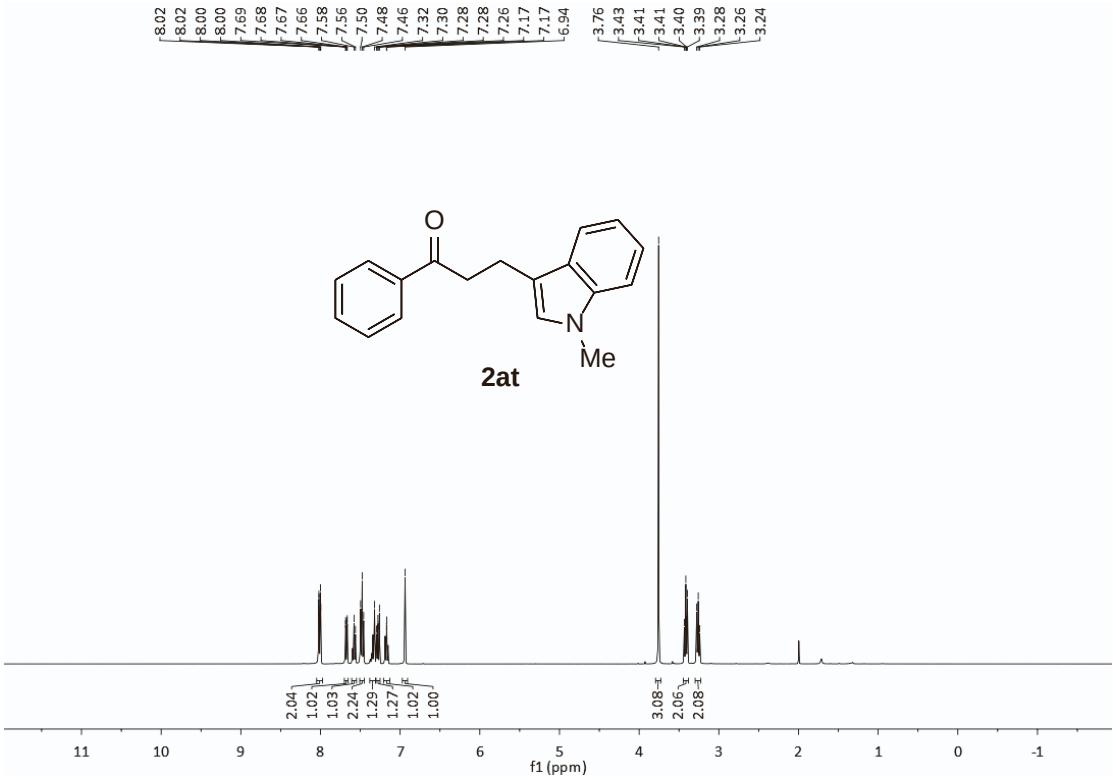
^{1}H NMR (400 MHz, $CDCl_3$)



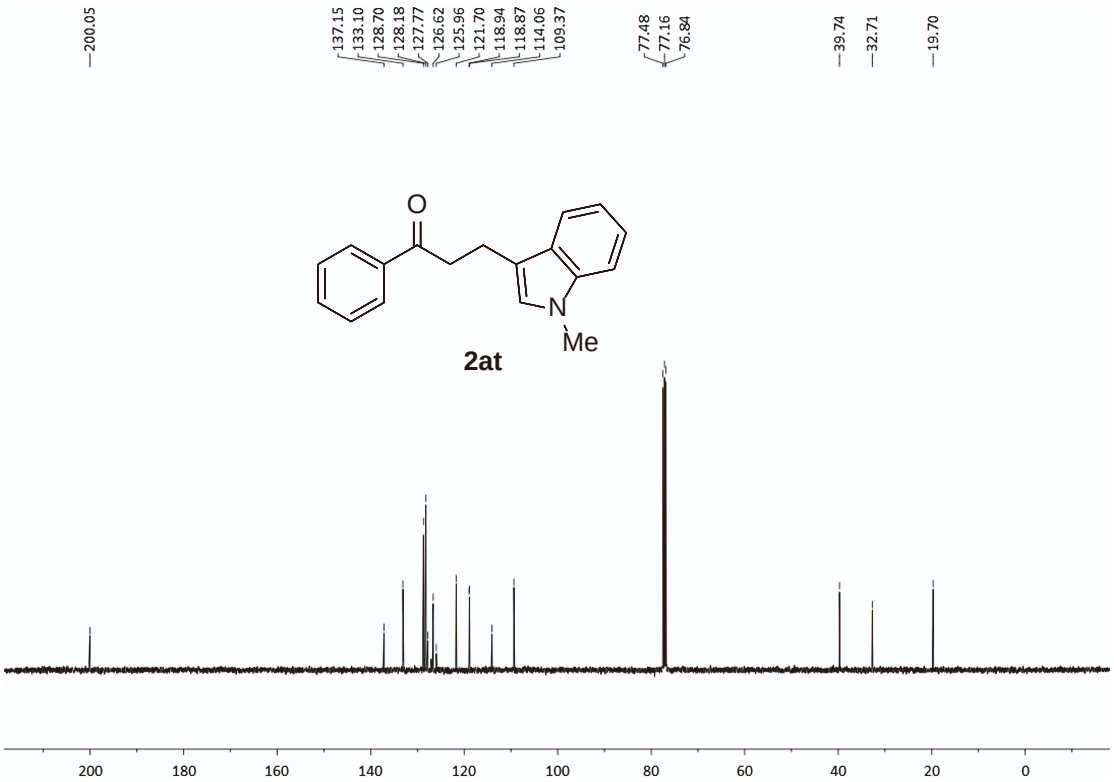
^{13}C NMR (101 MHz, $CDCl_3$)



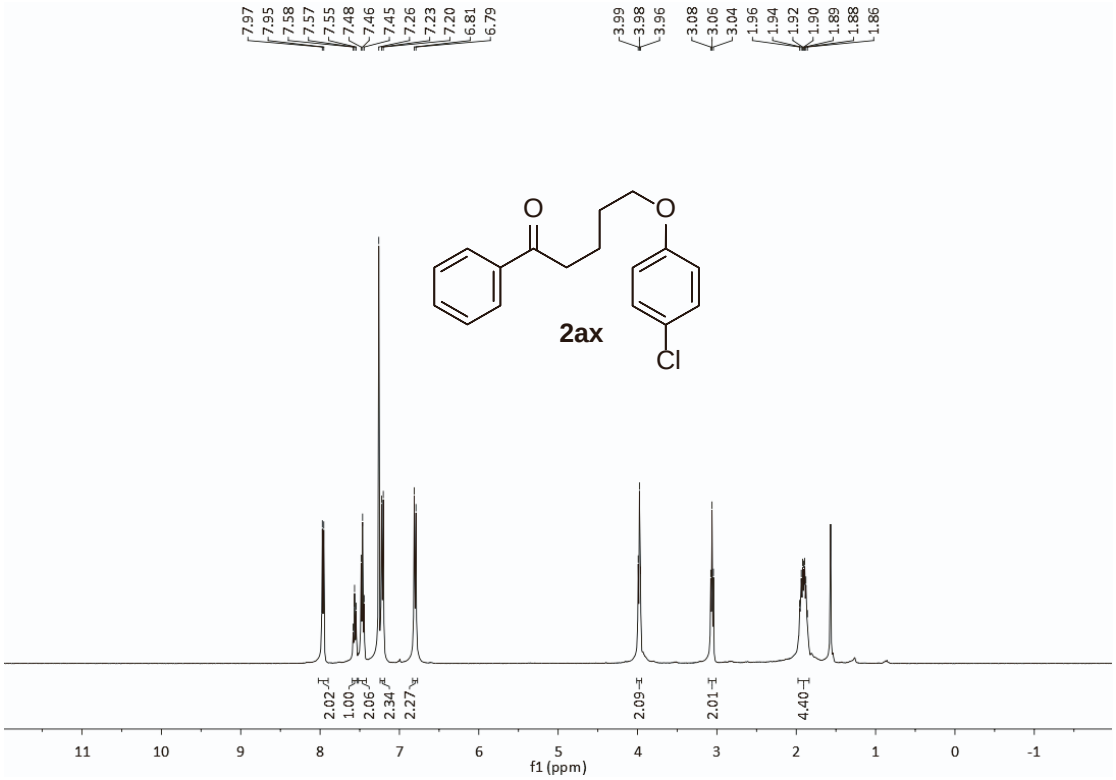
^{1}H NMR (400 MHz, $CDCl_3$)



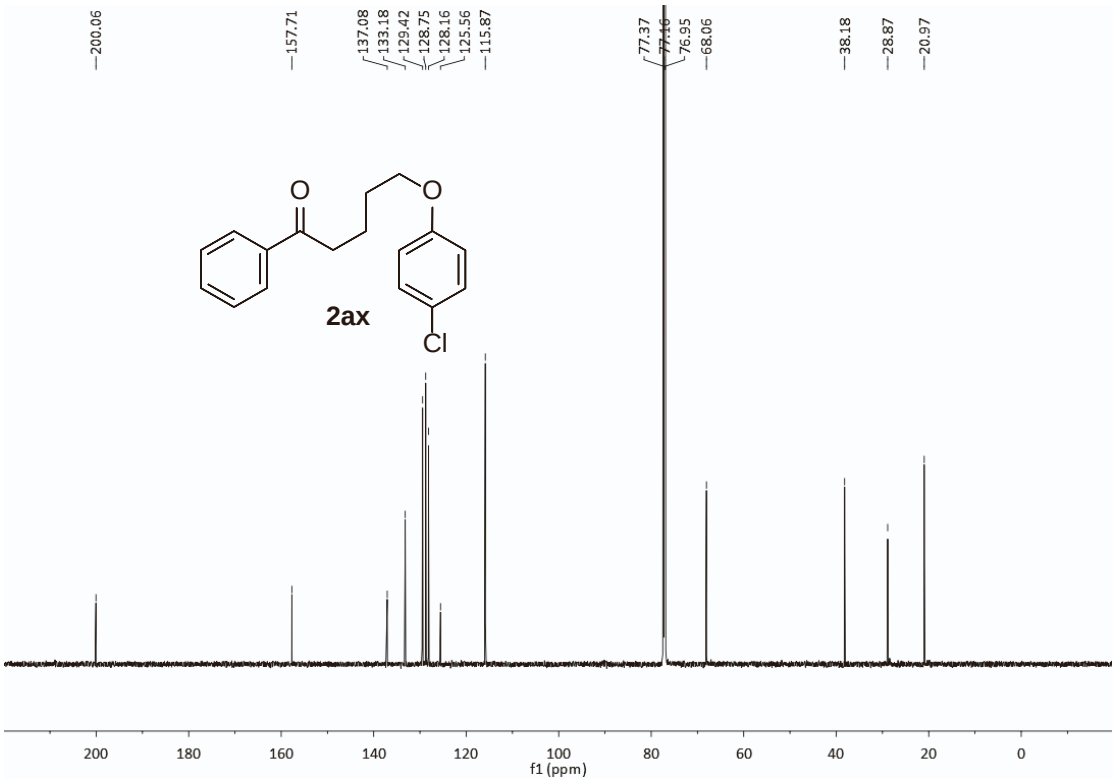
^{13}C NMR (101 MHz, $CDCl_3$)



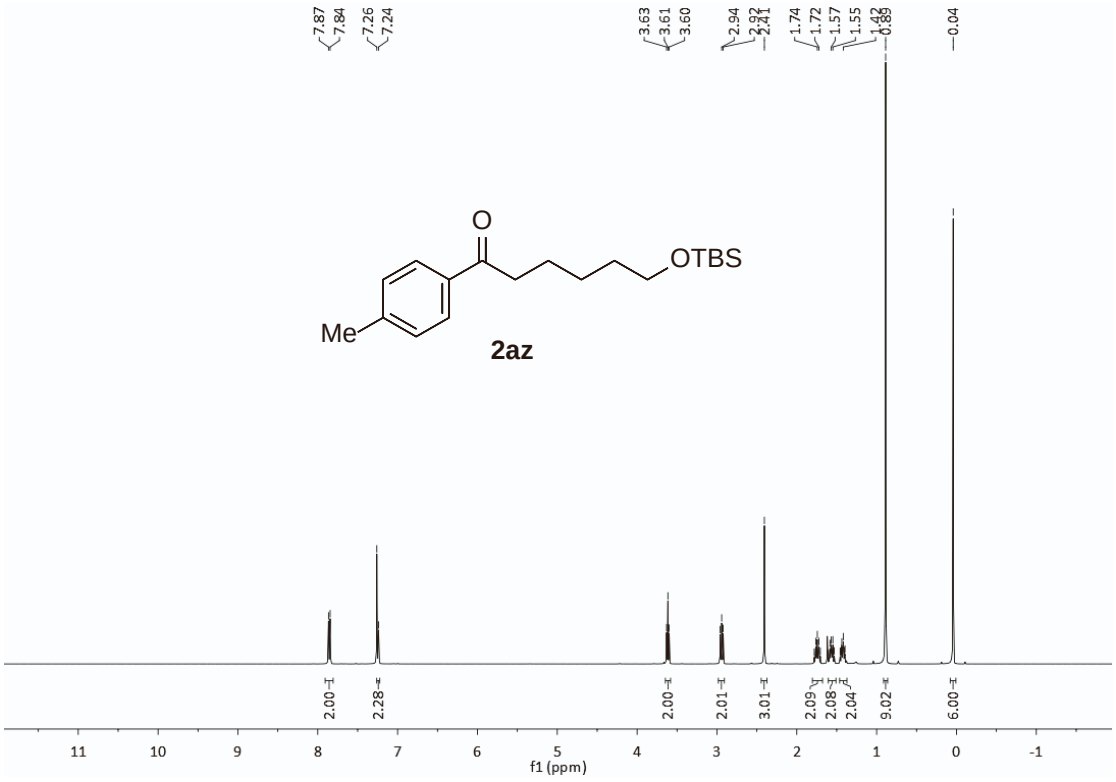
^{1}H NMR (400 MHz, $CDCl_3$)



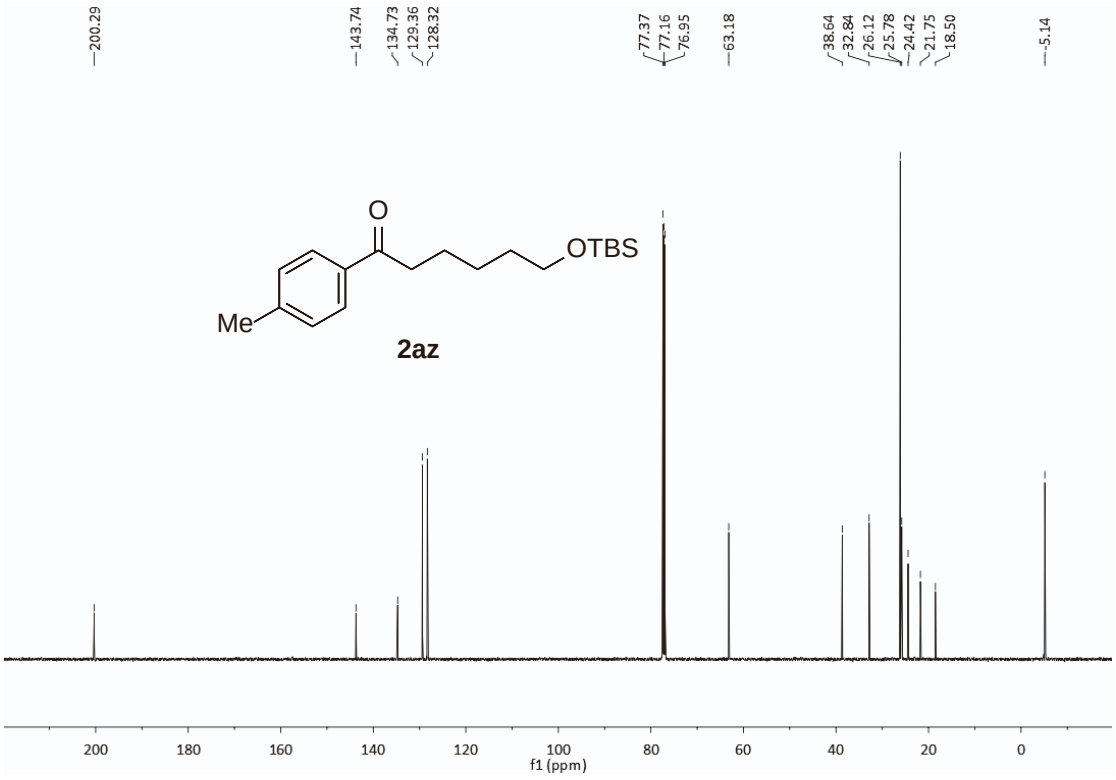
^{13}C NMR (151 MHz, $CDCl_3$)



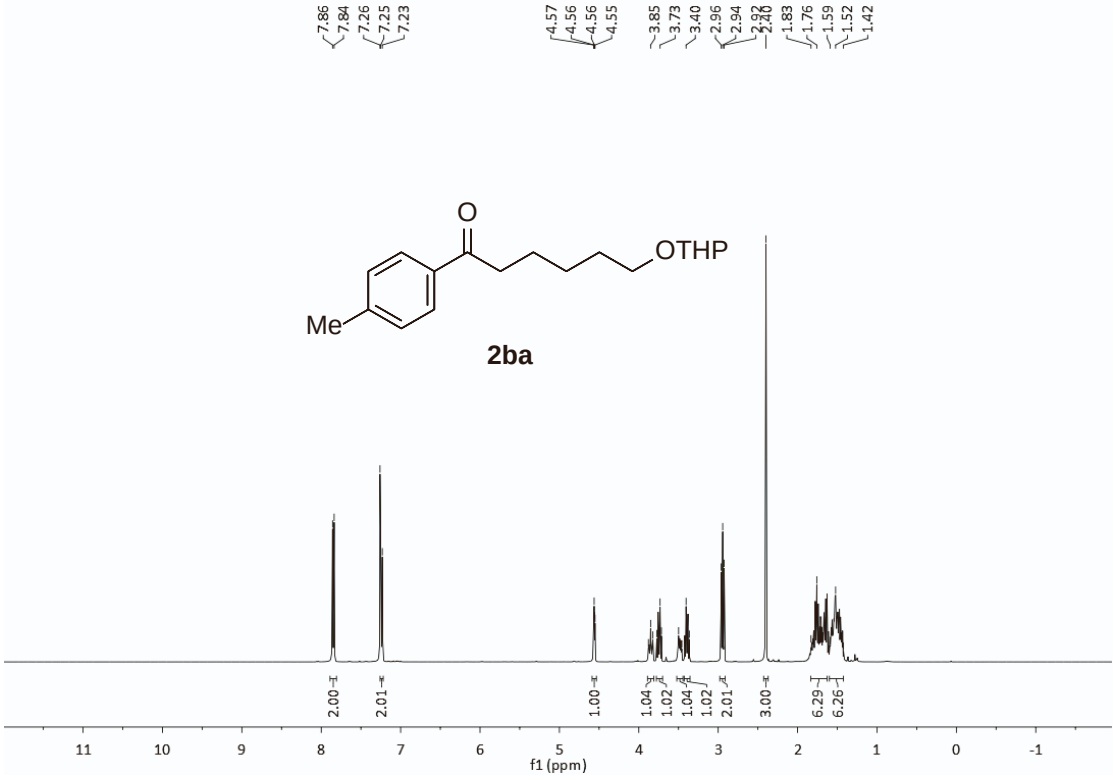
^{1}H NMR (400 MHz, $CDCl_3$)



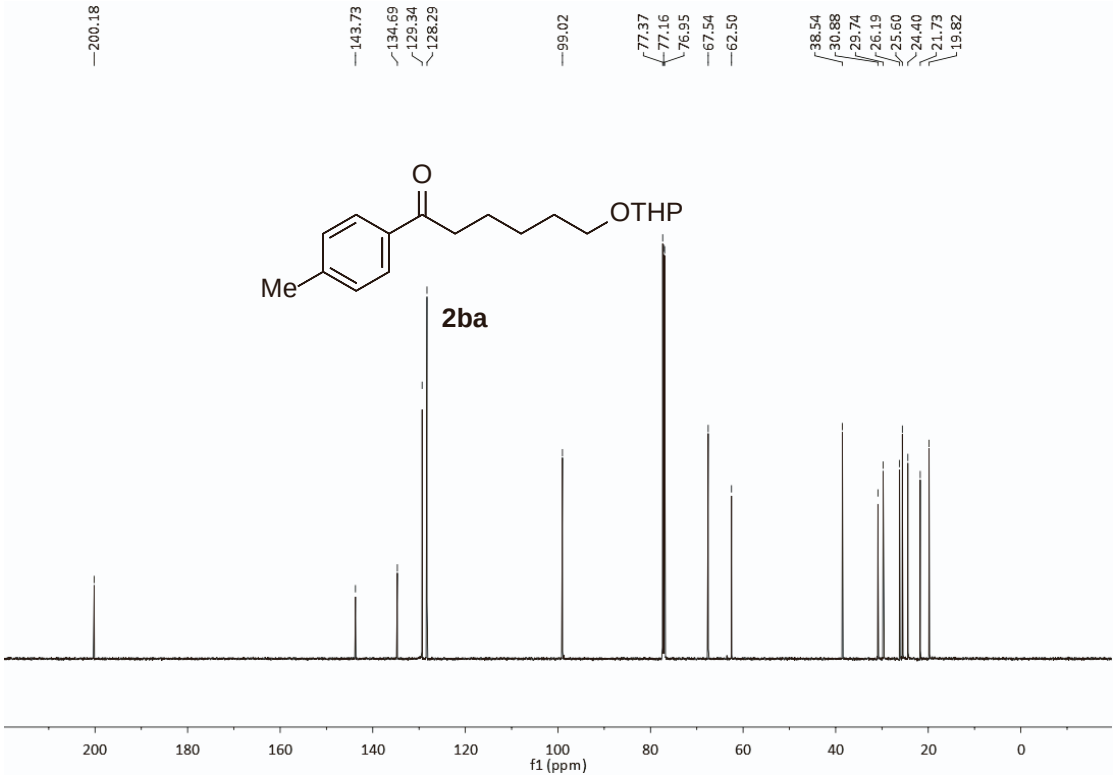
^{13}C NMR (151 MHz, $CDCl_3$)



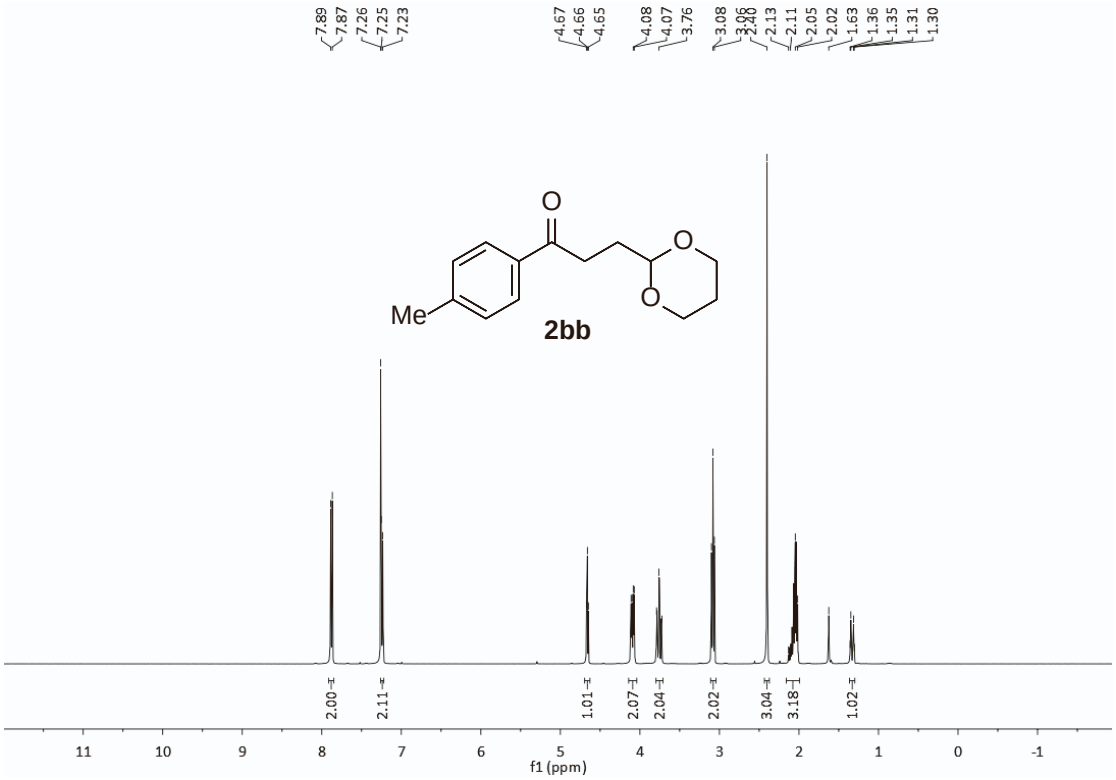
^{1}H NMR (400 MHz, $CDCl_3$)



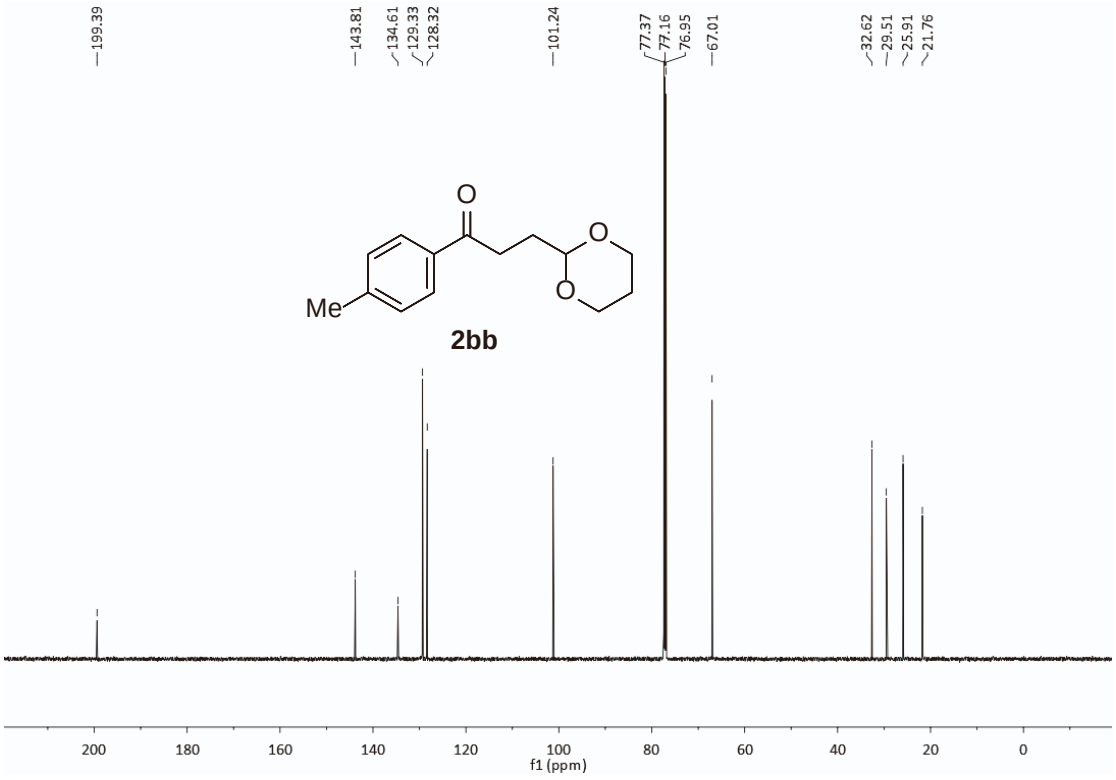
^{13}C NMR (151 MHz, $CDCl_3$)



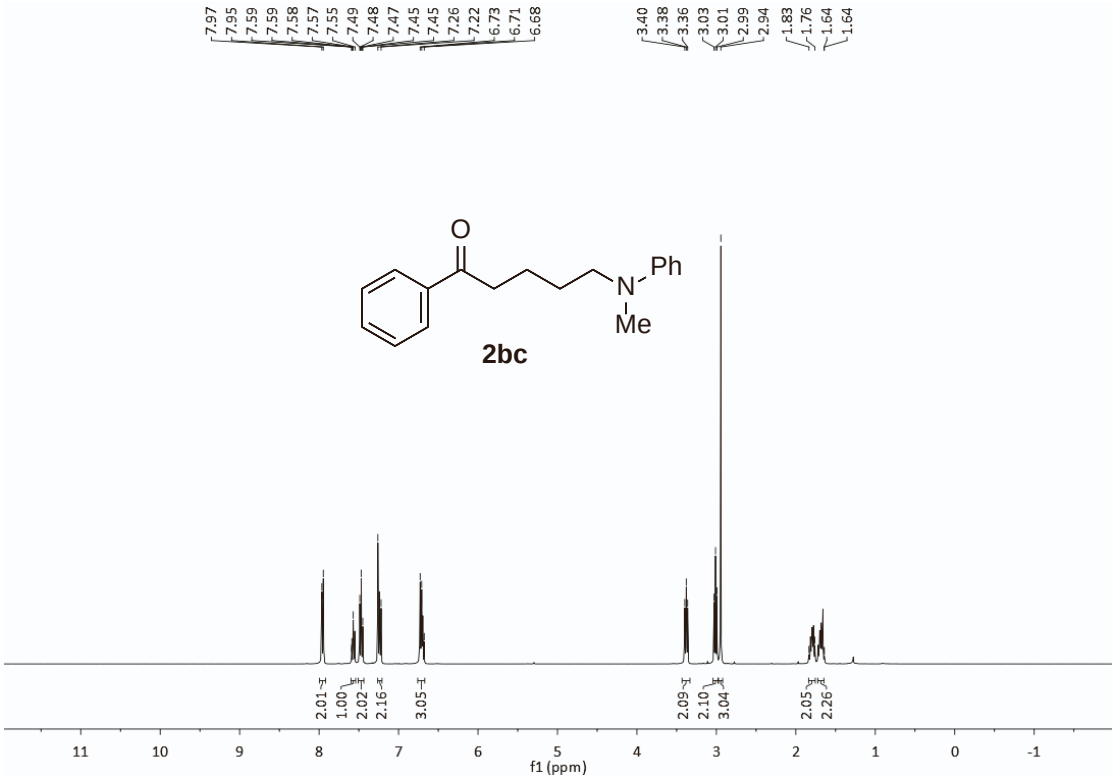
^{1}H NMR (400 MHz, $CDCl_3$)



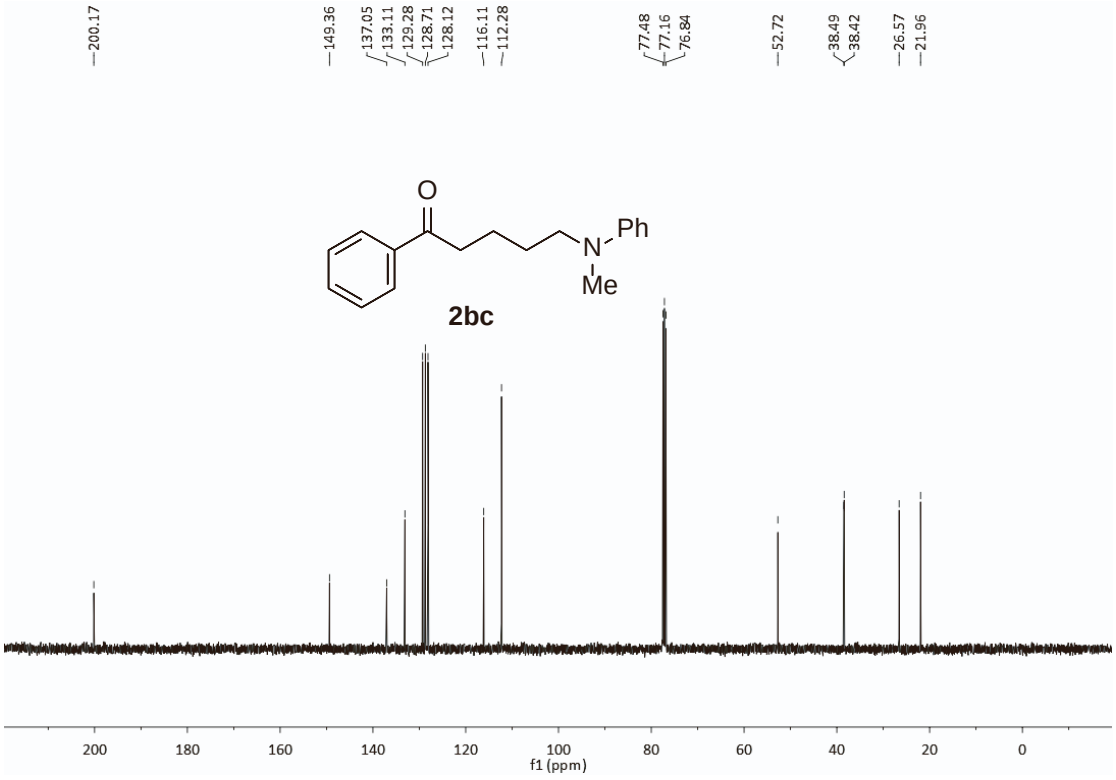
^{13}C NMR (151 MHz, $CDCl_3$)



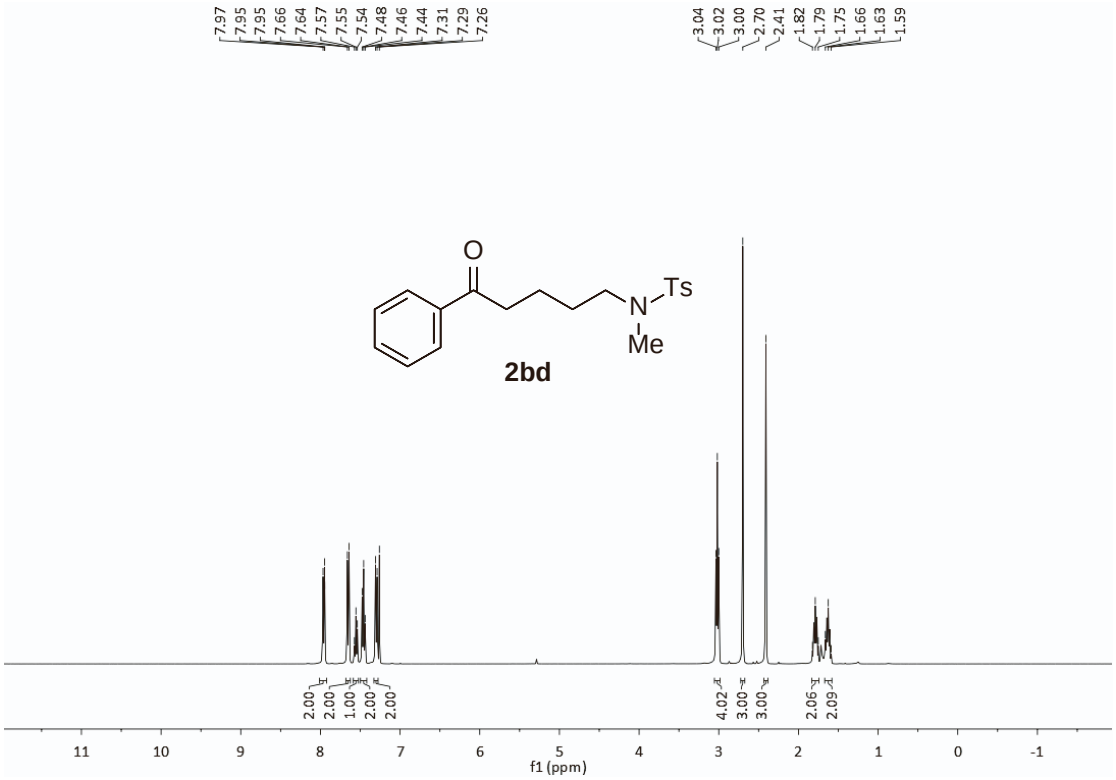
^{1}H NMR (400 MHz, $CDCl_3$)



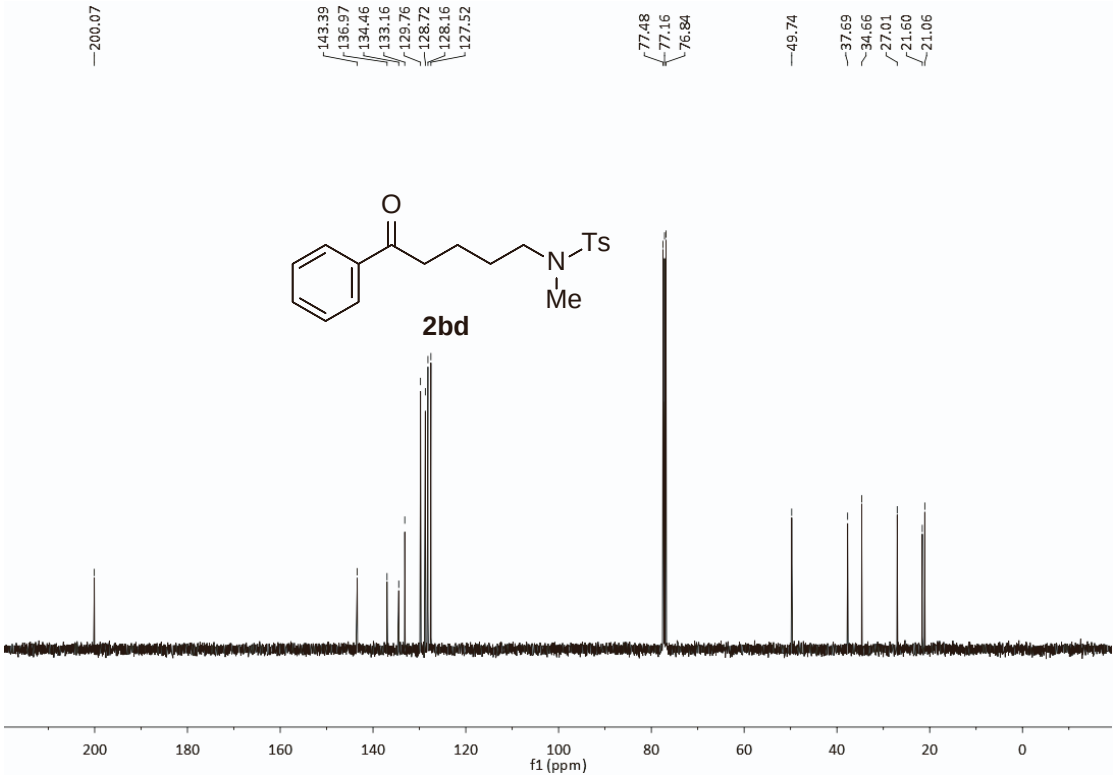
^{13}C NMR (101 MHz, $CDCl_3$)



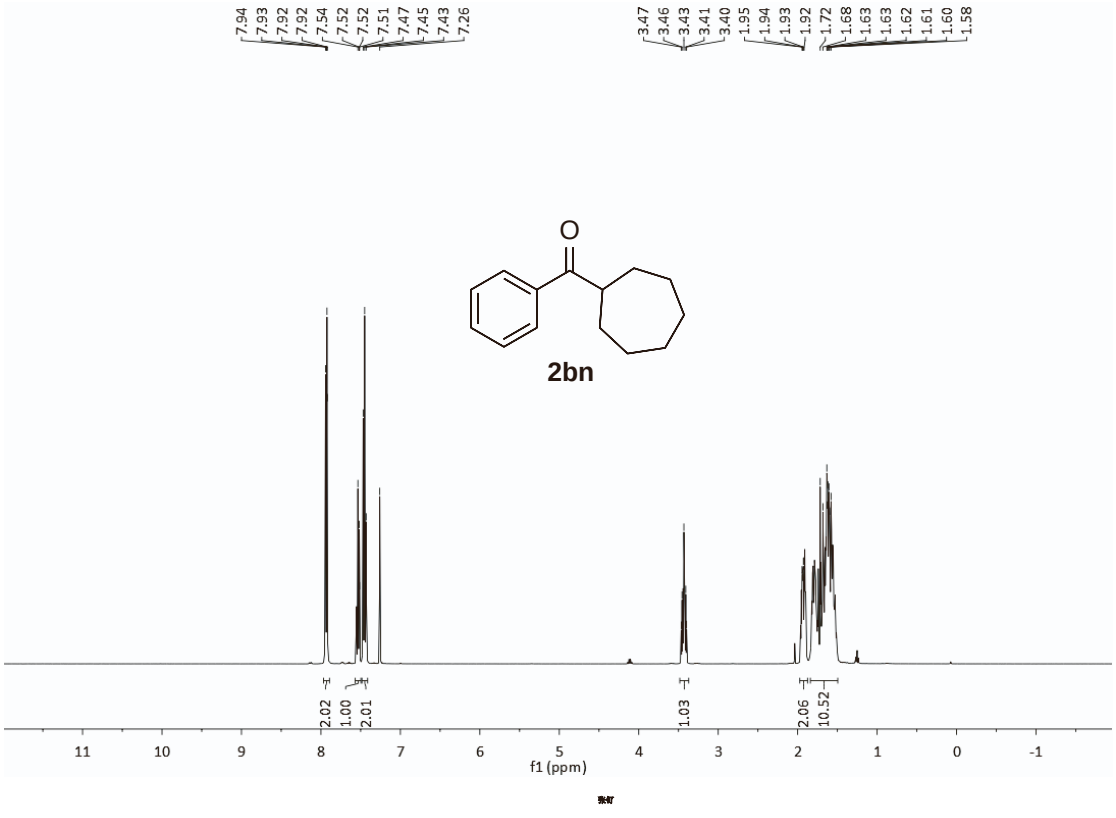
^{1}H NMR (400 MHz, $CDCl_3$)



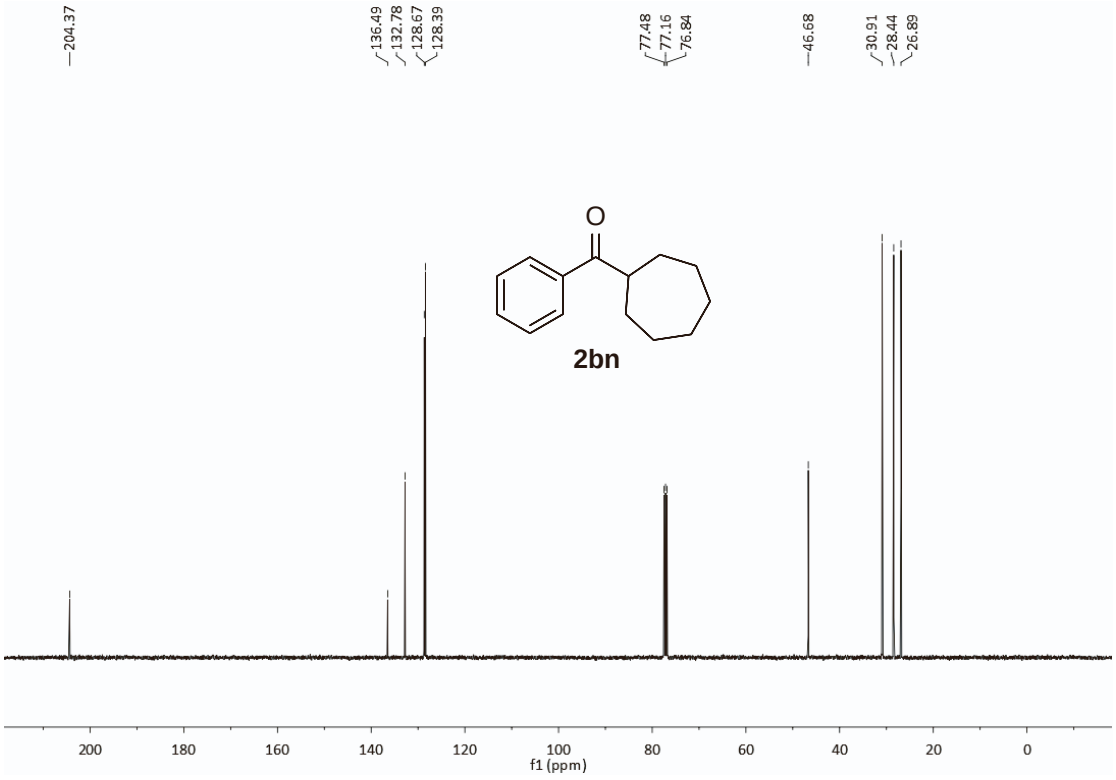
^{13}C NMR (101 MHz, $CDCl_3$)



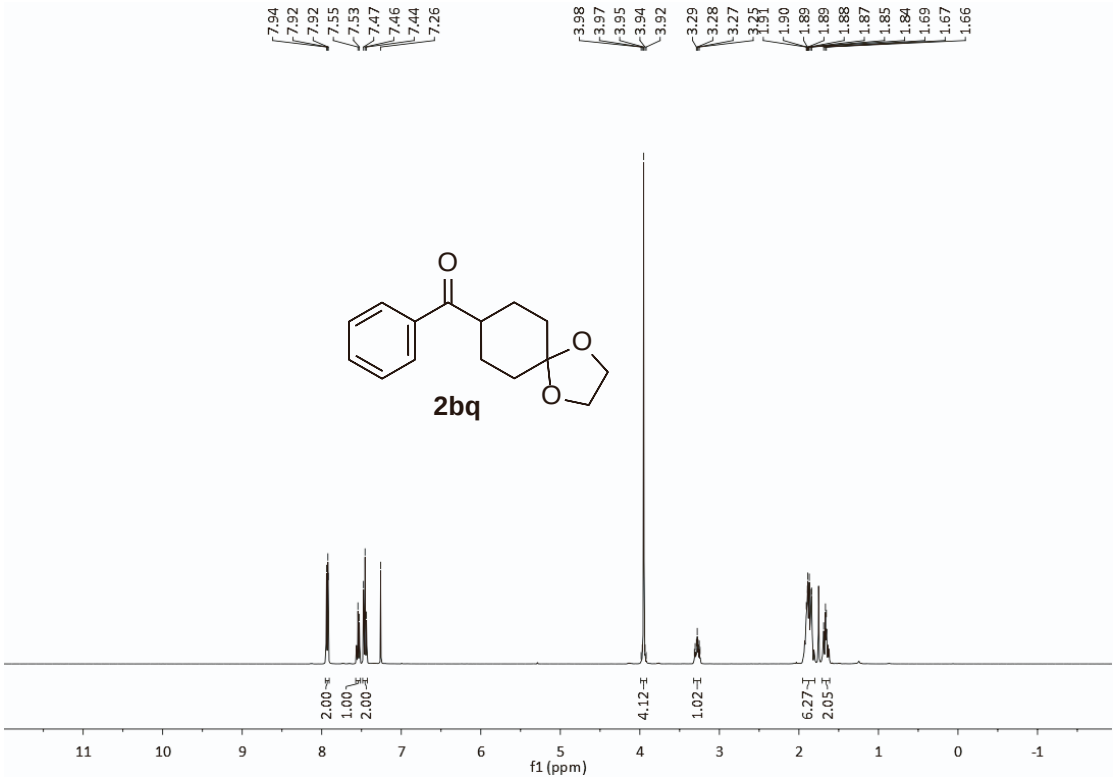
^{1}H NMR (400 MHz, $CDCl_3$)



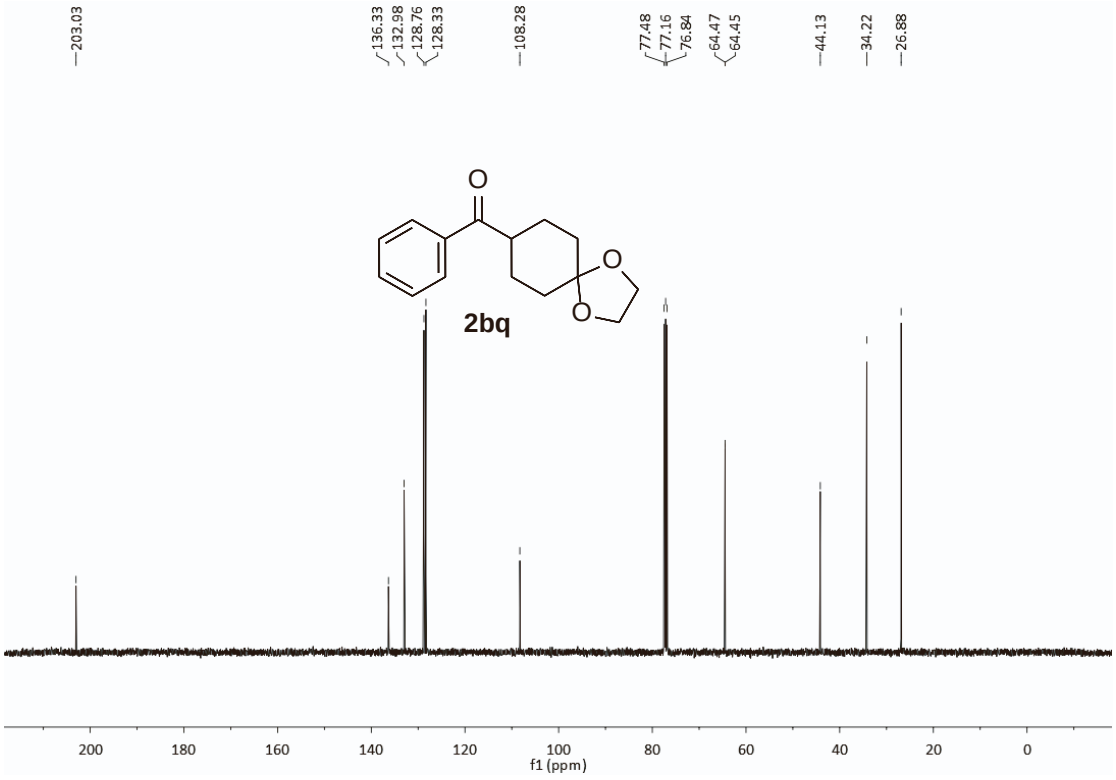
^{13}C NMR (101 MHz, $CDCl_3$)



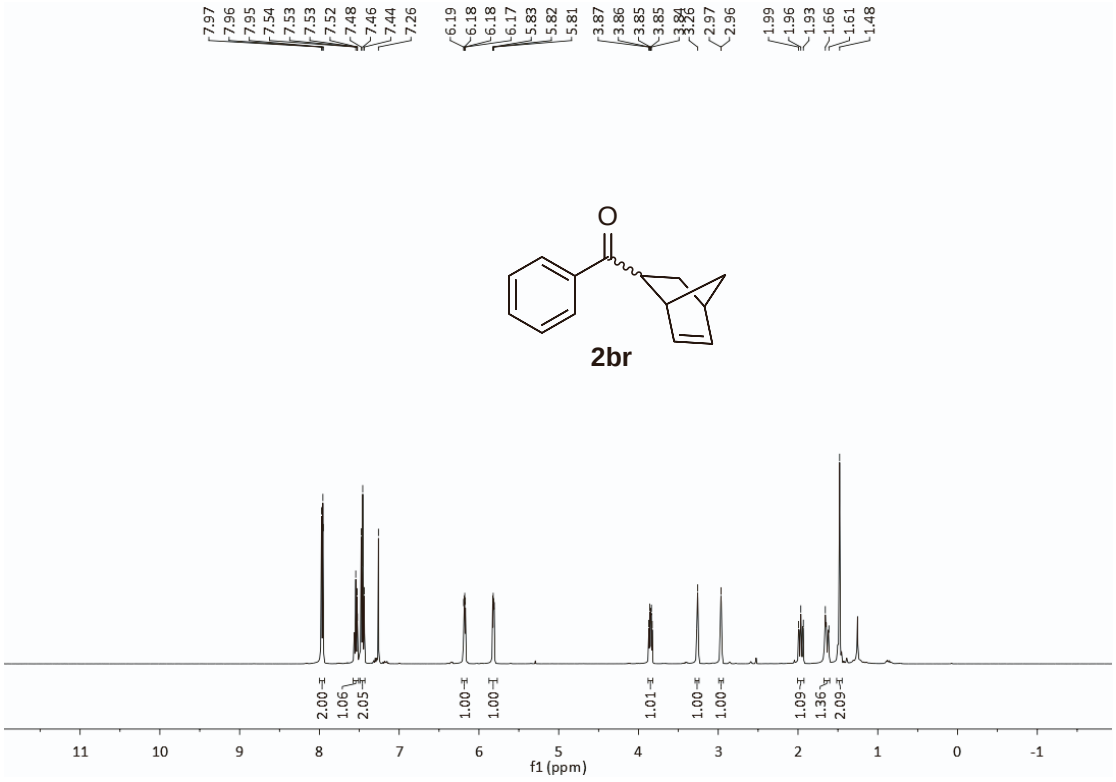
^{1}H NMR (400 MHz, $CDCl_3$)



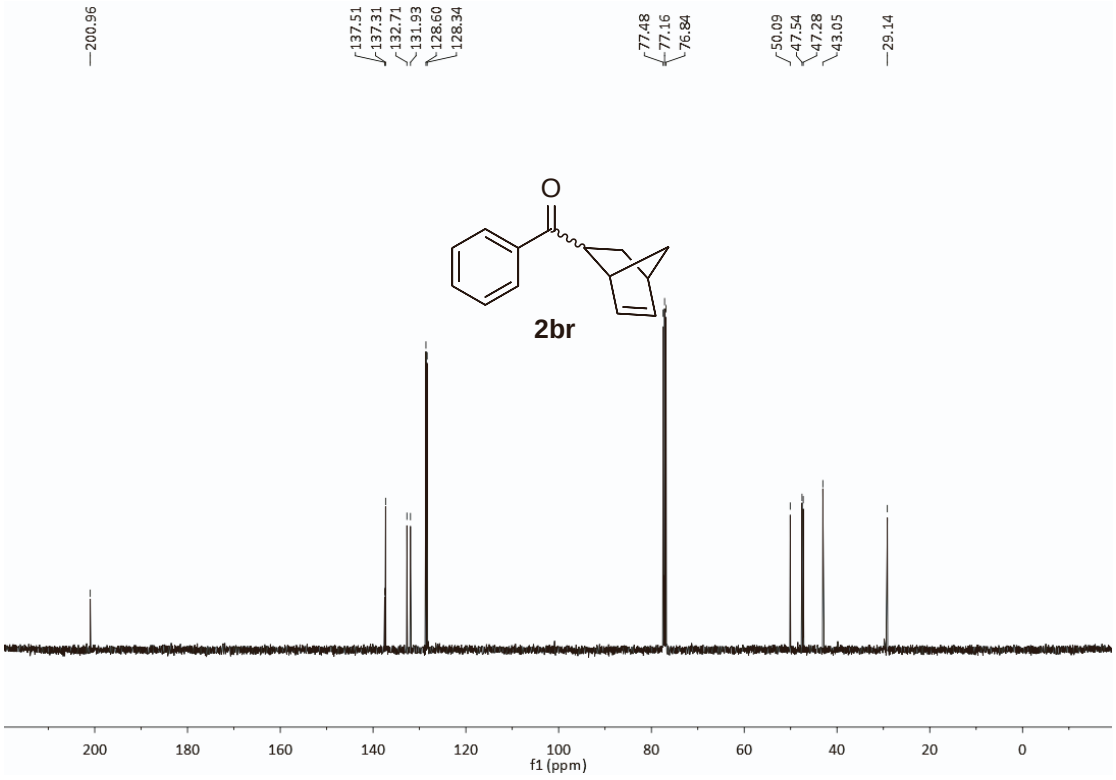
^{13}C NMR (101 MHz, $CDCl_3$)



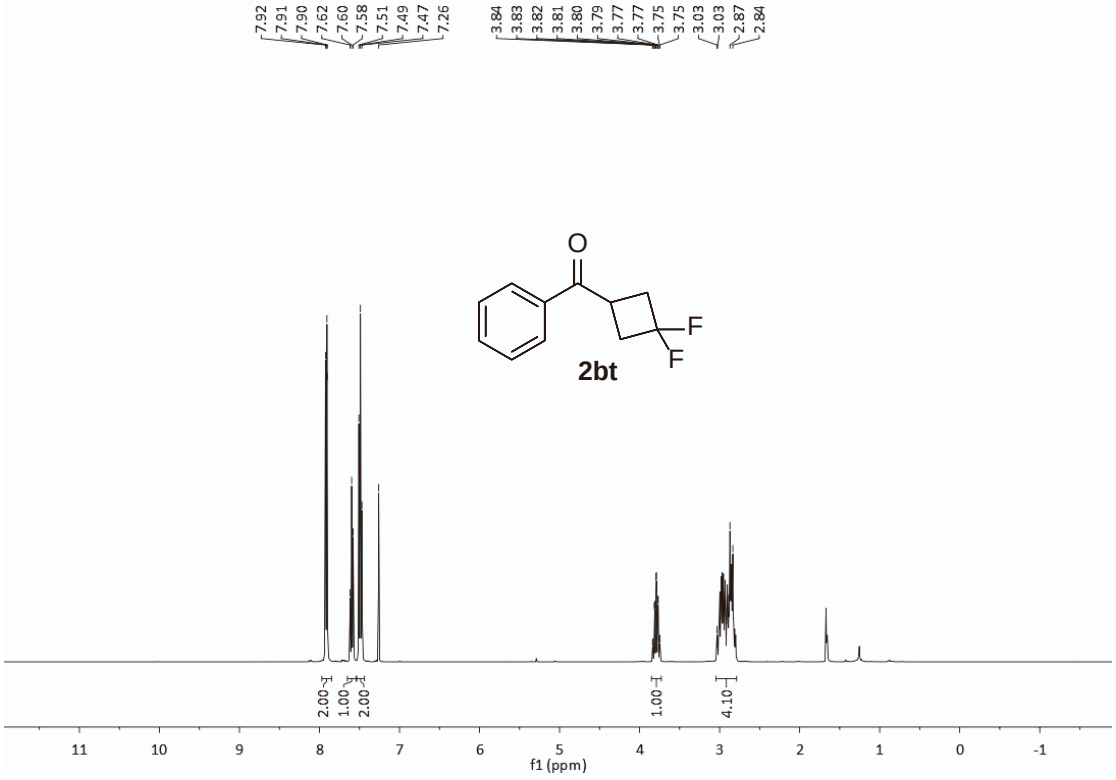
^{1}H NMR (400 MHz, $CDCl_3$)



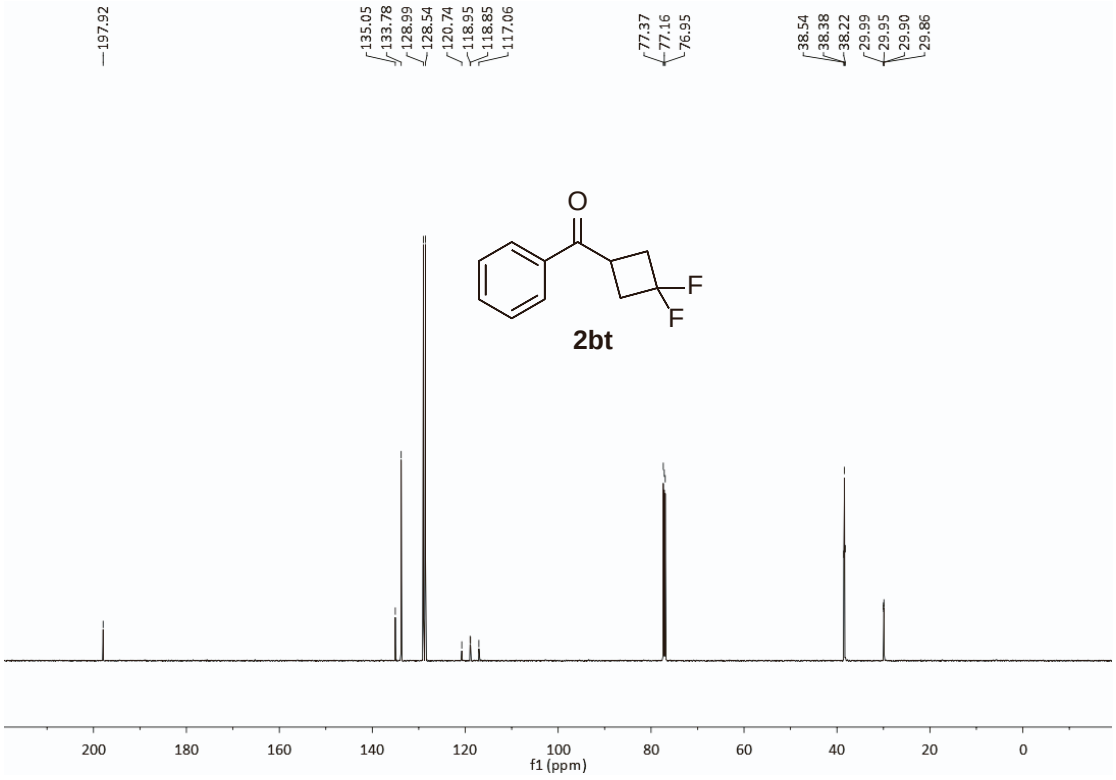
^{13}C NMR (101 MHz, $CDCl_3$)



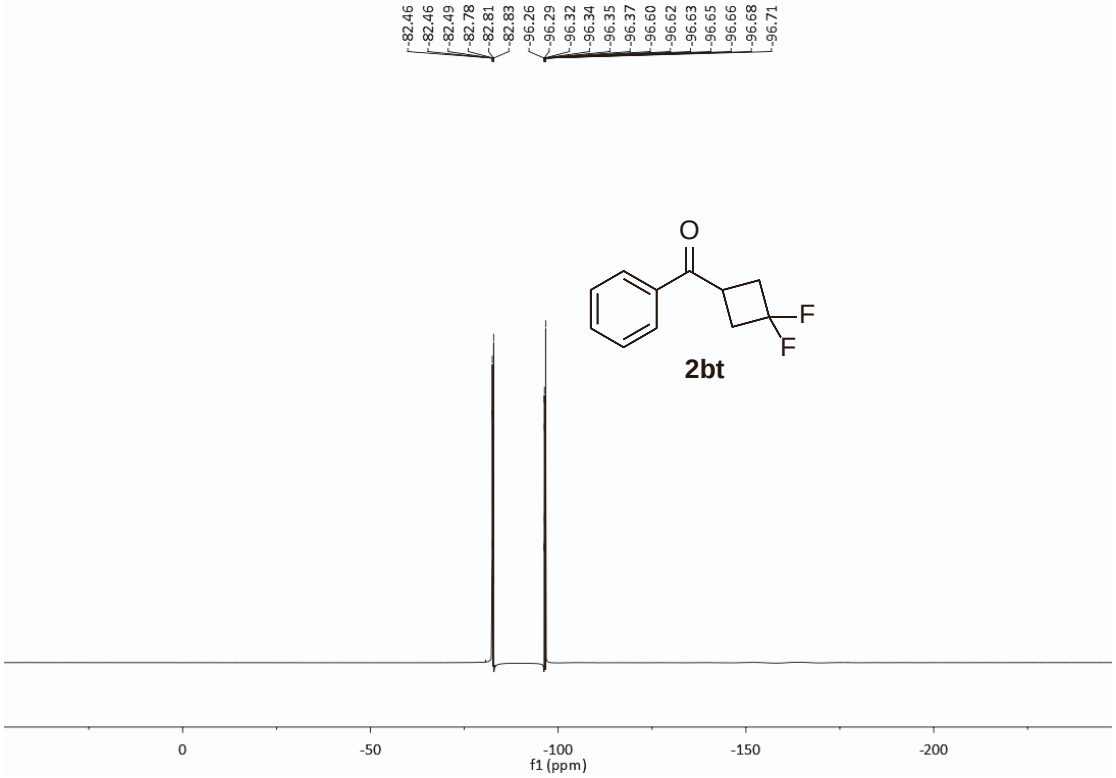
^{1}H NMR (400 MHz, $CDCl_3$)



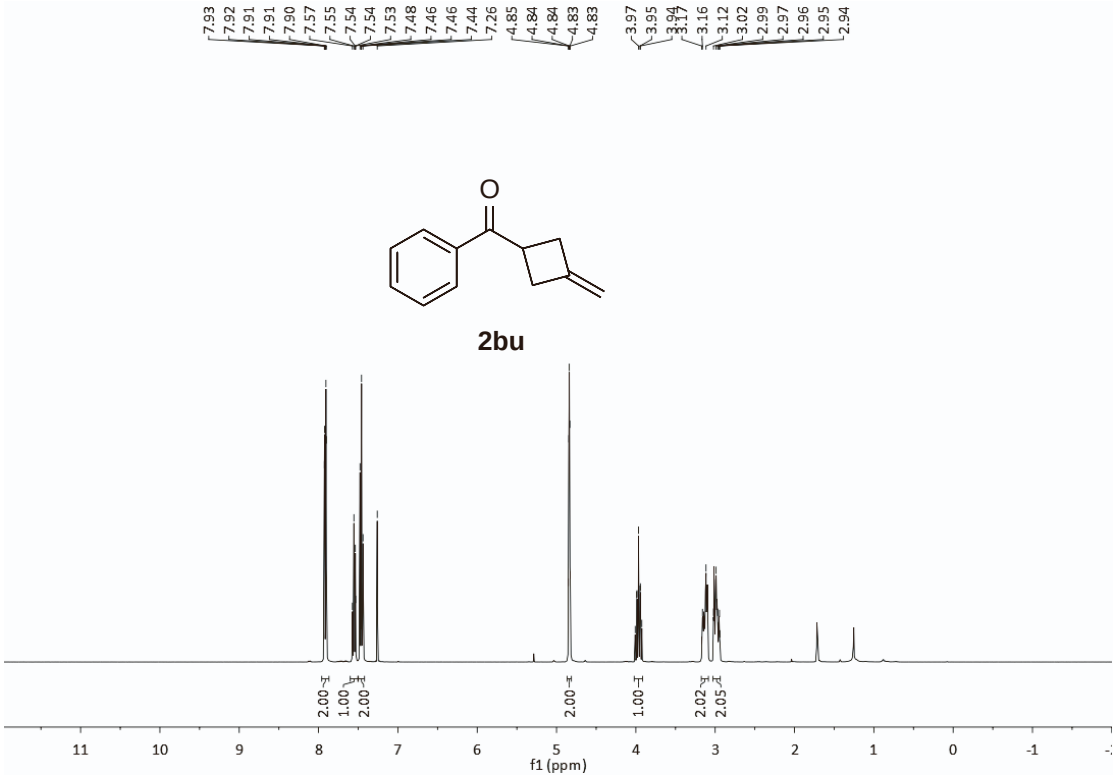
^{13}C NMR (151 MHz, $CDCl_3$)



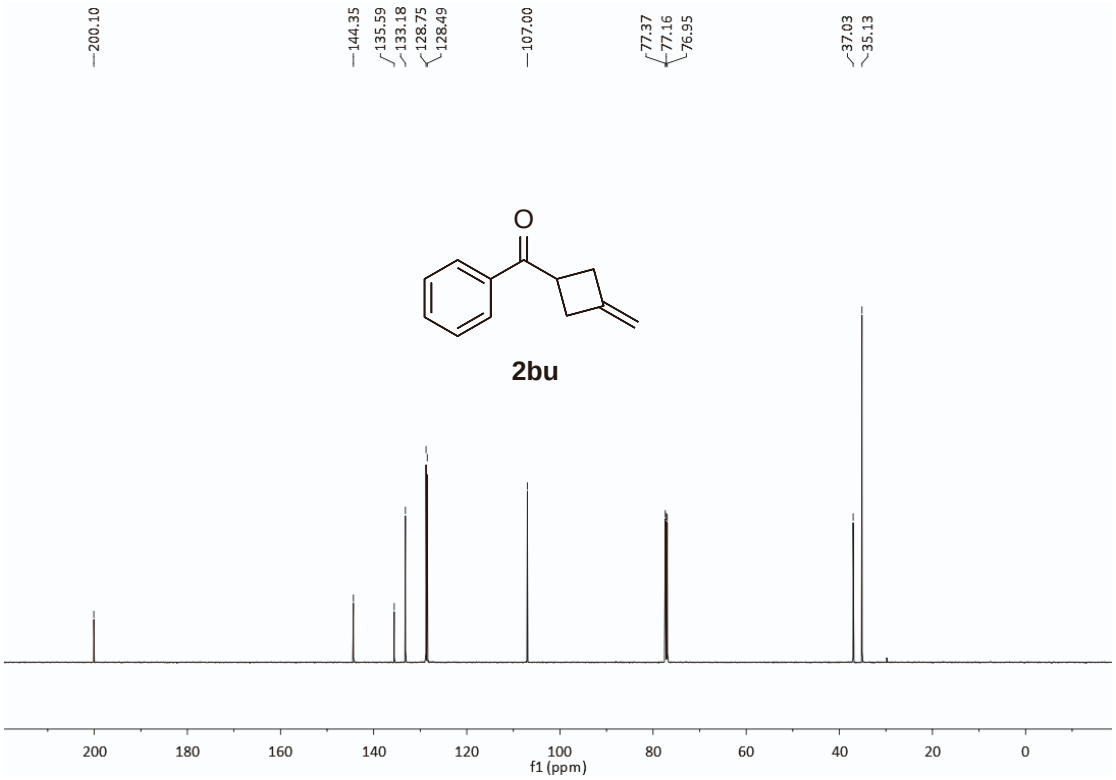
^{19}F NMR (565 MHz, $CDCl_3$)



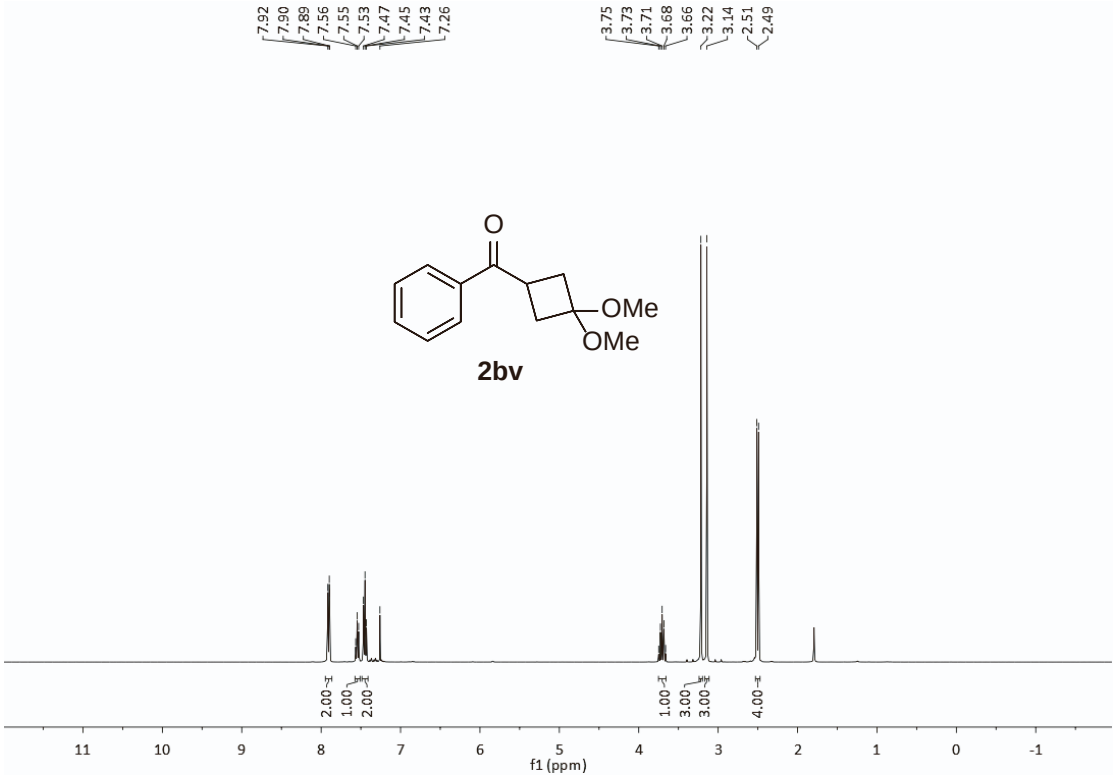
^{1}H NMR (400 MHz, $CDCl_3$)



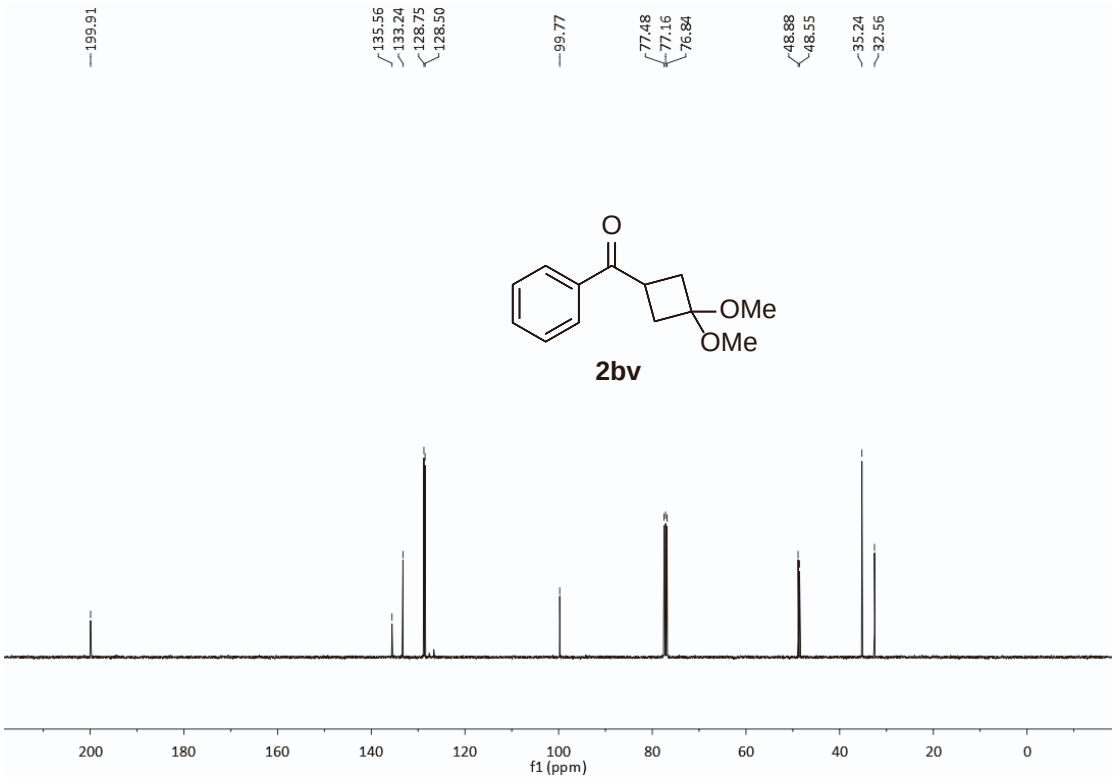
^{13}C NMR (151 MHz, $CDCl_3$)



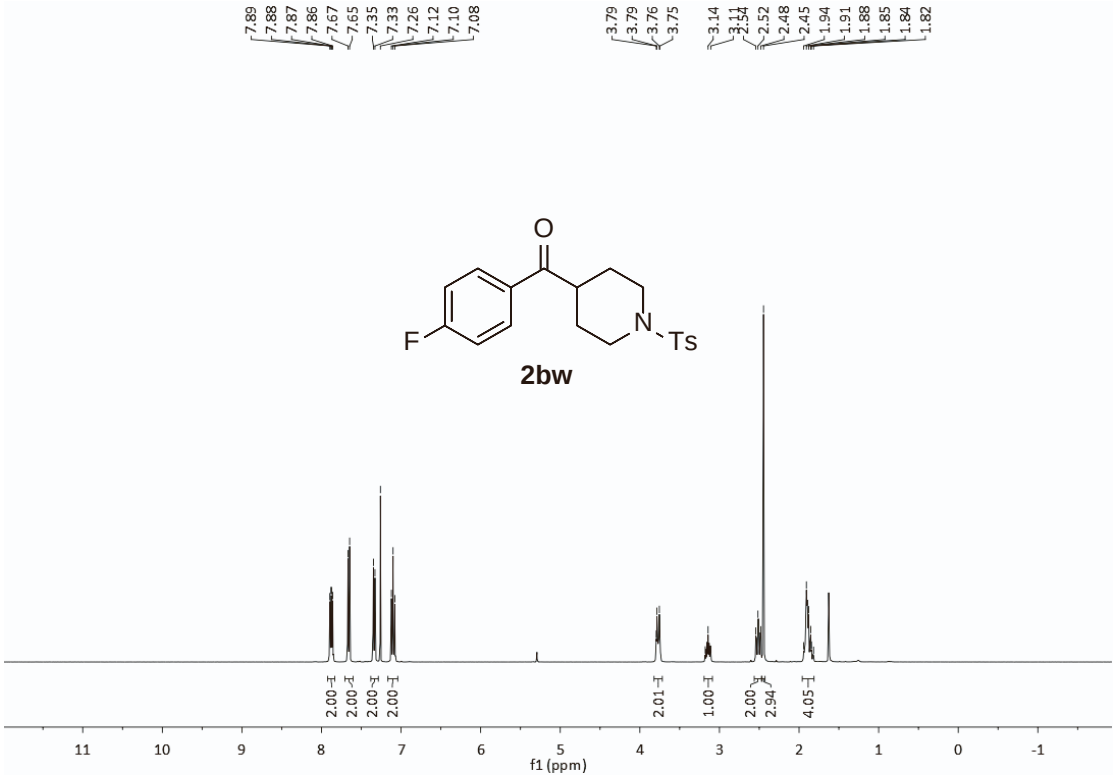
^{1}H NMR (400 MHz, $CDCl_3$)



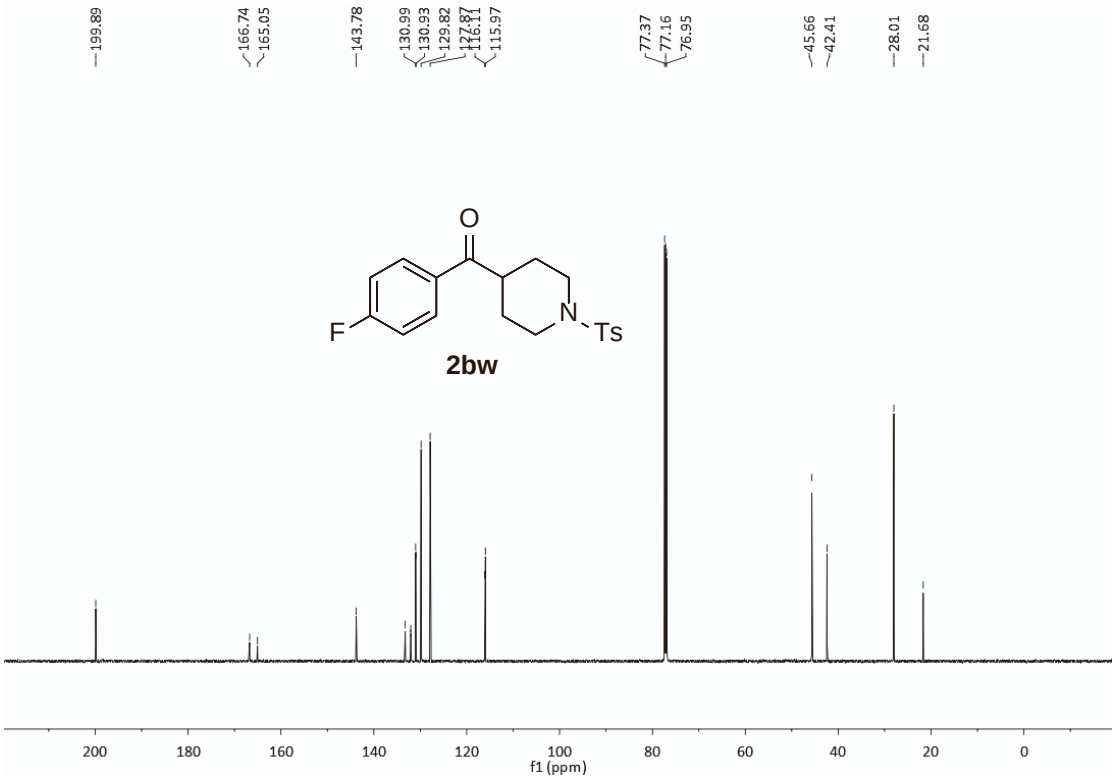
^{13}C NMR (101 MHz, $CDCl_3$)



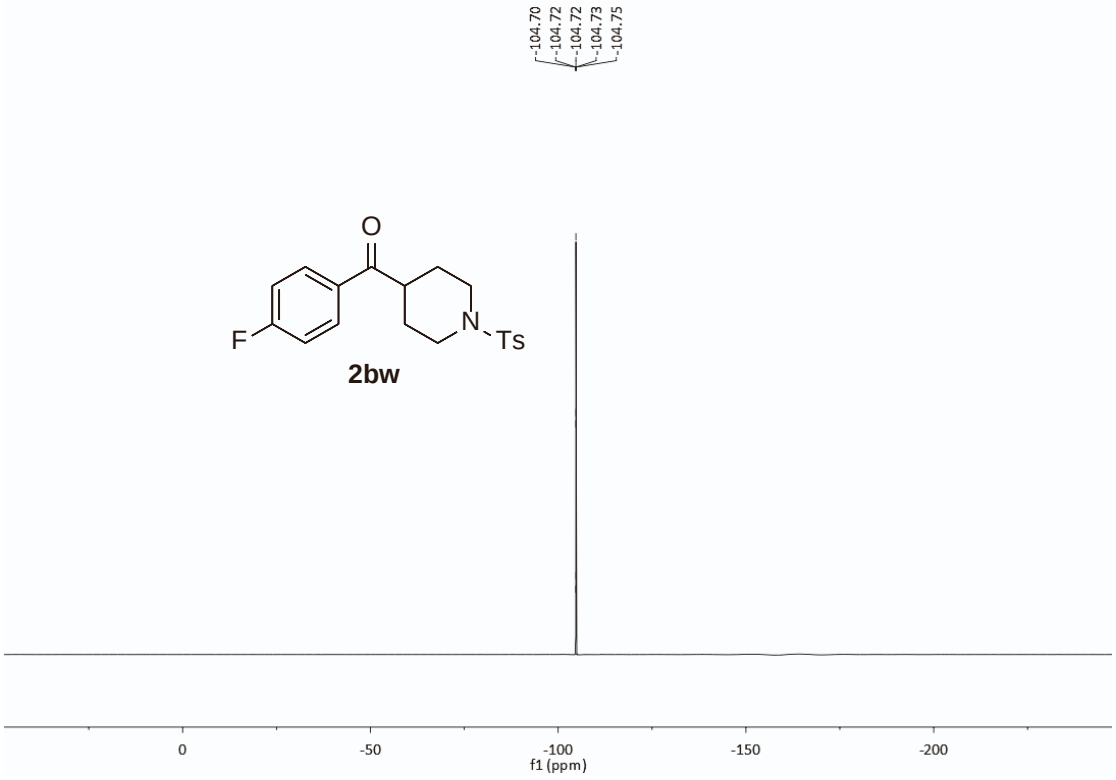
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (151 MHz, $CDCl_3$)

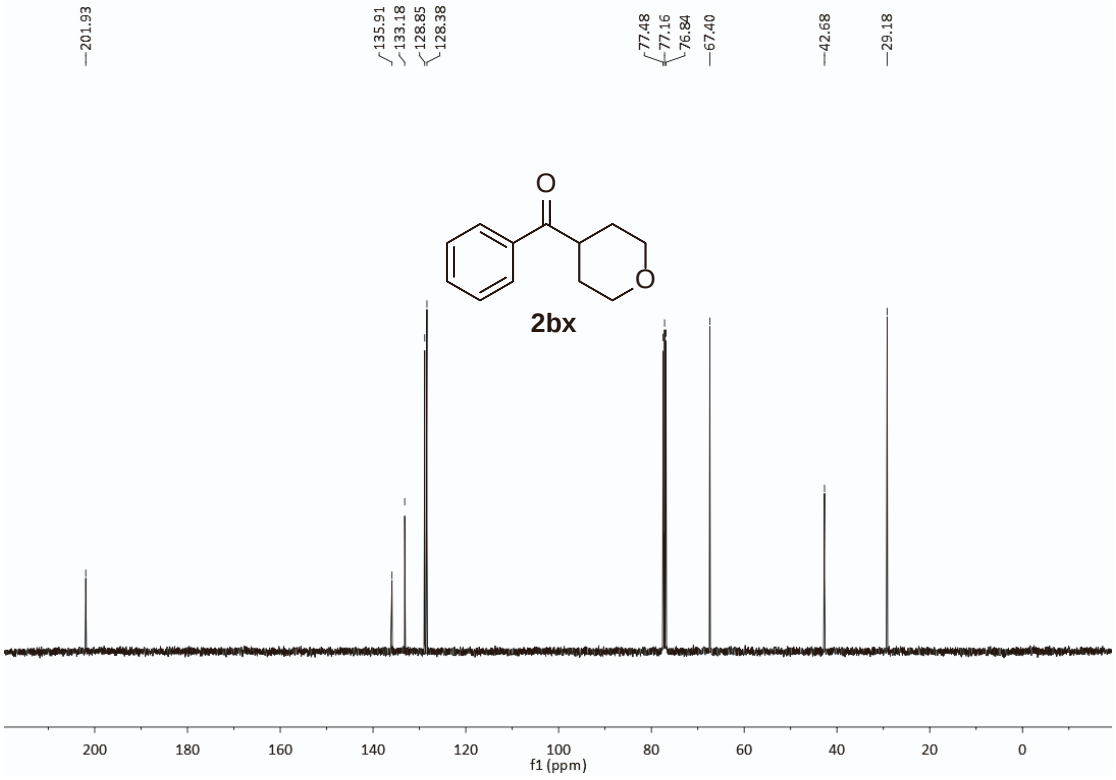


^{19}F NMR (565 MHz, $CDCl_3$)

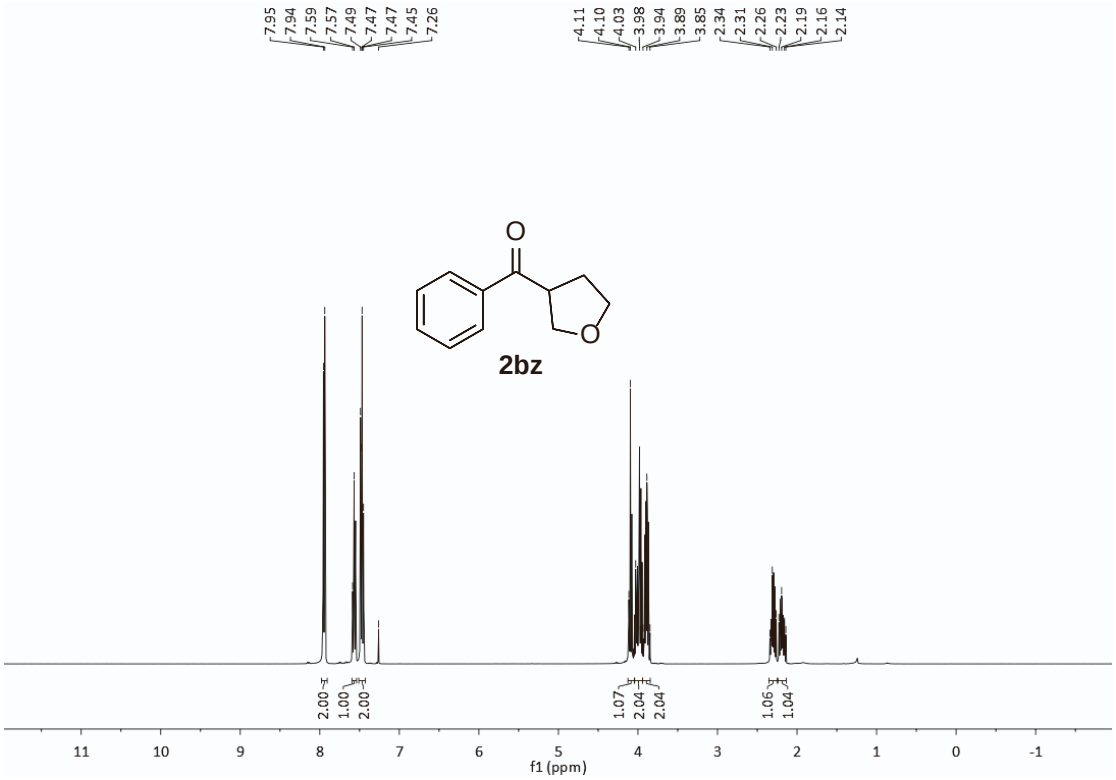


^{1}H NMR (400 MHz, $CDCl_3$)

^{13}C NMR (101 MHz, $CDCl_3$)

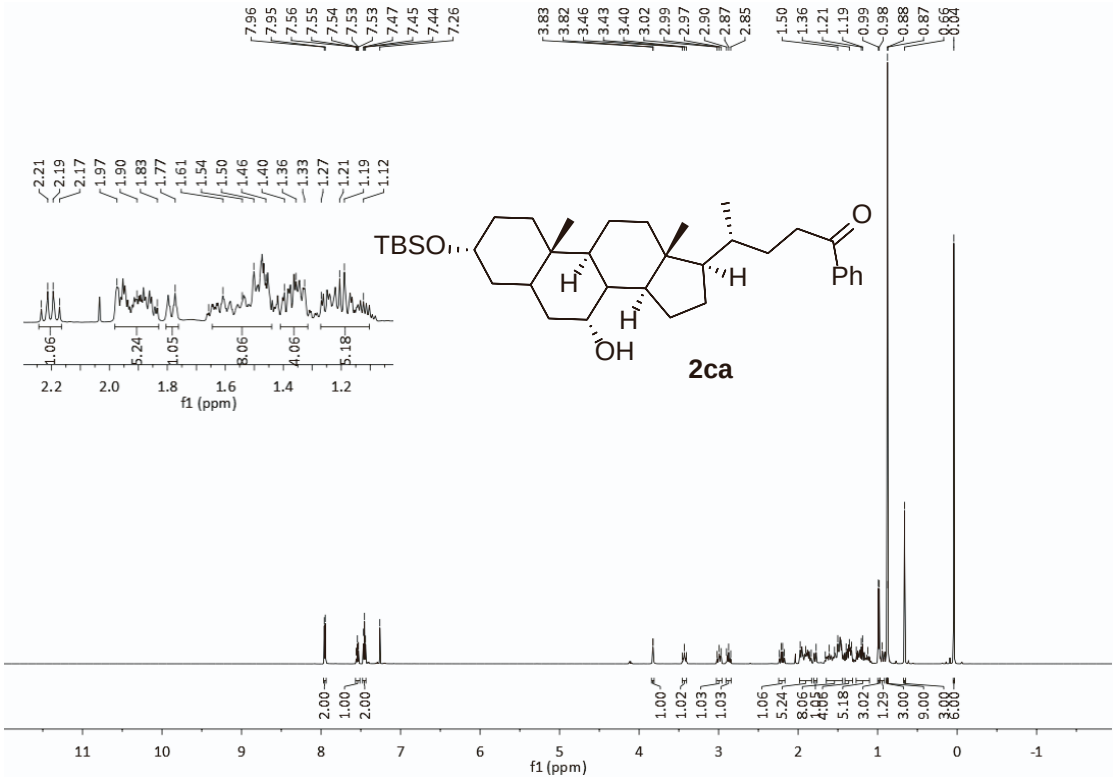


^{1}H NMR (400 MHz, $CDCl_3$)

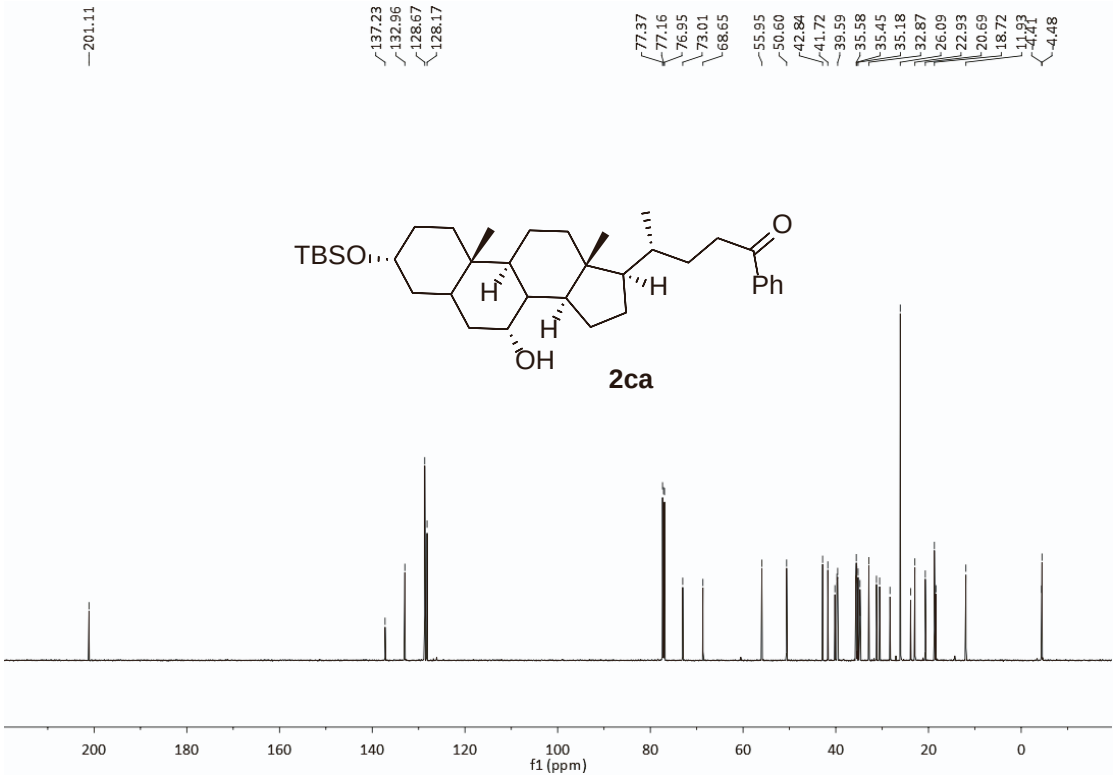


^{13}C NMR (101 MHz, $CDCl_3$)

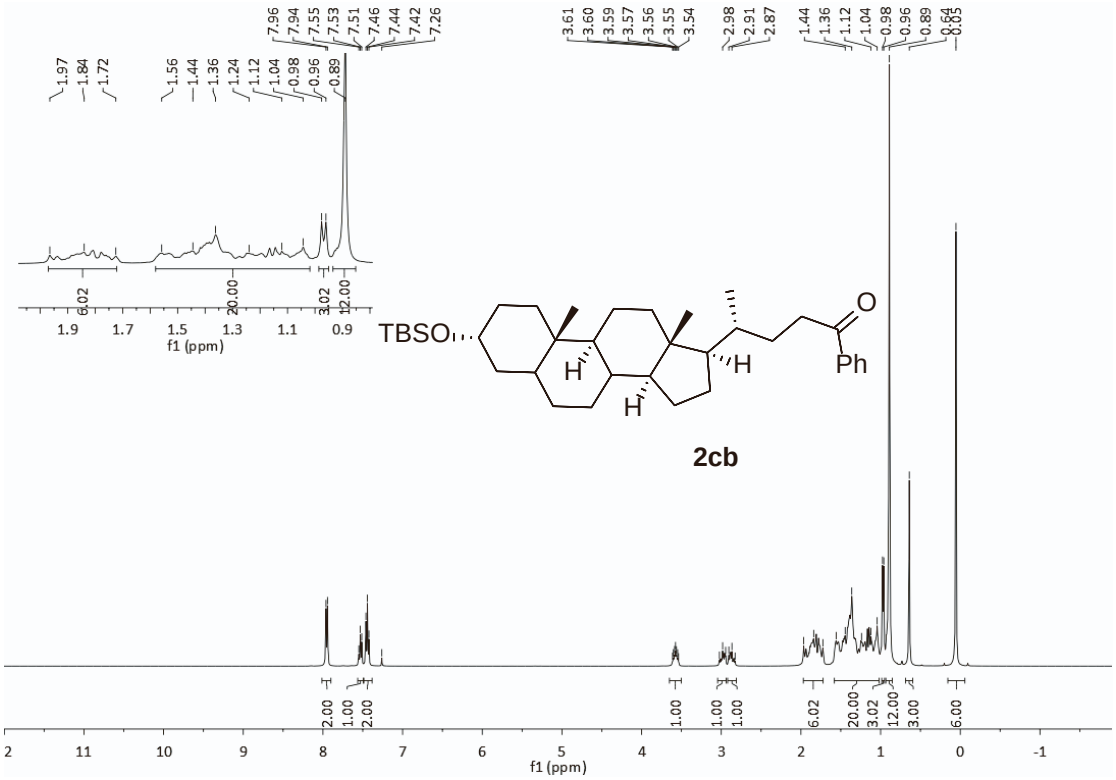
^{1}H NMR (600 MHz, $CDCl_3$)



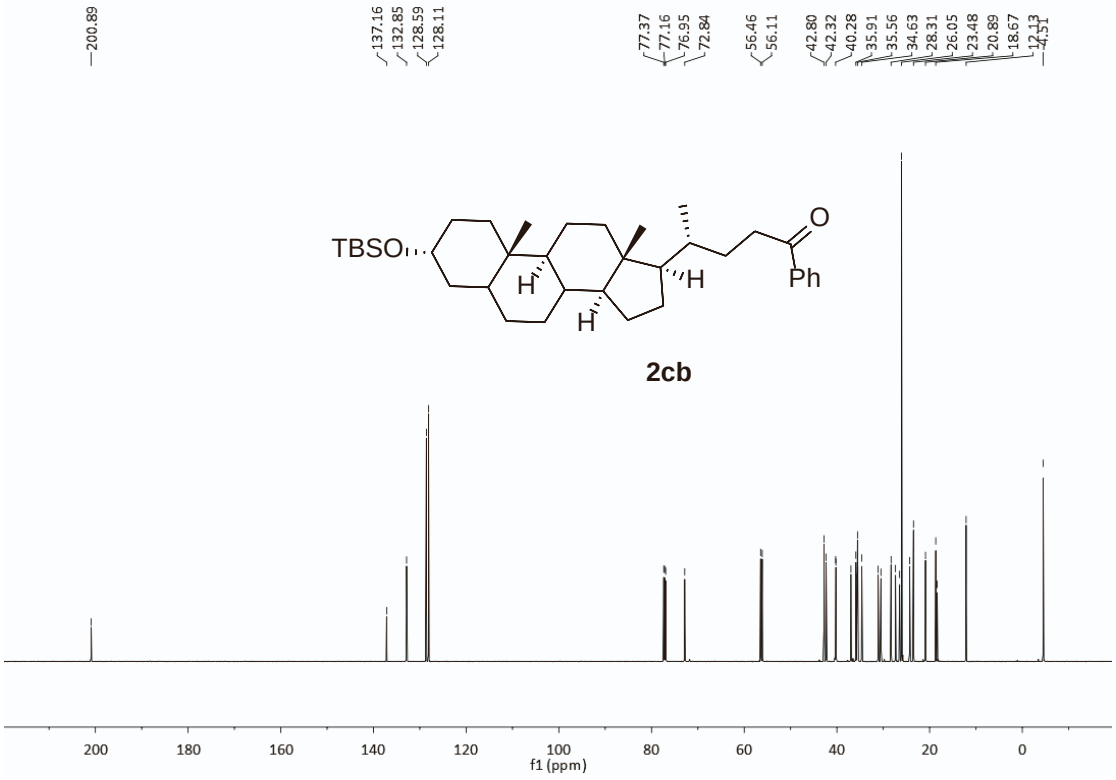
^{13}C NMR (151 MHz, $CDCl_3$)



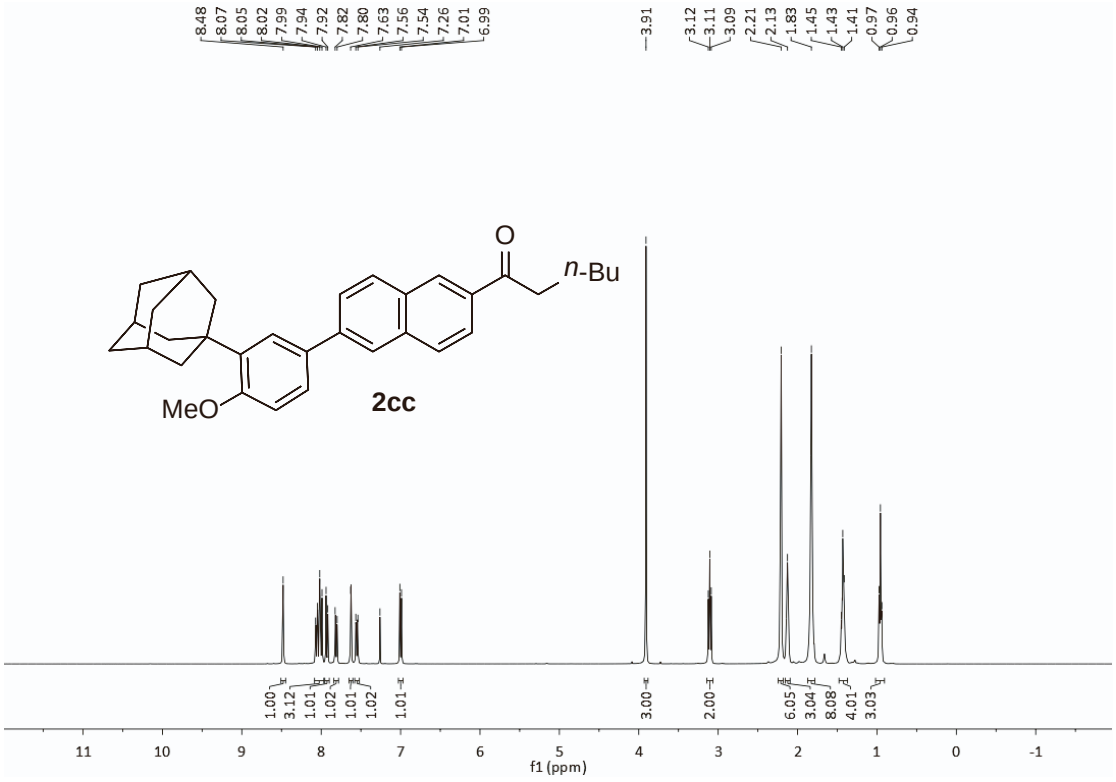
^{1}H NMR (400 MHz, $CDCl_3$)



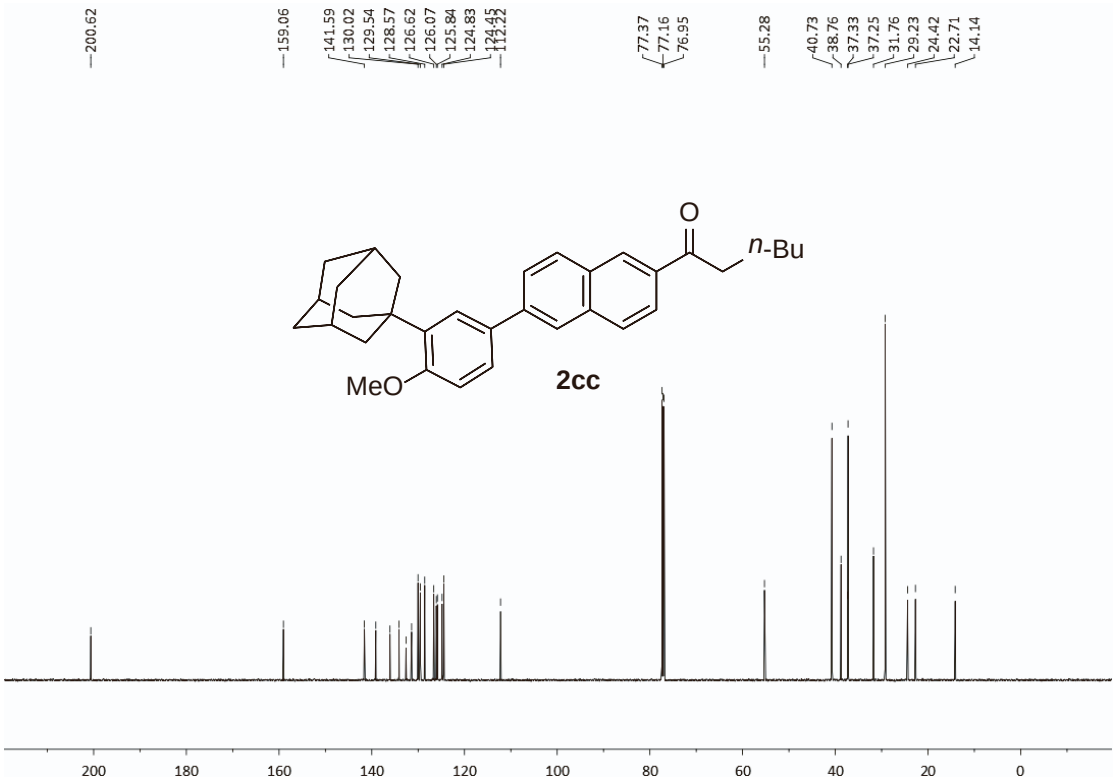
^{13}C NMR (151 MHz, $CDCl_3$)



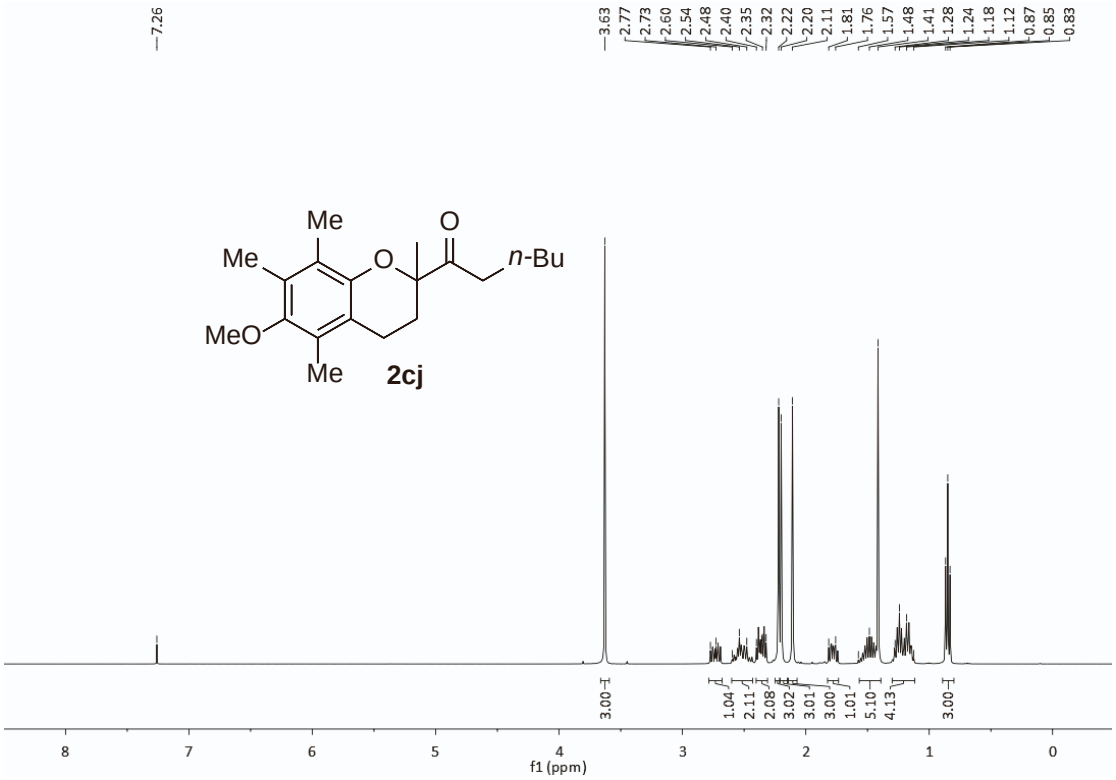
^{1}H NMR (400 MHz, $CDCl_3$)



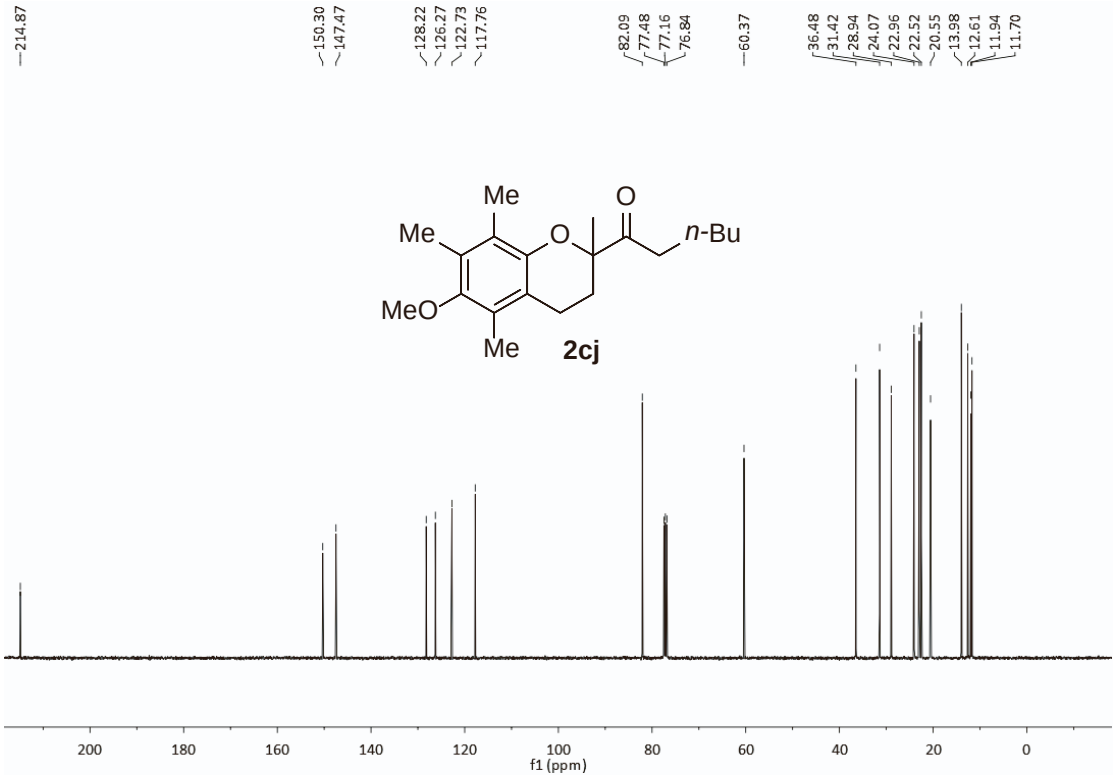
^{13}C NMR (151 MHz, $CDCl_3$)



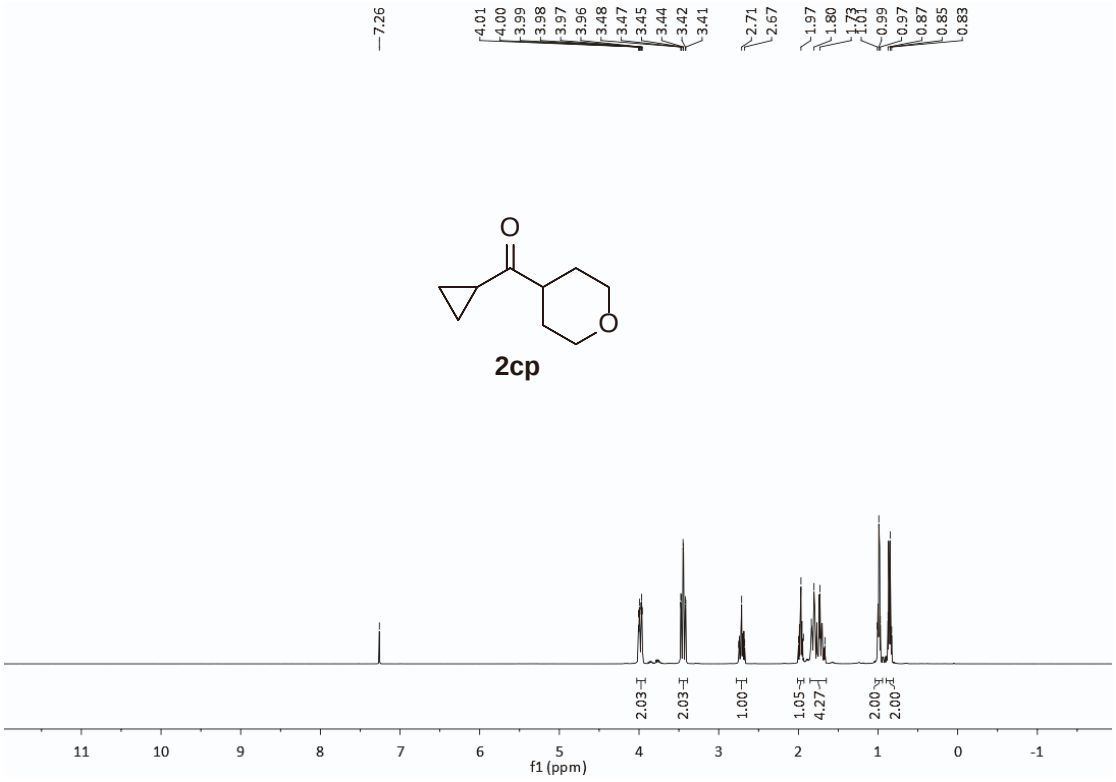
^{1}H NMR (400 MHz, $CDCl_3$)



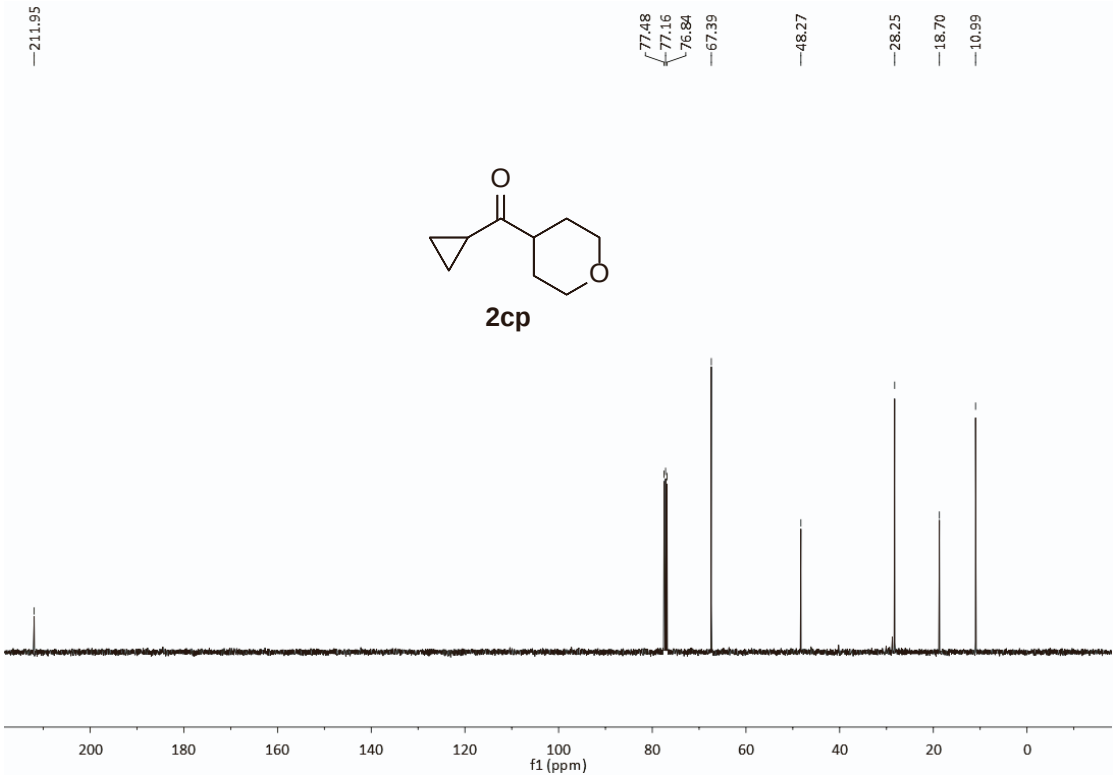
^{13}C NMR (101 MHz, $CDCl_3$)



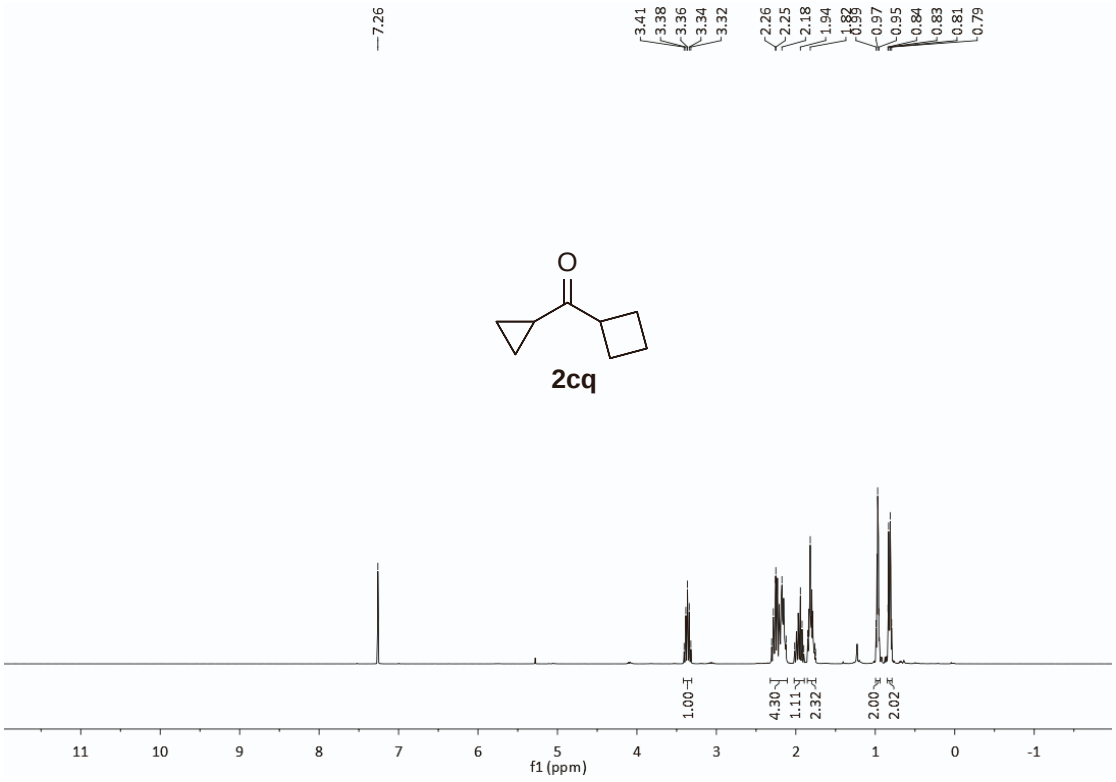
^{1}H NMR (400 MHz, $CDCl_3$)



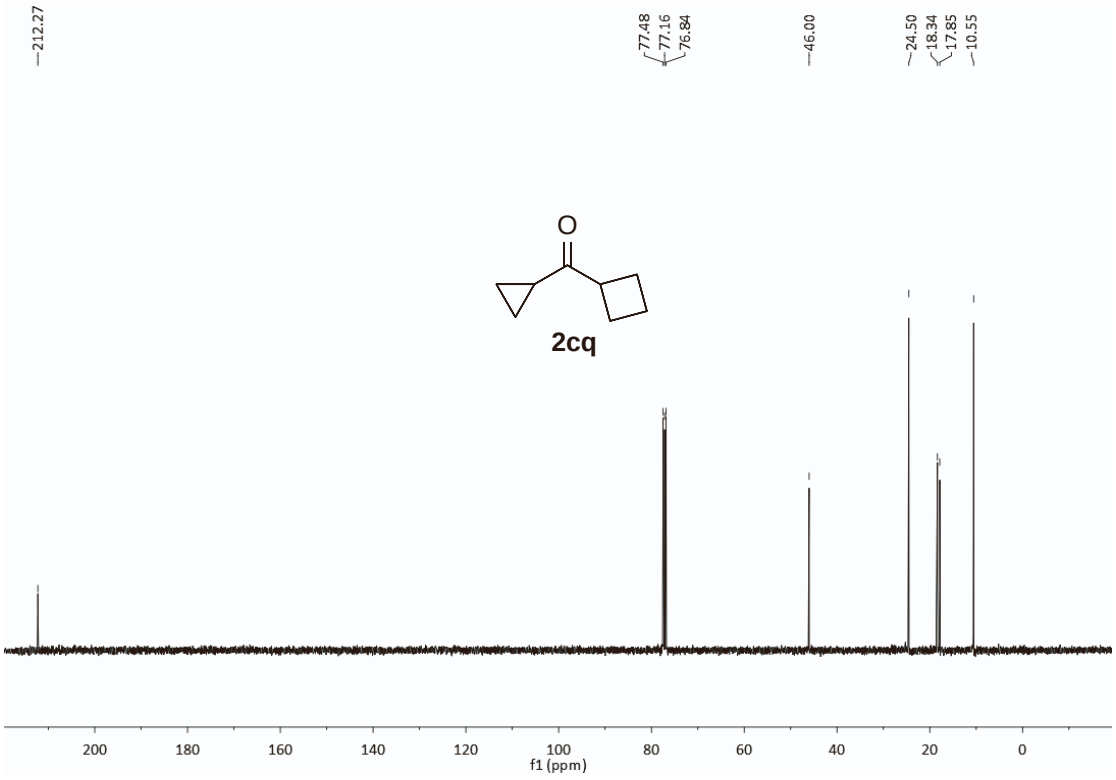
^{13}C NMR (101 MHz, $CDCl_3$)



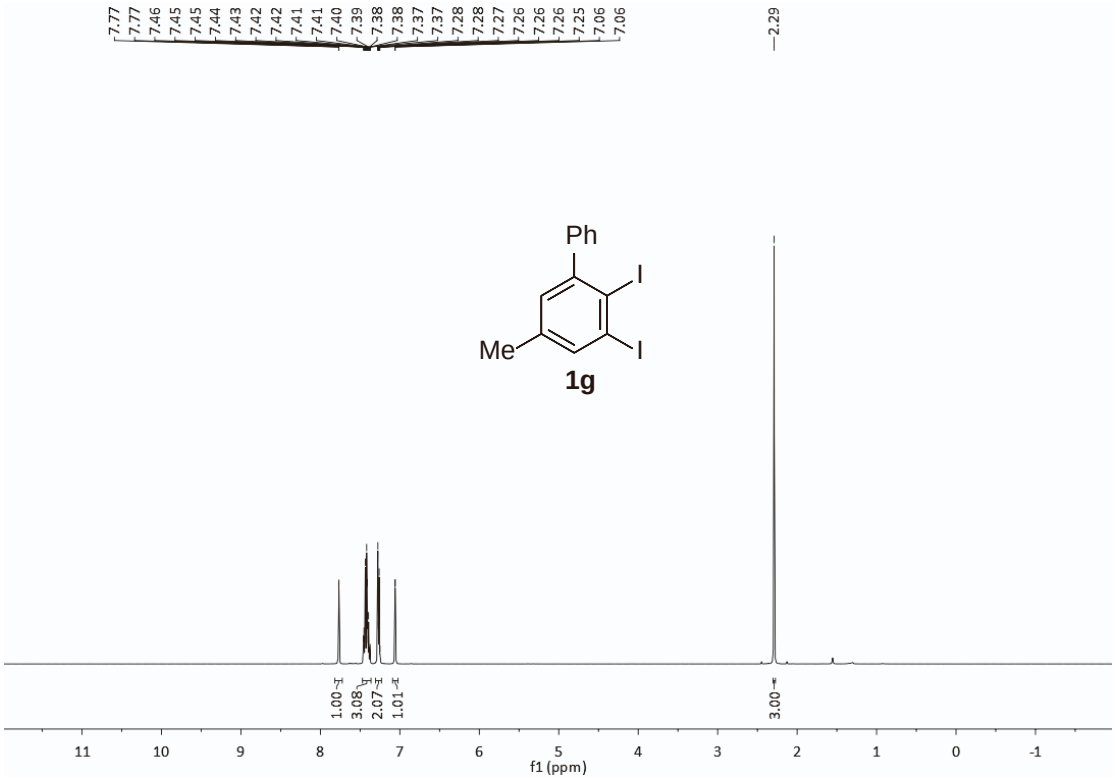
^{1}H NMR (400 MHz, $CDCl_3$)



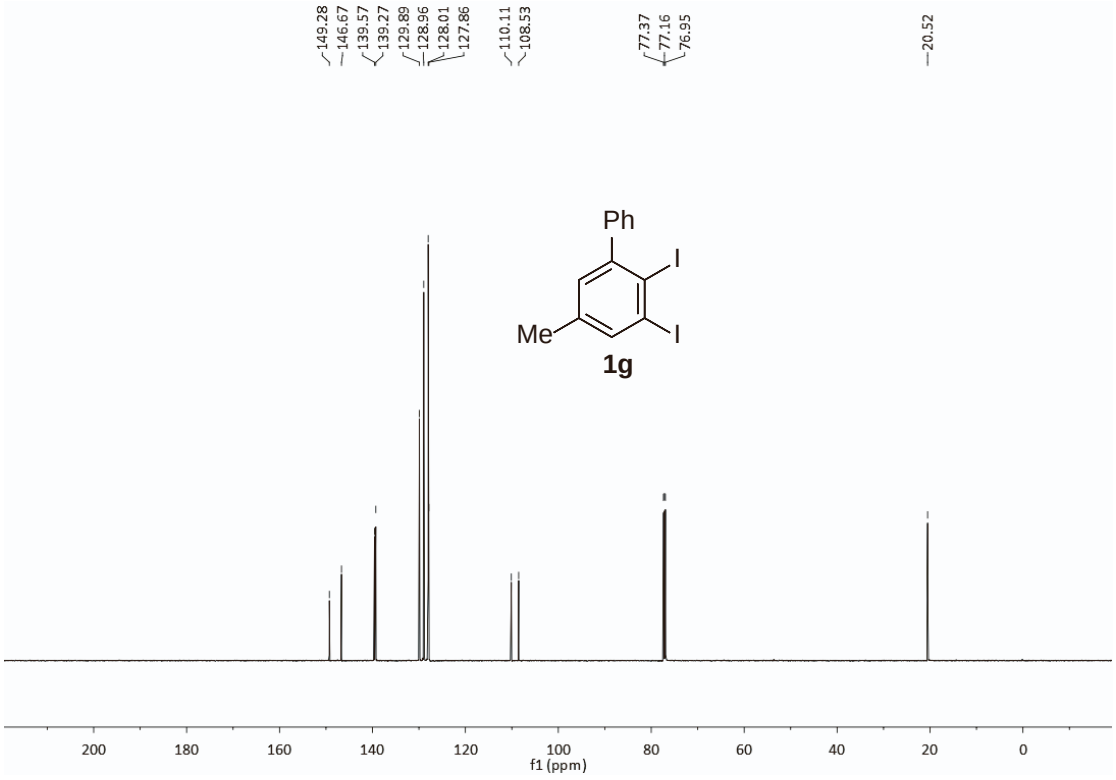
^{13}C NMR (101 MHz, $CDCl_3$)



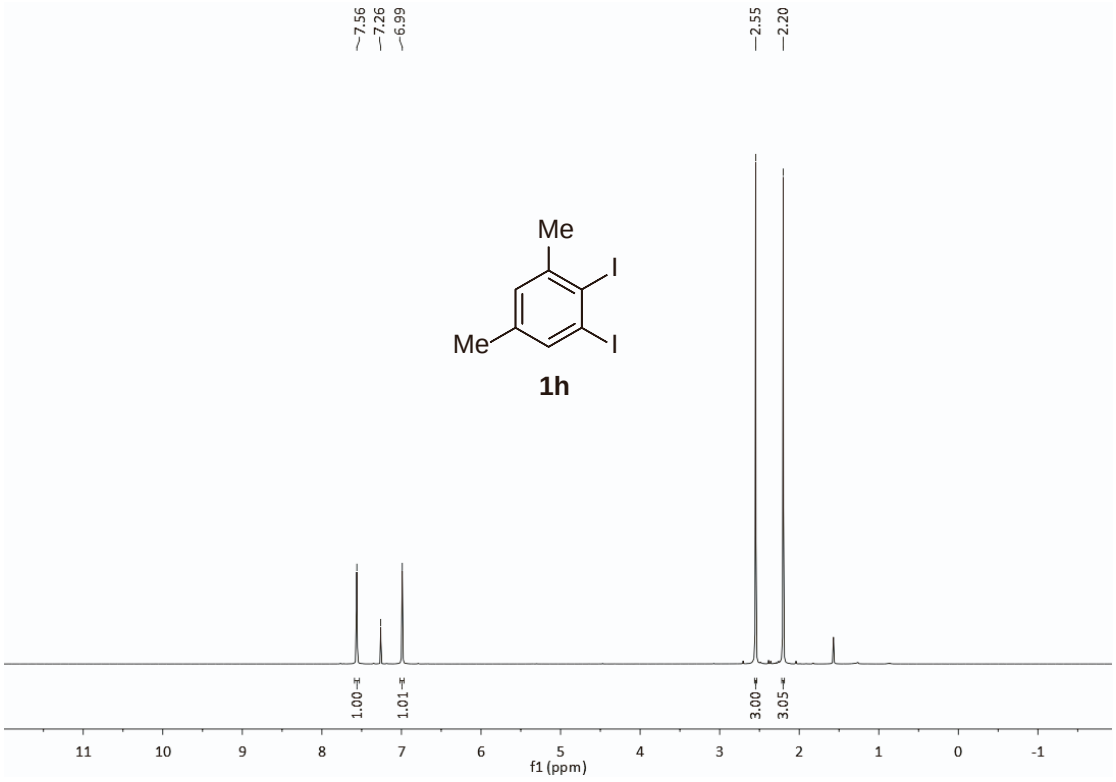
^{1}H NMR (400 MHz, $CDCl_3$)



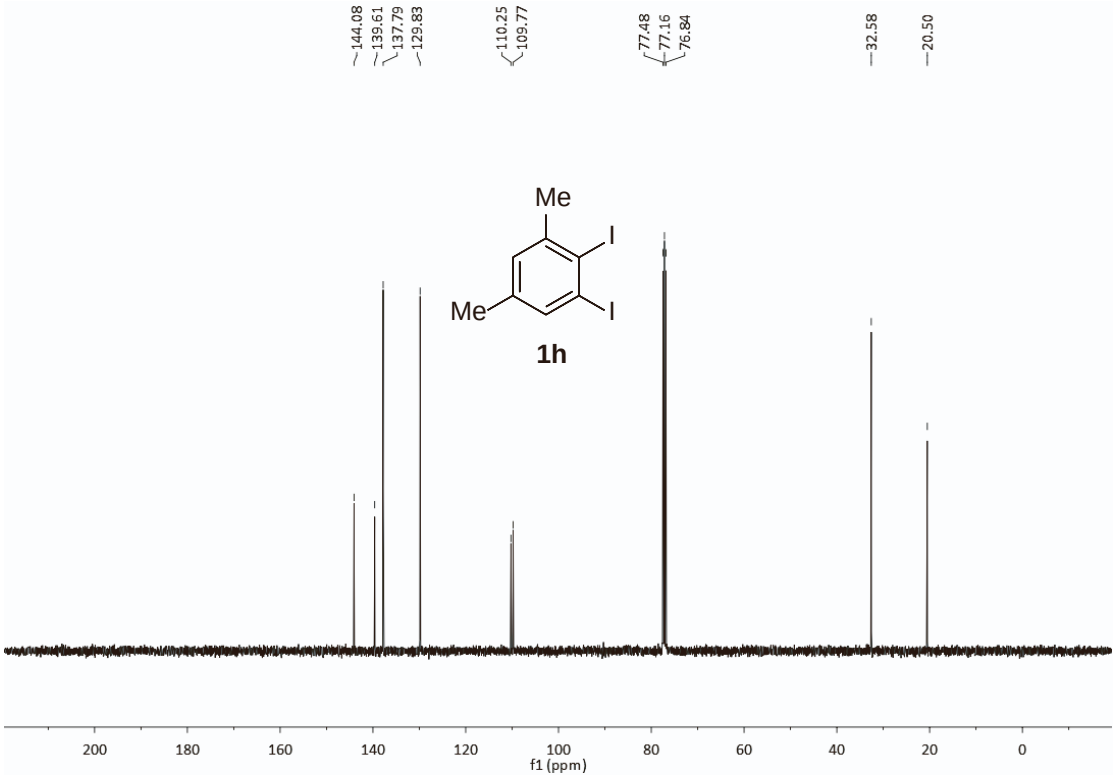
^{13}C NMR (151 MHz, $CDCl_3$)



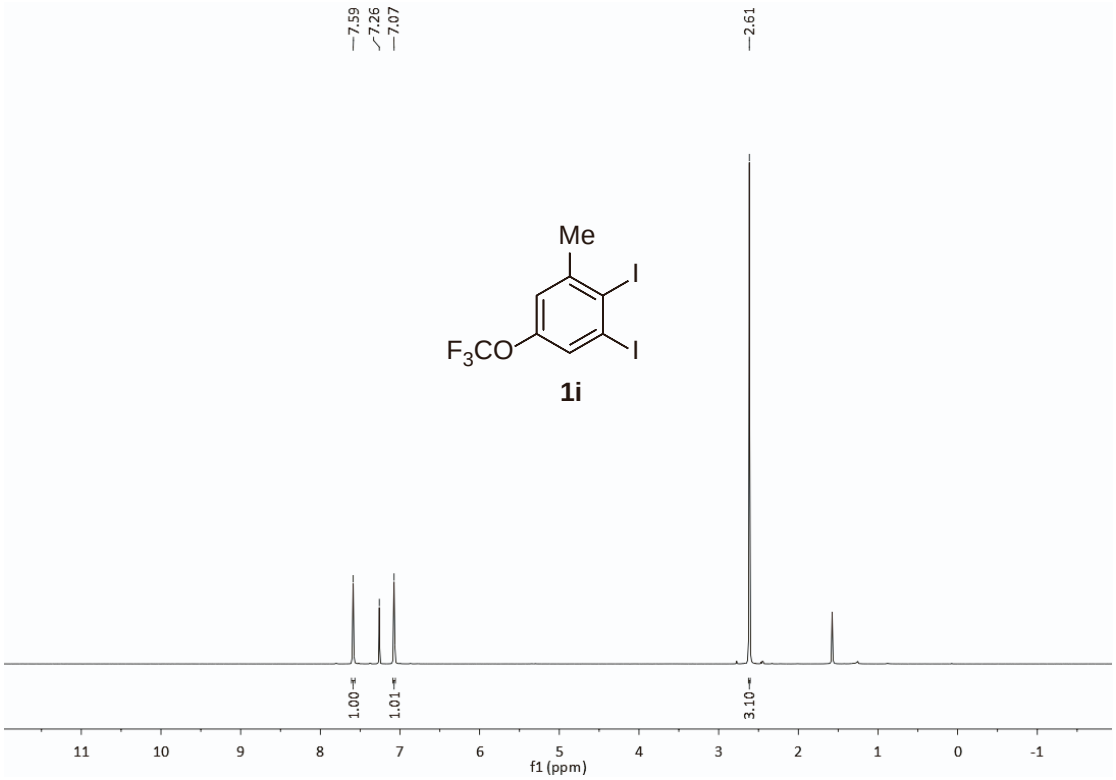
^{1}H NMR (400 MHz, $CDCl_3$)



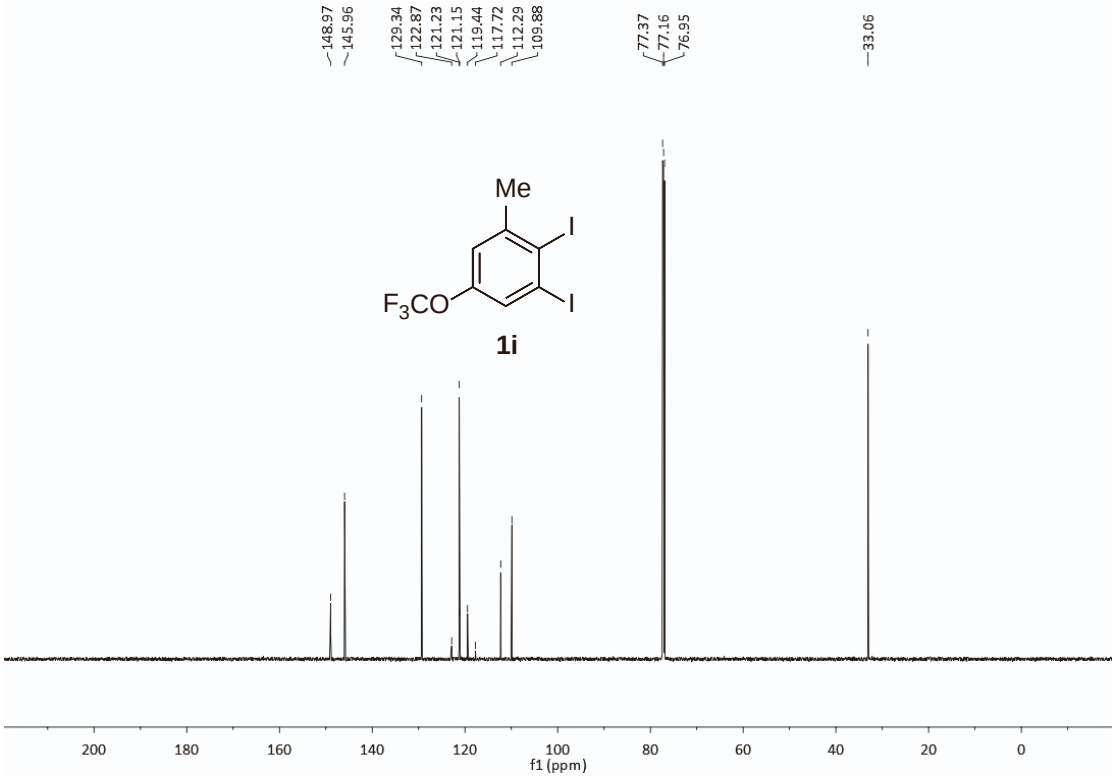
^{13}C NMR (101 MHz, $CDCl_3$)



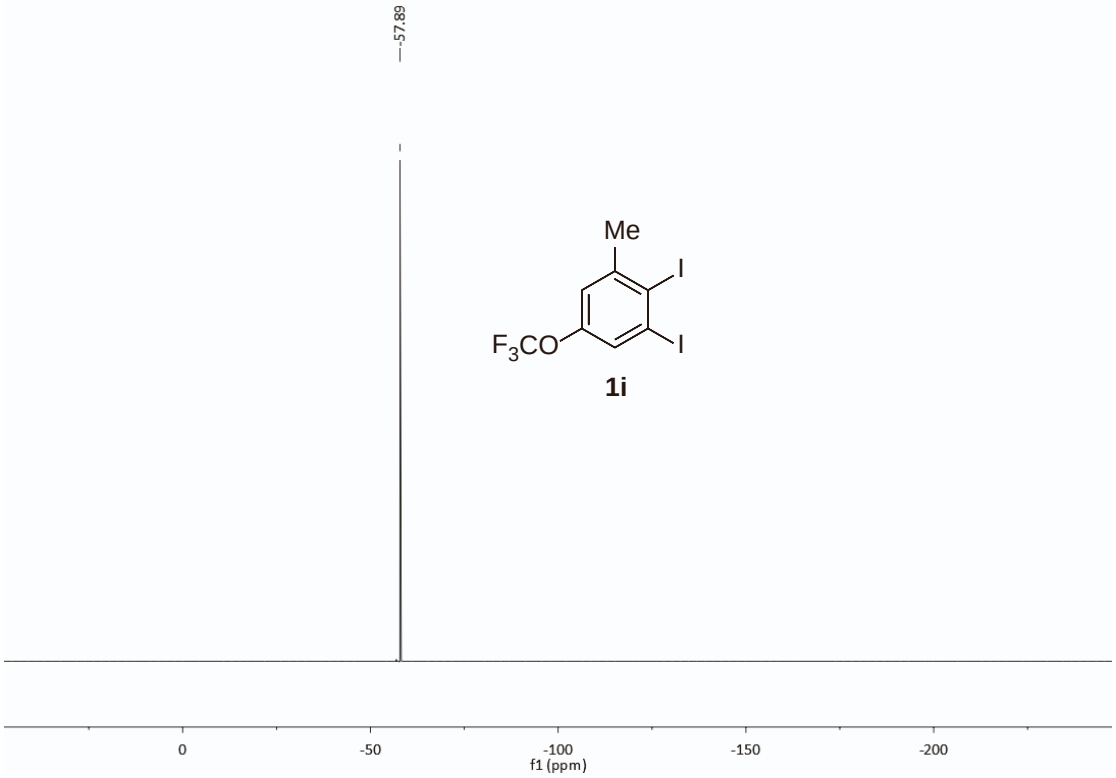
^{1}H NMR (400 MHz, $CDCl_3$)



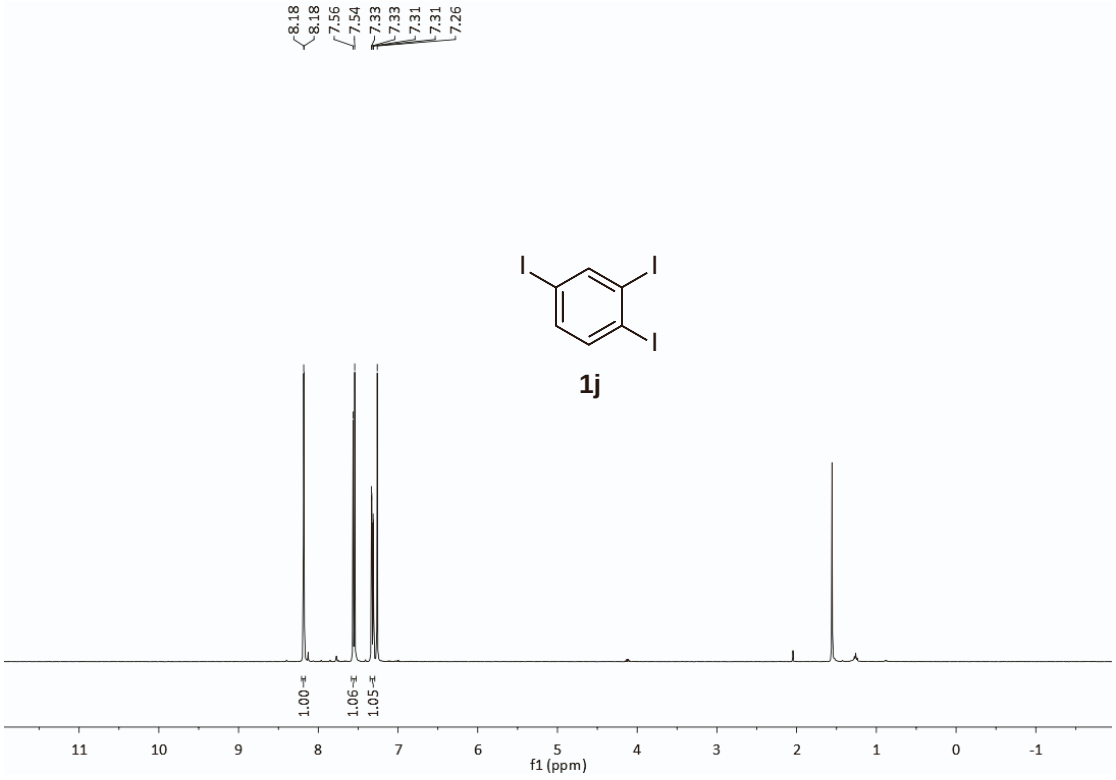
^{13}C NMR (151 MHz, $CDCl_3$)



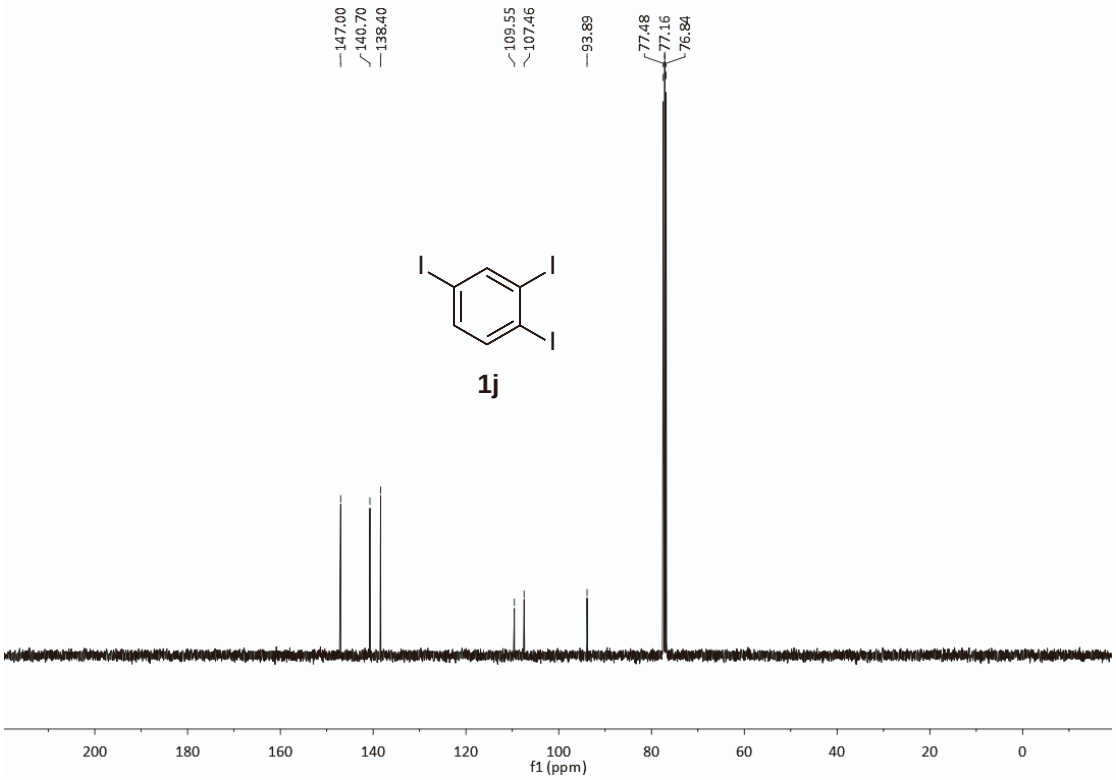
^{19}F NMR (565 MHz, $CDCl_3$)



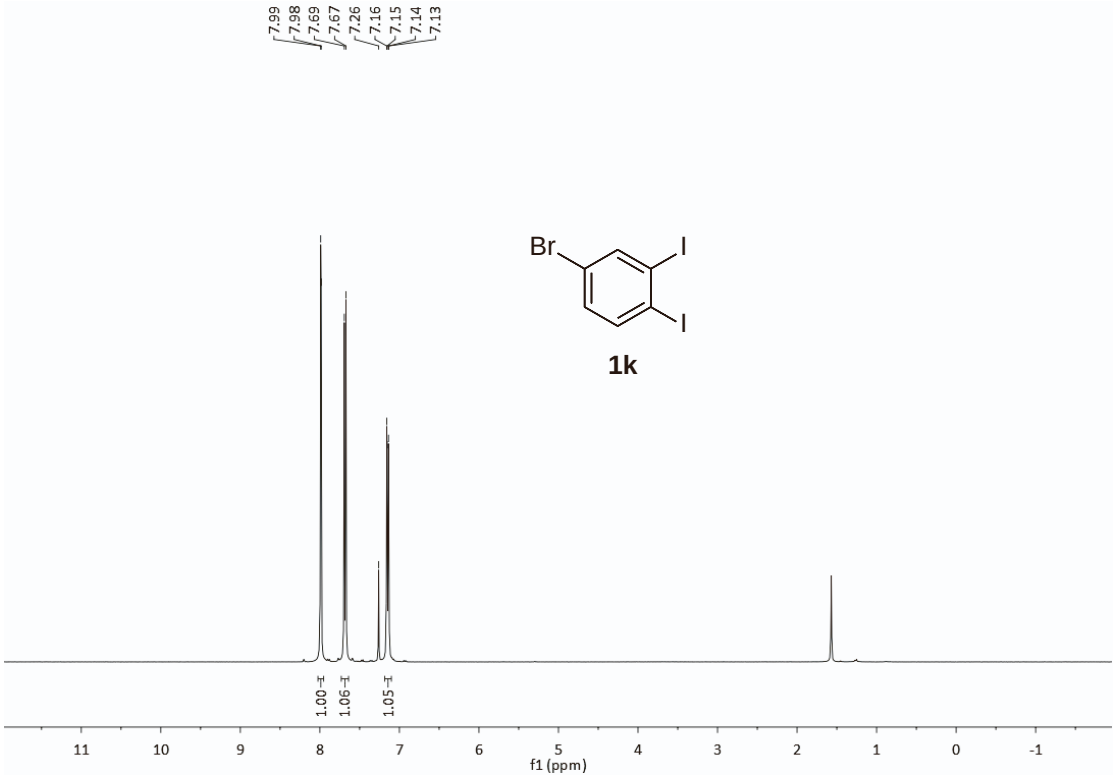
^{1}H NMR (400 MHz, $CDCl_3$)



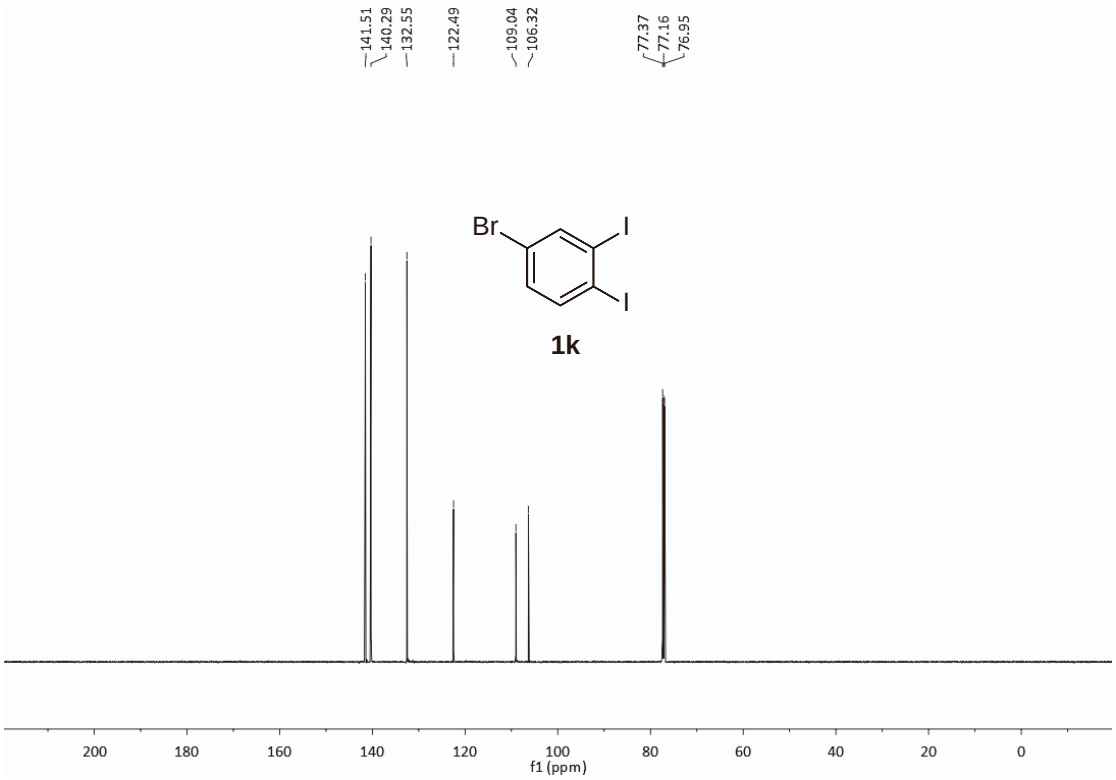
^{13}C NMR (101 MHz, $CDCl_3$)



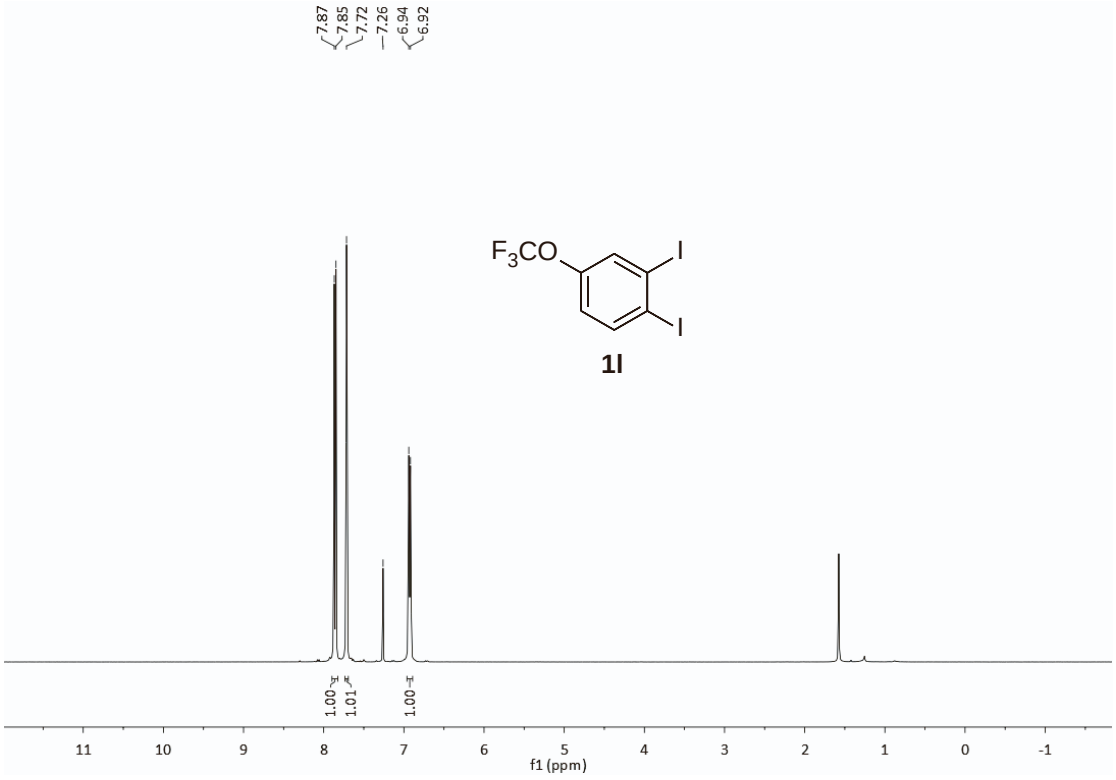
^{1}H NMR (400 MHz, $CDCl_3$)



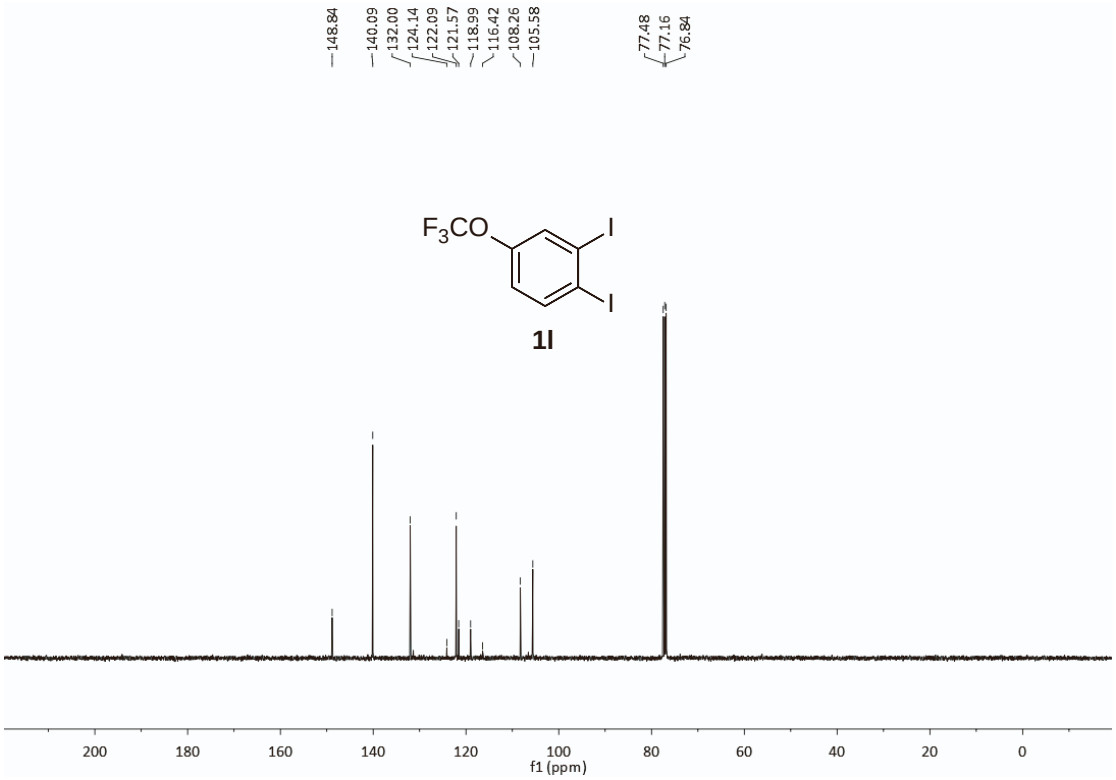
^{13}C NMR (151 MHz, $CDCl_3$)



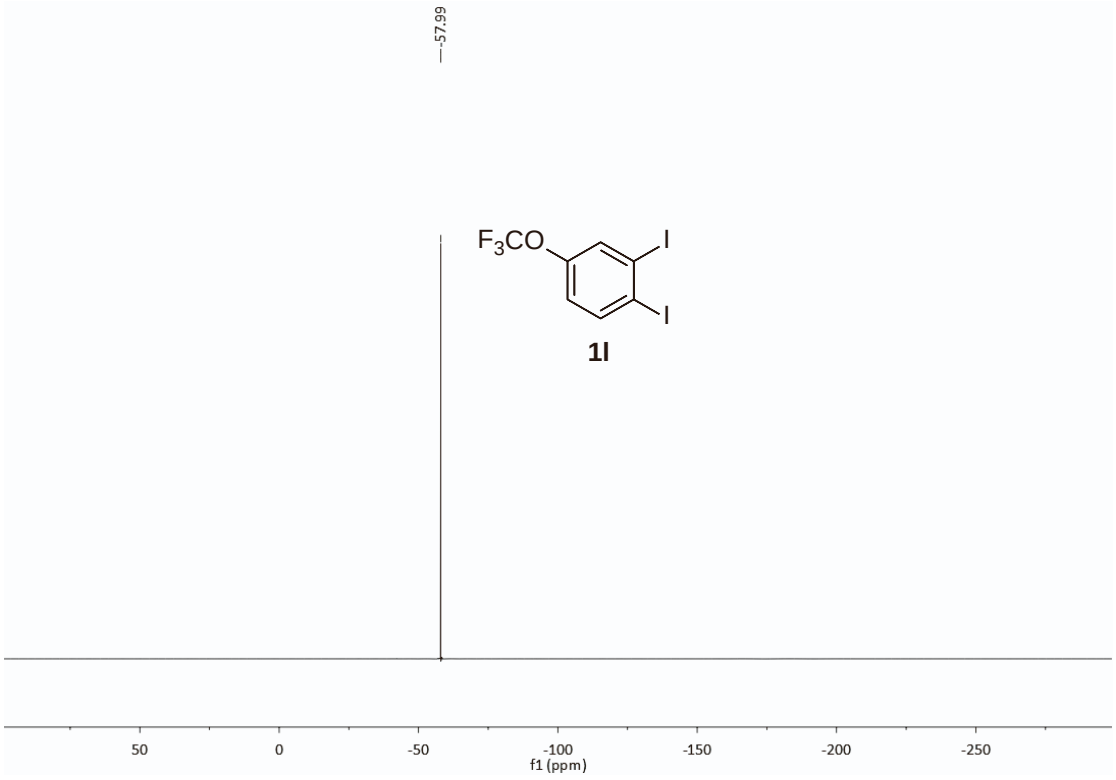
^{1}H NMR (400 MHz, $CDCl_3$)



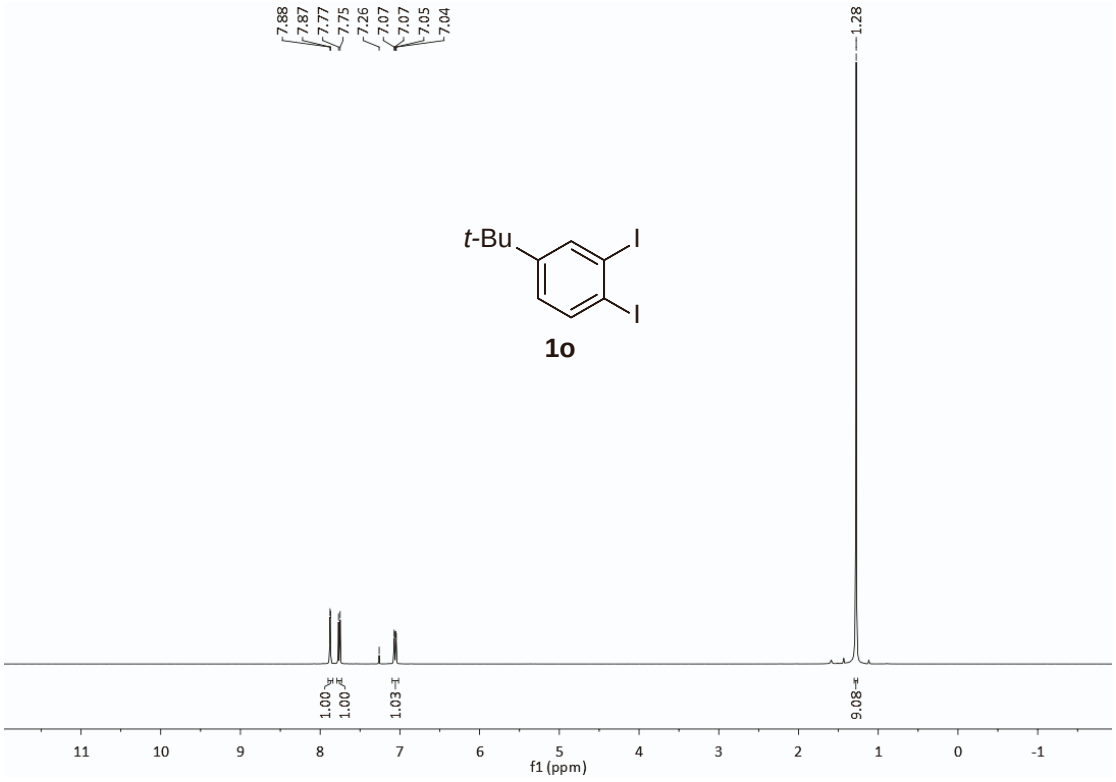
^{13}C NMR (101 MHz, $CDCl_3$)



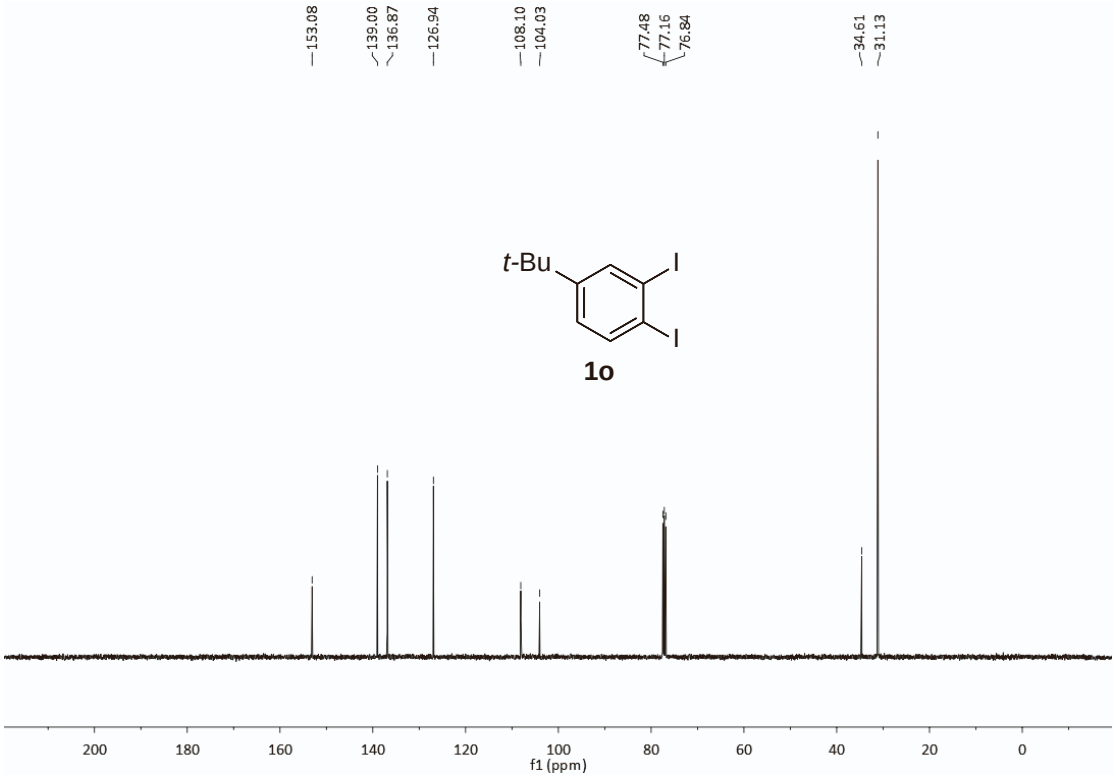
^{19}F NMR (565 MHz, $CDCl_3$)



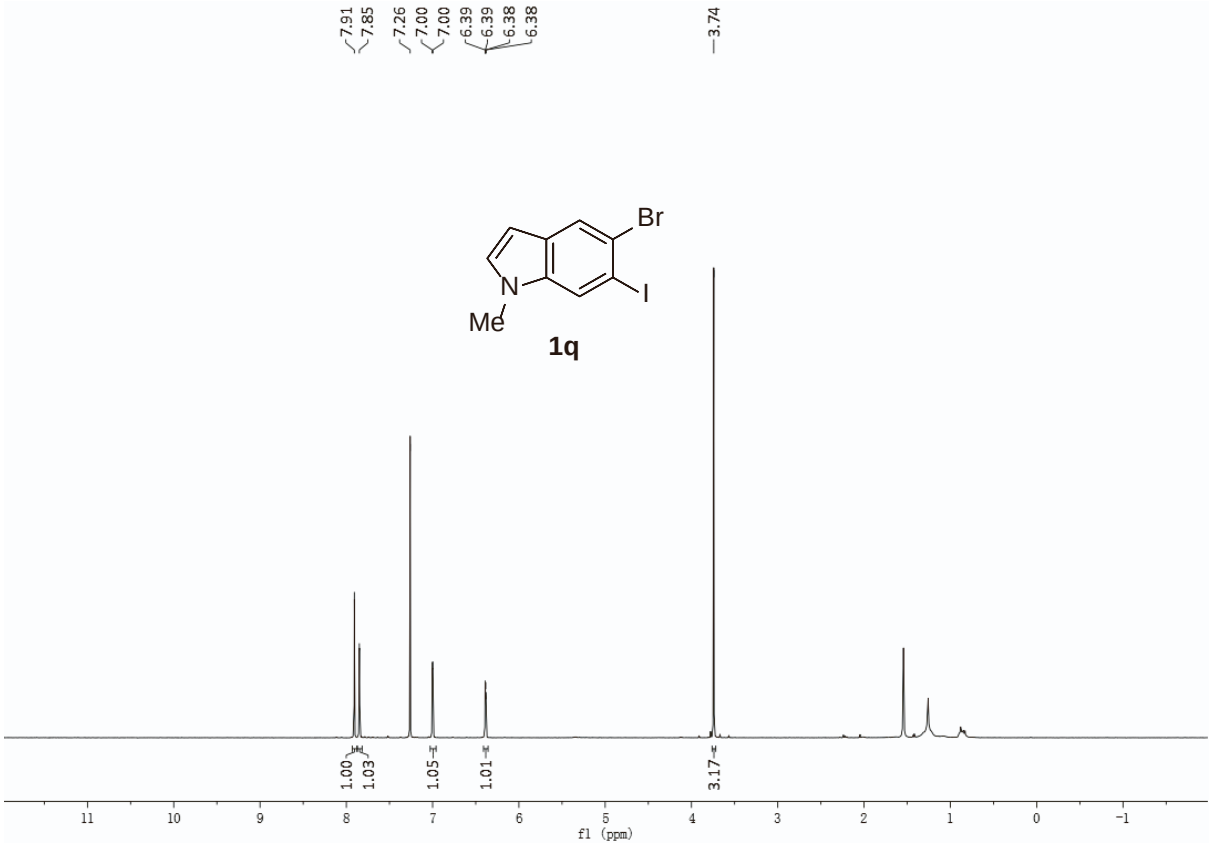
^{1}H NMR (400 MHz, $CDCl_3$)



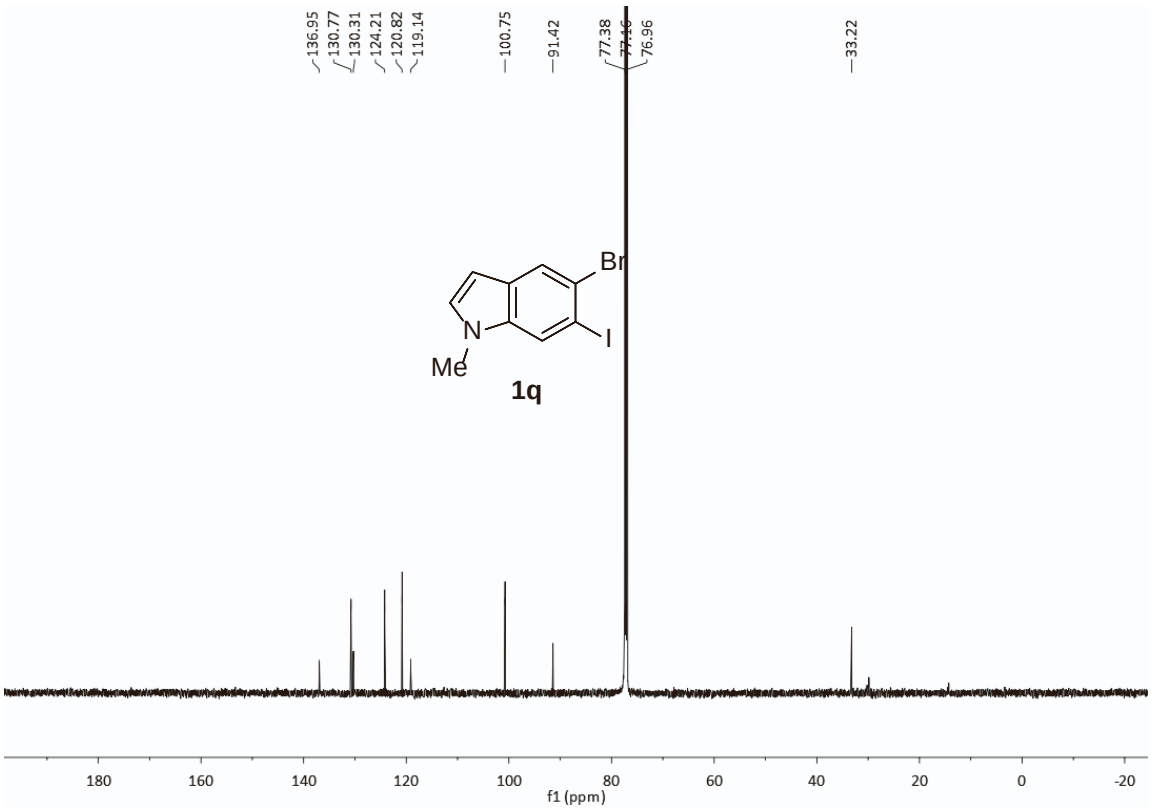
^{13}C NMR (151 MHz, $CDCl_3$)



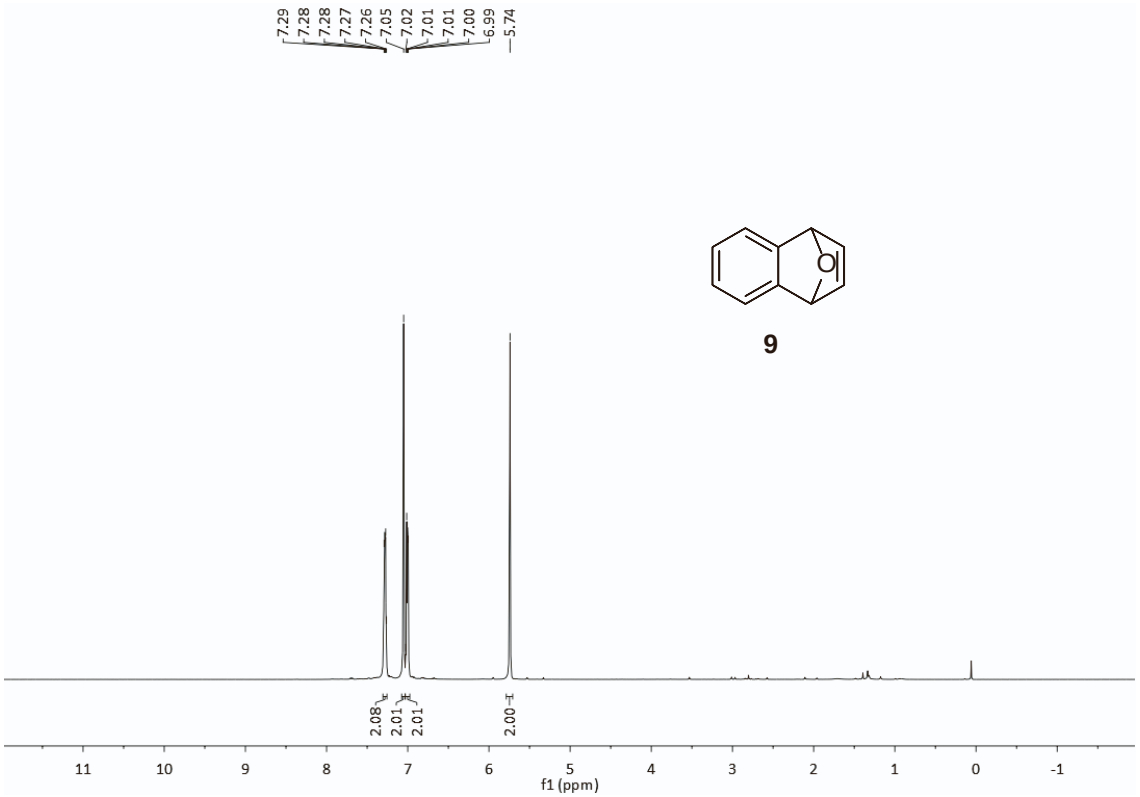
^{1}H NMR (400 MHz, $CDCl_3$)



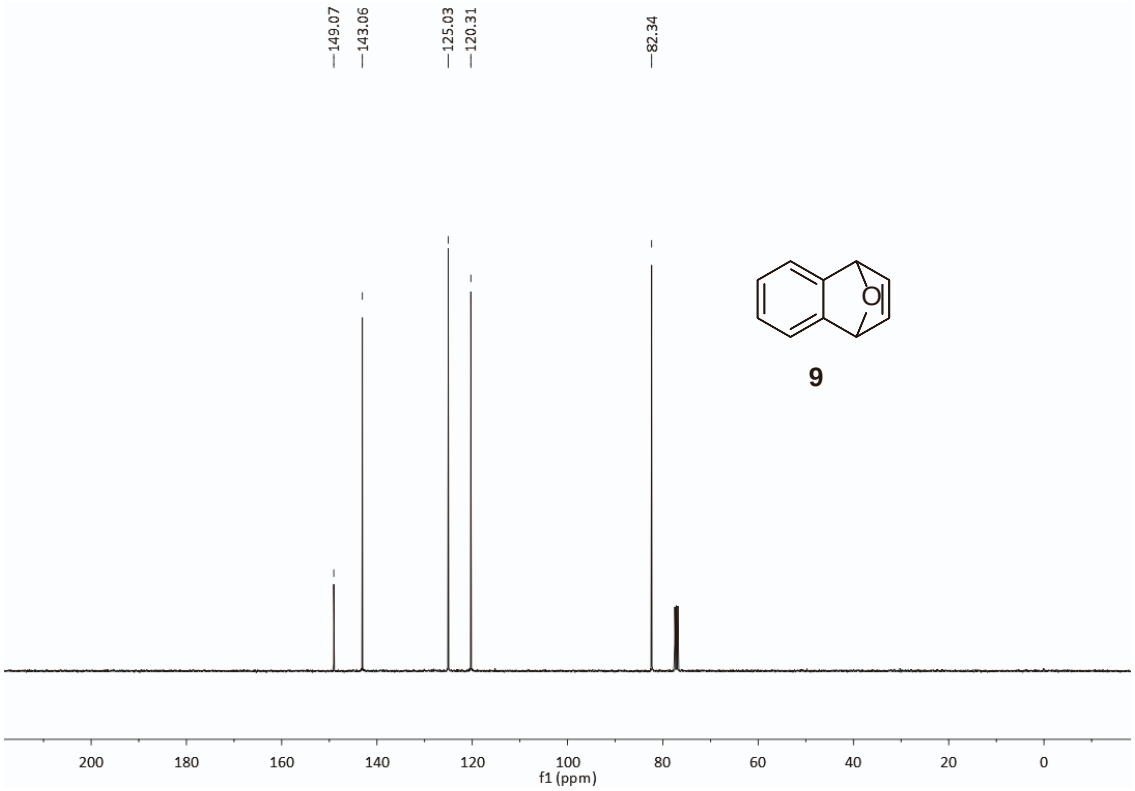
^{13}C NMR (151 MHz, $CDCl_3$)



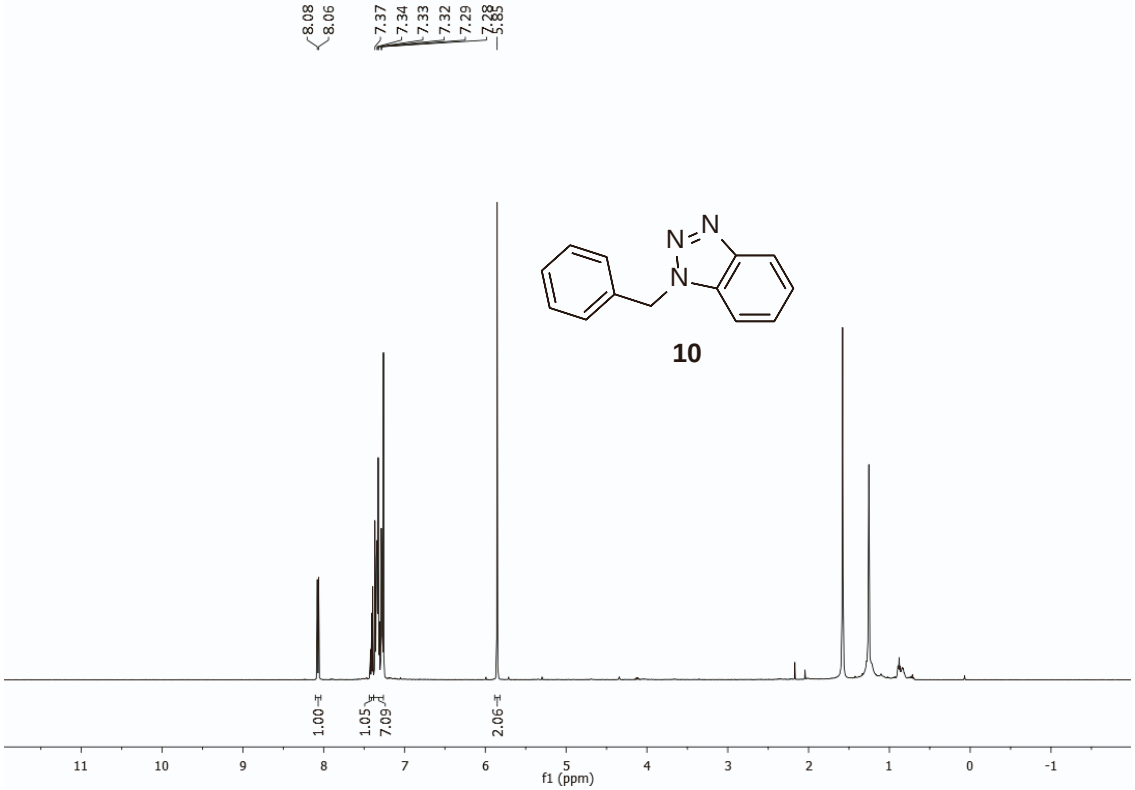
^{1}H NMR (400 MHz, $CDCl_3$)



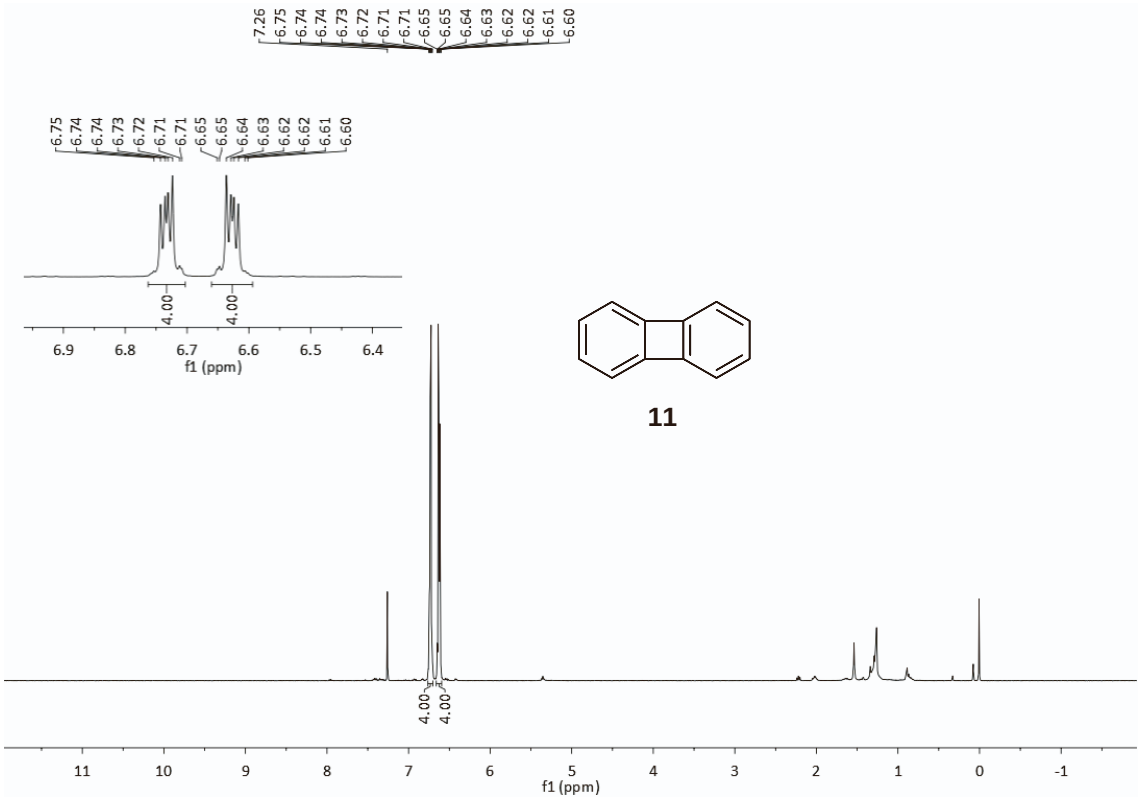
^{13}C NMR (101 MHz, $CDCl_3$)



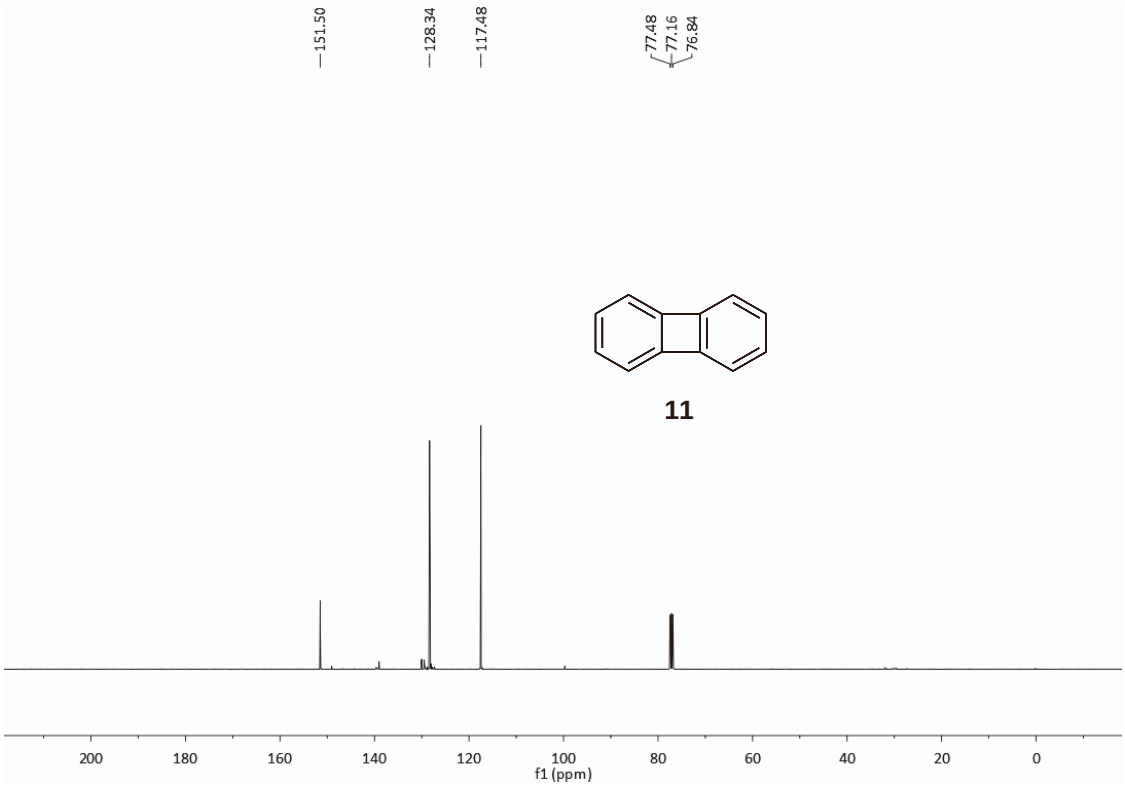
^{1}H NMR (500 MHz, $CDCl_3$)



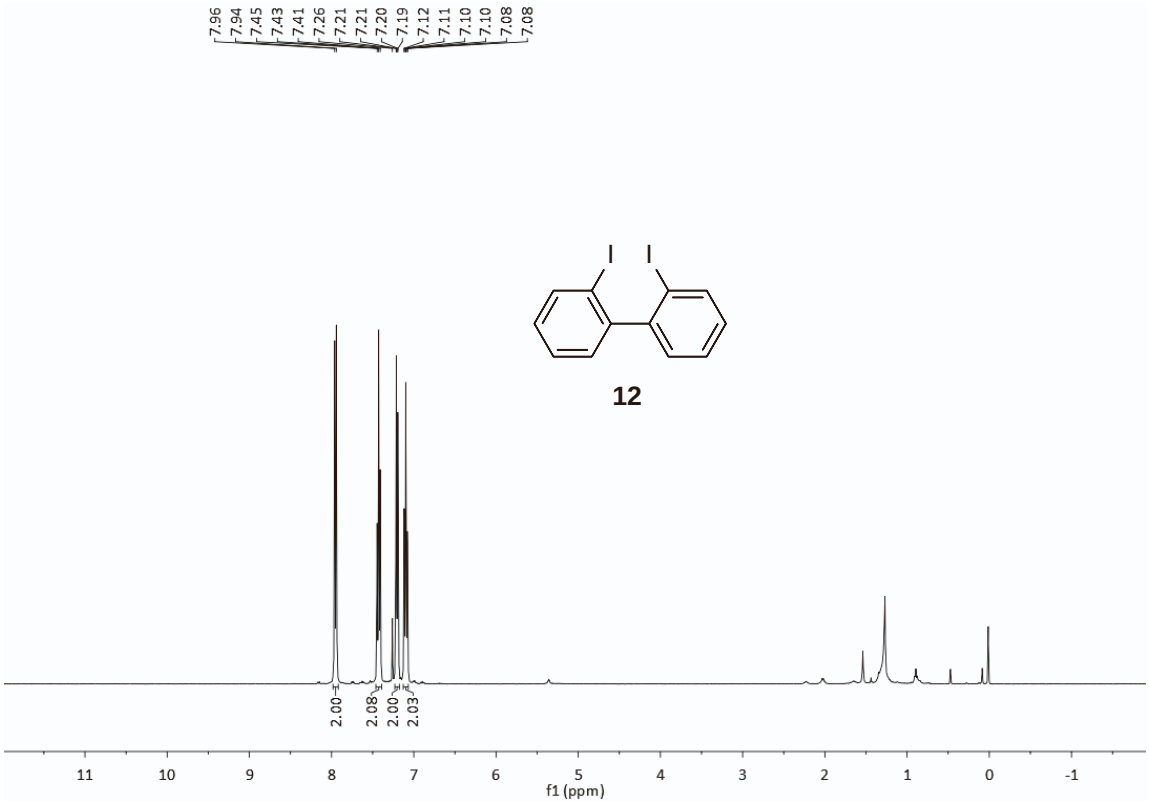
^{1}H NMR (400 MHz, $CDCl_3$)



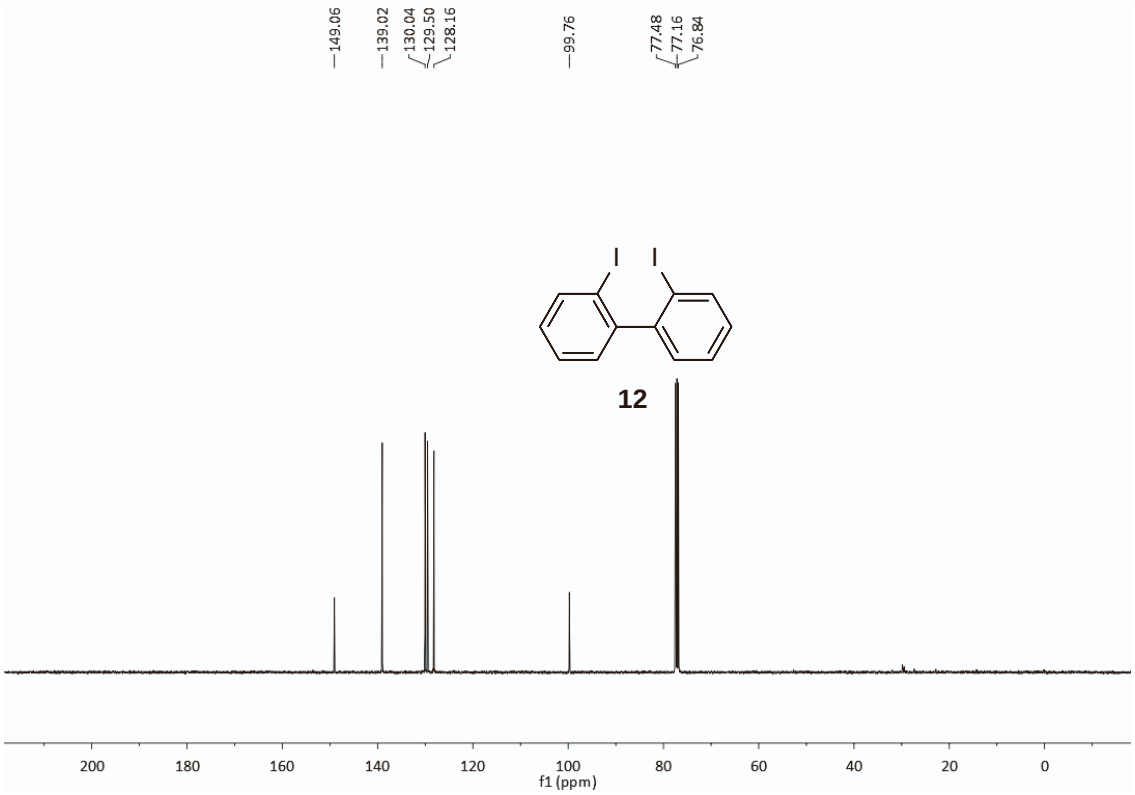
^{13}C NMR (101 MHz, $CDCl_3$)



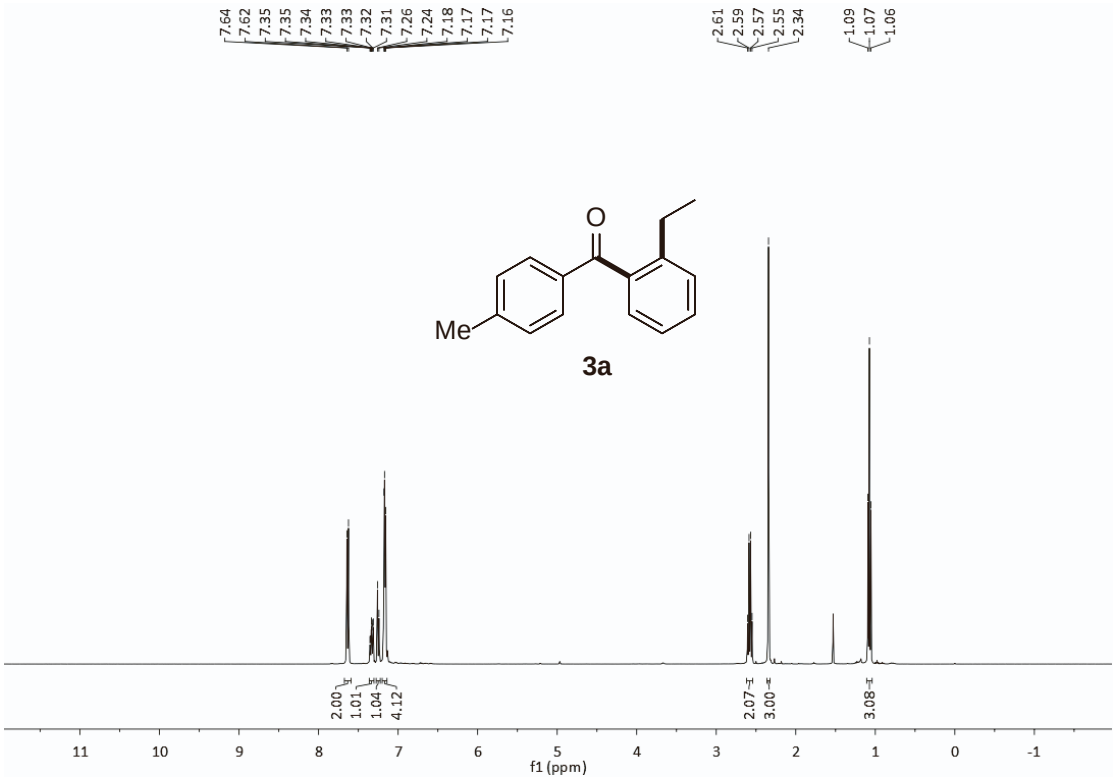
^{1}H NMR (400 MHz, $CDCl_3$)



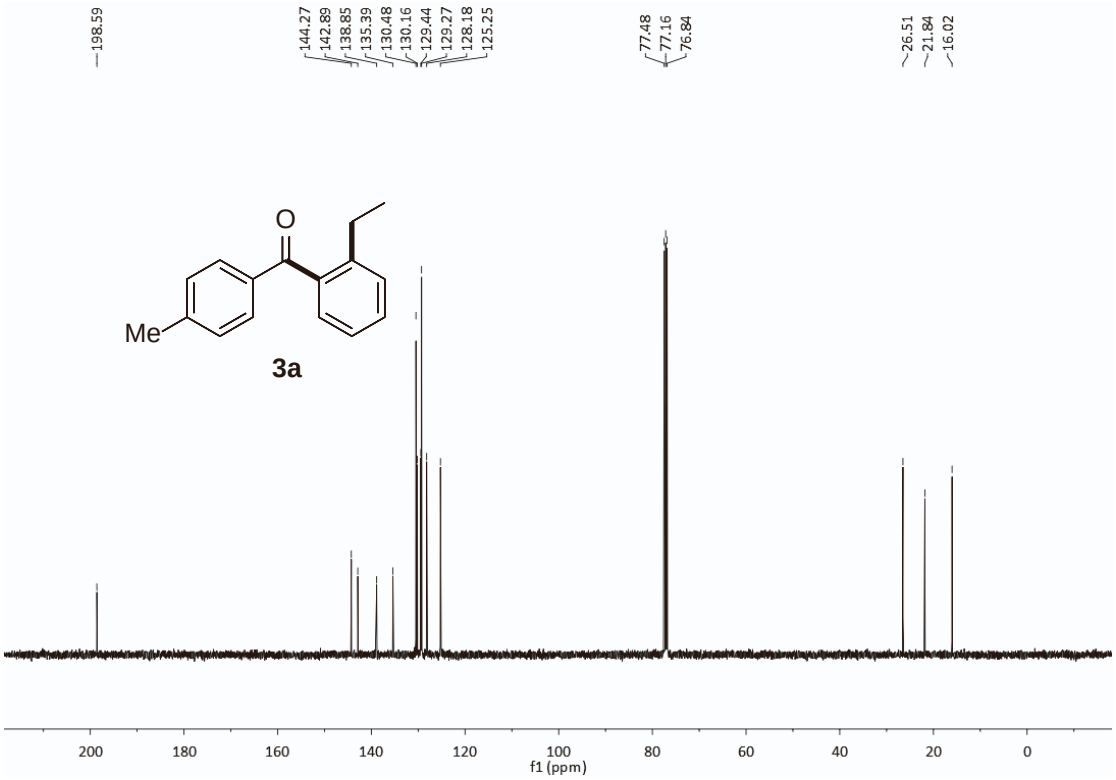
^{13}C NMR (101 MHz, $CDCl_3$)



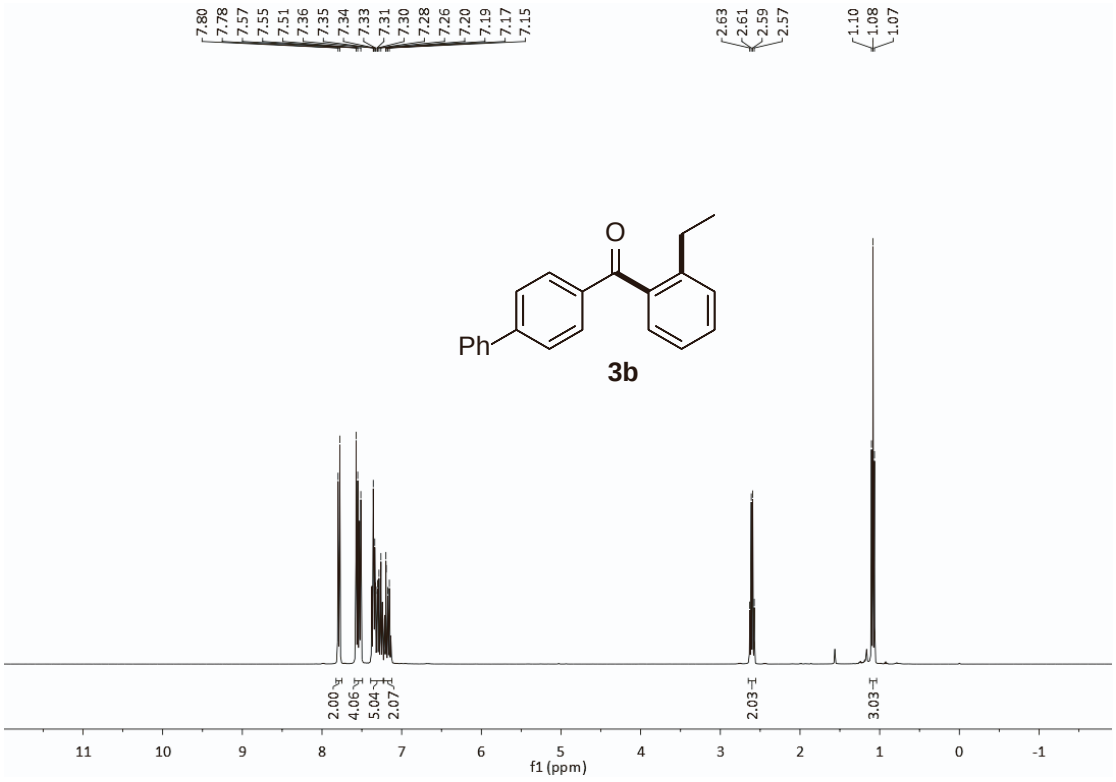
^{1}H NMR (400 MHz, $CDCl_3$)



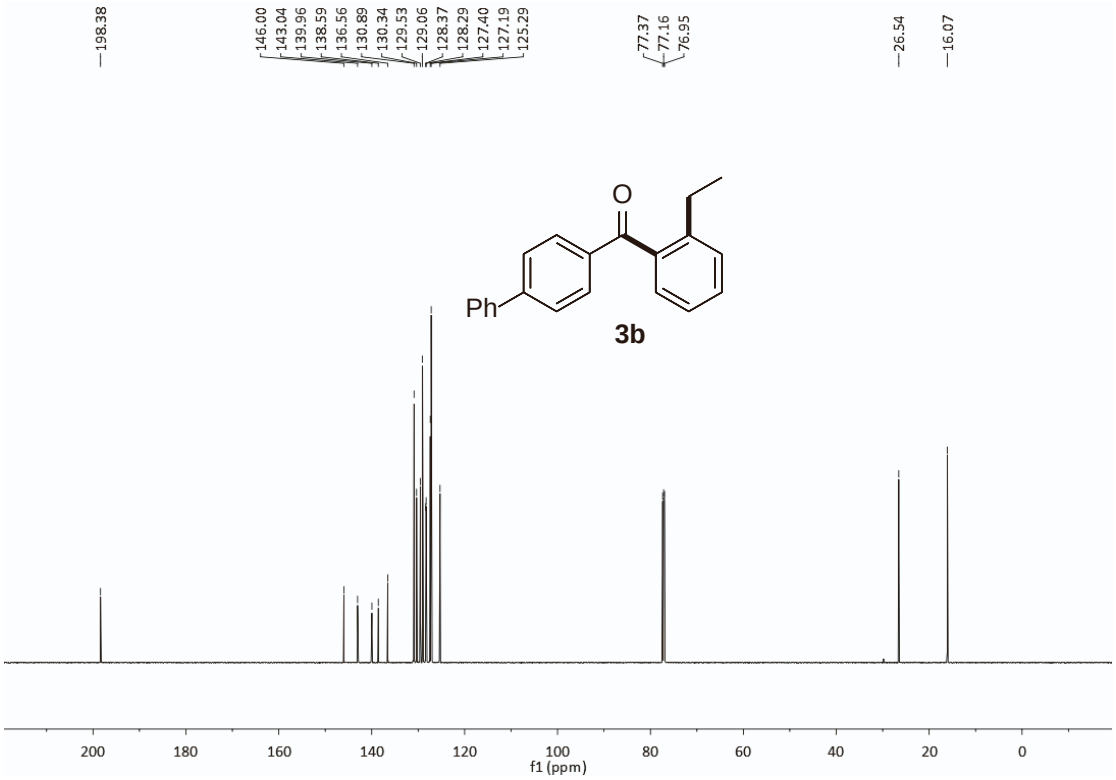
^{13}C NMR (101 MHz, $CDCl_3$)



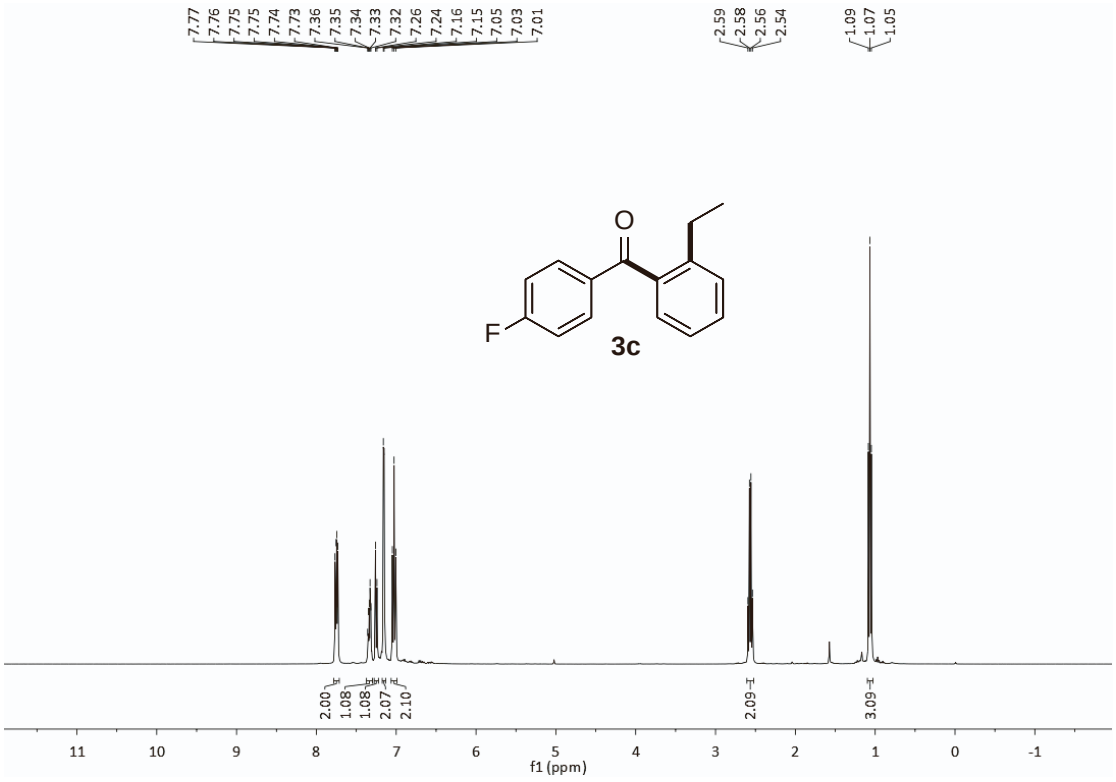
^{1}H NMR (400 MHz, $CDCl_3$)



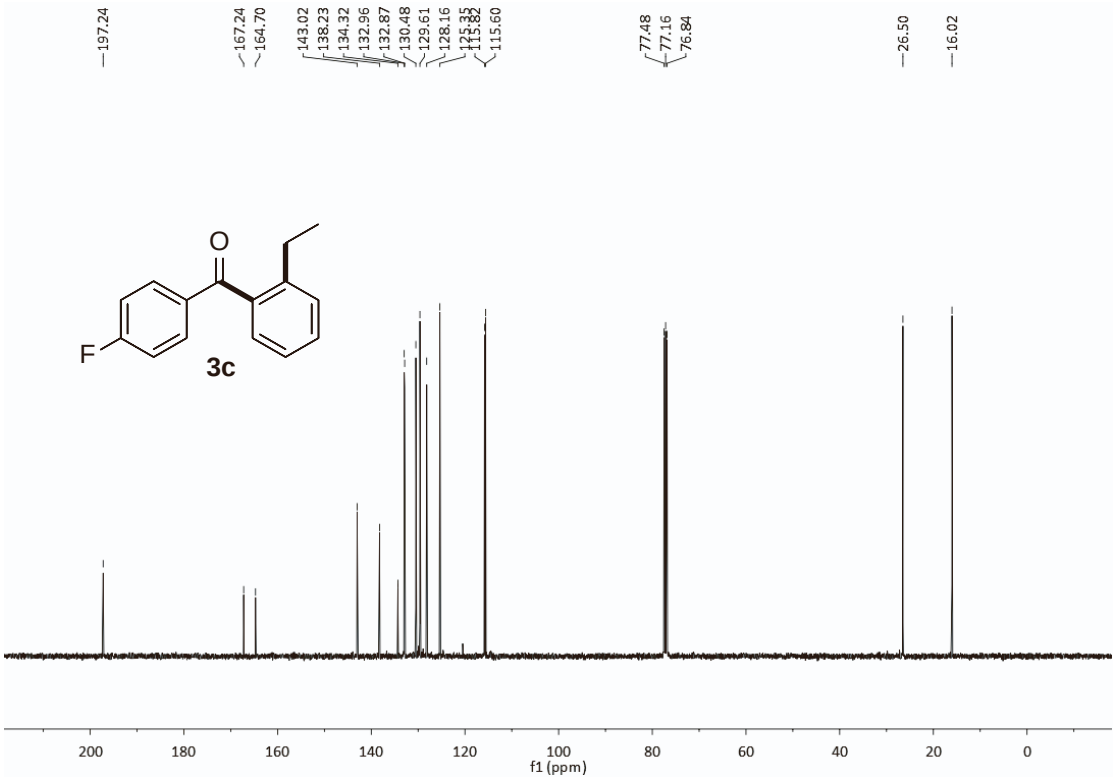
^{13}C NMR (151 MHz, $CDCl_3$)



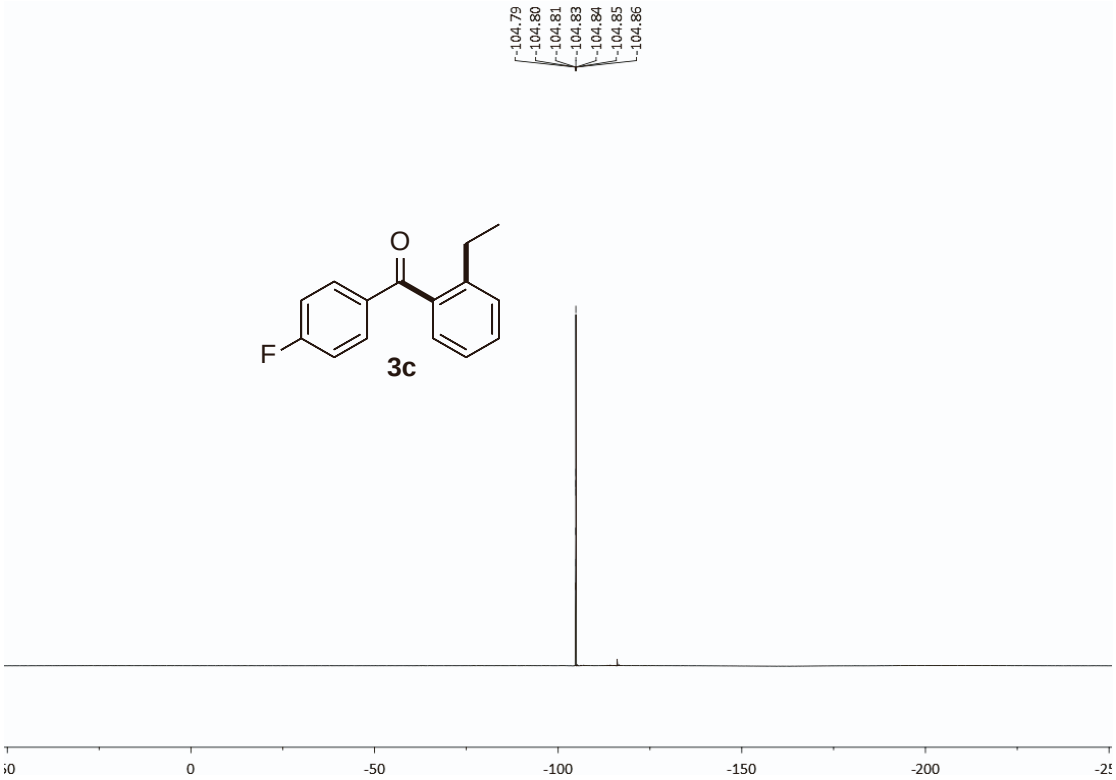
^{1}H NMR (400 MHz, $CDCl_3$)



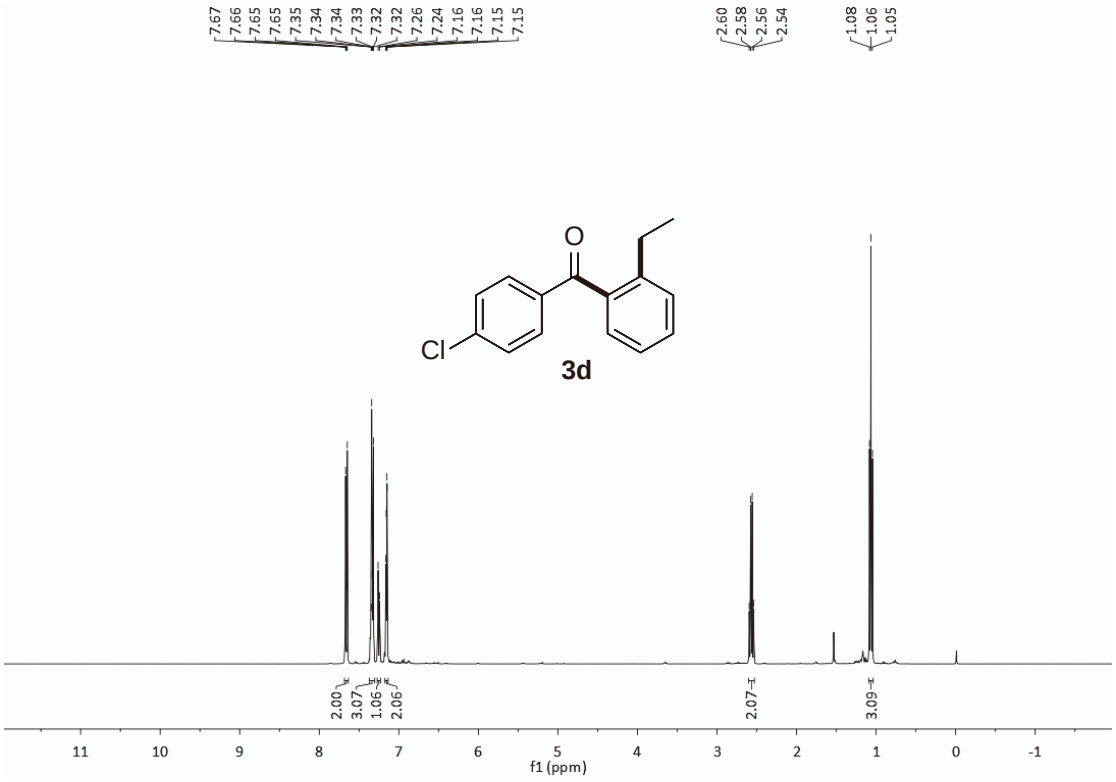
^{13}C NMR (101 MHz, $CDCl_3$)



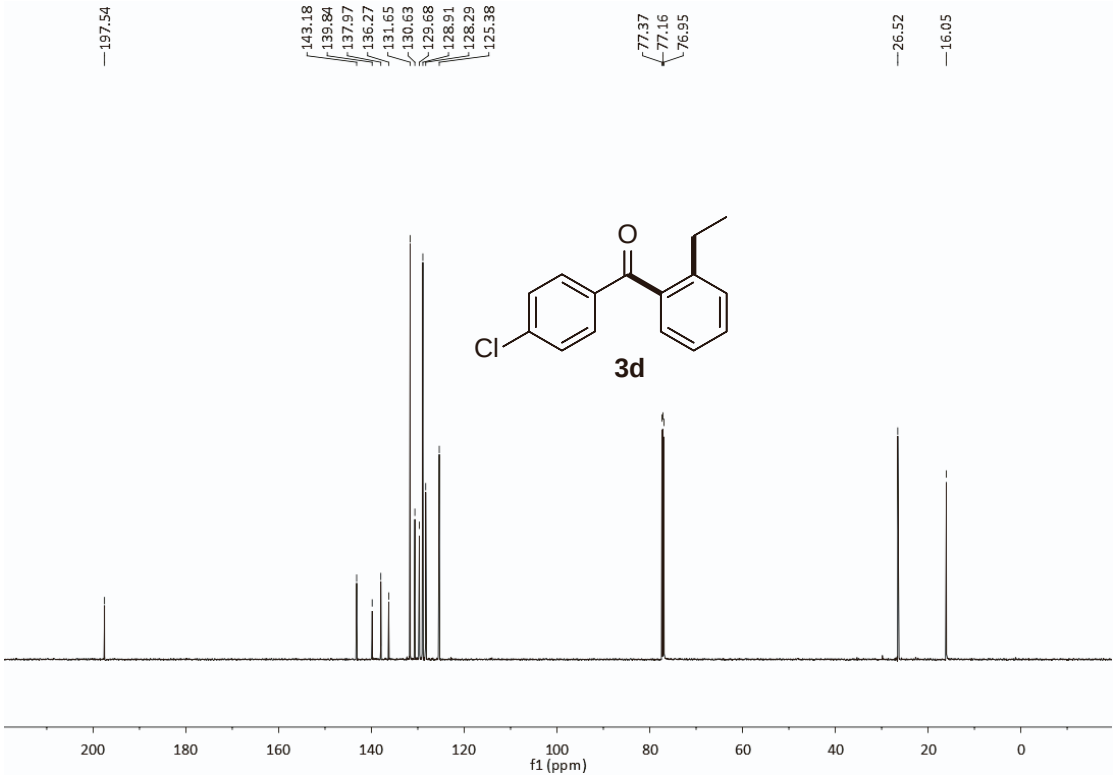
^{19}F NMR (377 MHz, $CDCl_3$)



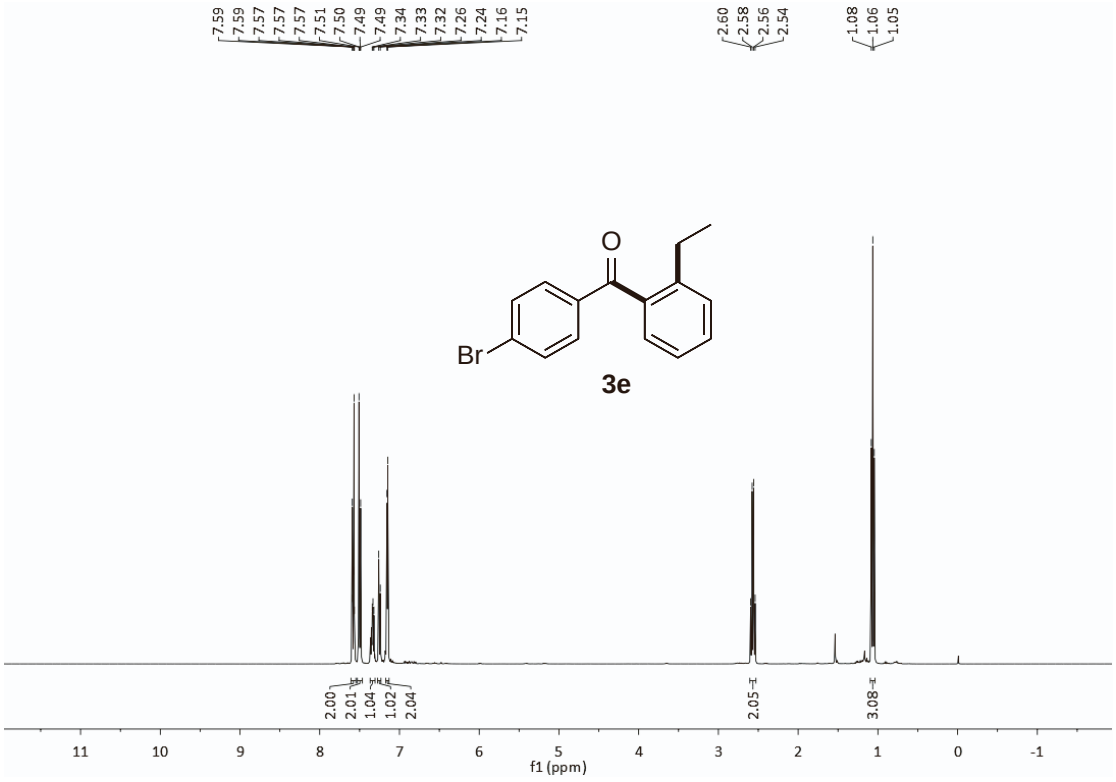
^{1}H NMR (400 MHz, $CDCl_3$)



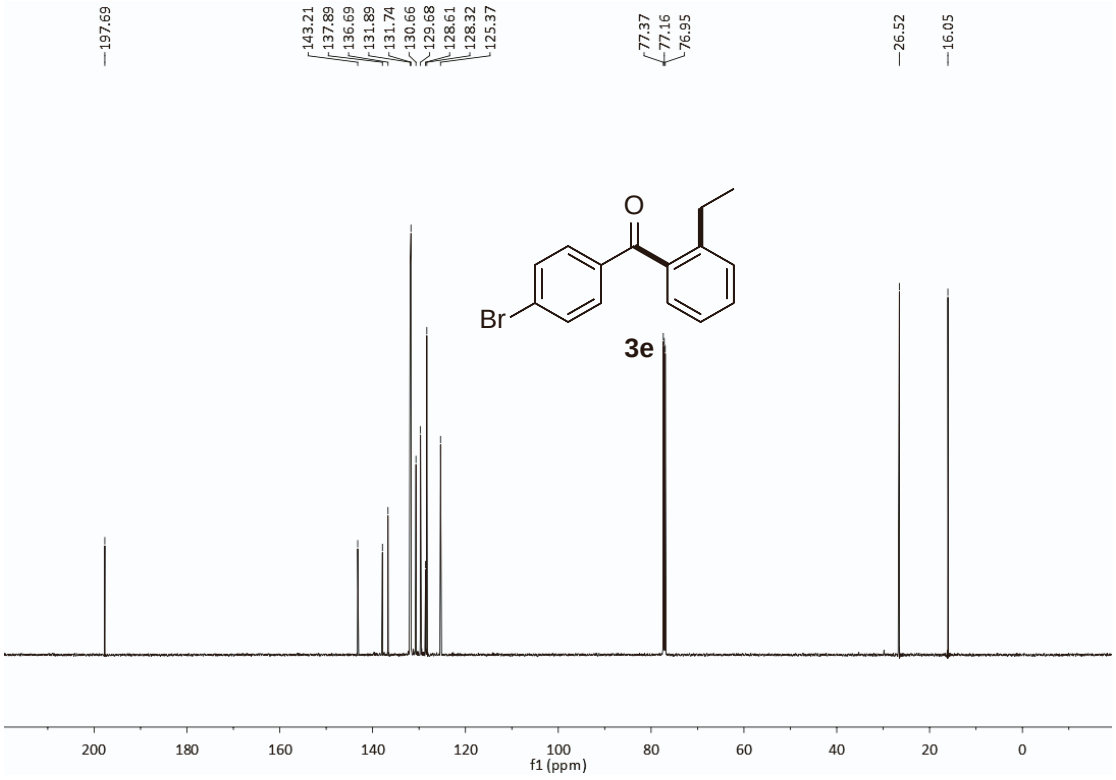
^{13}C NMR (151 MHz, $CDCl_3$)



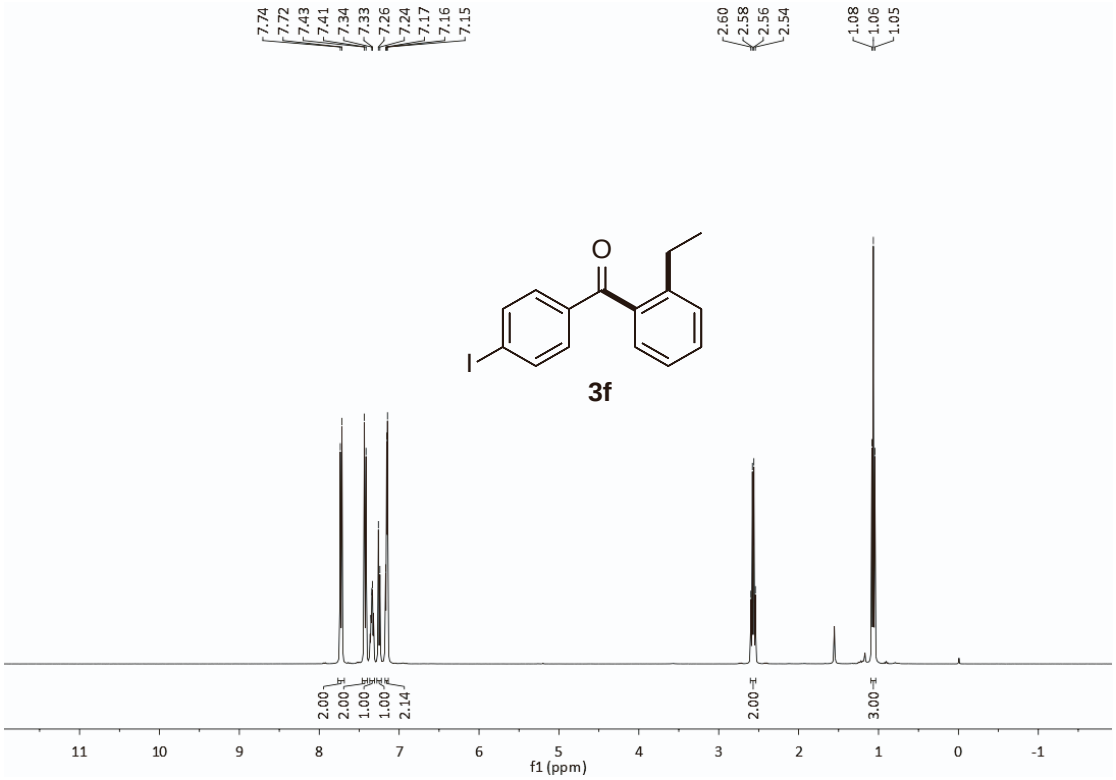
^{1}H NMR (400 MHz, $CDCl_3$)



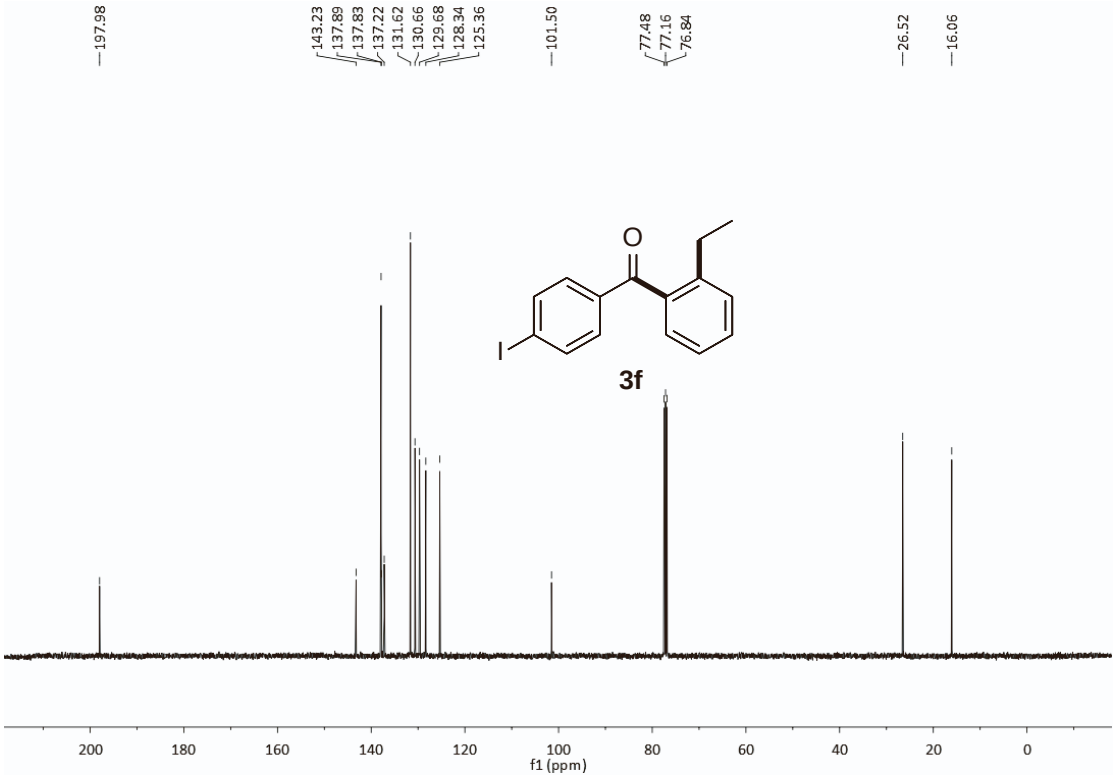
^{13}C NMR (151 MHz, $CDCl_3$)



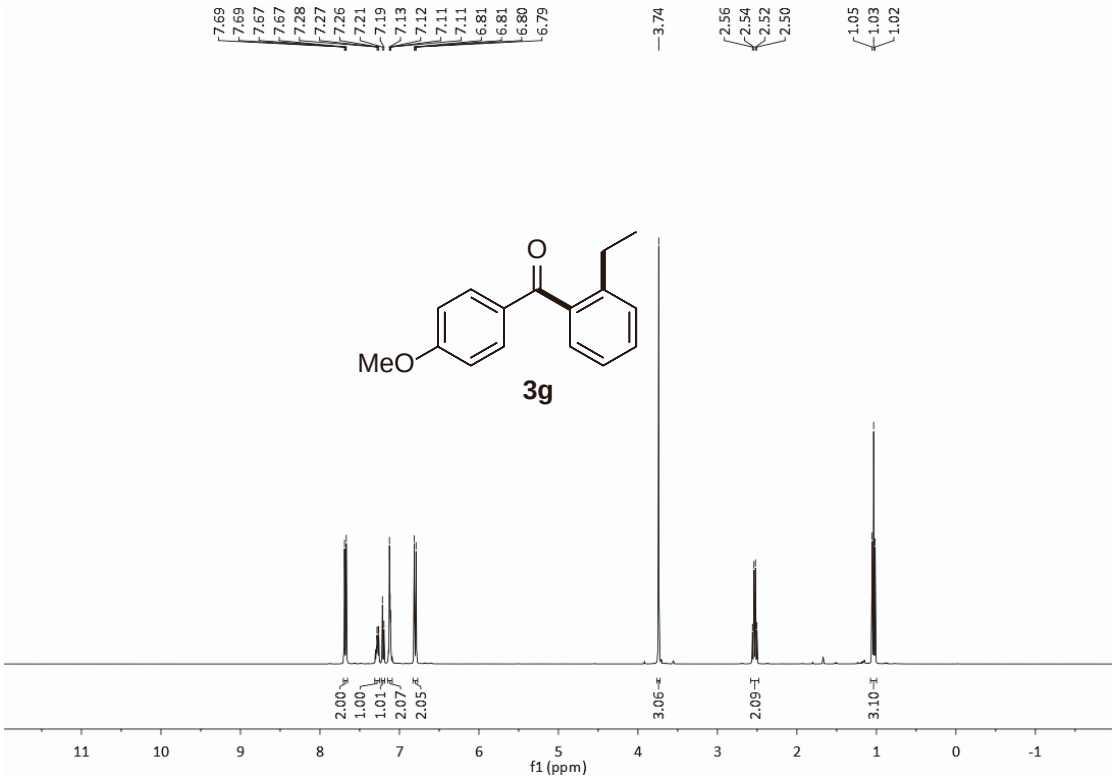
^{1}H NMR (400 MHz, $CDCl_3$)



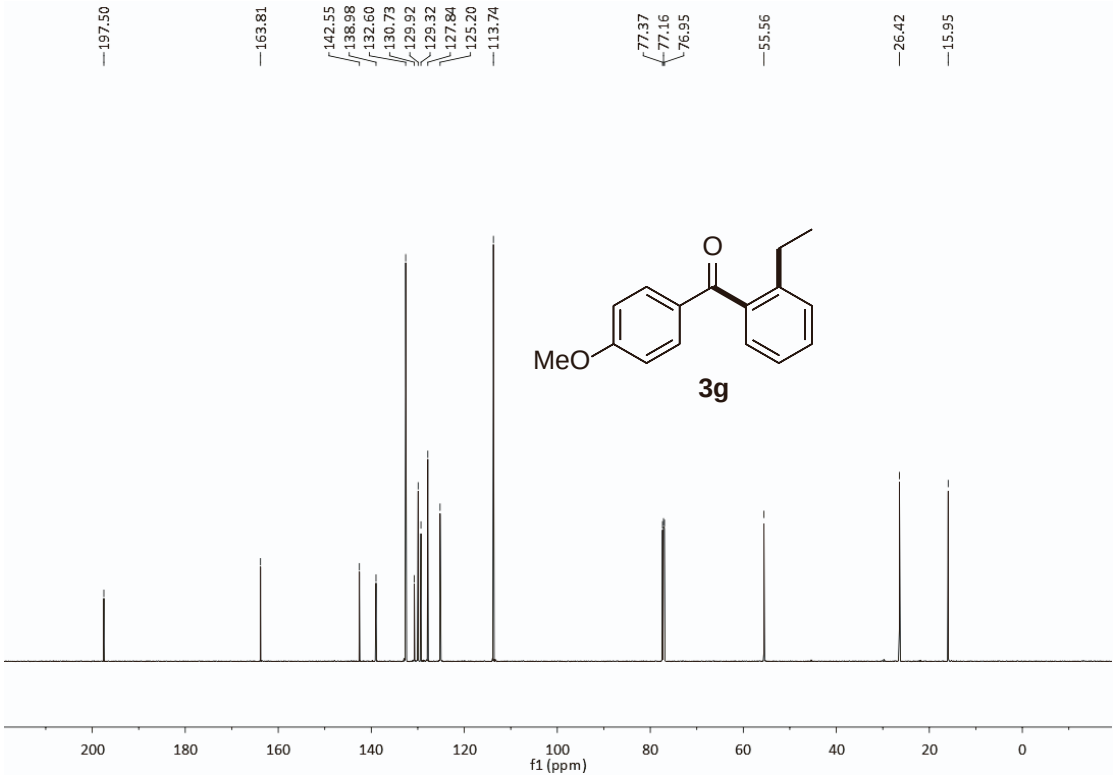
^{13}C NMR (101 MHz, $CDCl_3$)



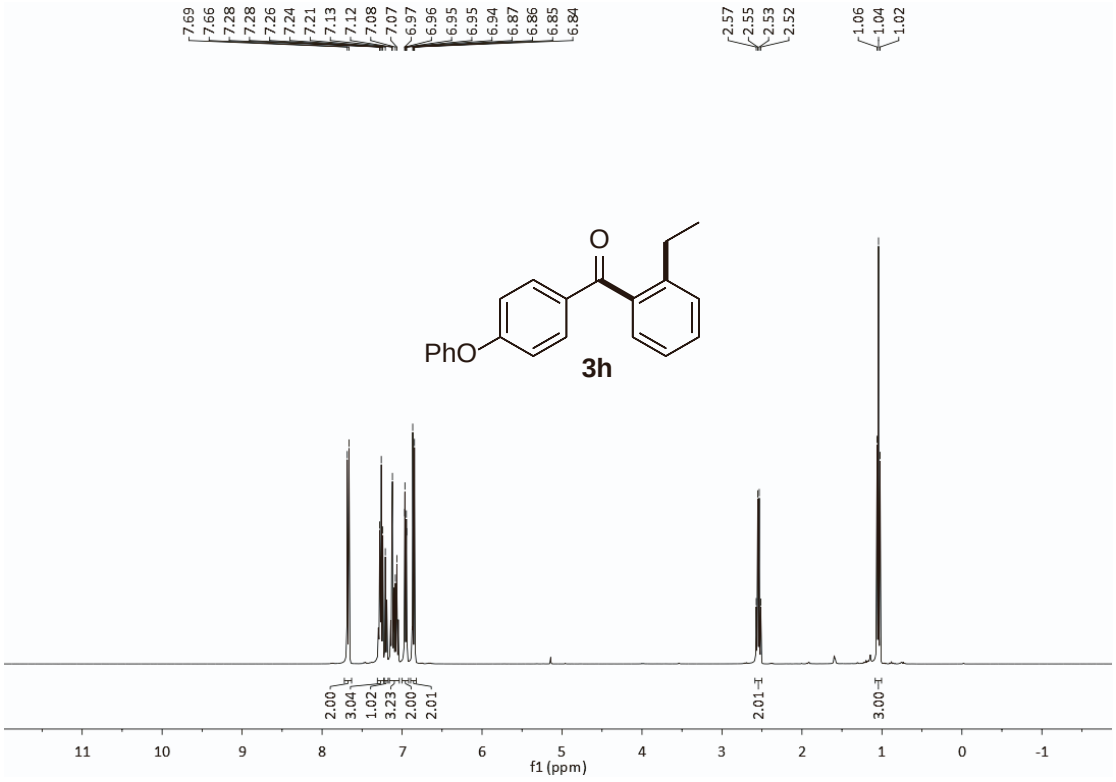
^{1}H NMR (400 MHz, $CDCl_3$)



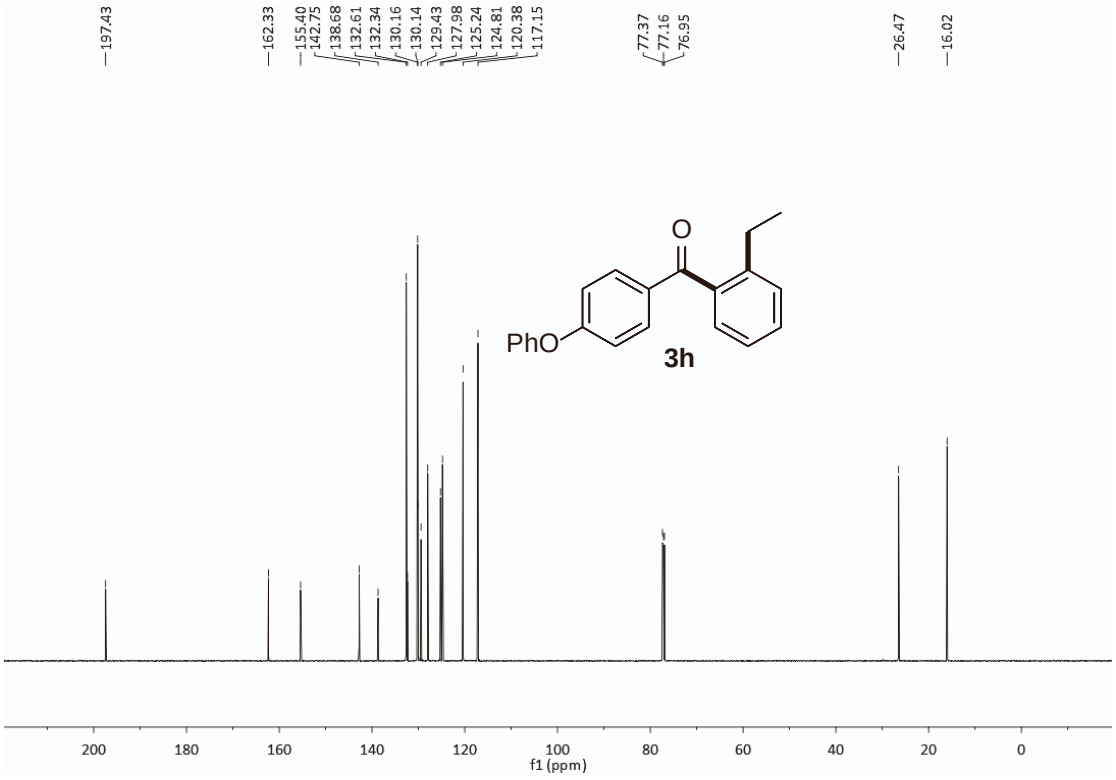
^{13}C NMR (151 MHz, $CDCl_3$)



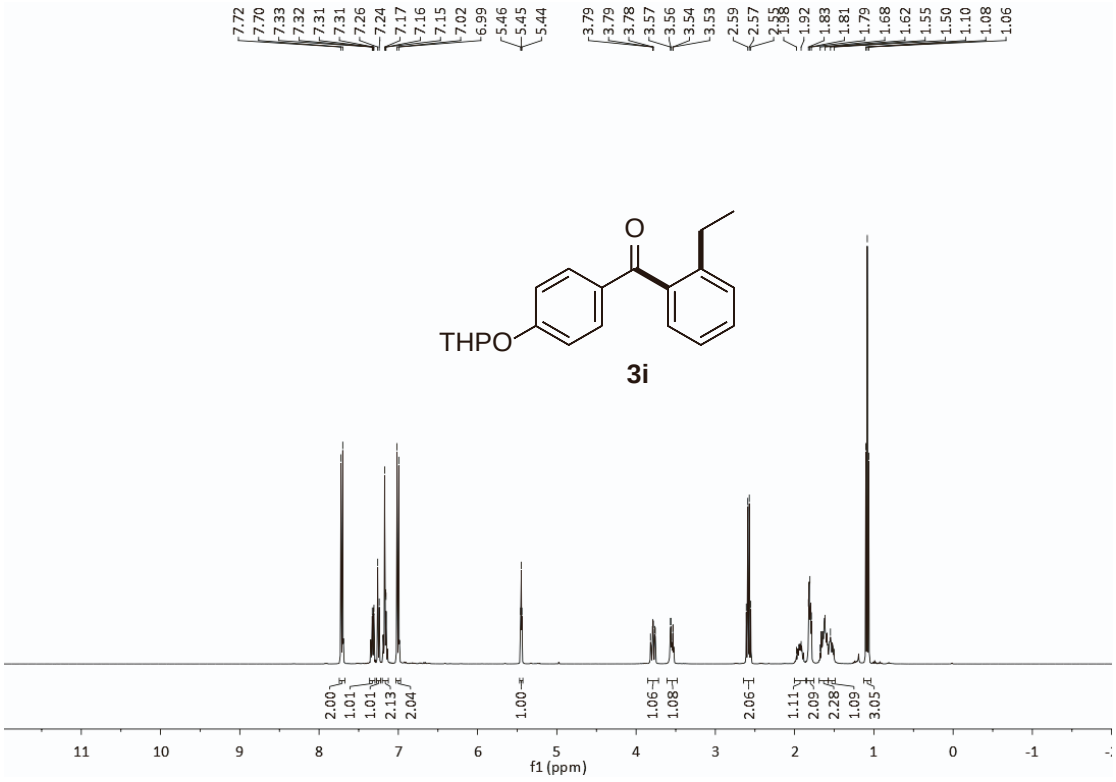
^{1}H NMR (400 MHz, $CDCl_3$)



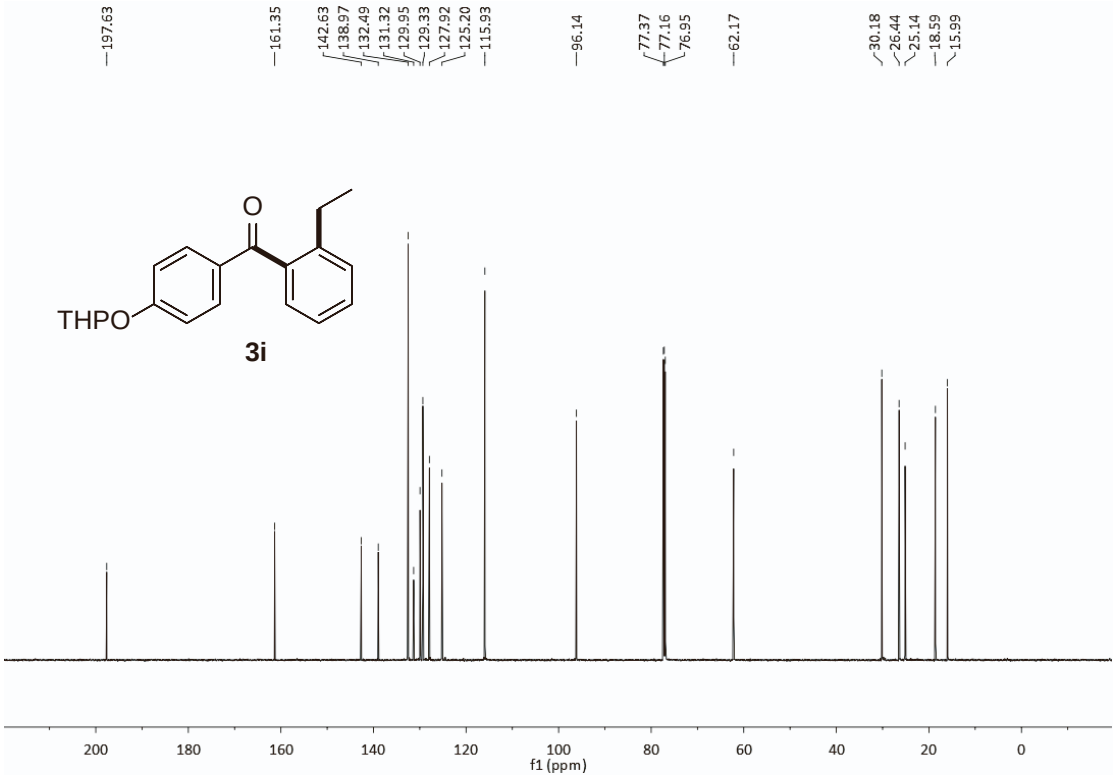
^{13}C NMR (151 MHz, $CDCl_3$)



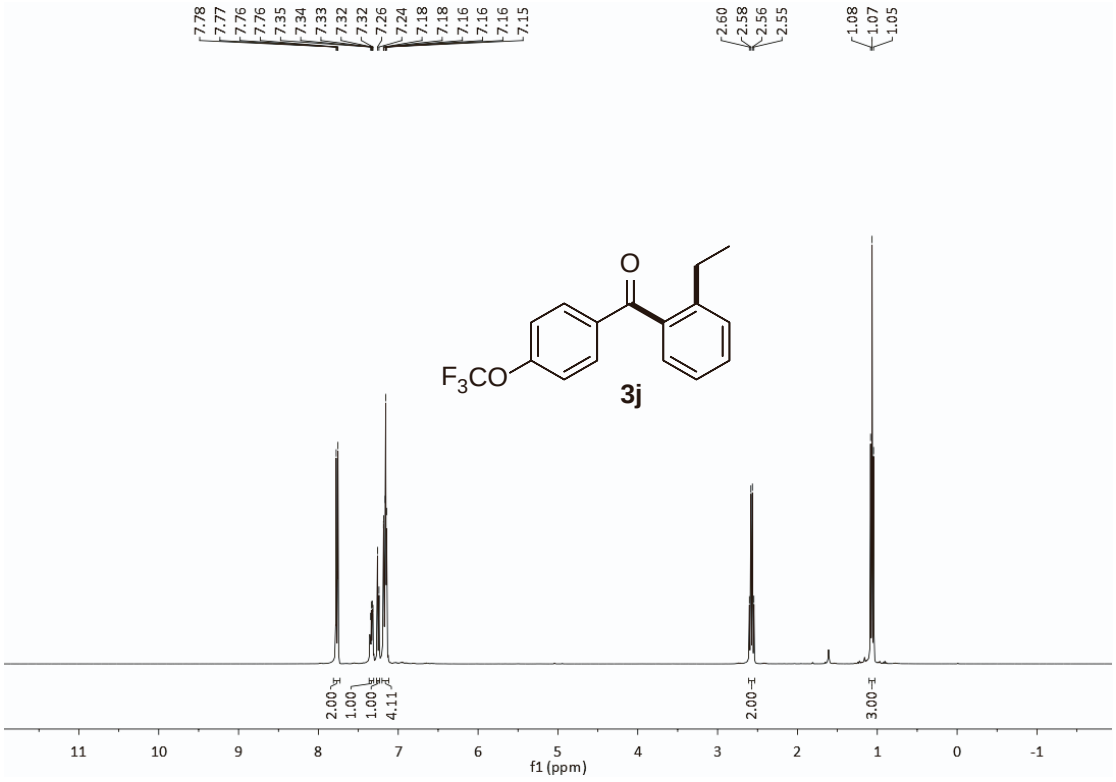
^{1}H NMR (400 MHz, $CDCl_3$)



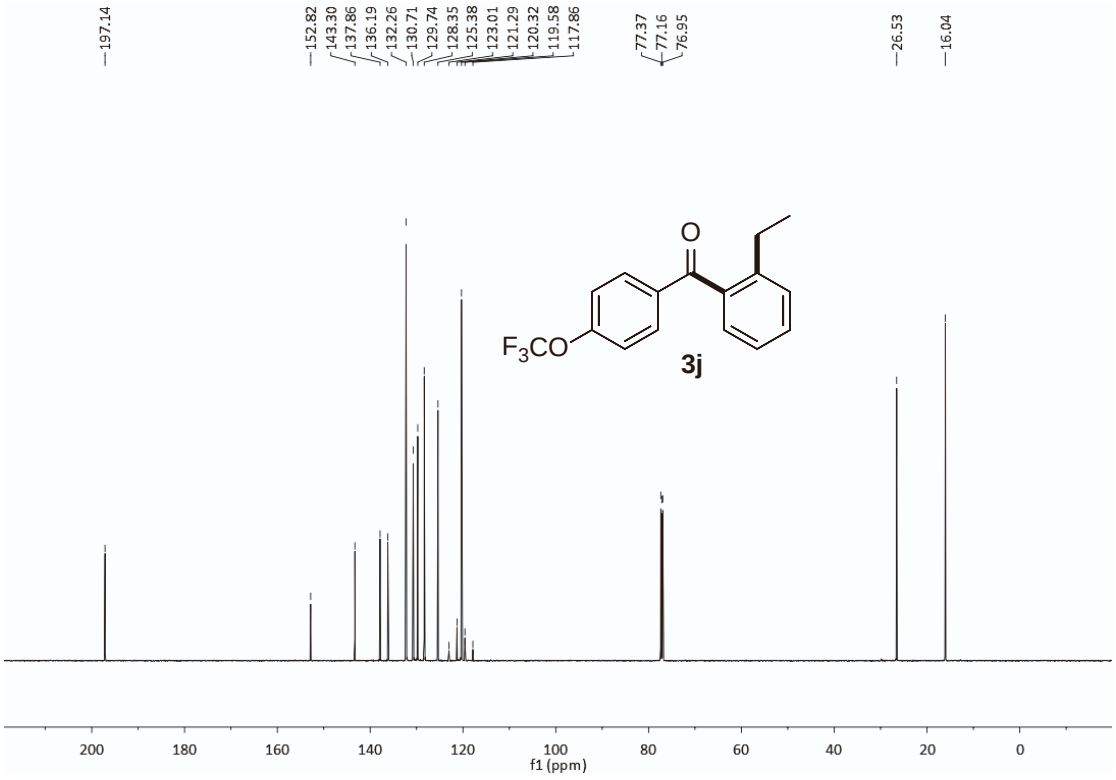
^{13}C NMR (151 MHz, $CDCl_3$)



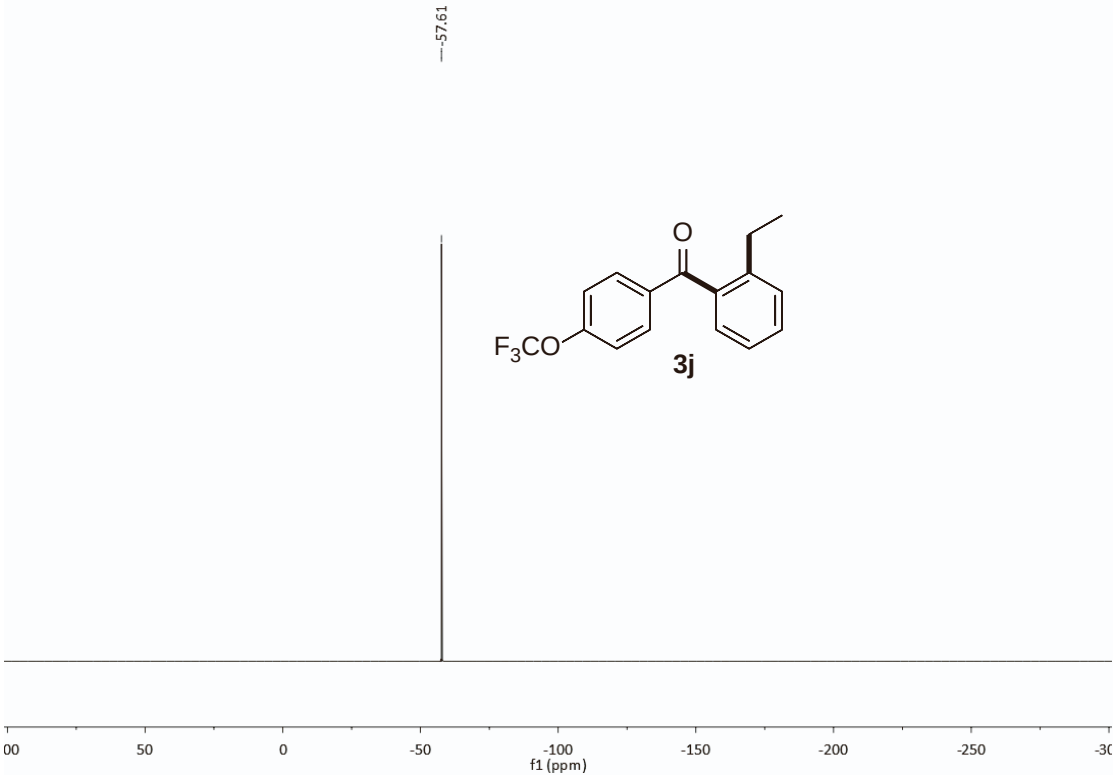
^{1}H NMR (400 MHz, $CDCl_3$)



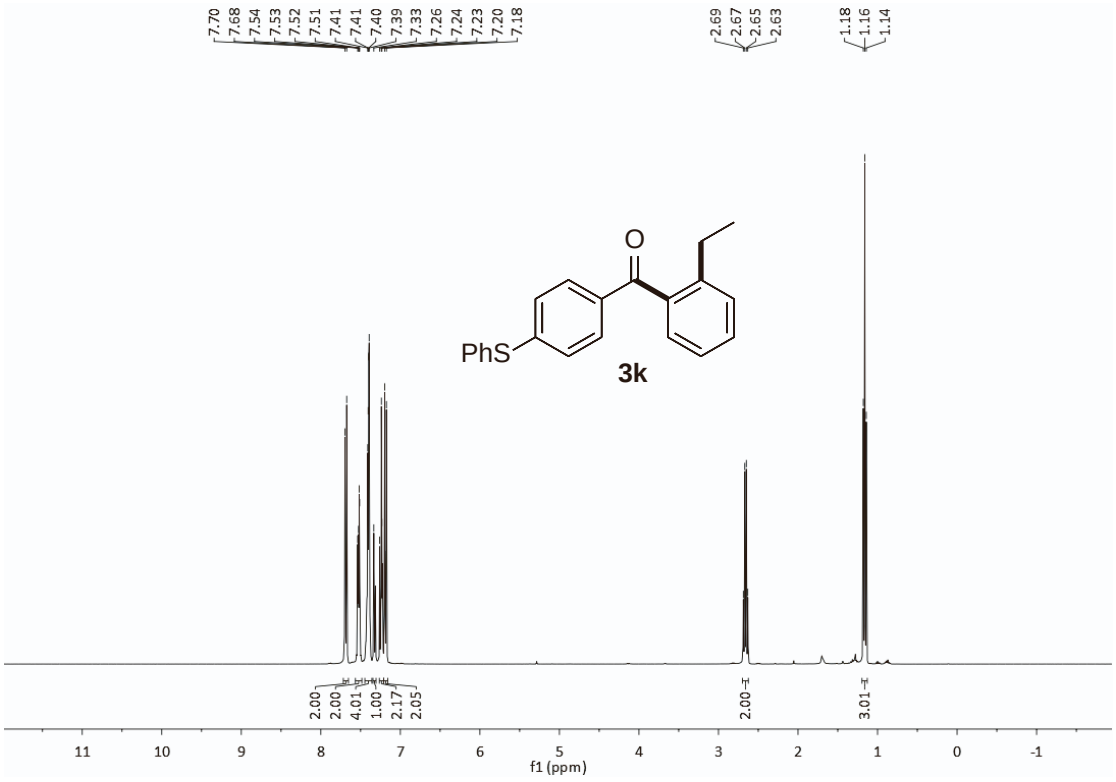
^{13}C NMR (151 MHz, $CDCl_3$)



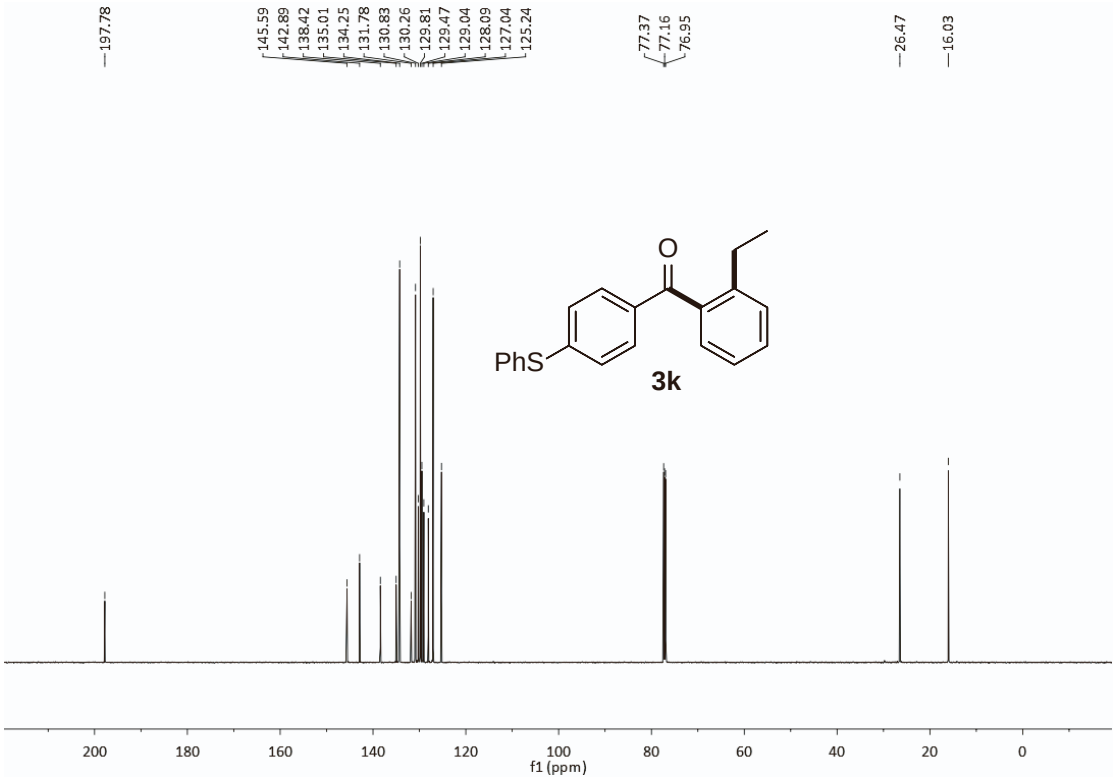
^{19}F NMR (565 MHz, $CDCl_3$)



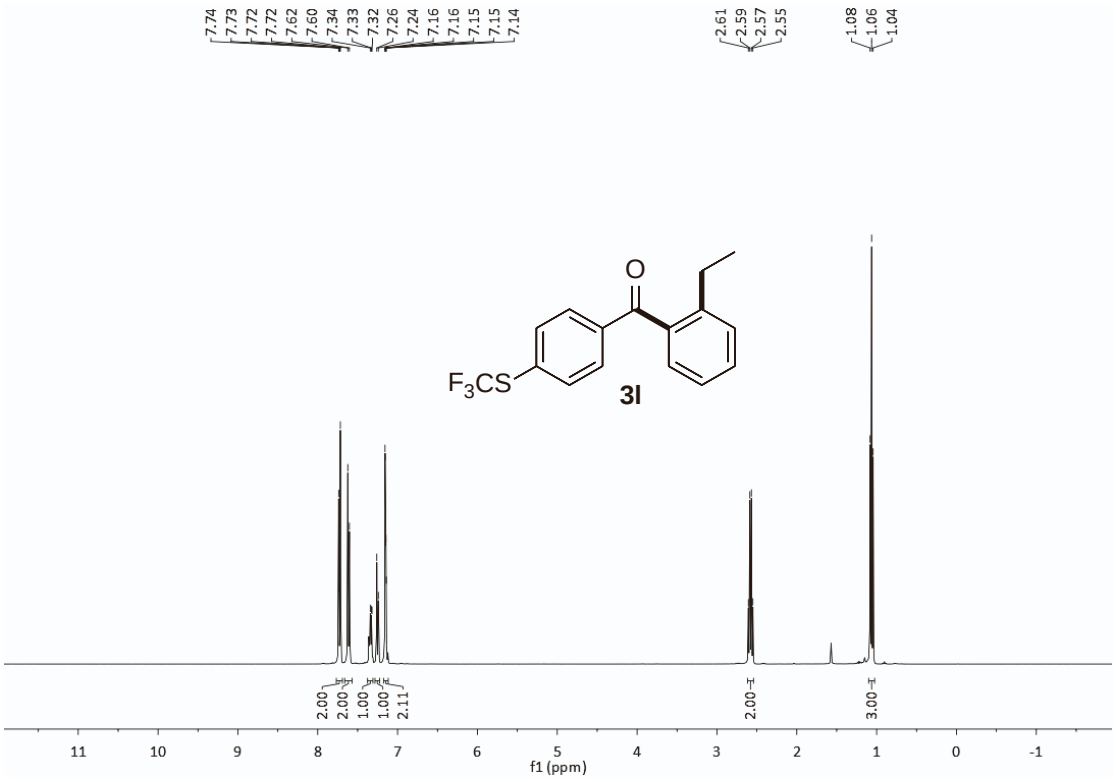
^{1}H NMR (400 MHz, $CDCl_3$)



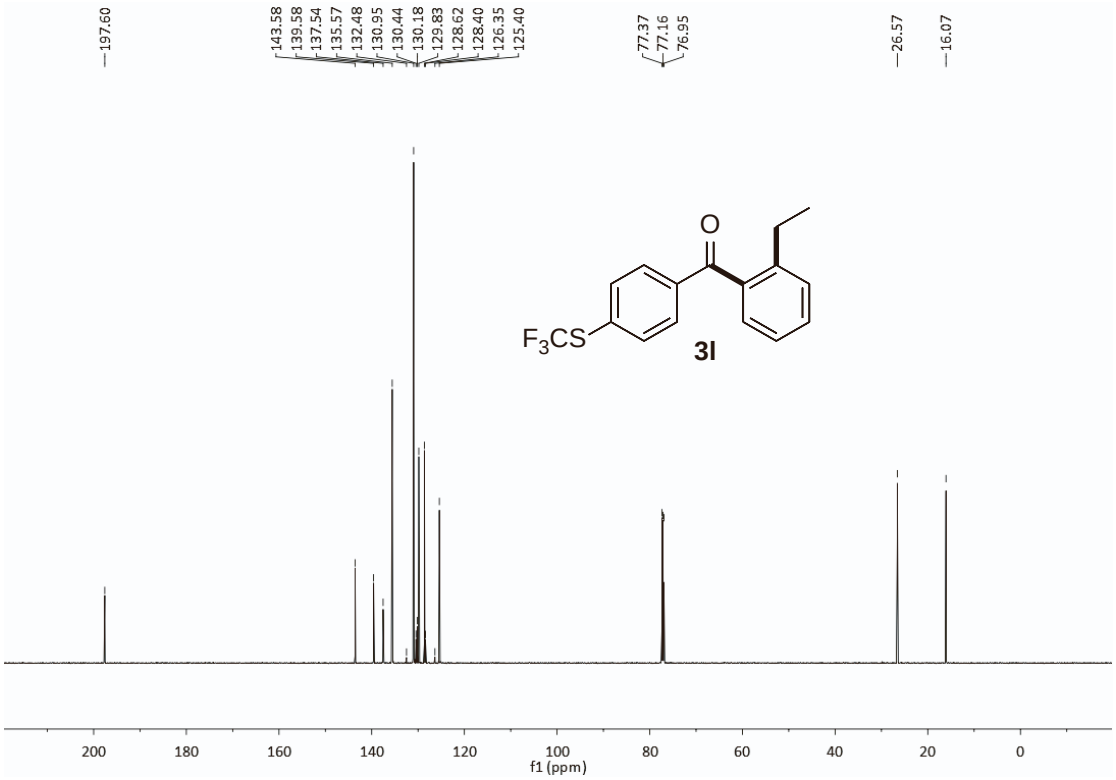
^{13}C NMR (151 MHz, $CDCl_3$)



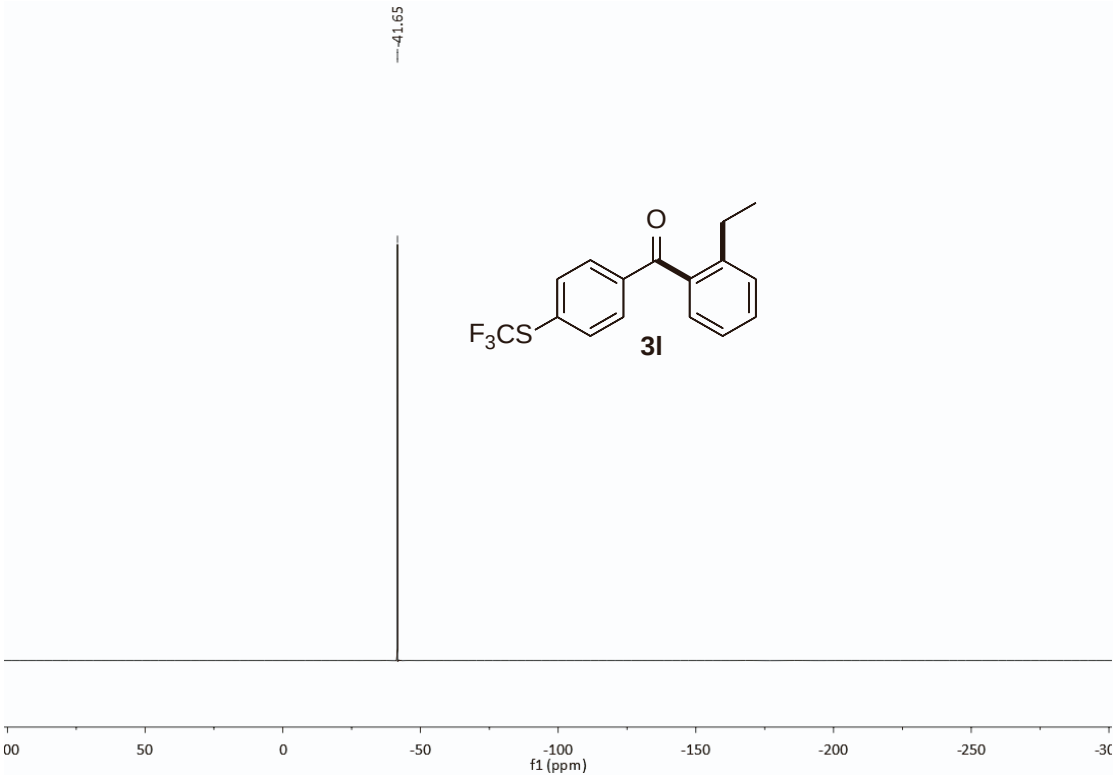
^{1}H NMR (400 MHz, $CDCl_3$)



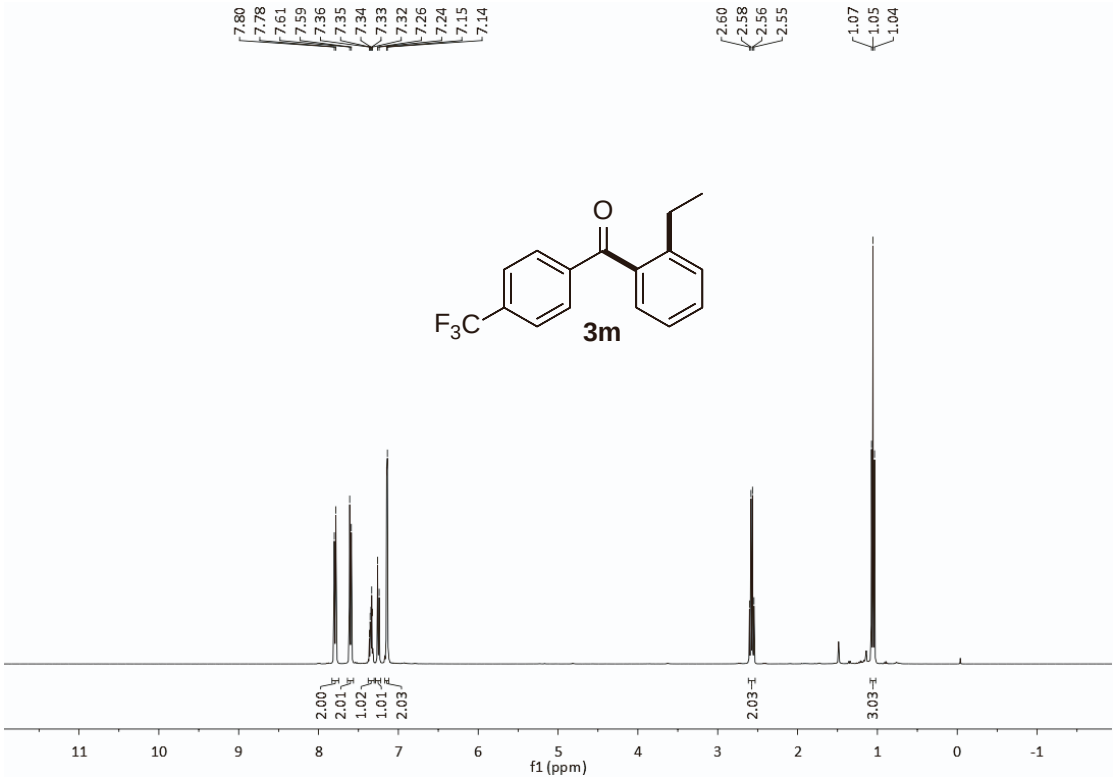
^{13}C NMR (151 MHz, $CDCl_3$)



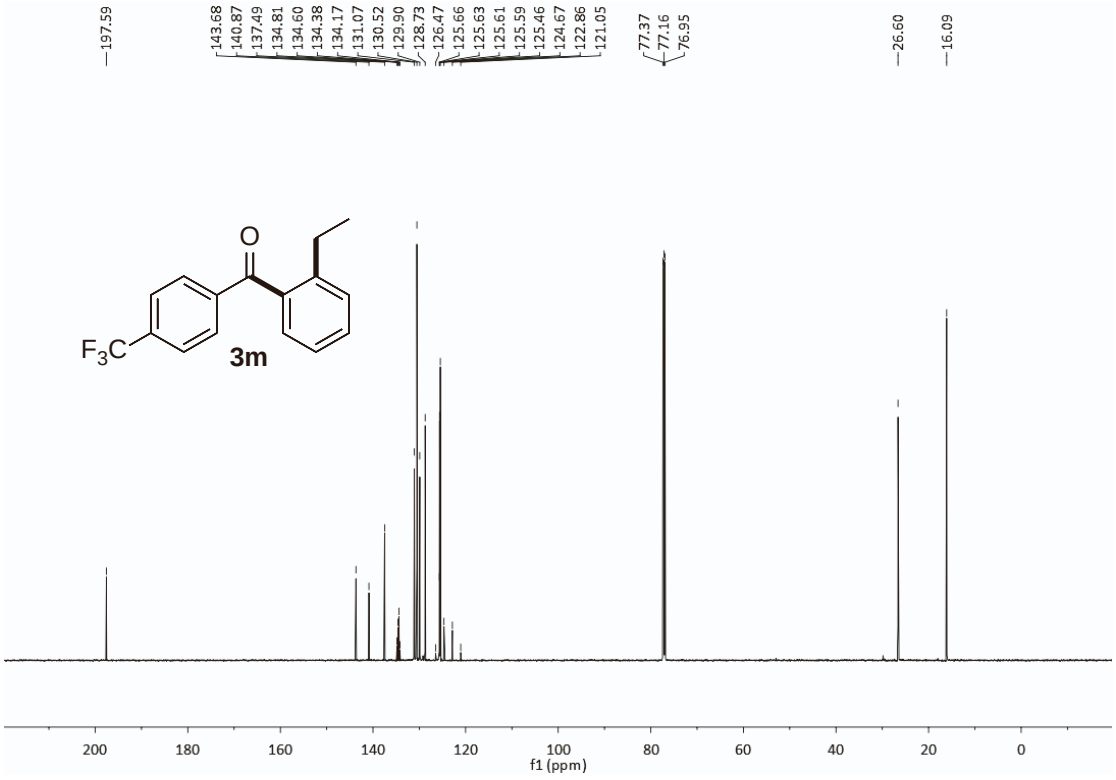
^{19}F NMR (565 MHz, $CDCl_3$)



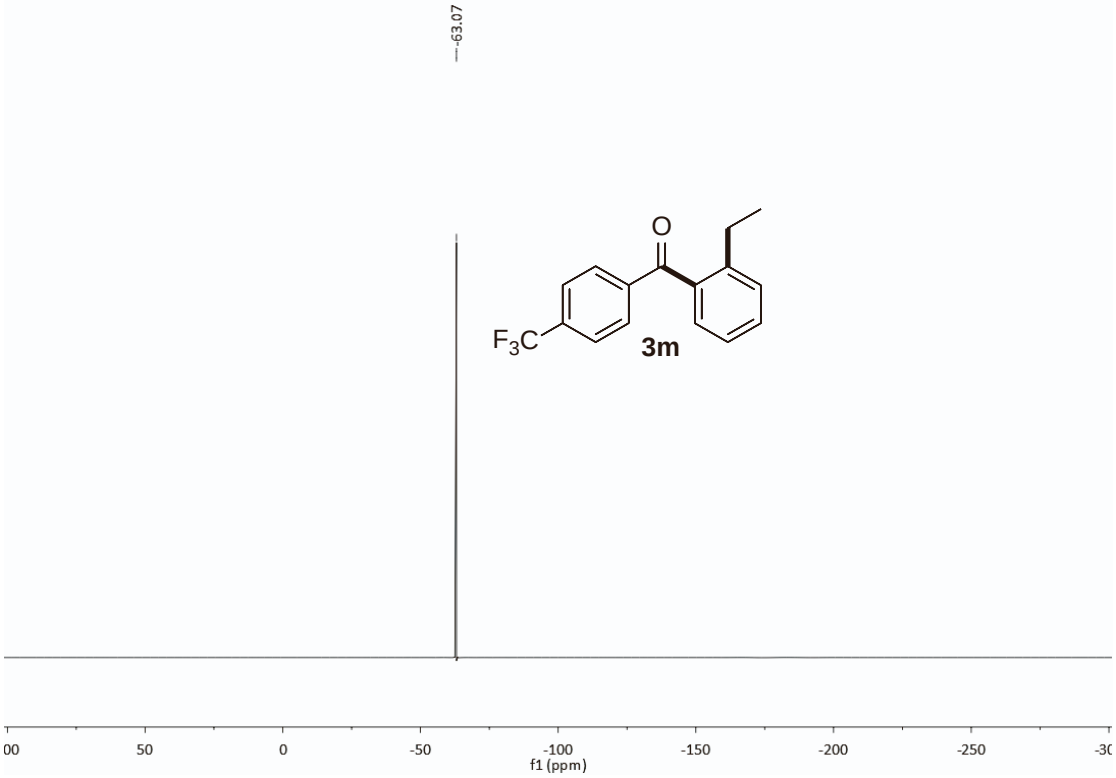
^{1}H NMR (400 MHz, $CDCl_3$)



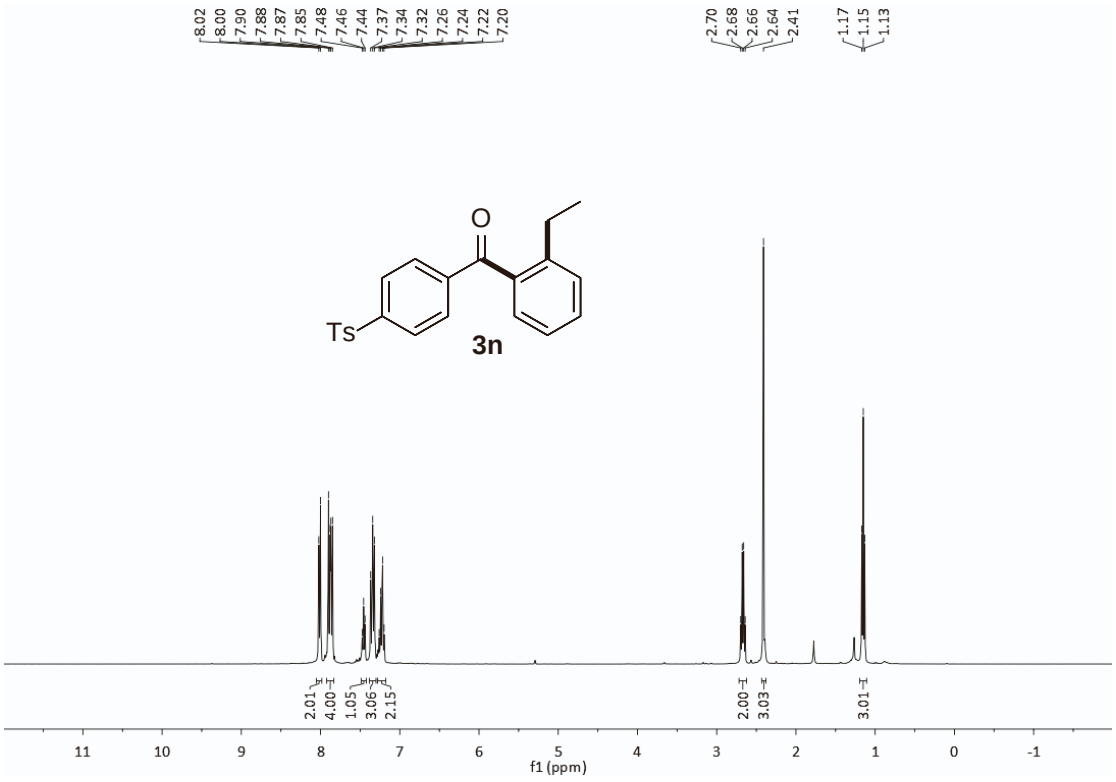
^{13}C NMR (151 MHz, $CDCl_3$)



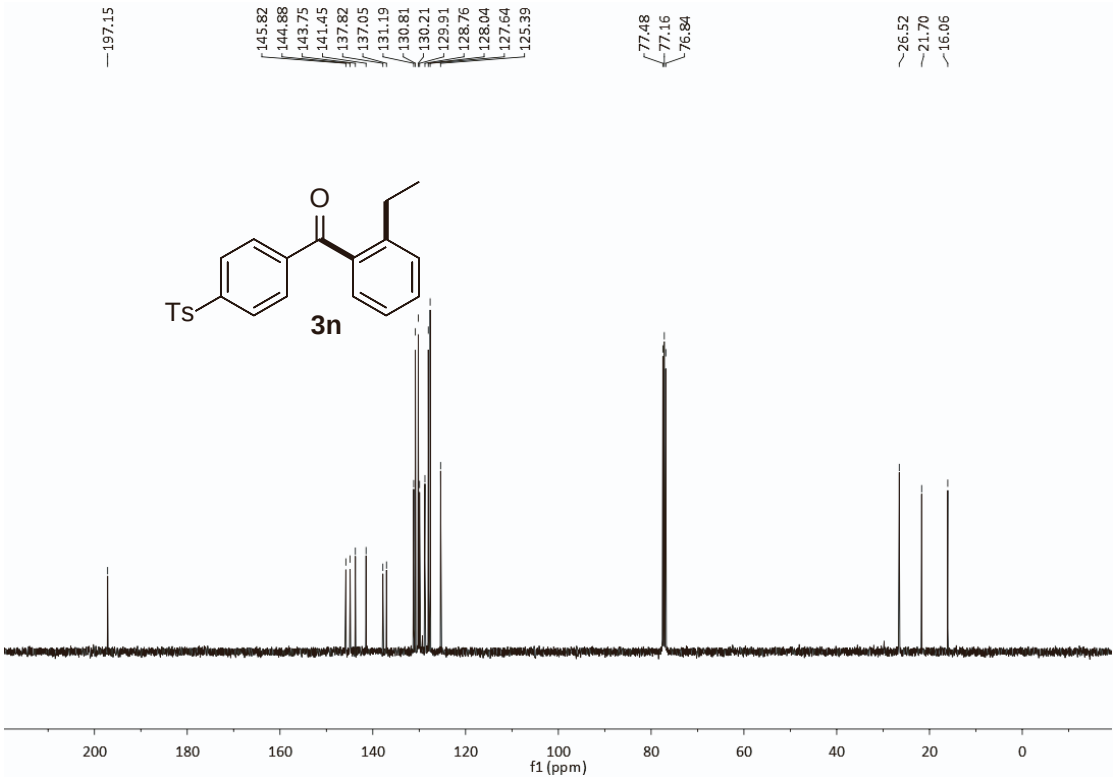
^{19}F NMR (565 MHz, $CDCl_3$)



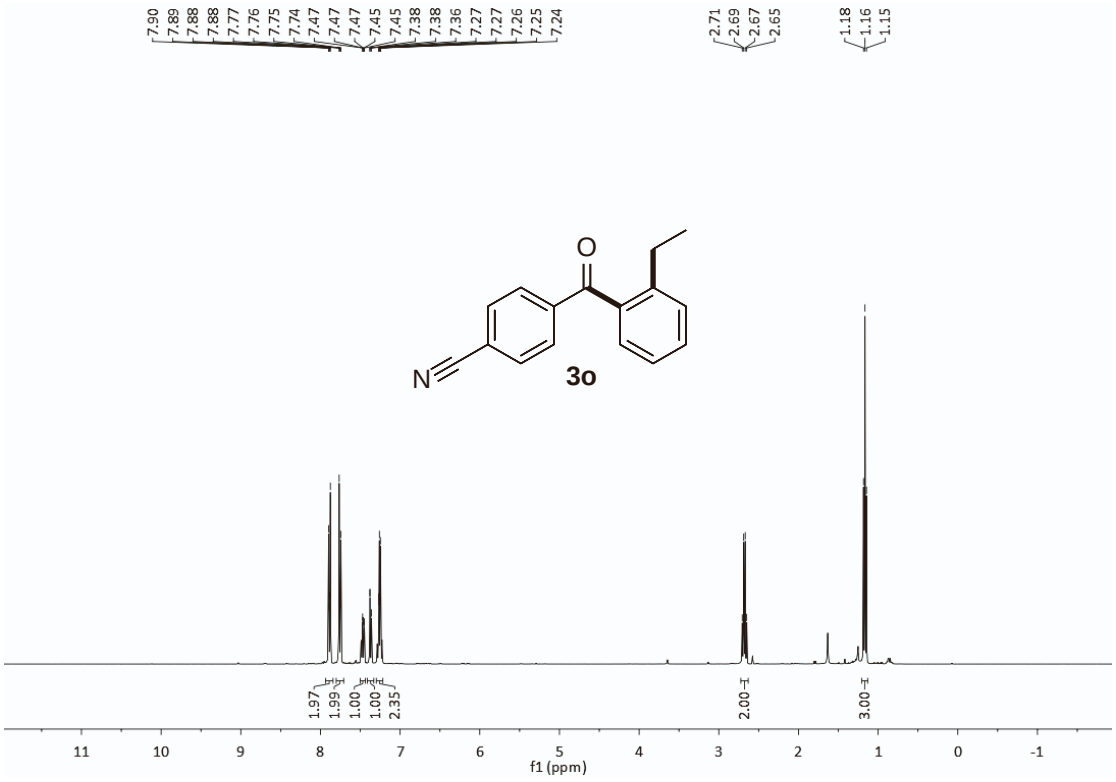
^{1}H NMR (400 MHz, $CDCl_3$)



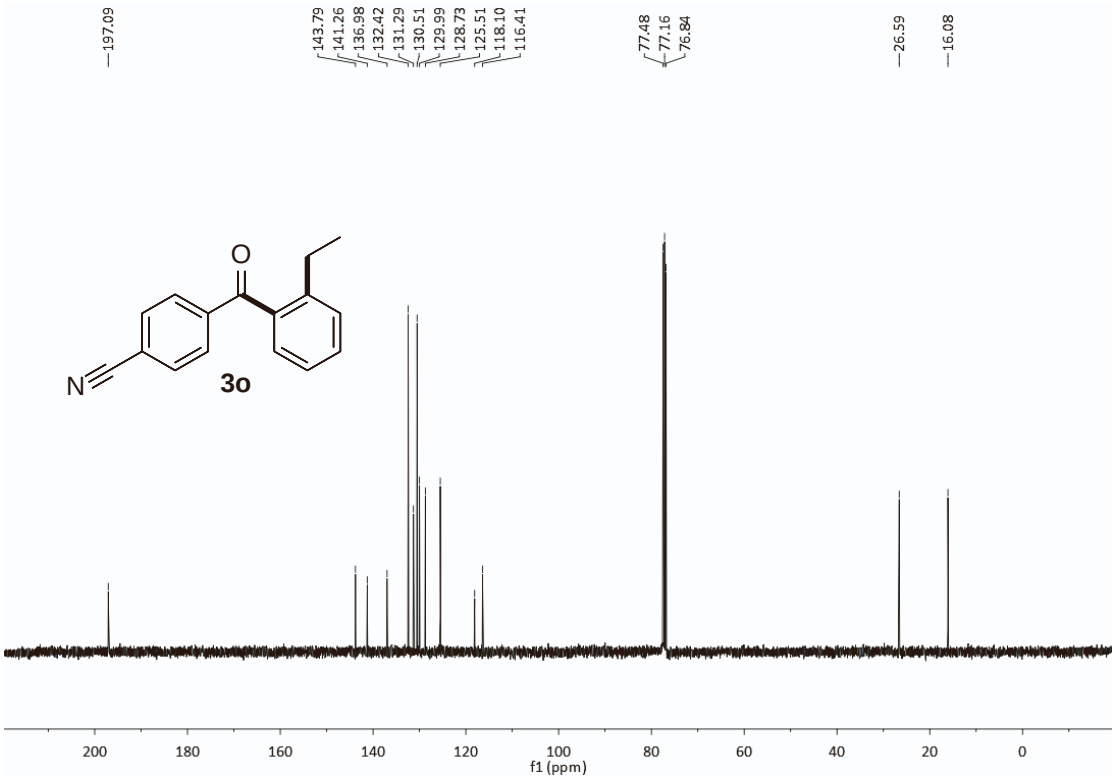
^{13}C NMR (101 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)



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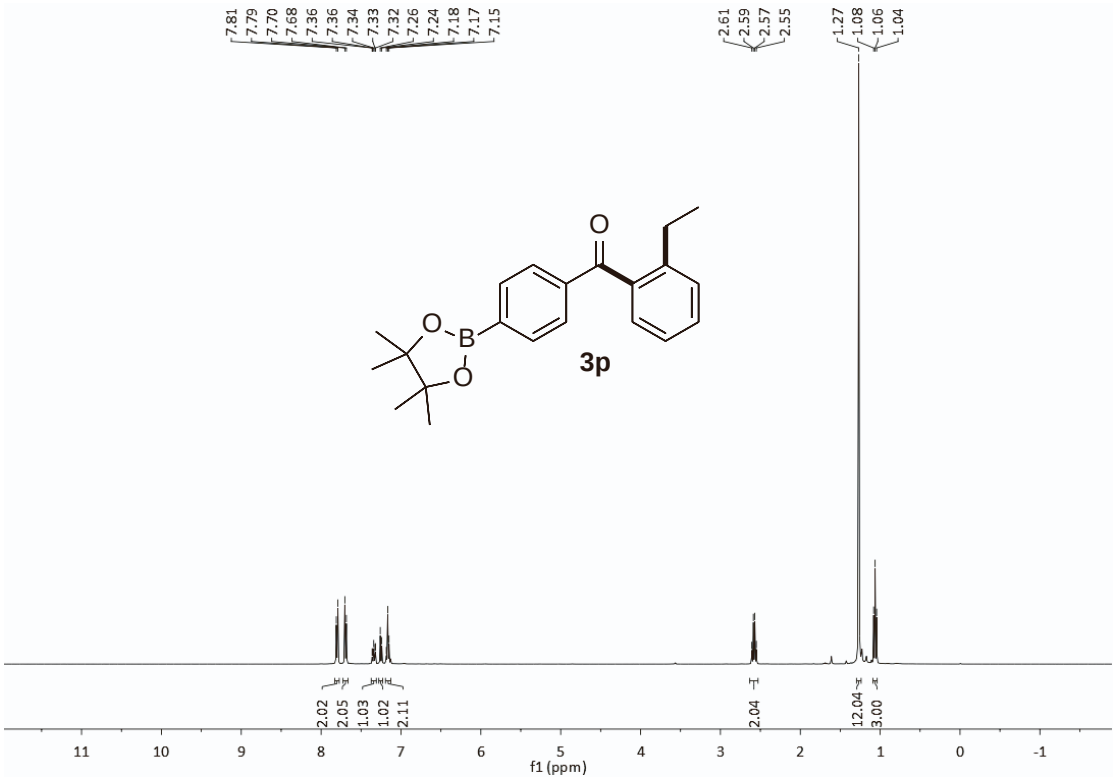
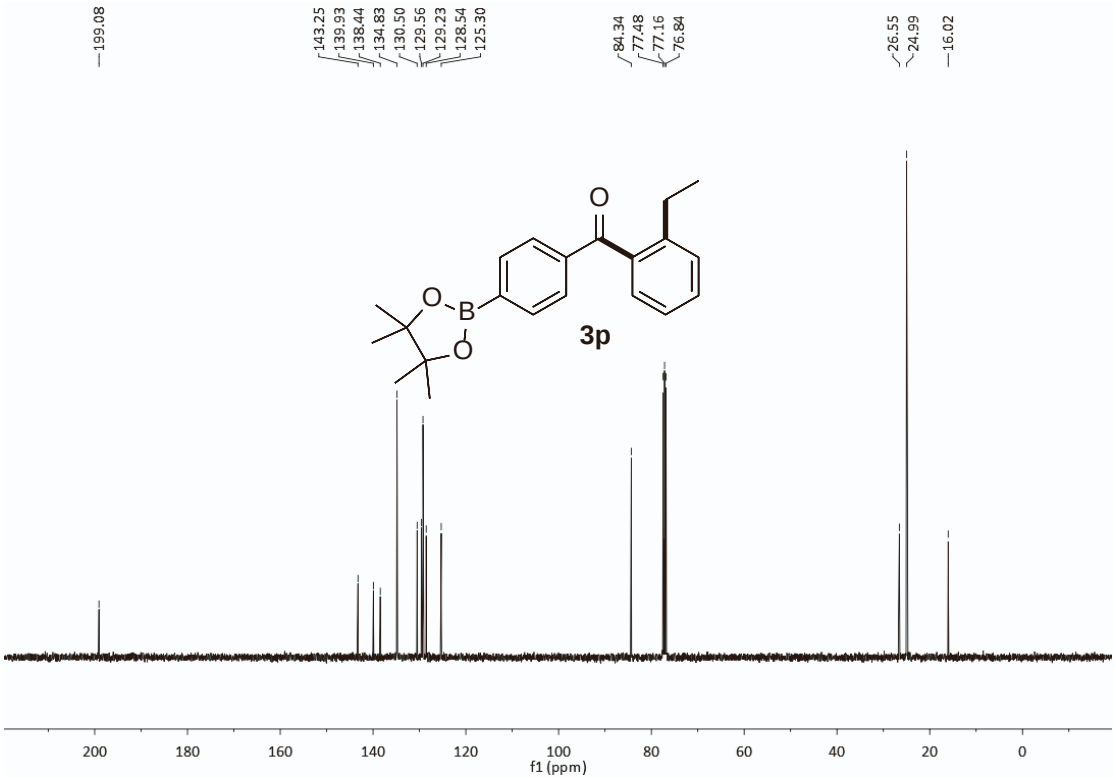
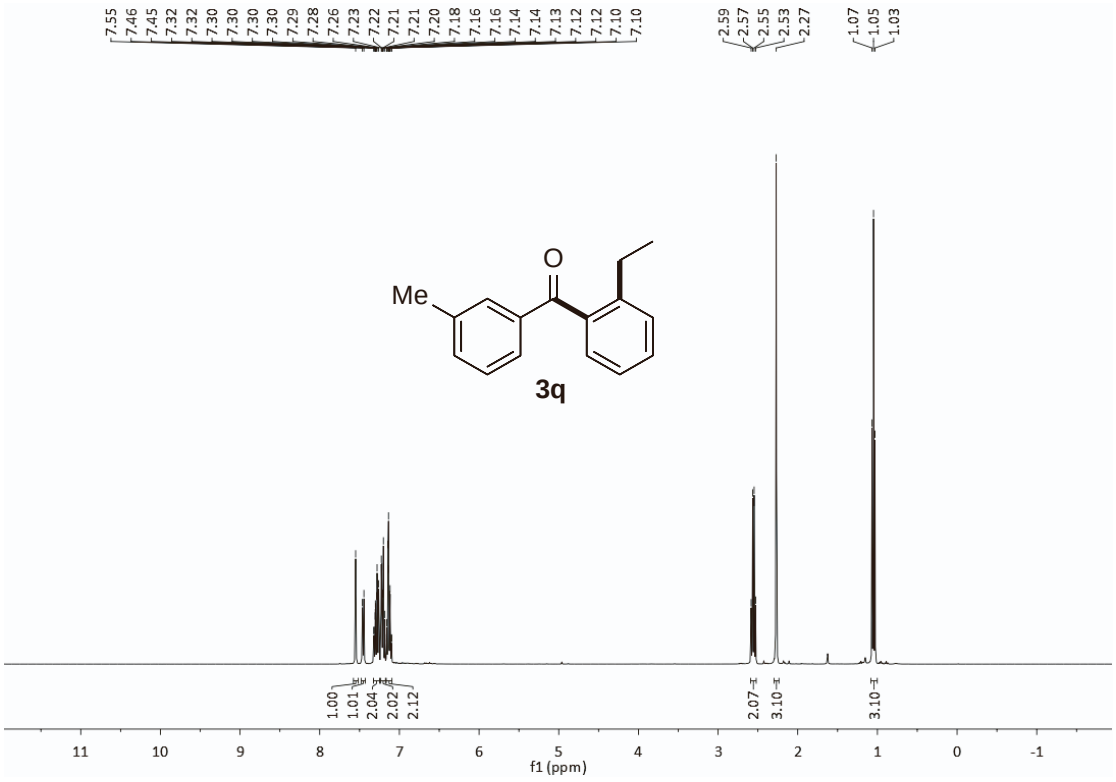


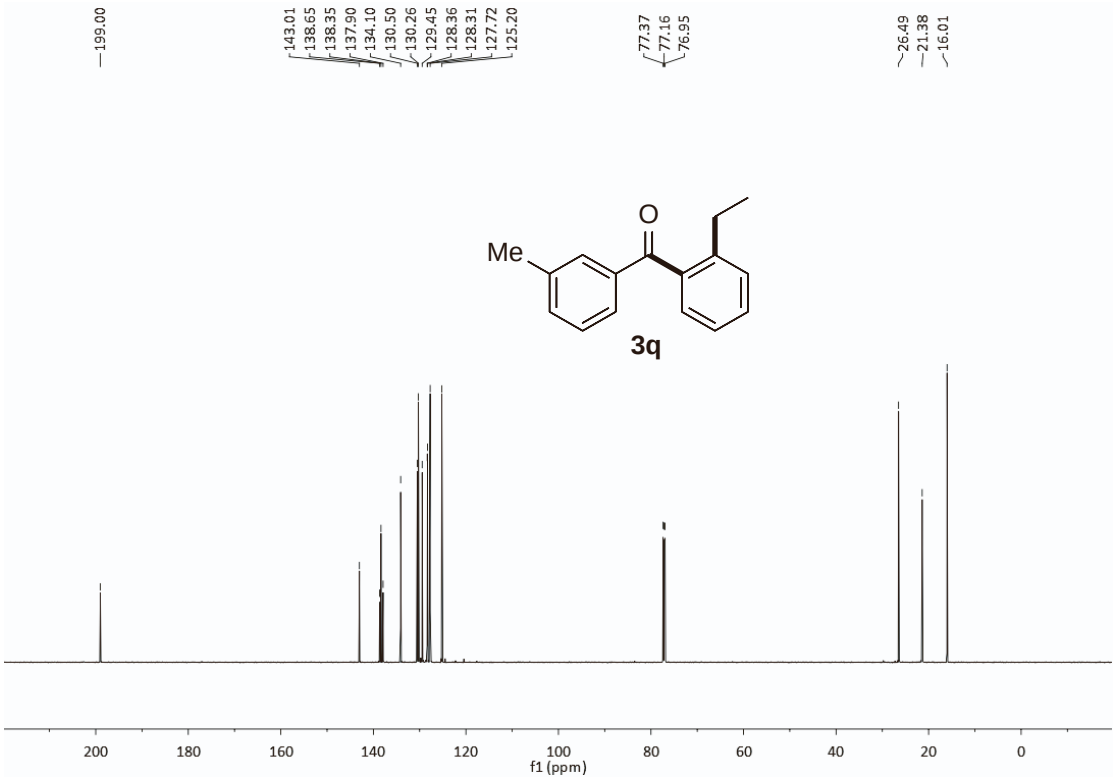
^{13}C NMR (101 MHz, $CDCl_3$)



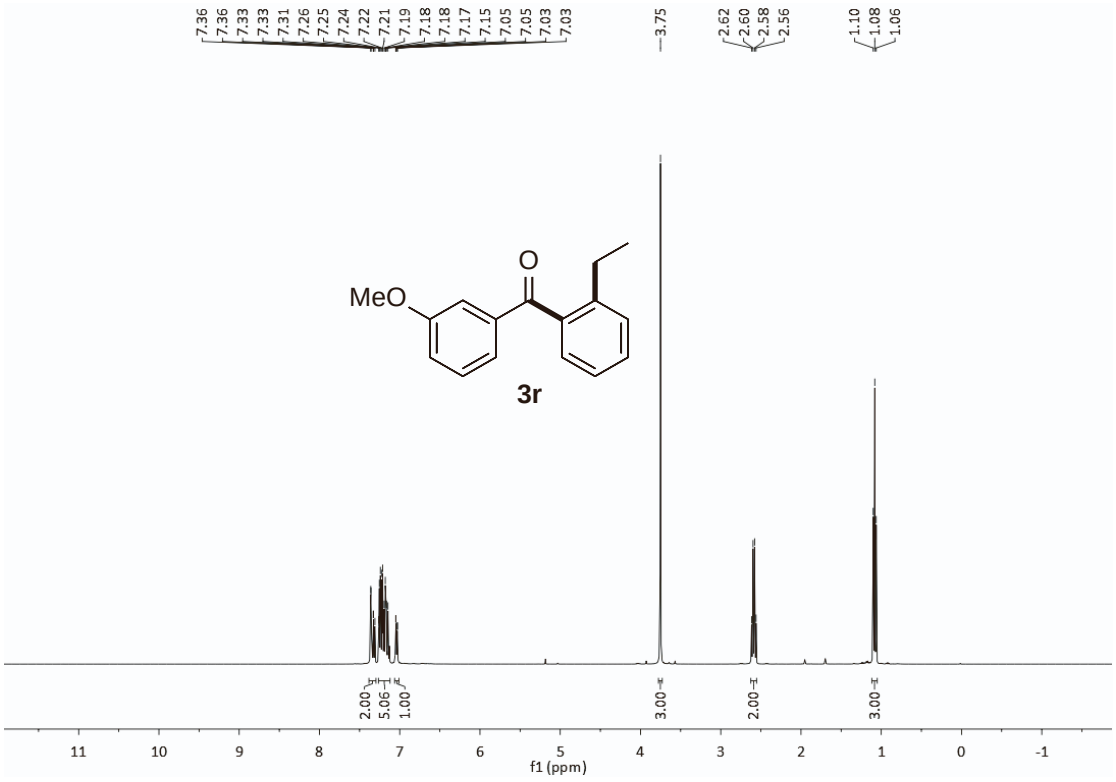
^{1}H NMR (400 MHz, $CDCl_3$)



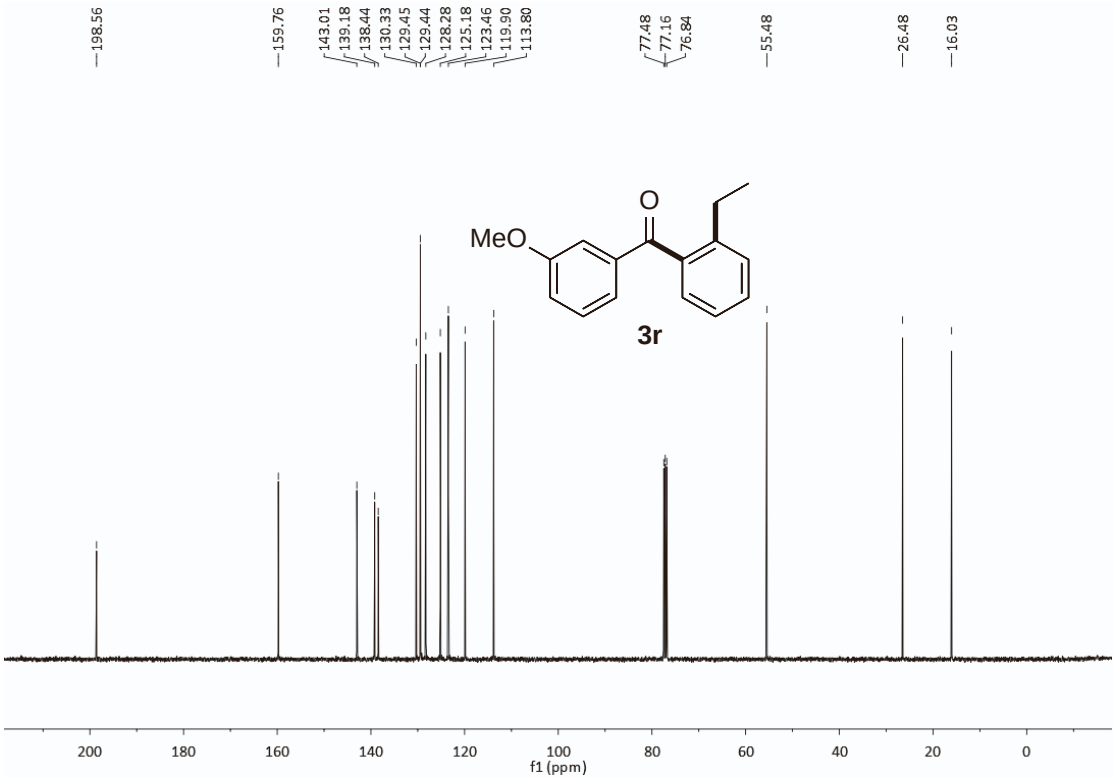
^{13}C NMR (151 MHz, $CDCl_3$)



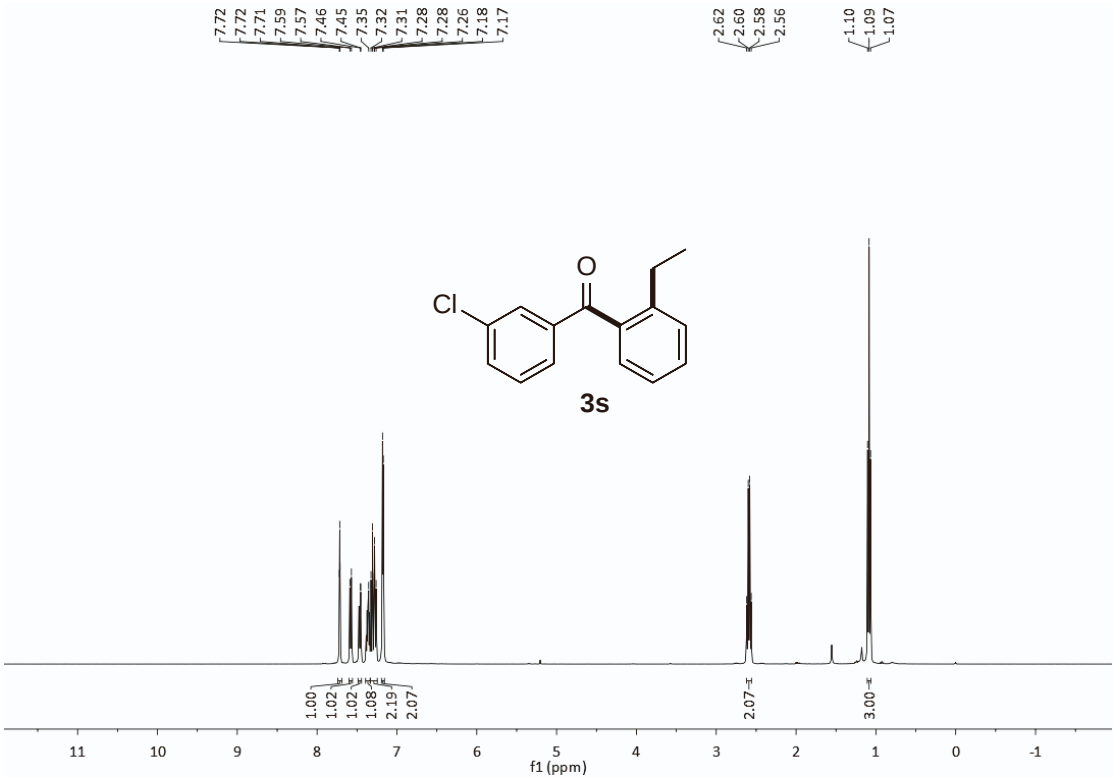
^{1}H NMR (400 MHz, $CDCl_3$)



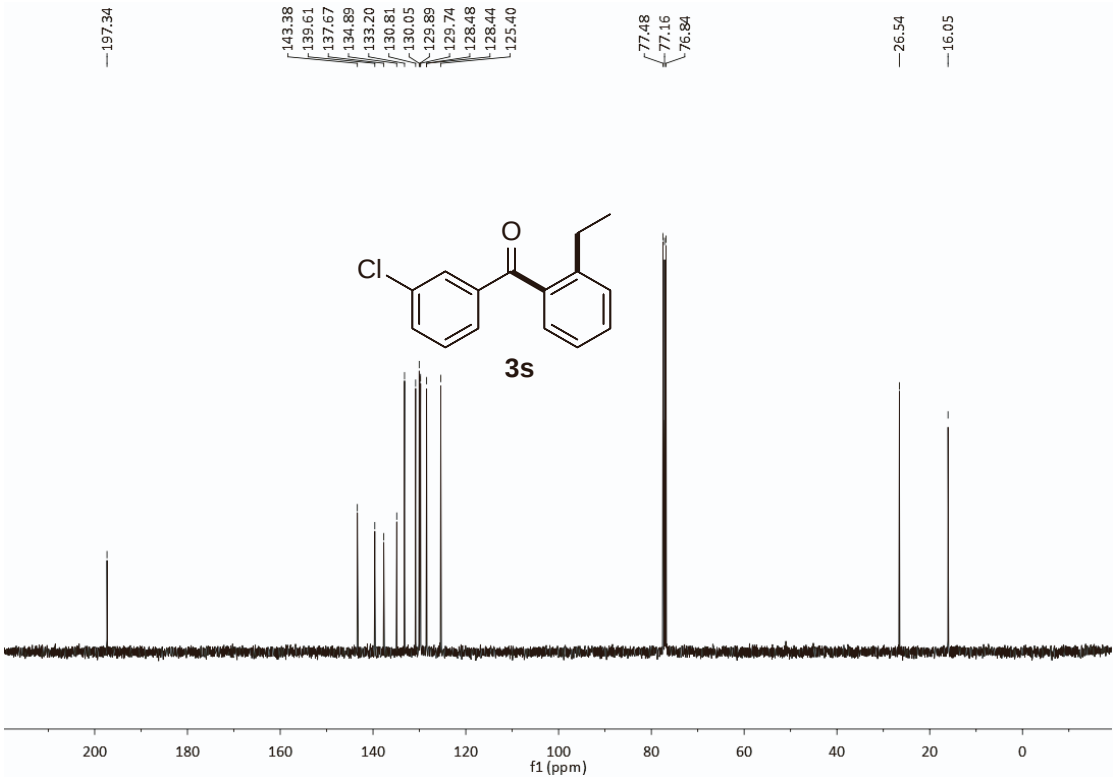
^{13}C NMR (101 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)



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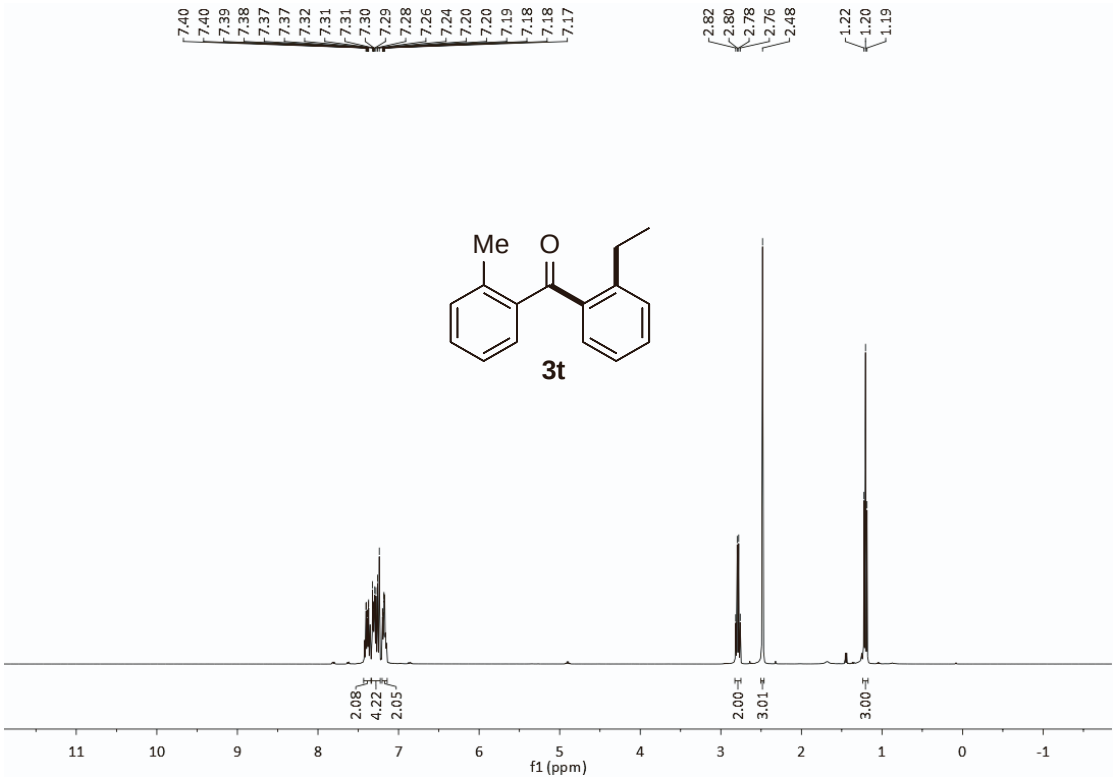
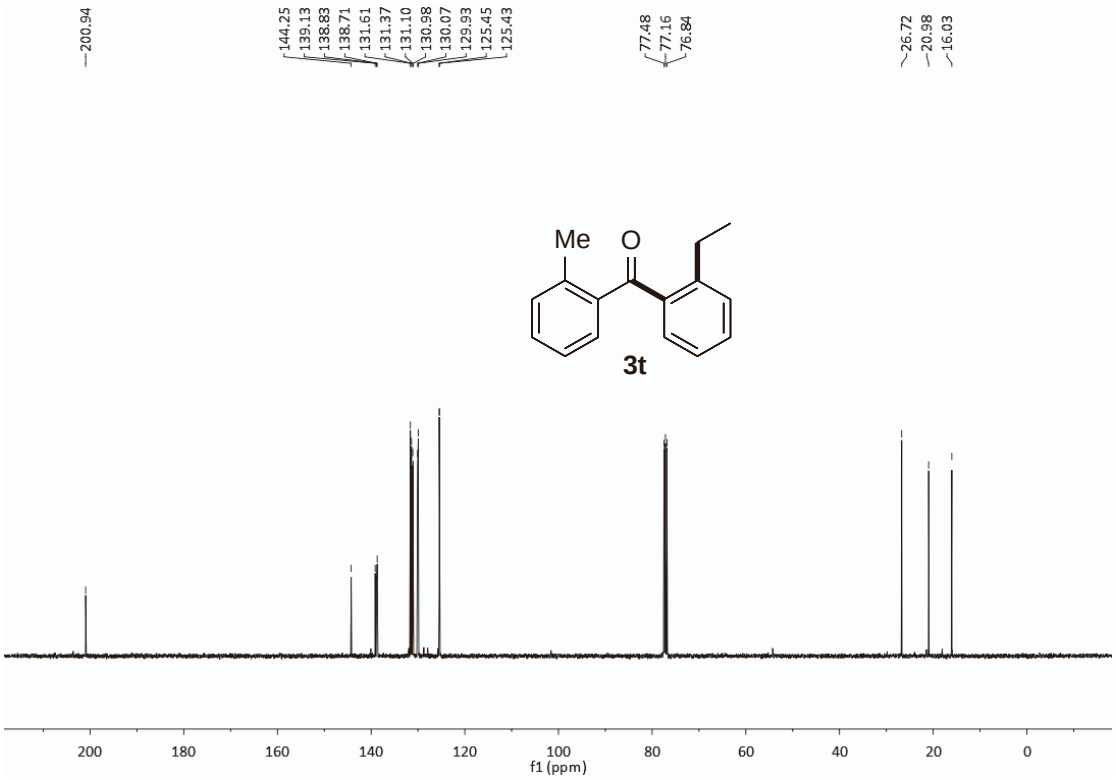
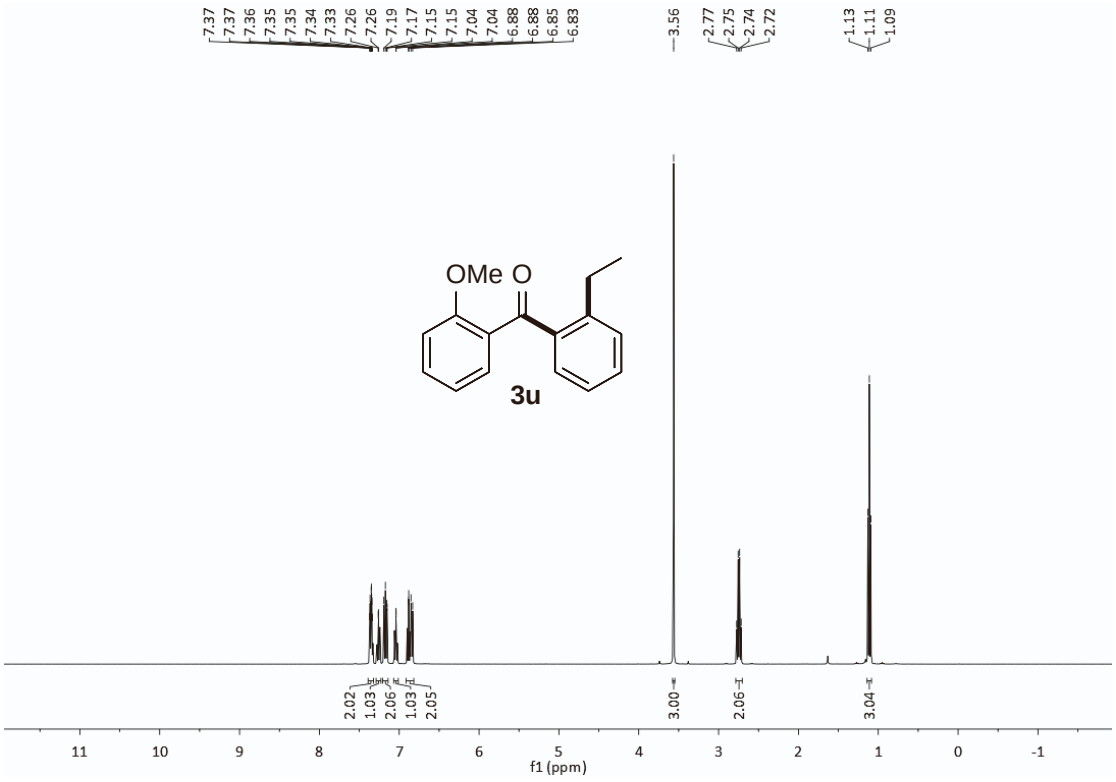


^{13}C NMR (101 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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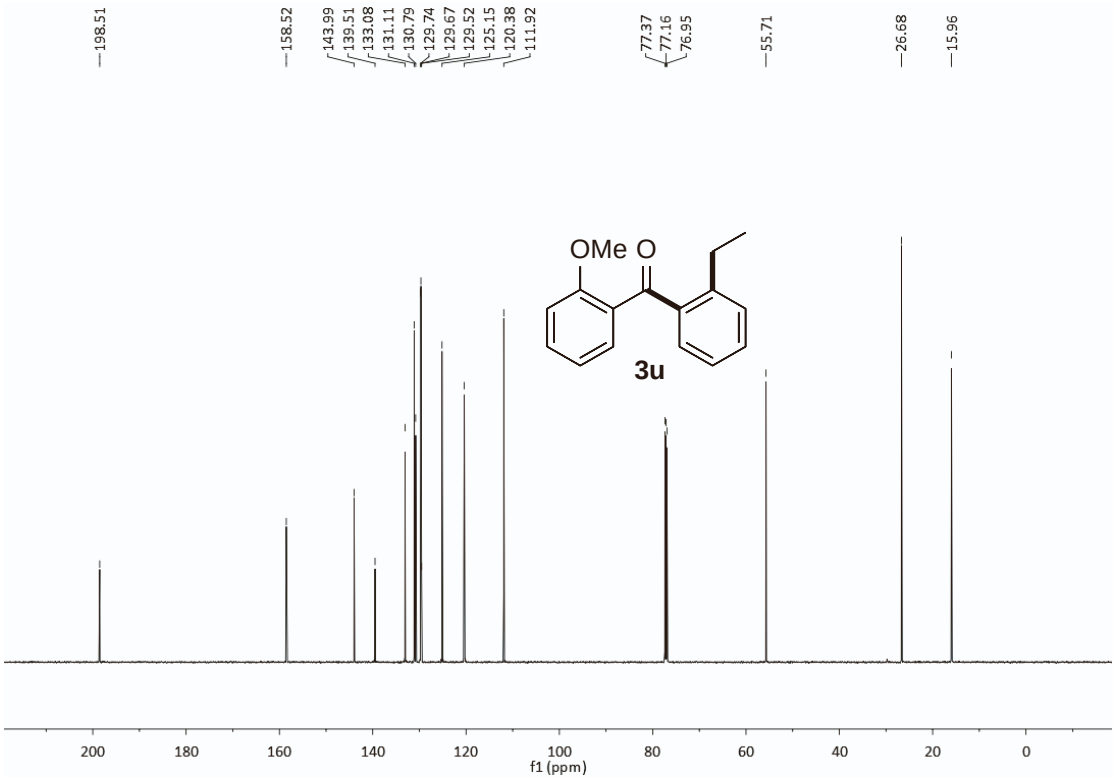
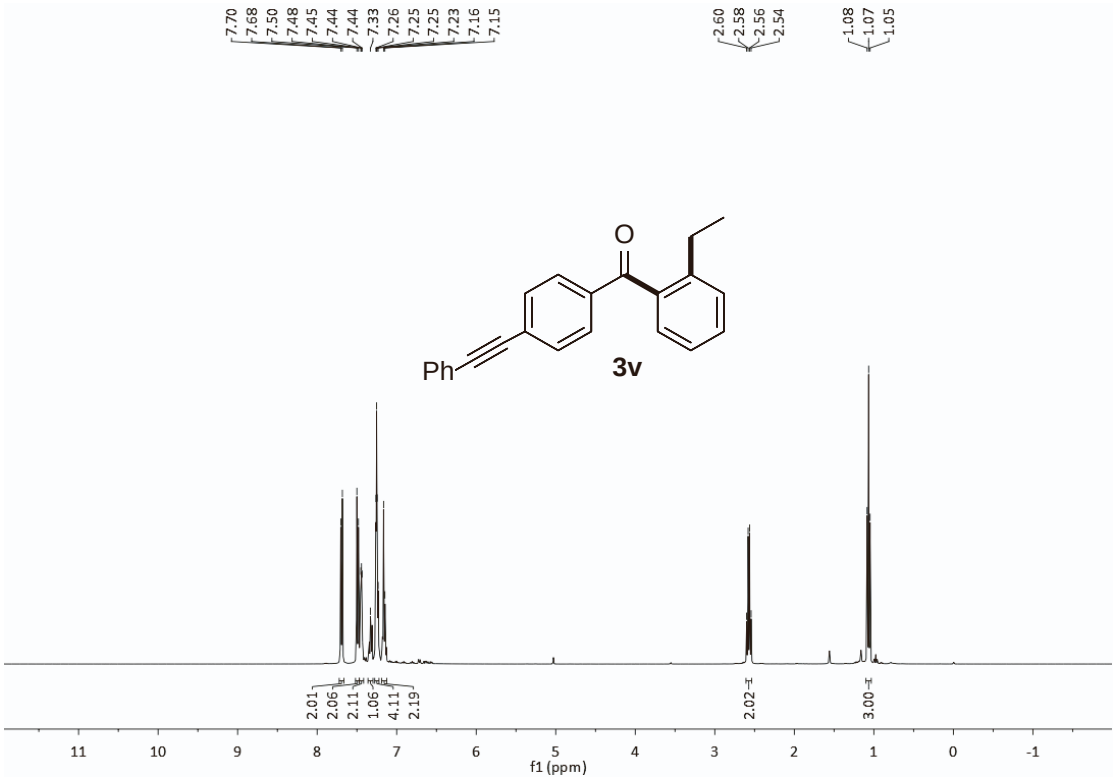
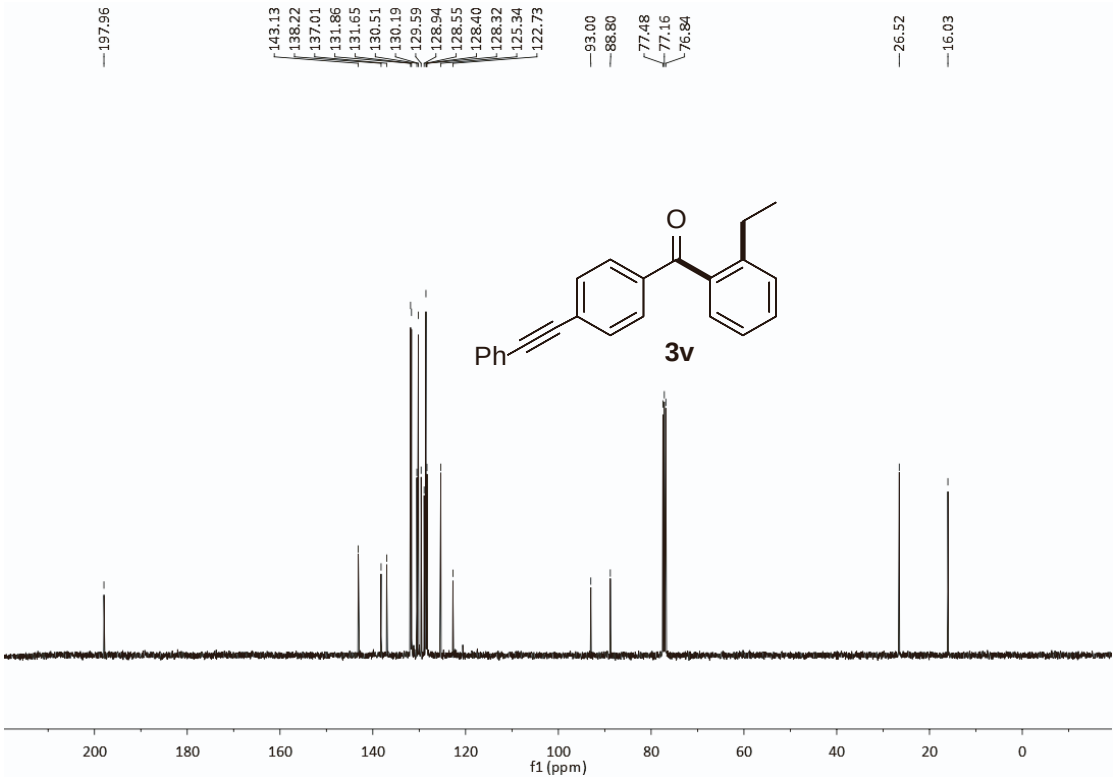


^{1}H NMR (400 MHz, $CDCl_3$)

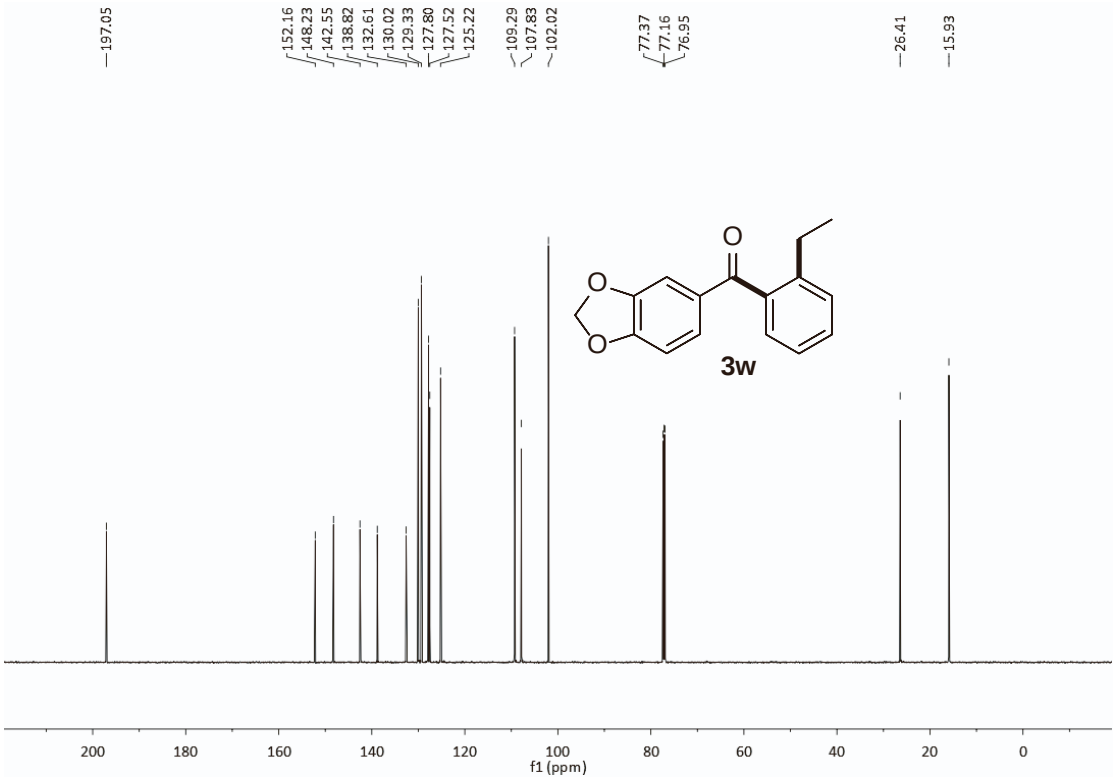


^{13}C NMR (101 MHz, $CDCl_3$)

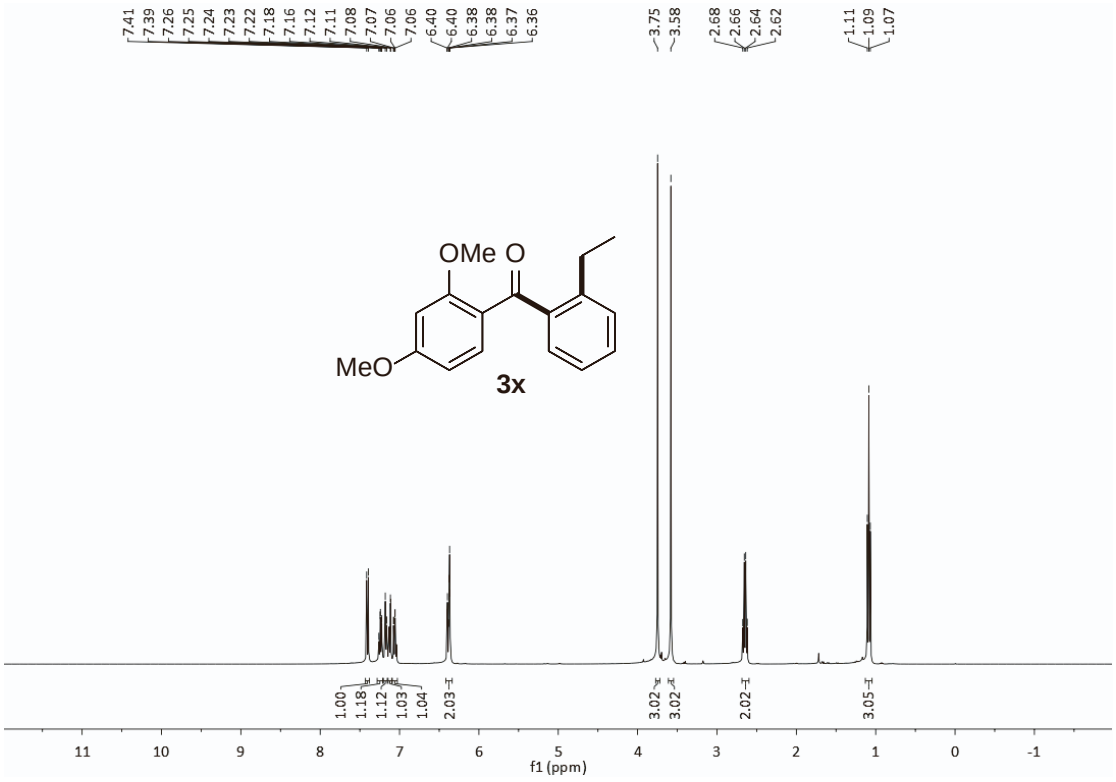


^{1}H NMR (400 MHz, $CDCl_3$)

^{13}C NMR (151 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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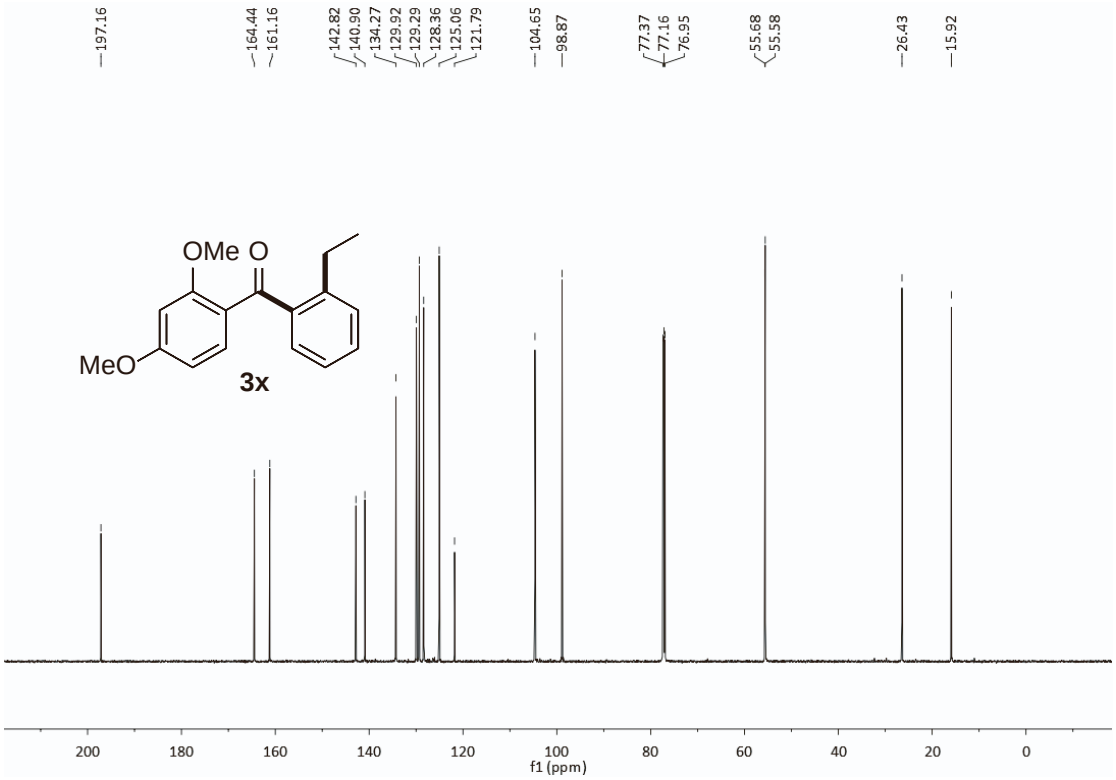

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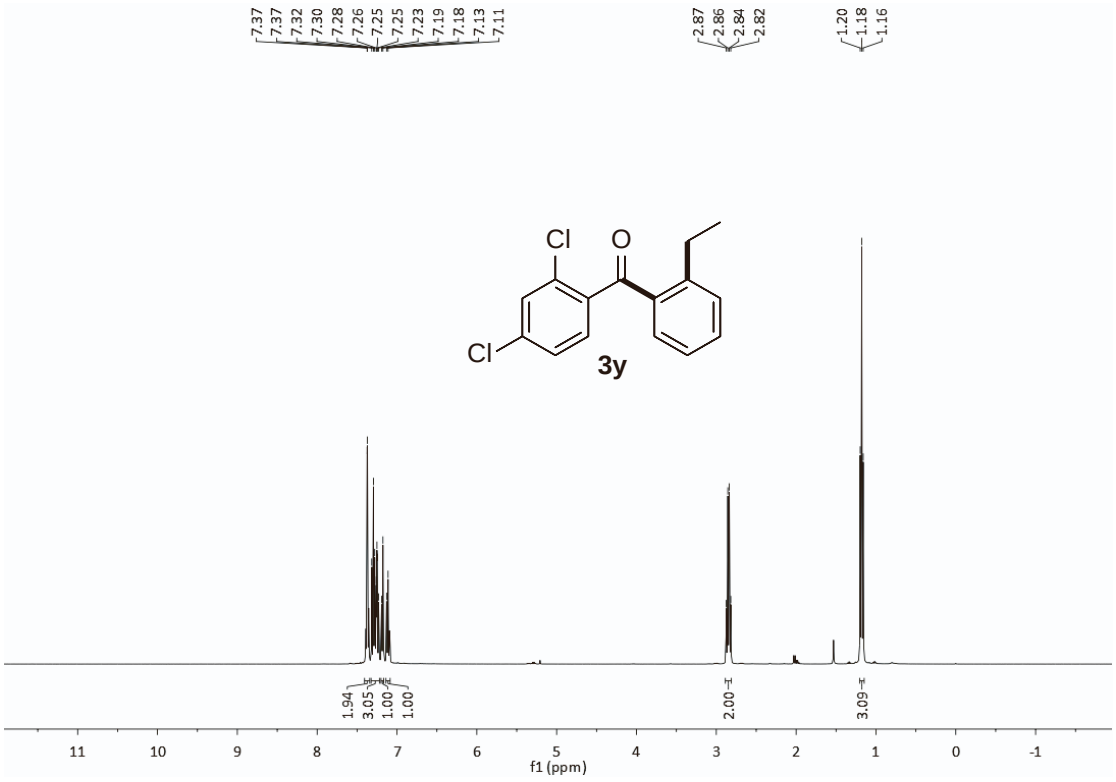

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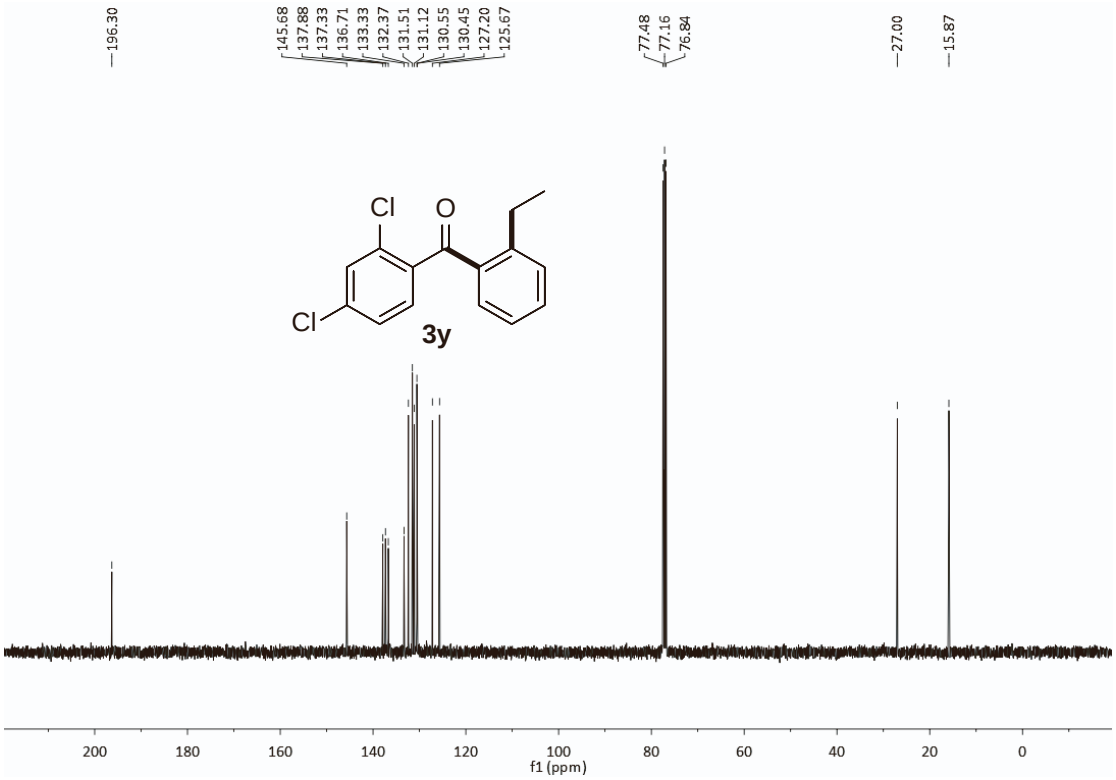

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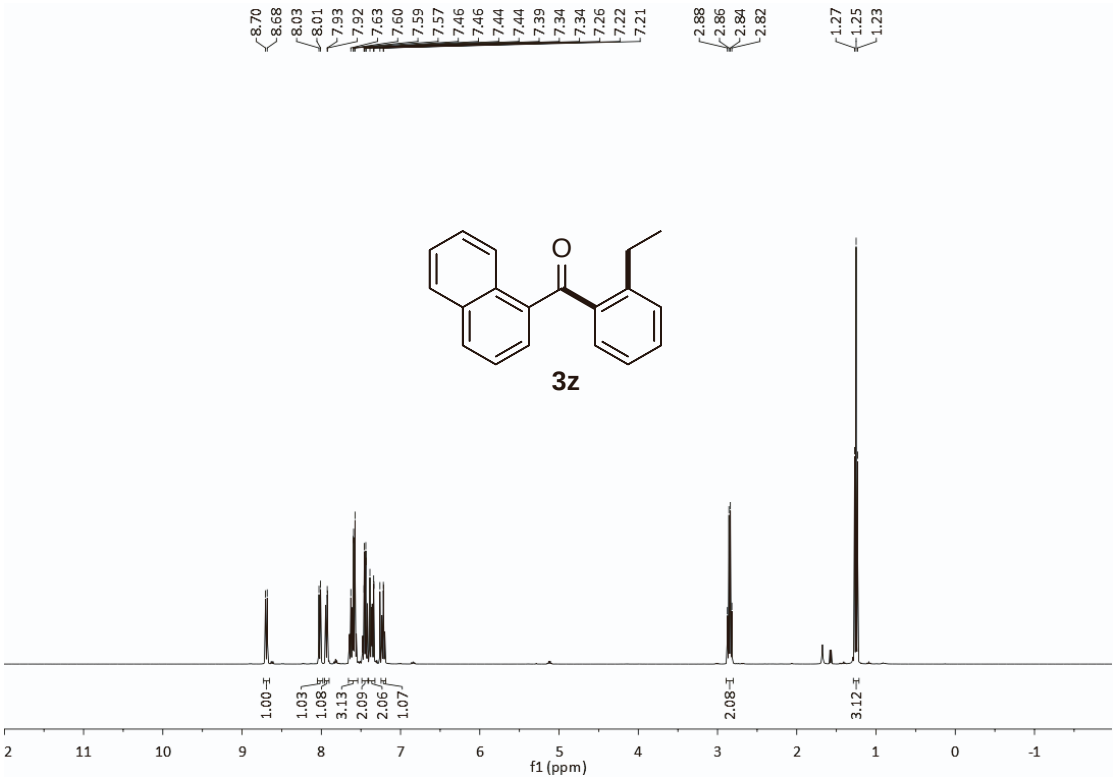

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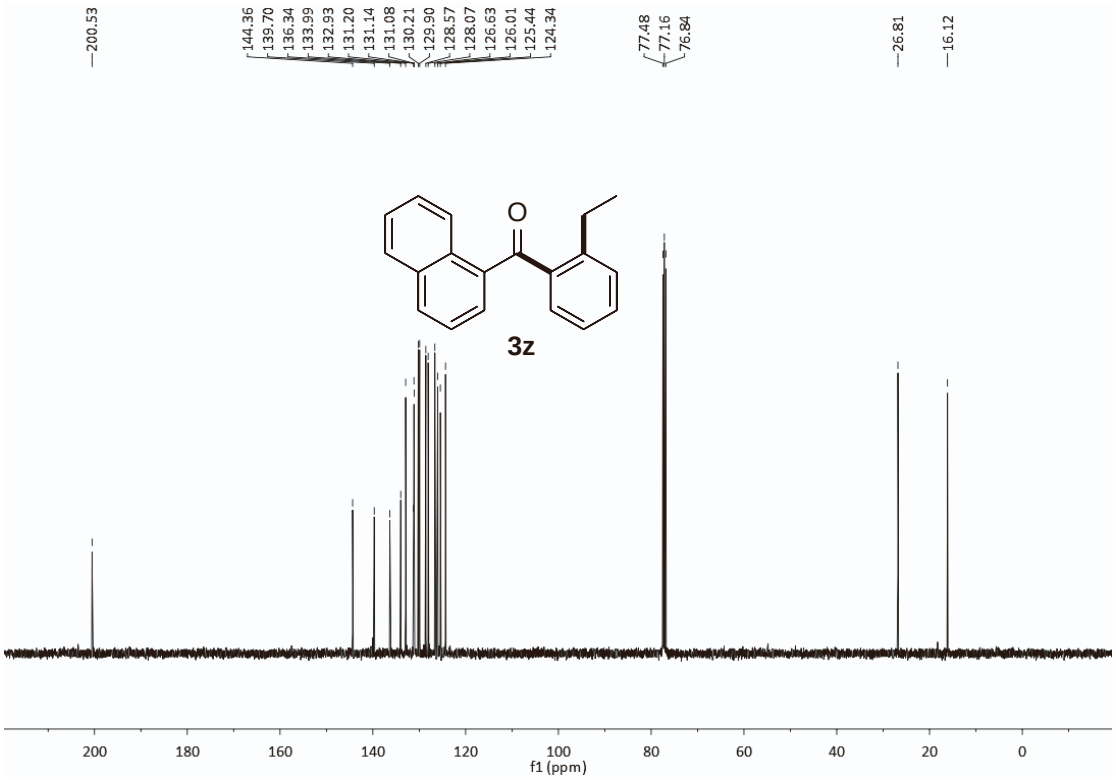

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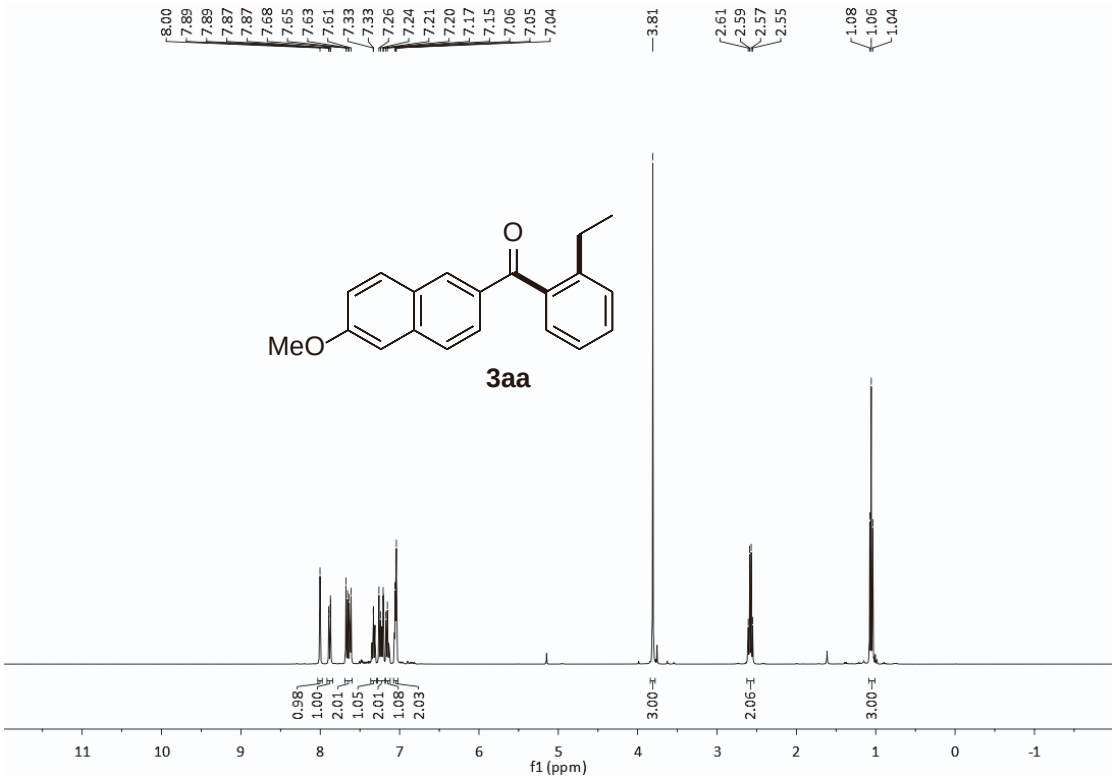
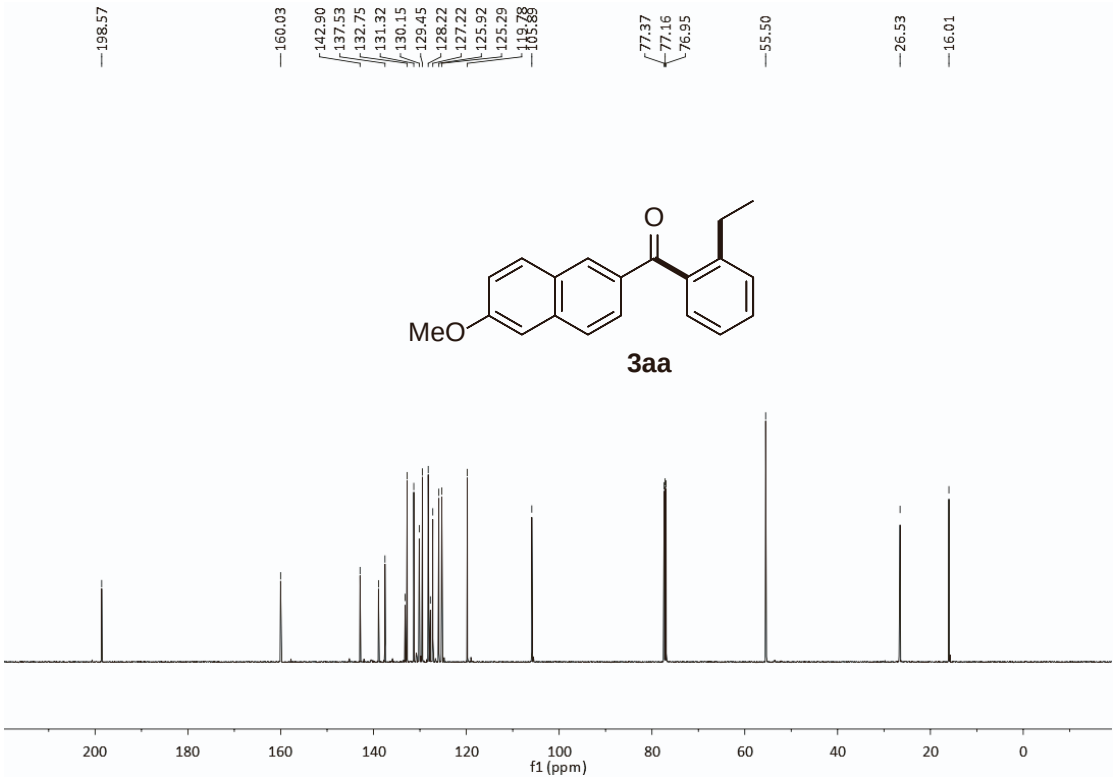


^{13}C NMR (151 MHz, $CDCl_3$)



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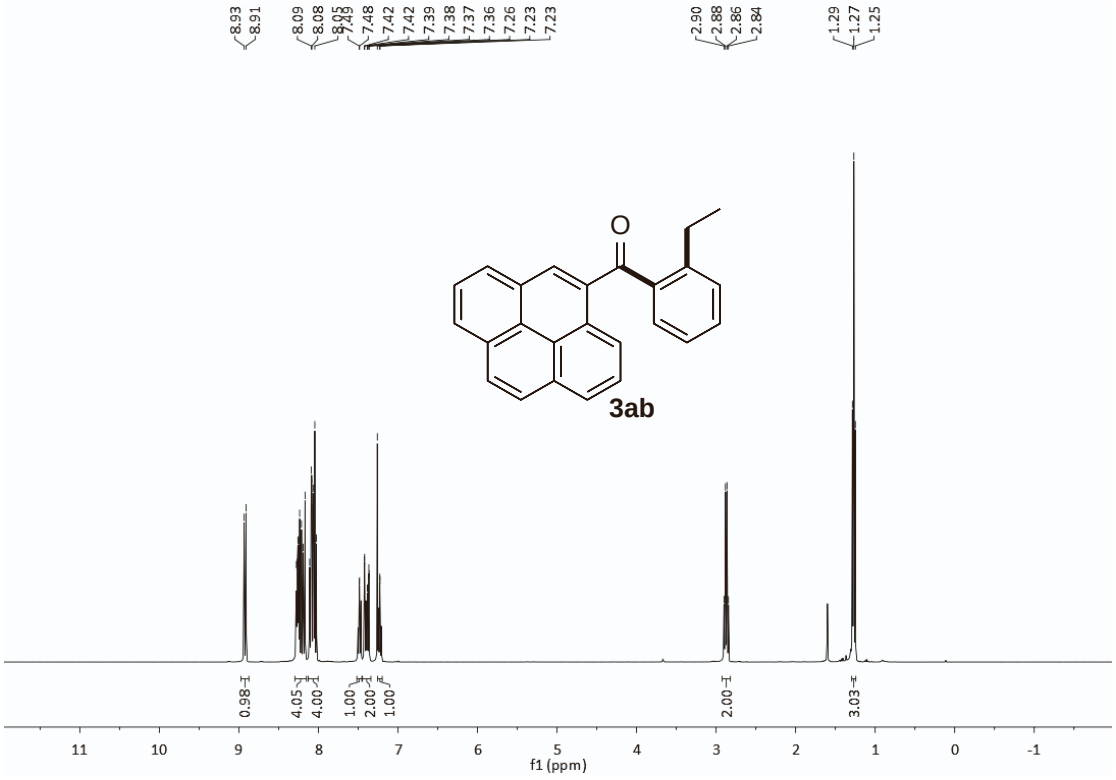
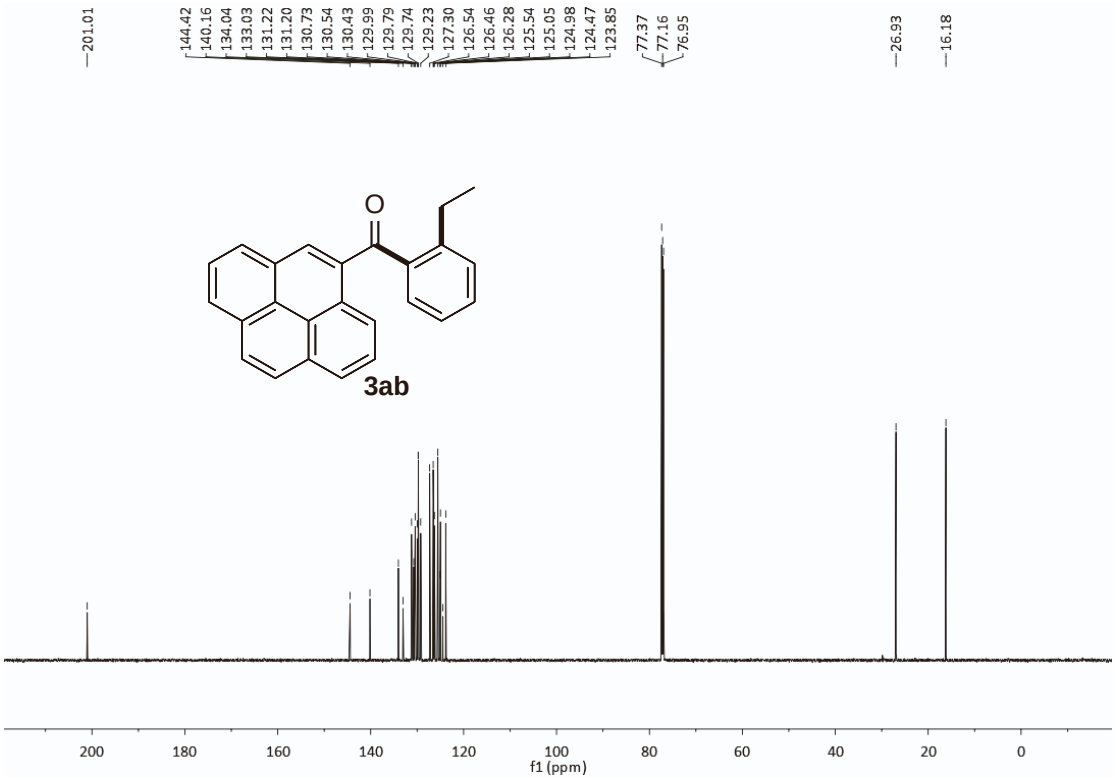


^{13}C NMR (151 MHz, $CDCl_3$)



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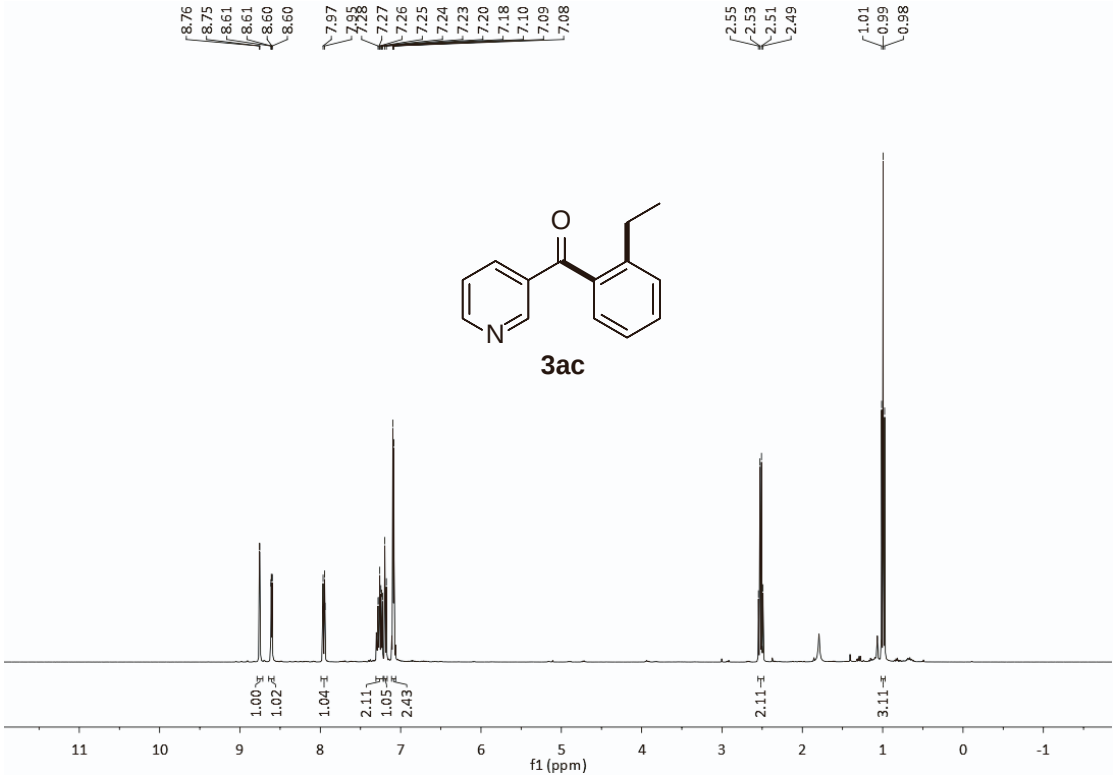
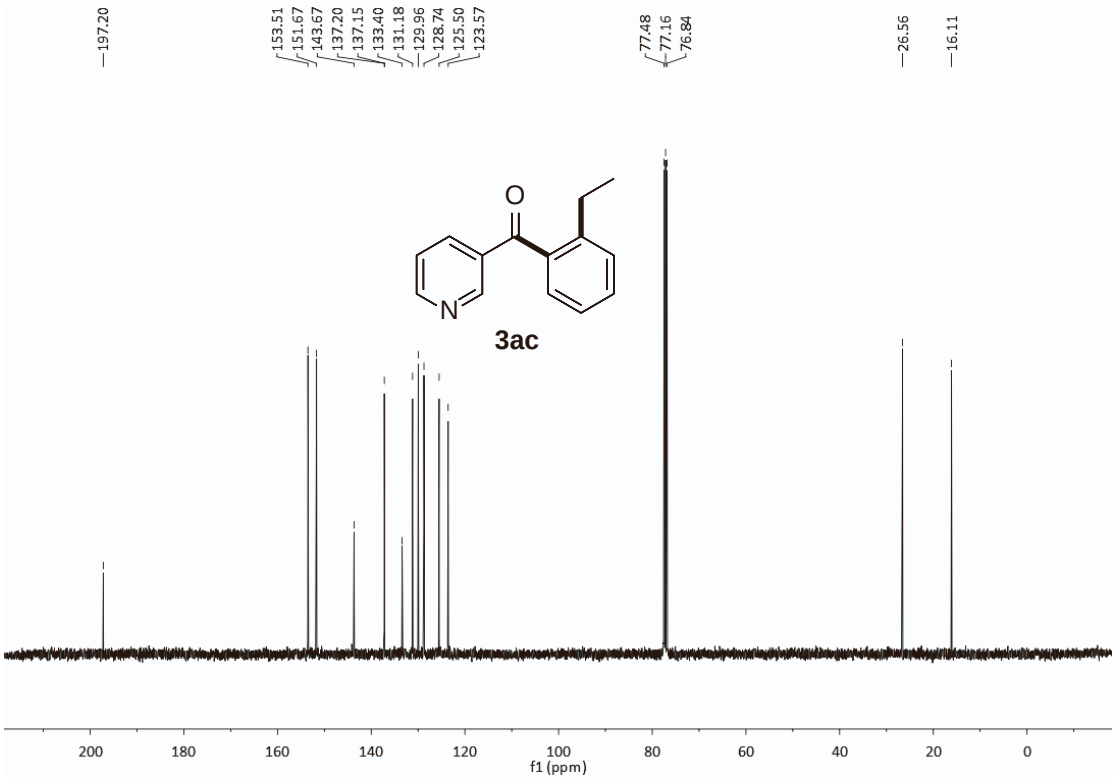


^{13}C NMR (101 MHz, $CDCl_3$)



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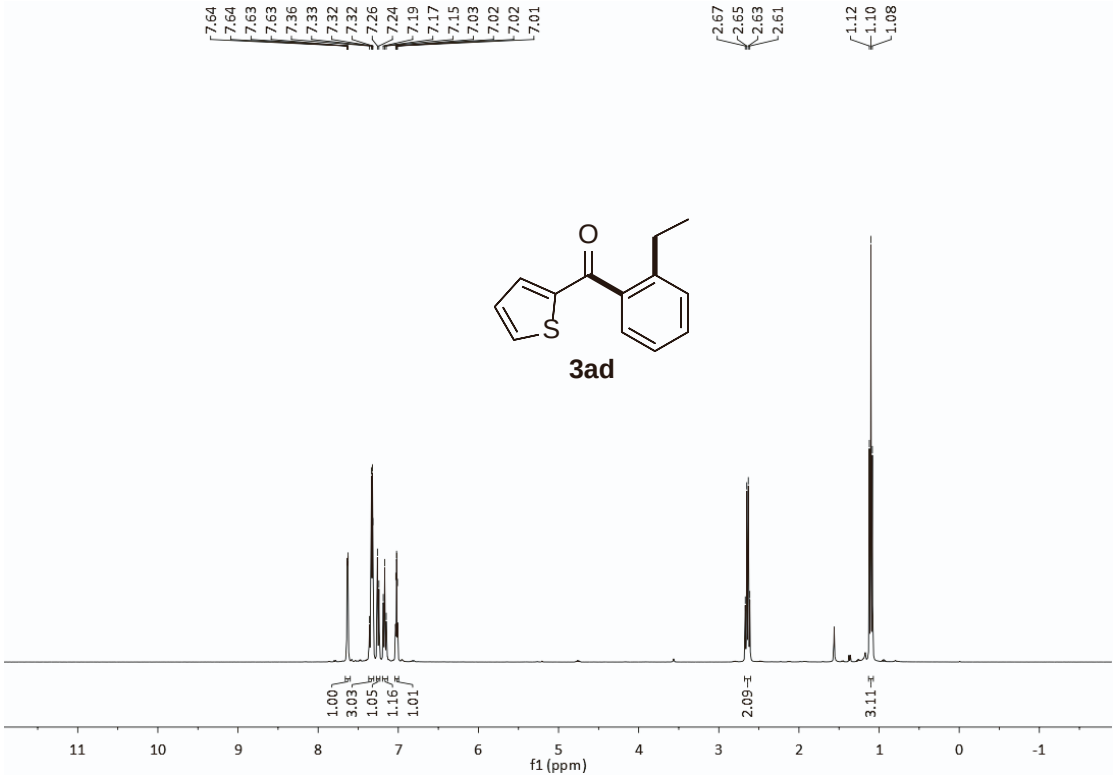
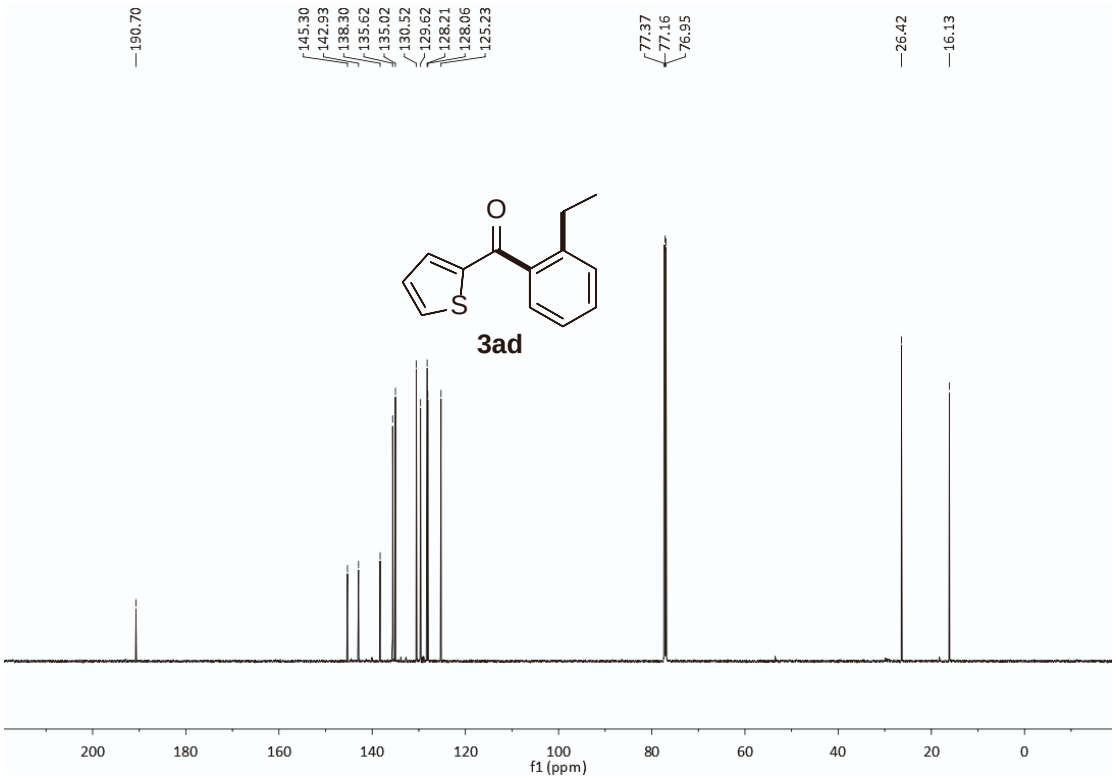
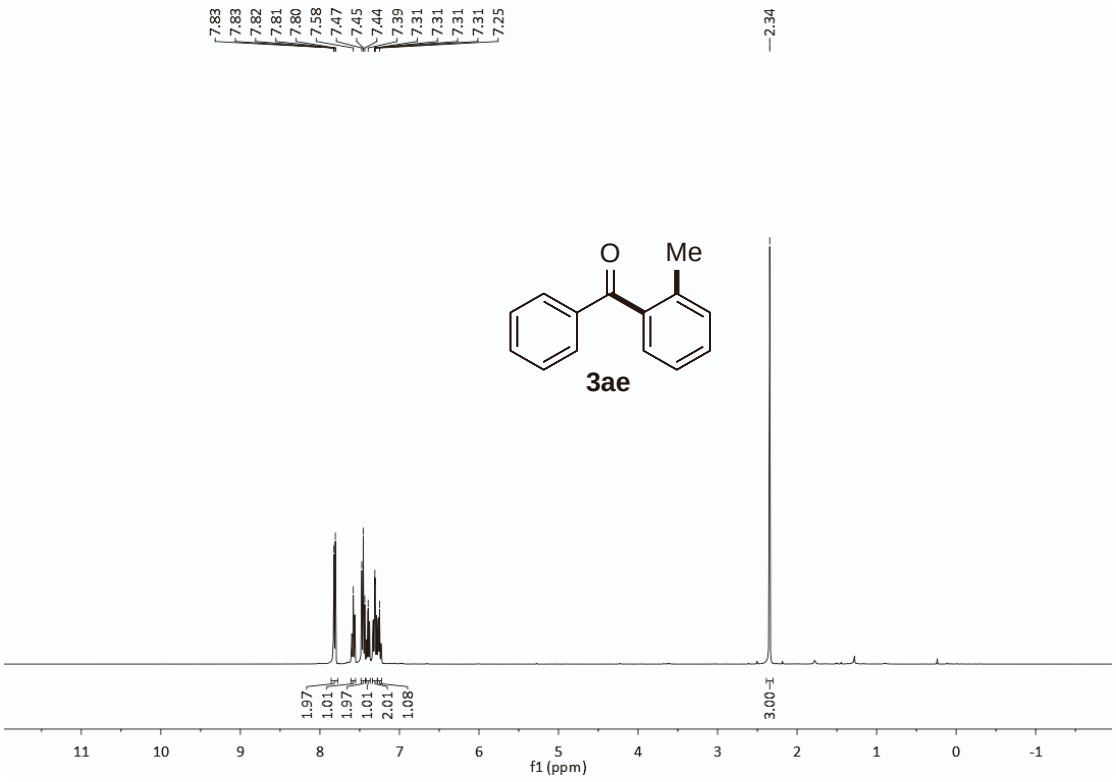


^{13}C NMR (151 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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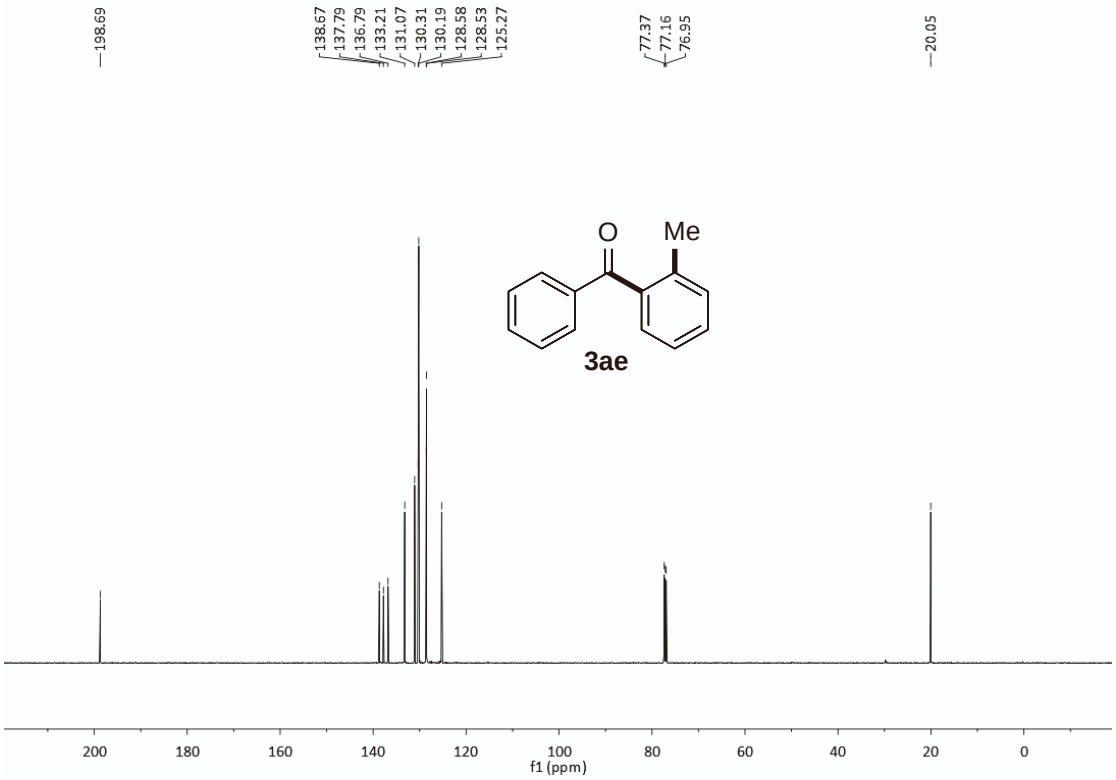

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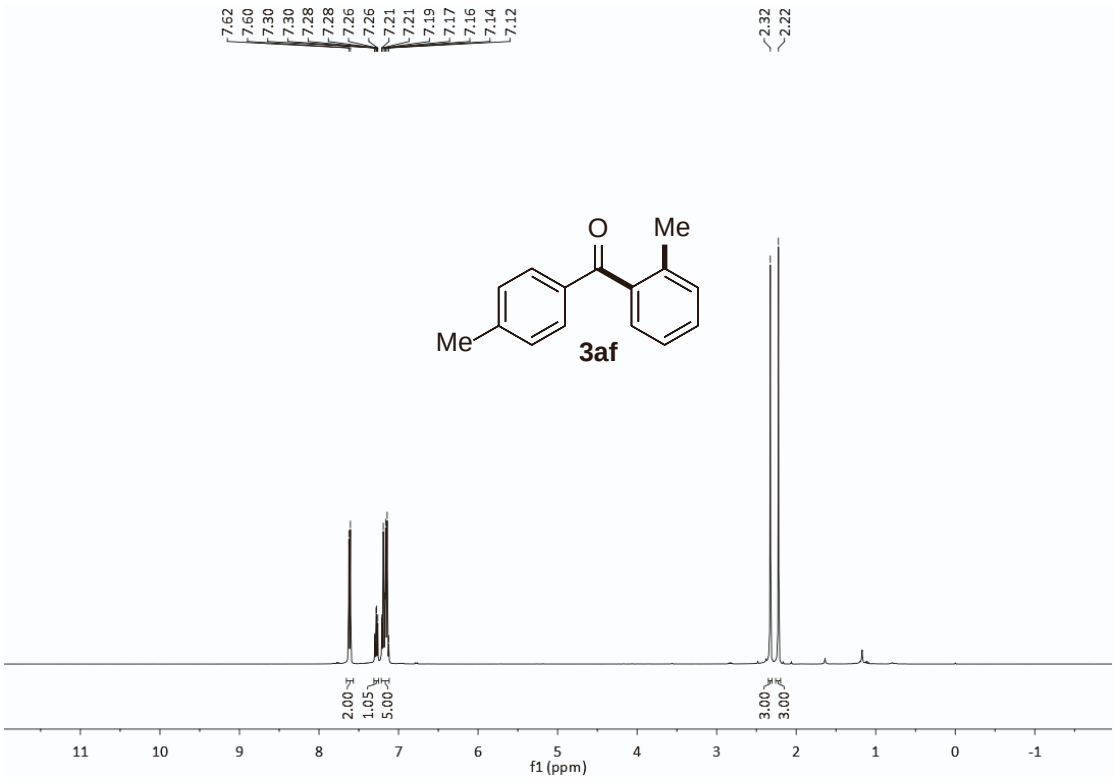

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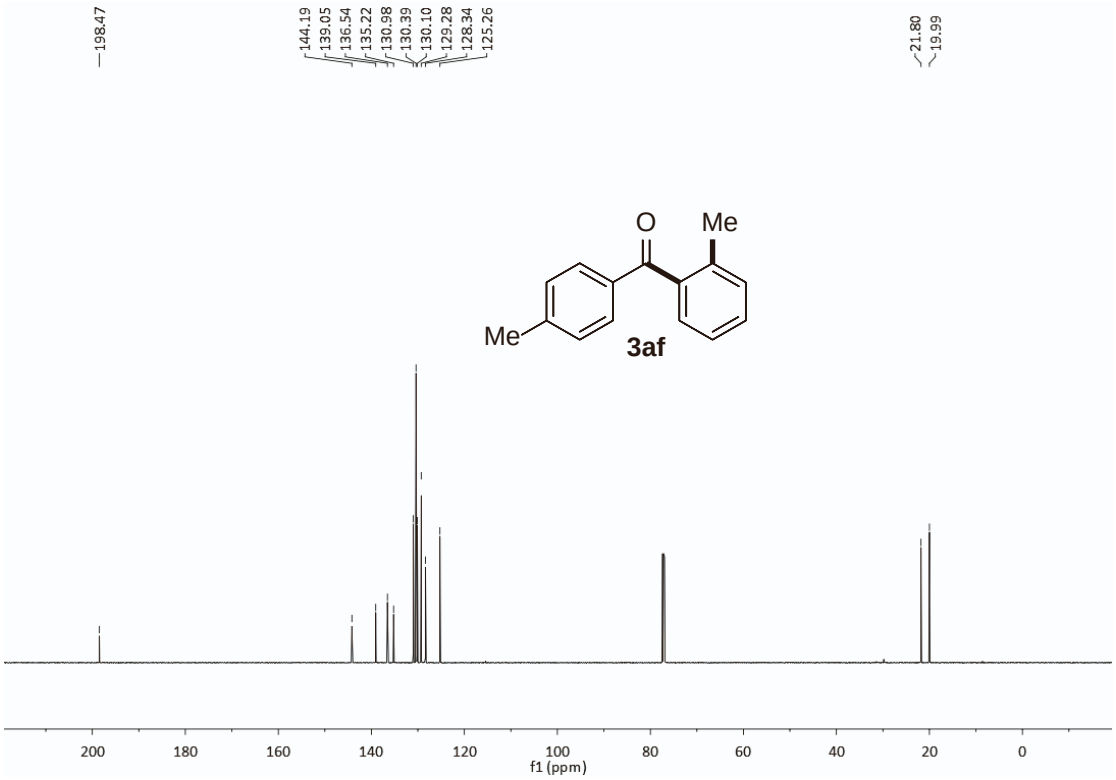
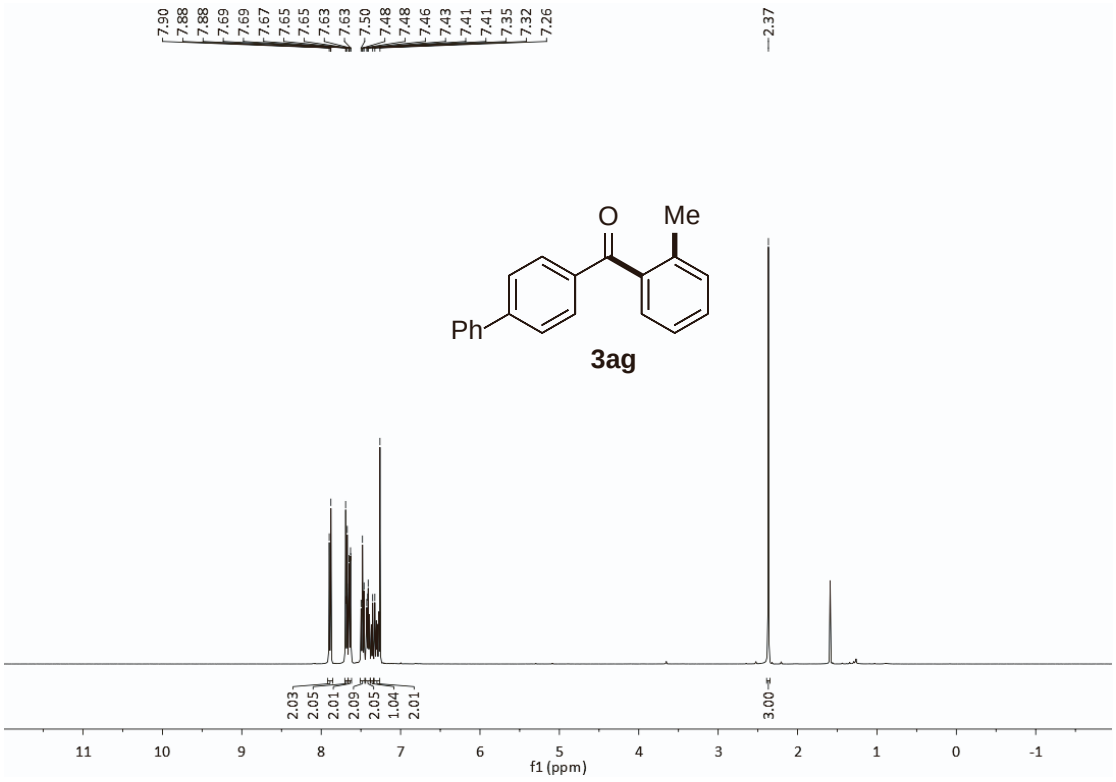


^{1}H NMR (400 MHz, $CDCl_3$)



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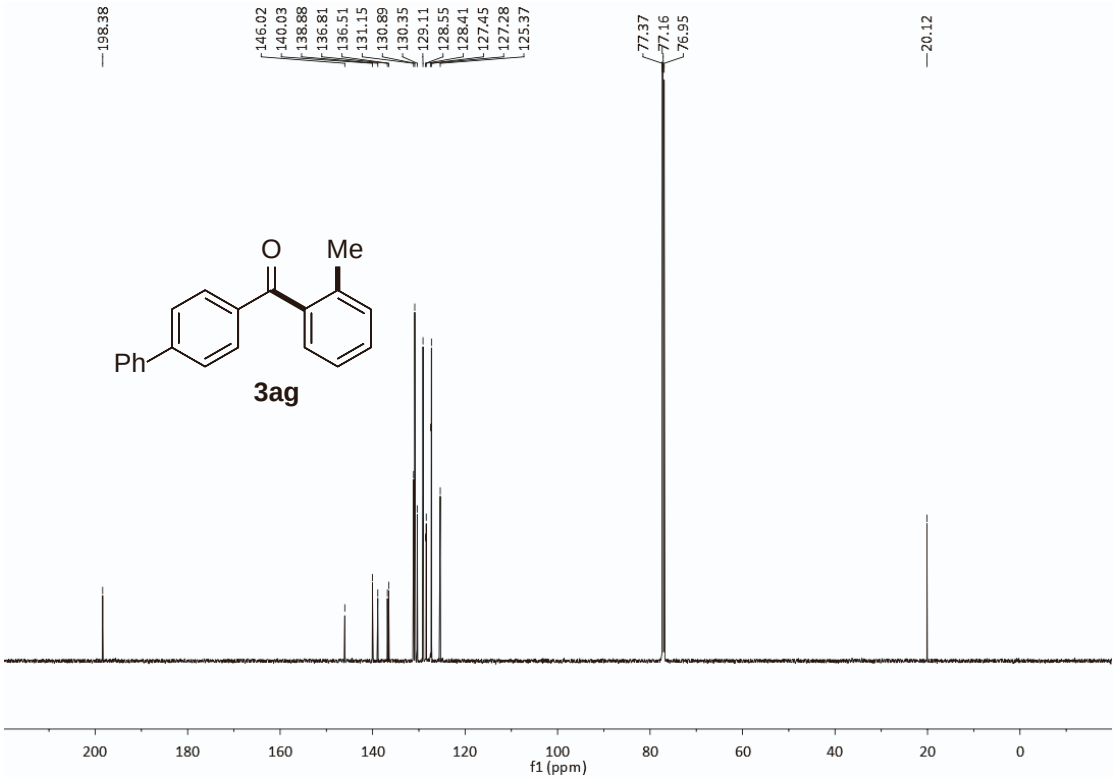

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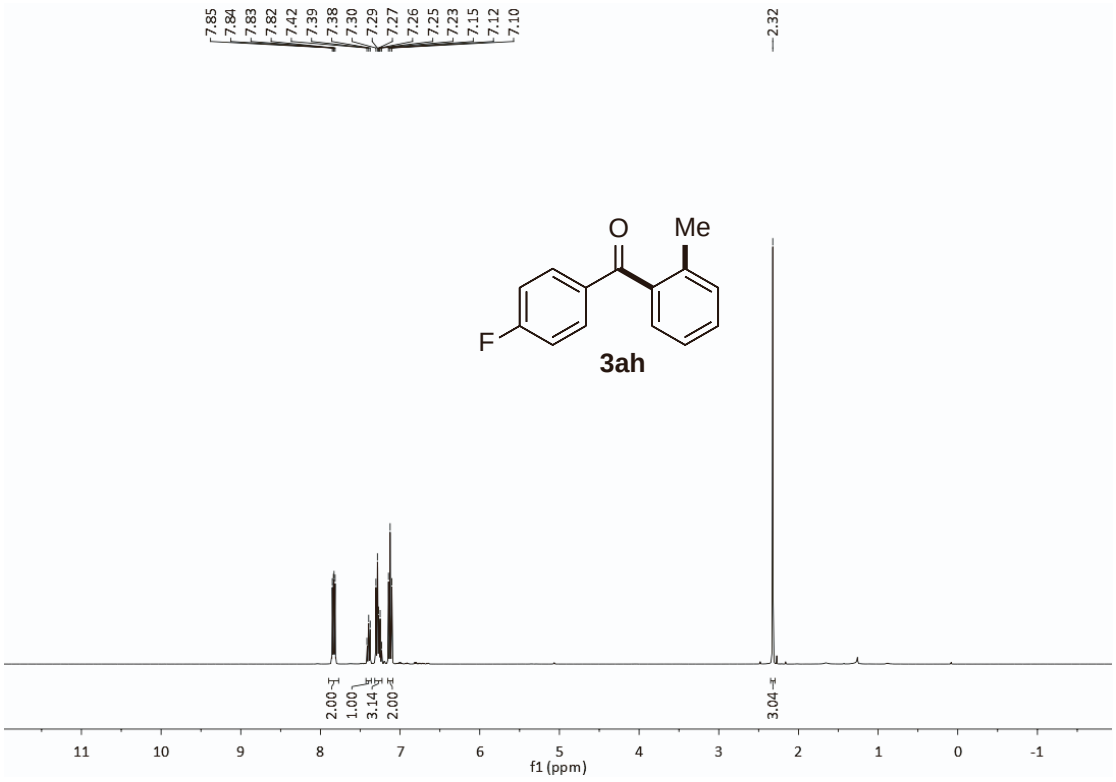
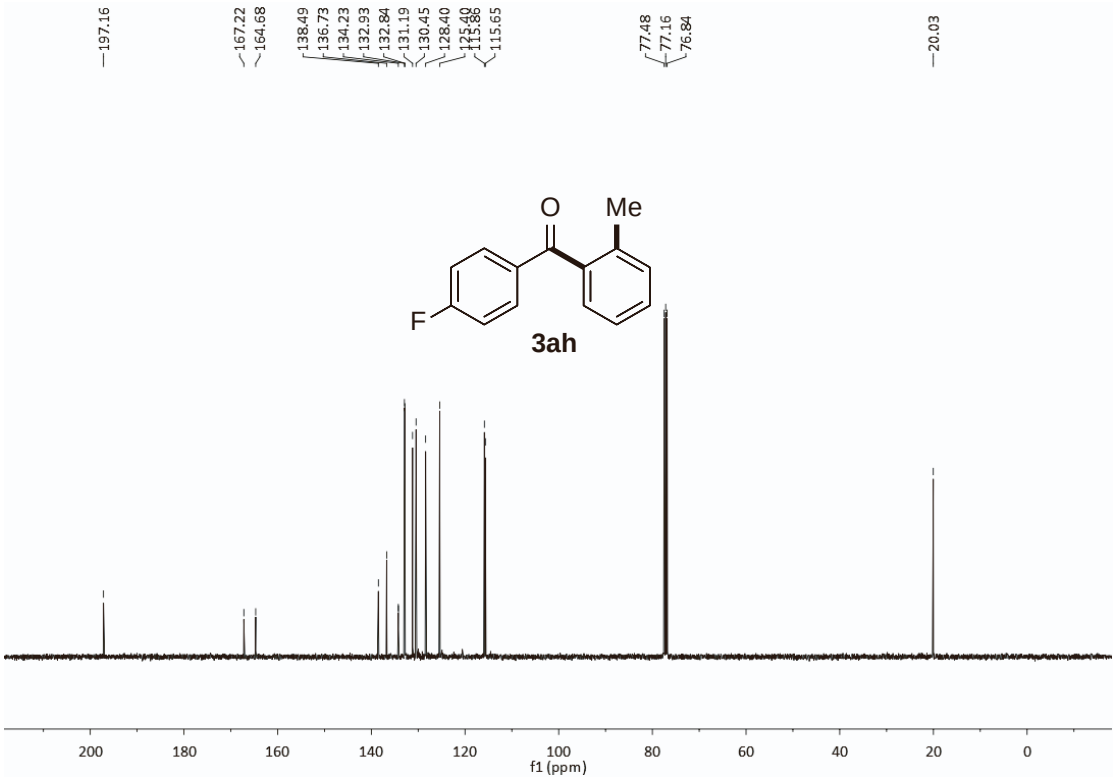
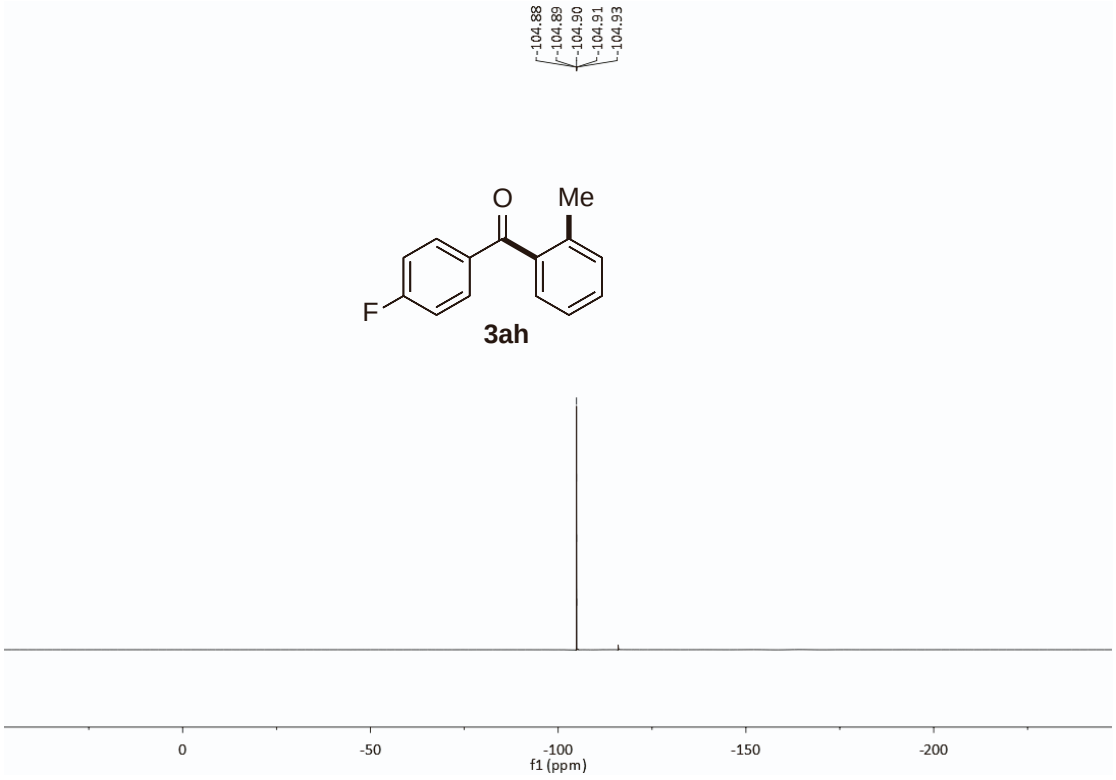


^{13}C NMR (101 MHz, $CDCl_3$)



^{19}F NMR (565 MHz, $CDCl_3$)



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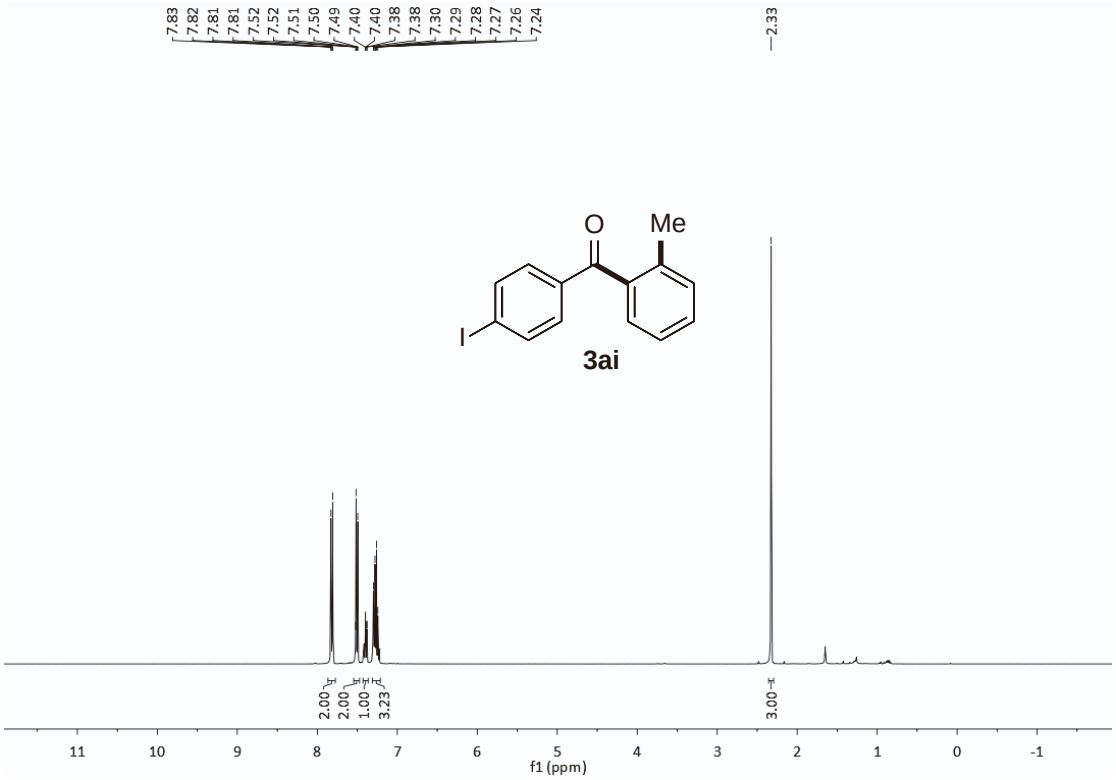
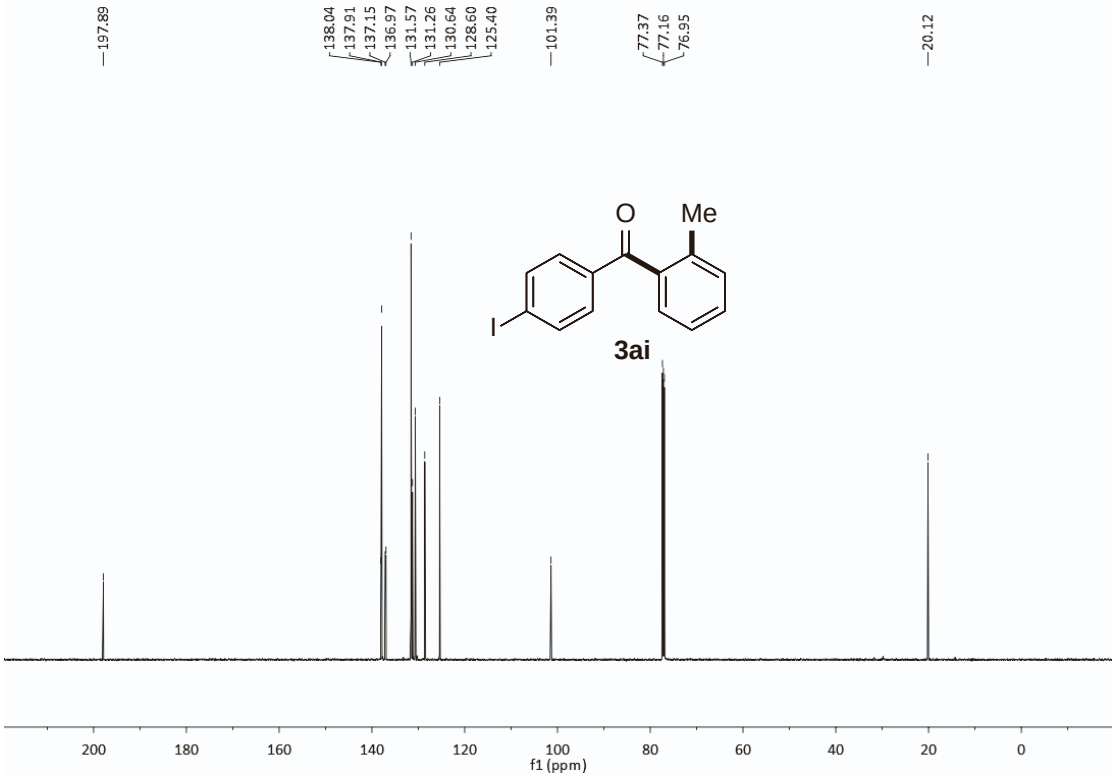


^{13}C NMR (151 MHz, $CDCl_3$)



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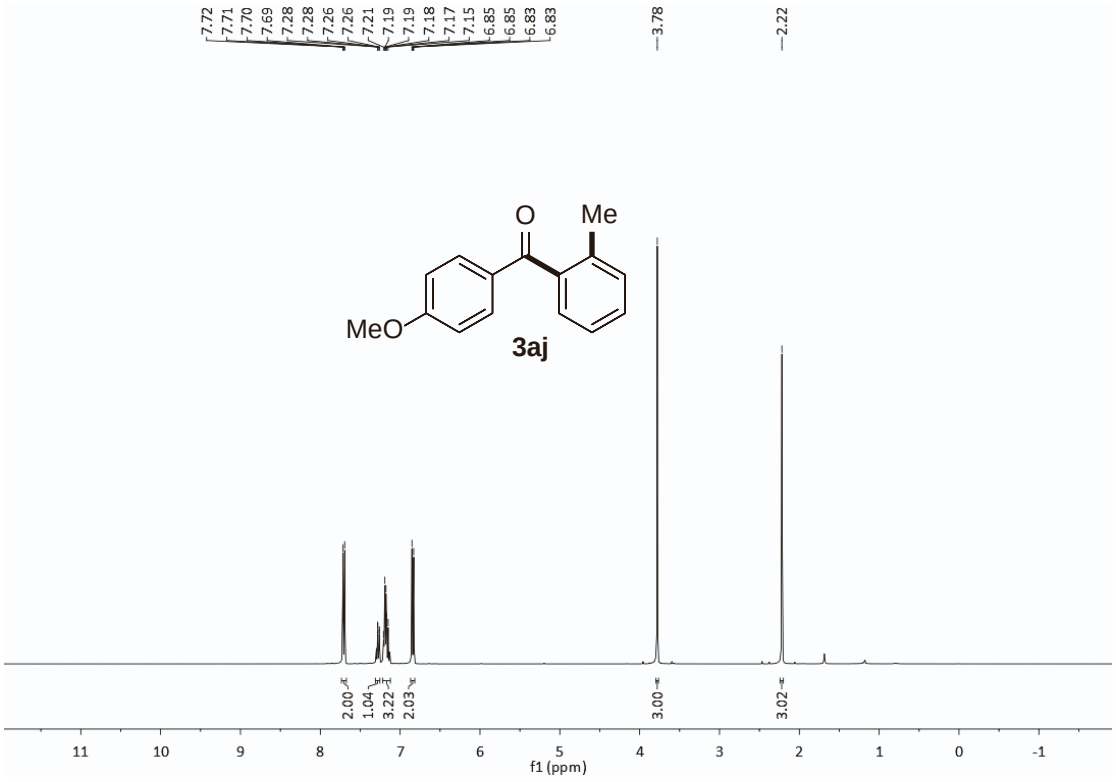
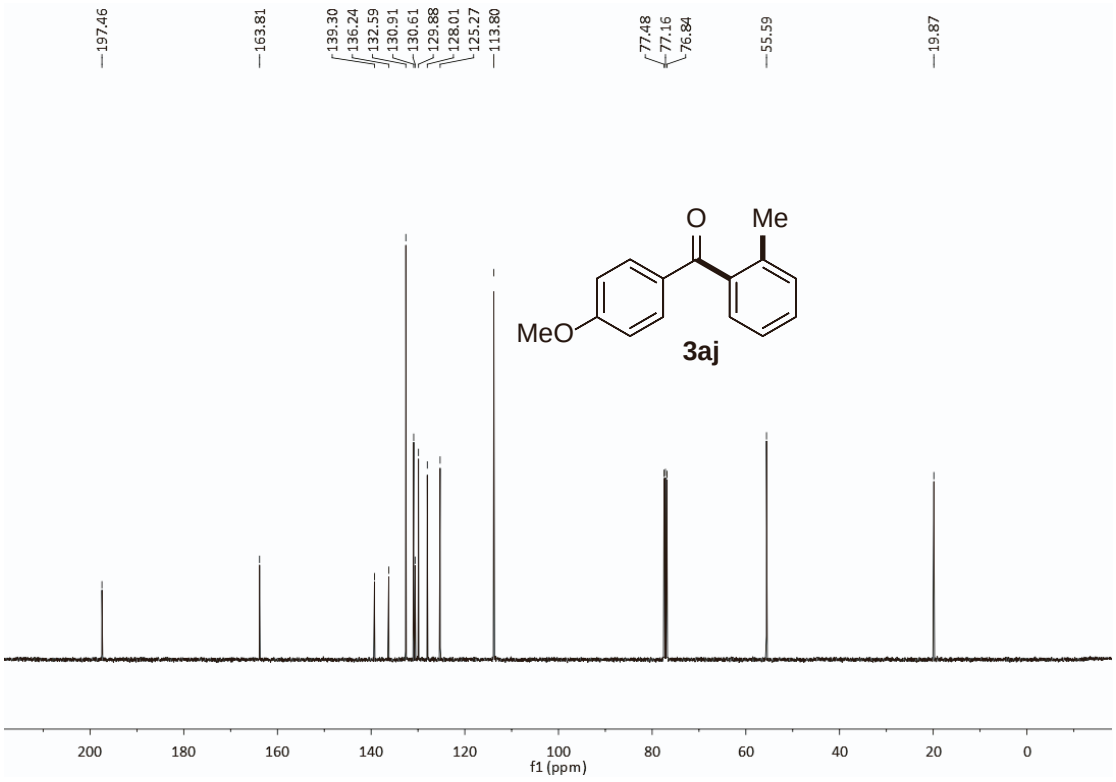
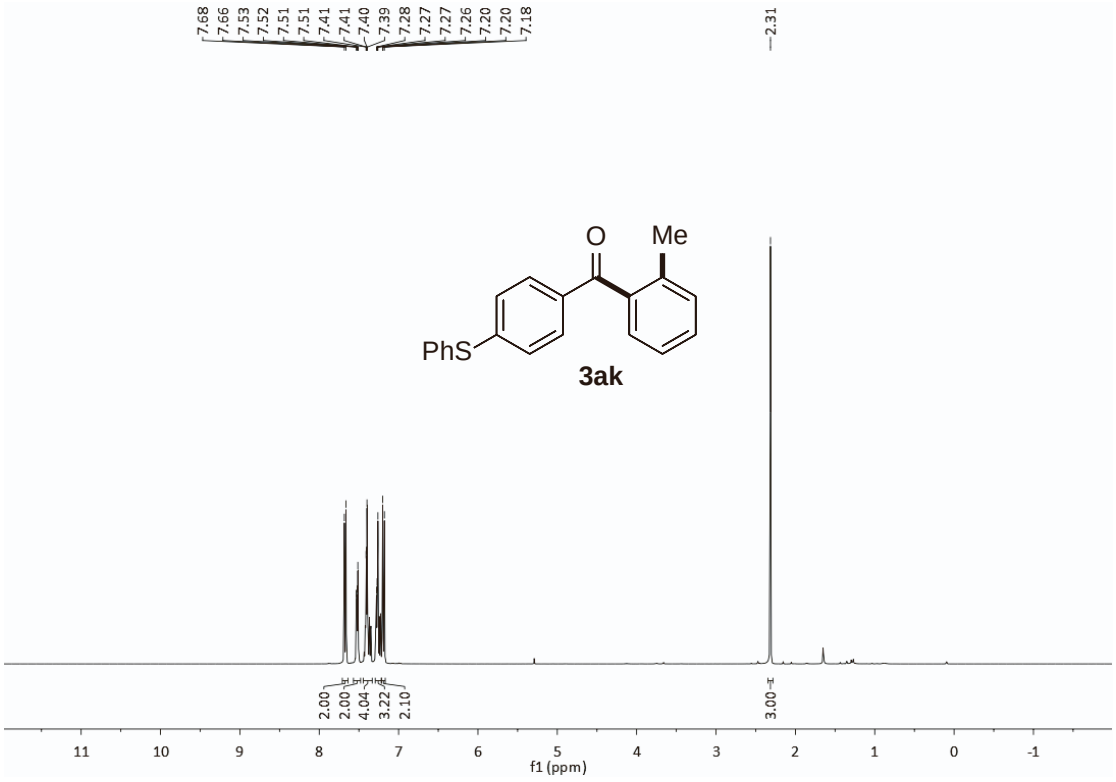


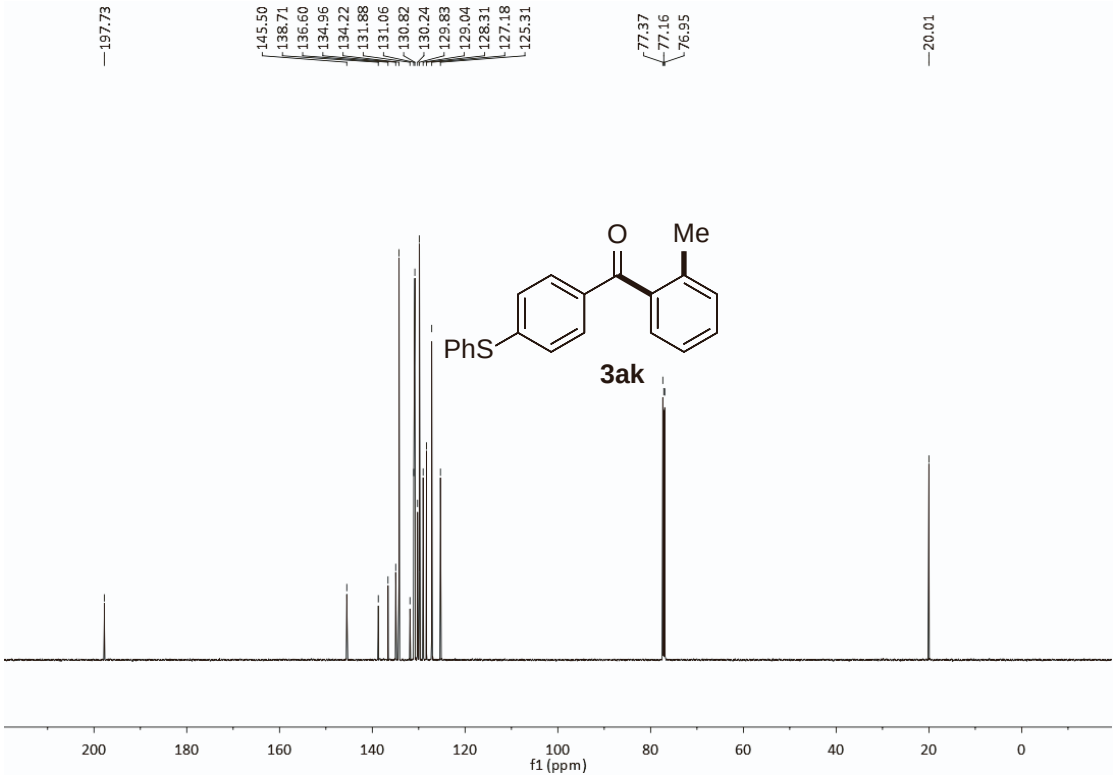
^{13}C NMR (101 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)

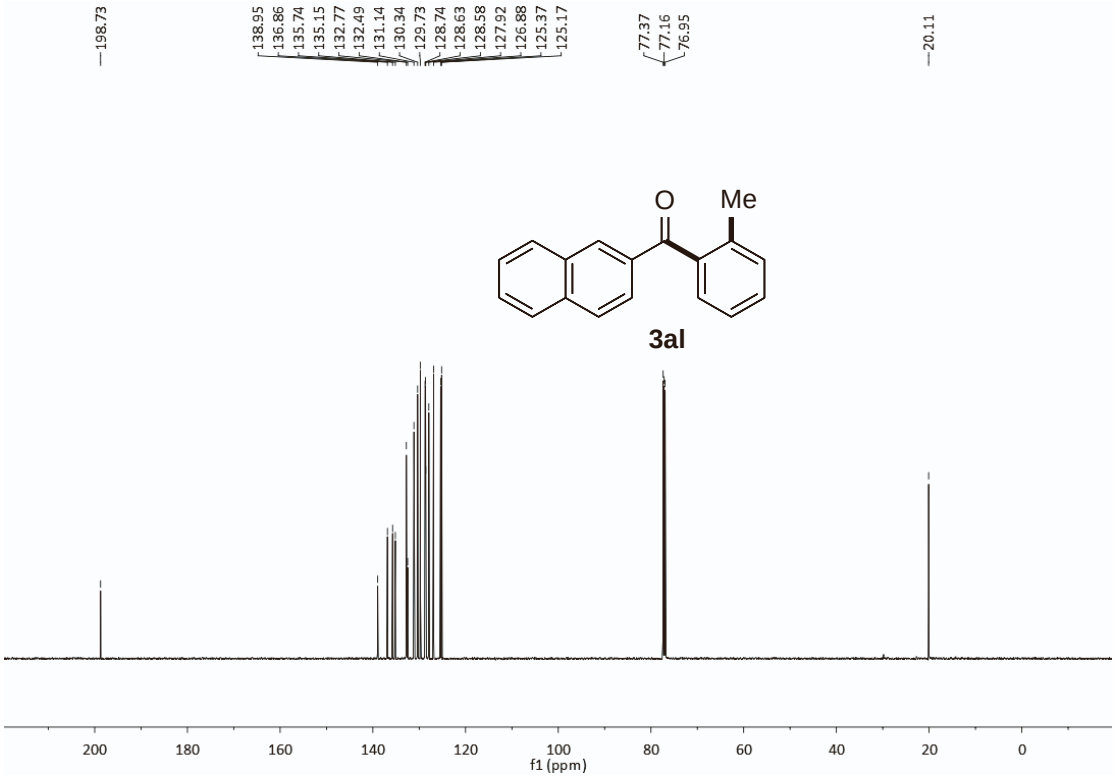


^{13}C NMR (151 MHz, $CDCl_3$)

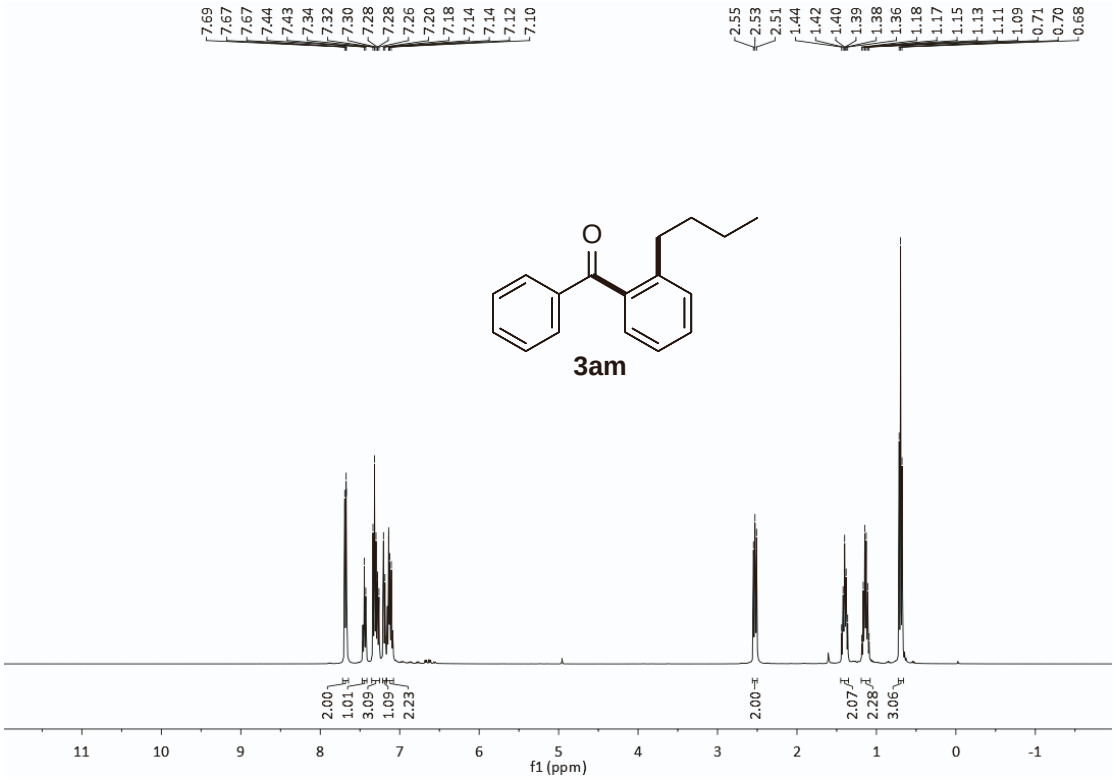


^{1}H NMR (400 MHz, $CDCl_3$)

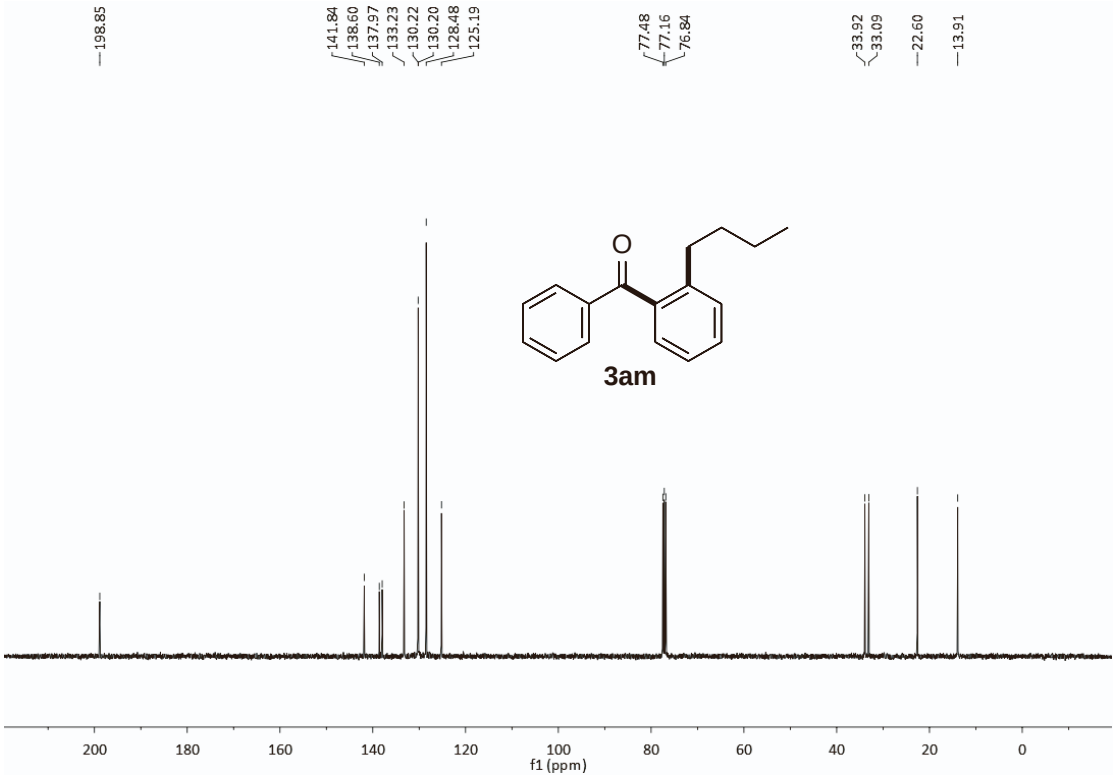
^{13}C NMR (151 MHz, $CDCl_3$)



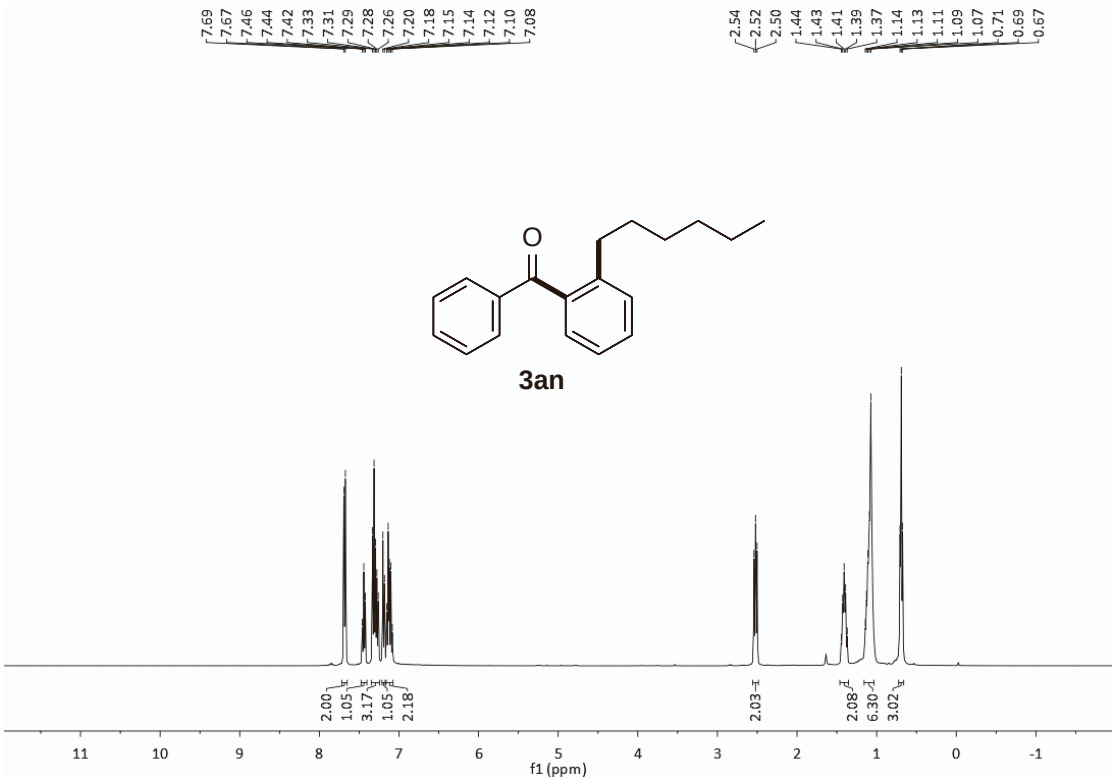
^{1}H NMR (400 MHz, $CDCl_3$)



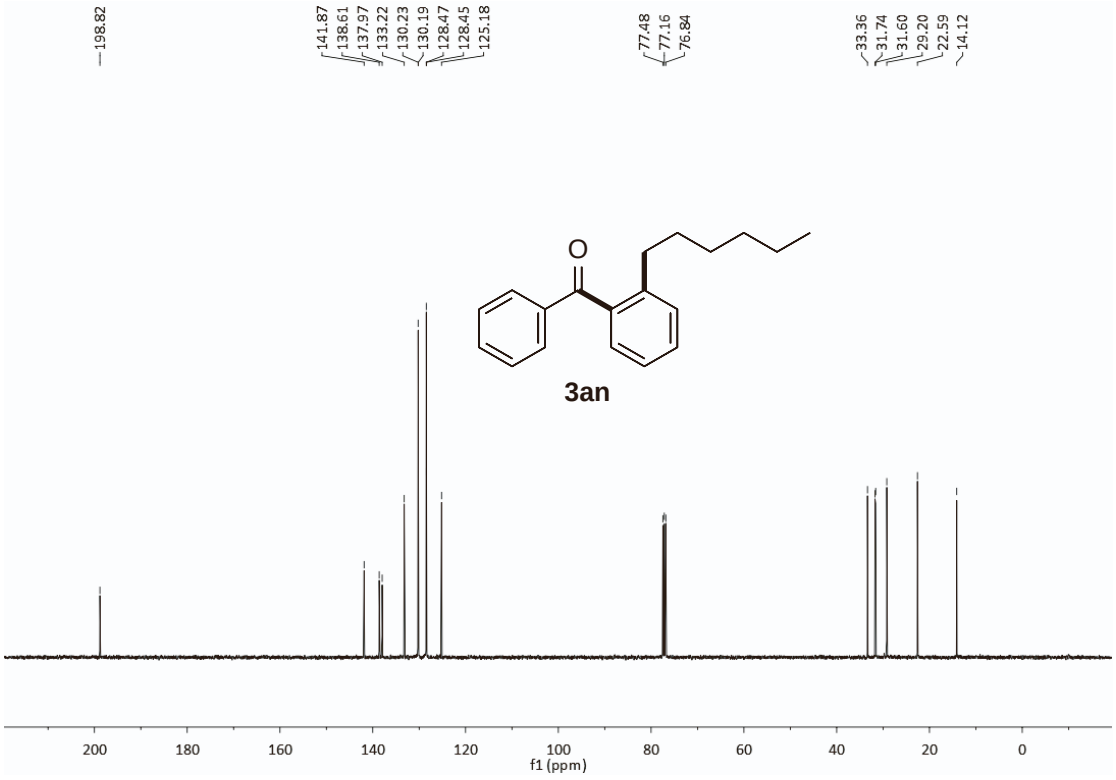
^{13}C NMR (101 MHz, $CDCl_3$)



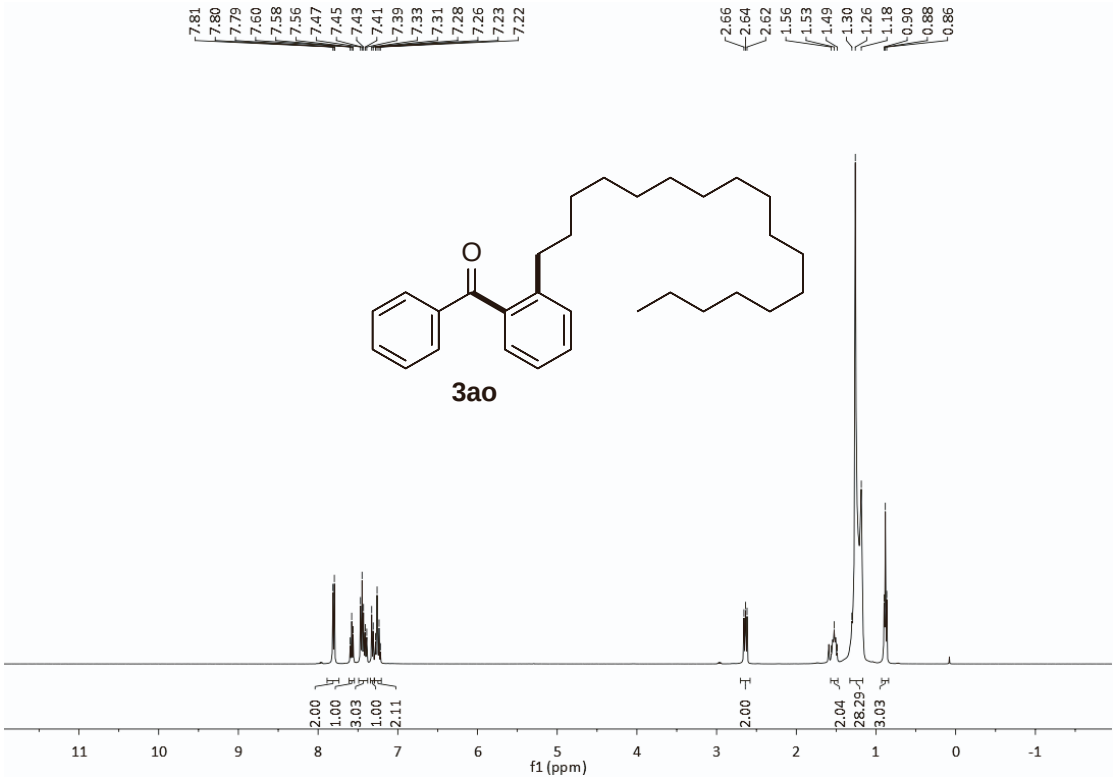
^{1}H NMR (400 MHz, $CDCl_3$)



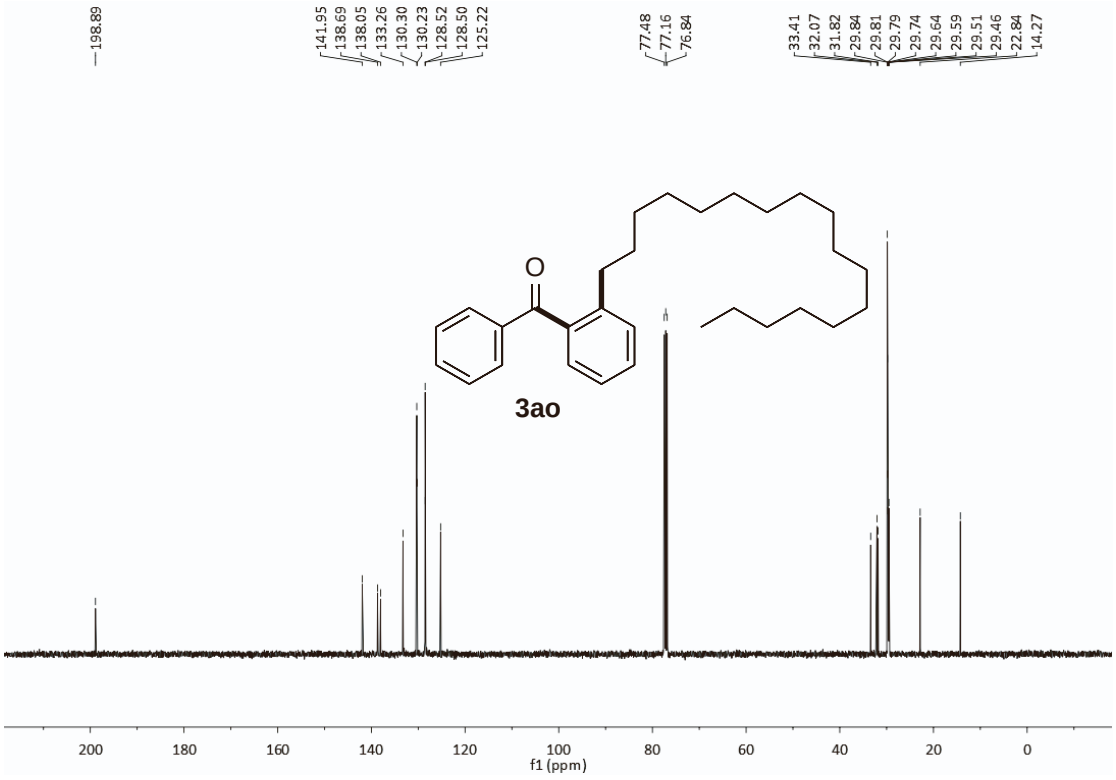
^{13}C NMR (101 MHz, $CDCl_3$)



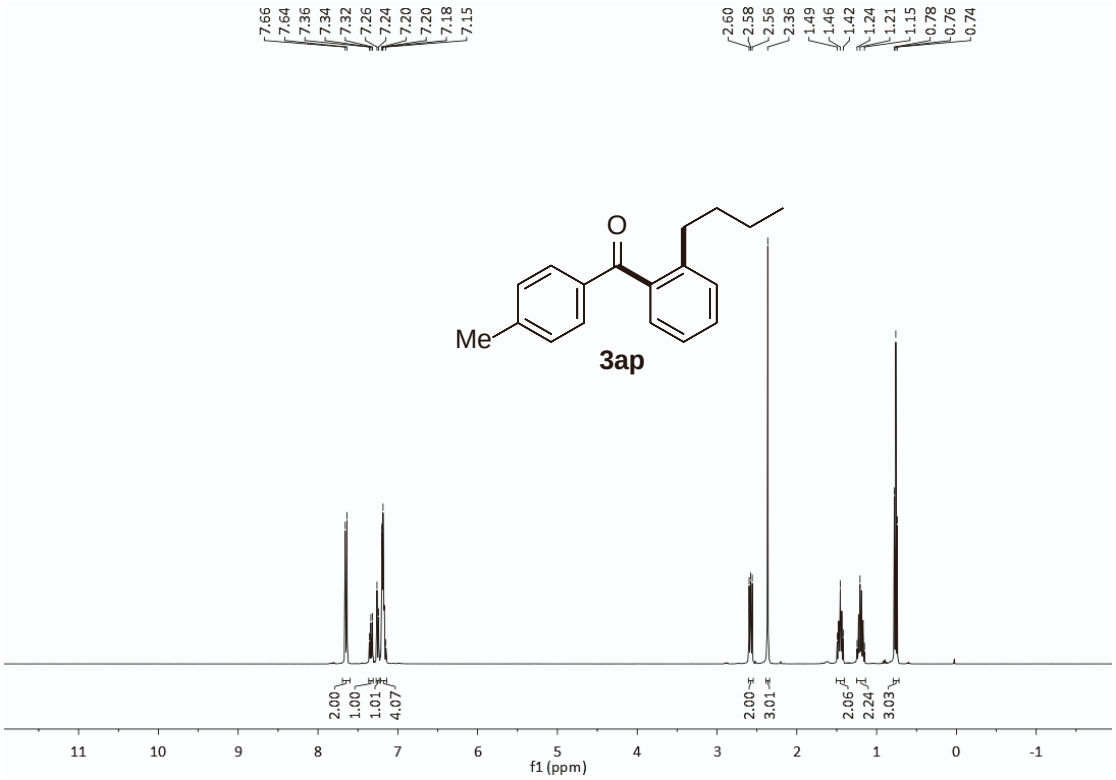
^{1}H NMR (400 MHz, $CDCl_3$)



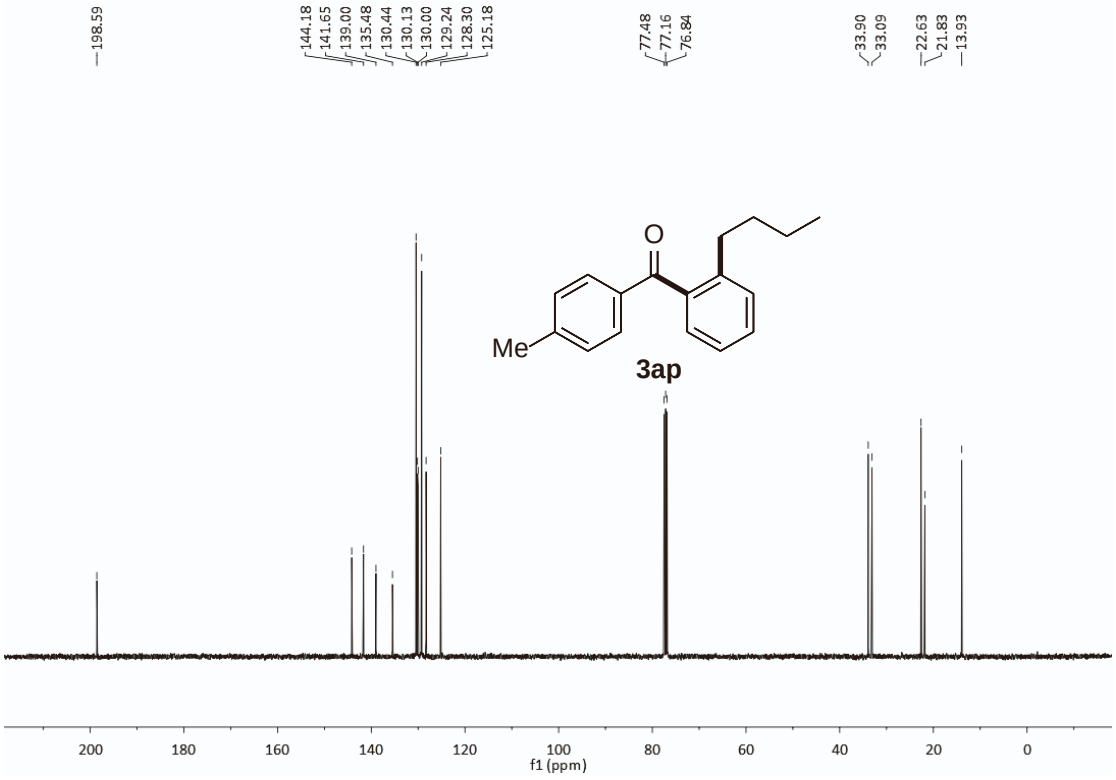
^{13}C NMR (101 MHz, $CDCl_3$)



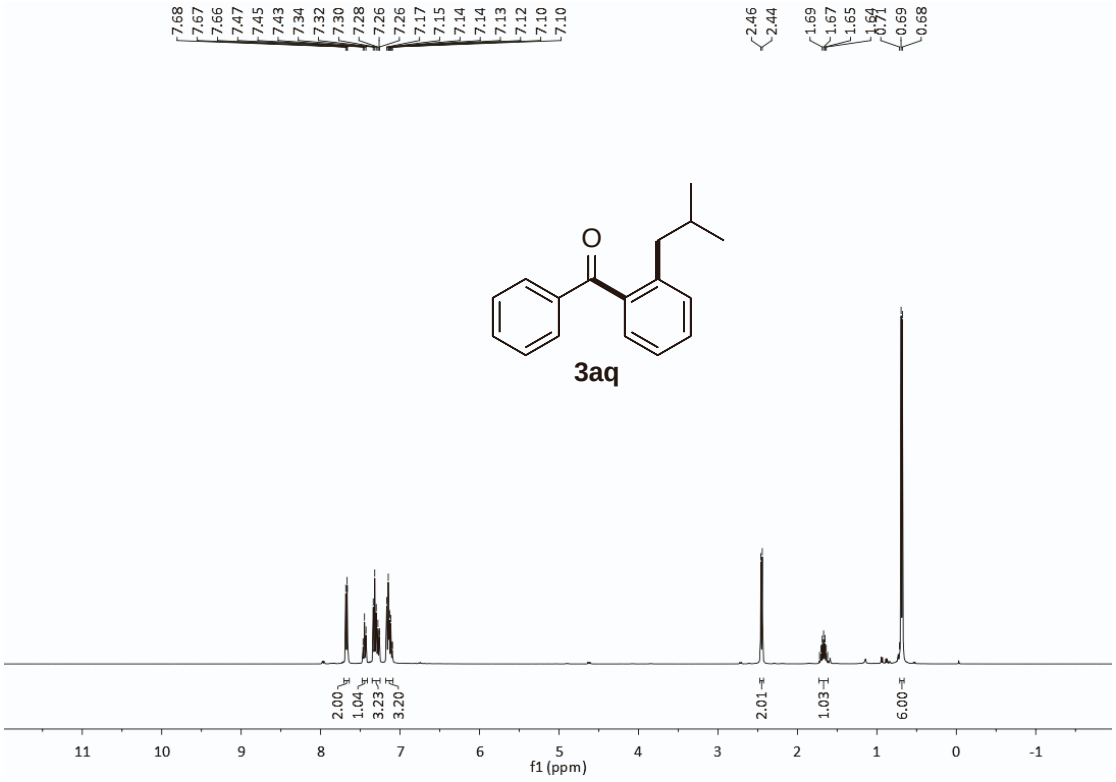
^{1}H NMR (400 MHz, $CDCl_3$)



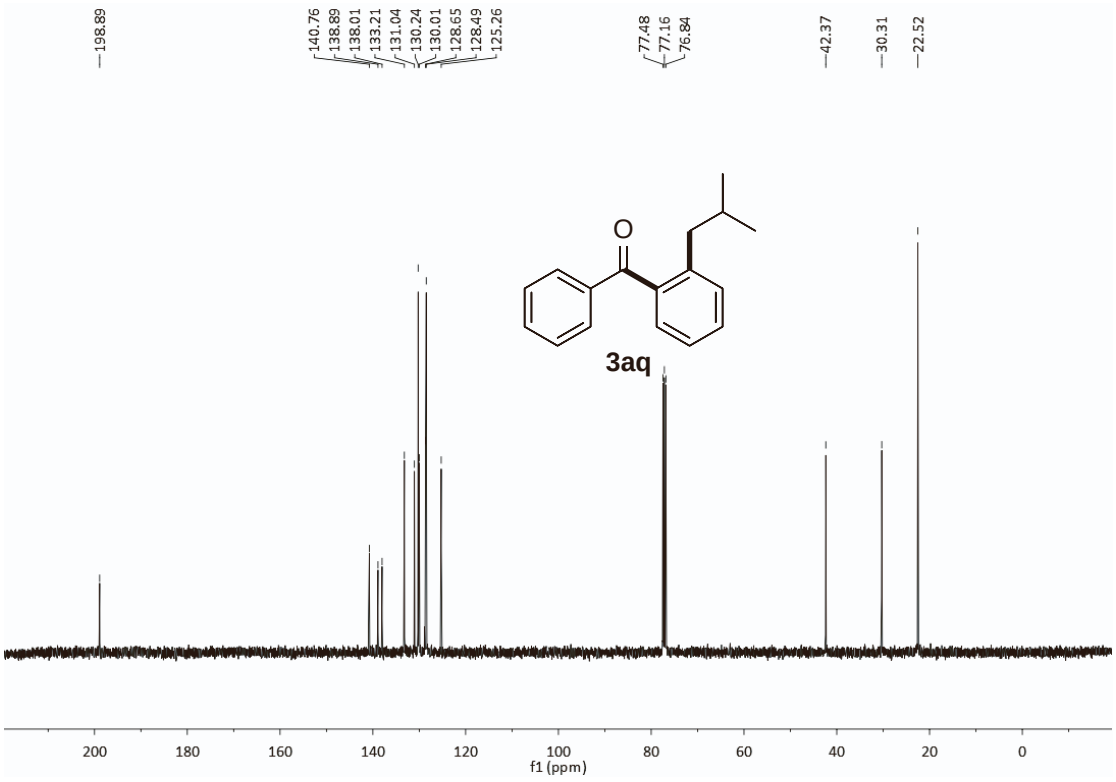
^{13}C NMR (101 MHz, $CDCl_3$)



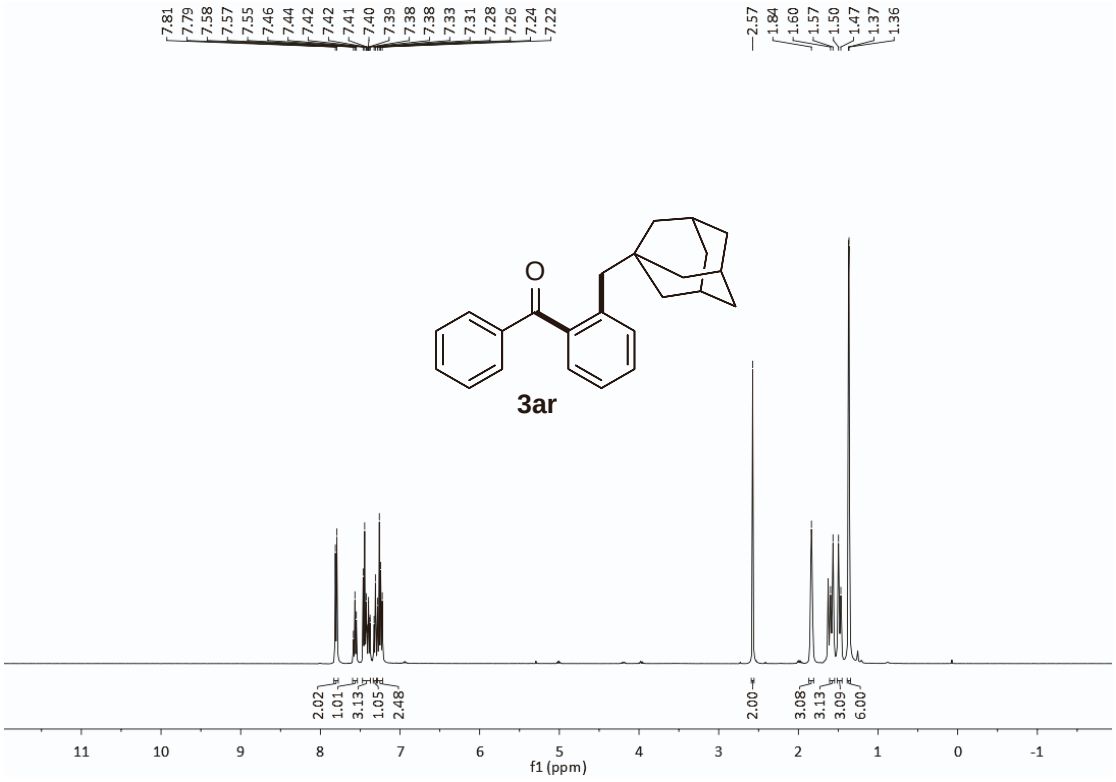
^{1}H NMR (400 MHz, $CDCl_3$)



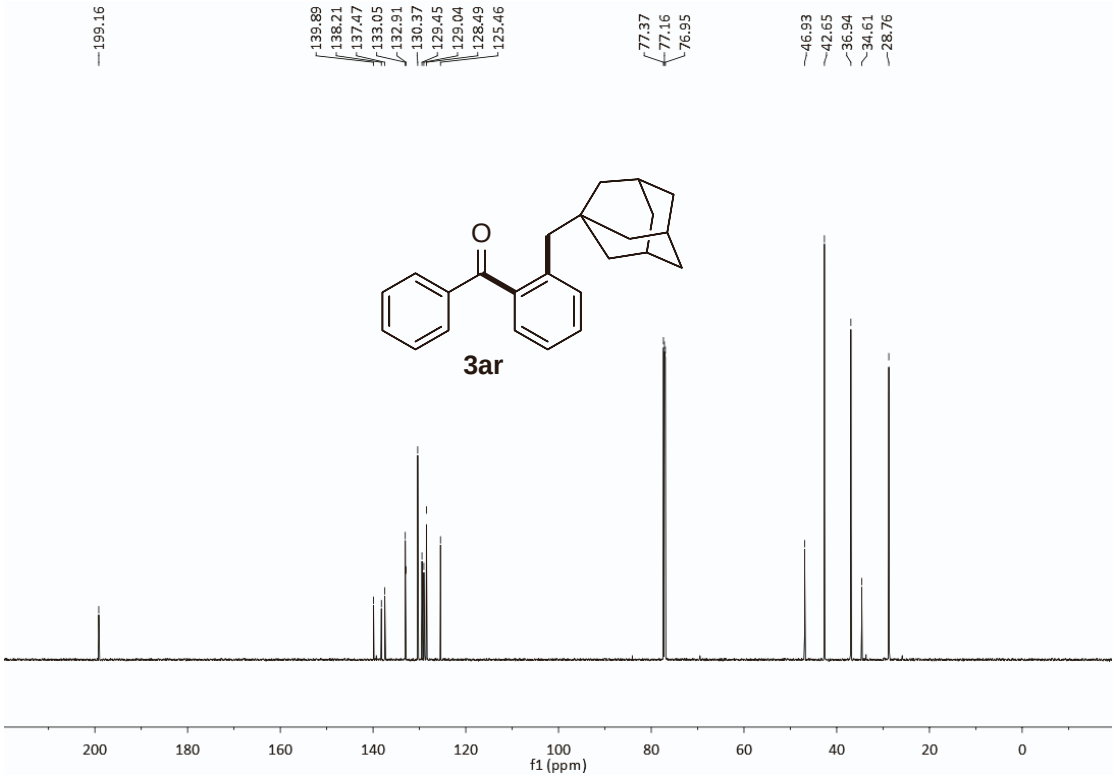
^{13}C NMR (101 MHz, $CDCl_3$)



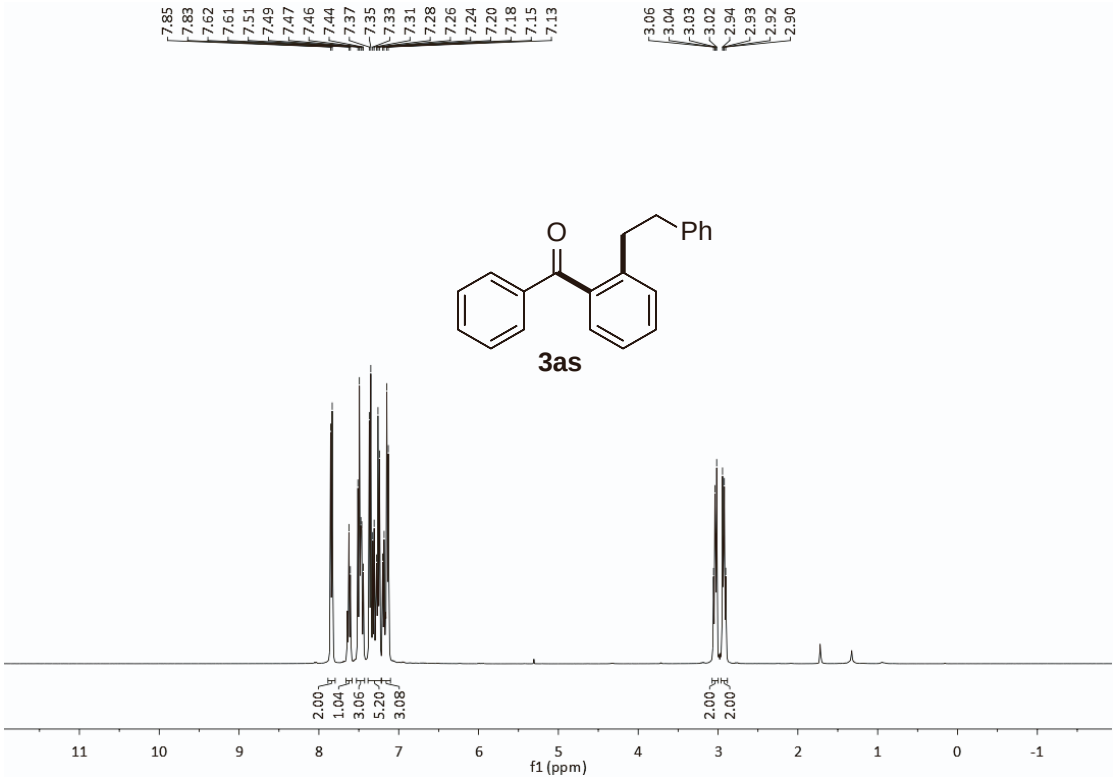
^{1}H NMR (400 MHz, $CDCl_3$)



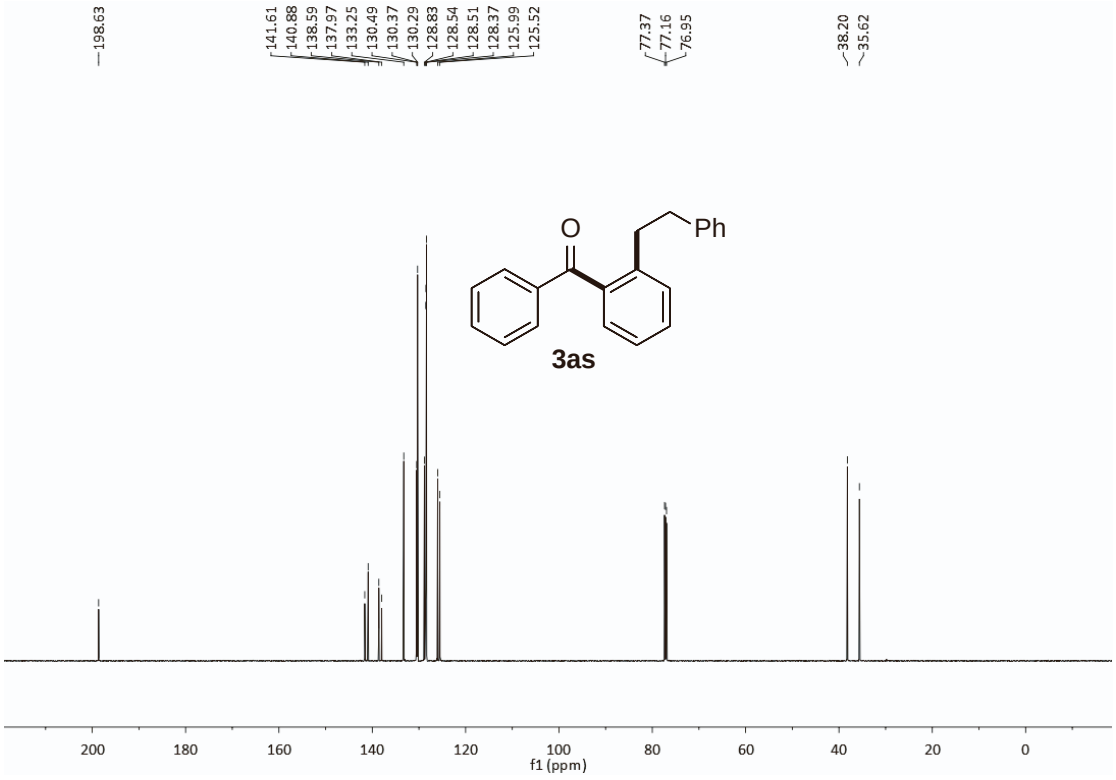
^{13}C NMR (151 MHz, $CDCl_3$)



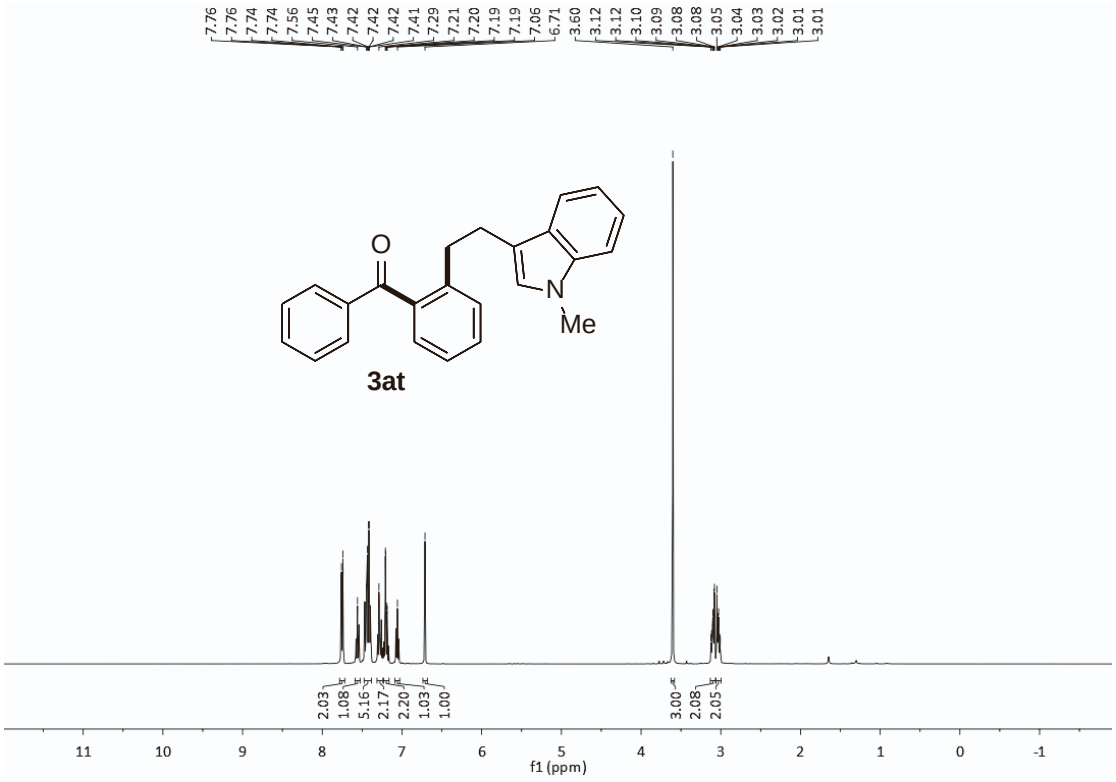
^{1}H NMR (400 MHz, $CDCl_3$)



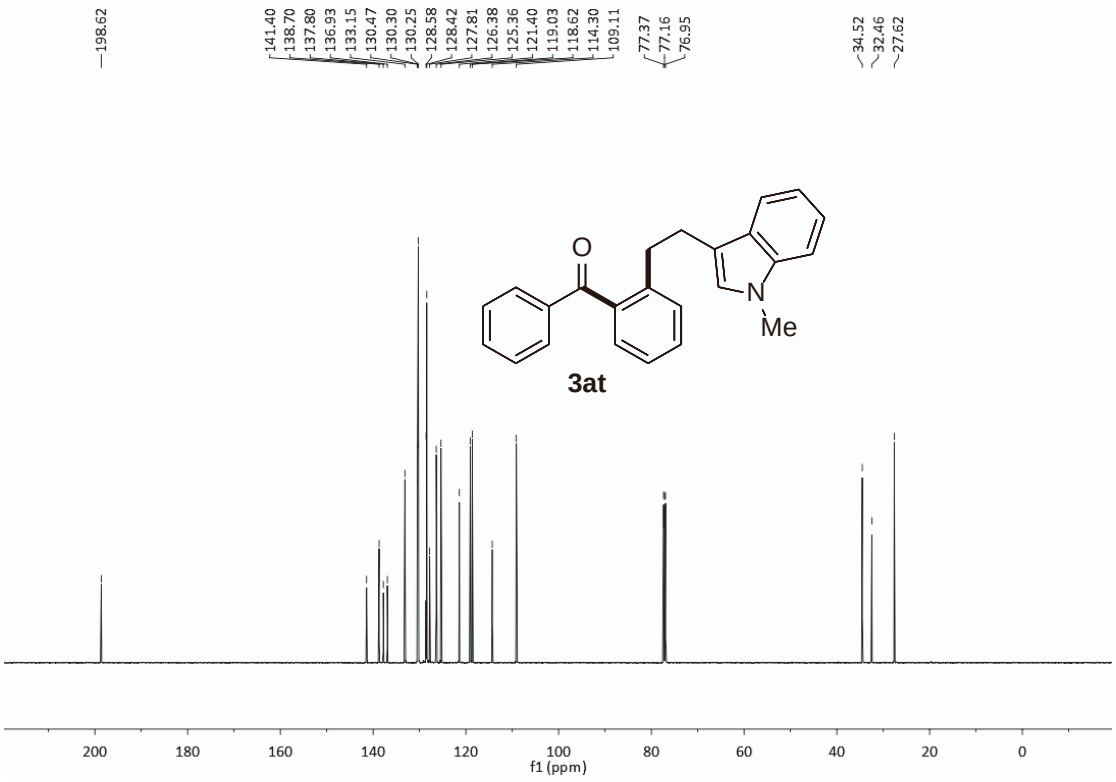
^{13}C NMR (151 MHz, $CDCl_3$)



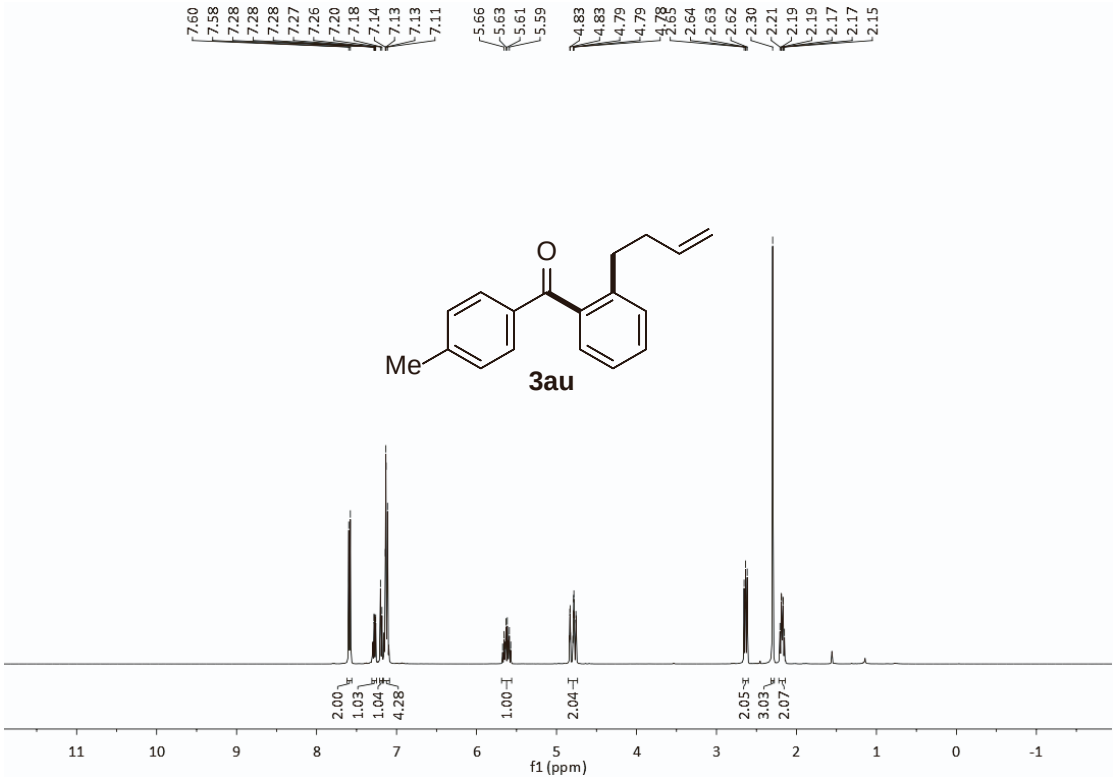
^{1}H NMR (400 MHz, $CDCl_3$)



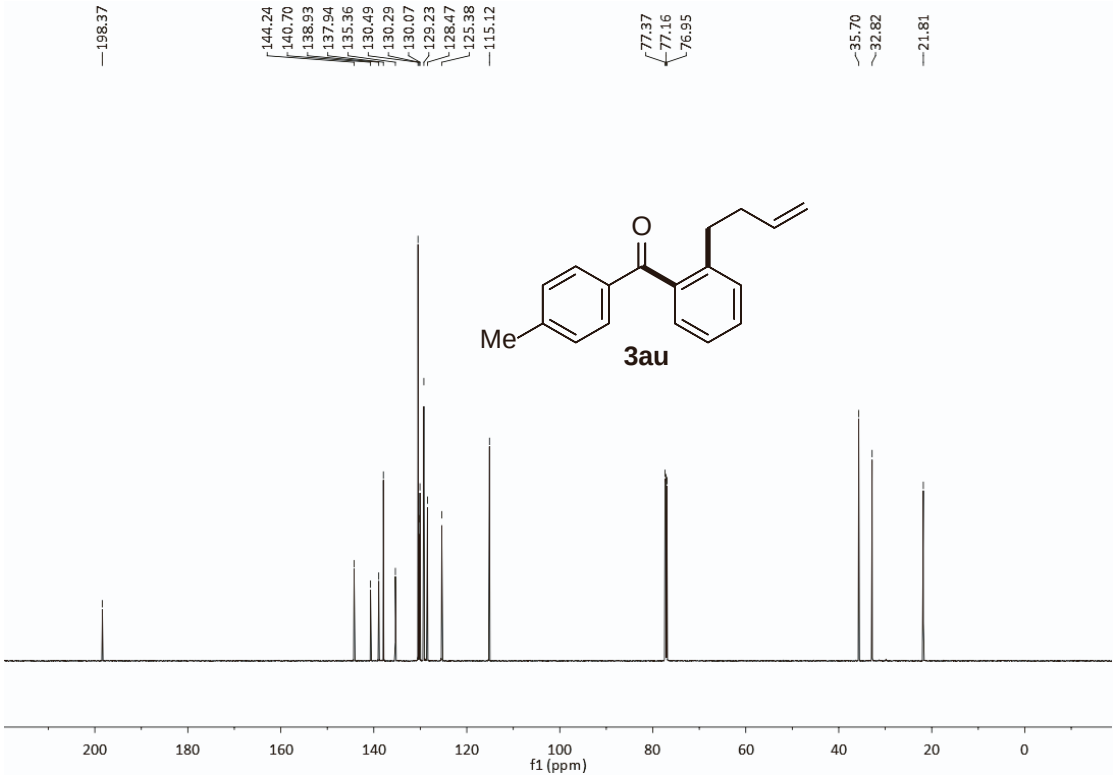
^{13}C NMR (151 MHz, $CDCl_3$)



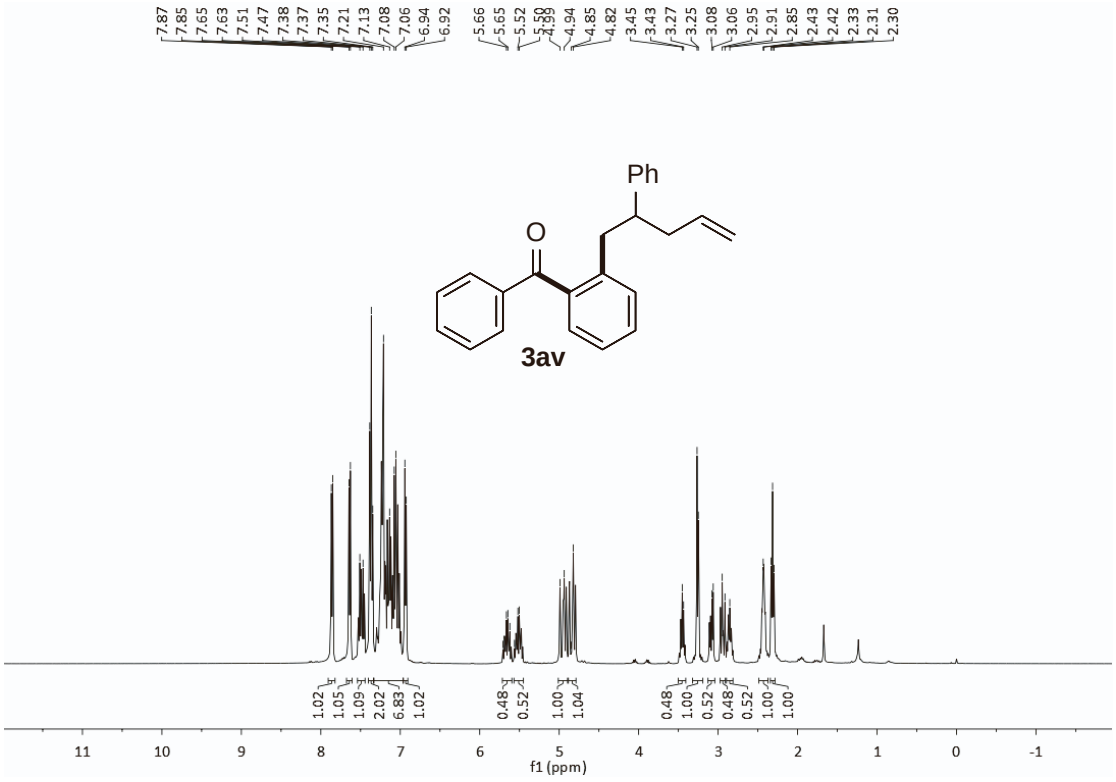
^{1}H NMR (400 MHz, $CDCl_3$)



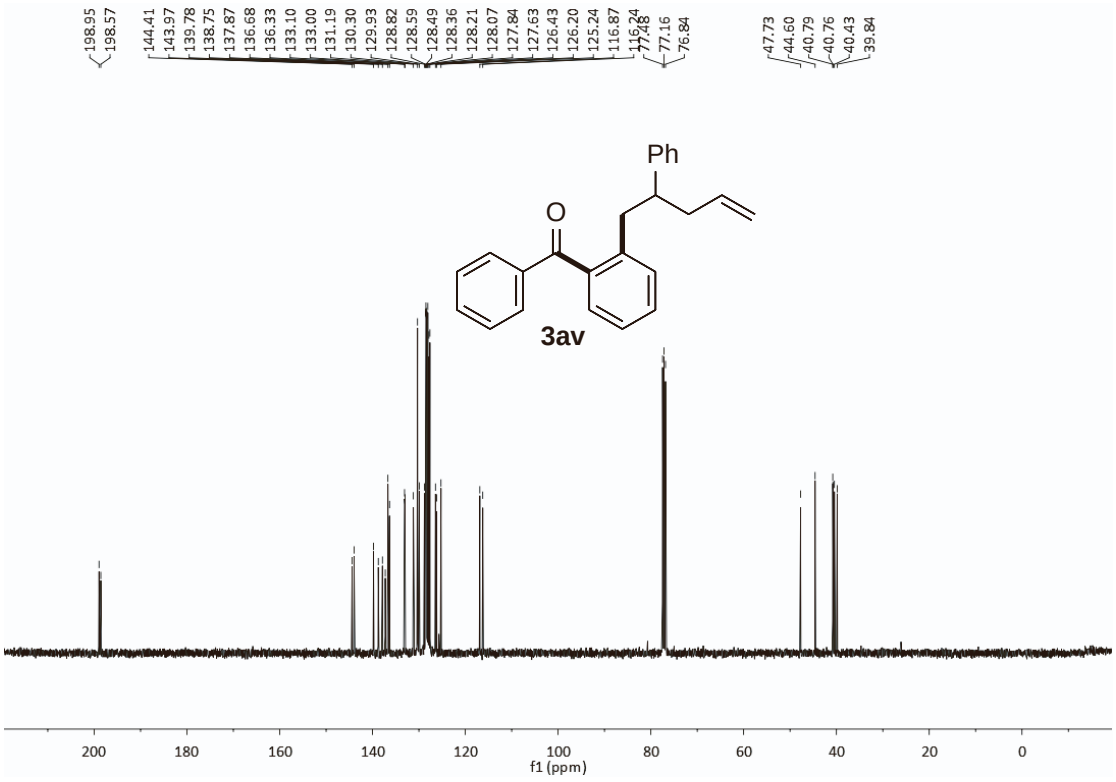
^{13}C NMR (151 MHz, $CDCl_3$)



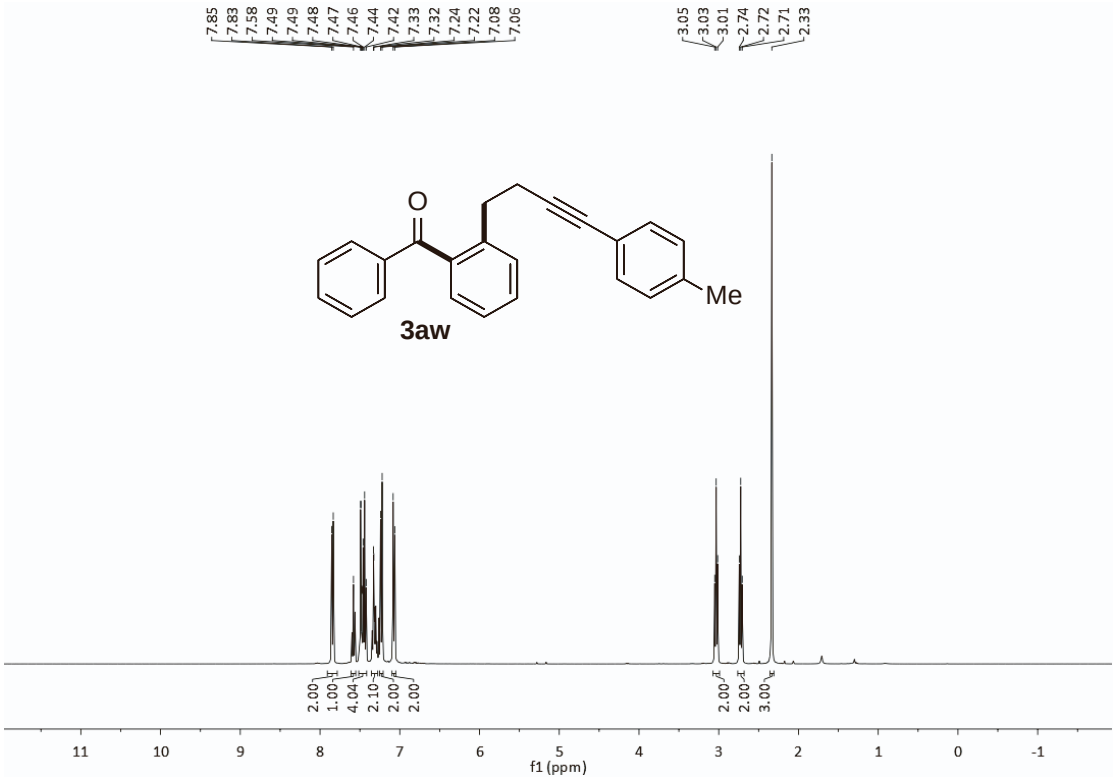
^{1}H NMR (400 MHz, $CDCl_3$)



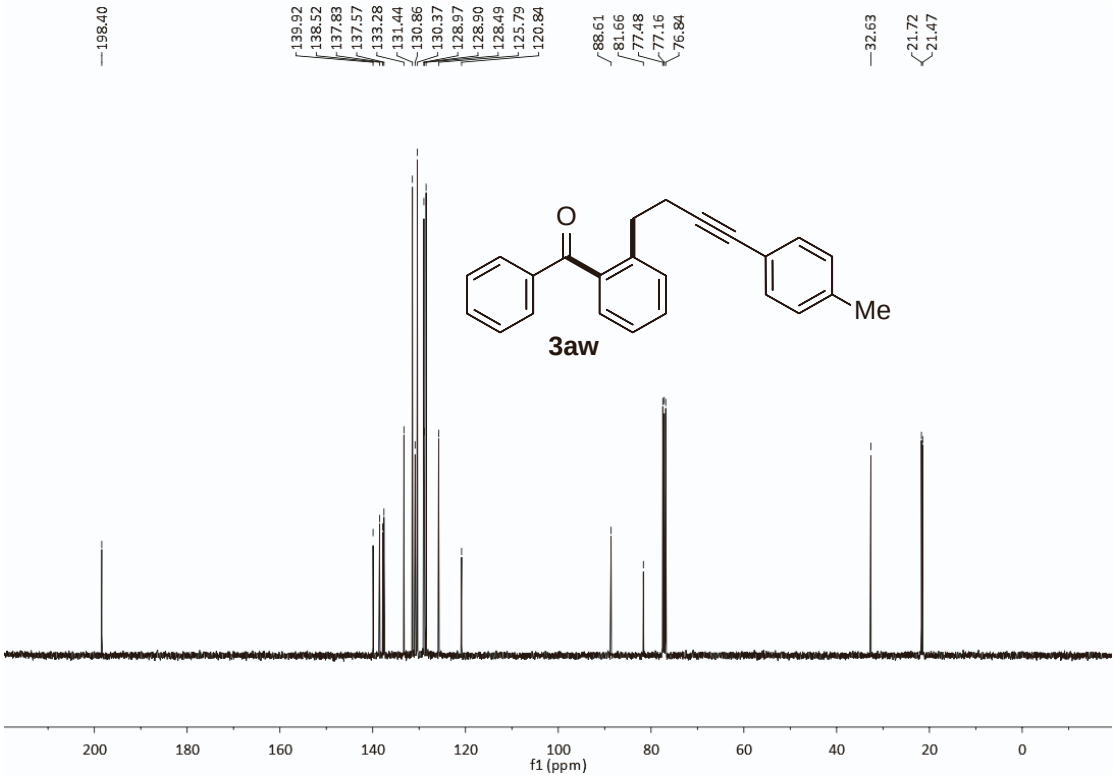
^{13}C NMR (101 MHz, $CDCl_3$)



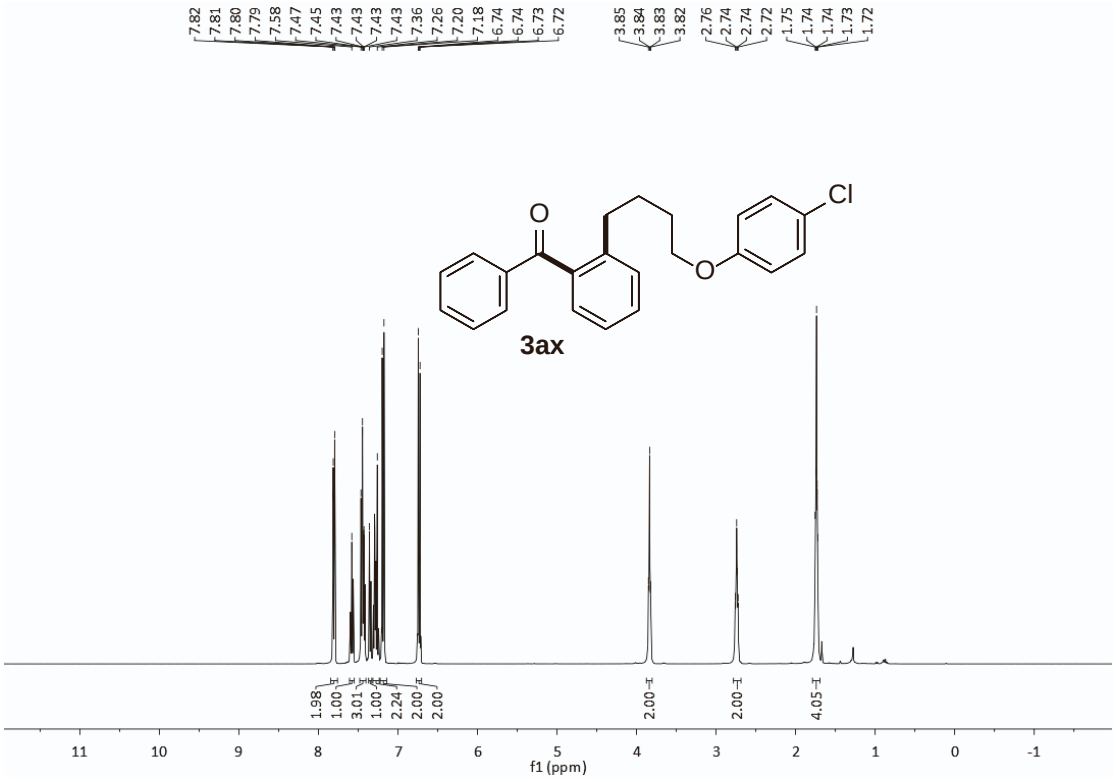
^{1}H NMR (400 MHz, $CDCl_3$)



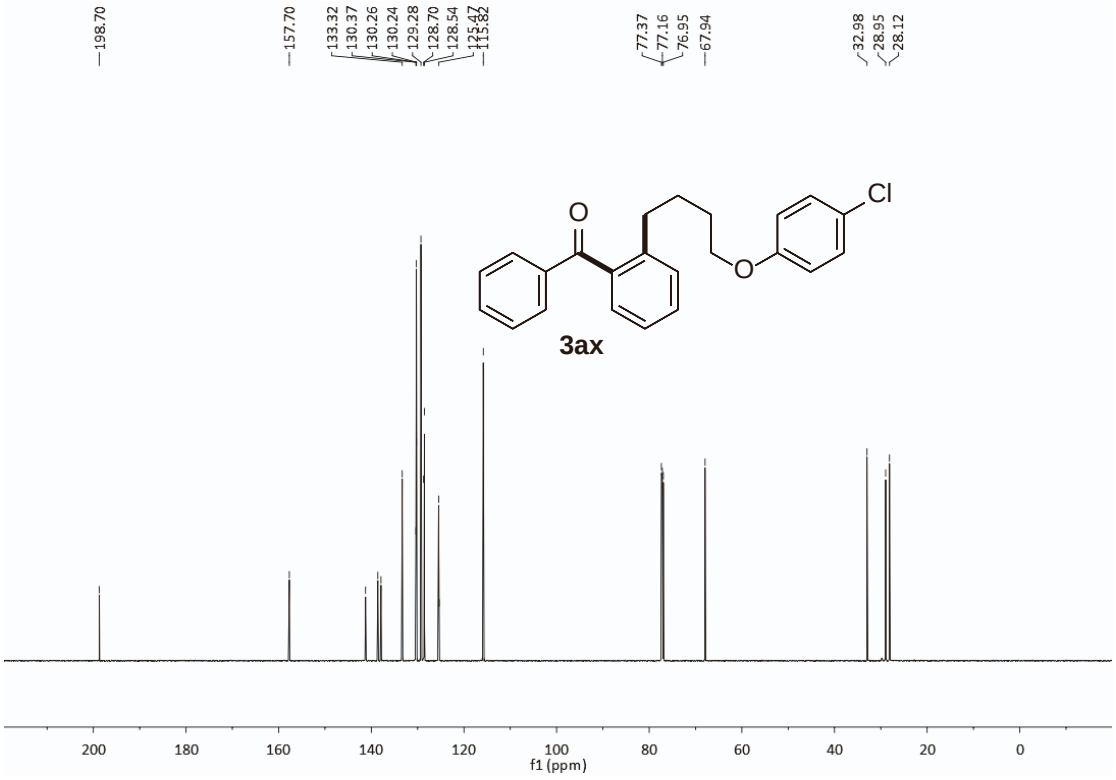
^{13}C NMR (101 MHz, $CDCl_3$)



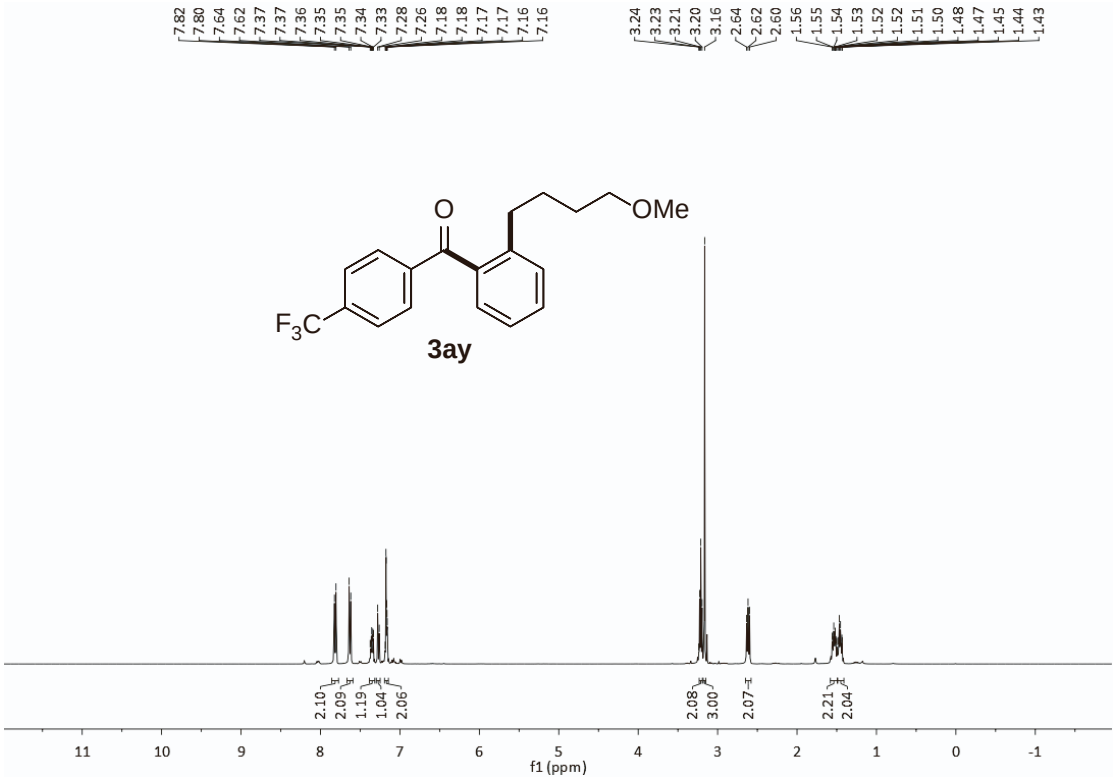
^{1}H NMR (400 MHz, $CDCl_3$)



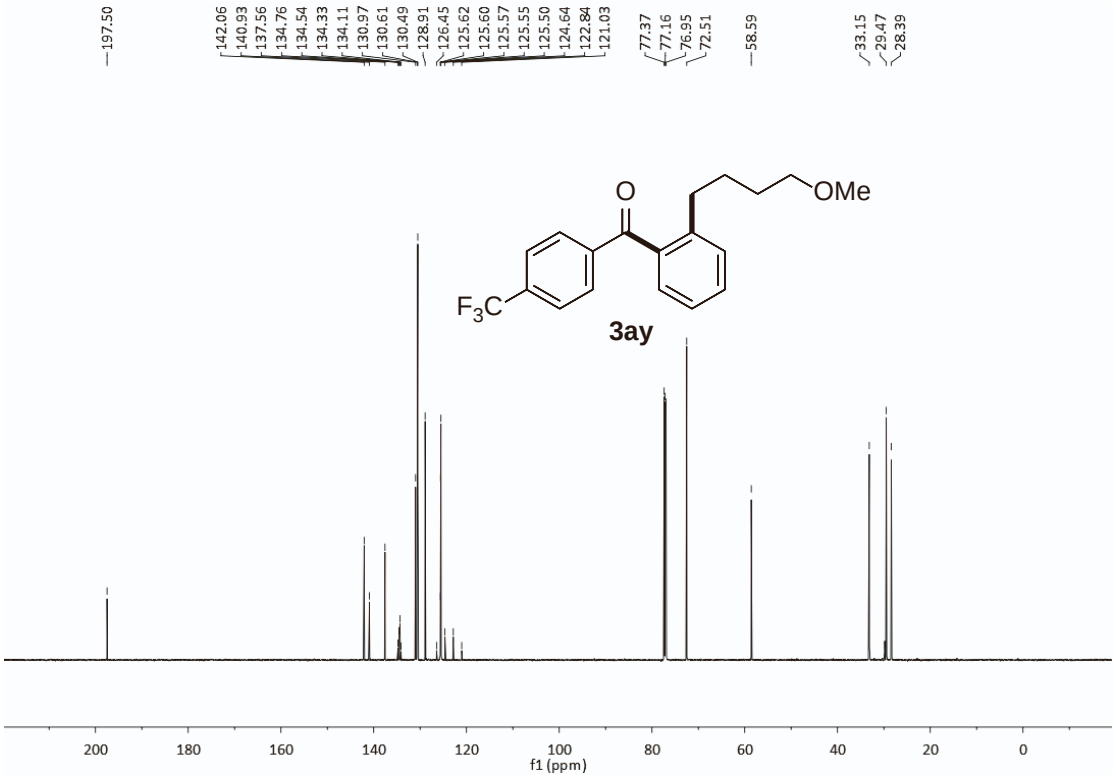
^{13}C NMR (151 MHz, $CDCl_3$)



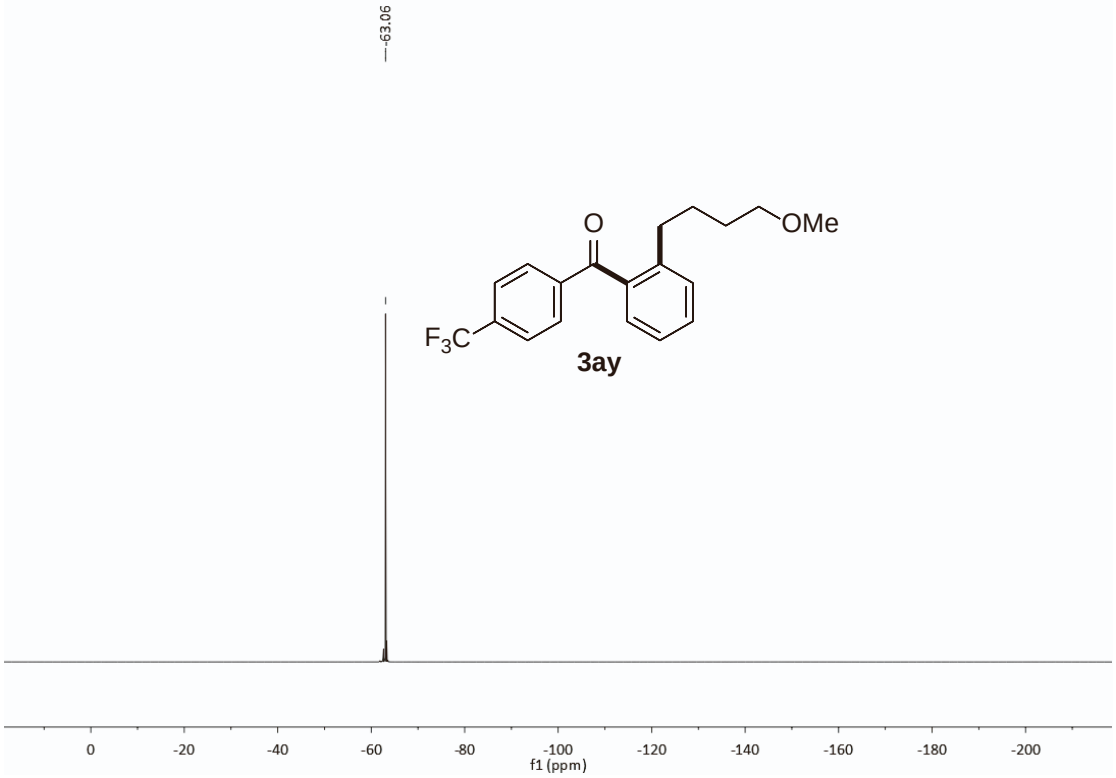
^{1}H NMR (400 MHz, $CDCl_3$)



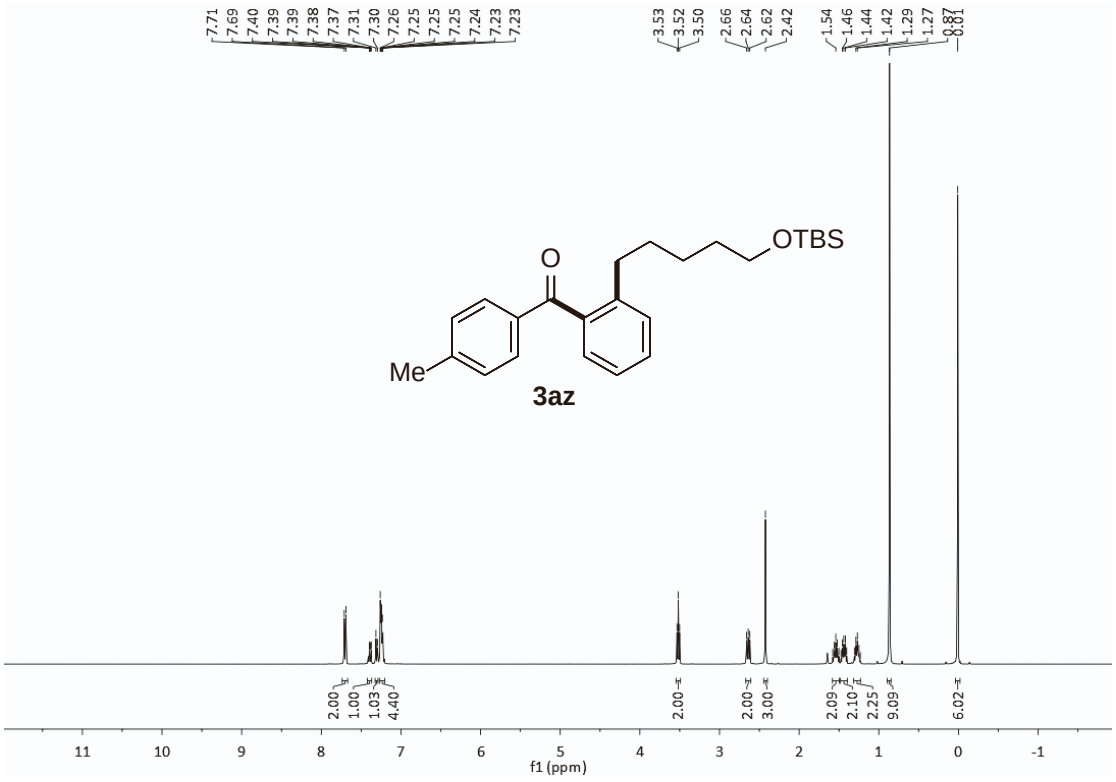
^{13}C NMR (151 MHz, $CDCl_3$)



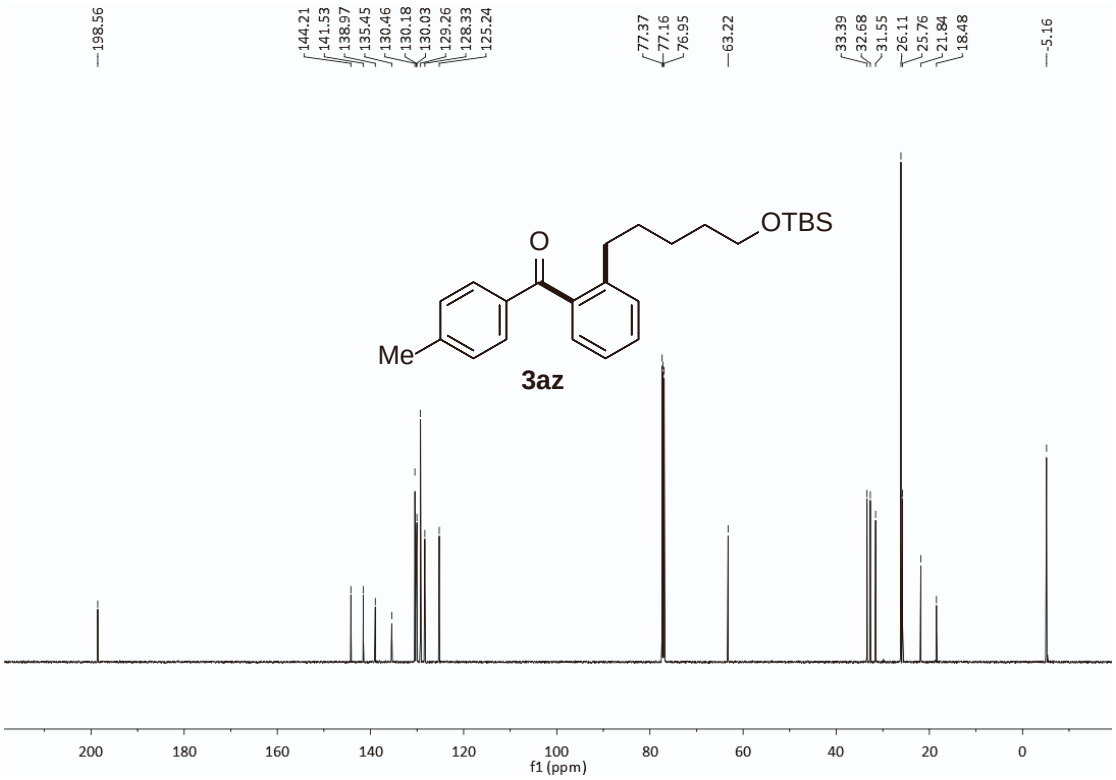
^{19}F NMR (376 MHz, $CDCl_3$)



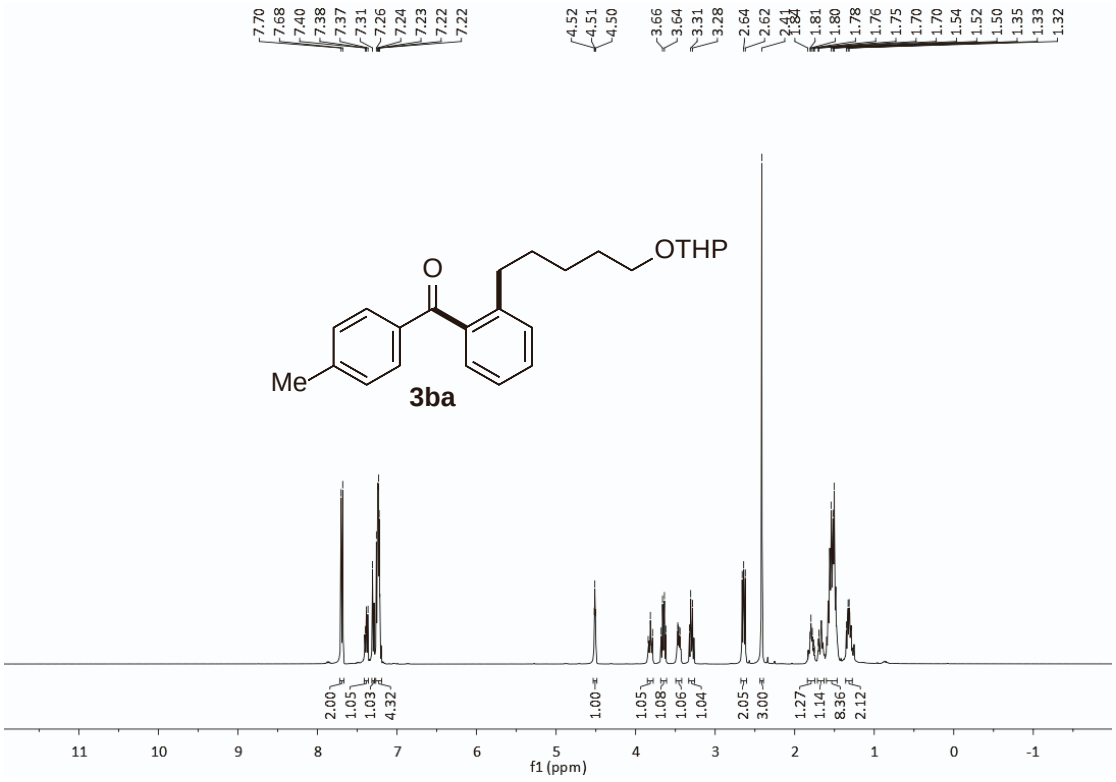
^{1}H NMR (400 MHz, $CDCl_3$)



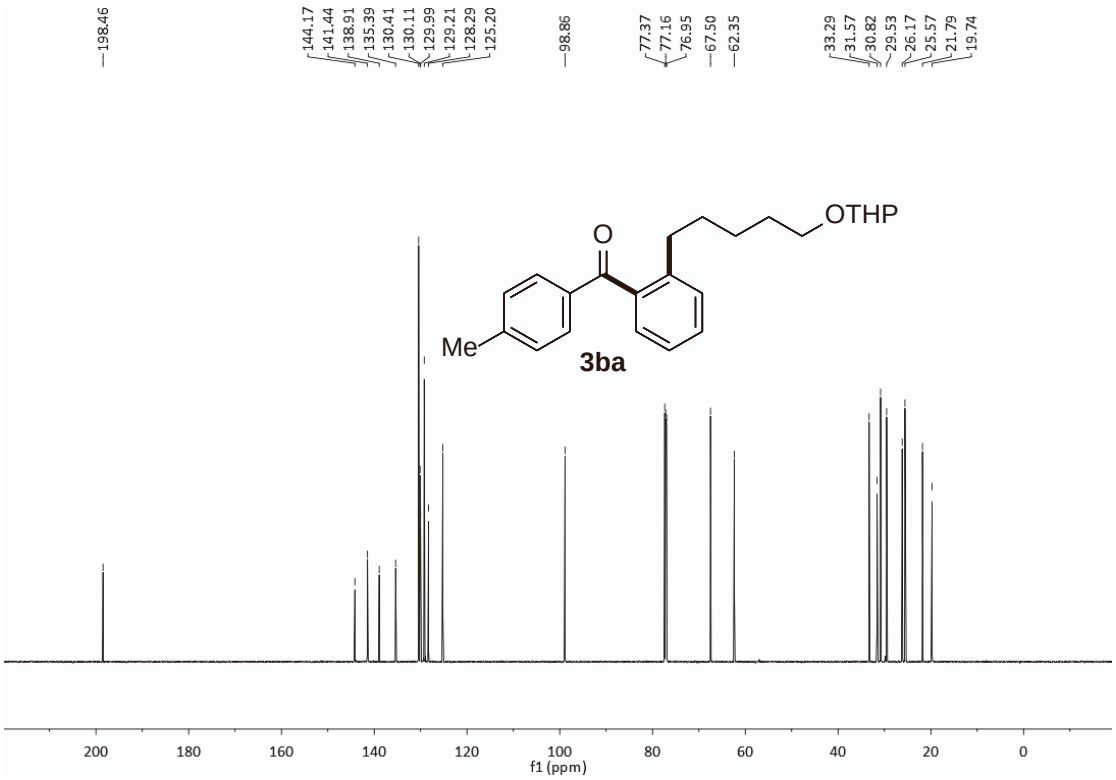
^{13}C NMR (151 MHz, $CDCl_3$)



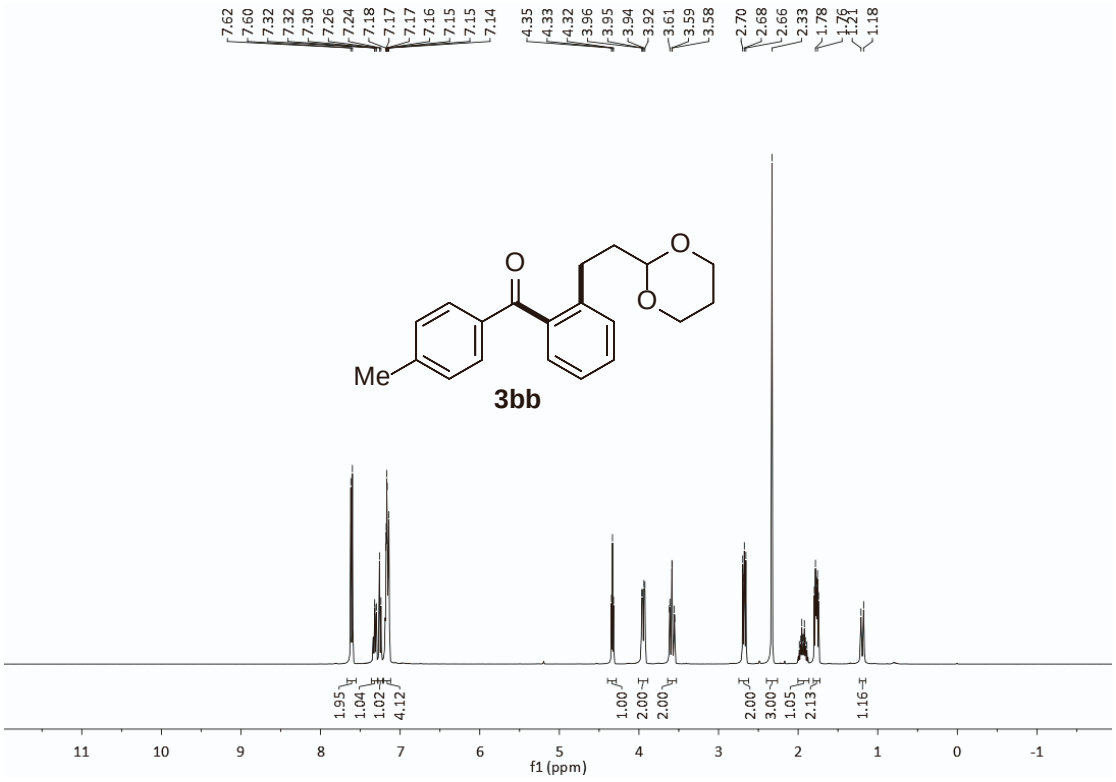
^{1}H NMR (400 MHz, $CDCl_3$)



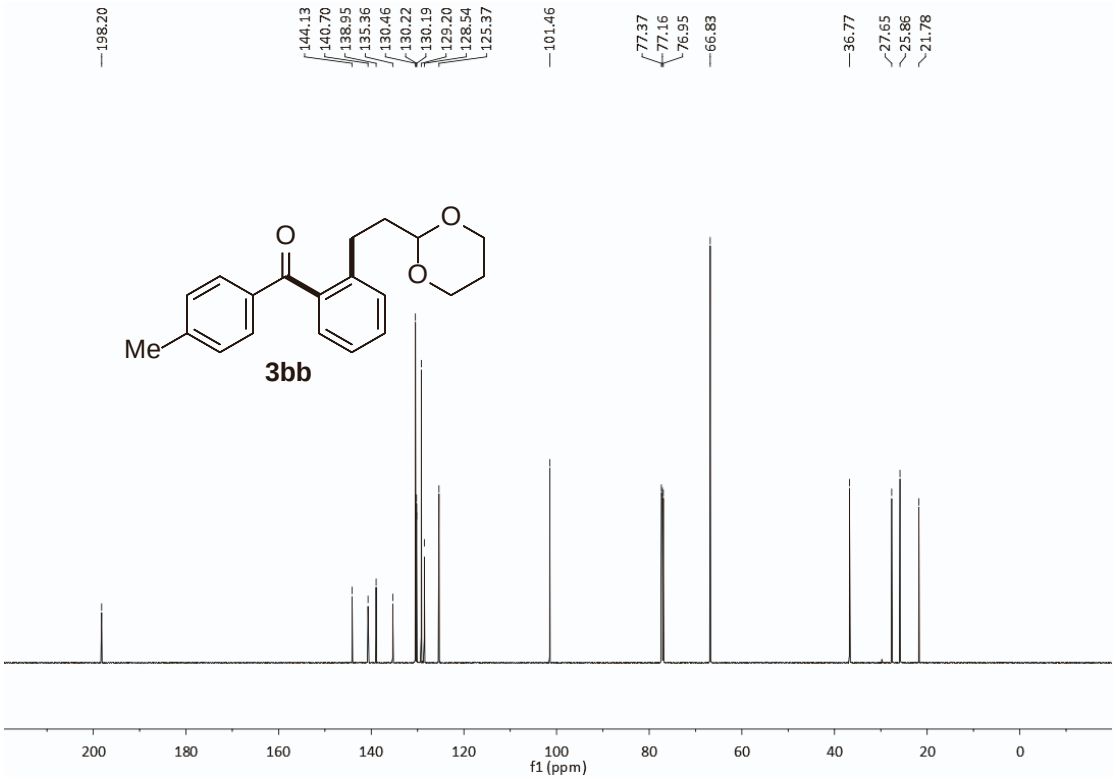
^{13}C NMR (151 MHz, $CDCl_3$)



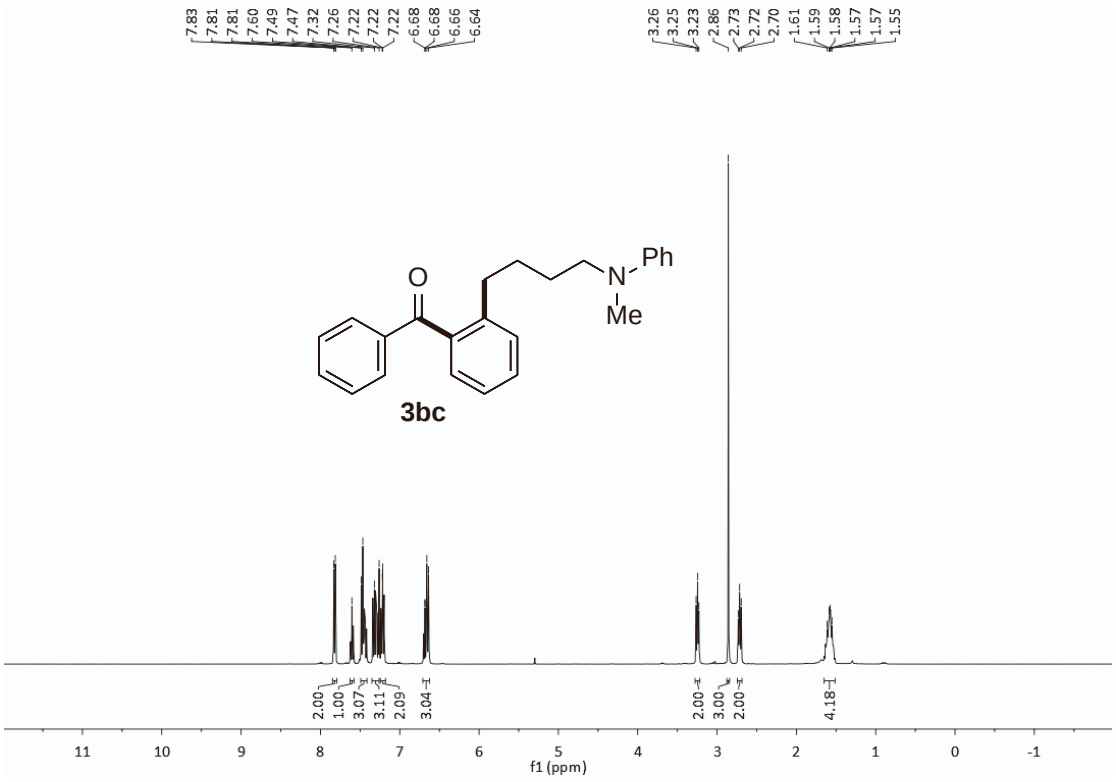
^{1}H NMR (400 MHz, $CDCl_3$)



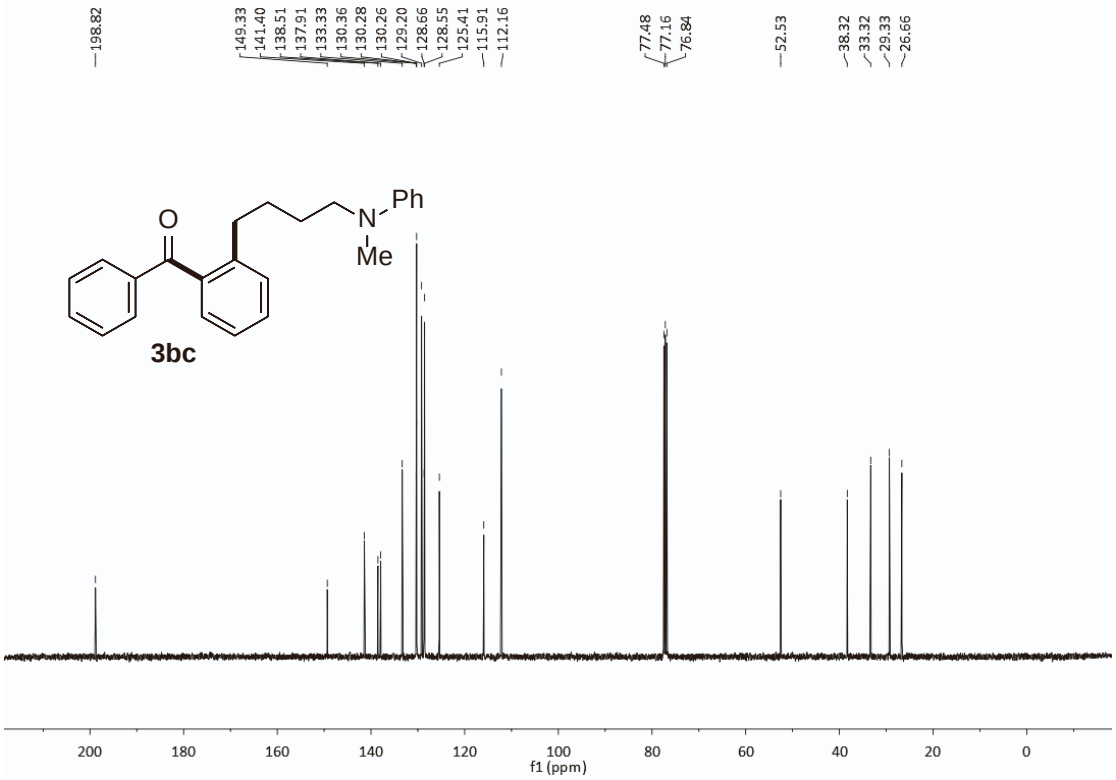
^{13}C NMR (151 MHz, $CDCl_3$)



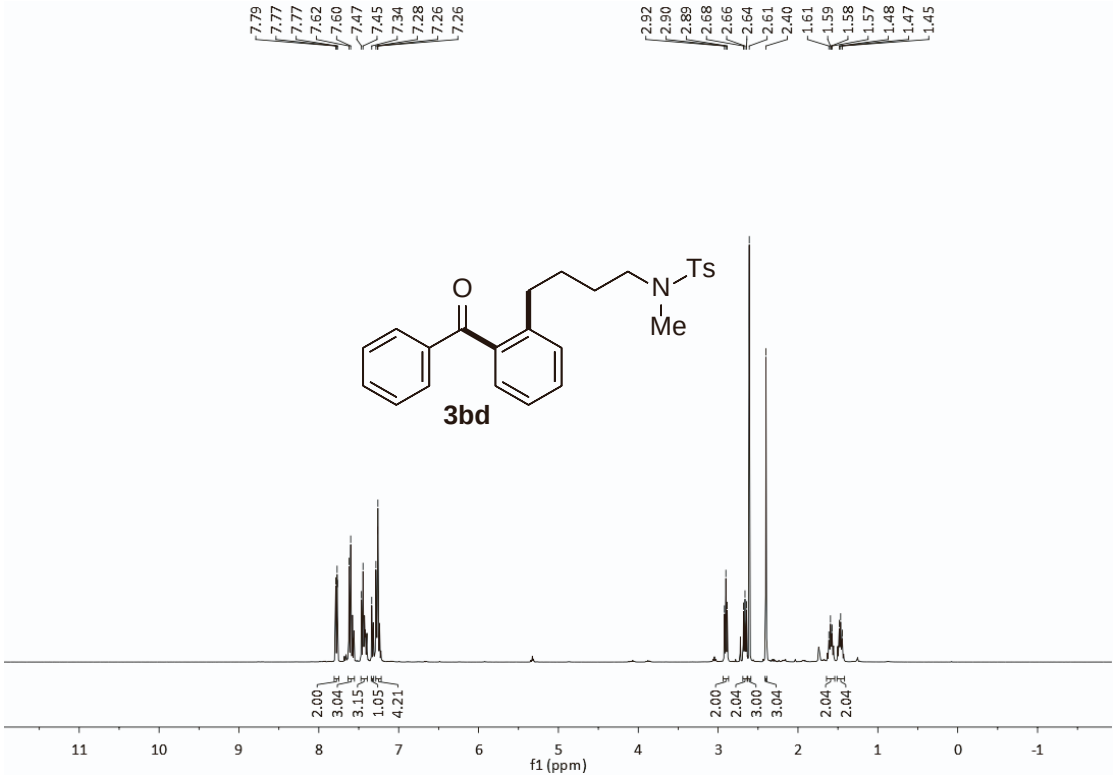
^{1}H NMR (400 MHz, $CDCl_3$)



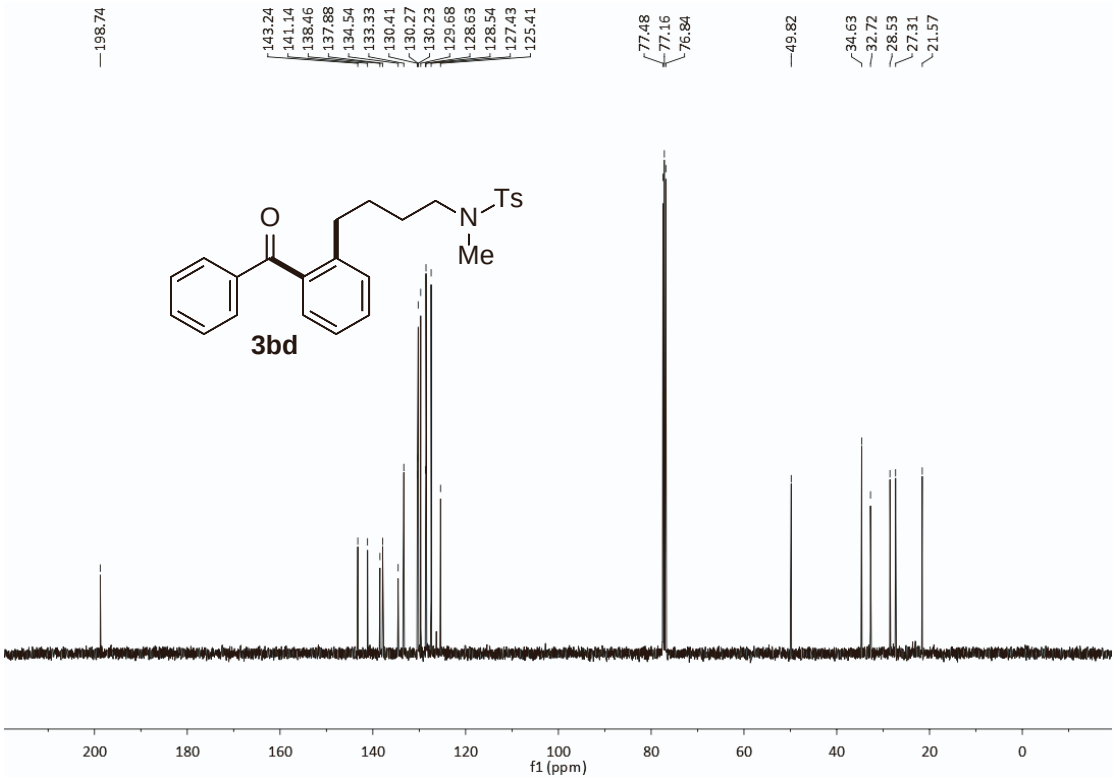
^{13}C NMR (101 MHz, $CDCl_3$)



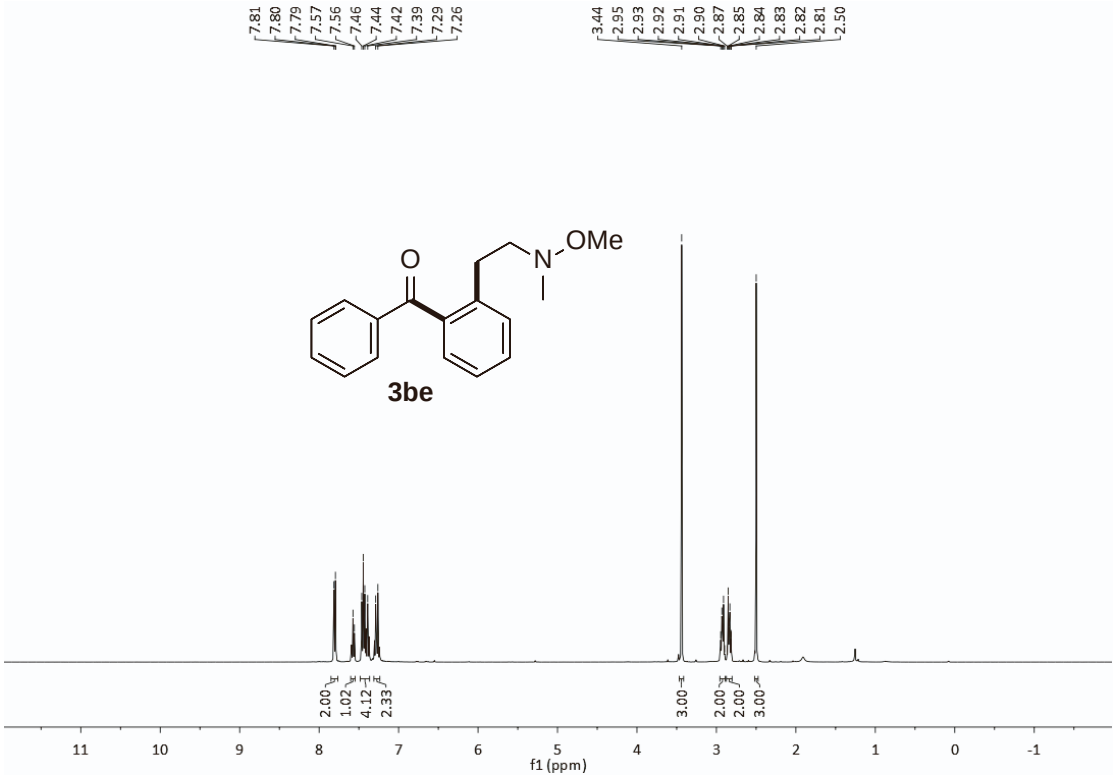
^{1}H NMR (400 MHz, $CDCl_3$)



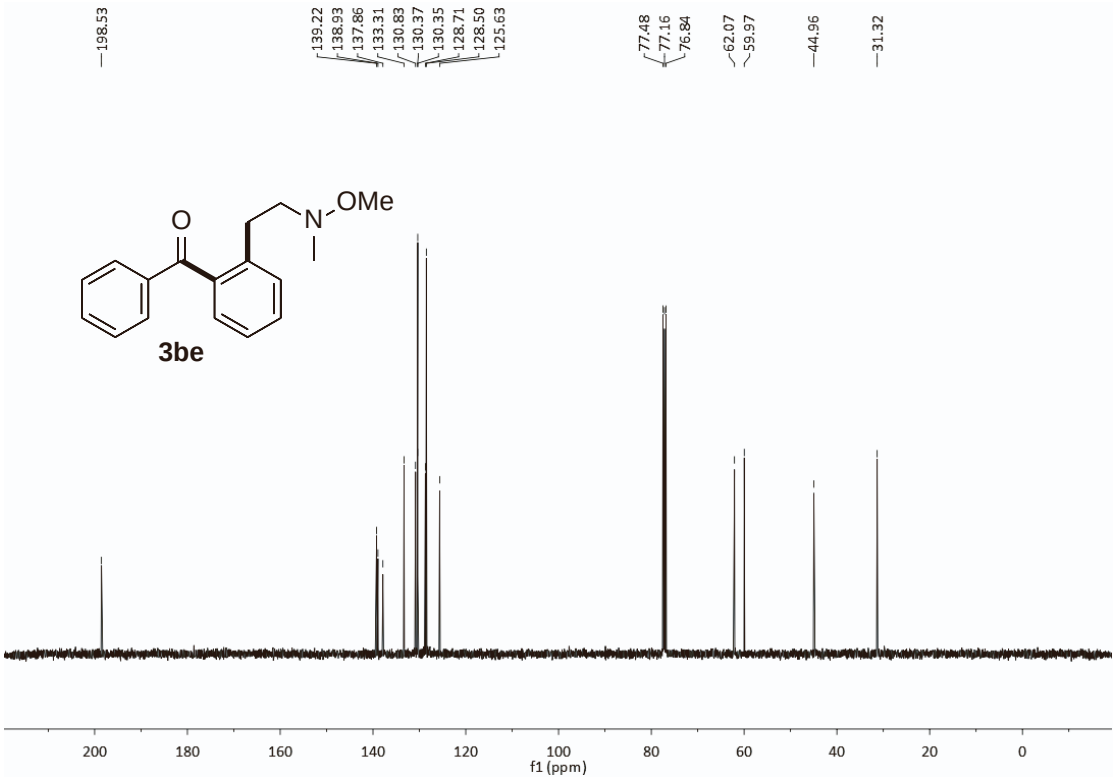
^{13}C NMR (101 MHz, $CDCl_3$)



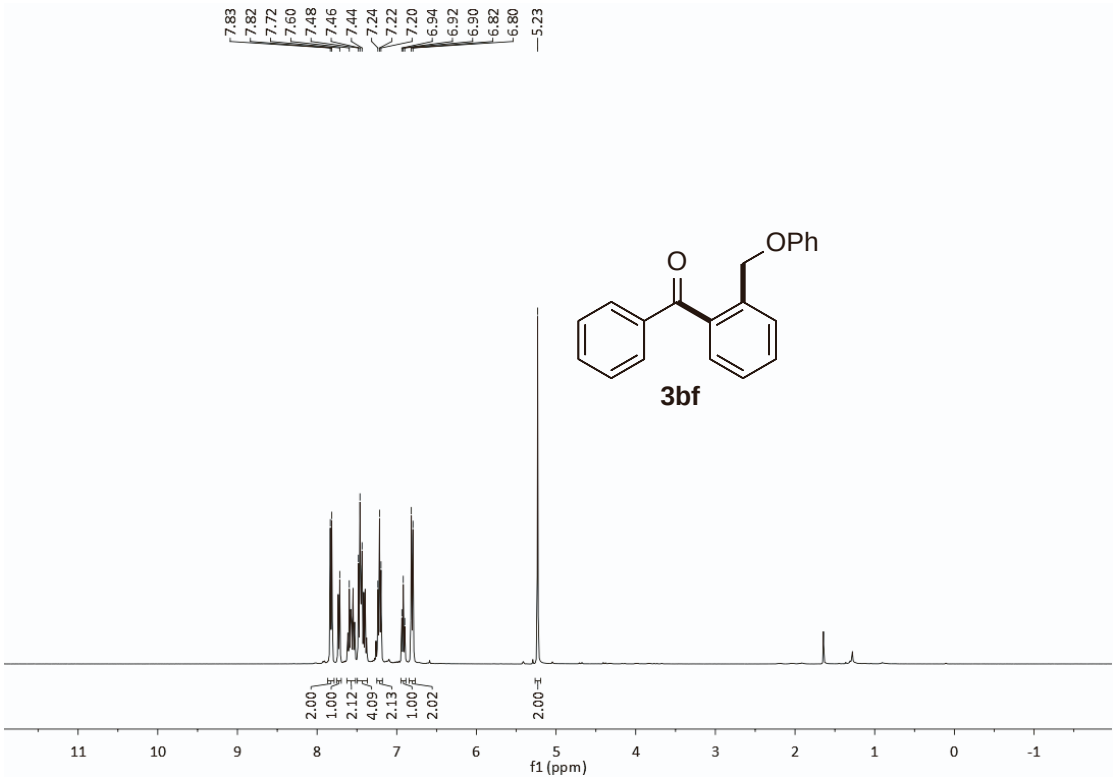
^{1}H NMR (400 MHz, $CDCl_3$)



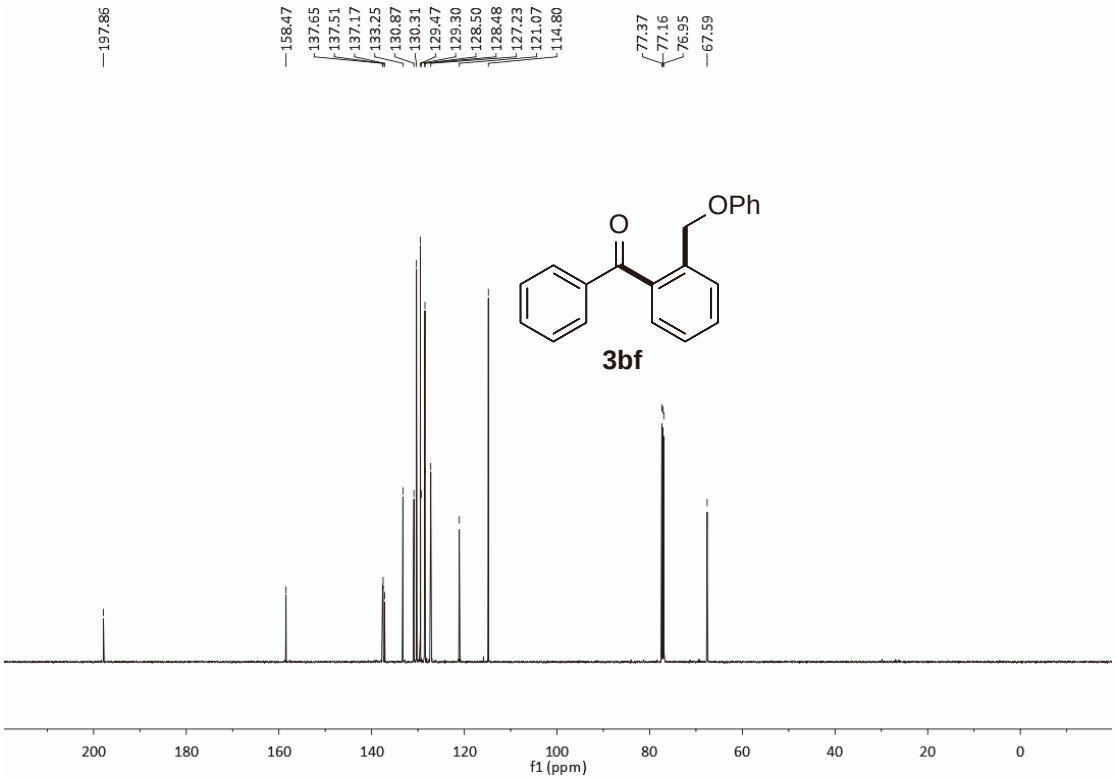
^{13}C NMR (101 MHz, $CDCl_3$)



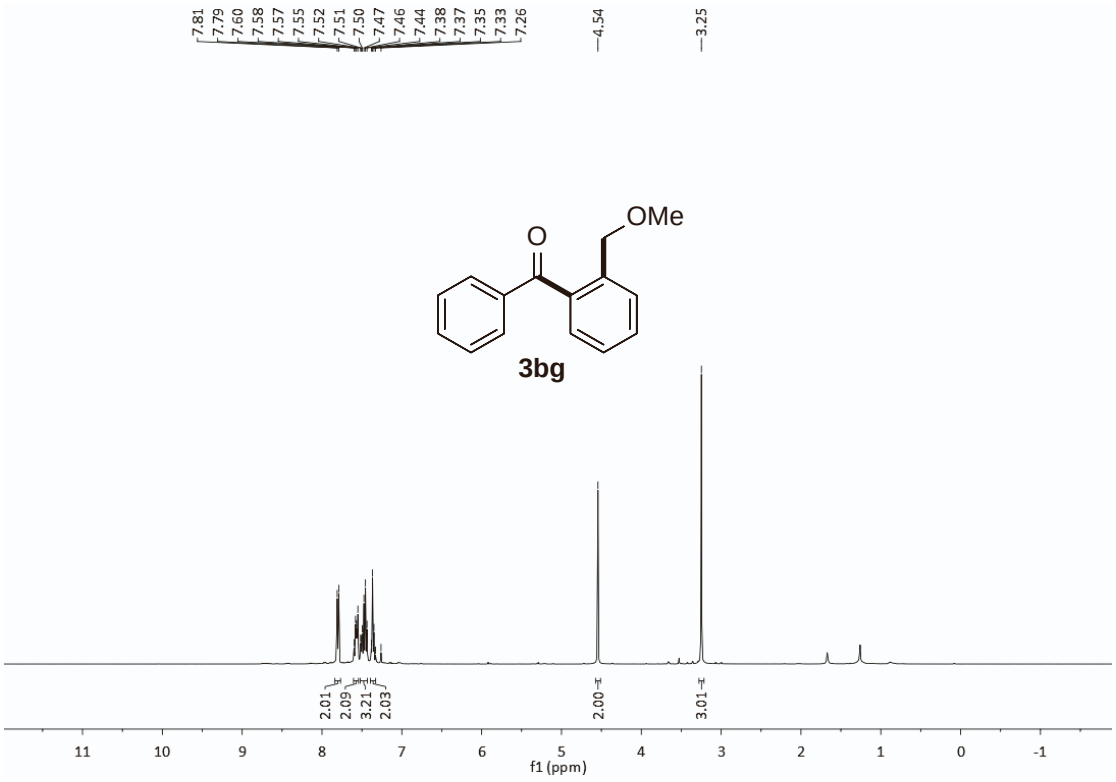
^{1}H NMR (400 MHz, $CDCl_3$)



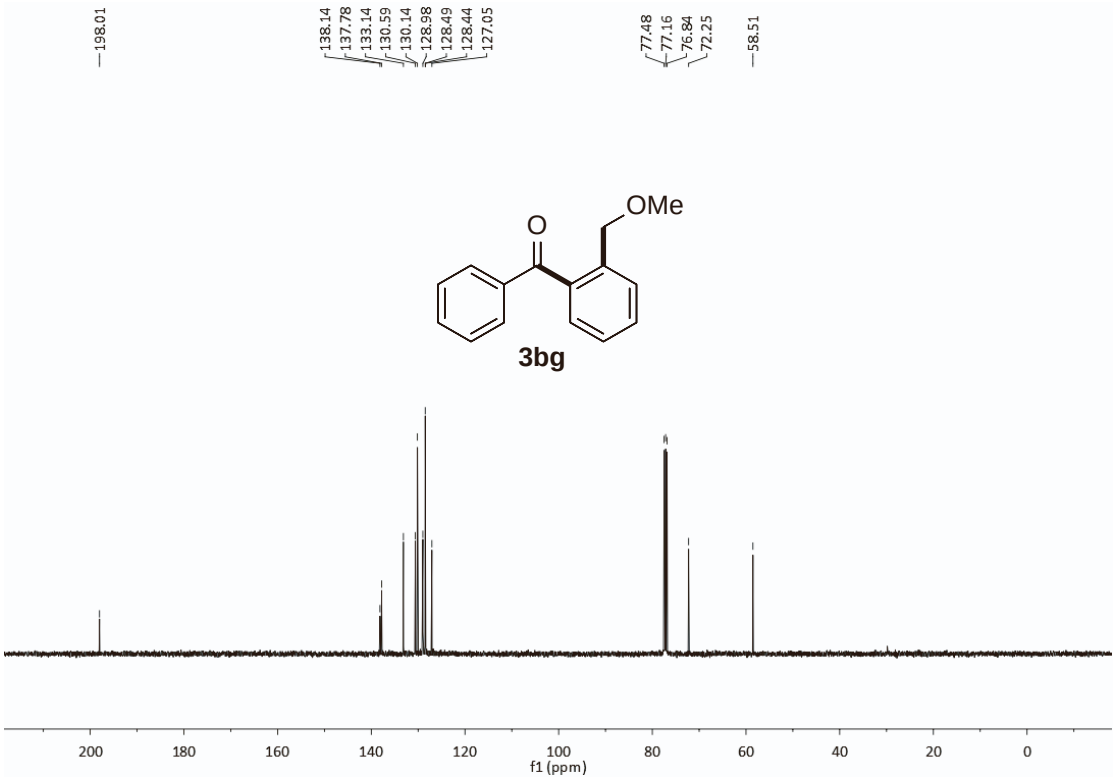
^{13}C NMR (151 MHz, $CDCl_3$)



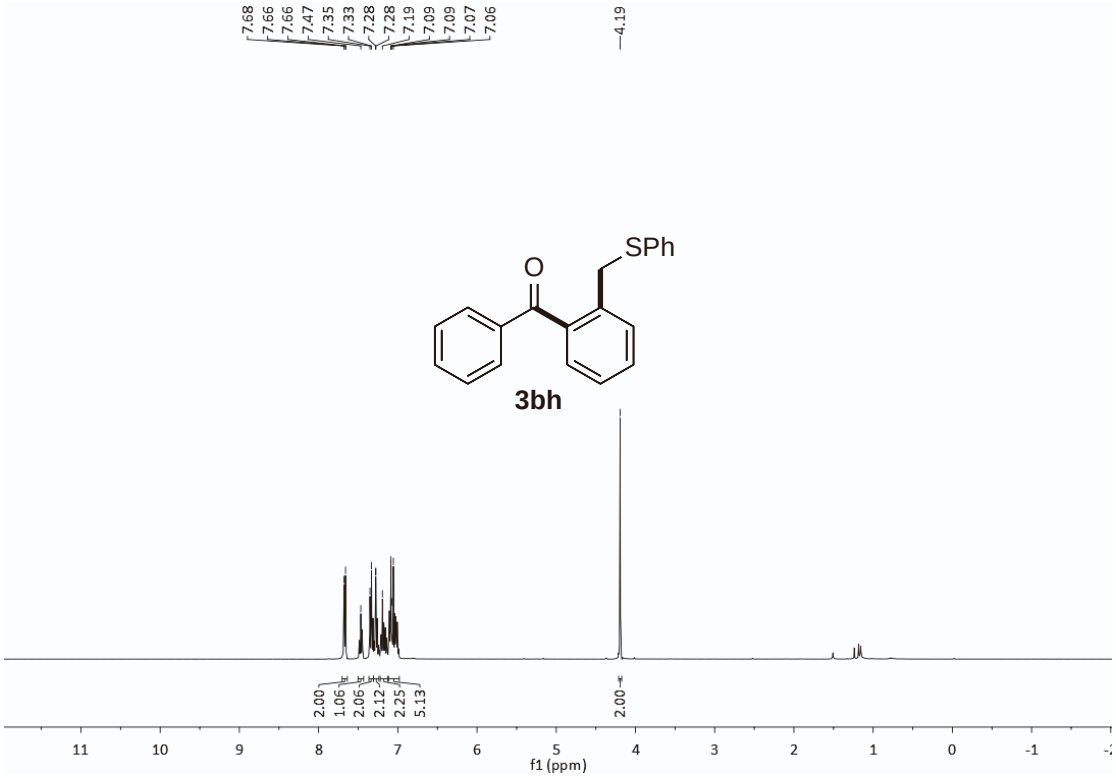
^{1}H NMR (400 MHz, $CDCl_3$)



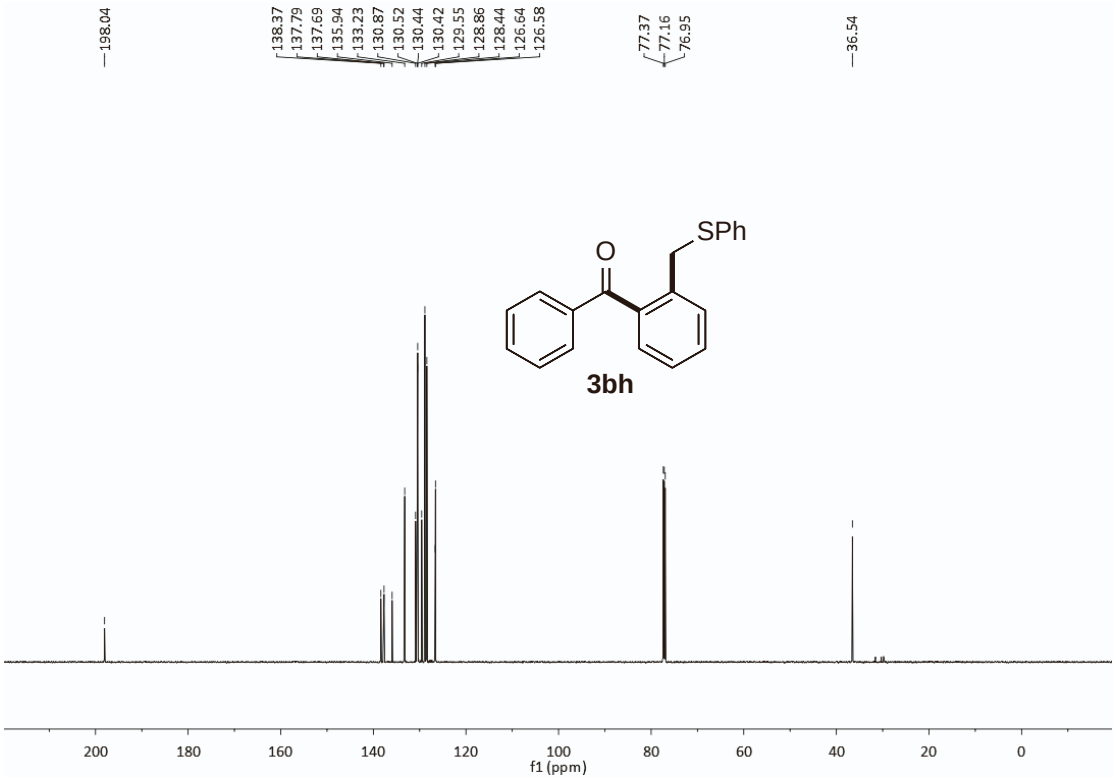
^{13}C NMR (101 MHz, $CDCl_3$)



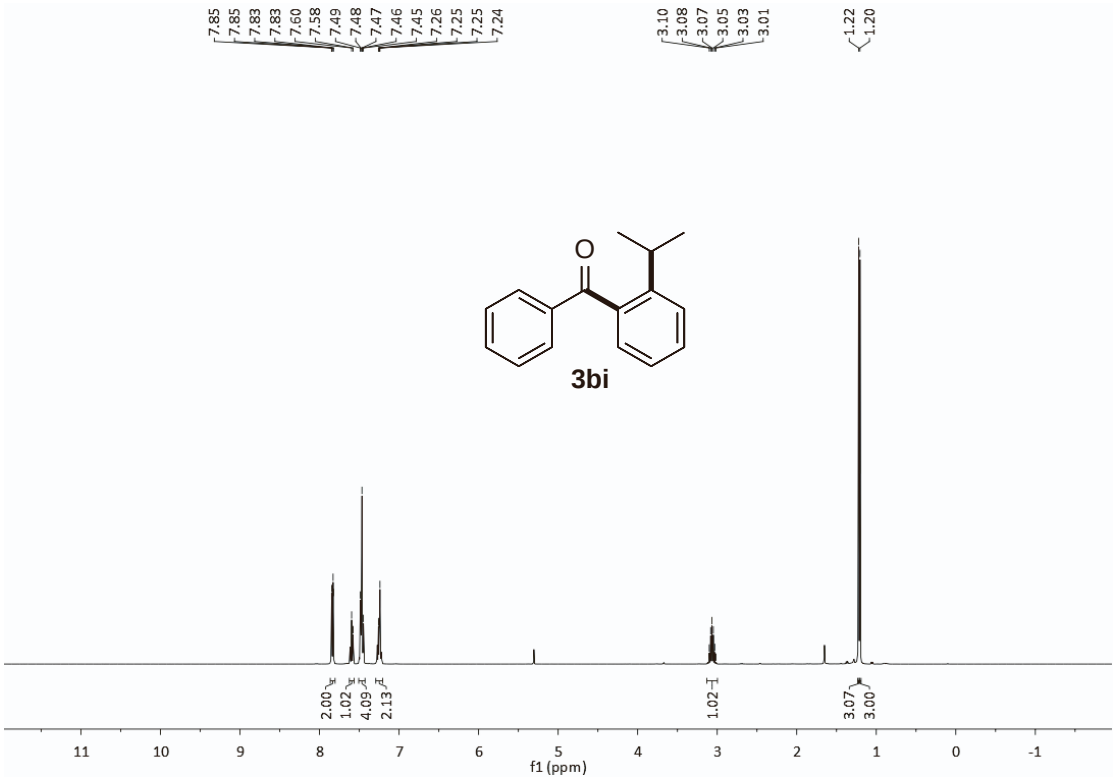
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (151 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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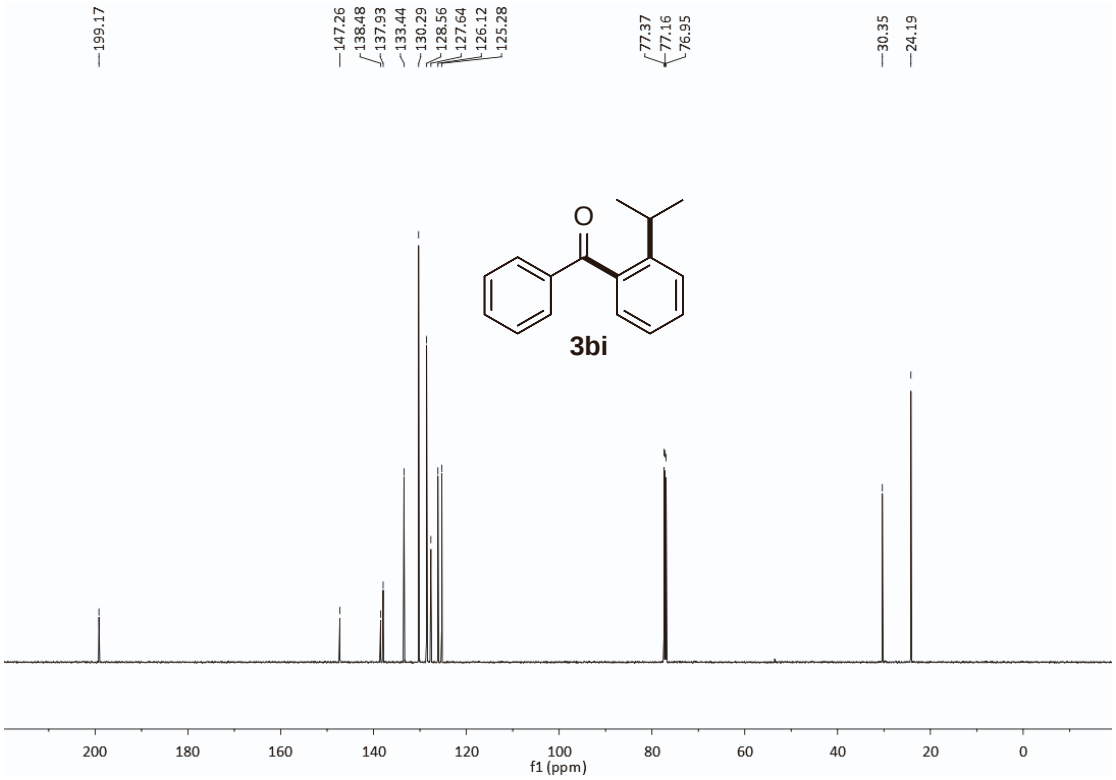
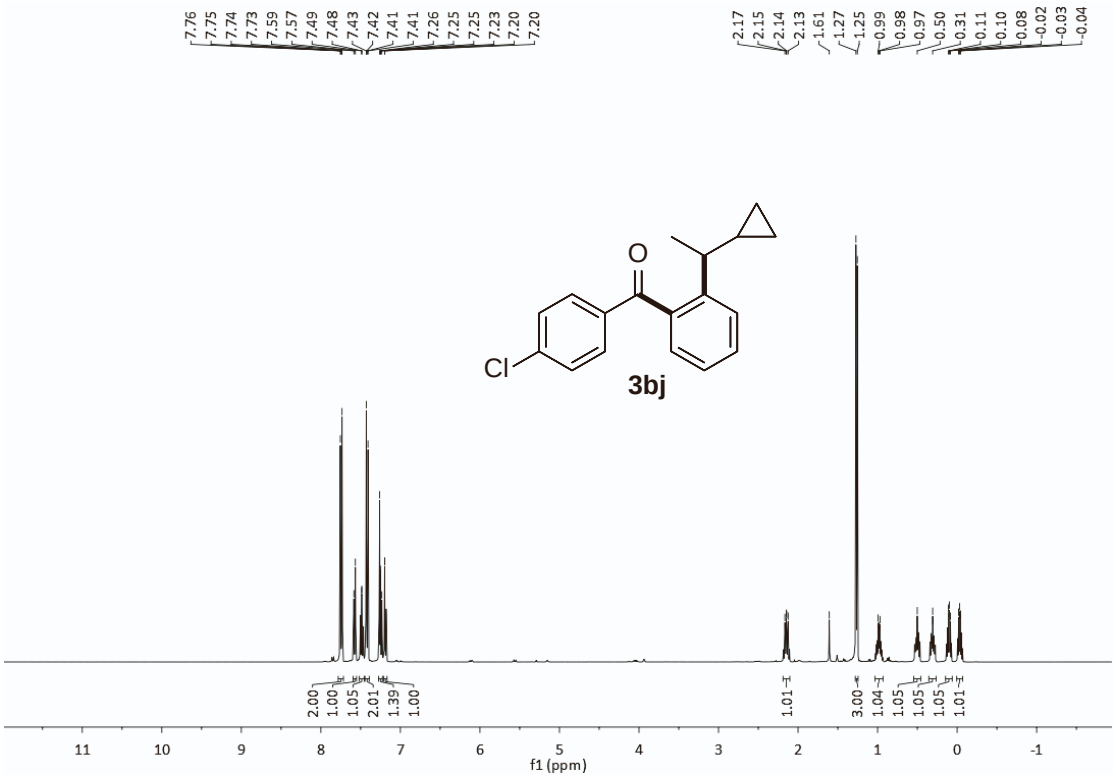
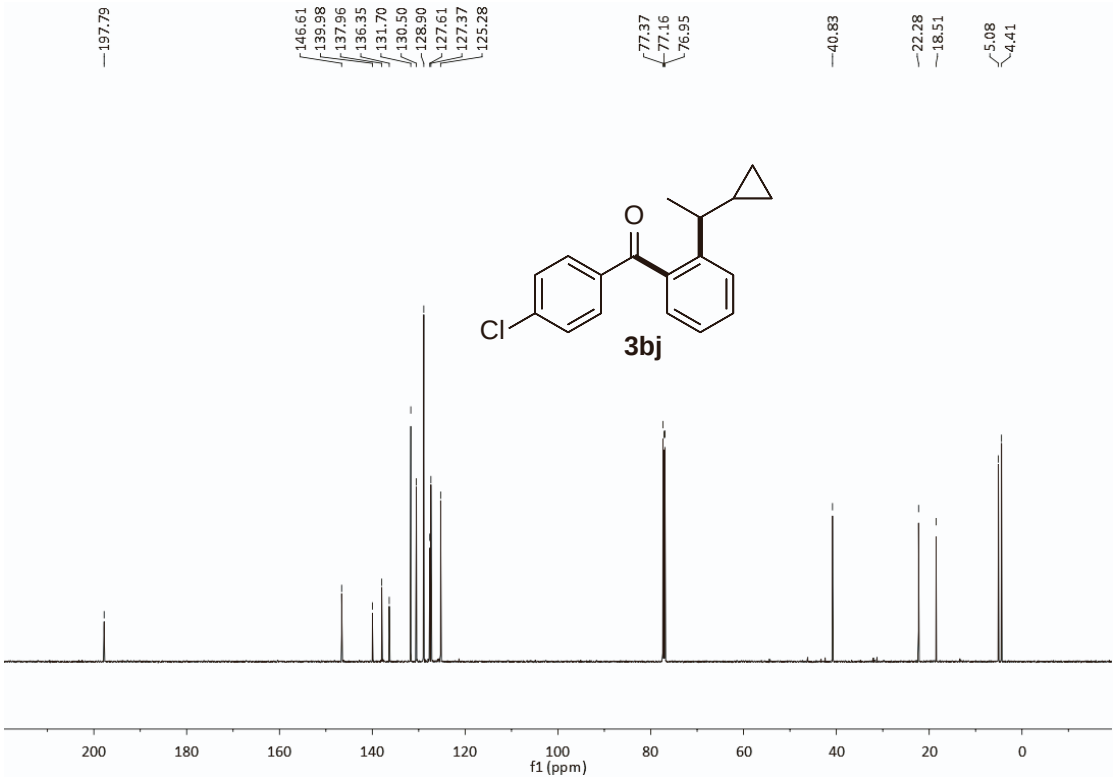


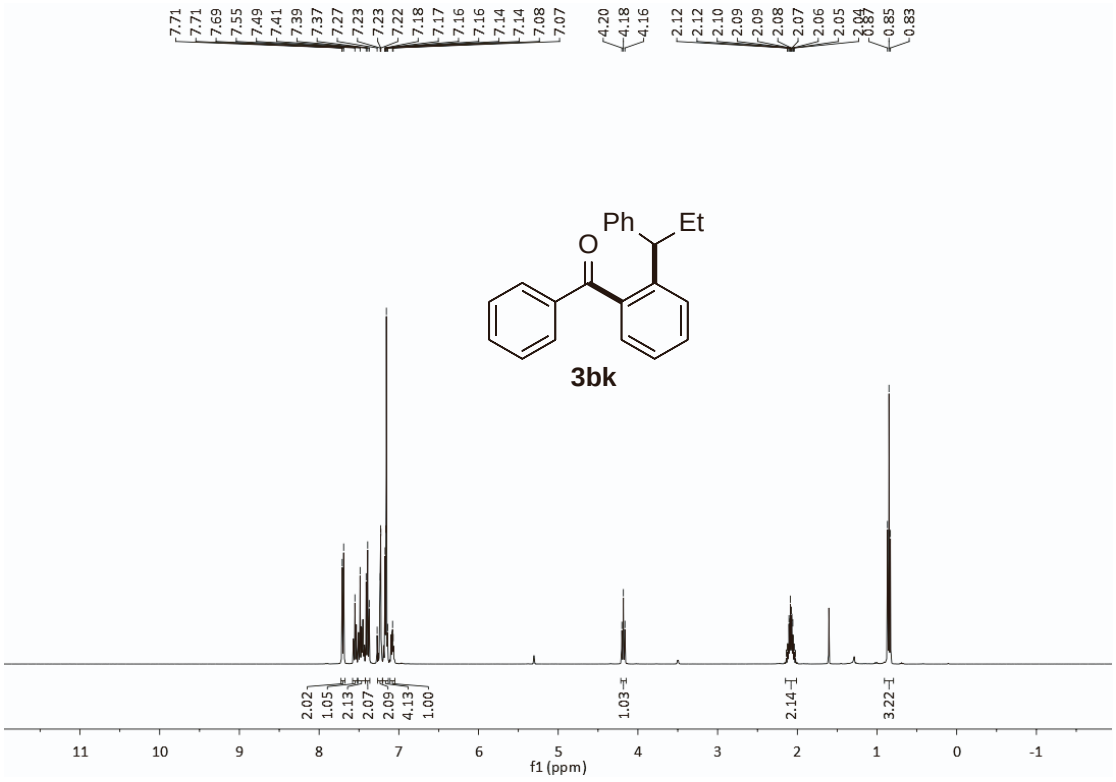
^{1}H NMR (400 MHz, $CDCl_3$)



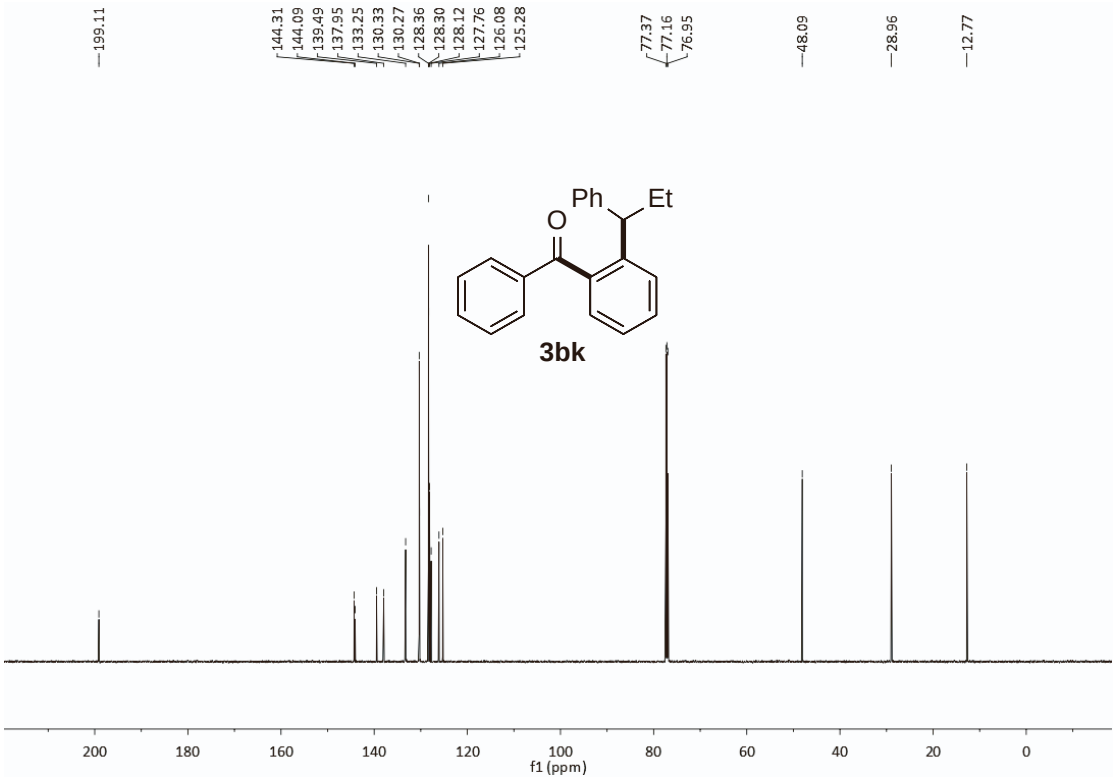
^{13}C NMR (151 MHz, $CDCl_3$)



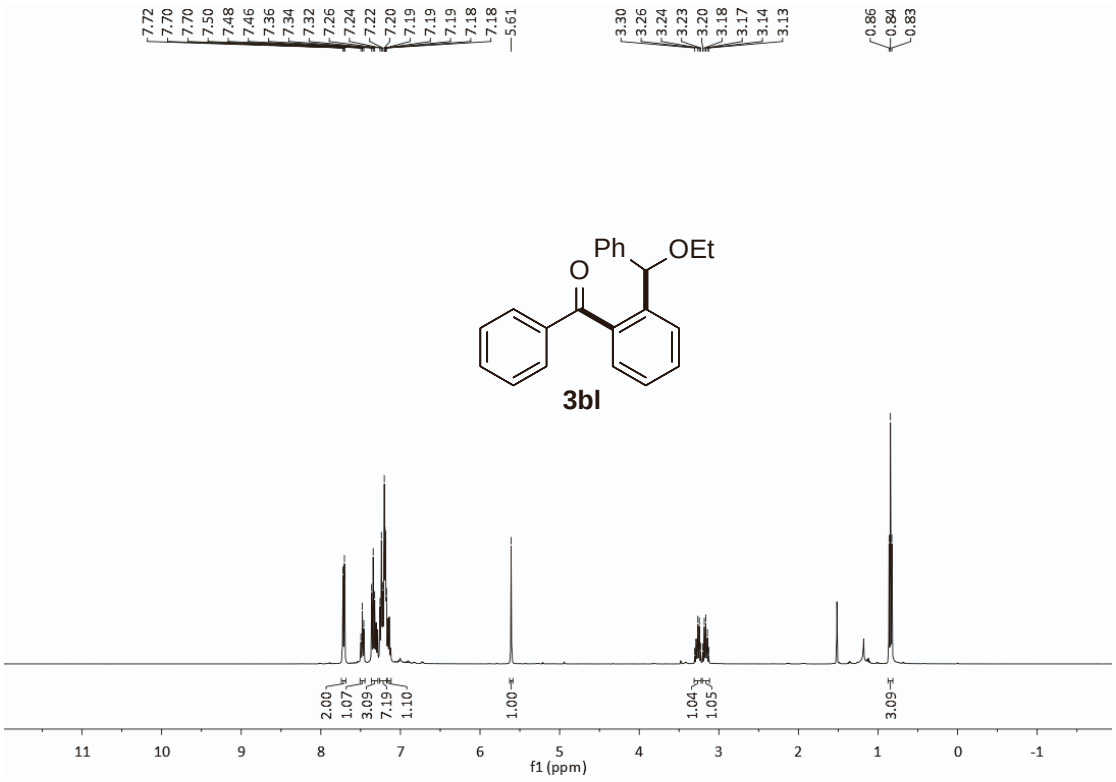
^{1}H NMR (400 MHz, $CDCl_3$)



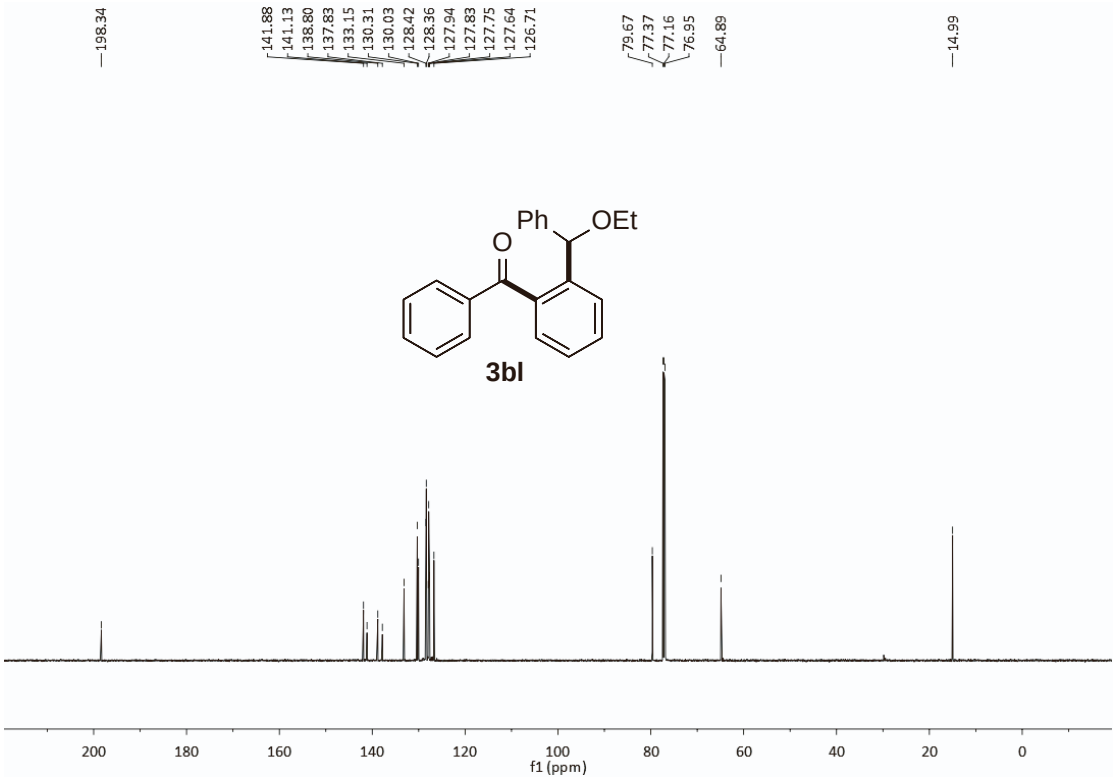
^{13}C NMR (151 MHz, $CDCl_3$)



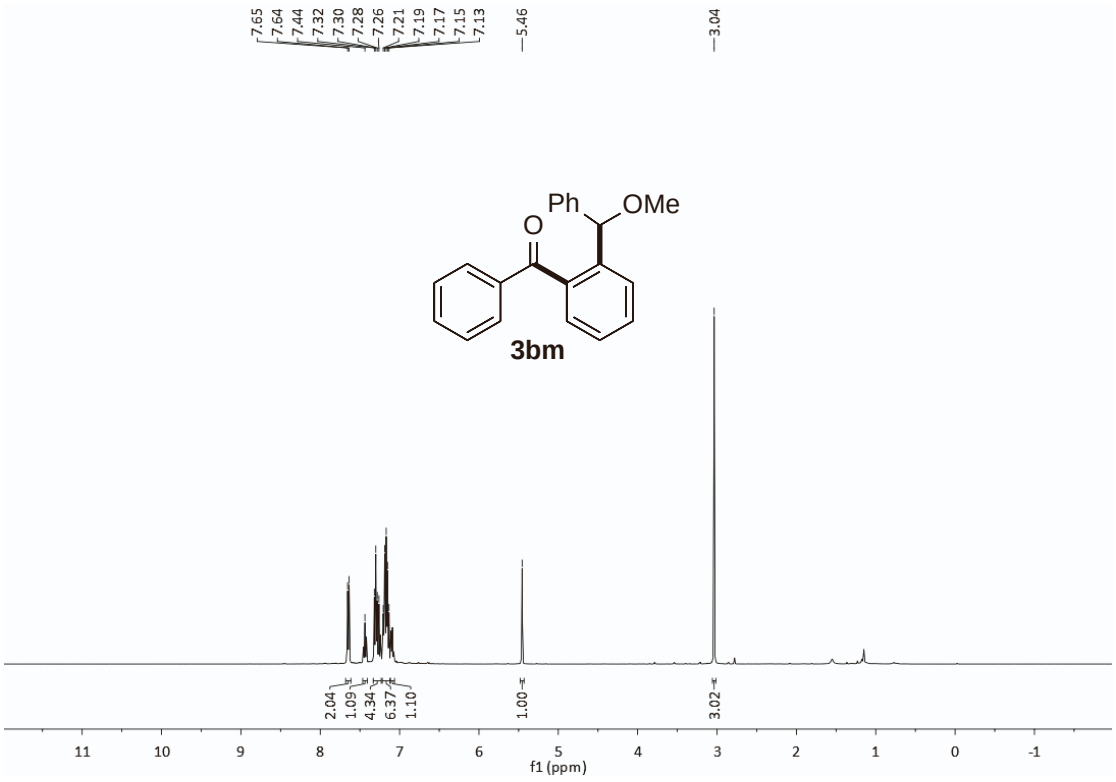
^{1}H NMR (400 MHz, $CDCl_3$)



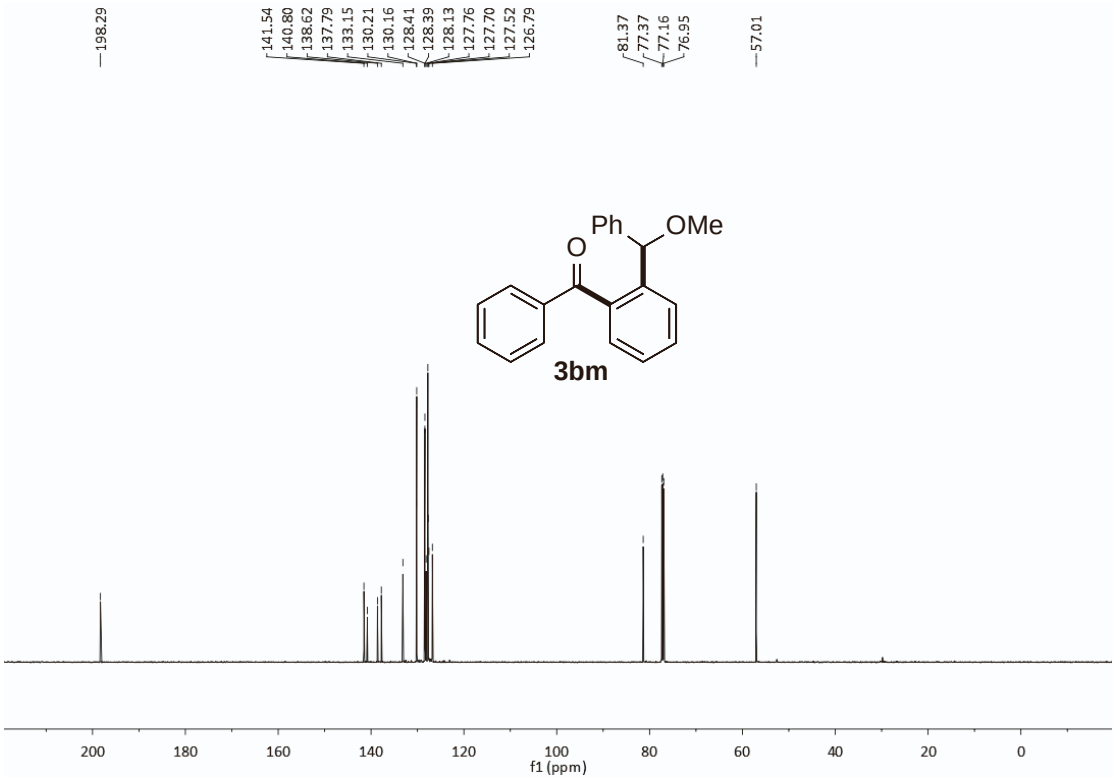
^{13}C NMR (151 MHz, $CDCl_3$)



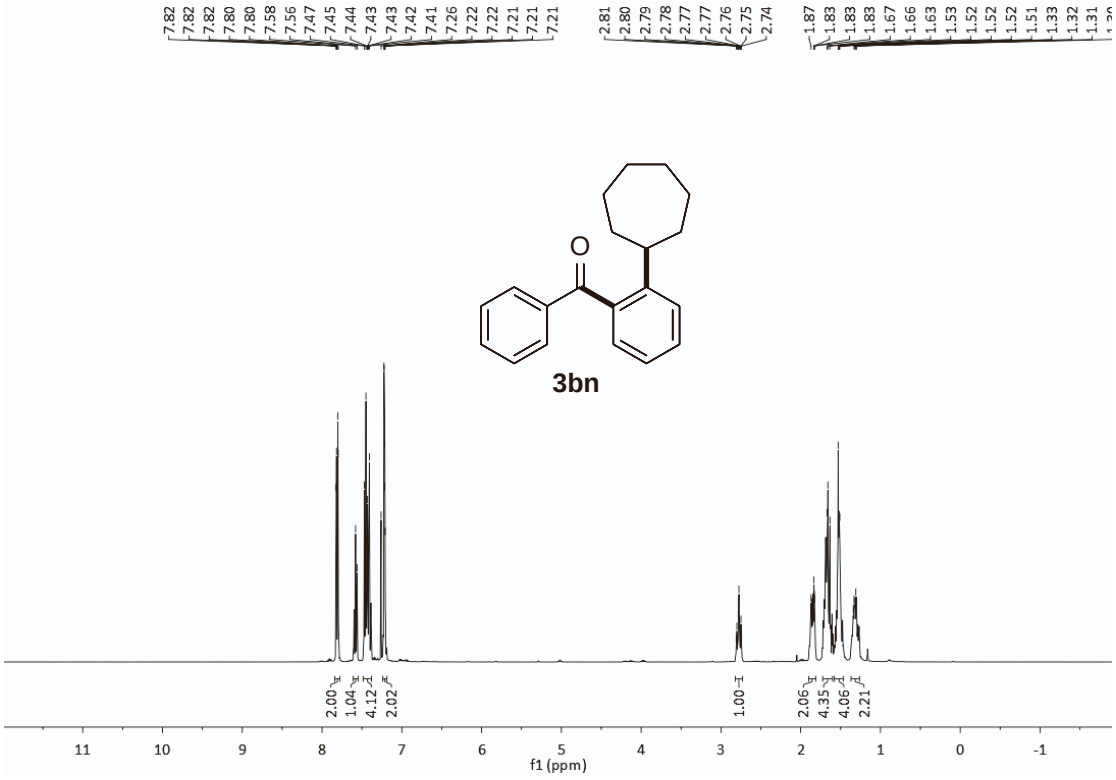
^{1}H NMR (400 MHz, $CDCl_3$)



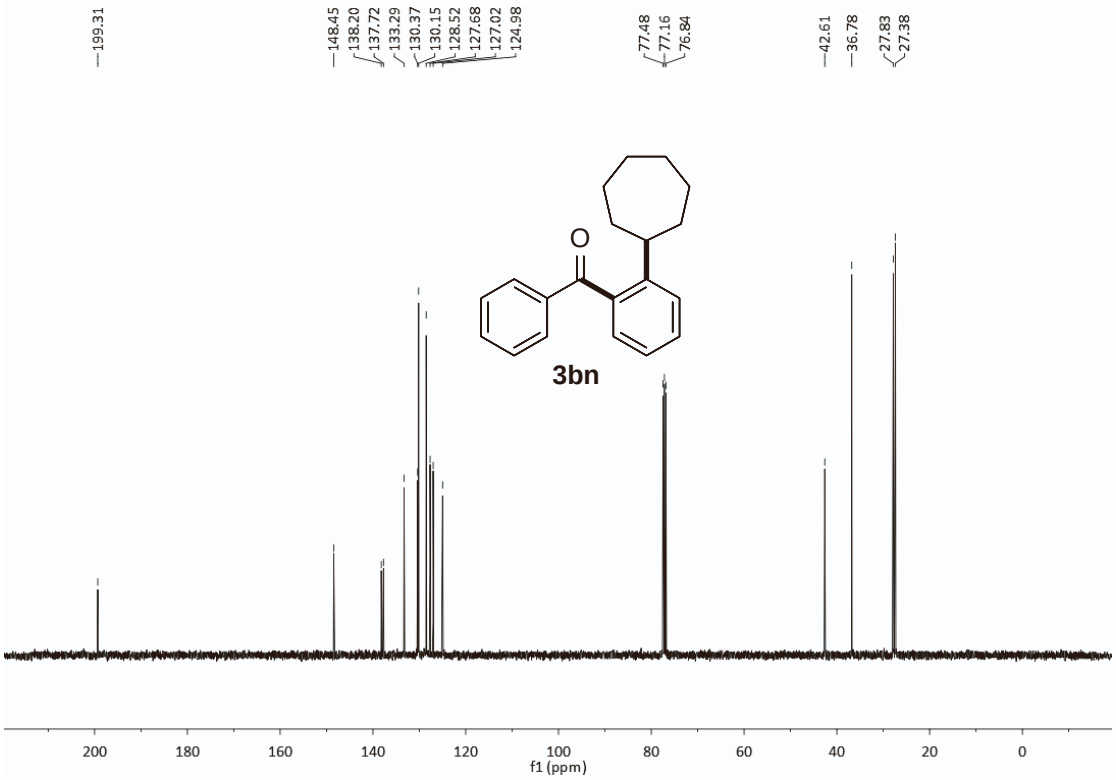
^{13}C NMR (151 MHz, $CDCl_3$)



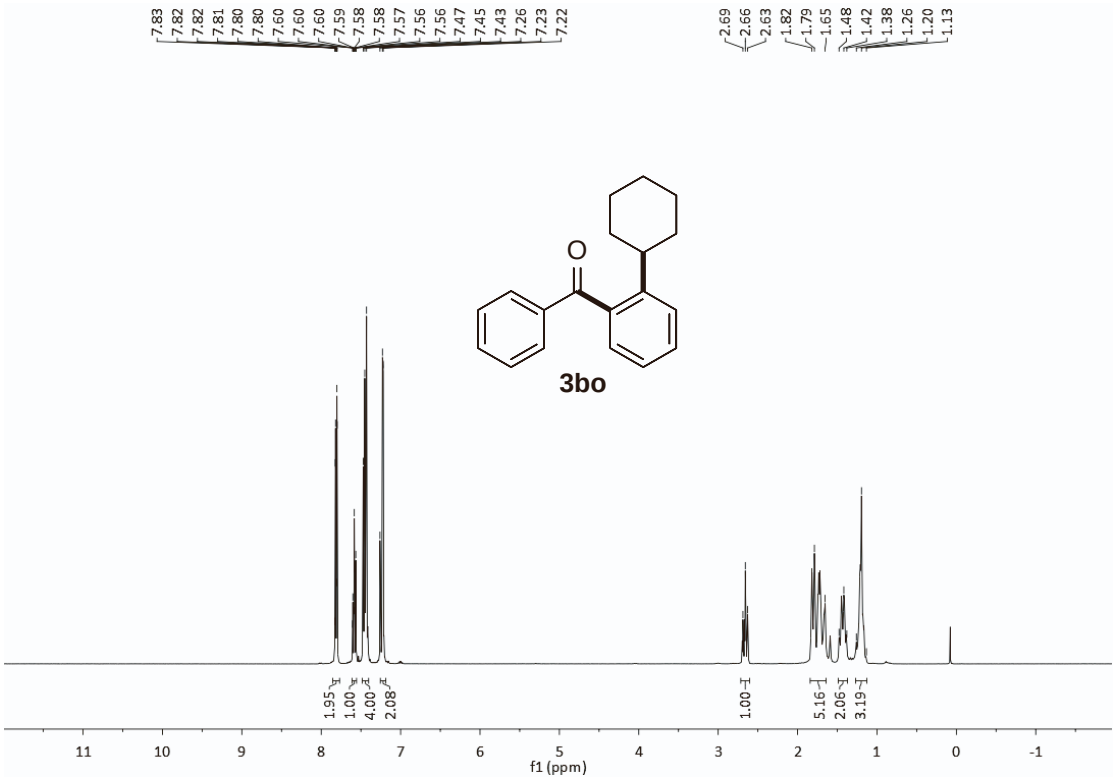
^{1}H NMR (400 MHz, $CDCl_3$)



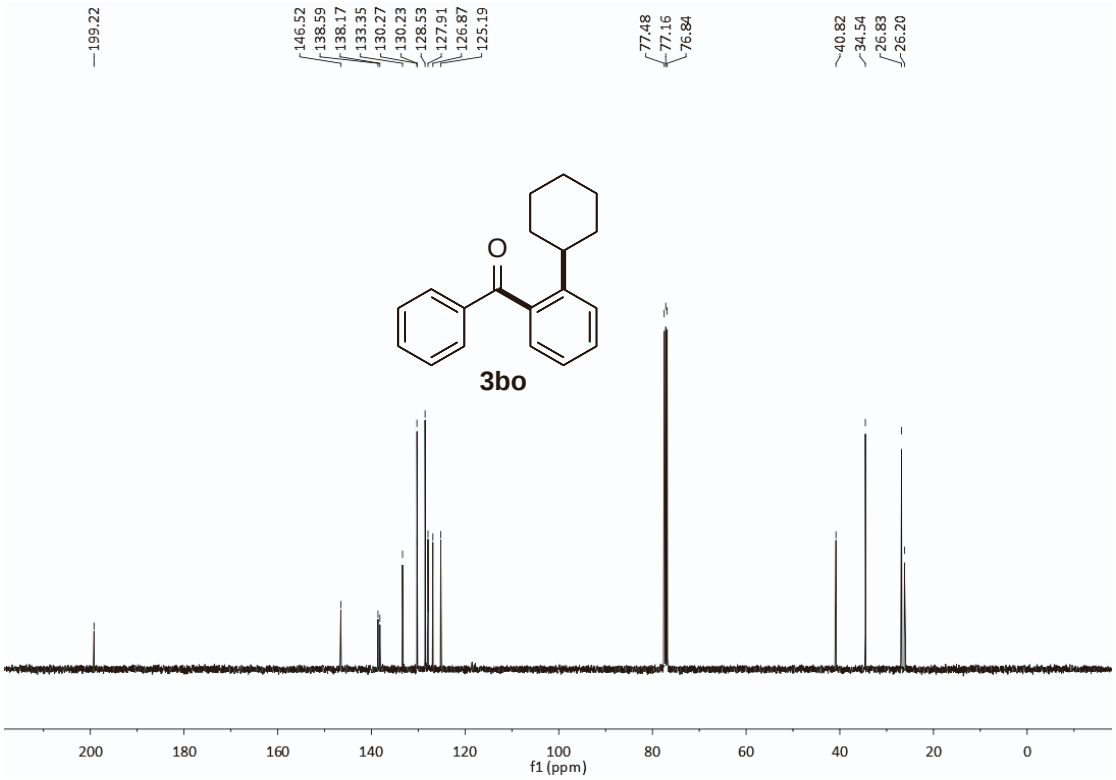
^{13}C NMR (101 MHz, $CDCl_3$)



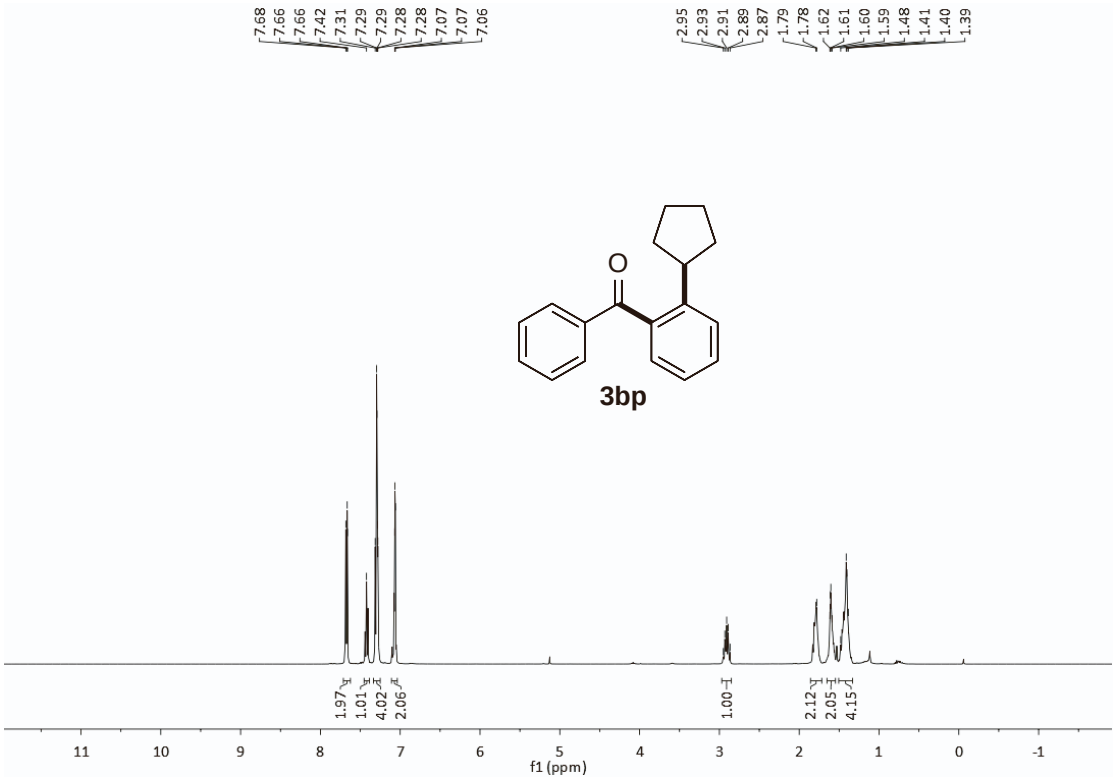
^{1}H NMR (400 MHz, $CDCl_3$)



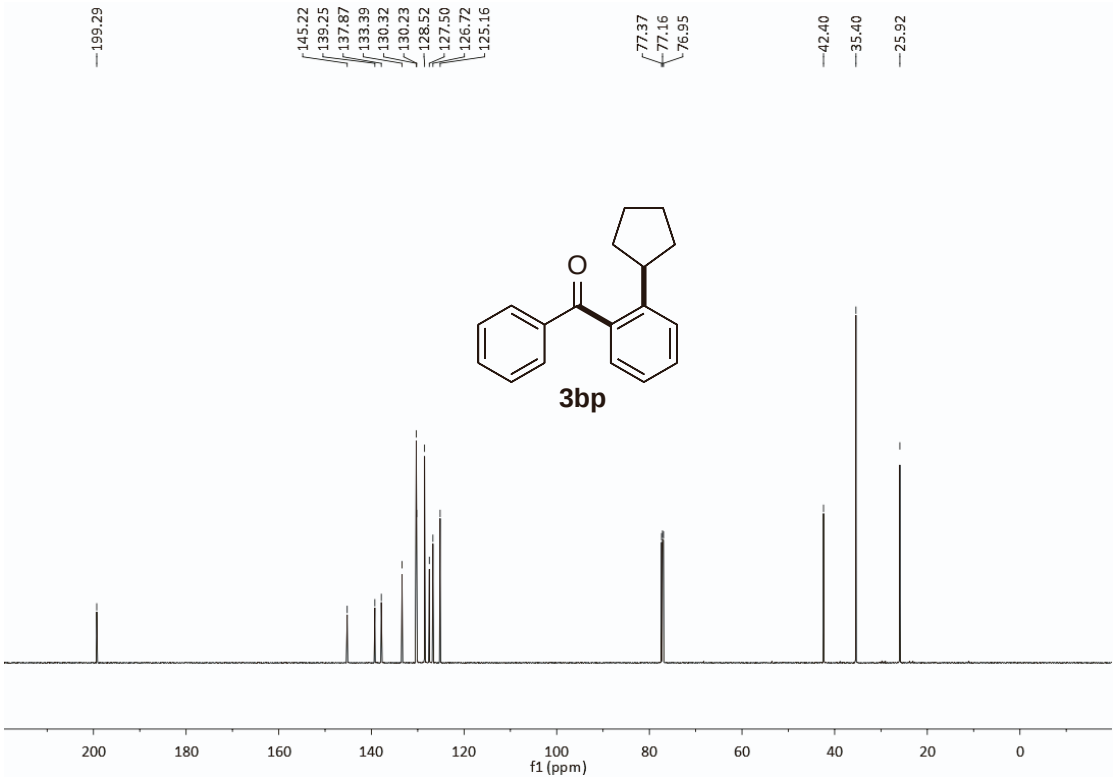
^{13}C NMR (101 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (151 MHz, $CDCl_3$)



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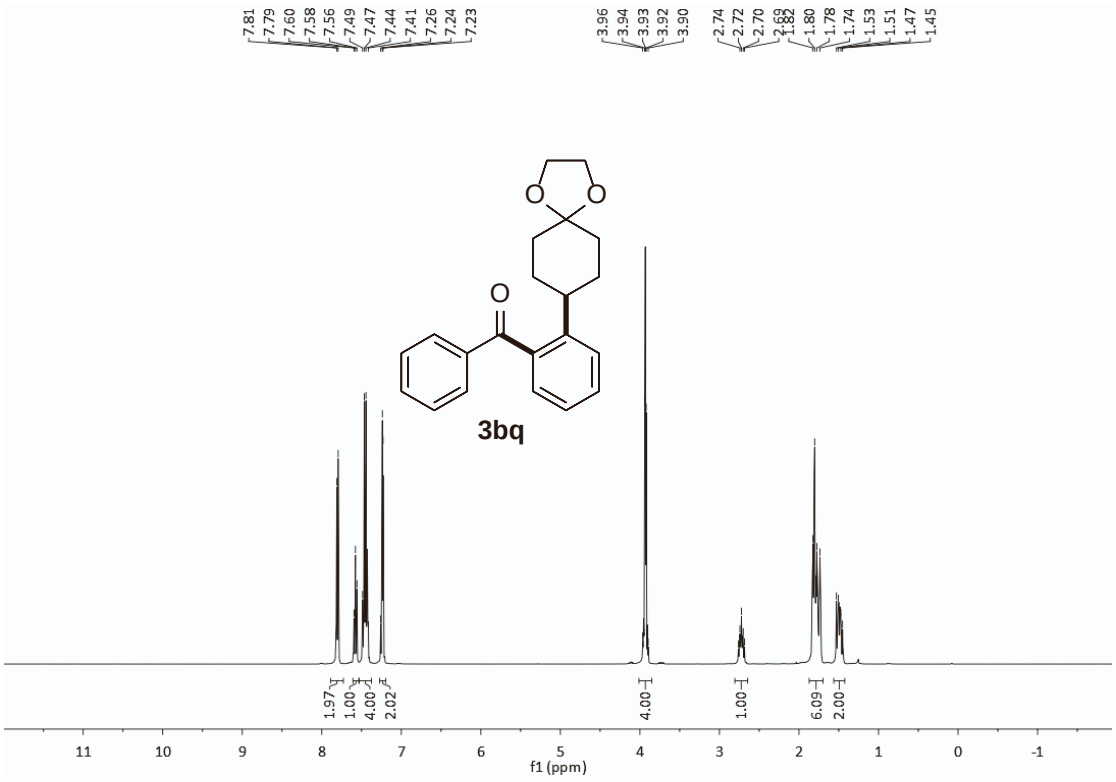
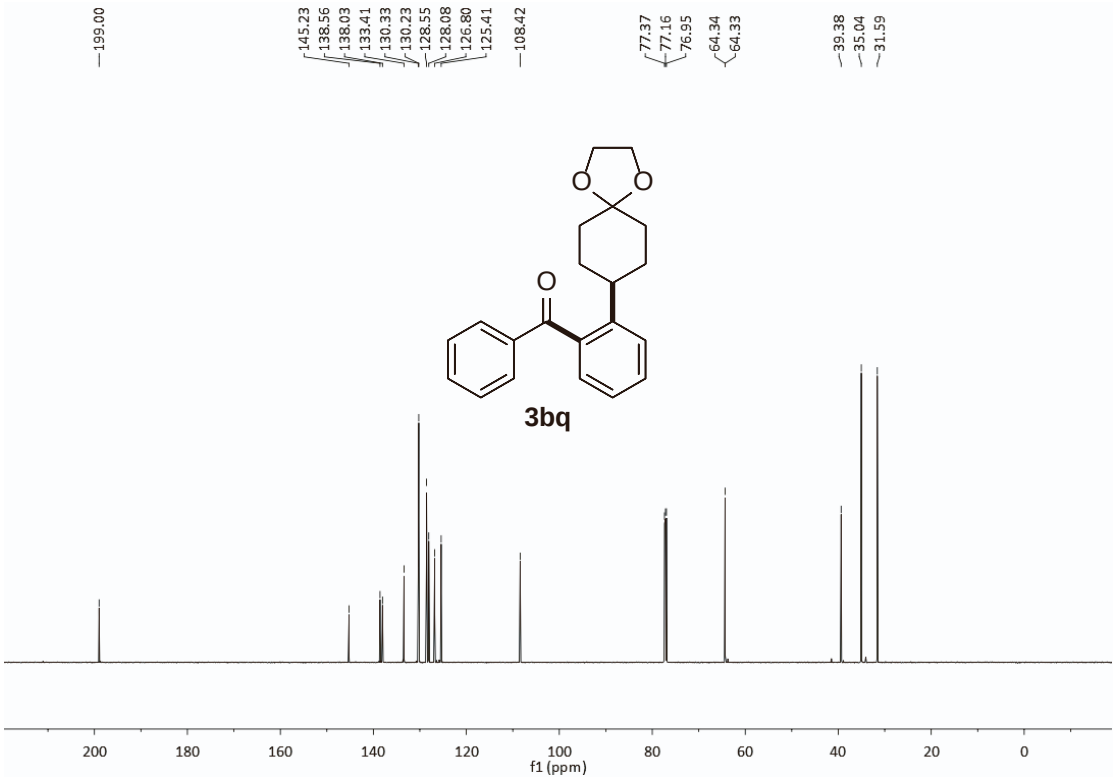


^{13}C NMR (151 MHz, $CDCl_3$)



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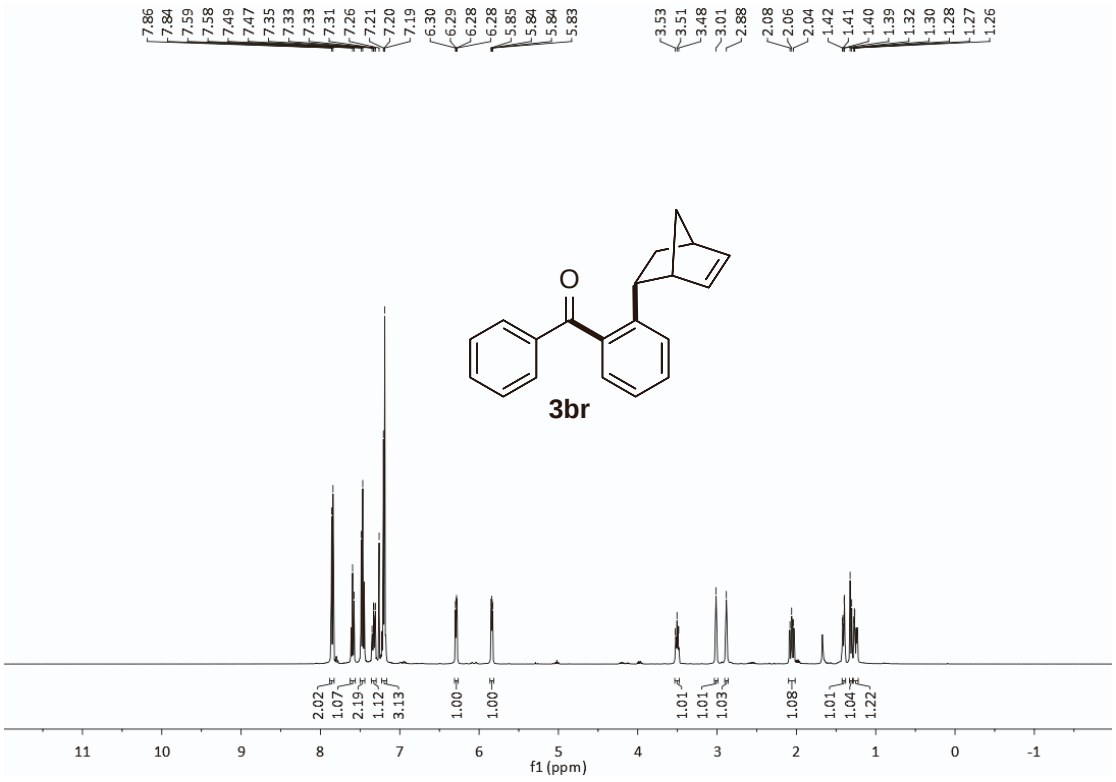

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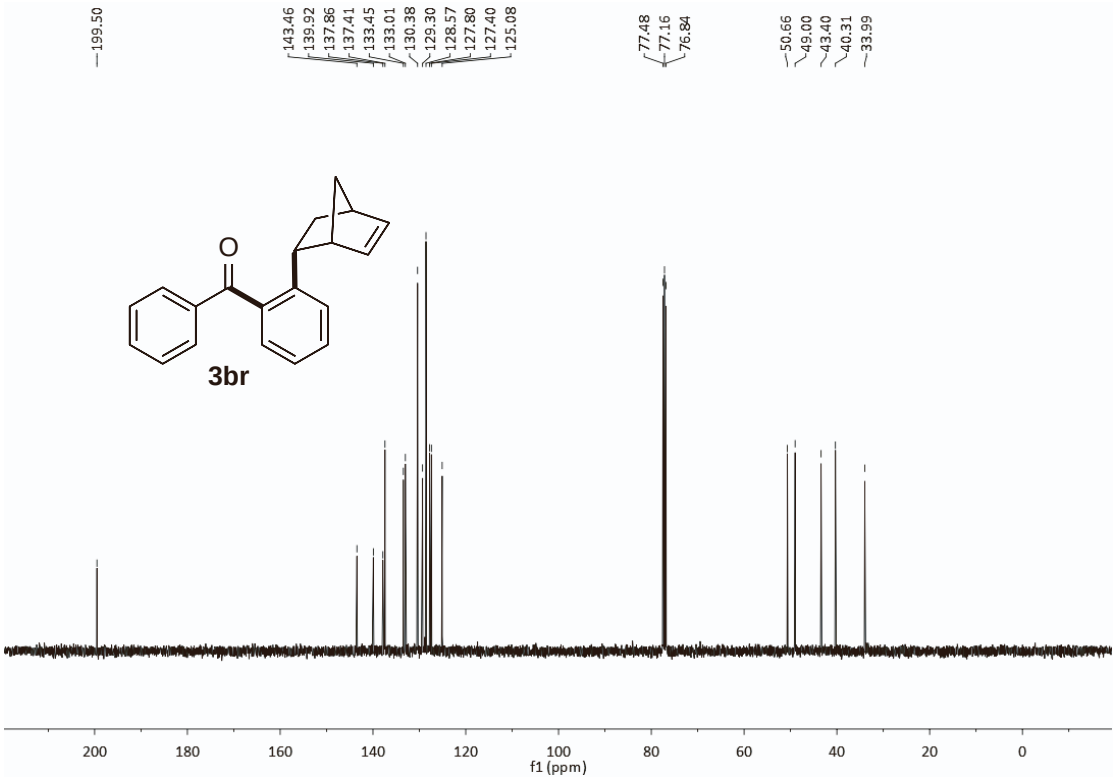

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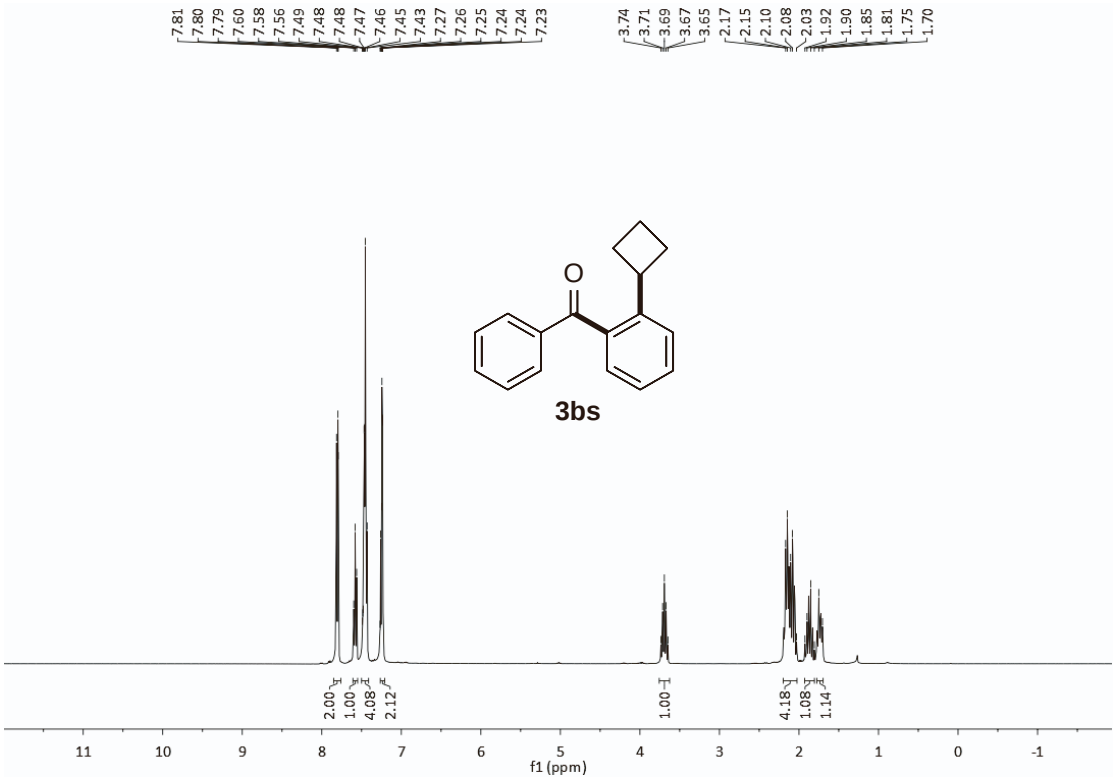
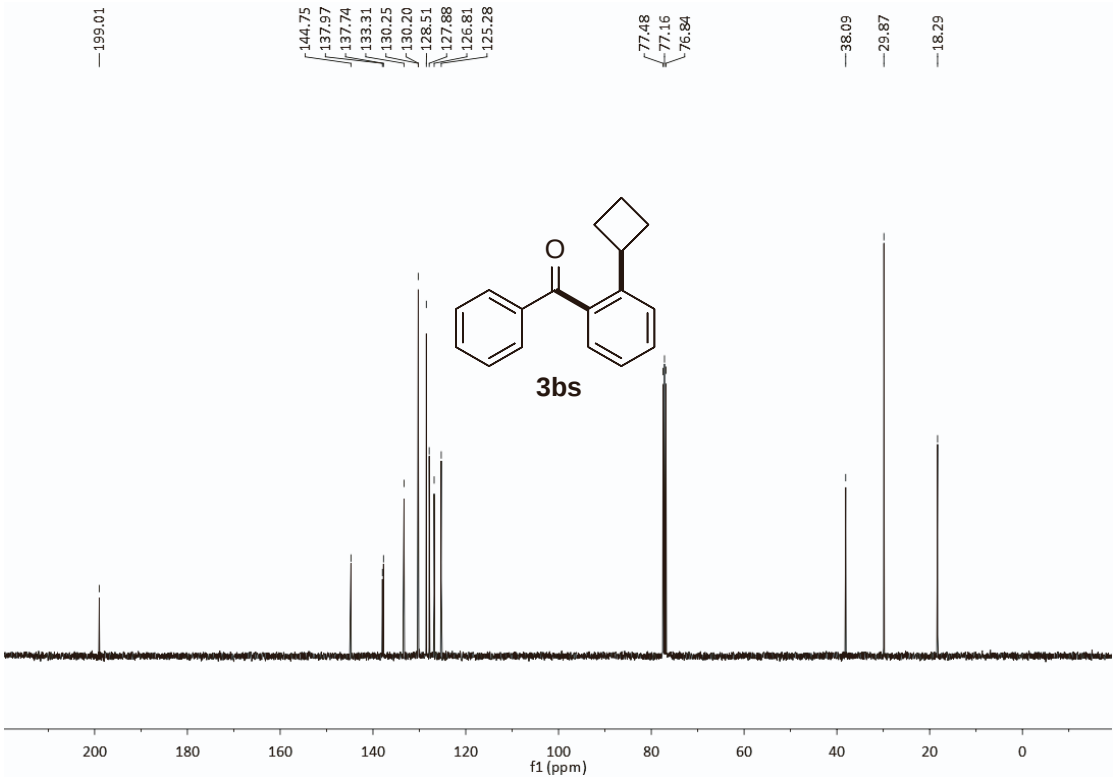


^{13}C NMR (101 MHz, $CDCl_3$)



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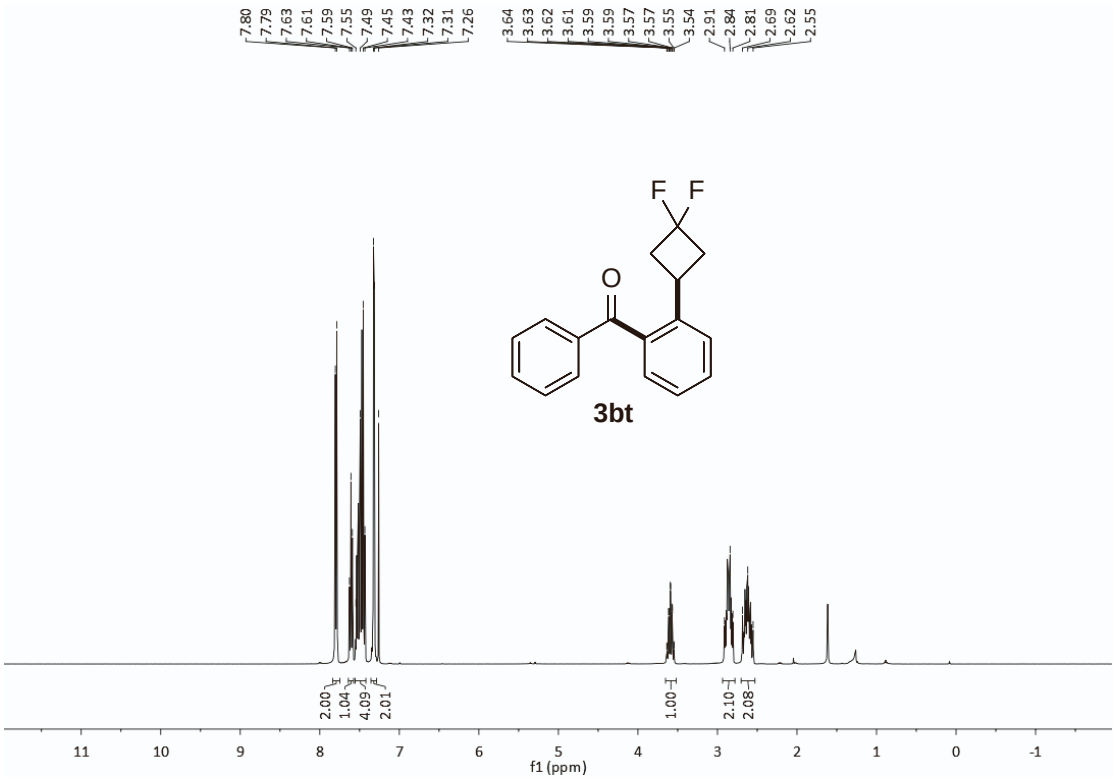
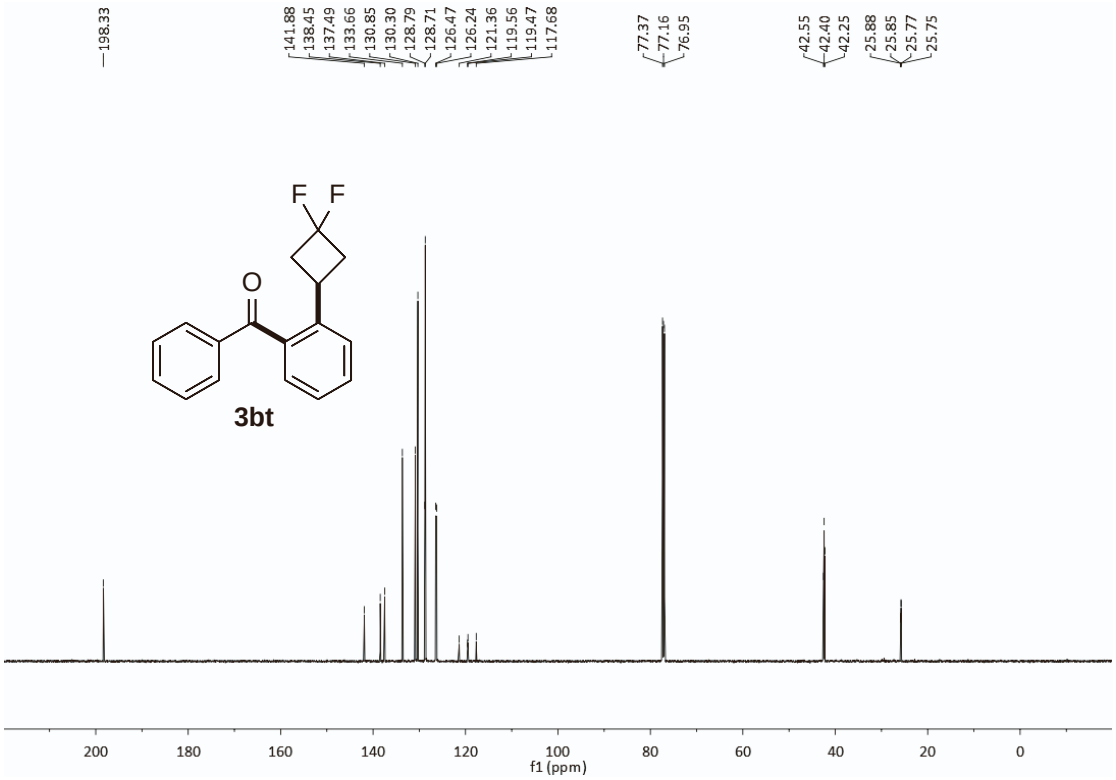
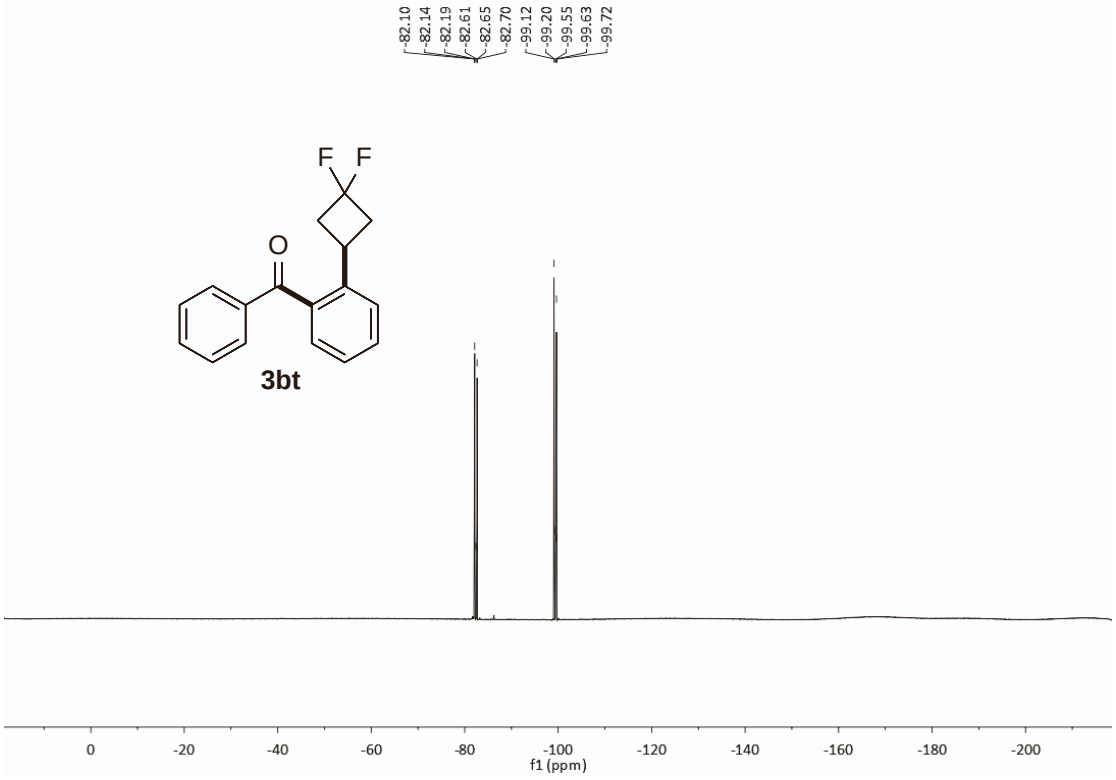


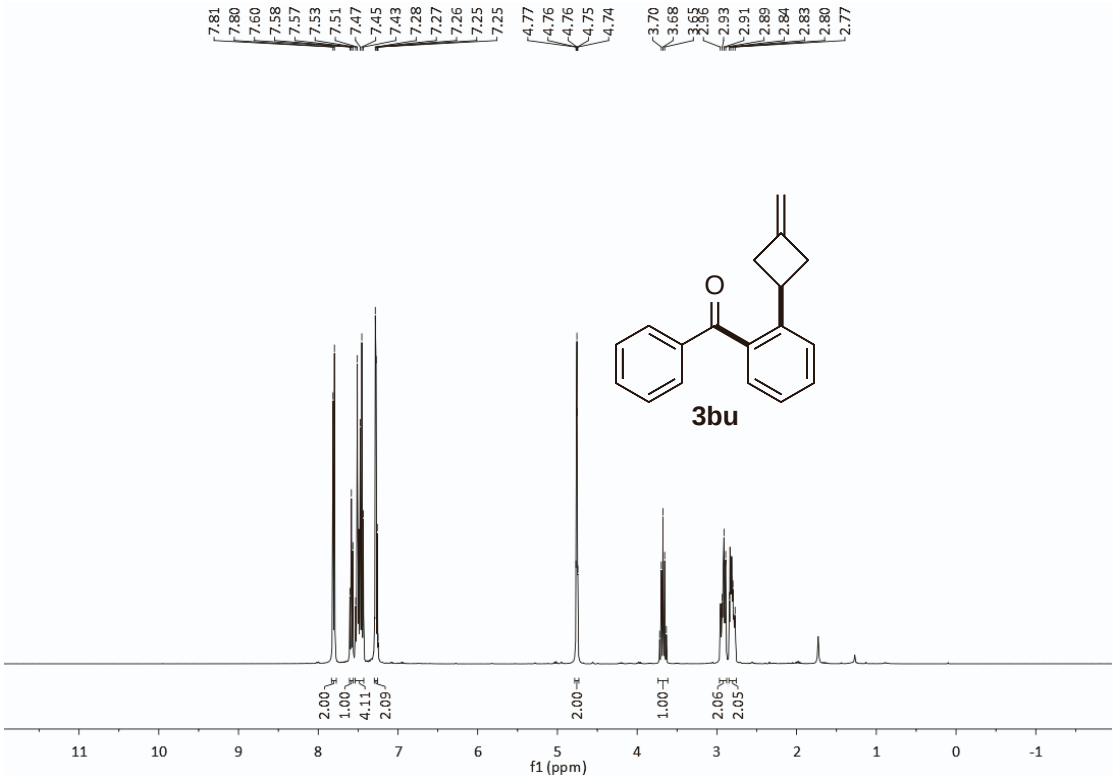
^{13}C NMR (151 MHz, $CDCl_3$)



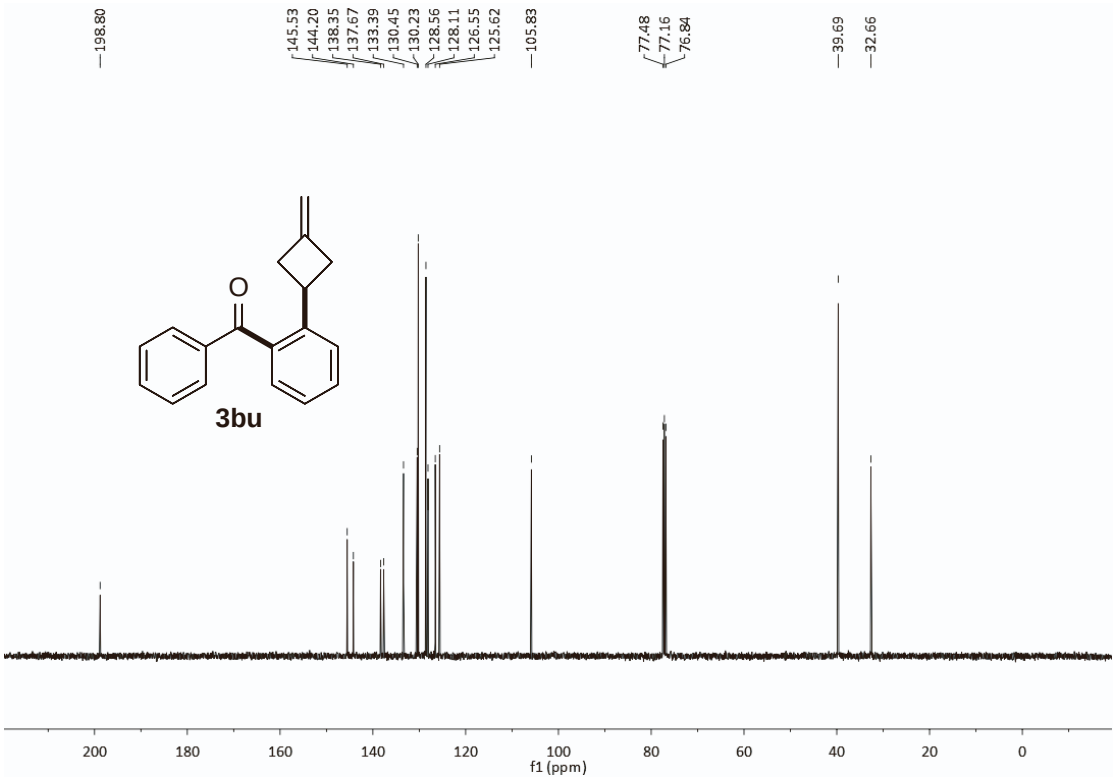
^{19}F NMR (376 MHz, $CDCl_3$)



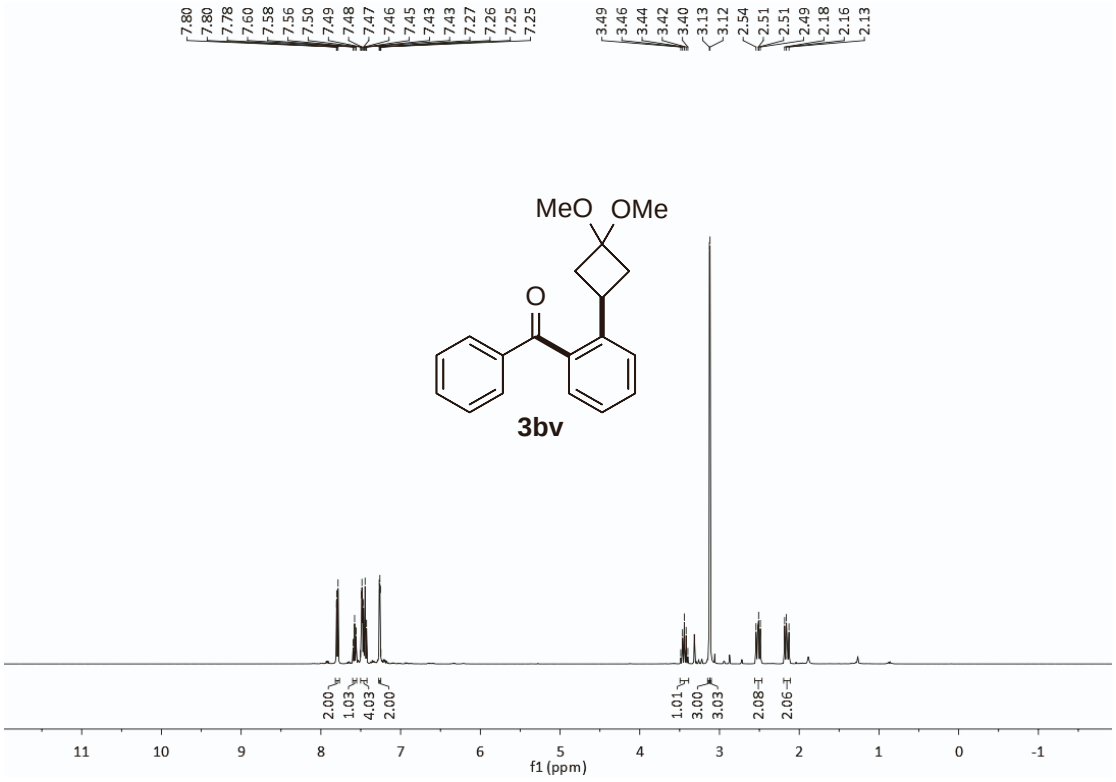
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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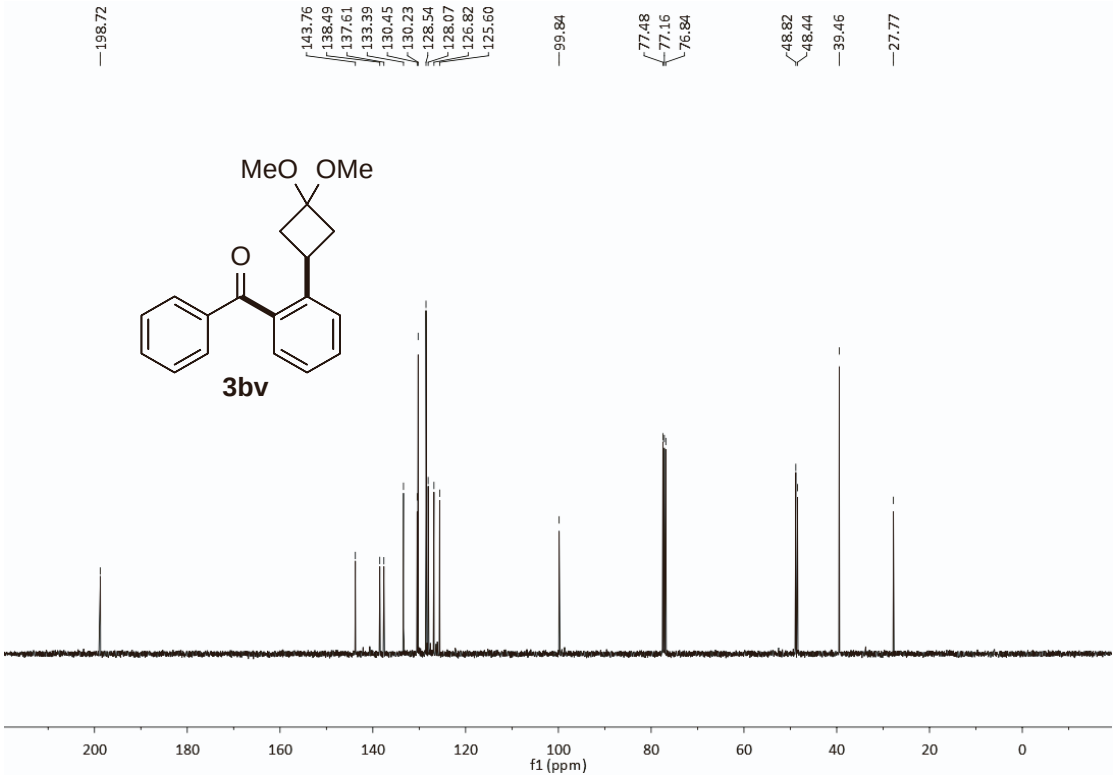

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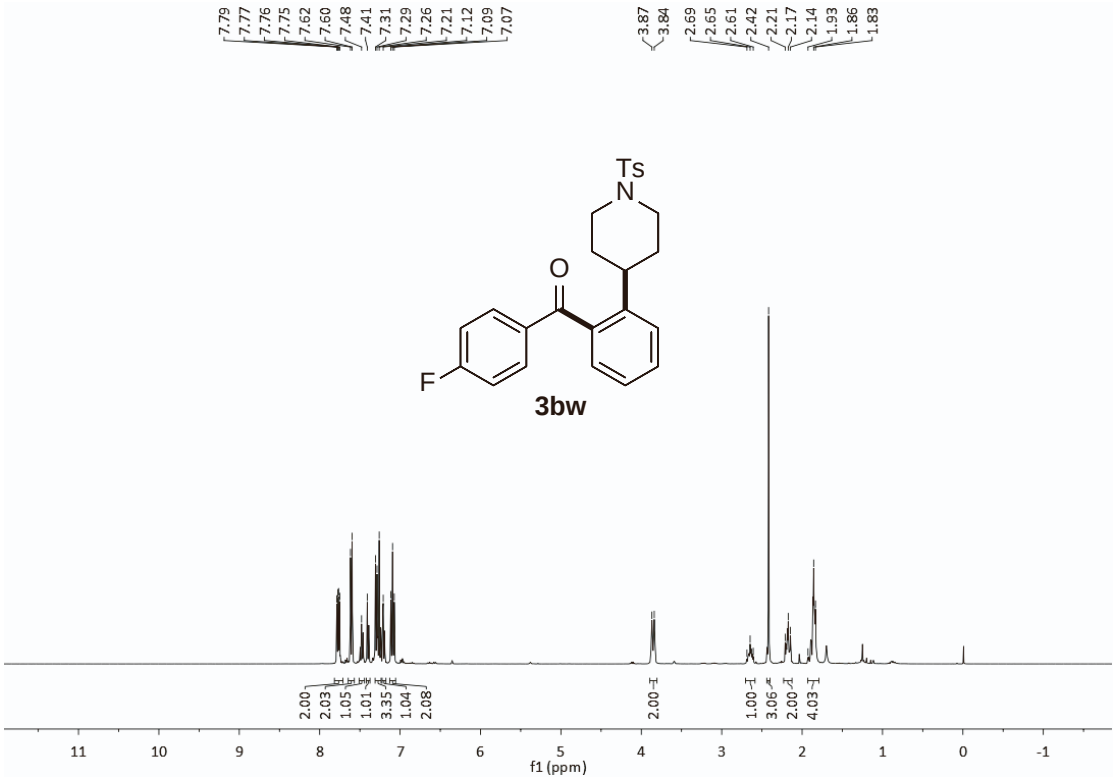
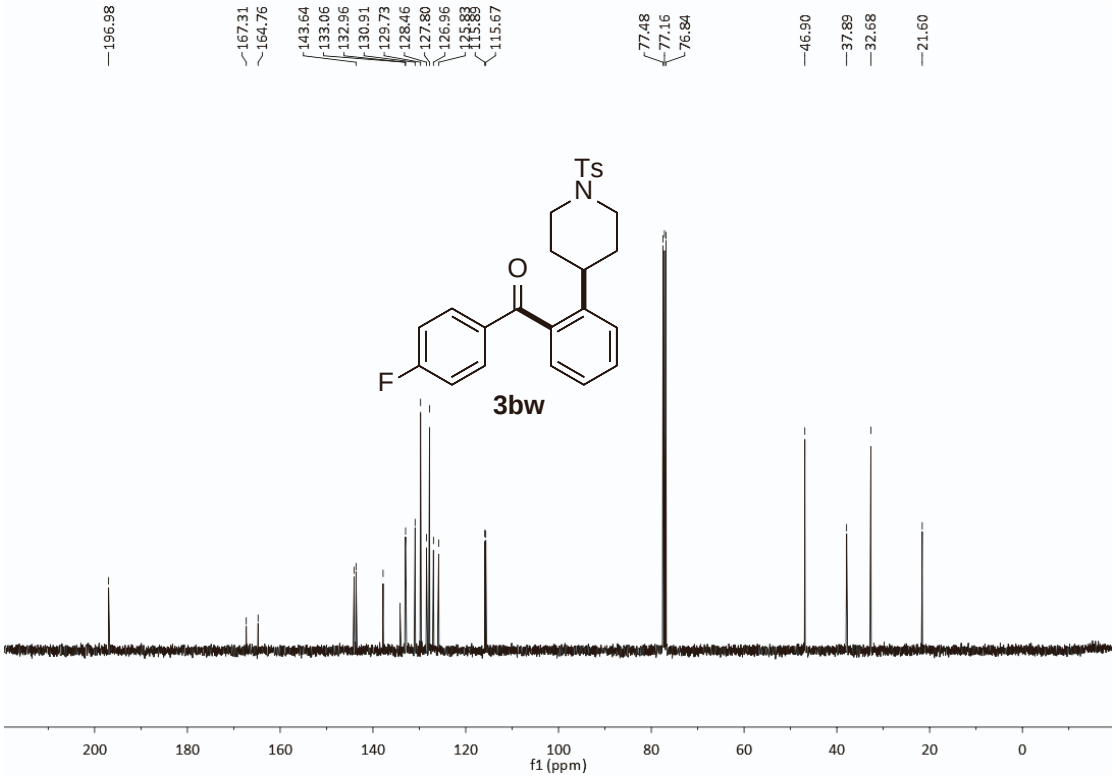
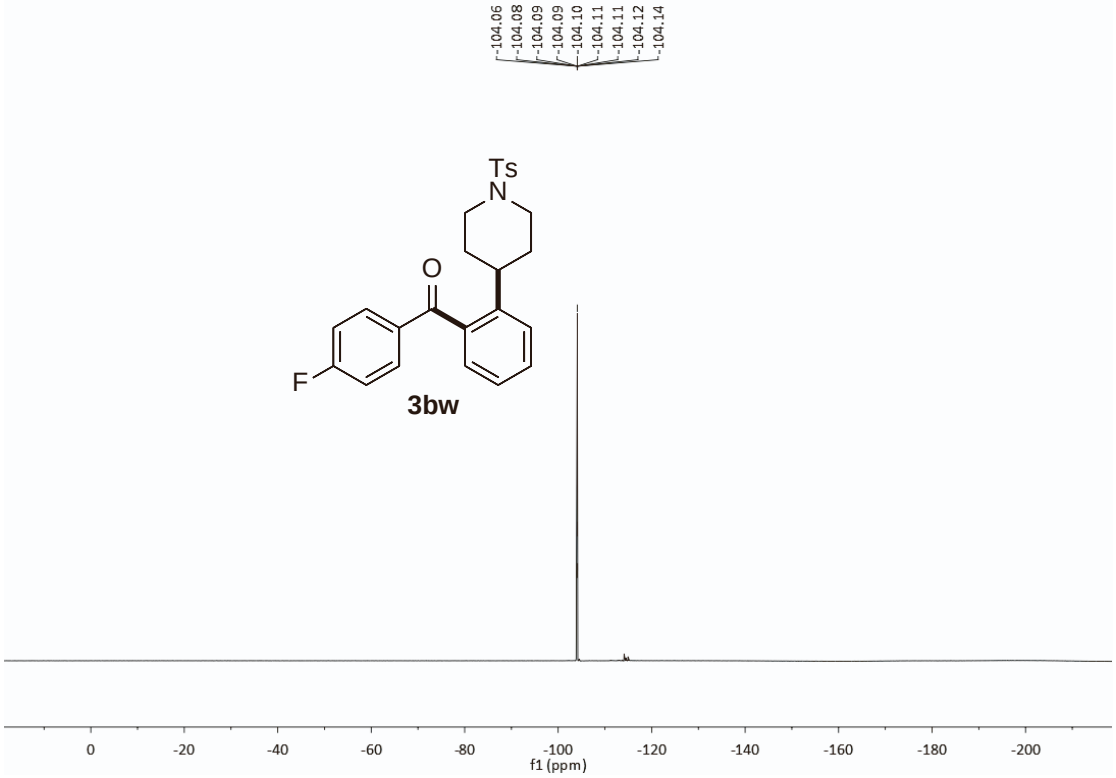


^{13}C NMR (101 MHz, $CDCl_3$)



^{19}F NMR (376 MHz, $CDCl_3$)



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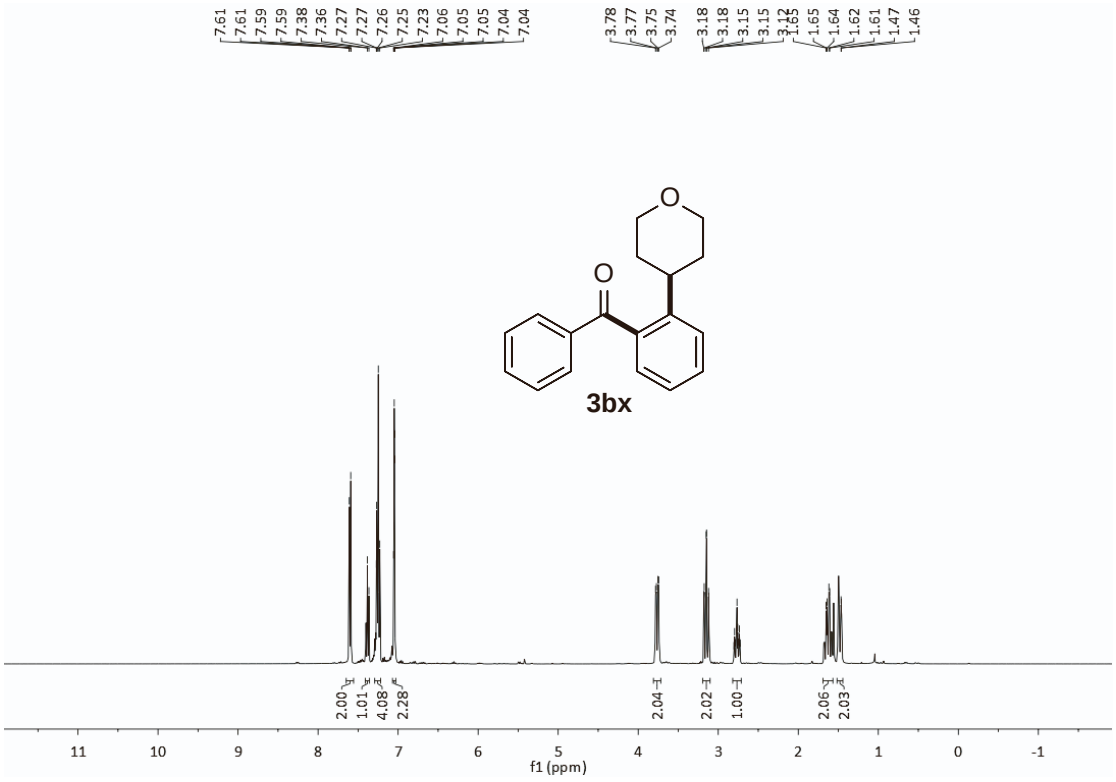

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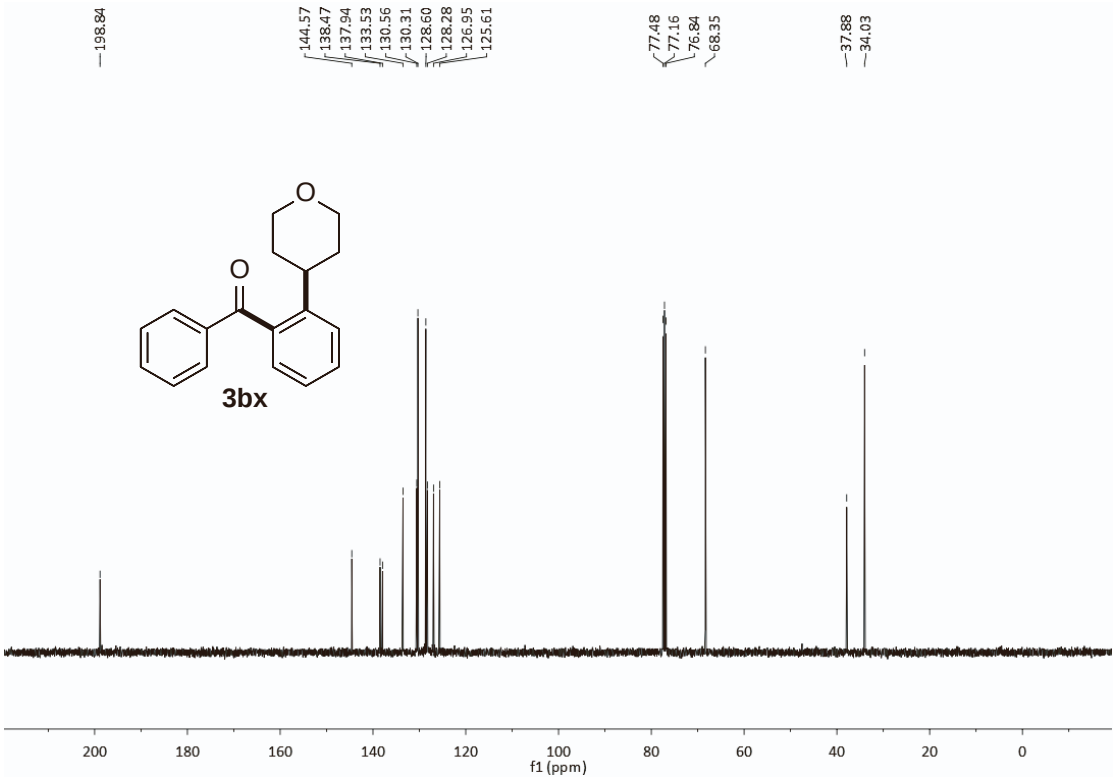

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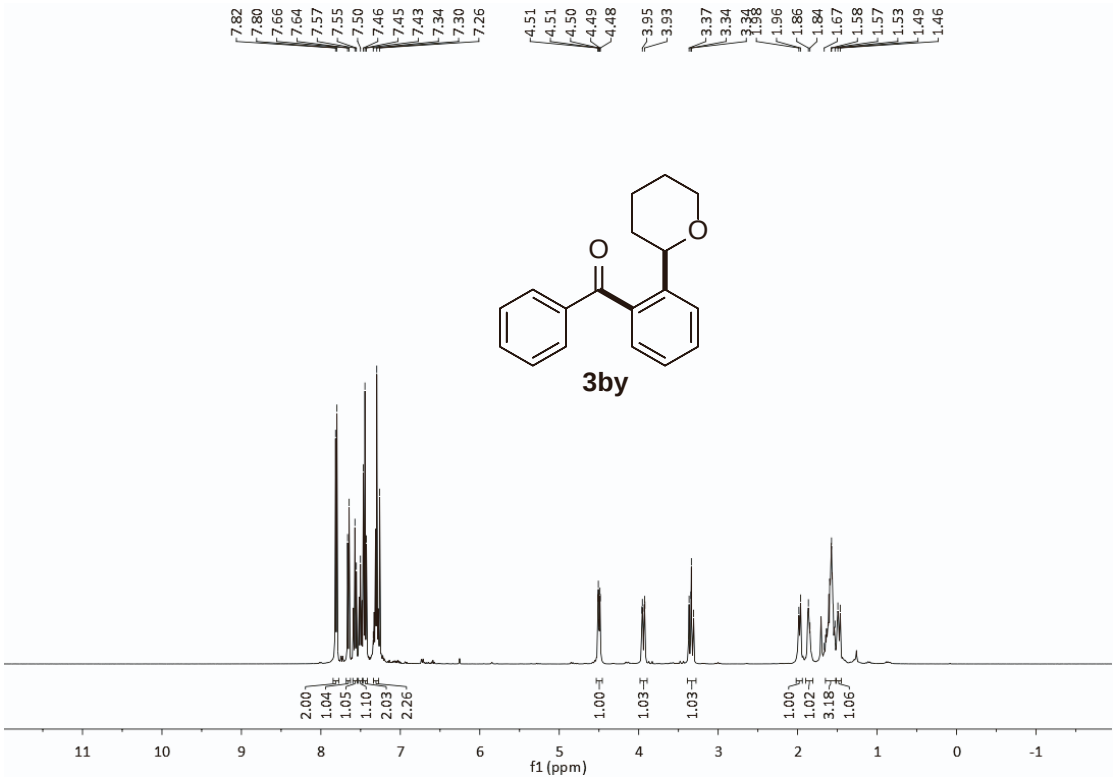

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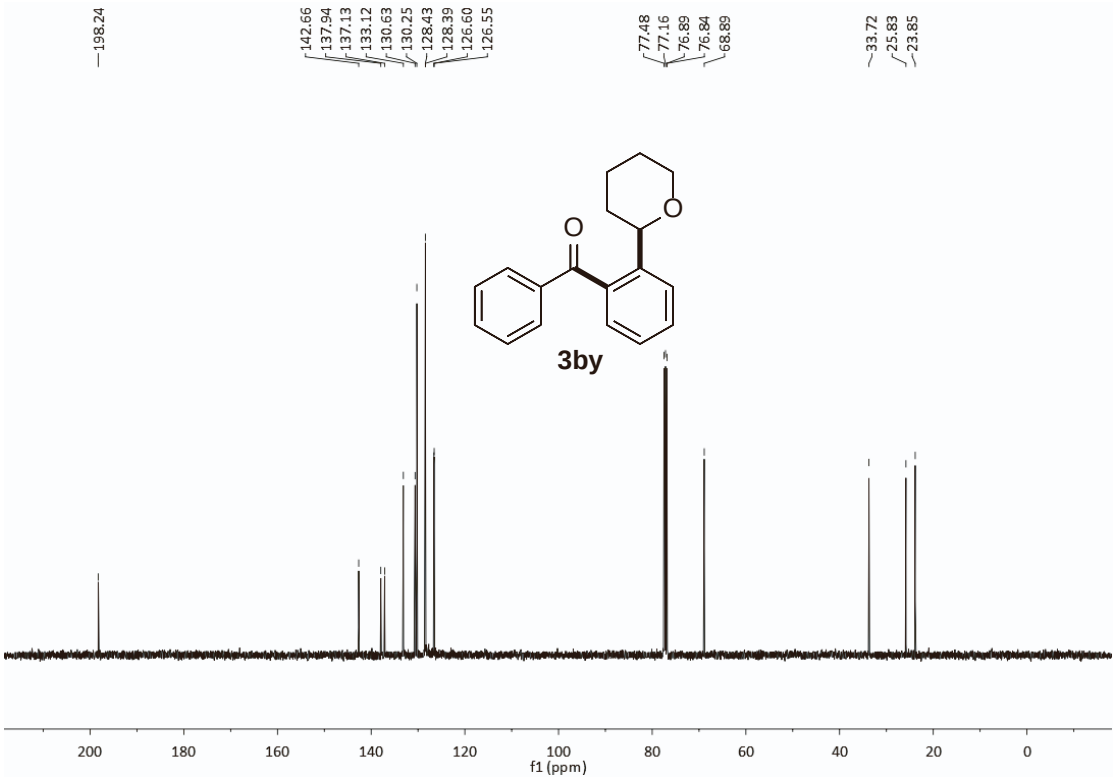

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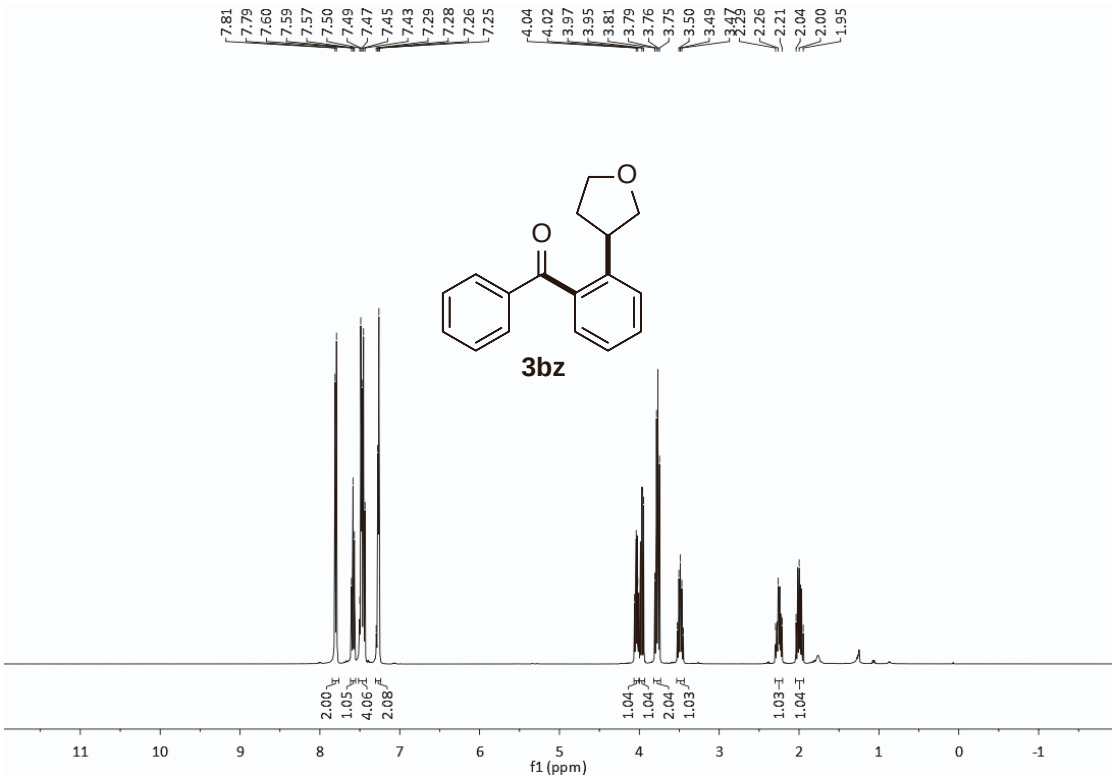

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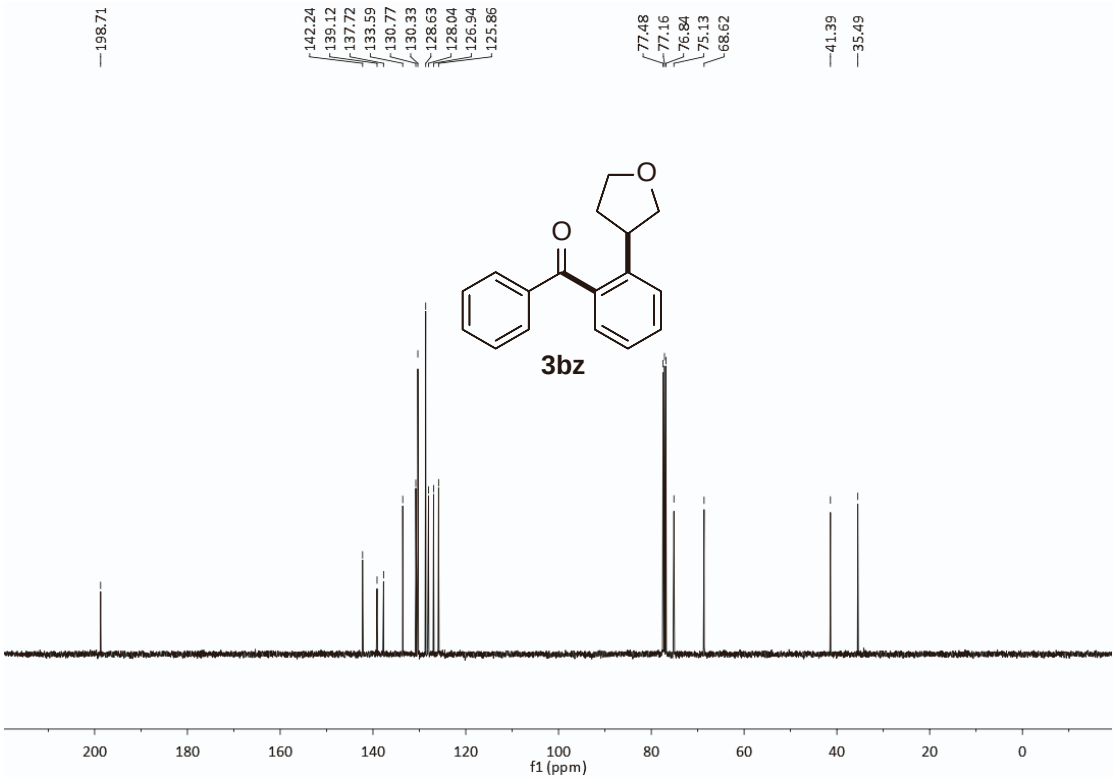

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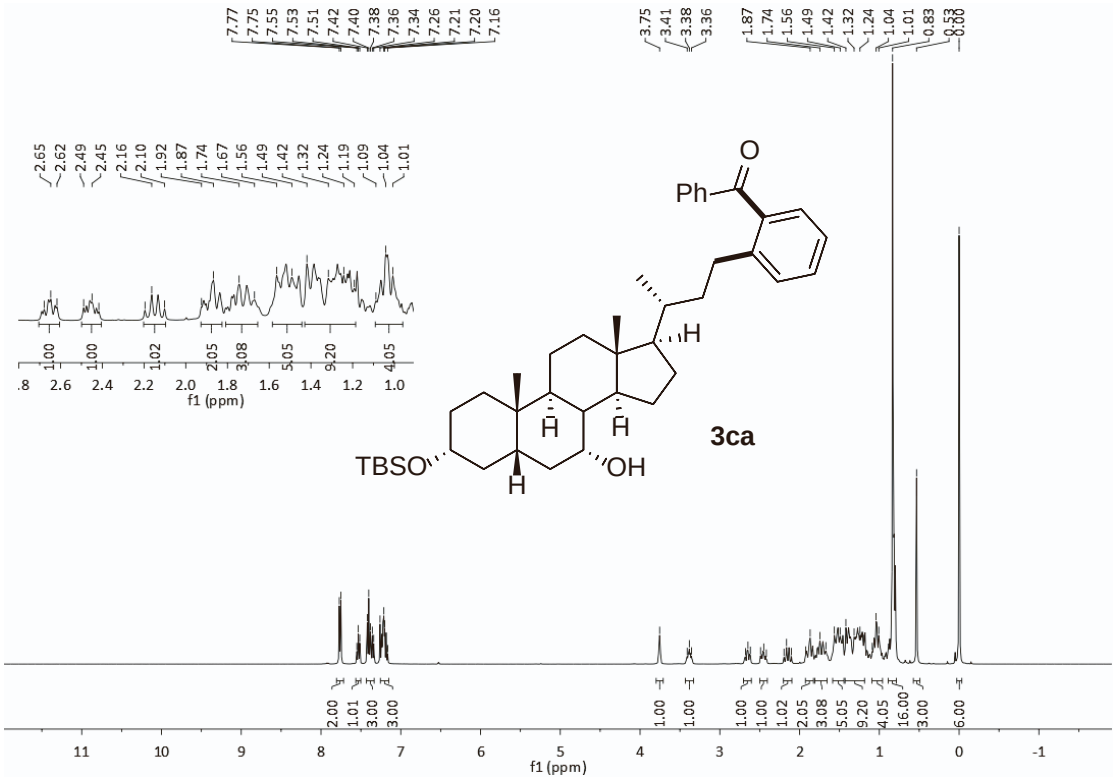
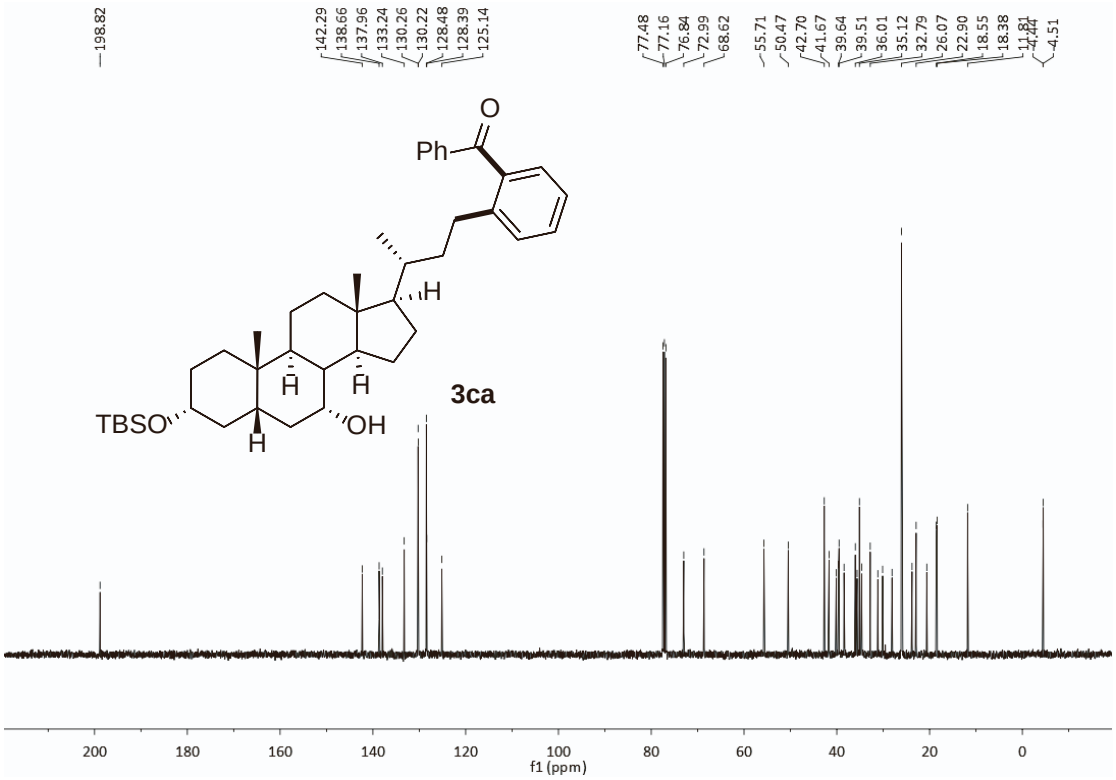


^{13}C NMR (101 MHz, $CDCl_3$)



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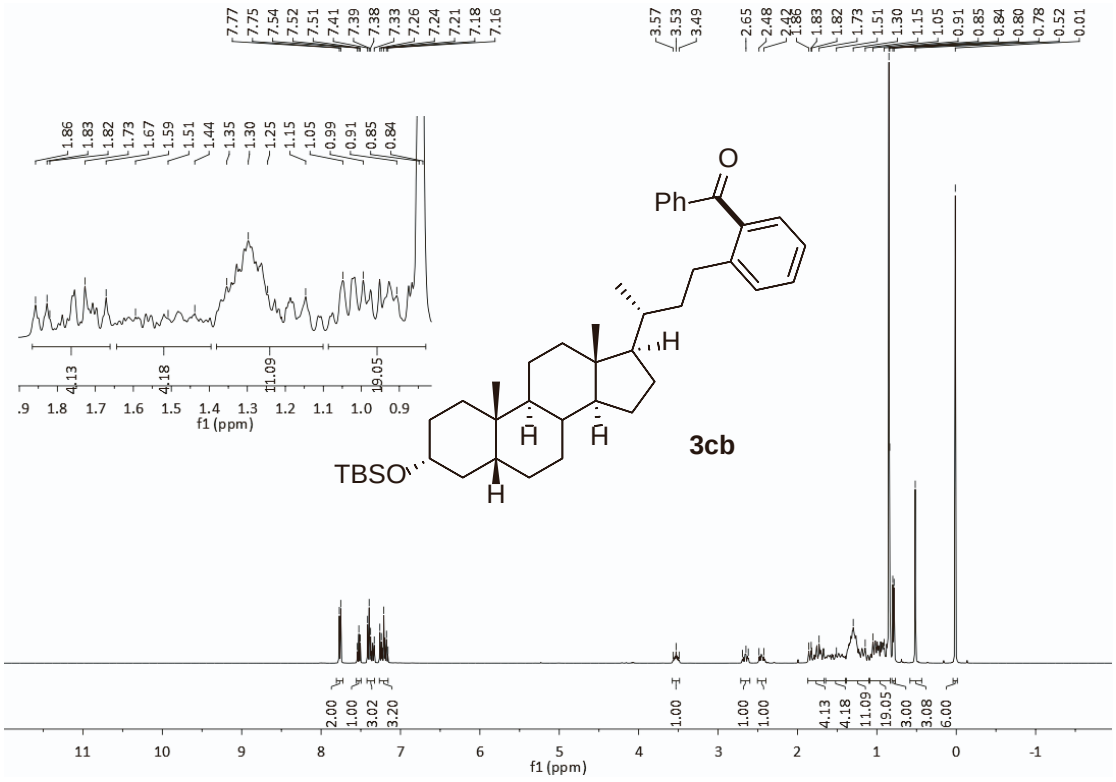
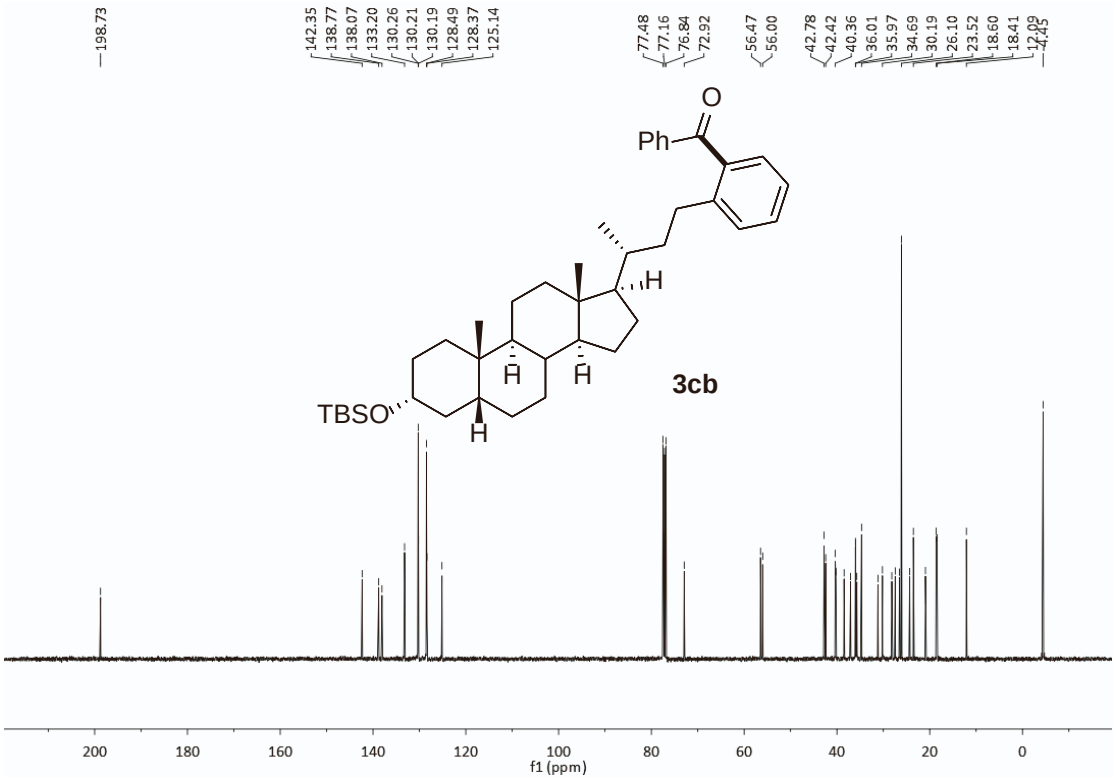
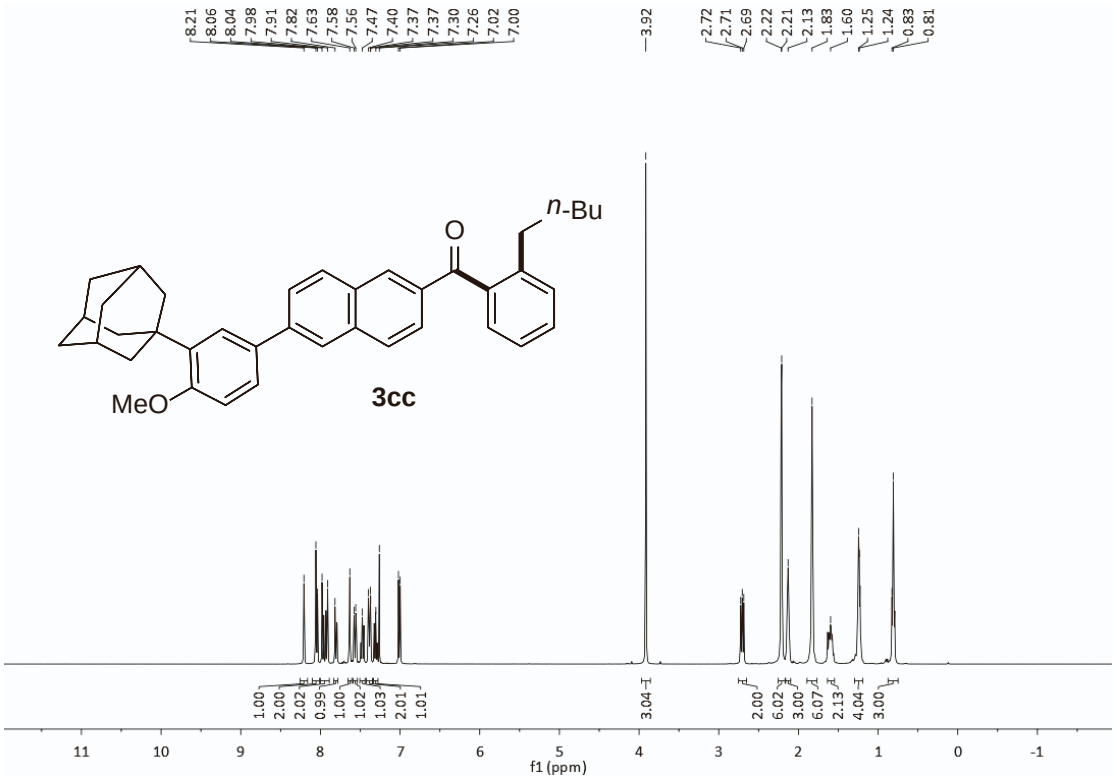


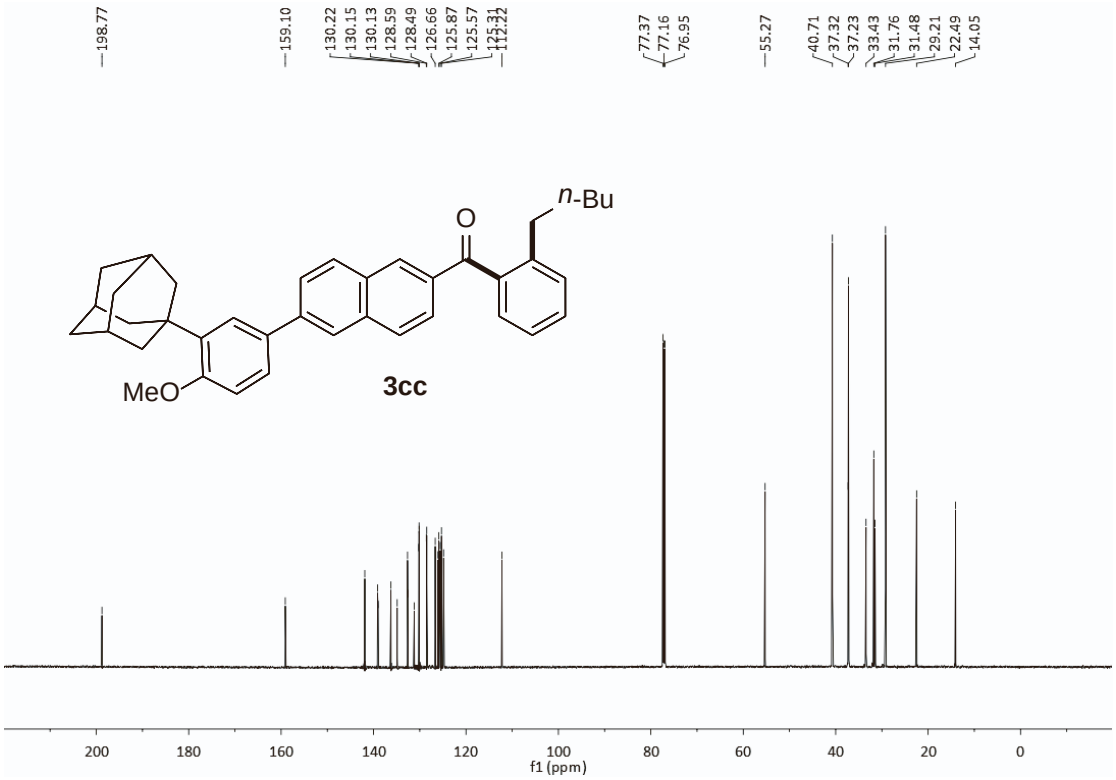
^{13}C NMR (101 MHz, $CDCl_3$)



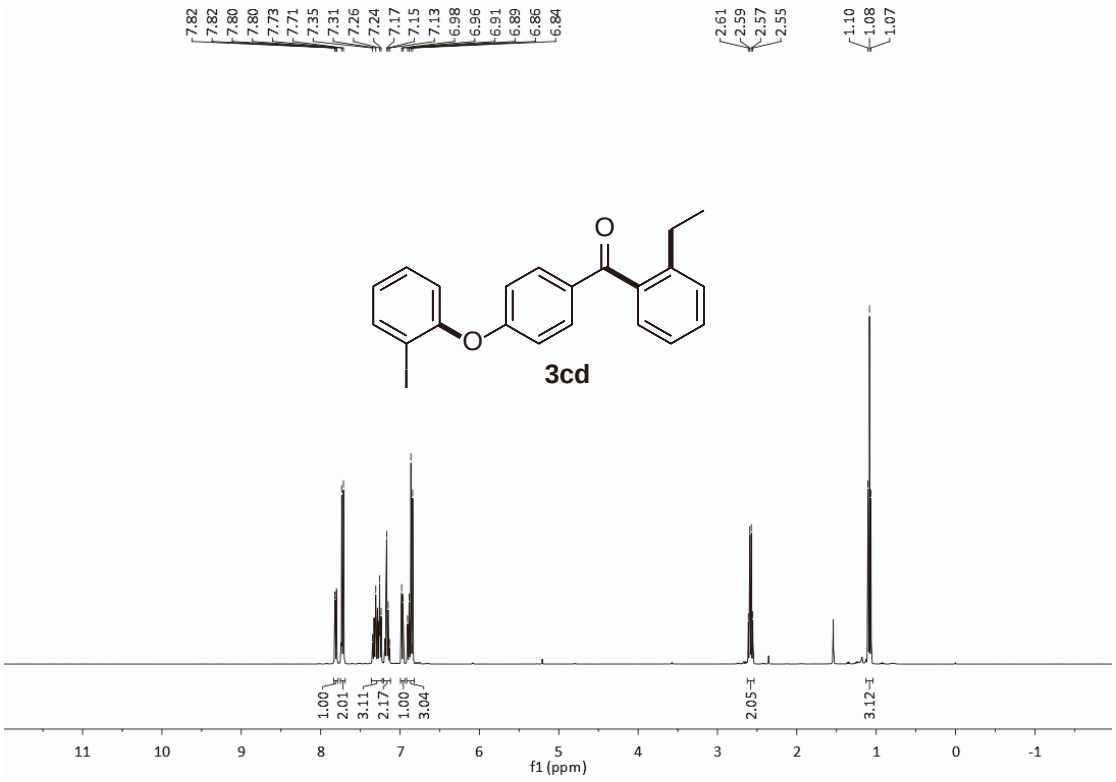
^{1}H NMR (400 MHz, $CDCl_3$)



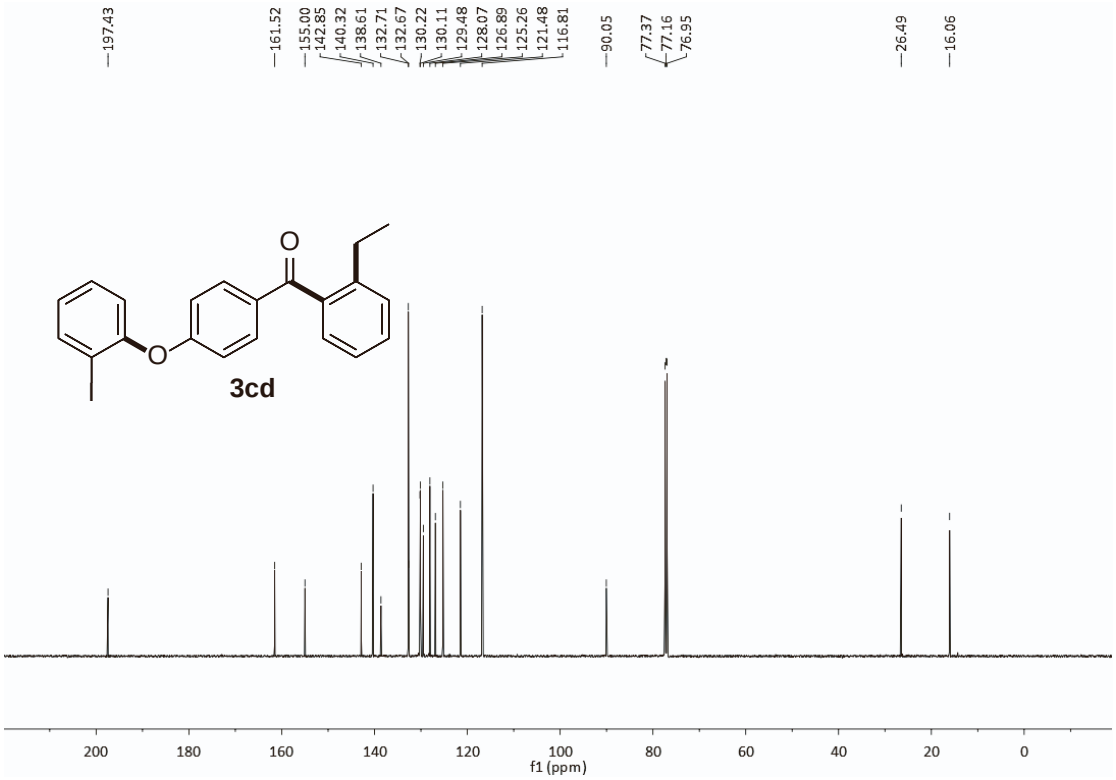
^{13}C NMR (151 MHz, $CDCl_3$)



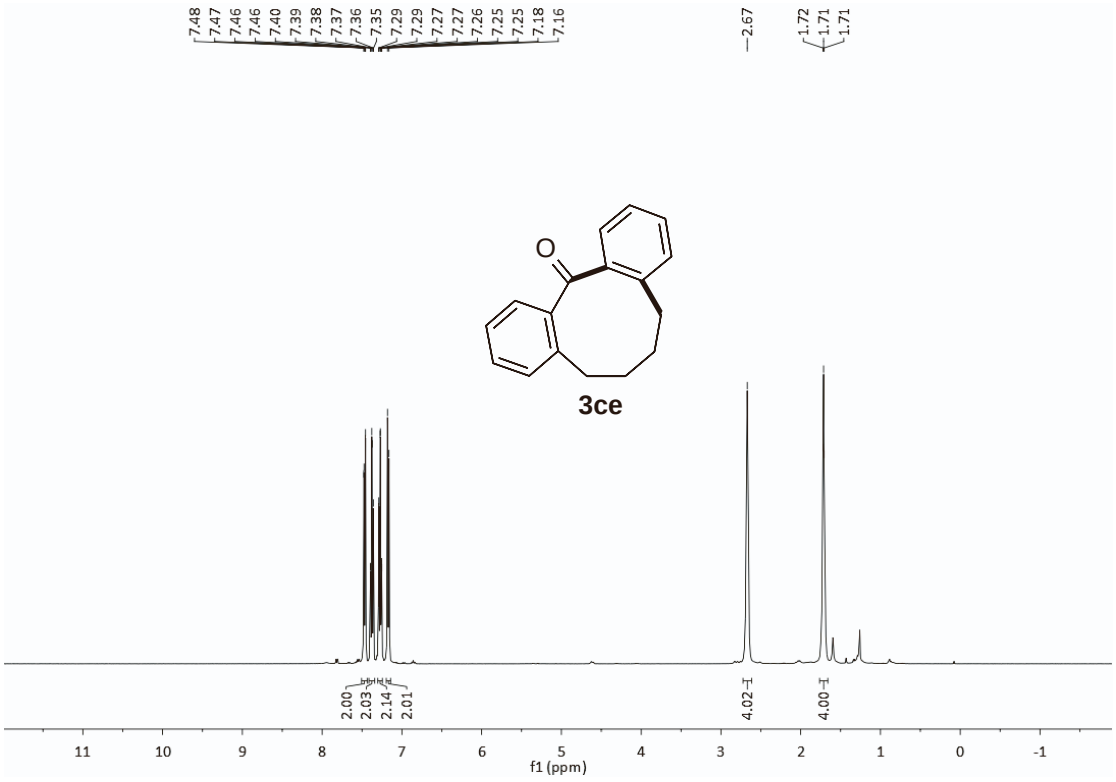
^{1}H NMR (400 MHz, $CDCl_3$)



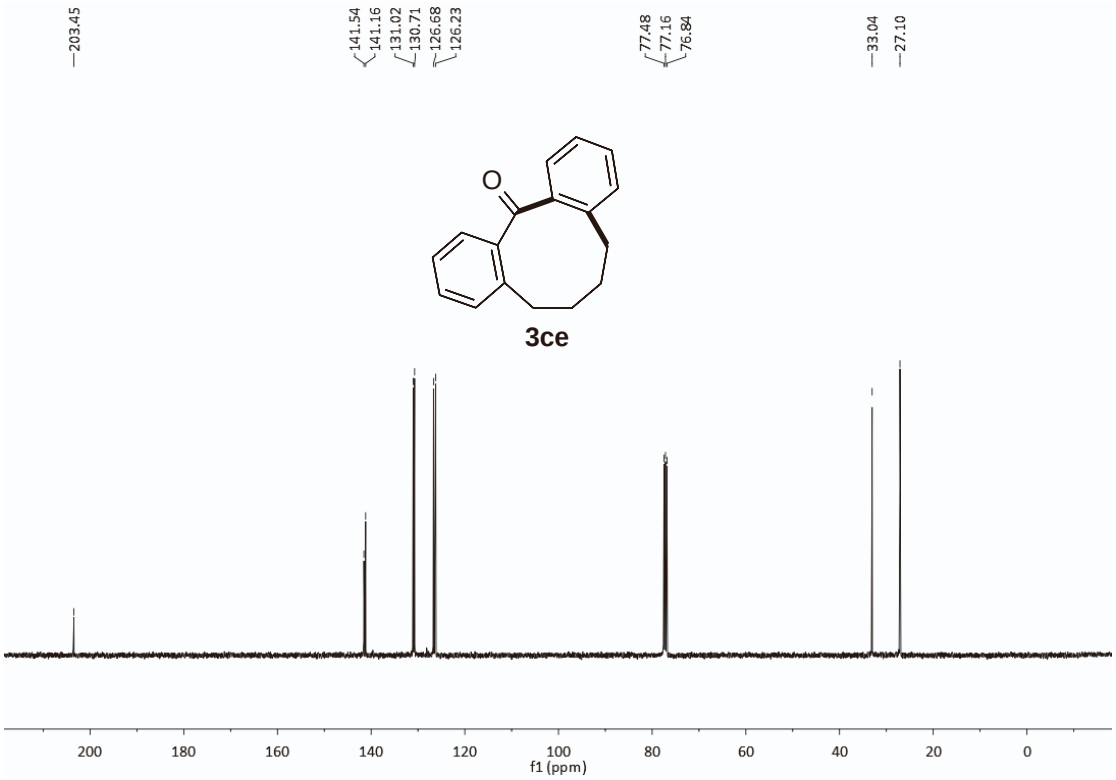
^{13}C NMR (151 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)



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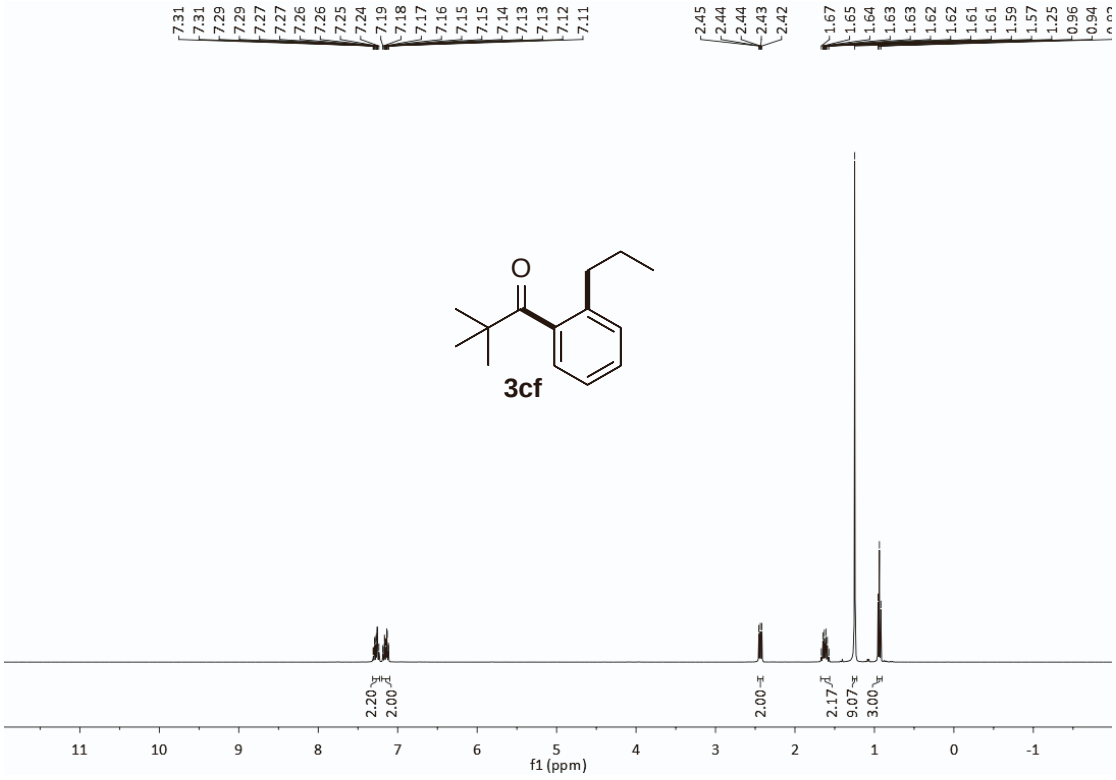

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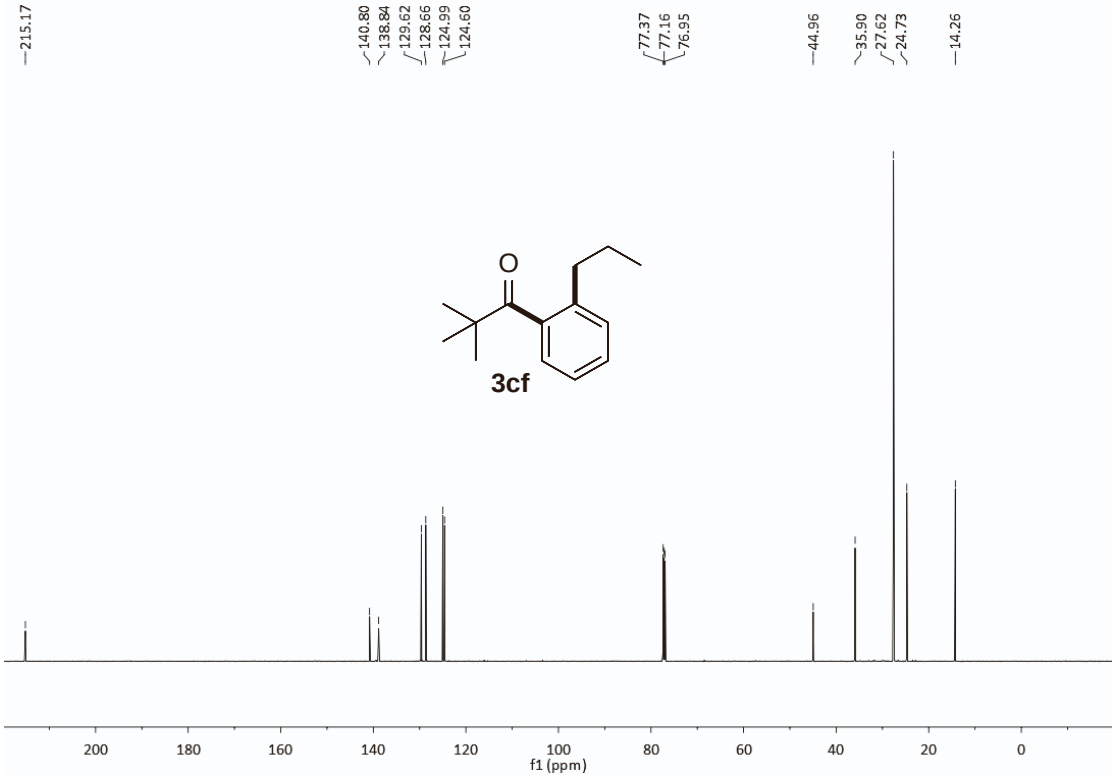

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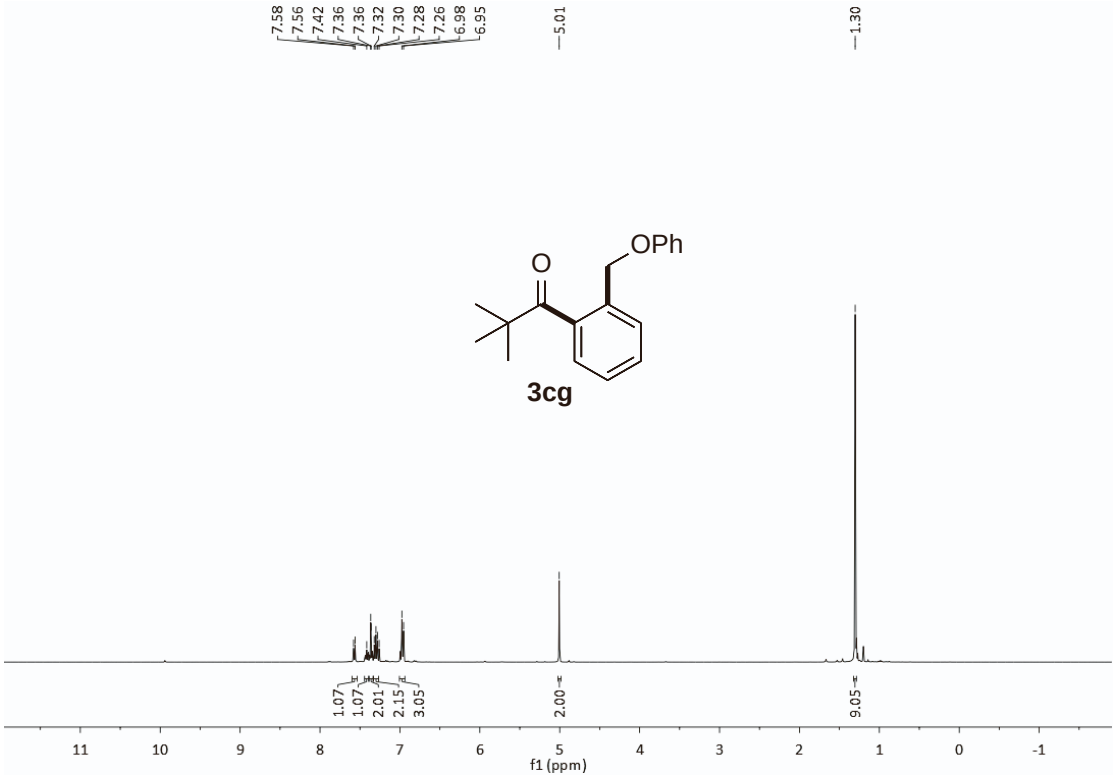

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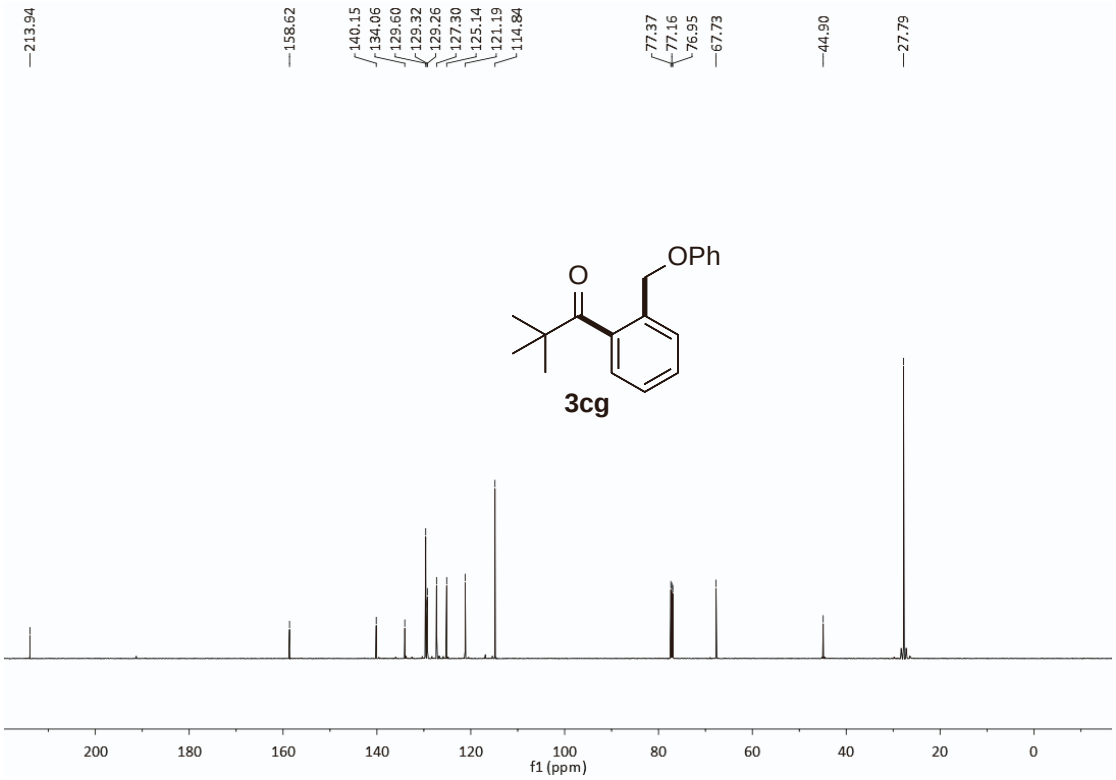

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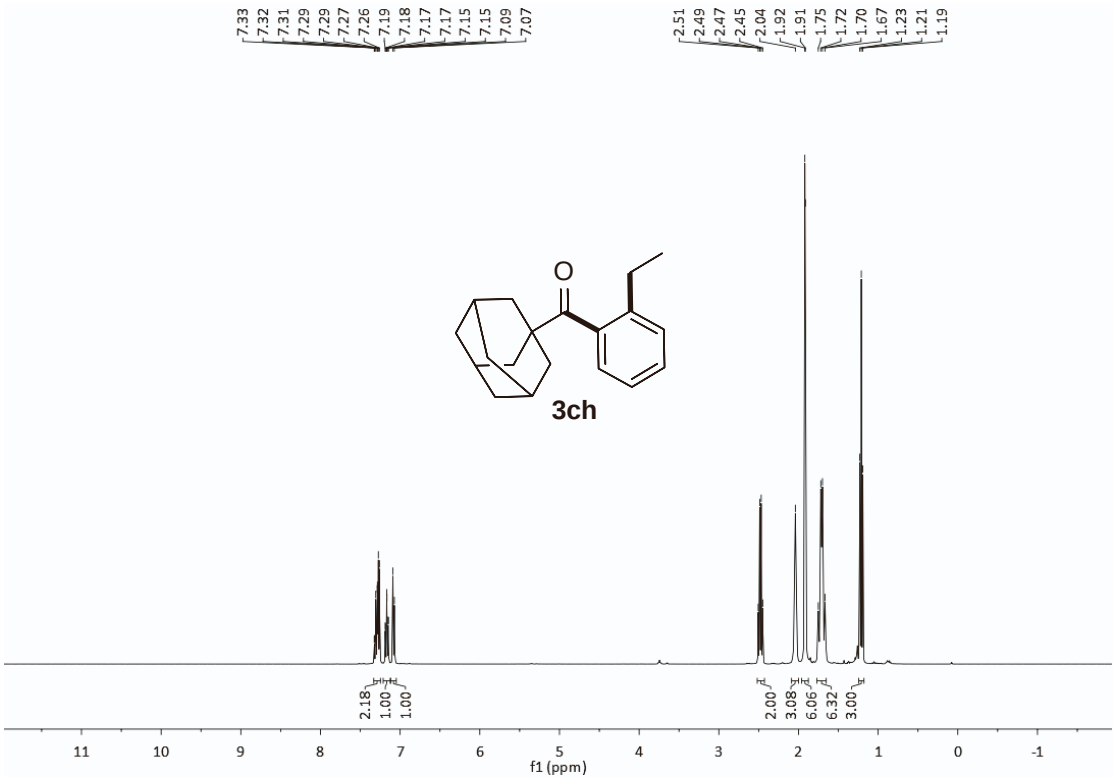
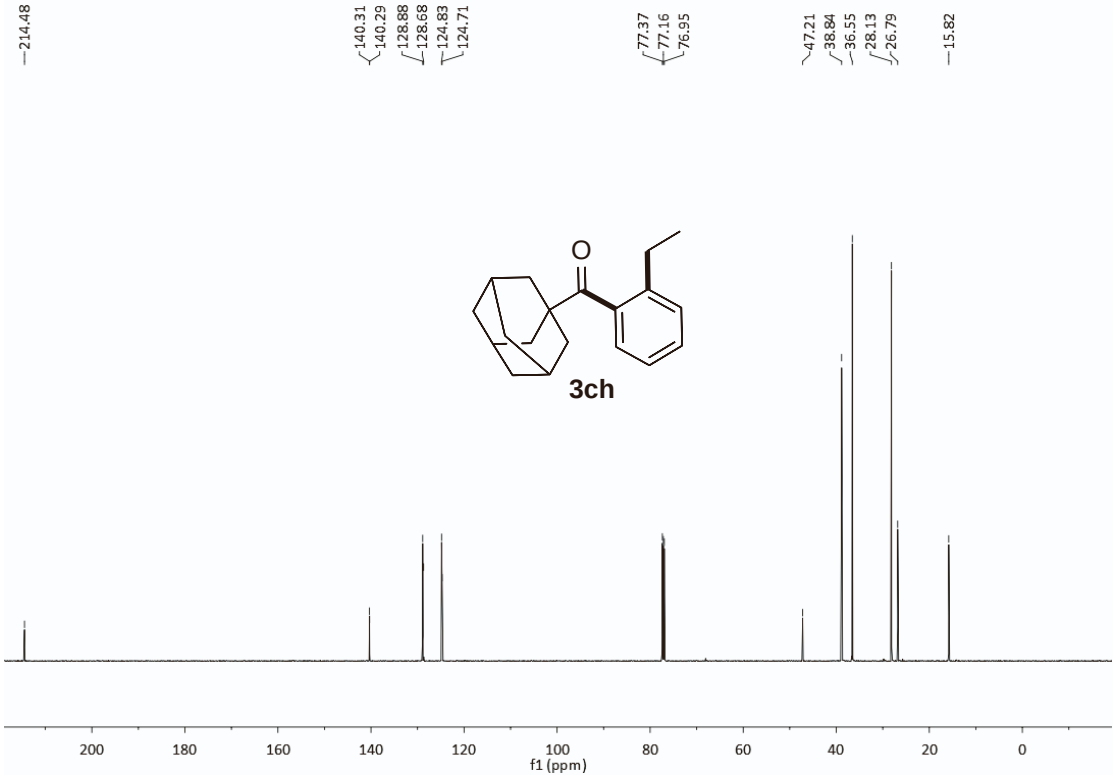


^{13}C NMR (151 MHz, $CDCl_3$)



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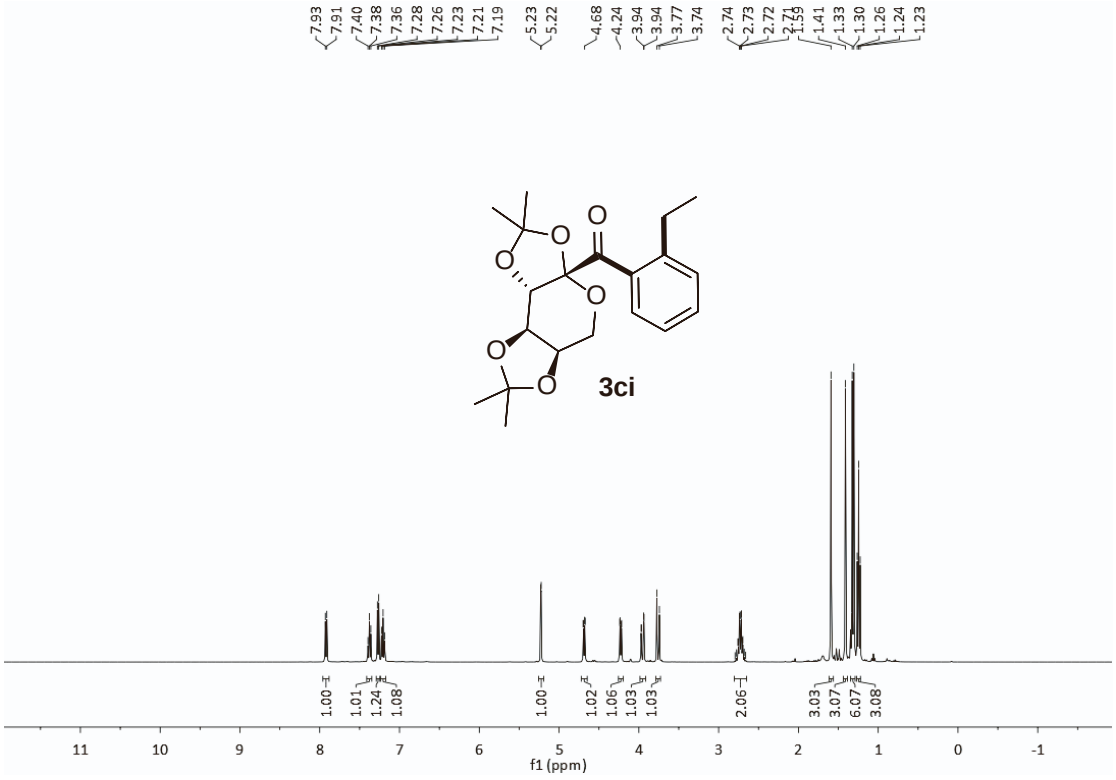

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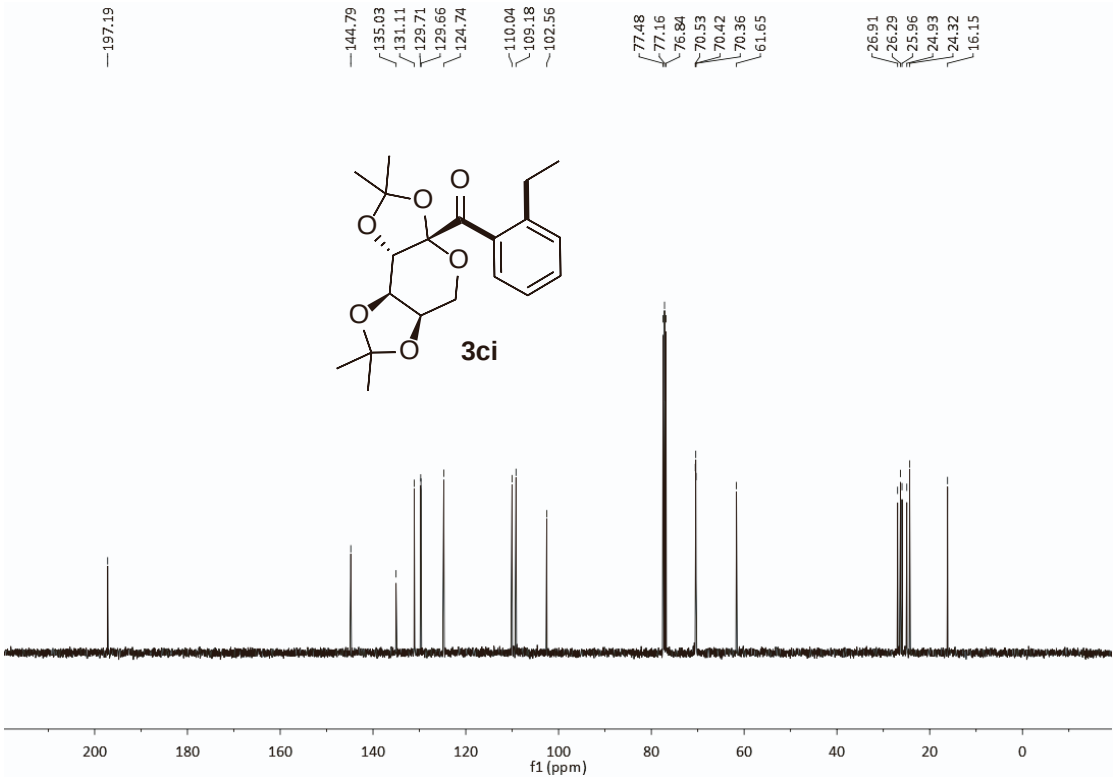

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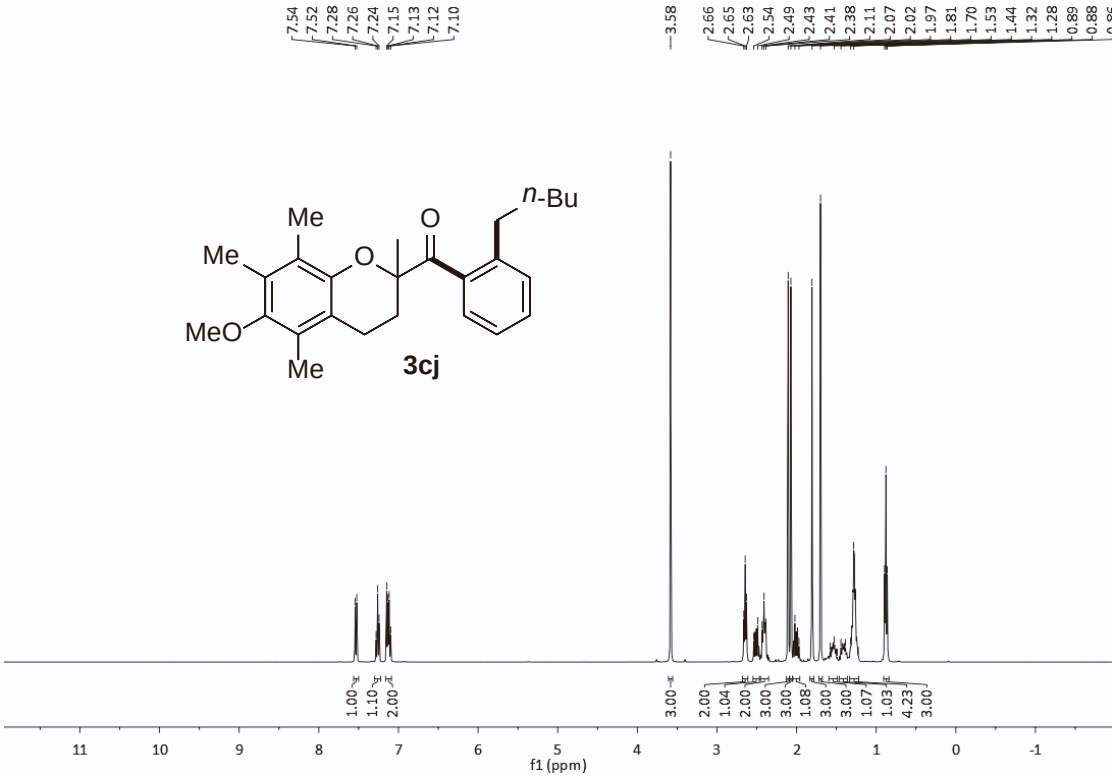

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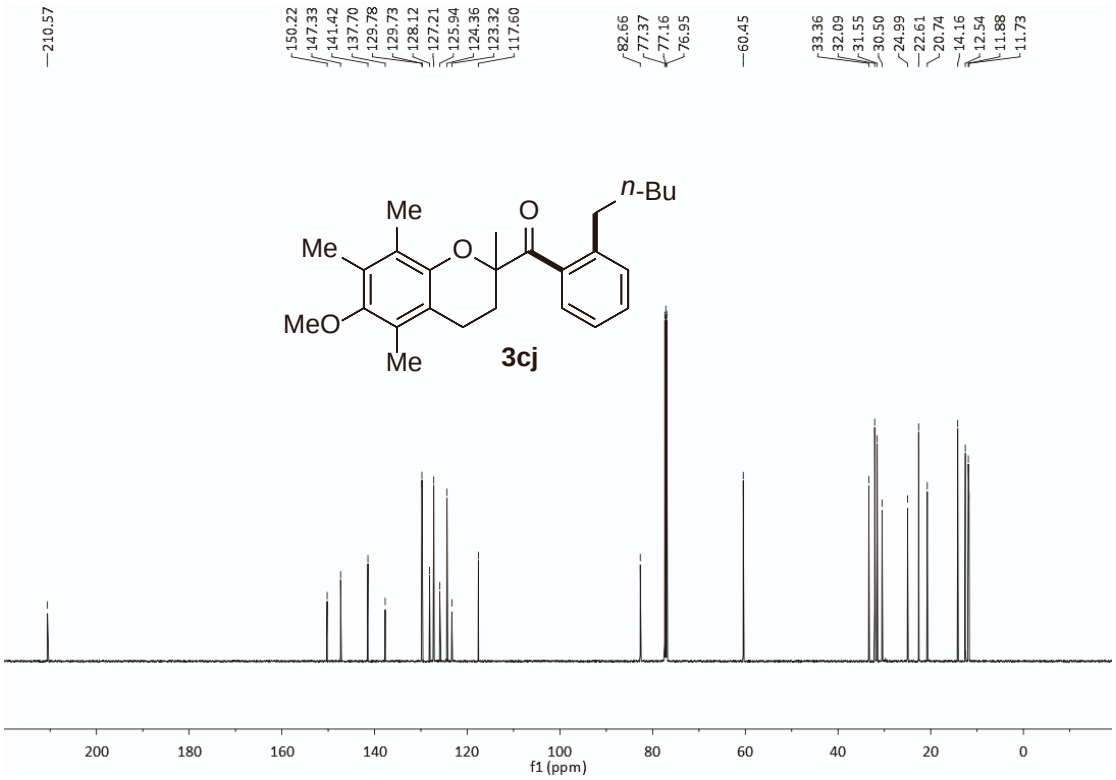

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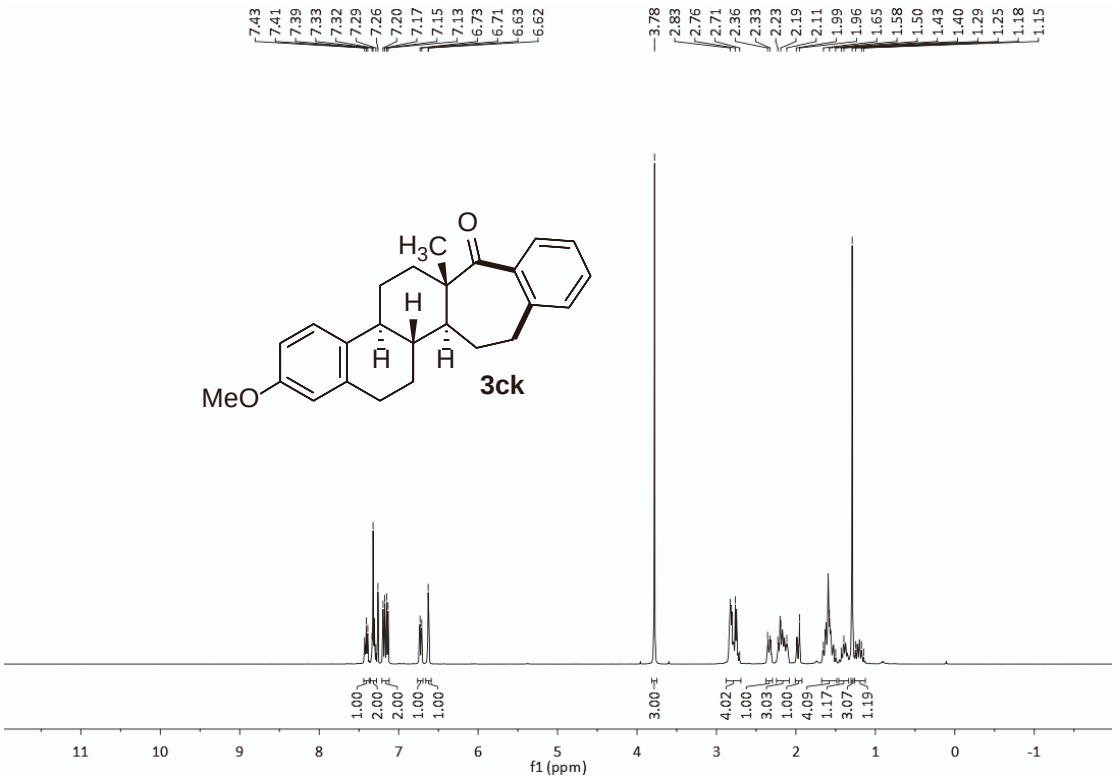
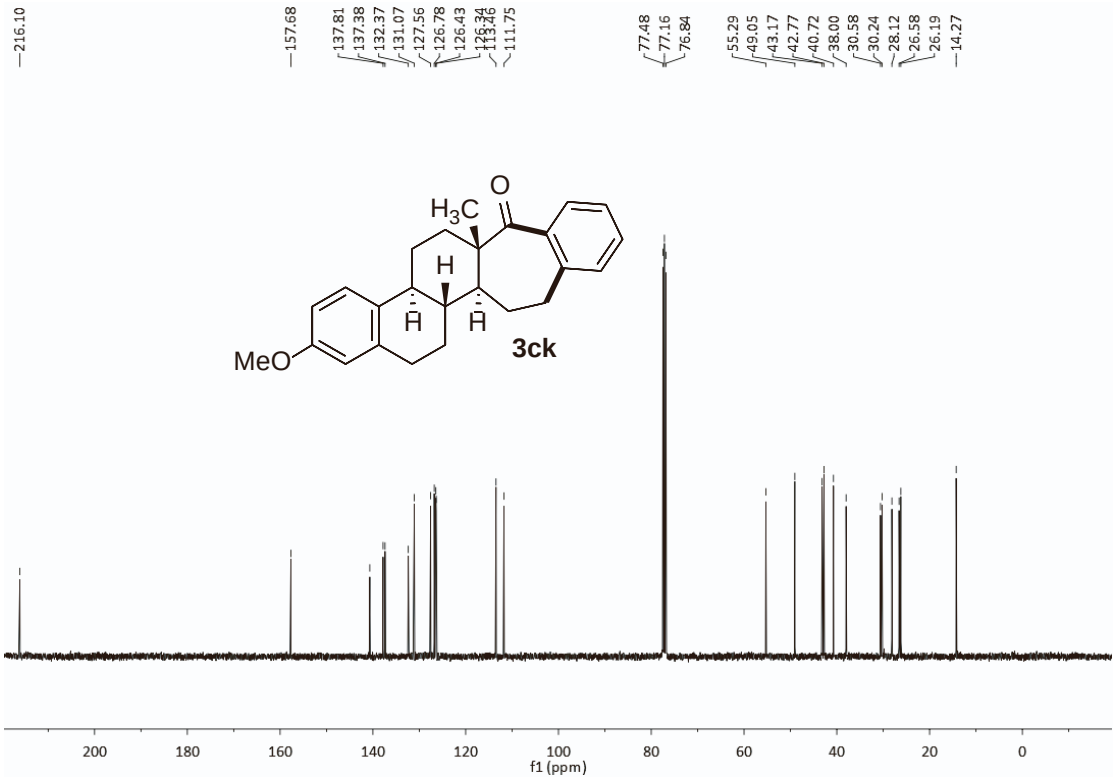
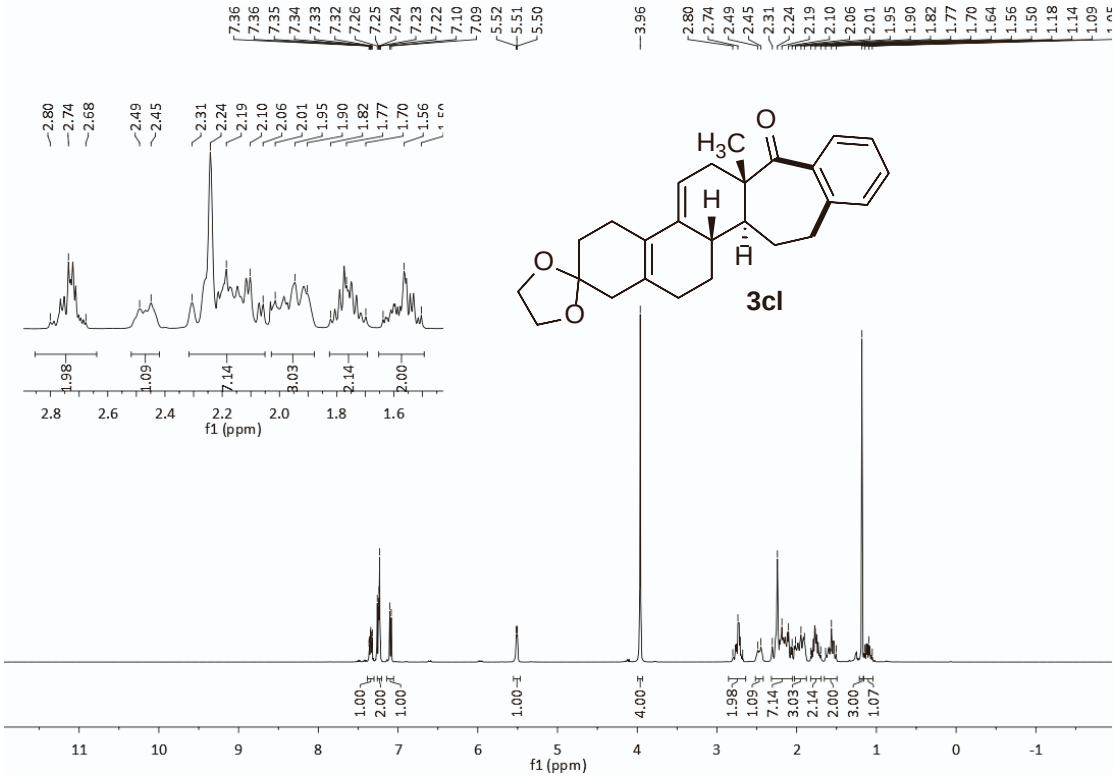


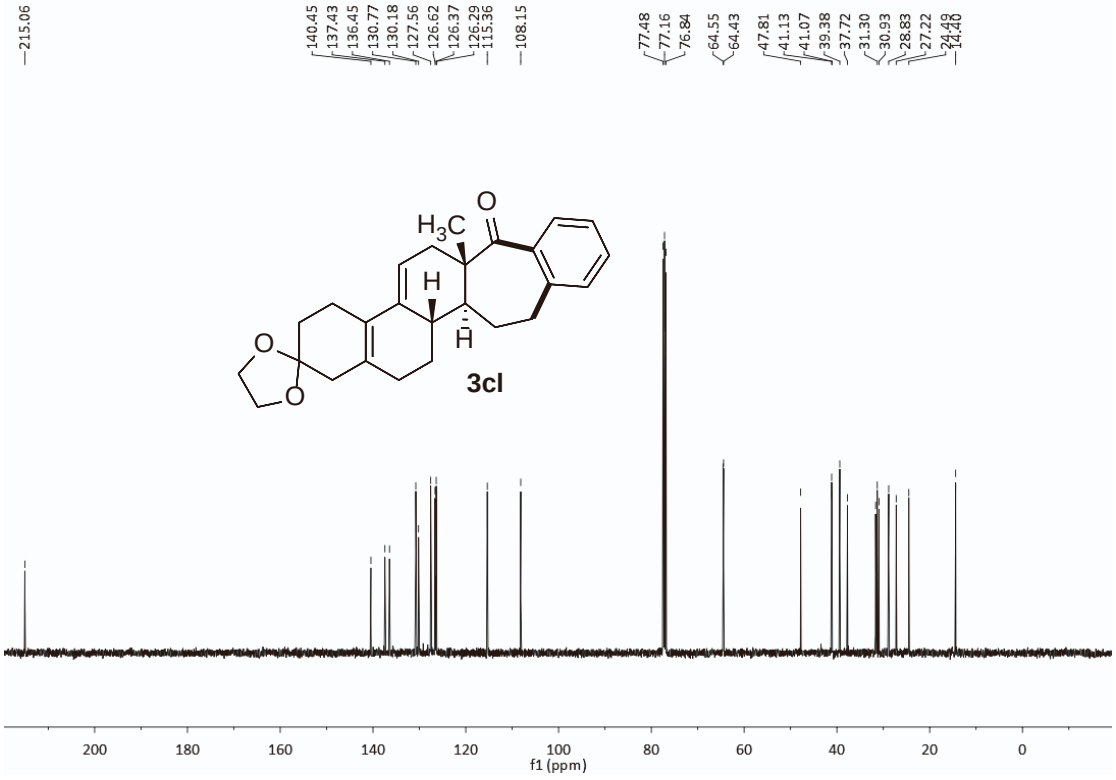
^{13}C NMR (101 MHz, $CDCl_3$)



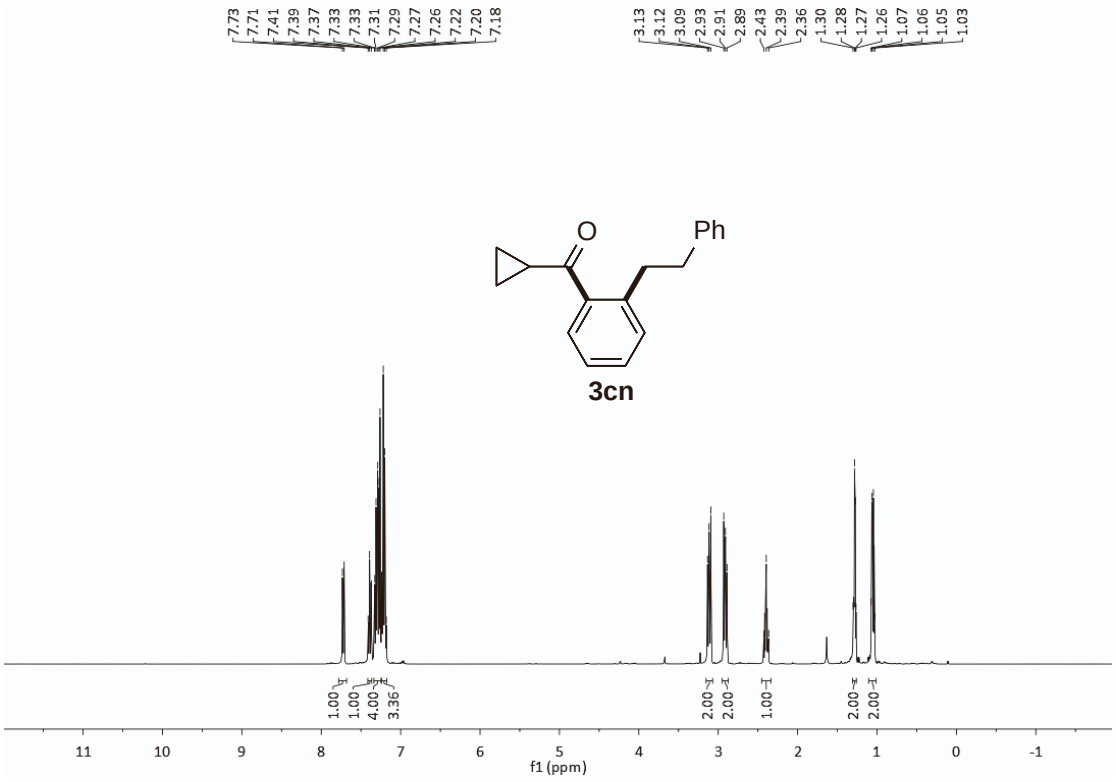
^{1}H NMR (400 MHz, $CDCl_3$)



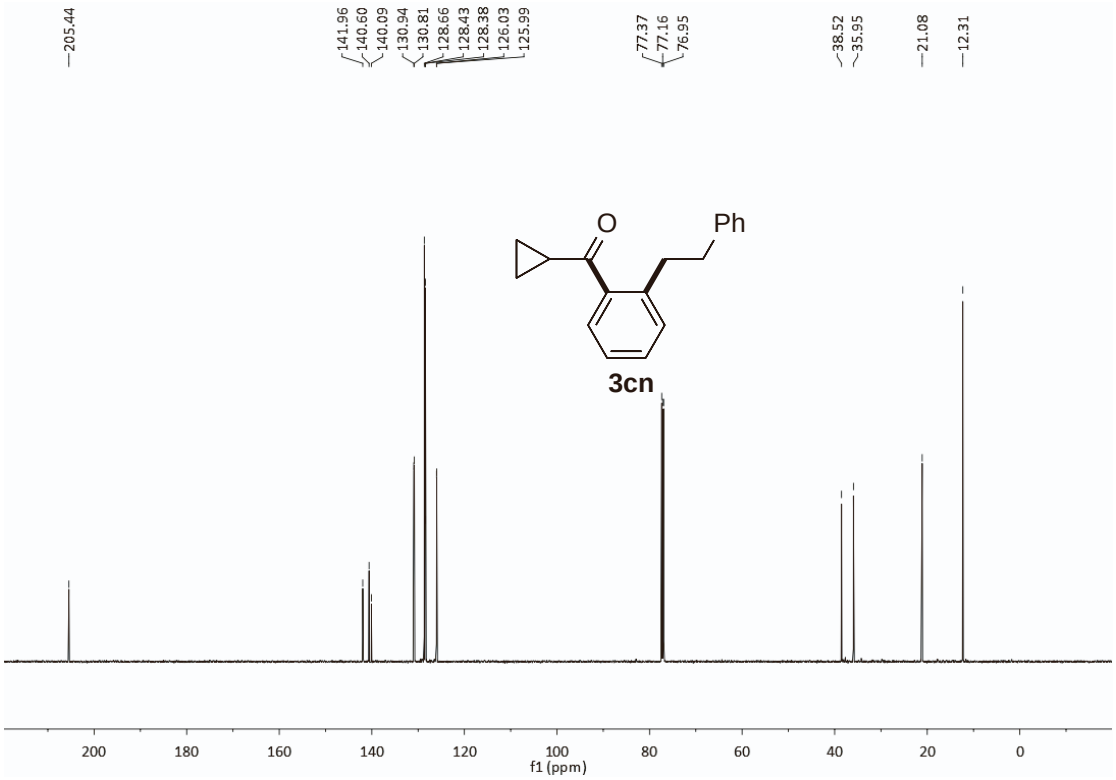
^{13}C NMR (101 MHz, $CDCl_3$)



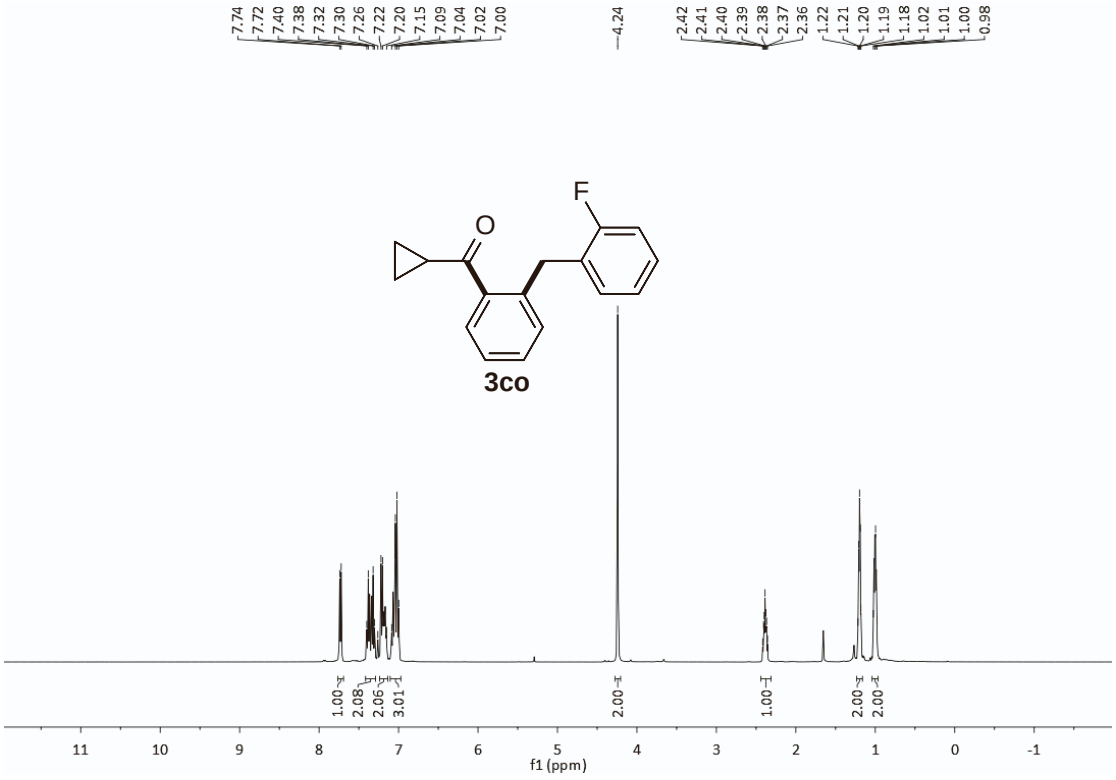
^{1}H NMR (400 MHz, $CDCl_3$)



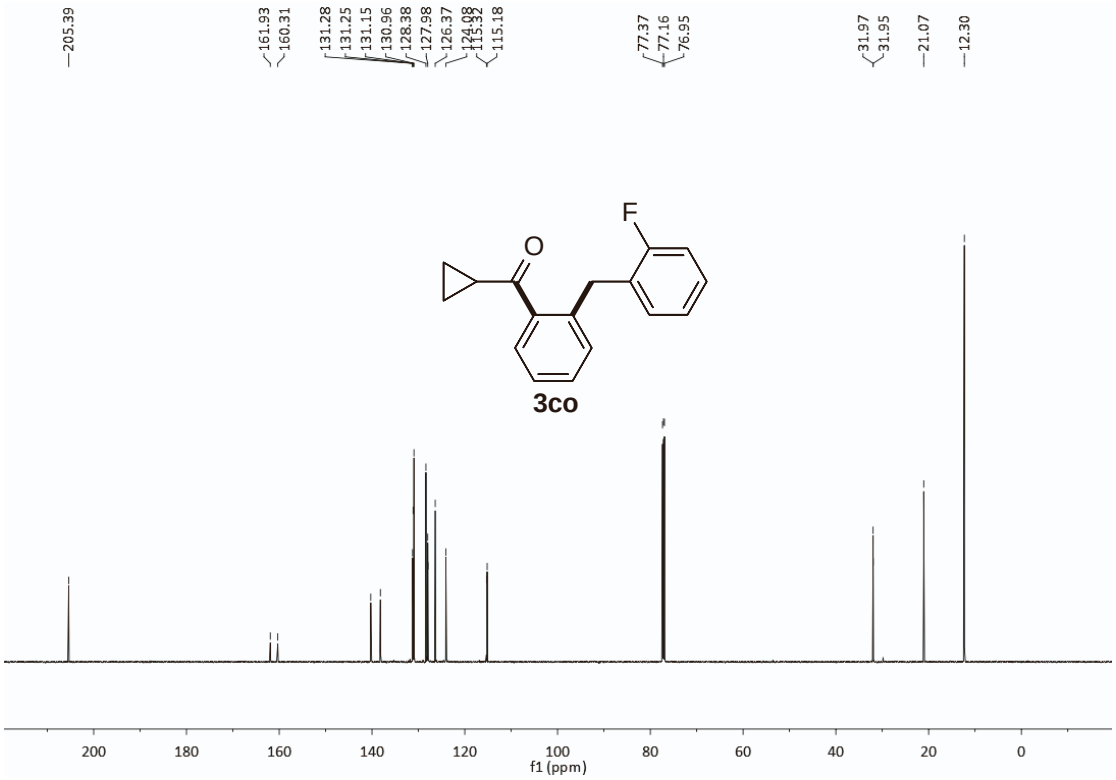
^{13}C NMR (151 MHz, $CDCl_3$)



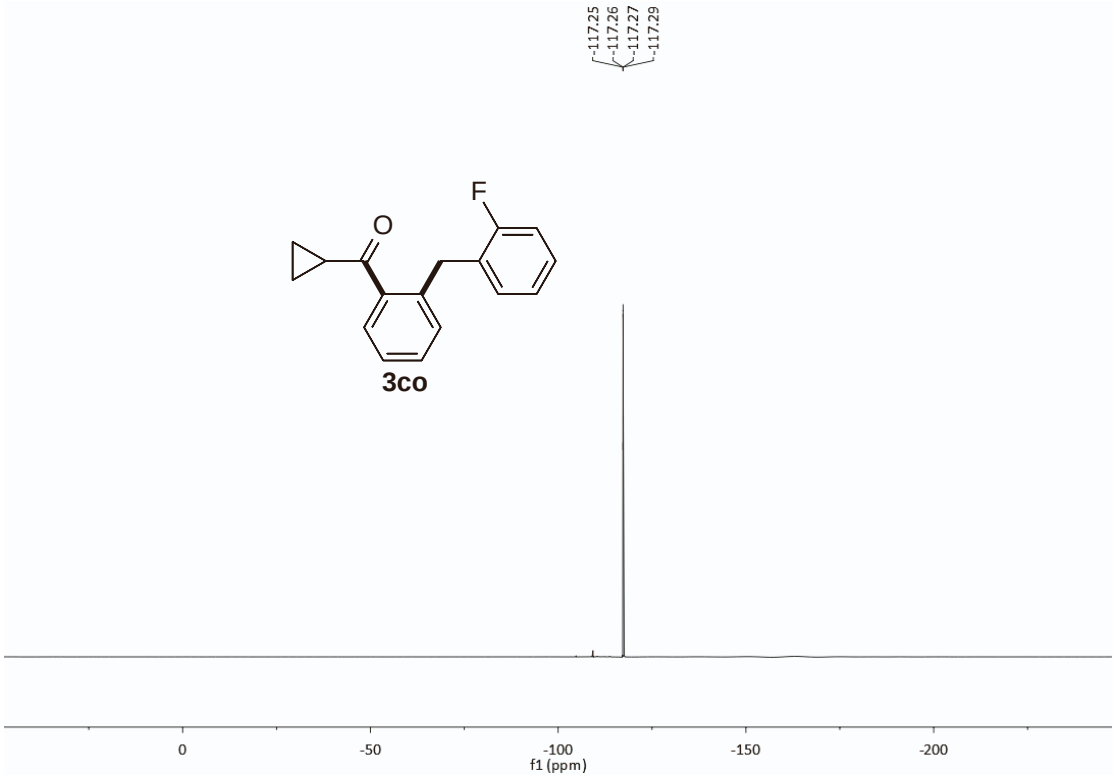
^{1}H NMR (400 MHz, $CDCl_3$)



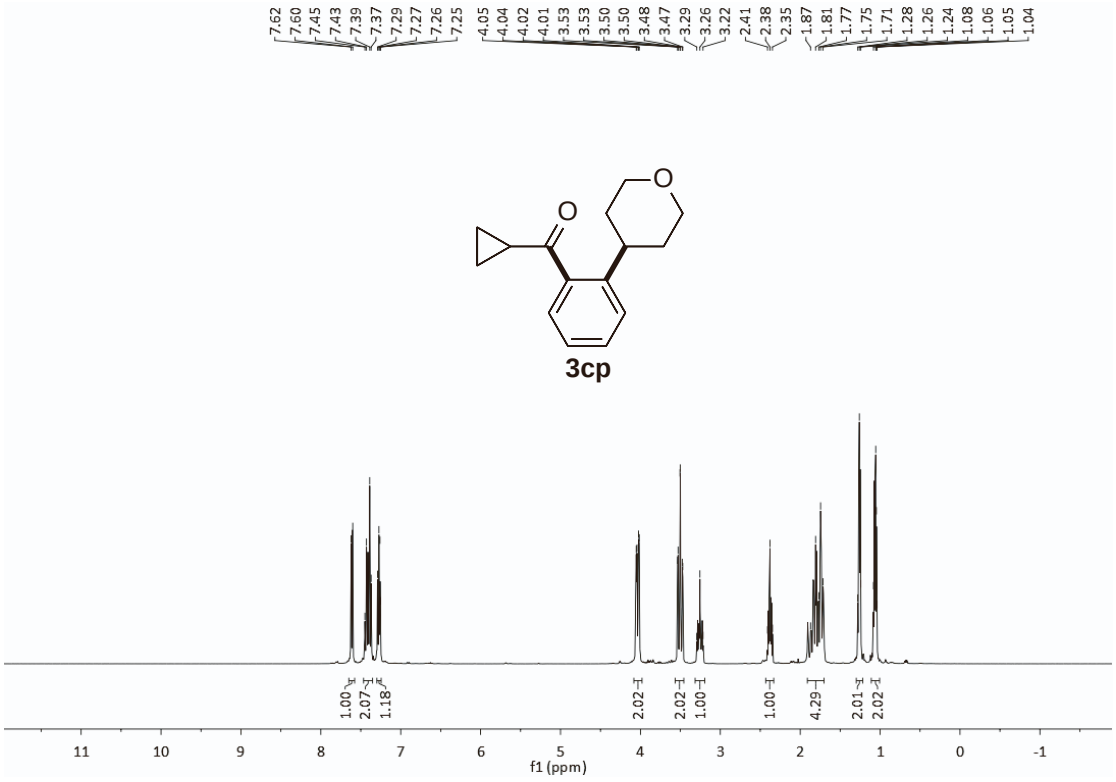
^{13}C NMR (151 MHz, $CDCl_3$)



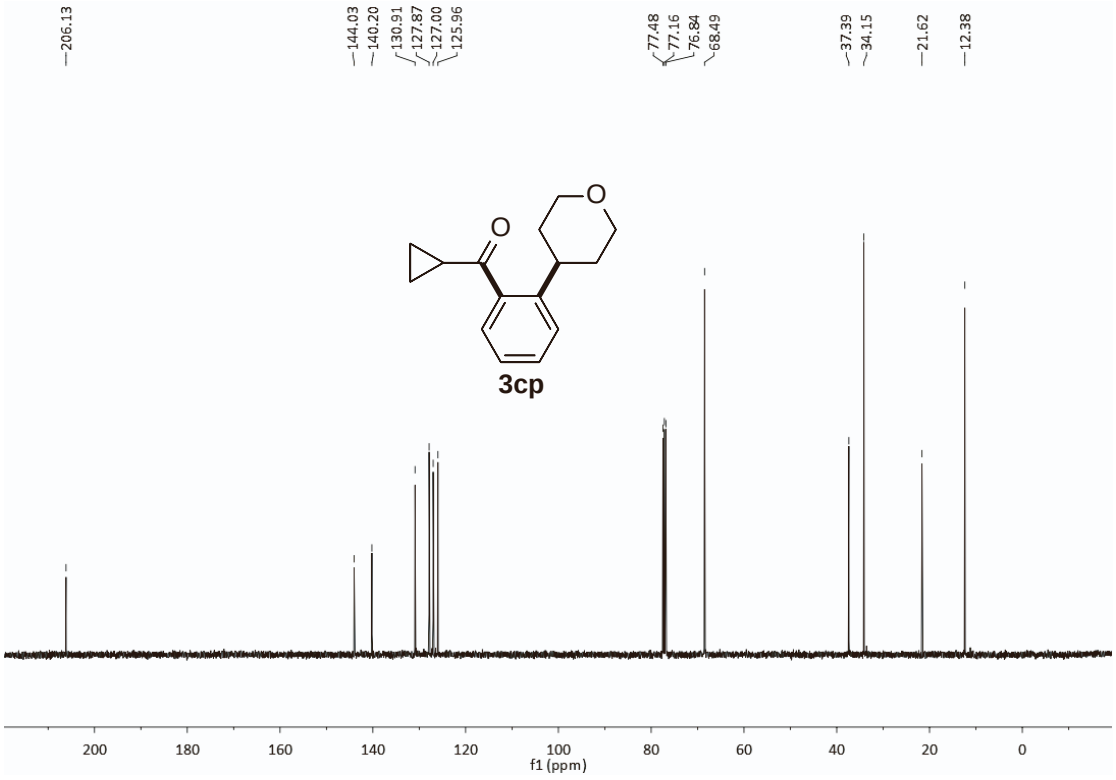
^{19}F NMR (565 MHz, $CDCl_3$)



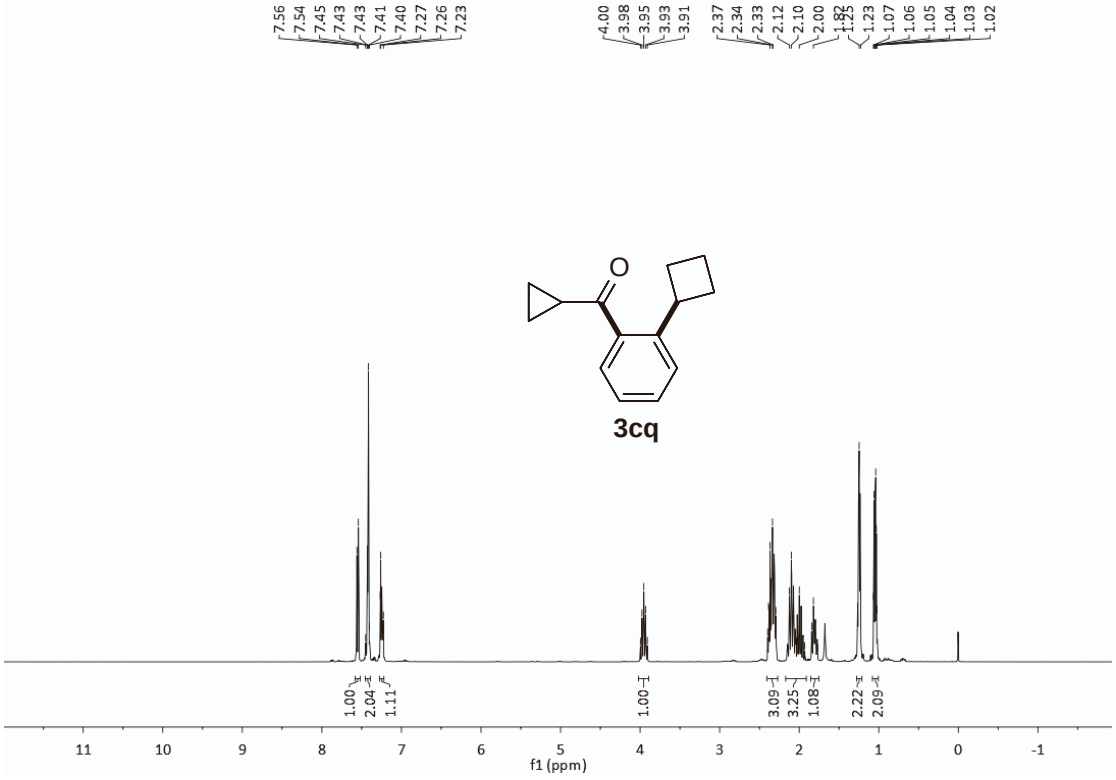
^{1}H NMR (400 MHz, $CDCl_3$)



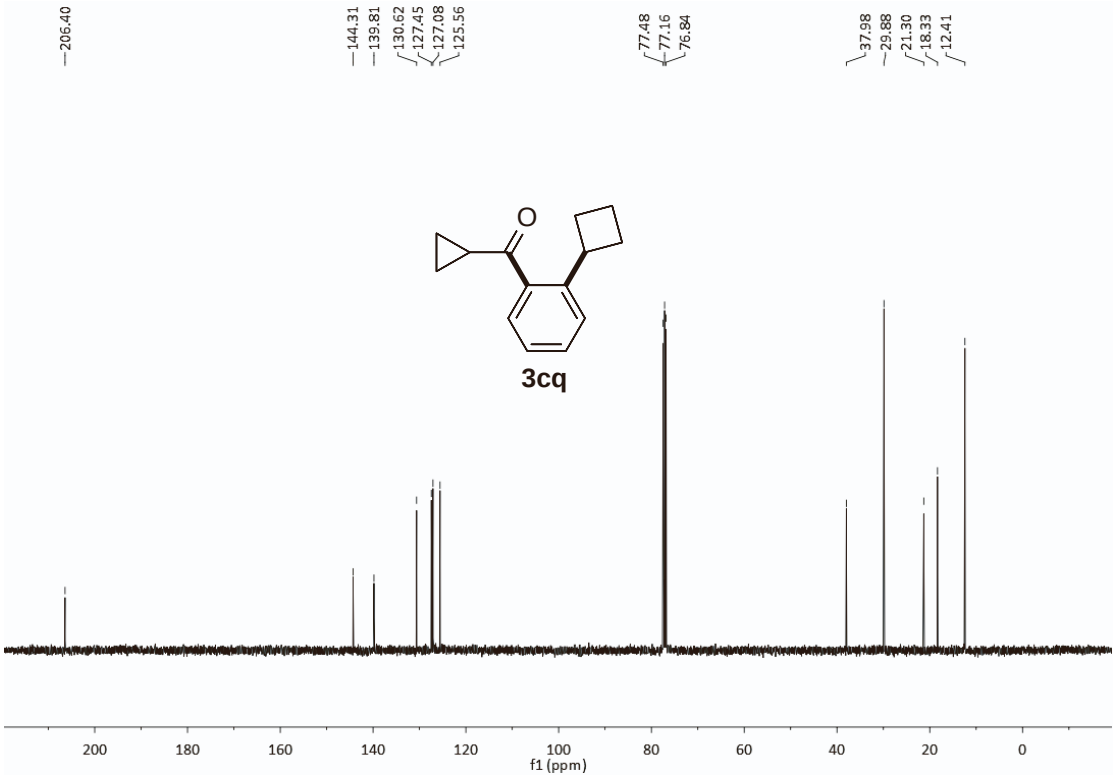
^{13}C NMR (101 MHz, $CDCl_3$)



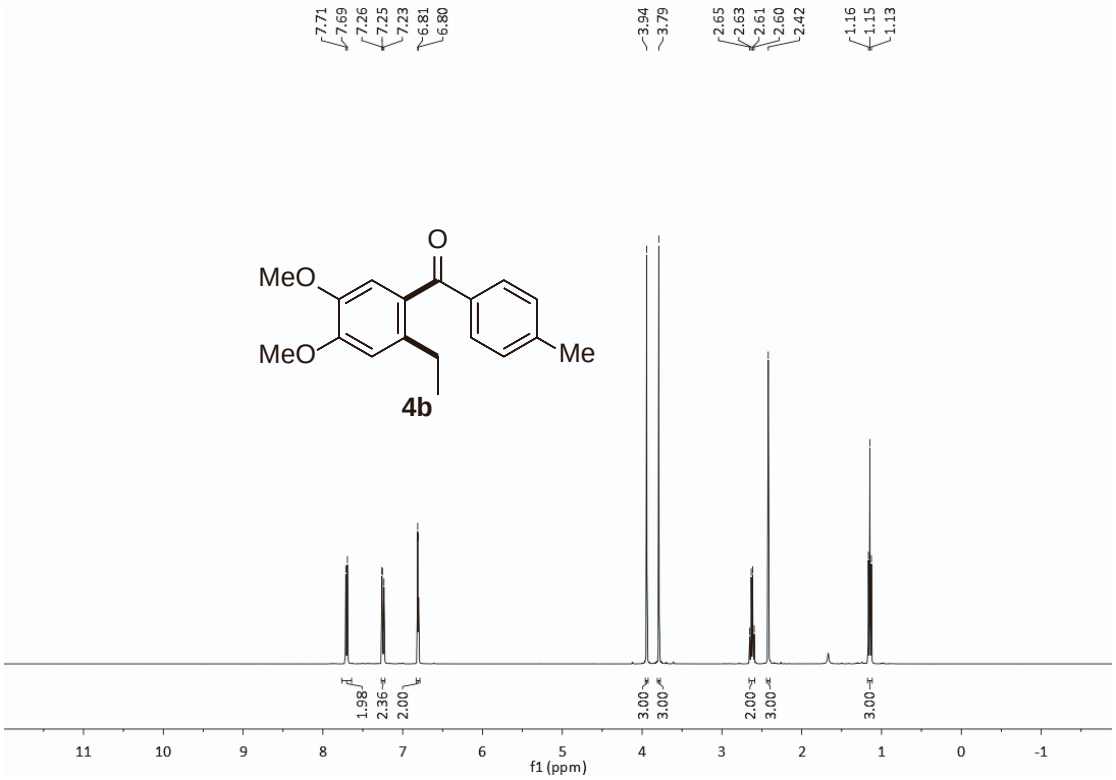
^{1}H NMR (400 MHz, $CDCl_3$)



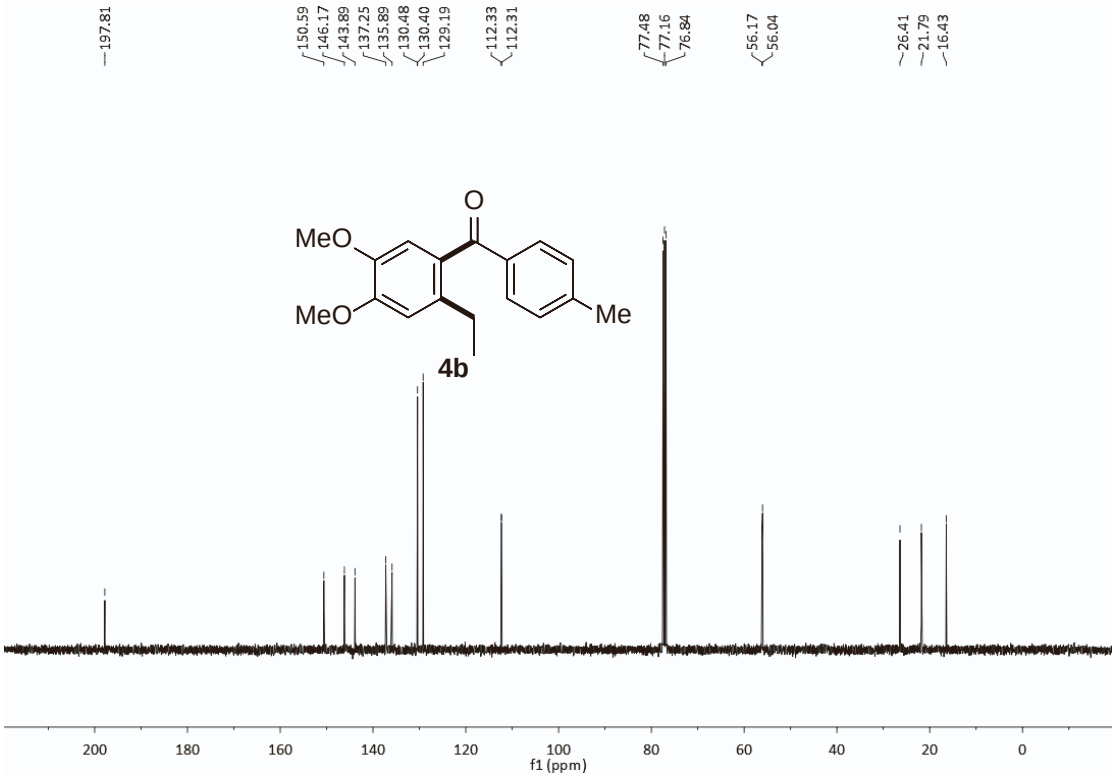
^{13}C NMR (101 MHz, $CDCl_3$)



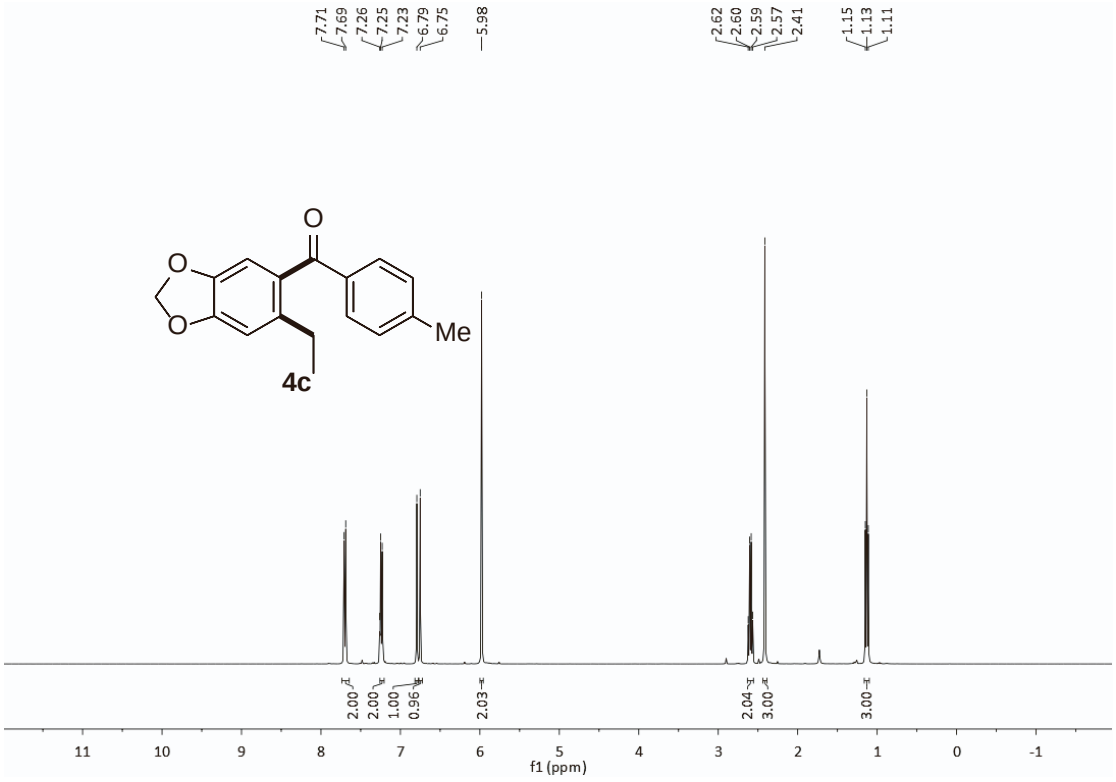
^{1}H NMR (400 MHz, $CDCl_3$)



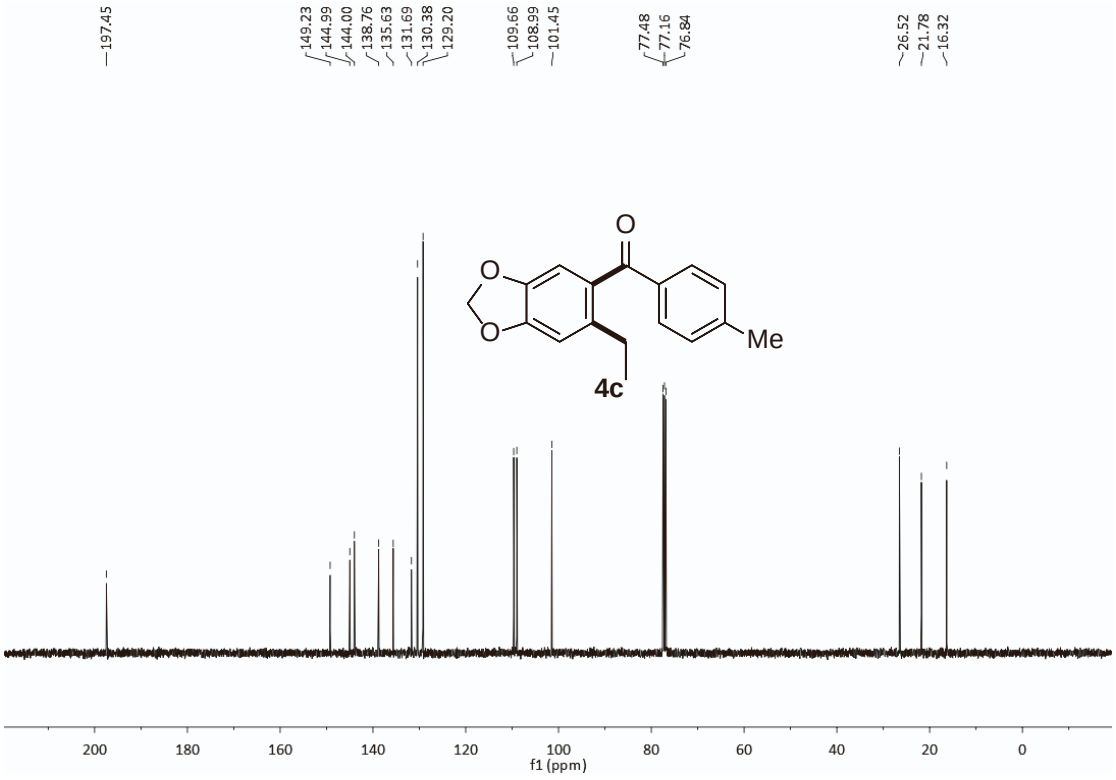
^{13}C NMR (101 MHz, $CDCl_3$)



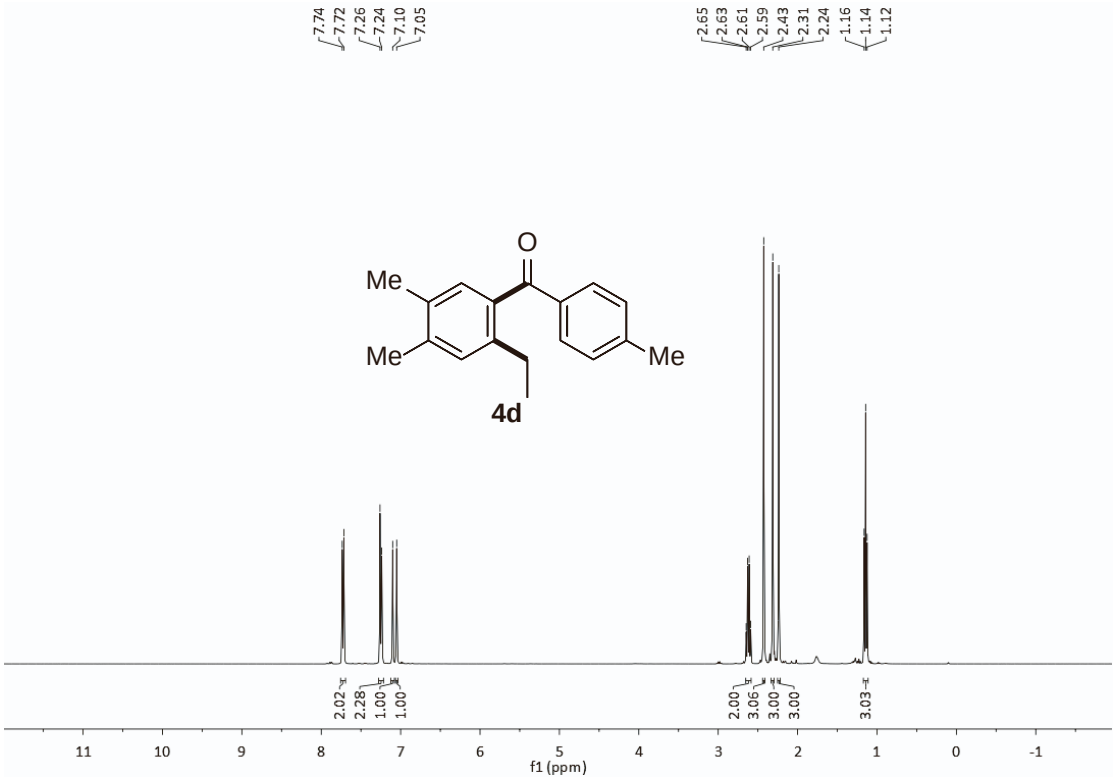
^{1}H NMR (400 MHz, $CDCl_3$)



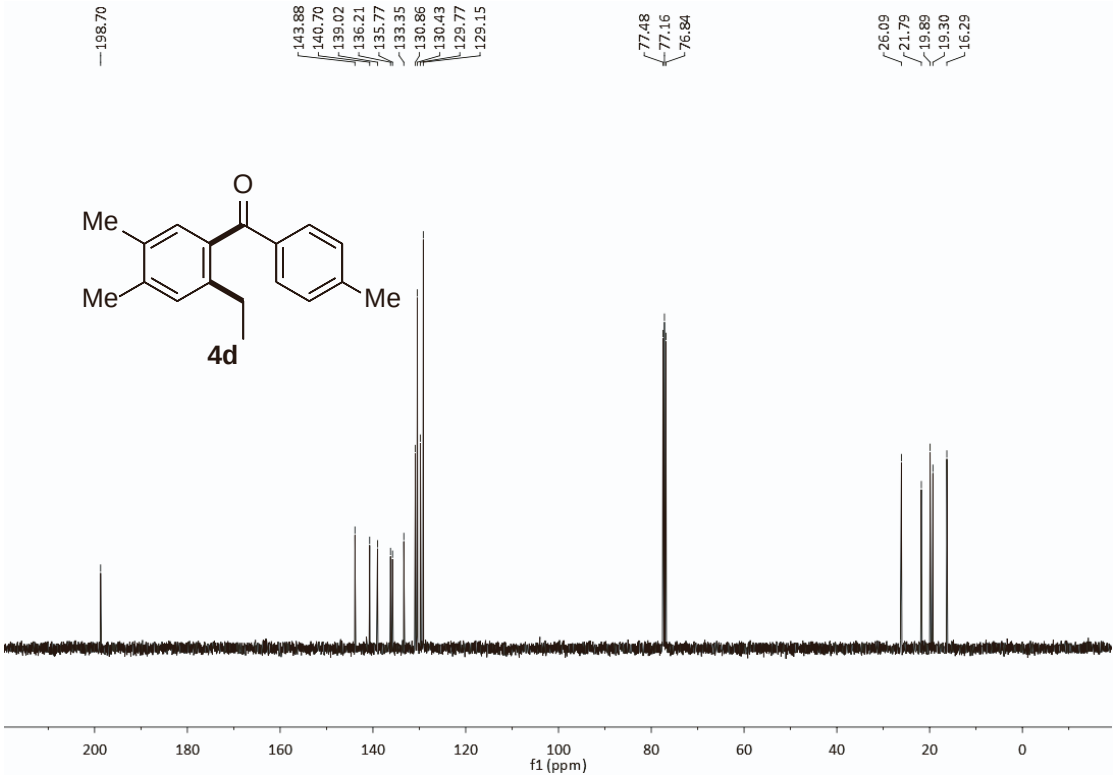
^{13}C NMR (101 MHz, $CDCl_3$)



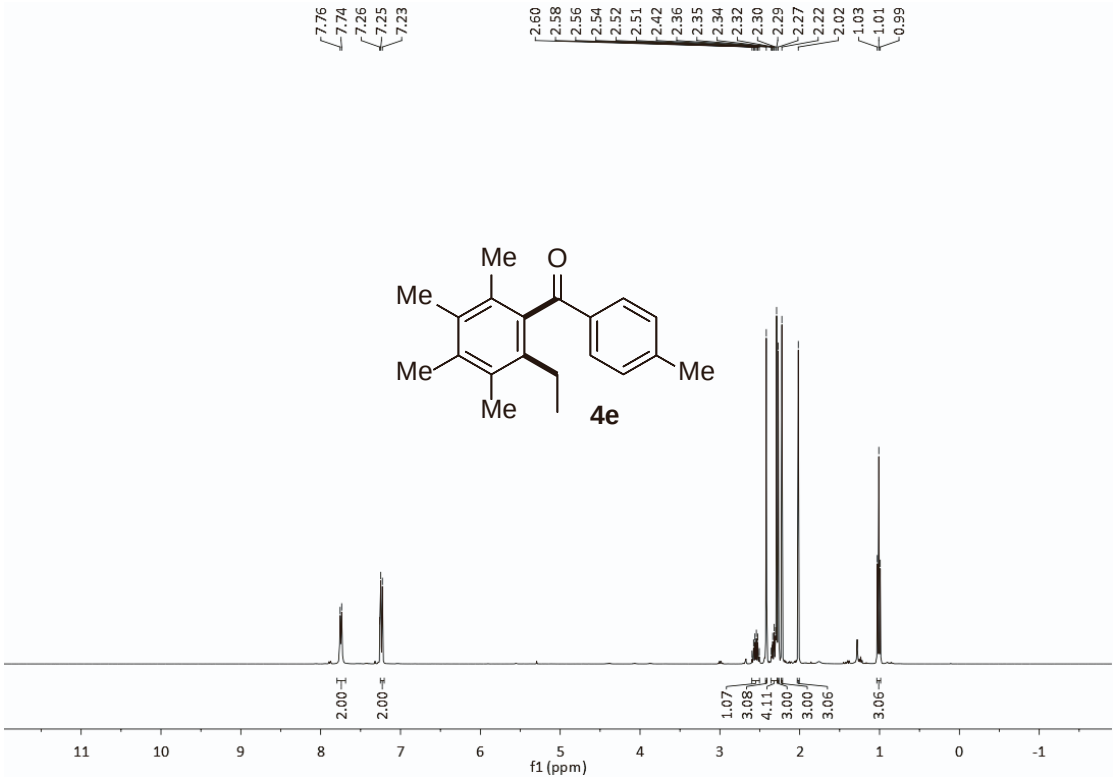
^{1}H NMR (400 MHz, $CDCl_3$)



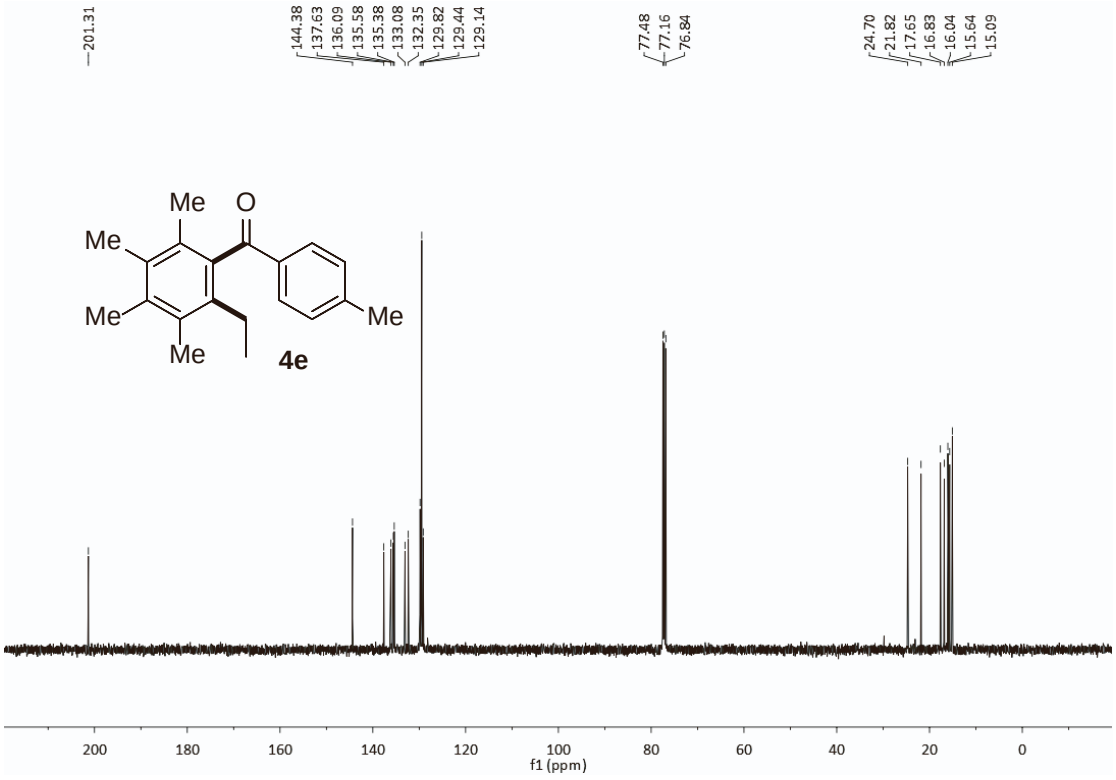
^{13}C NMR (101 MHz, $CDCl_3$)



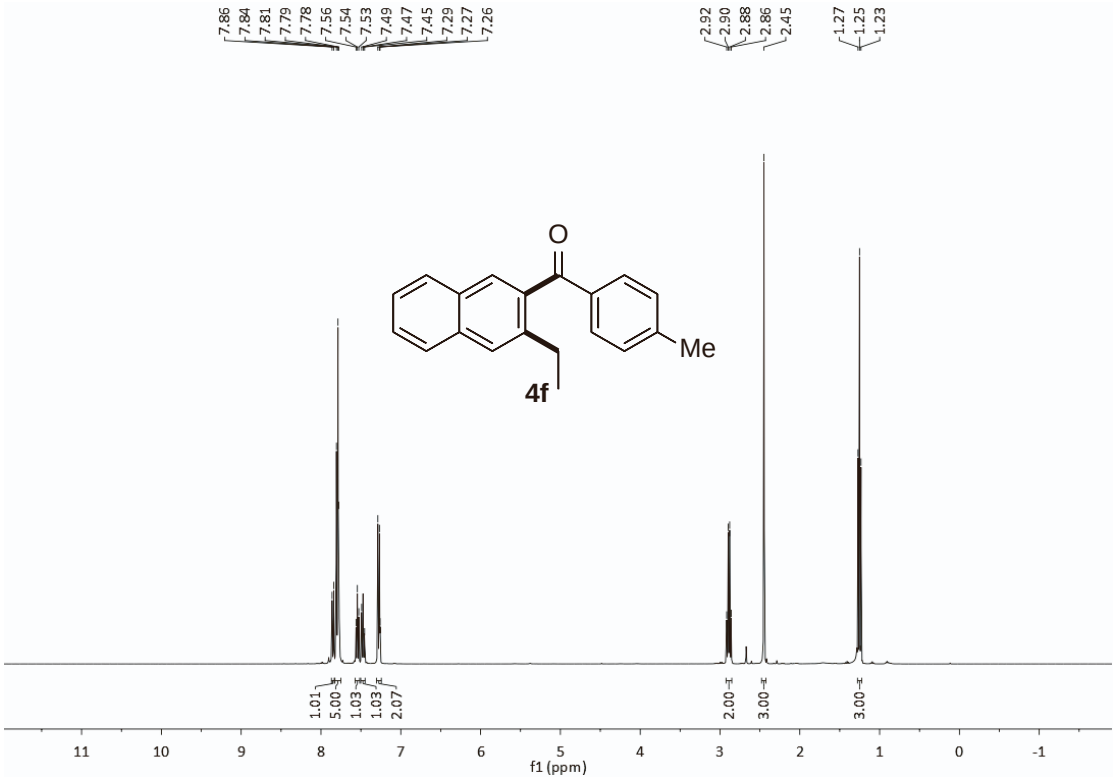
^{1}H NMR (400 MHz, $CDCl_3$)



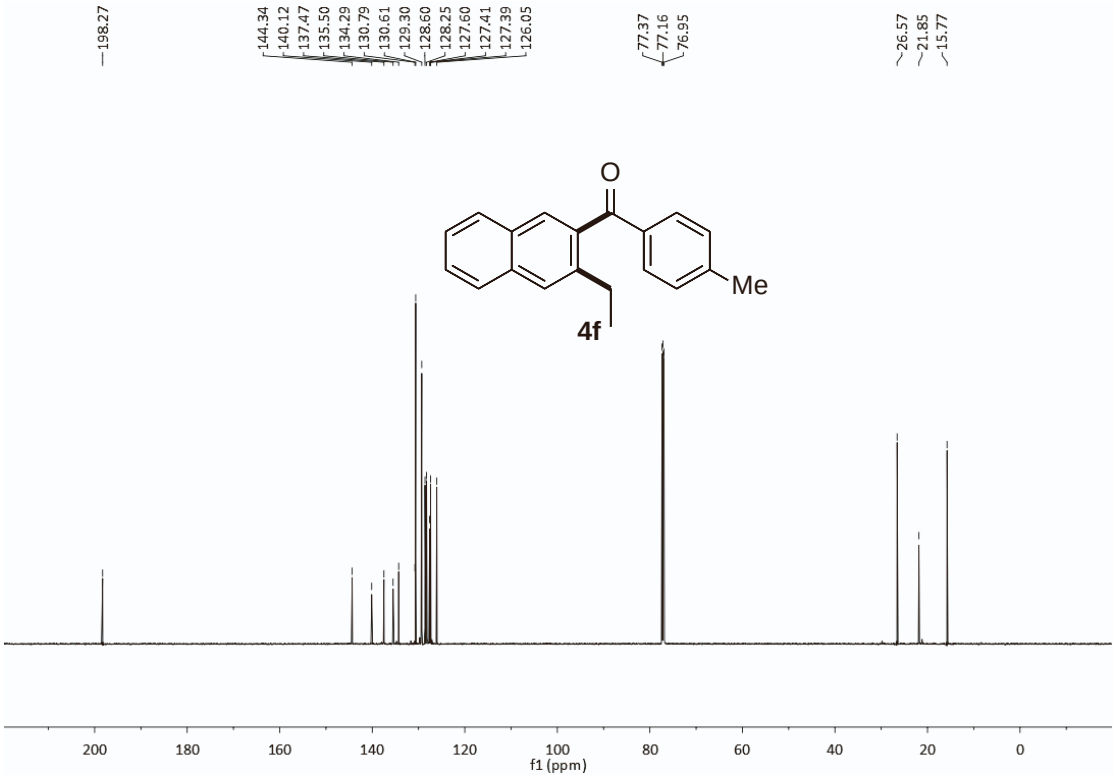
^{13}C NMR (101 MHz, $CDCl_3$)



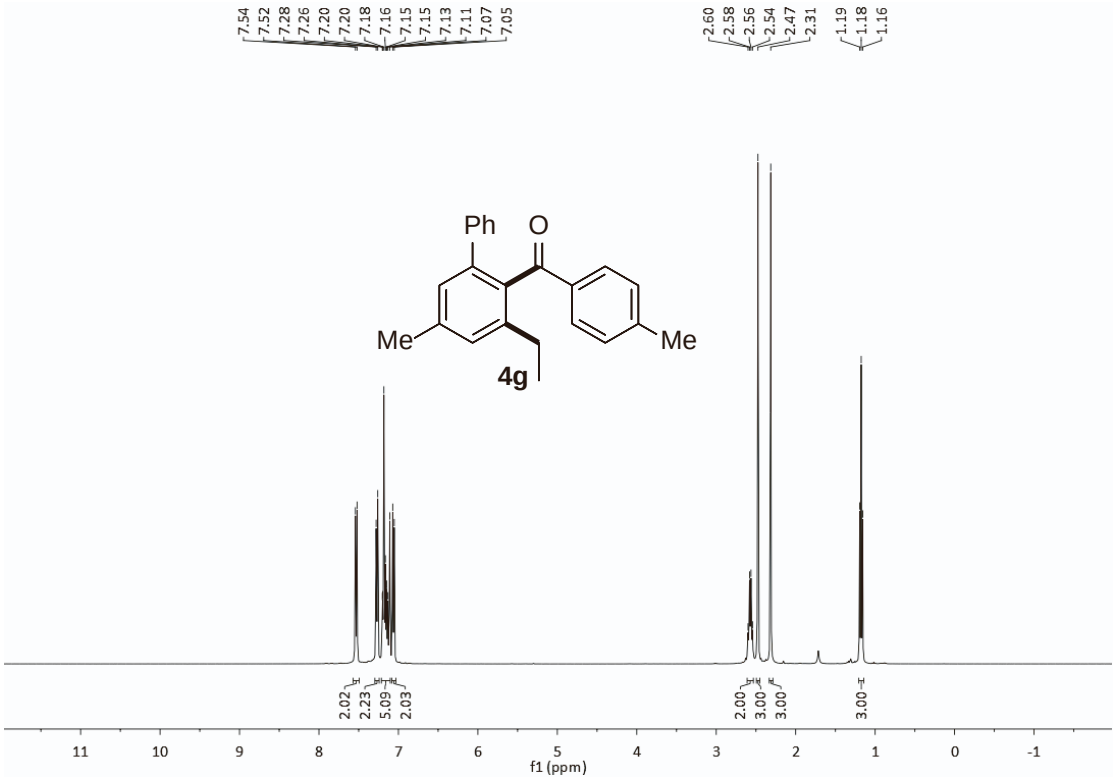
^{1}H NMR (400 MHz, $CDCl_3$)



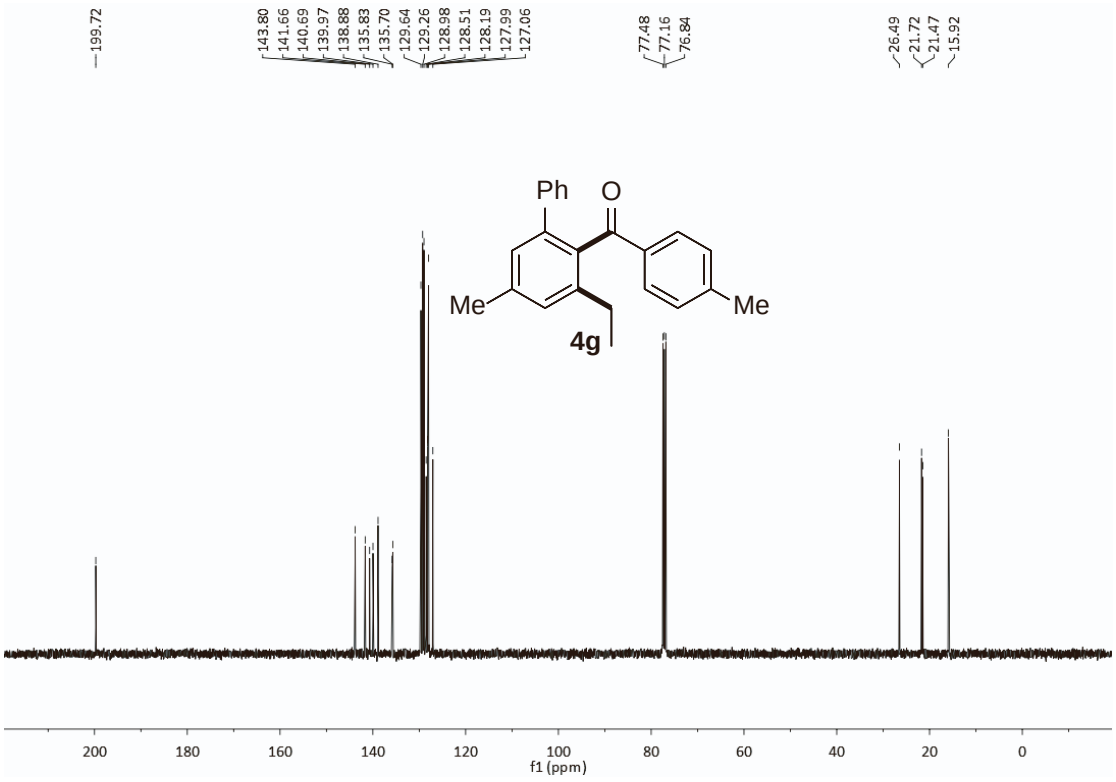
^{13}C NMR (151 MHz, $CDCl_3$)



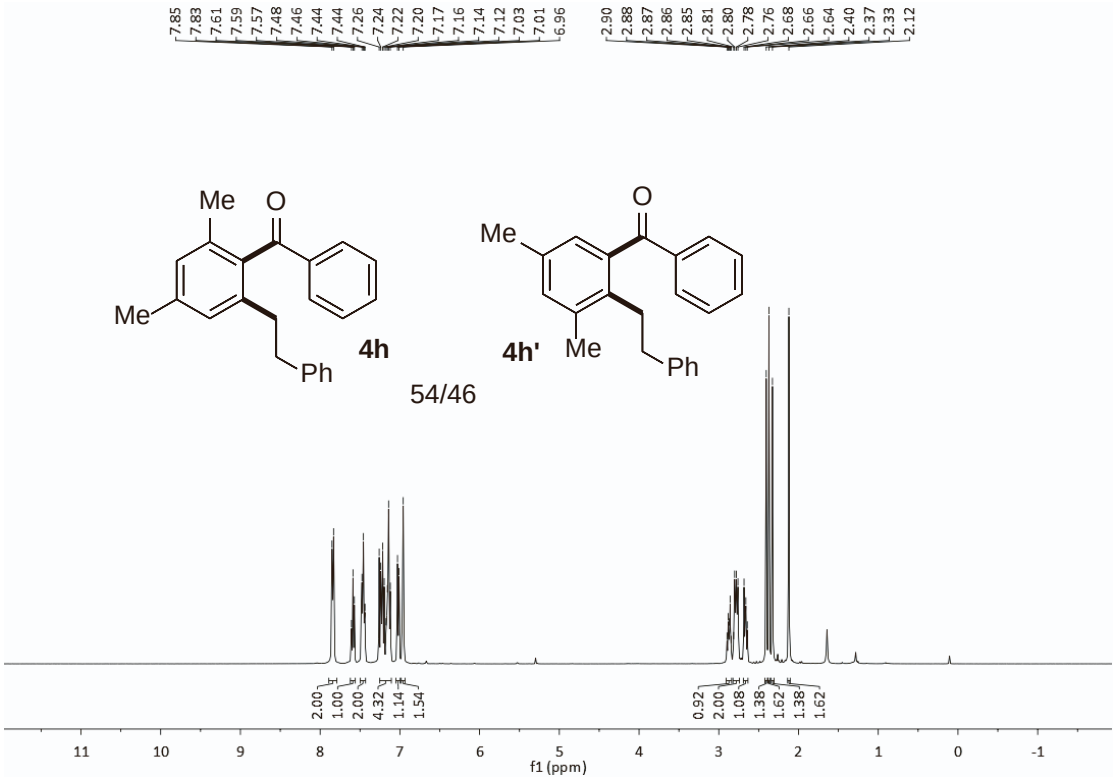
^{1}H NMR (400 MHz, $CDCl_3$)



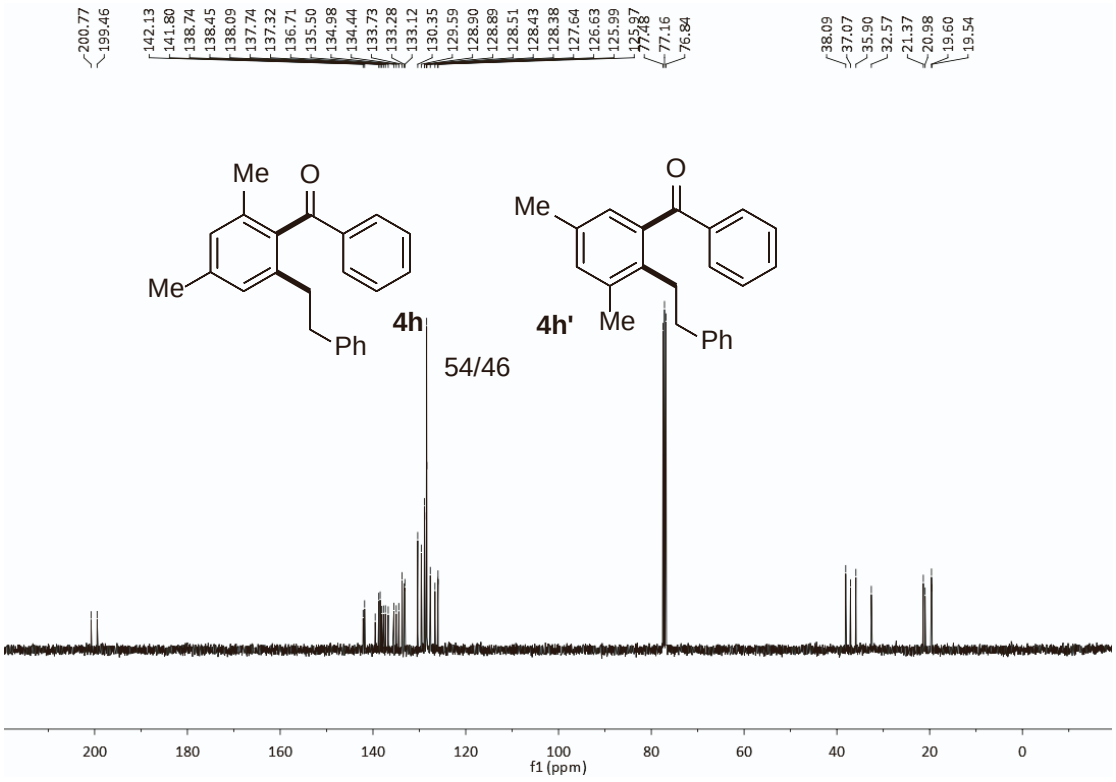
^{13}C NMR (101 MHz, $CDCl_3$)



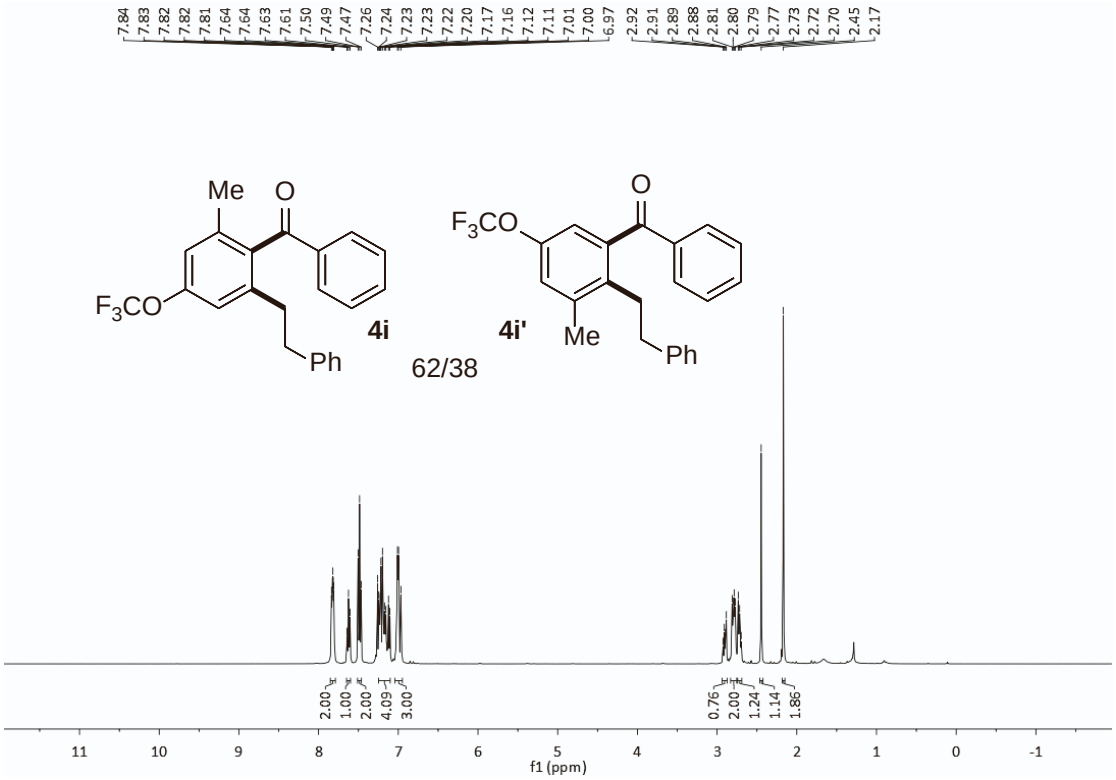
^{1}H NMR (400 MHz, $CDCl_3$)



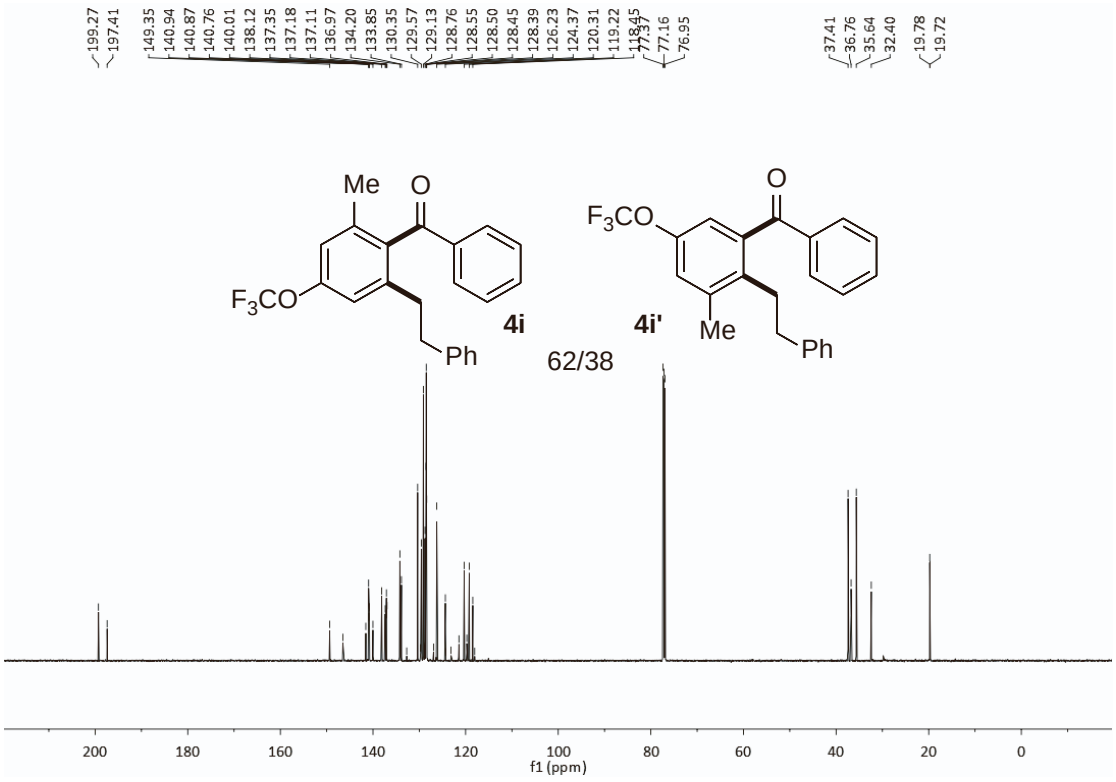
^{13}C NMR (101 MHz, $CDCl_3$)



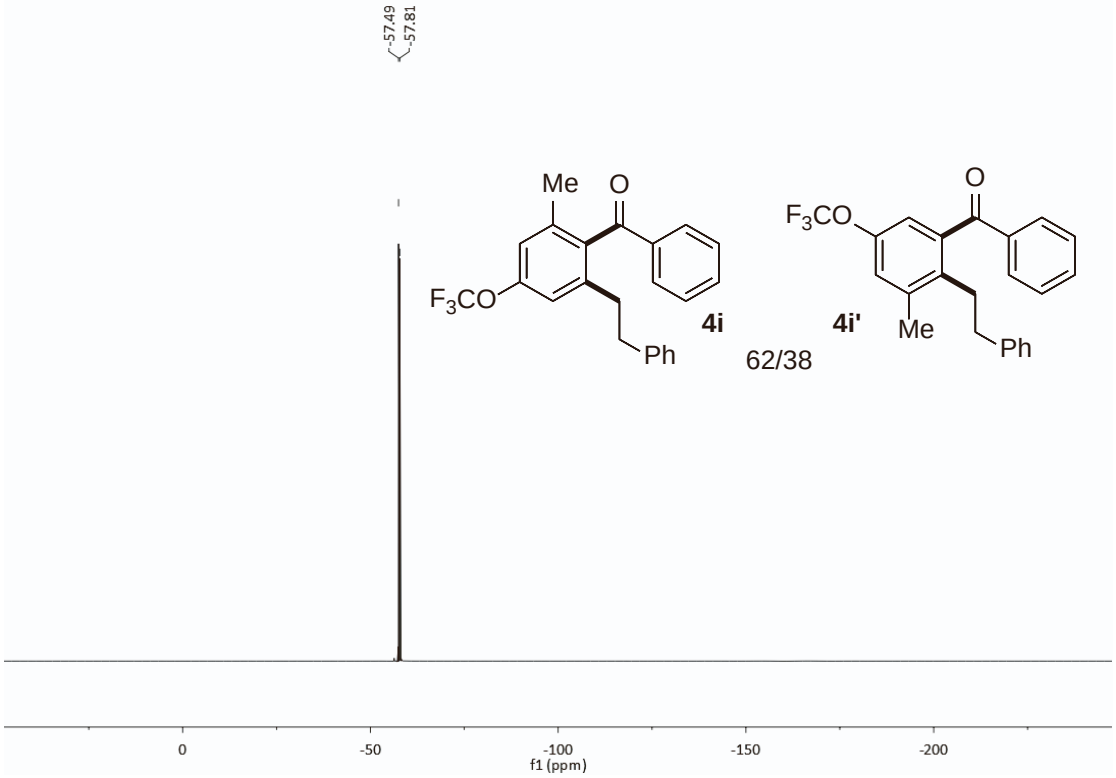
^{1}H NMR (400 MHz, $CDCl_3$)



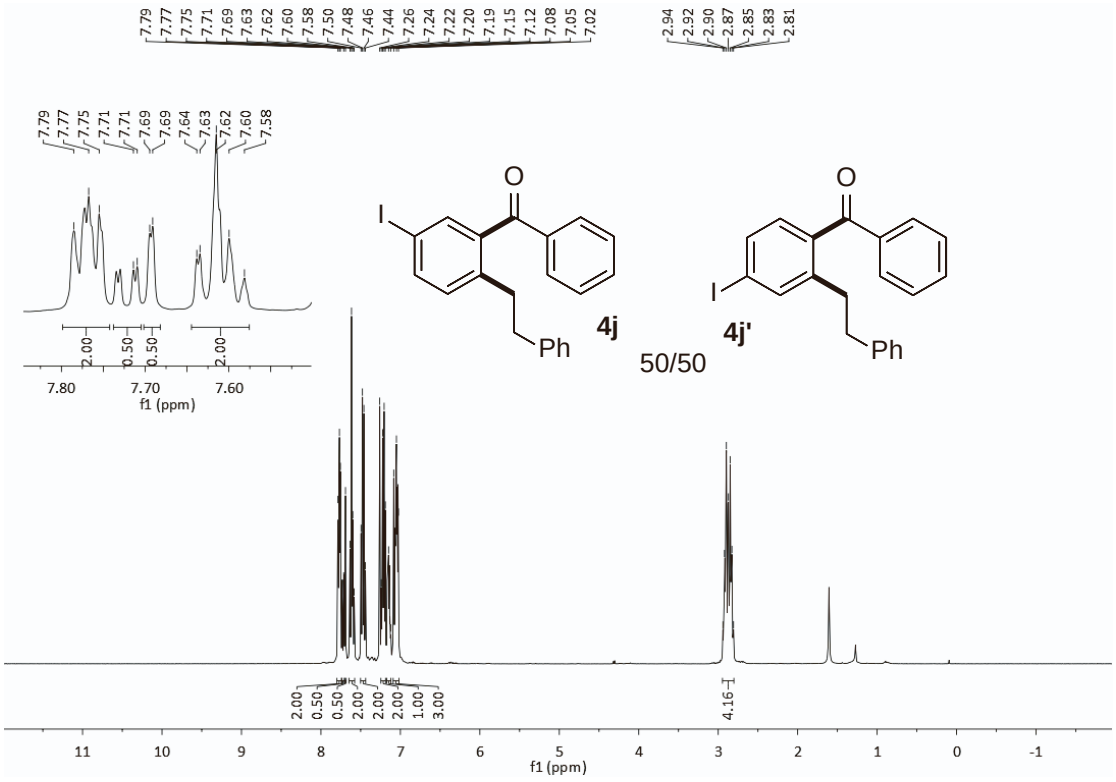
^{13}C NMR (151 MHz, $CDCl_3$)



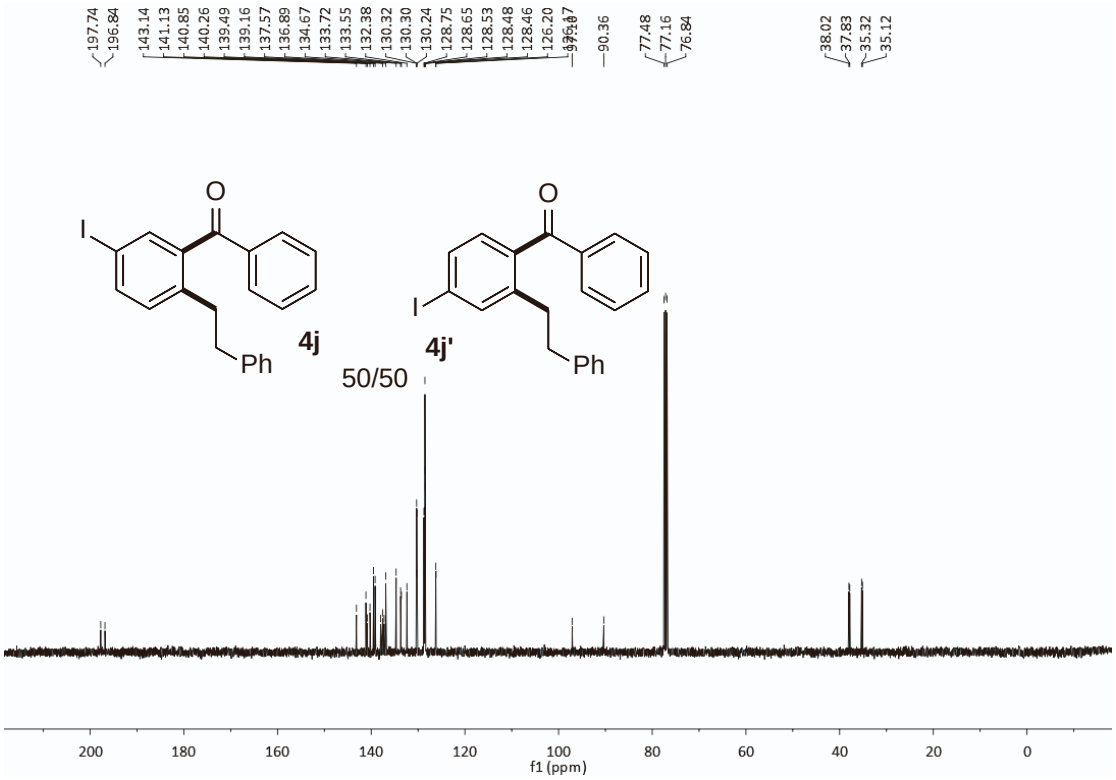
^{19}F NMR (565 MHz, $CDCl_3$)



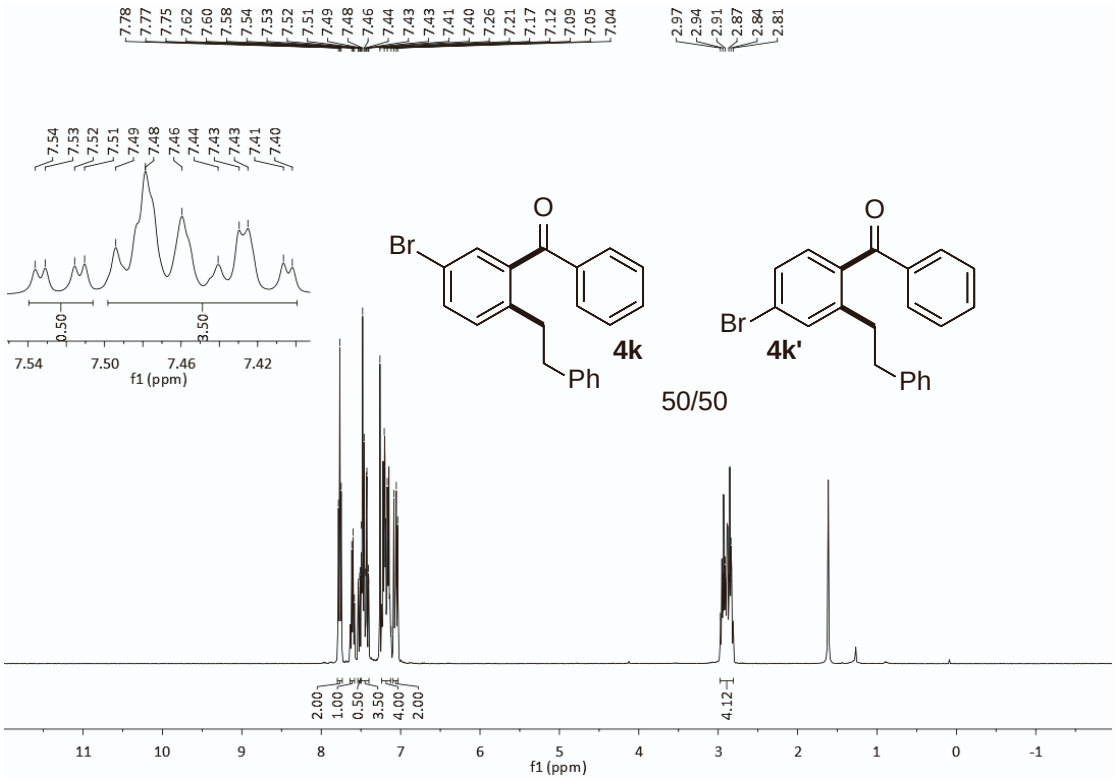
^{1}H NMR (400 MHz, $CDCl_3$)



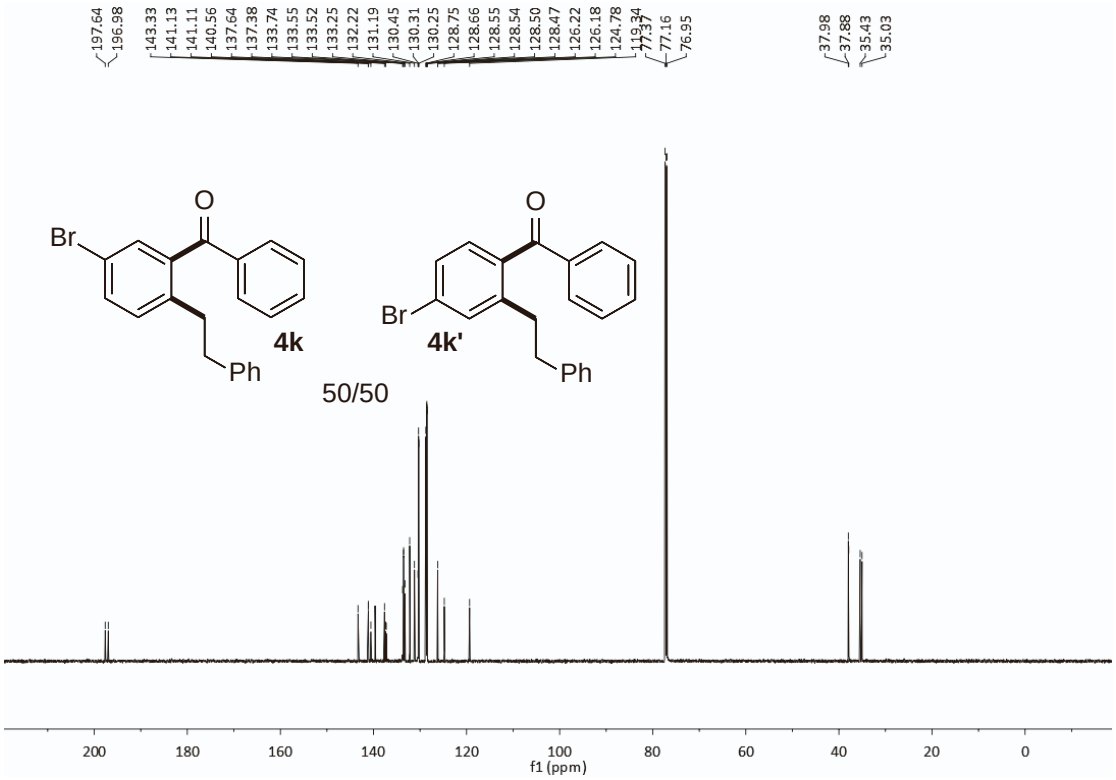
^{13}C NMR (101 MHz, $CDCl_3$)



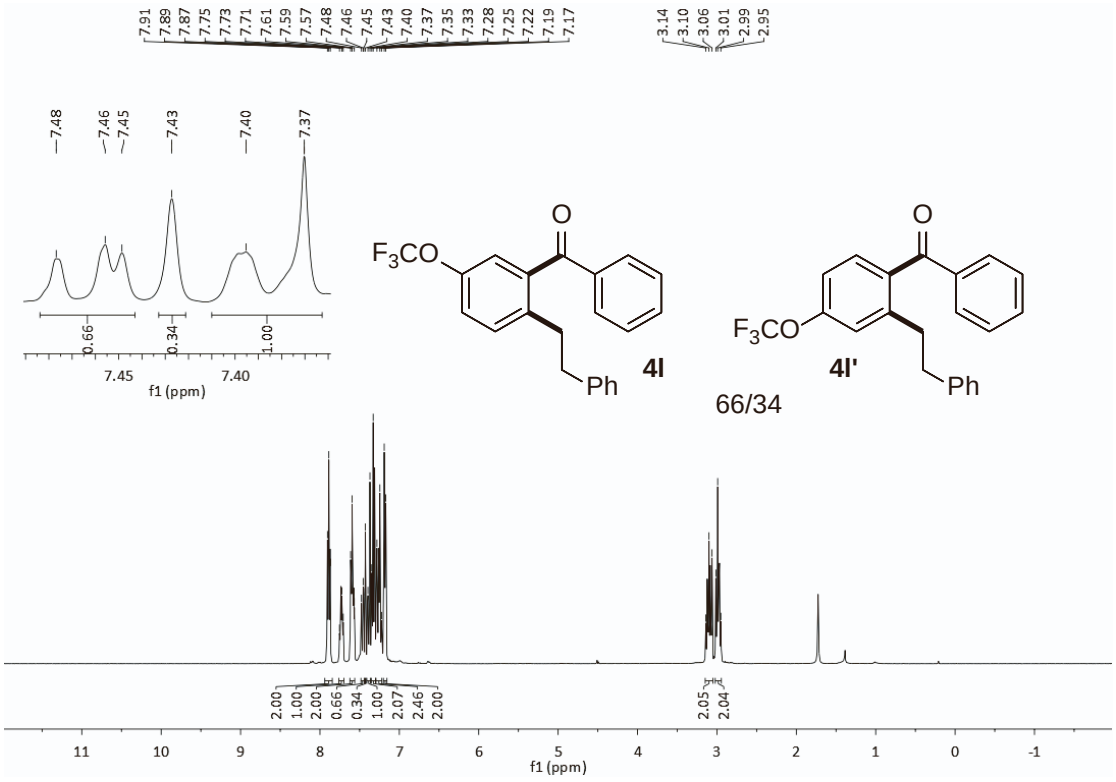
^{1}H NMR (400 MHz, $CDCl_3$)



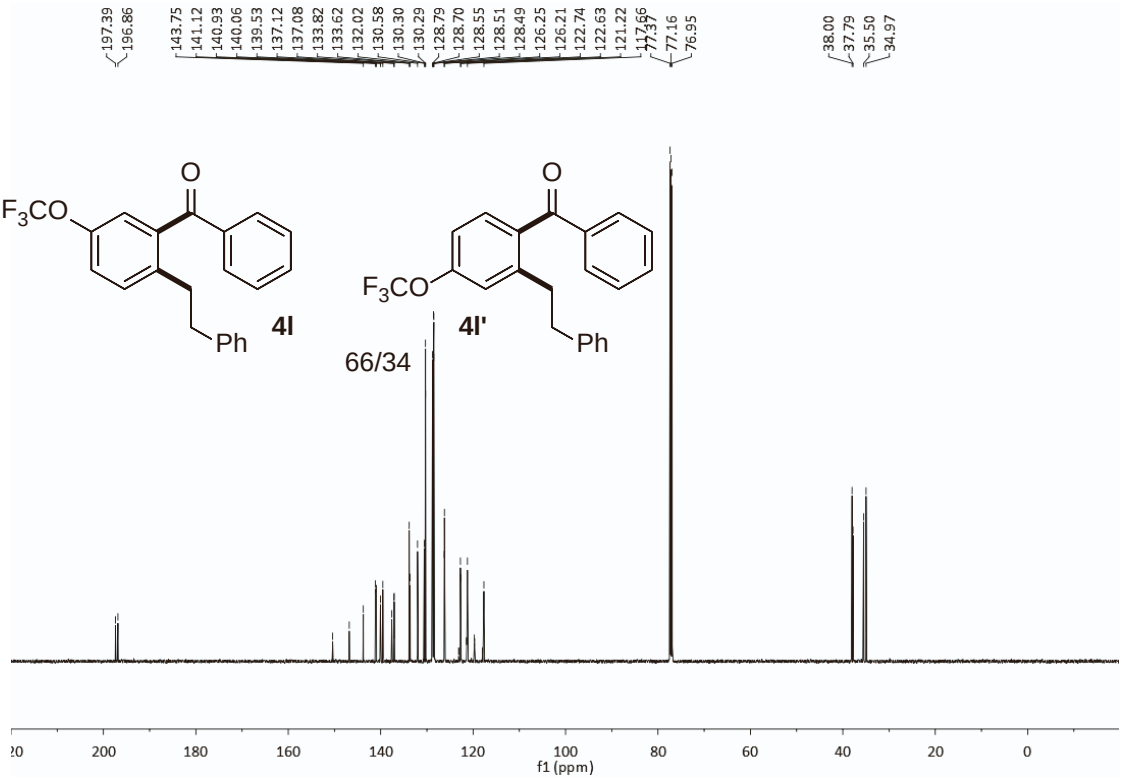
^{13}C NMR (151 MHz, $CDCl_3$)



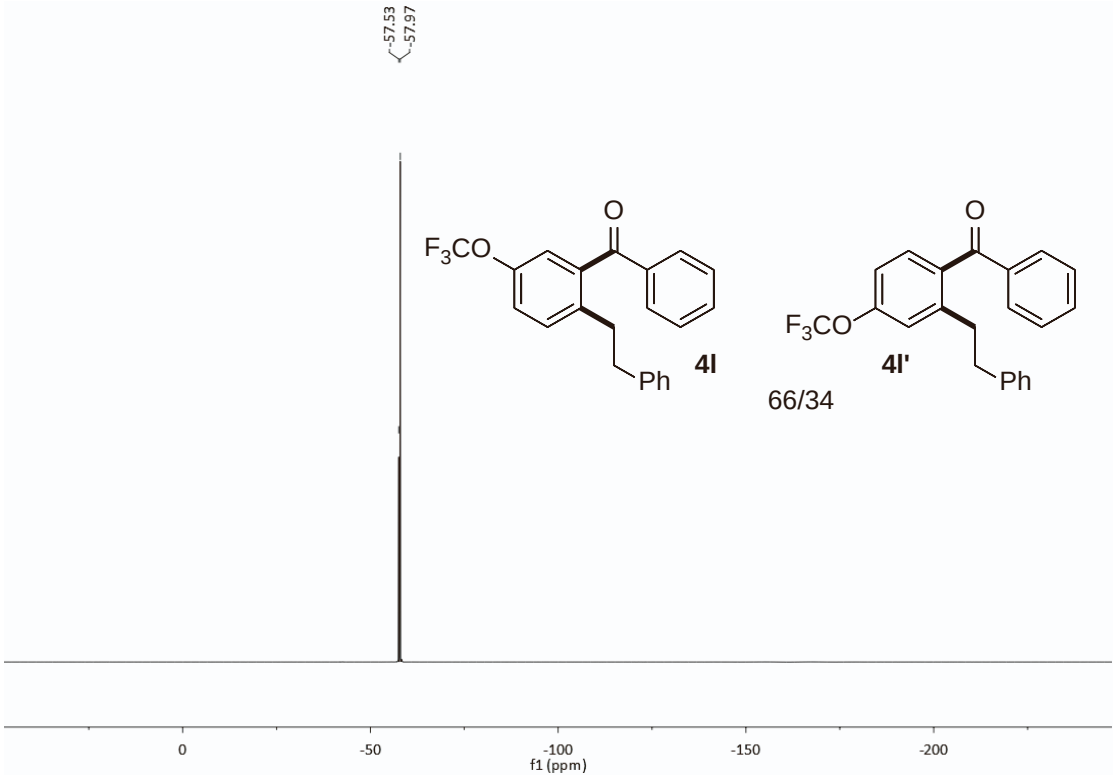
^{1}H NMR (400 MHz, $CDCl_3$)



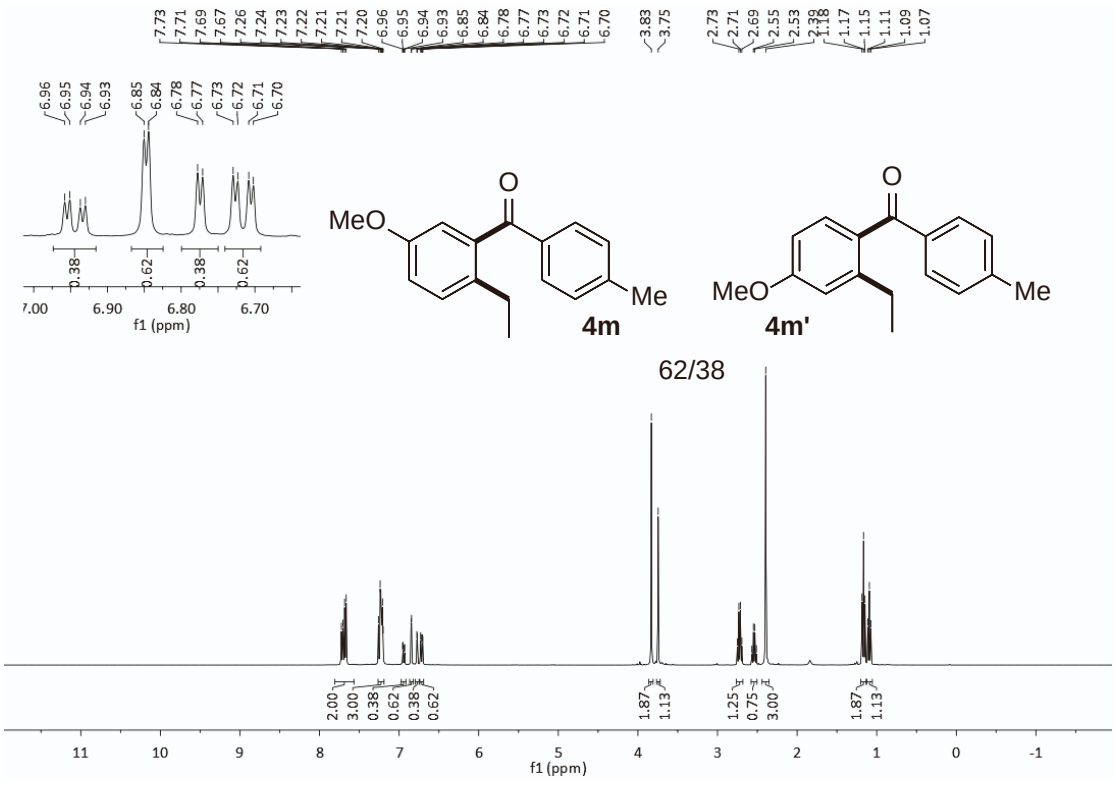
^{13}C NMR (151 MHz, $CDCl_3$)



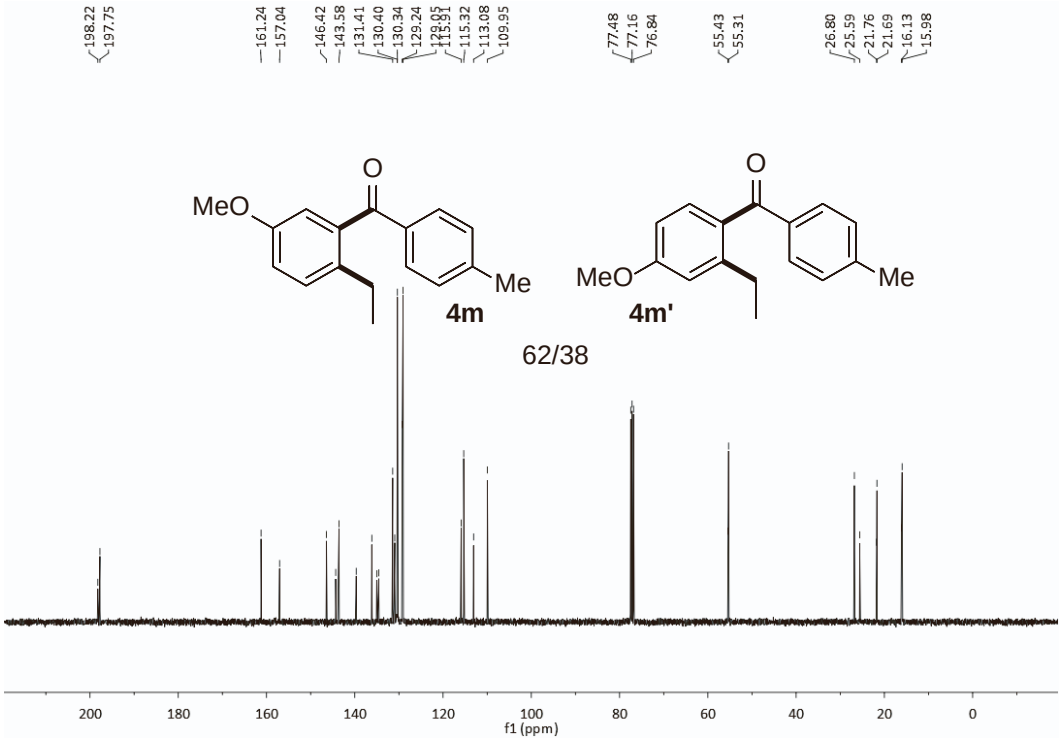
^{19}F NMR (565 MHz, $CDCl_3$)



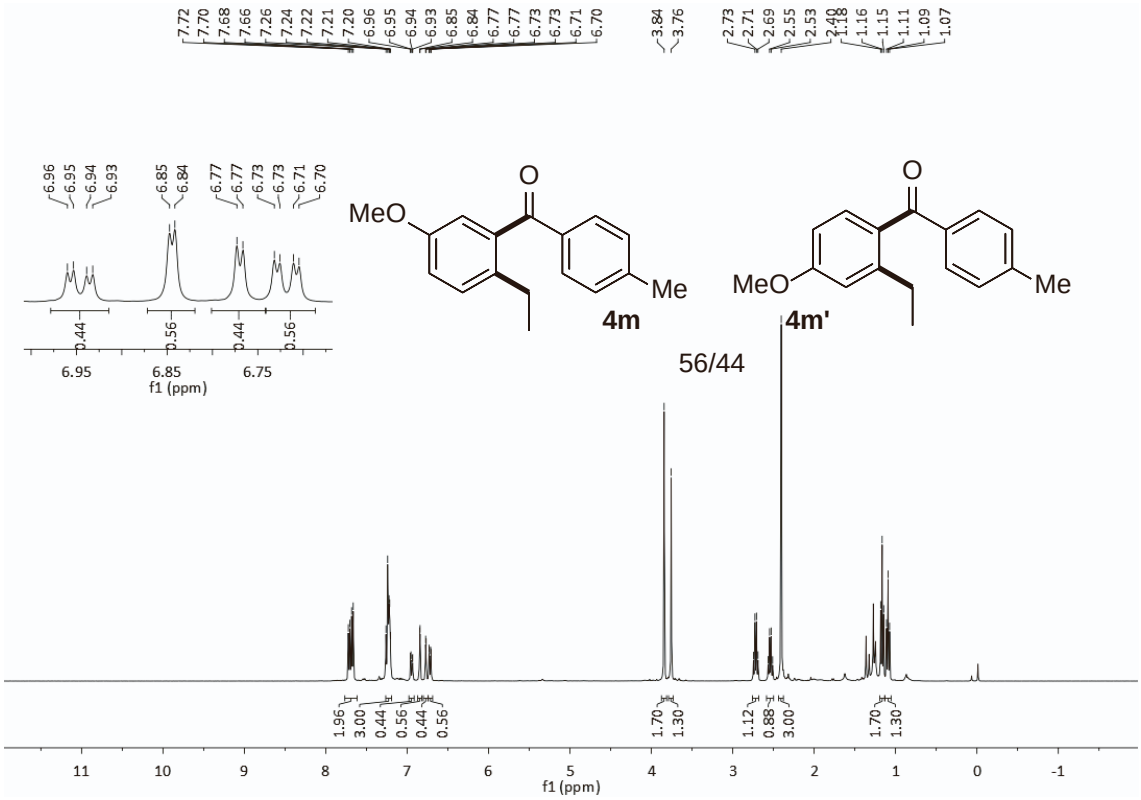
^{1}H NMR (400 MHz, $CDCl_3$)



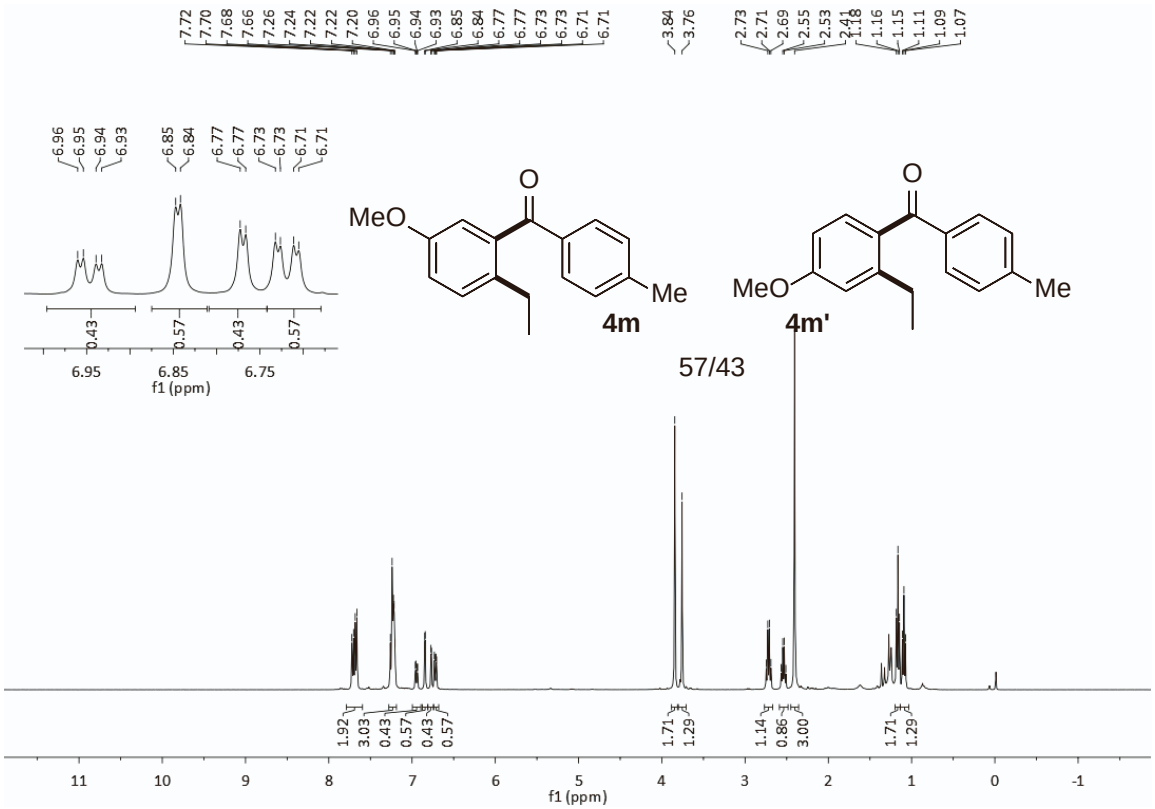
^{13}C NMR (101 MHz, $CDCl_3$)



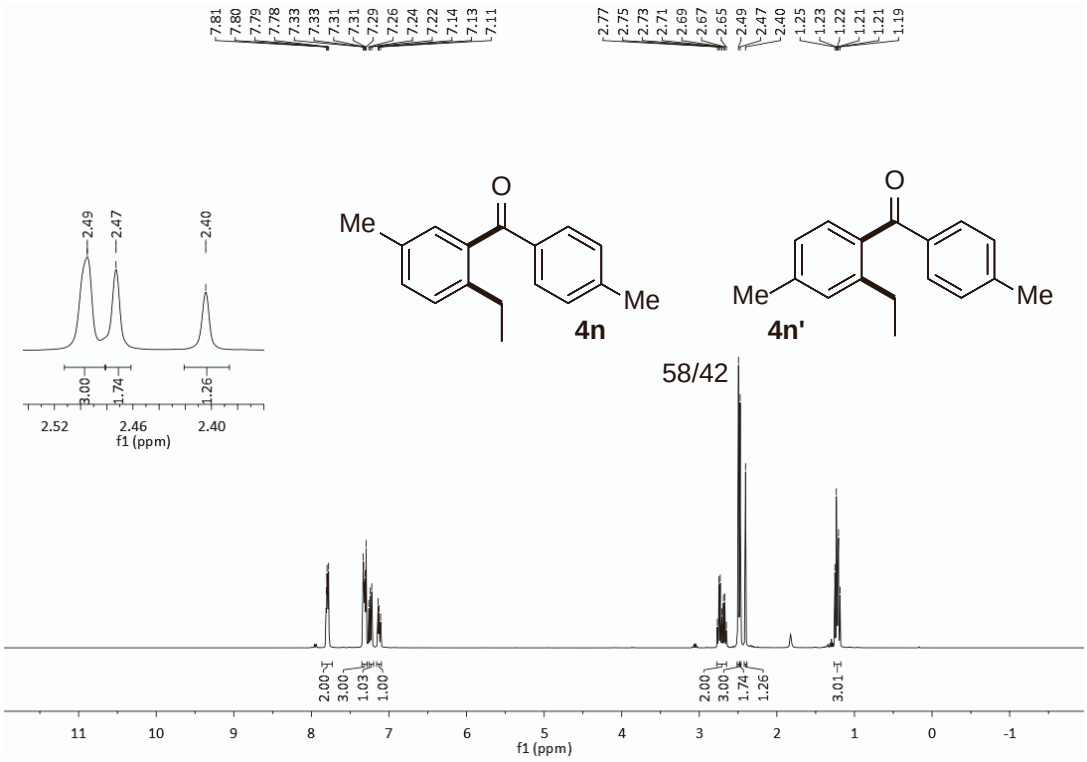
^{1}H NMR (400 MHz, $CDCl_3$) (2-bromo-1-iodo-4-methoxybenzene 1m' was used as the aryne precursor)



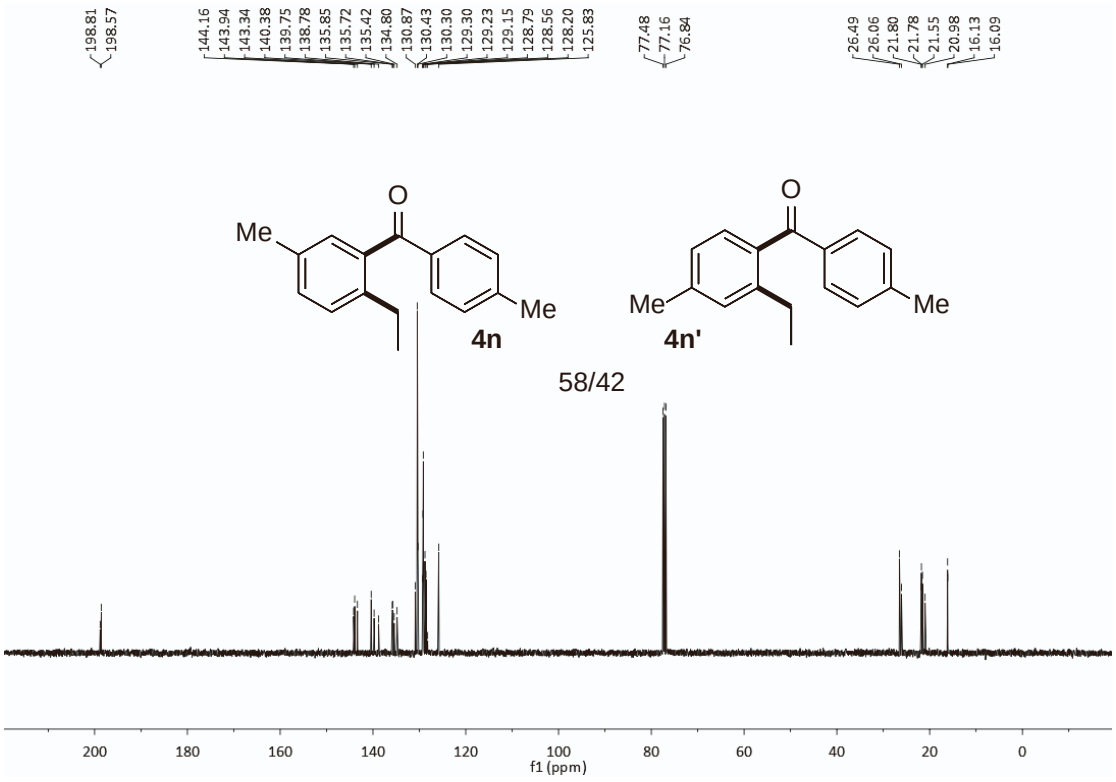
^{1}H NMR (400 MHz, $CDCl_3$) (1-bromo-2-iodo-4-methoxybenzene 1m" was used as the aryne precursor)



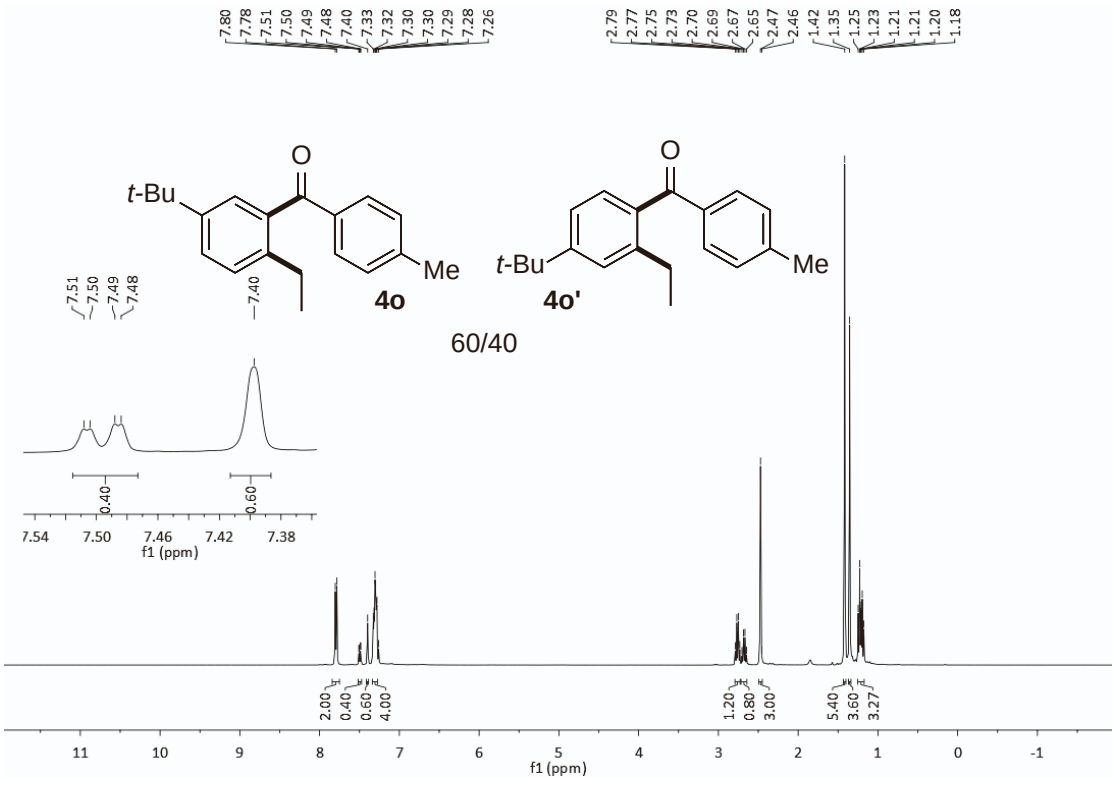
^{1}H NMR (400 MHz, $CDCl_3$)



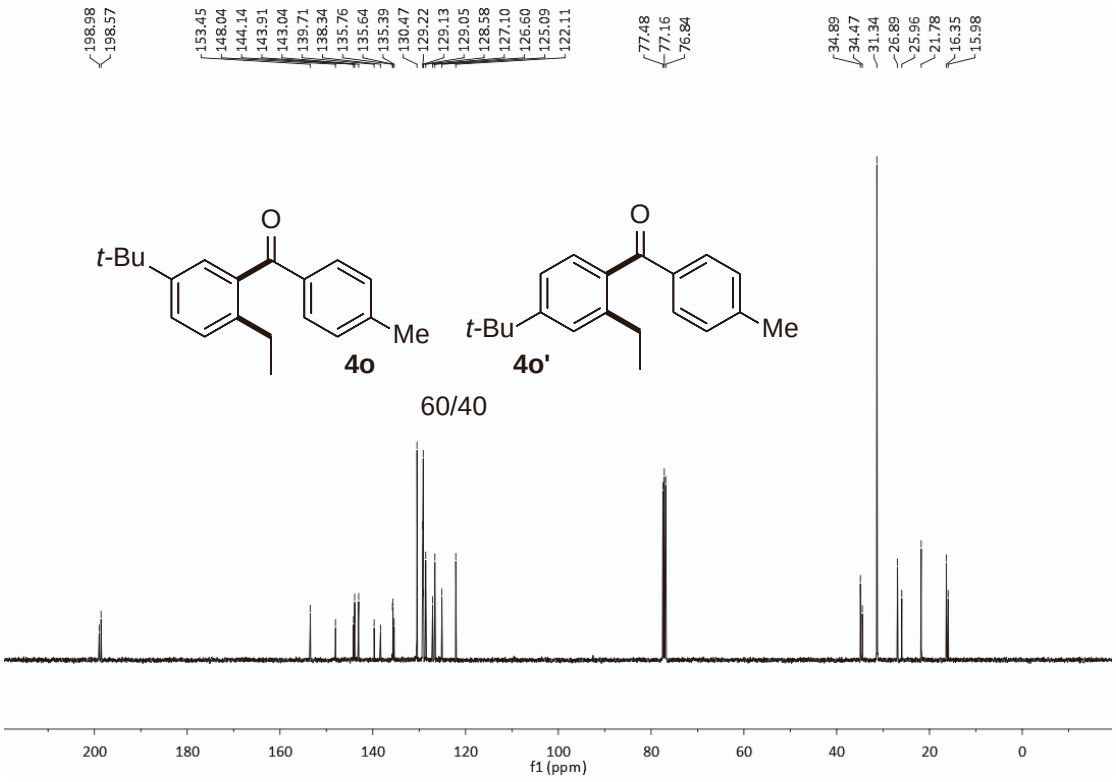
^{13}C NMR (101 MHz, $CDCl_3$)



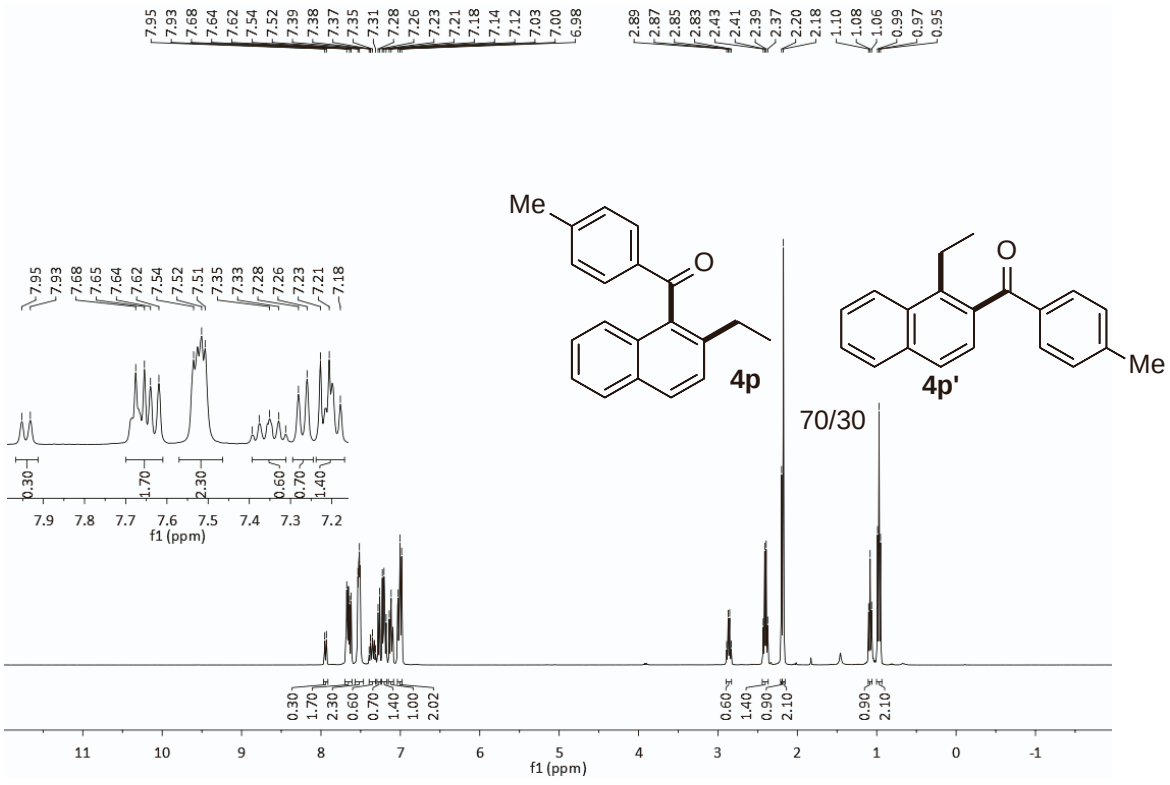
^{1}H NMR (400 MHz, $CDCl_3$)



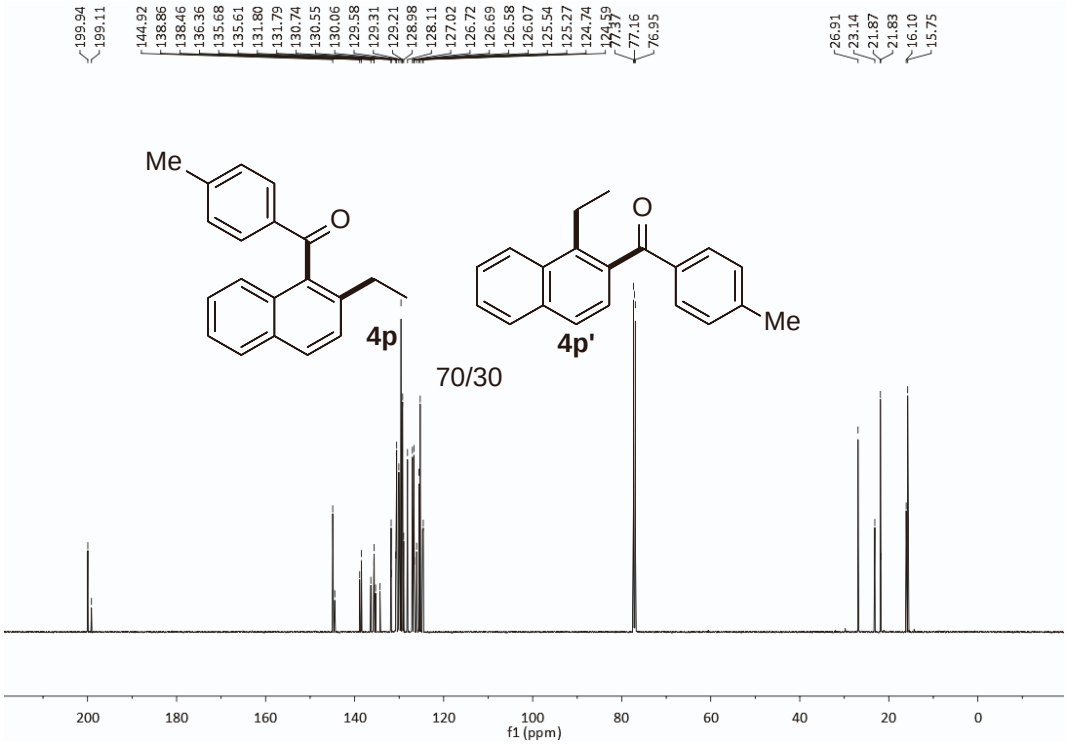
^{13}C NMR (101 MHz, $CDCl_3$)



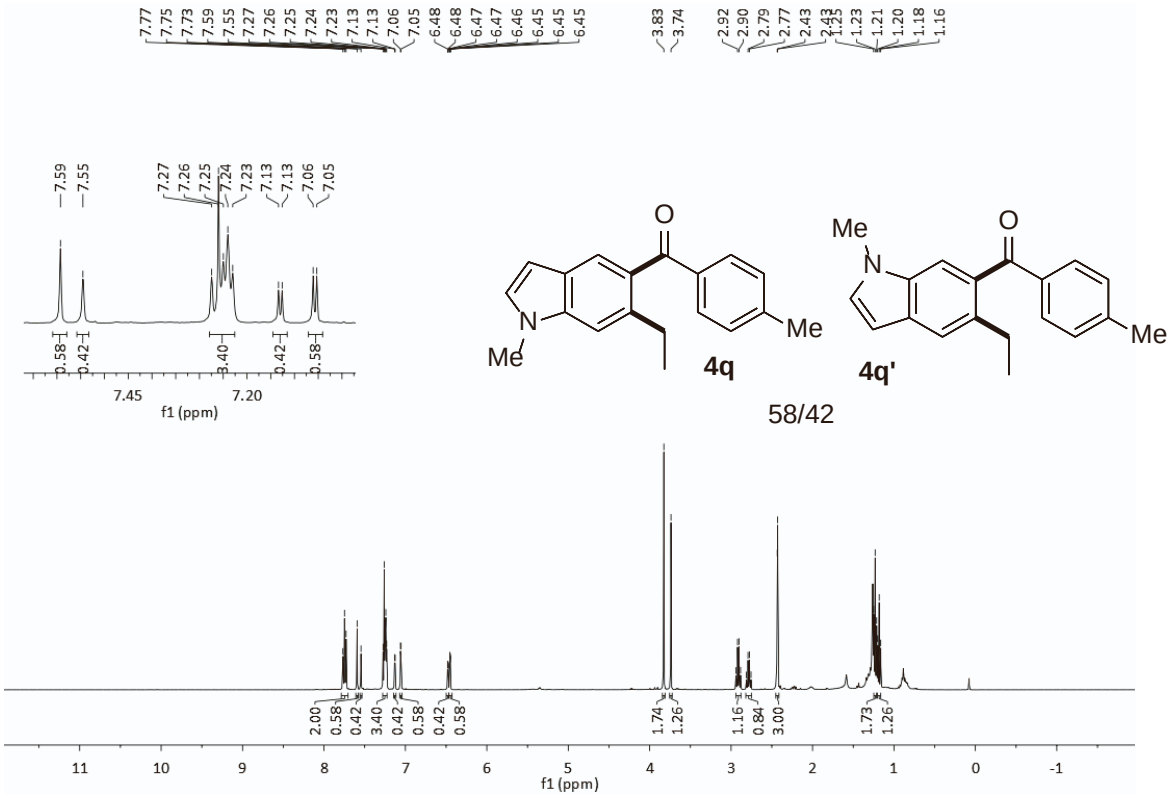
^{1}H NMR (400 MHz, $CDCl_3$)



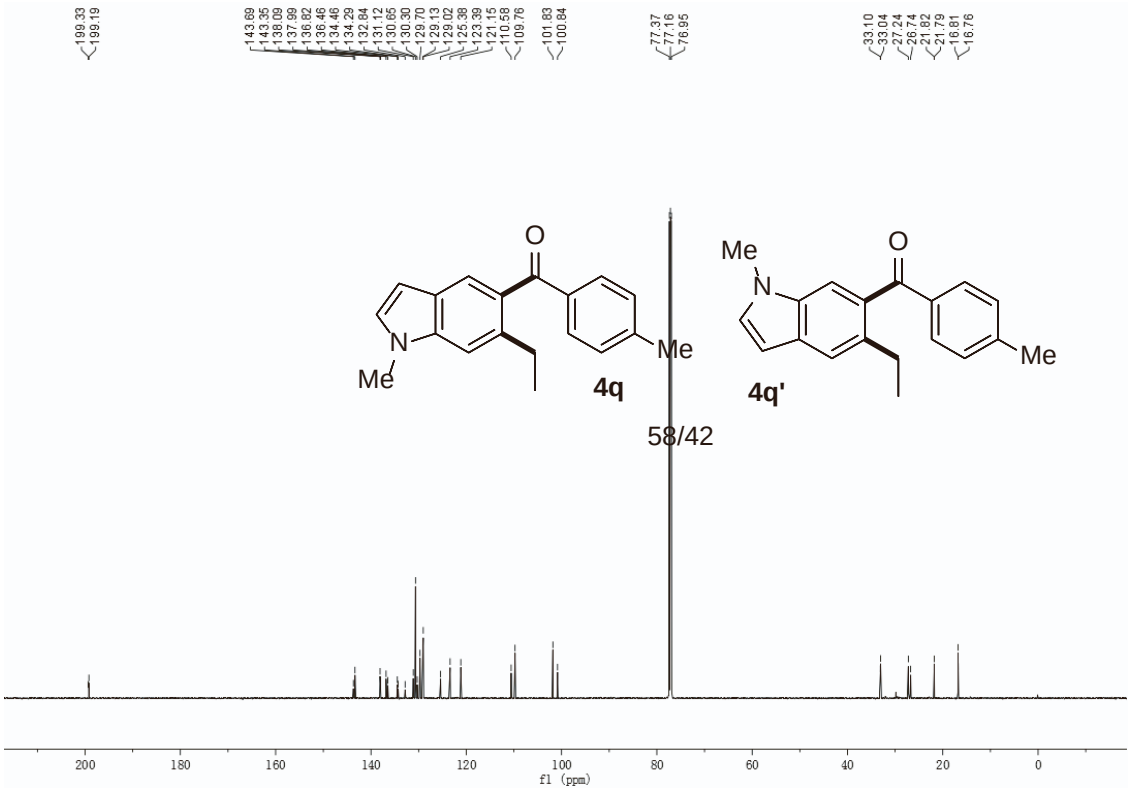
^{13}C NMR (151 MHz, $CDCl_3$)



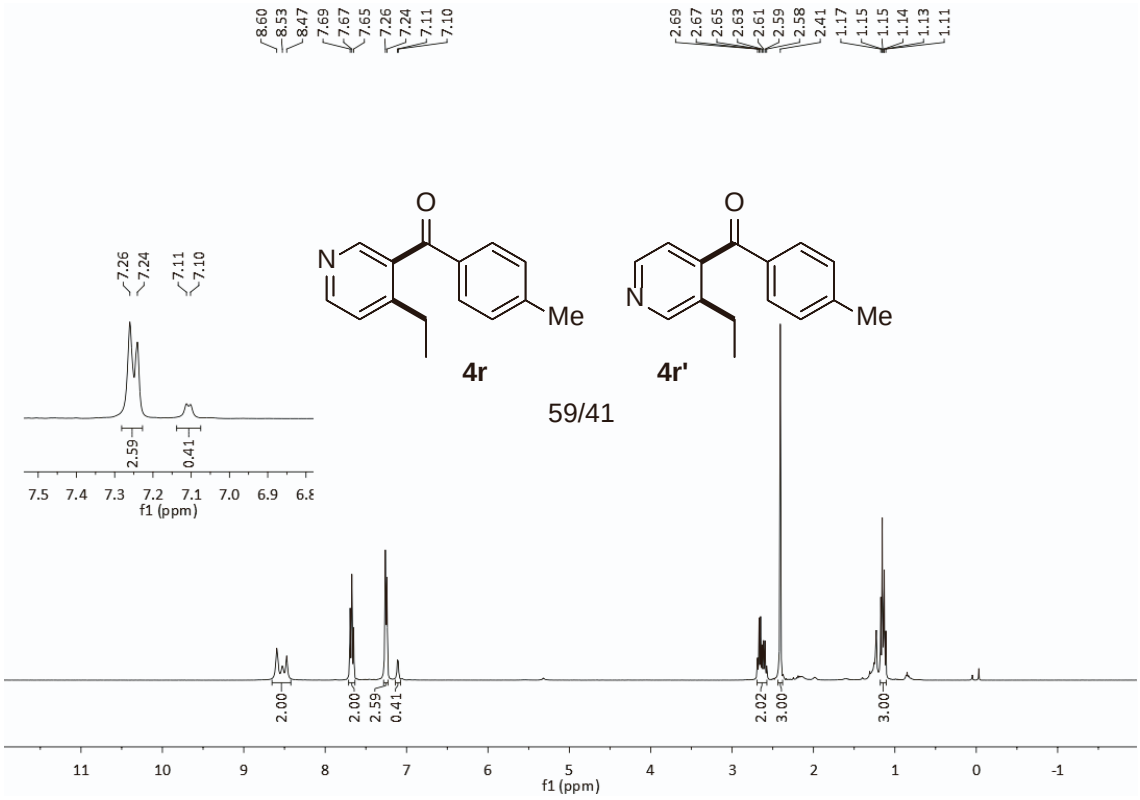
^{1}H NMR (400 MHz, $CDCl_3$)



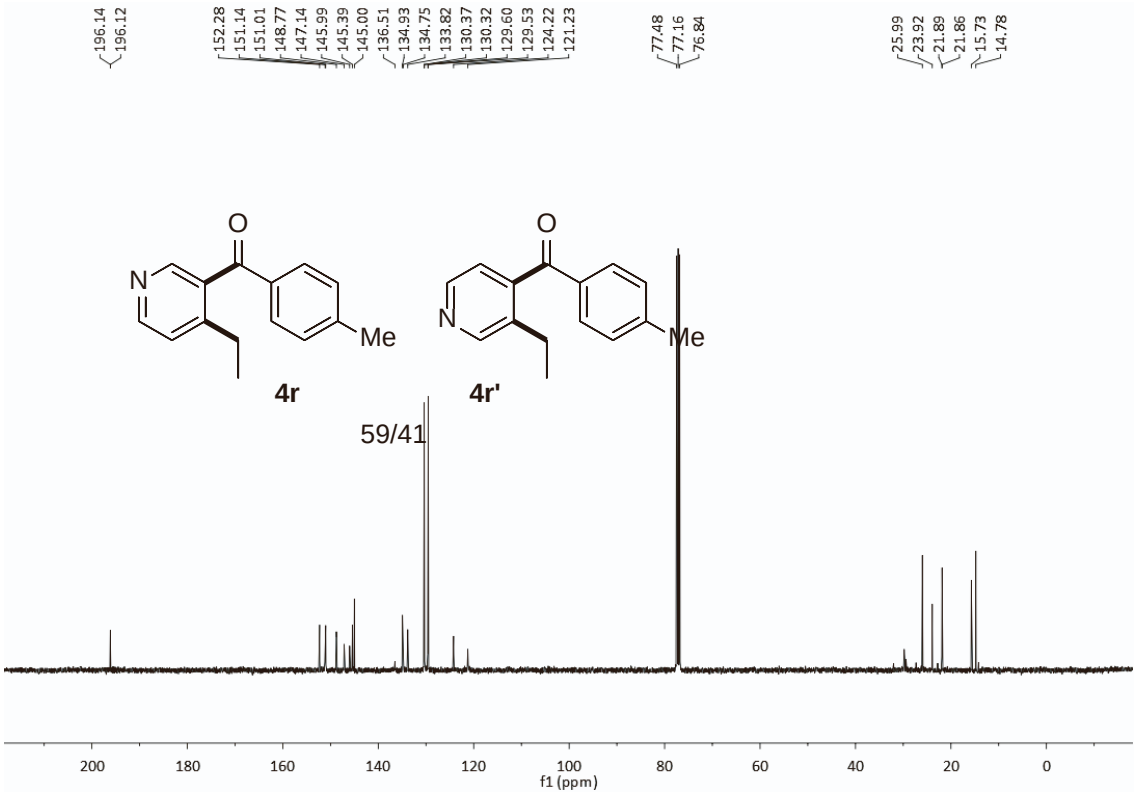
^{13}C NMR (151 MHz, $CDCl_3$)



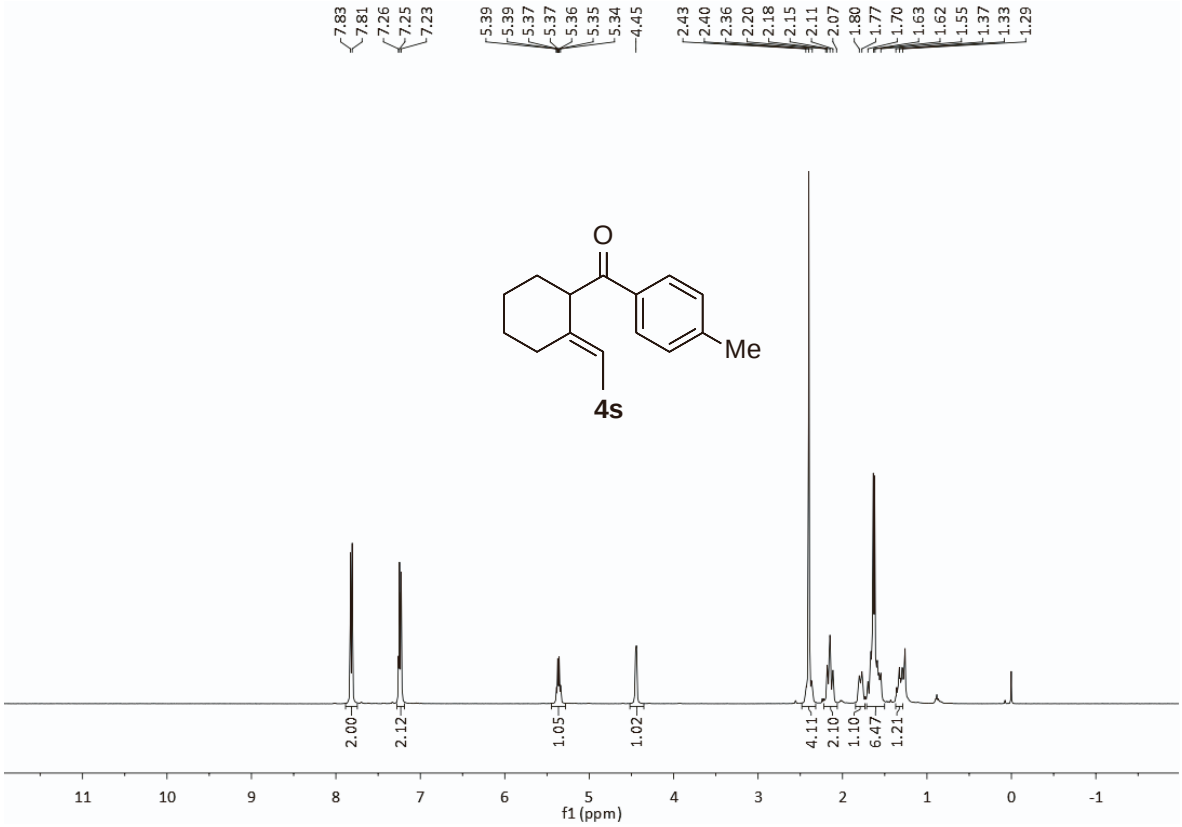
^{1}H NMR (400 MHz, $CDCl_3$)



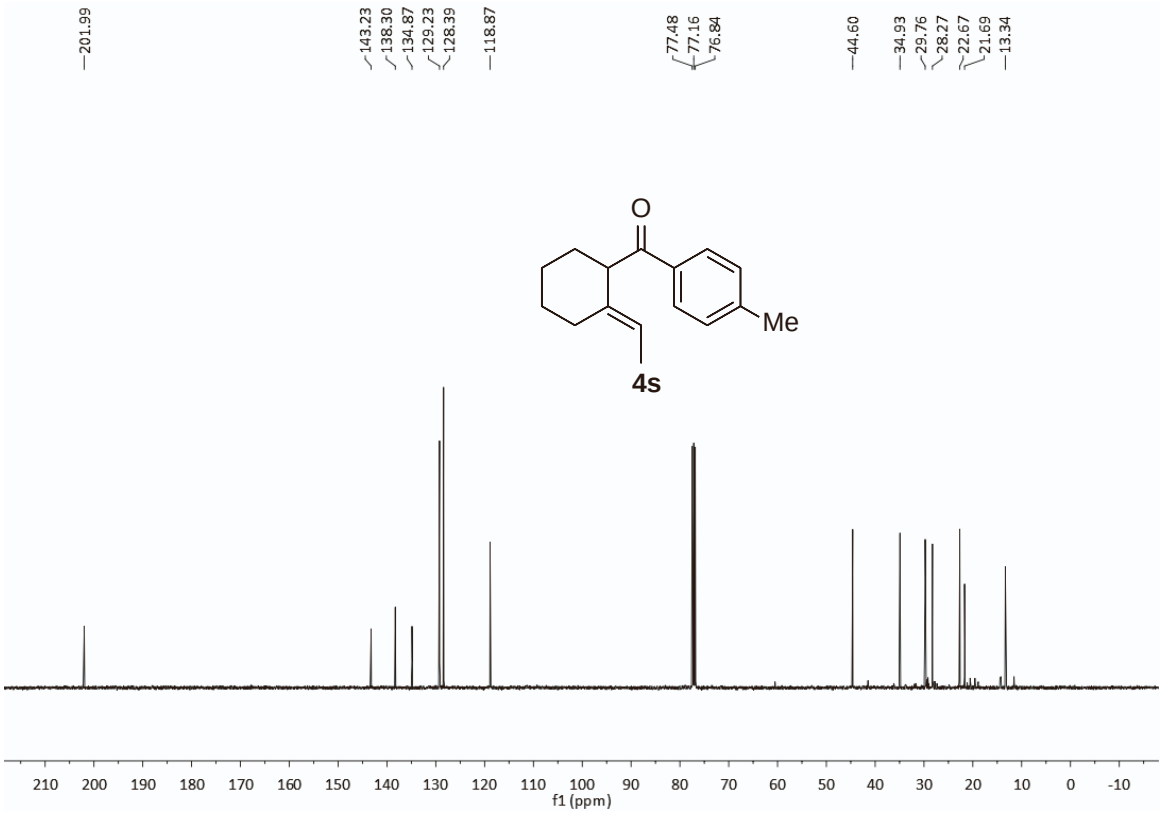
^{13}C NMR (101 MHz, $CDCl_3$)



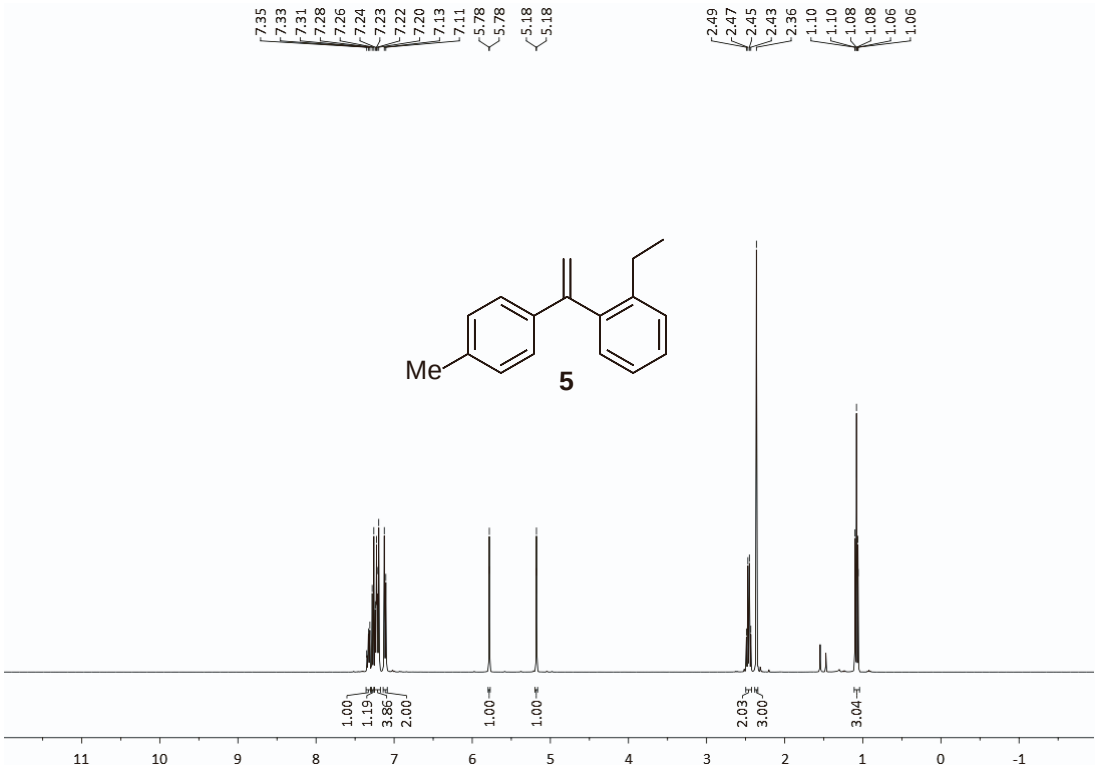
^{1}H NMR (400 MHz, $CDCl_3$)



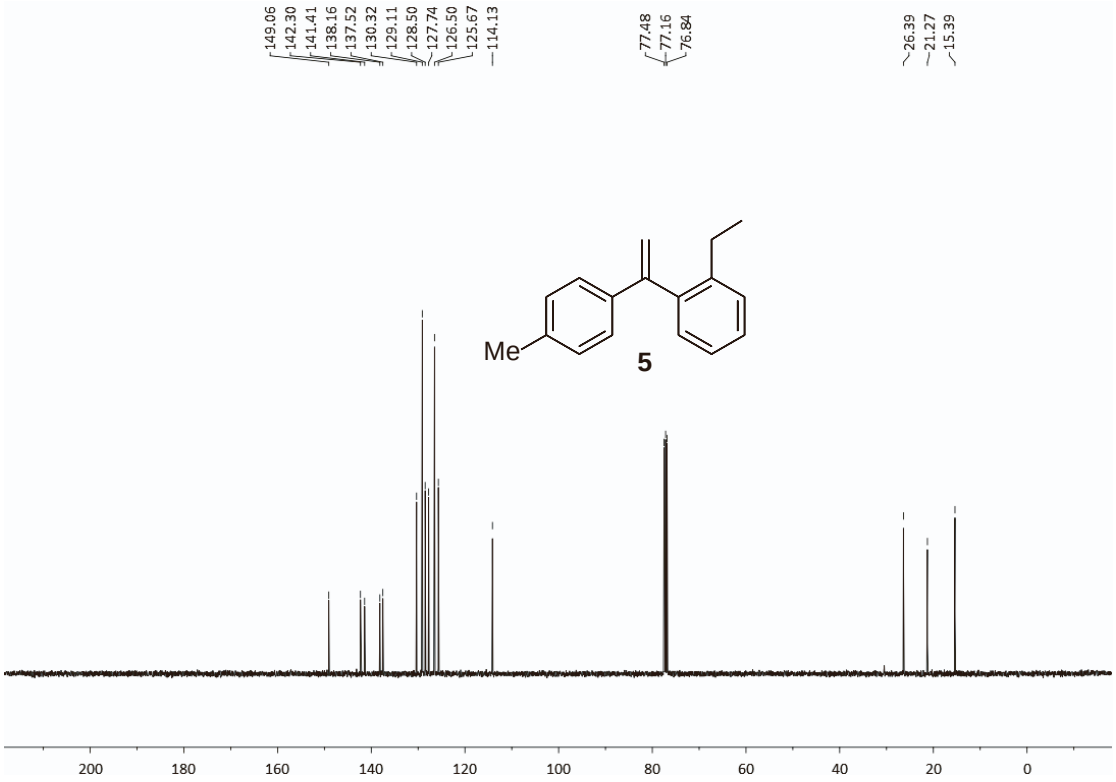
^{13}C NMR (101 MHz, $CDCl_3$)



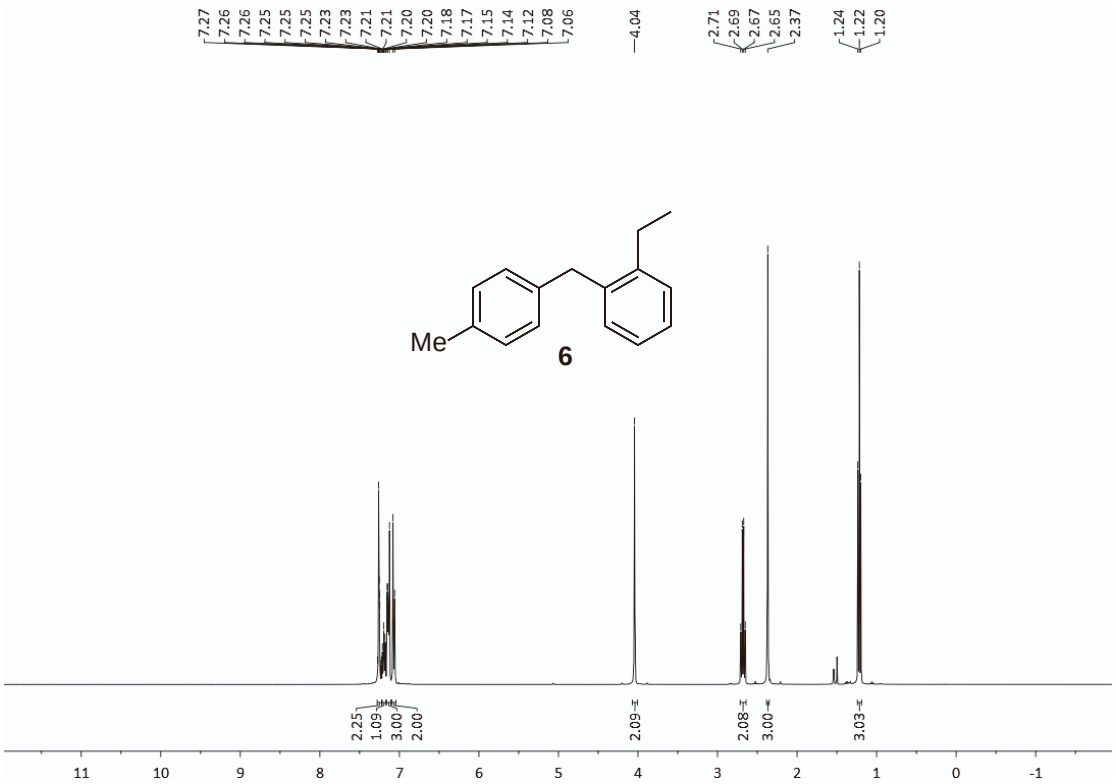
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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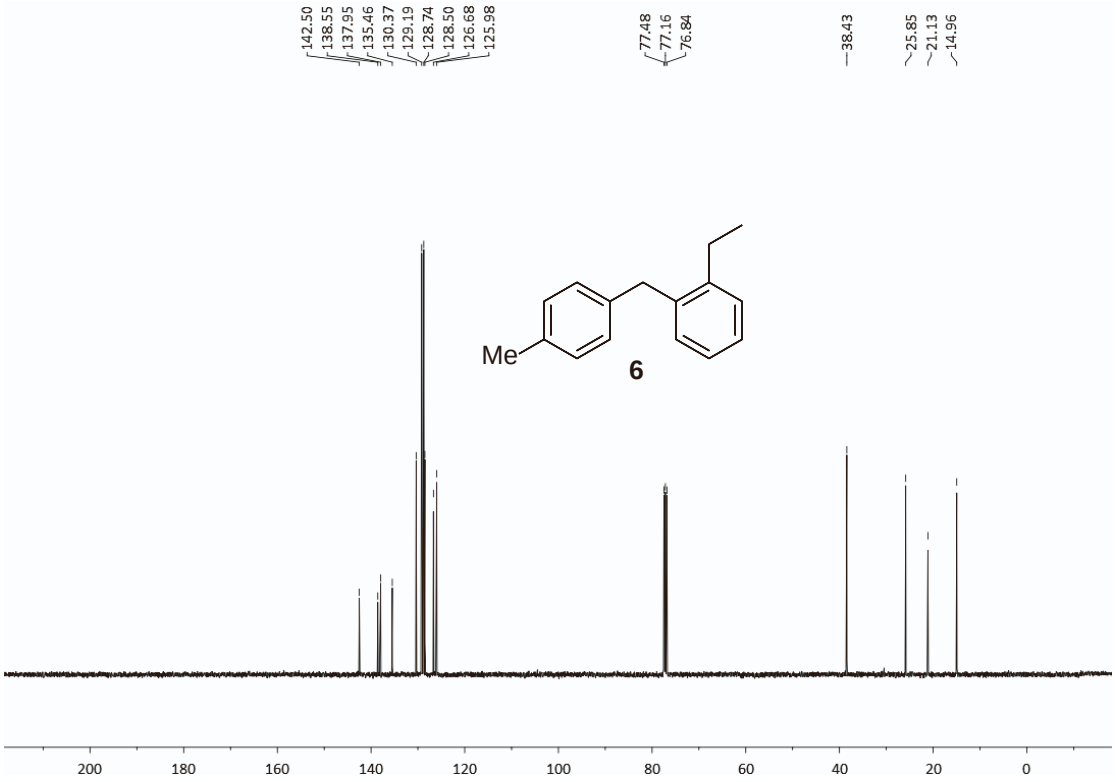

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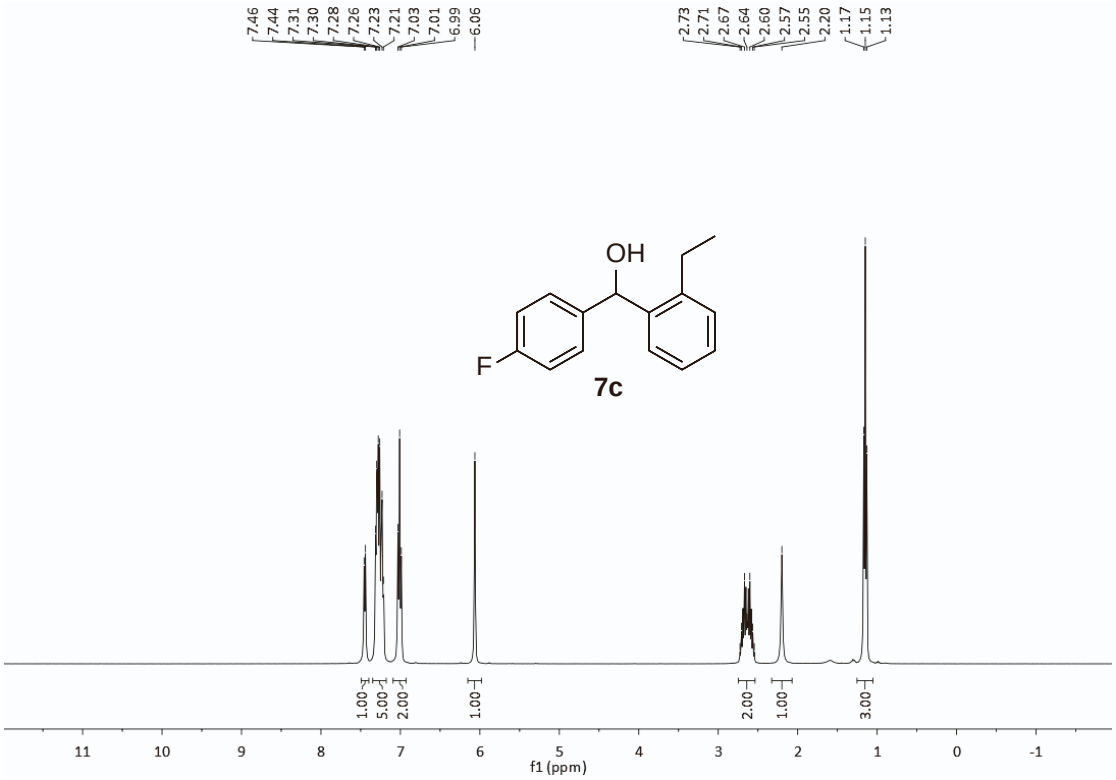

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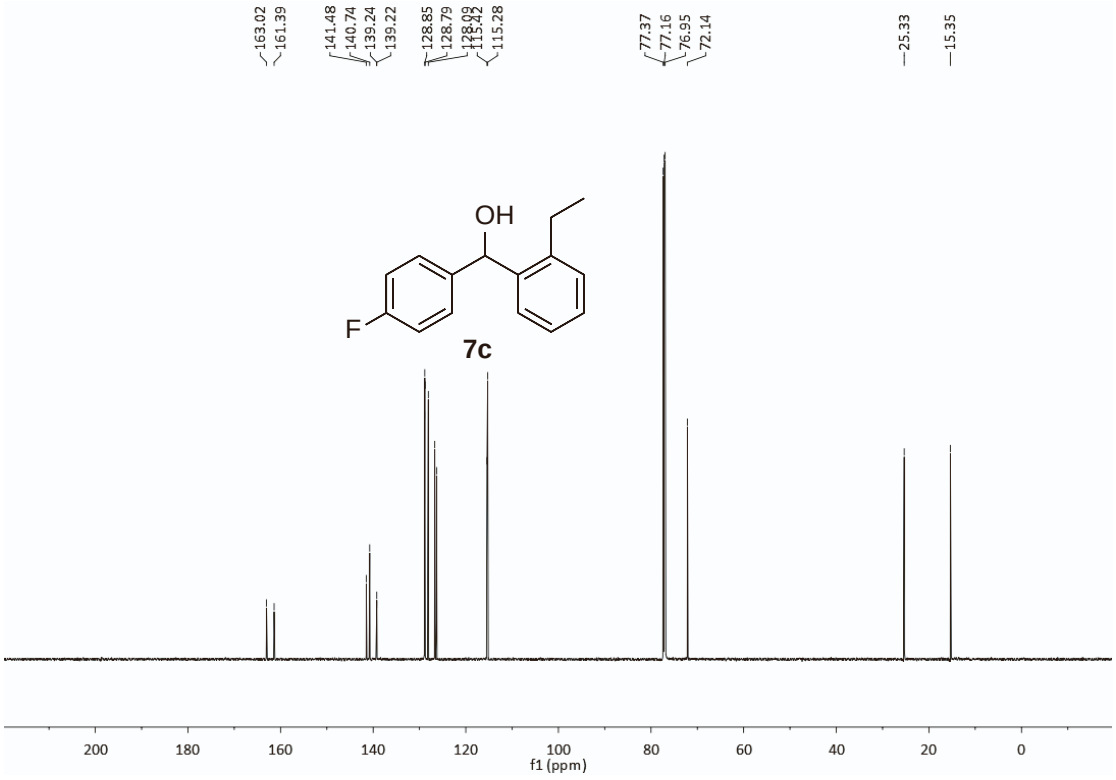

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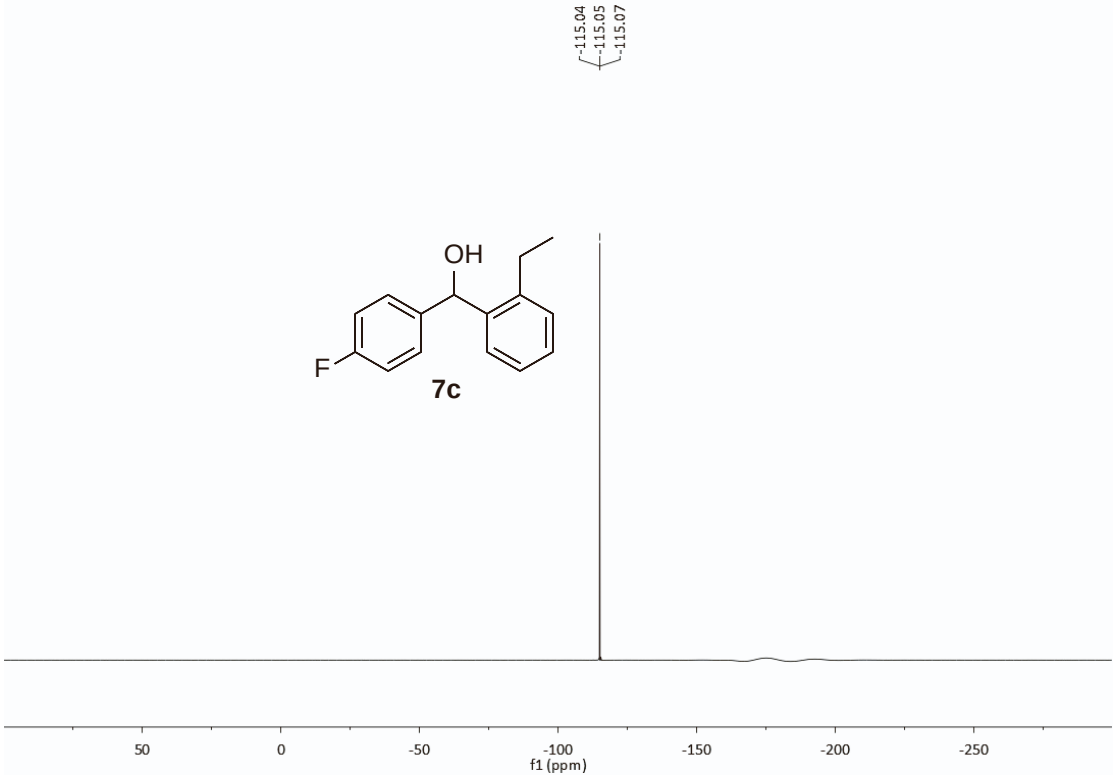

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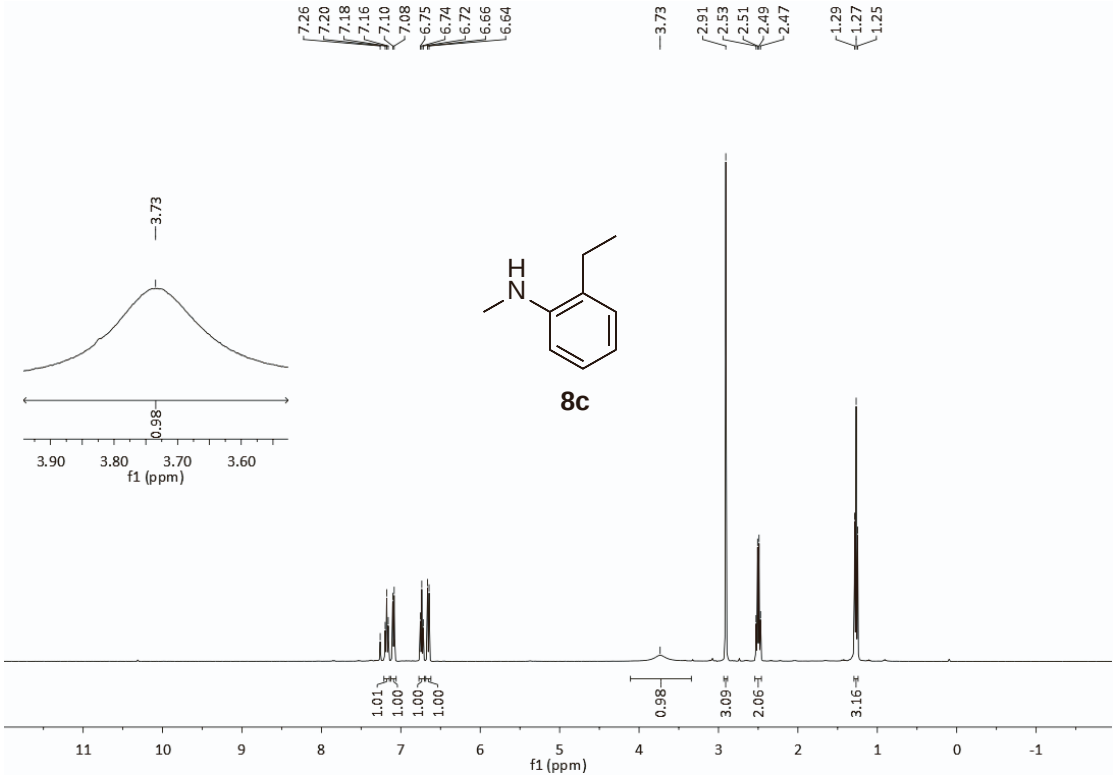

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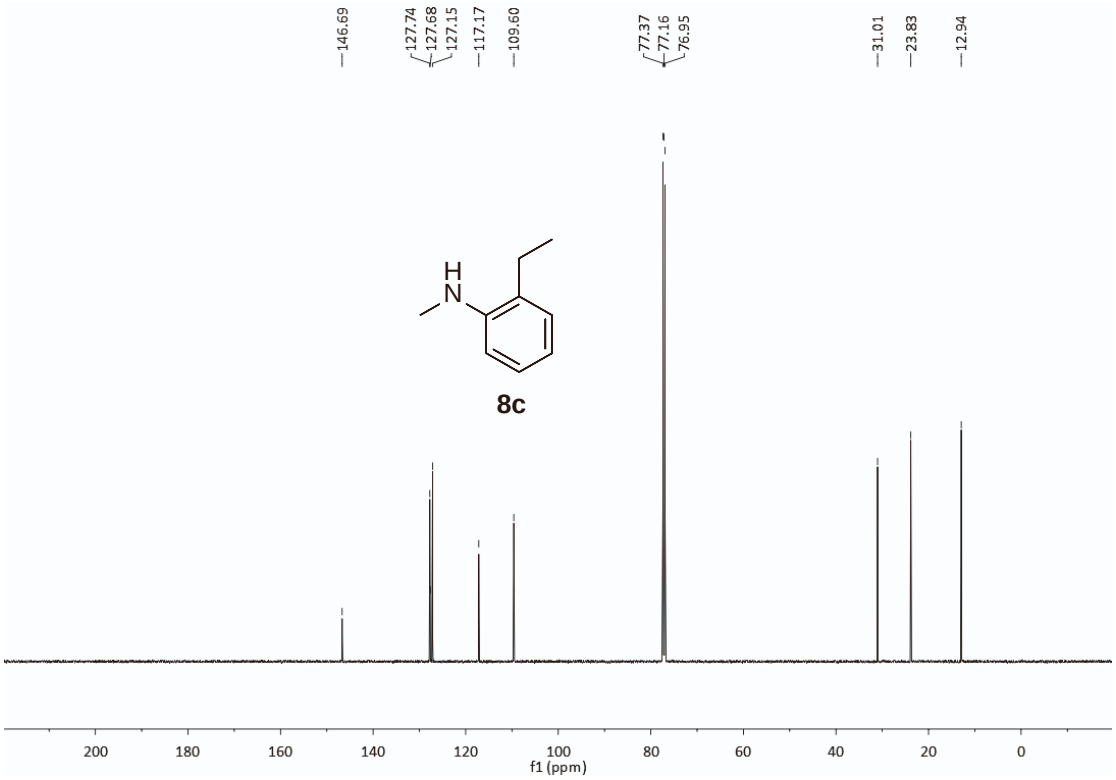

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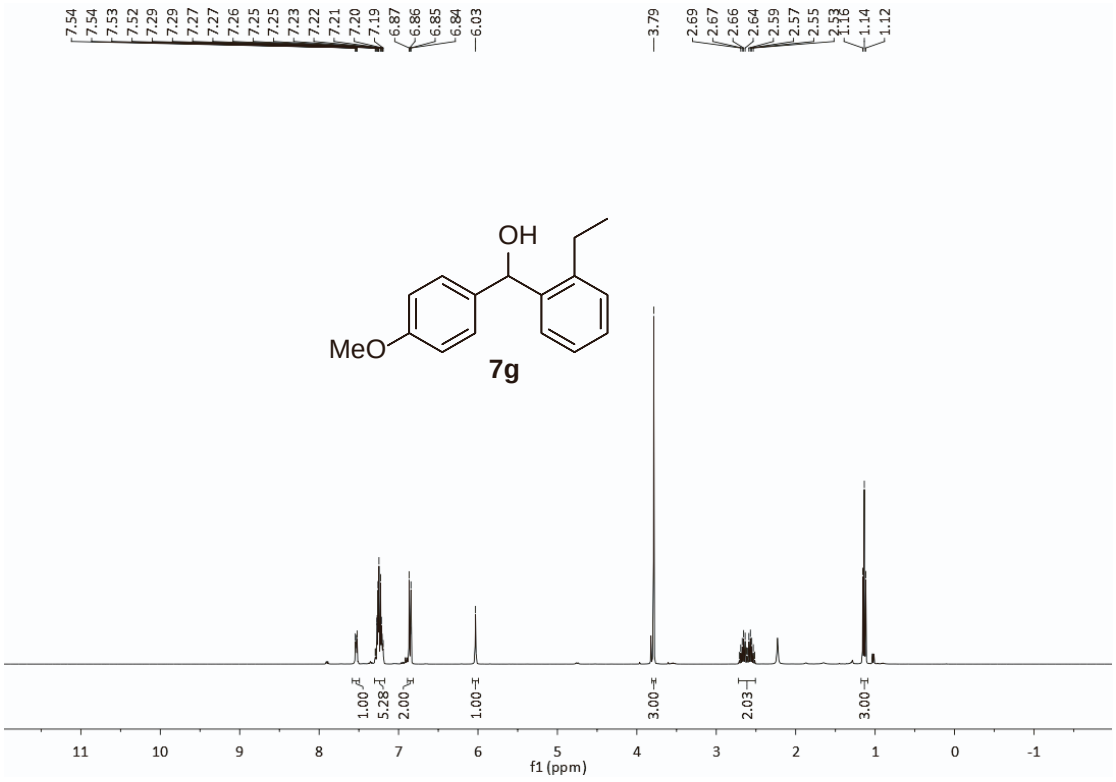

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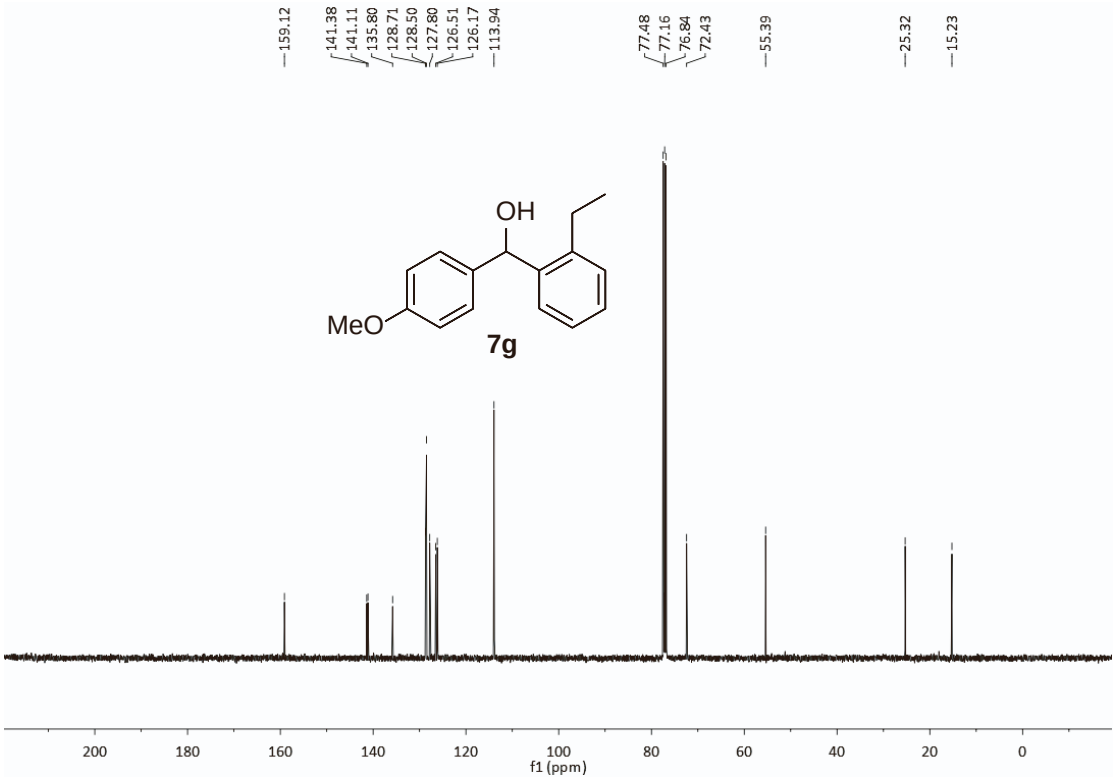

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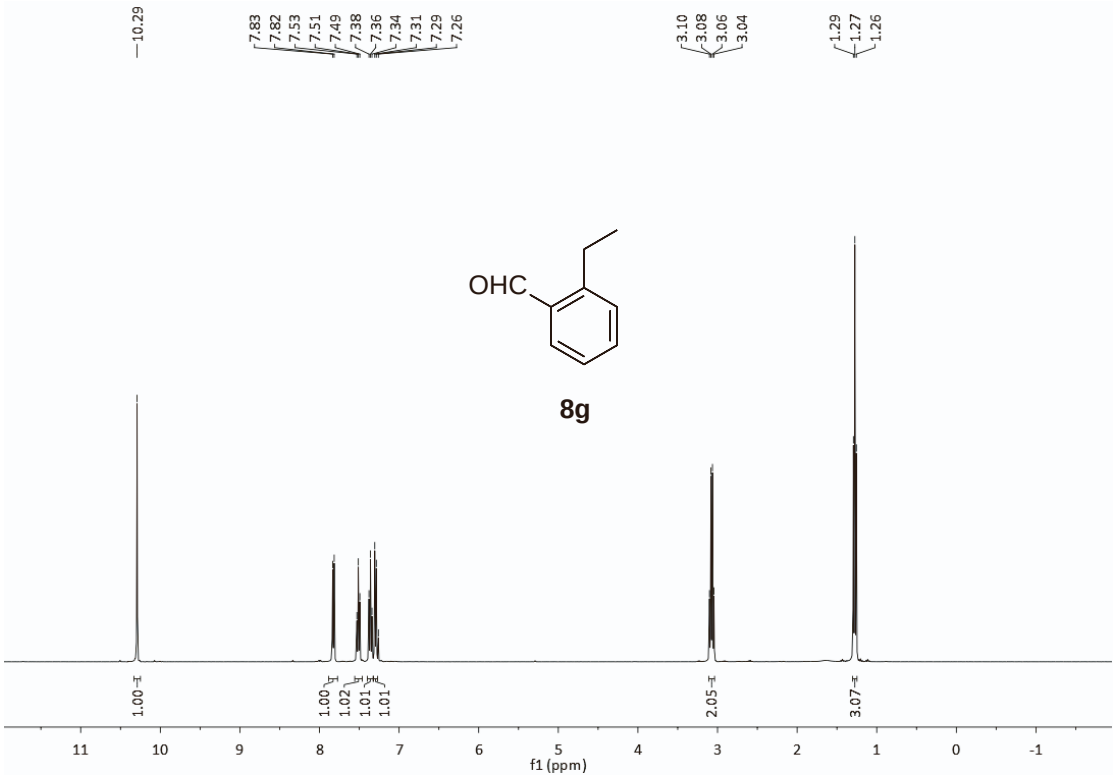

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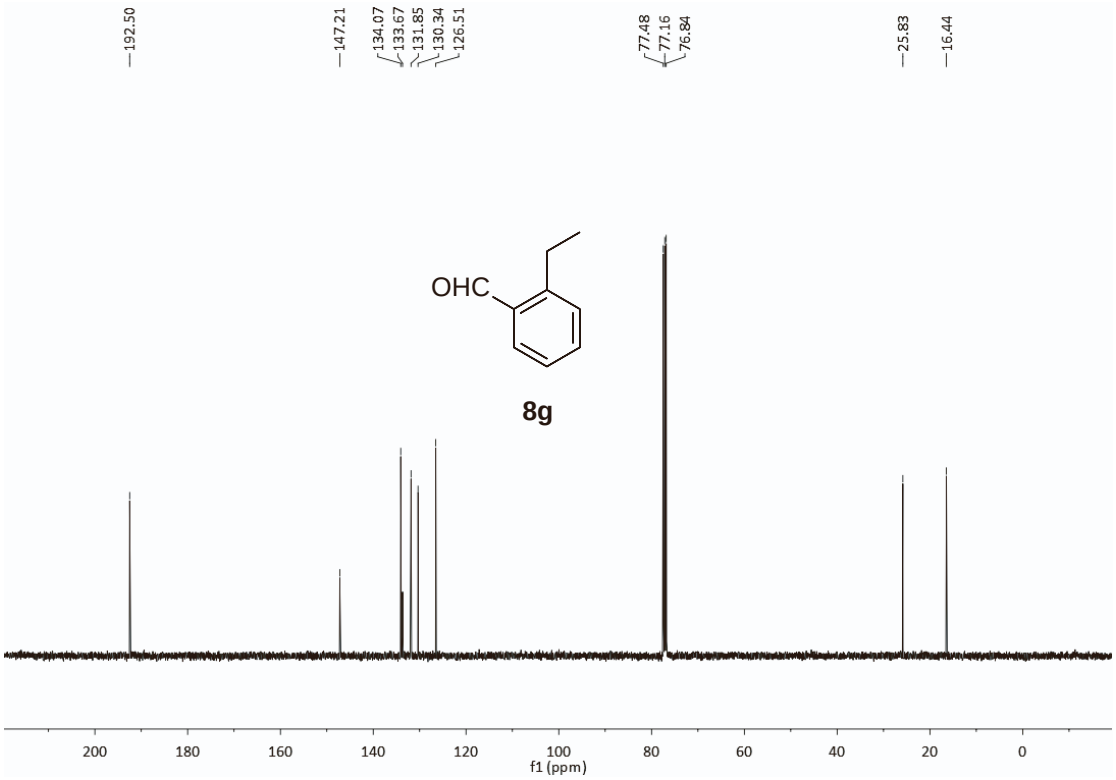

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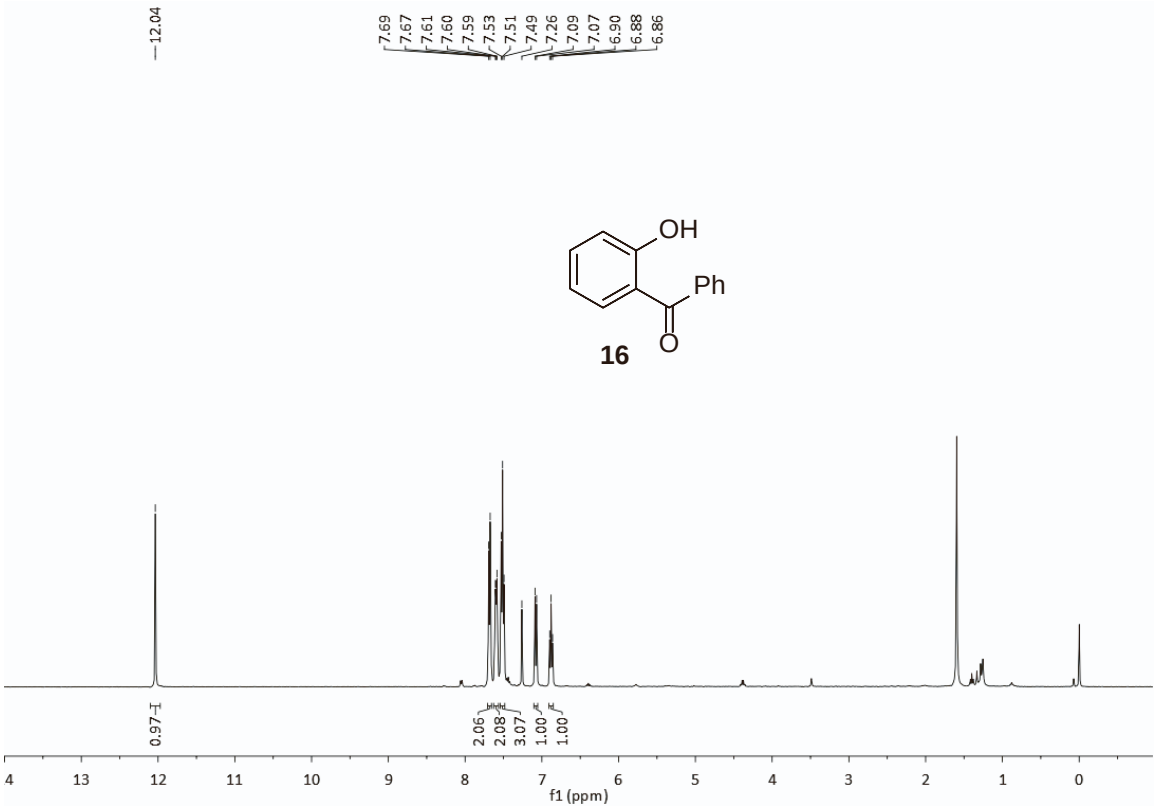

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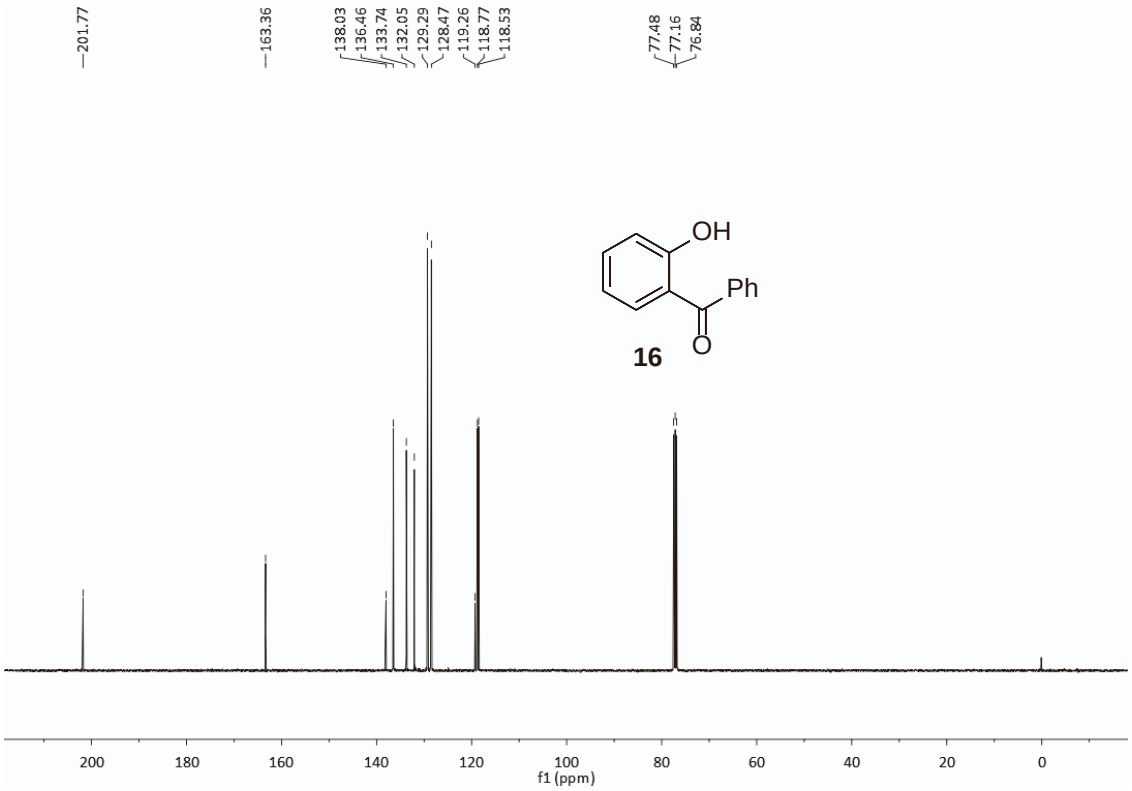

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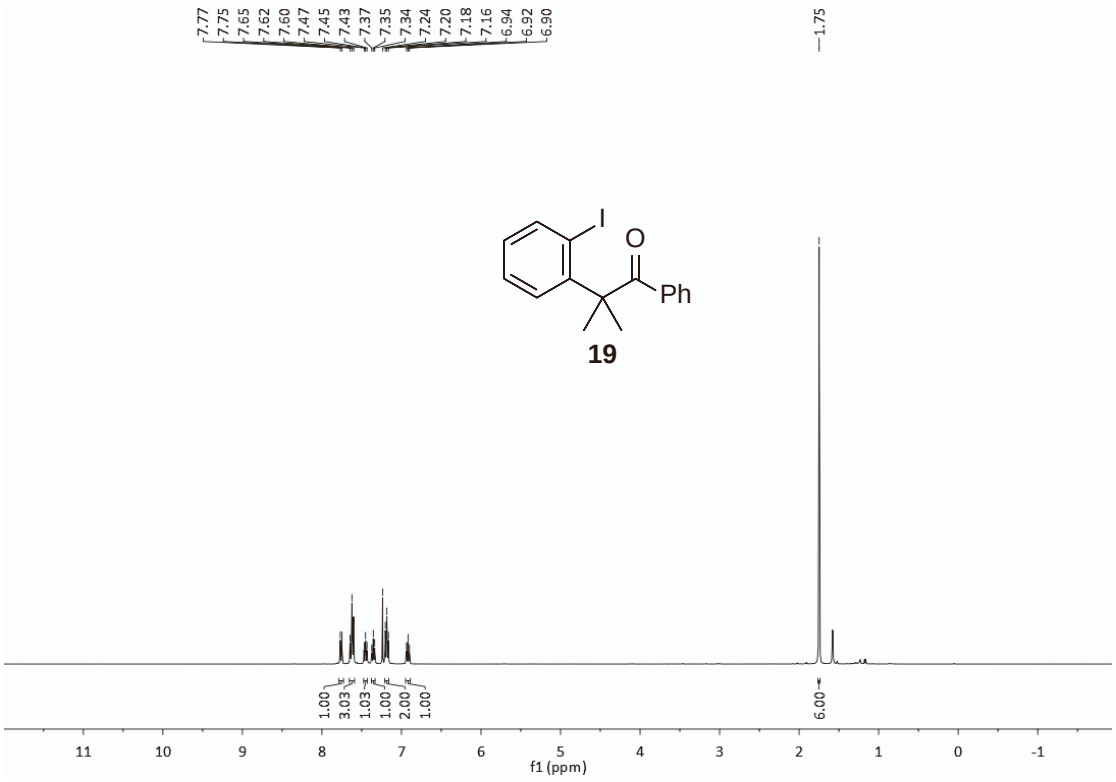

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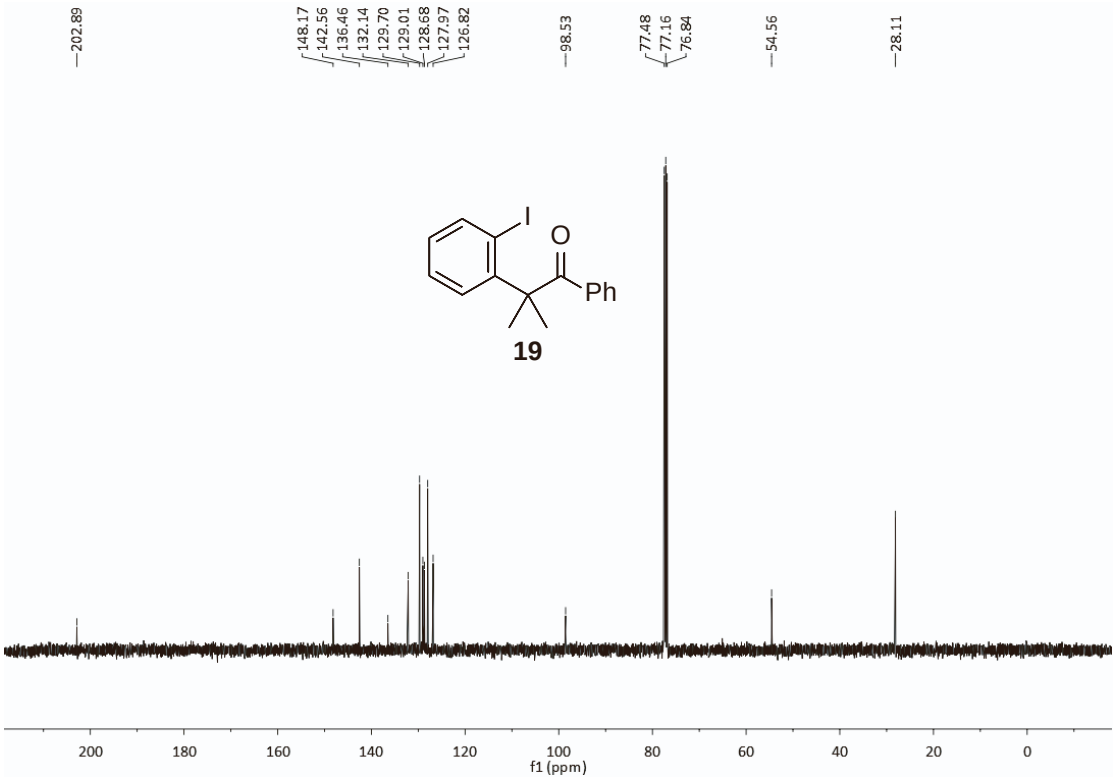

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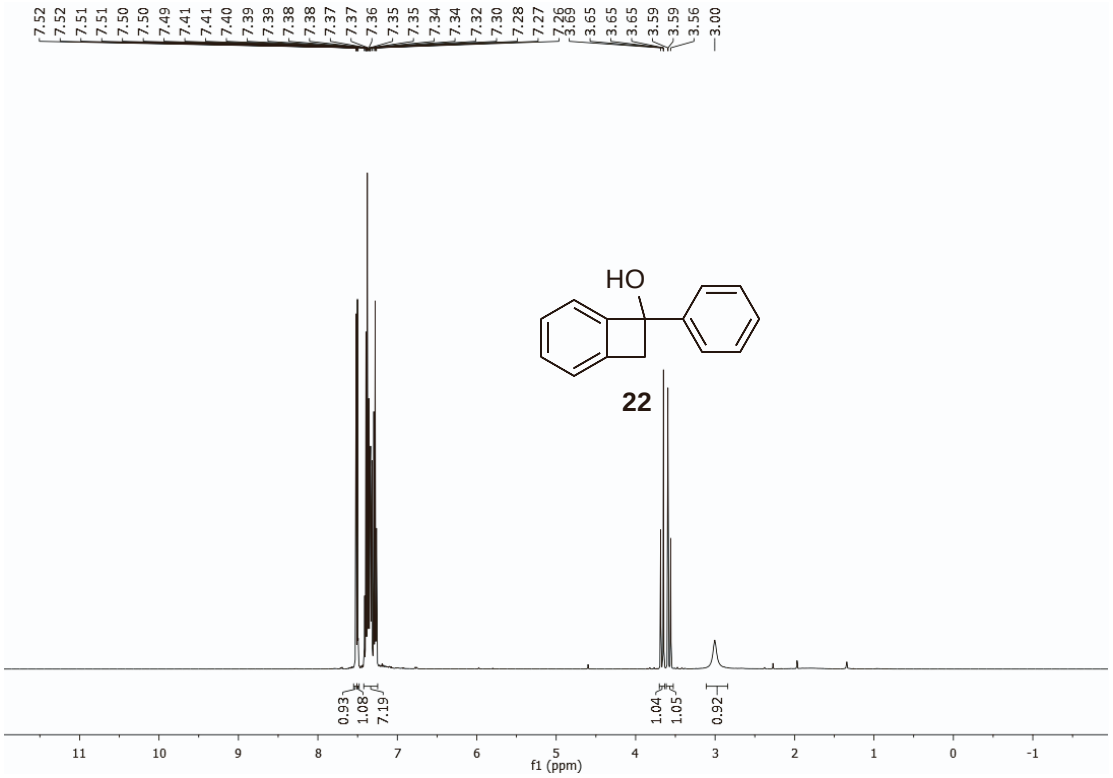

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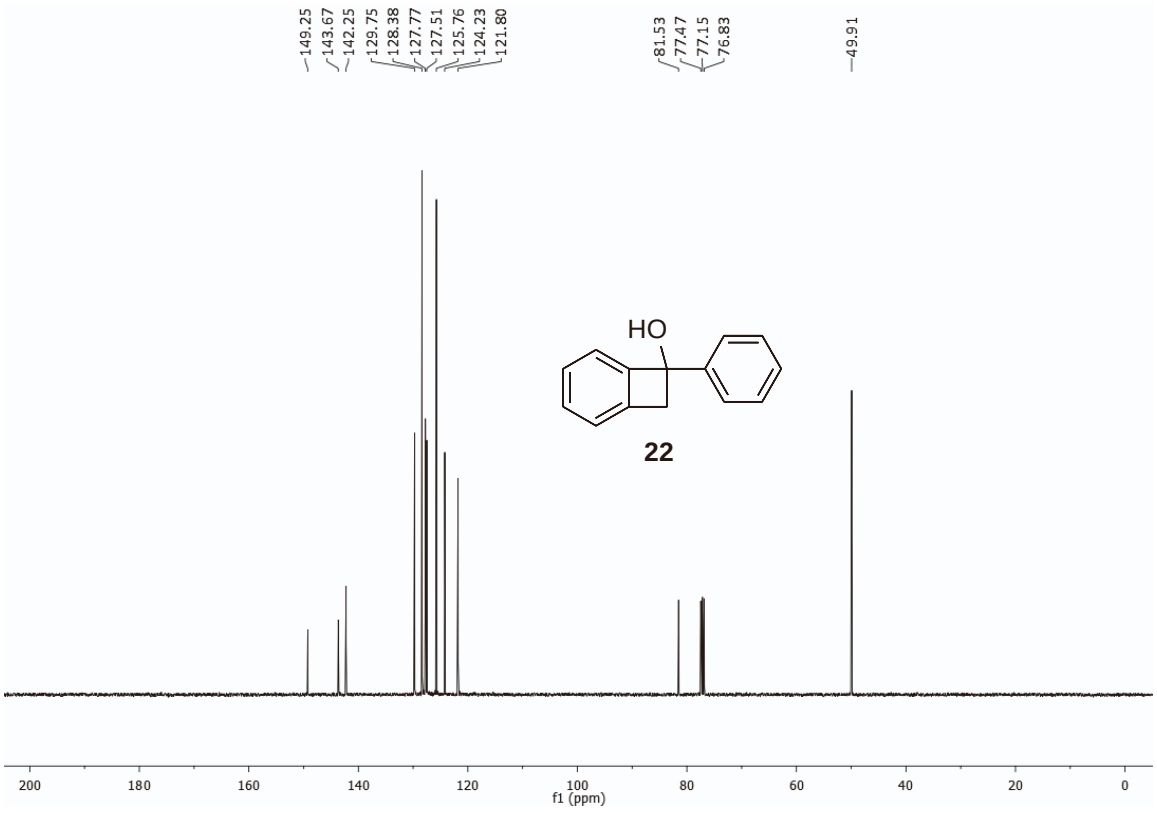

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