Supporting Information

Synthesis of Biologically Important Tetrahydroisoquinoline (THIQ) Motifs using Quantum Dot Photocatalyst and Evaluation of Their Anti-Bacterial Activity

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1. General Information

Unless otherwise indicated, all reagents and solvents were purchased from commercial distributors and used as received. THF was dried over sodium/benzophenone then distilled and stored under Ar gas for moisture sensitive reactions. Column chromatography was performed with silica gel (200 - 300 mesh). Thin layer chromatography (TLC) was measured on silica gel 60 F254 and was visualized under ultraviolet light (254 nm and 365 nm). NMR spectra were recorded on Brucker Avance operation, ^{1}H at 400 MHz & ^{13}C at 100MHz. All chemical shifts are given in ppm downfield relative to Tetramethylsilane (TMS) and were referenced to TMS as internal standard[1]. ^{1}H NMR chemical shifts are designated using the following abbreviations as well as their combinations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad signal. NMR data were processed using the TopSpin 3.6.2 software package. High resolution mass spectra (HRMS) were obtained on Waters Xevo G2-XS Q-TOF equipped with ESI.

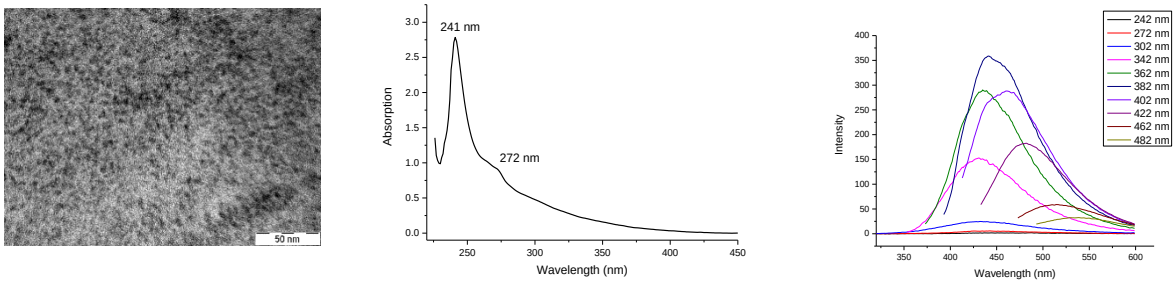
All visible light mediated reactions were carried out in 10 ml cylindrical Schlenk tube to get maximum exposer to light source. Blue LED of 10 W were use as light source for 420 nm. The distance from the Blue LED to the irradiation vessel maintain approx. 5 cm. No filter was used in the light-promoted reactions. During reactions, oxygen atmosphere was maintained through normal oxygen filled balloon.

Abbreviations:

EtOAc: ethyl acetate; MeCN: Acetonitrile; PTSA: p-Toluenesulfonic acid; DCM: dichloromethane; MeOH: methanol; THF: tetrahydrofurane; Et_2O: diethyl ether; Me: methyl; Et: ethyl; Bn: benzyl.

2. Synthesis and Characterization WS_2 Quantum Dots

In the laboratory, we prepared a suspension of WS_2 in N,N-Dimethylformamide (DMF) through a solution process. Initially, we added 10 mg of WS2 to 2.5 mL of DMF and subjected the mixture to sonication for 5 hours. After that, we centrifuged the mixture at 8000 rpm for 20 minutes at room temperature to remove any remaining WS_2 flakes. The obtained suspension was then transferred to a Teflon-lined stainless-steel autoclave and maintained at a temperature of 200 °C for 10 hours. It was then naturally cooled to room temperature. To purify the QD solution, we centrifuged the crude solution at 12000 rpm to separate the bulk material, and collected the QD in the supernatant. Finally, the collected QD in DMF was dried under reduced pressure using a rotary evaporator, dispersed in water, and stored under nitrogen.



1a. TEM image 1b. Absorption spectra 1c. Emission spectra

Figure S1. Characterization of MoS_2 QD (TEM, Absorption & Emission spectra).

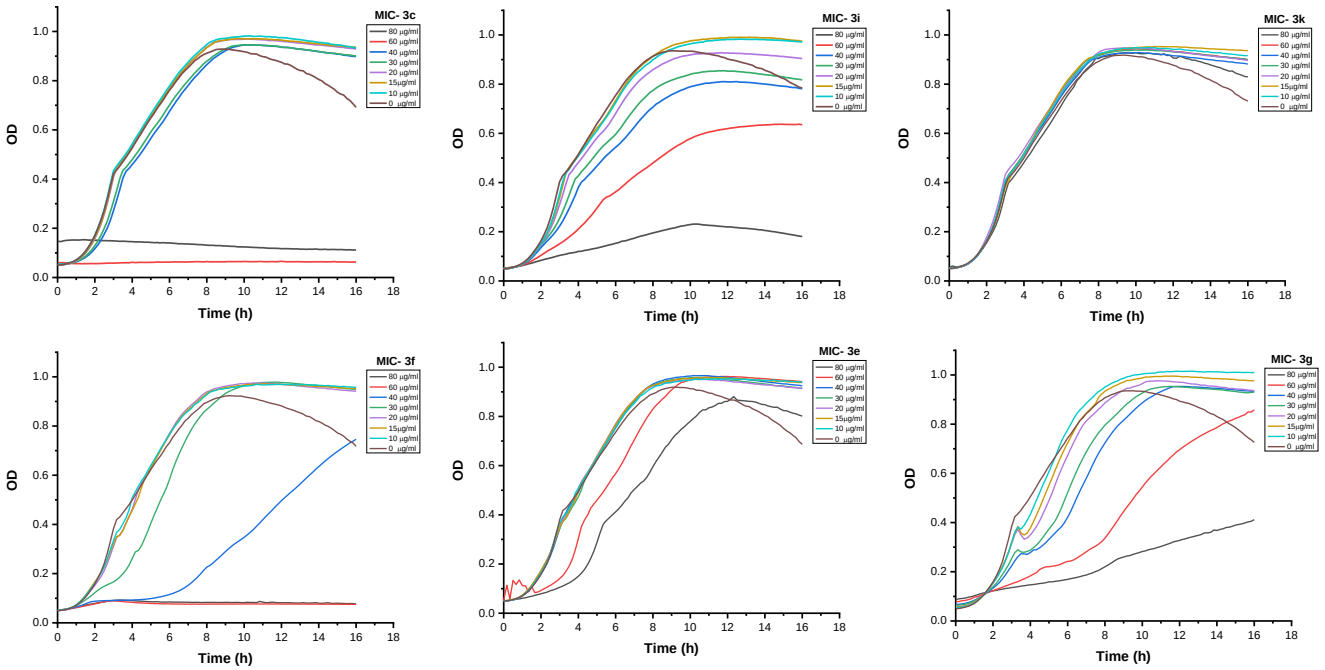
3. Optimization of reaction condition

After stirring for respective time at rt, reaction mixture was portioned between water layer (10 mL) and EtOAc layer (10 mL). The aqueous layer was extracted with EtOAc (10 mL x 3 times), and the combined organic phase was washed with a saturated solution of brine (10 mL), the combined organic layer was dried over anhydrous Na_2SO_4, concentrated to afford the residue. Obtained crude residue was recorded for NMR in $CDCl_3$ solvent. Yields and conversions were calculated from signal ratios relative to the internal standard Terephthalaldehyde.

4. Antibacterial assay

The antimicrobial efficacy of synthesized compounds was evaluated against Methicillin-Resistant *Staphylococcus aureus* (MRSA, USA300) representing Gram-positive bacteria. The frozen bacteria were reactivated on nutrient agar plates. A small number of bacterial colonies were then cultured in Luria broth media (LB, HiMedia – 20 g/L) overnight for approximately 10-12 hours to establish the primary culture. Subsequently, a secondary culture was initiated by transferring 50 µL from the primary culture into 5 mL of fresh LB media, allowing it to reach the mid-log growth phase (A600nm~0.3). For experimental purposes, the optical density (OD) was adjusted to A_{600nm}=0.01, resulting in a bacterial concentration of ~10^6 bacterial/mL.

The microbroth dilution method in 96-well plates was employed to determine the minimum inhibitory concentration (MIC) of synthesized compounds (which was taken into the 8% of MeCN in Water solution). Phosphate saline buffer (PBS) was utilized for sequential dilution of the working concentrations. A bacterial suspension of 100 µL with an A_{600nm} of 0.01 was combined with 100 µL of the prepared working concentration in the 96-well plate. The growth curve of the bacteria was monitored using a microplate reader (Eppendorf AF2200) equipped with a shaker, maintained at 37°C, for a duration of 16 hours. Optical density readings at 600 nm were taken at 10-minute intervals during a kinetic cycle, with concurrent shaking. The MIC, the lowest concentration at which the growth curve exhibited a 95% decline, was determined based on these measurements.



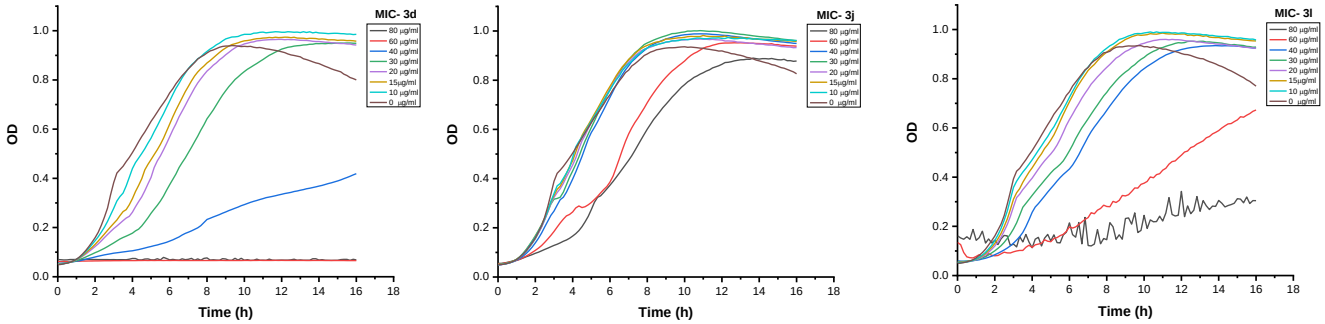


Figure S2. Evaluation of antibacterial efficacy of various C1-Substituted Tetrahydroisoquinoline (THIQ) Motifs. Growth kinetic curve of MRSA in presence of those derivatives.

5. Recyclability test for Catalyst

To check the recyclability of WS_2 QD catalyst, WS_2 QD catalyst were extracted into aqueous layer (10ml) against EtOAc layer (10ml) after the completion of reaction. The extracted aqueous layer was subsequently utilized as the reaction solvent for the next cycle. The combined organic layer was dried over anhydrous Na_2SO_4, concentrated to afford the residue and submitted for NMR. Reaction yield was determined by NMR against internal standard Terephthalaldehyde.

Table S3. Recyclability test for Catalyst.

Cycle	1	2	3	4	5
Yield (%)	82	81	79	78	75
Condition: Reactions were carried out on 0.5 mmol scale of 1a. Yield and selectivity were determined by crude NMR against Terephthaldehyde as internal standard.					

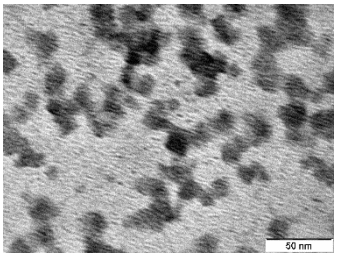
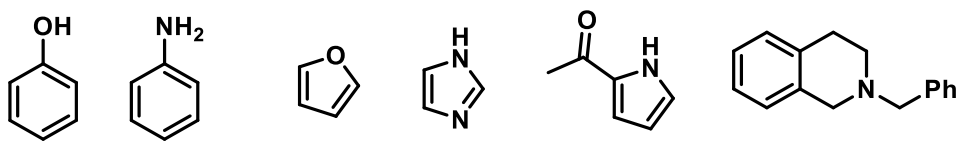


Figure S4. TEM image of recycled QD after 5th cycle.

6. Unsuccessful Substates



7. General Procedure for synthesis of C1 substituted THIQ

All Substrates were synthesised with standard optimized reaction conditions of 0.5 mmol of N-Ph THIQ with 0.75 mmol of Nucleophile (Naphthol, Indole, Pyrrole, or Phosphite) under catalytic loading of 5 w/w% WS_2 QD in 2ml of H_2O solvent inside Schlenk tube under Blue LED irradiation at room

temperature under oxygen atmosphere. After 24h of reaction, reaction mixture was portioned between water layer (30 mL) and EtOAc layer (30 mL). The aqueous layer was extracted with EtOAc (30 mL x 3 times) and the combined organic phase was washed with a saturated solution of brine (30 mL), the combined organic layer was dried over anhydrous Na_2SO_4, concentrated to afford the residue. The crude product was purified by column chromatography on silica gel using Pet. Ether / EtOAc as the eluent.

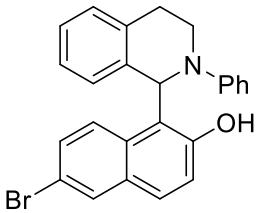
8. Procedure for reaction scale up

Reaction was scale up with same general procedure **7** under optimized reaction condition by increasing the loading of all reaction component (Nucleophile, Catalyst, Solvent) proportionally to the mmol of starting material N-Ph THIQ under Blue light irradiation at room temperature under oxygen atmosphere for 24h.

9. Photograph of reaction setup

10. Characterization of substrates

6-bromo-1-(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)naphthalen-2-ol (3a)



Purification: by column chromatography (Pet.ether/EtOAc = 96/04)

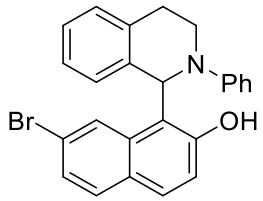
R_f (Pet. ether /EtOAc = 85/15)**:** 0.6

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 11.14 (bs, 1H), 8.10 – 8.08 (m, 1H), 7.90 – 7.89 (m, 1H), 7.65 – 7.63 (m, 1H), 7.52 – 7.49 (m, 1H), 7.32 – 7.30 (m, 2H), 7.23 – 7.15 (m, 4H), 7.04 – 6.93 (m, 3H), 6.68 – 6.66 (m, 1H), 6.37 (s, 1H), 3.73 – 3.69 (m, 1H), 3.66 – 3.58 (m, 1H), 3.46 – 3.39 (m, 1H), 3.06 – 3.02 (m, 1H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 155.04, 149.84, 135.98, 133.43, 132.16, 130.89, 130.30, 129.62, 129.19, 128.71, 128.47, 127.35, 126.88, 126.58, 125.78, 123.17, 122.91, 120.89, 118.73, 116.02, 59.63, 55.28, 30.57.

HRMS (ESI) m/z**:** $[M+H]^+$ Calcd for $C_{25}H_{20}BrNOH$ 430.0806; Found: 430.0808

7-bromo-1-(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)naphthalen-2-ol (3b)



Purification: by column chromatography (Pet.ether/EtOAc = 96/04)

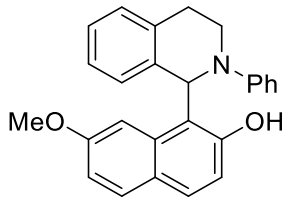
R_f (Pet. ether /EtOAc = 85/15)**:** 0.6

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 11.18 (bs, 1H), 8.36 (s, 1H), 7.61 – 7.55 (m, 2H), 7.43 – 7.40 (m, 1H), 7.33 – 7.31 (m, 2H), 7.23 – 7.16 (m, 4H), 7.05 – 6.94 (m, 3H), 6.70 – 6.68 (m, 1H), 6.31 (s, 1H), 3.73 – 3.68 (m, 1H), 3.65 – 3.57 (m, 1H), 3.46 – 3.39 (m, 1H), 3.06 – 3.02 (m, 1H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 155.58, 149.80, 135.88, 134.95, 133.46, 130.65, 129.59, 129.22, 128.47, 127.42, 126.91, 126.77, 126.62, 125.91, 125.80, 123.26, 123.21, 121.86, 120.15, 117.76, 59.65, 55.38, 30.55.

HRMS (ESI) m/z**:** $[M+H]^+$ Calcd for $C_{25}H_{20}BrNOH$ 430.0806; Found: 430.0804

7-methoxy-1-(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)naphthalen-2-ol (3c)



Purification: by column chromatography (Pet.ether/EtOAc = 96/03)

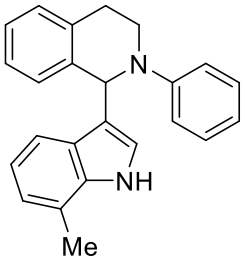
R_f (Pet. ether /EtOAc = 85/15)**:** 0.6

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 10.96 (bs, 1H), 7.64 – 7.61 (m, 1H), 7.50 – 7.48 (m, 2H), 7.30 – 7.25 (m, 2H), 7.20 – 7.11 (m, 4H), 7.01 – 6.92 (m, 3H), 6.77 – 6.75 (m, 2H), 6.30 (s, 1H), 3.96 (s, 3H), 3.73 – 3.69 (m, 1H), 3.64 – 3.55 (m, 1H), 3.44 – 3.37 (m, 1H), 3.03 – 2.99 (m, 1H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 159.02, 155.26, 150.01, 136.40, 134.85, 133.44, 130.57, 129.34, 129.08, 128.37, 127.45, 126.74, 126.60, 125.47, 123.91, 123.02, 117.74, 117.13, 114.14, 100.81, 59.61, 55.44, 30.61.

HRMS (ESI) m/z**:** $[M+H]^+$ Calcd for $C_{26}H_{23}NO_2H$ 382.1807; Found: 382.1804

1-(7-methyl-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (3d)



Purification: by column chromatography (Pet.ether/EtOAc = 94/06)

R_f (Pet. ether /EtOAc = 85/15)**:** 0.6

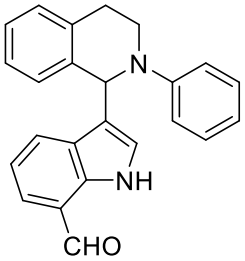
^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.86 (bs, 1H), 7.46 - 7.46 (m, 1H), 7.35 – 7.20 (m, 6H), 7.09 – 7.02 (m, 4H), 6.86 – 6.82 (m, 1H), 6.66 (s, 1H), 6.23 (s, 1H), 3.69 – 3.66 (m, 2H), 3.17 – 3.09 (m, 1H), 2.90 – 2.86 (m, 1H), 2.47 (s, 3H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 149.81, 137.50, 136.16, 135.57, 129.25, 128.83, 128.08, 126.72, 126.03, 125.78, 123.95, 122.67, 120.27, 119.90, 119.66, 118.10, 117.80, 115.83, 56.81, 42.37, 26.78, 16.63.

DEPT: +ve: 129.25, 128.83, 128.08, 126.72, 125.78, 123.95, 122.67, 119.90, 118.10, 117.80, 115.83, 56.81, 16.63.; -ve: 42.37, 26.78

HRMS (ESI) m/z**:** $[M+H]^+$ Calcd for $C_{24}H_{22}N_2H$ 339.1861; Found: 339.1865

3-(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)-1H-indole-7-carbaldehyde (3e)



Purification: by column chromatography (Pet.ether/EtOAc = 95/05)

R_f (Pet. ether /EtOAc = 90/10)**:** 0.4

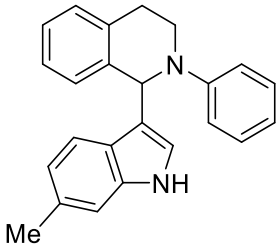
^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 10.10 (s, 1H), 9.96 (bs, 1H), 7.82 - 7.81 (m, 1H), 7.64 – 7.63 (m, 1H), 7.30 – 7.16 (m, 7H), 7.08 – 7.07 (m, 2H), 6.86 – 6.79 (m, 2H), 6.22 (s, 1H), 3.64 – 3.61 (m, 2H), 3.12 – 3.11 (m, 1H), 2.86 – 2.82 (m, 1H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 193.52, 136.93, 135.43, 134.41, 129.30, 129.03, 128.93, 128.00, 127.077, 127.67, 126.95, 126.02, 125.87, 120.34, 119.35, 118.69, 116.45, 56.78, 42.42, 26.66.

DEPT: +ve: 193.52, 129.30, 129.03, 128.93, 128.00, 127.077, 126.95, 125.87, 119.35, 118.69, 116.45, 56.78.; -ve: 42.42, 26.66.

HRMS (ESI) m/z**:** NA

1-(6-methyl-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (3f)



Purification: by column chromatography (Pet.ether/EtOAc = 96/04)

R_f (Pet. ether /EtOAc = 90/10)**:** 0.5

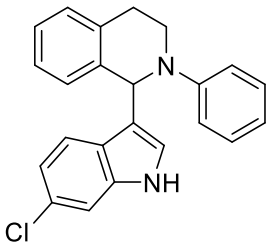
^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.80 (bs, 1H), 7.48 - 7.46 (m, 1H), 7.35 – 7.20 (m, 6H), 7.10 – 7.08 (m, 3H), 6.94 – 6.84 (m, 2H), 6.55 (s, 1H), 6.21 (s, 1H), 3.67 – 3.66 (m, 2H), 3.17 – 3.09 (m, 1H), 2.90 – 2.86 (m, 1H), 2.48 (s, 3H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 149.80, 137.54, 137.07, 135.54, 131.91, 131.05, 129.27, 128.83, 128.08, 126.72, 125.77, 124.34, 123.69, 121.42, 119.69, 118.17, 115.89, 111.13, 56.84, 42.36, 26.77, 21.72.

DEPT: +ve: 129.27, 128.83, 128.08, 126.72, 125.77, 123.69, 121.42, 119.69, 118.17, 115.89, 111.13, 56.84, 21.72.; -ve: 42.36, 26.77.

HRMS (ESI) m/z**:** $[M+H]^+$ Calcd for $C_{24}H_{22}N_2H$ 339.1861; Found: 339.1863

1-(6-chloro-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (3g)



Purification: by column chromatography (Pet.ether/EtOAc = 95/05)

R_f (Pet. ether /EtOAc = 90/10)**:** 0.5

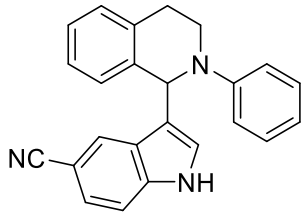
^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 8.00 (bs, 1H), 7.43 - 7.41 (m, 1H), 7.29 – 7.18 (m, 7H), 7.06 – 6.99 (m, 3H), 6.86 – 6.82 (m, 1H), 6.62 (s, 1H), 6.14 (s, 1H), 3.63 – 3.61 (m, 2H), 3.13 – 3.06 (m, 1H), 2.87 – 2.80 (m, 1H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 136.92, 135.46, 129.28, 128.94, 128.02, 127.98, 126.85, 125.81, 125.09, 124.85, 121.01, 120.37, 118.52, 116.21, 110.98, 56.67, 42.40, 26.64.

DEPT: +ve: 129.28, 128.94, 127.98, 126.85, 125.81, 124.85, 121.01, 120.37, 118.52, 116.21, 110.98, 56.67.; -ve: 42.40, 26.64.

HRMS (ESI) m/z**:** $[M+H]^+$ Calcd for $C_{23}H_{19}ClN_2H$ 359.1315; Found: 359.1316

3-(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)-1H-indole-5-carbonitrile (3h)



Purification: by column chromatography (Pet.ether/EtOAc = 85/15)

R_f (Pet. ether /EtOAc = 80/20)**:** 0.3

^{1}H NMR (400 MHz, DMSO – *d6*): δ (ppm) 11.55 (bs, 1H), 7.89 (s, 1H), 7.51 – 7.49 (m, 1H), 7.40 – 7.38 (m, 2H), 7.19 – 7.17 (m, 5H), 7.03 – 7.03 (m, 3H), 6.72 – 6.70 (m, 1H), 6.31 (s, 1H), 3.54 – 3.43 (m, 2H), 3.05 – 2.88 (m, 2H).

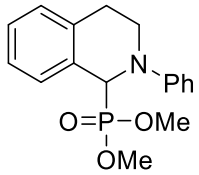
^{13}C NMR (100 MHz, DMSO – *d6*): δ (ppm) 149.60, 138.69, 137.78, 135.34, 129.51, 128.98, 128.17, 127.50, 127.14, 126.24, 126.19, 125.33, 124.19, 121.28, 115.58, 113.40, 102.56, 101.10, 55.73, 42.33, 27.03.

DEPT: +ve: 129.51, 128.98, 128.17, 127.50, 127.14, 126.24, 125.33, 124.19, 115.58, 113.40, 55.73.

-ve: 42.33, 27.03.

HRMS (ESI) m/z**:** $[M+H]^+$ Calcd for $C_{24}H_{19}N_3H$ 350.1657; Found: 350.1660

dimethyl(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)phosphonate (3i)



Purification: by column chromatography (Pet.ether/EtOAc = 68/32)

R_f (Pet. ether /EtOAc = 50/50)**:** 0.4

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.38 – 7.37 (m, 1H), 7.30 – 7.17 (m, 5H), 7.01 – 6.99 (m, 2H), 6.85 – 6.81 (m, 1H), 5.22 (d, J = 20.01 Hz, 1H), 4.12 – 4.00 (m, 2H), 3.69 – 3.65 (m, 6H), 3.12 – 3.02 (m, 2H).

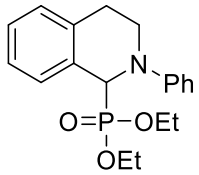
^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 136.45, 130.93, 129.27, 128.85, 127.99, 127.94, 127.59, 127.56, 126.10, 126.07, 118.72, 114.81, 58.77 (d, J = 159.59 Hz, 1C), 54.00, 53.93, 53.0152.94, 43.58, 26.68.

DEPT: +ve: 130.93, 129.27, 128.85, 127.99, 127.94, 127.59, 127.56, 126.10, 126.07, 118.72, 114.81, 58.77 (d, J = 159.59 Hz, 1C), 54.00, 53.93, 53.0152.94.; -ve: 43.58, 26.68.

^{31}P NMR (162 MHz, Chloroform – *d*): δ (ppm) 24.36.

HRMS (ESI) m/z**:** $[M+Na]^+$ Calcd for $C_{17}H_{20}NO_3PNa$ 340.1079; Found: 340.1078

diethyl (2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)phosphonate (3j)



Purification: by column chromatography (Pet.ether/EtOAc = 70/30)

R_f (Pet. ether /EtOAc = 50/50)**:** 0.5

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.30 – 7.28 (m, 1H), 7.18 – 7.15 (m, 2H), 7.10 – 7.07 (m, 2H), 6.91 – 6.89 (m, 2H), 6.72 – 6.69 (m, 1H), 5.11 (d, J = 20.07 Hz, 1H), 4.02 – 3.80 (m, 5H), 3.57 – 3.51 (m, 1H), 3.02 – 2.88 (m, 2H), 1.16 (t, J = 6.96 Hz, 3H), 1.05 (t, J = 7.05 Hz, 3H).

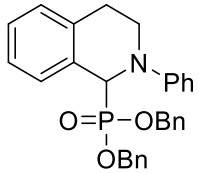
^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 149.51, 149.45, 136.55, 136.50, 130.73, 129.22, 128.84, 128.82, 128.24, 128.19, 127.53, 127.50, 125.96, 125.94, 118.55, 114.88, 63.43, 63.36, 62.46, 62.38, 58.91 (d, J = 159.19 Hz, 1C), 43.56, 26.85, 16.56, 16.50, 16.48, 16.42.

DEPT: +ve: 129.22, 128.84, 128.82, 128.24, 128.19, 127.53, 127.50, 125.96, 125.94, 118.55, 114.88, 58.91 (d, J = 159.19 Hz, 1C), 16.56, 16.50, 16.48, 16.42.; -ve: 63.43, 63.36, 62.46, 62.38, 43.56, 26.85.

^{31}P NMR (162 MHz, Chloroform – *d*): δ (ppm) 22.15.

HRMS (ESI) m/z**:** $[M+Na]^+$ Calcd for $C_{19}H_{24}NO_3PNa$ 368.1392; Found: 368.1391

dibenzyl(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)phosphonate (3k)



Purification: by column chromatography (Pet.ether/EtOAc = 82/18)

R_f (Pet. ether /EtOAc = 80/20)**:** 0.2

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.40 - 7.37 (m, 1H), 7.35 – 7.32 (m, 3H), 7.30 – 7.24 (m, 8H), 7.20 – 7.14 (m, 4H), 7.02 – 7.00 (m, 2H), 6.85 – 6.82 (m, 1H), 5.33 (d, J = 19.61 Hz, 1H), 5.07 – 5.03 (m, 1H), 4.99 – 4.89 (m, 2H), 4.83 – 4.79 (m, 1H), 4.09 – 4.03 (m, 1H), 3.69 – 3.63 (m, 1H), 3.15 – 2.98 (m, 2H).

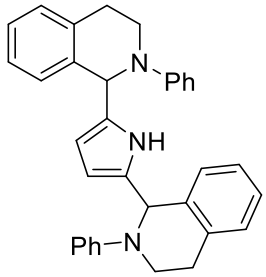
^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 130.39, 129.23, 128.85, 128.82, 128.47, 128.38, 128.29, 128.23, 128.19, 128.07, 128.02, 127.60, 127.57, 126.03, 126.00, 118.65, 114.90, 68.71, 68.64, 67.81, 67.73, 59.05 (d, J = 158.09 Hz, 1C), 43.59, 26.85.

DEPT: +ve: 129.23, 128.85, 128.82, 128.47, 128.38, 128.29, 128.23, 128.19, 128.07, 128.02, 127.60, 127.57, 126.03, 126.00, 118.65, 114.90, 59.05 (d, J = 158.09 Hz, 1C).; -ve: 68.71, 68.64, 67.81, 67.73, 43.59, 26.85.

^{31}P NMR (162 MHz, Chloroform – *d*): δ (ppm) 22.96.

HRMS (ESI) m/z**:** NA

2,5-bis(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)-1H-pyrrole (3l)



Purification: by column chromatography (Pet.ether/EtOAc = 96/03)

R_f (Pet. ether /EtOAc = 90/10)**:** 0.7

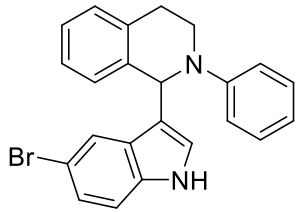
^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.84 (d, J = 11.95 Hz, 1H), 7.28 – 7.19 (m, 10H), 7.14 – 7.13 (m, 2H), 6.94 – 6.90 (m, 4H), 6.86 – 6.83 (m, 2H), 5.79 (d, J = 9.01 Hz, 2H), 5.52 (s, 1H), 5.45 (s, 1H), 3.52 – 3.44 (m, 2H), 3.38 – 3.24 (m, 2H), 3.00 – 2.93 (m, 2H), 2.74 – 2.66 (m, 2H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 150.07, 149.99, 135.67, 135.07, 135.05, 132.69, 132.58, 129.30, 129.23, 128.73, 128.68, 127.83, 126.93, 125.78, 125.74, 119.13, 119.05, 116.36, 116.25, 107.67, 107.53, 57.85, 57.80, 42.71, 42.38, 27.24, 27.20.

DEPT: +ve: 129.30, 129.23, 128.73, 128.68, 127.83, 126.93, 125.78, 125.74, 119.13, 119.05, 116.36, 116.25, 107.67, 107.53, 57.85, 57.80.; -ve: 42.71, 42.38, 27.24, 27.20.

HRMS (ESI) m/z**:** $[M]^+$ Calcd for $C_{34}H_{31}N_3$ 481.2518; Found: 481.2495

1-(5-bromo-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (3m)



Purification: by column chromatography (Pet.ether/EtOAc = 95/05)

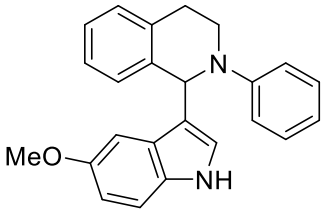
R_f (Pet. ether /EtOAc = 90/10)**:** 0.5

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.97 (bs, 1H), 7.59 (s, 1H), 7.24 – 7.13 (m, 8H), 7.00 – 6.98 (m, 2H), 6.82 – 6.78 (m, 1H), 6.61 (s, 1H), 6.06 (s, 1H), 3.59 – 3.52 (m, 2H), 3.08 – 3.00 (m, 1H), 2.81 – 2.76 (m, 1H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 149.81, 136.95, 135.39, 135.13, 129.17, 128.87, 128.08, 127.91, 126.78, 125.77, 125.34, 124.97, 122.65, 119.01, 118.73, 116.46, 112.95, 112.40, 56.65, 42.51, 26.55.

HRMS (ESI) m/z**:** NA

1-(5-methoxy-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (3n)



Purification: by column chromatography (Pet.ether/EtOAc = 95/05)

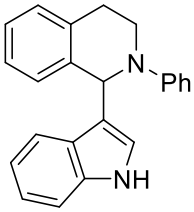
R_f (Pet. ether /EtOAc = 90/10)**:** 0.5

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.81 (bs, 1H), 7.27 – 7.25 (m, 1H), 7.22 – 7.14 (m, 6H), 7.02 – 7.00 (m, 2H), 6.87 – 6.86 (m, 1H), 6.80 – 6.74 (m, 2H), 6.57 – 6.56 (m, 1H), 6.13 (s, 1H), 3.64 (s, 3H), 3.60 – 3.57 (m, 2H), 3.10 – 3.02 (m, 1H), 2.83 – 2.77 (m, 1H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 153.83, 149.97, 137.47, 135.51, 131.55, 129.13, 128.73, 127.94, 126.88, 126.63, 125.62, 124.92, 118.69, 118.22, 116.15, 112.21, 111.58, 101.84, 56.79, 55.62, 42.07, 26.89.

HRMS (ESI) m/z**:** NA

1-(1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (3o)



Purification: by column chromatography (Pet.ether/EtOAc = 95/05)

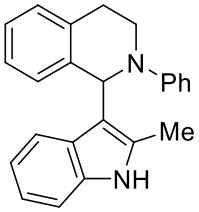
R_f (Pet. ether /EtOAc = 90/10)**:** 0.4

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.99 (bs, 1H), 7.61 - 7.59 (m, 1H), 7.34 – 7.27 (m, 4H), 7.24 – 7.17 (m, 4H), 7.09 – 7.07 (m, 3H), 6.85 – 6.81 (m, 1H), 6.64 (s, 1H), 6.22 (s, 1H), 3.68 – 3.65 (m, 2H), 3.15 – 3.07 (m, 1H), 2.87 – 2.83 (m, 1H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 149.80, 137.43, 136.61, 135.58, 129.26, 128.86, 128.08, 126.72, 126.47, 125.75, 124.28, 122.10, 120.06, 119.63, 119.16, 118.13, 115.83, 111.84, 56.68, 42.31, 26.65.

HRMS (ESI) m/z**:** $[M+H]^+$ Calcd for $C_{23}H_{20}N_2H$ 325.1704; Found: 325.1703

1-(2-methyl-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (3p)



Purification: by column chromatography (Pet.ether/EtOAc = 95/05)

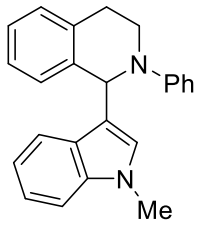
R_f (Pet. ether /EtOAc = 90/10)**:** 0.5

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.72 (bs, 1H), 7.29 (s, 1H), 7.22 – 7.18 (m, 4H), 7.11 – 7.03 (m, 6H), 6.95 – 6.91 (m, 1H), 6.88 – 6.85 (m, 1H), 6.00 (s, 1H), 3.75 – 3.61 (m, 2H), 3.16 – 3.00 (m, 2H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 150.92, 138.02, 135.29, 134.91, 133.27, 128.77, 128.67, 128.59, 128.19, 126.24, 126.02, 120.75, 120.18, 119.47, 119.42, 119.16, 113.44, 109.96, 57.13, 45.87, 27.95, 12.25.

HRMS (ESI) m/z**:** NA

1-(1-methyl-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (3q)



Purification: by column chromatography (Pet.ether/EtOAc = 97/03)

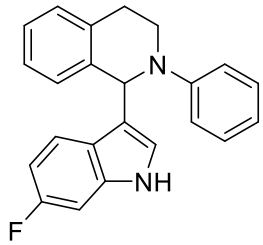
R_f (Pet. ether /EtOAc = 90/10)**:** 0.4

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.61 - 7.59 (m, 1H), 7.36 – 7.34 (m, 1H), 7.31 – 7.27 (m, 4H), 7.25 – 7.21 (m, 3H), 7.09 – 7.07 (m, 3H), 6.85 – 6.81 (m, 1H), 6.56 (s, 1H), 6.24 (s, 1H), 3.76 – 3.65 (m, 2H), 3.70 (s, 3H), 3.16 – 3.09 (m, 1H), 2.90 – 2.84 (m, 1H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 149.74, 137.60, 137.35, 135.54, 129.21, 128.80, 128.03, 126.87, 126.62, 125.69, 121.64, 119.11, 117.99, 117.61, 115.65, 109.13, 56.60, 42.18, 32.69, 26.61.

HRMS (ESI) m/z**:** NA

1-(6-fluoro-1H-indol-3-yl)-2-phenyl-1,2,3,4-tetrahydroisoquinoline (3r)



Purification: by column chromatography (Pet.ether/EtOAc = 94/06)

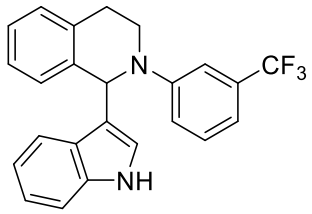
R_f (Pet. ether /EtOAc = 90/10)**:** 0.4

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.95 (bs, 1H), 7.22 – 7.11 (m, 8H), 7.01 – 6.99 (m, 2H), 6.90 – 6.85 (m, 1H), 6.80 – 6.76 (m, 1H), 6.66 (s, 1H), 6.07 (s, 1H), 3.62 – 3.53 (m, 2H), 3.09 – 3.01 (m, 1H), 2.80 – 2.76 (m, 1H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 149.73, 137.05, 136.92, 135.46, 129.21, 128.90, 128.03, 127.93, 126.78, 125.73, 125.07, 124.74, 121.04, 120.35, 119.45, 118.51, 116.20, 110.89, 56.64, 42.38, 26.63.

HRMS (ESI) m/z**:** NA

1-(1H-indol-3-yl)-2-(3-(trifluoromethyl)phenyl)-1,2,3,4-tetrahydroisoquinoline (3s)



Purification: by column chromatography (Pet.ether/EtOAc = 93/07)

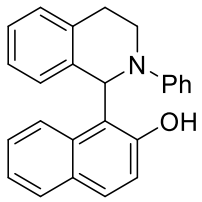
R_f (Pet. ether /EtOAc = 90/10)**:** 0.2

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.92 (bs, 1H), 7.54 - 7.52 (m, 1H), 7.33 – 7.30 (m, 3H), 7.24 – 7.14 (m, 6H), 7.07 – 6.98 (m, 2H), 6.66 – 6.65 (m, 1H), 6.20 (s, 1H), 3.71 – 3.62 (m, 2H), 3.11 – 3.03 (m, 1H), 2.90 – 2.84 (m, 1H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 149.66, 136.91, 136.60, 135.21, 129.68, 128.81, 127.96, 126.97, 126.14, 125.92, 124.11, 122.26, 119.78, 118.51, 118.02, 114.13, 111.36, 111.32, 111.17, 56.55, 42.21, 26.67.

HRMS (ESI) m/z**:** NA

1-(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)naphthalen-2-ol (3t)



Purification: by column chromatography (Pet.ether/EtOAc = 97/03)

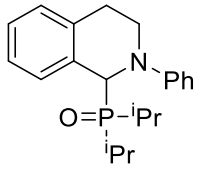
R_f (Pet. ether /EtOAc = 85/15)**:** 0.6

^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 11.09 (bs, 1H), 8.23 – 8.21 (m, 1H), 7.77 – 7.75 (m, 1H), 7.62 – 7.57 (m, 2H), 7.37 – 7.33 (m, 3H), 7.23 – 7.14 (m, 4H), 7.02 – 6.92 (m, 3H), 6.74 – 6.72 (m, 1H), 6.45 (s, 1H), 3.76 – 3.72 (m, 1H), 3.68 – 3.60 (m, 1H), 3.47 – 3.40 (m, 1H), 3.06 – 3.02 (m, 1H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 154.62, 149.86, 136.30, 133.62, 133.38, 129.62, 129.12, 129.03, 128.44, 128.37, 127.53, 127.21, 126.74, 126.54, 125.61, 123.13, 122.55, 121.03, 119.66, 118.37, 59.51, 55.45, 30.60.

HRMS (ESI) m/z**:** $[M+H]^+$ Calcd for $C_{25}H_{21}NOH$ 352.1701; Found: 352.1700

diisopropyl(2-phenyl-1,2,3,4-tetrahydroisoquinolin-1-yl)phosphine oxide (3u)



Purification: by column chromatography (Pet.ether/EtOAc = 65/35)

R_f (Pet. ether /EtOAc = 50/50)**:** 0.4

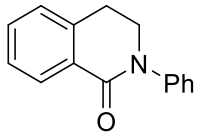
^{1}H NMR (400 MHz, , Chloroform – *d*): δ (ppm) 7.43 – 7.42 (m, 1H), 7.27 – 7.14 (m, 5H), 6.99 – 6.97 (m, 2H), 6.81 – 6.78 (m, 1H), 5.17 (d, J = 21.15 Hz, 1H), 4.69 – 4.61 (m, 2H), 4.10 – 4.03 (m, 1H), 3.71 – 3.65 (m, 1H), 3.05 – 2.99 (m, 2H), 1.33 (d, J = 6.65 Hz, 6H), 1.19 (d, J = 6.61 Hz, 3H), 0.97 (d, J = 6.62 Hz, 3H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 149.56, 149.50, 139.23, 136.42, 136.37, 135.13, 130.88, 128.96, 128.69, 128.67, 128.42, 128.37, 127.26, 127.23, 125.61, 125.58, 118.27, 115.04, 114.02, 72.29, 72.21, 70.93, 70.85, 58.73 (d, J = 161.38 Hz, 1C), 43.47, 26.55, 24.55, 24.52, 24.10, 24.07, 23.72, 23.66, 23.29, 23.24.

^{31}P NMR (162 MHz, Chloroform – *d*): δ (ppm) 20.15.

HRMS (ESI) m/z**: NA**

2-phenyl-3,4-dihydroisoquinolin-1(2H)-one (4a)



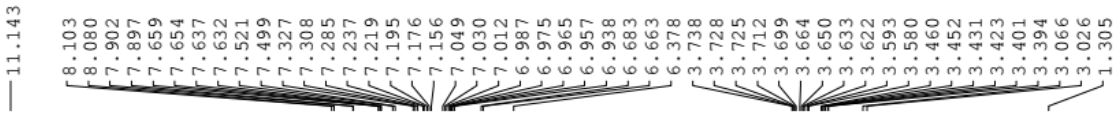
Purification: by column chromatography (Pet.ether/EtOAc = 90/10)

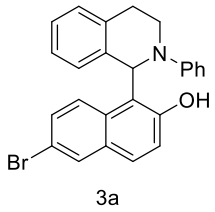
R_f (Pet. ether /EtOAc = 80/20)**:** 0.5

^{1}H NMR (400 MHz, Chloroform – *d*): δ (ppm) 8.19 – 8.17 (m, 1H), 7.51 – 7.38 (m, 6H), 7.29 – 7.26 (m, 2H), 4.02 (t, J = 6.45 Hz, 2H), 3.17 (t, J = 6.47 Hz, 2H).

^{13}C NMR (100 MHz, Chloroform – *d*): δ (ppm) 164.22, 143.13, 138.32, 132.05, 129.74, 128.93, 128.77, 127.21, 126.96, 126.27, 125.34, 49.44, 28.65.

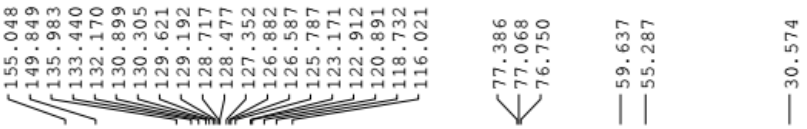
11. NMR and HRMS copies

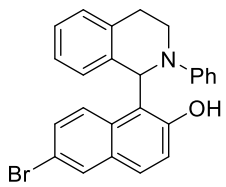




3a

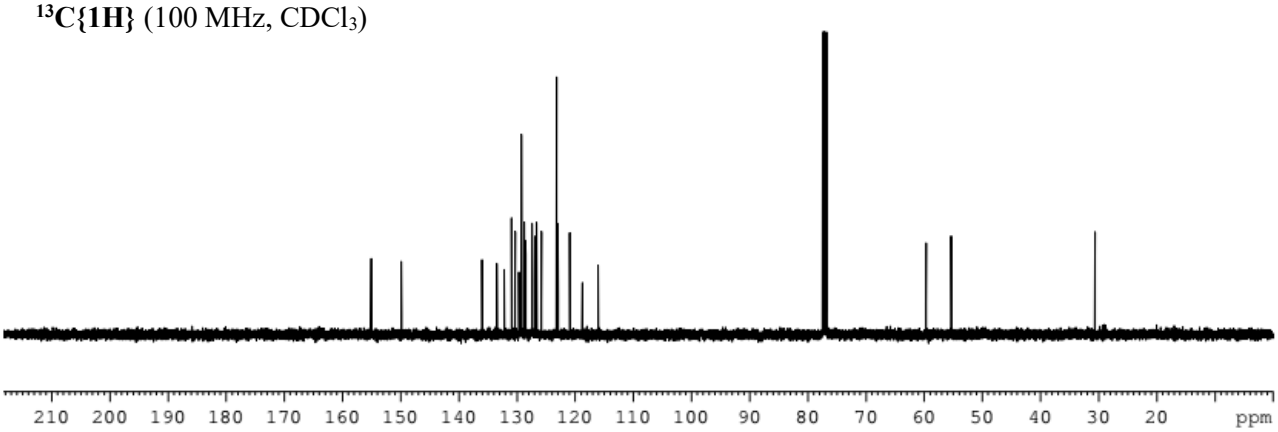
^{1}H (400 MHz, $CDCl_3$)

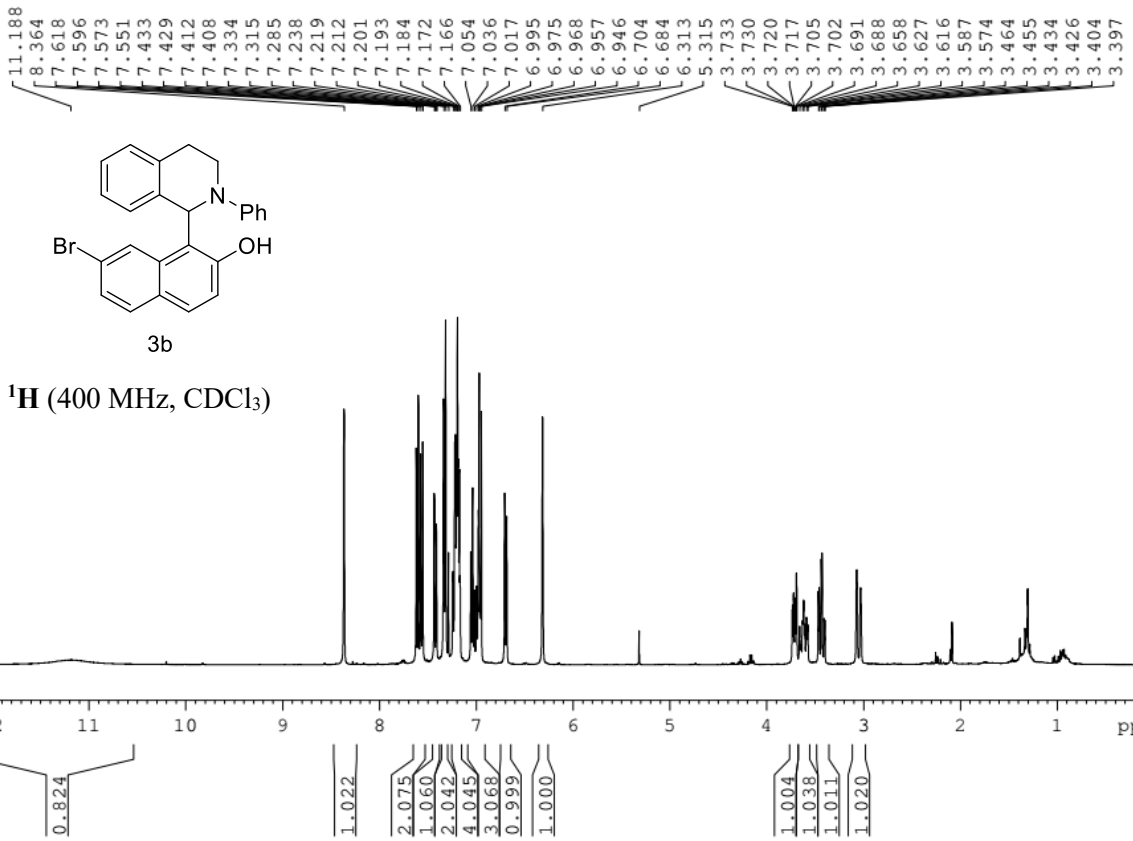




3a

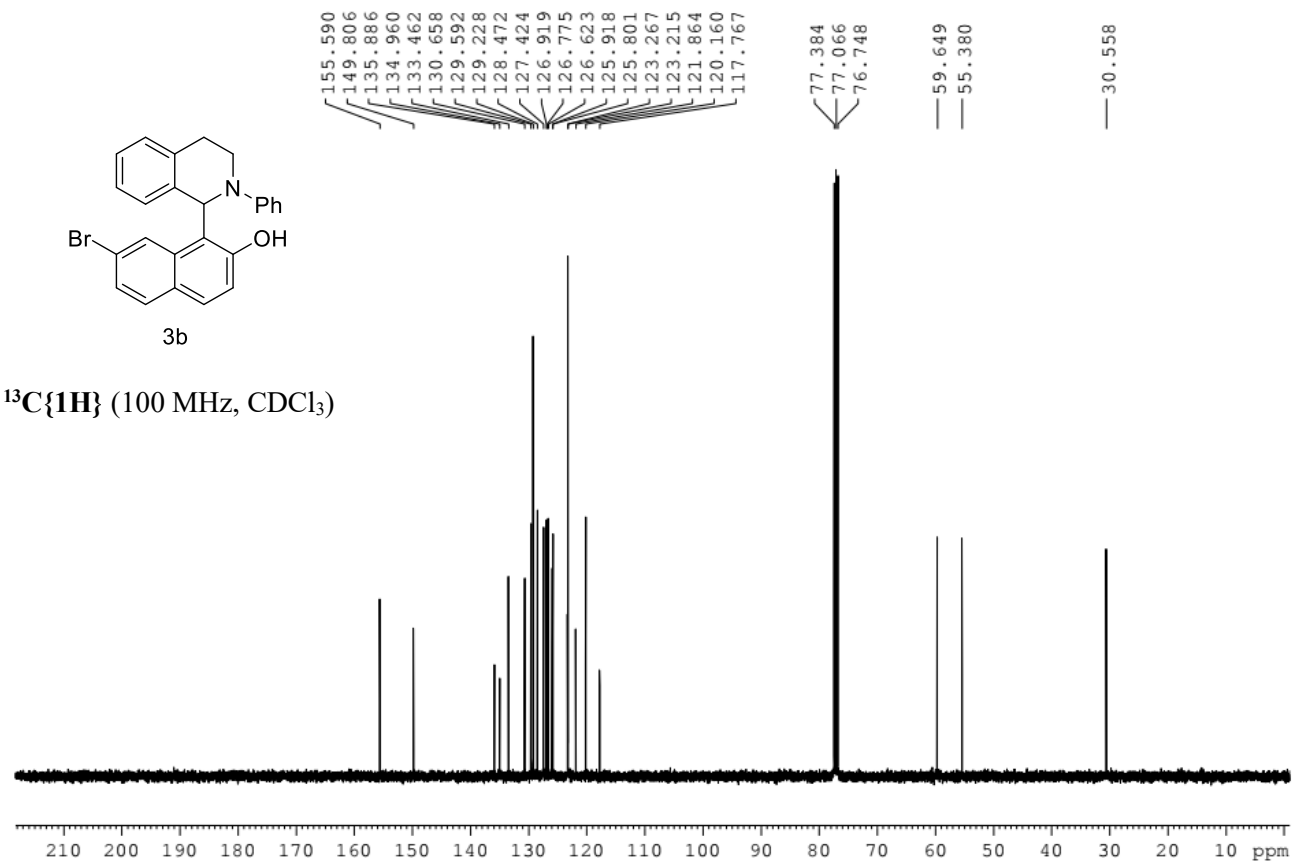
^{13}C{1H} (100 MHz, $CDCl_3$)





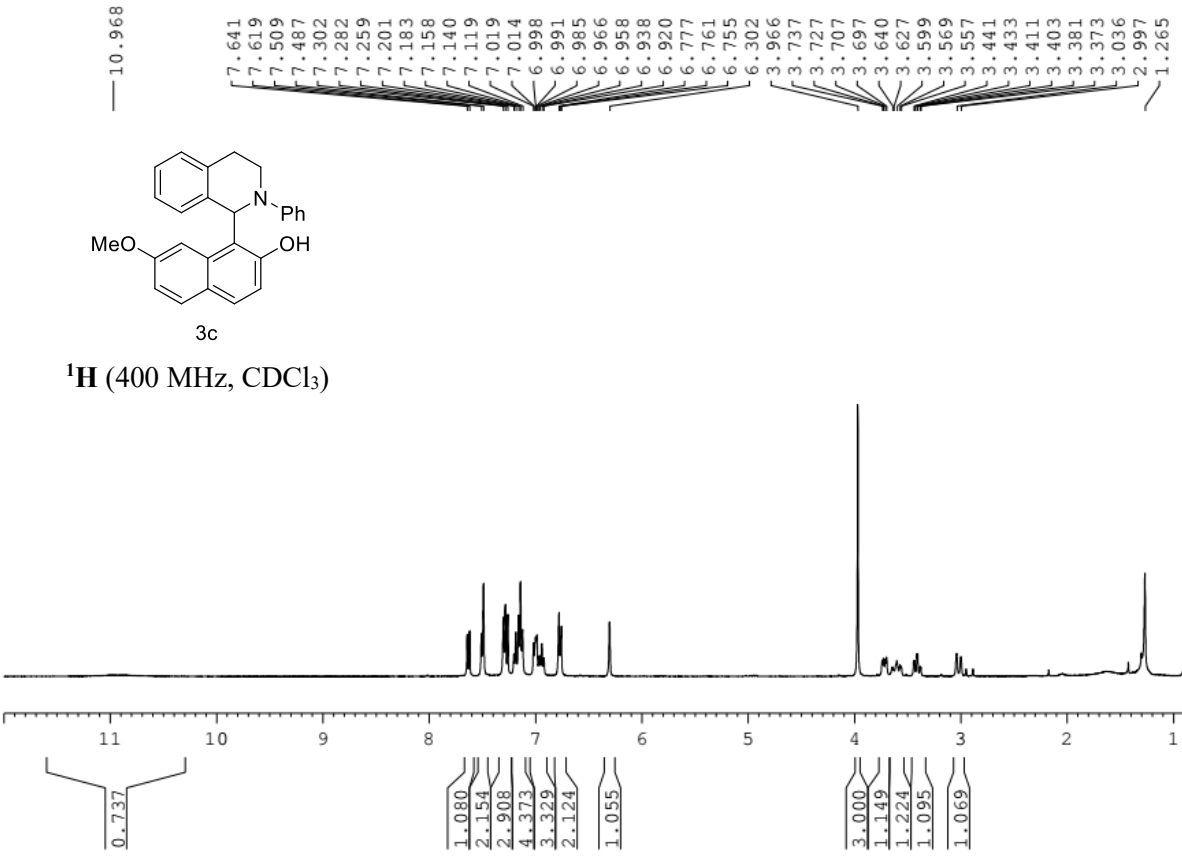
3b

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

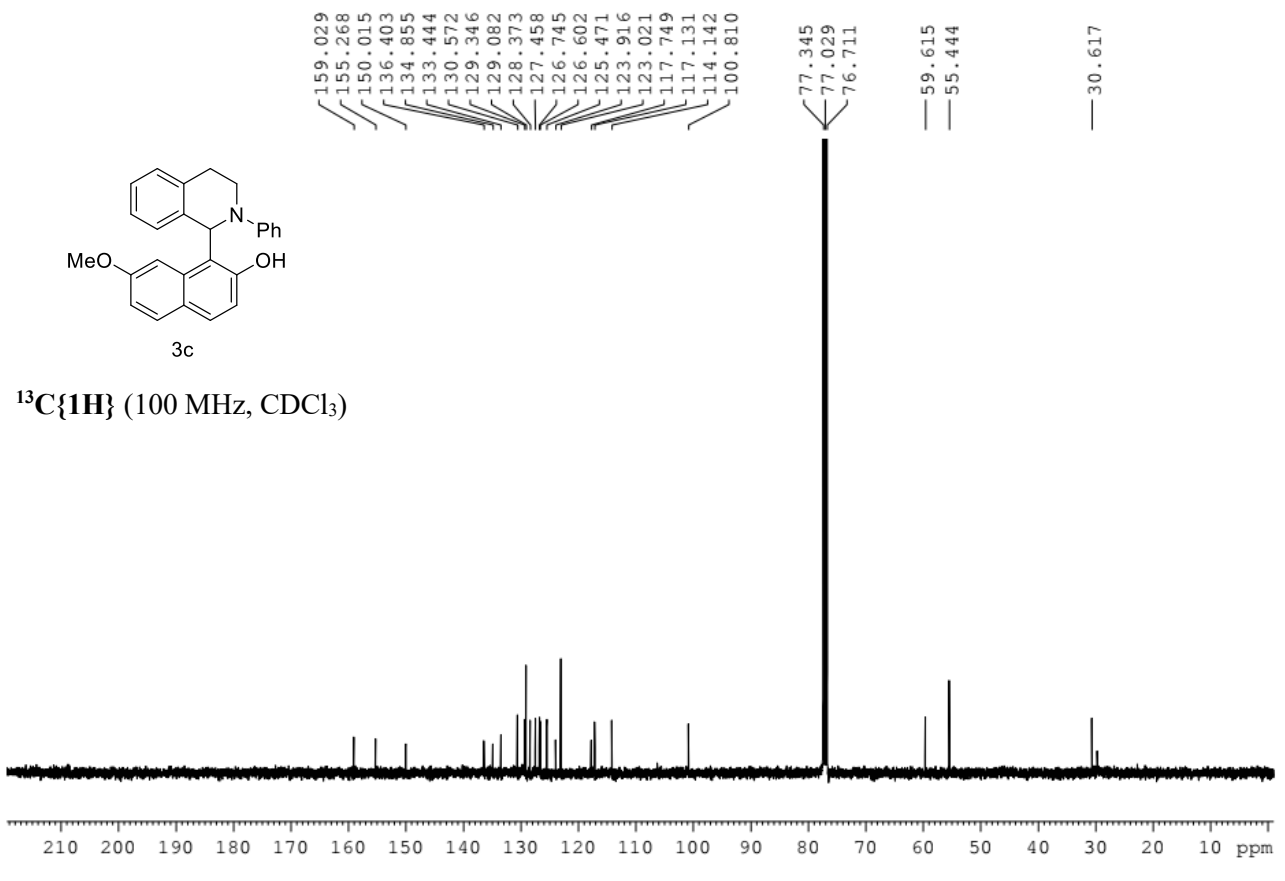


3b

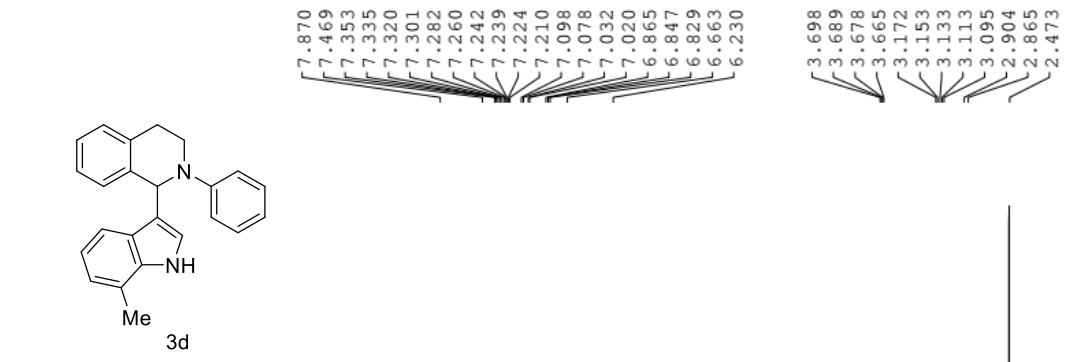
^{13}C{1H} (100 MHz, $CDCl_3$)



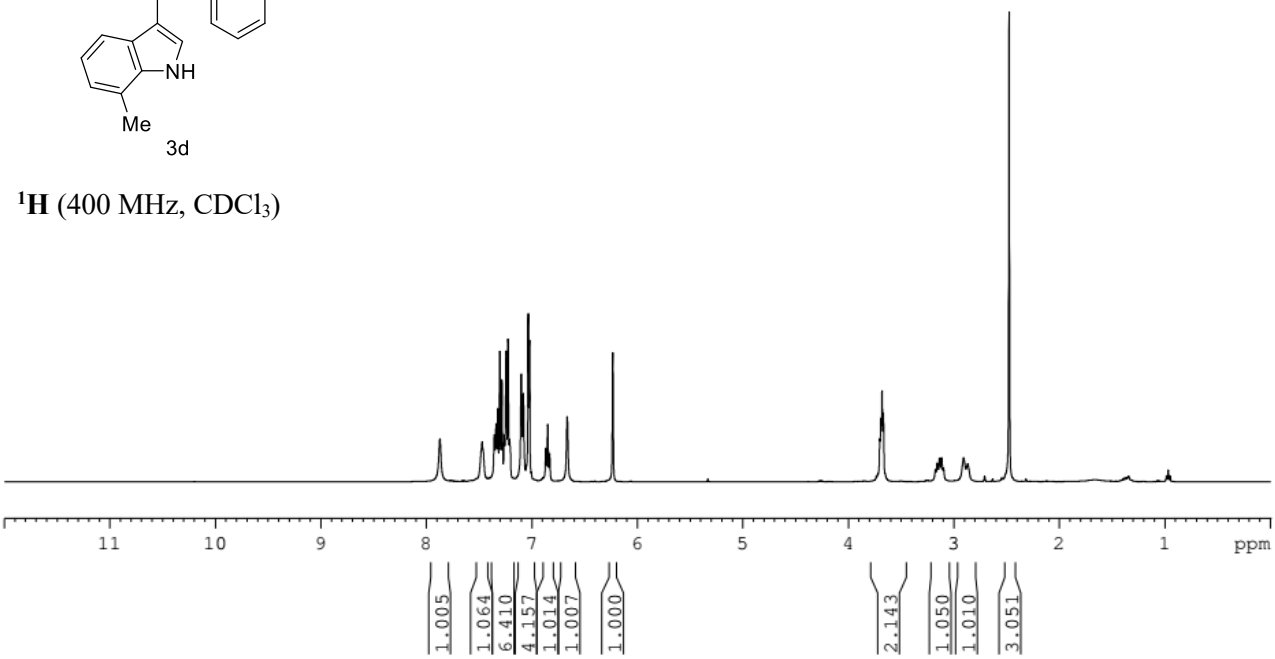
^{1}H (400 MHz, $CDCl_3$)

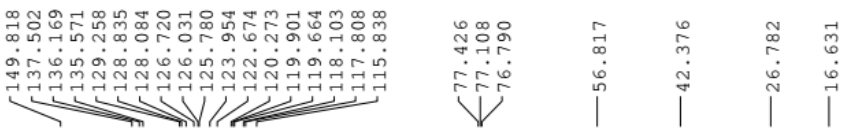


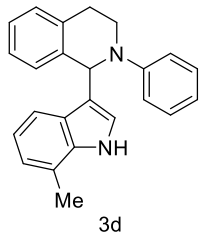
^{13}C{1H} (100 MHz, $CDCl_3$)



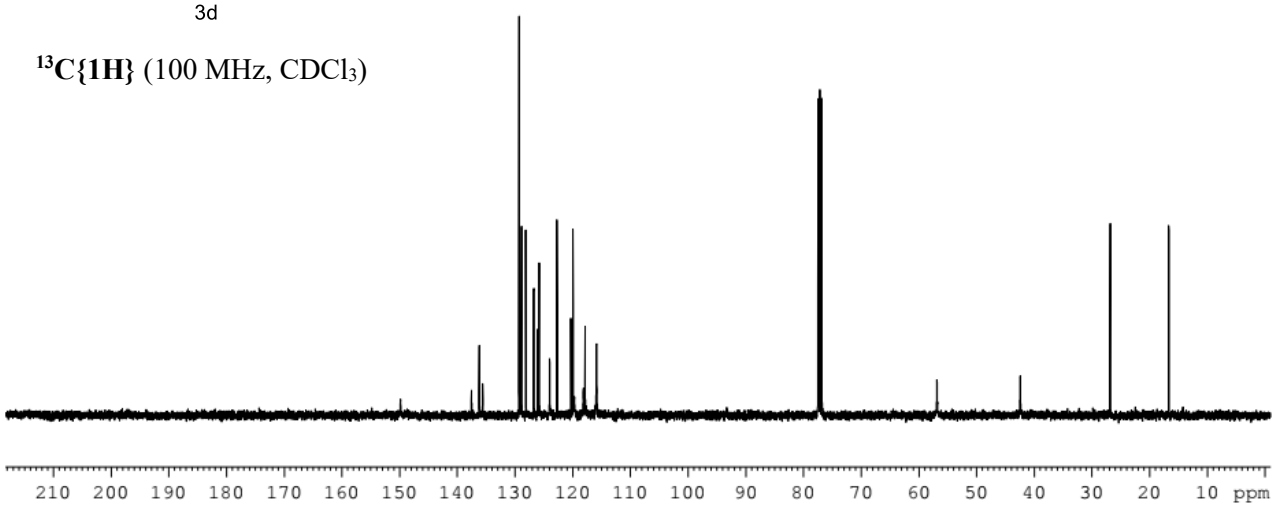
^{1}H (400 MHz, $CDCl_3$)

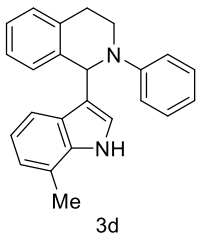






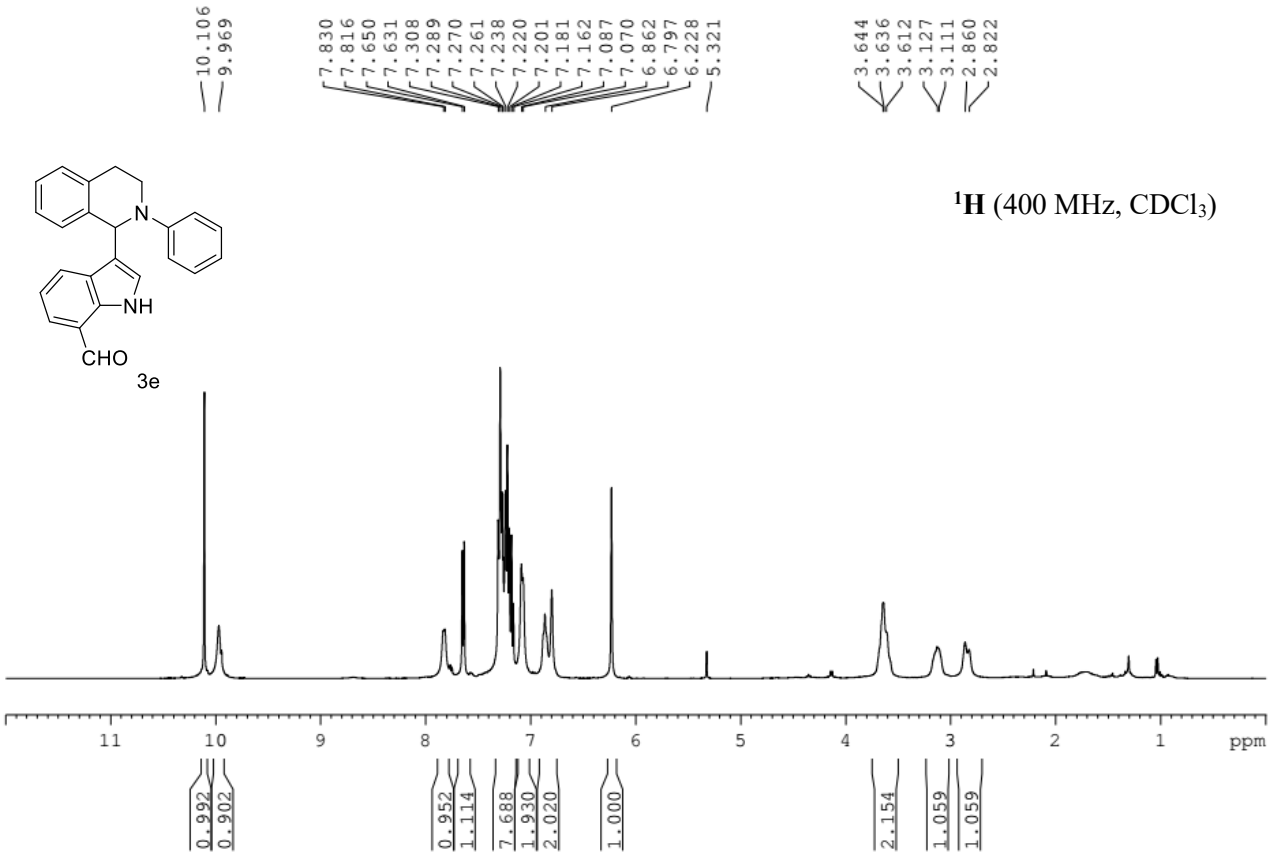
^{13}C{1H} (100 MHz, $CDCl_3$)



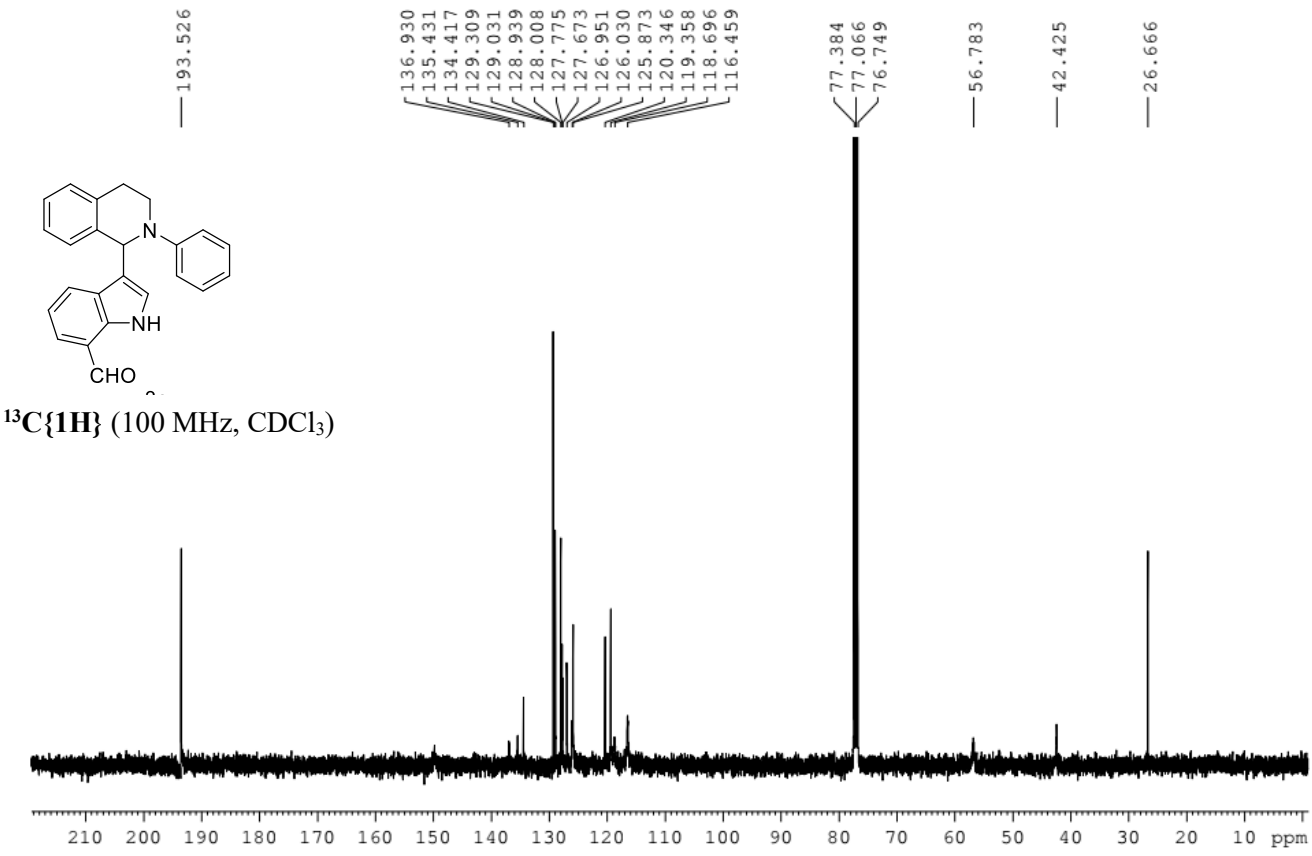


3d

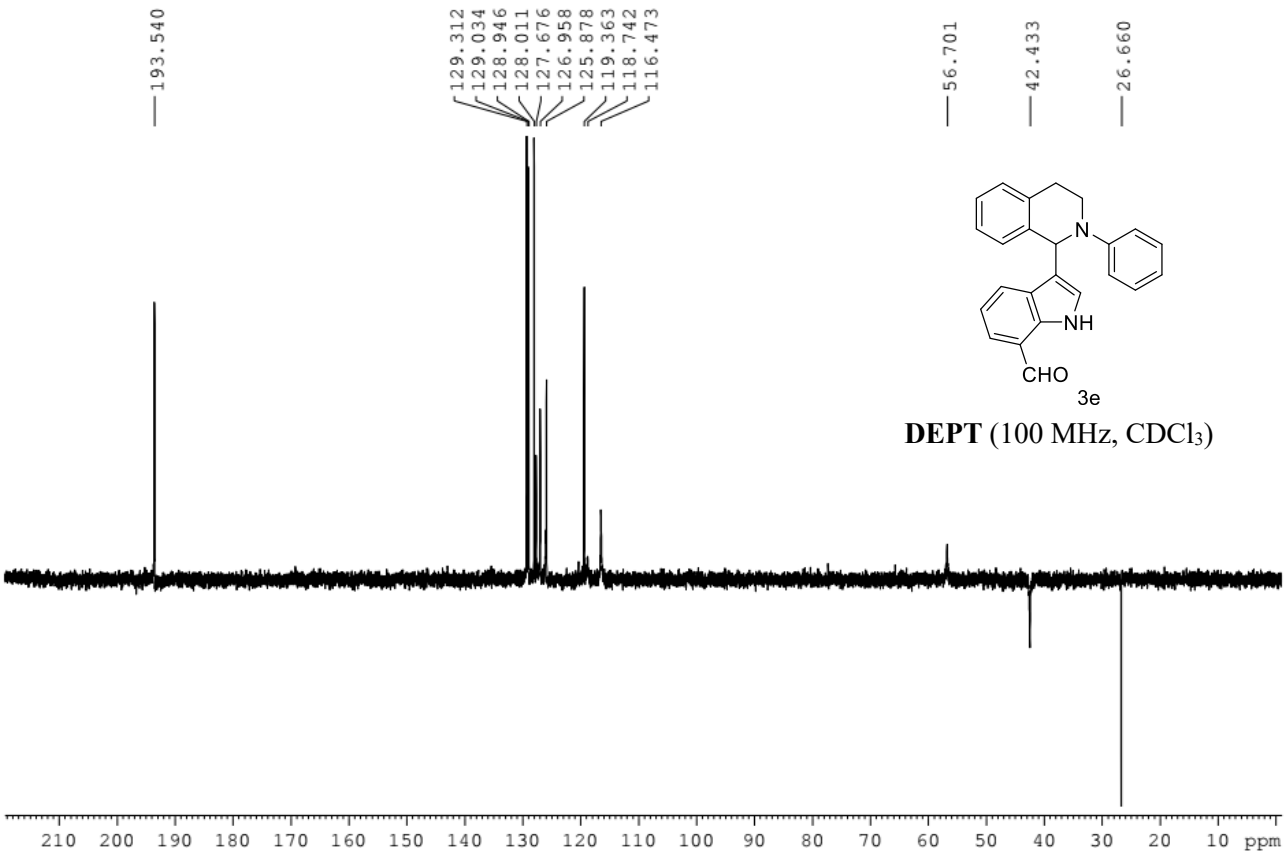
DEPT (100 MHz, $CDCl_3$)



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

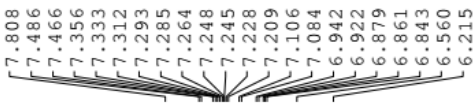


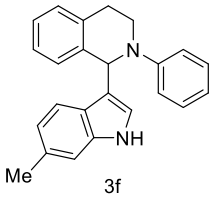
^{13}C{1H} (100 MHz, $CDCl_3$)



3e

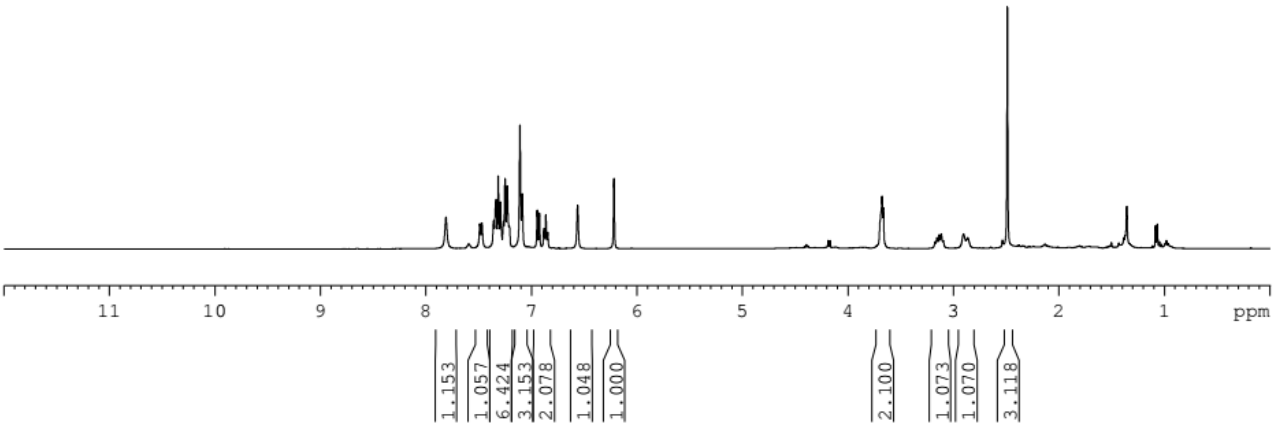
DEPT (100 MHz, $CDCl_3$)

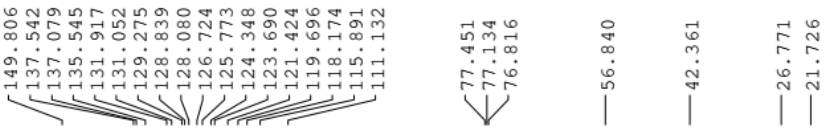


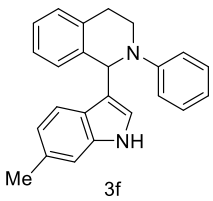


3f

[1]H (400 MHz, $CDCl_3$)

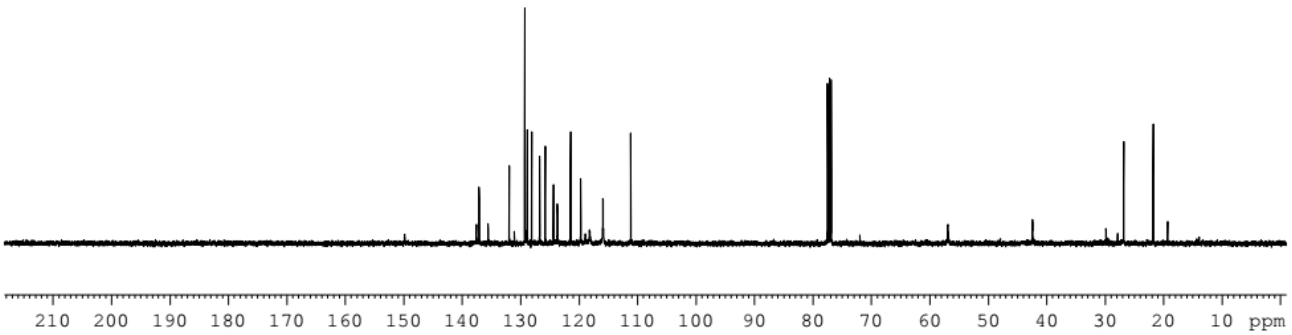


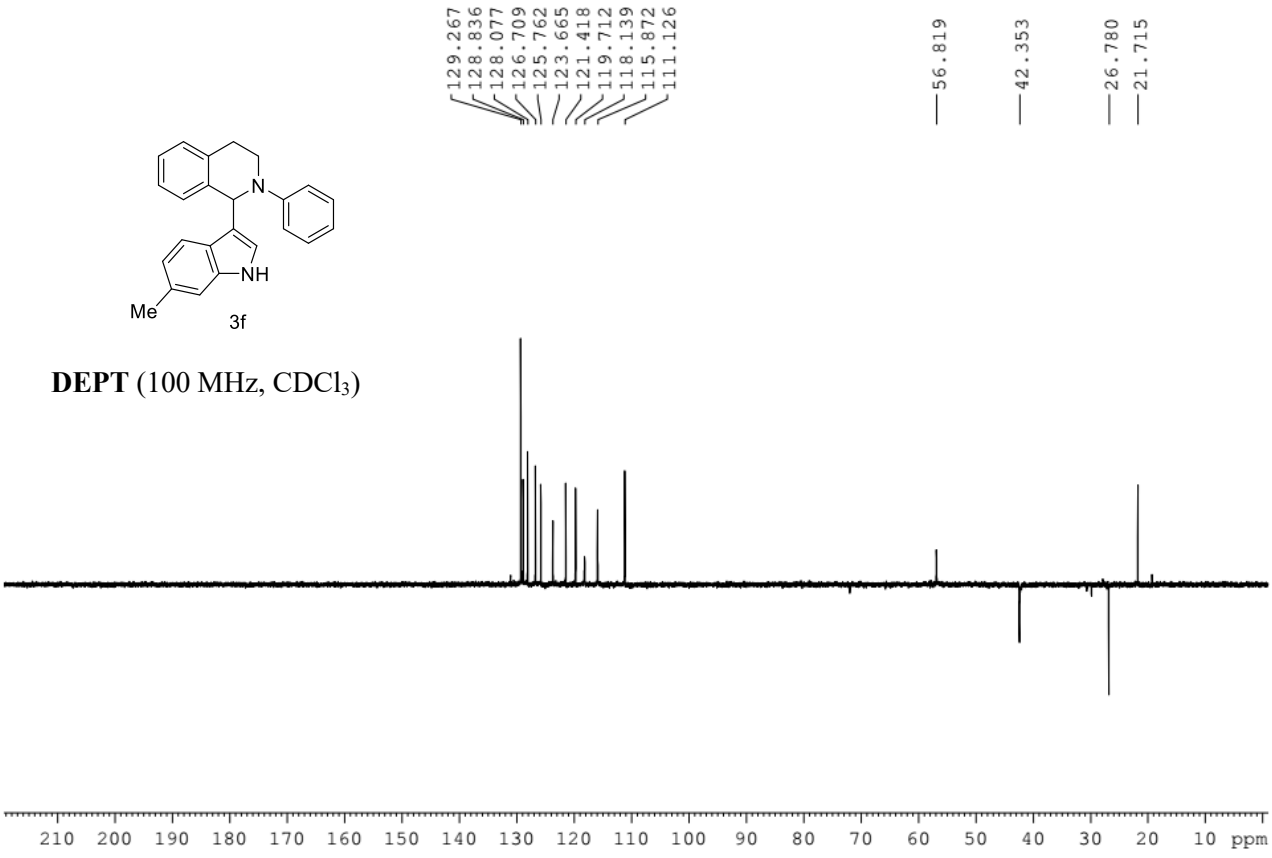




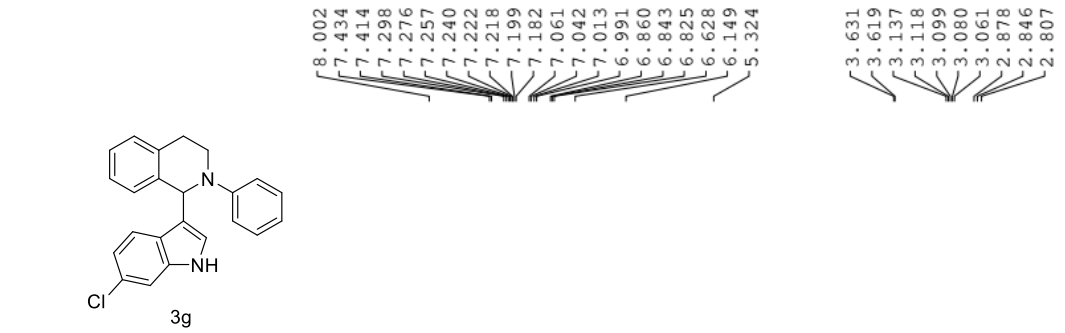
3f

[13]C{1H} (100 MHz, $CDCl_3$)



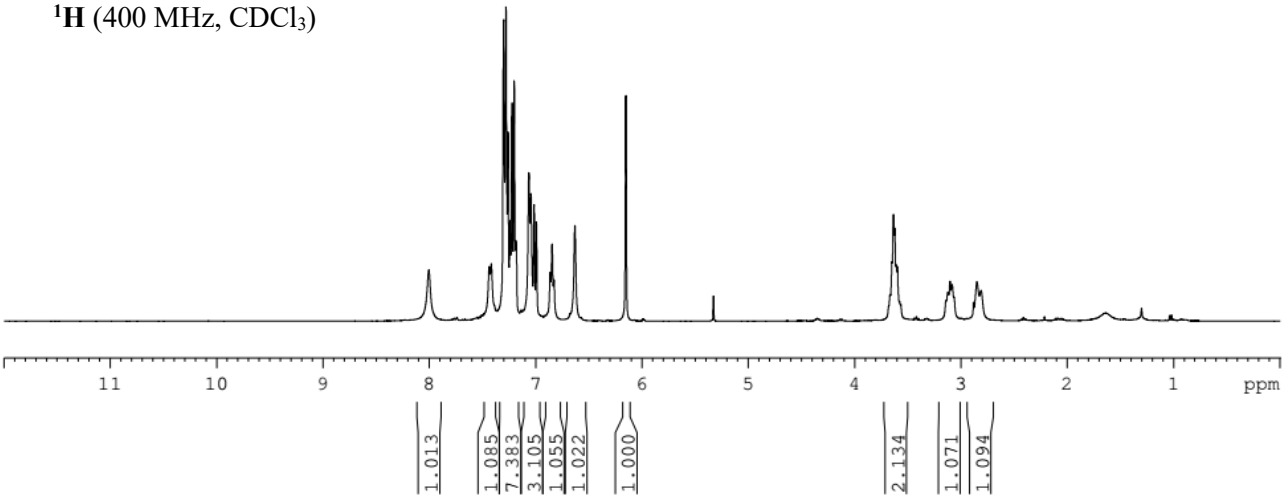


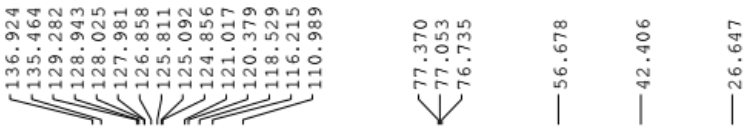
DEPT (100 MHz, $CDCl_3$)

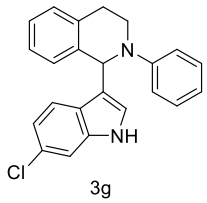


3g

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

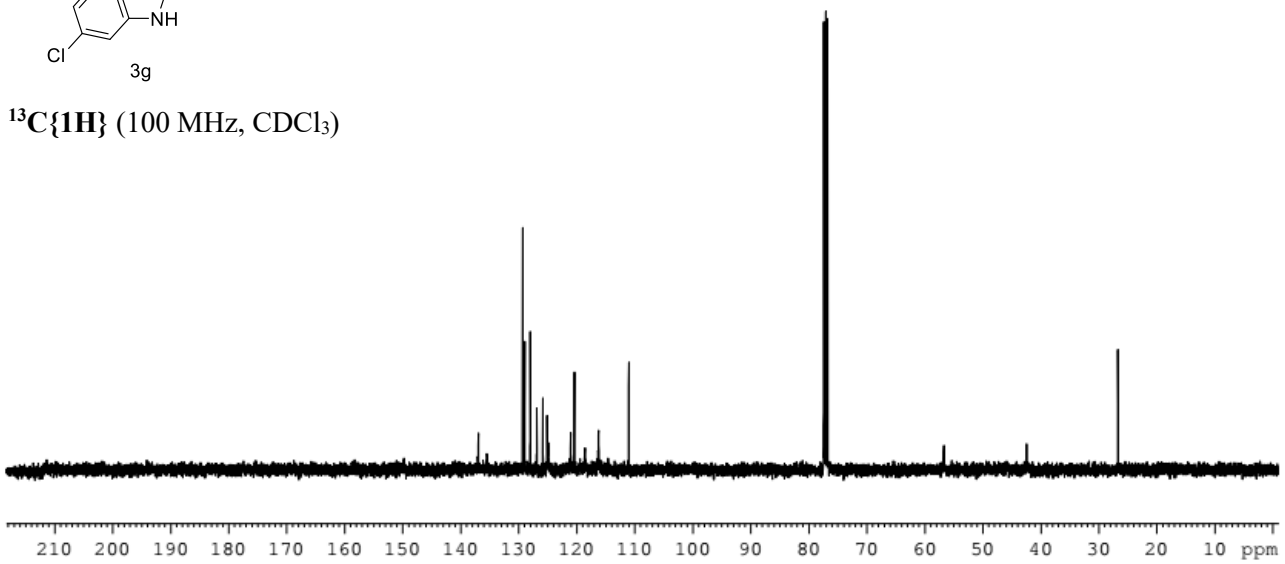


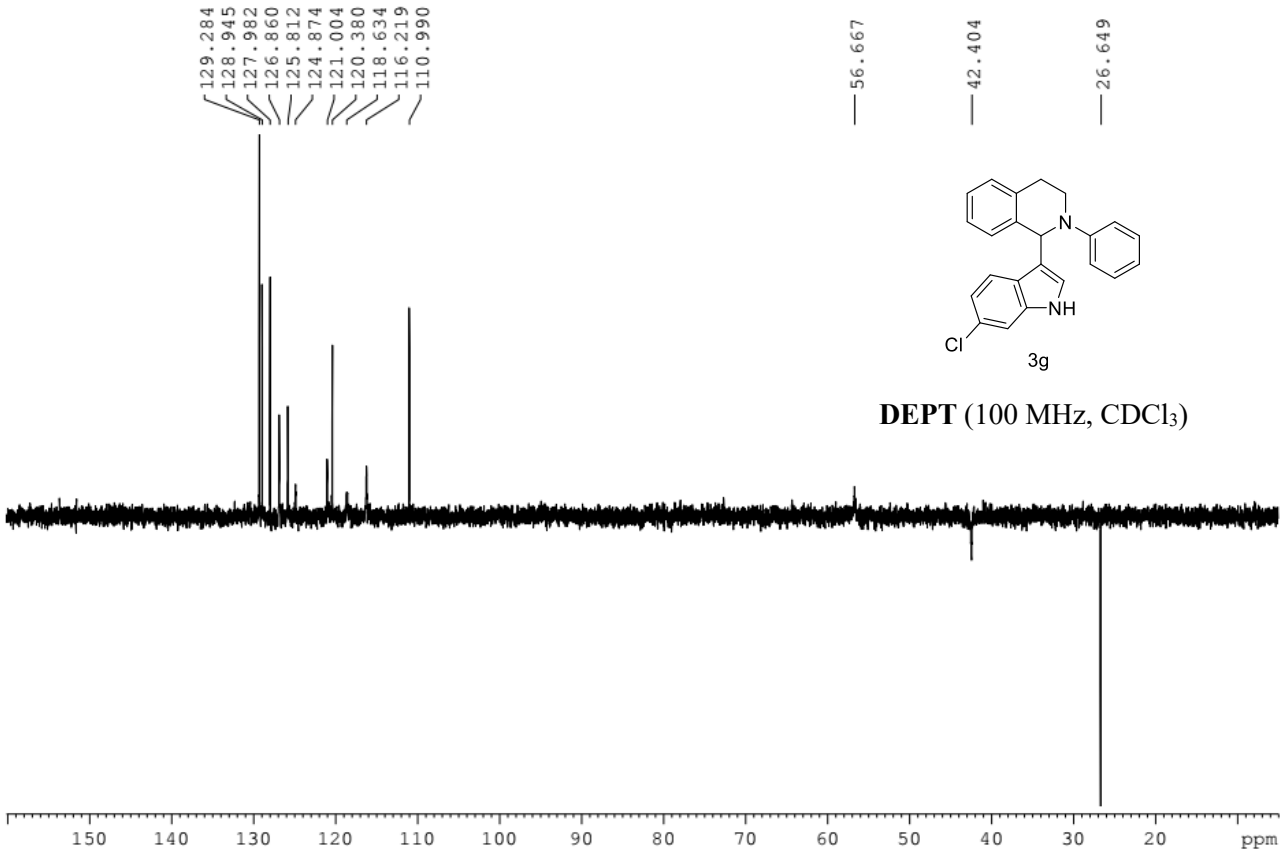




3g

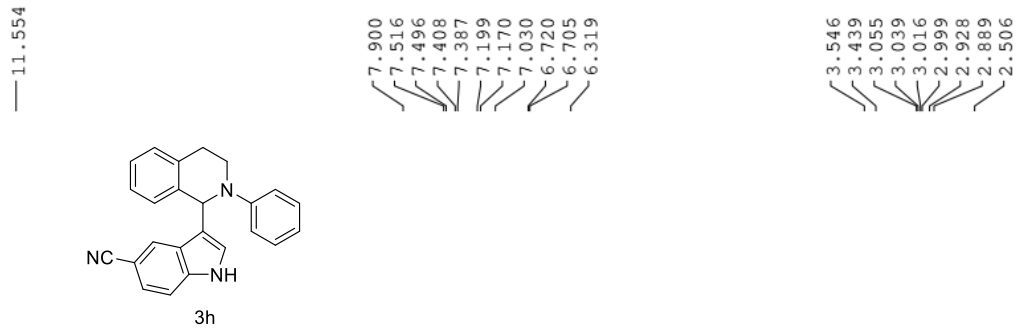
^{13}C{1H} (100 MHz, $CDCl_3$)



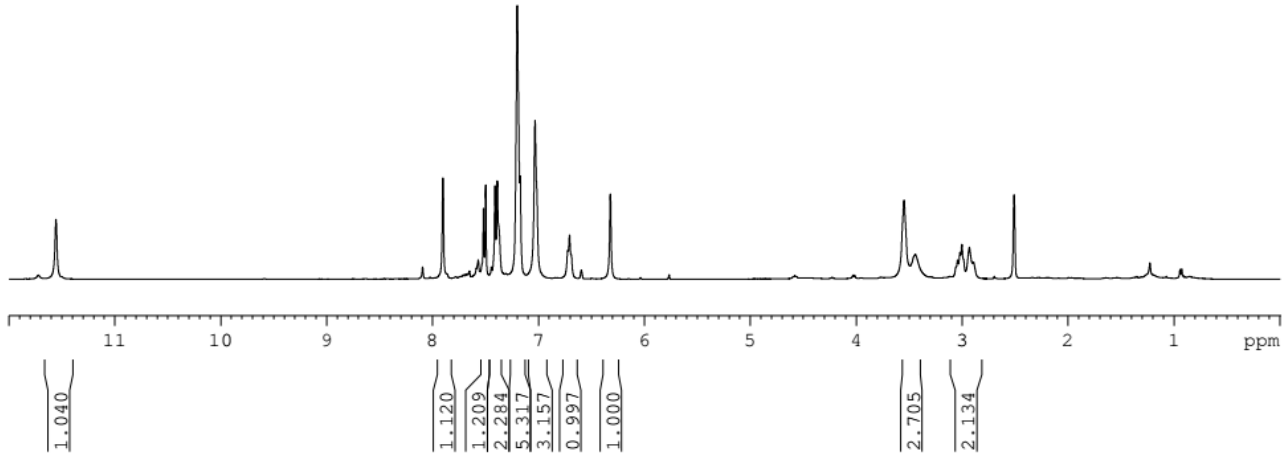


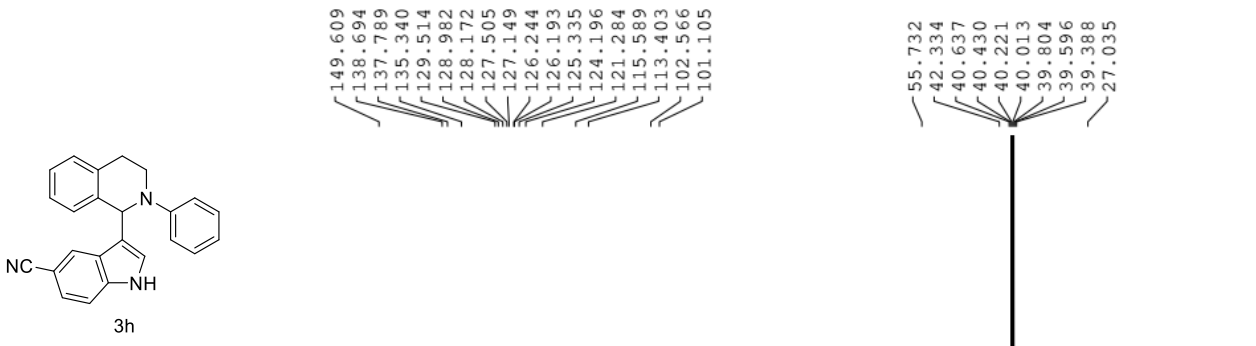
3g

DEPT (100 MHz, $CDCl_3$)

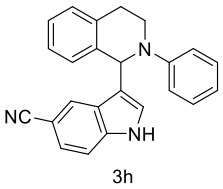


[1]H (400 MHz, DMSO – d6)



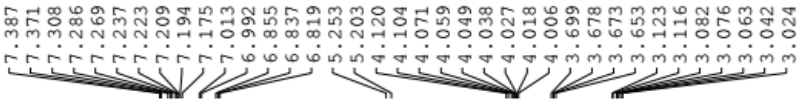


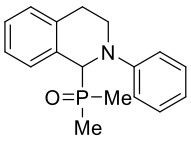
[13]C{1H} (100 MHz, DMSO – d6)



3h

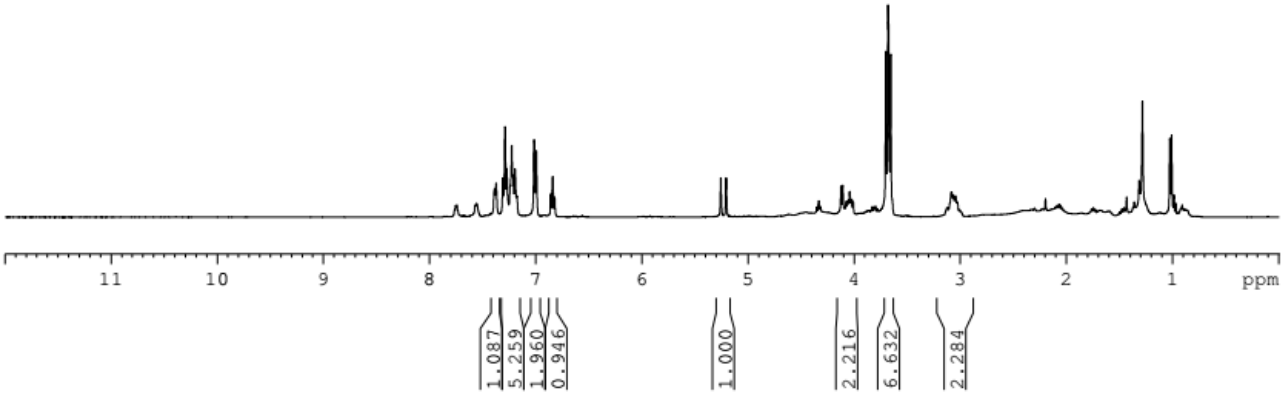
DEPT (100 MHz, DMSO – d6)

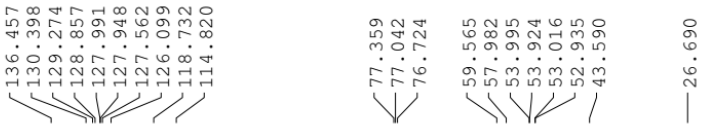


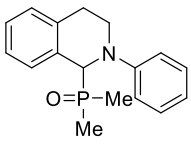


3i

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

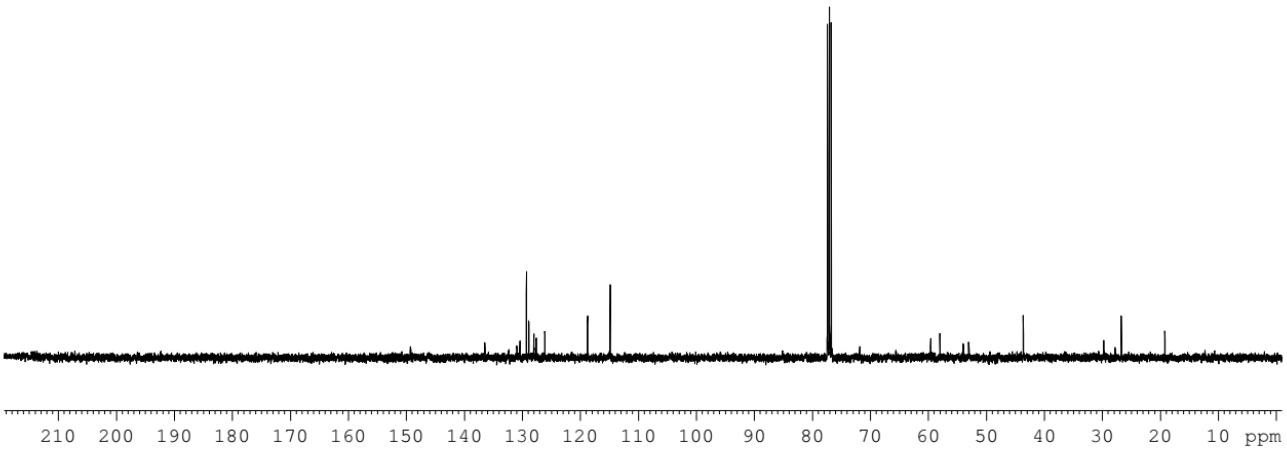


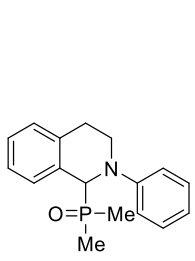




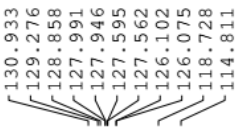
3i

^{13}C{1H} (100 MHz, $CDCl_3$)

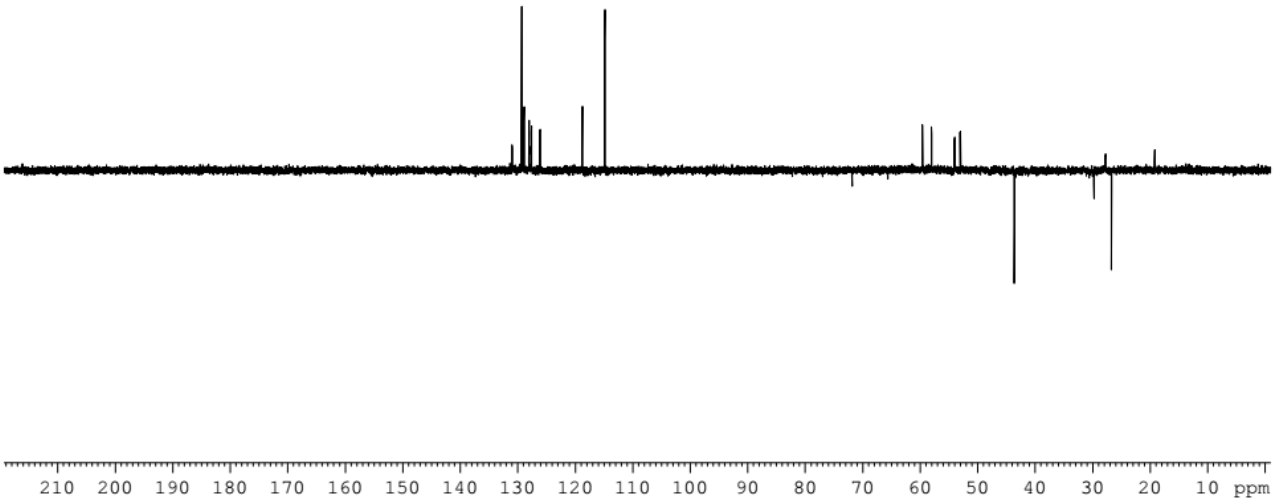


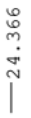


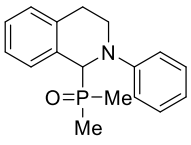
3i



DEPT (100 MHz, $CDCl_3$)

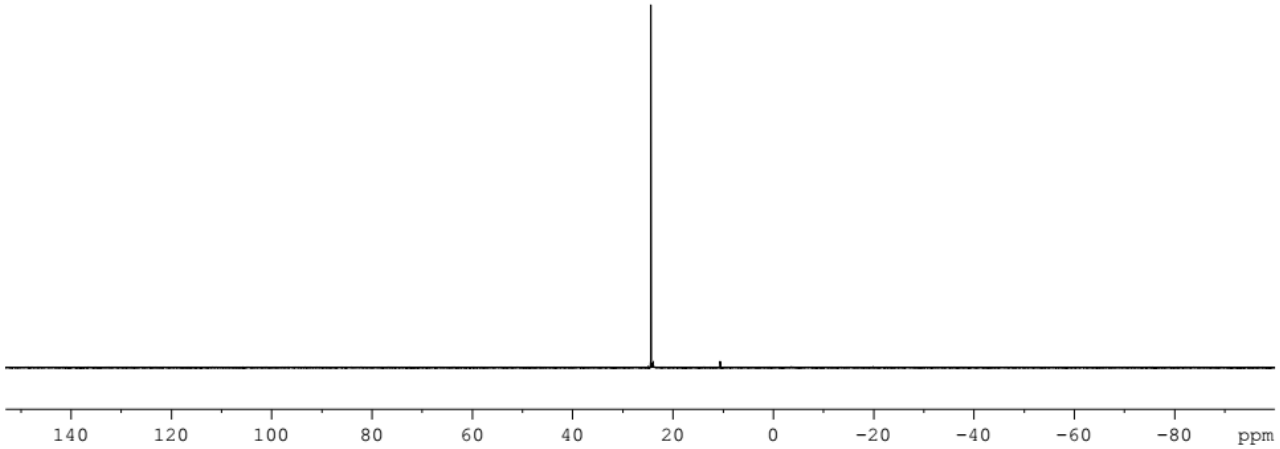


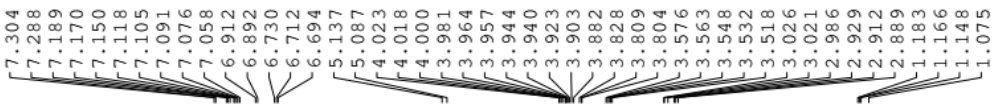


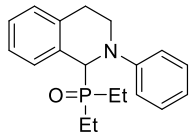


3i

^{31}P{1H} (162 MHz, $CDCl_3$)

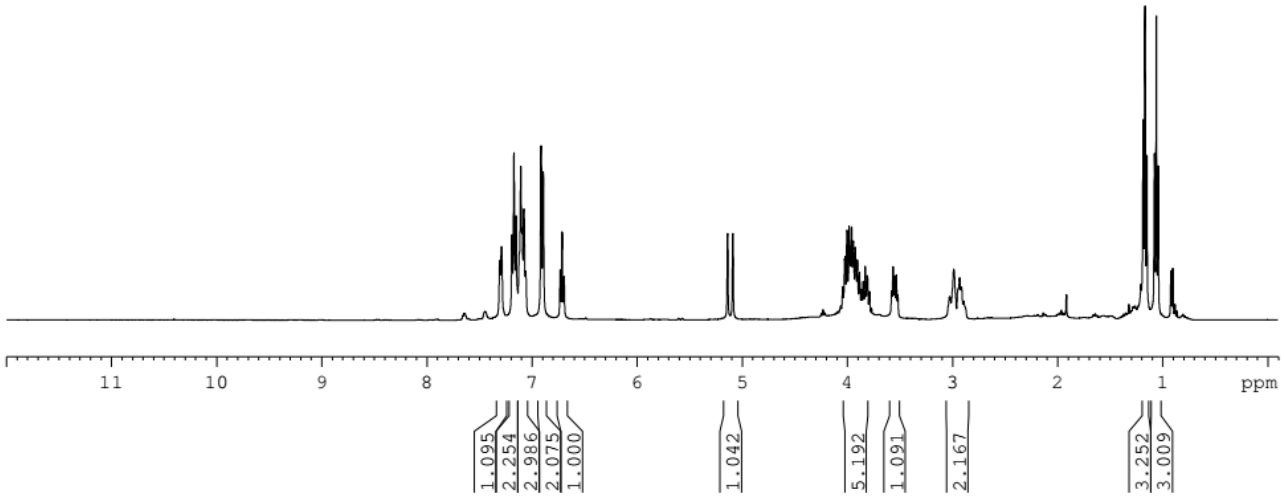


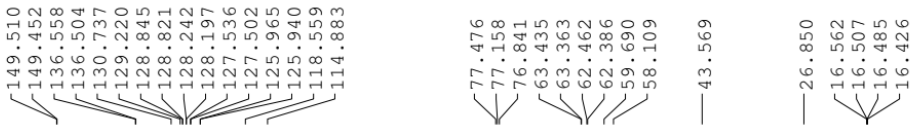


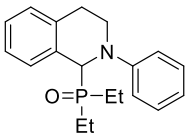


3j

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

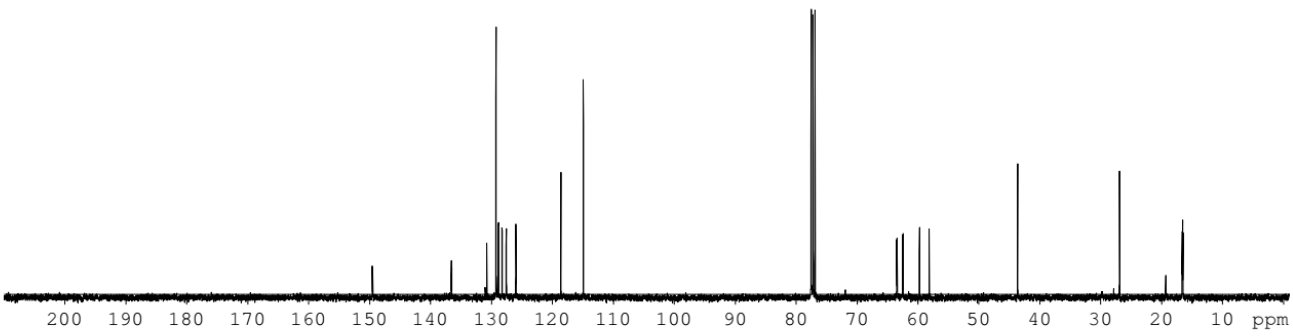


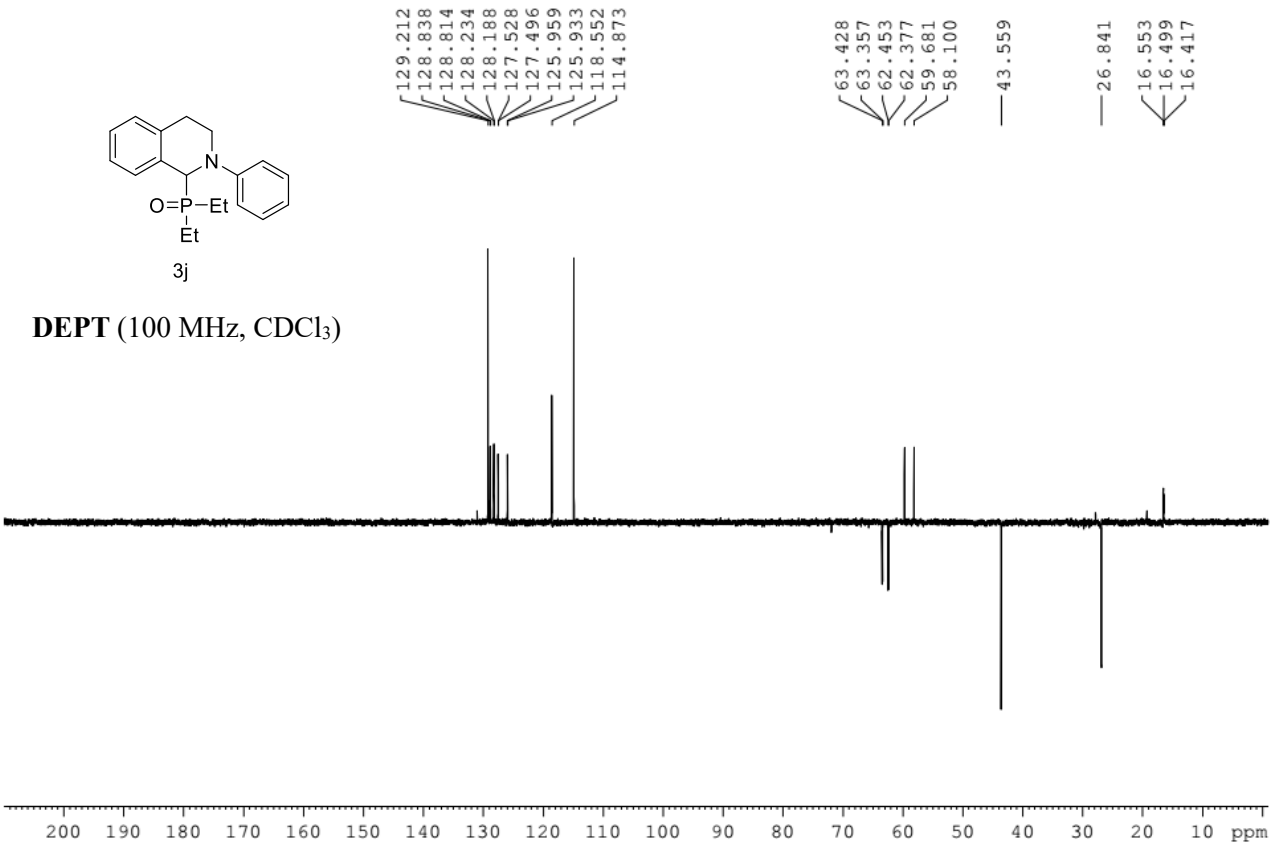




3j

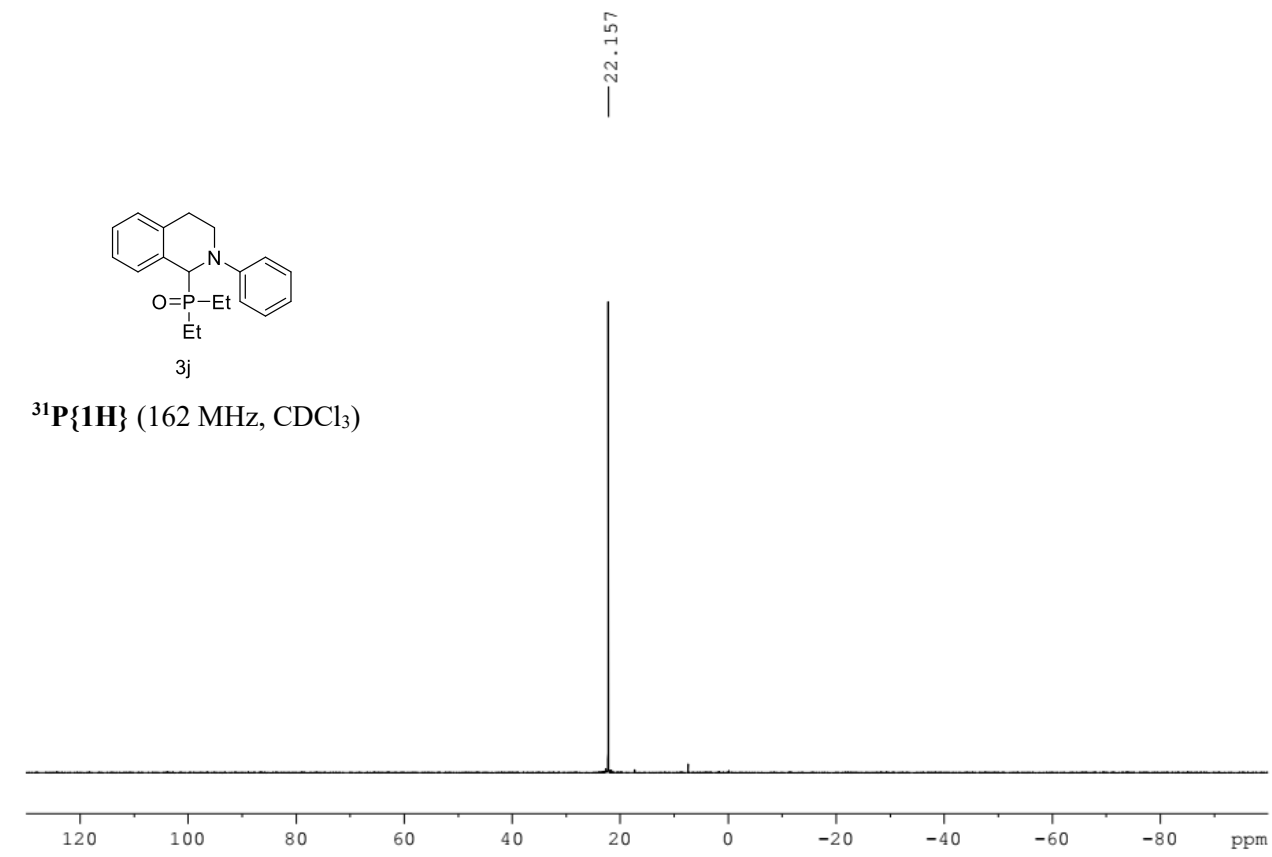
^{13}C{1H} (100 MHz, $CDCl_3$)





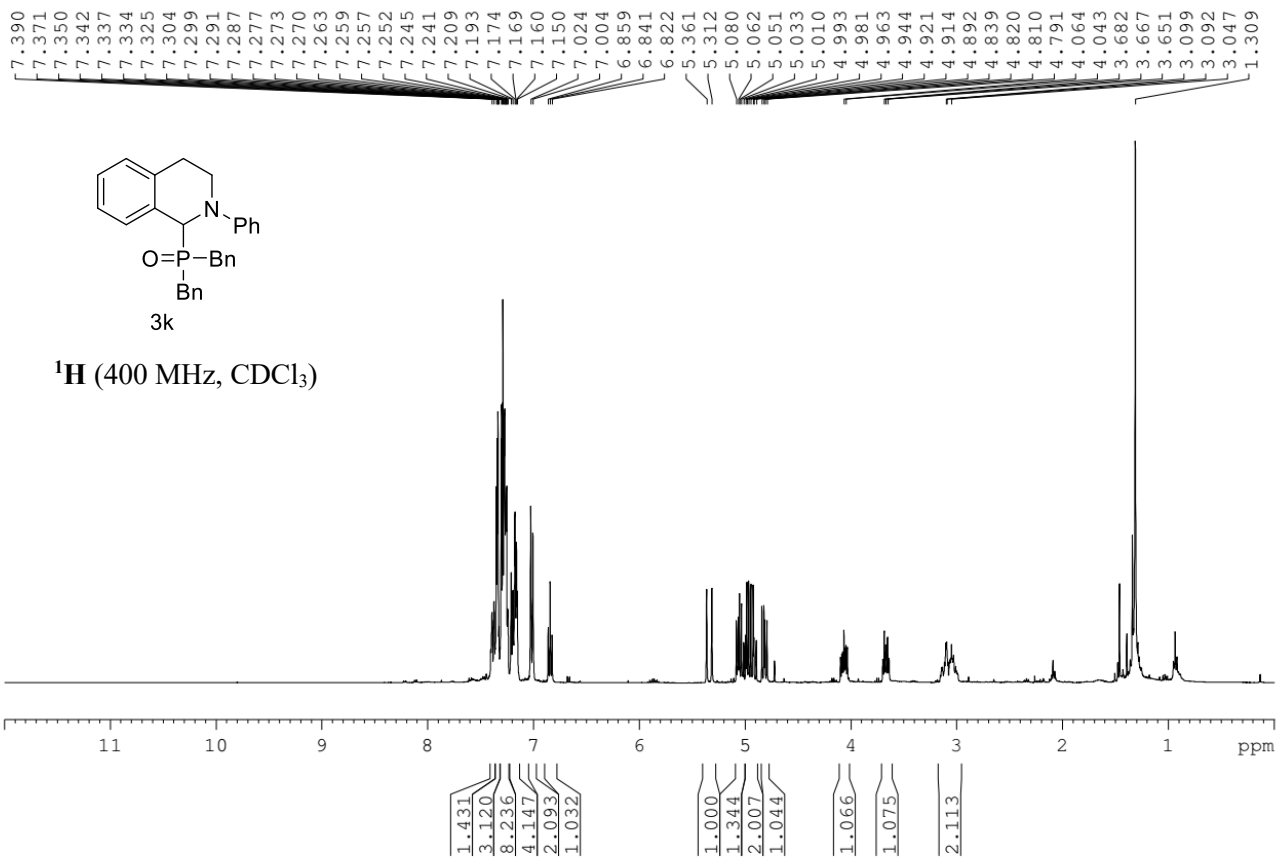
3j

DEPT (100 MHz, $CDCl_3$)

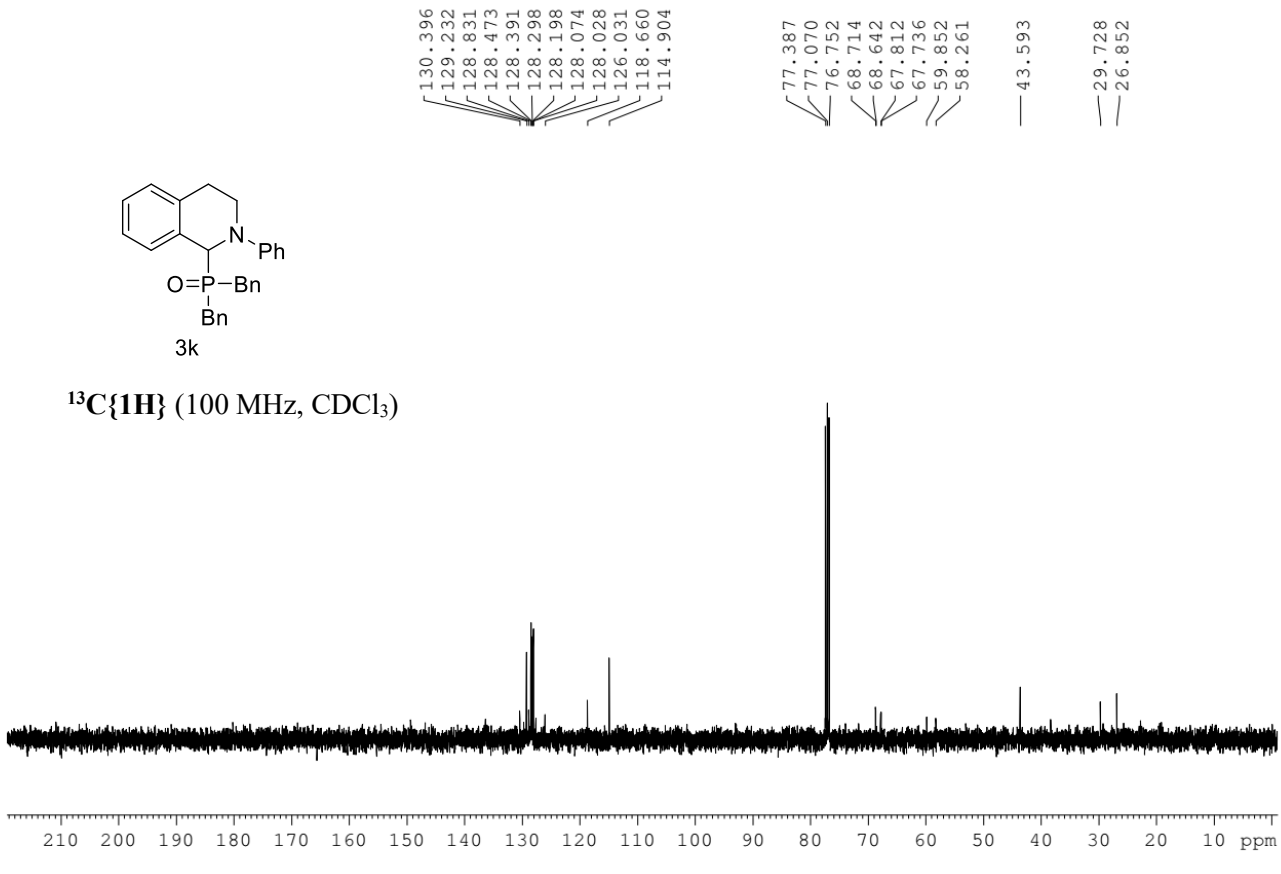


3j

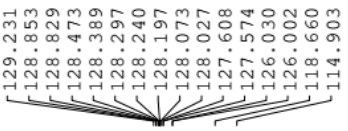
^{31}P{1H} (162 MHz, $CDCl_3$)

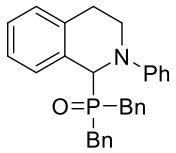


^{1}H (400 MHz, $CDCl_3$)



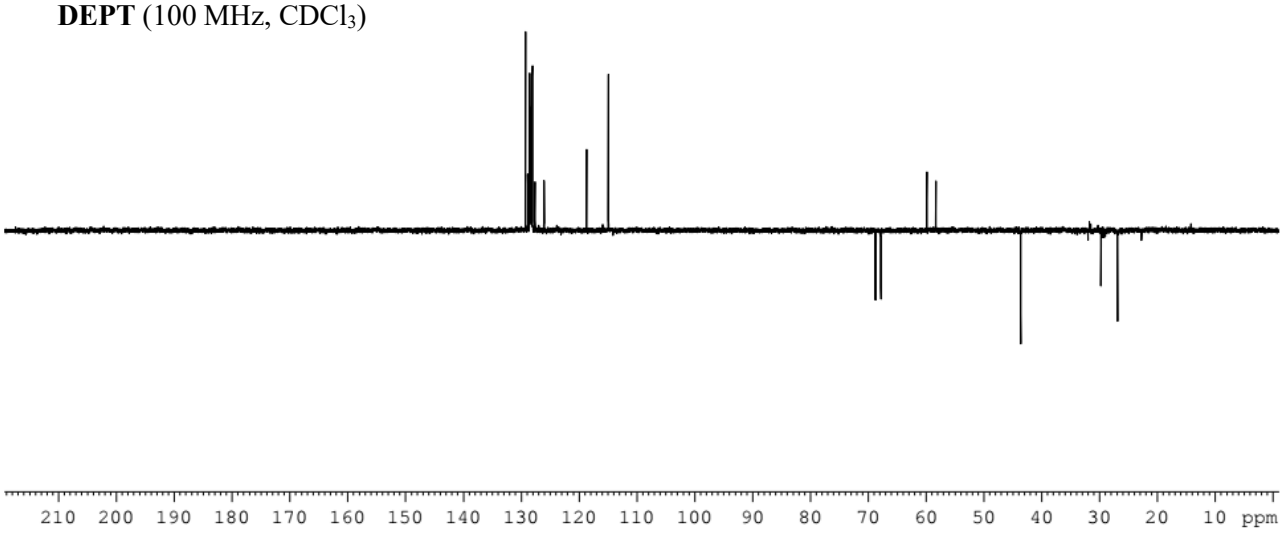
^{13}C{1H} (100 MHz, $CDCl_3$)

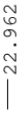


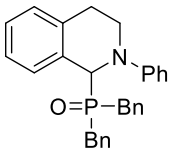


3k

DEPT (100 MHz, $CDCl_3$)

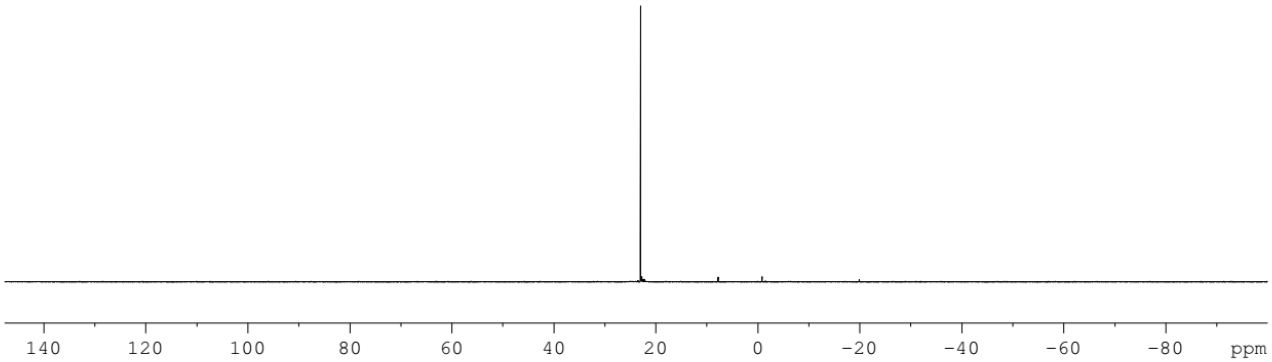


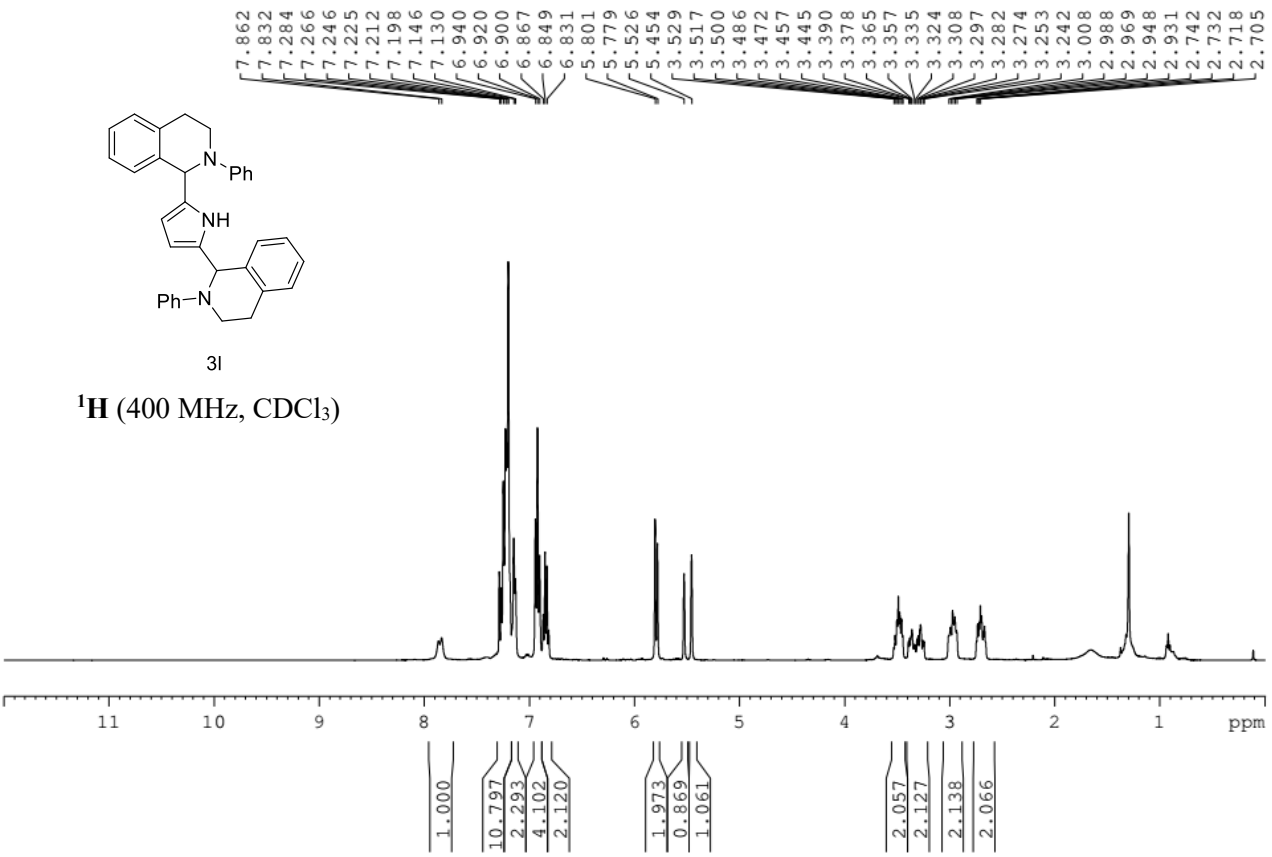




3k

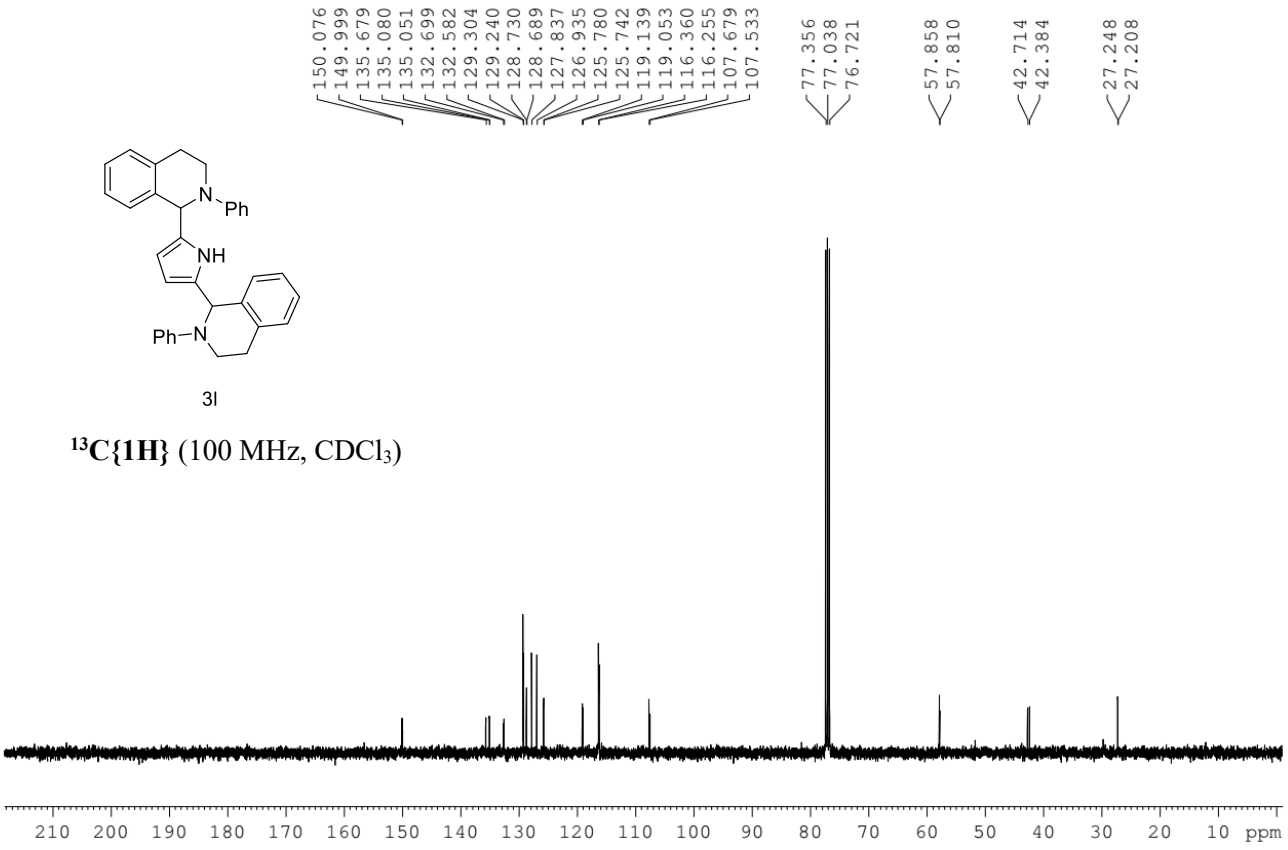
^{31}P{1H} (162 MHz, $CDCl_3$)





3l

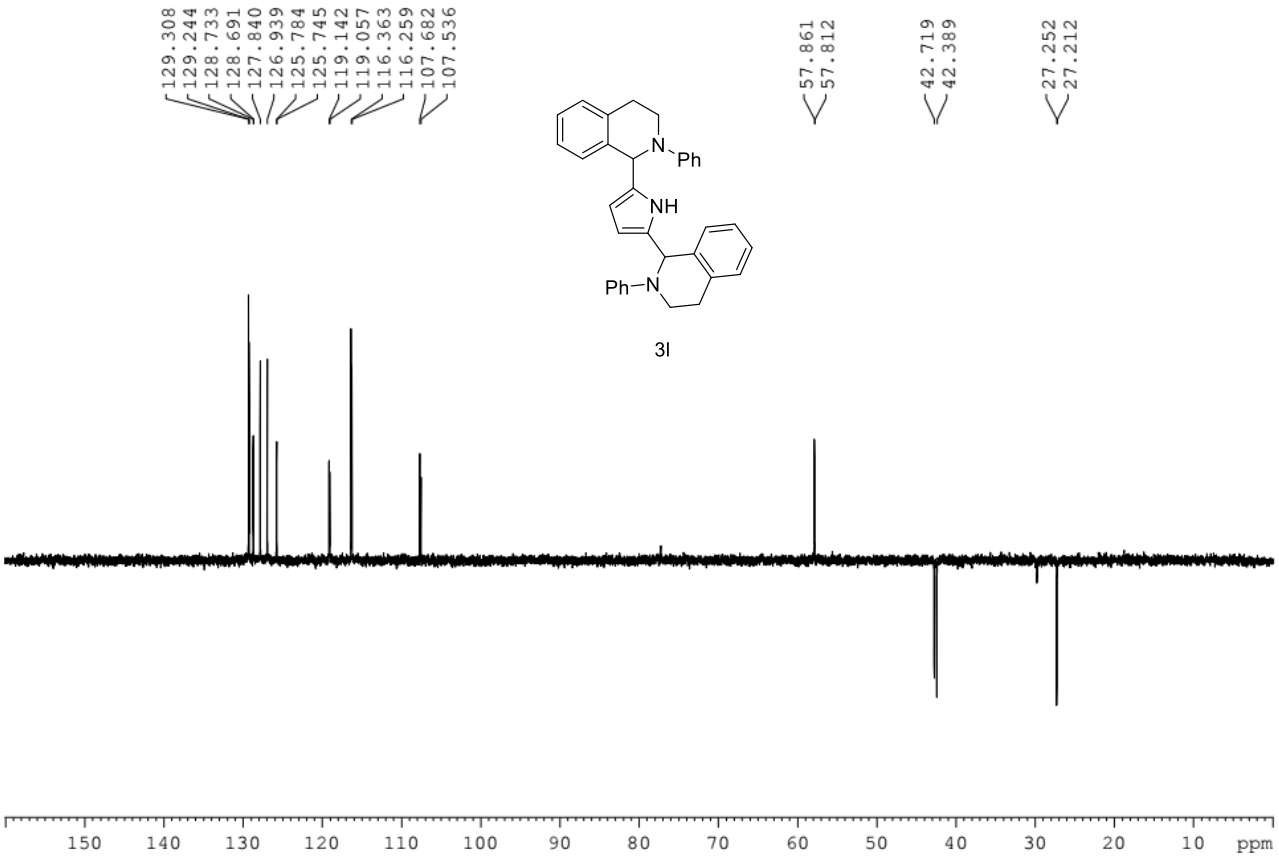
^{1}H (400 MHz, $CDCl_3$)

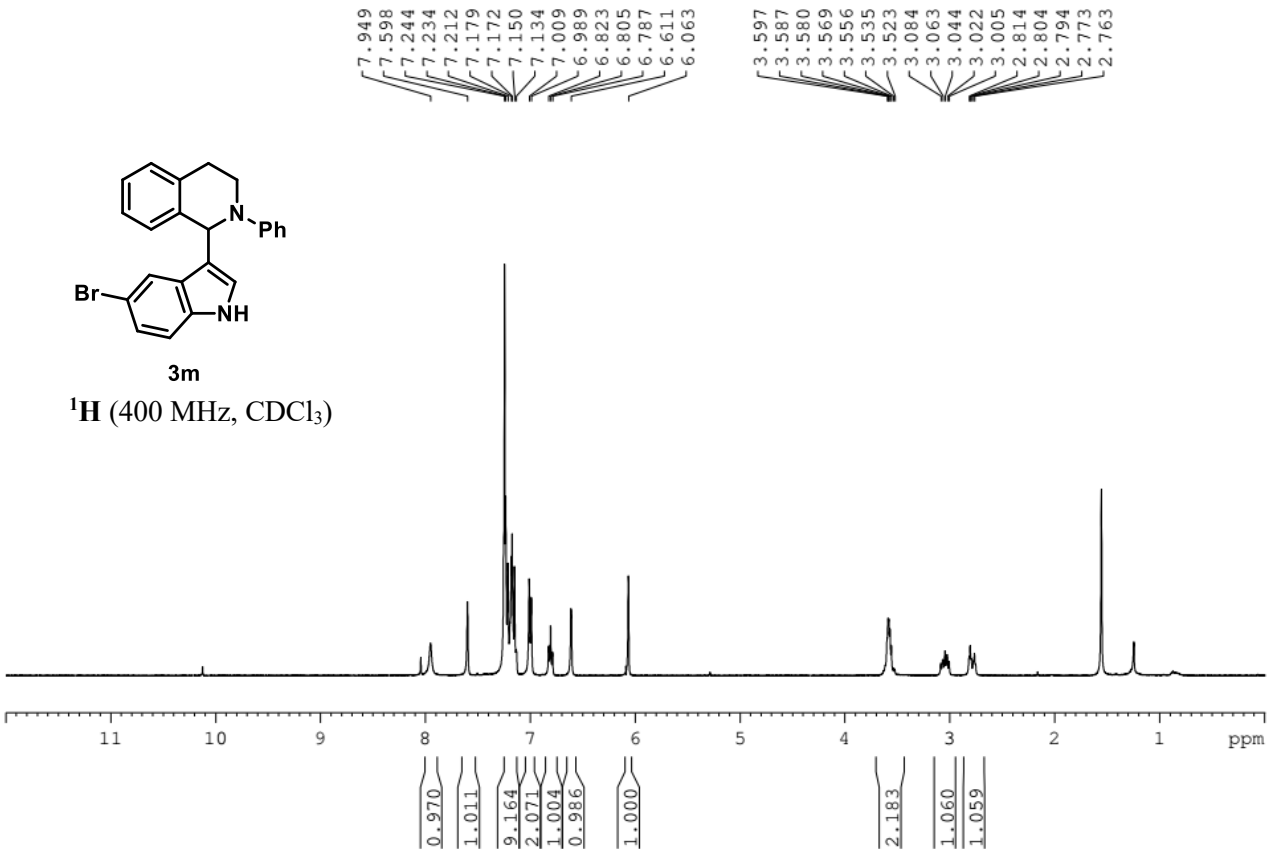


3l

^{13}C{1H} (100 MHz, $CDCl_3$)

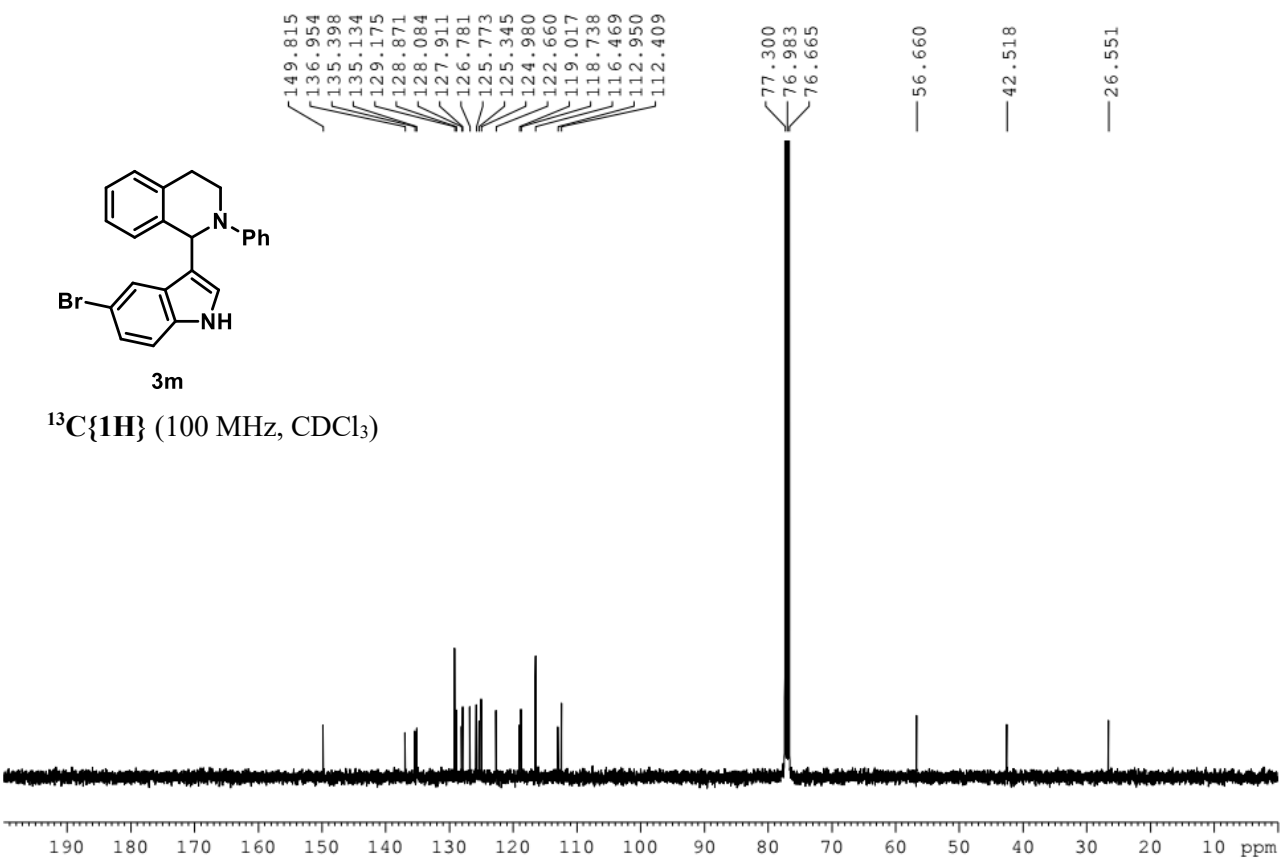
DEPT (100 MHz, $CDCl_3$)





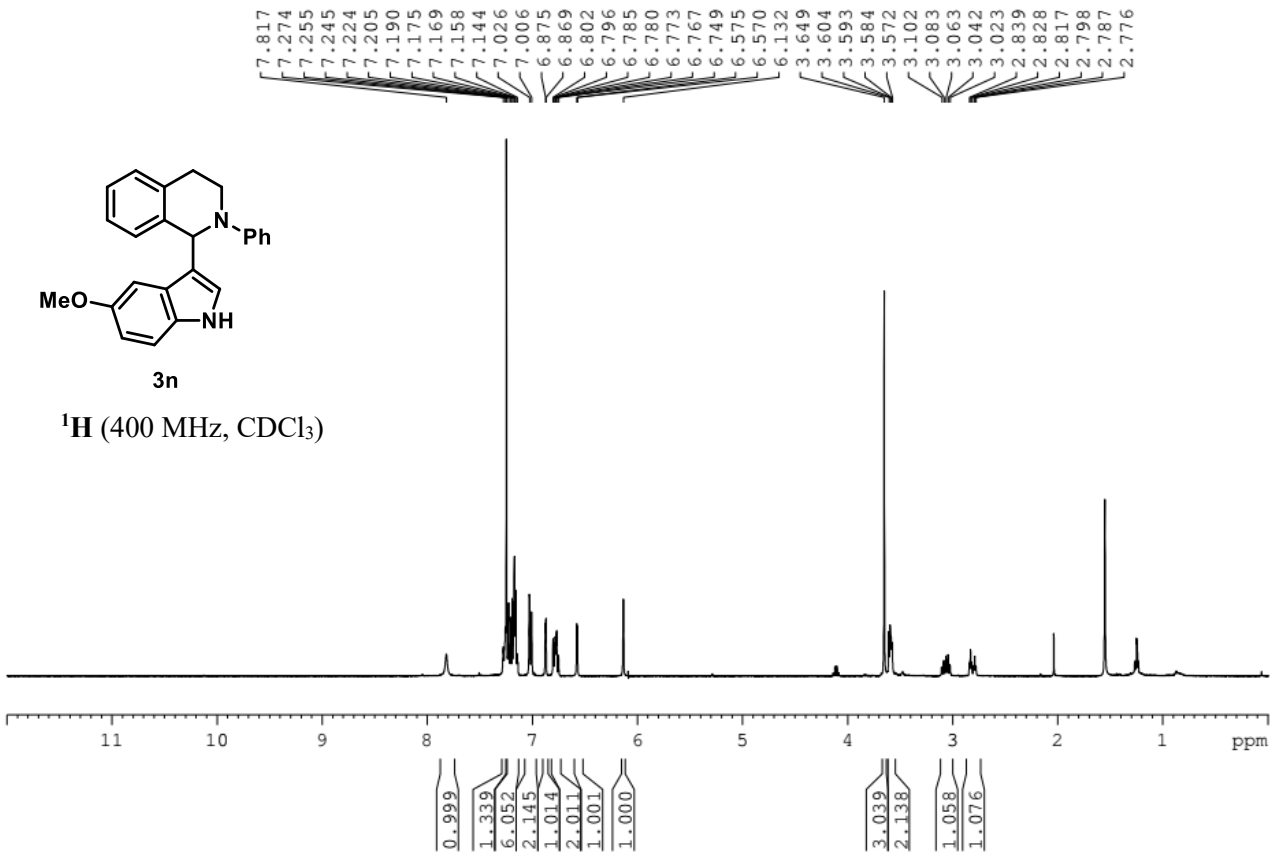
3m

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



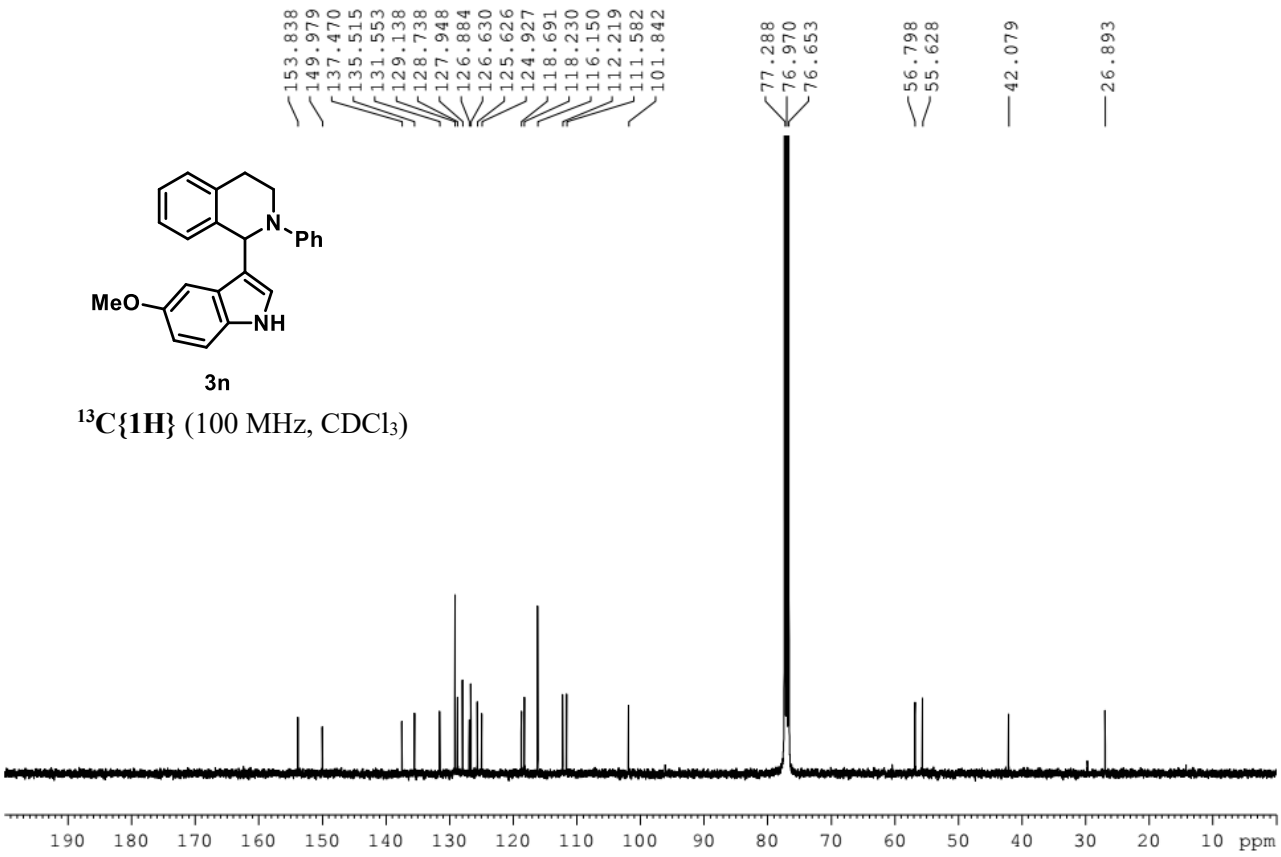
3m

^{13}C{1H} (100 MHz, $CDCl_3$)



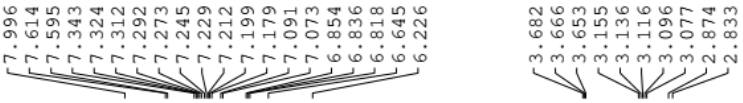
3n

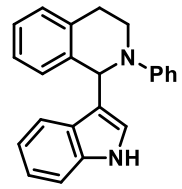
^{1}H (400 MHz, $CDCl_3$)



3n

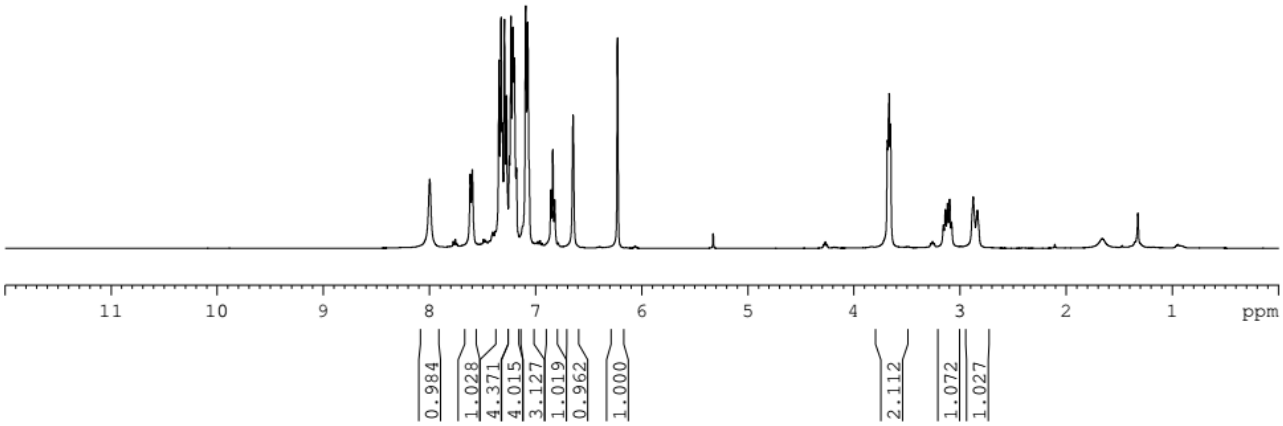
^{13}C{1H} (100 MHz, $CDCl_3$)

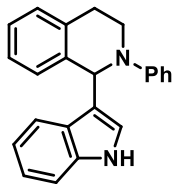




3o

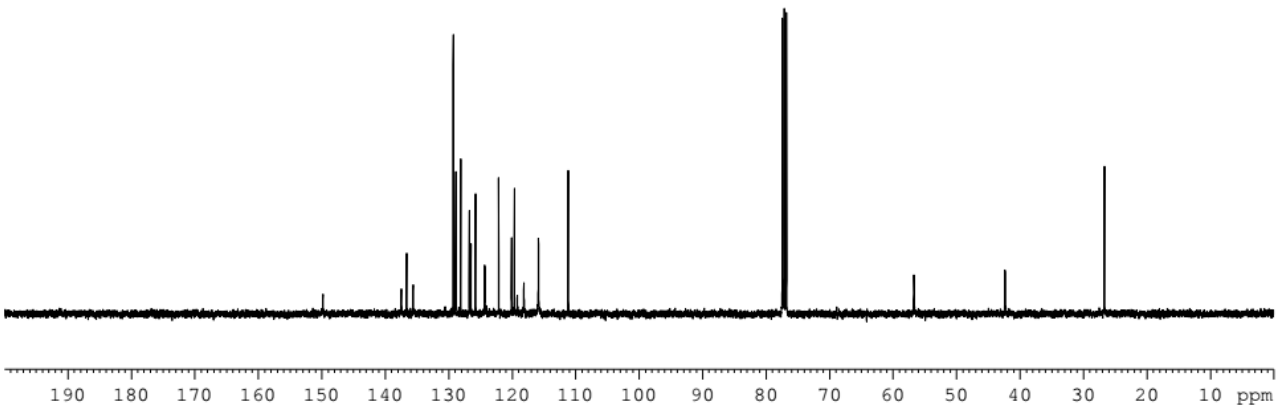
^{1}H (400 MHz, $CDCl_3$)

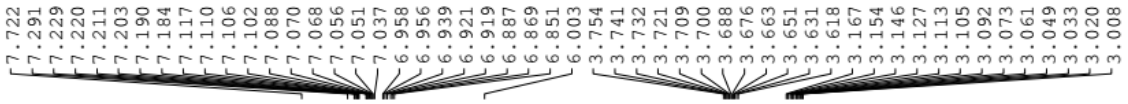


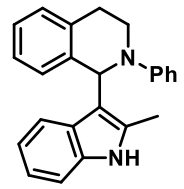


3o

^{13}C{1H} (100 MHz, $CDCl_3$)

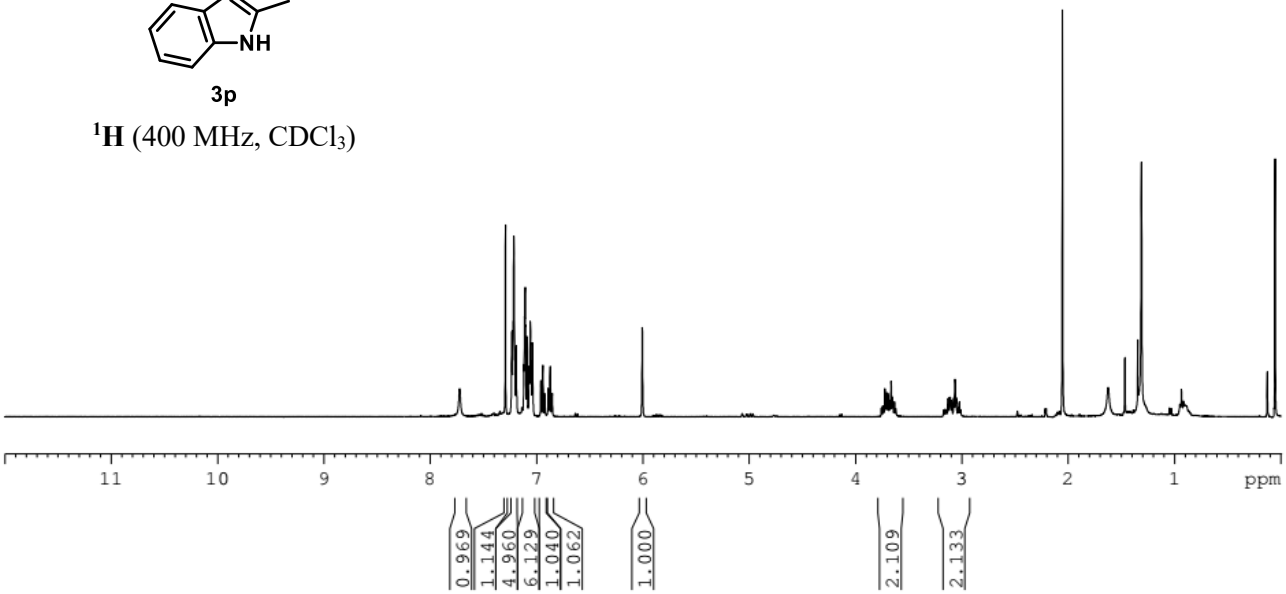


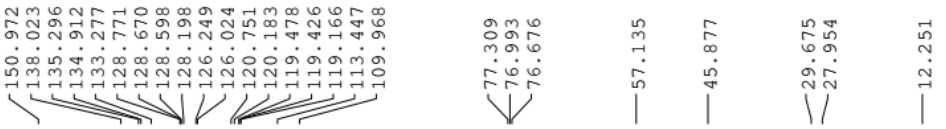


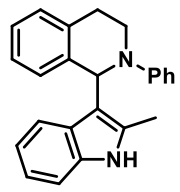


3p

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

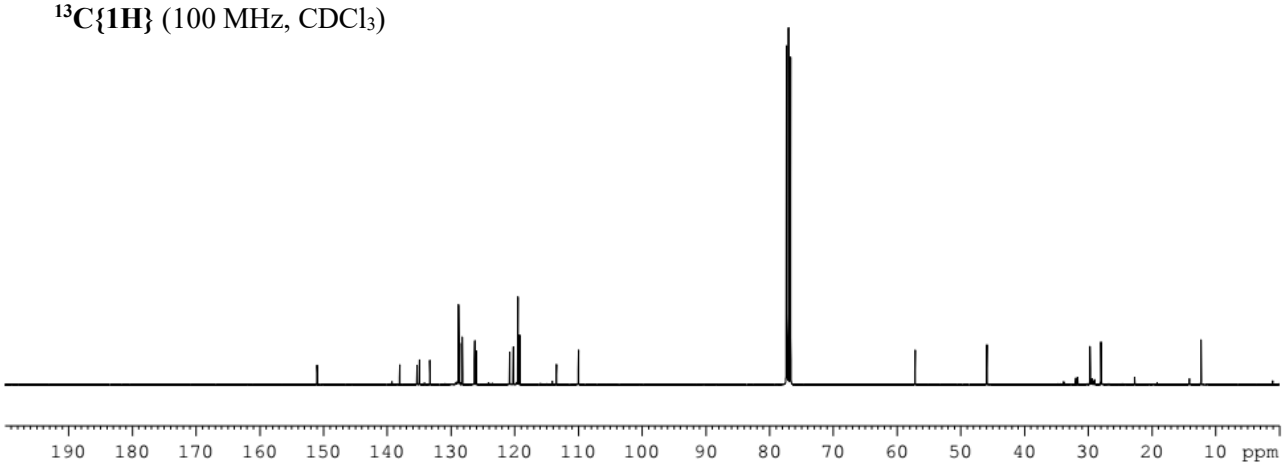


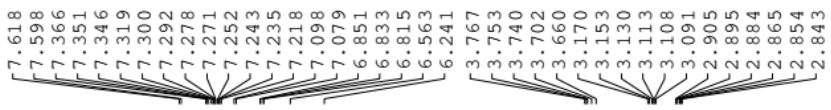


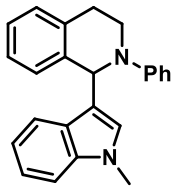


3p

^{13}C{1H} (100 MHz, $CDCl_3$)

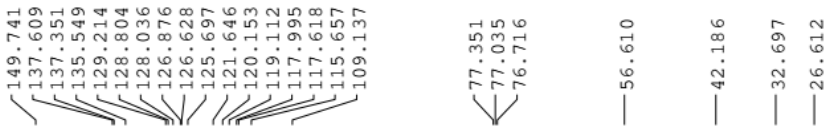


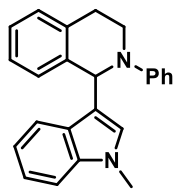




3q

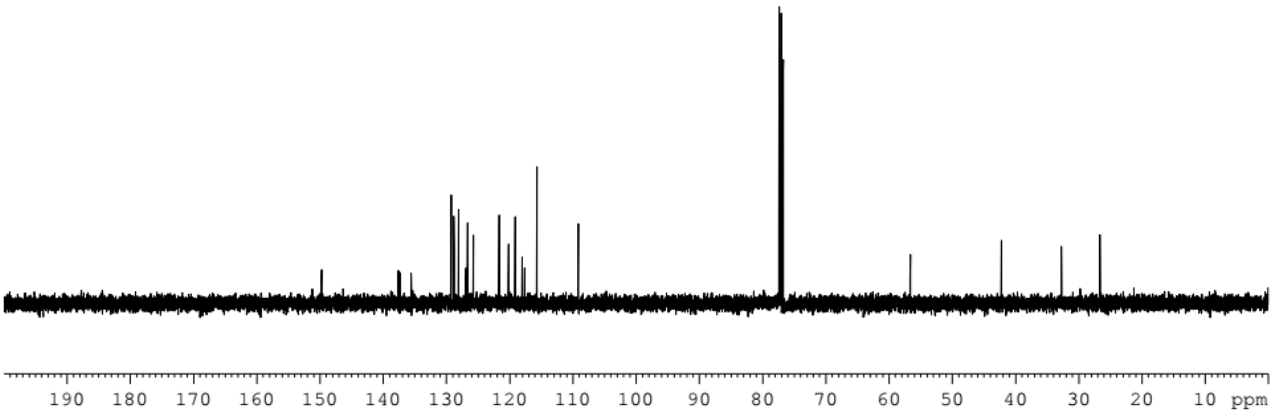
^{1}H (400 MHz, $CDCl_3$)

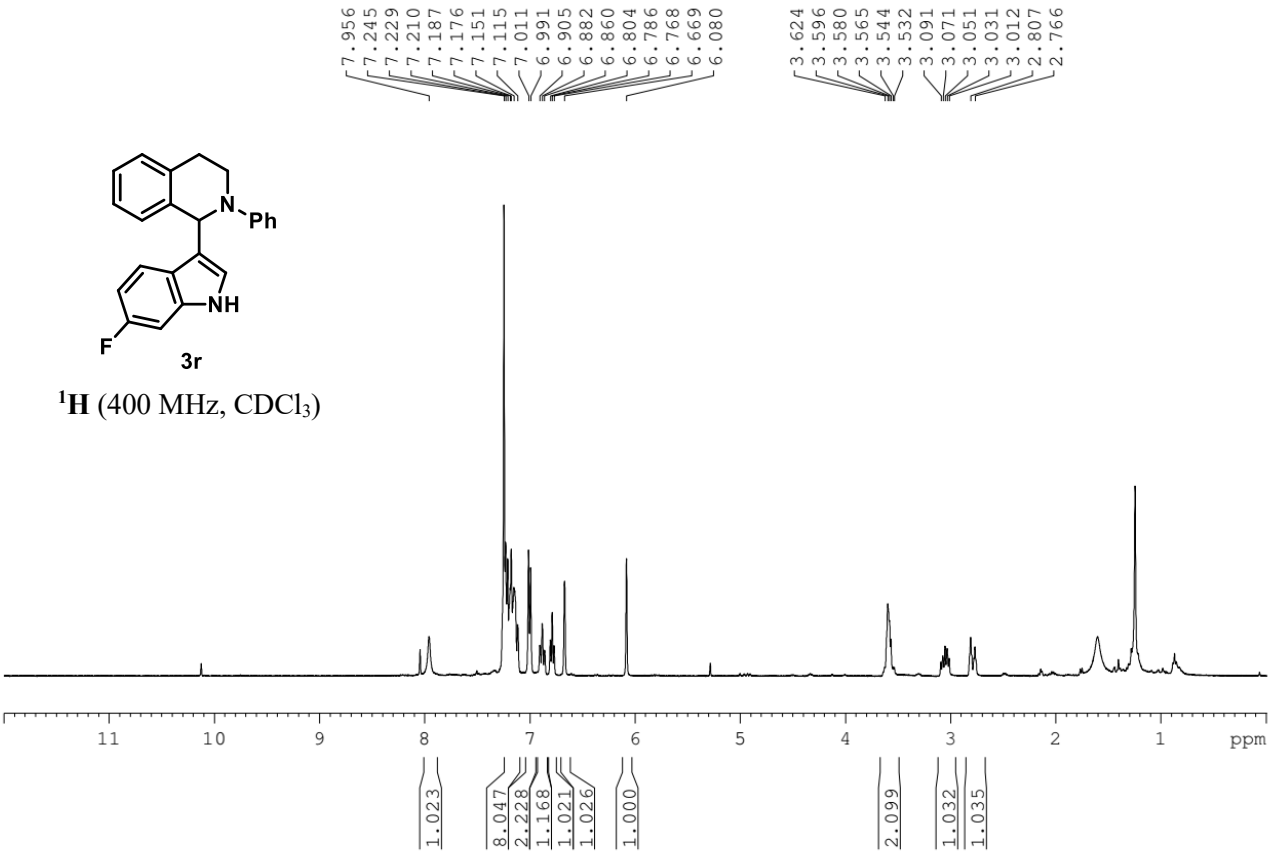




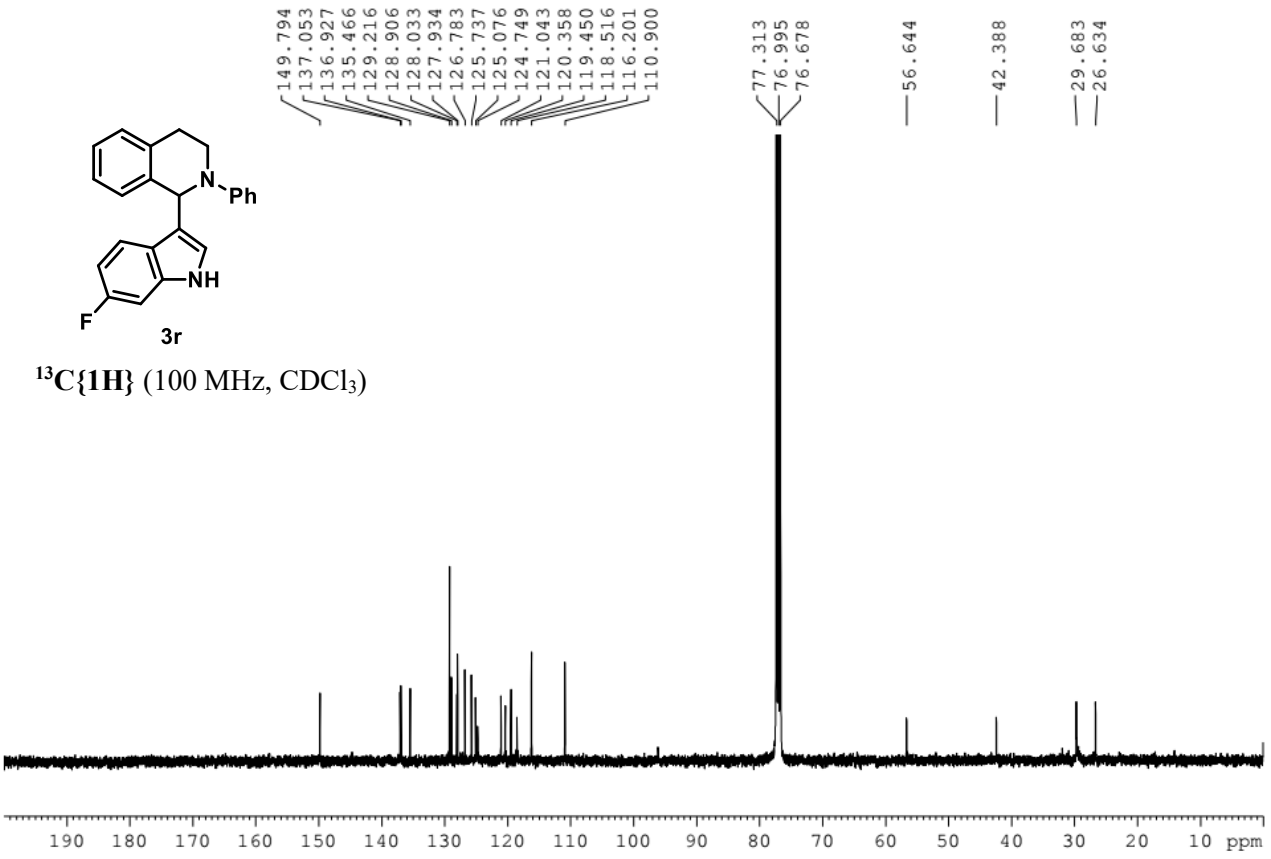
3q

^{13}C{1H} (100 MHz, $CDCl_3$)

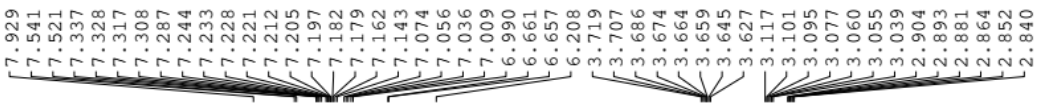


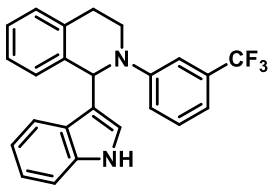


^{1}H (400 MHz, $CDCl_3$)



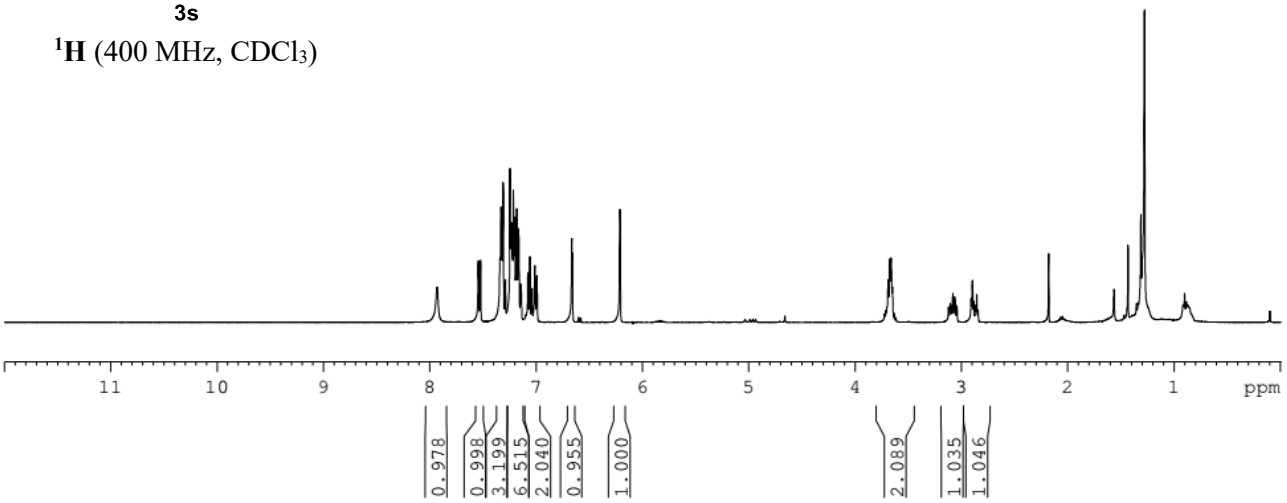
^{13}C{1H} (100 MHz, $CDCl_3$)

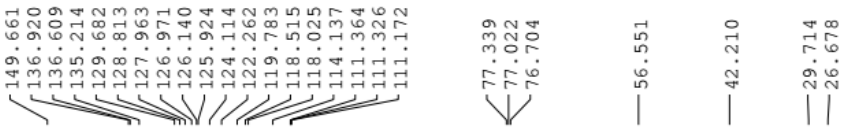


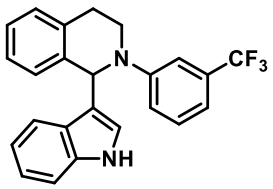


3s

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

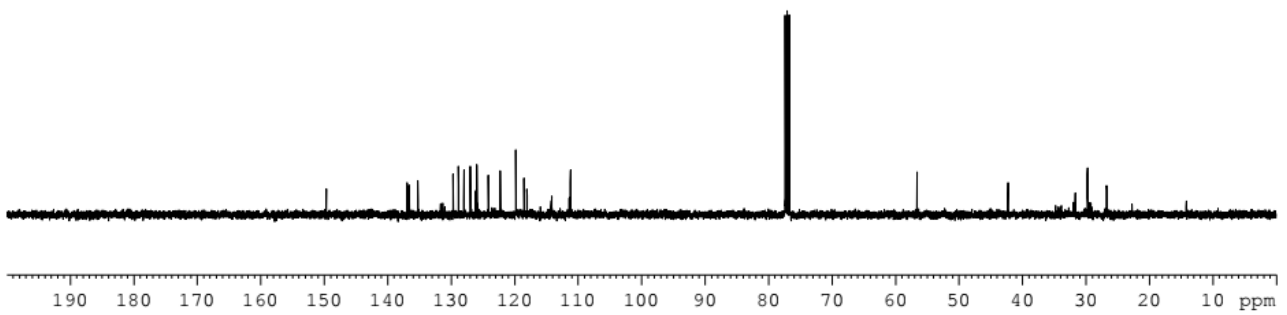


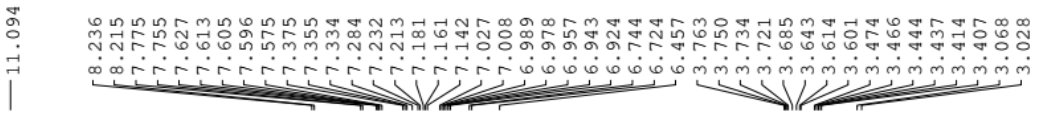


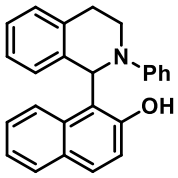


3s

^{13}C{1H} (100 MHz, $CDCl_3$)

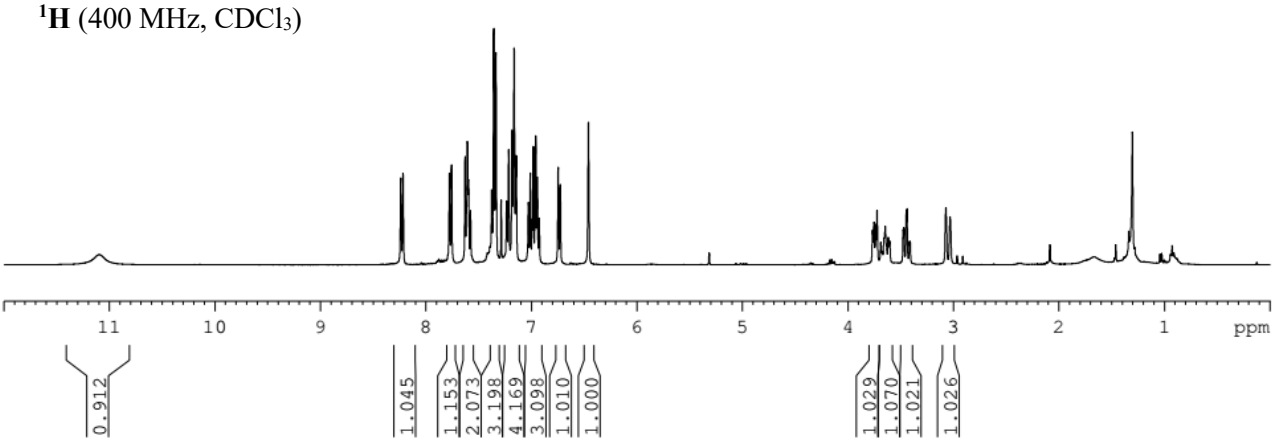


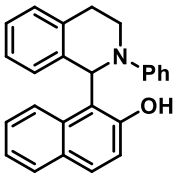




3t

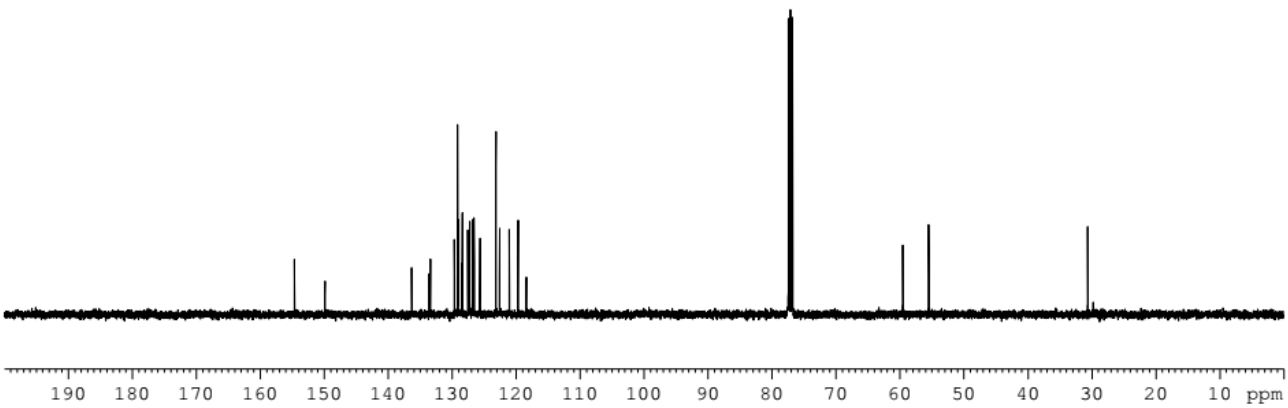
^{1}H (400 MHz, $CDCl_3$)

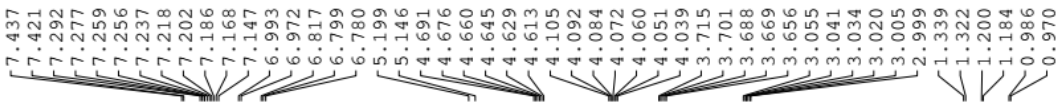


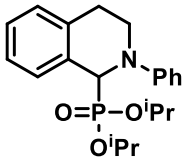


3t

^{13}C{1H} (100 MHz, $CDCl_3$)

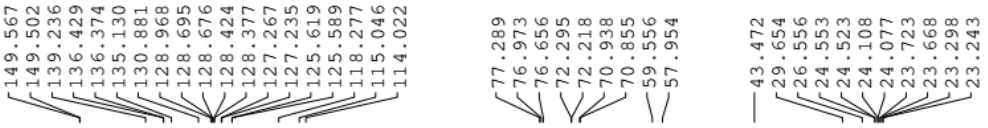


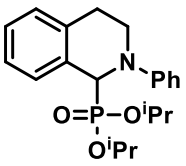




3u

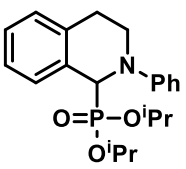
^{1}H (400 MHz, $CDCl_3$)





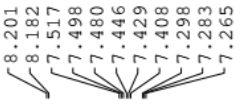
3u

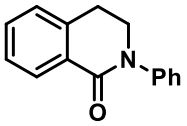
^{13}C{1H} (100 MHz, $CDCl_3$)



3u

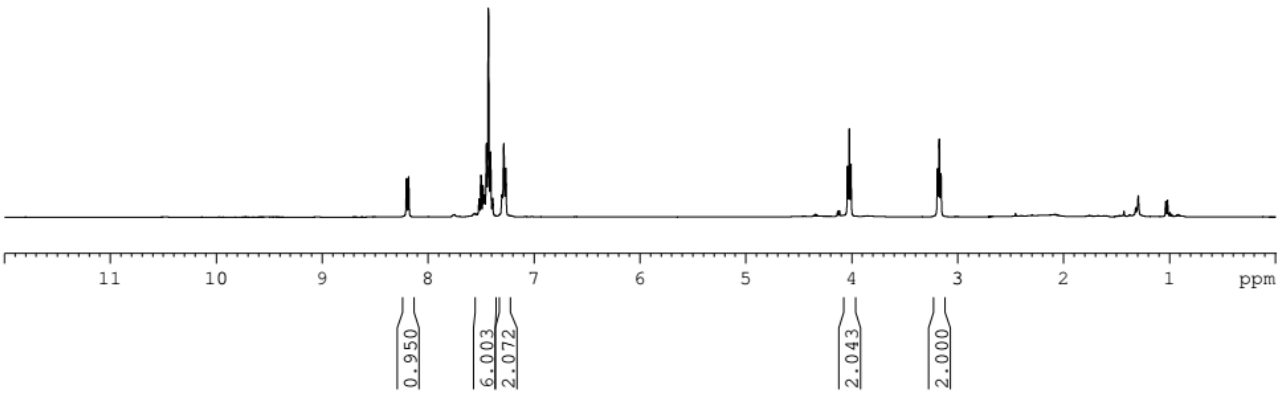
^{31}**P{1H}** (162 MHz, $CDCl_3$)

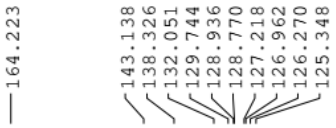


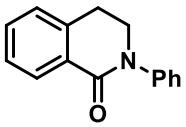


4a

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

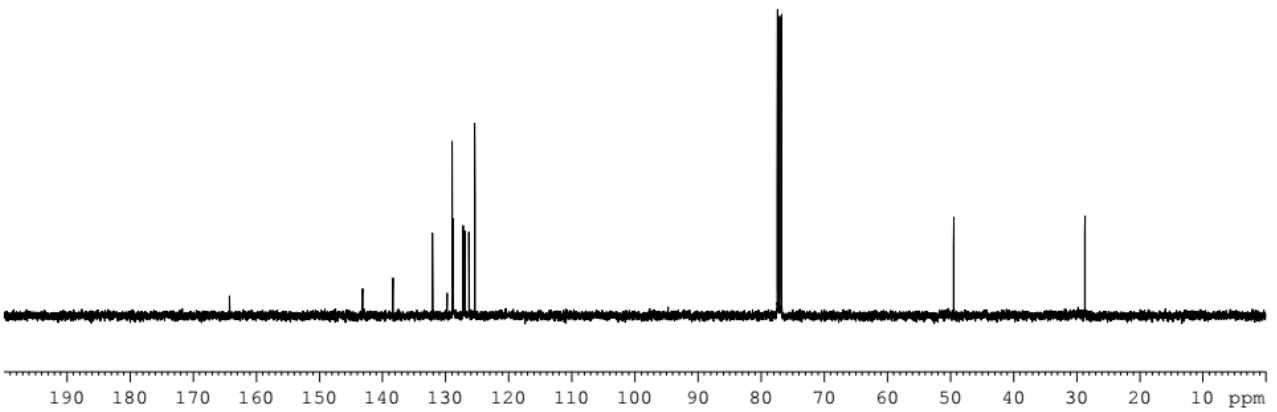


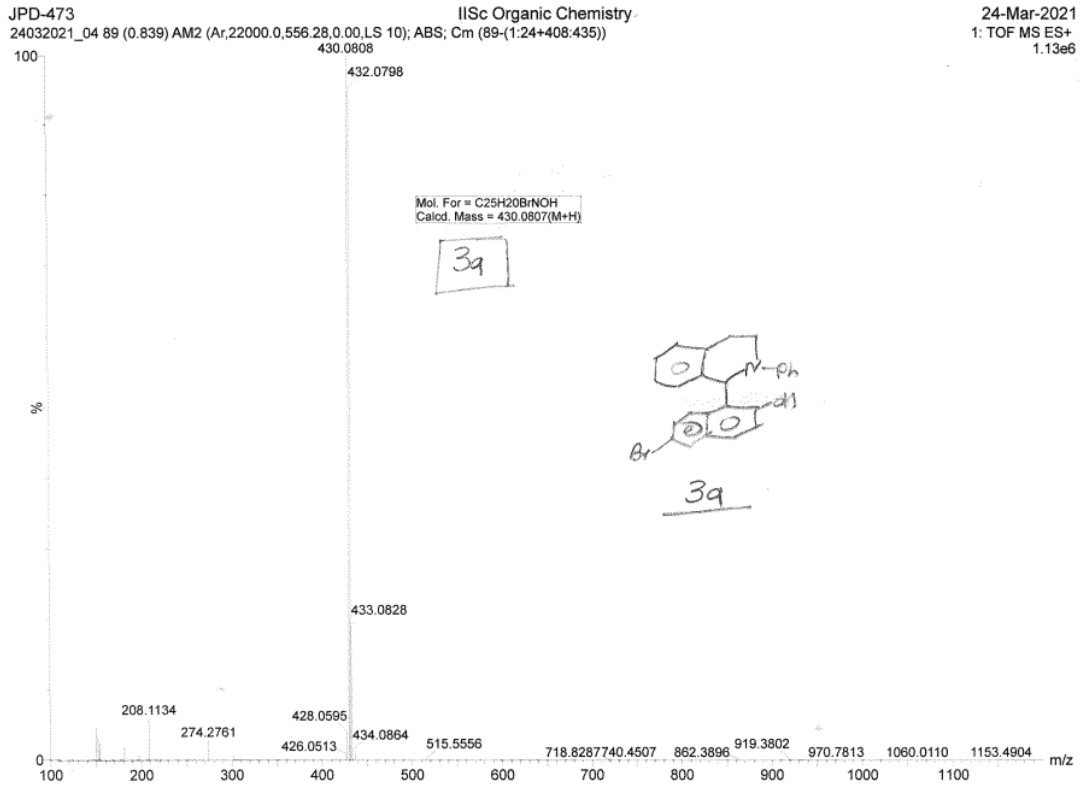


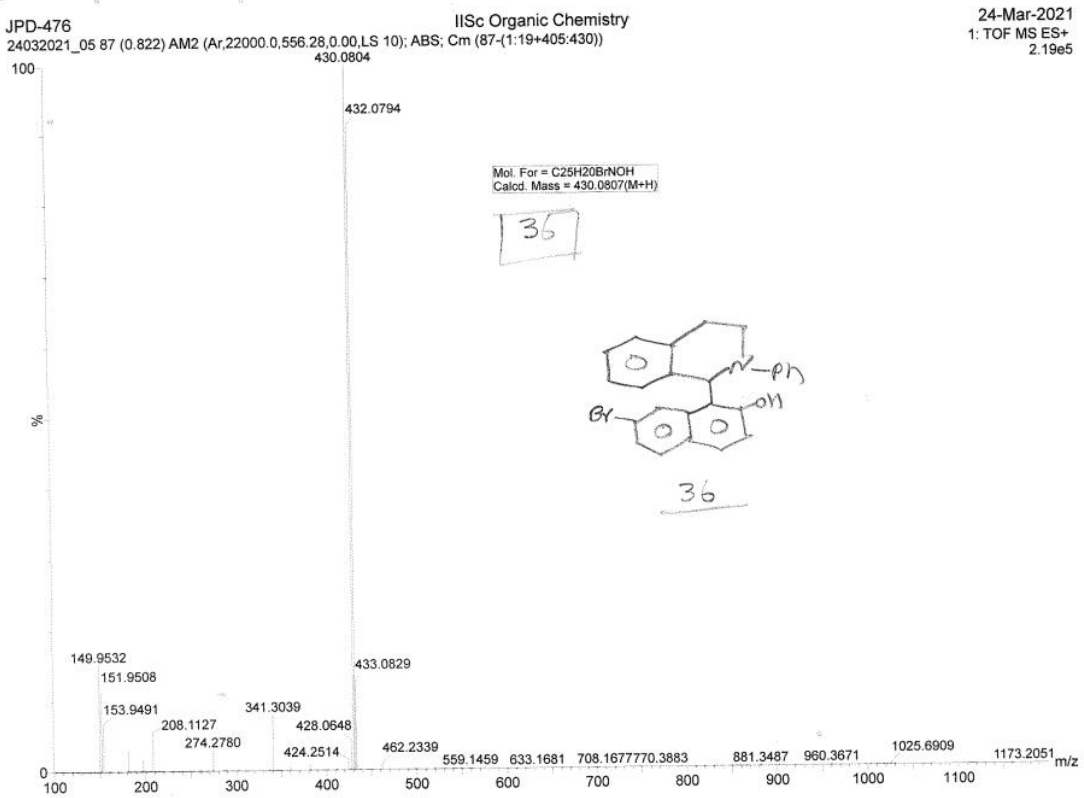


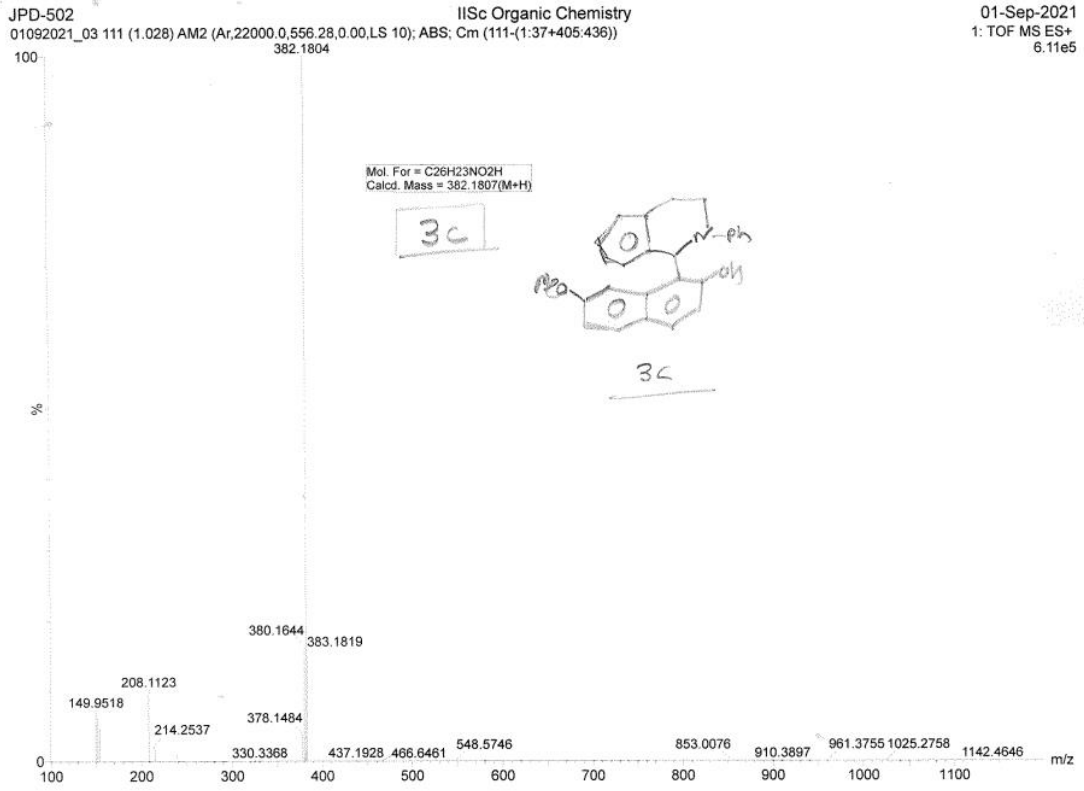
4a

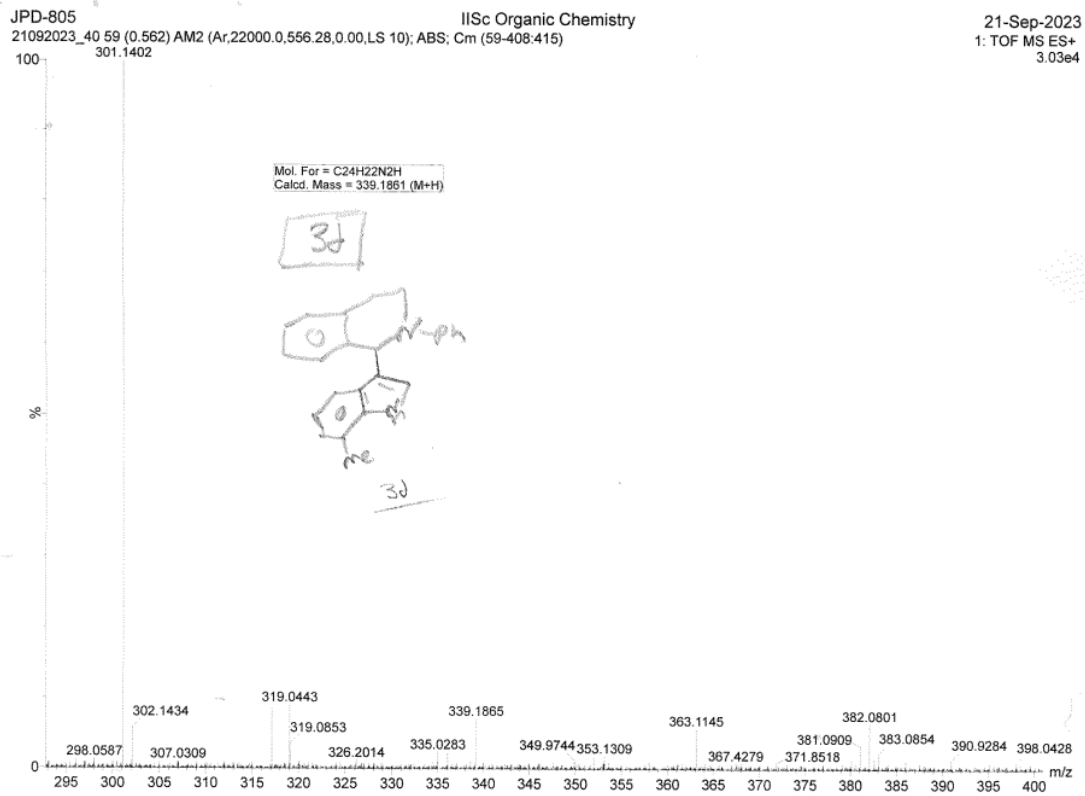
^{13}C{1H} (100 MHz, $CDCl_3$)

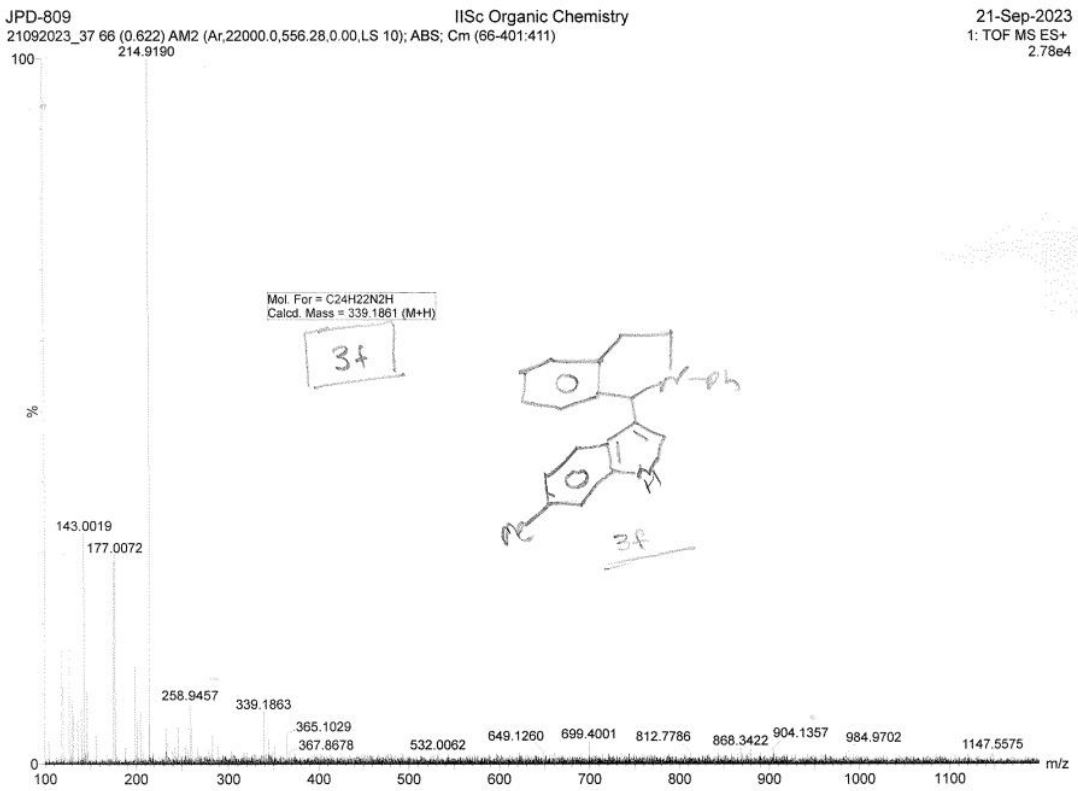


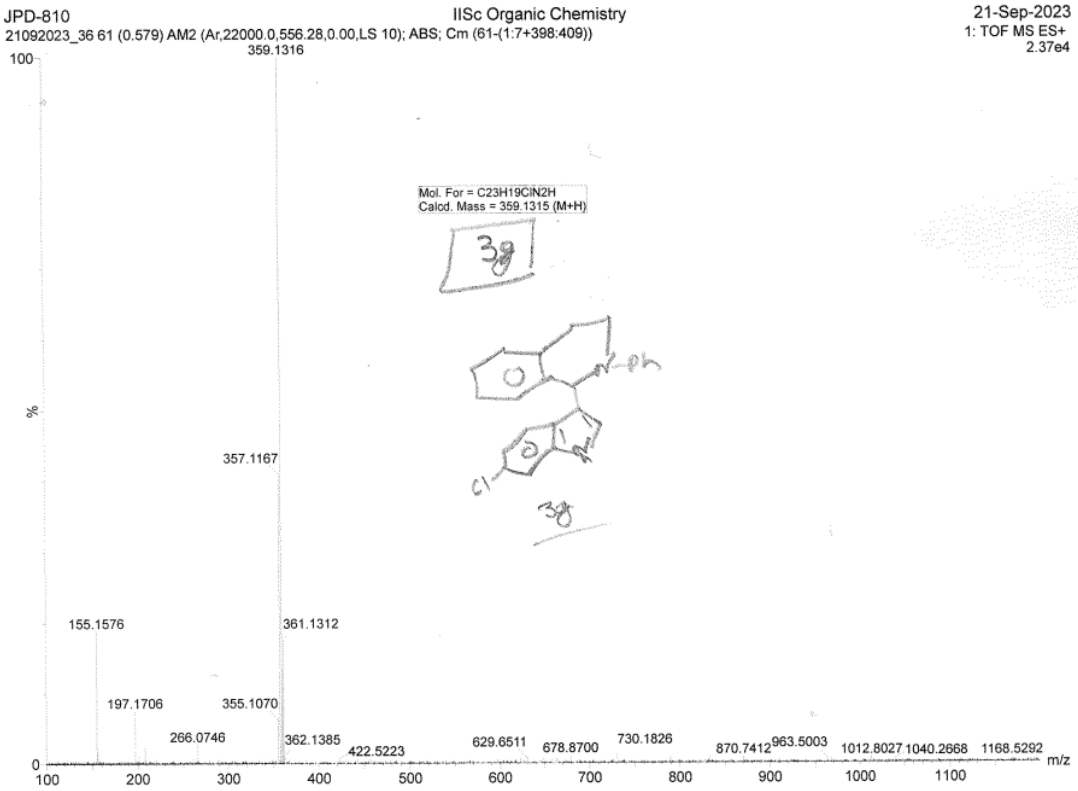

JPD-473
IISc Organic Chemistry
24-Mar-2021
24032021_04 89 (0.839) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS; Cm (89-(1:24+408:435))
1: TOF MS ES+
1.13e6
Mol. For = C25H20BrNOH
Calcd. Mass = 430.0807(M+H)
3a
3a
m/z

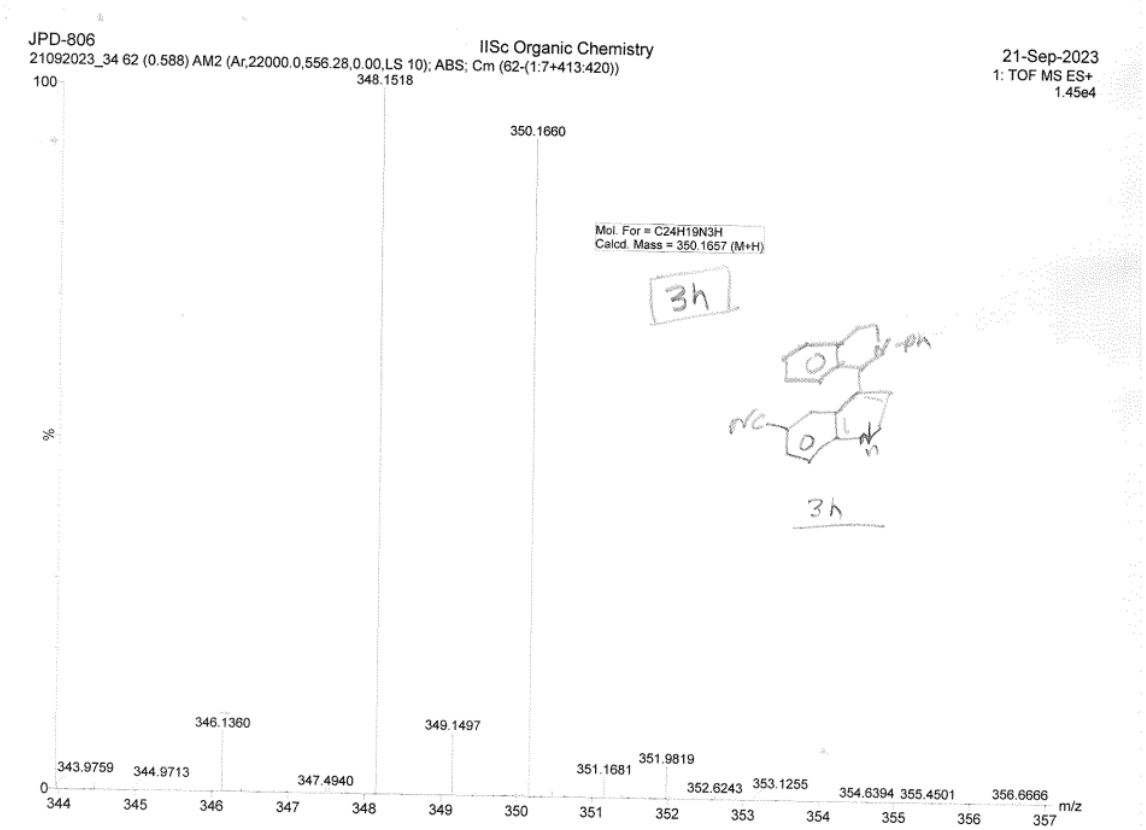

JPD-476
IISc Organic Chemistry
24-Mar-2021
24032021_05 87 (0.822) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS; Cm (87-(1:19+405:430))
1: TOF MS ES+
2.19e5
Mol. For = C25H20BrNOH
Calcd. Mass = 430.0807(M+H)
3b
3b
m/z

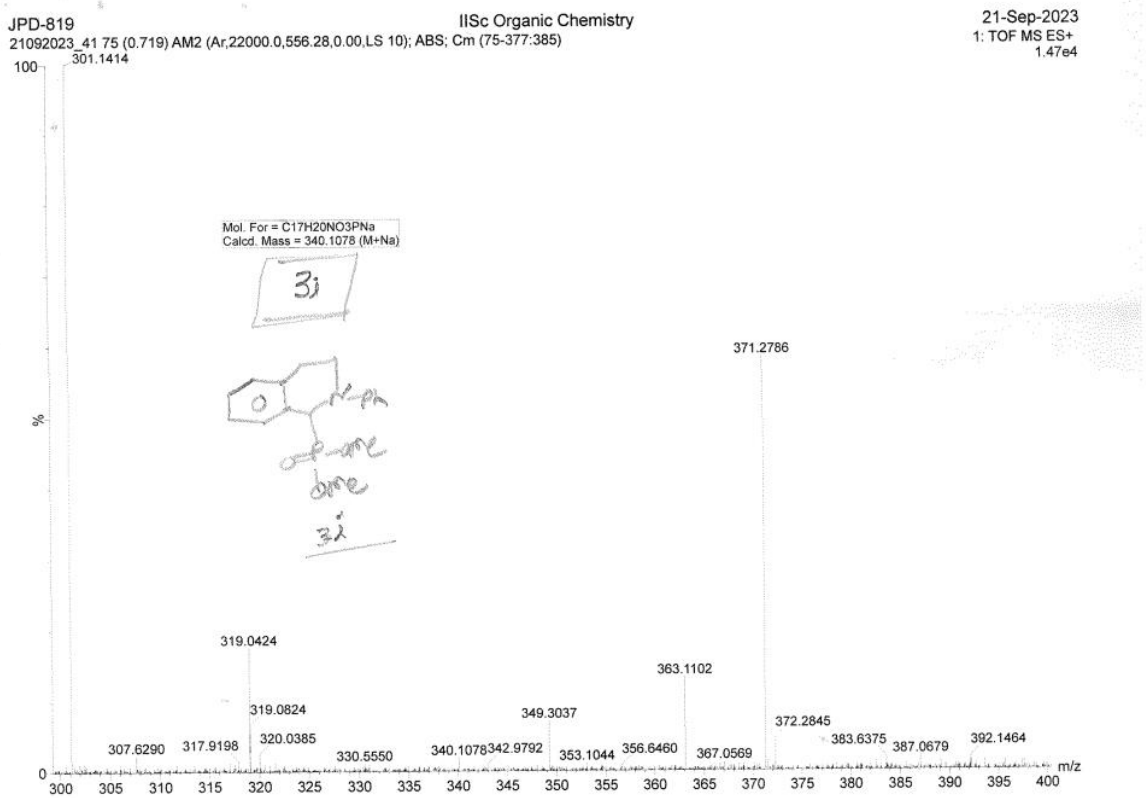

JPD-502
IISc Organic Chemistry
01-Sep-2021
01092021_03 111 (1.028) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS; Cm (111-(1:37+405:436))
1: TOF MS ES+
6.11e5
382.1804
Mol. For = C26H23NO2H
Calcd. Mass = 382.1807(M+H)
3c
3c
380.1644
383.1819
208.1123
149.9518
214.2537
378.1484
330.3368
437.1928
466.6461
548.5746
853.0076
910.3897
961.3755
1025.2758
1142.4646
%
m/z

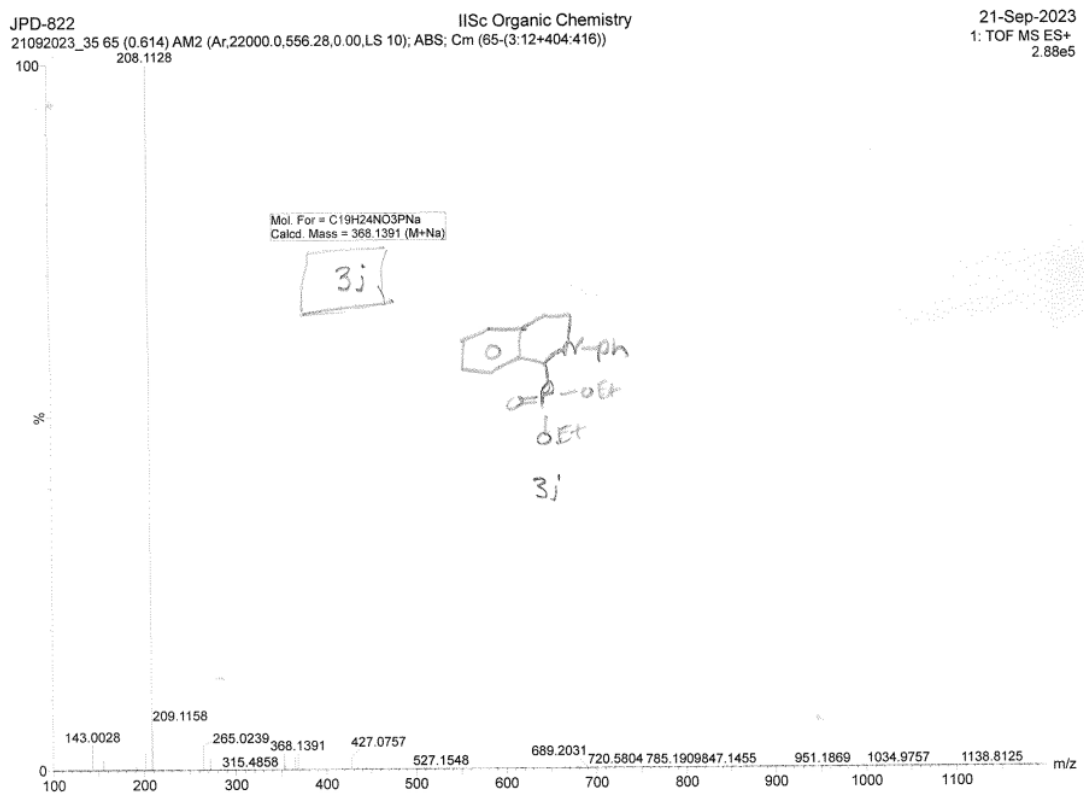

JPD-805
IISc Organic Chemistry
21-Sep-2023
21092023_40 59 (0.562) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS; Cm (59-408:415)
1: TOF MS ES+
3.03e4
301.1402
Mol. For = C24H22N2H
Calcd. Mass = 339.1861 (M+H)
3d
3d
319.0443
302.1434
319.0853
339.1865
298.0587
307.0309
326.2014
335.0283
349.9744
353.1309
363.1145
367.4279
371.8518
381.0909
382.0801
383.0854
390.9284
398.0428
%
m/z

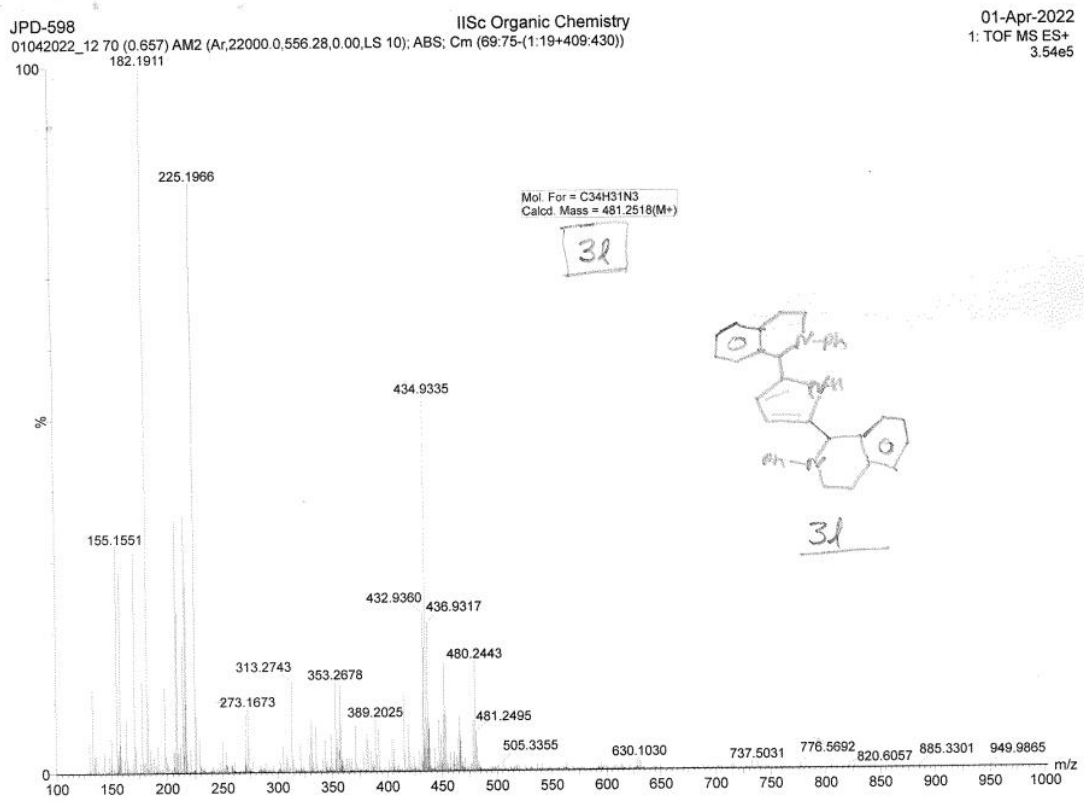

JPD-809
IISc Organic Chemistry
21-Sep-2023
21092023_37 66 (0.622) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS; Cm (66-401:411)
1: TOF MS ES+
2.78e4
214.9190
Mol. For = C24H22N2H
Calcd. Mass = 339.1861 (M+H)
3f
143.0019
177.0072
258.9457
339.1863
365.1029
367.8678
532.0062
649.1260
699.4001
812.7786
868.3422
904.1357
984.9702
1147.5575
%
m/z

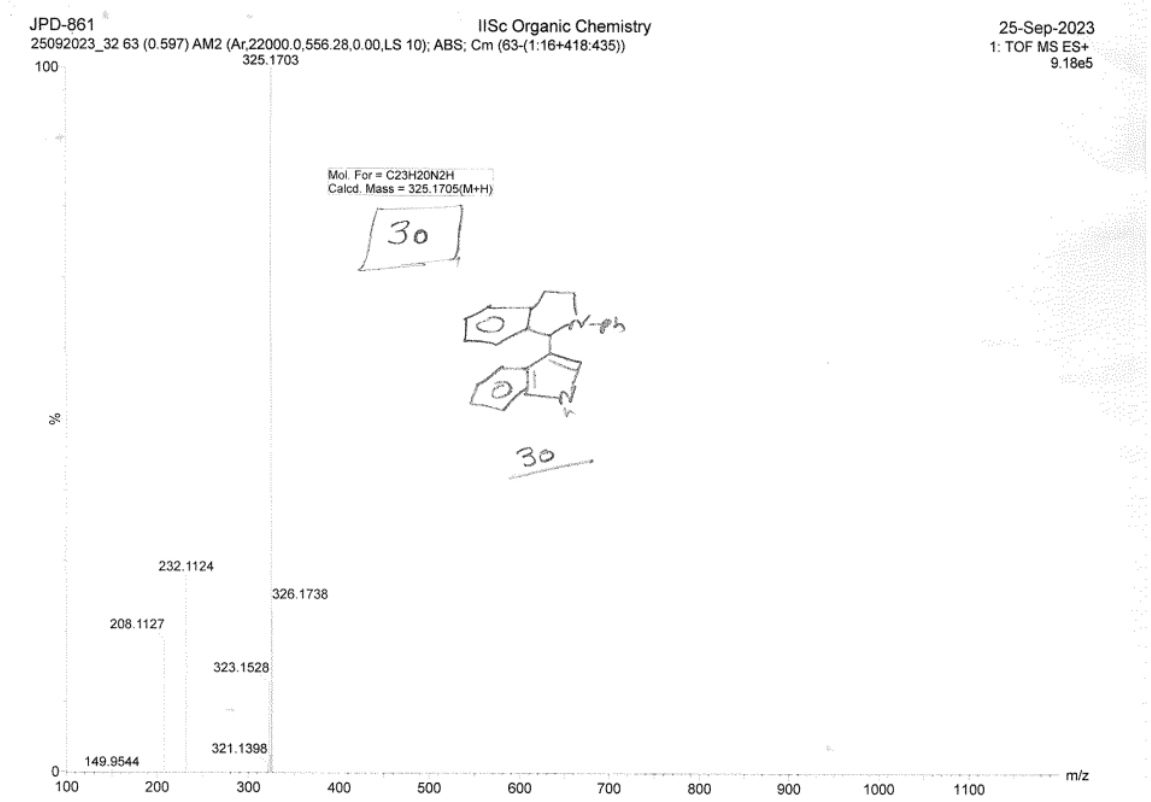

JPD-810
IISc Organic Chemistry
21-Sep-2023
21092023_36 61 (0.579) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS; Cm (61-(1:7+398:409))
1: TOF MS ES+
2.37e4
359.1316
Mol. For = C23H19ClN2H
Calcd. Mass = 359.1315 (M+H)
3g
357.1167
155.1576
361.1312
197.1706
355.1070
266.0746
362.1385
422.5223
629.6511
678.8700
730.1826
870.7412
963.5003
1012.8027
1040.2668
1168.5292
%
m/z

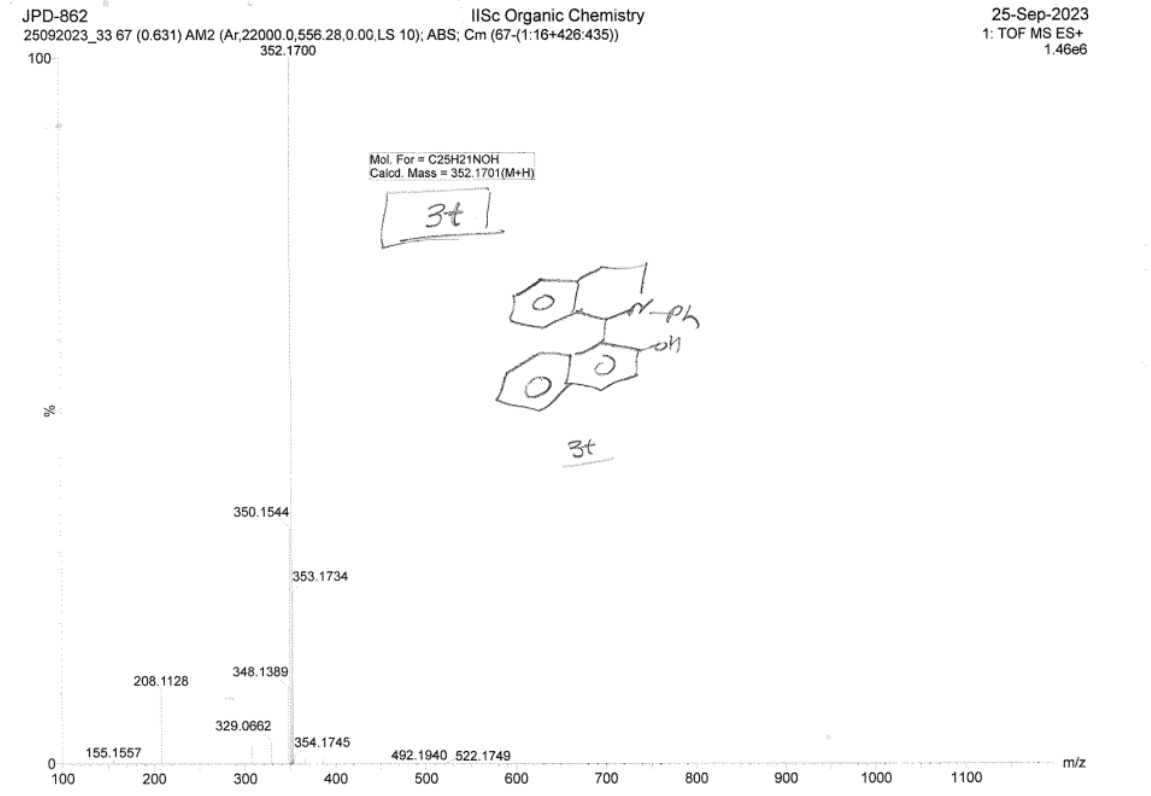

JPD-806
IISc Organic Chemistry
21092023_34 62 (0.588) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS; Cm (62-(1:7+413:420))
21-Sep-2023
1: TOF MS ES+
1.45e4
Mol. For = C24H19N3H
Calcd. Mass = 350.1657 (M+H)
3h
3h
m/z


JPD-819
IISc Organic Chemistry
21092023_41 75 (0.719) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS; Cm (75-377:385)
21-Sep-2023
1: TOF MS ES+
1.47e4
Mol. For = C17H20NO3PNa
Calcd. Mass = 340.1078 (M+Na)
3j
3j
m/z


JPD-822
IISc Organic Chemistry
21-Sep-2023
21092023_35 65 (0.614) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS; Cm (65-(3:12+404:416))
1: TOF MS ES+
2.88e5
Mol. For = C19H24NO3PNa
Calcd. Mass = 368.1391 (M+Na)
3j
3j
m/z


JPD-598
IISc Organic Chemistry
01-Apr-2022
01042022_12 70 (0.657) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS; Cm (69:75-(1:19+409:430))
1: TOF MS ES+
3.54e5
Mol. For = C34H31N3
Calcd. Mass = 481.2518(M+)
3l
3l
m/z


JPD-861
IISc Organic Chemistry
25-Sep-2023
25092023_32 63 (0.597) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS; Cm (63-(1:16+418:435))
1: TOF MS ES+
9.18e5
325.1703
Mol. For = C23H20N2H
Calcd. Mass = 325.1705(M+H)
30
30
232.1124
326.1738
208.1127
323.1528
321.1398
149.9544
%
m/z


JPD-862
IISc Organic Chemistry
25-Sep-2023
25092023_33 67 (0.631) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS; Cm (67-(1:16+426:435))
1: TOF MS ES+
1.46e6
352.1700
Mol. For = C25H21NOH
Calcd. Mass = 352.1701(M+H)
3t
3t
350.1544
353.1734
348.1389
208.1128
329.0662
354.1745
155.1557
492.1940
522.1749
%
m/z