Electronic Supplementary Information

Ligand Assisted Co(II) Catalyzed Direct C-H Alkylation of Aryl Ketones with Diverse Alkyl Halides

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1. Methods, Materials, and Reagents:

Analytical thin-layer chromatography (TLC) was performed on Merck 60 F254 silica gel plates. Thin-layer chromatography plates were visualised by exposure to ultraviolet light (UV) and/or by immersion in a staining solution of 2,4-DNP/I_2. Column chromatography was performed using 60-120 µm silica gel. Commercial reagents were purchased from Merck, TCI, and other commercial suppliers and were used without further purification. Anhydrous cobalt(III) 2,4-pentanedionate (CAS No. 21679-46-9) was purchased from Alfa Aesar and used as received. Deuterated solvents $CDCl_3$, CD_3OD, and DMSO-d_6 were used without purification.

Instrumentation: ^1H and ^{13}C nuclear magnetic resonance (NMR) spectra were recorded on Bruker AV-400 (400 MHz) NMR spectrometers. Chemical shifts of the NMR spectra are reported relative to residual signals of $CDCl_3$ (^1H NMR: δ = 7.26 ppm, ^{13}C NMR: δ = 77.16 ppm), CD_3OD (^1H-NMR: δ = 3.31 ppm, ^{13}C-NMR: δ = 49 ppm), DMSO-d_6 (^1H-NMR: δ = 2.50 ppm, ^{13}C-NMR: δ = 39.52 ppm). The data are presented as follows: chemical shift; multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet and/or multiplet resonances); and coupling constant in Hertz (Hz). High-resolution mass spectra (HRMS) were obtained with a Q-Tof Premier LC-HR mass spectrometer. Electron paramagnetic resonance (EPR) measurements were performed at room temperature using a Bruker A3000-9.5/12/S/W spectrometer at 9.85 GHz. Cyclic voltammetry (CV) was performed using the Gamry interface 1010E Potentiostat. A Thermogravimetric Analyser (DT-TGA) TGA 5500 by TA Instruments was used to analyse the catalyst composition over a temperature range of 25 °C to 1000 °C. The magnetic property was established by using a vibrating sample magnetometer (VSM), Model No.: Microsense, Model ADE-EV9. Organic solvents were concentrated on a rotary evaporator.

Abbreviations Used:

DFT = density functional theory, h = hours, m/z = mass to charge ratio, NMR = nuclear magnetic resonance, equiv. = equivalents, HRMS= High-resolution mass spectra, VSM= vibrating sample magnetometer, DT-TGA= Differential thermogravimetric analysis, Ph = phenyl, rt = room temperature, TLC = thin layer chromatography, 2,4-DNP = 2,4-dinitrophenyl hydrazine, $Co(acac)_3$ = Cobalt acetylacetonate, $Co(OAc)_3$ = Cobalt acetate.

2. General Experimental Procedures:

2.1. General Procedure for Preparation of $Co(OAc)_3$ from $Co(acac)_3$

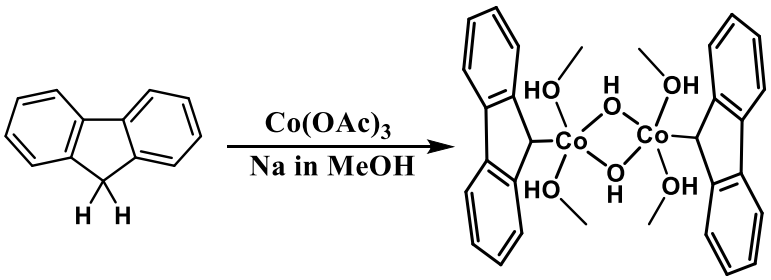
$Co(acac)_3$ (1.44 g, 4 mmol) was dissolved in methanol and stirred under ice-cold conditions. Then, glacial acetic acid (1.29 g, 20 mmol) was added at room temperature, and the reaction mixture was stirred for one hour. The resulting reaction mixture was refluxed for four hours and then cooled to room temperature. After the reaction was complete, the methanol and acetic acid were removed under vacuum using a rotary evaporator, yielding a green solid $Co(OAc)_3$ with a yield of 98%.

2.2. Synthesis of Cat-1

Fluorene (2.12 mmol, 0.351 g) was dissolved in 25 mL of dry methanol and stirred for 30 min under nitrogen to obtain a clear solution. Then, sodium (5 mmol, 115 mg) was added to the reaction mixture and stirred for one hour, followed by the addition of $Co(OAc)_3$ (2.12 mmol, 0.500 g), and the mixture was stirred until the solution changed from green to dark reddish-orange. The progress of the reaction was monitored using TLC. Once the **Cat-1** was formed, it was filtered to remove insoluble residues, then concentrated using a rotary vacuum, and purified by column chromatography using 10%, 20%, 30% and 50% DCM/hexanes mixture to eluate the catalyst. The eluents were concentrated using a rotary evaporator. Upon isolation and purification, the **Cat-1** (0.470 g) was obtained in 87% yield. The catalyst was dissolved in commercial-grade methanol and stored in a refrigerator for further use in C-H alkylation reactions. A small portion of the catalyst solution was taken, and the methanol was removed on a rotary evaporator to obtain the solid catalyst complex. This solid catalyst (48 mg, 5 mol%) was used in the C-H alkylation reactions as discussed in **Section 4**.

^{1}H NMR (400 MHz, CD_3OD): δ 7.82 (d, *J* = 7.5 Hz, 4H), 7.56 (d, *J* = 7.4 Hz, 4H), 7.37 (t, *J* = 7.4 Hz, 4H), 7.30 (td, *J* = 7.4, 1.0 Hz, 4H), 4.88 (s, 12H), 3.90 (s, 2H).
^{13}C NMR (101 MHz, CD_3OD): δ 143.0, 141.6, 126.4, 126.3, 124.6, 119.3, 48.2, 48.0, 47.8, 47.6, 47.40, 47.1, 46.9.

S. No	Catalyst Molecular formula and form	Theoretical Mass	Observed Mass
1.	$C_{13}H_{10}CoO$ (monomeric form)	$[M+H]^+$ = 242.0136	**242.0128**
2.	$C_{26}H_{20}Co_2O_2$ (active catalyst)	$[M+H]^+$ = 483.0200	**483.0171**
3.	$C_{28}H_{28}Co_2O_4$ (active catalyst with two moles of methanol)	$[M]^+$ = 546.0646	**546.0688**
4.	$C_{30}H_{36}Co_2O_6$ (dimer with solvent)	$[M+H]^+$ = 611.1249	**611.1238**



Fluorene **Cat-1**

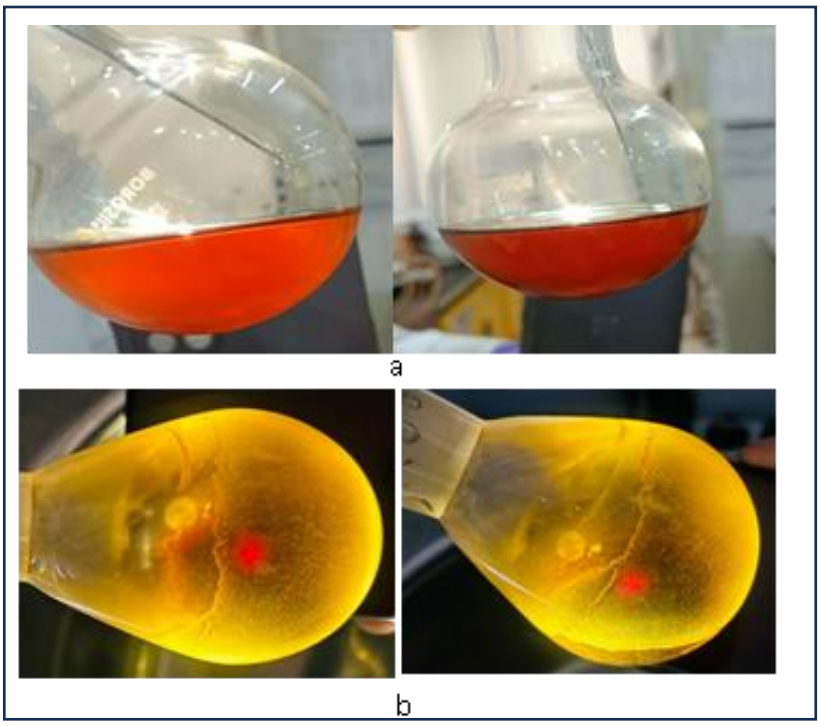


Figure S1. Cat-1 (a) in methanol **(b)** showing fluorescence under white light

3. Characterisation Details of Catalyst

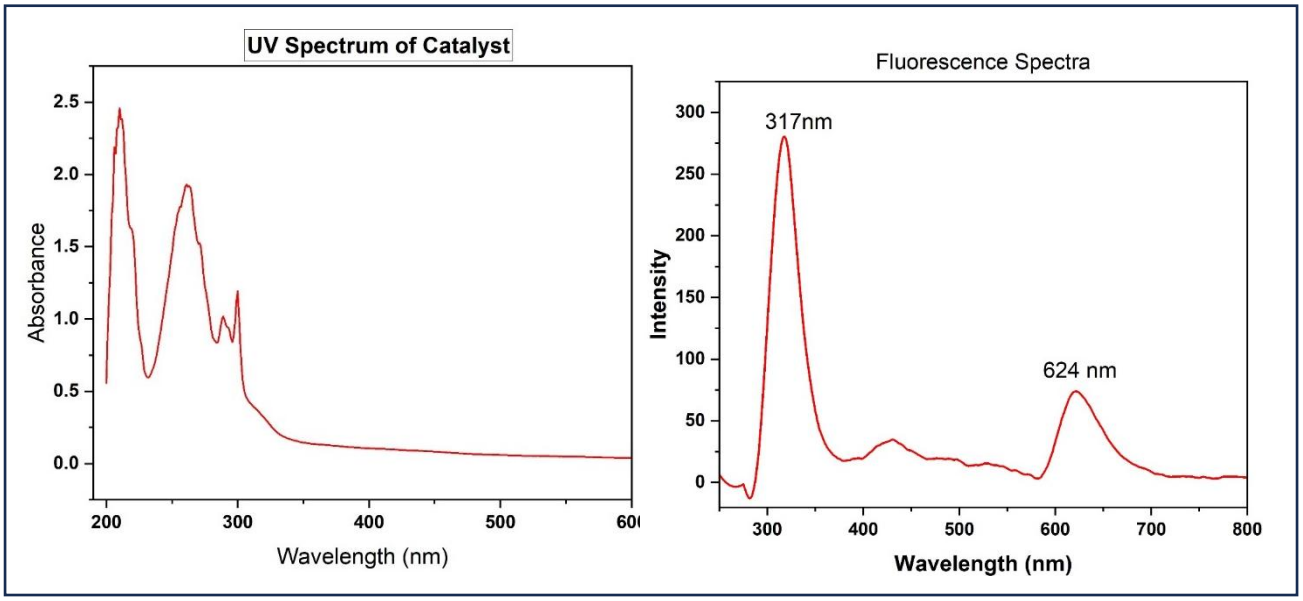


Figure S2. UV & Fluorescence spectrum of **Cat-1**

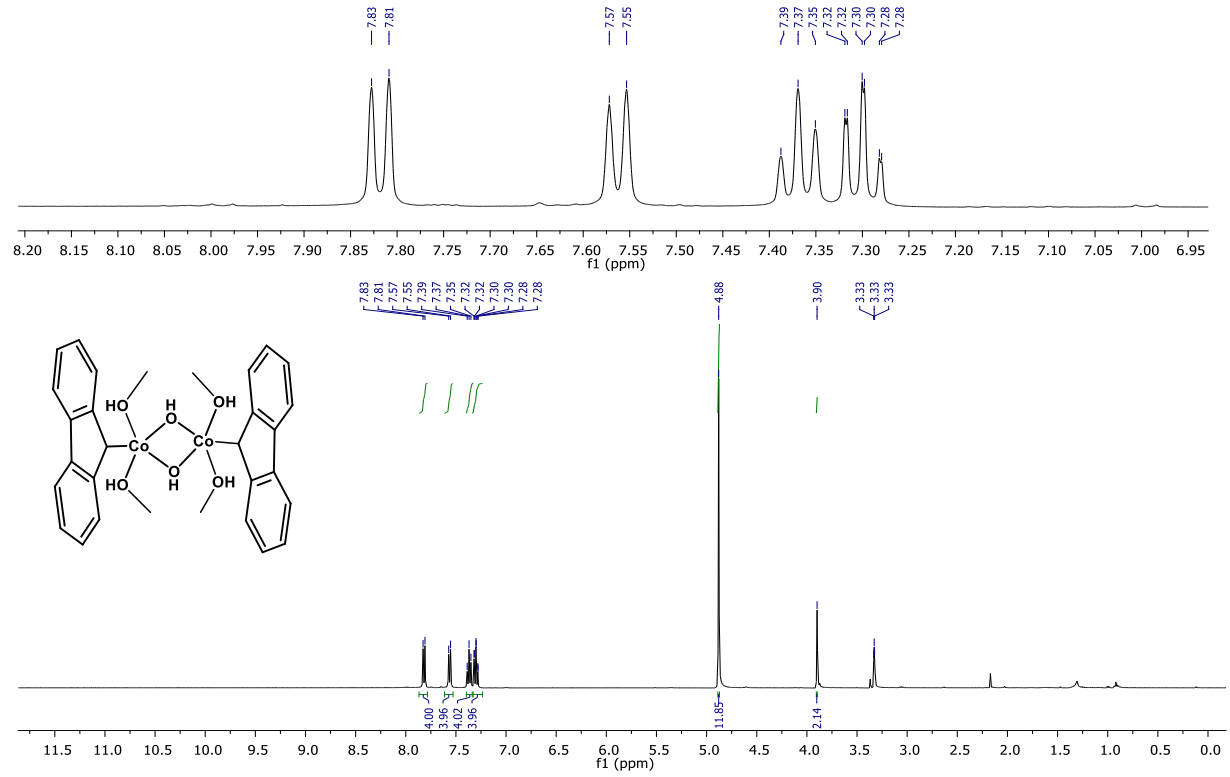


Figure S3. ^{1}H NMR spectrum of **Cat-1** (400 MHz, CD_3OD)

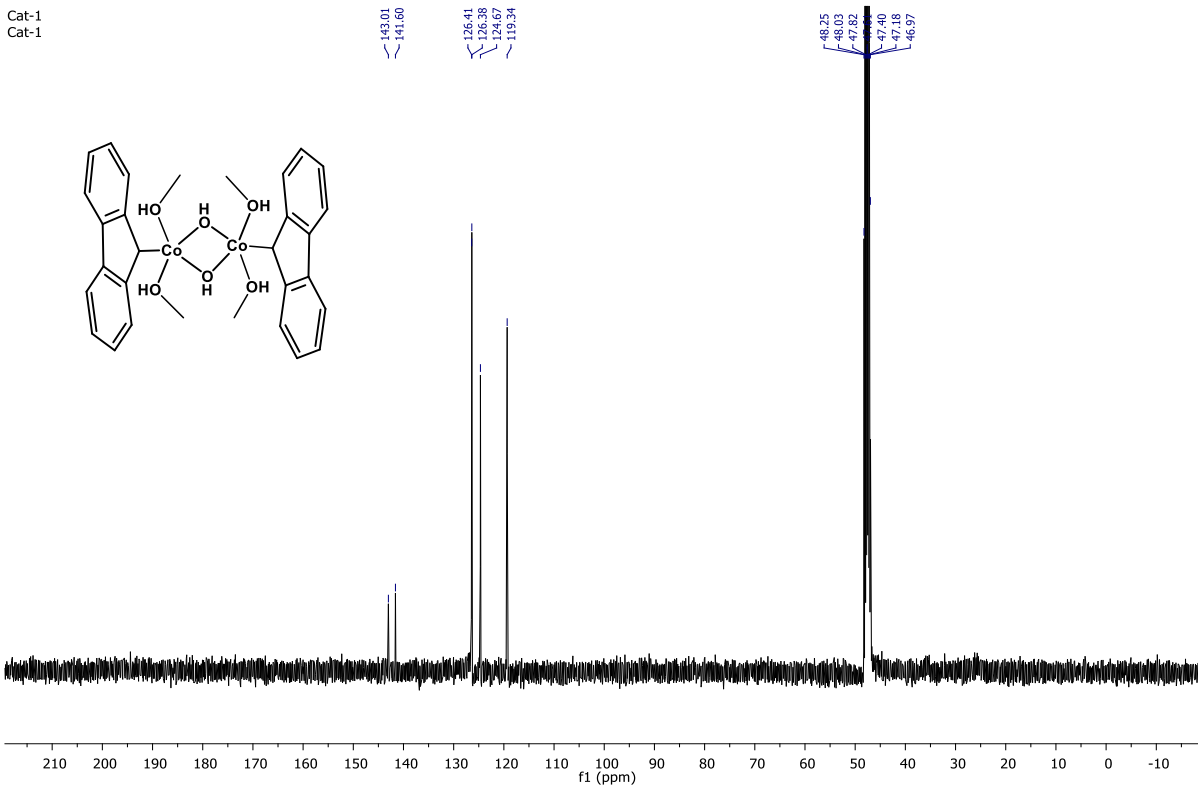


Figure S4. ^{13}C NMR spectrum of **Cat-1** (101 MHz, CD_3OD)

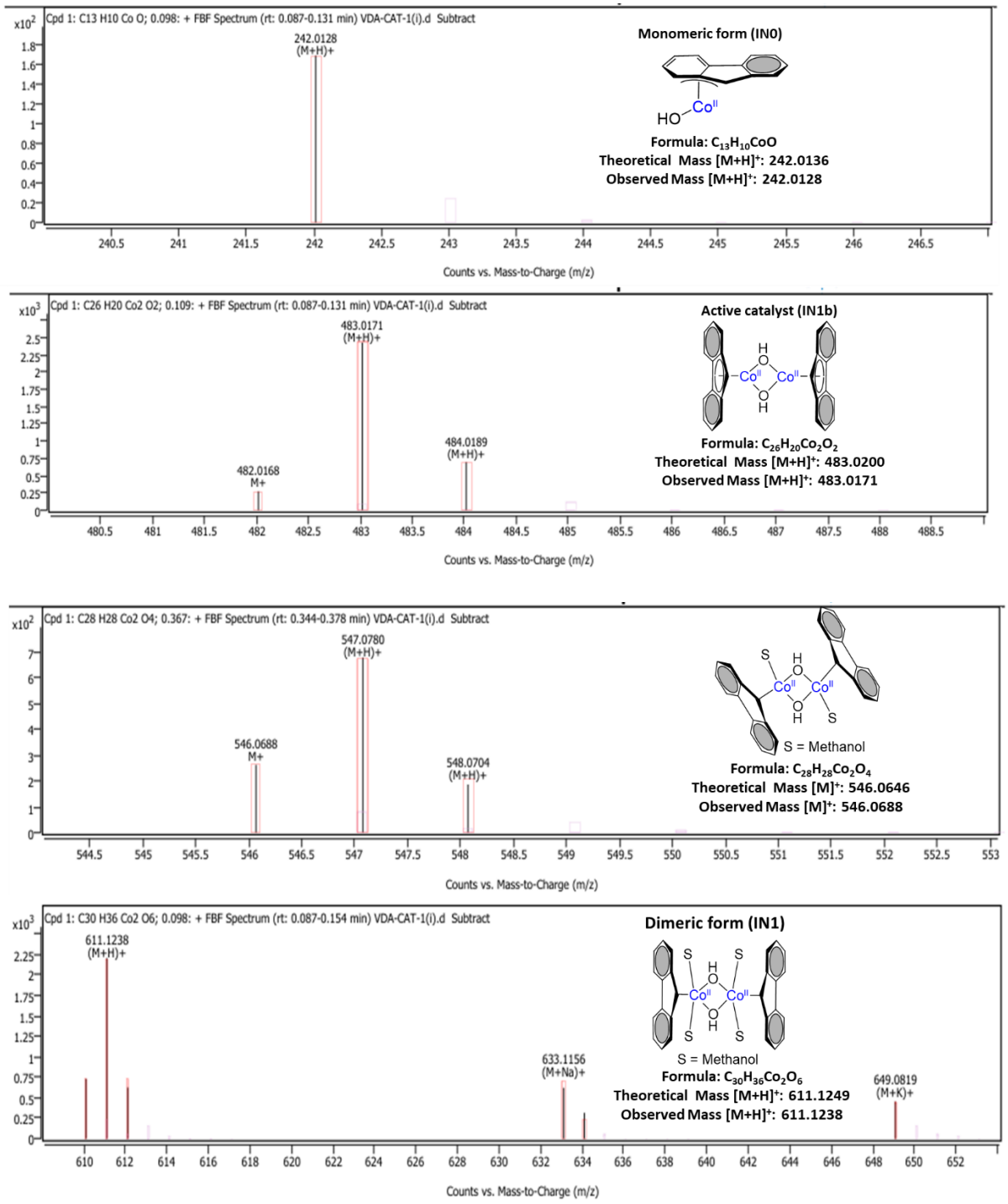


Figure S5. HRMS spectrum of **Cat-1**

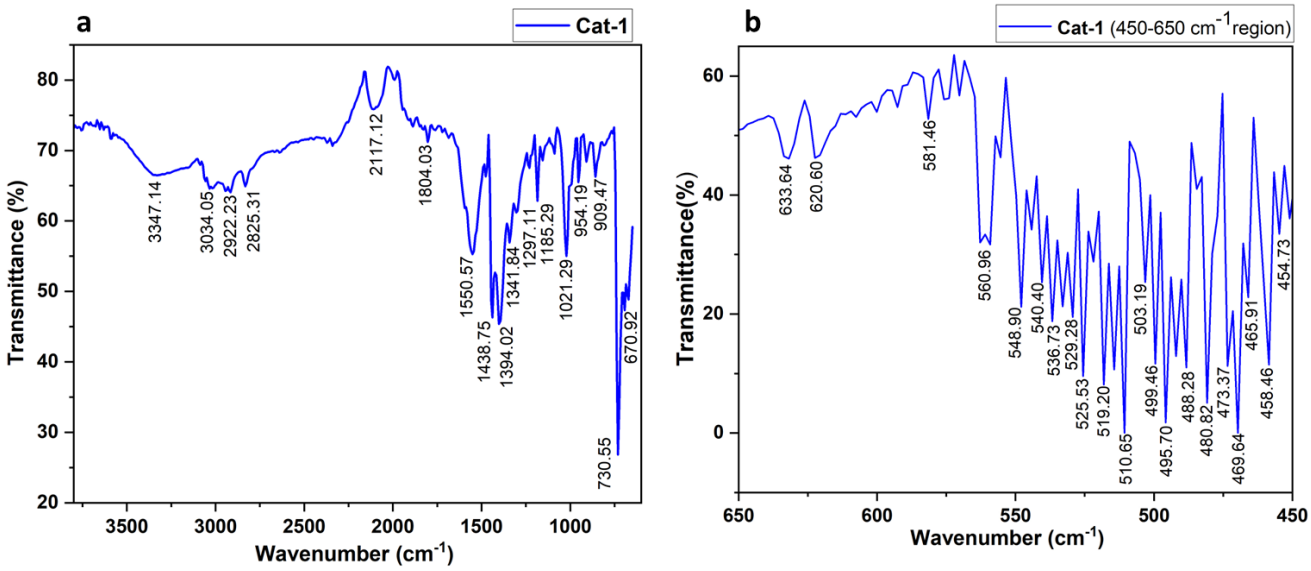


Figure S6. FT-IR spectrum of **Cat-1**

FT-IR Analysis: The above FT-IR spectrum clearly shows the presence of the following groups:

S.No.	IR Frequency	Vibrations
1.	3347 cm^{-1}	O-H stretching
2.	3034, 2922, 2825 cm^{-1}	Aliphatic and aromatic C-H stretching
3.	1438, 1550 cm^{-1}	Aromatic ring stretching
4.	581, 560, 548 cm^{-1}	Co-OH stretching
5.	540, 510, 495 cm^{-1}	Co-O(H)-Co bridging skeletal vibration

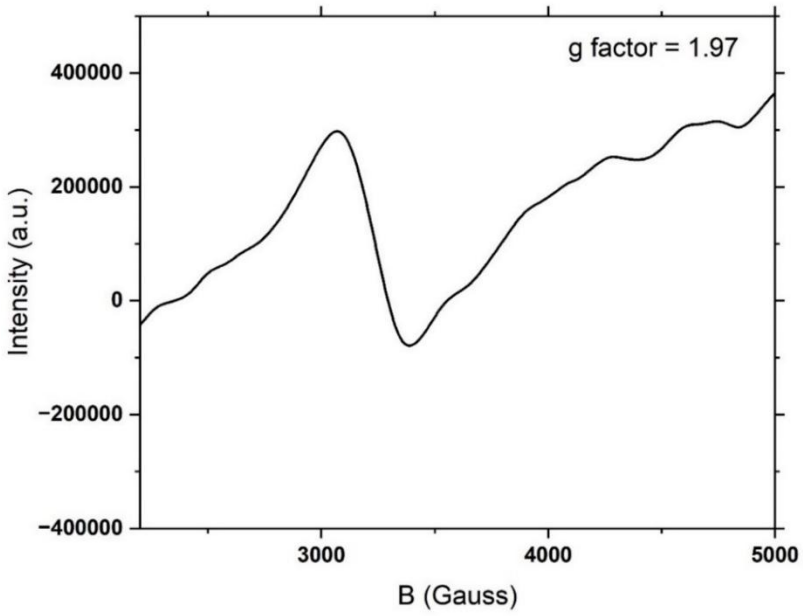


Figure S7. EPR of **Cat-1** in methanol (**Instrument Frequency**: 9.85 GHz, Temperature- RT)

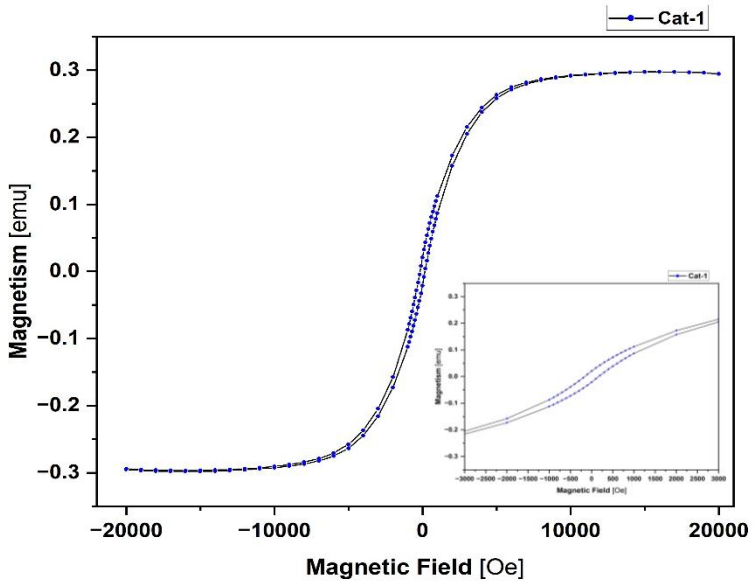


Figure S8. VSM analysis of **Cat-1**

The magnetic property of **Cat-1** was evaluated using a vibrating sample magnetometer (VSM) at room temperature. **Figure S8** shows the magnetization (M) versus applied magnetic field (H) plot recorded in the field range of -20,000 to +20,000 Oe. The magnetization curve exhibits a typical S-shaped hysteresis loop with saturation at higher applied fields. The saturation magnetization (Ms) was observed at ±0.30 emu, while the remanent magnetization (Mr) and coercivity (Hc) were negligible. These features indicate that **Cat-1** exhibits soft ferromagnetic behavior, with magnetization increasing rapidly with applied field and reaching a stable saturation value, with little remanence or coercivity.

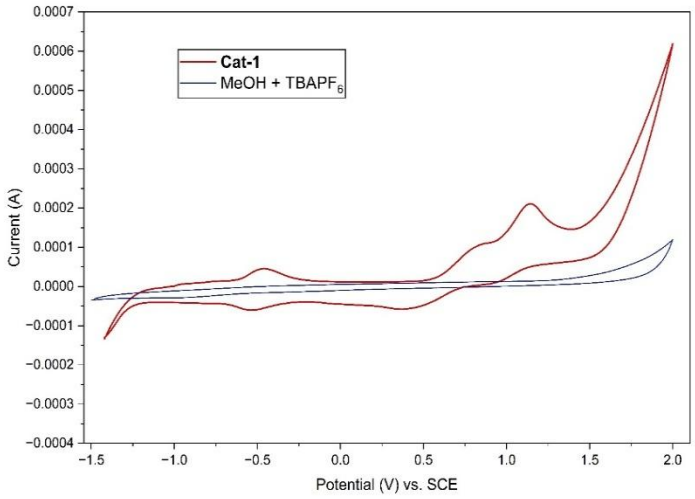


Figure S9. Cyclic voltammogram of Cat-1 (2mM) in methanol using Glassy Carbon, platinum wire, and Saturated Calomel Electrode as working, counter, and reference electrode, respectively. (Voltammograms recorded at 100 mV/s in 0.1 M TBAPF6).

Cyclic voltammetry of **Cat-1** was recorded in methanol with 0.1 M TBAPF6 (vs. SCE) using Gamry Interface 1010E potentiostat at a scan rate of 100 mV/s. Scanning anodically from 0 V reveals an irreversible oxidation peak at +1.14 V, attributed to the Co(II)/Co(III) oxidation. A weak reduction peak is observed at +0.36 V on the reverse sweep, with a significant peak separation of 780.1 mV, indicating electrochemical irreversibility of this oxidation.
In the cathodic region, a reduction peak at −0.54 V appears, followed by an anodic peak at −0.46 V during the reverse scan, giving a peak separation of ~80 mV, which is slightly larger than the ideal 57 mV expected for a fully Nernstian one-electron process. This behaviour suggests a near-reversible or quasi-reversible redox event, which is likely associated with the Co(II)/Co(I) redox couple.

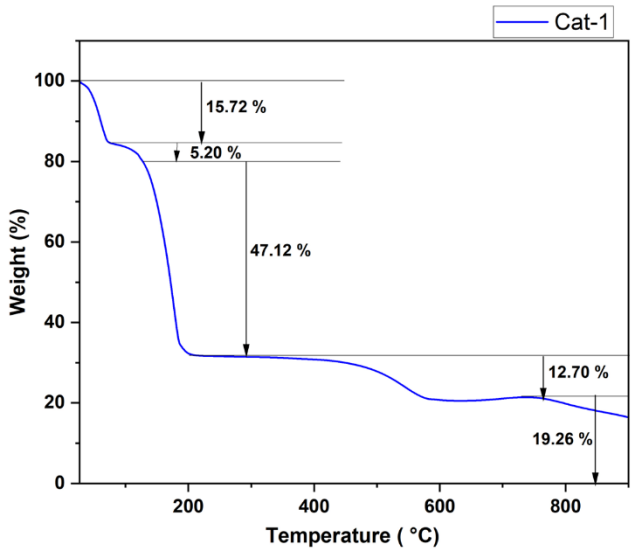


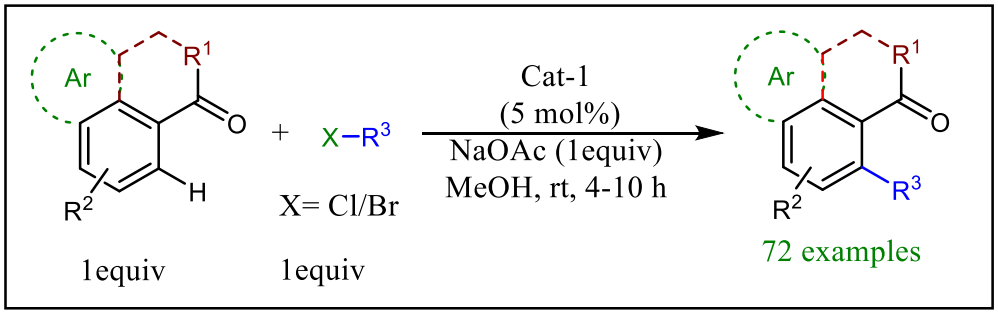
Figure S10. DT-TGA graph of **Cat-1**

The thermal stability and composition of **Cat-1** ($C_{30}H_{36}Co_2O_6$; MW = 610.12 g/mol) were examined by thermogravimetric analysis (TGA) at variable temperatures ranging from 30 °C to 1000 °C (Figure **S10**). The TGA profile exhibits four distinct weight-loss steps, consistent with the sequential elimination of coordinated ligands and the decomposition of the organic framework. The initial weight loss of **15.72%** (calcd 15.75%) at < 110 °C corresponds to the loss of three coordinated methanol, followed by a second step of **5.20%** (calcd 5.34%) between 110–160 °C, attributed to the loss of the fourth coordinated methanol. The third major decomposition event occurs between 160–330 °C and 450–750 °C, with a combined weight loss of 59.93% (calcd 60.41%), assigned to the elimination of two fluorene and two -OH ligands. The remaining residue of **19.26%** (calcd 19.16%) above 750 °C is attributed to the formation of cobalt residue species in close agreement with the theoretical cobalt content of the complex. Overall, the DT-TGA data strongly supported the proposed structure of the cobalt(II) catalyst, as shown in Cat-1 or IN1, comprising two cobalt centres bridged by two hydroxide ligands, with each Co centre coordinating one fluorenyl and two methanol molecules.

Interpretation of the DT-TGA graph

S.No.	Ligands	Weight loss %		Temperature (℃)
		Calculated	Experimental	
1.	Three methanol	**15.75**	15.72	0 - 110
2.	One methanol	**5.34**	5.20	110-160
3.	Hydroxyl and fluorene ligands	**60.41**	47.12 + 12.70 = 59.82	160 -330 450-750
4.	Cobalt residues	**19.16**	19.26	750 -900

4. General Procedure for C-H alkylation reaction:



In a round-bottom flask/reaction tube, sodium acetate (2.0 mmol, 0.164 g) was placed and dissolved in 5 mL of methanol, followed by the addition of **Cat-1** (48 mg, 5 mol%) (**Figure S9a**). Then, the corresponding aryl ketone (2 mmol) and an alkyl halide (2 mmol) were added to the above solution. The resulting reaction mixture was stirred for 4-10 hours at room temperature to get the C-H alkylated products in the absence of any dry/inert atmosphere. The progress of the reaction was monitored using thin-layer chromatography and 2,4-dinitrophenylhydrazine (2,4-DNP) as the staining agent. The reaction yields were determined by GC-MS. After the reaction was complete, the solvent was removed under vacuum, and the product was directly adsorbed onto silica for column chromatography. The crude product was then purified by column chromatography, using a mixture of hexanes and EtOAc as the eluent. **Note**: For light-sensitive alkyl halides, the reaction flask was covered with black tape to avoid contact with light to get the desired C-H alkylated products (**3x**-**3aa**, **3ae**-**3ap**, **3av**-**3ay,** and **3bo**-**3bt**) (**Figure S9b**).

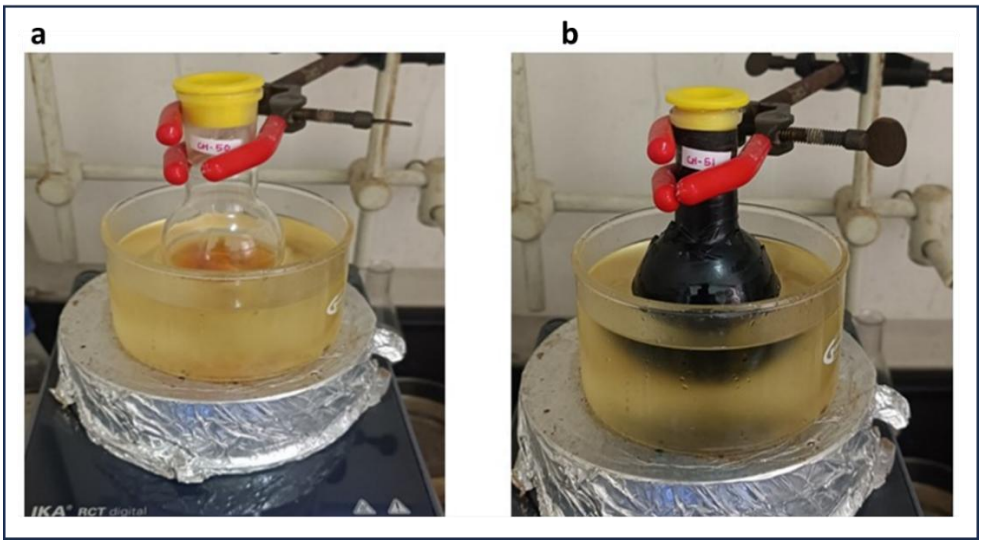
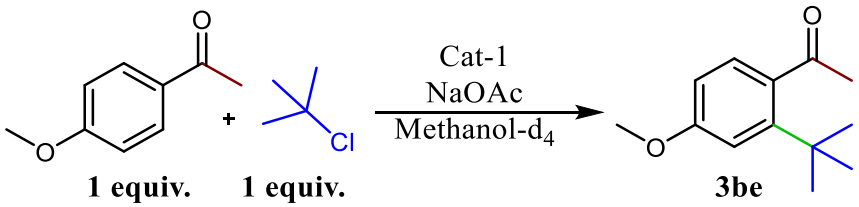


Figure S11. Experimental setup for C-H alkylation reaction: (a) General alkyl halides, (b) Light-sensitive alkyl halide. The oil bath temperature was maintained at 25-30 ℃.

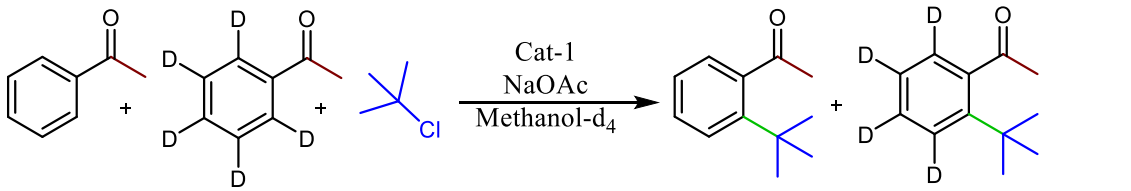
5. Kinetic study

5.1. Procedure for the time-dependent NMR study



The time-dependent NMR study was performed in the reaction tube at room temperature. 4-methoxyacetophenone (20 mg, 0.13 mmol) and **Cat-1** (40 mg, 0.82 mmol, 63 mol%) were dissolved in 2.5 mL of methanol-d_4 in the reaction tube. (**Note**: the excess catalyst was used to obtain better NMR signals and to identify intermediates.) Immediately, ^{1}H and ^{13}C NMR spectra of the reaction mixture (**1b + Cat-1**) were recorded. The reaction mixture was stirred for one hour, and NMR was recorded. The ^{1}H and ^{13}C NMR analyses revealed the formation of the intermediate **IN3a**. Following this confirmation, sodium acetate (11 mg, 0.13 mmol) and *tert*-butyl chloride (12 mg, 0.13 mmol) were added to the reaction mixture. Subsequent NMR measurements confirmed the formation of **IN4a**. Further stirred for another hour, and the NMR was recorded. The formation of **IN5a**, as evidenced by ^{1}H and ^{13}C NMR spectra. Continued stirring of the same reaction mixture up to 3 hours, and NMR was recorded. Which established the formation of d **IN6a**. Thus, all intermediates (**IN3a**, **IN4a**, **IN5a**, and **IN6a**) were thoroughly identified by ^{1}H and ^{13}C. We performed a similar experiment to record the 2D NMR (^{1}H-^{1}H COSY), which confirmed the formation of **IN3a, IN5a**, and **IN6a.** The formation of **IN3a** and **IN5a** was detected by high-resolution mass spectroscopy (HRMS). The respective spectrum was added in Page No. S109-S114.

5.2. Competitive reaction between acetophenone and acetophenone-d_5 with *tert*-butyl chloride



1 equiv. **1 equiv.** **1 equiv.** **3bg** **3bg' (*not observed*)**

To probe whether C-H bond metathesis is the rate-determining step (RDS) in the cobalt-catalysed alkylation reaction, a competitive kinetic isotope effect (KIE) experiment was conducted. Sodium acetate (20.50 mg, 0.25 mmol) was dissolved in methanol-d_4 (2 mL) in a reaction tube, followed by the addition of **Cat-1** (5 mol%). Subsequently, acetophenone (30.00 mg, 0.25 mmol), acetophenone-d_5 (31.29 mg, 0.25 mmol), and *tert*-butyl chloride (23.14 mg, 0.25 mmol) were added. The mixture was stirred at room temperature, and the reaction progress was monitored by GC-MS at hourly intervals. After seven h, the only single alkylated product, **3bg,** was obtained in 97% GC yield. The crude reaction mixture was further analysed by ^{1}H and ^{13}C NMR spectroscopy.

GC-MS and NMR analyses revealed that alkylation occurred exclusively with acetophenone, while no significant alkylated product derived from acetophenone-d_5 was detected. Moreover, no evidence of H/D scrambling was observed. These results show that the primary kinetic isotope effect, indicating that C-H bond cleavage is involved in the transition state of the RDS. The lack of reactivity of acetophenone-d_5 suggests a substantial rate difference (k_H/k_D >> 1), which is characteristic of a primary KIE. The absence of H/D exchange further supports the irreversibility of the C-H bond metathesis step.

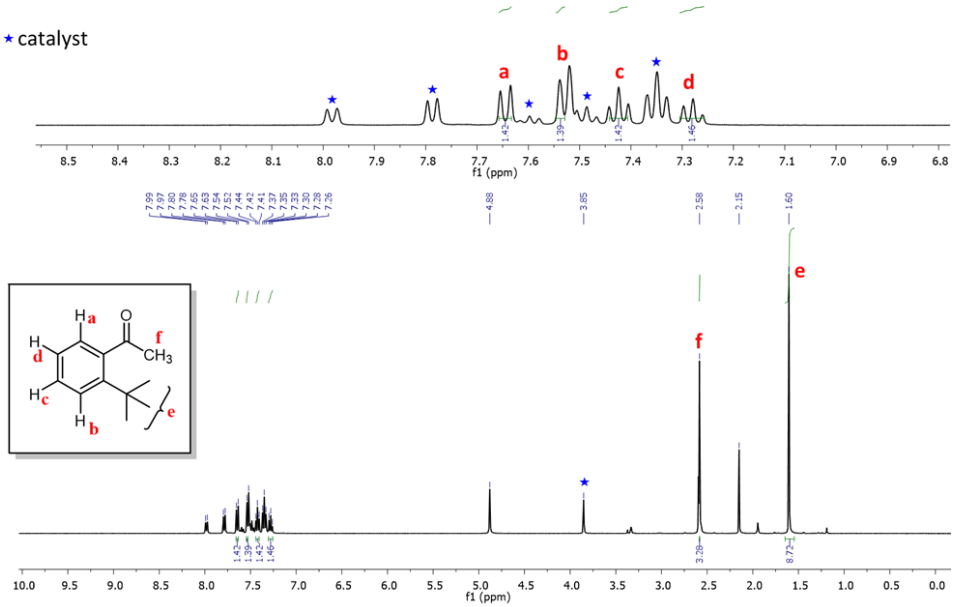


Figure S12. ^{1}H NMR spectrum of crude reaction mixture of acetophenone, acetophenone-d_5, and *tert*-butylchloride.

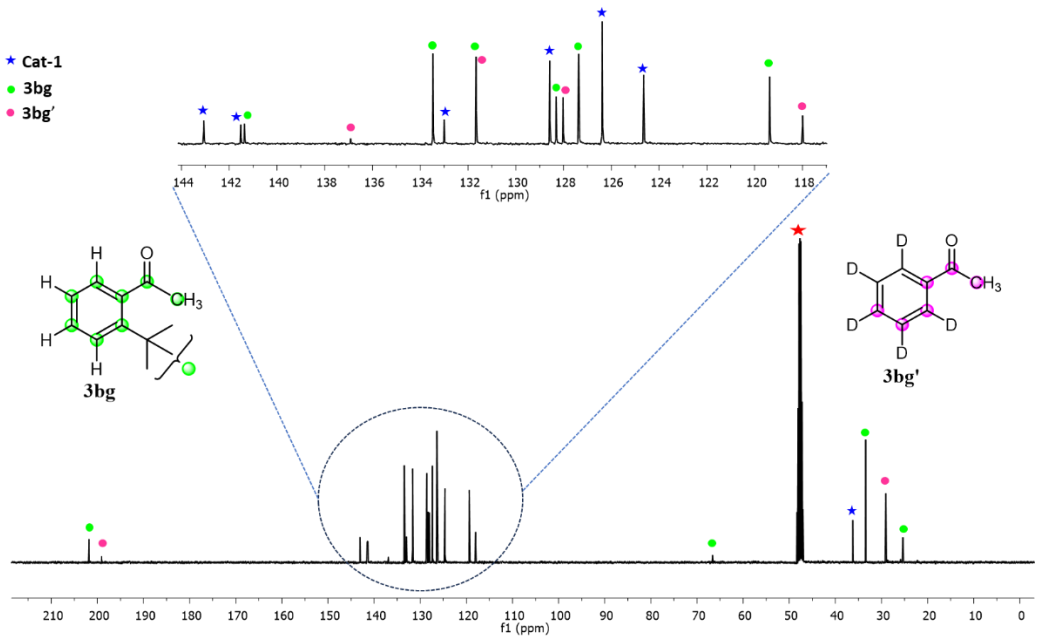
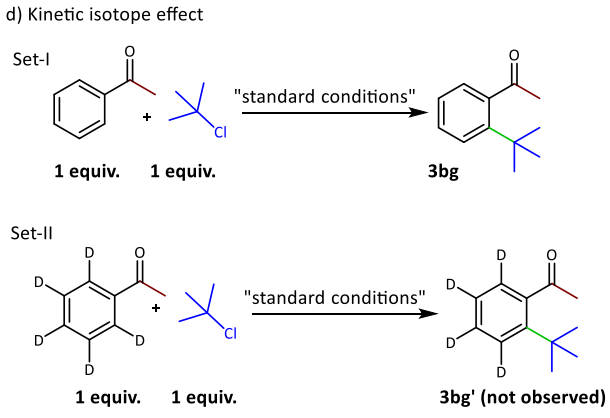
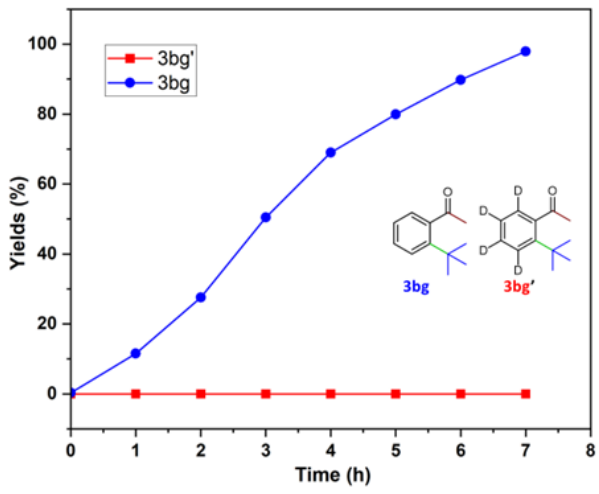


Figure S13. ^{13}C NMR spectrum of the crude reaction mixture of acetophenone, acetophenone-d5, and *tert*-butylchloride.

5.3. Kinetic isotope effect: To study KIE the following reactions were performed.

Set-I (with acetophenone): In a reaction tube, sodium acetate (0.25 mmol, 20 mg) was placed and dissolved in 1.5 mL of methanol, followed by the addition of **Cat-1 (**6.5 mg, 5 mol%). Acetophenone (0.25 mmol, 30 mg) and *tert*-butyl chloride (0.25 mmol, 25 mg) were added to the reaction mixture. The resulting mixture was stirred at room temperature. GC-MS monitored the reaction progress at hourly intervals. After 7 h, the product **3bg** was obtained with 97.71% GC yield.

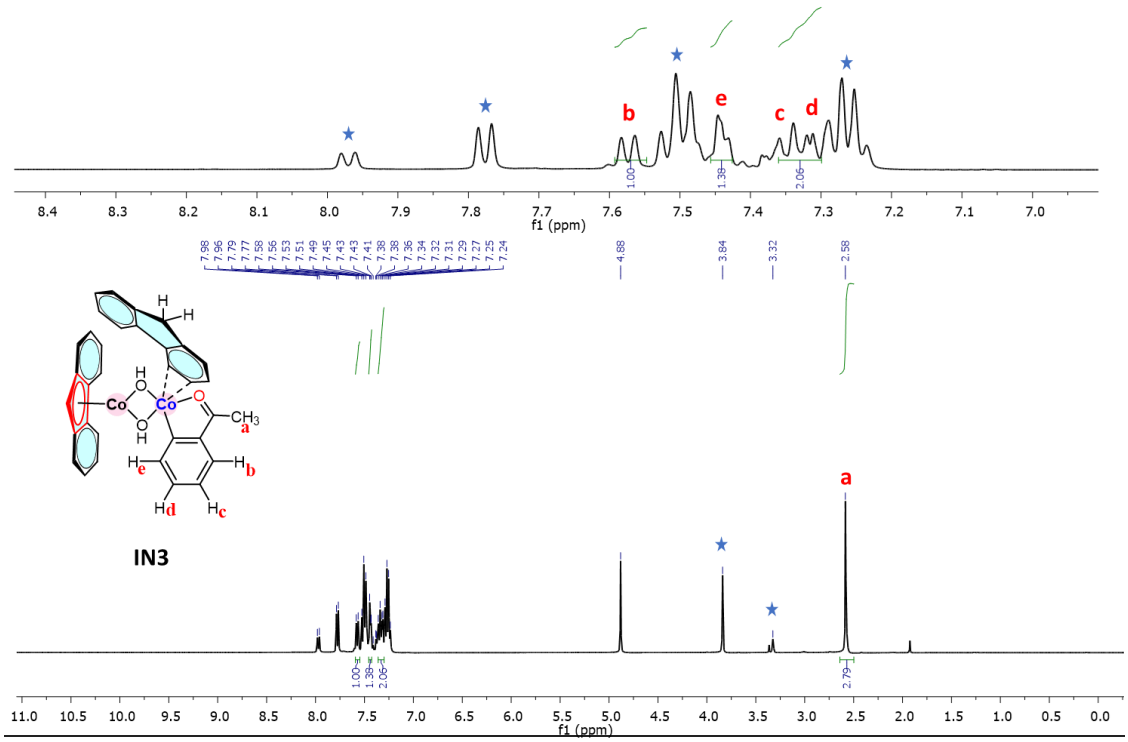


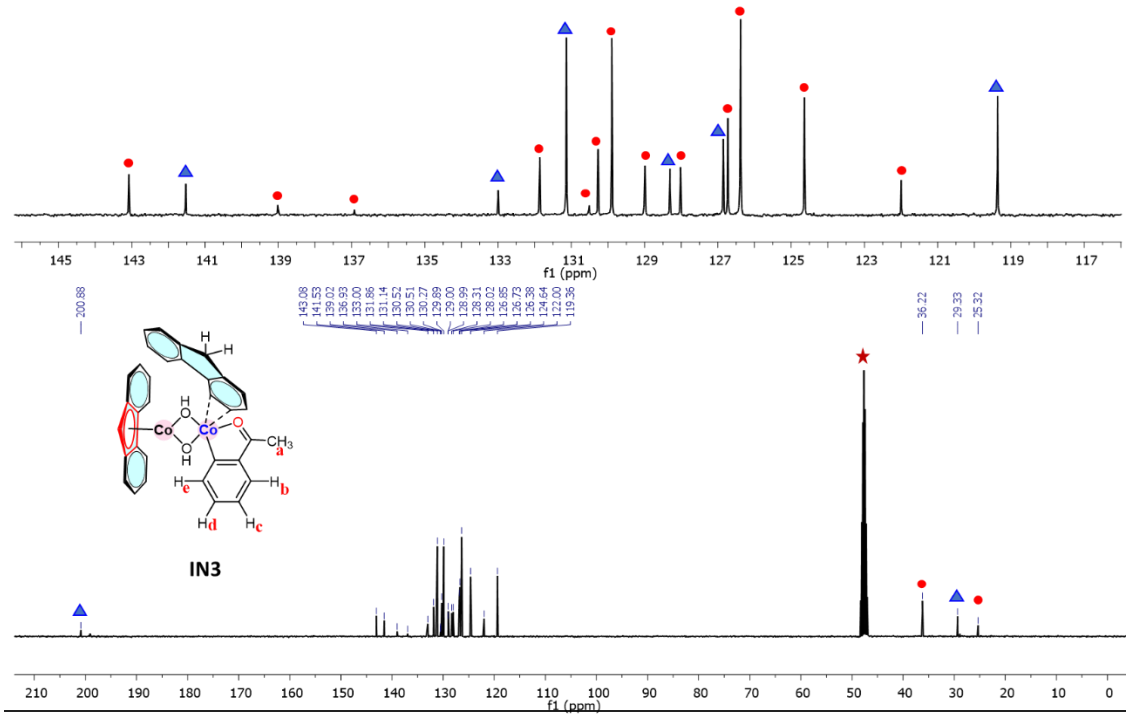


Set-II (with acetophenone-d_5): In a reaction tube, sodium acetate (0.25 mmol, 20 mg) was placed and dissolved in 1.5 mL of methanol, followed by the addition of **Cat-1 (**6.5 mg, 5 mol%). Acetophenone-d_5 (0.25 mmol, 31 mg) and *tert*-butyl chloride (0.25 mmol, 25 mg) were

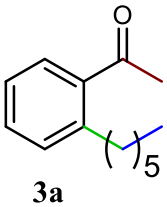
added to the reaction mixture. The resulting mixture was stirred at room temperature. The progress of the reaction was monitored by using GC-MS at hourly intervals. However, no expected **3bg** product was observed over the monitored period.

^{1}H and ^{13}C NMR spectrum of IN3



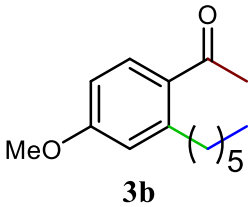


6. Experimental Details and Spectroscopic Data of 3a-3bq



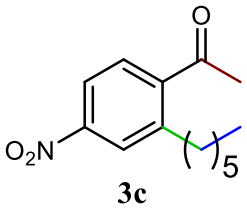
3a

1-(2-hexylphenyl)ethan-1-one (3a): General procedure as stated above was followed for the synthesis of **3a** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and 1-bromohexane (2 mmol, 0.330 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), and a light-yellow oil of 1-(2-hexylphenyl)ethan-1-one (0.39g, 95%) was obtained with a boiling point of 189 ℃. R_f = 0.48; TLC in 2.5% ethyl acetate in hexane with three runs and stained in 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.62 (d, *J* = 7.9 Hz, 1H), 7.48 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.33 – 7.27 (m, 1H), 3.42 (t, *J* = 6.9 Hz, 2H), 2.64 (s, 3H), 1.90 – 1.80 (m, 2H), 1.49 – 1.39 (m, 2H), 1.34 – 1.26 (m, 4H), 0.91 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.3, 141.3, 133.5, 131.7, 128.5, 127.6, 118.7, 34.1, 33.0, 30.95, 30.3, 27.8, 22.5, 13.8. **HRMS** (ESI-TOF) calculated for $C_{14}H_{20}O_3$ $[M+H]^+$ 205.1514, found 205.1519.



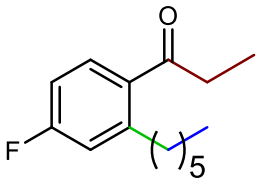
3b

1-(2-hexyl-4-methoxyphenyl)ethan-1-one (3b): General procedure as stated above was followed for the synthesis of **3b** from 4-methoxyacetophenone (0.300 g, 2 mmol, 1 equiv.) and 1-bromohexane (2 mmol, 0.330 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution with 2.5% and 5% ethyl acetate in hexanes), yielding a white solid of 1-(2-hexyl-4-methoxyphenyl)ethan-1-one (0.44g, 95%), with a melting point of 132 ℃. R_f = 0.36; TLC in 2.5% ethyl acetate in hexane with three runs and stained in 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 8.3 Hz, 1H), 6.99 – 6.98 (dd, *J* = 7.2, 2.4 Hz, 1H), 6.14 (s, 1H), 3.96 (s, 3H), 3.41 (t, *J* = 6.9 Hz, 2H), 2.57 (s, 3H), 2.02-1.82 (m, 2H), 1.44 (dt, *J* = 14.9, 7.5 Hz, 2H), 1.39-1.25 (m, 4H), 0.91 (t, *J* = 6.97 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.6, 150.4, 146.6, 130.2, 123.9, 113.7, 109.7, 56.0, 33.9, 32.8, 30.9, 27.8, 26.1, 22.4, 13.9. **HRMS** (ESI-TOF) calculated for $C_{15}H_{22}O_2$ $[M]^+$ 235.1614, found 235.1604.



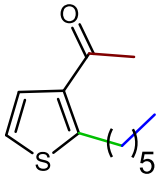
3c

1-(2-hexyl-4-nitrophenyl) ethan-1-one (3c): General procedure as stated above was followed for the synthesis of **3c** from 4-nitroacetophenone (0.330g, 2 mmol, 1 equiv.) and 1-bromohexane (2 mmol, 0.330 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, 10% ethyl acetate in hexanes), yielding a yellow solid of 1-(2-hexyl-4-nitrophenyl)ethan-1-one. (0.45g, 92%) with a melting point of 128 ℃. R_f = 0.45; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.00 (d, *J* = 2.1 Hz, 1H), 7.50 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.32 (d, *J* = 8.2 Hz, 1H), 3.43 (t, *J* = 6.9 Hz, 2H), 2.59 (s, 3H), 2.02 – 1.75 (m, 2H), 1.45 (m, 2H), 1.37 – 1.26 (m, 4H), 0.91 (t, J = 6.9 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.7, 150.4, 146.6, 130.2, 124.0, 113.7, 109.7, 56.0, 34.0, 32.8, 30.9, 27.8, 22.4, 13.9. **HRMS** (ESI-TOF) calculated for $C_{14}H_{19}NO_3$ $[M+H]^+$ 250.1438, found 250.1438.



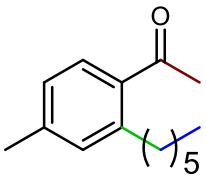
3d

1-(4-fluoro-2-hexylphenyl)propan-1-one (3d): General procedure as stated above was followed for the synthesis of **3d** from 4-fluoropropiophenone (0.304 g, 2 mmol, 1 equiv.) and 1-bromohexane (2 mmol, 0.330 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, 10% ethyl acetate in hexanes), yielding an oily liquid of 1-(4-fluoro-2-hexylphenyl)propan-1-one (0.38g, 87%) with a boiling point of 218 ℃. R_f = 0.30; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.03 – 8.01 (m, 1H), 8.00 – 7.97 (m, 1H), 7.17 – 7.08 (m, 1H), 3.42 (t, *J* = 7.2 Hz, 2H), 2.99 (q, *J* = 7.2 Hz, 2H), 1.92 – 1.80 (m, 2H), 1.49 – 1.38 (m, 2H), 1.37 – 1.27 (m, 4H), 1.23 (t, *J* = 7.2 Hz, 3H), 0.91 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 199.1, 165.61 (d, $J_{(C-F)}$ = 254.2 Hz), 164.3, 133.3 (d, $J_{(C-F)}$ = 3.0 Hz), 130.5 (d, $J_{(C-F)}$ = 9.2 Hz), 115.5 (d, $J_{(C-F)}$ = 21.8 Hz)., 34.0, 32.8, 31.7, 30.9, 27.8, 22.4, 13.9, 8.1. **^{19}F NMR** (377 MHz, $CDCl_3$) δ -104.88 – -106.39 (m). **HRMS** (ESI-TOF) calculated for $C_{15}H_{19}FO$ $[M+NH_4]^+$ 254.1915, found 254.1909.



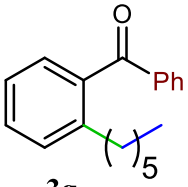
3e

1-(2-hexylthiophen-3-yl) ethan-1-one (3e): General procedure as stated above was followed for the synthesis of **3e** from 3-acetylthiophene (0.252 g, 2 mmol, 1 equiv.) and 1-bromohexane (2mmol, 0.330 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, 10% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-hexylthiophen-3-yl)ethan-1-one (0.36g, 88%) with a boiling point of 198 ℃. R_f = 0.30; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.01 (d, J = 5.6 Hz, 1H), 6.79 (d, *J* = 5.6 Hz, 1H), 2.63 – 2.44 (m, 2H), 2.14 (s, 3H), 1.53 (m, 2H), 1.28 (m, 6H), 0.87 (m, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 206.6, 139.1, 127.8, 121.9, 31.5, 30.7, 29.5, 28.8, 27.8, 22.5, 14.0. **HRMS** (ESI-TOF) calculated for $C_{12}H_{18}OS$ $[M+Na]^+$ 221.0971, found 221.0962.



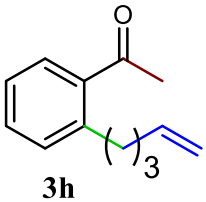
3f

1-(2-hexyl-4-methylphenyl)ethan-1-one (3f): General procedure as stated above was followed for the synthesis of **3f** from 4-methylacetophenone (0.268 g, 2 mmol, 1 equiv.) and 1-bromohexane (2 mmol, 0.330 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution with 2.5% and 5% ethyl acetate in hexanes). and pale-yellow oil of 1-(2-hexyl-4-methylphenyl)ethan-1-one was obtained (0.41g, 93%) with boiling of 232 ℃. R_f = 0.36; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.19 (d, *J* = 8.3 Hz, 1H), 7.12 (d, *J* = 8.3 Hz, 1H), 6.98 (d, *J* = 2.7 Hz, 1H), 3.44 (t, *J* = 6.9 Hz, 1H), 2.35 (s, 3H), 2.32 (s, 3H), 1.96 – 1.82 (m, 2H), 1.47 (d, *J* = 6.7 Hz, 2H), 1.38 – 1.30 (m, 4H), 0.93 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 203.4, 136.9, 133.9, 132.7, 130.6, 129.5, 127.3, 34.0, 32.8, 30.9, 27.8, 22.5, 20.6, 19.5, 13.9. **HRMS** (ESI-TOF) calculated for $C_{15}H_{22}O$ $[M+H]^+$ 219.1743, found 219.1741.



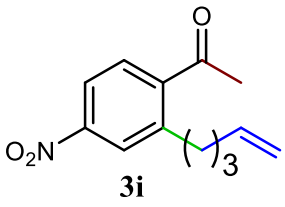
3g

(2-hexylphenyl) (phenyl)methanone (3g): General procedure as stated above was followed for the synthesis of **3g** from benzophenone (0.364 g, 2 mmol, 1 equiv.) and 1-bromohexane (2 mmol, 0.330 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, 10% ethyl acetate in hexanes), and a white solid of (2-hexylphenyl)(phenyl)methanone (0.50g, 93%) was obtained, with a melting point of 120 ℃. R_f = 0.52; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.82 – 7.77 (m, 2H), 7.73 – 7.68 (m, 2H), 7.67 – 7.61 (m, 3H), 7.51 (t, J = 7.6 Hz, 2H), 3.43 (t, J = 6.9 Hz, 2H), 1.93 – 1.80 (m, 2H), 1.45 (dt, J = 14.7, 7.4 Hz, 2H), 1.39 – 1.26 (m, 4H), 0.92 (t, J = 6.8 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 195.6, 137.1, 136.3, 132.6, 131.6, 131.5, 129.9, 128.4, 127.5, 34.0, 32.8, 30.9, 27.8, 22.4, 13.9. **HRMS** (ESI-TOF) calculated for $C_{18}H_{18}O$ $[M+H]^+$ 271.1693, found 271.1712.



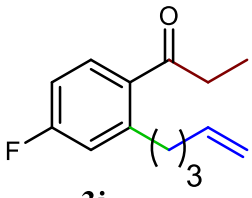
3h

1-(2-(pent-4-en-1-yl)phenyl) ethan-1-one (3h): General procedure as stated above was followed for the synthesis of **3h** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and 5-bromo-1-pentene (2 mmol, 0.286 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), and an oily liquid of 1-(2-(pent-4-en-1-yl)phenyl)ethan-1-one (0.32g, 85%) was obtained, boiling at 245 ℃. R_f = 0.43; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.62 (dd, J = 7.9, 0.9 Hz, 1H), 7.47 (dd, J = 7.6, 1.8 Hz, 1H), 7.37 (td, J = 7.5, 1.1 Hz, 1H), 7.30 (td, J = 7.7, 2.1 Hz, 1H), 5.82 – 5.70 (m, 1H), 5.16 – 4.98 (m, 2H), 3.49 – 3.38 (m, 2H), 2.64 (s, 3H), 2.28 – 2.12 (m, 2H), 2.01 – 1.88 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.2, 141.4, 136.7, 133.8, 131.7, 128.9, 127.4, 118.8, 115.8, 33.1, 32.0, 31.7, 30.3. **HRMS** (ESI-TOF) calculated for $C_{13}H_{16}O$ $[M+H]^+$ 189.1274, found 189.1278.



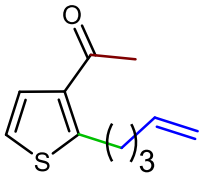
3i

1-(4-nitro-2-(pent-4-en-1-yl) phenyl) ethan-1-one (3i): General procedure as stated above was followed for the synthesis of **3i** from 4-nitroacetophenone (0.330 g, 2 mmol, 1 equiv.) and 5-bromo-1-pentene (2 mmol, 0.298 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution 5%,10%, 15% ethyl acetate in hexanes) and a yellow solid, 1-(4-nitro-2-(pent-4-en-1-yl)phenyl)ethan-1-one, was obtained (0.41g, 86%) with a melting point of 161 ℃. R_f = 0.26; TLC in 5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.30 (d, J = 2.1 Hz, 1H), 8.10 (dd, J = 8.2, 2.2 Hz, 1H), 7.28 (d, J = 8.2 Hz, 1H),), 5.82 – 5.70 (m, 1H), 5.16 – 4.98 (m, 2H), 3.42 (t, *J* = 6.9 Hz, 2H), 2.69 (s, 3H), 1.95 – 1.78 (m, 2H), 1.50 – 1.39 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.7, 150.4, 141.6, 136.2, 129.0, 127.6, 115.7, 109.7, 56.0, 34.0, 32.8, 30.9, 27.8, 22.4, 13.9. **HRMS** (ESI-TOF) calculated for $C_{13}H_{15}NO_3$ $[M+H]^+$ 234.1125, found 234.1126.



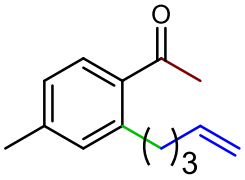
3j

1-(4-fluoro-2-(pent-4-en-1-yl)phenyl)propan-1-one (3j): General procedure as stated above was followed for the synthesis of **3j** from 4-fluoropropiophenone (0.304 g, 2 mmol, 1 equiv.) and 5-bromo-1-pentene (2 mmol, 0.298 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), and an oily liquid, 1-(4-fluoro-2-(pent-4-en-1-yl)phenyl)propan-1-one (0.40g, 90%), was obtained with a boiling point of 245 ℃. R_f = 0.43; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.05 – 8.01 (m, 1H), 8.01 – 7.96 (m, 1H), 7.15 (t, *J* = 8.6 Hz, 1H), 5.84 – 5.73 (m, 1H), 5.14 – 4.98 (m, 2H), 3.44 (t, *J* = 6.7 Hz, 2H), 3.00 (q, *J* = 7.2 Hz, 2H), 2.23 (q, *J* = 7.0 Hz, 2H), 2.05 – 1.90 (m, 2H), 1.24 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 199.0, 165.6 (d, $J_{(C-F)}$ = 254.2 Hz), 164.0, 136.9, 133.3 (d, $J_{(C-F)}$ = 3.1 Hz), 130.5 (d, $J_{(C-F)}$ = 9.2 Hz), 115.8 (d, $J_{(C-F)}$ = 16.1 Hz)., 115.5, 33.1, 32.0, 31.7, 31.7, 8.21. **^{19}F NMR** (377 MHz, $CDCl_3$) δ -105.48 – -105.99 (m). **HRMS** (ESI-TOF) calculated for $C_{14}H_{17}FO$ $[M+Na]^+$ 204.0921, found 204.0911.



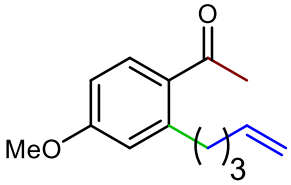
3k

1-(2-(pent-4-en-1-yl)thiophen-3-yl)ethan-1-one (3k): General procedure as stated above was followed for the synthesis of **3k** from 1-(thiophen-3-yl)ethan-1-one (0.252 g, 2 mmol, 1 equiv.) and 5-bromo-1-pentene (2 mmol, 1 equiv. 0.298 g). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), and the oil liquid of 1-(2-(pent-4-en-1-yl)thiophen-3-yl)ethan-1-one was obtained (0.35g, 88%) with a boiling point of 215 ℃. R_f = 0.43; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.59 (d, *J* = 3.6 Hz, 1H), 7.26 (d, *J* = 3.6 Hz, 1H), 5.78 (ddt, *J* = 17.0, 10.2, 6.7 Hz, 1H), 5.18 – 4.95 (m, 2H), 3.47 – 3.38 (m, 2H), 2.22 (d, *J* = 7.0 Hz, 2H), 2.17 (s, 3H), 2.00 – 1.91 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 206.9, 152.0, 141.6, 136.7, 121.1, 115.8, 33.1, 32.0, 31.7, 30.9. **HRMS** (ESI-TOF) calculated for $C_{15}H_{23}O_3$ $[M+Na]^+$: 273.1284; found: 273.1289.



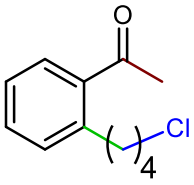
3l

1-(4-methyl-2-(pent-4-en-1-yl)phenyl)ethan-1-one (3l): General procedure as stated above was followed for the synthesis of **3l** from 4-methylacetophenone (0.268 g, 2 mmol, 1 equiv.) and 5-bromo-1-pentene (2 mmol, 0.298 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding an oily liquid of 1-(4-methyl-2-(pent-4-en-1yl)phenyl)ethan-1-one (0.38g, 94%) with a boiling point of 235 ℃. R_f = 0.56; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.19 (d, *J* = 8.3 Hz, 1H), 7.12 (d, *J* = 8.3 Hz, 1H), 6.98 (d, *J* = 2.7 Hz, 1H), 5.82 – 5.70 (m, 1H), 5.16 – 4.98 (m, 2H), 3.49 – 3.38 (m, 2H), 2.35 (s, 3H), 2.32 (s, 3H), 2.28 – 2.12 (m, 2H), 2.01 – 1.88 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 200.4, 136.9, 136.7, 133.9, 132.7, 130.6, 129.5, 127.3, 115.9, 33.1, 32.0, 31.7, 20.6, 19.5. **HRMS** (ESI-TOF) calculated for $C_{14}H_{18}O$ $[M+Na]^+$ 225.1252, found 225.1250.



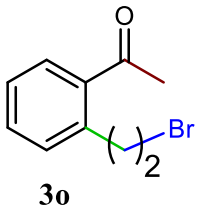
3m

1-(4-methoxy-2-(pent-4-en-1-yl)phenyl)ethan-1-one (3m): General procedure as stated above was followed for the synthesis of **3m** from 4-methoxyacetophenone (0.300 g, 2 mmol, 1 equiv.) and 5-bromo-1-pentene (2 mmol, 0.298 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a white solid of 1-(4-methoxy-2-(pent-4-en-1yl)phenyl)ethan-1-one (0.40g, 92%), with a melting point of 155 ℃. R_f = 0.56; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 8.3 Hz, 1H), 6.99 – 6.98 (dd, *J* = 7.2, 2.4 Hz, 1H), 6.14 (s, 1H), 5.82 – 5.70 (m, 1H), 5.16 – 4.98 (m, 2H), 3.49 – 3.38 (m, 2H), 3.96 (s, 3H), 2.64 (s, 3H), 2.28 – 2.12 (m, 2H), 2.01 – 1.88 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): 196.7, 150.4, 146.6, 136.7, 130.2, 124.0, 115.8, 113.7, 109.7, 56.0, 33.1, 32.0, 31.7, 26.1. **HRMS** (ESI-TOF) calculated for $C_{14}H_{18}O_2$ $[M+H]^+$ 219.1380, found 219.1399.



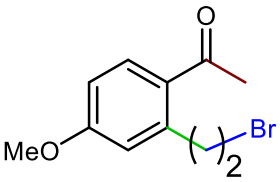
3n

1-(2-(4-chlorobutyl)phenyl)ethan-1-one (3n): General procedure as stated above was followed for the synthesis of **3n** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and 1-chloro-4-dibromobutane (2 mmol, 0.342 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution with 2.5% and 5% ethyl acetate in hexanes), yielding a yellow liquid, 1-(2-(4-chlorobutyl)phenyl)ethan-1-one (0.48g, 94%), with a boiling point of 218 ℃. R_f = 0.39; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.62 (d, *J* = 7.9 Hz, 1H), 7.47 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.41 – 7.34 (m, 1H), 7.30 (td, *J* = 7.8, 1.9 Hz, 1H), 3.58 (t, *J* = 6.2 Hz, 2H), 3.45 (t, *J* = 6.4 Hz, 2H), 2.63 (s, 3H), 2.10 – 1.98 (m, 2H), 1.99 – 1.87 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.2, 141.4, 133.8, 131.7, 128.9, 127.4, 118.8, 44.0, 32.7, 30.8, 30.3, 29.7. **HRMS** (ESI-TOF) calculated for $C_{12}H_{15}ClO$ $[M]^+$ 210.0806, found 210.0807.



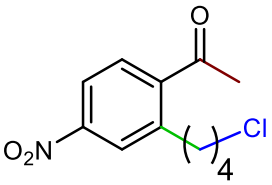
3o

1-(2-(2-bromoethyl) phenyl) ethan-1-one (3o): General procedure as stated above was followed for the synthesis of **3o** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and 1,2-dibromoethane (2 mmol, 0.375 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution with 2.5% and 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-(2-bromoethyl)phenyl)ethan-1-one (0.43g, 95%) with a boiling point of 250 ℃. R_f = 0.39; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.62 (dd, *J* = 7.9, 0.8 Hz, 1H), 7.47 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.38 (td, *J* = 7.5, 1.0 Hz, 1H), 7.30 (td, *J* = 7.7, 1.7 Hz, 1H), 3.44 (t, *J* = 2.2 Hz, 2H), 2.64 (s, 3H), 2.03 (t, *J* = 3.1 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.3, 141.4, 133.84, 131.8, 128.9, 127.4, 118.8, 32.5, 30.9, 30.3. **HRMS** (ESI-TOF) calculated for $C_{10}H_{11}BrO$ $[M+NH_4]^+$ 246.0312, found 246.0325.



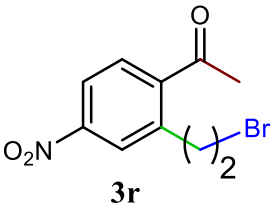
3p

1-(2-(2-bromoethyl)-4-methoxyphenyl)ethan-1-one (3p): General procedure as stated above was followed for the synthesis of **3p** from 4-methoxyacetophenone (0.300 g, 2 mmol, 1 equiv.) and 1,4-dibromobutane (2 mmol, 0.375 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, ethyl acetate in hexanes), and a colourless liquid, 1-(2-(2-bromoethyl)-4-methoxyphenyl)ethan-1-one (0.47g, 94%), was obtained with a boiling point of 224 ℃. R_f = 0.61; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 8.3 Hz, 1H), 6.99 – 6.98 (dd, *J* = 7.2, 2.4 Hz, 1H), 6.14 (s, 1H), 3.96 (s, 3H), 3.44 (t, *J* = 2.2 Hz, 2H), 2.64 (s, 3H), 2.37 (t, *J* = 3.1 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): 196.8, 150.4, 146.6, 130.3, 124.0, 113.8, 109.7, 56.0, 34.9, 31.1, 26.2. **HRMS** (ESI-TOF) calculated for $C_{11}H_{13}BrO_2$ $[M]^+$ 258.0074, found 258.0078.



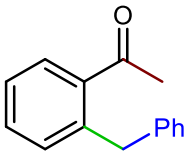
3q

1-(2-(4-chlorobutyl)-4-nitrophenyl)ethan-1-one (3q): General procedure as stated above was followed for the synthesis of **3q** from 4-nitroacetophenone (0.330 g, 2 mmol, 1 equiv.) and 1-chloro-4-dibromobutane (2 mmol, 0.342 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 5%, 10%, 15% ethyl acetate in hexanes), yielding a yellow solid, 1-(2-(4-chlorobutyl)-4-nitrophenyl)ethan-1-one (0.40g, 85%), with a melting point of 188 ℃. R_f = 0.26; TLC in 5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.00 (d, *J* = 2.1 Hz, 1H), 7.50 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.32 (d, *J* = 8.2 Hz, 1H), 3.60 (t, *J* = 6.2 Hz, 2H), 3.47 (t, *J* = 6.3 Hz, 2H), 2.60 (s, 3H), 2.11 – 2.02 (m, 2H), 1.97 (tt, *J* = 6.7, 3.6 Hz, 2H)..**^{13}C NMR** (101 MHz, $CDCl_3$): δ 200.36, 133.8, 133.0, 132.0, 124.7, 43.9, 32.71, 30.8, 29.7, 20.0. **HRMS** (ESI-TOF) calculated for $C_{12}H_{14}ClNO_3$ $[M+K]^+$ 294.0294, found 294.0291.



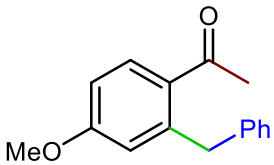
3r

1-(2-(2-bromoethyl)-4-nitrophenyl)ethan-1-one (3r): General procedure as stated above was followed for the synthesis of **3r** from 4-nitroacetophenone (0.330 g, 2 mmol, 1 equiv.) and 1,2-dibromoethane (2 mmol, 0.375 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution with 2.5% and 5% ethyl acetate in hexanes), yielding a yellow liquid, 1-(2-(2-bromoethyl)-4-nitrophenyl)ethan-1-one (0.42g, 90%), with a boiling point of 250 ℃. R_f = 0.39; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.00 (d, *J* = 2.1 Hz, 1H), 7.50 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.32 (d, *J* = 8.2 Hz, 1H), 3.58 (t, *J* = 2.2 Hz, 2H), 2.64 (s, 3H), 2.38 (t, *J* = 3.1 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.8, 133.8, 133.0, 132.4, 132.0, 124.7, 34.8, 31.1, 20.0. **HRMS** (ESI-TOF) calculated for $C_{10}H_{10}BrNO_3$ $[M+Na]^+$[-H_2O] 277.9611, found 277.9589.



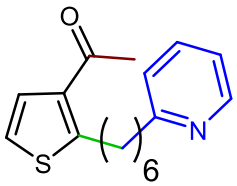
3s

1-(2-benzylphenyl) ethan-1-one (3s): General procedure as stated above was followed for the synthesis of **3s** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and benzyl bromide (2 mmol, 0.342 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution with 2.5% and 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-benzylphenyl)ethan-1-one (0.40g, 95%) with a boiling point of 236 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.63 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.49 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.41 (m, 2H), 7.37 (ddd, *J* = 7.1, 3.9, 1.9 Hz, 2H), 7.34 – 7.30 (m, 2H), 7.29 (dd, *J* = 3.6, 1.8 Hz, 1H), 4.52 (s, 2H), 2.65 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.3, 141.4, 137.8, 133.8, 131.8, 129.0, 128.9, 128.8, 128.4, 127.4, 118.9, 33.6, 30.3. **HRMS** (ESI-TOF) calculated for $C_{15}H_{14}O$ $[M+H]^+$ 211.1117, found 211.1116.



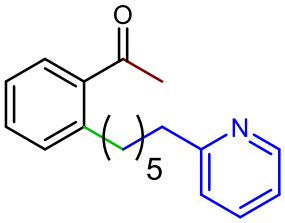
3t

1-(2-benzyl-4-methoxyphenyl) ethan-1-one (3t): General procedure as stated above was followed for the synthesis of **3t** from 4-methoxyacetophenone (0.300 g, 2 mmol, 1 equiv.) and benzyl bromide (2 mmol, 0.342 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid, 1-(2-benzyl-4-methoxyphenyl)ethan-1-one (0.45g, 93%), with a boiling point of 202 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.62 – 7.52 (m, 1H), 7.46 – 7.39 (m, 2H), 7.40 – 7.36 (m, 2H), 7.36 – 7.32 (m, 1H), 7.01 – 6.96 (m, 1H), 6.20 (s, 1H), 4.53 (s, 3H), 3.97 (s, 3H), 2.59 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.8, 150.4, 146.6, 137.80, 130.2, 129.0, 128.8, 128.4, 124.0, 113.8, 109.7, 56.0, 33.6, 26.2. **HRMS** (ESI-TOF) calculated for $C_{16}H_{16}O_2$ $[M]^+$ 240.1145, found 240.1140.



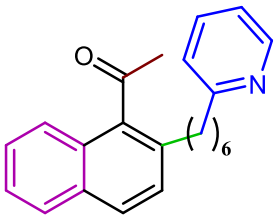
3u

1-(2-(6-(pyridin-2-yl)hexyl)thiophen-3-yl)ethan-1-one (3u): General procedure as stated above was followed for the synthesis of **3u** from 3-acetylthiophene (0.252 g, 2 mmol, 1 equiv.) and 2-(bromohexyl)pyridine (2 mmol, 0.394 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution 5%,10%, 15% ethyl acetate in hexanes) and a yellow liquid of 1-(2-(6-(pyridin-2-yl)hexyl)thiophen-3-yl) ethan-1-one was obtained (0.50g, 86%) with a boiling point of 242 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.31 (dd, *J* = 4.7, 1.5 Hz, 1H), 7.54 – 7.47 (m, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.25 – 7.15 (m, 1H), 6.96 (d, *J* = 5.7 Hz, 1H), 6.74 (d, J = 5.7 Hz, 1H), 3.35 (t, *J* = 6.9 Hz, 2H), 2.57 – 2.41 (m, 2H), 2.11 (s, 3H), 1.87 – 1.71 (m, 2H), 1.57 – 1.45 (m, 1H), 1.36 (dd, *J* = 14.6, 6.9 Hz, 1H), 1.24 (dd, *J* = 6.7, 2.9 Hz, 2H), 0.86 – 0.80 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 206.6, 150.1, 142.22, 139.1, 138.4, 128.2, 127.8, 124.2, 122.5, 121.9, 33.9, 32.7, 31.5, 30.9, 30.8, 29.5, 28.8, 27.8, 22.5, 14.0, 13.9. **HRMS** (ESI-TOF) calculated for $C_{17}H_{21}NOS$ $[M+Na]^+$ 310.1236, found 310.1230.



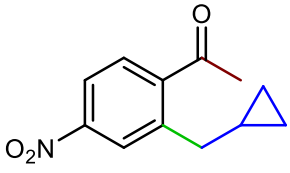
3v

1-(2-(6-(pyridin-2-yl) hexyl) phenyl) ethan-1-one (3v): General procedure as stated above was followed for the synthesis of **3v** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and 2-(bromohexyl)pyridine (2 mmol, 0.394 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution 5%,10%, 15% ethyl acetate in hexanes) and a yellow liquid of 1-(2-(6-(pyridin-2-yl)hexyl)phenyl)ethan-1-one was obtained (0.49g, 86%) with a boiling point of 245 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.63 (dd, *J* = 7.9, 0.9 Hz, 2H), 7.48 (dd, *J* = 7.6, 1.7 Hz, 2H), 7.38 (td, *J* = 7.5, 1.1 Hz, 2H), 7.34 – 7.28 (m, 2H), 3.42 (t, *J* = 6.9 Hz, 2H), 2.65 (s, 3H), 1.93 – 1.80 (m, 2H), 1.49 – 1.40 (m, 2H), 1.36 – 1.25 (m, 4H), 0.91 (t, *J* = 6.9 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.3, 141.5, 133.8, 131.8, 128.2, 127.8, 118.9, 33.9, 32.7, 31.5, 30.9, 27.8, 22,4, 13.9. **HRMS** (ESI-TOF) calculated for $C_{19}H_{23}NO$ $[M]^+$ 281.1779, found 281.1777.



3w

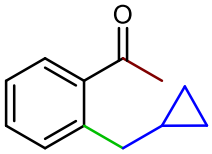
1-(2-(6-(pyridin-2-yl)hexyl)naphthalen-1-yl)ethan-1-one (3w): General procedure as stated above was followed for the synthesis of **3w** from 1'-Acetonapthone (0.340 g, 2 mmol, 1 equiv.) and 2-(6-bromohexyl)pyridine (2 mmol, 0.394 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution 5%,10%, 15% ethyl acetate in hexanes) and a yellow liquid of 1-(2-(6-(pyridin-2-yl)hexyl)naphthalen-1-yl)ethan-1-one was obtained (0.54g, 82%) with a boiling point of 248 ℃. R_f = 0.26; TLC in 5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.77 (d, *J* = 8.6 Hz, 1H), 8.41 (dd, *J* = 4.8, 1.6 Hz, 1H), 8.02 (d, *J* = 8.2 Hz, 1H), 7.96 (d, *J* = 7.2 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.70 – 7.60 (m, 2H), 7.60 – 7.46 (m, 2H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.24 (dd, *J* = 7.4, 4.9 Hz, 1H), 3.42 (t, *J* = 6.9 Hz, 2H), 2.77 (s, 3H), 1.88 (dd, *J* = 14.5, 7.3 Hz, 2H), 1.45 (dt, *J* = 14.7, 7.4 Hz, 3H), 1.36 – 1.27 (m, 3H), 0.92 (t, *J* = 6.8 Hz, 2H).**^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.8, 151.61, 149.8, 138.7, 135.4, 133.9, 133.0, 130.1, 128.6, 128.4, 128.0, 126.4, 126.0, 124.4, 124.3, 122.2, 34.0, 32.8, 30.9, 29.9, 27.8, 22.4, 13.9. **HRMS** (ESI-TOF) calculated for $C_{23}H_{25}NO$ $[M+K]^+$ 370.1936, found 370.1621.



3x

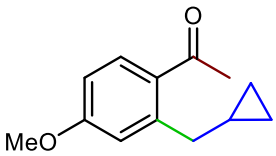
1-(2-(cyclopropylmethyl)-4-nitrophenyl)ethan-1-one (3x): General procedure as stated above was followed for the synthesis of **3x** from 4-nitroacetophenone (0.330 g, 2 mmol, 1 equiv.) and (chloromethyl)cyclopropane (2 mmol, 0.180 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution 5%, 10%, 15% ethyl acetate in hexanes) and a yellow solid of 1-(2-(cyclopropylmethyl)-4-nitrophenyl)ethan-1-one was obtained (0.37g, 84%) with a melting point of 157 ℃. R_f = 0.28; TLC in 5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.00 (d, *J* = 2.1 Hz, 1H), 7.50 (dd, *J* = 8.2, 2.2 Hz, 1H),

7.32 (d, *J* = 8.2 Hz, 1H), 3.46 (d, *J* = 7.4 Hz, 2H), 2.59 (s, 3H), 1.25 (tt, *J* = 7.7, 4.8 Hz, 1H), 0.77 – 0.61 (m, 2H), 0.37 (q, *J* = 4.8 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.2, 149.9, 141.3, 136.69, 136.1, 129.3, 123.8, 50.7, 26.9, 13.8, 5.7. **HRMS** (ESI-TOF) calculated for $C_{12}H_{13}NO_3$ $[M+H]^+$ 220.0895, found 220.0915.



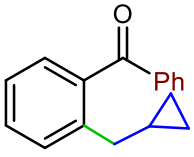
3y

1-(2-(cyclopropylmethyl) phenyl) ethan-1-one (3y): General procedure as stated above was followed for the synthesis of **3y** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and (bromomethyl)cyclopropane (2 mmol, 0.180 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution with 2.5% and 5% hexanes), yielding a yellow, oily liquid of 1-(2-cyclopropylphenyl)ethan-1-one (0.33g, 94%), with a boiling point of 250 ℃. R_f = 0.23; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.62 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.48 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.38 (td, *J* = 7.5, 1.2 Hz, 1H), 7.32 (dd, *J* = 7.8, 1.8 Hz, 1H), 3.44 (d, *J* = 7.4 Hz, 2H), 2.64 (s, 3H), 1.24 (m, 1H), 0.75 – 0.64 (m, 2H), 0.40 – 0.31 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): 201.2, 141.4, 133.8, 131.7, 128.9, 127.4, 118.8, 50.6, 34.9, 30.3, 13.8, 5.7. **HRMS** (ESI-TOF) calculated for $C_{12}H_{14}O$ $[M+H]^+$ 174.1044, found 174.1030.



3z

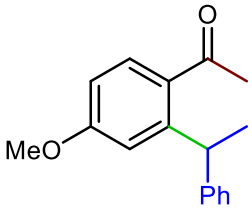
1-(2-(cyclopropylmethyl)-4-methoxyphenyl)ethan-1-one (3z): General procedure as stated above was followed for the synthesis of **3z** from 4-methoxyacetophenone (0.300 g, 2 mmol, 1 equiv.) and (chloromethyl)cyclopropane (2 mmol, 0.180 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-(cyclopropylmethyl)-4-methoxyphenyl)ethan-1-one (0.34g, 85%) with a boiling point of 211 ℃. R_f = 0.5; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 8.3 Hz, 1H), 6.99 – 6.98 (dd, *J* = 7.2, 2.4 Hz, 1H), 6.14 (s, 1H), 3.96 (s, 3H), 3.44 (d, *J* = 7.4 Hz, 2H), 2.64 (s, 3H), 1.24 (m, 1H), 0.75 – 0.64 (m, 2H), 0.40 – 0.31 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): 196.7, 150.3, 146.6, 130.2, 123.9, 113.7, 109.7, 56.0, 50.6, 26.1, 13.8, 5.7. **HRMS** (ESI-TOF) calculated for $C_{13}H_{16}O_2$ $[M]^+$ 204.1150, found 204.1130.



3aa

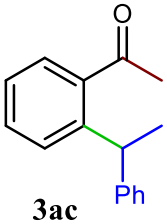
(2(cyclopropylmethyl)phenyl)(phenyl)methanone (3aa): General procedure as stated above was followed for the synthesis of **3aa** from benzophenone (0.364 g, 2 mmol, 1 equiv.) and 2-Chloro-2-methyl cyclopropane (2 mmol, 0.180 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, 10% ethyl acetate in hexanes), yielding a brown solid of (2(cyclopropylmethyl)phenyl)(phenyl)methanone (0.39g, 85%) with a melting point of 90 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.80 – 7.71 (m, 2H), 7.69 – 7.64 (m, 2H), 7.64 – 7.60 (m, 2H), 7.60 – 7.55 (m, 2H), 7.47 (dd, *J* = 10.6, 4.6 Hz, 1H), 3.46 (d, *J* = 7.4 Hz, 2H), 2.59 (s, 3H), 1.25 (tt, *J* =

7.7, 4.8 Hz, 1H), 0.77 – 0.61 (m, 2H), 0.37 (q, *J* = 4.8 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 195.3, 137.1, 136.3, 132.5, 131.5, 131.50, 129.8, 128.3, 127.3, 50.5, 34.9, 13.7, 5.68 **HRMS** (ESI-TOF) calculated for $C_{17}H_{16}O$ $[M+H]^+$ 236.1201, found 236.1197.



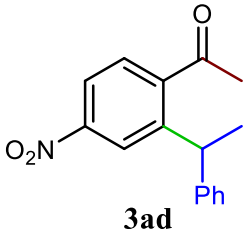
3ab

1-(4-methoxy-2-(1-phenylethyl)phenyl)ethan-1-one (3ab): General procedure as stated above was followed for the synthesis of **3ab** from 4-methoxyacetophenone (0.300 g, 2 mmol, 1 equiv.) and (1-chloroethyl)benzene (2 mmol, 0.281 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 5%, 10%, 15% ethyl acetate in hexanes), yielding a yellow liquid of 1-(4-methoxy-2-(1-phenylethyl)phenyl)ethan-1-one (0.46g, 91%) with a boiling point of 220 ℃. R_f = 0.2; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 2.5 Hz, 1H), 7.49 – 7.43 (m, 2H), 7.39 (t, *J* = 4.3 Hz, 2H), 7.36 – 7.32 (m, 1H), 6.99 (d, *J* = 8.7 Hz, 1H), 6.20 (s, 1H), 5.13 (q, *J* = 6.8 Hz, 1H), 3.97 (s, 3H), 2.59 (s, 3H), 1.89 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.8, 150.4, 146.6, 142.8, 130.2, 128.6, 128.2, 126.5, 124.0, 113.8, 109.7, 58.8, 56.0, 26.5, 26.2. **HRMS** (ESI-TOF) calculated for $C_{17}H_{18}O_2$ $[M+H]^+$ 254.1307, found 254.1308.



3ac

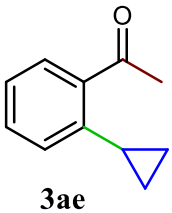
1-(2-(1-phenylethyl)phenyl)ethan-1-one (3ac): General procedure as stated above was followed for the synthesis of **3ac** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and (1-chloroethyl)benzene (2 mmol, 0.281 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution with 2.5% and 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-(1-phenylethyl)phenyl)ethan-1-one (0.43g, 95%) with a boiling point of 215 ℃. R_f = 0.40; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.65 (dd, *J* = 7.2, 3.3 Hz, 1H), 7.65 – 7.57 (m, 1H), 7.54 – 7.49 (m, 1H), 7.47 (m, 2H), 7.43 – 7.38 (m, 2H), 7.37 – 7.32 (m, 2H), 5.14 (q, *J* = 6.8 Hz, 1H), 2.64 (s, 3H), 1.90 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.3, 142.8, 141.4, 133.8, 131.8, 128.9, 128.6, 127.4, 126.5, 118.9, 58.7, 30.3, 26.5. **HRMS** (ESI-TOF) calculated for $C_{16}H_{16}O$ $[M+H]^+$ 225.1201, found 225.1241,



3ad

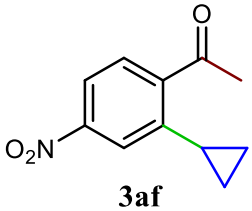
1-(4-nitro-2-(1-phenylethyl)phenyl)ethan-1-one (3ad): General procedure as stated above was followed for the synthesis of **3ad** from 4-nitroacetophenone (0.330 g, 2 mmol, 1 equiv.) and (1-chloroethyl)benzene (2 mmol, 0.281 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 5%, 10%, 15% ethyl acetate in hexanes), yielding a yellow liquid of 1-(4-nitro-2-(1-phenylethyl)phenyl)ethan-1-one (0.47g, 87%) with a boiling point of 210 ℃. R_f = 0.26; TLC in 5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.02 (d, *J* = 2.1 Hz, 1H), 7.50 – 7.43 (m, 2H), 7.40 (dd, *J* = 9.9, 4.8 Hz, 3H), 7.37 – 7.31 (m, 2H), 5.14 (q, *J* = 6.8 Hz, 1H), 2.61 (s, 3H), 1.90 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (101 MHz,

$CDCl_3$): δ 196.2, 150.4, 146.6, 142.8, 130.2, 128.6, 128.2, 126.5, 124.0, 113.8, 109.7, 58.8, 27.01, 26.6. **HRMS** (ESI-TOF) calculated for $C_{16}H_{15}NO_3$ $[M+H]^+$ 270.1052, found 270.1122.



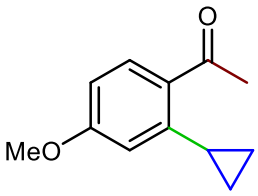
3ae

1-(2-cyclopropylphenyl) ethan-1-one (3ae): General procedure as stated above was followed for the synthesis of **3ae** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and bromocyclopropane (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow, oily liquid of 1-(2-cyclopropylphenyl)ethan-1-one (0.35g, 94%) with a boiling point of 228 ℃. R_f = 0.43; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.63 (dd, *J* = 7.9, 0.7 Hz, 1H), 7.48 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.38 (td, *J* = 7.5, 1.0 Hz, 1H), 7.33 – 7.27 (m, 1H), 2.92 – 2.83 (m, 1H), 2.64 (s, 3H), 1.02 – 0.95 (m, 2H), 0.90 – 0.85 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.2, 141.4, 133.8, 131.7, 128.9, 127.4, 118.8, 30.3, 14.3, 9.0. **HRMS** (ESI-TOF) calculated for $C_{11}H_{12}O$ $[M+Na]^+$ 183.0888, found 183.0882.



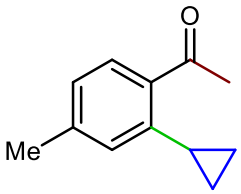
3af

1-(2-cyclopropyl-4-nitrophenyl) ethan-1-one (3af): General procedure as stated above was followed for the synthesis of **3af** from 4-nitroacetophenone (0.330 g, 2 mmol, 1 equiv.) and bromocyclopropane (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, 10% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-cyclopropyl-4-nitrophenyl)ethan-1-one (0.34g, 84%) with a boiling point of 231 ℃. R_f = 0.48; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.00 (d, *J* = 2.1 Hz, 1H), 7.50 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.32 (d, *J* = 8.2 Hz, 1H), 2.96 – 2.83 (m, 1H), 2.60 (s, 3H), 1.03 – 0.96 (m, 2H), 0.91 – 0.86 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.7, 150.4, 146.6, 130.2, 123.9, 113.7, 109.7, 56.0, 26.1, 14.3, 9.0. **HRMS** (ESI-TOF) calculated for $C_{11}H_{11}NO_3$ $[M+H]^+$: 206.0739; found: 206.1016.



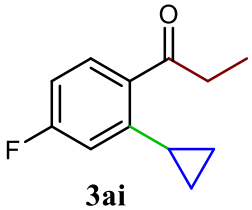
3ag

1-(2-cyclopropyl-4-methoxyphenyl) ethan-1-one (3ag): General procedure as stated above was followed for the synthesis of **3ag** from 4-methoxyacetophenone (0.300 g, 2 mmol, 1 equiv.) and bromocyclopropane (2 mmol, 0.241g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-cyclopropyl-4-methoxyphenyl)ethan-1-one (0.34g, 91%) with a boiling point of 185 ℃. R_f = 0.6; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.3 Hz, 1H), 6.97 (d, *J* = 8.7 Hz, 1H), 6.11 (s, 1H), 3.91 (s, 3H), 2.86 (td, *J* = 7.1, 3.6 Hz, 1H), 2.63 (s, 3H), 1.03 – 0.94 (m, 2H), 0.90 – 0.81 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.7, 150.4, 146.6, 130.2, 123.9, 113.7, 109.7, 56.0, 26.1, 14.3, 9.0. **HRMS** (ESI-TOF) calculated for $C_{12}H_{14}O_2$ $[M+H]^+$: 190.0994; found: 190.0986.



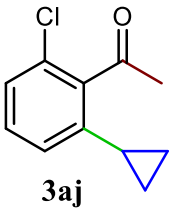
3ah

1-(2-cyclopropyl-4-methylphenyl) ethan-1-one (3ah): General procedure as stated above was followed for the synthesis of **3ah** from 4-methylacetophenone (0.268 g, 2 mmol, 1 equiv.) and bromocyclopropane (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-cyclopropyl-4-methylphenyl)ethan-1-one (0.33g, 94%) with a boiling point of 218 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.3 Hz, 1H), 6.97 (d, *J* = 8.7 Hz, 1H), 6.11 (s, 1H), 3.91 (s, 3H), 3.00 – 2.82 (m, 2H), 2.51 (s, 3H), 1.07 – 0.97 (m, 3H), 0.93 – 0.81 (m, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.7, 150.4, 146.6, 130.2, 123.9, 113.7, 109.7, 56.0, 26.1, 14.34, 9.0. **HRMS** (ESI-TOF) calculated for $C_{12}H_{14}O$ $[M+H]^+$ 174.1045, found 174.1039.



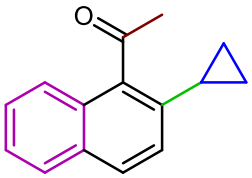
3ai

1-(2-cyclopropyl-4-fluorophenyl)propan-1-one (3ai): General procedure as stated above was followed for the synthesis of **3ai** from 4-fluoropropiophenone (0.304 g, 2 mmol, 1 equiv.) and bromocyclopropane (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-cyclopropyl-4-fluorophenyl)propane-1-one (0.40g, 90%) with a boiling point of 244 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.10 – 7.90 (m, 2H), 7.22 – 7.06 (m, 1H), 2.99 (q, *J* = 7.2 Hz, 2H), 2.91 – 2.83 (m, 1H), 1.27 – 1.20 (m, 3H), 1.02 – 0.94 (m, 2H), 0.92 – 0.85 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 199.1, 165.6(d, $J_{(C-F)}$ = 254.2 Hz), 133.3 (d, $J_{(C-F)}$ = 3.0 Hz), 130.5 (d, $J_{(C-F)}$ = 9.3 Hz), 130.5, 115.7, 115.4, 31.7, 14.3, 9.0, 8.2. **^{19}F NMR** (377 MHz, $CDCl_3$) δ -105.70 – -105.96 (m). **HRMS** (ESI-TOF) calculated for $C_{12}H_{13}FO$ $[M]^+$ 192.0950, found 192.0944.



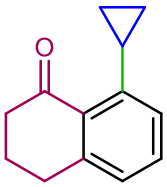
3aj

1-(2-chloro-6-cyclopropylphenyl) ethan-1-one (3aj): General procedure as stated above was followed for the synthesis of **3aj** from 2-chloroacetophenone (0.309 g, 2 mmol, 1 equiv.) and bromocyclopropane (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-chloro-6-cyclopropylphenyl)ethan-1-one (0.34g, 87%) with a boiling point of 165 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.61 (t, *J* = 9.9 Hz, 1H), 7.48 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.35 – 7.28 (m, 1H), 2.92 – 2.83 (m, 1H), 2.64 (s, 3H), 1.02 – 0.95 (m, 2H), 0.90 – 0.85 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.2, 141.4, 133.8, 131.7, 128.9, 127.4, 118.8, 30.3, 14.3, 9.0. **HRMS** (ESI-TOF) calculated for $C_{11}H_{11}ClO$ $[M+H]^+$ 194.0448, found 194.1170.



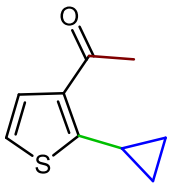
3ak

1-(2-cyclopropylnaphthalen-1-yl)ethan-1-one (3ak): General procedure as stated above was followed for the synthesis of **3ak** from 1'-acetonaphthone (0.340 g, 2 mmol, 1 equiv.) and bromocyclopropane (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-cyclopropylnaphthalen-1-yl)ethan-1-one (0.40g, 92%) with a boiling point of 246 ℃. R_f = 0.61; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.78 (d, *J* = 8.6 Hz, 1H), 8.00 (t, *J* = 10.3 Hz, 1H), 7.98 – 7.91 (m, 1H), 7.91 (t, *J* = 7.7 Hz, 1H), 7.66 – 7.56 (m, 1H), 7.59 – 7.46 (m, 1H), 2.95 – 2.81 (m, 1H), 2.77 (s, 3H), 1.08 – 0.95 (m, 2H), 0.93 – 0.78 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.8, 135.4, 133.9, 133.0, 130.1, 128.6, 128.4, 128.0, 126.4, 126.0, 124.3, 30.0, 14.4, 9.0. **HRMS** (ESI-TOF) calculated for $C_{15}H_{14}O$ $[M+H]^+$ 211.1044, found 211.1118.



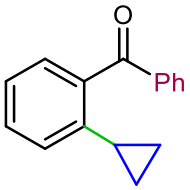
3al

8-cyclopropyl-3,4-dihydronaphthalen-1(2*H*)-one (3al): General procedure as stated above was followed for the synthesis of **3al** from α-tetralone (0.292 g, 2 mmol, 1 equiv.) and bromocyclopropane (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid of 8-cyclopropyl-3,4-dihydronaphthalen-1 (2H)-one (0.33g, 89%) with a boiling point of 185 ℃. R_f = 0.48; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.04 (d, *J* = 7.8 Hz, 1H), 7.47 (m, 1H), 7.33 – 7.26 (m, 1H), 2.95 – 2.81 (m, 1H), 2.97 (t, *J* = 6.1 Hz, 2H), 2.73 – 2.62 (m, 2H), 2.15 (dt, *J* = 12.7, 6.4 Hz, 2H), 1.08 – 0.95 (m, 2H), 0.93 – 0.78 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 198.3, 144.4, 133.3, 132.6, 128.7, 127.1, 126.6, 39.1, 29.7, 23.3, 14.3, 9.0. **HRMS** (ESI-TOF) calculated for $C_{13}H_{14}O$ $[M+H]^+$ 187.1045, found 187.0842.



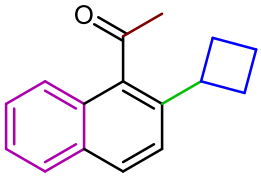
3am

1-(2-cyclopropylthiophen-3-yl)ethan-1-one (3 am): General procedure as stated above was followed for the synthesis of **3am** from 3-acetylthiophene (0.252 g, 2 mmol, 1 equiv.) and bromocyclopropane (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 5%, 10%, 15% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-cyclopropylthiophen-3-yl)ethan-1-one (0.29g, 87%) with a boiling point of 189 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 3.6 Hz, 1H), 7.26 (d, *J* = 3.6 Hz, 1H), 2.94 – 2.78 (m, 1H), 2.17 (s, 3H), 1.02 – 0.96 (m, 2H), 0.93 – 0.81 (m, 2H).**^{13}C NMR** (101 MHz, $CDCl_3$): δ 206.9, 152.0, 141.5, 121.1, 30.9, 14.3, 9.0. **HRMS** (ESI-TOF) calculated for $C_9H_{10}OS$ $[M+H]^+$: 167.2380; found: 167.0705.



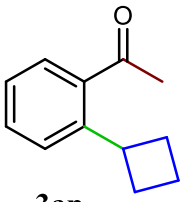
3an

(2-cyclopropylphenyl)(phenyl)methanone (3an): General procedure as stated above was followed for the synthesis of **3an** from benzophenone (0.364 g, 2 mmol, 1 equiv.) and bromocyclopropane (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 5%, 10%, 15% ethyl acetate in hexanes), and a brown solid of (2-cyclopropylphenyl)(phenyl)methanone (0.43g, 84%) was obtained, with a melting point of 90 ℃. R_f = 0.26; TLC in 5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.80 – 7.71 (m, 2H), 7.69 – 7.64 (m, 2H), 7.64 – 7.60 (m, 2H), 7.60 – 7.55 (m, 2H), 7.47 (dd, *J* = 10.6, 4.6 Hz, 1H), 2.94 – 2.78 (m, 1H), 1.02 – 0.96 (m, 2H), 0.93 – 0.81 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 195.5, 137.1, 136.3, 132.6, 131.6, 131.5, 129.9, 128.4, 127.4, 14.3, 9.0. **HRMS** (ESI-TOF) calculated for $C_{16}H_{14}O$ $[M+H]^+$ 225.1201, found 225.1941.



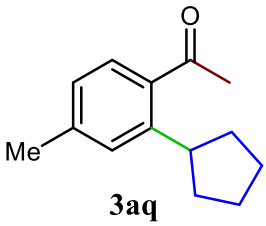
3ao

1-(2-cyclobutylnaphthalen-1-yl)ethan-1-one (3ao): General procedure as stated above was followed for the synthesis of **3ao** from 1'-acetonaphthone (0.340 g, 2 mmol, 1 equiv.) and bromocyclobutane (2 mmol, 0.267 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, 15% ethyl acetate in hexanes) as a yellow liquid, and 1-(2-cyclobutylnaphthalen-1-yl)ethan-1-one (0.42g, 85%) was obtained, with a boiling point of 257 ℃. R_f = 0.52; (TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.62 (d, *J* = 8.4 Hz, 1H), 8.15 (dd, *J* = 7.8, 2.7 Hz, 2H), 8.04 – 7.97 (m, 1H), 7.68 – 7.55 (m, 2H), 3.55 (m,1H), 2.73 (s, 3H), 2.59 – 2.41 (m, 1H), 1.29 – 1.06 (m, 1H), 0.65 – 0.57 (m, 2H), 0.36 – 0.27 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 202.2, 135.3, 133.9, 133.2, 129.8, 129.6, 128.9, 128.3, 126.8, 125.9, 125.3, 51.3, 30.5, 14.1, 6.1. **HRMS** (ESI-TOF) calculated for $C_{16}H_{16}O$ $[M+Na]^+$ 247.1201, found 247.1095.



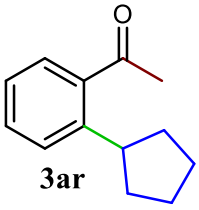
3ap

1-(2-cyclobutylphenyl) ethan-1-one (3ap): General procedure as stated above was followed for the synthesis of **3ap** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and bromocyclobutane (2 mmol, 0.267 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-cyclobutylphenyl)ethan-1-one (0.30g, 85%) with a boiling point of 228 ℃. R_f = 0.32; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.63 (dd, *J* = 7.9, 0.7 Hz, 1H), 7.48 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.38 (td, *J* = 7.5, 1.0 Hz, 1H), 7.33 – 7.27 (m, 1H), 3.45 – 3.43 (m, 1H), 2.64 (s, 3H), 0.90 – 0.85 (m, 2H), 0.65 – 0.57 (m, 2H), 0.36 – 0.27 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.2, 141.4, 133.8, 131.7, 128.9, 127.4, 118.8, 30.3, 14.3, 9.0. **HRMS** (ESI-TOF) calculated for $C_{12}H_{14}O$ $[M+H]^+$ 174.1509, found 174.1569.



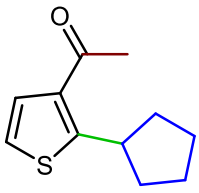
3aq

1-(2-cyclopentyl-4-methylphenyl) ethan-1-one (3aq): General procedure as stated above was followed for the synthesis of **3aq** from 4-methylacetophenone (0.268 g, 2 mmol, 1 equiv.) and chlorocyclopentane (2 mmol, 0.209 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow, oily liquid of 1-(2-cyclopentyl-4-methylphenyl)ethan-1-one (0.39g, 95%) with a boiling point of 233 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.19 (s, 1H), 7.12 (d, *J* = 7.7 Hz, 1H), 6.98 (d, *J* = 2.7 Hz, 1H), 4.51 – 4.43 (m, 1H), 2.35 (s, 3H), 2.32 (s, 3H), 2.15 – 2.05 (m, 4H), 1.98 – 1.87 (m, 2H), 1.76 – 1.60 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 200.9, 136.9, 133.9, 132.7, 130.6, 129.5, 127.3, 53.7, 37.8, 23.23, 20.6, 19.5. **HRMS** (ESI-TOF) calculated for $C_{14}H_{18}O$ $[M+H]^+$ 203.1358, found 203.0517.



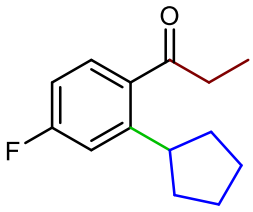
3ar

1-(2-cyclopentylphenyl)ethan-1-one (3ar): General procedure as stated above was followed for the synthesis of **3ar** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and chlorocyclopentane (2 mmol, 0.209 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow, oily liquid of 1-(2-cyclopentylphenyl)ethan-1-one (0.34g, 90%) with a boiling point of 232 ℃. R_f = 0.52; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.61 (d, *J* = 7.9 Hz, 1H), 7.48 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.38 (td, *J* = 7.5, 0.9 Hz, 1H), 7.35 – 7.28 (m, 1H), 4.49 – 4.43 (m, 1H), 2.64 (s, 3H), 2.12 – 2.04 (m, 4H), 1.95 – 1.86 (m, 2H), 1.72 – 1.60 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.3, 141.4, 133.8, 131.7, 128.9, 127.4, 118.9, 53.7, 37.8, 30.3, 23.2. **HRMS** (ESI-TOF) calculated for $C_{13}H_{16}O$ $[M+H]^+$ 190.1201, found 190.0466.



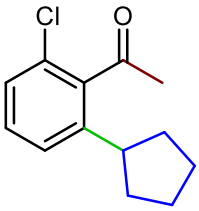
3as

1-(2-cyclopentylthiophen-3-yl)ethan-1-one (3as): General procedure as stated above was followed for the synthesis of **3as** from 3-acetylthiophene (0.252 g, 2 mmol, 1 equiv.) and chlorocyclopentane (2 mmol, 0.209 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 5%, 10%, 15% ethyl acetate in hexanes), and a yellow liquid, 1-(2-cyclopentylthiophen-3-yl)ethan-1-one (0.35g, 85%), was obtained, boiling at 132 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, DMSO-d_6): δ 7.76 (d, *J* = 3.6 Hz, 1H), 7.70 (d, *J* = 3.6 Hz, 1H), 4.52 (dq, *J* = 8.9, 3.0 Hz, 1H), 2.09 (s, 3H), 2.01 (ddd, *J* = 17.1, 11.6, 5.9 Hz, 2H), 1.85 – 1.70 (m, 4H), 1.62 (td, *J* = 7.1, 3.1 Hz, 2H).**^{13}C NMR** (101 MHz, DMSO-d_6): δ 207.0, 150.9, 142.1, 124.1, 63.1, 37.0, 31.1, 22.9. **HRMS** (ESI-TOF) calculated for $C_{11}H_{14}OS$ $[M+H]^+$ 194.0229, found 194.0229.



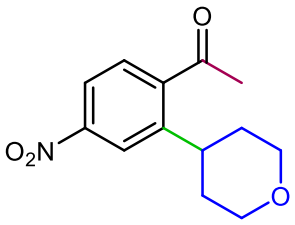
3at

1-(2-cyclopentyl-4-fluorophenyl) propan-1-one (3at): General procedure as stated above was followed for the synthesis of **3at** from 4-fluoropropiophenone (0.304 g, 2 mmol, 1 equiv.) and chlorocyclopentane (2 mmol, 0.209 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow, oily liquid of 1-(2-cyclopentyl-4-fluorophenyl)propan-1-one (0.37g, 84%) with a boiling point of 245 °C. R_f = 0.34; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.03 – 8.00 (m, 1H), 8.01 – 7.97 (m, 1H), 7.13 (t, *J* = 8.7 Hz, 1H), 4.54 – 4.24 (m, 1H), 2.99 (q, *J* = 7.2 Hz, 2H), 2.06 – 1.97 (m, 4H), 1.92 – 1.76 (m, 2H), 1.71 – 1.55 (m, 2H), 1.23 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 199.1, 166.8, 164.3, 133.3 (d, $J_{(C-F)}$ = 3.0 Hz), 130.5 (d, $J_{(C-F)}$ = 9.2 Hz), 115.6, 115.4, 62.0, 37.0, 31.6, 22.9. **HRMS** (ESI-TOF) calculated for $C_{14}H_{17}FO$ $[M+H]^+$ 220.1263, found 220.0940.



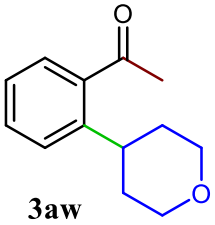
3au

1-(2-chloro-6-cyclopentylphenyl)ethan-1-one (3au): General procedure as stated above was followed for the synthesis of **3au** from 2-chloroacetophenone (0.309 g, 2 mmol, 1 equiv.) and chlorocyclopentane (2 mmol, 0.209 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow, oily liquid of 1-(2-chloro-6-cyclopentylphenyl)ethan-1-one (0.42g, 86%) with a boiling point of 185 °C. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.61 (t, *J* = 9.9 Hz, 1H), 7.48 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.35 – 7.28 (m, 1H), 4.49 – 4.43 (m, 2H), 2.64 (s, 3H), 2.12 – 2.04 (m, 7H), 1.95 – 1.86 (m, 3H), 1.72 – 1.60 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.3, 141.4, 133.8, 131.7, 128.9, 127.4, 118.9, 77.3, 77.0, 76.7, 53.7, 37.8, 30.3, 23.2. **HRMS** (ESI-TOF) calculated for $C_{13}H_{15}ClO$ $[M+H]^+$ 223.0811, found 223.0840.



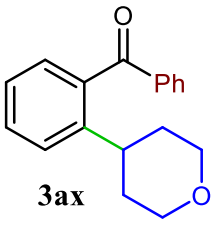
3av

1-(4-nitro-2-(tetrahydro-2*H*-pyran-4-yl)phenyl)ethan-1-one (3av): General procedure as stated above was followed for the synthesis of **3av** from 4-nitroacetophenone (0.330 g, 2 mmol, 1 equiv.) and chlorotetrahydro-2*H*-pyran (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, 10% ethyl acetate in hexanes), yielding a yellow solid of 1-(4-nitro-2-(tetrahydro-2H-pyran-4-yl)phenyl)ethan-1-one (0.44g, 88%) with a melting point of 251 °C. R_f = 0.44; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 2.1 Hz, 1H), 7.49 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.31 (d, *J* = 8.2 Hz, 1H), 4.29 – 4.18 (m, 1H), 4.01 – 3.93 (m, 2H), 3.54 (ddd, *J* = 11.6, 8.5, 3.0 Hz, 2H), 2.59 (s, 3H), 2.11 (ddd, *J* = 12.6, 4.8, 3.1 Hz, 2H), 1.96 – 1.80 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.8, 150.6, 146.7, 130.0, 123.9, 113.9, 109.8, 65.5, 56.0, 55.7, 36.1, 26.1. **HRMS** (ESI-TOF) calculated for $C_{13}H_{15}NO_4$ $[M+H]^+$: 250.1001; found: 250.0248.



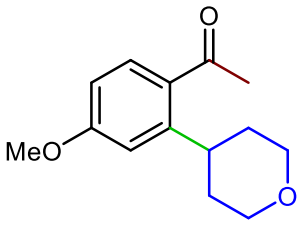
3aw

1-(2-(tetrahydro-2*H*-pyran-4-yl) phenyl) ethan-1-one (3aw): General procedure as stated above was followed for the synthesis of **3aw** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and 4-chlorotetrahydro-2*H*-pyran (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-(tetrahydro-2H-pyran-4-yl)phenyl)ethan-1-one (0.38g, 94%) with a boiling point of 182 ℃. R_f = 0.63; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.63 (dd, *J* = 7.9, 0.8 Hz, 1H), 7.48 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.38 (td, *J* = 7.5, 1.0 Hz, 1H), 7.33 – 7.29 (m, 1H), 4.22 (dt, *J* = 12.7, 4.2 Hz, 1H), 4.00 – 3.92 (m, 2H), 3.53 (ddd, *J* = 11.6, 8.5, 3.0 Hz, 2H), 2.64 (s, 3H), 2.17 – 2.07 (m, 2H), 1.95 – 1.81 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.3, 141.4, 133.8, 131.7, 128.9, 127.4, 118.9, 65.6, 55.8, 36.2, 30.3. **HRMS** (ESI-TOF) calculated for $C_{13}H_{16}O_2$ $[M+H]^+$ 205.1150, found 205.1125.



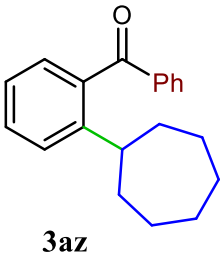
3ax

Phenyl (2-(tetrahydro-2*H*-pyran-4-yl)phenyl)methanone (3ax): General procedure as stated above was followed for the synthesis of **3ax** from benzophenone (0.364 g, 2 mmol, 1 equiv.) and 4-chlorotetrahydro-2*H*-pyran (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, ethyl acetate in hexanes), yielding a yellow liquid of phenyl(2-(tetrahydro-2H-pyran-4-yl)phenyl)methanone (0.45g, 86%) with a boiling point of 236 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.79 – 7.75 (m, 2H), 7.70 – 7.65 (m, 2H), 7.65 – 7.61 (m, 2H), 7.59 (d, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 4.20 (dt, *J* = 12.7, 4.2 Hz, 1H), 4.01 – 3.89 (m, 2H), 3.51 (ddd, *J* = 11.6, 8.5, 3.0 Hz, 2H), 2.17 – 2.04 (m, 2H), 1.92 – 1.80 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 195.5, 137.1, 136.3, 132.6, 131.5, 131.5, 129.9, 128.3, 127.4, 65.5, 55.8, 36.2. **HRMS** (ESI-TOF) calculated for $C_{18}H_{18}O_2$ $[M+H]^+$ 267.1307, found 267.0158.



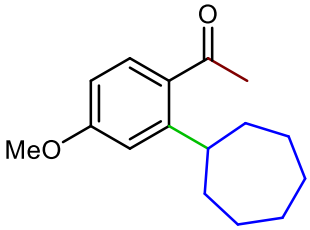
3ay

1-(4-methoxy-2-(tetrahydro-2*H*-pyran-4-yl) phenyl) ethan-1-one (3ay): General procedure as stated above was followed for the synthesis of **3ay** from 4-methoxyacetophenone (0.300 g, 2 mmol, 1 equiv.) and 4-chlorotetrahydro-2*H*-pyran (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, ethyl acetate in hexanes), and a white solid of 1-(4-methoxy-2-(tetrahydro-2H-pyran-4-yl)phenyl)ethan-1-one (0.41g, 92%) was obtained, with a melting point of 118 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.53 (dd, *J* = 8.2, 2.4 Hz, 2H), 6.92 (s, 1H), 4.24 – 4.14 (m, 2H), 4.03 – 3.87 (m, 3H), 3.56 – 3.44 (m, 1H), 2.55 (s, 3H), 2.12 – 2.05 (m, 2H), 1.93 – 1.81 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.8, 150.6, 146.7, 130.0, 123.9, 113.9, 109.8, 65.5, 56.0, 55.7, 36.1, 26.4. **HRMS** (ESI-TOF) calculated for $C_{14}H_{18}O_3$ $[M+H]^+$ 225.1201, found 225.1941.



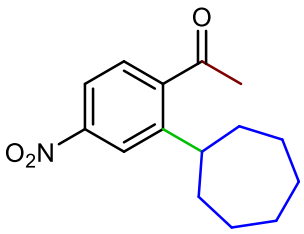
3az

(2-cycloheptylphenyl)(phenyl)methanone (3az): General procedure as stated above was followed for the synthesis of **3az** from benzophenone (0.364 g, 2 mmol, 1 equiv.) and chlorocyclohepatane (2 mmol, 0.264g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, ethyl acetate in hexanes), yielding a yellow liquid of (2-cycloheptylphenyl)(phenyl)methanone (0.48g, 86%) with a boiling point of 213 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.79 – 7.75 (m, 2H), 7.70 – 7.65 (m, 2H), 7.65 – 7.61 (m, 2H), 7.59 (d, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 4.20 (dt, *J* = 12.7, 4.2 Hz, 1H), 4.01 – 3.89 (m, 2H), 3.51 (ddd, *J* = 11.6, 8.5, 3.0 Hz, 2H), 2.17 – 2.04 (m, 2H), 1.92 – 1.80 (m, 2H), 1.78 – 1.69 (m, 2H), 1.63 – 1.54 (m, 3H), 1.52 – 1.38 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 195.5, 137.1, 136.0, 132.64, 131.5, 131.5, 129.9, 128.3, 127.4, 63.0, 38.9, 27.6, 23.8. **HRMS** (ESI-TOF) calculated for $C_{20}H_{22}O$ $[M+H]^+$ 279.3950, found 279.0876.



3ba

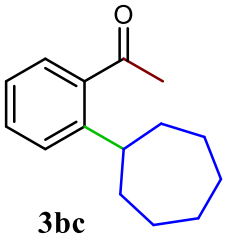
1-(2-cycloheptyl-4-methoxyphenyl)ethan-1-one (3ba): General procedure as stated above was followed for the synthesis of **3ba** from 4-methoxyacetophenone (0.300 g, 2 mmol, 1 equiv.) and chlorocyclohepatane (2 mmol, 0.264 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), and a light-yellow liquid of 1-(2-cycloheptyl-4-methoxyphenyl)ethan-1-one (0.45g, 91%) was obtained, with a boiling point of 205 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 8.3, 1H), 6.96 (d, *J* = 8.7 Hz, 1H), 6.25 (s, 1H), 4.18 (m, 1H), 3.96 (s, 3H), 2.57 (s, 3H), 2.23 – 2.11 (m, 2H), 1.91 (m, 2H), 1.78 – 1.69 (m, 2H), 1.63 – 1.54 (m, 3H), 1.52 – 1.38 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.8, 150.4, 146.6, 130.1, 124.0, 113.8, 109.7, 63.0, 56.0, 38.9, 27.6, 26.1, 23.8. **HRMS** (ESI-TOF) calculated for $C_{16}H_{22}O_2$ $[M+H]^+$ 246.1001, found 246.9936.



3bb

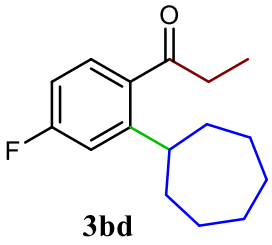
1-(2-cycloheptyl-4-nitrophenyl)ethan-1-one (3bb): General procedure as stated above was followed for the synthesis of **3bb** from 4-nitroacetophenone (0.330 g, 2 mmol, 1 equiv.) and chlorocyclohepatane (2 mmol, 0.264 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), and a light-yellow liquid of 1-(2-cycloheptyl-4-nitrophenyl)ethan-1-one (0.47g, 91%) was obtained with a boiling point of 221℃. R_f = 0.25; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 2.1 Hz, 1H), 7.49 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.31 (d, *J* = 8.2 Hz, 1H), 4.19 (tt, *J* = 8.6, 4.3 Hz, 1H), 2.59 (s, 3H), 2.16 (ddd, *J* = 12.7, 7.9, 3.9 Hz, 2H), 1.99 – 1.83 (m, 2H), 1.82 – 1.68 (m, 2H), 1.62 – 1.56 (m, 4H), 1.51 – 1.37 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.8, 150.4, 146.6, 130.1, 124.0, 113.8,

109.7, 63.0, 56.0, 38.9, 27.6, 26.1, 23.8. **HRMS** (ESI-TOF) calculated for $C_{15}H_{19}NO_3$ $[M+H]^+$ 262.3210, found 262.2516.



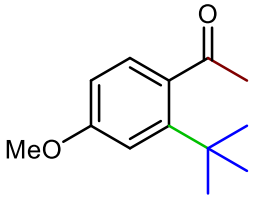
3bc

1-(2-cycloheptylphenyl) ethan-1-one (3bc): General procedure as stated above was followed for the synthesis of **3bc** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and chlorocyclohepatane (2 mmol, 0.264 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-cycloheptylphenyl)ethan-1-one (0.41g, 95%) with a boiling point of 226 ℃. R_f = 0.43; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.58 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.45 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.34 (td, *J* = 7.5, 1.2 Hz, 1H), 7.27 (td, *J* = 7.7, 1.8 Hz, 1H), 4.77 – 3.89 (m, 1H), 2.60 (s, 3H), 2.22 – 2.02 (m, 2H), 1.95 – 1.80 (m, 2H), 1.75 – 1.64 (m, 2H), 1.60 – 1.50 (m, 4H), 1.47 – 1.36 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.1, 141.4, 133.8, 131.7, 128.9, 127.4, 118.8, 63.0, 38.8, 30.2, 27.6, 23.7. **HRMS** (ESI-TOF) calculated for $C_{15}H_{20}O$ $[M+H]^+$ 215.1514, found 215.0822.



3bd

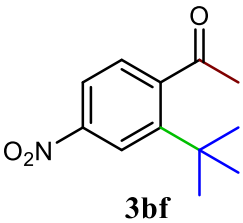
1-(2-cycloheptyl-4-fluorophenyl) propan-1-one (3bd): General procedure as stated above was followed for the synthesis of **3bd** from 4-fluoropropiophenone (0.304 g, 2 mmol, 1 equiv.) and chlorocyclohepatane (2 mmol, 0.264 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, ethyl acetate in hexanes), and a pale-yellow liquid of 1-(2-cycloheptyl-4-fluorophenyl) propan-1-one (0.48g, 86%) was obtained, with a boiling point of 240 ℃. R_f = 0.25; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.03 – 8.00 (m, 1H), 7.99 (s, 1H), 7.14 (t, *J* = 8.7 Hz, 1H), 4.18 (tt, *J* = 8.6, 4.3 Hz, 1H), 2.99 (q, *J* = 7.2 Hz, 2H), 2.21 – 2.12 (m, 2H), 1.98 – 1.86 (m, 2H), 1.78 – 1.69 (m, 2H), 1.61 – 1.55 (m, 4H), 1.50 – 1.41 (m, 2H), 1.23 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 199.1, 165.61 (d, $J_{(C-F)}$ = 254.2 Hz), 133.33 (d, $J_{(C-F)}$ = 3.0 Hz), 130.55 (d, $J_{(C-F)}$ = 9.2 Hz), 115.60 (d, $J_{(C-F)}$ = 21.8 Hz), 115.7, 63.1, 38.9, 31.7, 27.6, 23.8. **HRMS** (ESI-TOF) calculated for $C_{16}H_{21}FO$ $[M+H]^+$: 250.1576; found: 250.0248.



3be

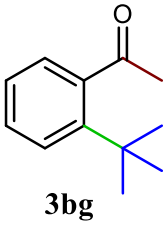
1-(2-(*tert*-butyl)-4-methoxyphenyl)ethan-1-one (3be): General procedure as stated above was followed for the synthesis of **3be** from 4-methoxyacetophenone (0.300 g, 2 mmol, 1 equiv.) and 2-Chloro-2-methylpropane (2 mmol, 0.185 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-(tert-butyl)-4-methoxyphenyl) ethanone (0.37g, 92%) with a boiling point of 245 ℃. R_f = 0.41; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.3 Hz, 1H), 6.97 (d, *J* = 8.7 Hz, 1H), 6.11 (s, 1H), 3.97 (s, 3H), 2.58 (s, 3H), 1.64 (s,

9H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.7, 150.3, 146.6, 130.2, 123.9, 113.7, 109.6, 67.4, 56.0, 34.4, 26.1. **HRMS** (ESI-TOF) calculated for $C_{13}H_{18}O_2$ $[M+H]^+$ 206.1307, found 206.1299.



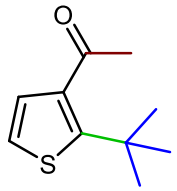
3bf

1-(2-(*tert*-butyl)-4-nitrophenyl)ethan-1-one (3bf): General procedure as stated above was followed for the synthesis of **3bf** from 4-nitroacetophenone (0.330 g, 2 mmol, 1 equiv.) and 2-Chloro-2-methylpropane (2 mmol, 0.185 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, 15% ethyl acetate in hexanes), yielding a yellow solid of 1-(2-(tert-butyl)-4-nitrophenyl)ethan-1-one (0.34g, 84%) with a melting point of 156 ℃. R_f = 0.30; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.50 (dd, *J* = 8.2, 2.2 Hz, 1H), 6.98 (d, *J* = 8.2 Hz, 1H), 6.10 (s, 1H), 3.97 (s, 3H), 2.58 (s, 3H), 1.64 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.7, 150.3, 146.6, 130.2, 123.9, 113.7, 109.6, 56.0, 34.4, 26.1. **HRMS** (ESI-TOF) calculated for $C_{12}H_{15}NO_3$ $[M+H]^+$ 221.2560, found 221.1095.



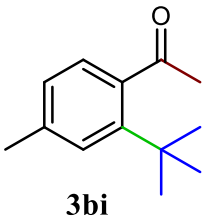
3bg

1-(2-(tert-butyl) phenyl) ethan-1-one (3bg): General procedure as stated above was followed for the synthesis of **3bg** from acetophenone (0.240 g, 2 mmol, 1 equiv.) and 2-chloro-2-methyl propane (2 mmol, 0.184 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-(tert-butyl)phenyl)ethan-1-one (0.33g, 92%) with a boiling point of 226 ℃. R_f = 0.5; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.61 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.47 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.37 (td, *J* = 7.5, 1.2 Hz, 1H), 7.29 (td, *J* = 7.7, 1.8 Hz, 1H), 2.63 (s, 3H), 1.62 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.2, 141.4, 133.8, 131.7, 128.9, 127.4, 118.8, 67.4, 34.4, 30.3. **HRMS** (ESI-TOF) calculated for $C_{12}H_{16}O$ $[M+H]^+$ 178.1201, found 178.1305.



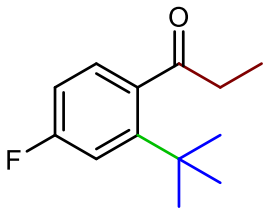
3bh

1-(2-(tert-butyl)thiophen-3-yl)ethan-1-one **(3bh):** *General procedure as* stated above was followed for the synthesis of **3bh** from 1-(thiophen-3-yl)ethan-1-one (0.252 g, 2 mmol, 1 equiv.) and 2-chloro-2-methyl propane (2 mmol, 0.184 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), and an oily liquid, 1-(2-(tert-butyl)thiophen-3-yl)ethan-1-one (0.30g, 85%), was obtained with a boiling point of 245 ℃. R_f = 0.43; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.59 (d, *J* = 3.6 Hz, 1H), 7.26 (d, *J* = 3.6 Hz, 1H), 2.18 (s, 3H), 1.63 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 206.9, 152.0, 141.6, 121.1, 34.4, 30.9. **HRMS** (ESI-TOF) calculated for $C_{10}H_{14}OS$ $[M+H]^+$ 183.0765, found 183.0823.



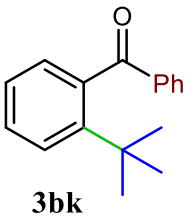
3bi

1-(2-(*tert*-butyl)-4-methylphenyl)ethan-1-one (3bi): General procedure as stated above was followed for the synthesis of **3bi** from 4-methylacetophenone (0.268 g, 2 mmol, 1 equiv.) and 2-Chloro-2-methylpropane (2 mmol, 0.185 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5% to 5% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-(tert-butyl)-4-methylphenyl)ethan-1-one (0.32g, 85%) with a boiling point of 245 ℃. R_f = 0.41; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, DMSO): δ 7.22 (s, 1H), 7.20 (s, 1H), 7.04 (d, *J* = 7.6 Hz, 1H), 2.27 (s, 3H), 2.26 (s, 3H), 1.60 (s, 3H).**^{13}C NMR** (101 MHz, DMSO): δ 198.4, 137.5, 133.3, 132.5, 131.3, 129.5, 128.2, 34.5, 20.6, 19.5. **HRMS** (ESI-TOF) calculated for $C_{13}H_{18}O$ $[M+H]^+$ 190.1358, found 190.1466.



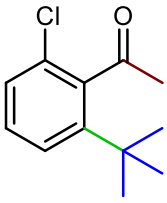
3bj

1-(2-(*tert*-butyl)-4-fluorophenyl)propan-1-one (3bj): General procedure as stated above was followed for the synthesis of **3bj** from 4-fluoropropiophenone (0.304 g, 2 mmol, 1 equiv.) and 2-chloro-2-methyl propane (2 mmol, 0.185 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 5%, 10%, 15% ethyl acetate in hexanes), and a yellow liquid, 1-(2-(tert-butyl)-4-fluorophenyl)propan-1-one (0.34g, 87%), was obtained with a boiling point of 257 ℃. R_f = 0.52; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.04 – 8.01 (m, 1H), 8.01 – 7.98 (m, 1H), 7.14 (t, *J* = 8.6 Hz, 1H), 3.00 (q, *J* = 7.2 Hz, 2H), 1.64 (s, 9H), 1.24 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 199.1, 165.62 (d, $J_{(C-F)}$ = 254.2 Hz), 133.3 (d, $J_{(C-F)}$ = 3.0 Hz), 130.5 (d, $J_{(C-F)}$ = 9.3 Hz), 115.7, 115.5, 34.4, 31.7, 8.2. **^{19}F NMR** (377 MHz, $CDCl_3$) δ -105.45 – -106.17 (m). **HRMS** (ESI-TOF) calculated for $C_{12}H_{15}FO$ $[M+H]^+$ 194.011, found 194.1101.



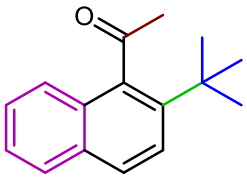
3bk

(2-(*tert*-butyl)phenyl)(phenyl)methanone (3bk): General procedure as stated above was followed for the synthesis of **3bk** from benzophenone (0.364 g, 2 mmol, 1 equiv.) and 2-chloro-2-methyl propane (2 mmol, 0.185 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, 10% ethyl acetate in hexanes), yielding a yellow liquid of (2-(tert-butyl)phenyl)(phenyl)methanone (0.40g, 83%) with a boiling point of 125 ℃. R_f = 0.52; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.83 – 7.76 (m, 2H), 7.73 – 7.68 (m, 2H), 7.67 – 7.65 (m, 1H), 7.65 – 7.60 (m, 2H), 7.54 – 7.48 (m, 2H), 1.62 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 195.3, 137.1, 136.8, 136.3, 133.2, 132.6, 131.6, 131.5, 129.9, 128.4, 127.5, 34.4, 30.3. **HRMS** (ESI-TOF) calculated for $C_{17}H_{18}O$ $[M+H]^+$ 238.3300, found 238.3303.



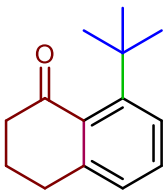
3bl

1-(2-(*tert*-butyl)-6-chlorophenyl)ethan-1-one (3bl): General procedure as stated above was followed for the synthesis of **3bl** from 2-chloroacetophenone (0.309 g, 2 mmol, 1 equiv.) and 2-methylpropane (2 mmol, 0.185 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 5%, 10%, 15% ethyl acetate in hexanes), yielding a yellow liquid of 1-(2-(tert-butyl)-6-chlorophenyl)ethan-1-one (0.30g, 80%) with a boiling point of 256 ℃. R_f = 0.26; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.61 (t, *J* = 9.9 Hz, 1H), 7.48 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.35 – 7.28 (m, 1H), 2.62 (s, 3H), 1.62 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.2, 141.4, 133.8, 131.7, 128.9, 127.4, 118.8, 67.4, 34.4, 30.3. **HRMS** (ESI-TOF) calculated for $C_{12}H_{15}ClO$ $[M+H]^+$ 225.1201, found 225.1221.



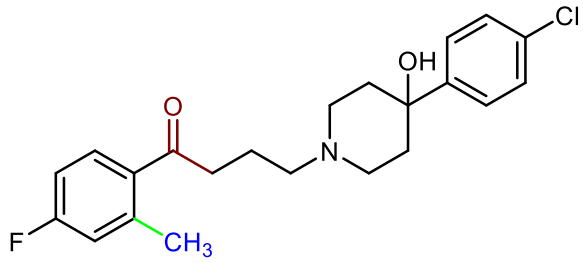
3bm

1-(2-(*tert*-butyl)naphthalen-1-yl)ethan-1-one (3bm): General procedure as stated above was followed for the synthesis of **3bm** from 1'-acetonaphthone (0.340 g, 2 mmol, 1 equiv.) and 2-chloro-2-methyl propane (2 mmol, 0.185 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 5%, 10%, 15% ethyl acetate in hexanes), and yellow liquid 1-(2-(tert-butyl)naphthalen-1-yl)etha-1-one (0.40g, 89%) was obtained, with a boiling point of 257 ℃. R_f = 0.52; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.78 (d, *J* = 8.6 Hz, 1H), 8.04 – 7.95 (m, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.63 (ddd, *J* = 8.5, 6.9, 1.4 Hz, 1H), 7.58 – 7.48 (m, 2H), 2.77 (s, 3H), 1.65 (s, 9H) **^{13}C NMR** (101 MHz, $CDCl_3$): δ 201.8, 135.4, 133.99, 133.0, 130.1, 128.6, 128.4, 128.0, 126.4, 126.0, 124.3, 67.5, 34.4, 30.0. **HRMS** (ESI-TOF) calculated for $C_{16}H_{18}O$ $[M+H]^+$ 227.1358, found 227.0902.



3bn

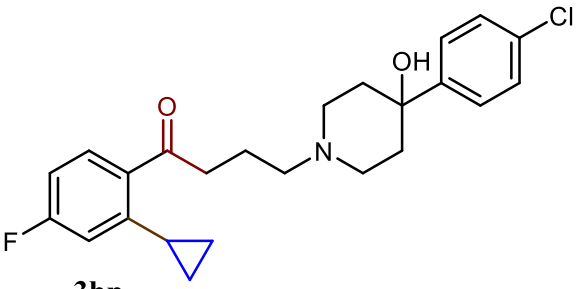
8-(*tert*-butyl)-3,4-dihydronaphthalen-1(2*H*)-one (3bn): General procedure as stated above was followed for the synthesis of **3bn** from α-tetralone (0.292 g, 2 mmol) and 2-chloro-2-methyl propane (2 mmol, 0.185 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution: 2.5%, 5%, 10% ethyl acetate in hexanes), yielding a yellow liquid of 8-(tert-butyl)-3,4-dihydronaphthalen-1-(2H)-one (0.39g, 85%) with a boiling point of 155 ℃. R_f = 0.60; TLC in 2.5% ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.04 (d, *J* = 7.8 Hz, 1H), 7.47 (m, 1H), 7.33 – 7.26 (m, 1H), 2.97 (t, *J* = 6.1 Hz, 2H), 2.73 – 2.62 (m, 2H), 2.15 (dt, *J* = 12.7, 6.4 Hz, 2H), 1.63 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 198.3, 144.4, 133.3, 132.6, 128.7, 127.1, 126.6, 67.4, 39.1, 34.4, 29.7, 23.2. **HRMS** (ESI-TOF) calculated for $C_{14}H_{18}O$ $[M+H]^+$ 203.1358, found 203.1350.



3bo

4-(4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl)-1-(4-fluoro-2-methylphenyl)butan-1-one (3bo)

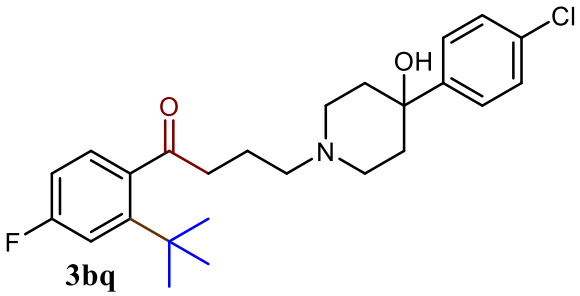
The general procedure stated above was followed for the synthesis of **3bo** from haloperidol (0.751 g, 2 mmol) and methyl iodide (2 mmol, 0.283 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution 2.5%, 5%, 10% ethyl acetate in hexanes) and a colourless solid of 4-(4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl)-1-(4-fluoro-2-methylphenyl)butan-1-one was obtained (0.61g, 79%) with melting point of 155 ℃. R_f = 0.60; TLC in 5%, 10 % ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): 7.91 (m , 2H), 7.53 (dt, *J* = 23.5, 11.8 Hz, 2H), 7.27 (d, *J* = 9.3 Hz, 1H), 7.08 (dd, *J* = 26.6, 18.3 Hz, 2H), 4.27 (s, 1H), 3.91 (t, *J* = 12.2 Hz, 1H), 3.60 (m, 4H), 3.37 – 3.10 (m, 4H), 3.22 – 2.89 (m, 1H), 2.17 (s, 3H), 2.07 – 1.81 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 196.8, 165.5 (d, $J_{(C-F)}$ = 254.3 Hz), 146.9, 133.7 (d, $J_{(C-F)}$ = 3.1 Hz), 132.7, 130.6 (d, $J_{(C-F)}$ = 9.2 Hz), 128.3, 126.0, 115.5 (d, $J_{(C-F)}$ = 21.8 Hz), 115.8, 77.4, 77.0, 76.7, 68.4, 68.3, 67.6, 57.6, 45.1, 34.4, 32.6, 16.7. **HRMS** (ESI-TOF) calculated for $C_{23}H_{26}O_2ClF$ $[M+H]^+$ 388.1838, found 388.1809.



3bp

4-(4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl)-1-(2-cyclopropyl-4-fluorophenyl)butan-1-one (3bp)

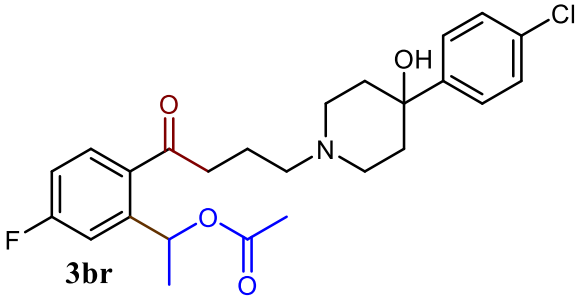
The general procedure stated above was followed for the synthesis of **3bp** from haloperidol (0.751 g, 2 mmol) and bromocyclopropane (2 mmol, 0.241 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution 2.5%, 5%, 10% ethyl acetate in hexanes) and colourless solid of 4-(4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl)-1-(2-cyclopropyl-4-fluorophenyl)butan-1-one was obtained (0.66g, 81%) with melting point of 187 ℃. R_f = 0.60; TLC in 5%, 10 % ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.03 (dd, *J* = 8.5, 5.6 Hz, 2H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.33 – 7.27 (m, 1H), 7.15 (t, *J* = 8.5 Hz, 2H), 3.00 (t, *J* = 7.0 Hz, 2H), 2.88 (tt, *J* = 7.3, 3.8 Hz, 1H), 2.80 (d, *J* = 11.5 Hz, 2H), 2.54 – 2.38 (m, 4H), 2.00 (dt, *J* = 14.1, 7.1 Hz, 4H), 1.68 (d, *J* = 12.5 Hz, 2H), 1.04 – 0.93 (m, 2H), 0.93 – 0.78 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 198.2, 165.5 (*d*, $J_{(C-F)}$ = 254.3 Hz), 146.9, 133.7 (d, $J_{(C-F)}$ = 3.1 Hz), 132.7, 130.6 (d, $J_{(C-F)}$ = 9.2 Hz), 128.3, 126.0, 115.5 (d, $J_{(C-F)}$ = 21.8 Hz) 71.0, 57.8, 49.3, 38.3, 36.2, 21.9, 14.3, 9.0, 1.0. **HRMS** (ESI-TOF) calculated for $C_{25}H_{28}O_2ClF$ $[M+H]^+$ 415.1835, found 415.1846.



3bq

1-(2-(tert-butyl)-4-fluorophenyl)-4-(4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl)butan-1-one (3bq)

The general procedure stated above was followed for the synthesis of **3bq** from haloperidol (0.751 g, 2 mmol) and *tert*-butyl chloride (2 mmol, 0.185 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution 2.5%, 5%, 10% ethyl acetate in hexanes) and colourless solid of 1-(2-(*tert*-butyl)-4-fluorophenyl)-4-(4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl)butan-1-one was obtained (0.70g, 80%) with melting point of 136 ℃. R_f = 0.60; TLC in 5%, 10 % ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.03 (dd, *J* = 8.4, 5.6 Hz, 2H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.36 – 7.25 (m, 1H), 7.15 (t, *J* = 8.5 Hz, 2H), 3.00 (t, *J* = 7.0 Hz, 2H), 2.81 (d, *J* = 11.3 Hz, 2H), 2.54 – 2.37 (m, 4H), 2.01 (dt, *J* = 13.1, 6.5 Hz, 4H), 1.64 (s, 9H), 1.28 (d, *J* = 5.2 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 198.2, 165.5 (d, $J_{(C-F)}$ = 254.3 Hz), 146.92, 133.7 (d, $J_{(C-F)}$ = 3.1 Hz), 132.7, 130.6 (d, $J_{(C-F)}$ = 9.2 Hz), 128.3, 126.0, 115.5 (d, $J_{(C-F)}$ = 21.8 Hz), 71.0, 67.4, 57.8, 49.3, 38.3, 36.2, 34.4, 21.8. **HRMS** (ESI-TOF) calculated for $C_{14}H_{18}O$ $[M+NH_4]^+$ 448.2413, found 448.2401.

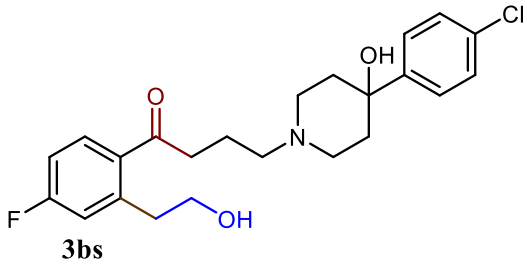


3br

1-(2-(4-(4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl)butanoyl)-5-fluorophenyl)ethyl acetate (3br)

General procedure as stated above was followed for the synthesis of **3br** from haloperidol (0.751 g, 2 mmol) and 2-bromo-methylpropionate (2 mmol, 0.334 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution 2.5%, 5%, 10% ethyl acetate in hexanes) and colourless solid of 1-(2-(4-(4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl)butanoyl)-5-fluorophenyl)ethyl acetate was obtained (0.77g, 78%) with melting point of 136 ℃. R_f = 0.60; TLC in 5%, 10 % ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.08 – 7.98 (m, 2H), 7.57 (dd, *J* = 21.0, 8.6 Hz, 1H), 7.45 – 7.39 (m, 1H), 7.34 – 7.28 (m, 2H), 7.18 – 7.11 (m, 2H), 4.71 (d, *J* = 7.5 Hz, 1H), 4.05 (s, 1H), 3.97 (d, *J* = 8.8 Hz, 1H), 3.92 (d, *J* = 7.8 Hz, 1H), 3.89 (s, 1H), 3.85 (s, 3H), 3.80 (s, 3H), 3.06 (dd, *J* = 15.2, 8.3 Hz, 3H), 2.72 (s, 2H), 2.25 (d, *J* = 14.8 Hz, 1H), 2.15 – 2.01 (m, 1H), 1.79 (d, *J* = 12.9 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 197.8, 167.7, 165.5 (d, $J_{(C-F)}$ = 254.3 Hz), 146.9, 133.7 (d, $J_{(C-F)}$ = 3.1 Hz), 132.7, 130.6 (d, $J_{(C-F)}$ = 9.2 Hz), 128.3, 126.0, 115.5 (d, $J_{(C-F)}$ = 21.8 Hz)., 115.6, 77.3, 77.0, 77.7, 67.9, 57.3, 53.1, 49.0, 37.3, 36.0, 25.5, 20.6.
HRMS (ESI-TOF) calculated for $C_{25}H_{29}ClFNO_4$ $[M]^+$: 461.9584; found: 461.9374.

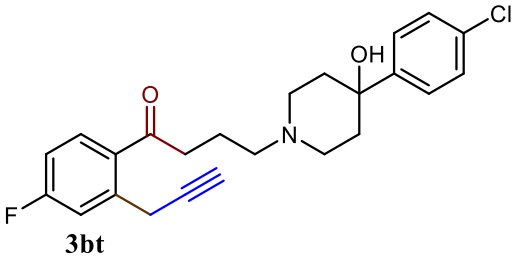
4-(4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl)-1-(4-fluoro-2-(2-hydroxyethyl)phenyl)butan-1-one (3bs)



3bs

The general procedure stated above was followed for the synthesis of **3bs** from haloperidol (0.751 g, 2 mmol) and 2-bromoethanol (2 mmol, 0.249 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution 2.5%, 5%, 10% ethyl acetate in hexanes) and a colourless solid of 4-(4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl)-1-(4-fluoro-2-(2-hydroxyethyl)phenyl)butan-1-one was obtained (0.79g, 76%) with melting point of 136 ℃. R_f = 0.60; TLC in 5%, 10 % ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$):) δ 8.06 – 7.99 (m, 2H), 7.45 – 7.38 (m, 2H), 7.34 – 7.29 (m, 1H), 7.15 (t, *J* = 8.6 Hz, 2H), 3.97 – 3.89 (m, 2H), 3.87 – 3.80 (m, 1H), 3.74 – 3.69 (m, 1H), 3.69 – 3.63 (m, 1H), 3.58 – 3.53 (m, 1H), 3.07 (t, *J* = 6.9 Hz, 2H), 2.68 (dd, *J* = 17.9, 10.2 Hz, 2H), 2.33 – 2.20 (m, 3H), 2.09 (dt, *J* = 14.1, 6.9 Hz, 2H), 1.77 (d, *J* = 12.2 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 198.2, 165.5 (d, $J_{(C-F)}$ = 254.3 Hz), 146.9, 133.7 (d, $J_{(C-F)}$ = 3.1 Hz), 132.7, 130.6 (d, $J_{(C-F)}$ = 9.2 Hz), 128.3, 126.0, 115.5 (d, $J_{(C-F)}$ = 21.8 Hz), 77.3, 77.2, 77.0, 76.7, 72.1, 70.9, 70.6, 67.0, 62.7, 61.6, 57.5, 49.2, 37.4, 36.0, 35.8, 29.5, 20.8.
HRMS (ESI-TOF) calculated for $C_{23}H_{27}ClFNO_3$ $[M]^+$ 419.9214, found 419.9013.

4-(4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl)-1-(2-ethynyl-4-fluorophenyl)butan-1-one (3bt)

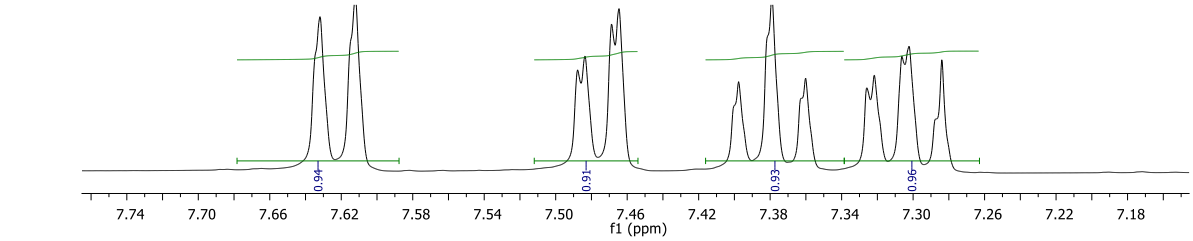


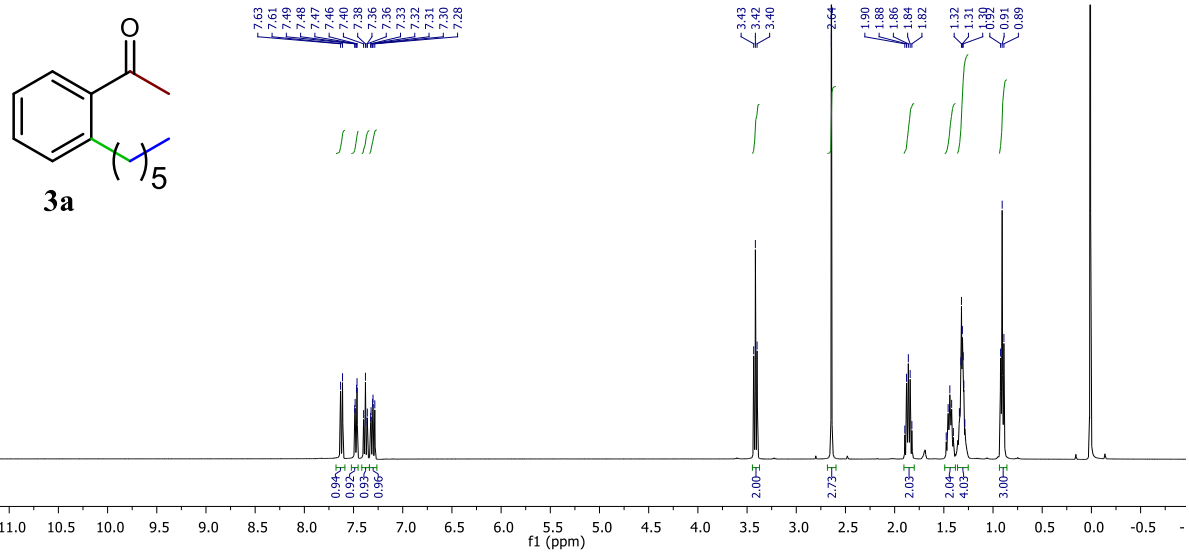
3bt

General procedure as stated above was followed for the synthesis of **3bq** from haloperidol (0.751 g, 2 mmol) and *tert*-butyl chloride (2 mmol, 0.209 g, 1 equiv.). The product was purified by column chromatography (silica gel, gradient elution 2.5%, 5%, 10% ethyl acetate in hexanes) and a colourless solid of 4-(4-(4-chlorophenyl)-4-hydroxypiperidin-1-yl)-1-(2-ethynyl-4-fluorophenyl)butan-1-one was obtained (0.70g, 78%) with a melting point of 136 ℃. R_f = 0.60; TLC in 5%, 10 % ethyl acetate in hexane with three runs and stained with 2,4-DNP. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.05 – 7.98 (m, 1H), 7.96 – 7.90 (m, 1H), 7.62 (d, *J* = 8.6 Hz, 1H), 7.55 (d, *J* = 8.6 Hz, 1H), 7.43 – 7.37 (m, 1H), 7.32 – 7.23 (m, 1H), 7.18 – 7.08 (m, 1H), 5.27 (d, *J* = 23.2 Hz, 1H), 4.66 (dd, *J* = 11.7, 1.7 Hz, 1H), 4.21 – 4.13 (m, 1H), 4.11 – 4.04 (m, 1H), 3.89 (d, *J* = 2.6 Hz, 1H), 3.80 – 3.61 (m, 1H), 3.29 (t, *J* = 6.0 Hz, 1H), 3.16 (t, *J* = 6.4 Hz, 1H), 3.03 (dt, *J* = 14.1, 4.6 Hz, 1H), 2.91 (t, *J* = 2.2 Hz, 1H), 2.54 (t, *J* = 2.6 Hz, 2H), 2.51 – 2.43 (m, 1H), 2.35 – 2.25 (m, 2H), 2.24 – 2.13 (m, 1H), 2.09 – 1.87 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ 197.0, 165.5 (d, $J_{(C-F)}$ = 254.3 Hz), 146.9, 133.3 (d, $J_{(C-F)}$ = 3.1 Hz), 132.7, 130.6 (d, $J_{(C-F)}$ = 9.2 Hz), 128.3, 126.0, 115.5 (d, $J_{(C-F)}$ = 21.8 Hz). 115.7, 115.5, 82.2, 81.7, 78.7, 77.3, 77.0, 76.7, 74.8, 70.8, 70.8, 68.2, 68.0, 64.6, 55.5, 55.1, 49.2, 36.1, 34.8, 34.4, 32.7, 32.4, 13.4.
HRMS (ESI-TOF) calculated for $C_{24}H_{25}ClFNO_2$ $[M]^+$ 413.9174, found 413.9051.

7. ^{1}H and ^{13}C NMR Spectra (3a-3bt)

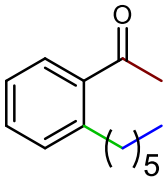
^{1}H NMR of 3a (400 MHz, 32 scans, RT, $CDCl_3$)



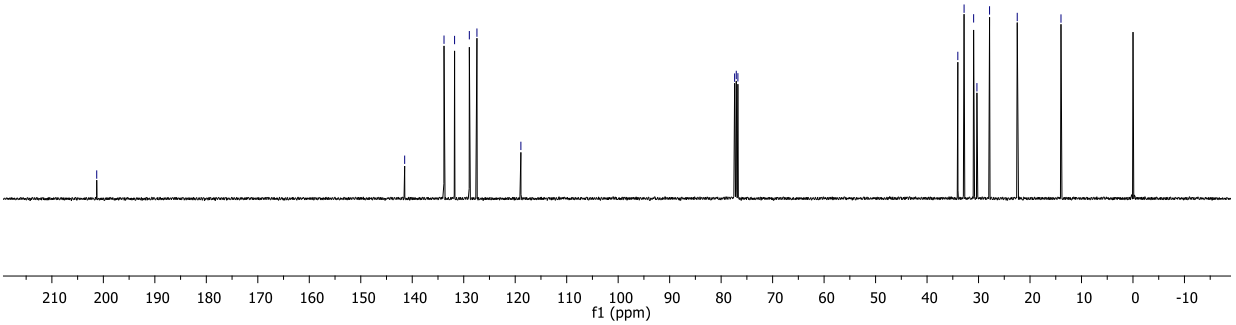


3a

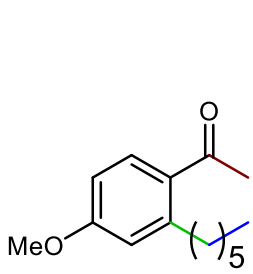
^{13}C NMR of 3a (101 MHz, 512 scans, RT, $CDCl_3$)



3a

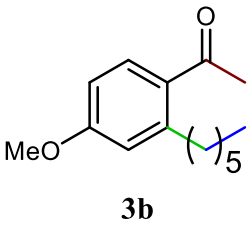


^{1}H NMR of 3b (400 MHz, 32 scans, RT, $CDCl_3$)



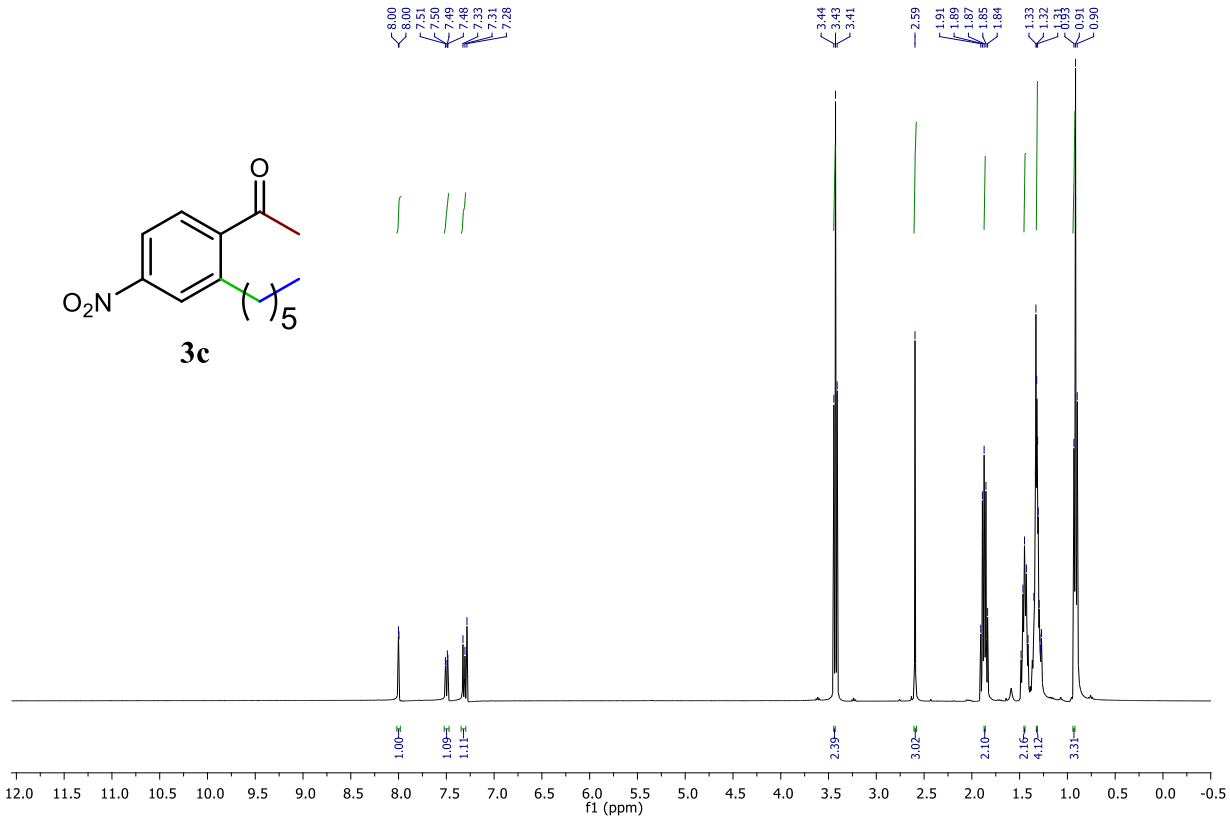
3b

^{13}C NMR of 3b (101 MHz, 512 scans, RT, $CDCl_3$)



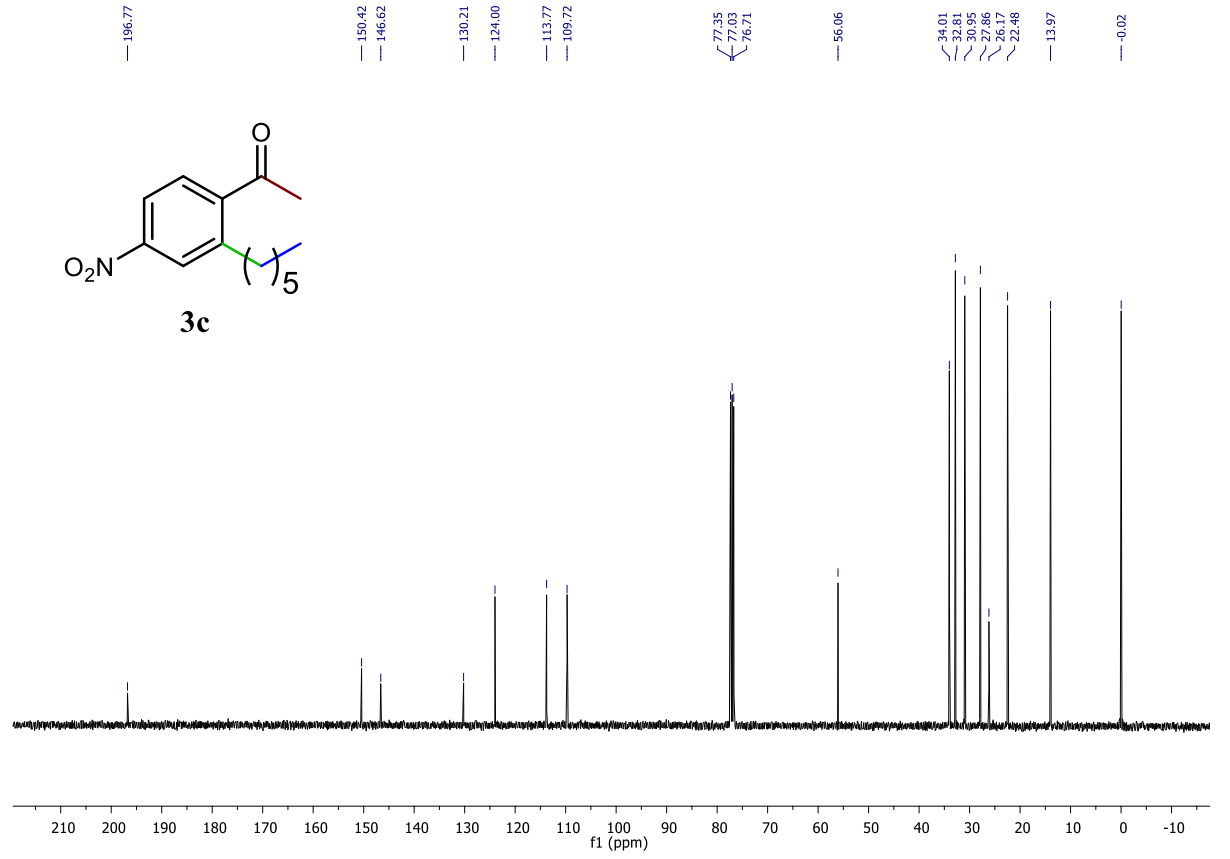
3b

^{1}H NMR of 3c (400 MHz, 32 scans, RT, $CDCl_3$)



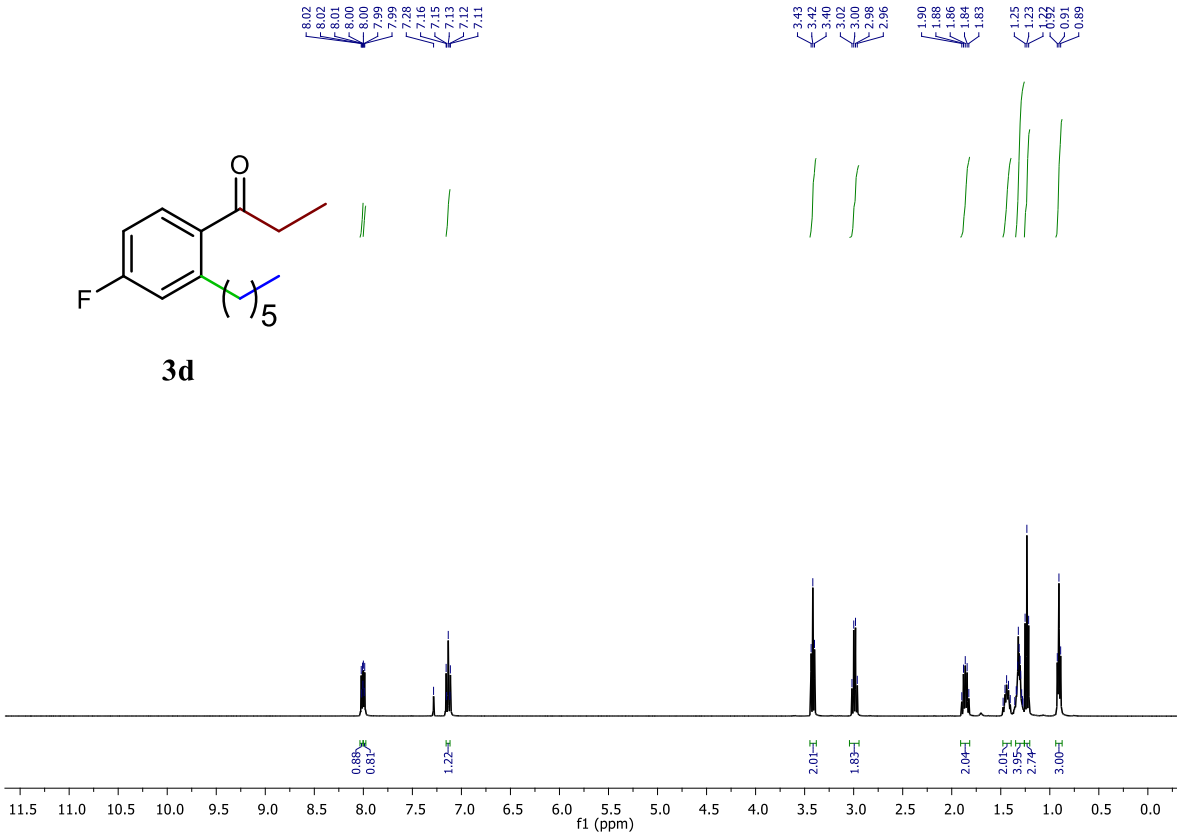
3c

^{13}C NMR of 3c (101 MHz, 512 scans, RT, $CDCl_3$)



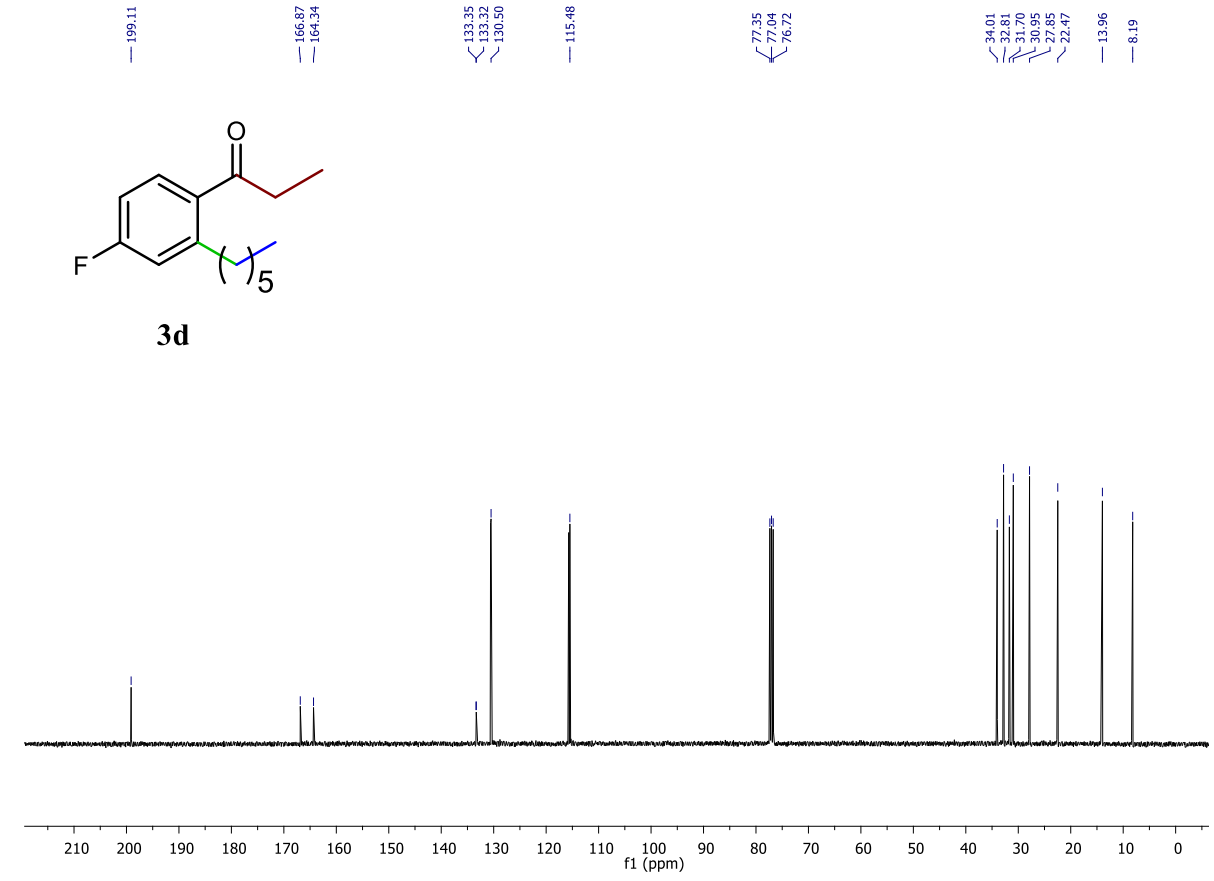
3c

^{1}H NMR of 3d (400 MHz, 32 scans, RT, $CDCl_3$)



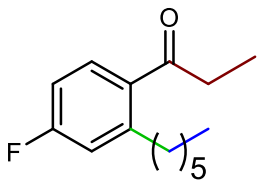
3d

^{13}C NMR of 3d (101 MHz, 512 scans, RT, $CDCl_3$)

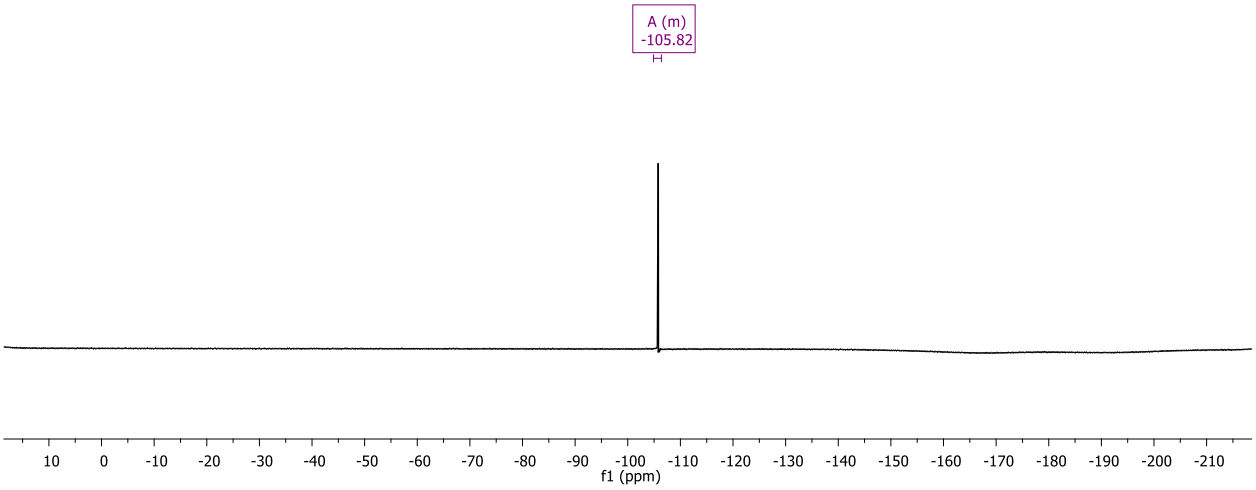


3d

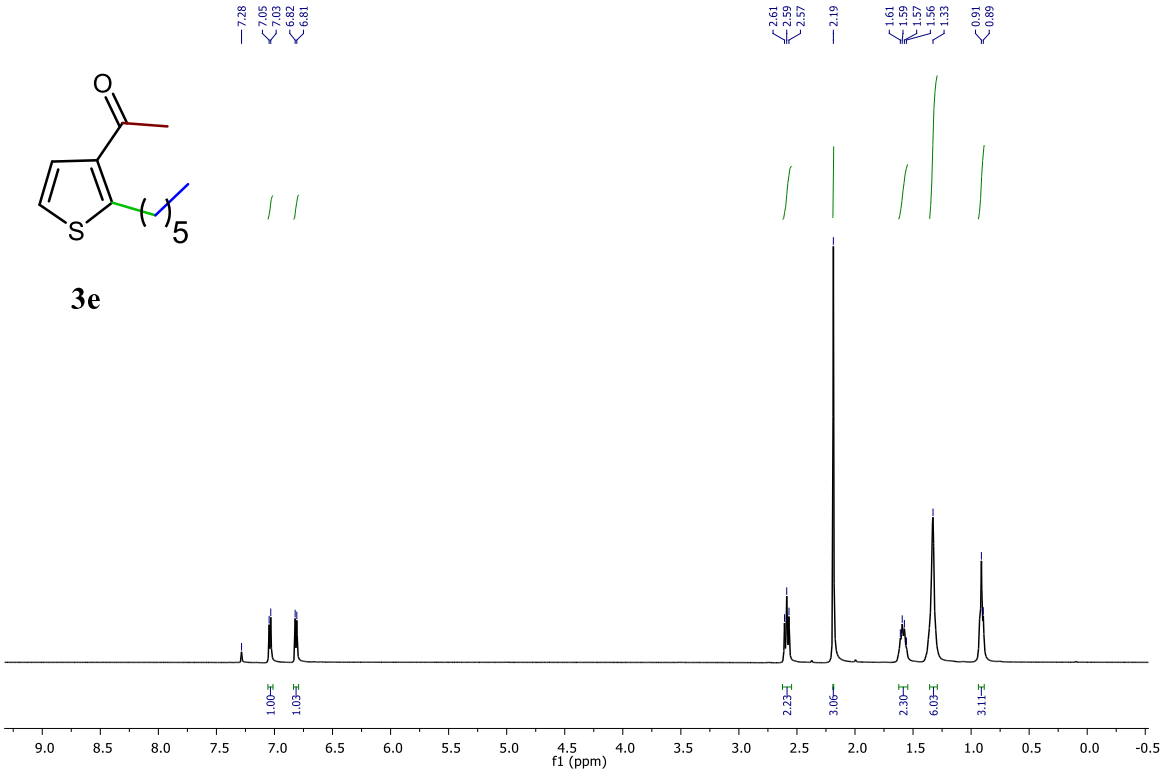
^{19}F NMR of **3d (377 MHz, RT, $CDCl_3$)**



3d

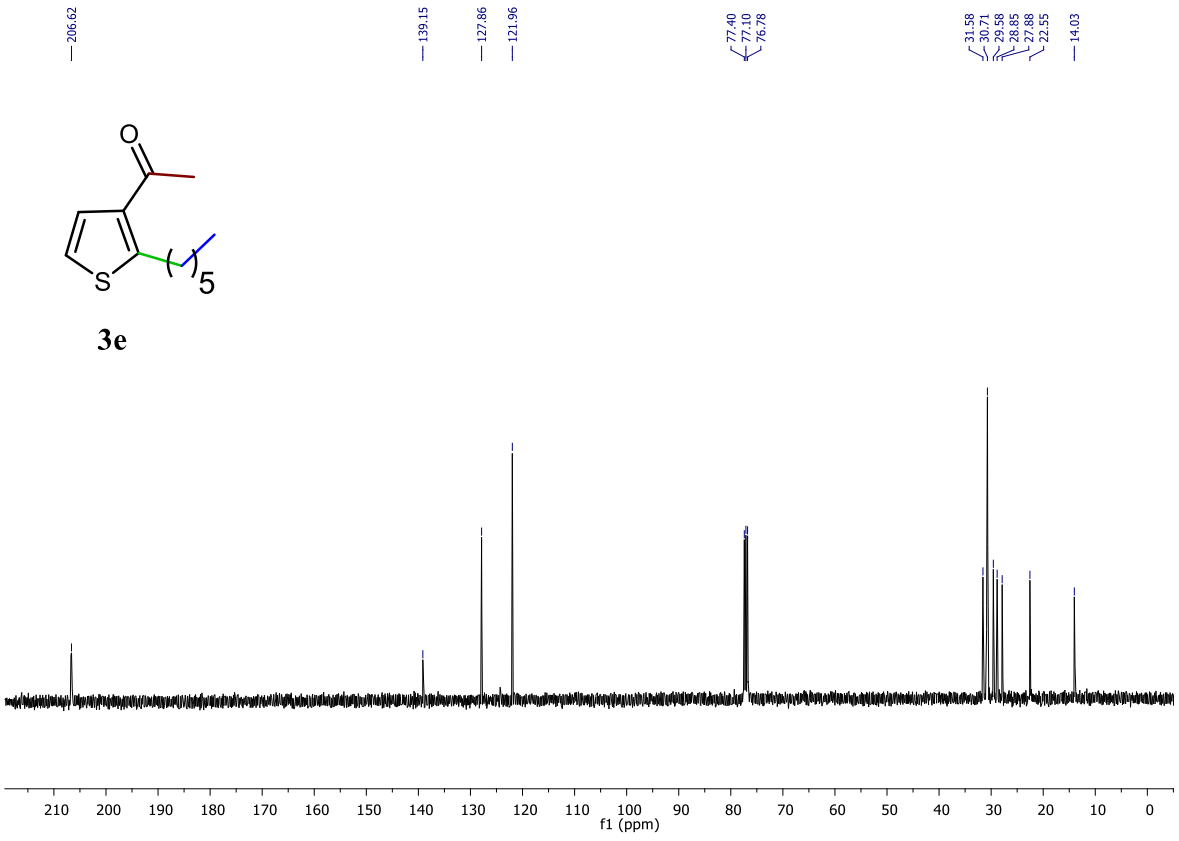


^{1}H NMR of 3e (400 MHz, 32 scans, RT, $CDCl_3$)



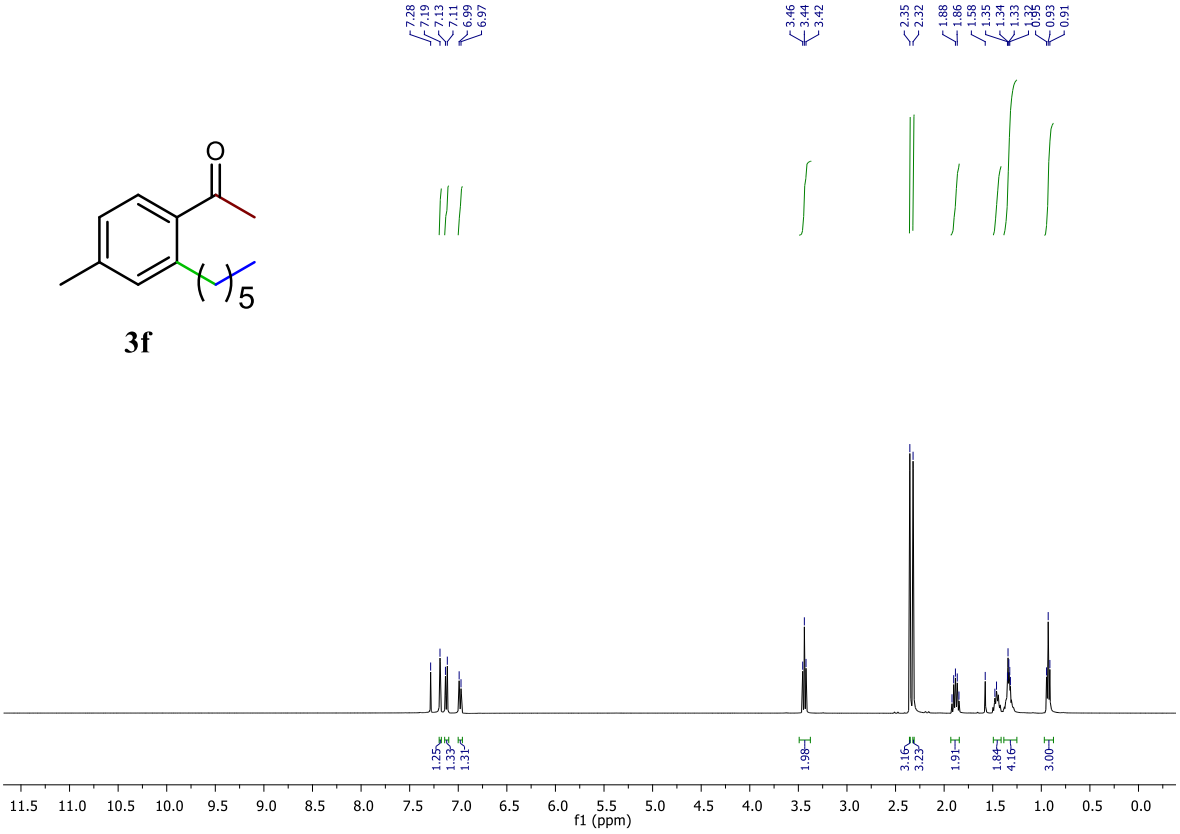
3e

^{13}C NMR of 3e (101 MHz, 512 scans, RT, $CDCl_3$)



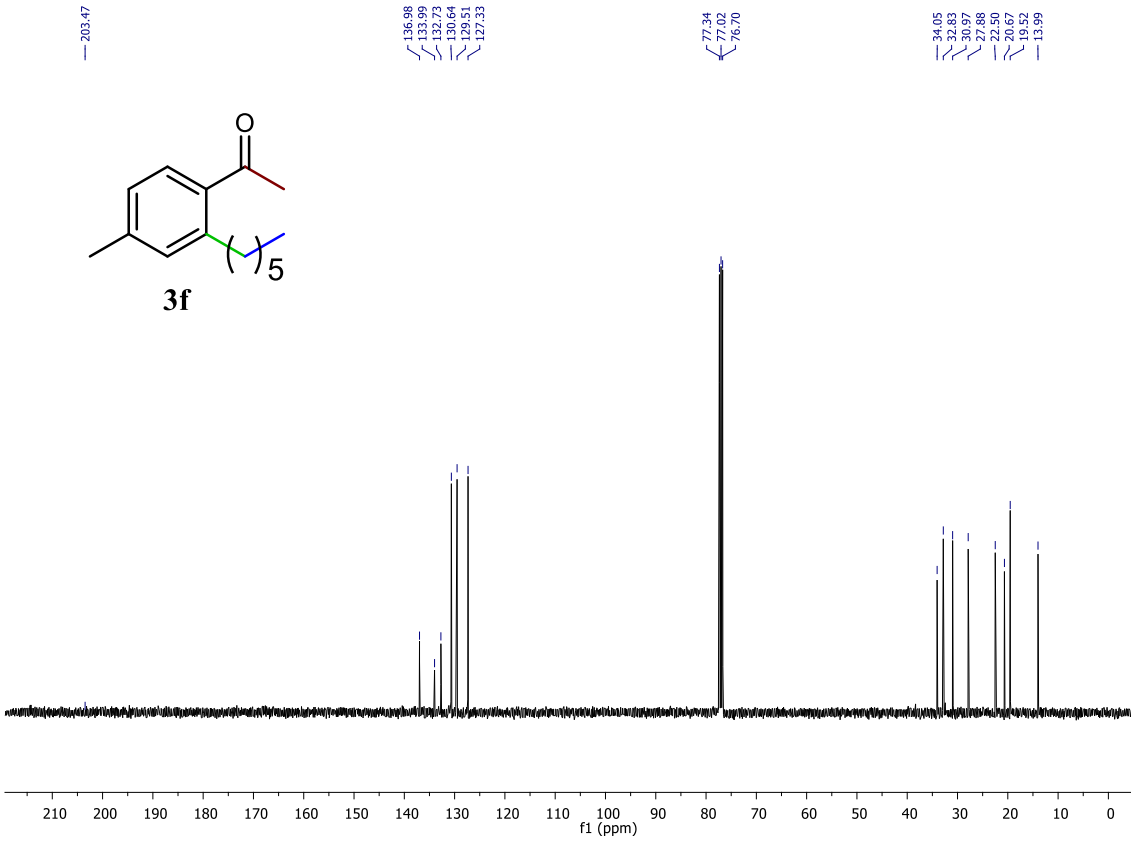
3e

^{1}H NMR of 3f (400 MHz, 32 scans, RT, $CDCl_3$)



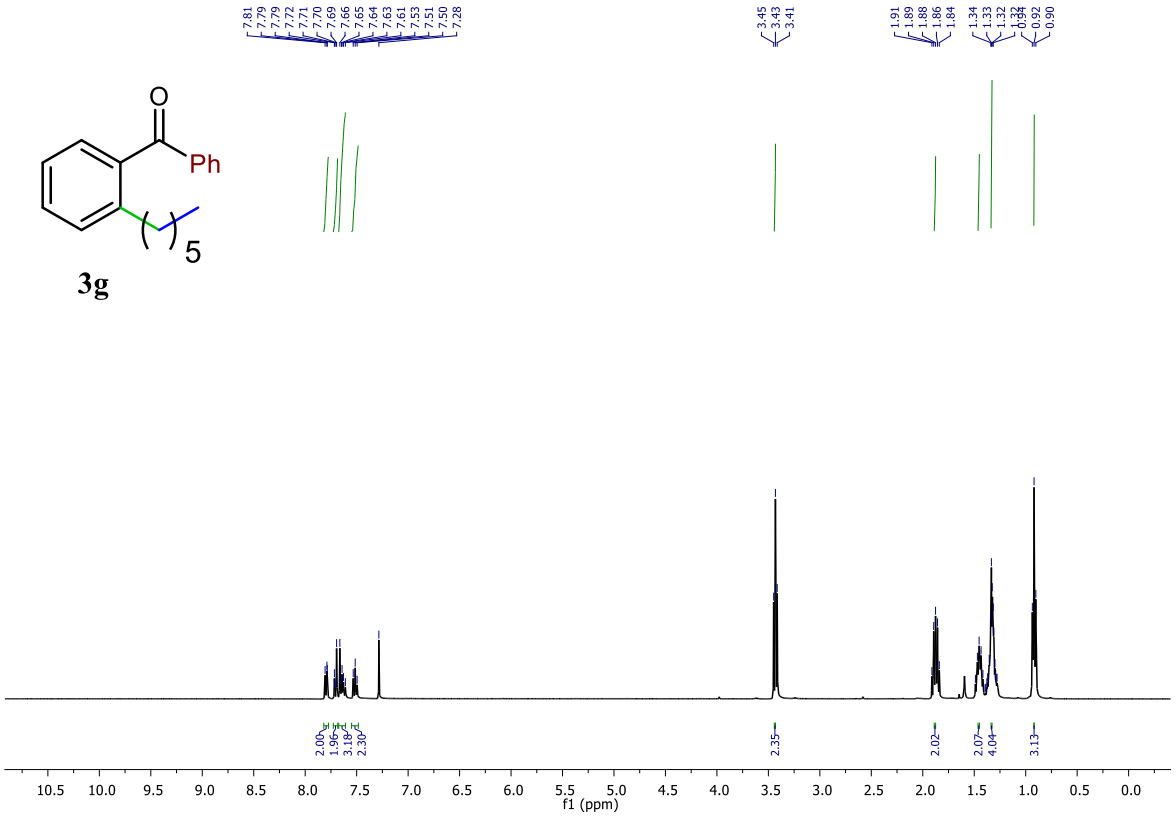
3f

^{13}C NMR of 3f (101 MHz, 512 scans, RT, $CDCl_3$)

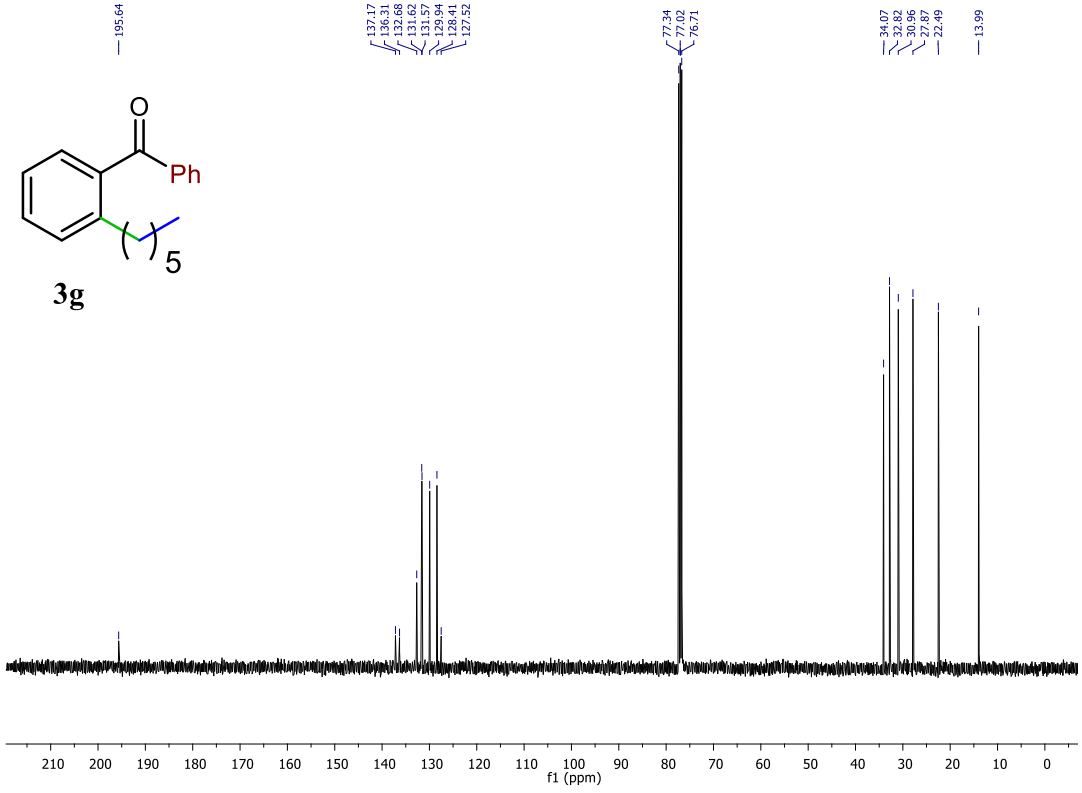


3f

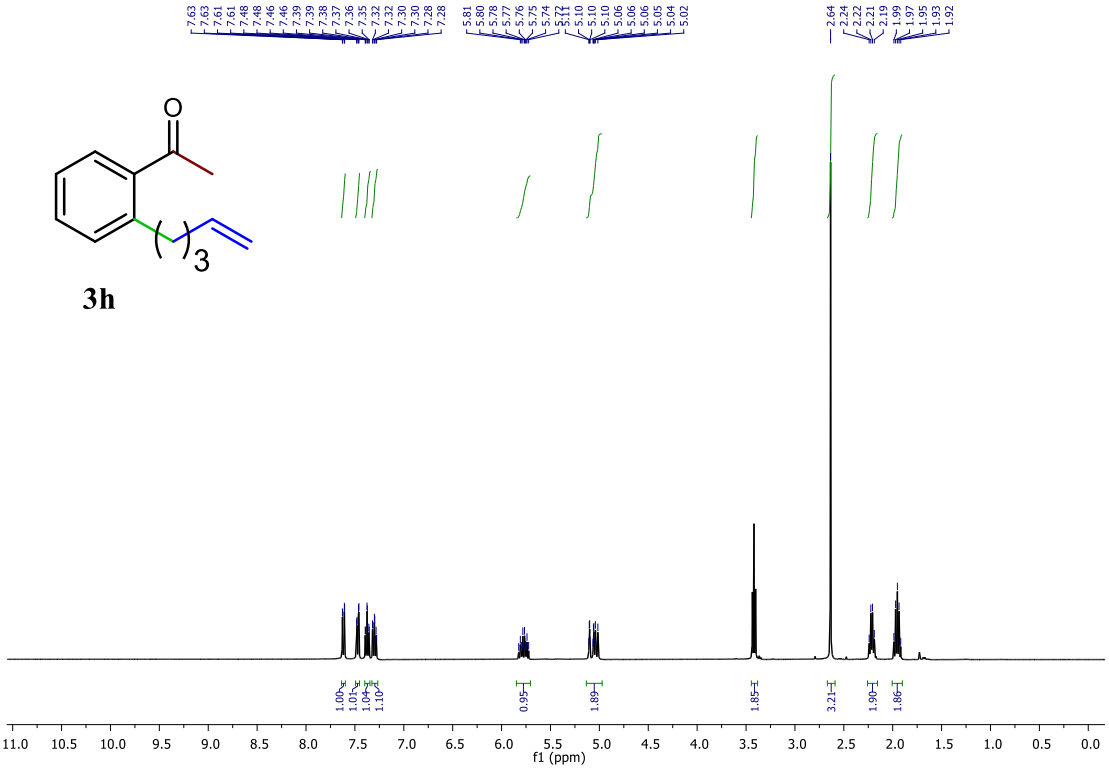
^{1}H NMR of 3g (400 MHz, 32 scans, RT, $CDCl_3$)



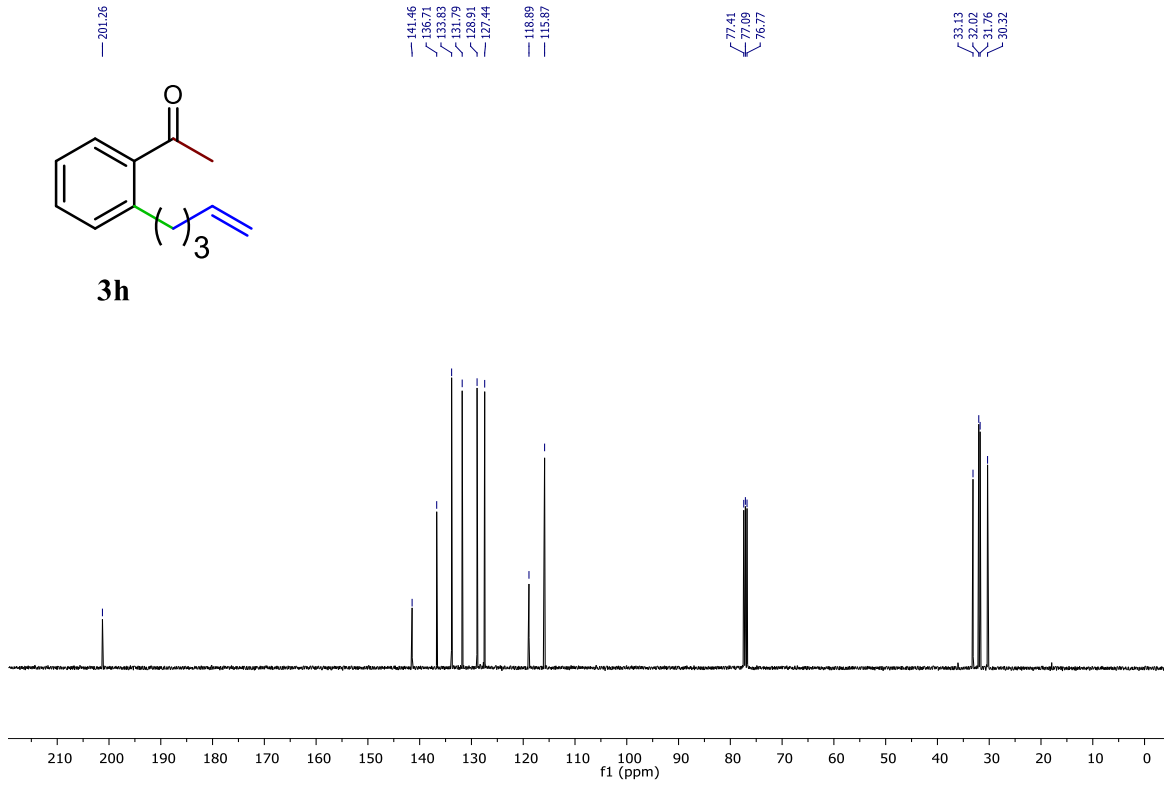
^{13}C NMR of 3g (101 MHz, 512 scans, RT, $CDCl_3$)



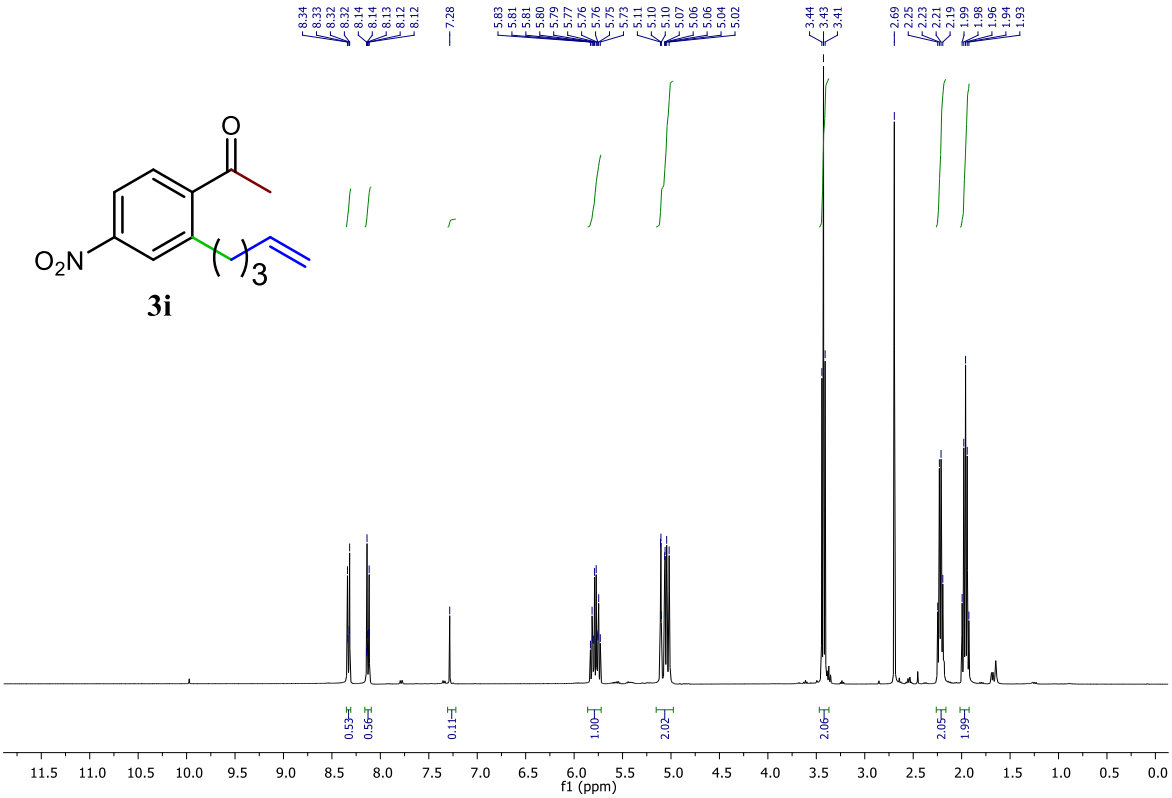
^{1}H NMR of 3h (400 MHz, 32 scans, RT, $CDCl_3$)



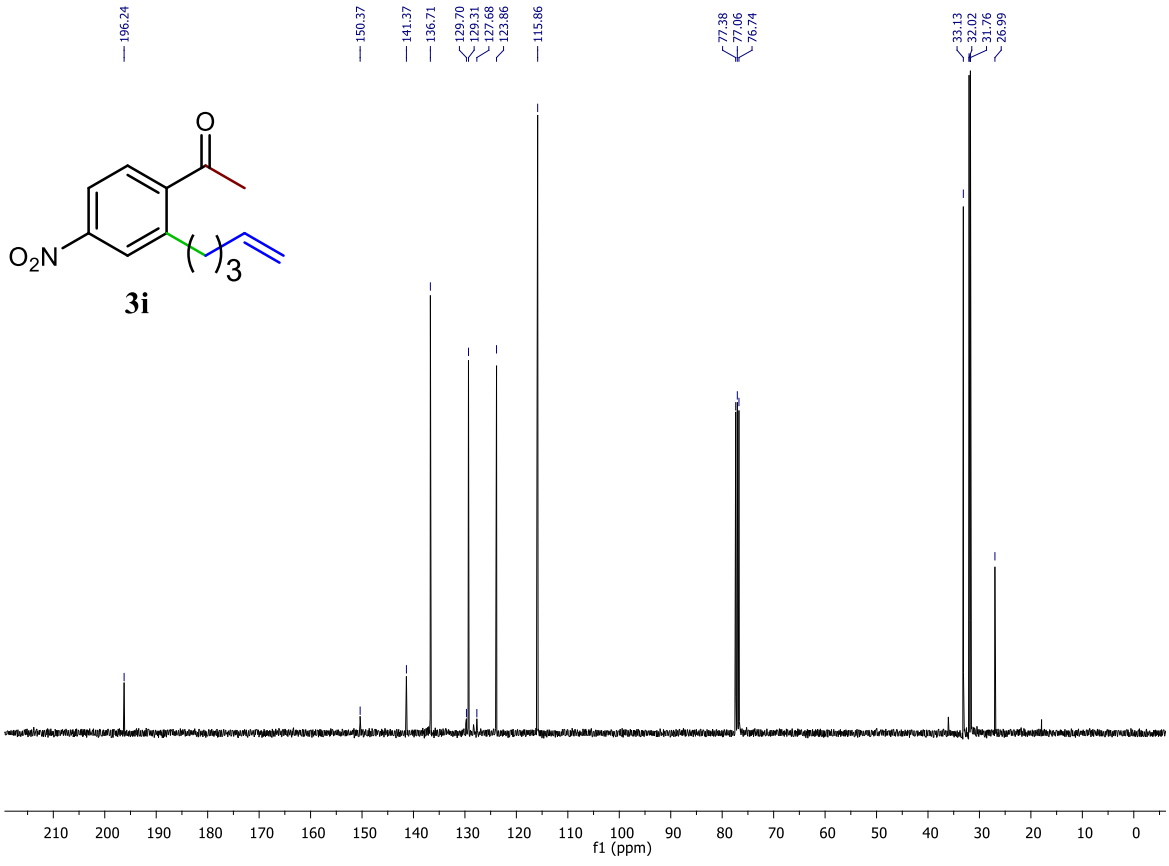
^{13}C NMR of 3h (101 MHz, 512 scans, RT, $CDCl_3$)



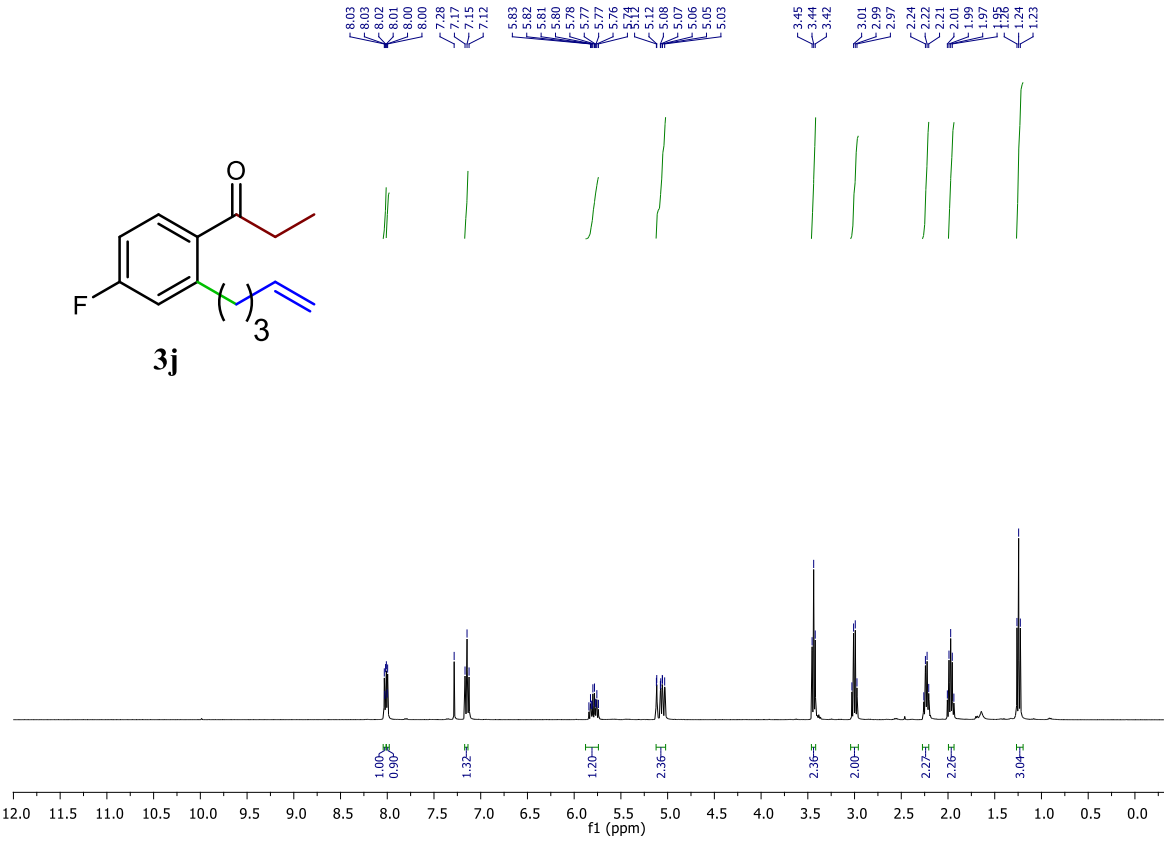
^{1}H NMR of 3i (400 MHz, 32 scans, RT, $CDCl_3$)



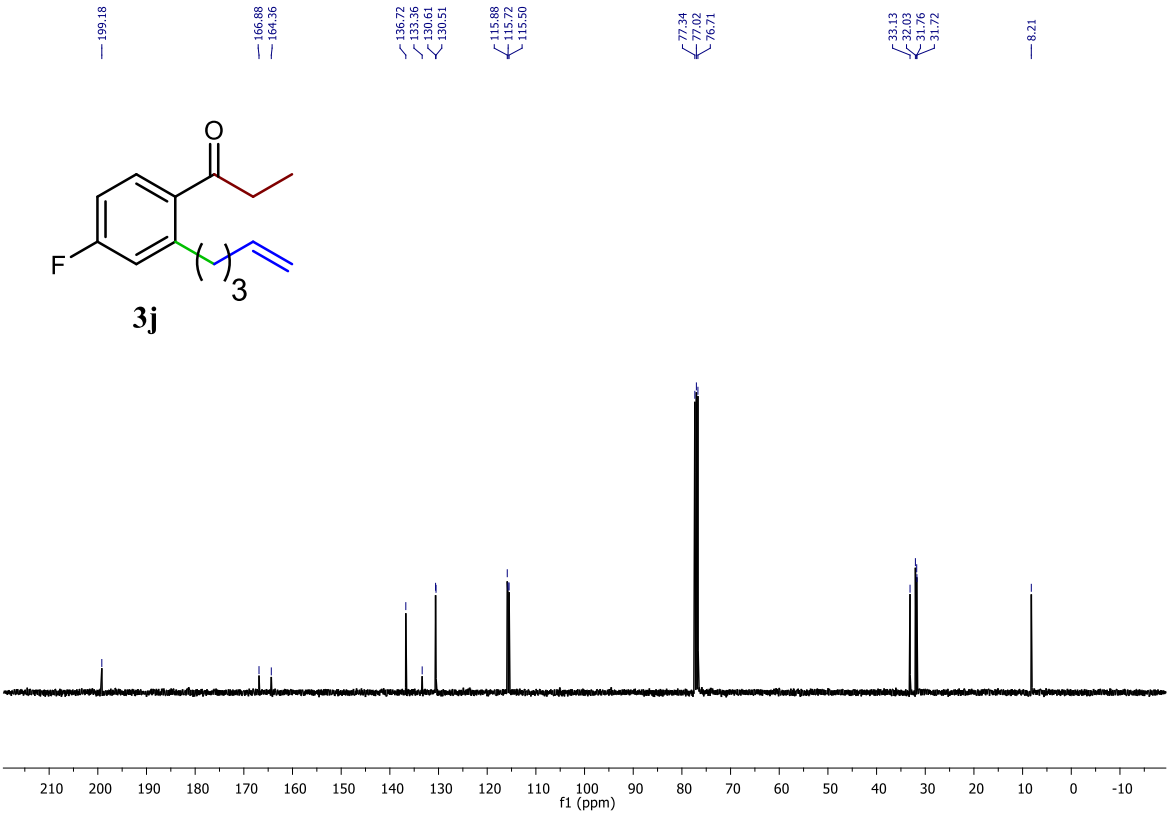
^{13}C NMR of 3h (101 MHz, 512 scans, RT, $CDCl_3$)



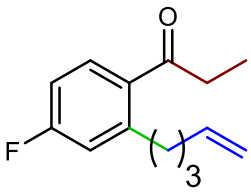
^{1}H NMR of 3j (400 MHz, 32 scans, RT, $CDCl_3$)



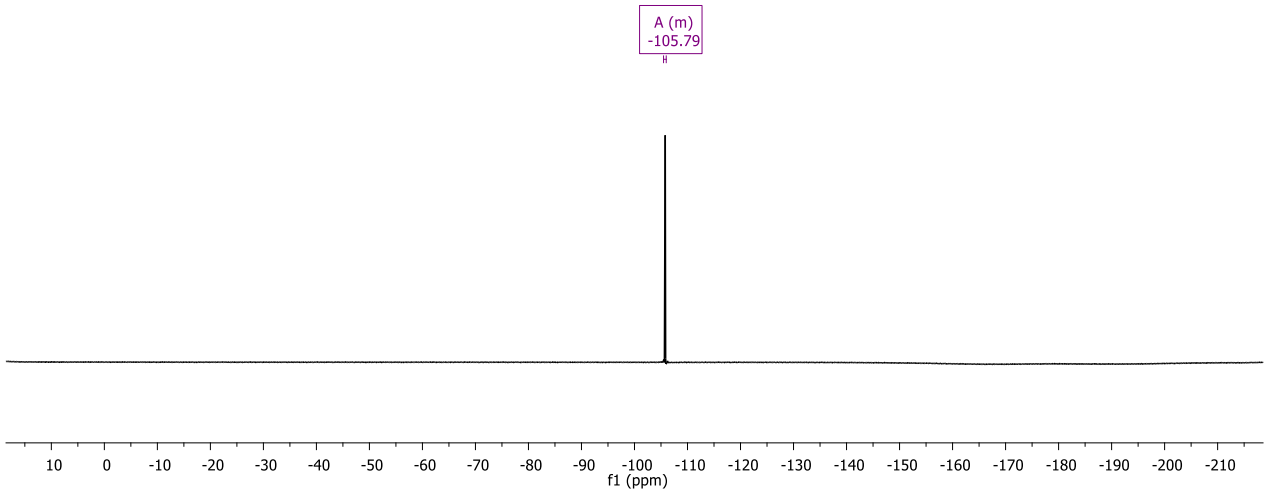
^{13}C NMR of 3j (101 MHz, 512 scans, RT, $CDCl_3$)



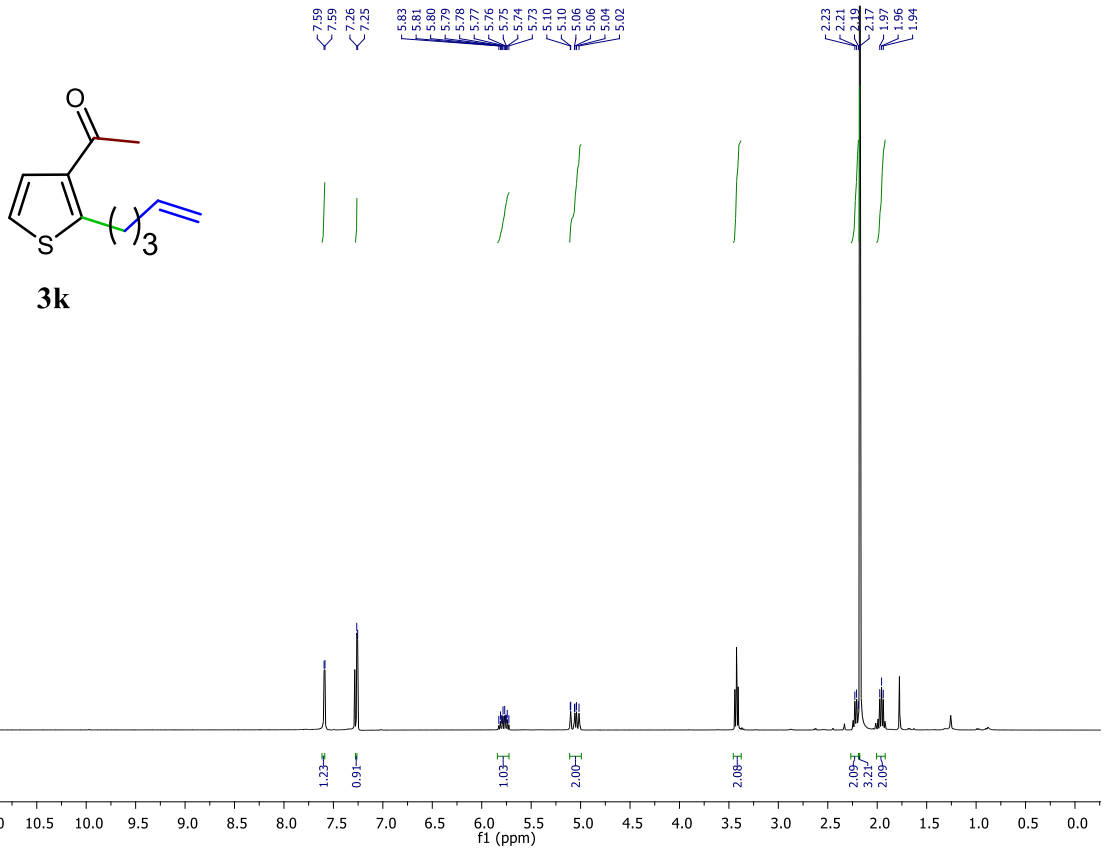
^{19}F NMR of **3j (377 MHz, CDCl3)**



3j

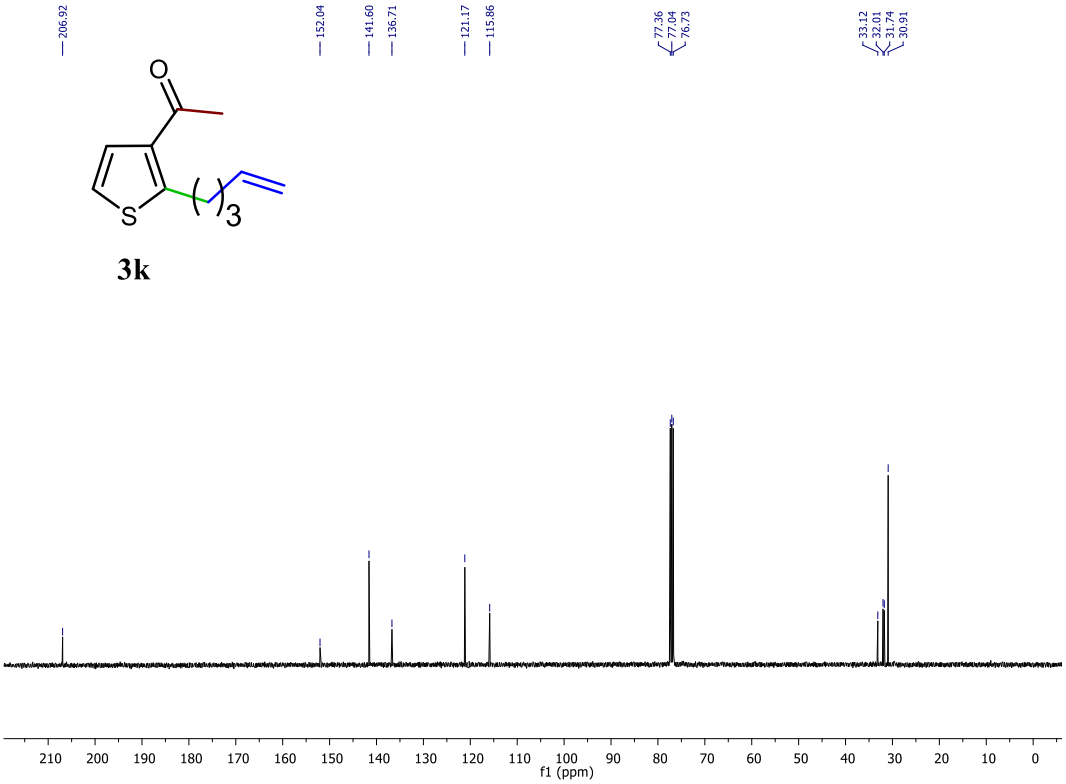


^{1}H NMR of 3k (400 MHz, 32 scans, RT, $CDCl_3$)



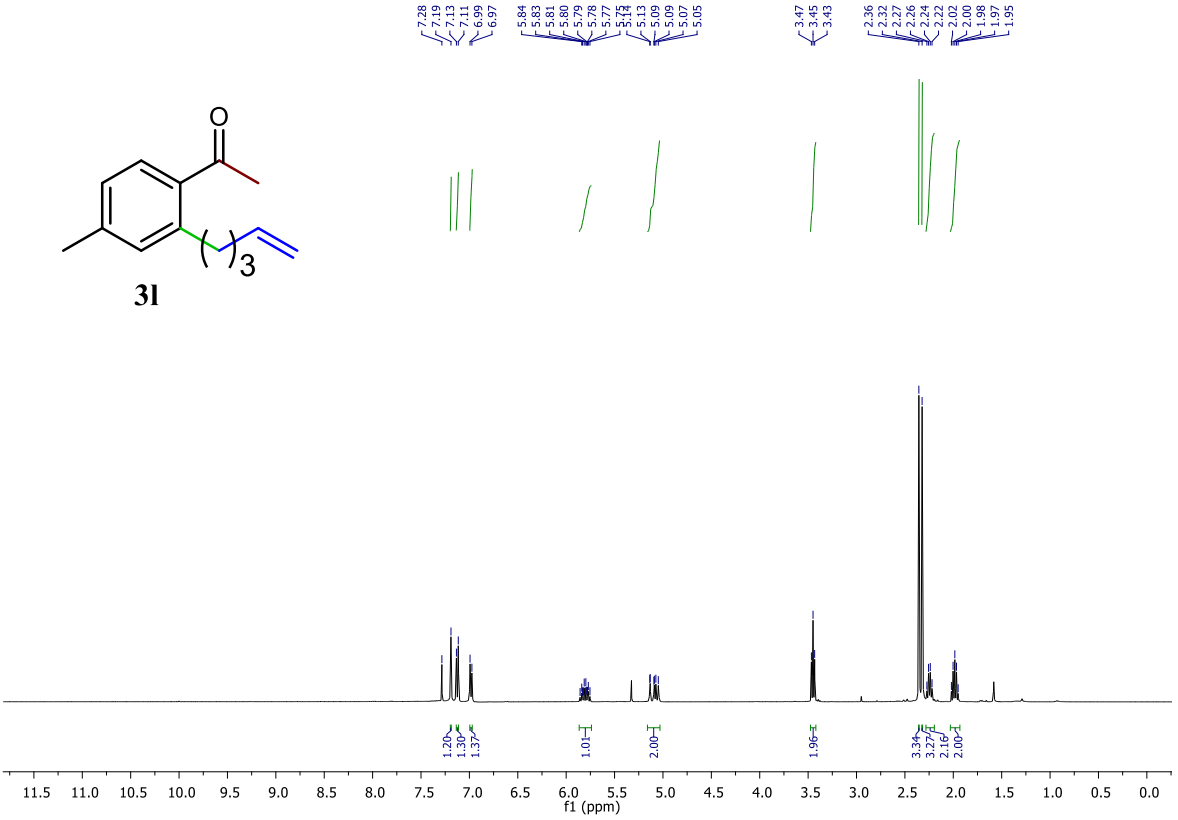
3k

^{13}C NMR of 3k (101 MHz, 512 scans, RT, $CDCl_3$)

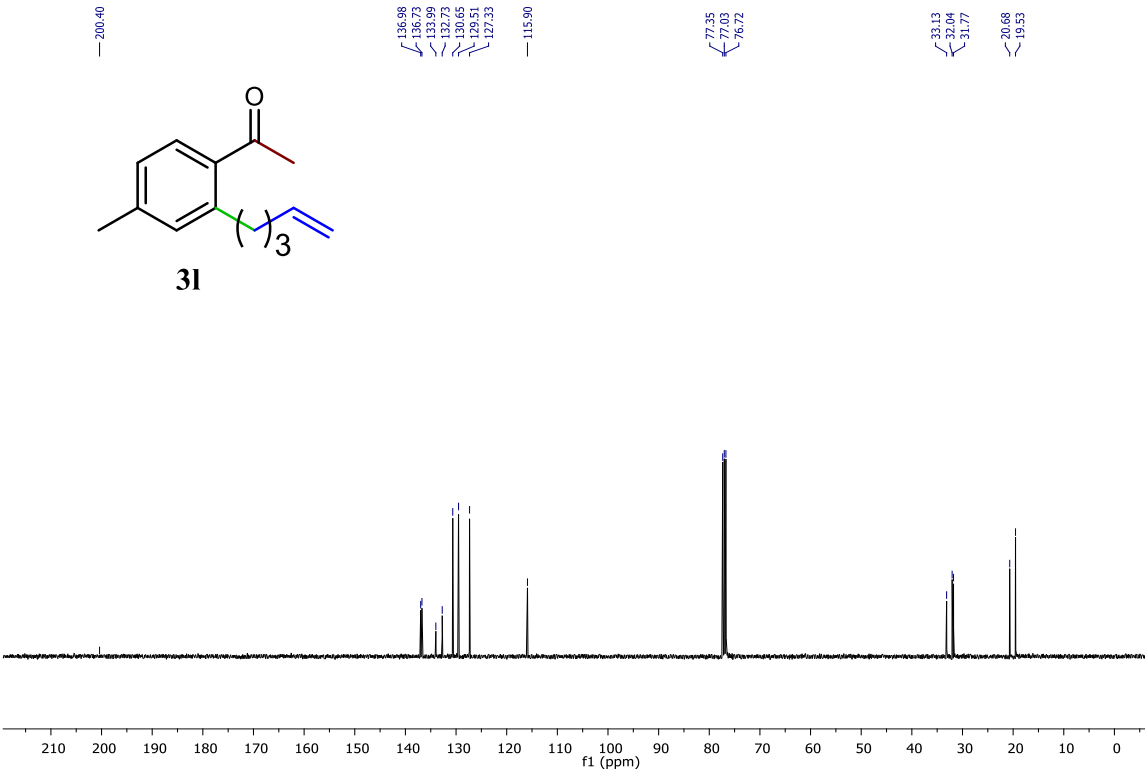


3k

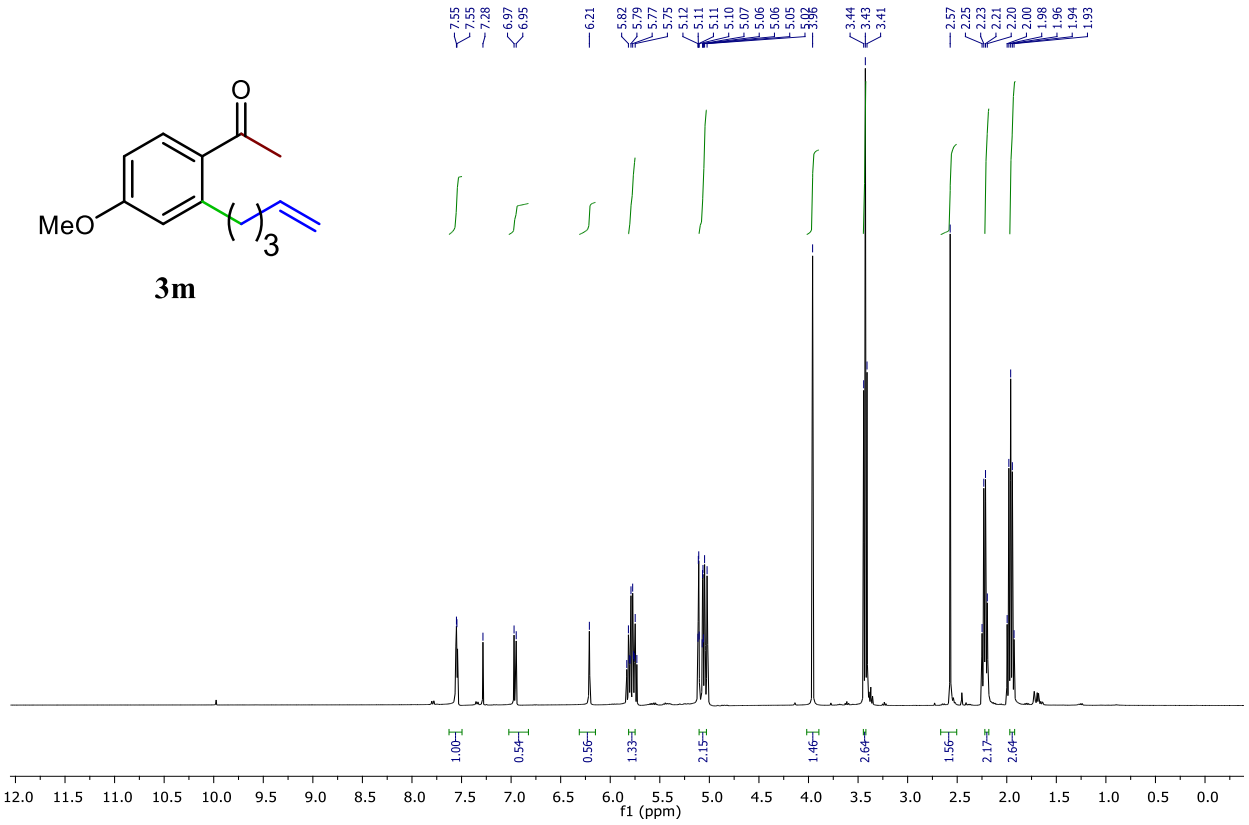
^{1}H NMR of 3l (400 MHz, 32 scans, RT, $CDCl_3$)



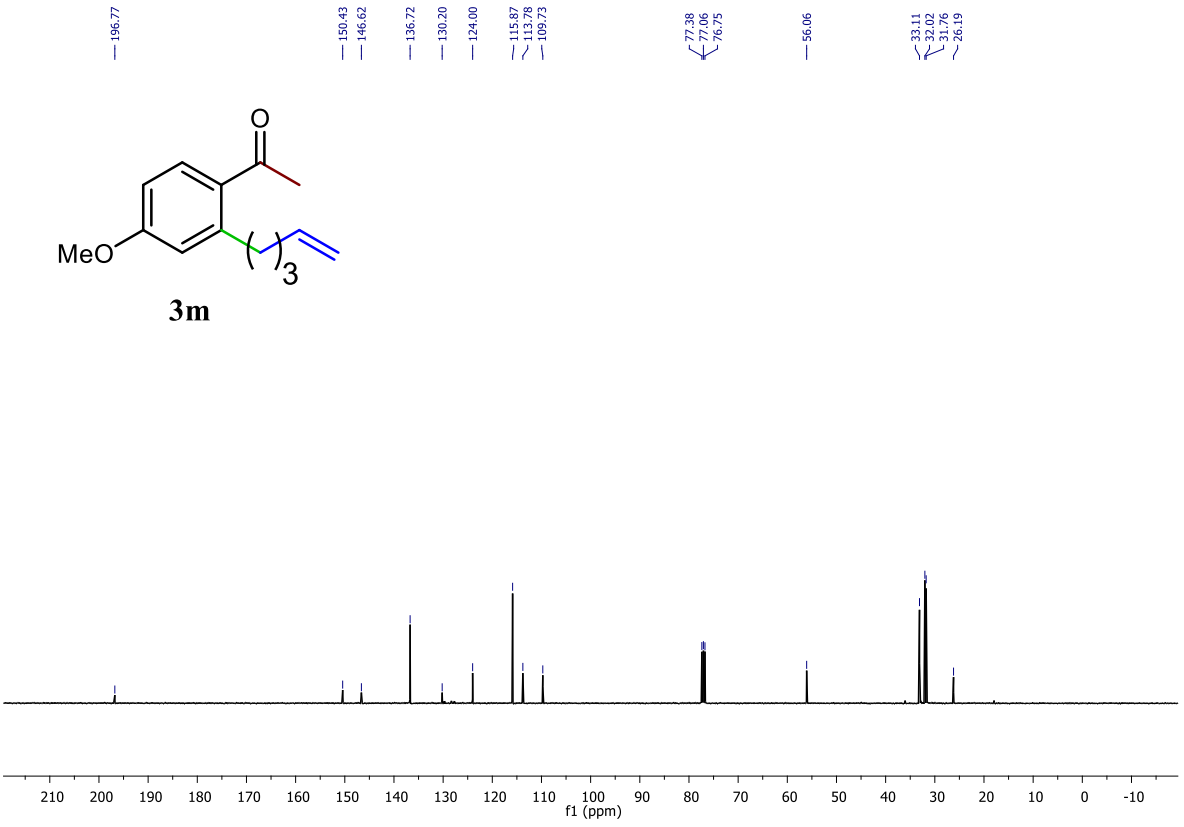
^{13}C NMR of 3l (101 MHz, 512 scans, RT, $CDCl_3$)



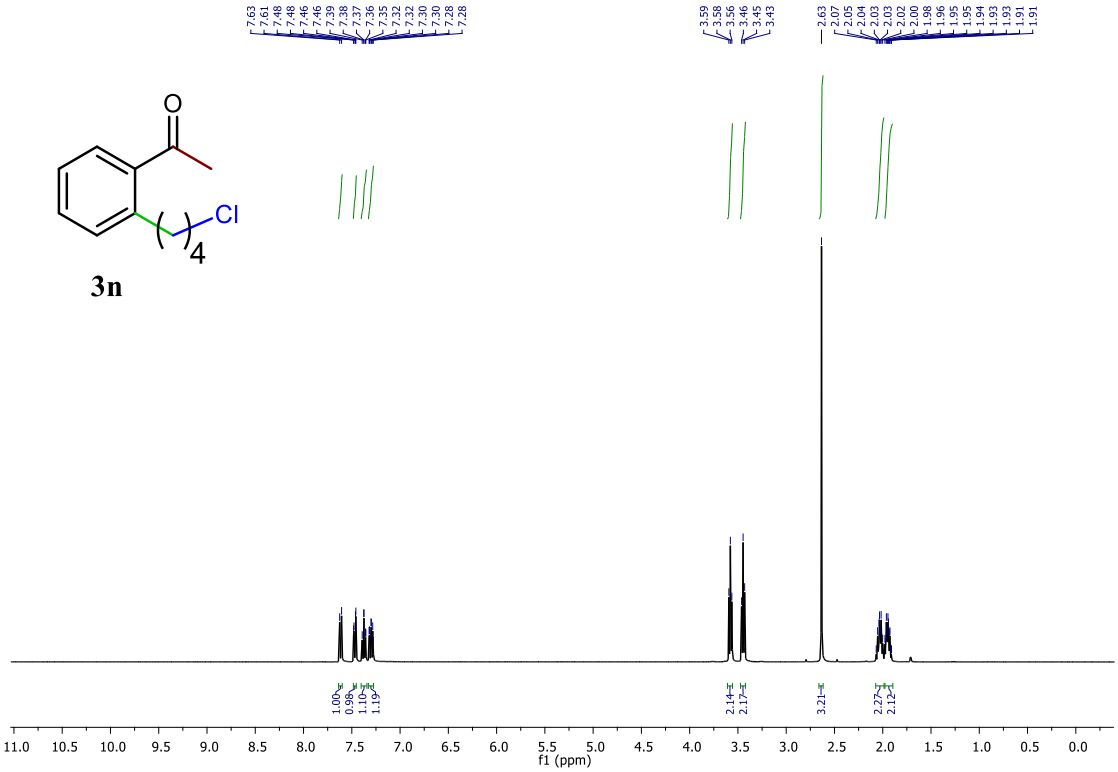
^{1}H NMR of 3m (400 MHz, 32 scans, RT, $CDCl_3$)



^{13}C NMR of 3m (101 MHz, 512 scans, RT, $CDCl_3$)

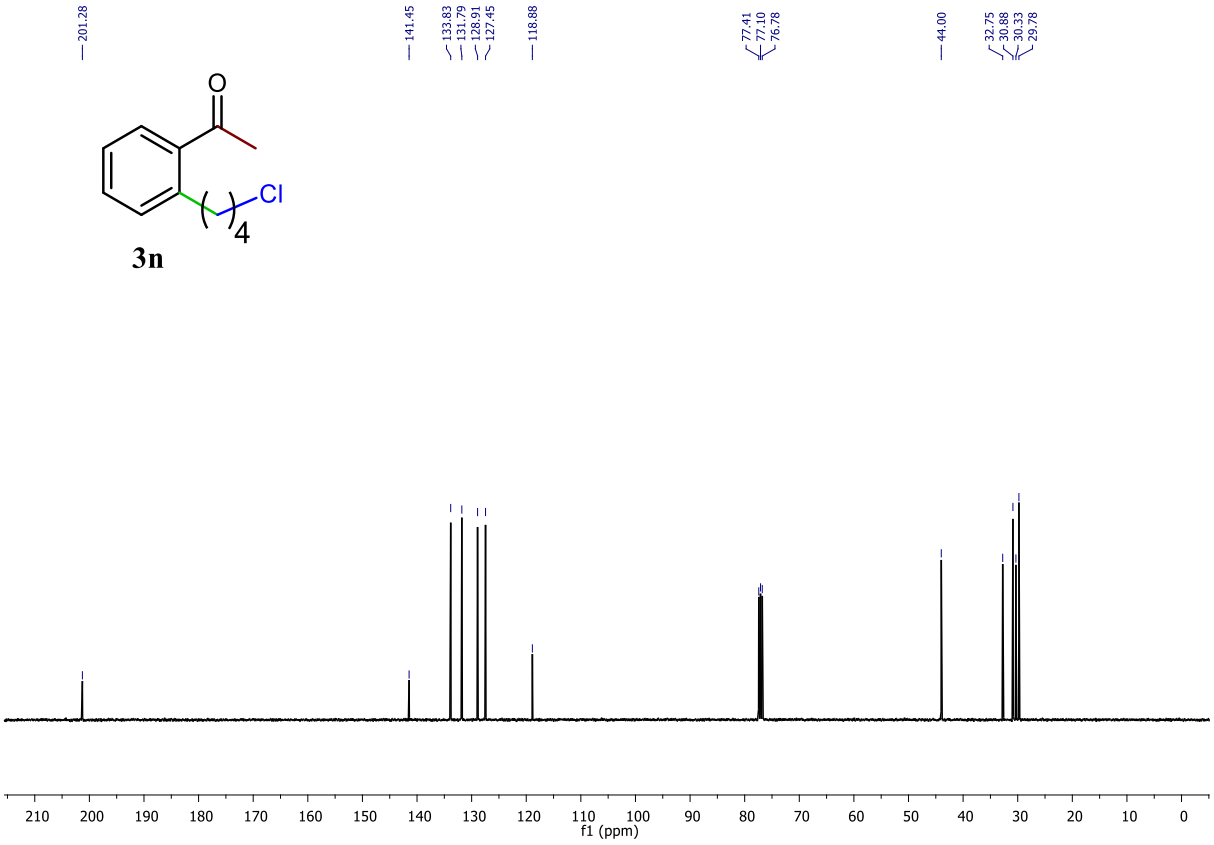


^{1}H NMR of 3n (400 MHz, 32 scans, RT, $CDCl_3$)



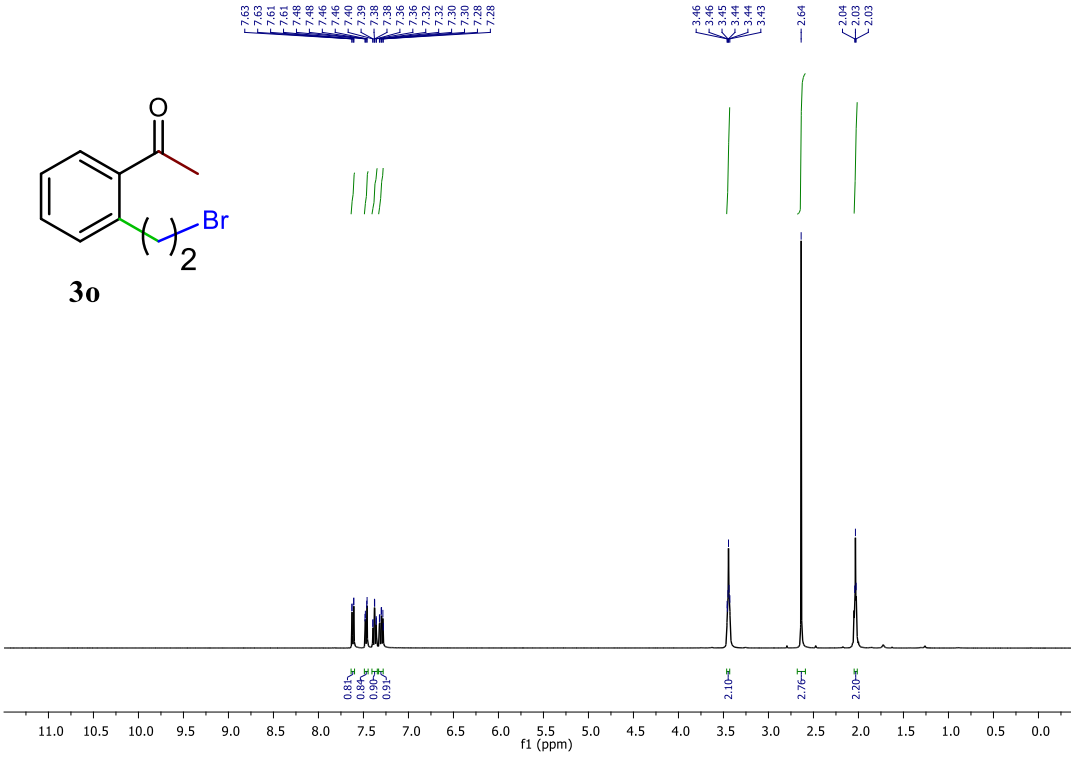
3n

^{13}C NMR of 3n (101 MHz, 512 scans, RT, $CDCl_3$)



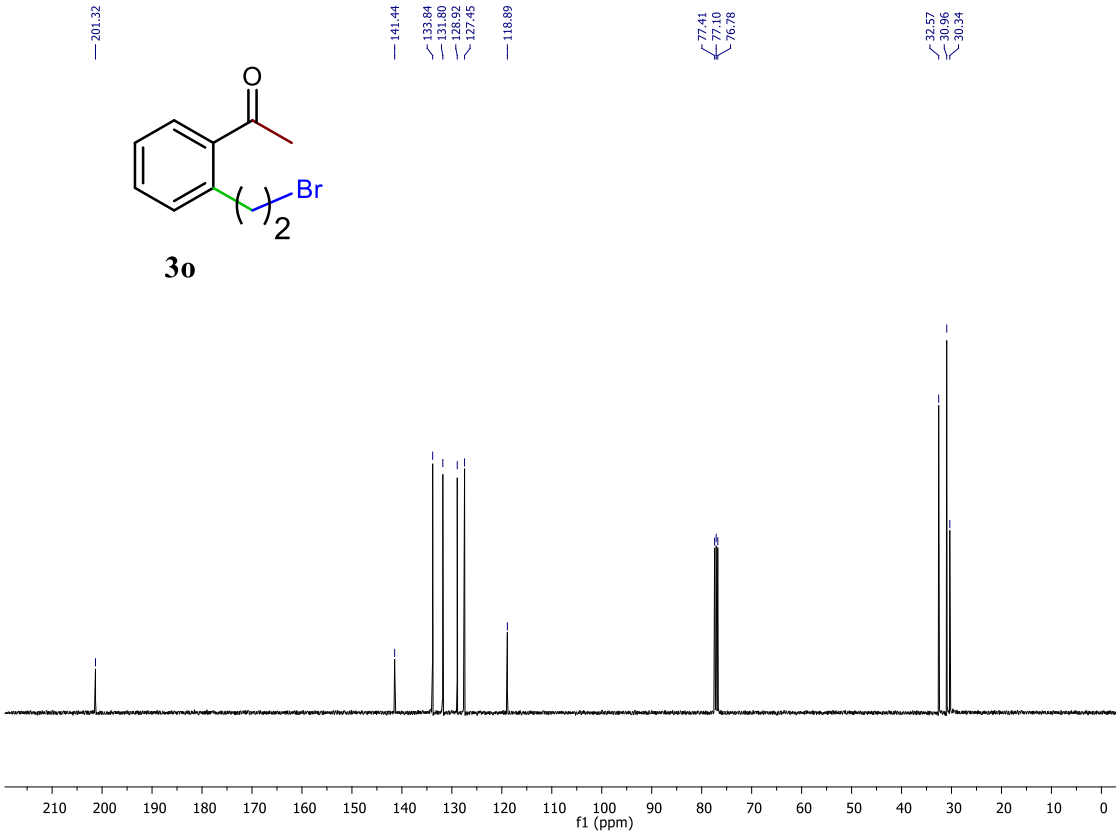
3n

^{1}H NMR of 3o (400 MHz, 32 scans, RT, $CDCl_3$)



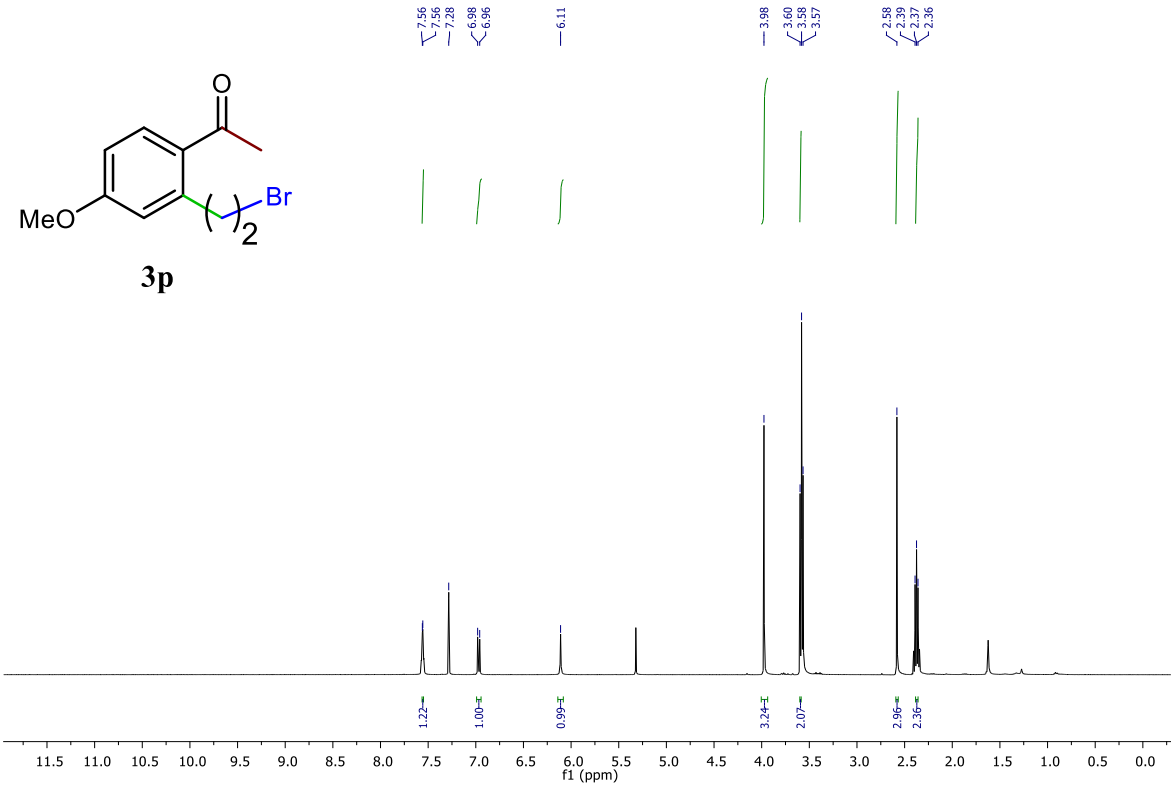
3o

^{13}C NMR of 3o (101 MHz, 512 scans, RT, $CDCl_3$)



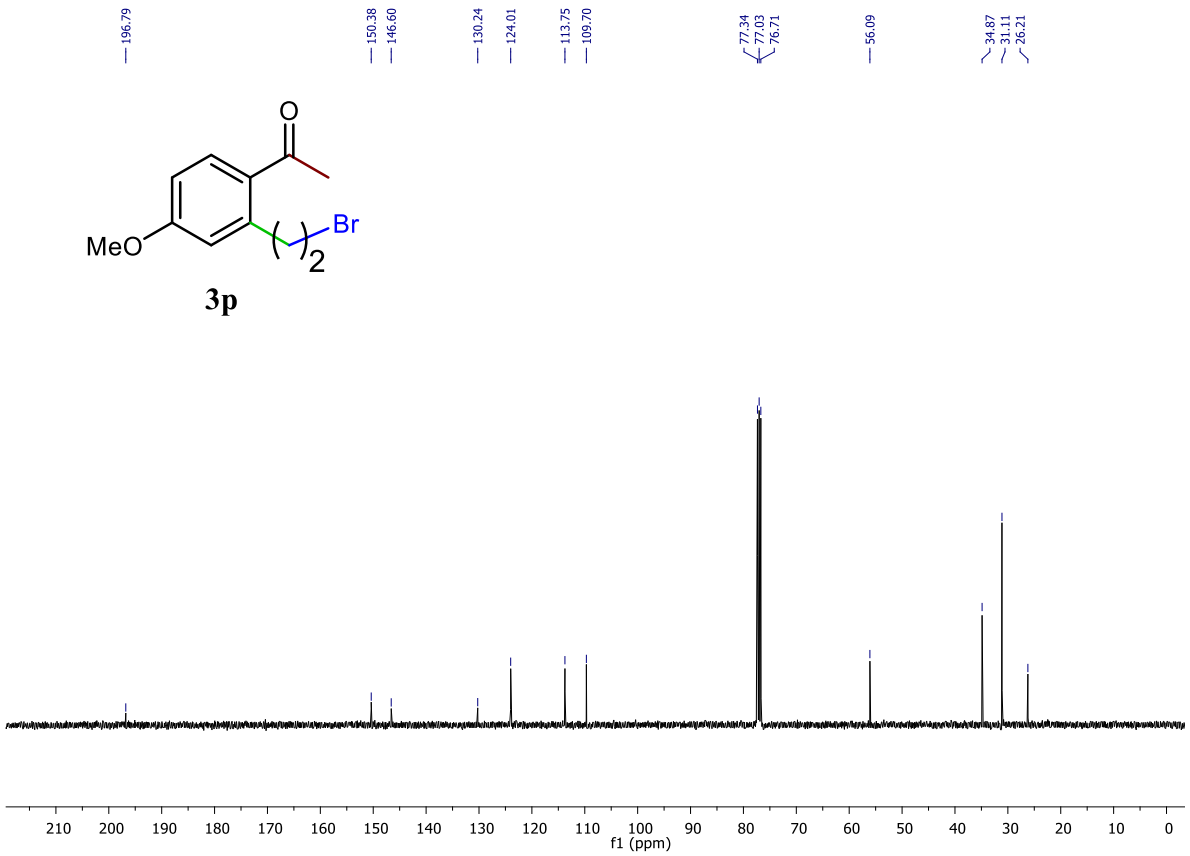
3o

^{1}H NMR of 3p (400 MHz, 32 scans, RT, $CDCl_3$)



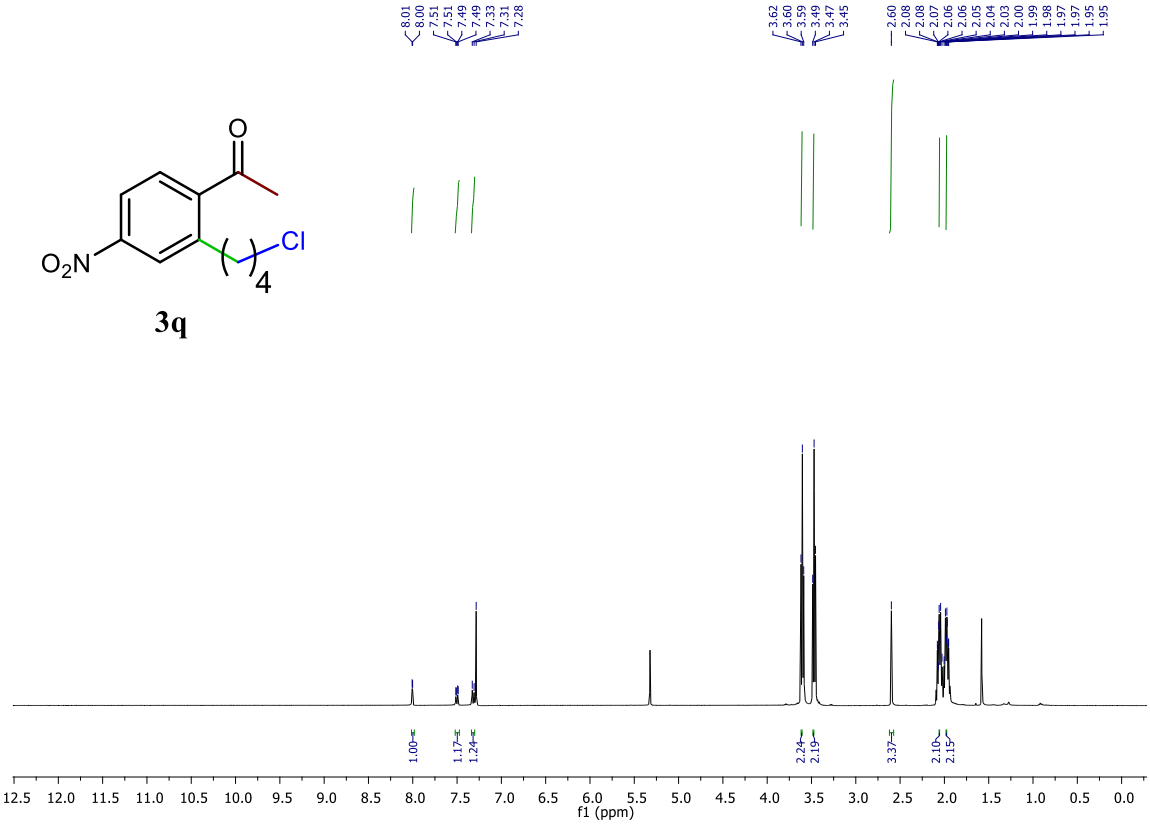
3p

^{13}C NMR of 3p (101 MHz, 512 scans, RT, $CDCl_3$)

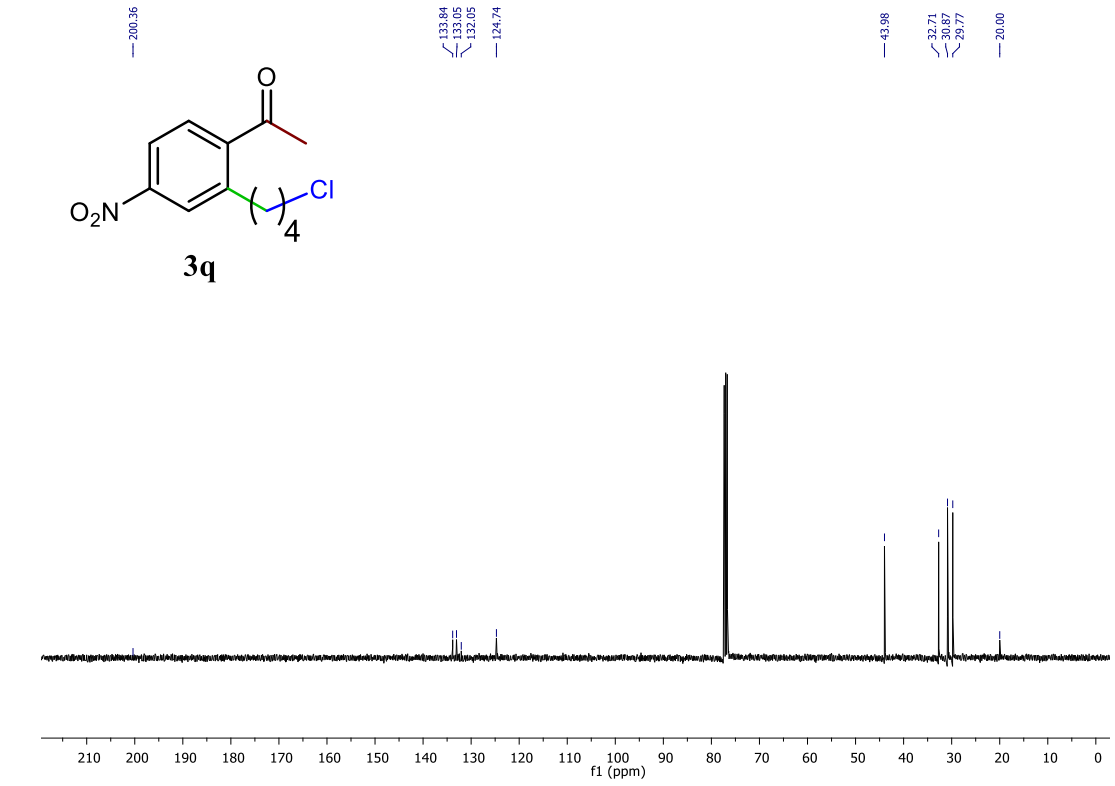


3p

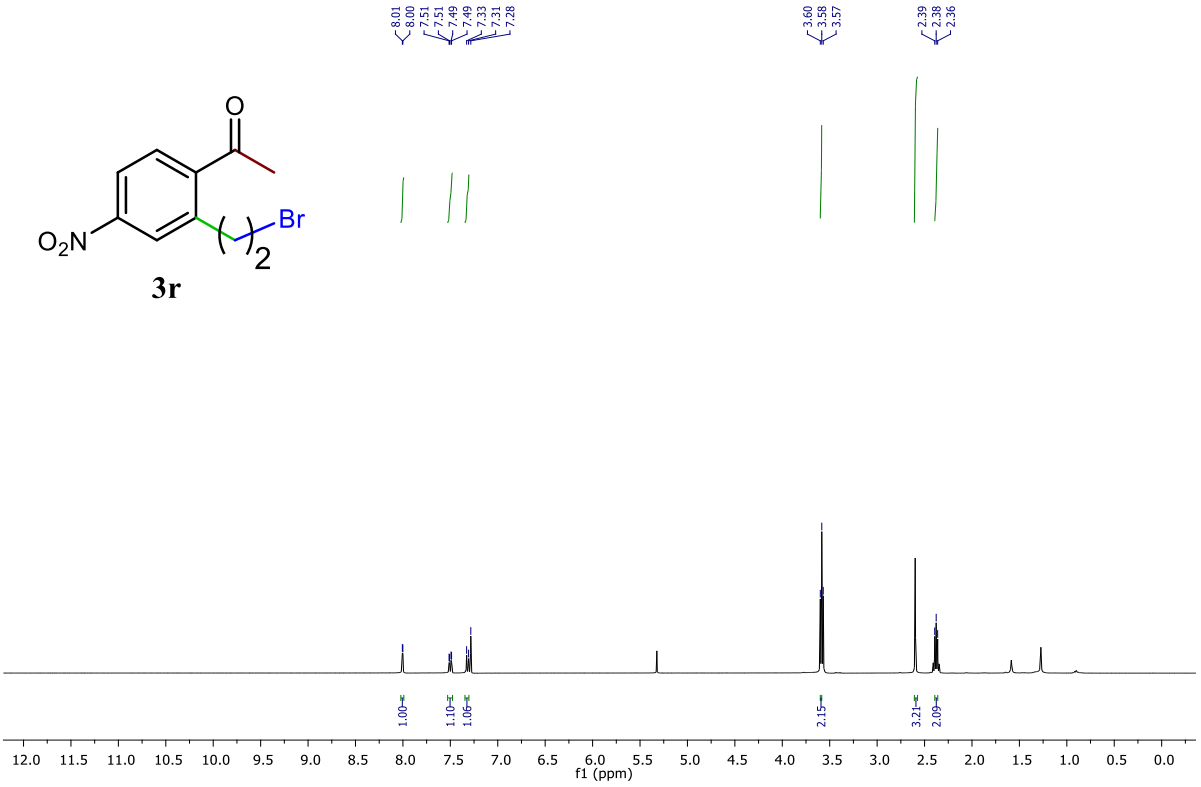
^{1}H NMR of 3q (400 MHz, 32 scans, RT, $CDCl_3$)



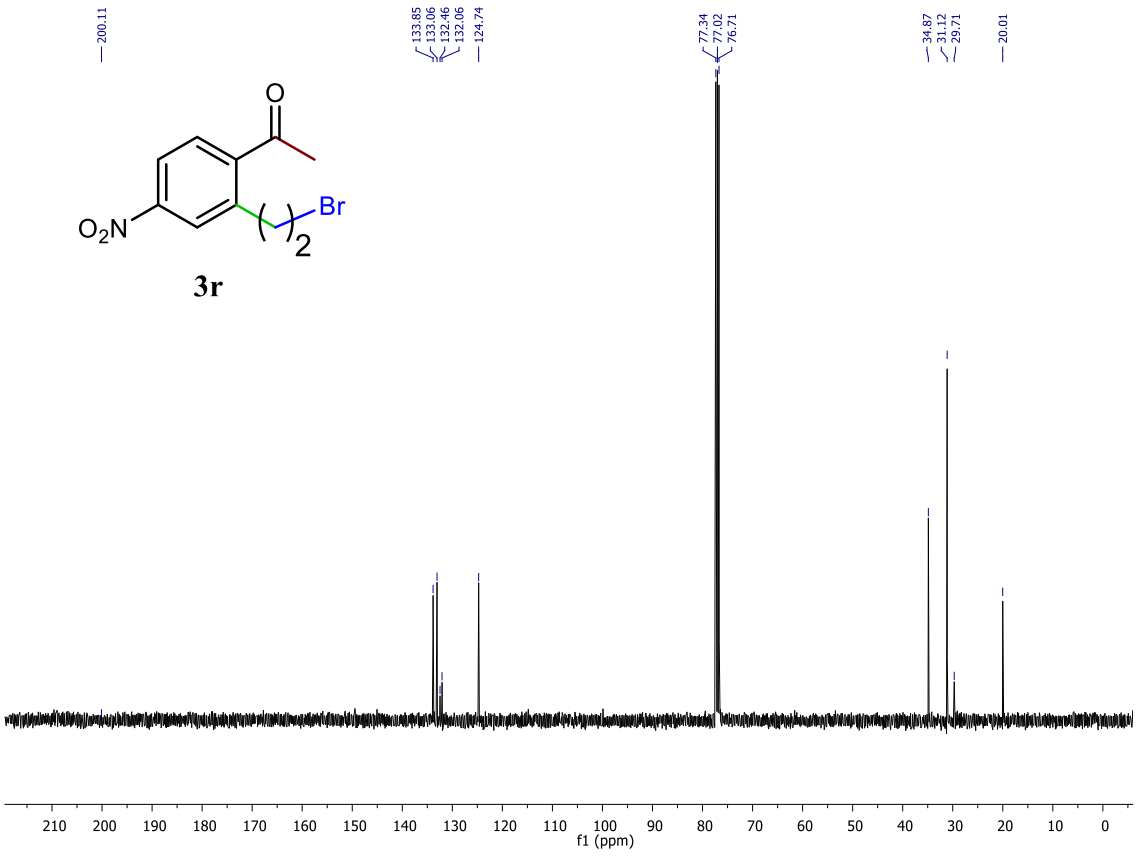
^{13}C NMR of 3q (101 MHz, 512 scans, RT, $CDCl_3$)



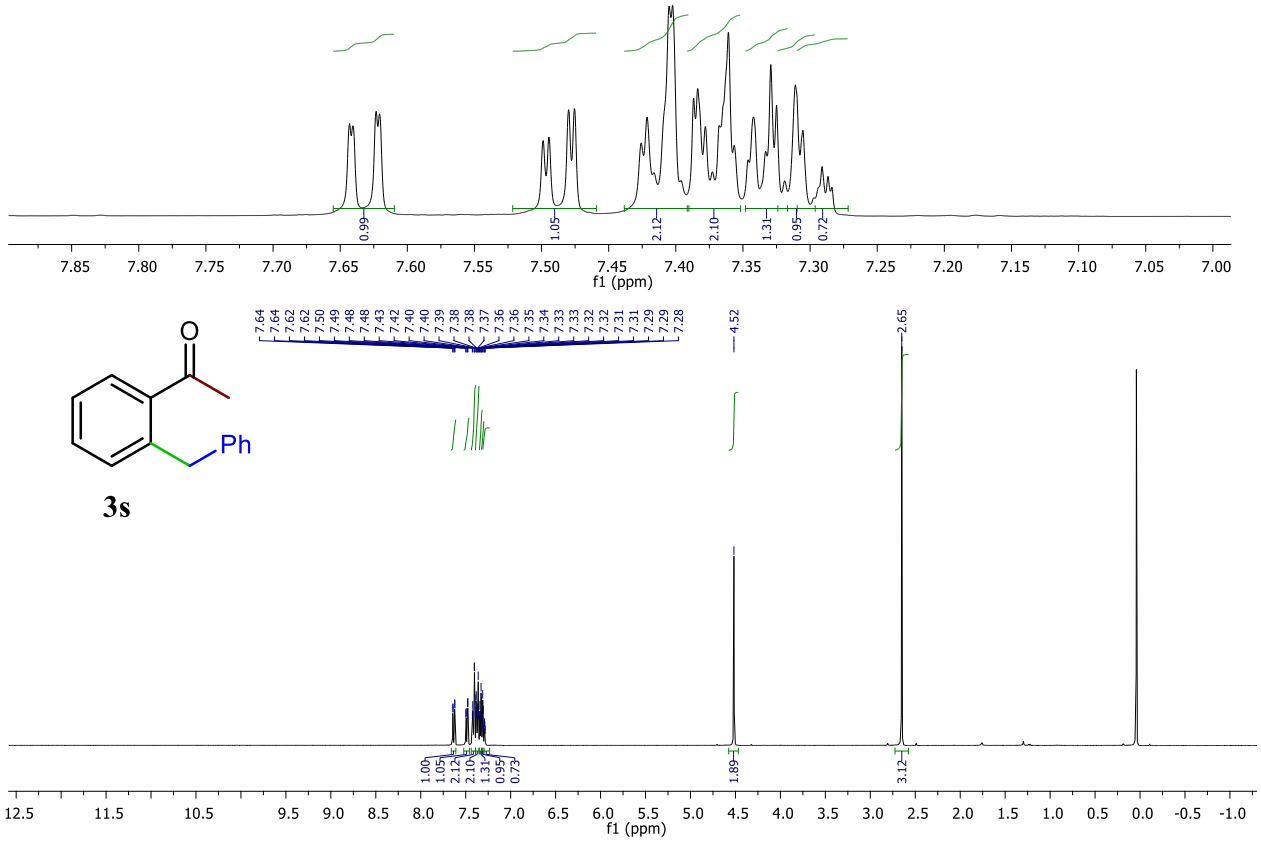
^{1}H NMR of 3r (400 MHz, 32 scans, RT, $CDCl_3$)



^{13}C NMR of 3r (101 MHz, 512 scans, RT, $CDCl_3$)

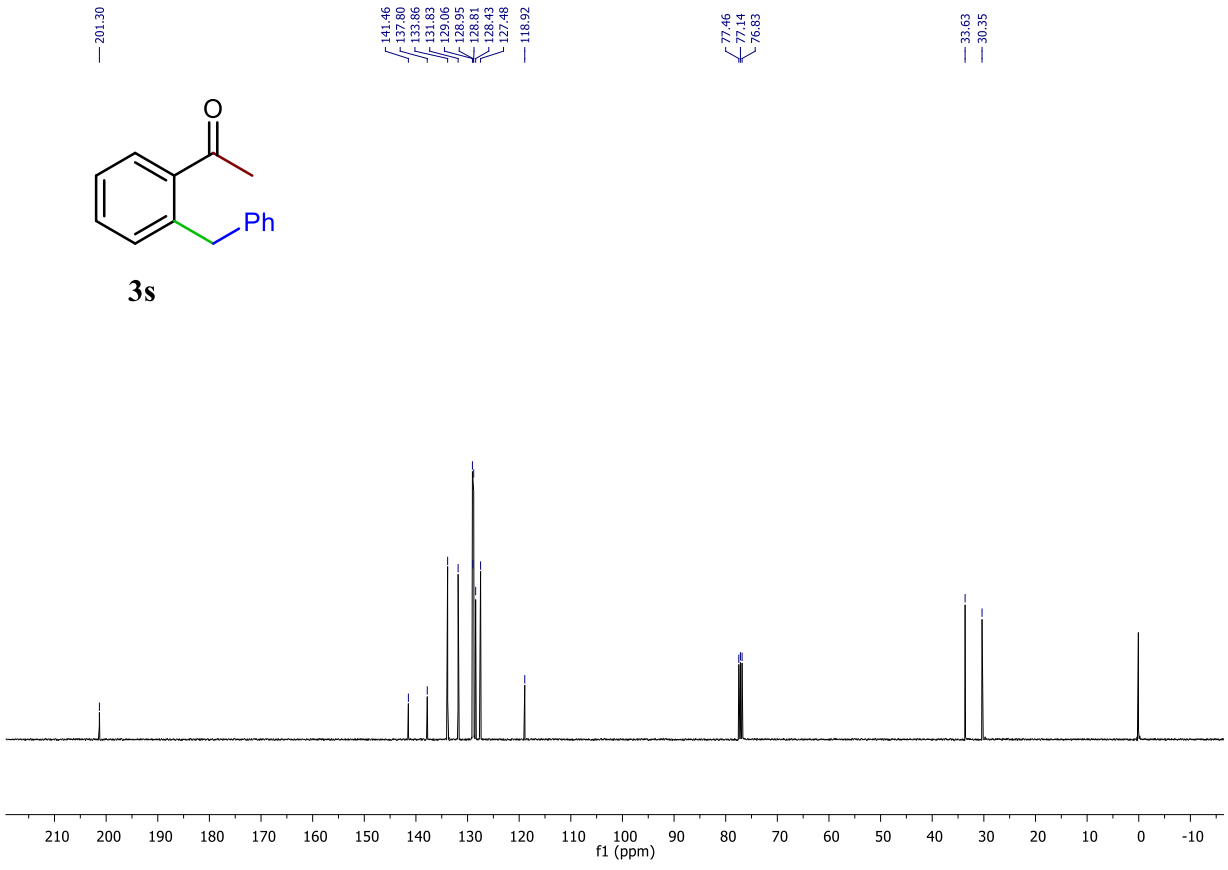


^{1}H NMR of 3s (400 MHz, 32 scans, RT, $CDCl_3$)



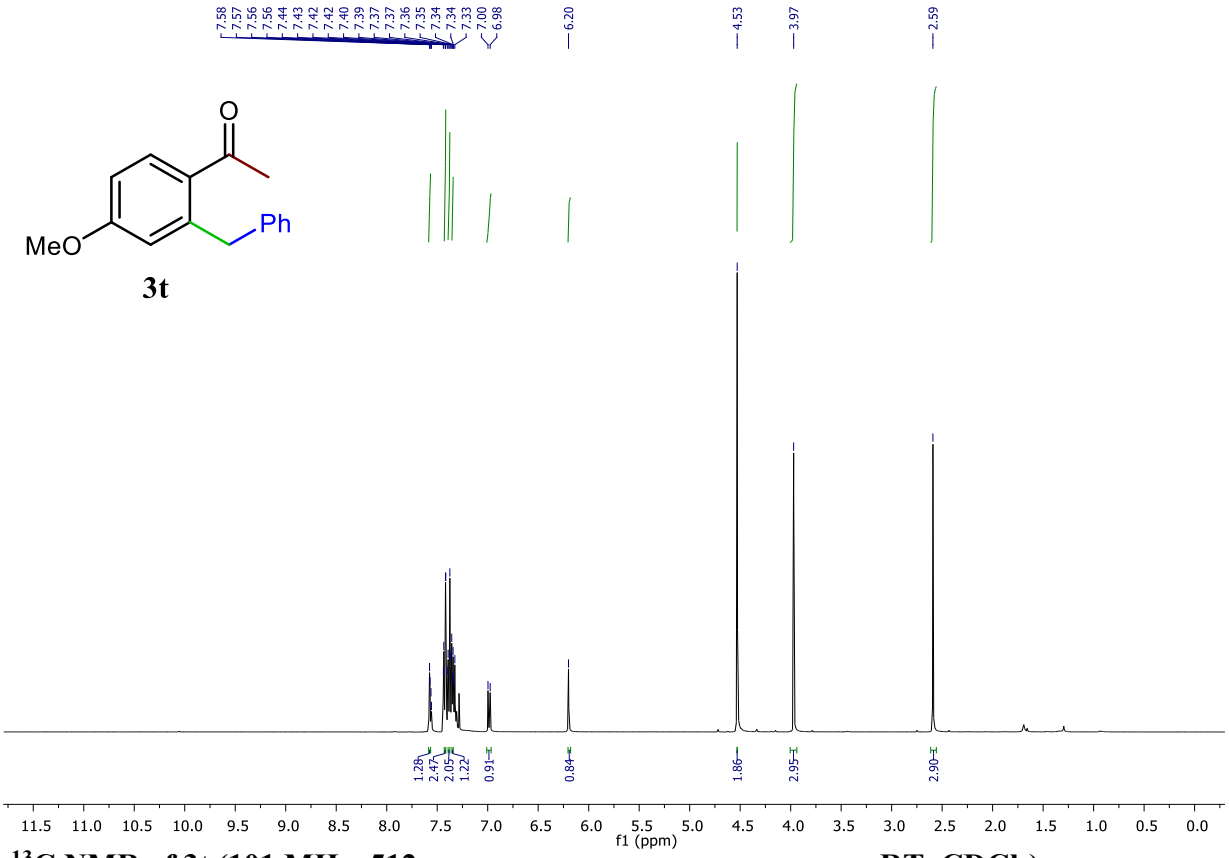
3s

^{13}C NMR of 3s (101 MHz, 512 scans, RT, $CDCl_3$)



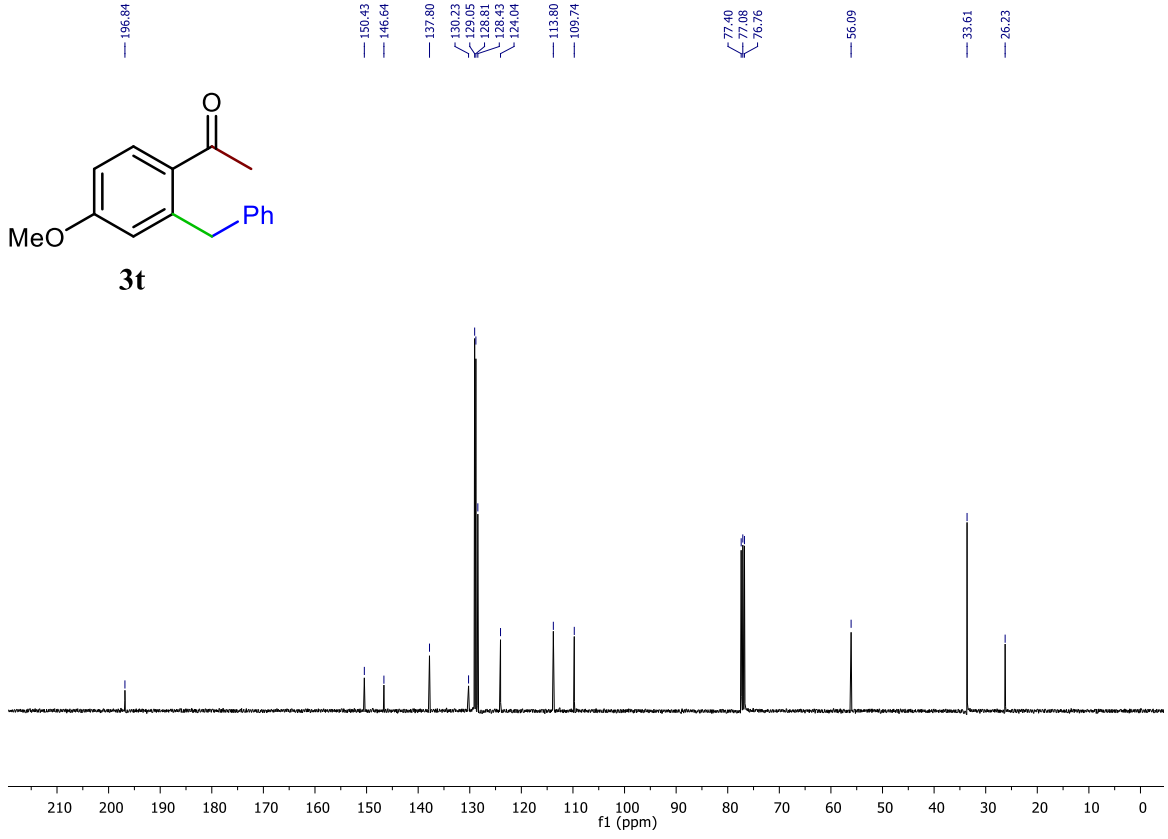
3s

^{1}H NMR of 3t (400 MHz, 32 scans, RT, $CDCl_3$)



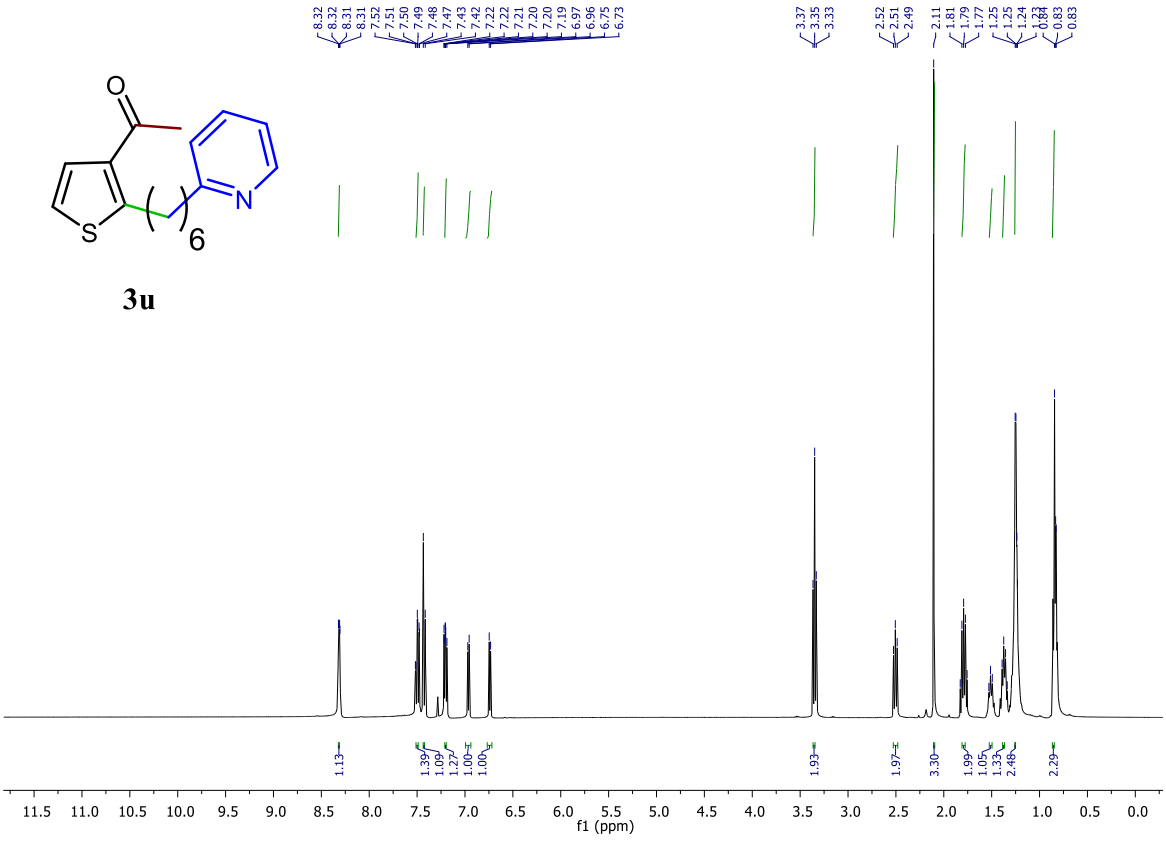
3t

^{13}C NMR of 3t (101 MHz, 512 scans, RT, $CDCl_3$)



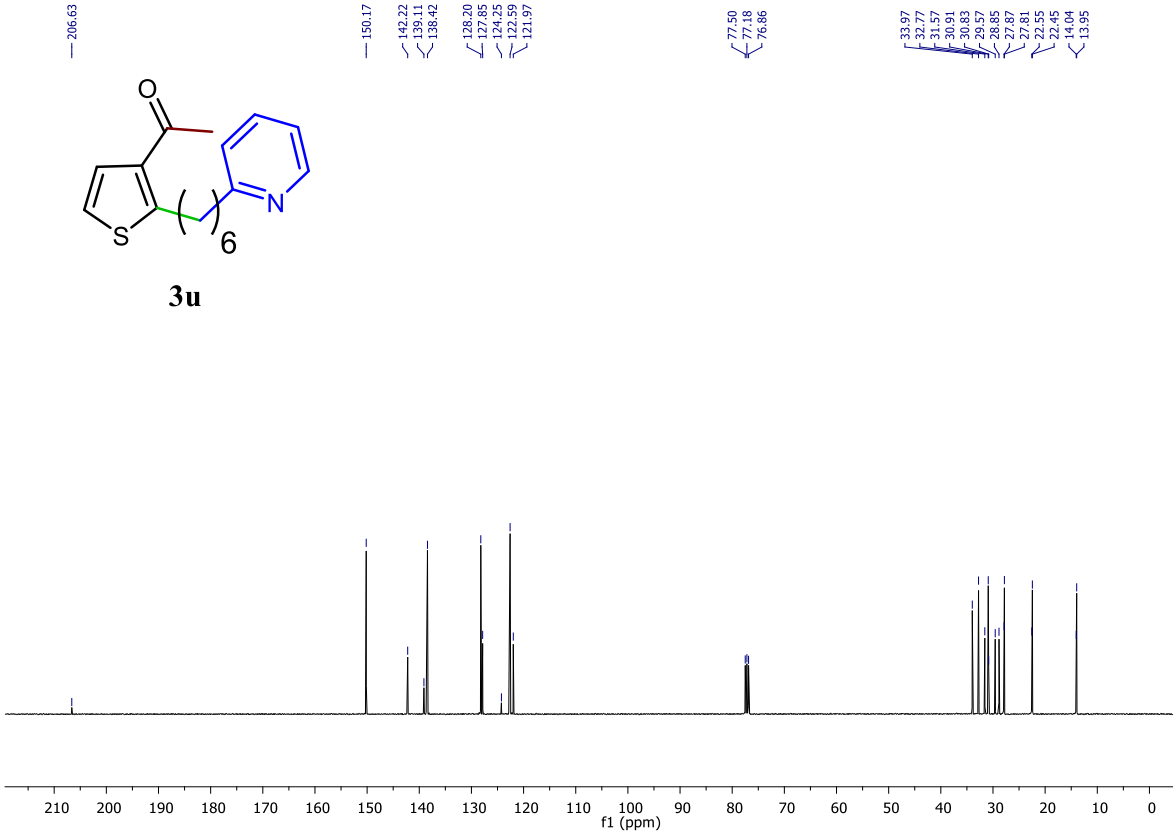
3t

^{1}H NMR of 3u (400 MHz, 32 scans, RT, $CDCl_3$)



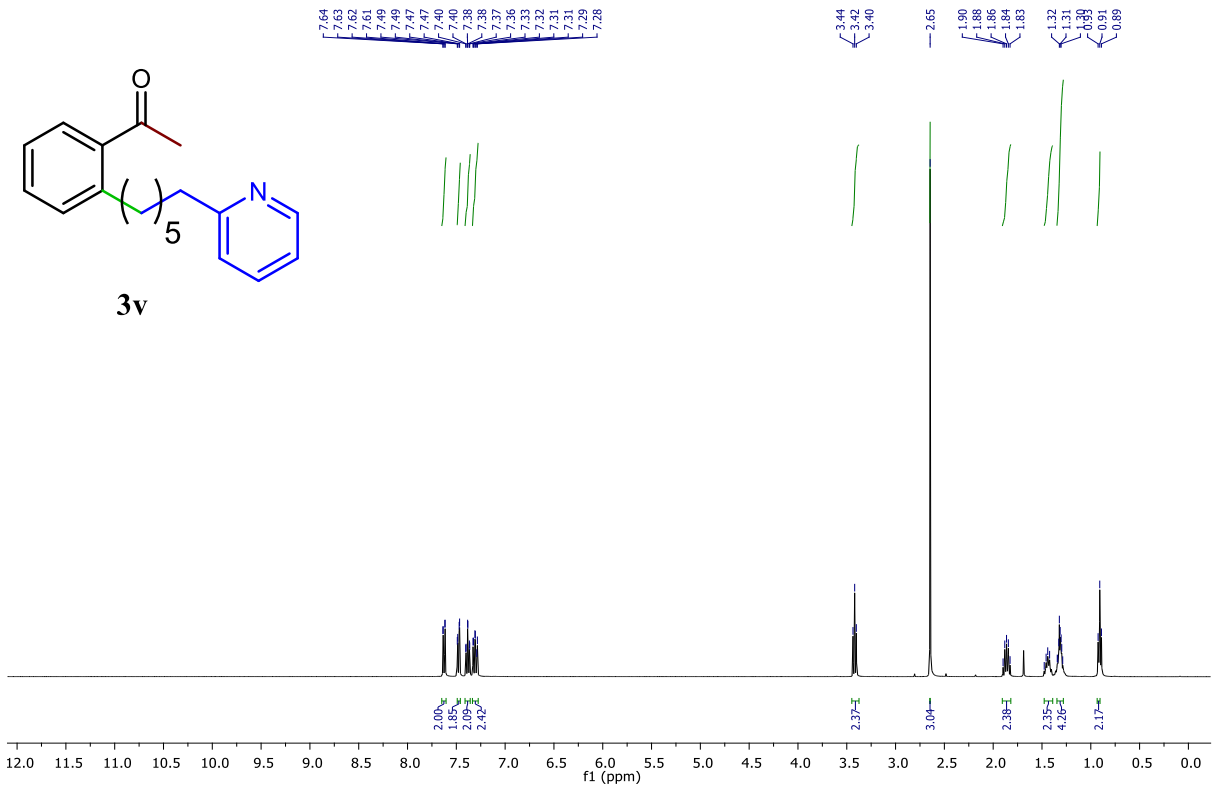
3u

^{13}C NMR of 3u (101 MHz, 512 scans, RT, $CDCl_3$)



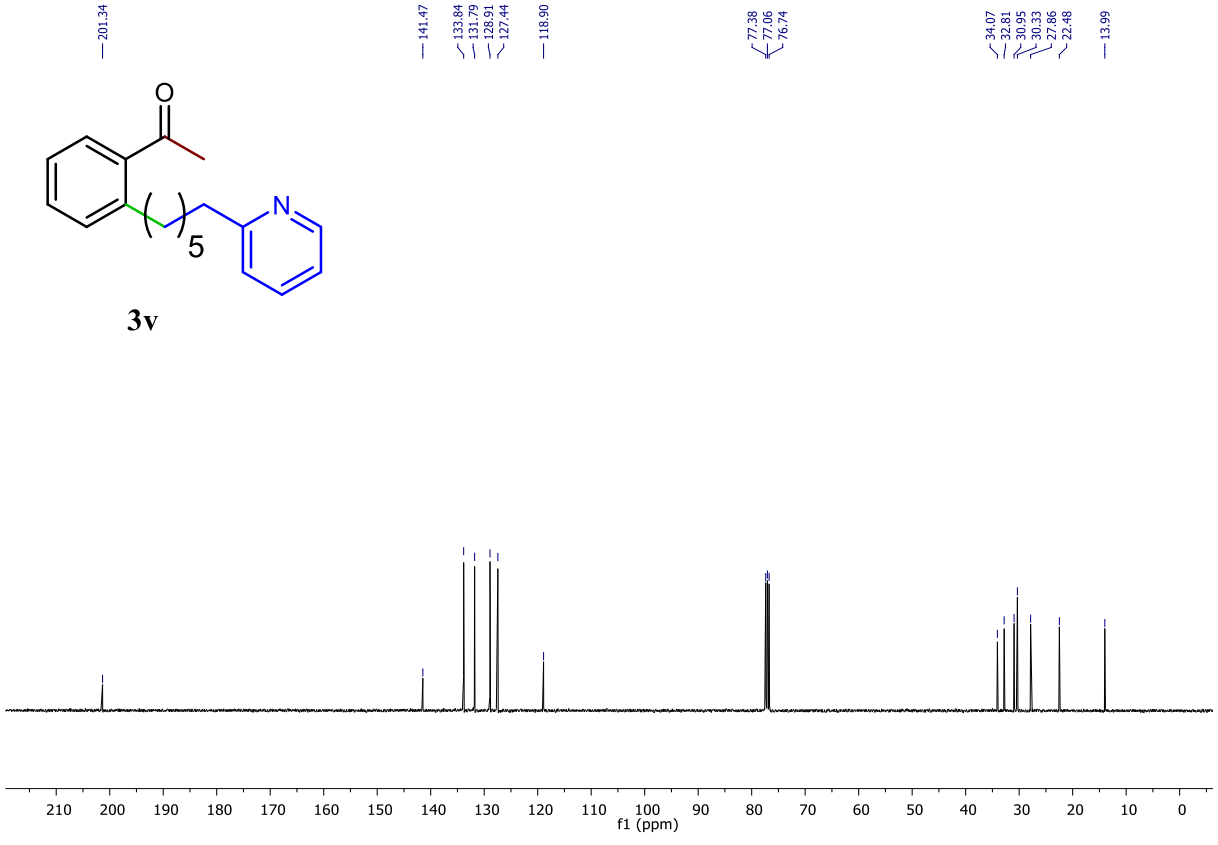
3u

^{1}H NMR of 3v (400 MHz, 32 scans, RT, $CDCl_3$)



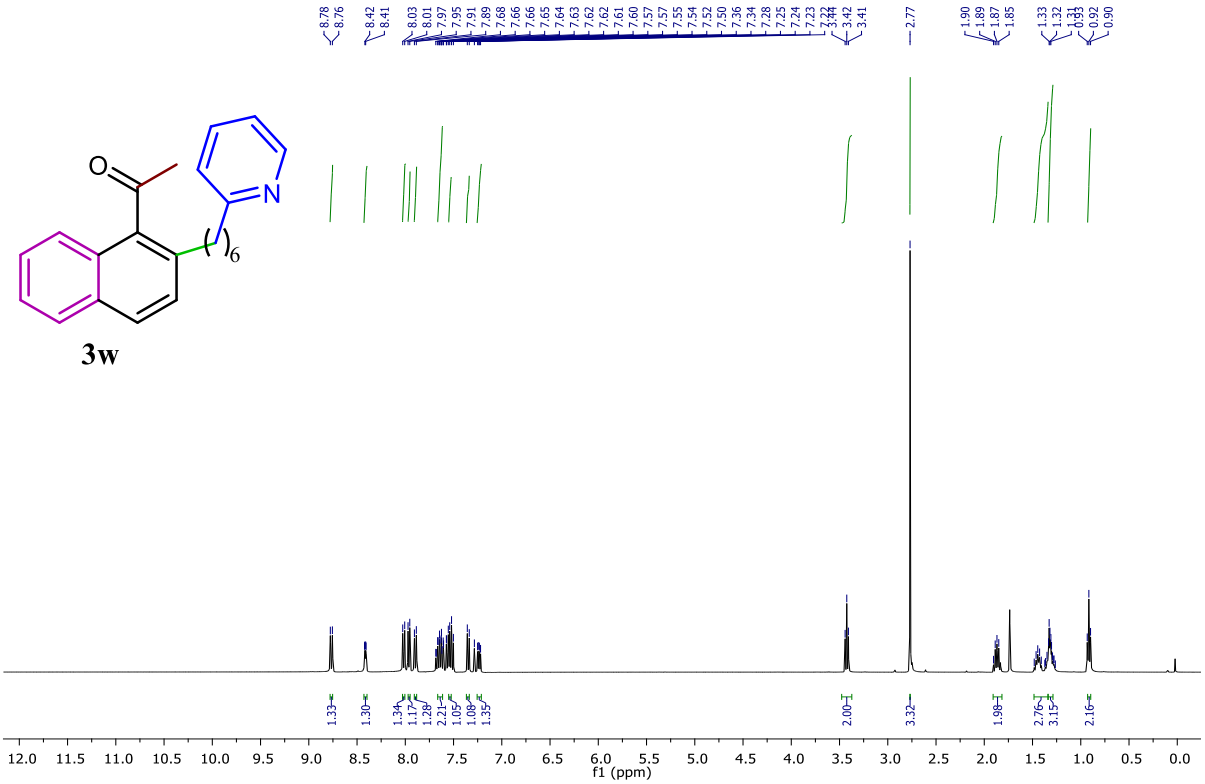
3v

^{13}C NMR of 3v (101 MHz, 512 scans, RT, $CDCl_3$)

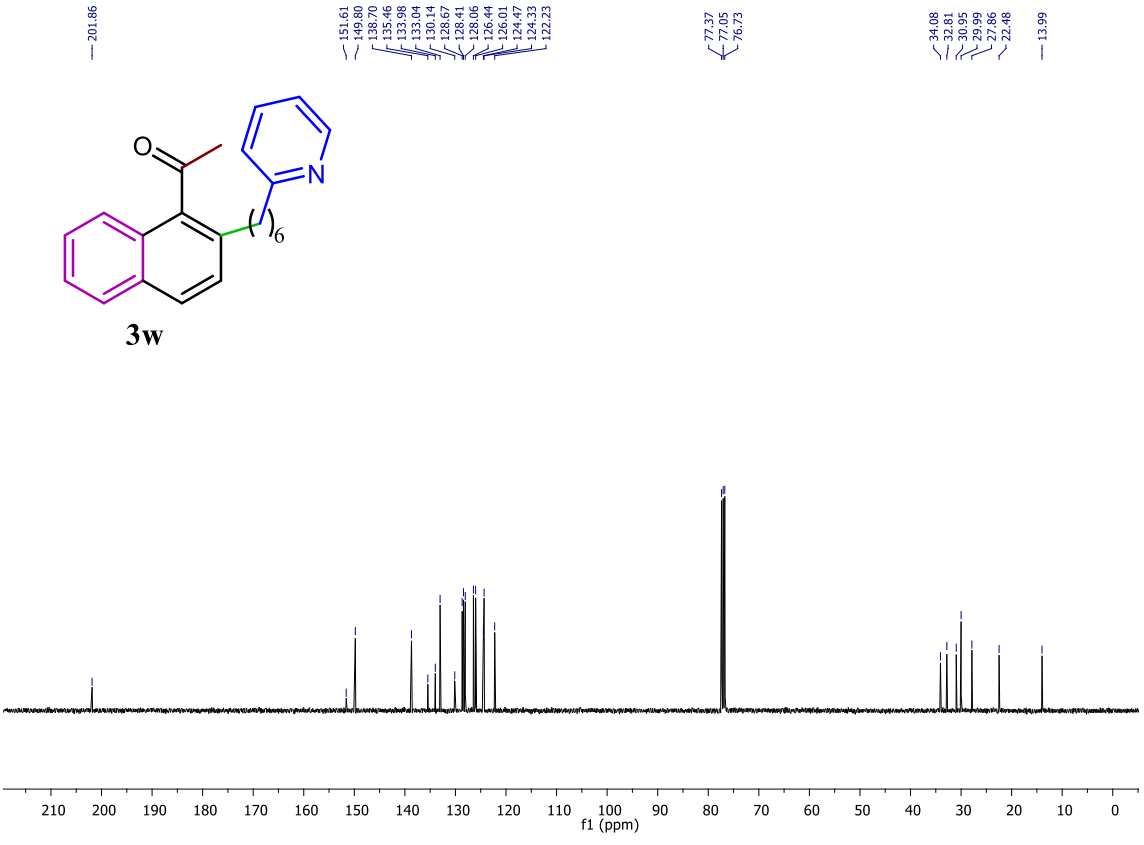


3v

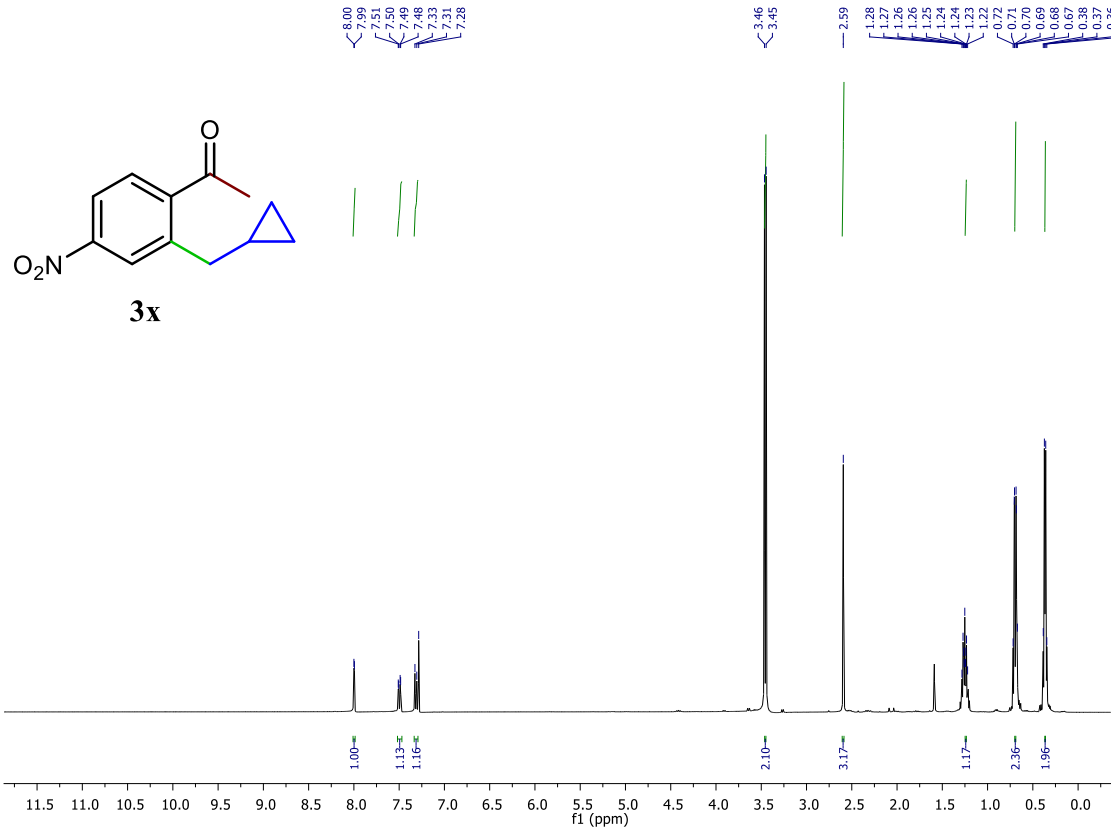
^{1}H NMR of 3w (400 MHz, 32 scans, RT, $CDCl_3$)



^{13}C NMR of 3w (101 MHz, 512 scans, RT, $CDCl_3$)

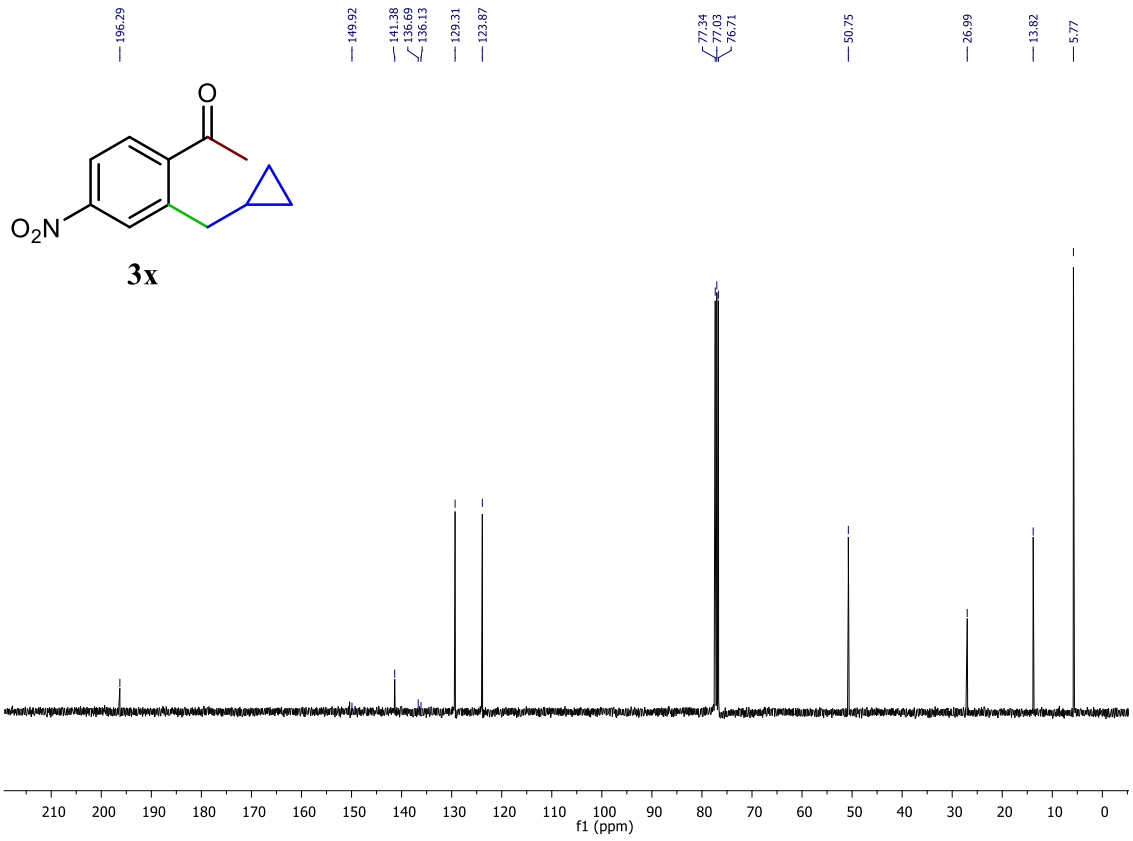


^{1}H NMR of 3x (400 MHz, 32 scans, RT, $CDCl_3$)



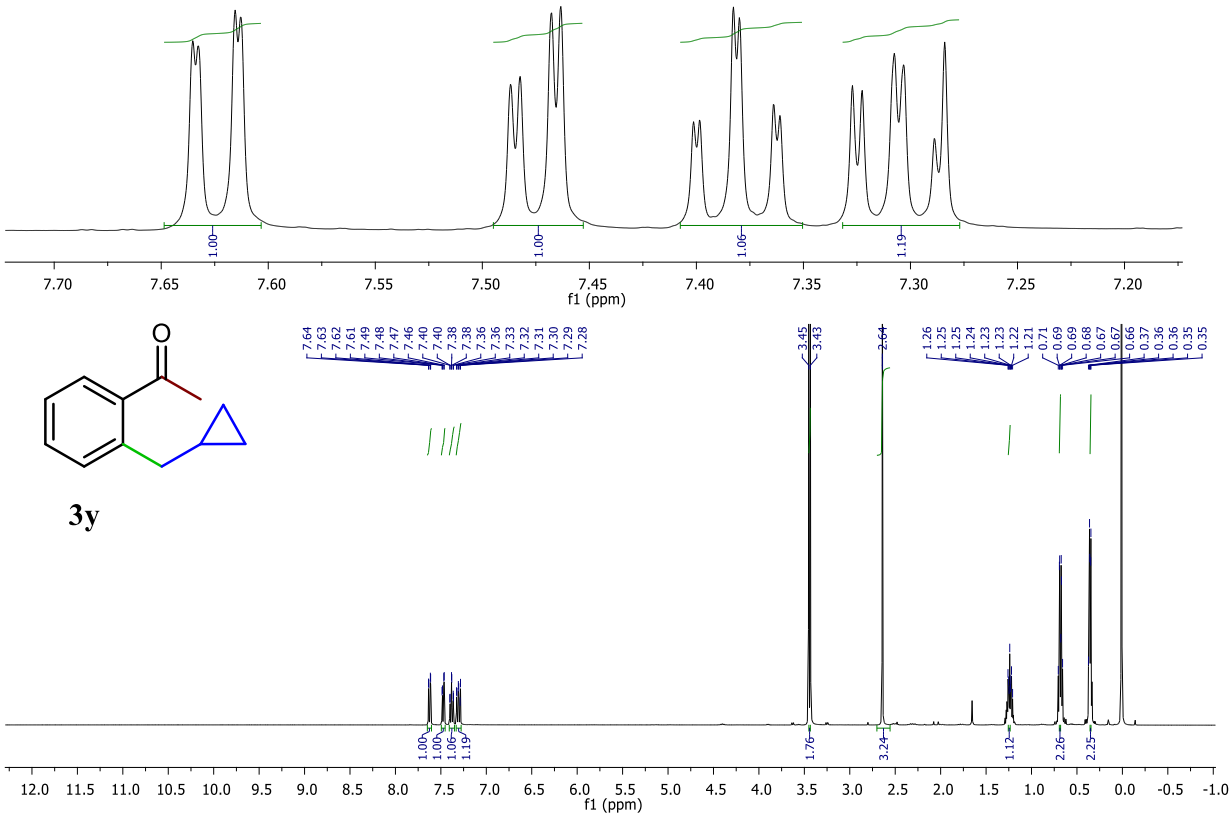
3x

^{13}C NMR of 3x (101 MHz, 512 scans, RT, $CDCl_3$)



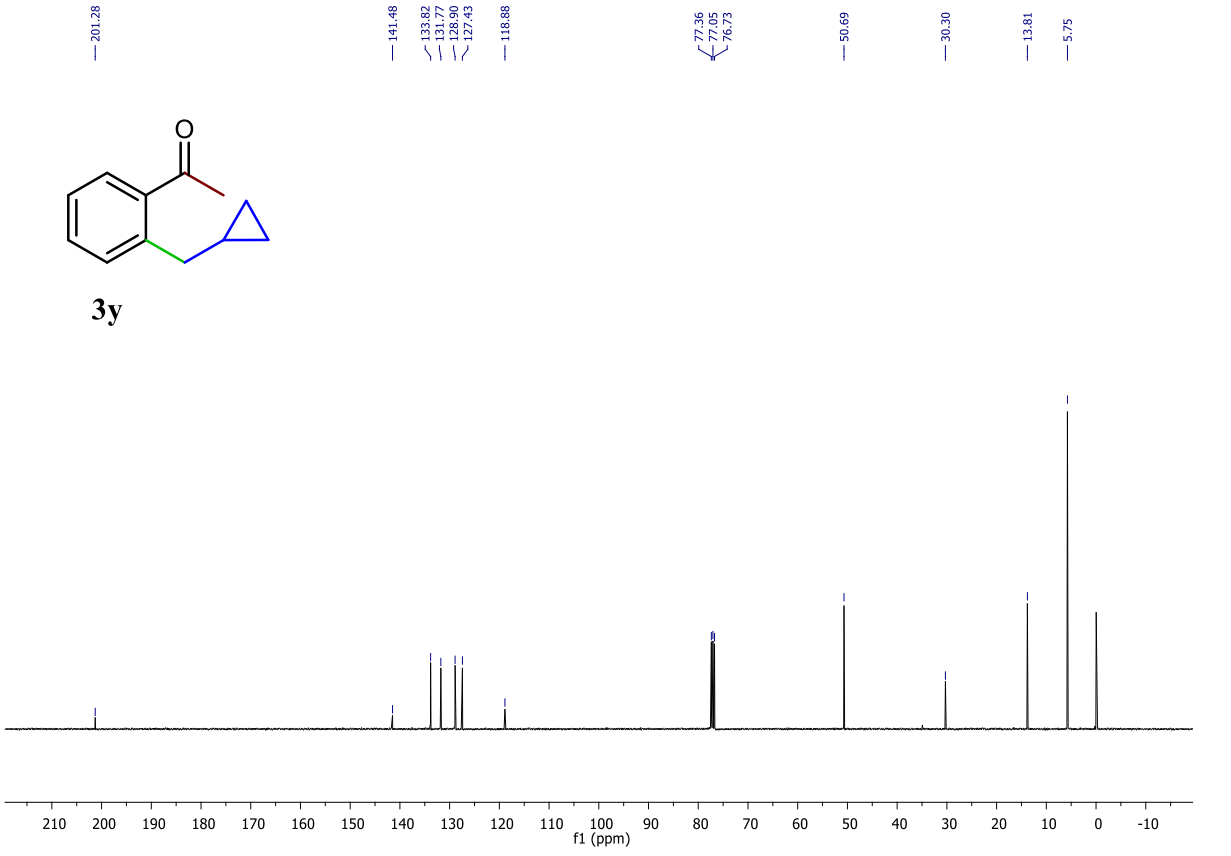
3x

^{1}H NMR of 3y (400 MHz, 32 scans, RT, $CDCl_3$)



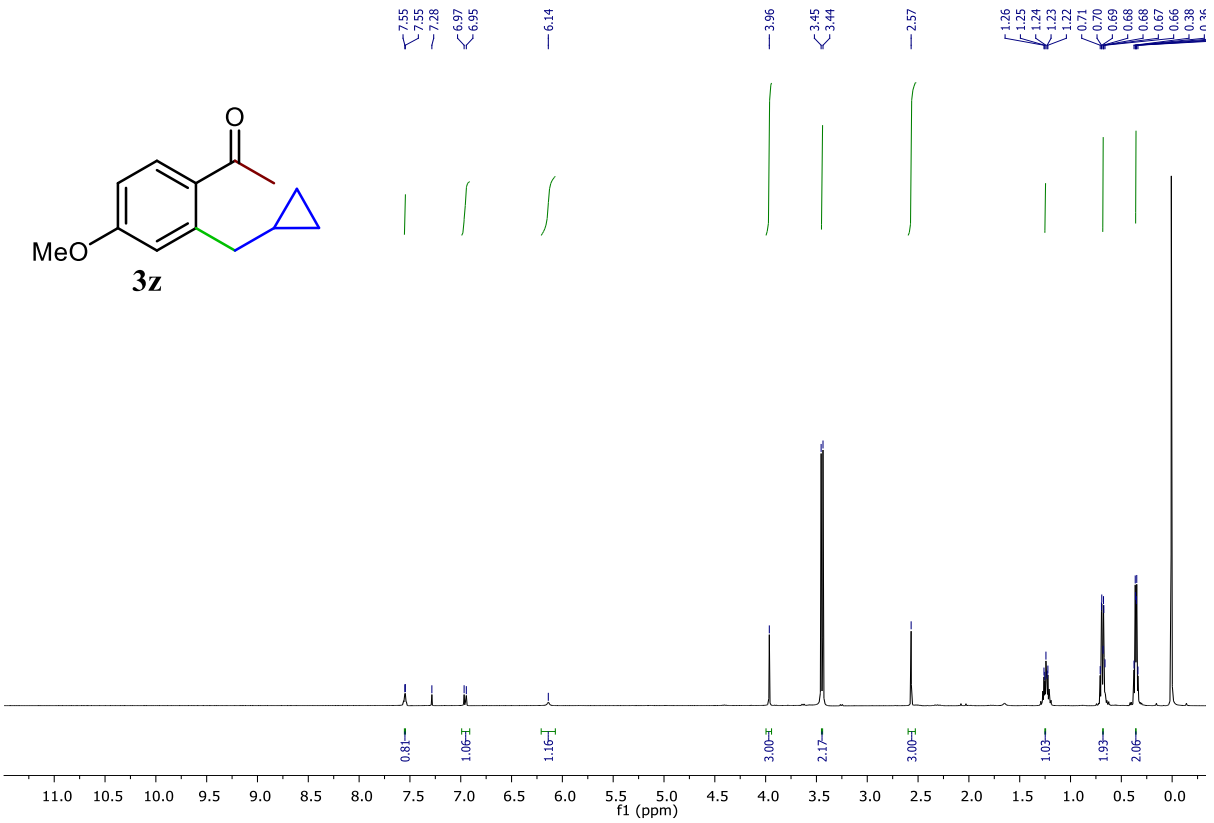
3y

^{13}C NMR of 3y (101 MHz, 512 scans, RT, $CDCl_3$)

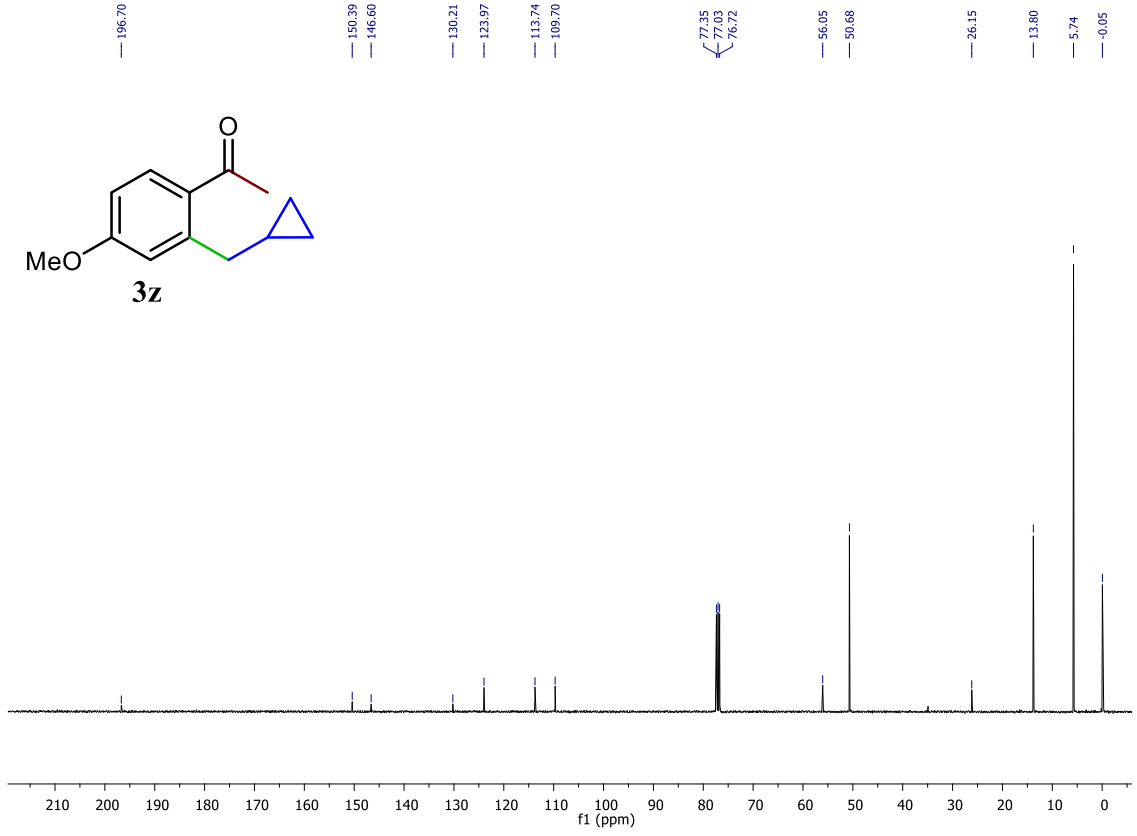


3y

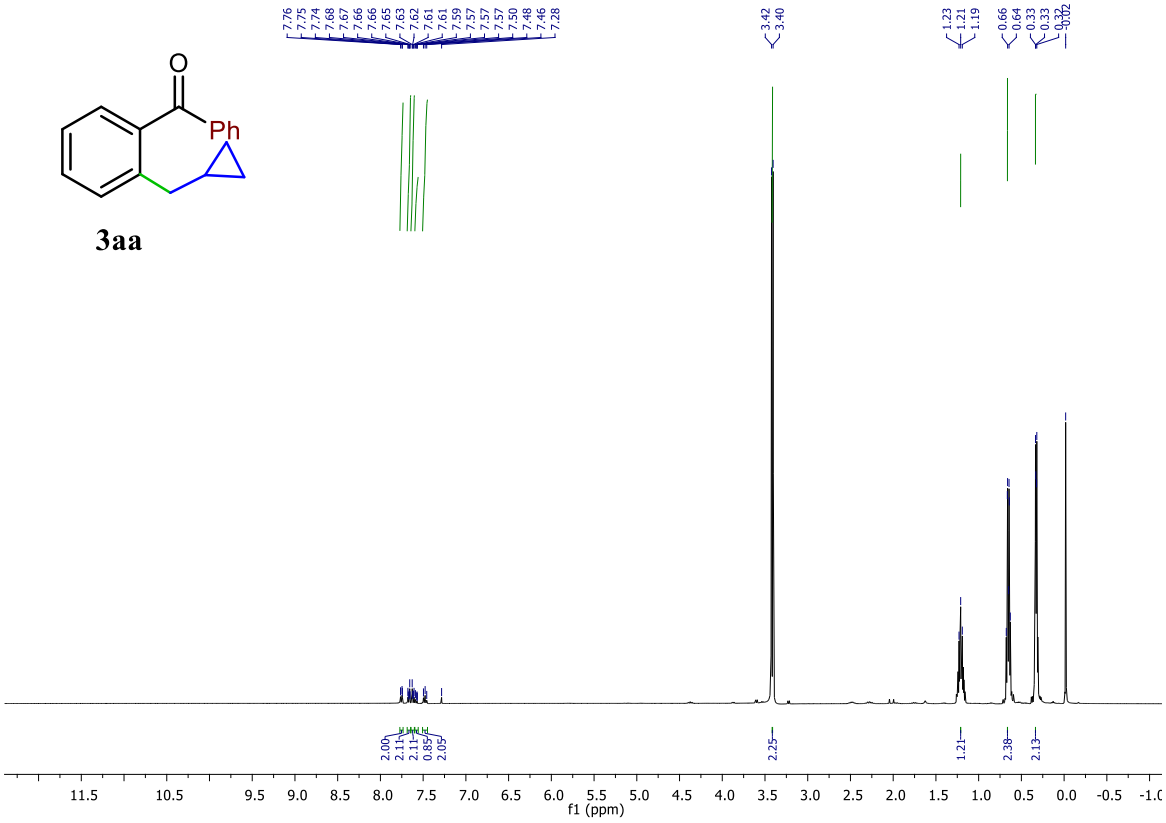
^{1}H NMR of 3z (400 MHz, 32 scans, RT, $CDCl_3$)



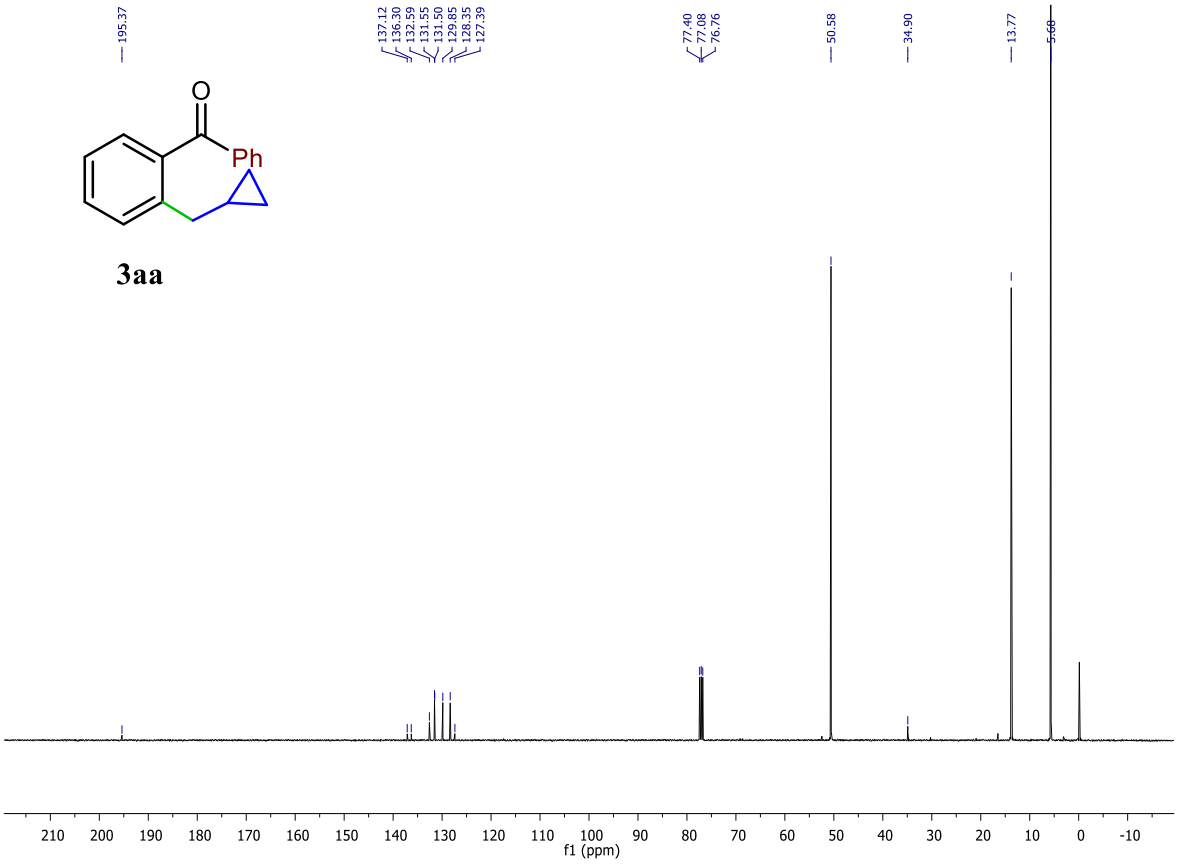
^{13}C NMR of 3z (101 MHz, 512 scans, RT, $CDCl_3$)



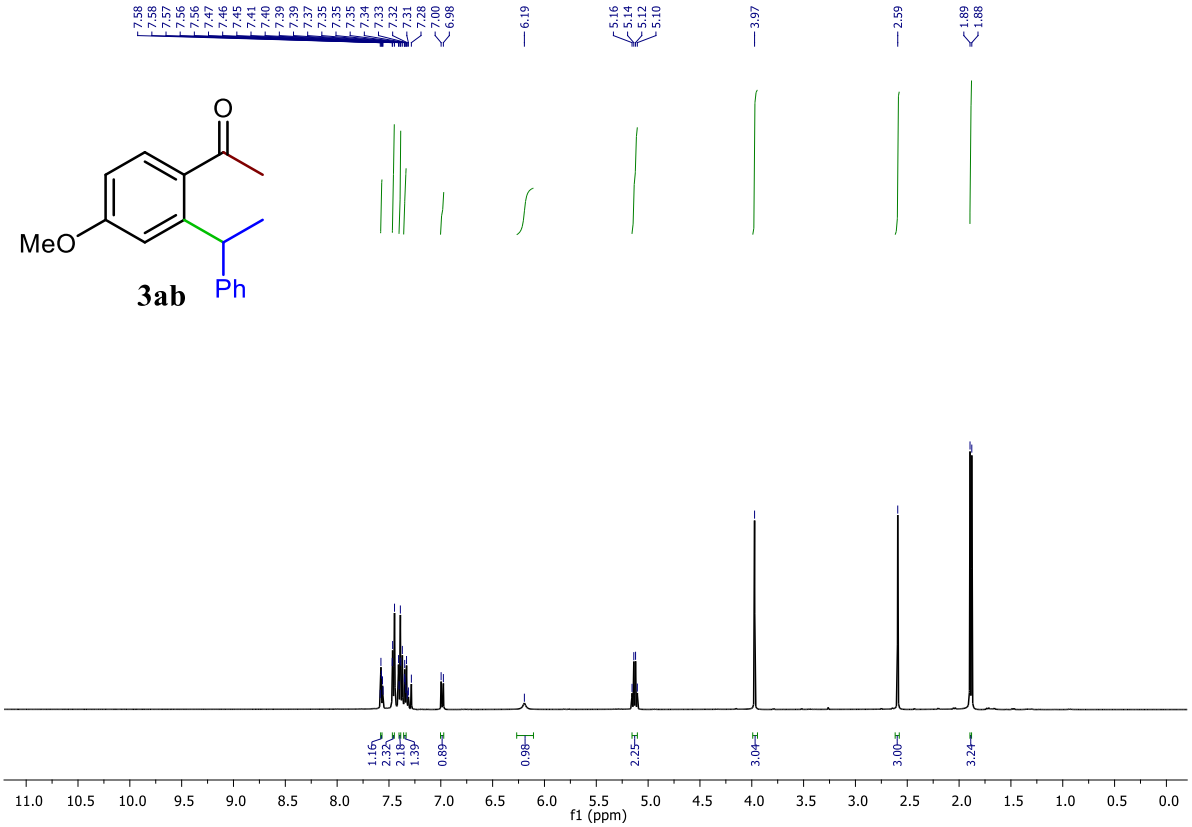
^{1}H NMR of 3aa (400 MHz, 32 scans, RT, $CDCl_3$)



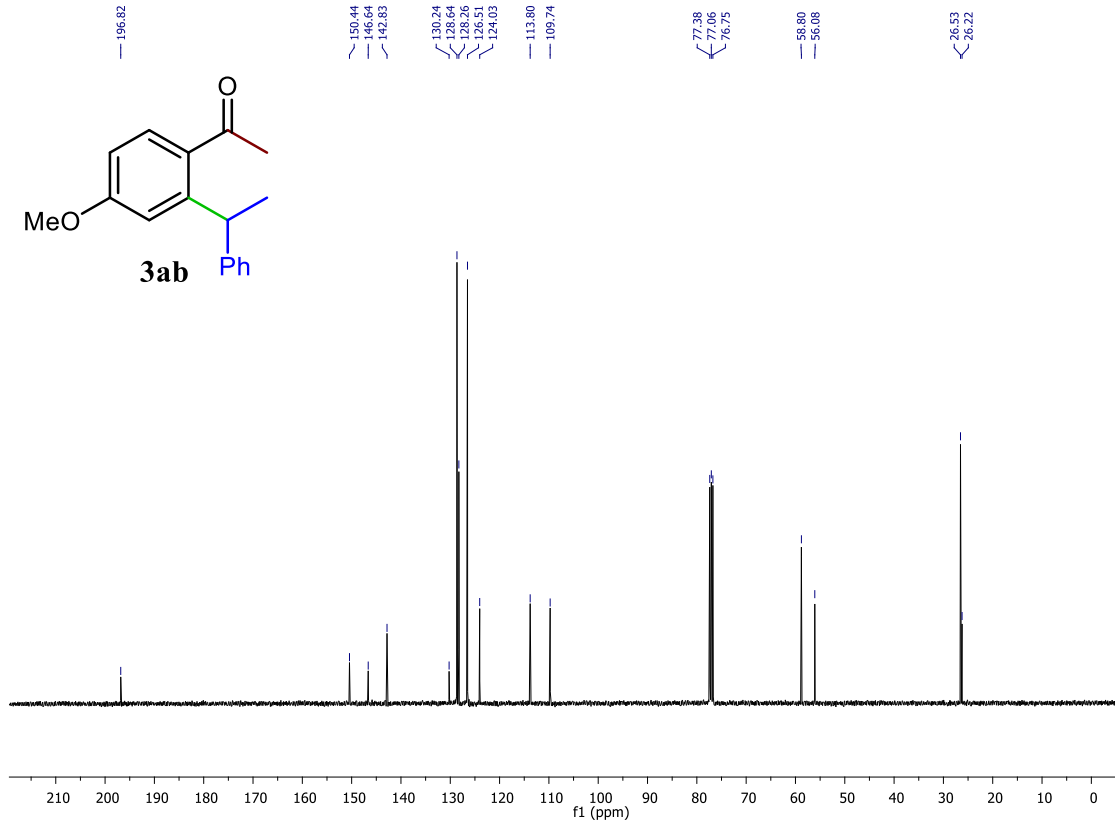
^{13}C NMR of 3aa (101 MHz, 512 scans, RT, $CDCl_3$)



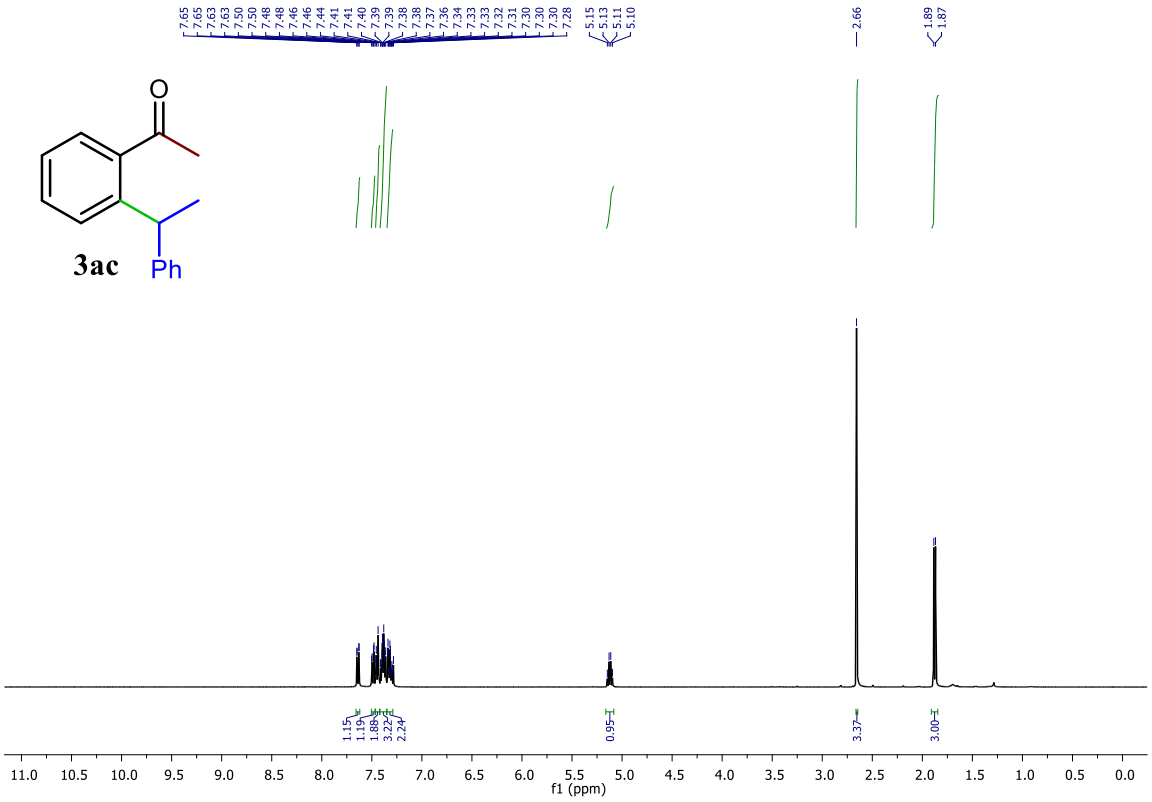
^{1}H NMR of 3ab (400 MHz, 32 scans, RT, $CDCl_3$)



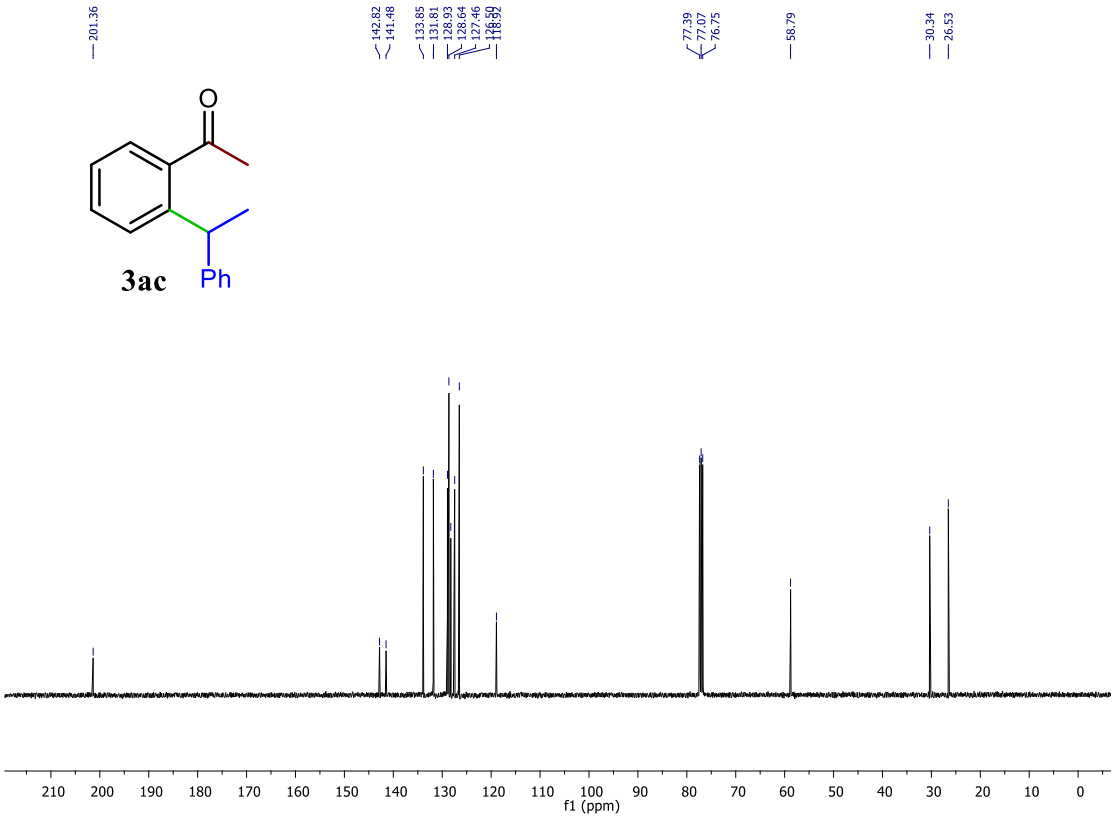
^{13}C NMR of 3ab (101 MHz, 512 scans, RT, $CDCl_3$)



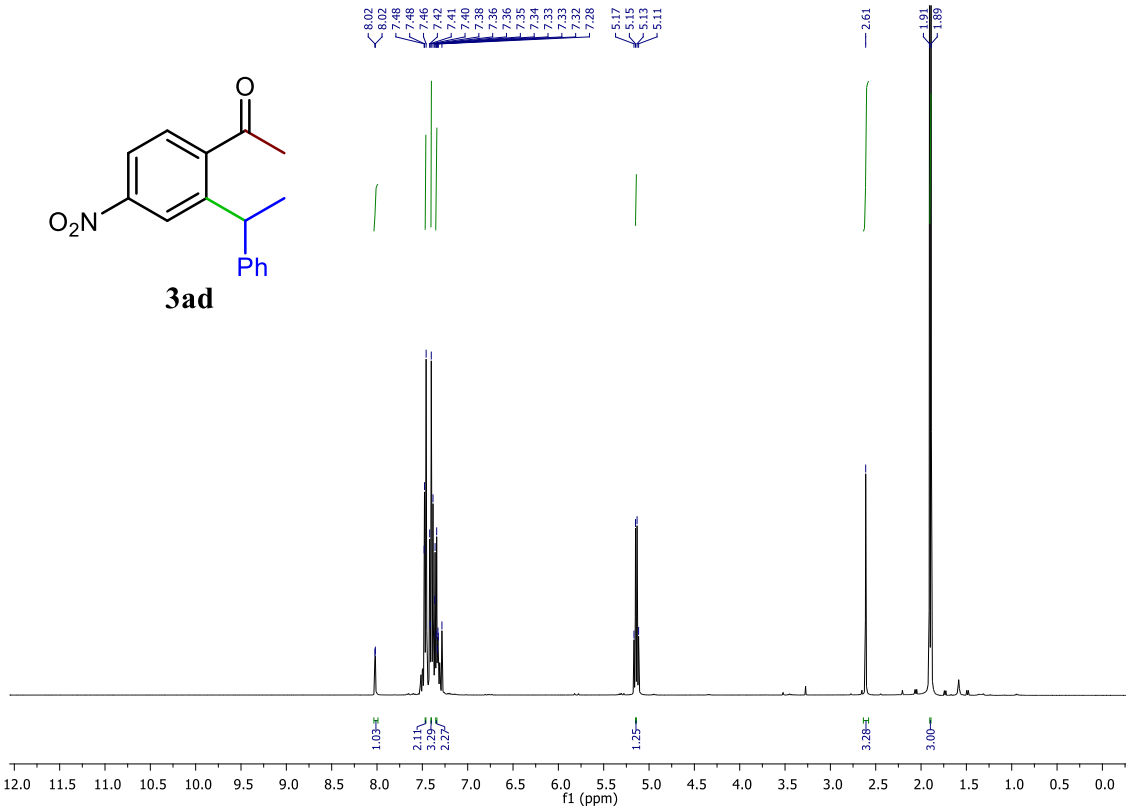
^{1}H NMR of 3ac (400 MHz, 32 scans, RT, $CDCl_3$)



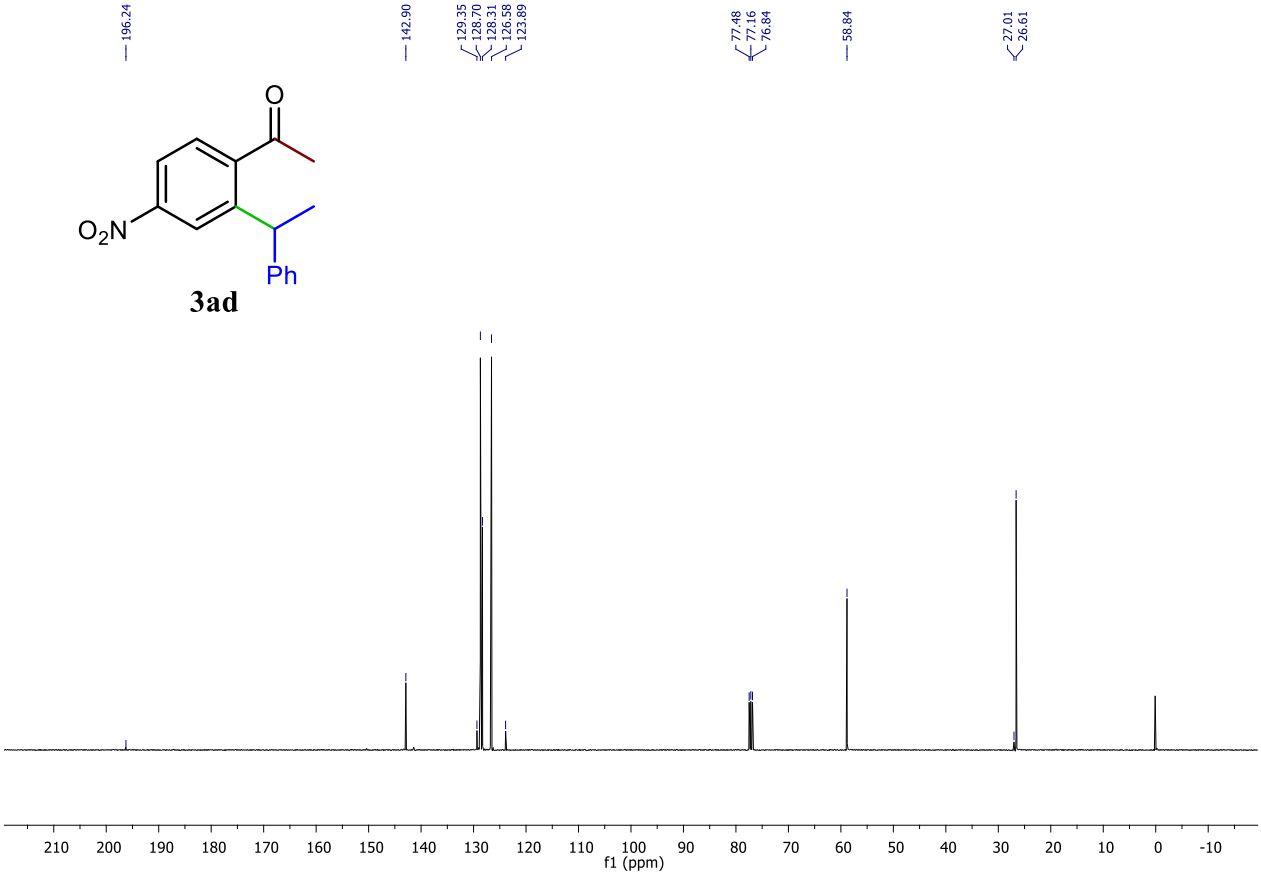
^{13}C NMR of 3ac (101 MHz, 512 scans, RT, $CDCl_3$)



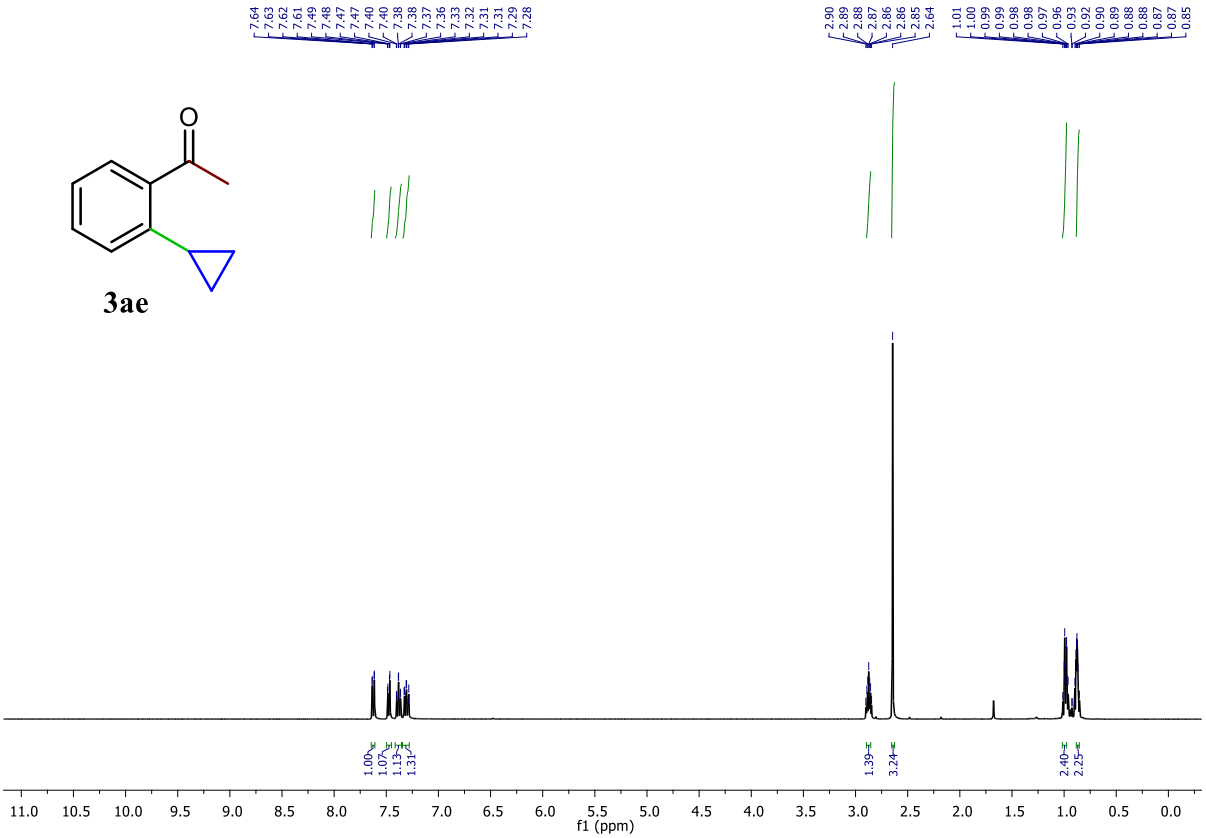
^{1}H NMR of 3ad (400 MHz, 32 scans, RT, $CDCl_3$)



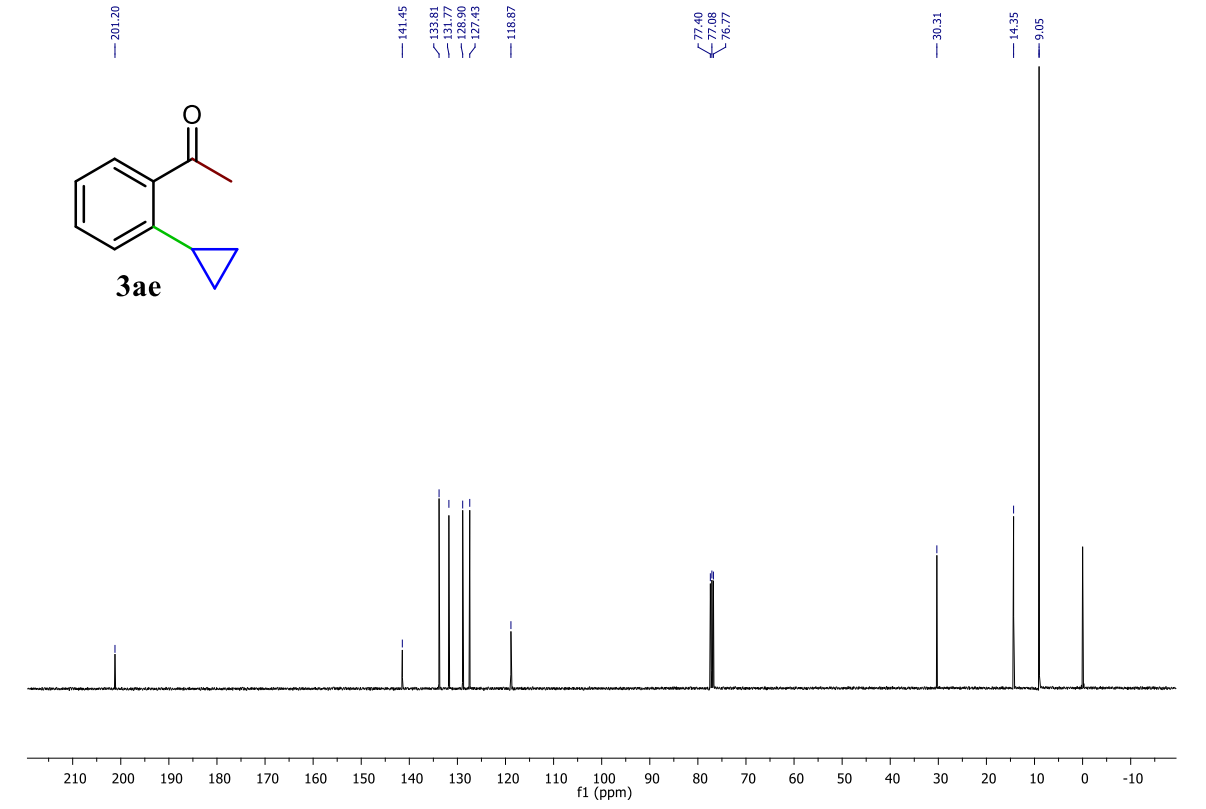
^{13}C NMR of 3ad (101 MHz, 512 scans, RT, $CDCl_3$)



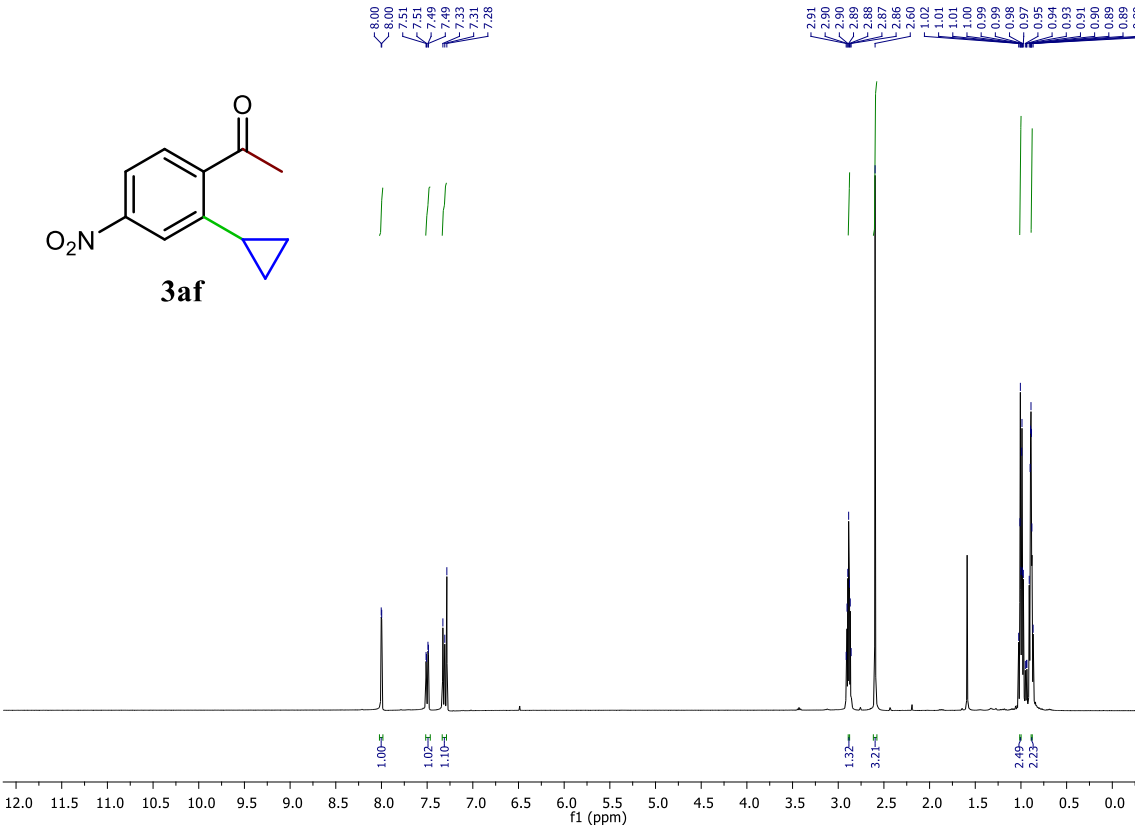
^{1}H NMR of 3ae (400 MHz, 32 scans, RT, $CDCl_3$)



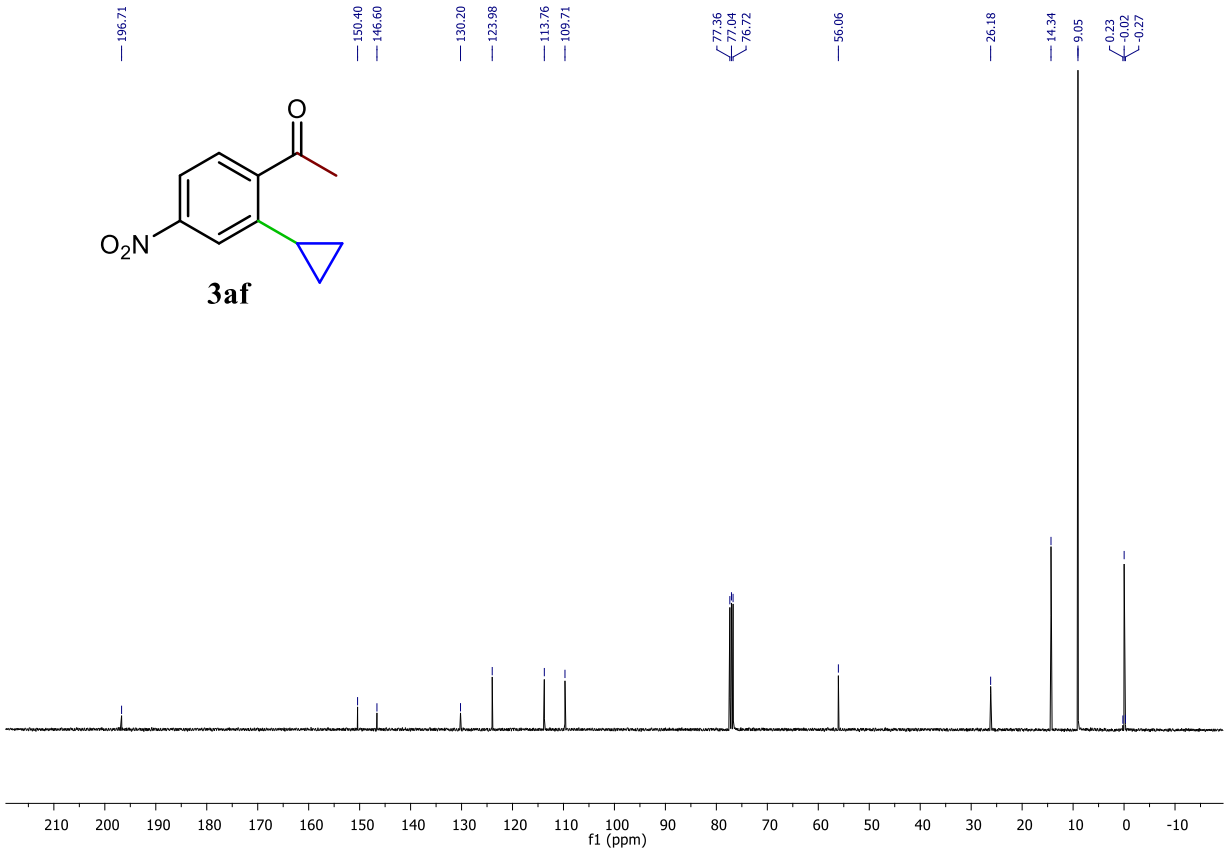
^{13}C NMR of 3ae (101 MHz, 512 scans, RT, $CDCl_3$)



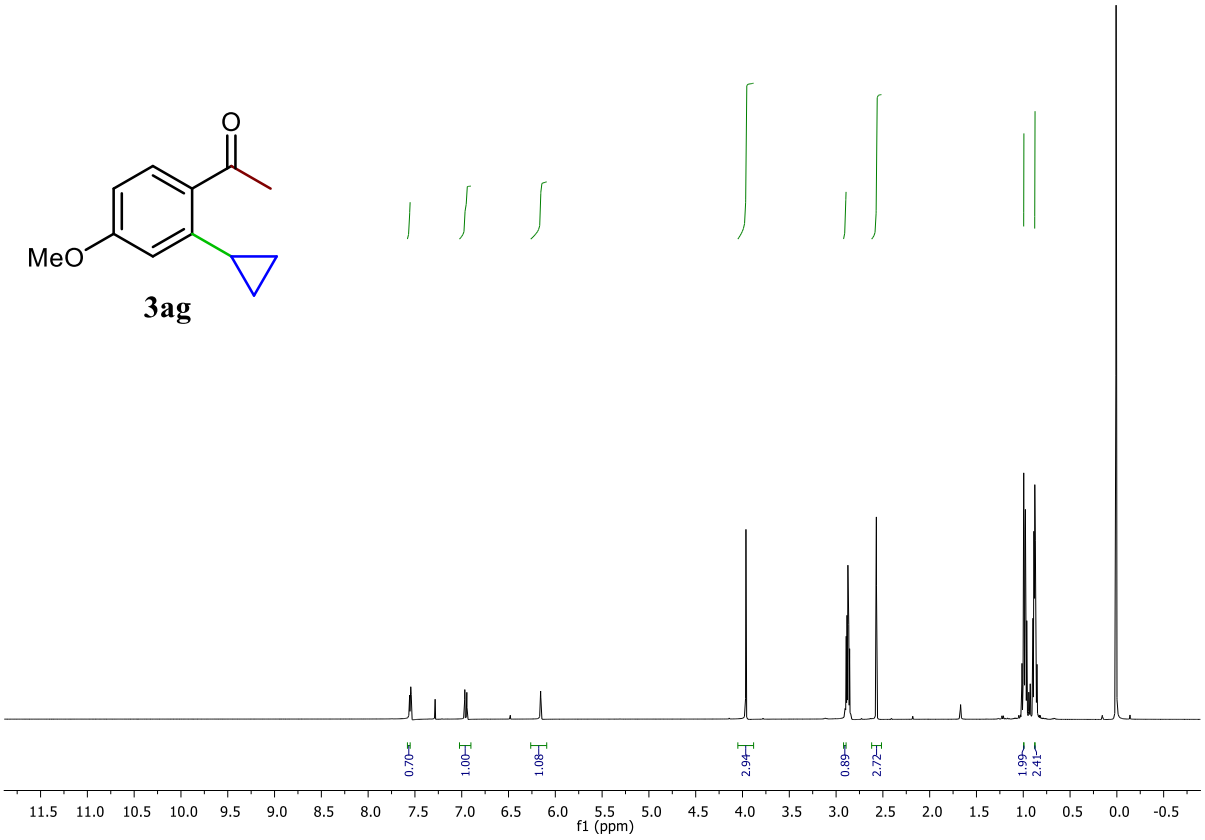
^{1}H NMR of 3af (400 MHz, 32 scans, RT, $CDCl_3$)



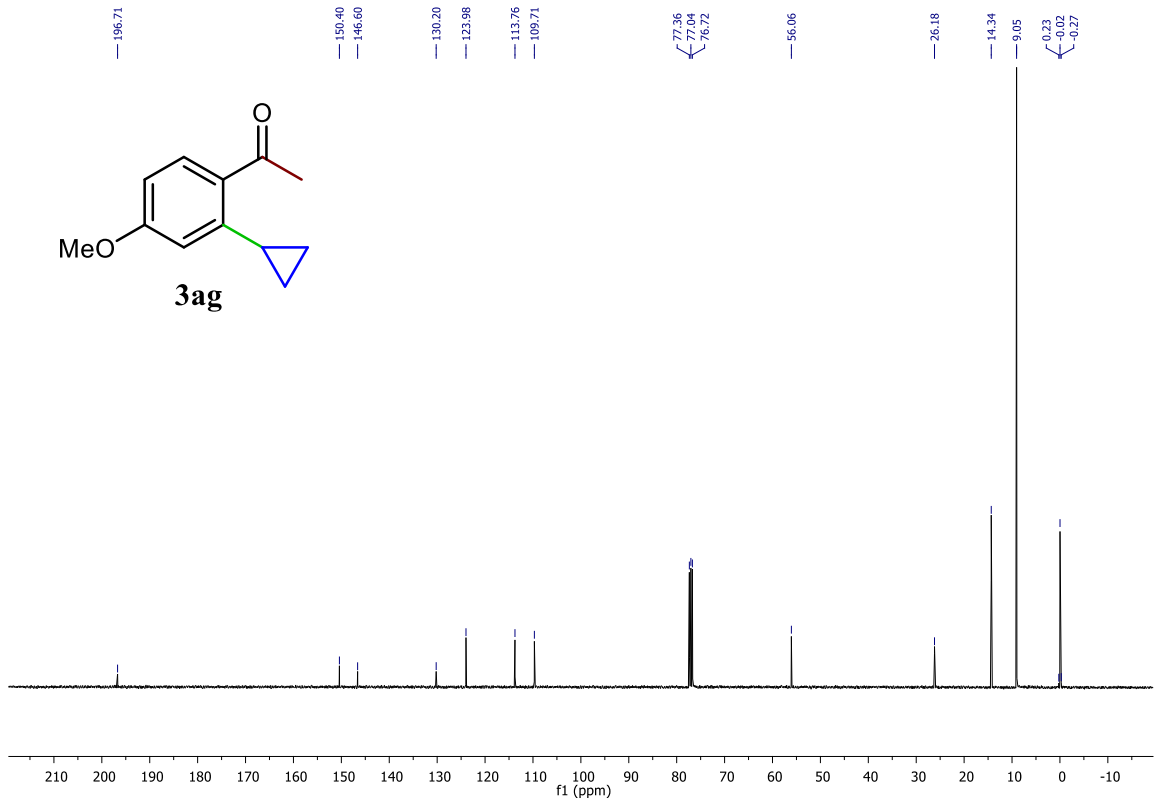
^{13}C NMR of 3af (101 MHz, 512 scans, RT, $CDCl_3$)



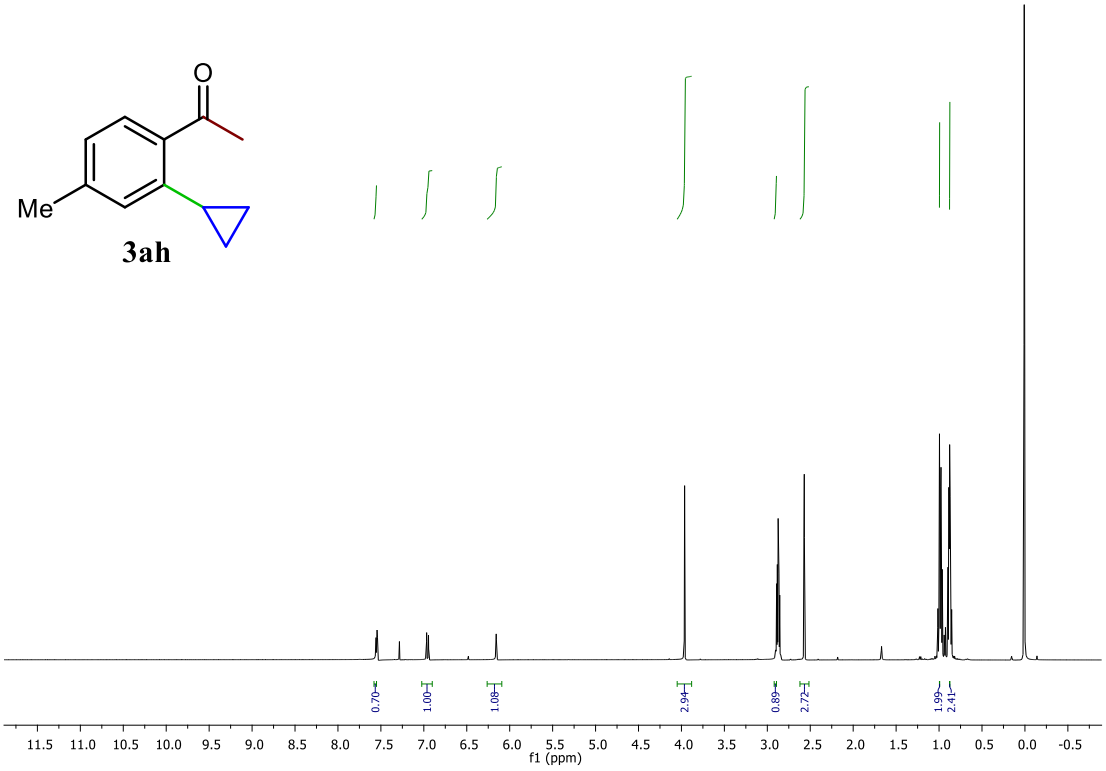
^{1}H NMR of 3ag (400 MHz, 32 scans, RT, $CDCl_3$)



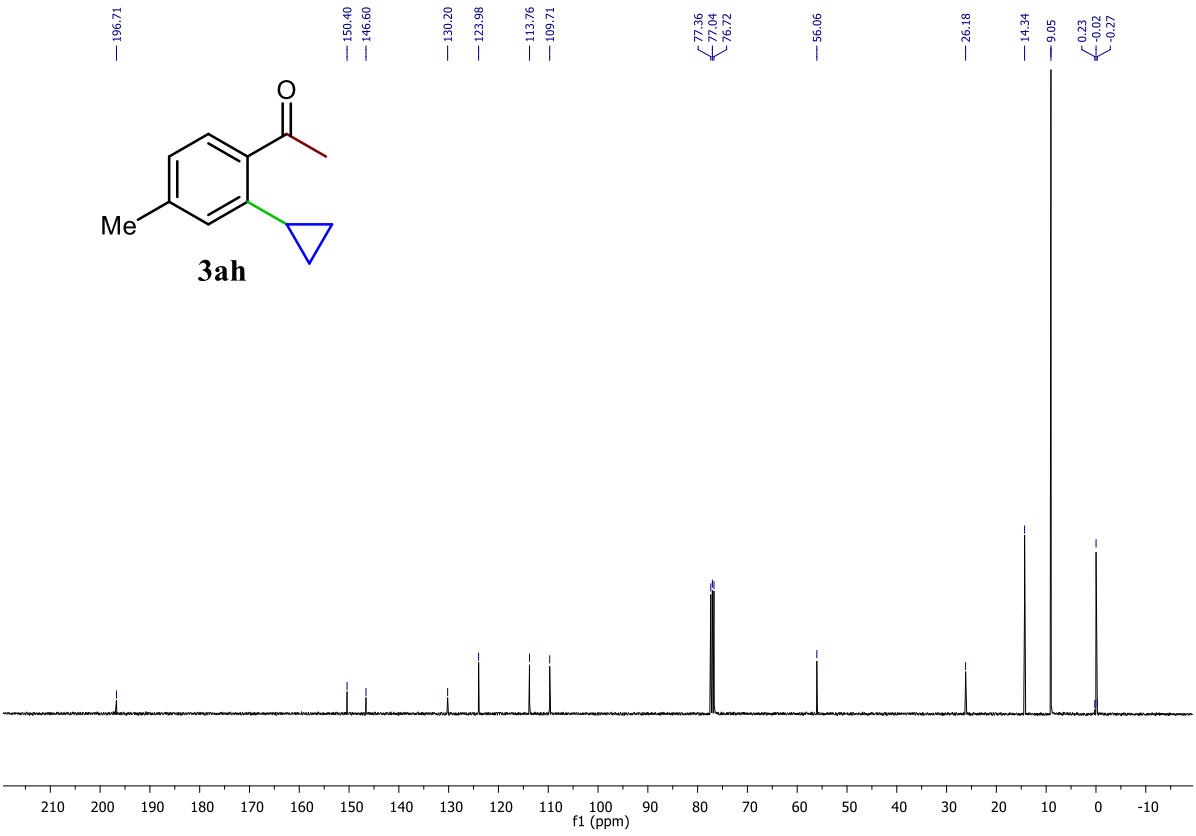
^{13}C NMR of 3ag (101 MHz, 512 scans, RT, $CDCl_3$)



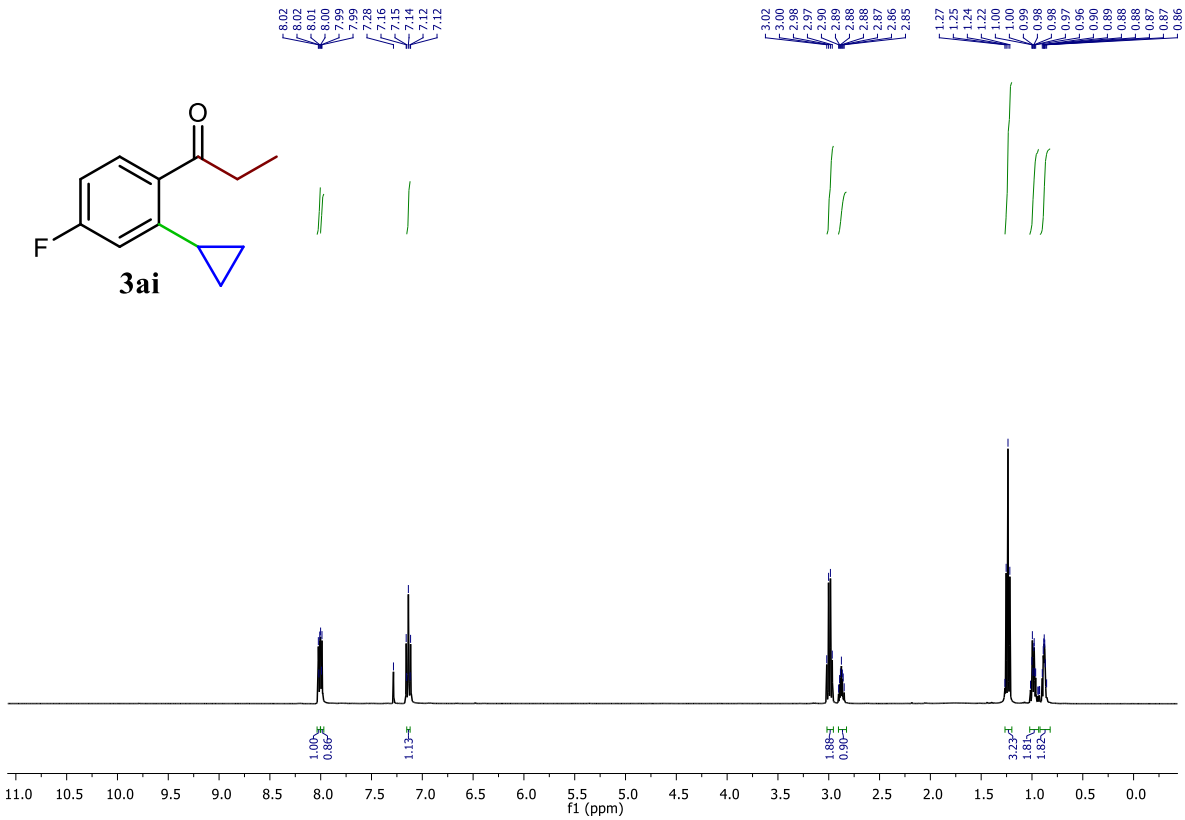
^{1}H NMR of 3ah (400 MHz, 32 scans, RT, $CDCl_3$)



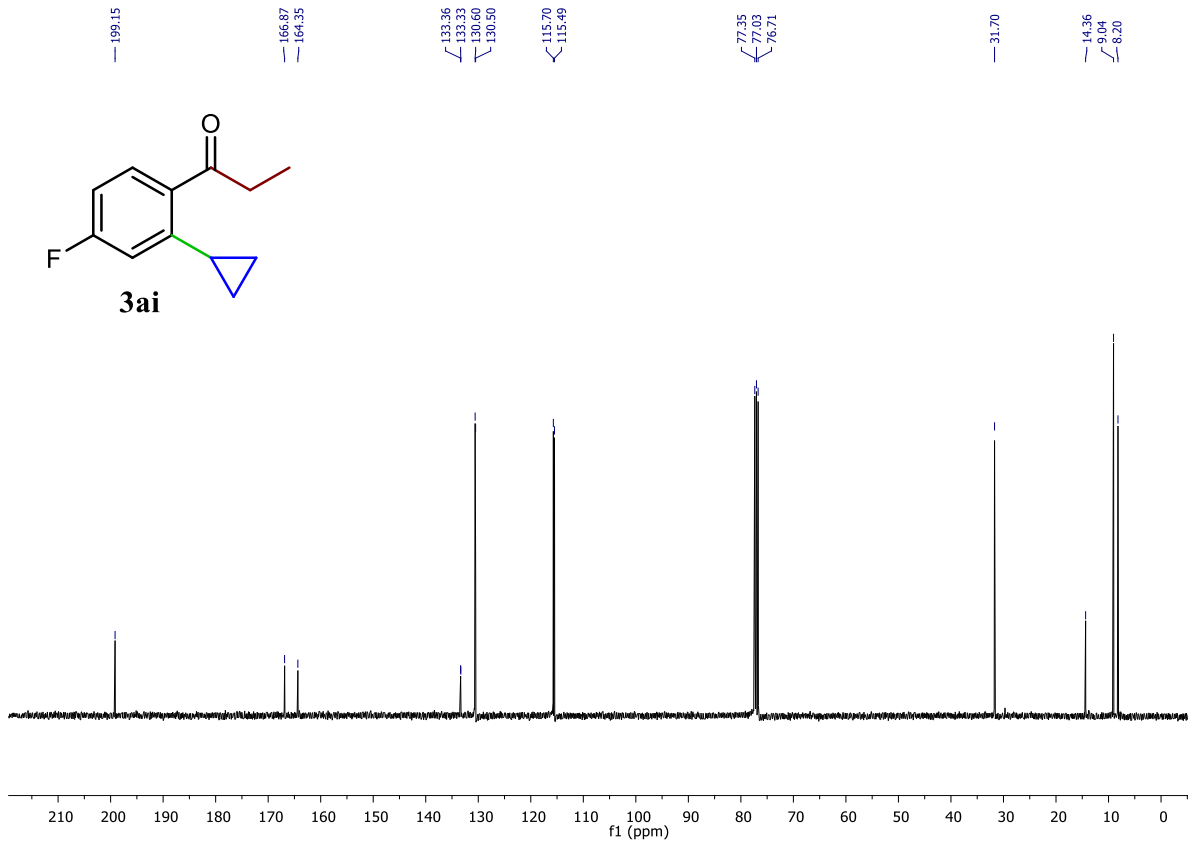
^{13}C NMR of 3ah (101 MHz, 512 scans, RT, $CDCl_3$)



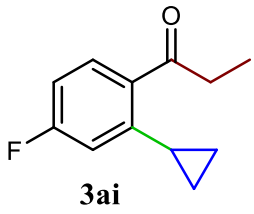
^{1}H NMR of 3ai (400 MHz, 32 scans, RT, $CDCl_3$)



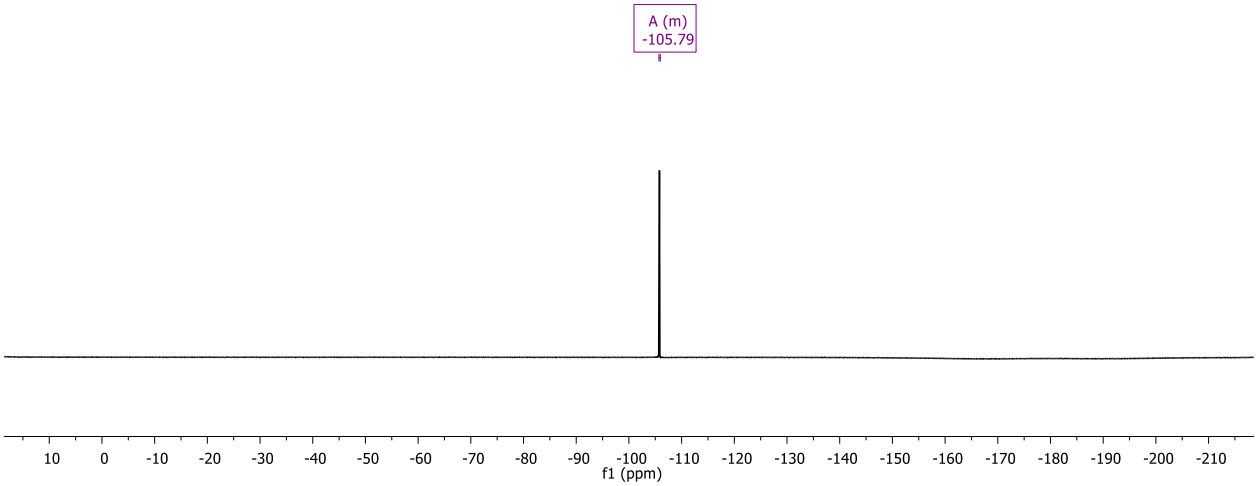
^{13}C NMR of 3ai (101 MHz, 512 scans, RT, $CDCl_3$)



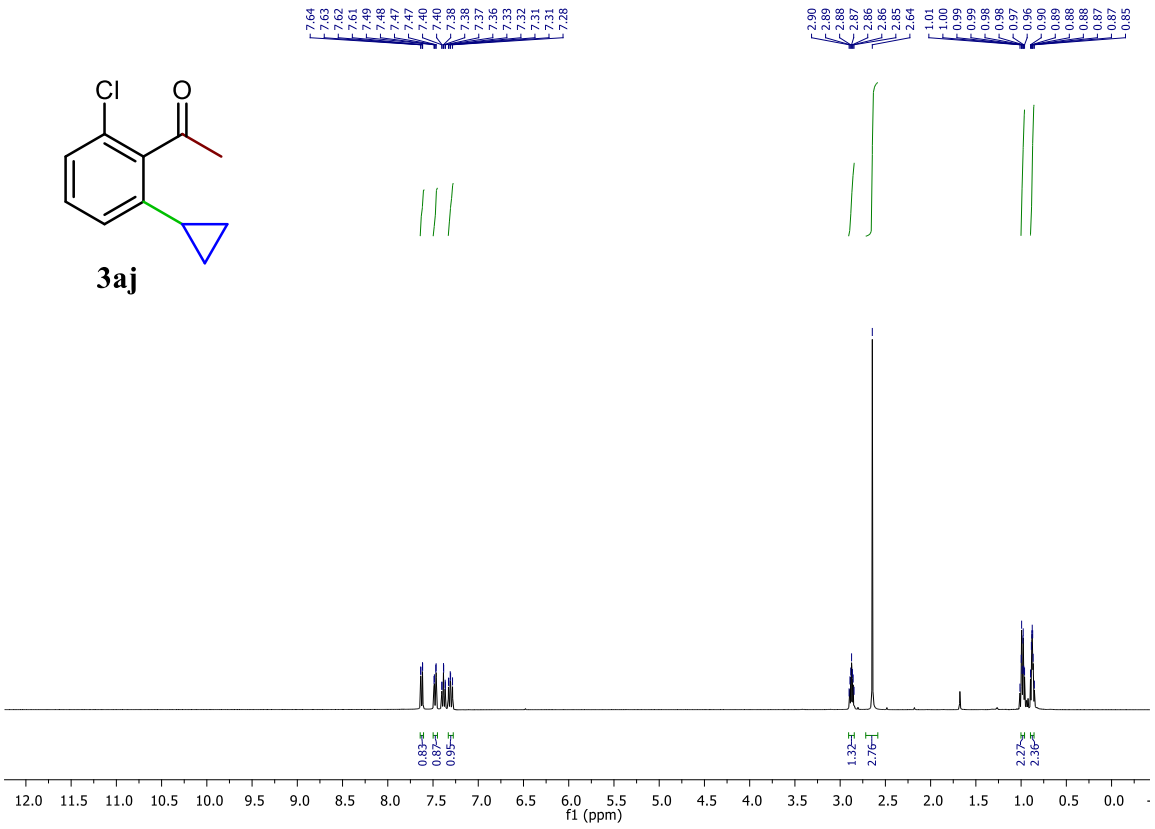
^{19}F NMR of **3ai (377 MHz, $CDCl_3$)**



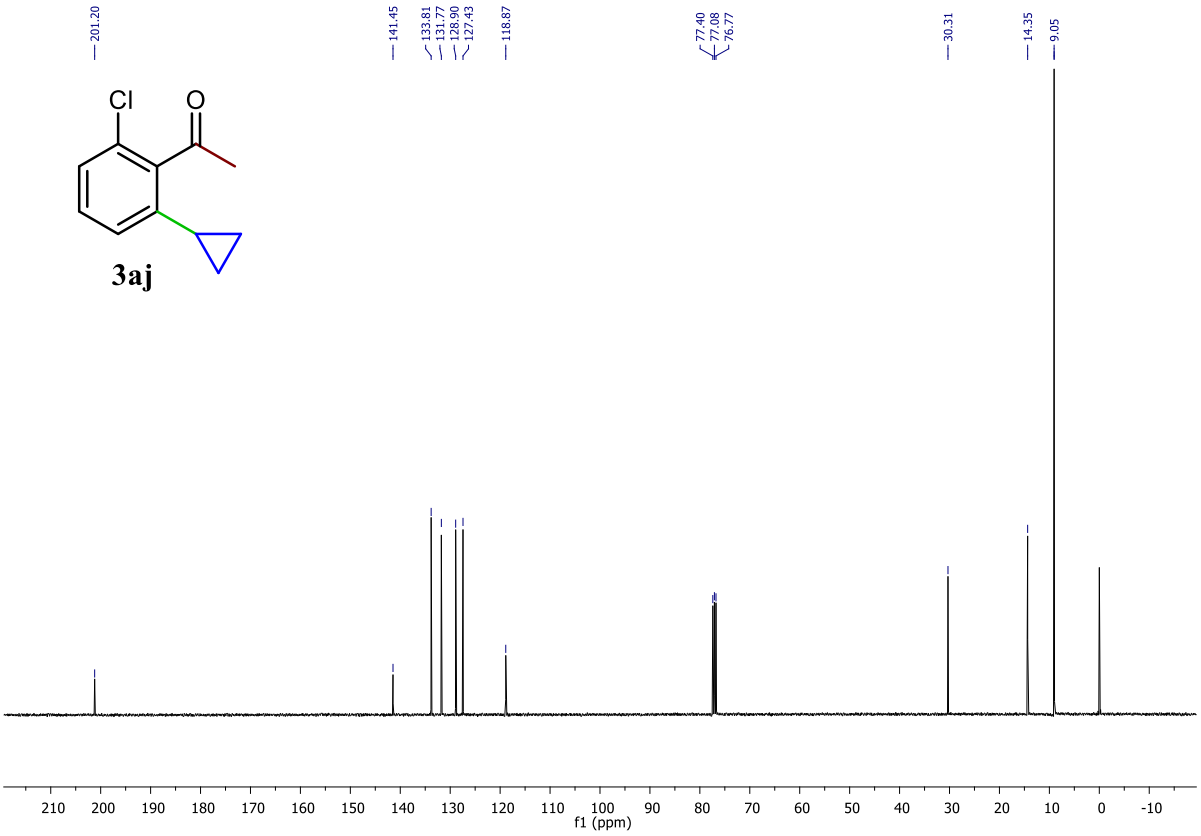
3ai



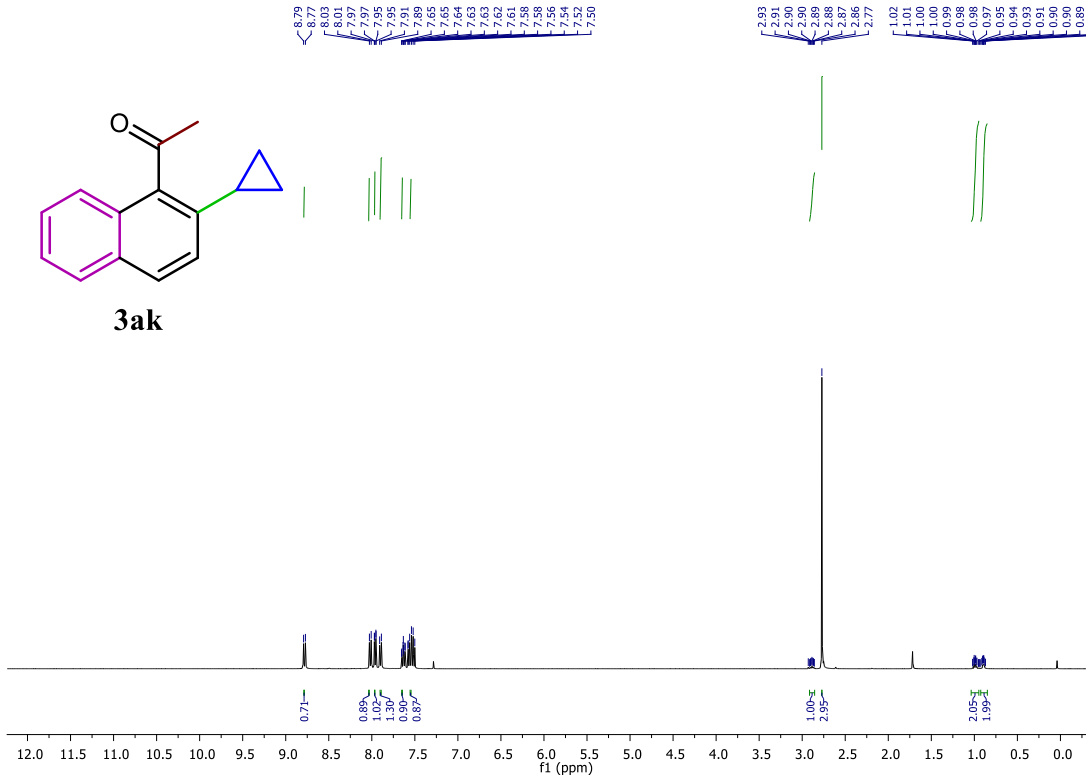
^{1}H NMR of 3aj (400 MHz, 32 scans, RT, $CDCl_3$)



^{13}C NMR of 3aj (101 MHz, 512 scans, RT, $CDCl_3$)

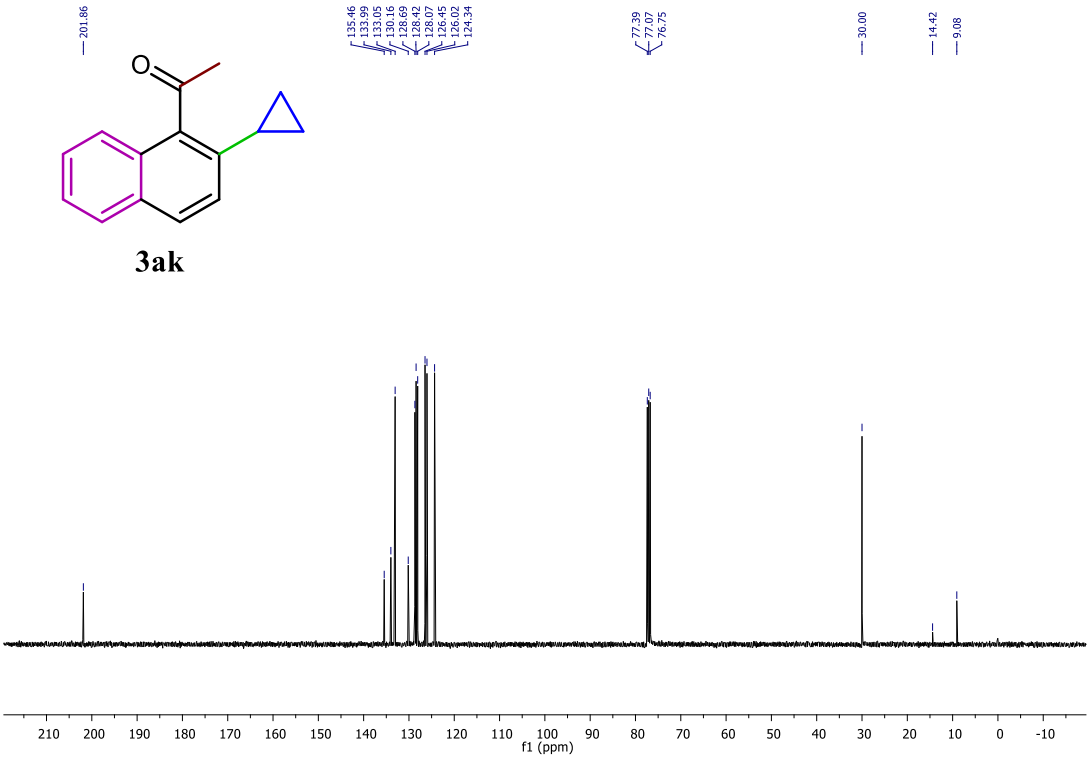


^{1}H NMR of 3ak (400 MHz, 32 scans, RT, $CDCl_3$)



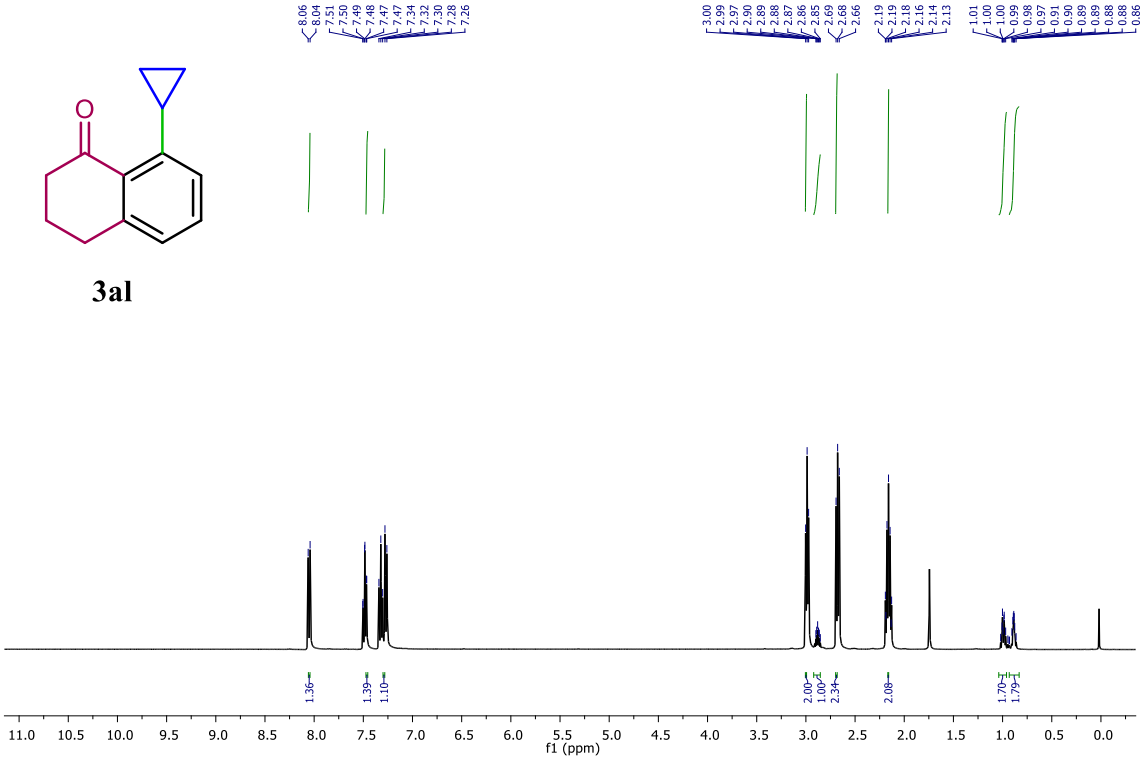
3ak

^{13}C NMR of 3ak (101 MHz, 512 scans, RT, $CDCl_3$)



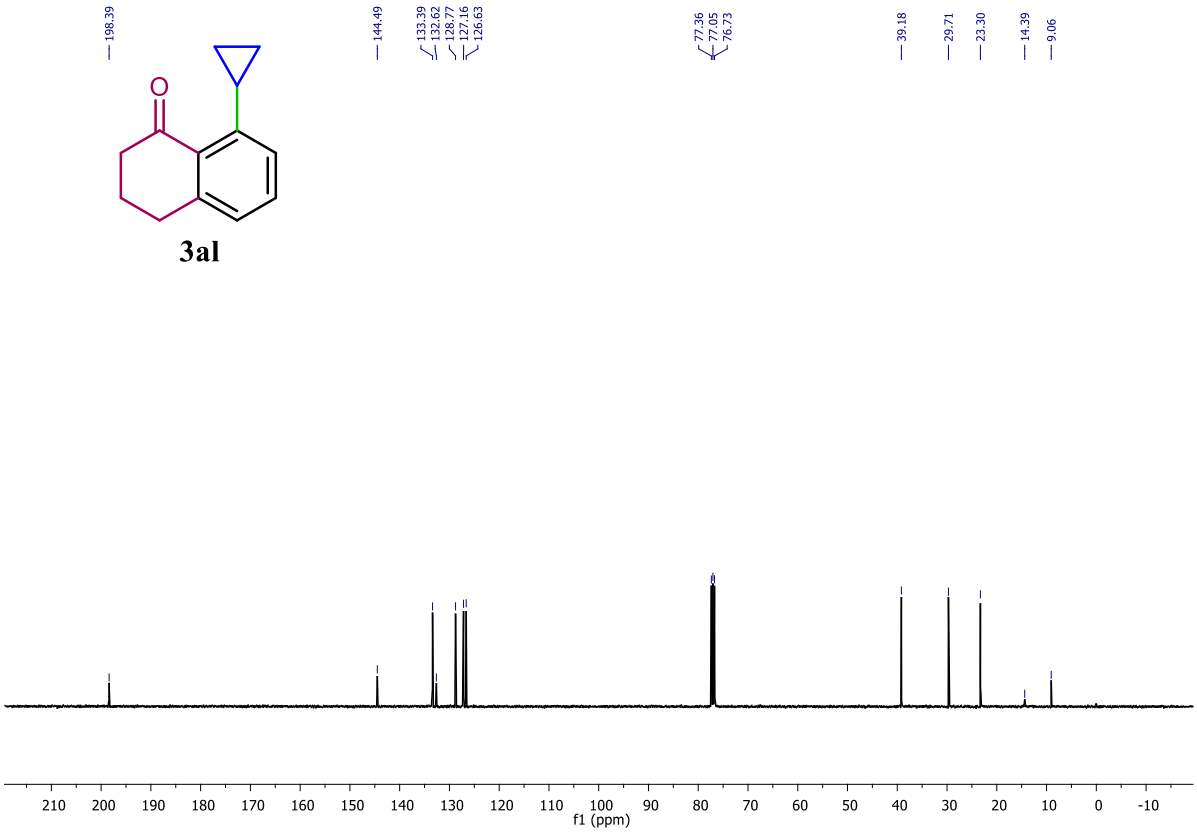
3ak

^{1}H NMR of 3al (400 MHz, 32 scans, RT, $CDCl_3$)



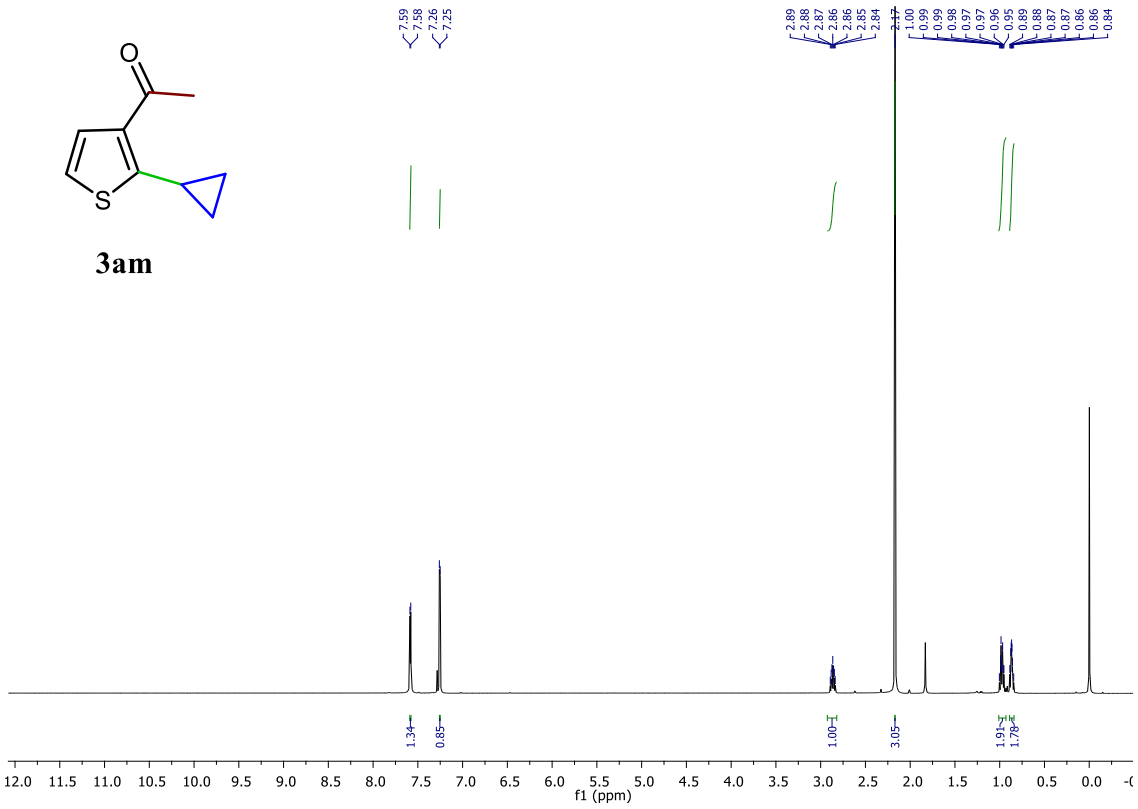
3al

^{13}C NMR of 3al (101 MHz, 512 scans, RT, $CDCl_3$)

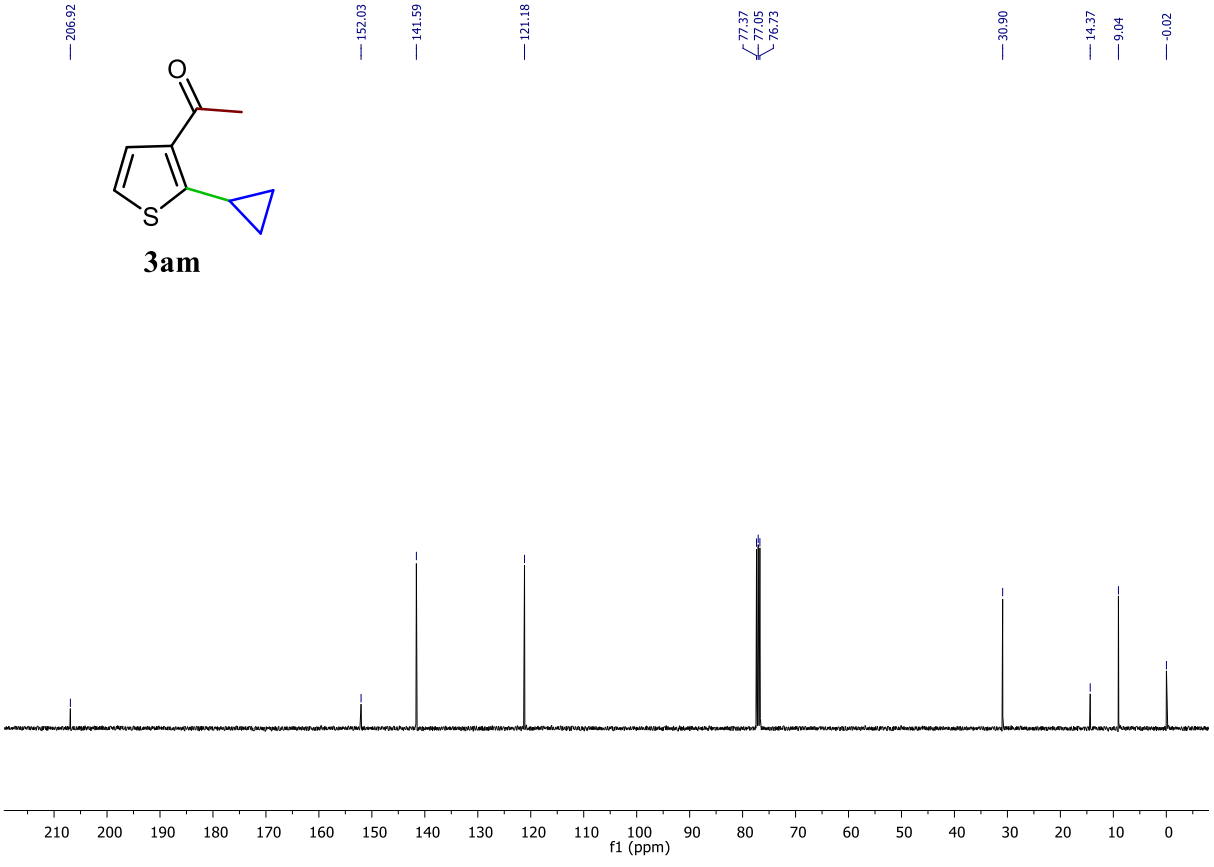


3al

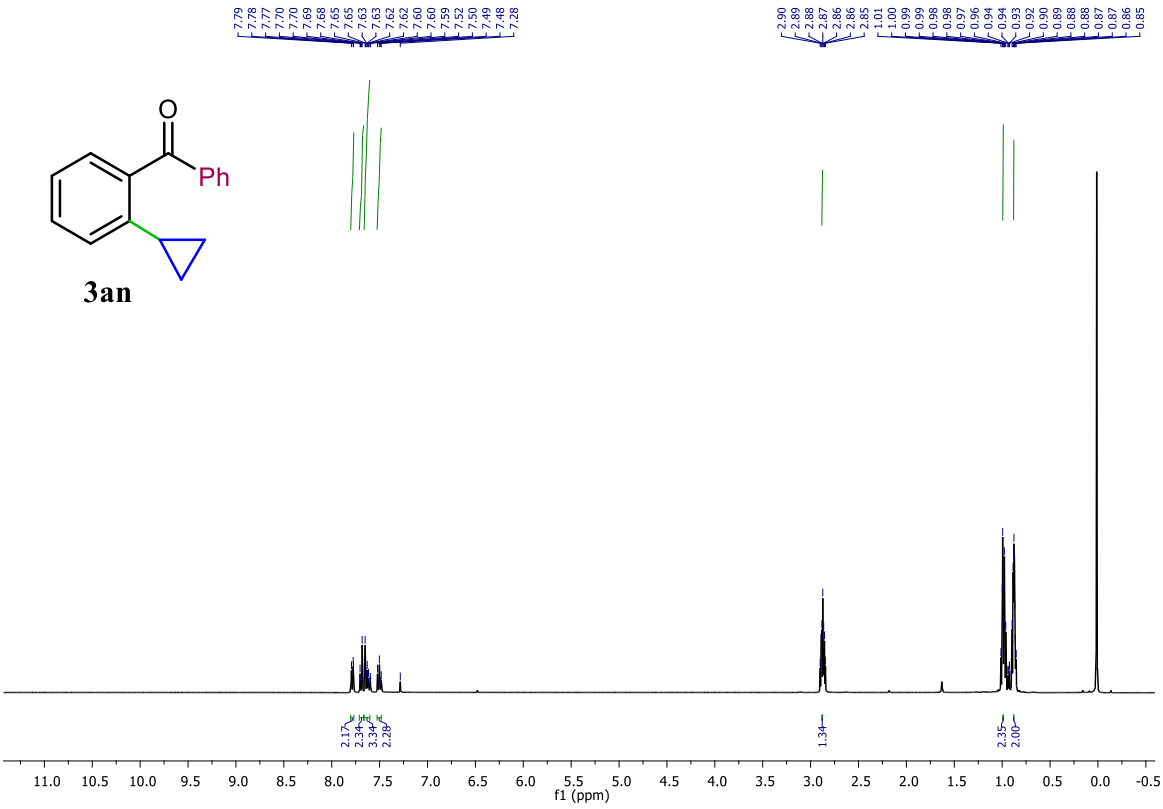
^{1}H NMR of 3am (400 MHz, 32 scans, RT, $CDCl_3$)



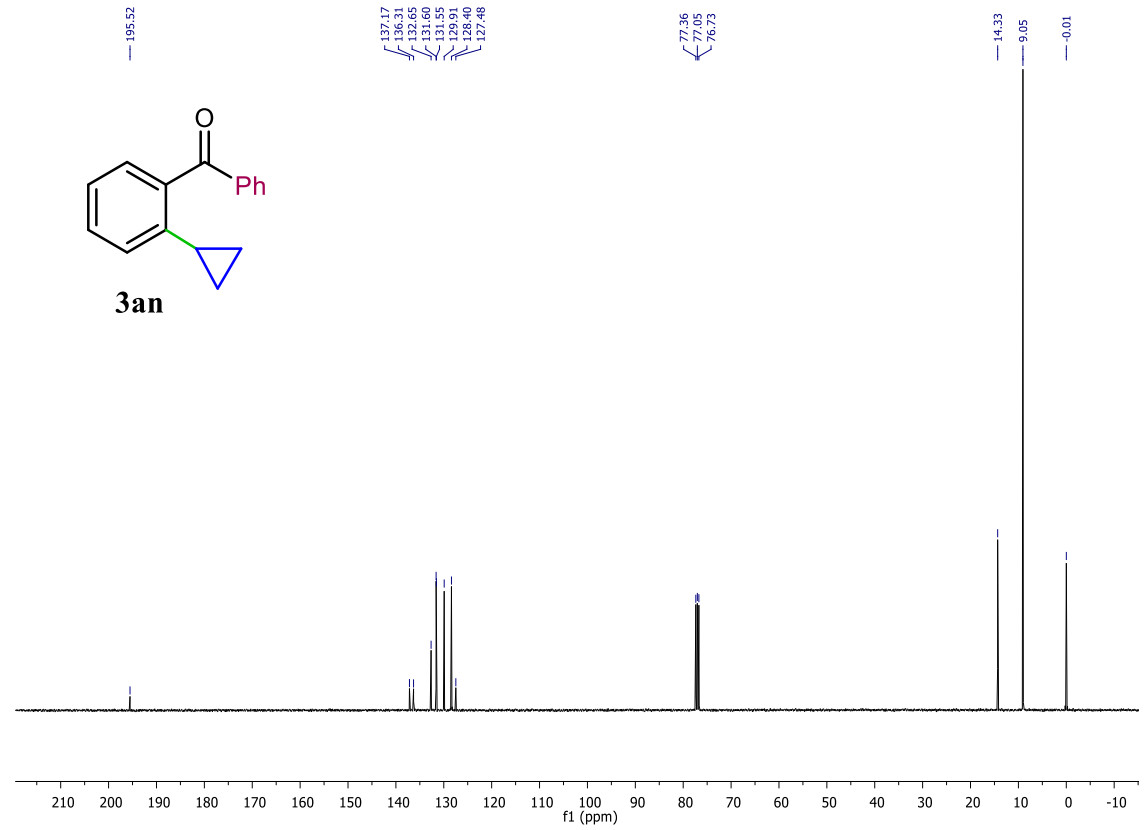
^{13}C NMR of 3am (101 MHz, 512 scans, RT, $CDCl_3$)



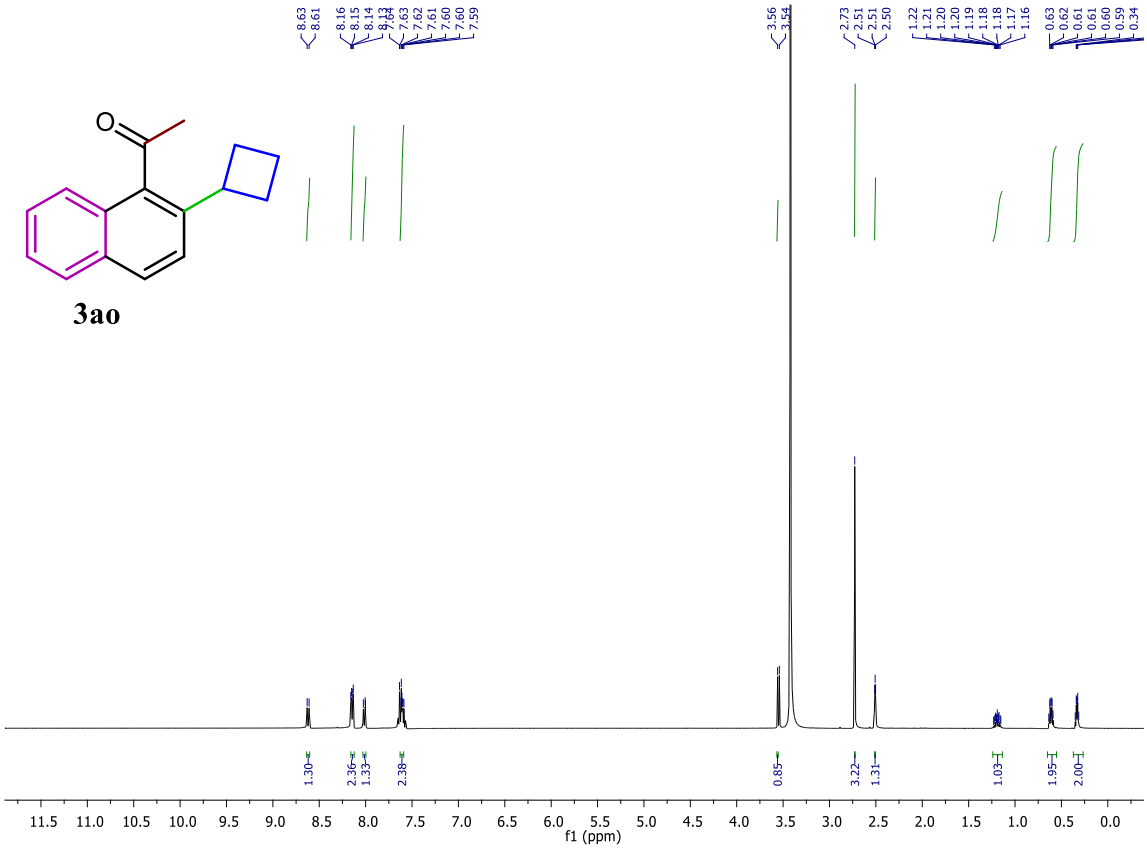
^{1}H NMR of 3an (400 MHz, 32 scans, RT, $CDCl_3$)



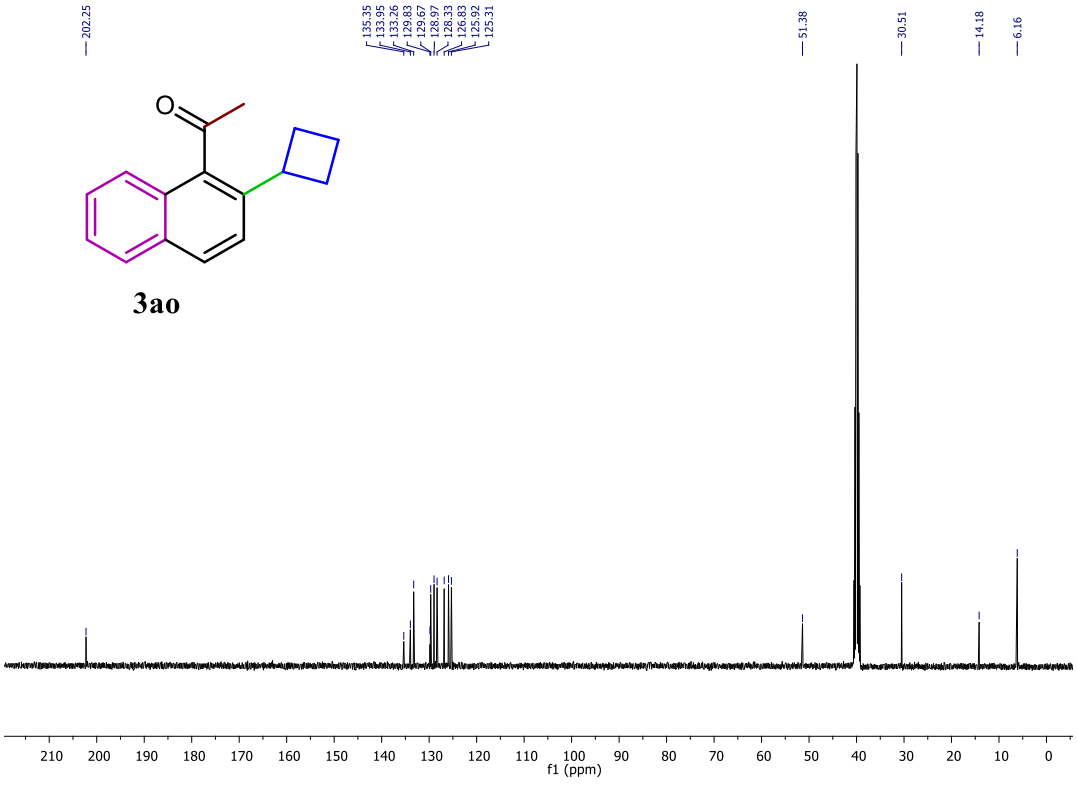
^{13}C NMR of 3an (101 MHz, 512 scans, RT, $CDCl_3$)



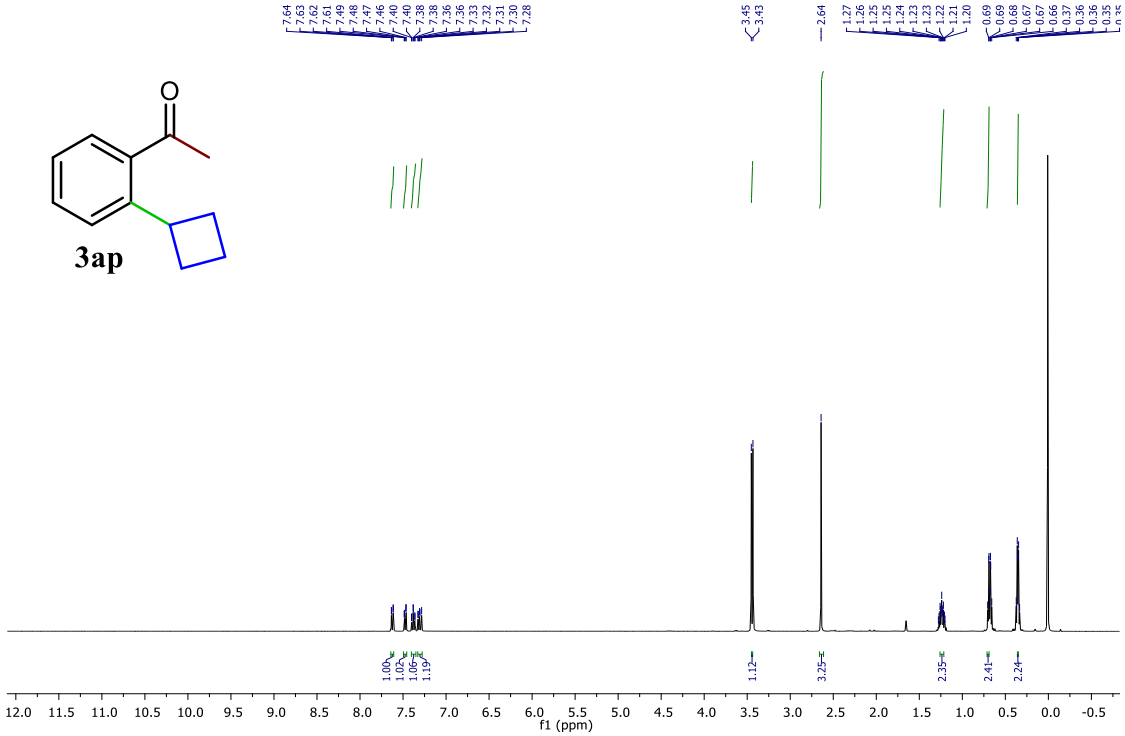
^{1}H NMR of 3ao (400 MHz, 32 scans, RT, DMSO-d$_6$)



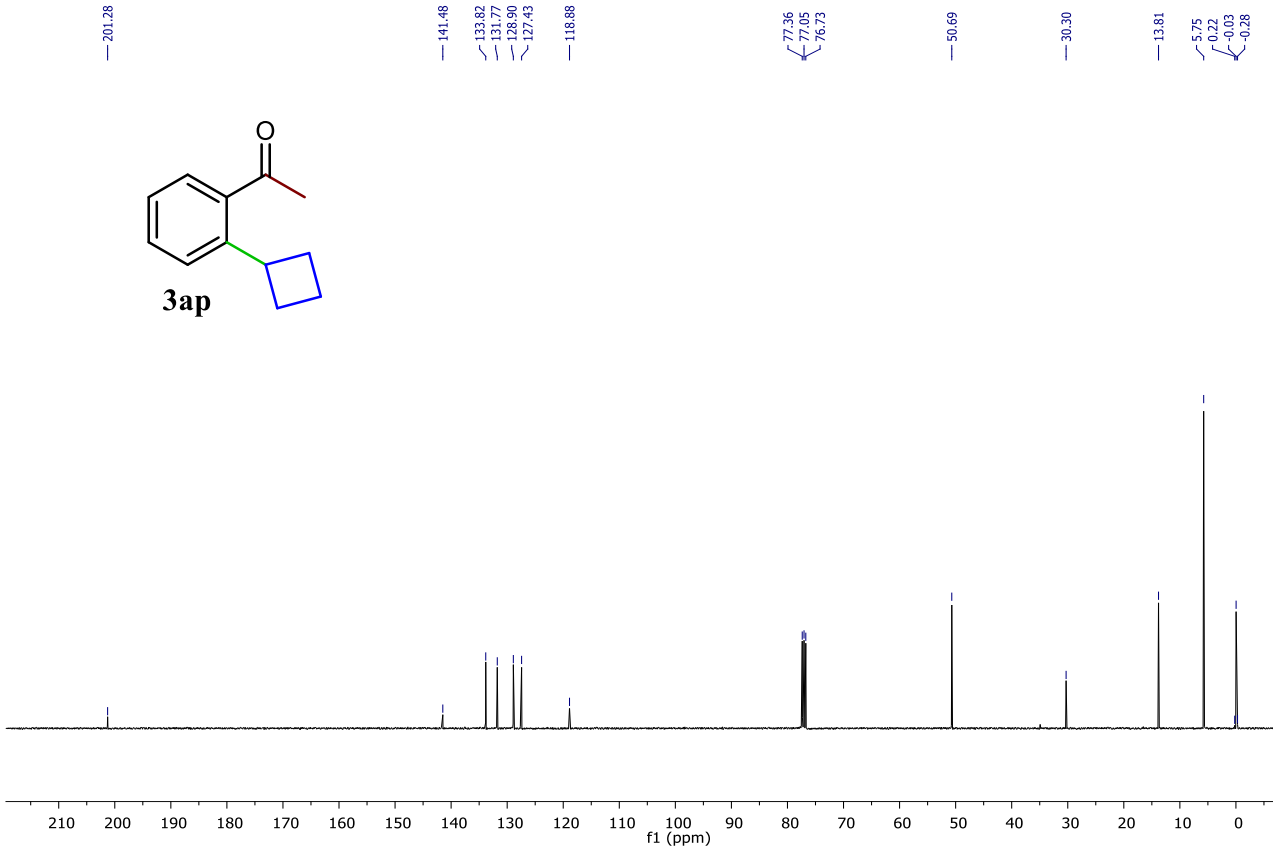
^{13}C NMR of 3ao (101 MHz, 512 scans, RT, DMSO-d$_6$)



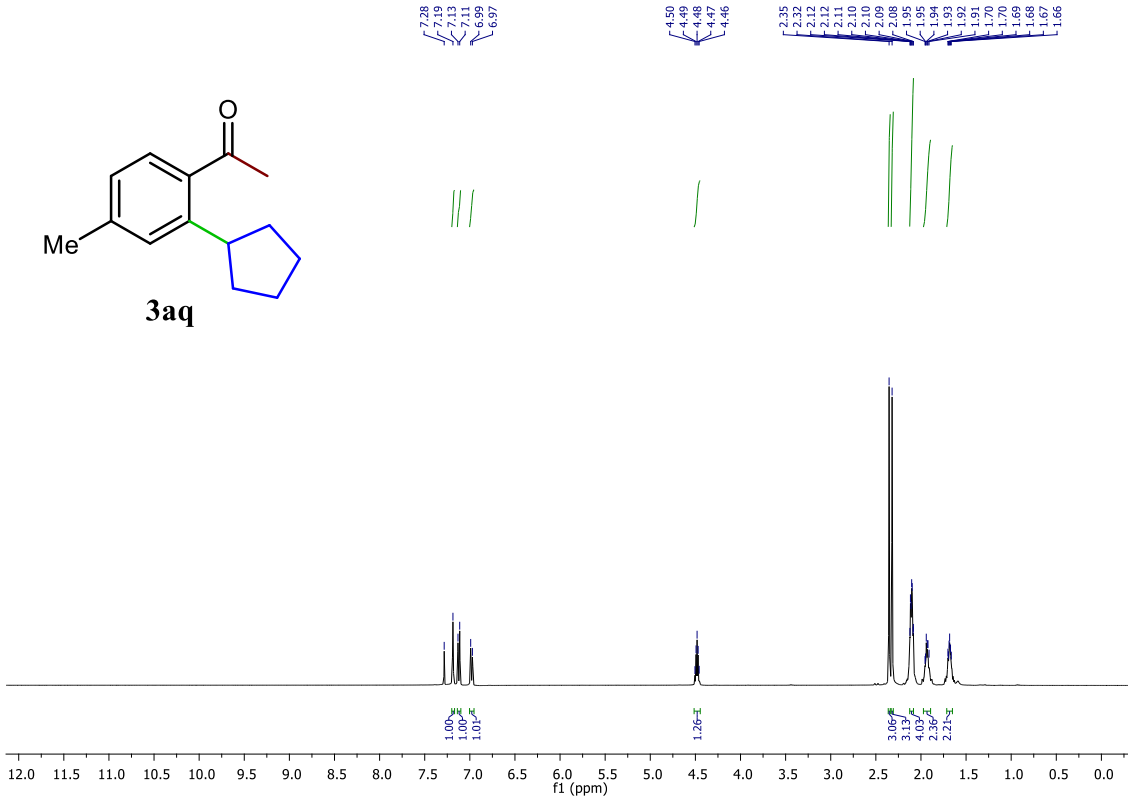
^{1}H NMR of 3ap (400 MHz, 32 scans, RT, $CDCl_3$)



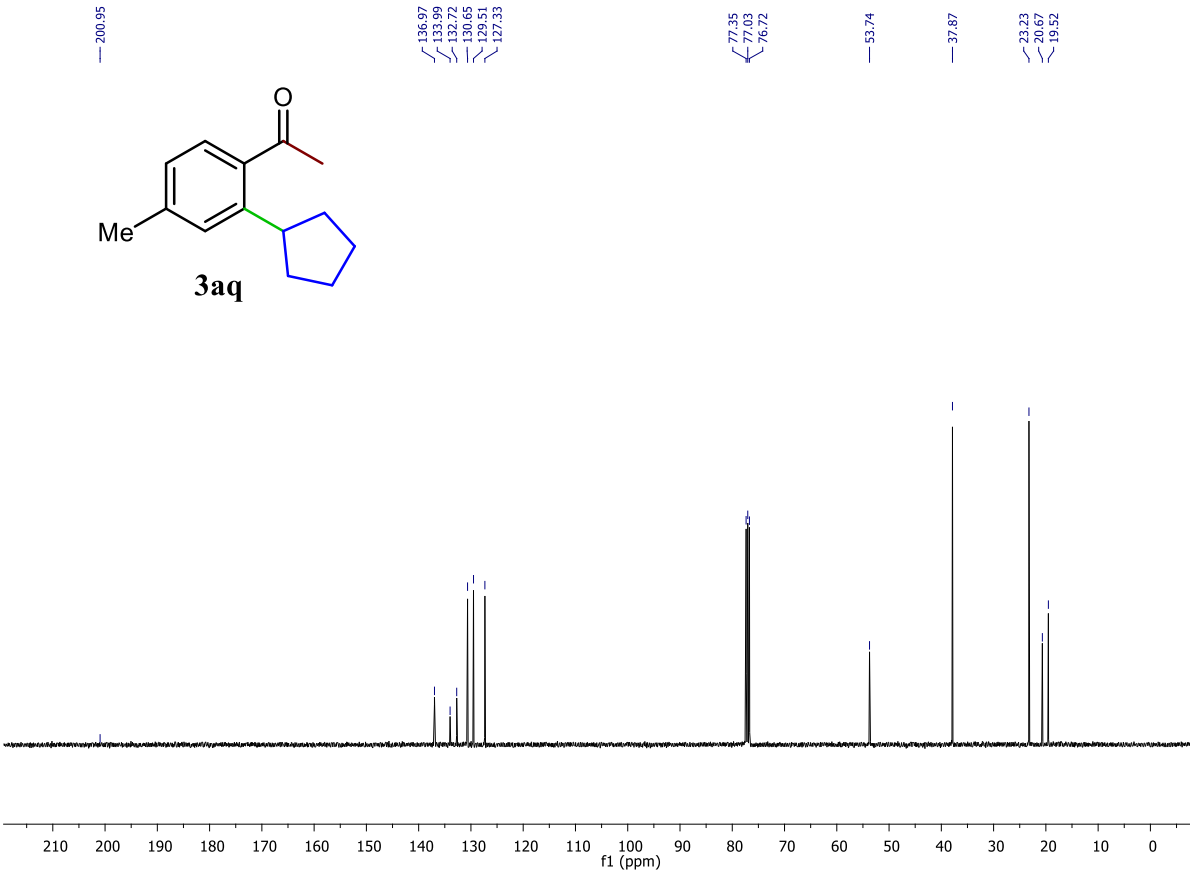
^{13}C NMR of 3ap (101 MHz, 512 scans, RT, $CDCl_3$)



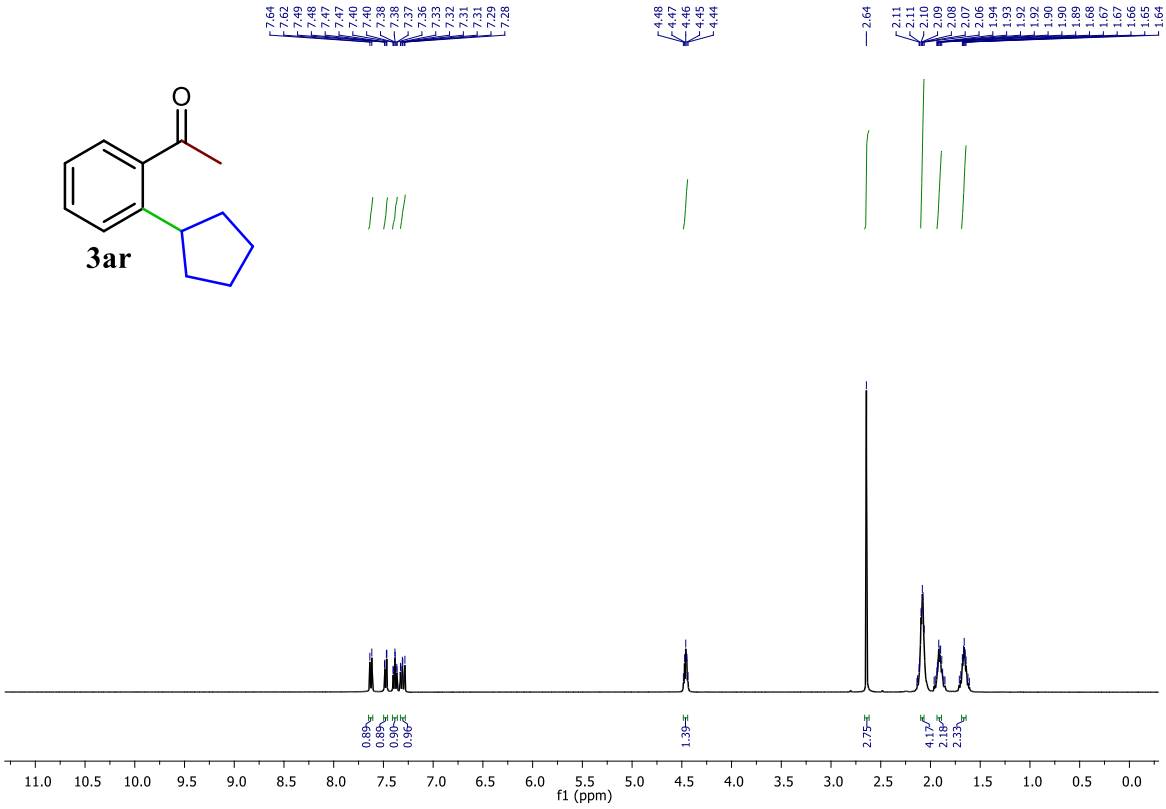
^{1}H NMR of 3aq (400 MHz, 32 scans, RT, $CDCl_3$)



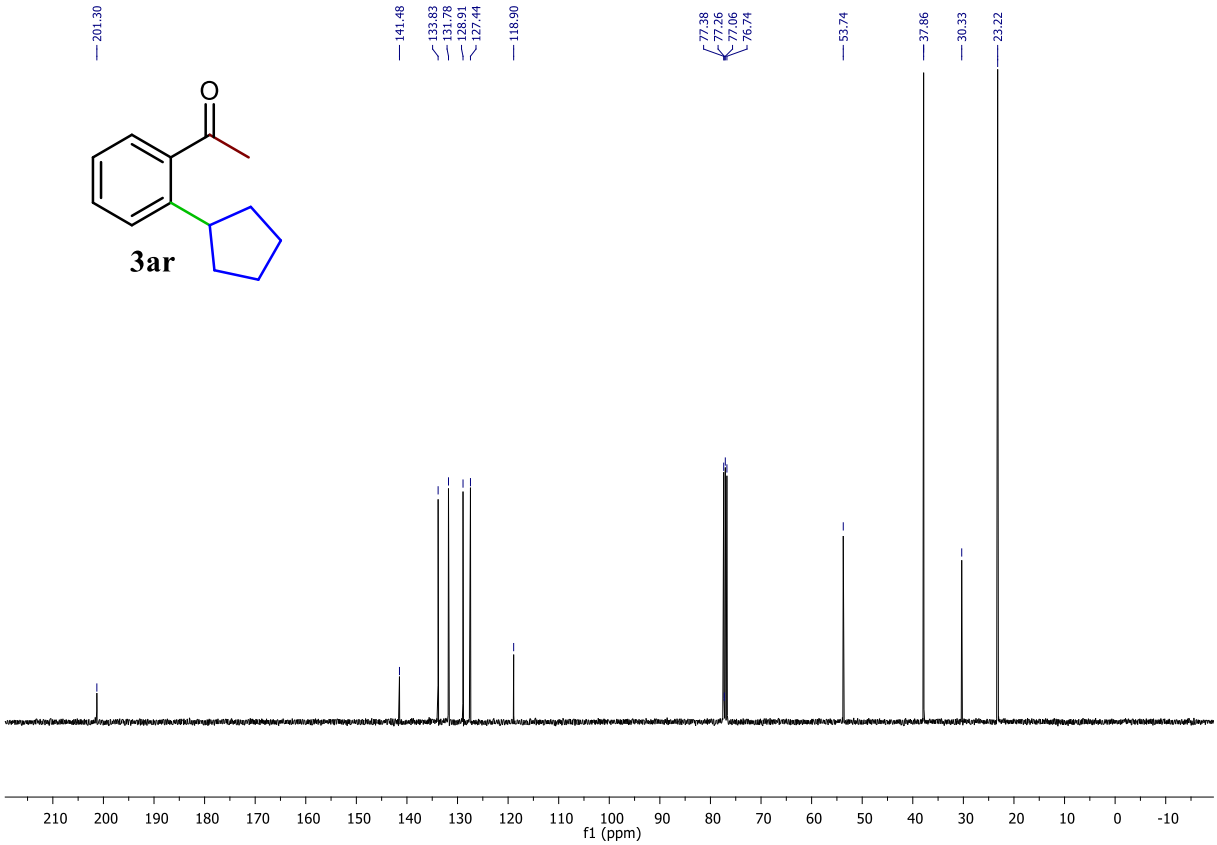
^{13}C NMR of 3aq (101 MHz, 512 scans, RT, $CDCl_3$)



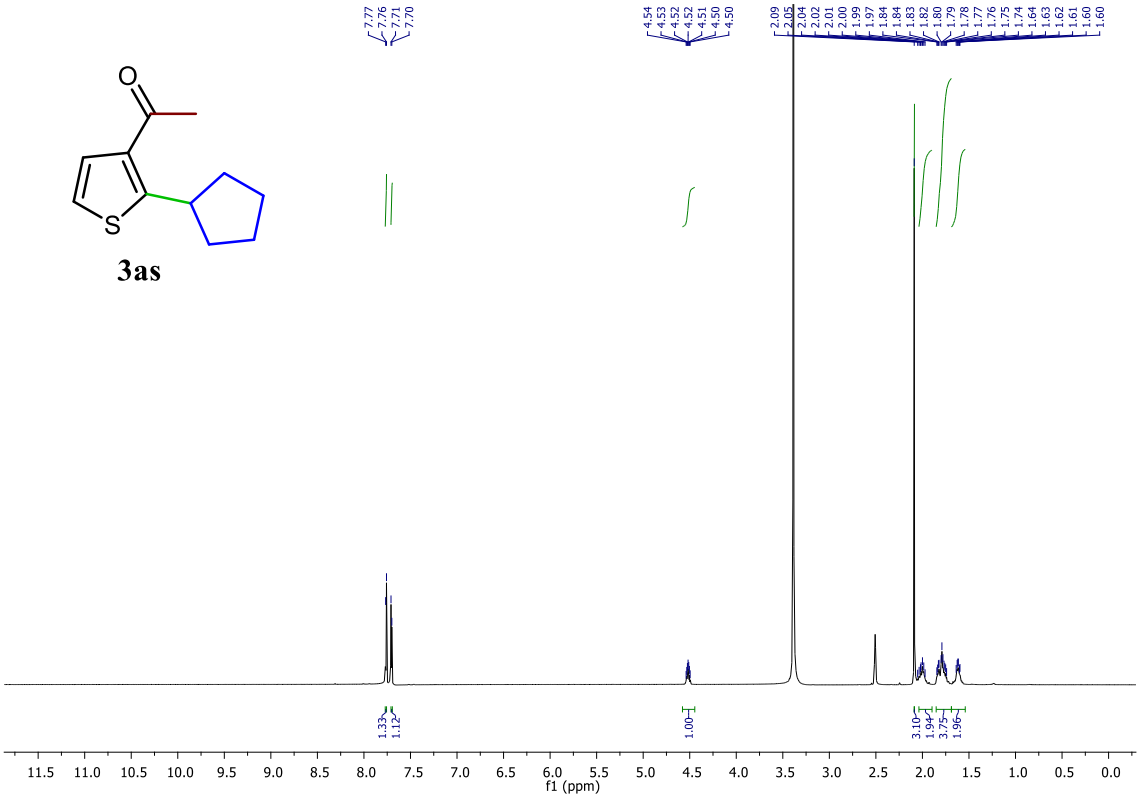
^{1}H NMR of 3ar (400 MHz, 32 scans, RT, $CDCl_3$)



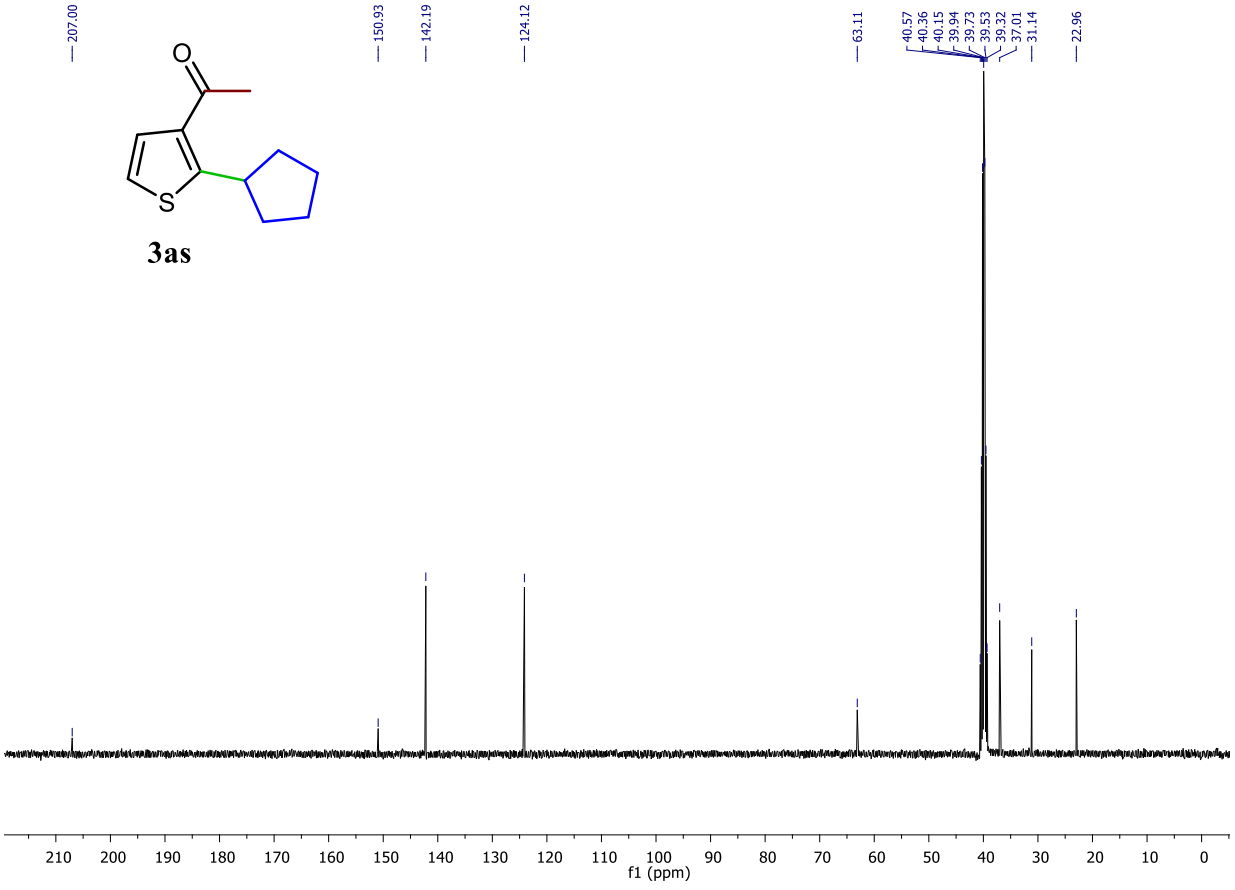
^{13}C NMR of 3ar (101 MHz, 512 scans, RT, $CDCl_3$)



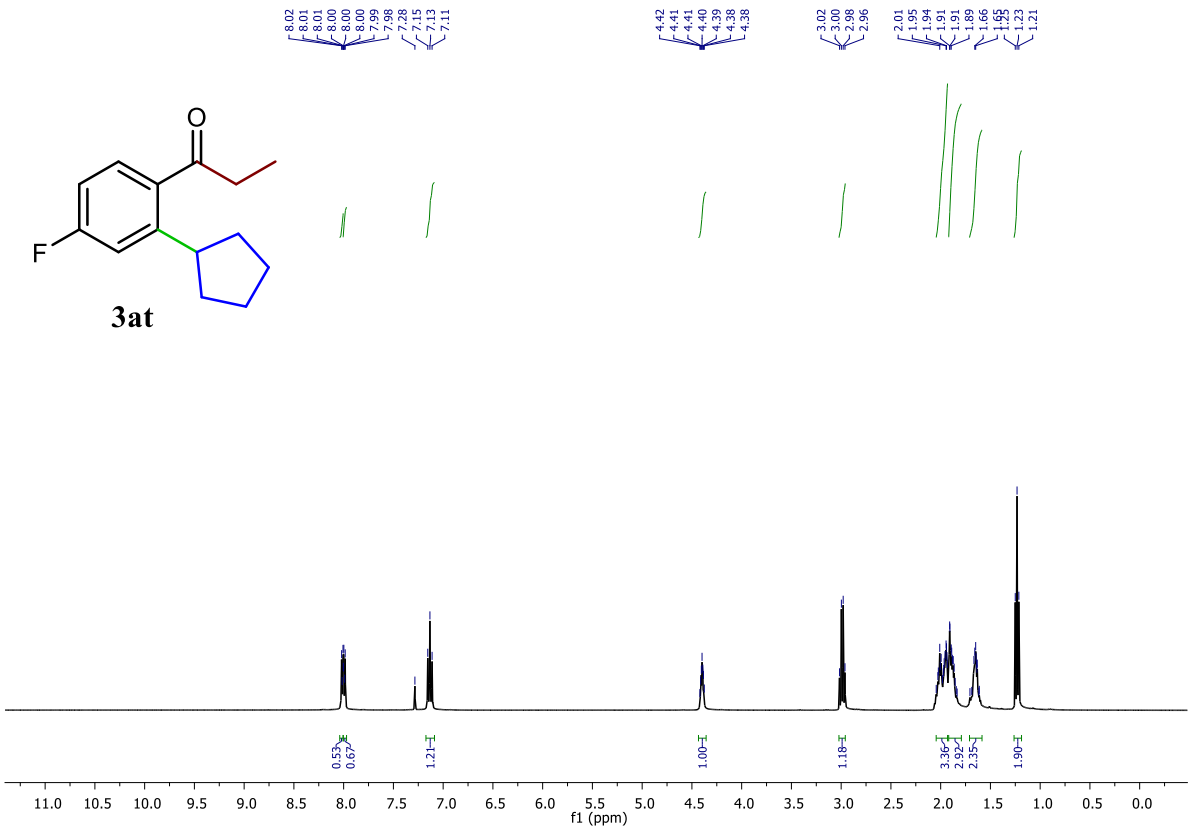
^{1}H NMR of 3as (400 MHz, 32 scans, RT, DMSO-d$_6$)



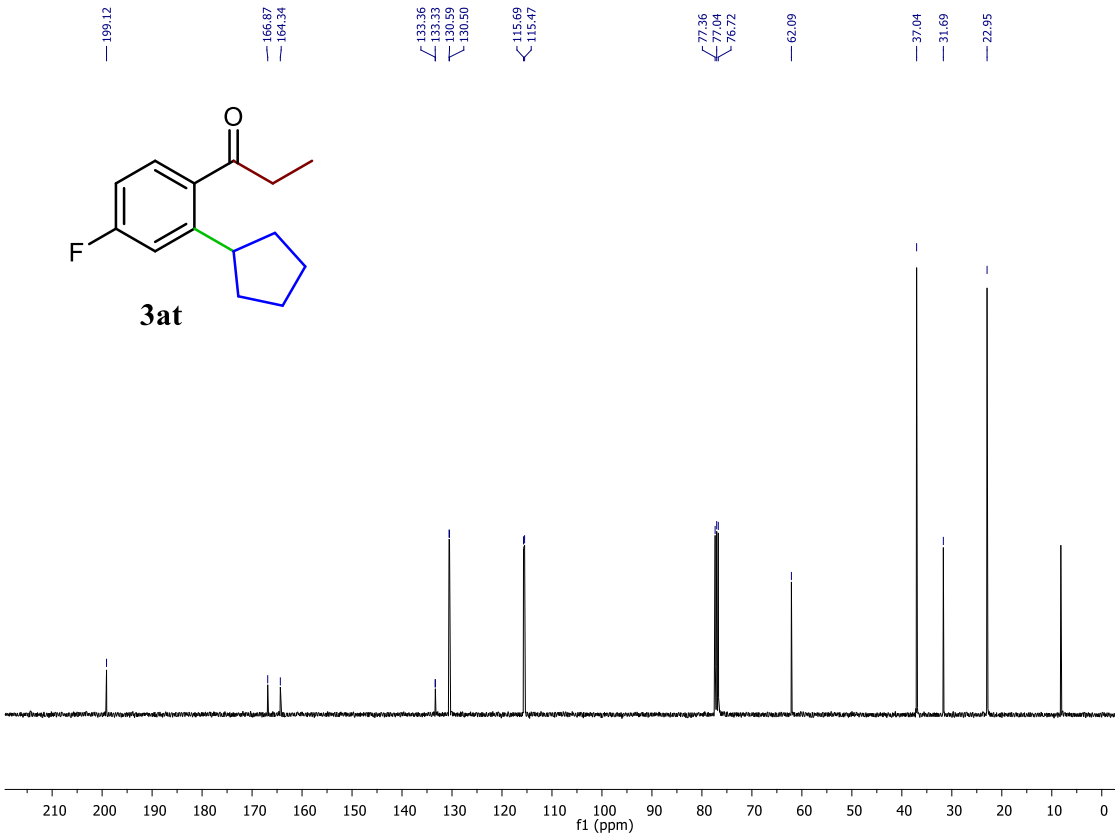
^{13}C NMR of 3as (101 MHz, 512 scans, RT, DMSO-d$_6$)



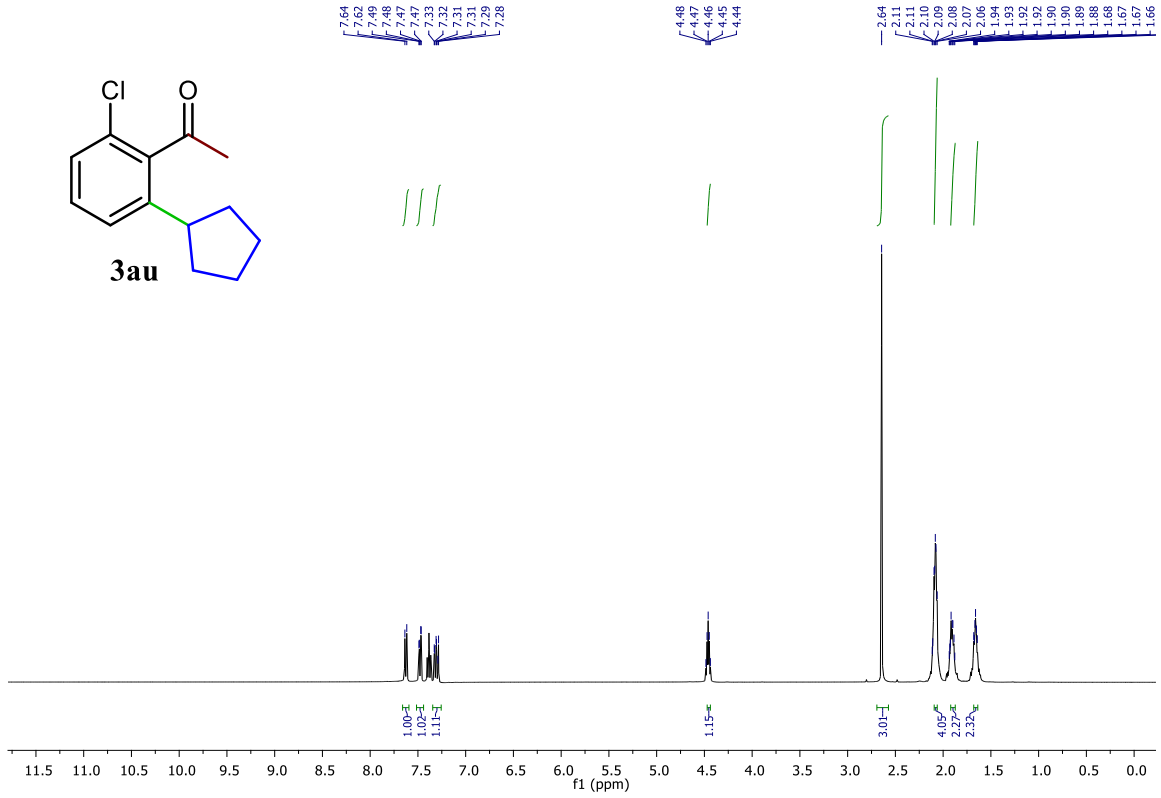
^{1}H NMR of 3at (400 MHz, 32 scans, RT, $CDCl_3$)



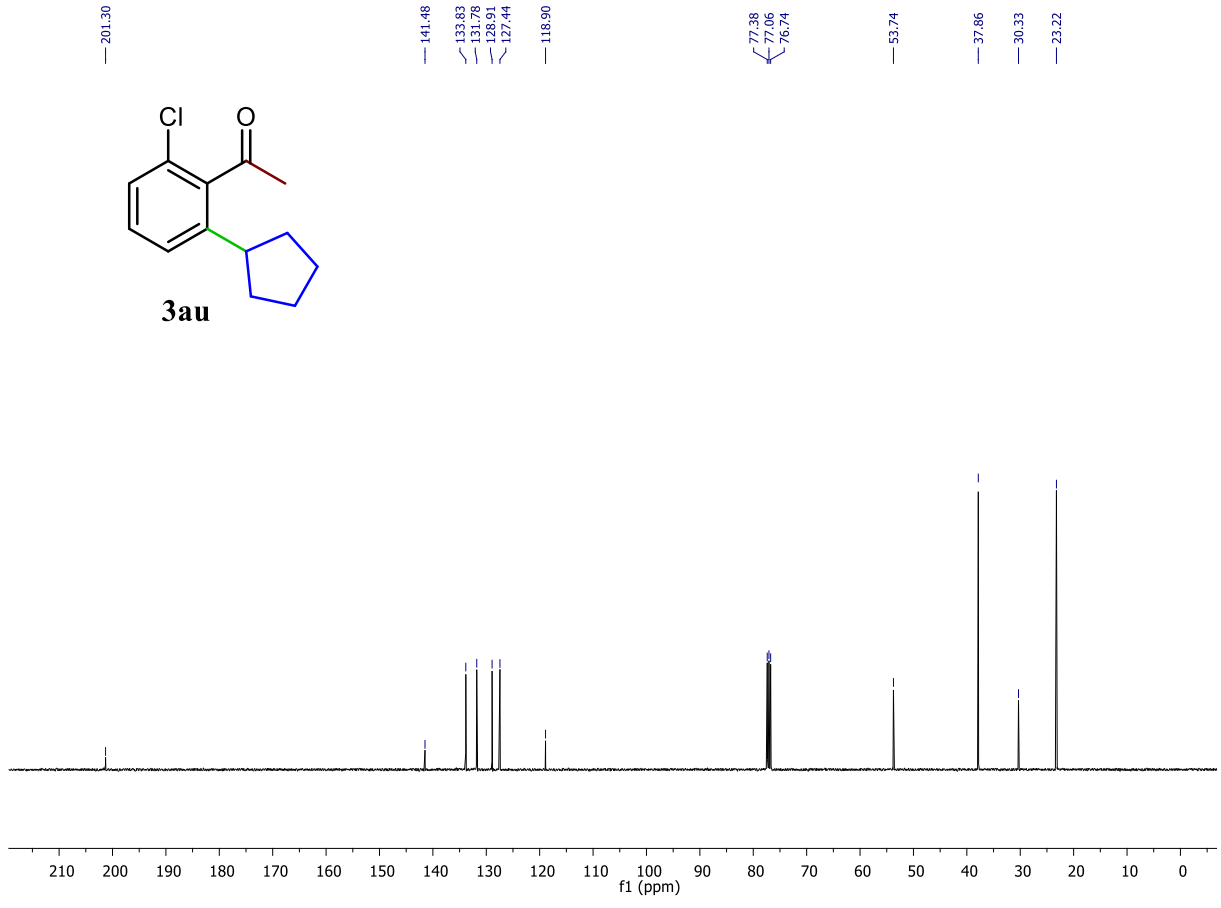
^{13}C NMR of 3at (101 MHz, 512 scans, RT, $CDCl_3$)



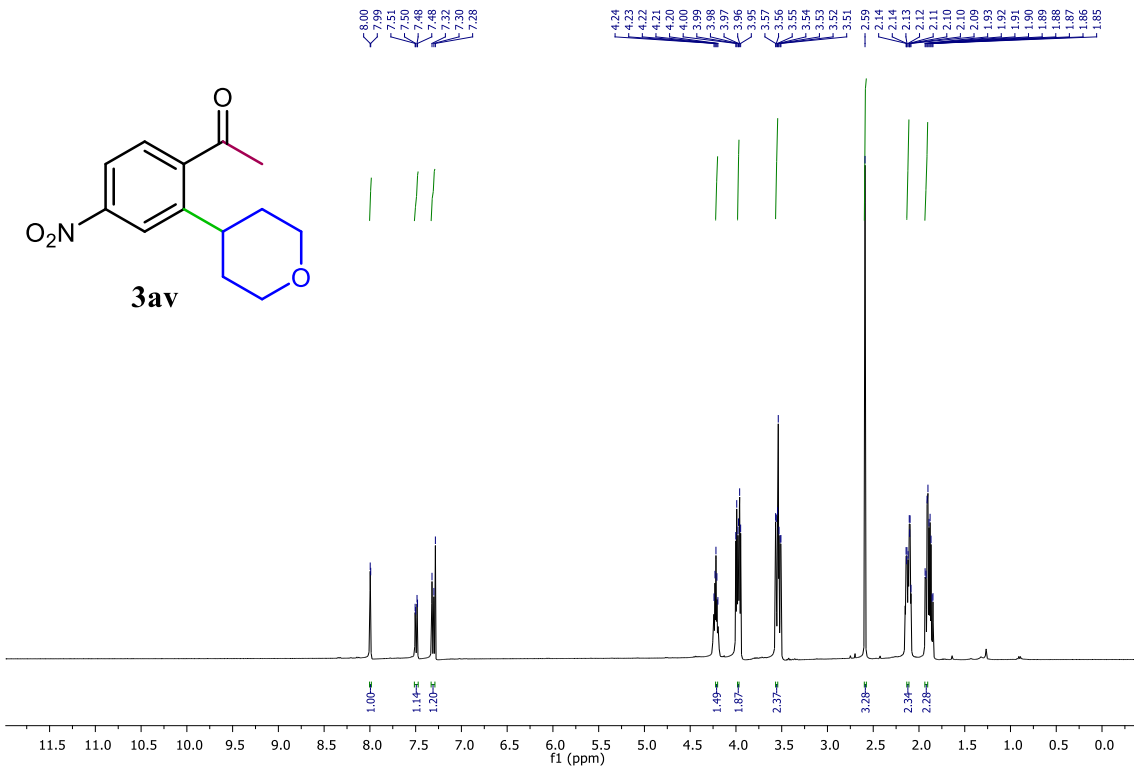
^{1}H NMR of 3au (400 MHz, 32 scans, RT, $CDCl_3$)



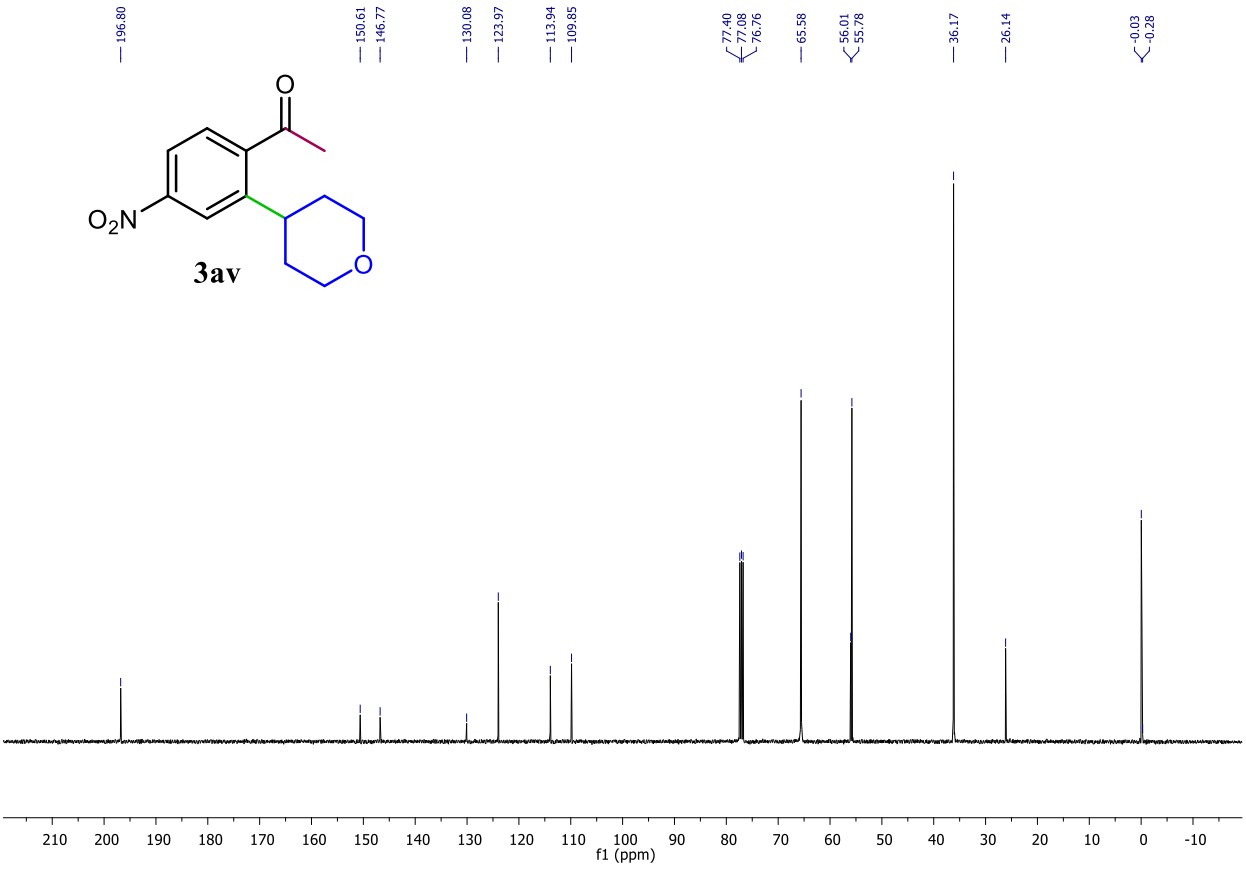
^{13}C NMR of 3au (101 MHz, 512 scans, RT, $CDCl_3$)



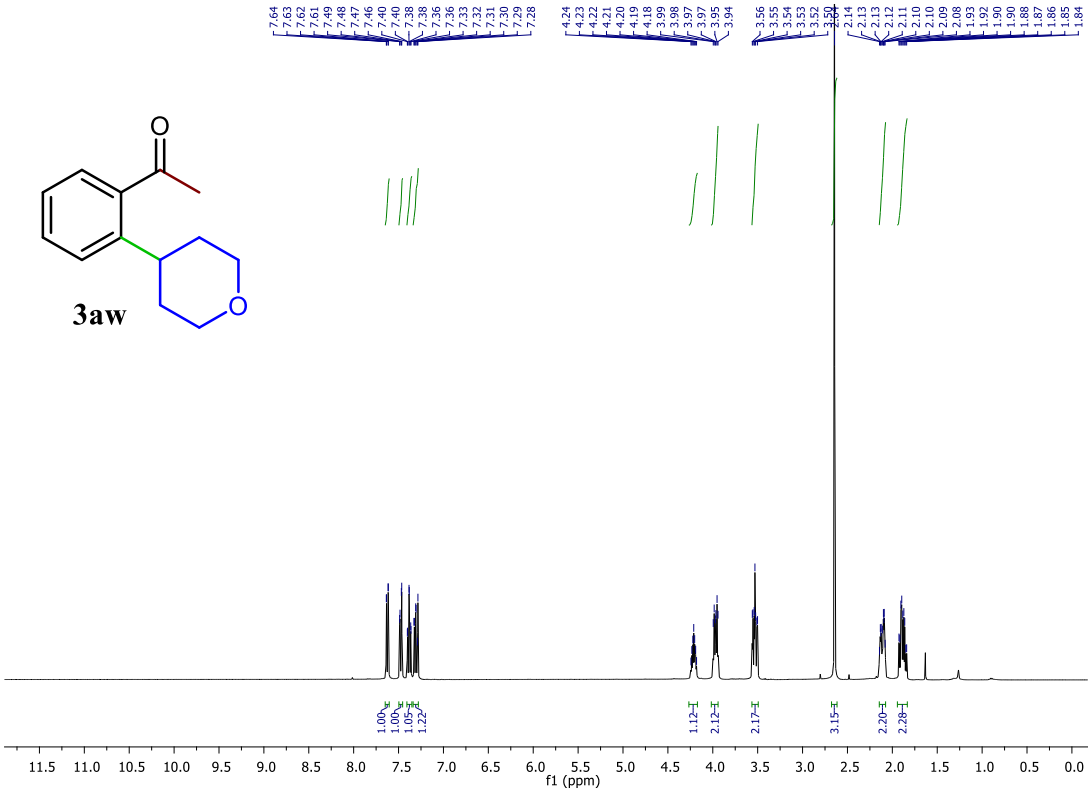
^{1}H NMR of 3av (400 MHz, 32 scans, RT, $CDCl_3$)



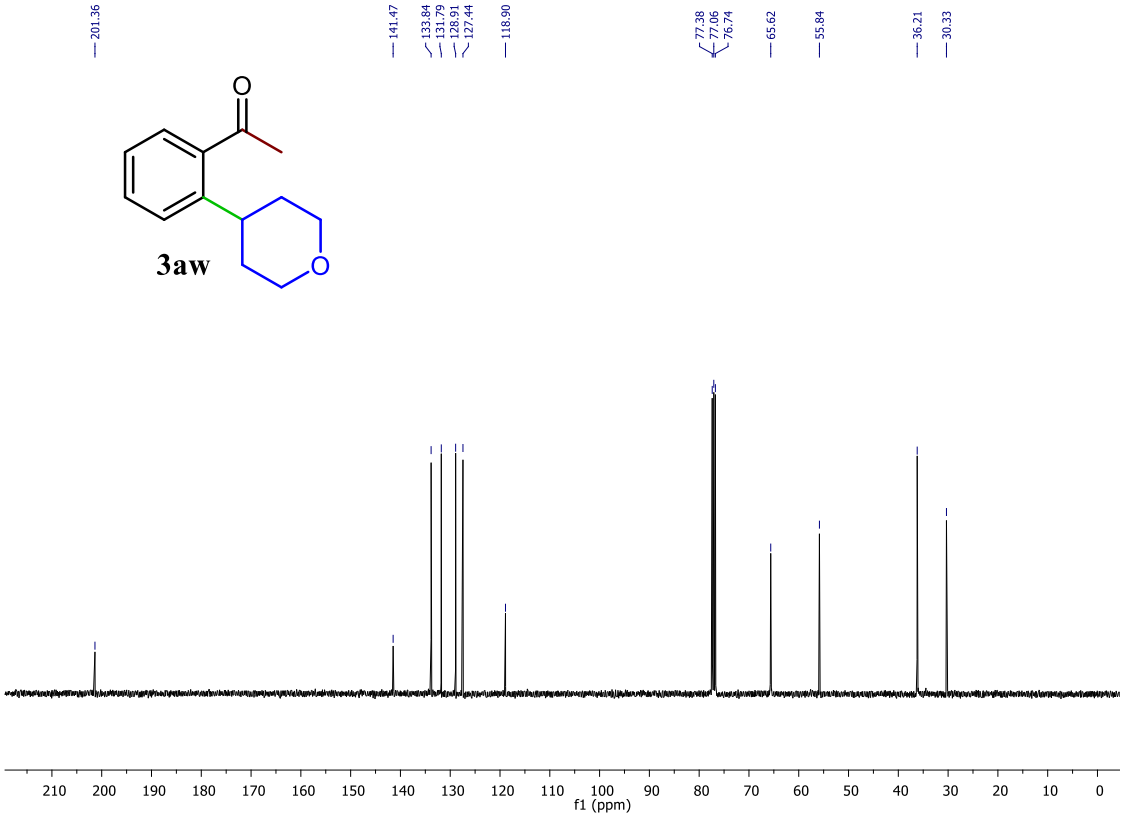
^{13}C NMR of 3av (101 MHz, 512 scans, RT, $CDCl_3$)



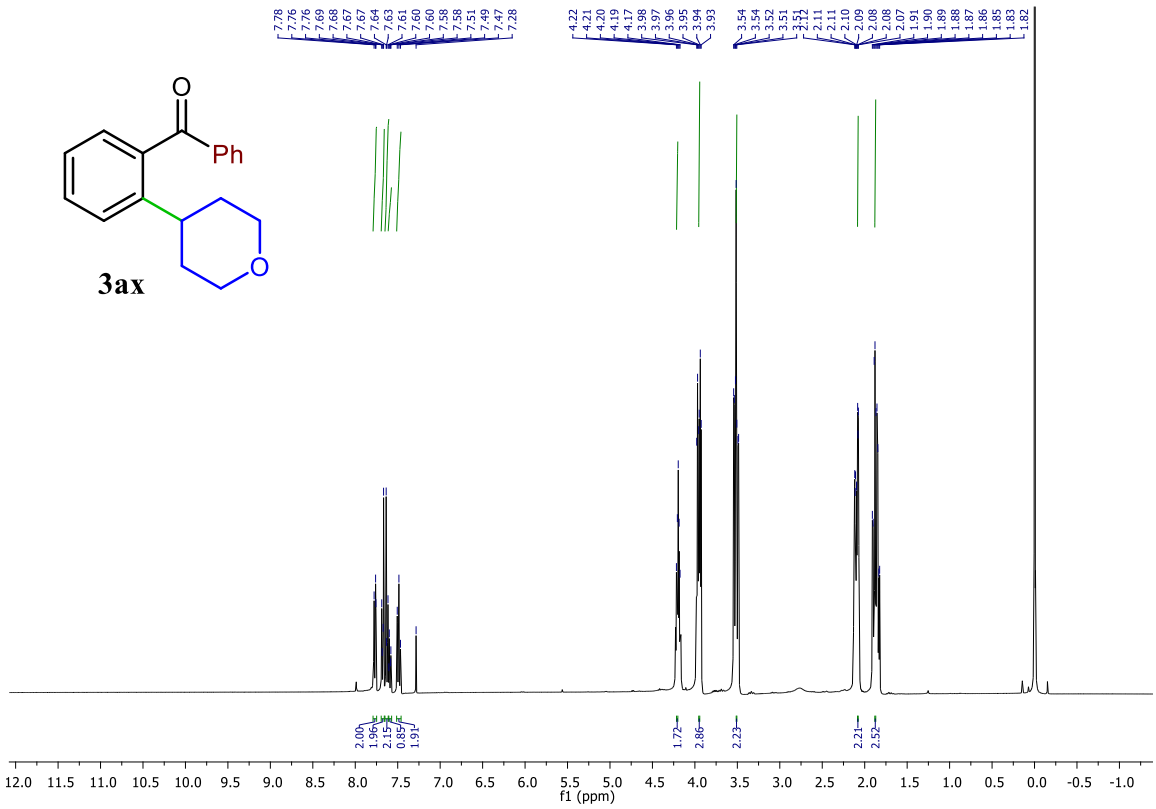
^{1}H NMR of 3aw (400 MHz, 32 scans, RT, $CDCl_3$)



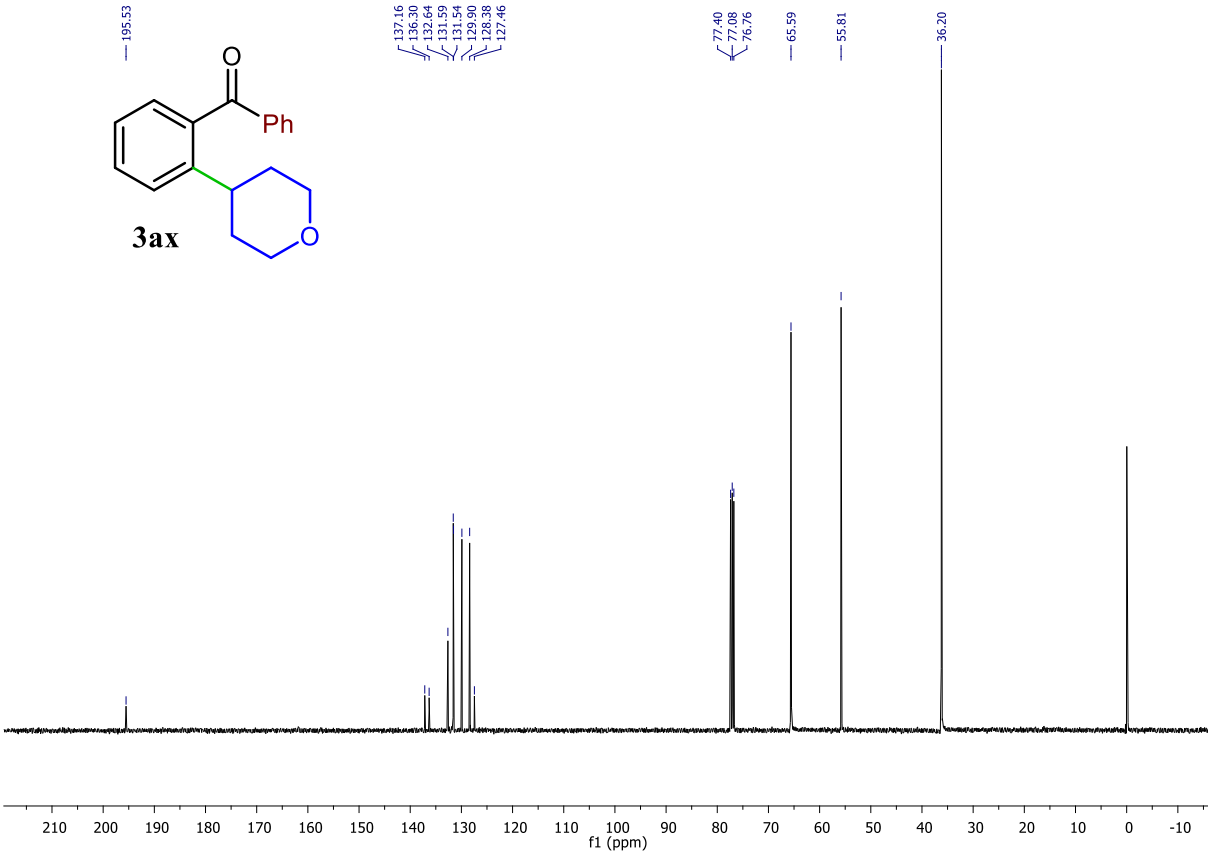
^{13}C NMR of 3aw (101 MHz, 512 scans, RT, $CDCl_3$)



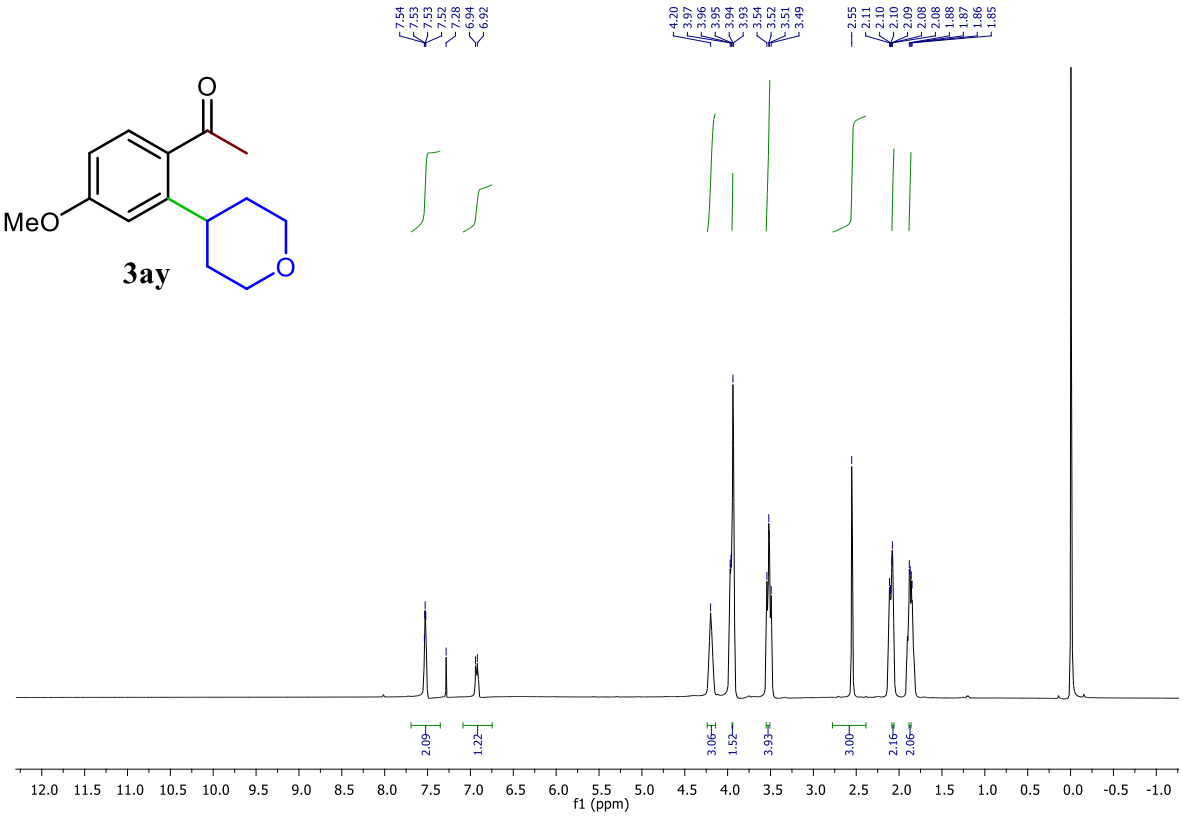
^{1}H NMR of 3ax (400 MHz, 32 scans, RT, $CDCl_3$)



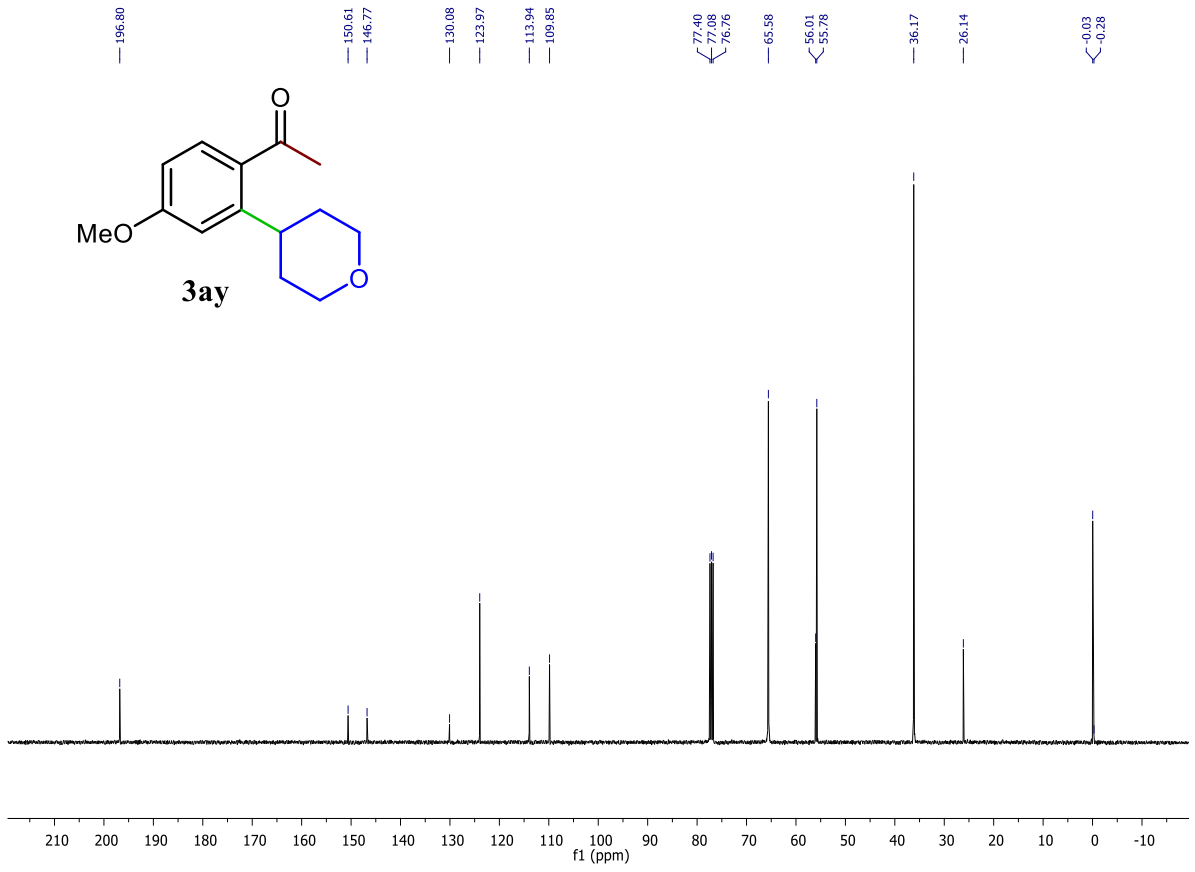
^{13}C NMR of 3ax (101 MHz, 512 scans, RT, $CDCl_3$)



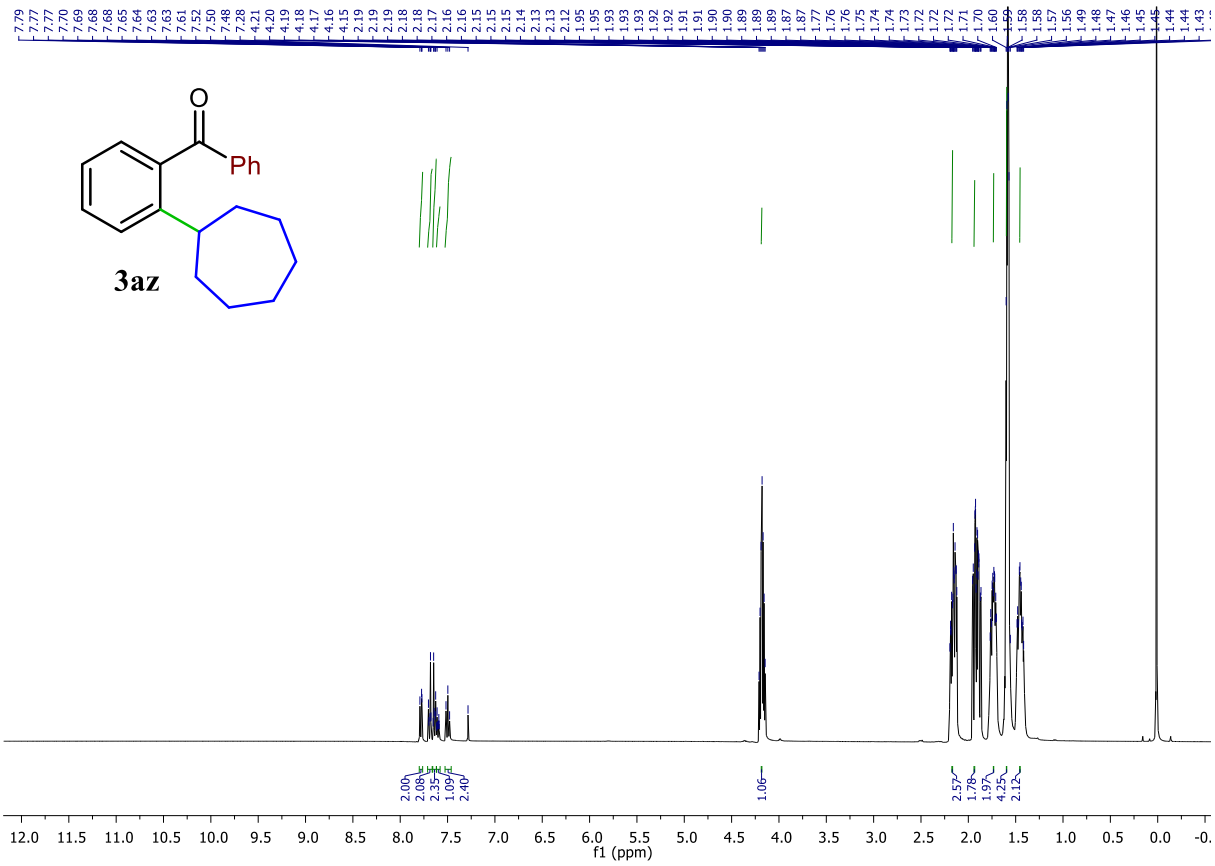
^{1}H NMR of 3ay (400 MHz, 32 scans, RT, $CDCl_3$)



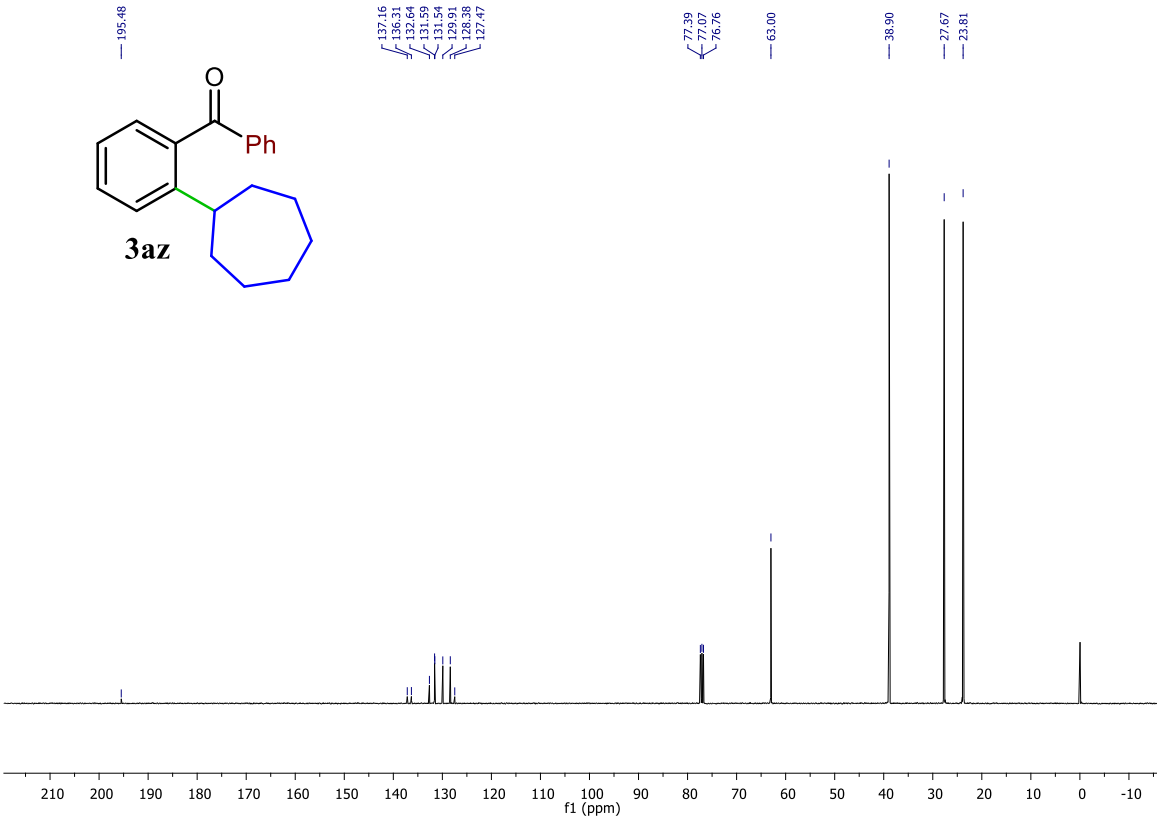
^{13}C NMR of 3ay (101 MHz, 512 scans, RT, $CDCl_3$)



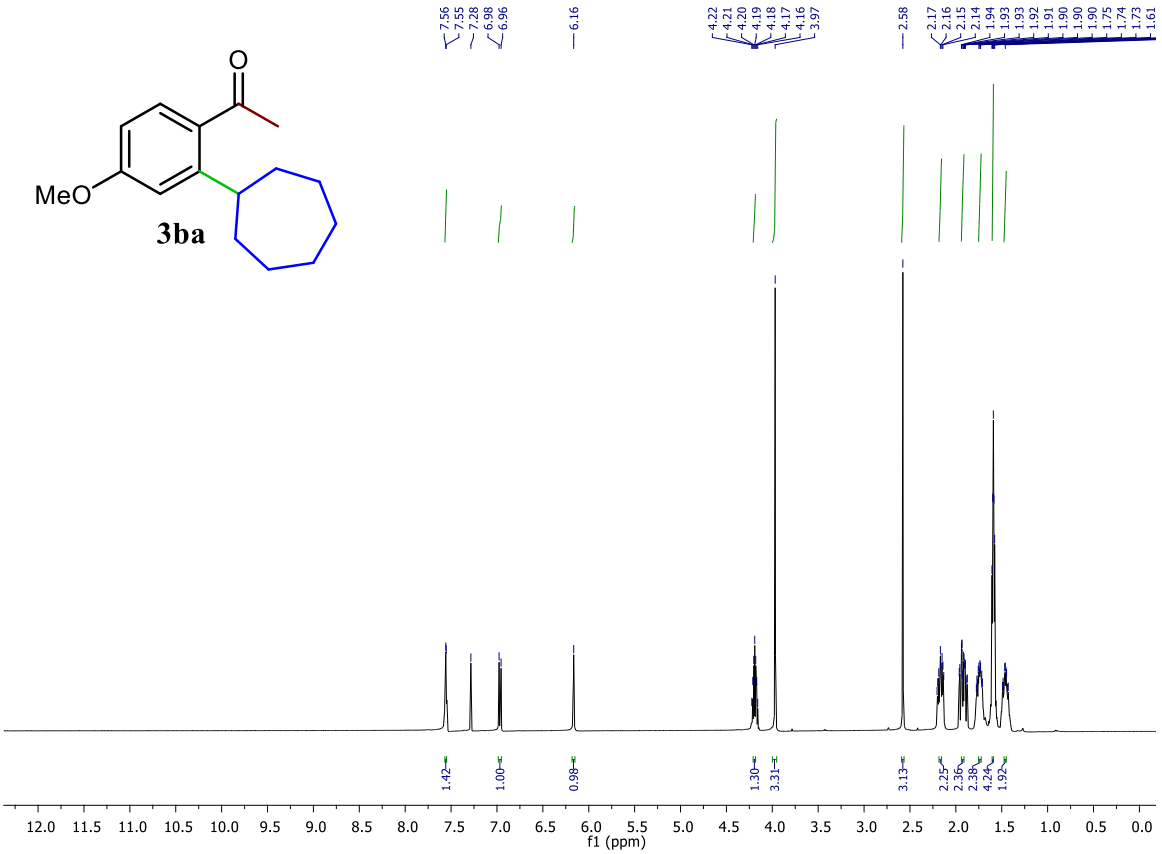
^{1}H NMR of 3az (400 MHz, 32 scans, RT, $CDCl_3$)



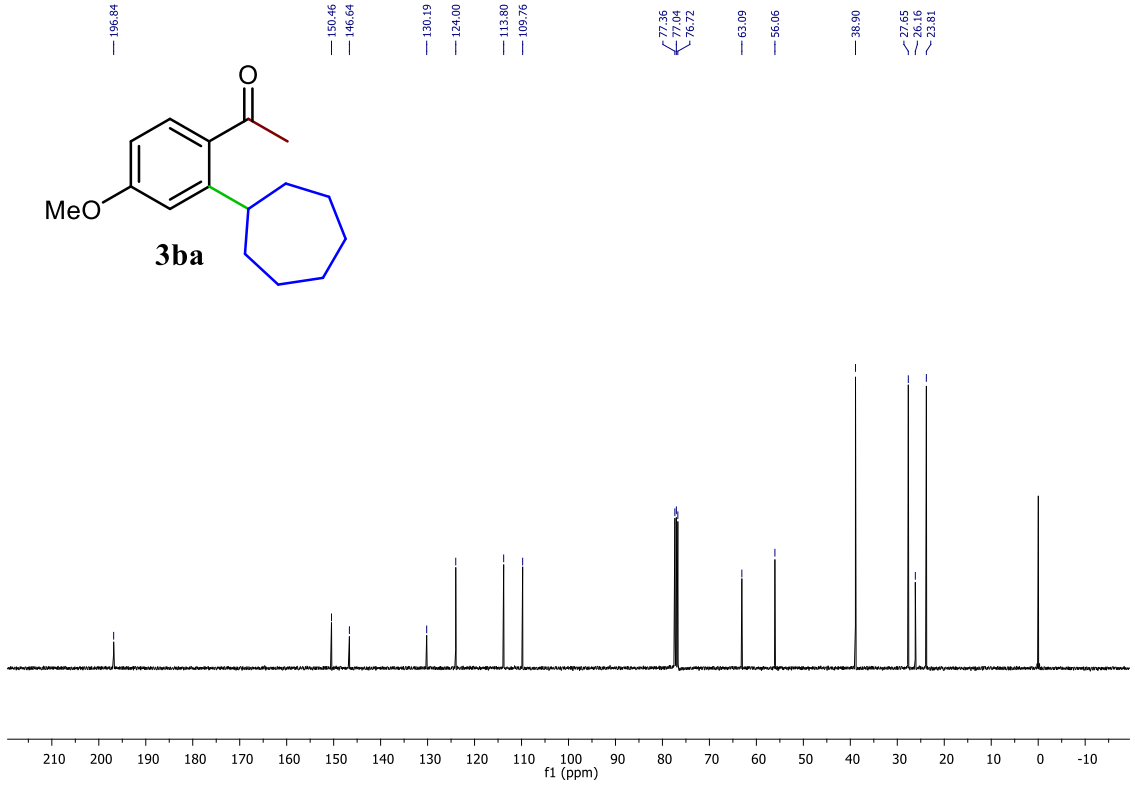
^{13}C NMR of 3az (101 MHz, 512 scans, RT, $CDCl_3$)



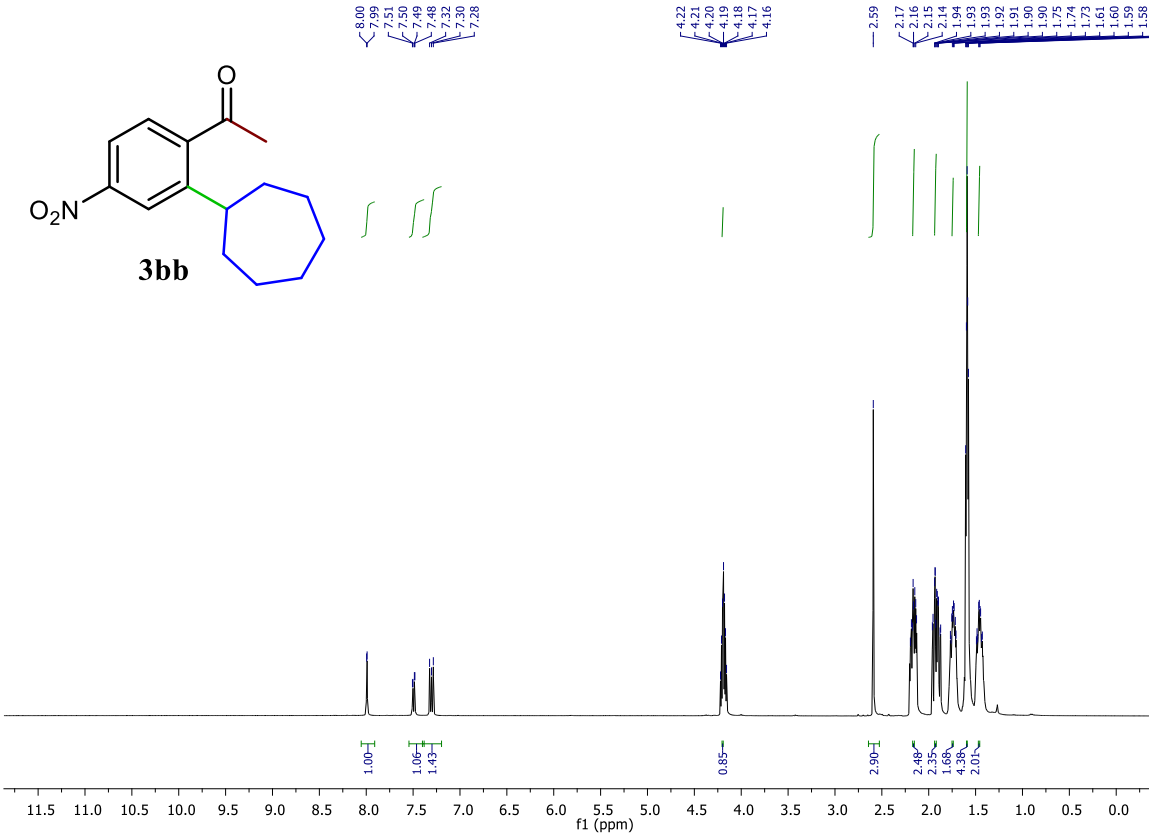
^{1}H NMR of 3ba (400 MHz, 32 scans, RT, $CDCl_3$)



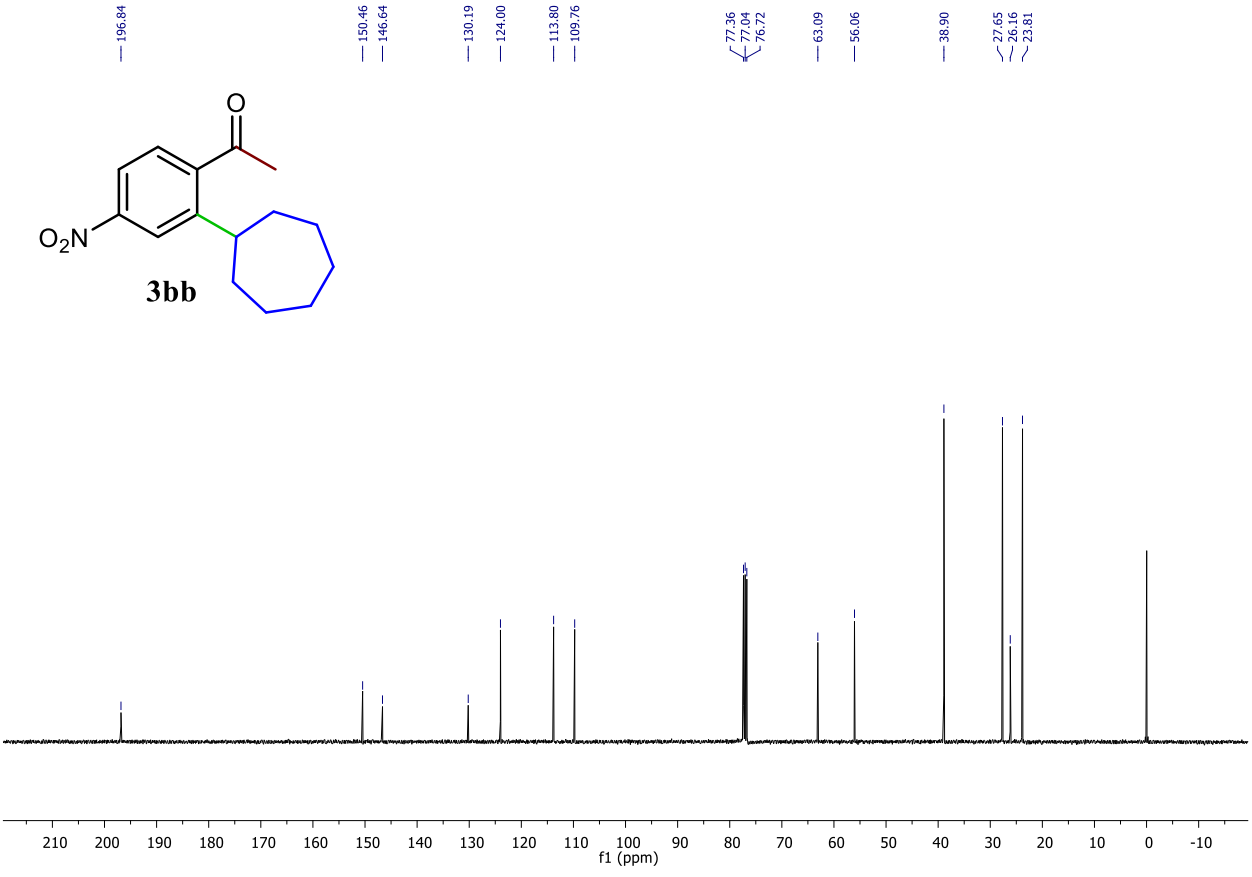
NMR of 3ba (101 MHz, 512 scans, RT, $CDCl_3$)



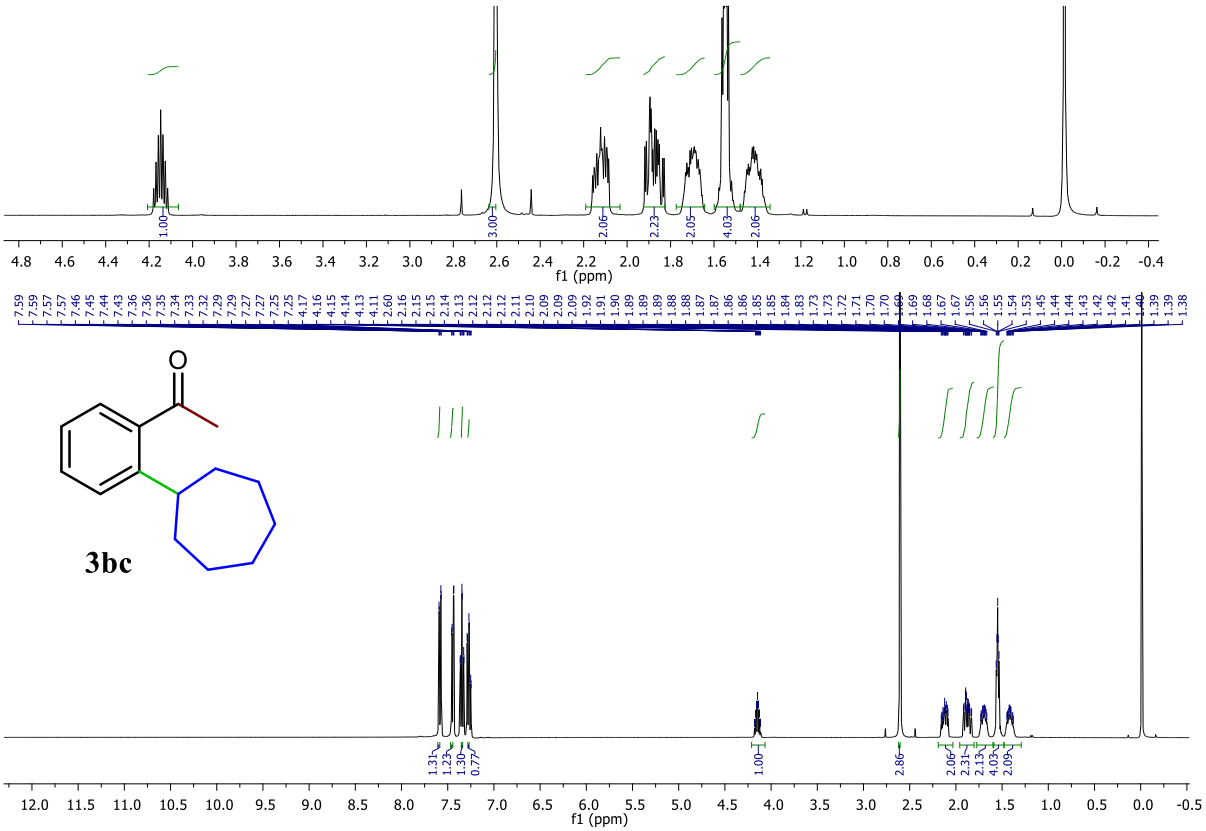
^{1}H NMR of 3bb (400 MHz, 32 scans, RT, $CDCl_3$)



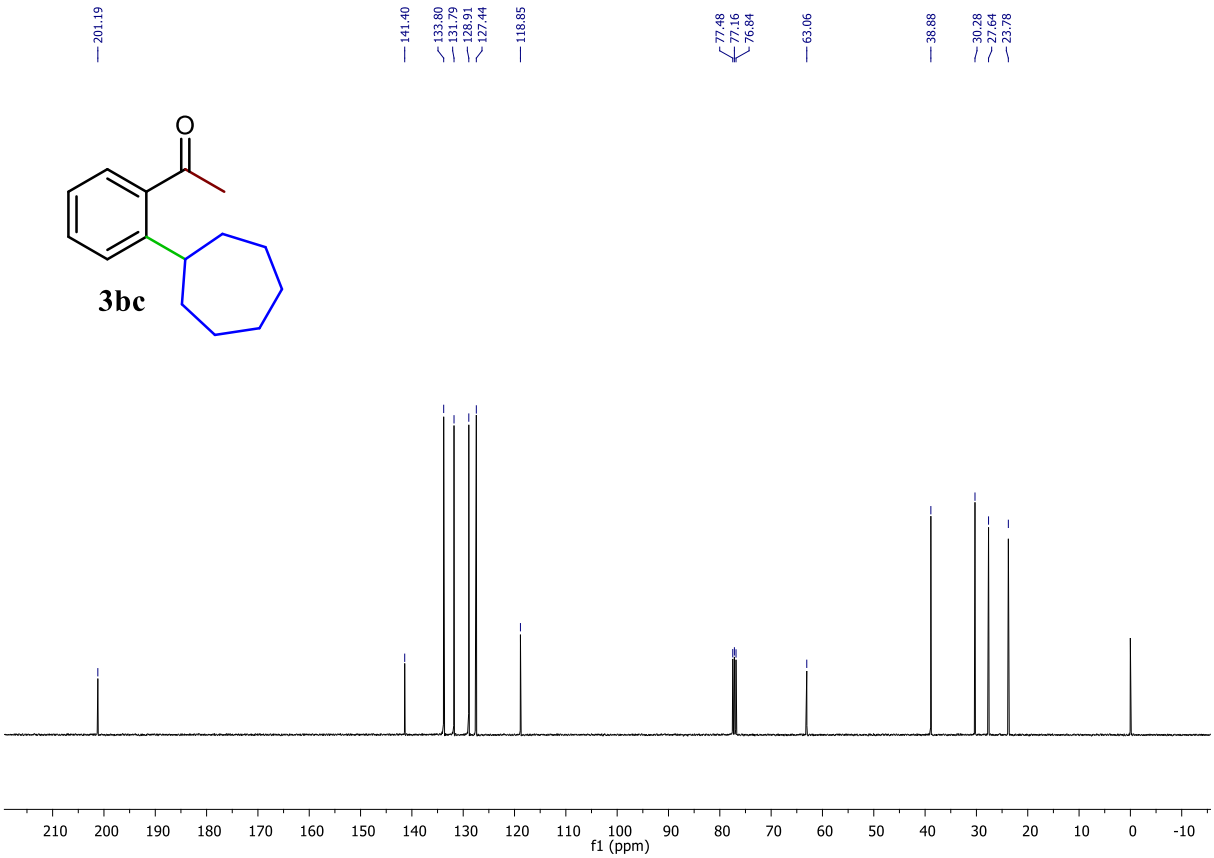
NMR of 3bb (101 MHz, 512 scans, RT, $CDCl_3$)



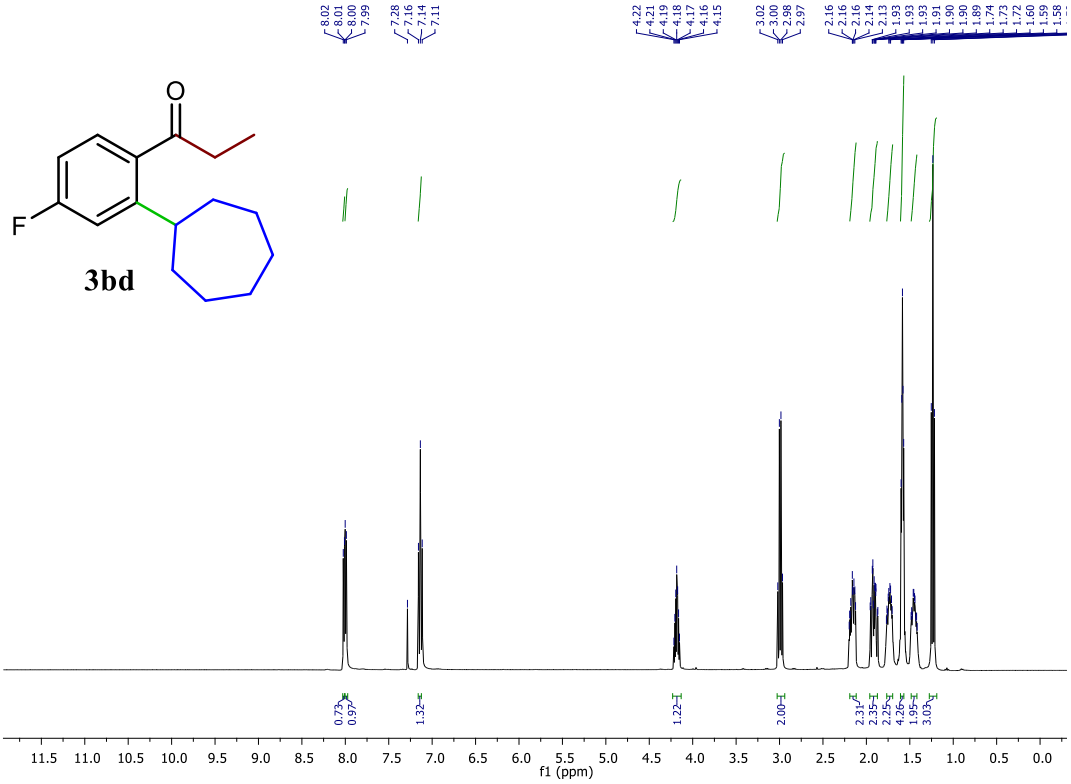
^{1}H NMR of 3bc (400 MHz, 32 scans, RT, $CDCl_3$)



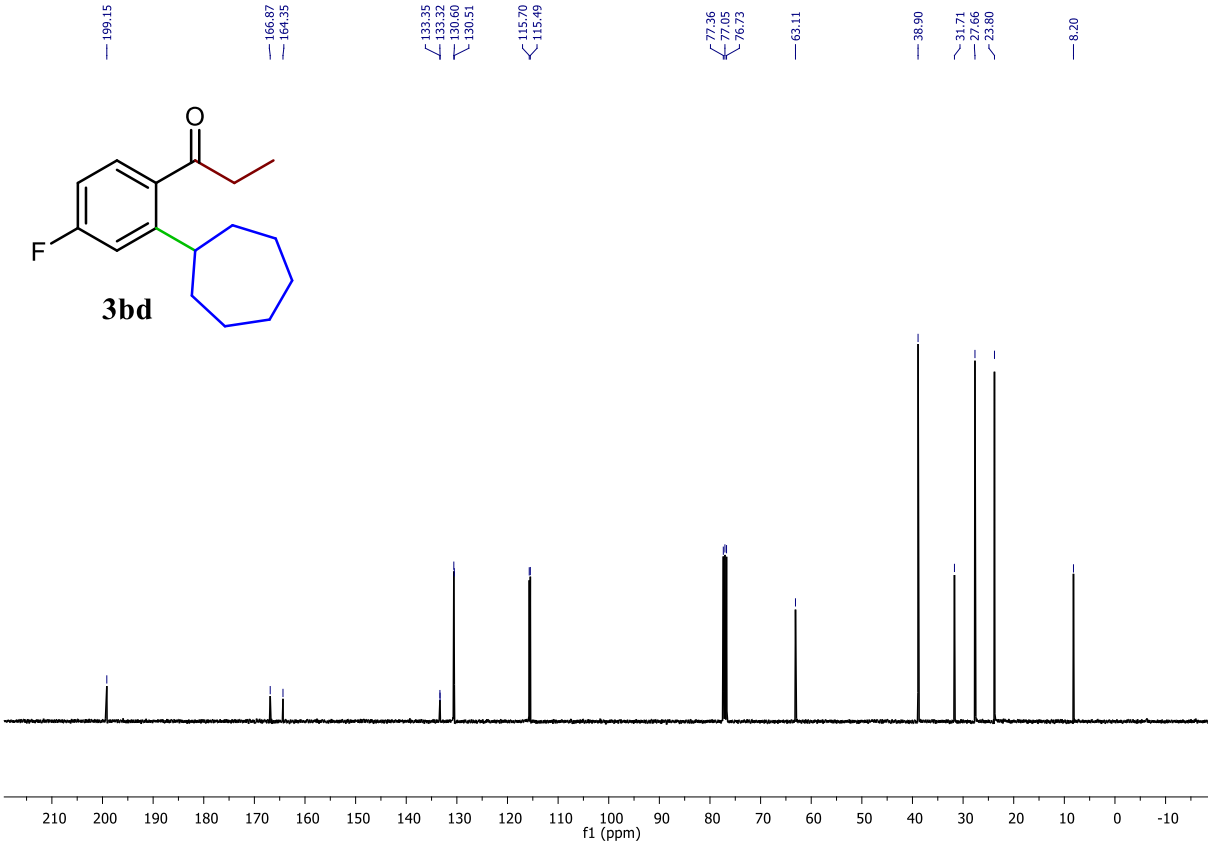
NMR of 3bc (101 MHz, 512 scans, RT, $CDCl_3$)



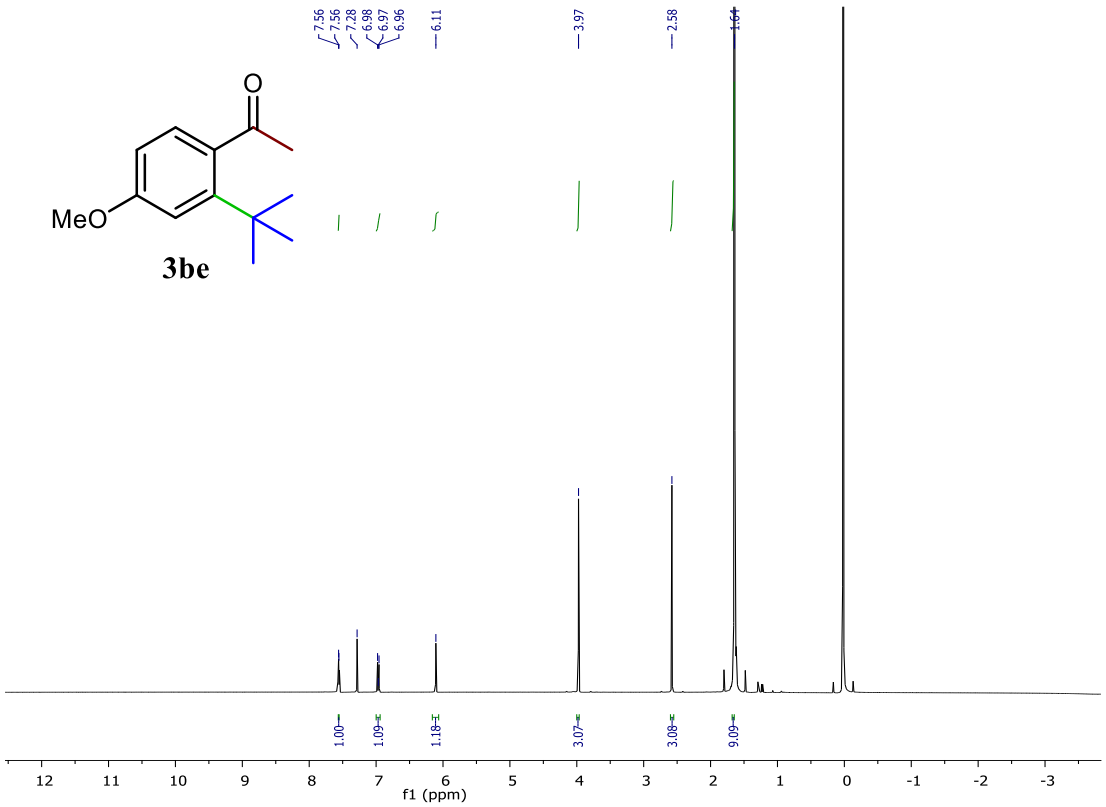
^{1}H NMR of 3bd (400 MHz, 32 scans, RT, $CDCl_3$)



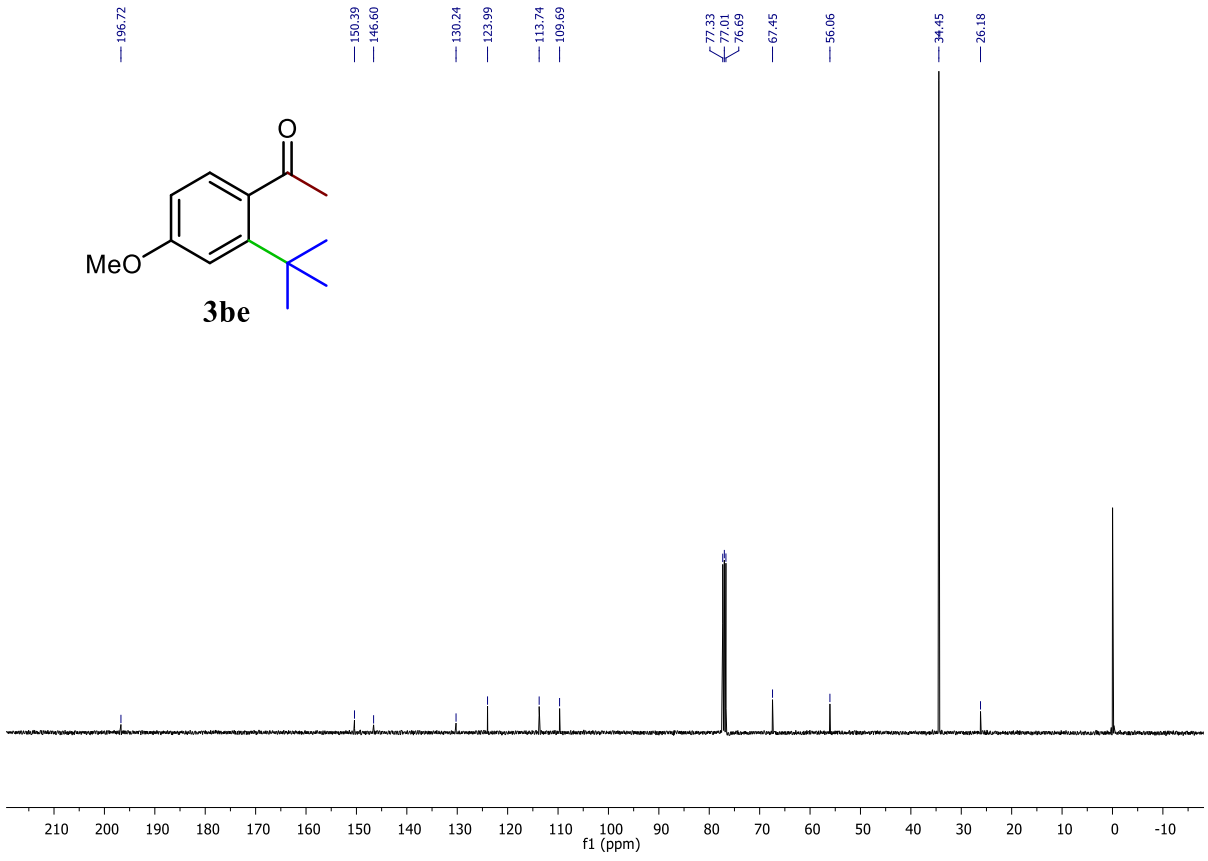
NMR of 3bd (101 MHz, 512 scans, RT, $CDCl_3$)



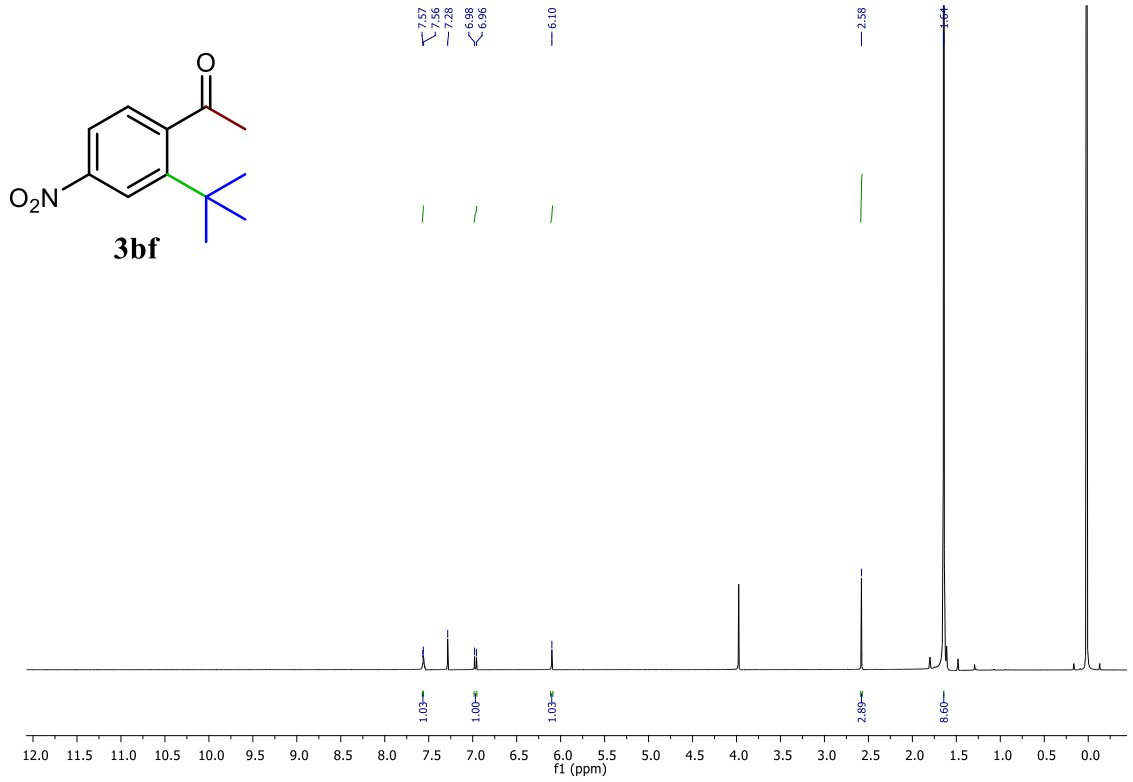
^{1}H NMR of 3be (400 MHz, 32 scans, RT, $CDCl_3$)



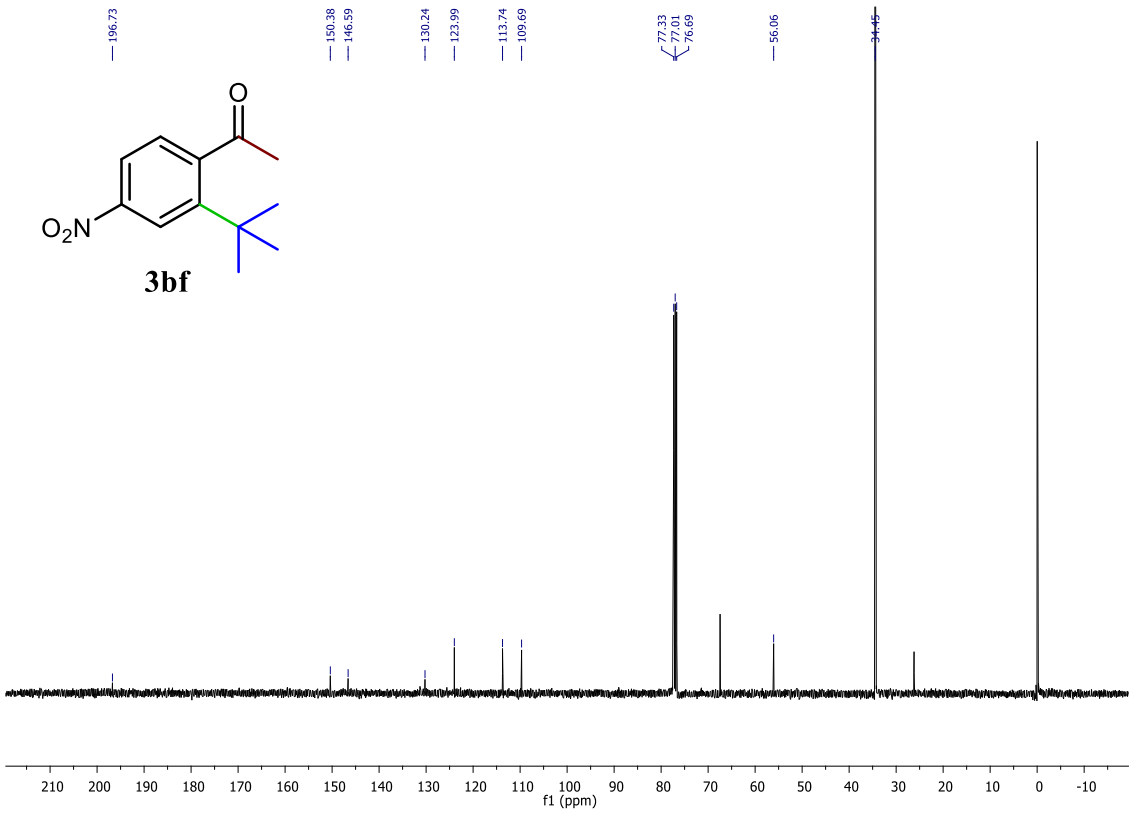
NMR of 3be (101 MHz, 512 scans, RT, $CDCl_3$)



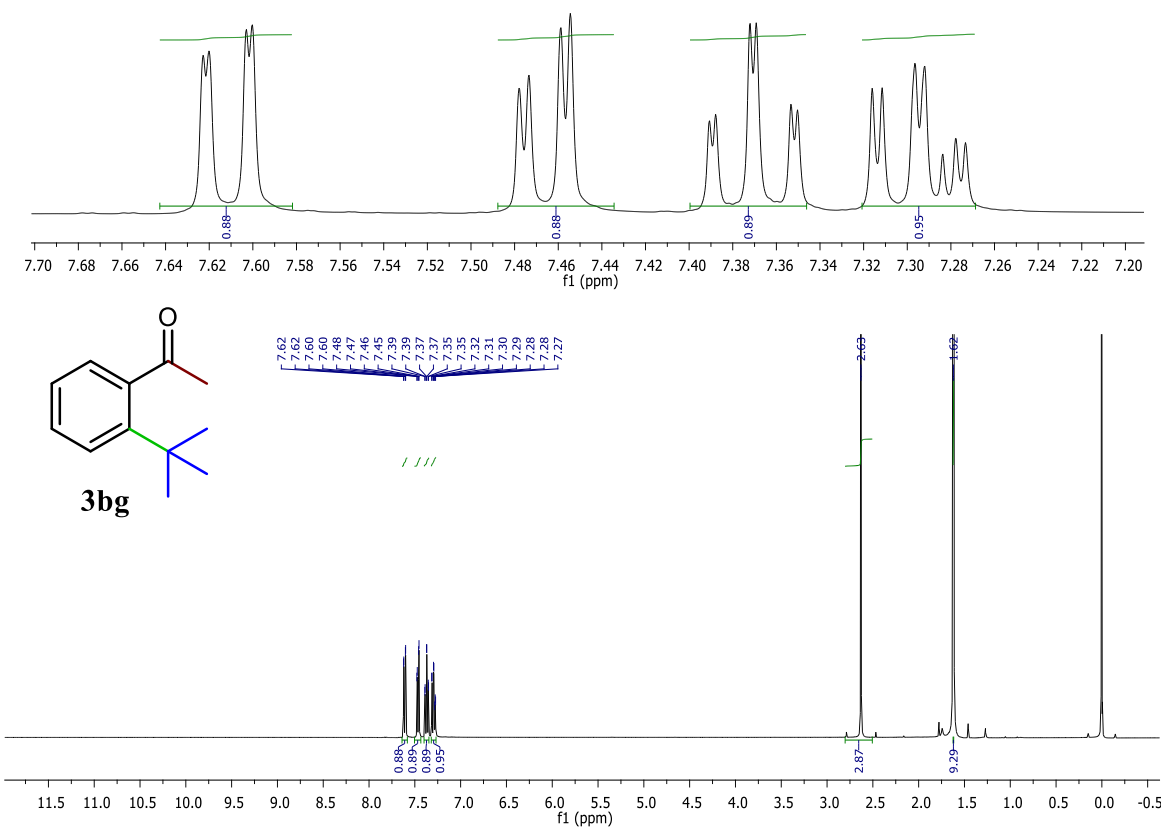
^{1}H NMR of 3bf (400 MHz, 32 scans, RT, $CDCl_3$)



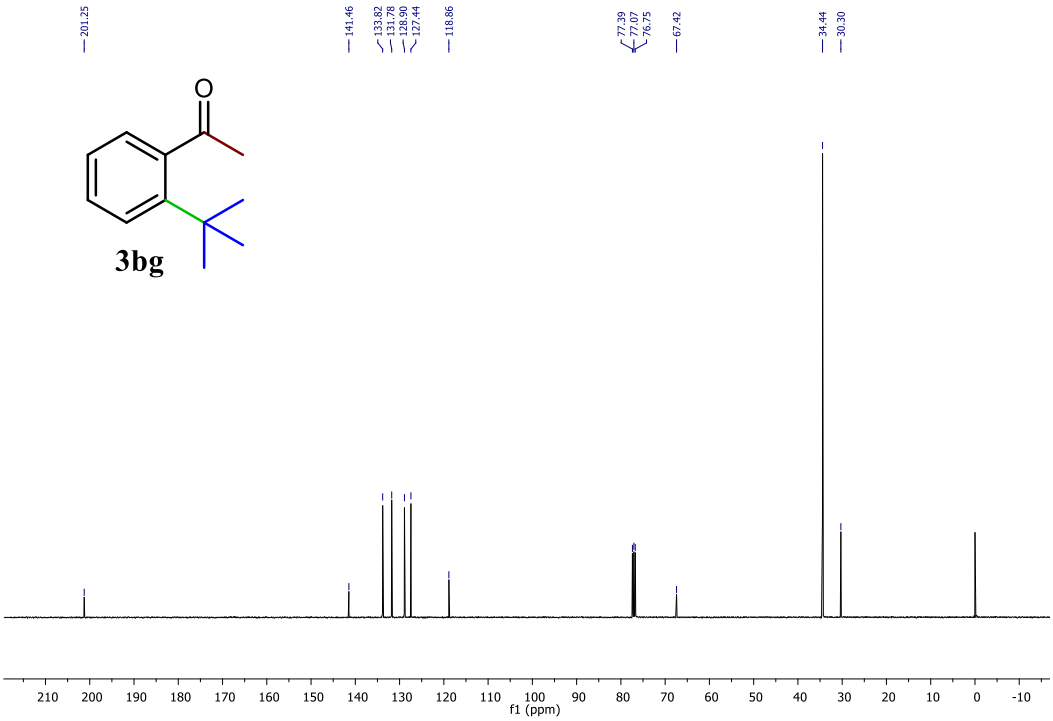
^{13}C NMR of 3bf (101 MHz, 512 scans, RT, $CDCl_3$)



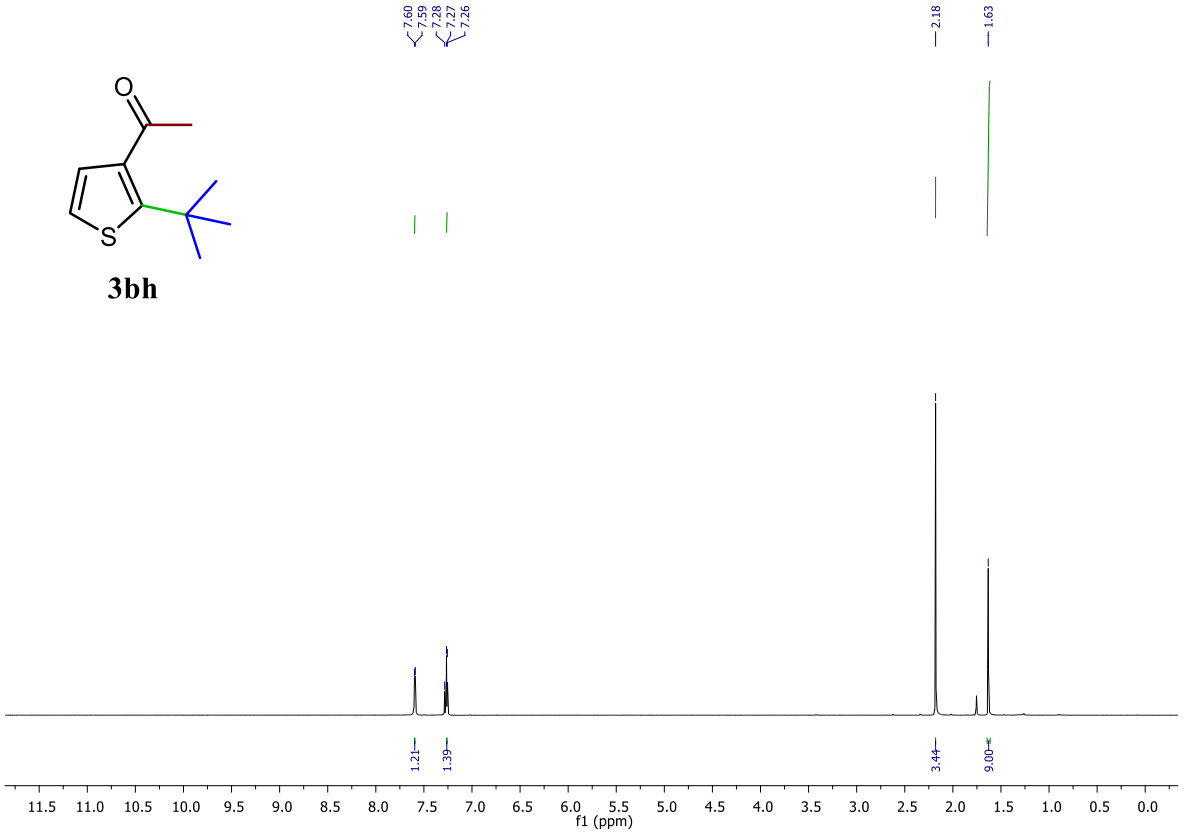
^{1}H NMR of 3bg (400 MHz, 32 scans, RT, $CDCl_3$)



^{13}C NMR of 3bg (101 MHz, 512 scans, RT, $CDCl_3$)

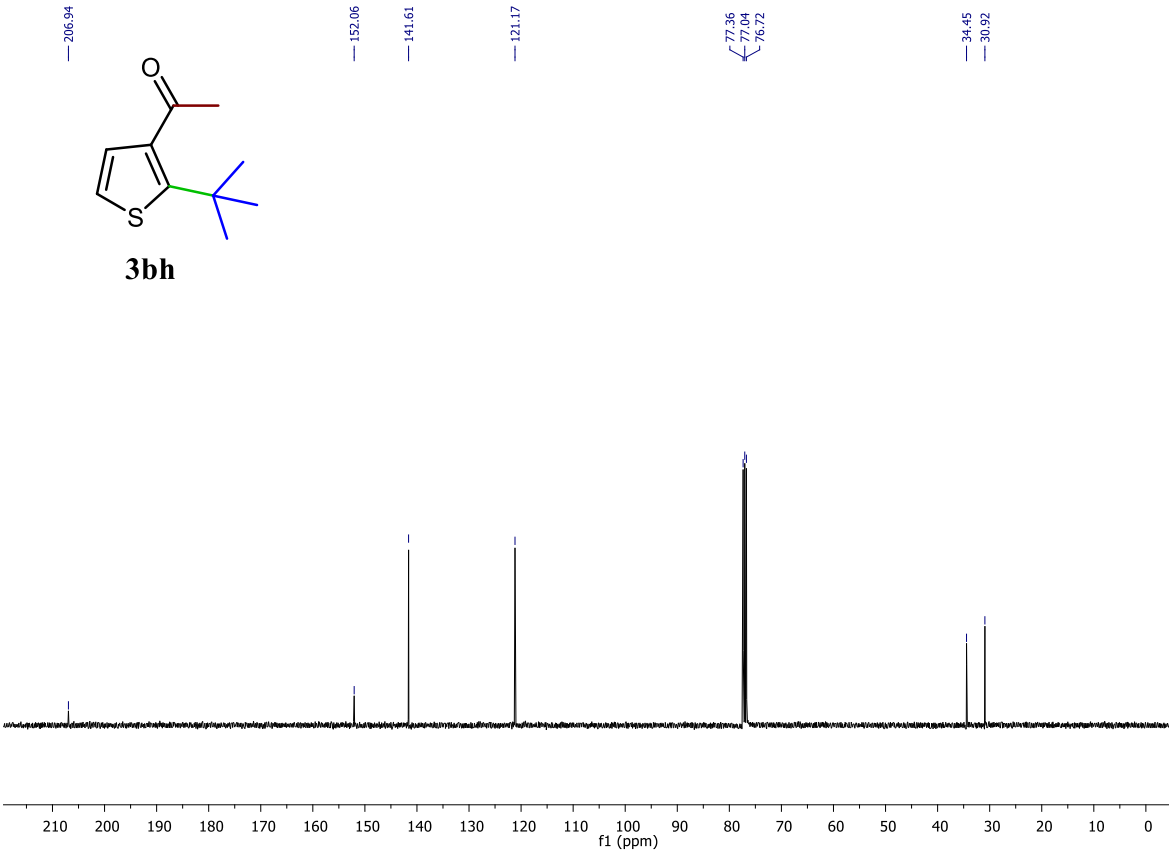


^{1}H NMR of 3bh (400 MHz, 32 scans, RT, $CDCl_3$)



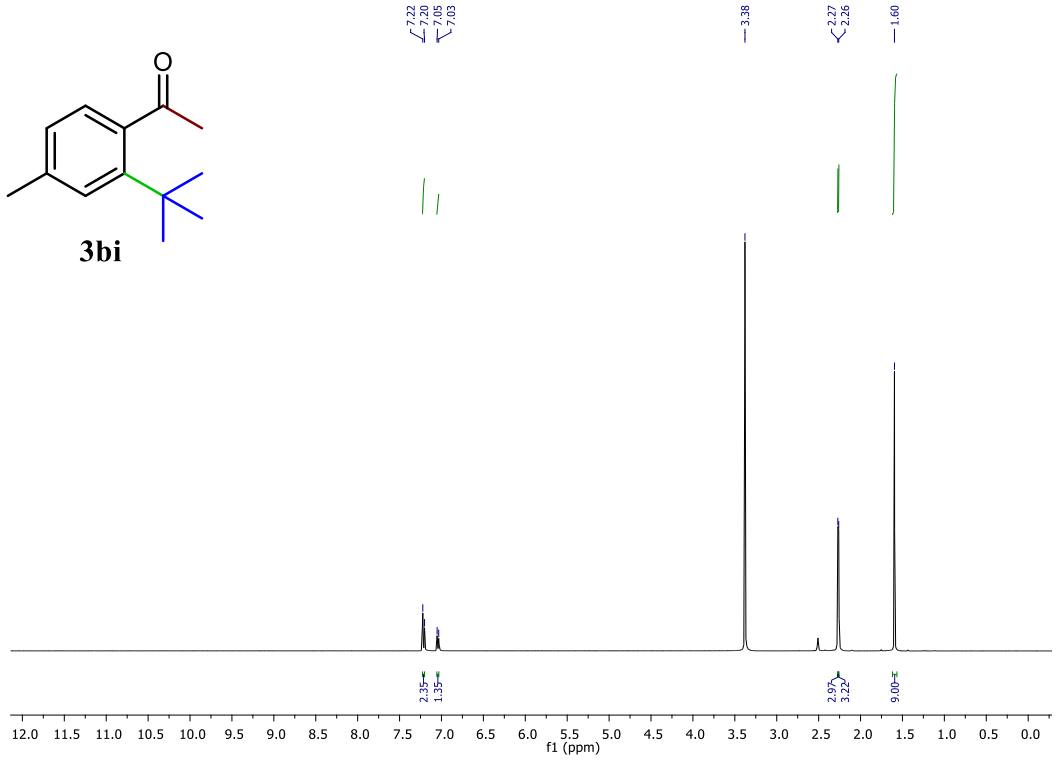
3bh

NMR of 3bh (101 MHz, 512 scans, RT, $CDCl_3$)



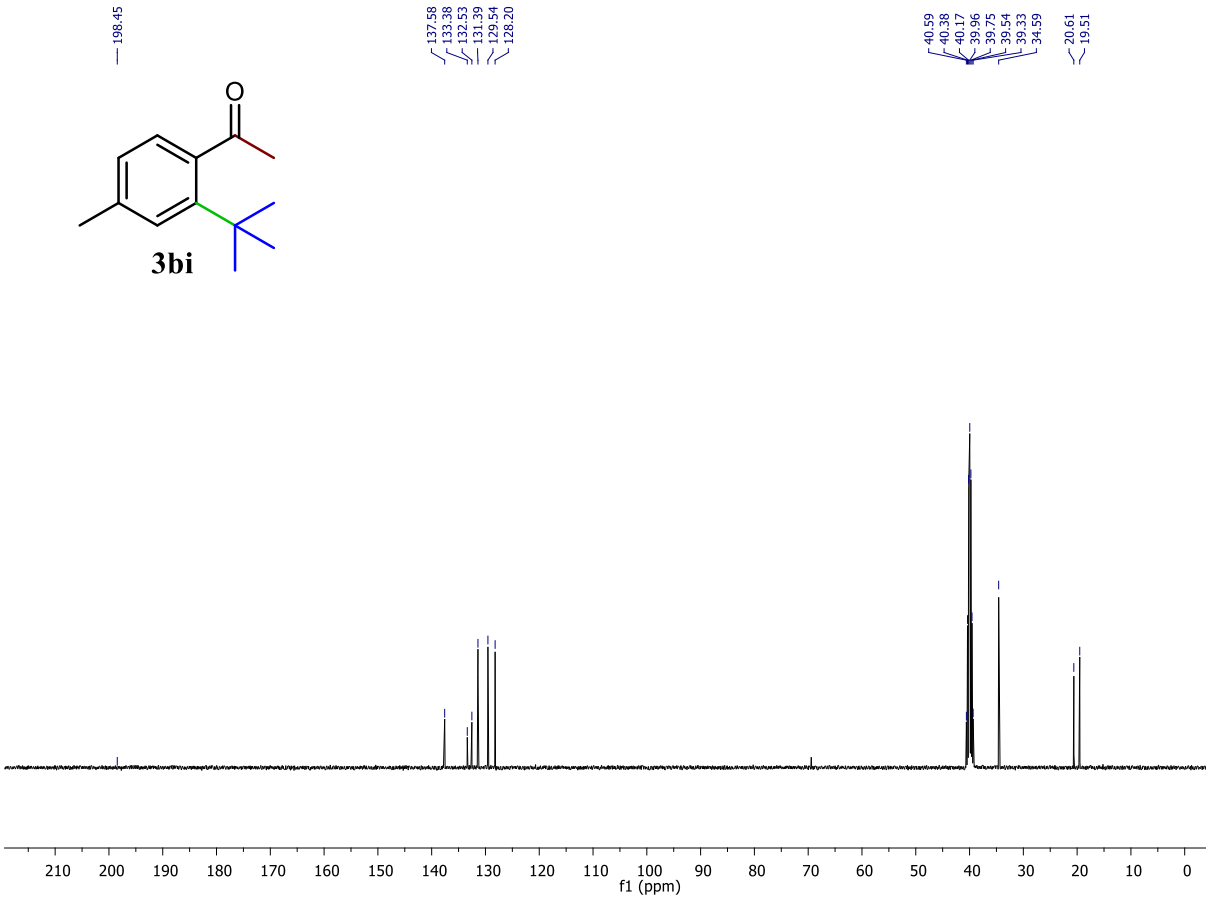
3bh

^{1}H NMR of 3bi (400 MHz, 32 scans, RT, DMSO-d$_6$)



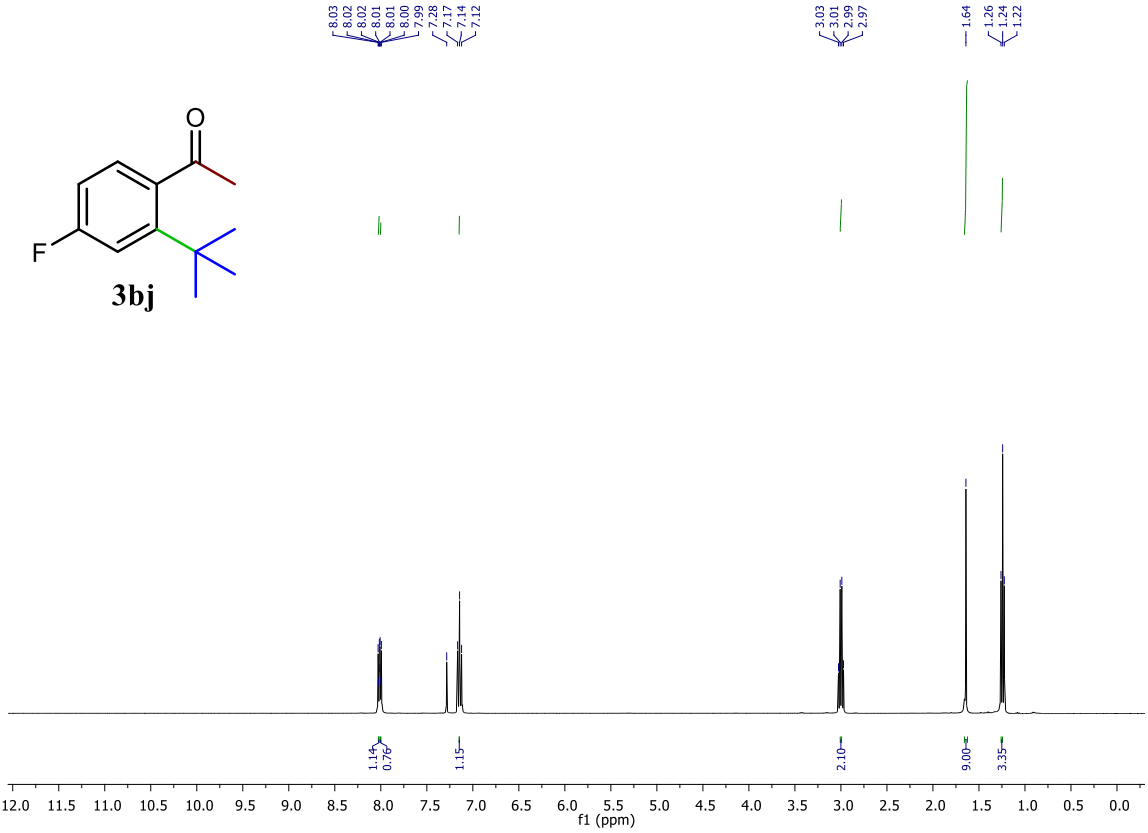
3bi

^{13}CNMR of 3bi (101 MHz, 512 scans, RT, DMSO-d$_6$)

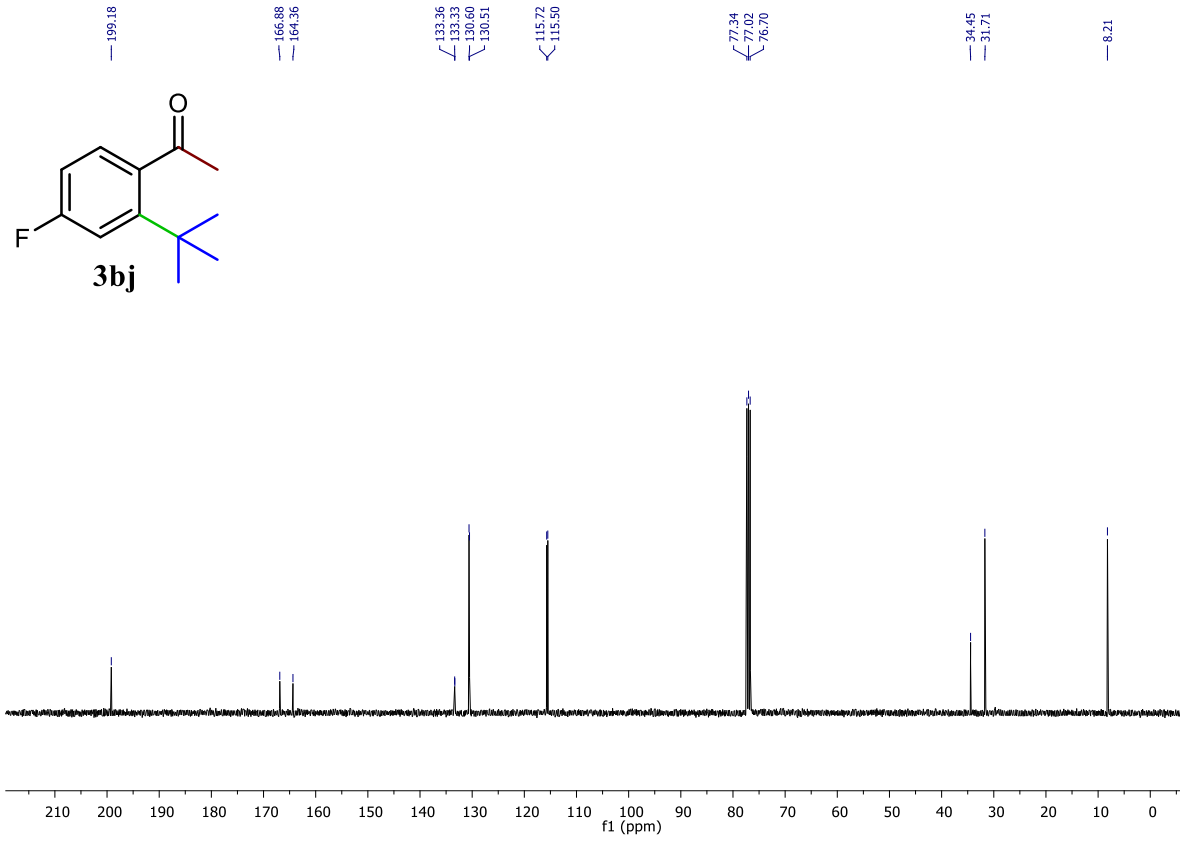


3bi

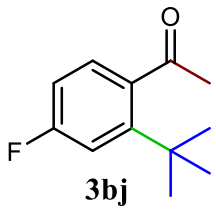
^{1}H NMR of 3bj (400 MHz, 32 scans, RT, $CDCl_3$)



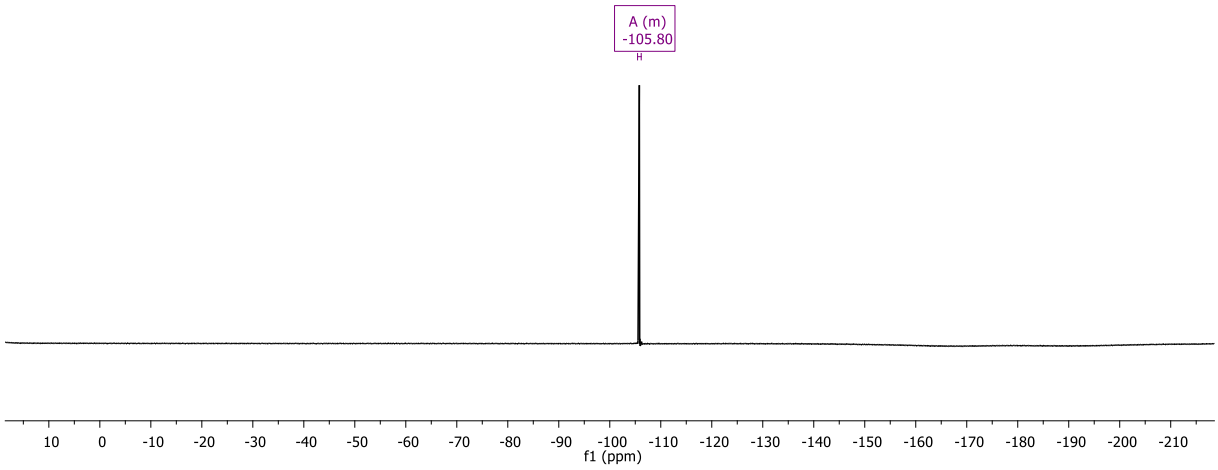
^{13}C NMR of 3bj (101 MHz, 512 scans, RT, $CDCl_3$)



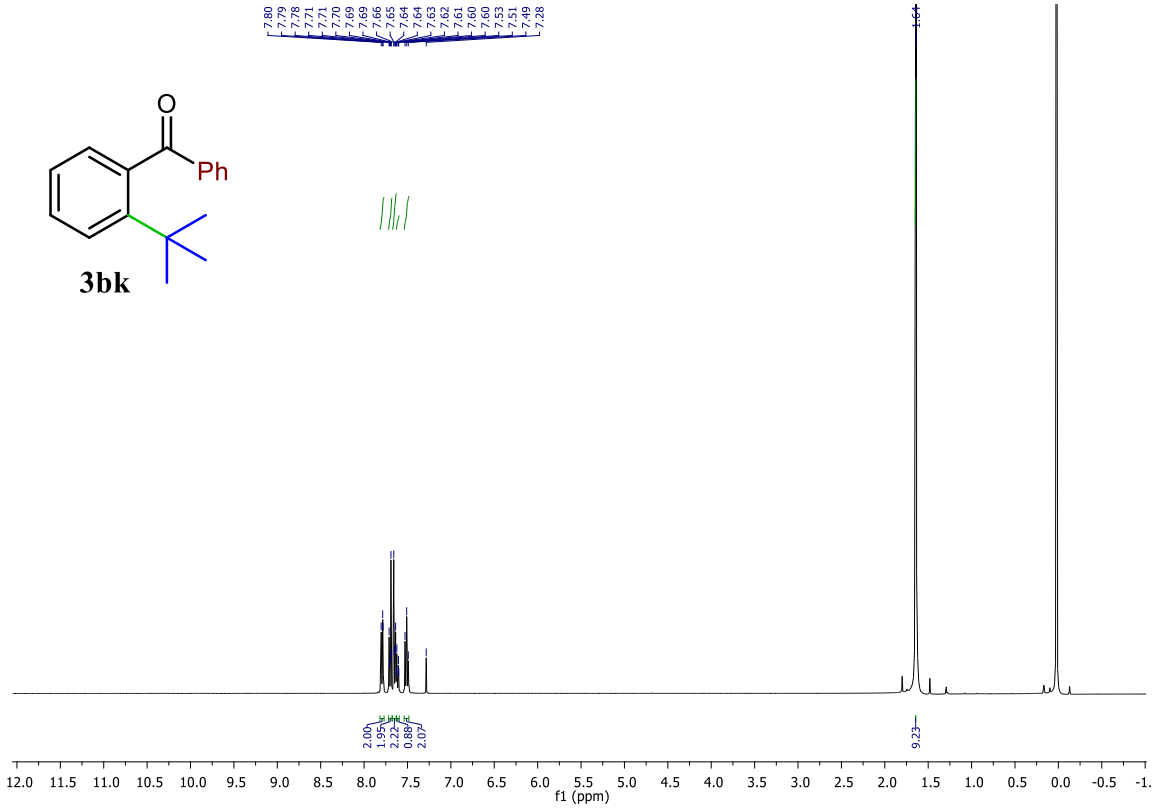
^{19}F NMR of **3bj (377 MHz, $CDCl_3$)**



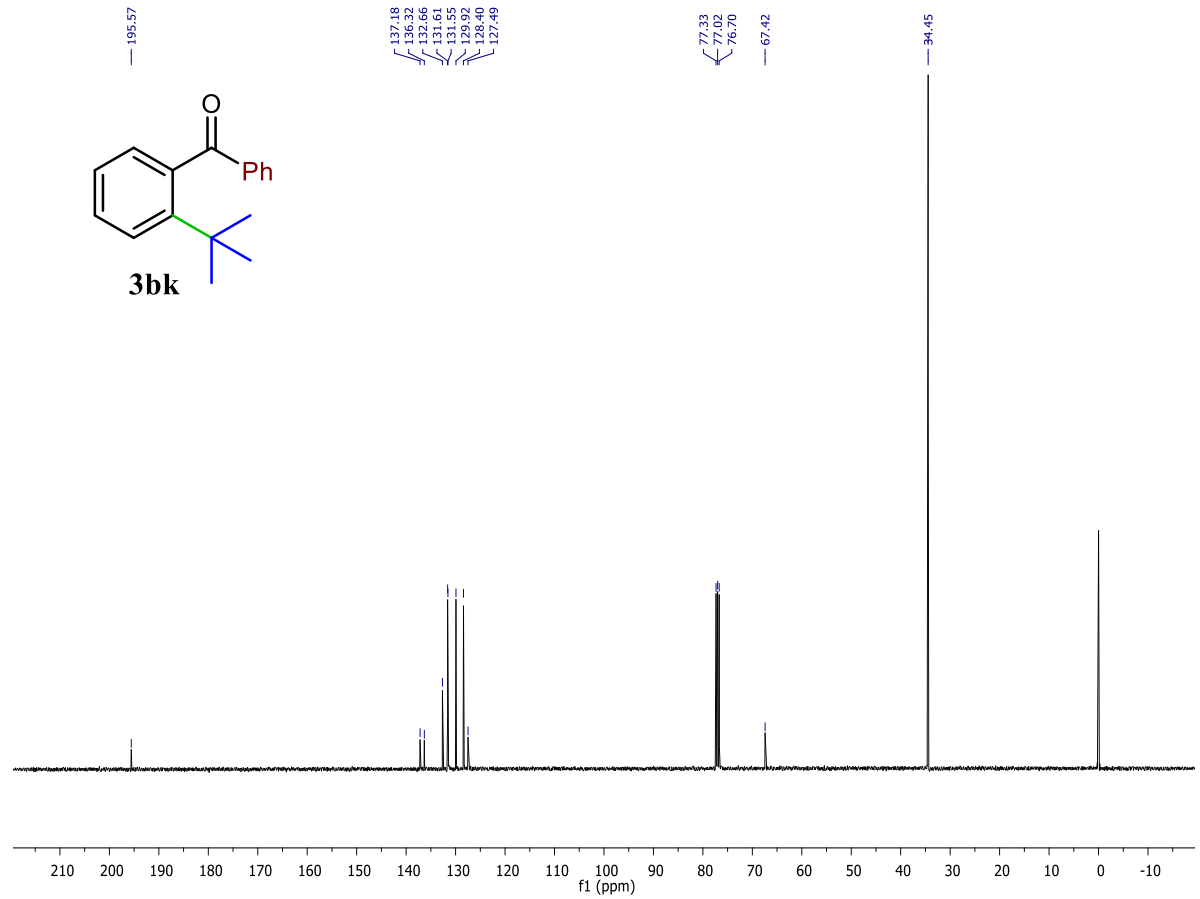
3bj



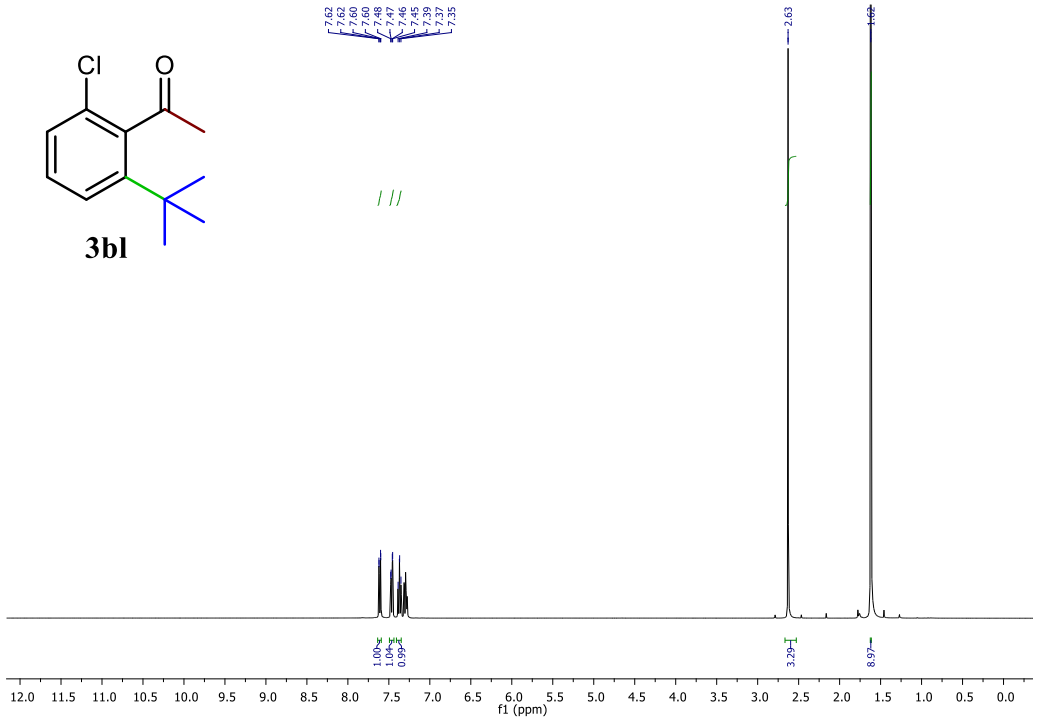
^{1}H NMR of 3bk (400 MHz, 32 scans, RT, $CDCl_3$)



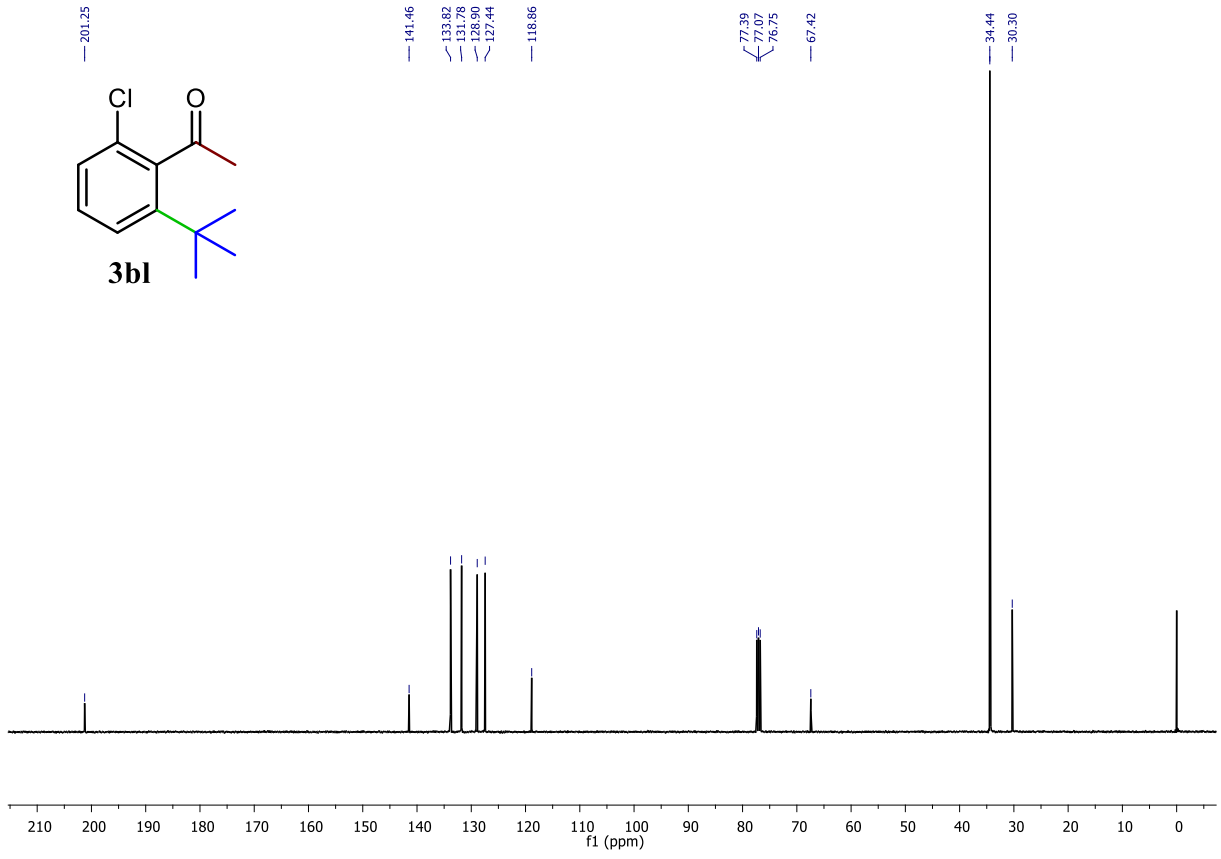
^{13}CNMR of 3bk (101 MHz, 512 scans, RT, $CDCl_3$)



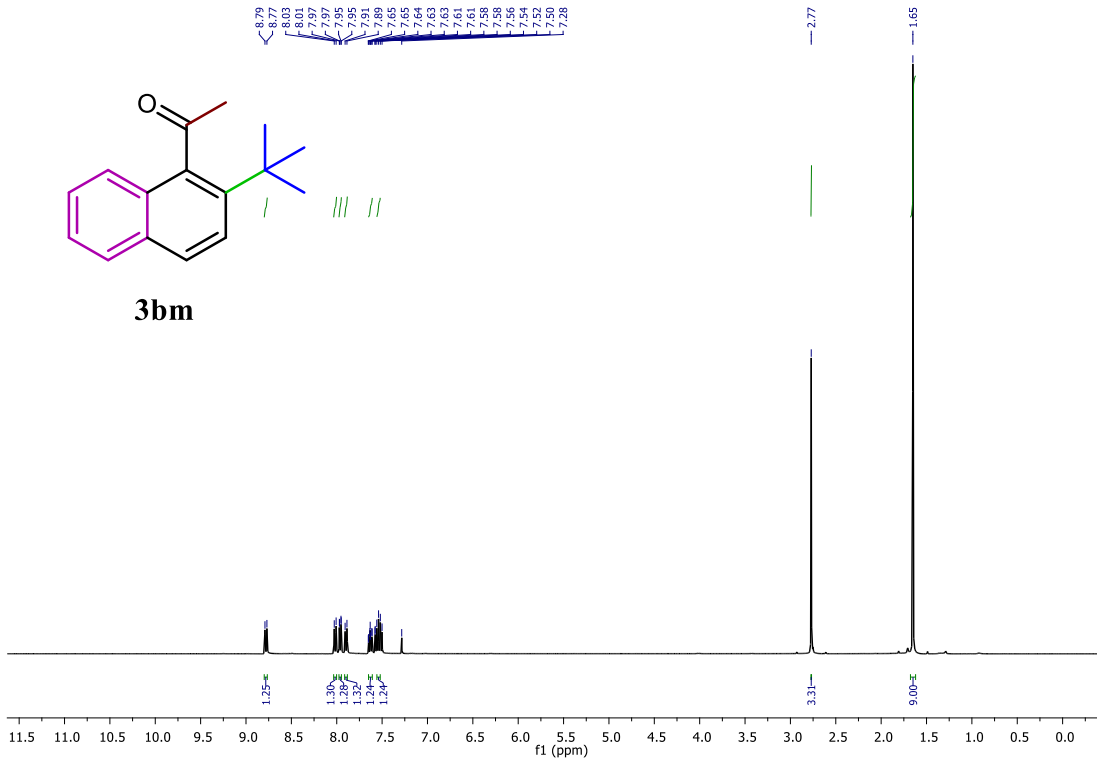
^{1}H NMR of 3bl (400 MHz, 32 scans, RT, $CDCl_3$)



^{13}CNMR of 3bl (101 MHz, 512 scans, RT, $CDCl_3$)

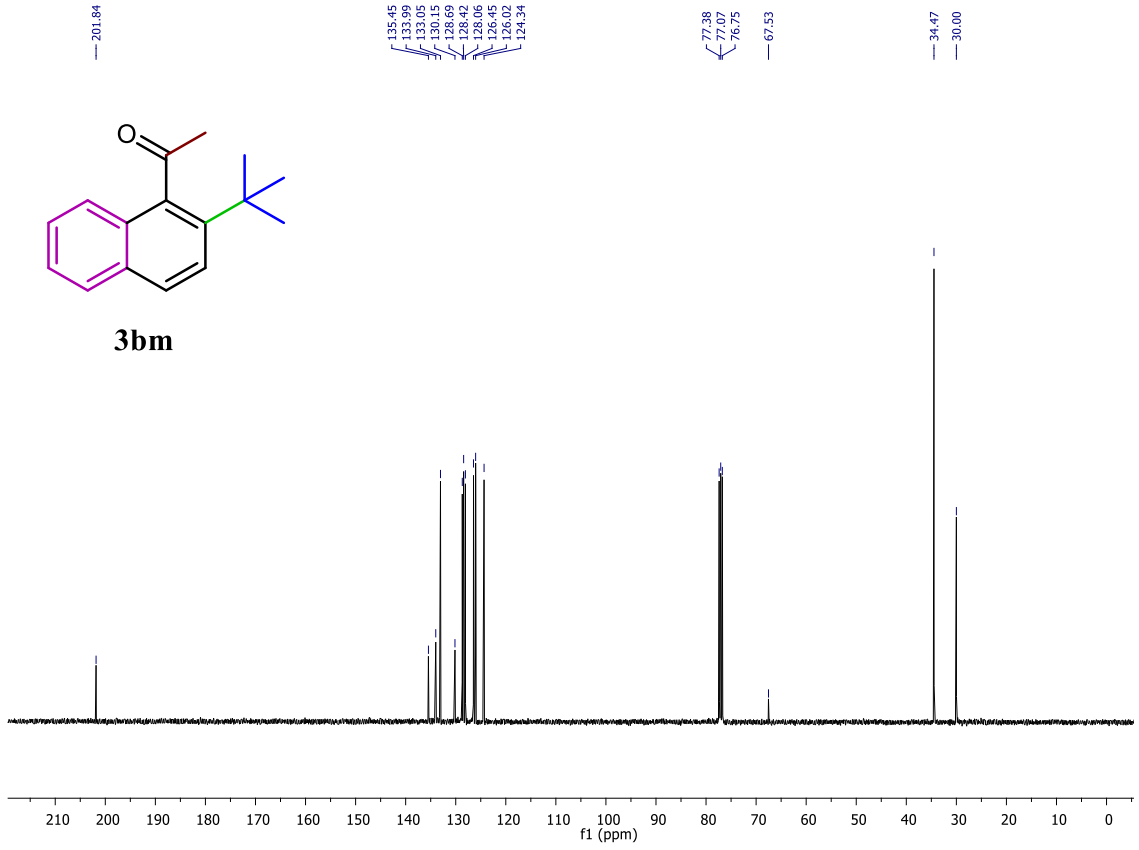


^{1}H NMR of 3bm (400 MHz, 32 scans, RT, $CDCl_3$)



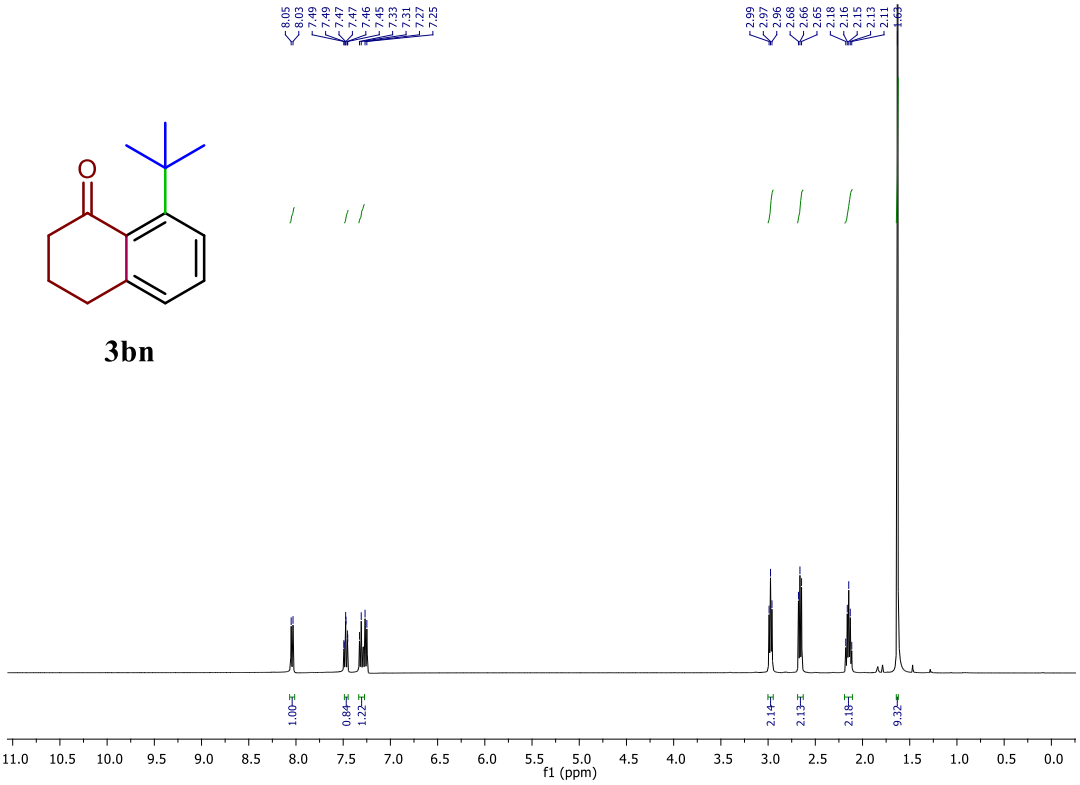
3bm

^{13}CNMR of 3bm (101 MHz, 512 scans, RT, $CDCl_3$)



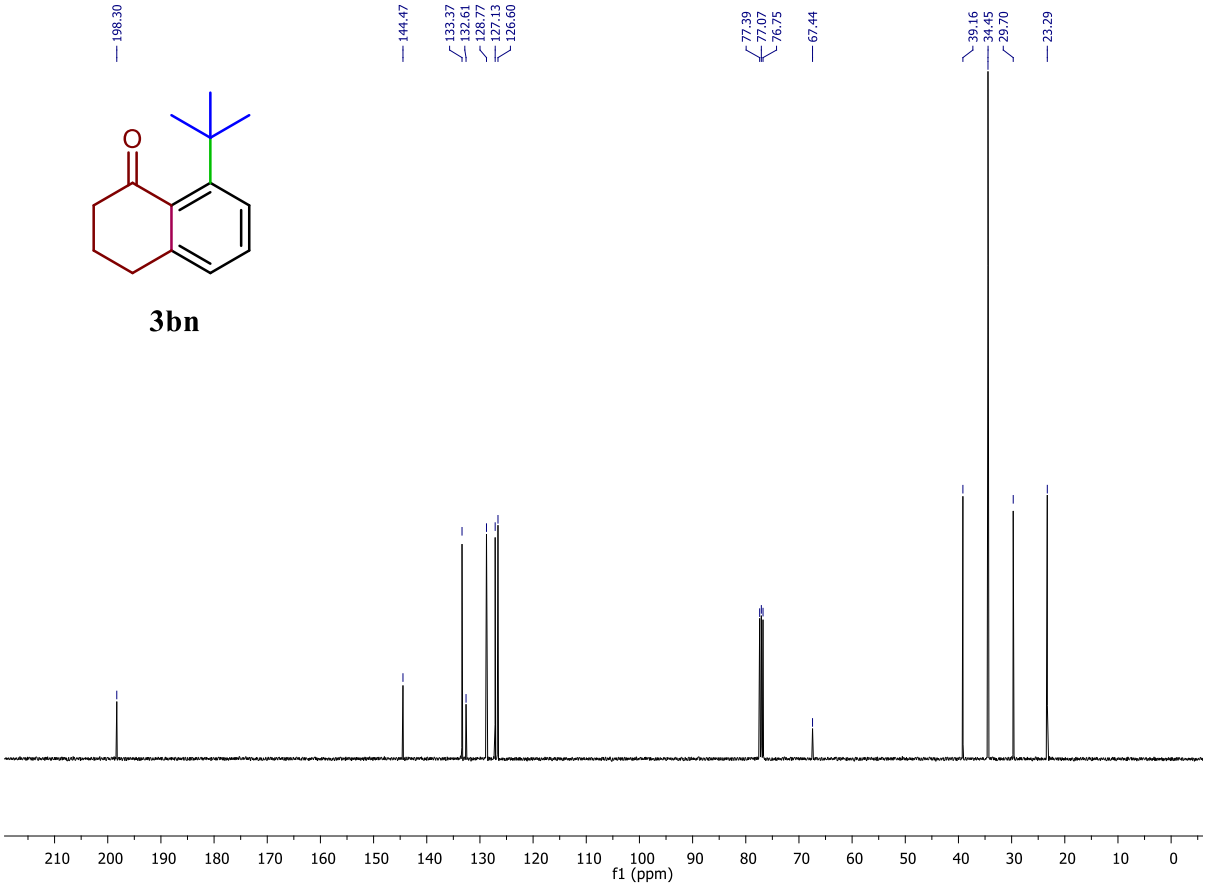
3bm

^{1}H NMR of 3bn (400 MHz, 32 scans, RT, $CDCl_3$)



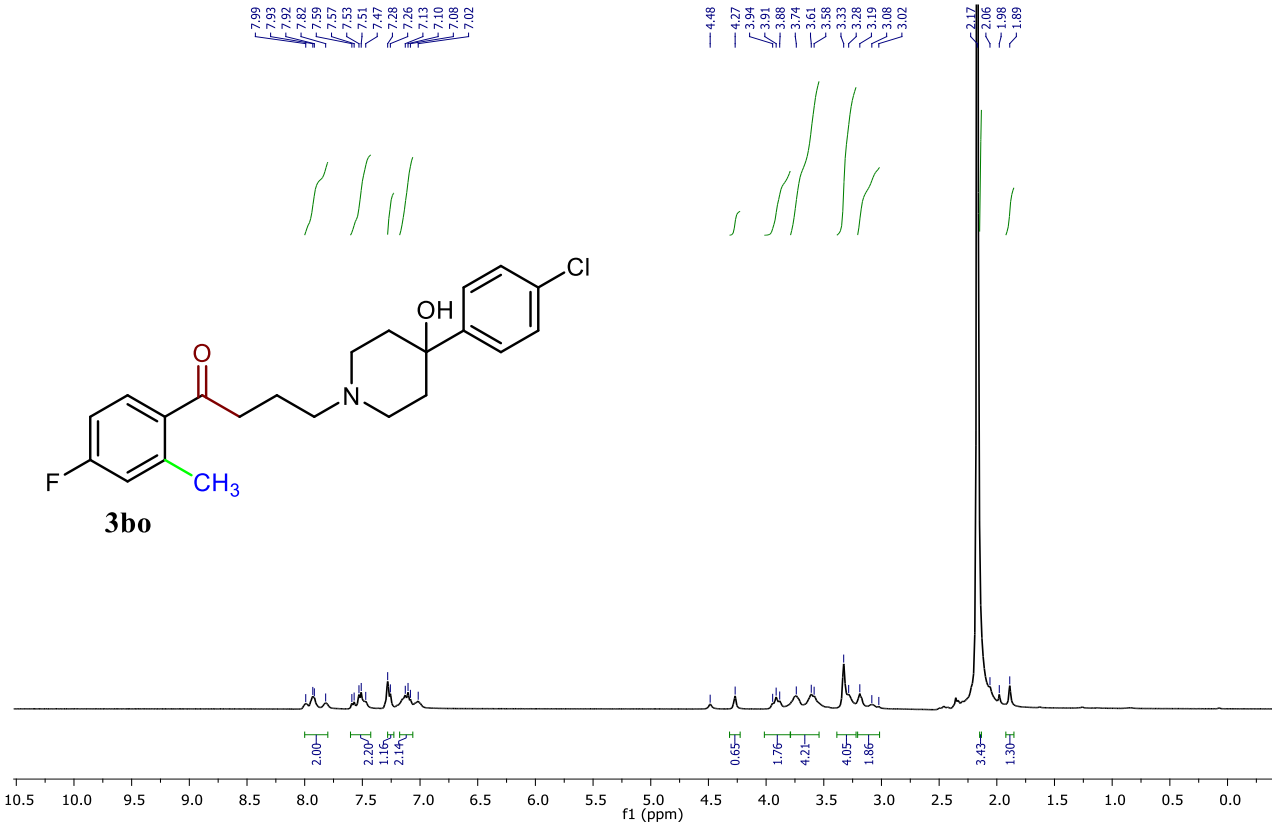
3bn

^{13}CNMR of 3bn (101 MHz, 512 scans, RT, $CDCl_3$)

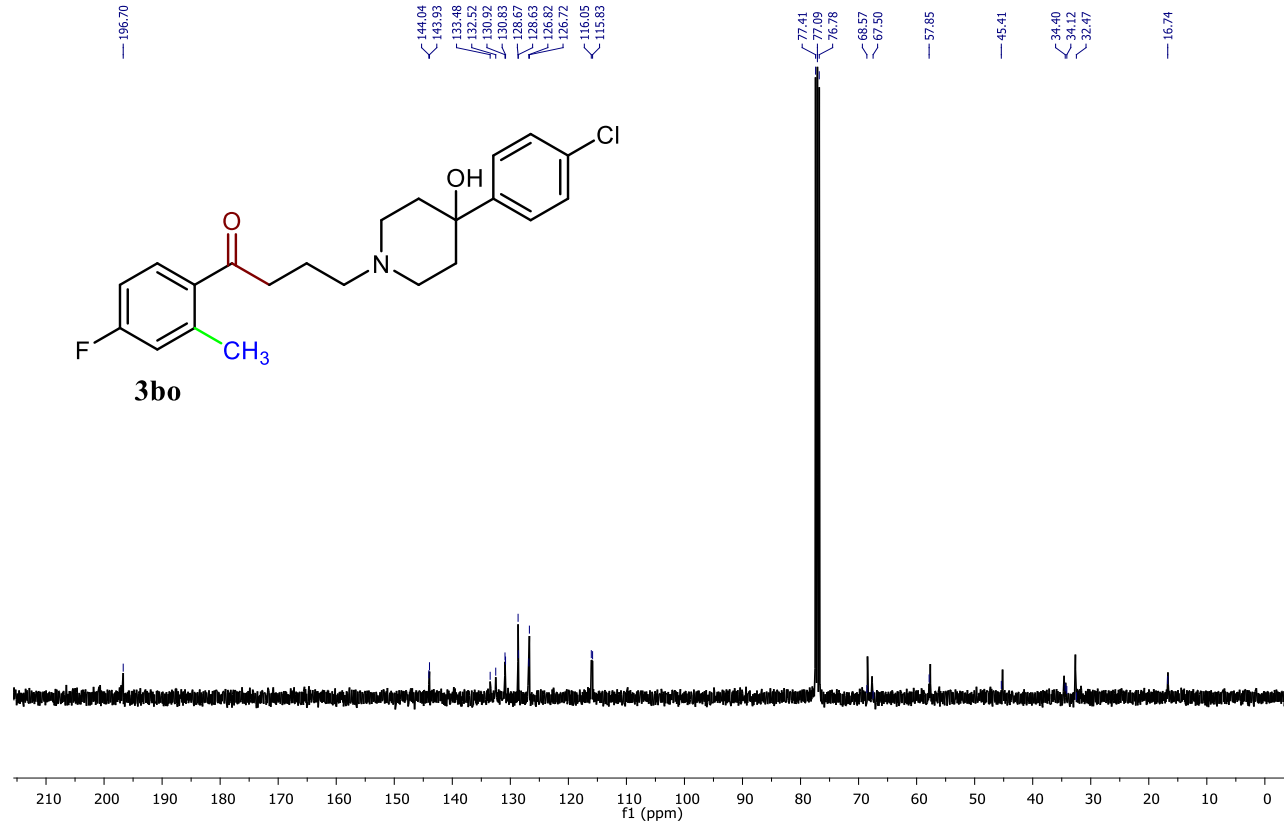


3bn

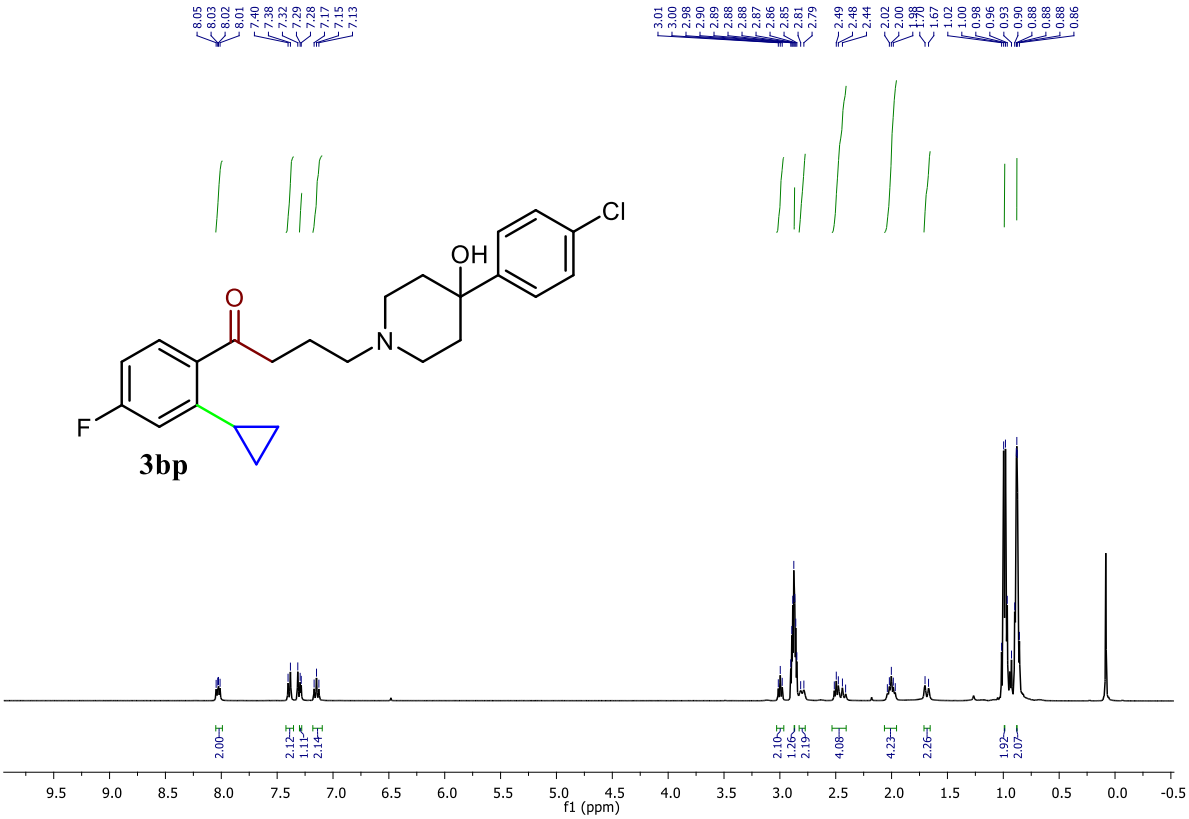
^{1}H NMR of 3bo (400 MHz, 32 scans, RT, $CDCl_3$)



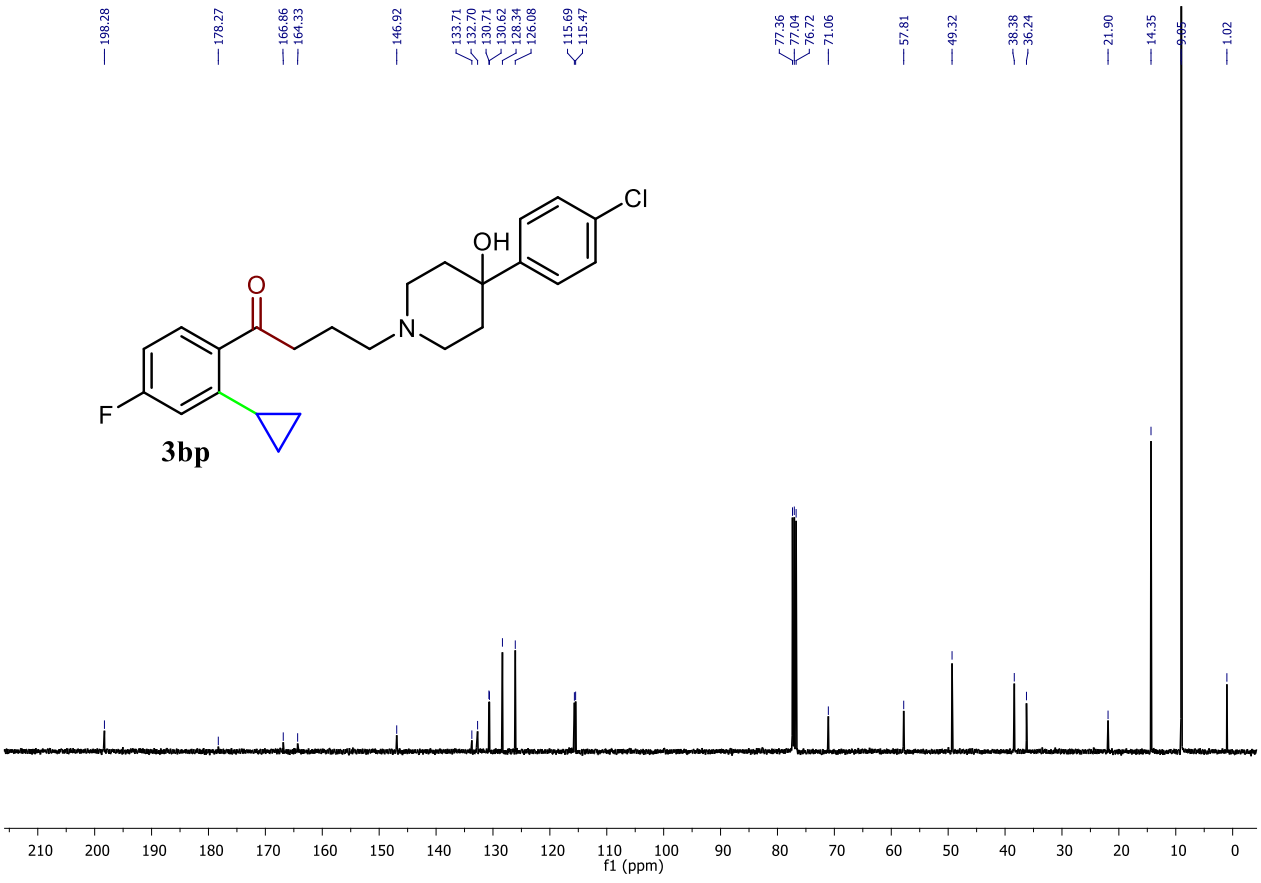
^{13}CNMR of 3bo (101 MHz, 512 scans, RT, $CDCl_3$)



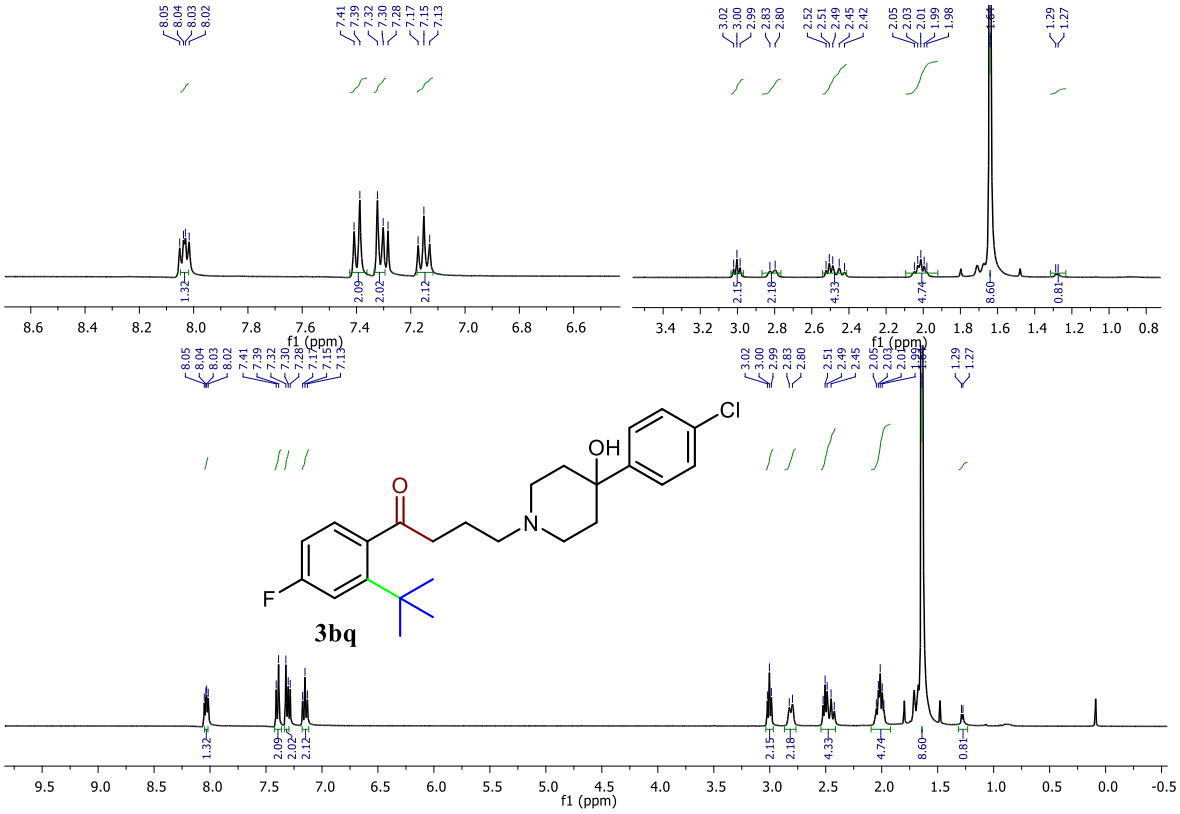
^{1}H NMR of 3bp (400 MHz, 32 scans, RT, $CDCl_3$)



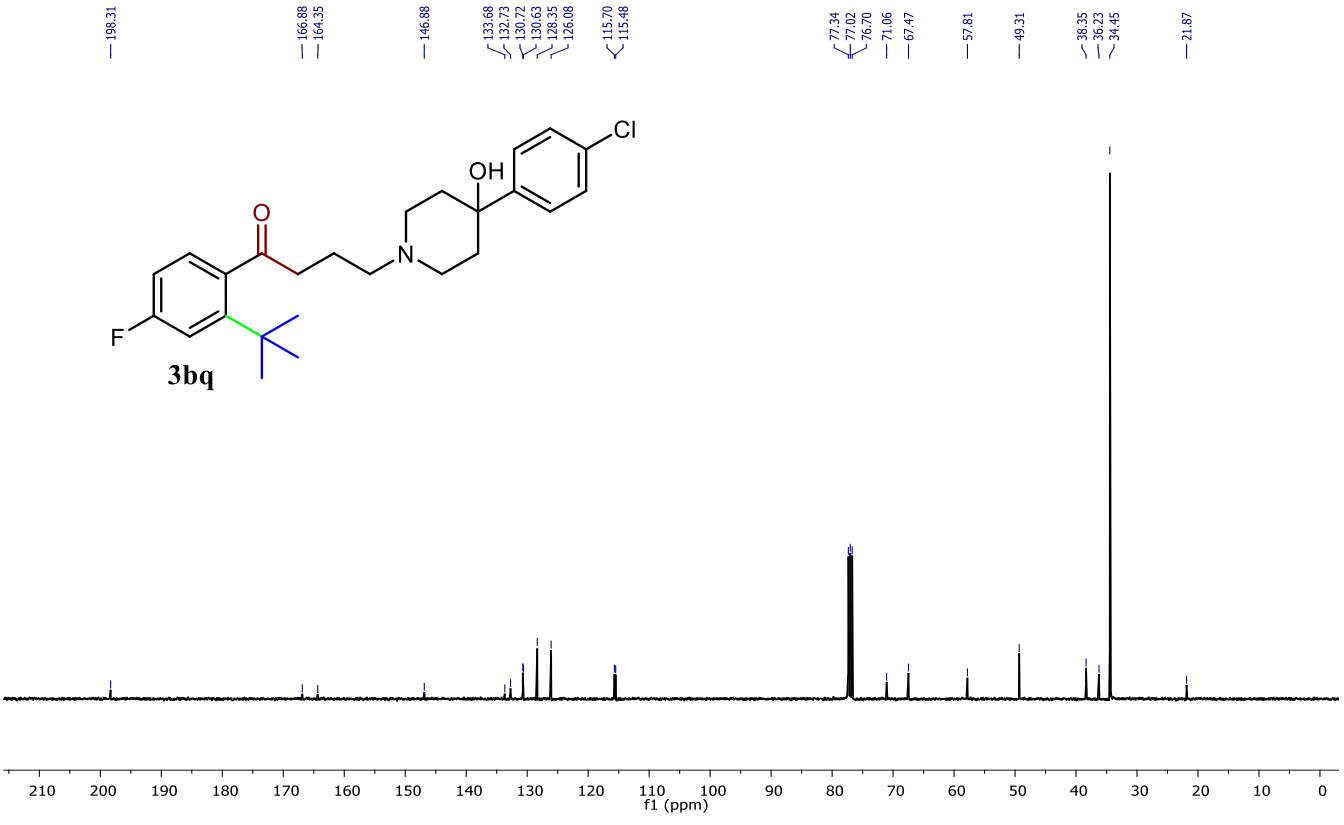
^{13}CNMR of 3bo (101 MHz, 512 scans, RT, $CDCl_3$)



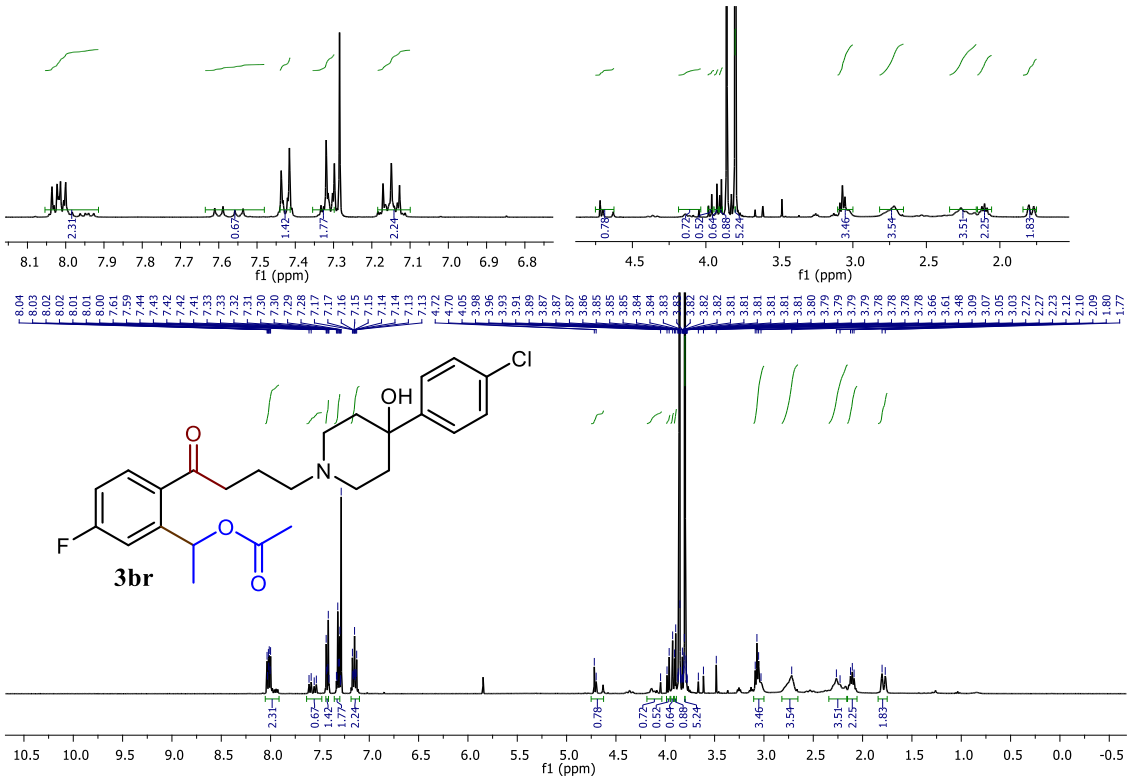
^{1}H NMR of 3bq (400 MHz, 32 scans, RT, $CDCl_3$)



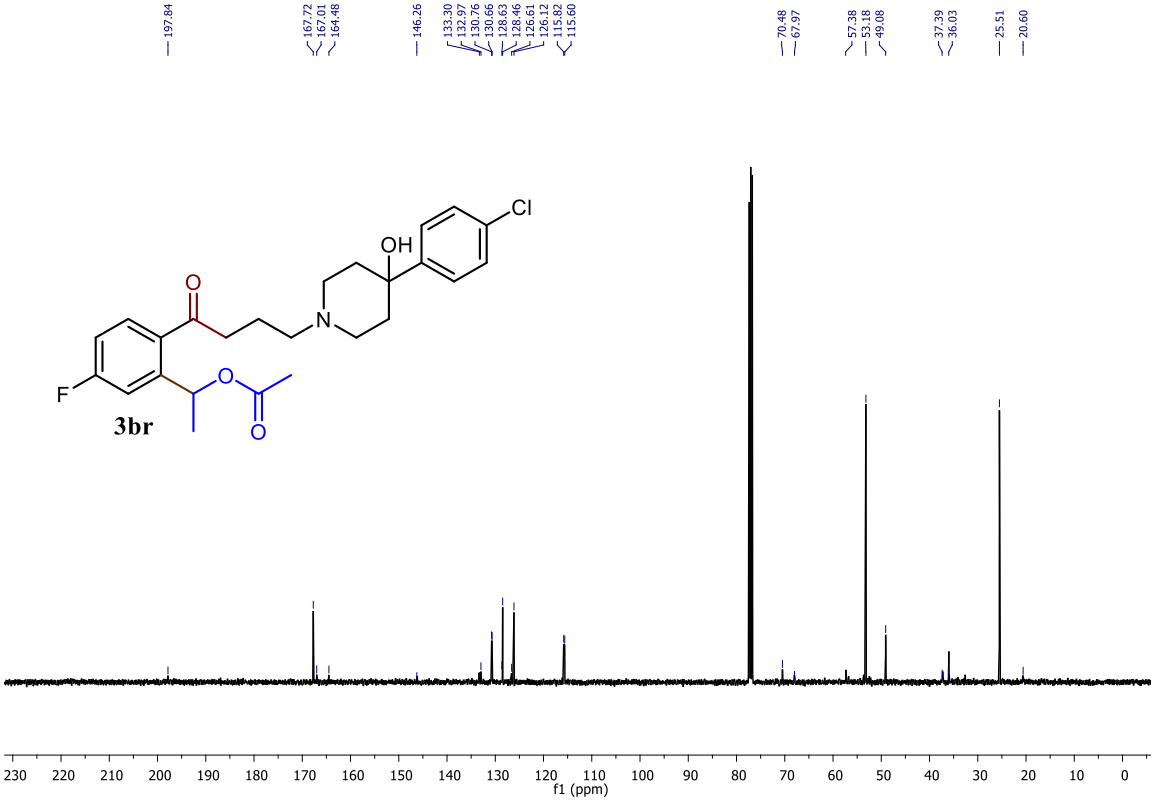
^{13}CNMR of 3bq (101 MHz, 512 scans, RT, $CDCl_3$)



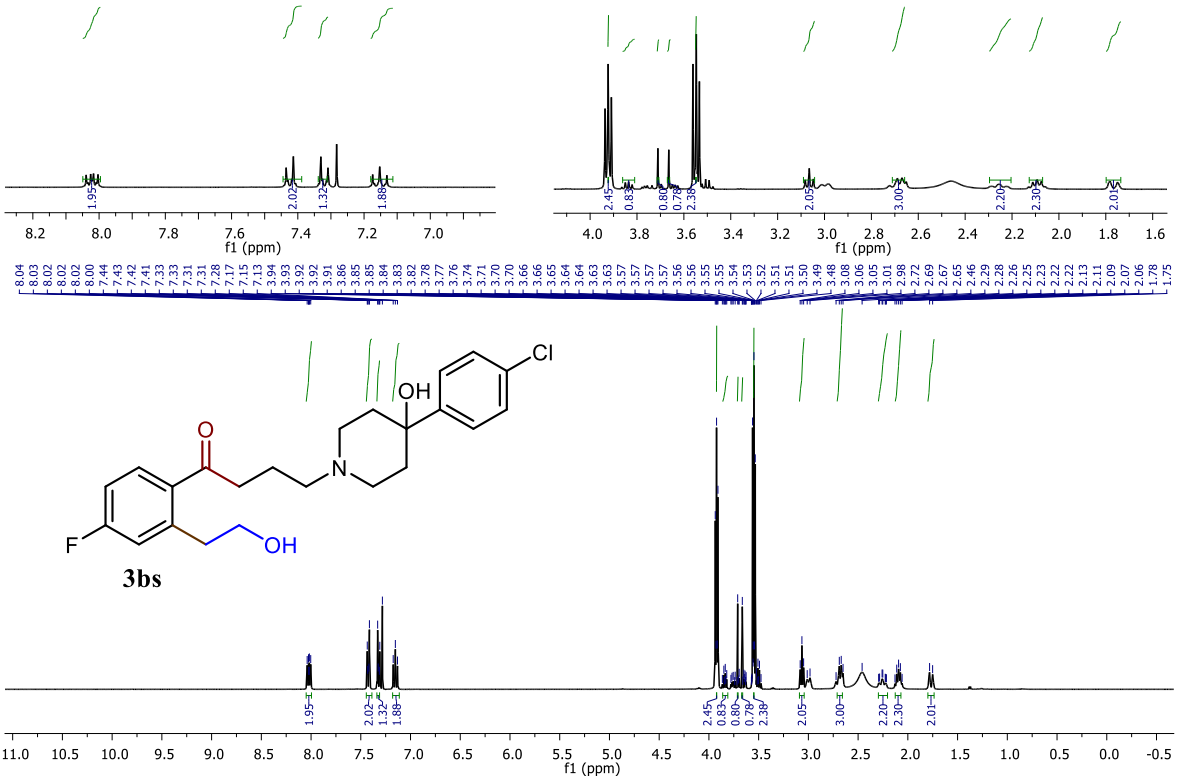
^{1}H NMR of 3br (400 MHz, 32 scans, RT, $CDCl_3$)



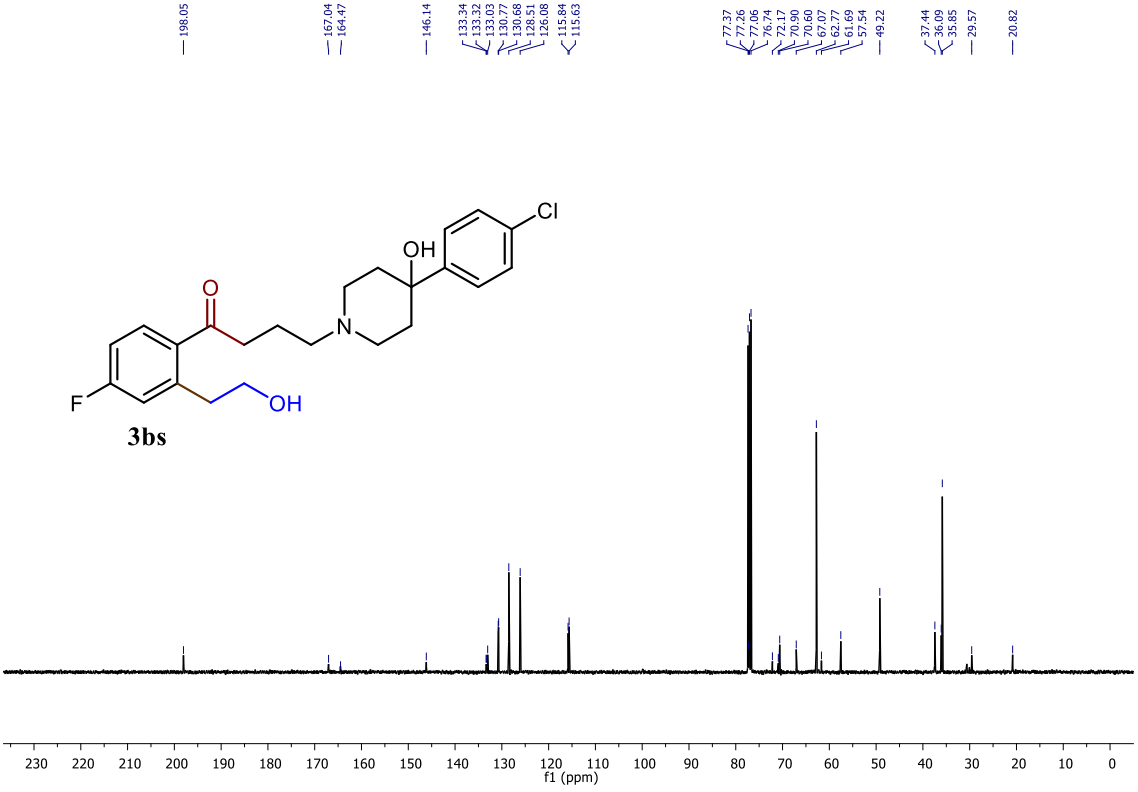
^{13}C NMR of 3br (101 MHz, 512 scans, RT, $CDCl_3$)



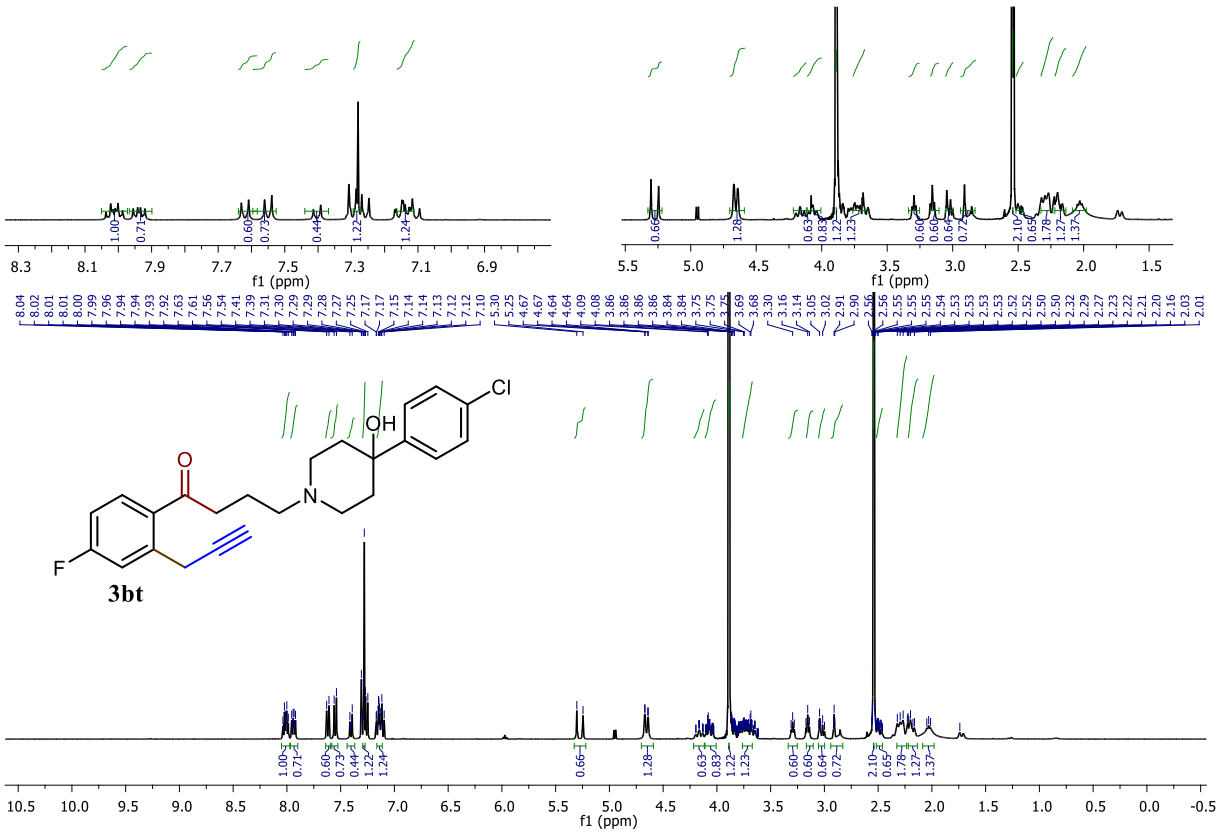
^{1}H NMR of 3bs (400 MHz, 32 scans, RT, $CDCl_3$)



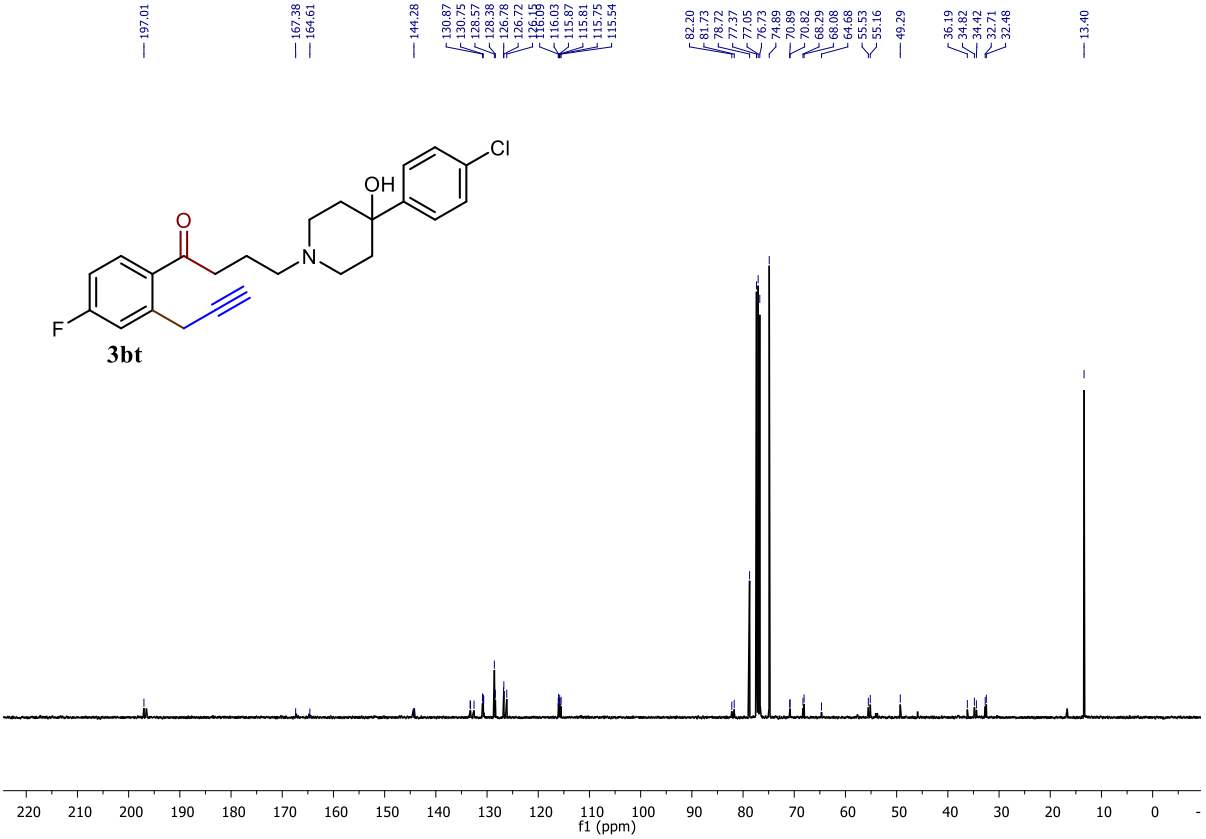
^{13}C NMR of 3bs (101 MHz, 512 scans, RT, $CDCl_3$)



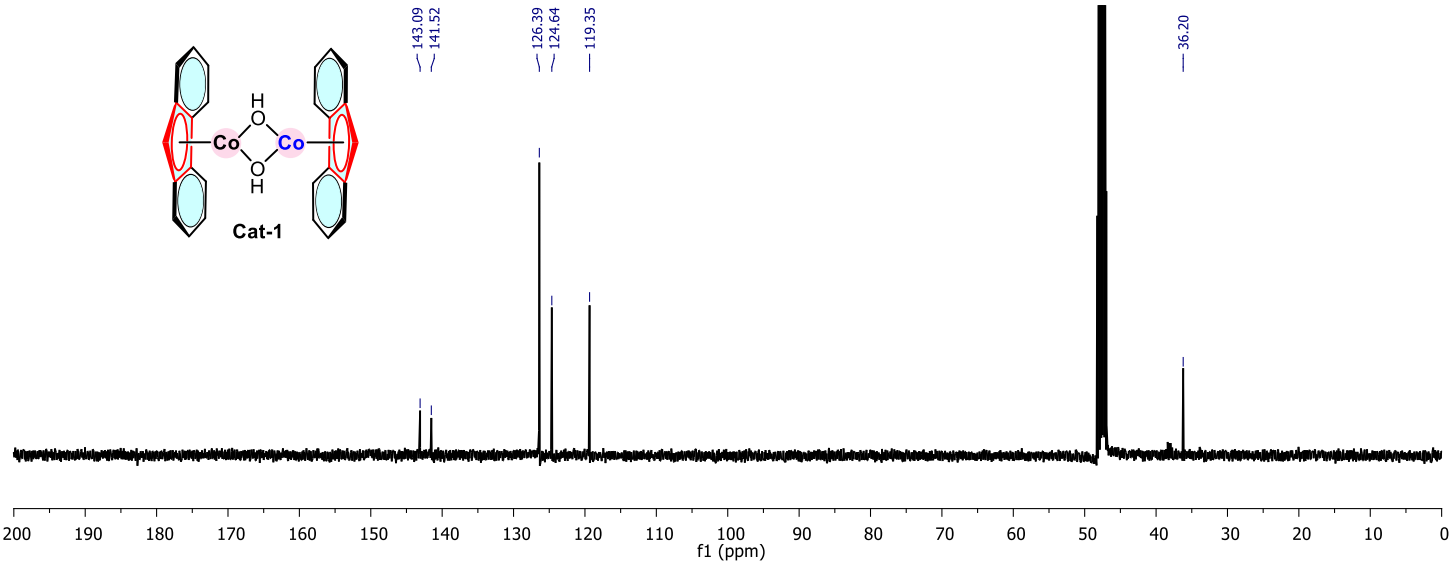
^{1}H NMR of 3bt (400 MHz, 32 scans, RT, $CDCl_3$)

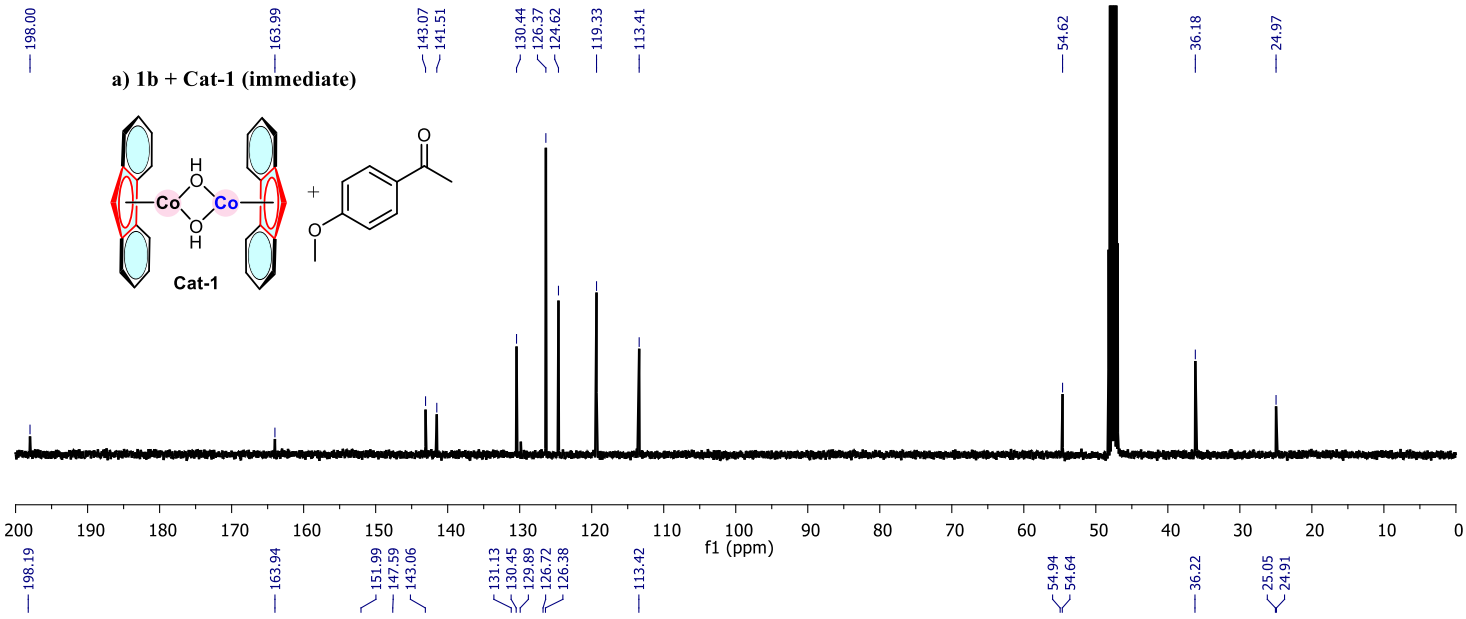


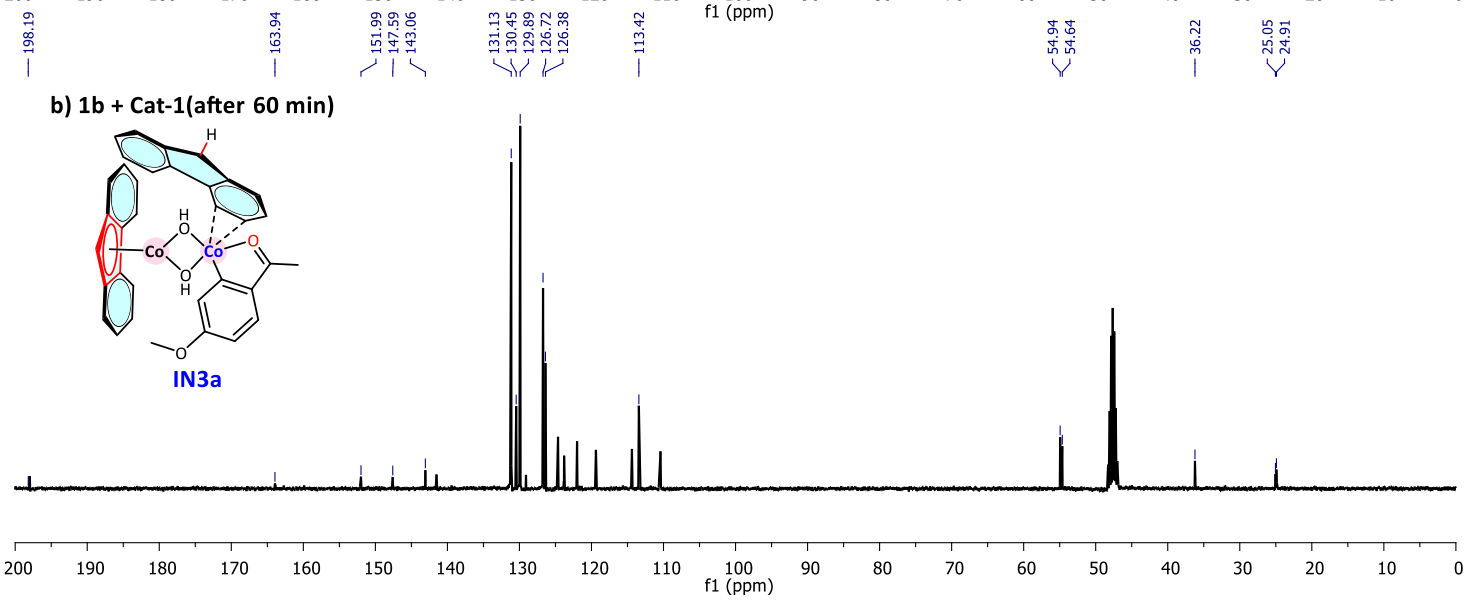
^{13}C NMR of 3bt (101 MHz, 512 scans, RT, $CDCl_3$)

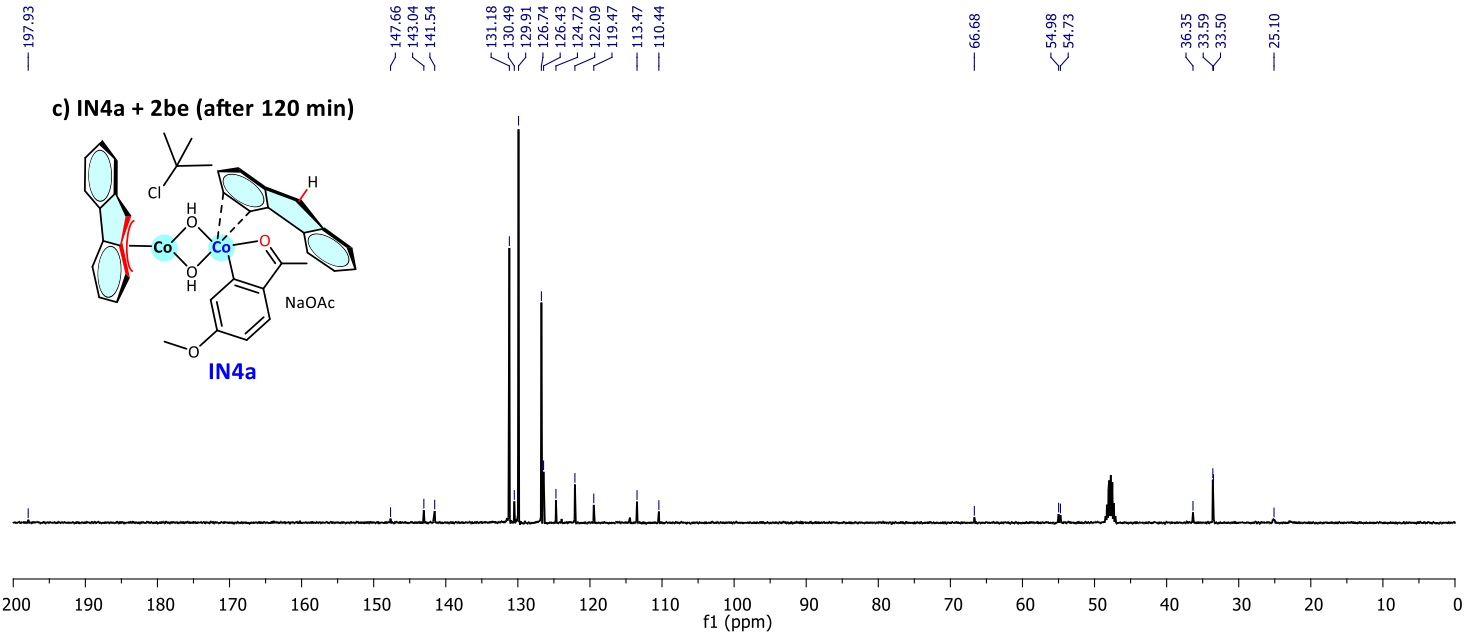


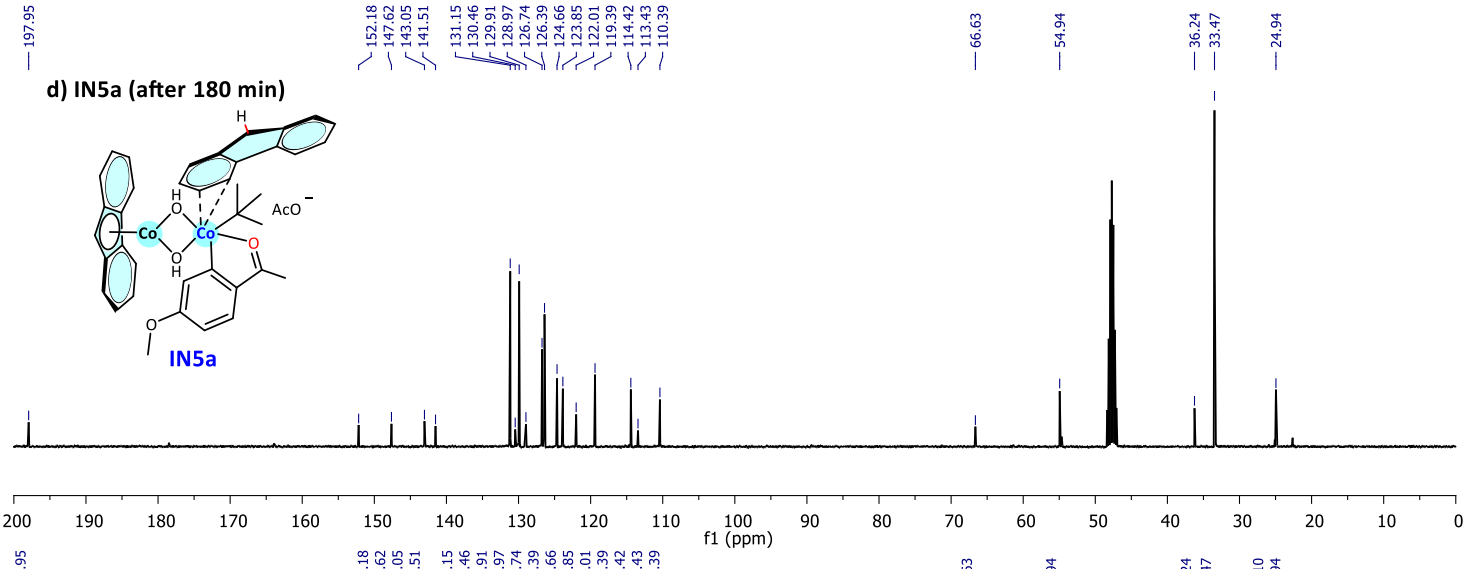
8. ^{1}H and ^{13}C NMR and ^{1}H-^{1}H COSY Spectra of Time-dependent NMR Study

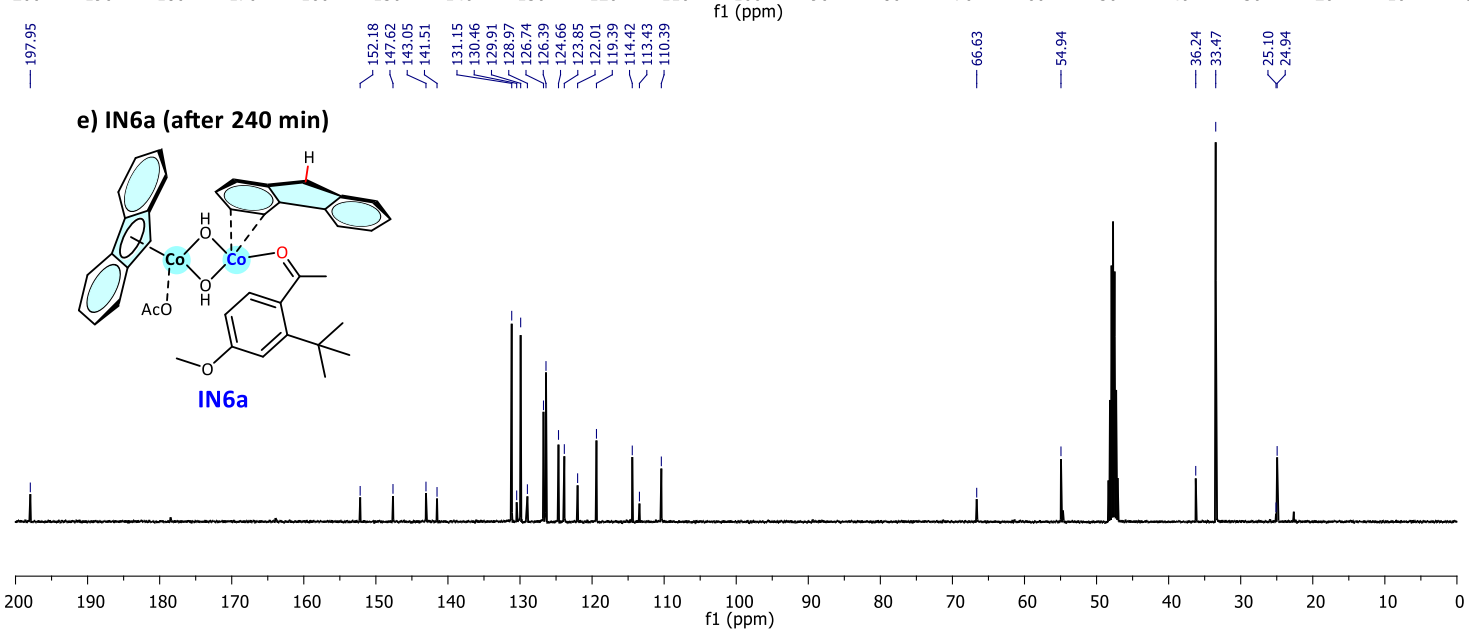




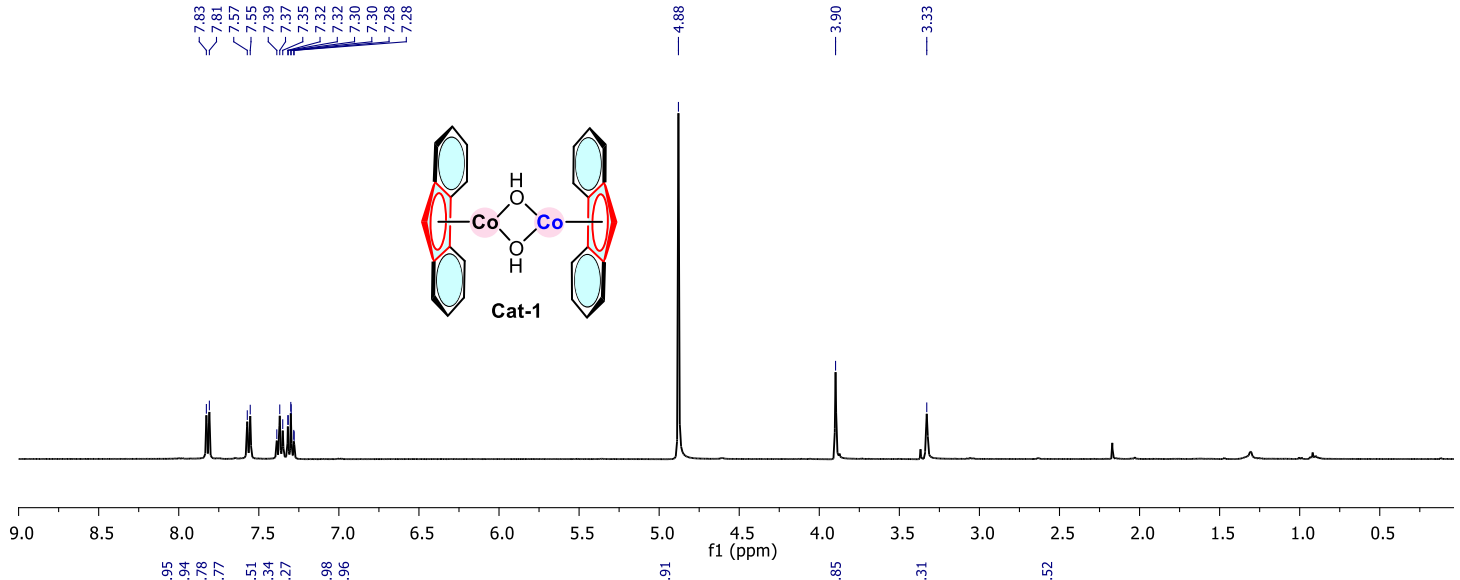


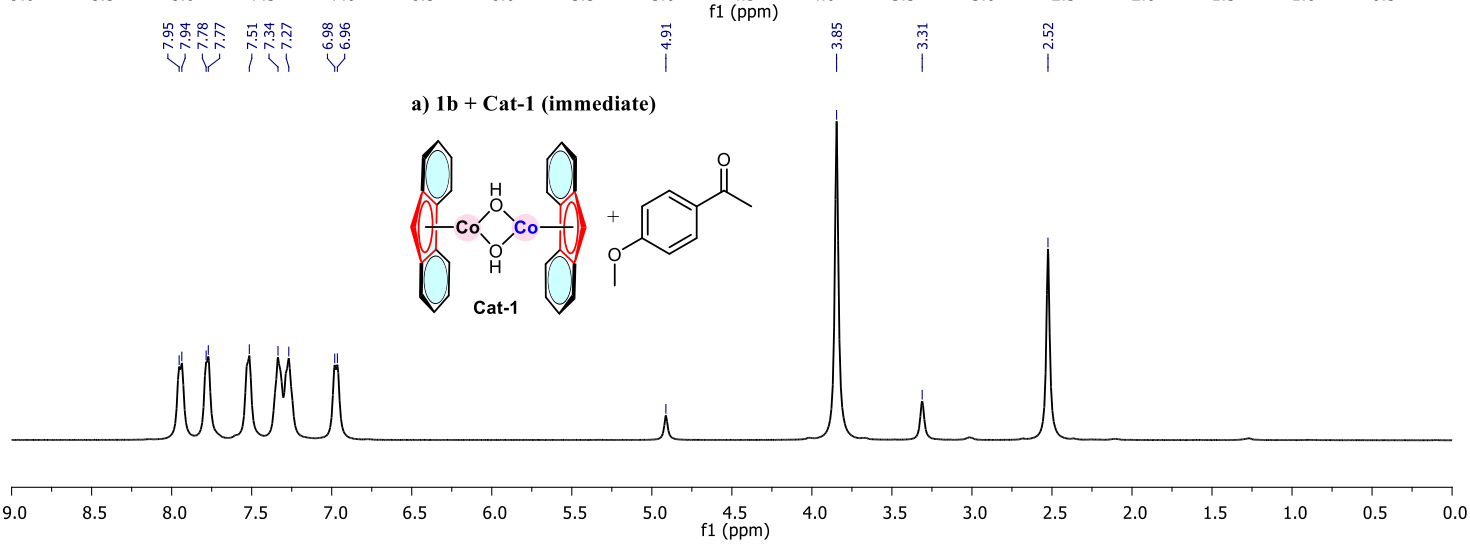

197.93
147.66
143.04
141.54
131.18
130.49
129.91
126.74
126.43
124.72
122.09
119.47
113.47
110.44
66.68
54.98
54.73
36.35
33.59
33.50
25.10
c) IN4a + 2be (after 120 min)
Cl
H
Co
Co
O
NaOAc
IN4a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

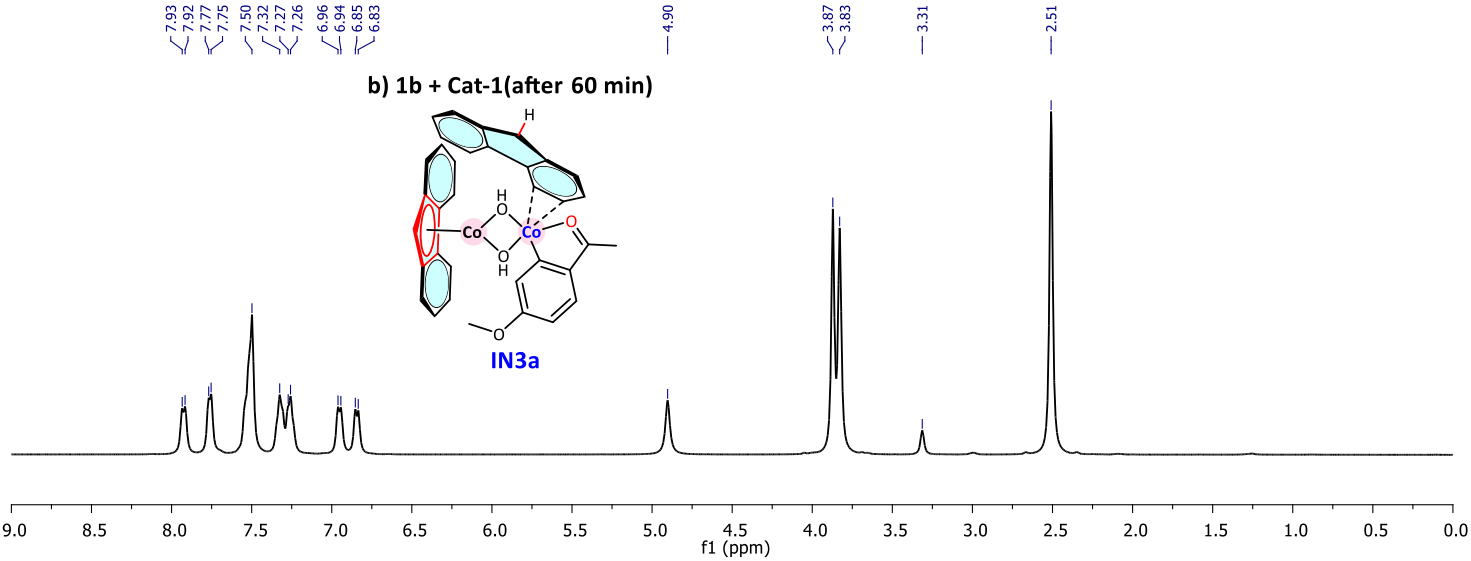

197.95
152.18
147.62
143.05
141.51
131.15
130.46
129.91
128.97
126.74
126.39
124.66
123.85
122.01
119.39
114.42
113.43
110.39
66.63
54.94
36.24
33.47
24.94
d) IN5a (after 180 min)
H
AcO
Co
Co
O
IN5a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


197.95
152.18
147.62
143.05
141.51
131.15
130.46
129.91
128.97
126.74
126.39
124.66
123.85
122.01
119.39
114.42
113.43
110.39
66.63
54.94
36.24
33.47
25.10
24.94
e) IN6a (after 240 min)
H
Co
Co
O
AcO
IN6a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

^{1}H NMR of the ring slippage mechanism







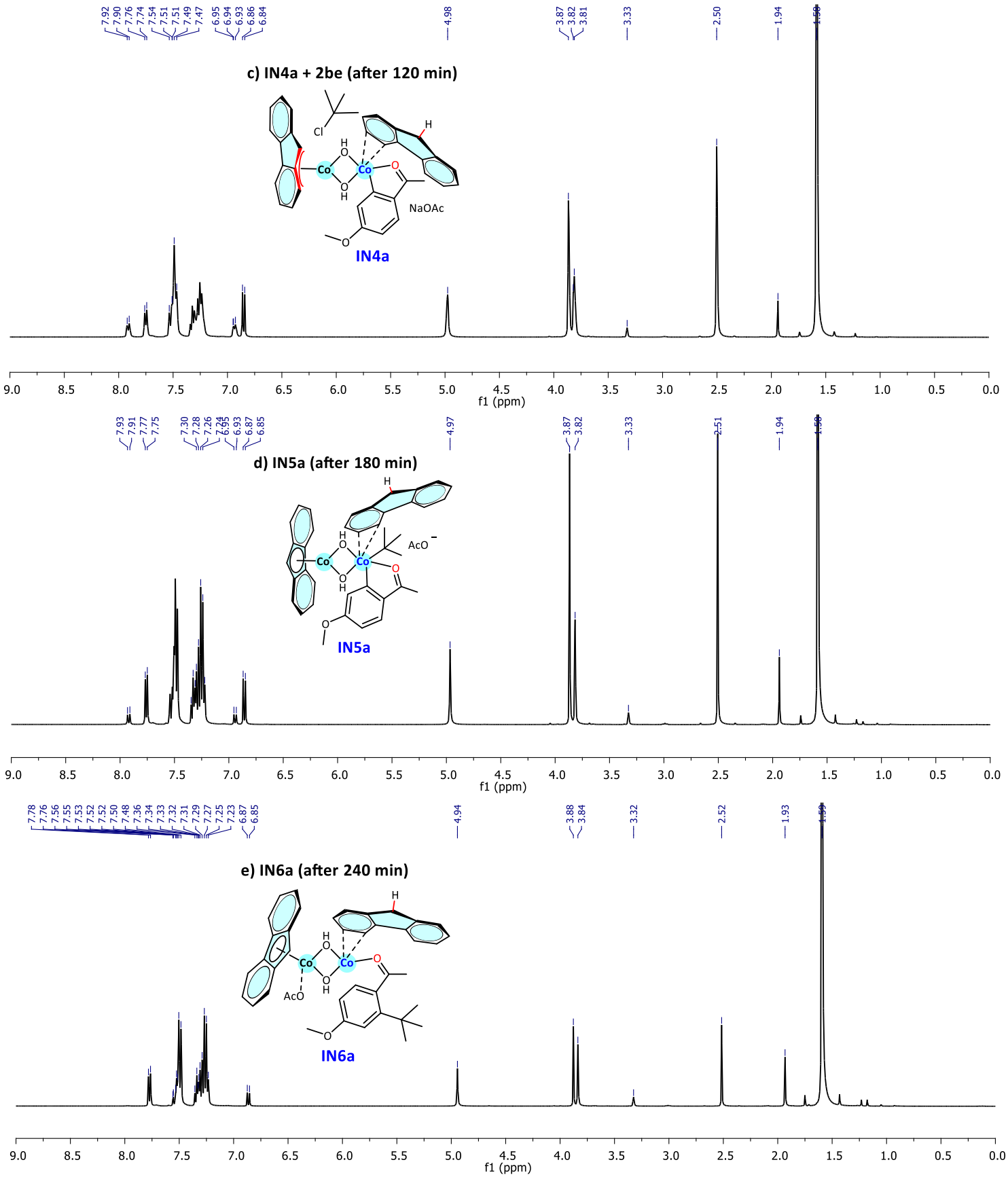
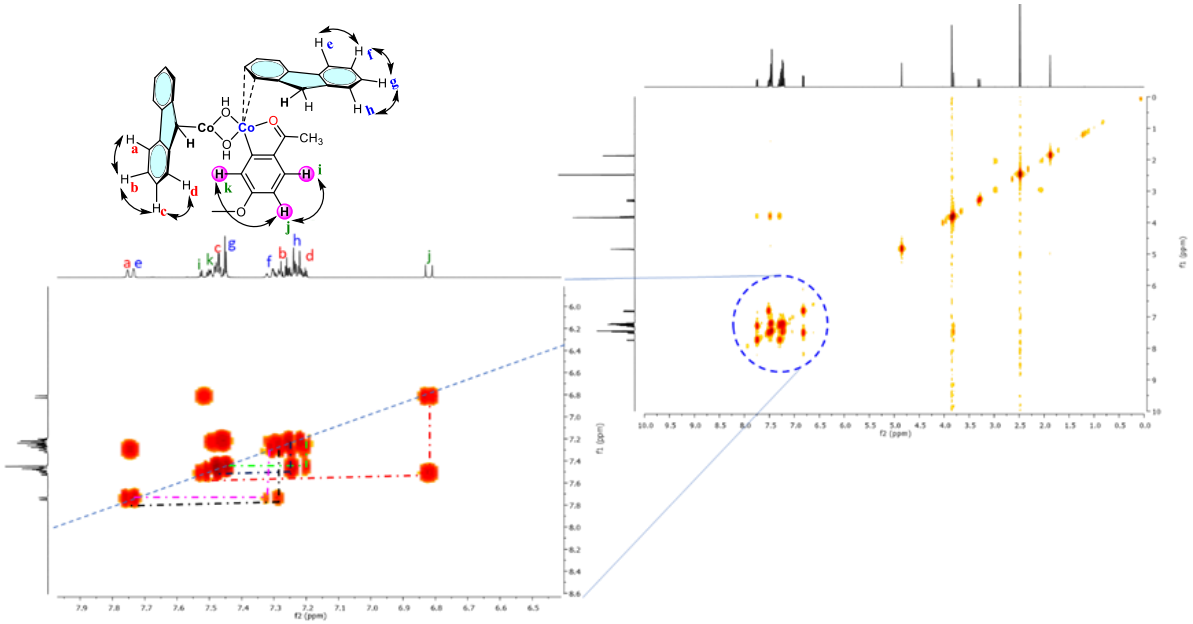


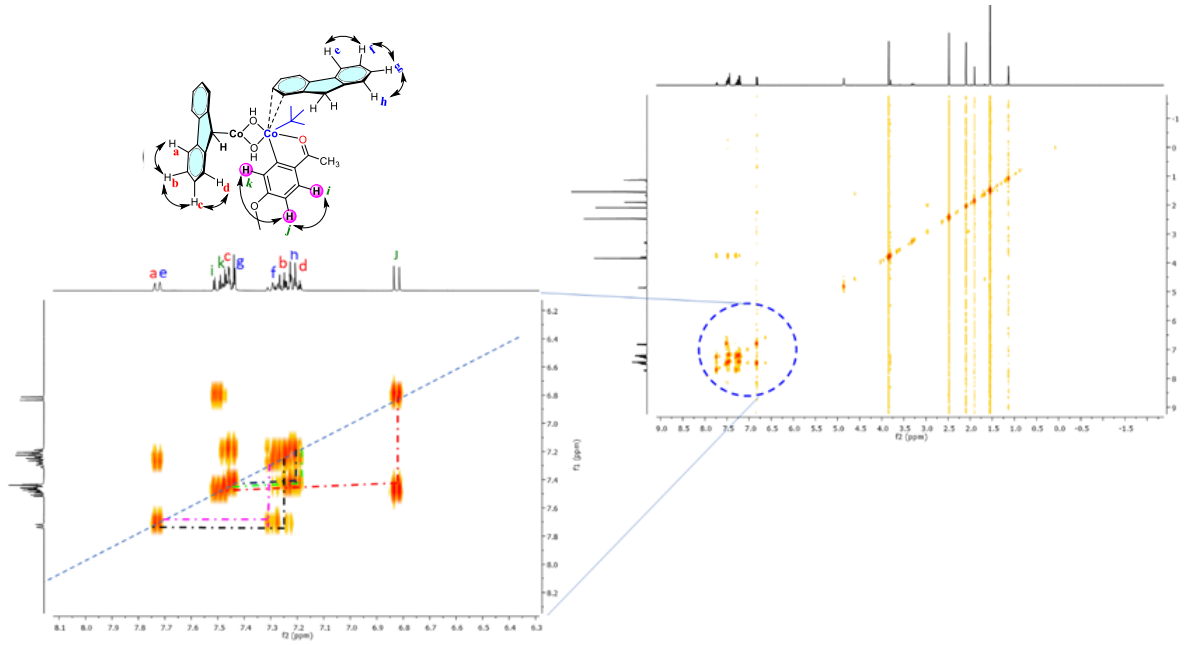
Figure S14. Evidence of ring slippage by time-dependent ^{13}C and ^{1}H NMR study

2D NMR of reaction intermediates (^{1}H-^{1}H COSY)

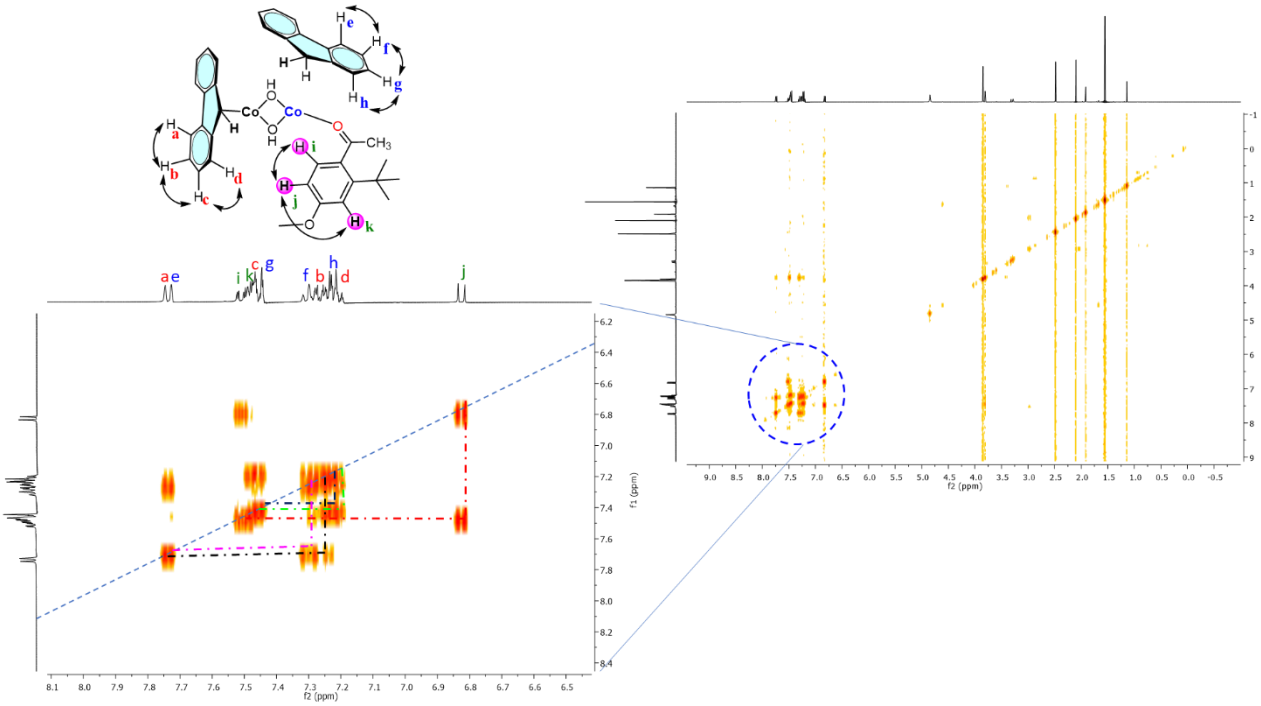
^{1}H-^{1}H COSY of **IN3a**



^{1}H-^{1}H COSY of **IN5a**



^{1}H-^{1}H COSY of **IN6a**



9. GC-MS snapshots (3a-3bq)

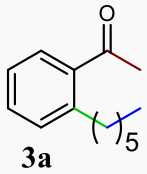
Area Percent Report

Data File : CH-1.D
Acq On : 07 Aug 2024 14:49
Operator :
Sample : CH-1
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-1.D\data.ms



3a

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	331	339	348	BV	97412	1092740	0.51%	0.275%
2	1.386	361	439	378	BV	99412	192740	0.41%	0.168%
3	4.826	451	549	598	GV	81412	1292740	1.31%	1.275%
4	7.362	648	655	879	VB	4049752	31174554	100.00%	97.764%
5	8.623	2231	2242	2275	BB	57609	1094240	1.51%	1.080%

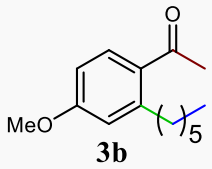
Area Percent Report

Data File : CH-2.D
Acq On : 03 Aug 2024 15:30
Operator :
Sample : CH-2
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-2.D\data.ms



3b

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	321	329	348	BV	87412	1142740	0.41%	0.175%
2	1.376	351	429	378	BV	89412	192740	0.21%	0.108%
3	4.826	541	769	798	GV	91412	1092740	1.43%	1.353%
4	7.362	648	655	879	VB	4049752	43174554	100.00%	98.004%
5	8.623	2231	2242	2275	BB	57609	1294240	0.71%	0.880%

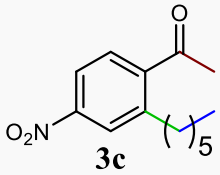
Area Percent Report

Data File : CH-3.D
Acq On : 03 Aug 2024 12:30
Operator :
Sample : CH-3
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-3.D\data.ms



3c

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	97412	142740	0.41%	0.175%
2	1.376	351	429	378	BV	89412	192740	0.21%	0.108%
3	4.826	641	769	788	GV	91412	118274	1.43%	1.353%
4	8.362	748	655	879	VB	4049752	41174554	100.00%	97.110%
5	8.623	2231	2242	2275	BB	57609	1294240	0.71%	0.880%

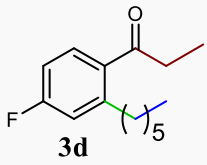
Area Percent Report

Data File : CH-4.D
Acq On : 02 Aug 2024 12:43
Operator :
Sample : CH-4
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-4.D\data.ms



3d

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	96712	202640	1.41%	1.175%
2	1.376	351	429	378	BV	89412	202740	2.21%	2.178%
3	4.826	641	769	788	GV	91412	118274	1.43%	1.353%
4	7.326	741	709	798	GV	1191412	118274	3.73%	5.353%
5	8.662	748	655	879	VB	4049752	41174554	100.00%	90.050%
6	8.673	2231	2242	2275	BB	57609	1294240	0.71%	0.980%

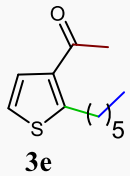
Area Percent Report

Data File : CH-5.D
Acq On : 03 Aug 2024 12:01
Operator :
Sample : CH-5
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-5.D\data.ms



3e

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	96712	202640	1.11%	1.115%
2	1.376	351	429	378	BV	79412	232740	2.71%	3.178%
3	4.826	641	769	788	GV	91412	118274	2.43%	2.153%
4	5.326	641	719	798	GV	1291412	118274	3.73%	3.353%
5	7.662	748	655	879	VB	4049752	41174554	100.00%	90.150%
6	8.573	2231	2242	2275	BB	457609	1194240	0.81%	0.880%

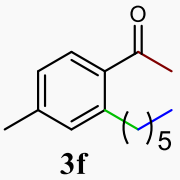
Area Percent Report

Data File : CH-6.D
Acq On : 02 Aug 2024 12:12
Operator :
Sample : CH-6
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-6.D\data.ms

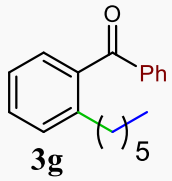


3f

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	86712	202640	0.11%	0.115%
2	1.376	351	429	378	BV	78412	222740	1.71%	2.178%
3	4.826	641	769	788	GV	91412	118274	2.43%	2.153%
4	8.112	748	655	879	VB	4149752	53174554	100.00%	95.750%
5	8.573	2231	2242	2275	BB	497609	1794240	0.91%	0.980%

Area Percent Report

Data File : CH-7.D
Acq On : 02 Aug 2024 12:20
Operator :
Sample : CH-7
Misc :
ALS Vial : 1 Sample Multiplier: 1



3g

Integration Parameters: autoint1.e
Integrator: ChemStation

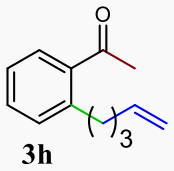
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-7.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	86712	202640	0.11%	0.115%
2	1.376	351	429	378	BV	78412	222740	1.71%	2.178%
3	4.826	641	769	788	GV	91412	118274	2.43%	2.153%
4	8.673	2231	2242	2275	BB	497609	1794240	0.91%	0.780%
5	10.112	748	655	879	VB	4349752	55574554	100.00%	95.050%

Area Percent Report

Data File : CH-8.D
Acq On : 02 Aug 2024 10:12
Operator :
Sample : CH-8
Misc :
ALS Vial : 1 Sample Multiplier: 1



3h

Integration Parameters: autoint1.e
Integrator: ChemStation

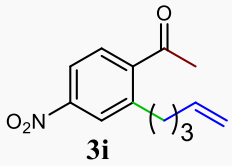
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-8.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	86712	202640	1.11%	1.115%
2	1.376	351	429	378	BV	78412	222740	1.71%	1.178%
3	5.826	741	769	788	GV	91412	118274	2.43%	2.153%
4	6.776	751	769	788	GV	91412	118274	2.43%	5.153%
5	8.112	788	655	879	VB	4149752	53174554	100.00%	90.010%
6	8.573	2231	2242	2275	BB	497609	1794240	0.91%	0.980%

Area Percent Report

Data File : CH-9.D
Acq On : 02 Aug 2024 11:09
Operator :
Sample : CH-9
Misc :
ALS Vial : 1 Sample Multiplier: 1



3i

Integration Parameters: autoint1.e
Integrator: ChemStation

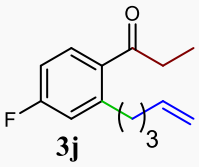
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-9.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	86712	202640	2.11%	2.115%
2	1.376	351	429	378	BV	78412	222740	2.71%	2.178%
3	5.826	741	769	788	GV	91412	118274	2.43%	2.153%
4	7.776	751	769	788	GV	91412	118274	2.43%	5.153%
5	8.332	788	655	879	VB	4249752	43174554	100.00%	88.001%
6	8.573	2231	2242	2275	BB	497609	1794240	0.91%	0.980%

Area Percent Report

Data File : CH-10.D
Acq On : 02 Aug 2024 11:20
Operator :
Sample : CH-10
Misc :
ALS Vial : 1 Sample Multiplier: 1



3j

Integration Parameters: autoint1.e
Integrator: ChemStation

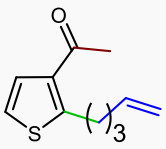
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-10.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	86712	202640	2.11%	2.115%
2	1.376	351	429	378	BV	78412	222740	2.71%	2.178%
3	5.826	741	769	788	GV	91412	118274	2.73%	3.153%
4	7.132	888	855	879	VB	4249752	43174554	100.00%	92.001%
5	8.673	2231	2242	2275	BB	497609	1794240	0.91%	0.980%

Area Percent Report

Data File : CH-11.D
Acq On : 03 Aug 2024 11:10
Operator :
Sample : CH-11
Misc :
ALS Vial : 1 Sample Multiplier: 1



3k

Integration Parameters: autoint1.e
Integrator: ChemStation

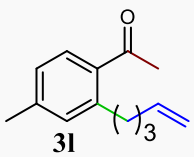
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-11.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	86712	202640	2.11%	2.115%
2	1.376	351	429	378	BV	78412	222740	2.71%	2.178%
3	5.826	741	769	788	GV	91412	118274	3.73%	5.153%
4	6.332	888	855	879	VB	4249752	43174554	100.00%	90.001%
5	8.673	2231	2242	2275	BB	497609	1794240	1.81%	1.020%

Area Percent Report

Data File : CH-12.D
Acq On : 03 Aug 2024 12:03
Operator :
Sample : CH-12
Misc :
ALS Vial : 1 Sample Multiplier: 1



3l

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-12.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.11%	1.115%
2	1.376	351	429	378	BV	78412	222740	2.71%	2.178%
3	5.826	741	769	788	GV	91412	118274	1.73%	1.153%
4	8.332	888	855	879	VB	4249752	43174554	100.00%	95.131%
5	8.673	2231	2242	2275	BB	497609	1794240	1.81%	1.020%

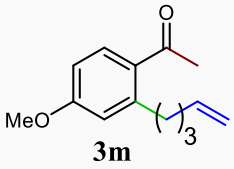
Area Percent Report

Data File : CH-13.D
Acq On : 02 Aug 2024 10:13
Operator :
Sample : CH-13
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-13.D\data.ms



peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.11%	1.115%
2	1.376	351	429	378	BV	78412	222740	2.71%	1.118%
3	5.826	741	769	788	GV	91412	118274	1.73%	1.153%
4	7.632	888	855	879	VB	4249752	43174554	100.00%	95.703%
5	8.473	2231	2242	2275	BB	497609	1794240	1.81%	1.020%

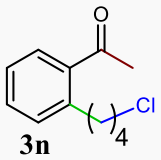
Area Percent Report

Data File : CH-14.D
Acq On : 05 Aug 2024 11:11
Operator :
Sample : CH-14
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-14.D\data.ms



peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	0.11%	0.015%
2	1.376	351	429	378	BV	78412	222740	2.71%	0.218%
3	5.826	741	769	788	GV	91412	118274	1.73%	1.153%
4	8.312	788	855	879	VB	4249752	43174554	100.00%	98.103%
5	8.473	2231	2242	2275	BB	497609	1794240	1.81%	0.820%

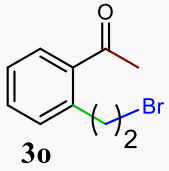
Area Percent Report

Data File : CH-15.D
Acq On : 04 Aug 2024 10:01
Operator :
Sample : CH-15
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-15.D\data.ms



peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	0.11%	0.215%
2	1.376	351	429	378	BV	78412	222740	2.71%	0.118%
3	7.826	741	769	788	GV	91412	118274	1.03%	1.053%
4	8.312	788	855	879	VB	4249752	43174554	100.00%	98.103%
5	8.473	2231	2242	2275	BB	497609	1794240	1.81%	0.820%

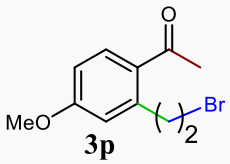
Area Percent Report

Data File : CH-15.D
Acq On : 04 Aug 2024 10:01
Operator :
Sample : CH-15
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-15.D\data.ms



peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	0.011%	0.115%
2	1.376	351	429	378	BV	78412	222740	1.71%	1.118%
3	7.826	741	769	788	GV	91412	118274	1.03%	1.053%
4	8.112	778	855	879	VB	4249752	43174554	100.00%	97.103%
5	8.674	2231	2242	2275	BB	4497609	1894240	1.81%	0.720%

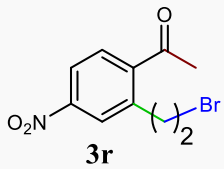
Area Percent Report

Data File : CH-18.D
Acq On : 07 Aug 2024 11:01
Operator :
Sample : CH-18
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-18.D\data.ms



peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	0.011%	2.115%
2	1.376	351	429	378	BV	78412	222740	2.71%	3.118%
3	7.826	741	769	788	GV	91412	118274	1.03%	2.053%
4	7.912	878	875	879	VB	4249752	43174554	100.00%	92.103%
5	8.674	2231	2242	2275	BB	4497609	1894240	1.81%	1.020%

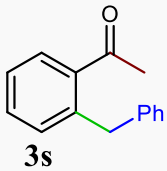
Area Percent Report

Data File : CH-19.D
Acq On : 05 Aug 2024 12:00
Operator :
Sample : CH-19
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-19.D\data.ms



peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	0.011%	0.115%
2	1.376	351	429	378	BV	78412	222740	2.71%	0.118%
3	7.826	741	769	788	GV	91412	118274	1.03%	1.053%
4	8.512	878	875	879	VB	4249752	43174554	100.00%	98.003%
5	8.674	2231	2242	2275	BB	4497609	1894240	1.81%	1.020%

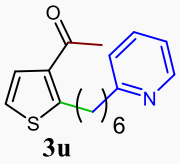
Area Percent Report

Data File : CH-21.D
Acq On : 04 Aug 2024 11:01
Operator :
Sample : CH-21
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-21.D\data.ms



3u

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	2.011%	2.115%
2	1.376	351	429	378	BV	78412	222740	1.71%	2.118%
3	7.826	741	769	788	GV	91412	118274	1.03%	1.053%
4	8.512	878	875	879	VB	4249752	43174554	1.00%	4.003%
5	8.674	2231	2242	2275	BB	4497609	1894240	1.81%	1.020%
6	9.512	978	875	879	VB	4249752	43174554	100.00%	90.003%

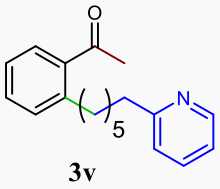
Area Percent Report

Data File : CH-22.D
Acq On : 04 Aug 2024 09:11
Operator :
Sample : CH-22
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-22.D\data.ms



3v

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	2.011%	3.115%
2	1.376	351	429	378	BV	78412	222740	1.71%	2.118%
3	7.826	741	769	788	GV	91412	118274	1.03%	1.053%
4	8.512	878	875	879	VB	4249752	43174554	2.70%	3.103%
5	8.674	2231	2242	2275	BB	4497609	1894240	1.81%	0.920%
6	8.924	978	875	879	VB	4249752	43174554	100.00%	90.003%

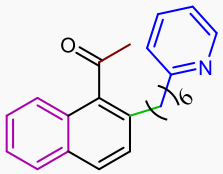
Area Percent Report

Data File : CH-23.D
Acq On : 04 Aug 2024 11:45
Operator :
Sample : CH-23
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-23.D\data.ms



3w

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	2.011%	3.115%
2	1.376	351	429	378	BV	78412	222740	1.71%	2.118%
3	7.826	741	769	788	GV	91412	118274	1.03%	1.053%
4	8.512	878	875	879	VB	4249752	43174554	3.70%	4.103%
5	8.674	2231	2242	2275	BB	4497609	1894240	1.81%	0.920%
6	8.714	978	875	879	VB	4249752	43174554	100.00%	88.103%

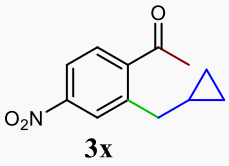
Area Percent Report

Data File : CH-24.D
Acq On : 06 Aug 2024 11:30
Operator :
Sample : CH-24
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-24.D\data.ms



3x

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	0.011%	2.115%
2	1.376	351	429	378	BV	78412	222740	2.71%	1.118%
3	5.376	351	429	378	BV	78412	222740	2.31%	1.118%
4	7.426	741	769	788	GV	91412	1118274	5.03%	5.053%
5	8.512	878	875	879	VB	4249752	43174554	100.00%	90.007%
6	8.674	2231	2242	2275	BB	4497609	1894240	1.81%	1.020%

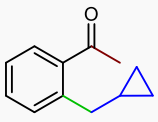
Area Percent Report

Data File : CH-25.D
Acq On : 07 Aug 2024 11:01
Operator :
Sample : CH-25
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-25.D\data.ms



3y

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	0.011%	0.115%
2	1.376	351	429	378	BV	78412	222740	1.71%	0.118%
3	5.376	351	429	378	BV	78412	222740	1.31%	1.118%
4	7.426	741	769	788	GV	91412	1118274	5.03%	1.053%
5	7.512	878	875	879	VB	4249752	43174554	100.00%	97.107%
6	8.674	2231	2242	2275	BB	4497609	1894240	1.81%	0.920%

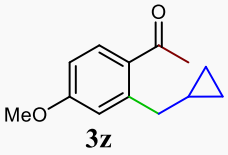
Area Percent Report

Data File : CH-26.D
Acq On : 04 Aug 2024 9:27
Operator :
Sample : CH-26
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-26.D\data.ms

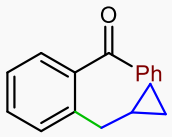


3z

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	0.011%	1.115%
2	1.376	351	429	378	BV	78412	222740	1.71%	2.118%
3	5.376	351	429	378	BV	78412	222740	1.31%	1.118%
4	6.126	741	769	788	GV	91412	1118274	5.03%	4.753%
5	7.512	878	875	879	VB	4249752	43174554	100.00%	89.907%
6	8.674	2231	2242	2275	BB	4497609	2094240	1.91%	1.920%\

Area Percent Report

Data File : CH-27.D
Acq On : 02 Aug 2024 10:27
Operator :
Sample : CH-27
Misc :
ALS Vial : 1 Sample Multiplier: 1



3aa

Integration Parameters: autoint1.e
Integrator: ChemStation

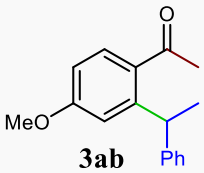
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-27.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	0.011%	1.115%
2	2.376	351	429	378	BV	78412	222740	1.71%	2.118%
3	5.316	351	429	378	BV	78412	222740	1.31%	1.118%
4	5.626	741	769	788	GV	91412	1118274	5.03%	4.953%
5	8.512	878	875	879	VB	4249752	43174554	100.00%	90.017%
6	8.674	2231	2242	2275	BB	4497609	2094240	0.91%	0.920%

Area Percent Report

Data File : CH-28.D
Acq On : 01 Aug 2024 11:27
Operator :
Sample : CH-28
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ab

Integration Parameters: autoint1.e
Integrator: ChemStation

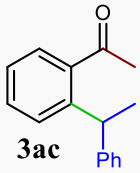
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-28.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	0.011%	1.315%
2	2.376	351	429	378	BV	78412	222740	1.71%	2.018%
3	5.316	351	429	378	BV	78412	222740	1.31%	1.218%
4	7.512	878	875	879	VB	4249752	43174554	100.00%	95.107%
5	8.674	2231	2242	2275	BB	4497609	2094240	0.91%	0.920%

Area Percent Report

Data File : CH-29.D
Acq On : 01 Aug 2024 10:17
Operator :
Sample : CH-29
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ac

Integration Parameters: autoint1.e
Integrator: ChemStation

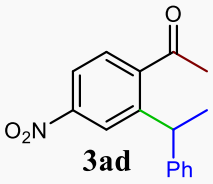
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-29.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	0.011%	0.315%
2	2.376	351	429	378	BV	78412	222740	0.71%	0.018%
3	5.316	351	429	378	BV	78412	222740	1.31%	1.218%
4	8.512	878	875	879	VB	4249752	43174554	100.00%	98.004%
5	8.674	2231	2242	2275	BB	4497609	2094240	0.91%	0.920%

Area Percent Report

Data File : CH-30.D
Acq On : 08 Aug 2024 12:17
Operator :
Sample : CH-30
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ad

Integration Parameters: autoint1.e
Integrator: ChemStation

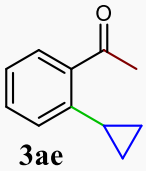
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-29.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	2.315%
2	2.376	351	429	378	BV	78412	222740	2.71%	2.018%
3	5.316	351	429	378	BV	78412	222740	1.31%	3.218%
4	6.316	351	429	378	BV	78412	222740	1.31%	2.218%
5	8.512	878	875	879	VB	4249752	43174554	100.00%	89.804%
6	8.674	2231	2242	2275	BB	4497609	2094240	0.91%	0.920%

Area Percent Report

Data File : CH-31.D
Acq On : 07 Aug 2024 10:17
Operator :
Sample : CH-31
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ae

Integration Parameters: autoint1.e
Integrator: ChemStation

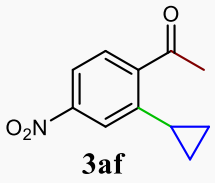
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-31.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	0.015%
2	2.376	351	429	378	BV	78412	222740	0.71%	0.018%
3	7.316	351	429	378	BV	78412	222740	1.31%	2.218%
4	8.512	878	875	879	VB	4249752	43174554	100.00%	97.304%
5	8.674	2231	2242	2275	BB	4497609	2094240	0.91%	0.920%

Area Percent Report

Data File : CH-32.D
Acq On : 06 Aug 2024 10:15
Operator :
Sample : CH-32
Misc :
ALS Vial : 1 Sample Multiplier: 1



3af

Integration Parameters: autoint1.e
Integrator: ChemStation

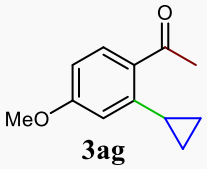
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-32.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	2.315%
2	2.376	351	429	378	BV	78412	222740	2.71%	2.018%
3	4.216	351	429	378	BV	78412	222740	1.31%	3.218%
4	4.316	351	429	378	BV	78412	222740	1.31%	2.218%
5	8.772	878	875	879	VB	4249752	43174554	100.00%	90.204%
6	8.674	2231	2242	2275	BB	4497609	2094240	0.91%	1.120%

Area Percent Report

Data File : CH-33.D
Acq On : 04 Aug 2024 10:12
Operator :
Sample : CH-33
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ag

Integration Parameters: autoint1.e
Integrator: ChemStation

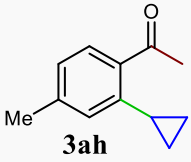
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-33.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	0.715%
2	2.376	351	429	378	BV	78412	222740	2.71%	2.018%
3	4.316	351	429	378	BV	78412	222740	1.31%	1.218%
4	8.772	878	875	879	VB	4249752	43174554	100.00%	95.007%
5	8.674	2231	2242	2275	BB	4497609	2094240	0.91%	0.920%

Area Percent Report

Data File : CH-34.D
Acq On : 03 Aug 2024 10:11
Operator :
Sample : CH-34
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ah

Integration Parameters: autoint1.e
Integrator: ChemStation

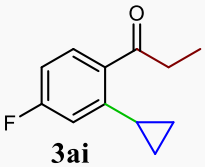
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-34.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	1.715%
2	2.376	351	429	378	BV	78412	222740	2.71%	2.018%
3	4.316	351	429	378	BV	78412	222740	1.31%	1.218%
4	7.673	878	875	879	VB	4249752	43174554	100.00%	96.107%
5	8.674	2231	2242	2275	BB	4497609	2094240	0.91%	1.320%

Area Percent Report

Data File : CH-35.D
Acq On : 01 Aug 2024 11:11
Operator :
Sample : CH-35
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ai

Integration Parameters: autoint1.e
Integrator: ChemStation

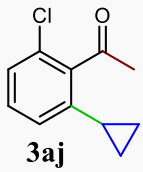
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-35.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	1.715%
2	2.376	351	429	378	BV	78412	222740	2.71%	1.018%
3	4.316	351	429	378	BV	78412	222740	2.31%	2.318%
4	7.673	878	875	879	VB	4249752	43174554	100.00%	95.417%
5	8.674	2231	2242	2275	BB	4497609	2094240	0.91%	1.320%

Area Percent Report

Data File : CH-36.D
Acq On : 08 Aug 2024 10:09
Operator :
Sample : CH-36
Misc :
ALS Vial : 1 Sample Multiplier: 1



3aj

Integration Parameters: autoint1.e
Integrator: ChemStation

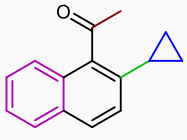
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-36.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	1.715%
2	2.376	351	429	378	BV	78412	222740	1.71%	1.018%
3	4.316	351	429	378	BV	78412	222740	2.31%	2.318%
4	7.313	678	875	879	VB	4249752	43174554	4.80%	5.417%
5	8.573	878	875	879	VB	4249752	43174554	100.00%	90.017%
6	8.674	2231	2242	2275	BB	4497609	2094240	1.01%	1.020%

Area Percent Report

Data File : CH-37.D
Acq On : 10 Aug 2024 10:09
Operator :
Sample : CH-37
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ak

Integration Parameters: autoint1.e
Integrator: ChemStation

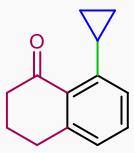
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-37.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	0.715%
2	2.376	351	429	378	BV	78412	222740	1.71%	1.018%
3	4.316	351	429	378	BV	78412	222740	2.31%	2.318%
4	8.673	878	875	879	VB	4249752	43174554	100.00%	96.017%
5	8.774	2231	2242	2275	BB	4497609	2094240	1.01%	1.020%

Area Percent Report

Data File : CH-38.D
Acq On : 8 Aug 2024 10:12
Operator :
Sample : CH-38
Misc :
ALS Vial : 1 Sample Multiplier: 1



3al

Integration Parameters: autoint1.e
Integrator: ChemStation

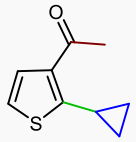
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-38.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	0.715%
2	2.376	351	429	378	BV	78412	222740	1.71%	1.018%
3	4.316	351	429	378	BV	78412	222740	2.31%	2.318%
4	7.673	878	875	879	VB	4249752	43174554	100.00%	95.017%
5	8.774	2231	2242	2275	BB	4497609	2094240	1.01%	1.020%

Area Percent Report

Data File : CH-39.D
Acq On : 7 Aug 2024 10:35
Operator :
Sample : CH-39
Misc :
ALS Vial : 1 Sample Multiplier: 1



3am

Integration Parameters: autoint1.e
Integrator: ChemStation

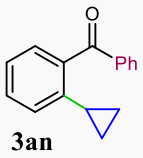
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-39.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	0.715%
2	2.376	351	429	378	BV	78412	222740	1.71%	1.018%
3	4.316	351	429	378	BV	78412	222740	2.31%	2.318%
4	5.016	351	429	378	BV	78412	222740	4.31%	5.318%
5	7.673	878	875	879	VB	4249752	43174554	100.00%	90.017%
6	8.774	2231	2242	2275	BB	4497609	2094240	1.01%	1.020%

Area Percent Report

Data File : CH-40.D
Acq On : 8 Aug 2024 11:35
Operator :
Sample : CH-40
Misc :
ALS Vial : 1 Sample Multiplier: 1



3an

Integration Parameters: autoint1.e
Integrator: ChemStation

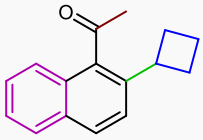
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-39.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	0.715%
2	2.376	351	429	378	BV	78412	222740	1.71%	1.118%
3	4.316	351	429	378	BV	78412	222740	2.31%	2.118%
4	4.716	351	429	378	BV	78412	222740	4.31%	4.918%
5	8.573	878	875	879	VB	4249752	43174554	100.00%	90.017%
6	8.774	2231	2242	2275	BB	4497609	2094240	1.01%	1.020%

Area Percent Report

Data File : CH-41.D
Acq On : 5 Aug 2024 10:25
Operator :
Sample : CH-41
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ao

Integration Parameters: autoint1.e
Integrator: ChemStation

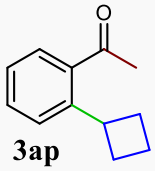
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-41.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	0.715%
2	2.396	351	429	378	BV	78412	222740	1.71%	1.118%
3	3.316	351	429	378	BV	78412	222740	2.31%	2.118%
4	6.516	351	429	378	BV	78412	222740	4.31%	5.118%
5	8.663	878	875	879	VB	4249752	43174554	100.00%	89.817%
6	8.794	2231	2242	2275	BB	4497609	2094240	1.01%	1.020%

Area Percent Report

Data File : CH-42.D
Acq On : 3 Aug 2024 11:20
Operator :
Sample : CH-42
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ap

Integration Parameters: autoint1.e
Integrator: ChemStation

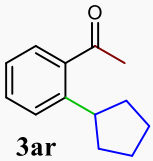
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-42.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	0.715%
2	2.396	351	429	378	BV	78412	222740	1.71%	1.118%
3	3.316	351	429	378	BV	78412	222740	2.31%	2.118%
4	6.516	351	429	378	BV	78412	222740	4.31%	4.788%
5	8.663	878	875	879	VB	4249752	43174554	100.00%	89.997%
6	8.794	2231	2242	2275	BB	4497609	2094240	1.01%	0.720%

Area Percent Report

Data File : CH-44.D
Acq On : 3 Aug 2024 11:37
Operator :
Sample : CH-44
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ar

Integration Parameters: autoint1.e
Integrator: ChemStation

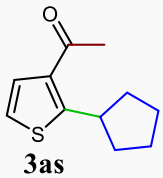
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-44.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	0.715%
2	2.396	351	429	378	BV	78412	222740	1.71%	1.118%
3	3.316	351	429	378	BV	78412	222740	2.31%	2.118%
4	6.516	351	429	378	BV	78412	222740	100.00%	95.788%
5	8.794	2231	2242	2275	BB	4497609	2094240	1.01%	0.720%

Area Percent Report

Data File : CH-45.D
Acq On : 4 Aug 2024 10:37
Operator :
Sample : CH-45
Misc :
ALS Vial : 1 Sample Multiplier: 1



3as

Integration Parameters: autoint1.e
Integrator: ChemStation

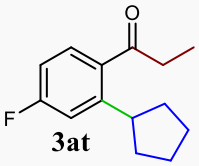
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-45.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	1.715%
2	2.396	351	429	378	BV	78412	222740	1.71%	1.118%
3	3.316	351	429	378	BV	78412	222740	2.31%	2.718%
4	5.016	351	429	378	BV	78412	222740	2.31%	2.118%
5	6.516	351	429	378	BV	78412	222740	100.00%	90.168%
6	8.694	2231	2242	2275	BB	4497609	2094240	1.01%	1.020%

Area Percent Report

Data File : CH-46.D
Acq On : 4 Aug 2024 11:37
Operator :
Sample : CH-46
Misc :
ALS Vial : 1 Sample Multiplier: 1



3at

Integration Parameters: autoint1.e
Integrator: ChemStation

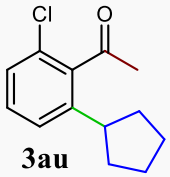
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-46.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	1.915%
2	2.296	351	429	378	BV	78412	222740	1.71%	2.118%
3	3.316	351	429	378	BV	78412	222740	2.31%	1.718%
4	5.026	351	429	378	BV	78412	222740	2.31%	3.118%
5	8.386	351	429	378	BV	78412	222740	100.00%	90.168%
6	8.694	2231	2242	2275	BB	4497609	2094240	1.01%	1.020%

Area Percent Report

Data File : CH-47.D
Acq On : 12 Aug 2024 11:37
Operator :
Sample : CH-47
Misc :
ALS Vial : 1 Sample Multiplier: 1



3au

Integration Parameters: autoint1.e
Integrator: ChemStation

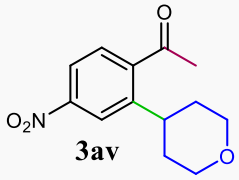
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-47.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	1.915%
2	2.296	351	429	378	BV	78412	222740	1.71%	2.518%
3	3.316	351	429	378	BV	78412	222740	2.31%	2.318%
4	5.026	351	429	378	BV	78412	222740	2.31%	2.918%
5	7.386	351	429	378	BV	78412	222740	100.00%	90.468%
6	8.694	2231	2242	2275	BB	4497609	2094240	1.31%	1.420%

Area Percent Report

Data File : CH-48.D
Acq On : 12 Aug 2024 11:56
Operator :
Sample : CH-48
Misc :
ALS Vial : 1 Sample Multiplier: 1



3av

Integration Parameters: autoint1.e
Integrator: ChemStation

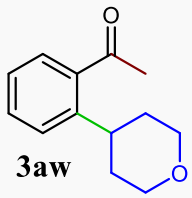
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-48.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.306	221	219	378	BV	87712	212640	1.011%	1.915%
2	2.296	351	429	378	BV	78412	222740	1.71%	2.518%
3	3.316	351	429	378	BV	78412	222740	2.31%	0.718%
4	6.826	351	429	378	BV	78412	222740	2.31%	2.018%
5	8.228	351	429	378	BV	78412	222740	100.00%	92.138%
6	8.694	2231	2242	2275	BB	4497609	2094240	1.31%	0.870%

Area Percent Report

Data File : CH-49.D
Acq On : 11 Aug 2024 11:50
Operator :
Sample : CH-49
Misc :
ALS Vial : 1 Sample Multiplier: 1



3aw

Integration Parameters: autoint1.e
Integrator: ChemStation

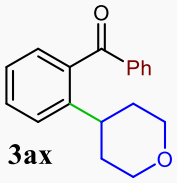
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-49.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	0.215%
2	2.396	351	429	378	BV	78412	222740	1.71%	1.118%
3	3.216	351	429	378	BV	78412	222740	2.31%	0.718%
4	7.658	351	429	378	BV	78412	222740	100.00%	98.038%
5	8.694	2231	2242	2275	BB	4497609	2094240	0.31%	0.570%

Area Percent Report

Data File : CH-50.D
Acq On : 11 Aug 2024 10:41
Operator :
Sample : CH-50
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ax

Integration Parameters: autoint1.e
Integrator: ChemStation

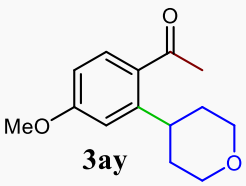
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-50.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	1.215%
2	2.396	351	429	378	BV	78412	222740	1.71%	2.118%
3	4.216	351	429	378	BV	78412	222740	2.31%	2.718%
4	7.858	351	429	378	BV	78412	222740	100.00%	92.148%
5	8.644	2231	2242	2275	BB	4497609	2094240	1.31%	1.570%

Area Percent Report

Data File : CH-51.D
Acq On : 11 Aug 2024 10:41
Operator :
Sample : CH-51
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ay

Integration Parameters: autoint1.e
Integrator: ChemStation

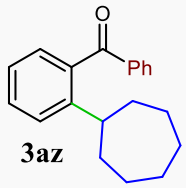
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-51.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	1.215%
2	2.396	351	429	378	BV	78412	222740	1.71%	1.118%
3	4.216	351	429	378	BV	78412	222740	2.31%	1.318%
4	7.858	351	429	378	BV	78412	244740	100.00%	96.248%
5	8.644	2231	2242	2275	BB	4497609	2094240	1.71%	1.970%

Area Percent Report

Data File : CH-52.D
Acq On : 10 Aug 2024 11:41
Operator :
Sample : CH-52
Misc :
ALS Vial : 1 Sample Multiplier: 1



3az

Integration Parameters: autoint1.e
Integrator: ChemStation

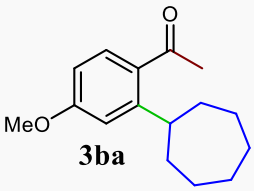
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-52.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	0.615%
2	2.396	351	429	378	BV	78412	222740	1.71%	1.118%
3	4.216	332	429	378	BV	78412	222740	2.31%	1.818%
4	5.216	363	429	378	BV	78412	222740	2.31%	5.318%
5	8.548	385	429	378	BV	78412	244740	100.00%	90.118%
6	8.644	2231	2242	2275	BB	4497609	2094240	1.71%	1.970%

Area Percent Report

Data File : CH-53.D
Acq On : 10 Aug 2024 09:41
Operator :
Sample : CH-53
Misc :
ALS Vial : 1 Sample Multiplier: 1



3ba

Integration Parameters: autoint1.e
Integrator: ChemStation

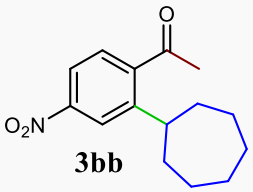
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-53.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	0.085%
2	2.396	351	429	378	BV	78412	222740	1.71%	1.118%
3	5.216	333	429	378	BV	78412	222740	2.31%	1.318%
4	7.848	395	429	378	BV	78412	244740	100.00%	96.218%
5	8.674	2231	2242	2275	BB	4497609	2094240	1.71%	1.970%

Area Percent Report

Data File : CH-54.D
Acq On : 11 Aug 2024 11:45
Operator :
Sample : CH-54
Misc :
ALS Vial : 1 Sample Multiplier: 1



3bb

Integration Parameters: autoint1.e
Integrator: ChemStation

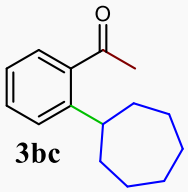
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-54.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	0.985%
2	2.396	351	429	378	BV	78412	222740	1.71%	1.118%
3	5.216	333	439	378	BV	78412	222740	2.31%	1.318%
4	8.448	305	419	378	BV	78412	244740	100.00%	95.118%
5	8.674	2231	2242	2275	BB	4497609	2094240	1.71%	1.970%

Area Percent Report

Data File : CH-55.D
Acq On : 11 Aug 2024 13:40
Operator :
Sample : CH-55
Misc :
ALS Vial : 1 Sample Multiplier: 1



3bc

Integration Parameters: autoint1.e
Integrator: ChemStation

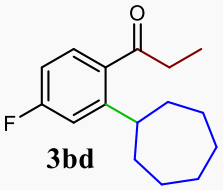
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-55.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	0.985%
2	2.396	351	429	378	BV	78412	222740	1.71%	0.118%
3	5.216	333	439	378	BV	78412	222740	2.31%	1.318%
4	6.448	305	419	378	BV	78412	244740	100.00%	98.008%
5	8.674	2231	2242	2275	BB	4497609	2094240	1.71%	0.670%

Area Percent Report

Data File : CH-56.D
Acq On : 10 Aug 2024 12:40
Operator :
Sample : CH-56
Misc :
ALS Vial : 1 Sample Multiplier: 1



3bd

Integration Parameters: autoint1.e
Integrator: ChemStation

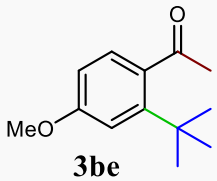
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-56.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	0.985%
2	2.396	351	429	378	BV	78412	222740	1.71%	1.118%
3	5.216	333	439	378	BV	78412	222740	2.31%	5.318%
4	8.348	305	419	378	BV	78412	244740	100.00%	92.108%
5	8.674	2231	2242	2275	BB	4497609	2094240	1.71%	1.370%

Area Percent Report

Data File : CH-57.D
Acq On : 16 Aug 2024 11:40
Operator :
Sample : CH-57
Misc :
ALS Vial : 1 Sample Multiplier: 1



3be

Integration Parameters: autoint1.e
Integrator: ChemStation

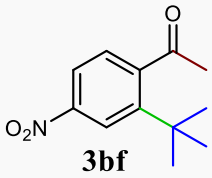
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-57.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	0.985%
2	2.396	351	429	378	BV	78412	222740	1.71%	0.318%
3	5.216	333	439	378	BV	78412	222740	2.31%	3.318%
4	7.778	405	419	378	BV	78412	244740	100.00%	96.108%
5	8.674	2231	2242	2275	BB	4497609	2094240	1.71%	1.370%

Area Percent Report

Data File : CH-58.D
Acq On : 16 Aug 2024 11:56
Operator :
Sample : CH-58
Misc :
ALS Vial : 1 Sample Multiplier: 1



3bf

Integration Parameters: autoint1.e
Integrator: ChemStation

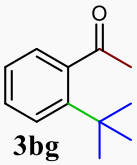
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-58.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	0.985%
2	2.396	351	429	378	BV	78412	222740	1.71%	1.318%
3	4.216	333	439	378	BV	78412	222740	2.31%	7.318%
4	6.778	405	419	378	BV	78412	244740	100.00%	90.008%
5	8.674	2231	2242	2275	BB	4497609	2094240	1.71%	1.270%

Area Percent Report

Data File : CH-59.D
Acq On : 12 Aug 2024 10:52
Operator :
Sample : CH-59
Misc :
ALS Vial : 1 Sample Multiplier: 1



3bg

Integration Parameters: autoint1.e
Integrator: ChemStation

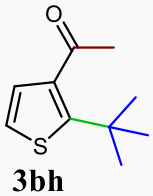
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-59.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	0.085%
2	2.396	351	429	378	BV	78412	222740	1.71%	0.318%
3	4.216	363	439	378	BV	78412	222740	2.31%	1.318%
4	6.778	445	419	378	BV	78412	244740	100.00%	98.208%
5	8.674	2231	2242	2275	BB	4497609	2094240	1.71%	1.670%

Area Percent Report

Data File : CH-60.D
Acq On : 12 Aug 2024 10:52
Operator :
Sample : CH-60
Misc :
ALS Vial : 1 Sample Multiplier: 1



3bh

Integration Parameters: autoint1.e
Integrator: ChemStation

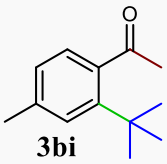
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-60.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	0.785%
2	2.396	351	429	378	BV	78412	222740	1.71%	1.318%
3	4.216	363	439	378	BV	78412	222740	2.31%	6.318%
4	5.778	445	419	378	BV	78412	244740	100.00%	90.208%
5	8.674	2231	2242	2275	BB	4497609	2094240	1.81%	1.870%

Area Percent Report

Data File : CH-61.D
Acq On : 10 Aug 2024 00:52
Operator :
Sample : CH-61
Misc :
ALS Vial : 1 Sample Multiplier: 1



3bi

Integration Parameters: autoint1.e
Integrator: ChemStation

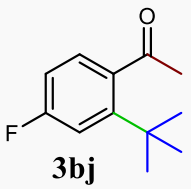
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-61.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	0.785%
2	2.396	351	429	378	BV	78412	222740	1.71%	1.318%
3	4.216	363	439	378	BV	78412	222740	6.31%	7.318%
4	7.778	445	419	378	BV	78412	244740	100.00%	90.088%
5	8.674	2231	2242	2275	BB	4497609	2094240	1.41%	1.570%

Area Percent Report

Data File : CH-62.D
Acq On : 11 Aug 2024 10:52
Operator :
Sample : CH-62
Misc :
ALS Vial : 1 Sample Multiplier: 1



3bj

Integration Parameters: autoint1.e
Integrator: ChemStation

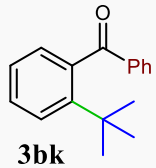
Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-62.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	0.785%
2	2.396	351	429	378	BV	78412	222740	1.71%	0.318%
3	4.216	363	439	378	BV	78412	222740	6.31%	8.318%
4	8.178	445	419	378	BV	78412	244740	100.00%	90.088%
5	8.474	2231	2242	2275	BB	4497609	2094240	1.51%	1.670%

Area Percent Report

Data File : CH-63.D
Acq On : 10 Aug 2024 11:52
Operator :
Sample : CH-63
Misc :
ALS Vial : 1 Sample Multiplier: 1



3bk

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-63.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	1.785%
2	2.396	351	429	378	BV	78412	222740	1.71%	2.318%
3	4.216	363	439	378	BV	78412	222740	6.31%	6.318%
4	7.578	445	419	378	BV	78412	244740	100.00%	90.088%
5	8.674	2231	2242	2275	BB	4497609	2094240	1.211%	1.370%

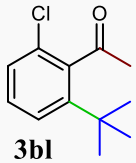
Area Percent Report

Data File : CH-64.D
Acq On : 10 Aug 2024 09:52
Operator :
Sample : CH-64
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-64.D\data.ms



3bl

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	1.785%
2	2.396	351	429	378	BV	78412	233740	1.71%	1.318%
3	4.216	363	439	378	BV	78412	242740	6.31%	5.318%
3	6.316	363	439	378	BV	78412	2212740	5.31%	5.318%
4	8.178	445	419	378	BV	78412	244740	100.00%	85.798%
5	8.674	2231	2242	2275	BB	4497609	2094240	1.311%	1.470%

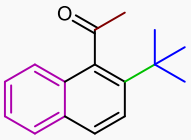
Area Percent Report

Data File : CH-65.D
Acq On : 08 Aug 2024 11:52
Operator :
Sample : CH-65
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-65.D\data.ms



3bm

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	0.785%
2	2.396	351	429	378	BV	78412	233740	1.71%	1.318%
3	4.216	363	439	378	BV	78412	242740	3.31%	3.318%
4	8.178	445	419	378	BV	78412	244740	100.00%	95.198%
5	8.674	2231	2242	2275	BB	4497609	2094240	1.311%	1.470%

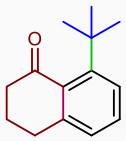
Area Percent Report

Data File : CH-66.D
Acq On : 05 Aug 2024 11.56
Operator :
Sample : CH-66
Misc :
ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: autoint1.e
Integrator: ChemStation

Method : C:\MassHunter\GCMS\3\methods\Method 11_H2_CO_DETECTION.M
Title :

Signal : TIC: CH-65.D\data.ms



3bn

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.316	221	219	378	BV	87712	212640	0.11%	1.785%
2	2.396	351	429	378	BV	78412	233740	1.71%	3.318%
3	4.216	363	439	378	BV	78412	242740	3.31%	3.318%
4	7.178	445	419	378	BV	78412	244740	100.00%	92.138%
5	8.674	2231	2242	2275	BB	4497609	2094240	1.311%	1.470%

10. Computational details

All DFT computations were carried out using the Gaussian 16, Revision C.01 program.[1] All structures were optimized at the B3LYP-D3[2-5] functional with LANL2DZ[6,7] for Co and 6-31G(d,p) basis set for other elements.[8,9] Single point calculations were performed at the PBE1PBE/6-311++G(d,p)[10-12], def2tzvpp (Co) level of theory and Grimme's dispersion correction[13] with universal solvation model (SMD) in methanol.[14] All transition states are confirmed to be first-order saddle points and optimized at the same level of theory. Intrinsic reaction coordinate (IRC) calculations were also carried out for the key reaction step connecting the reactant and product adducts to obtain the minimum energy path.[15] Optimized structures were illustrated with CYLview20.[16]

NBO analysis was carried out using the NBO 3.1 suite as implemented in Gaussian-16.[17,18.] The second-order perturbative estimation of donor–acceptor stabilization energy (E_s) was calculated using the following equation,

$$E_s = \Delta E_{ij} = q_i \frac{F_{ij}^2}{\Delta \varepsilon_{ji}} \qquad (1)$$

where q_i is the donor orbital occupancy number, and F_{ij} is the off-diagonal element of the Fock matrix in the NBO basis. $\Delta\varepsilon_{ji} = \varepsilon_j - \varepsilon_i$ is the orbital energy difference between the acceptor (j) and donor (i) NBO.

The turnover frequency (TOF), turnover-determining intermediate (TDI), transition state (TDTS), and the energetics-determining factors can be obtained from the reaction profile of a computed catalytic cycle.[19-21]

The energetic span of the cycle, ∂*E,* can be calculated as;

$$\partial E = T_{TDTS} - I_{TDI} \qquad \text{(If the TDTS is after the TDI)}$$

$$\partial E = T_{TDTS} - I_{TDI} + \Delta G_r \text{ (If the TDTS is before the TDI)}$$

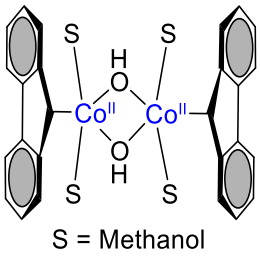
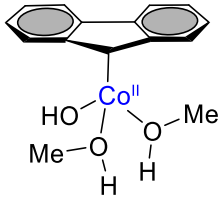
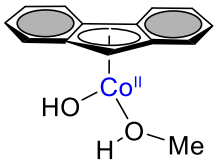
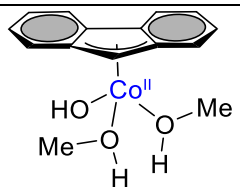
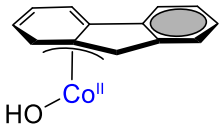
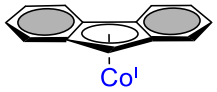
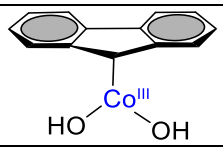
ΔG_r is the global energy of the reaction,

This ∂E value was used to find the turnover frequency (TOF)[19-21] for each catalytic cycle, using the formula-

$$TOF \approx (k_B T/h)\, e^{-\delta E/RT}$$

Where kB is the Boltzmann constant, T is the temperature in kelvin, h is Planck's constant, R is the gas constant, and ∂E is the energy span of the reaction.

Table S1: Stability study of possibilities of monomer Co-complexes w.r.t **IN1**.

Sr. No.	Catalyst structure	Energy	Hapticity of fluorenyl
1.	 S = Methanol **IN2a** (now **IN1**)	0.0 kcal/mol	η^1
2.		221.0 kcal/mol	η^1
3.		224.1 kcal/mol	η^5
4.		231.0 kcal/mol	endocyclic-η^3
5.	 **IN0**	381.9 kcal/mol	exocyclic-η^3
6.		34.9 kcal/mol	η^5
7.		71.4 kcal/mol	η^1

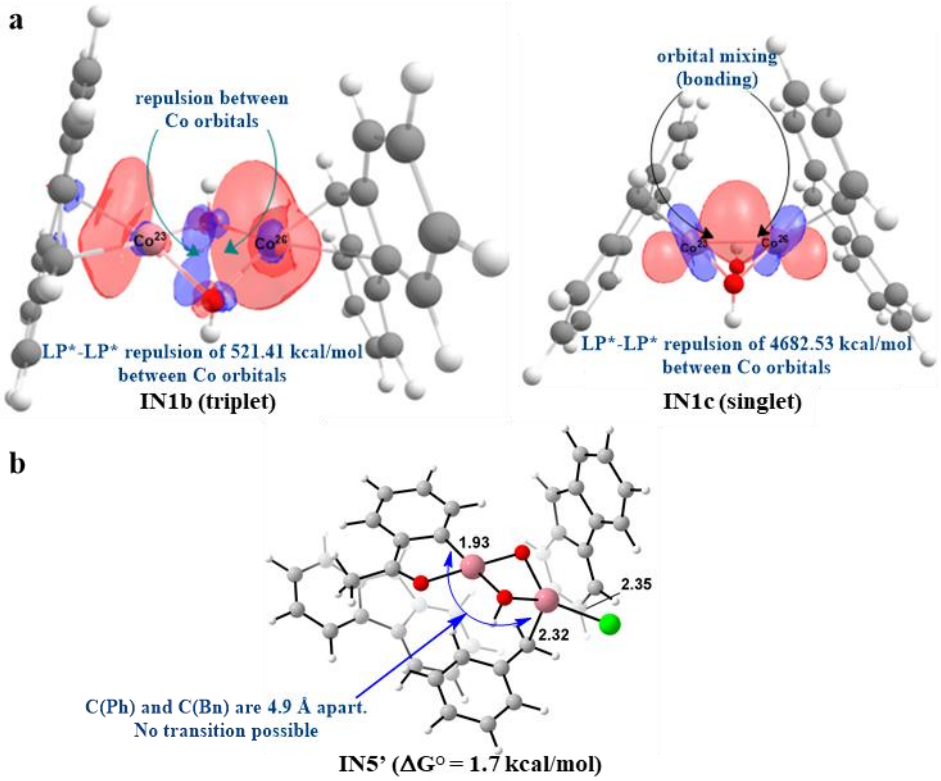


Figure S15. (a) NBO diagram for **IN1b** and **IN1c**. Opposite colour lobes in the NBO represent repulsion (isovalue = 0.062). (b) Optimised geometry of **IN5'** (Gibbs free energy given in comparison with **IN1**)**.**

11. TOF calculations.

Experimental

$$TON = \frac{\text{moles of substrate}}{\text{moles of catalyst}} \times \%\text{yield}$$

for product **3s**, yield = 98%

$$TON = \frac{2.0 \text{ mmoles}}{0.05 \text{ mmoles}} \times 98\%$$

$TON = 3920$

$$TOF = \frac{TON}{\text{reaction time}}$$

$$= \frac{3920}{5}$$

$TOF = 789\ h^{-1}$

Computational

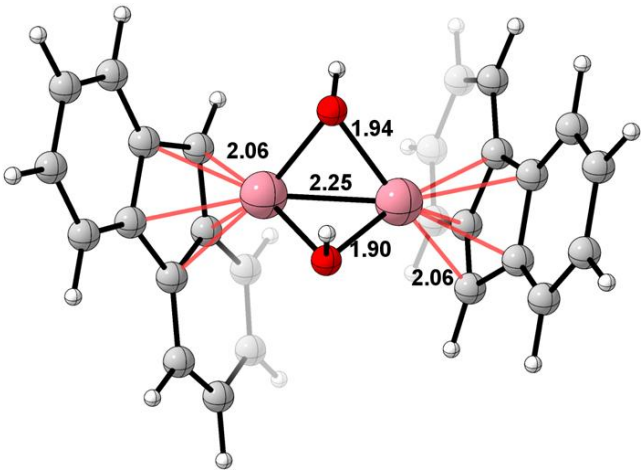
$$TOF = \frac{(k_B T)\, e^{-\Delta E/RT}}{h}$$

$\Delta E = TDTS - TDI$

$\Delta E =$ **22.0** kcal/mol for **3s**,

$TOF = 558.01\ h^{-1}$

Figure S16. Experimental and computational calculations for the formation of **3s**.



IN1c (singlet)
ΔG° = 38.8 kcal/mol

Figure S17. Optimized geometries and Gibbs free energies of singlet Co-complex, **IN1c** (the number of red bonds indicates the hapticity of fluorenyl).

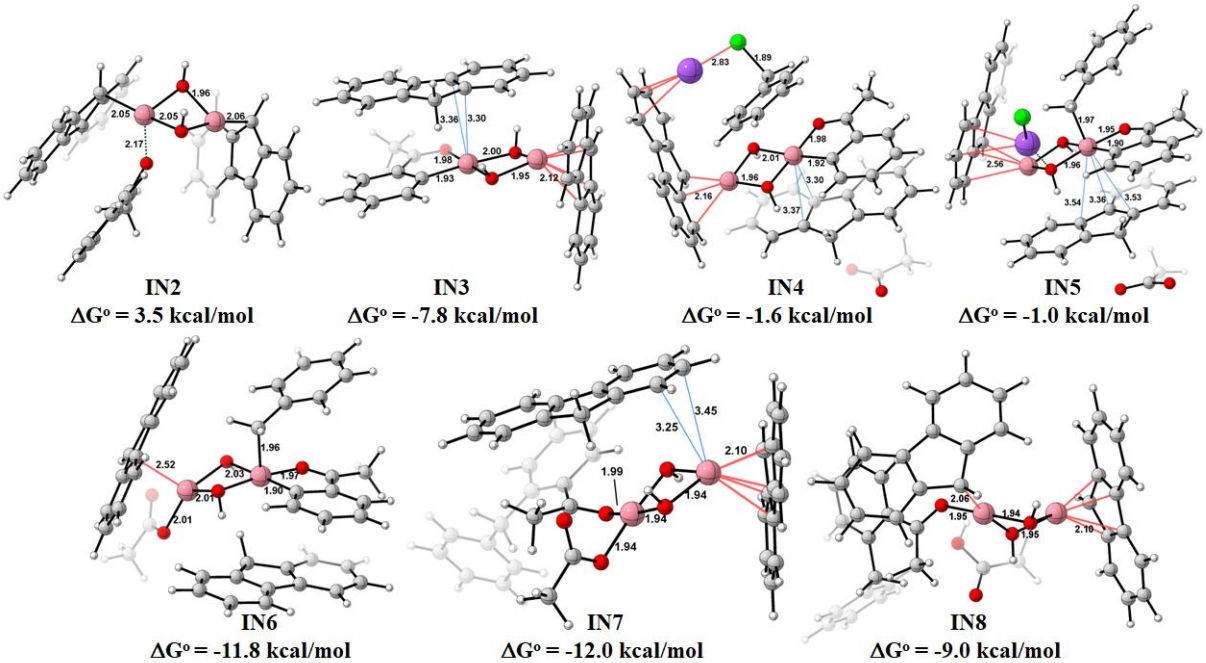


Figure S18. Optimized geometries and Gibbs free energies of intermediates (the number of red bonds indicates the hapticity of fluorenyl).

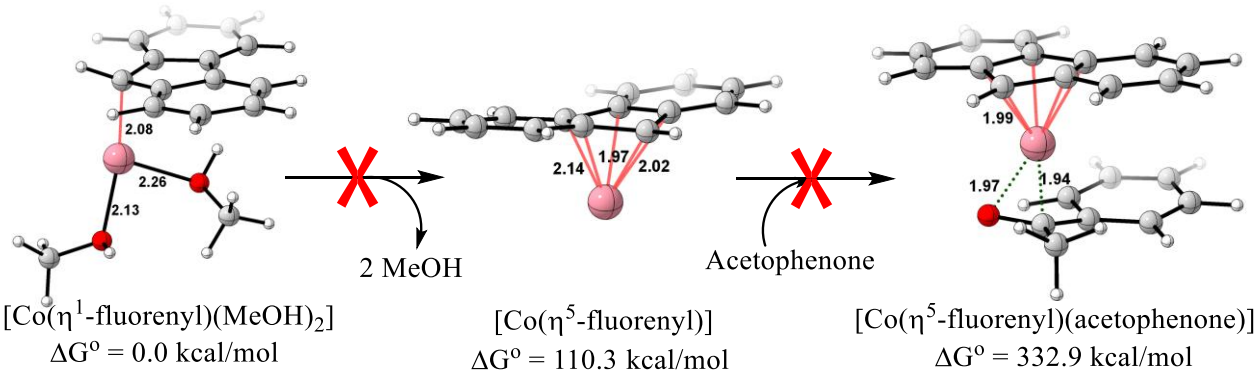


Figure S19. DFT study of Co(I)-acetophenone complex formation (the number of red bonds indicates the hapticity of fluorenyl).

Although the [Co(η^1-fluorenyl)$(MeOH)_2$] is stable compared to **IN1**, the activation of [Co(η^1-fluorenyl)$(MeOH)_2$] to [Co(η^5-fluorenyl)] requires 110.3 kcal/mol, which is highly unfavourable under the given reaction conditions. Also, the formation of [Co(η^5-fluorenyl)(acetophenone)] seems highly undesirable as the complex is highly unstable ($\Delta G°$ = 332.9 kcal/mol) when compared with the [Co(η^1-fluorenyl)$(MeOH)_2$] catalyst.

12. Comparison between Lanl2tz(f) and def2tzvpp basis sets[22]

Basis set: LANL2TZ(f)
BASIS "ao basis"
Primitive Gaussian functions to contracted basis functions
BASIS SET: (5s,5p,5d,1f) to [5s,5p,3d,1f]

s = 1 primitive function
p = 3 primitive functions
d = 5 primitive functions
f = 7 primitive functions

Total contracted basis functions = 5(1) + 5(3) + 3(5) + 1(7)
= 42

Basis set: def2-TZVPP
BASIS "ao basis"
Primitive Gaussian functions to contracted basis functions
BASIS SET: (17s,12p,7d,2f,1g) to [6s,5p,4d,2f,1g]
g = 9 primitive functions

Total contracted basis functions = 6(1) + 5(3) + 4(5) + 2(7) + 1(9)
= 64

Thus, proving def2tzvpp to be equivalent to lanl2tz(f), if not better.

13. Coordinates of Intermediates and Transition states:

IN0

Energy: -1958.417865 Hartree

Charge: 0

Spin Multiplicity: 2

H	-1.43498	-0.97886	1.0185
C	-0.25285	3.62341	-0.62696
C	-0.49036	3.3042	0.70935
C	-0.77591	1.98002	1.09631
C	-0.84072	0.98457	0.09198
C	-0.55525	1.32291	-1.28589
C	-0.27593	2.63433	-1.63173
H	-0.0373	4.65206	-0.90024
H	-0.46979	4.08559	1.4629
H	-1.04342	1.75281	2.12469
H	-0.06707	2.90254	-2.66362
C	-0.90608	-0.45753	0.22489
C	-0.81157	-0.9935	-1.13946
C	-0.89232	-2.3054	-1.60721
C	-0.74391	-2.54539	-2.97696
C	-0.51594	-1.49192	-3.87295
C	-0.43674	-0.17234	-3.41594
C	-0.58904	0.07699	-2.05308
H	-1.05934	-3.12789	-0.91719
H	-0.80474	-3.56318	-3.35198
H	-0.40417	-1.70222	-4.93261
H	-0.2683	0.64316	-4.1141
Co	0.91496	0.20585	0.94651
O	2.35419	-0.77848	1.35603
H	2.27149	-1.30331	2.16499

IN1

Energy: -4379.859869 Hartree

Charge: 0

Spin Multiplicity: 3

H	0.22437	-2.0213	-2.04464
C	-0.21407	-0.13766	2.55484
C	0.78766	-1.04189	2.1586
C	0.93237	-1.41432	0.82095
C	0.05233	-0.88916	-0.13952
C	-0.97158	0.01887	0.27078
C	-1.09425	0.3987	1.61281
H	-0.30053	0.14536	3.60054
H	1.46872	-1.44528	2.90353
H	1.72503	-2.09556	0.52674
H	-1.87219	1.09411	1.92041
C	0.01559	-1.04551	-1.60444
C	-1.18433	-0.31563	-2.0262
C	-1.76872	-0.1712	-3.29324
C	-2.88374	0.65699	-3.44474
C	-3.42139	1.35281	-2.34626
C	-2.85597	1.21486	-1.07645
C	-1.74836	0.37532	-0.91045
H	-1.34972	-0.69136	-4.15225
H	-3.34063	0.76986	-4.42499
H	-4.28491	1.99742	-2.48769
H	-3.27637	1.74844	-0.22686
Co	1.69746	0.0415	-2.09824
O	2.82841	-1.58478	-1.99144
O	3.43188	1.08328	-2.17526
Co	4.2499	-0.40166	-1.14773

C	4.56306	1.22949	1.01305
C	5.0289	0.59255	2.2037
C	5.45922	0.89924	-0.10966
C	6.5735	0.17007	0.51025
C	6.29127	-0.06511	1.89
C	3.37207	1.97284	1.05373
C	4.30307	0.68623	3.39724
H	5.68131	1.66242	-0.85723
C	7.75993	-0.33111	-0.04387
C	7.17077	-0.81161	2.68331
C	2.66631	2.07366	2.2538
H	2.99891	2.45938	0.15791
C	3.1226	1.43173	3.41883
H	4.66022	0.19482	4.29968
C	8.63697	-1.0637	0.75855
H	7.98695	-0.16236	-1.09396
C	8.34396	-1.31072	2.11215
H	6.94784	-0.99572	3.73196
H	1.7433	2.64698	2.2858
H	2.55096	1.51575	4.33929
H	9.55842	-1.45261	0.33165
H	9.03836	-1.88796	2.71714
H	3.10521	-1.80085	-2.89408
C	1.33439	1.02748	-5.11278
H	0.30086	1.35315	-4.95798
H	2.01479	1.80745	-4.76601
H	1.506	0.85011	-6.18106
C	5.59534	-0.58344	-4.00417
H	5.91439	0.45528	-3.89394
H	6.23629	-1.07613	-4.74406
H	4.55523	-0.60798	-4.35125
O	1.6313	-0.1495	-4.34492
O	5.733	-1.20045	-2.71381
H	0.97922	-0.83128	-4.56323
H	5.46403	-2.12705	-2.79867
O	4.37612	-2.12832	0.02357
O	1.02279	1.9732	-1.75217
C	5.51058	-3.00842	0.13478
H	6.14101	-2.63114	0.93801
H	5.16878	-4.0182	0.38516
H	6.08924	-3.03629	-0.79362
C	0.11637	2.84675	-2.45019
H	-0.76553	2.27062	-2.72028
H	-0.17598	3.67375	-1.79384
H	0.58048	3.24911	-3.35523
H	1.93751	2.30603	-1.84264
H	3.71879	-2.51751	-0.59239
H	3.75595	1.09313	-3.08641

IN1a

Energy: -4148.685235 Hartree

Charge: 0

Spin Multiplicity: 3

H	-0.35147	-2.1037	-0.34394
C	-0.83571	2.74943	0.89841
C	-0.21502	1.77064	1.69778
C	-0.11203	0.44718	1.26663
C	-0.64304	0.09566	-0.00128
C	-1.27795	1.10523	-0.8107
C	-1.36831	2.42302	-0.3519
H	-0.90764	3.7708	1.26176
H	0.18392	2.0481	2.66992

H	0.37288	-0.30527	1.88252
H	-1.85212	3.18467	-0.95842
C	-0.50471	-1.12082	-0.77919
C	-1.27133	-0.90231	-2.00166
C	-1.53481	-1.74738	-3.08942
C	-2.24916	-1.25119	-4.18249
C	-2.69562	0.08294	-4.2141
C	-2.42638	0.94289	-3.14737
C	-1.72306	0.45555	-2.04071
H	-1.19517	-2.78046	-3.07726
H	-2.46536	-1.90602	-5.02309
H	-3.24959	0.44506	-5.07583
H	-2.76866	1.97487	-3.1718
Co	1.30972	-0.07536	-1.02613
O	2.63292	-1.51875	-0.48115
O	2.77868	1.21895	-1.02956
Co	3.96959	-0.11475	-0.14692
C	4.88685	0.40166	1.88164
C	5.82181	-0.67621	2.06108
C	5.3045	1.22039	0.75641
C	6.61377	0.72265	0.3646
C	6.92006	-0.45339	1.12646
C	3.67901	0.40598	2.61339
C	5.55251	-1.69784	2.97726
H	4.98753	2.24856	0.60542
C	7.49799	1.14137	-0.64388
C	8.09019	-1.17942	0.875
C	3.43282	-0.62386	3.52305
H	2.95399	1.2018	2.46393
C	4.36155	-1.66395	3.7084
H	6.26124	-2.5101	3.11959
C	8.65903	0.40365	-0.88264
H	7.27922	2.03148	-1.22955
C	8.95863	-0.74651	-0.12888
H	8.32129	-2.0683	1.45786
H	2.51011	-0.61932	4.09787
H	4.14771	-2.45149	4.42585
H	9.34966	0.72732	-1.6575
H	9.87156	-1.30008	-0.33097
H	2.57901	1.94869	-0.42422
H	2.86321	-1.97278	-1.30246
C	1.05884	0.40449	-4.11786
H	0.0164	0.16376	-4.32586
H	1.12714	1.4066	-3.69604
H	1.63827	0.37065	-5.0495
C	5.73618	-1.8418	-2.14736
H	4.9941	-2.62615	-1.99242
H	6.15475	-1.93807	-3.15603
H	6.53447	-1.95508	-1.41008
O	1.62291	-0.49538	-3.15038
O	5.0604	-0.57863	-1.99742
H	1.33173	-1.39909	-3.34011
H	5.72241	0.12349	-2.09696

IN1b

Energy: -3917.503963 Hartree

Charge: 0

Spin Multiplicity: 3

H	-1.15608	-1.04211	1.10642
C	-0.25285	3.62341	-0.62696
C	-0.49036	3.3042	0.70935
C	-0.77591	1.98002	1.09631

C	-0.84072	0.98457	0.09198
C	-0.55525	1.32291	-1.28589
C	-0.27593	2.63433	-1.63173
H	-0.0373	4.65206	-0.90024
H	-0.46979	4.08559	1.4629
H	-1.04342	1.75281	2.12469
H	-0.06707	2.90254	-2.66362
C	-0.90608	-0.45753	0.22489
C	-0.81157	-0.9935	-1.13946
C	-0.89232	-2.3054	-1.60721
C	-0.74391	-2.54539	-2.97696
C	-0.51594	-1.49192	-3.87295
C	-0.43674	-0.17234	-3.41594
C	-0.58904	0.07699	-2.05308
H	-1.05934	-3.12789	-0.91719
H	-0.80474	-3.56318	-3.35198
H	-0.40417	-1.70222	-4.93261
H	-0.2683	0.64316	-4.11411
Co	1.0118	0.00922	-0.52088
O	2.45104	-0.97511	-0.11136
O	2.60909	0.88082	-0.48351
Co	3.90398	0.04136	0.42564
C	4.94242	-0.34177	2.30543
C	5.47255	-1.21435	1.27973
C	5.0732	1.03587	1.87346
C	5.84376	0.99574	0.62355
C	6.07755	-0.36092	0.25617
C	4.20202	-0.88133	3.38454
C	5.30602	-2.585	1.38479
H	4.82802	1.94054	2.42374
C	6.32055	2.02966	-0.18273
C	6.76974	-0.67101	-0.91321
C	4.05288	-2.2801	3.46134
H	3.84766	-0.24507	4.19099
C	4.59979	-3.11234	2.48548
H	5.70542	-3.25129	0.62526
C	7.01889	1.70901	-1.35121
H	6.14464	3.06693	0.08866
C	7.23989	0.37375	-1.71562
H	6.94997	-1.70518	-1.19403
H	3.51634	-2.71228	4.30049
H	4.4732	-4.18769	2.56846
H	7.39434	2.50628	-1.98654
H	7.78524	0.14866	-2.6275
H	2.46429	1.73065	-0.06112
H	2.70618	-1.46968	-0.8936

IN2

Energy: -4302.076145 Hartree

Charge: 0

Spin Multiplicity: 3

H	-0.47659	0.5951	-2.63156
C	3.47936	2.06196	-5.30738
C	2.87813	2.82292	-4.28842
C	1.85836	2.28979	-3.49795
C	1.42278	0.97745	-3.73197
C	2.01946	0.2177	-4.78308
C	3.05247	0.75638	-5.55785
H	4.27867	2.49504	-5.90288
H	3.21768	3.84016	-4.1101
H	1.42233	2.87651	-2.69386
H	3.51356	0.16857	-6.34804

C	0.44178	0.14483	-3.0186
C	0.38275	-1.10903	-3.78225
C	-0.38891	-2.26442	-3.58893
C	-0.17161	-3.37754	-4.40566
C	0.80567	-3.35197	-5.41506
C	1.58178	-2.20871	-5.62266
C	1.37308	-1.08794	-4.81315
H	-1.14094	-2.29599	-2.80336
H	-0.76349	-4.27695	-4.25658
H	0.96275	-4.23152	-6.0333
H	2.33987	-2.19313	-6.40217
Co	1.3487	-0.49957	-1.29259
O	1.61326	-1.43369	0.50938
O	1.72464	1.20594	-0.30841
Co	2.7923	0.10497	0.90619
C	4.85368	0.23979	2.03445
C	5.76521	-0.4126	1.13101
C	4.30325	1.42609	1.38891
C	5.04007	1.56552	0.12881
C	5.89753	0.43453	-0.04812
C	4.51982	-0.38806	3.25405
C	6.32414	-1.649	1.46038
H	3.92221	2.2831	1.94057
C	4.95758	2.53181	-0.88358
C	6.65377	0.28504	-1.2145
C	5.09622	-1.62143	3.56628
H	3.82989	0.09297	3.94317
C	5.99069	-2.24622	2.68035
H	7.01021	-2.14278	0.77652
C	5.72441	2.37504	-2.03998
H	4.29683	3.38807	-0.77432
C	6.57025	1.26415	-2.20671
H	7.29918	-0.58011	-1.34606
H	4.85283	-2.10262	4.50998
H	6.42532	-3.20599	2.94632
H	5.66406	3.12142	-2.82731
H	7.15589	1.16519	-3.11654
H	0.91523	1.47926	0.15138
H	2.07816	-3.02908	-0.88416
C	2.36787	-3.76724	-1.62518
C	1.87903	-5.06852	-1.5385
C	3.25871	-3.41145	-2.65456
C	2.26933	-6.03085	-2.47516
H	1.19534	-5.33464	-0.73717
C	3.65792	-4.39034	-3.58334
C	3.16185	-5.68961	-3.49499
H	1.88333	-7.04424	-2.40756
H	4.34216	-4.14101	-4.3864
H	3.46895	-6.43435	-4.22326
C	3.76226	-2.0179	-2.74588
C	4.88472	-1.69574	-3.69436
H	5.765	-2.309	-3.47401
H	4.57794	-1.91726	-4.72184
H	5.13513	-0.6393	-3.61142
O	3.28791	-1.10366	-2.05191
H	0.80096	-1.33369	1.02884

TS[2-3]

Energy: -4302.046447 Hartree

Imaginary Frequency: -1232.52

Charge: 0

Spin Multiplicity: 3

H	0.21941 -3.07983 -1.88285	C	3.84906 0.50141 3.94688
C	1.10162 0.31774 1.72768	C	5.51816 -1.74246 3.39121
C	1.29888 -1.07217 1.85359	H	4.75777 2.63481 1.99018
C	1.04206 -1.93451 0.78838	C	7.18734 1.87426 0.34593
C	0.58261 -1.40503 -0.4288	C	7.75032 -0.81851 1.0777
C	0.34436 0.0058 -0.54012	C	3.70706 -0.6884 4.63967
C	0.61903 0.85985 0.53391	H	3.21317 1.35427 4.1658
H	1.325 0.96756 2.56827	C	4.52796 -1.81065 4.35846
H	1.67578 -1.47073 2.7913	H	6.15806 -2.59679 3.18712
H	1.22698 -3.00137 0.88834	C	8.24428 1.17881 -0.22948
H	0.46003 1.93195 0.44115	H	6.97071 2.89849 0.05466
C	0.38352 -2.01732 -1.72972	C	8.52516 -0.15825 0.13033
C	-0.14 -0.98337 -2.5951	H	7.96334 -1.84846 1.35137
C	-0.50178 -1.00985 -3.95155	H	2.94927 -0.76935 5.41446
C	-0.85636 0.18485 -4.58622	H	4.38175 -2.72987 4.9187
C	-0.82638 1.40859 -3.89718	H	8.86845 1.67085 -0.97086
C	-0.45206 1.45408 -2.54866	H	9.35862 -0.67339 -0.3392
C	-0.12201 0.26766 -1.89279	H	3.05854 1.5943 -0.67176
H	-0.51302 -1.94807 -4.50073	H	1.91419 -1.94868 -2.27885
H	-1.1478 0.16858 -5.63331	C	2.89777 -2.18859 -3.02426
H	-1.09501 2.32519 -4.41536	C	3.316 -3.52933 -2.87528
H	-0.42169 2.4041 -2.01962	C	2.80812 -1.66986 -4.35457
Co	3.35401 -0.53203 -1.82721	C	3.60929 -4.31737 -3.9825
O	4.06753 -1.50568 -0.31663	H	3.37968 -3.94975 -1.87447
O	3.86132 1.07847 -0.84585	C	3.06404 -2.48311 -5.47293
Co	4.4012 0.10092 0.75912	C	3.46532 -3.80126 -5.28434
C	4.85112 0.60211 2.94961	H	3.9441 -5.34263 -3.84742
C	5.69898 -0.5362 2.68194	H	2.98511 -2.07874 -6.47772
C	5.1727 1.63444 1.99728	H	3.67929 -4.43075 -6.14302
C	6.39801 1.23356 1.3227	C	2.57958 -0.23319 -4.45233
C	6.68827 -0.12821 1.68578	C	2.30941 0.46792 -5.74674

H	3.26739	0.63575	-6.2565
H	1.67471	-0.12434	-6.40791
H	1.84587	1.4358	-5.54953
O	2.70456	0.4601	-3.40424
H	4.91173	-1.90136	-0.58137

IN3

Energy: -4302.094146 Hartree

Charge: 0

Spin Multiplicity: 3

H	-0.63023	-1.84037	0.51947
C	0.96109	2.70375	-0.21007
C	1.31742	1.96277	0.92584
C	1.05915	0.5865	0.99471
C	0.433	-0.03436	-0.08232
C	0.06089	0.71544	-1.22053
C	0.33407	2.08443	-1.29519
H	1.17447	3.76858	-0.24556
H	1.80805	2.45748	1.75717
H	1.3588	0.01992	1.87202
H	0.0588	2.65686	-2.17662
C	0.04548	-1.48566	-0.26907
C	-0.61063	-1.48429	-1.63238
C	-1.15573	-2.54122	-2.35297
C	-1.69498	-2.28981	-3.62167
C	-1.68531	-0.99605	-4.15922
C	-1.13156	0.06904	-3.44257
C	-0.59332	-0.18257	-2.17843
H	-1.15843	-3.5483	-1.94453
H	-2.1206	-3.10766	-4.1964
H	-2.10715	-0.82039	-5.14508
H	-1.11462	1.07058	-3.86328
Co	3.15601	-0.37144	-1.92474
O	3.82136	-1.211	-0.3213
O	3.90961	1.28961	-1.10648
Co	4.24848	0.44471	0.61365
C	4.56128	1.03391	2.75455
C	5.27853	-0.21251	2.60211
C	5.10141	1.97441	1.80771
C	6.32916	1.40177	1.27809
C	6.41438	0.03409	1.71413
C	3.45377	1.09165	3.63969
C	4.87026	-1.36259	3.31543
H	4.80646	3.01194	1.71233
C	7.29079	1.90407	0.37882
C	7.44542	-0.80012	1.25307
C	3.08426	-0.04806	4.3311
H	2.91815	2.02598	3.77918
C	3.78081	-1.27411	4.16475
H	5.41471	-2.29601	3.20118
C	8.31425	1.06681	-0.0502
H	7.23179	2.93294	0.03406
C	8.39348	-0.27592	0.38053
H	7.50269	-1.83438	1.58179
H	2.24417	-0.00733	5.01938
H	3.4582	-2.14825	4.72337
H	9.07016	1.45116	-0.73013
H	9.20674	-0.90341	0.02657
H	3.23052	1.97328	-1.00546
H	0.92428	-2.14271	-0.25233
C	2.56002	-1.96939	-2.8289
C	2.56428	-3.31915	-2.44648

C	2.04241	-1.67615	-4.12084
C	2.07046	-4.31649	-3.29529
H	2.95253	-3.60137	-1.46932
C	1.54528	-2.67084	-4.98343
C	1.5614	-3.99753	-4.56389
H	2.07787	-5.35525	-2.97121
H	1.14847	-2.41231	-5.96145
H	1.17921	-4.78142	-5.21143
C	2.05747	-0.25505	-4.43857
C	1.56306	0.30338	-5.73554
H	2.20843	-0.04435	-6.55121
H	0.55135	-0.05555	-5.94463
H	1.57247	1.39428	-5.70592
O	2.52858	0.53198	-3.57082
H	3.13043	-1.72125	0.12459

IN4

Energy: -5423.452704 Hartree

Charge: 0

Spin Multiplicity: 3

H	-1.55572	-1.5586	0.71563
C	1.2279	2.40234	0.43478
C	1.34922	1.50281	1.50488
C	0.73959	0.24128	1.44965
C	0.01159	-0.10847	0.31563
C	-0.10158	0.79384	-0.76573
C	0.50585	2.05283	-0.71093
H	1.70409	3.37705	0.49634
H	1.92073	1.78646	2.38363
H	0.84121	-0.45311	2.27942
H	0.41745	2.74746	-1.54176
C	-0.73674	-1.38595	0.00723
C	-1.27454	-1.12981	-1.3807
C	-2.04601	-1.95515	-2.19149
C	-2.43295	-1.49232	-3.45552
C	-2.05642	-0.21576	-3.89524
C	-1.2882	0.62174	-3.0799
C	-0.90247	0.15877	-1.81953
H	-2.34347	-2.9431	-1.85153
H	-3.03065	-2.12885	-4.10201
H	-2.36555	0.12695	-4.8789
H	-0.9942	1.61004	-3.42268
Co	2.53012	-0.91244	-1.77698
O	2.96913	-1.74848	-0.0885
O	3.57204	0.65888	-1.07851
Co	3.91107	-0.18959	0.62791
C	5.21162	-0.02886	2.3399
C	6.4375	-0.73897	2.05501
C	5.17033	1.19862	1.57158
C	6.47939	1.30385	0.92962
C	7.25338	0.13357	1.22187
C	4.17056	-0.69142	3.03426
C	6.61815	-2.04244	2.50031
H	4.57874	2.07156	1.83353
C	7.03019	2.30764	0.11988
C	8.55749	-0.00688	0.73473
C	4.38274	-2.01307	3.47107
H	3.25645	-0.16546	3.2966
C	5.58488	-2.67561	3.21334
H	7.54026	-2.57628	2.28481
C	8.33425	2.16256	-0.36424
H	6.45485	3.19827	-0.11887

C	9.10379	1.02062	-0.05218
H	9.15119	-0.88235	0.98713
H	3.59783	-2.51857	4.02684
H	5.72147	-3.69549	3.56105
H	8.77224	2.94854	-0.97354
H	10.1346	0.95365	-0.39352
H	2.98123	1.41323	-0.93124
H	-0.08481	-2.26784	0.03369
C	1.63328	-2.41326	-2.5794
C	1.36852	-3.70649	-2.10508
C	1.20316	-2.11891	-3.9029
C	0.69874	-4.64593	-2.89685
H	1.68206	-3.98543	-1.1008
C	0.53243	-3.05749	-4.70946
C	0.27902	-4.32632	-4.19852
H	0.49703	-5.64007	-2.50304
H	0.20937	-2.79856	-5.71419
H	-0.24116	-5.06581	-4.8005
C	1.50605	-0.75778	-4.3183
C	1.16585	-0.21286	-5.66897
H	1.74486	-0.746	-6.43278
H	0.10687	-0.37381	-5.89056
H	1.39747	0.85255	-5.71594
O	2.10447	-0.01538	-3.4912
H	2.16125	-1.96519	0.39685
C	5.12175	0.0598	-3.82886
H	4.64834	0.71482	-3.09978
C	5.38265	-1.30205	-3.27449
C	5.70596	-1.4513	-1.91156
C	5.31662	-2.44076	-4.087
C	5.96567	-2.71372	-1.37303
H	5.68248	-0.58038	-1.26023
C	5.56707	-3.70486	-3.54633
H	5.06258	-2.33495	-5.13818
C	5.89797	-3.84365	-2.19487
H	6.19227	-2.80916	-0.31521
H	5.50575	-4.58302	-4.18246
H	6.08955	-4.82922	-1.78088
H	4.57819	0.04768	-4.77099
Cl	6.7489	0.92203	-4.24379
C	-3.96462	-0.25484	0.16594
O	-4.01941	-1.43172	0.63155
O	-3.25101	0.687	0.62058
C	-4.83828	0.07368	-1.05404
H	-5.60421	0.80591	-0.77042
H	-4.22565	0.53392	-1.83631
H	-5.33056	-0.81562	-1.45658
Na	8.10429	-0.30253	-2.08038

TS[4-5]

Energy: -5423.434554 Hartree

Imaginary Frequency: -170.67

Charge: 0

Spin Multiplicity: 3

H	3.4907	-2.95925	1.47076
C	0.59978	-2.86496	-2.42557
C	0.25762	-3.59678	-1.27863
C	0.95463	-3.40701	-0.07549
C	1.99895	-2.48752	-0.03749
C	2.34483	-1.75475	-1.1956
C	1.64471	-1.93727	-2.3926
H	0.04562	-3.02152	-3.34694

H	-0.55513 -4.31576 -1.32191	H	-5.90171 -1.03622 2.13621
H	0.68308 -3.97556 0.81028	C	-4.86685 0.9799 -2.86015
H	1.91113 -1.37183 -3.28142	H	-3.41276 -0.39674 -3.67717
C	2.9085 -2.10329 1.10999	C	-5.68249 1.3157 -1.76518
C	3.81193 -1.06545 0.4856	H	-6.32657 0.77394 0.2264
C	4.86621 -0.35864 1.05428	H	-3.32044 -4.43122 2.79306
C	5.5792 0.54846 0.26044	H	-5.07102 -2.8736 3.59534
C	5.24132 0.73945 -1.08661	H	-4.8677 1.6164 -3.74144
C	4.1856 0.02777 -1.66474	H	-6.30314 2.2063 -1.80976
C	3.47578 -0.87763 -0.87176	H	-0.58746 -0.45689 -2.11449
H	5.13592 -0.50982 2.09561	H	2.35849 -1.69912 1.96968
H	6.40355 1.1089 0.69236	C	1.511 1.40438 1.26212
H	5.80741 1.44541 -1.6879	C	1.67688 1.18743 2.62931
H	3.92322 0.1765 -2.70852	C	2.34465 2.35143 0.62088
Co	0.32996 0.55126 0.0006	C	2.65458 1.89732 3.33832
O	-0.48865 -0.66914 1.24517	H	1.04986 0.46622 3.14753
O	-0.9625 -0.11488 -1.29028	C	3.32176 3.07116 1.32893
Co	-1.7316 -1.4477 -0.10916	C	3.47123 2.83823 2.69362
C	-3.68373 -2.55354 -0.03065	H	2.78373 1.72033 4.40344
C	-4.66001 -1.61212 0.46766	H	3.95728 3.79078 0.82121
C	-3.22999 -2.12766 -1.34054	H	4.22381 3.37998 3.25854
C	-4.05328 -0.96617 -1.68991	C	2.09795 2.47465 -0.80782
C	-4.89215 -0.62826 -0.58471	C	2.81623 3.4416 -1.68655
C	-3.17537 -3.55104 0.83059	H	2.61753 4.46217 -1.34162
C	-5.15552 -1.73298 1.76279	H	3.89556 3.27469 -1.61648
H	-2.81485 -2.80083 -2.08678	H	2.48788 3.3313 -2.72096
C	-4.05088 -0.1546 -2.83083	O	1.21601 1.72055 -1.3036
C	-5.69976 0.51283 -0.62246	H	0.19706 -1.29468 1.52141
C	-3.68456 -3.64781 2.13406	C	-1.37754 2.112 0.91505
H	-2.43673 -4.26157 0.46971	H	-0.93643 2.16471 1.89782
C	-4.6757 -2.76513 2.58886	C	-1.25118 3.20042 0.00142

C	-0.45099	4.3218	0.32733
C	-1.87026	3.13662	-1.27104
C	-0.26808	5.34079	-0.59822
H	0.02711	4.36562	1.30116
C	-1.68554	4.16178	-2.18847
H	-2.47273	2.26947	-1.52347
C	-0.88065	5.26047	-1.85697
H	0.35054	6.19771	-0.34928
H	-2.16075	4.11012	-3.16351
H	-0.73127	6.05717	-2.58014
H	-2.01268	1.2707	0.67696
Cl	-3.65569	2.66173	2.39119
C	5.79571	-3.55582	0.00084
O	5.91466	-3.59233	1.26176
O	4.84988	-4.06665	-0.66794
C	6.88157	-2.82091	-0.79962
H	7.34848	-3.51008	-1.51313
H	6.42212	-2.01545	-1.38281
H	7.65329	-2.39726	-0.1514
Na	-2.27282	-0.38657	3.72842

IN5

Energy: -5423.451825 Hartree

Charge: 0

Spin Multiplicity: 3

H	4.52985	-1.00983	1.53337
C	1.20771	-4.04973	-0.20804
C	1.50952	-4.02932	1.16046
C	2.25982	-2.97911	1.7086
C	2.69165	-1.94696	0.87871
C	2.3605	-1.95036	-0.49449
C	1.62679	-3.00631	-1.04743
H	0.64348	-4.87897	-0.62439
H	1.17051	-4.8406	1.79815
H	2.50753	-2.97655	2.76685
H	1.39293	-3.02473	-2.10868
C	3.52023	-0.7267	1.21046
C	3.57771	0.00407	-0.11071
C	4.21467	1.19869	-0.43263
C	4.15352	1.66519	-1.75122
C	3.46542	0.94287	-2.73701
C	2.83621	-0.26468	-2.42428
C	2.89925	-0.73127	-1.10642
H	4.7516	1.76055	0.32627
H	4.64534	2.59689	-2.01495
H	3.42979	1.32136	-3.75468
H	2.3217	-0.83666	-3.19247
Co	0.12832	0.72379	0.11881
O	-0.41902	-0.89154	1.0833
O	-0.51359	-0.16912	-1.60581
Co	-0.9429	-1.77873	-0.63567
C	-3.04858	-2.99103	-0.62924
C	-3.92627	-1.99192	-0.06626
C	-2.88182	-2.70627	-2.03255
C	-3.64541	-1.52673	-2.33964
C	-4.28613	-1.06806	-1.14412
C	-2.51801	-4.0141	0.189
C	-4.28015	-2.05114	1.27509
H	-2.32404	-3.31157	-2.7379
C	-3.78564	-0.81014	-3.53696
C	-5.05079	0.09058	-1.15164
C	-2.86424	-4.0372	1.54336

H	-1.85521	-4.76303	-0.23257
C	-3.74238	-3.08028	2.07627
H	-4.96942	-1.32706	1.70183
C	-4.56269	0.35132	-3.53375
H	-3.29598	-1.15077	-4.44475
C	-5.1853	0.79749	-2.35833
H	-5.52988	0.44975	-0.24546
H	-2.46417	-4.81479	2.18623
H	-4.02033	-3.13608	3.12504
H	-4.68145	0.92101	-4.45049
H	-5.77489	1.70905	-2.37865
H	0.22425	-0.26057	-2.22653
H	3.07426	-0.11906	2.00577
C	0.86768	1.62378	1.61432
C	0.90647	1.28088	2.96881
C	1.51467	2.82386	1.22335
C	1.55618	2.10583	3.89625
H	0.45335	0.35619	3.31782
C	2.1685	3.65693	2.14767
C	2.18272	3.29354	3.49143
H	1.5794	1.82049	4.94538
H	2.65973	4.56928	1.82132
H	2.68056	3.92295	4.22292
C	1.44756	3.07443	-0.20807
C	2.02613	4.28179	-0.86601
H	1.45832	5.1622	-0.54133
H	3.06559	4.42955	-0.56013
H	1.96301	4.18926	-1.95088
O	0.83569	2.22334	-0.90881
H	0.37458	-1.30634	1.45941
C	-1.65282	1.49588	0.47607
H	-1.75451	1.65554	1.55324
C	-1.89394	2.74817	-0.27209
C	-1.68931	4.00188	0.33378
C	-2.28361	2.71777	-1.62443
C	-1.85623	5.18328	-0.38979
H	-1.3854	4.04221	1.3768
C	-2.45733	3.89805	-2.34637
H	-2.43606	1.7584	-2.10792
C	-2.23875	5.13722	-1.73475
H	-1.69081	6.14142	0.09628
H	-2.76544	3.85117	-3.38788
H	-2.37081	6.05715	-2.29769
H	-2.29358	0.67816	0.1266
Cl	-3.22654	0.43193	4.55926
C	6.30328	-1.73268	-0.62978
O	6.7505	-0.96692	0.2747
O	5.61197	-2.77609	-0.4398
C	6.58858	-1.35204	-2.08991
H	6.89958	-2.23247	-2.66248
H	5.66428	-0.97813	-2.54583
H	7.35274	-0.5738	-2.16775
Na	-2.06568	-0.54844	2.53845

IN6

Energy: -4801.154161 Hartree

Charge: 0

Spin Multiplicity: 3

H	-0.35487	-3.17196	2.28431
C	-4.98635	-2.73291	0.84146
C	-4.53557	-2.17538	2.04556
C	-3.16488	-2.09658	2.32708

C	-2.25852 -2.58307 1.39132	C	4.62171 -2.17608 -1.84381
C	-2.71212 -3.13242 0.17213	H	4.90875 -2.06393 0.3012
C	-4.07849 -3.2143 -0.10654	C	4.24518 -1.48702 -3.00615
H	-6.05282 -2.784 0.63976	H	3.58335 0.38942 -3.86872
H	-5.25539 -1.80067 2.76786	C	2.89153 4.26707 -0.01122
H	-2.81819 -1.65904 3.25989	H	3.44869 3.25132 1.81913
H	-4.42927 -3.63091 -1.0465	C	2.75094 4.16736 -1.40327
C	-0.74803 -2.59587 1.43741	H	2.94125 2.90984 -3.15925
C	-0.3757 -3.19736 0.09995	H	4.89598 -3.22505 -1.90755
C	0.88372 -3.40601 -0.45935	H	4.23149 -2.01131 -3.95741
C	0.9705 -3.91646 -1.76187	H	2.63197 5.19575 0.48821
C	-0.18844 -4.22447 -2.48724	H	2.38595 5.02154 -1.96632
C	-1.45377 -4.02415 -1.92769	H	0.1379 0.8206 2.55108
C	-1.54245 -3.50523 -0.63309	H	-0.34727 -1.57953 1.54638
H	1.78019 -3.15626 0.09914	C	-2.04856 0.11659 -1.10018
H	1.94727 -4.06549 -2.21395	C	-1.92612 -0.4555 -2.37097
H	-0.10257 -4.61721 -3.49678	C	-3.35976 0.38766 -0.62957
H	-2.35188 -4.25046 -2.49586	C	-3.06186 -0.76203 -3.12895
Co	-0.73143 0.60598 0.17842	H	-0.94122 -0.67449 -2.77657
O	0.76894 -0.21923 -0.68255	C	-4.50582 0.09057 -1.38906
O	0.53178 1.05984 1.69997	C	-4.35099 -0.48976 -2.6441
Co	1.84219 -0.25528 1.0205	H	-2.94758 -1.21939 -4.10931
C	4.28126 -0.1732 -0.54817	H	-5.4986 0.30338 -1.00281
C	3.89677 0.5262 -1.73895	H	-5.22194 -0.73329 -3.24546
C	4.12834 0.71788 0.57706	C	-3.385 0.98936 0.69368
C	3.67736 1.99138 0.07241	C	-4.63992 1.39377 1.39563
C	3.52426 1.89187 -1.3484	H	-5.07011 2.25679 0.87288
C	4.64296 -1.52829 -0.60522	H	-5.3782 0.58799 1.36997
C	3.88039 -0.12923 -2.96136	H	-4.42223 1.67175 2.4282
C	3.35226 3.18176 0.73939	O	-2.2732 1.20474 1.24841
C	3.06458 2.97633 -2.08188	H	0.52059 -1.09516 -1.01247

C	-0.3539	2.27758	-0.78149
C	-1.23568	3.37515	-0.33523
C	-2.42335	3.68656	-1.02409
C	-0.94004	4.10151	0.83511
C	-3.28997	4.67392	-0.55349
H	-2.66989	3.13403	-1.92721
C	-1.80214	5.09205	1.30409
H	-0.03133	3.86303	1.38154
C	-2.98577	5.38002	0.61553
H	-4.20375	4.89501	-1.09966
H	-1.55258	5.64095	2.2089
H	-3.66005	6.1493	0.98213
H	0.68629	2.42333	-0.48693
C	3.04044	-1.62503	3.12188
O	2.47595	-1.89603	1.98987
O	3.10713	-0.47143	3.59863
C	3.65281	-2.80818	3.84477
H	4.52718	-3.1538	3.28108
H	3.96358	-2.53506	4.85484
H	2.93921	-3.63671	3.88287
H	-0.42254	2.07478	-1.85203
H	4.41648	0.50682	1.60113

TS[6-7]

Energy: -4801.123586 Hartree

Imaginary Frequency: -327.02

Charge: 0

Spin Multiplicity: 3

H	0.63533	2.87181	-0.73746
C	-4.23179	3.90923	-1.05382
C	-3.46444	3.65099	-2.20105
C	-2.18331	3.10102	-2.09321
C	-1.6757	2.82246	-0.82692
C	-2.44273	3.08629	0.32734
C	-3.72774	3.62894	0.21809
H	-5.22764	4.33147	-1.15808
H	-3.87325	3.87645	-3.18227
H	-1.59795	2.88261	-2.98273
H	-4.32217	3.82778	1.10585
C	-0.37138	2.19445	-0.43707
C	-0.40163	2.20969	1.07317
C	0.60784	1.96965	2.00582
C	0.32807	2.12651	3.36799
C	-0.93427	2.55915	3.79677
C	-1.92268	2.88356	2.86441
C	-1.64757	2.72691	1.50358
H	1.60503	1.68701	1.68337
H	1.10562	1.92189	4.09898
H	-1.13493	2.67083	4.85872
H	-2.88629	3.26616	3.18988
Co	-0.60892	-0.09061	-0.54683
O	1.11213	-0.49945	0.33777
O	0.69577	-0.19734	-2.31825
Co	2.2403	0.26578	-1.11102
C	4.72197	-0.472	0.09051
C	4.29954	-1.2689	1.20498
C	4.2704	-1.10743	-1.12328
C	3.59386	-2.32873	-0.75766
C	3.59304	-2.43975	0.66956
C	5.38523	0.74779	0.29683
C	4.54513	-0.84186	2.50213
H	4.54351	-0.81445	-2.13015

C	2.92414	-3.27511	-1.54567
C	2.93608	-3.49178	1.28986
C	5.62907	1.16278	1.60859
H	5.68142	1.36009	-0.55004
C	5.21371	0.3803	2.6964
H	4.22462	-1.43345	3.35519
C	2.26149	-4.32841	-0.90839
H	2.90725	-3.1776	-2.6275
C	2.26859	-4.43674	0.48999
H	2.92351	-3.58282	2.37242
H	6.14033	2.10381	1.78954
H	5.40939	0.72481	3.70786
H	1.7336	-5.07003	-1.50066
H	1.74616	-5.26246	0.96454
H	0.51999	0.46054	-3.00582
H	-0.00522	1.43327	-1.14182
C	-1.88855	-0.57201	0.96194
C	-1.65495	-0.80019	2.33181
C	-3.21637	-0.24957	0.55571
C	-2.69615	-0.71612	3.24802
H	-0.65182	-1.04221	2.67232
C	-4.27204	-0.19292	1.48973
C	-4.0122	-0.41972	2.83236
H	-2.49521	-0.87757	4.30462
H	-5.2791	0.04783	1.16042
H	-4.81372	-0.36828	3.56319
C	-3.37458	0.00764	-0.85845
C	-4.71181	0.18383	-1.50971
H	-5.35505	-0.67568	-1.29524
H	-5.20461	1.07654	-1.11007
H	-4.58992	0.29455	-2.5883
O	-2.33223	0.06944	-1.57212
H	1.18892	-0.10857	1.21594
C	-1.07589	-2.19297	-0.09734
C	-2.30857	-2.95745	-0.37734
C	-2.99662	-3.62967	0.65127
C	-2.84818	-3.00332	-1.67619
C	-4.18058	-4.31769	0.39123
H	-2.59939	-3.59434	1.66237
C	-4.03507	-3.68922	-1.93728
H	-2.33266	-2.48338	-2.47878
C	-4.70996	-4.34679	-0.90414
H	-4.69487	-4.83042	1.20012
H	-4.43336	-3.7108	-2.94846
H	-5.63495	-4.87996	-1.10612
H	-0.40388	-2.20639	-0.96392
C	3.13796	2.52542	-1.89196
O	2.48284	2.43238	-0.79747
O	3.37196	1.48328	-2.57941
C	3.59228	3.88257	-2.36298
H	4.08697	4.41219	-1.54352
H	4.26524	3.80212	-3.21815
H	2.71092	4.46783	-2.64943
H	-0.52456	-2.52217	0.77718

IN7

Energy: -4801.154526 Hartree

Charge: 0

Spin Multiplicity: 3

H	-3.80834	0.96267	-2.93622
C	-6.98879	-0.33303	0.7619
C	-6.80879	-1.04759	-0.44906

C	-5.92672 -0.60809 -1.42199	C	1.2895 -4.02716 1.69385
C	-5.19808 0.5891 -1.20438	C	2.22816 -3.19129 -0.84091
C	-5.39023 1.31524 0.03018	C	-2.77948 -2.18939 -2.45651
C	-6.29029 0.83878 1.00649	H	-3.62106 -2.77323 -0.55007
H	-7.68922 -0.70933 1.50229	C	-1.61502 -2.01362 -3.21463
H	-7.38 -1.95688 -0.6168	H	0.54343 -2.16759 -3.25769
H	-5.80611 -1.15717 -2.35076	C	2.65736 -4.05581 1.39163
H	-6.43528 1.39181 1.93056	H	0.93506 -4.34183 2.6718
C	-4.13017 1.22618 -1.93647	C	3.12095 -3.64175 0.13557
C	-3.84585 2.49057 -1.27271	H	2.5895 -2.86116 -1.81037
C	-2.9322 3.52064 -1.57236	H	-3.74403 -1.95657 -2.89519
C	-2.76189 4.55715 -0.66019	H	-1.68908 -1.64582 -4.23456
C	-3.47181 4.58459 0.5597	H	3.36663 -4.3978 2.14043
C	-4.36914 3.5704 0.88319	H	4.18605 -3.66273 -0.07904
C	-4.56812 2.52414 -0.03029	H	-2.55308 -0.84687 1.81046
H	-2.37216 3.50139 -2.50354	H	-1.01181 1.15577 -1.23769
H	-2.07017 5.36357 -0.88969	C	2.35449 0.15712 -2.06596
H	-3.3168 5.40869 1.25042	C	3.03262 -0.00155 -3.2683
H	-4.91124 3.58726 1.82497	C	4.42937 -0.04236 -3.26144
Co	-3.16459 0.43553 -0.24768	C	5.13026 0.0929 -2.06278
O	-1.29072 0.37175 -0.74179	C	4.4711 0.24051 -0.83535
O	-2.49833 0.0874 1.56174	C	3.05667 0.25362 -0.84637
Co	-0.65625 0.48835 1.08826	H	1.26981 0.161 -2.04355
C	-1.46618 -2.95538 -0.5925	H	2.47993 -0.0978 -4.19799
C	-0.29312 -2.78084 -1.35952	H	4.97674 -0.16952 -4.19129
C	-1.11283 -3.47314 0.78424	H	6.21563 0.09553 -2.08039
C	0.3944 -3.59084 0.72188	C	2.19801 0.27497 0.36258
C	0.86215 -3.17264 -0.54311	O	1.11825 0.89464 0.28402
C	-2.71258 -2.65653 -1.13584	C	5.29198 0.41905 0.43825
C	-0.36096 -2.30619 -2.67188	H	4.68568 0.91059 1.20313
H	-1.59422 -4.43569 1.00018	H	5.55347 -0.57049 0.83286

C	6.55799	1.22948	0.24031
C	7.81876	0.62093	0.25401
C	6.47972	2.61401	0.02584
C	8.97906	1.37716	0.05915
H	7.89264	-0.45127	0.41909
C	7.63488	3.37178	-0.16763
H	5.5048	3.09596	0.00985
C	8.89031	2.75436	-0.15232
H	9.94988	0.88888	0.07402
H	7.55727	4.44373	-0.32932
H	9.7907	3.34375	-0.30279
C	-0.05298	-0.27972	3.70238
O	-0.10112	0.75162	2.92629
O	-0.31147	-1.44723	3.34106
C	0.40885	-0.00581	5.12164
H	0.11679	0.99475	5.4496
H	0.0114	-0.75896	5.8059
H	1.50396	-0.06539	5.14714
C	2.52331	-0.51515	1.59226
H	3.40447	-1.14048	1.48058
H	2.65196	0.17056	2.43645
H	1.65977	-1.14618	1.81879
H	-1.4211	-2.78207	1.57688

TS[7-8]

Energy: -4801.135008 Hartree

Imaginary Frequency: -270.39

Charge: 0

Spin Multiplicity: 3

H	3.87834	-0.3318	-3.08677
C	6.98816	0.86794	0.69783
C	6.71757	1.68482	-0.42959
C	5.86625	1.26461	-1.43689
C	5.26302	-0.01566	-1.34142
C	5.54514	-0.84489	-0.1916
C	6.41344	-0.38641	0.8225
H	7.66198	1.23229	1.46823
H	7.19457	2.65852	-0.50362
H	5.67496	1.89086	-2.30334
H	6.62988	-1.01649	1.68085
C	4.25073	-0.67345	-2.1289
C	4.10637	-2.0246	-1.60745
C	3.295	-3.10283	-2.01296
C	3.24952	-4.24634	-1.22207
C	3.983	-4.3359	-0.01923
C	4.7781	-3.27662	0.41007
C	4.85217	-2.12037	-0.3815
H	2.71788	-3.03796	-2.93154
H	2.63894	-5.08931	-1.5352
H	3.9272	-5.24392	0.57455
H	5.33701	-3.342	1.33972
Co	3.26917	-0.18533	-0.33963
O	1.38713	-0.23569	-0.79595
O	2.61933	-0.06813	1.50884
Co	0.85239	-0.71624	1.00372
C	0.89034	2.98526	0.03911
C	-0.15806	2.82896	-0.89789
C	0.31519	3.1585	1.4143
C	-1.1672	3.19396	1.17874
C	-1.43764	2.95085	-0.18816
C	2.21896	2.96433	-0.37964
C	0.12144	2.62815	-2.25264

H	0.7257	3.98304	2.00247
C	-2.21013	3.39795	2.07798
C	-2.75475	2.88491	-0.65171
C	2.49457	2.78936	-1.74241
H	3.03077	3.07683	0.33471
C	1.45567	2.61351	-2.66734
H	-0.68396	2.49685	-2.96992
C	-3.52879	3.34911	1.60831
H	-2.00583	3.58545	3.12904
C	-3.79786	3.08585	0.25709
H	-2.96585	2.67763	-1.69673
H	3.52481	2.77985	-2.08271
H	1.6925	2.46773	-3.7179
H	-4.35236	3.50796	2.29916
H	-4.82711	3.03723	-0.08778
H	2.5236	0.85942	1.77302
H	1.17846	-0.97196	-1.39006
C	-2.10794	-0.31631	-2.10107
C	-2.76464	-0.00537	-3.2858
C	-4.15798	0.08212	-3.28664
C	-4.8775	-0.15359	-2.11382
C	-4.24081	-0.45529	-0.90393
C	-2.8249	-0.52393	-0.90447
H	-1.02452	-0.34706	-2.06992
H	-2.19655	0.17596	-4.19319
H	-4.69044	0.32949	-4.20086
H	-5.9609	-0.10588	-2.14099
C	-1.97715	-0.68698	0.30125
O	-0.87779	-1.26397	0.16218
C	-5.07647	-0.70469	0.34772
H	-4.56565	-1.43043	0.98686
H	-5.13134	0.22946	0.91917
C	-6.4824	-1.19913	0.07969
C	-7.58316	-0.34276	0.20697
C	-6.70351	-2.5267	-0.31629
C	-8.87862	-0.80062	-0.05209
H	-7.42361	0.68908	0.51117
C	-7.99485	-2.98771	-0.57501
H	-5.85542	-3.19936	-0.42174
C	-9.08786	-2.1245	-0.444
H	-9.72173	-0.123	0.05355
H	-8.14972	-4.02016	-0.87714
H	-10.09395	-2.48293	-0.64412
C	0.29691	-0.63753	3.7862
O	0.42126	-1.4074	2.75808
O	0.38779	0.60866	3.76148
C	-0.02853	-1.35402	5.08443
H	0.59048	-2.24886	5.19519
H	0.11176	-0.69181	5.94096
H	-1.0759	-1.67727	5.05442
C	-2.33817	-0.08604	1.62448
H	-3.12457	0.65988	1.55059
H	-2.65874	-0.88606	2.30262
H	-1.44508	0.36855	2.05454
H	0.59447	2.02675	2.18211

IN8

Energy: -4801.149725 Hartree

Charge: 0

Spin Multiplicity: 3

H	-2.88666	-2.35953	2.24838
C	-6.17477	1.20467	0.86465

C	-5.37842	1.2354	2.03974	H	-1.72957	2.78199	-2.20335
C	-4.51172	0.20358	2.35207	C	1.13163	3.31444	-2.88571
C	-4.44073	-0.92274	1.48957	C	2.11368	4.6256	-0.57882
C	-5.25405	-0.94925	0.2937	C	-2.415	3.46029	2.05574
C	-6.11903	0.1282	-0.00409	H	-3.26435	2.4525	0.34393
H	-6.83855	2.03782	0.65175	C	-1.30869	4.14678	2.5855
H	-5.45226	2.0917	2.70423	H	0.67238	4.92525	2.20487
H	-3.89824	0.24001	3.24793	C	2.39667	3.90767	-2.88395
H	-6.73564	0.10069	-0.89844	H	0.76735	2.80316	-3.77428
C	-3.56672	-2.06661	1.45831	C	2.89041	4.55325	-1.73652
C	-4.0329	-2.93902	0.38987	H	2.49343	5.12616	0.30871
C	-3.60584	-4.21012	-0.03794	H	-3.28335	3.27678	2.68265
C	-4.1786	-4.76567	-1.17835	H	-1.33078	4.48871	3.61694
C	-5.16025	-4.07218	-1.91684	H	3.00976	3.86815	-3.7811
C	-5.58786	-2.80731	-1.52029	H	3.88027	5.00165	-1.7541
C	-5.03679	-2.23805	-0.36327	H	-3.20889	1.14752	-1.60865
H	-2.84759	-4.7495	0.52266	H	-0.87577	-1.71701	-0.9842
H	-3.86665	-5.75393	-1.50638	C	3.10787	1.88832	1.23277
H	-5.58916	-4.53368	-2.80201	C	4.17779	2.25097	2.04051
H	-6.34364	-2.27242	-2.08952	C	5.37805	1.5463	1.9334
Co	-2.9424	-0.80361	-0.10454	C	5.48479	0.48043	1.04059
O	-1.02582	-1.11854	-0.23726	C	4.42438	0.09687	0.20783
O	-2.61364	0.38404	-1.60925	C	3.21684	0.83831	0.29671
Co	-0.84364	0.76114	-0.91104	H	2.1723	2.43065	1.29758
C	-1.28894	3.24048	-0.07181	H	4.07748	3.07505	2.74056
C	-0.17404	3.95122	0.46698	H	6.23013	1.81626	2.55127
C	-0.96139	2.75458	-1.42752	H	6.41377	-0.07804	0.99665
C	0.34546	3.3645	-1.72773	C	2.01427	0.61059	-0.54367
C	0.84105	4.04269	-0.57595	O	0.90712	0.93104	-0.06601
C	-2.41173	3.00175	0.73563	C	4.60599	-1.10838	-0.71202
C	-0.18338	4.39391	1.7944	H	3.64933	-1.61421	-0.84476

H	4.91566	-0.7545	-1.70276
C	5.60536	-2.13289	-0.21411
C	6.87951	-2.24249	-0.78438
C	5.26216	-2.99383	0.84015
C	7.79404	-3.19055	-0.31477
H	7.15678	-1.5814	-1.60208
C	6.172	-3.94121	1.31058
H	4.27463	-2.91635	1.28796
C	7.44292	-4.04237	0.7345
H	8.77821	-3.26298	-0.77021
H	5.88988	-4.60306	2.12532
H	8.15145	-4.78067	1.10016
C	1.11984	-2.94988	0.36362
O	1.35103	-3.10274	-0.82539
O	1.83783	-2.03686	1.04559
H	1.55842	-1.97891	1.97402
C	0.11425	-3.74778	1.14684
H	0.64449	-4.39849	1.85166
H	-0.53547	-3.08027	1.71814
H	-0.4822	-4.35367	0.46555
C	2.07436	0.08027	-1.94482
H	3.0287	0.27829	-2.43239
H	1.89955	-1.00147	-1.91745
H	1.26095	0.53455	-2.51612

Benzyl chloride

Energy: -730.780726 Hartree

Charge: 0

Spin Multiplicity: 1

C	-0.39300	-2.2236	0.06595
C	-0.99553	-2.67335	-1.10728
C	-0.64728	-2.88872	1.26391
C	-1.84307	-3.77192	-1.08308
H	-0.79633	-2.15397	-2.04238
C	-1.49491	-3.98714	1.28920
H	-0.17576	-2.53745	2.17933
C	-2.09321	-4.43031	0.11534
H	-2.31275	-4.11437	-2.00063
H	-1.69213	-4.49810	2.22720
H	-2.75838	-5.28890	0.13506
C	0.52044	-1.05304	0.03776
H	0.28640	-0.35791	-0.76908
H	0.55279	-0.52305	0.99017
Cl	2.24993	-1.58643	-0.27470

NaOAc

Energy: -390.587774 Hartree

Charge: 0

Spin Multiplicity: 1

C	0.6244	-1.06525	0.10592
O	1.84157	-1.1444	0.10589
O	-0.02591	0.11535	0.1059
C	-0.32684	-2.22668	0.10597
H	-0.972	-2.17367	0.98879
H	-0.97209	-2.17367	-0.77679
H	0.23038	-3.16332	0.10594
Na	1.37327	1.62727	0.10583

Acetophenone

Energy: -384.55969 Hartree

Charge: 0

Spin Multiplicity: 1

C	0.20815	-0.88263	-0.39549
O	0.8417	-0.71154	-1.42685
C	0.19931	0.15915	0.67609
H	-0.82317	0.49306	0.88228
H	0.60049	-0.24693	1.61099
H	0.80399	1.01166	0.36356
C	-0.57005	-2.13205	-0.18547
C	-0.58343	-3.09966	-1.19324
C	-1.28843	-2.36269	0.98986
C	-1.30085	-4.27224	-1.03072
H	-0.02467	-2.91974	-2.10666
C	-2.00624	-3.53842	1.15245
H	-1.29145	-1.62524	1.78634
C	-2.01392	-4.49276	0.14341
H	-1.30684	-5.01868	-1.81939
H	-2.56176	-3.71024	2.06938
H	-2.57714	-5.41273	0.27139

Methanol

Energy: -115.584488 Hartree

Charge: 0

Spin Multiplicity: 1

C	0.26522	0.11324	0.00000
H	0.62187	-0.89557	0.00000
H	0.62189	0.61764	-0.87365
H	-0.80478	0.11325	0.00000
O	0.74189	0.78734	1.16759
H	0.42356	1.69302	1.16714

IN5'

Energy: -5423.447983 Hartree

Charge: 0

Spin Multiplicity: 3

H	-0.14583	-3.64572	-2.26459
C	-0.66847	-0.38935	1.24896
C	0.34291	-1.35622	1.30424
C	0.67505	-2.10907	0.16922
C	-0.01446	-1.87855	-1.01667
C	-1.01386	-0.88168	-1.07860
C	-1.35079	-0.13884	0.05513
H	-0.91666	0.17993	2.13958
H	0.87489	-1.52475	2.23559
H	1.45612	-2.86229	0.22068
H	-2.12088	0.62573	0.00778
C	0.10153	-2.57899	-2.35289
C	-0.90663	-1.84211	-3.20686
C	-1.22611	-2.01785	-4.54924
C	-2.18295	-1.17848	-5.13481
C	-2.81266	-0.17818	-4.38118
C	-2.50201	-0.00251	-3.02888
C	-1.54727	-0.84062	-2.44561
H	-0.73528	-2.78711	-5.13950
H	-2.43747	-1.30182	-6.18395
H	-3.55022	0.46591	-4.85227
H	-2.99181	0.77190	-2.44460
Co	3.16524	2.26448	-1.77459
O	4.58991	1.49870	-0.73345
O	3.49308	3.89689	-0.64215
Co	4.20040	2.68943	0.78020
C	7.20421	-0.67618	-0.54841
C	6.96024	0.02378	0.67956
C	6.27594	-1.76255	-0.64722

C	5.43917	-1.74413	0.51645
C	5.84394	-0.64938	1.35274
C	8.20567	-0.22913	-1.42503
C	7.70160	1.14906	1.01155
H	6.21021	-2.47278	-1.46328
C	4.37103	-2.56830	0.90494
C	5.17818	-0.38760	2.54319
C	8.94680	0.90406	-1.07874
H	8.39543	-0.75216	-2.35855
C	8.69900	1.58600	0.12300
H	7.49967	1.69641	1.92731
C	3.71966	-2.30251	2.11271
H	4.05904	-3.39874	0.27756
C	4.11347	-1.22455	2.92051
H	5.46342	0.45682	3.16379
H	9.72408	1.26340	-1.74736
H	9.28573	2.46651	0.37019
H	2.89605	-2.93567	2.42867
H	3.58502	-1.03077	3.84963
H	2.65381	4.31054	-0.39395
H	1.11128	-2.53253	-2.77691
C	2.91234	0.77234	-2.97344
C	3.61366	-0.43259	-3.12789
C	1.84441	1.01087	-3.88269
C	3.27473	-1.34332	-4.13587
H	4.44678	-0.66702	-2.46837
C	1.48573	0.09516	-4.88866
C	2.21285	-1.08441	-5.01672
H	3.84145	-2.26630	-4.23982
H	0.65430	0.29854	-5.55709
H	1.95697	-1.80331	-5.78922
C	1.18982	2.29587	-3.67987
C	-0.01379	2.73505	-4.44978
H	0.20466	2.73747	-5.52337
H	-0.83166	2.02301	-4.28925
H	-0.32367	3.73273	-4.13443
O	1.67187	3.06124	-2.79923
H	4.46940	0.55366	-0.56977
C	2.39353	1.64691	1.78946
H	2.48436	0.74735	1.18608
H	2.79584	1.60125	2.79730
C	1.35765	2.58293	1.48759
C	1.03419	3.64175	2.37820
C	0.65804	2.50553	0.25295
C	0.05814	4.57158	2.04376
H	1.56595	3.71567	3.32287
C	-0.30872	3.44273	-0.07827
H	0.90669	1.70534	-0.43642
C	-0.61522	4.47984	0.81593
H	-0.18331	5.37464	2.73423
H	-0.82535	3.37109	-1.03087
H	-1.37397	5.21293	0.55775
Cl	5.28306	3.49488	2.69996

[Co(η^1-fluorenyl)(MeOH)$_2$]

Energy: -877.154844 Hartree

Charge: 0

Spin Multiplicity: 1

Co	0.740988	-3.33548	-3.8844
O	1.85889	-1.42643	-4.32559
O	2.329888	-3.85527	-2.56478
H	1.209767	-0.92514	-4.84669
C	2.164513	-0.66808	-3.14372
H	2.868767	-1.26372	-2.56062

H	2.631365	0.289555	-3.40328
H	1.266068	-0.4833	-2.54488
C	2.763244	-5.22881	-2.57295
H	3.672506	-5.34766	-1.97424
H	1.978892	-5.89397	-2.19436
H	2.977483	-5.48196	-3.61271
H	-1.75809	-4.04765	-4.2861
C	-1.77595	0.312229	-1.7956
C	-1.9571	-0.96022	-1.20637
C	-1.82323	-2.12442	-1.95539
C	-1.50603	-2.03869	-3.32823
C	-1.37231	-0.73964	-3.93239
C	-1.48614	0.42318	-3.15312
H	-1.8744	1.206353	-1.18541
H	-2.20028	-1.02771	-0.1484
H	-1.94914	-3.09825	-1.48636
H	-1.36073	1.402849	-3.60991
C	-1.26946	-3.07299	-4.33484
C	-1.10293	-2.35396	-5.59367
C	-0.94834	-2.80862	-6.92078
C	-0.76538	-1.88796	-7.94714
C	-0.72449	-0.49909	-7.68675
C	-0.90173	-0.02253	-6.39045
C	-1.1171	-0.93455	-5.34221
H	-0.9614	-3.87536	-7.13553
H	-0.64528	-2.24157	-8.96867
H	-0.56656	0.197918	-8.50562
H	-0.89139	1.047195	-6.19113
H	2.132219	-3.59448	-1.65349

[Co(η^5-fluorenyl)]

Energy: -645.714452 Hartree

Charge: 0

Spin Multiplicity: 1

Co	0.508418	-1.03947	1.127521
C	-1.29921	-0.61033	-0.58836
C	-0.90675	0.692518	-0.12446
C	-0.09309	-1.41344	-0.76955
C	1.049879	-0.51779	-0.68881
C	0.556302	0.718564	-0.08761
C	-2.66032	-0.92558	-0.69868
C	-1.87348	1.641351	0.226042
H	-0.0834	-2.39815	-1.22572
C	2.439552	-0.66164	-0.96762
C	1.476335	1.765365	0.205773
C	-3.61476	0.039776	-0.35821
H	-2.96972	-1.9084	-1.04676
C	-3.22736	1.309439	0.101134
H	-1.5766	2.625517	0.580496
C	3.295933	0.386305	-0.6775
H	2.807583	-1.57418	-1.42994
C	2.816337	1.591156	-0.08718
H	1.119149	2.69864	0.63465
H	-4.67201	-0.19523	-0.45393
H	-3.98719	2.044166	0.354883
H	4.356666	0.289549	-0.89446
H	3.522043	2.389707	0.127767

[Co(η^5-fluorenyl)(acetophenone)]

Energy: -1029.897016 Hartree

Charge: 0

Spin Multiplicity: 1

Co	-1.6699	2.094145	0.240495
C	-1.63381	3.649607	-1.00061
C	-2.32709	2.620593	-1.71859
C	-3.45613	2.225884	-0.91333
C	-3.57293	3.16097	0.197881
C	-2.46697	4.069161	0.109477
H	-0.7118	4.133444	-1.31101
C	-1.99184	1.869008	-2.87074
C	-4.25668	1.12651	-1.30313
C	-4.4693	3.236066	1.280177
C	-2.26866	5.031832	1.121871
H	-1.13054	2.15265	-3.47323
C	-2.78022	0.794985	-3.2127
C	-3.91015	0.428445	-2.43551
H	-5.12723	0.8444	-0.71301
H	-5.3059	2.542055	1.348595
C	-4.27004	4.209159	2.238788
H	-1.42281	5.714654	1.068155
C	-3.17534	5.09861	2.159511
H	-2.54101	0.214488	-4.10124
H	-4.51243	-0.42149	-2.75005
H	-4.96317	4.293016	3.073039
H	-3.04662	5.848671	2.937197
C	-3.4286	-1.20888	1.198812
C	-3.08472	-0.13968	1.994314
C	-1.87707	0.562868	1.780581
C	-1.02175	0.160764	0.708769
C	-1.37574	-0.97898	-0.06792
C	-2.54912	-1.64528	0.181432
H	-4.35886	-1.74492	1.372816

H	-3.72961	0.160787	2.818333
H	-1.51911	1.255673	2.539979
H	-0.7091	-1.32064	-0.85694
H	-2.81	-2.51793	-0.41423
C	0.006746	1.117741	0.310574
C	0.938233	0.899431	-0.83489
H	1.809377	0.312253	-0.51386
H	0.463222	0.365485	-1.66446
H	1.297227	1.869524	-1.19629
O	0.119085	2.175306	1.058731

IN3a

H -0.51047700 0.36864700 -2.56267700

C 3.32437900 2.08441400 -5.26153600

C 2.69126300 2.80091700 -4.22967300

C 1.71406600 2.20251500 -3.43226900

C 1.35511500 0.86822500 -3.67159300

C 1.98564100 0.15163300 -4.73304900

C 2.97369400 0.75736700 -5.51694700

H 4.08885900 2.56890400 -5.86314000

H 2.97175100 3.83531000 -4.04733400

H 1.25168500 2.75710800 -2.62014200

H 3.45984700 0.20326800 -6.31642000

C 0.43176100 -0.02431300 -2.95523500

C 0.44512400 -1.27800900 -3.72165000

C -0.24450700 -2.48283200 -3.51842100

C 0.04128000 -3.58165300 -4.33384000

C 1.00583700 -3.49257200 -5.35172300

C 1.70020400 -2.29933300 -5.56923800

C 1.42278200 -1.19241500 -4.76120200

H -0.98491200 -2.56312500 -2.72529100

H -0.48558700 -4.51930500 -4.17636100

H 1.21868300 -4.36167000 -5.96809000

H 2.44991500 -2.23515100 -6.35434600

Co 1.37189200 -0.63639600 -1.24004000

O 1.69110700 -1.56408000 0.55500200

O 1.70370700 1.07754000 -0.25966400

Co 2.83513600 0.01055800 0.92105100

C 4.93796200 0.19699800 1.96023700

C 5.86987600 -0.37111100 1.02176900

C 4.31155800 1.37423000 1.36727500

C 5.01679200 1.59403300 0.09939500

C 5.93504500 0.52244000 -0.12815900

C 4.65267800 -0.49368200 3.15678200

C 6.49725800 -1.58696700 1.29655400

H 3.91281900 2.19643700 1.95887500

C 4.86686900 2.59046800 -0.87496200

C 6.68531600 0.46061300 -1.30610700

C 5.29682500 -1.70704300 3.41476900

H 3.94816600 -0.07604000 3.87206100

C 6.21124500 -2.24820200 2.49628500

H 7.19855900 -2.01770400 0.58601800

C 5.62679500 2.52117300 -2.04482200

H 4.16053100 3.40331700 -0.72614500

C 6.53301200 1.46822300 -2.26110200

H 7.37964600 -0.35894500 -1.47491500

H 5.09049800 -2.23607700 4.34151700

H 6.69951000 -3.19296900 2.71943200

H 5.51384000 3.29153200 -2.80278600

H 7.11224400 1.43631600 -3.17982000

H 0.89652400 1.31923200 0.22133500

H 2.26408100 -3.13361300 -0.89233900

C 2.62334300 -3.84245100 -1.63134300

C 2.22606400 -5.17157900 -1.54100500

C 3.49953300 -3.40617900 -2.64097300

C 2.70447600 -6.10079900 -2.47957000

H 1.55454000 -5.47455900 -0.74684800
C 3.98610600 -4.35881400 -3.56231800
C 3.59339800 -5.68395200 -3.48724700
H 4.66422300 -4.06259000 -4.35475400
H 3.95486700 -6.41899300 -4.19932400
C 3.88139700 -1.98603300 -2.72495600
C 4.95717600 -1.56144500 -3.69022500
H 5.89299700 -2.09191000 -3.48430700
H 4.65782500 -1.80770200 -4.71411900
H 5.11368400 -0.48739900 -3.60689900
O 3.34347400 -1.11529100 -2.01521400
H 0.88504800 -1.48349400 1.08730900
C 1.46439900 -7.90995800 -1.50533300
H 1.34678100 -8.97356100 -1.71827400
H 1.86853100 -7.78234700 -0.49482400
H 0.49113500 -7.41205400 -1.58079300
O 2.37649700 -7.41571000 -2.49508200

IN4a

H -1.62345300 -1.84830300 0.61351000
C 1.21855900 2.08981100 0.76756000
C 1.26290000 1.10234600 1.76324200
C 0.63608800 -0.13642800 1.56891400
C -0.04343900 -0.36841100 0.37655300
C -0.09029000 0.62688800 -0.62420900
C 0.54555100 1.85861300 -0.43581400
H 1.71663200 3.04112000 0.93304800
H 1.79358000 1.29771100 2.69021300
H 0.68081300 -0.90083500 2.34024300
H 0.51255300 2.62303500 -1.20732700
C -0.80667600 -1.59495300 -0.07429700
C -1.31153300 -1.19086000 -1.44162600
C -2.07311400 -1.91564200 -2.35227700
C -2.40103200 -1.32691700 -3.58022800
C -1.96650600 -0.03120400 -3.89082200
C -1.19739500 0.70050600 -2.98116700
C -0.87561000 0.11513200 -1.75419200
H -2.40123000 -2.92562300 -2.12121900
H -2.99090600 -1.88361500 -4.30309600
H -2.22777900 0.40778400 -4.84974000
H -0.85295000 1.70130200 -3.22656200
Co 2.55319400 -0.96352800 -1.85963500
O 2.99754700 -1.89015400 -0.22210500
O 3.60537100 0.54262300 -1.07052800
Co 3.87529000 -0.35576700 0.62849900
C 5.16491400 -0.25195200 2.33071300
C 6.44739300 -0.79788700 1.93949100
C 4.98720700 1.04580600 1.71873300
C 6.26247200 1.35660000 1.06845500
C 7.14501200 0.23944300 1.18874800
C 4.20576000 -1.09531700 2.94172200
C 6.75931400 -2.12094900 2.21741000
H 4.31435600 1.81466000 2.08906600
C 6.67822800 2.49055700 0.36042100
C 8.40879400 0.25768200 0.59223400
C 4.55563800 -2.43499600 3.21218600
H 3.25437100 -0.69690100 3.28421100
C 5.80913800 -2.93641200 2.86286500
H 7.72064500 -2.53413700 1.92229500
C 7.94633800 2.49998700 -0.22754900
H 6.01999400 3.35076600 0.26342300
C 8.80641100 1.39376200 -0.11701300

H 9.07200400 -0.59957900 0.67870900
H 3.83694200 -3.07877900 3.71201700
H 6.05436400 -3.97175800 3.08209100
H 8.27353700 3.37724400 -0.78010900
H 9.78720800 1.42517300 -0.58354800
H 3.05292800 1.32815200 -0.94549100
H -0.15904200 -2.47892100 -0.13422300
C 1.60230500 -2.40576500 -2.72209000
C 1.27611800 -3.68892600 -2.29256000
C 1.18872500 -2.03447700 -4.03638000
C 0.55069900 -4.57247600 -3.11382500
H 1.56902500 -4.04219000 -1.30593000
C 0.47936100 -2.91925200 -4.86747200
C 0.15404200 -4.19107800 -4.41236400
H 0.17139000 -2.61973000 -5.86573900
H -0.39904100 -4.86904900 -5.05022500
C 1.54105800 -0.67905700 -4.39467600
C 1.21527500 -0.06561000 -5.72121200
H 1.76810000 -0.58639700 -6.51209400
H 0.14924000 -0.17413700 -5.94135800
H 1.48756900 0.99128700 -5.72577000
O 2.16549400 0.01362700 -3.53729900
H 2.18877000 -2.16103700 0.23437500
C 6.14510100 -2.67697300 -2.74974100
Cl 5.54537700 -1.76890500 -4.30351800
C 6.25091000 -1.62859700 -1.65115700
H 5.29641300 -1.12488400 -1.49111700
H 6.53729800 -2.12529000 -0.71774200
H 7.00829100 -0.87661800 -1.88651200
C 7.49727000 -3.28699000 -3.09618100
H 7.87570000 -3.81541700 -2.21278700
H 7.41376400 -4.00607500 -3.91594200
H 8.22351000 -2.51705800 -3.37121000
C 5.09572000 -3.73527700 -2.43743200
H 5.40241100 -4.27497000 -1.53332200
H 4.12074700 -3.28190900 -2.25243000
H 5.00272500 -4.45695600 -3.25428600
C -0.47855300 -6.73727800 -3.33034300
H 0.05074200 -7.01861400 -4.24794800
H -0.58332900 -7.61455000 -2.68965400
H -1.47246700 -6.34952800 -3.58183400
O 0.27239500 -5.78629000 -2.56659800

IN5a

H -4.06742200 -0.24084900 -1.98232400
C 0.11030500 -2.55784900 -2.71864900
C -0.22678600 -1.43884900 -3.49190100
C -1.29354500 -0.60879300 -3.11565000
C -2.00495300 -0.89536400 -1.95407000
C -1.64566400 -2.00195100 -1.15248000
C -0.59263500 -2.84807700 -1.53367700
H 0.92301900 -3.20760300 -3.02961800
H 0.33445500 -1.22072900 -4.39559700
H -1.56109600 0.24874300 -3.72745700
H -0.34683200 -3.73056800 -0.94780600
C -3.18095300 -0.17234700 -1.33957400
C -3.40389300 -0.93501900 -0.05489400
C -4.34560600 -0.72311800 0.94748400
C -4.36292600 -1.58308500 2.05194300
C -3.45315100 -2.64645500 2.15039700
C -2.51758000 -2.87683800 1.13861700
C -2.50370300 -2.01741800 0.03488900

H -5.05038600 0.10022000 0.87826600
H -5.08958600 -1.42589200 2.84352300
H -3.48308700 -3.30121000 3.01673800
H -1.82170700 -3.70941800 1.20337100
Co -0.21610400 0.56072700 1.30856700
O 0.63074300 0.50095400 -0.46975800
O 0.58102600 -1.31553900 1.65673400
Co 1.20540400 -1.44061500 -0.18899500
C 4.20932100 -1.45958500 -1.46004600
C 4.86721900 -0.42185300 -0.71588900
C 4.10192800 -2.62287300 -0.62104500
C 4.66472400 -2.30377100 0.65669000
C 5.15007500 -0.95467100 0.62045100
C 3.77403500 -1.22147700 -2.77459000
C 5.11077700 0.81633700 -1.29897900
H 3.66773900 -3.57364600 -0.90879900
C 4.77419600 -3.06083000 1.83473000
C 5.73401600 -0.38419100 1.74218300
C 4.02104200 0.03017000 -3.35005000
H 3.25959100 -1.99696000 -3.33454900
C 4.69287100 1.03358400 -2.62790300
H 5.61867200 1.60397100 -0.74909100
C 5.35661500 -2.47153100 2.95962000
H 4.41014800 -4.08410600 1.86893200
C 5.83240600 -1.15174500 2.91555200
H 6.10202000 0.63758800 1.72137000
H 3.70050100 0.22896800 -4.36839300
H 4.89268000 1.99042800 -3.10112900
H 5.44579900 -3.04146000 3.87987700
H 6.28288100 -0.71543100 3.80233700
H -0.16227500 -1.90515600 1.85562400
H -2.97793000 0.88959000 -1.16637400
C -1.39155400 2.00196300 0.92883900
C -1.46167600 2.84176000 -0.18375700
C -2.43172500 2.07286700 1.89354900
C -2.54242600 3.72929600 -0.33062700
H -0.68411100 2.81070000 -0.93716700
C -3.50714300 2.97655100 1.75281700
C -3.56078500 3.80287300 0.64759800
H -4.29835600 3.01746800 2.49619400
H -4.37557500 4.50383200 0.49755700
C -2.30846300 1.10123000 2.94995000
C -3.26170100 0.98938000 4.09573700
H -3.13272300 1.86129300 4.74935300
H -4.29724400 0.99233700 3.74651100
H -3.06354700 0.08041200 4.66572000
O -1.31695500 0.31393400 2.89991300
H -0.11697200 0.49954100 -1.09075200
C 1.21065200 1.68178700 2.13283300
Cl 1.88180800 3.87534100 -2.82190100
C -5.46938900 -2.72856500 -1.81966300
O -6.12180400 -1.64453300 -1.87258800
O -4.49119800 -3.03884000 -2.56165900
C -5.87090700 -3.75510700 -0.75079100
H -6.01536700 -4.74019600 -1.20859700
H -5.05699600 -3.85362000 -0.02356100
H -6.78188500 -3.46211800 -0.22200400
Na 2.20147000 1.74997900 -1.46573700
C 2.48732200 0.86421000 1.92200200
H 2.62697400 0.54928100 0.88344400
H 3.36669600 1.46293000 2.20080300
H 2.49247500 -0.04114700 2.53029100

C 1.33721100 3.05877400 1.48511900
H 2.27034800 3.54248700 1.81311600
H 1.35107700 3.02141500 0.39309200
H 0.50721100 3.71464500 1.75846300
C 0.93095800 1.83810000 3.62391000
H 0.82455900 0.87088000 4.12289800
H 1.77009100 2.36981100 4.10090400
H 0.02416700 2.42186500 3.80680000
C -1.76137500 4.49640900 -2.46528500
H -1.75475900 3.49853600 -2.91919600
H -2.10243100 5.22816600 -3.19950100
H -0.75030300 4.74849000 -2.13225200
O -2.70698200 4.56144400 -1.38719200

IN6a

H -3.30371900 -2.57263200 -1.81195200
C -6.55064600 -0.31794000 1.32582600
C -6.11966300 -1.66543000 1.42501300
C -5.24281200 -2.21247200 0.50422200
C -4.77416500 -1.40885200 -0.56754200
C -5.22282500 -0.03881600 -0.66602300
C -6.11369500 0.49299500 0.29141700
H -7.23917100 0.07617900 2.06807500
H -6.49202000 -2.28114100 2.23954200
H -4.93283800 -3.24982600 0.58185200
H -6.45378900 1.52151500 0.20663600
C -3.77732300 -1.62543400 -1.58621200
C -3.81383100 -0.47516400 -2.47857600
C -3.09127400 -0.17603000 -3.64978300
C -3.22634300 1.08564500 -4.22143700
C -4.05523200 2.06862900 -3.64007700
C -4.76589100 1.80009500 -2.47271800
C -4.65790300 0.52841000 -1.89120200
H -2.44059400 -0.92266800 -4.09735000
H -2.68451900 1.32030900 -5.13404600
H -4.14036800 3.04369700 -4.11154100
H -5.39792100 2.55937200 -2.01978700
Co -2.89240600 -0.25661300 -0.25585400
O -0.98863700 -0.37067600 -0.62047900
O -2.40095200 1.35065700 0.74142800
Co -0.63503700 1.45866500 -0.06230200
C -0.62916800 -1.74103200 2.43054200
C 0.58360800 -2.17158900 1.84863600
C -0.35933300 -0.65145200 3.44474700
C 1.14475400 -0.49937300 3.38152300
C 1.68422700 -1.39558200 2.43273400
C -1.83717100 -2.31492100 2.04448900
C 0.59455100 -3.18398300 0.88562900
H -0.70402100 -0.93050000 4.44898300
C 1.97775500 0.36384600 4.08727800
C 3.06006200 -1.43043400 2.18574800
C -1.82384000 -3.33231100 1.07937300
H -2.77865000 -1.97901900 2.47199700
C -0.62004100 -3.76126000 0.50630700
H 1.52873900 -3.51551700 0.44286100
C 3.35737300 0.32214900 3.84599200
H 1.56590600 1.06247900 4.81068900
C 3.89189700 -0.56649500 2.90321800
H 3.47410700 -2.10904400 1.44585900
H -2.75637000 -3.79294500 0.77140800
H -0.63202800 -4.55174800 -0.23944100
H 4.01900200 0.99078100 4.38996900

H 4.96302000 -0.57757800 2.72045300
H -2.30022400 1.20251200 1.69269800
H -0.80239400 -0.47389800 -1.56542200
C 2.53188300 -1.07642100 -1.29104300
C 3.24931500 -2.23716400 -1.55117800
C 4.64075900 -2.14101800 -1.64953900
C 5.26309700 -0.88639500 -1.56053700
C 4.56097200 0.29680300 -1.32787300
C 3.15558100 0.17751900 -1.12676800
H 1.46016800 -1.14650600 -1.13745900
H 2.73036100 -3.18262700 -1.64438600
H 6.33665600 -0.87022400 -1.70683900
C 2.22241900 1.17521500 -0.55478100
O 1.09059500 1.29022800 -1.07104900
C 5.35299300 1.62528400 -1.41447100
C -0.22363400 3.52553300 1.74580700
O -0.36397600 3.30123700 0.47975500
O -0.22057700 2.63775300 2.62401700
C 0.00501600 4.97570400 2.13032500
H -0.46834800 5.65791100 1.42028900
H -0.36540600 5.16502900 3.14061300
H 1.08461500 5.17031100 2.12236800
C 2.50975000 1.83681600 0.75910500
H 3.54212400 1.72277000 1.07617400
H 2.22094700 2.88833300 0.71987700
H 1.86135500 1.35119200 1.49607200
H -0.86338600 0.28722100 3.19006200
O 5.47557800 -3.19332400 -1.85511500
C 6.29402300 1.57955400 -2.64615700
H 6.81713000 2.53721900 -2.73923100
H 7.05775900 0.80185600 -2.56997800
H 5.72679600 1.41121000 -3.56811600
C 4.45503800 2.86422900 -1.61105500
H 3.73928500 2.71666600 -2.42711600
H 3.90857500 3.14789400 -0.71295000
H 5.08129300 3.72325500 -1.87291900
C 6.21499600 1.79703700 -0.14404700
H 6.91475700 0.96244400 -0.02976400
H 6.79825100 2.72292400 -0.20615000
H 5.60073600 1.84573900 0.75999800
C 4.90341100 -4.50307600 -1.95333900
H 4.22569500 -4.57758800 -2.81154100
H 5.74422800 -5.18401700 -2.09459300
H 4.36682300 -4.77066700 -1.03556700

14. Electronic energies and transition frequencies for all intermediates, transition states, and substrates.

Catalyst Structures			**Oxidative Addition**			**Catalyst Regeneration**	
IN0	-1958.417865		IN4	-5423.452704		TS[7-8]	-4801.135008
IN1	-4379.859869		TS[4-5]	-5423.434554		Imaginary frequency	-270.39
IN1a	-4148.685235		Imaginary frequency	-170.67		IN8	-4801.149725
IN1b	-3917.503963		IN5	-5423.451825		**Other Substrates**	
			IN5’	-5423.447983			
C-H Activation			**Reductive Elimination**			MeOH	-115.584488
IN2	-4302.076145		IN6	-4801.154161		Benzyl chloride	-730.780726
TS[2-3]	-4302.046447		TS[6-7]	-4801.123586		Acetophenone	-384.55969
Imaginary frequency	-1232.52		Imaginary frequency	-327.02		Sodium acetate	-390.587774
IN3	-4302.094146		IN7	-4801.154526		NaCl	-622.314724

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