Supporting Information for

Nitrogen atom insertion into indenes to access isoquinolines

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Contents

1. General information

Chemicals: All used reagents were purchased from common suppliers and used as received unless noted otherwise. Solvents used for syntheses were of puriss grade and technical grade solvents were used for column chromatography. All reactions were carried out in round-bottomed flasks or vials under air unless stated otherwise.

TLC: Analytical thin-layer chromatography (TLC) was performed using silica gel 60 F254 coated aluminum sheets (Merck). Visualization was achieved by ultraviolet fluorescence (λ = 254 nm) and/or staining with potassium permanganate ($KMnO_4$).

FCC: Flash column chromatography was performed using silica gel 60 (pore size = 60 Å, mesh: 40-63 µm from Sigma-Aldrich or SiliCycle).

HPLC: Preparative RP-HPLC was performed on an Agilent infinity II 1260 with C18 column (7 µm, 250x21 mm) using a gradient of MeCN in H_2O with 0.1% TFA.

HRMS: High-resolution mass spectrometry data were obtained by the mass spectrometry service in the Laboratorium für Organische Chemie at ETH Zürich on VG-TRIBRIB for electron impact ionization (EI) or a Varian IonSpec Spectrometer for electrospray ionization (ESI) and are reported as (m/z).

NMR: ^{1}H-, ^{13}C-, ^{15}N-NMR, and ^{19}F-NMR spectra were recorded on a Bruker AVIII 400 MHz, a Bruker Neo 400 MHz or a Bruker Neo 500 MHz spectrometer and are reported in parts per million (ppm). ^{1}H-NMR spectra are calibrated with respect to the corresponding solvent residual peak ($CHCl_3$: 7.26 ppm; CH_3OH: 3.31 ppm; DMSO: 2.50 ppm). ^{13}C-NMR spectra are calibrated with respect to the corresponding solvent residual peak ($CHCl_3$: 77.16 ppm; CH_3OH: 49.00 ppm; DMSO: 39.52 ppm). Multiplet signals are reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, or combinations thereof. ^{13}C signals are acquired with proton decoupling and are singlets unless otherwise stated. NMR yields were determined using 1,1,2,2-tetrachloroethane as an internal standard.

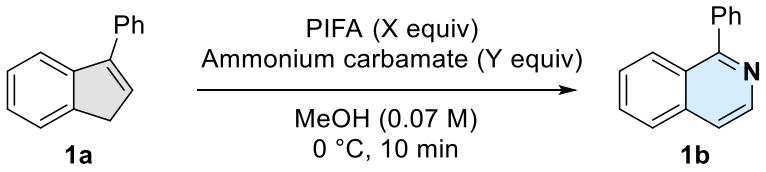
X-Ray analysis: Single crystalline samples were measured on a Riguka Oxford Diffraction XtaLAB Synergy-S Dualflex kappa diffractometer equipped with a Dectris Pilatus 300 HPAD detector and using microfocus sealed tube Cu-Kα radiation with mirror optics (λ = 1.54178 Å). All measurements were carried out at 100 K (unless otherwise noted) using an Oxford Cryosystems Cryostream 800 sample cryostat. Data collected on the Rigaku instrument were integrated using CrysAlisPro and corrected for absorption effects using a combination of empirical (ABSPACK) and numerical corrections.[1] The structures were solved using SHELXT[2] or SHELXS[3] and refined by full-matrix least-squares analysis (SHELXL),[4] using the program package OLEX2.[5] Unless otherwise indicated below, all non-hydrogen atoms were refined anisotropically and hydrogen atoms were constrained to ideal geometries and refined with fixed isotropic displacement parameters (in terms of a riding model).

2. Optimization of reaction conditions

General procedure for the optimization of reaction conditions

In a 4 mL screw-cap vial equipped with a magnetic stirring bar, 3-phenyl-1*H*-indene indene (**1a**) (9.6 mg, 0.050 mmol, 1.0 equiv) was dissolved in 0.7 mL of a stock solution containing deuterated methanol (CD_3OD) and internal standard (1,1,2,2-tetrachloroethane) and cooled in an ice bath. The ammonia source was added in one portion and the mixture was stirred for 1 minute before the oxidant was added in one portion and the reaction was stirred for 10 minutes at 0 °C. The crude reaction mixture was analyzed by ^{1}H NMR. The yield was determined by integration of the peak corresponding to the H at the 3-position of the product (400 MHz, methanol-d_4 δ 8.49 (d, *J* = 5.8 Hz, 1H)), relative to the internal standard (δ 6.48 (s, 1H)) and the conversion was determined by integration of the H at the 2-position of the starting material (δ 6.60 (t, *J* = 2.2 Hz, 1H)), relative to the internal standard and subtracting the value from 100%.

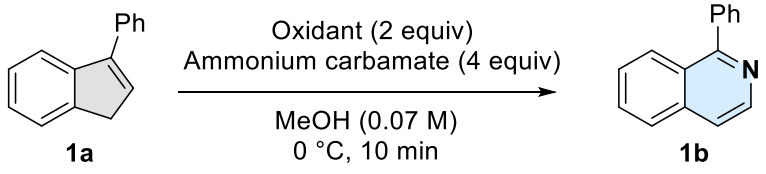
Equivalent optimization



1a **1b**

Entry	PIFA [X equiv]	Ammonium carbamate [Y equiv]	Conversion of **1a** [%]	NMR yield of **1b** [%]
1	2	1	**27**	**0**
2	2	2	**61**	**61**
3	2	4	**90**	**77**
4	3	1.5	**32**	**0**
5	3	3	**85**	**82**
6	3	6	**100**	**84**
7	4	2	**92**	**0**
8	4	4	**100**	**92**
9	4	6	**100**	**72**

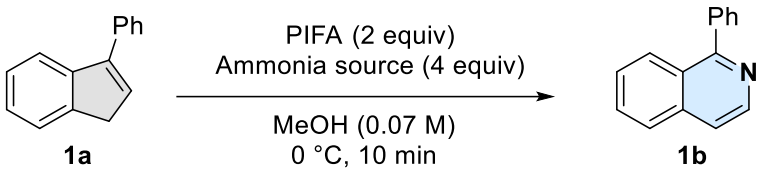
Oxidant optimization



1a **1b**

Entry	Oxidant	Conversion of **1a** [%]	NMR yield of **1b** [%]
1	**PIFA** phenyliodine(III)-bis(trifluoroacetate)	**90**	**77**
2	Bis(*tert*-butylcarbonyloxy)iodobenzene	**91**	**91**
3	**PIDA** phenyliodine(III) diacetate	**94**	**93**

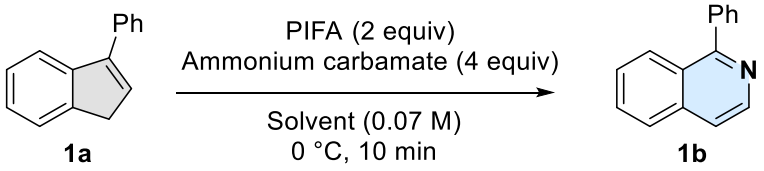
Ammonia source optimization



1a **1b**

Entry	Ammonia source	Conversion of **1a** [%]	NMR yield of **1b** [%]
1	Ammonium carbamate	**90**	**77**
2	Ammonium acetate	**70**	**70**
3	Ammonium bicarbonate	**95**	**91**
4	Ammonium formate	**46**	**46**
5	NH_3 in methanol (7M)	**15**	**12**

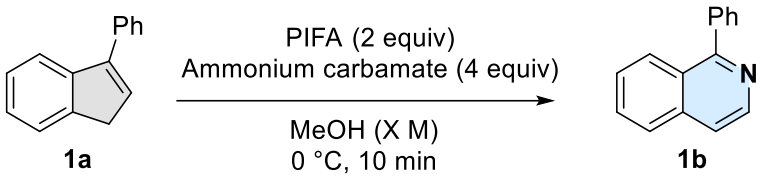
Solvent optimization



1a **1b**

Entry	Solvents	Conversion of **1a** [%]	NMR yield of **1b** [%]
1	MeOH	**90**	**77**
2	EtOH	**90**	**67**
3	MeCN	**100**	**62**
4	HFIP	**100**	**0**
5	$CHCl_3$	**100**	**0**
6	DCM	**100**	**10**
7	DMF	**69**	**31**
8	THF	**68**	**19**
9	toluene	**81**	**21**
10	dioxane	**87**	**25**

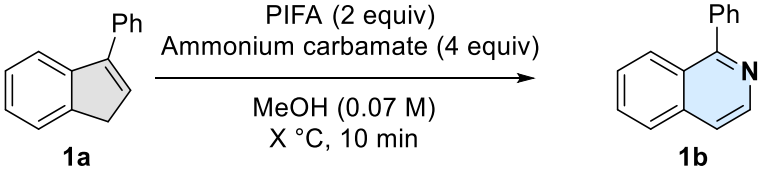
Concentration optimization



1a **1b**

Entry	Concentration	Conversion of **1a** [%]	NMR yield of **1b** [%]
1	0.033 M	**88**	**80**
2	0.066 M	**90**	**77**
3	0.1 M	**85**	**77**
4	0.2 M	**97**	**75**

Temperature optimization



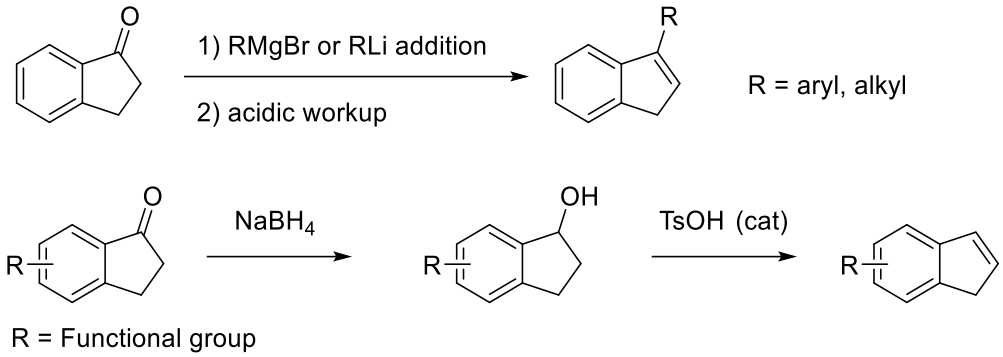
1a **1b**

Entry	Temperature	Conversion of **1a** [%]	NMR yield of **1b** [%]
1	0 °C	**90**	**77**
2	rt	**92**	**73**
3	50 °C	**86**	**61**

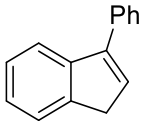
3. Preparation of starting materials

Starting materials for the corresponding isoquinoline products **2b**, **4b**, **7b, 8b, 12b**, **26b**, and **27b** were commercially available.

General preparation of the starting materials



3-Phenyl-1*H*-indene (1a)

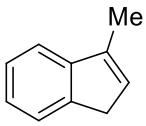


3-Phenyl-1*H*-indene (**1a**) was prepared according to a reported literature procedure.[6]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.59 (m, 3H), 7.58 – 7.54 (m, 1H), 7.50 – 7.43 (m, 2H), 7.42 – 7.38 (m, 1H), 7.38 – 7.31 (m, 1H), 7.31 – 7.24 (m, 1H), 6.60 (t, *J* = 2.2 Hz, 1H), 3.53 (d, *J* = 2.2 Hz, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.3, 144.9, 144.0, 136.3, 131.0, 128.7, 127.8, 127.7, 126.3, 125.0, 124.2, 120.4, 38.3.
HRMS (EI, m/z): $[M]^+$ calc. 192.0934; found 192.0931

The spectral data are consistent with those reported in the literature.[6]

3-Methyl-1*H*-indene (3a)

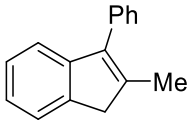


3-Methyl-1*H*-indene (**3a**) was prepared according to a reported literature procedure.[6]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.44 (m, 1H), 7.39 – 7.29 (m, 2H), 7.25 – 7.18 (m, 1H), 6.24 – 6.20 (m, 1H), 3.38 – 3.30 (m, 2H), 2.23 – 2.16 (m, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 146.3, 144.5, 140.1, 128.9, 126.2, 124.6, 123.7, 119.0, 37.8, 13.2.
HRMS (EI, m/z): $[M]^+$ calc. 130.0777; found 130.0773

The spectral data are consistent with those reported in the literature.[6]

2-Methyl-3-phenyl-1*H*-indene (5a)

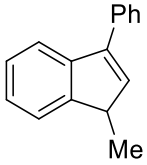


2-Methyl-3-phenyl-1*H*-indene (**5a**) was prepared according to a reported literature procedure.[7]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.39 (m, 5H), 7.39 – 7.33 (m, 1H), 7.25 – 7.22 (m, 2H), 7.19 – 7.14 (m, 1H), 3.48 – 3.45 (m, 2H), 2.17 – 2.13 (m, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 146.5, 142.6, 140.8, 138.8, 135.7, 129.3, 128.5, 127.1, 126.3, 124.1, 123.5, 119.4, 43.3, 15.0
HRMS (EI, m/z): $[M]^+$ calc. 206.1090; found 206.1086

The spectral data are consistent with those reported in the literature.[8]

1-Methyl-3-phenyl-1*H*-indene (6a)

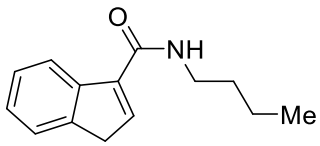


1-Methyl-3-phenyl-1*H*-indene (**6a**) was prepared with the same procedure as **5a**, but with 3-methyl-2,3-dihydro-1*H*-inden-1-one as the starting material.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.59 (m, 2H), 7.58 – 7.54 (m, 1H), 7.51 – 7.43 (m, 3H), 7.41 – 7.27 (m, 3H), 6.54 – 6.52 (m, 1H), 3.66 – 3.56 (m, 1H), 1.44 – 1.39 (m, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 150.4, 143.4, 143.1, 138.2, 136.2, 128.7, 127.8, 127.7, 126.5, 125.2, 123.1, 120.5, 44.2, 16.4.
HRMS (EI, m/z): $[M]^+$ calc. 206.1090; found 206.1088

The spectral data are consistent with those reported in the literature.[9]

***N*-Butyl-*1H*-indene-3-carboxamide (9a)**

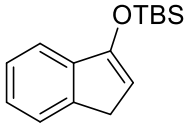


In a 100 mL round bottom flask charged with a stir bar, 1*H*-indene-3-carboxylic acid (1.24 g, 7.74 mmol, 1.0 equiv) was dissolved in anhydrous DCM (15 mL). Thionyl chloride (0.57 mL, 7.74 mmol, 1.0 equiv) was added dropwise at 0 °C, followed by 3 drops of DMF. The mixture was warmed to room temperature and stirred for 30 minutes, followed by evaporation of the solvent. The residue was dissolved in anhydrous

DCM (15 mL) and butylamine (1.50 mL, 15.48 mmol, 2.0 equiv) was added and the reaction progress monitored by TLC. After completion, the reaction mixture was washed with saturated aq. $NaHCO_3$ and brine. The organic phase was dried over Na_2SO_4 and concentrated. Flash column chromatography (0–50% EtOAc in hexanes) gave the product as a dark red solid (346 mg, 21% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.86 (m, 1H), 7.50 – 7.44 (m, 1H), 7.37 – 7.31 (m, 1H), 7.25 (tdd, *J* = 7.4, 1.2, 0.4 Hz, 1H), 6.92 (t, *J* = 2.1 Hz, 1H), 6.03 (s, 1H), 3.48 – 3.42 (m, 4H), 1.65 – 1.56 (m, 2H), 1.48 – 1.37 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 165.1, 143.8, 141.5, 140.8, 135.9, 126.8, 125.7, 124.0, 122.0, 39.4, 38.3, 31.9, 20.3, 13.9.
HRMS (ESI, m/z): $[M+Na]^+$ calc. 238.1202; found 238.1204

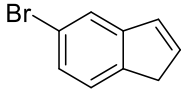
((1*H*-Inden-3-yl)oxy)(*tert*-butyl)dimethylsilane (10a)



In a 100 mL round bottom flask charged with a stir bar, 1-indanone (1.23 g, 10.0 mmol, 1.0 equiv) and *tert*-butyldimethylsilyl chloride (1.66 g, 11.0 mmol, 1.1 equiv) were dissolved in 10 mL toluene, then DBU (2.0 mL, 13.0 mmol, 1.3 equiv) was added to the solution at 0 °C and the resulting mixture was stirred at room temperature for 16 hours. Diethyl ether was added, the mixture was washed with water and then the organic phase was dried over Na_2SO_4, filtered, and concentrated. Flash column chromatography (pentane) gave the product as a colourless oil (518 mg, 21%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.38 (m, 2H), 7.35 – 7.29 (m, 1H), 7.27 – 7.21 (m, 1H), 5.44 (t, *J* = 2.4 Hz, 1H), 3.32 – 3.27 (m, 2H), 1.06 (s, 9H), 0.28 (s, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 153.9, 142.9, 142.1, 126.1, 125.2, 123.9, 118.3, 106.0, 34.1, 25.9, 18.4, -4.6.
HRMS (ESI, m/z): $[M+H]^+$ calc. 247.1513; found 247.1508

5-Bromo-1*H*-indene (11a)

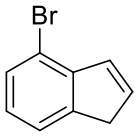


5-Bromo-1*H*-indene (11a) was prepared with the same procedure as **14a**, but with 6-bromo-1-indanone as the starting material.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.53 (m, 1H), 7.33 – 7.31 (m, 2H), 6.84 – 6.80 (m, 1H), 6.60 (dt, *J* = 5.6, 2.0 Hz, 1H), 3.36 (td, *J* = 2.0, 0.7 Hz, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.1, 142.5, 136.1, 131.4, 127.4, 125.1, 124.2, 120.4, 38.9.
HRMS (EI, m/z): $[M]^+$ calc. 193.9726; found 193.9723

The spectral data are consistent with those reported in the literature.[10]

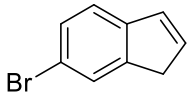
4-Bromo-1*H*-indene (13a)



4-Bromo-1*H*-indene (**13a**) was prepared with the same procedure as **14a**, but with 7-bromo-1-indanone as the starting material.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.37 (m, 2H), 7.08 – 7.03 (m, 1H), 7.00 – 6.96 (m, 1H), 6.66 – 6.62 (m, 1H), 3.51 – 3.49 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.4, 145.1, 135.4, 131.8, 129.6, 126.2, 122.7, 115.4, 40.5.
HRMS (EI, m/z): $[M]^+$ calc. 193.9726; found 193.9724

6-Bromo-1*H*-indene (14a)

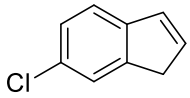


6-Bromo-1*H*-indene (**14a**) was prepared according to a reported literature procedure.[11]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.59 (m, 1H), 7.43 – 7.39 (m, 1H), 7.28 – 7.24 (m, 1H), 6.86 – 6.82 (m, 1H), 6.57 – 6.53 (m, 1H), 3.40 – 3.38 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.9, 143.9, 134.7, 131.6, 129.4, 127.1, 122.2, 118.8, 39.2.
HRMS (EI, m/z): $[M]^+$ calc. 193.9726; found 193.9724

The spectral data are consistent with those reported in the literature.[12]

6-Chloro-1*H*-indene (15a)

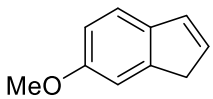


6-Chloro-1*H*-indene (**15a**) was prepared according to a reported literature procedure.[11]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.44 (m, 1H), 7.32 – 7.29 (m, 1H), 7.27 – 7.23 (m, 1H), 6.87 – 6.83 (m, 1H), 6.58 – 6.54 (m, 1H), 3.41 – 3.39 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.5, 143.5, 134.7, 131.5, 130.8, 126.6, 124.3, 121.8, 39.2.
HRMS (EI, m/z): $[M]^+$ calc. 150.0231; found 150.0232

The spectral data are consistent with those reported in the literature.[13]

6-Methoxy-1*H*-indene (16a)

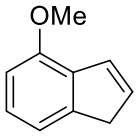


6-Methoxy-1*H*-indene (**16a**) was prepared according to a reported literature procedure.[14]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.28 (m, 1H), 7.10 – 7.07 (m, 1H), 6.87 – 6.80 (m, 2H), 6.44 – 6.40 (m, 1H), 3.86 – 3.83 (m, 3H), 3.40 – 3.37 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 158.0, 145.7, 138.2, 132.1, 131.6, 121.2, 112.1, 110.4, 55.7, 39.3.
HRMS (ESI, m/z): $[M+H]^+$ calc. 147.0804; found 147.0801

The spectral data are consistent with those reported in the literature.[15]

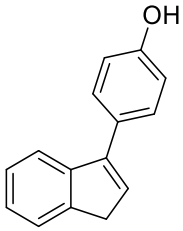
4-Methoxy-1*H*-indene (17a)



4-Methoxy-1*H*-indene (**17a**) was prepared according to an adapted reported literature procedure. The reduction of the ketone starting material 7-methoxy-2,3-dihydro-1*H*-inden-1-one was achieved according to literature.[16] Then, a solution of the crude 5-methoxy-1-indanol (510 mg, 3.14 mmol, 1.0 equiv), *p*-toluenesulfonic acid monohydrate (12.0 mg, 62.9 µmol, 0.02 equiv) and tetrahydrofuran (30 mL) was stirred and heated at reflux temperature overnight. The reaction solution was cooled and saturated aqueous bicarbonate solution was added. Most of the THF was removed under reduced pressure, then water was added and the mixture was extracted with ethyl acetate. The combined organic extracts were washed with brine and dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure and the crude product was purified by flash column chromatography (0–5% EtOAc in hexanes) to yield the product as a yellow oil (170 mg, 37%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 – 7.10 (m, 2H), 7.07 – 7.03 (m, 1H), 6.82 – 6.78 (m, 1H), 6.49 – 6.44 (m, 1H), 3.92 – 3.89 (m, 3H), 3.44 – 3.41 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 153.3, 146.0, 133.6, 132.4, 128.4, 126.0, 116.8, 108.3, 55.6, 39.7.
HRMS (ESI, m/z): $[M+H]^+$ calc. 147.0804; found 147.0800

4-(1*H*-Inden-3-yl)phenol (18a)

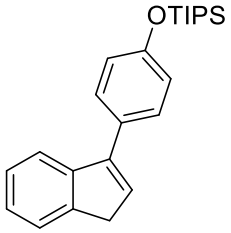


To a 100 mL flask, tetra-*n*-butylammonium fluoride (10.0 mL, 1M in THF, 10 mmol, 1.2 equiv) was added dropwise over 5 min to a solution of (4-(1*H*-inden-3-yl)phenoxy)triisopropylsilane (**19a**) (3.0 g, 8.2 mmol, 1.0 equiv) in THF (30 mL) at room temperature. After stirring for 15 min, brine (100 mL) and EtOAc (200 mL) were added to the mixture and the organic layers were separated, dried over Na_2SO_4, filtered

and concentrated in vacuo. Purification by flash column chromatography (0–10% EtOAC in hexanes, dry loading) afforded 4-(1*H*-inden-3-yl)phenol as a white solid (1.53 g, 89 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.56 (m, 1H), 7.56 – 7.52 (m, 1H), 7.52 – 7.48 (m, 2H), 7.35 – 7.30 (m, 1H), 7.28 – 7.23 (m, 1H), 6.95 – 6.88 (m, 2H), 6.51 (t, *J* = 2.2 Hz, 1H), 4.82 (s, 1H), 3.49 (d, *J* = 2.2 Hz, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 155.2, 145.0, 144.7, 144.2, 130.1, 129.2, 129.1, 126.3, 124.9, 124.2, 120.4, 115.6, 38.2.
HRMS (EI, m/z): $[M]^+$ calc. 208.0883; found 208.0881

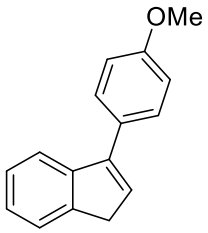
(4-(1*H*-Inden-3-yl)phenoxy)triisopropylsilane (19a)



Under a nitrogen atmosphere, *n*-BuLi (11.4 mL, 1.6 M in hexanes, 18.3 mmol, 1.0 equiv) was added dropwise over 5 min to a solution of (4-bromophenoxy)triisopropylsilane[17] (6.00 g, 18.3 mmol, 1.0 equiv) in anhydrous THF (30 mL) at -78 °C in an oven-dried 100 mL round bottom flask. After stirring for 15 min, 1-indanone (2.40 g, 18.3 mmol, 1.0 equiv) was added as a powder to the reaction mixture. After 5 min of stirring at –78 °C, the reaction mixture was warmed to room temperature and stirred for 30 min. The mixture was treated with concentrated HCl 37% (2 mL) and stirred for an additional 15 min. Brine (100 mL) and EtOAc (200 mL) were added to the mixture and the organic layers were separated, dried over Na_2SO_4, filtered, and concentrated in vacuo. Purification by flash column chromatography (0–5% EtOAC in hexanes, dry loading) afforded (4-(1*H*-inden-3-yl)phenoxy)triisopropylsilane as a colorless oil (3.12 g, 47%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.58 (m, 1H), 7.55 – 7.50 (m, 1H), 7.50 – 7.45 (m, 2H), 7.35 – 7.29 (m, 1H), 7.28 – 7.23 (m, 1H), 6.99 – 6.94 (m, 2H), 6.52 (t, *J* = 2.2 Hz, 1H), 3.49 (d, *J* = 1.9 Hz, 2H), 1.36 – 1.26 (m, 3H), 1.18 – 1.13 (m, 18H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 155.8, 145.0, 144.9, 144.3, 129.9, 129.1, 128.9, 126.2, 124.8, 124.2, 120.5, 120.1, 38.2, 18.1, 12.9.
HRMS (EI, m/z): $[M]^+$ calc. 364.2217; found 364.2214

3-(4-Methoxyphenyl)-1*H*-indene (20a)

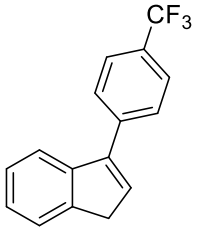


3-(4-Methoxyphenyl)-1*H*-indene (**20a**) was prepared with the same procedure as **5a** using 1-indanone as the starting material.[7]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.55 (m, 4H), 7.39 – 7.34 (m, 1H), 7.31 – 7.27 (m, 1H), 7.05 – 7.01 (m, 2H), 6.55 (t, *J* = 2.2 Hz, 1H), 3.89 (s, 3H), 3.54 – 3.51 (m, 2H).
^{13}C NMR ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.3, 144.9, 144.8, 144.3, 130.0, 129.0, 128.8, 126.2, 124.9, 124.2, 120.4, 114.1, 55.4, 38.2.
HRMS (ESI, m/z): $[M+H]^+$ calc. 223.1117; found 223.1115

The spectral data are consistent with those reported in the literature.[18]

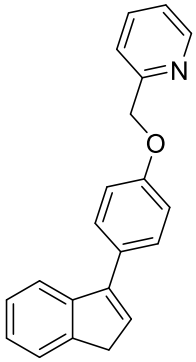
3-(4-(Trifluoromethyl)phenyl)-1*H*-indene (21a)



An oven-dry flask was charged with Mg turnings (547 mg, 22.5 mmol, 2.25 equiv) and purged with N_2. THF (2.5 mL) and dibromoethane (2 drops) were added and the mixture was stirred for 10 minutes. 1-Bromo-4-(trifluoromethyl)benzene (2.63 mL, 18.8 mmol, 1.88 equiv) in THF (17.5 mL) was added dropwise. After the addition, the reaction was heated to reflux, then allowed to cool to room temperature and stirred for 3 hours at room temperature. 1-Indanone (1.32 g, 10.0 mmol, 1.00 equiv) in THF (6.5 mL) was added dropwise. The reaction was stirred at room temperature overnight. The reaction was quenched by dropwise addition of conc. HCl at 0 °C. The solution was allowed to warm to room temperature and stirred until full conversion was indicated. The organic layer was separated, and the aqueous layer was extracted with EtOAc. The organic layers were combined and washed with saturated $NaHCO_3$ (15 mL), H_2O (15 mL), and brine (15 mL). The organic layer was then dried over Na_2SO_4, filtered, and concentrated under reduced pressure. Purification by flash column chromatography (0–5% EtOAc in hexanes) gave the product as a light yellow oil (2.44 g; 94%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (s, 4H), 7.63 – 7.57 (m, 2H), 7.41 – 7.37 (m, 1H), 7.36 – 7.32 (m, 1H), 6.69 (t, *J* = 2.2 Hz, 1H), 3.58 (d, *J* = 2.2 Hz, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 144.8, 144.3, 143.4, 139.9 (d, *J* = 1.5 Hz), 132.6, 129.8 (q, *J* = 32.5 Hz), 128.1, 126.5, 125.7 (q, *J* = 3.8 Hz), 125.4, 124.5 (q, *J* = 271.9 Hz), 124.4, 120.2, 38.5.
^{19}F NMR (376 MHz, $CDCl_3$) δ -62.45 (d, *J* = 1.5 Hz).
HRMS (EI, m/z): $[M]^+$ calc. 260.0807; found 260.0803

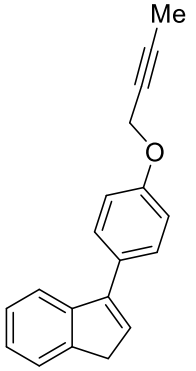
2-((4-(1*H*-inden-3-yl)phenoxy)methyl)pyridine (22a)



In a 50 mL flask, 4-(1*H*-indene-3-yl)phenol (**18a**) (388.2 mg, 1.86 mmol, 1.0 equiv) was dissolved in anhydrous THF (18.6 mL) and cooled in an ice bath to 0 °C. NaH (164 mg, 60% in mineral oil, 4.10 mmol, 2.2 equiv) was added and stirred at 0 °C for 5 minutes. Then, 2-bromomethylpyridine hydrochloride (472 mg, 1.86 mmol, 1.0 equiv) was added and the resulting mixture was stirred at room temperature overnight under N_2 atmosphere. The conversion was monitored by TLC. Water was added and the crude was extracted with EtOAc three times. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated. The crude product was purified by flash column chromatography (0–15% EtOAc in hexanes) to yield the product as a beige solid (342 mg, 61%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 – 8.61 (m, 1H), 7.74 (td, *J* = 7.7, 1.8 Hz, 1H), 7.60 – 7.51 (m, 5H), 7.34 – 7.29 (m, 1H), 7.28 – 7.22 (m, 2H), 7.11 – 7.05 (m, 2H), 6.52 (t, *J* = 2.2 Hz, 1H), 5.28 (s, 2H), 3.49 (d, *J* = 2.3 Hz, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 157.5, 149.4, 144.9, 144.7, 144.2, 137.0, 130.2, 129.4, 129.0, 126.3, 124.9, 124.2, 122.8, 121.5, 120.4, 115.1, 70.9, 38.2.
HRMS (ESI, m/z): $[M+H]^+$ calc. 300.1383; found 300.1380

3-(4-(But-2-yn-1-yloxy)phenyl)-1*H*-indene (23a)

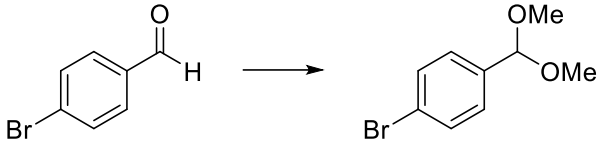


4-(1*H*-Inden-3-yl)phenol (**18a**) (500 mg, 2.40 mmol, 1.00 equiv) was dissolved in acetonitrile (2.0 mL). Then, 1-bromobut-2-yne (0.32 mL, 3.6 mmol, 1.5 equiv) and potassium carbonate (664 mg, 4.80 mmol, 2.00 equiv) were added. The mixture was stirred at 50 °C overnight. Then, the reaction was cooled to room temperature and water was added. The organic layer was separated and the aqueous layer was washed with EtOAc three times. The combined organic layers were washed with brine, dried over Na_2SO_4,

filtered, and concentrated under reduced pressure. The crude product was purified by flash column chromatography (0–5% EtOAc in hexanes) to yield the product as an orange oil (247 mg, 40%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.57 (m, 1H), 7.57 – 7.51 (m, 3H), 7.35 – 7.30 (m, 1H), 7.28 – 7.23 (m, 1H), 7.08 – 7.03 (m, 2H), 6.52 (t, *J* = 2.2 Hz, 1H), 4.71 (q, *J* = 2.4 Hz, 2H), 3.51 – 3.47 (m, 2H), 1.92 – 1.88 (m, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6, 145.0, 144.7, 144.2, 130.2, 129.4, 128.9, 126.3, 124.9, 124.2, 120.4, 115.1, 84.0, 74.2, 56.7, 38.2, 3.9.
HRMS (ESI, m/z): $[M+H]^+$ calc. 261.1274; found 261.1267

1-Bromo-4-(dimethoxymethyl)benzene (S1)

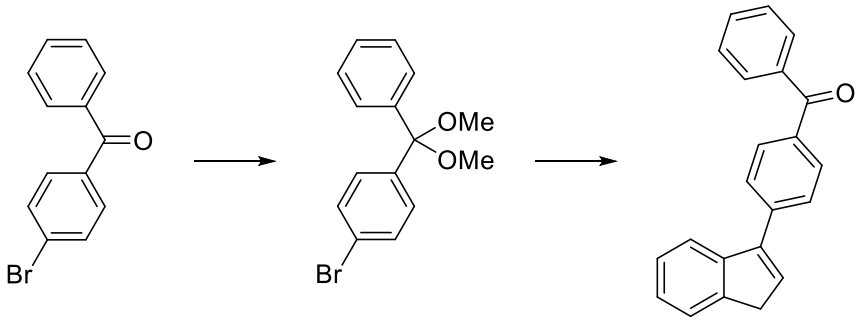


In a 100 mL round bottom flask charged with a stir bar, 4-bromobenzaldehyde (925 mg, 5.00 mmol, 1.0 equiv) was dissolved in MeOH (10 mL), then *para*-toluenesulfonic acid monohydrate (95.0 mg, 0.500 mmol, 0.1 equiv) and trimethyl orthoformate (6.6 mL, 60 mmol, 12 equiv) were added to the solution, which was stirred at reflux for 48 hours. The mixture was then washed with 1 M NaOH solution, the aqueous phase was extracted with DCM, and the combined organic phases were dried over Na_2SO_4, filtered, and concentrated. The product was used without any further purification (867 mg, 75%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 2H), 7.36 – 7.28 (m, 2H), 5.35 (s, 1H), 3.30 (s, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 137.2, 131.4, 128.6, 122.6, 102.4, 52.6.

The spectral data are consistent with those reported in the literature.[19]

(4-(1*H*-inden-3-yl)phenyl)(phenyl)methanone (24a)



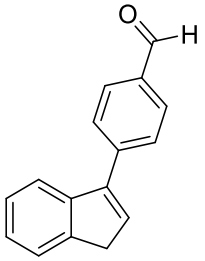
21a

To a 100 mL flask 4-bromobenzophenone (3.00 g, 11.5 mmol, 1.0 equiv), methyl orthoformate (6.76 mL, 57.4 mmol, 5.0 equiv), and MeOH (50 mL) were added. Then, H_2SO_4 (98%, 100 µL) was added to the mixture which was stirred at 50 °C and monitored by TLC. After full conversion of the starting material, saturated aqueous $NaHCO_3$ (50 mL) and EtOAc (200 mL) were added and the organic layer was separated,

washed with brine (3 X 50 mL), dried over Na_2SO_4 and filtered. The mixture was then concentrated, transferred to a 100 mL flask and dried in vacuo for 30 min.
Under a N_2 atmosphere, anhydrous THF (30 mL) was added to the flask and the mixture was cooled to -78 °C. *n*-BuLi (7.20 mL, 1.6 M in hexanes, 11.5 mmol, 1.0 equiv) was added and the reaction mixture was stirred for 15 min before 1-indanone (1.50 g, 11.5 mmol, 1.0 equiv) was added as a powder to the reaction mixture. After 5 min of stirring at -78 °C, the reaction mixture was warmed to rt and stirred for an additional 30 min. The mixture was treated with concentrated HCl 37% (5 mL) and stirred for an additional 30 min. Brine and EtOAc were added to the mixture and the organic layers were separated, dried over Na_2SO_4, filtered and concentrated in vacuo. Purification by flash column chromatography (0–5% EtOAC in hexanes, dry loading) afforded the product as a yellow oil (465 mg, 14 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 – 7.90 (m, 2H), 7.89 – 7.85 (m, 2H), 7.76 – 7.71 (m, 2H), 7.65 – 7.56 (m, 3H), 7.55 – 7.49 (m, 2H), 7.40 – 7.34 (m, 1H), 7.33 – 7.28 (m, 1H), 6.72 (t, *J* = 2.2 Hz, 1H), 3.57 (d, *J* = 2.2 Hz, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 196.4, 144.8, 144.5, 143.4, 140.5, 137.9, 136.7, 132.7, 132.5, 130.7, 130.1, 128.4, 127.6, 126.4, 125.3, 124.4, 120.3, 38.5.
HRMS (ESI, m/z): $[M+Na]^+$ calc. 319.1093; found 319.1089

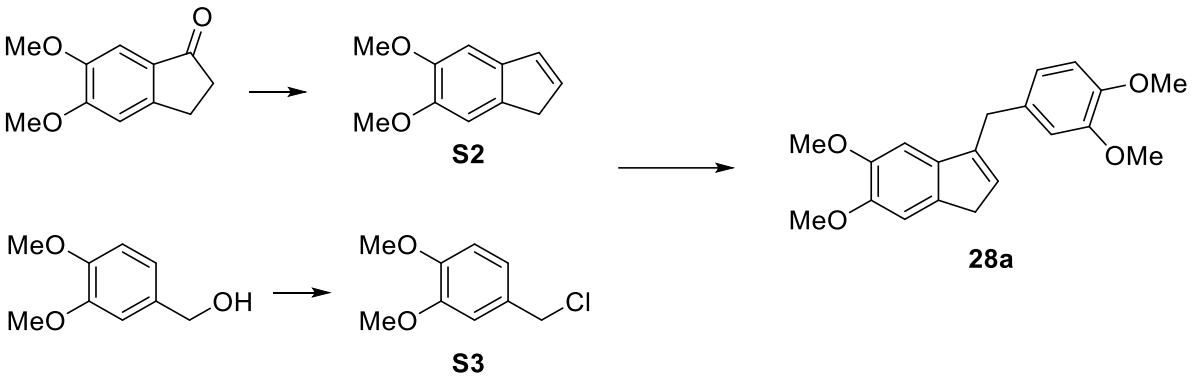
4-(1*H*-Inden-3-yl)benzaldehyde (25a)



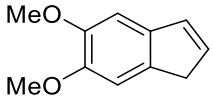
In a flame-dried 100 mL round bottom flask charged with a stir bar, 1-bromo-4-(dimethoxymethyl)benzene (**S1**) (867 mg, 3.75 mmol, 1.0 equiv) was dissolved in anhydrous THF (15 mL) under N_2 atmosphere. *n*-BuLi (2.60 mL, 1.6 M solution in hexanes, 4.12 mmol, 1.1 equiv) was added dropwise at -78 °C, then the mixture was stirred at -78 °C for 30 minutes. A solution of 2,3-dihydro-1*H*-inden-1-one (495 mg, 3.75 mmol, 1.0 equiv) in anhydrous THF (5 mL) was added dropwise to the mixture, then it was allowed to warm up over 2 hours from -78 °C to 25 °C. The mixture was quenched with water, extracted with DCM, and concentrated. The concentrate was dissolved in a water-acetone mixture, then conc. HCl was added, and the mixture was stirred for 60 minutes at room temperature. It was then neutralized with 1 M NaOH solution, extracted with DCM, and the combined organic phases were washed with brine, dried over Na_2SO_4, filtered, and then concentrated. Flash column chromatography (10–20% EtOAc in pentane) gave the product as a pale yellow oil (270.8 mg, 32%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 7.96 – 7.92 (m, 2H), 7.74 (d, *J* = 8.2 Hz, 2H), 7.62 – 7.55 (m, 2H), 7.40 – 7.35 (m, 1H), 7.35 – 7.30 (m, 1H), 6.68 (t, *J* = 2.2 Hz, 1H), 3.52 (d, *J* = 2.3 Hz, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 191.6, 144.5, 144.0, 142.8, 142.0, 135.4, 133.1, 129.9, 128.0, 126.2, 125.2, 124.2, 120.0, 38.3.
HRMS (ESI, m/z): $[M+Na]^+$ calc. 243.0780; found 243.0780

Synthesis of 3-(3,4-dimethoxybenzyl)-5,6-dimethoxy-1*H*-indene (28a)



5,6-Dimethoxy-1*H*-indene (S2)

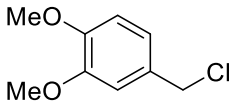


5,6-Dimethoxy-1H-indene (**S2**) was prepared according to a reported literature procedure.[20]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.09 – 7.07 (m, 1H), 6.98 (s, 1H), 6.82 – 6.78 (m, 1H), 6.46 (dt, *J* = 5.5, 1.9 Hz, 1H), 3.91 (s, 3H), 3.91 (s, 3H), 3.35 (td, *J* = 2.0, 0.8 Hz, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 148.4, 147.3, 137.7, 136.3, 133.0, 131.8, 108.2, 104.7, 56.4, 56.3, 39.3.

The spectral data are consistent with those reported in the literature.[21]

4-(Chloromethyl)-1,2-dimethoxybenzene (S3)

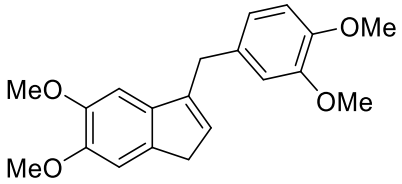


4-(Chloromethyl)-1,2-dimethoxybenzene (**S3**) was prepared according to a reported literature procedure.[22]

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 – 6.89 (m, 2H), 6.83 (d, *J* = 8.0 Hz, 1H), 4.57 (d, *J* = 0.5 Hz, 2H), 3.90 (s, 3H), 3.88 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 149.4, 149.3, 130.2, 121.3, 111.9, 111.1, 56.1, 56.0, 46.8.

The spectral data are consistent with those reported in the literature.[22]

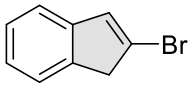
3-(3,4-Dimethoxybenzyl)-5,6-dimethoxy-1*H*-indene (28a)



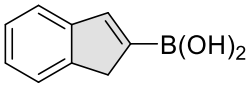
3-(3,4-Dimethoxybenzyl)-5,6-dimethoxy-1*H*-indene (**28a**) was prepared by adapting a reported literature procedure.[23] A Schlenk flask equipped with a stirring bar was filled with LDA (2.4 ml, 2M in THF/heptane/ethylbenzene, 4.8 mmol, 2.0 equiv). To this, a solution of 5,6-dimethoxy-1H-indene (**S2**) (426 mg, 2.40 mmol, 1.0 equiv) and HMPA (0.84 mL, 4.8 mmol, 2.0 equiv) in anhydrous THF (12 mL) was added dropwise. The mixture was stirred for 5 minutes. Then, a solution of 4-(chloromethyl)-1,2-dimethoxybenzene (**S3**) (676 mg, 3.60 mmol, 1.5 equiv) in anhydrous THF (12 mL) was added dropwise and the mixture was stirred at room temperature for 2 h. The reaction progress was determined by TLC. After completion, the reaction mixture was quenched with saturated NH_4Cl solution and extracted with DCM. The combined organic phases were washed with brine, dried over $MgSO_4$, and concentrated. Flash column chromatography of the crude reaction mixture (30% EtOAc in DCM → 100% DCM → 5% MeOH in DCM) afforded the product as a light yellow solid (243 mg, 31%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07 – 7.06 (m, 1H), 6.84 (s, 1H), 6.83 – 6.81 (m, 3H), 6.02 – 6.00 (m, 1H), 3.90 (s, 3H), 3.86 (s, 3H), 3.85 (s, 3H), 3.84 (s, 3H), 3.82 (q, *J* = 2.0 Hz, 2H), 3.30 – 3.27 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 149.0, 148.2, 147.6, 147.4, 143.6, 138.1, 137.1, 132.0, 128.5, 121.0, 112.5, 111.3, 108.2, 103.4, 56.4, 56.3, 56.1, 56.0, 37.7, 34.4.
HRMS (ESI, m/z): $[M+Na]^+$ calc. 349.1410; found 349.1408

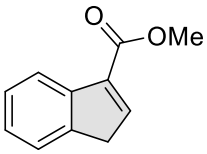
4. Unsuccessful examples



no reaction



no product formation



no reaction

5. Substrate scope

General procedure A: 1.0 mmol reaction

A 100 mL round bottom flask equipped with a Teflon stir bar was charged with the indene (1.0mmol) and MeOH (15 mL) and cooled in an ice bath to 0 °C, while stirring vigorously. Ammonium carbamate (312 mg, 4.00 mmol, 4.0 equiv) was added in one portion. After 1 minute, PIDA (805 mg, 2.50 mmol, 2.5 equiv)[1] was added in one portion and the reaction mixture was stirred for 20 minutes at 0 °C. The ice bath was removed, and the mixture was warmed to room temperature. The reaction progress was monitored by TLC (usually 10–30 minutes).

The solvent was evaporated, the mixture was dissolved in DCM (30 mL), and the organic layer was washed with 1M NaOH (30 mL). The aqueous phase was extracted again with DCM (10 mL) and the combined organic layers were dried over $MgSO_4$ or Na_2SO_4, filtered, and concentrated under reduced pressure.

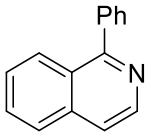
The product was purified by flash column chromatography unless stated otherwise.

General procedure B: 0.05 mmol reaction

In a 4 mL screw-cap vial equipped with a magnetic stirring bar, the indene (0.05 mmol) was dissolved in 0.7 mL of a stock solution containing deuterated methanol and internal standard (1,1,2,2-tetrachloroethane) and cooled in an ice bath to 0 °C, while stirring vigorously. Ammonium carbamate (15.6 mg, 0.200 mmol, 4.00 equiv) was added and the mixture was stirred for 1 minute before PIDA (32 mg, 0.10 mmol, 2.0 equiv) was added in one portion and the reaction was stirred for 10 minutes at 0 °C. The crude reaction mixture was analyzed by recording a ^1H NMR spectrum and the yield was determined by comparing the integration areas corresponding to the product relative to the internal standard 1,1,2,2-tetrachloroethane (^1H NMR 400 MHz, CD_3OD δ 6.48, s, 2H) which was set to 1.0. Unless stated otherwise, the peak corresponding to the H at the 3-position of the isoquinoline product was integrated and compared to the internal standard.

[1] 2.5 equivalents of PIDA were used for the larger scale reactions as remaining starting material was detected when only using 2 equivalents, while oxidative byproducts were obtained when using 3 or more equivalents of PIDA.

1-Phenylisoquinoline (1b)



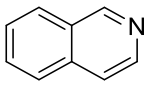
1-Phenylisoquinoline (**1b**) was prepared according to the general procedure A using 3-phenyl indene (**1a**). Preparative RP-HPLC afforded the product as a beige solid (129 mg, 63% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 5.7 Hz, 1H), 8.13 – 8.09 (m, 1H), 7.91 – 7.86 (m, 1H), 7.73 – 7.67 (m, 3H), 7.65 (dd, *J* = 5.7, 0.9 Hz, 1H), 7.57 – 7.49 (m, 4H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 160.9, 142.4, 139.7, 137.0, 130.1, 130.1, 128.7, 128.5, 127.7, 127.3, 127.1, 126.9, 120.0.
HRMS (ESI, m/z): $[M+H]^+$ calc. 206.0964; found 206.0964

The spectral data are consistent with those reported in the literature.[24]

The NMR yield was determined by general procedure B using 0.90 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.52 relative to the internal standard, which corresponds to 93% yield.

Isoquinoline (2b)



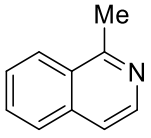
Isoquinoline (**2b**) was prepared according to the general procedure A using 3-*H* indene as the starting material. Flash column chromatography (25% EtOAc in hexanes) afforded the product as a brown oil (55 mg, 43 % yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.26 (t, *J* = 1.0 Hz, 1H), 8.53 (d, *J* = 5.7 Hz, 1H), 7.99 – 7.96 (m, 1H), 7.84 – 7.81 (m, 1H), 7.72 – 7.68 (m, 1H), 7.65 (dt, *J* = 5.8, 1.1 Hz, 1H), 7.63 – 7.59 (m, 1H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 152.7, 143.3, 135.9, 130.5, 128.8, 127.8, 127.4, 126.6, 120.6.
HRMS (ESI, m/z): $[M+H]^+$ calc. 130.0651; found 130.0655

The spectral data are consistent with those reported in the literature.[25]

The NMR yield was determined by general procedure B using 0.69 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.42 relative to the internal standard, which corresponds to 58% yield.

1-Methylisoquinoline (3b)



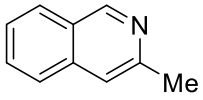
1-Methylisoquinoline (**3b**) was prepared according to the general procedure A using 3-methyl indene (**3a**) as the starting material. Flash column chromatography (25% EtOAc in hexanes) afforded the product as a brown oil (92 mg, 64% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (d, *J* = 5.8 Hz, 1H), 8.14 – 8.10 (m, 1H), 7.82 – 7.79 (m, 1H), 7.69 – 7.65 (m, 1H), 7.61 – 7.58 (m, 1H), 7.52 – 7.50 (m, 1H), 2.97 (d, *J* = 0.6 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 158.8, 142.0, 136.1, 130.0, 127.7, 127.4, 127.2, 125.8, 119.4, 22.6.
HRMS (ESI, m/z): $[M+H]^+$ calc. 144.0808; found 144.0809

The spectral data are consistent with those reported in the literature.[26]

The NMR yield was determined by general procedure B using 0.69 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.64 relative to the internal standard, which corresponds to 88% yield.

3-Methylisoquinoline (4b)



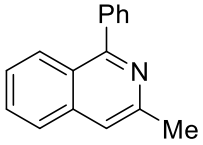
3-Methylisoquinoline (**4b**) was prepared according to the general procedure A using 2-methyl indene (**4a**) as the starting material. Flash column chromatography (30% EtOAc in hexanes) afforded the product as a beige solid (71 mg, 50% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.18 (s, 1H), 7.94 – 7.90 (m, 1H), 7.74 – 7.71 (m, 1H), 7.66 – 7.62 (m, 1H), 7.54 – 7.49 (m, 1H), 7.49 – 7.47 (m, 1H), 2.71 – 2.69 (m, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 152.1, 151.8, 136.7, 130.4, 127.6, 127.0, 126.4, 126.1, 118.6, 24.3.
HRMS (ESI, m/z): $[M+H]^+$ calc. 144.0808; found 144.0808

The spectral data are consistent with those reported in the literature.[27]

The NMR yield was determined by general procedure B using 0.70 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 1-H peak was 0.39 relative to the internal standard, which corresponds to 54% yield.

3-Methyl-1-phenylisoquinoline (5b)



3-Methyl-1-phenylisoquinoline (**5b**) was prepared according to the general procedure A using 2-methyl-3-phenyl-1H-indene (**5a**) as the starting material. Flash column chromatography (0–10% EtOAc in hexanes) afforded the product as a light yellow oil (122 mg, 56% yield).

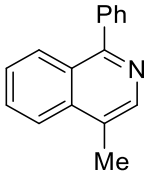
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 – 7.99 (m, 1H), 7.80 – 7.77 (m, 1H), 7.69 – 7.66 (m, 2H), 7.65 – 7.61 (m, 1H), 7.55 – 7.46 (m, 4H), 7.46 – 7.42 (m, 1H), 2.76 – 2.74 (m, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 160.5, 151.0, 139.9, 137.7, 130.1 (2C), 128.6, 128.5, 127.7, 126.5, 126.3, 125.1, 118.1, 24.6.
HRMS (ESI, m/z): $[M+H]^+$ calc. 220.1121; found 220.1123

The spectral data are consistent with those reported in the literature.[28]

The NMR yield was determined by general procedure B using 1.12 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-Me peak (corresponds to 3H) was 0.87 relative to the internal standard, which corresponds to 65% yield.

4-Methyl-1-phenylisoquinoline (6b)



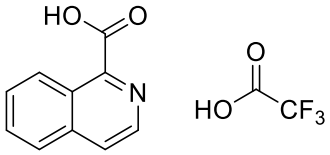
4-Methyl-1-phenylisoquinoline (**6b**) was prepared according to the general procedure A using 1-methyl-3-phenyl-1*H*-indene (**6a**) as the starting material. Flash column chromatography (0–10% EtOAc in hexanes) afforded the product as a light yellow oil (129 mg, 59% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.47 – 8.46 (m, 1H), 8.13 – 8.10 (m, 1H), 8.04 – 8.00 (m, 1H), 7.76 – 7.72 (m, 1H), 7.69 – 7.66 (m, 2H), 7.56 – 7.46 (m, 4H), 2.68 (d, *J* = 0.9 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 159.5, 142.3, 139.9, 136.3, 130.1, 129.9, 128.5, 128.4, 128.2, 126.8, 126.6, 126.3, 123.6, 16.2.
HRMS (ESI, m/z): $[M+H]^+$ calc. 220.1121; found 220.1120

The spectral data are consistent with those reported in the literature.[29]

The NMR yield was determined by general procedure B using 0.70 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.49 relative to the internal standard, which corresponds to 68% yield.

Isoquinoline-1-carboxylic acid (7b · TFA)



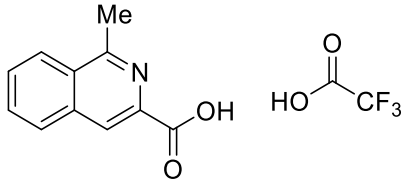
Isoquinoline-1-carboxylic acid (**7b** · **TFA**) was prepared according to the general procedure A using 1*H*-indene-3-carboxylic acid. Preparative RP-HPLC afforded the product as the TFA salt as a white solid (86 mg, 30% yield).

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.62 – 8.59 (m, 1H), 8.57 (d, *J* = 5.6 Hz, 1H), 8.11 – 8.07 (m, 2H), 7.89 – 7.85 (m, 1H), 7.81 – 7.77 (m, 1H).
^{13}C NMR (126 MHz, DMSO-d_6) δ 167.0, 158.4 (q, *J* = 37.6 Hz), 150.0, 140.7, 136.6, 131.2, 129.0, 127.4, 126.0, 125.2, 123.8, 115.3 (q, *J* = 289.6 Hz).

^{19}F NMR (471 MHz, DMSO) δ -75.01.
HRMS (ESI, m/z): $[M+H]^+$ calc. 174.0550; found 174.0550

The NMR yield was determined by general procedure B using 0.69 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.42 relative to the internal standard, which corresponds to 58% yield.

1-Methylisoquinoline-3-carboxylic acid (8b · TFA)

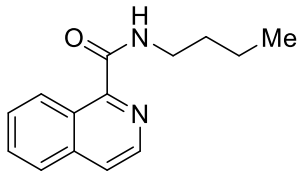


1-Methylisoquinoline-3-carboxylic acid (**8b** · **TFA**) was prepared according to the general procedure A using 3-methyl-1*H*-indene-2-carboxylic acid. Preparative RP-HPLC afforded the product as the TFA salt as a white solid (87 mg, 29% yield).

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.55 (s, 1H), 8.38 – 8.34 (m, 1H), 8.23 – 8.20 (m, 1H), 7.96 – 7.91 (m, 1H), 7.90 – 7.85 (m, 1H), 3.01 – 3.00 (m, 3H).
^{13}C NMR (126 MHz, DMSO-d_6) δ 165.7, 159.2, 138.9, 135.4, 132.0, 130.2, 128.9, 128.1, 126.4, 122.8, 21.3. (*The two carbon quartets referring to the TFA were not fully resolved and were thus omitted*)
^{19}F NMR (471 MHz, DMSO) δ -74.60.
fHRMS (ESI, m/z): $[M+H]^+$ calc 188.0706.; found 188.0709

The NMR yield was determined by general procedure B using 0.60 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the methyl peak (corresponds to 3H) was 1.35 relative to the internal standard, which corresponds to 54% yield.

***N*-Butylisoquinoline-1-carboxamide (9b)**



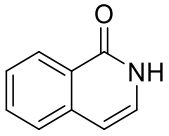
N-Butylisoquinoline-1-carboxamide (**9b**) was prepared according to the general procedure A using *N*-butyl-1*H*-indene-3-carboxamide (**9a**). Flash column chromatography (20% EtOAc in hexanes) afforded the product as a yellow oil (52 mg, 23% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.64 – 9.59 (m, 1H), 8.46 – 8.43 (m, 1H), 8.20 (s, 1H), 7.85 – 7.81 (m, 1H), 7.79 – 7.76 (m, 1H), 7.73 – 7.64 (m, 2H), 3.57 – 3.47 (m, 2H), 1.71 – 1.62 (m, 2H), 1.52 – 1.41 (m, 2H), 1.01 – 0.95 (m, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2, 148.7, 140.3, 137.6, 130.6, 128.7, 128.1, 127.2, 126.9, 124.3, 39.4, 31.9, 20.4, 14.0.

HRMS (ESI, m/z): $[M+H]^+$ calc. 229.1335; found 229.1342

The NMR yield was determined by general procedure B using 1.22 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.13 relative to the internal standard, which corresponds to 32% yield.

Isoquinolin-1(2H)-one (10b)

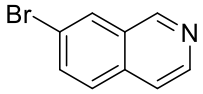


Isoquinolin-1(2H)-one (**10b**) was prepared according to the general procedure A using ((1*H*-inden-3-yl)oxy)(*tert*-butyl)dimethylsilane (**10a**). Flash column chromatography (20–50% EtOAc in pentane), followed by recrystallization from methanol, afforded the product as a white solid (54 mg, 37% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 11.37 (s, 1H), 8.47 – 8.40 (m, 1H), 7.72 – 7.64 (m, 1H), 7.62 – 7.48 (m, 2H), 7.19 (d, *J* = 7.2 Hz, 1H), 6.61 – 6.55 (m, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 164.5, 138.3, 132.8, 127.8, 127.5, 127.0, 126.4, 126.3, 106.9.
HRMS (ESI, m/z): $[M+H]^+$ calc. 146.0600; found 146.0604

The NMR yield was determined by general procedure B using 0.95 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 4-H peak was 0.27 relative to the internal standard, which corresponds to 52% yield.

7-Bromoisoquinoline (11b)

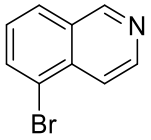


7-Bromoisoquinoline (**11b**) was prepared according to the general procedure A using 5-bromo-1*H*-indene (**11a**) as the starting material. Flash column chromatography (25% EtOAc in hexanes) afforded the product as a beige solid (60 mg, 29% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 – 9.16 (m, 1H), 8.55 (d, *J* = 5.8 Hz, 1H), 8.13 – 8.11 (m, 1H), 7.75 (dd, *J* = 8.8, 1.9 Hz, 1H), 7.71 – 7.67 (m, 1H), 7.63 – 7.59 (m, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 151.6, 143.6, 134.3, 134.0, 129.9, 129.6, 128.4, 121.0, 120.4.
HRMS (ESI, m/z): $[M+H]^+$ calc. 207.9756; found 207.9754

The NMR yield was determined by general procedure B using 0.71 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.24 relative to the internal standard, which corresponds to 34% yield.

5-Bromoisoquinoline (12b)



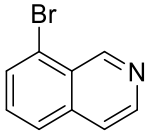
5-Bromoisoquinoline (**12b**) was prepared according to the general procedure using 7-bromo-1*H*-indene (**12a**) as the starting material. Flash column chromatography (25% EtOAc in hexanes) afforded the product as a beige solid (62 mg, 30% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.23 (d, *J* = 0.9 Hz, 1H), 8.65 (d, *J* = 5.9 Hz, 1H), 8.00 – 7.98 (m, 1H), 7.97 (dd, *J* = 2.5, 1.0 Hz, 1H), 7.97 – 7.93 (m, 1H), 7.47 (dd, *J* = 8.2, 7.4 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 152.9, 144. 7, 135.2, 134.1, 129.8, 127.9, 127.6, 121.7, 119.5.
HRMS (ESI, m/z): $[M+H]^+$ calc. 207.9756; found 207.9753

The spectral data are consistent with those reported in the literature.[30]

The NMR yield was determined by general procedure B using 0.70 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.22 relative to the internal standard, which corresponds to 31% yield.

8-Bromoisoquinoline (13b)



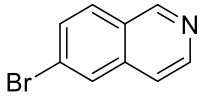
8-Bromoisoquinoline (**13b**) was prepared according to the general procedure using 4-bromo-1*H*-indene (**13a**) as the starting material. Flash column chromatography (20% EtOAc in hexanes) afforded the product as a beige solid (62 mg, 30% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.64 – 9.58 (m, 1H), 8.64 – 8.59 (m, 1H), 7.87 – 7.81 (m, 1H), 7.80 – 7.76 (m, 1H), 7.63 – 7.59 (m, 1H), 7.54 – 7.49 (m, 1H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 152.2, 144.1, 137.4, 131.4, 130.8, 127.0, 126.6, 122.7, 120.2.
HRMS (ESI, m/z): $[M+H]^+$ calc. 207.9756; found 207.9758

The spectral data are consistent with those reported in the literature.[31]

The NMR yield was determined by general procedure B using 0.95 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.18 relative to the internal standard, which corresponds to 34% yield.

6-Bromoisoquinoline (14b)



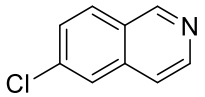
6-Bromoisoquinoline (**14b**) was prepared according to the general procedure A using 6-bromo-1*H*-indene (**14a**) as the starting material. Flash column chromatography (0–20% EtOAc in hexanes) afforded the product as a brown solid (78 mg, 37% yield). Single-crystals suitable for X-ray analysis were obtained as the hydrate by slow evaporation from chloroform.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.24 – 9.21 (m, 1H), 8.57 – 8.54 (m, 1H), 8.02 – 7.99 (m, 1H), 7.87 – 7.82 (m, 1H), 7.71 – 7.67 (m, 1H), 7.58 – 7.55 (m, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 152.6, 144.2, 136.9, 131.1, 129.4, 128.9, 127.2, 125.3, 119.5.
HRMS (ESI, m/z): $[M+H]^+$ calc. 207.9756; found 207.9756

The spectral data are consistent with those reported in the literature.[11]

The NMR yield was determined by general procedure B using 0.70 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.35 relative to the internal standard, which corresponds to 49% yield.

6-Chloroisoquinoline (15b)

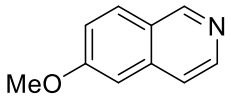


6-Chloroisoquinoline (**15b**) was prepared according to the general procedure A using 6-chloro-1*H*-indene (**15a**) as the starting material. Flash column chromatography (30% EtOAc in pentane) afforded the product as a brown solid (60 mg, 37% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (s, 1H), 8.51 (d, *J* = 5.8 Hz, 1H), 7.85 (d, *J* = 8.8 Hz, 1H), 7.75 (d, *J* = 2.0 Hz, 1H), 7.54 – 7.45 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 152.3, 144.1, 136.6, 136.5, 129.3, 128.4, 126.8, 125.4, 119.6.
HRMS (ESI, m/z): $[M+H]^+$ calc. 164.0262; found 164.0263

The NMR yield was determined by general procedure B using 0.82 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.29 relative to the internal standard, which corresponds to 47% yield.

6-Methoxyisoquinoline (16b)



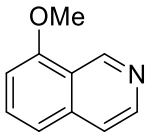
6-Methoxyisoquinoline (**16b**) was prepared according to the general procedure A using 6-methoxy-1*H*-indene (**16a**) as the starting material. Flash column chromatography (40–50% EtOAc in pentane) afforded the product as a brown oil (45 mg, 29% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.06 (t, *J* = 0.9 Hz, 1H), 8.40 (d, *J* = 5.7 Hz, 1H), 7.80 (d, *J* = 9.0 Hz, 1H), 7.49 (d, *J* = 5.8 Hz, 1H), 7.18 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.00 (d, *J* = 2.5 Hz, 1H), 3.89 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 161.0, 151.6, 143.5, 137.8, 129.4, 124.5, 120.4, 119.8, 104.0, 55.5.
HRMS (ESI, m/z): $[M+H]^+$ calc. 160.0757; found 160.0756

The spectral data are consistent with those reported in the literature.[32]

The NMR yield was determined by general procedure B using 1.05 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.24 relative to the internal standard, which corresponds to 50% yield.

8-Methoxyisoquinoline (17b)

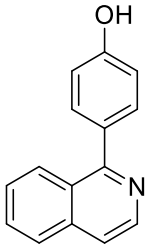


8-Methoxyisoquinoline (**17b**) was prepared according to the general procedure A using 4-methoxy-1*H*-indene (**17a**) as the starting material. Flash column chromatography (30% EtOAc in pentane) afforded the product as a brown oil (82 mg, 52% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.59 (t, *J* = 1.0 Hz, 1H), 8.49 (d, *J* = 5.7 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.28 (d, *J* = 8.2 Hz, 1H), 6.80 (d, *J* = 7.7 Hz, 1H), 3.94 (s, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 156.4, 147.6, 143.6, 136.9, 130.9, 120.8, 119.9, 118.4, 105.1, 55.5.
HRMS (ESI, m/z): $[M+H]^+$ calc. 160.0757; found 160.0758

The NMR yield was determined by general procedure B using 1.08 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.31 relative to the internal standard, which corresponds to 67% yield.

4-(Isoquinolin-1-yl)phenol (18b)

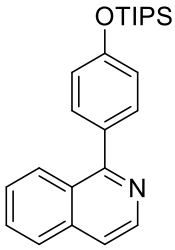


4-(Isoquinolin-1-yl)phenol (**18b**) was prepared according to the general procedure A using 4-(1*H*-inden-3-yl)phenol (**18a**) as the starting material. Flash column chromatography (50% EtOAc in hexanes) afforded the product as a brown solid (80 mg, 36% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.77 (s, 1H), 8.53 (d, *J* = 5.7 Hz, 1H), 8.11 – 8.06 (m, 1H), 8.04 – 7.99 (m, 1H), 7.80 – 7.74 (m, 2H), 7.67 – 7.60 (m, 1H), 7.55 – 7.49 (m, 2H), 6.97 – 6.91 (m, 2H).
^{13}C NMR (101 MHz, DMSO-d_6) δ 159.7, 157.9, 142.0, 136.4, 131.3, 130.1, 130.0, 127.5, 127.1, 126.9, 125.8, 119.2, 115.0.
HRMS (ESI, m/z): $[M+H]^+$ calc. 222.0913; found 222.0914

The NMR yield was determined by general procedure B using 0.70 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.36 relative to the internal standard, which corresponds to 50% yield.

1-(4-((Triisopropylsilyl)oxy)phenyl)isoquinoline (19b)

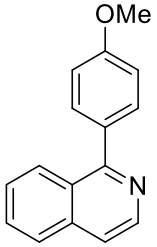


1-(4-((Triisopropylsilyl)oxy)phenyl)isoquinoline (**19b**) was prepared according to the general procedure A using 4-(1*H*-inden-3-yl)phenoxy)triisopropylsilane (**19a**) as the starting material. Flash column chromatography (0–5% EtOAc in hexanes) afforded the product as a yellow oil (209 mg, 55% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 (d, *J* = 5.7 Hz, 1H), 8.16 – 8.13 (m, 1H), 7.87 – 7.84 (m, 1H), 7.69 – 7.65 (m, 1H), 7.62 – 7.58 (m, 3H), 7.55 – 7.51 (m, 1H), 7.06 – 7.03 (m, 2H), 1.37 – 1.28 (m, 3H), 1.18 – 1.14 (m, 18H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 160.7, 156.8, 142.3, 137.0, 132.5, 131.4, 130.0, 127.8, 127.1, 127.1, 126.9, 119.9, 119.6, 18.1, 12.9.
HRMS (ESI, m/z): $[M+H]^+$ calc. 378.2248; found 378.2248

The NMR yield was determined by general procedure B using 0.70 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.62 relative to the internal standard, which corresponds to 87% yield.

1-(4-Methoxyphenyl)isoquinoline (20b)



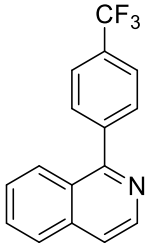
1-(4-Methoxyphenyl)isoquinoline (**20b**) was prepared according to the general procedure A using 3-(4-methoxyphenyl)-1*H*-indene (**20a**) as the starting material. Flash column chromatography (20% EtOAc in pentane) afforded the product as an orange oil (107 mg, 45% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, *J* = 5.7 Hz, 1H), 8.17 – 8.13 (m, 1H), 7.89 – 7.85 (m, 1H), 7.71 – 7.65 (m, 3H), 7.63 – 7.60 (m, 1H), 7.56 – 7.51 (m, 1H), 7.09 – 7.05 (m, 2H), 3.90 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 160.5, 160.2, 142.3, 137.1, 132.2, 131.4, 130.1, 127.8, 127.2, 127.1, 126.9, 119.7, 114.0, 55.5.
HRMS (ESI, m/z): $[M+H]^+$ calc. 236.1070; found 236.1069

The spectral data are consistent with those reported in the literature.[33]

The NMR yield was determined by general procedure B using 1.05 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.32 relative to the internal standard, which corresponds to 67% yield.

1-(4-(Trifluoromethyl)phenyl)isoquinoline (21b)



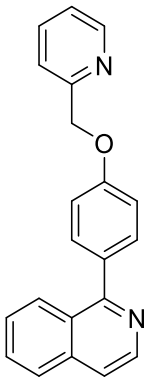
1-(4-(Trifluoromethyl)phenyl)isoquinoline (**21b**) was prepared according to the general procedure A using 3-(4-(trifluoromethyl)phenyl)-1*H*-indene (**21a**) as the starting material. Flash column chromatography (0–10% EtOAc in hexanes) afforded the product as a white solid (179 mg, 66% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 5.7 Hz, 1H), 8.04 – 8.01 (m, 1H), 7.94 – 7.90 (m, 1H), 7.85 – 7.79 (m, 4H), 7.75 – 7.69 (m, 2H), 7.60 – 7.55 (m, 1H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 159.3, 143.3 (d, *J* = 1.4 Hz), 142.4, 137.0, 130.8 (q, *J* = 32.6 Hz), 130.5, 130.4, 127.8, 127.3, 127.1, 126.7, 125.5 (q, *J* = 3.8 Hz), 124.3 (q, *J* = 272.2 Hz), 120.7.
^{19}F NMR (471 MHz, $CDCl_3$) δ -62.55.
HRMS (ESI, m/z): $[M+H]^+$ calc. 274.0838; found 274.0836

The spectral data are consistent with those reported in the literature.[28]

The NMR yield was determined by general procedure B using 0.89 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.52 relative to the internal standard, which corresponds to 93% yield.

1-(4-(Pyridin-2-ylmethoxy)phenyl)isoquinoline (22b)



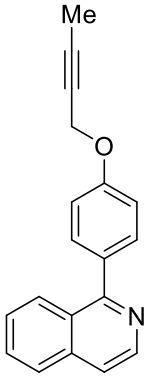
1-(4-(Pyridin-2-ylmethoxy)phenyl)isoquinoline (**22b**) was prepared according to the general procedure A using 2-((4-(1*H*-inden-3-yl)phenoxy)methyl)pyridine (**22a**) as the starting material. Flash column

chromatography (10% EtOAc in hexanes, with NH_3-neutralized silica[2]) afforded the product as an off-white solid (191 mg, 61% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 – 8.61 (m, 1H), 8.58 (d, *J* = 5.7 Hz, 1H), 8.15 – 8.12 (m, 1H), 7.88 – 7.85 (m, 1H), 7.73 (td, *J* = 7.7, 1.8 Hz, 1H), 7.69 – 7.65 (m, 3H), 7.60 (dd, *J* = 5.7, 0.9 Hz, 1H), 7.58 – 7.55 (m, 1H), 7.55 – 7.51 (m, 1H), 7.25 – 7.22 (m, 1H), 7.17 – 7.13 (m, 2H), 5.31 (s, 2H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 160.4, 158.9, 157.3, 149.4, 142.3, 137.1, 137.0, 132.8, 131.5, 130.1, 127.7, 127.2, 127.1, 126.8, 122.8, 121.5, 119.7, 114.9, 70.9.
HRMS (ESI, m/z): $[M+H]^+$ calc. 313.1335; found 313.1334

The NMR yield was determined by general procedure B using 0.71 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.59 relative to the internal standard, which corresponds to 83% yield.

1-(4-(But-2-yn-1-yloxy)phenyl)isoquinoline (23b)



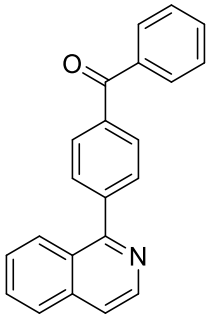
1-(4-(But-2-yn-1-yloxy)phenyl)isoquinoline (**23b**) was prepared according to the general procedure A using 3-(4-(but-2-yn-1-yloxy)phenyl)-1*H*-indene (**23a**) as the starting material. Flash column chromatography (5–15% EtOAc in hexanes) afforded the product as a light yellow solid (95 mg, 35% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 (d, *J* = 5.7 Hz, 1H), 8.17 – 8.14 (m, 1H), 7.88 – 7.86 (m, 1H), 7.70 – 7.65 (m, 3H), 7.63 – 7.60 (m, 1H), 7.56 – 7.52 (m, 1H), 7.15 – 7.11 (m, 2H), 4.74 (q, *J* = 2.3 Hz, 2H), 1.89 (td, *J* = 2.3, 0.5 Hz, 3H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 160.5, 158.4, 142.4, 137.1, 132.8, 131.4, 130.1, 127.8, 127.2, 127.1, 126.9, 119.7, 114.9, 84.1, 74.0, 56.7, 3.9.
HRMS (ESI, m/z): $[M+H]^+$ calc. 274.1226; found 274.1220

The NMR yield was determined by general procedure B using 1.07 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.26 relative to the internal standard, which corresponds to 56% yield.

[2] Silica gel was treated at room temperature for at least 5 h with an equal volume of a solution consisting of 6:2:2 CH_2Cl_2:MeOH:25 % $NH_{3(aq.)}$; the slurry was then filtered and dried using compressed air.[34]

(4-(Isoquinolin-1-yl)phenyl)(phenyl)methanone (24b)

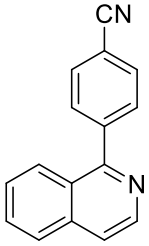


(4-(Isoquinolin-1-yl)phenyl)(phenyl)methanone (**24b**) was prepared according to the general procedure A using (4-(1*H*-inden-3-yl)phenyl)(phenyl)methanone (**24a**) as the starting material. Flash column chromatography (20% EtOAc in pentane) afforded the product as an orange solid (186 mg, 60% yield). Single-crystals suitable for X-ray analysis were obtained by slow evaporation from chloroform.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 5.7 Hz, 1H), 8.11 – 8.07 (m, 1H), 7.99 – 7.95 (m, 2H), 7.92 – 7.86 (m, 3H), 7.85 – 7.81 (m, 2H), 7.73 – 7.67 (m, 2H), 7.63 – 7.54 (m, 2H), 7.53 – 7.48 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 196.5, 159.6, 143.6, 142.4, 137.7, 137.6, 136.9, 132.7, 130.3, 130.2, 130.2, 130.0, 128.5, 127.6, 127.3, 127.2, 126.7, 120.6.
HRMS (ESI, m/z): $[M+H]^+$ calc. 310.1226; found 310.1226

The NMR yield was determined by general procedure B using 0.38 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.72 relative to the internal standard, which corresponds to 54% yield.

4-(Isoquinolin-1-yl)benzonitrile (25b)



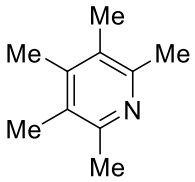
4-(Isoquinolin-1-yl)benzonitrile (**25b**) was prepared according to the general procedure using 4-(1*H*-inden-3-yl)benzaldehyde (**25a**) as the starting material. Flash column chromatography (20% EtOAc in pentane) afforded the product as an off-white solid (120 mg, 54% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, *J* = 5.7 Hz, 1H), 7.95 – 7.91 (m, 1H), 7.89 – 7.85 (m, 1H), 7.76 (s, 4H), 7.70 – 7.64 (m, 2H), 7.55 – 7.50 (m, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 158.2, 143.9, 142.2, 136.7, 132.0, 130.6, 130.3, 127.7, 127.2, 126.4, 126.2, 120.8, 118.6, 112.2.
HRMS (ESI, m/z): $[M+H]^+$ calc. 231.0917; found 231.0914

The spectral data are consistent with those reported in the literature.[35]

The NMR yield was determined by general procedure B using 0.90 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 3-H peak was 0.25 relative to the internal standard, which corresponds to 45% yield.

2,3,4,5,6-Pentamethylpyridine (26b)

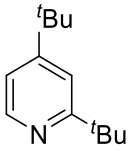


2,3,4,5,6-Pentamethylpyridine (**26b**) was prepared according to the general procedure A using 1,2,3,4,5-pentamethyl cyclopentadiene as the starting material. Flash column chromatography (30–80% EtOAc in hexanes) afforded the product as an orange oil (77 mg, 52% yield), which upon exposure to atmospheric moisture solidified as the hydrate.

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.46 (s, 6H), 2.18 (s, 3H), 2.17 (s, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 152.4, 143.9, 127.2, 23.3, 15.9, 15.4
HRMS (ESI, m/z): $[M+H]^+$ calc. 150.1277; found 150.1276

The NMR yield was determined by general procedure B using 1.06 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 2-Me peak (corresponds to 6H) was 2.70 relative to the internal standard, which corresponds to 95% yield.

2,4-Di-*tert*-butylpyridine (27b)



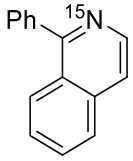
2,4-Di-*tert*-butylpyridine (**27b**) was prepared according to the general procedure A using di-*tert*-butyl-1,3-cyclopentadiene. Flash column chromatography (0–5% EtOAc in hexanes) afforded the product as a colourless oil (116 mg, 65% yield).

^{1}H NMR ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (dd, *J* = 5.3, 0.8 Hz, 1H), 7.32 (dd, *J* = 1.9, 0.8 Hz, 1H), 7.08 (dd, *J* = 5.3, 1.9 Hz, 1H), 1.37 (s, 9H), 1.31 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 169.2, 160.1, 148.5, 117.9, 115.9, 37.6, 34.9, 30.8, 30.5.
HRMS (ESI, m/z): $[M+H]^+$ calc. 192.1747; found 192.1745

The spectral data are consistent with those reported in the literature.[36]

The NMR yield was determined by general procedure B using 0.98 equivalents of the internal standard 1,1,2,2-tetrachloroethane. The integral of the 2-H peak was 0.47 relative to the internal standard, which corresponds to 92% yield.

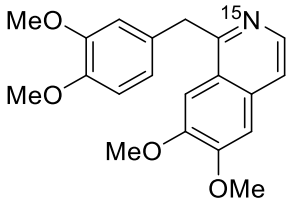
1-Phenylisoquinoline-^{15}N (15N-1b)



A 100ml round bottom flask equipped with a Teflon stir bar was charged with 3-phenyl indene (**1a**) (192 mg, 1.00 mmol, 1.0 equiv) and MeOH (15mL) and cooled in an ice bath while stirring vigorously. $^{15}NH_4Cl$ (109 mg, 2.00 mmol, 2.0 equiv) was added in one portion, followed by K_2CO_3 (276 mg, 2.00 mmol, 2.0 equiv). After 1 minute, PIDA (805 mg, 2.50 mmol, 2.5 equiv) was added in one portion and the reaction mixture was stirred for 20 minutes at 0 °C. The ice bath was removed and the mixture was warmed to room temperature. The reaction progress was monitored by TLC. The solvent was evaporated and the mixture was dissolved in DCM (30 mL). The organic layer was washed with 1M NaOH (30 mL) and the aqueous phase was extracted once with DCM (10 mL). The combined organic layers were dried over $MgSO_4$, filtered, and evaporated. Flash column chromatography (20% EtOAc in hexanes) afforded the product as a beige solid (106 mg, 51% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (dd, *J* = 10.9, 5.7 Hz, 1H), 8.11 (dq, *J* = 8.6, 0.9 Hz, 1H), 7.93 – 7.85 (m, 1H), 7.72 – 7.67 (m, 3H), 7.66 – 7.64 (m, 1H), 7.56 – 7.47 (m, 4H).
^{13}C NMR. (126 MHz, $CDCl_3$) δ 160.9 (d, *J* = 2.6 Hz), 142.4, 139.8 (d, *J* = 7.5 Hz), 137.0 (d, *J* = 2.3 Hz), 130.1, 130.1 (d, *J* = 1.7 Hz), 128.7, 128.5, 127.7 (d, *J* = 1.2 Hz), 127.3, 127.1, 126.9 (d, *J* = 2.0 Hz), 120.0 (d, *J* = 2.5 Hz).
^{15}N NMR (51 MHz, $CDCl_3$) δ 306.7 (dd, *J* = 10.8, 1.9 Hz).
HRMS (ESI, m/z): $[M+H]^+$ calc. 207.0935; found 207.0937

Papaverine-^{15}N (15N-28b)



A 50 mL round bottom flask equipped with a Teflon stir bar was charged with **28a** (163 mg, 0.500 mmol, 1.0 equiv) and MeOH (7.5mL) and cooled in an ice bath while stirring vigorously. $^{15}NH_4Cl$ (55 mg, 1.00 mmol, 2.0 equiv) was added in one portion, followed by K_2CO_3 (138 mg, 1.00 mmol, 2.0 equiv). After 1 minute, PIDA (403 mg, 1.25 mmol, 2.5 equiv) was added in one portion and the reaction mixture was stirred for 20 minutes at 0 °C. The ice bath was removed and the mixture was warmed to room temperature. The reaction progress was determined by TLC. The solvent was evaporated and the mixture was dissolved in DCM (30 mL). The organic layer was washed with 1M NaOH (30 mL) and the aqueous phase was extracted once with DCM (10 mL). The combined organic layers were dried over $MgSO_4$, filtered, and evaporated. Flash column chromatography (0–100% EtOAc in hexanes) afforded the product as an off-white solid (64 mg, 38% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (dd, *J* = 10.7, 5.7 Hz, 1H), 7.43 – 7.41 (m, 1H), 7.34 (d, *J* = 0.8 Hz, 1H), 7.04 (s, 1H), 6.82 – 6.80 (m, 2H), 6.77 – 6.74 (m, 1H), 4.53 (d, *J* = 3.3 Hz, 2H), 3.99 (s, 3H), 3.90 (s, 3H), 3.81 (s, 3H), 3.76 (s, 3H).
^{13}C NMR. (126 MHz, $CDCl_3$) δ 157.9 (d, *J* = 2.5 Hz), 152.6 (d, *J* = 0.6 Hz), 149.9, 149.2, 147.7, 141.2, 133.6 (d, *J* = 2.4 Hz), 132.4 (d, *J* = 1.0 Hz), 123.1 (d, *J* = 2.5 Hz), 120.6, 118.8 (d, *J* = 2.6 Hz), 112.0, 111.3, 105.4, 104.4 (d, *J* = 1.1 Hz), 56.1, 56.0, 56.0, 55.9, 42.4 (d, *J* = 9.2 Hz).
^{15}N NMR (51 MHz, $CDCl_3$) δ 299.9 (d, *J* = 10.8 Hz).
HRMS (ESI, m/z): $[M+H]^+$ calc. 341.1514; found 341.1519

6. Crystal data

	6-Bromoisoquinoline hydrate (14b)	**(4-(Isoquinolin-1-yl)phenyl)(phenyl)methanone (24b)**
CCDC #	2221959	2221960
Empirical formula	C_9H_8BrNO	$C_{22}H_{15}NO$
Formula weight	226.07	309.35
Temperature/K	100.0(1)	100.0(1)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$
a/Å	12.0681(5)	9.8089(3)
b/Å	4.8252(2)	8.7371(2)
c/Å	15.0066(7)	18.3869(5)
α/°	90	90
β/°	94.654(4)	104.498(3)
γ/°	90	90
Volume/Å^3	870.97(7)	1525.60(7)
Z	4	4
ρ_{calc}g/cm^3	1.724	1.347
μ/mm^{-1}	4.666	0.646
F(000)	448.0	648.0
Crystal size/mm^3	0.261 × 0.08 × 0.077	0.154 × 0.133 × 0.058
Radiation	Mo Kα (λ = 0.71073)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.644 to 66.216	9.312 to 160.654
Index ranges	-17 ≤ h ≤ 17 -6 ≤ k ≤ 7 -22 ≤ l ≤ 22	-11 ≤ h ≤ 12 -11 ≤ k ≤ 10 -23 ≤ l ≤ 22
Reflections collected	14713	21147
Independent reflections	2985 R_{int} = 0.0510 R_{sigma} = 0.0472	3303 R_{int} = 0.0557 R_{sigma} = 0.0365
Data/restraints/parameters	2985/0/112	3303/0/217
Goodness-of-fit on F^2	1.037	1.143
Final R indexes [I>=2σ (I)]	R_1 = 0.0391 wR_2 = 0.0875	R_1 = 0.0752 wR_2 = 0.2394
Final R indexes [all data]	R_1 = 0.0618 wR_2 = 0.0948	R_1 = 0.0803 wR_2 = 0.2429
Largest diff. peak/hole / e Å^{-3}	1.10/-1.57	0.56/-0.40

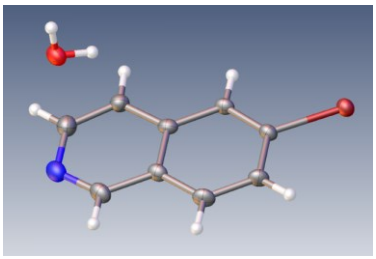


Fig. S1: Asymmetric unit of the crystal structure of product **14b**, ellipsoids depicted at 50% probability.

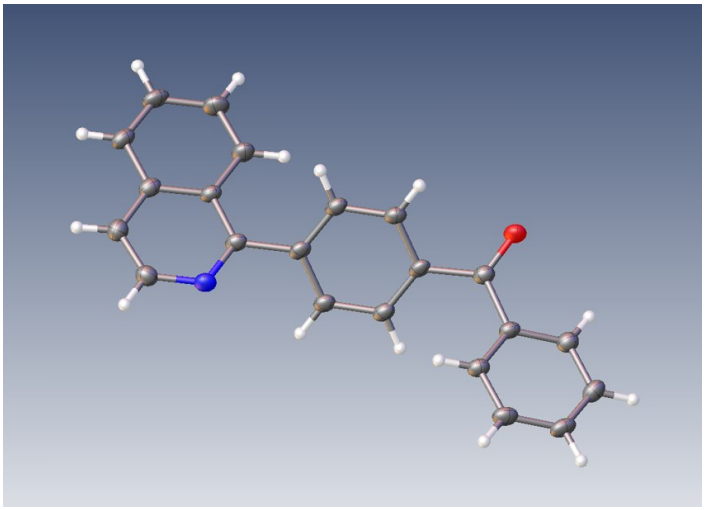


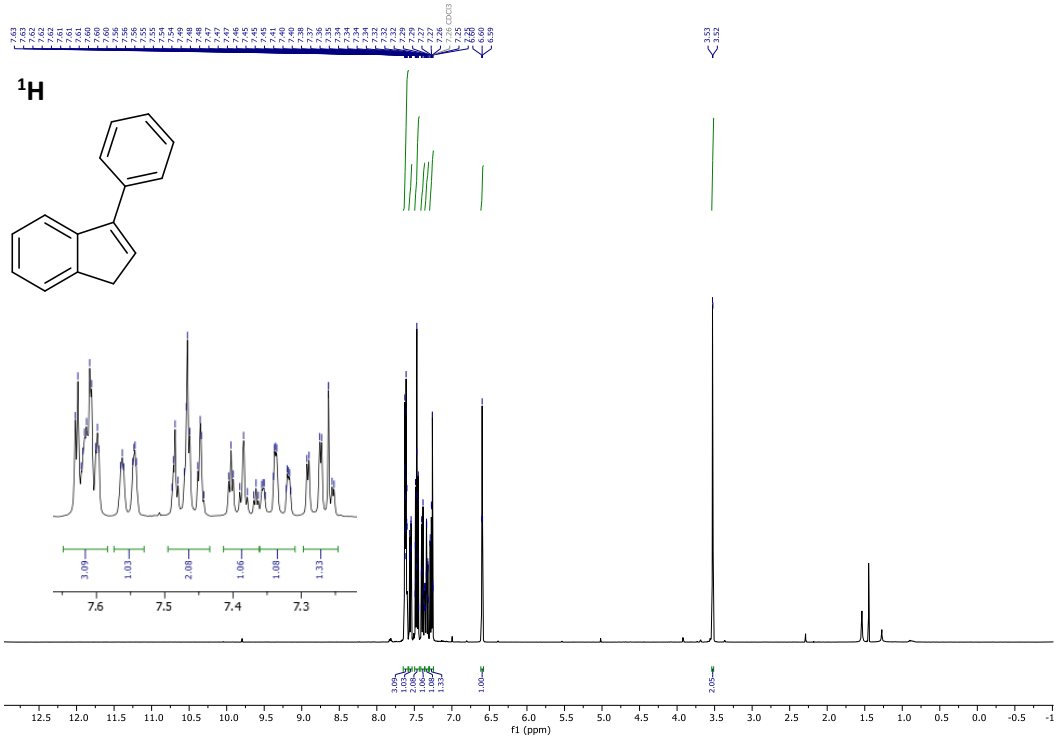
Fig. S2: Asymmetric unit of the crystal structure of product **24b**, ellipsoids depicted at 50% probability.

CCDC 2221959 and CCDC 2221960 contain the supplementary crystallographic data for this paper, including structure factors and refinement instructions. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44(1223)-336-033; e-mail: deposit@ccdc.cam.ac.uk), or via https://www.ccdc.cam.ac.uk/structures.

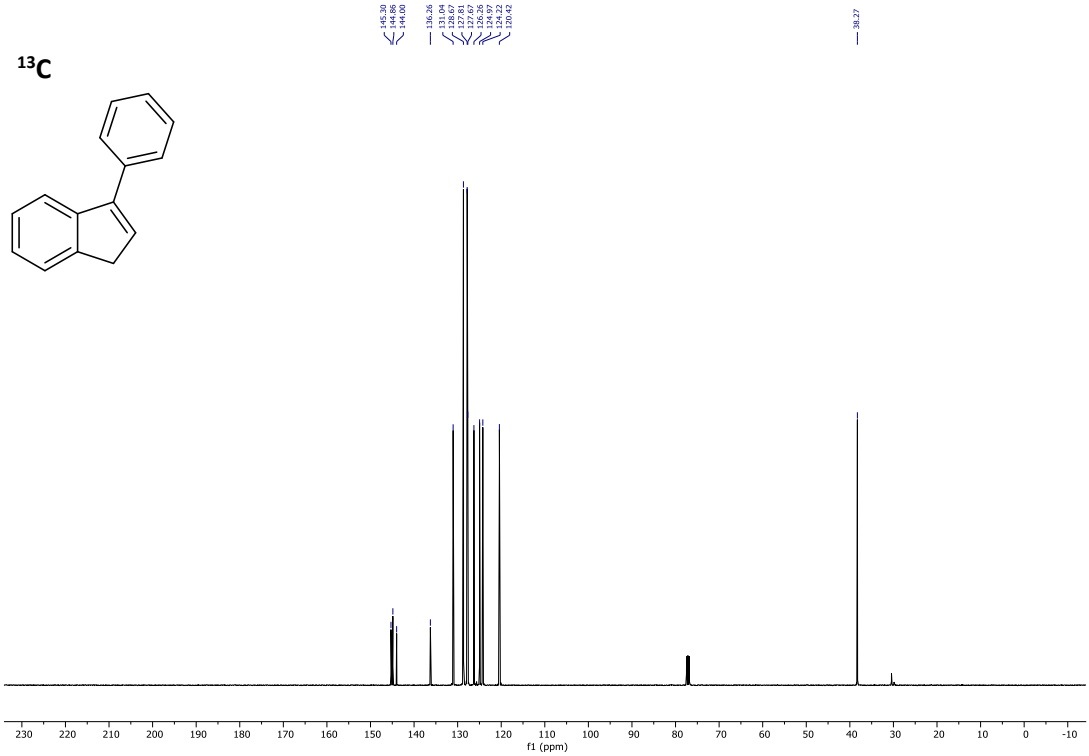
7. NMR Spectra

3-Phenyl-1*H*-indene (1a)

^{1}H

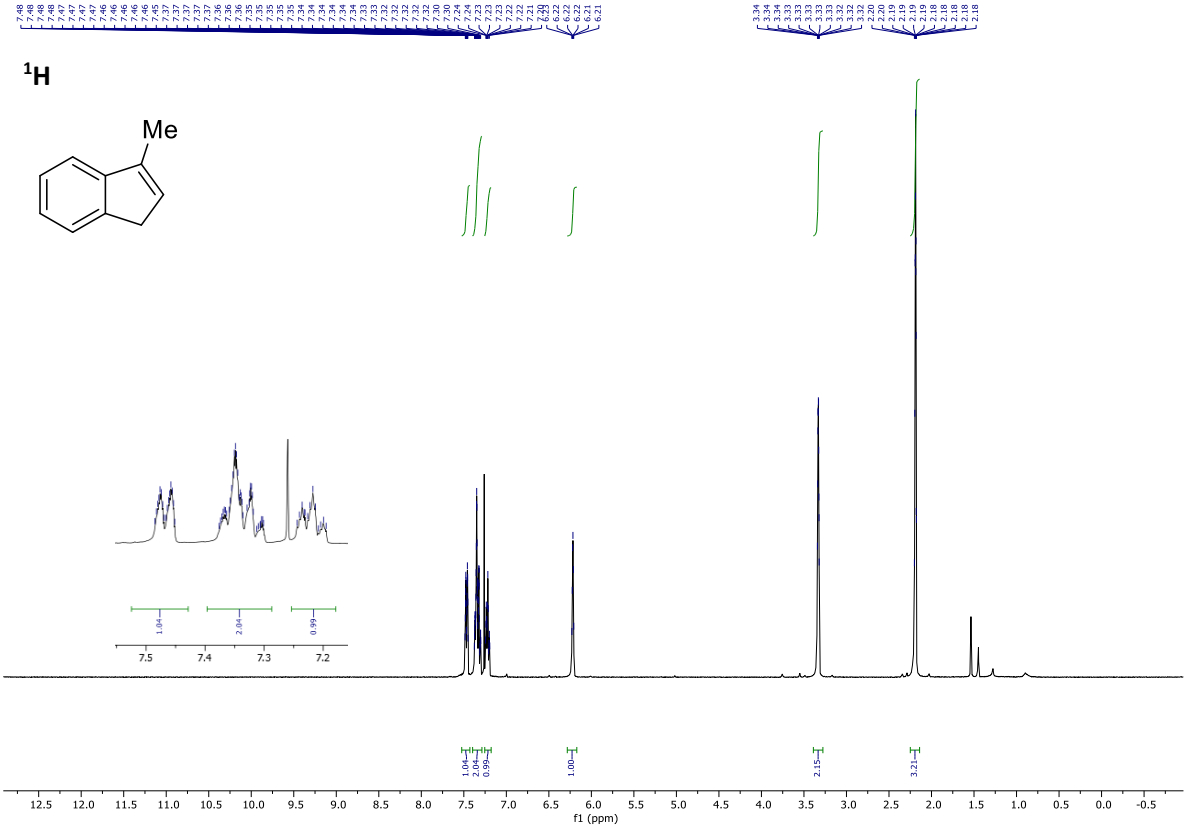


^{13}C

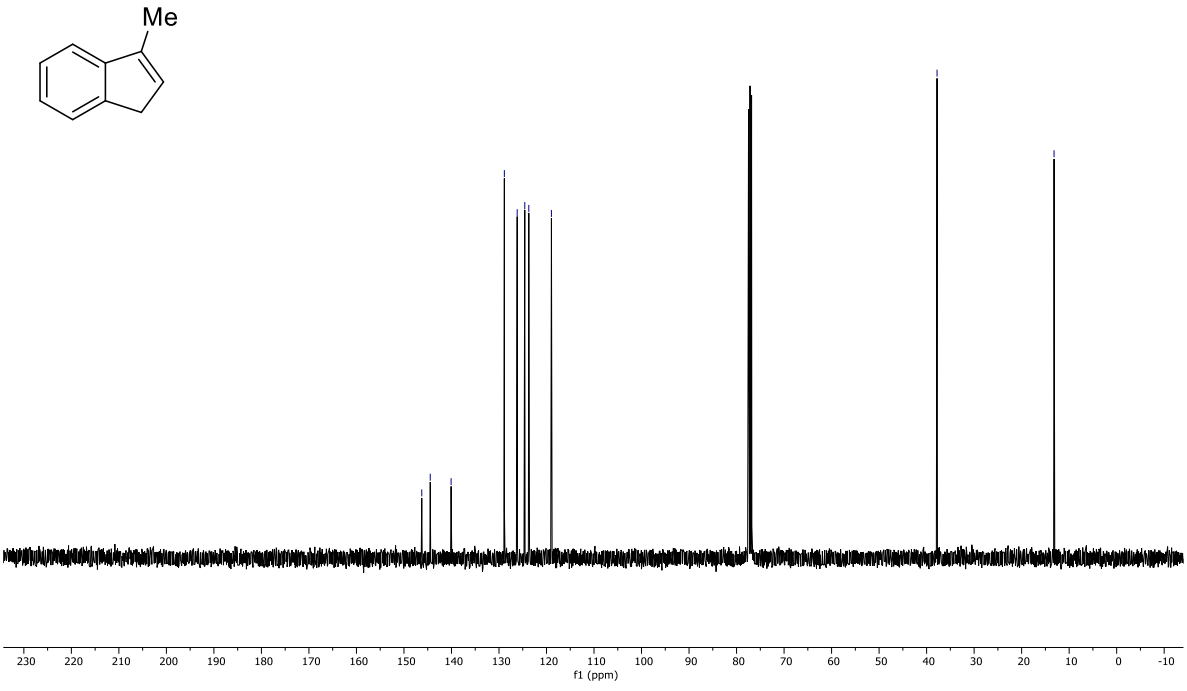


3-Methyl-1*H*-indene (3a)

^{1}H

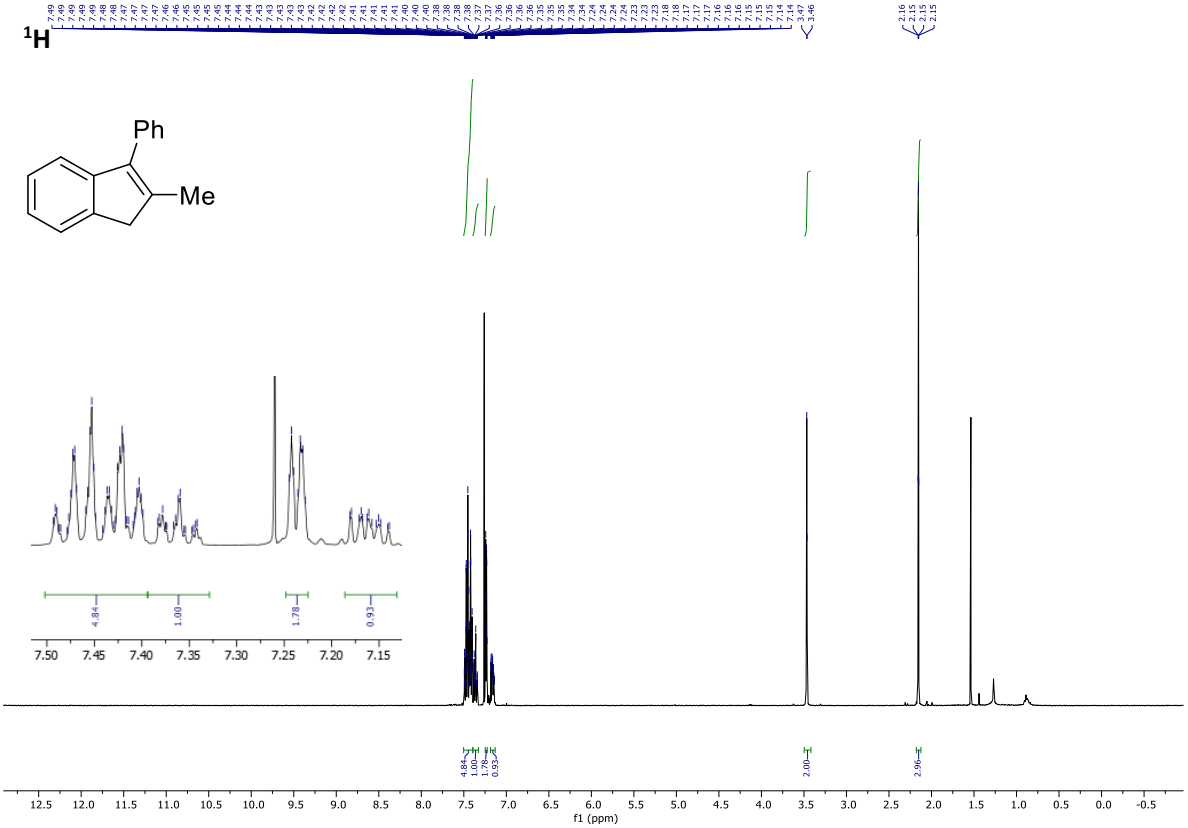


^{13}C

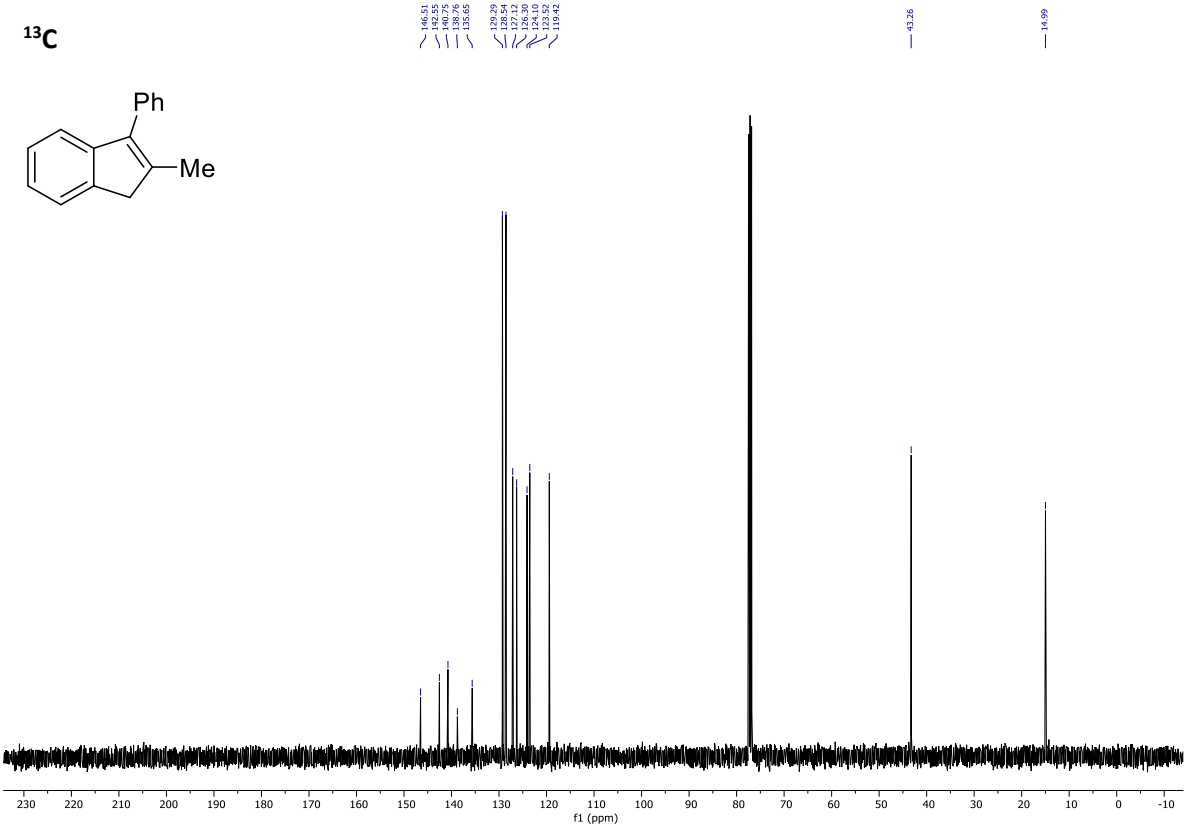


2-Methyl-3-phenyl-1*H*-indene (5a)

^{1}H

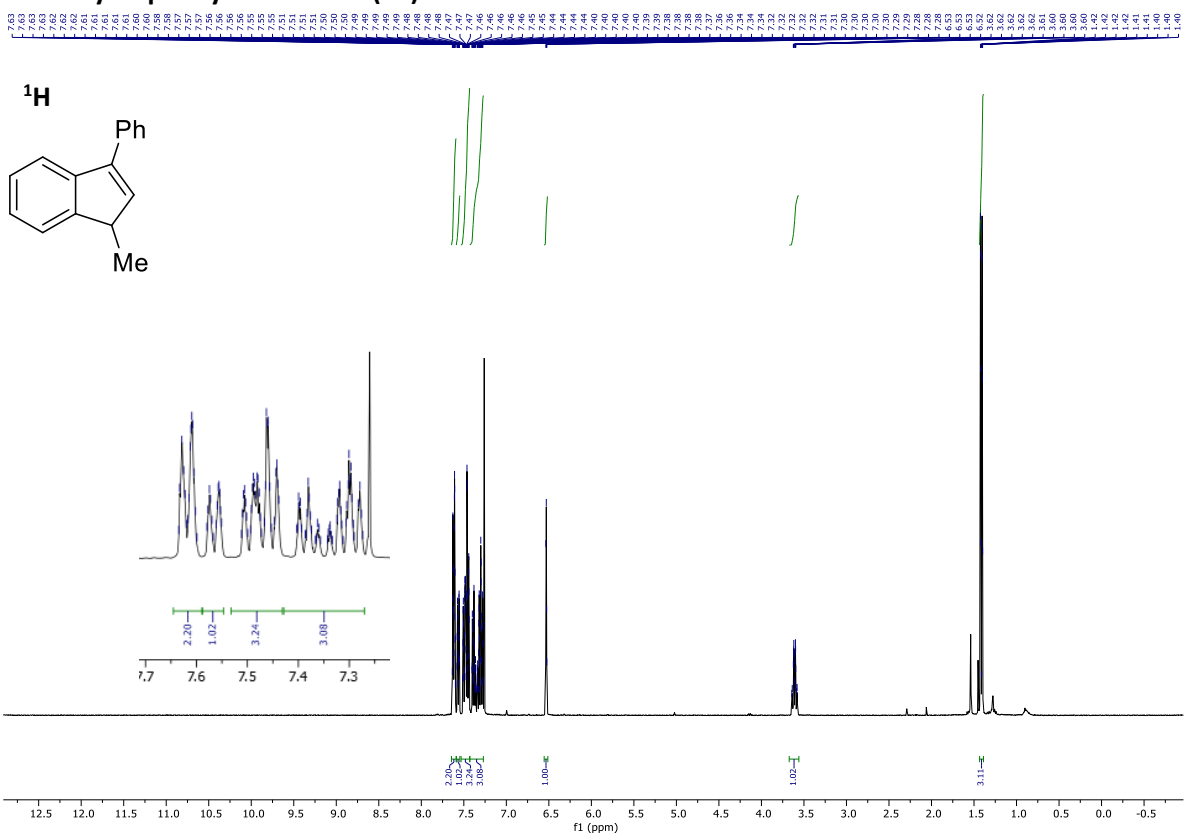


^{13}C

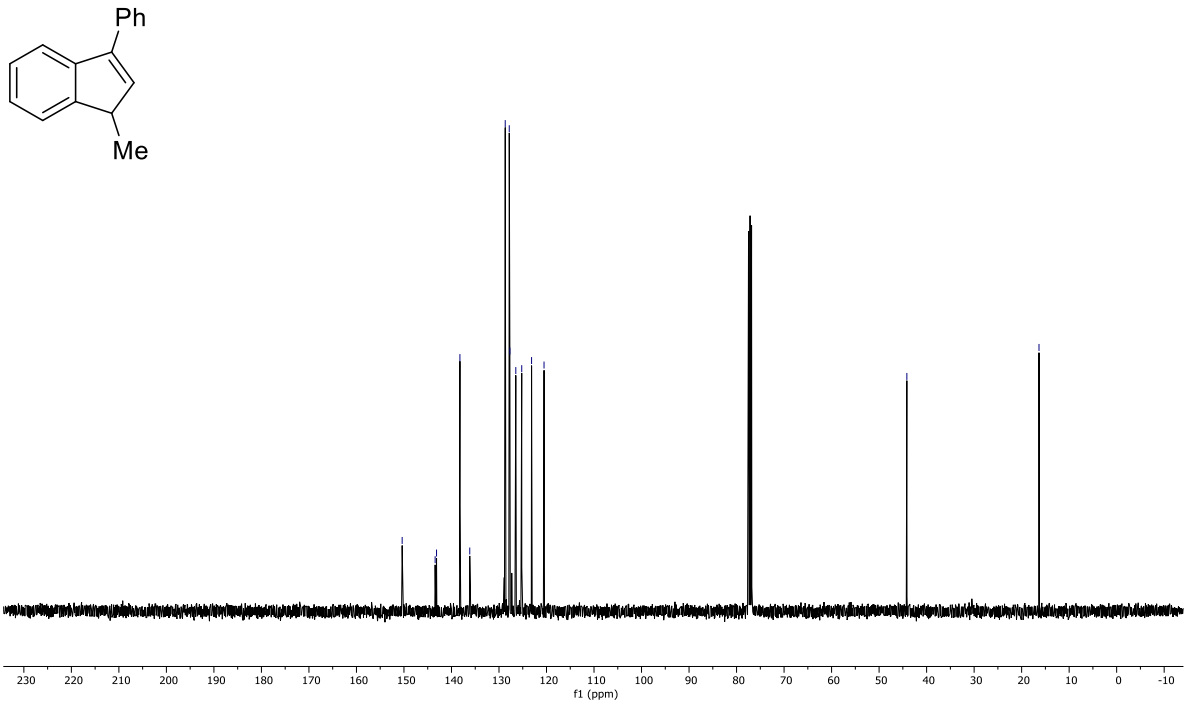


1-Methyl-3-phenyl-1*H*-indene (6a)

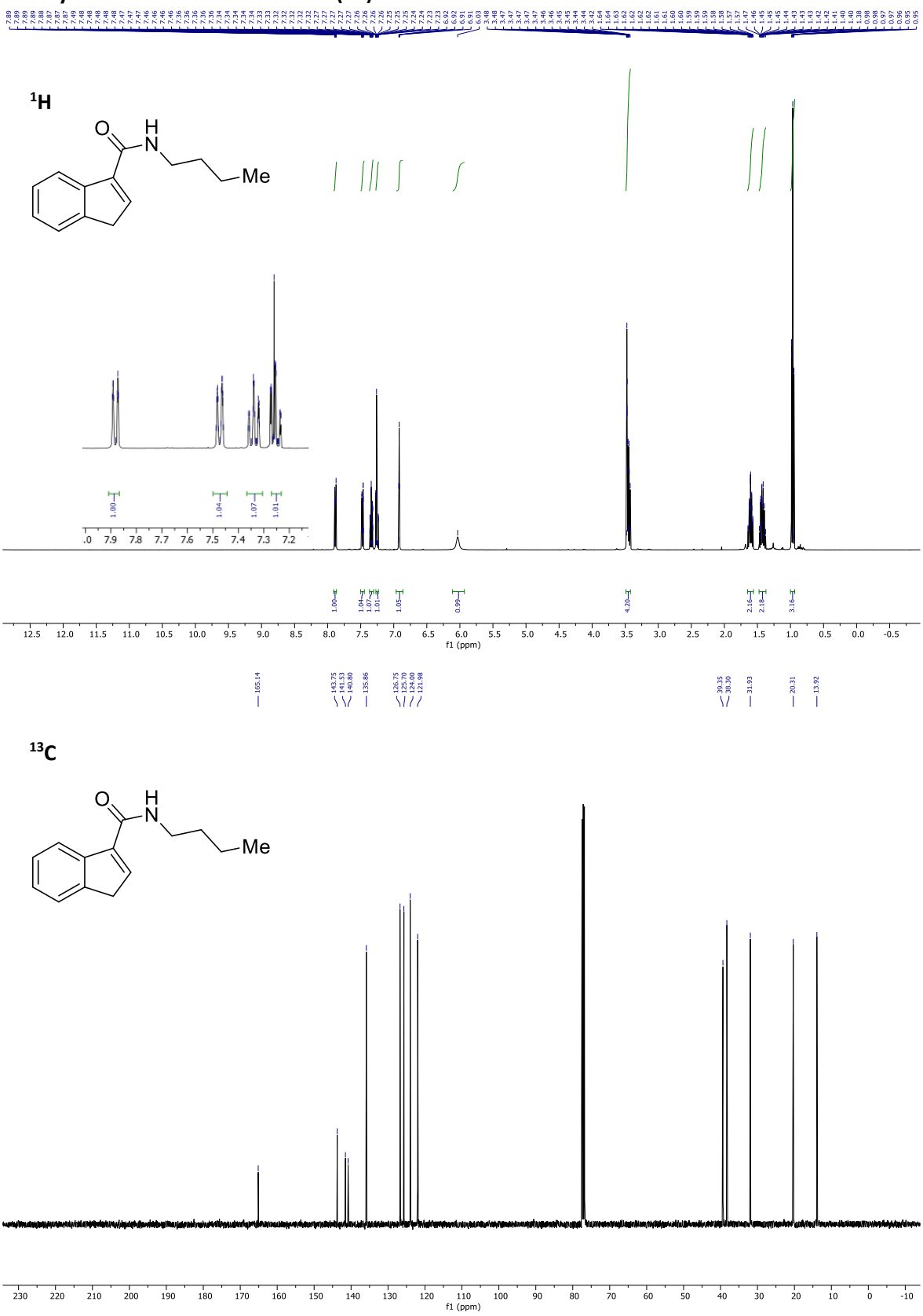
^{1}H



^{13}C

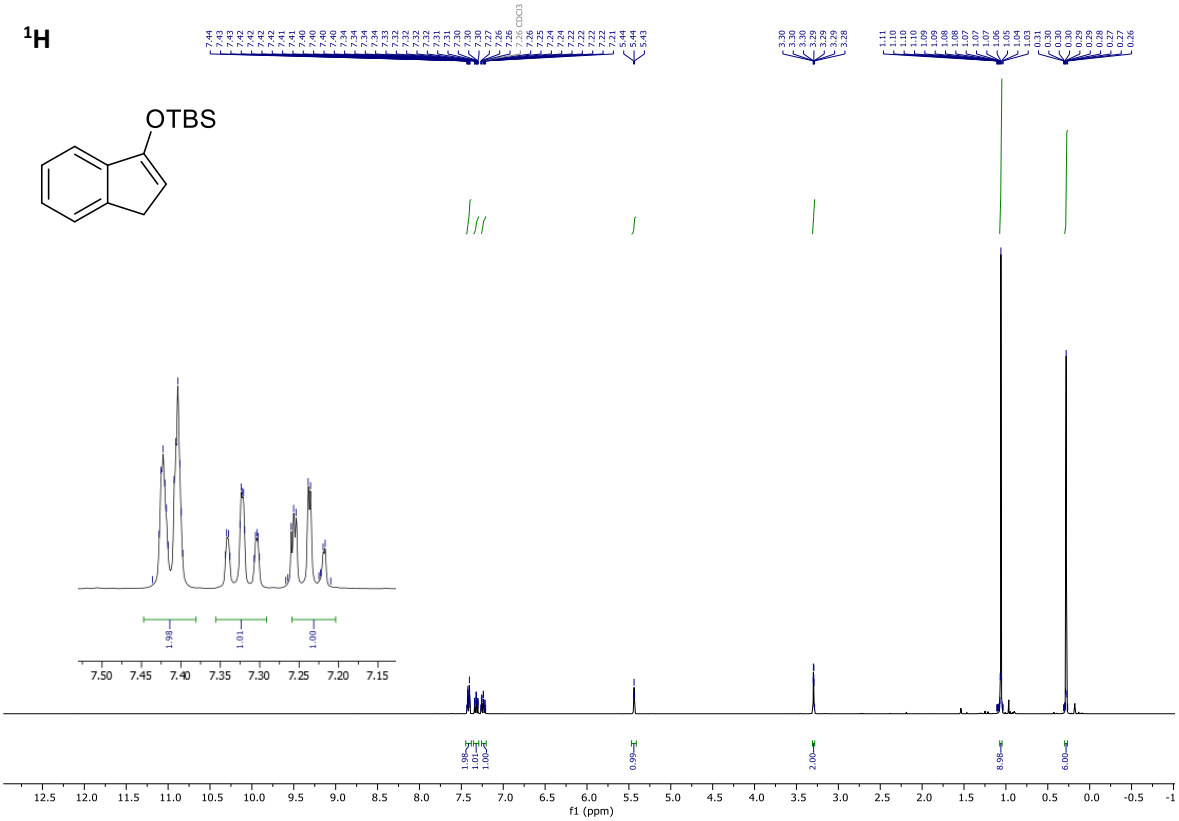


***N*-Butyl-*1H*-indene-3-carboxamide (9a)**

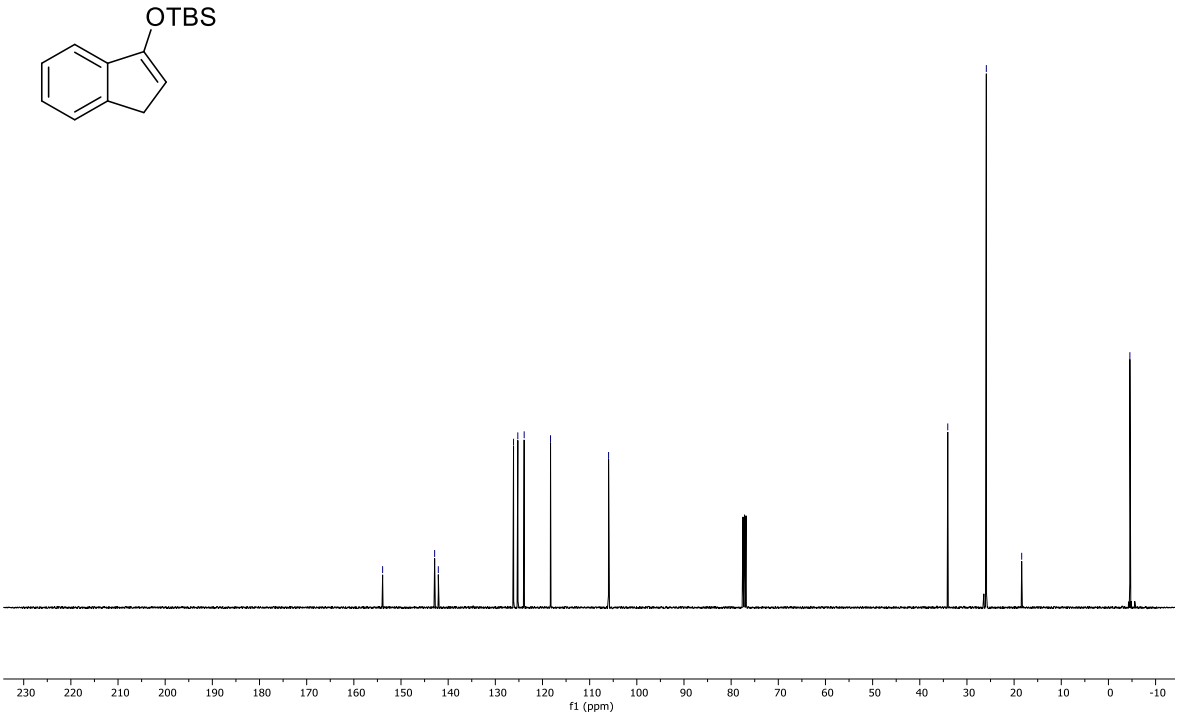


((1*H*-Inden-3-yl)oxy)(tert-butyl)dimethylsilane (10a)

^{1}H

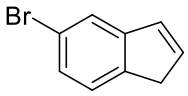


^{13}C

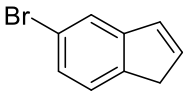


5-Bromo-1*H*-indene (11a)

^{1}H

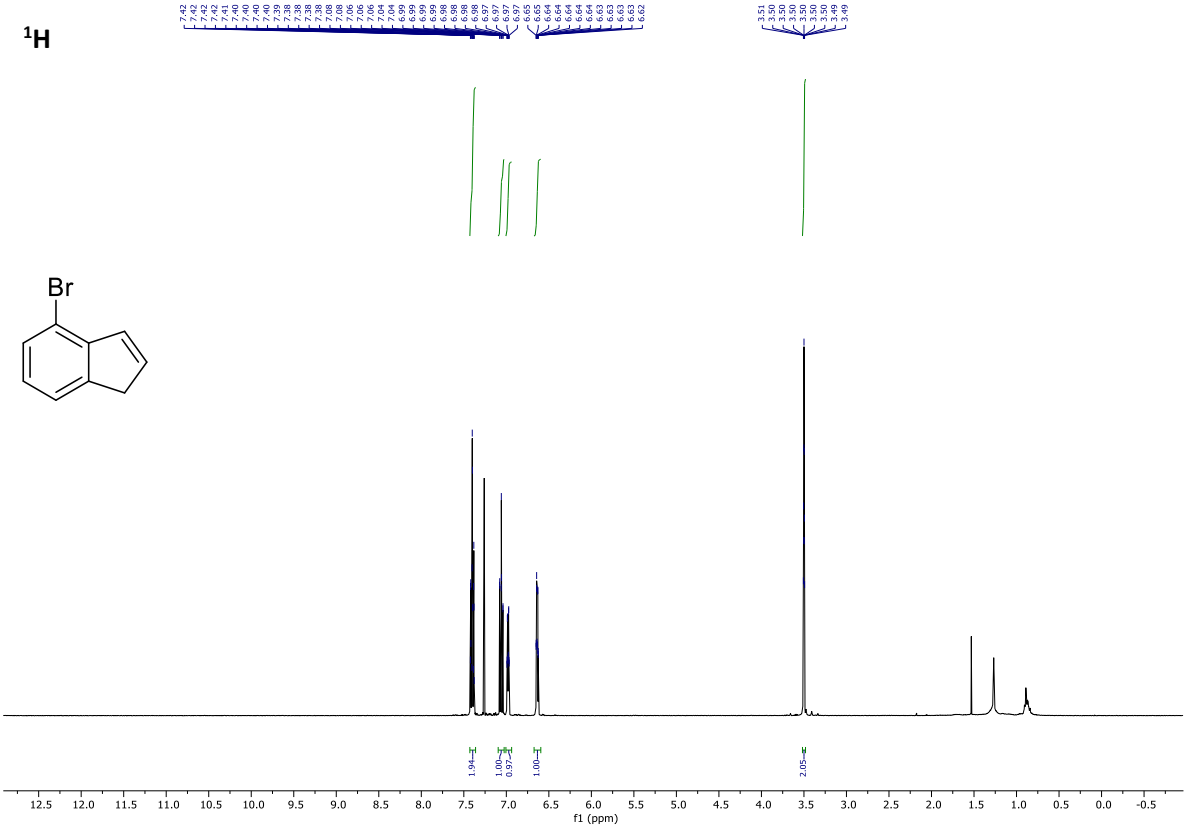


^{13}C

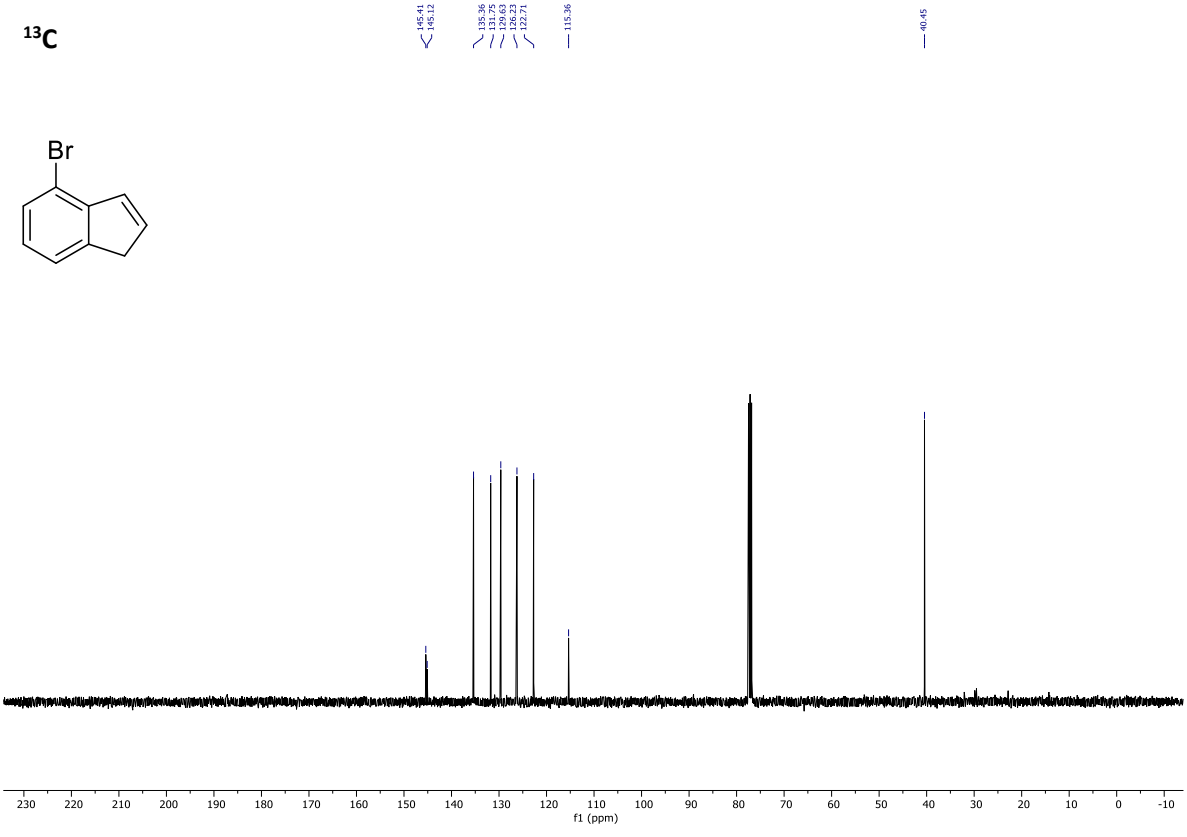


4-Bromo-1*H*-indene (13a)

^{1}H

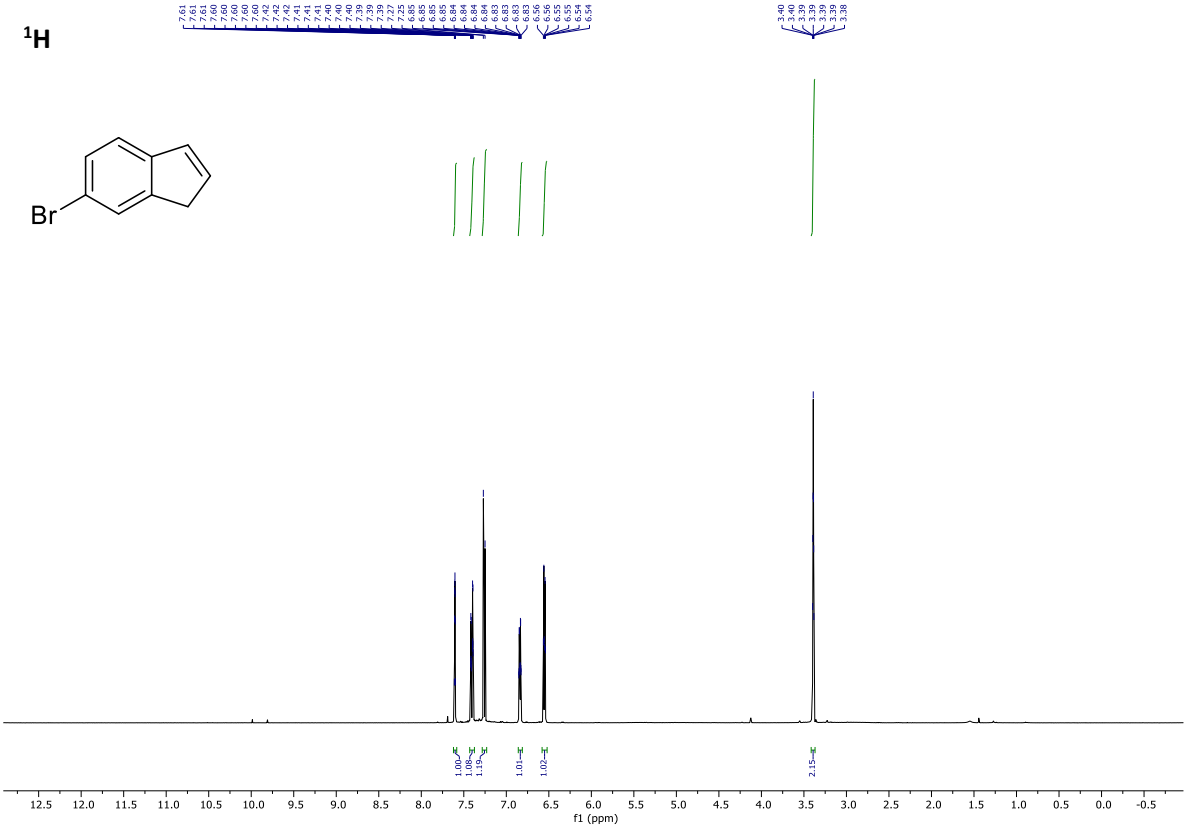


^{13}C

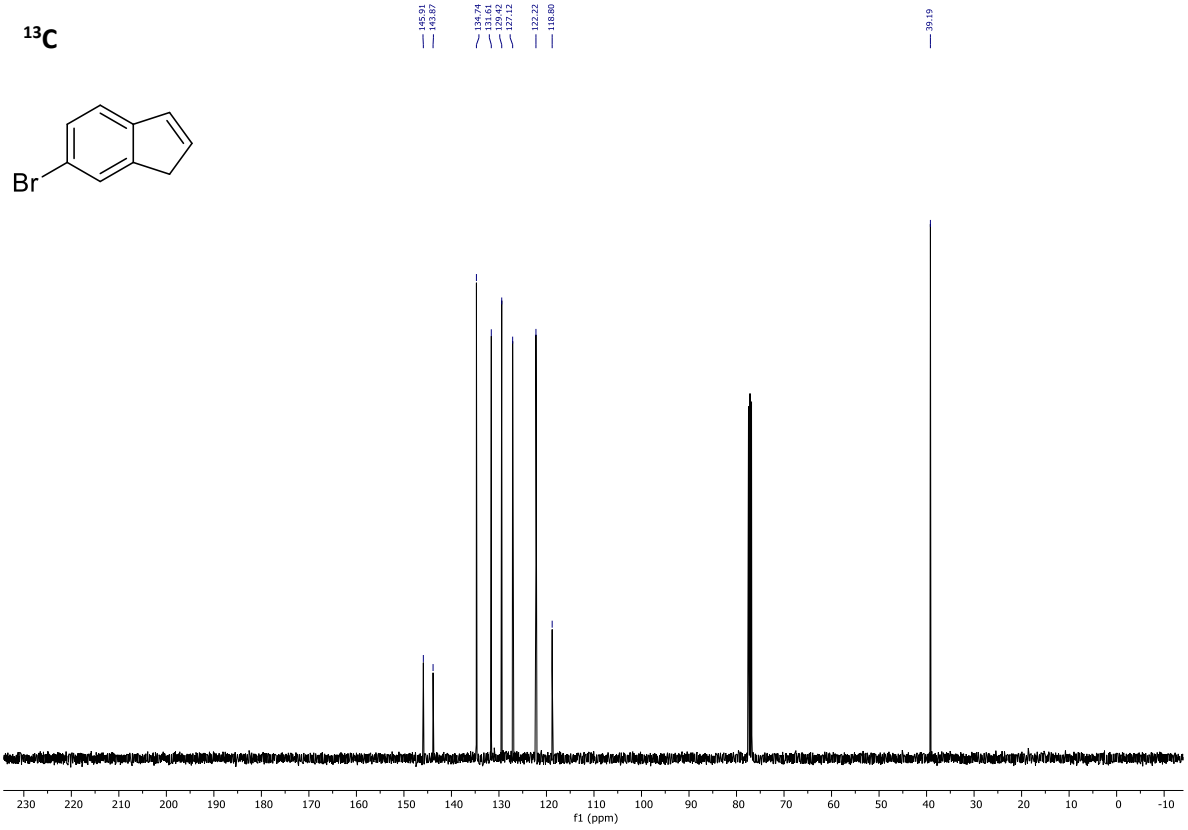


6-Bromo-1*H*-indene (14a)

^{1}H

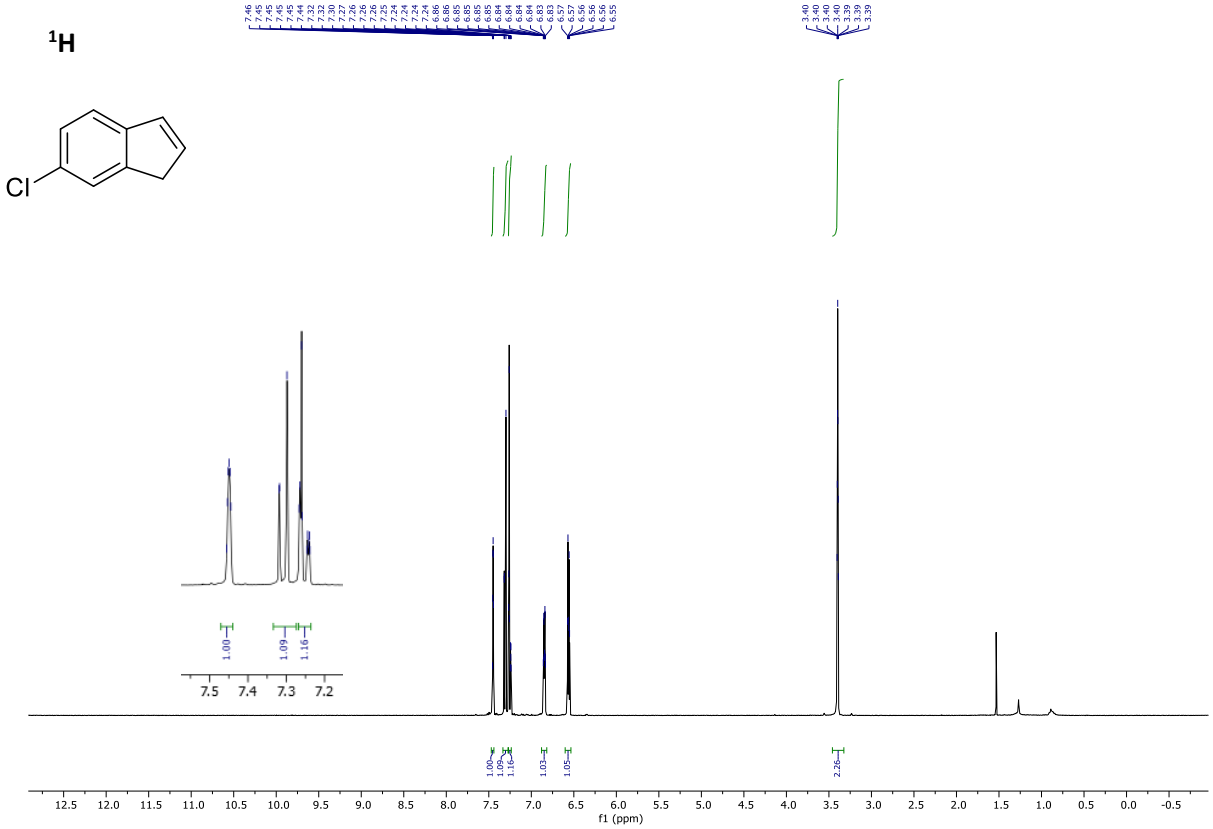


^{13}C

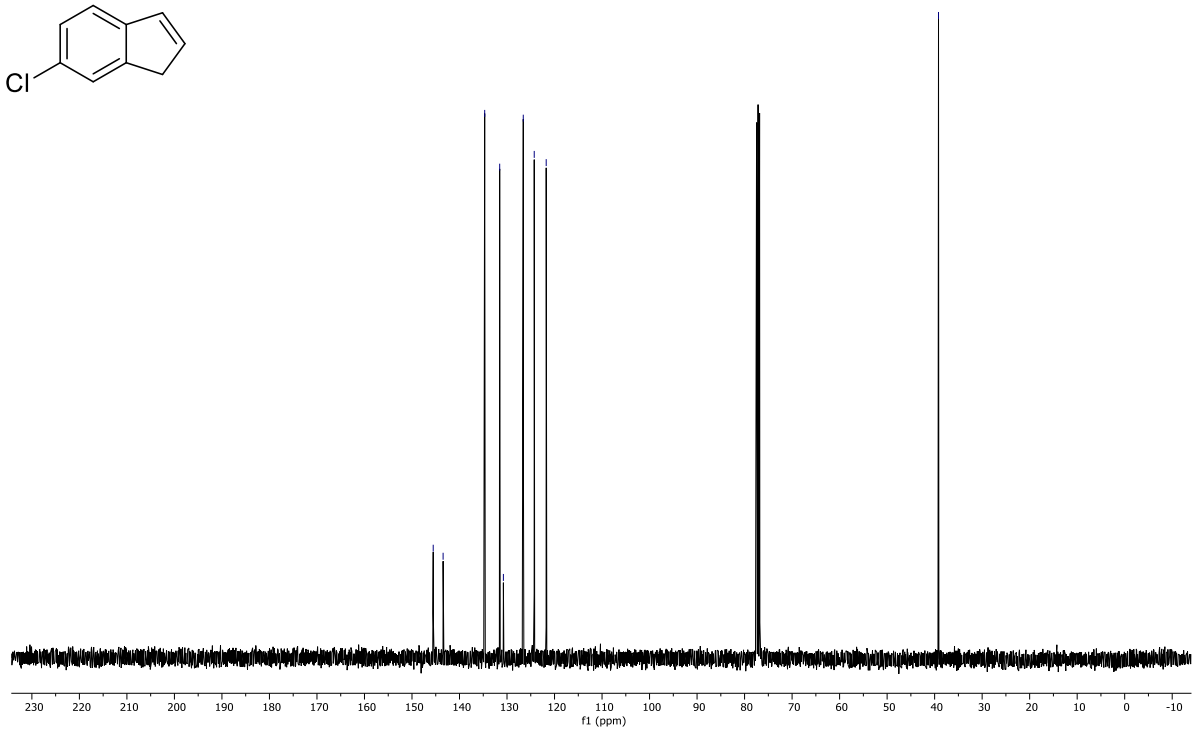


6-Chloro-1*H*-indene (15a)

^{1}H

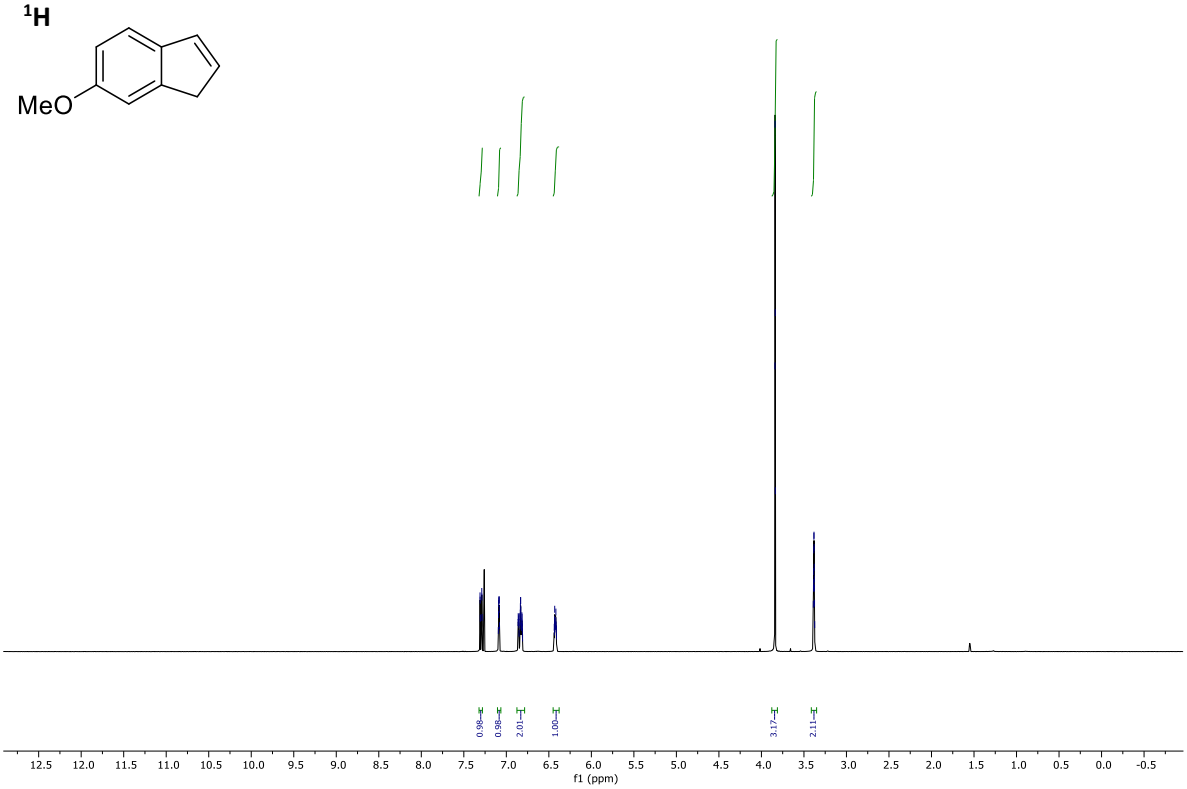


^{13}C

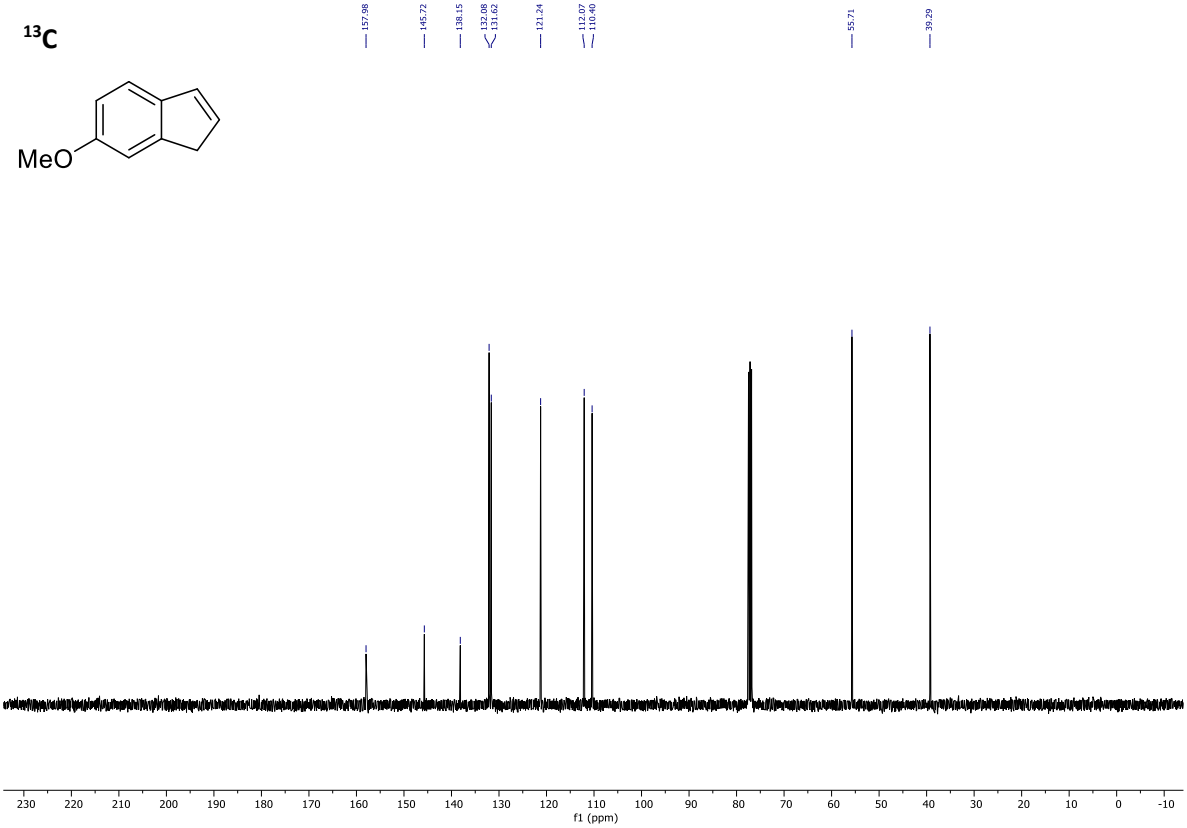


6-Methoxy-1*H*-indene (16a)

^{1}H

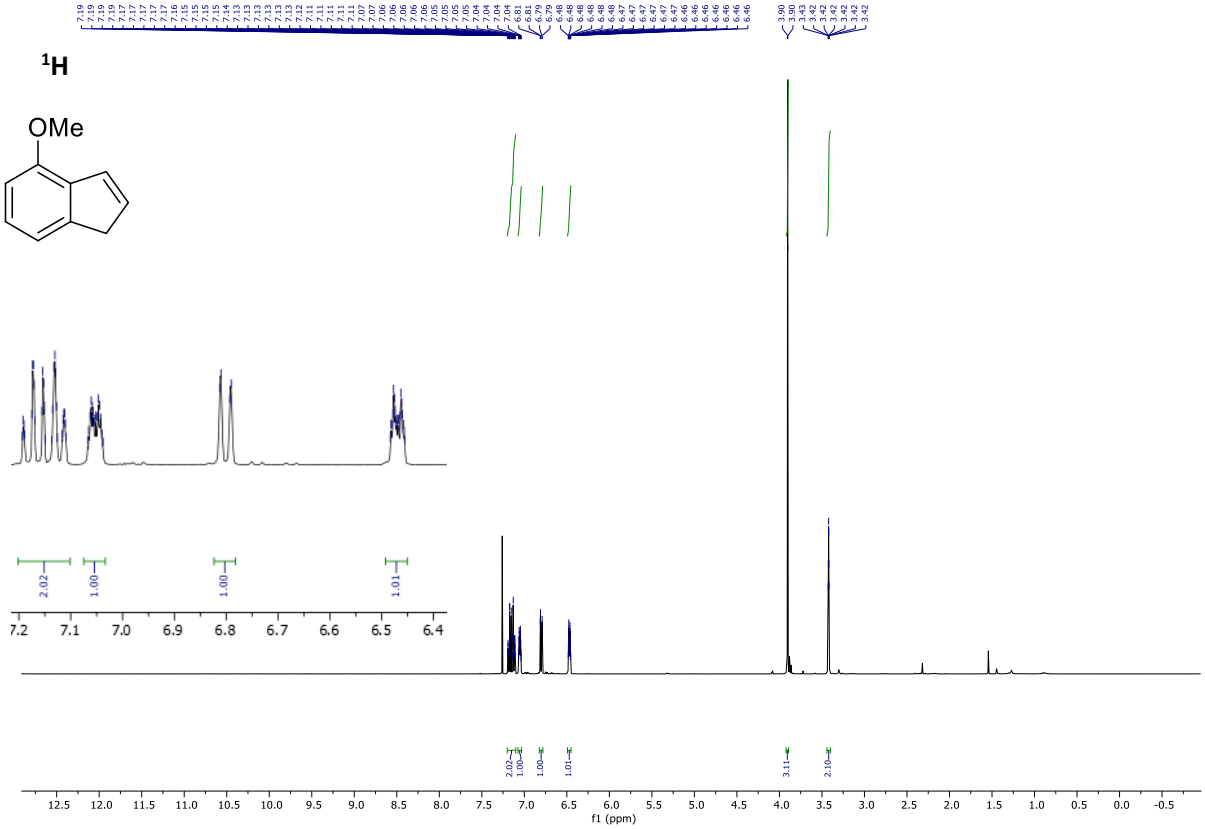


^{13}C

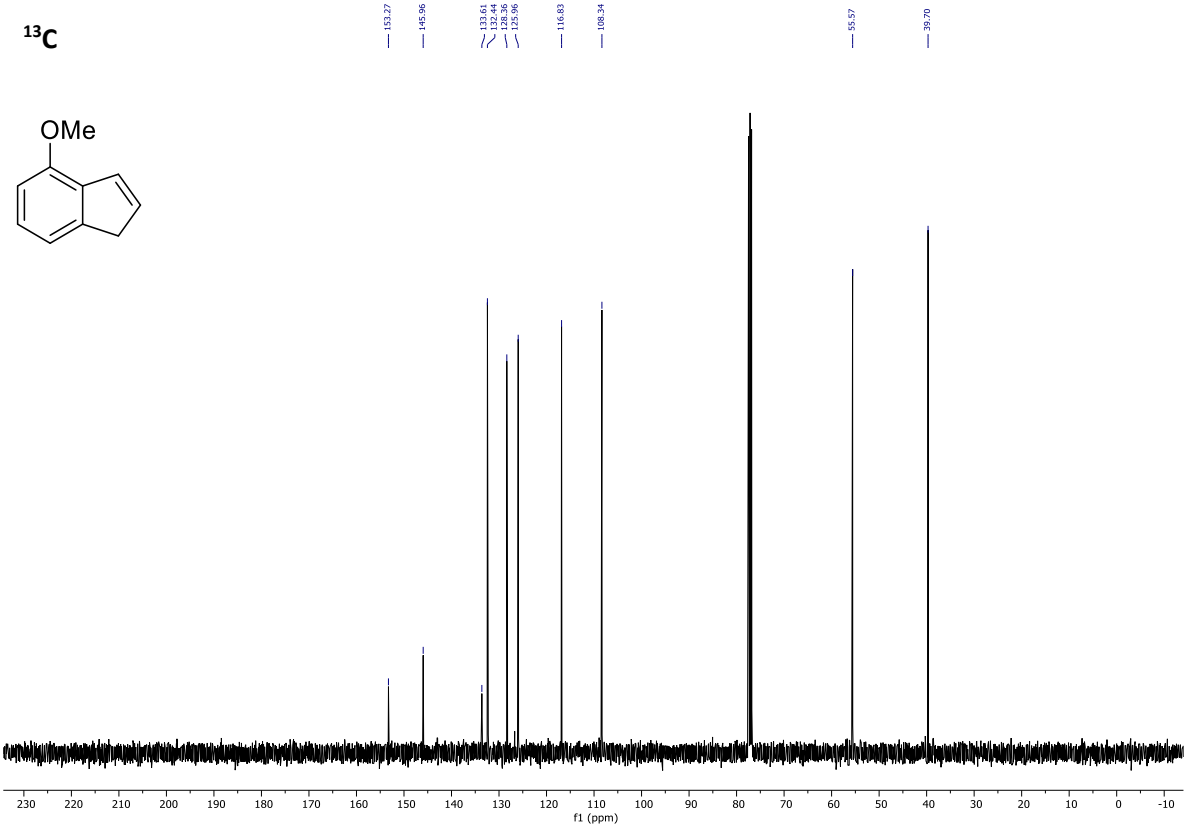


4-Methoxy-1*H*-indene (17a)

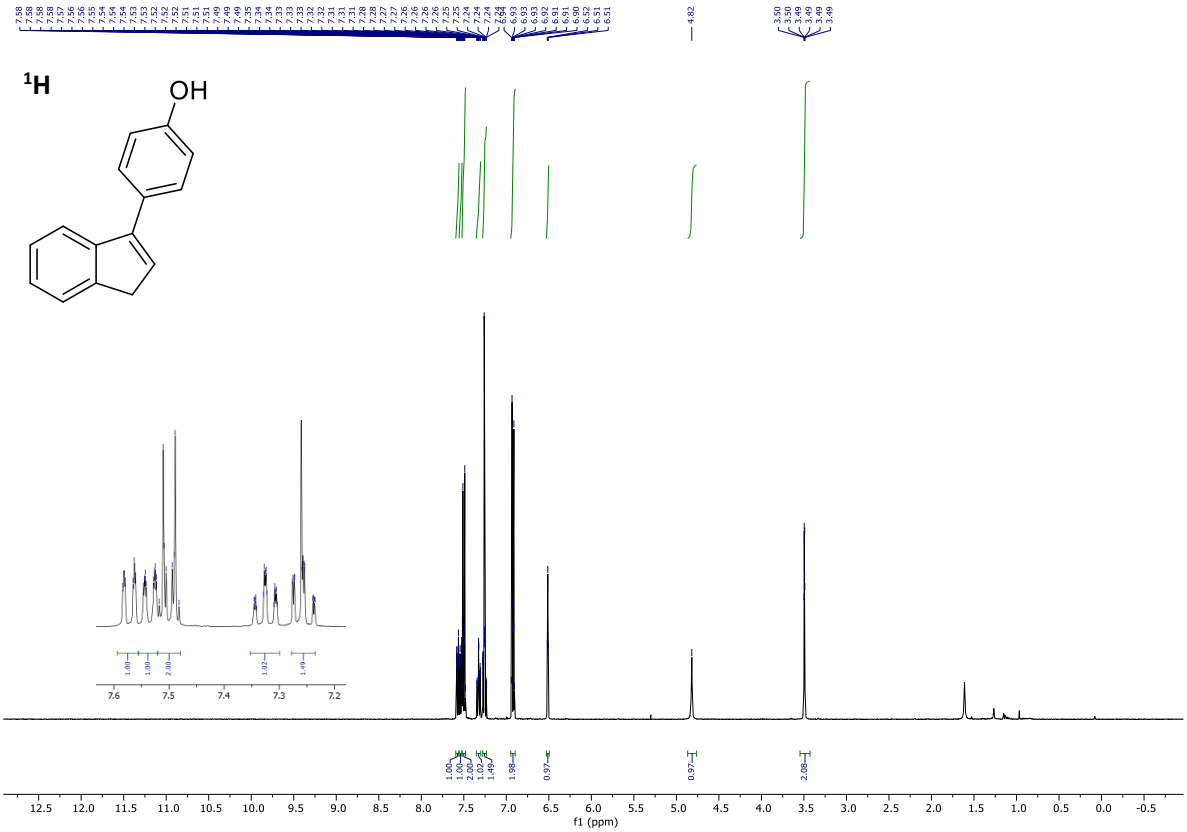
^{1}H

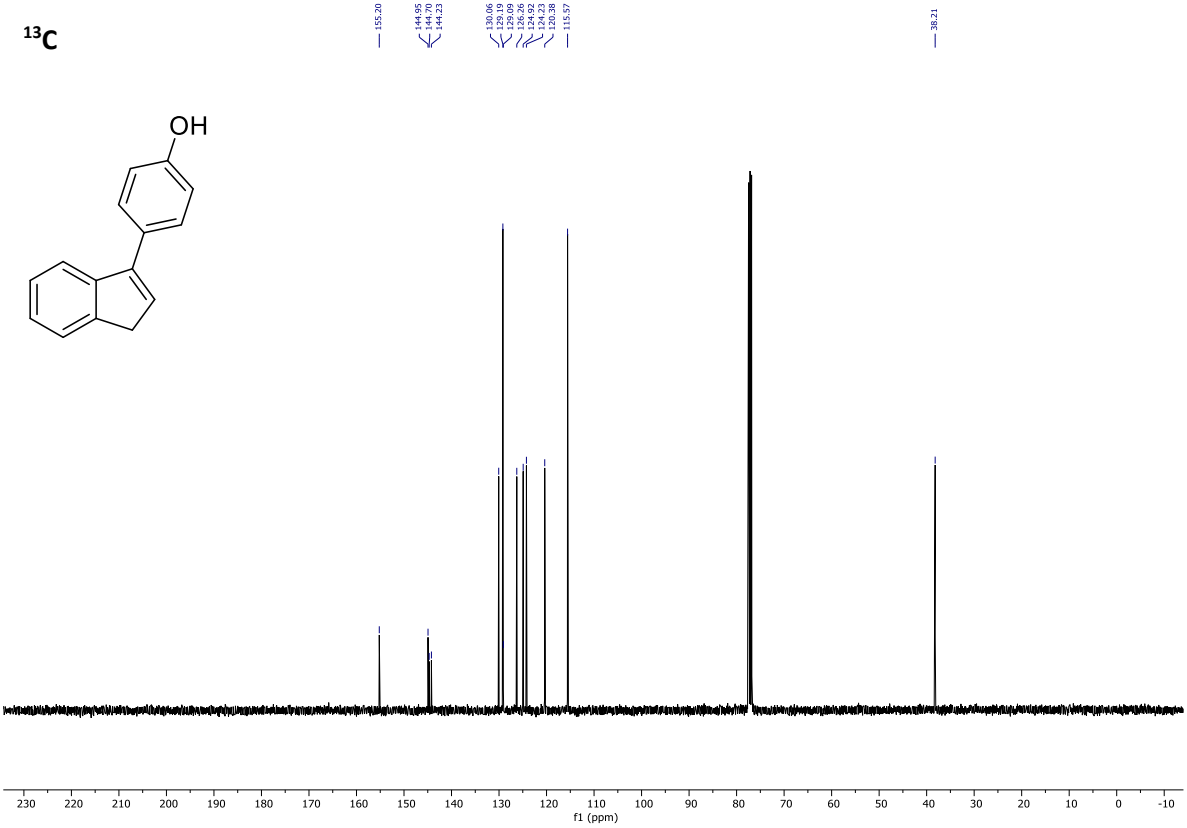


^{13}C

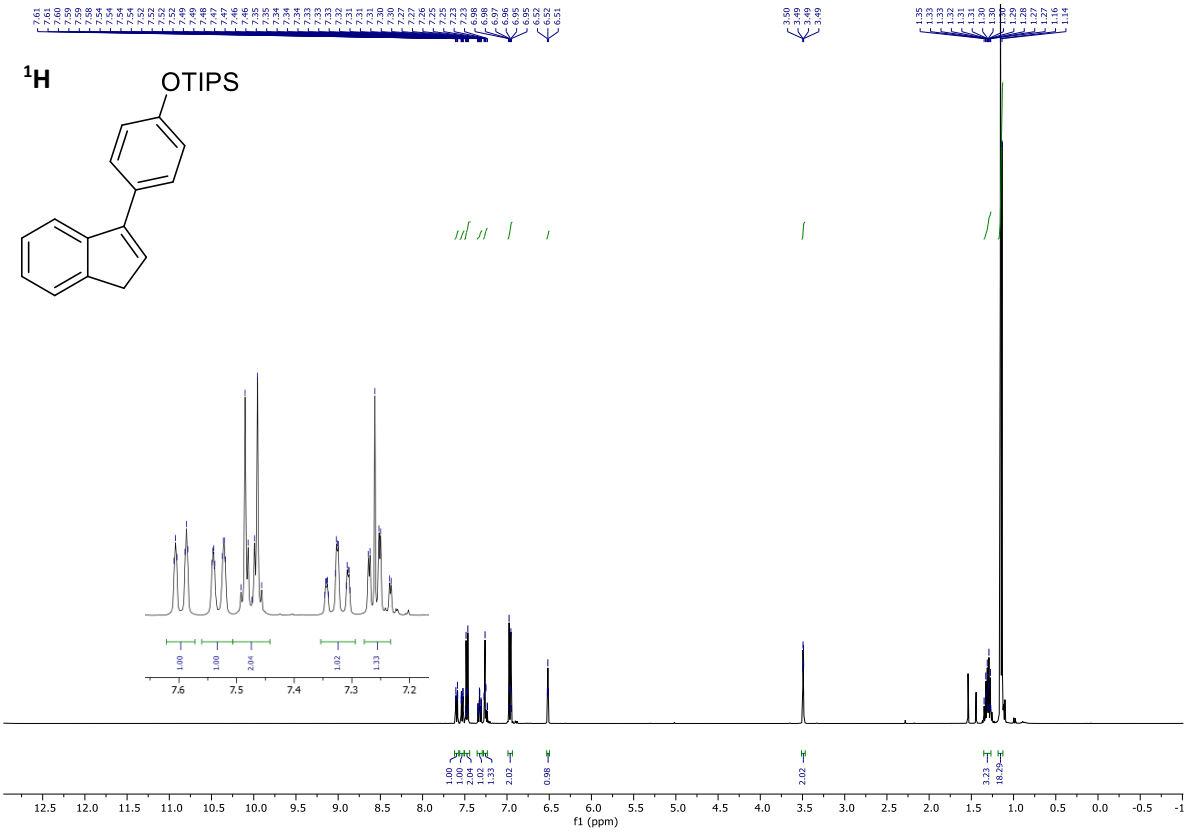


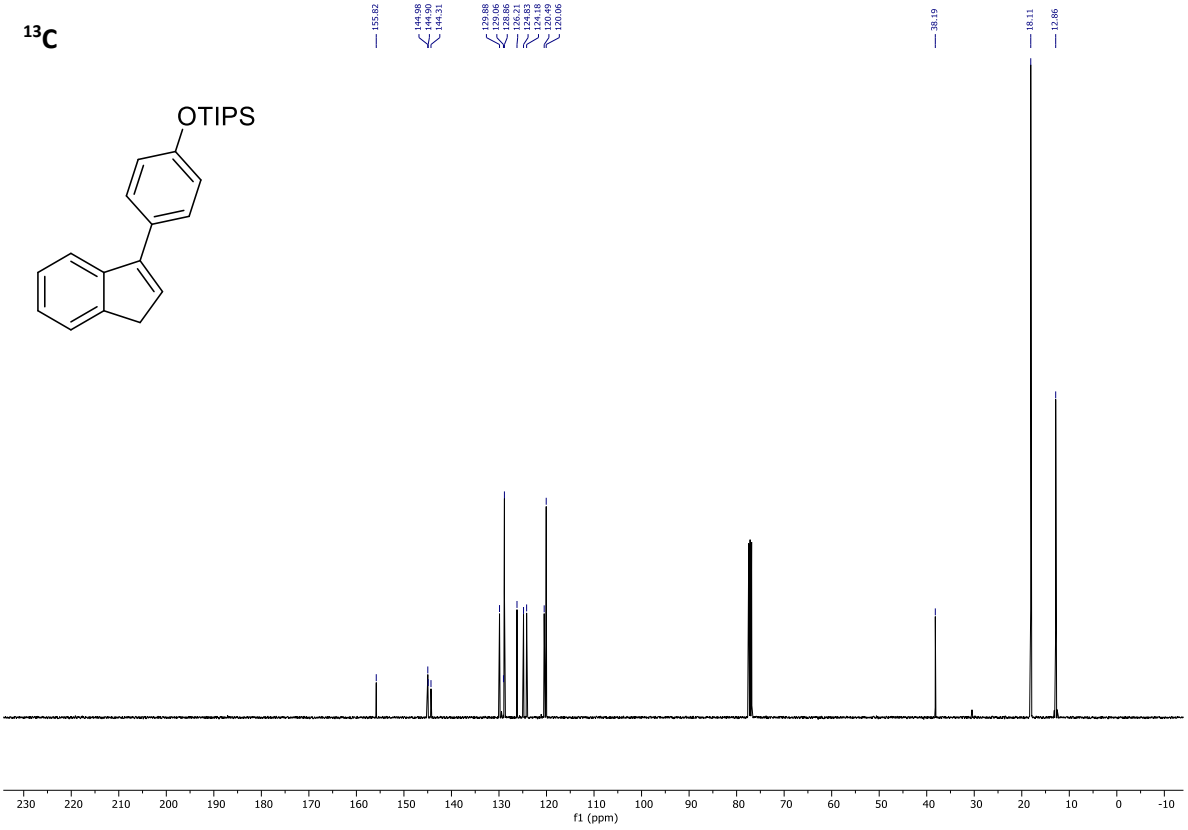
4-(1*H*-inden-3-yl)phenol (18a)



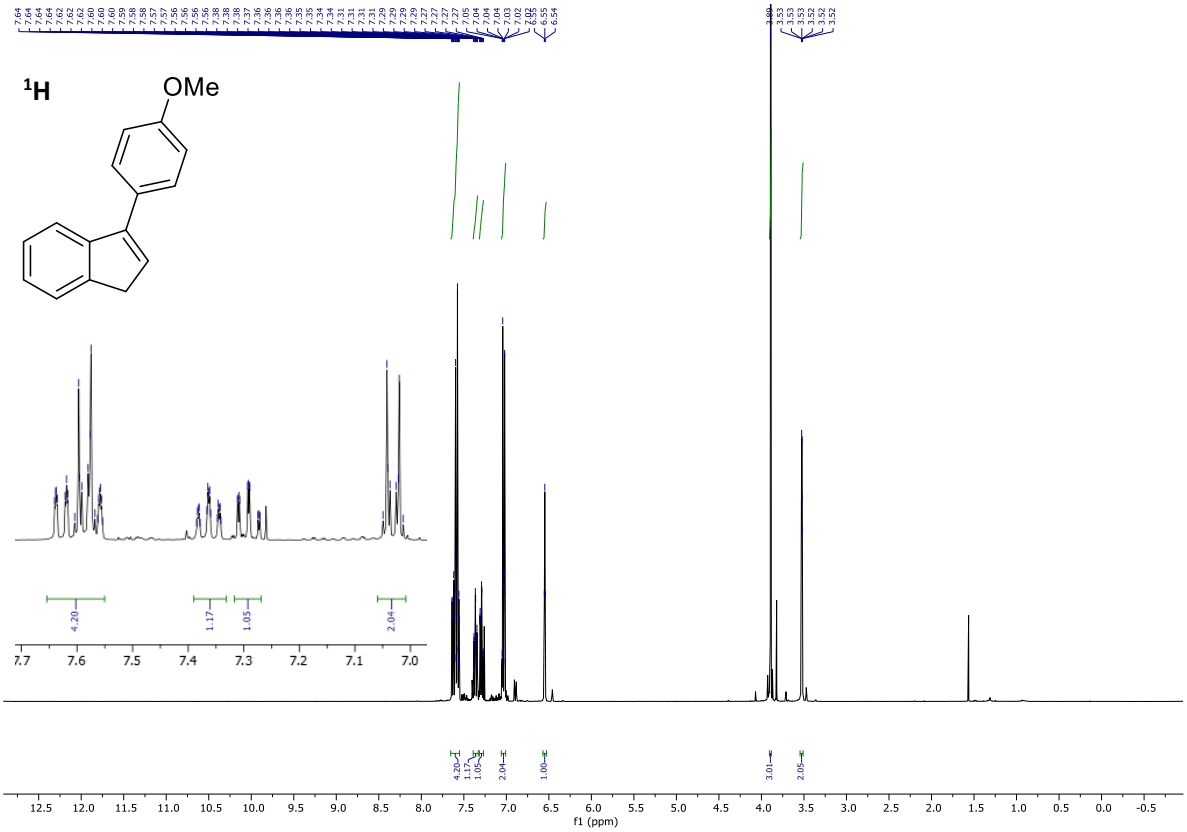


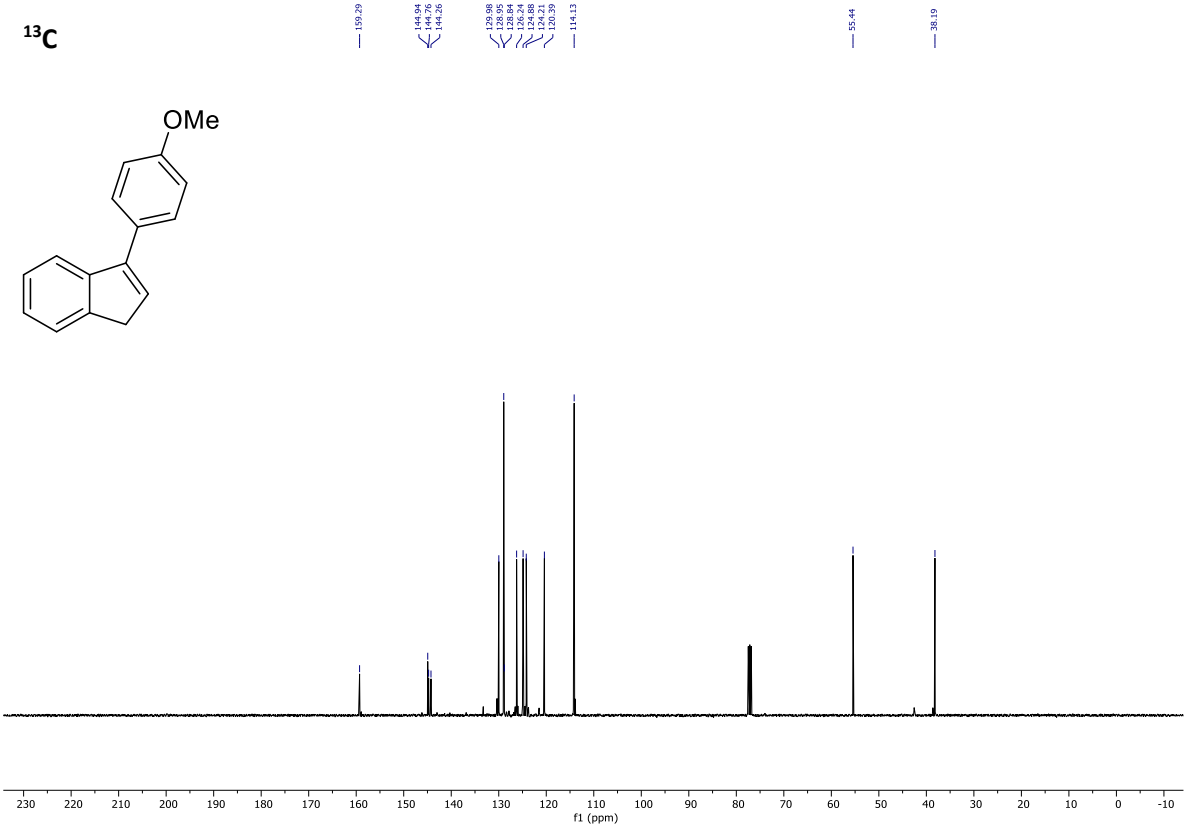
(4-(1*H*-inden-3-yl)phenoxy)triisopropylsilane (19a)





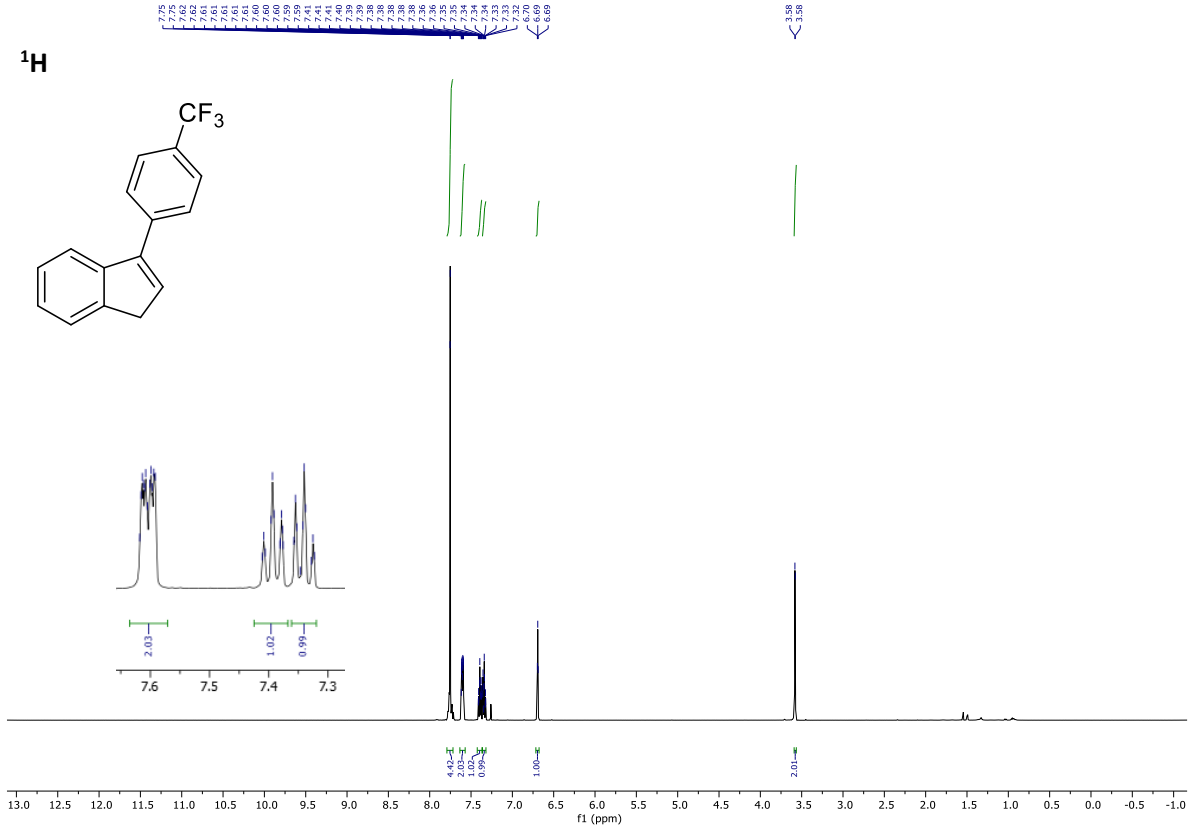
3-(4-Methoxyphenyl)-1*H*-indene (20a)



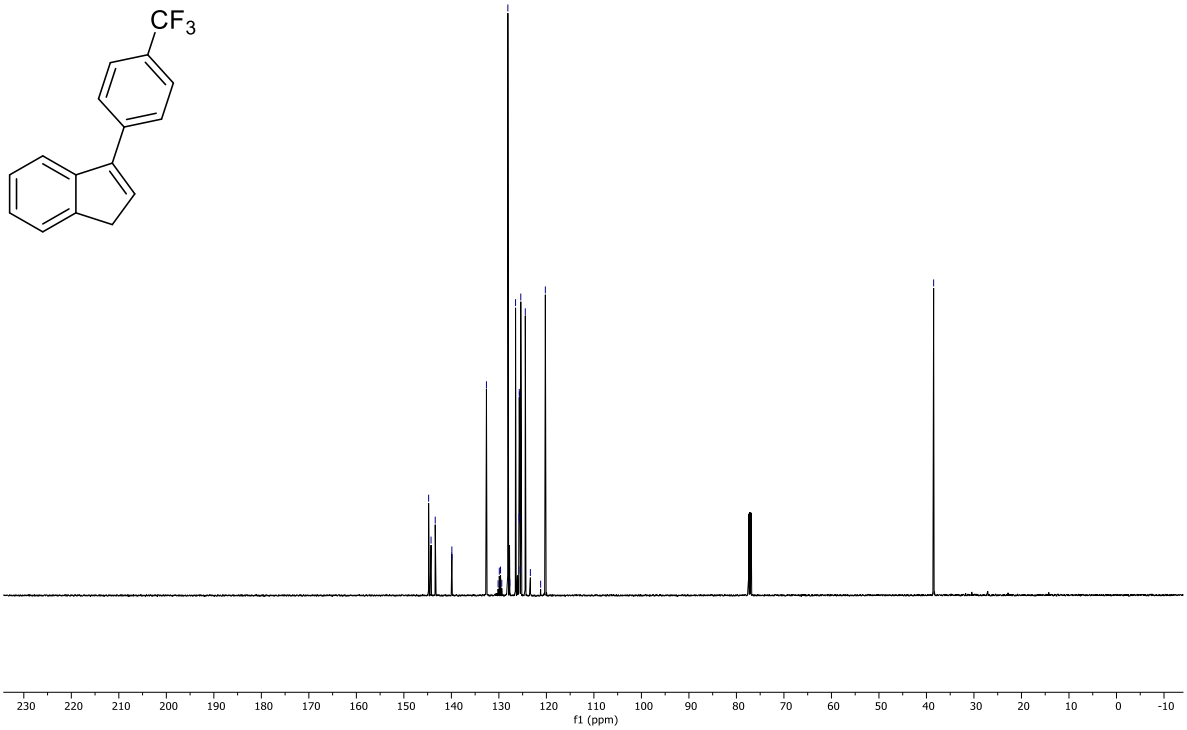


3-(4-(Trifluoromethyl)phenyl)-1*H*-indene (21a)

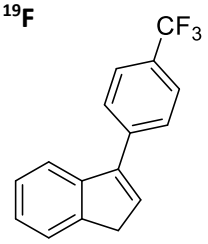
^{1}H



^{13}C



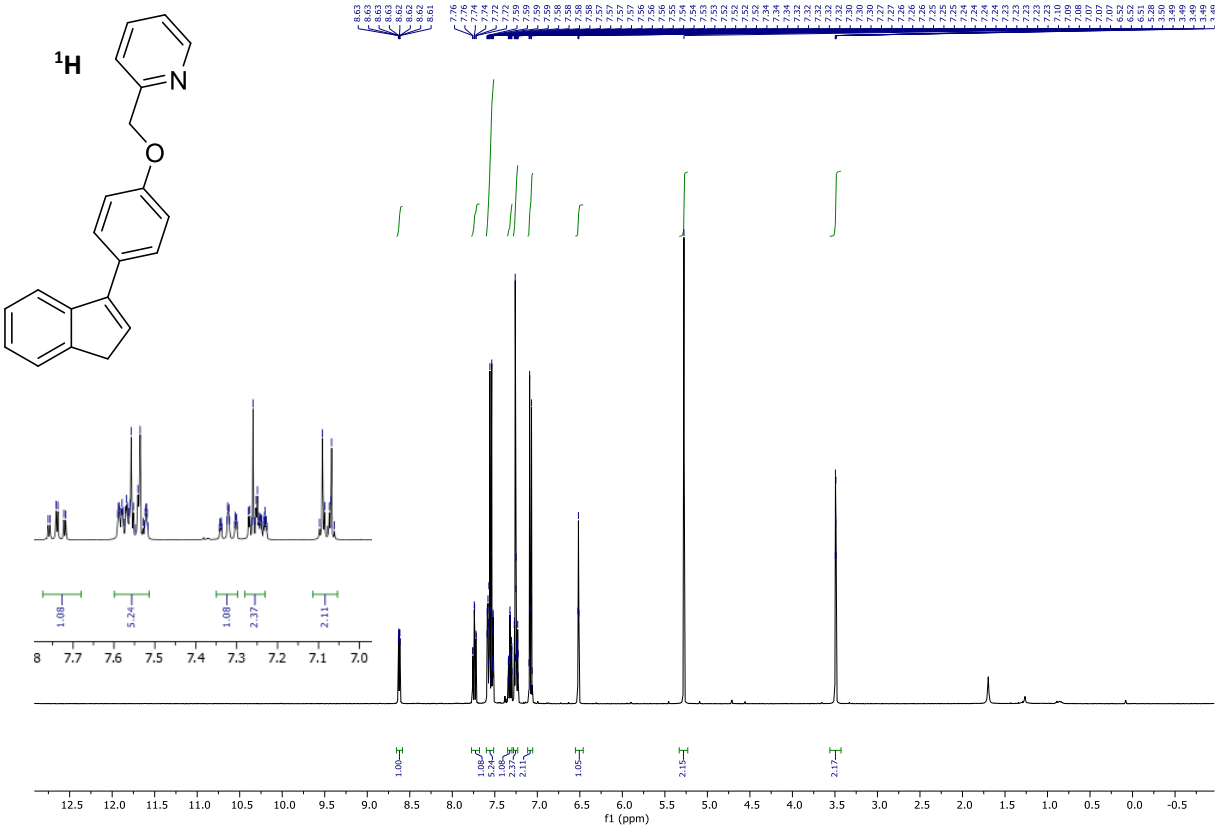
^{19}F


CF3

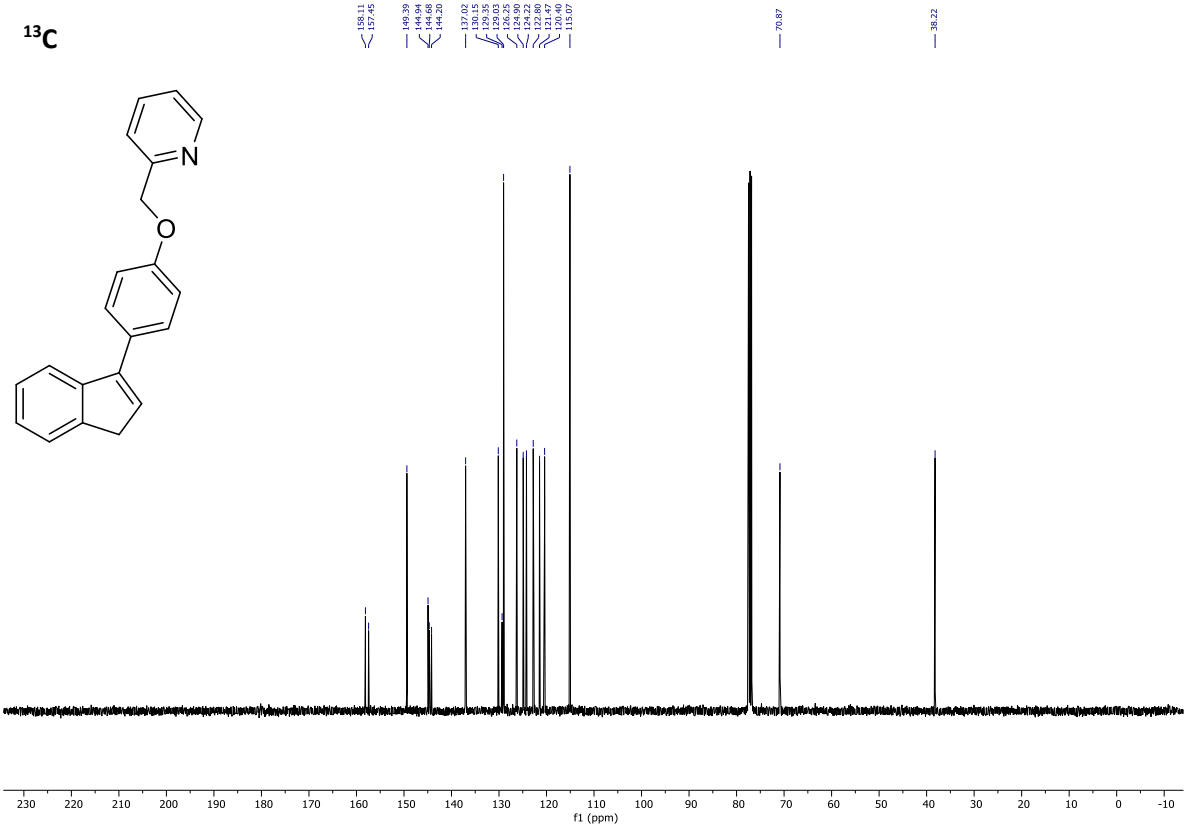
-62.45
-62.46
50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)

2-((4-(1*H*-inden-3-yl)phenoxy)methyl)pyridine (22a)

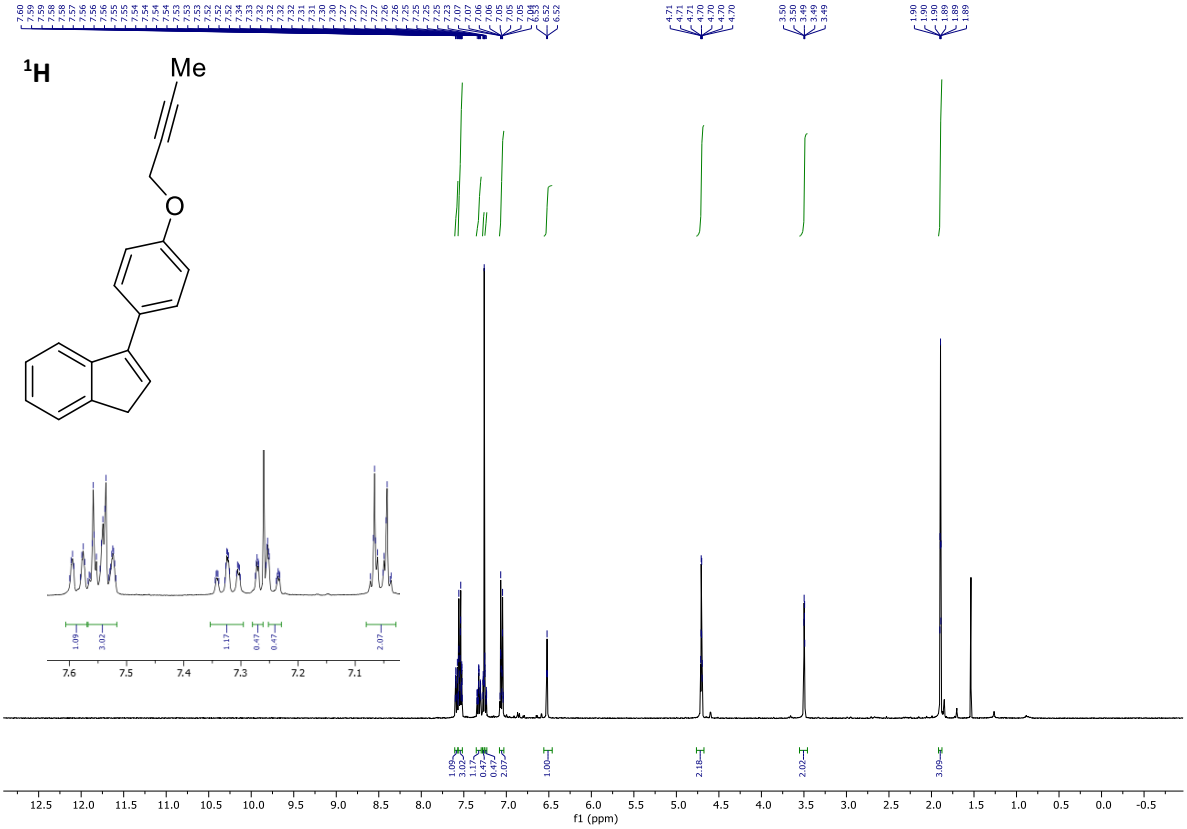
^{1}H

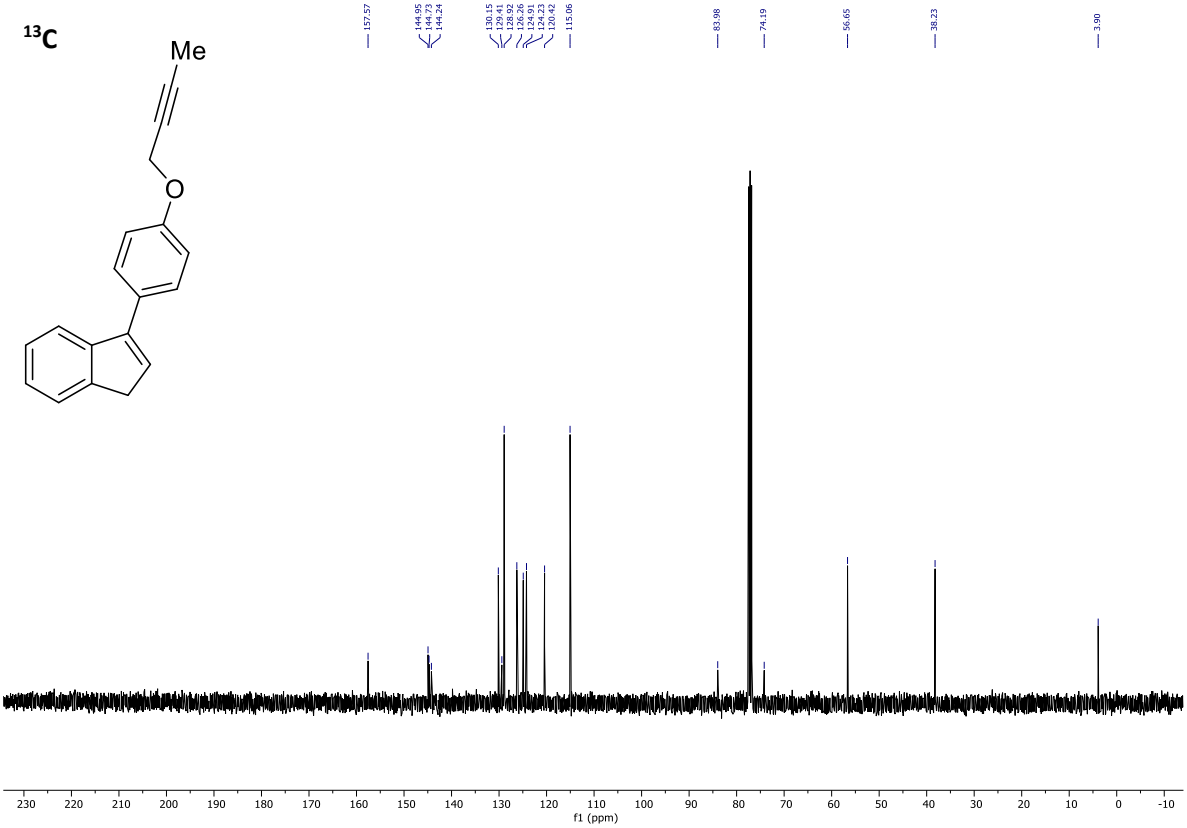


^{13}C

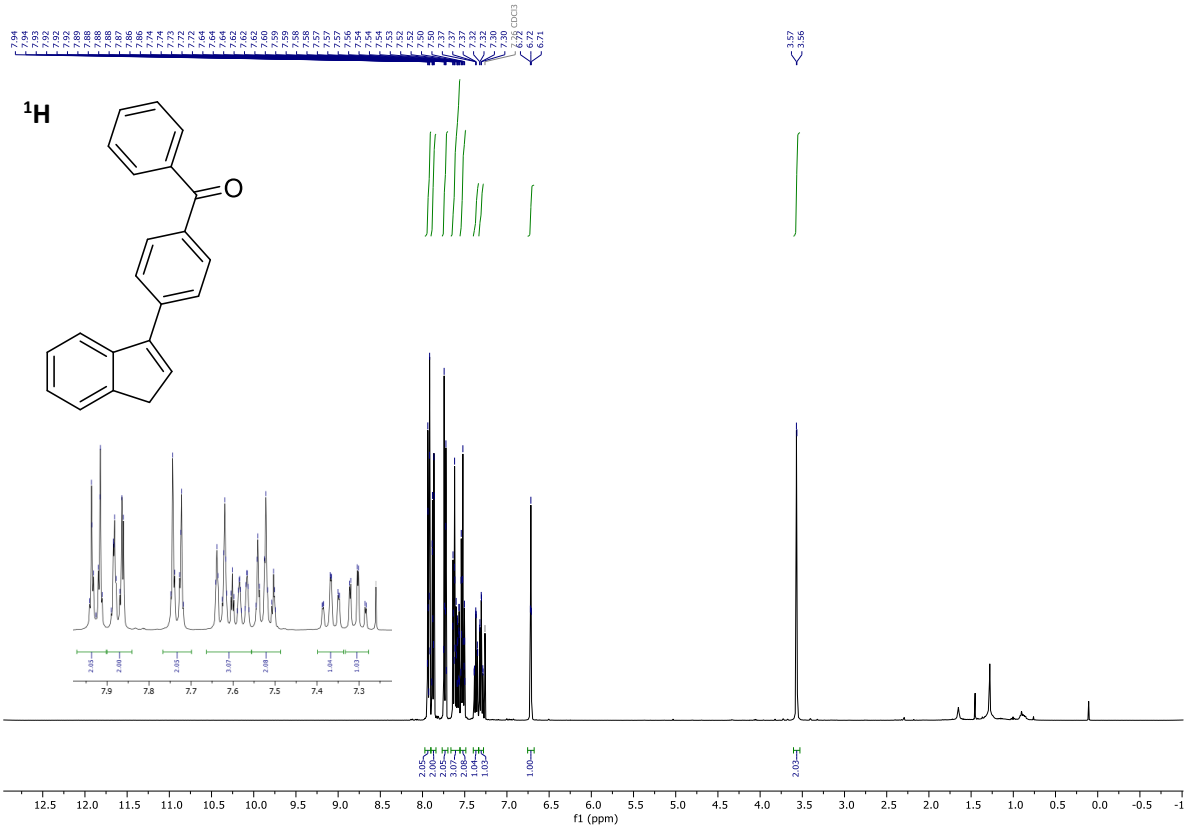


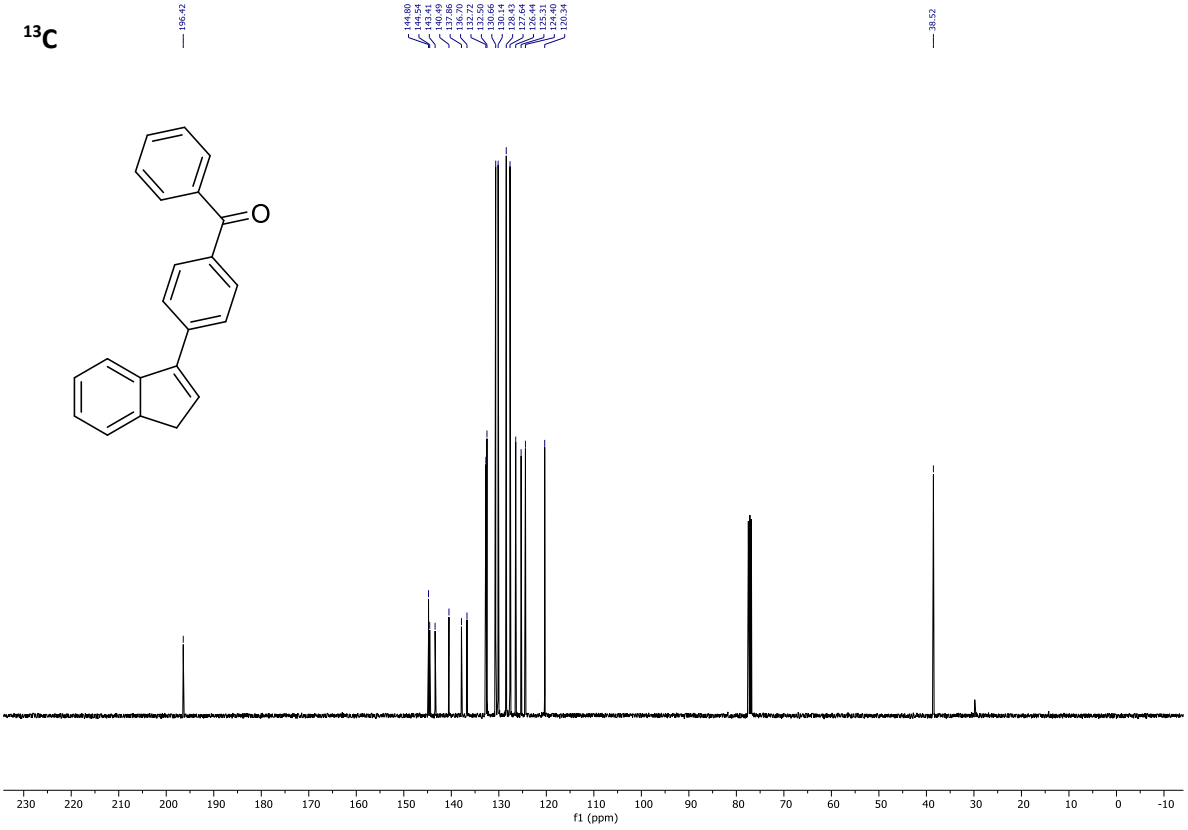
3-(4-(But-2-yn-1-yloxy)phenyl)-1*H*-indene (23a)





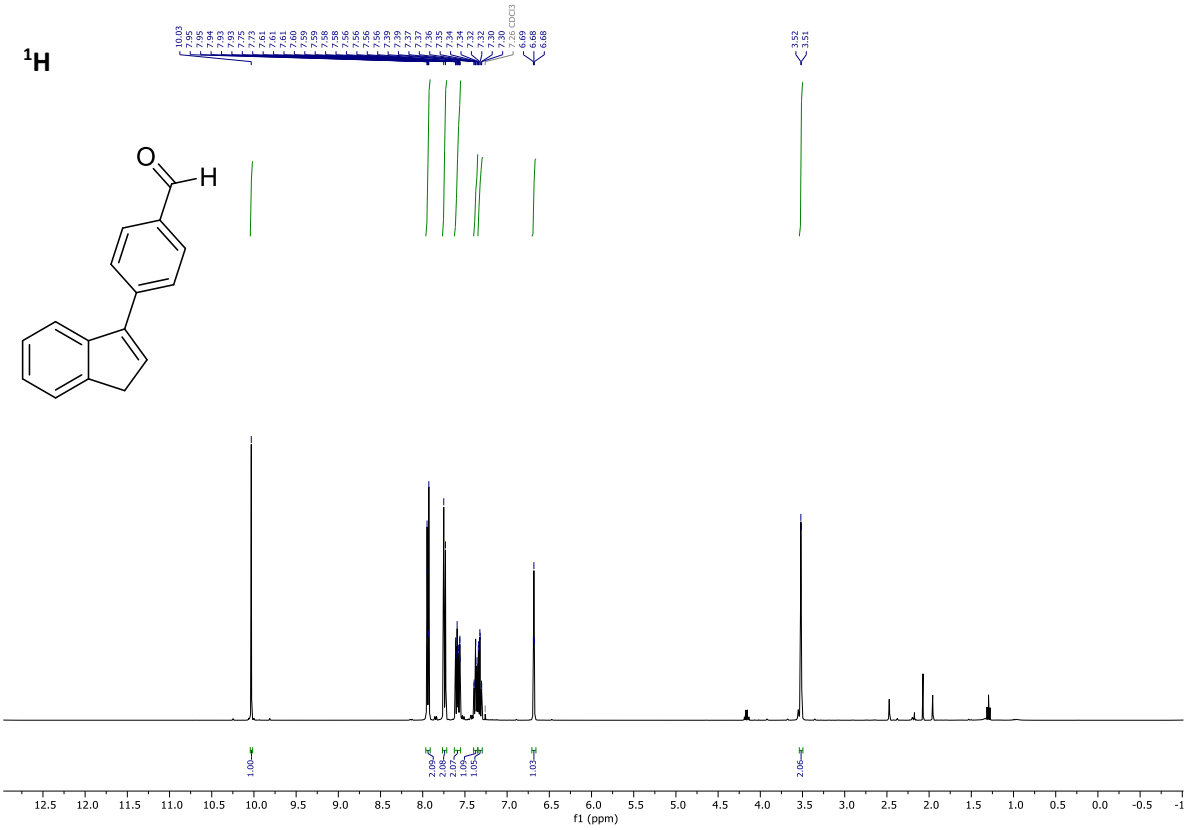
(4-(1*H*-inden-3-yl)phenyl)(phenyl)methanone (24a)



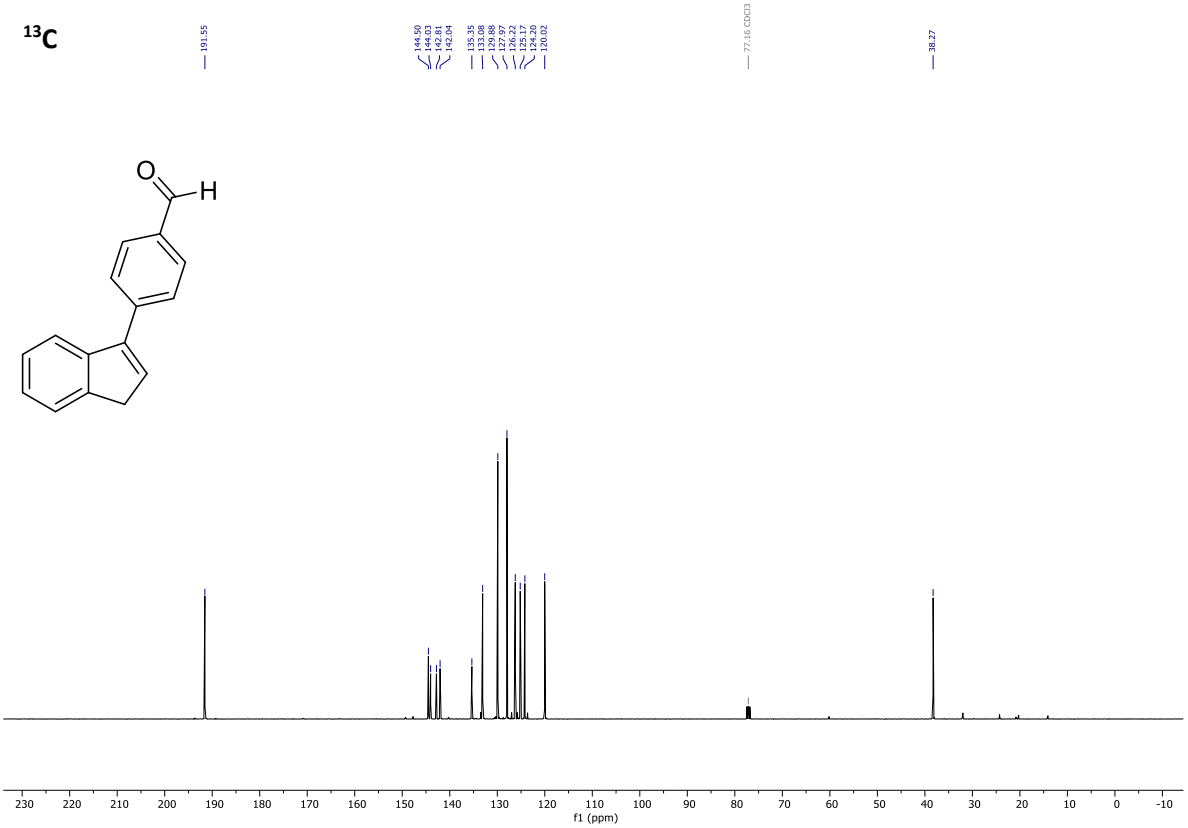


4-(1*H*-inden-3-yl)benzaldehyde (25a)

^{1}H

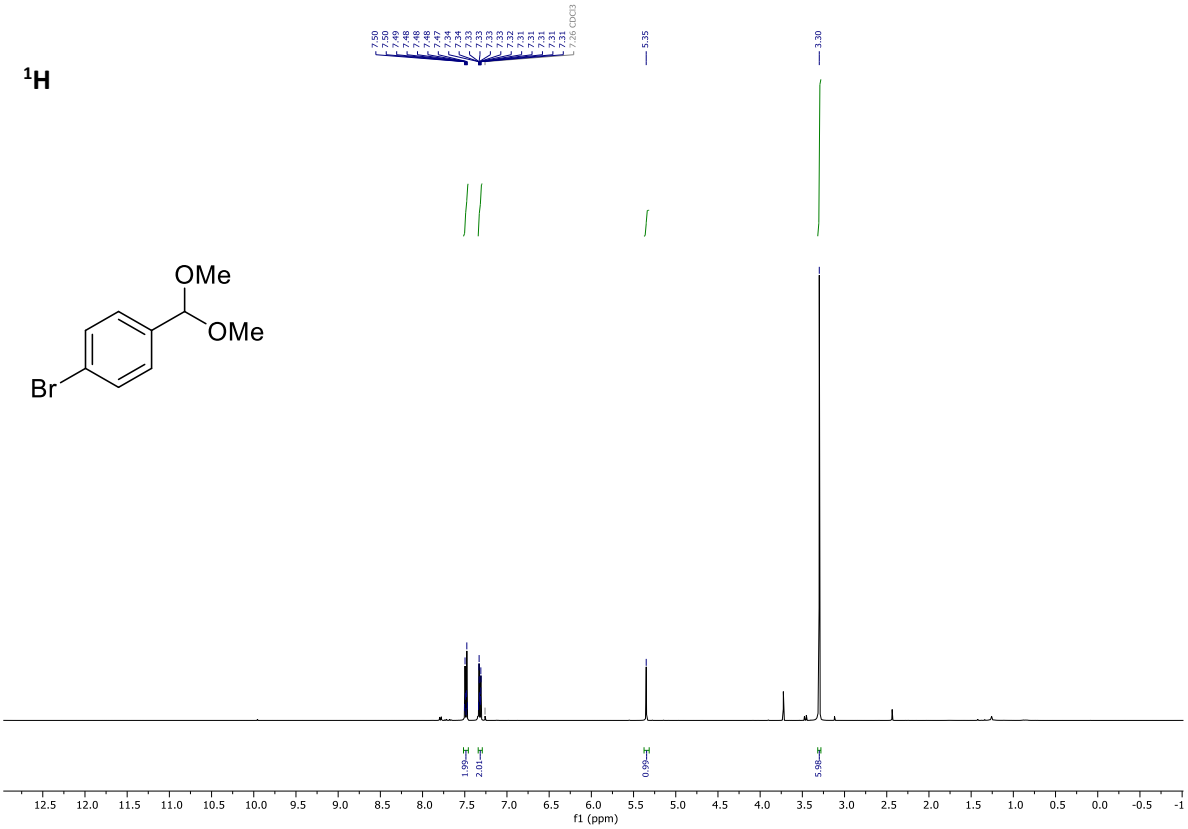


^{13}C

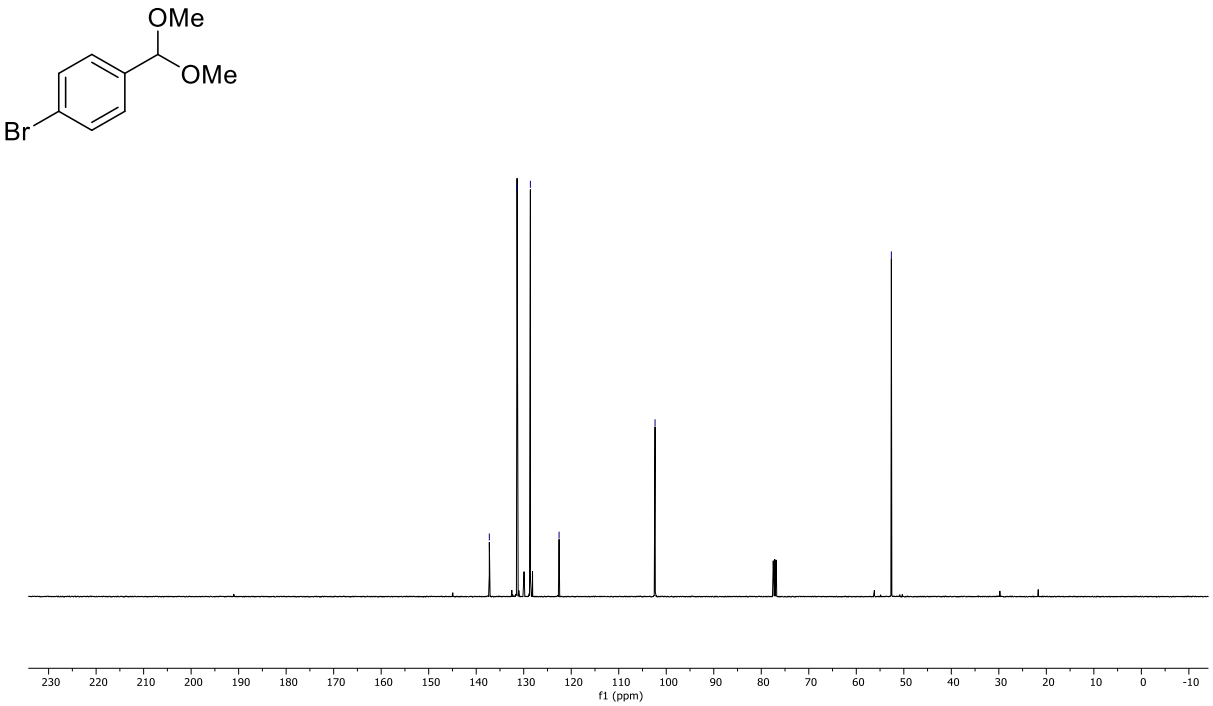


1-Bromo-4-(dimethoxymethyl)benzene (S1)

^{1}H

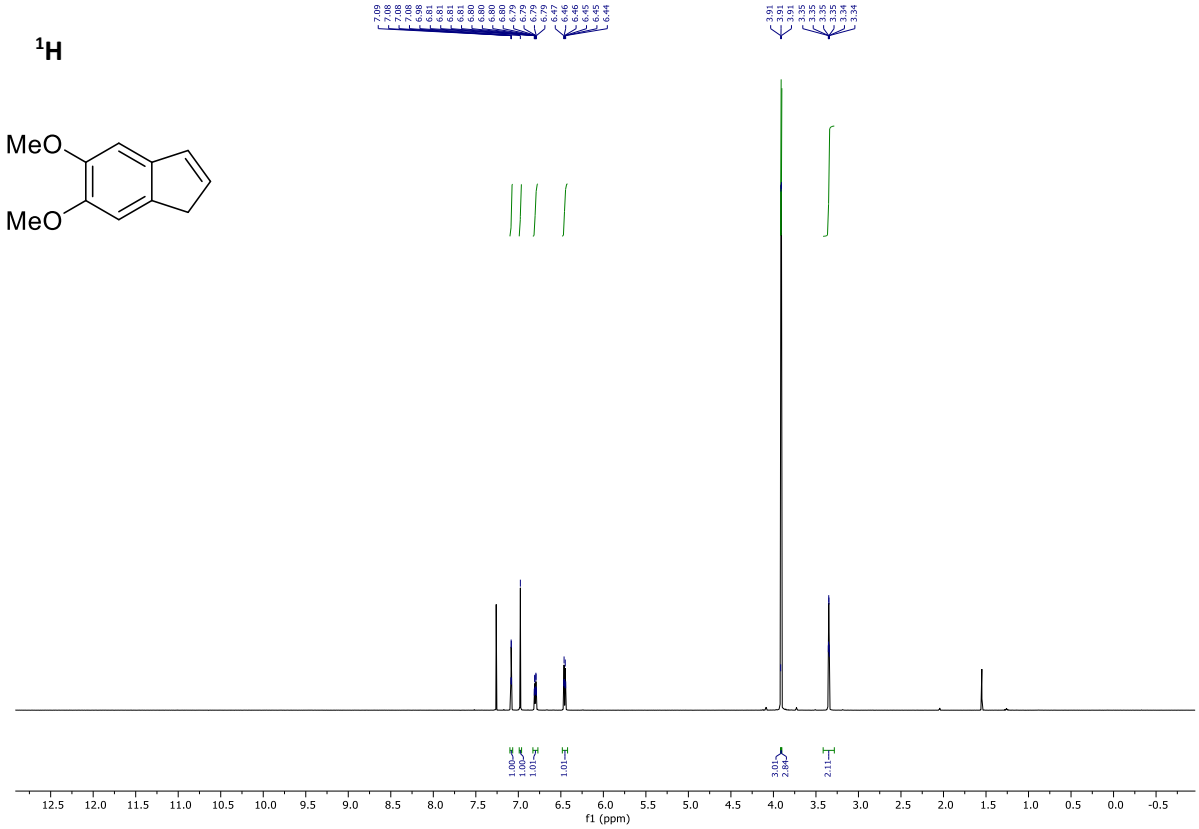


^{13}C

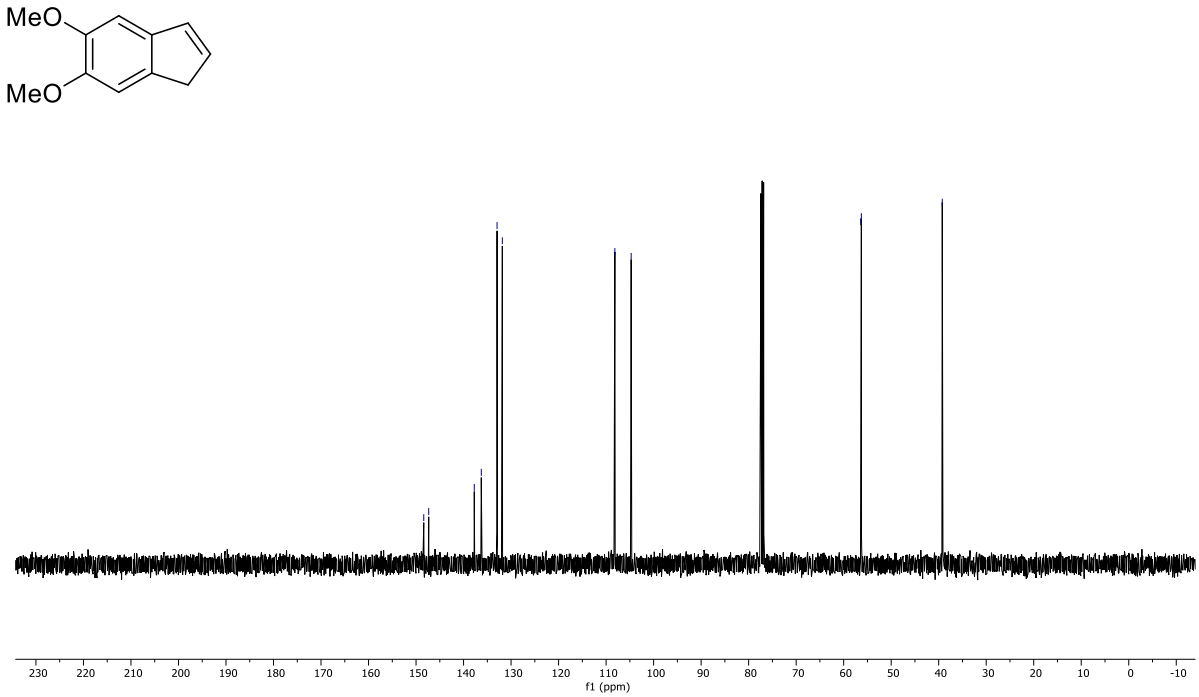


5,6-Dimethoxy-1*H*-indene (S2)

^{1}H

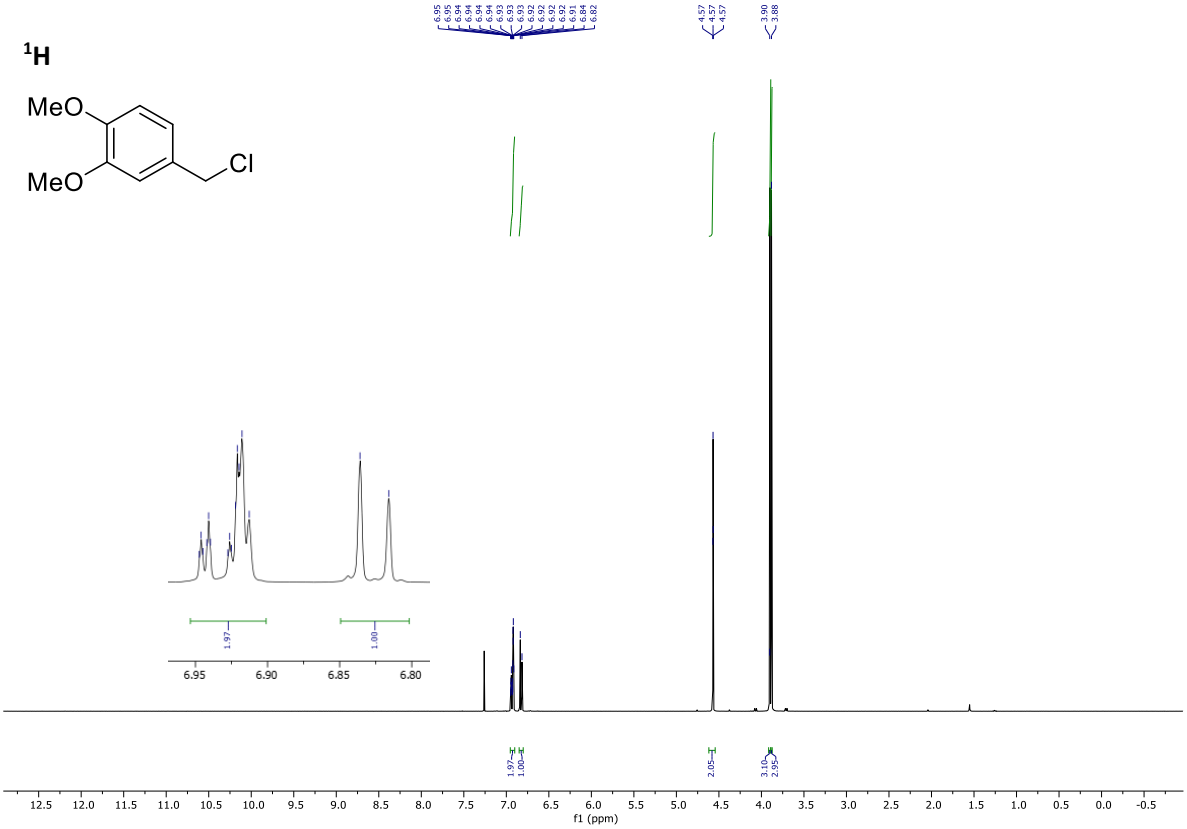


^{13}C

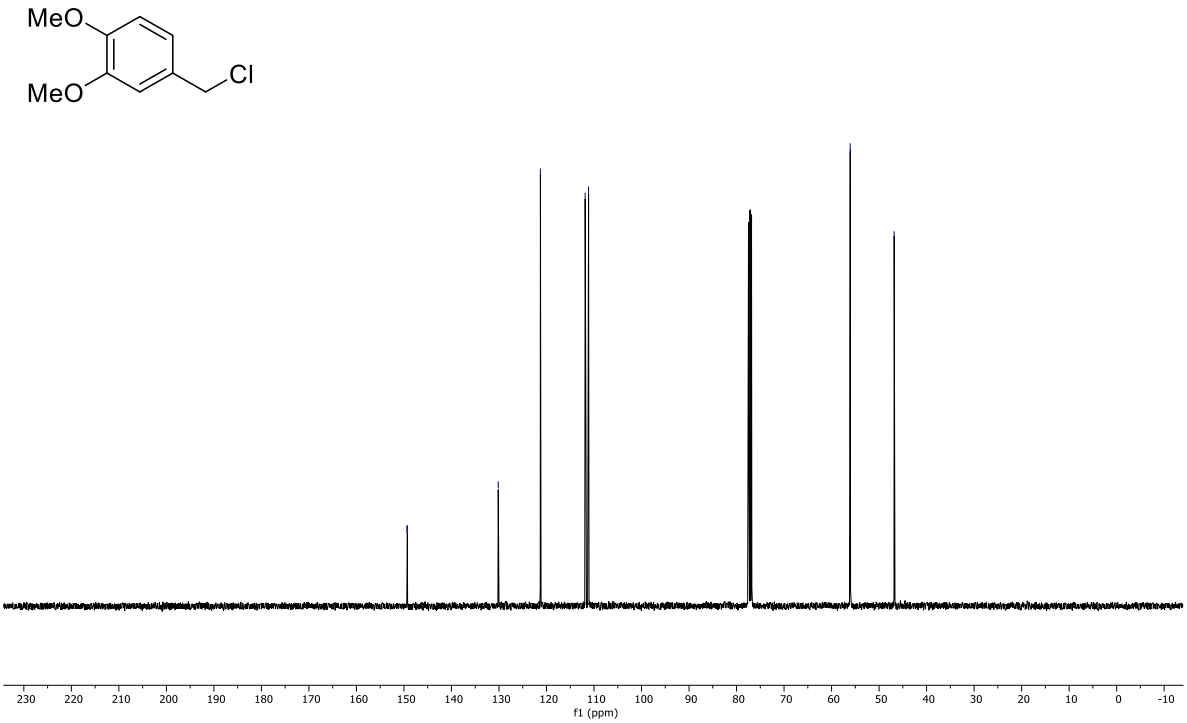


4-(Chloromethyl)-1,2-dimethoxybenzene (S3)

^{1}H

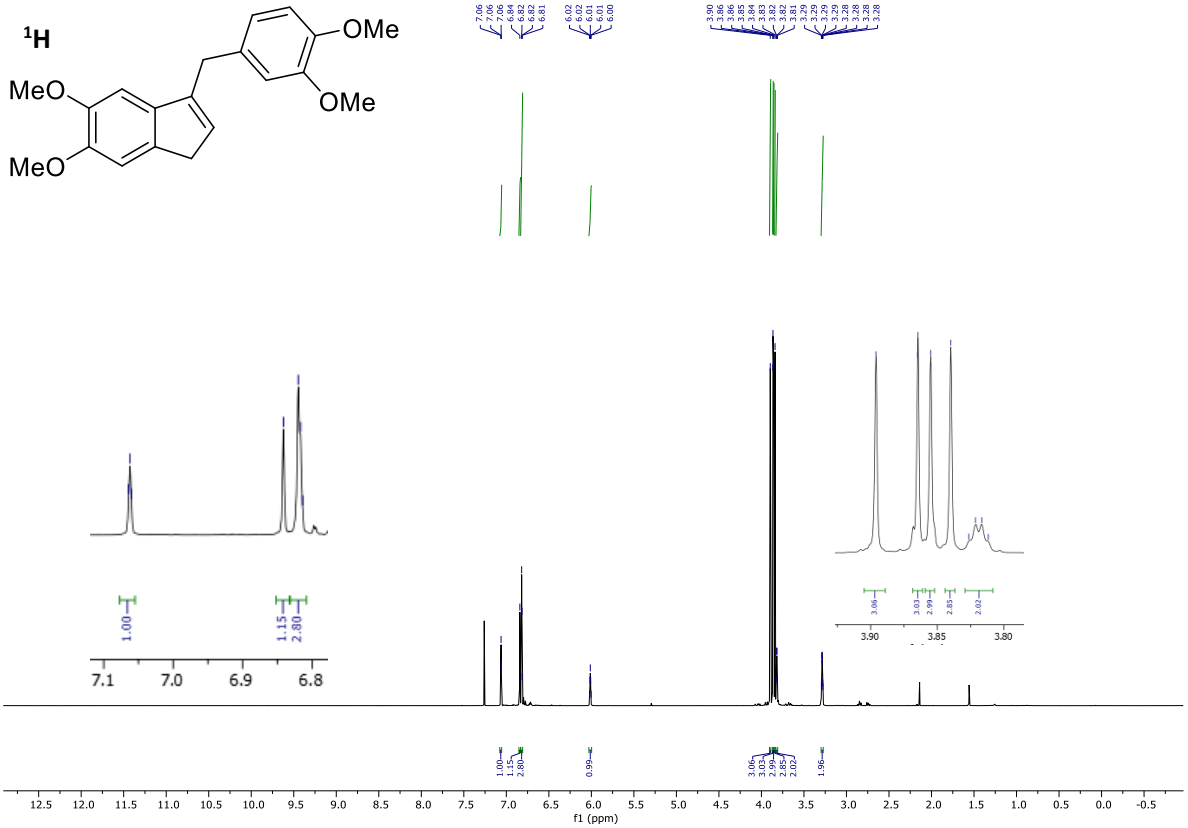


^{13}C

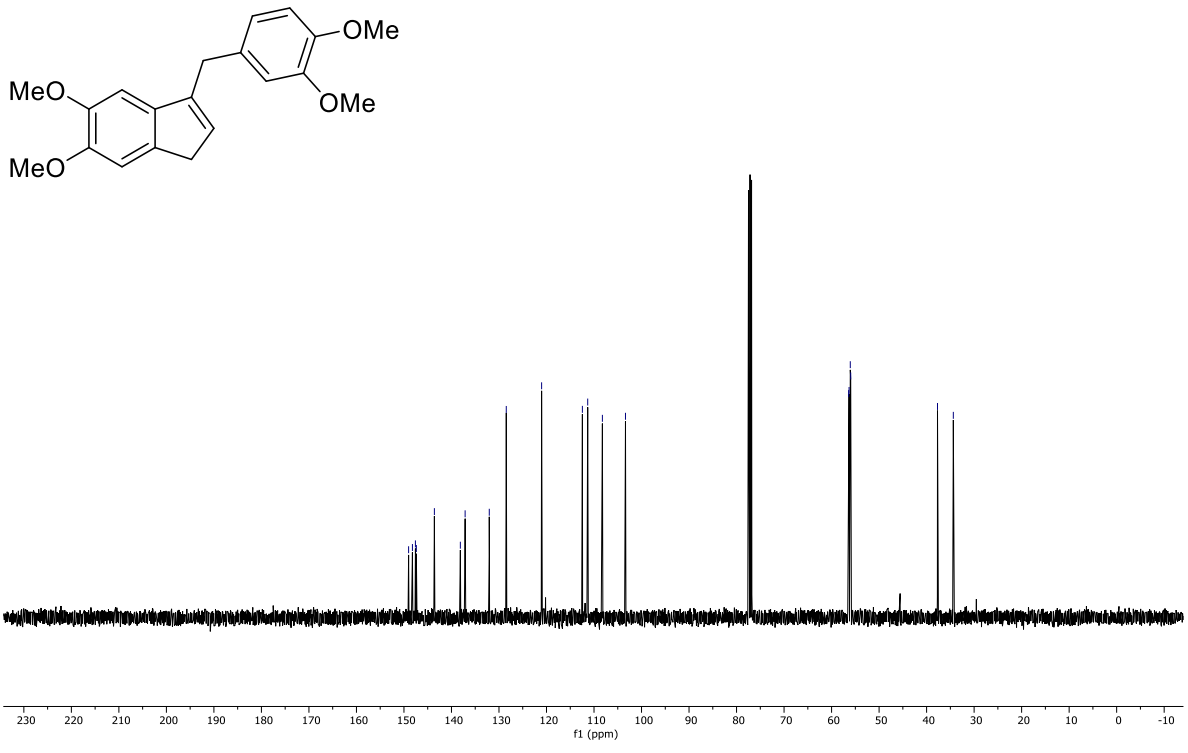


3-(3,4-Dimethoxybenzyl)-5,6-dimethoxy-1*H*-indene (28a)

^{1}H

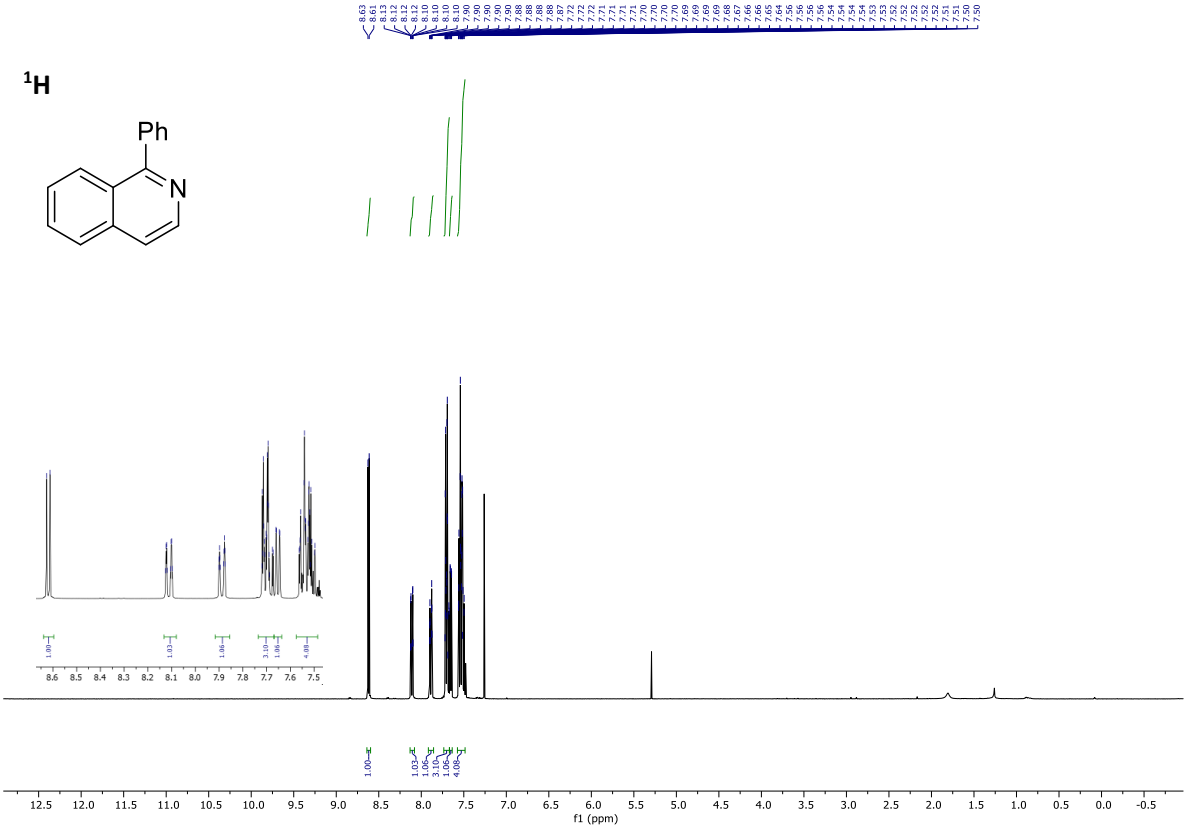


^{13}C

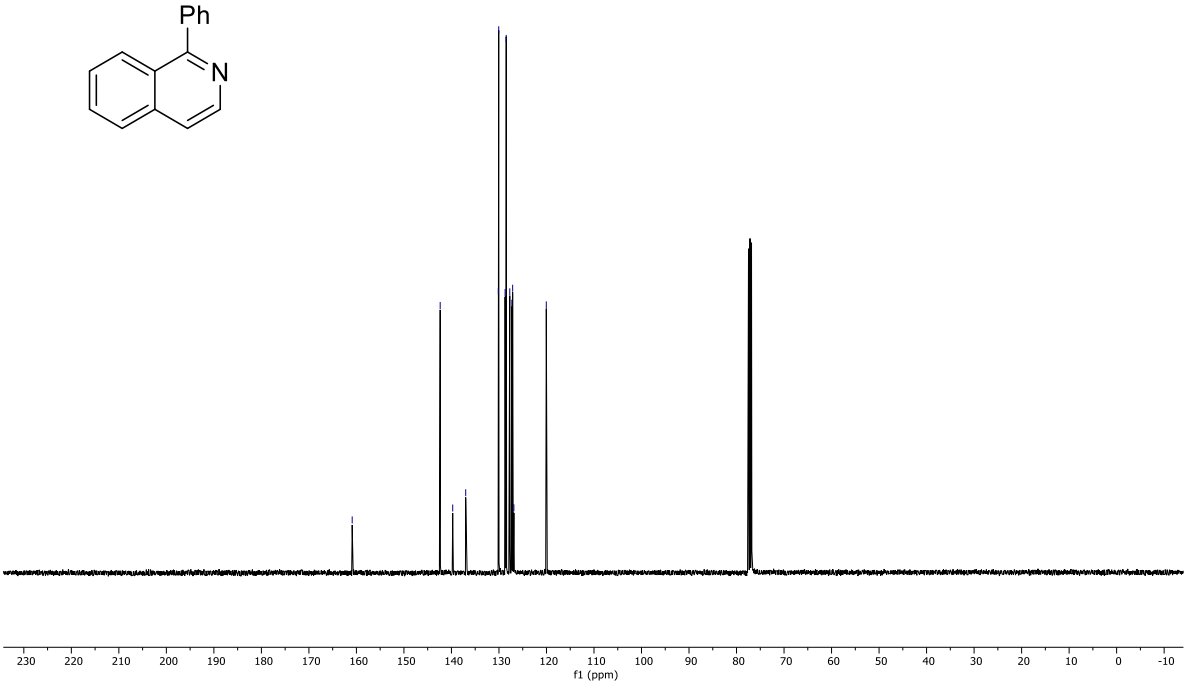


1-Phenylisoquinoline (1b)

^{1}H

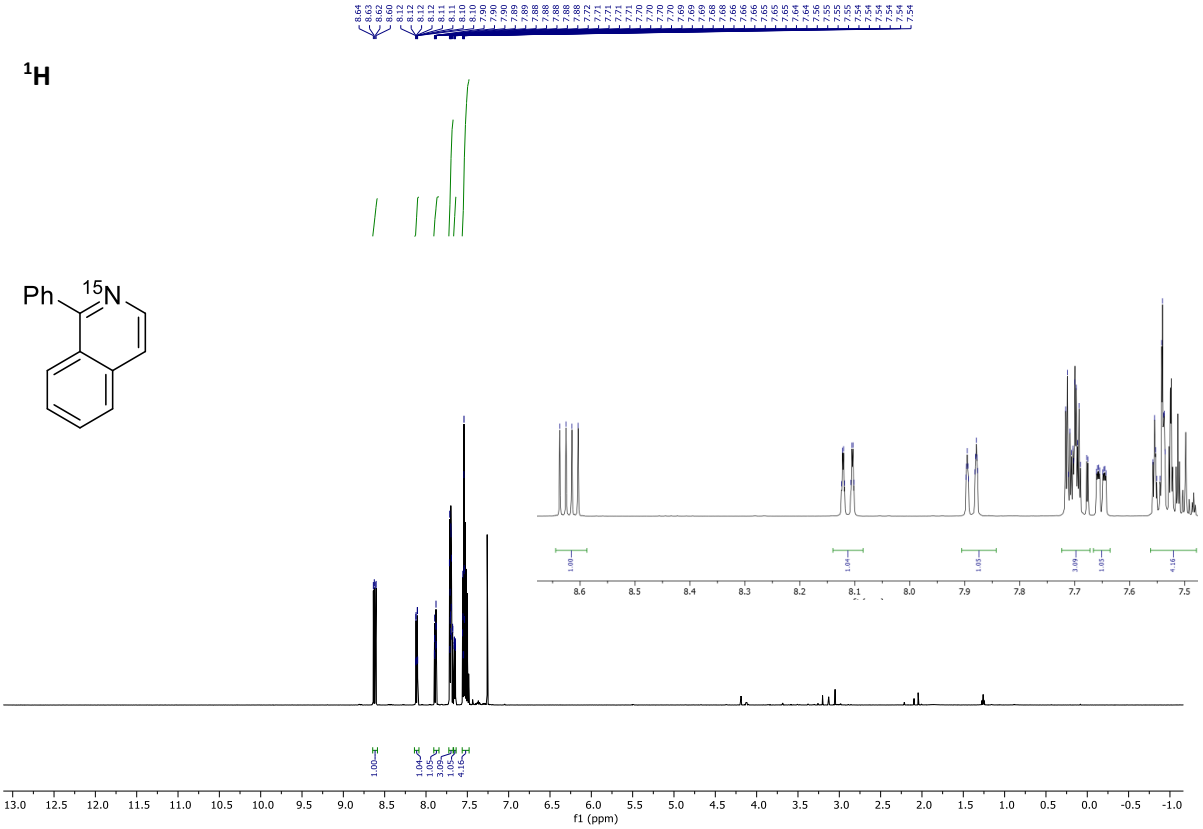


^{13}C

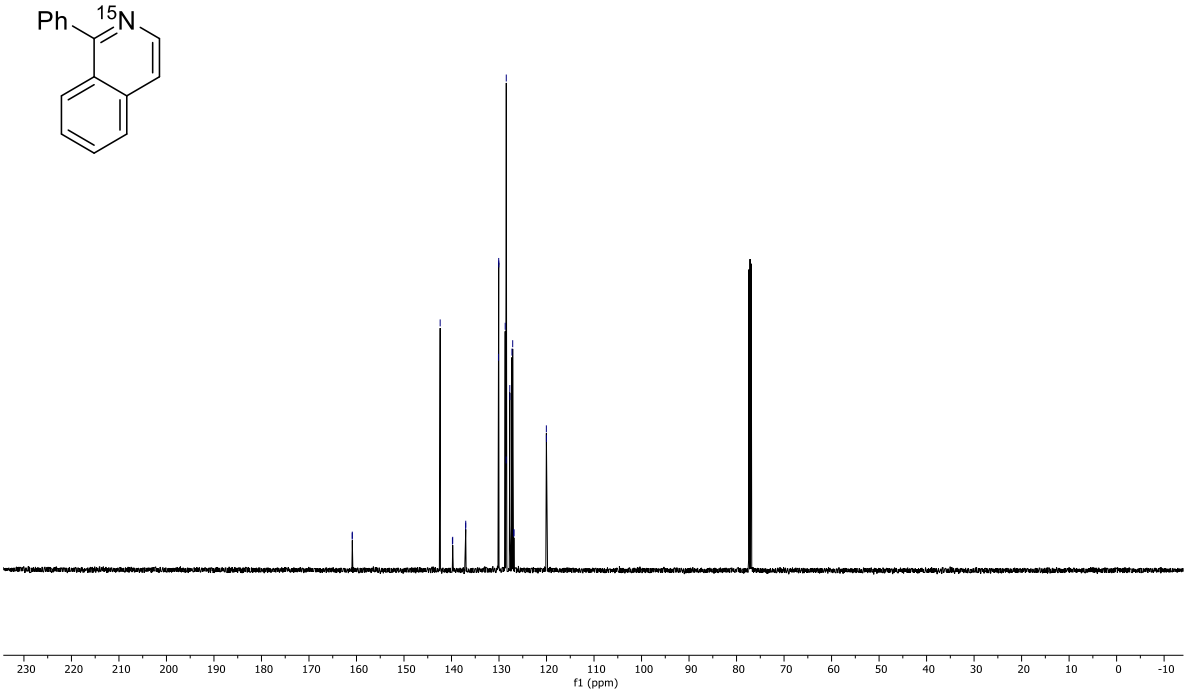


1-Phenylisoquinoline-^{15}N (15N-1b)

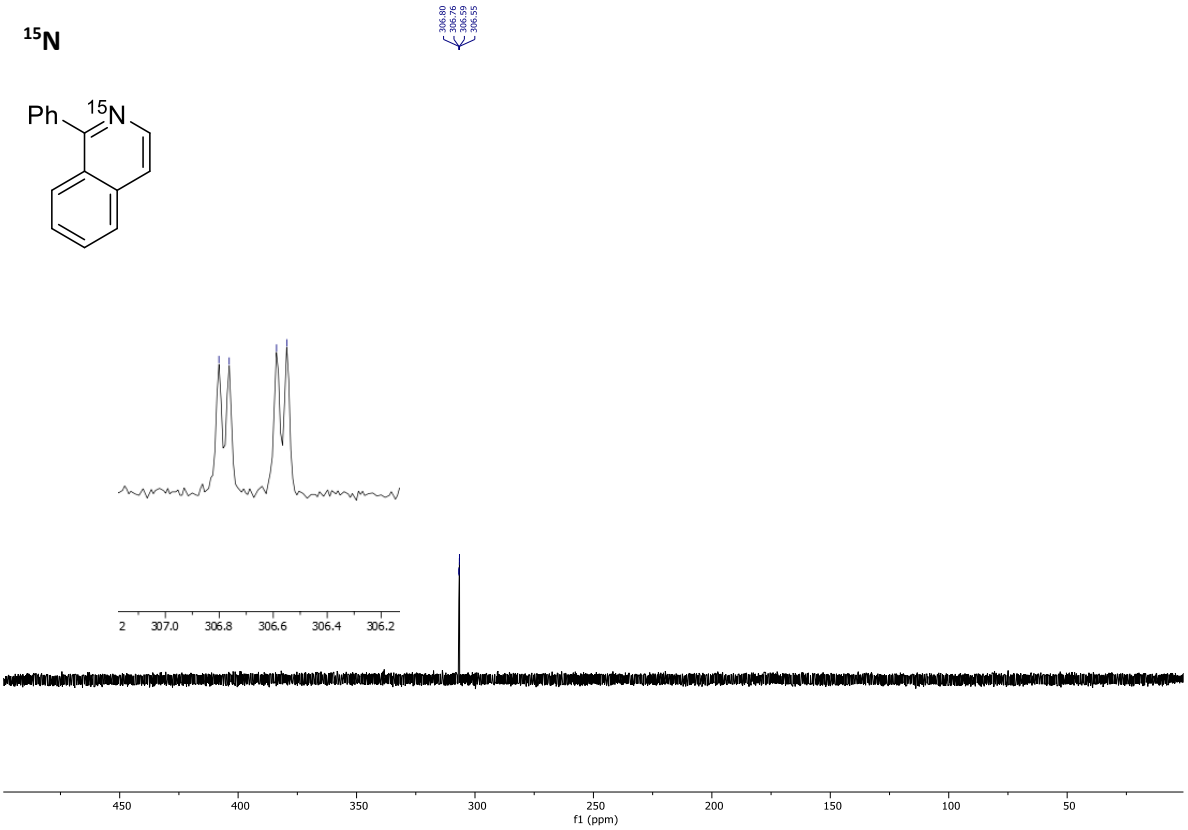
^{1}H



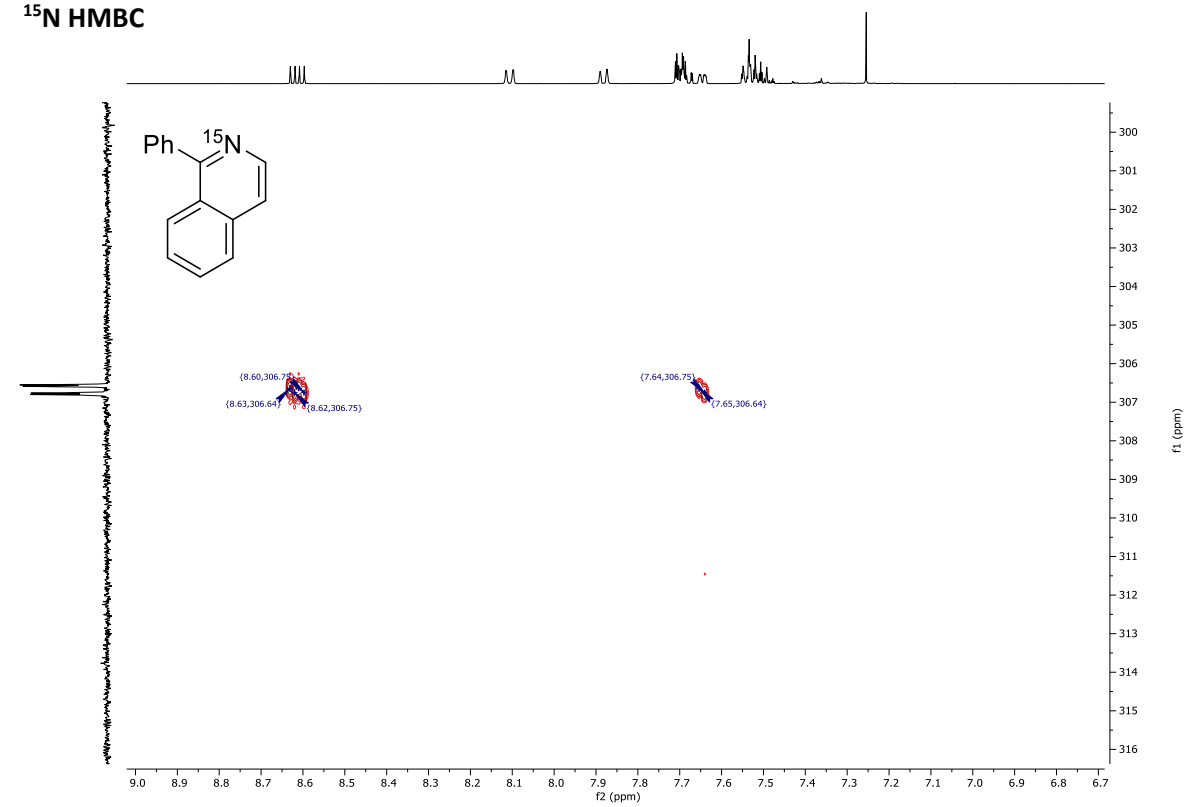
^{13}C



^{15}N

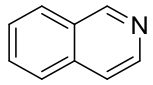

306.80
306.75
306.59
306.55
Ph
15N
2
307.0
306.8
306.6
306.4
306.2
450
400
350
300
250
200
150
100
50
f1 (ppm)

^{15}N HMBC

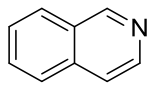

Ph
15N
{8.60,306.75}
{8.63,306.64}
{8.62,306.75}
{7.64,306.75}
{7.65,306.64}
9.0
8.9
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
f2 (ppm)
300
301
302
303
304
305
306
307
308
309
310
311
312
313
314
315
316
f1 (ppm)

Isoquinoline (2b)

^{1}H

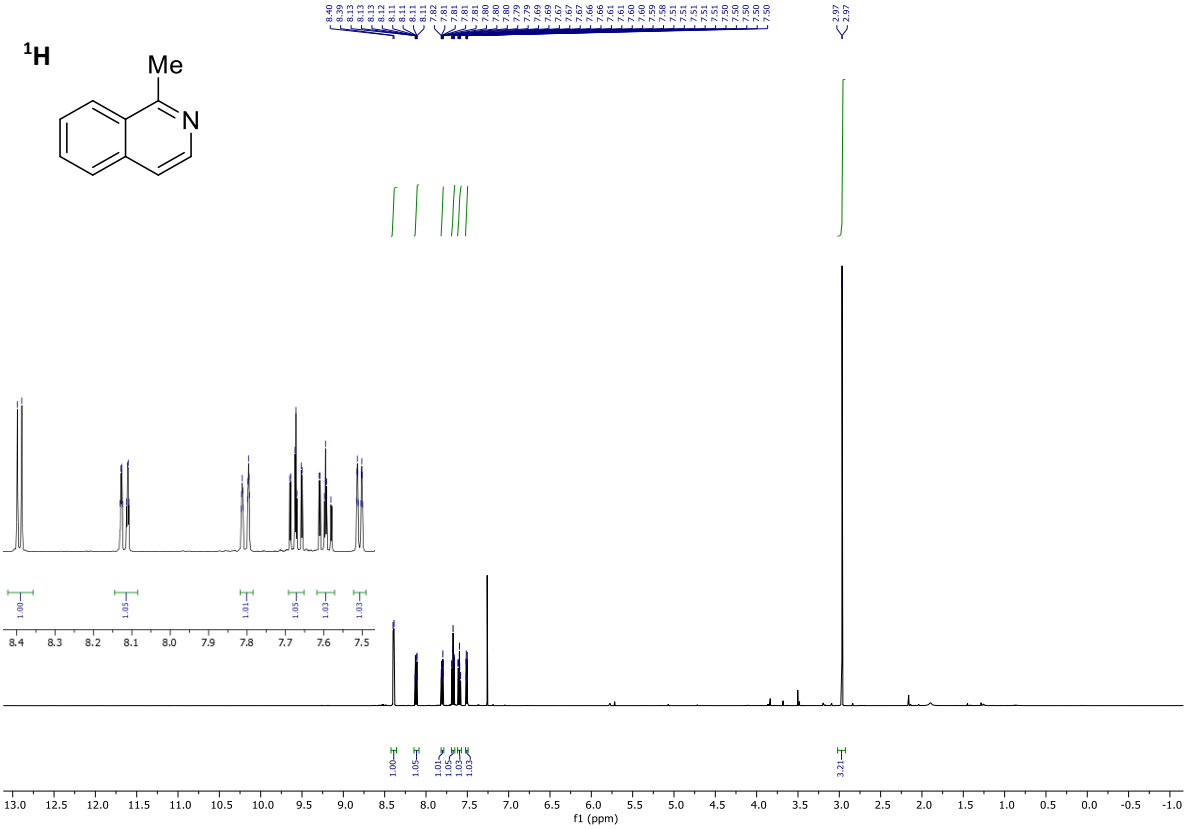


^{13}C

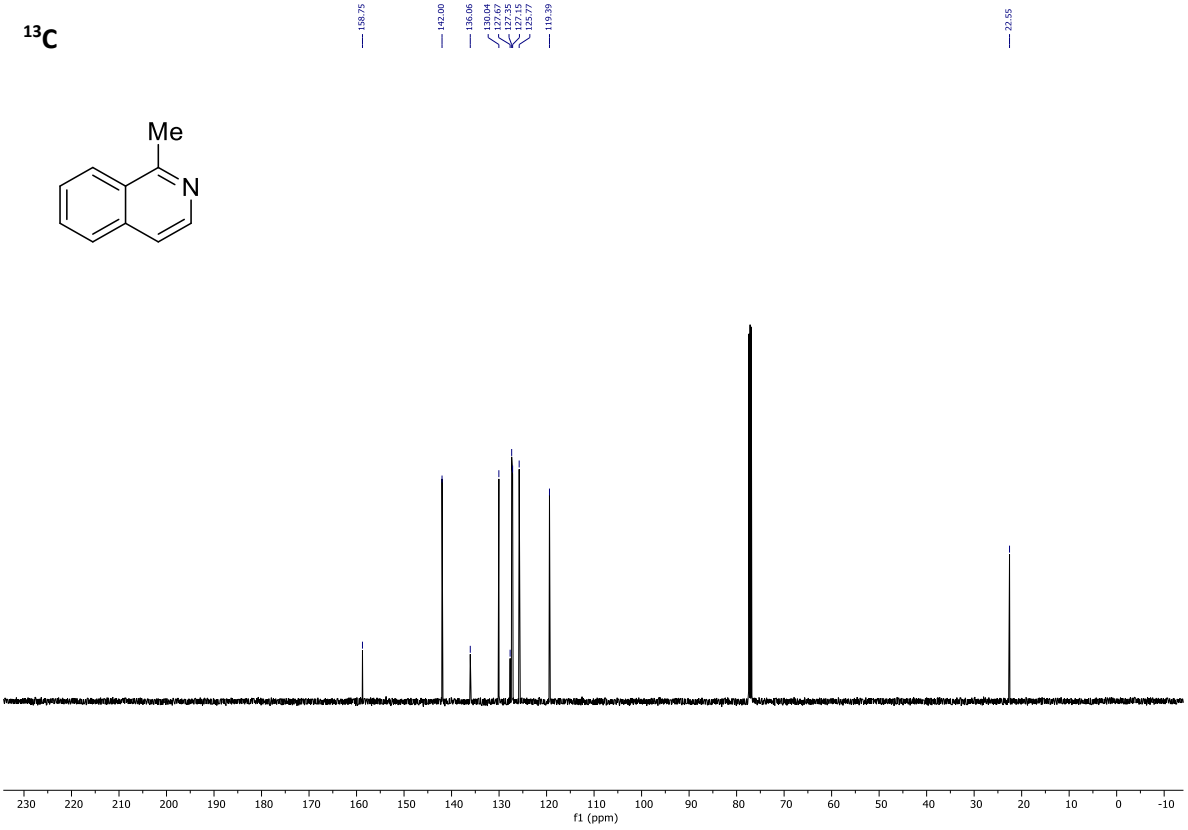


1-Methylisoquinoline (3b)

^{1}H

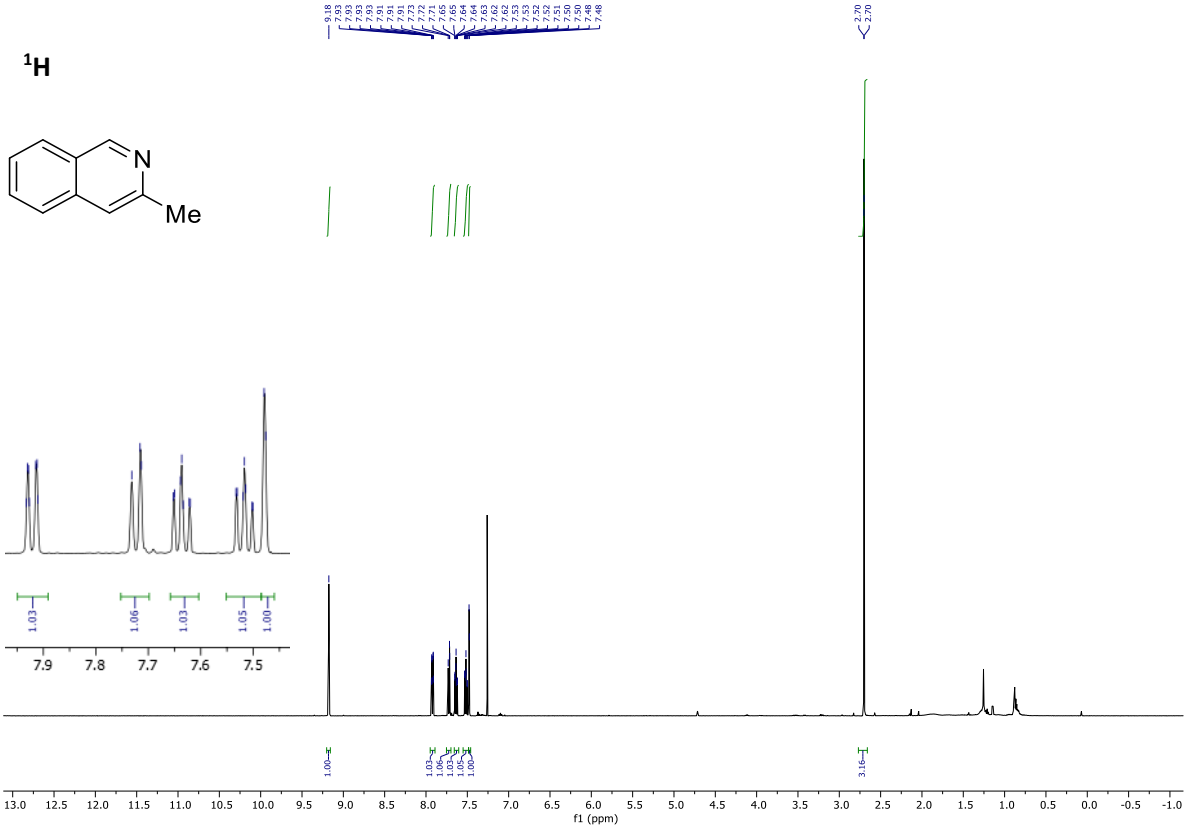


^{13}C

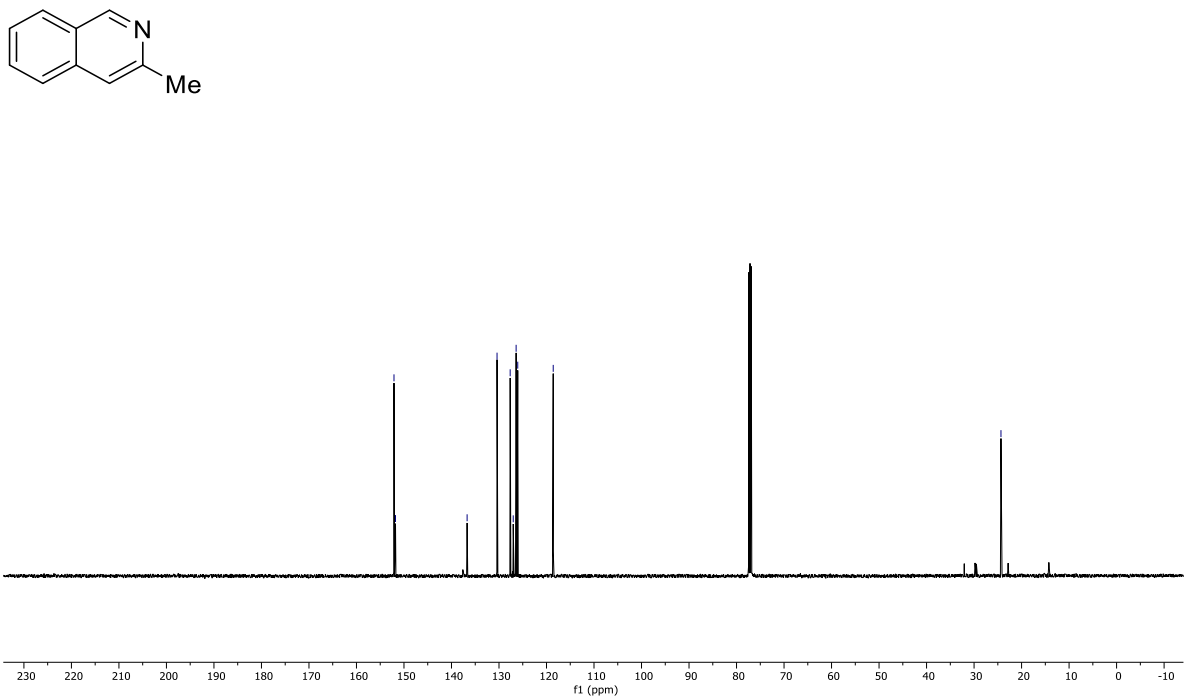


3-Methylisoquinoline (4b)

^{1}H

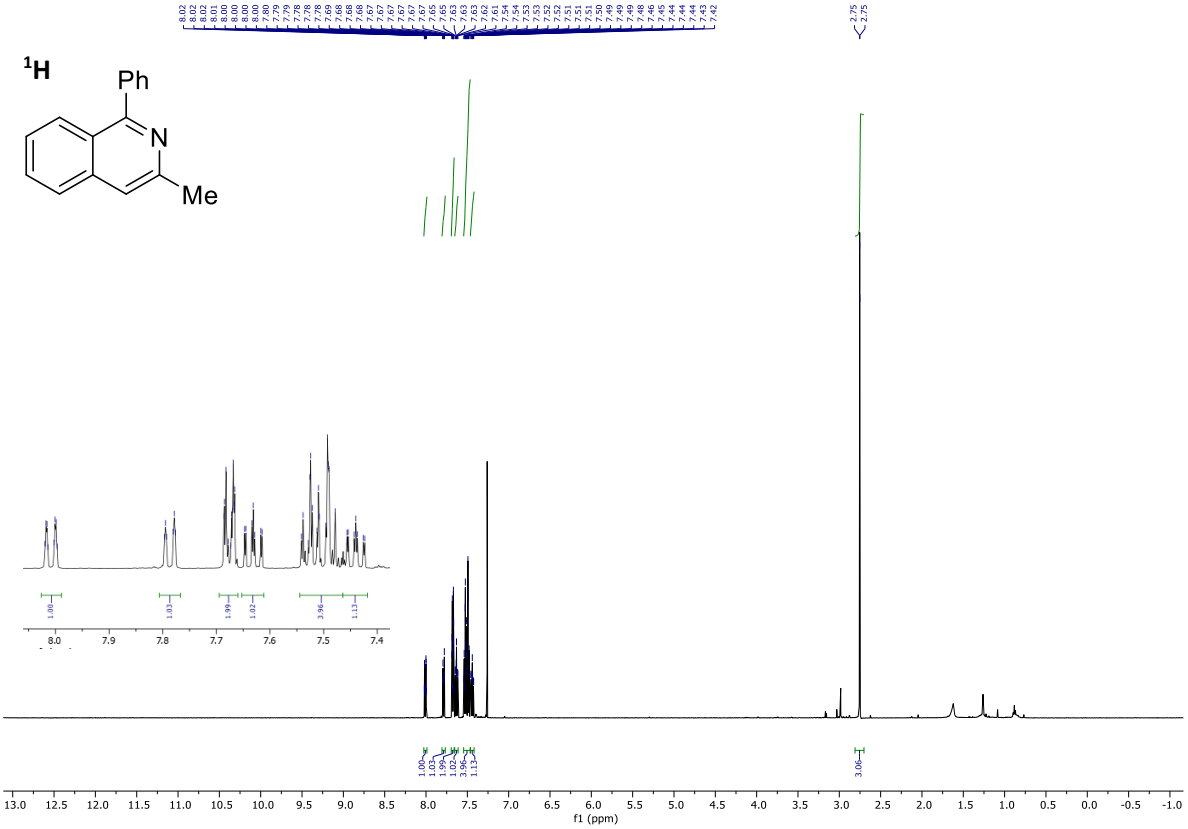


^{13}C

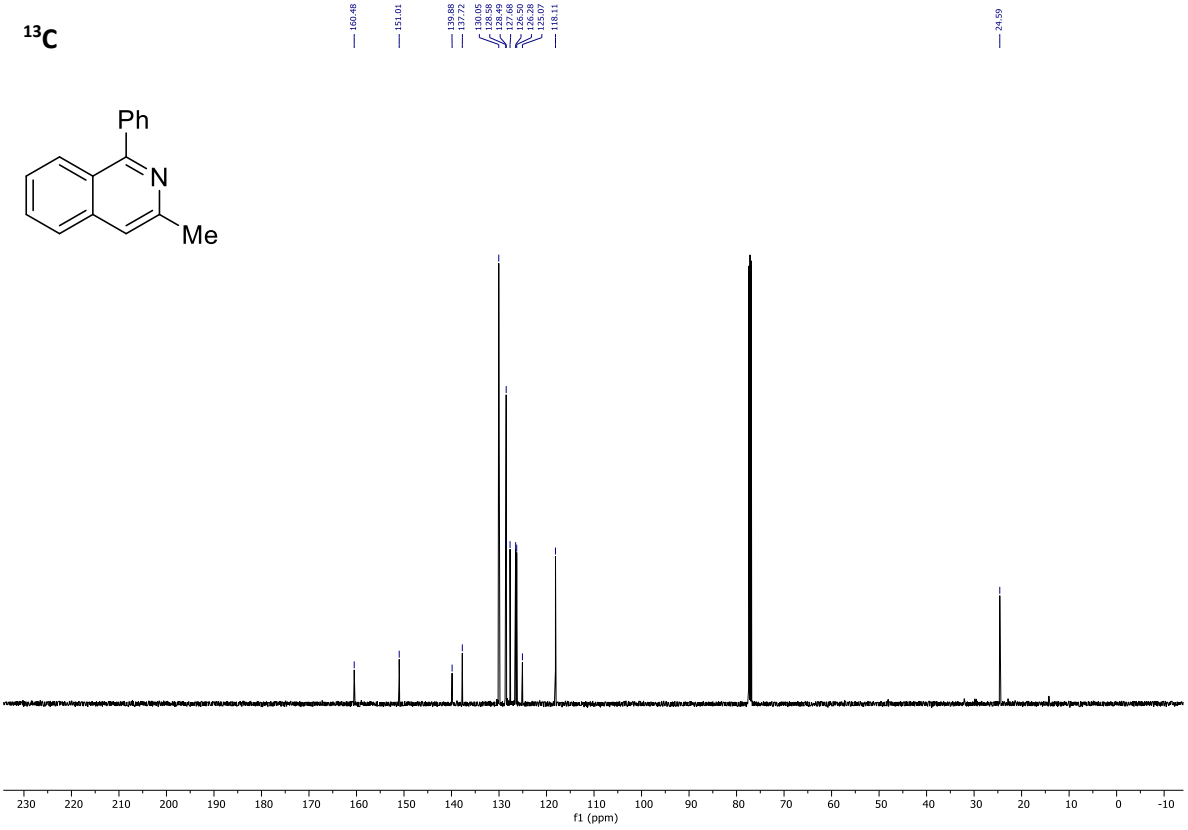


3-Methyl-1-phenylisoquinoline (5b)

^{1}H

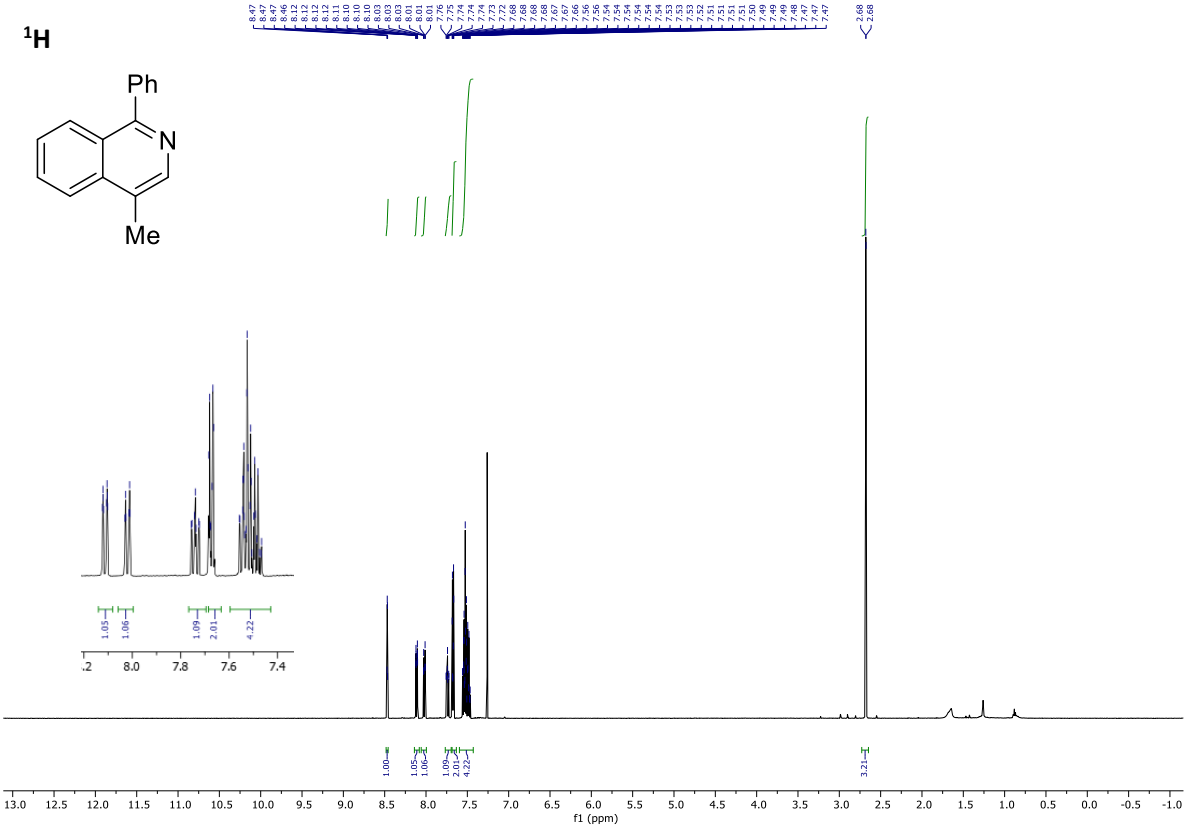


^{13}C

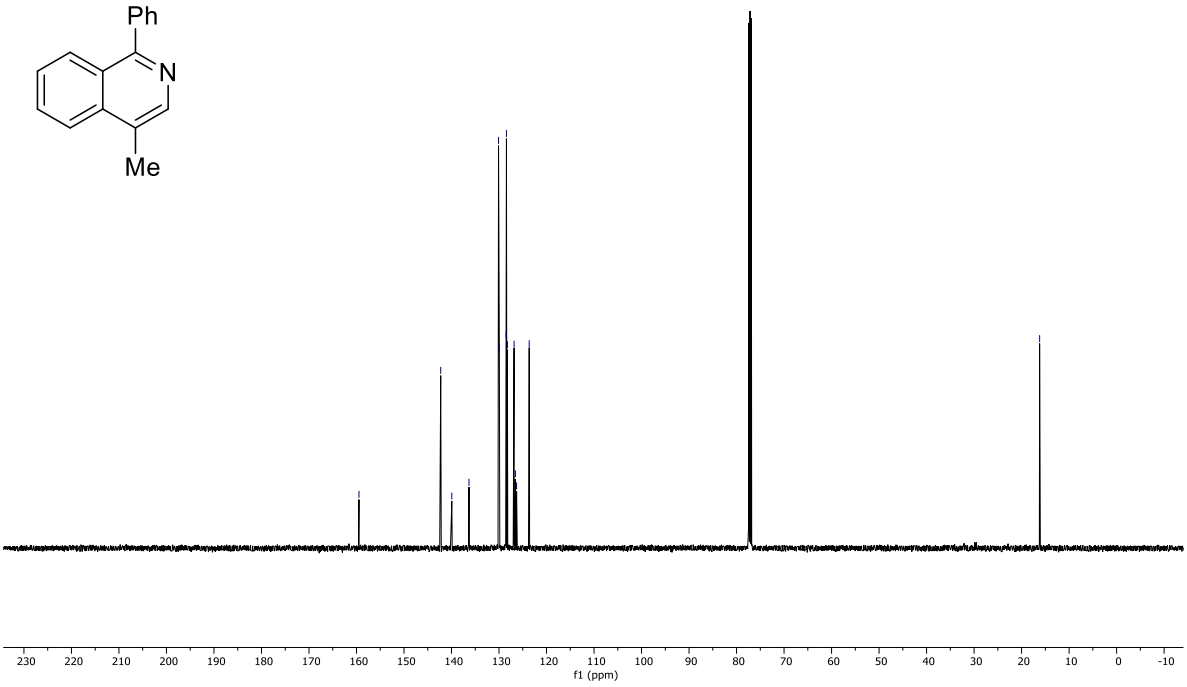


4-Methyl-1-phenylisoquinoline (6b)

^{1}H

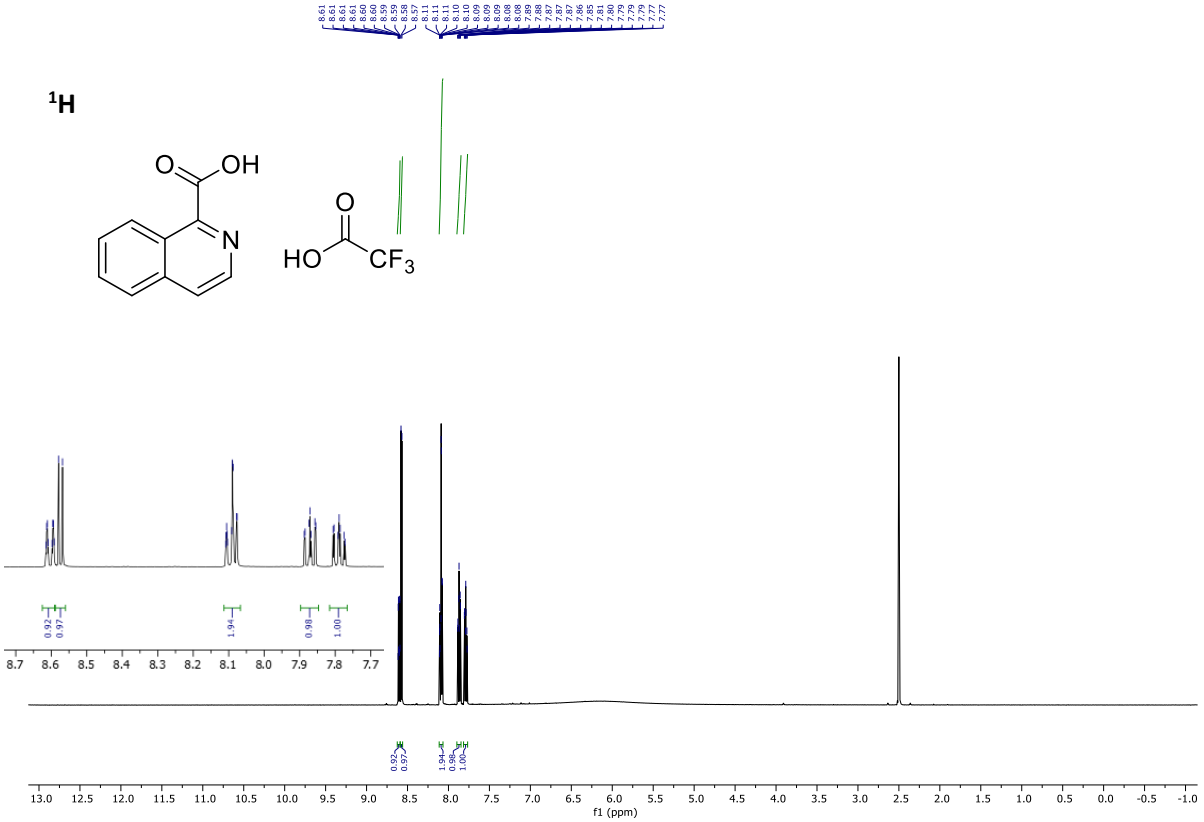


^{13}C

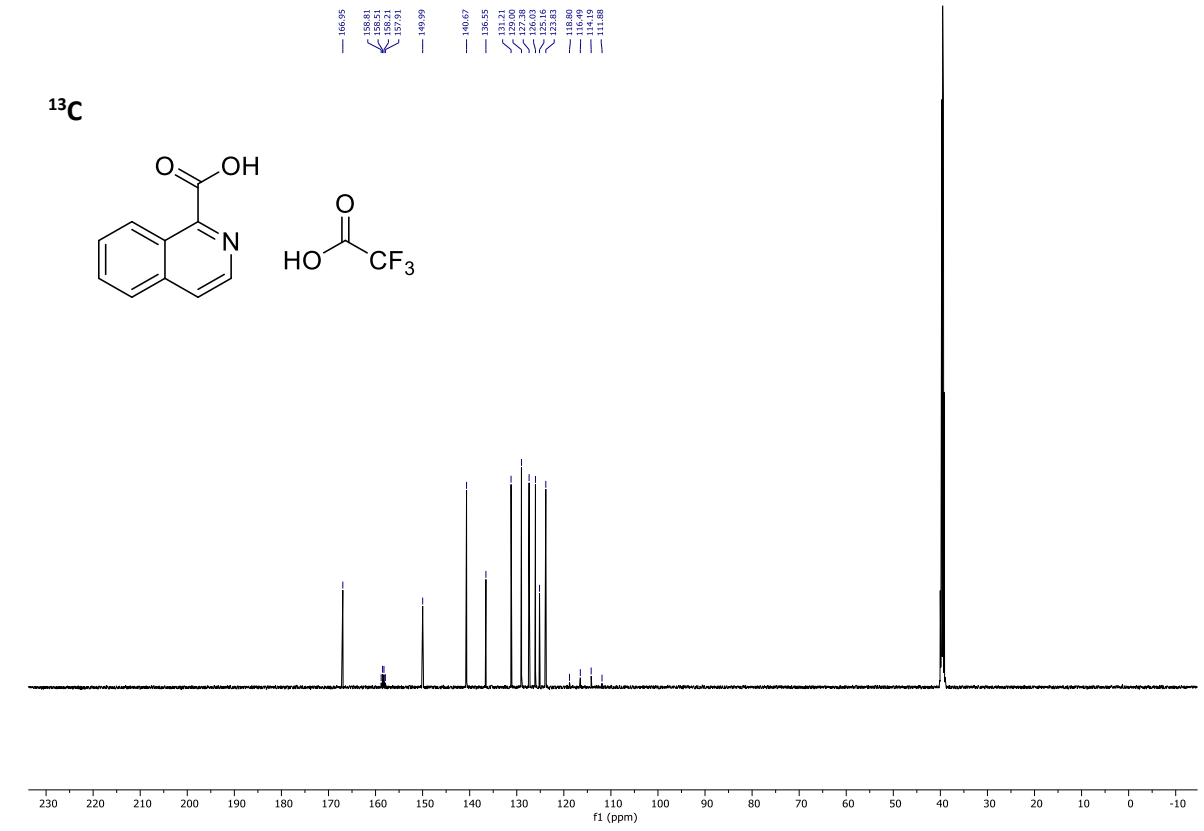


Isoquinoline-1-carboxylic acid (7b · TFA)

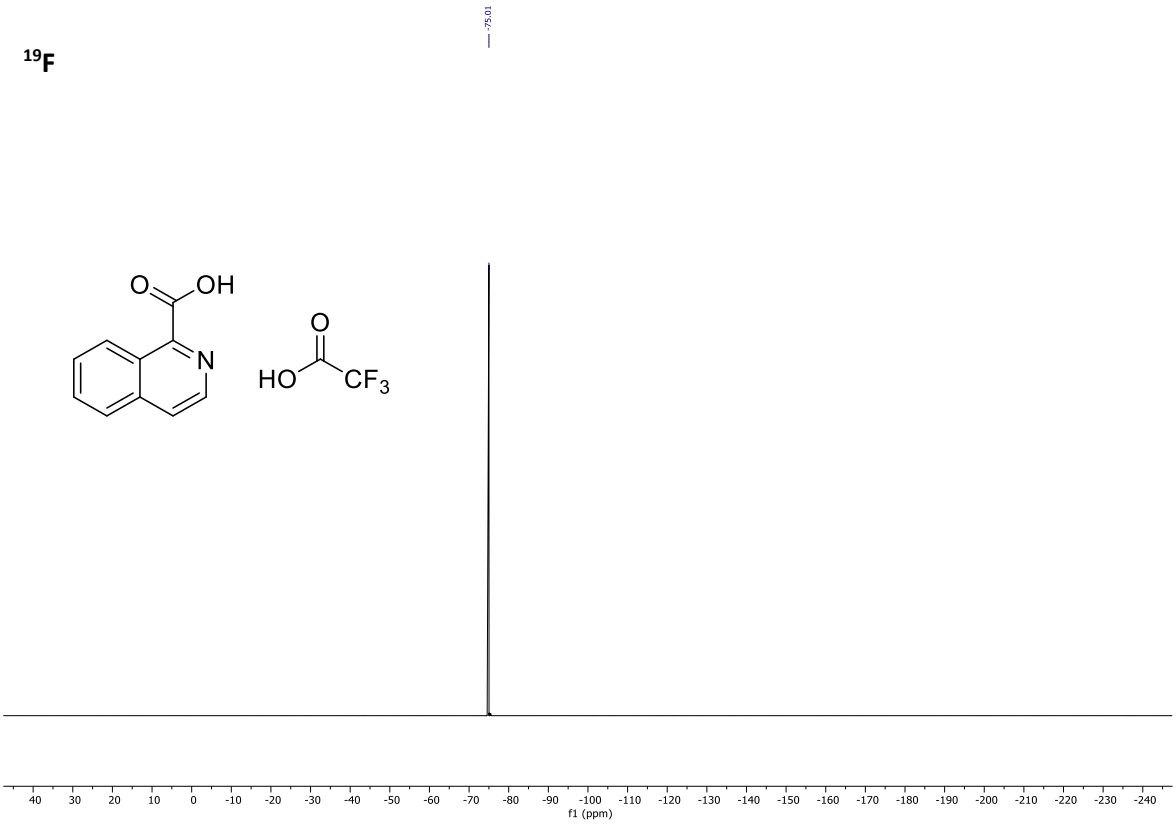
^{1}H



^{13}C

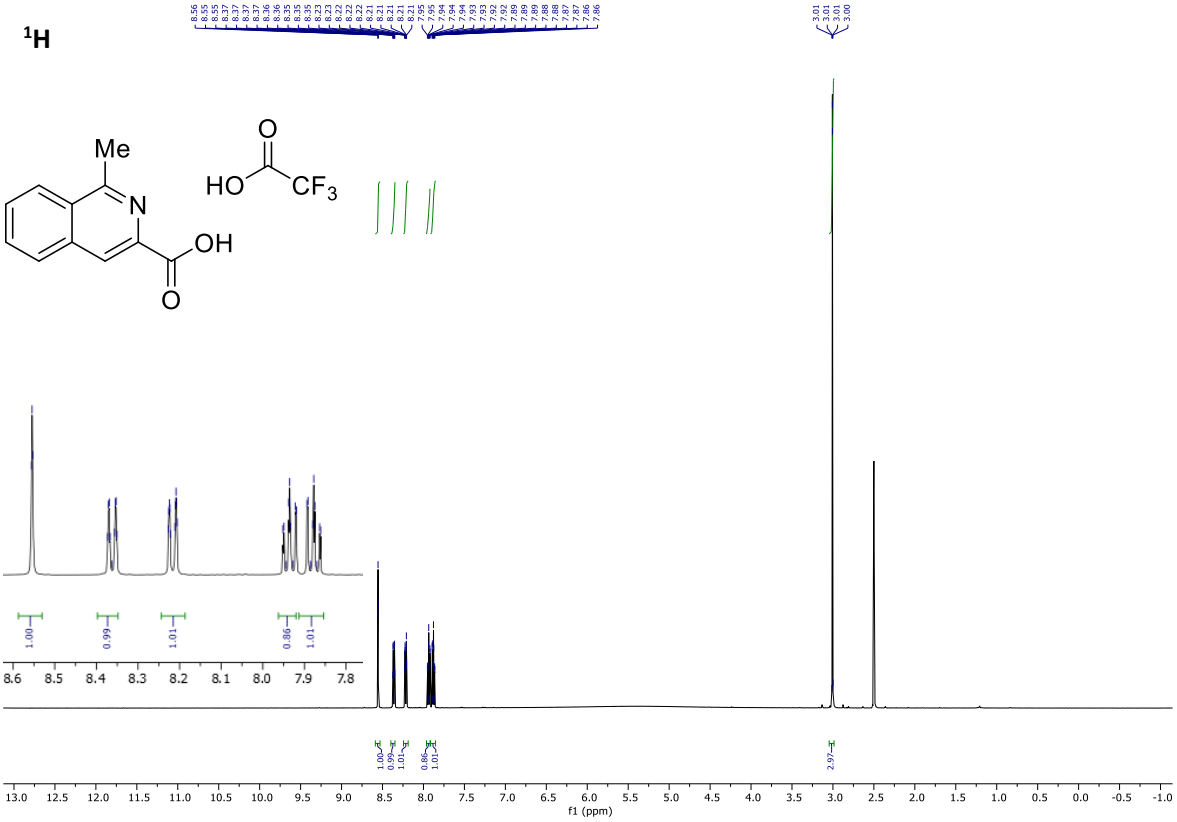


^{19}F

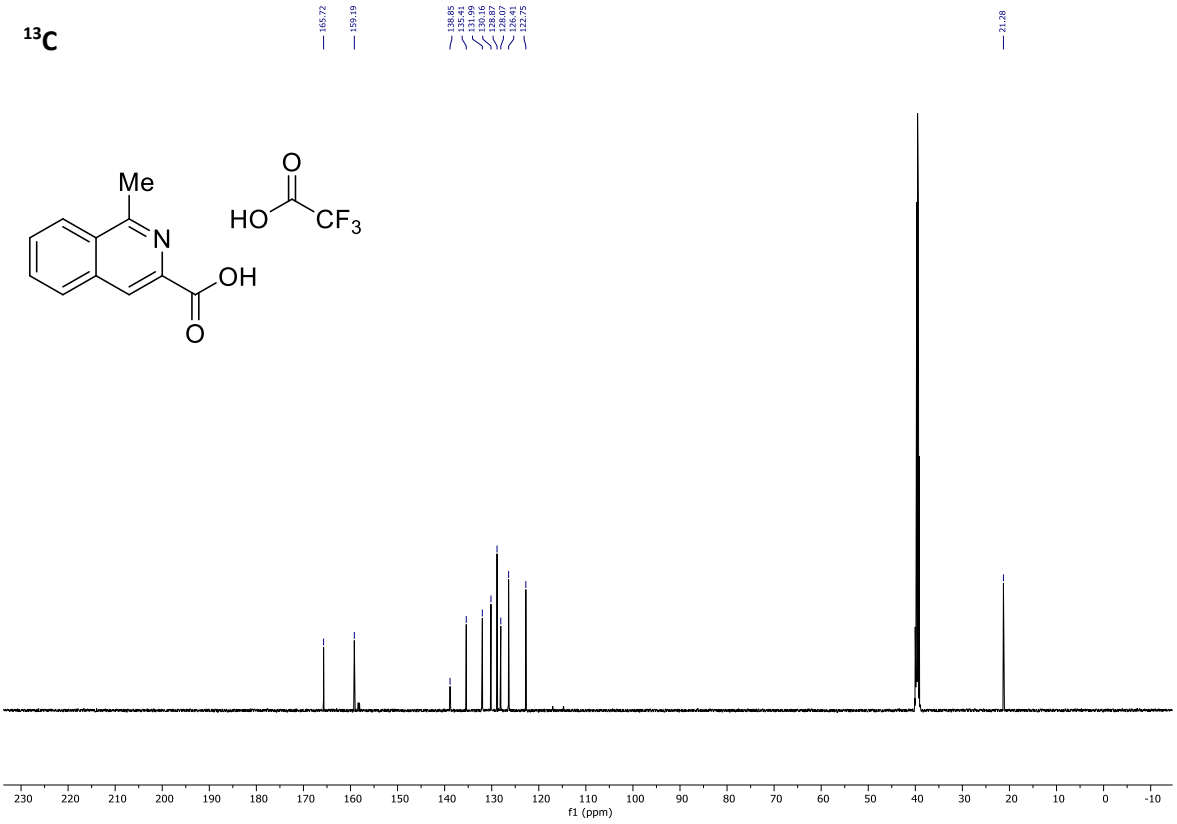

-75.01
O
OH
N
HO
O
CF3
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)

1-Methylisoquinoline-3-carboxylic acid (8b · TFA)

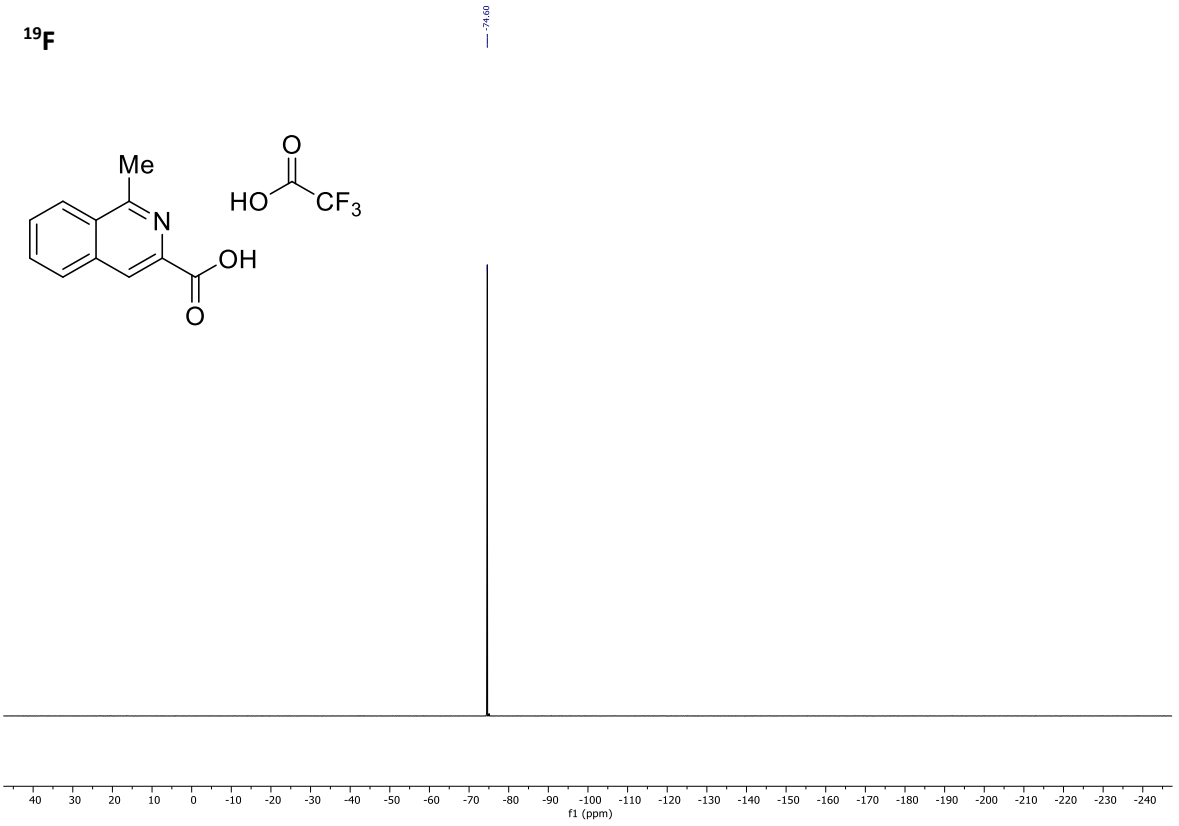
^{1}H



^{13}C

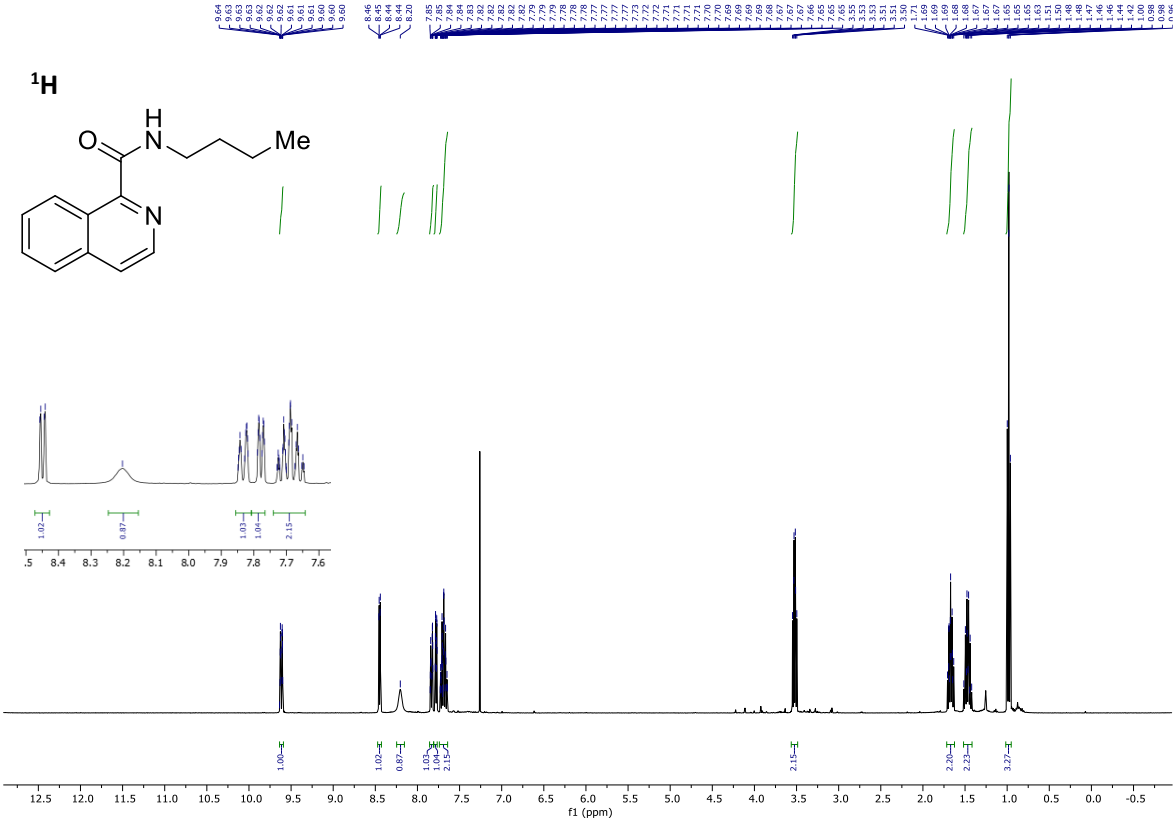


^{19}F

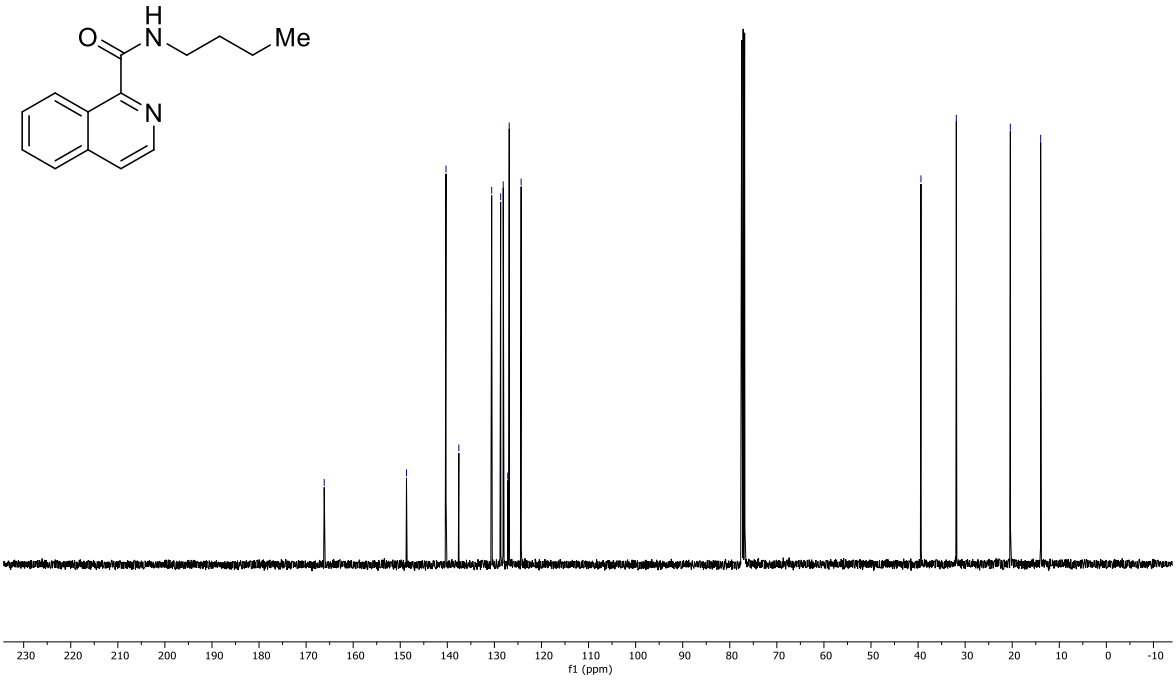

-74.60
Me
N
OH
O
HO
O
CF3
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)

N-Butylisoquinoline-1-carboxamide (9b)

^{1}H

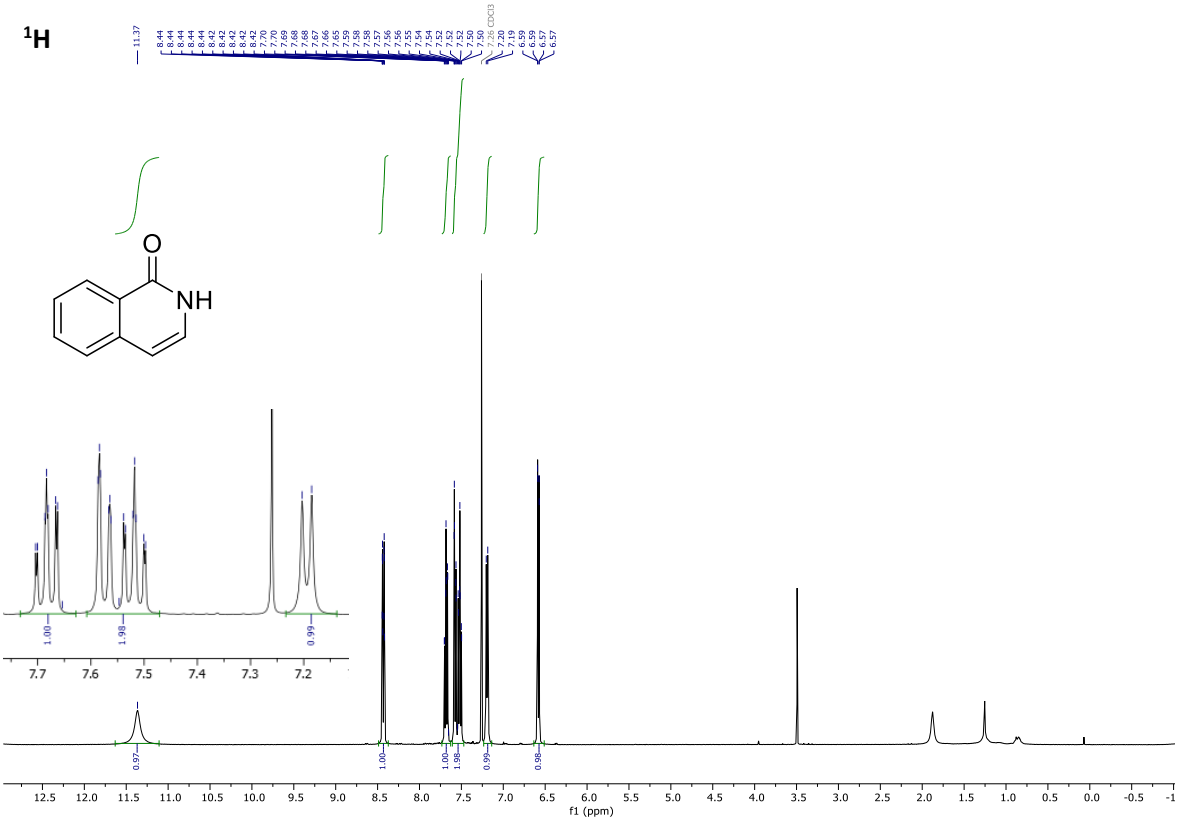


^{13}C

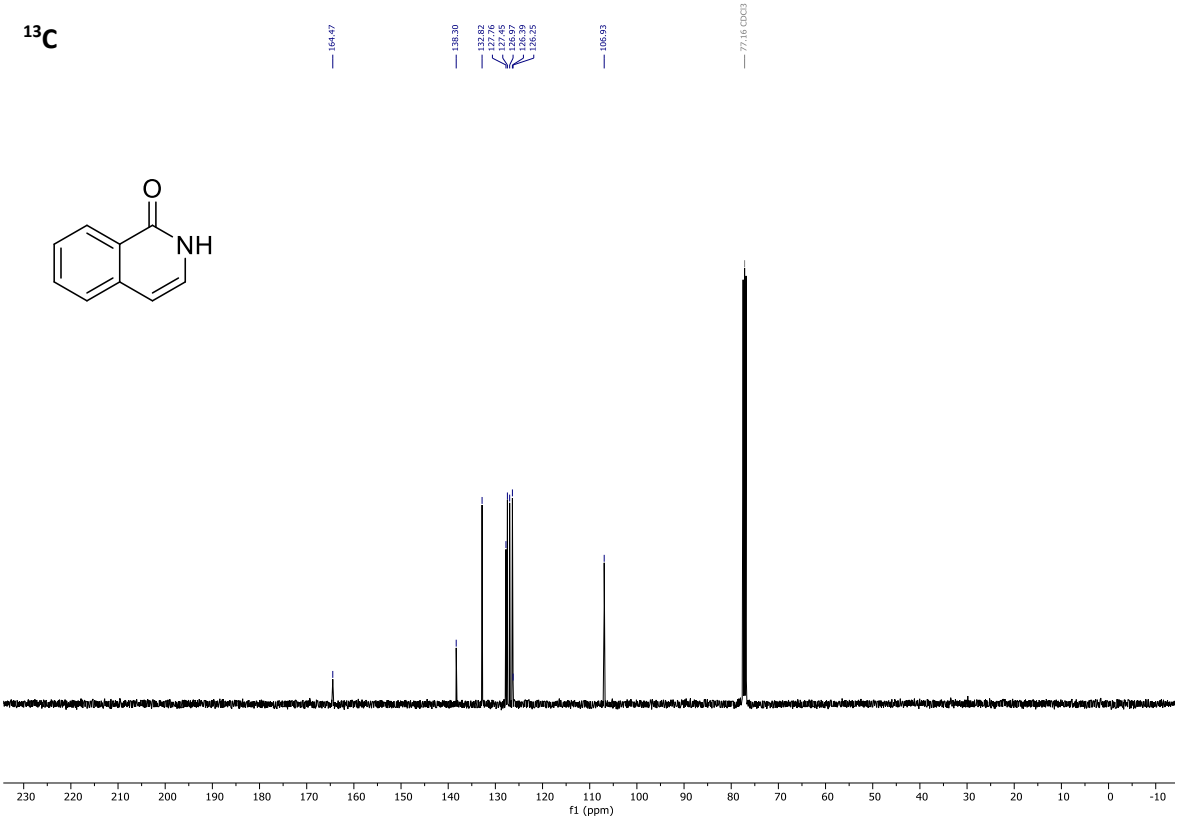


Isoquinolin-1(2*H*)-one (10b)

^{1}H

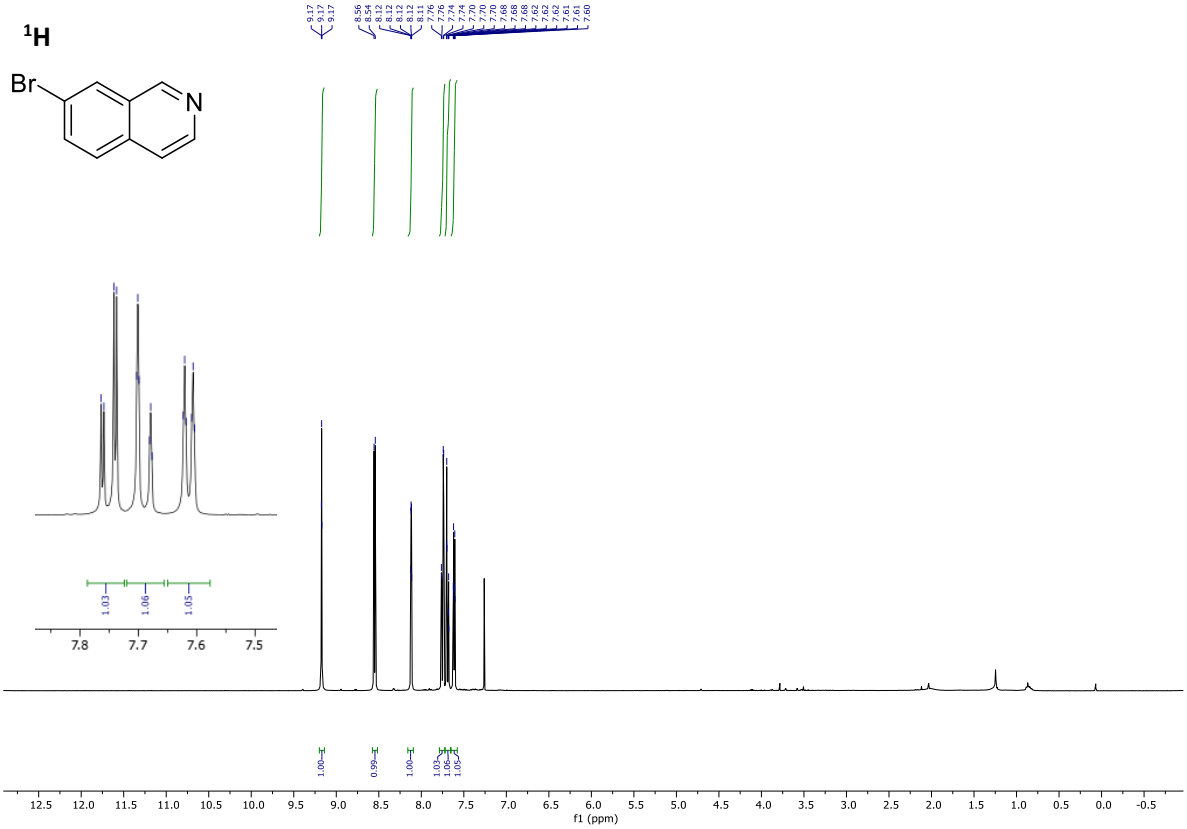


^{13}C

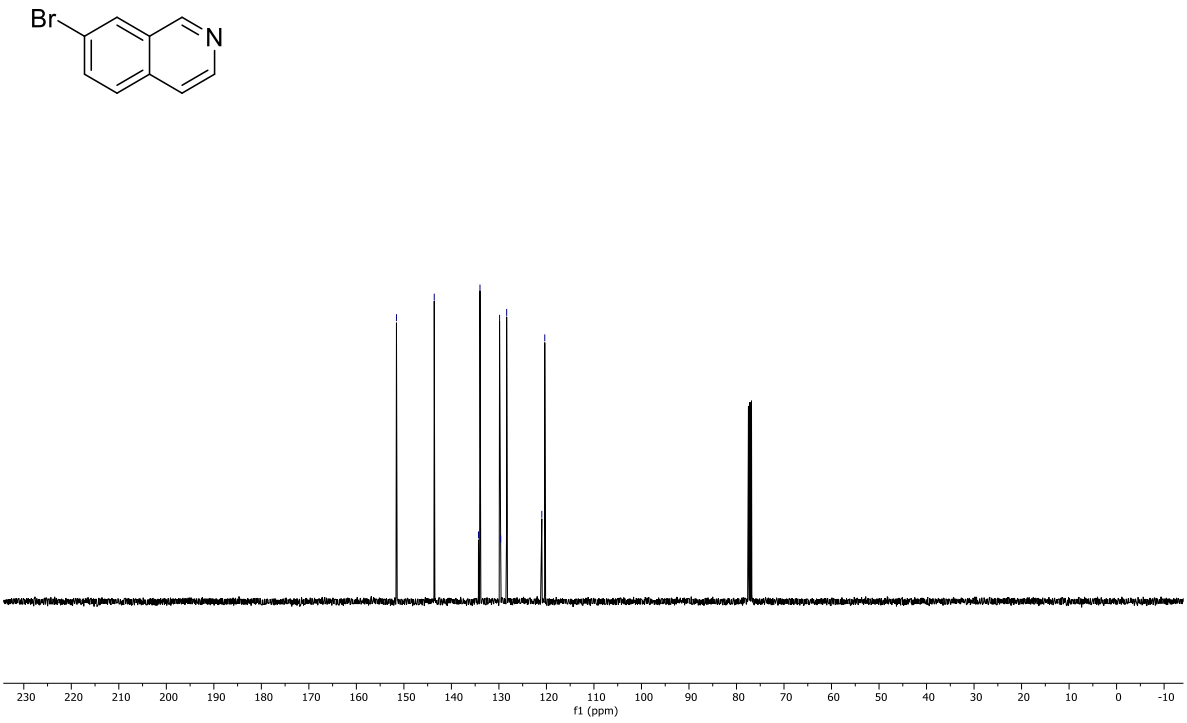


7-Bromoisoquinoline (11b)

^{1}H

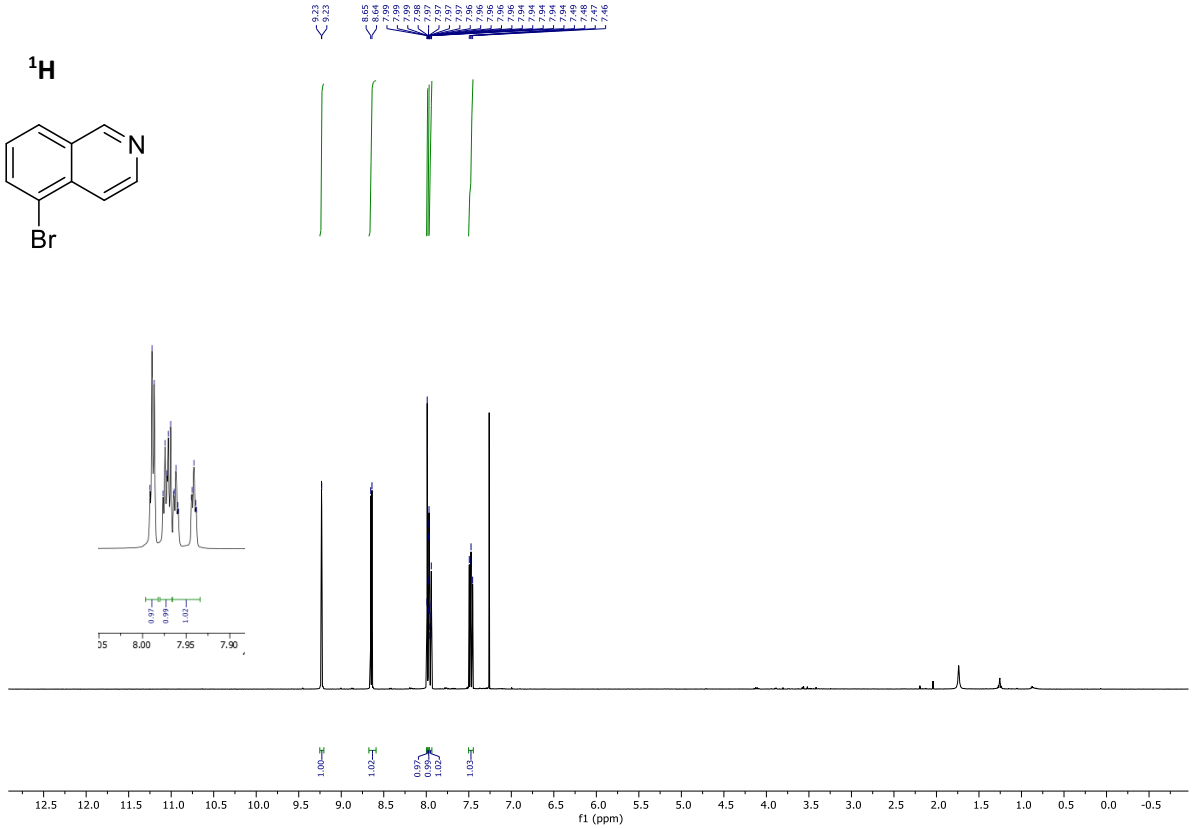


^{13}C

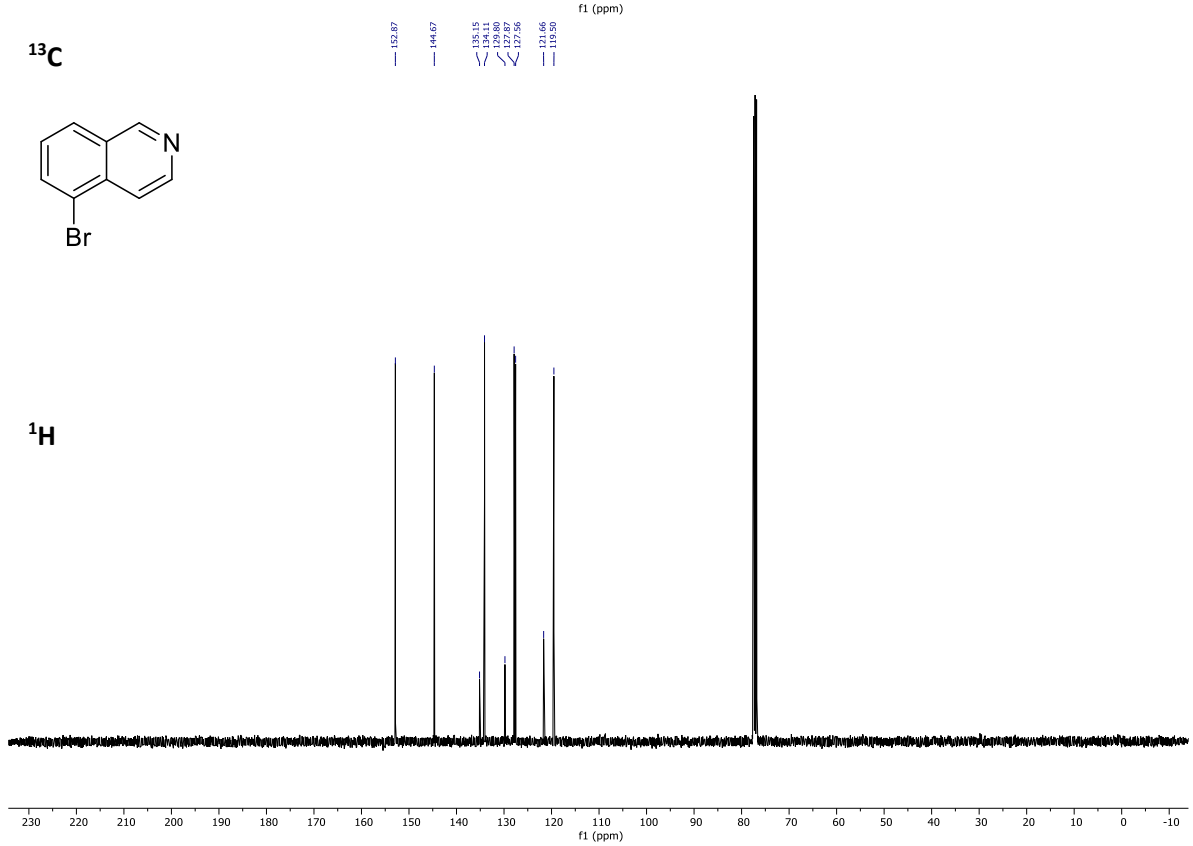


5-Bromoisoquinoline (12b)

^{1}H



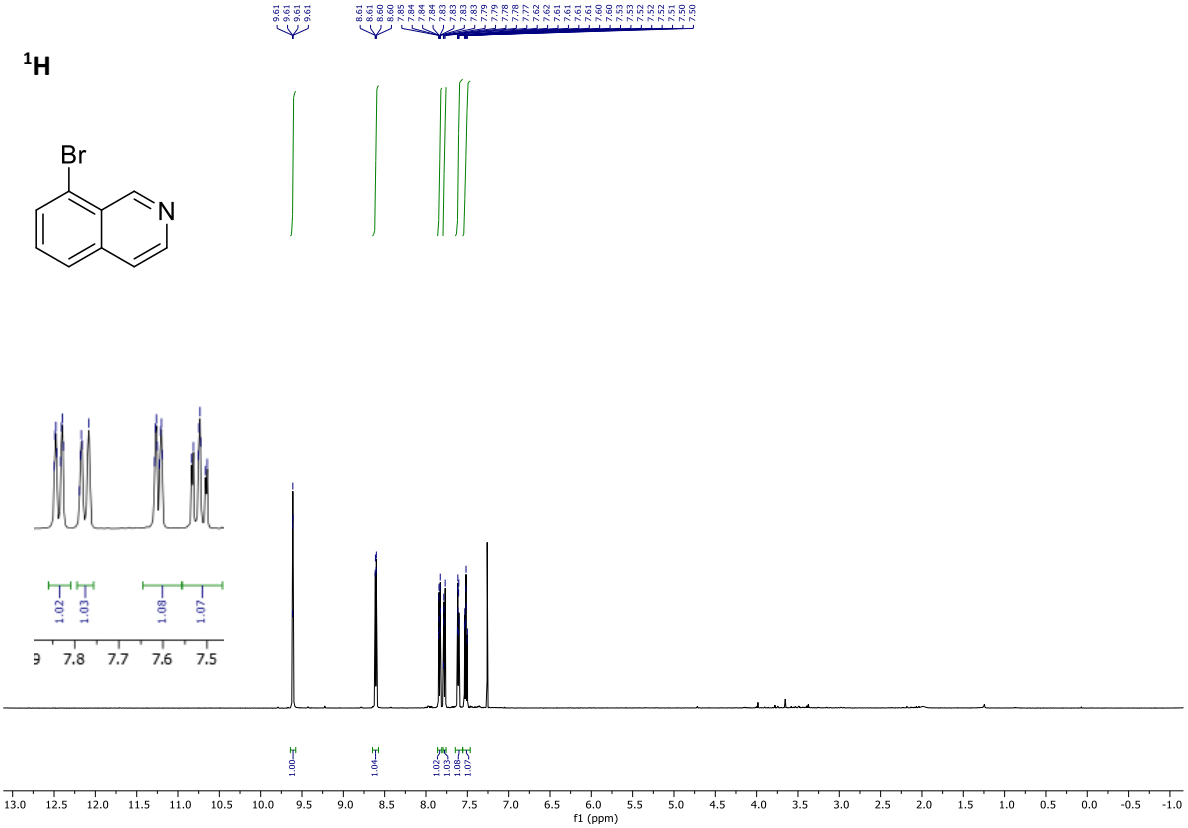
^{13}C



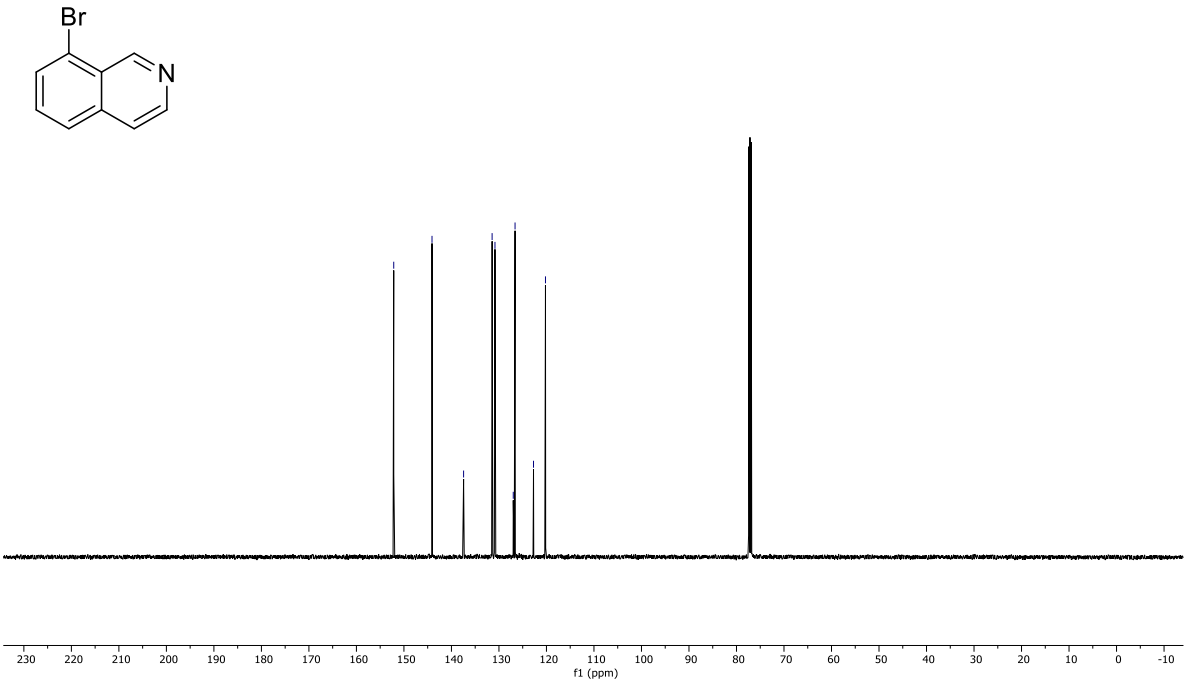
^{1}H

8-Bromoisoquinoline (13b)

^{1}H

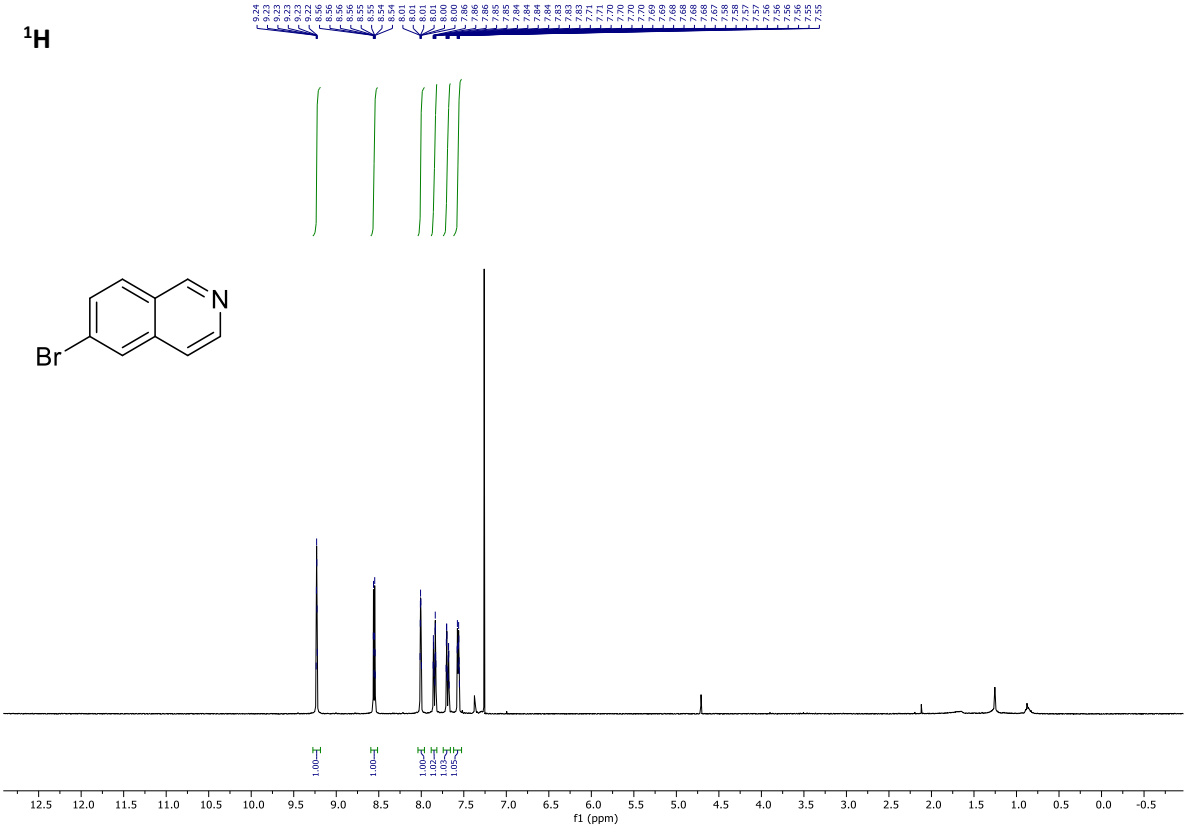


^{13}C

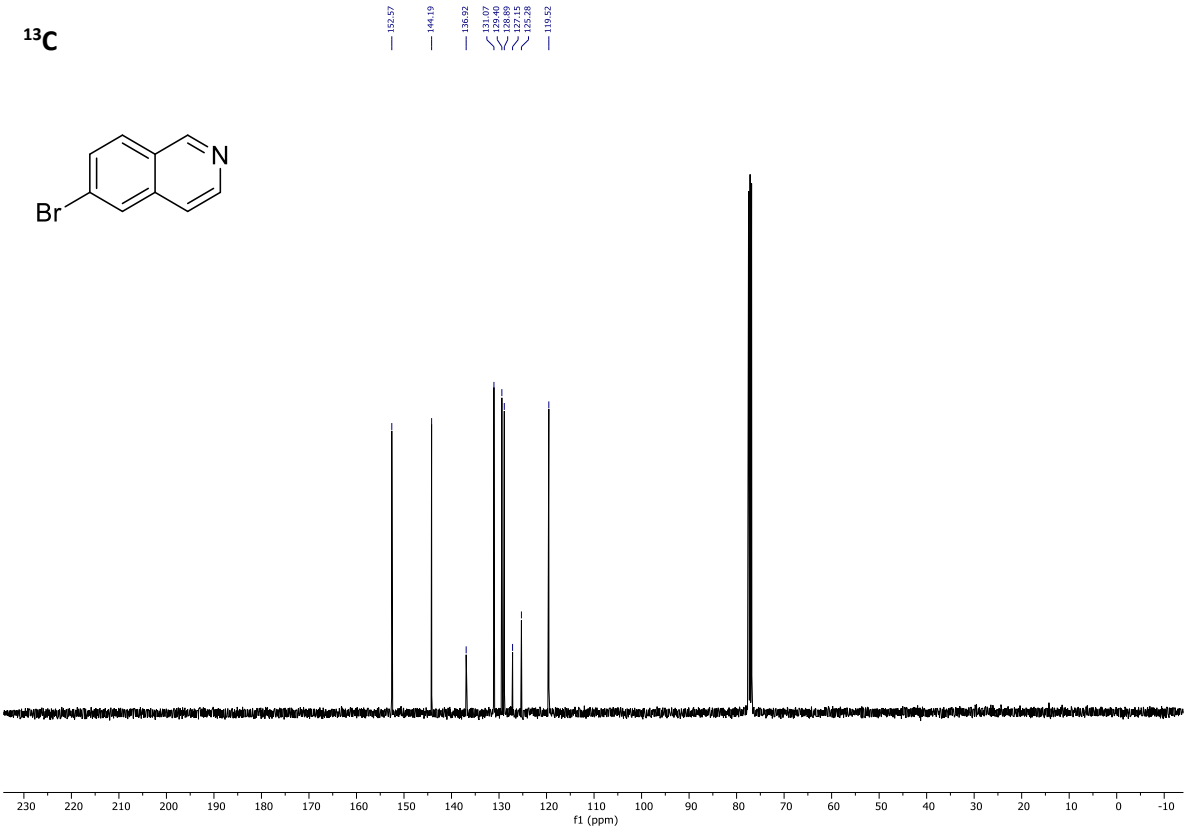


6-Bromoisoquinoline (14b)

^{1}H

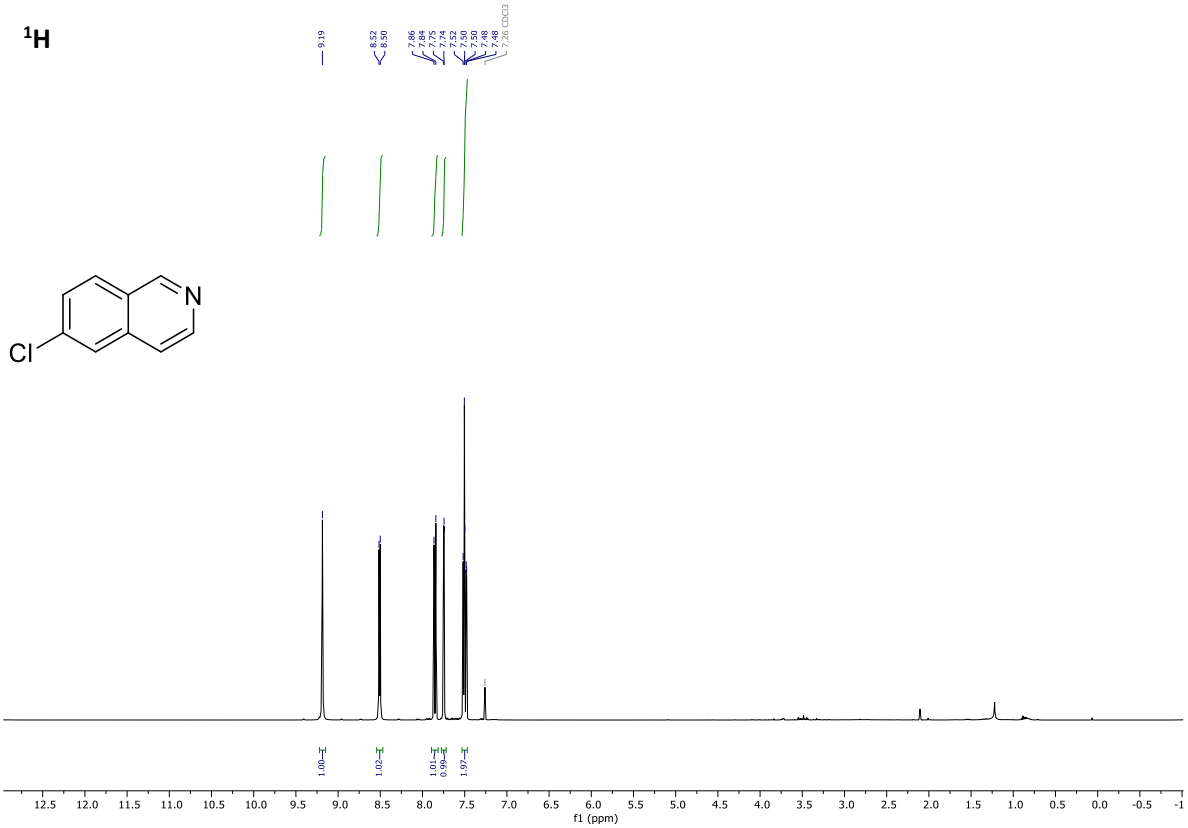


^{13}C

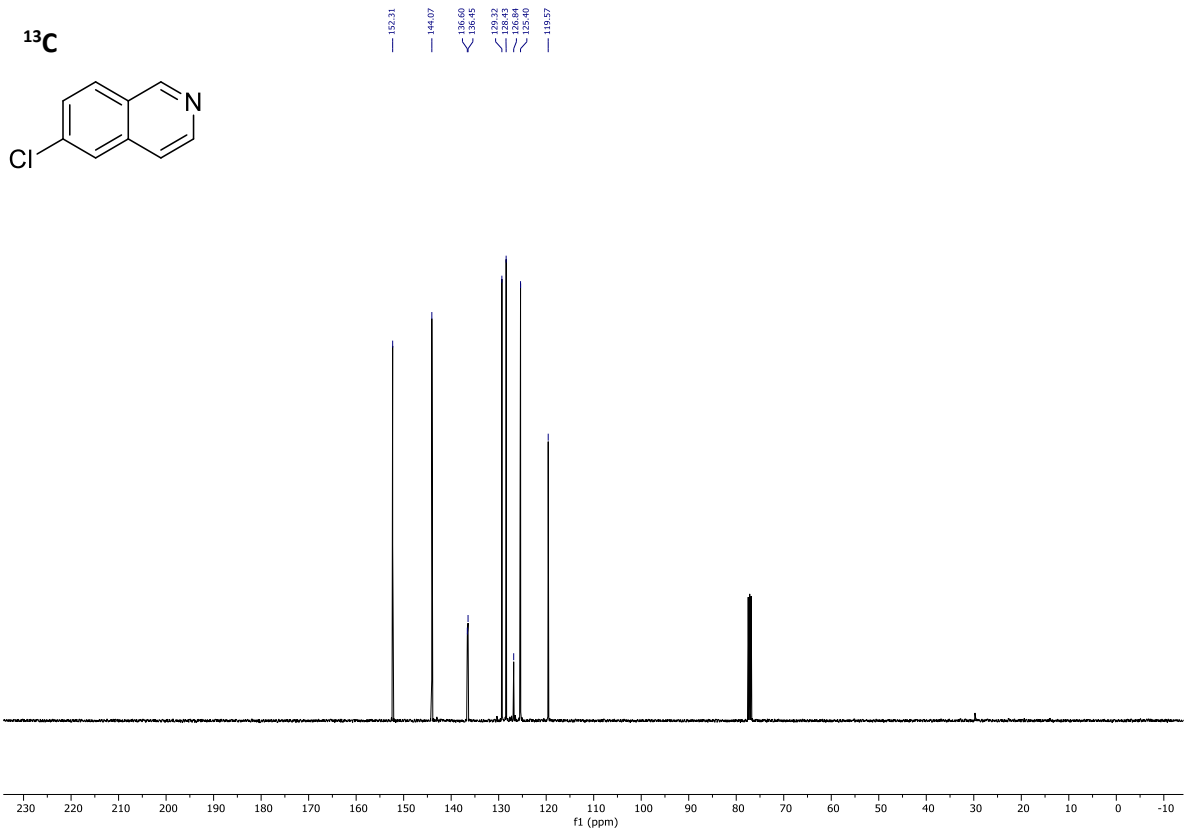


6-Chloroisoquinoline (15b)

^{1}H

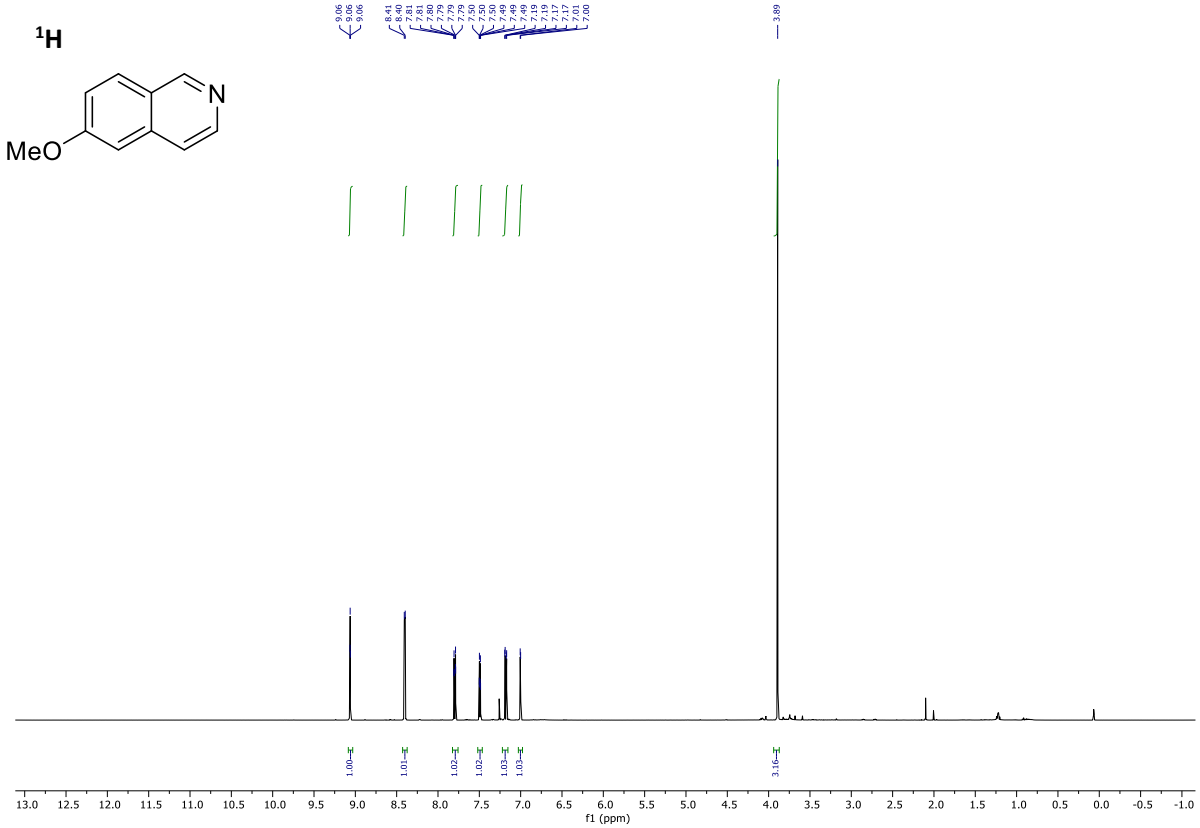


^{13}C

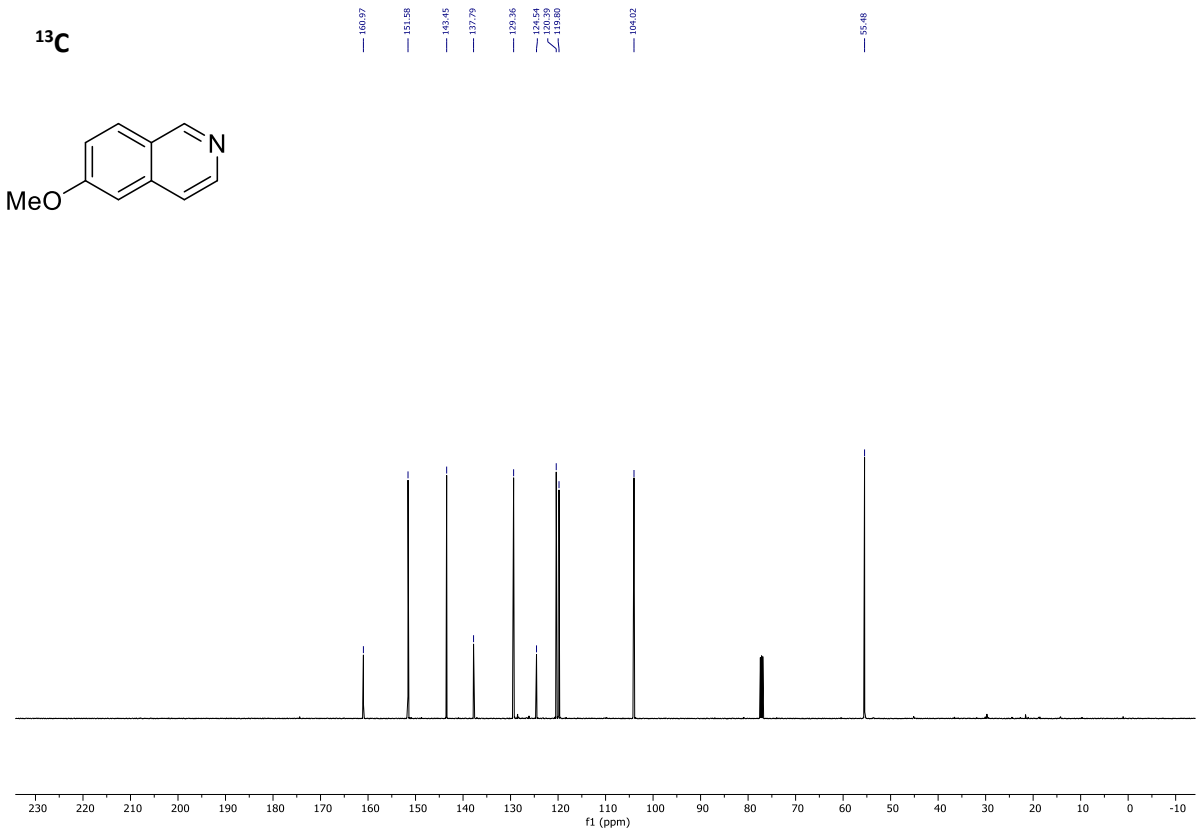


6-Methoxyisoquinoline (16b)

^{1}H

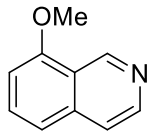


^{13}C

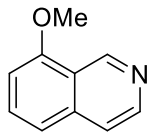


8-Methoxyisoquinoline (17b)

^{1}H

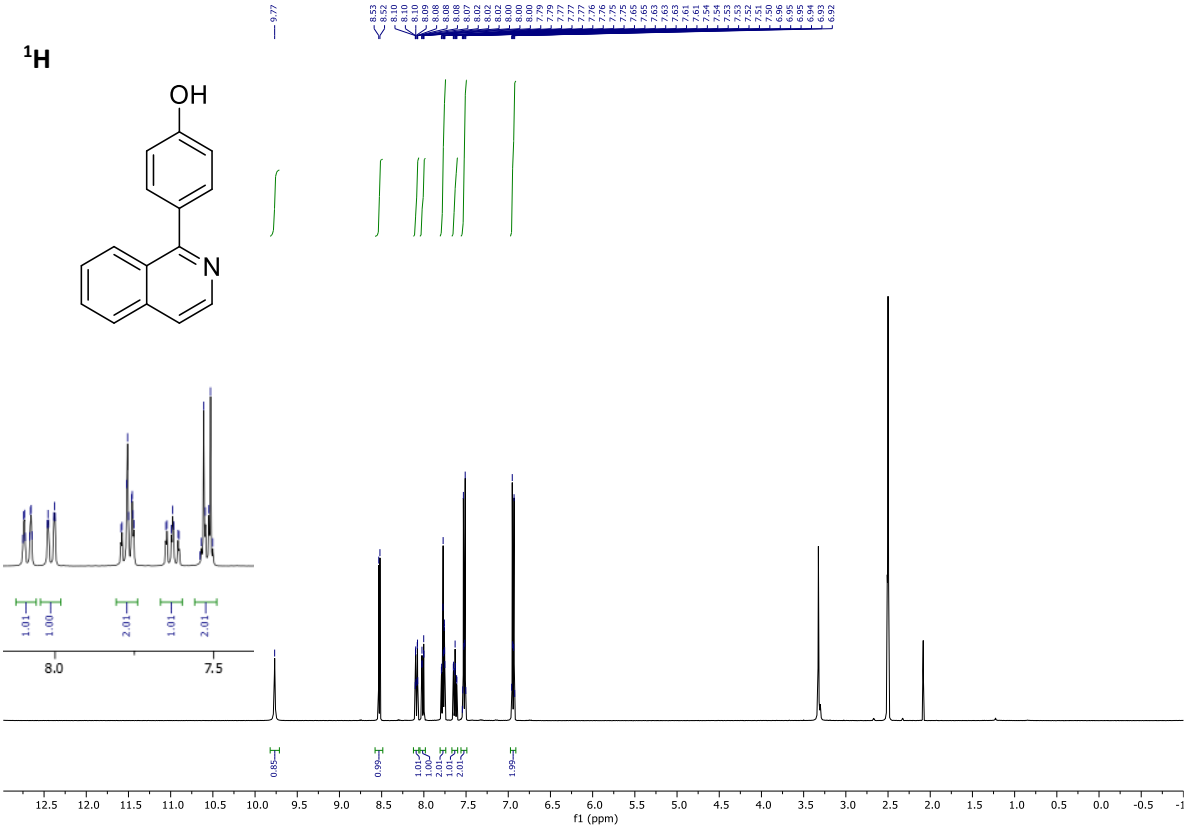


^{13}C

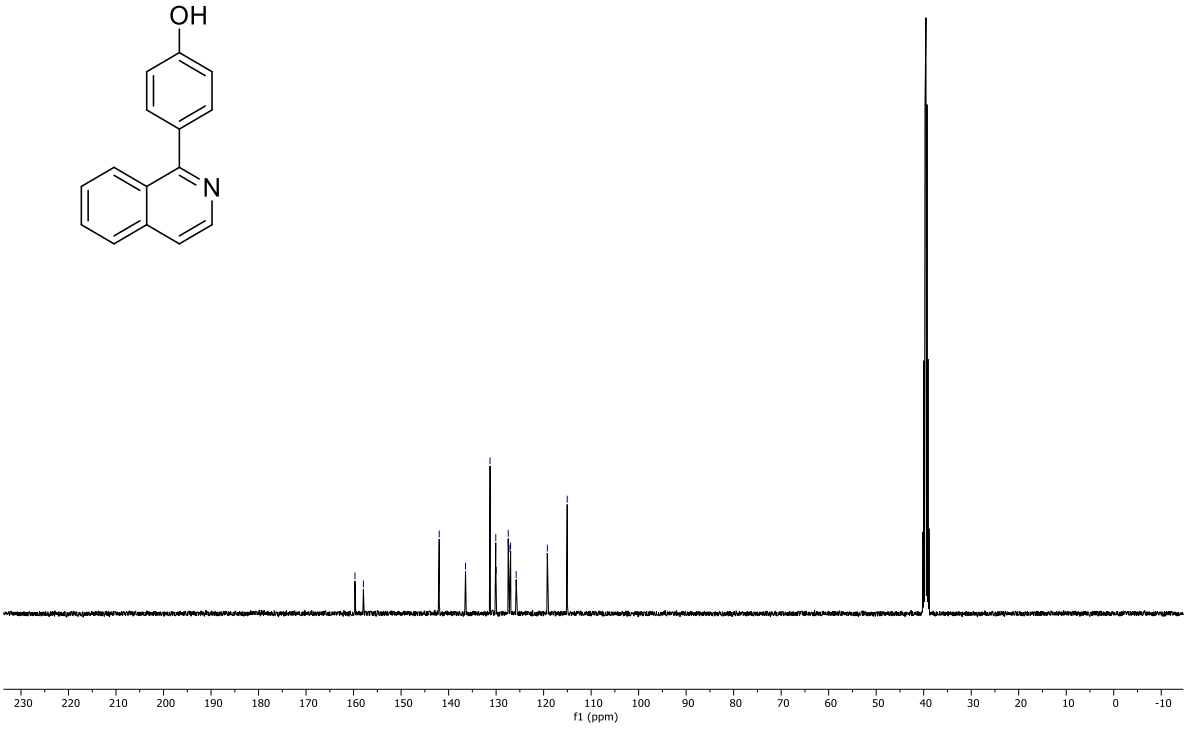


4-(Isoquinolin-1-yl)phenol (18b)

^{1}H

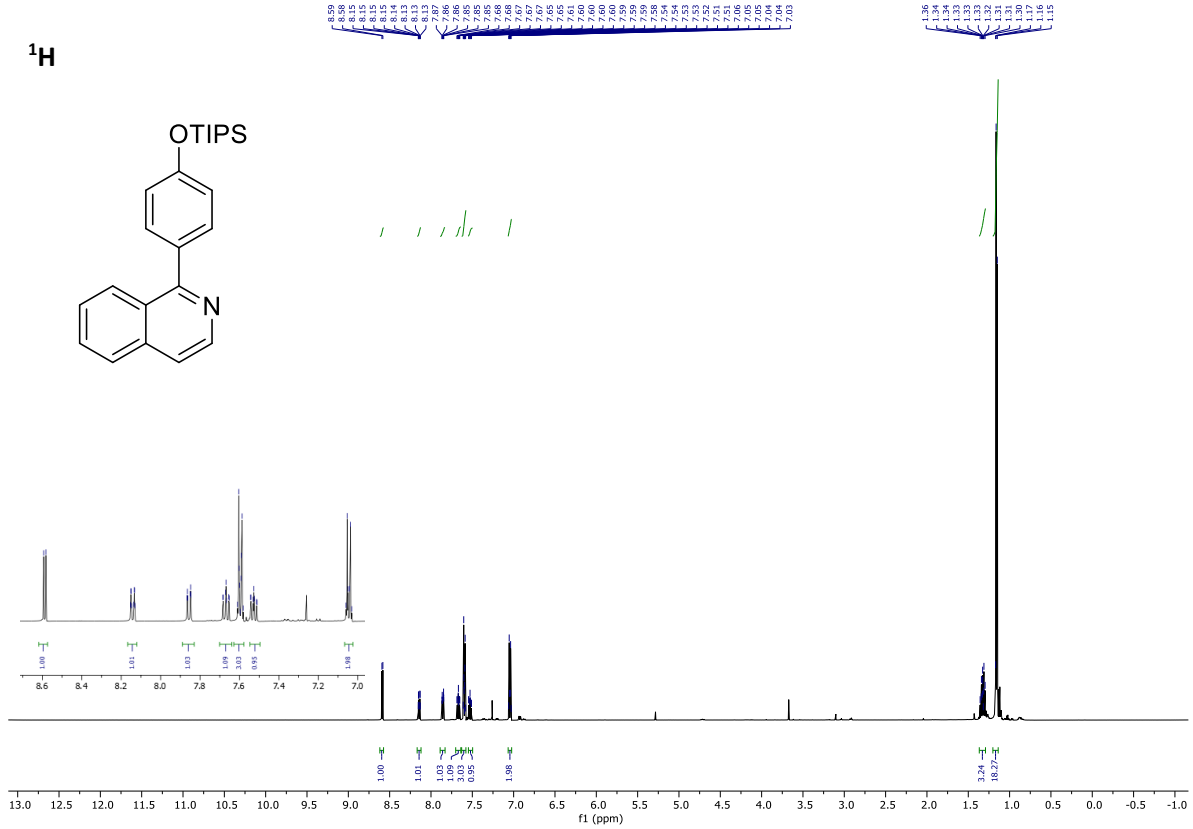


^{13}C

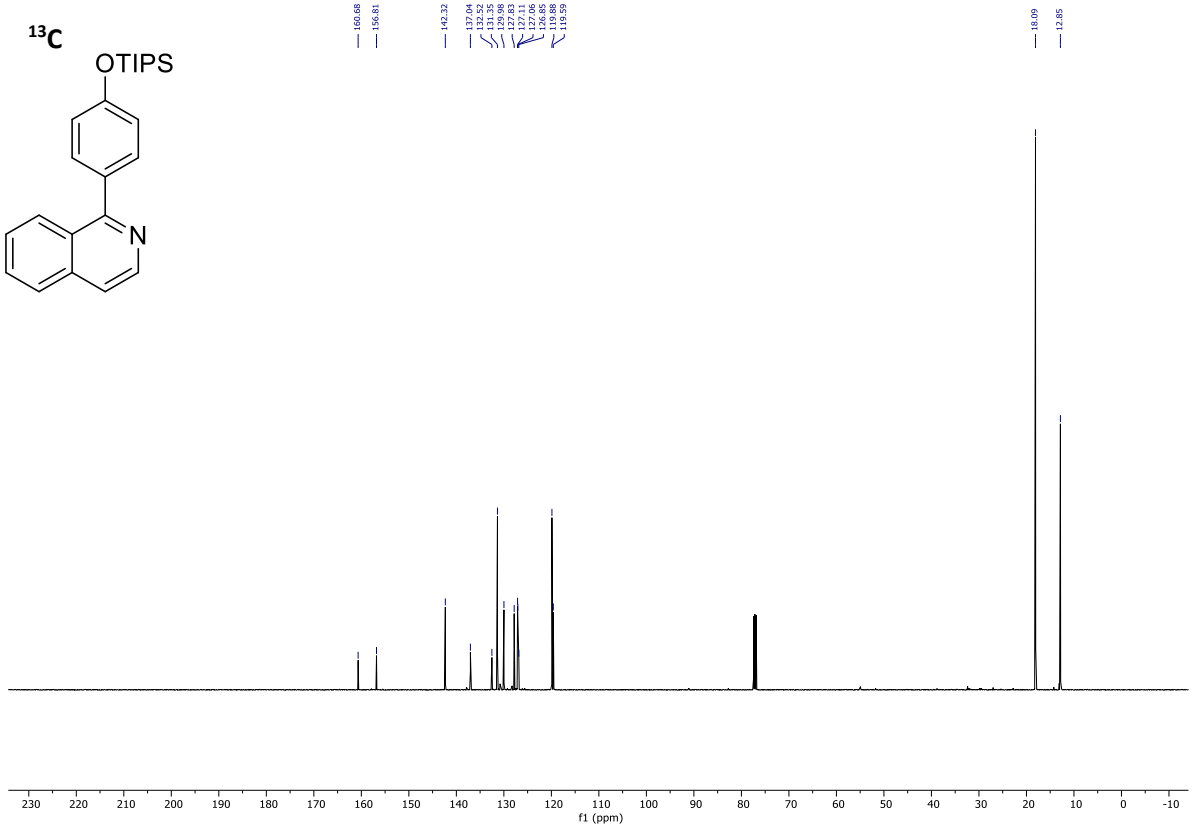


1-(4-((Triisopropylsilyl)oxy)phenyl)isoquinoline (19b)

^{1}H

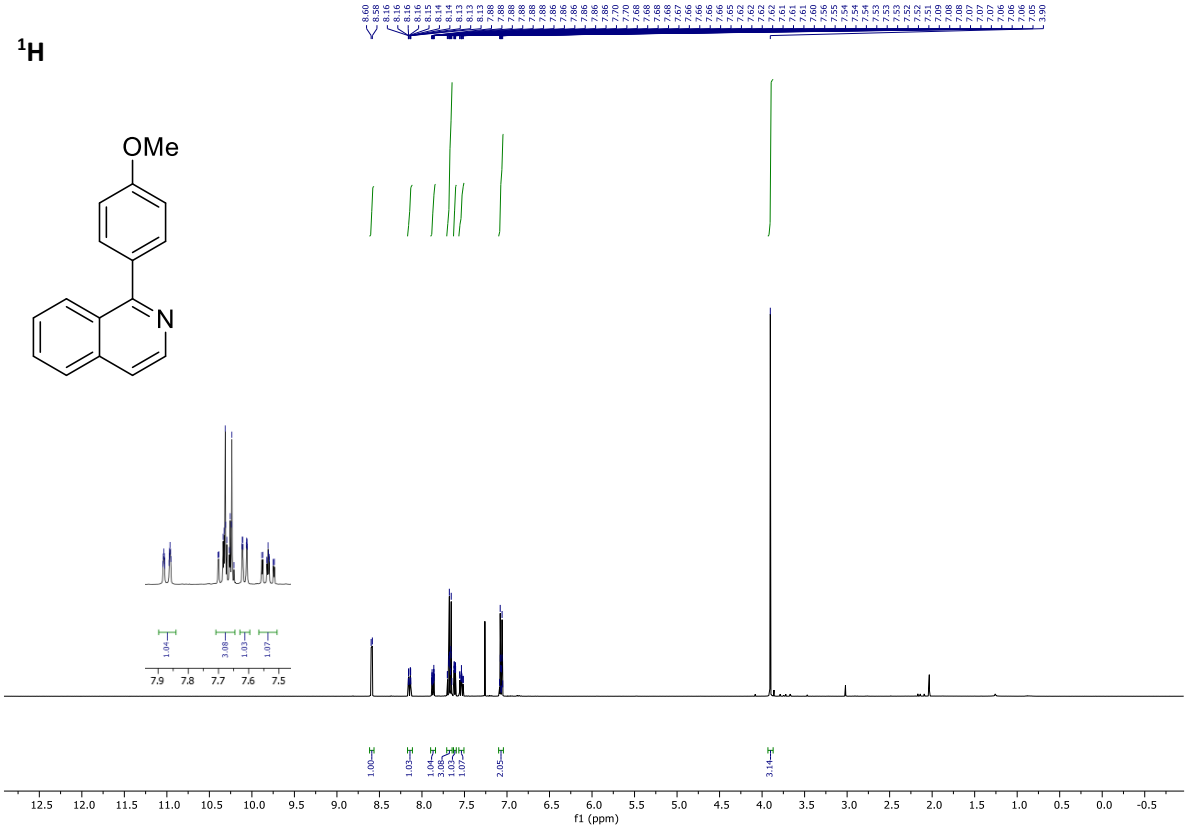


^{13}C

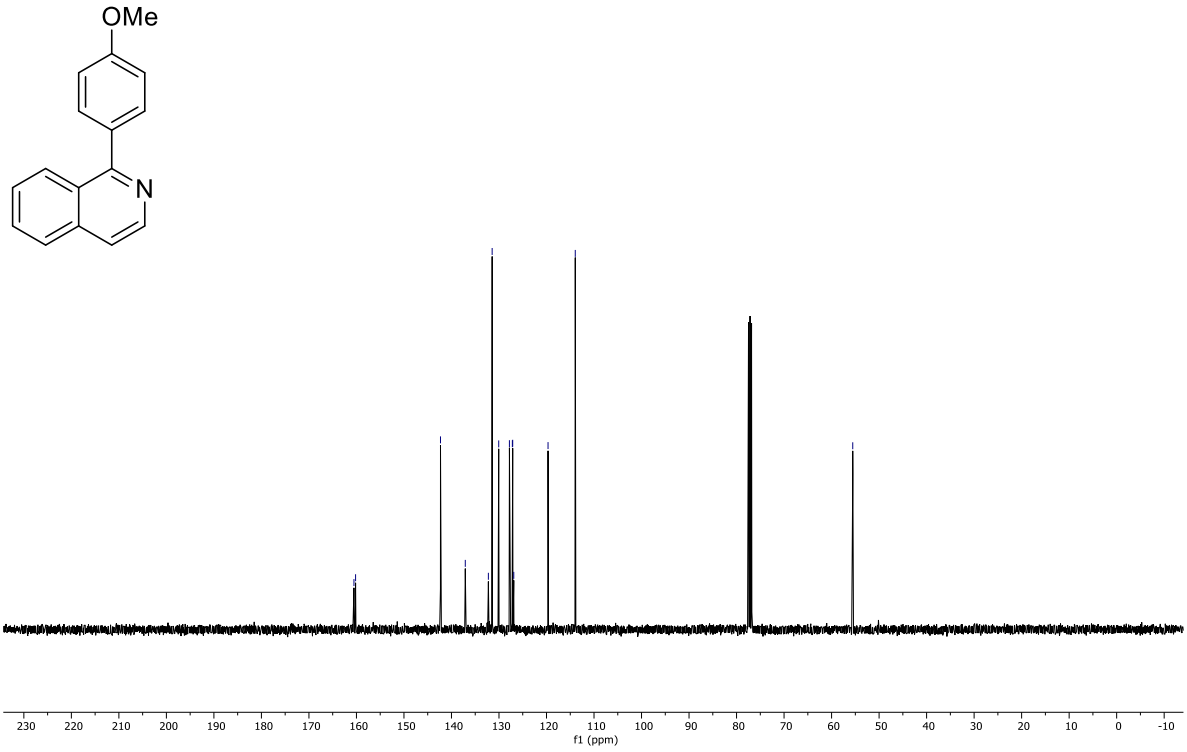


1-(4-Methoxyphenyl)isoquinoline (20b)

^{1}H

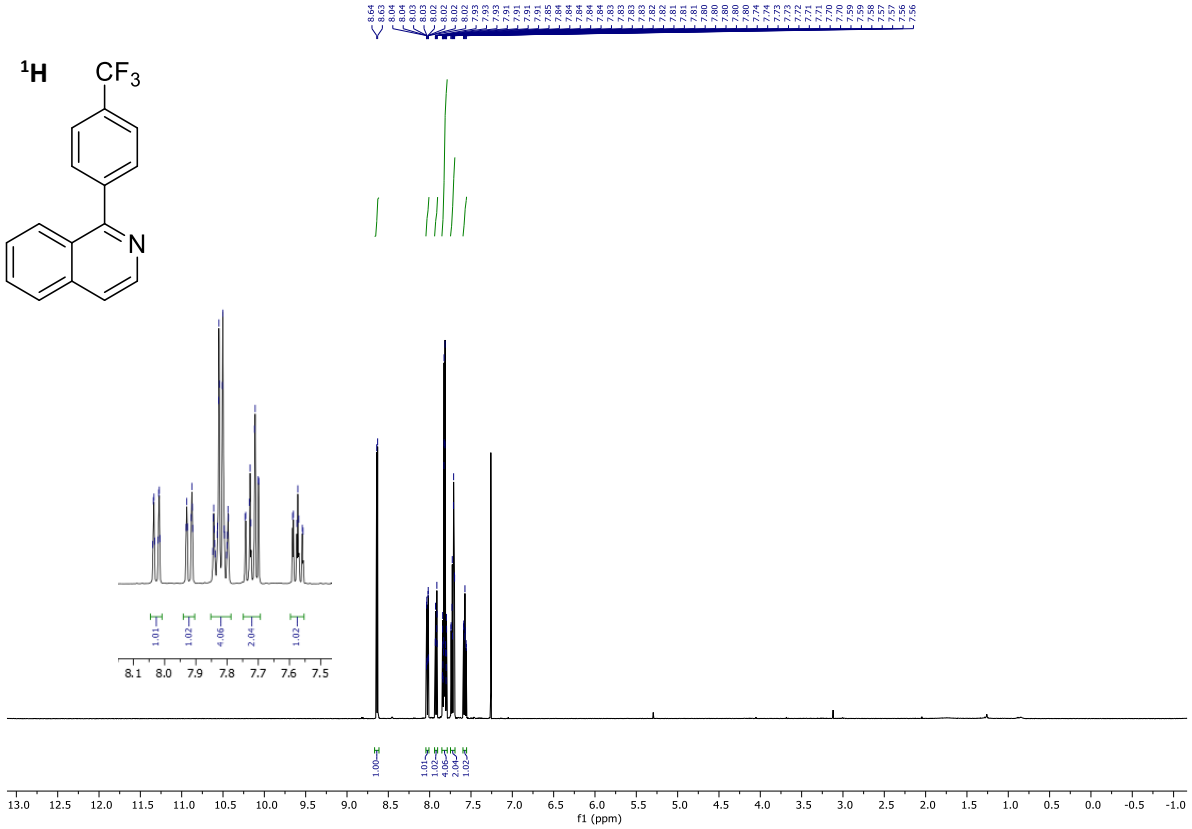


^{13}C

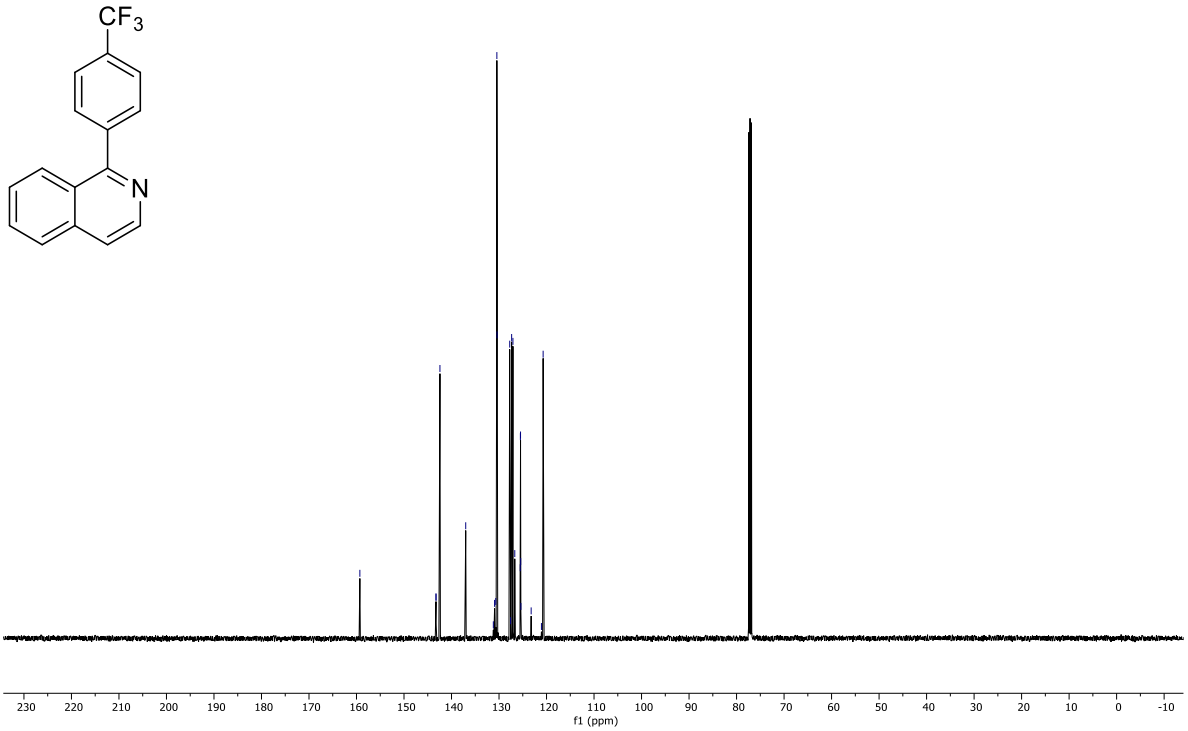


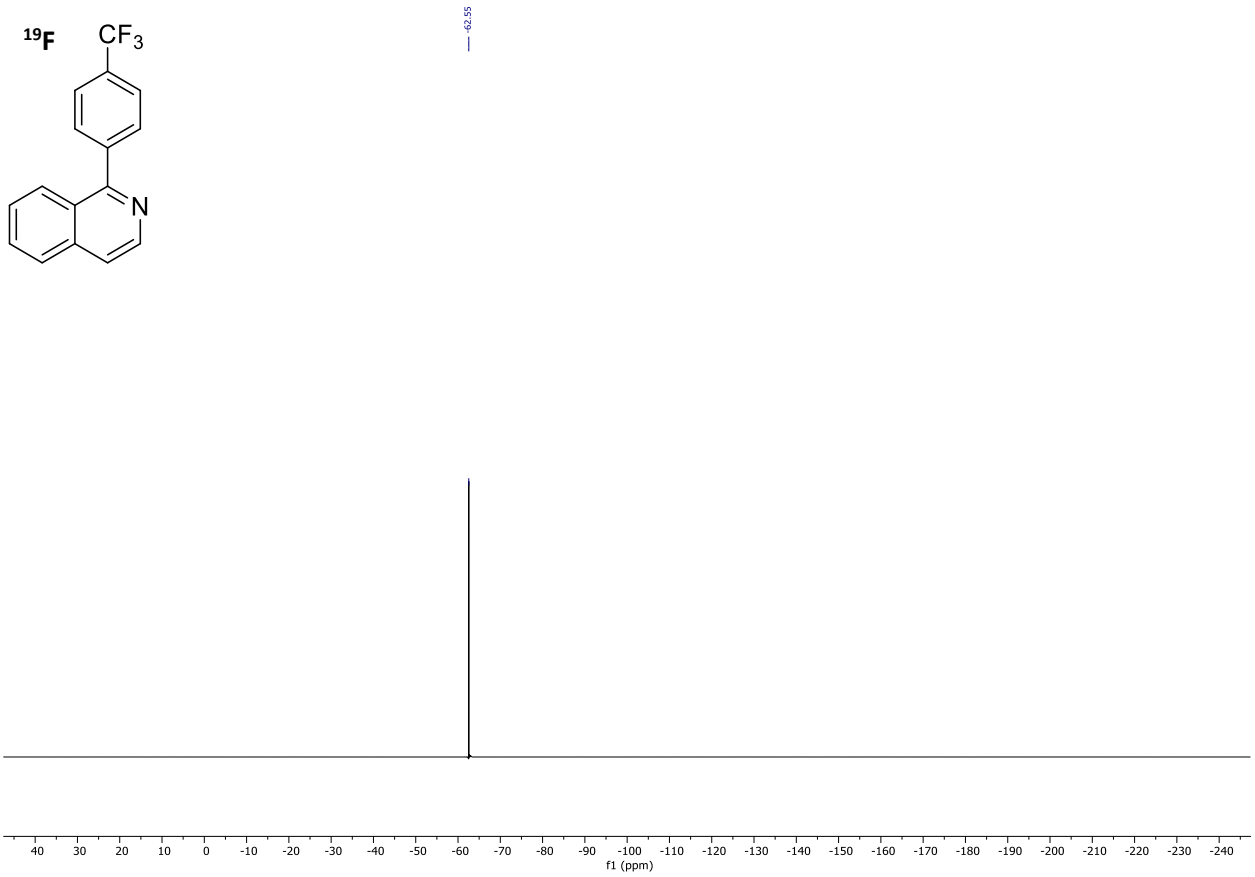
1-(4-(Trifluoromethyl)phenyl)isoquinoline (21b)

^{1}H



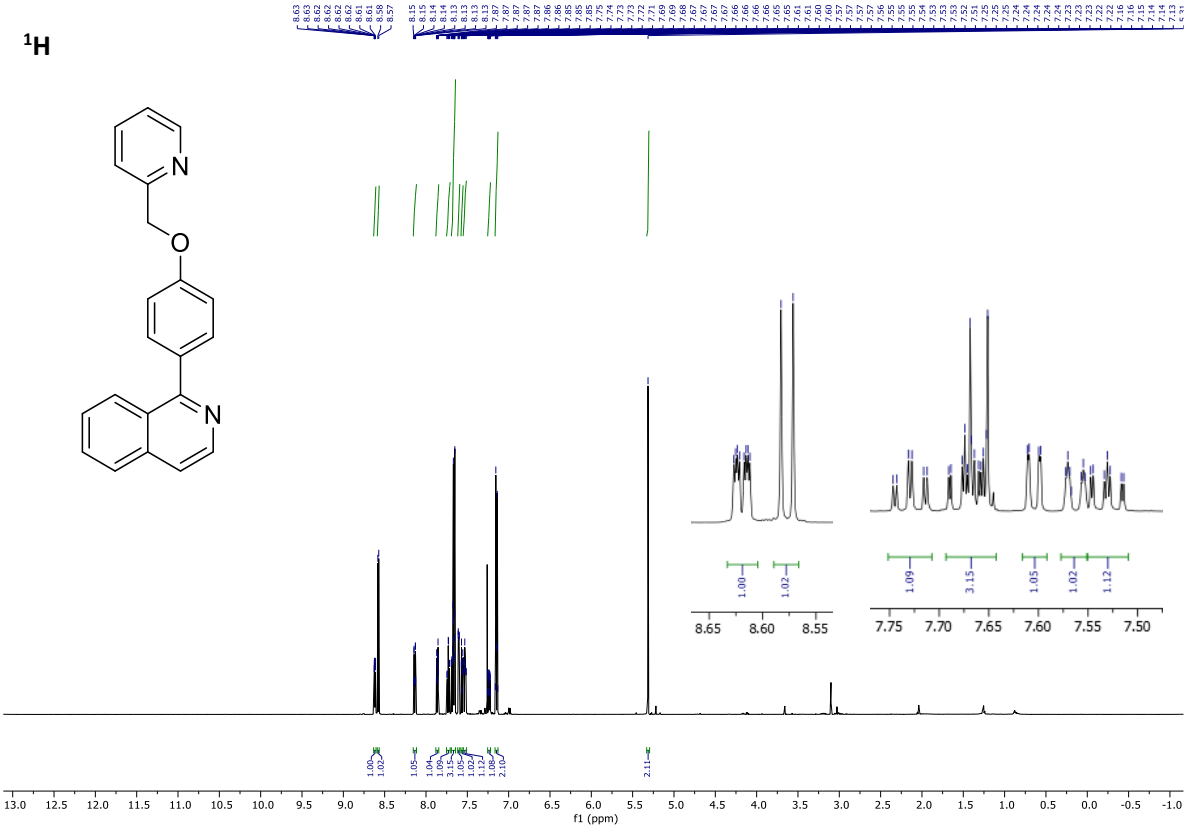
^{13}C



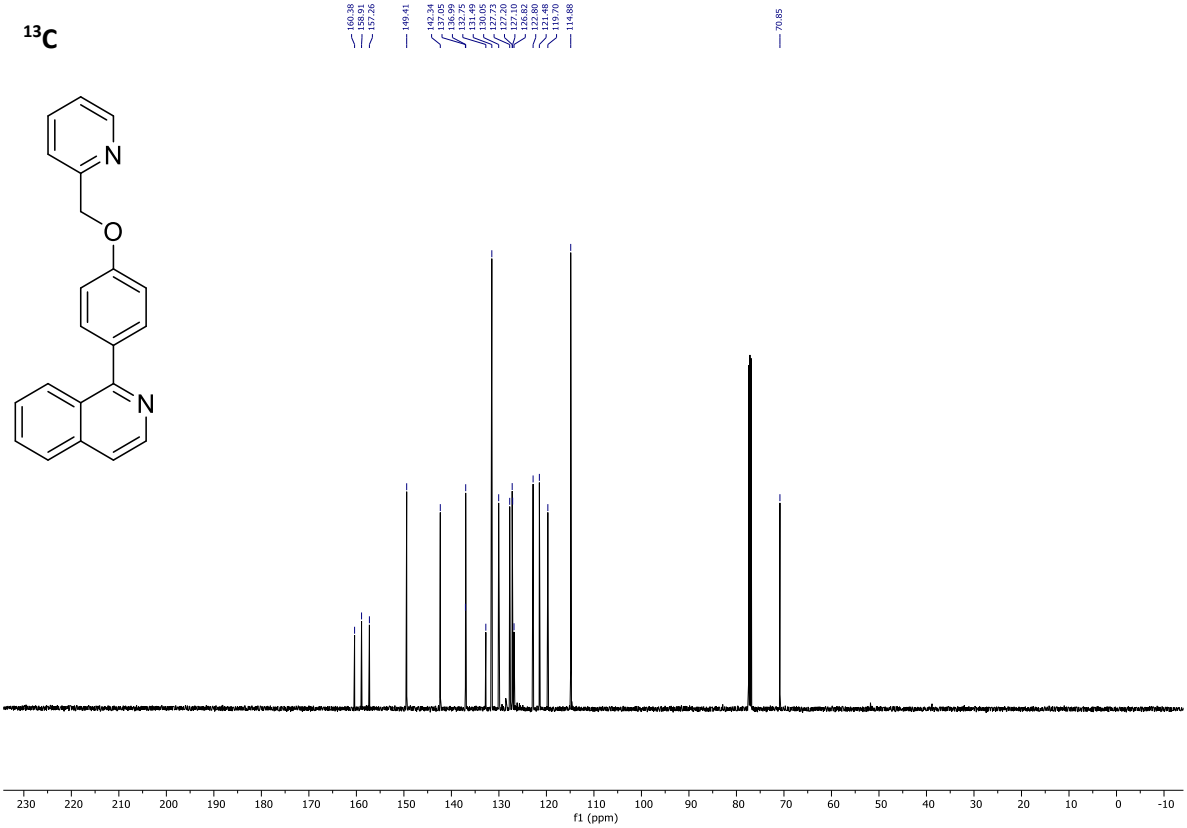

19F
CF3
N
-62.55
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)

1-(4-(Pyridin-2-ylmethoxy)phenyl)isoquinoline (22b)

^{1}H

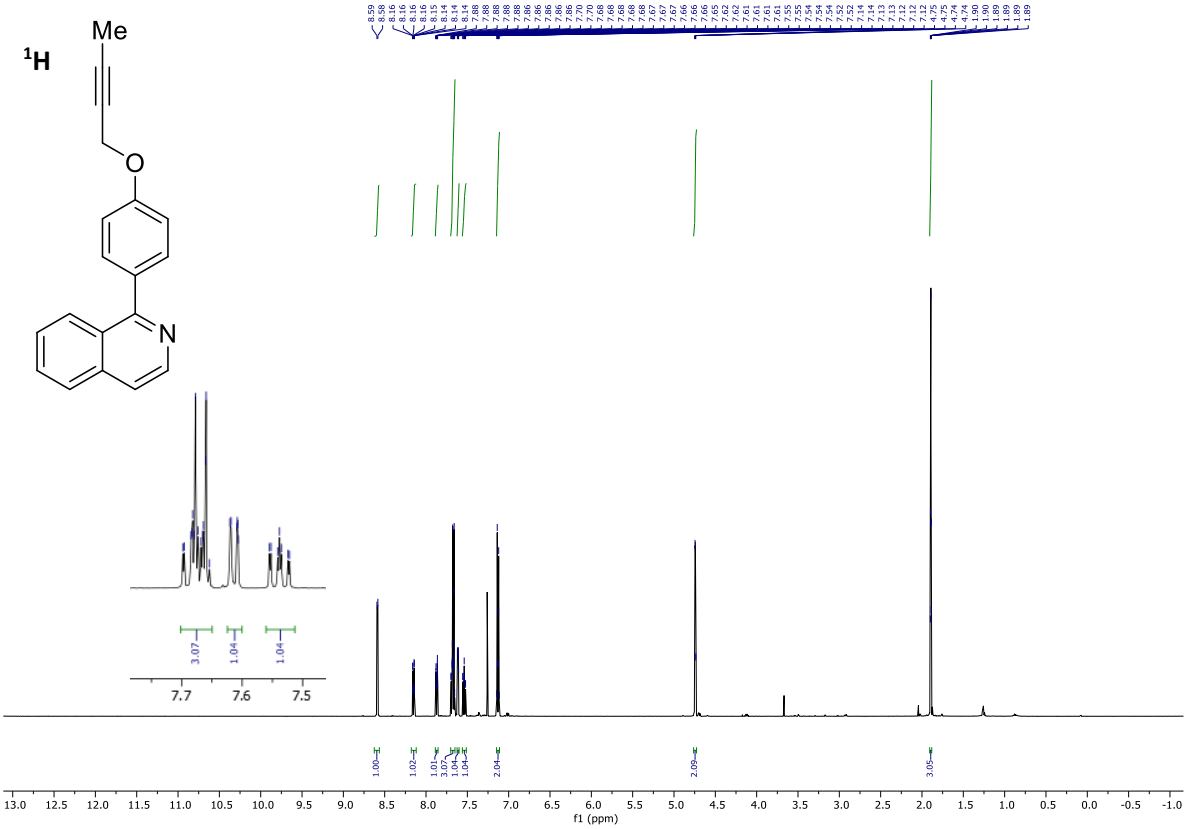


^{13}C

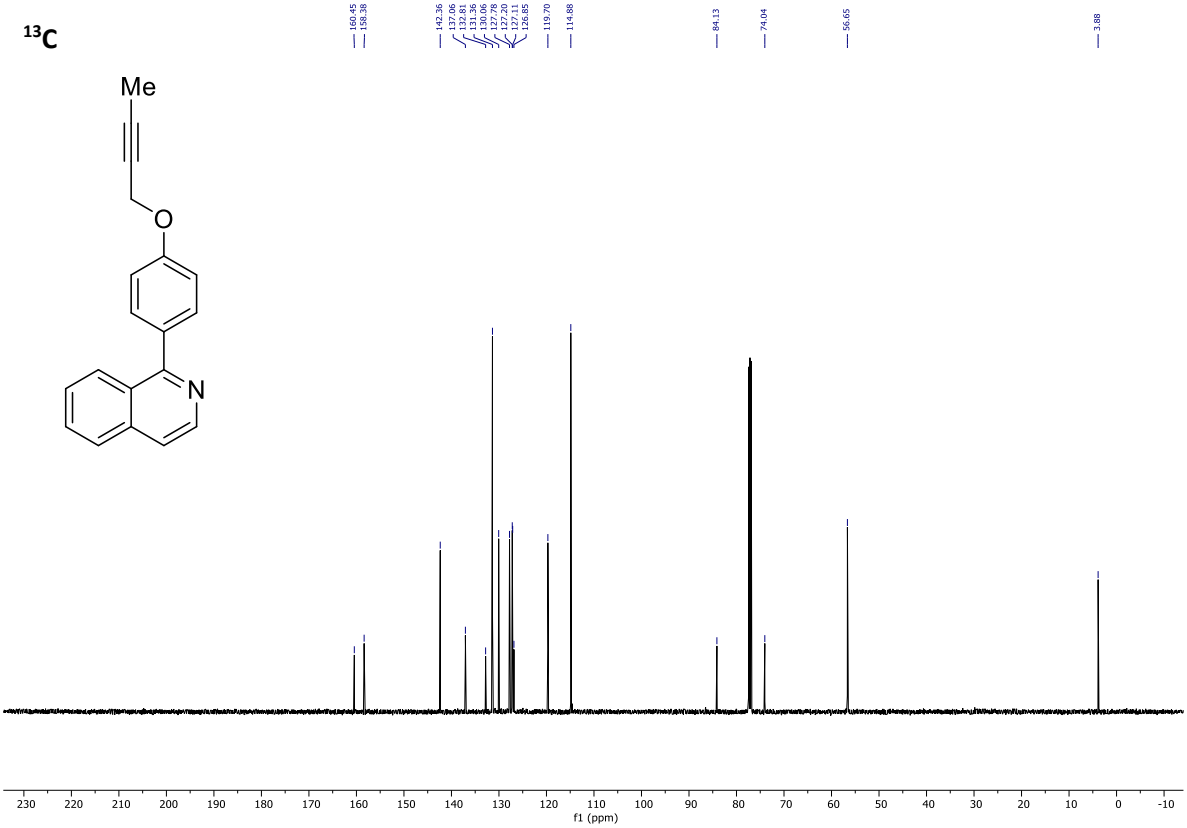


1-(4-(But-2-yn-1-yloxy)phenyl)isoquinoline (23b)

^{1}H

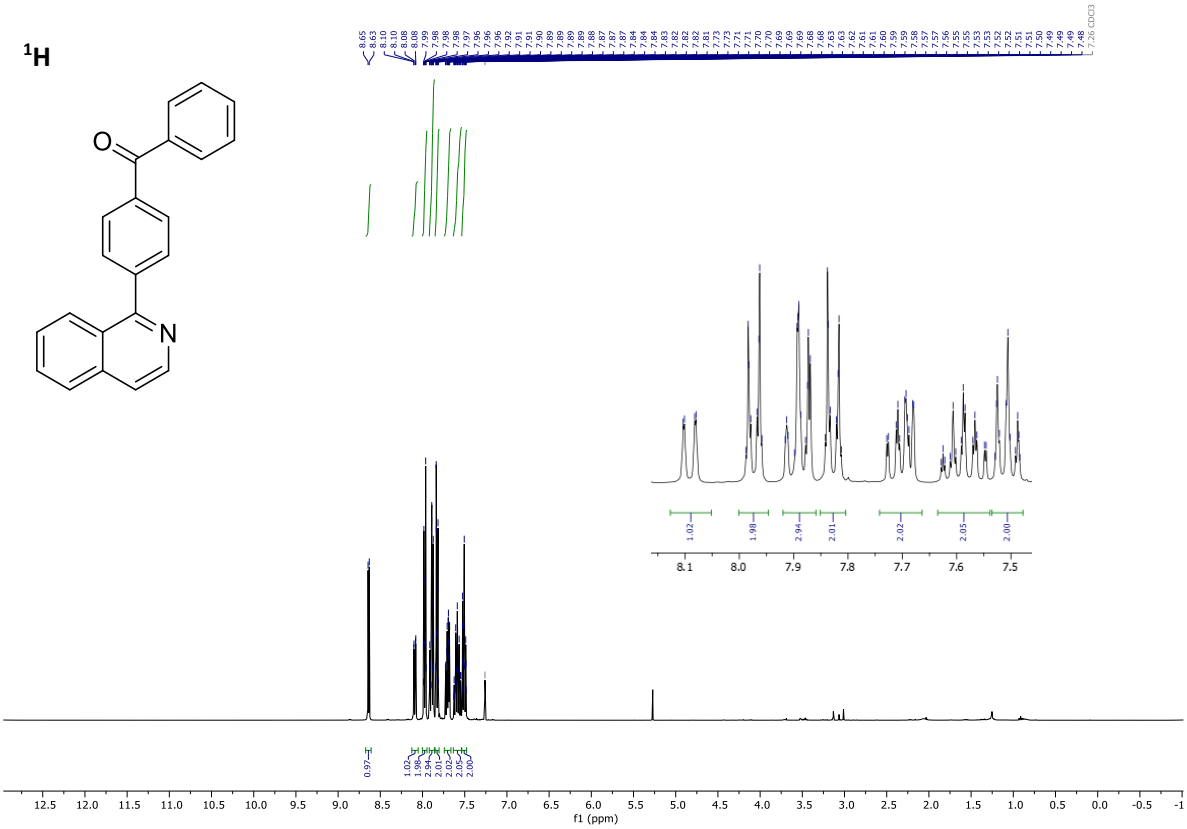


^{13}C

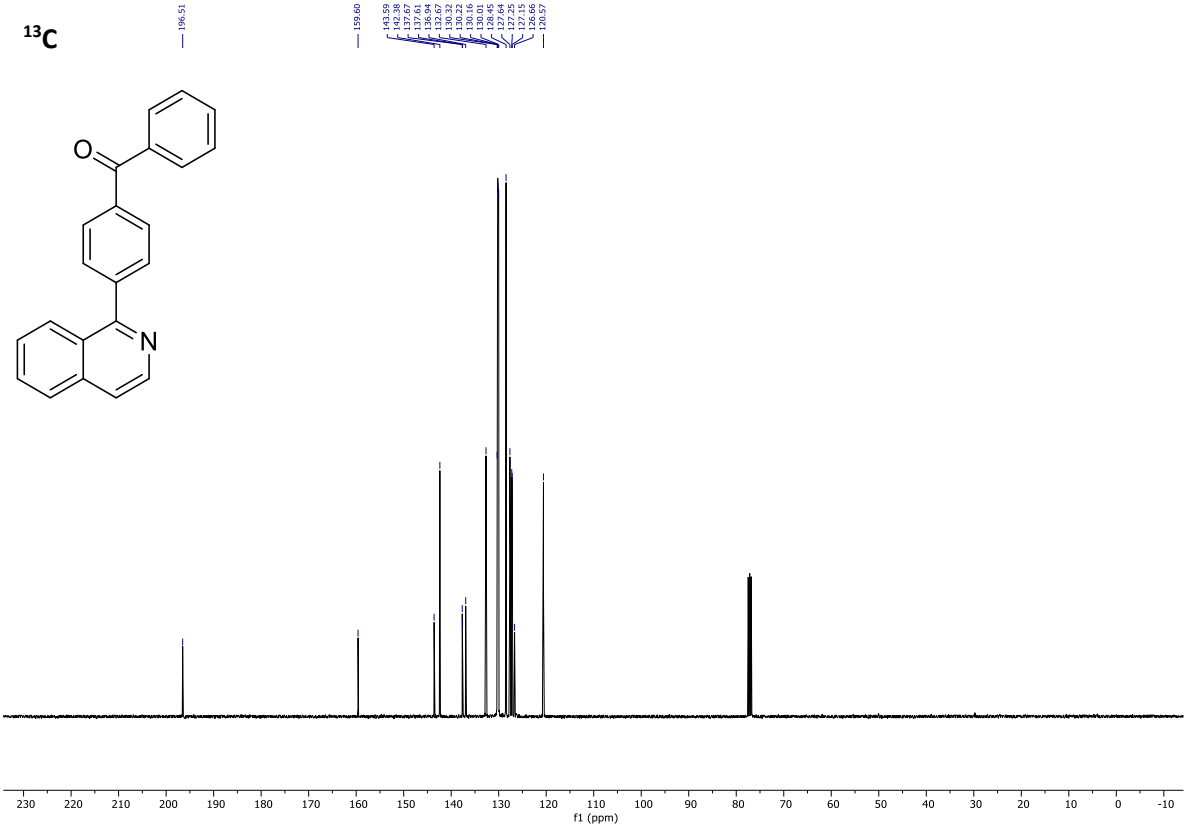


(4-(Isoquinolin-1-yl)phenyl)(phenyl)methanone (24b)

^{1}H

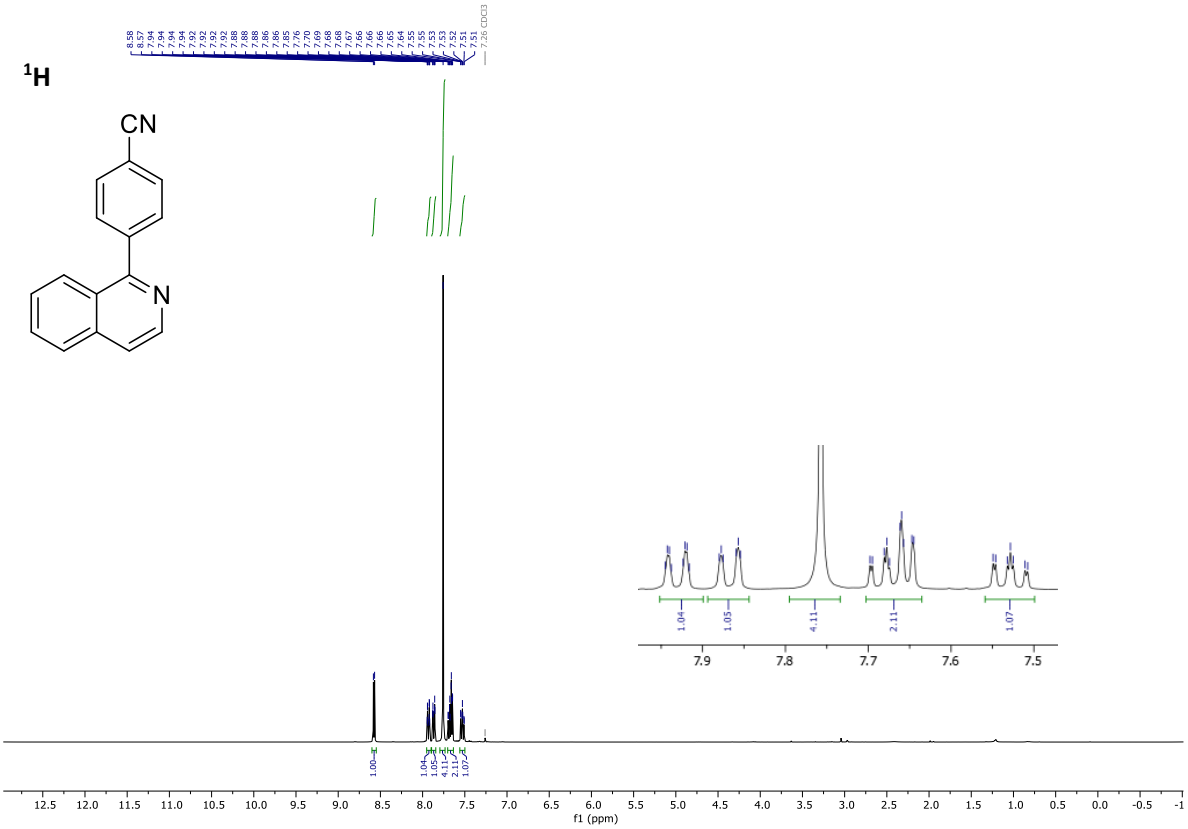


^{13}C

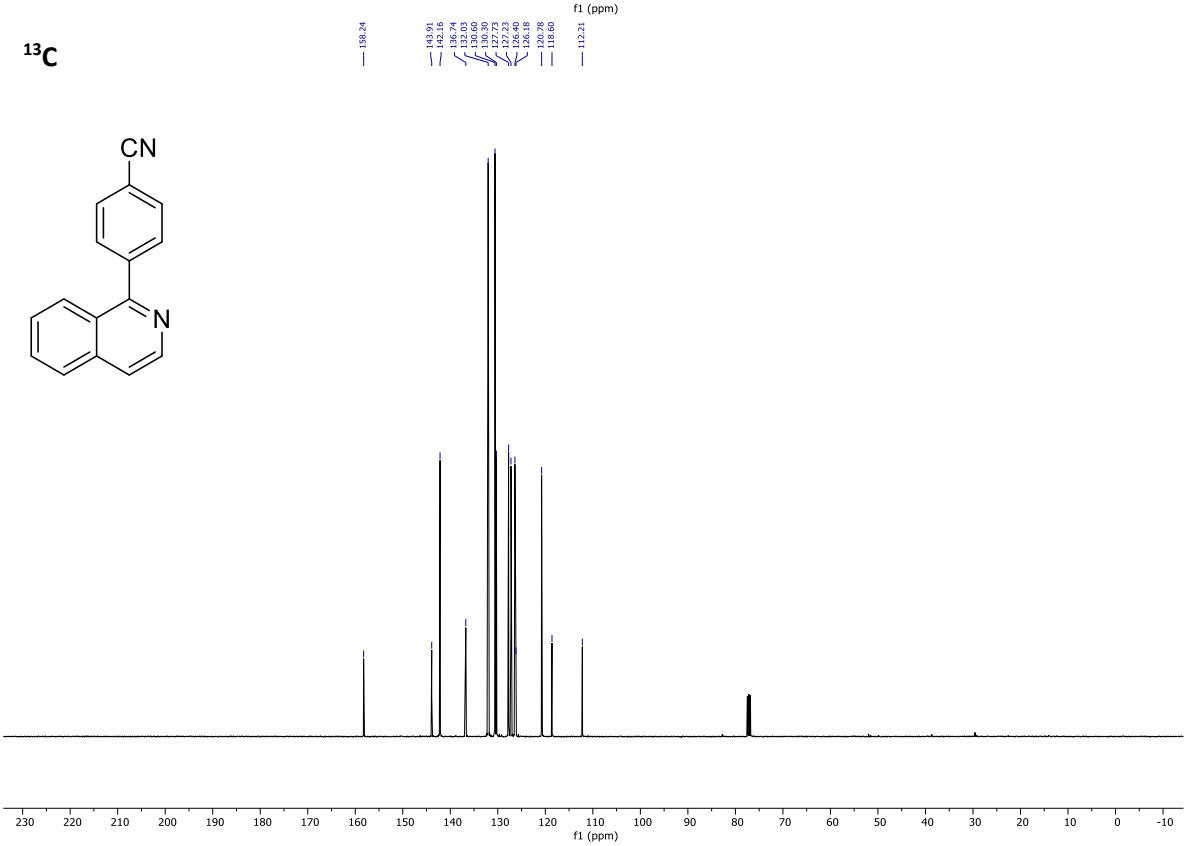


4-(Isoquinolin-1-yl)benzonitrile (25b)

^{1}H

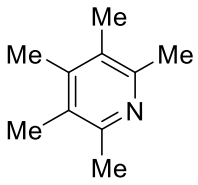


^{13}C

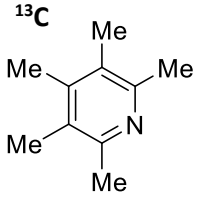


2,3,4,5,6-Pentamethylpyridine (26b)

^{1}H

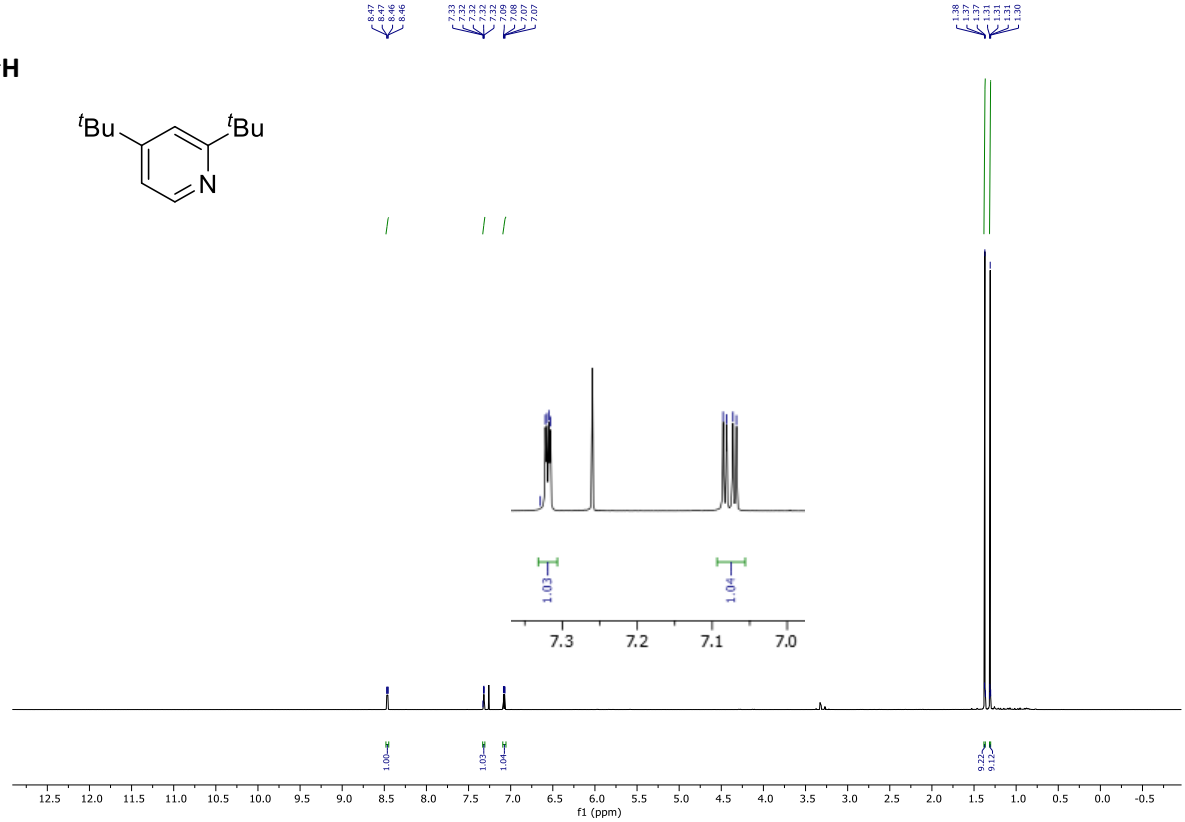


^{13}C

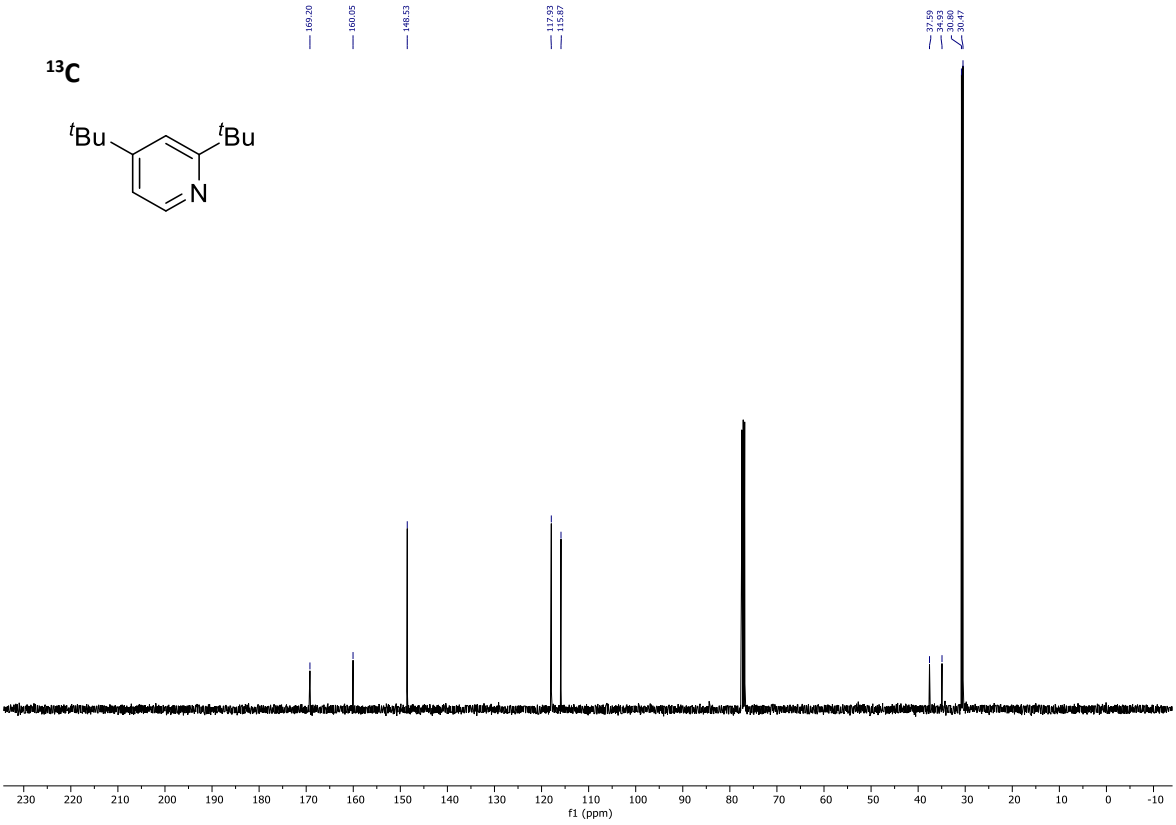


2,4-Di-*tert*-butylpyridine (27b)

^{1}H

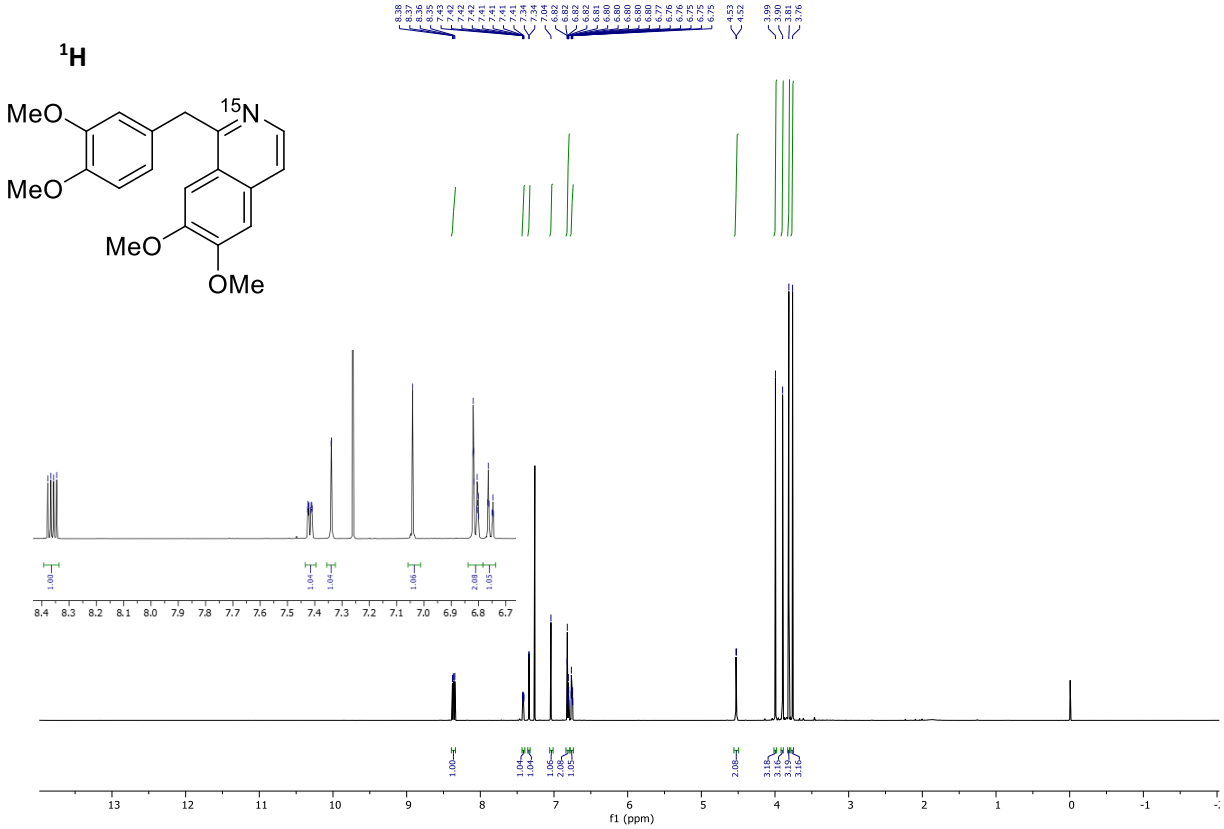


^{13}C

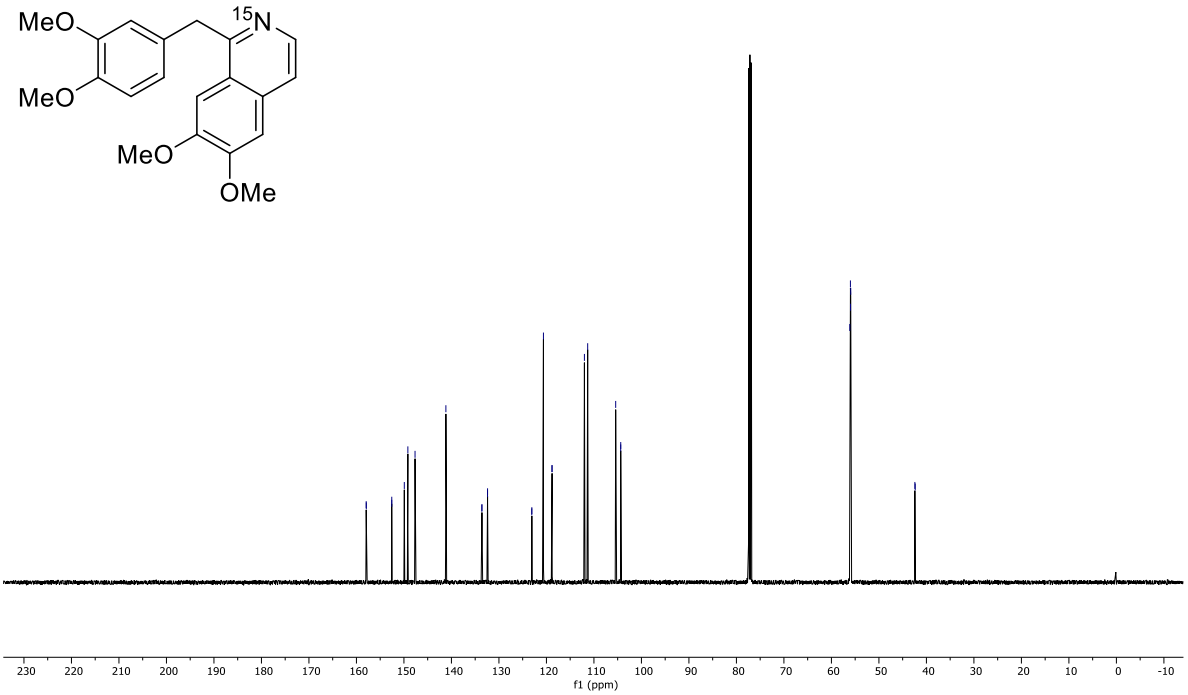


Papaverine-^{15}N (15N-28b)

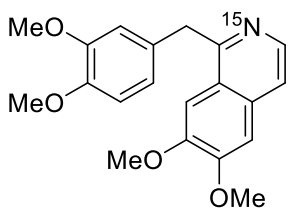
^{1}H



^{13}C

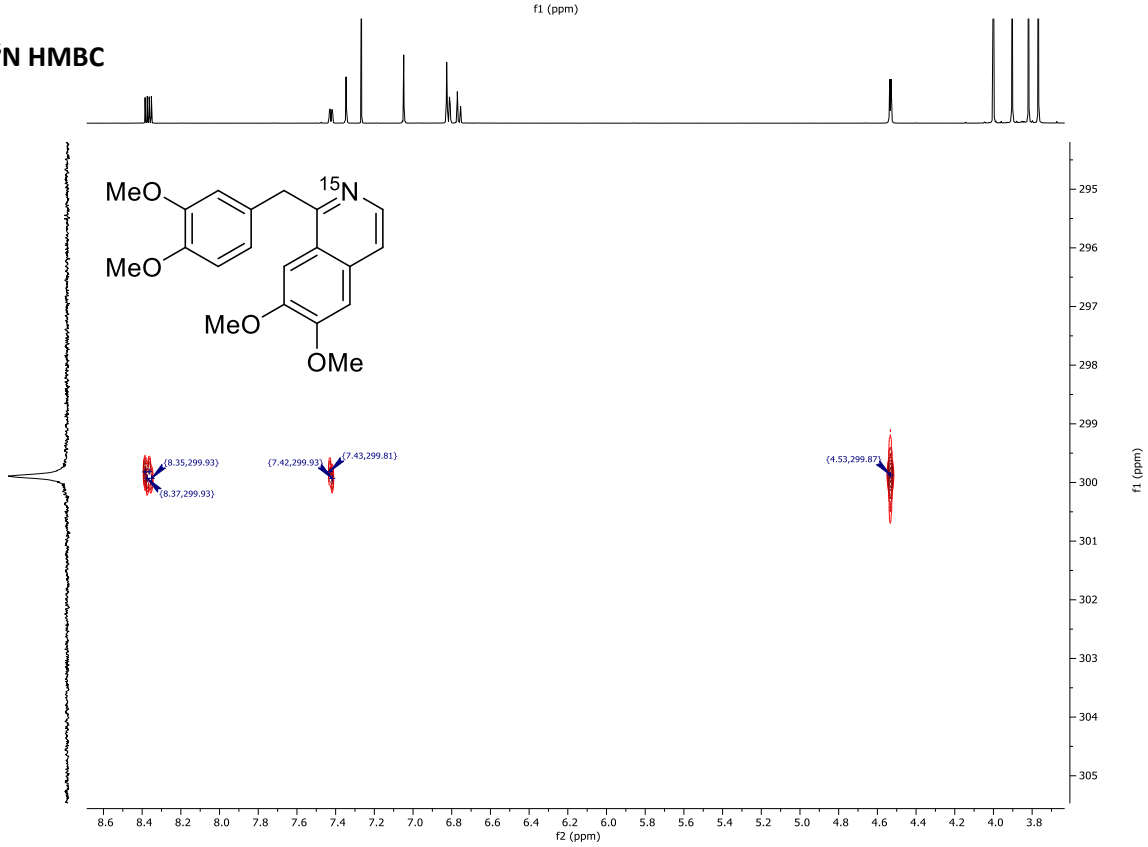


^{15}N

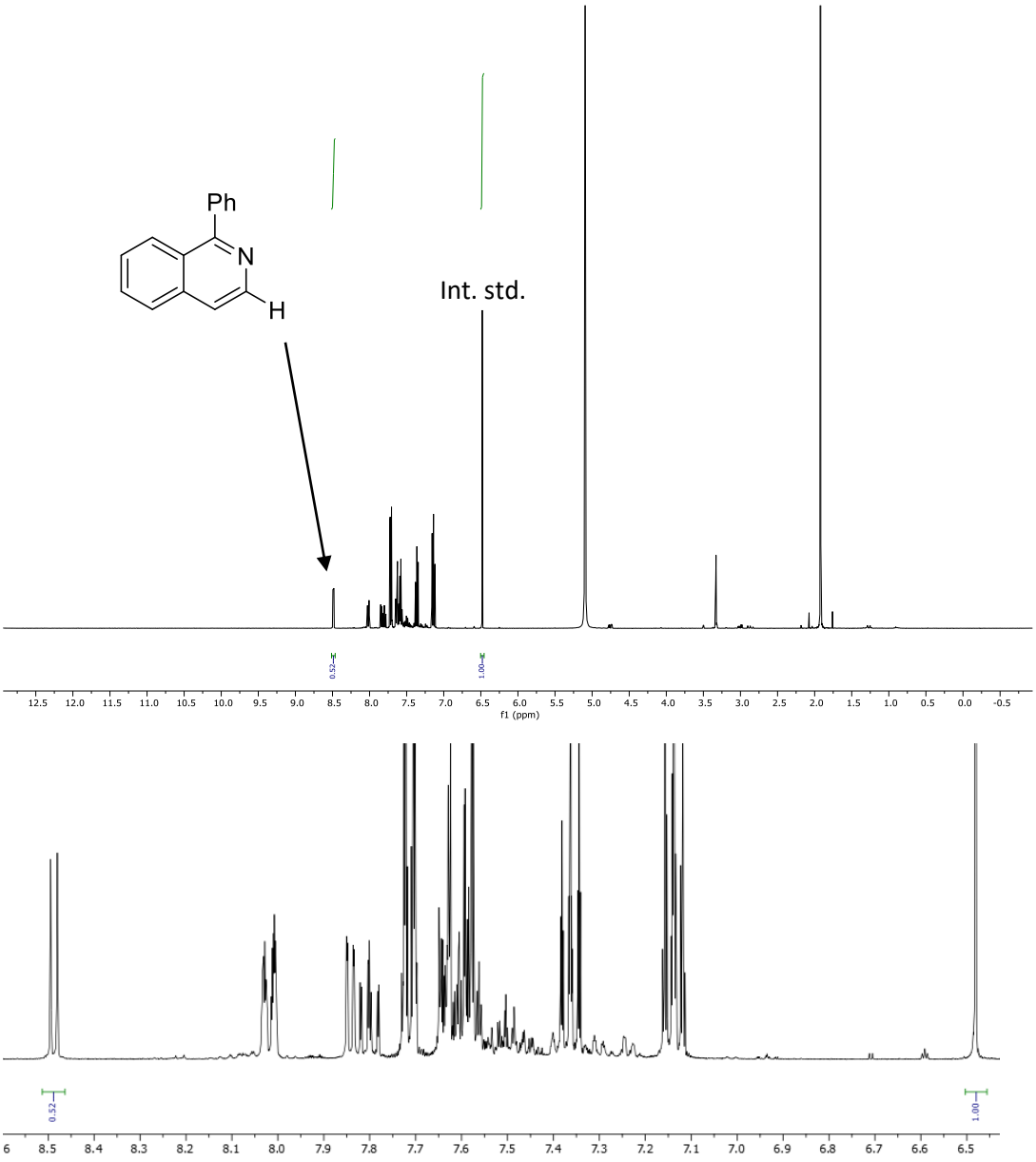

MeO
MeO
MeO
OMe
15N

300.01
299.79
301
300
299
298
450
400
350
300
250
200
150
100
50
f1 (ppm)

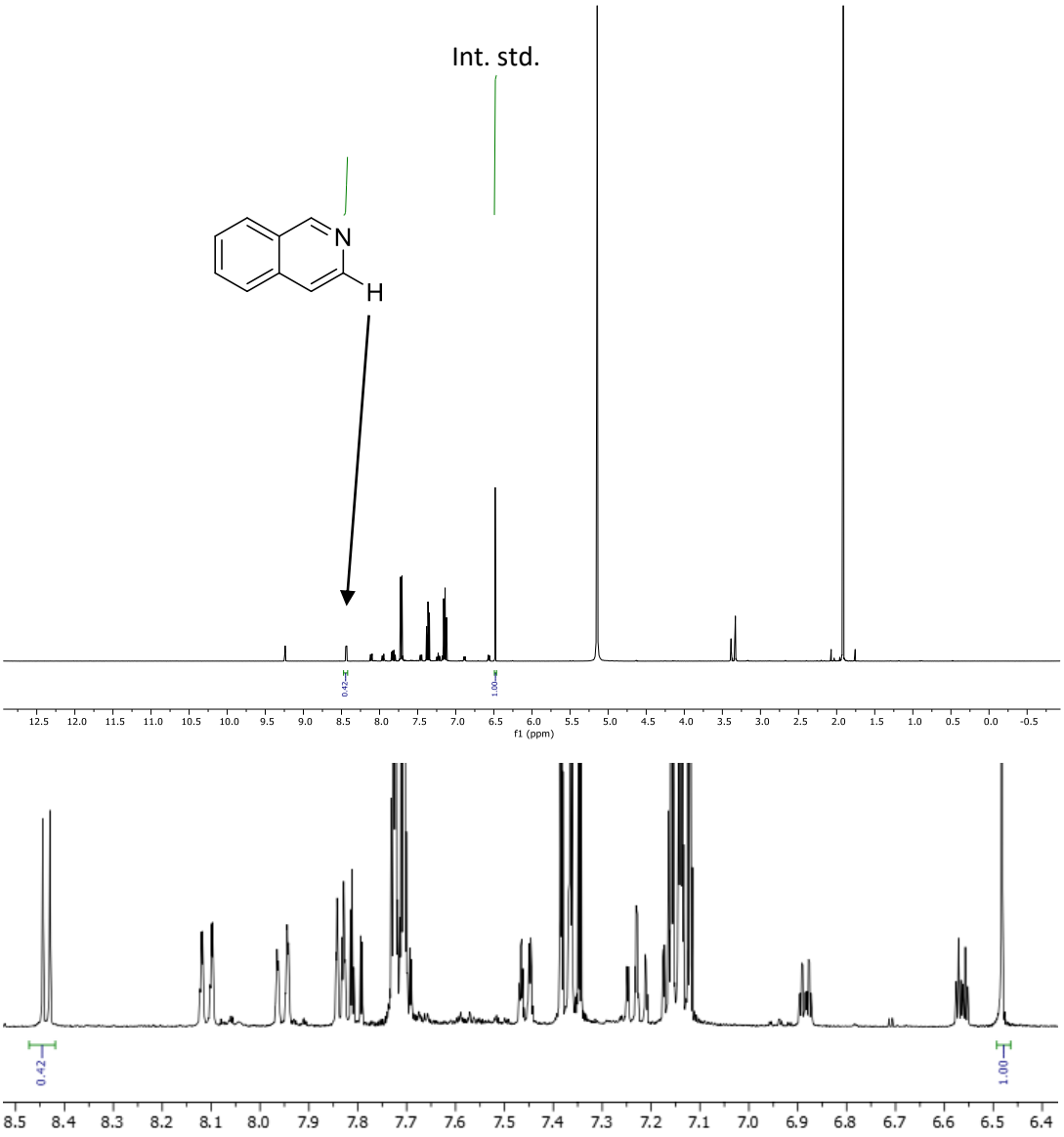
^{15}N HMBC


MeO
MeO
MeO
OMe
15N
{8.35,299.93}
{8.37,299.93}
{7.42,299.93}
{7.43,299.81}
{4.53,299.87}
f1 (ppm)
f2 (ppm)

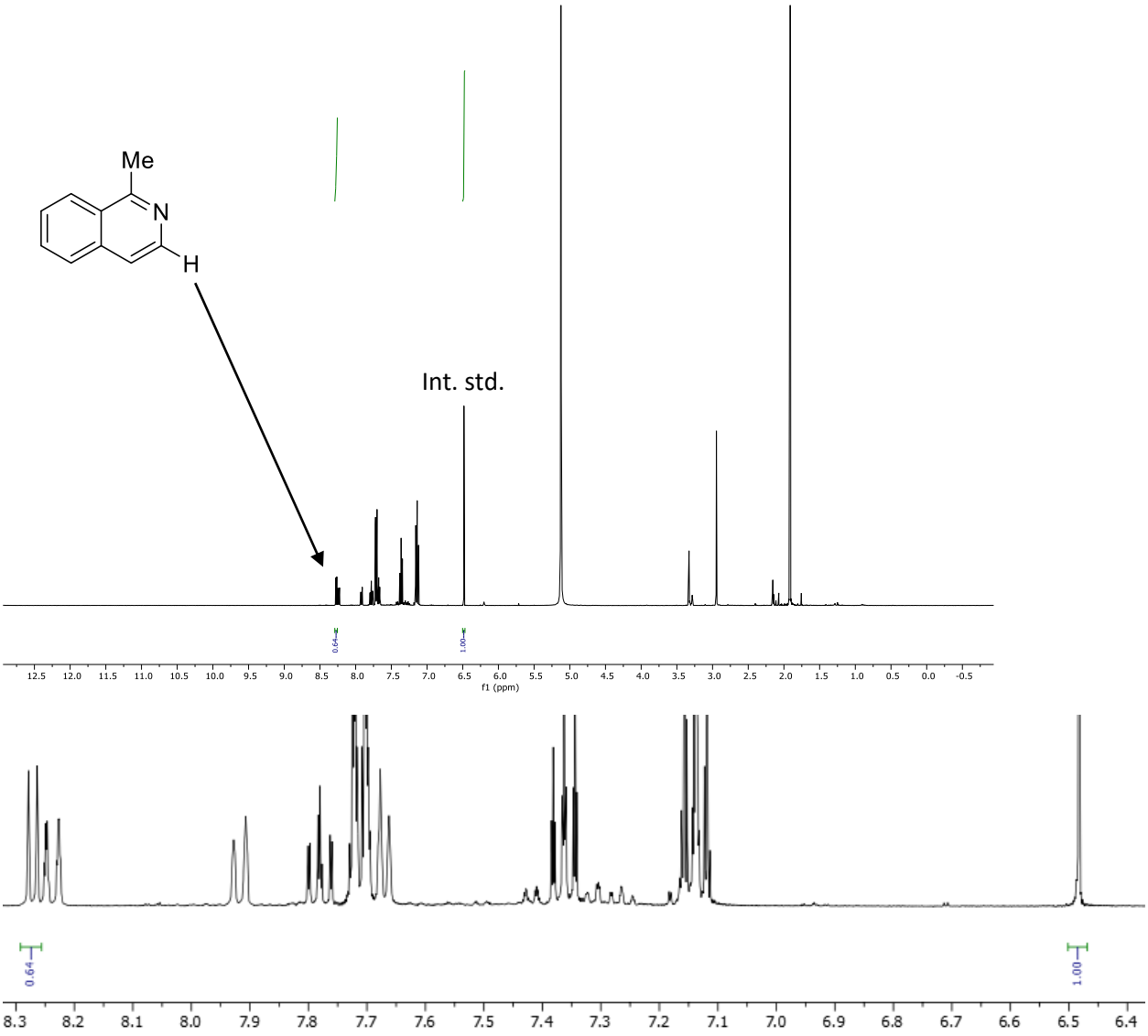
NMR yield: 1-Phenylisoquinoline (1b)



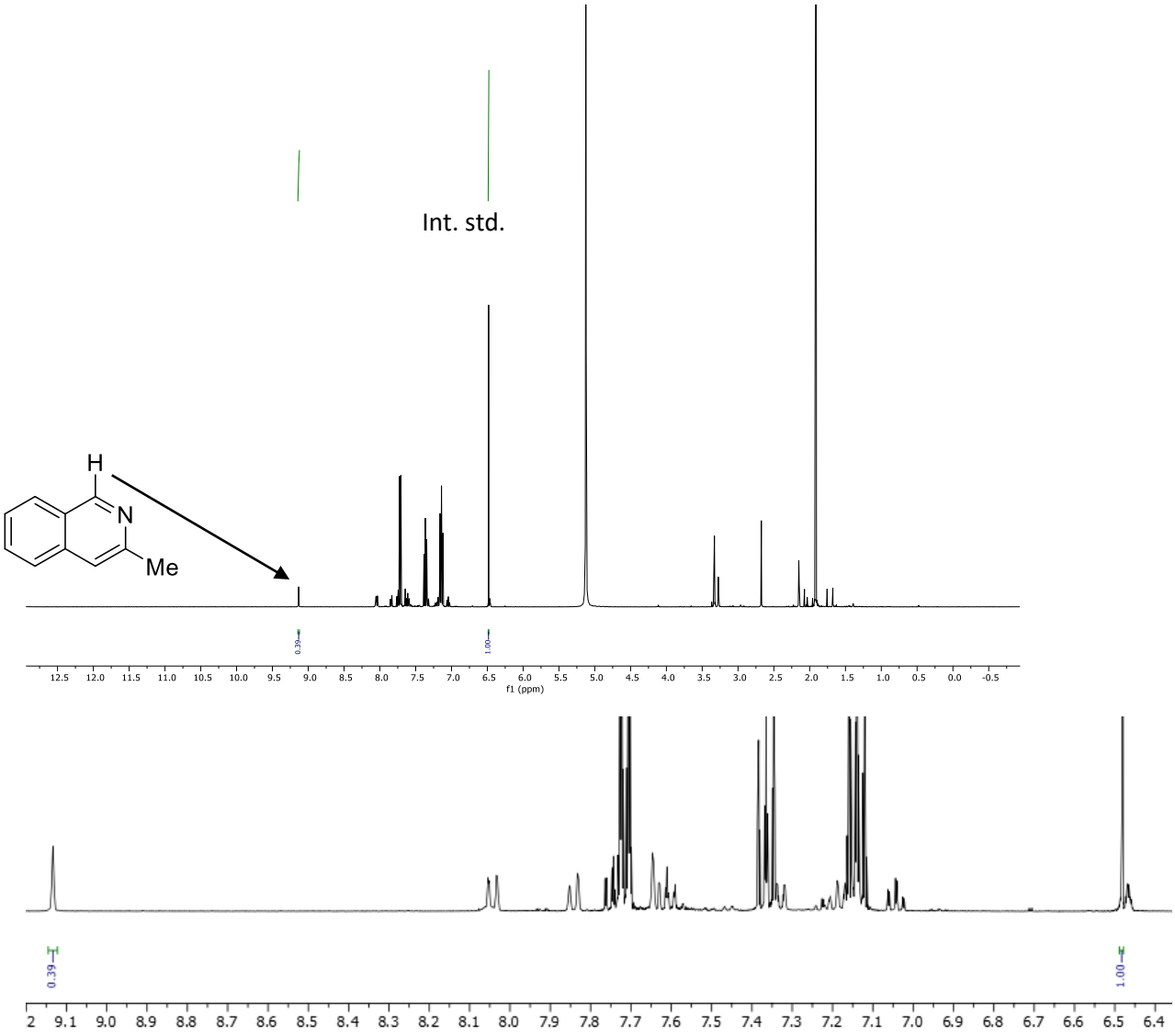
NMR yield: Isoquinoline (2b)



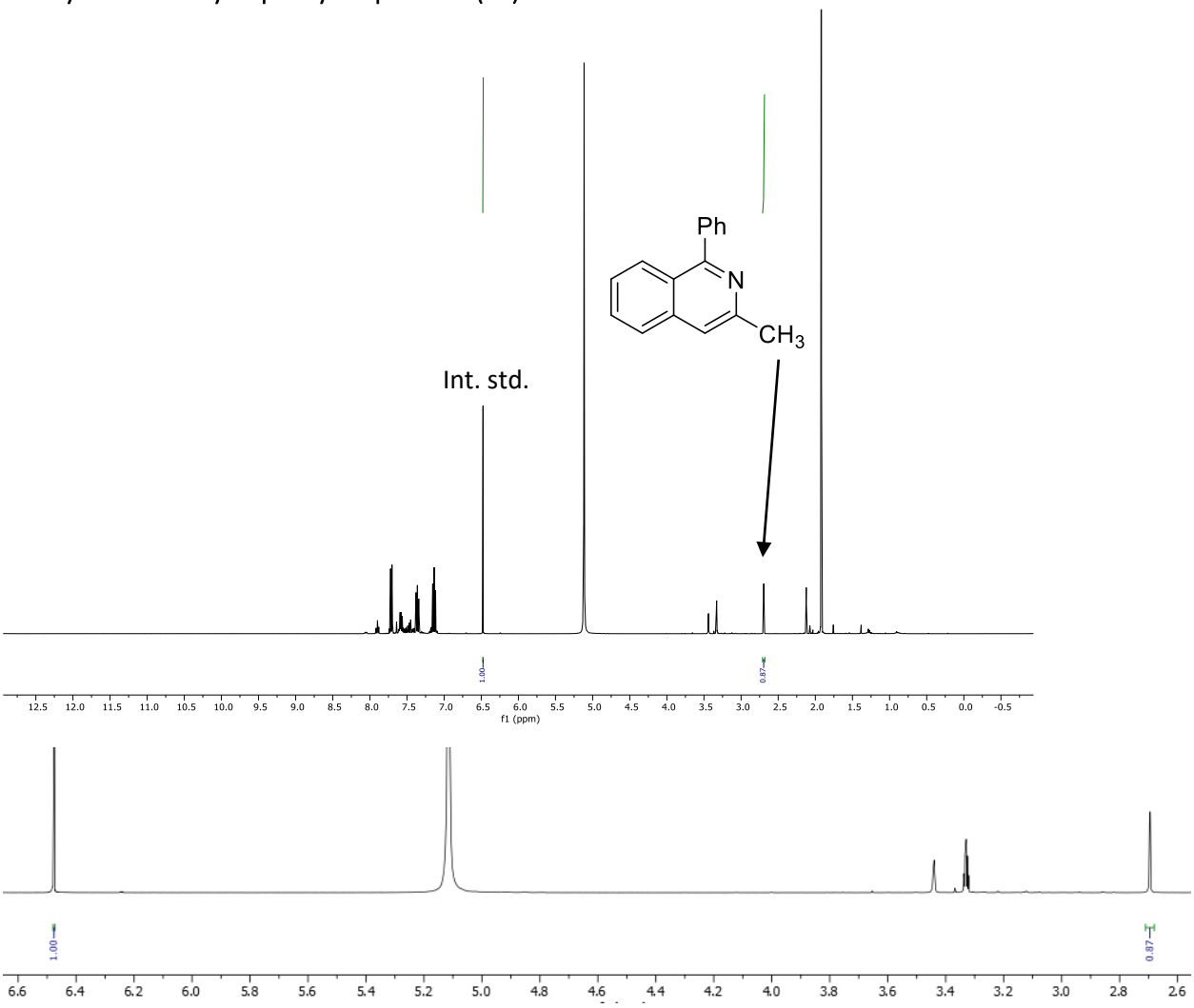
NMR yield: 1-Methylisoquinoline (3b)



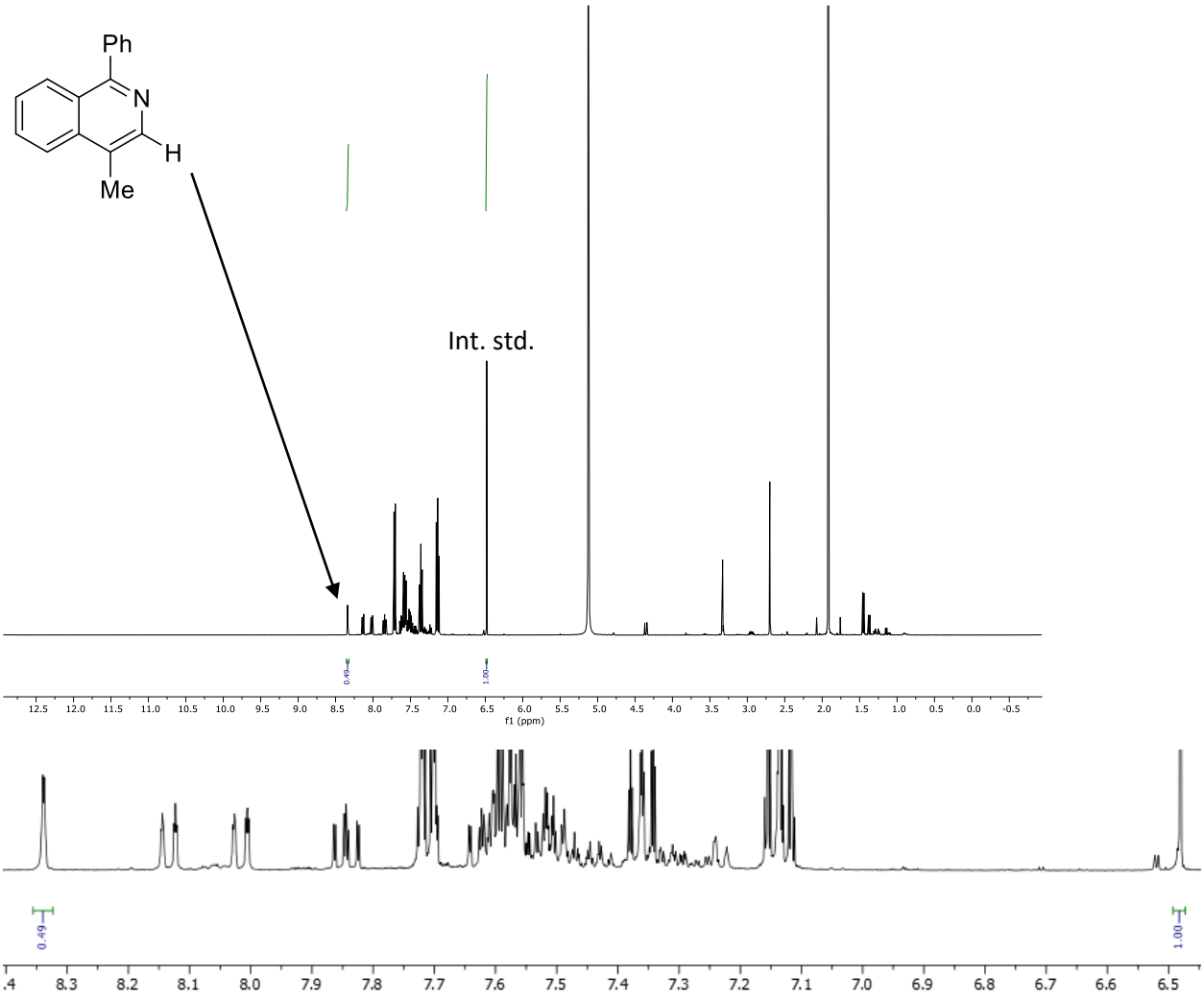
NMR yield: 3-Methylisoquinoline (4b)



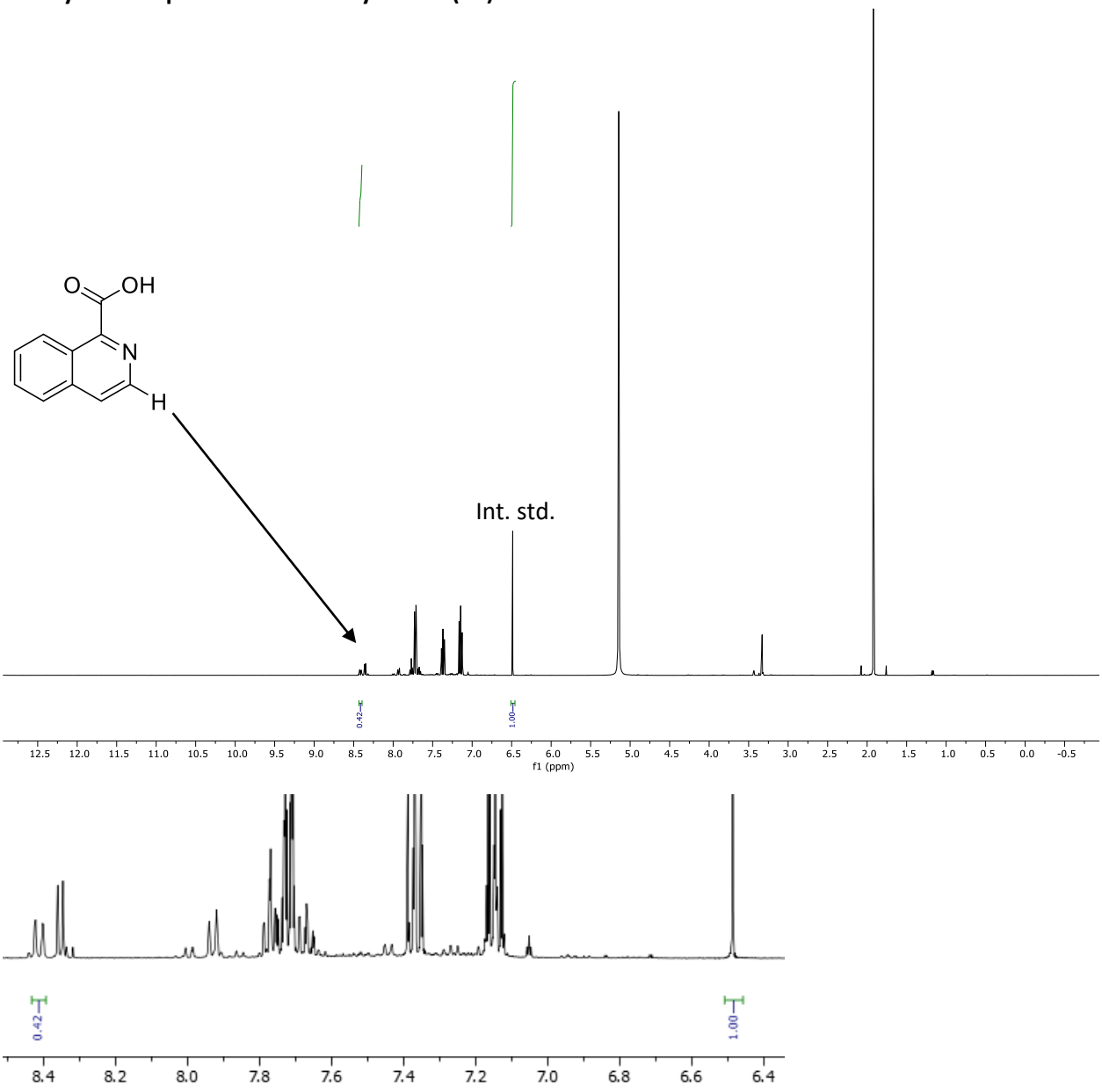
NMR yield: 3-Methyl-1-phenylisoquinoline (5b)



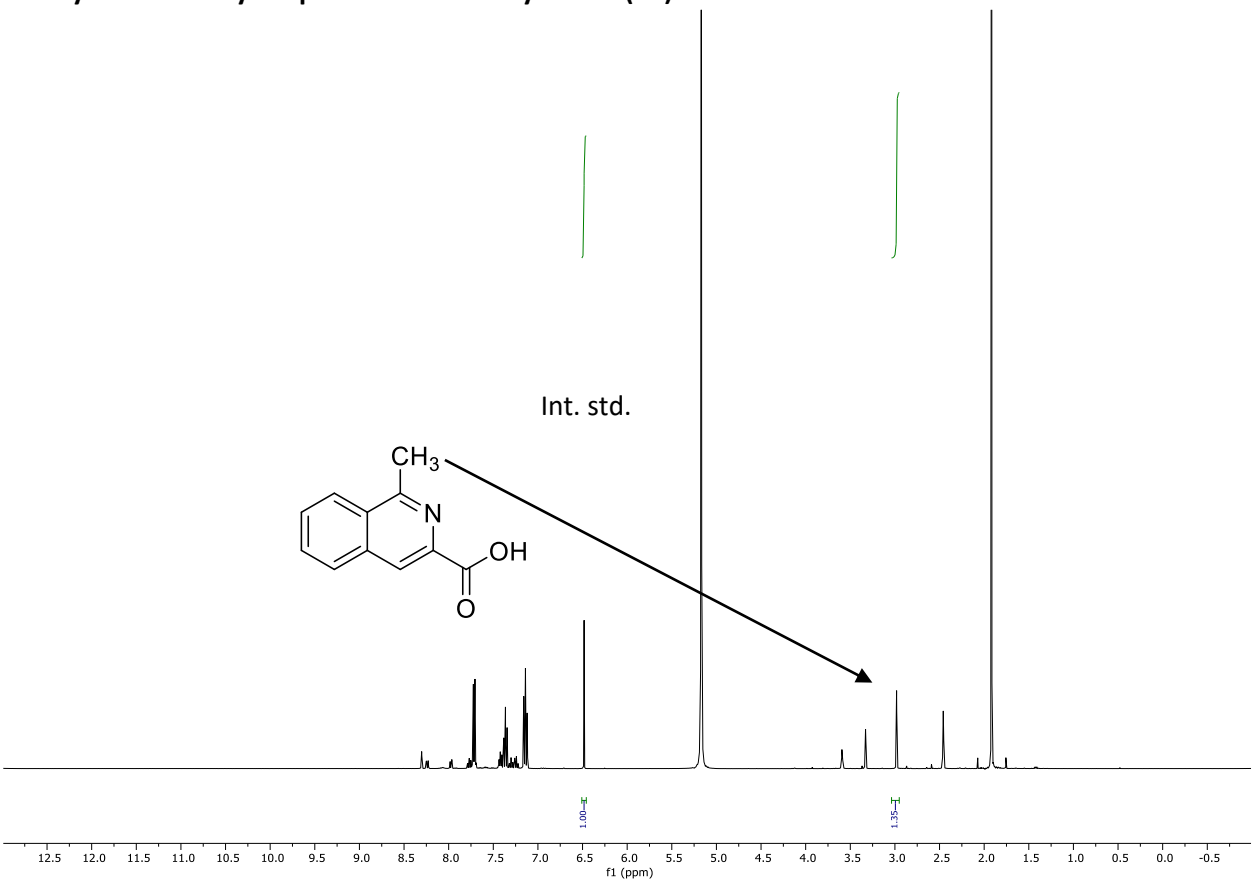
NMR yield: 4-Methyl-1-phenylisoquinoline (6b)



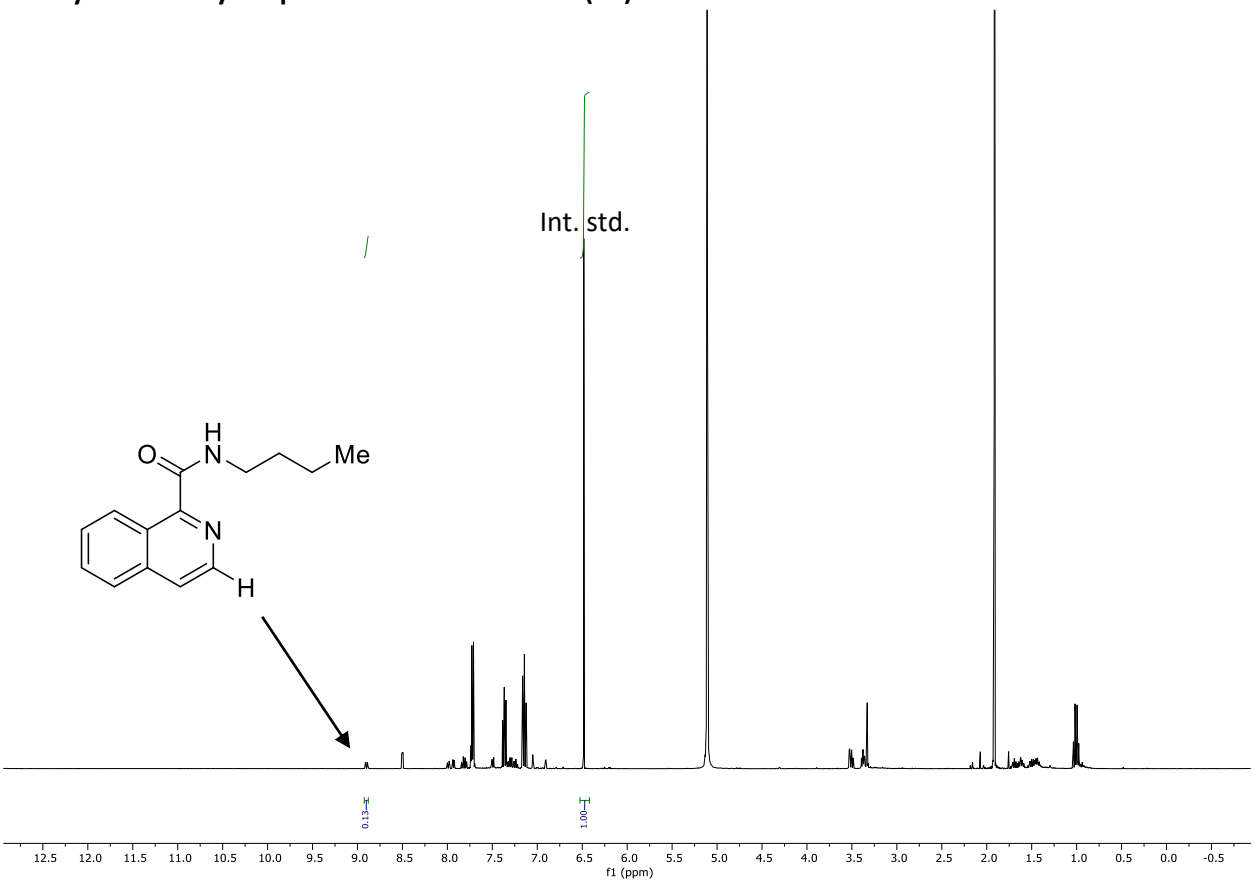
NMR yield: Isoquinoline-1-carboxylic acid (7b)

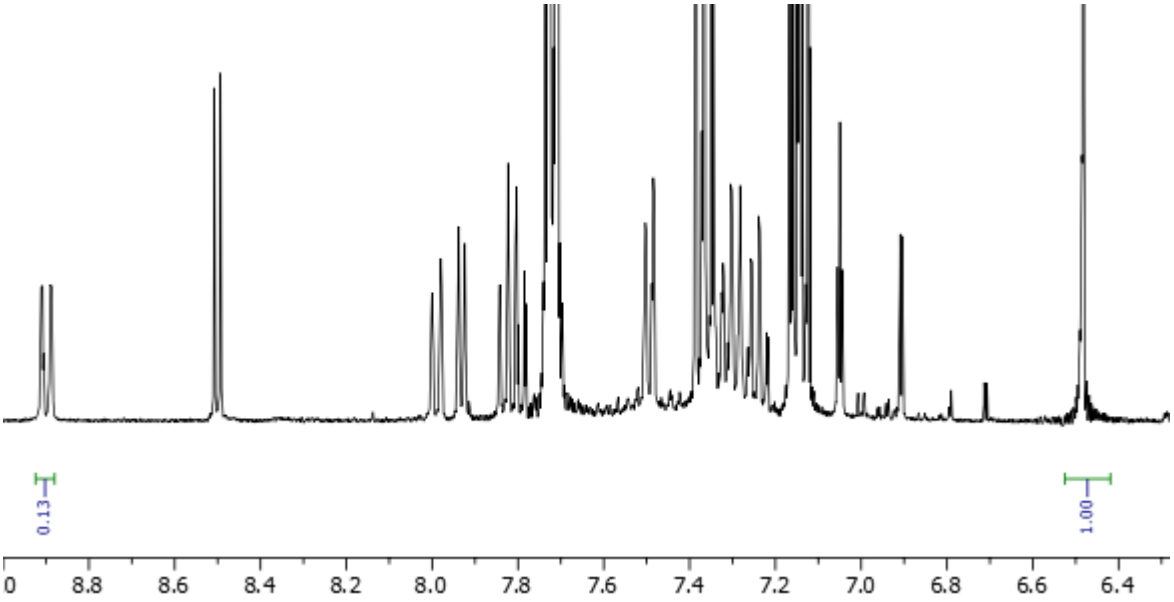


NMR yield: 1-Methylisoquinoline-3-carboxylic acid (8b)

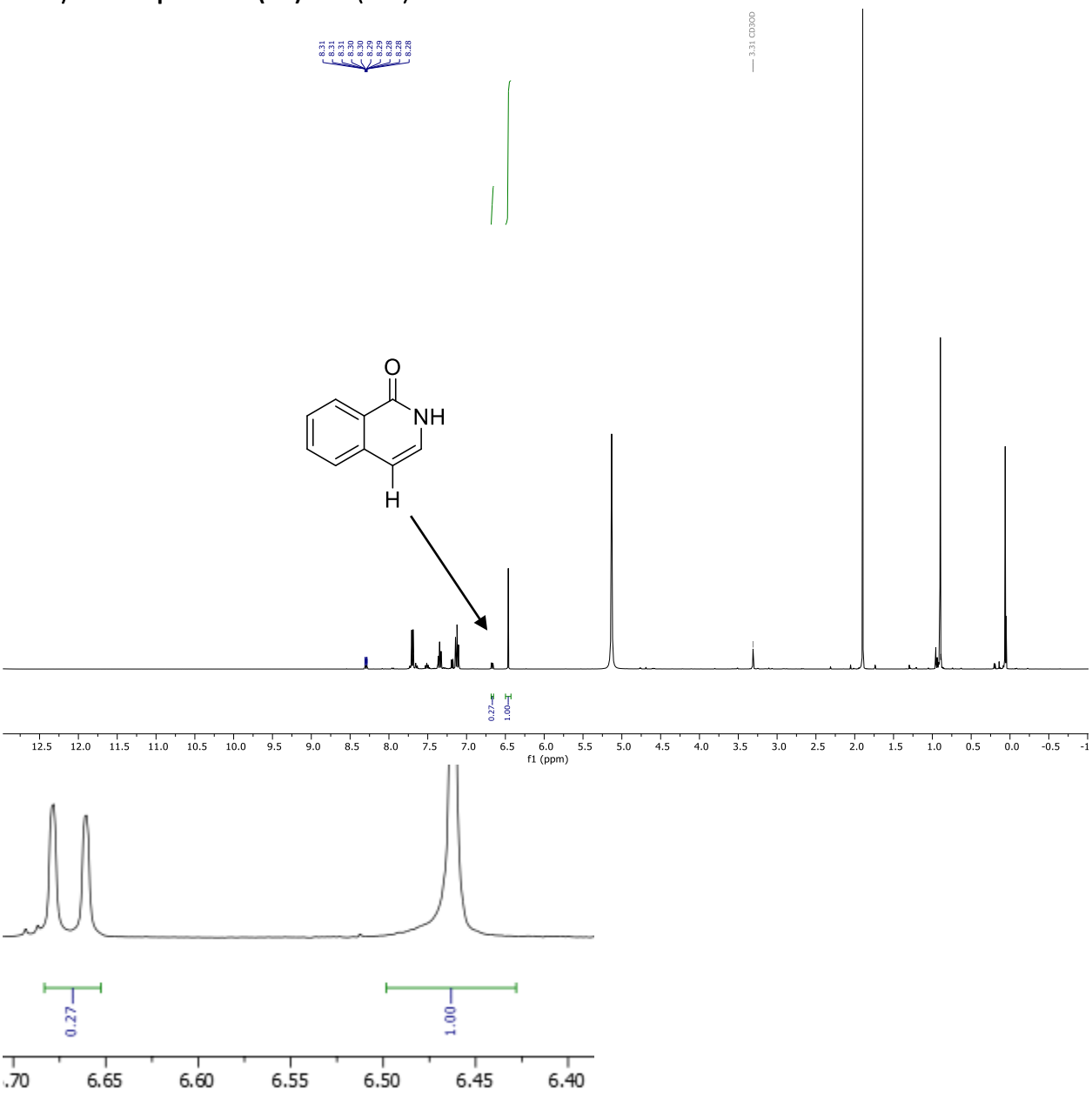


NMR yield: *N*-Butylisoquinoline-1-carboxamide (9b)

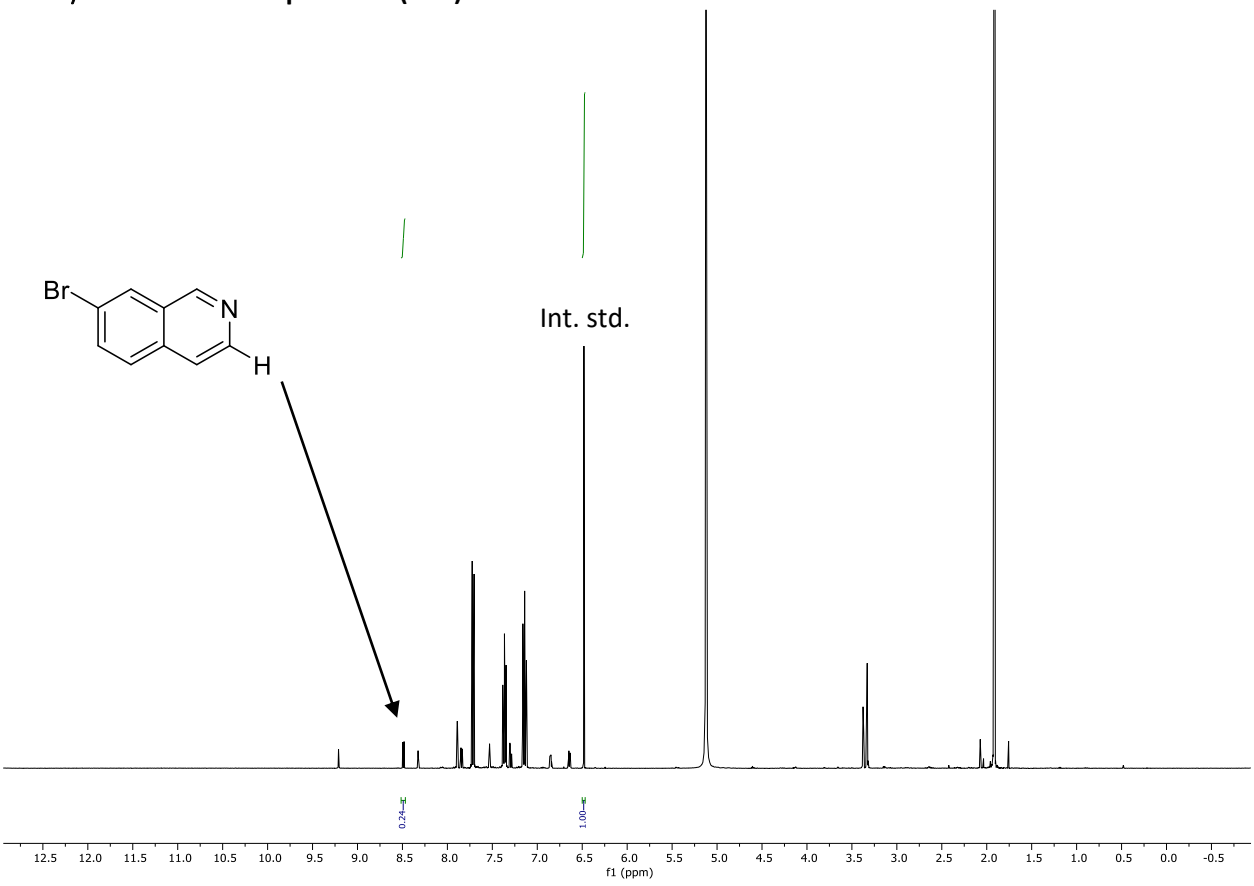


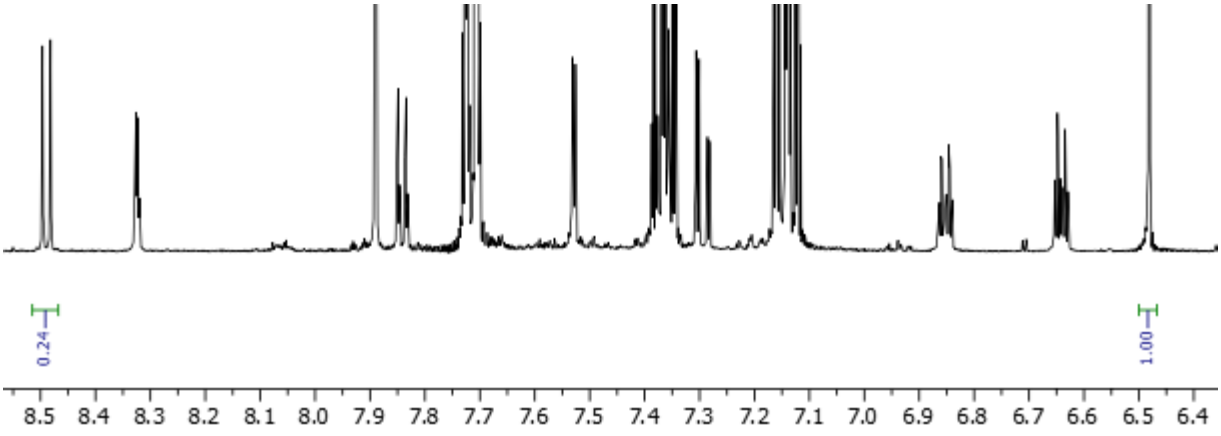


NMR yield: **Isoquinolin-1(2*H*)-one** (10b)

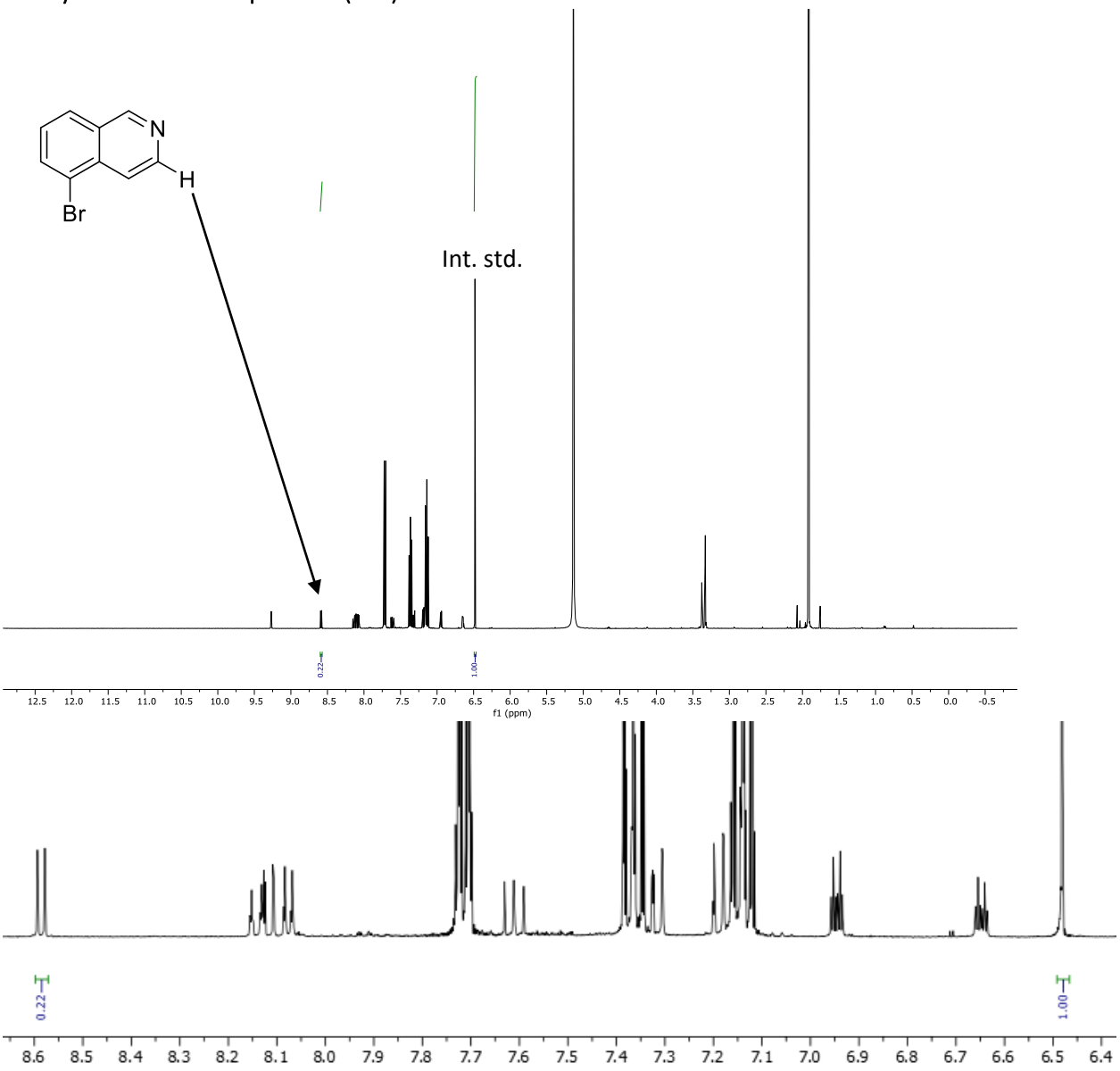


NMR yield: **7-Bromoisoquinoline (11b)**

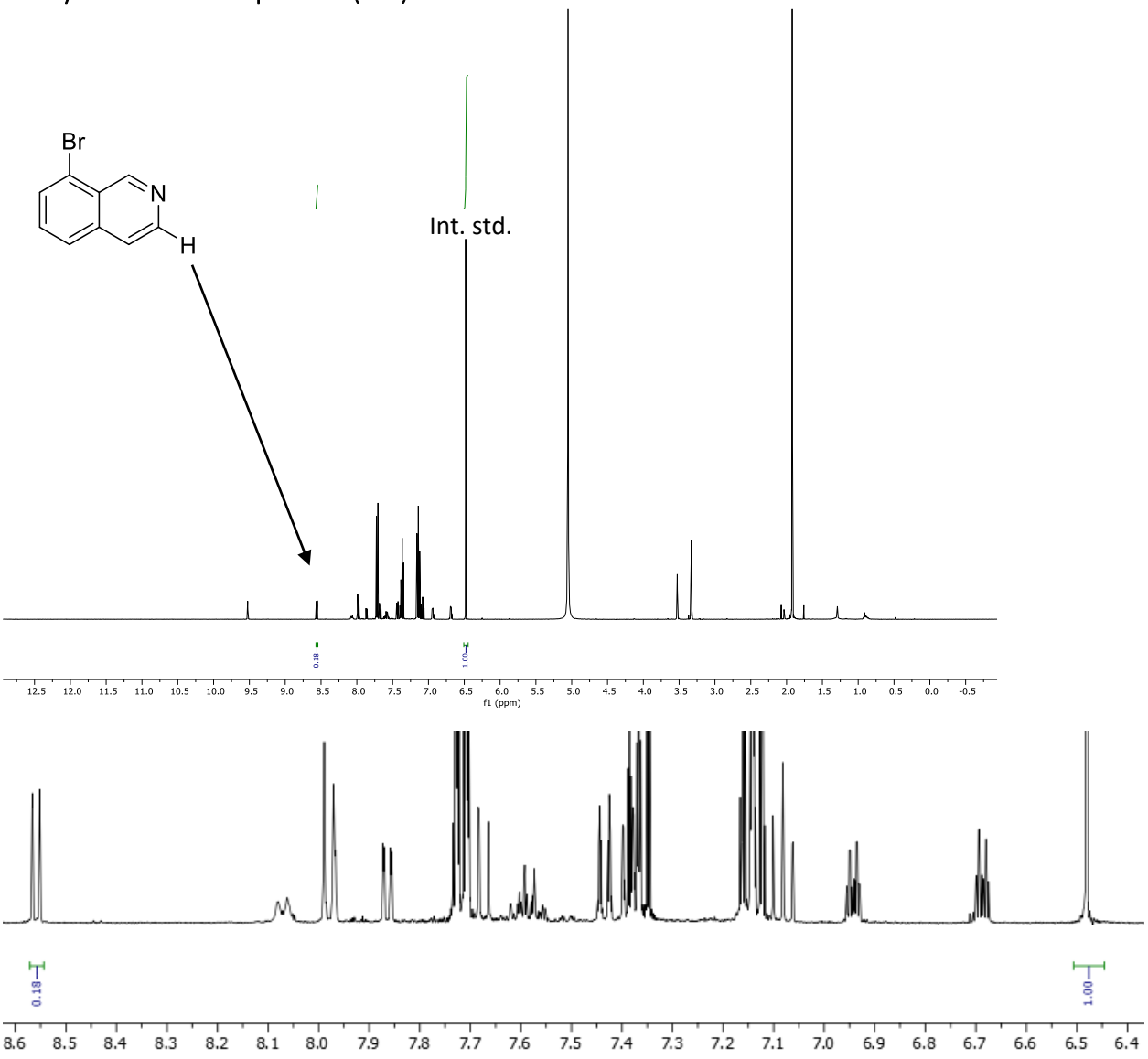




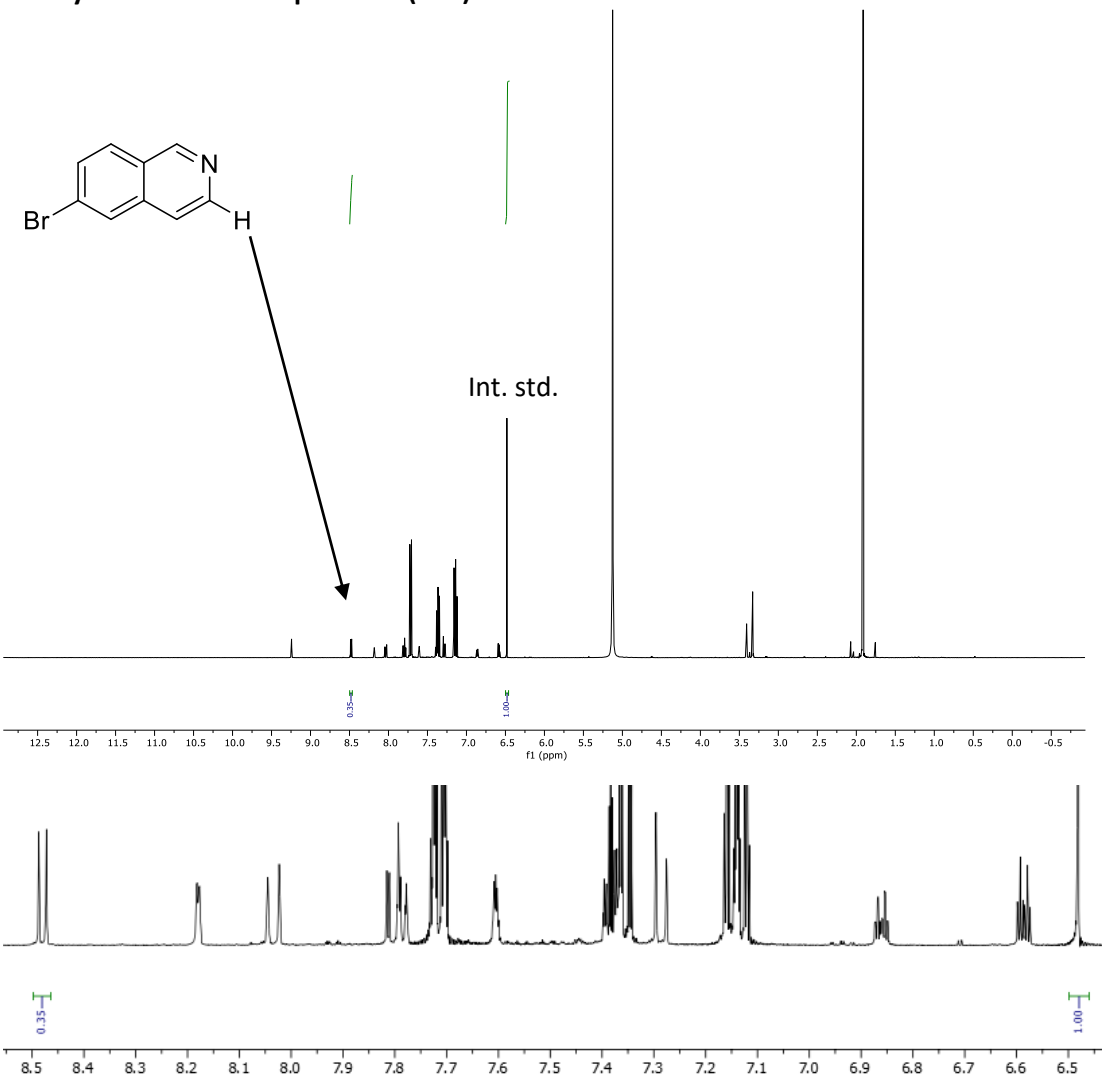
NMR yield: 5-Bromoisoquinoline (12b)



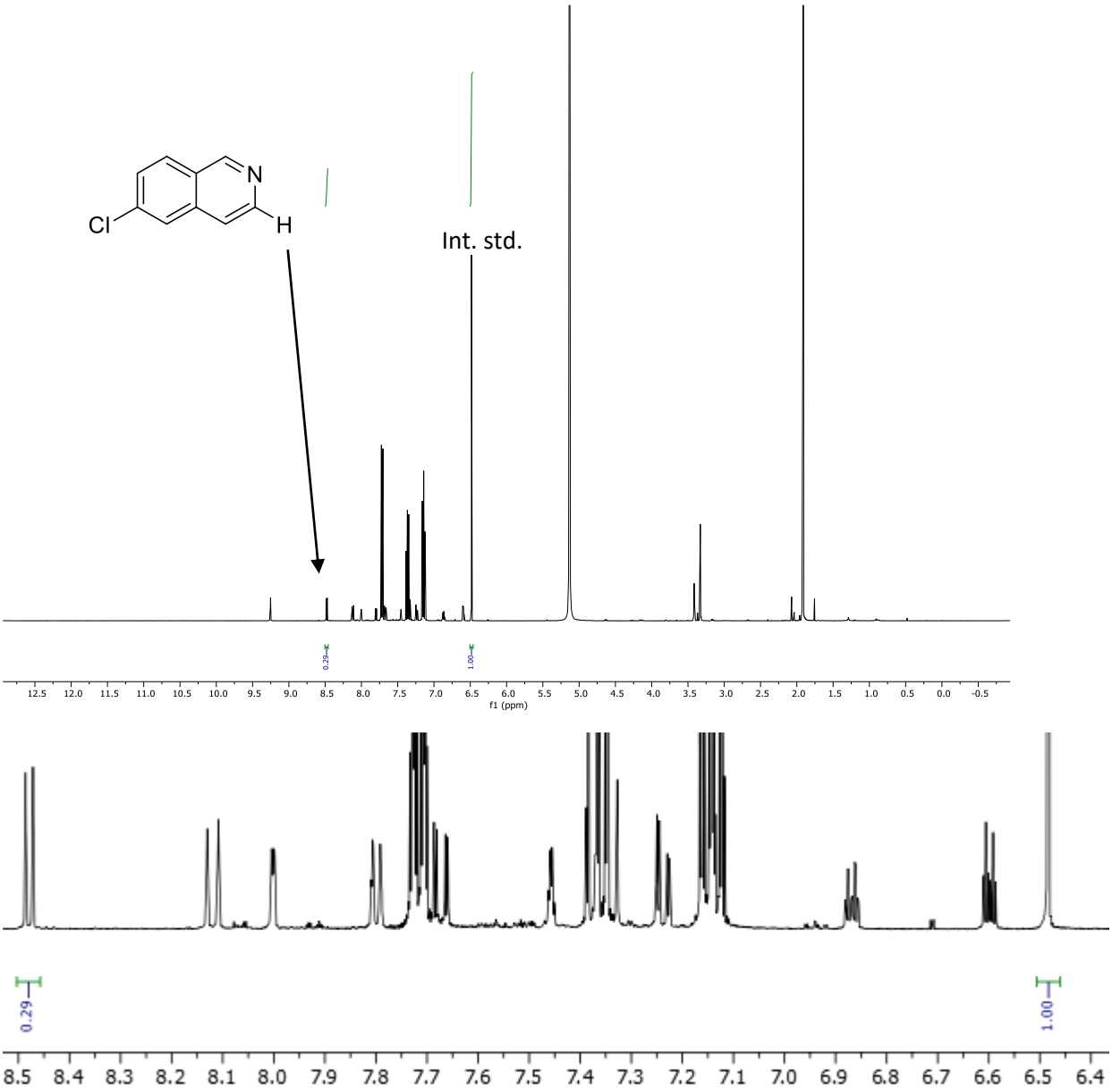
NMR yield: 8-Bromoisoquinoline (13b)



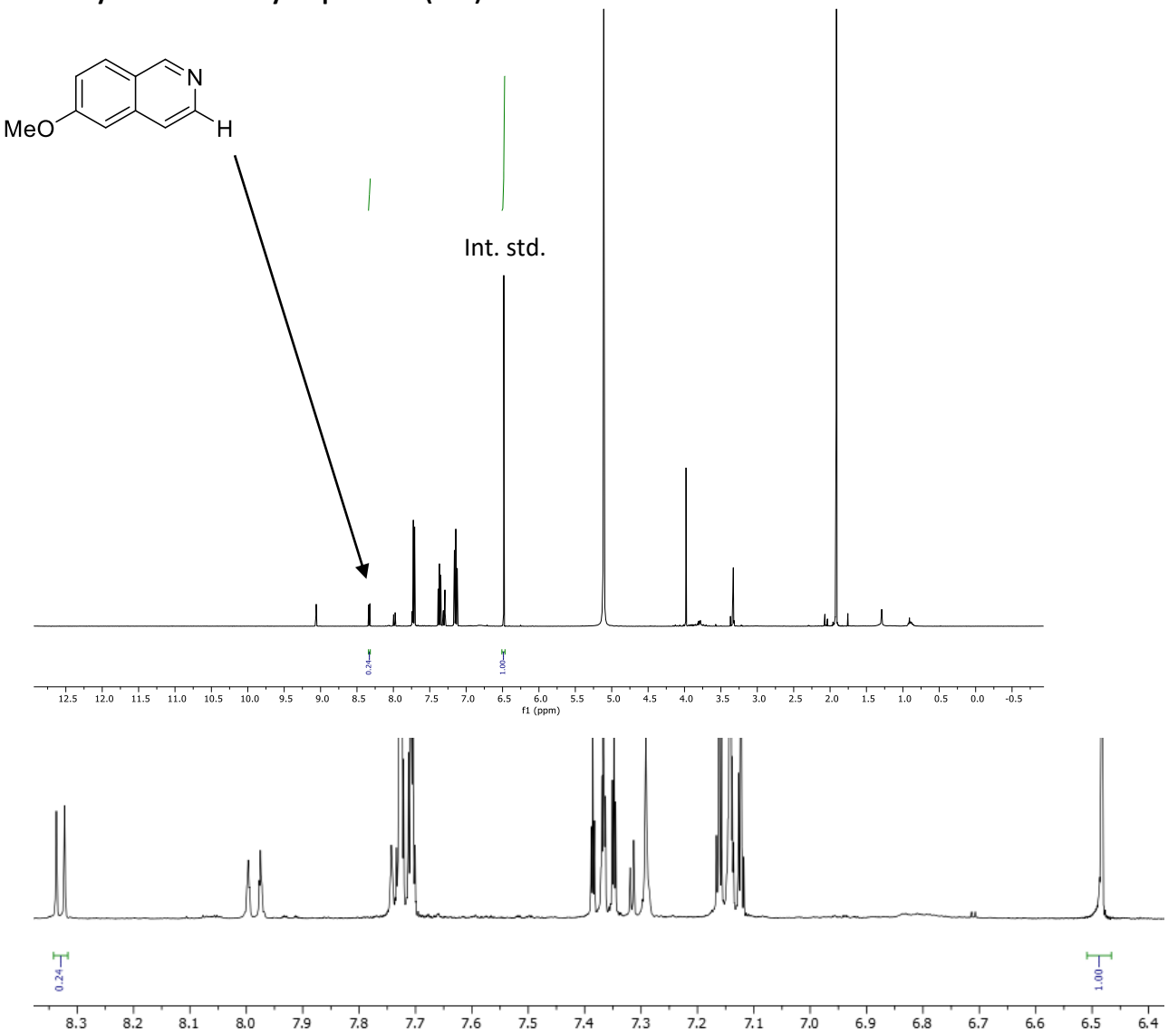
NMR yield: 6-Bromoisoquinoline (14b)



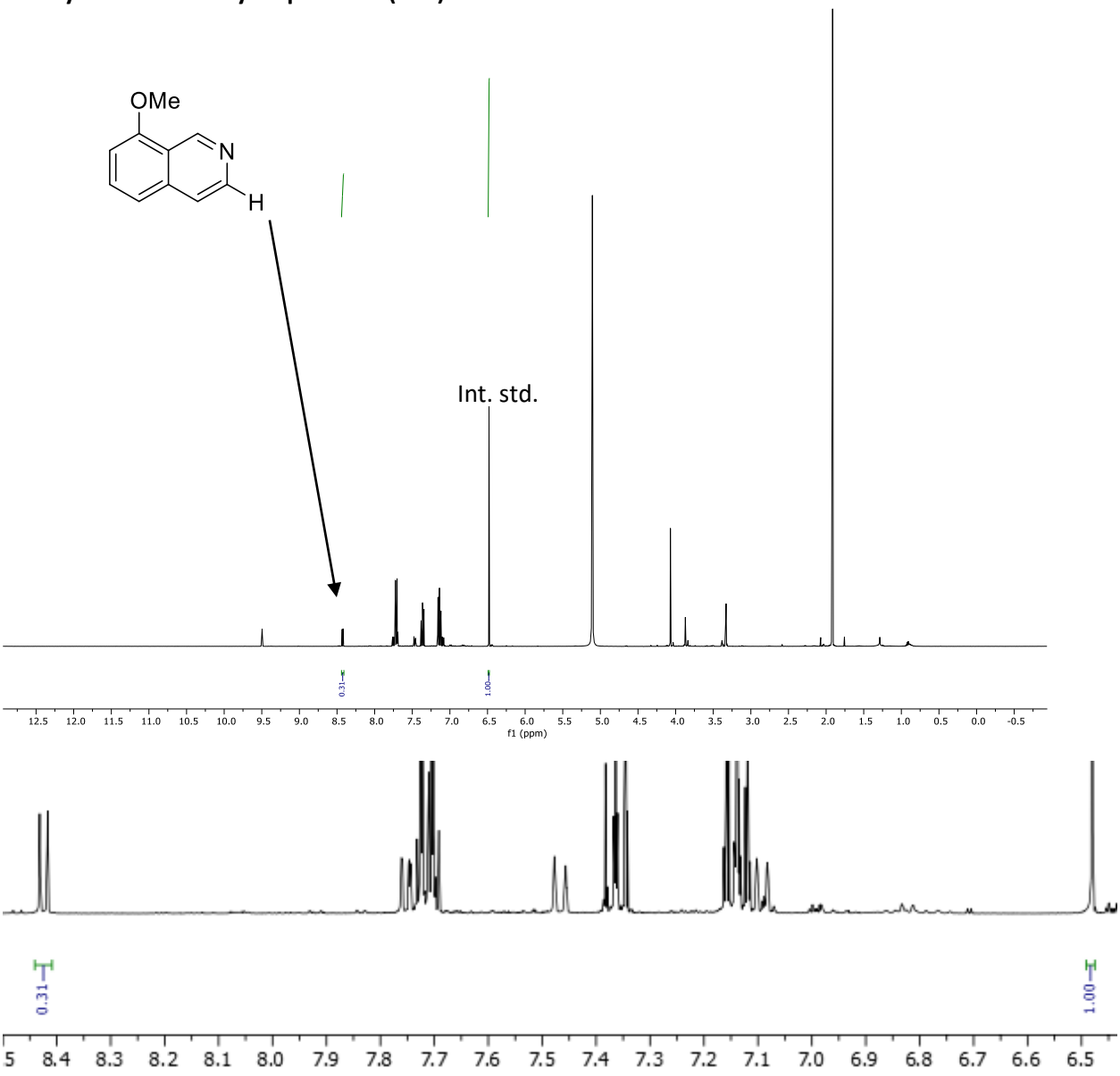
NMR yield: 6-Chloroisoquinoline (15b)



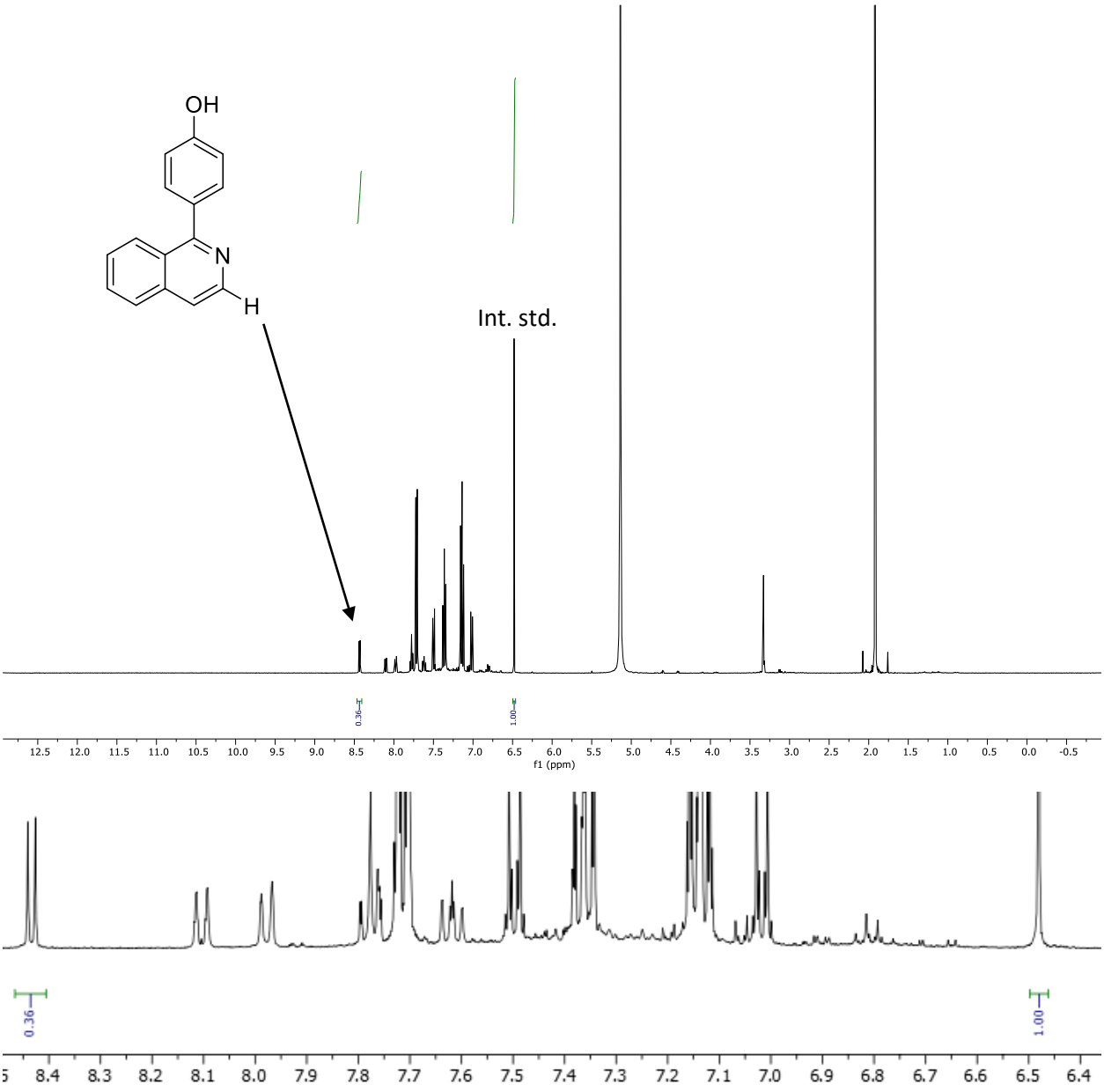
NMR yield: 6-Methoxyisoquinoline (16b)



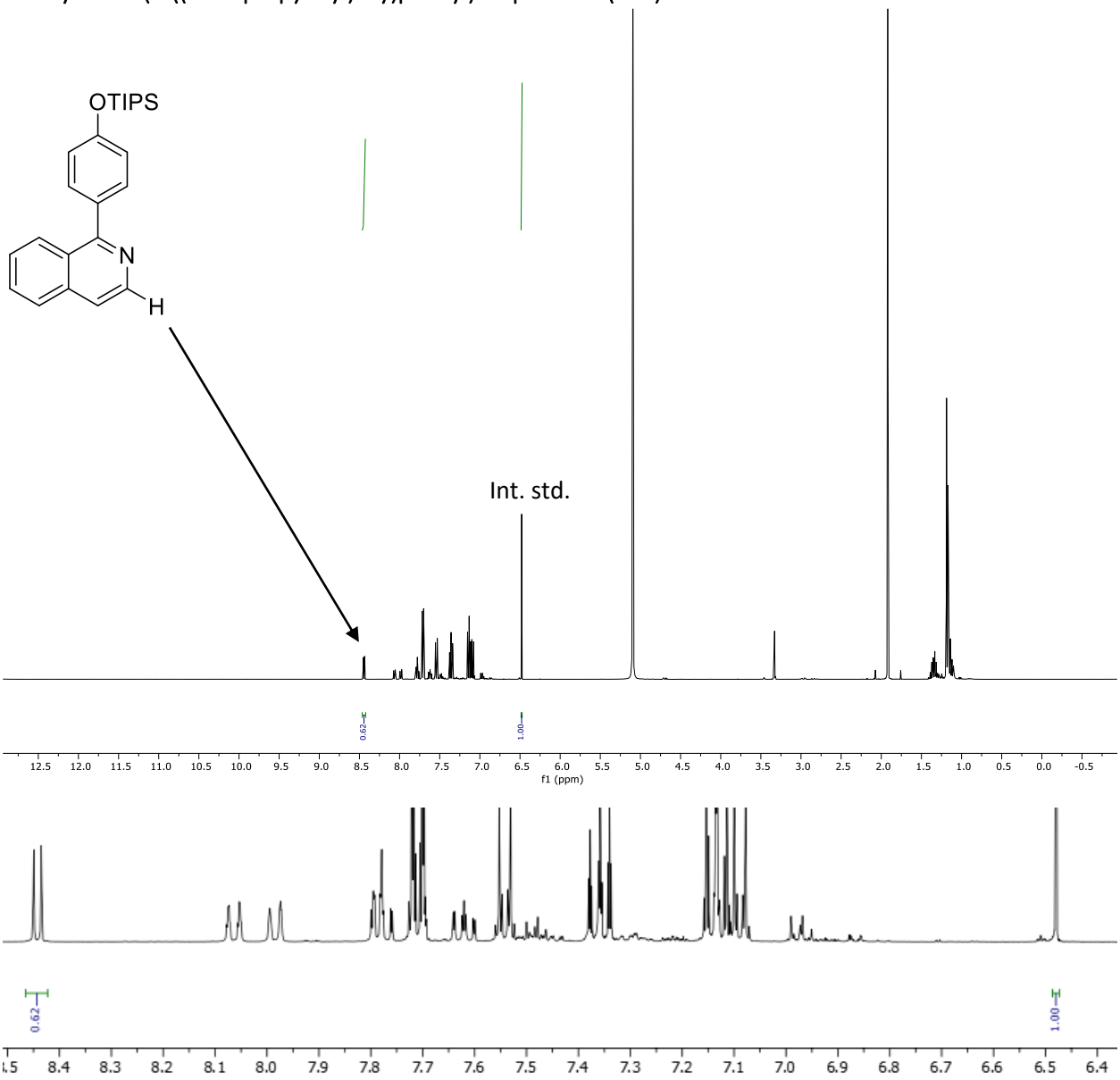
NMR yield: 8-Methoxyisoquinoline (17b)



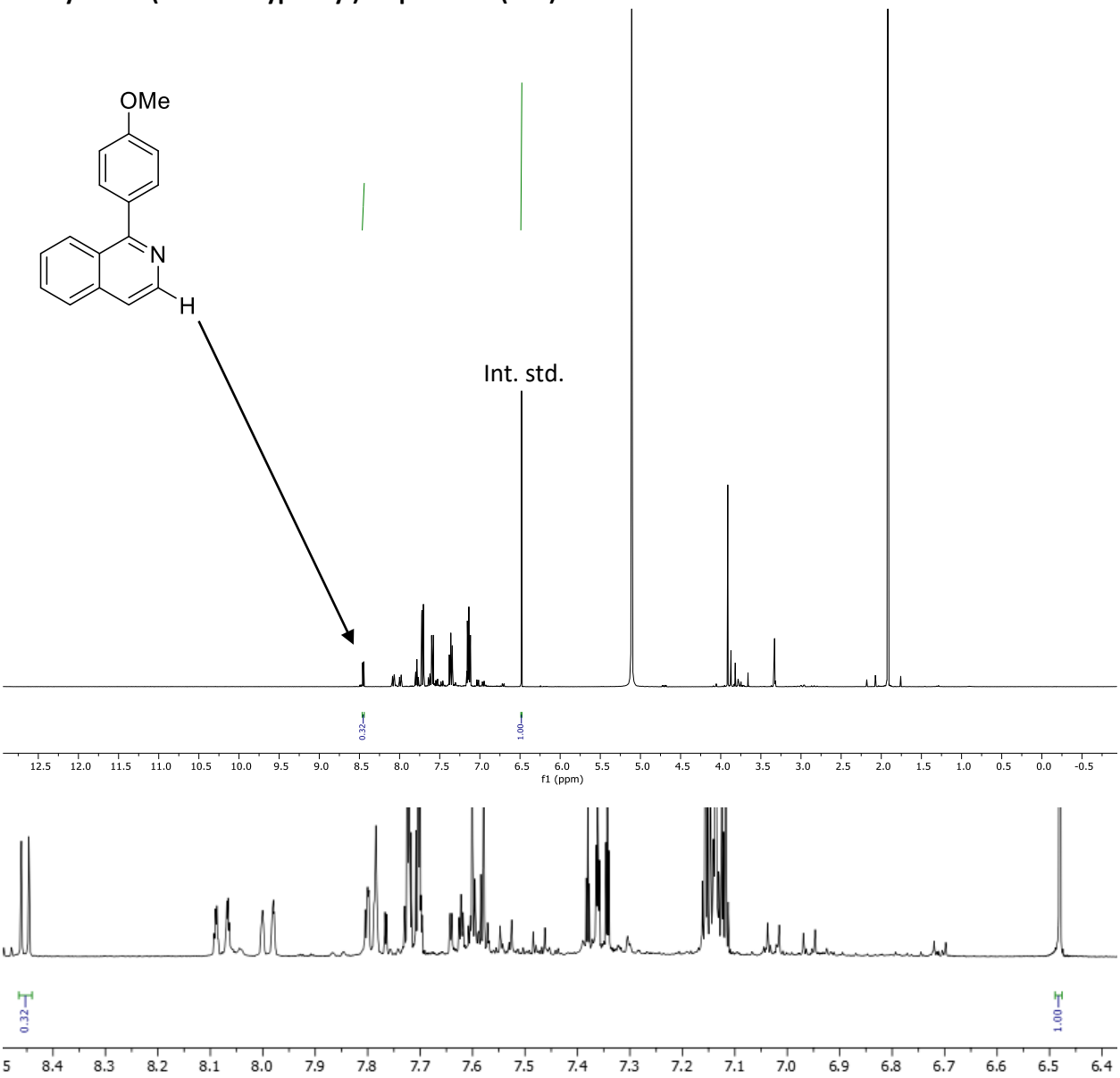
NMR yield: 4-(Isoquinolin-1-yl)phenol (18b)



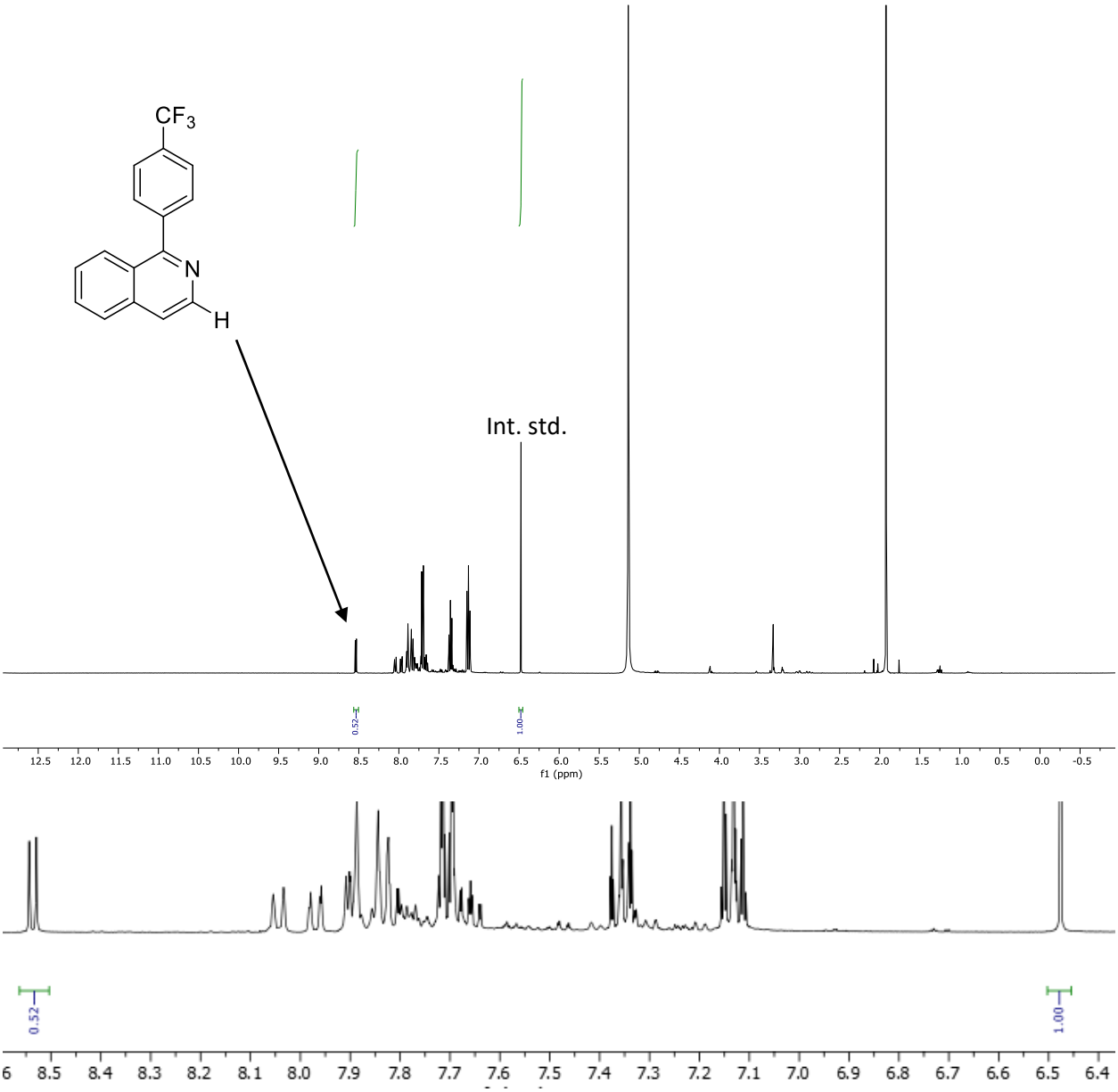
NMR yield: 1-(4-((Triisopropylsilyl)oxy)phenyl)isoquinoline (19b)



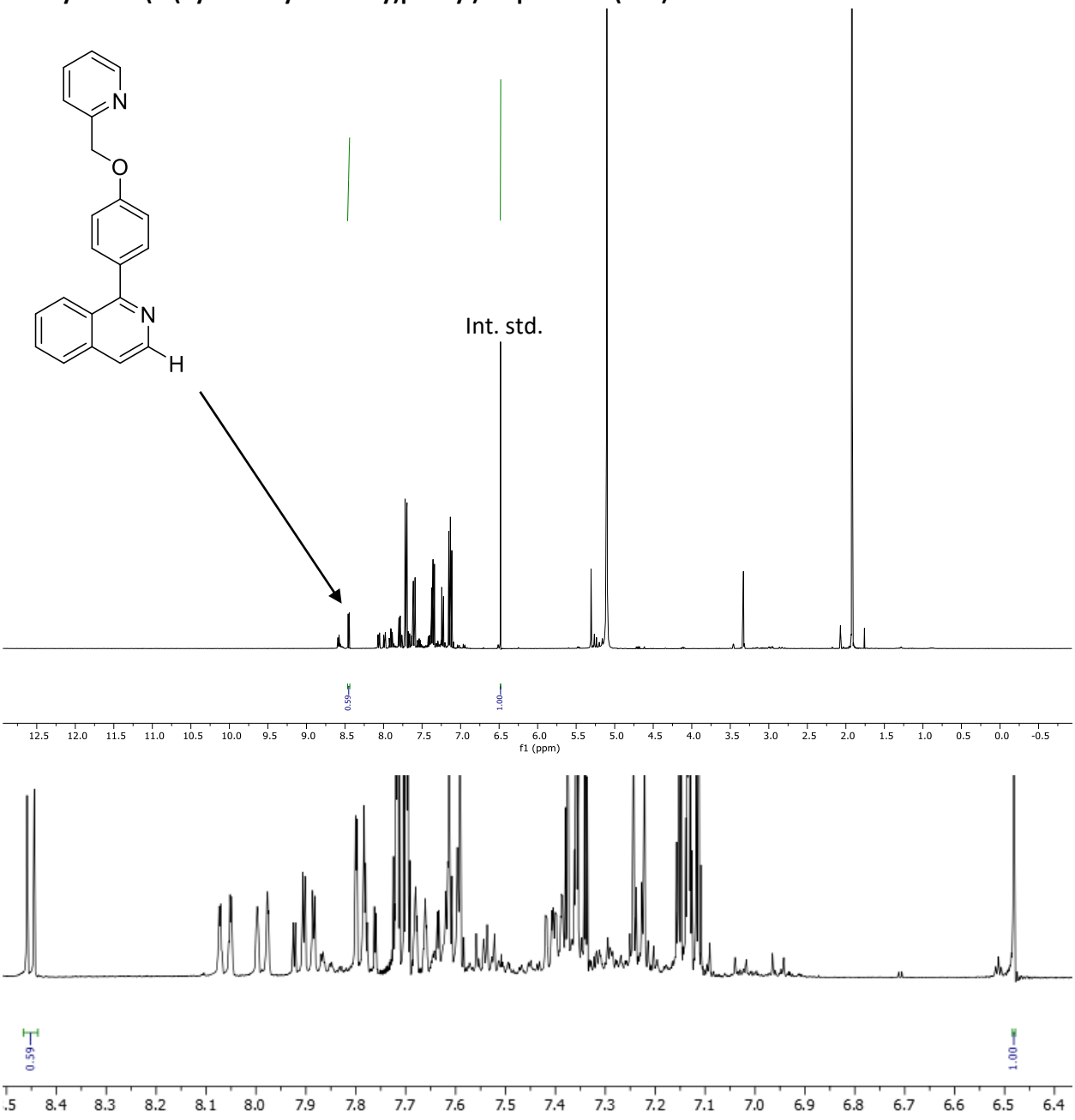
NMR yield: 1-(4-Methoxyphenyl)isoquinoline (20b)



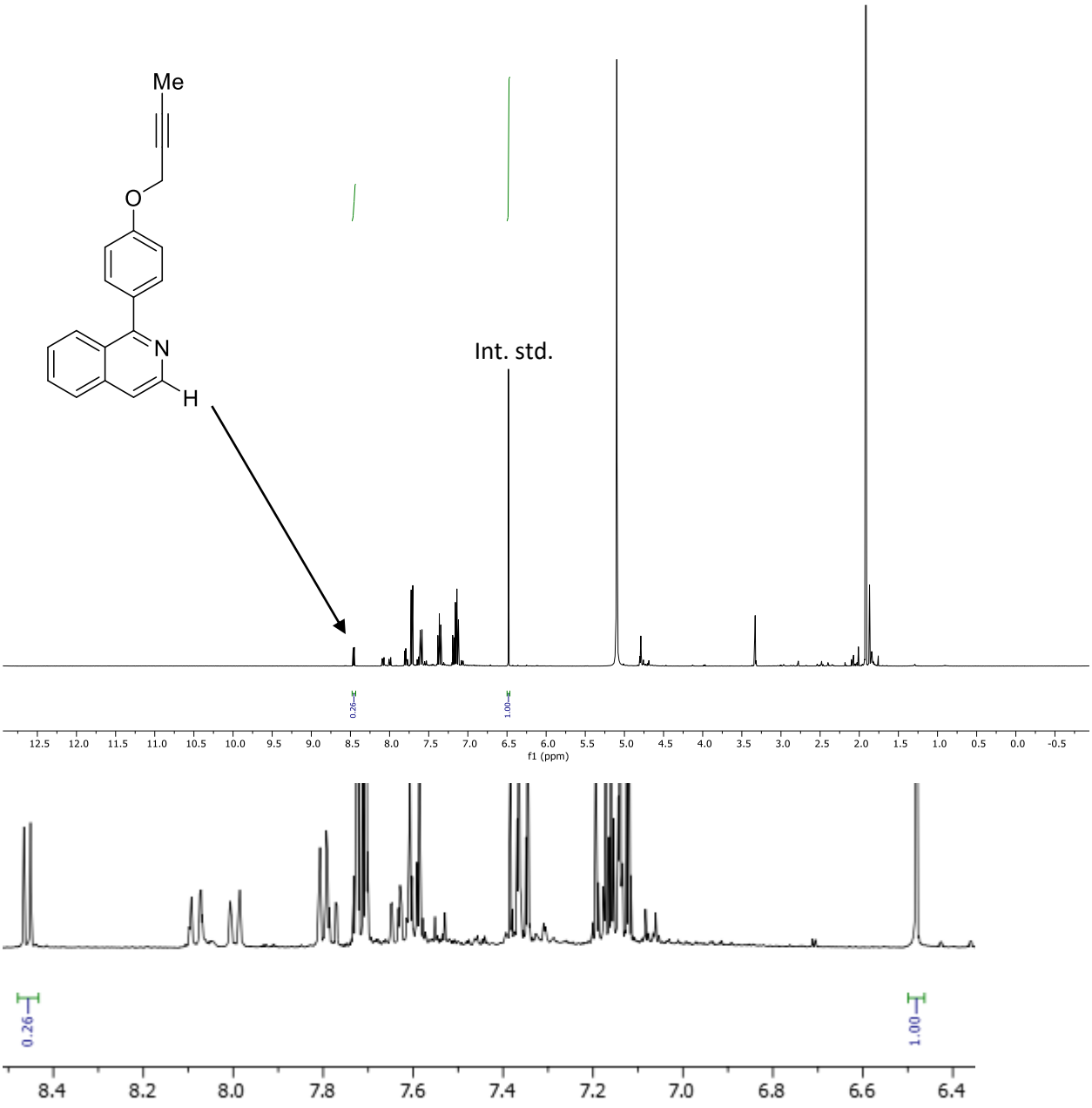
NMR yield: 1-(4-(Trifluoromethyl)phenyl)isoquinoline (21b)



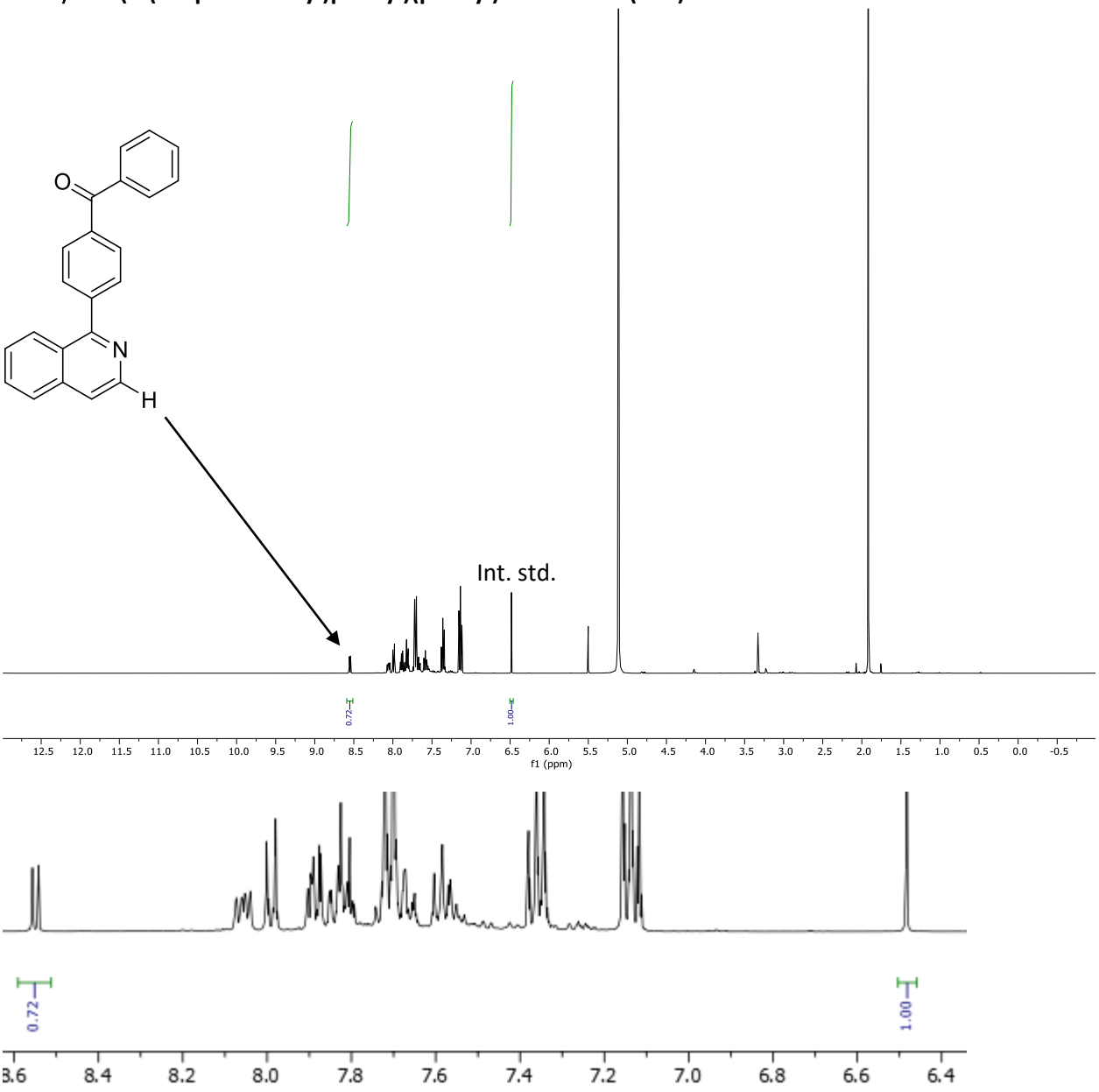
NMR yield: 1-(4-(Pyridin-2-ylmethoxy)phenyl)isoquinoline (22b)



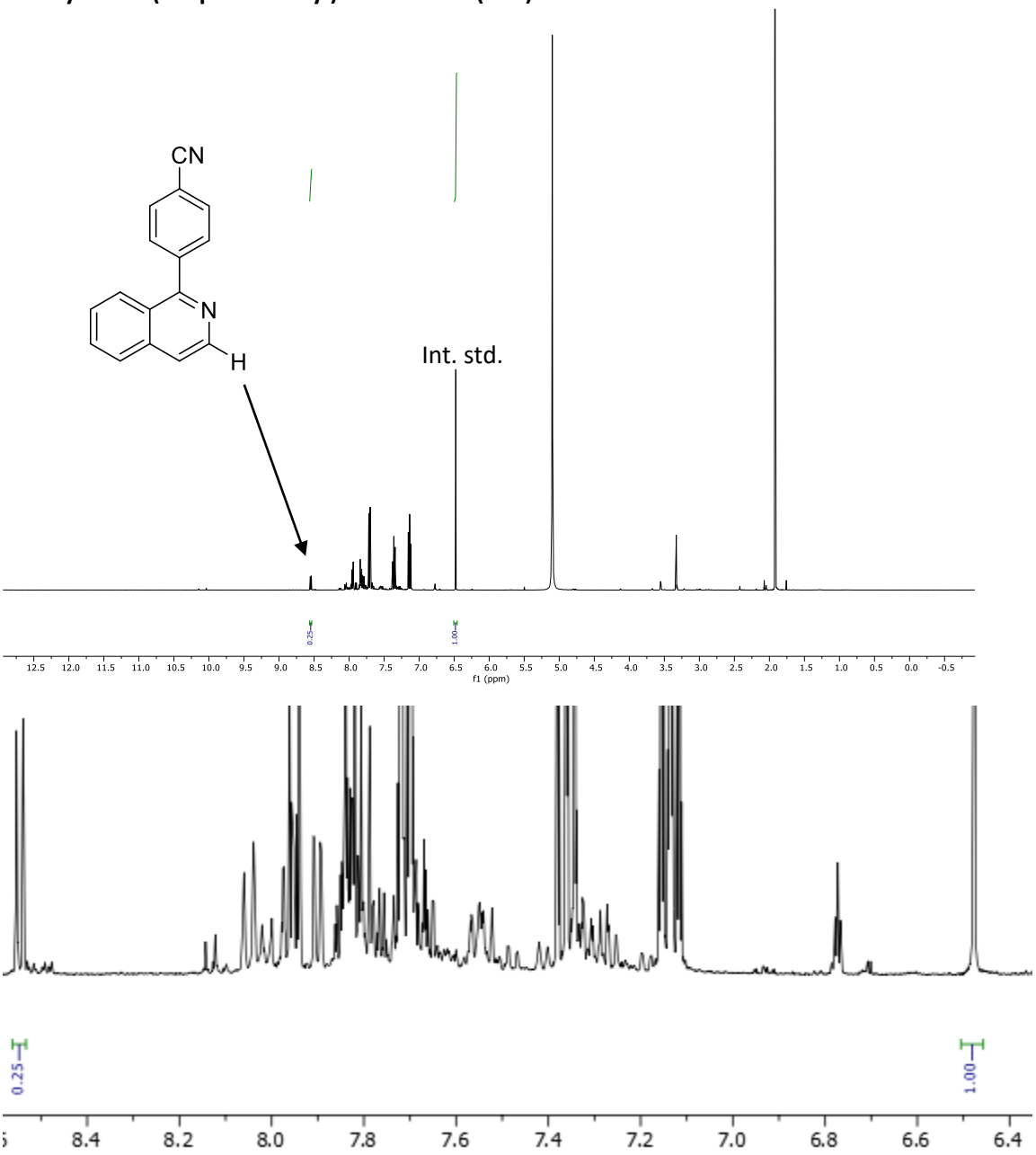
NMR yield: 1-(4-(But-2-yn-1-yloxy)phenyl)isoquinoline (23b)



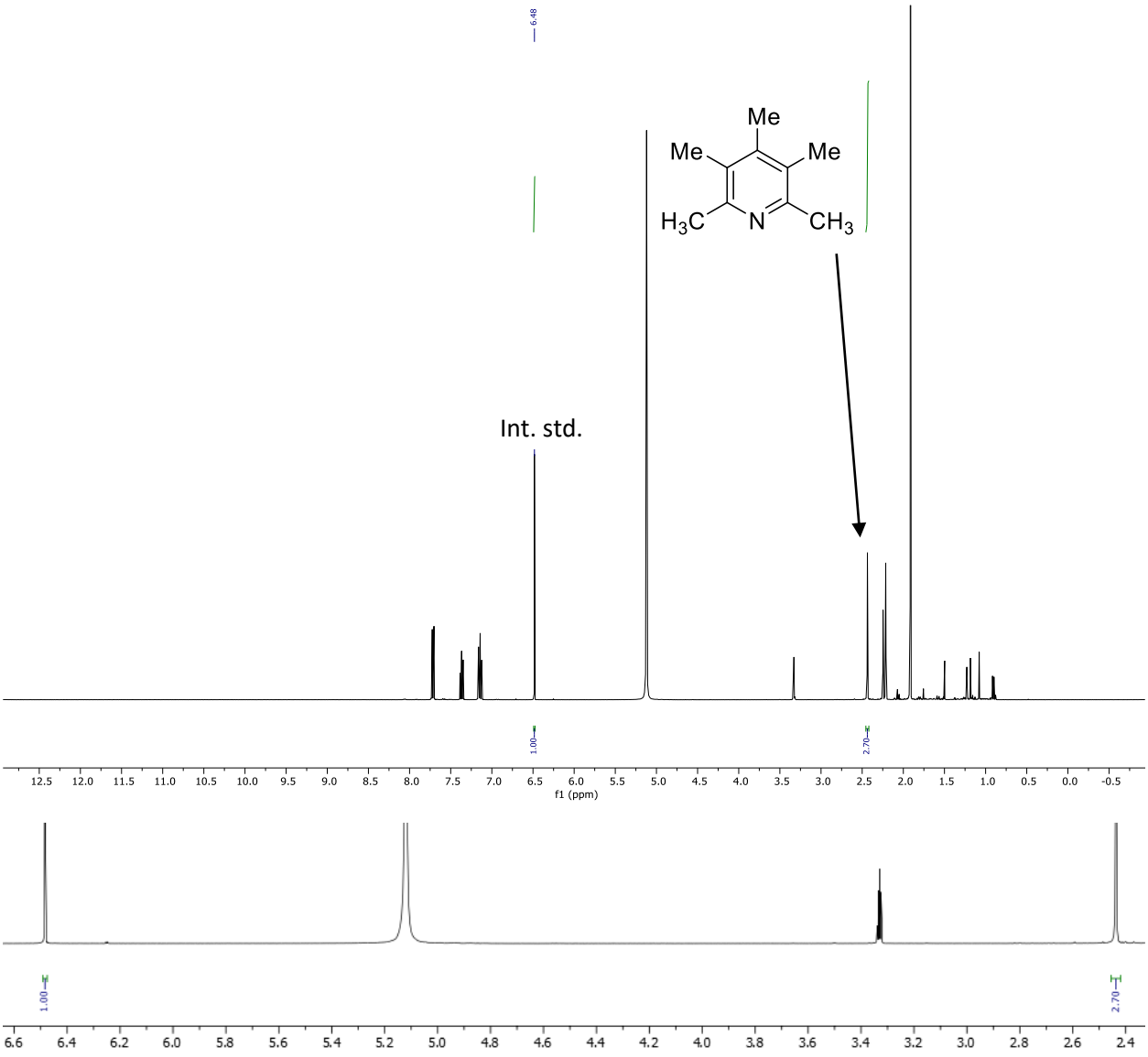
NMR yield: **(4-(Isoquinolin-1-yl)phenyl)(phenyl)methanone (24b)**



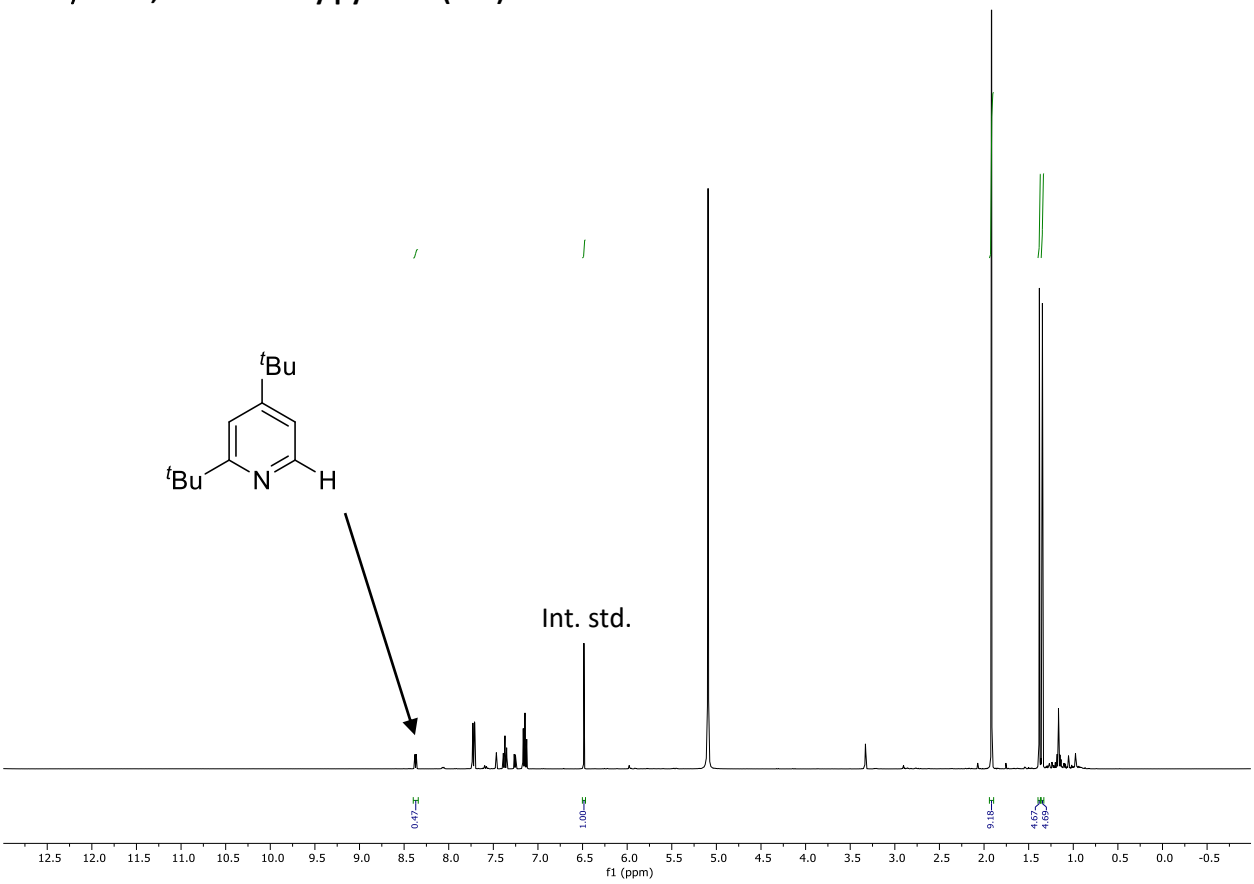
NMR yield: 4-(Isoquinolin-1-yl)benzonitrile (25b)

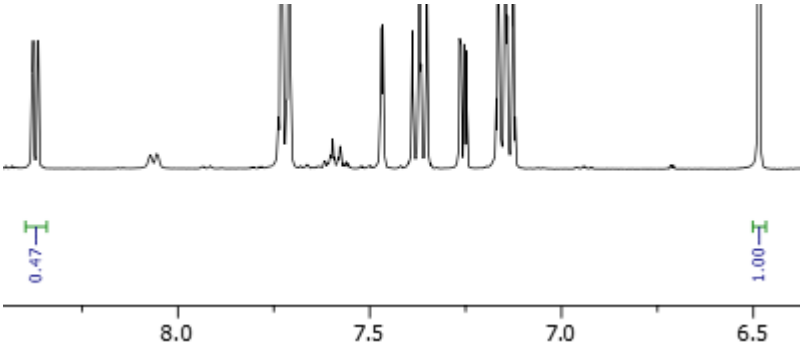


NMR yield: 2,3,4,5,6-Pentamethylpyridine (26b)



NMR yield: **2,4-Di-*tert*-butylpyridine (27b)**





8. References

[1] "CrysAlis Pro | Rigaku Global Website," can be found under https://rigaku.com/products/crystallography/crysalis, **n.d.**
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