Inherent directing group enabled Co(III)-catalyzed C-H allylation/vinylation of isoquinolones

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Supporting Information

1. General Information.

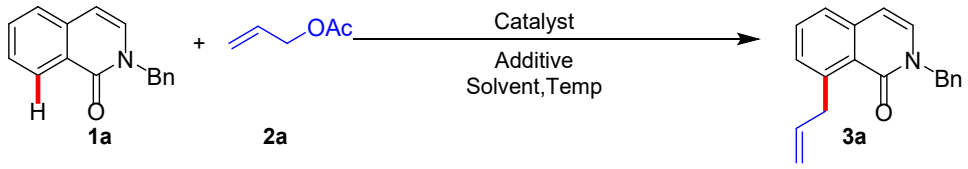
All Chemicals were purchased from the Sigma- Aldrich, TCI and AVRA chemicals. TLC plates (Aluminium Sheet Silica gel 60 F_{254}) were purchased from Merck. Column chromatography was performed over silica gel (230−400 mesh) using *n*-hexane and ethyl acetate as eluents. All products were characterized by ^{1}H NMR, ^{13}C NMR, FT-IR and high-resolution mass spectrometry (HRMS) and melting points. NMR spectra were recorded in on Bruker Advance at 400 MHz or 500 MHz (^{1}H) and 100 MHz and 125 MHz (^{13}C) respectively. Chemical shifts (δ) are reported in ppm, using the residual solvent peak in $CDCl_3$ (δH = 7.26 and δC = 77.16) (H_2O, δH = 1.56) ppm, and coupling constants (J) are given in Hz. HRMS were recorded Mass spectra were recorded on Water Q-ToF Micromass, maXis Impact mass spectrometers, and a high-resolution 6560 Ion Mobility Q-TOF LC/MS (Agilent, Santa Clara, USA). IR was analyzed using a Shimadzu IR Prestige-21 with a ZnSe single reflection ATR accessory. X-ray photoelectron spectra (XPS) was analysed using Thermo Scientific NEXSA Surface Analysis. The melting points were recorded on a Brønsted Electrothermal 9100 and Labindia visual melting range.

2. General procedure for the synthesis of Isoquinolone.

Isoquinolone 1a-1m [S1], 1n [S2], 1o [S3], 1p [S4], 1q [S3], 1a-d_1 [S1] were prepared according to known literature method.

3. Optimization study:

3.1 Optimization table for allylation of Isoquinolone with allyl acetate (Table S1):

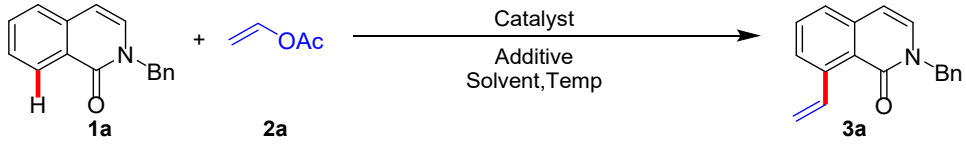


Entry	Catalyst (10 mol%)	Ag salt (30 mol%)	Solvent (0.2 M)	Additive (0.5 equiv)	Temp (°C)	Yield[a] (%)
1	$[CoCp^*(CO)I_2]$	$AgSbF_6$	HFIP	-	120	ND
2	$[CoCp^*(CO)I_2]$	$AgSbF_6$	DCE	-	120	ND
3	$[CoCp^*(CO)I_2]$	$AgSbF_6$	TFE	-	120	ND
4	$[CoCp^*(CO)I_2]$	$AgSbF_6$	HFIP	Cu_2O	120	26
5	$[CoCp^*(CO)I_2]$	$AgSbF_6$	TFE	Cu_2O	120	54
6	$[CoCp^*(CO)I_2]$	$AgSbF_6$	PhCl	Cu_2O	120	54
7	$[CoCp^*(CO)I_2]$	$AgSbF_6$	DCE	Cu_2O	120	89 (81)[b]
8	[CoCp*-	-	DCE	Cu_2O	120	46

	$(MeCN)_3(SbF_6)_2]$					
9	$[CoCp^*(CO)I_2]$	$AgSbF_6$	DCE	$Cu(OAc)_2$	120	61
10	$[CoCp^*(CO)I_2]$	$AgSbF_6$	DCE	Ag_2O	120	32
11	$[CoCp^*(CO)I_2]$	$AgSbF_6$	DCE	Ag_2CO_3	120	28
12[c]	$[CoCp^*(CO)I_2]$	$AgSbF_6$	DCE	$Cu(OAc)_2$	120	32
13	$[CoCp^*(CO)I_2]$	$AgSbF_6$	DCE	Cu_2O	100	70
14	$[CoCp^*(CO)I_2]$	$AgSbF_6$	DCE	Cu_2O	60	54
15	-	$AgSbF_6$	DCE	Cu_2O	120	ND
16	$[CoCp^*(CO)I_2]$	-	DCE	Cu_2O	120	ND
17	$[CoCp^*(CO)I_2]$	$AgSbF_6$	DCE	CuO	120	46

a = Yields are calculated using GC and *n*-decane as internal standard; b = isolated yield; c = $AgSbF_6$ (20 mol%), nd = not detected

3.2 Optimization table for vinylation of Isoquinolone with vinyl acetate (Table S2):



Entry	Catalyst (x mol%)	Ag salt (x mol%)	Solvent (0.2 M)	Additive (0.5 equiv)	Temp (°C)	Yield[a] (%)
1	$[CoCp^*(CO)I_2]$	$AgSbF_6$ (30)	DCE	Cu_2O	120	37
2	$[CoCp^*(CO)I_2]$	$AgNTf_2$ (30)	DCE	Cu_2O	120	30
3	$[CoCp^*(CO)I_2]$	$AgNTf_2$ (30)	TFE	Cu_2O	120	90 (84)[b]
4	$[CoCp^*(CO)I_2]$	$AgNTf_2$ (30)	PhCl	Cu_2O	120	17
5	$[CoCp^*(CO)I_2]$	$AgNTf_2$ (30)	DMC	Cu_2O	120	52
6	$[CoCp^*(CO)I_2]$	$AgSbF_6$ (30)	TFE	Cu_2O	120	63
7	$[CoCp^*$-$(MeCN)_3(SbF_6)_2]$	-	TFE	Cu_2O	120	33
8	$[CoCp^*(CO)I_2]$	$AgSbF_6$ (20)	TFE	Cu_2O (2.0)	120	23
9	$[CoCp^*(CO)I_2]$	$AgNTf_2$ (20)	TFE	Cu_2O (2.0)	120	58
10	-	$AgNTf_2$ (30)	TFE	Cu_2O	120	ND
11	$[CoCp^*(CO)I_2]$	-	TFE	Cu_2O	120	ND
12	$[CoCp^*(CO)I_2]$	$AgNTf_2$ (30)	TFE	-	120	ND
13	$[CoCp^*(CO)I_2]$	$AgNTf_2$ (30)	TFE	CuO	120	41

a = Yields are calculated using GC and *n*-decane as internal standard; b = isolated yield, nd = not detected

4. General Procedure for the allylation of isoquinolone.

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar isoquinolone (**1a**) (0.2 mmol), allyl acetate (0.6 mmol) (**2a**) $[CoCp^*(CO)I_2]$ (10 mol%), $AgSbF_6$ (30 mol%), Cu_2O (50 mol%) were added followed by the addition of DCE (1.0 mL). The subsequent reaction mixture was stirred at 120°C in a preheated block for 24 h. Reaction mixture was cooled to room temperature and diluted with ethyl acetate. Solvent was evaporated under reduced pressure and the crude mixture was purified by column chromatography using silica gel (230−400 mesh size) and hexane/EtOAc as the eluent.

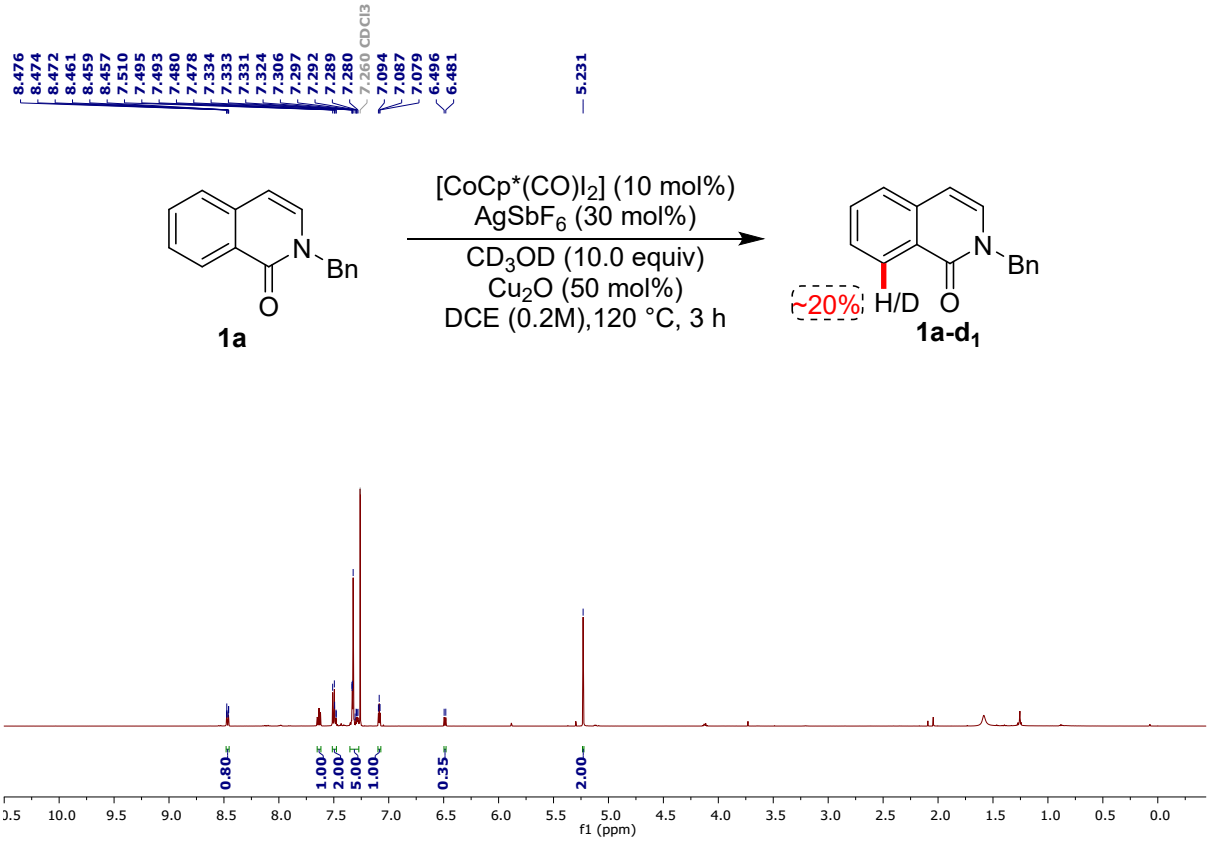
5. General Procedure for the vinylation of isoquinolone.

To an oven-dried screw cap reaction vial charged with a spin vane magnetic stir-bar isoquinolone **1** (0.2 mmol), vinyl acetate (0.6 mmol) (**2b**) [CoCp*(CO)I_2] (10 mol%), $AgNTf_2$ (30 mol%), Cu_2O (50 mol%) were added followed by the addition of TFE (1.0 mL). The subsequent reaction mixture was stirred at 120 °C in a preheated block for 24 h. Reaction mixture was allowed to cool to room temperature and diluted with ethyl acetate. Solvent was evaporated under reduced pressure and the crude mixture was purified by column chromatography using silica gel (230−400 mesh size) and hexane/EtOAc as the eluent.

6. Mechanistic studies

6.1. Deuterium labelling experiments without allyl acetate (2a) :

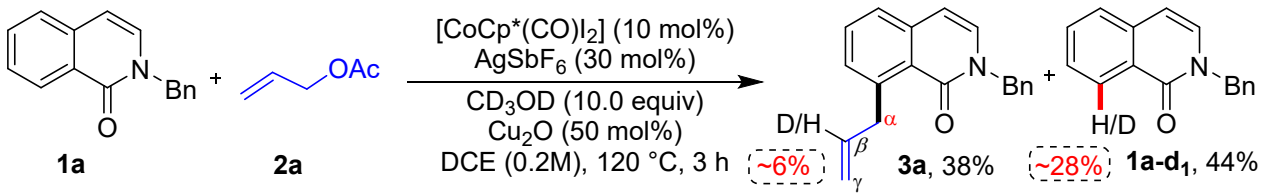
The substrate **1a** (0.1 mmol), [CoCp*(CO)I_2] (10 mol%), $AgSbF_6$ (30 mol%), Cu_2O (50 mol%),CD_3OD (10.0 equiv) and DCE (500 µL) were added to a screw-cap tube equipped with magnetic stirring bar and the mixture was stirred at preheated block maintained at 120 °C for 3 h. The reaction mixture was then allowed to cool to room temperature. The deuterium incorporation at C8 of **1a** was determined by ^{1}H NMR.

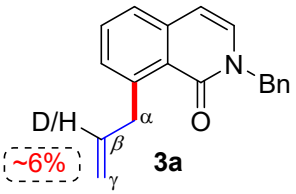


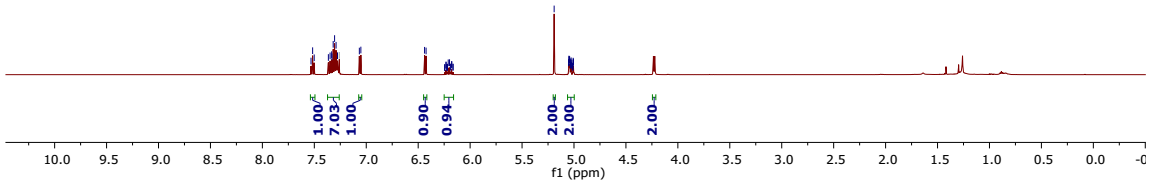
6.2 Deuterium labelling experiments with allyl acetate (2a) :

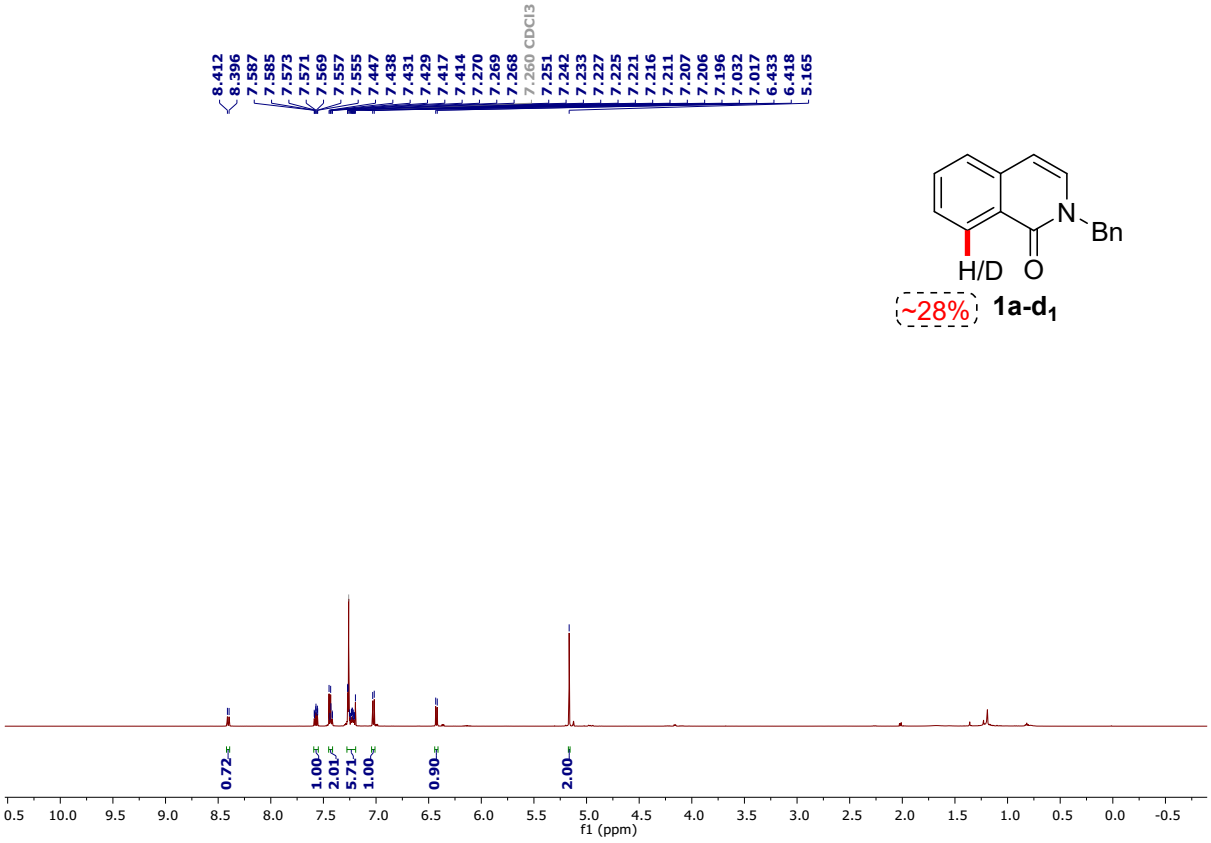
The substrate **1a** (0.1 mmol), **2a** (0.3 mmol), [CoCp*(CO)I_2] (10 mol%), $AgSbF_6$ (30 mol%), Cu_2O (50 mol%), CD_3OD (10.0 equiv) and DCE (500 µL) were added to a screw-cap tube equipped with magnetic stirring bar and the mixture was stirred at 120 °C for 3 h. The reaction

mixture was then allowed to cool to room temperature. The deuterium incorporation was determined by ^{1}H NMR.





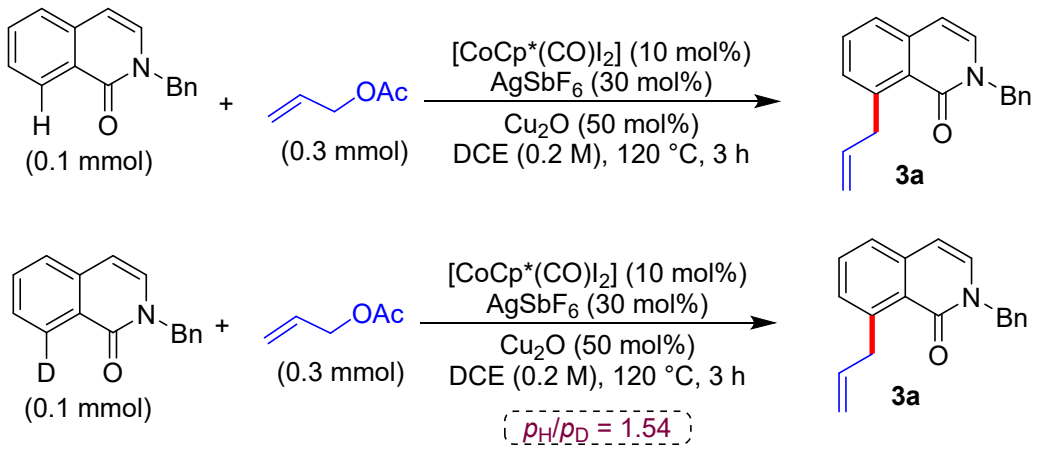




6.3 Determination of Kinetic Isotope Effect through parallel reactions :

In two different screwcapped vials with a stir bar separately placed **1a** and **1a-d$_2$** (0.1 mmol), were reacted with allyl acetate **2a** (0.3 mmol) under standard reaction conditions. Yield of product in both reaction was analyzed by GC after 3 hours.

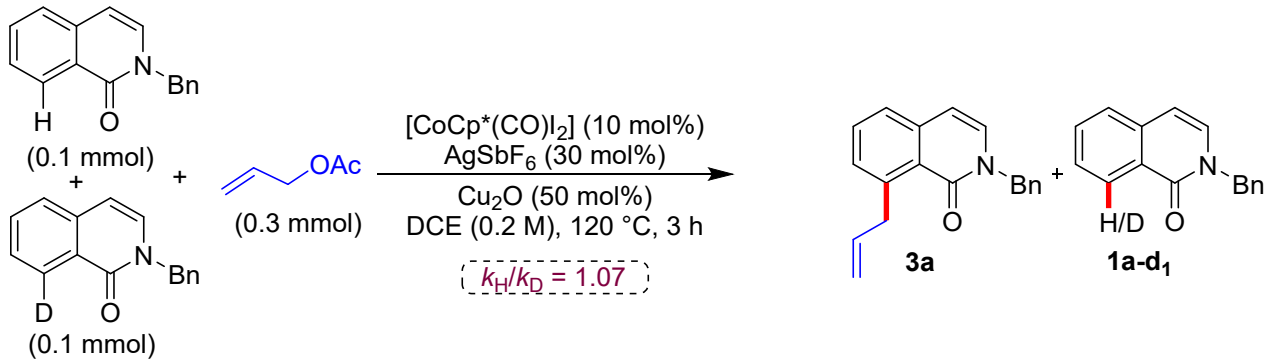
Conclusions: p_H/p_D=1.54 for parallel reactions.

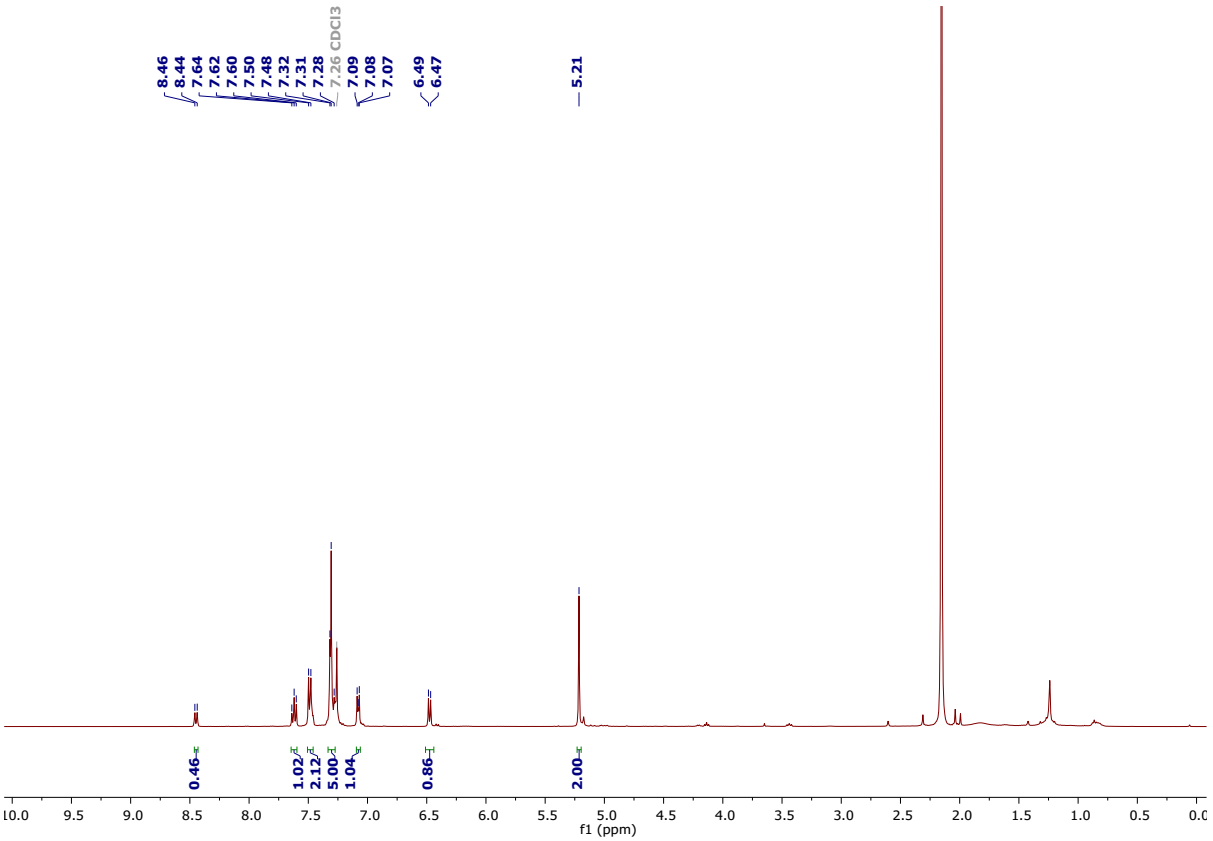


6.4 Determination of Kinetic Isotope Effect from an intermolecular competition experiment:

In a screwcapped vials with a stir bar **1a** (0.1 mmol) and **1a-d$_2$** (0.1 mmol), were reacted with allyl acetate **2a** (3 equiv.) under standard reaction conditions for 3 hours. The k_H/k_D was calculated by ^{1}H NMR.

Conclusions: k_H/k_D=1.07 for competitive experiments.





6.5 Recovery of Cu from crude reaction mixture for XPS analysis

In a screwcapped vials with a stir bar **1a** (0.1 mmol) was reacted with allyl acetate **2a** (3 equiv.) under standard reaction conditions for 12 hours. The reaction mixture were cooled to room temperature and filtered using whatman filter paper. The residue was submitted for XPS analysis.

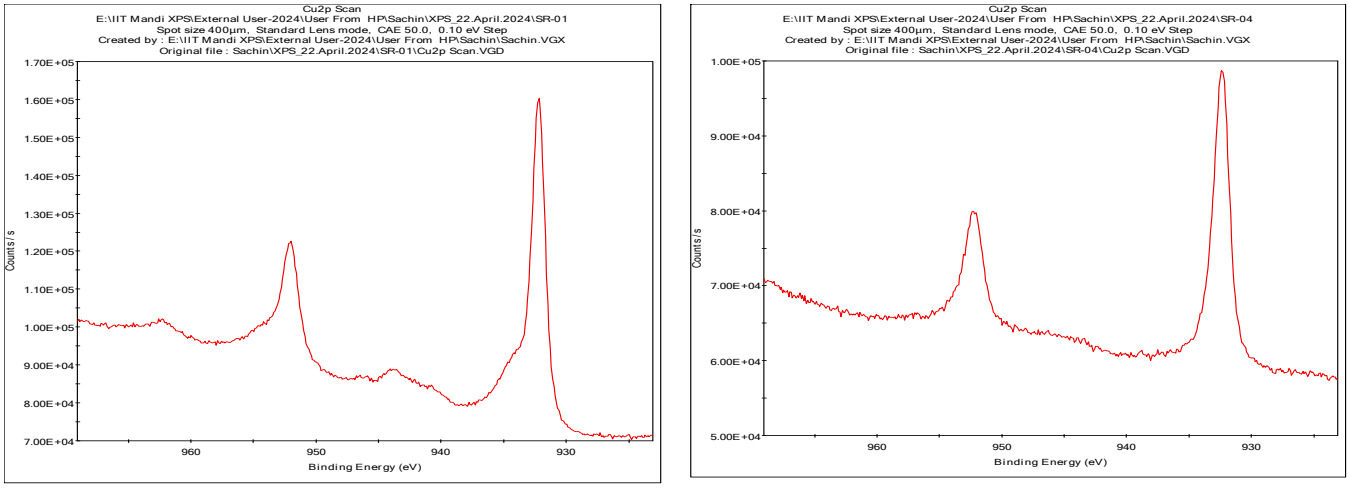


Figure S1: XPS spectra of Cu2p of standard Cu_2O (left) and recovered Cu from reaction mixture (right)

7.0 Procedure for the scale-up synthesis and post-transformations

7.1 Scale-up synthesis : In a round-bottom flask, equipped with a magenetic stir bar were added *N*- benzylisoquinolone **1a** (1175 mg, 5.0 mmol), vinyl acetate **2b** (1.38 ml, 3.0 equiv.), [CoCp*(CO)I_2] (240 mg, 10.0 mol%), $AgNTf_2$ (582 mg, 30 mol%) and Cu_2O (358 mg, 50 mol%) in TFE (25 ml, 0.2 M). The subsequent reaction mixture was stirred at 120°C for 24 h. Reaction mixture was allowed to cool to room temperature and diluted with ethyl acetate. Solvent was evaporated under reduced pressure and the crude mixture was purified by column chromatography using silica gel (230−400 mesh size) and hexane/EtOAc as the eluent to obtain 801 mg of **3r,** yield 61%.

7.2 Post transformation of 3a to 1-chloroisoquinoline (4) : The following general procedure was adopted for the synthesis of 1-chloroisoquinoline **4** , In a round-bottom flask, equipped with a magenetic stir bar was added **3a** (137.5 mg, 0.5 mmol), trifluoromethanesulfonic acid (8.0 mL). The resulting mixture was heated to reflux while being stirred and monitored by TLC until the starting materials were consumed (about 10 h). The mixture was neutralized by addition of a 10% sodium hydroxide solution, then extracted with ethyl acetate (20.0 mL × 4). The organic layer was washed with brine, dried over Na_2SO_4 and concentrated. To a flask was added crude Isoquinolinone was dissolved in dry toluene (3 mL) and phosphoryl trichloride (6.8 equiv.) was added dropwise via the syringe to the stirred mixture. The reaction mixture was allowed to stir at 90 °C in an oil bath for 2 h. After cooling to ambient temperature, the solvent was removed under vacuum. and crude mixture was purified by column chromatography using silica gel (230−400 mesh size) and hexane/EtOAc as the eluent.

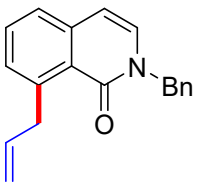
7.3 Post transformation of 3r to aldehyde (5) : The following general procedure was adopted for the synthesis of **5**, which were carried out with 0.2 mmol isoquinolone **3r** . The substrate was

dissolved in a mixture of degassed DMF (2 mL) and degassed water (0.2 mL). Once dissolution was complete, the palladium(II) source (2.0 equiv) was added, and the reaction mixture stirred at room temperature. Solvent was evaporated under reduced pressure and the crude mixture was purified by column chromatography using silica gel (230−400 mesh size) and hexane/EtOAc as the eluent.

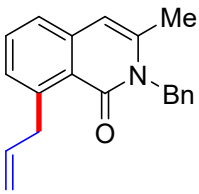
7.4 Post transformation of 3r to nitrile (6) : To an oven-dried screw cap reaction vial charged with NH_4HCO_3 (1.2 mmol) and CH_3OH/H_2O (2 mL/0.5 mL). The mixture was stirred at room temperature until the solid was completely dissolved. Then alkene isoquinolone **3r** was added. After stirring for 2 min, $PhI(OAc)_2$ (1.1 mmol) was added, and the reaction mixture was stirred at 36 °C for 12 h. After cooling to room temperature, the reaction mixture was diluted by addition of 20 mL ethyl acetate, dried over Na_2SO_4, filtered, and concentrated under vacuum. The crude residue was purified by column chromatography on silica gel to afford the desired product.

8. Characterization Data

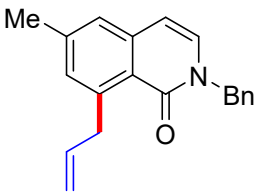
*8-allyl-2-benzylisoquinolin-1(2H)-one (Scheme 2, **3a**).* White solid, yield = 44.5 mg (81%). Mp = 38-40 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.51 (t, J = 7.5 Hz, 1H), 7.35 (dd, J = 8.0, 1.0 Hz, 1H), 7.33 – 7.26 (m, 6H), 7.05 (d, J = 7.0 Hz, 1H), 6.43 (d, J = 7.0 Hz, 1H), 6.23-6.15 (m, 1H), 5.18 (s, 2H), 5.04-5.03 (m, 1H), 5.02 – 5.00 (m, 1H), 4.23 (dt, J = 6.0, 2.0 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.5, 143.8, 139.1, 138.7, 137.2, 131.8, 131.3, 129.5, 128.9, 127.9, 127.8, 125.0, 124.2, 115.0, 106.8, 51.7, 40.1. IR (ZnSe): ν_{max} (cm^{-1}) 2978, 2940, 2904, 1651, 1619, 1435, 1367, 1283, 1024, 915, 816, 704, 697.; HRMS (ESI-TOF) m/z calcd for $C_{19}H_{18}NO$ $[M+H]^+$ 276.1383; found 276.1383.



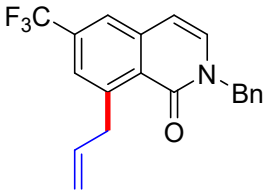
*8-allyl-2-benzyl-3-methylisoquinolin-1(2H)-one (Scheme 2, **3b**).* White solid, yield = 45.1 mg (78%). Mp = 78-80 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.51 (t, J = 7.5 Hz, 1H), 7.30 – 7.27 (m, 3H), 7.24 – 7.20 (m, 2H), 7.15 – 7.12 (m, 2H), 6.32-6.31 (m, 1H), 6.23 – 6.15 (m, 1H), 5.38 (s, 2H), 5.04 – 5.03 (m, 1H), 5.01-4.99 (m, 1H), 4.20 (d, J = 6.5 Hz, 2H), 2.30 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 163.5, 143.7, 139.4, 138.8, 138.7, 137.5, 131.9, 128.8, 128.5, 127.1, 126.2, 124.1, 122.3, 114.9, 106.6, 47.0, 40.1, 20.6. IR (ZnSe): ν_{max} (cm^{-1}) 2940, 2921, 1651, 1612, 1571, 1411, 1398, 1370, 1313, 1295, 1235, 1072, 963, 920, 747, 703, 688.; HRMS (ESI-TOF) m/z calcd for $C_{20}H_{20}NO$ $[M+H]^+$ 290.1539; found 290.1539.



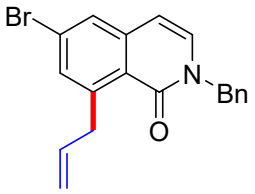
*8-allyl-2-benzyl-6-methylisoquinolin-1(2H)-one (Scheme 2, **3c**).* yellow oil, yield = 32.3 mg (56%).1H NMR (500 MHz, $CDCl_3$, δ): 7.33 – 7.26 (m, 5H), 7.14 (s, 1H), 7.10 (s, 1H), 7.02 (d, J = 7.5 Hz, 1H), 6.36 (d, J = 7.0 Hz, 1H), 6.23 – 6.15 (m, 1H), 5.17 (s, 2H), 5.05 – 5.01 (m, 2H), 4.19 (d, J = 6.5 Hz, 2H), 2.41 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.5, 143.6, 142.2, 139.3, 138.8, 137.4, 131.3, 131.0, 128.8, 127.8, 127.7, 124.8, 121.9, 114.9, 106.6, 51.6, 40.1, 21.5. IR (ZnSe): ν_{max} (cm^{-1}) 2942, 2831, 1652, 1607, 1450, 1121, 1022, 741, 703.; HRMS (ESI-TOF) m/z calcd for $C_{20}H_{20}NO$ $[M+H]^+$ 290.1539; found 290.1537.



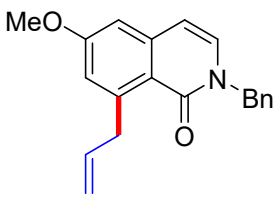
*8-allyl-2-benzyl-6-(trifluoromethyl)isoquinolin-1(2H)-one (Scheme 2, **3d**).* liquid red, yield = 43.9 mg (64%). ^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.63-7.64 (m, 1H), 7.48-7.45 (m, 1H), 7.35 – 7.32 (m, 2H), 7.30 – 7.28 (m, 3H), 7.16 (d, J = 7.5 Hz, 1H), 6.49 (d, J = 7.5 Hz, 1H), 6.20-6.12 (m, 1H), 5.19 (s, 2H), 5.10 – 5.033 (m, 2H), 4.25 (d, J = 6.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 161.8, 145.5, 139.1, 137.4, 136.7, 132.7, 129.0, 128.0 ($J_{C\text{-}F}$ = 11.25 Hz, 1C), 126.1, 125.0 ($J_{C\text{-}F}$ = 1.25 Hz, 1C), 122.06 ($J_{C\text{-}F}$ = 3.75 Hz, 1C), 116.1, 106.5, 52.0, 40.1 . ^{19}F NMR (471 MHz, $CDCl_3$, δ): -63.11. IR (ZnSe): ν_{max} (cm^{-1}) 2942, 2867, 1656, 1629, 1569, 1450, 1436, 1351, 1323, 1166, 1123, 923, 892, 822, 699.; HRMS (ESI-TOF) m/z calcd for $C_{20}H_{17}F_3NO$ $[M+H]^+$ 344.1257; found 344.1256.



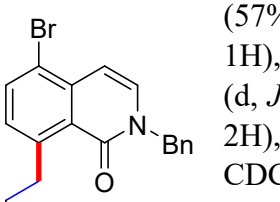
*8-allyl-2-benzyl-6-bromoisoquinolin-1(2H)-one (Scheme 2, **3e**).* White solid, yield = 52.1 mg (73%). Mp = 90-92 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.51 (d, J = 2.0 Hz, 1H), 7.38 (d, J = 2.0 Hz, 1H), 7.35 – 7.32 (m, 2H), 7.30 – 7.27 (m, 3H), 7.08 (d, J = 7.0 Hz, 1H), 6.33 (d, J = 7.0 Hz, 1H), 6.18 – 6.10 (m, 1H), 5.15 (s, 2H), 5.09 – 5.03 (m, 2H), 4.17 (d, J = 6.5 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.1, 146.1, 140.4, 137.6, 136.9, 132.5, 132.0, 128.98, 128.96, 127.98, 127.95, 127.2, 126.6, 122.8, 115.9, 105.6, 51.8, 39.8. IR (ZnSe): ν_{max} (cm^{-1}) 3063, 2970, 1645, 1628, 1611, 1592, 1581, 1397, 1162, 908, 850, 723, 689, 681.; HRMS (ESI-TOF) m/z calcd for $C_{19}H_{17}BrNO$ $[M+H]^+$ 354.0488; found 354.0483.



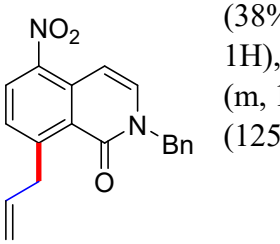
*8-allyl-2-benzyl-6-methoxyisoquinolin-1(2H)-one (Scheme 2, **3f**).* White solid, yield = 45.8 mg (75%). Mp = 69-71 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.34 – 7.31 (m, 4H), 7.29 – 7.27 (m, 1H), 7.03 (d, J = 7.0 Hz, 1H), 6.87 (d, J = 2.5 Hz, 1H), 6.72 (d, J = 2.5 Hz, 1H), 6.35 (d, J = 7.0 Hz, 1H), 6.21 – 6.13 (m, 1H), 5.16 (s, 2H), 5.06-5.02 (m, 2H), 4.18 (dd, J = 6.4 , 1.5 Hz, 2H), 3.85 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.2, 161.7, 146.2, 141.3, 138.3, 137.4, 131.9, 128.8, 127.8, 127.7, 118.4, 118.2, 115.3, 106.6, 105.7, 55.4, 51.5, 40.2. IR (ZnSe): ν_{max} (cm^{-1}) 2976, 2900, 1650, 1631, 1596, 1504, 1381, 1260, 1205, 777, 732, 707, 694.; HRMS (ESI-TOF) m/z calcd for $C_{20}H_{20}NO_2$ $[M+H]^+$ 306.1489; found 306.1489.



*8-allyl-2-benzyl-5-bromoisoquinolin-1(2H)-one (Scheme 2, **3g**).* White solid, yield = 40.3 mg (57%). Mp = 65-67 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.77 (d, J = 8.5 Hz, 1H), 7.35 – 7.32 (m, 2H), 7.30-7.27 (m, 3H), 7.16 (d, J = 8.0 Hz, 1H), 7.13 (d, J = 8.0 Hz, 1H), 6.86 (d, J = 7.5 Hz, 1H), 6.19 – 6.11 (m, 1H), 5.18 (s, 2H), 5.05 – 4.98 (m, 2H), 4.16 (dt, J = 6.0, 1.5 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, δ): 161.8, 143.7, 138.0, 137.8, 136.7, 135.7, 132.5, 130.0, 129.0, 128.0, 127.9, 125.6, 119.0, 115.4, 105.3, 51.9, 40.1 . IR (ZnSe): ν_{max} (cm^{-1}) 3076, 2922, 1649, 1619, 1474, 1425, 1360, 1322, 869, 836, 783, 743, 728, 707, 696.; HRMS (ESI-TOF) m/z calcd for $C_{19}H_{17}BrNO$ $[M+H]^+$ 354.0488; found 354.0486.

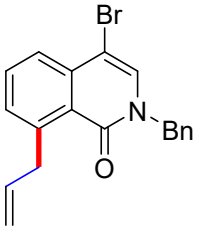


*8-allyl-2-benzyl-5-nitroisoquinolin-1(2H)-one (Scheme 2, **3h**).* Yellow solid, yield = 24.3 mg (38%). Mp = 71-73 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.19 (d, J = 8.0 Hz, 1H), 7.35-728 (m, 6H), 7.24-7.23 (m, 1H), 7.19 (d, J = 8.0 Hz, 1H), 6.15-6.07 (m, 1H), 5.17 (s, 2H), 5.09 – 5.02 (m, 2H), 4.23 (d, J = 6.5 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, δ): 161.1, 151.3, 143.9, 136.7, 136.2, 134.8, 132.6, 129.1,

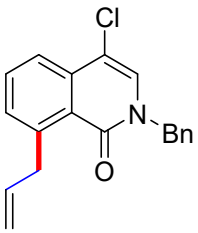


128.5, 128.4, 128.2, 128.0, 125.5, 116.5, 100.5, 52.1, 40.8. IR (ZnSe): ν_{max} (cm^{-1}) 3068, 2989, 2952, 1648, 1632, 1622, 1540, 1505, 1374, 1317, 1301, 1226, 757, 695.; HRMS (ESI-TOF) m/z calcd for $C_{19}H_{17}N_2O_3$ $[M+H]^+$ 321.1234; found 321.1231.

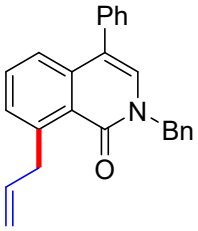
8-allyl-2-benzyl-4-chloroisoquinolin-1(2H)-one (Scheme 2, ***3i****).* White solid, yield = 43.1 mg (61%). Mp = 98-100 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.75(dd, J = 8.0 Hz, 1.5 Hz, 1H), 7.65 (t, J = 8.0 Hz , 1H), 7.38 – 7.33 (m, 4H), 7.33 – 7.30 (m, 3H), 6.21– 6.13(m, 1H), 5.16 (s, 2H), 5.06 – 4.98 (m, 2H), 4.22 (d, J = 6.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 161.6, 144.3, 138.3, 137.1, 136.6, 132.6, 132.0, 130.8, 129.0, 128.1, 128.0, 125.1, 124.4, 115.3, 100.3, 51.8, 40.1. IR (ZnSe): ν_{max} (cm^{-1}) 3068, 3000, 1644, 1623, 1607, 1481, 1372, 1179, 1154, 913, 896, 786, 752, 732, 695.; HRMS (ESI-TOF) m/z calcd for $C_{19}H_{17}BrNO$ $[M+H]^+$ 354.0488; found 354.0484.



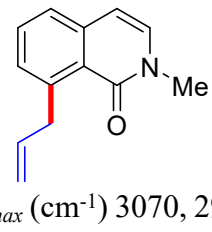
8-allyl-2-benzyl-4-chloroisoquinolin-1(2H)-one (Scheme 2, ***3j****).* White solid, yield = 41.4 mg (67%). Mp = 99-101 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.79 (dd, J = 8.0, 1.0 Hz, 1H), 7.64 (t, J = 8.0 Hz, 1H), 7.39 – 7.33 (m, 3H), 7.32 – 7.28 (m, 3H), 7.23 (s, 1H), 6.22-6.14 (m, 1H), 5.16 (s, 2H), 5.06 – 4.99 (m, 2H), 4.23 (dt, J = 1.5, 6.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 161.4, 144.3, 138.2, 136.5, 136.4, 132.4, 130.8, 129.3, 129.0, 128.1, 128.0, 124.1, 122.4, 115.3, 111.5, 51.7, 40.0. IR (ZnSe): ν_{max} (cm^{-1}) 3069, 1648, 1626, 1609, 1507, 1373, 1151, 1000, 955, 913, 903, 831, 786, 760, 714, 695.; HRMS (ESI-TOF) m/z calcd for $C_{19}H_{17}ClNO$ $[M+H]^+$ 310.0993; found 310.0990.



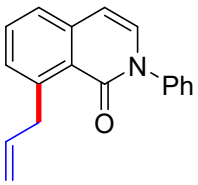
8-allyl-2-benzyl-4-phenylisoquinolin-1(2H)-one (Scheme 3, ***3k****).* colourless oil, yield = 39.3 mg (56%). 1H NMR (500 MHz, $CDCl_3$, δ) 7.40 – 7.33 (m, 4H), 7.32 – 7.29 (m, 2H), 7.27 – 7.26 (m, 2H), 7.25 – 7.17 (m, 5H), 6.95 (s, 1H), 6.20 – 6.12 (m, 1H), 5.15 (s, 2H), 5.00 – 4.98 (m, 1H), 4.97 (t, J = 1.5 Hz, 1H), 4.21 (dt, J = 6.5, 1.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.0, 144.1, 138.7, 138.5, 137.2, 137.0, 131.7, 130.5, 130.3, 129.8, 128.9, 128.7, 127.9, 127.8, 127.7, 124.0, 123.8, 119.9, 115.0, 51.8, 40.4. IR (ZnSe): ν_{max} (cm^{-1}) 2942, 2830, 1652, 1621, 1598, 1426, 1243, 1045, 1023, 862, 787, 701.; HRMS (ESI-TOF) m/z calcd for $C_{25}H_{22}NO$ $[M+H]^+$ 352.1696; found 352.1692.



8-allyl-2-methylisoquinolin-1(2H)-one (Scheme 2, ***3l****).* White solid, yield = 26.6 mg (67%). Mp = 34-36 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.50 (t, J = 7.5 Hz, 1H), 7.35 (dd, J = 8.0, 1.0 Hz, 1H), 7.25 – 7.24 (m, 1H), 7.04 (d, J = 7.5 Hz, 1H), 6.41 (d, J = 7.5 Hz, 1H), 6.23-6.15 (m, 1H), 5.03 – 4.97 (m, 2H), 4.19 (d, J = 6.5 Hz, 2H), 3.53 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.9, 143.2, 139.3, 138.7, 132.3, 131.6, 129.4, 124.9, 123.9, 114.9, 106.3, 40.0, 37.5. IR (ZnSe): ν_{max} (cm^{-1}) 3070, 2924, 1774, 1648, 1631, 1595, 1567, 1504, 1489, 1460, 1437, 1364, 1345, 1327, 1293, 1152, 1015, 944, 903, 854, 813, 790, 690, 654, 643.; HRMS (ESI-TOF) m/z calcd for $C_{13}H_{14}NO$ $[M+H]^+$ 200.1070; found 200.1070.

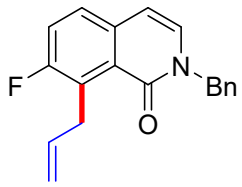


8-allyl-2-phenylisoquinolin-1(2H)-one (Scheme 2, ***3m****).* White solid, yield = 31.3 mg (60%). Mp = 96-98 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 7.56 (t, J = 7.5 Hz, 1H), 7.51 – 7.48 (m, 2H), 7.42 – 7.39 (m, 4H), 7.32 (dd, J = 7.0, 1Hz, 1H), 7.15 (d, J = 7.5 Hz, 1H), 6.51 (d, J = 7.5 Hz, 1H), 6.23 – 6.15 (m, 1H), 5.04-7.01 (m, 1H), 5.00 (t, J = 1.5 Hz, 1H), 4.18 (d, J = 6.5 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$,

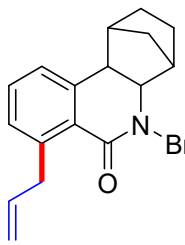


δ): 162.5, 144.2, 141.8, 139.2, 138.6, 132.1, 132.0, 129.7, 129.4, 128.1, 127.2, 125.0, 124.3, 115.0, 106.6, 40.1. IR (ZnSe): ν_{max} (cm^{-1}) 2984, 2919, 1651, 1633, 1603, 1592, 1508, 1348, 1269, 1059, 776, 759, 714, 693.; HRMS (ESI-TOF) m/z calcd for $C_{18}H_{16}NO$ $[M+H]^+$ 262.1226; found 262.1228.

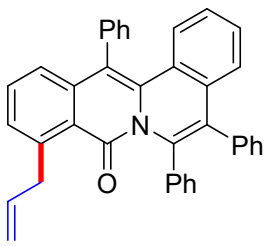
8-allyl-2-benzyl-7-fluoroisoquinolin-1(2H)-one (Scheme 2, ***3n****).* White solid, yield = 20.5 mg (35%). Mp = 60-62 °C. 1H NMR (500 MHz, $CDCl_3$, δ): 7.35 – 7.28 (m, 5H), 7.24 – 7.18 (m, 2H), 7.12 (d, J = 7.5 Hz, 1H), 6.68 (d, J = 7.5 Hz, 1H), 6.20 – 6.12 (m, 1H), 5.19 (s, 2H), 5.05 – 4.97 (m, 2H), 4.16 (d, J = 6.5 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$, δ): 161.70 ($J_{C\text{-}F}$ = 2.5 Hz, 1C), 157.2, 155.2, 139.28 ($J_{C\text{-}F}$ = 5.0 Hz, 1C), 138.48 ($J_{C\text{-}F}$ = 1.25 Hz, 1C), 136.9, 132.09 ($J_{C\text{-}F}$ = 2.5 Hz, 1C), 129.24 ($J_{C\text{-}F}$ = 7.5 Hz, 1C), 128.9, 128.2 , 128.0, 127.96 ($J_{C\text{-}F}$ = 1.25 Hz, 1C), 125.15 ($J_{C\text{-}F}$ = 3.75 Hz, 1C), 116.67 ($J_{C\text{-}F}$ = 20.0 Hz, 1C) , 115.2, 98.8 ($J_{C\text{-}F}$ = 7.5 Hz, 1C), 51.9, 39.5. ^{19}F NMR (125 MHz, $CDCl_3$, δ): -124.29. IR (ZnSe): ν_{max} (cm^{-1}) 3067, 2972, 2926, 1648, 1632, 1609, 1572, 1559, 1516, 1490, 1387, 1372, 1338, 1192, 1180, 1090, 1044, 913, 858, 744, 696.; HRMS (ESI-TOF) m/z calcd for $C_{19}H_{17}FNO$ $[M+H]^+$ 294.1289; found 294.1288.



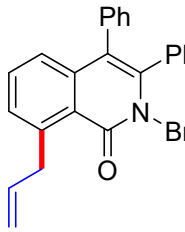
7-allyl-5-benzyl-1,3,4,4a,5,10b-hexahydro-1,4-methanophenanthridin-6(2H)-one (Scheme 2, ***3o****).* colourless oil, yield = 50.1 mg (73%). 1H NMR (500 MHz, $CDCl_3$, δ) 7.35 – 7.25 (m, 5H), 7.13 (d, J = 7.5 Hz, 1H), 7.08 (d, J = 7.5 Hz, 1H), 6.18 – 6.12 (m, 1H), 5.49 (d, J = 15.0 Hz, 1H), 5.02 – 4.98 (m, 2H), 4.16 – 4.12 (m, 2H), 4.07 – 3.99 (m, 1H), 3.55 (dd, J = 9.0, 1.0 Hz, 1H), 3.18 (d, J = 9.5 Hz, 1H), 2.52 (d, J = 3.0 Hz, 1H), 2.28 (d, J = 2.5 Hz, 1H), 1.67 – 1.43 (m, 5H), 1.22 – 1.78 (m, 1H), 1.11 (dt, J = 10.5, 1.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 163.2, 143.1, 141.6, 138.9, 137.7, 131.5, 130.0, 128.6, 127.9, 127.1, 127.1, 124.4, 114.6, 62.4, 49.4, 48.7, 45.3, 42.4, 40.6, 32.3, 29.2, 26.8. IR (ZnSe): ν_{max} (cm^{-1}) 2967, 2889, 1642, 1593, 1475, 1455, 1359, 1332, 1289, 1267, 1076, 1035, 982, 909, 788, 757, 699.; HRMS (ESI-TOF) m/z calcd for $C_{24}H_{26}NO$ $[M+H]^+$ 344.2009; found 344.2010.



9-allyl-5,6,13-triphenyl-8H-isoquinolino[3,2-a]isoquinolin-8-one (Scheme 2, ***3p****).* yellow solid, yield = 30.78 mg (30%), Mp = 169-171 °C. 1H NMR (500 MHz, $CDCl_3$, δ): 7.67 – 7.50 (m, 3H), 7.48 – 7.43 (m, 3H), 7.27 – 7.21 (m, 4H), 7.17 – 7.10 (m, 7H), 7.07 – 7.05 (m, 3H), 7.03 (d, J = 8.5 Hz, 1H), 6.88 – 6.84 (m, 1H), 5.80 – 5.72 (m, 1H), 4.93 – 4.89 (m, 1H), 4.86 – 4.83 (m, 1H), 3.77 (d, J = 6.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 163.7, 142.4, 139.3, 138.2, 137.4, 136.6, 136.4, 133.5, 133.4, 132.3, 131.7, 131.6, 129.8, 129.2, 128.9, 128.56, 128.54, 128.1, 128.0, 127.4, 127.0, 126.9, 126.3, 126.0, 125.7, 124.4, 123.8, 116.2, 115.2, 39.4. IR (ZnSe): ν_{max} (cm^{-1}) 2926, 2852, 1678, 1664, 1515, 1477, 1381, 1290, 944, 942, 750, 716, 694.; HRMS (ESI-TOF) m/z calcd for $C_{38}H_{28}NO$ $[M+H]^+$ 514.2165; found 514.2162.



8-allyl-2-benzyl-3,4-diphenylisoquinolin-1(2H)-one (Scheme 2, ***3q****).* White solid, yield = 52.09 mg (61%). Mp = 64-66 °C. 1H NMR (500 MHz, $CDCl_3$, δ): 7.44 (t, J = 7.5 Hz, 1H), 7.33 (d, J = 6.5 Hz, 1H), 7.18 – 7.15 (m, 4H), 7.14 – 7.09 (m, 3H), 7.05 – 7.02 (m, 5H), 6.91-6.89 (m, 4H), 6.31-6.23 (m, 1H), 5.22 – 5.05 (m, 4H), 4.32 (d, J = 6.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.2, 143.8, 141.5, 139.4, 138.8, 138.0, 137.2, 134.7, 131.7, 130.3, 129.4, 128.3, 128.1, 127.0, 127.7, 126.8, 124.6, 123.1, 119.4, 115.0, 49.1, 40.6 . IR (ZnSe): ν_{max}



(cm^{-1}) 3067, 2972, 1645, 1619, 1591, 1507, 1491, 1476, 1430, 1390, 1309, 1091, 1071, 1042, 903, 857, 783, 758, 696.; HRMS (ESI-TOF) m/z calcd for $C_{31}H_{26}NO$ $[M+H]^+$ 428.2009; found 428.2009.

*2-benzyl-8-vinylisoquinolin-1(2H)-one (Scheme 2, **3r**).* White solid, yield = 43.8 mg (84%). Mp = 120-122 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.16 (dd, J = 17.5, 11.0 Hz, 1H), 7.56 (t, J = 7.5 Hz, 1H), 7.50 (d, J = 7.0 Hz, 1H), 7.41 (d, J = 7.5 Hz, 1H), 7.31-7.29 (m, 4H), 7.29-7.27 (m, 1H), 7.07 (d, J = 7.5 Hz, 1H), 6.44 (d, J = 7.5 Hz, 1H), 5.51 (dd, J = 17.0 Hz,1.5 Hz, 1H), 5.35 (dd, J = 11.0 Hz,1.5 Hz, 1H), 5.18 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.7, 142.2, 139.3, 138.5, 137.16, 131.9, 131.4, 128.9, 128.0, 127.8, 127.0, 126.1, 123.4, 115.3, 106.7, 51.8. IR (ZnSe): ν_{max} (cm^{-1}) 2922, 2857, 1652, 1624, 1579, 1366, 1274, 826, 731, 695.; HRMS (ESI-TOF) m/z calcd for $C_{18}H_{16}NO$ $[M+H]^+$ 262.1226; found 262.1226.

*2-benzyl-6-methyl-8-vinylisoquinolin-1(2H)-one (Scheme 2, **3s**).* White solid, yield = 41.0 mg (74%). Mp = 60-62 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ) 8.13 (dd, J = 17.5, 11.0 Hz, 1H), 7.33 – 7.29 (m, 6H), 7.20 (s, 1H), 7.04 (d, J = 7.5 Hz, 1H), 6.37 (d, J = 7.0 Hz, 1H), 5.50 (dd, J = 17.5, 1.5 Hz, 1H), 5.33 (dd, J = 11.0, 1.5 Hz, 1H), 5.17 (s, 2H), 2.44 (s, 3H).); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.6, 142.3, 142.0, 139.3, 138.7, 137.2, 131.4, 128.9, 128.5, 128.0, 127.8, 125.9, 121.2, 115.1, 106.5, 51.6, 21.7. IR (ZnSe): ν_{max} (cm^{-1}) 2944, 2920, 1647, 1633, 1610, 1507, 876, 859, 834, 729, 730, 681, 670, 635.; HRMS (ESI-TOF) m/z calcd for $C_{19}H_{18}NO$ $[M+H]^+$ 276.1383; found 276.1383.

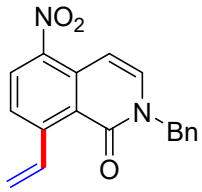
*2-benzyl-6-phenyl-8-vinylisoquinolin-1(2H)-one (Scheme 2, **3t**).* White solid, yield = 27.7 mg (41%). Mp = 71-73 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ) 8.19 (dd, J = 17.0, 10.5 Hz, 1H), 7.73-7.72 (m, 1H), 7.70 – 7.68 (m, 2H), 7.61 (d, J = 2.0 Hz, 1H), 7.50-7.47 (m, 2H), 7.43-7.41 (m, 1H), 7.35 – 7.32 (m, 5H), 7.10 (d, J = 7.5 Hz, 1H), 6.50 (d, J = 7.0 Hz, 1H), 5.59 (dd, J = 17.0, 1.5 Hz, 1H), 5.40 (dd, J = 11.0, 1.5 Hz, 1H), 5.20 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.6, 144.5, 142.8, 139.9, 139.3, 139.0, 137.1, 131.8, 129.0, 128.9, 128.3, 128.0, 127.9, 127.5, 126.2, 124.1, 122.2, 115.6, 106.8, 51.8. IR (ZnSe): ν_{max} (cm^{-1}) 3000, 2929, 1648, 1615, 1517, 1363, 1263, 1269, 1074, 881, 764, 695.; HRMS (ESI-TOF) m/z calcd for $C_{24}H_{20}NO$ $[M+H]^+$ 338.1539; found 338.1538.

*2-benzyl-6-(trifluoromethyl)-8-vinylisoquinolin-1(2H)-one (Scheme 2, **3u**).* White solid, yield = 43.2 mg (66%). Mp = 85-87 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ) 8.12 (dd, J = 17.5, 11.0 Hz, 1H), 7.68 – 7.65 (m, 2H), 7.36 - 729 (m, 5H), 7.16 (d, J = 7.5 Hz, 1H), 6.49 (d, J = 7.5 Hz, 1H), 5.58 (dd, J = 17.5 Hz, 1.5, 1H), 5.44 (dd, J = 10.5 Hz, 1.0 Hz, 1H), 5.19 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.0, 143.6, 138.6, 138.2, 136.6, 133.4 (J_{C-F} = 32.5 Hz, q, 1C), 132.8, 129.0, 128.1, 125.2, 124.7, 122.8 (q, m), 116.9, 106.3, 52.1, ^{19}F NMR (471 MHz, Chloroform-d) δ -63.28. IR (ZnSe): ν_{max} (cm^{-1}) 2926, 2855, 2154, 1648, 1635, 1616, 1572, 1200, 1159, 1140, 1111, 1083, 733, 708, 697.; HRMS (ESI-TOF) m/z calcd for $C_{19}H_{15}F_3NO$ $[M+H]^+$ 330.1100; found 330.1100.

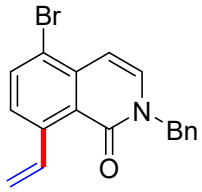
*2-benzyl-6-bromo-8-vinylisoquinolin-1(2H)-one (Scheme 2, **3v**).* White solid, yield = 47.4 mg (70%). Mp = 115-117 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ) 8.06 (dd, J = 17.5, 11.0 Hz, 1H), 7.57 (d, J = 14.5, 1.5 Hz, 2H), 7.35– 7.28 (m, 5H),

7.09 (d, J = 7.5 Hz, 1H), 6.34 (d, J = 7.5 Hz, 1H), 5.53 (dd, J = 17.5 Hz, 1.5 Hz, 1H), 5.39 (d, J = 10.5 Hz, 1.5Hz, 1H), 5.15 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.31, 144.21, 139.93, 138.06, 136.81, 132.65, 129.78, 129.01, 128.21, 128.11, 128.04, 126.74, 122.11, 116.62, 105.57, 51.93. IR (ZnSe): ν_{max} (cm^{-1}) 3079, 2927, 1645, 1629, 1611, 1586, 1573, 1502, 1267, 770, 750, 721, 703, 673, 688.; HRMS (ESI-TOF) m/z calcd for $C_{18}H_{15}NO$ $[M+H]^+$ 340.0332; found 340.0329.

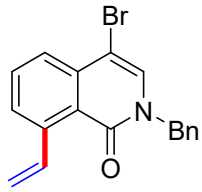
2-benzyl-5-nitro-8-vinylisoquinolin-1(2H)-one (Scheme 2, ***3w****).* White solid, yield = 17.7 mg (29%). Mp = 155-157 °C. 1H NMR (500 MHz, $CDCl_3$, δ) 8.26 (dd, J = 8.5, 0.5 Hz, 1H), 8.02 (dd, J = 17.0, 10.0 Hz, 1H), 7.49 (dd, J = 8.5, 0.5 Hz, 1H), 7.32-7.27 (m, 5H), 7.24 (d, J = 6.0 Hz, 1H), 7.21 (d, J = 7.5, 1H), 5.57 (dd, J = 17.0, 1.5 Hz, 1H), 5.48 (dd, J = 11.0, 1.5 Hz, 1H), 5.17 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 161.3, 148.5, 144.2, 138.5, 136.1, 134.9, 132.2, 129.1, 128.8, 128.3, 128.2, 126.2, 124.7, 118.1, 100.6, 52.2. IR (ZnSe): ν_{max} (cm^{-1}) 2953, 2939, 1655, 1639, 1627, 1598, 1531, 1501, 1416, 1338, 1312, 754, 729, 709.; HRMS (ESI-TOF) m/z calcd for $C_{18}H_{15}N_2O_3[M+H]^+$ 307.1077; found 307.1075.



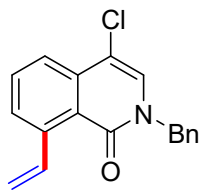
2-benzyl-5-bromo-8-vinylisoquinolin-1(2H)-one (Scheme 2, ***3x****).* White solid, yield = 35.3 mg (52%). Mp = 82-84 °C ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.02 (dd, J = 17.5, 11.0 Hz, 1H), 7.82 (d, J = 8.0 Hz, 1H), 7.35 – 7.27 (m, 6H), 7.17 (d, J = 7.5 Hz, 1H), 6.85 (d, J = 7.5 Hz, 1H), 5.48 (dd, J = 17.0, 1.5 Hz, 1H), 5.38 dd, J = 10.5, 1.5 Hz, 1H), 5.17 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.0, 142.0, 138.8, 137.3, 136.7, 135.8, 132.6, 129.0, 128.1, 120.0, 127.6, 124.7, 120.2, 115.7, 105.2, 52.0. IR (ZnSe): ν_{max} (cm^{-1}) 3066, 2946, 1644, 1630, 1611, 1410, 863, 835, 789, 742, 726, 717, 697, 641.; HRMS (ESI-TOF) m/z calcd for $C_{18}H_{15}BrNO$ $[M+H]^+$ 340.0332; found 340.0328.



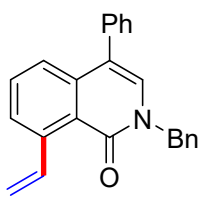
2-benzyl-4-bromo-8-vinylisoquinolin-1(2H)-one (Scheme 2, ***3y****).* White solid, yield = 42.1 mg (62%). Mp = 156-158 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ) 8.07 (dd, J = 17.5, 11.0, 1H), 7.80 (dd, J = 8.0, 1.0 Hz, 1H), 7.69-7.65(m, 1H), 7.57-7.55 (m, 1H), 7.36 (s, 1H), 7.35 – 7.29 (m, 5H), 5.51 (dd, J = 17.0, 1.5 Hz, 1H), 5.38 (dd, J = 11.0, 1.5 Hz, 1H), 5.15 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 161.8, 142.7, 139.0, 136.6, 136.4, 132.7, 132.1, 129.0, 128.4, 128.2, 126.0, 123.6, 115.9, 100.2, 51.9. IR (ZnSe): ν_{max} (cm^{-1}) 2934, 1673, 1545, 1486, 1452, 1380, 1351, 1293, 1214, 1110, 1074, 1029, 919, 861, 822, 754, 699.; HRMS (ESI-TOF) m/z calcd for $C_{18}H_{15}BrNO$ $[M+H]^+$ 340.0332; found 340.0320.



2-benzyl-4-chloro-8-vinylisoquinolin-1(2H)-one (Scheme 2, ***3z****).* White solid, yield = 25.3 mg (43%). Mp = 154-156 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.08 (dd, J = 17.5, 11.0 Hz, 1H), 7.83 (d, J = 8.0 Hz, 1H), 7.69 (t, J = 8.0 Hz, 1H), 7.57 (d, J = 7.5, 1H), 7.40-7.28 (m, 5H), 7.23 (s, 1H), 5.52 (dd, J = 17.0, 1.5 Hz, 1H), 5.39 (dd, J = 11.0, 1.5 Hz, 1H), 5.16 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 161.6, 142.7, 138.9, 136.4, 135.9, 132.6, 129.4, 129.1, 128.4, 128.2, 128.2, 123.4, 123.3, 115.9, 111.5, 51.9. IR (ZnSe): ν_{max} (cm^{-1}) 3079, 2826, 1644, 1623, 1603, 1504, 937, 907, 853, 761, 744, 733, 713, 698, 648.; HRMS (ESI-TOF) m/z calcd for $C_{18}H_{15}ClNO$ $[M+H]^+$ 296.0837; found 296.0837.

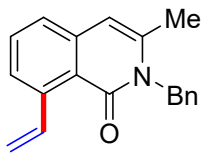


2-benzyl-4-phenyl-8-vinylisoquinolin-1(2H)-one (Scheme 2, ***3za****).* White solid, yield = 35.5 mg (52%). Mp = 125-127 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ) 8.18 (dd, J = 17.0,

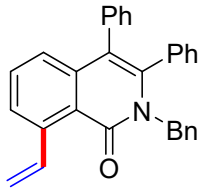


11.0 Hz, 1H), 7.52 – 7.51 (m, 2H), 7.45 – 7.39 (m, 4H), 7.36 – 7.31 (m, 6H), 7.29 – 7.27 (m, 1H), 7.05 (s, 1H), 5.52 (dd, J = 17.5, 1.5 Hz, 1H), 5.38 (dd, J = 10.5, 1.5 Hz, 1H), 5.23 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 162.2, 142.6, 137.9, 137.0, 136.8, 136.8, 130.6, 130.3, 128.9, 128.7, 128.1, 127.9, 127.8, 127.4, 124.8, 123.2, 119.8, 115.2, 51.9. IR (ZnSe): ν_{max} (cm^{-1}) 3047, 2951, 1648, 1630, 1607, 1507, 1414, 1365, 1230, 799, 761, 737, 724, 715, 696, 627.; HRMS (ESI-TOF) m/z calcd for $C_{24}H_{20}NO$ $[M+H]^+$ 338.1539; found 338.1539.

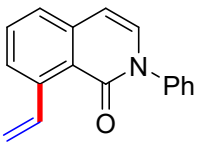
2-benzyl-3-methyl-8-vinylisoquinolin-1(2H)-one (Scheme 2, ***3zb****).* White solid, yield = 48.5 mg (88%). Mp = 117-119 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.13 (dd, J = 17.0, 10.5 Hz, 1H), 7.54 (t, J = 7.5 Hz, 1H), 7.45 (d, J = 7.5 Hz, 1H), 7.35 (dd, J = 7.5, 1.0 Hz, 1H), 7.30-7.27 (m, 2H), 7.24-7.20 (m, 1H), 7.16-7.14 (m, 2H), 6.34 (s, 1H), 5.51 (dd, J = 17.5, 1.5 Hz, 1H), 5.39-5.35 (m, 2H), 5.32 (dd, J = 11.0, 1.5 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, δ): 163.7, 142.1, 139.6, 139.3, 138.2, 137.4, 132.0, 128.8, 127.2, 126.2, 126.1, 125.2, 121.5, 115.1, 106.5, 47.1, 20.6 . IR (ZnSe): ν_{max} (cm^{-1}) 2988, 2956, 1651, 1634, 1611, 1464, 1399, 1345, 1276, 1160, 1075, 964, 856, 835, 751, 715, 683.; HRMS (ESI-TOF) m/z calcd for $C_{19}H_{18}NO$ $[M+H]^+$ 276.1383; found 276.1383.



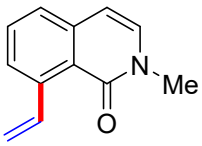
2-benzyl-3,4-diphenyl-8-vinylisoquinolin-1(2H)-one (Scheme 2, ***3zc****).* White solid, yield = 55.1 mg (66%). Mp = 144-146 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ): 8.21 (dd, J = 17.5, 11.0 Hz, 1H), 7.53 – 7.51 (m, 1H), 7.49-7.46 (m, 1H), 7.18-7.14 (m, 5H), 7.13 – 7.08 (m, 3H), 7.06 – 7.03 (m, 4H), 6.91 – 6.87 (m, 4H), 5.54 (dd, J = 17.0, 2.0 Hz, 1H), 5.38 (dd, J = 10.5, 2.0 Hz, 1H), 5.25 – 5.09 (m, 2H), ^{13}C NMR (125 MHz, $CDCl_3$, δ): 163.0, 142.3, 141.6, 139.8, 138.8, 137.9, 137.0, 134.5, 131.8, 131.7, 130.4, 128.3, 128.1, 128.0, 127.7, 127.1, 126.9, 126.8, 125.6, 122.4, 119.3, 115.1, 49.2. IR (ZnSe): ν_{max} (cm^{-1}) 3058, 2956, 1640, 1619, 1589, 1508, 1492, 1477, 1391, 1309, 1100, 718, 695, 628.; HRMS (ESI-TOF) m/z calcd for $C_{30}H_{24}NO$ $[M+H]^+$ 414.1852; found 414.1852.

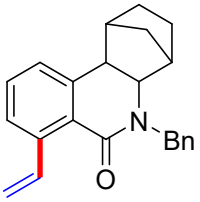


2-phenyl-8-vinylisoquinolin-1(2H)-one (Scheme 2, ***3zd****).* White solid, yield = 37.05 mg (75%). Mp = 138-140 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ) 8.08 (dd, J = 17.0, 10.0 Hz, 1H), 7.63-7.59 (m, 1H), 7.53 – 7.46 (m, 4H), 7.42 – 7.39 (m, 3H), 7.16 (d, J = 7.5 Hz, 1H), 6.53 (d, J = 7.5 Hz, 1H), 5.50 (dd, J = 17.5, 1.5 Hz, 1H), 5.30 (dd, J = 11.0, 1.5 Hz, 1H). ^{13}CNMR (125 MHz, $CDCl_3$, δ): 162.6, 142.6, 141.73, 139.2, 138.7, 132.3, 132.1, 129.4, 128.2, 127.3, 127.2, 126.1, 123.5, 115.4, 106.5. IR (ZnSe): ν_{max} (cm^{-1}) 2931, 1656, 1651, 1622, 1492, 1352, 1272, 868, 759, 715, 693.; HRMS (ESI-TOF) m/z calcd for $C_{17}H_{14}NO$ $[M+H]^+$ 248.1070; found 248.1072.

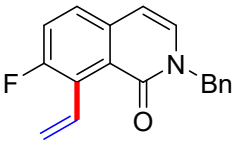


2-methyl-8-vinylisoquinolin-1(2H)-one (Scheme 2, ***3ze****).* White solid, yield = 23.7 mg (64%). Mp = 65-67 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ) 8.15 (dd, J = 17.5, 10.5 Hz, 1H), 7.55 – 7.52 (m, 1H), 7.47-7.46 (m, 1H), 7.41 (dd, J = 8.0, 1.5 Hz, 1H), 7.04 (d, J = 7.0 Hz, 1H), 6.43 (d, J = 7.5 Hz, 1H), 5.48 (dd, J = 17.0, 1.5 Hz, 1H), 5.34 (dd, J = 11.0, 1.5 Hz ,1H) 3.54 (s, 3H). ^{13}C NMR (125 MHz, Chloroform-d) δ 163.1, 141.9, 139.2, 138.6, 132.4, 131.7, 126.9, 126.0, 123.1, 115.3, 106.2, 37.4. IR (ZnSe): ν_{max} (cm^{-1}) 3074, 2951, 1650, 1610, 1362, 1345, 840, 820, 801, 785, 722, 681, 487.; HRMS (ESI-TOF) m/z calcd for $C_{12}H_{12}NO$ $[M+H]^+$ 186.0913; found 186.0913.

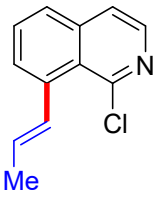


*5-benzyl-7-vinyl-1,3,4,4a,5,10b-hexahydro-1,4-methanophenanthridin-6(2H)-one (Scheme 2, **3zf**).* 

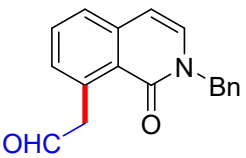
White solid, yield = 42.1 mg (64%). Mp = 105-107 °C. ^{1}H NMR (500 MHz, $CDCl_3$, δ) δ 7.87 (dd, J = 17.5, 11.0 Hz, 1H), 7.39 (t, J = 8.0 Hz, 1H), 7.32 – 7.27 (m, 5H), 7.14 (d, J = 7.5 Hz, 1H), 5.52 (d, J = 10.0 Hz, 1H), 5.41 (dd, J = 17.5, 2.0 Hz, 1H), 5.26 (dd, J = 11.0, 2.0 Hz, 1H), 4.12 (d, J = 15.0 Hz, 1H), 3.53 (dd, J = 9.0, 1.5 Hz, 1H), 3.17 (d, J = 9.0 Hz, 1H), 2.53 (d, J = 3.0 Hz, 1H), 2.29 (d, J = 2.5 Hz, 1H), 1.65 – 1.55 (m, 4H), 1.47 – 1.43 (m, 1H), 1.21 – 1.18 (m, 1H), 1.11 (dt, J = 10.5, 1.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 163.0, 141.6, 141.0, 140.1, 137.6, 131.7, 128.6, 128.1, 127.6, 127.2, 123.8, 113.9, 62.3, 49.3, 48.5, 45.2, 42.3, 32.4, 29.1, 26.9. IR (ZnSe): ν_{max} (cm^{-1}) 2960, 2926, 1621, 1516, 1470, 1369, 1256, 1209, 936, 907, 836, 717, 701, 632.; HRMS (ESI-TOF) m/z calcd for $C_{23}H_{24}NO$ $[M+H]^+$ 330.1852; found 330.1853.

*2-benzyl-7-fluoro-8-vinylisoquinolin-1(2H)-one (Scheme 2, **3zg**).* 

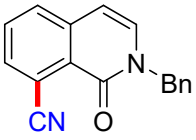
White solid, yield = 32.9 mg (59%). Mp = 51-53°C. ^{1}H NMR ((500 MHz, $CDCl_3$, δ) 8.05 (dd, J = 17.5, 11.0 Hz, 1H), 7.43 (dd, J = 8.5, 5.5 Hz, 1H), 7.35-7.30 (m, 5H), 7.29 – 7.27 (m, 1H), 7.14 (d, J = 7.5 Hz, 1H), 6.67 (d, J = 7.5 Hz, 1H), 5.46 (dd, J = 17.5, 1.5 Hz, 1H), 5.34 (dd, J = 11.0, 1.5 Hz, 1H), 5.18 (s, 2H).); ^{13}C NMR (125 MHz, $CDCl_3$, δ): 161.8, δ 158.1, 156.1, 138.4, 138.15 ($J_{C\text{-}F}$ = 5.0 Hz, 1C), 136.7, 132.21 ($J_{C\text{-}F}$ = 1.25 Hz, 1C) , 129.0, 128.0, 127.08 ($J_{C\text{-}F}$ = 7.0 Hz, 1C), 116.94 ($J_{C\text{-}F}$ = 22.5 Hz, 1C), 115.44 ($J_{C\text{-}F}$ = 2.5 Hz, 1C), 98.81($J_{C\text{-}F}$ = 7.5 Hz, 1C), 52.03, ^{19}F NMR (471 MHz, , $CDCl_3$, δ) -122.44. IR (ZnSe): ν_{max} (cm^{-1}) 3066, 2939, 1650, 1636, 1613, 1572, 1260, 1243, 1194, 745, 724, 706, 695, 633.; HRMS (ESI-TOF) m/z calcd for $C_{18}H_{15}NO$ $[M+H]^+$ 280.1132; found 280.1133.

*(E)-1-chloro-8-(prop-1-en-1-yl)isoquinoline (Scheme 5, **4**).* 

White solid, yield = 52.9 mg (52%). Mp = 44-46°C. ^{1}H NMR ((400 MHz, $CDCl_3$, δ) 8.21 (d, J = 5.6 Hz, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.64 - 7.59 (m, 1H), 7.56 – 7.43 (m, 3H), 5.90 (dq, J = 20.4, 6.8 Hz, 1H), 1.97 (dd, J = 6.8, 1.6 Hz, 3H).;^{13}C NMR (100 MHz, $CDCl_3$, δ): δ 197.0, 162.5, 139.1, 136.7, 136.2, 132.1, 131.6, 131.3, 129.0, 128.0, 127.9, 126.4, 124.1, 107.2, 51.8, 50.2. HRMS (ESI-TOF) m/z calcd for $C_{12}H_{11}ClN$ $[M+H]^+$ 204.0575; found 204.0582.

*2-(2-benzyl-1-oxo-1,2-dihydroisoquinolin-8-yl)acetaldehyde (Scheme 5, **5**).* 

White solid, yield = 34.3 mg (62%). Mp = 98-100°C. ^{1}H NMR ((500 MHz, $CDCl_3$, δ) 9.83 (s, 1H), 7.5(t, J = 7.5, 1H), 7.46 (dd, J = 8.0, 1.0 Hz, 1H), 7.35 – 7.31 (m, 3H), 7.29 - 7.27 (m, 2H), 7.24 - 7.21 (m, 1H), 7.09 (d, J = 7.5 Hz, 1H), 6.50 (d, J = 7.5 Hz, 1H), 5.17 (s, 2H), 4.33 (s, 2H).; ^{13}C NMR (125 MHz, $CDCl_3$, δ): δ 197.0, 162.5, 139.1, 136.7, 136.2, 132.1, 131.6, 131.3, 129.0, 128.0, 127.9, 126.4, 124.1, 107.2, 51.8, 50.2.;HRMS (ESI-TOF) m/z calcd for $C_{18}H_{16}NO_2$ $[M+H]^+$ 278.1176; found 278.1181.

*2-benzyl-1-oxo-1,2-dihydroisoquinoline-8-carbonitrile (Scheme 5, **6**).* 

White solid, yield = 35.36 mg (68%). Mp = 100-102°C. ^{1}H NMR ((500 MHz, $CDCl_3$, δ) 7.86 (dd, J = 7.0 Hz, 2.0 Hz, 1H), 7.70 - 7.65 (m, 2H), 7.37 - 7.29 (m, 5H), 7.19 (d, J = 7.5 Hz, 1H), 6.49 (d, J = 7.5 Hz, 1H), 5.23 (s, 2H).; ^{13}C NMR (125 MHz, $CDCl_3$, δ): 160.0 138.4, 136.3, 134.8, 133.1, 131.7, 130.6, 129.0, 128.4, 128.3, 118.7,

112.6, 105.7, 51.9.; HRMS (ESI-TOF) m/z calcd for $C_{17}H_{13}N_2O$ $[M+H]^+$ 261.1022; found 261.1026.

9.0 References

S1. Chandra, D., Kumar, N., Parmar, D., Gupta, P. and Sharma, U., **2021**. Co (iii)-catalysed regioselective linear C (8)–H olefination of isoquinolone with terminal aromatic and aliphatic alkynes. *Chemical Communications*, 57(88), 11613-11616.

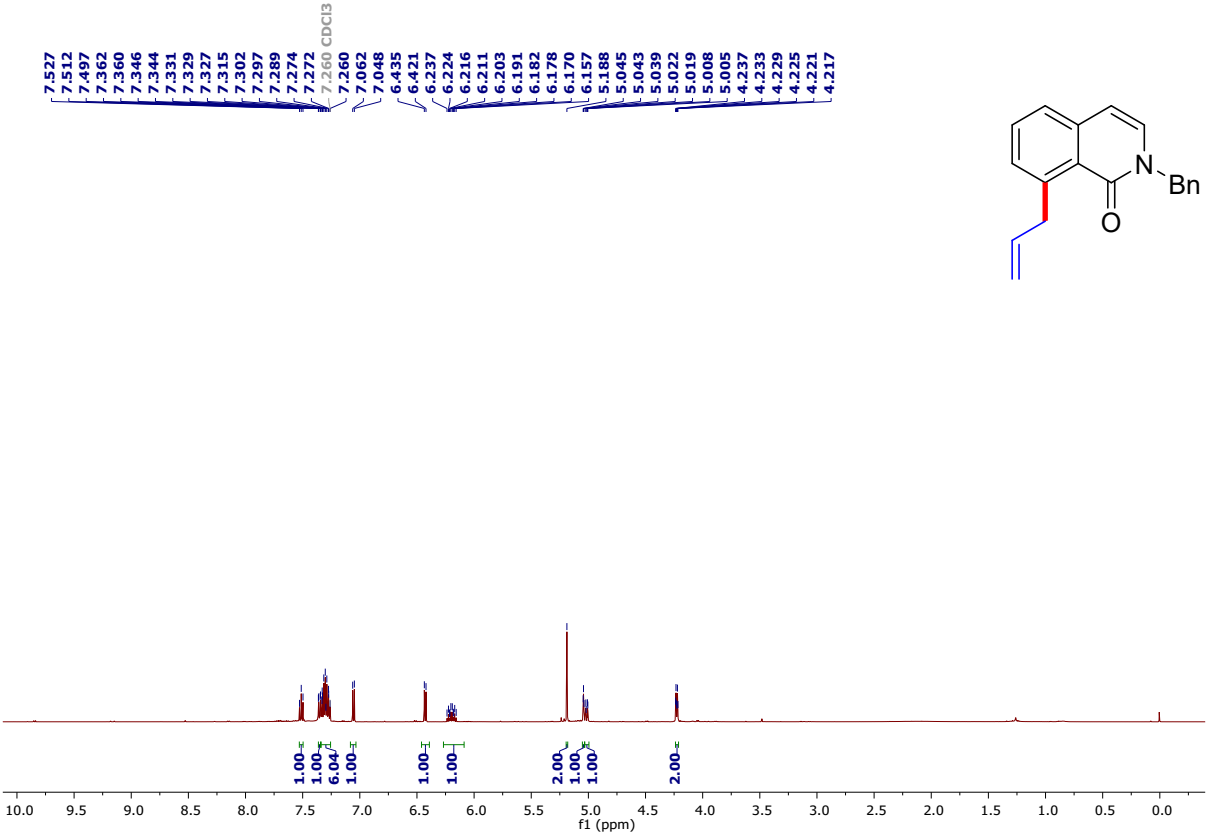
S2. Chandra, D., Sachin and Sharma, U., **2024**. Co (III)-Catalyzed Regioselective [4+ 2]-Annulation of N-Chlorobenzamide with Allenes and Vinyl Acetate. *Asian Journal of Organic Chemistry*, 13(1), e202300536.

S3. Guimond, N., Gorelsky, S.I. and Fagnou, K., **2011**. Rhodium (III)-catalyzed heterocycle synthesis using an internal oxidant: improved reactivity and mechanistic studies. *Journal of the American Chemical Society*, 133(16), 6449-6457.

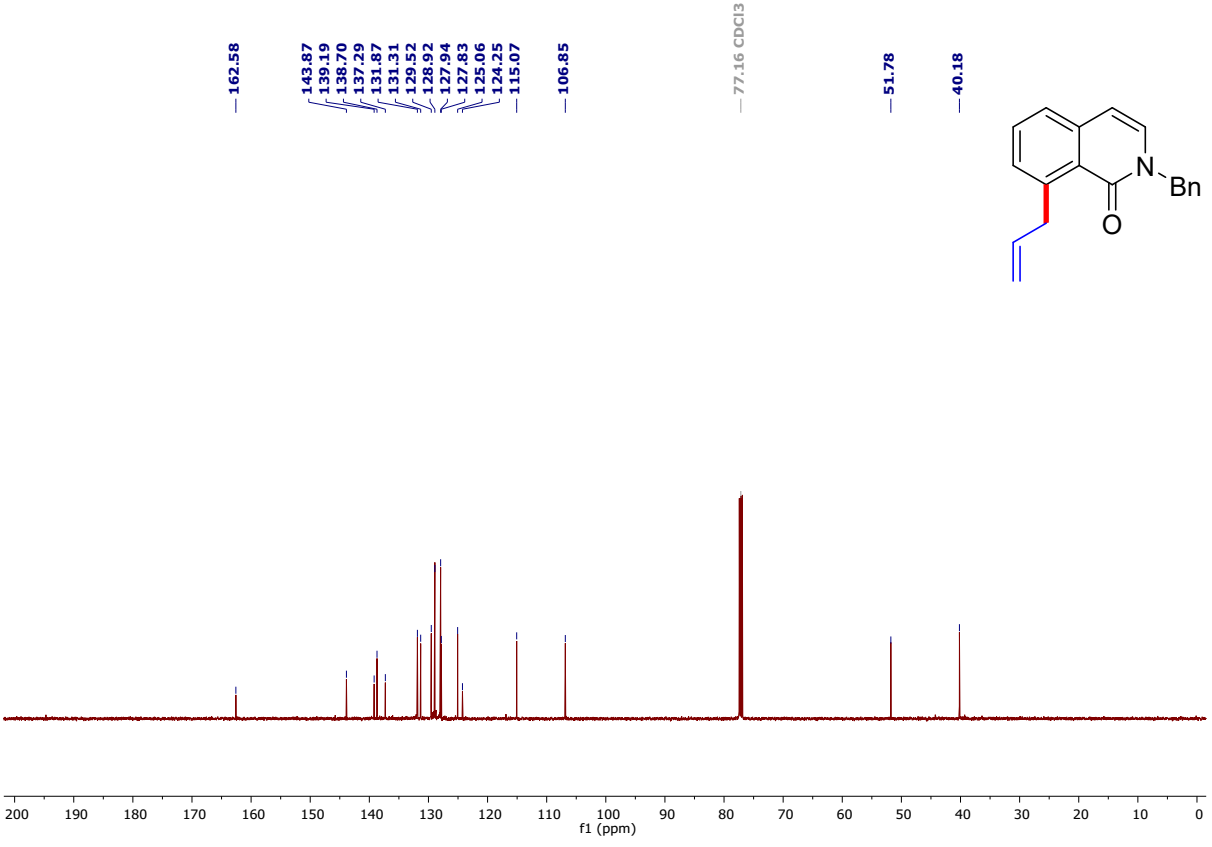
S4. Song, G., Chen, D., Pan, C.L., Crabtree, R.H. and Li, X., **2010**. Rh-catalyzed oxidative coupling between primary and secondary benzamides and alkynes: synthesis of polycyclic amides. *The Journal of Organic Chemistry*, 75(21), 7487-7490.

10 Copy of ^{1}H and ^{13}C NMR

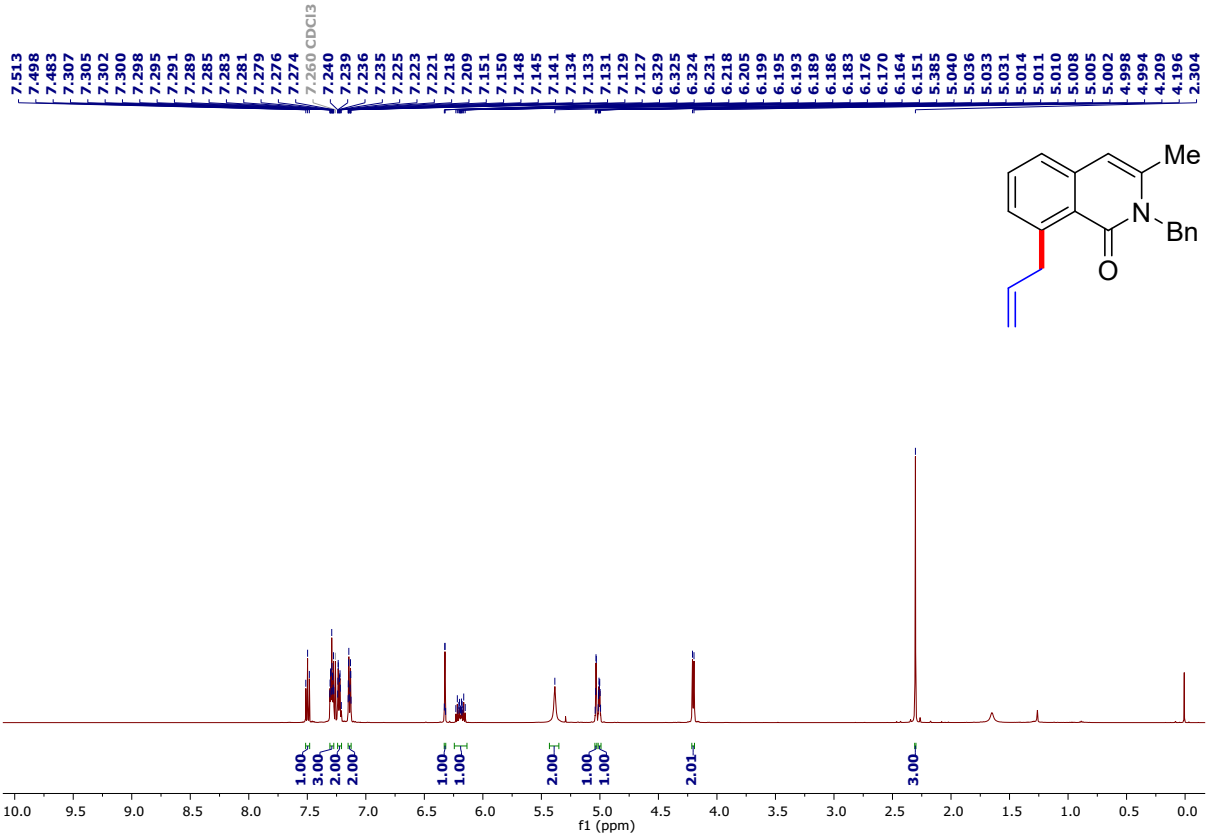
^{1}H NMR spectrum of 3a



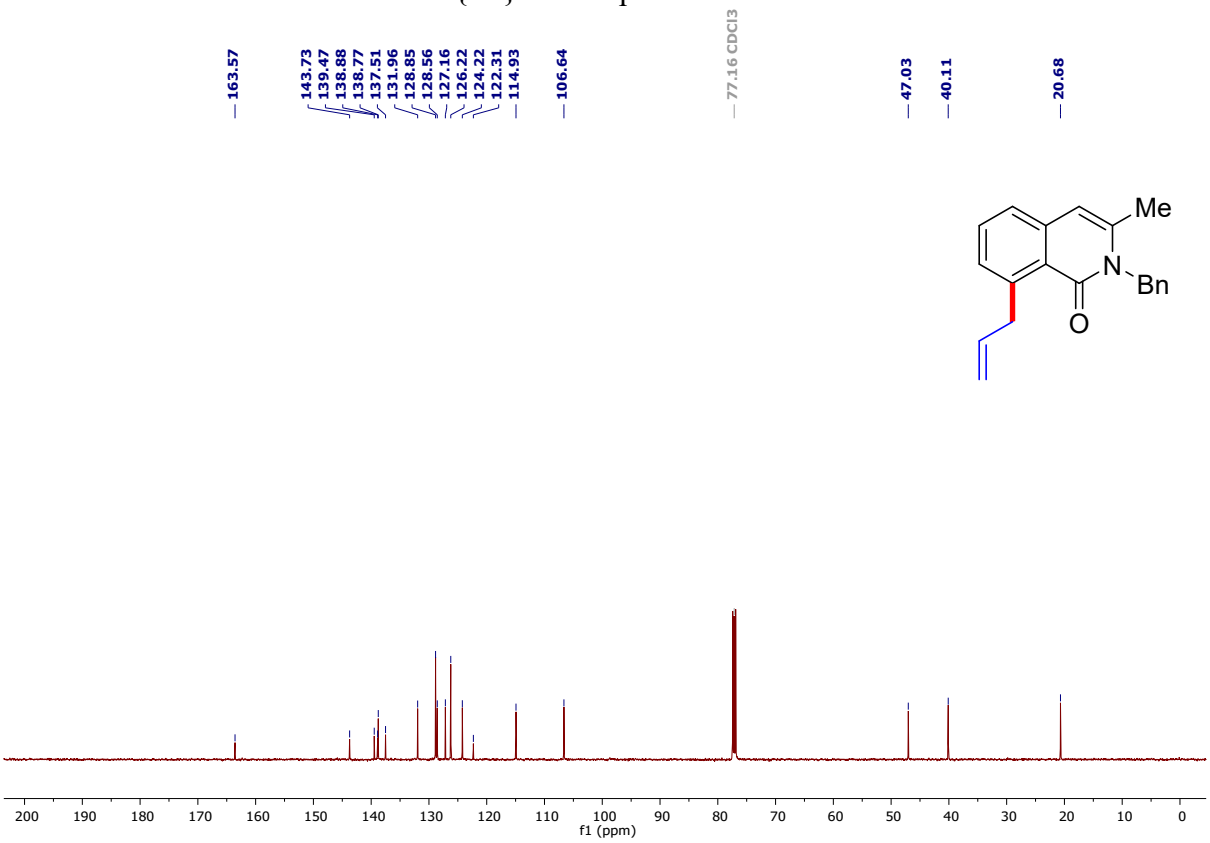
^{13}C{^{1}H} NMR spectrum of 3a



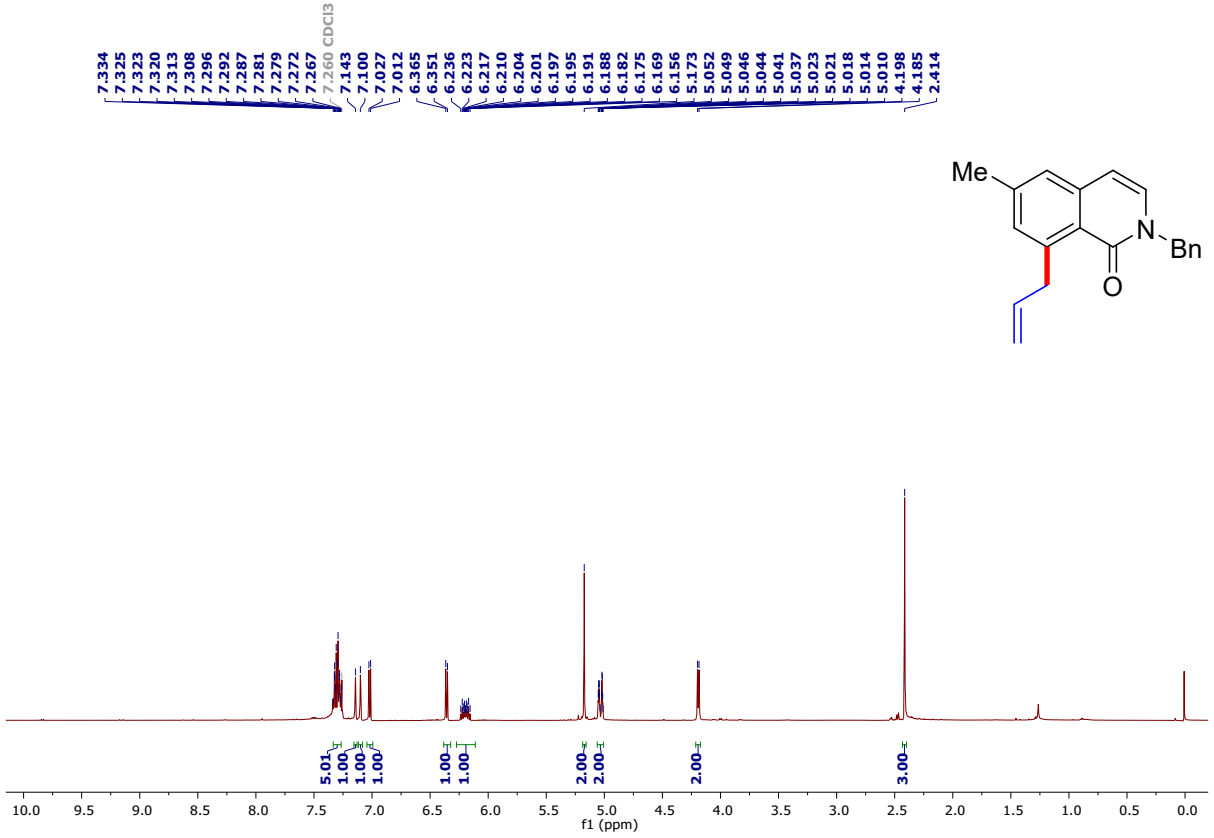
^{1}H NMR spectrum of 3b



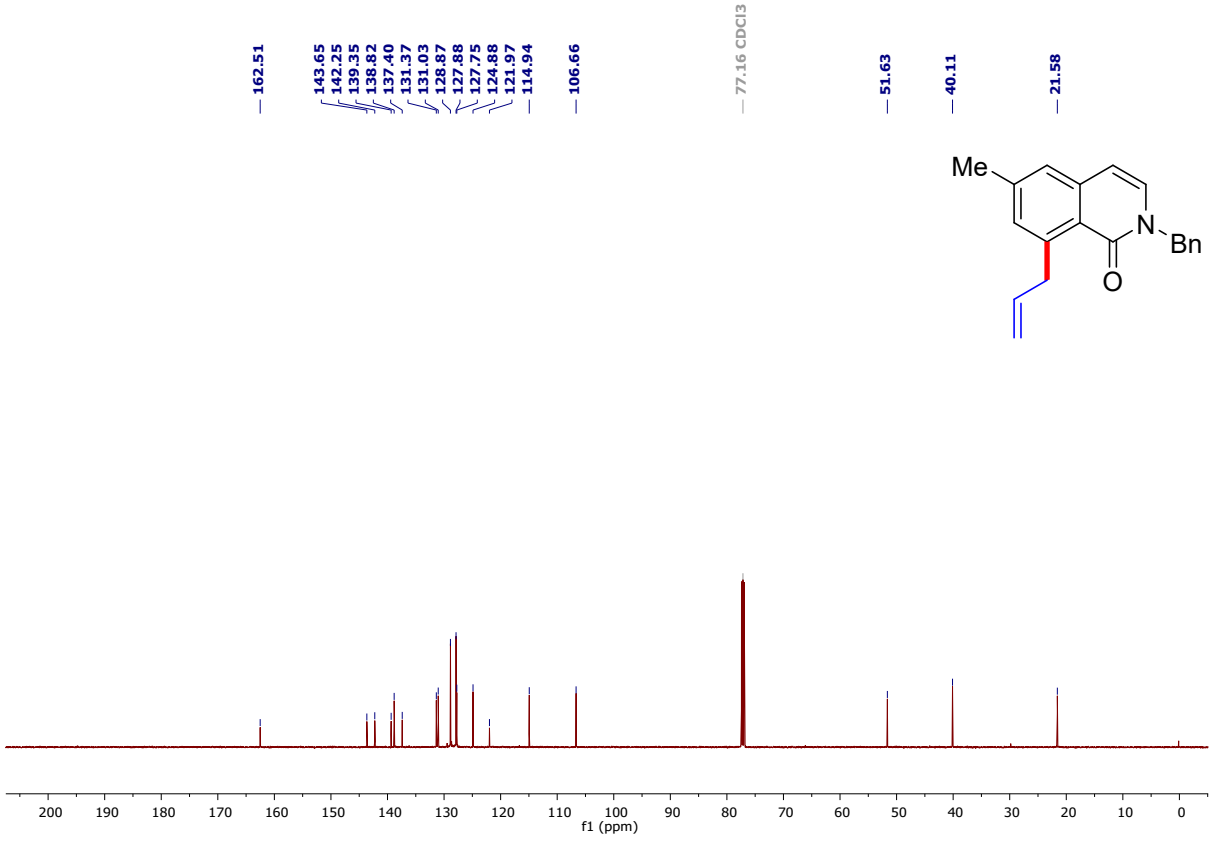
$^{13}C\{^{1}H\}$ NMR spectrum of 3b



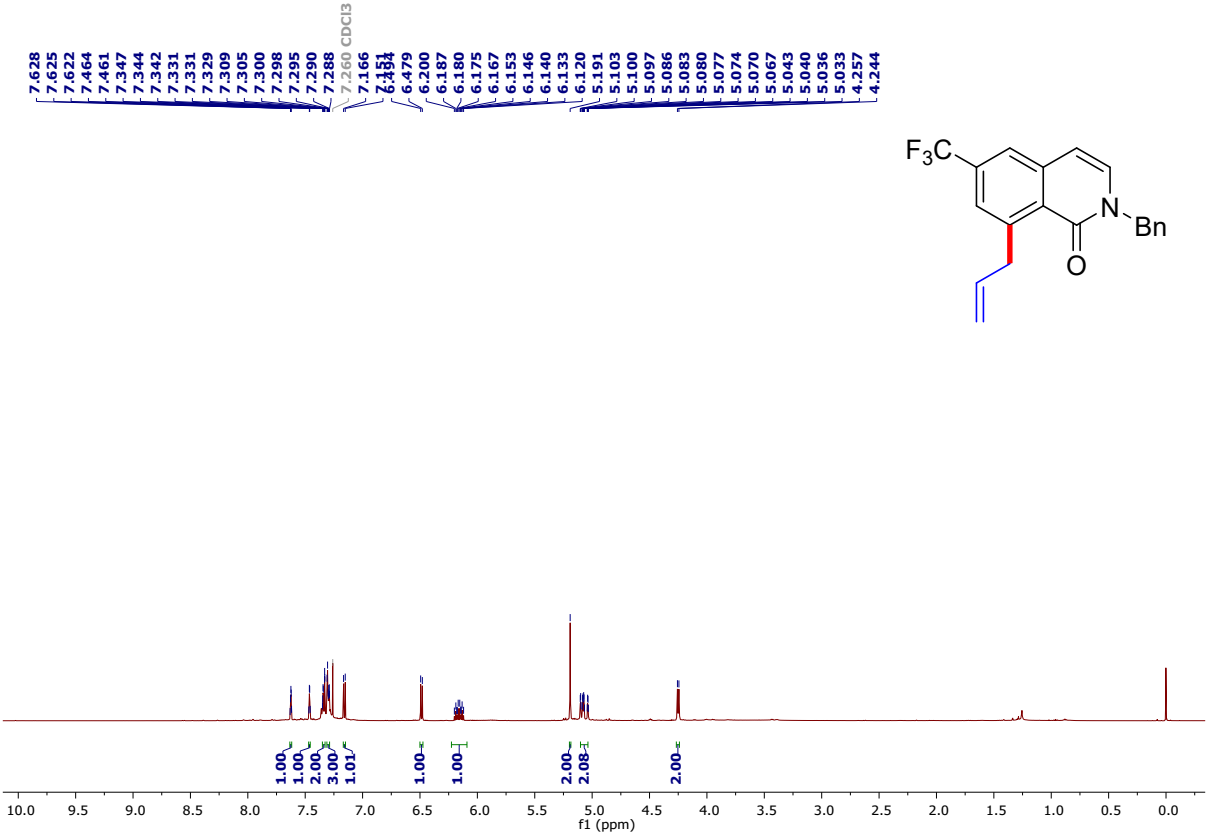
^{1}H NMR spectrum of 3c



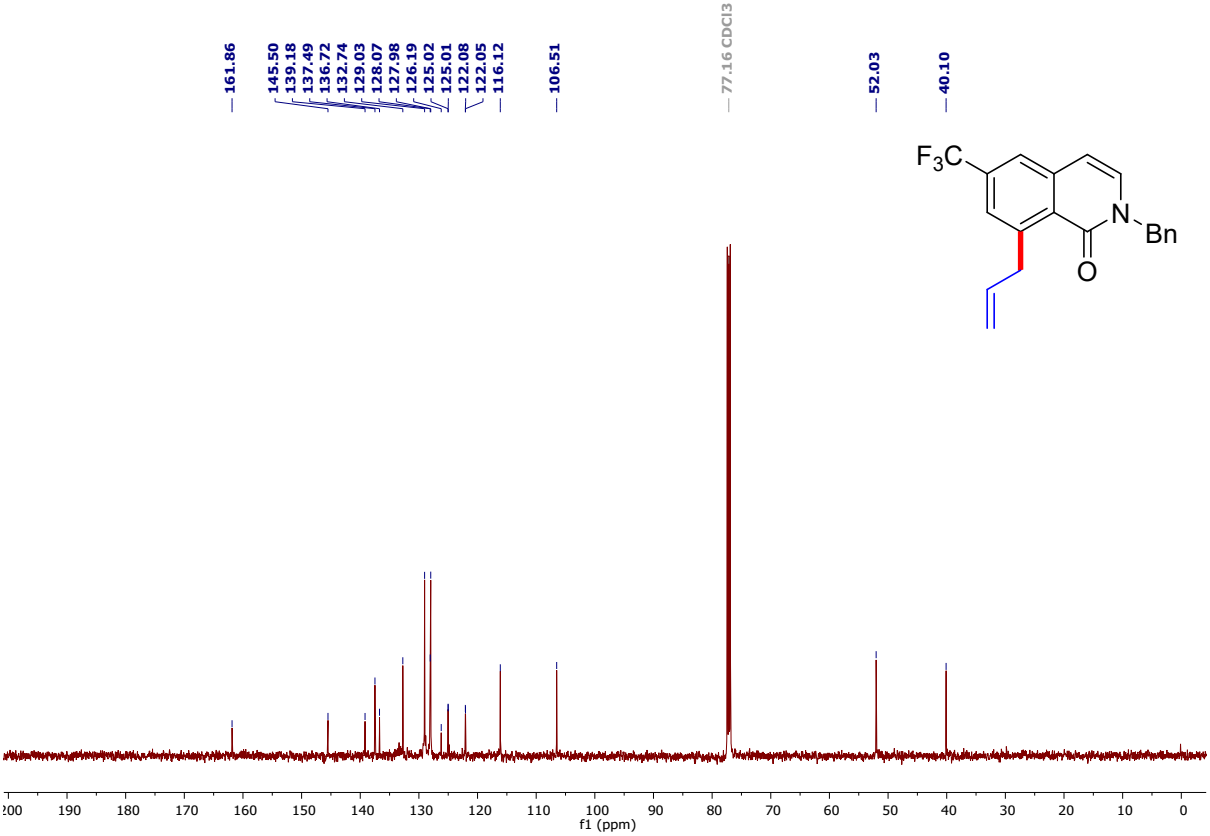
^{13}C{^{1}H} NMR spectrum of 3c



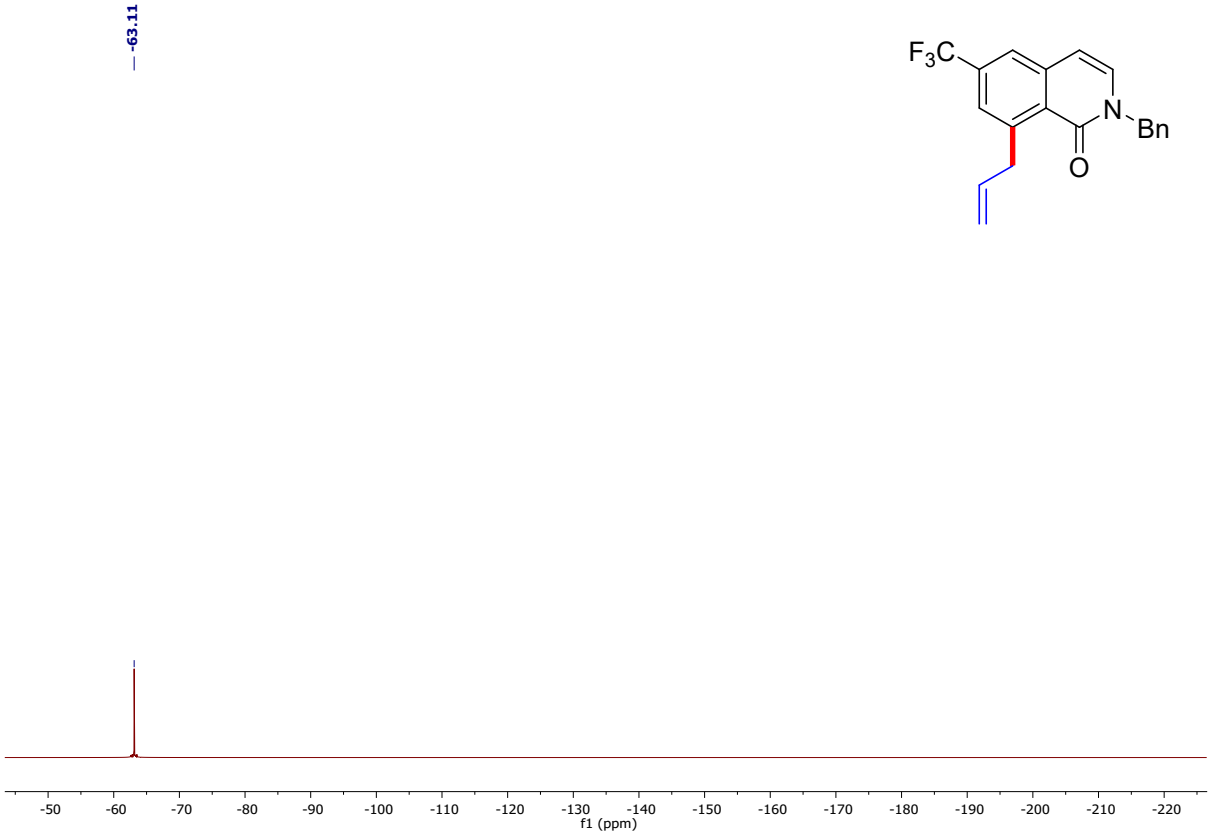
^{1}H NMR spectrum of 3d



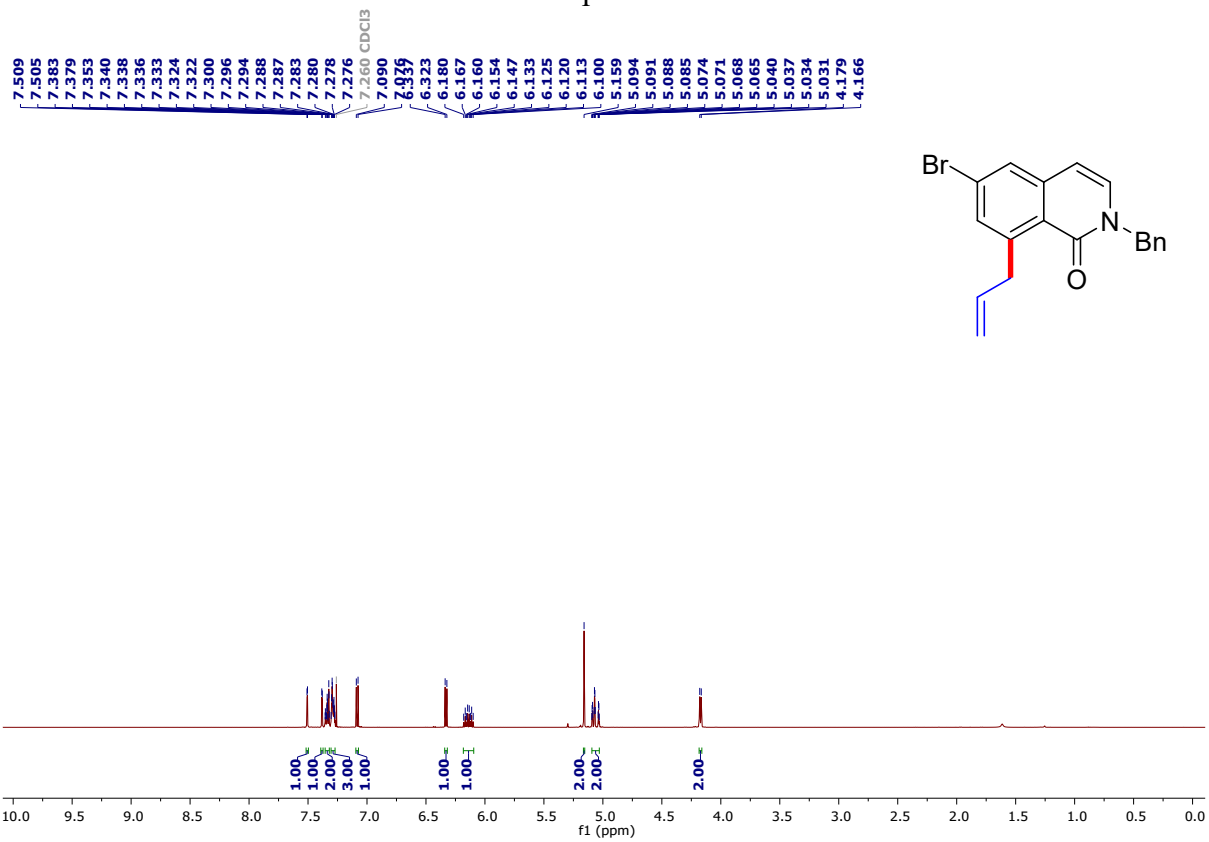
^{13}C{^{1}H} NMR spectrum of 3d



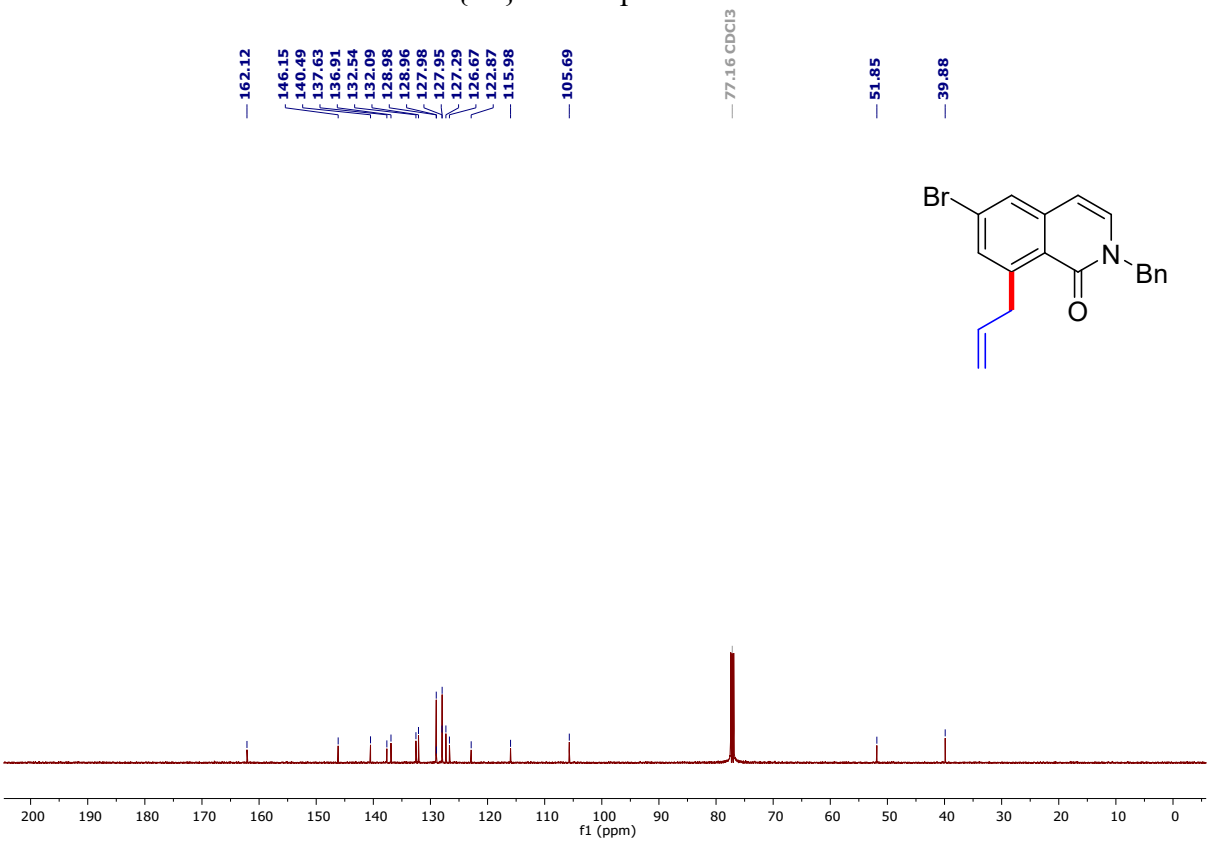
^{19}F NMR spectrum of 3d



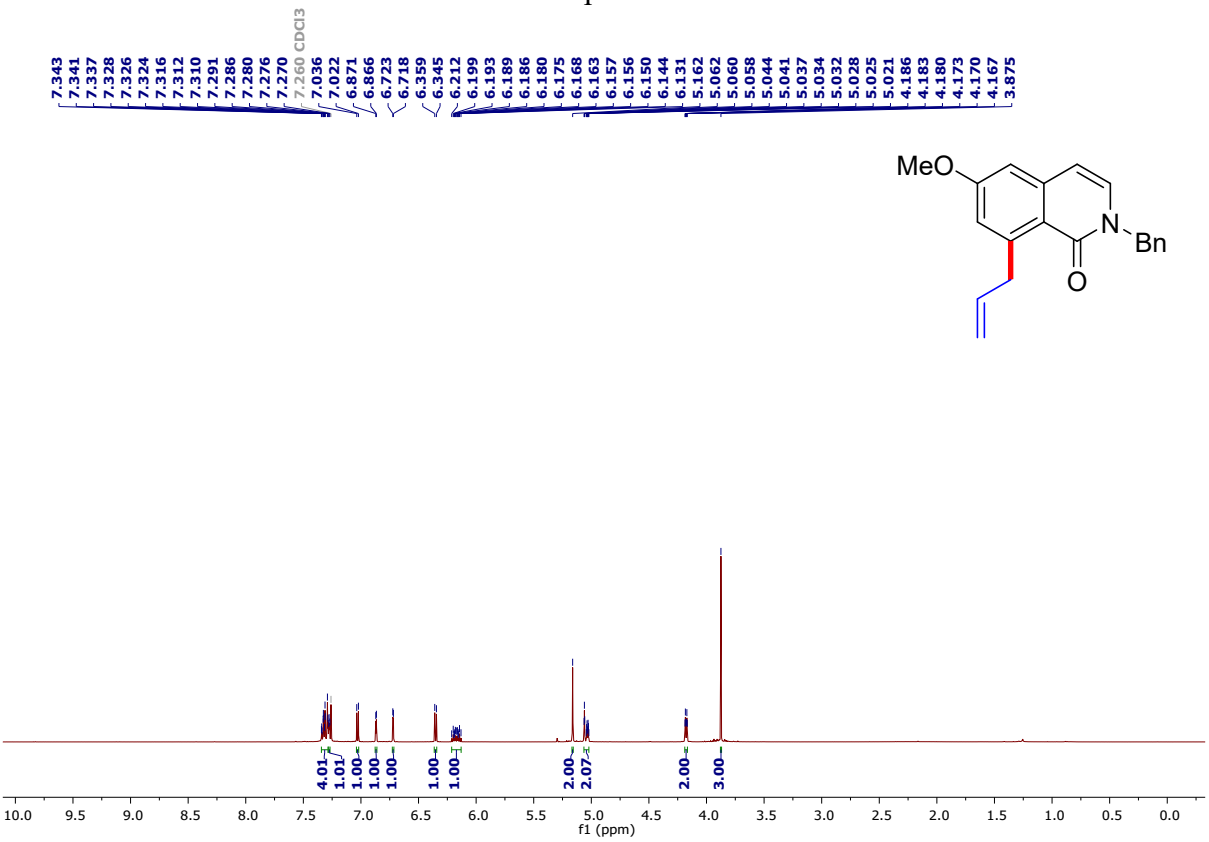
^{1}H NMR spectrum of 3e



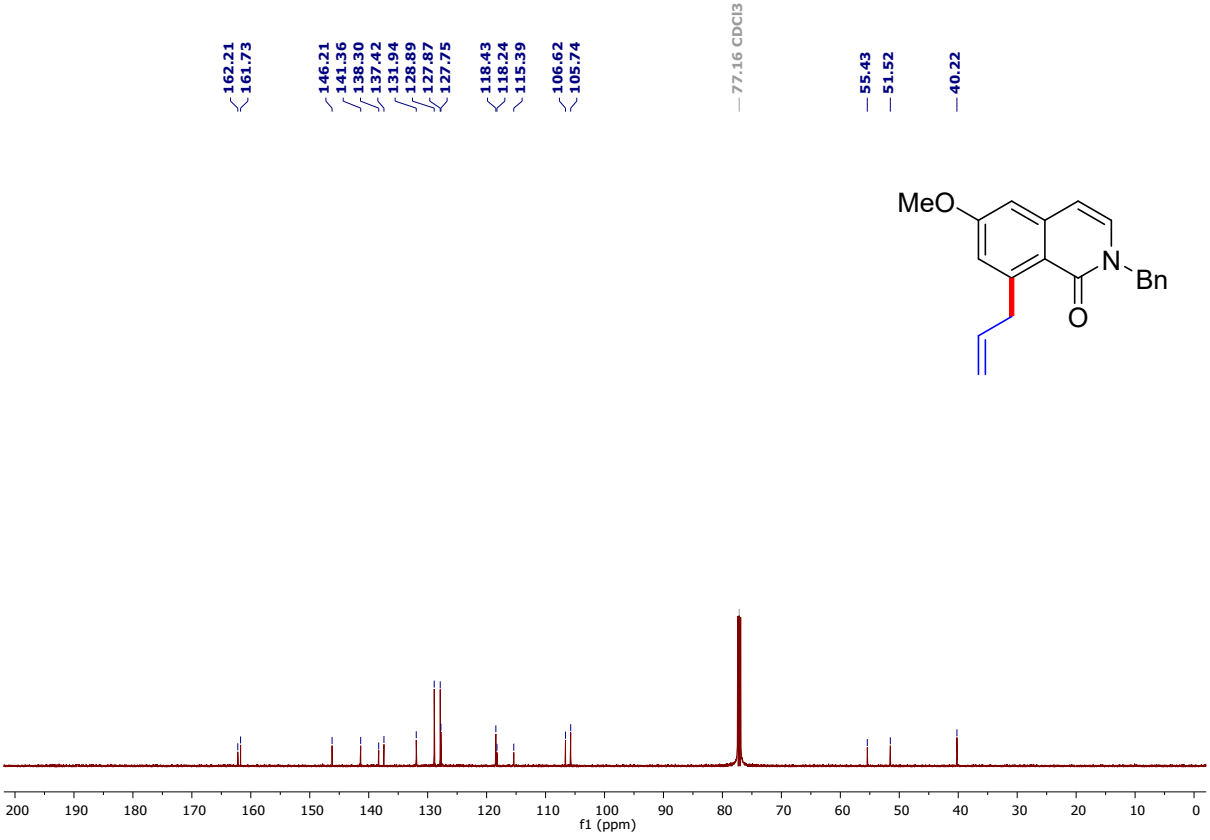
^{13}C{^{1}H} NMR spectrum of 3e



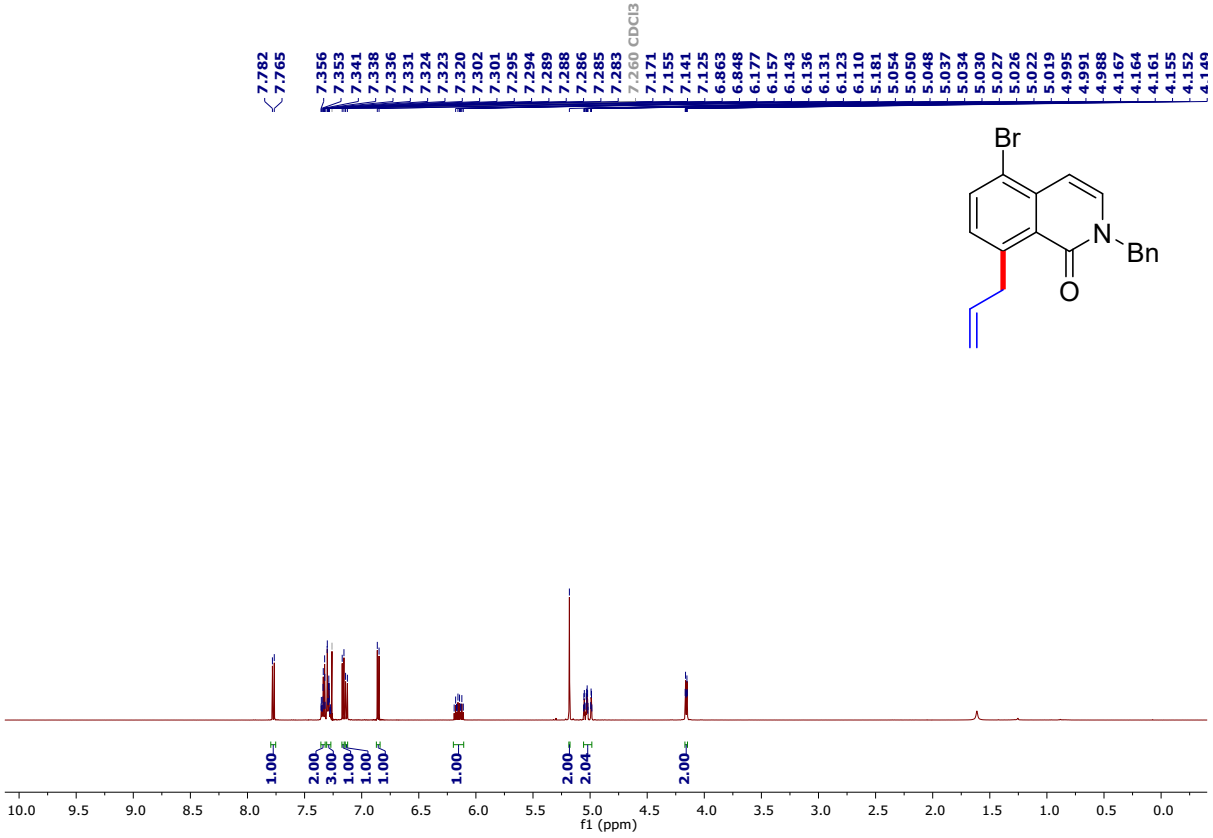
^{1}H NMR spectrum of 3f



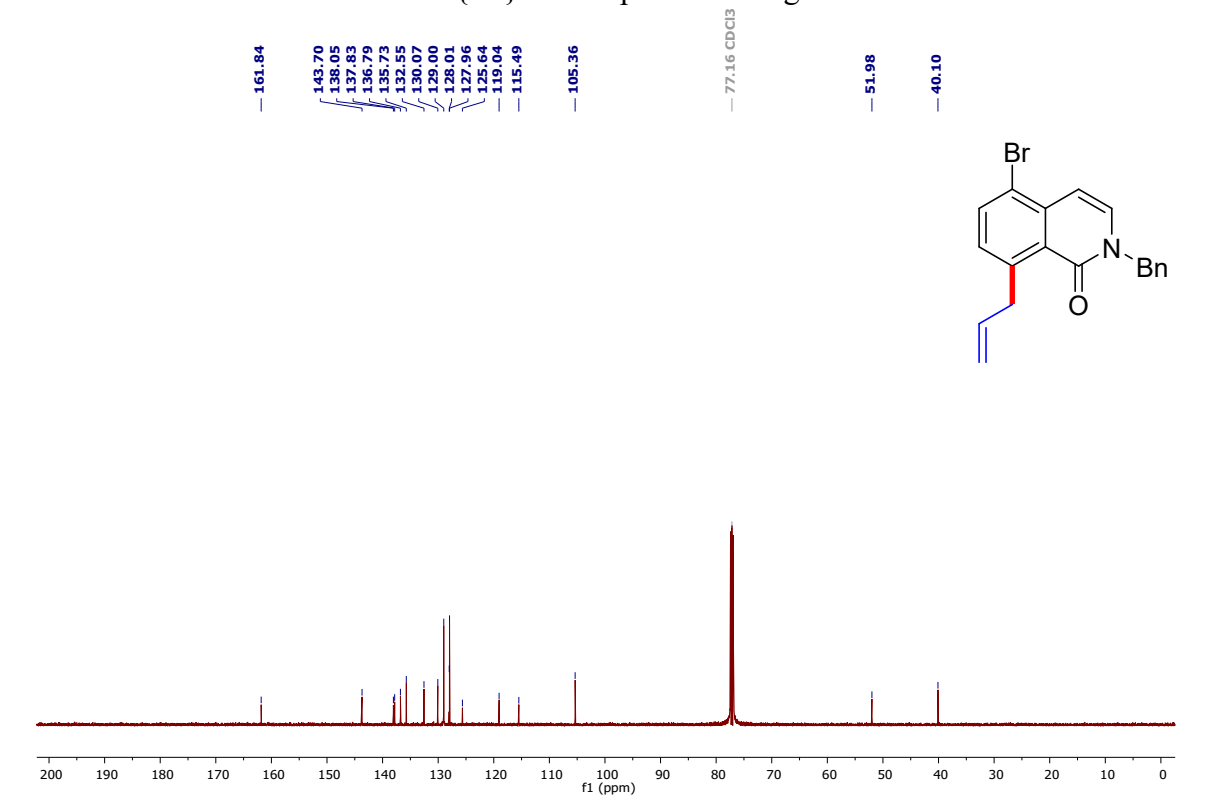
^{13}C{^{1}H} NMR spectrum of 3f



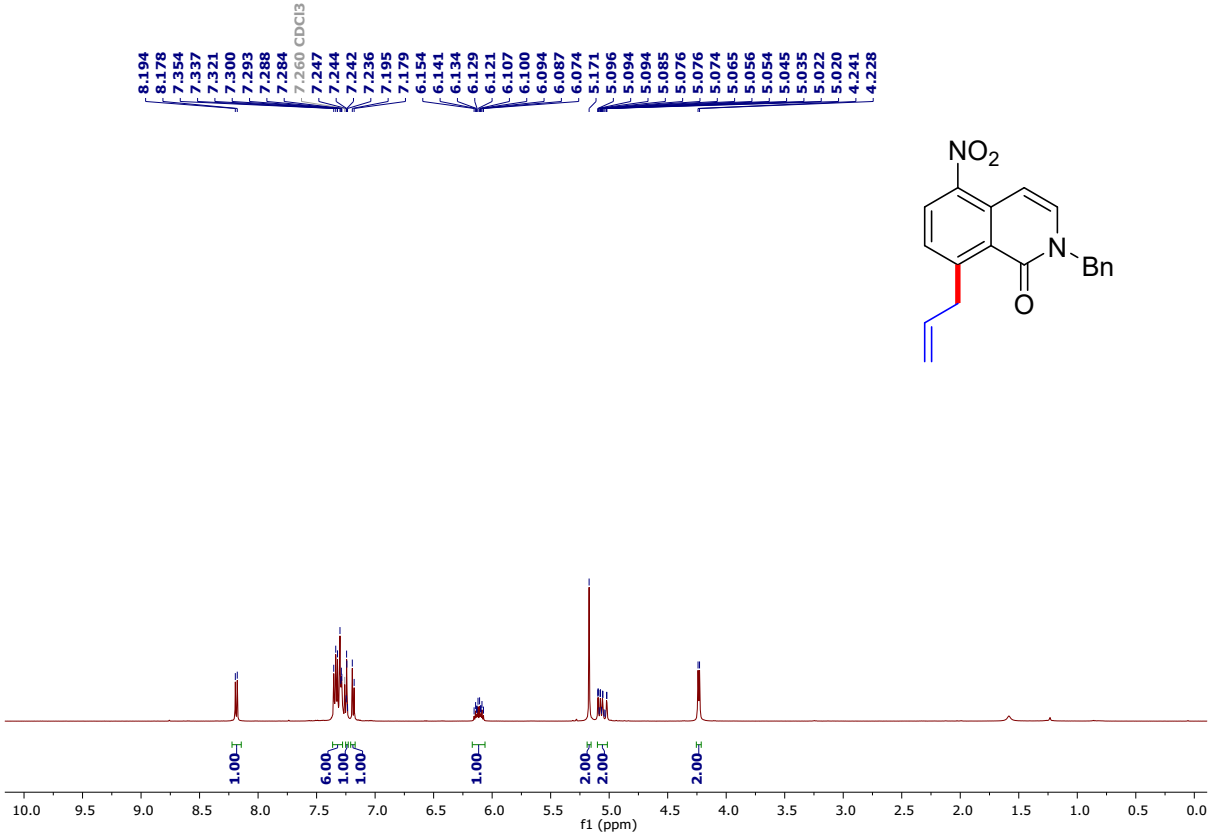
^{1}H NMR spectrum of 3g



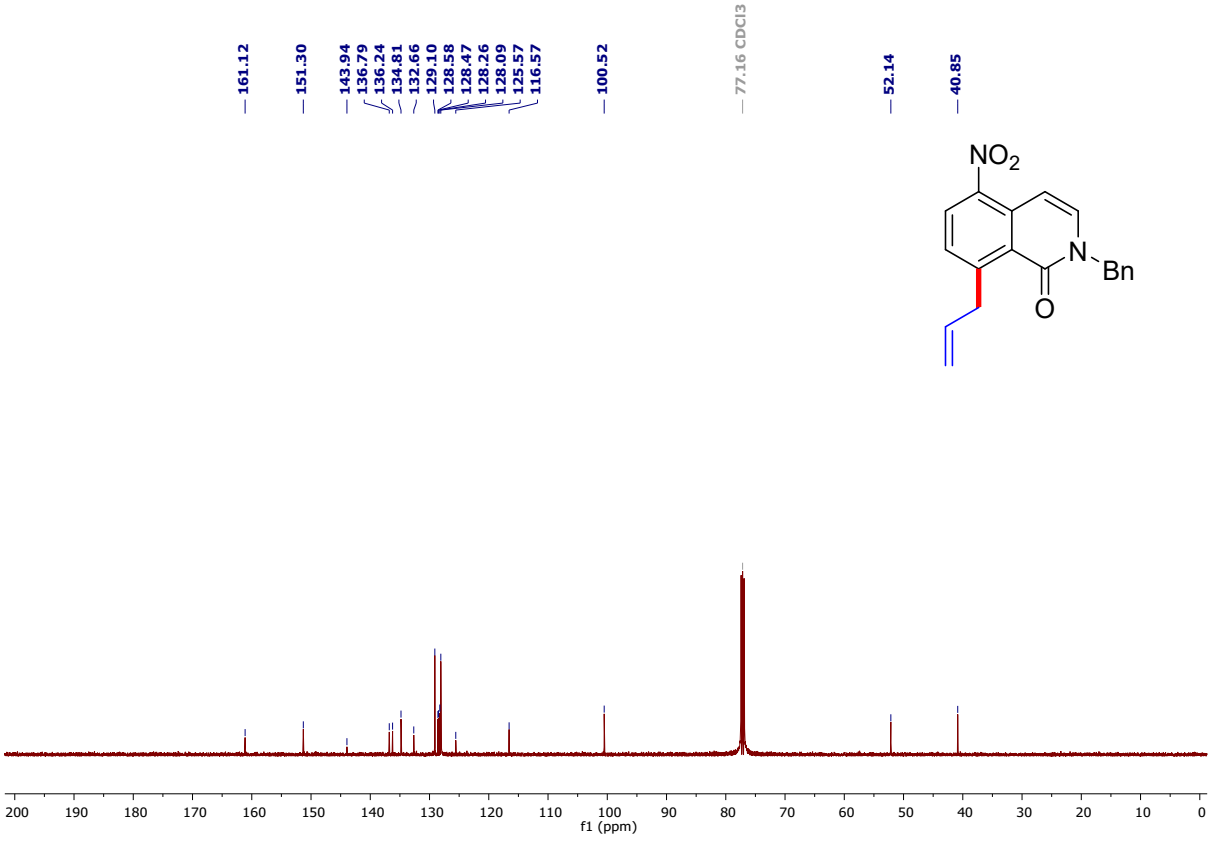
^{13}C{^{1}H} NMR spectrum of 3g



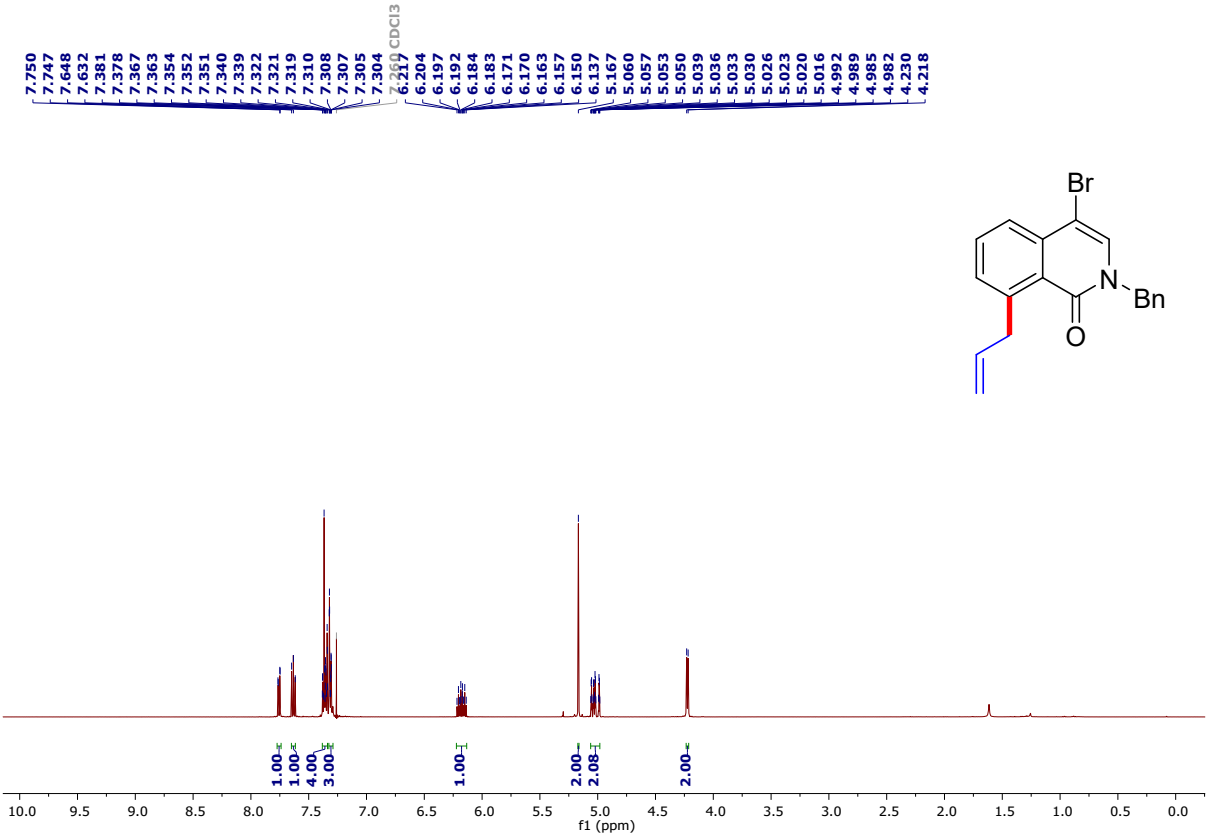
^{1}H NMR spectrum of 3h



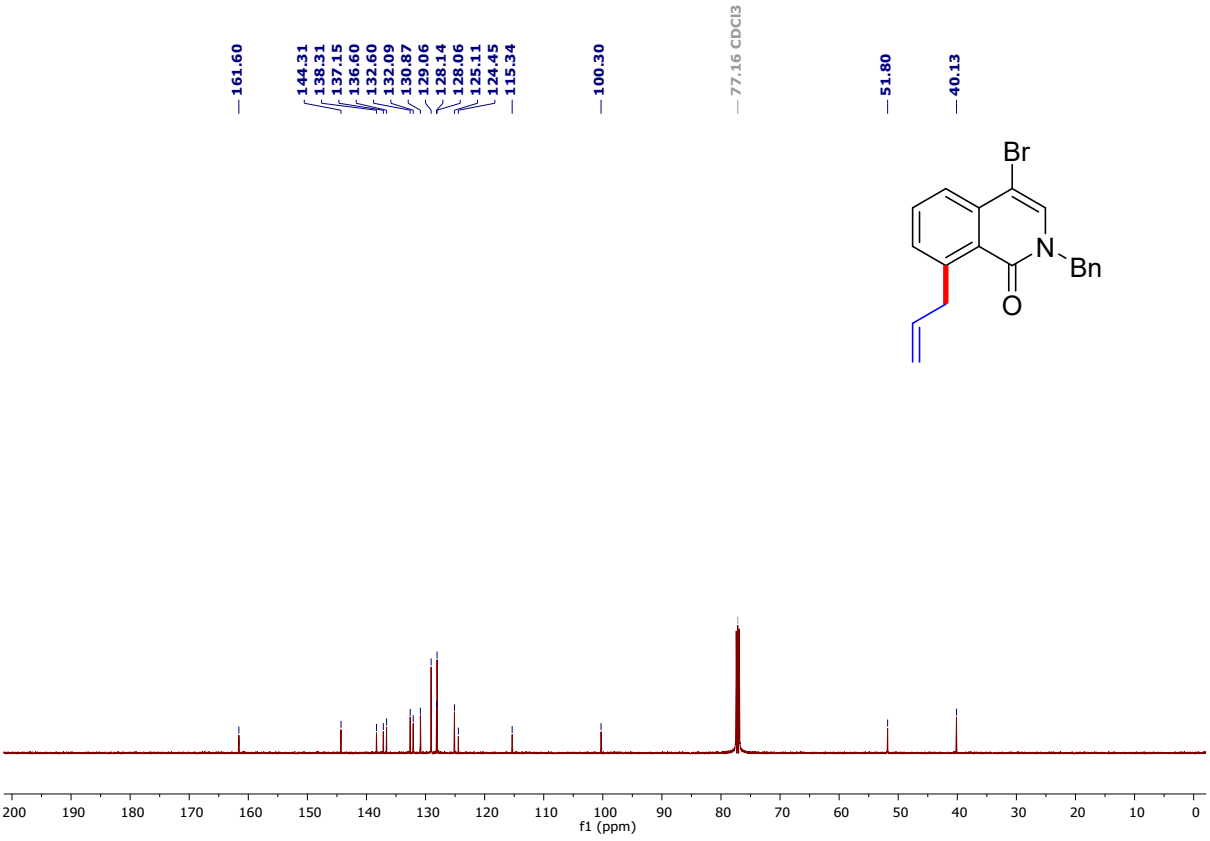
^{13}C{^{1}H} NMR spectrum of 3h



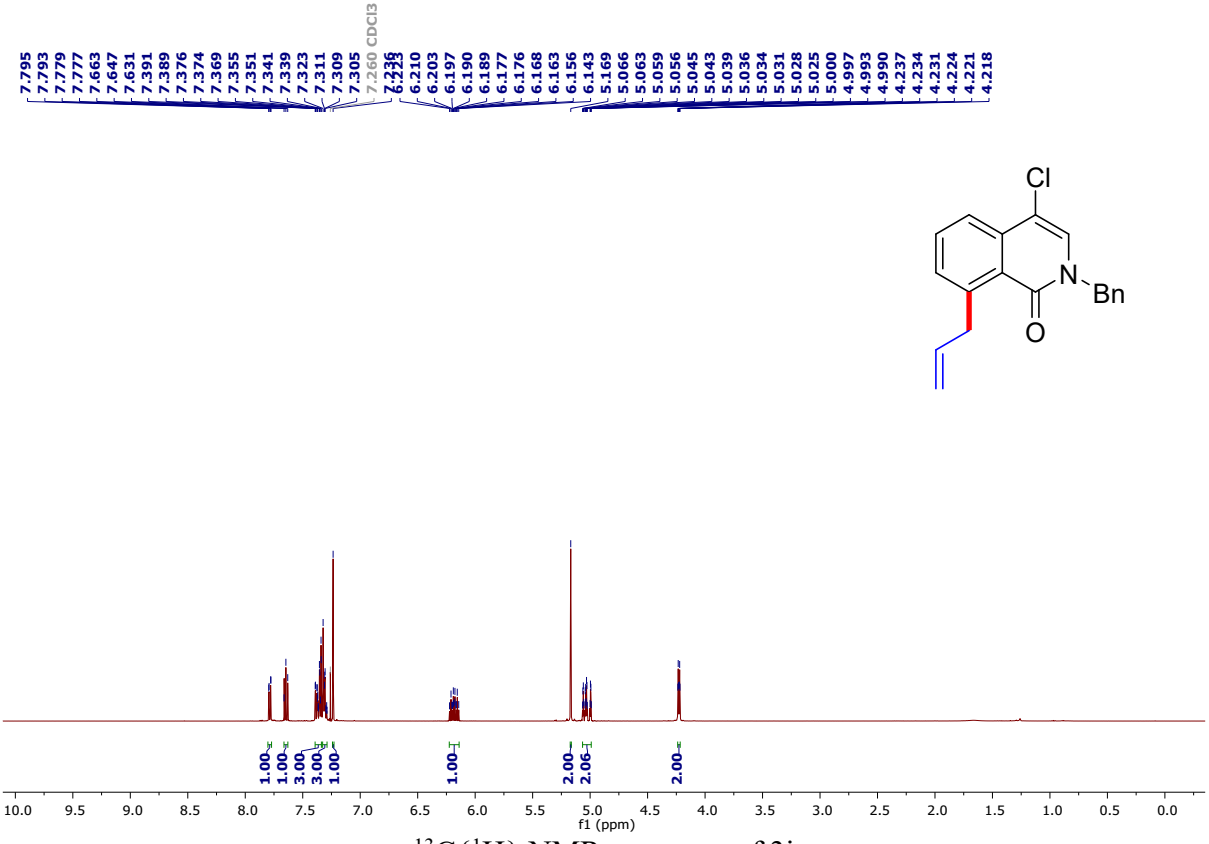
^{1}H NMR spectrum of 3i



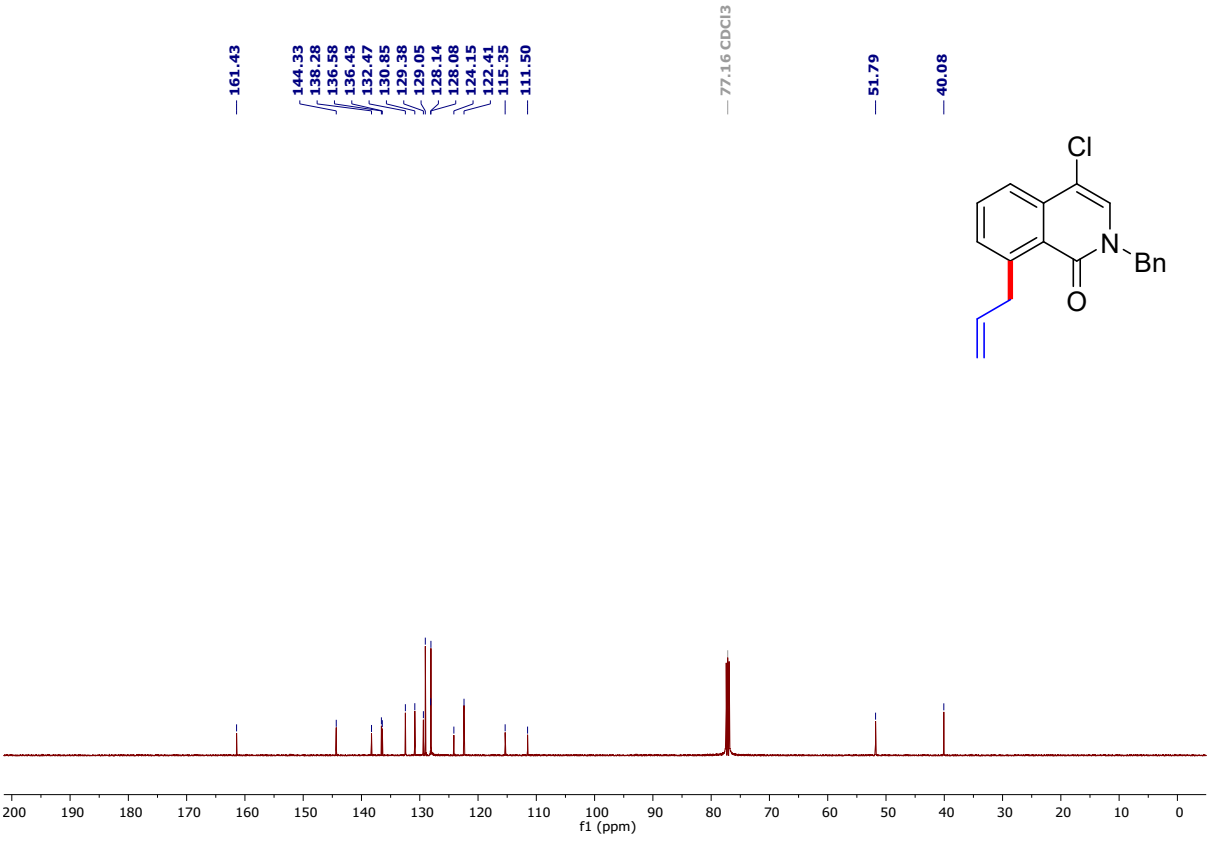
^{13}C{^{1}H} NMR spectrum of 3i



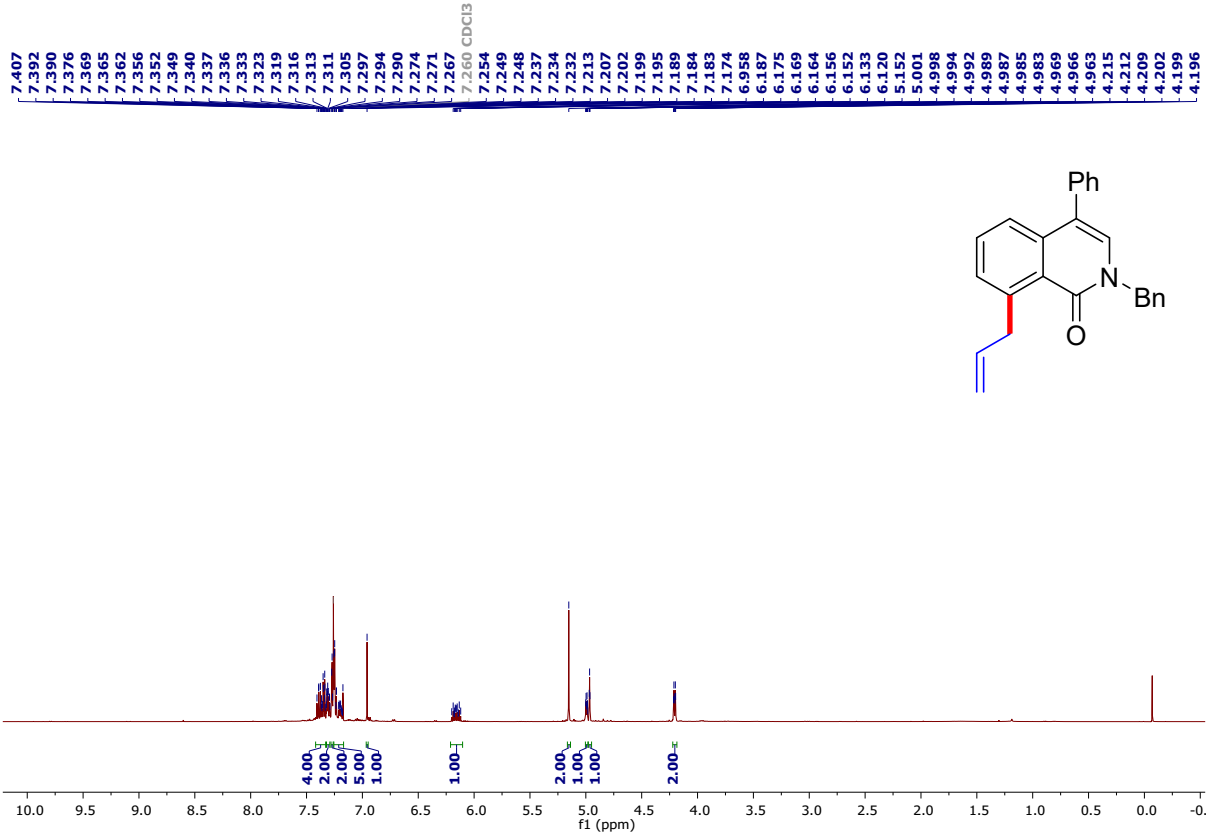
^{1}H NMR spectrum of 3j



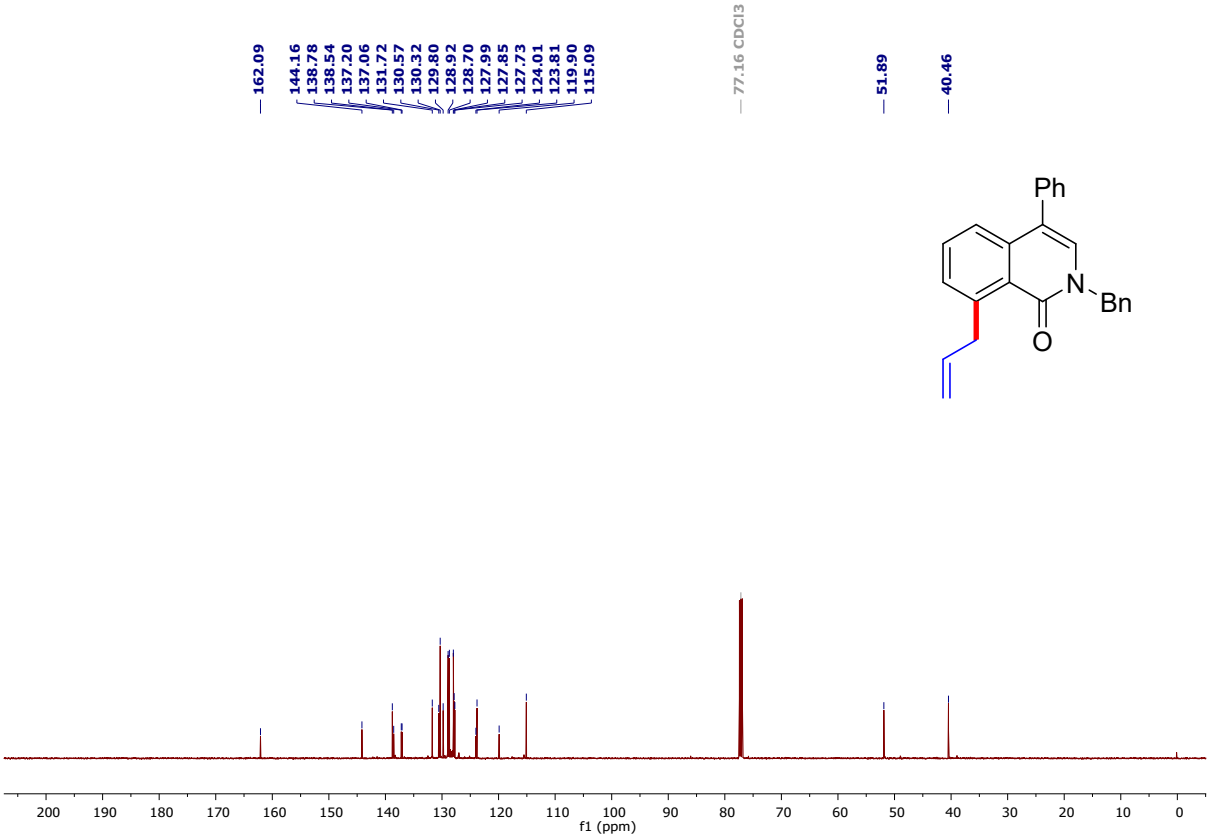
^{13}C{^{1}H} NMR spectrum of 3j



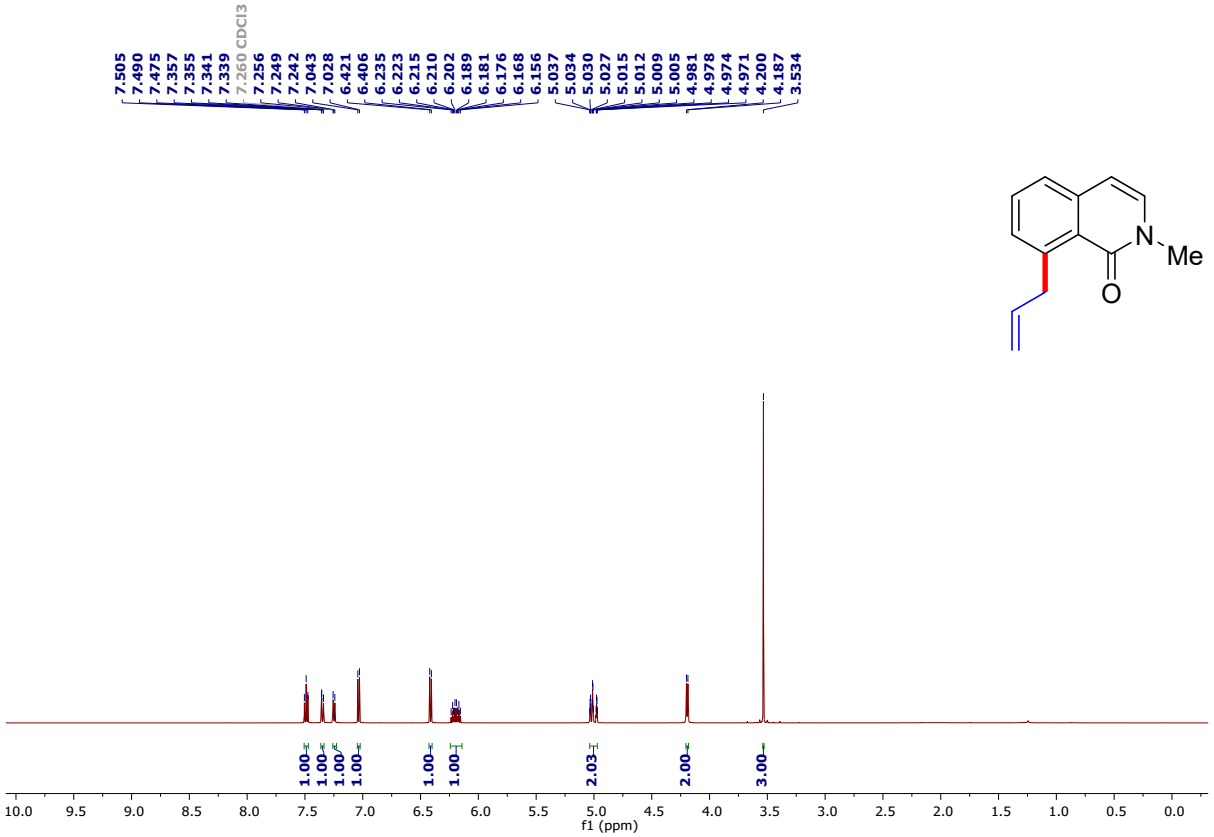
^{1}H NMR spectrum of 3k



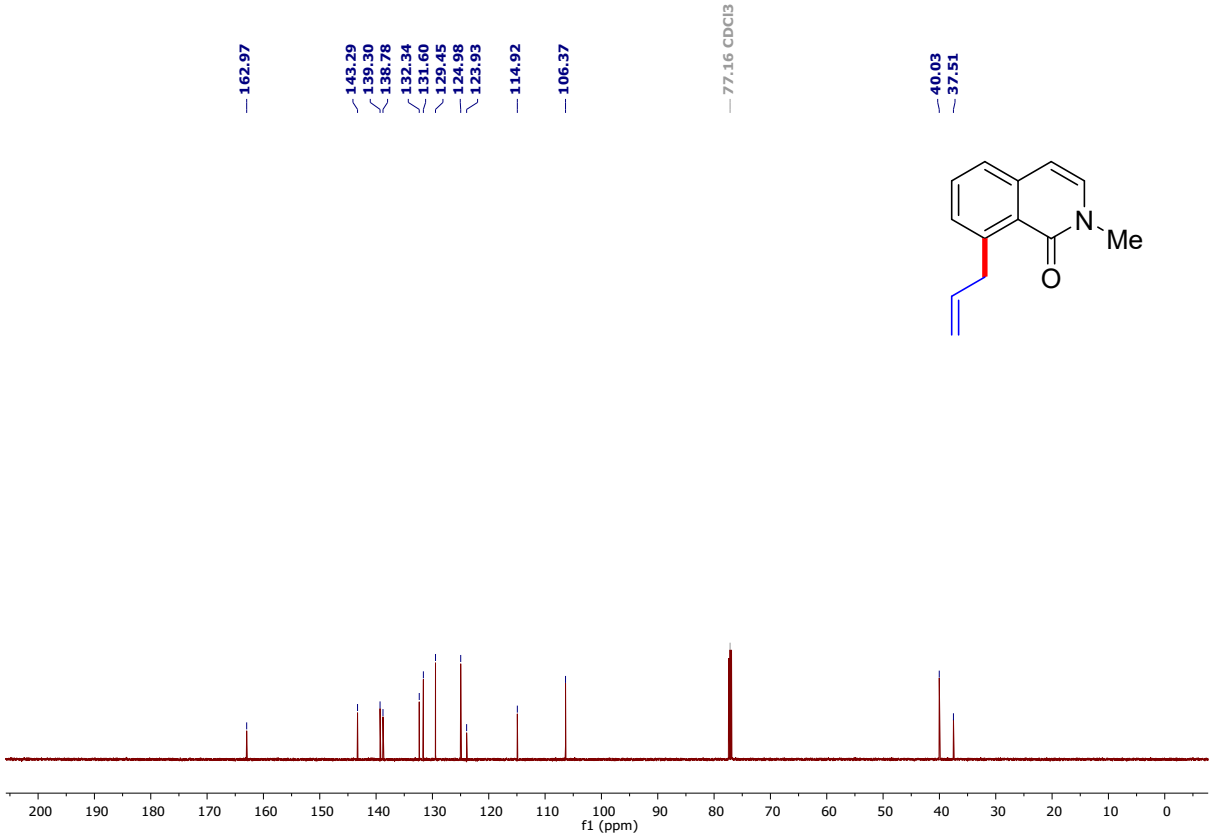
^{13}C{^{1}H} NMR spectrum of 3k



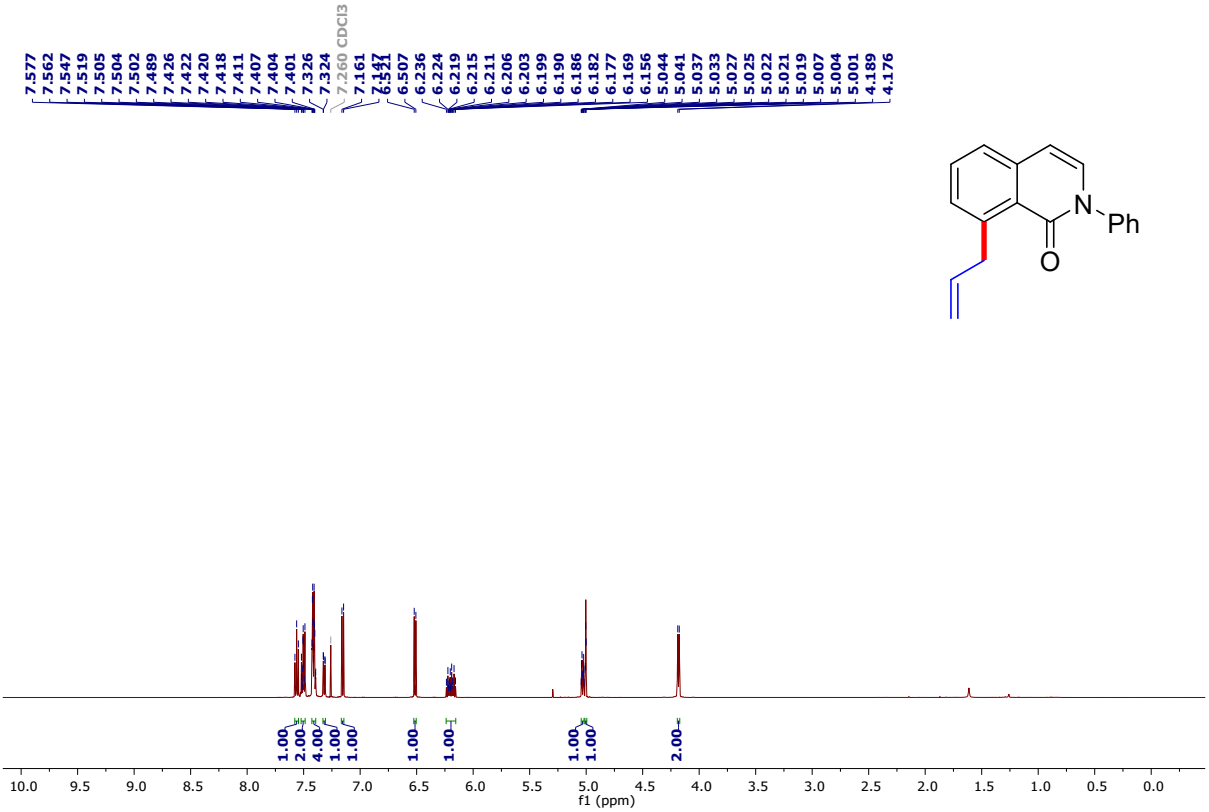
^{1}H NMR spectrum of 3l



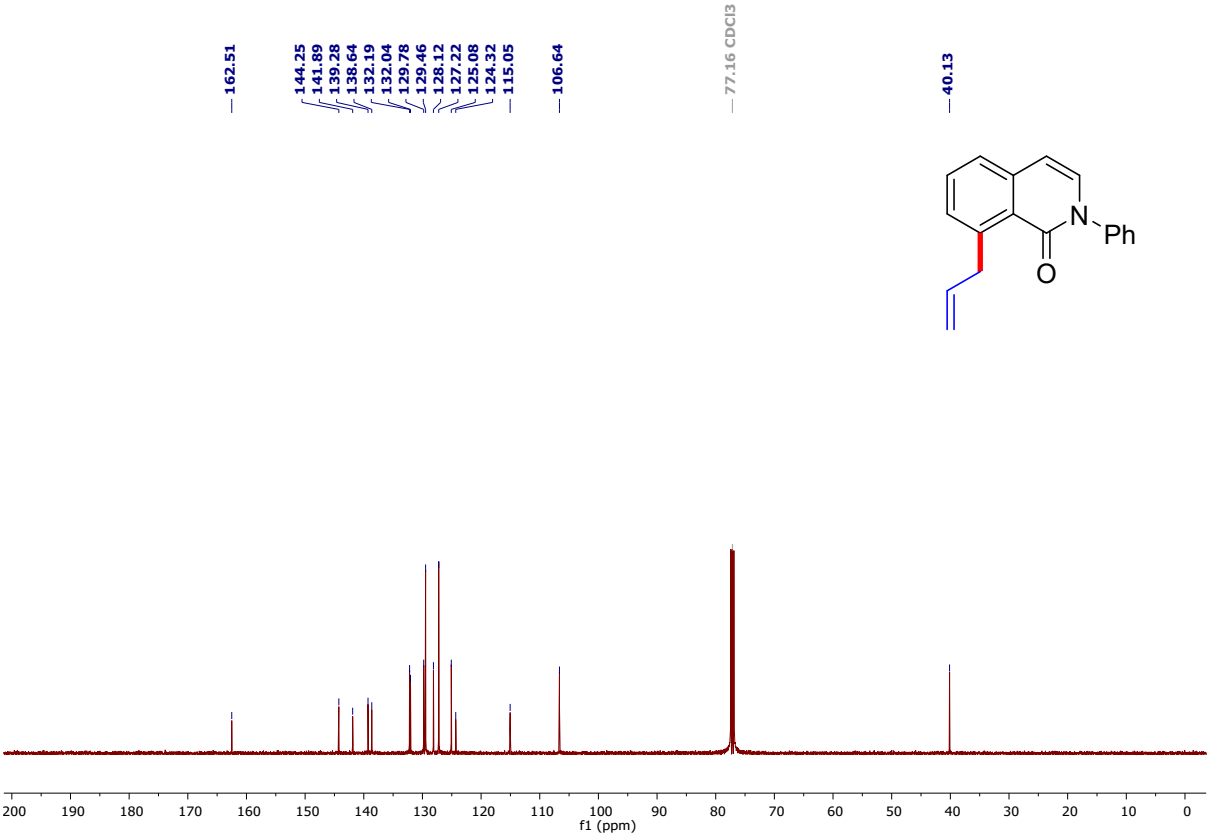
^{13}C{^{1}H} NMR spectrum of 3l



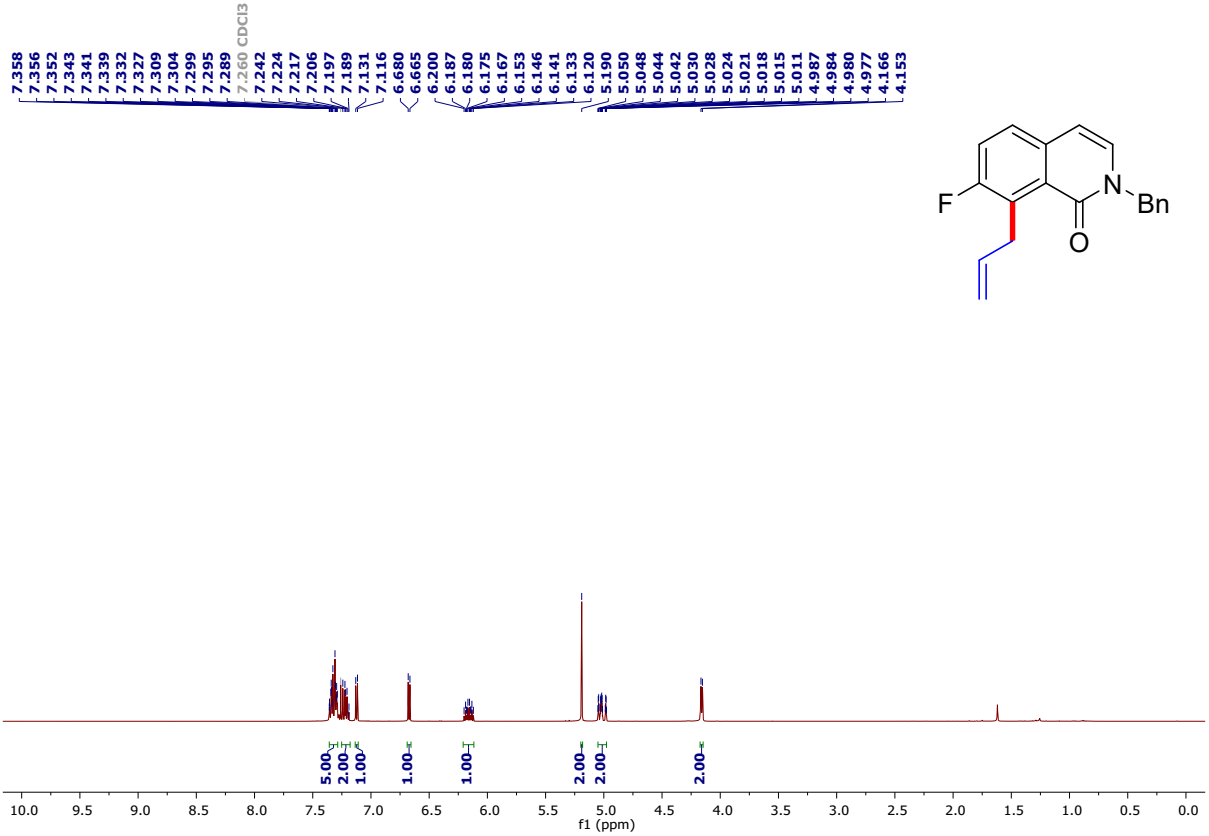
^{1}H NMR spectrum of 3m



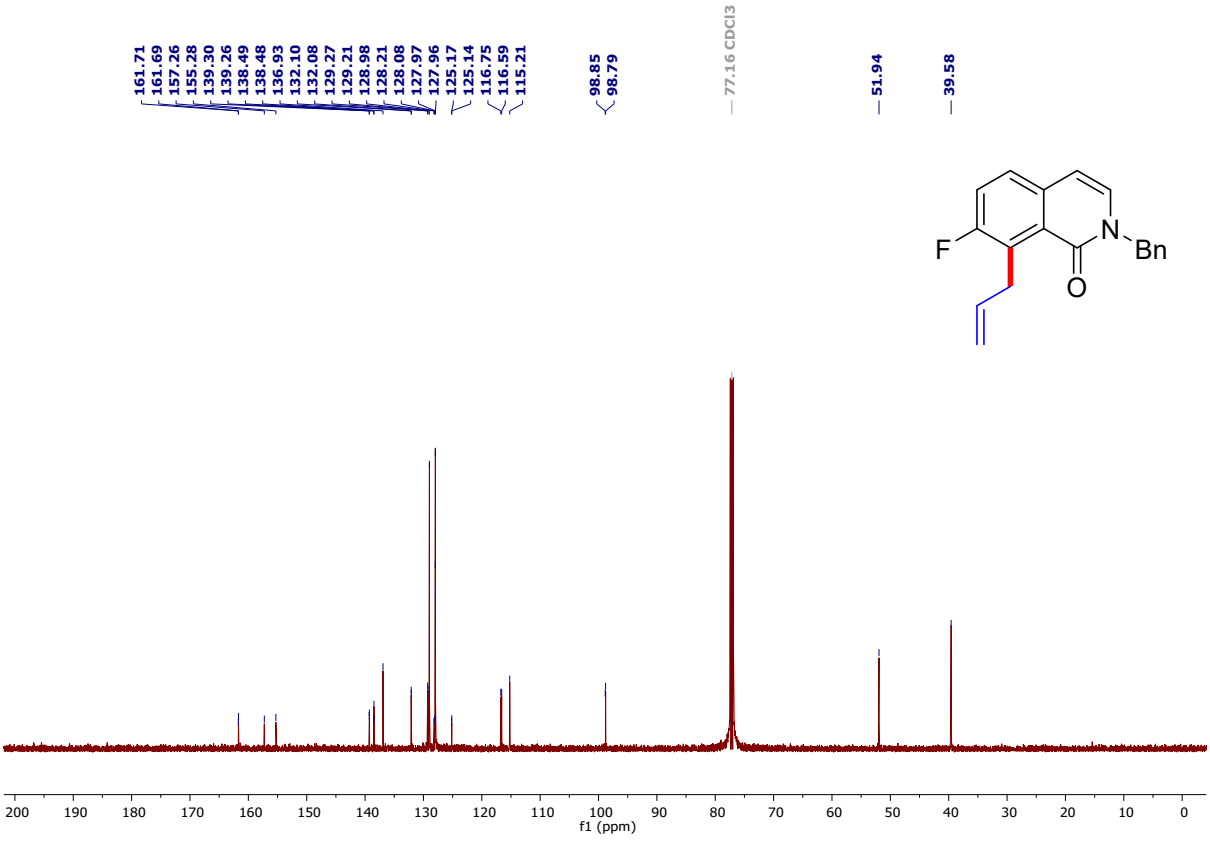
^{13}C NMR spectrum of 3m



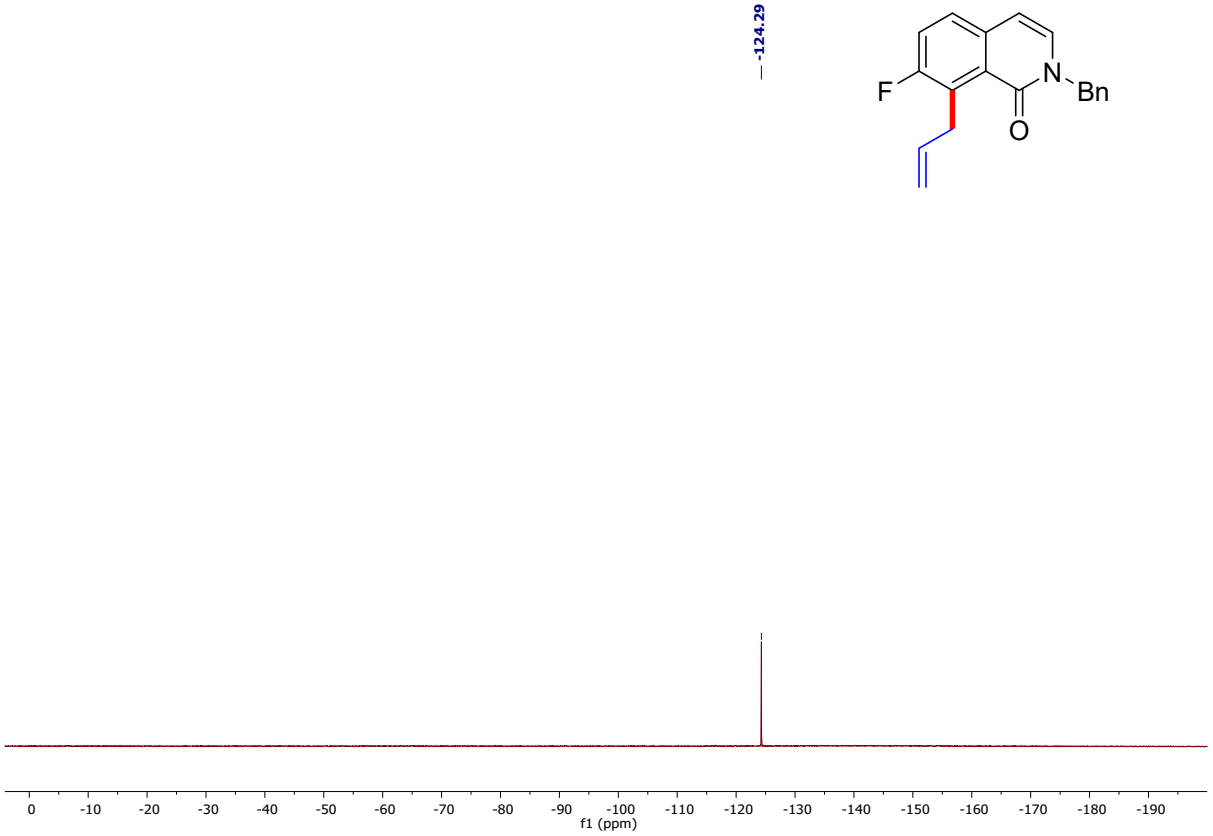
^{1}H NMR spectrum of 3n



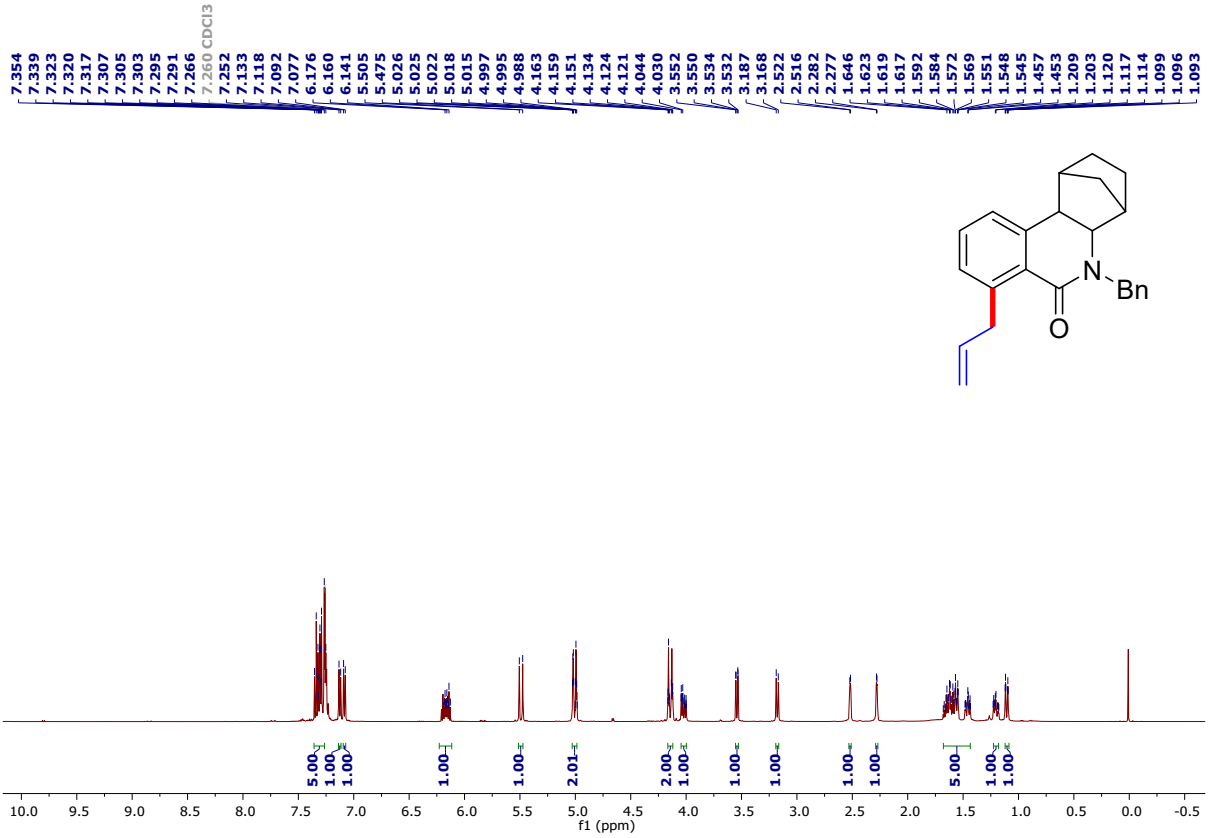
^{13}C{^{1}H} NMR spectrum of 3n



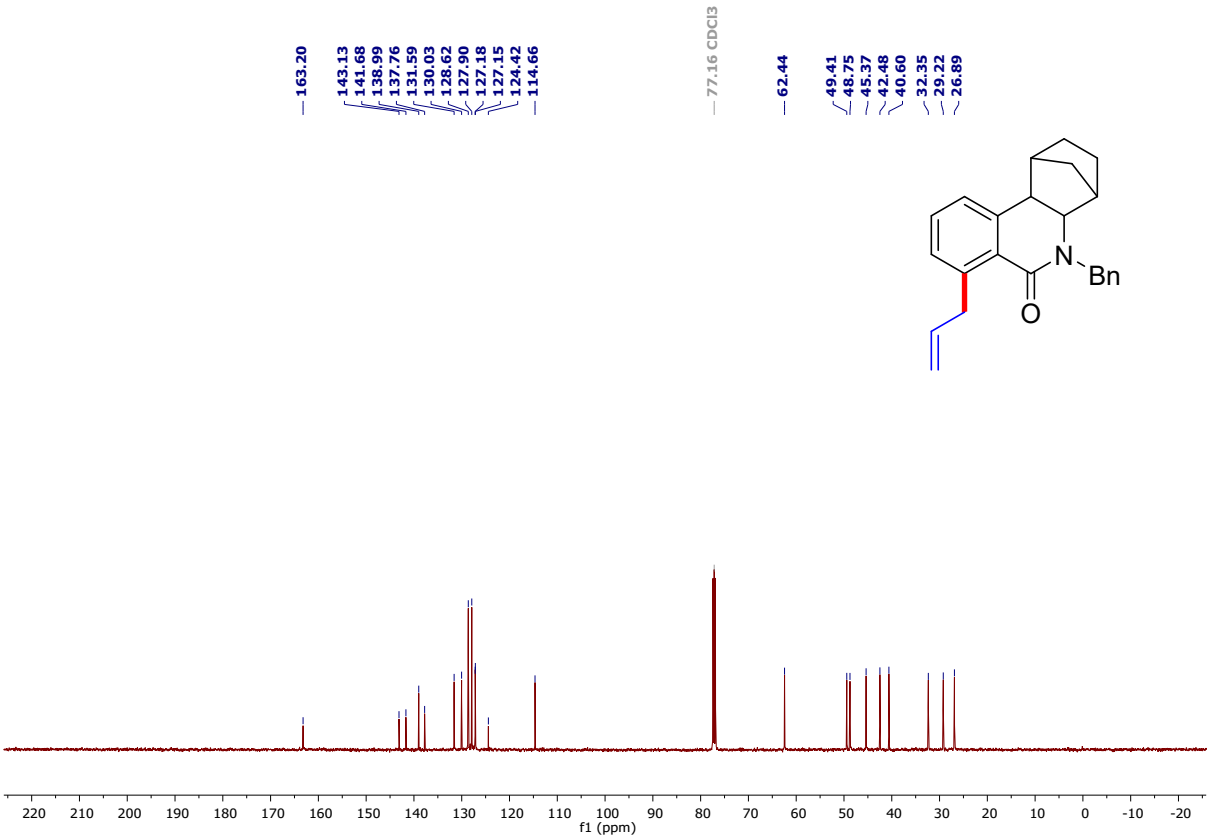
^{19}F NMR spectrum of 3n



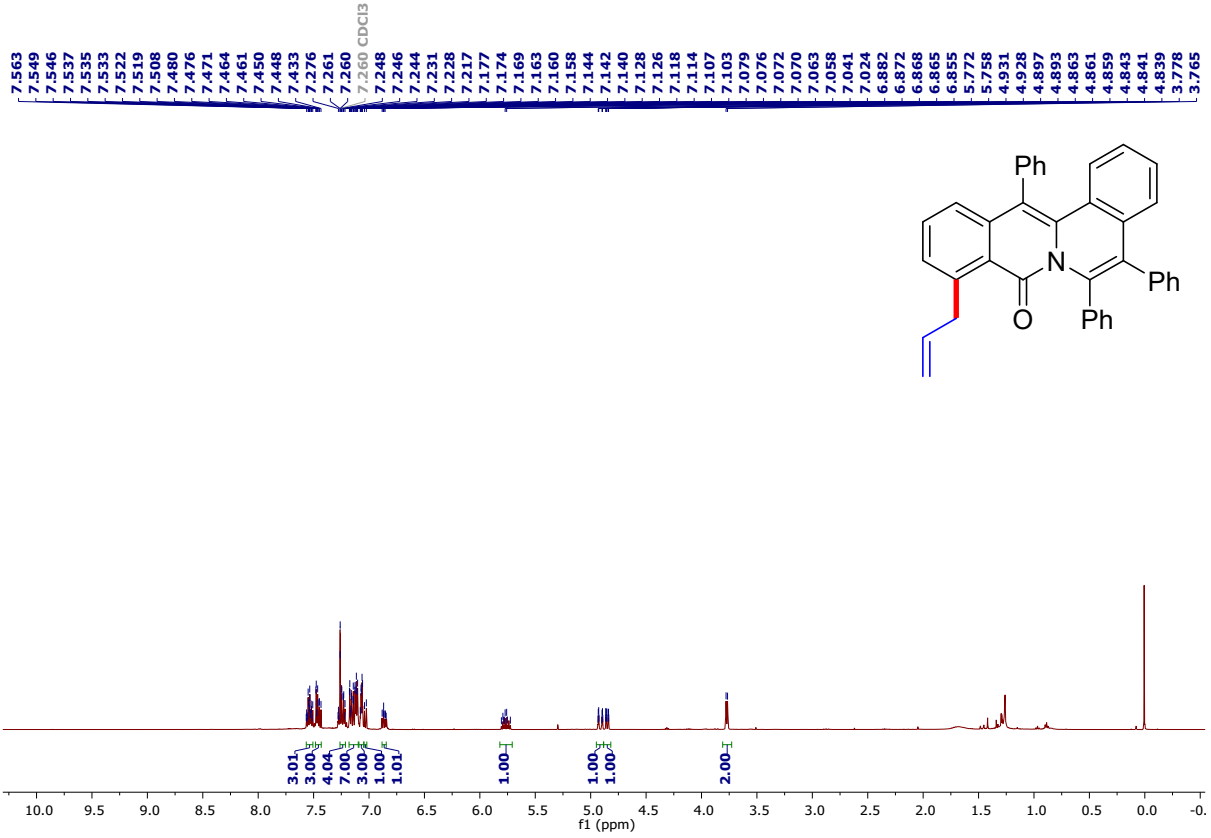
^{1}H NMR spectrum of 3o



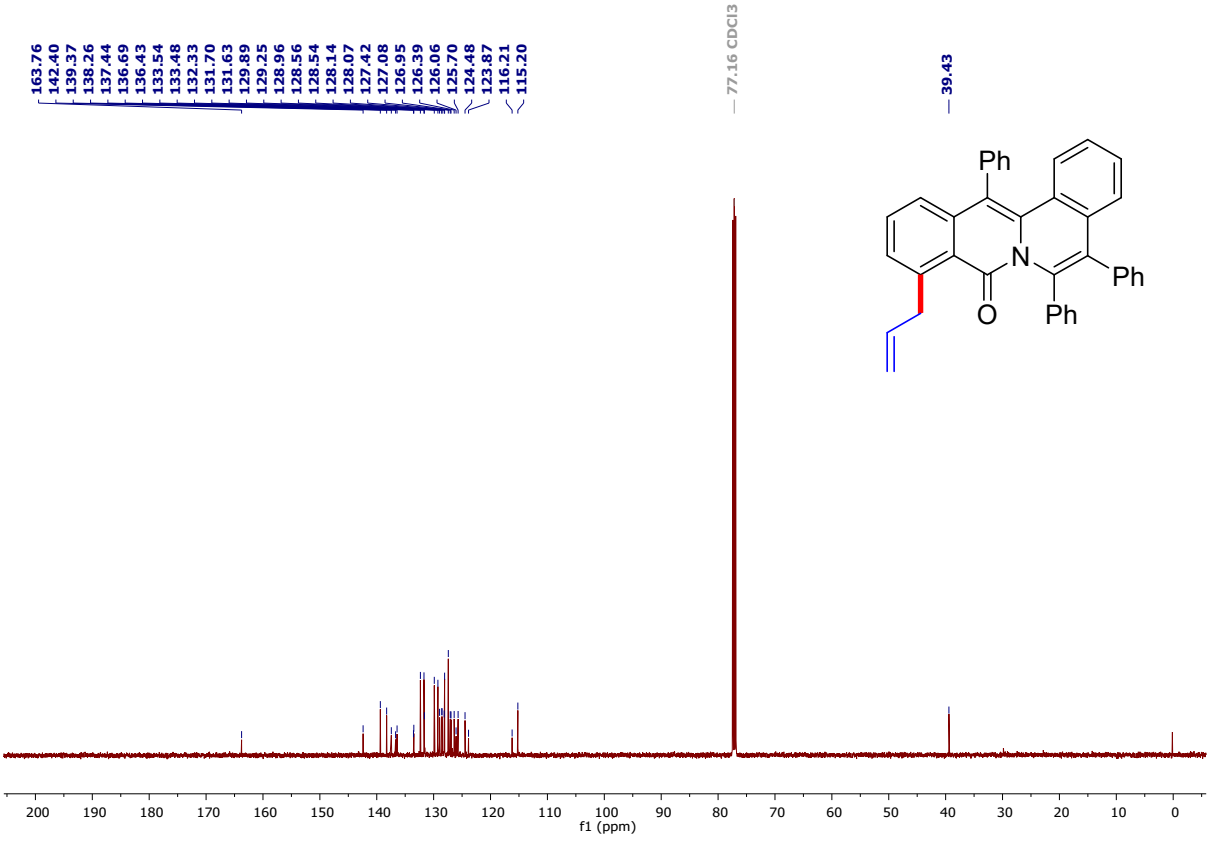
^{13}C{^{1}H} NMR spectrum of 3o



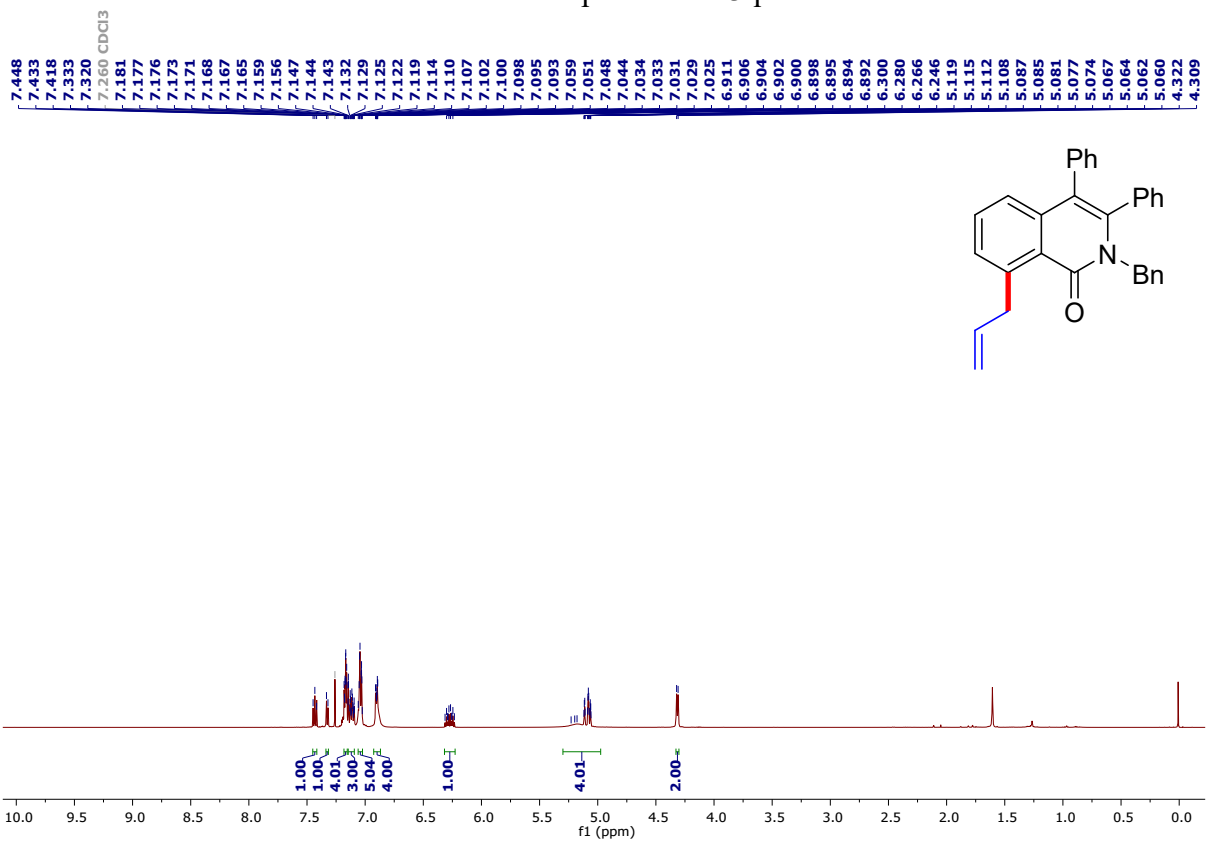
^{1}H NMR spectrum of 3p



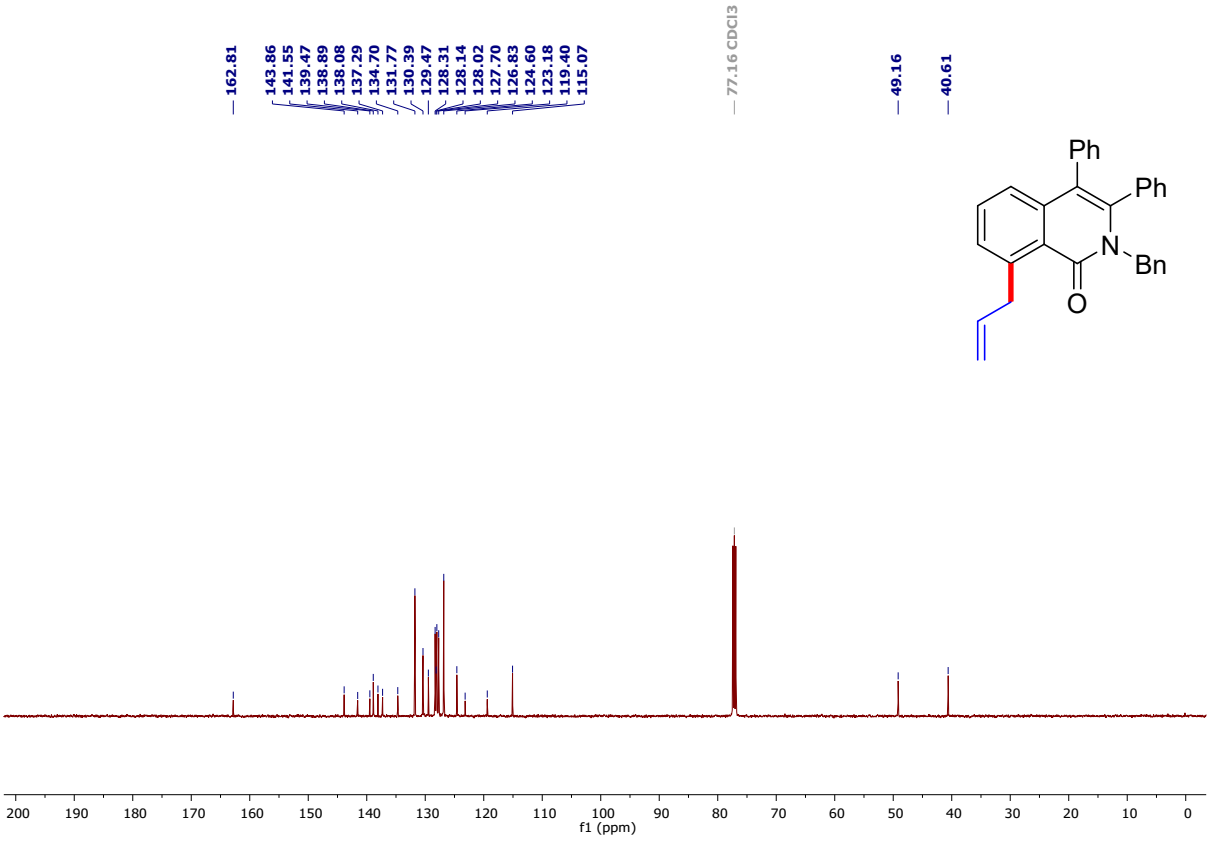
^{13}C{^{1}H} NMR spectrum of 3p



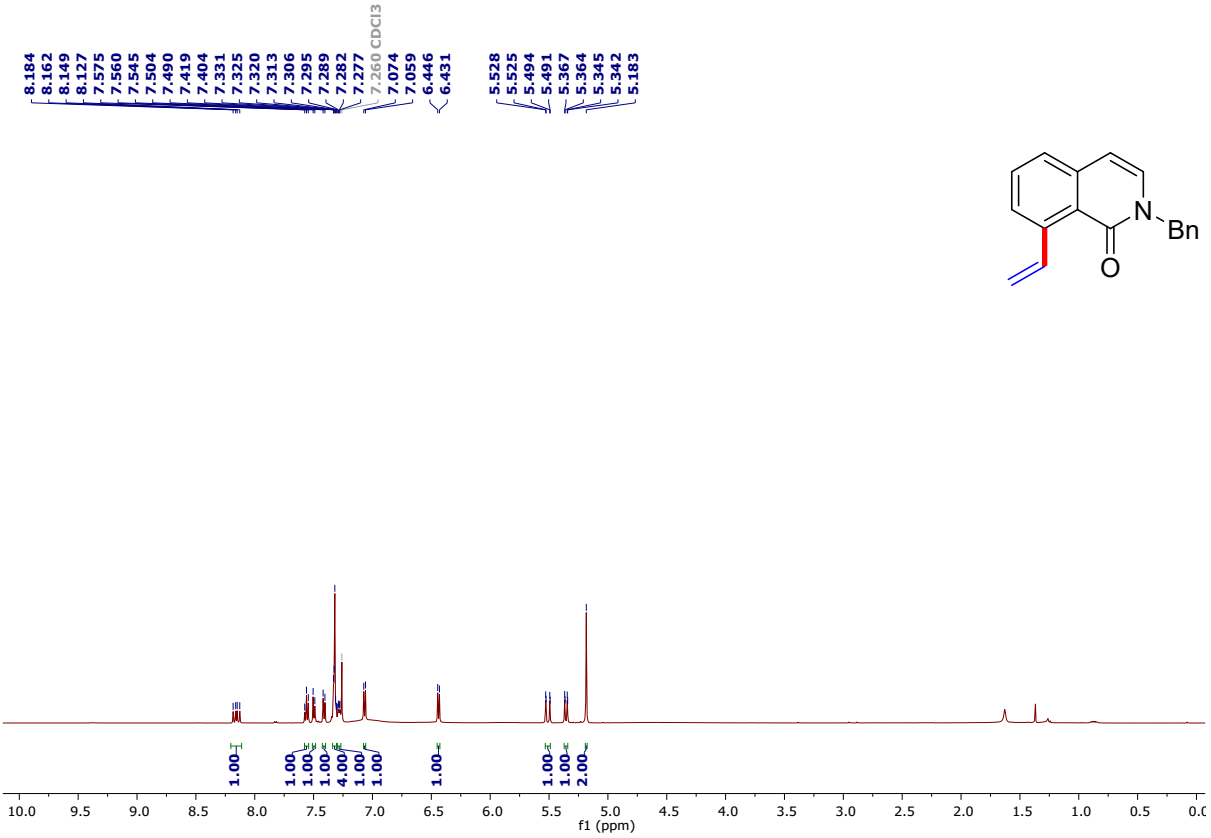
^{1}H NMR spectrum of 3q



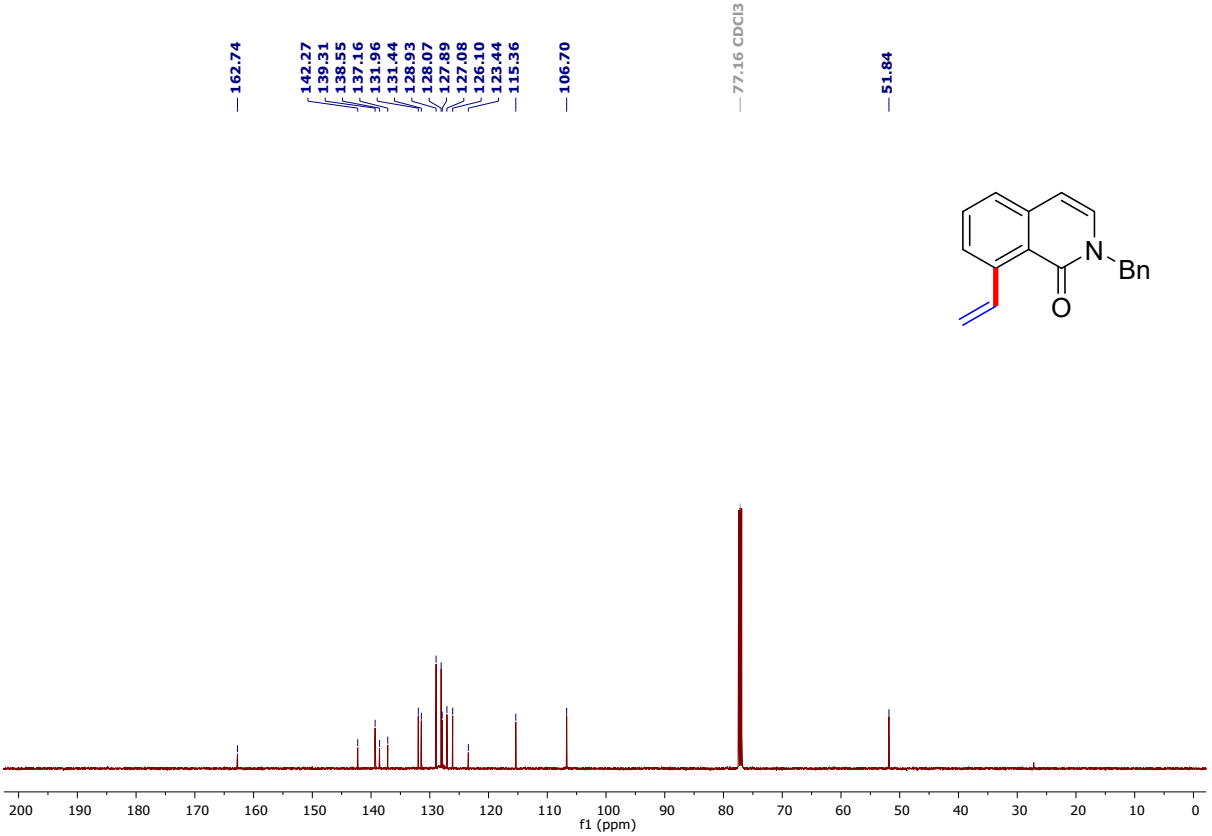
^{13}C{^{1}H} NMR spectrum of 3q



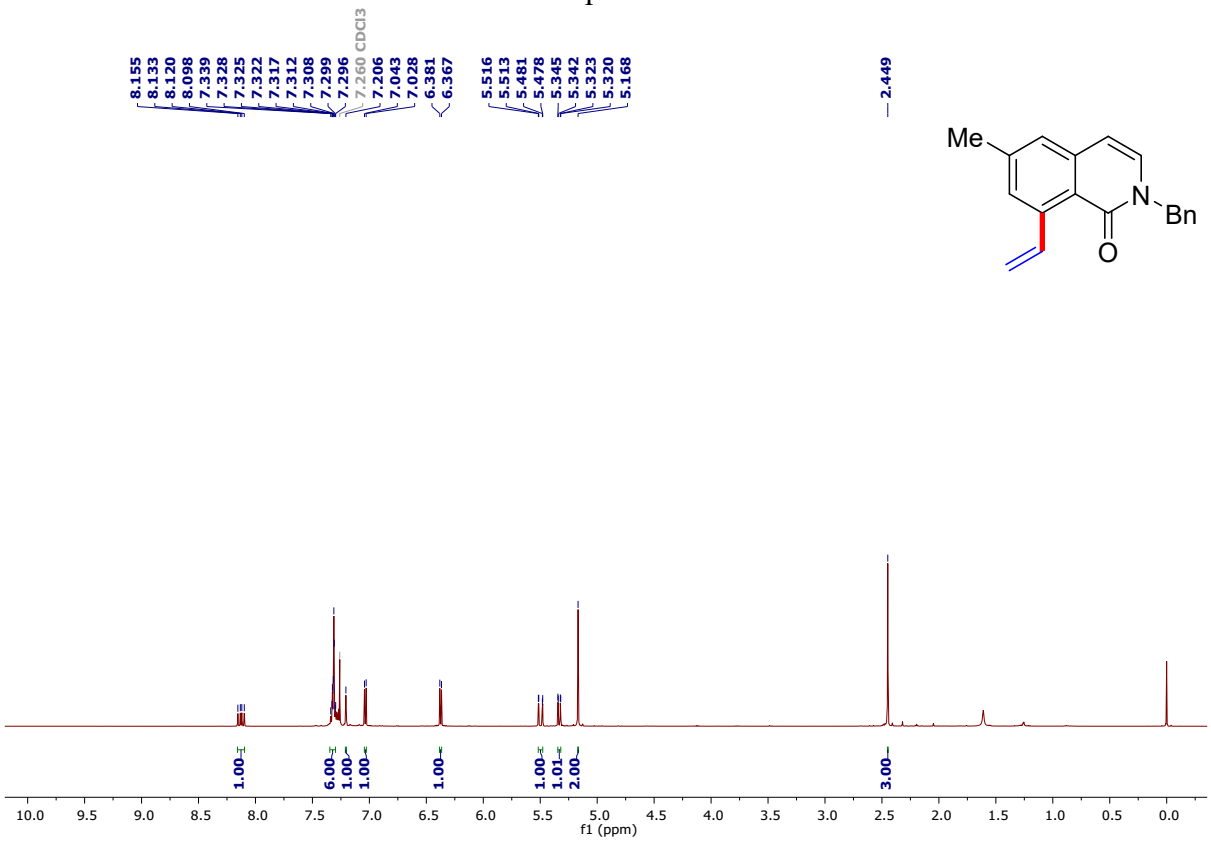
^{1}H NMR spectrum of 3r



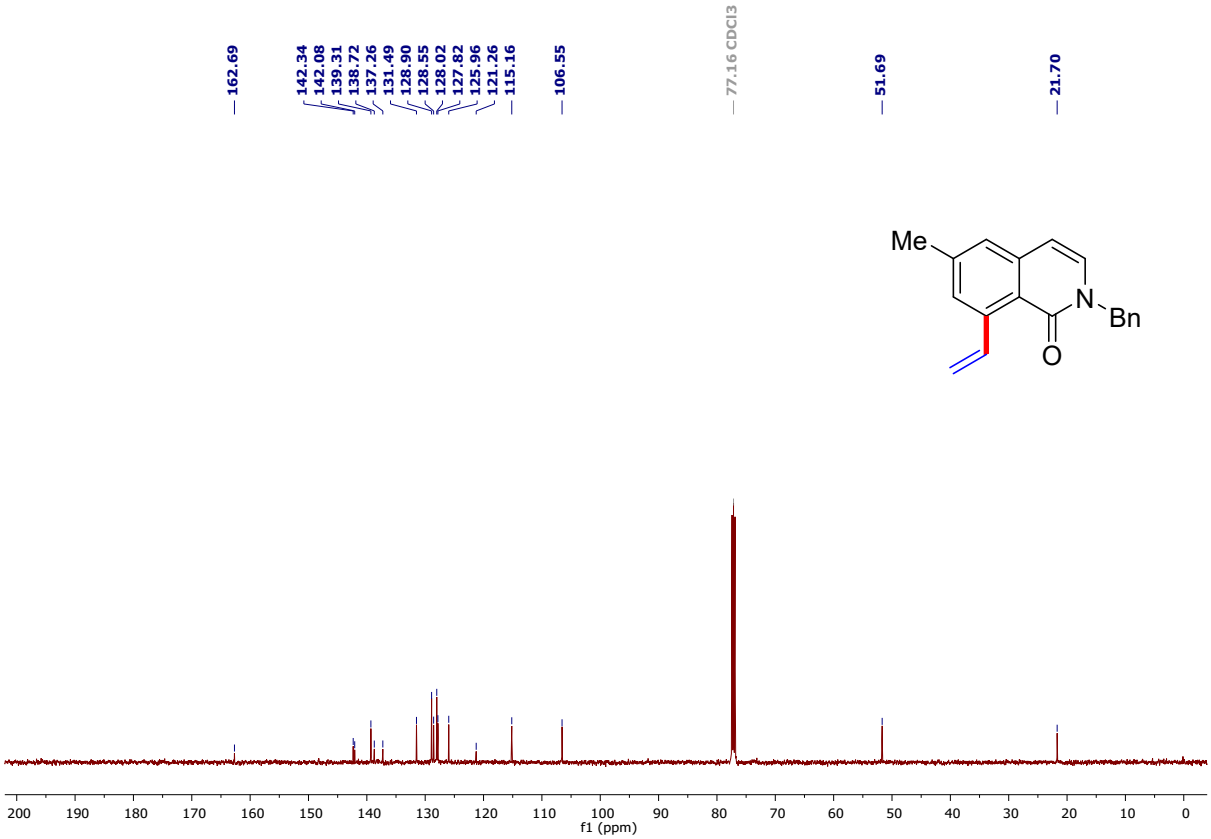
^{13}C{^{1}H} NMR spectrum of 3r



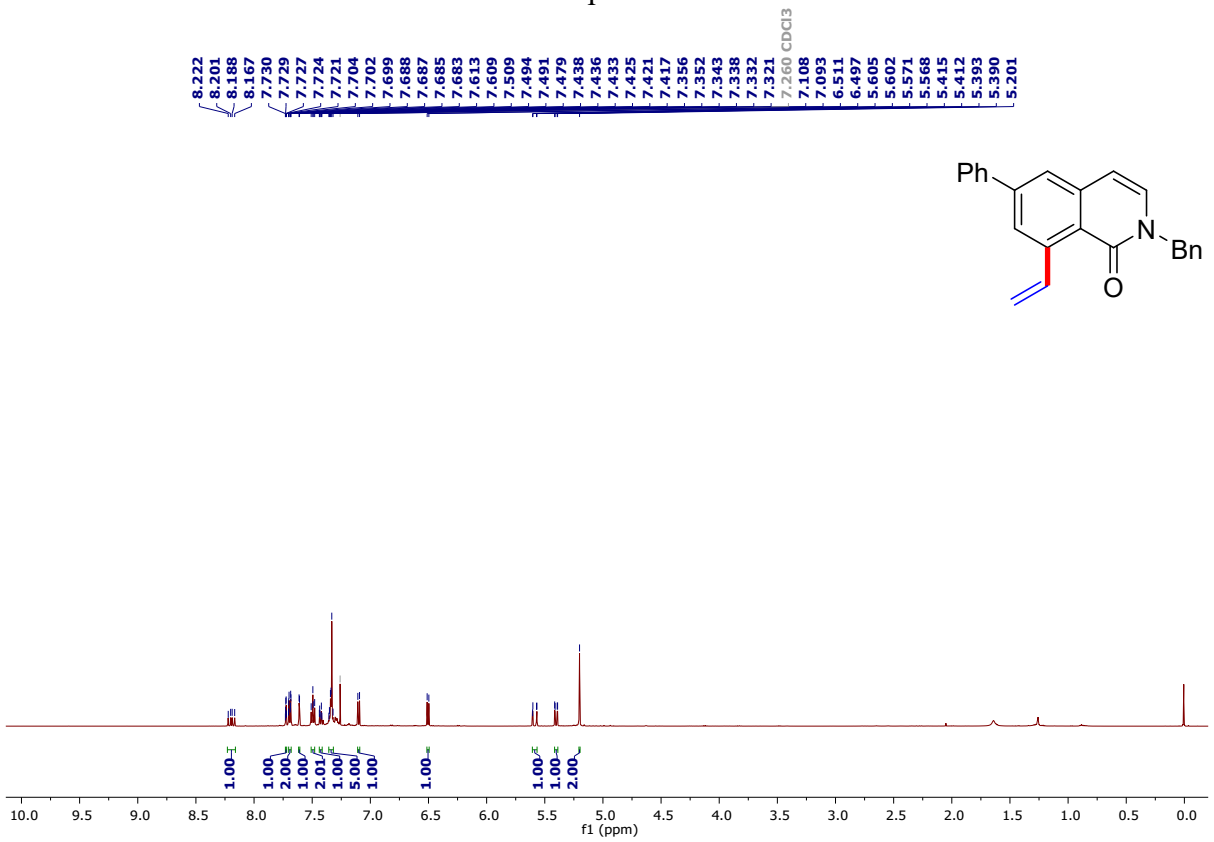
^{1}H NMR spectrum of 3s



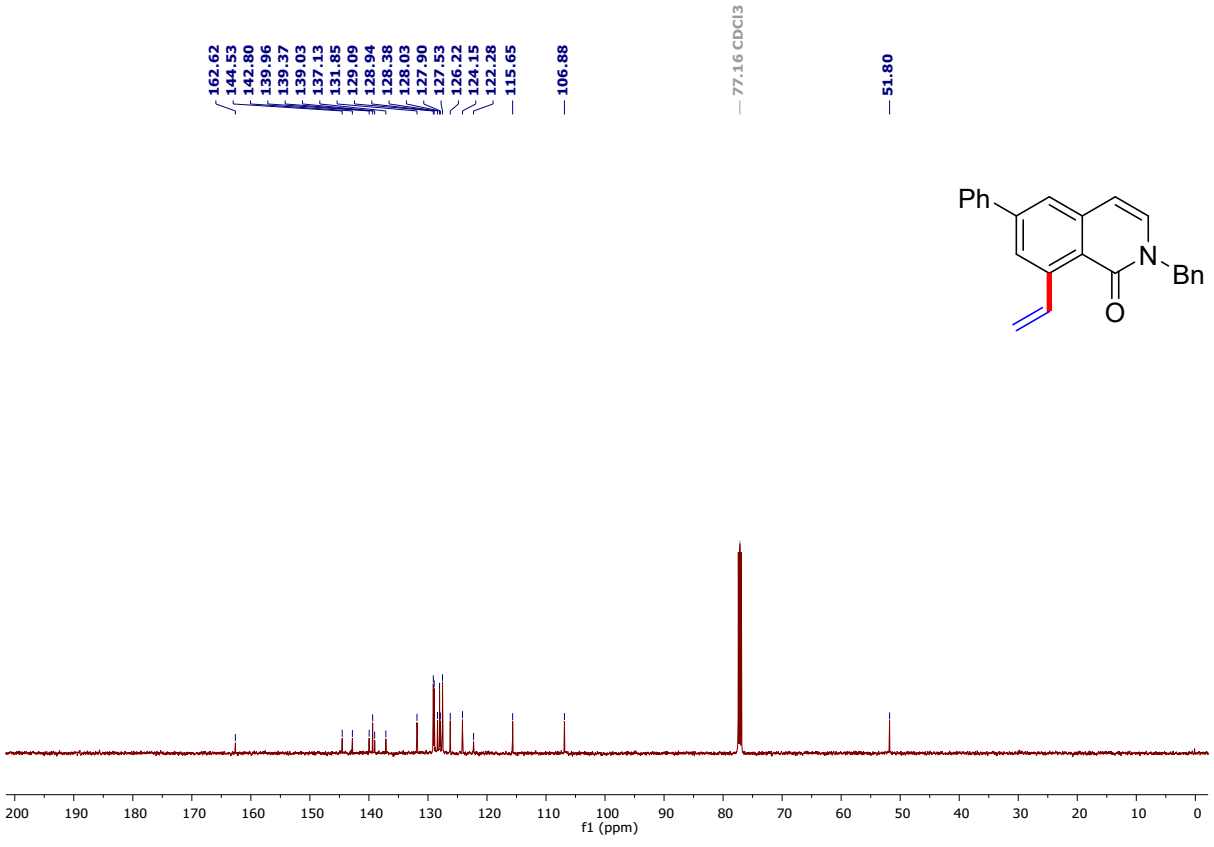
^{13}C{^{1}H} NMR spectrum of 3s



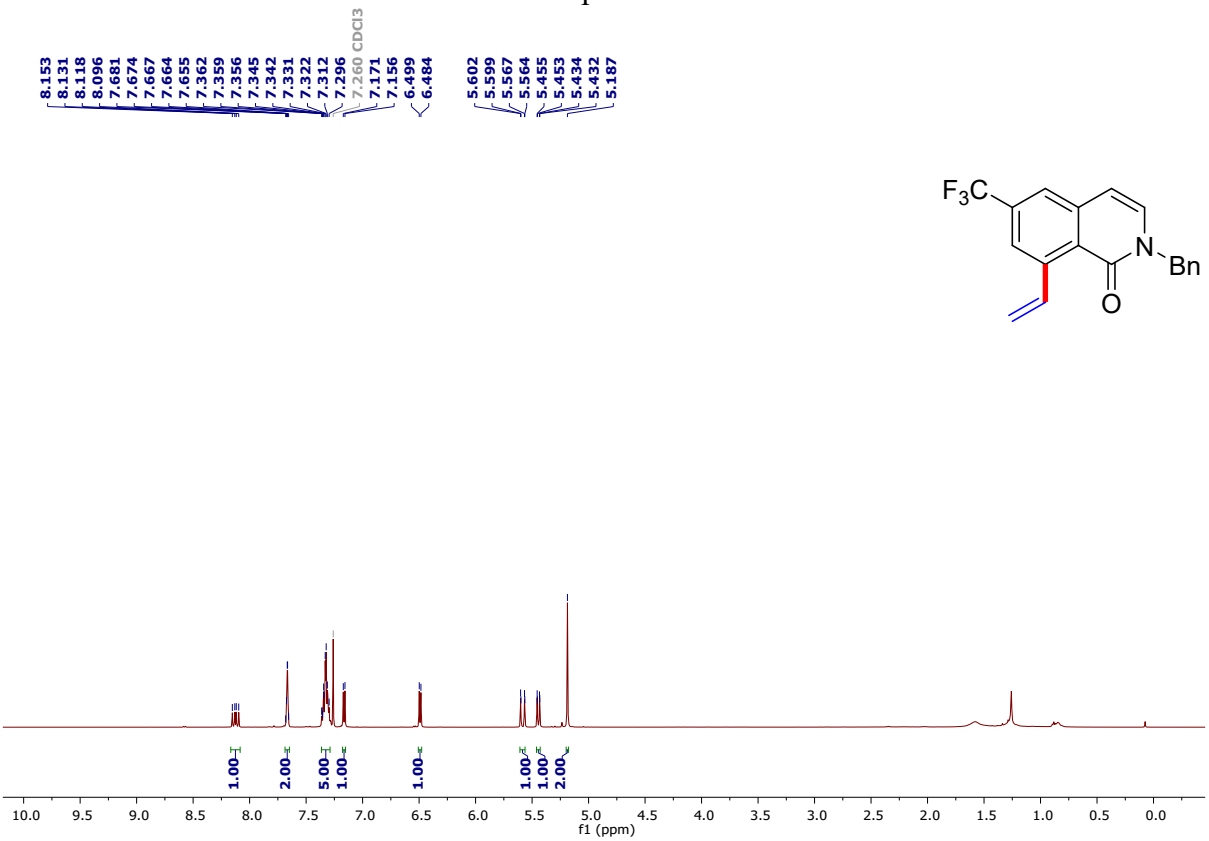
^{1}H NMR spectrum of 3t



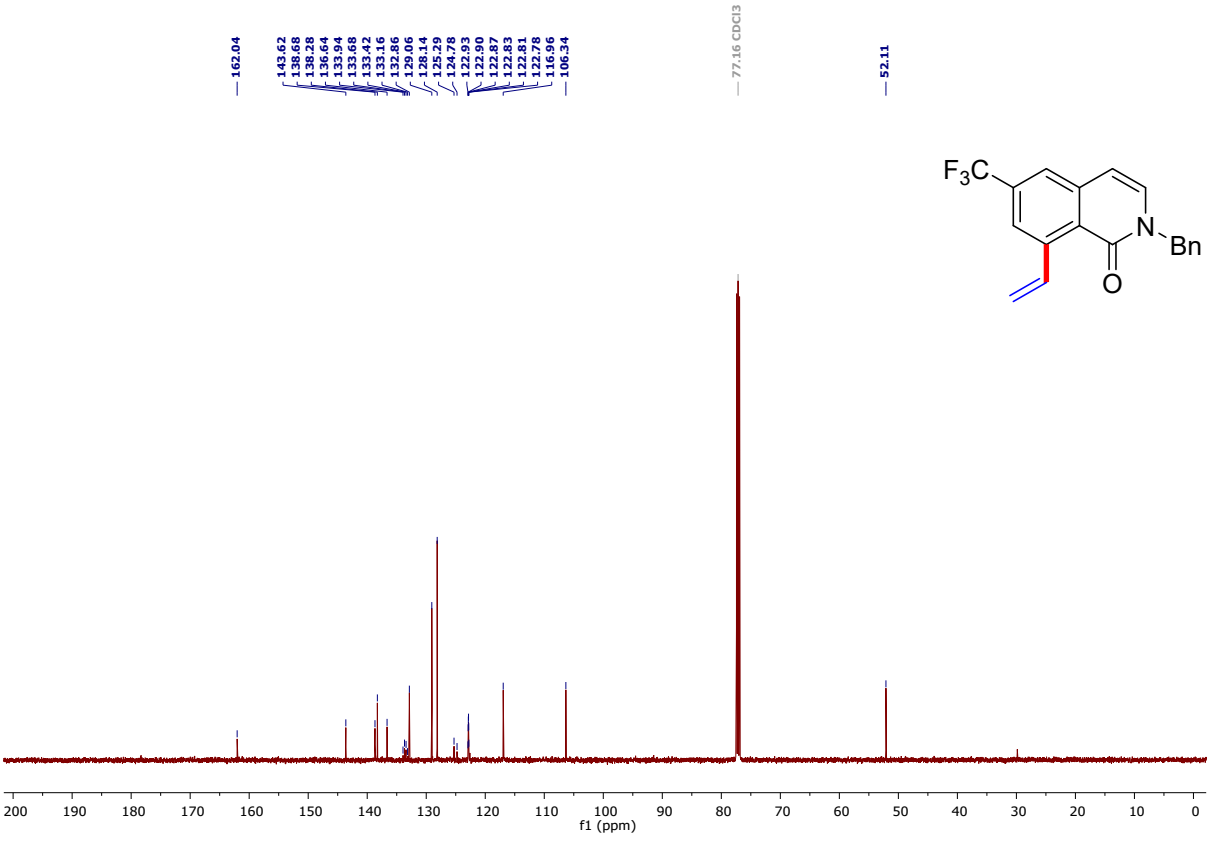
^{13}C{^{1}H} NMR spectrum of 3t



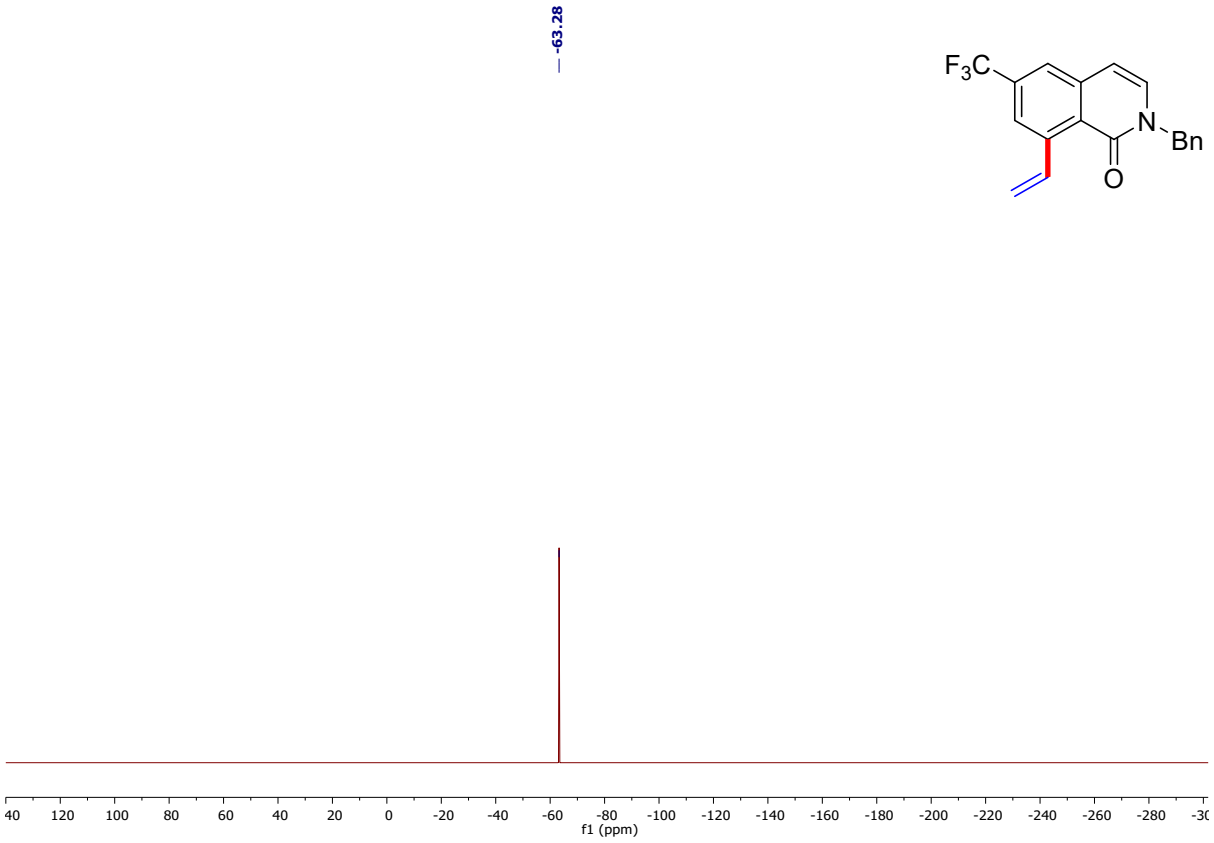
^{1}H NMR spectrum of 3u



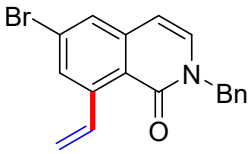
^{13}C{^{1}H} NMR spectrum of 3u

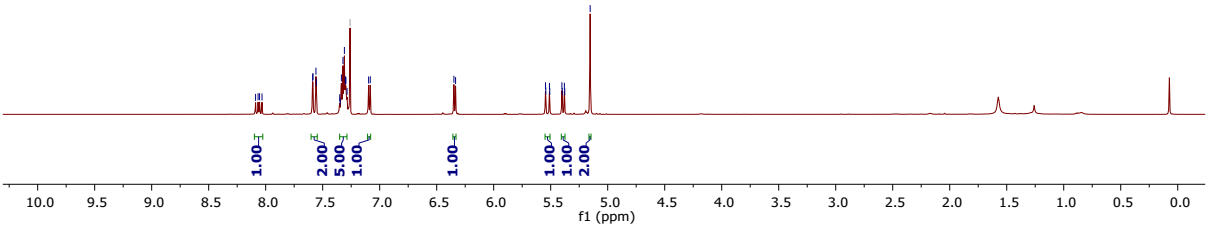


^{19}F NMR spectrum of 3u

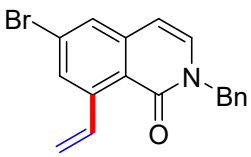


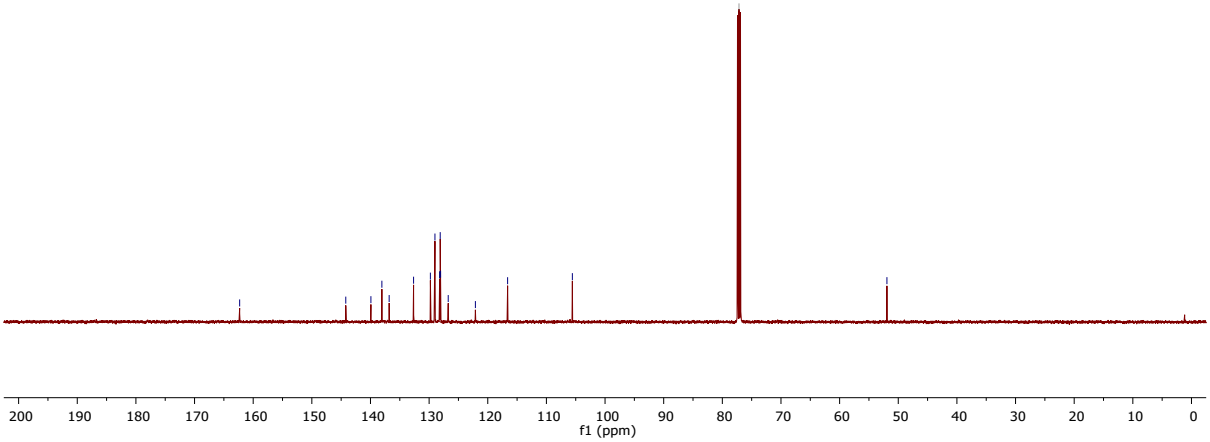
^{1}H NMR spectrum of 3v



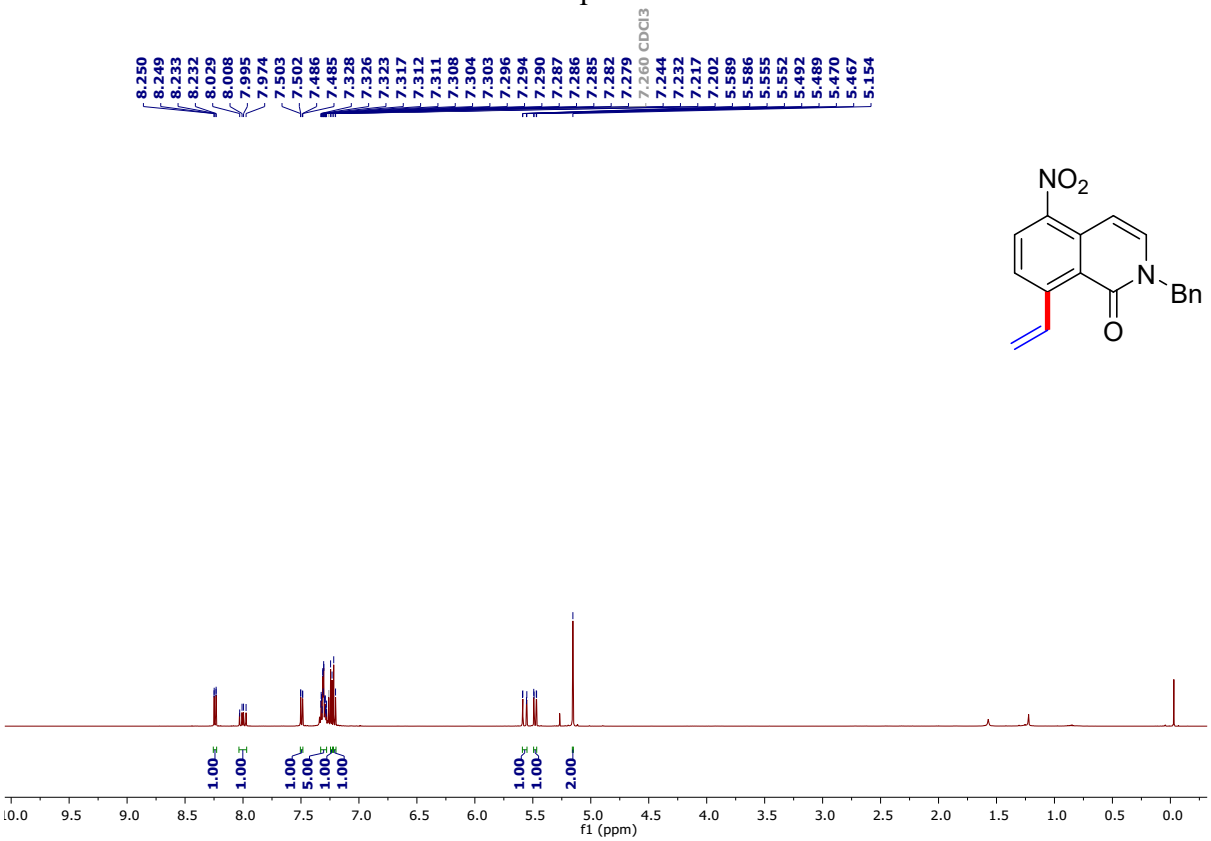


^{13}C{^{1}H} NMR spectrum of 3v

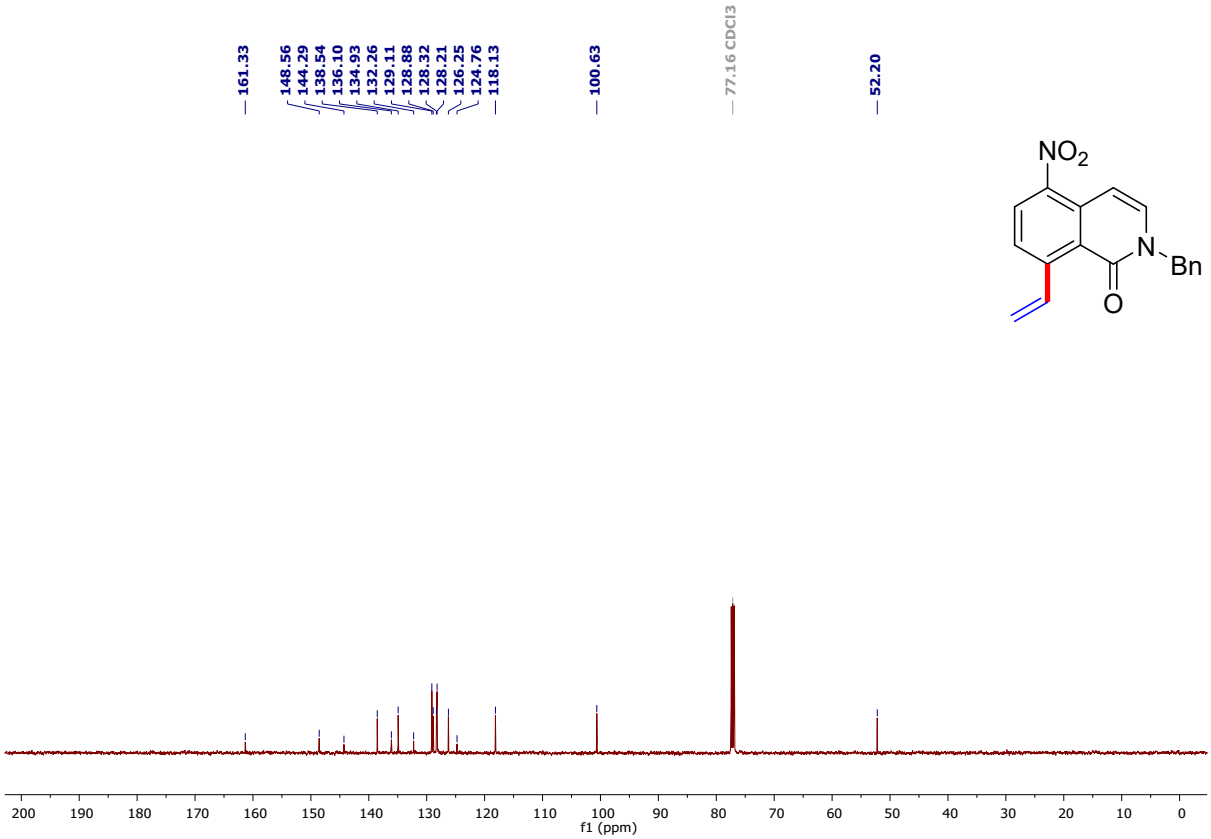




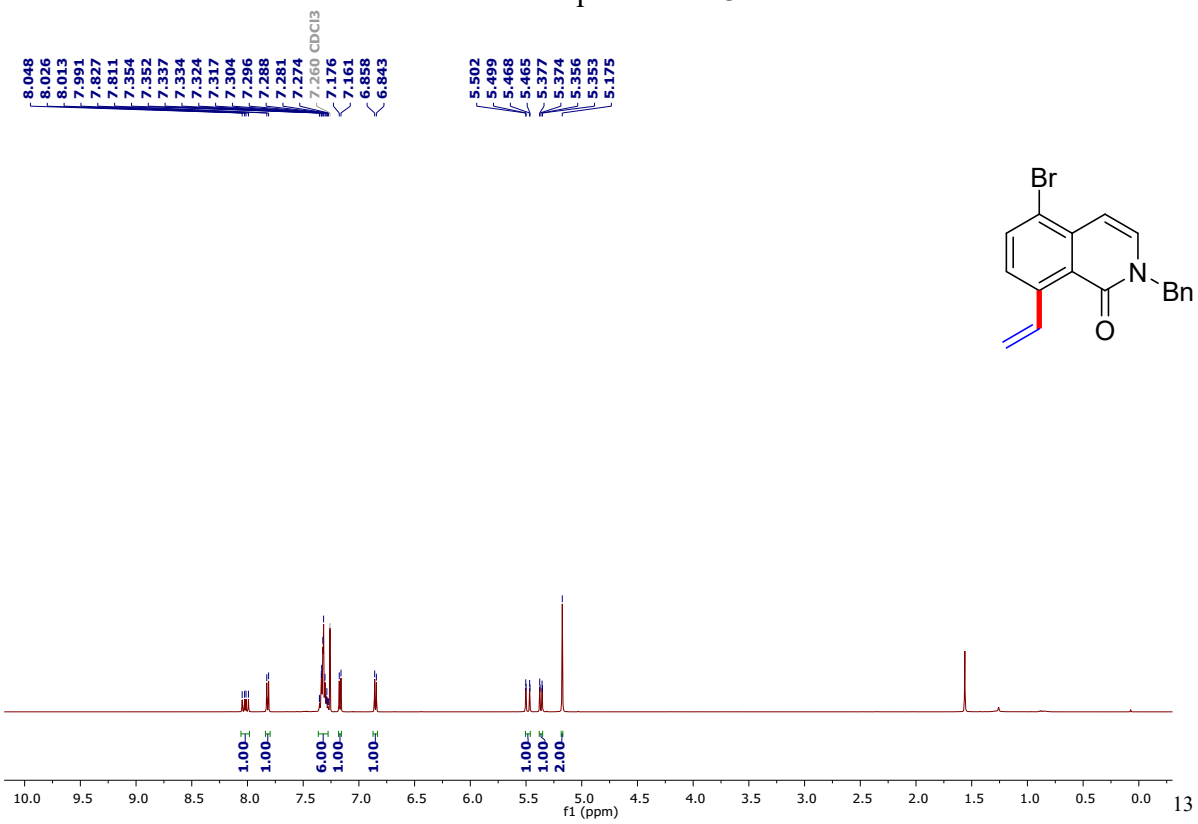
^{1}H NMR spectrum of 3w



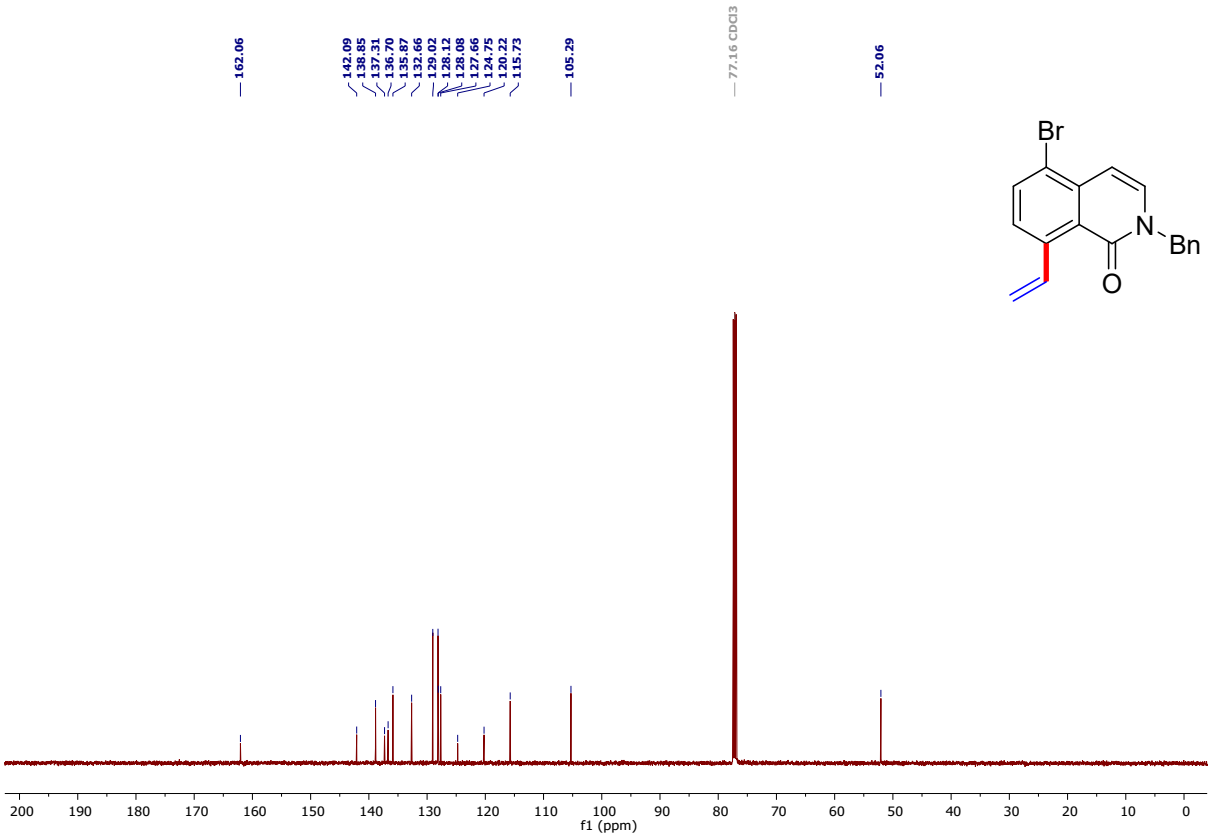
^{13}C{^{1}H} NMR spectrum of 3w



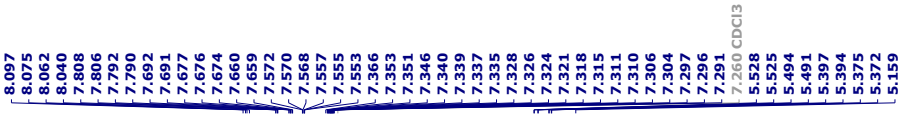
^{1}H NMR spectrum of 3x

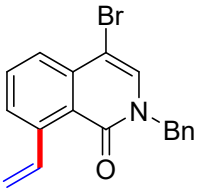


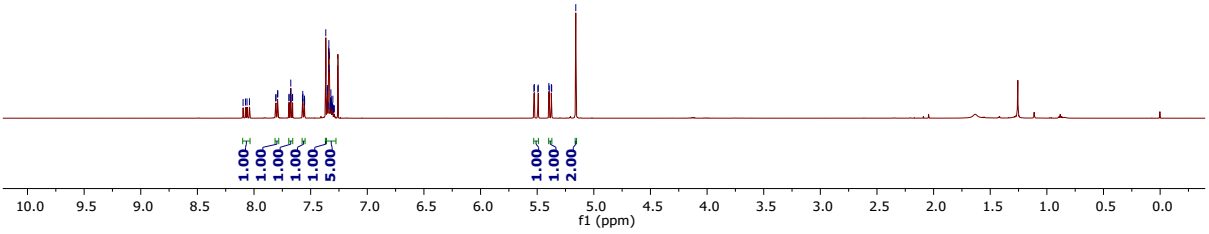
C{^{1}H} NMR spectrum of 3x



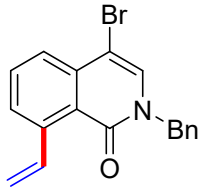
^{1}H NMR spectrum of 3y

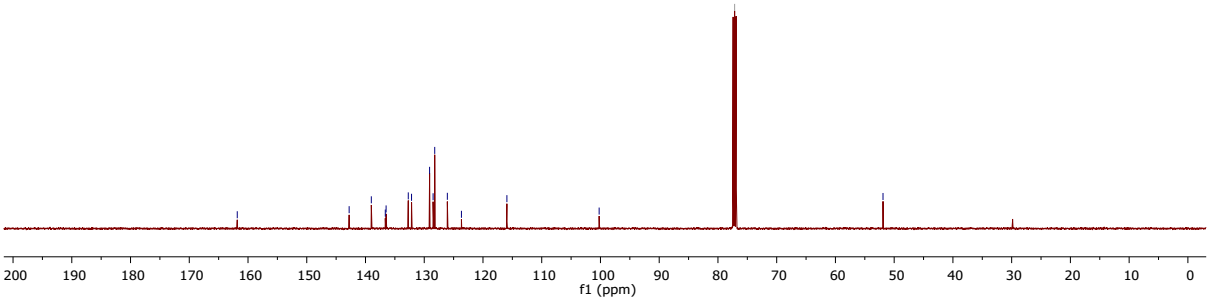




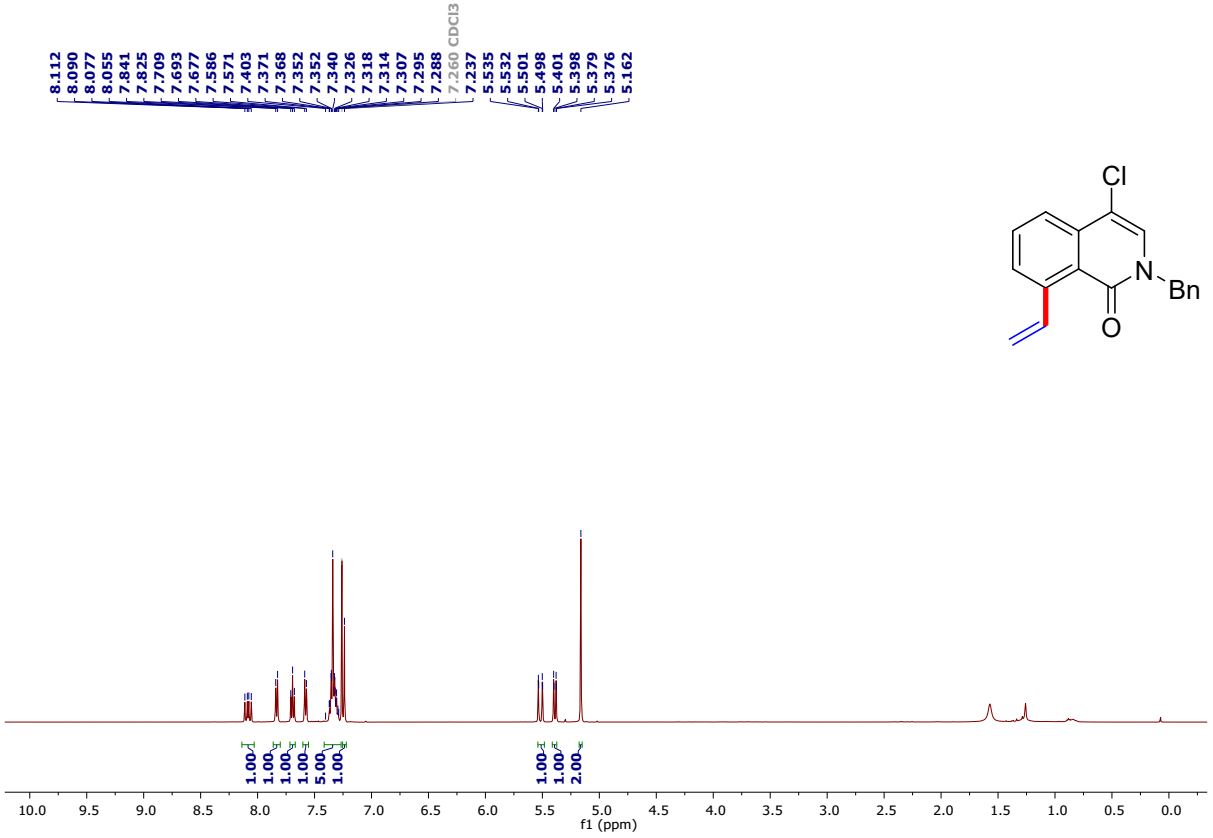


^{13}C{^{1}H} NMR spectrum of 3y

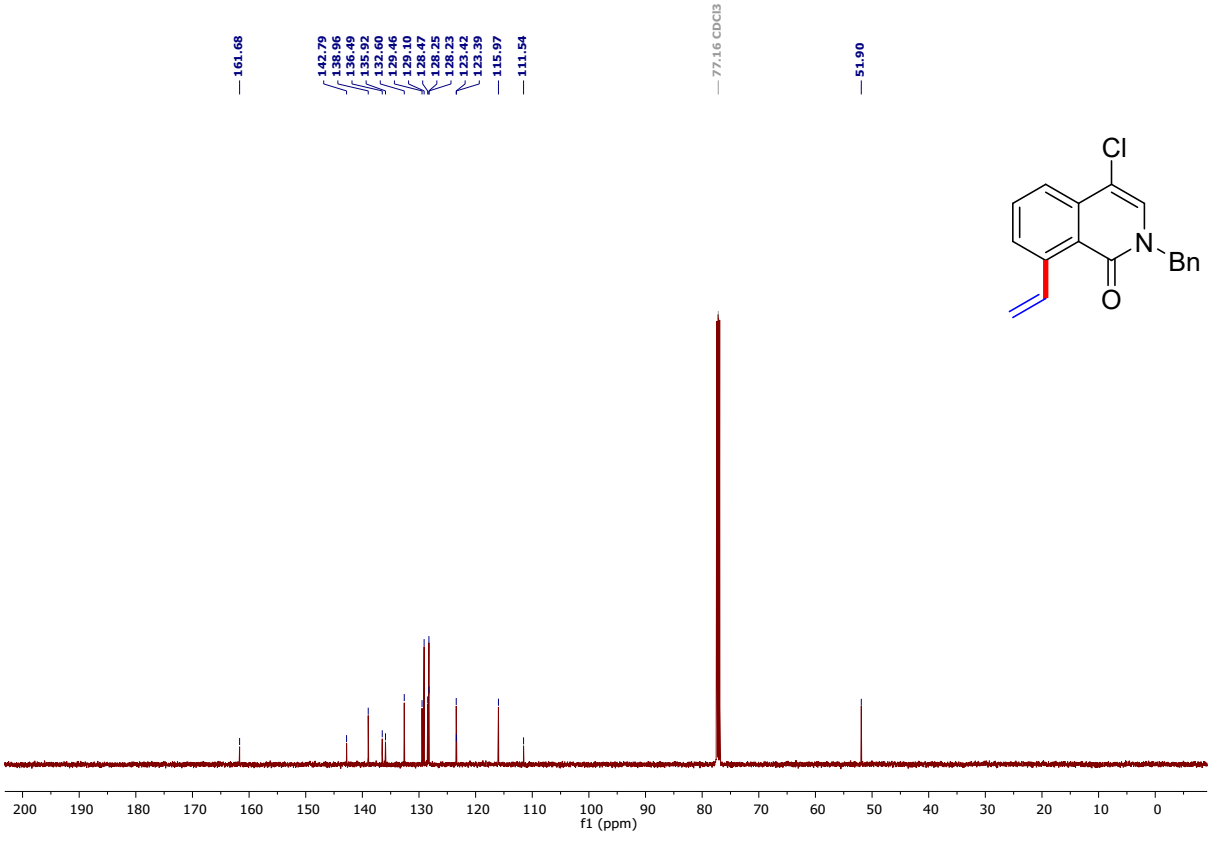




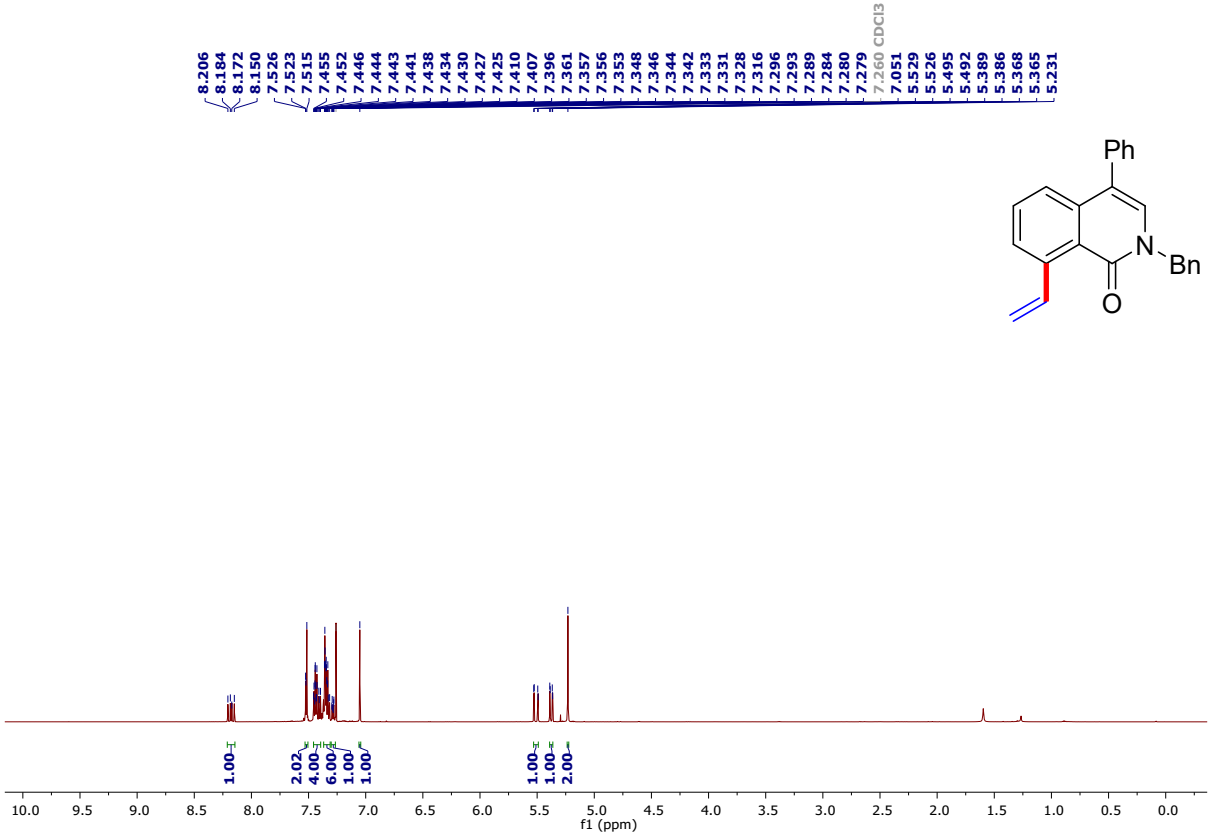
^{1}H NMR spectrum of 3z



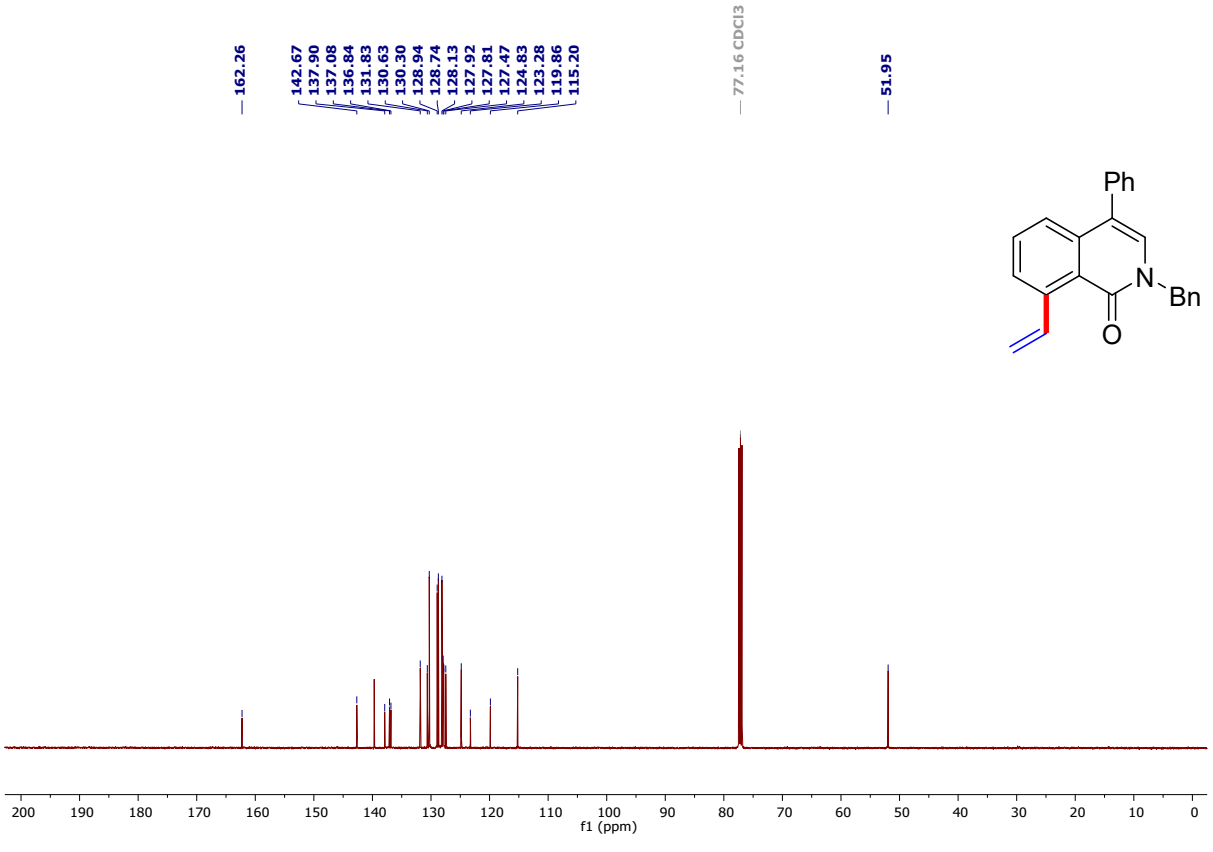
^{13}C{^{1}H} NMR spectrum of 3z



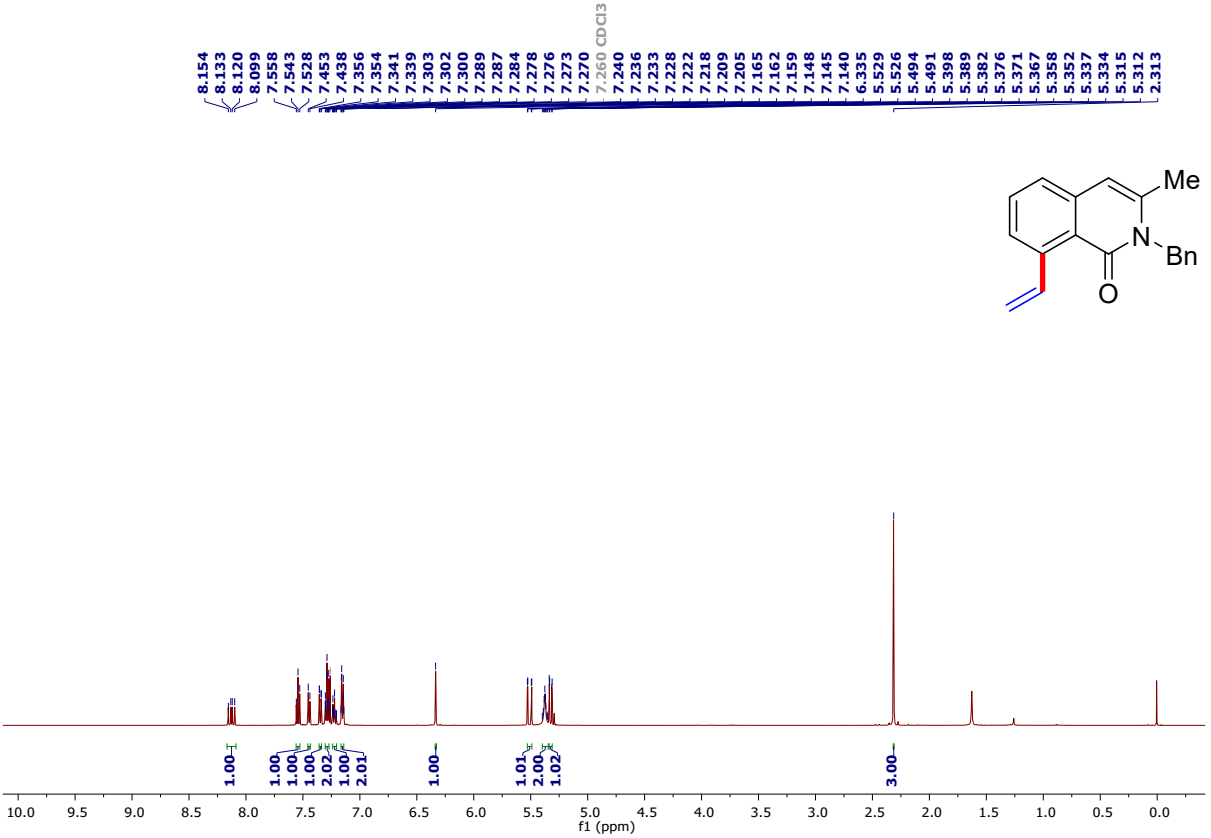
^{1}H NMR spectrum of 3za



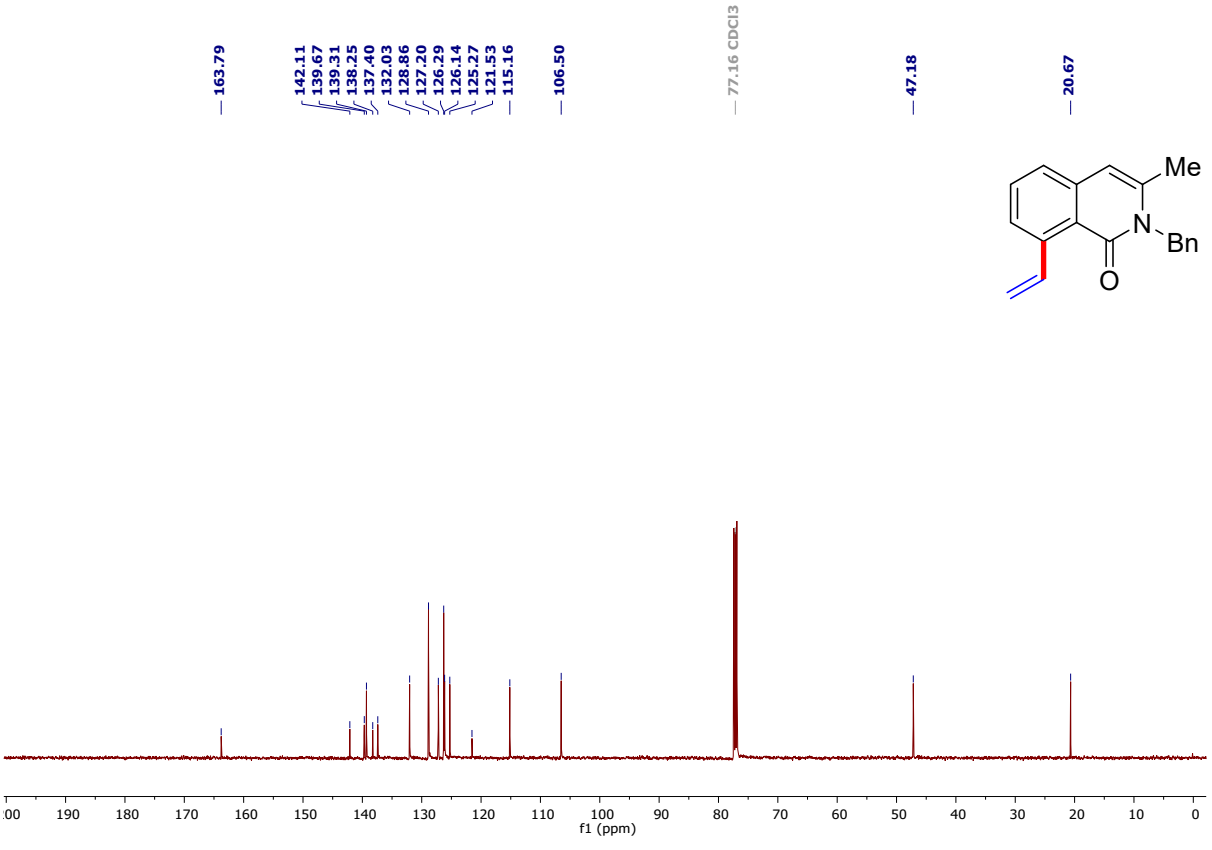
^{13}C{^{1}H} NMR spectrum of 3za



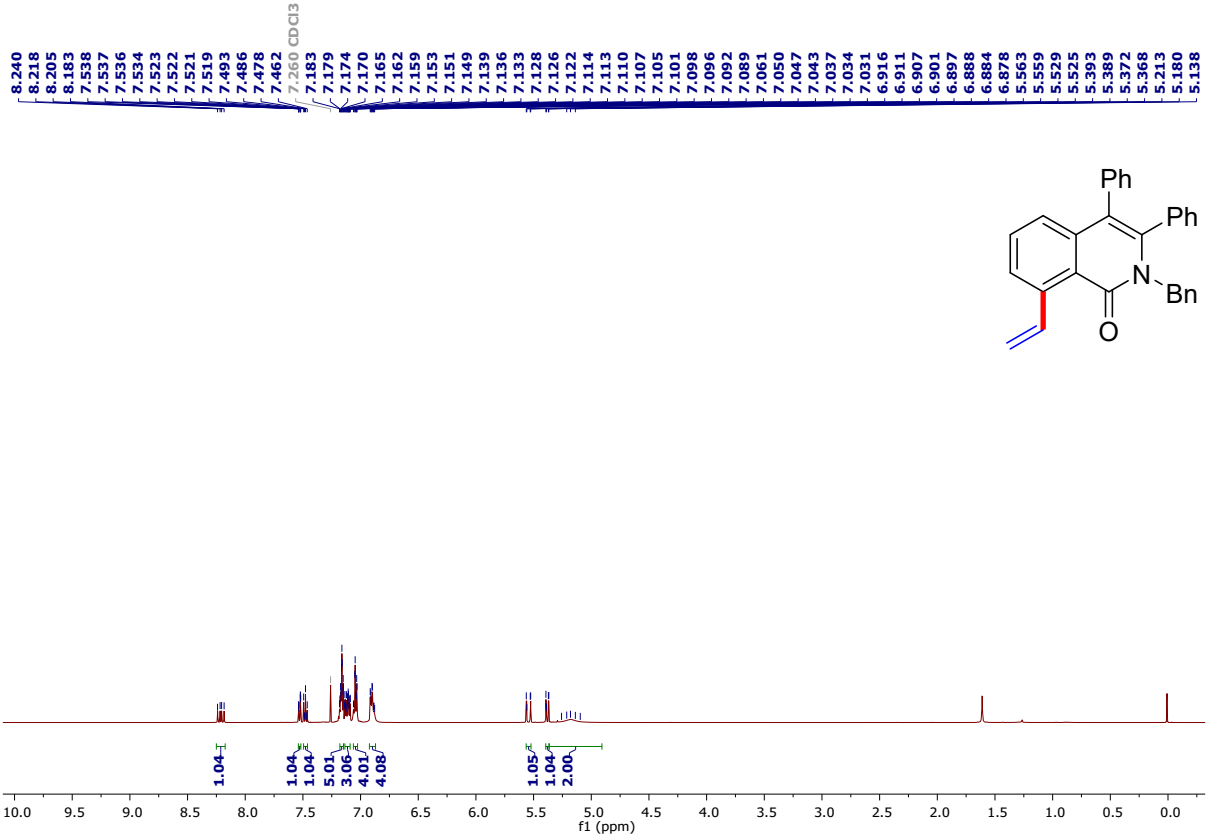
^{1}H NMR spectrum of 3zb



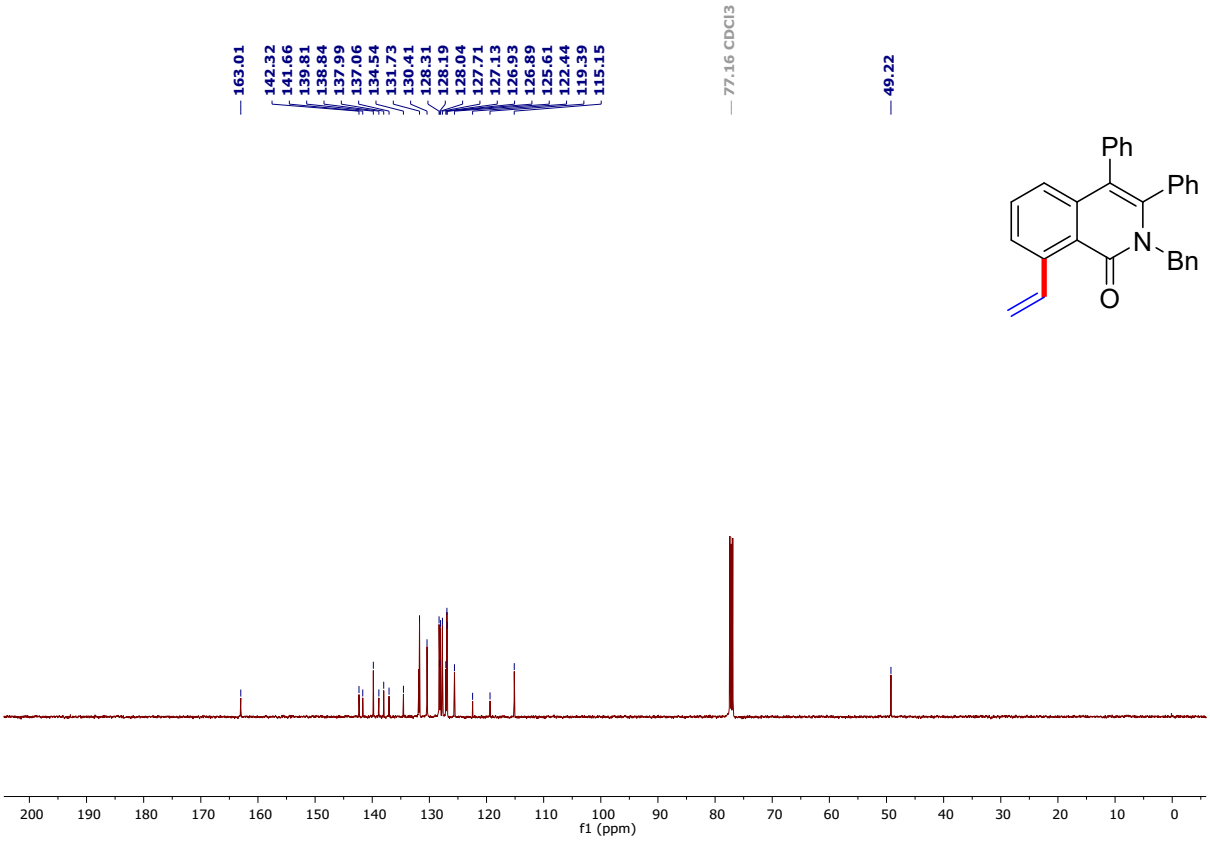
^{13}C{^{1}H} NMR spectrum of 3zb



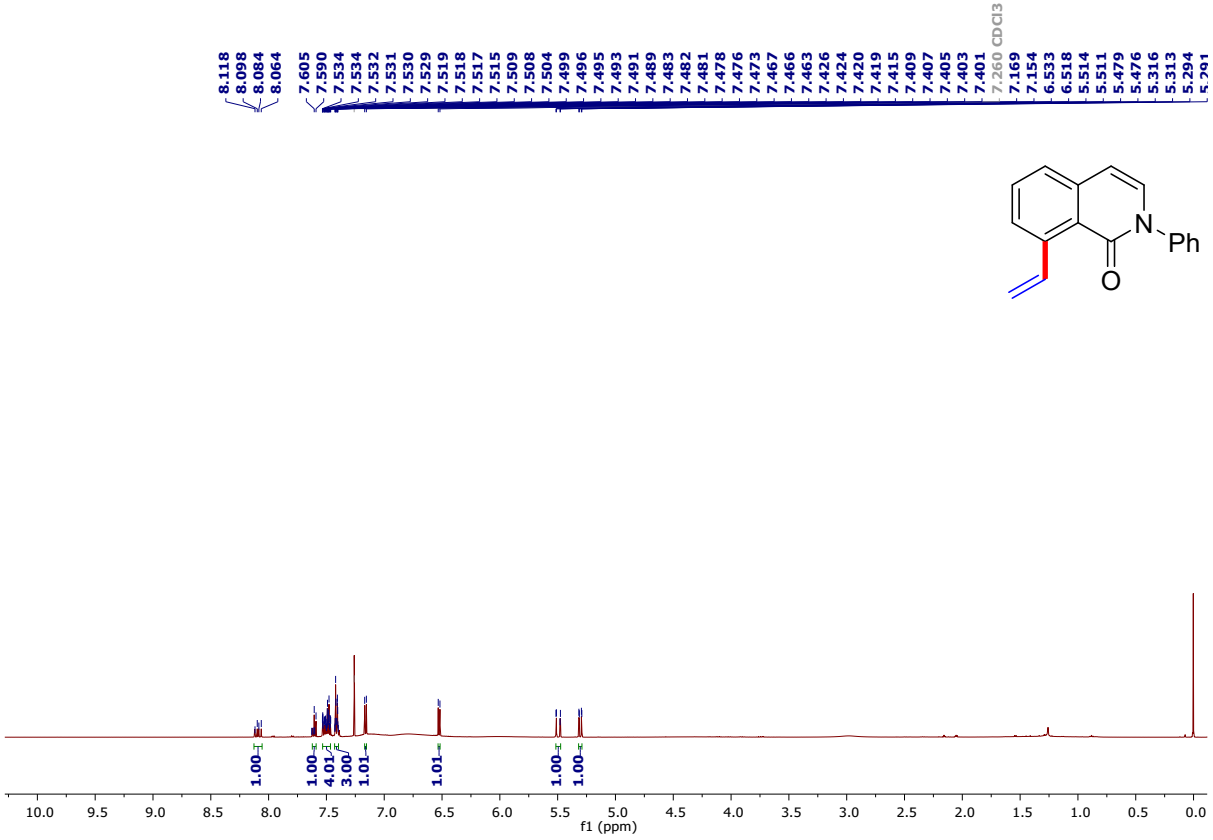
^{1}H NMR spectrum of 3zc



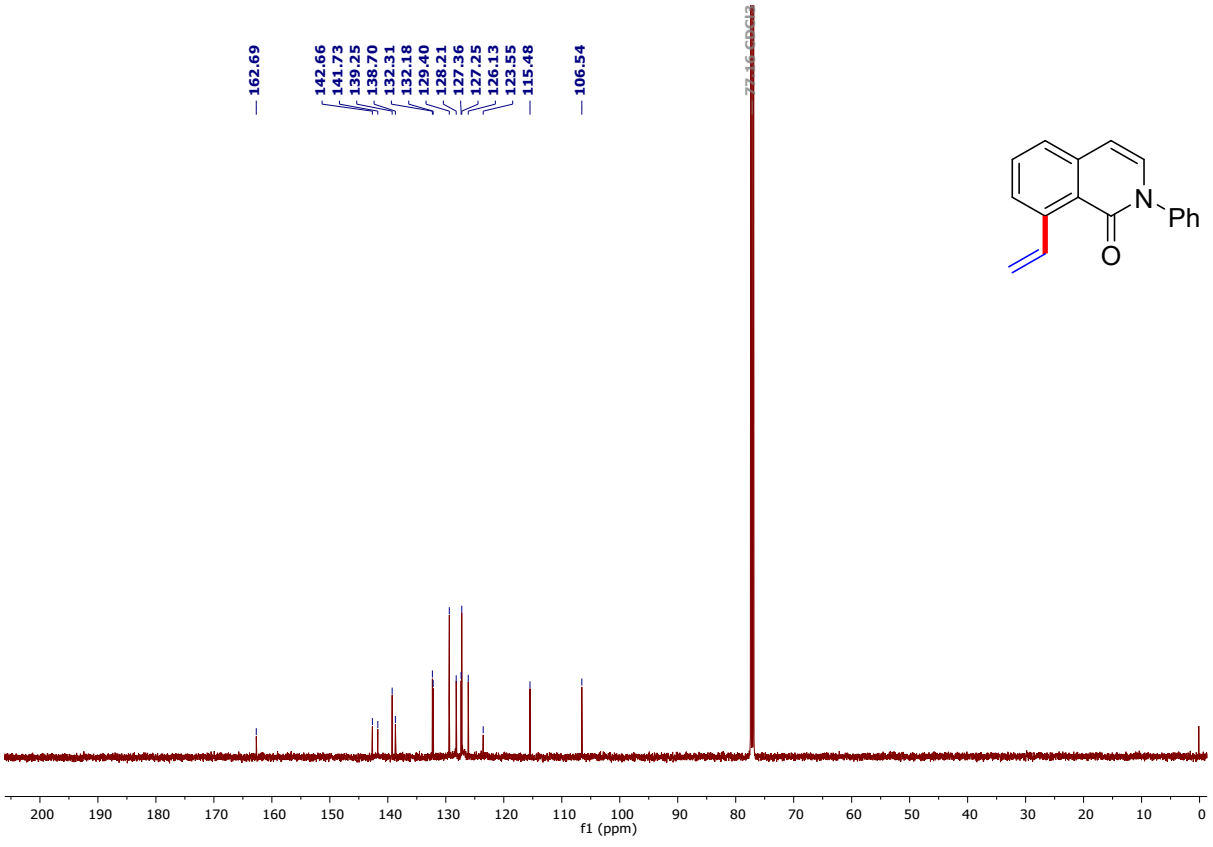
^{13}C{^{1}H} NMR spectrum of 3zc



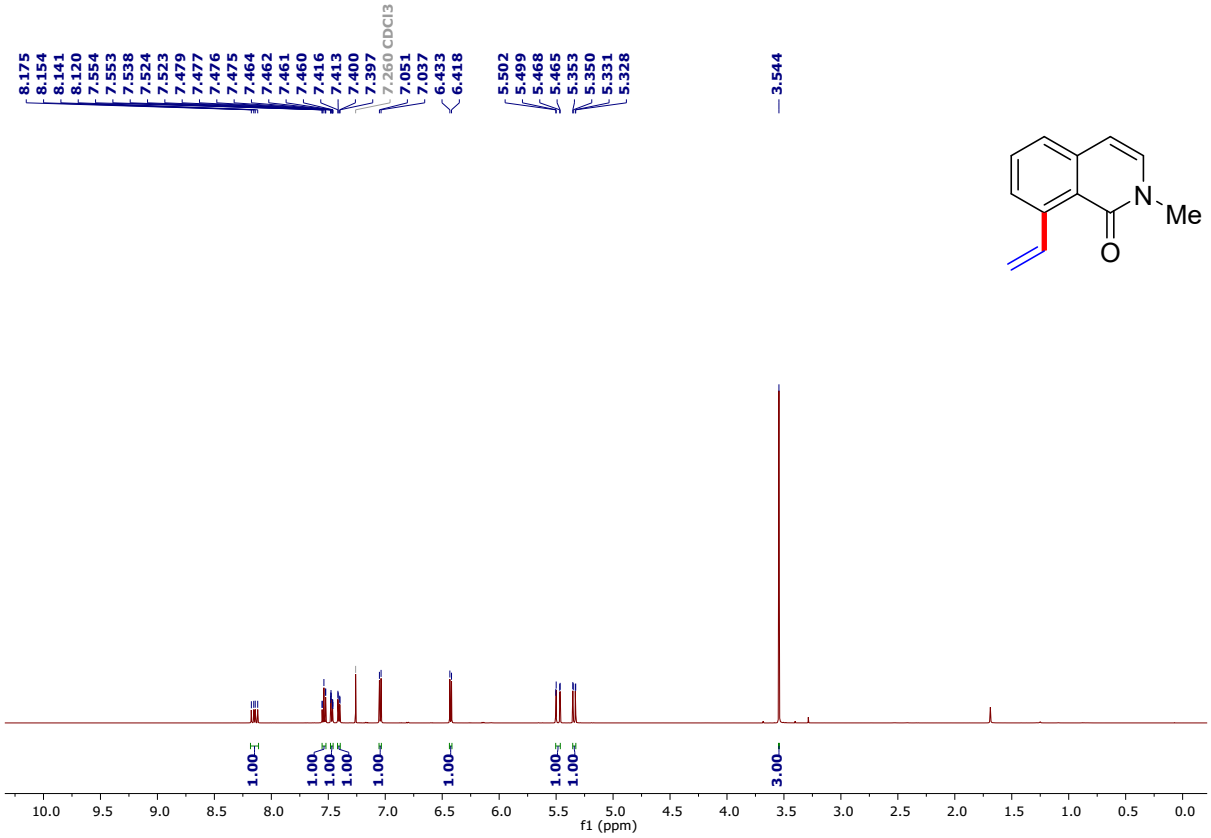
^{1}H NMR spectrum of 3zd



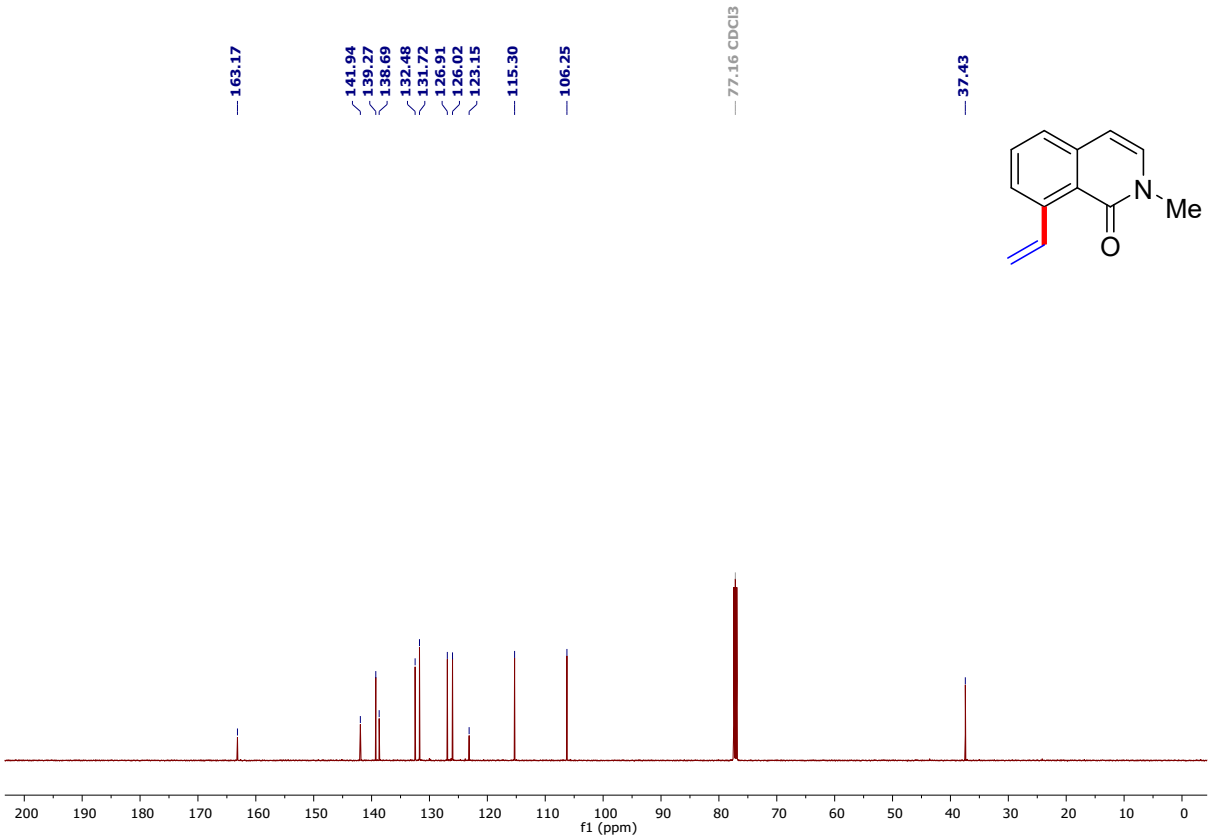
^{13}C{^{1}H} NMR spectrum of 3zd



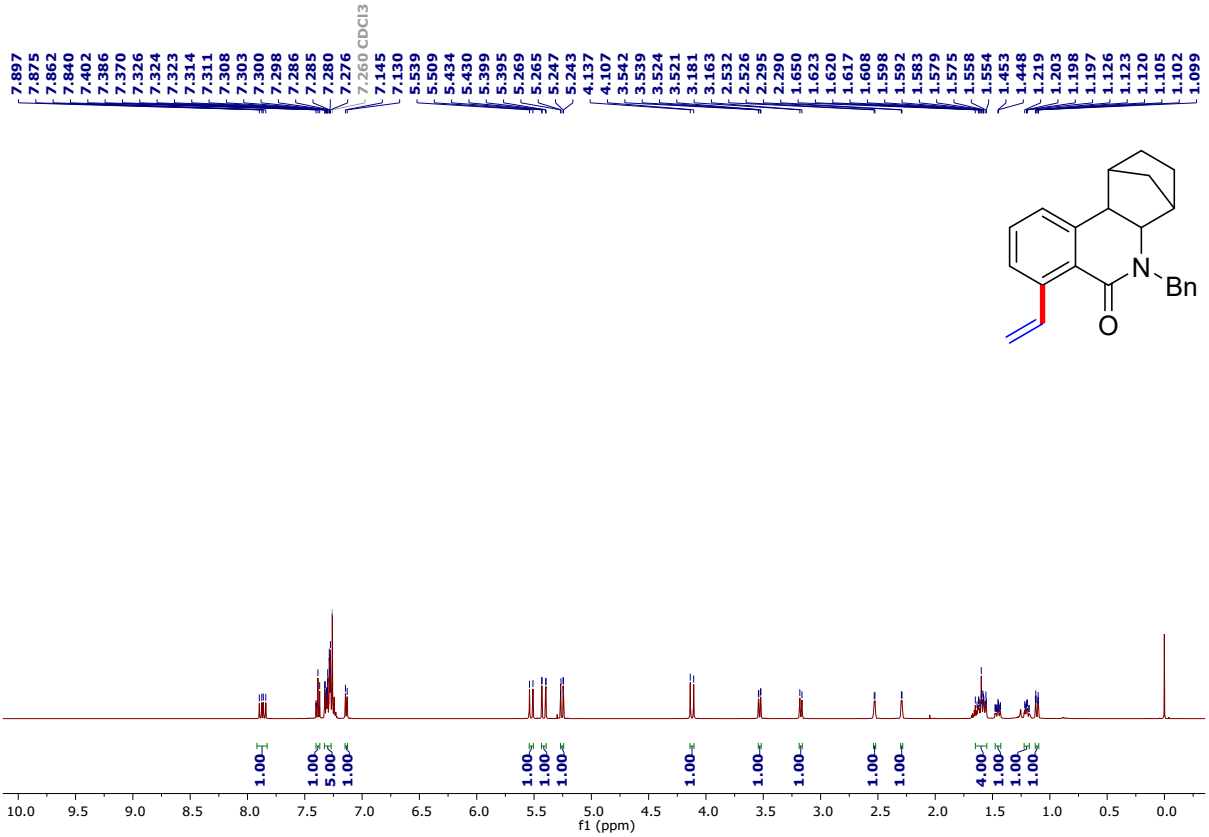
^{1}H NMR spectrum of 3ze



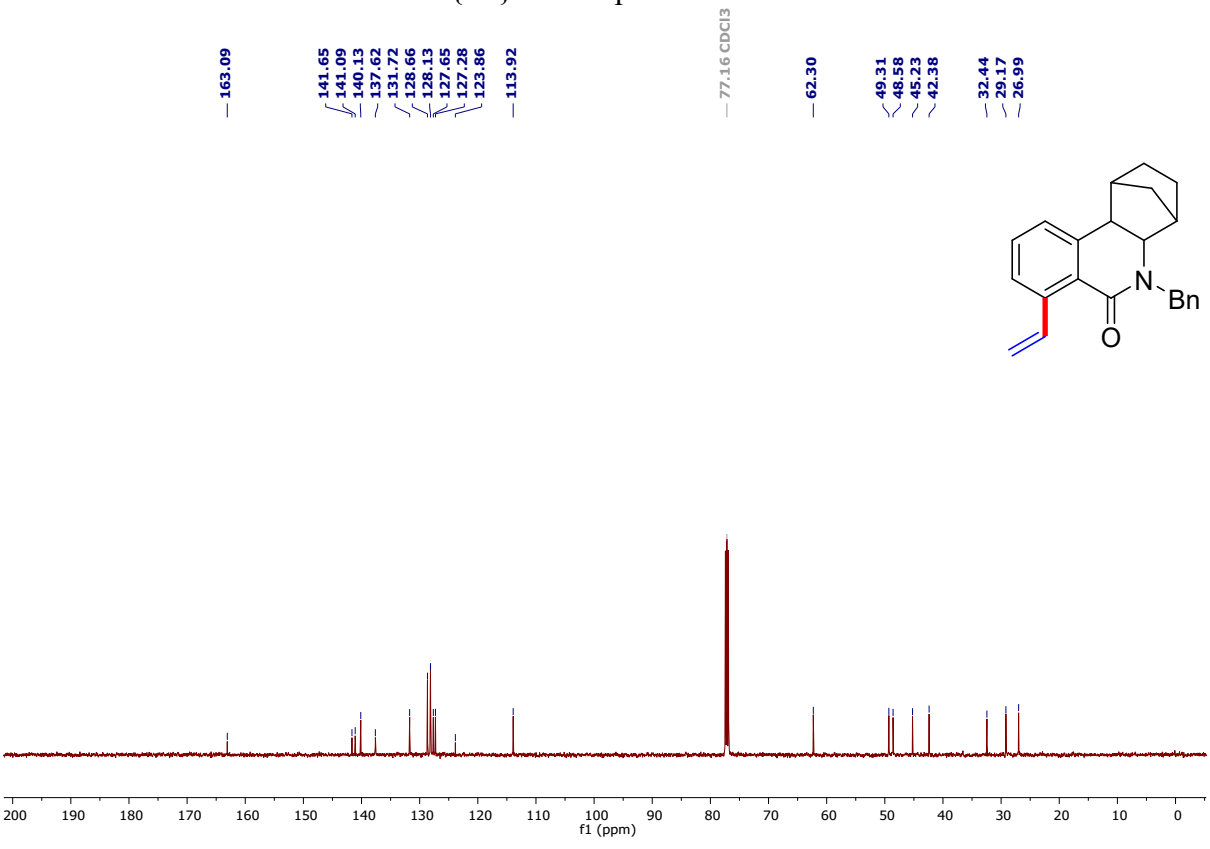
^{13}C{^{1}H} NMR spectrum of 3ze



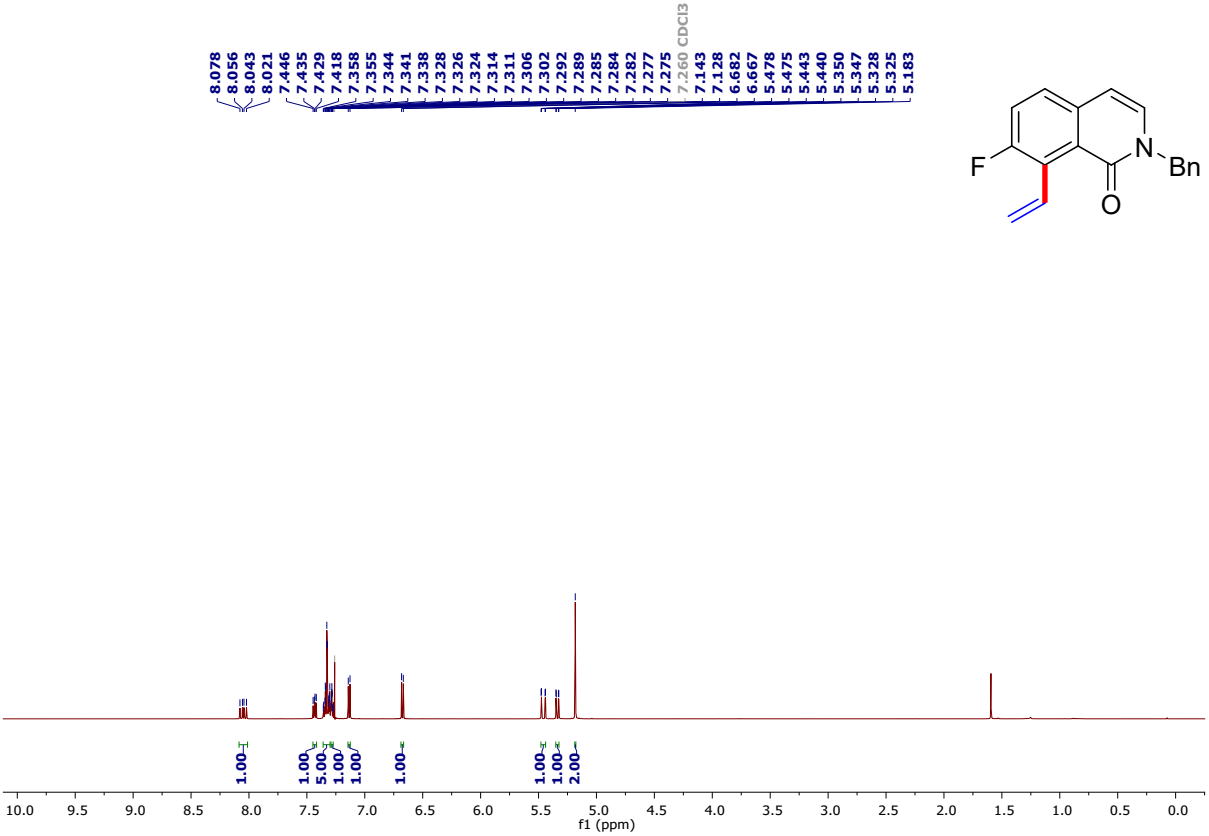
^{1}H NMR spectrum of 3zf



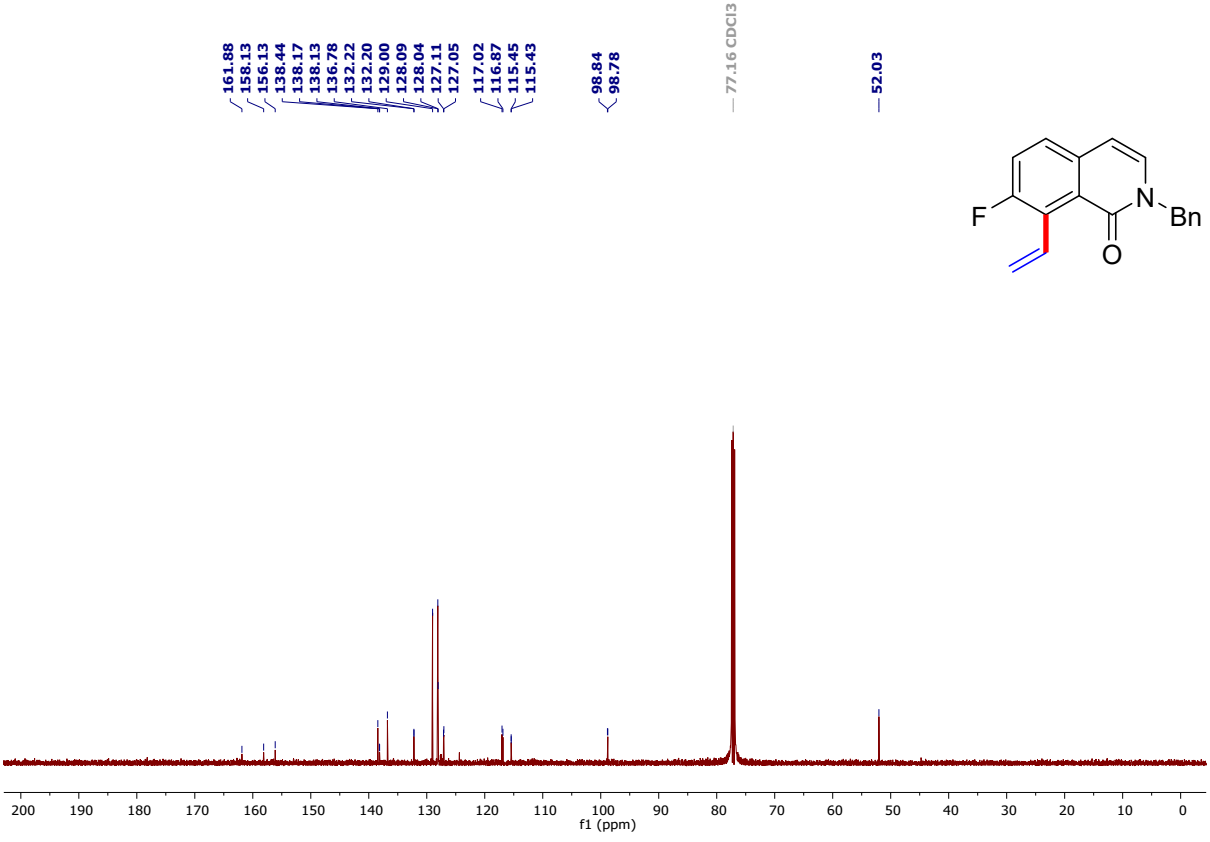
^{13}C{^{1}H} NMR spectrum of 3zf



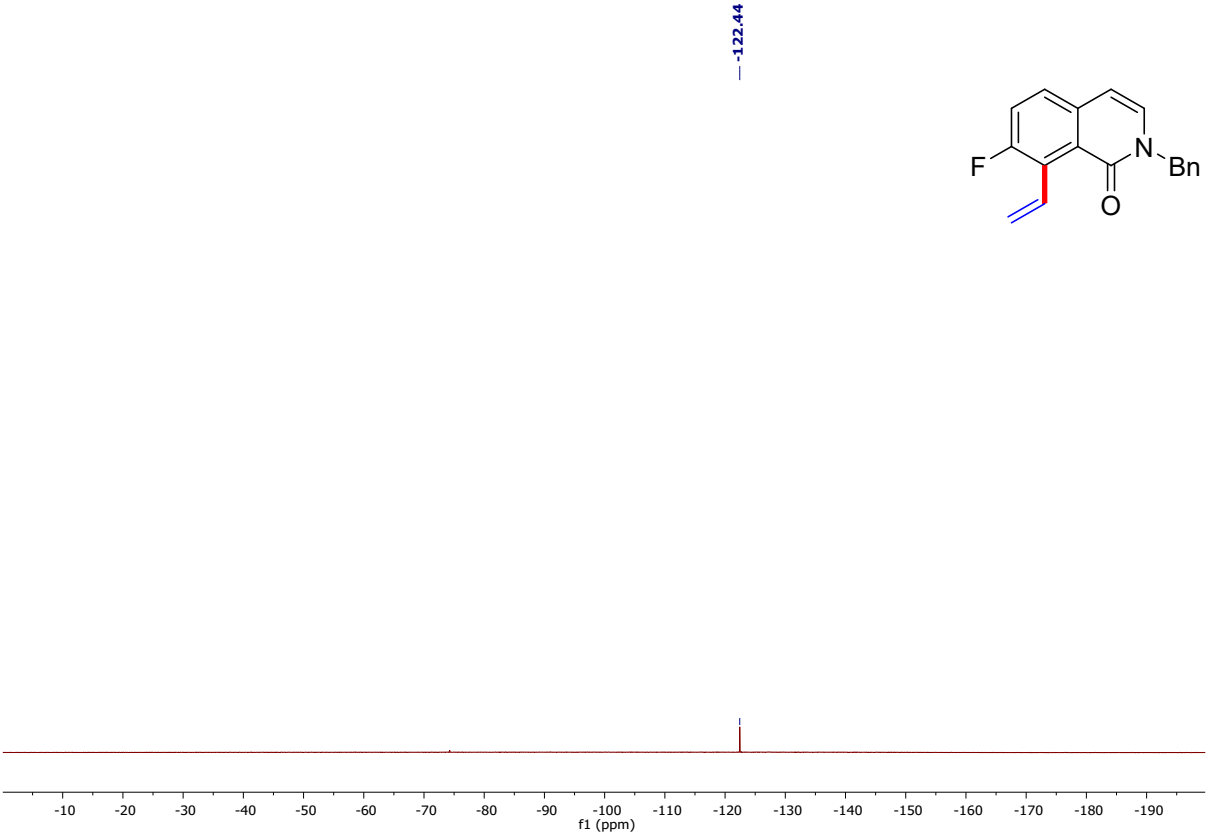
^{1}H NMR spectrum of 3zg



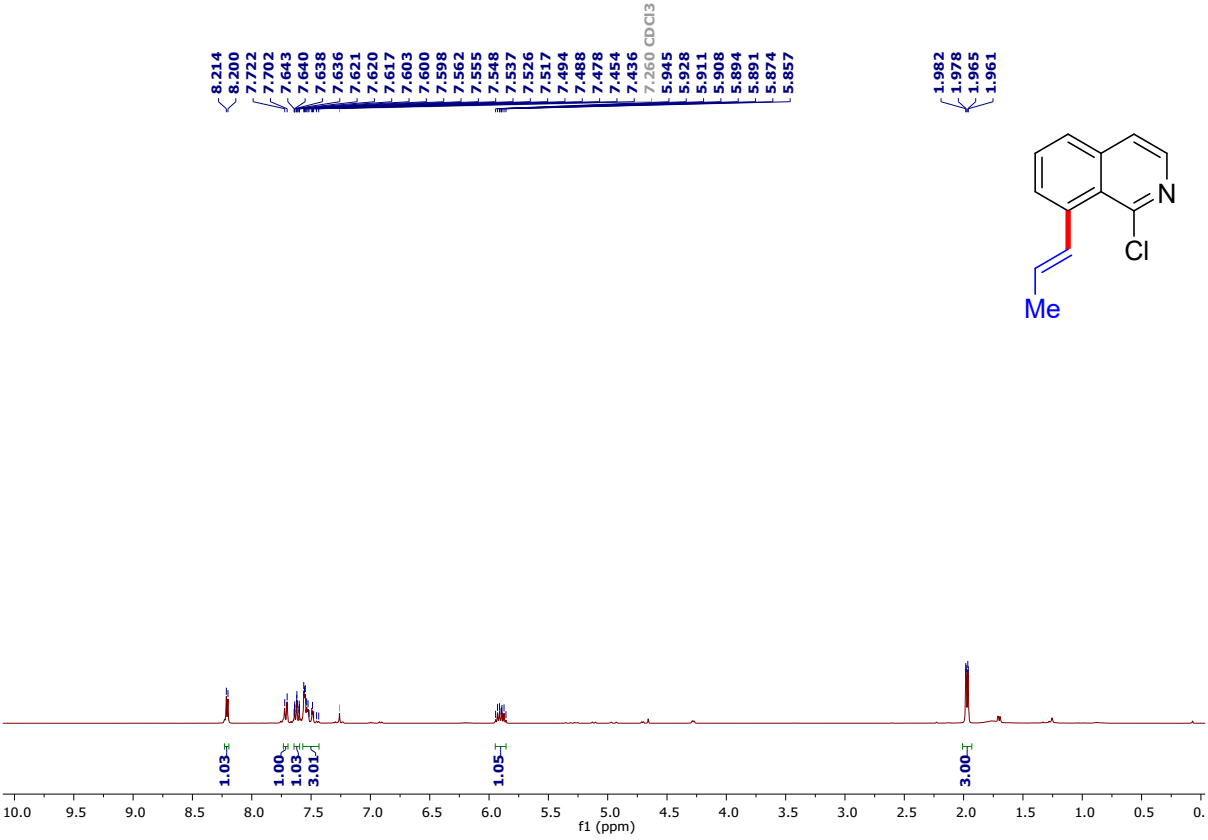
^{13}C{^{1}H} NMR spectrum of 3zg



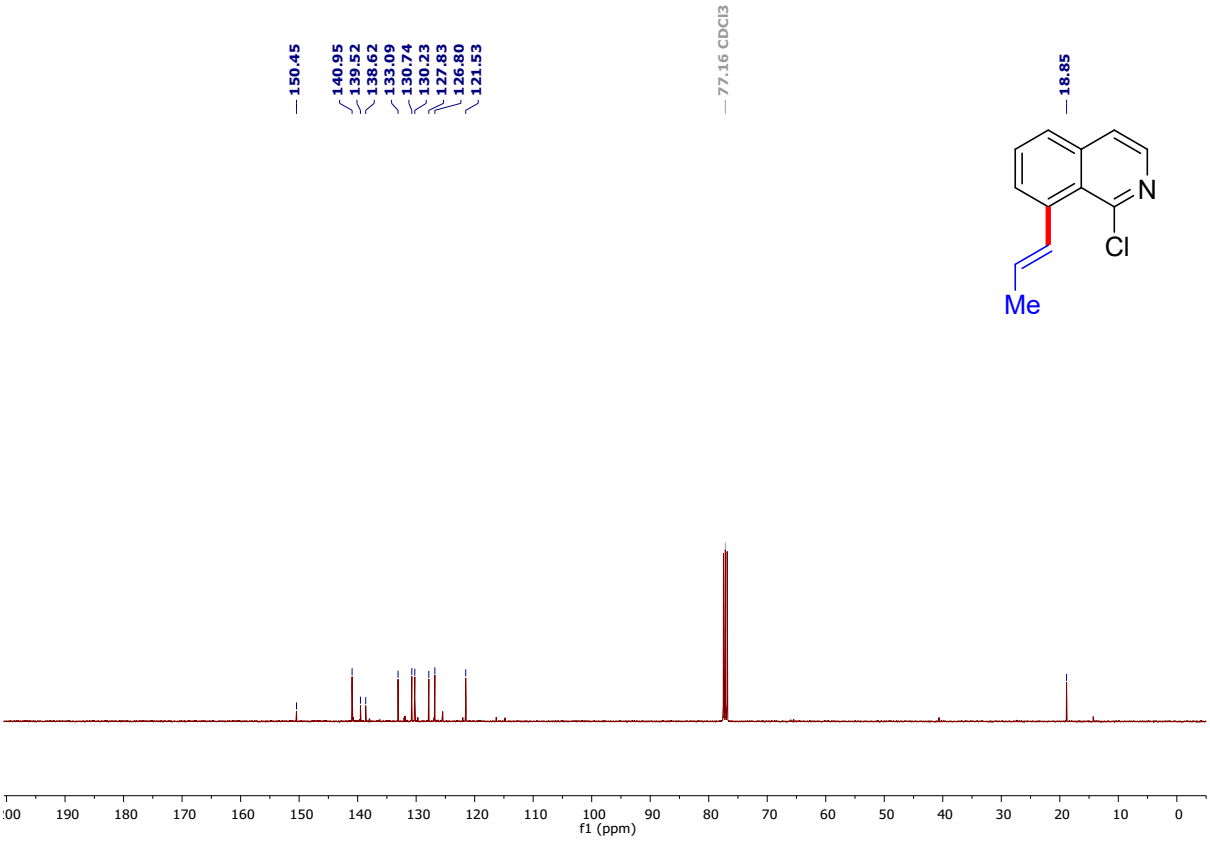
^{1}F NMR spectrum of 3zg



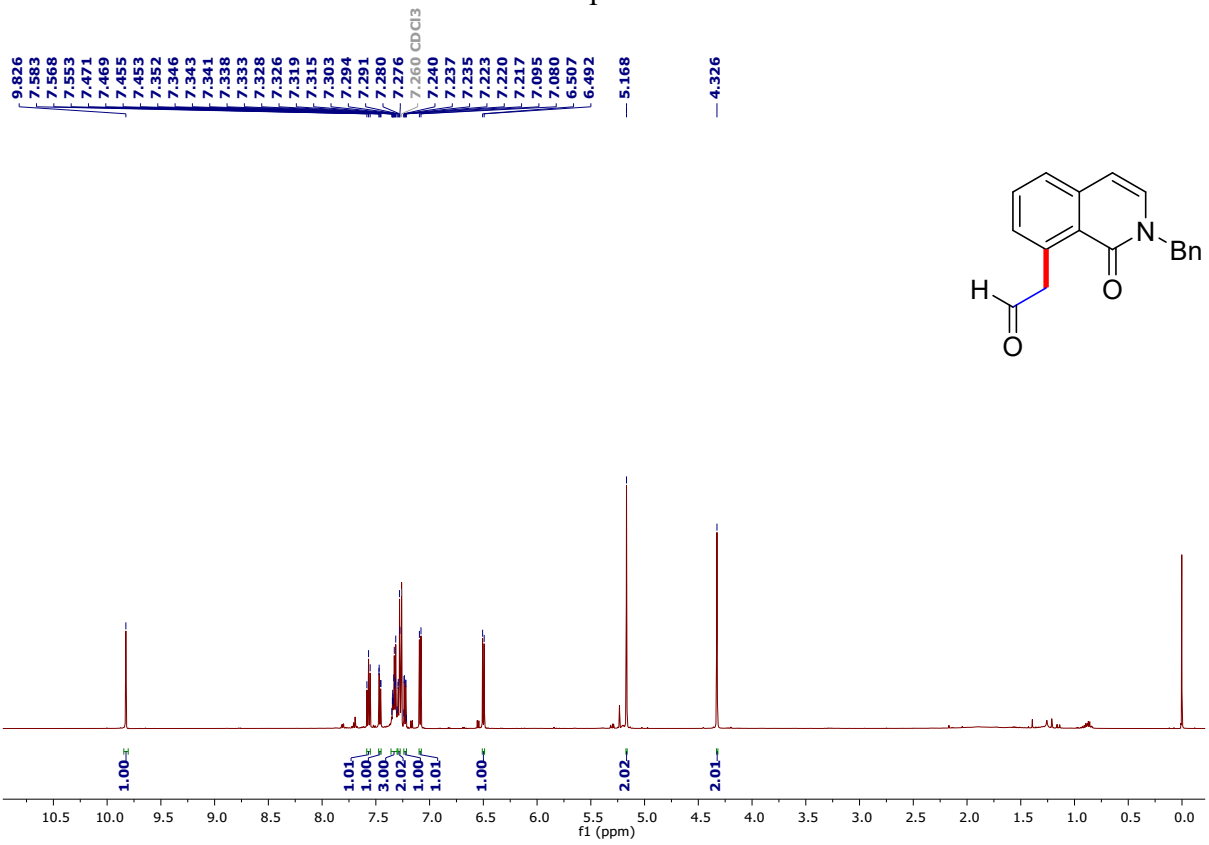
^{1}H NMR spectrum of 4



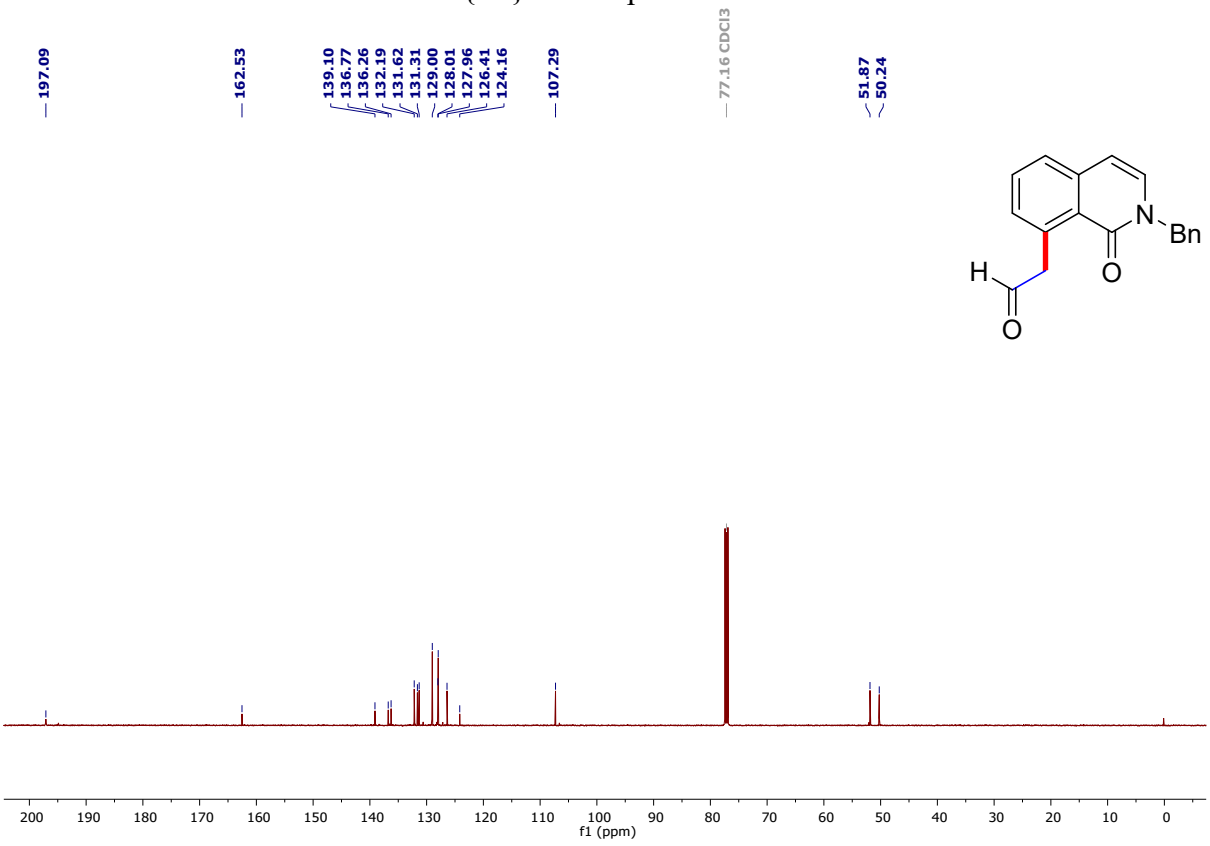
^{13}C{^{1}H} NMR spectrum of 4



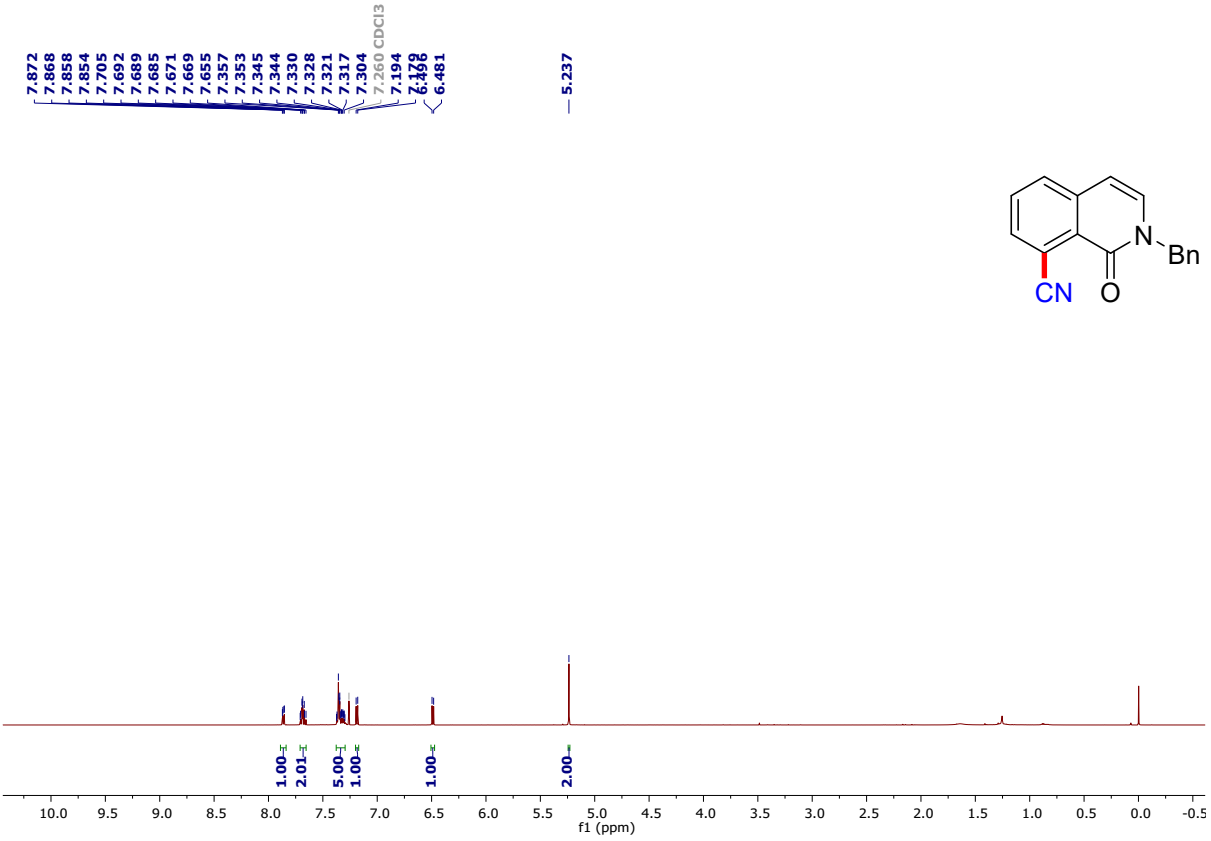
^{1}H NMR spectrum of 5



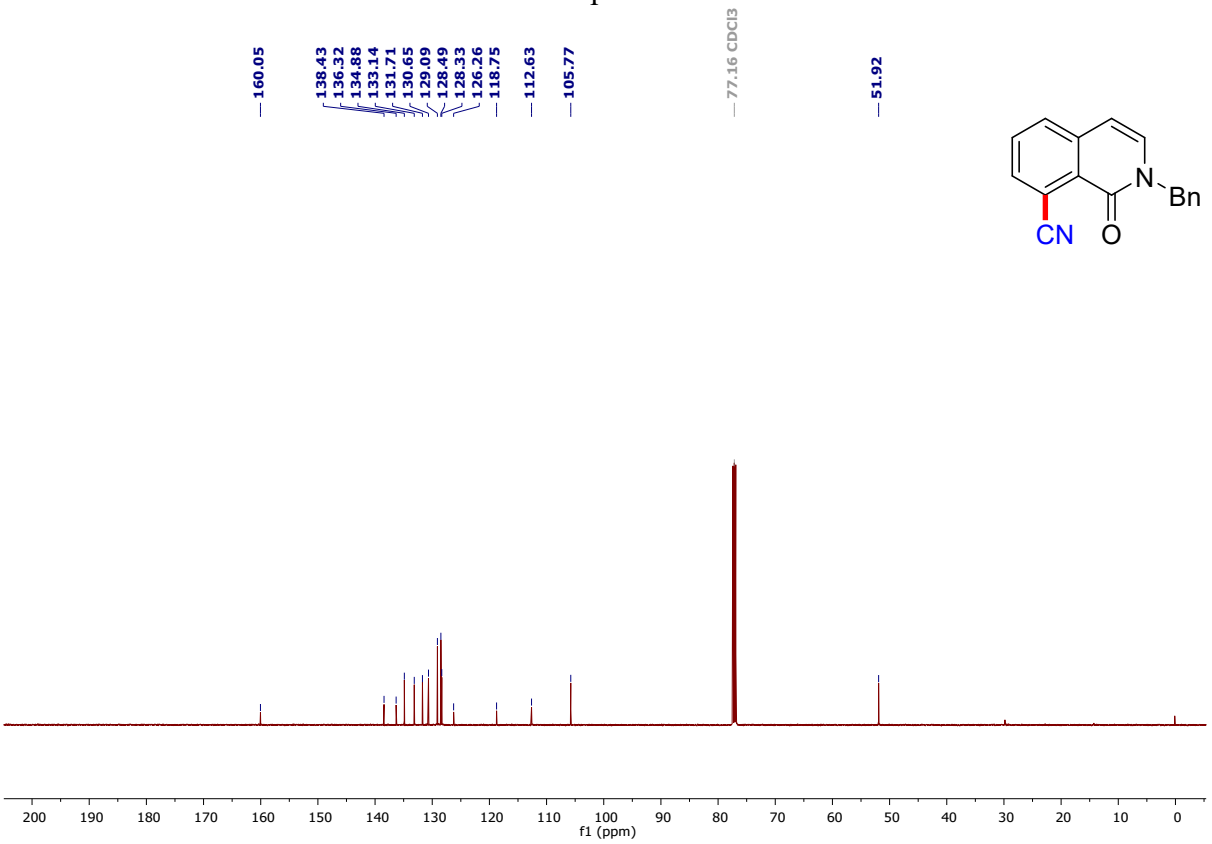
^{13}C{^{1}H} NMR spectrum of 5



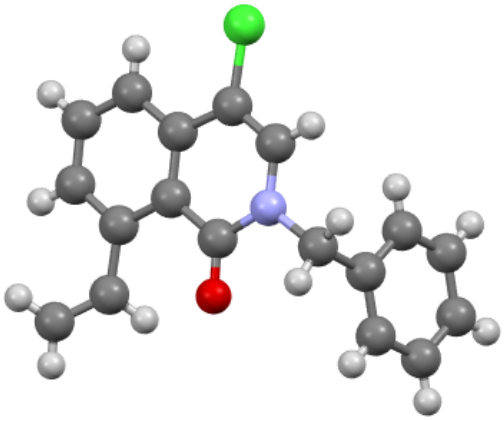
^{1}H NMR spectrum of 6



^{1}H NMR spectrum of 6



11.0 X-ray data (3z)



CCDC: 2300817

Table 1 Crystal data.

Identification code	USSRNB1_134_1_Rt_Cu_auto
Empirical formula	$C_{18}H_{14}ClNO$
Formula weight	295.75
Temperature/K	293(2)
Crystal system	Monoclinic
Space group	$P2_1/c$
a/Å	7.8569(6)
b/Å	16.8285(13)
c/Å	11.2120(8)
α/°	90
β/°	104.254(7)
γ/°	90
Volume/Å^3	1436.81(19)
Z	4
ρ_{calc}g/cm^3	1.367
μ/mm^{-1}	2.323
F(000)	616.0
Crystal size/mm^3	0.635 × 0.387 × 0.143
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.688 to 137.948
Index ranges	$-9 \le h \le 9$, $-20 \le k \le 9$, $-10 \le l \le 13$
Reflections collected	4102
Independent reflections	2554 [R_{int} = 0.0256, R_{sigma} = 0.0384]
Data/restraints/parameters	2554/0/191
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0510, wR_2 = 0.1395

Final R indexes [all data] $R_1 = 0.0614$, $wR_2 = 0.1540$
Largest diff. peak/hole / e Å^{-3} 0.19/-0.26

Table 2 Bond Lengths for USSRNB1_134_1_Rt_Cu_auto.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C9	1.736(2)	C10	C11	1.408(3)
O1	C16	1.225(2)	C6	C7	1.509(3)
N1	C16	1.381(3)	C6	C5	1.386(3)
N1	C8	1.369(3)	C6	C1	1.377(3)
N1	C7	1.480(3)	C17	C18	1.293(4)
C15	C16	1.479(3)	C11	C12	1.373(4)
C15	C14	1.416(3)	C5	C4	1.377(3)
C15	C10	1.411(3)	C13	C12	1.379(4)
C8	C9	1.337(3)	C1	C2	1.387(4)
C14	C17	1.496(3)	C4	C3	1.367(4)
C14	C13	1.392(3)	C3	C2	1.375(4)
C10	C9	1.433(3)			

Table 5 Bond Angles for USSRNB1_134_1_Rt_Cu_auto.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C16	N1	C7	117.68(17)	C5	C6	C7	120.4(2)
C8	N1	C16	124.06(18)	C1	C6	C7	121.4(2)
C8	N1	C7	118.26(17)	C1	C6	C5	118.2(2)
C14	C15	C16	120.42(19)	N1	C7	C6	112.99(17)
C10	C15	C16	119.77(19)	C8	C9	Cl1	118.32(18)
C10	C15	C14	119.80(19)	C8	C9	C10	121.3(2)
O1	C16	N1	119.65(18)	C10	C9	Cl1	120.34(18)
O1	C16	C15	124.59(19)	C18	C17	C14	123.6(3)
N1	C16	C15	115.76(17)	C12	C11	C10	119.6(2)
C9	C8	N1	120.7(2)	C4	C5	C6	121.0(2)
C15	C14	C17	124.29(19)	C12	C13	C14	122.1(2)
C13	C14	C15	118.0(2)	C6	C1	C2	120.8(2)
C13	C14	C17	117.6(2)	C11	C12	C13	120.6(2)
C15	C10	C9	118.27(19)	C3	C4	C5	120.3(3)
C11	C10	C15	119.9(2)	C4	C3	C2	119.7(2)
C11	C10	C9	121.8(2)	C3	C2	C1	120.0(3)