Supporting Information

Phosphite mediated molecular editing *via* switch to *meta*-C−H alkylation of isoquinolines: emergence of a distinct photochemical [1,3] N to C rearrangement

Soniya Rani,[a,b†] Anuj Kumar Ray,[c†] Devendra Kumar Dewangan,[a,b†] Nita Aruna Ramchandra Patil,[a] M Aarthika,[a,b] Ankan Paul,*[c] and Pradip Maity*[a,b]

[a]Organic Chemistry Division, CSIR-National Chemical Laboratory, Pune-411008, India. [b]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India. CSIR-National Chemical Laboratory, Pune 411008, India. [c]School of Chemical Sciences, Indian Association for the Cultivation of Science, Kolkata 700032, India

Table of Contents

1. General Information

Unless otherwise mentioned, all the chemicals and reagents were purchased from commercial sources and used without further purification. The rearrangement reactions were carried out with anhydrous solvents in flame-dried borosilicate's Schleck tube under anhydrous argon and oxygen-free conditions. All other reactions were carried out under anhydrous solvent and argon atmosphere. Anhydrous tetrahydrofuran (THF) solvent was used from MBRAUN (MB-SPS-COMPACT) solvent purification system. All other solvents were purchased anhydrous from Sigma and stored under argon over 4 Å molecular sieves. Analytical thin-layer chromatography was performed on glass plates pre-coated with silica gel (Silica Gel 60 F_{254}; Merck). Silica plates were visualized using UV light (λ = 254 nm) and then stained with either aqueous basic potassium permanganate ($KMnO_4$) and developed upon heating in Hitachi heat gun. Flash chromatography was performed using silica gel (Merck and Spectrochem, 230-400 mesh) to isolate products with suitable eluent as determined by TLC. Flash column was performed using Sebo aquarium air pump (SB-548A). ^{1}H, ^{13}C, and ^{31}P spectrum were acquired in deuterated solvents at room temperature on Bruker: Ultrashield 400 MHz, Ultrashield 500 MHz, and Chemical shifts (δ) are reported for ^{1}H NMR in parts per million (ppm) from TMS as internal standard at δ 0.00 ppm. ^{1}H NMR spectra are reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz), and integration. Data for ^{13}C NMR spectra are reported in terms of chemical shift (δ ppm). Melting points were recorded in Buchi Melting Point B-540 instrument and reported in ^{o}C. FT-IR was analyzed using the Bruker ALPHA instrument and reported as wave numbers (cm^{-1}). High resolution mass spectral (HRMS) analyses were recorded by high- resolution mass spectrometry using ESI TOF mass analyzer. UV-Vis absorption spectra were recorded on Shimadzu 1800 spectrophotometer, while all emission spectra were performed using PTI Quanta Master™ Steady State Spectrofluorometer.

2. Materials

Commercially available reagents were purchased and used as obtained. Substituted analogs of isoquinolines 6,7-dimethoxyisoquinoline[1] and 6-methoxyisoquinoline[2] were synthesized following the literature procedure. Alkyl halides were purchased or synthesized following literature procedures.[3] Isoquinolinium salts were synthesized following the literature procedure.[4,5,6]

3. Light Sources and Graphical Representation

Photochemical reactions were performed in a metal condenser (aluminium) to maintain the reaction temperature at 40 °C using LED (30 W, λ_{max} = 365 nm).

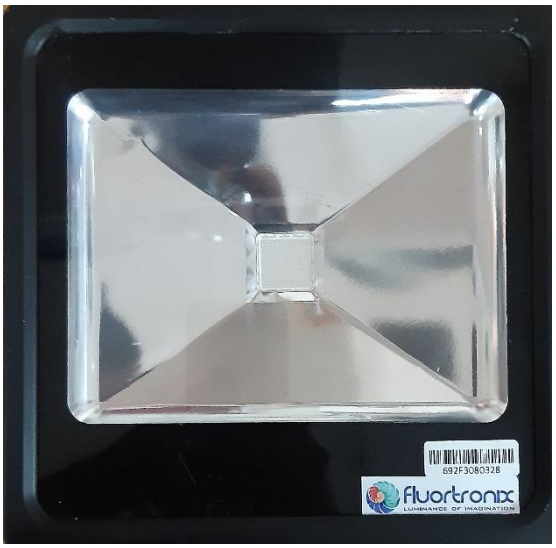
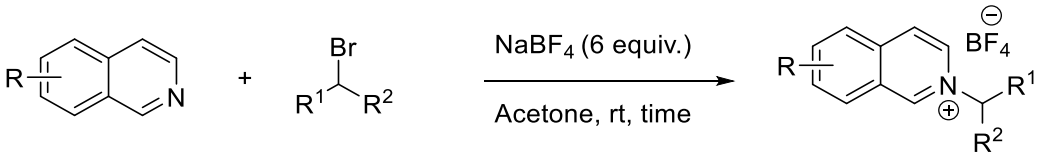


Figure. 1a LED (30W, λ_{max} = 365 nm)

Figure. 1b Metal Condenser (aluminium)

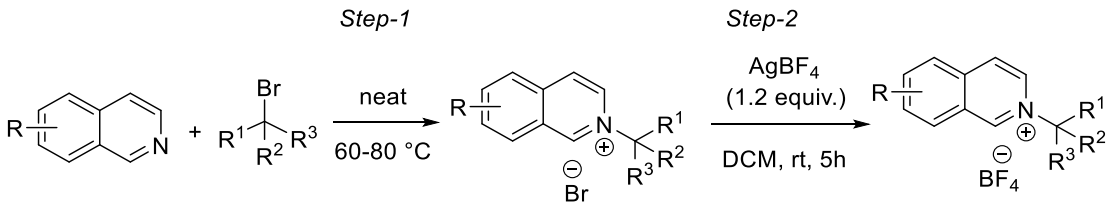
4. Preparation of *N*-alkyl Isoquinolinium Salts

4a. General Procedure (GP-A) for the Synthesis of N-alkyl Isoquinolinium Salts



Unless otherwise specified, in a flame dried 50 mL round bottom flask with a magnetic bar, isoquinoline (2 mmol, 1 equiv.) was taken, and anhydrous acetone (10 mL, 0.2 M) was added by syringe at room temperature under a stream of Ar atmosphere. Substituted alkyl halide (3 mmol, 1.5 equiv.) was added to this solution. Subsequently, the cap was opened and solid sodium tetrafluoroborate was added quickly in one portion. Reaction mixture was allowed to stir at ambient temperature till the consumption of isoquinoline. Upon complete consumption of the starting material (monitored by TLC), the precipitate was removed through filtration. The solvent was removed under reduced pressure, and the solid residual was purified via silica gel column chromatography using 05:95 MeOH/DCM as an eluent to obtain the pure product.

4b. General Procedure (GP-B) for the Synthesis of N-alkyl Isoquinolinium Salts



Step-1:

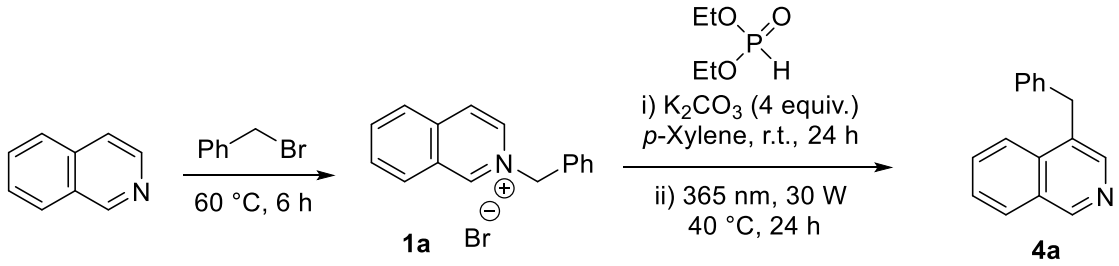
Unless otherwise specified, in a flame dried 10 mL pressure tube with a magnetic bar, isoquinoline (3 mmol, 1 equiv.) was mixed neat with a slight excess (1.2 equiv.) of alkyl bromide and the mixture heated to 60-80 ℃ until the reaction mixture solidified (7-12 h). Upon complete consumption of the starting material (monitored by TLC), the solid mass was washed with diethyl ether to obtain pure bromo salt.

Step-2:

To obtain tetrafluoroborate salt, the bromide salt was dissolved in DCM and treated with $AgBF_4$ (1.2 equiv) at room temperature for 5 h. The solvent was removed under reduced pressure, and the tetrafluoroborate product was purified via silica gel column chromatography using 05:95 MeOH/DCM as an eluent.

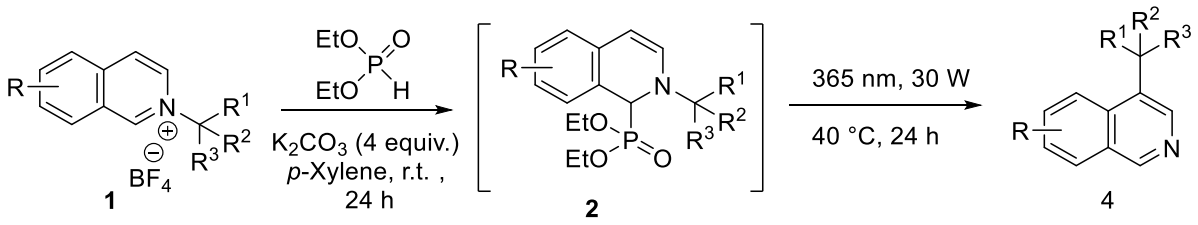
5. Optimization of Reaction Conditions

5a. Reaction Procedure (GP-C) for One-pot *meta*-Alkylation



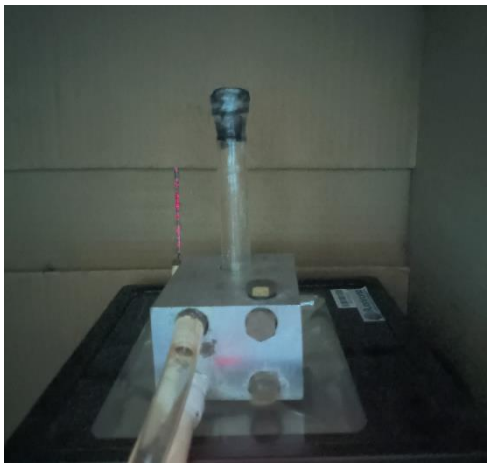
In a flame dried 25 mL schlenk tube with a magnetic bar, isoquinoline (0.2 mmol, 1 equiv.) was mixed neat with a slight excess (1.2 equiv.) of benzyl bromide and the reaction mixture was allowed to stir at 60 °C. Upon complete consumption of the starting material (monitored by TLC), the solid mass was washed with diethyl ether to obtain pure bromo salt. Anhydrous *p*-xylene (2.5 mL) was added by syringe under the stream of argon atmosphere. To this solution, diethyl hydrogen phosphite (0.24 mmol, 1.2 equiv.) was added by micro syringe, and solid K_2CO_3 (0.8 mmol, 4 equiv.) was quickly added in one portion via opening the cap. The vial was re-capped with septa, packed with insulating tape, and covered with aluminium foil. The reaction mixture was degassed with argon for 10 minutes, and then the reaction mixture was stirred for 24 h at 25 °C. After this time, the aluminium foil was removed, and this solution was exposed to a 365 nm LED (30W) at 40 °C for 24 h. Lithium tert-butoxide (1 mL, 0.1M) solution was added (using a syringe without opening the reaction tube) at room temperature to quench the reaction. The crude was extracted with ethyl acetate (three times), and the organic layer was combined and dried over sodium sulfate. The solvent was removed under reduced pressure to obtain the crude product, which was further purified by flash column chromatography on silica gel using ethyl acetate-pet ether as an eluent.

5b. General Reaction Procedure (GP-D) for Phosphite Mediated Photochemical *meta*-Alkylation

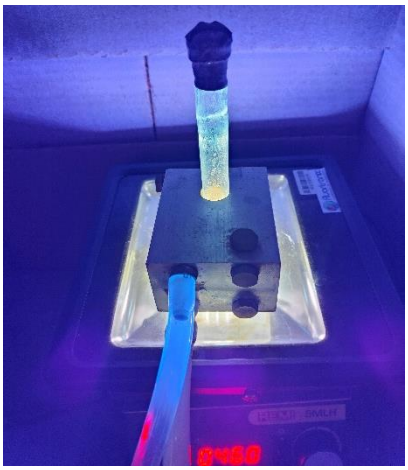


Unless otherwise specified, in a flame dried 25 mL schlenk tube with a magnetic bar, isoquinolinium salt **1** (0.2 mmol, 1 equiv.) was added, followed by anhydrous *p*-xylene (2.5 mL) by syringe under the stream of argon atmosphere. To this solution, diethyl hydrogen phosphite (0.24 mmol, 1.2 equiv.) was added by micro syringe, and solid K_2CO_3 (0.8 mmol, 4 equiv.) was quickly added in one portion via opening the cap. The vial was re-capped with septa, packed with insulating tape, and covered with aluminium foil. The reaction mixture was degassed with argon for 10 minutes, and then the reaction mixture was stirred for 24 h at 25 °C. After this time, the aluminium foil was removed, and this solution was exposed to a 365 nm LED (30W) at 40 °C for 24 h. Lithium tert-butoxide (1 mL, 0.1M) solution was added (using a syringe without opening the reaction tube) at room temperature to quench the reaction. The ethyl acetate extract contained product while the phosphite remained in aqueous solution. The organic layer was combined and dried over sodium sulfate. The solvent was removed under reduced pressure to obtain the crude product, which was further purified by flash column chromatography on silica gel using ethyl acetate-pet ether as an eluent. The phosphite could be extracted from the aqueous solution via neutralization with dilute HCl and extraction in ethyl acetate (Note: the phosphite anion is prone to air oxidation, and the extraction under inert conditions led to near quantitative phosphite recovery).

Graphical Procedure for Phosphite Mediated Photochemical [1,3] N to C Rearrangement

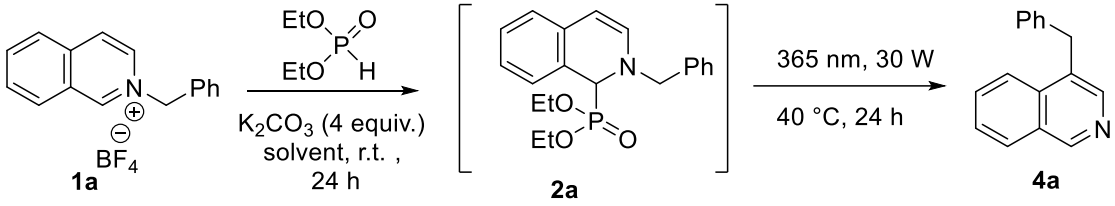


Reaction setup before turn on the light



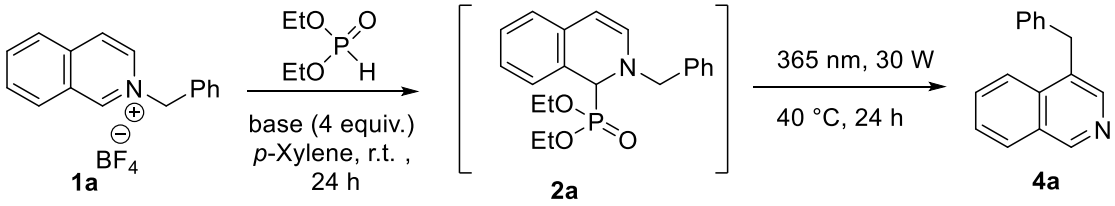
Reaction setup after turn on the light

Figure-2. Reaction setup for photochemical *meta*-alkylation



Entry	Solvent	yield (%)
1	PhMe	35
2	***p*-Xylene**	**60**
3	mesitylene	12
4	Hexane	13
5	Ph^{t}Bu	44
6	$PhCF_3$	46
7	THF	43
8	DCM	13
9	ACN	20
10	DMSO	37

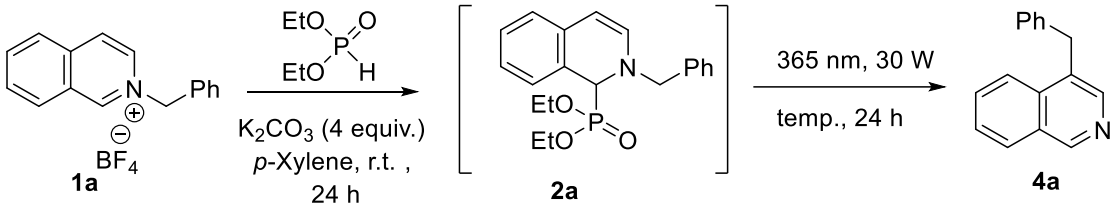
Figure-3. Solvent optimization for photochemical *meta*-alkylation



Entry	Base	yield (%)
1	**K_2CO_3**	**60**
2[a]	K_2CO_3	54
3[b]	K_2CO_3	60
4	Cs_2CO_3	35
5	Et_3N	19
6	DBU	10
7	TMG	15
8	Na_3PO_4	50
9	NaOH	25
10	NaO^{t}Bu	20

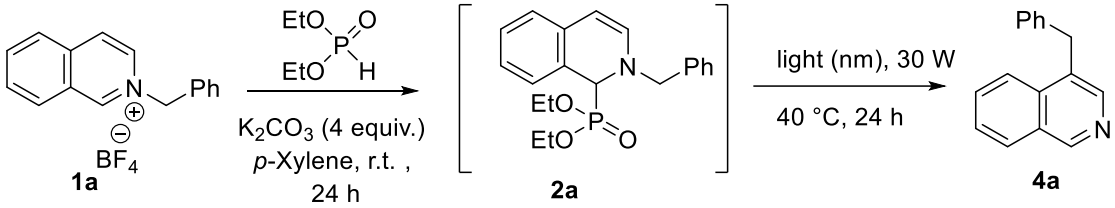
[a]3.0 equiv. of K_2CO_3. [b]5.0 equiv. of K_2CO_3

Figure-4. Base optimization for photochemical *meta*-alkylation



Entry	Temperature (°C)	yield (%)
1	25	47
2	**40**	**60**
3	10	27
4	50	44

Figure-5. Temperature screening for photochemical *meta*-alkylation

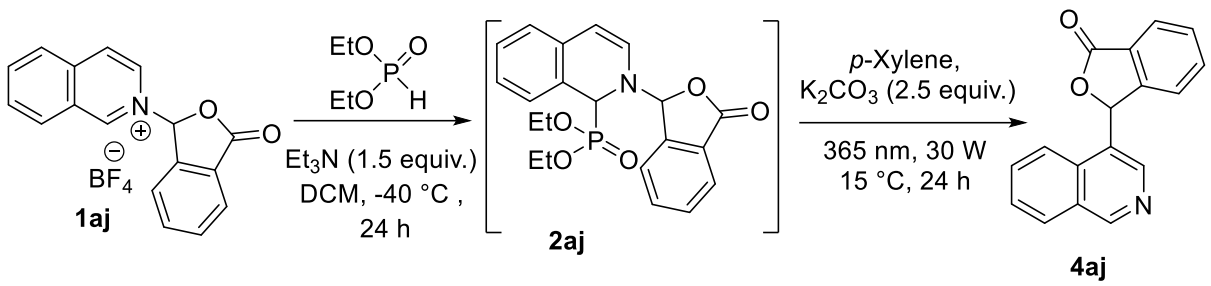


Entry	Light (nm)	yield (%)
1	320	<5
2	**365**	**60**
3	380	40
4[a]	395	29
5[b]	410	10
6[c]	450	n.d.
7[d]	365	34

[a]30% intermediate **2a** remaining. [b]80% intermediate **2a** remaining. [c]More that 95% intermediate **2a** remaining. [d]18 W 365 nm light was used. n.d. - not detected

Figure-6. Light screening for photochemical *meta*-alkylation

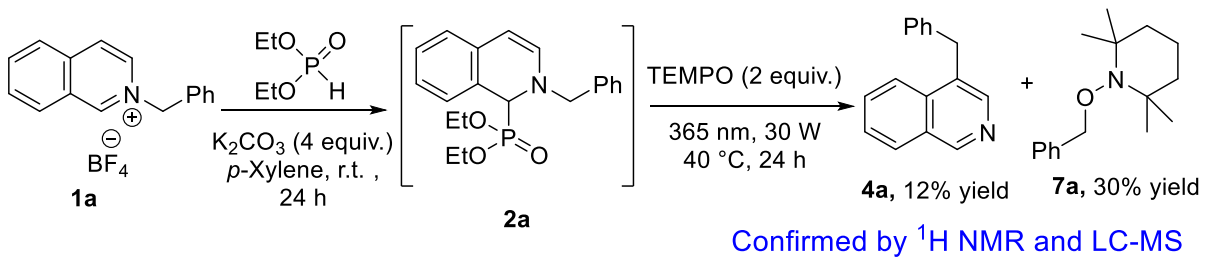
5c. Reaction Procedure (GP-E) for Phosphite Mediated Photochemical *meta*-Alkylation of Compound 4aj



In a flame dried 25 mL schlenk tube with a magnetic bar 2-(3-oxo-1,3-dihydroisobenzofuran-1-yl)isoquinolin-2-ium tetrafluoroborate **1aj** (0.2 mmol, 1 equiv.) was charged and subsequently anhydrous DCM (2.5 mL) was added by syringe under the stream of argon atmosphere. To this solution, diethyl hydrogen phosphite (0.24 mmol, 1.2 equiv.) was added by micro syringe, then Et_3N (0.3 mmol, 1.5 equiv.) was added by micro syringe at -40 °C. The reaction vessel was packed with insulating tape and covered with aluminium foil. The reaction mixture was degassed with argon atmosphere for 10 minutes, and stirred for 24 h at -40 °C. DCM solvent was evaporated at reduced pressure, and anhydrous *p*-xylene (2.5 mL) and K_2CO_3 (2.5 equiv.) were added under the stream of argon atmosphere. The reaction mixture was degassed with argon for 10 minutes and exposed to a 365 nm LED (30W) at 15 °C for 24 h. Lithium tert-butoxide (1 mL, 0.1M) solution was added (using a syringe without opening the reaction tube) at room temperature to quench the reaction. The crude was extracted with ethyl acetate (three times), and the organic layer was combined and dried over sodium sulfate. The solvent was removed under reduced pressure to obtain the crude product, which was further purified by flash column chromatography on silica gel using ethyl acetate-pet ether as an eluent.

6. Mechanistic Studies

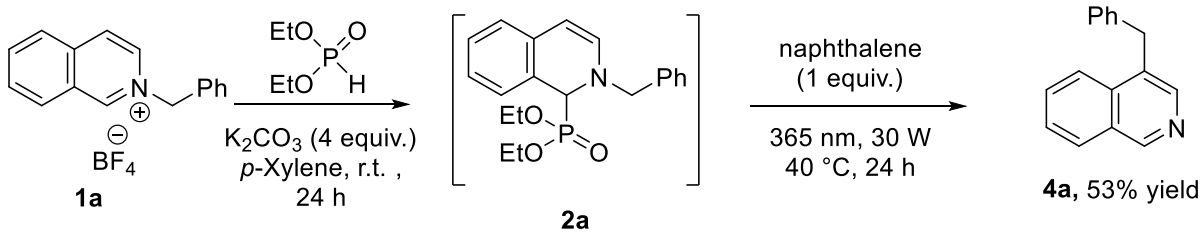
6a. Reaction with TEMPO as Radical Trapping Reagent



In a flame dried 25 mL schlenk tube with a magnetic bar, isoquinolinium salt **1a** (0.2 mmol, 1 equiv.) was added, followed by anhydrous *p*-xylene (2.5 mL) by syringe under the stream of argon atmosphere. To this solution, diethyl hydrogen phosphite (0.24 mmol, 1.2 equiv.) was added by micro syringe, and solid K_2CO_3 (0.8 mmol, 4 equiv.) was quickly added in one portion via opening the cap. The vial was

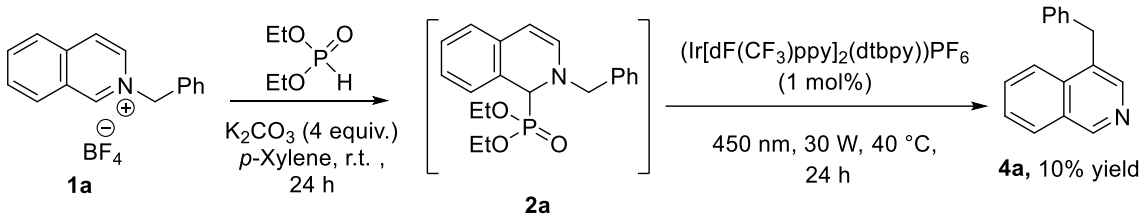
re-capped with septa, packed with insulating tape, and covered with aluminium foil. The reaction mixture was degassed with argon for 10 minutes, and then the reaction mixture was stirred for 24 h at 25 °C. After this time, degassed TEMPO solution in 0.5 mL *p*-xylene (0.4 mmol, 2 equiv.) was added to the reaction mixture at 25 °C. The aluminium foil was removed, and this solution was exposed to a 365 nm LED (30W) at 40 °C for 24 h. Lithium tert-butoxide (1 mL, 0.1M) solution was added (using a syringe without opening the reaction tube) at room temperature to quench the reaction. The crude was extracted with ethyl acetate (three times), and the organic layer was combined and dried over sodium sulfate. The solvent was removed under reduced pressure to obtain the crude product which was first analysed by HRMS and ^{1}H-NMR, followed by further purification via column chromatography on silica gel using 1.5 - 2% EtOAc-Pet ether as eluent to obtain TEMPO-trapped benzyl compound (**7a**) 30% yield and rearrangement product (**4a**) 12% yield in pure form. Presence of TEMPO-trapped benzyl compound indicates the reaction proceeds via radical pathway.

6b. Experimental Procedure for Reaction with a Triplet Quencher



In a flame dried 25 mL schlenk tube with a magnetic bar, isoquinolinium salt **1a** (0.2 mmol, 1 equiv.) was added, followed by anhydrous *p*-xylene (2.5 mL) by syringe under the stream of argon atmosphere. To this solution, diethyl hydrogen phosphite (0.24 mmol, 1.2 equiv.) was added by micro syringe, and solid K_2CO_3 (0.8 mmol, 4 equiv.) was quickly added in one portion via opening the cap. The vial was re-capped with septa, packed with insulating tape, and covered with aluminium foil. The reaction mixture was degassed with argon for 10 minutes, and then the reaction mixture was stirred for 24 h at 25 °C. After this time, degassed naphthalene solution in 0.5 mL *p*-xylene (0.2 mmol, 1 equiv.) was added to the reaction mixture at 25 °C. After this time, the aluminium foil was removed, and this solution was exposed to a 365 nm LED (30W) at 40 °C for 24 h. Lithium tert-butoxide (1 mL, 0.1M) solution was added (using a syringe without opening the reaction tube) at room temperature to quench the reaction. The crude was extracted with ethyl acetate (three times), and the organic layer was combined and dried over sodium sulphate. Solvent was removed under reduced pressure to obtain the crude product which was further purified by flash column chromatography on silica gel using ethyl acetate-pet ether as an eluent.

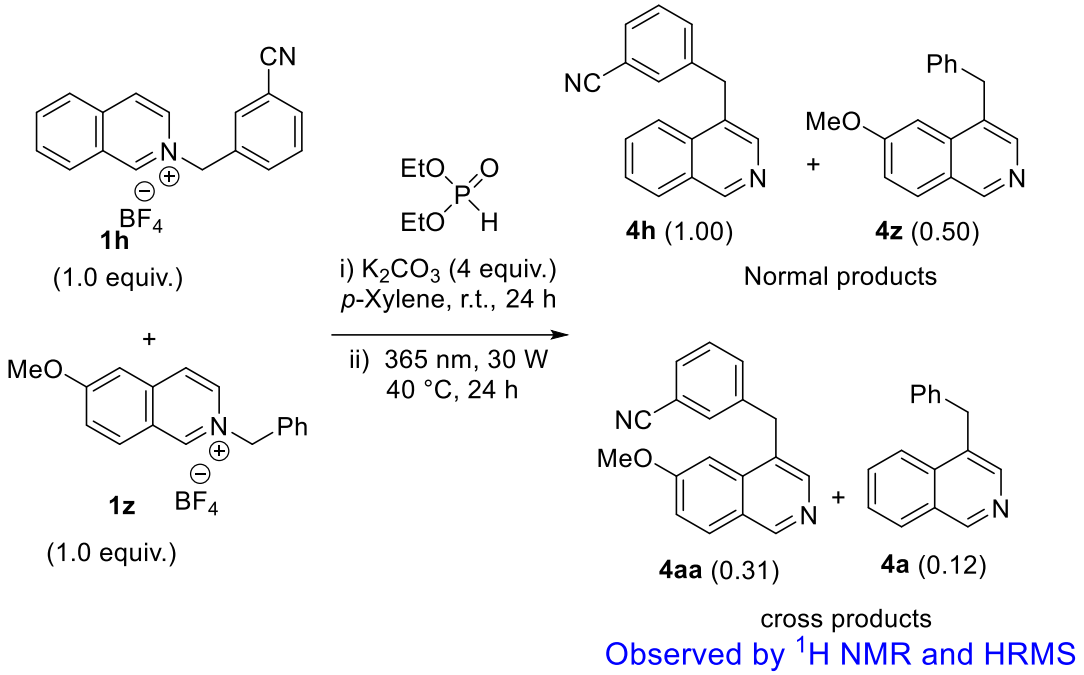
6c. Experimental Procedure for Reaction with a Triplet Photosensitizer



In a flame dried 25 mL schlenk tube with a magnetic bar, isoquinolinium salt **1a** (0.2 mmol, 1 equiv.) was added, followed by anhydrous *p*-xylene (2.5 mL) by syringe under the stream of argon atmosphere. To this solution, diethyl hydrogen phosphite (0.24 mmol, 1.2 equiv.) was added by micro syringe, and solid K_2CO_3 (0.8 mmol, 4 equiv.) was quickly added in one portion via opening the cap. The vial was re-capped with septa, packed with insulating tape, and covered with aluminium foil. The reaction mixture was degassed with argon for 10 minutes, and then the reaction mixture was stirred for 24 h at 25 °C. After this time, triplet photosensitizer ($Ir[dF(CF_3)ppy]_2(dtbpy))PF_6$ (1 mol%) was added to the reaction mixture at 25 °C under the stream of argon atmosphere. Reaction mixture was degassed for 5 min. After this time, the aluminium foil was removed, and this solution was exposed to a 450 nm LED (30W) at 40 °C for 24 h. Lithium tert-butoxide (1 mL, 0.1M) solution was added (using a syringe without opening the reaction tube) at room temperature to quench the reaction. The crude was extracted with ethyl acetate (three times), and the organic layer was combined and dried over sodium sulphate. Solvent was removed under reduced pressure to obtain the crude product which was further purified by flash column chromatography on silica gel using ethyl acetate-pet ether as an eluent.

More than 95% of the intermediate **2a** remained unreacted throughout the direct excitation process at 450 nm LED (30W). However, using a triplet photosensitizer at 450 nm LED (30W) resulted in 10% yield of *meta*-alkylated product, leaving 15% unreacted intermediate **2a**. This explains that 10% product formed via triplet state in presence of triplet photosensitizer at 450 nm.

6d. Experimental Procedure for Crossover Experiment



In a flame dried 25 mL schlenk tube with a magnetic bar, isoquinolinium salt **1h** and **1z** (1 equiv. and 0.1 mmol each) was added followed by anhydrous *p*-xylene (2.5 mL) by syringe under the stream of argon atmosphere. To this solution, diethyl hydrogen phosphite (0.24 mmol, 1.2 equiv.) was added by micro syringe, and solid K_2CO_3 (0.8 mmol, 4 equiv.) was quickly added in one portion via opening the cap. The vial was re-capped with septa, packed with insulating tape, and covered with aluminium foil. The reaction mixture was degassed with argon for 10 minutes, and then the reaction mixture was stirred for 24 h at 25 °C. After this time, the aluminium foil was removed, and this solution was exposed to a 365 nm LED (30W) at 40 °C for 24 h. Lithium tert-butoxide (1 mL, 0.1M) solution was added (using a syringe without opening the reaction tube) at room temperature to quench the reaction. The crude was extracted with ethyl acetate (three times), and the organic layer was combined and dried over sodium sulfate. The solvent was removed under reduced pressure to obtain the crude product. ^{1}H NMR and HRMS confirmed the normal products (**4h**, **4z**) and cross products (**4a**, **4aa**) formation. The ratio of normal products and cross products was analysed by ^{1}H NMR (**4h** : **4aa** : **4z** : **4a** = 1.00 : 0.31 : 0.50 : 0.12). (See analysis below)

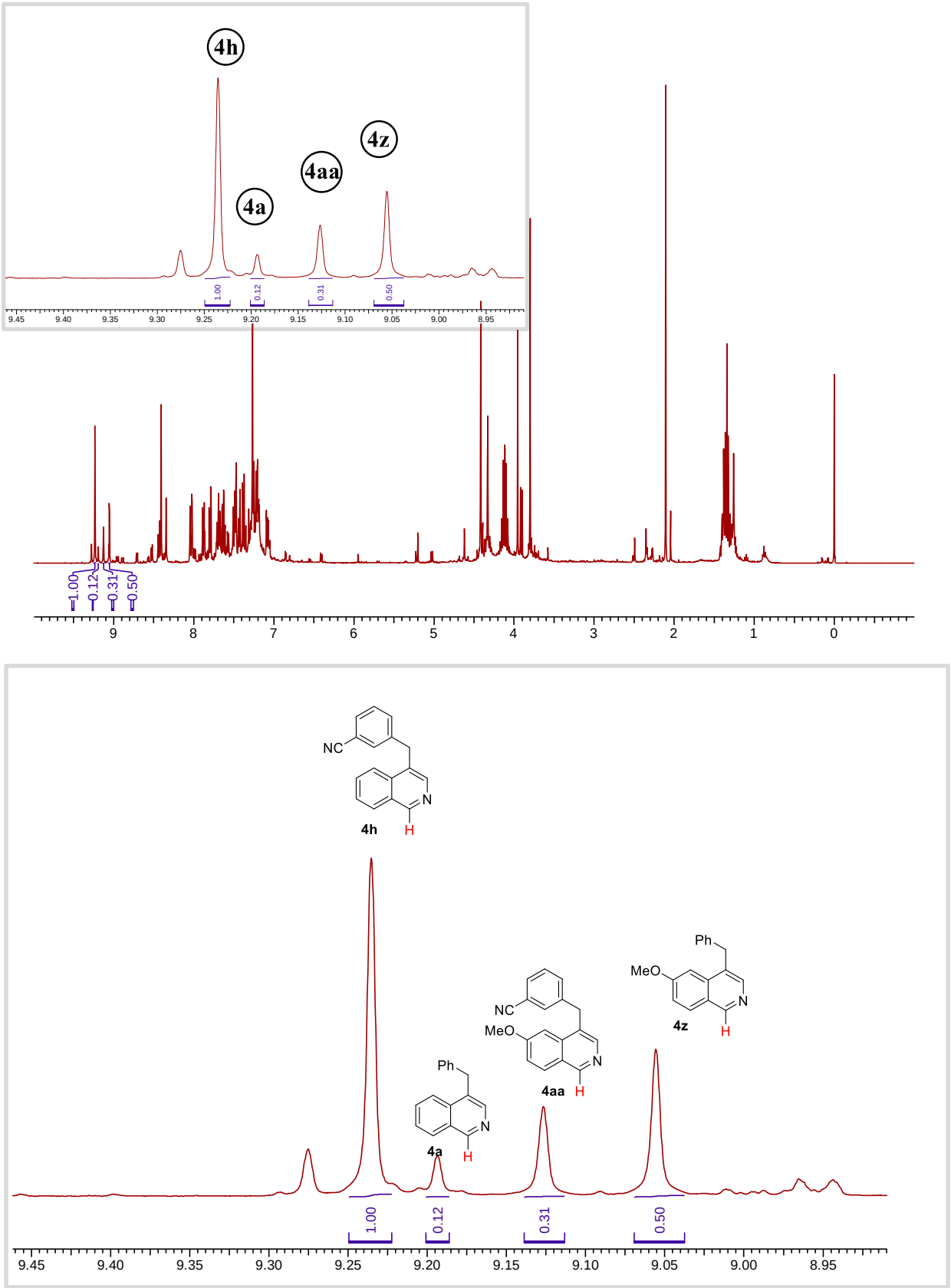
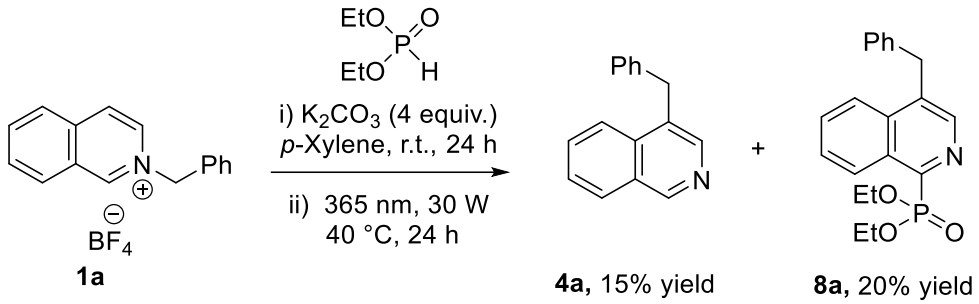


Figure-7. ^{1}H NMR of reaction crude from the crossover experiment

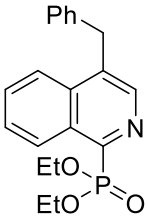
6e. Experimental Procedure for Reaction under Aerobic Condition:



Confirmed by ^{1}H NMR and LC-MS

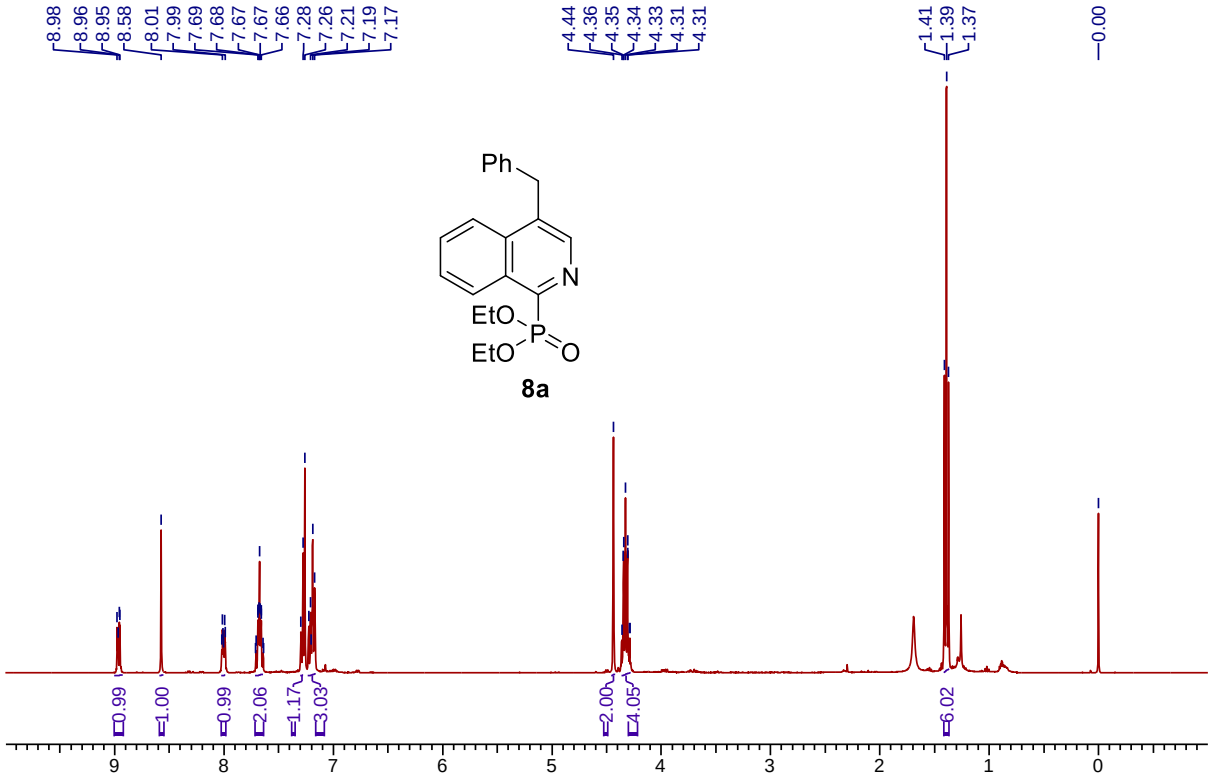
In a flame dried 25 mL schlenk tube with a magnetic bar, isoquinolinium salt **1a** (0.2 mmol, 1 equiv.) was added followed by anhydrous *p*-xylene (2.5 mL) by syringe under the stream of argon atmosphere. To this solution, diethyl hydrogen phosphite (0.24 mmol, 1.2 equiv.) was added by micro syringe, and solid K_2CO_3 (0.8 mmol, 4 equiv.) was quickly added in one portion via opening the cap. The vial was re-capped with septa, packed with insulating tape, and covered with aluminium foil and then the reaction mixture was stirred for 24 h at 25 °C. After this time, the aluminium foil was removed, and this solution was exposed to a 365 nm LED (30W) at 40 °C for 24 h. Lithium tert-butoxide (1 mL, 0.1M) solution was added (using a syringe without opening the reaction tube) at room temperature to quench the reaction. The crude was extracted with ethyl acetate (three times), and the organic layer was combined and dried over sodium sulphate. Solvent was removed under reduced pressure to obtain the crude product, which was further purified by flash column chromatography on silica gel using ethyl acetate-pet ether as an eluent. After purification compound **4a** was obtained in 15% yield along with compound **8a** in 20% yield. Compound **8a** formation support the proposed mechanism.

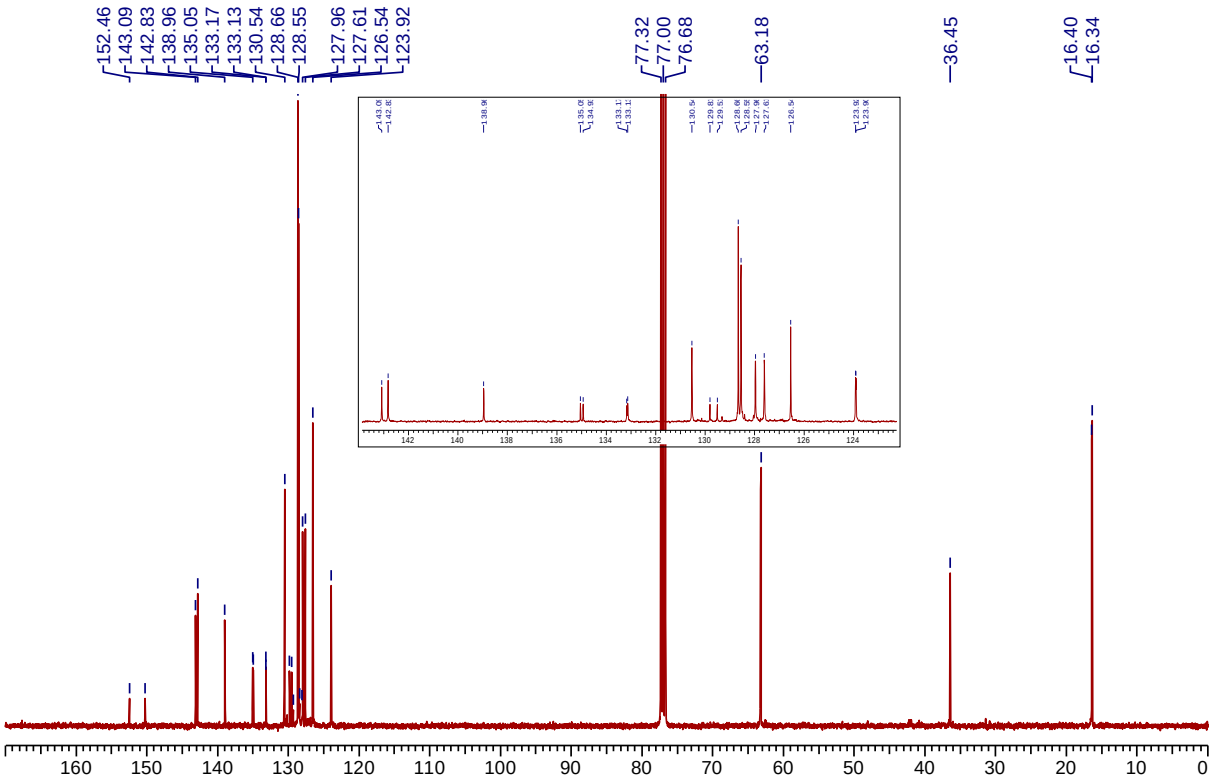
Diethyl (4-benzylisoquinolin-1-yl)phosphonate (8a)

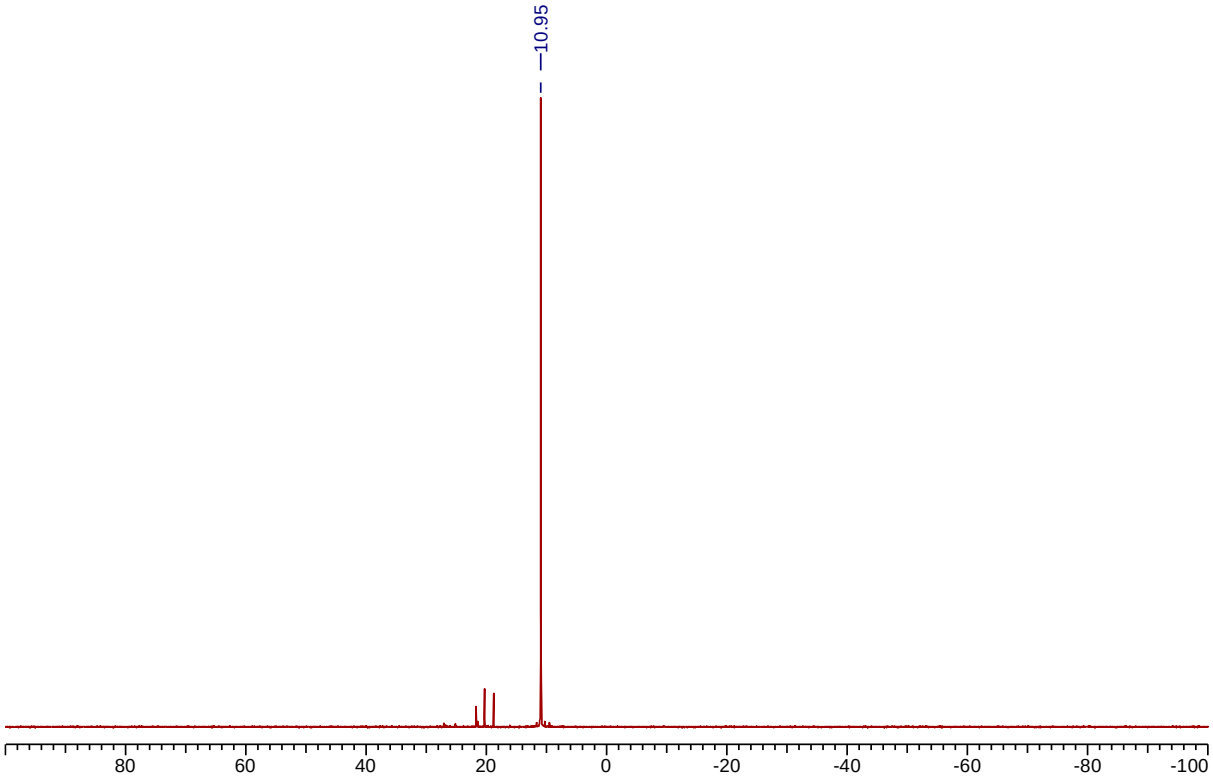


The title compound was isolated via flash column chromatography using 80-90% Ethyl acetate/Pet. ether, obtained as a sticky solid (14.2 mg, 20% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.00 – 8.92 (m, 1H), 8.58 (s, 1H), 8.03 – 7.98 (m, 1H), 7.71 – 7.64 (m, 2H), 7.30 - 7.27 (m, 1H), 7.23 - 7.16 (m, 3H), 4.44 (s, 2H), 4.37 - 4.28 (m, 4H), 1.39 (t, *J* = 7.1 Hz, 6H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.3 (d, *J* = 224.3 Hz), 143.1, 142.8, 139.0, 135.0 (d, *J* = 11.4 Hz), 133.2 (d, *J* = 4.6 Hz), 130.5, 129.7 (d, *J* = 29.8 Hz), 128.7, 128.6, 127.8 (d, *J* = 35.9 Hz), 126.5, 123.9 (d, *J* = 1.5 Hz), 63.2 (d, *J* = 6.1 Hz), 36.5 (d, *J* = 1.5 Hz), 16.4 (d, *J* = 6.1 Hz). **^{31}P NMR (162 MHz, $CDCl_3$)** δ 10.95. **FTIR (cm^{-1}):** 3028, 2960, 2921, 2854, 1726, 1639, 1499, 1396, 1296, 1035, 890, 762.

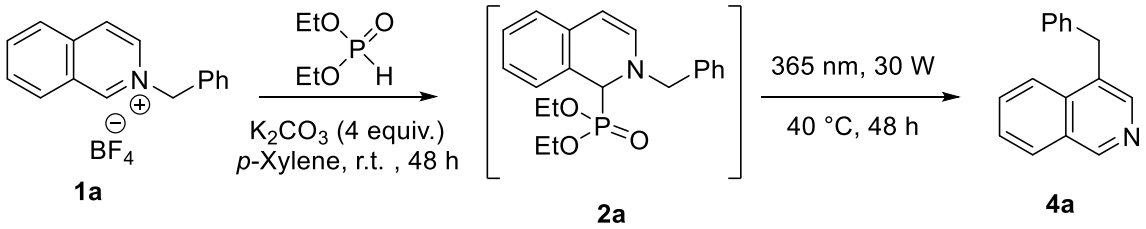
HRMS (ESI) *m/z* Calculated for $C_{20}H_{23}O_3NP$ $[M+H]^+$: 356.1410, found: 356.1409.


8.98
8.96
8.95
8.58
8.01
7.99
7.69
7.68
7.67
7.67
7.66
7.28
7.26
7.21
7.19
7.17
4.44
4.36
4.35
4.34
4.33
4.31
4.31
1.41
1.39
1.37
0.00
Ph
N
EtO
P
O
EtO
8a
0.99
1.00
0.99
2.06
1.17
3.03
2.00
4.05
6.02
9
8
7
6
5
4
3
2
1
0


152.46
143.09
142.83
138.96
135.05
133.17
133.13
130.54
128.66
128.55
127.96
127.61
126.54
123.92
77.32
77.00
76.68
63.18
36.45
16.40
16.34
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



7. Reaction Scale-up – 1 mmole Scale Reaction



Unless otherwise specified, in a flame dried 55 mL schlenk tube with a magnetic bar, isoquinolinium salt **1** (1.0 mmol, 1 equiv.) was added, followed by anhydrous *p*-xylene (11 mL) by syringe under the stream of argon atmosphere. To this solution, diethyl hydrogen phosphite (12 mmol, 1.2 equiv.) was added by micro syringe, and solid K_2CO_3 (4 mmol, 4 equiv.) was quickly added in one portion via opening the cap. The vial was re-capped with septa, packed with insulating tape, and covered with aluminium foil. The reaction mixture was degassed with argon for 20 minutes, and then the reaction mixture was stirred for 48 h at 25 °C. After this time, the aluminium foil was removed, and this solution was exposed to a 365 nm LED (30W) at 40 °C for 48 h. Lithium tert-butoxide (5 mL, 0.1M) solution was added (using a syringe without opening the reaction tube) at room temperature to quench the reaction. The crude was extracted with ethyl acetate (three times), and the organic layer was combined and dried over sodium sulphate. The solvent was removed under reduced pressure to obtain the crude product, which was further purified by flash column chromatography on silica gel using ethyl acetate-pet ether as an eluent to obtain **4a** in pure form with 61% yield.

7.1 Graphical Procedure of Scale-up Reaction

***Image S1**: Flame dried schleck tube by heat gun under vacuum*

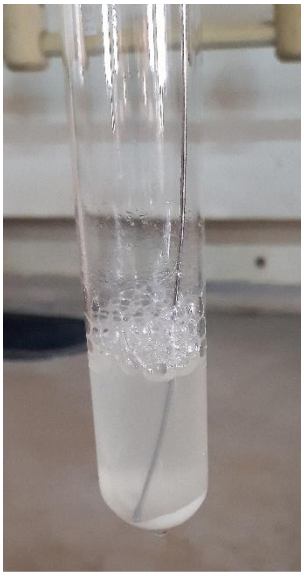


***Image S2**: Degassing the reaction mixture using argon*

***Image S3**: Reaction mixture before intermediate formation*

***Image S4**: Reaction covered with aluminium foil*

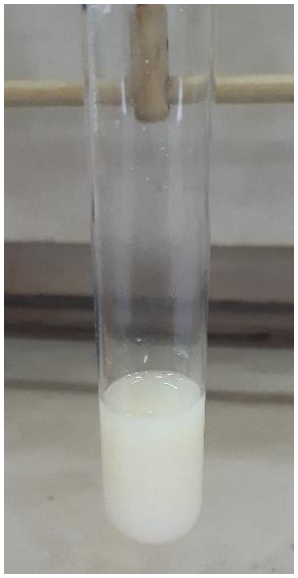


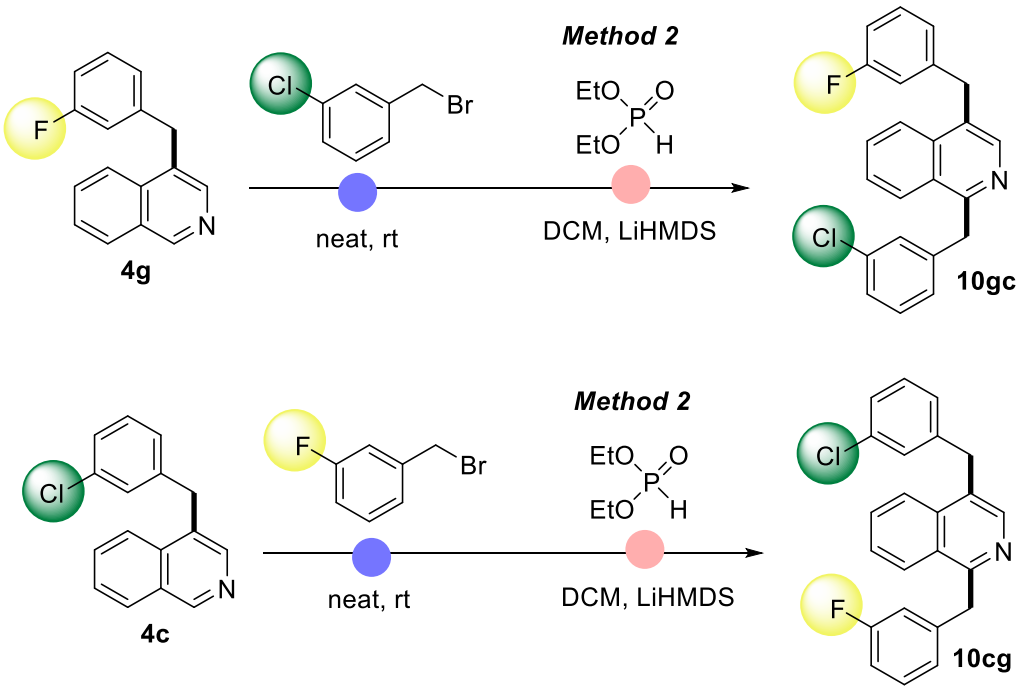
***Image S5**: Reaction mixture after intermediate formation*

***Image S6**: Reaction mixture in presence of light*

***Image S7**: Reaction mixture after completing light reaction*

8. Reaction Procedure for Molecular Editing via Phosphite Mediated Sequential Functionalization of Isoquinoline

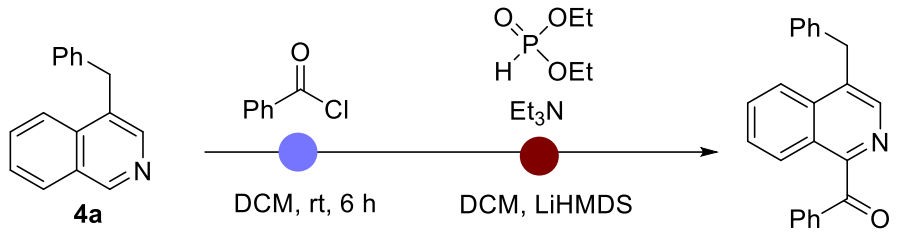
8a. Reaction Procedure (GP-F) for one-pot regiodivergent double C−H alkylation



In a flame dried 25 mL peared-shaped flask with a magnetic bar, preformed *meta*-alkylated isoquinoline (0.3 mmol, 1 equiv.) following the general procedure for *meta*-alkylation (**GP-D**) was taken. Substituted alkyl halide (0.45 mmol, 1.5 equiv.) was added. Reaction mixture was allowed to stir at 60 °C till the consumption of starting material. Upon complete consumption of the starting material (monitored by TLC), the solid mass was washed with diethyl ether to obtain pure bromo salt. Anhydrous DCM (4 mL) was added by syringe under the stream of argon atmosphere. To this solution, diethyl hydrogen phosphite (0.3 mmol, 1.2 equiv.) was added by micro syringe, and solid K_2CO_3 (0.75 mmol, 2.5 equiv.) was quickly added in one portion via opening the cap. The vial was re-capped with septa, packed with insulating tape, and covered with aluminium foil. The reaction mixture was degassed with argon for 15 minutes, and then the reaction mixture was stirred for 24 h at 25 °C. After this time, LiHMDS (2.5 equiv., 1M in Hexane) was added dropwise over the period of 5 minutes at 0 °C and stirred it for 12 h at 0 °C. After completion, the reaction mixture was quenched with aq. NH_4Cl, and the crude was extracted with DCM (three times), the organic layer was combined and dried over sodium sulphate. The solvent was removed under reduced pressure to obtain the crude product, which was further purified by flash column chromatography on silica gel using ethyl acetate-pet ether as an eluent.

8b. Reaction Procedure (GP-G) for one-pot *ortho*-Acylation of *meta*-Alkylated Isoquinoline

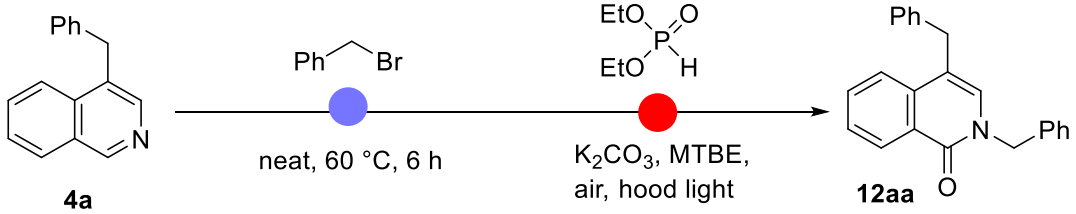
Method 3



In a flame dried 25 mL peared shaped flask with a magnetic bar preformed *meta*-alkylated isoquinoline (0.3 mmol, 1 equiv.) following the general procedure for *meta*-alkylation (**GP-D**) was taken in anhydrous DCM (4 mL, 0.1 M). To this solution, substituted acyl halide (0.3 mmol, 1 equiv.) was added at 0 °C. The flask was capped with septa, packed with insulating tape. The reaction mixture was allowed to stir for 30 minutes. After this time, diethyl hydrogen phosphite (0.3 mmol, 1 equiv.) and Et_3N (0.45 mmol, 1.5 equiv.) was added at 0 °C. Reaction mixture was allowed to stir for 6 h. Upon complete consumption of starting material (monitored by TLC). The reaction mixture was degassed with argon atmosphere for the period of 10 minutes. After this time, LiHMDS (3.0 equiv., 1M in Hexane) was added dropwise over the period of 5 minutes at 0 °C and allowed to stir for 6 h at 0 °C. After completion, the reaction mixture was quenched with NH_4Cl, and the crude was extracted with ethyl acetate (three times), the organic layer was combined and dried over sodium sulphate. The solvent was removed under reduced pressure to obtain the crude product, which was further purified by flash column chromatography on silica gel using ethyl acetate-pet ether as an eluent.

8c. Reaction Procedure (GP-H) for one-pot Aerobic Oxidation

Method 4



In a flame dried 25 mL schlenk tube with a magnetic bar, preformed *meta*-alkylated isoquinoline (0.3 mmol, 1 equiv.) following the general procedure for *meta*-alkylation (**GP-D**) was taken. Substituted alkyl halide (0.45 mmol, 1.5 equiv.) was added. Reaction mixture was allowed to stir at 60 °C till the consumption of starting material. Upon complete consumption of the starting material (monitored by TLC), the solid mass was washed with diethyl ether to obtain pure bromo salt. Anhydrous MTBE (3

mL) was added by syringe under the stream of argon atmosphere. To this solution, diethyl hydrogen phosphite (5.5 µl, 0.06 mmol, 20 mol %) was added by micro syringe, and solid K_2CO_3 (0.9 mmol, 3 equiv.) was quickly added in one portion via opening the cap. The vial was re-capped, and heated at 40 °C for 16 h in presence of air. The reaction was monitored by TLC for the consumption of starting material. After completion, the reaction mixture was quenched with NH_4Cl, and the crude was extracted with ethyl acetate (three times), the organic layer was combined and dried over sodium sulphate. The solvent was removed under reduced pressure to obtain the crude product, which was further purified by flash column chromatography on silica gel using ethyl acetate-pet ether as an eluent.

9. Absorption and Emission Spectroscopy

9a. UV/Vis Absorption Spectroscopy

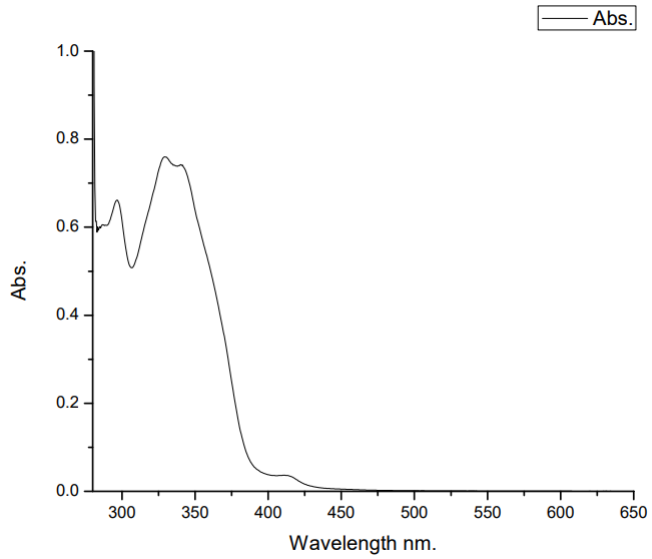


Figure-8. UV/vis absorption spectra of the starting material intermediate **2a**

The UV/vis spectrum of starting material intermediate **2a** was recorded on Shimadzu 1800 spectrophotometer. To record the spectra intermediate **2a** was dissolved in toluene to make the solution with concentration of 10^{-5} M. The intermediate **2a** shows two maxima around 330-340 nm and at 415 nm. The maximum absorption is situated between 320 and 370 nm.

9b. Fluorescence Spectroscopy

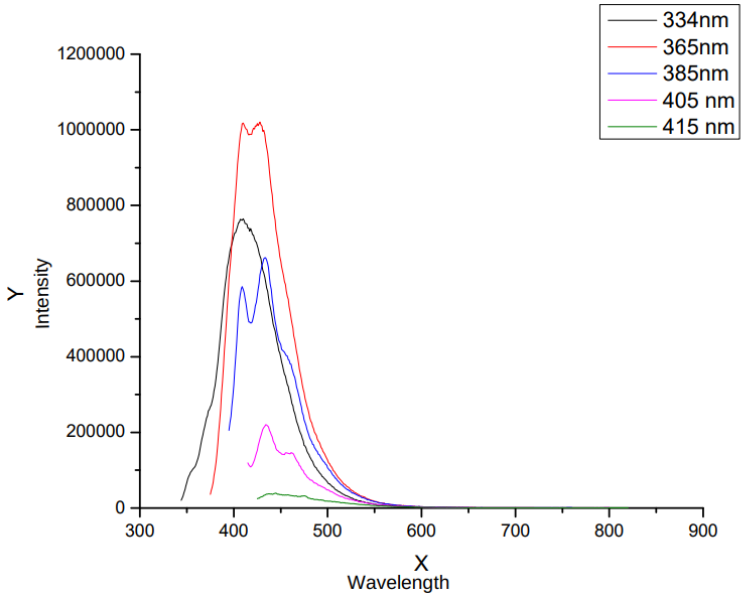


Figure-9. Fluorescence spectra of the starting material intermediate **2a**

The Fluorescence spectrum of starting material intermediate **2a** was recorded using PTI Quanta Master™ Steady State Spectrofluorometer. To record the emission spectra intermediate **2a** solution was made in toluene with concentration 10^{-5} M. From emission spectra, maximum emission was observed at 365 nm. From lower wavelength to higher wavelength, we observed a pattern of decrease in emission. Emission spectra shows the 365 nm is the best wavelength for the reaction condition.

10. Computational Method:

All density functional calculations were conducted using the Gaussian16 package.[7] All molecular geometries were optimized in vacuum with M062X density functional[8] paired with 6–31++G (d,p) basis set at room temperature (298 K). Each intermediate and transition state is characterized by all real frequencies and a single imaginary frequency, respectively. For obtaining solvent phase corrected free energy, we included the standard entropic correction to the ideal gas phase model.[9,10] Single-point solvent phase calculations were carried using the CPCM[11] solvent model for *p*-xylene using M062X functional and 6-31++G (d,p) basis set. The first excited singlet state S_1 was found to be the bright state (oscillator strength = 0.1278). TD-DFT calculations were used to optimize S_1 excited state intermediates and transition states using 20 singlet excited states (keyword: nstates = 20). The strongly contracted n-electron valence state perturbation theory (SC-NEVPT)[12] and spin-orbit coupling matrix elements calculations were carried out using ORCA 5.0 package.[13] The SC-NEVPT2 calculations were performed on converged CASSCF solutions with 8 electrons in 8 active orbitals (CAS [8,8]) over DFT optimized geometries. cc-pVTZ basis set was used to calculate SC-NEVPT2 energies and def2-TZVP

basis set with def2/JK and RI-JK approximation was used to calculate spin-orbit coupling matrix. The molecular orbital pictures were generated using iboview.[14]

10a. Relaxed Potential Energy Scans along N-C Bond using DFT:

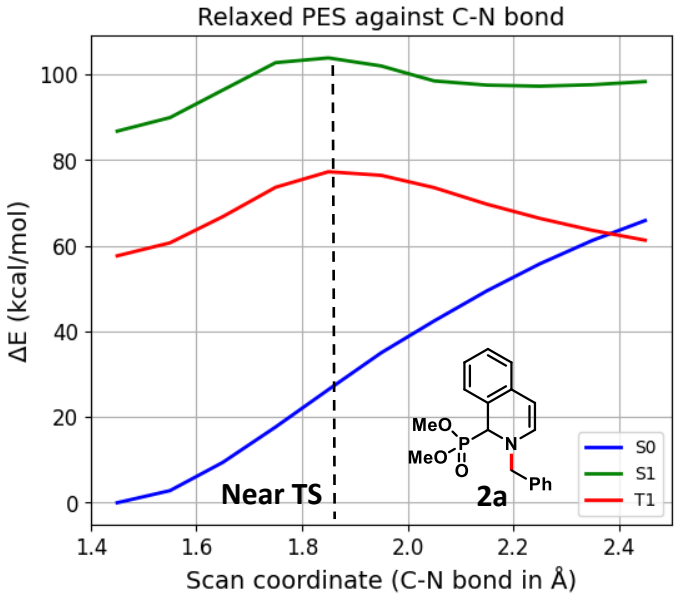


Figure-10. Relaxed potential energy scans along C-N bond (marked in red) of the initial substrate **2a** at three different states S_0 (blue), S_1 (green), T_1 (red). The black dashed line represents the near TS geometry.

In order to gain more insight on the C-N bond dissociation process under light, we performed relaxed potential energy scans considering the singlet ground state (S_0) and two most important excited states namely, first excited singlet (S_1) and triplet states (T_1) using DFT/TDDFT (M062X/6-31++G(d,p)). The C-N bond (indicated in red) distance was elongated starting from equilibrium distance 1.45 Å to 2.45 Å, with regular interval of +0.05 Å at the S_0 surface. The scan points obtained on the S_0 surface were then used for single point calculations to generate the S_1 and T_1 surfaces. Note that the dotted black line is the C-N bond distance corresponding to the transition state at T_1 (1.87 Å). Interestingly, there is less difference between the relative S_1 and T_1 energies till the geometry reaches TS. The barrier for C-N bond dissociation appears similar in S_1 and T_1 surfaces. After the TS geometry is reached the S_1 and T_1 surfaces diverge with the elongation of C-N bond. The S_1 state does not gain any stability while the T_1 state gains stability with increasing C-N bond length. From this result we infer that TDDFT cannot provide conclusive result regarding the active photochemical pathway. Since, such bond dissociation scenarios require multireference treatment; thus we perform state average NEVPT2-CASSCF to provide reliable results.

10b. NEVPT2-CASSCF (8,8) Relative Energies at DFT Optimized Geometries

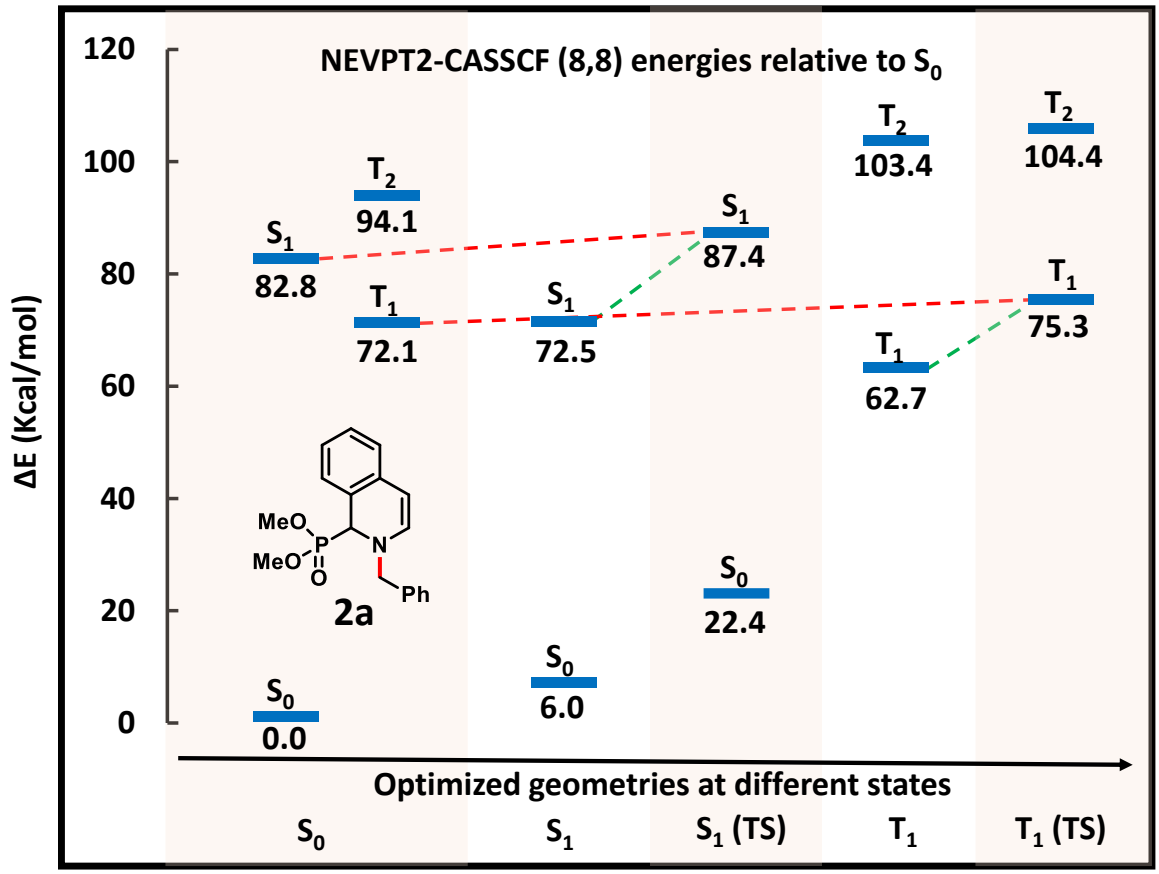


Figure-11. NEVPT2-CASSCF (8,8) energies using cc-pVTZ basis set over DFT optimized geometries of **2a**

In order to confirm the validity of the TDDFT scans and provide reliable insights for such intricate photochemical path, we perform NEVPT2-CASSCF single point energy calculations over DFT optimized geometries. The calculations include two states for each multiplicity i.e. S_0, S_1 for singlet case and T_1, T_2 for triplet case at equal weightage. The computations were conducted over five DFT optimized geometries namely S_0 equilibrium, S_1 equilibrium, S_1 transition state, T_1 equilibrium and T_1 transition states. The red dashed lines connect the difference between S_1 and T_1 states at the Franck-Condon region to their respective transition states at S_1 and T_1. The relative energies are 4.6 and 3.2 kcal/mol for S_1 and T_1 respectively, which are very low. The green dashed lines connect the S_1 and T_1 equilibrium to their respective transition states, which are found to be 14.9 and 12.6 kcal/mol respectively. According to Figure 11, the most probable case that may lead to the photoproduct via C-N bond dissociation is if the molecule at S_1 state tumbles to cross the 4.6 kcal/mol barrier to find the S_1 transition state before relaxing to the S_1 equilibrium. If the molecule relaxes to S_1 equilibrium then it has to overcome a higher barrier of 14.9 kcal/mol, which is possible but will lead to a slower rate. The energy barrier at triplet state T_1 is comparable (12.6 kcal/mol) but the molecule has to undergo singlet to triplet intersystem crossing before the C-N bond breaking.

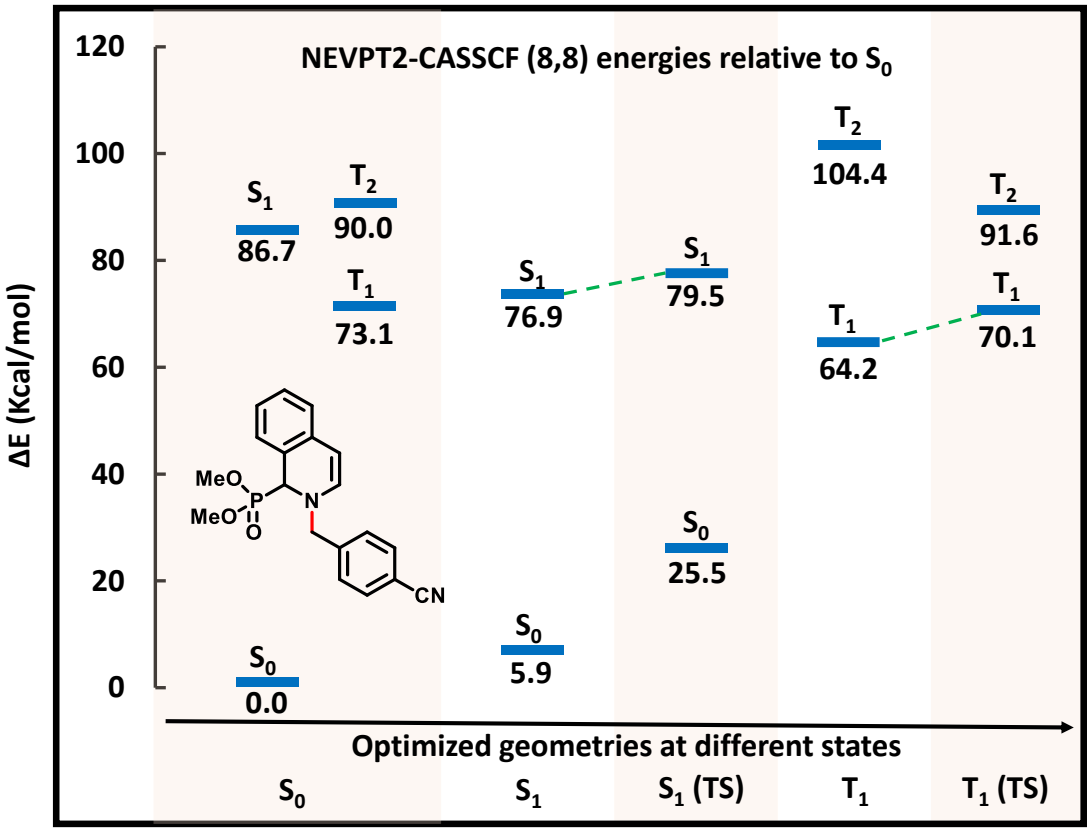


Figure-12. NEVPT2-CASSCF (8,8) energies using cc-pVTZ basis set over DFT optimized geometries of substrate **2a** with *p*-CN substitution at migrating group

For comparison, we also computed the NEVPT2 total energies at important DFT optimized geometries for a model having *p*-CN substitution at phenyl ring in the migrating group (see Figure 12). The effect of incorporating electron withdrawing group on the migrating group substantially reduces the transition state barrier for the C-N photo-dissociation on the S_1 surface. The TS at S_1 for this case is mere 2.6 kcal/mol, which is much lower than for the case of unsubstituted **2a**. This fact is in line with the experimental observation which shows higher yield for the reactions where electron withdrawing substituents were present on the migrating group (see main manuscript). The photon driven homolytic bond dissociation leads to radical character on the corresponding fragments. It is expected that both electron donating and electron withdrawing groups will stabilize the fragments developing radical character due to extended delocalization. The spin-orbit coupling matrix elements (SOCME) were still negligible after CN substitution, which suggests that there is no change in the nature of mechanism and it still proceeds through the S_1 channel.

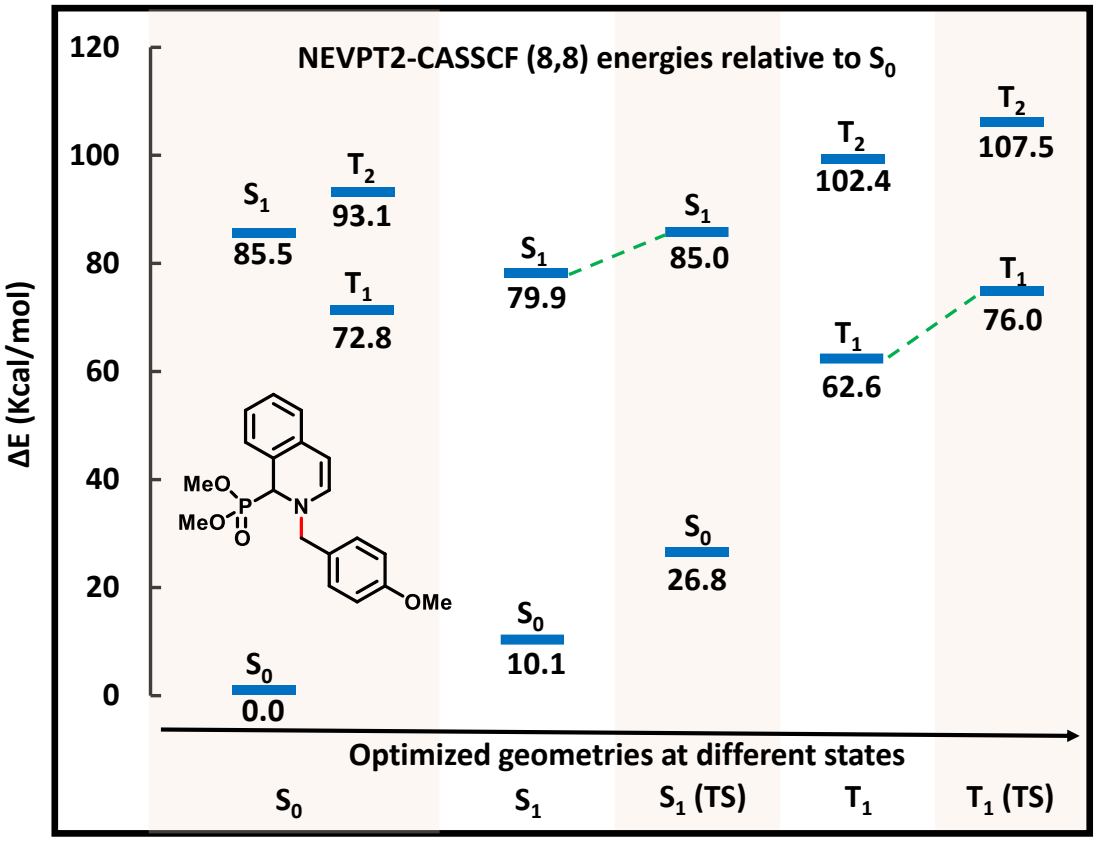


Figure-13. NEVPT2-CASSCF (8,8) energies using cc-pVTZ basis set over DFT optimized geometries of substrate **2a** with *p*-OMe substitution at migrating group.

For the case of *p*-OMe substitution at phenyl ring in migrating group the calculated NEVPT2 energies depict similar trend for the reaction. The TS for the C-N photo-dissociation is found to be 5.1 kcal/mol above the S_1 minimum, which is lower than the one predicted for **2a**. Unfortunately, the major photo-products could not be experimentally characterized. There may be a case that the photo-excited state at S_1 is still able to expel the migrating group but later reaction goes through some unknown channel due to which we are not able to get [1,3] migrated photoproduct. Currently, we have not been able to identify the exact reason behind this anomalous behaviour for the *p*-OMe substituted case.

10c. Spin Orbit Coupling Matrix of the System at S_0 Optimized Geometry

In order to clarify our doubts whether the reaction occurs through S_1 or T_1, we calculated spin orbit coupling (SOC) matrix of the system at S_0, S_1 and T_1 optimized DFT geometry using def2-TZVP basis set with def2/JK and RI-JK approximation. The SOC calculation was performed at the CASSCF[8,8] level involving 3 singlet (S_0, S_1 and S_2) and 2 triplet (T_1 and T_2) states using equal weightage for each state. The output below shows the non-zero SOC matrix elements S_0 state (The output for S_1 and T_1 optimized geometries are similar). Since all the values are very low (less than 1 cm^{-1}) there is very low possibility of intersystem crossing in this system. Hence, we suggest that the reaction is likely to occur on the S_1 surface.

NONZERO SOC MATRIX ELEMENTS (cm^{-1})

Bra				Ket					
<Block	Root	S	Ms	| HSOC | Block	Root	S	Ms>	= Real-part	Imaginary part
0	1	1.0	1.0	0	0	1.0	1.0	0.000	-0.217
0	0	1.0	0.0	0	1	1.0	1.0	-0.102	-0.041
0	1	1.0	0.0	0	0	1.0	1.0	0.102	0.041
0	0	1.0	-1.0	0	1	1.0	0.0	-0.102	-0.041
0	1	1.0	-1.0	0	0	1.0	0.0	0.102	0.041
0	1	1.0	-1.0	0	0	1.0	-1.0	-0.000	0.217
1	0	0.0	0.0	0	0	1.0	1.0	-0.672	0.264
1	0	0.0	0.0	0	1	1.0	1.0	-0.527	0.090
1	0	0.0	0.0	0	0	1.0	0.0	-0.000	-2.617
1	0	0.0	0.0	0	1	1.0	0.0	-0.000	-2.131
1	0	0.0	0.0	0	0	1.0	-1.0	-0.672	-0.264
1	0	0.0	0.0	0	1	1.0	-1.0	-0.527	-0.090
1	1	0.0	0.0	0	0	1.0	1.0	-0.215	-0.029
1	1	0.0	0.0	0	1	1.0	1.0	0.188	-0.015
1	1	0.0	0.0	0	0	1.0	0.0	-0.000	-0.716
1	1	0.0	0.0	0	1	1.0	0.0	-0.000	0.652
1	1	0.0	0.0	0	0	1.0	-1.0	-0.215	0.029
1	1	0.0	0.0	0	1	1.0	-1.0	0.188	0.015
1	2	0.0	0.0	0	0	1.0	1.0	-0.151	0.017
1	2	0.0	0.0	0	1	1.0	1.0	-0.118	-0.066
1	2	0.0	0.0	0	0	1.0	0.0	-0.000	-0.544
1	2	0.0	0.0	0	1	1.0	0.0	-0.000	-0.326
1	2	0.0	0.0	0	0	1.0	-1.0	-0.151	-0.017
1	2	0.0	0.0	0	1	1.0	-1.0	-0.118	0.066

Figure-14. Non-zero Spin orbit coupling matrix elements (cm^{-1}) calculated at CASSCF(8,8) level over ground state DFT optimized geometry.

10d. CASSCF [8,8] Molecular Orbital Pictures

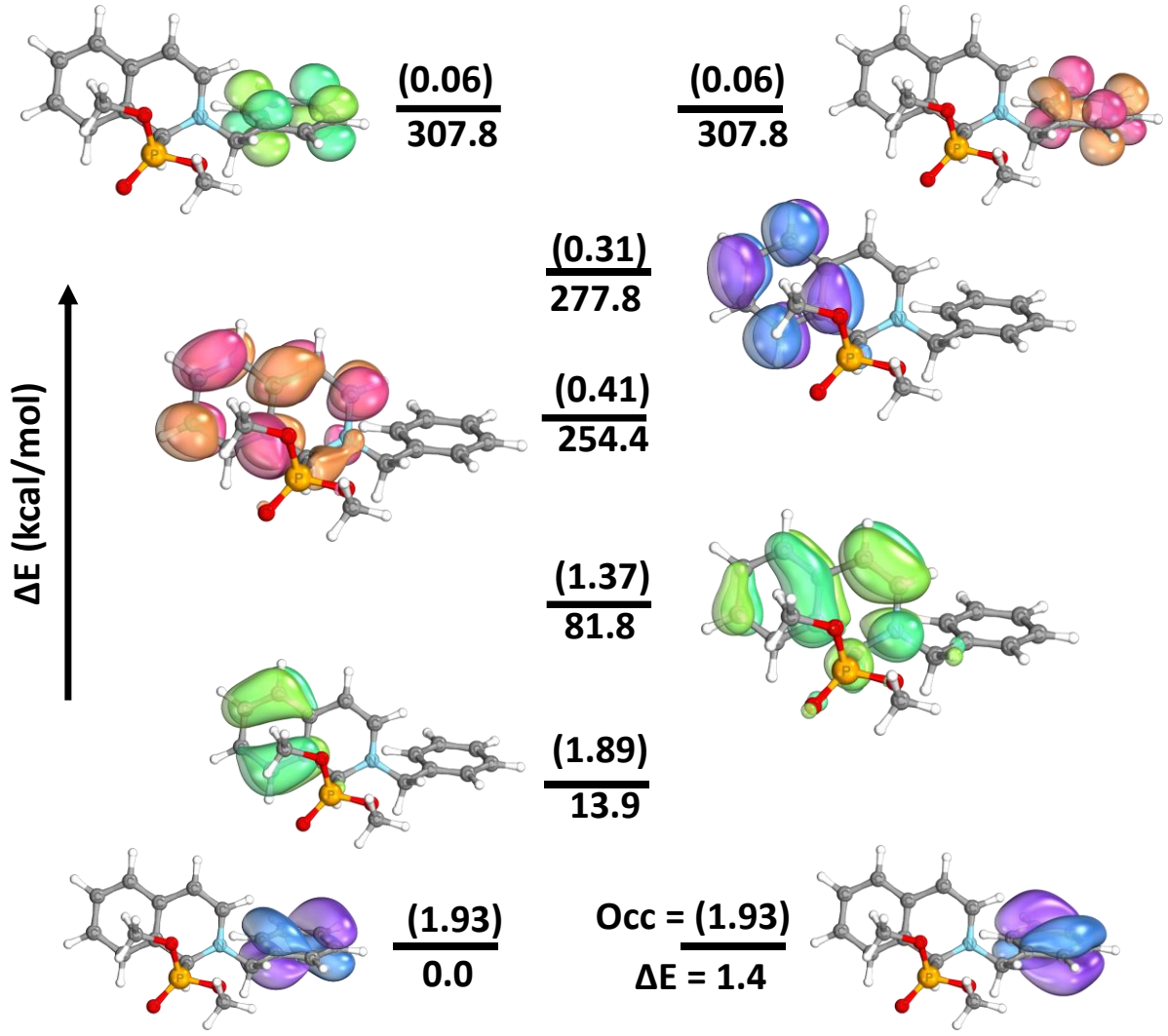


Figure-15. The molecular orbital diagram obtained from state average CASSCF [8,8] method including 3 roots (S_0, S_1 and S_2) over ground state DFT optimized geometry of model **2a**. The relative energies are reported with respect to lowest orbital in the active space. The occupation numbers of the orbitals are shown in parenthesis.

10e. Optimised Cartesian Coordinates:

2a

0, 1

C -3.13218600 -2.62815700 1.24294600

C -2.27093000 -1.55708700 1.48239500

C -1.34915800 -1.16636900 0.51445500

C -1.27297500 -1.84481900 -0.71751800

C -2.13638200 -2.92655500 -0.93842400

C -3.06209000 -3.31017100 0.02796000

H -0.24838200 0.19024100 1.76787700

H -3.85586200 -2.92080800 1.99628800

H -2.33638200 -0.99866000 2.41273900

C -0.51131700 0.08293300 0.70847000

C -0.28311500 -1.41910900 -1.69650700

H -2.07685700 -3.46333000 -1.88141900

H -3.72923800 -4.14443200 -0.16587600

C 0.66767300 -0.53655600 -1.32750200

H -0.26593900 -1.86163900 -2.68453500

H 1.49177100 -0.26767700 -1.98227200

N 0.70686500 0.03577000 -0.07394800

C 1.80593800 0.92857400 0.25525100

H 1.80196300 1.81502000 -0.39387600

H 1.63195800 1.29629500 1.27262400

C 3.15733400 0.24378900 0.18902800

C 4.29065600 0.98453900 -0.15262100

C 3.29921500 -1.11195000 0.49591500

C 5.55036300 0.38797700 -0.17197200

H 4.18556300 2.03654200 -0.40770100

C 4.55682300 -1.71138500 0.47247500

H 2.41596600 -1.69629700 0.73935800

C 5.68621900 -0.96326300 0.14141100

H 6.42276900 0.97589900 -0.43984200

H 4.65422600 -2.76625000 0.70977400

H 6.66480200 -1.43231000 0.12061900

P -1.61437400 1.53406100 0.36576500

O -2.54692300 1.84719200 1.47616300

O -0.55586200 2.67638700 -0.02777200

O -2.34631800 1.27711200 -1.04345900

C -3.66307500 0.70531500 -1.07124500

H -4.23119600 1.02290300 -0.19383600

H -4.13957200 1.06809100 -1.98225300

H -3.58832300 -0.38550800 -1.09787300

C -1.06641300 3.99274500 -0.28103900

H -0.20050400 4.63952900 -0.41725800

H -1.67345200 3.98735900 -1.19014800

H -1.66239900 4.33549000 0.56845100

2^{*}_{s}

0, 1

C -2.73597900 -2.63308600 1.45751100

C -1.86454800 -1.56283800 1.55606500

C -1.10957000 -1.14896100 0.45146300

C -1.23580100 -1.84534100 -0.81824000

C -2.16406000 -2.92914600 -0.88924600

C -2.89375500 -3.31198000 0.20741700

H 0.21860400 0.22906400 1.45631800

H -3.30042400 -2.95479300 2.32549900

H -1.77492400 -1.01761600 2.49306600

C -0.28965500 0.09172600 0.49225000

C -0.45407900 -1.41802800 -1.90289800

H -2.28155100 -3.44824200 -1.83777500

H -3.59307600 -4.13825800 0.13053900

C 0.47994200 -0.37368400 -1.77344700

H -0.54480100 -1.90417600 -2.86877100

H 1.11695700 -0.03947800 -2.58314000

N 0.65104700 0.25392700 -0.57530700

C 1.80839400 1.10310600 -0.37895100

H 1.94663400 1.71911100 -1.27855100

H 1.58927200 1.79155200 0.44152200

C 3.07135400 0.30932300 -0.08395200

C 4.29940000 0.97618300 -0.09795800

C 3.03301800 -1.04827800 0.23781800

C 5.47524800 0.29722700 0.21112900

H 4.33449600 2.03306400 -0.35307700

C 4.21181300 -1.72806600 0.54570100

H 2.08542600 -1.58088200 0.24096200

C 5.43377600 -1.05905300 0.53402600

H 6.42340700 0.82556500 0.19664800

H 4.17134100 -2.78430600 0.79230200

H 6.34922400 -1.59066500 0.77295700

P -1.54032000 1.48249300 0.43159700

O -2.27840000 1.67689500 1.69976900

O -0.63554800 2.72677700 -0.03590100

O -2.43599300 1.23833400 -0.86980100

C -3.68239200 0.52556600 -0.74655400

H -4.16020100 0.77025200 0.20466500

H -4.30086900 0.85503900 -1.58128000

H -3.49976400 -0.54966900 -0.81173000

C -1.25703600 4.02217100 -0.05766000

H -0.46829700 4.73623600 -0.29171500

H -2.02691900 4.05063900 -0.83310600

H -1.69394100 4.24557800 0.91849400

2^{*}_{T}

0,3

C -2.34764800 -2.68111000 1.62723600

C -1.49144400 -1.57481600 1.56922100

C -0.95769800 -1.15281400 0.36412200

C -1.28517800 -1.84611000 -0.86987400

C -2.19332700 -2.96727600 -0.77776300

C -2.70029400 -3.36409500 0.42809700

H 0.51530600 0.21473400 1.12932800

H -2.74510100 -3.01030800 2.58014800

H -1.26040800 -1.02112500 2.47586900

C -0.16785800 0.12587700 0.27467300

C -0.73664100 -1.41055800 -2.05510800

H -2.46190500 -3.48967700 -1.69233200

H -3.37811800 -4.21086300 0.47622400

C 0.21888800 -0.33147200 -2.10950300

H -0.99291800 -1.90595200 -2.98679700

H 0.71610800 -0.02072300 -3.01674500

N 0.58702600 0.29147500 -0.94604400

C 1.80136000 1.07826200 -0.88627300

H 2.03647100 1.40544500 -1.90524700

H 1.61201100 1.98218400 -0.29865700

C 2.97309000 0.30928600 -0.29682200

C 4.09758700 1.01573400 0.13915800

C 2.95743800 -1.08227200 -0.18536800

C 5.19677100 0.34302600 0.66633100

H 4.11022700 2.10109300 0.06717700

C 4.05599700 -1.75608300 0.34912500

H 2.08493600 -1.64046500 -0.51456000

C 5.17810200 -1.04775600 0.77288600

H 6.06371700 0.90384200 1.00147800

H 4.03092700 -2.83786900 0.43511400

H 6.03104700 -1.57414400 1.18912900

P -1.40730000 1.48720700 0.48608900

O -1.92967200 1.62850100 1.86491700

O -0.61957700 2.75834900 -0.09807700

O -2.52748600 1.26158000 -0.63951500

C -3.72907500 0.54130800 -0.31525100

H -4.00260300 0.71551000 0.72798700

H -4.50424700 0.92251900 -0.98014600

H -3.57515400 -0.52656200 -0.49149700

C -1.27119700 4.03394700 -0.01063500

H -0.54641000 4.77340500 -0.34886800

H -2.14826800 4.04778200 -0.66296100

H -1.56465600 4.23682400 1.02219600

$TS^*_S{}^{CN}$

0, 1

C -2.36944400 2.33765800 -1.88947200

C -1.42498500 1.35502300 -1.61866400

C -1.02753300 1.10322000 -0.30411700

C -1.62234600 1.83143100 0.76882000

C -2.58000300 2.83224200 0.46635000

C -2.95093200 3.07647500 -0.83906500

H 0.81415900 -0.00701600 -0.64008500

H -2.65246000 2.54200000 -2.91647100

H -0.99129200 0.77393100 -2.42689300

C -0.07484900 -0.01866600 0.00868400

C -1.21913100 1.54134400 2.09317300

H -3.02065400 3.39728100 1.28299900

H -3.68831400 3.84107100 -1.06002600

C -0.22035600 0.57900600 2.32280600

H -1.61365000 2.10896600 2.92903800

H 0.15860700 0.40511900 3.33033500

N 0.37701000 -0.09277000 1.36515100

C 1.98253400 -0.71511400 1.58462700

H 2.09370100 -0.45017900 2.63866000

H 1.84400000 -1.78329000 1.43501700

C 2.86954900 -0.06299800 0.65582800

C 3.33105000 -0.71984500 -0.52323200

C 3.22096100 1.31056600 0.82754100

C 4.09912300 -0.05339900 -1.45547500

H 3.07535300 -1.76682200 -0.67591600

C 3.99058700 1.96590400 -0.12318300

H 2.88964200 1.83895200 1.71873600

C 4.43823200 1.30676500 -1.27414800

H 4.44777000 -0.58337200 -2.33722600

H 4.24967300 3.00992300 0.03208100

H 5.04019300 1.82735400 -2.01008400

P -0.96501200 -1.59833600 -0.41437800

O -1.28993100 -1.74943900 -1.84965100

O -0.00722400 -2.70395700 0.22486900

O -2.23749000 -1.63424600 0.56498200

C -3.50884800 -1.15688600 0.09257500

H -3.63643300 -1.40598300 -0.96312800

H -4.26661200 -1.65527900 0.69660700

H -3.57213900 -0.07399100 0.23301600

C -0.27749900 -4.08336500 -0.07710600

H 0.55239400 -4.65310400 0.33794100

H -1.21391000 -4.38972000 0.39605400

H -0.33342900 -4.22645200 -1.15830600

$TS^*_T{}^{CN}$

0, 3

C 0.81695300 -3.23267000 -1.55136000

C 0.74823900 -1.84396100 -1.46614100

C 0.35807700 -1.22652500 -0.27949100

C 0.04618200 -2.01740600 0.86694000

C 0.11976700 -3.43523000 0.75279100

C 0.50214100 -4.02652200 -0.43050700

H -0.25459700 0.70129500 -1.00581200

H 1.10640100 -3.70146600 -2.48562700

H 1.00955100 -1.23122900 -2.32408300

C 0.31955600 0.27933400 -0.16954600

C -0.31648900 -1.37031200 2.05500300

H -0.12703900 -4.04046700 1.62073400

H 0.55693600 -5.10812500 -0.50275600

C -0.39376800 0.07045400 2.10053000

H -0.60095800 -1.94276400 2.93133900

H -0.69137200 0.56840800 3.02100900

N -0.19014900 0.84349800 1.06055200

C -1.44840400 2.18434200 0.68066200

H -1.52241600 2.57116000 1.69398600

H -0.86486400 2.81183000 0.01133700

C -2.59331600 1.49358900 0.14540700

C -2.79274200 1.35197800 -1.24840900

C -3.48179900 0.81326100 1.01119700

C -3.82896500 0.57681900 -1.74661300

H -2.13194000 1.87870900 -1.93428800

C -4.51442200 0.03372800 0.50406400

H -3.35517500 0.91601300 2.08619500

C -4.69616900 -0.09347600 -0.87462000

H -3.96871800 0.49293500 -2.82018000

H -5.18699000 -0.47657800 1.18734800

H -5.50503400 -0.70054900 -1.26719500

P 2.03176200 0.92942200 -0.40665400

O 2.62438700 0.62858000 -1.73083300

O 1.84820600 2.47622300 -0.04951800

O 2.88504900 0.38370700 0.83949400

C 3.59793300 -0.85736000 0.71397900

H 4.01360100 -0.95433900 -0.29169000

H 4.39700400 -0.82887600 1.45448000

H 2.92428300 -1.69321400 0.92380500

C 2.97076900 3.34546100 -0.26030400

H 2.61294800 4.35652100 -0.07152000

H 3.77053200 3.09758300 0.44251000

H 3.33006400 3.25623000 -1.28826800

R1

0, 2

C -2.77505500 -1.69004900 -0.72699700

C -1.55717300 -1.16925000 -1.15993500

C -1.13325100 0.08296100 -0.71847000

C -1.94290100 0.82907900 0.16806600

C -3.17361200 0.28887600 0.59593700

C -3.58115300 -0.95998900 0.15571300

H 0.45233100 0.43265700 -2.14271300

H -3.09490700 -2.66811200 -1.07104000

H -0.91417900 -1.74872100 -1.81621800

C 0.22448700 0.63443300 -1.08719500

C -1.48592500 2.12040000 0.57024200

H -3.79568600 0.86635100 1.27427300

H -4.52716700 -1.37180400 0.49231000

C -0.30627000 2.65378600 -0.00453600

H -2.07548400 2.71959000 1.25560300

H -0.04059400 3.68697700 0.21684300

N 0.49521000 2.02562500 -0.81768300

P 1.46123900 -0.40972300 -0.18918200

O 1.47678200 -1.82679500 -0.62488700

O 2.81626800 0.40794000 -0.36417600

O 1.13068500 -0.21697000 1.37505700

C 0.33792900 -1.19873100 2.05818800

H 0.56554300 -2.19827600 1.68128300

H 0.59539200 -1.12201000 3.11465100

H -0.72532800 -0.98084600 1.91876800

C 4.02529400 -0.19015200 0.12186700

H 4.83529200 0.46748600 -0.18979600

H 3.99813900 -0.25360300 1.21319300

H 4.15750100 -1.18480400 -0.31086600

R2

0, 2

C 2.40130700 -0.00005700 0.00017900

H 2.95833900 -0.92910100 0.00012300

H 2.95788800 0.92928200 0.00035700

C 0.98848400 -0.00006500 -0.00018200

C 0.25291200 1.21430800 -0.00009500

C 0.25273500 -1.21438000 -0.00009900

C -1.13253500 1.20937300 0.00005300

H 0.79550100 2.15569200 -0.00033000

C -1.13266100 -1.20932600 0.00005700

H 0.79528000 -2.15579300 -0.00028900

C -1.83642700 0.00008800 0.00005900

H -1.67413000 2.15028900 0.00002600

H -1.67437700 -2.15017200 0.00008700

H -2.92139800 0.00014900 0.00018700

3

0,1

C 0.29645000 2.93708400 -1.68428100

C -0.23889900 1.68423100 -1.39884100

C 0.09024300 1.02692900 -0.20498400

C 0.98955500 1.63067600 0.68003100

C 1.50486000 2.89778400 0.39447000

C 1.15996200 3.55683000 -0.78030900

H 0.00212400 -1.11819700 -0.46421500

H 0.03317700 3.43186500 -2.61386500

H -0.92027600 1.21248200 -2.09968700

C -0.48080400 -0.34030800 0.15008700

C 1.48118700 0.86954100 1.88202100

H 2.19520800 3.35946600 1.09742800

H 1.56718100 4.53995600 -0.99456500

C 0.49142800 -0.18728400 2.29067200

H 0.54537500 -0.54182800 3.32448100

N -0.35867300 -0.75553200 1.54279200

P -2.26901100 -0.45872200 -0.25698200

O -2.62654300 -0.18411200 -1.67131700

O -2.64255300 -1.91281600 0.27744100

O -3.02445200 0.50078500 0.79350200

C -3.27765000 1.86591500 0.44104800

H -3.55075700 1.94239300 -0.61458200

H -4.10328000 2.20057400 1.06931400

H -2.39011100 2.47375900 0.64061300

C -3.96243900 -2.39814900 0.00529600

H -3.98114600 -3.43378400 0.34185300

H -4.69866700 -1.81427500 0.56469700

H -4.17473100 -2.34408300 -1.06539800

H 1.63009200 1.55711300 2.72375800

C 2.86323600 0.19583800 1.59691500

H 3.58621700 0.99212900 1.38969500

H 3.19235600 -0.31938700 2.50692000

C 2.80581700 -0.77325500 0.44252000

C 2.94390100 -0.32180900 -0.87522200

C 2.52591900 -2.12598400 0.66154100

C 2.78455600 -1.19624400 -1.94788800

H 3.15402600 0.72923500 -1.06104700

C 2.36803800 -3.00530100 -0.40809600

H 2.41160300 -2.49029000 1.67956400

C 2.48996300 -2.54002200 -1.71696100

H 2.88317400 -0.82661500 -2.96371300

H 2.14218000 -4.04997800 -0.21908300

H 2.35858300 -3.22067200 -2.55211800

$TS_D^{C\text{-}C}$

0, 2

C 0.72487900 -4.15715700 -1.22982500

C 1.08398300 -3.09878700 -0.39743400

C 0.56650400 -1.82158700 -0.61691800

C -0.30131600 -1.58027800 -1.69563600

C -0.65183600 -2.65385200 -2.52435700

C -0.15204600 -3.93178700 -2.29154100

H 1.93213800 -0.76801700 0.66150400

H 1.12373600 -5.14939400 -1.04732500

H 1.74554900 -3.26679700 0.44876100

C 0.87172200 -0.71404000 0.37430000

C -0.78622000 -0.21602700 -1.94518000

H -1.32262400 -2.47337400 -3.36055900

H -0.43957400 -4.75066200 -2.94364200

C -0.14948200 0.80918600 -1.26960900

H -1.16346800 0.01439200 -2.93542600

H -0.28332700 1.84726500 -1.55469000

N 0.59096100 0.61537000 -0.13537000

C 1.39097600 1.70101800 0.39816900

H 0.91164400 2.63857300 0.09560100

H 1.35241100 1.66649200 1.49203400

C 2.83816500 1.67630000 -0.06845600

C 3.80879500 2.34942900 0.67831500

C 3.22079400 1.00825900 -1.23374600

C 5.13730200 2.37103200 0.26112700

H 3.52084800 2.85798100 1.59571400

C 4.55235800 1.02280000 -1.64883900

H 2.47708300 0.47021500 -1.81675500

C 5.51284500 1.70590100 -0.90588300

H 5.88064500 2.89794000 0.85123300

H 4.83794000 0.49604000 -2.55403400

H 6.54869600 1.71490200 -1.22957700

P -0.03352900 -1.12625100 1.93849700

O 0.65034200 -2.16000800 2.75094400

O -0.25347700 0.31105200 2.61457200

O -1.54766500 -1.50979600 1.54715300

C -1.91558200 -2.88318100 1.33581800

H -1.30584600 -3.53652800 1.96404100

H -2.96800500 -2.96716700 1.60841200

H -1.77853000 -3.14058800 0.28069900

C -0.97030600 0.36602600 3.85719700

H -0.88923400 1.39207700 4.21376300

H -2.01995900 0.11040200 3.68974600

H -0.52392700 -0.31985600 4.58169300

C -2.86812400 -0.32550800 -1.21836200

H -2.66483700 -1.00777000 -0.40186800

H -3.31300500 -0.76179000 -2.10958900

C -3.17580500 1.04193700 -0.89234600

C -3.75433400 1.91932900 -1.83274800

C -2.76260100 1.58404500 0.34470100

C -3.93024600 3.26769500 -1.54286800

H -4.07071600 1.52633500 -2.79628900

C -2.94028600 2.93283400 0.62999700

H -2.29212700 0.92635500 1.07159300

C -3.52593500 3.78551700 -0.30940600

H -4.38555700 3.92147200 -2.28108700

H -2.61769600 3.32495400 1.59090000

H -3.66487300 4.83811200 -0.08488600

2-R2

0, 2

C 3.79565200 -0.59437800 2.76253200

C 3.12116900 -1.26112500 1.74610700

C 1.91176600 -0.76151600 1.25232700

C 1.37240600 0.42526300 1.76005800

C 2.05229600 1.07213500 2.79899200

C 3.25276300 0.57551000 3.29632500

H 1.36687300 -2.55738600 0.22079900

H 4.73348700 -0.98747400 3.14106900

H 3.53543600 -2.16837200 1.31376100

C 1.21706000 -1.47678100 0.11552000

C 0.09787300 1.02659500 1.20031700

H 1.63101700 1.98082500 3.22228000

H 3.76287100 1.09721900 4.09994900

C -0.57877900 0.13210600 0.20396400

H -0.58630200 1.19207600 2.05206400

H -1.60975400 0.33884200 -0.06032500

N -0.20031000 -1.19752100 0.10683800

C -1.06821700 -2.06680700 -0.67252800

H -1.23146900 -1.65233500 -1.67770600

H -0.54950100 -3.02320400 -0.80566000

C -2.40155100 -2.30523300 0.00889600

C -3.53934000 -2.54220100 -0.76430000

C -2.51058900 -2.33017800 1.40159000

C -4.76564500 -2.81571500 -0.15988600

H -3.46541100 -2.50782600 -1.84874100

C -3.73578800 -2.59788900 2.00802900

H -1.62944900 -2.12521900 2.00349400

C -4.86667200 -2.84446500 1.22957500

H -5.64226100 -2.99688700 -0.77415200

H -3.80897900 -2.61107900 3.09122800

H -5.82130500 -3.05052900 1.70323300

P 2.14293000 -1.02406200 -1.42514800

O 3.40544600 -1.78438000 -1.59675600

O 1.03246900 -1.20248600 -2.56681200

O 2.35560700 0.57547900 -1.43218500

C 3.58700800 1.13121100 -0.94466100

H 4.41789700 0.45537800 -1.15899200

H 3.72596700 2.08003600 -1.46408900

H 3.51149200 1.30347000 0.13385800

C 1.43170400 -0.97589000 -3.92575100

H 0.58628500 -1.26678300 -4.54793000

H 1.65671600 0.08351100 -4.07423300

H 2.30534700 -1.58571600 -4.16932500

C 0.38054200 2.42402800 0.58129200

H 1.10950300 2.28936700 -0.22322900

H 0.82948400 3.06852000 1.34542000

C -0.86842400 3.07377000 0.04120100

C -1.75152500 3.74132300 0.89537600

C -1.19041900 2.98261700 -1.31660700

C -2.92852200 4.30646800 0.40801100

H -1.51138200 3.82122400 1.95374100

C -2.36566400 3.54730900 -1.80942700

H -0.51246100 2.45361600 -1.98257800

C -3.23876500 4.21046900 -0.94800800

H -3.60161600 4.82332100 1.08522500

H -2.60062800 3.46907100 -2.86663500

H -4.15384700 4.65127200 -1.33081300

$TS_D^{C\text{-}N}$

0, 2

C -4.31684800 2.43315400 -0.70752000

C -3.82879800 1.16083900 -0.97784400

C -2.45211700 0.90959400 -0.94329000

C -1.56053000 1.94124600 -0.64453100

C -2.06255400 3.21977500 -0.37915200

C -3.43003200 3.46808800 -0.40199200

H -2.56693500 -1.03033100 -1.86717700

H -5.38577300 2.61755000 -0.73156300

H -4.51383300 0.34381400 -1.18281700

C -1.92715900 -0.50206500 -1.14664200

C -0.06970700 1.69857700 -0.65919600

H -1.36560800 4.02647000 -0.16141400

H -3.80496800 4.46521600 -0.19395000

C 0.25605700 0.45002100 -1.42504400

H 0.38756900 2.52828200 -1.21696700

H 1.24470400 0.36831200 -1.87421100

N -0.56193300 -0.53934000 -1.66557000

C 0.27313400 -2.28315700 -1.88273600

H -0.55372500 -2.89324800 -1.54321600

H 0.37363200 -2.20861200 -2.96163300

C 1.50841700 -2.34656100 -1.13828800

C 1.54134200 -2.68085700 0.23545000

C 2.73092300 -1.99094000 -1.75067700

C 2.74317600 -2.72770500 0.93140800

H 0.61092400 -2.91894400 0.73902800

C 3.93043300 -2.03843100 -1.05041800

H 2.73003400 -1.70591700 -2.80044700

C 3.94864800 -2.41762300 0.29419200

H 2.74324800 -3.00420700 1.98177100

H 4.85658300 -1.77802900 -1.55487000

H 4.88510600 -2.46074000 0.84139700

P -2.32869900 -1.34342400 0.44962200

O -3.78051800 -1.34268100 0.74729700

O -1.67628100 -2.80053000 0.33169000

O -1.43180600 -0.64832500 1.59017000

C -2.04524000 0.30885500 2.47216800

H -2.97203900 -0.09791000 2.87996700

H -1.32157800 0.49294600 3.26639500

H -2.25508600 1.23862200 1.93487900

C -1.96713200 -3.74296500 1.37567000

H -1.50605200 -4.68289500 1.07407500

H -1.53110300 -3.40033100 2.31881200

H -3.04740700 -3.86334500 1.48096900

C 0.57787700 1.73888400 0.75964400

H 0.37700800 0.78953400 1.26364000

H 0.09315500 2.53885800 1.33305700

C 2.06060000 2.00362300 0.68346300

C 2.54095500 3.31782200 0.66440000

C 2.97496500 0.95228100 0.57539900

C 3.90391500 3.57955600 0.54509900

H 1.83754700 4.14408600 0.75000100

C 4.34005800 1.21082800 0.45410500

H 2.61622600 -0.07408100 0.58617500

C 4.80885800 2.52317500 0.43945700

H 4.25983900 4.60530800 0.53844000

H 5.03394400 0.37941000 0.37331400

H 5.87200100 2.72313000 0.34901100

p-CN substitution at **2a**

0 1

C	-3.20708000	2.93327600	-1.30153400
C	-2.48160700	1.76013200	-1.50934800
C	-1.66484500	1.25184400	-0.50254900

C	-1.56070100	1.91243100	0.73678700
C	-2.28618100	3.09608300	0.92635400
C	-3.10720100	3.59848700	-0.07944700
H	-0.68420500	-0.22543400	-1.71689000
H	-3.84997900	3.31887300	-2.08559000
H	-2.57510400	1.21662400	-2.44601700
C	-0.98586900	-0.09399000	-0.67073700
C	-0.68364600	1.35892400	1.76030600
H	-2.20296800	3.61856300	1.87551400
H	-3.66898600	4.51187000	0.08937900
C	0.15796900	0.35875700	1.43289300
H	-0.66326000	1.78900300	2.75377400
H	0.89899100	-0.02517100	2.12879800
N	0.18632500	-0.20871700	0.17439300
C	1.18113100	-1.22392400	-0.10872200
H	1.09457000	-2.06751900	0.59042100
H	0.96655400	-1.63447700	-1.10117600
C	2.59879200	-0.68339300	-0.09017400
C	3.66297700	-1.55868500	0.14624100
C	2.86625600	0.66591000	-0.33502000
C	4.97612100	-1.10578000	0.12352500
H	3.46077200	-2.60674700	0.35160100
C	4.17564900	1.13337300	-0.35667400
H	2.03979000	1.35097200	-0.49893300
C	5.23372600	0.24668800	-0.12918600
H	5.80152000	-1.78535100	0.30655200
H	4.38493900	2.18086700	-0.54544800
P	-2.27424700	-1.39734500	-0.39570400
O	-3.19911900	-1.57118800	-1.54149900
O	-1.37592300	-2.66746100	0.00501700
O	-3.01057300	-1.07201200	0.99587900
C	-4.25011000	-0.34582500	0.99558300
H	-4.83444500	-0.59736200	0.10763600
H	-4.78382100	-0.64519600	1.89764100
H	-4.04621400	0.72839000	1.02144000
C	-2.05185800	-3.91622300	0.21439400
H	-1.27640900	-4.66838300	0.35379200

H	-2.67609500	-3.85458400	1.10951200
H	-2.66360500	-4.16369000	-0.65665600
C	6.59131900	0.72676900	-0.14700300
N	7.68332400	1.11087400	-0.16141000

p-OMe substitution at **2a**

0 1

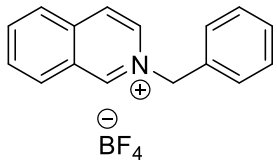
C	-3.28356300	3.00885000	-1.22756400
C	-2.59773400	1.81941800	-1.47467600
C	-1.76263400	1.27465400	-0.50272100
C	-1.59784500	1.91461600	0.74134100
C	-2.28419900	3.11508800	0.97010800
C	-3.12472800	3.65322300	-0.00040700
H	-0.87658400	-0.22406100	-1.76513500
H	-3.94186600	3.42252900	-1.98411400
H	-2.73710600	1.29137200	-2.41454800
C	-1.12988900	-0.08855500	-0.70664400
C	-0.69918900	1.32449000	1.72289100
H	-2.15494500	3.62200600	1.92263100
H	-3.65574300	4.57875500	0.19978100
C	0.10737400	0.31010200	1.34798700
H	-0.62505200	1.74398100	2.71831100
H	0.87214000	-0.09310300	2.00568400
N	0.07238500	-0.24257100	0.08602500
C	1.02029700	-1.29534900	-0.24678700
H	0.86363800	-2.17998100	0.38606300
H	0.80053900	-1.61312300	-1.27220800
C	2.46049800	-0.83544300	-0.14663400
C	3.46311100	-1.74565400	0.20735200
C	2.82982100	0.47629700	-0.43217900
C	4.79523400	-1.36284500	0.25685900
H	3.19499300	-2.77147400	0.44934100
C	4.16497400	0.88227600	-0.38219000
H	2.06080600	1.20135300	-0.68540200
C	5.15346800	-0.04293100	-0.04007400
H	5.57743900	-2.06254400	0.53146800

H	4.41410800	1.91266000	-0.60558400
P	-2.45322600	-1.34989400	-0.39444900
O	-3.40920600	-1.49617300	-1.51943300
O	-1.59607200	-2.65093500	-0.00509000
O	-3.15371300	-0.99663400	1.01022400
C	-4.36508700	-0.22626100	1.03058400
H	-4.96929200	-0.44925800	0.14817100
H	-4.89908500	-0.51273800	1.93689300
H	-4.12191900	0.83970600	1.06179100
C	-2.31319300	-3.87082900	0.22939700
H	-1.56352800	-4.65095000	0.35626500
H	-2.91338100	-3.77986000	1.13849600
H	-2.95464100	-4.10113600	-0.62499200
O	6.48035300	0.24453600	0.04059800
C	6.88457100	1.56547100	-0.25135300
H	7.96756900	1.58252400	-0.13472300
H	6.62367500	1.84183100	-1.27997500
H	6.43131400	2.28186300	0.44422400

11. Compound Characterization Data:

11a. Compound Characterization Data for N-alkyl Isoquinolinium Salts:

2-benzylisoquinolin-2-ium tetrafluoroborate (1a)

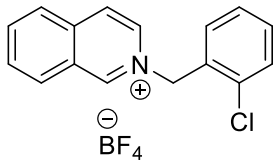


The titled compound **1a** was prepared by exactly following the general procedure **A (GP-A)**. $\mathbf{R_f}$ (MeOH/DCM = 10:90) = 0.41. The title compound was isolated via flash column chromatography using 4-5% MeOH/DCM, obtained as a white solid (0.54 g, 89% yield).

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.27 (s, 1H), 8.84 (dd, *J* = 6.8, 1.2 Hz, 1H), 8.61 (d, *J* = 6.8 Hz, 1H), 8.55 (d, *J* = 8.3 Hz, 1H), 8.37 (d, *J* = 8.3 Hz, 1H), 8.32 - 8.25 (m, 1H), 8.14 - 8.08 (m, 1H), 7.65 - 7.57 (m, 2H), 7.52 - 7.41 (m, 3H), 5.99 (s, 2H).

The spectral data match the previously reported structure.[15]

2-(2-chlorobenzyl)isoquinolin-2-ium tetrafluoroborate (1b)

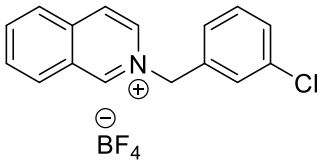


The titled compound **1b** was prepared by exactly following the general procedure **A (GP-A).** $\mathbf{R_f}$ (MeOH/DCM = 10:90) = 0.43. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM obtained as brown solid (0.58 g, 85% yield). MP = 85.4 – 87.3 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.18 (s, 1H), 8.76 (dd, *J* = 6.8, 1.4 Hz, 1H), 8.63 (d, *J* = 6.9 Hz, 1H), 8.59 (d, *J* = 8.3 Hz, 1H), 8.41 - 8.36 (m, 1H), 8.31 (td, *J* = 7.7, 1.1 Hz, 1H), 8.11 (td, *J* = 7.6, 1.0 Hz, 1H), 7.64 - 7.60 (m, 1H), 7.56 - 7.45 (m, 3H), 6.12 (s, 2H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 150.8, 137.4, 137.2, 135.0, 133.3, 131.6, 131.5, 131.4, 131.4, 130.8, 130.1, 128.2, 127.4, 127.2, 126.3, 61.3. **FTIR (cm^{-1}):** 3103, 2957, 2923, 2854, 1715, 1640, 1446, 1369, 1238, 1208, 937, 819.

HRMS (ESI) *m/z* Calculated for $C_{16}H_{13}NCl$ $[M]^+$: 254.0731, found: 254.0730.

2-(3-chlorobenzyl)isoquinolin-2-ium tetrafluoroborate (1c)



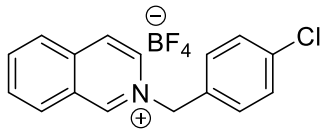
The titled compound **1c** was prepared by exactly following the general procedure **A (GP-A).** $\boldsymbol{R_f}$ (MeOH/DCM; 10:90) = 0.42. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a yellow solid (0.56 g, 82% yield). MP = 96.2 – 98.5 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.26 (s, 1H), 8.85 (dd, *J* = 6.9, 1.4 Hz, 1H), 8.63 (d, *J* = 6.9 Hz, 1H), 8.56 (d, *J* = 8.3 Hz, 1H), 8.42 - 8.34 (m, 1H), 8.30 (td, *J* = 7.6, 1.1 Hz, 1H), 8.12 (td, *J* = 7.6, 1.0

Hz, 1H), 7.79 (s, 1H), 7.63 - 7.56 (m, 1H), 7.56 - 7.48 (m, 2H), 6.00 (s, 2H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 150.5, 137.2, 137.1, 136.4, 134.7, 133.7, 131.4, 131.1, 130.7, 129.3, 128.9, 127.7, 127.4, 127.3, 126.4, 62.6. **FTIR (cm^{-1}):** 3069, 2959, 2920, 2854, 1718, 1641, 1474, 1397, 1285, 1043, 876, 737.

HRMS (ESI) *m/z* Calculated for $C_{16}H_{13}NCl$ $[M]^+$: 254.0731, found: 254.0738.

2-(4-chlorobenzyl)isoquinolin-2-ium tetrafluoroborate (1d)

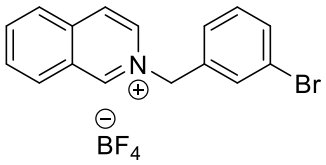


The titled compound **1d** was prepared by exactly following the general procedure **A (GP-A).** ***R$_f$*** (MeOH/DCM; 10:90) = 0.43. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a yellow solid (0.52 g, 76% yield). MP = 132.1 – 134.6 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.23 (s, 1H), 8.82 (dd, *J* = 6.9, 1.4 Hz, 1H), 8.62 (d, *J* = 6.9 Hz, 1H), 8.54 (d, *J* = 8.3 Hz, 1H), 8.40 - 8.34 (m, 1H), 8.29 (td, *J* = 7.6, 1.1 Hz, 1H), 8.11 (ddd, *J* = 8.2, 7.1, 1.0 Hz, 1H), 7.67 - 7.61 (m, 2H), 7.58 - 7.51 (m, 2H), 5.99 (s, 2H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 150.3, 137.2, 137.1, 134.7, 134.2, 133.1, 131.4, 130.9, 130.7, 129.2, 127.3, 126.4, 62.6. **FTIR (cm^{-1}):** 2957, 2922, 2852, 1641, 1512, 1493, 1466, 1397, 1057, 885, 811, 765.

HRMS (ESI) *m/z* Calculated for $C_{16}H_{13}NCl$ $[M]^+$: 254.0731, found: 254.0734.

2-(3-bromobenzyl)isoquinolin-2-ium tetrafluoroborate (1e)

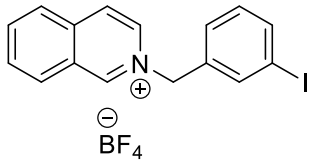


The titled compound **1e** was prepared by exactly following the general procedure **A (GP-A).** ***R$_f$*** (MeOH/DCM; 10:90) = 0.43. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a brown solid (0.63 g, 82% yield). MP = 111.9 – 113.2 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.25 (s, 1H), 8.84 (dd, *J* = 6.9, 1.4 Hz, 1H), 8.62 (d, *J* = 6.9 Hz, 1H), 8.55 (d, *J* = 8.1 Hz, 1H), 8.40 - 8.34 (m, 1H), 8.30 (td, *J* = 7.6, 1.1 Hz, 1H), 8.11 (ddd, *J* = 8.2, 7.0, 1.0 Hz, 1H), 7.92 (t, *J* = 1.7 Hz, 1H), 7.70 - 7.59 (m, 2H), 7.48 - 7.40 (m, 1H), 5.98 (s, 2H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 150.5, 137.2, 137.1, 136.6, 134.7, 132.2, 131.8, 131.3, 131.3, 130.7, 128.1, 127.3, 126.4, 122.2, 62.5. **FTIR (cm^{-1}):** 3005, 2956, 2922, 2865, 1642, 1512, 1470, 1396, 1063, 885, 756, 695.

HRMS (ESI) *m/z* Calculated for $C_{16}H_{13}NBr$ $[M]^+$: 298.0226, found: 298.0226.

2-(3-iodobenzyl)isoquinolin-2-iumtetrafluoroborate (1f)

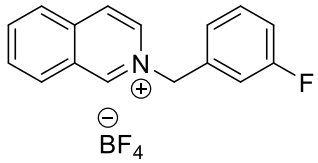


The titled compound **1f** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.45. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a brown solid (0.62 g, 72% yield). MP = 119.4 – 121.6 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.24 (s, 1H), 8.82 (d, *J* = 6.8 Hz, 1H), 8.61 (d, *J* = 6.8 Hz, 1H), 8.55 (d, *J* = 8.4 Hz, 1H), 8.37 (d, *J* = 8.3 Hz, 1H), 8.29 (t, *J* = 7.6 Hz, 1H), 8.11 (t, *J* = 7.6 Hz, 1H), 8.07 (s, 1H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.27 (t, *J* = 7.8 Hz, 1H), 5.94 (s, 2H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 150.4, 138.0, 137.4, 137.2, 137.1, 136.5, 134.7, 131.3, 131.2, 130.7, 128.4, 127.3, 126.4, 95.5, 62.5. **FTIR (cm^{-1}):** 3097, 3066, 2922, 2853, 1735, 1643, 1570, 1453, 1282, 1069, 823, 728.

HRMS (ESI) *m/z* Calculated for $C_{16}H_{13}NI$ $[M]^+$: 346.0087, found: 346.0088.

2-(3-fluorobenzyl)isoquinolin-2-ium tetrafluoroborate (1g)

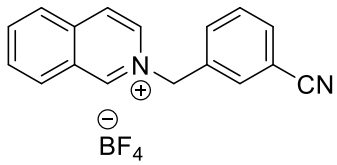


The titled compound **1g** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.42. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a brown solid (0.53 g, 81% yield). MP = 79.9 – 80.6 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.25 (s, 1H), 8.84 (dd, *J* = 6.9, 1.4 Hz, 1H), 8.62 (d, *J* = 6.8 Hz, 1H), 8.55 (d, *J* = 8.3 Hz, 1H), 8.41 - 8.35 (m, 1H), 8.30 (td, *J* = 7.6, 1.1 Hz, 1H), 8.12 (ddd, *J* = 8.2, 7.0, 1.1 Hz, 1H), 7.59 - 7.50 (m, 2H), 7.50 - 7.42 (m, 1H), 7.35 - 7.25 (m, 1H), 6.01 (s, 2H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 162.2 (d, *J* = 244.9 Hz), 150.5, 137.2, 137.1, 136.6 (d, *J* = 7.6 Hz), 134.8, 131.4, 131.3, 130.7, 127.4, 127.4, 126.4, 125.1 (d, *J* = 3.1 Hz), 116.2 (d, *J* = 20.6 Hz), 116.0 (d, *J* = 22.1 Hz), 62.7 (d, *J* = 1.53 Hz). **FTIR (cm^{-1}):** 3097, 3063, 2921, 2854, 1731, 1638, 1589, 1446, 1284, 1026, 837, 729.

HRMS (ESI) *m/z* Calculated for $C_{16}H_{13}NF$ $[M]^+$: 238.1027, found: 238.1036.

2-(3-cyanobenzyl)isoquinolin-2-ium tetrafluoroborate (1h)

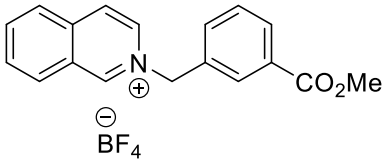


The titled compound **1h** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.35. The title compound was isolated via flash column chromatography using 4-5% MeOH/DCM, obtained as a yellow solid (0.57 g, 86% yield). MP = 127.3 – 128.7 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.25 (s, 1H), 8.84 (dd, *J* = 6.8, 1.4 Hz, 1H), 8.63 (d, *J* = 6.9 Hz, 1H), 8.56 (d, *J* = 8.3 Hz, 1H), 8.42 - 8.36 (m, 1H), 8.31 (td, *J* = 7.6, 1.1 Hz, 1H), 8.18 - 8.09 (m, 2H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.96 - 7.91 (m, 1H), 7.74 - 7.68 (m, 1H), 6.06 (s, 2H).**^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 150.7, 137.2, 137.2, 135.6, 134.8, 133.9, 133.0, 132.8, 131.3, 130.8, 130.4, 127.4, 127.3, 126.4, 118.3, 112.1, 62.3. **FTIR (cm^{-1}):** 3075, 3011, 2921, 2852, 2229, 1643, 1513, 1445, 1286, 1036, 872, 755.

HRMS (ESI) *m/z* Calculated for $C_{17}H_{13}N_2$ $[M]^+$: 245.1073, found: 245.1076.

2-(3-(methoxycarbonyl)benzyl)isoquinolin-2-ium tetrafluoroborate (1i)

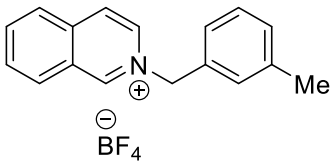


The titled compound **1i** was prepared by exactly following the general procedure **A (GP-A).** ***R**$_f$* (MeOH/DCM; 10:90) = 0.34. The title compound was isolated via flash column chromatography using 4-5% MeOH/DCM, obtained as a white solid (0.60 g, 82% yield). MP = 150.3 – 151.2 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.30 (s, 1H), 8.89 (dd, *J* = 6.8, 1.2 Hz, 1H), 8.64 (d, *J* = 6.8 Hz, 1H), 8.57 (d, *J* = 8.4 Hz, 1H), 8.42 - 8.35 (m, 1H), 8.35 - 8.26 (m, 2H), 8.16 - 8.10 (m, 1H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.65 (t, *J* = 7.8 Hz, 1H), 6.10 (s, 2H), 3.90 (s, 3H).**^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 165.8, 150.4, 137.2, 137.1, 134.8, 134.7, 133.9, 131.4, 130.7, 130.5, 130.0, 129.9, 129.8, 127.4, 126.4, 62.8, 52.3. **FTIR (cm^{-1}):** 3066, 3026, 2957, 2852, 1712, 1641, 1513, 1437, 1283, 1161, 880, 762.

HRMS (ESI) *m/z* Calculated for $C_{18}H_{16}O_2N$ $[M]^+$:278.1176, found: 278.1171.

2-(3-methylbenzyl)isoquinolin-2-ium tetrafluoroborate (1j)

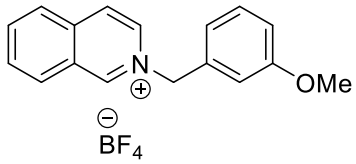


The titled compound **1j** was prepared by exactly following the general procedure **A (GP-A).** ***R**$_f$* (MeOH/DCM; 10:90) = 0.42. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a brown solid (0.50 g, 78% yield). MP = 97.2 – 99.2 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.25 (s, 1H), 8.82 (dd, *J* = 6.8, 1.3 Hz, 1H), 8.60 (d, *J* = 6.8 Hz, 1H), 8.55 (d, *J* = 8.3 Hz, 1H), 8.34 - 8.39 (m, 1H), 8.29 (td, *J* = 7.6, 1.1 Hz, 1H), 8.11 (td, *J* = 7.6, 1.0 Hz, 1H), 7.43 (s, 1H), 7.41 - 7.33 (m, 2H), 7.25 (d, *J* = 7.1 Hz, 1H), 5.94 (s, 2H), 2.32 (s, 3H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 150.2, 138.6, 137.2, 137.0, 134.8, 134.2, 131.4, 130.6, 129.9, 129.3, 129.1, 127.4, 127.3, 126.3, 125.9, 63.5, 20.9. **FTIR (cm^{-1}):** 3067, 2920, 2853, 1728, 1641, 1456, 1394, 1281, 1043, 879, 756, 657.

HRMS (ESI) *m/z* Calculated for $C_{17}H_{16}N$ $[M]^+$:234.1277, found: 234.1274.

2-(3-methoxybenzyl)isoquinolin-2-ium tetrafluoroborate (1k)

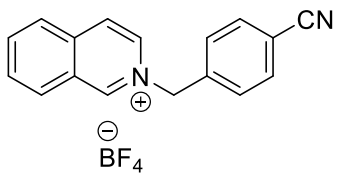


The titled compound **1k** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.37. The title compound was isolated via flash column chromatography using 4-5% MeOH/DCM, obtained as a brown solid (0.51 g, 76% yield). MP = 86.8 – 88.9 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.25 (s, 1H), 8.84 (dd, *J* = 6.8, 1.3 Hz, 1H), 8.61 (d, *J* = 6.9 Hz, 1H), 8.55 (d, *J* = 8.3 Hz, 1H), 8.40 - 8.34 (m, 1H), 8.29 (td, *J* = 7.6, 1.1 Hz, 1H), 8.11 (ddd, *J* = 8.2, 7.0, 1.1 Hz, 1H), 7.42 - 7.36 (m, 1H), 7.27 - 7.23 (m, 1H), 7.16 (d, *J* = 7.8 Hz, 1H), 7.02 (dd, *J* = 8.0, 2.3 Hz, 1H), 5.94 (s, 2H), 3.79 (s, 3H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 159.7, 150.2, 137.2, 137.1, 135.6, 134.7, 131.4, 130.7, 130.5, 127.4, 127.3, 126.3, 120.9, 114.8, 114.7, 63.4, 55.3. **FTIR (cm^{-1}):** 3095, 2923, 2848, 1730, 1639, 1456, 1360, 1268, 1159, 1053, 876, 747.

HRMS (ESI) *m/z* Calculated for $C_{17}H_{16}ON$ $[M]^+$:250.1226, found: 250.1229.

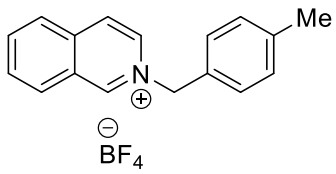
2-(4-cyanobenzyl)isoquinolin-2-ium tetrafluoroborate (1l)



The titled compound **1l** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.37. The title compound was isolated via flash column chromatography using 4-5% MeOH/DCM, obtained as a white solid (0.53 g, 80% yield). MP = 169.9 – 171.4 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.25 (s, 1H), 8.82 (dd, *J* = 6.8, 1.3 Hz, 1H), 8.63 (d, *J* = 6.9 Hz, 1H), 8.55 (d, *J* = 8.3 Hz, 1H), 8.41 - 8.35 (m, 1H), 8.31 (td, *J* = 7.6, 1.1 Hz, 1H), 8.16 - 8.09 (m, 1H), 7.96 (d, *J* = 8.4 Hz, 2H), 7.76 (d, *J* = 8.4 Hz, 2H), 6.09 (s, 2H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 150.8, 139.4, 137.3, 137.2, 134.9, 133.0, 131.4, 130.7, 129.7, 127.4, 127.4, 126.4, 118.3, 112.0, 62.6. **FTIR (cm^{-1}):** 3001, 2959, 2922, 2853, 2229, 1644, 1554, 1461, 1398, 1057, 825, 768. **HRMS** (ESI) *m/z* Calculated for $C_{17}H_{13}N_2$ $[M]^+$:245.1073, found: 245.1071.

2-(4-methylbenzyl)isoquinolin-2-ium tetrafluoroborate (1m)

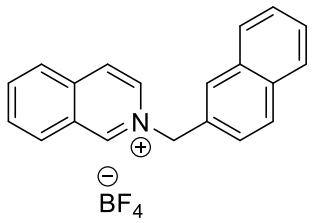


The titled compound **1m** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.43. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as brown solid (0.51 g, 79% yield). MP = 125.1 – 126.7 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.25 (s, 1H), 8.83 (dd, *J* = 6.8, 1.2 Hz, 1H), 8.61 (d, *J* = 6.8 Hz, 1H), 8.56 (d, *J* = 8.3 Hz, 1H), 8.37 (d, *J* = 8.3 Hz, 1H), 8.26 - 8.32 (m, 1H), 8.15 - 8.08 (m, 1H), 7.53 (d, *J* = 7.9 Hz, 2H) 7.29 (d, *J* = 7.9 Hz, 2H), 5.95 (s, 2H), 2.33 (s, 3H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 150.0, 139.0, 137.1, 137.0, 134.7, 131.4, 131.3, 130.6, 129.8, 128.9, 127.3, 127.3, 126.3, 63.3, 20.7. **FTIR (cm^{-1}):** 3063, 2920, 2853, 1728, 1640, 1513, 1446, 1394, 1282, 1052, 888, 758.

HRMS (ESI) *m/z* Calculated for $C_{17}H_{16}N$ $[M]^+$: 234.1277, found: 234.1278.

2-(naphthalen-2-ylmethyl)isoquinolin-2-ium tetrafluoroborate (1n)

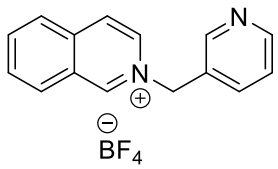


The titled compound **1n** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.45. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a white solid (0.57 g, 80% yield). MP = 159.1 – 160.9 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.32 (s, 1H), 8.90 (dd, *J* = 6.8, 1.3 Hz, 1H), 8.63 (d, *J* = 6.9 Hz, 1H), 8.57 (d, *J* = 8.4 Hz, 1H), 8.42 - 8.35 (m, 1H), 8.30 (td, *J* = 7.6, 1.0 Hz, 1H), 8.17 (s, 1H), 8.15 - 8.09 (m, 1H), 8.03 (d, *J* = 8.6 Hz, 1H), 8.00 – 7.94 (m, 2H), 7.70 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.64 - 7.56 (m, 2H), 6.17 (s, 2H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 150.3, 137.2, 137.1, 134.9, 132.9, 132.7, 131.7, 131.3, 130.7, 129.0, 128.5, 128.1, 127.7, 127.4, 127.4, 127.1, 126.9, 126.3, 125.9, 63.6. **FTIR (cm^{-1}):** 3064, 2965, 2919, 2854, 1643, 1473, 1394, 1283, 1154, 1033, 876, 760.

HRMS (ESI) *m/z* Calculated for $C_{20}H_{16}N$ $[M]^+$:270.1277, found: 270.1282.

2-(pyridin-3-ylmethyl)isoquinolin-2-ium tetrafluoroborate (1o)



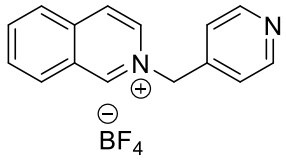
The titled compound **1o** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.28. The title compound was isolated via flash column chromatography using 8-10% MeOH/DCM, obtained as a liquid (0.44 g, 72% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ. 10.23 (s, 1H), 8.86 (d, *J* = 1.9 Hz, 1H), 8.83 (dd, *J* = 6.8, 1.3 Hz, 1H), 8.62 (dd, *J* = 4.8, 1.4 Hz, 1H), 8.59 (d, *J* = 6.8 Hz, 1H), 8.52 (d, *J* = 8.3 Hz, 1H), 8.36 - 8.32 (m,

1H), 8.26 (td, *J* = 7.6, 1.0 Hz, 1H), 8.11 - 8.05 (m, 1H), 8.00 (dt, *J* = 7.9, 1.8 Hz, 1H), 7.47 (dd, *J* = 7.9, 4.8 Hz, 1H), 6.02 (s, 2H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 150.5, 150.5, 150.1, 137.3, 137.2, 136.9, 134.8, 131.5, 130.8, 130.1, 127.5, 127.4, 126.5, 124.2, 61.1. **FTIR (cm^{-1}):** 3068, 2924, 2859, 1733, 1644, 1551, 1460, 1386, 1268, 1075, 878, 740.

HRMS (ESI) *m/z* Calculated for $C_{15}H_{13}N_2$ $[M]^+$:221.1073, found: 221.1072.

2-(pyridin-4-ylmethyl)isoquinolin-2-ium tetrafluoroborate (1p)

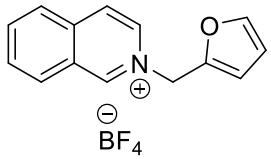


The titled compound **1p** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.30. The title compound was isolated via flash column chromatography using 8-10% MeOH/DCM, obtained as a white solid (0.43 g, 70% yield). MP = 143.4 – 147.4 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.37 (s, 1H), 8.87 (dd, *J* = 6.9, 1.4 Hz, 1H), 8.66 (d, *J* = 6.9 Hz, 1H), 8.64 - 8.60 (m, 2H), 8.54 (d, *J* = 8.0 Hz, 1H), 8.39 (d, *J* = 8.1 Hz, 1H), 8.29 (ddd, *J* = 8.3, 7.1, 1.2 Hz, 1H), 8.10 (ddd, *J* = 8.3, 7.1, 1.1 Hz, 1H), 7.54 - 7.47 (m, 2H), 6.10 (s, 2H).**^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 151.0, 150.3, 143.0, 137.4, 137.3, 135.1, 131.4, 130.8, 127.4, 126.5, 123.0, 61.8. **FTIR (cm^{-1}):** 3054, 2959, 2920, 2852, 1727, 1642, 1605, 1464, 1282, 1070, 882, 770.

HRMS (ESI) *m/z* Calculated for $C_{15}H_{13}N_2$ $[M]^+$: 221.1073, found: 221.1074.

2-(furan-2-ylmethyl)isoquinolin-2-ium tetrafluoroborate (1q):

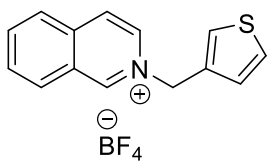


The titled compound **1q** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.45. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a brown solid (0.45 g, 75 % yield). MP = 125.4 – 126.0 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.18 (s, 1H), 8.81 (d, *J* = 6.9 Hz, 1H), 8.63 (d, *J* = 6.9 Hz, 1H), 8.58 (d, *J* = 8.4 Hz, 1H), 8.37 (d, *J* = 8.3 Hz, 1H), 8.30 (t, *J* = 7.6 Hz, 1H), 8.11 (t, *J* = 7.6 Hz, 1H), 7.80 (s, 1H), 6.91 (d, *J* = 3.0 Hz, 1H), 6.63 - 6.55 (m, 1H), 6.07 (s, 2H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 150.0, 146.7, 145.2, 137.3, 137.2, 134.5, 131.5, 130.6, 127.4, 127.2, 126.4, 112.6, 111.3, 56.2. **FTIR (cm^{-1}):** 2963, 2920, 2852, 1640, 1506, 1467, 1389, 1282, 1152, 1052, 876, 755.

HRMS (ESI) *m/z* Calculated for $C_{14}H_{12}ON$ $[M]^+$:210.0913 found: 210.0912.

2-(thiophen-3-ylmethyl)isoquinolin-2-ium tetrafluoroborate (1r)



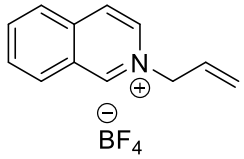
The titled compound **1r** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.46. The title compound

was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a yellow solid (0.46 g, 73% yield). MP = 120.9 – 122.7 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.21 (s, 1H), 8.83 (dd, *J* = 6.8, 1.2 Hz, 1H), 8.61 (d, *J* = 6.8 Hz, 1H), 8.54 (d, *J* = 8.3 Hz, 1H), 8.36 (d, *J* = 8.3 Hz, 1H), 8.32 - 8.24 (m, 1H), 8.14 - 8.06 (m, 1H), 7.87 (d, *J* = 1.9 Hz, 1H), 7.67 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.34 (dd, *J* = 5.0, 1.1 Hz, 1H), 5.99 (s, 2H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 150.0, 137.1, 137.0, 134.6, 131.3, 130.6, 128.2, 127.6, 127.3, 127.3, 126.9, 126.3, 58.6. **FTIR (cm^{-1}):** 3068, 2960, 2920, 2853, 1735, 1640, 1516, 1472, 1284, 1028, 889, 737.

HRMS (ESI) *m/z* Calculated for $C_{14}H_{12}NS$ $[M]^+$: 226.0685, found: 226.0683.

2-allylisoquinolin-2-ium tetrafluoroborate (1s)

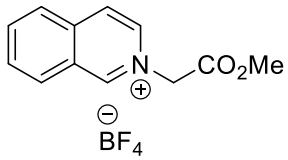


The titled compound **1s** was prepared by exactly following the general procedure **A (GP-A).** ***R$_f$*** (MeOH/DCM; 05:95) = 0.40. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a brown solid (0.41 g, 80% yield).

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.04 (s, 1H), 8.76 - 8.69 (m, 1H), 8.62 (d, *J* = 6.9 Hz, 1H), 8.54 (d, *J* = 8.4 Hz, 1H), 8.37 (d, *J* = 8.3 Hz, 1H), 8.33 - 8.25 (m, 1H), 8.14 - 8.05 (m, 1H), 6.26 (ddt, *J* = 16.8, 10.5, 6.2, 6.2 Hz, 1H), 5.55 - 5.46 (m, 2H), 5.39 (d, *J* = 6.1 Hz, 2H).

The spectral data match the previously reported structure.[4]

2-(2-methoxy-2-oxoethyl)isoquinolin-2-ium tetrafluoroborate (1u)

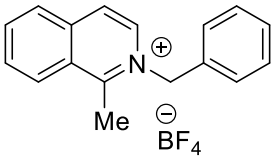


The titled compound **1u** was prepared by exactly following the general procedure **A (GP-A).** ***R$_f$*** (MeOH/DCM; 10:90) = 0.40. The title compound was isolated via flash column chromatography using 4-5% MeOH/DCM, obtained as a white solid (0.47 g, 82% yield). MP = 93.5 – 94.3 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.03 (s, 1H), 8.75 (dd, *J* = 6.9, 1.3 Hz, 1H), 8.65 (d, *J* = 6.9 Hz, 1H), 8.54 (d, *J* = 8.3 Hz, 1H), 8.42 - 8.36 (m, 1H), 8.36 - 8.29 (m, 1H), 8.16 - 8.08 (m, 1H), 5.80 (s, 2H), 3.81 (s, 3H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 167.1, 151.8, 137.8, 137.4, 136.2, 131.6, 130.7, 127.4, 126.8, 125.6, 60.3, 53.2. **FTIR (cm^{-1}):** 2956, 2921, 2854, 1749, 1643, 1513, 1433, 1397, 1297, 1051, 830, 768.

HRMS (ESI) *m/z* Calculated for $C_{12}H_{12}O_2N$ $[M]^+$: 202.0863, found: 202.0861.

2-benzyl-1-methylisoquinolin-2-ium tetrafluoroborate (1v)

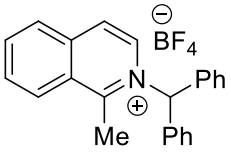


The titled compound **1v** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.37. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a white solid (0.52 g, 81% yield). MP = 129.8. – 131.3 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.82 (d, *J* = 6.9 Hz, 1H), 8.77 (d, *J* = 8.6 Hz, 1H), 8.51 (d, *J* = 6.9 Hz, 1H), 8.35 (d, *J* = 8.1 Hz, 1H), 8.26 (t, *J* = 7.5 Hz, 1H), 8.11 - 8.04 (m, 1H), 7.48 - 7.38 (m, 3H), 7.32 (d, *J* = 6.8 Hz, 2H), 6.10 (s, 2H), 3.25 (s, 3H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 160.6, 136.7, 136.3, 136.3, 133.8, 131.1, 129.2, 128.9, 128.7, 128.0 127.7, 127.3, 124.2, 60.8, 17.0. **FTIR (cm^{-1}):** 3097, 2956, 2921. 2852, 1633, 1568, 1492, 1382, 1284, 1053, 882, 730.

HRMS (ESI) *m/z* Calculated for $C_{17}H_{16}N$ $[M]^+$: 234.1277, found: 234.1282.

2-benzhydryl-1-methylisoquinolin-2-ium tetrafluoroborate (1w)

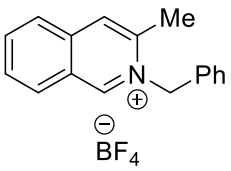


The titled compound **1w** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.44. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a white solid (0.58 g, 74% yield). MP = 168.4 – 169.6 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 8.6 Hz, 1H), 8.14 - 8.08 (m, 2H), 8.08 - 8.02 (m, 1H), 7.97 (d, *J* = 7.1 Hz, 1H), 7.96 - 7.90 (m, 1H), 7.78 (s, 1H), 7.43 - 7.38 (m, 6H), 7.19 (dd, *J* = 6.4, 3.0 Hz, 4H), 3.34 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.3, 137.0, 136.8, 135.2, 132.4, 131.7, 129.8, 129.7, 129.1, 128.5, 128.3, 128.2, 124.0, 73.9, 17.5. **FTIR (cm^{-1}):** 3096, 2963, 2927, 1630, 1565, 1497, 1452, 1383, 1277, 1057, 818, 753.

HRMS (ESI) *m/z* Calculated for $C_{23}H_{20}O_2N$ $[M]^+$: 310.1590, found: 310.1595.

2-benzyl-3-methylisoquinolin-2-ium tetrafluoroborate (1x)

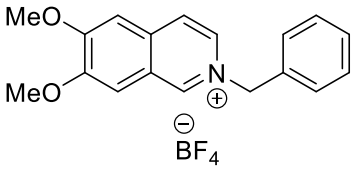


The titled compound **1x** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.38. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a white solid (0.55 g, 86% yield). MP = 137.1 – 138.6 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.36 (s, 1H), 8.54 (s, 1H), 8.52 (d, *J* = 8.5 Hz, 1H), 8.26 (d, *J* = 3.8 Hz, 2H), 8.04 (dt, *J* = 8.3, 4.1 Hz, 1H), 7.48 - 7.39 (m, 3H), 7.37 - 7.32 (m, 2H), 6.11 (s, 2H), 2.76 (s, 3H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 151.7, 144.3, 138.0, 137.2, 133.4, 130.5, 130.3, 129.2, 128.8, 127.5, 126.7, 126.4, 126.2, 60.6, 19.1. **FTIR (cm^{-1}):** 3063, 2924, 2853, 1726, 1648, 1519, 1498, 1345, 1294, 1059, 826, 740.

HRMS (ESI) *m/z* Calculated for $C_{17}H_{16}N$ $[M]^+$: 234.1277, found: 234.1283.

2-benzyl-6,7-dimethoxyisoquinolin-2-ium tetrafluoroborate (1y)

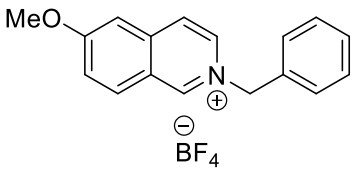


The titled compound **1y** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.35. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a brown solid (0.54 g, 73% yield). MP = 138.4 – 141.5 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.72 (s, 1H), 8.66 (dd, *J* = 6.8, 1.4 Hz, 1H), 8.31 (d, *J* = 6.8 Hz, 1H), 7.81 (s, 1H), 7.76 (s, 1H), 7.57 - 7.51 (m, 2H), 7.49 - 7.42 (m, 3H), 5.87 (s, 2H), 4.07 (s, 3H), 4.01 (s, 3H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 157.8, 152.6, 145.0, 135.4, 134.7, 133.6, 129.2, 128.6, 124.0, 123.7, 107.3, 105.8, 62.7, 56.9, 56.3. **FTIR (cm^{-1}):** 3080, 2949, 2923, 2850, 1636, 1613, 1497, 1460, 1219, 1062, 870, 749.

HRMS (ESI) *m/z* Calculated for $C_{18}H_{18}O_2N$ $[M]^+$:280.1332, found: 280.1336.

2-benzyl-6-methoxyisoquinolin-2-ium tetrafluoroborate (1z)

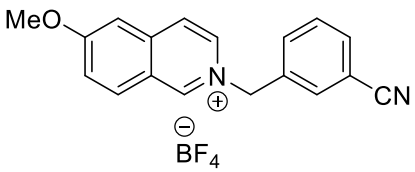


The titled compound **1z** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.36. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a brown solid (0.49 g, 73% yield). MP = 117.4 – 119.9 °C.

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.01 (s, 1H), 8.70 (d, *J* = 6.6 Hz, 1H), 8.42 (d, *J* = 9.3 Hz, 1H), 8.37 (d, *J* = 6.9 Hz, 1H), 7.76 (d, *J* = 2.3 Hz, 1H), 7.68 (dd, *J* = 9.1, 2.4 Hz, 1H), 7.60 - 7.53 (m, 2H), 7.49 - 7.40 (m, 3H), 5.89 (s, 2H), 4.06 (s, 3H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 165.8, 148.2, 140.0, 135.1, 134.6, 132.5, 129.2, 128.7, 124.3, 124.1, 122.7, 105.9, 62.7, 56.6. **FTIR (cm^{-1}):** 2923, 2853, 1719, 1640, 1621, 1491, 1457, 1284, 1216, 1049, 866, 741.

HRMS (ESI) *m/z* Calculated for $C_{17}H_{16}ON$ $[M]^+$:250.1226, found: 250.1229.

2-(3-cyanobenzyl)-6-methoxyisoquinolin-2-ium tetrafluoroborate (1aa)

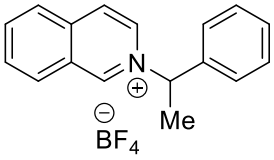


The titled compound **1aa** was prepared by exactly following the general procedure **A (GP-A).** R_f (MeOH/DCM; 10:90) = 0.34. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a sticky solid (0.51 g, 70% yield).

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.95 (s, 1H), 8.68 (dd, *J* = 6.9, 1.2 Hz, 1H), 8.41 (d, *J* = 9.1 Hz, 1H), 8.36 (d, *J* = 6.9 Hz, 1H), 8.09 (s, 1H), 7.94 - 7.86 (m, 2H), 7.76 (d, *J* = 2.4 Hz, 1H), 7.71 - 7.67

(m, 2H), 5.92 (s, 2H), 4.06 (s, 3H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 165.8, 148.6, 140.2, 135.9, 135.0, 133.7, 132.9, 132.7, 132.6, 130.4, 124.4, 124.1, 122.8, 118.3, 112.1, 105.9, 61.6, 56.7. **FTIR (cm^{-1}):** 3067, 2926, 2859, 2231, 1728, 1635, 1458, 1371, 1279, 1075, 862, 737.
HRMS (ESI) *m/z* Calculated for $C_{18}H_{15}ON_2$ $[M]^+$: 275.1179, found 275.1170.

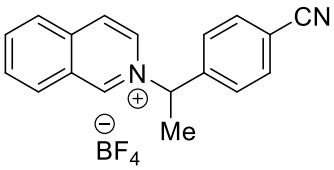
2-(1-phenylethyl)isoquinolin-2-ium tetrafluoroborate (1ab)



The titled compound **1ab** was prepared by exactly following the general procedure **B (GP-B).** ***R**$_f$* (MeOH/DCM; 10:90) = 0.6. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a brown solid (0.43 g, 67% yield).

The spectral values were matched favourably with previously reported literature values.[6]

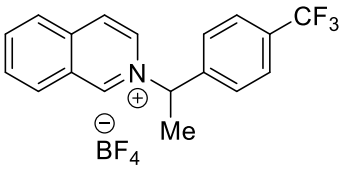
2-(1-(4-cyanophenyl)ethyl)isoquinolin-2-ium tetrafluoroborate (1ac)



The titled compound **1ac** was prepared by exactly following the general procedure **B (GP-B).** ***R**$_f$* (MeOH/DCM; 10:90) = 0.37. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM, obtained as a sticky liquid (0.48 g, 70% yield).

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.28 (s, 1H), 8.80 (d, *J* = 6.9 Hz, 1H), 8.61 - 8.53 (m, 2H), 8.36 (d, *J* = 8.3 Hz, 1H), 8.29 (t, *J* = 7.6 Hz, 1H), 8.11 (t, *J* = 7.6 Hz, 1H), 7.94 (d, *J* = 8.1 Hz, 2H), 7.75 (d, *J* = 8.0 Hz, 2H), 6.42 (q, *J* = 6.8 Hz, 1H), 2.16 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 149.3, 143.2, 137.4, 137.3, 133.5, 133.1, 131.4, 131.0, 128.5, 127.5, 127.3, 126.5, 118.3, 112.0, 68.7, 19.6. **FTIR (cm^{-1}):** 2958, 2921, 2854, 2230, 1724, 1639, 1508, 1460, 1268, 1030, 881, 753.
HRMS (ESI) *m/z* Calculated for $C_{18}H_{15}N_2$ $[M]^+$: 259.1230, found: 259.1228.

2-(1-(4-(trifluoromethyl)phenyl)ethyl)isoquinolin-2-ium tetrafluoroborate (1ad)



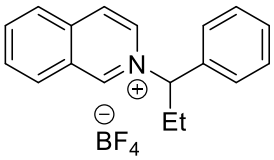
The titled compound **1ad** was prepared by exactly following the general procedure **B (GP-B).** ***R**$_f$* (MeOH/DCM; 10:90) = 0.44. The title compound was isolated via flash column chromatography using 2-3% MeOH/DCM, obtained as a sticky liquid (0.50 g, 64% yield).

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.31 (s, 1H), 8.83 (dd, *J* = 6.9, 1.4 Hz, 1H), 8.62 - 8.54 (m, 2H), 8.38 - 8.33 (m, 1H), 8.29 (td, *J* = 7.6, 1.0 Hz, 1H), 8.15 - 8.09 (m, 1H), 7.85 - 7.77 (m, 4H), 6.44 (q, *J* = 6.9 Hz, 1H), 2.19 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 149.3, 142.6, 137.4, 137.3, 133.6, 131.4, 130.9, 129.6 (q, *J* = 32.04 Hz), 128.4, 127.5, 127.3, 126.5, 126.0 (q, *J* = 3.81 Hz), 123.9

(q, *J* = 272.4 Hz), 68.7, 19.8. **FTIR (cm^{-1}):** 2995, 2795, 2726, 1645, 1468, 1406, 1324, 1070, 886, 842, 709, 760.

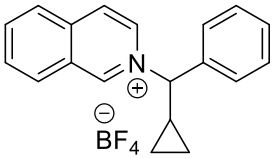
HRMS (ESI) *m/z* Calculated for $C_{18}H_{15}NF_3$ $[M]^+$: 302.1151, found: 302.1149.

2-(1-phenylpropyl)isoquinolin-2-ium tetrafluoroborate (1ae)



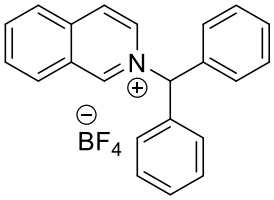
The titled compound **1ae** was used from the library of salts used in our previous report.[6]

2-(cyclopropyl(phenyl)methyl)isoquinolin-2-ium tetrafluoroborate (1af)



The titled compound **1af** was used from the library of salts used in our previous report.[6]

2-benzhydrylisoquinolin-2-ium tetrafluoroborate (1ag)

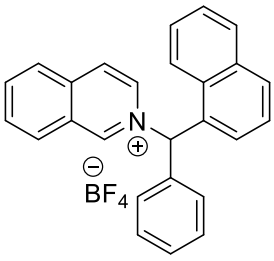


The titled compound **1ag** was prepared by exactly following the general procedure **B (GP-B).** R_f (MeOH/DCM; 10:90) = 0.46. The title compound was isolated via flash column chromatography using 4-5% MeOH/DCM, obtained as a white solid (0.73 g, 95% yield). MP = 179.2 – 185.3 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.18 (s, 1H), 8.82 (dd, *J* = 6.9, 1.5 Hz, 1H), 8.67 (d, *J* = 7.0 Hz, 1H), 8.61 (d, *J* = 8.3 Hz, 1H), 8.43 (d, *J* = 8.1 Hz, 1H), 8.32 (ddd, *J* = 8.3, 7.1, 1.1 Hz, 1H), 8.10 (ddd, *J* = 8.2, 7.1, 1.0 Hz, 1H), 7.91 (s, 1H), 7.57 - 7.46 (m, 6H), 7.45 - 7.37 (m, 4H). **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 149.8, 137.5, 137.5, 136.0, 134.5, 131.3, 131.2, 129.4, 129.3, 128.9, 127.4, 127.3, 126.5, 75.9. **FTIR (cm^{-1}):** 3059, 2970, 2923, 2859, 1640, 1498, 1455, 1399, 1285, 1063, 873, 755.

HRMS (ESI) *m/z* Calculated for $C_{22}H_{18}N$ $[M]^+$: 296.1434, found: 296.1436.

2-(naphthalen-1-yl(phenyl)methyl)isoquinolin-2-ium tetrafluoroborate (1ah)



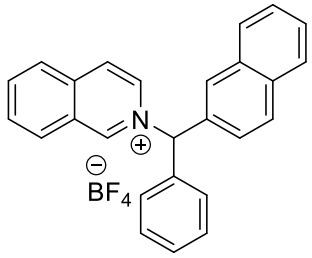
The titled compound **1ah** was prepared by exactly following the general procedure **B (GP-B).** R_f (MeOH/DCM; 10:90) = 0.53. The title compound was isolated via flash column chromatography using 2-3% MeOH/DCM, obtained as a yellow solid (0.56 g, 65% yield). MP = 183.5 – 186.7 °C.

^{1}H NMR (400 MHz, CDCl$_3$) δ 9.84 (s, 1H), 8.40 - 8.35 (m, 2H), 8.31 - 8.25 (m, 2H), 8.13 – 8.09 (m, 1H), 8.06 (t, *J* = 7.6 Hz, 1H), 7.97 (d, *J* = 7.9 Hz,

1H), 7.91 (d, *J* = 8.3 Hz, 1H), 7.88 - 7.81 (m, 2H), 7.45 - 7.36 (m, 6H), 7.33 - 7.28 (m, 2H), 6.90 (d, *J* = 7.3 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.8, 137.9, 137.8, 135.3, 134.0, 133.5, 131.7, 131.4, 131.1, 131.0, 130.5, 130.0, 129.7, 129.0, 129.0, 128.2, 127.8, 127.4, 127.3, 126.8, 126.4, 125.0, 123.0, 74.9. **FTIR (cm^{-1}):** 3063, 2961, 2925, 2856, 1666, 1641, 1460, 1399, 1286, 1060, 876, 789.

HRMS (ESI) *m/z* Calculated for $C_{26}H_{20}N$ $[M]^+$: 346.1590, found: 346.1584.

2-(naphthalen-2-yl(phenyl)methyl)isoquinolin-2-ium tetrafluoroborate (1ai)

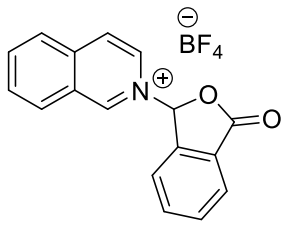


The titled compound **1ai** was prepared by exactly following the general procedure **B (GP-B).** R_f (MeOH/DCM; 10:90) = 0.50. The title compound was isolated via flash column chromatography using 2-3% MeOH/DCM, obtained as a sticky liquid (0.59 g, 68% yield). MP = 91.5 – 92.6 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.91 (s, 1H), 8.42 - 8.35 (m, 2H), 8.28 (d, *J* = 7.0 Hz, 1H), 8.13 - 8.04 (m, 2H), 7.88 - 7.82 (m, 3H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.71 (s, 1H), 7.53 - 7.43 (m, 2H), 7.42 - 7.37 (m, 4H), 7.36 - 7.30 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 149.8, 137.8, 135.2, 133.4, 133.2, 133.0, 132.6, 131.7, 131.4, 129.9, 129.7, 129.7, 128.9, 128.9, 128.5, 127.7, 127.7, 127.6, 127.3, 127.1, 126.4, 125.4, 77.7. **FTIR (cm^{-1}):** 3061, 2921, 2854, 1728, 1639, 1503, 1459, 1395, 1270, 1057, 879, 734.

HRMS (ESI) *m/z* Calculated for $C_{26}H_{20}N$ $[M]^+$: 346.1590, found: 346.1585.

2-(3-oxo-1,3-dihydroisobenzofuran-1-yl)isoquinolin-2-ium tetrafluoroborate (1aj)

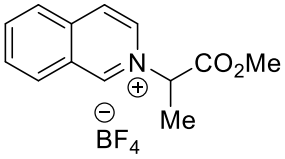


In a flame dried 50 mL round bottom flask with a magnetic bar, starting material Isoquinoline (2 mmol, 1 equiv.) was charged and anhydrous acetone 10 mL was added by syringe at room temperature under a stream of Ar atmosphere. To this solution 3-bromoisobenzofuran-1(3H)-one (3 mmol, 1.5 equiv.) was added. Subsequently, the cap was opened and solid sodium tetrafluroborate was added quickly in one portion. Reaction mixture was allowed to stir at ambient temperature till completion of reaction. Upon complete consumption of starting material (monitored by TLC), the precipitate was removed through filtration. The filtrate solvent was removed under reduced pressure obtained as a white solid (0.59 g, 85% yield). R_f (MeOH/DCM; 10:90) = 0.36. MP = 218.5 – 220.5 °C (becomes red at 195 °C).

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.56 (s, 1H), 8.86 (dd, *J* = 6.9, 1.6 Hz, 1H), 8.69 (d, *J* = 6.9 Hz, 1H), 8.65 (d, *J* = 8.4 Hz, 1H), 8.45 (d, *J* = 8.1 Hz, 1H), 8.38 (ddd, *J* = 8.2, 7.0, 1.1 Hz, 1H), 8.31 (s, 1H), 8.21 - 8.13 (m, 2H), 7.98 - 7.94 (m, 2H), 7.94 - 7.87 (m, 1H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 166.8, 150.4, 142.6, 138.5, 138.4, 135.9, 132.5, 131.7, 131.6, 131.6, 127.5, 126.9, 126.5, 126.0, 125.8,

124.8, 92.0. **FTIR (cm^{-1}):** 2956, 2921, 2854, 1784, 1638, 1517, 1464, 1409, 1284, 1050, 975, 816. **HRMS** (ESI) *m/z* Calculated for $C_{17}H_{12}O_2N$ $[M]^+$: 262.0863, found 262.0870.

2-(1-methoxy-1-oxopropan-2-yl)isoquinolin-2-ium tetrafluoroborate (1ak)

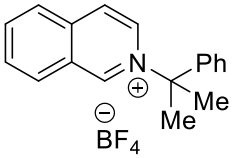


The titled compound **1ak** was prepared by exactly following the general procedure **A (GP-A).** $\mathbf{R_f}$ (MeOH/DCM = 10:90) = 0.47. The title compound was isolated via flash column chromatography using 3-4% MeOH/DCM obtained as white solid (0.49 g, 82% yield). MP = 96.2-97.8°C.

^{1}H NMR (400MHz, DMSO-d$_6$) δ = 10.16 (s, 1H), 8.88 (dd, *J* = 1.4, 6.9 Hz, 1H), 8.66 (d, *J* = 6.9 Hz, 1H), 8.56 (d, *J* = 8.3 Hz, 1H), 8.42 - 8.37 (m, 1H), 8.37 - 8.29 (m, 1H), 8.16 - 8.09 (m, 1H), 6.05 (q, *J* = 7.3 Hz, 1H), 3.79 (s, 3H), 2.04 (d, *J* = 7.4 Hz, 3H). **^{13}C NMR (100MHz, DMSO-d$_6$)** δ 168.9, 150.5, 137.7, 137.6, 134.8, 131.4, 130.8, 127.3, 127.0, 125.5, 67.2, 53.5, 40.1, 39.9, 39.7, 39.3, 39.1, 38.9, 17.3. **FTIR (cm^{-1}):** 3134, 3069, 3010, 2960, 1749, 1646, 1458, 1399, 1234, 1036, 827, 729.

HRMS (ESI) *m/z* Calculated for $C_{13}H_{14}O_2N$ $[M]^+$: 216.1019, found: 216.1020.

2-(2-phenylpropan-2-yl)isoquinolin-2-ium tetrafluoroborate (1al)



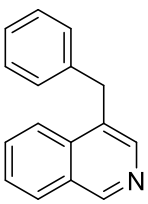
The titled compound **1al** was prepared by exactly following the general procedure **B (GP-B).** $\boldsymbol{R_f}$ (MeOH/DCM; 10:90) = 0.41. The title compound was isolated via flash column chromatography using 4-5% MeOH/DCM, obtained as a brown solid (0.46 g, 69% yield). MP = 127.2 – 127.6 °C.

^{1}H NMR (400 MHz, DMSO-*d$_6$*) δ 10.29 (s, 1H), 8.70 (d, *J* = 8.3 Hz, 1H), 8.54 - 8.49 (m, 1H), 8.49 – 8.44 (m, 1H), 8.37 - 8.27 (m, 2H), 8.13 (t, *J* = 7.5 Hz, 1H), 7.48 - 7.37 (m, 5H), 2.24 (s, 6H). **^{13}C NMR (100 MHz, DMSO-*d$_6$*)** δ 148.3, 143.0, 137.3, 136.7, 133.5, 131.5, 131.1, 129.0, 128.6, 127.0, 127.0, 126.0, 125.6, 73.7, 28.8. **FTIR (cm^{-1}):** 3062, 2993, 2917, 2850, 1732, 1641, 1469, 1448, 1261, 1054, 880, 737.

HRMS (ESI) *m/z* Calculated for $C_{18}H_{18}N$ $[M]^+$: 248.1434, found: 248.1441.

11b. Compound Characterization Data for *meta*-Alkylated Isoquinoline:

4-benzylisoquinoline (4a)

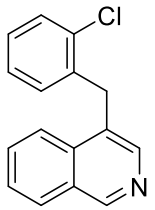


The titled compound **4a** was prepared by exactly following the general procedure **D (GP-D).** $\boldsymbol{R_f}$ (Ethyl acetate/Pet. ether; 30:70) = 0.34. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. ether, obtained as a white solid (26 mg, 60% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.18 (s, 1H), 8.42 (s, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.3 Hz, 1H), 7.63 (t, *J* = 7.3 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H) 7.29 - 7.22 (m, 2H), 7.22 – 7.15 (m, 3H), 4.38 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.9, 143.7, 139.7, 134.8, 130.4, 129.6, 128.5, 128.5, 128.2, 126.9, 126.3, 123.4, 36.2.

The spectral data match the previously reported structure. [16]

4-(2-chlorobenzyl)isoquinoline (4b)



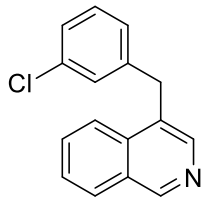
The titled compound **4b** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.35. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. ether, obtained as a white solid (35 mg, 69% yield). MP = 55.5 – 56.8 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.32 (s, 1H), 8.01 (d, *J* = 8.1 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.68 (td, *J* = 7.6, 1.3 Hz, 1H), 7.63 - 7.58 (m, 1H), 7.46 - 7.42 (m, 1H), 7.20 - 7.14 (m, 1H), 7.10 - 7.05 (m, 1H), 6.90 - 6.84 (m, 1H) 4.48 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 152.0, 143.5, 137.0, 134.8, 133.9, 130.7, 130.3, 129.5, 128.6, 128.4, 128.3, 127.8, 127.1, 126.9, 123.2, 33.4.

FTIR (cm^{-1}): 3057, 3024, 2923, 2854, 1725, 1623, 1472, 1439, 1387, 1041, 747, 624.

HRMS (ESI) *m/z* Calculated for $C_{16}H_{13}NCl$ $[M+H]^+$: 254.0731, found: 254.0738.

4-(3-chlorobenzyl)isoquinoline (4c)

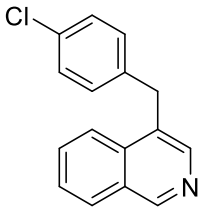


The titled compound **4c** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.35. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. ether, obtained as a white solid (36 mg, 70% yield). MP = 82.5 – 84.4 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.41 (s, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.3 Hz, 1H), 7.69 - 7.64 (m, 1H), 7.62 - 7.57 (m, 1H), 7.22 - 7.16 (m, 3H), 7.09 - 7.05 (m, 1H), 4.36 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 152.3, 143.7, 141.8, 134.7, 134.5, 130.6, 129.8, 128.8, 128.6, 128.6, 128.4, 127.1, 126.7, 126.6, 123.2, 35.9. **FTIR (cm^{-1})**: 3058, 2924, 2854, 1709, 1629, 1472, 1434, 1388, 1028, 781, 624.

HRMS (ESI) *m/z* Calculated for $C_{16}H_{13}NCl$ $[M+H]^+$: 254.0731, found: 254.0737.

4-(4-chlorobenzyl)isoquinoline (4d)

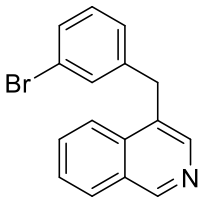


The titled compound **4d** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.36. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. ether, obtained as a white solid (34 mg, 67% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (s, 1H), 8.40 (s, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.84 (d, *J* = 8.5 Hz, 1H), 7.68 - 7.62 (m, 1H), 7.62 - 7.57 (m, 1H), 7.25 - 7.20 (m, 2H), 7.15 – 7.09 (m, 2H), 4.35 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 152.0, 143.4, 138.1, 134.8, 132.2, 130.7, 129.8, 129.3, 128.7, 128.6, 128.4, 127.2, 123.3, 35.6.

The spectral data match the previously reported structure. [16]

4-(3-bromobenzyl)isoquinoline (4e)

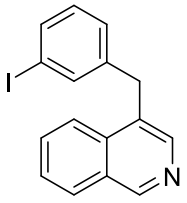


The titled compound **4e** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.37. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. Ether, obtained as a white solid (39 mg, 65% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.41 (s, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.69 - 7.64 (m, 1H), 7.62 - 7.57 (m, 1H), 7.36 (s, 1H) 7.33 (dt, *J* = 6.9, 2.0 Hz, 1H), 7.16 - 7.08 (m, 2H), 4.35 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 152.2, 143.7, 142.0, 134.7, 131.5, 130.6, 130.1, 129.6, 128.8, 128.6, 128.4, 127.1, 123.2, 122.7, 35.9.

The spectral data match the previously reported structure. [17]

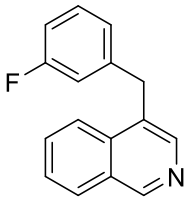
4-(3-iodobenzyl)isoquinoline (4f)



The titled compound **4f** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.36. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. Ether, obtained as a sticky liquid (46 mg, 67% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.21 (s, 1H), 8.40 (s, 1H), 8.00 (d, *J* = 7.9 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.70 - 7.65 (m, 1H), 7.61 (d, *J* = 7.9 Hz, 1H), 7.58 (s, 1H), 7.53 (d, *J* = 7.9 Hz, 1H), 7.13 (d, *J* = 7.8 Hz, 1H), 6.99 (t, *J* = 7.8 Hz, 1H), 4.33 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 152.2, 143.7, 142.1, 137.4, 135.5, 134.7, 130.6, 130.3, 128.4, 127.8, 127.1, 123.2, 94.7, 35.8. **FTIR (cm^{-1}):** 3055, 3033, 2923, 2858, 1626, 1498, 1449, 1386, 1029, 787, 750, 624.

HRMS (ESI) *m/z* Calculated for $C_{16}H_{13}NI$ $[M+H]^+$: 346.0087, found: 346.0094.

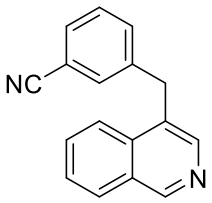
4-(3-fluorobenzyl)isoquinoline (4g)



The titled compound **4g** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.37. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. Ether, obtained as a white solid (32 mg, 68% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.41 (s, 1H), 7.99 (d, *J* = 8.3 Hz, 1H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.65 (td, *J* = 7.6, 1.4 Hz, 1H), 7.61 - 7.56 (m, 1H), 7.25 - 7.19 (m, 1H), 6.98 (d, *J* = 7.5, Hz, 1H), 6.92 - 6.84 (m, 2H), 4.37 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 163.0 (d, *J* = 246.4 Hz), 152.2, 143.7, 142.3 (d, *J* = 6.9 Hz), 134.7, 130.5, 130.0 (d, *J* = 8.4 Hz), 128.9, 128.6, 128.3, 127.1, 124.2 (d, *J* = 2.3 Hz), 123.3, 115.4 (d, *J* = 21.4 Hz), 113.3 (d, *J* = 21.4 Hz), 35.9 (d, *J* = 1.5 Hz). The spectral data match the previously reported structure. [16]

3-(isoquinolin-4-ylmethyl)benzonitrile (4h)

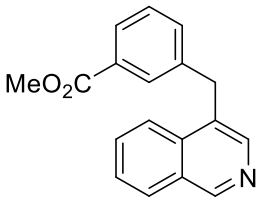


The titled compound **4h** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 50:50) = 0.40. The title compound was isolated via flash column chromatography using 35-40% Ethyl acetate/Pet. Ether, obtained as a yellow solid (35 mg, 71% yield). MP = 116.3 – 118.8 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.23 (s, 1H), 8.41 (s, 1H), 8.03 (d, *J* = 7.6 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.71 - 7.66 (m, 1H), 7.65 - 7.60 (m, 1H), 7.52 - 7.48 (m, 1H), 7.48 - 7.46 (m, 1H), 7.45 - 7.42 (m, 1H), 7.40 - 7.35 (m, 1H), 4.42 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 152.5, 143.8, 141.2, 134.5, 132.9, 131.9, 130.8, 130.2, 129.4, 128.6, 128.5, 128.1, 127.3, 122.9, 118.7, 112.7, 35.7. **FTIR (cm^{-1}):** 3056, 2926, 2853, 2229, 1724, 1622, 1483, 1435, 1388, 1022, 785, 688.

HRMS (ESI) *m/z* Calculated for $C_{17}H_{13}N_2$ $[M+H]^+$: 245.1073, found: 245.1079.

methyl 3-(isoquinolin-4-ylmethyl)benzoate (4i)

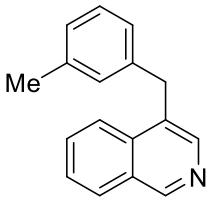


The titled compound **4i** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 50:50) = 0.37. The title compound was isolated via flash column chromatography using 35-40% Ethyl acetate/Pet. Ether, obtained as a sticky solid (40 mg, 72% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.42 (s, 1H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.95 (s, 1H), 7.91 - 7.85 (m, 2H), 7.68 - 7.63 (m, 1H), 7.61 - 7.56 (m, 1H), 7.37 - 7.30 (m, 2H), 4.43 (s, 2H), 3.88 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 167.0, 152.2, 143.7, 140.1, 134.7, 133.0 130.6, 130.5, 129.6, 129.1, 128.7, 128.6, 128.3, 127.7, 127.0, 123.2, 52.1, 36.1. **FTIR (cm^{-1}):** 3056, 3031, 2951, 2851, 1720, 1623, 1487, 1437, 1199, 1021, 781, 689.

HRMS (ESI) *m/z* Calculated for $C_{18}H_{16}O_2N$ $[M+H]^+$: 278.1176, found: 278.1172.

4-(3-methylbenzyl)isoquinoline (4j)

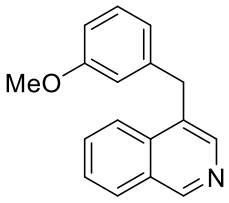


The titled compound **4j** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.37. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. Ether, obtained as a sticky solid (27 mg, 57% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.18 (s, 1H), 8.41 (s, 1H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.93 (d, *J* = 8.3 Hz, 1H), 7.65 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.61 - 7.55 (m, 1H), 7.18 - 7.13 (m, 1H), 7.03 – 6.97 (m, 3H), 4.35 (s, 2H), 2.28 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.8, 143.6, 139.6, 138.2, 134.9, 130.4, 129.9, 129.3, 128.6, 128.4, 128.3, 127.1, 127.0, 125.6, 123.5, 36.2, 21.4. **FTIR (cm^{-1}):** 3019, 2922, 2856, 1724, 1615, 1496, 1451, 1386, 1031, 953, 757, 624.

HRMS (ESI) *m/z* Calculated for $C_{17}H_{16}N$ $[M+H]^+$: 234.1277, found: 234.1274.

4-(3-methoxybenzyl)isoquinoline (4k)

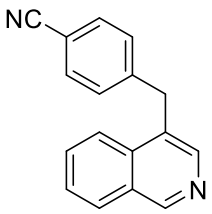


The titled compound **4k** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.25. The title compound was isolated via flash column chromatography using 20-25% Ethyl acetate/Pet. Ether, obtained as a sticky liquid (26 mg, 52% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (s, 1H), 8.42 (s, 1H), 7.99 (d, *J* = 7.9 Hz, 1H), 7.92 (d, *J* = 8.5 Hz, 1H), 7.65 (ddd, *J* = 8.4, 7.0, 1.3 Hz, 1H), 7.61 - 7.56 (m, 1H), 7.18 (dd, *J* = 8.9, 7.8 Hz, 1H), 6.79 (d, *J* = 7.6 Hz, 1H), 6.75 - 6.72 (m, 2H), 4.36 (s, 2H) 3.73 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.8, 151.9, 143.5, 141.3, 134.9, 130.5, 129.6, 129.5, 128.6, 128.3, 127.0, 123.5, 121.0, 114.5, 111.4, 55.1, 36.3.

The spectral data match the previously reported structure. [17]

4-(isoquinolin-4-ylmethyl)benzonitrile (4l)



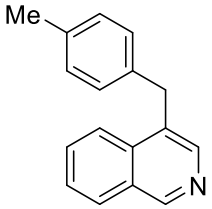
The titled compound **4l** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 50:50) = 0.41. The title compound was isolated via flash column chromatography using 35-40% Ethyl acetate/Pet. Ether, obtained as a white solid (31 mg, 63% yield). MP = 102.6 – 104.4 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.22 (s, 1H), 8.42 (s, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.67 (td, *J* = 7.60, 1.3 Hz, 1H), 7.64 - 7.59 (m, 1H), 7.56 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 4.45 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 152.5, 145.3, 143.8, 134.5, 132.4,

130.8, 129.2, 128.6, 128.5, 128.1, 127.3, 123.0, 118.7, 110.4, 36.3. **FTIR (cm^{-1}):** 3057, 3008, 2924, 2855, 2227, 1614, 1503, 1389, 1261, 1062, 853, 787.

HRMS (ESI) *m/z* Calculated for $C_{17}H_{13}N_2$ $[M+H]^+$: 245.1073, found: 245.1070.

4-(4-methylbenzyl)isoquinoline (4m)

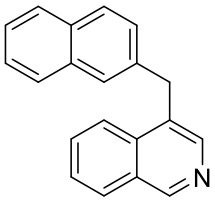


The titled compound **4m** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.37. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. Ether, obtained as a white solid (11 mg, 24% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (br. s., 1H), 8.42 (br. s., 1H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.65 (ddd, *J* = 8.4, 7.0, 1.3 Hz, 1H), 7.61 - 7.55 (m, 1H), 7.10 - 7.05 (m, 4H), 4.35 (s, 2H), 2.29 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.8, 143.5, 136.6, 135.9, 134.9, 130.4, 129.3, 128.4, 128.3, 127.0, 123.5, 35.8, 21.0.

The spectral data match the previously reported structure. [16]

4-(naphthalen-2-ylmethyl)isoquinoline (4n)

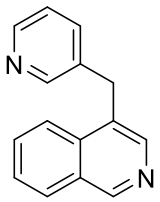


The titled compound **4n** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.31. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. Ether, obtained as a white solid (37 mg, 68% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (s, 1H), 8.39 (s, 1H), 7.89 (d, *J* = 7.9 Hz, 1H), 7.85 (d, *J* = 8.3 Hz, 1H), 7.70 - 7.64 (m, 2H), 7.62 - 7.58 (m, 1H), 7.53 - 7.44 (m, 3H), 7.35 – 7.29 (m, 2H), 7.26 (d, *J* = 8.4 Hz, 1H), 4.44 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 152.0, 143.8, 137.2, 134.9, 133.5, 132.1, 130.4, 129.5, 128.6, 128.2, 128.2, 127.6, 127.5, 126.9, 126.8, 126.1, 125.5, 123.5, 36.4.

The spectral data match the previously reported structure. [17]

4-(pyridin-3-ylmethyl)isoquinoline (4o)



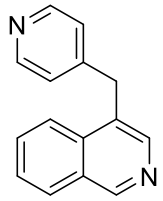
The titled compound **4o** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate) = 0.21. The title compound was isolated via flash column chromatography using 3-5% Methanol/Ethyl acetate, obtained as a sticky liquid (25 mg, 57% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.62 - 8.56 (m, 1H), 8.46 (d, *J* = 3.6 Hz, 1H), 8.43 (s, 1H), 8.01 (d, *J* = 7.9 Hz, 1H), 7.90 - 7.83 (m, 1H), 7.71 - 7.65 (m, 1H), 7.64 - 7.57 (m, 1H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.17 (dd, *J* = 7.8, 4.8 Hz, 1H), 4.39 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)**

δ 152.4, 149.9, 147.9, 143.7, 135.9, 135.2, 134.5, 130.7, 128.6, 128.4, 127.2, 123.5, 123.1, 33.5. **FTIR (cm^{-1}):** 2926, 2857, 1724, 1665, 1624, 1472, 1428, 1229, 1029, 754, 625.

HRMS (ESI) *m/z* Calculated for $C_{15}H_{13}N_2$ $[M+H]^+$: 221.1073, found: 221.1072.

4-(pyridin-4-ylmethyl)isoquinoline (4p)



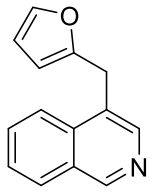
The titled compound **4p** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate) = 0.21. The title compound was isolated via flash column chromatography using 3-5% Methanol/Ethyl acetate, obtained as a white solid (24 mg, 55% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.23 (s, 1H), 8.48 (d, *J* = 5.6 Hz, 2H), 8.44 (s, 1H), 8.02 (d, *J* = 7.6 Hz, 1H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.70 - 7.57 (m, 2H), 7.11 (d, *J* = 5.8 Hz, 2H), 4.38 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 152.5, 149.9, 148.8, 143.8, 134.5, 130.7, 128.6, 128.4, 127.7, 127.2, 123.7, 123.0, 35.6.

The spectral data match the previously reported structure. [17]

.

4-(furan-2-ylmethyl)isoquinoline (4q)

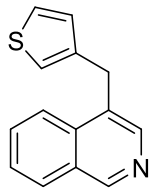


The titled compound **4q** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.36. The title compound was isolated via flash column chromatography using 15-18% Ethyl acetate/Pet. ether, obtained as a sticky liquid (14 mg, 33% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (s, 1H), 8.42 (s, 1H), 8.00 (d, *J* = 8.4 Hz, 2H), 7.72 (td, *J* = 7.7, 1.3 Hz, 1H), 7.64 - 7.59 (m, 1H), 7.35 - 7.30 (m, 1H), 6.27 (dd, *J* = 3.1, 1.9 Hz, 1H), 5.93 (d, *J* = 3.1 Hz, 1H), 4.37 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 153.1, 152.0, 143.0, 141.5, 134.8, 130.7, 128.5, 128.3, 127.6, 127.2, 123.2, 110.4, 106.8, 29.2.

The spectral data match the previously reported structure. [18]

4-(thiophen-3-ylmethyl)isoquinoline (4r)



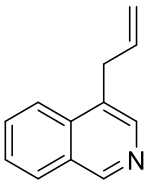
The titled compound **4r** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.35. The title compound was isolated via flash column chromatography using 15-18% Ethyl acetate/Pet. ether, obtained as a sticky liquid (16 mg, 35% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.43 (s, 1H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.95 (d, *J* = 8.5 Hz, 1H), 7.69 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H), 7.63 - 7.58 (m, 1H), 7.26 - 7.24 (m, 1H), 6.94 (dd, *J* = 4.9, 1.2

Hz, 1H), 6.87 (dd, *J* = 2.9, 1.1 Hz, 1H), 4.38 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.9, 143.2, 140.1, 134.8, 130.5, 129.6, 128.5, 128.3, 128.1, 127.0, 125.8, 123.3, 121.5, 31.1.

The spectral data match the previously reported structure. [16]

4-allylisoquinoline (4s)

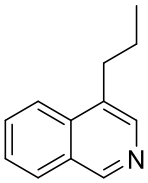


The titled compound **4s** was prepared by exactly following the general procedure **D (GP-D).** ***R*$_f$** (Ethyl acetate/Pet. ether; 20:80) = 0.43. The title compound was isolated via flash column chromatography using 15-18% Ethyl acetate/Pet. Ether, obtained as a colourless liquid (16 mg, 46% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.16 (s, 1H), 8.39 (s, 1H), 7.99 (d, *J* = 8.3 Hz, 2H), 7.72 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H), 7.64 - 7.57 (m, 1H), 6.09 (ddt, *J* = 16.9, 10.4, 6.3, 6.3 Hz, 1H), 5.18 - 5.05 (m, 2H), 3.79 (d, *J* = 6.1 Hz, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.6, 142.9, 136.0, 134.8, 130.3, 129.1, 128.4, 128.2, 126.9, 123.2, 116.8, 34.3.

The spectral data match the previously reported structure. [19]

4-propylisoquinoline (4t)

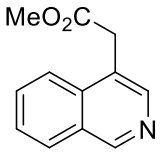


The titled compound **4t** was prepared from **4s** (0.1 mmol) by exactly following the literature known procedure.[20] ***R*$_f$** (Ethyl acetate/Pet. ether; 20:80) = 0.44. The title compound was isolated via flash column chromatography using 15-18% Ethyl acetate/Pet. Ether, obtained as a colourless liquid (7 mg, 42% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.13 (s, 1H), 8.38 (s, 1H), 7.99 (t, *J* = 9.2 Hz, 2H), 7.73 (t, *J* = 7.6 Hz, 1H), 7.66 - 7.54 (m, 1H), 3.00 (t, *J* = 7.5 Hz, 2H), 1.82 - 1.76 (m, 2H), 1.03 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.1, 142.6, 134.8, 130.1, 128.3, 126.7, 123.0, 32.1, 23.7, 14.1. **FTIR (cm^{-1}):** 3020, 2954, 2928, 2866, 1623, 1580, 1458, 1385, 1262, 1024, 906, 745.

HRMS (ESI) *m/z* Calculated for $C_{12}H_{14}N$ $[M+H]^+$: 172.1121, found: 172.1119.

methyl 2-(isoquinolin-4-yl)acetate (4u)

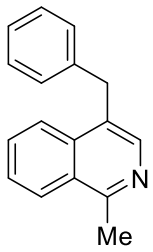


The titled compound **4u** was prepared by exactly following the general procedure **D (GP-D).** ***R*$_f$** (Ethyl acetate/Pet. ether; 50:50) = 0.25. The title compound was isolated via flash column chromatography using 35-40% Ethyl acetate/Pet. ether, obtained as a sticky liquid (23 mg, 58% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.22 (s, 1H), 8.45 (s, 1H), 8.02 (d, *J* = 8.1 Hz, 1H), 7.98 (d, *J* = 8.3 Hz, 1H), 7.78 (ddd, *J* = 8.4, 7.00, 1.4 Hz, 1H), 7.68 - 7.63 (m, 1H), 4.04 (s, 2H), 3.70 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 171.2, 152.4, 143.7, 134.9, 131.0, 128.4, 128.4, 127.4, 124.3, 123.0, 52.3, 36.1. **FTIR (cm^{-1}):** 3001, 2954, 2924, 2853, 1736, 1624, 1436, 1391, 1268, 1056, 885, 771.

HRMS (ESI) *m/z* Calculated for $C_{12}H_{12}O_2N$ $[M+H]^+$: 202.0863, found: 202.0862.

4-benzyl-1-methylisoquinoline (4v)

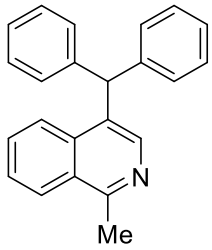


The titled compound **4v** was prepared by exactly following the general procedure **D (GP-D)** with 72 h reaction time in light. R_f (Ethyl acetate/Pet. ether; 30:70) = 0.25. The title compound was isolated via flash column chromatography using 15-16% Ethyl acetate/Pet. ether, obtained as a sticky liquid (19 mg, 41% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 8.14 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.1 Hz, 1H), 7.64 - 7.54 (m, 2H), 7.28 - 7.22 (m, 2H), 7.22 - 7.16 (m, 3H), 4.35 (s, 2H), 2.97 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.8, 142.4, 140.0, 135.0, 129.9, 128.5, 128.4, 128.0, 127.4, 126.6, 126.2, 126.2, 124.2, 36.2, 22.4. **FTIR (cm^{-1}):** 3062, 2956, 2924, 1602, 1450 1390, 1185, 1032, 957, 835, 765, 729.

HRMS (ESI) *m/z* Calculated for $C_{17}H_{16}N$ $[M+H]^+$: 234.1277, found: 234.1282.

4-benzhydryl-1-methylisoquinoline (4w)

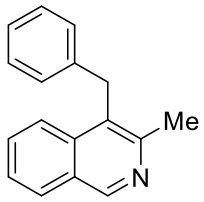


The titled compound **4w** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.33. The title compound was isolated via flash column chromatography using 3-5% Methanol/Ethyl acetate, obtained as a white solid (34 mg, 55% yield). MP = 148.4 – 150.2 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 - 8.19 (m, 1H), 7.91 (d, *J* = 7.9 Hz, 1H), 7.83 (s, 1H), 7.62 - 7.52 (m, 2H), 7.32 - 7.19 (m, 6H), 7.13 (d, *J* = 7.3 Hz, 4H), 6.12 (s, 1H), 2.95 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 157.7, 143.0, 142.7, 134.7, 131.4, 130.1, 129.5, 128.5, 127.2, 126.6, 126.5, 126.2, 124.0, 51.3, 22.4. **FTIR (cm^{-1}):** 3060, 3026, 2924, 2853, 1660, 1586, 1494, 1390, 1255, 1030, 963, 734.

HRMS (ESI) *m/z* Calculated for $C_{23}H_{20}N$ $[M+H]^+$: 310.1590, found: 310.1597.

4-benzyl-3-methylisoquinoline (4x)



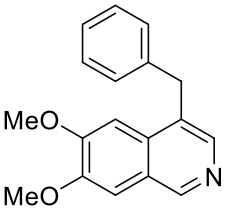
The titled compound **4x** was prepared by exactly following the general procedure **D (GP-D)** with 72 h reaction time in light. R_f (Ethyl acetate/Pet. ether; 30:70) = 0.25. The title compound was isolated via flash column chromatography using 3-5% Methanol/Ethyl acetate, obtained as a sticky liquid (14 mg, 30% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.16 (s, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.90 (d, *J* = 8.5 Hz, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.23 (d, *J* = 7.5 Hz, 2H), 7.18 (d, *J* = 7.1 Hz, 1H), 7.07 (d, *J* = 7.3 Hz, 2H), 4.46 (s, 2H), 2.71 (s, 3H). 1.47 - 0.75 (some unknown solvent impurity)

HRMS (ESI) *m/z* Calculated for $C_{17}H_{16}N$ $[M+H]^+$: 234.1277, found: 234.1282.

The spectral data match the previously reported structure. [21]

4-benzyl-6,7-dimethoxyisoquinoline (4y)

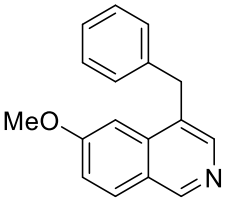


The titled compound **4y** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 50:50) = 0.33. The title compound was isolated via flash column chromatography using 30-35% Ethyl acetate/Pet. Ether, obtained as a sticky solid (35 mg, 63% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.98 (s, 1H), 8.30 (s, 1H), 7.29 - 7.24 (m, 2H), 7.23 - 7.16 (m, 4H), 7.07 (s, 1H), 4.32 (s, 2H), 4.01 (s, 3H), 3.85 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 152.9, 150.0, 149.0, 142.1, 139.7, 131.6, 128.7, 128.6, 128.5, 126.4, 124.8, 105.9, 102.2, 56.0, 55.9, 36.8.

The spectral data match the previously reported structure. [16]

4-benzyl-6-methoxyisoquinoline (4z)

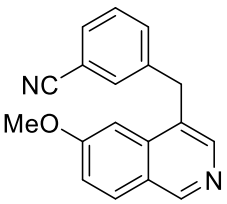


The titled compound **4z** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 50:50) = 0.37. The title compound was isolated via flash column chromatography using 30-35% Ethyl acetate/Pet. Ether, obtained as a sticky solid (27 mg, 55% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.04 (s, 1H), 8.35 (s, 1H), 7.87 (d, *J* = 8.9 Hz, 1H), 7.30 - 7.25 (m, 2H), 7.23 - 7.17 (m, 4H), 7.08 (d, *J* = 2.4 Hz, 1H), 4.33 (s, 2H), 3.80 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.9, 150.9, 143.9, 139.6, 136.8, 130.0, 128.9, 128.6, 128.5, 126.4, 124.4, 119.7, 101.8, 55.3, 36.7. **FTIR (cm^{-1}):** 3062, 2957, 2928, 2853, 1725, 1623, 1498, 1405, 1269, 1029, 844, 756.

HRMS (ESI) *m/z* Calculated for $C_{17}H_{16}ON$ $[M+H]^+$: 250.1226, found: 250.1225.

3-((6-methoxyisoquinolin-4-yl)methyl)benzonitrile (4aa)



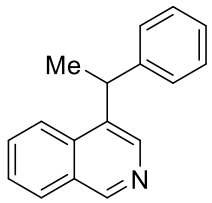
The titled compound **4aa** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 50:50) = 0.32. The title compound was isolated via flash column chromatography using 35-40% Ethyl acetate/Pet. Ether, obtained as a white solid (33 mg, 61% yield). MP = 96.3 – 97.9 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (s, 1H), 8.33 (s, 1H), 7.91 (d, *J* = 9.0 Hz, 1H), 7.52 - 7.47 (m, 2H), 7.47 – 7.43 (m, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.23 (dd, *J* = 9.0, 2.4 Hz, 1H), 6.95 (d, *J* = 2.0 Hz, 1H), 4.35 (s, 2H), 3.82 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.2, 151.5, 144.2, 141.2, 136.4, 132.9,

131.9, 130.3, 130.2, 129.4, 127.1, 124.3, 119.7, 118.6, 112.7, 101.4, 55.3, 36.0. **FTIR (cm^{-1}):** 3063, 3017, 2929, 2845, 2229, 1660, 1621, 1487, 1402, 1222, 1031, 772, 624.

HRMS (ESI) *m/z* Calculated for $C_{18}H_{15}ON_2$ $[M+H]^+$:275.1179, found: 275.1177.

4-(1-phenylethyl)isoquinoline (4ab)

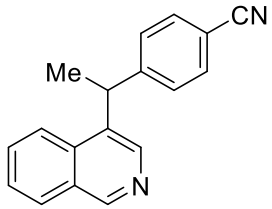


The titled compound **4ab** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.37. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. ether, obtained as a white solid (31 mg, 66% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.53 (s, 1H), 7.98 - 7.91 (m, 2H), 7.64 - 7.58 (m, 1H), 7.57 - 7.52 (m, 1H), 7.29 - 7.22 (m, 4H), 7.20 - 7.15 (m, 1H), 4.81 (q, *J* = 7.3 Hz, 1H), 1.81 (d, *J* = 7.3 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.6, 145.5, 141.1, 134.4, 134.3, 130.4, 128.6, 128.5, 128.4, 127.5, 126.7, 126.3, 123.2, 39.4, 22.0.

The spectral data match the previously reported structure. [22]

4-(1-(isoquinolin-4-yl)ethyl)benzonitrile (4ac)

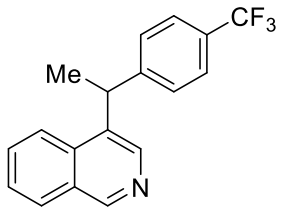


The titled compound **4ac** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 50:50) = 0.32. The title compound was isolated via flash column chromatography using 30-35% Ethyl acetate/Pet. ether, obtained as a sticky liquid (36 mg, 69% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.50 (s, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.66 - 7.61 (m, 1H), 7.61 - 7.53 (m, 3H), 7.34 (d, *J* = 8.1 Hz, 2H), 4.85 (q, *J* = 7.2 Hz, 1H), 1.83 (d, *J* = 7.3 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 152.3, 151.1, 141.4, 134.0, 132.7, 132.5, 130.7, 128.6, 128.5, 128.2, 127.0, 122.7, 118.7, 110.3, 39.5, 21.6. **FTIR (cm^{-1}):** 3062, 2969, 2928, 2871, 2226, 1616, 1453, 1386, 1255, 1023, 751, 624.

HRMS (ESI) *m/z* Calculated for $C_{18}H_{15}N_2$ $[M+H]^+$: 259.1230, found: 259.1229.

4-(1-(4-(trifluoromethyl)phenyl)ethyl)isoquinoline (4ad)



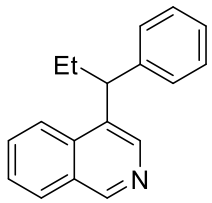
The titled compound **4ad** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.38. The title compound was isolated via flash column chromatography using 15-18% Ethyl acetate/Pet. ether, obtained as a sticky liquid (42 mg, 70% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.52 (s, 1H), 7.99 (d, *J* = 7.5 Hz, 1H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.66 - 7.61 (m, 1H), 7.60 - 7.55 (m, 1H), 7.52 (d, *J* = 8.1 Hz, 2H),

7.35 (d, *J* = 8.4 Hz, 2H), 4.86 (q, *J* = 7.3 Hz, 1H), 1.83 (d, *J* = 7.3 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 152.1, 149.7, 141.3, 134.2, 133.2, 130.6, 128.7 (q, *J* = 32.0 Hz), 128.5, 127.8, 126.9, 125.6 (q, *J* = 3.8 Hz), 124.1 (q, *J* = 271.6 Hz), 122.9, 39.3, 21.8. **FTIR (cm^{-1}):** 3057, 2973, 2934, 2884, 1619, 1455, 1408, 1324, 1068, 791, 750, 624.

HRMS (ESI) *m/z* Calculated for $C_{18}H_{15}NF_3$ $[M+H]^+$: 302.1151, found: 302.1146.

4-(1-phenylpropyl)isoquinoline (4ae)

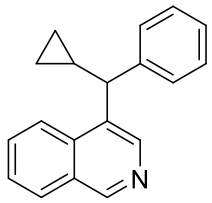


The titled compound **4ae** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.33. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. ether, obtained as a white solid (35 mg, 71% yield). MP = 93.3 – 95.4 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.15 (s, 1H), 8.58 (s, 1H), 8.03 (d, *J* = 8.5 Hz, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.66 - 7.61 (m, 1H), 7.56 - 7.52 (m, 1H), 7.31 - 7.23 (m, 4H), 7.18 - 7.13 (m, 1H), 4.48 (t, *J* = 7.6 Hz, 1H), 2.31 - 2.20 (m, 2H), 1.00 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.5, 144.0, 141.4, 134.7, 133.3, 130.3, 128.6, 128.5, 128.4, 128.0, 126.6, 126.3, 122.9, 47.0, 28.6, 12.8. **FTIR (cm^{-1}):** 3059, 3027, 2964, 2932, 2874, 1622, 1498, 1452, 1392, 1028, 751, 634.

HRMS (ESI) *m/z* Calculated for $C_{18}H_{18}N$ $[M+H]^+$: 248.1434, found: 248.1440.

4-(cyclopropyl(phenyl)methyl)isoquinoline (4af)

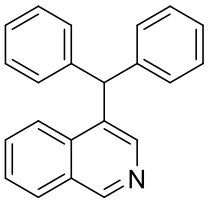


The titled compound **4af** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.32. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. ether, obtained as a white solid (34 mg, 65% yield). MP = 117.2 – 119.7 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.19 (s, 1H), 8.84 (s, 1H), 7.98 - 7.93 (m, 1H), 7.80 - 7.76 (m, 1H), 7.56 - 7.48 (m, 2H), 7.28 - 7.22 (m, 4H), 7.20 - 7.14 (m, 1H), 3.85 (d, *J* = 9.3 Hz, 1H), 1.62 - 1.52 (m, 1H), 0.84 - 0.76 (m, 1H), 0.74 - 0.66 (m, 1H), 0.51 (dq, *J* = 9.6, 4.9 Hz, 1H), 0.28 - 0.21 (m, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.8, 144.0, 142.4, 134.5, 133.3, 130.1, 128.6, 128.4, 128.3, 127.9, 126.6, 126.4, 123.4, 50.6, 16.7, 6.3, 5.0. **FTIR (cm^{-1}):** 3068, 3011, 2928, 2864, 1725, 1618, 1496, 1453, 1222, 1024, 749, 624.

HRMS (ESI) *m/z* Calculated for $C_{19}H_{18}N$ $[M+H]^+$: 260.1434, found: 260.1439.

4-benzhydrylisoquinoline (4ag)

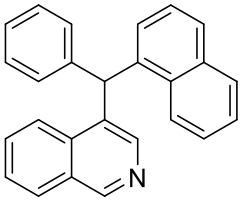


The titled compound **4ag** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.38. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. ether, obtained as a white solid (46 mg, 78% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.04 – 7.95 (m, 2H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.64 - 7.54 (m, 2H), 7.34 - 7.27 (m, 4H), 7.26 - 7.21 (m, 2H), 7.16 - 7.07 (m, 4H), 6.16 (s, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.9, 144.2, 142.5, 134.6, 133.0, 130.6, 129.5, 128.6, 128.4, 128.3, 126.8, 126.7, 123.4, 51.4.

The spectral data match the previously reported structure.[23]

4-(naphthalen-1-yl(phenyl)methyl)isoquinoline (4ah)

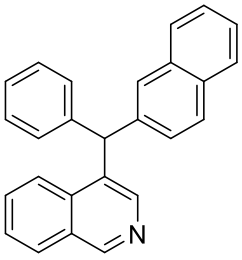


The titled compound **4ah** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.40. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. ether, obtained as a white solid (44.9 mg, 65% yield). MP = 204.6 – 206.8 °C (become red at 196.1 °C).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.18 (s, 1H), 8.03 – 7.98 (m, 1H), 7.96 - 7.91 (m, 2H), 7.91 - 7.82 (m, 2H), 7.77 (d, *J* = 8.3 Hz, 1H), 7.60 - 7.55 (m, 2H), 7.48 - 7.43 (m, 1H), 7.38 (td, *J* = 7.6, 1.3 Hz, 1H), 7.34 - 7.24 (m, 4H), 7.20 - 7.15 (m, 2H), 6.93 (d, *J* = 7.3 Hz, 1H), 6.84 (s, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 151.9, 144.2, 142.0, 138.5, 134.5, 134.1, 133.0, 131.5, 130.8, 129.7, 128.9, 128.7, 128.5, 128.4, 127.7, 127.0, 126.9, 126.4, 125.6, 125.3, 123.7, 123.3, 47.7. **FTIR (cm^{-1}):** 3058, 2927, 2859, 1722, 1628, 1590, 1451, 1388, 1219, 1071, 774, 624.

HRMS (ESI) *m/z* Calculated for $C_{26}H_{20}N$ $[M+H]^+$: 346.1590, found: 346.1593.

4-(naphthalen-2-yl(phenyl)methyl)isoquinoline (4ai)



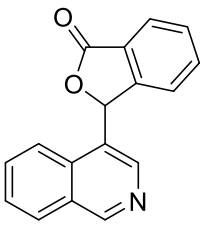
The titled compound **4ai** was prepared by exactly following the general procedure **D (GP-D).** R_f (Ethyl acetate/Pet. ether; 30:70) = 0.29. The title compound was isolated via flash column chromatography using 18-20% Ethyl acetate/Pet. ether, obtained as a yellow solid (49.0 mg, 71% yield). MP = 169.5 – 171.2 °C

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.06 – 7.98 (m, 2H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.84 - 7.77 (m, 2H), 7.69 - 7.64 (m, 1H), 7.59 (ddd, *J* = 7.7, 6.6, 1.4 Hz, 2H), 7.48 - 7.39 (m, 3H), 7.36 - 7.24 (m, 4H), 7.21 - 7.14 (m, 2H), 6.32 (s, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 152.0,

144.3, 142.3, 140.1, 134.7, 133.4, 132.9, 132.3, 130.6, 129.6, 128.6, 128.5, 128.3, 128.3, 128.0, 127.9, 127.9, 127.6, 126.9, 126.8, 126.1, 125.8, 123.5, 51.6. **FTIR (cm^{-1}):** 3056, 2957, 2923, 2852, 1623, 1584, 1497, 1389, 1217, 1061, 752, 727.

HRMS (ESI) *m/z* Calculated for $C_{26}H_{20}N$ $[M+H]^+$: 346.1590, found: 346.1585.

3-(isoquinolin-4-yl)isobenzofuran-1(3H)-one (4aj)

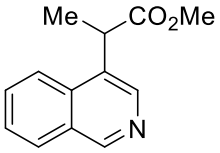


The titled compound **4aj** was prepared by exactly following the general procedure **E (GP-E).** ***R**$_f$* (Ethyl acetate/Pet. ether; 50:50) = 0.24. The title compound was isolated via flash column chromatography using 30-35% Ethyl acetate/Pet. Ether, obtained as a white solid (36 mg, 68% yield). MP = 152.3 – 153.9 °C.

^{1}H NMR (400 MHz, CDCl$_3$) δ 9.30 (s, 1H), 8.34 (s, 1H), 8.11 - 8.04 (m, 3H), 7.82 (ddd, *J* = 8.4, 7.0, 1.3 Hz, 1H), 7.75 - 7.69 (m, 2H), 7.68 - 7.62 (m, 1H), 7.49 - 7.44 (m, 1H), 7.10 (s, 1H). **^{13}C NMR (100 MHz, CDCl$_3$)** δ 170.0, 154.6, 148.0, 141.8, 134.4, 134.1, 131.7, 129.9, 128.7, 128.5, 127.8, 126.3, 126.3, 125.4, 123.2, 122.4, 78.8. **FTIR (cm^{-1}):** 3058, 2958, 2924, 2854, 1765, 1620, 1467, 1379, 1262, 1097, 859, 754.

HRMS (ESI) *m/z* Calculated for $C_{17}H_{12}O_2N$ $[M+H]^+$:262.0863, found: 262.0866.

methyl 2-(isoquinolin-4-yl)propanoate (4ak)

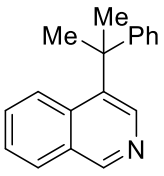


The titled compound **4ak** was prepared by exactly following the general procedure **D (GP-D).** **R$_f$** (Ethyl acetate/Pet ether: 30:70) = 0.21. The title compound was isolated via flash column chromatography using 22-25% Ethyl acetate/Pet ether, obtained as sticky liquid (19 mg, 44 % yield).

^{1}H NMR (400MHz, CDCl$_3$) δ 9.19 (s, 1H), 8.50 (s, 1H), 8.02 (t, *J* = 7.8 Hz, 2H), 7.78 - 7.73 (m, 1H), 7.66 - 7.60 (m, 1H), 4.38 (q, *J* = 7.2 Hz, 1H), 3.67 (s, 3H), 1.71 (d, *J* = 7.1 Hz, 3H). **^{13}C NMR (100MHz, CDCl$_3$)** δ = 174.3, 152.0, 141.6, 133.7, 130.4, 129.7, 128.2, 126.7, 122.0, 52.0, 39.8, 17.4 **FTIR (cm^{-1}):** 2984, 2950, 2850, 1730, 1622, , 1504, 1455, 1392, 1199, 1093, 959, 846, 751.

HRMS (ESI) *m/z* Calculated for $C_{13}H_{14}O_2N$ $[M+H]^+$: 216.1019, found: 216.1021.

4-(2-phenylpropan-2-yl)isoquinoline (4al)



The titled compound **4al** was prepared by exactly following the general procedure **D (GP-D).** ***R**$_f$* (Ethyl acetate/Pet. ether; 30:70) = 0.31. The title compound was isolated via flash column chromatography using 20-22% Ethyl acetate/Pet. ether, obtained as a white solid (18 mg, 40% yield). MP = 104.7 – 106.7 °C.

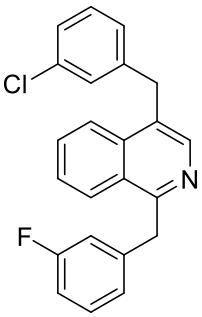
^{1}H NMR (400 MHz, CDCl$_3$) δ 9.19 (s, 1H), 8.77 (s, 1H), 7.95 - 7.92 (m, 1H), 7.47 - 7.41 (m, 2H), 7.37 - 7.31 (m, 1H), 7.26 - 7.21 (m, 4H), 7.19 - 7.14 (m, 1H), 1.87 (s, 6H). **^{13}C NMR (100 MHz, CDCl$_3$)**

δ 152.6, 150.3, 140.6, 137.8, 133.9, 129.3, 129.2, 128.6, 128.5, 126.2, 126.1, 125.8, 125.8, 42.7, 31.3. **FTIR (cm^{-1}):** 3057, 2967, 2930, 2875, 1724, 1619, 1494, 1451, 1389, 1223, 1024, 757.

HRMS (ESI) *m/z* Calculated for $C_{18}H_{18}N$ $[M+H]^+$: 248.1434, found: 248.1443.

12. Compound Characterization Data for Sequential Functionalization of Isoquinolines:

4-(3-chlorobenzyl)-1-(3-fluorobenzyl)isoquinoline (10cg)

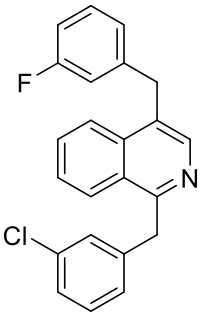


The titled compound **10cg** was prepared by exactly following the reaction procedure **F (GP-F)**. **R$_f$** (Ethyl acetate/Pet ether: 20:80) = 0.41. The title compound was isolated via flash column chromatography using 8-10% Ethyl acetate/Pet ether, obtained as sticky liquid (46.5 mg, 43% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.37 (s, 1H), 8.14 (d, *J* = 8.1 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.62 (ddd, *J* = 1.3, 6.9, 8.3 Hz, 1H), 7.55 - 7.50 (m, 1H), 7.24 - 7.16 (m, 4H), 7.09 - 7.05 (m, 2H), 6.97 (d, *J* = 10.0 Hz, 1H), 6.87 (dt, *J* = 2.2, 8.4 Hz, 1H), 4.66 (s, 2H), 4.34 (s, 2H). **^{13}C NMR (100 MHz, CDCl$_3$)** δ 162.9 (d, *J* = 245.6 Hz), 158.9, 142.8, 141.8 (d, *J* = 9.4 Hz), 135.4, 134.4, 130.1, 130.0, 129.9, 129.9 (d, *J* = 7.9 Hz), 128.0, 127.1, 127.0, 126.7, 126.6, 126.2, 124.3 (d, *J* = 2.9 Hz), 124.1, 115.6 (d, *J* = 21.1 Hz), 113.3 (d, *J* = 21.1 Hz), 41.7 (d, *J* = 1.4 Hz), 36.0. **FTIR (cm^{-1}):** 3062, 3004, 2924, 2853, 1732, 1587, 1486, 1385, 1245, 1019, 870, 762.

HRMS (ESI) *m/z* Calculated for $C_{23}H_{18}ClFN$ $[M+H]^+$: 362.1106, found: 362.1113.

1-(3-chlorobenzyl)-4-(3-fluorobenzyl)isoquinoline (10gc)

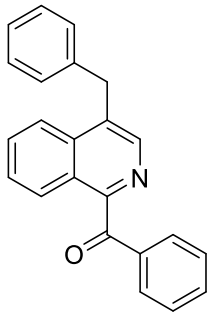


The titled compound **10gc** was prepared by exactly following the reaction procedure **F (GP-F)**. **R$_f$** (Ethyl acetate/Pet ether: 20:80) = 0.45. The title compound was isolated via flash column chromatography using 8-10% Ethyl acetate/Pet ether, obtained as sticky liquid (48.8 mg, 45% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.37 (s, 1H), 8.13 (d, *J* = 8.3 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.64 - 7.58 (m, 1H), 7.55 - 7.50 (m, 1H), 7.29 (s, 1H), 7.25 - 7.12 (m, 4H), 7.00 (d, *J* = 7.9 Hz, 1H), 6.94 - 6.84 (m, 2H), 4.63 (s, 2H), 4.37 (s, 2H). **^{13}C NMR (100 MHz, CDCl$_3$)** δ 163.0 (d, *J* = 246.3 Hz), 158.8, 142.8, 142.3 (d, *J* = 7.3 Hz), 141.4, 135.4, 134.3, 130.1, 130.1, 130.0 (d, *J* = 8.7 Hz), 128.7, 128.1, 127.1, 127.0, 126.8, 126.6, 126.2, 124.2 (d, *J* = 3.6 Hz), 115.5 (d, *J* = 21.1 Hz), 113.3 (d, *J* = 21.1 Hz), 41.6, 36.1 (d, *J* = 2.2 Hz). **FTIR (cm^{-1}):** 3062, 3005, 2924, 2853, 1589, 1487, 1384, 1247, 1134, 1078, 868, 771.

HRMS (ESI) *m/z* Calculated for $C_{23}H_{18}ClFN$ $[M+H]^+$: 362.1106, found: 362.1111.

(4-benzylisoquinolin-1-yl)(phenyl)methanone (11aa)

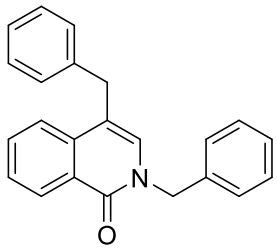


The titled compound **11aa** was prepared by exactly following the reaction procedure **G (GP-G)**. $\mathbf{R_f}$ (Ethyl acetate/Pet ether: 20:80) = 0.41. The title compound was isolated via flash column chromatography using 8-10% Ethyl acetate/Pet ether, obtained as sticky liquid (66 mg, 68% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.26 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 8.5 Hz, 1H), 8.00 - 7.95 (m, 2H), 7.70 (ddd, *J* = 1.3, 7.0, 8.4 Hz, 1H), 7.64 - 7.57 (m, 2H), 7.51 - 7.46 (m, 2H), 7.33 - 7.28 (m, 2H), 7.25 - 7.20 (m, 3H), 4.48 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 194.9, 155.7, 141.9, 139.2, 136.8, 135.7, 133.6, 132.0, 130.8, 130.7, 128.7, 128.6, 128.4, 127.9, 126.8, 126.6, 126.4, 123.9, 36.5. **FTIR (cm^{-1}):** 3061, 2924, 2856, 1730, 1669, 1499, 1240, 1166, 1023, 883, 763, 701.

HRMS (ESI) *m/z* Calculated for $C_{23}H_{18}NO$ $[M+H]^+$: 324.1383, found: 324.1388.

2,4-dibenzylisoquinolin-1(2H)-one (12aa)



The titled compound **12aa** was prepared by exactly following the reaction procedure **H (GP-H)**. $\mathbf{R_f}$ (Ethyl acetate/Pet ether: 20:80) = 0.45. The title compound was isolated via flash column chromatography using 8-10% Ethyl acetate/Pet ether, obtained as yellow solid (46 mg, 48% yield). MP = 98.1-98.8 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 - 8.49 (m, 1H), 7.59 (ddd, *J* = 1.4, 6.9, 8.1 Hz, 1H), 7.53 (d, *J* = 7.0 Hz, 1H), 7.48 (dt, *J* = 1.4, 7.4 Hz, 1H), 7.35 - 7.32 (m, 1H), 7.32 - 7.28 (m, 4H), 7.27 (t, *J* = 1.6 Hz, 1H), 7.21 (d, *J* = 7.3 Hz, 1H), 7.19 - 7.16 (m, 2H), 5.20 (s, 2H), 4.00 (s, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 162.0, 139.1, 136.9, 136.6, 132.2, 130.6, 128.8, 128.6, 128.6, 128.4, 127.9, 127.8, 126.8, 126.4, 126.4, 123.4, 115.2, 51.7, 35.7. **FTIR (cm^{-1}):** 3064, 3009, 2924, 2852, 1730, 1654, 1491, 1319, 1076, 1030, 983, 754.

HRMS (ESI) *m/z* Calculated for $C_{23}H_{20}NO$ $[M+H]^+$: 326.1539, found: 326.1536.

13. References

1. B. M. Reeves, H. B. Hepburn, A. Grozavu, P. J. Lindsay-Scott, T. J. Donohoe, *Angew. Chem. Int. Ed.*, 2019, **58**, 15697–15701.
2. J. M. M. Grandjean, A. Y. Jiu, J. W. West, A. Aoyagi, D. G. Droege, M. Elepano, M. Hirasawa, M. Hirouchi, R. Murakami, J. Lee, K. Sasaki, S. Hirano, T. Ohyama, B. C. Tang, R. J. Vaz, M.

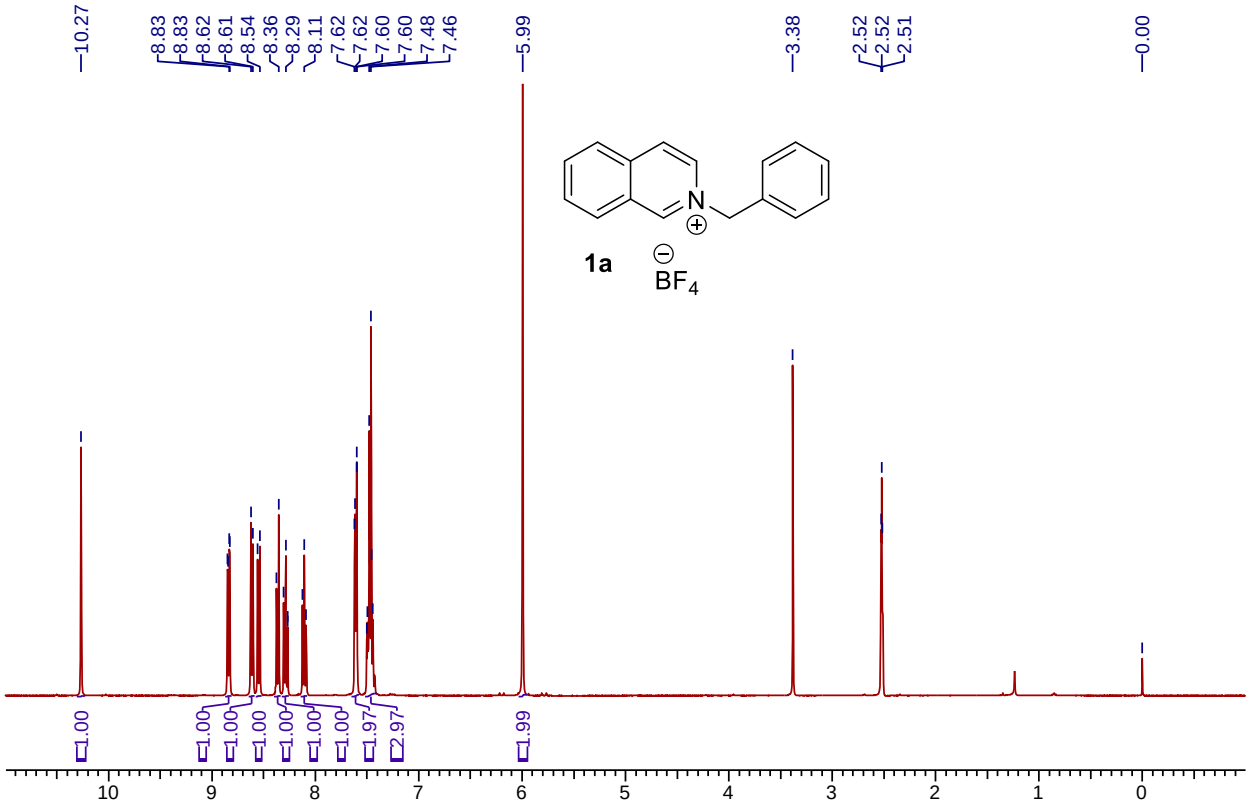
Inoue, S. H. Olson, S. B. Prusiner, J. Conrad, N. A. Paras, *ACS Med. Chem. Lett.*, 2020, **11**, 127–132.

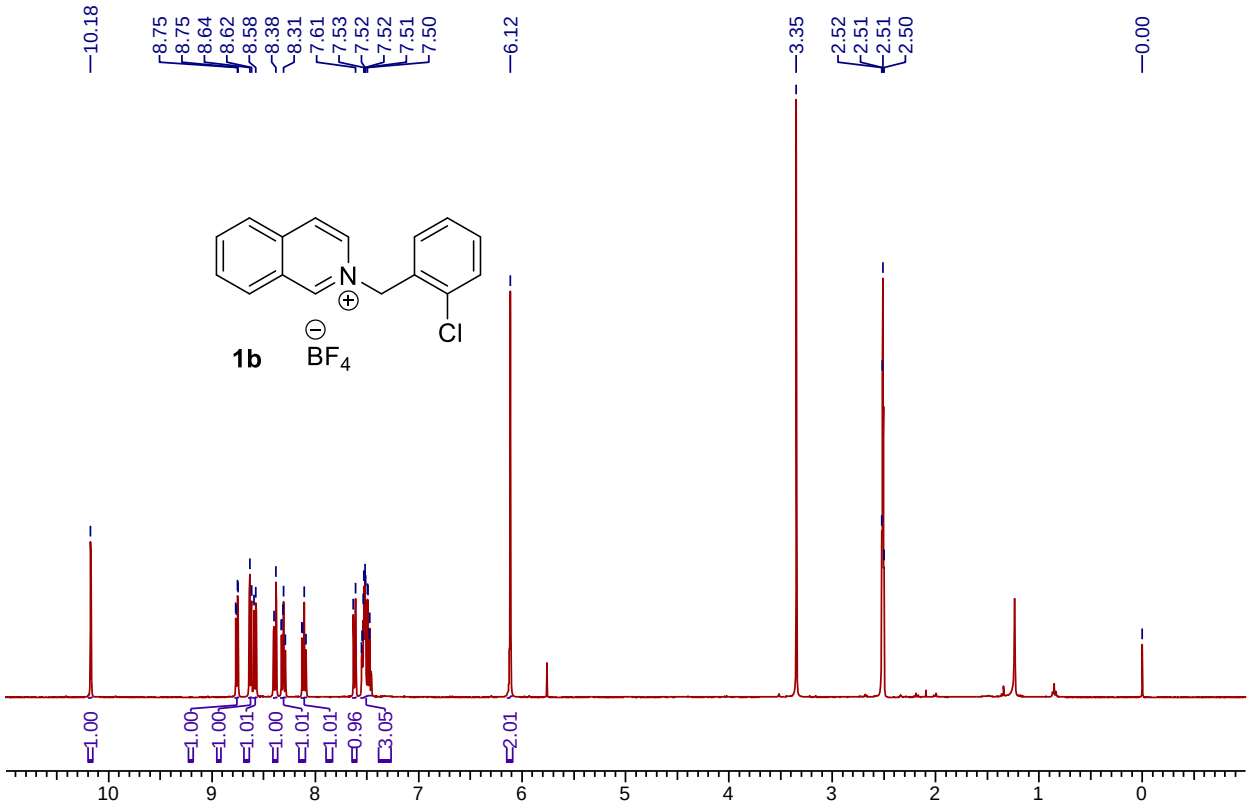
3. J. Holz, C. Pfeffer, H. Zuo, D. Beierlein, G. Richter, E. Elias Klemm, R. Peters, *Angew. Chem., Int. Ed.*, 2019, **58**, *10330-10334.*
4. A. Motaleb, A. Bera, P. Maity, *Org. Biomol. Chem*., 2018, **16**, 5081−5085.
5. A. Motaleb, S. Rani, T. Das, R. G. Gonnade, P. Maity, *Angew. Chem., Int. Ed*., 2019, **58**, 14104−14109.
6. S. Rani, S. R. Dash, A. Bera, Md. N. Alam, K. Vanka, P. Maity, *Chem. Sci*., 2021, **12**, 8996–9003.
7. Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A.V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, Jr. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. Fox, J. Gaussian, Inc., Wallingford CT (2016) GaussView 5.0. Wallingford, E.U.A.
8. Y. Zhao, D. G. Truhlar, *Theory Chem. Account*, 2008, **120**, 215–241.
9. Spickermann, Entropies of Condensed Phases and Complex Systems a first Principles. Approach, Berlin, Heidelberg, NewYork : Springer, 2011**.**
10. D. H. Wertz, *J. Am. Chem. Soc*., 1980, **102**, 5316–5322.
11. Y. Takano, K. N. Houk, *J. Chem. Theory Comput.*, 2005, **1**, 70–77.
12. C. Angeli, R. Cimiraglia, S. Evangelisti, T. Leininger, J.-P. *J. Chem. Phys.*, 2001, **114**, 10252–10264.
13. F. Neese, *WIREs Comput. Mol. Sci*., 2022, 12:e1606.
14. Available at www.iboview.org. a) G. Knizia, *J. Chem. Theory Comput*., 2013, **9**, 4834−4843; b) G. Knizia, J. E. M. N. Klein, *Angew. Chem., Int. Ed*., 2015, **54**, 5518−5522.
15. Q. Sun, Y. Y. Zhang, J. Sun, Y. Han, X. Jia, C. G. Yan, *Org. Lett.*, 2018, **20**, 987–990.
16. X. Xu, H. Feng, E. V. Van Der Eycken, *Org. Lett.*, 2021, **23**, 6578–6582.
17. A. Y. Platonova, D. Seidel, *Tetrahedron Lett.*, 2015, **56**, 3147–3150.
18. D. E. Minter, M. A. Re, *J. Org. Chem.*, 1988, **53**, 2653–2655.

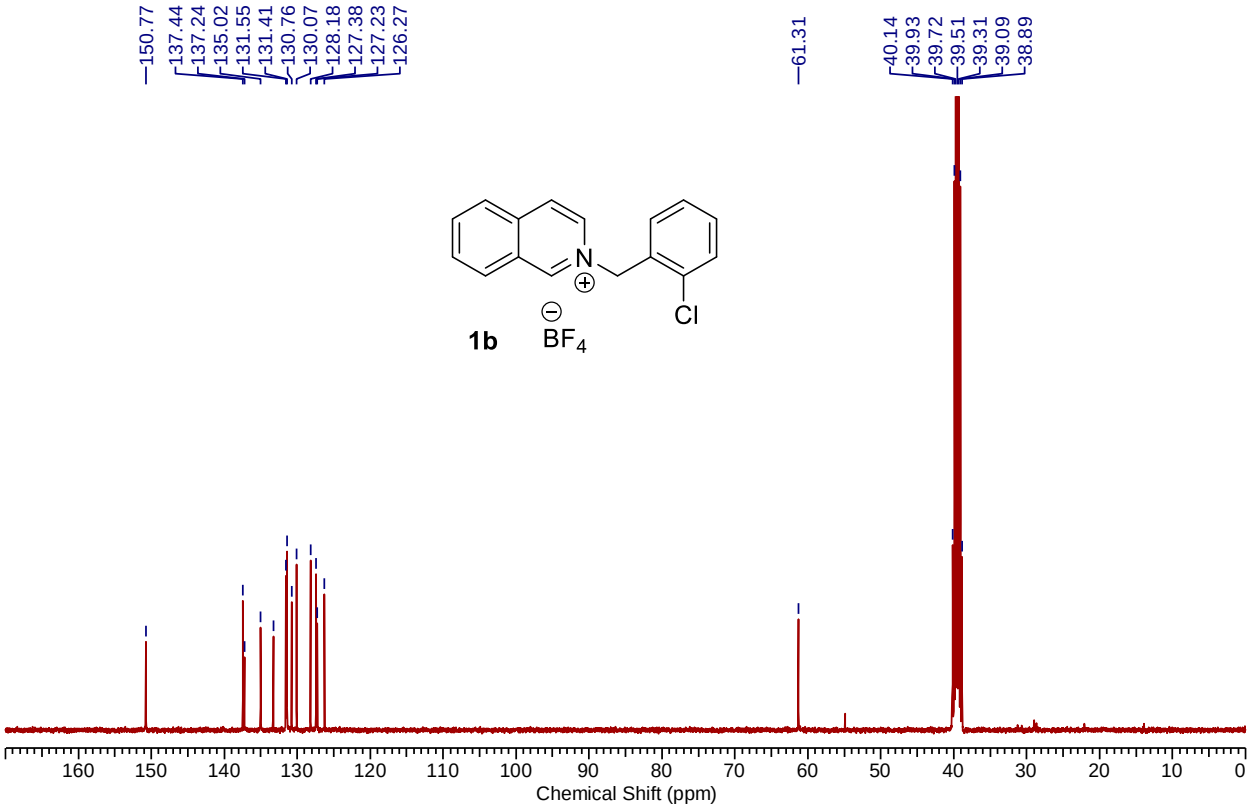
19. T. Heilmann, J. M. Lopez-Soria, J. Ulbrich, J. Kircher, Z. Li, B. Worbs, C. Golz, R. A. Mata, M. Alcarazo, *Angew. Chem. Int. Ed*., 2024, **63**, e202403826.
20. Z. Liu, Z.-J. Shi, L. Liu, M. Zhang, M.-C. Zhang, H.-Y. Gou, X.-C. Wang, *J. Am. Chem. Soc*., 2023, **145**, 11789−11797.
21. Y. Liu, X. Yi, X. Luo, C. Xi, *J. Org. Chem.* 2017, 82, **21**, 11391–11398
22. S. D. Friis, M. T. Pirnot, S. L. Buchwald, *J. Am. Chem. Soc*., 2016, **138**, 8372-8375.
23. A. Mondal, P. Kundu, M. Jash, C. Chowdhury, *Org. Biomol. Chem*., 2018, **16**, 963-980.

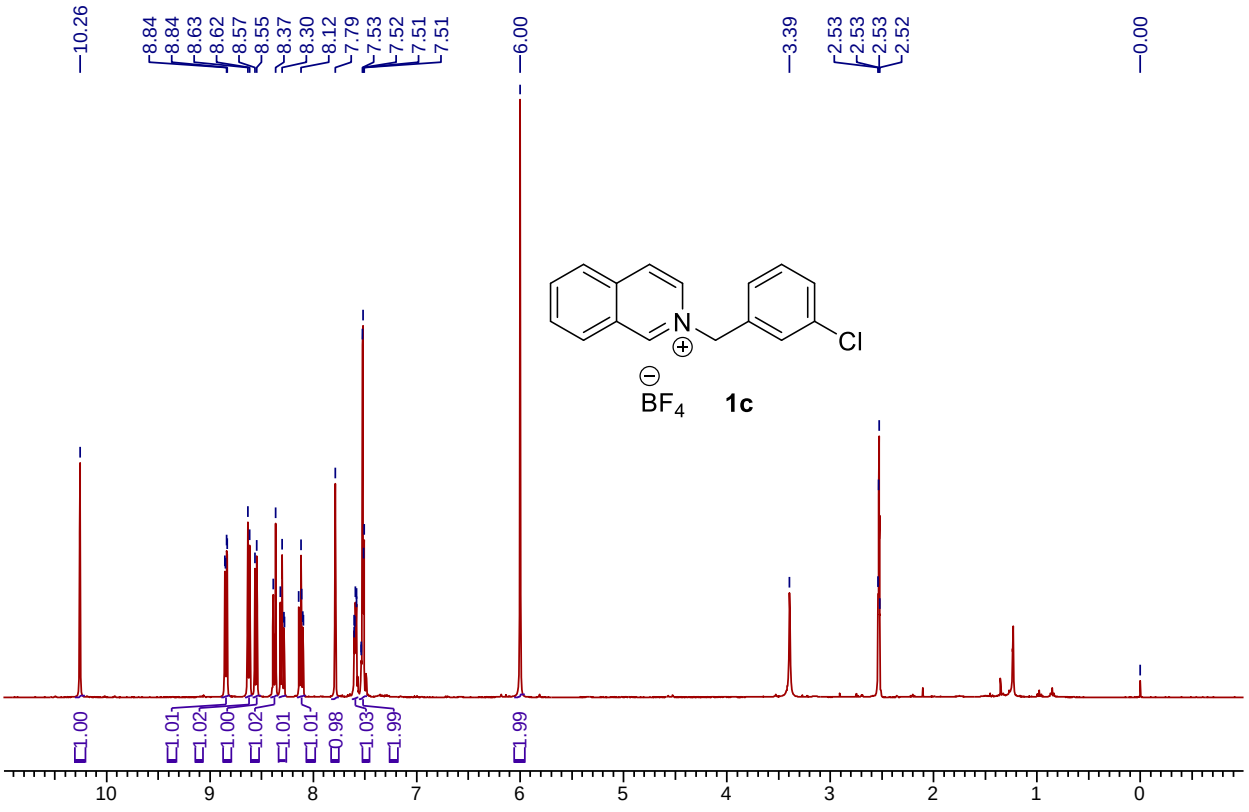
14. NMR Spectra:

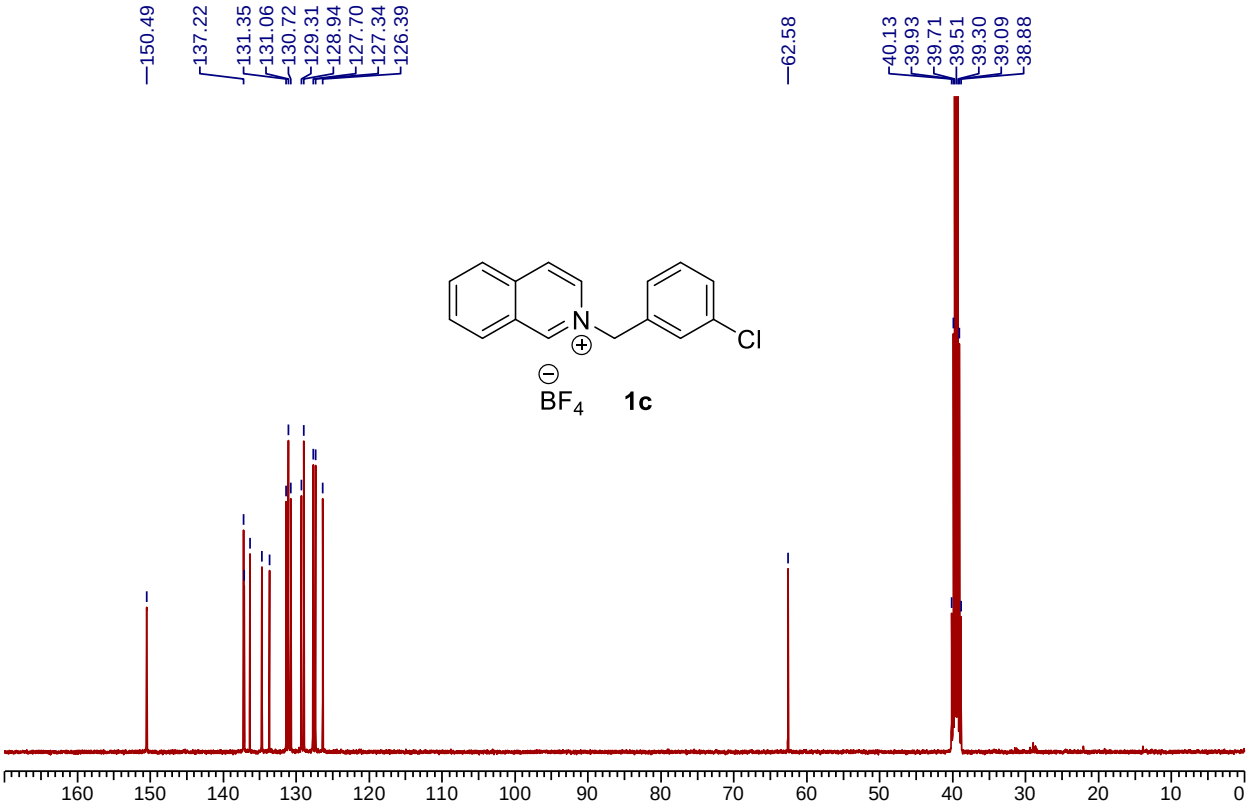
14a. NMR Spectra for *N*-alkyl Isoquinolinium Salts:

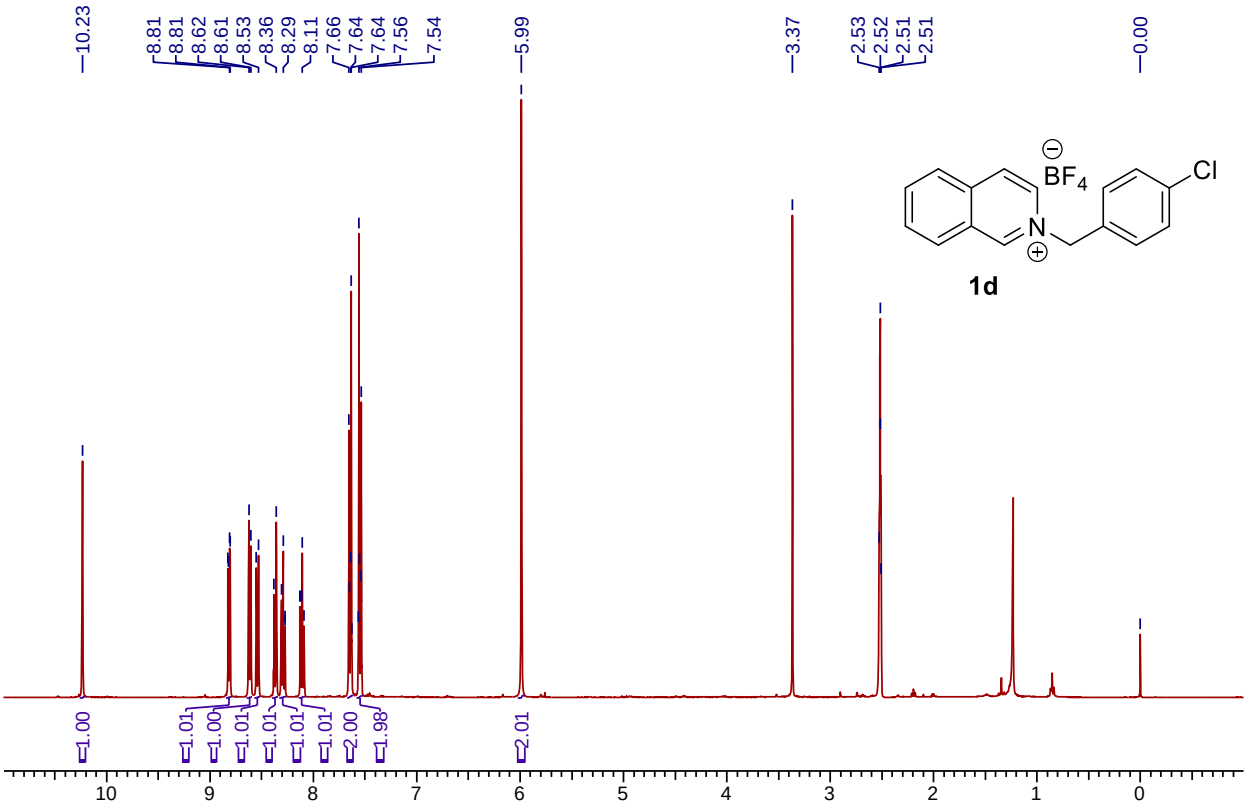


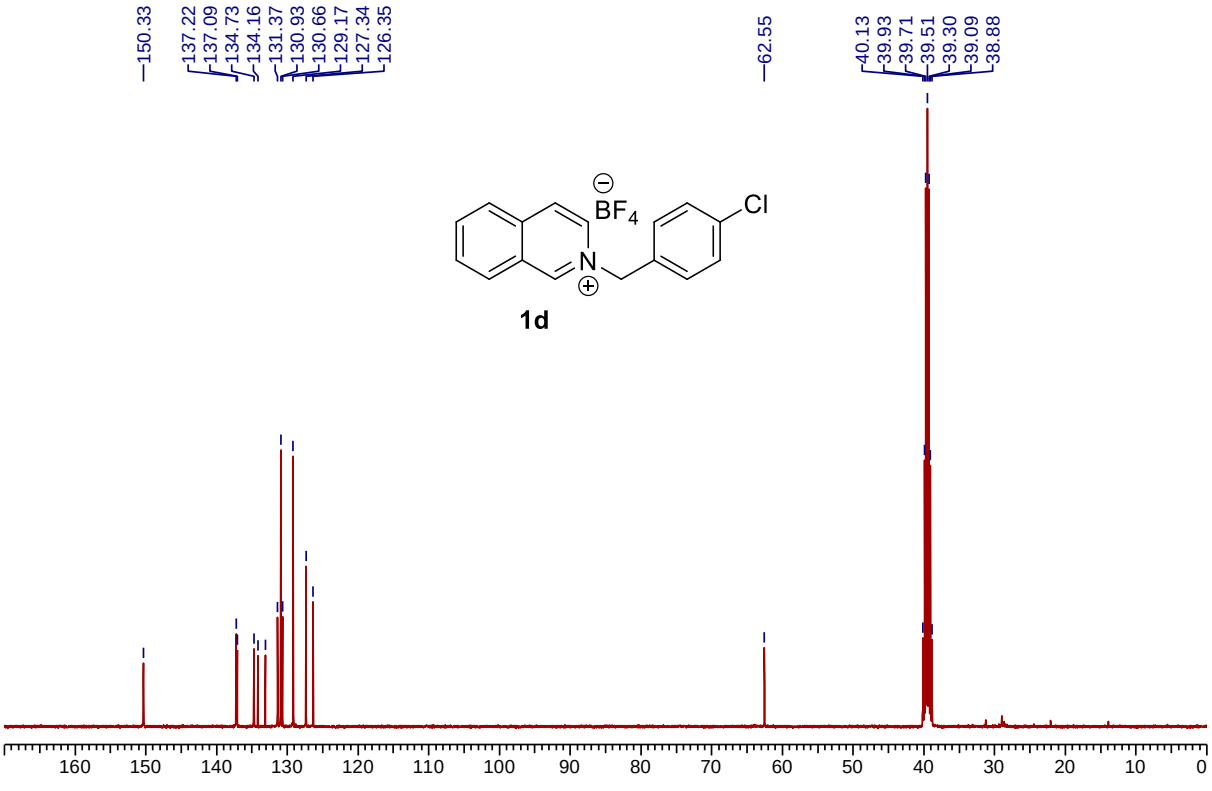

10.18
8.75
8.75
8.64
8.62
8.58
8.38
8.31
7.61
7.53
7.52
7.52
7.51
7.50
6.12
3.35
2.52
2.51
2.51
2.50
0.00
1.00
1.00
1.00
1.01
1.00
1.01
1.01
0.96
3.05
2.01
1b
BF4
Cl
10
9
8
7
6
5
4
3
2
1
0

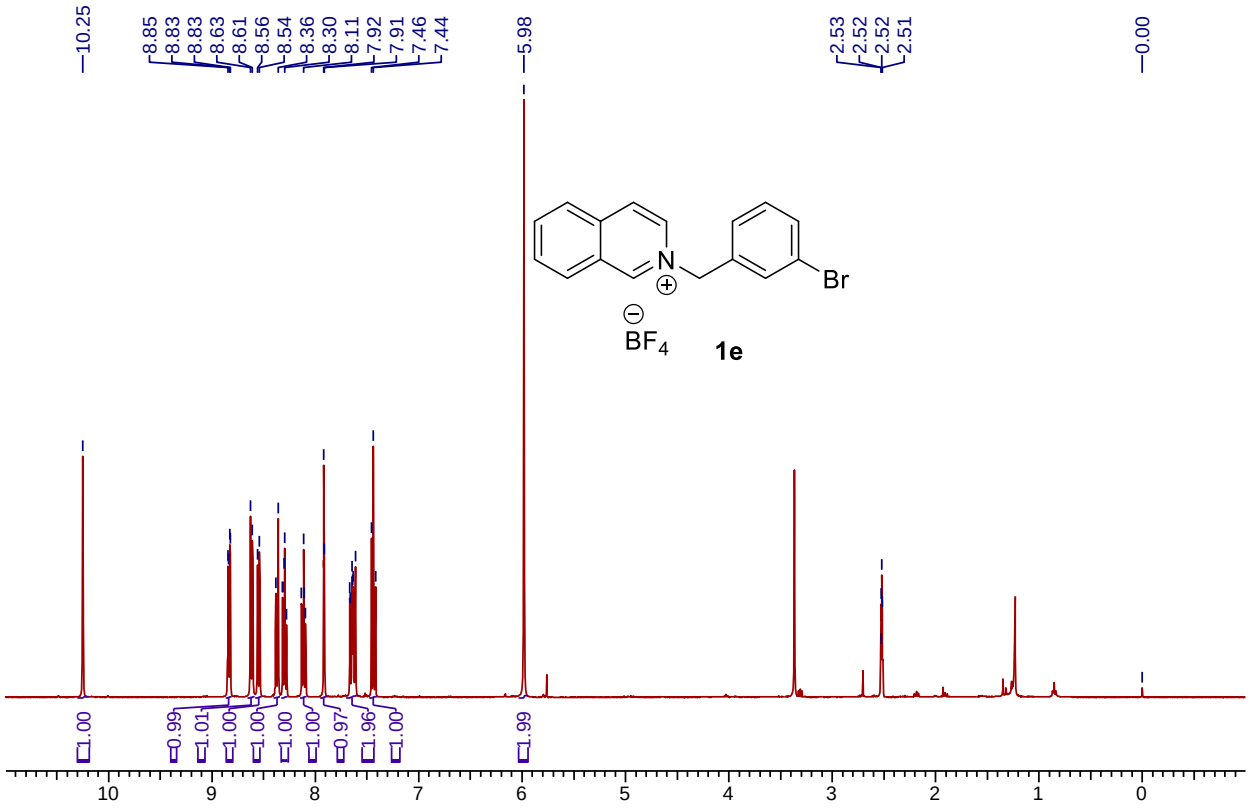

150.77
137.44
137.24
135.02
131.55
131.41
130.76
130.07
128.18
127.38
127.23
126.27
61.31
40.14
39.93
39.72
39.51
39.31
39.09
38.89
1b
BF4
Cl
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

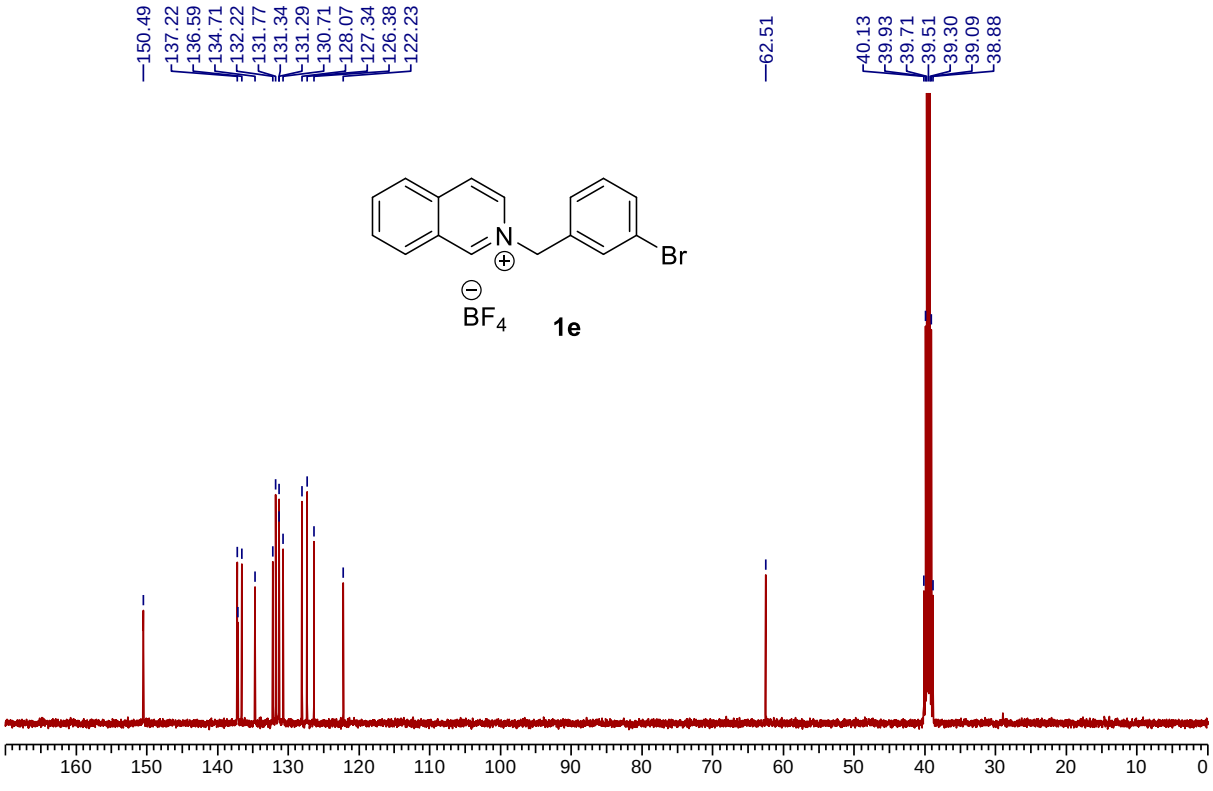

10.26
8.84
8.84
8.63
8.62
8.57
8.55
8.37
8.30
8.12
7.79
7.53
7.52
7.51
7.51
6.00
3.39
2.53
2.53
2.53
2.52
0.00
1.00
1.01
1.02
1.00
1.02
1.01
1.01
0.98
1.03
1.99
1.99
N
Cl
BF4
1c

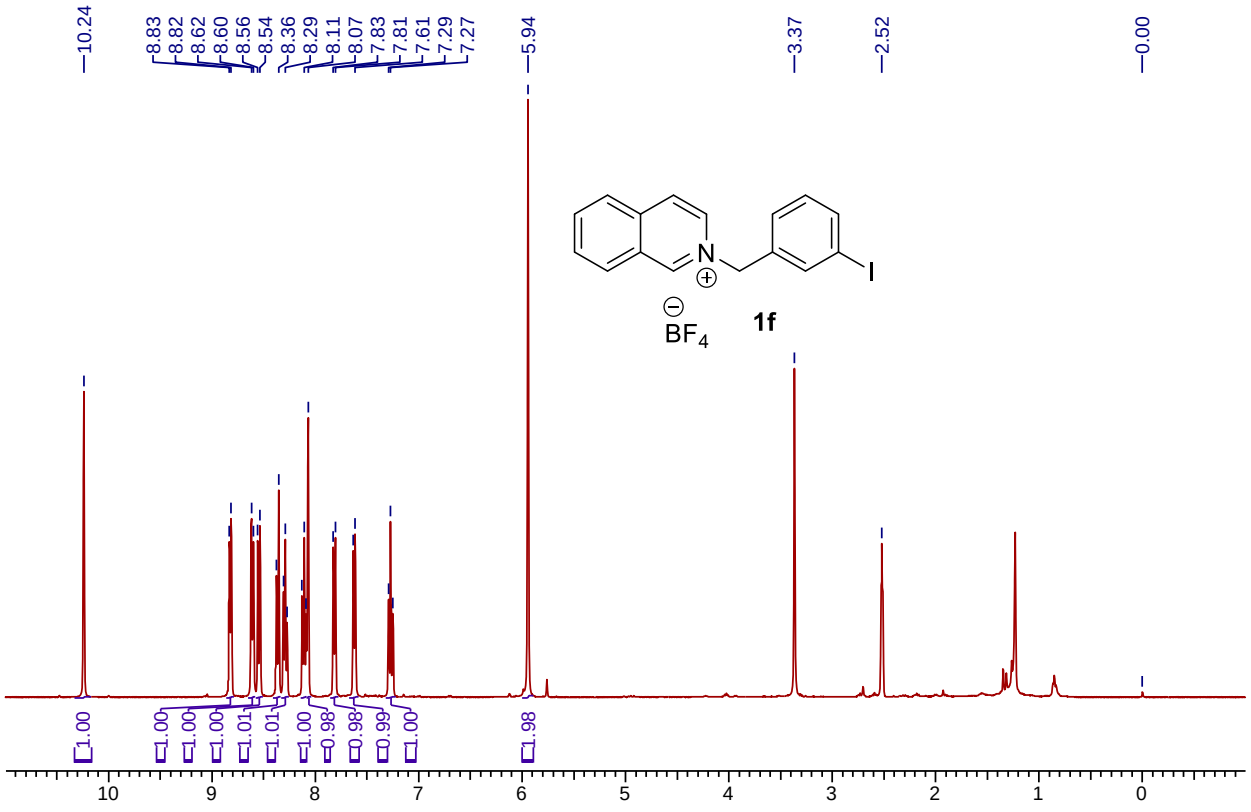

150.49
137.22
131.35
131.06
130.72
129.31
128.94
127.70
127.34
126.39
62.58
40.13
39.93
39.71
39.51
39.30
39.09
38.88
N
Cl
BF4
1c

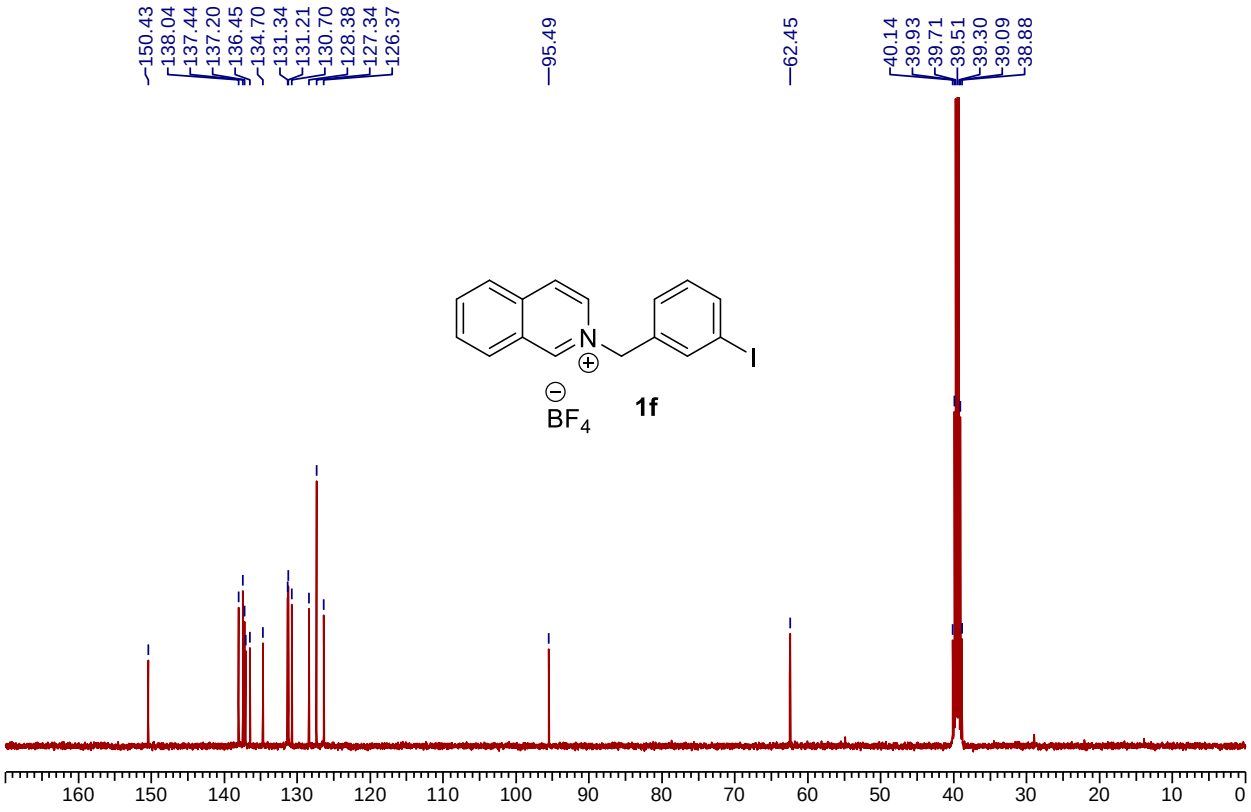

10.23
8.81
8.81
8.62
8.61
8.53
8.36
8.29
8.11
7.66
7.64
7.64
7.56
7.54
5.99
3.37
2.53
2.52
2.51
2.51
0.00
1.00
1.01
1.00
1.01
1.01
1.01
1.01
2.00
1.98
2.01
BF4
Cl
N
1d
10
9
8
7
6
5
4
3
2
1
0

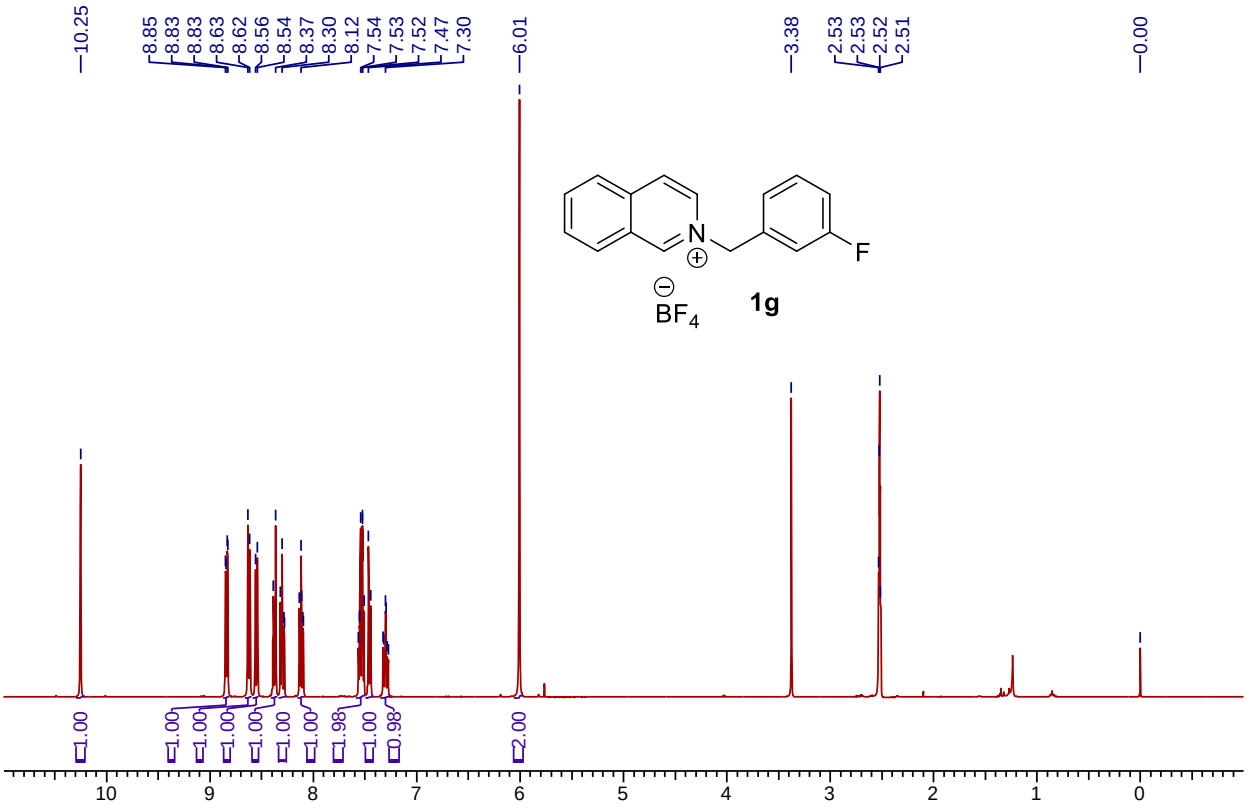

150.33
137.22
137.09
134.73
134.16
131.37
130.93
130.66
129.17
127.34
126.35
62.55
40.13
39.93
39.71
39.51
39.30
39.09
38.88
BF4
Cl
N
1d
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

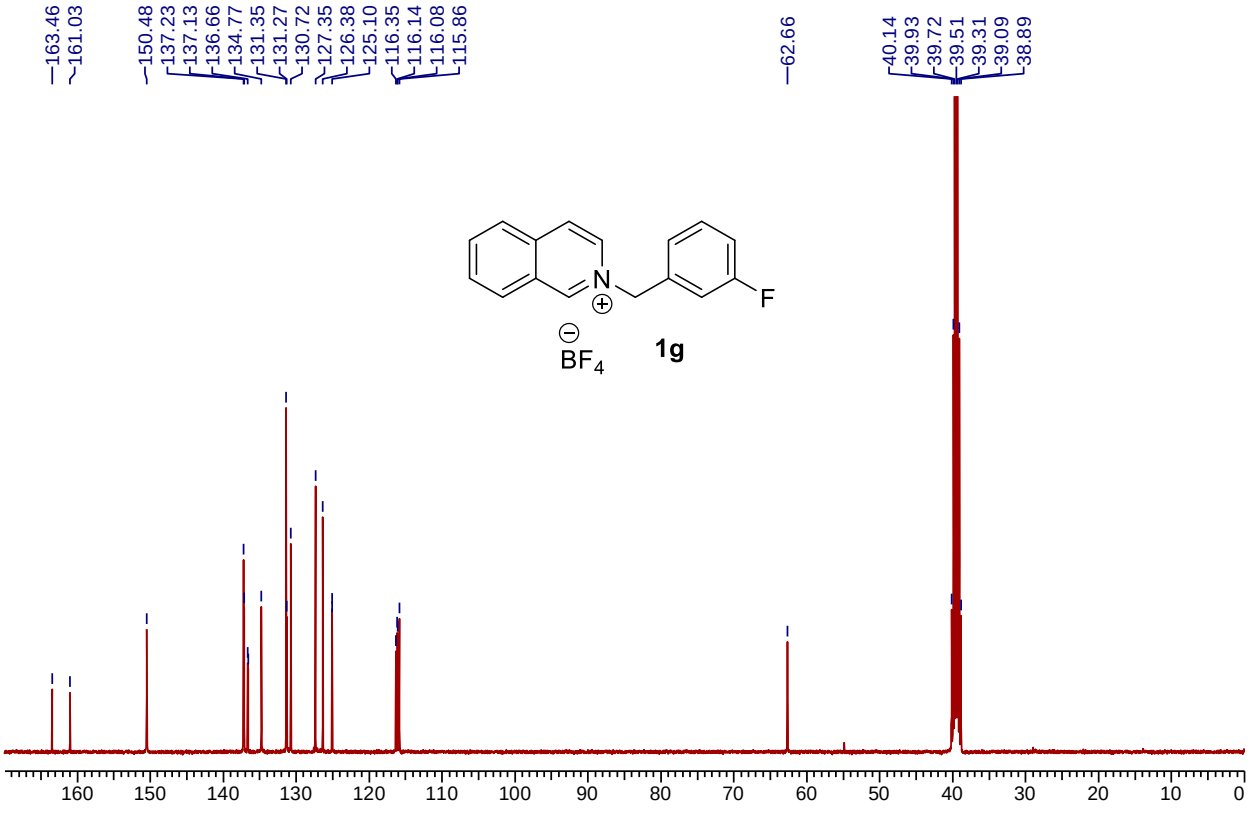

10.25
8.85
8.83
8.83
8.63
8.61
8.56
8.54
8.36
8.30
8.11
7.92
7.91
7.46
7.44
5.98
2.53
2.52
2.52
2.51
0.00
Br
BF4
1e
1.00
0.99
1.01
1.00
1.00
1.00
1.00
0.97
1.96
1.00
1.99

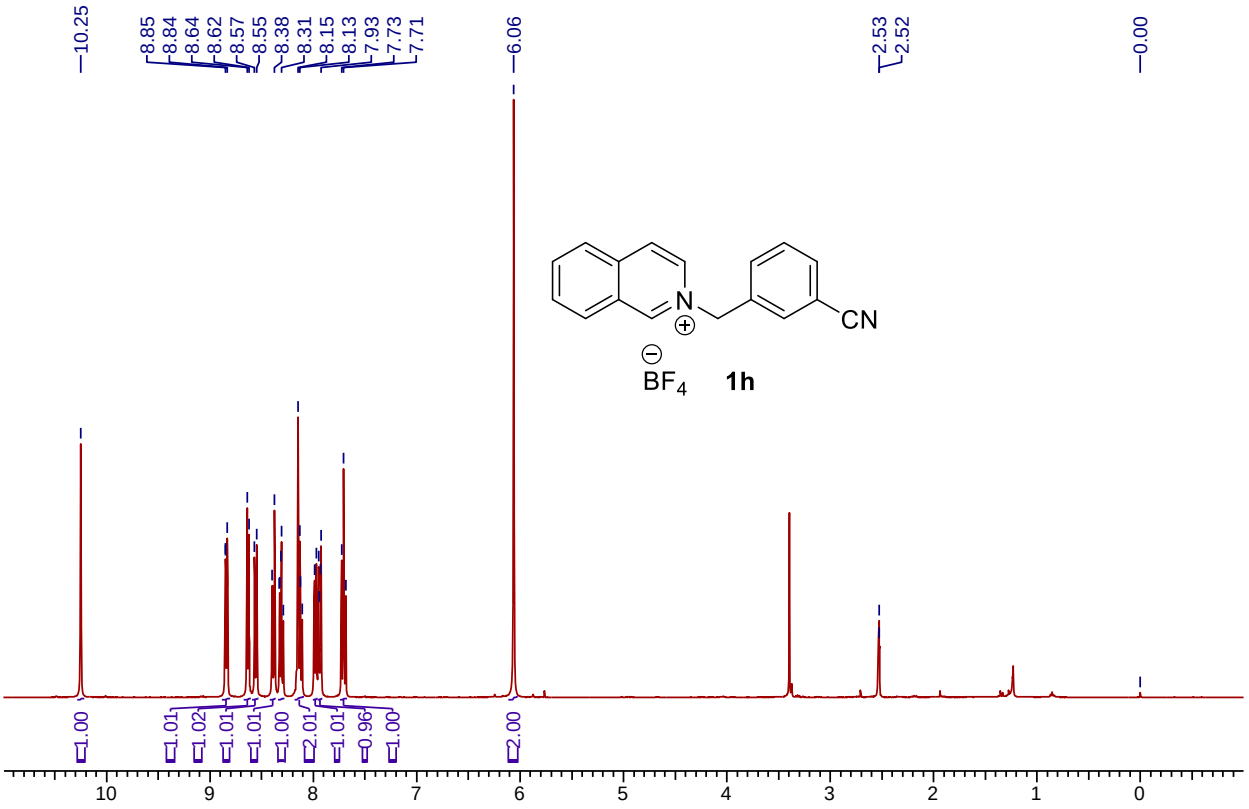

150.49
137.22
136.59
134.71
132.22
131.77
131.34
131.29
130.71
128.07
127.34
126.38
122.23
62.51
40.13
39.93
39.71
39.51
39.30
39.09
38.88
Br
BF4
1e

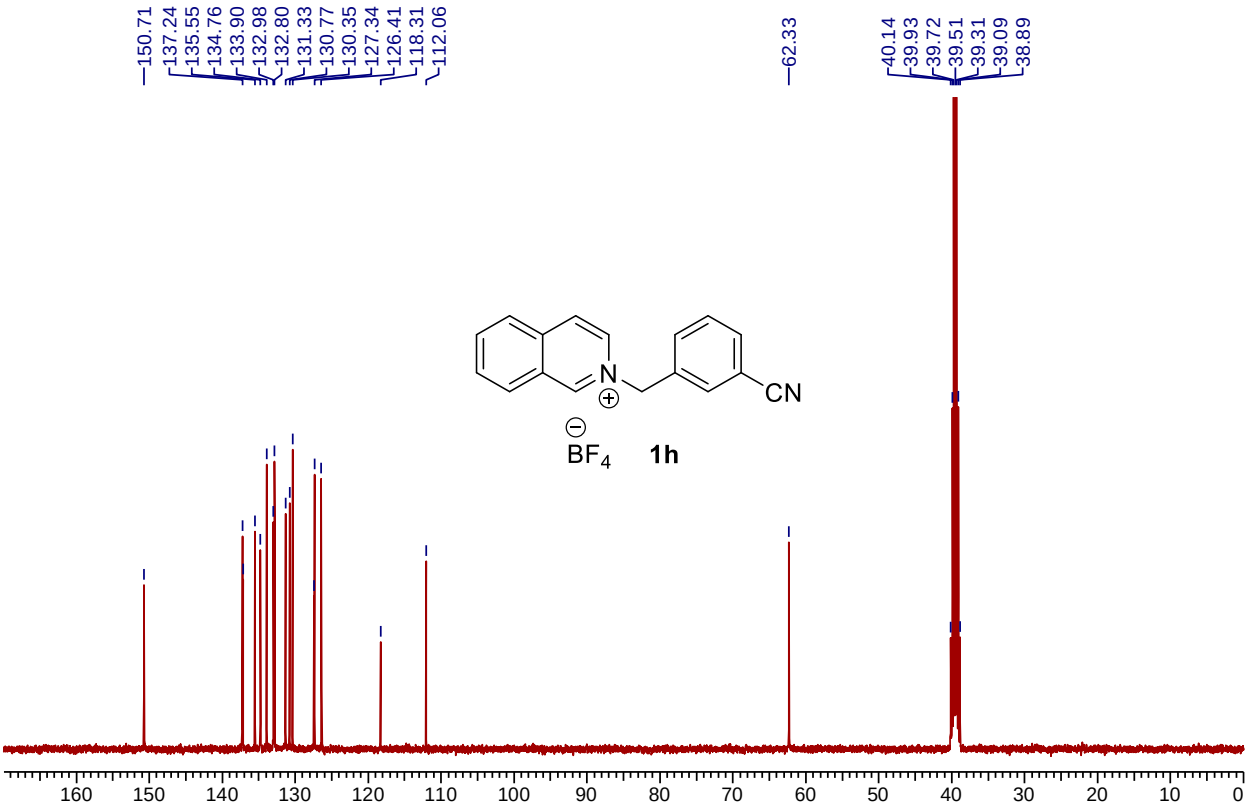

10.24
8.83
8.82
8.62
8.60
8.56
8.54
8.36
8.29
8.11
8.07
7.83
7.81
7.61
7.29
7.27
5.94
3.37
2.52
0.00
1.00
1.00
1.00
1.01
1.01
1.00
0.98
0.98
0.99
1.00
1.98
N
I
BF4
1f
10
9
8
7
6
5
4
3
2
1
0

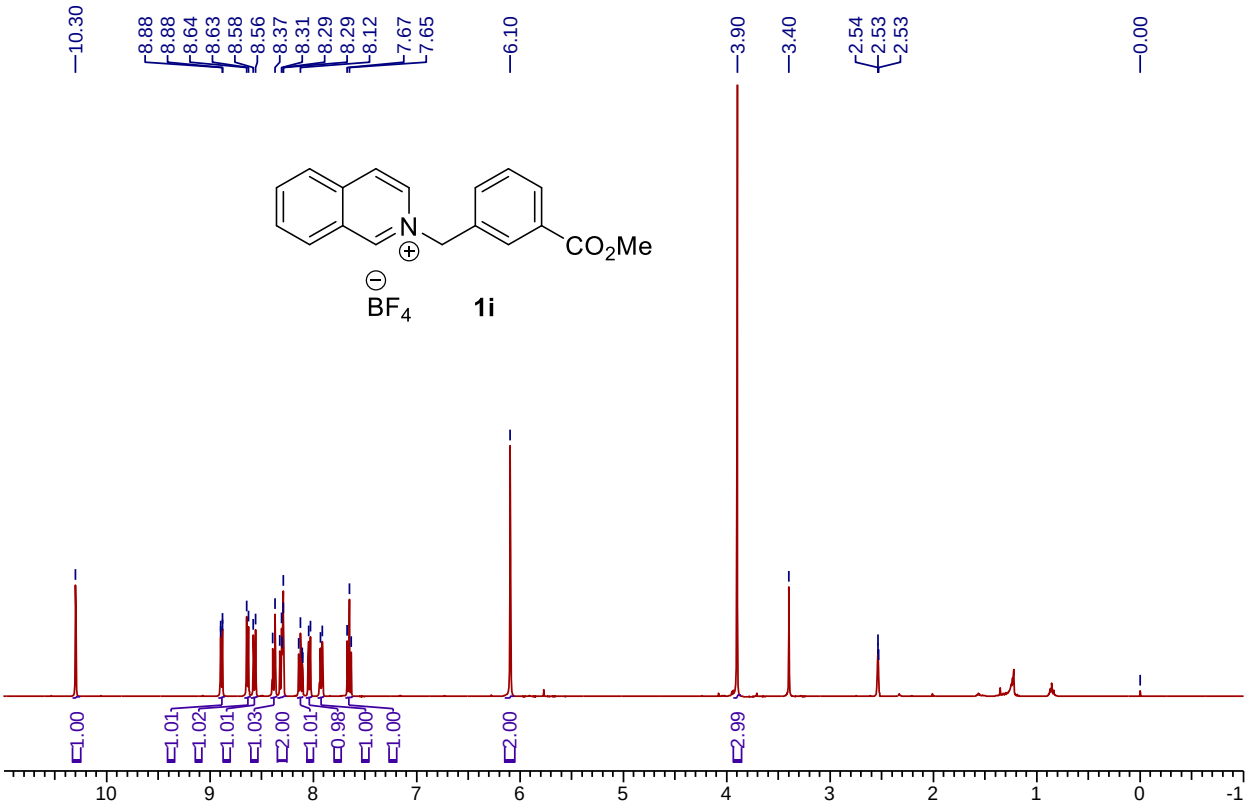

150.43
138.04
137.44
137.20
136.45
134.70
131.34
131.21
130.70
128.38
127.34
126.37
95.49
62.45
40.14
39.93
39.71
39.51
39.30
39.09
38.88
N
I
BF4
1f
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

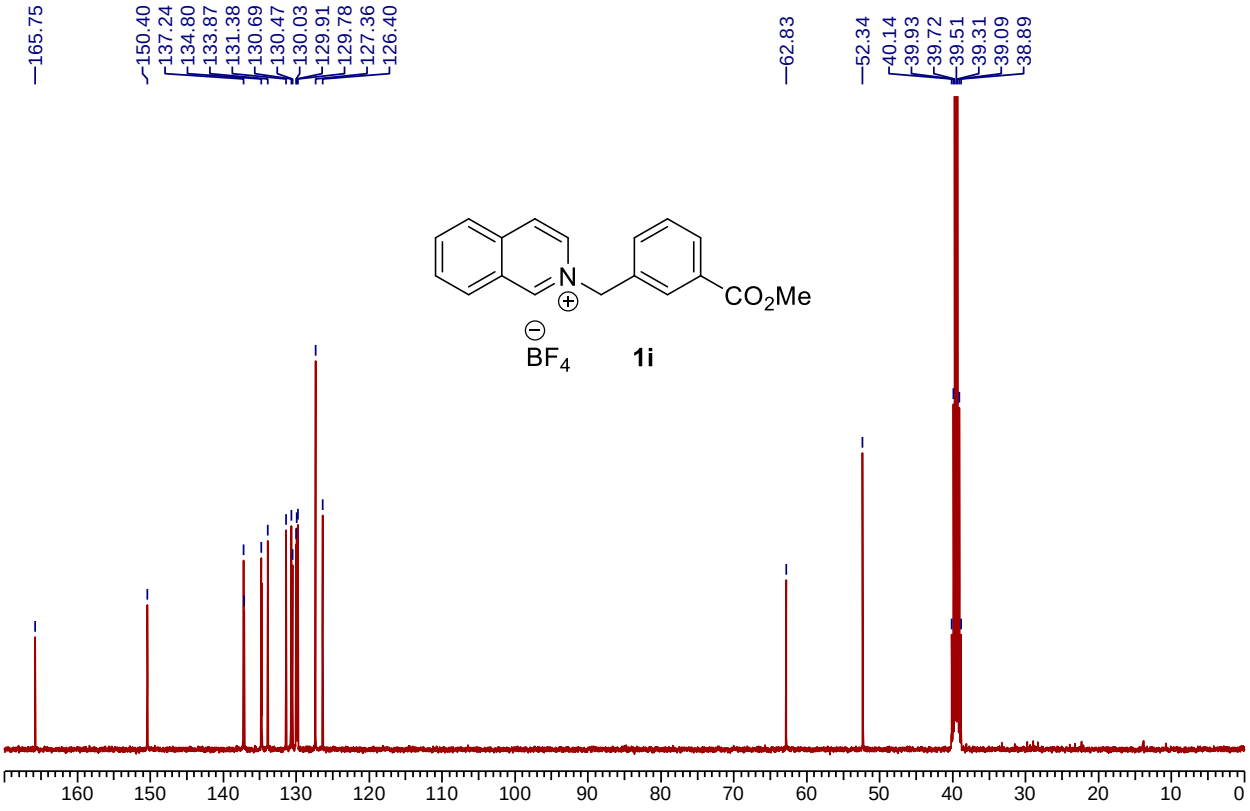

10.25
8.85
8.83
8.83
8.63
8.62
8.56
8.54
8.37
8.30
8.12
7.54
7.53
7.52
7.47
7.30
6.01
3.38
2.53
2.53
2.52
2.51
0.00
N
F
BF4
1g
1.00
1.00
1.00
1.00
1.00
1.00
1.00
1.98
1.00
0.98
2.00
10
9
8
7
6
5
4
3
2
1
0

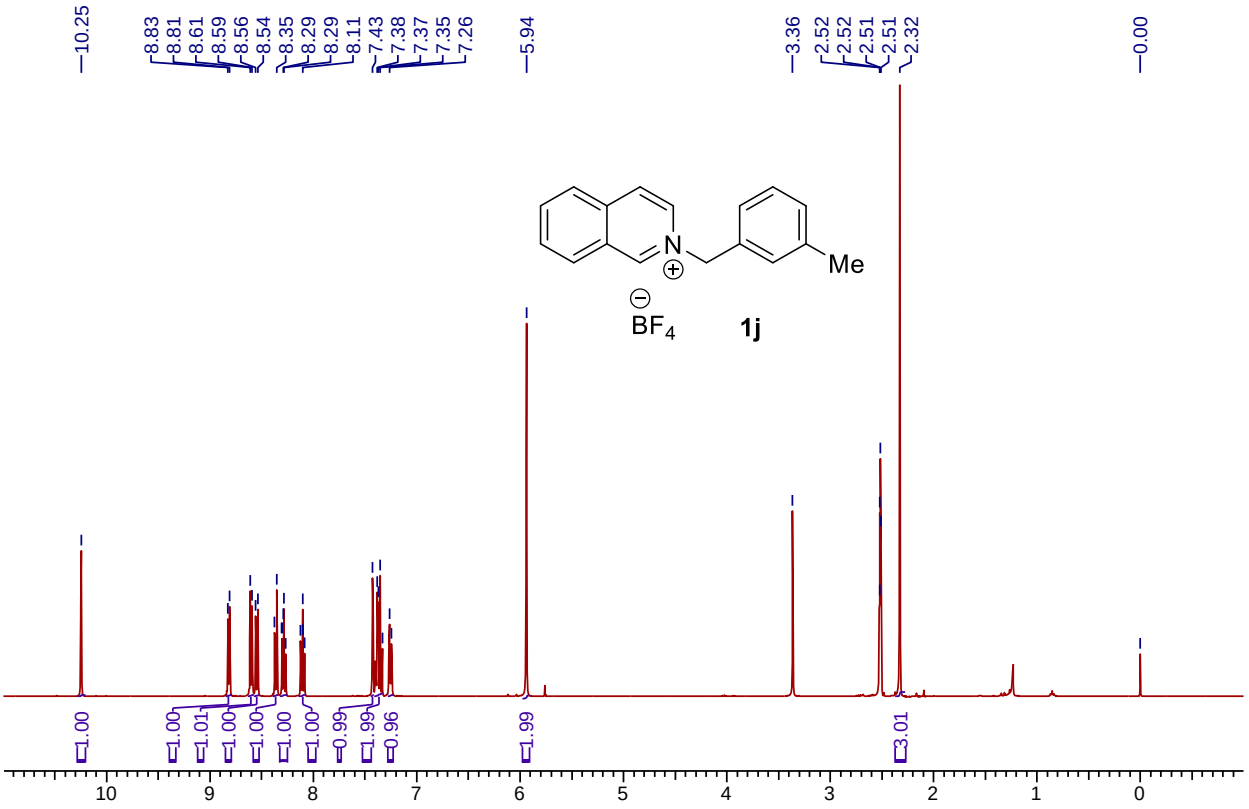

163.46
161.03
150.48
137.23
137.13
136.66
134.77
131.35
131.27
130.72
127.35
126.38
125.10
116.35
116.14
116.08
115.86
62.66
40.14
39.93
39.72
39.51
39.31
39.09
38.89
N
F
BF4
1g
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

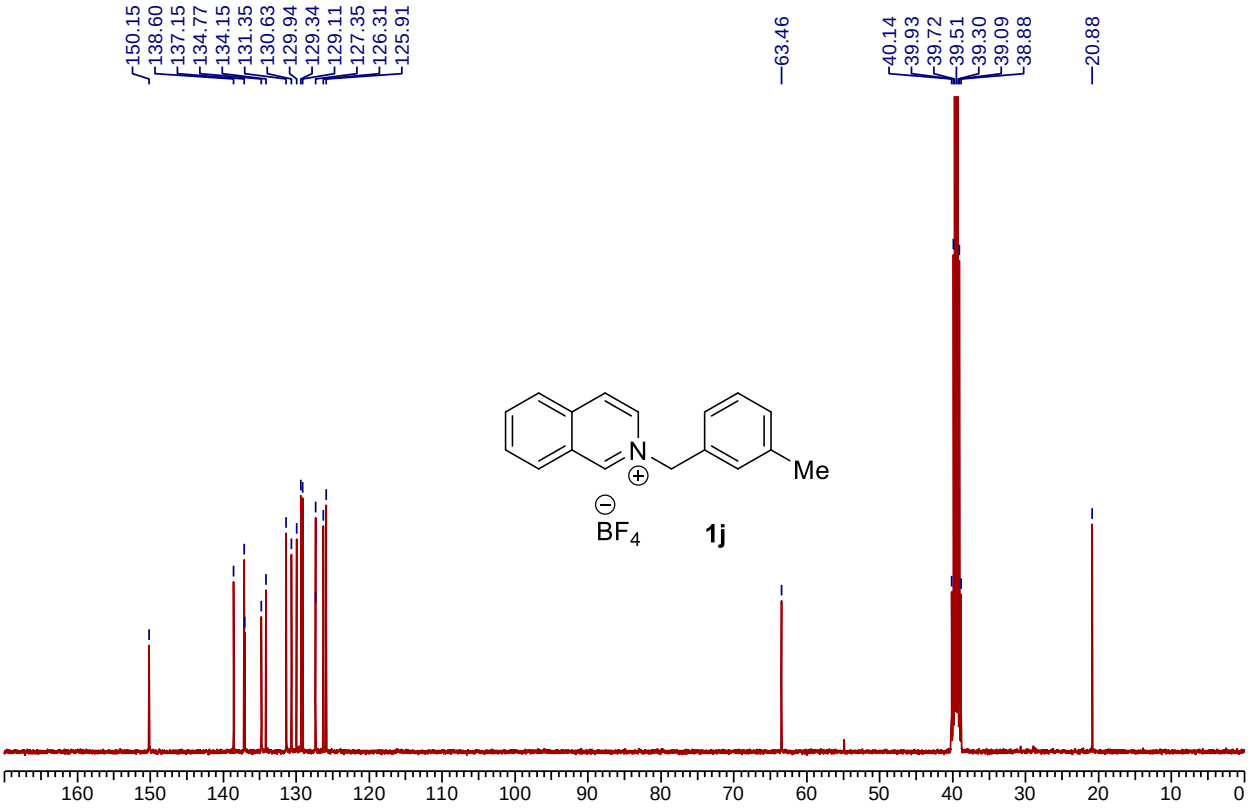

10.25
8.85
8.84
8.64
8.62
8.57
8.55
8.38
8.31
8.15
8.13
7.93
7.73
7.71
6.06
2.53
2.52
0.00
1.00
1.01
1.02
1.01
1.01
1.00
2.01
1.01
0.96
1.00
2.00
N
CN
BF4
1h
10
9
8
7
6
5
4
3
2
1
0

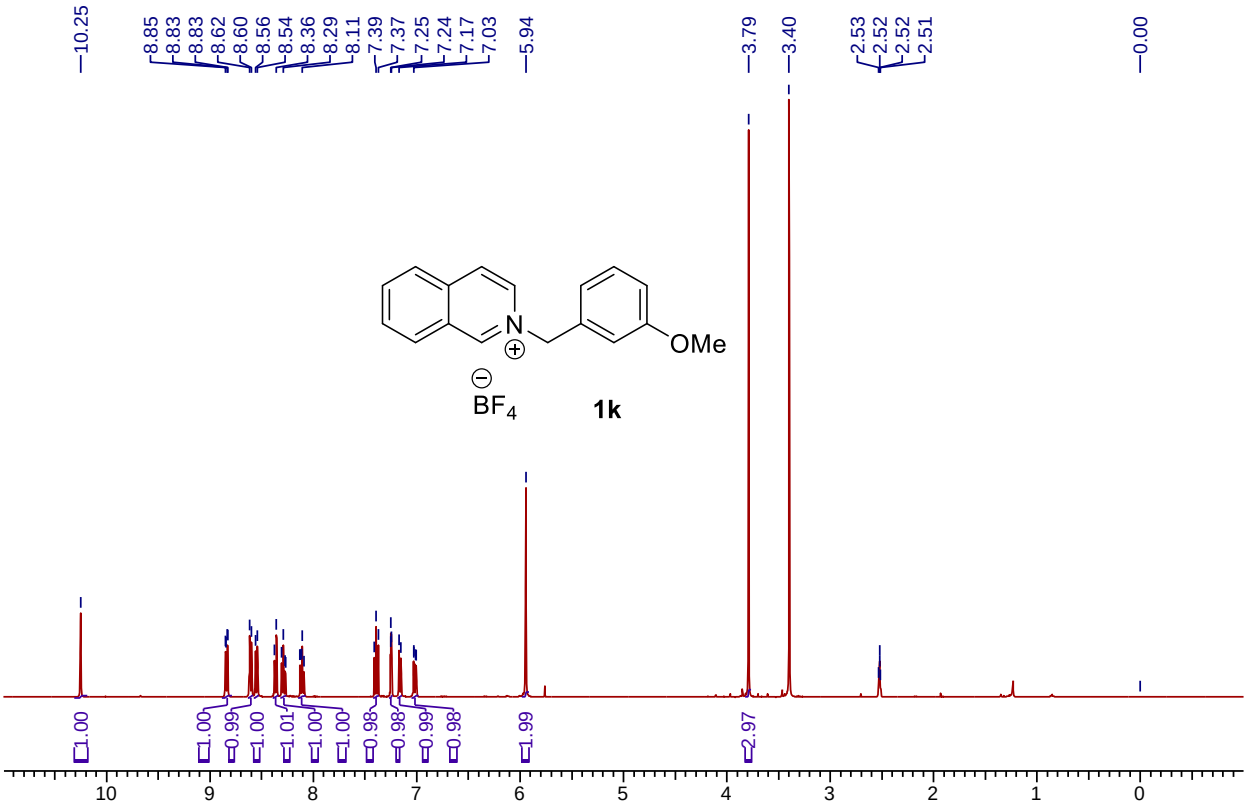

150.71
137.24
135.55
134.76
133.90
132.98
132.80
131.33
130.77
130.35
127.34
126.41
118.31
112.06
62.33
40.14
39.93
39.72
39.51
39.31
39.09
38.89
N
CN
BF4
1h
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

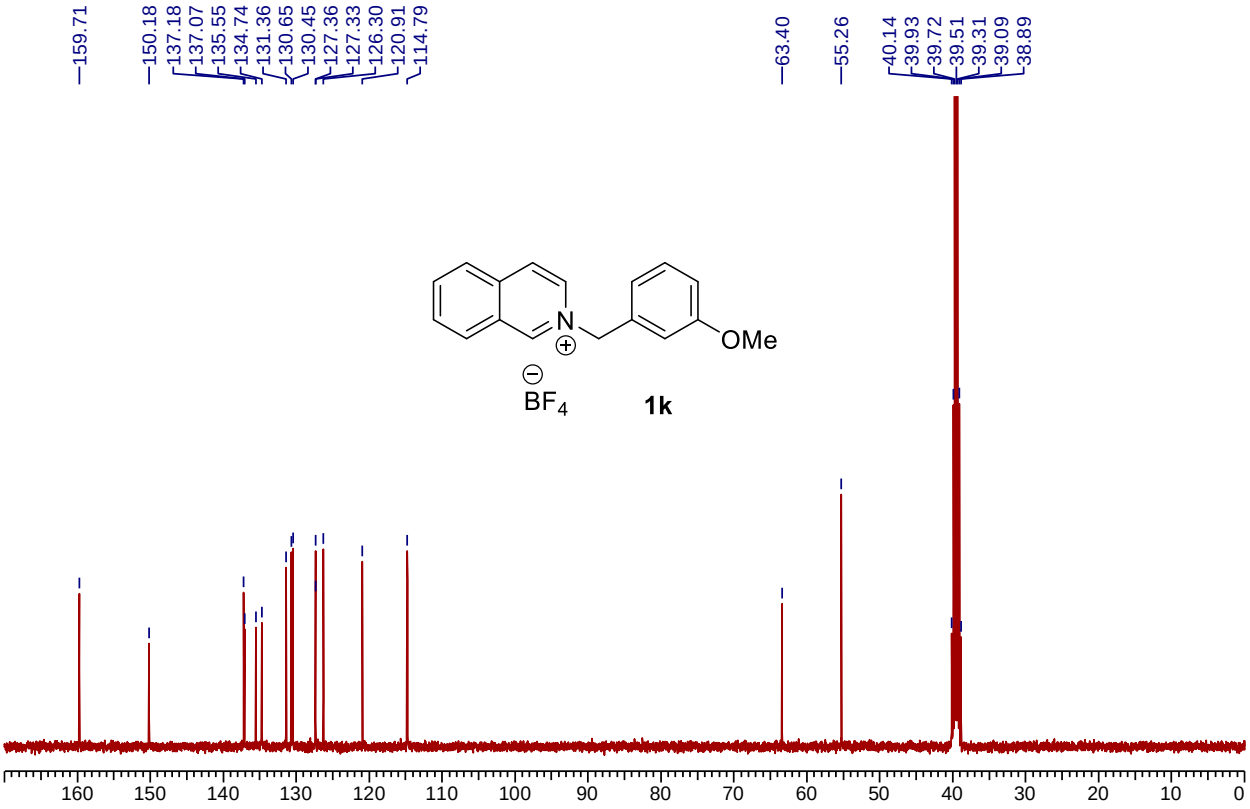

10.30
8.88
8.88
8.64
8.63
8.58
8.56
8.37
8.31
8.29
8.29
8.12
7.67
7.65
6.10
3.90
3.40
2.54
2.53
2.53
0.00
1.00
1.01
1.02
1.01
1.03
2.00
1.01
0.98
1.00
1.00
2.00
2.99
N
CO2Me
BF4
1i

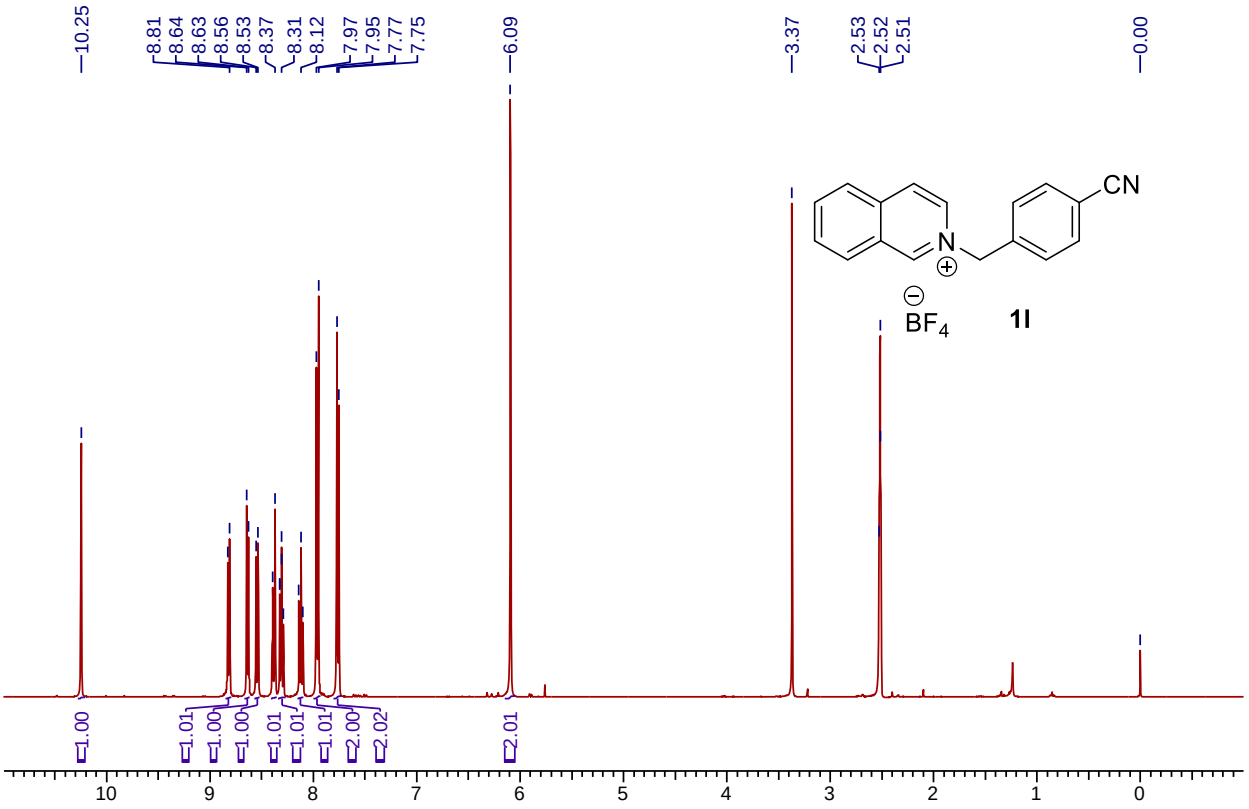

165.75
150.40
137.24
134.80
133.87
131.38
130.69
130.47
130.03
129.91
129.78
127.36
126.40
62.83
52.34
40.14
39.93
39.72
39.51
39.31
39.09
38.89
N
CO2Me
BF4
1i

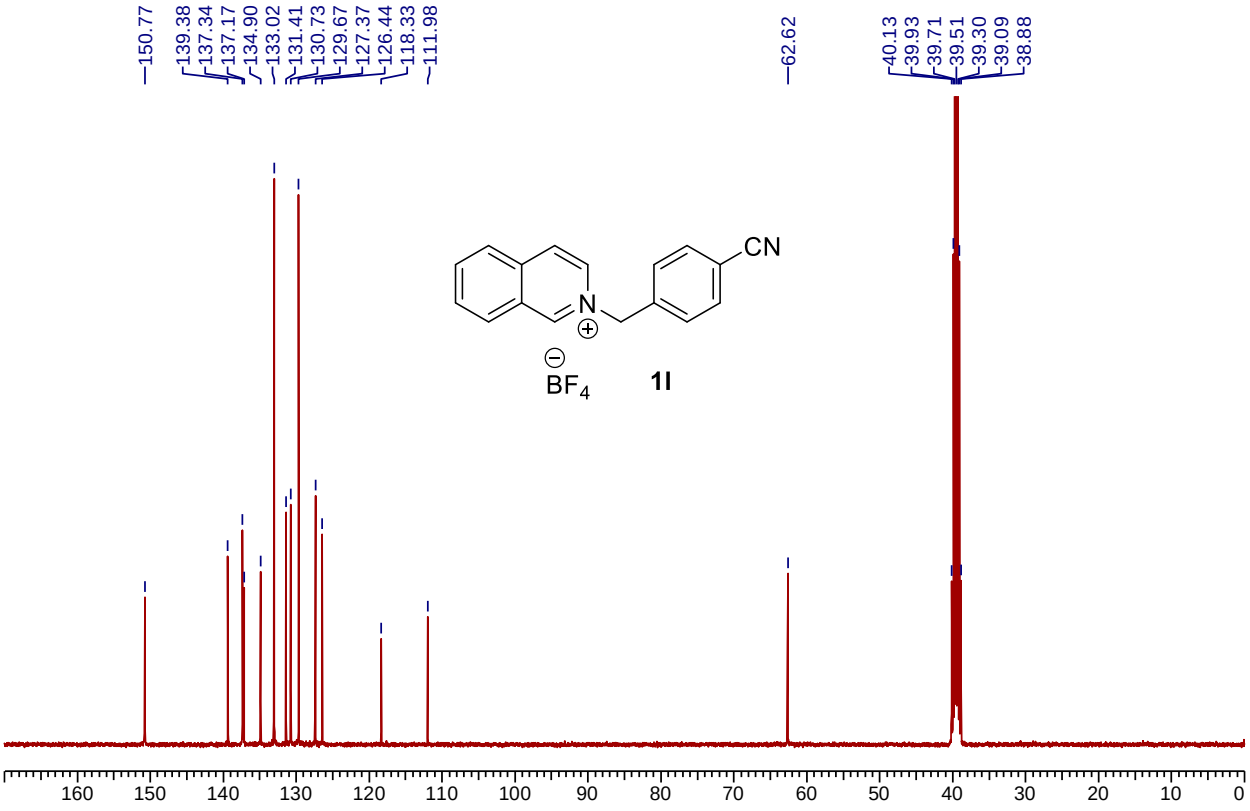

10.25
8.83
8.81
8.61
8.59
8.56
8.54
8.35
8.29
8.29
8.11
7.43
7.38
7.37
7.35
7.26
5.94
3.36
2.52
2.52
2.51
2.51
2.32
0.00
Me
BF4
1j
1.00
1.00
1.01
1.00
1.00
1.00
0.99
1.99
0.96
1.99
3.01

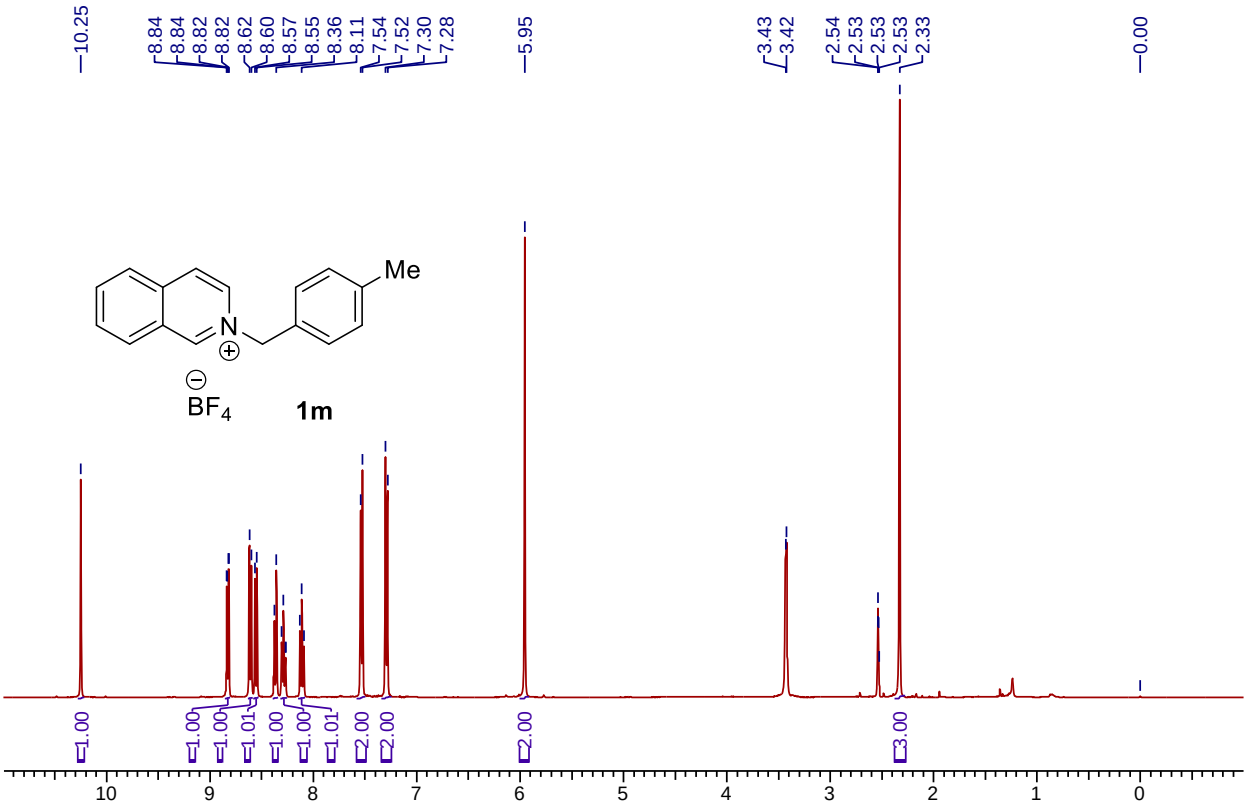

150.15
138.60
137.15
134.77
134.15
131.35
130.63
129.94
129.34
129.11
127.35
126.31
125.91
63.46
40.14
39.93
39.72
39.51
39.30
39.09
38.88
20.88
Me
BF4
1j

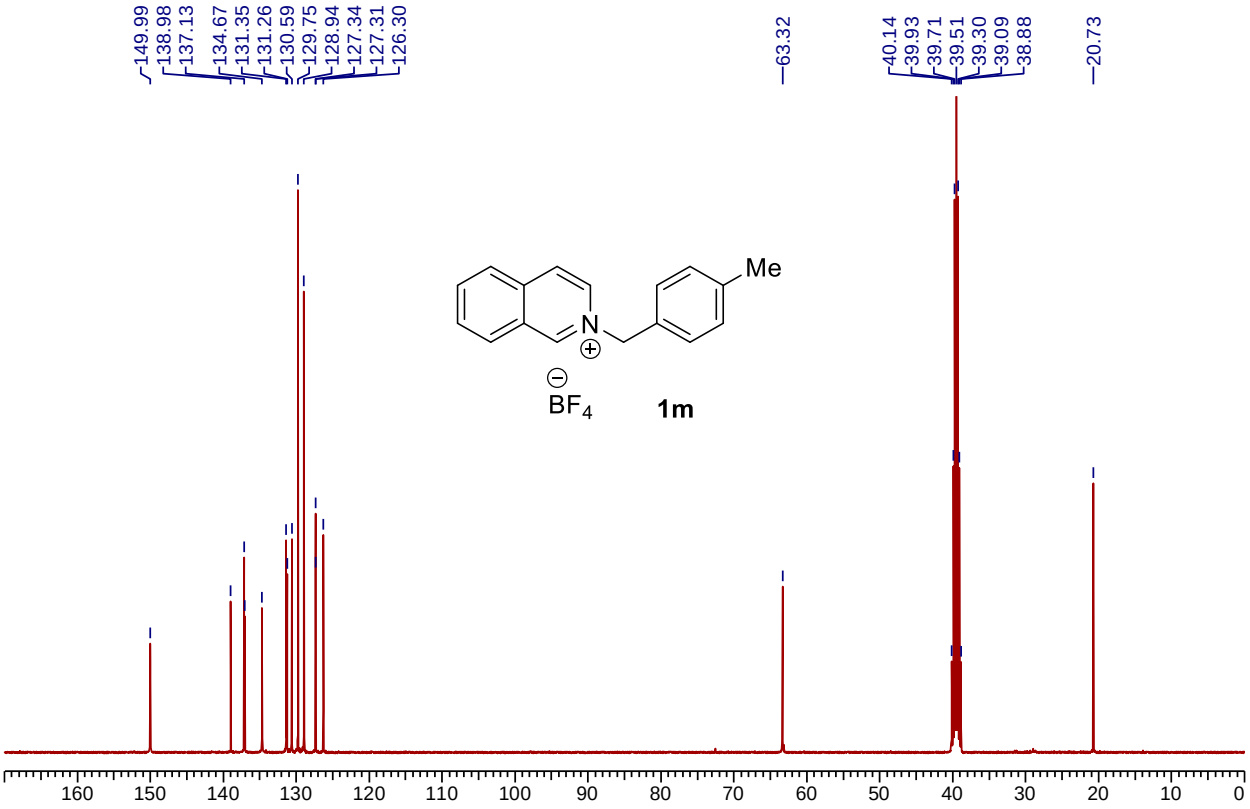

10.25
8.85
8.83
8.83
8.62
8.60
8.56
8.54
8.36
8.29
8.11
7.39
7.37
7.25
7.24
7.17
7.03
5.94
3.79
3.40
2.53
2.52
2.52
2.51
0.00
OMe
BF4
1k
1.00
0.99
1.00
1.01
1.00
1.00
0.98
0.98
0.99
0.98
1.99
2.97

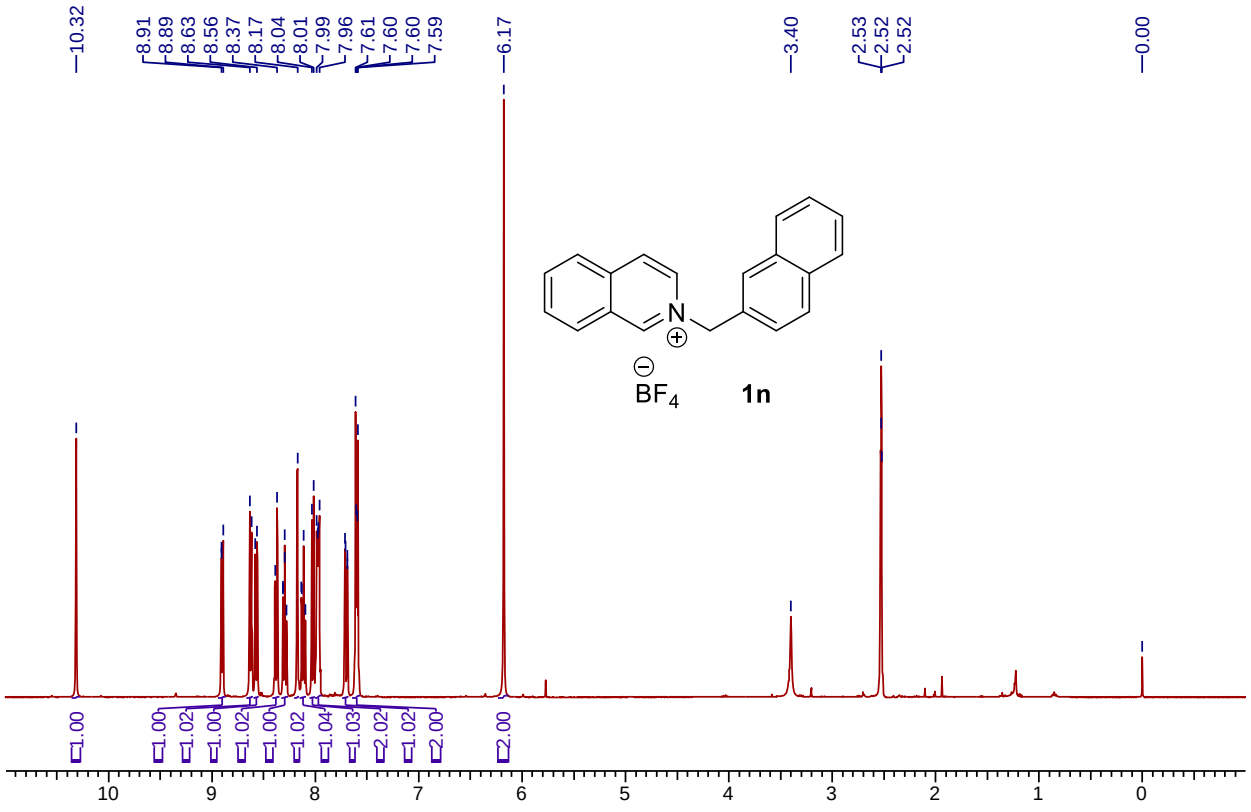

159.71
150.18
137.18
137.07
135.55
134.74
131.36
130.65
130.45
127.36
127.33
126.30
120.91
114.79
63.40
55.26
40.14
39.93
39.72
39.51
39.31
39.09
38.89
OMe
BF4
1k

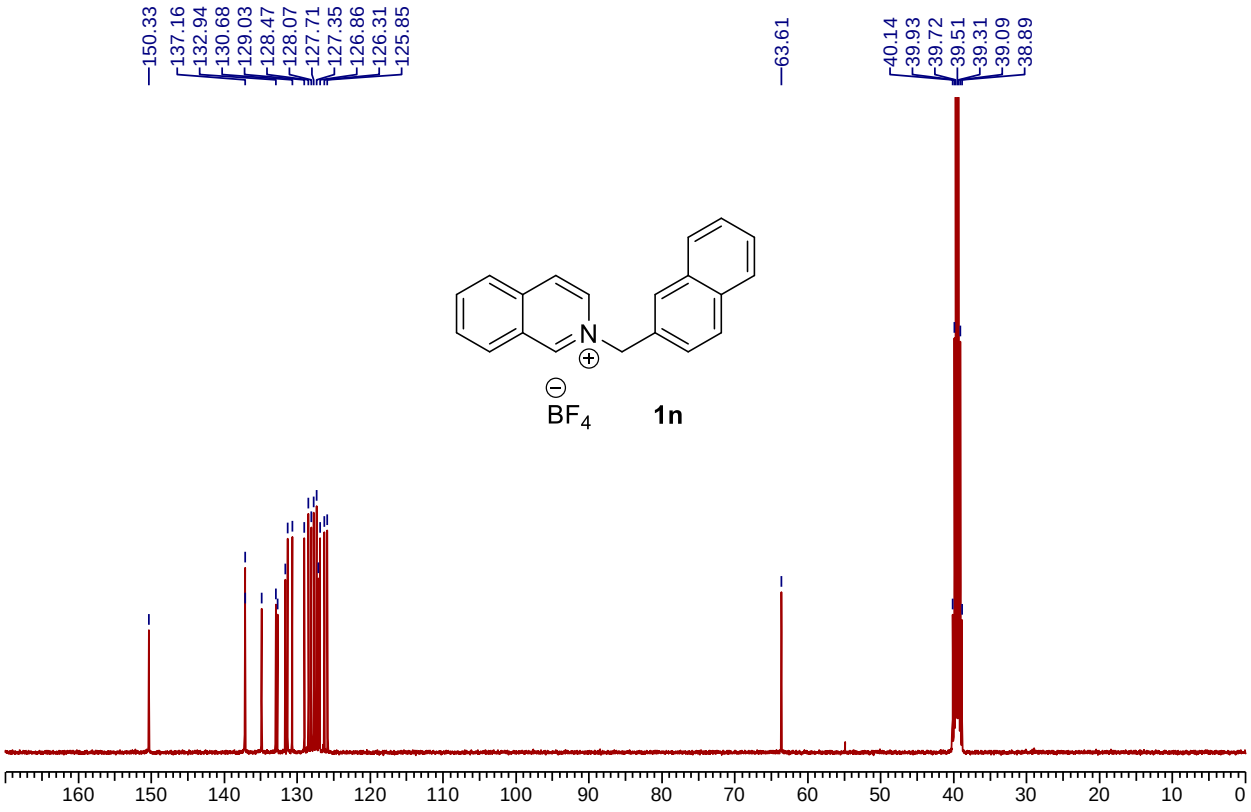

10.25
8.81
8.64
8.63
8.56
8.53
8.37
8.31
8.12
7.97
7.95
7.77
7.75
6.09
3.37
2.53
2.52
2.51
0.00
CN
N
BF4
1l
1.00
1.01
1.00
1.00
1.01
1.01
1.01
2.00
2.02
2.01

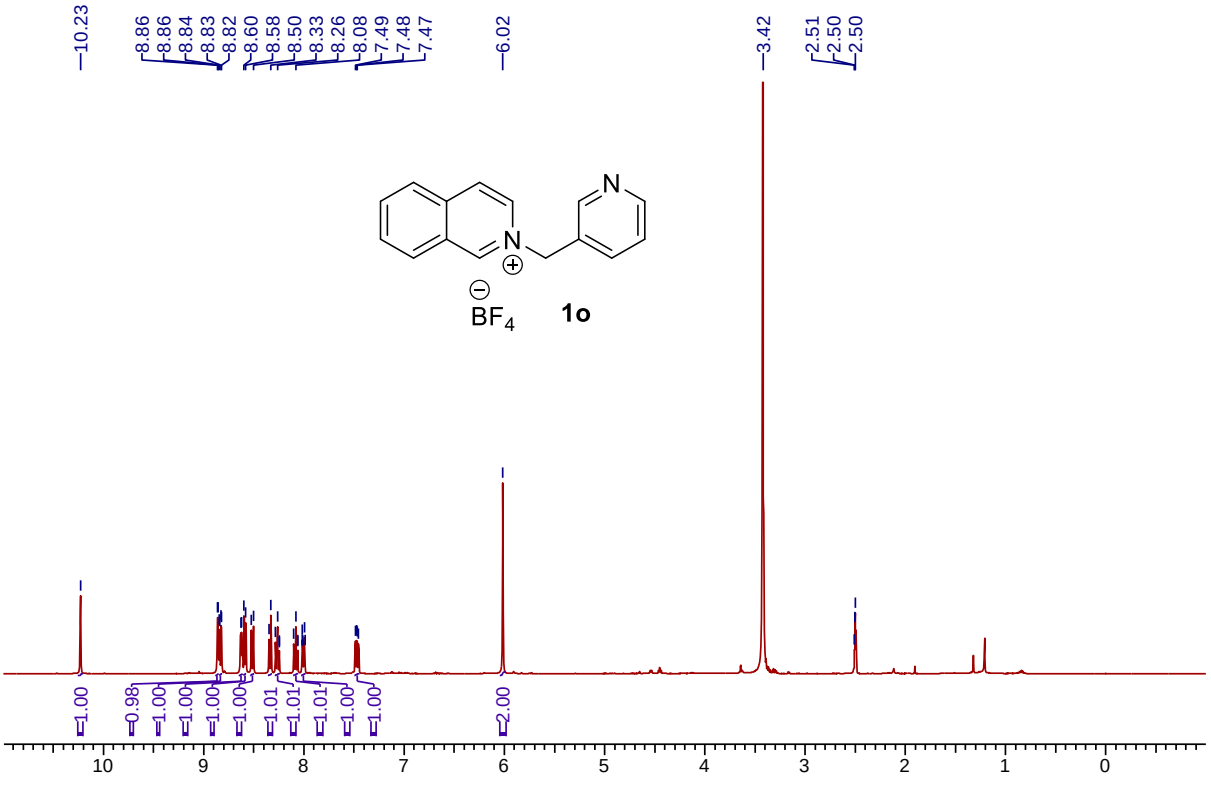

150.77
139.38
137.34
137.17
134.90
133.02
131.41
130.73
129.67
127.37
126.44
118.33
111.98
62.62
40.13
39.93
39.71
39.51
39.30
39.09
38.88
CN
N
BF4
1l

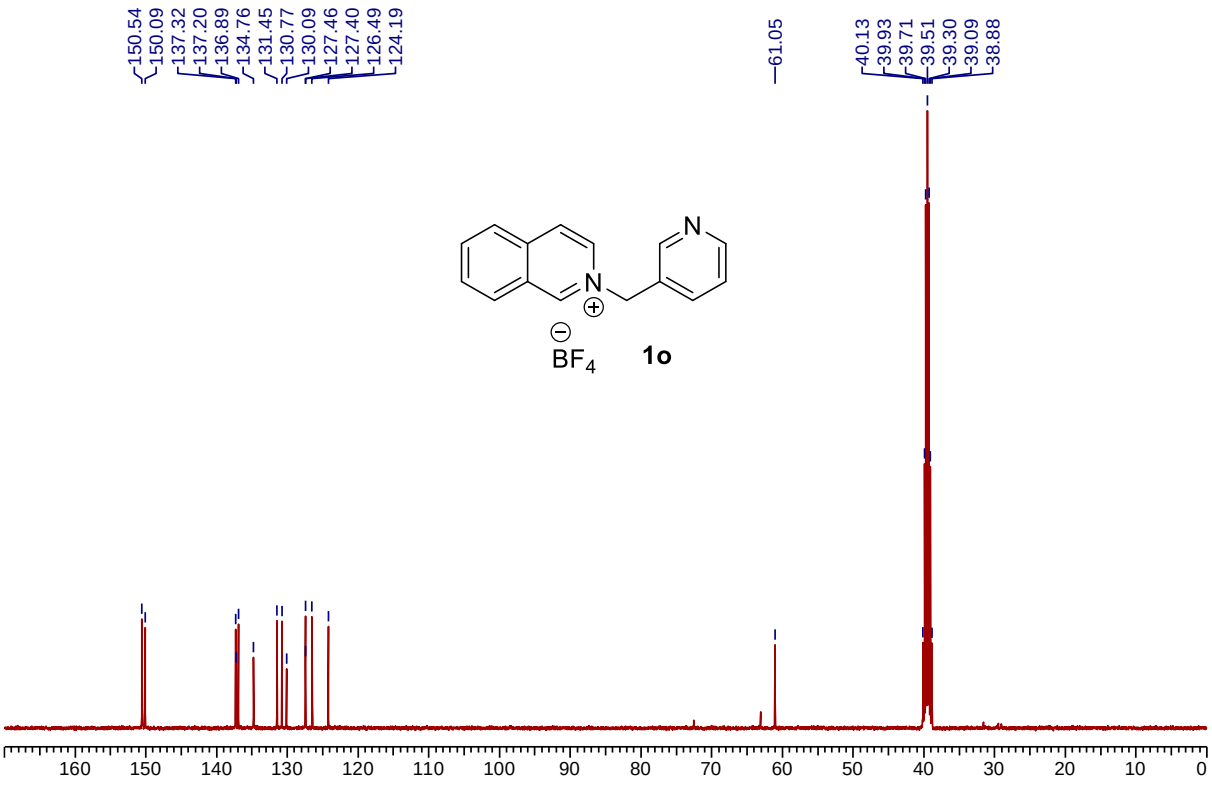

10.25
8.84
8.84
8.82
8.82
8.62
8.60
8.57
8.55
8.36
8.11
7.54
7.52
7.30
7.28
5.95
3.43
3.42
2.54
2.53
2.53
2.53
2.33
0.00
Me
N
BF4
1m
1.00
1.00
1.00
1.01
1.00
1.00
1.01
2.00
2.00
2.00
3.00
10
9
8
7
6
5
4
3
2
1
0

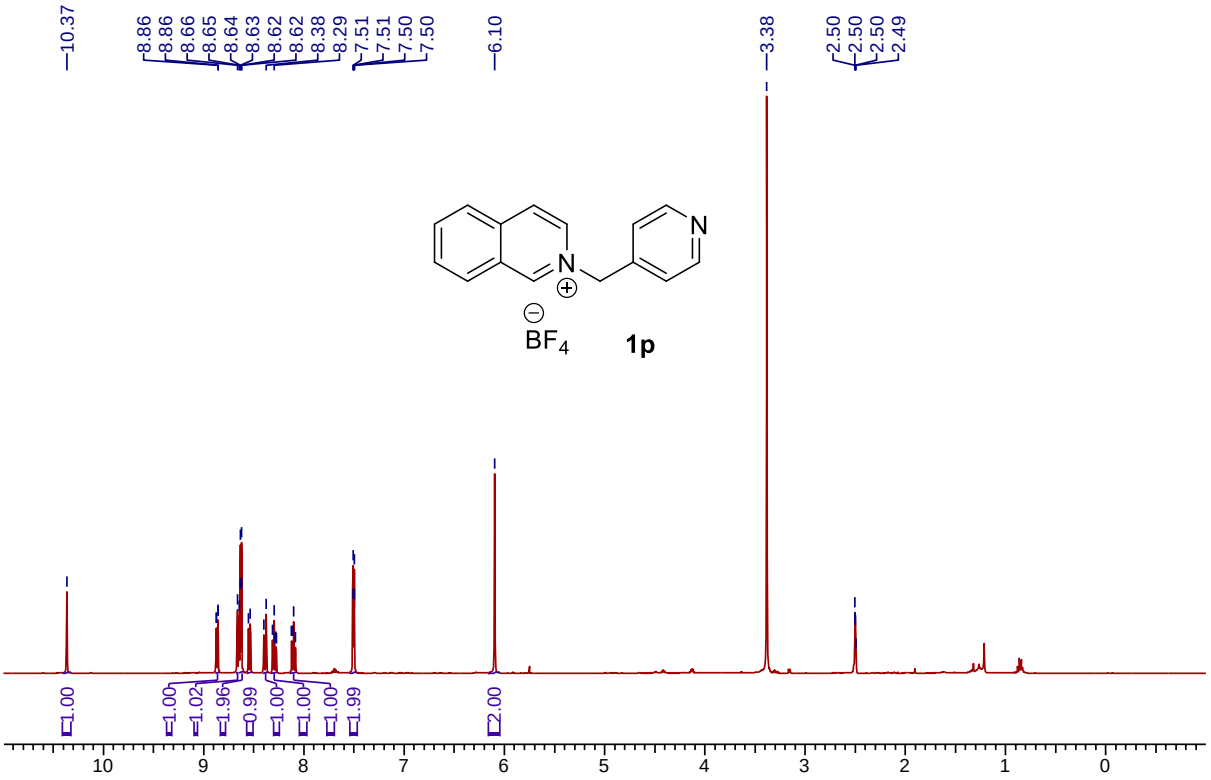

149.99
138.98
137.13
134.67
131.35
131.26
130.59
129.75
128.94
127.34
127.31
126.30
63.32
40.14
39.93
39.71
39.51
39.30
39.09
38.88
20.73
Me
N
BF4
1m
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

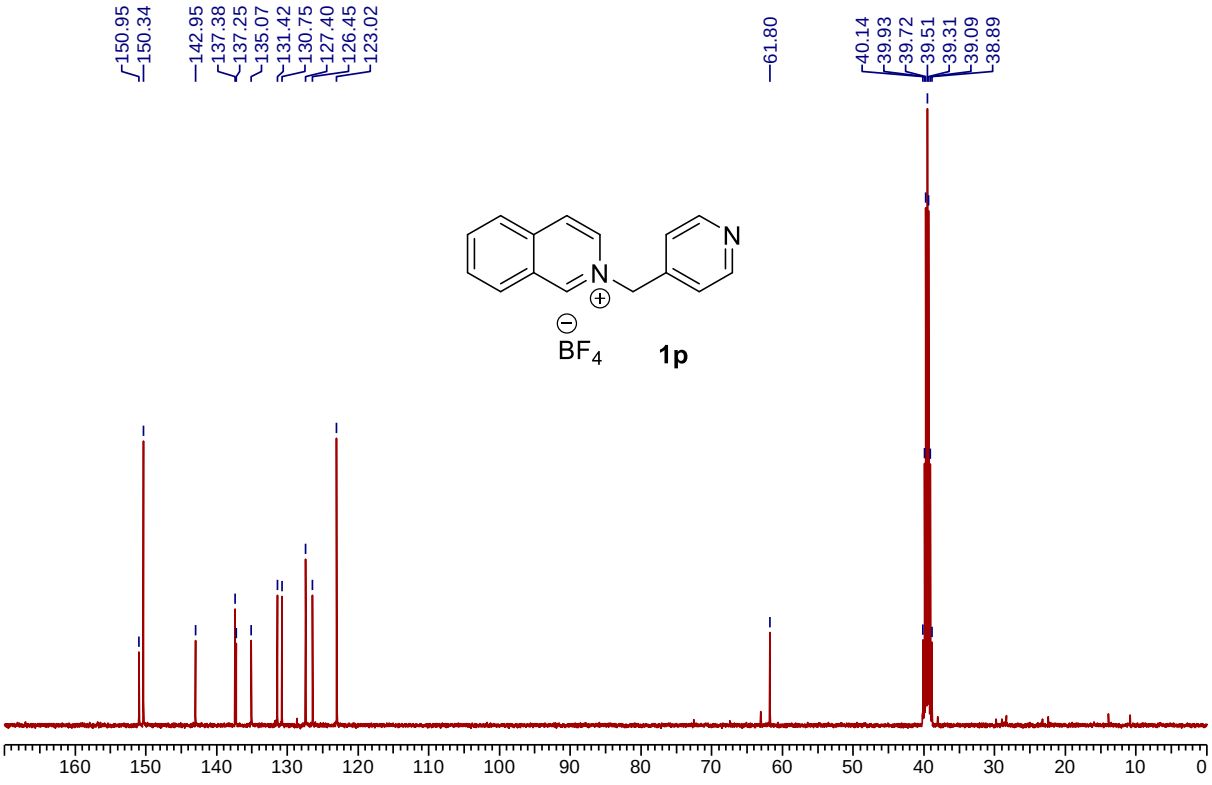

10.32
8.91
8.89
8.63
8.56
8.37
8.17
8.04
8.01
7.99
7.96
7.61
7.60
7.60
7.59
6.17
3.40
2.53
2.52
2.52
0.00
1.00
1.00
1.02
1.00
1.02
1.00
1.02
1.04
1.03
2.02
1.02
2.00
2.00
N
BF4
1n

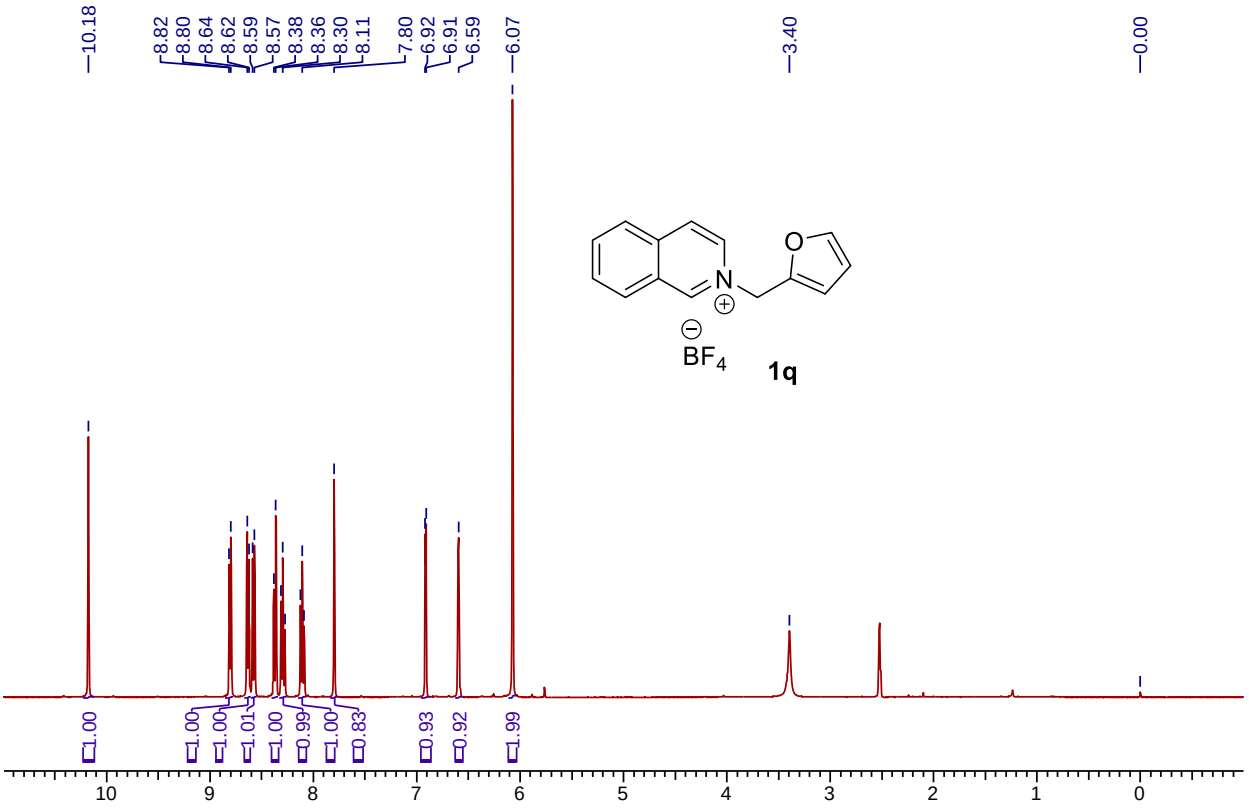

150.33
137.16
132.94
130.68
129.03
128.47
128.07
127.71
127.35
126.86
126.31
125.85
63.61
40.14
39.93
39.72
39.51
39.31
39.09
38.89
N
BF4
1n

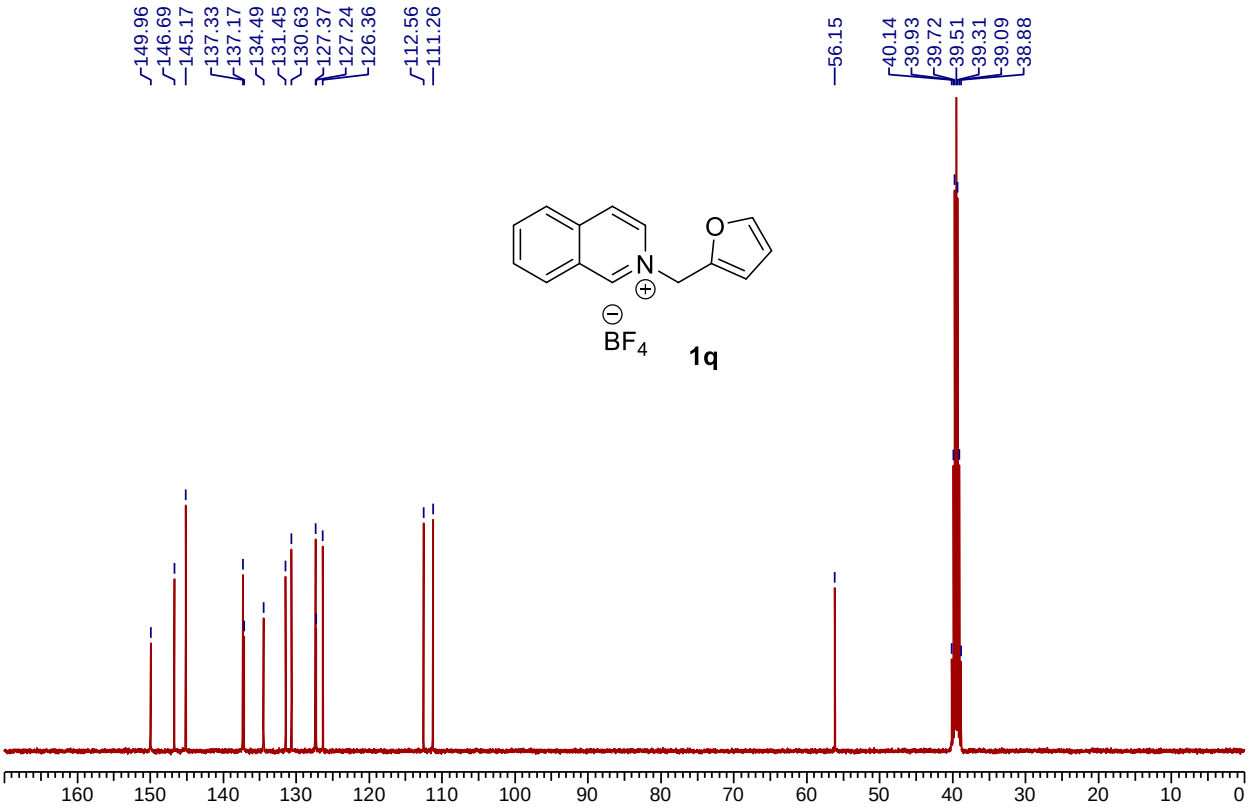

10.23
8.86
8.86
8.84
8.83
8.82
8.60
8.58
8.50
8.33
8.26
8.08
7.49
7.48
7.47
6.02
3.42
2.51
2.50
2.50
N
N
BF4
1o
1.00
0.98
1.00
1.00
1.00
1.00
1.01
1.01
1.01
1.00
1.00
2.00
10
9
8
7
6
5
4
3
2
1
0

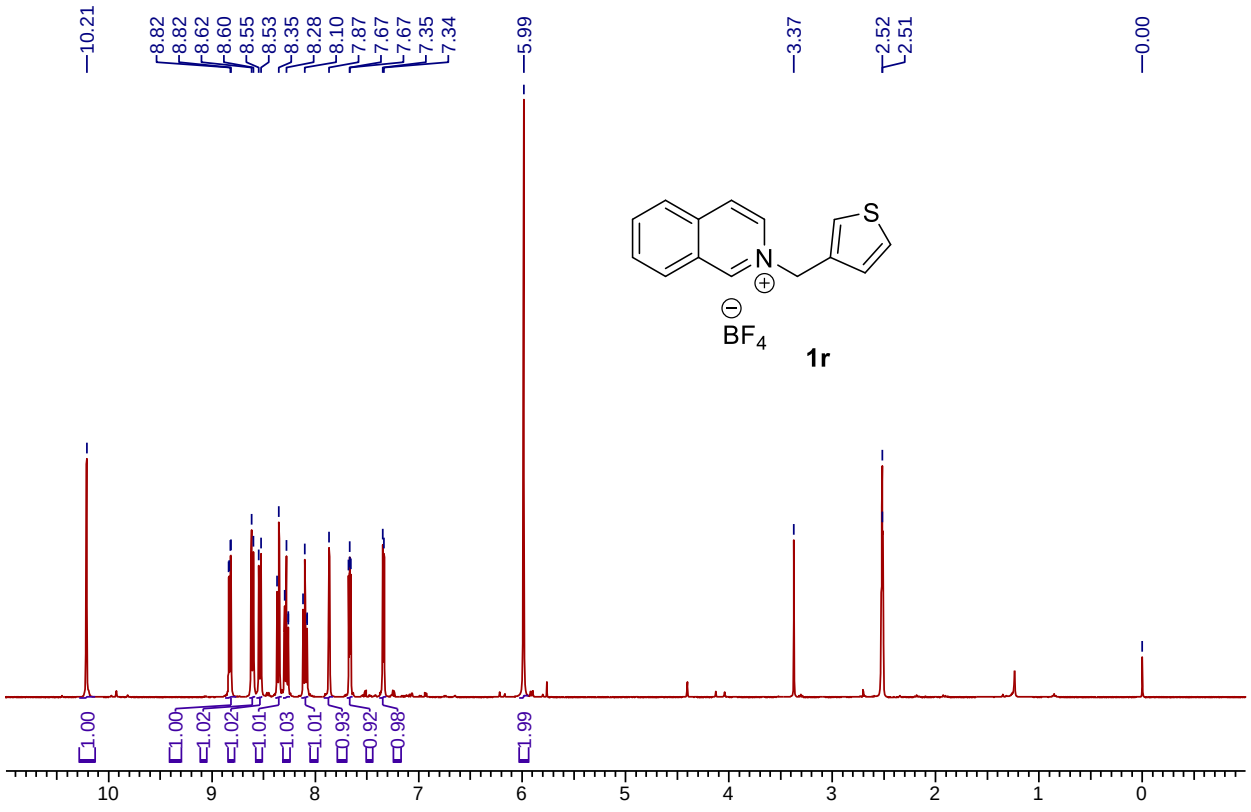

150.54
150.09
137.32
137.20
136.89
134.76
131.45
130.77
130.09
127.46
127.40
126.49
124.19
61.05
40.13
39.93
39.71
39.51
39.30
39.09
38.88
N
N
BF4
1o
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

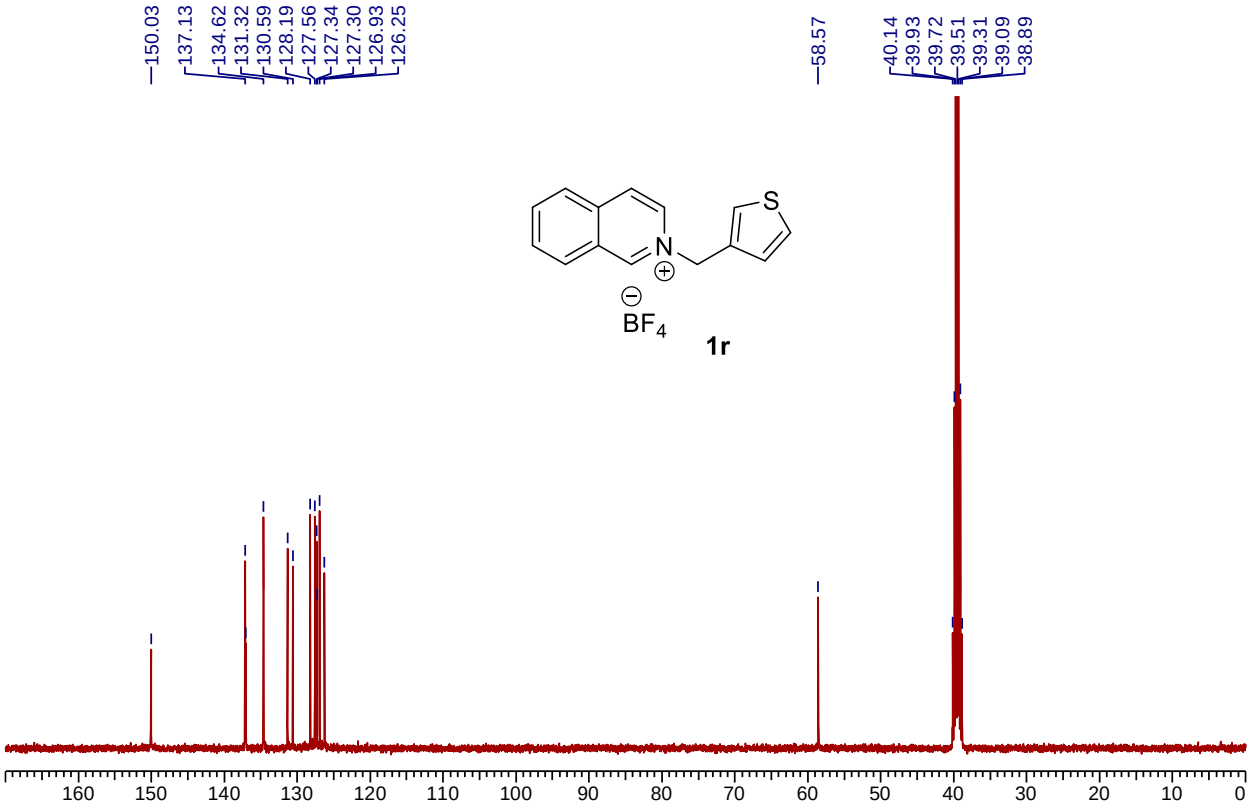

10.37
8.86
8.86
8.66
8.65
8.64
8.63
8.62
8.62
8.38
8.29
7.51
7.51
7.50
7.50
6.10
3.38
2.50
2.50
2.50
2.49
N
N
BF4
1p
1.00
1.00
1.02
1.96
0.99
1.00
1.00
1.00
1.99
2.00
10
9
8
7
6
5
4
3
2
1
0

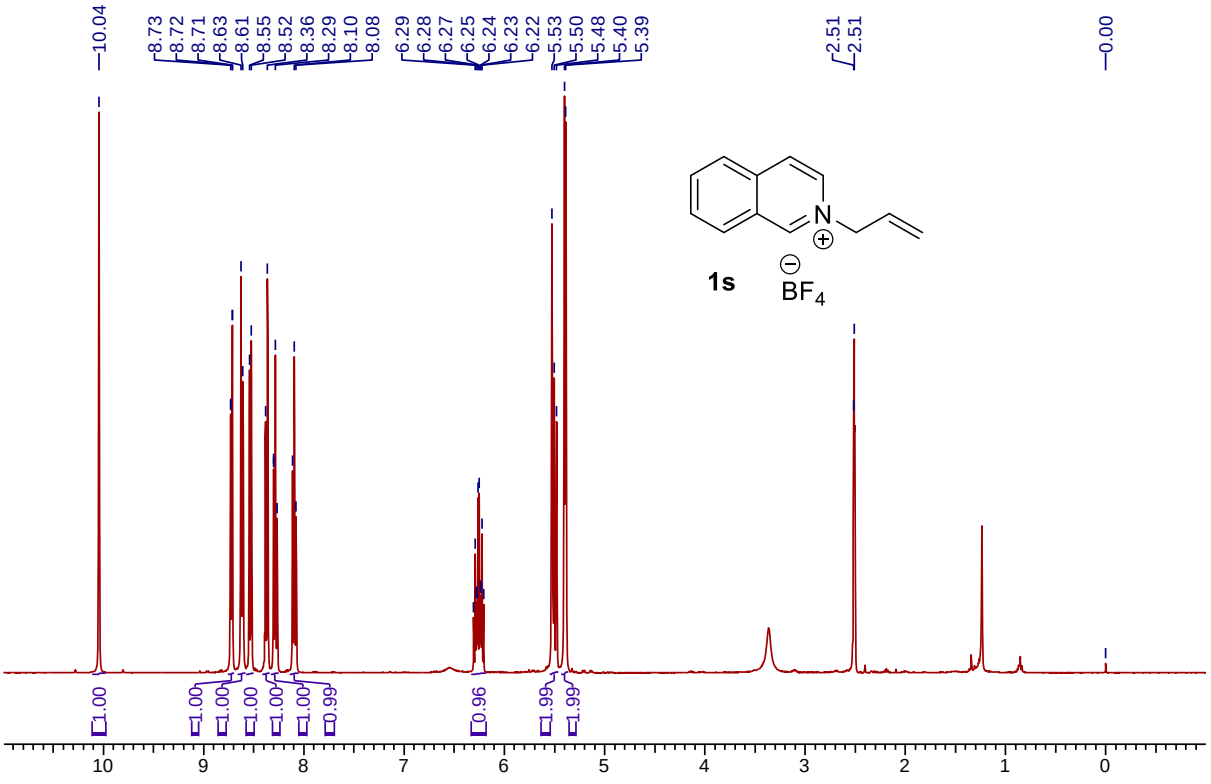

150.95
150.34
142.95
137.38
137.25
135.07
131.42
130.75
127.40
126.45
123.02
61.80
40.14
39.93
39.72
39.51
39.31
39.09
38.89
N
N
BF4
1p
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

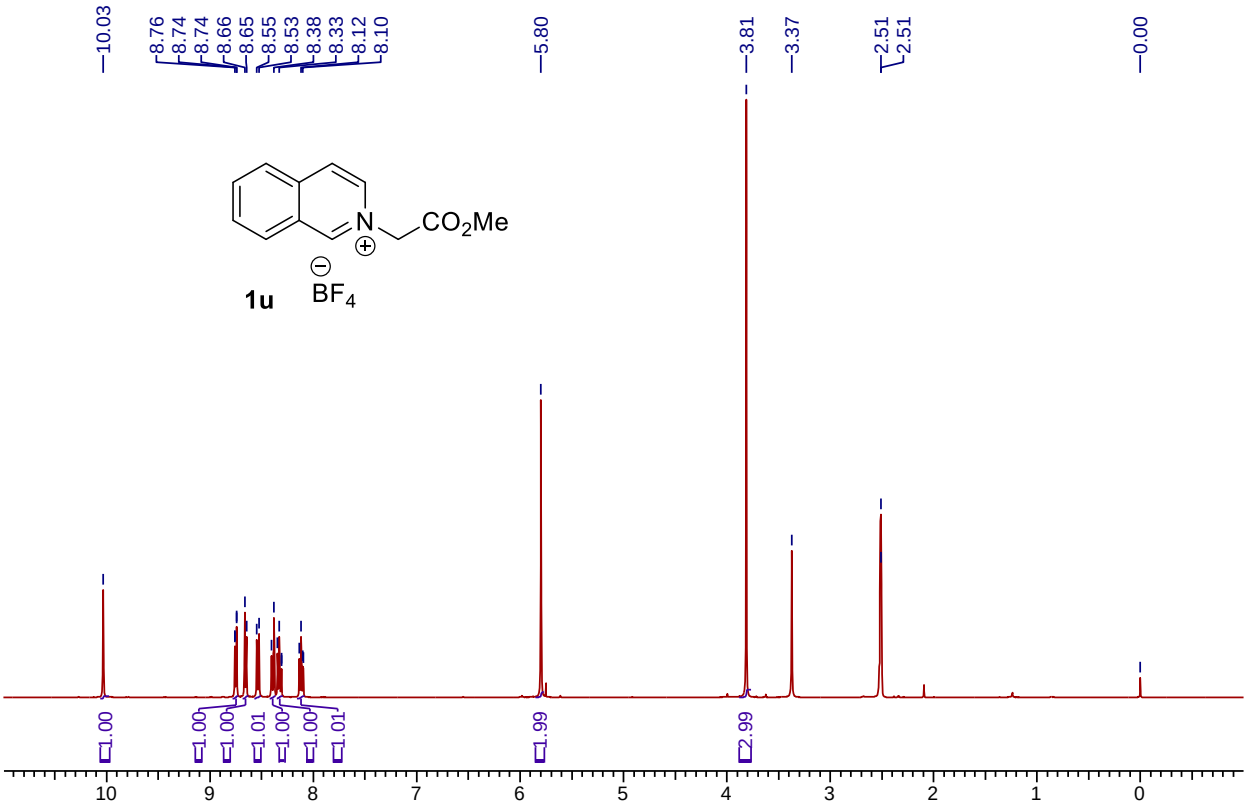

10.18
8.82
8.80
8.64
8.62
8.59
8.57
8.38
8.36
8.30
8.11
7.80
6.92
6.91
6.59
6.07
3.40
0.00
O
N
BF4
1q
1.00
1.00
1.01
1.00
0.99
1.00
0.83
0.93
0.92
1.99
10
9
8
7
6
5
4
3
2
1
0

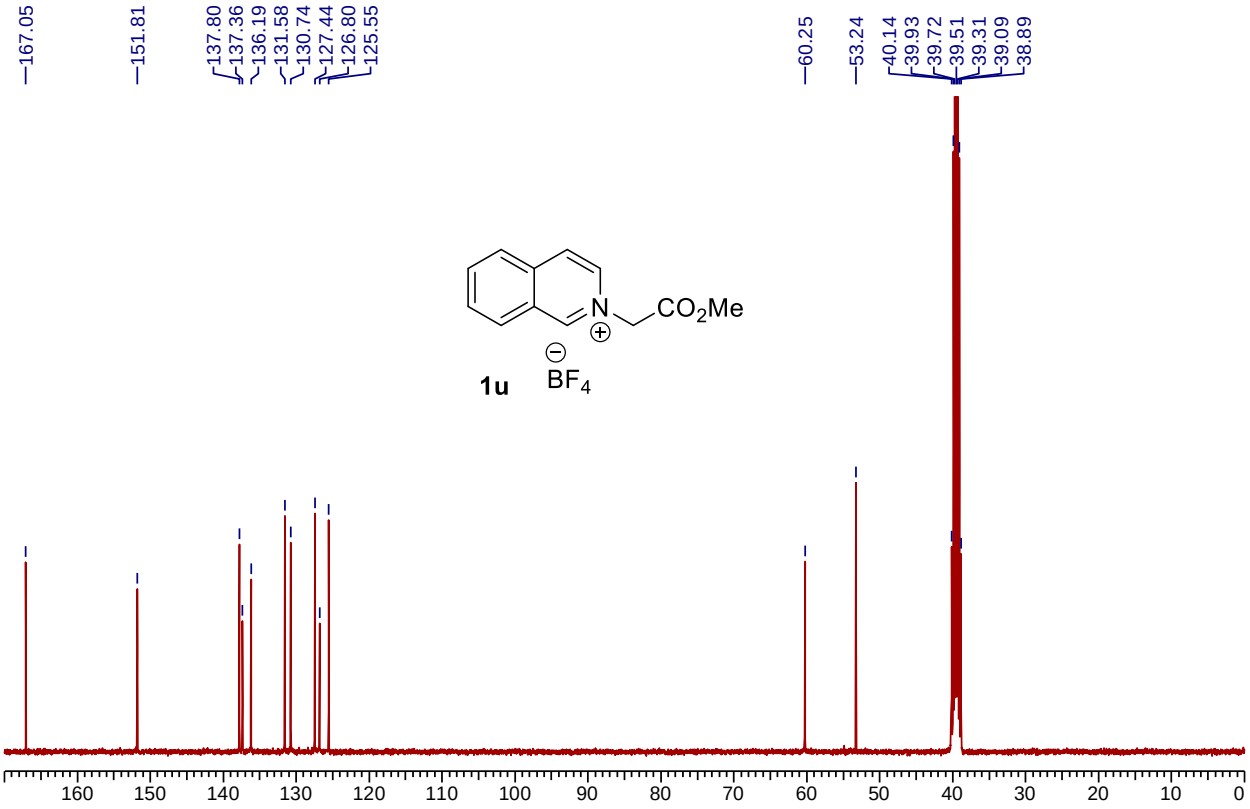

149.96
146.69
145.17
137.33
137.17
134.49
131.45
130.63
127.37
127.24
126.36
112.56
111.26
56.15
40.14
39.93
39.72
39.51
39.31
39.09
38.88
O
N
BF4
1q
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

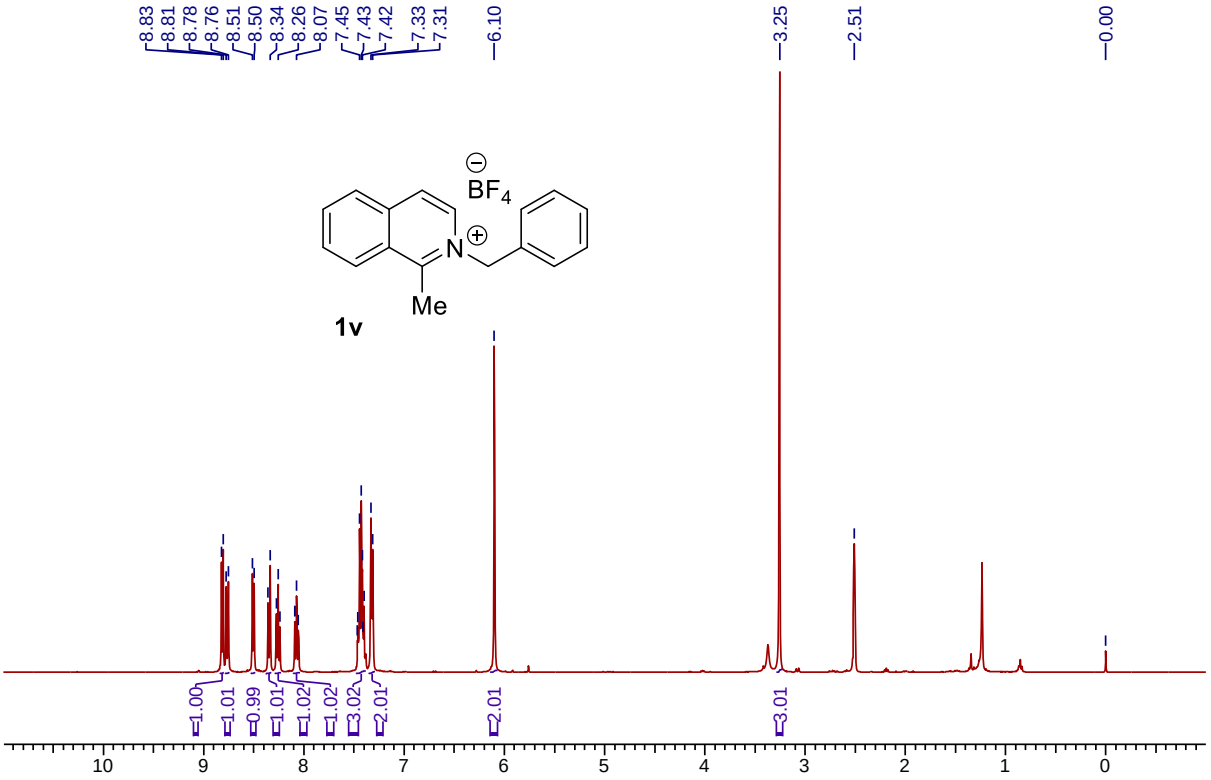

10.21
8.82
8.82
8.62
8.60
8.55
8.53
8.35
8.28
8.10
7.87
7.67
7.67
7.35
7.34
5.99
3.37
2.52
2.51
0.00
S
N
BF4
1r
1.00
1.00
1.02
1.02
1.01
1.03
1.01
0.93
0.92
0.98
1.99
10
9
8
7
6
5
4
3
2
1
0

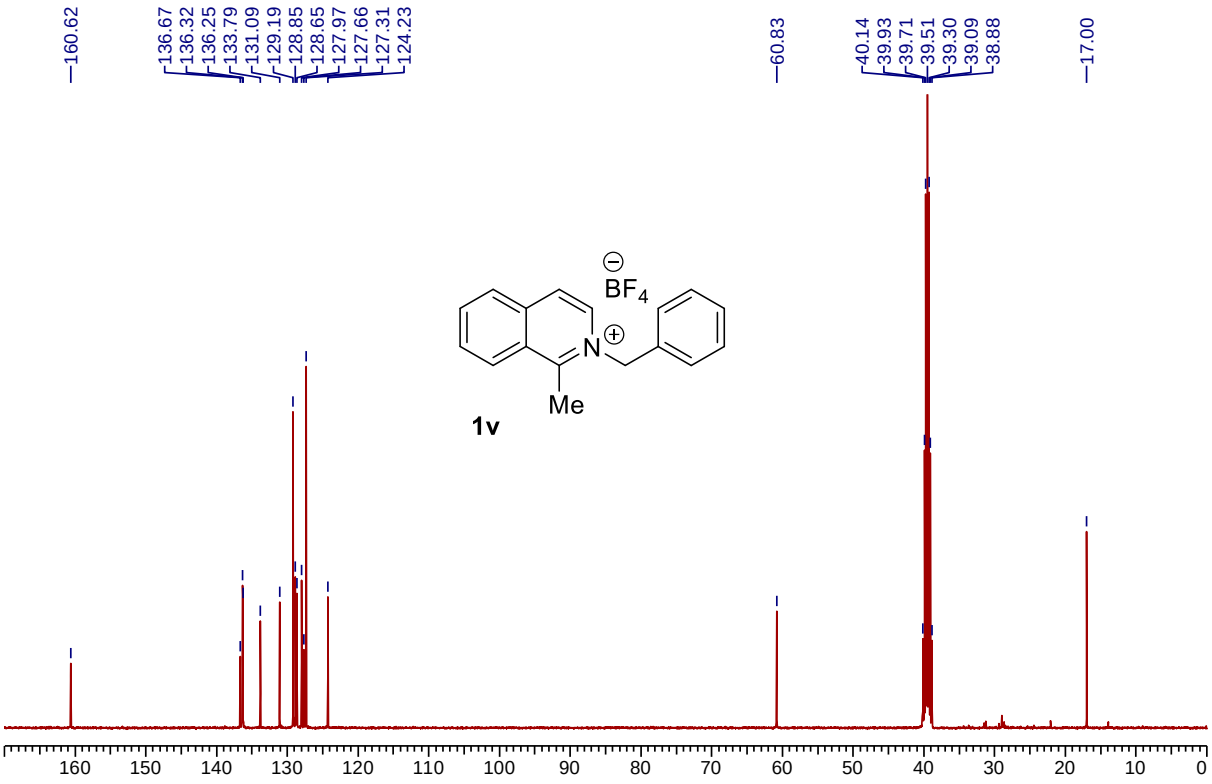

150.03
137.13
134.62
131.32
130.59
128.19
127.56
127.34
127.30
126.93
126.25
58.57
40.14
39.93
39.72
39.51
39.31
39.09
38.89
S
N
BF4
1r
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

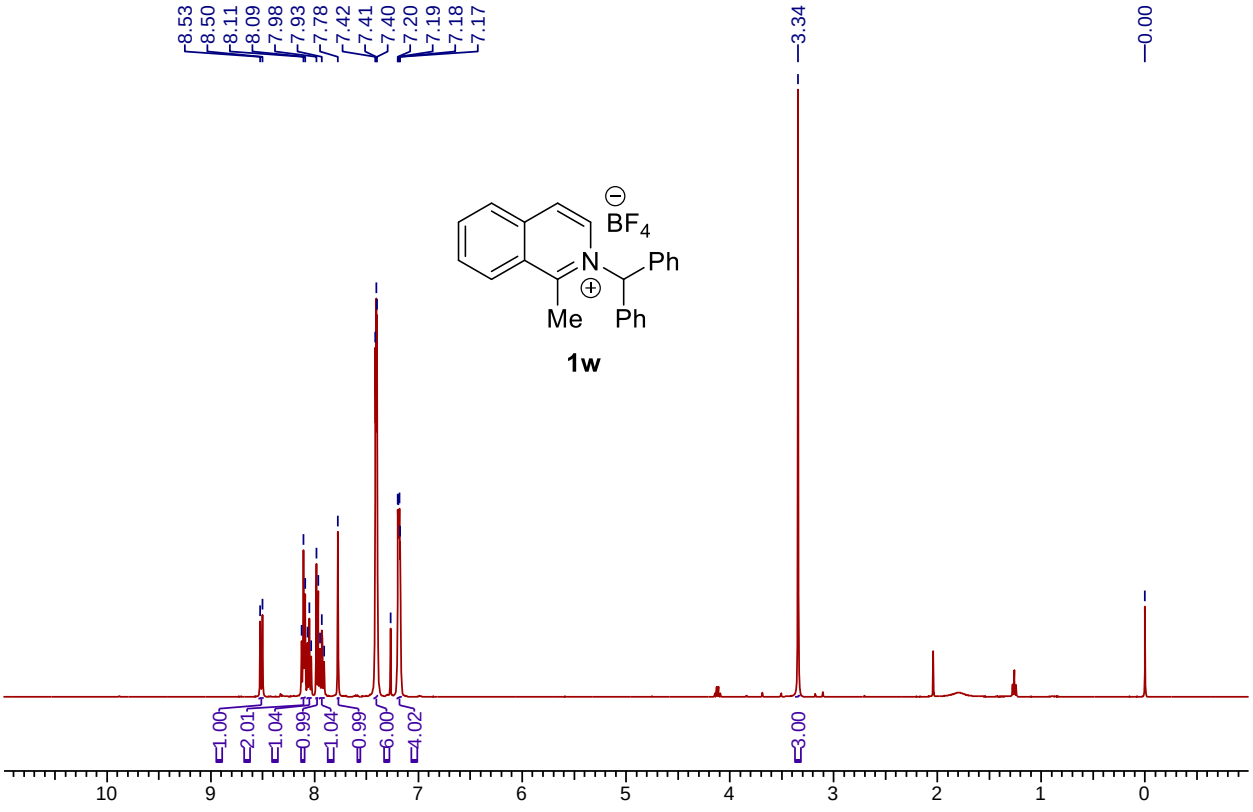

10.04
8.73
8.72
8.71
8.63
8.61
8.55
8.52
8.36
8.29
8.10
8.08
6.29
6.28
6.27
6.25
6.24
6.23
6.22
5.53
5.50
5.48
5.40
5.39
2.51
2.51
0.00
1.00
1.00
1.00
1.00
1.00
0.99
0.96
1.99
1.99
10
9
8
7
6
5
4
3
2
1
0
N
1s
BF4

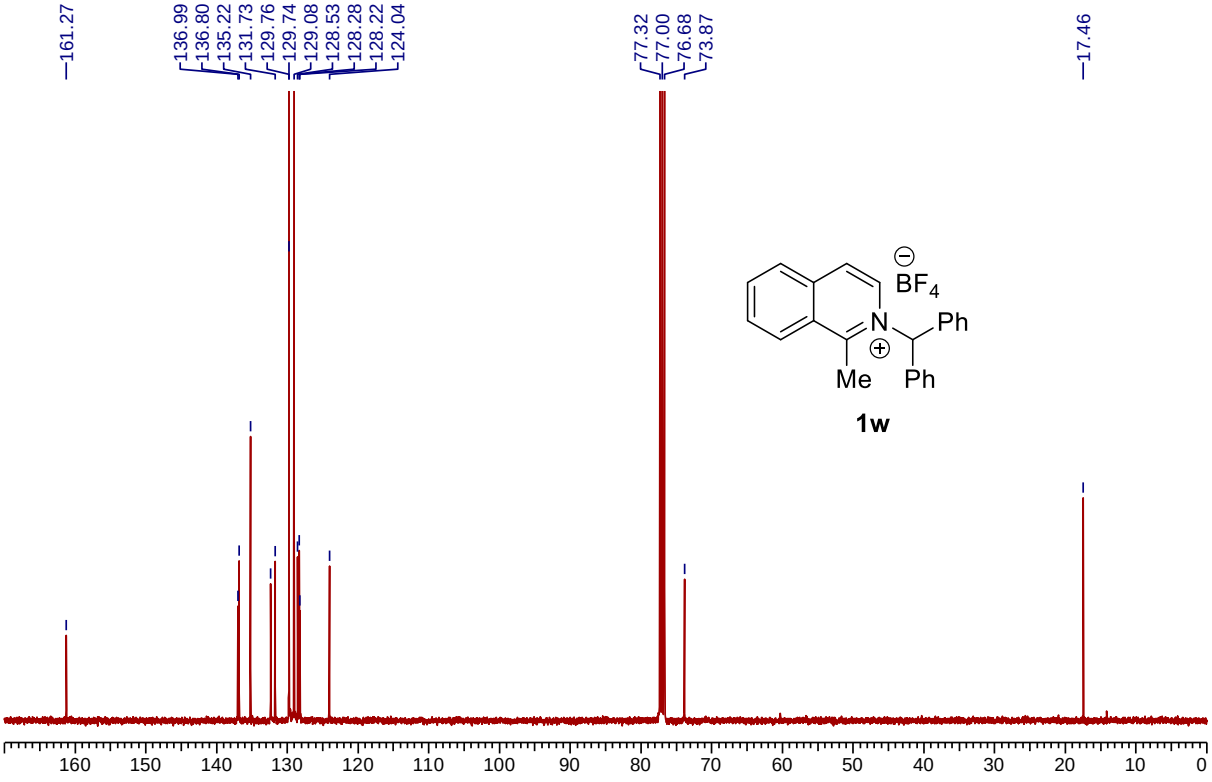

10.03
8.76
8.74
8.74
8.66
8.65
8.55
8.53
8.38
8.33
8.12
8.10
5.80
3.81
3.37
2.51
2.51
0.00
N
CO2Me
1u
BF4
1.00
1.00
1.00
1.01
1.00
1.00
1.01
1.99
2.99
10
9
8
7
6
5
4
3
2
1
0

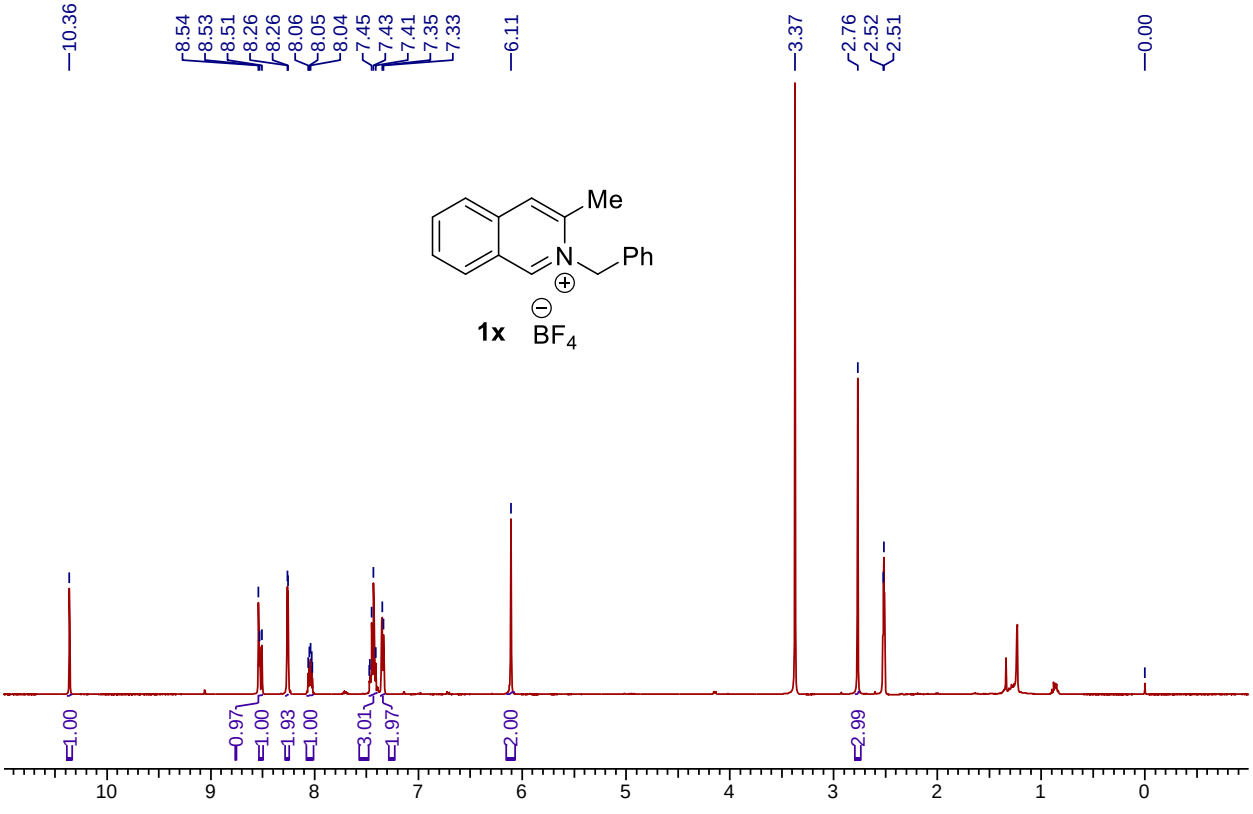

167.05
151.81
137.80
137.36
136.19
131.58
130.74
127.44
126.80
125.55
60.25
53.24
40.14
39.93
39.72
39.51
39.31
39.09
38.89
N
CO2Me
1u
BF4
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

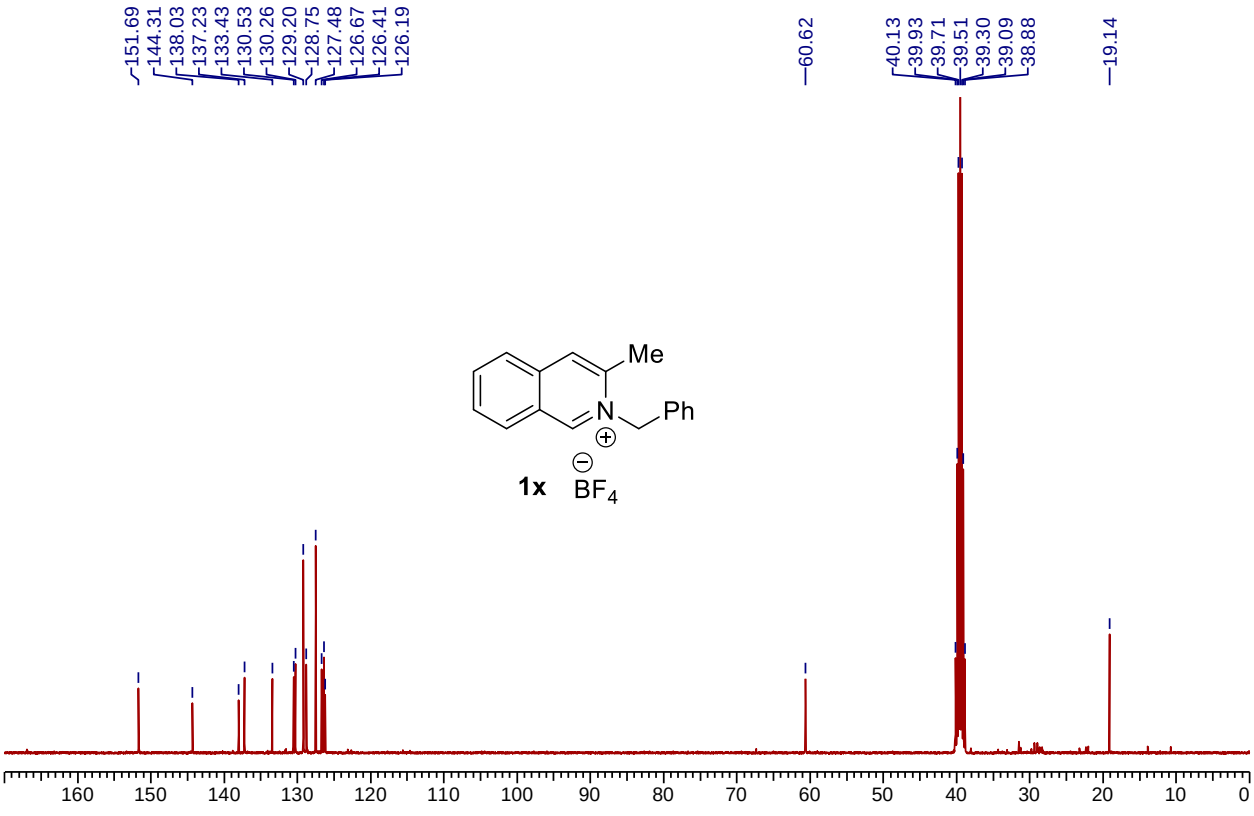

8.83
8.81
8.78
8.76
8.51
8.50
8.34
8.26
8.07
7.45
7.43
7.42
7.33
7.31
6.10
3.25
2.51
0.00
BF4
N
Me
1v
1.00
1.01
0.99
1.01
1.02
1.02
3.02
2.01
2.01
3.01
10
9
8
7
6
5
4
3
2
1
0

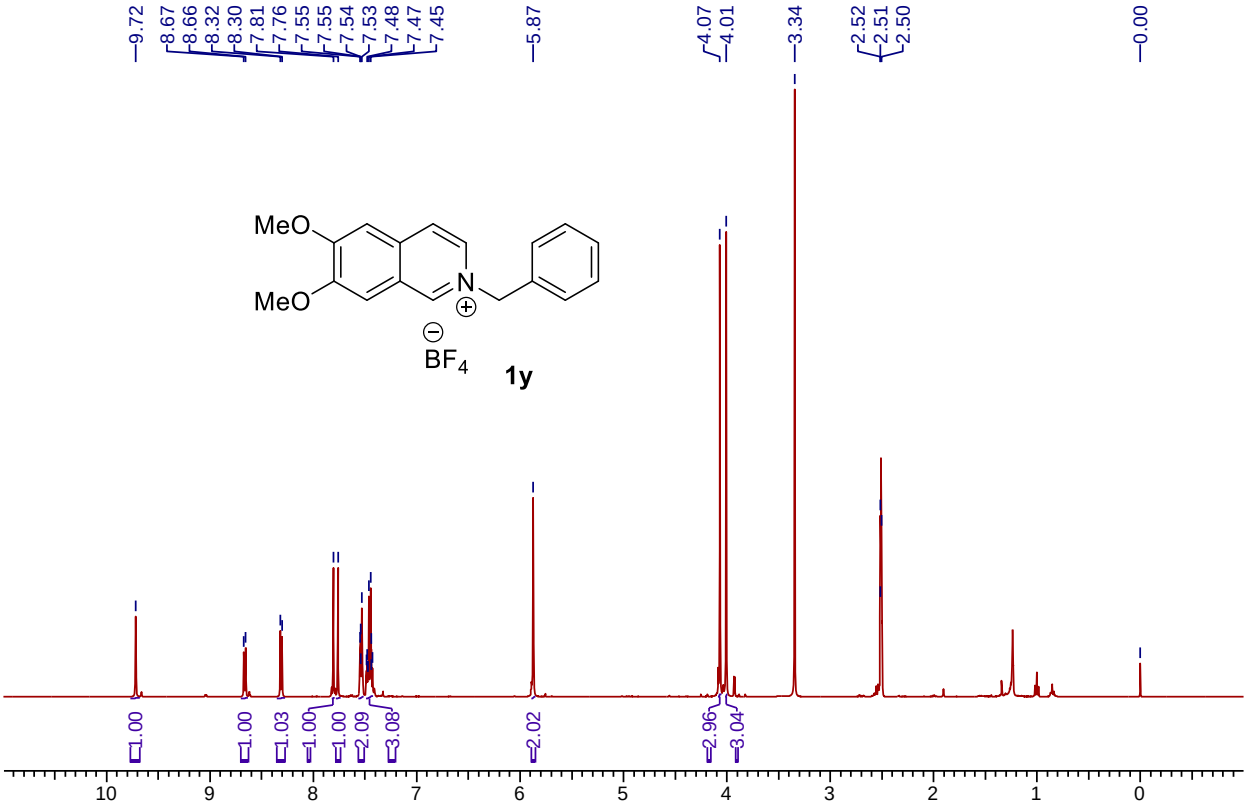

160.62
136.67
136.32
136.25
133.79
131.09
129.19
128.85
128.65
127.97
127.66
127.31
124.23
60.83
40.14
39.93
39.71
39.51
39.30
39.09
38.88
17.00
BF4
N
Me
1v
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

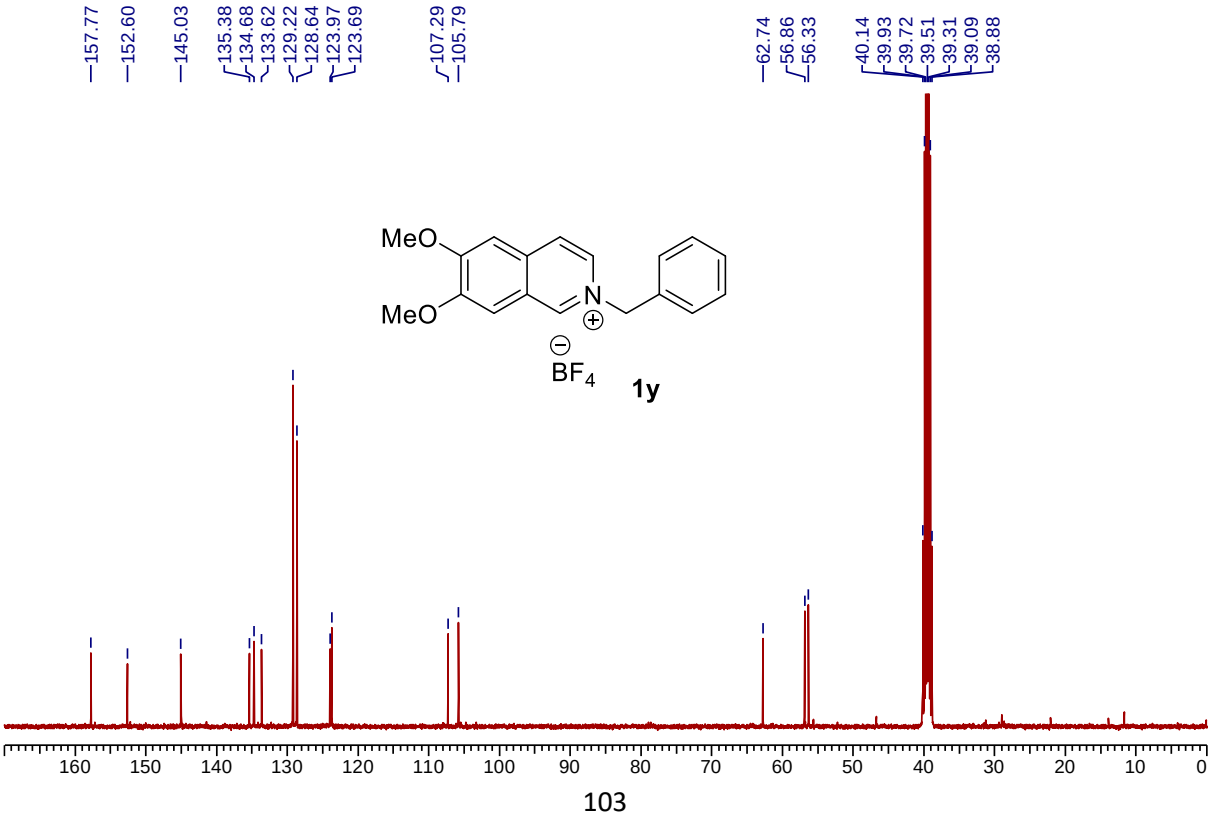

8.53
8.50
8.11
8.09
7.98
7.93
7.78
7.42
7.41
7.40
7.20
7.19
7.18
7.17
3.34
0.00
BF4
N
Ph
Me
Ph
1w
1.00
2.01
1.04
0.99
1.04
0.99
6.00
4.02
3.00
10
9
8
7
6
5
4
3
2
1
0

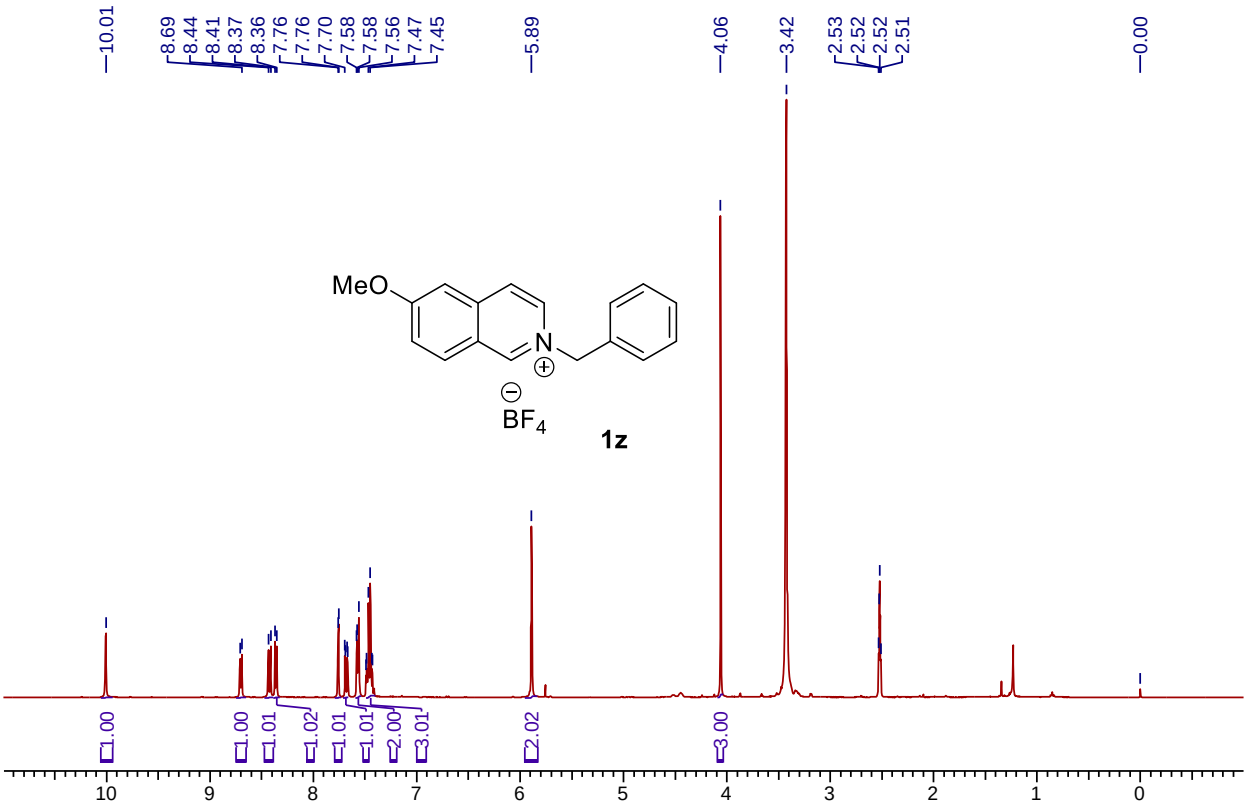

161.27
136.99
136.80
135.22
131.73
129.76
129.74
129.08
128.53
128.28
128.22
124.04
77.32
77.00
76.68
73.87
17.46
BF4
N
Ph
Me
Ph
1w
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

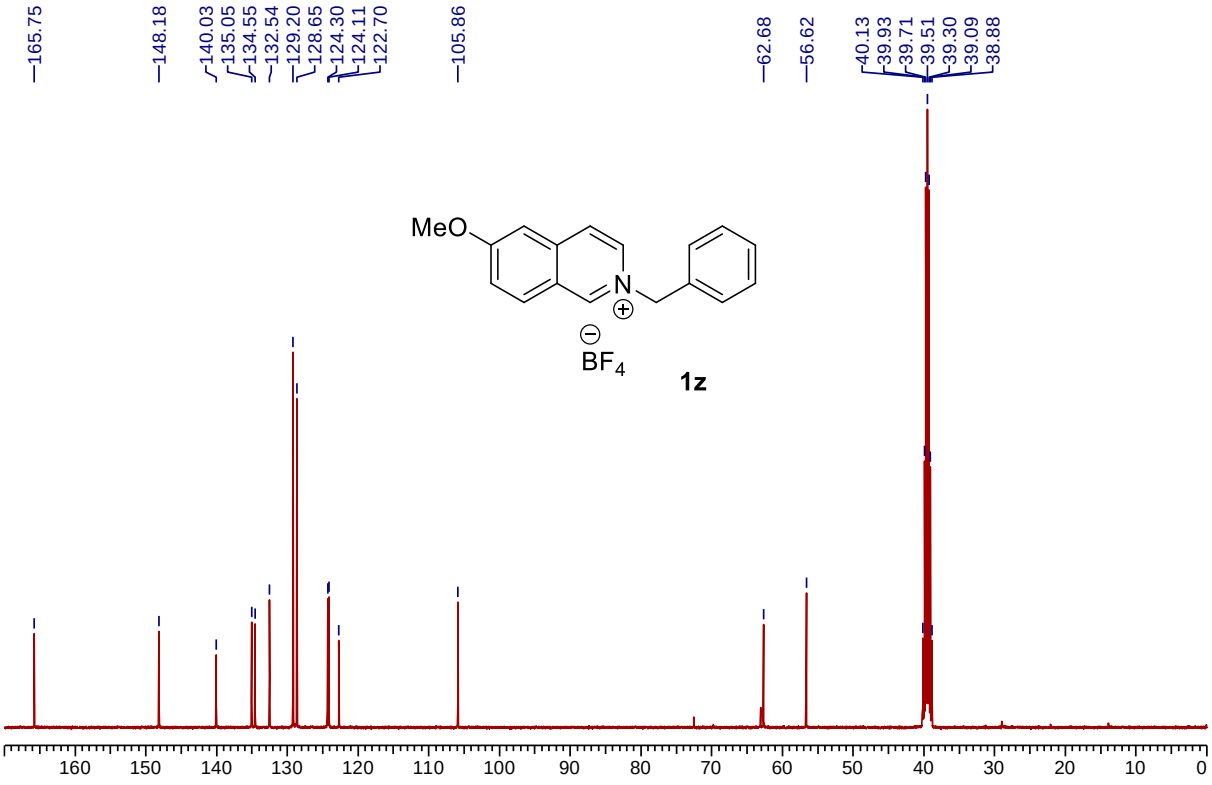

10.36
8.54
8.53
8.51
8.26
8.26
8.06
8.05
8.04
7.45
7.43
7.41
7.35
7.33
6.11
3.37
2.76
2.52
2.51
0.00
Me
N
Ph
1x
BF4
1.00
0.97
1.00
1.93
1.00
3.01
1.97
2.00
2.99

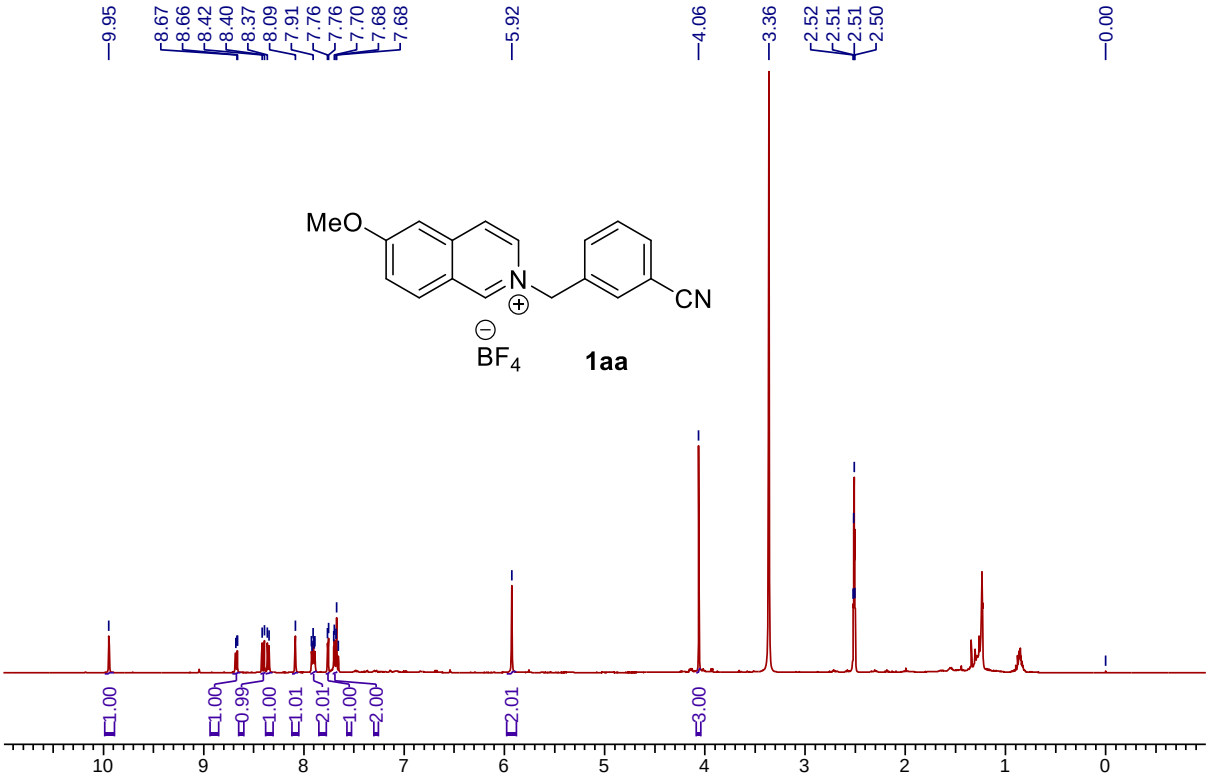

151.69
144.31
138.03
137.23
133.43
130.53
130.26
129.20
128.75
127.48
126.67
126.41
126.19
60.62
40.13
39.93
39.71
39.51
39.30
39.09
38.88
19.14
Me
N
Ph
1x
BF4

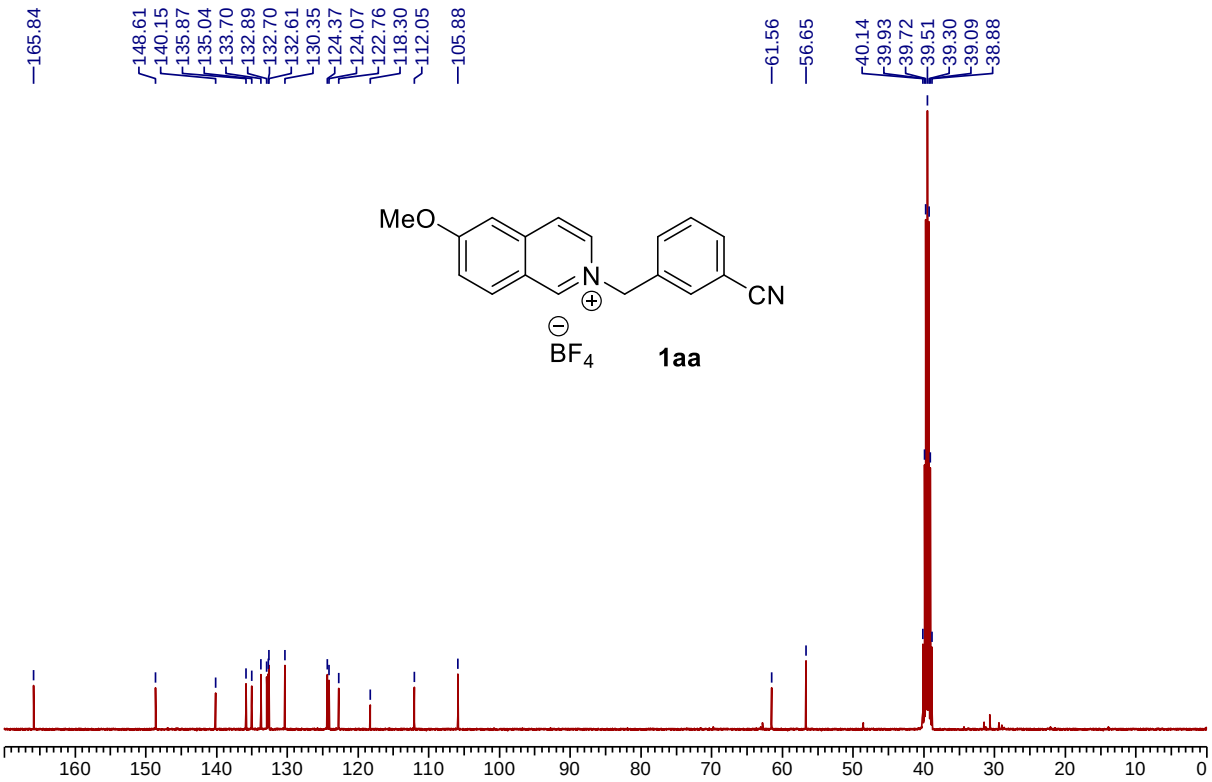

9.72
8.67
8.66
8.32
8.30
7.81
7.76
7.55
7.55
7.54
7.53
7.48
7.47
7.45
5.87
4.07
4.01
3.34
2.52
2.51
2.50
0.00
MeO
MeO
N
BF4
1y
1.00
1.00
1.03
1.00
1.00
2.09
3.08
2.02
2.96
3.04
10
9
8
7
6
5
4
3
2
1
0

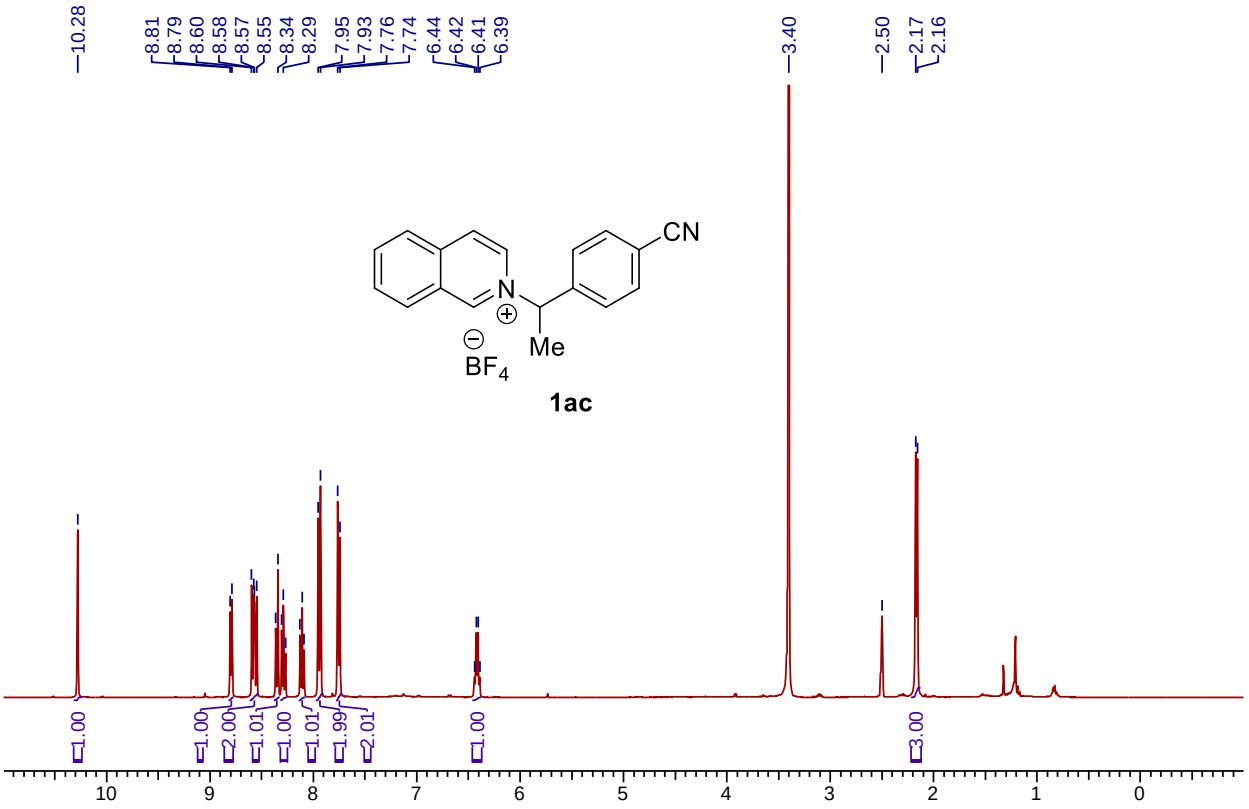

157.77
152.60
145.03
135.38
134.68
133.62
129.22
128.64
123.97
123.69
107.29
105.79
62.74
56.86
56.33
40.14
39.93
39.72
39.51
39.31
39.09
38.88
MeO
MeO
N
BF4
1y
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

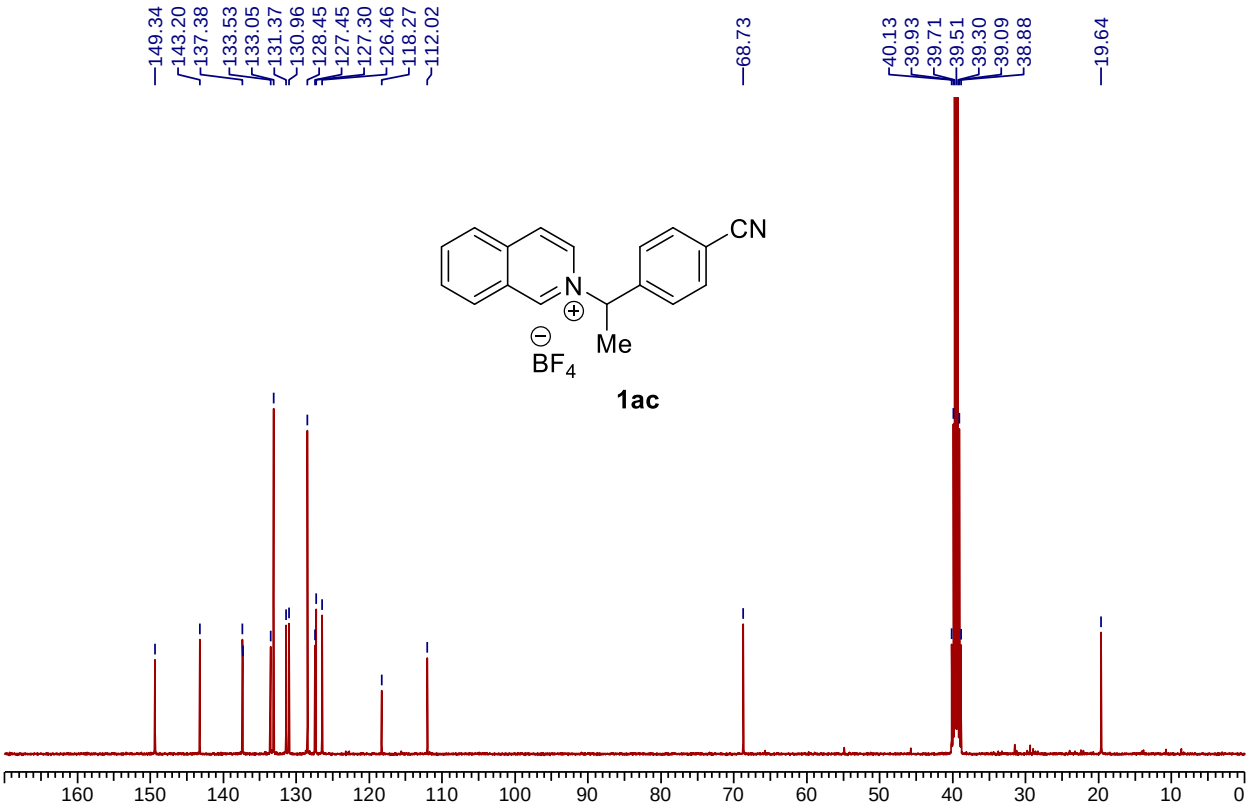

10.01
8.69
8.44
8.41
8.37
8.36
7.76
7.76
7.70
7.58
7.58
7.56
7.47
7.45
5.89
4.06
3.42
2.53
2.52
2.52
2.51
0.00
MeO
N
BF4
1z
1.00
1.00
1.01
1.02
1.01
1.01
2.00
3.01
2.02
3.00
10
9
8
7
6
5
4
3
2
1
0

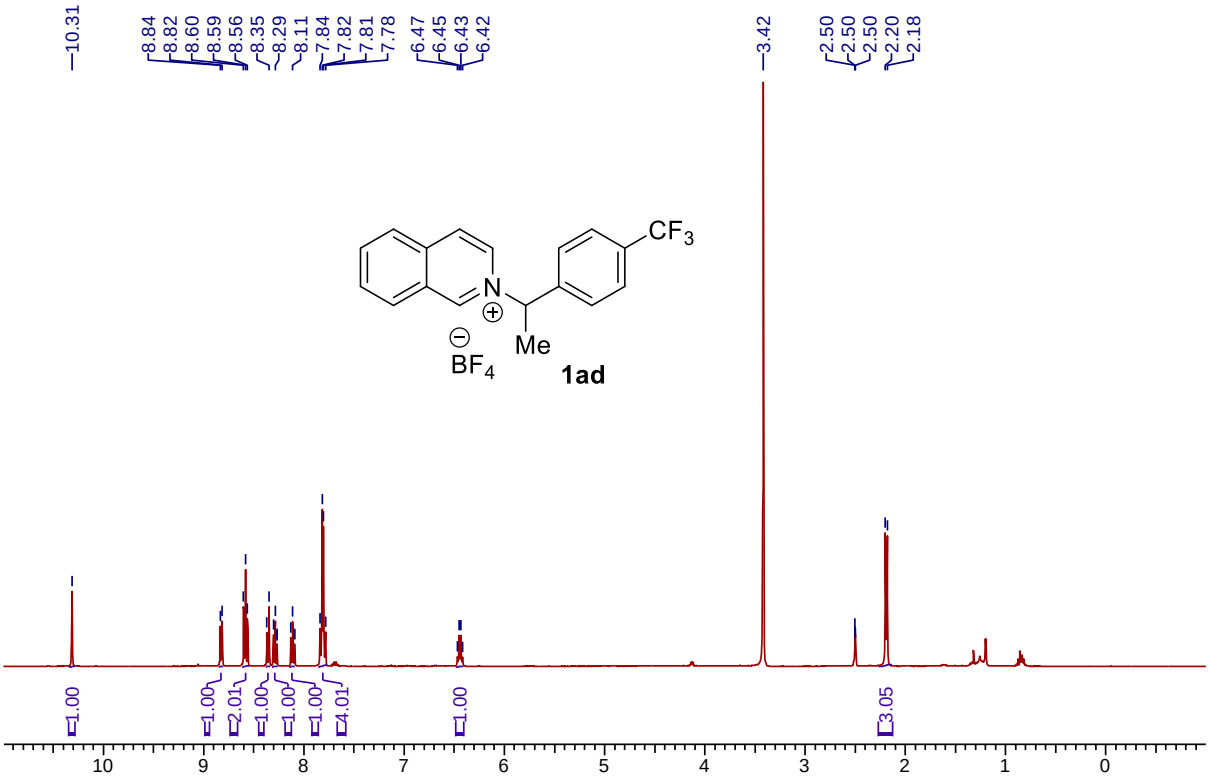

165.75
148.18
140.03
135.05
134.55
132.54
129.20
128.65
124.30
124.11
122.70
105.86
62.68
56.62
40.13
39.93
39.71
39.51
39.30
39.09
38.88
MeO
N
BF4
1z
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

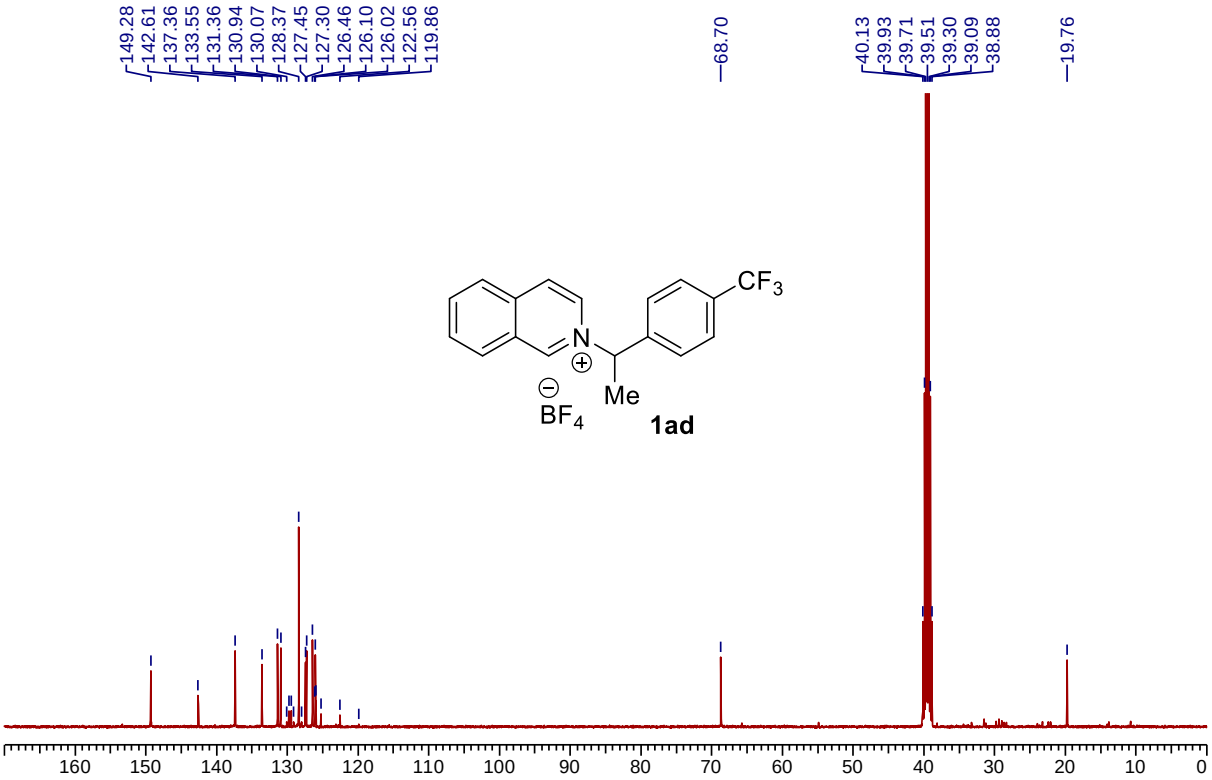

9.95
8.67
8.66
8.42
8.40
8.37
8.09
7.91
7.76
7.76
7.70
7.68
7.68
5.92
4.06
3.36
2.52
2.51
2.51
2.50
0.00
MeO
N
CN
BF4
1aa
1.00
0.99
1.00
1.01
2.01
1.00
2.00
2.01
3.00
10
9
8
7
6
5
4
3
2
1
0

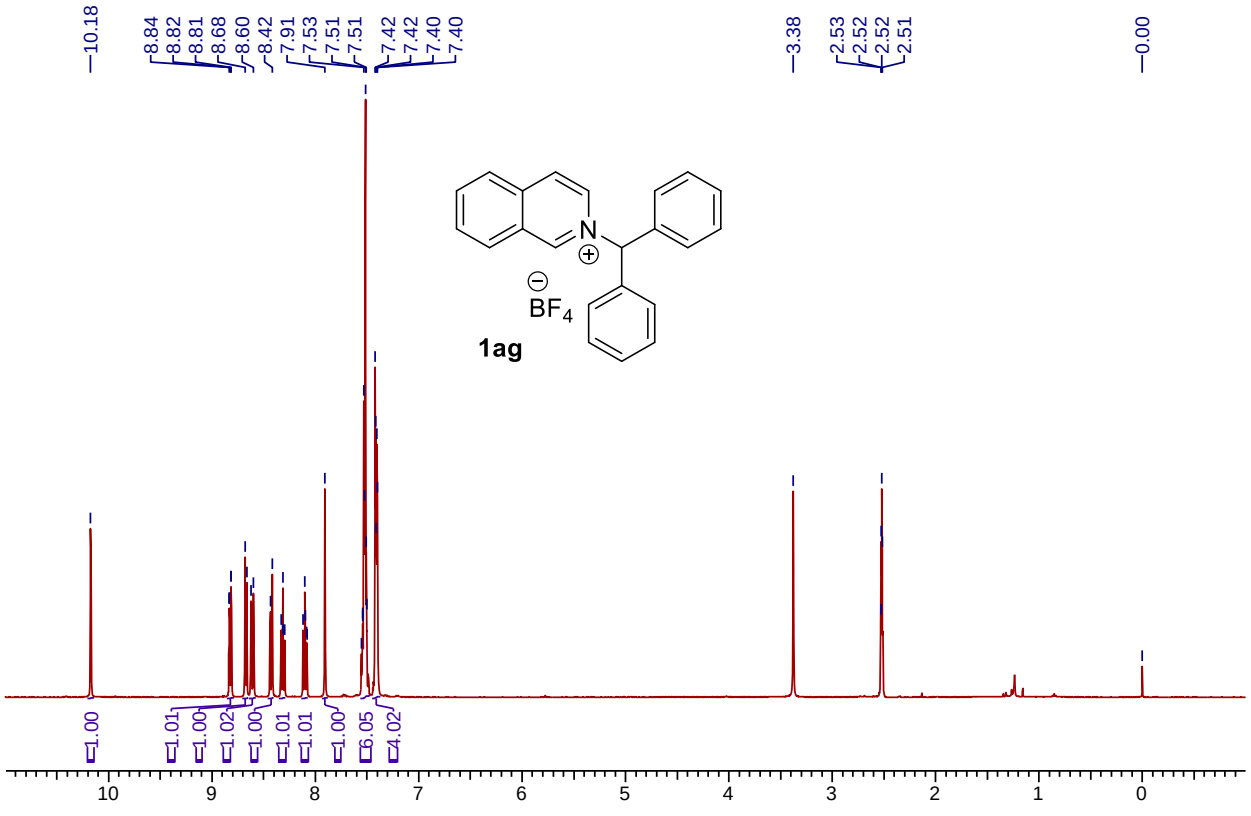

165.84
148.61
140.15
135.87
135.04
133.70
132.89
132.70
132.61
130.35
124.37
124.07
122.76
118.30
112.05
105.88
61.56
56.65
40.14
39.93
39.72
39.51
39.30
39.09
38.88
MeO
N
CN
BF4
1aa
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

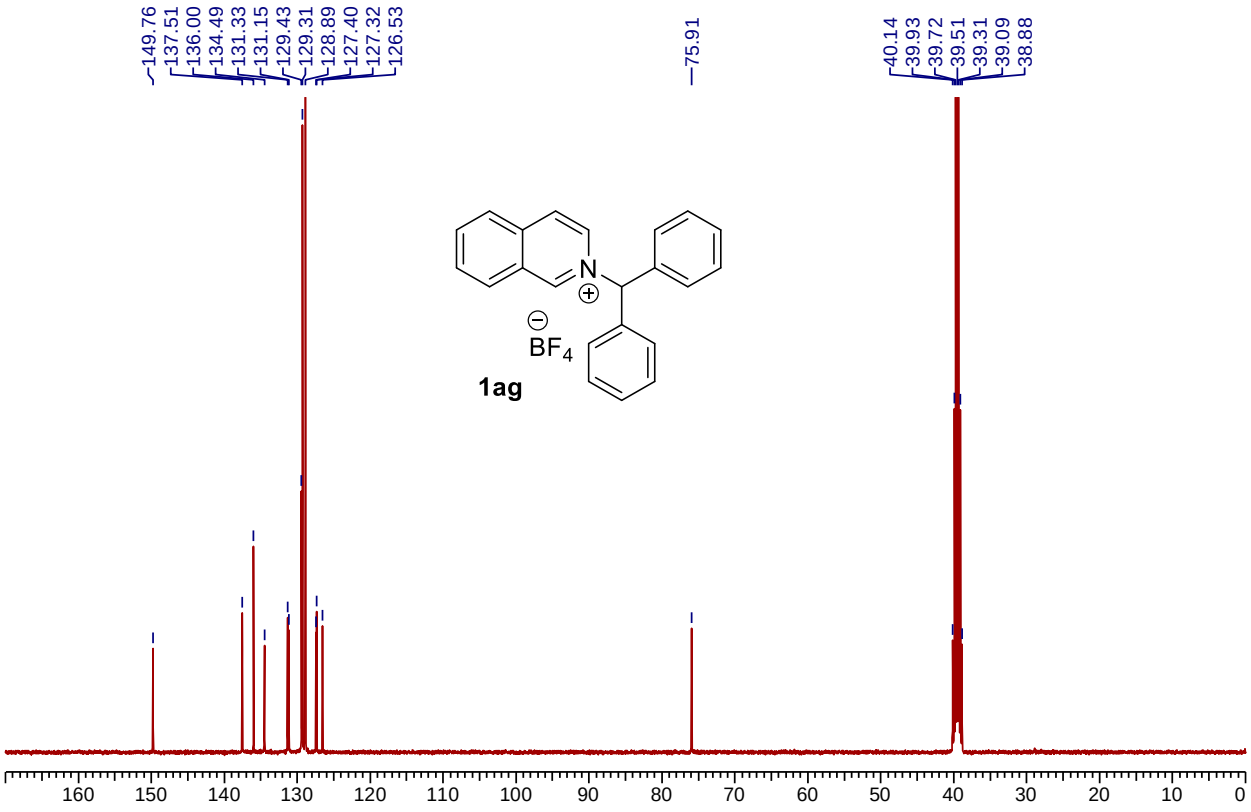

10.28
8.81
8.79
8.60
8.58
8.57
8.55
8.34
8.29
7.95
7.93
7.76
7.74
6.44
6.42
6.41
6.39
3.40
2.50
2.17
2.16
CN
N
Me
BF4
1ac
1.00
1.00
2.00
1.01
1.00
1.01
1.99
2.01
1.00
3.00

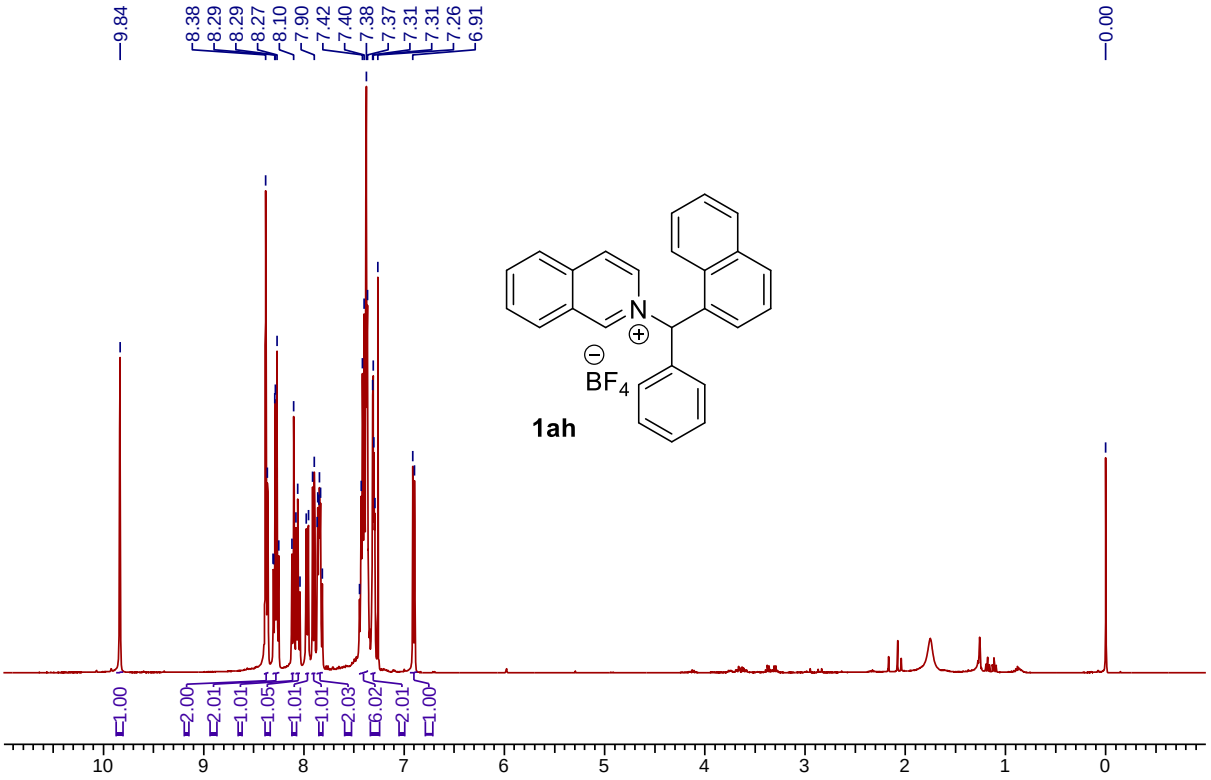

149.34
143.20
137.38
133.53
133.05
131.37
130.96
128.45
127.45
127.30
126.46
118.27
112.02
68.73
40.13
39.93
39.71
39.51
39.30
39.09
38.88
19.64
CN
N
Me
BF4
1ac

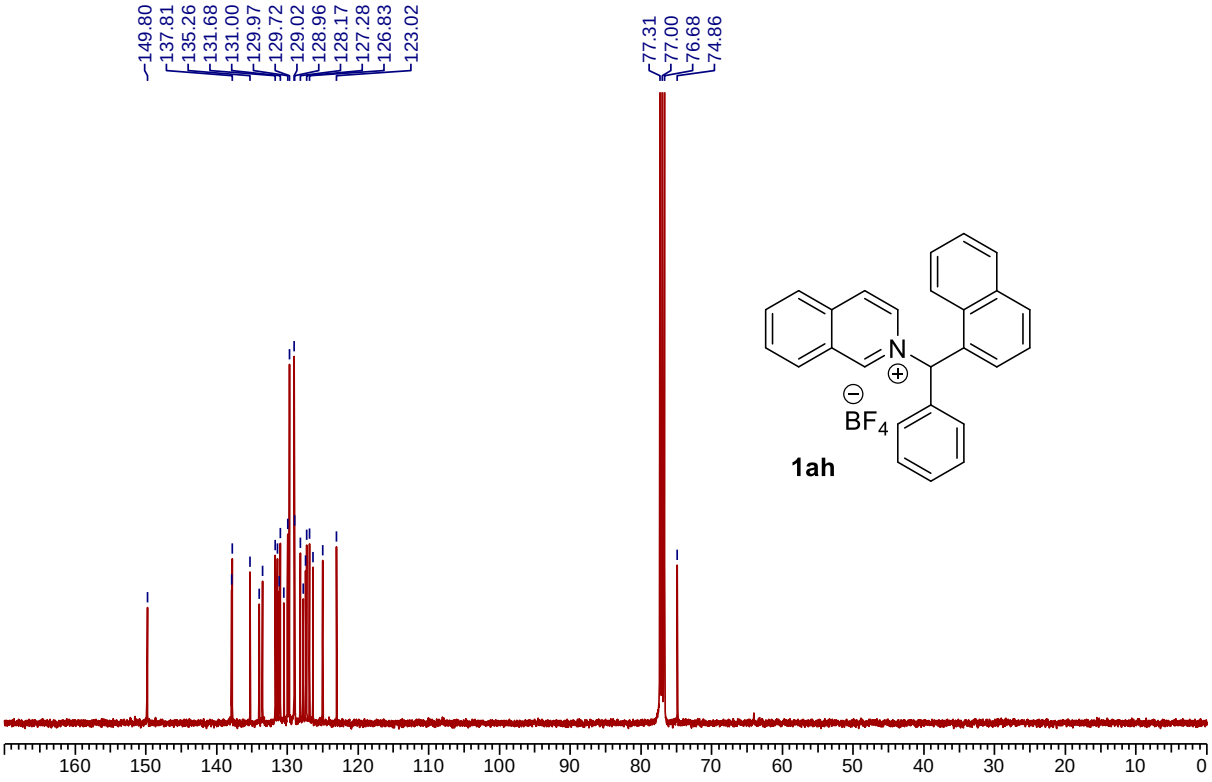

10.31
8.84
8.82
8.60
8.59
8.56
8.35
8.29
8.11
7.84
7.82
7.81
7.78
6.47
6.45
6.43
6.42
3.42
2.50
2.50
2.50
2.20
2.18
CF3
N
Me
BF4
1ad
1.00
1.00
2.01
1.00
1.00
4.01
1.00
3.05

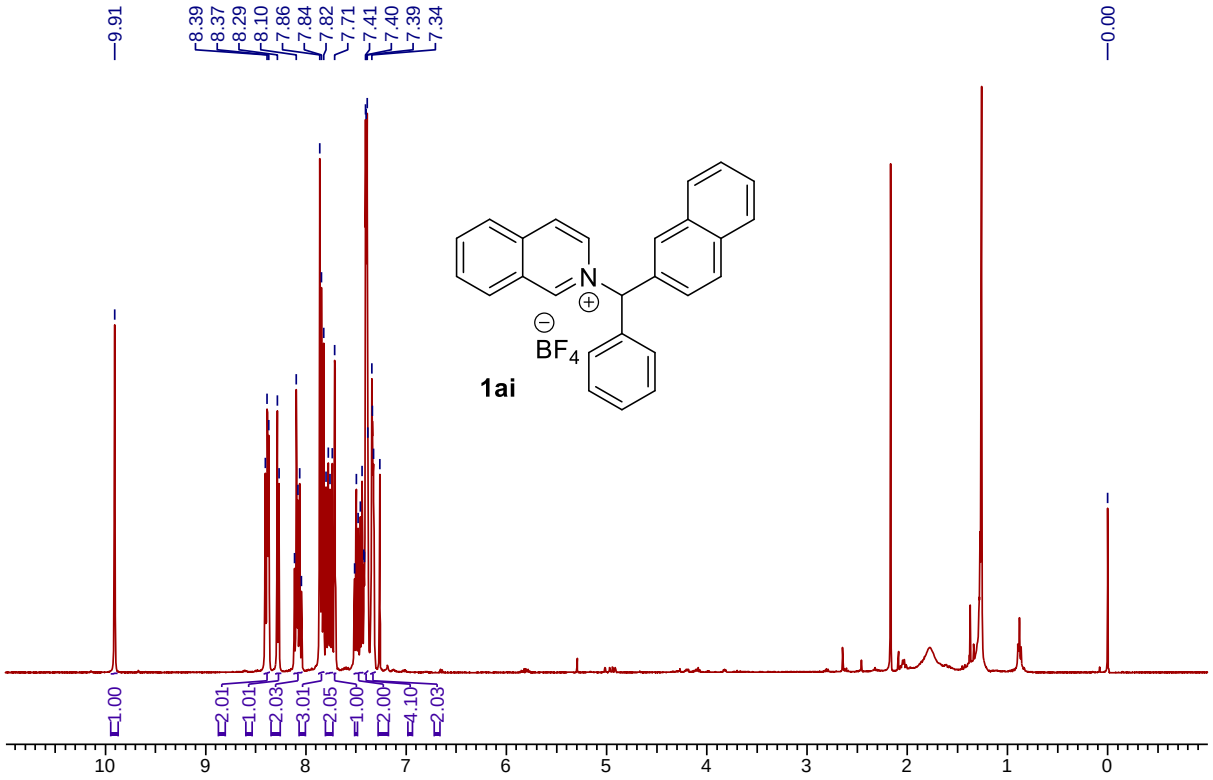

149.28
142.61
137.36
133.55
131.36
130.94
130.07
128.37
127.45
127.30
126.46
126.10
126.02
122.56
119.86
68.70
40.13
39.93
39.71
39.51
39.30
39.09
38.88
19.76
CF3
N
Me
BF4
1ad

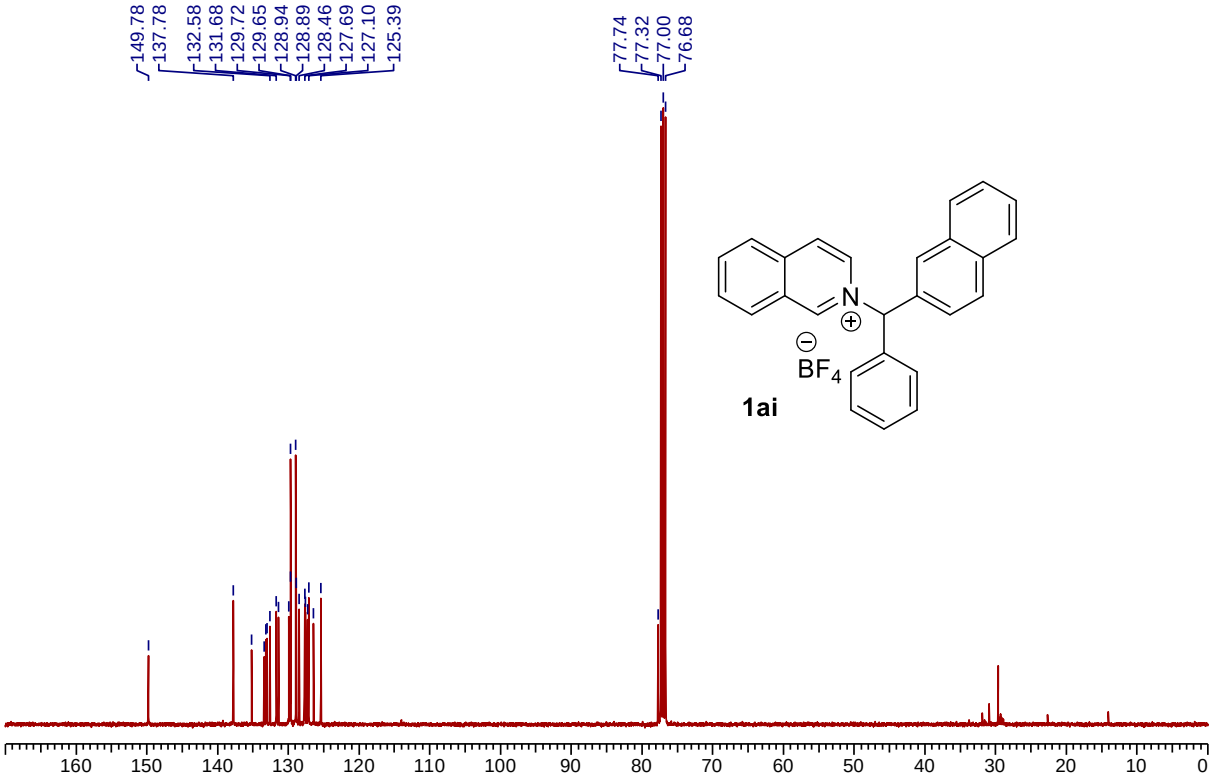

10.18
8.84
8.82
8.81
8.68
8.60
8.42
7.91
7.53
7.51
7.51
7.42
7.42
7.40
7.40
3.38
2.53
2.52
2.52
2.51
0.00
1.00
1.01
1.00
1.02
1.00
1.01
1.01
1.00
6.05
4.02
BF4
1ag

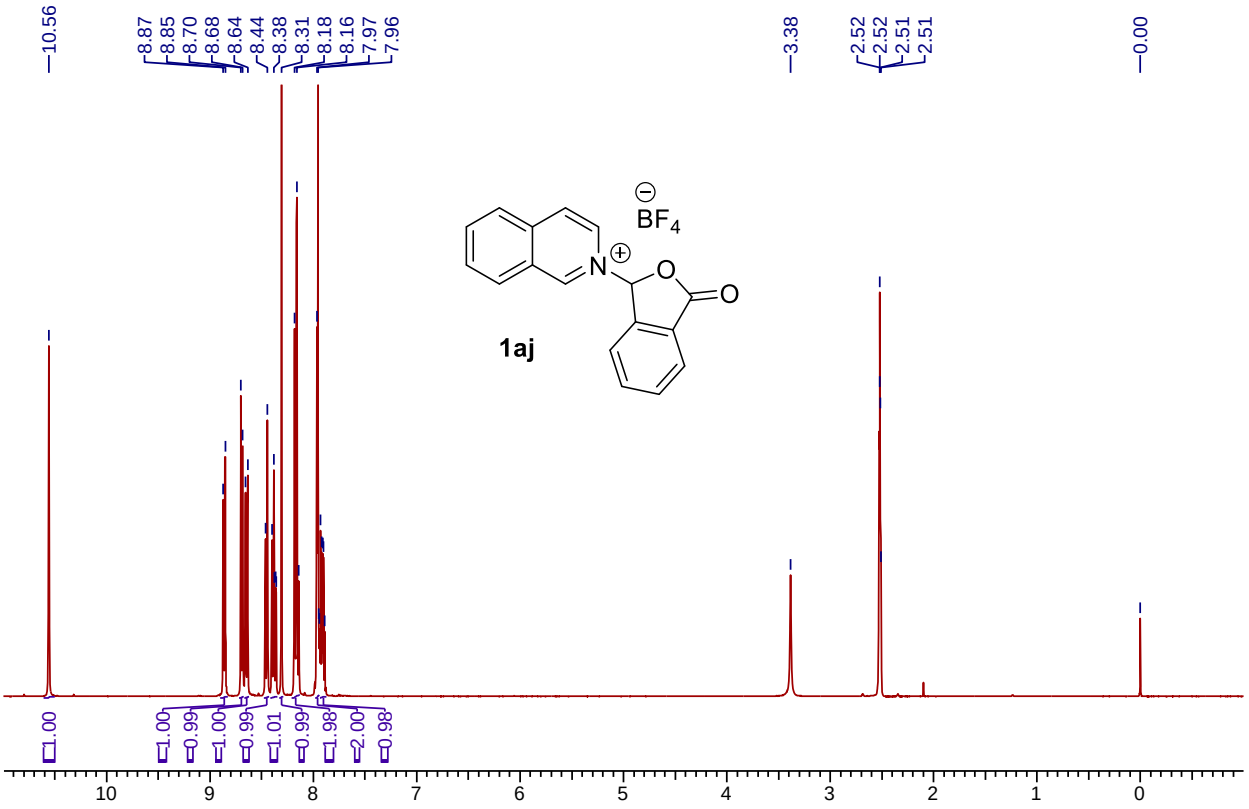

149.76
137.51
136.00
134.49
131.33
131.15
129.43
129.31
128.89
127.40
127.32
126.53
75.91
40.14
39.93
39.72
39.51
39.31
39.09
38.88
BF4
1ag

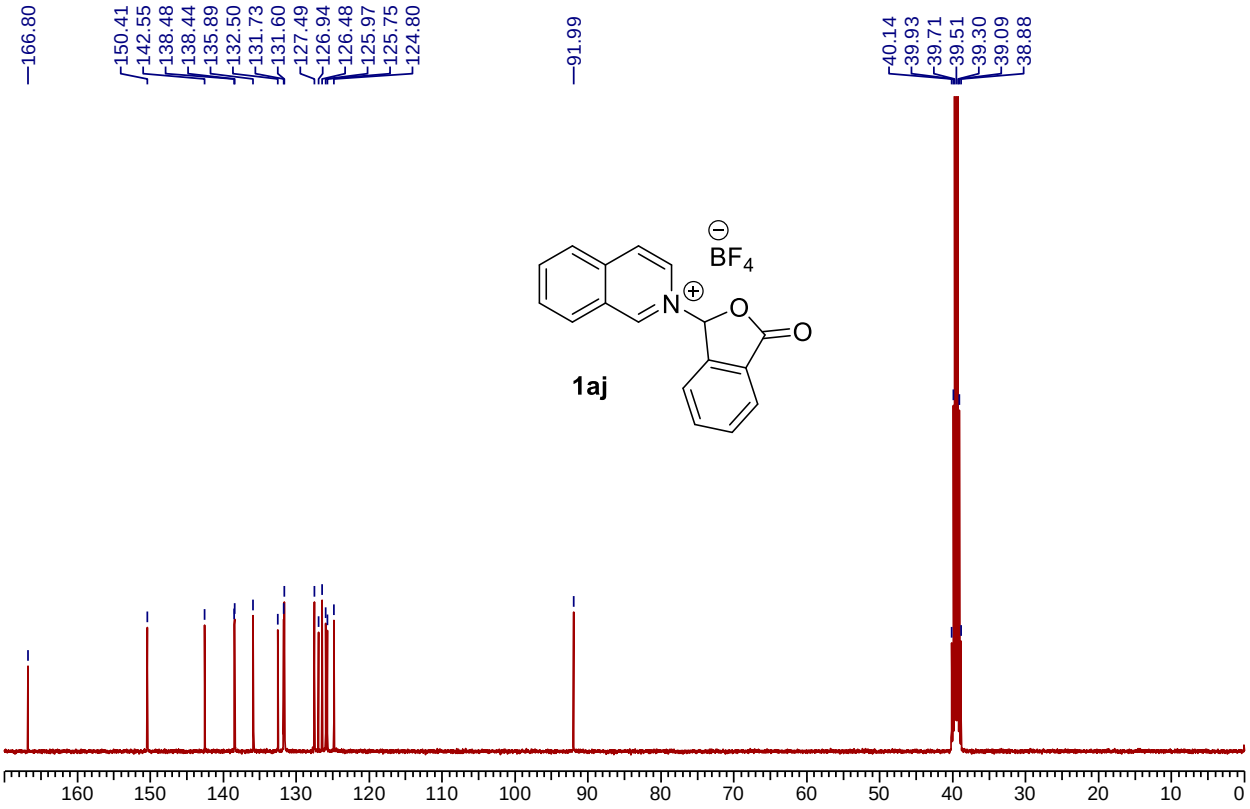

9.84
8.38
8.29
8.29
8.27
8.10
7.90
7.42
7.40
7.38
7.37
7.31
7.31
7.26
6.91
0.00
1.00
2.00
2.01
1.01
1.05
1.01
1.01
2.03
6.02
2.01
1.00
N
BF4
1ah
10
9
8
7
6
5
4
3
2
1
0

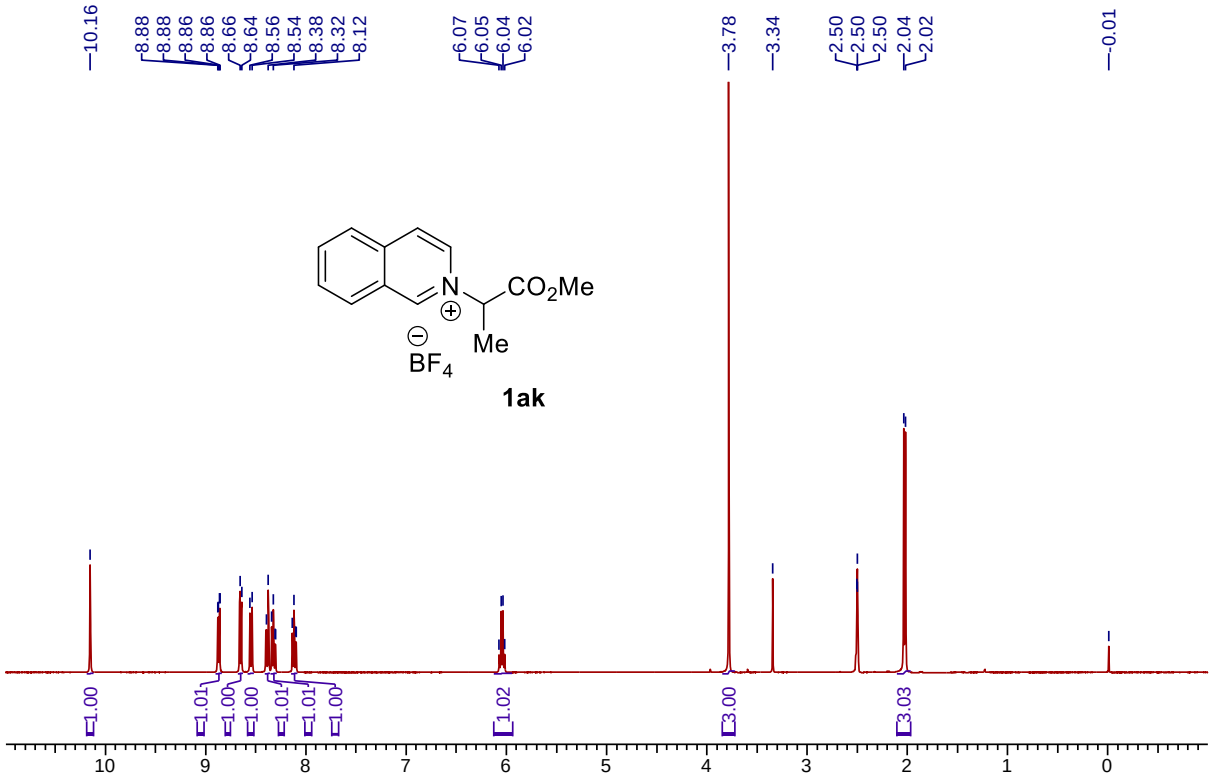

149.80
137.81
135.26
131.68
131.00
129.97
129.72
129.02
128.96
128.17
127.28
126.83
123.02
77.31
77.00
76.68
74.86
N
BF4
1ah
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

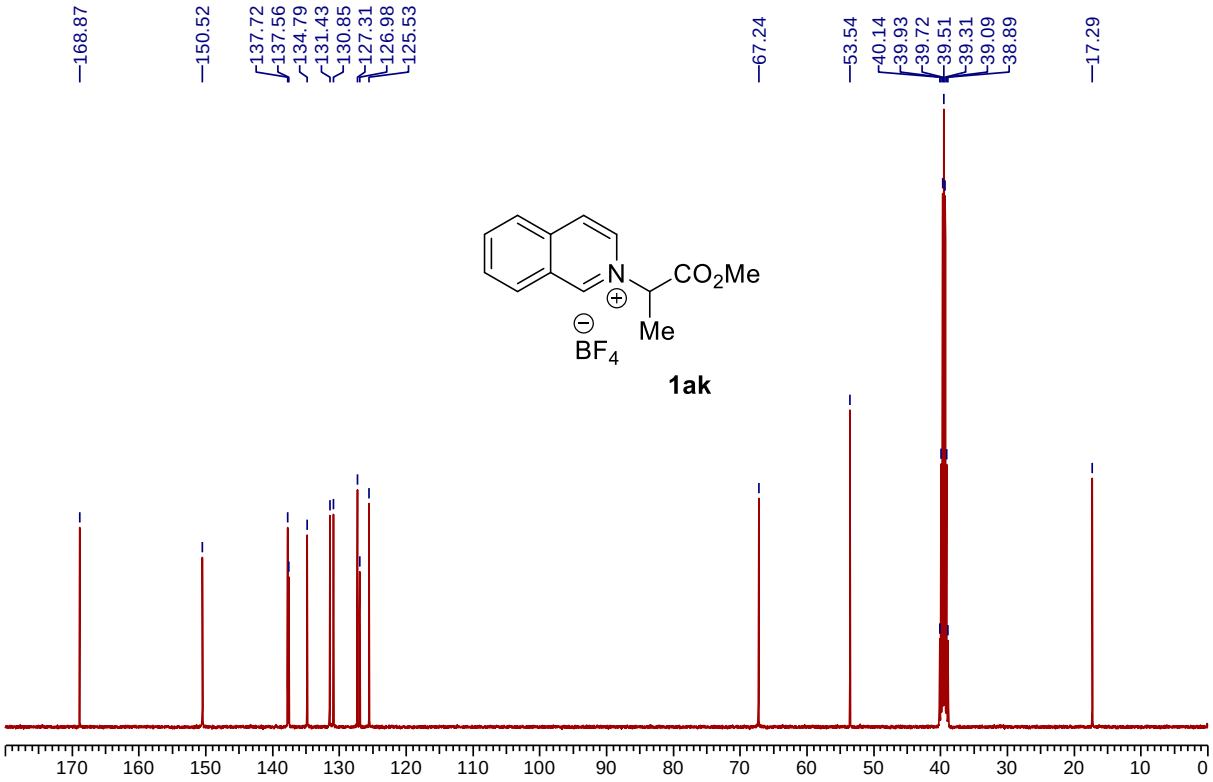

9.91
8.39
8.37
8.29
8.10
7.86
7.84
7.82
7.71
7.41
7.40
7.39
7.34
0.00
1.00
2.01
1.01
2.03
3.01
2.05
1.00
2.00
4.10
2.03
N
BF4
1ai

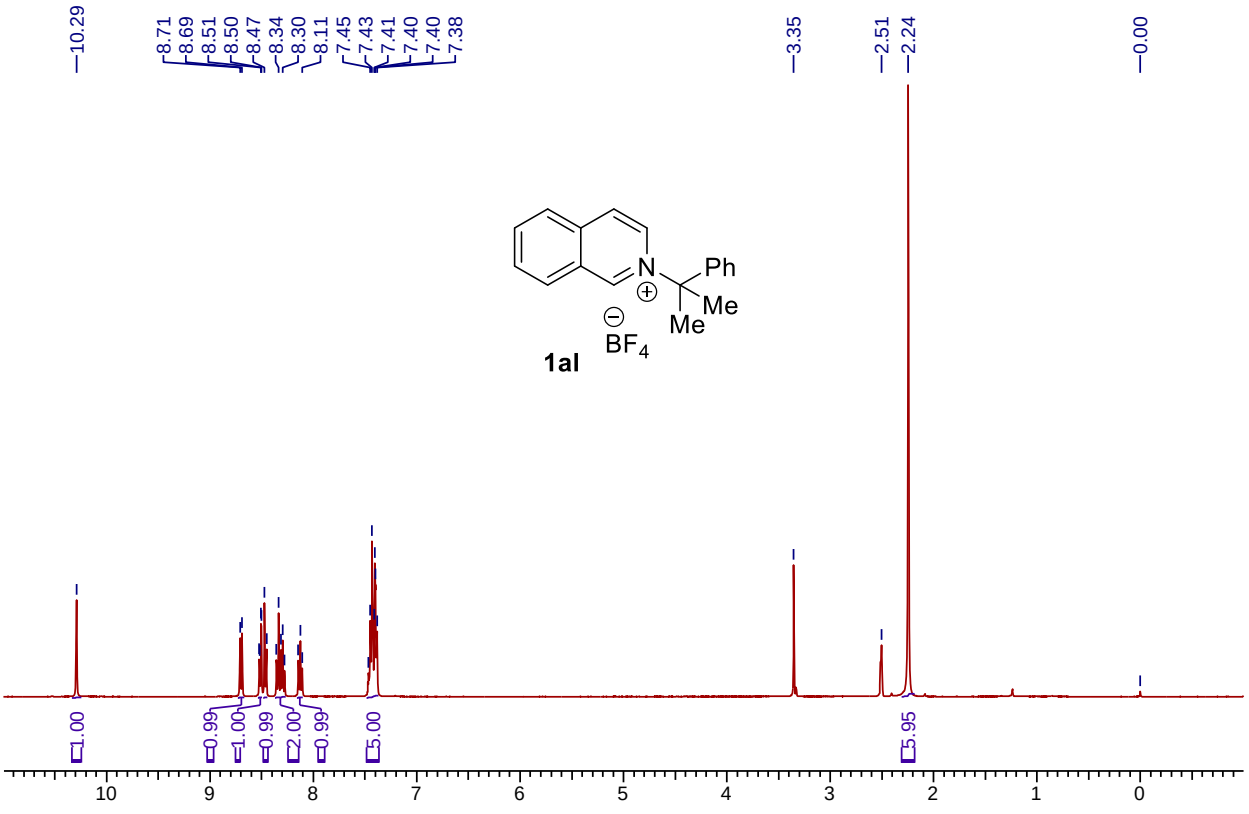

149.78
137.78
132.58
131.68
129.72
129.65
128.94
128.89
128.46
127.69
127.10
125.39
77.74
77.32
77.00
76.68
N
BF4
1ai

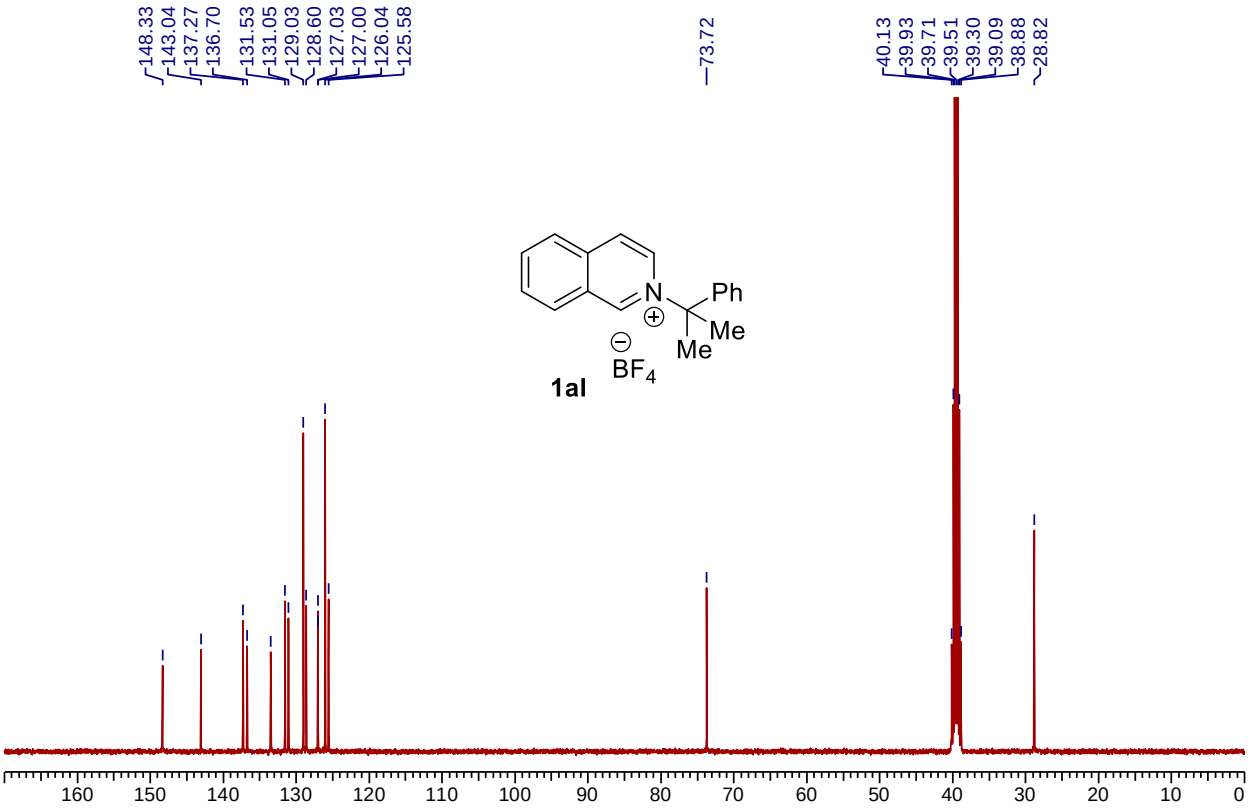

10.56
8.87
8.85
8.70
8.68
8.64
8.44
8.38
8.31
8.18
8.16
7.97
7.96
3.38
2.52
2.52
2.51
2.51
0.00
1.00
1.00
0.99
1.00
0.99
1.01
0.99
1.98
2.00
0.98
BF4
N
O
O
1aj
10
9
8
7
6
5
4
3
2
1
0


166.80
150.41
142.55
138.48
138.44
135.89
132.50
131.73
131.60
127.49
126.94
126.48
125.97
125.75
124.80
91.99
40.14
39.93
39.71
39.51
39.30
39.09
38.88
BF4
N
O
O
1aj
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

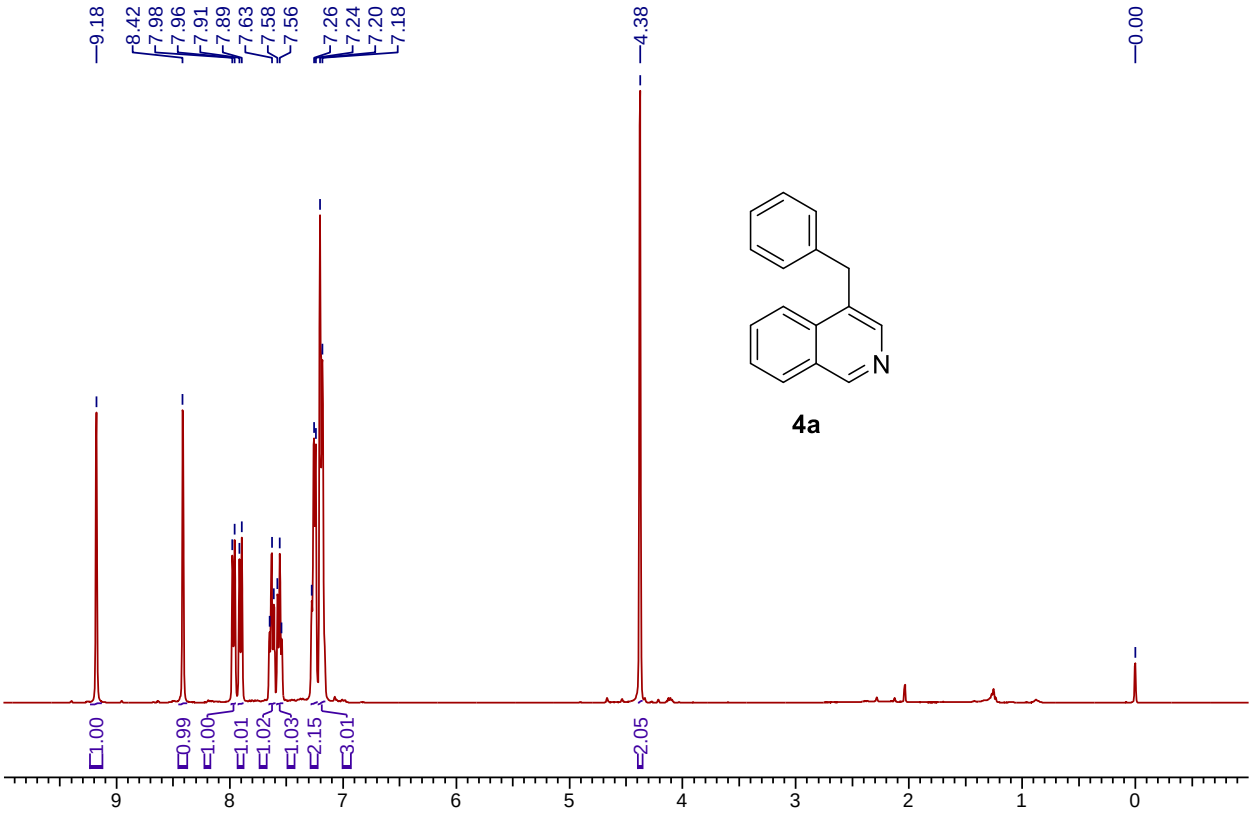

10.16
8.88
8.88
8.86
8.86
8.66
8.64
8.56
8.54
8.38
8.32
8.12
6.07
6.05
6.04
6.02
3.78
3.34
2.50
2.50
2.50
2.04
2.02
0.01
CO2Me
N
Me
BF4
1ak
1.00
1.01
1.00
1.00
1.01
1.01
1.00
1.02
3.00
3.03

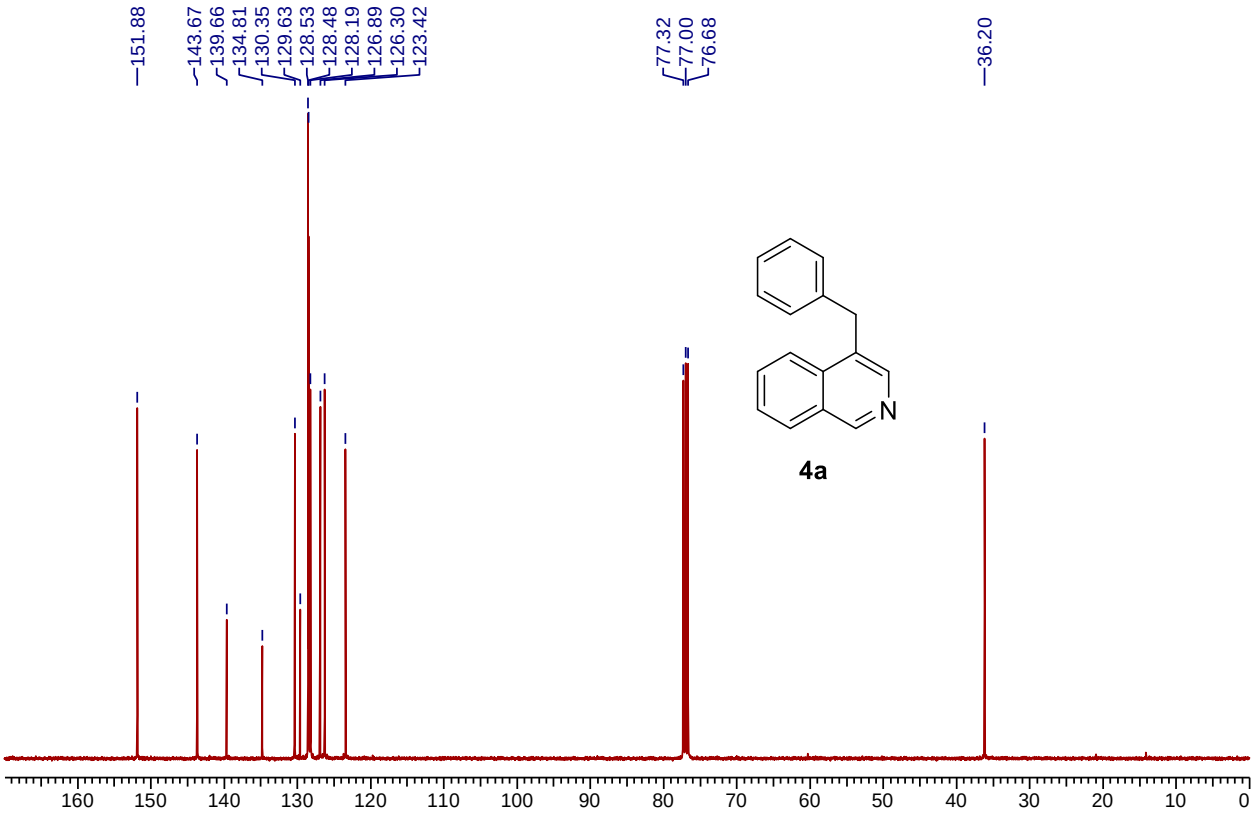

168.87
150.52
137.72
137.56
134.79
131.43
130.85
127.31
126.98
125.53
67.24
53.54
40.14
39.93
39.72
39.51
39.31
39.09
38.89
17.29
CO2Me
N
Me
BF4
1ak

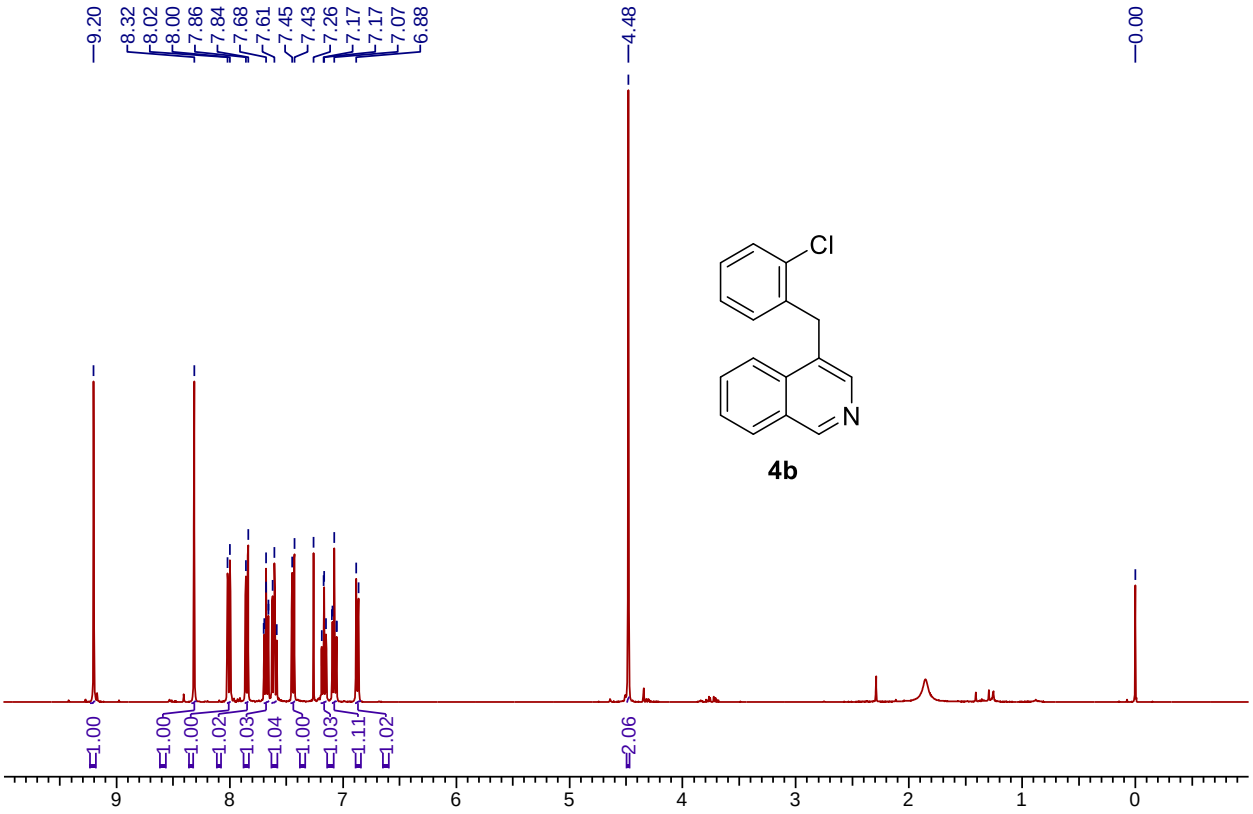

10.29
8.71
8.69
8.51
8.50
8.47
8.34
8.30
8.11
7.45
7.43
7.41
7.40
7.40
7.38
3.35
2.51
2.24
0.00
Ph
Me
Me
N
BF4
1al
1.00
0.99
1.00
0.99
2.00
0.99
5.00
5.95
10
9
8
7
6
5
4
3
2
1
0

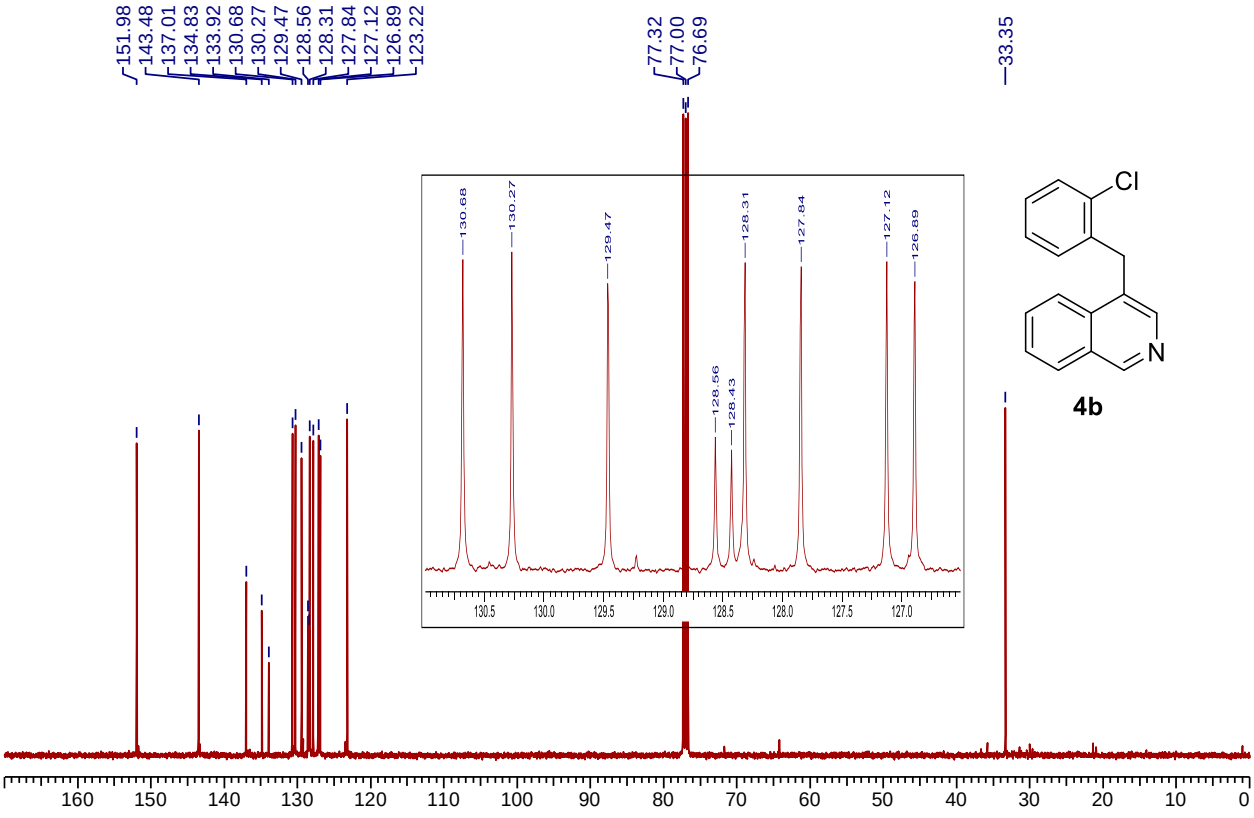

148.33
143.04
137.27
136.70
131.53
131.05
129.03
128.60
127.03
127.00
126.04
125.58
73.72
40.13
39.93
39.71
39.51
39.30
39.09
38.88
28.82
Ph
Me
Me
N
BF4
1al
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

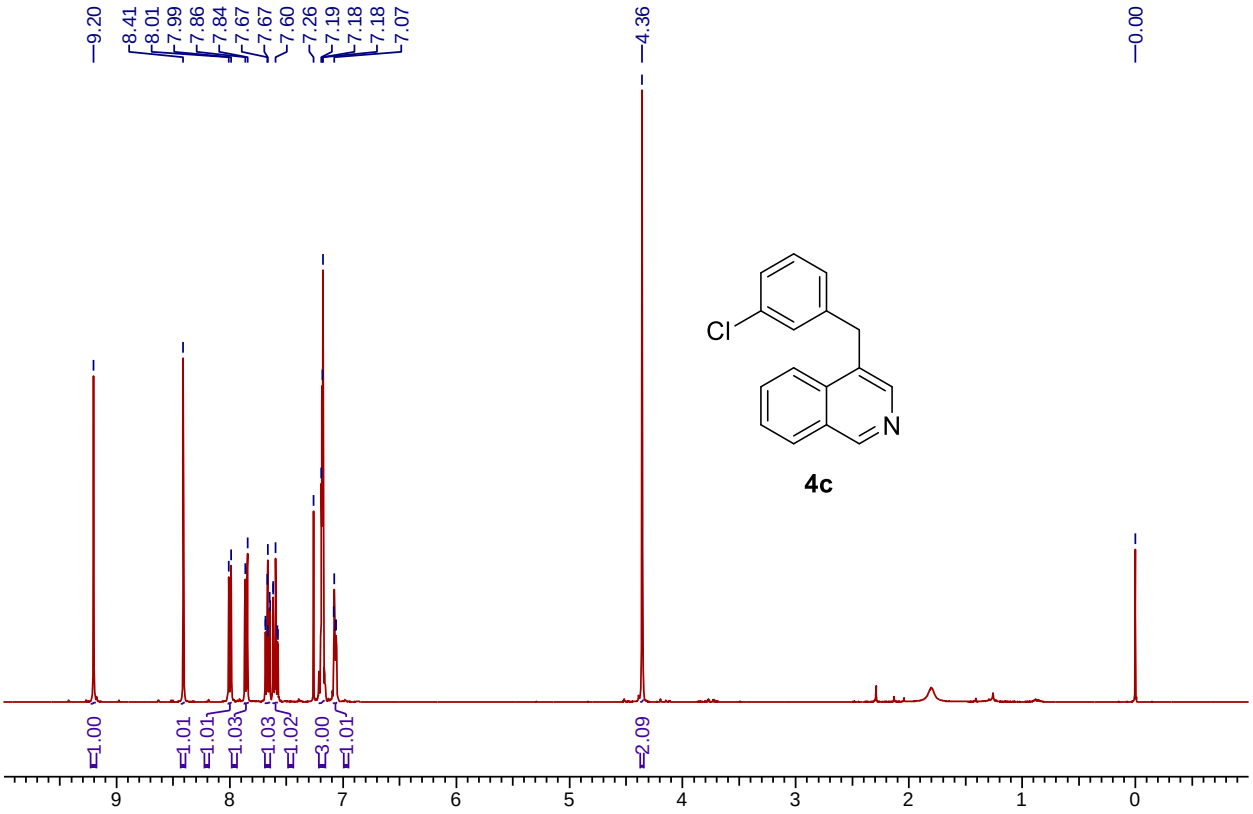
14b. NMR Spectra for *meta*-Alkylated Isoquinoline:

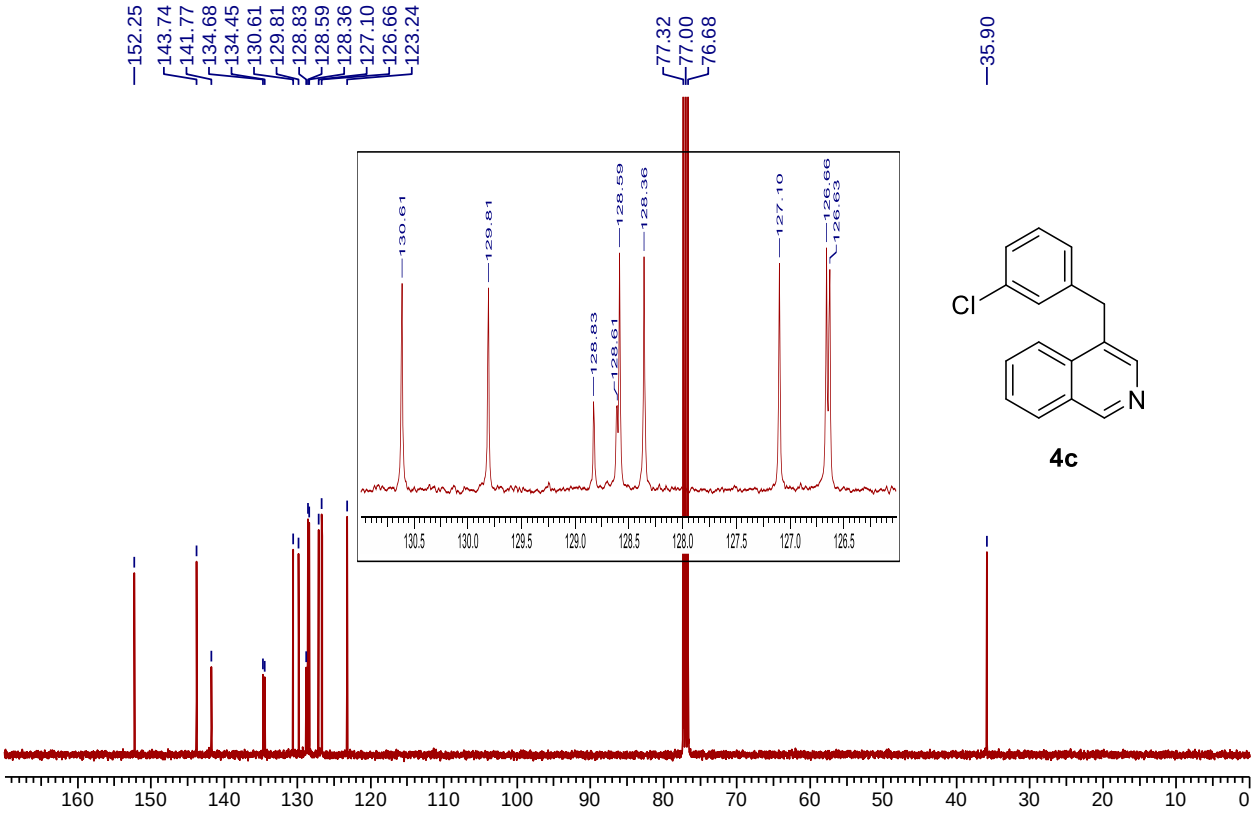


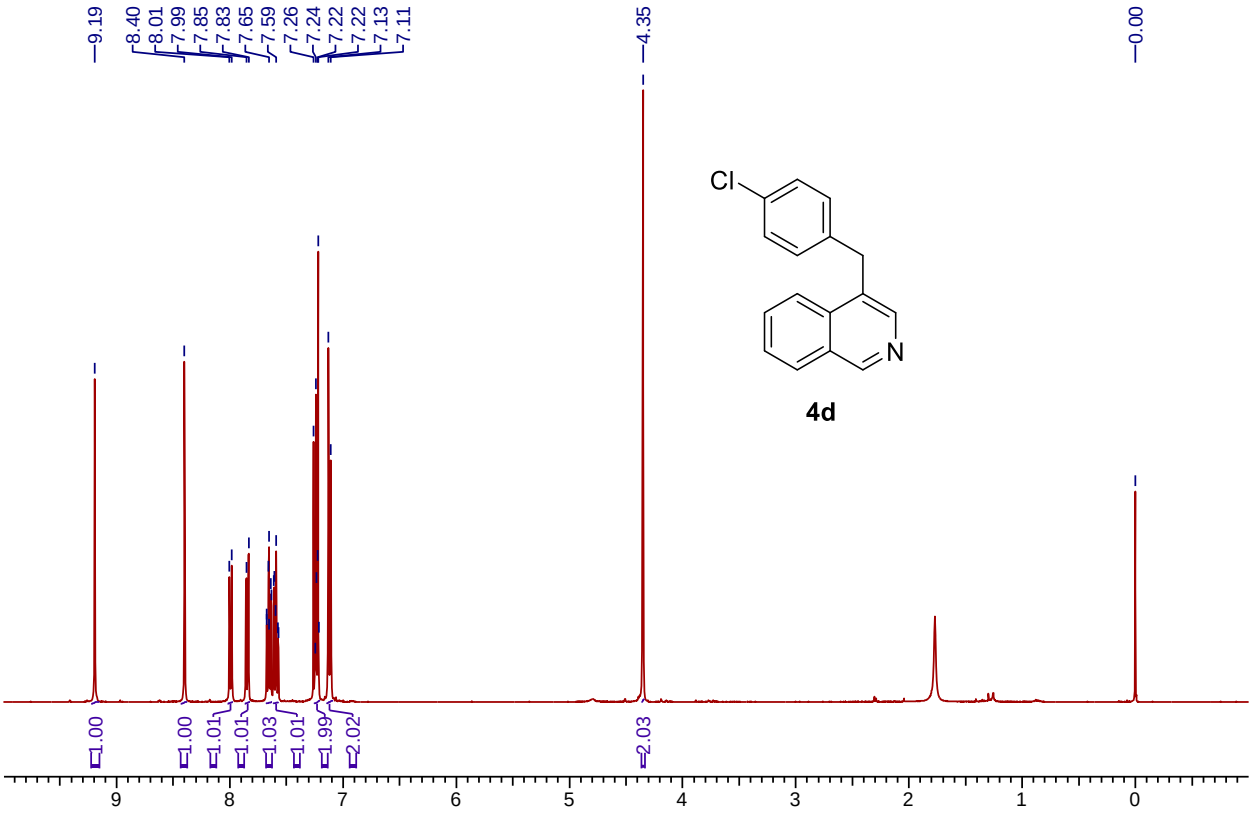


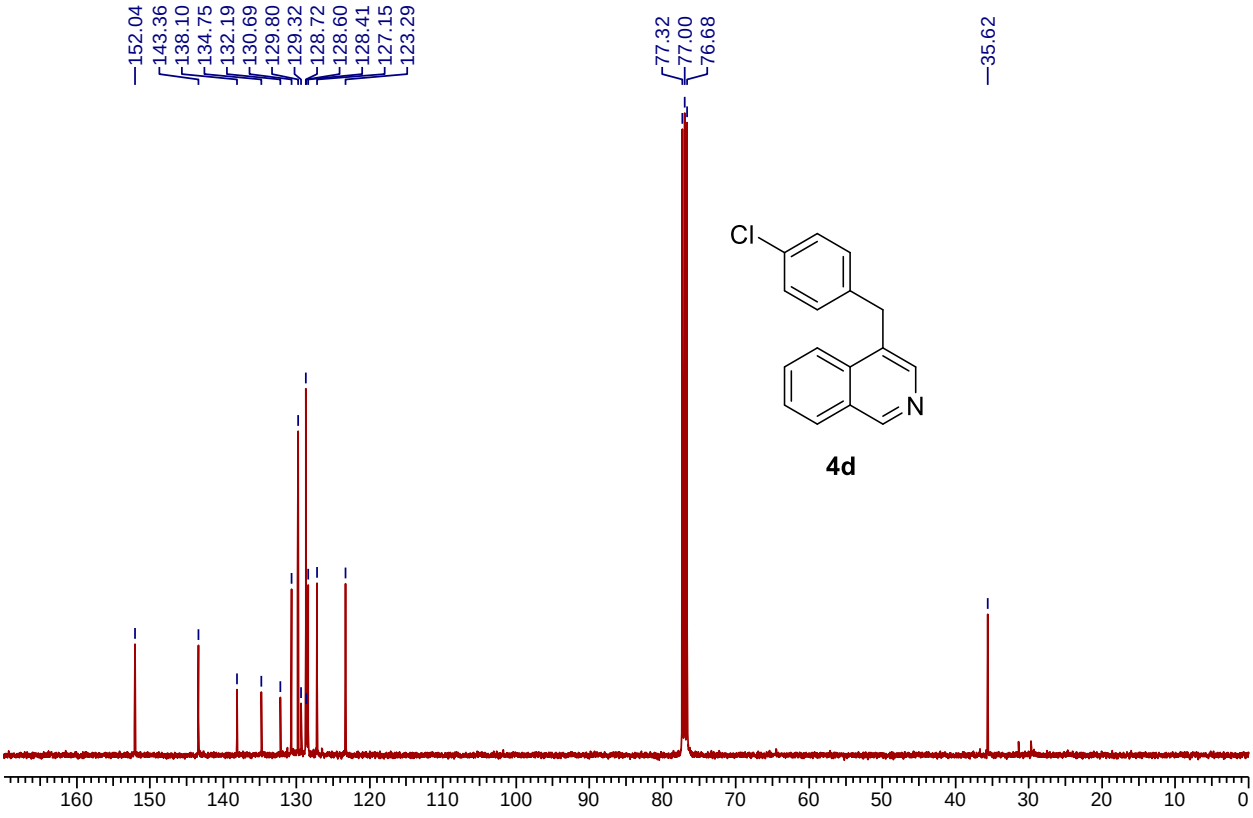

9.20
8.32
8.02
8.00
7.86
7.84
7.68
7.61
7.45
7.43
7.26
7.17
7.17
7.07
6.88
4.48
0.00
Cl
N
4b
1.00
1.00
1.00
1.02
1.03
1.04
1.00
1.03
1.11
1.02
2.06

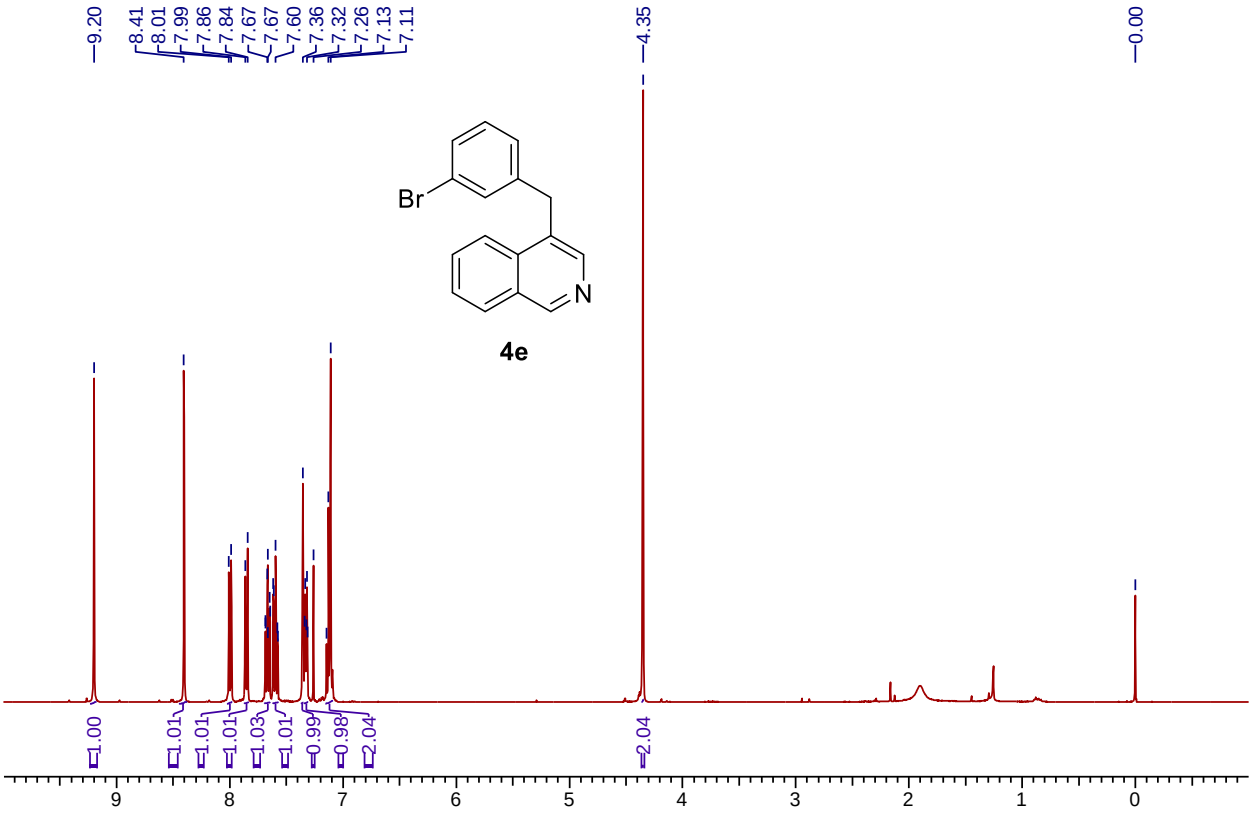

151.98
143.48
137.01
134.83
133.92
130.68
130.27
129.47
128.56
128.31
127.84
127.12
126.89
123.22
77.32
77.00
76.69
33.35
130.68
130.27
129.47
128.56
128.43
128.31
127.84
127.12
126.89
Cl
N
4b

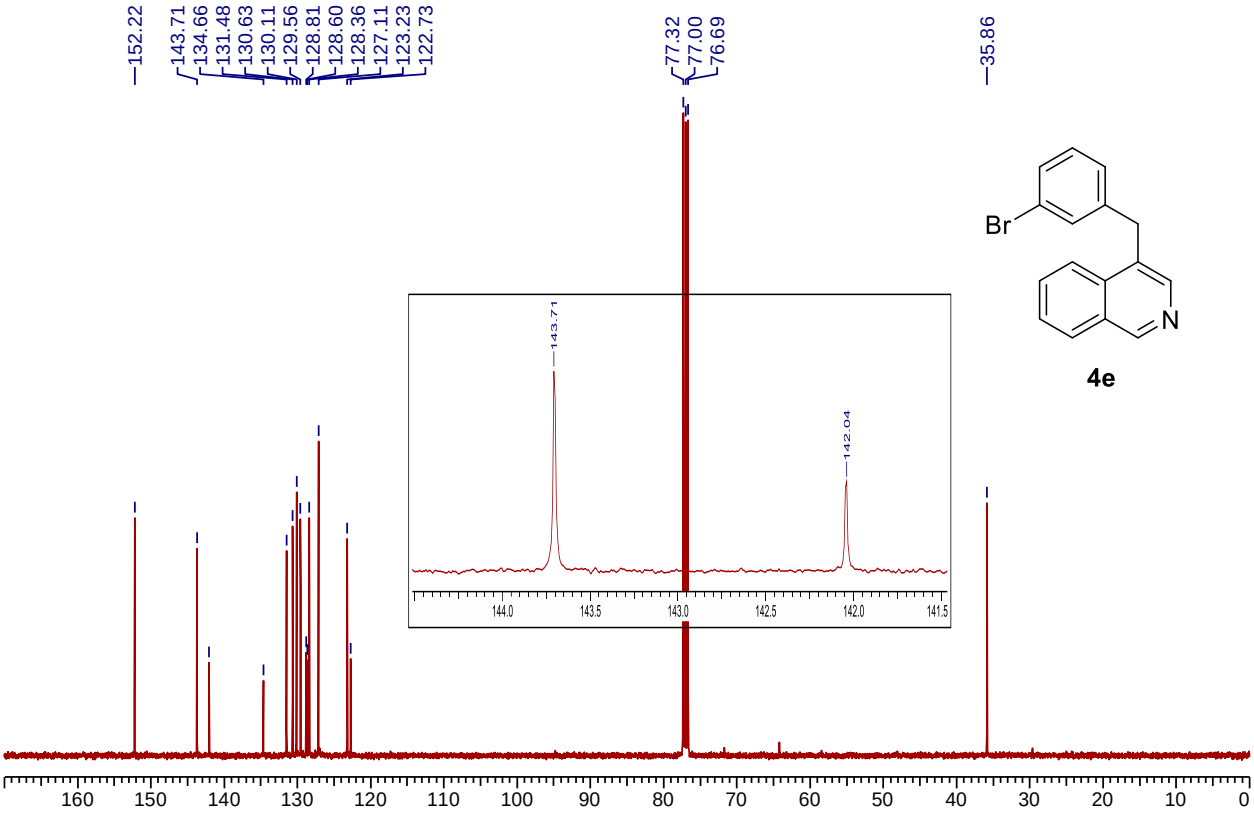

9.20
8.41
8.01
7.99
7.86
7.84
7.67
7.67
7.60
7.26
7.19
7.18
7.18
7.07
4.36
0.00
1.00
1.01
1.01
1.03
1.03
1.02
3.00
1.01
2.09
Cl
N
4c

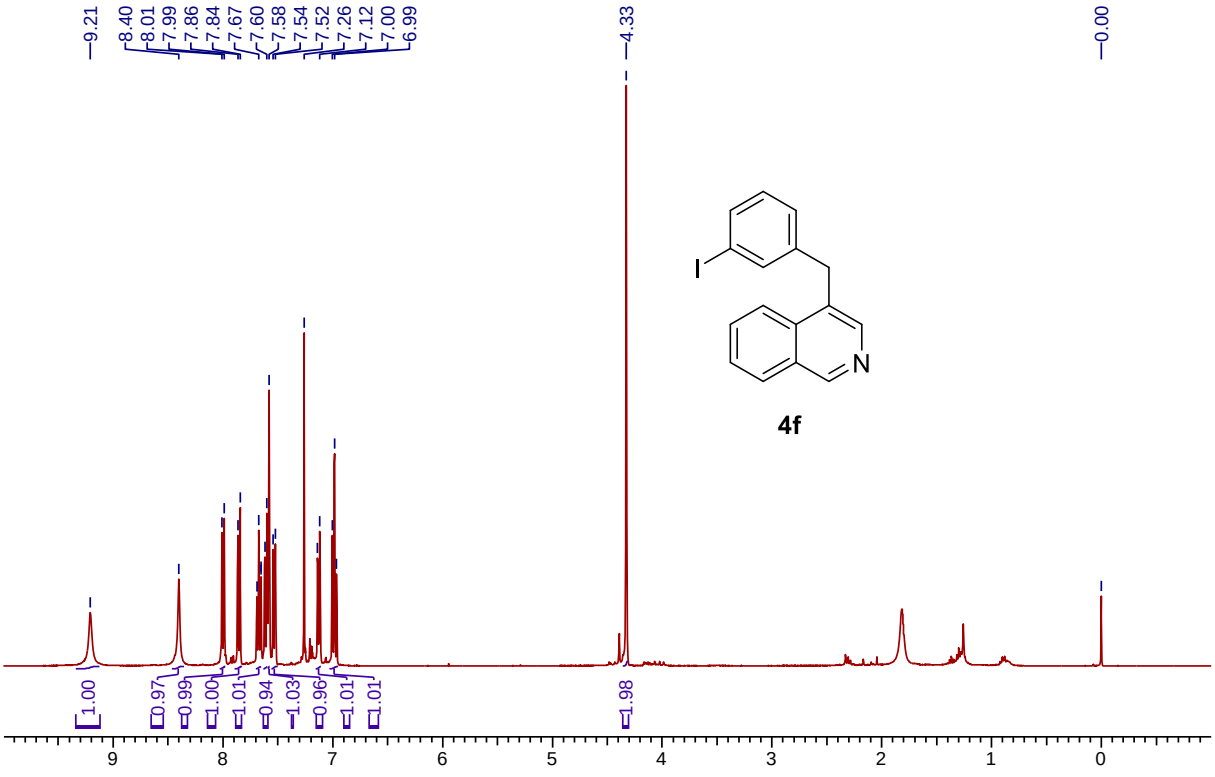

152.25
143.74
141.77
134.68
134.45
130.61
129.81
128.83
128.59
128.36
127.10
126.66
123.24
77.32
77.00
76.68
35.90
130.61
129.81
128.83
128.61
128.59
128.36
127.10
126.66
126.63
Cl
N
4c

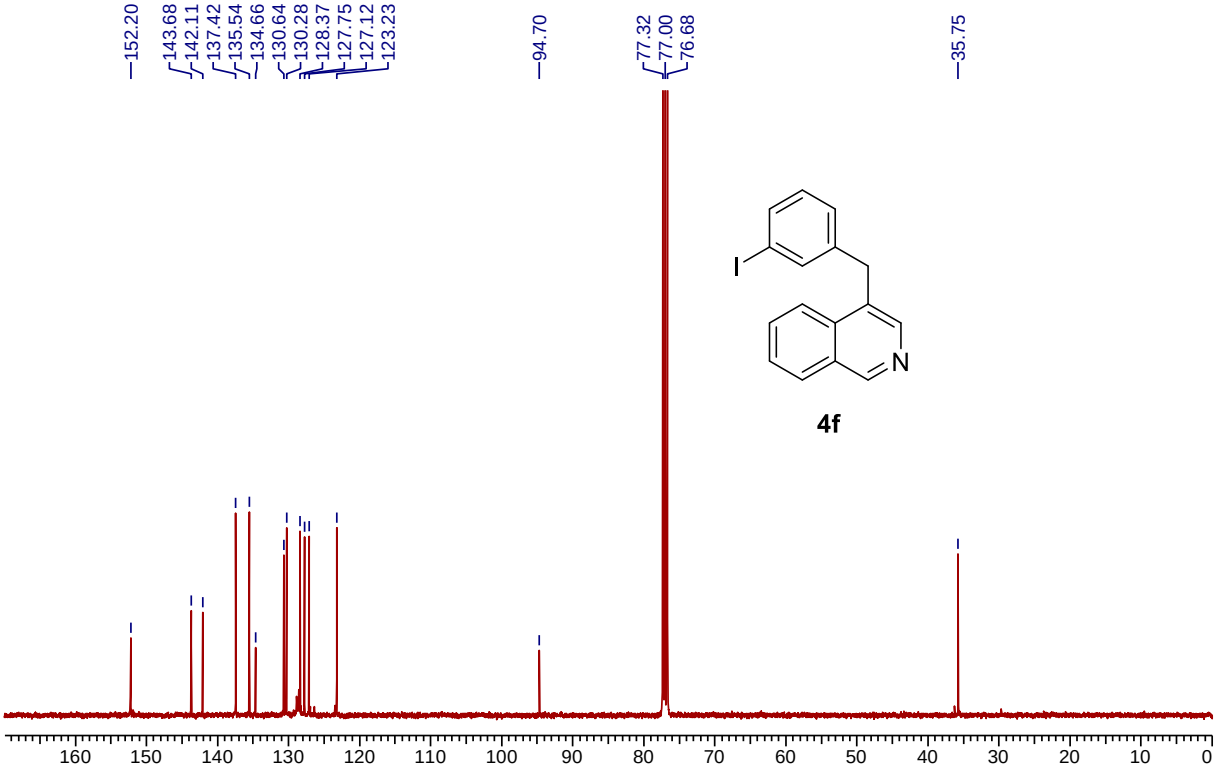

9.19
8.40
8.01
7.99
7.85
7.83
7.65
7.59
7.26
7.24
7.22
7.22
7.13
7.11
4.35
0.00
Cl
N
4d
1.00
1.00
1.01
1.01
1.03
1.01
1.99
2.02
2.03
9
8
7
6
5
4
3
2
1
0

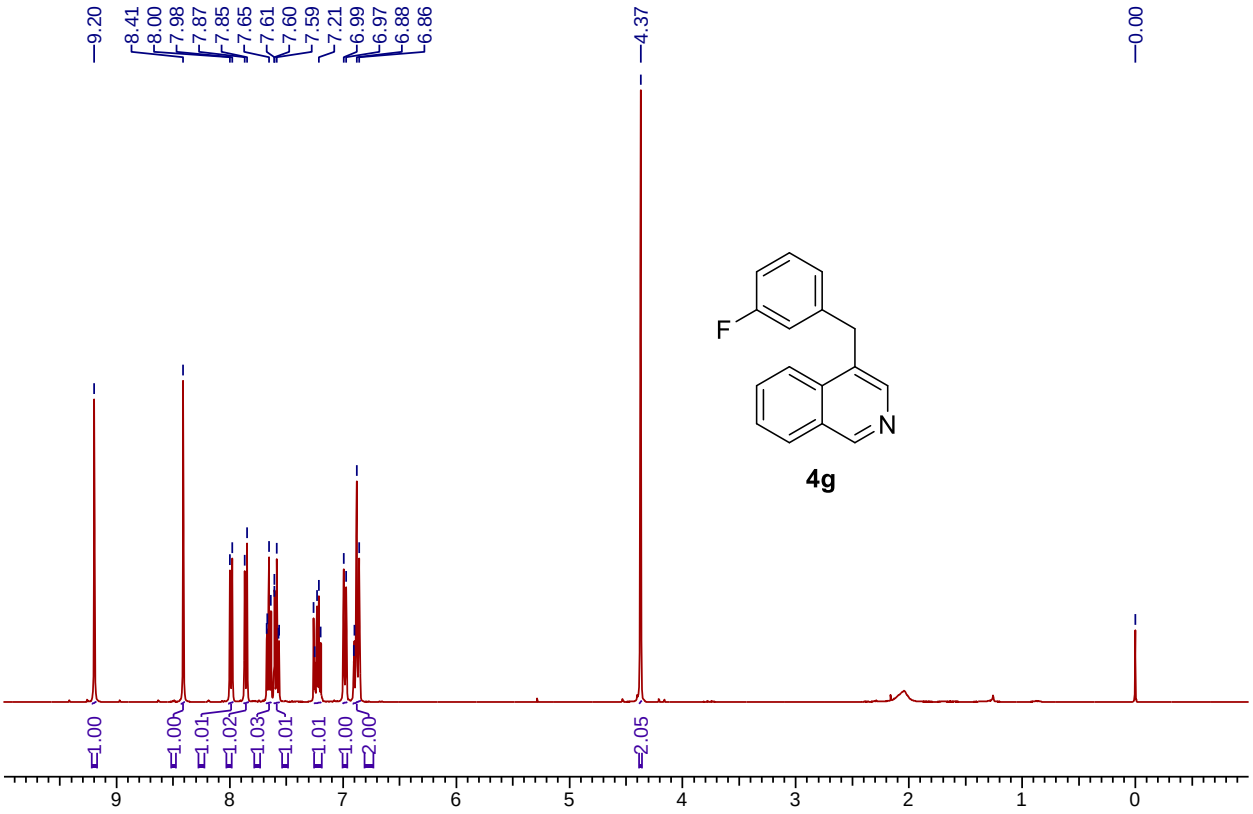

152.04
143.36
138.10
134.75
132.19
130.69
129.80
129.32
128.72
128.60
128.41
127.15
123.29
77.32
77.00
76.68
35.62
Cl
N
4d
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

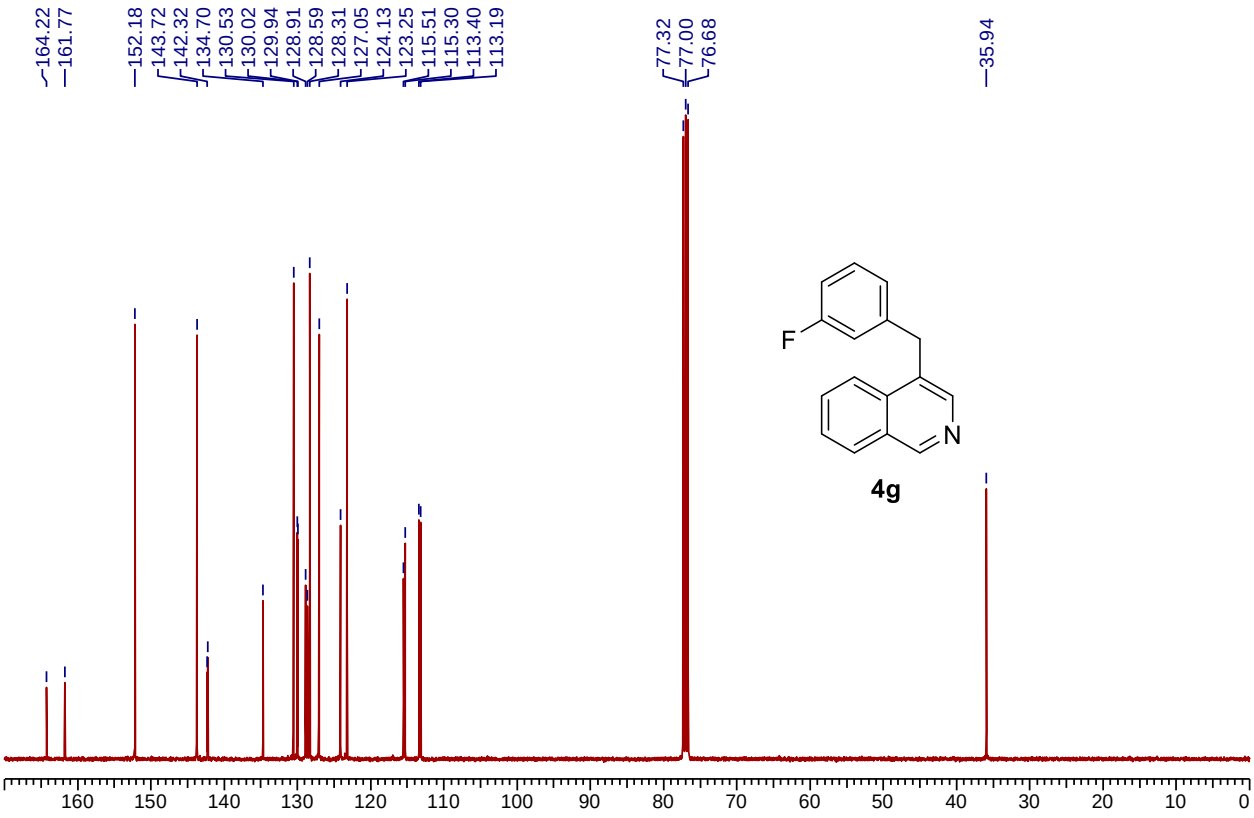

9.20
8.41
8.01
7.99
7.86
7.84
7.67
7.67
7.60
7.36
7.32
7.26
7.13
7.11
4.35
0.00
Br
N
4e
1.00
1.01
1.01
1.01
1.03
1.01
0.99
0.98
2.04
2.04
9
8
7
6
5
4
3
2
1
0

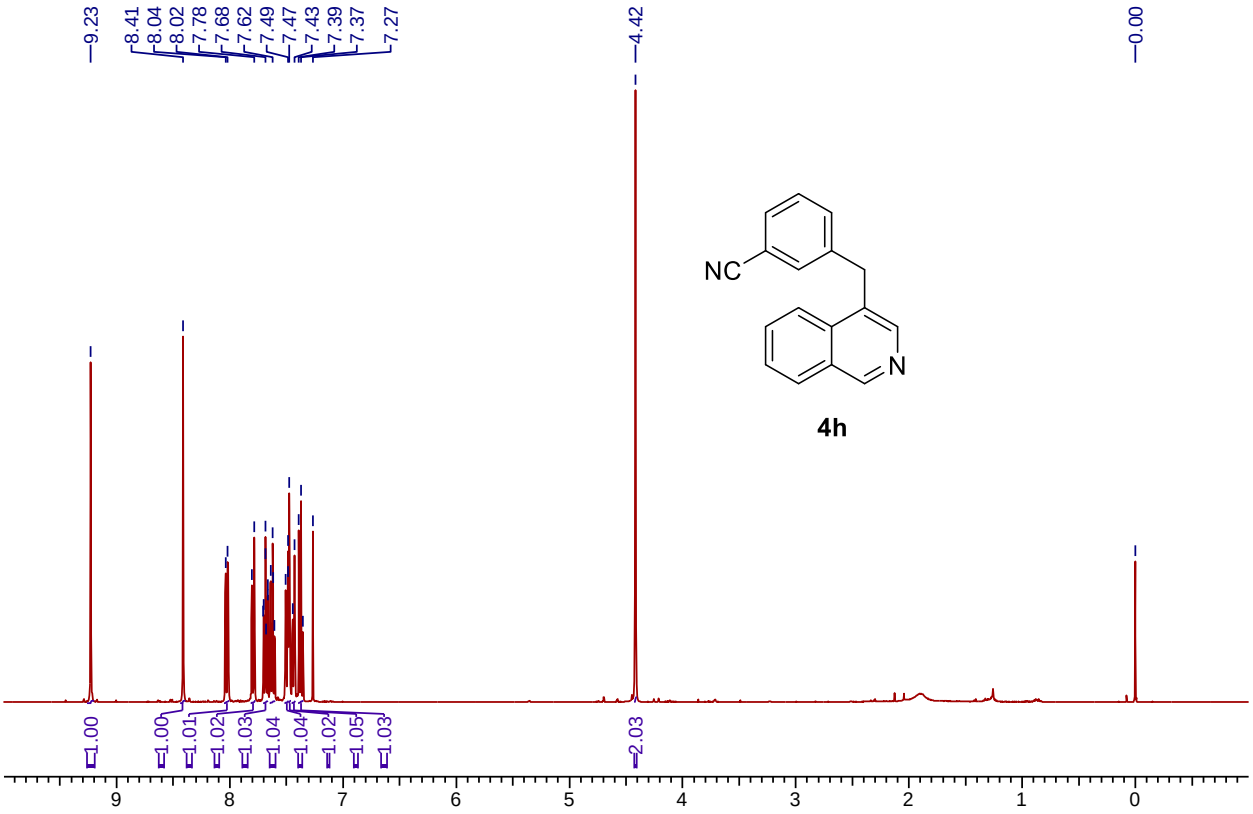

152.22
143.71
134.66
131.48
130.63
130.11
129.56
128.81
128.60
128.36
127.11
123.23
122.73
77.32
77.00
76.69
35.86
Br
N
4e
143.71
142.04
144.0
143.5
143.0
142.5
142.0
141.5
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

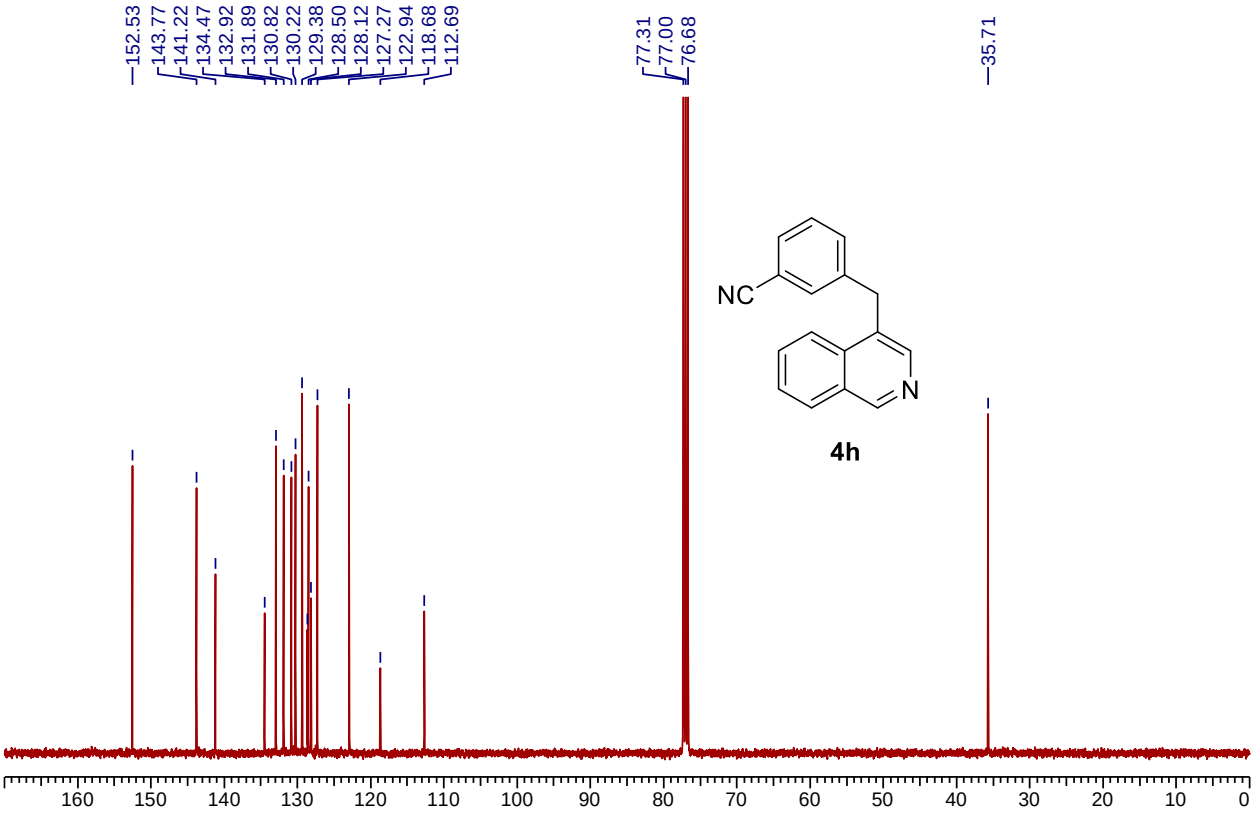

9.21
8.40
8.01
7.99
7.86
7.84
7.67
7.60
7.58
7.54
7.52
7.26
7.12
7.00
6.99
4.33
0.00
I
N
4f
1.00
0.97
0.99
1.00
1.01
0.94
1.03
0.96
1.01
1.01
1.98
9
8
7
6
5
4
3
2
1
0

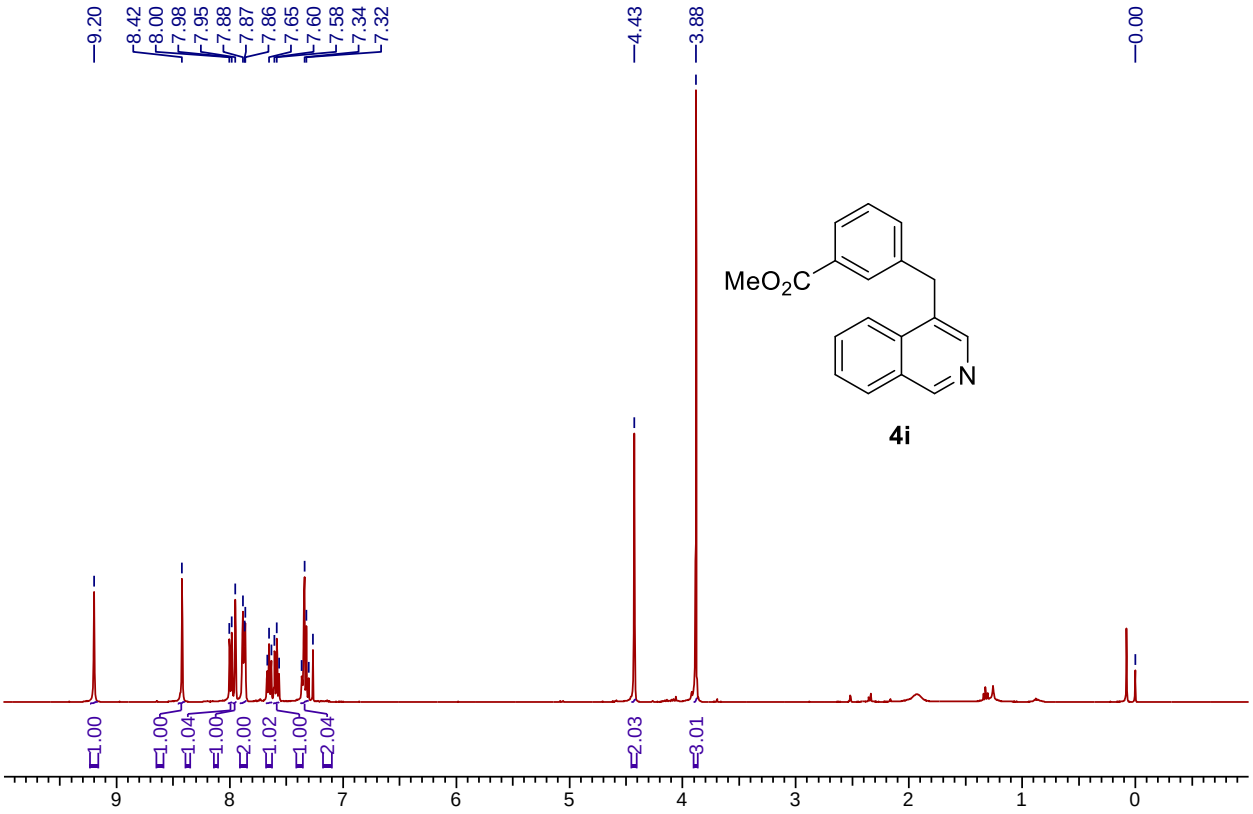

152.20
143.68
142.11
137.42
135.54
134.66
130.64
130.28
128.37
127.75
127.12
123.23
94.70
77.32
77.00
76.68
35.75
I
N
4f
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

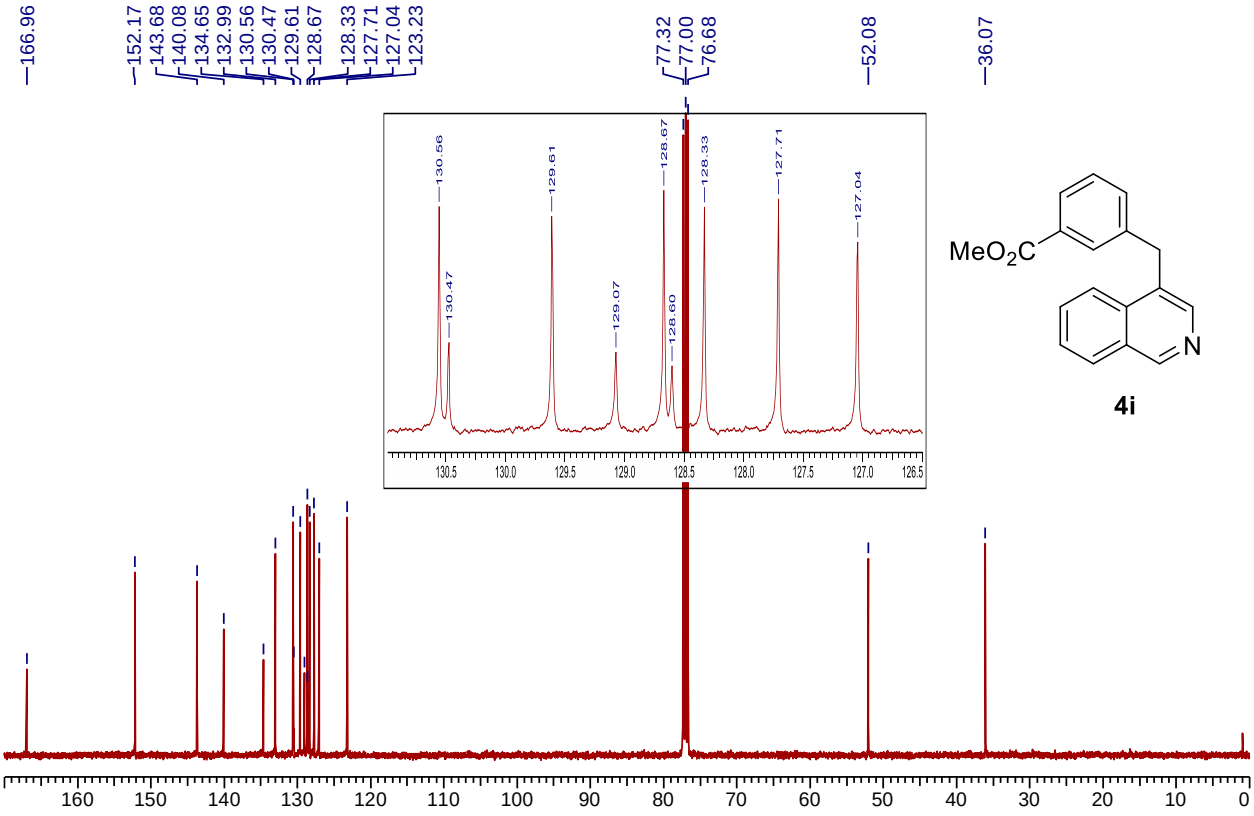

9.20
8.41
8.00
7.98
7.87
7.85
7.65
7.61
7.60
7.59
7.21
6.99
6.97
6.88
6.86
4.37
0.00
1.00
1.00
1.01
1.02
1.03
1.01
1.01
1.00
2.00
2.05
F
N
4g

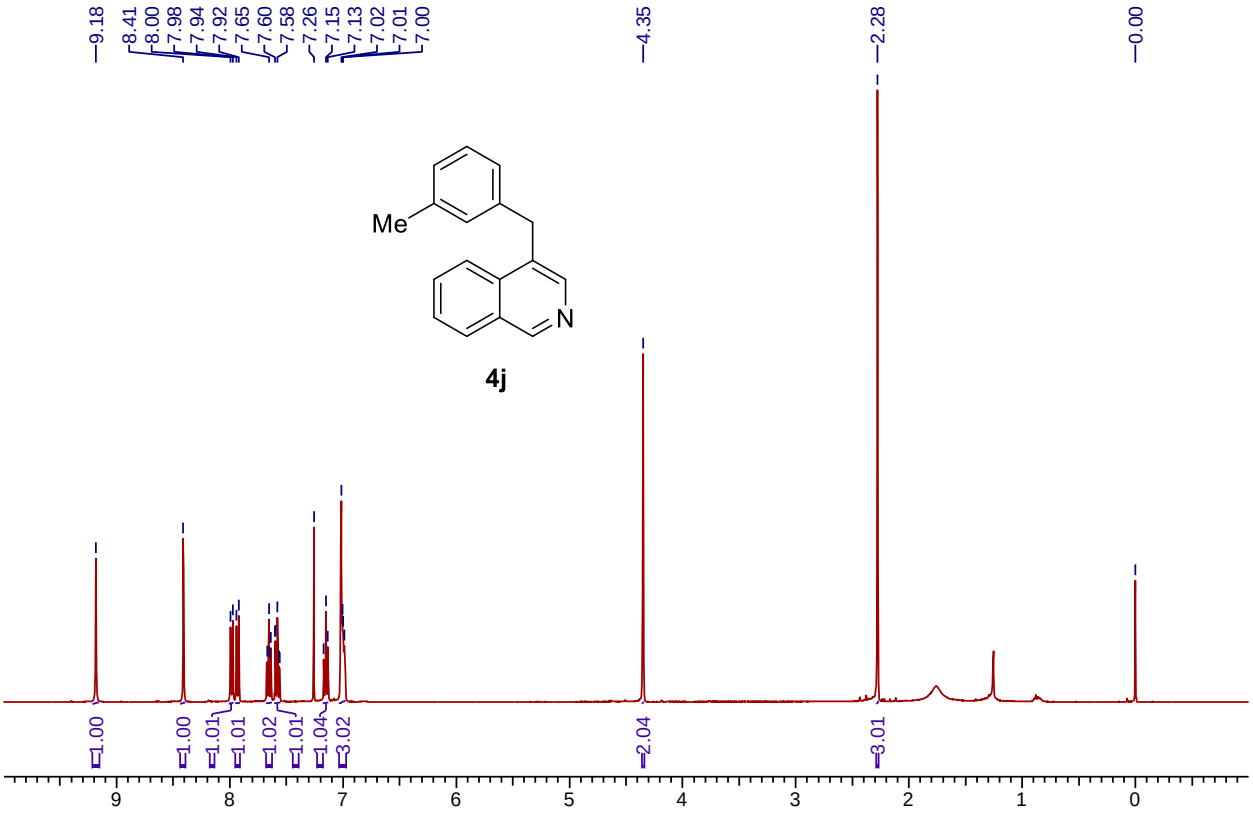

164.22
161.77
152.18
143.72
142.32
134.70
130.53
130.02
129.94
128.91
128.59
128.31
127.05
124.13
123.25
115.51
115.30
113.40
113.19
77.32
77.00
76.68
35.94
F
N
4g

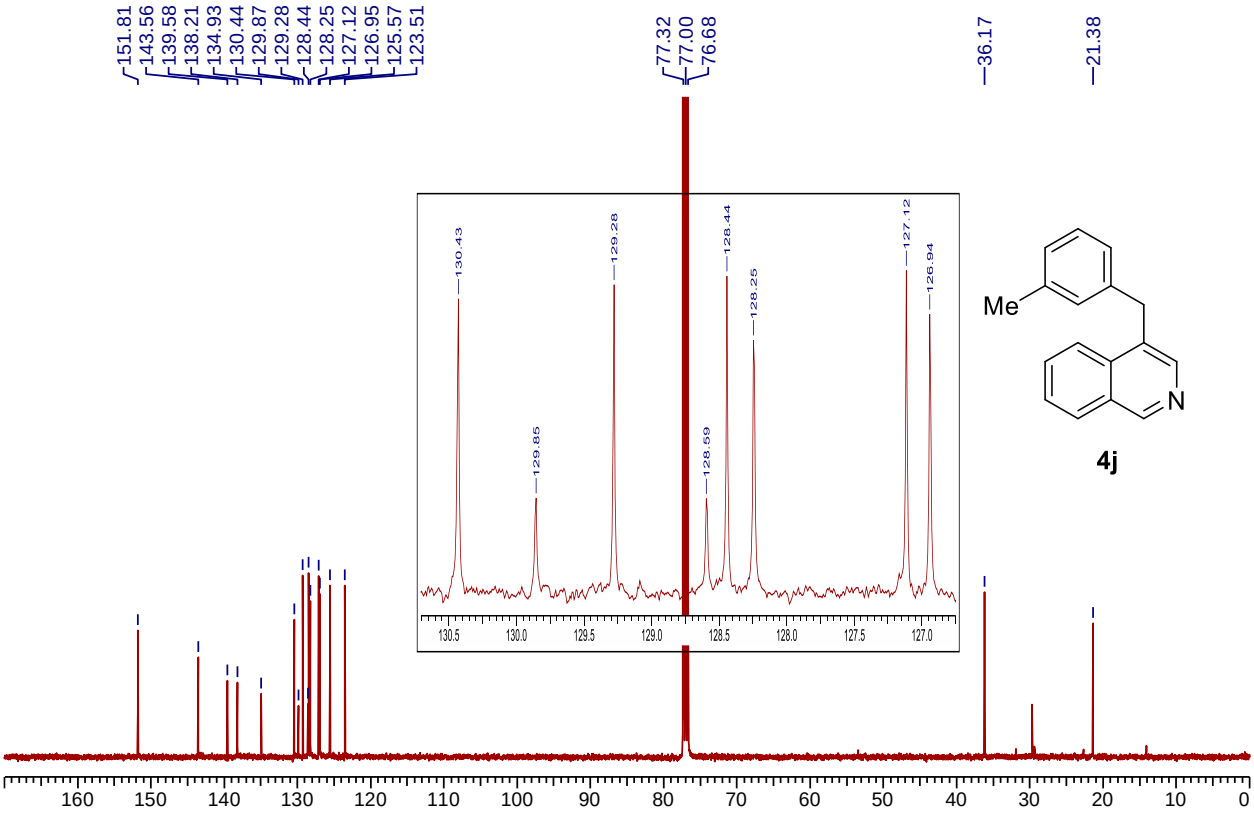

9.23
8.41
8.04
8.02
7.78
7.68
7.62
7.49
7.47
7.43
7.39
7.37
7.27
4.42
0.00
NC
N
4h
1.00
1.00
1.01
1.02
1.03
1.04
1.04
1.02
1.05
1.03
2.03
9
8
7
6
5
4
3
2
1
0

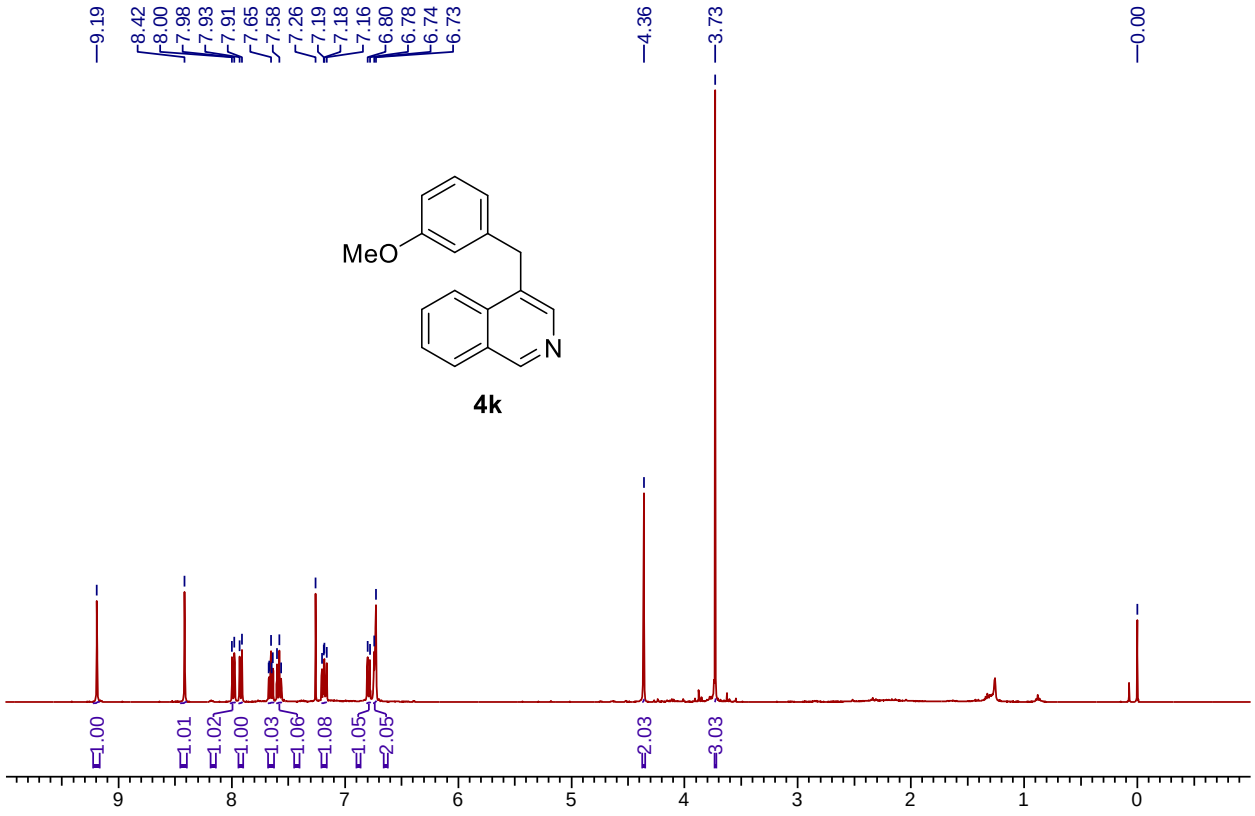

152.53
143.77
141.22
134.47
132.92
131.89
130.82
130.22
129.38
128.50
128.12
127.27
122.94
118.68
112.69
77.31
77.00
76.68
35.71
NC
N
4h
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

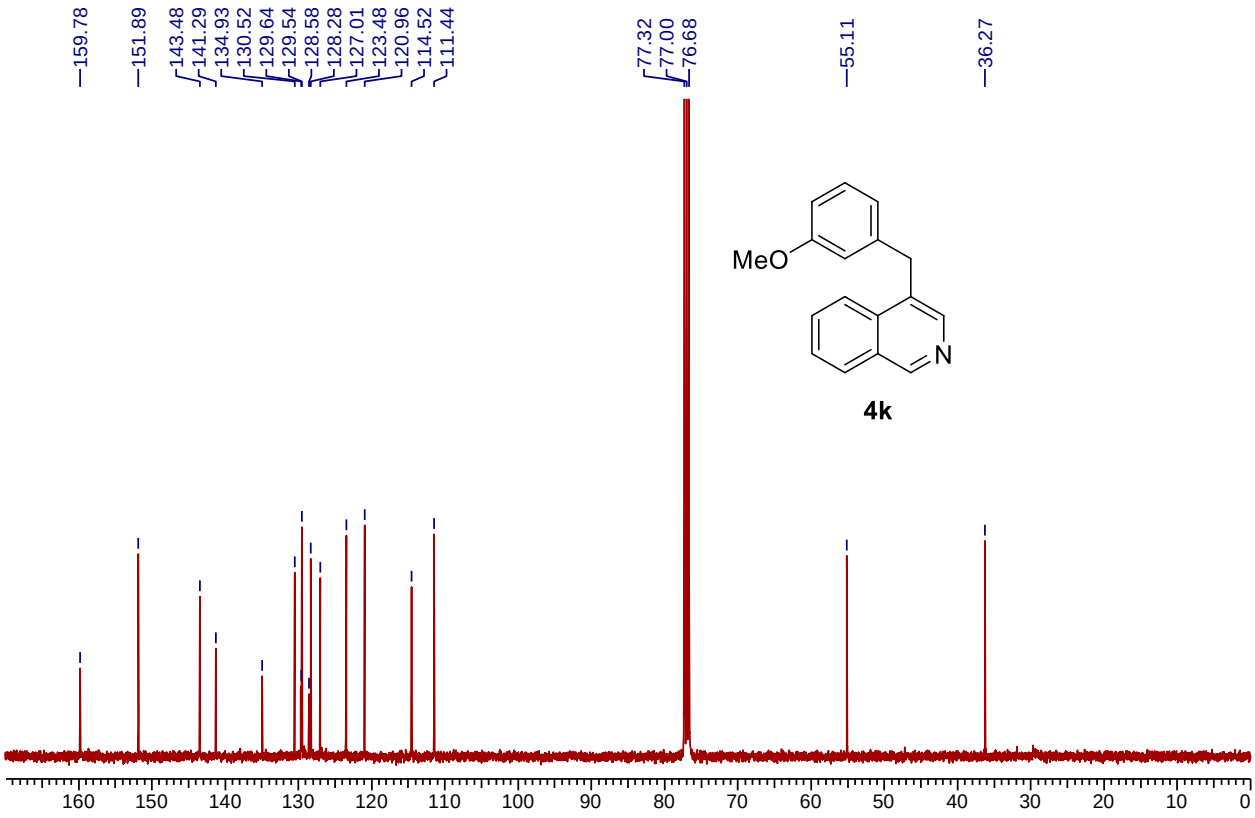

9.20
8.42
8.00
7.98
7.95
7.88
7.87
7.86
7.65
7.60
7.58
7.34
7.32
4.43
3.88
0.00
1.00
1.00
1.04
1.00
2.00
1.02
1.00
2.04
2.03
3.01
MeO2C
N
4i

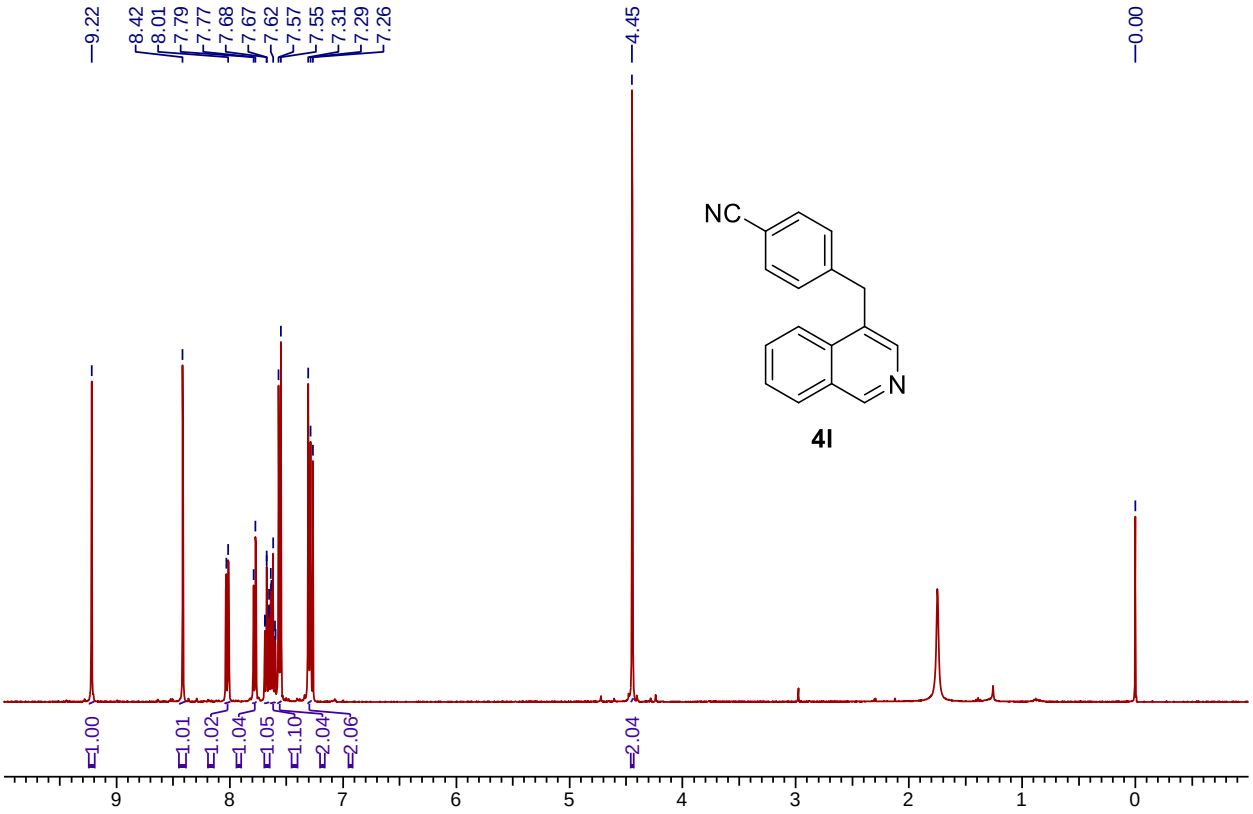

166.96
152.17
143.68
140.08
134.65
132.99
130.56
130.47
129.61
128.67
128.33
127.71
127.04
123.23
77.32
77.00
76.68
52.08
36.07
130.56
130.47
129.61
129.07
128.67
128.60
128.33
127.71
127.04
MeO2C
N
4i

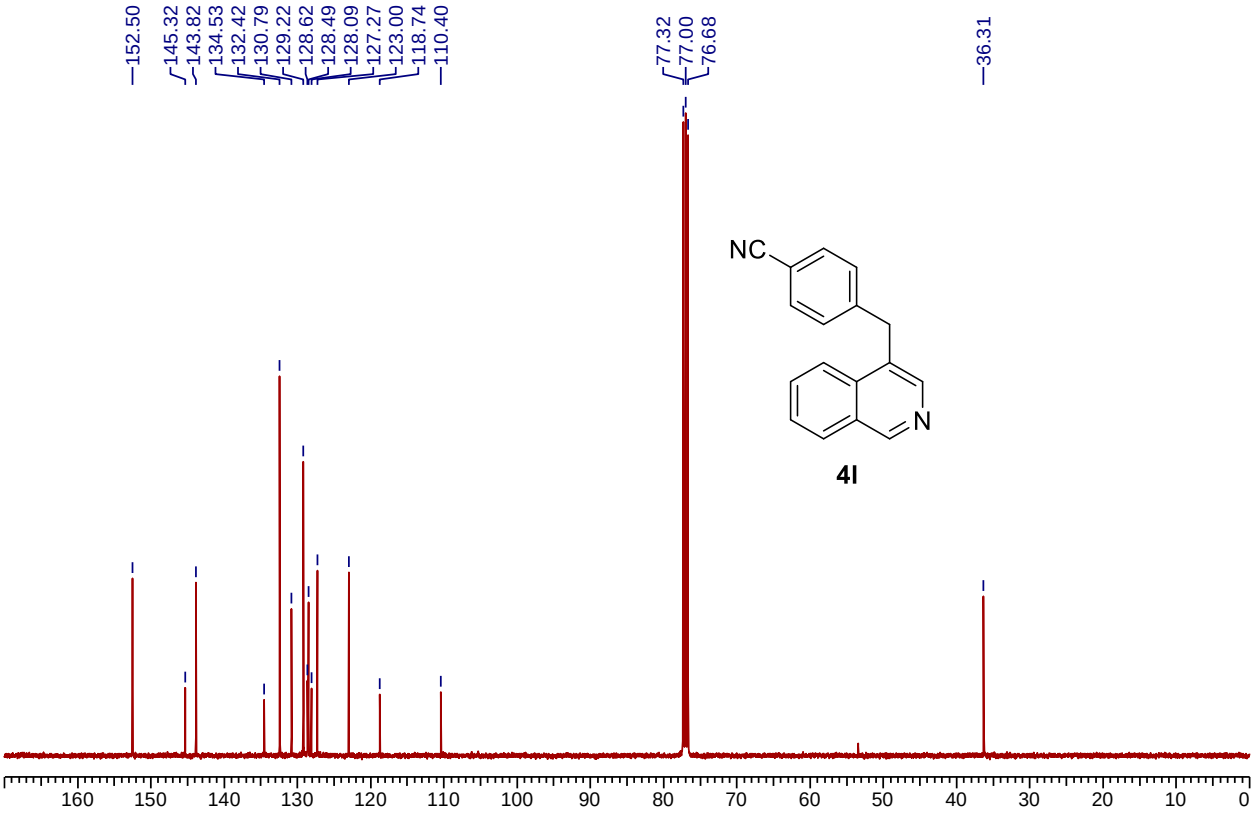

9.18
8.41
8.00
7.98
7.94
7.92
7.65
7.60
7.58
7.26
7.15
7.13
7.02
7.01
7.00
4.35
2.28
0.00
Me
N
4j
1.00
1.00
1.01
1.01
1.02
1.01
1.04
3.02
2.04
3.01

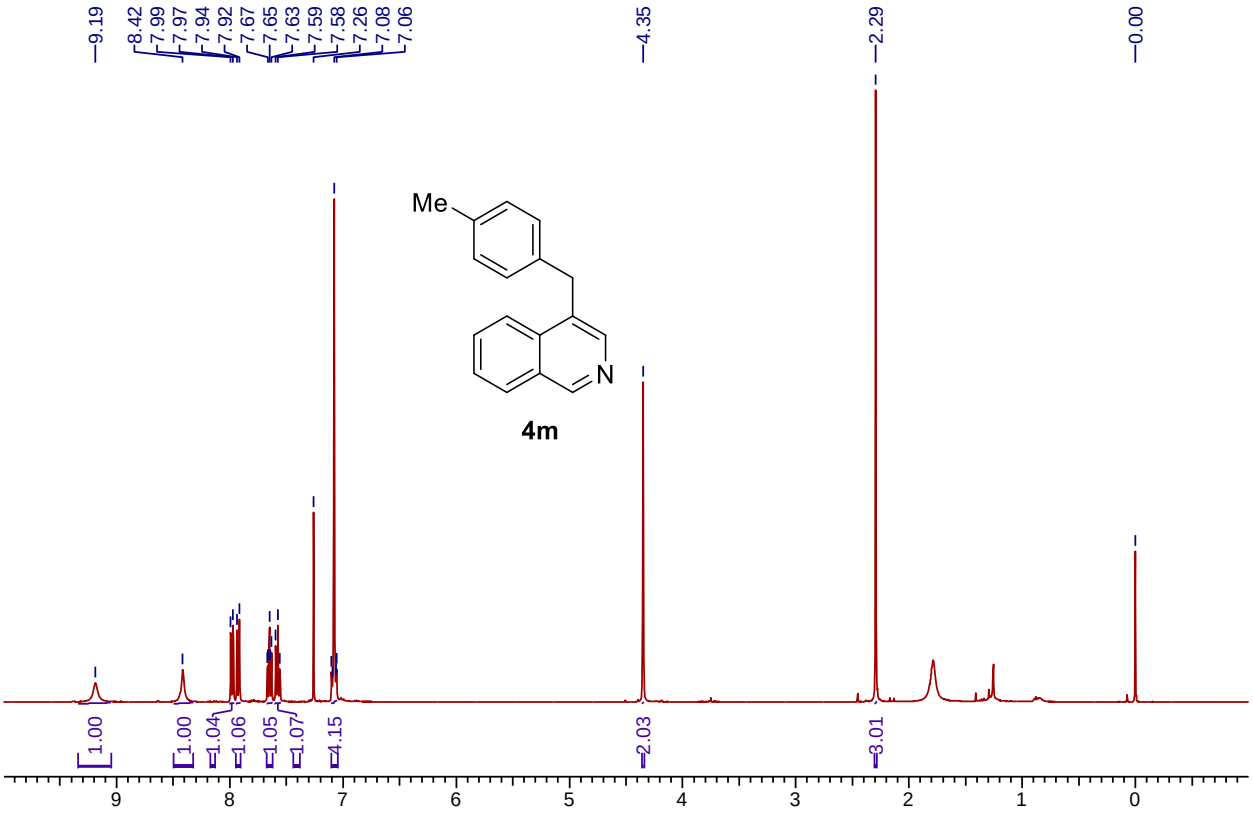

151.81
143.56
139.58
138.21
134.93
130.44
129.87
129.28
128.44
128.25
127.12
126.95
125.57
123.51
77.32
77.00
76.68
36.17
21.38
130.43
129.85
129.28
128.59
128.44
128.25
127.12
126.94
Me
N
4j

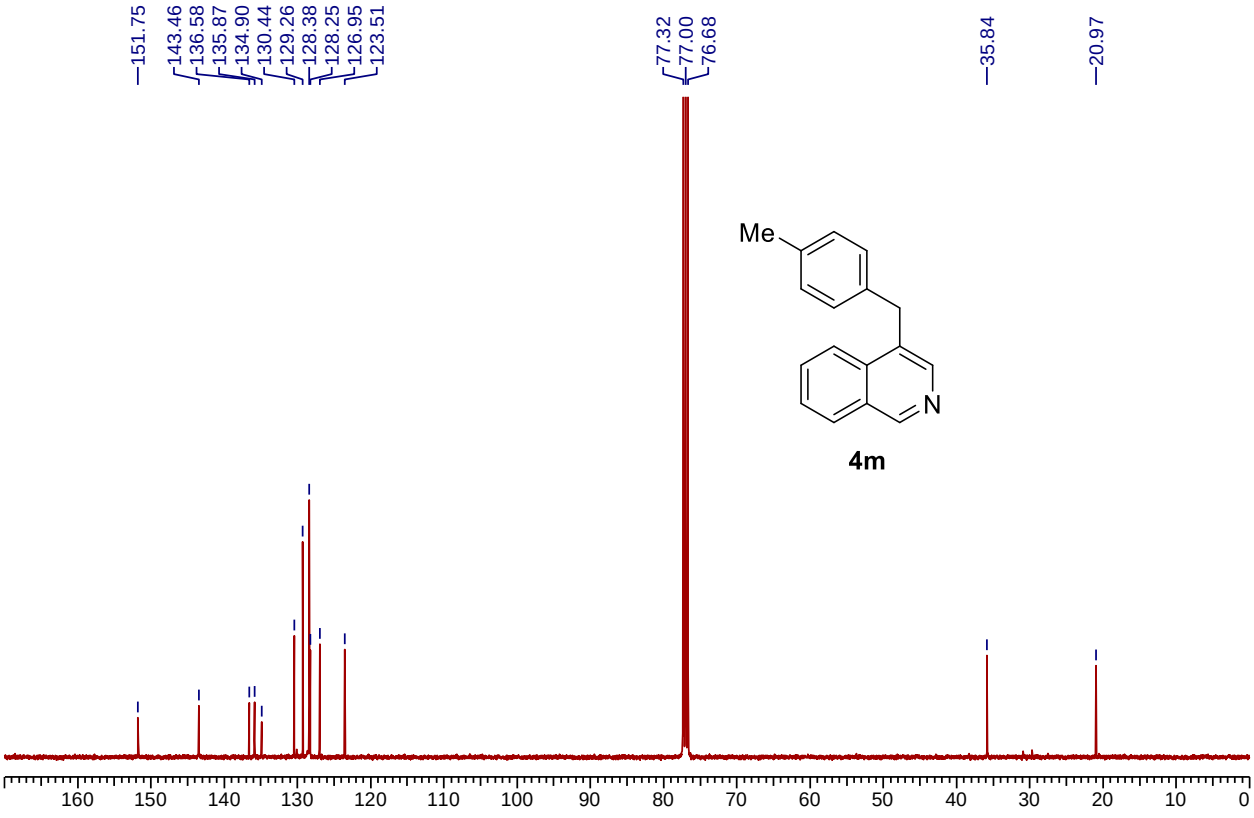

9.19
8.42
8.00
7.98
7.93
7.91
7.65
7.58
7.26
7.19
7.18
7.16
6.80
6.78
6.74
6.73
4.36
3.73
0.00
MeO
N
4k
1.00
1.01
1.02
1.00
1.03
1.06
1.08
1.05
2.05
2.03
3.03

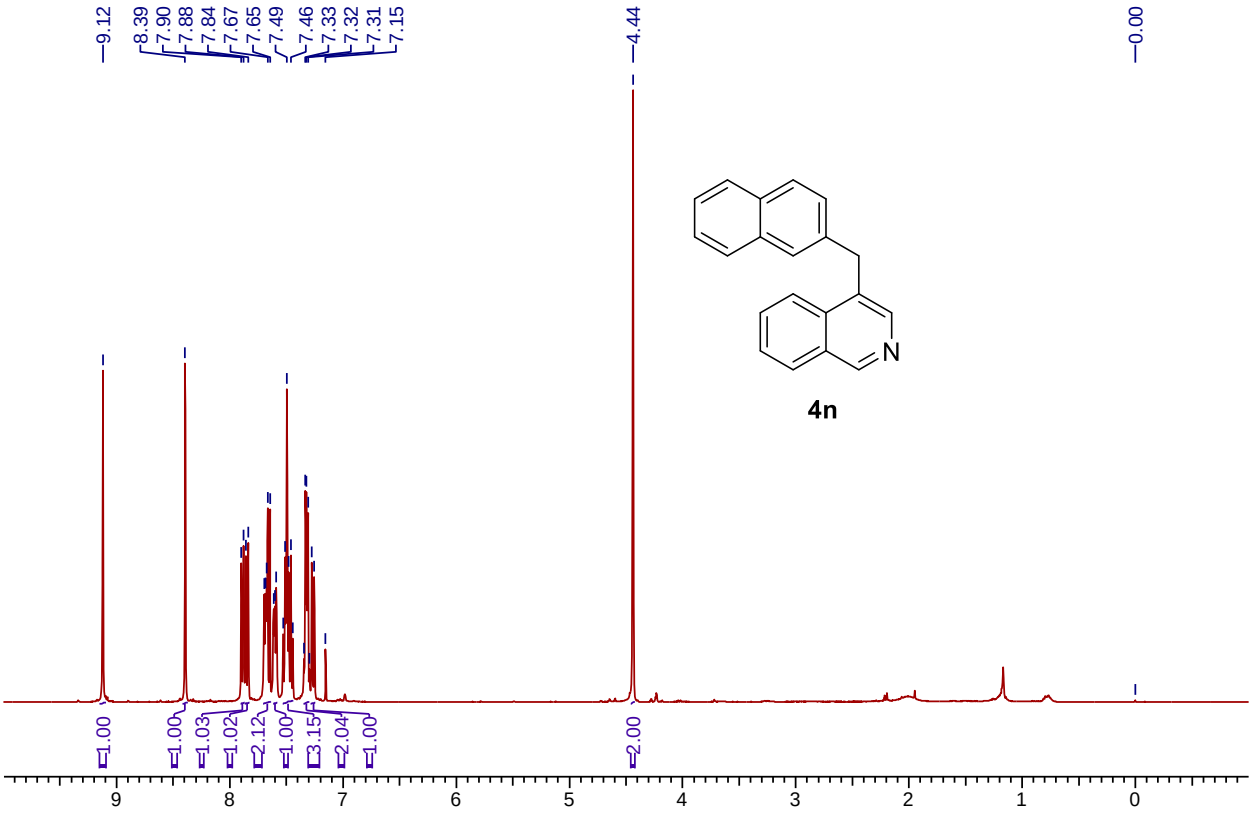

159.78
151.89
143.48
141.29
134.93
130.52
129.64
129.54
128.58
128.28
127.01
123.48
120.96
114.52
111.44
77.32
77.00
76.68
55.11
36.27
MeO
N
4k

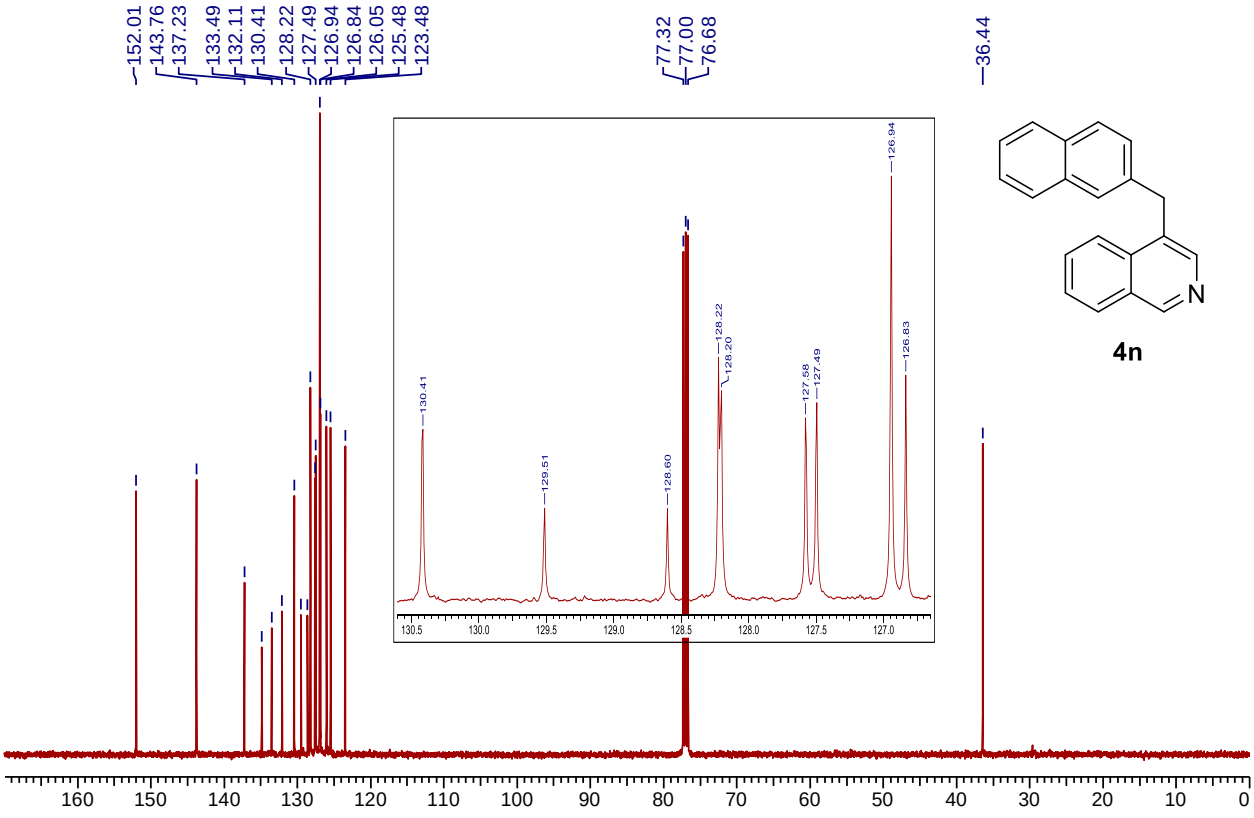

9.22
8.42
8.01
7.79
7.77
7.68
7.67
7.62
7.57
7.55
7.31
7.29
7.26
4.45
0.00
NC
N
4l
1.00
1.01
1.02
1.04
1.05
1.10
2.04
2.06
2.04
9
8
7
6
5
4
3
2
1
0

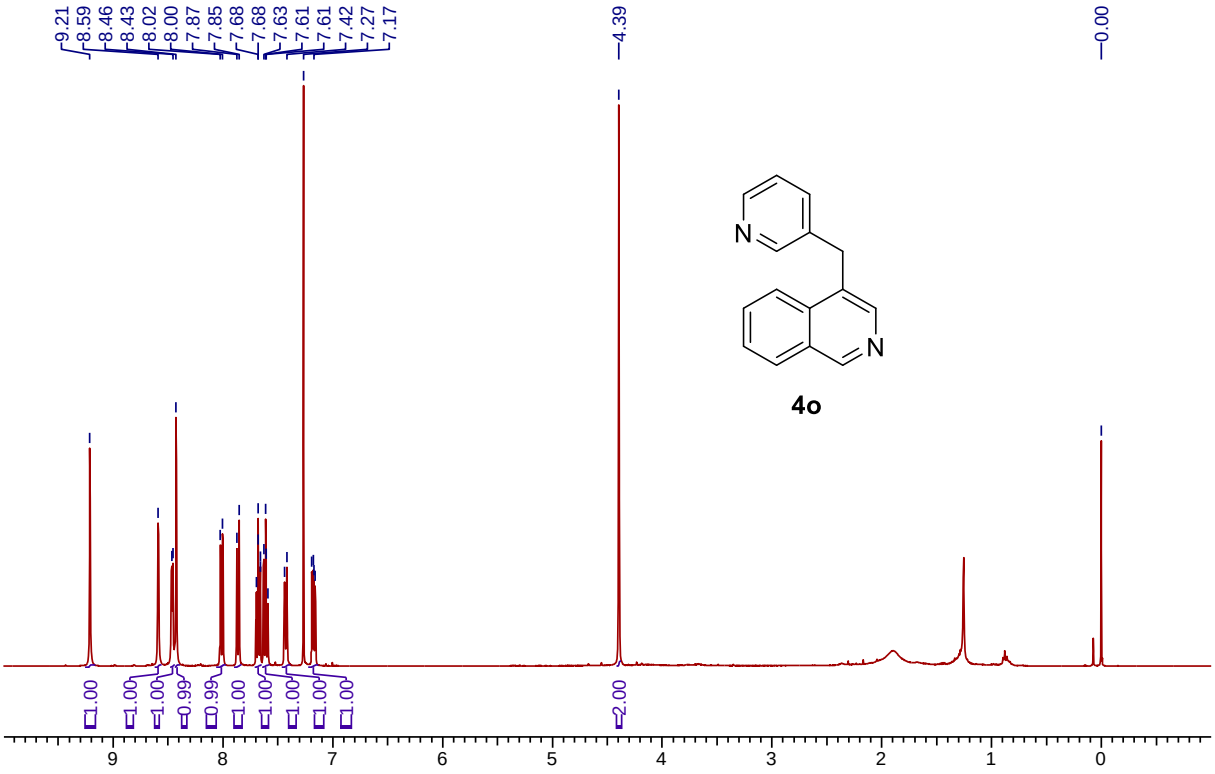

152.50
145.32
143.82
134.53
132.42
130.79
129.22
128.62
128.49
128.09
127.27
123.00
118.74
110.40
77.32
77.00
76.68
36.31
NC
N
4l
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

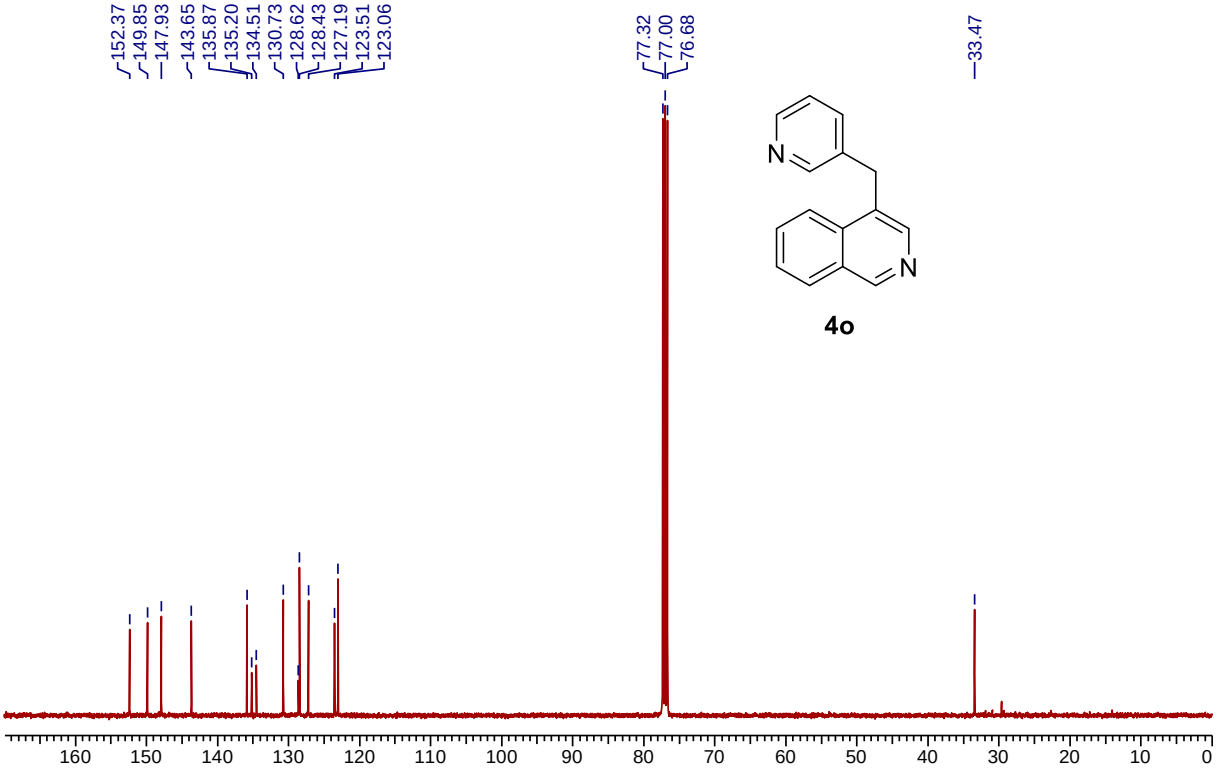

9.19
8.42
7.99
7.97
7.94
7.92
7.67
7.65
7.63
7.59
7.58
7.26
7.08
7.06
4.35
2.29
0.00
Me
N
4m
1.00
1.00
1.04
1.06
1.05
1.07
4.15
2.03
3.01
9
8
7
6
5
4
3
2
1
0

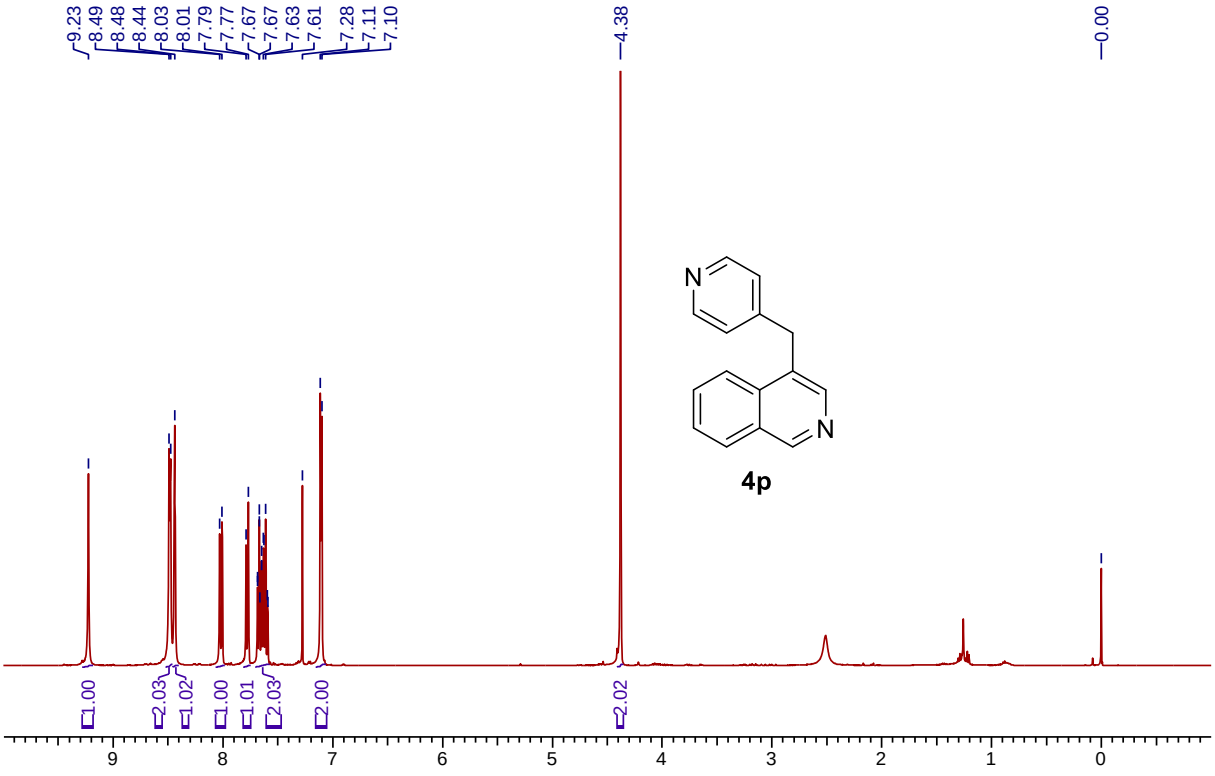

151.75
143.46
136.58
135.87
134.90
130.44
129.26
128.38
128.25
126.95
123.51
77.32
77.00
76.68
35.84
20.97
Me
N
4m
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

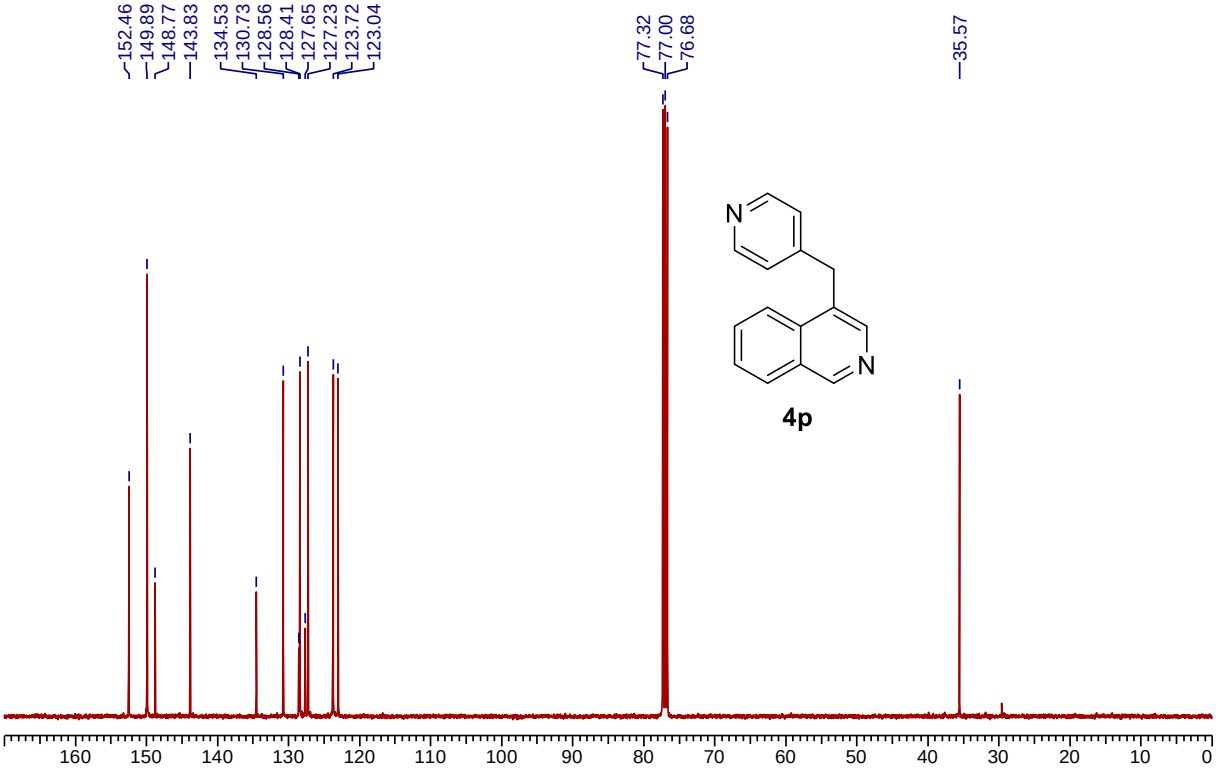

9.12
8.39
7.90
7.88
7.84
7.67
7.65
7.49
7.46
7.33
7.32
7.31
7.15
4.44
0.00
1.00
1.00
1.03
1.02
2.12
1.00
3.15
2.04
1.00
2.00
N
4n

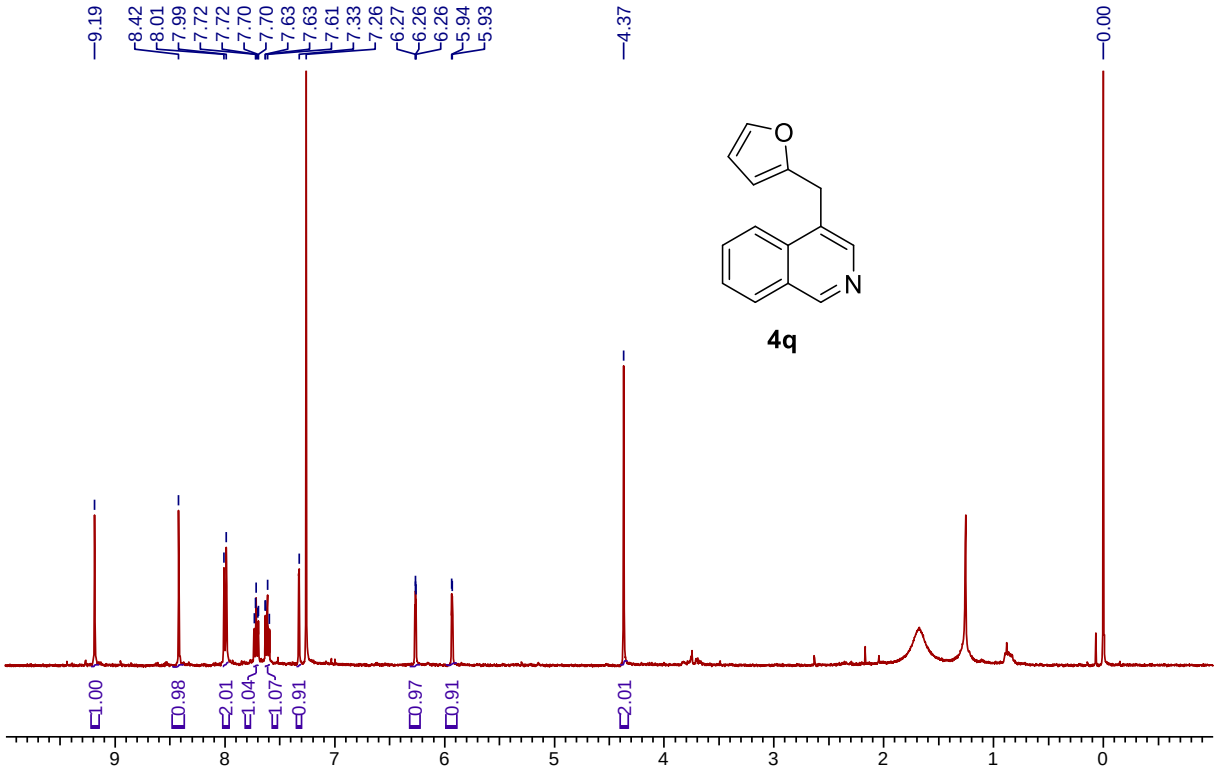

152.01
143.76
137.23
133.49
132.11
130.41
128.22
127.49
126.94
126.84
126.05
125.48
123.48
77.32
77.00
76.68
36.44
130.41
129.51
128.60
128.22
128.20
127.59
127.49
126.94
126.83
N
4n

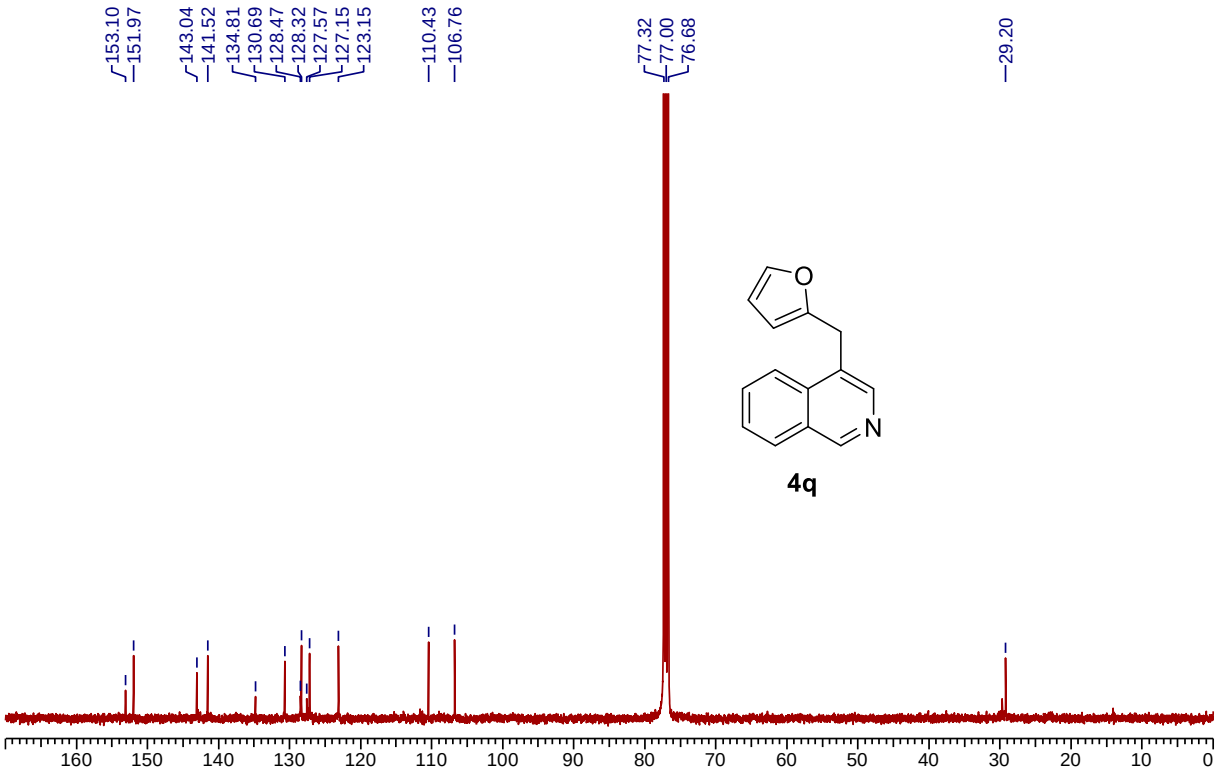

9.21
8.59
8.46
8.43
8.02
8.00
7.87
7.85
7.68
7.68
7.63
7.61
7.61
7.42
7.27
7.17
4.39
0.00
1.00
1.00
1.00
0.99
0.99
1.00
1.00
1.00
1.00
1.00
2.00
N
N
4o

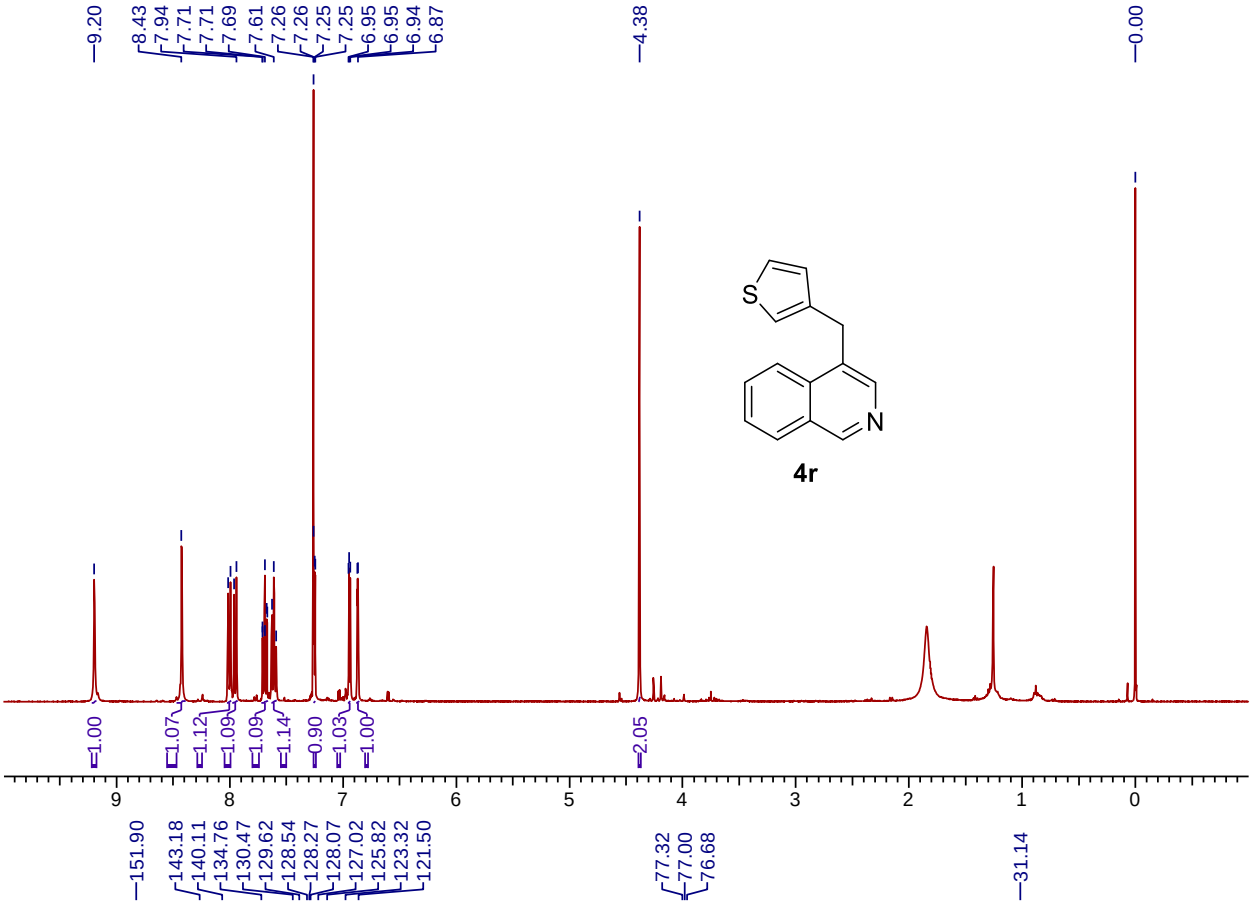

152.37
149.85
147.93
143.65
135.87
135.20
134.51
130.73
128.62
128.43
127.19
123.51
123.06
77.32
77.00
76.68
33.47
N
N
4o

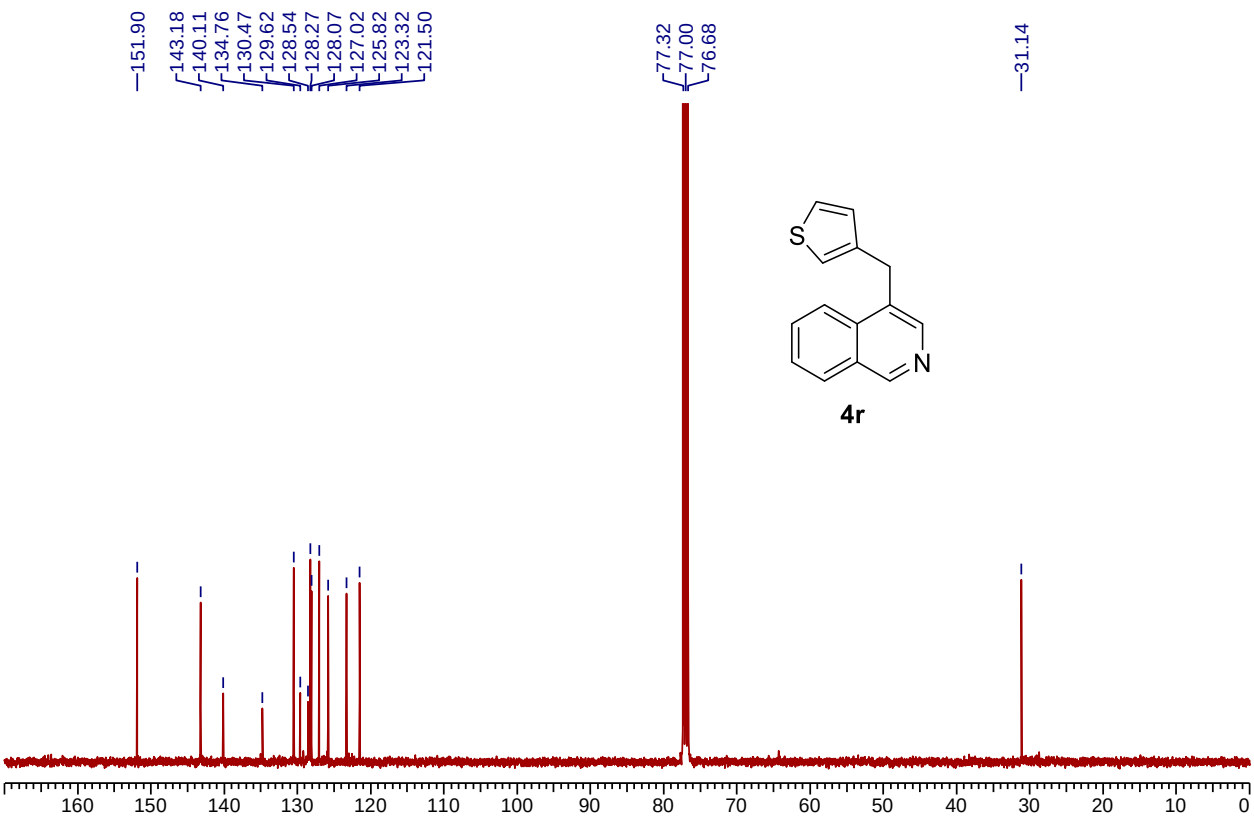

9.23
8.49
8.48
8.44
8.03
8.01
7.79
7.77
7.67
7.67
7.63
7.61
7.28
7.11
7.10
4.38
0.00
1.00
2.03
1.02
1.00
1.01
2.03
2.00
2.02
N
N
4p

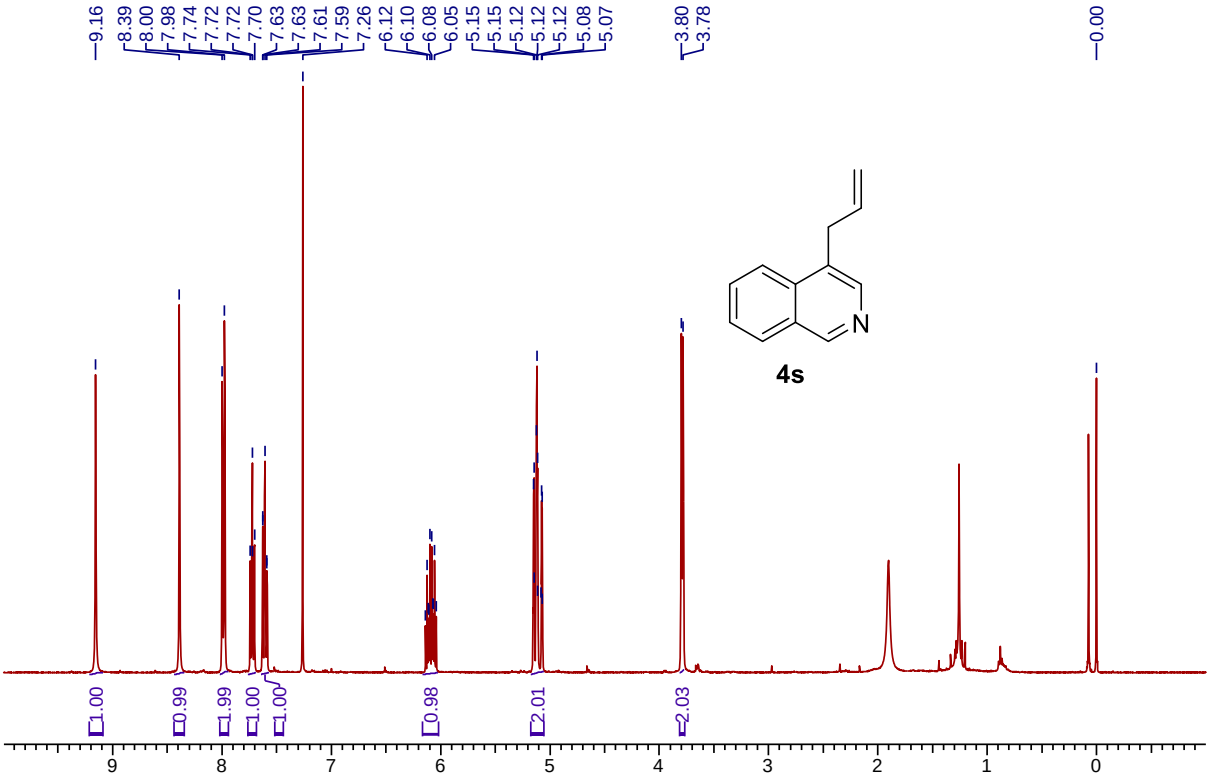

152.46
149.89
148.77
143.83
134.53
130.73
128.56
128.41
127.65
127.23
123.72
123.04
77.32
77.00
76.68
35.57
N
N
4p

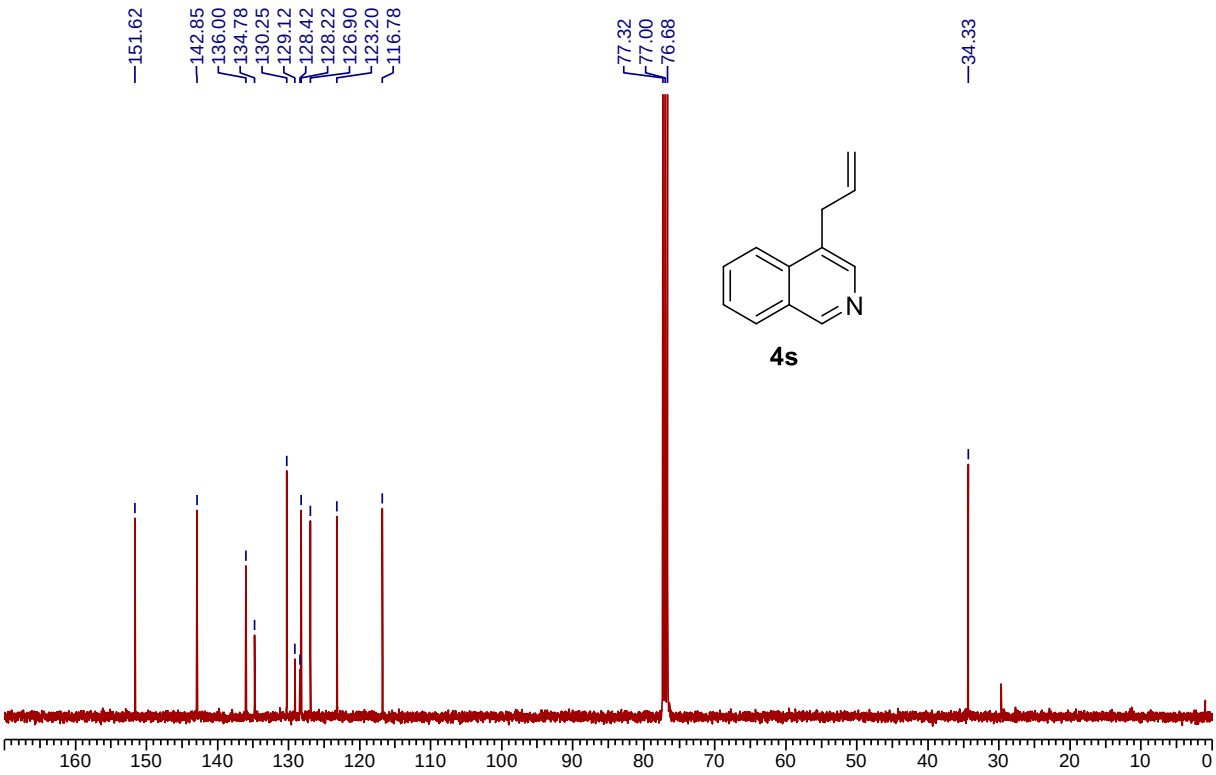

9.19
8.42
8.01
7.99
7.72
7.72
7.70
7.70
7.63
7.63
7.61
7.33
7.26
6.27
6.26
6.26
5.94
5.93
4.37
0.00
O
N
4q
1.00
0.98
2.01
1.04
1.07
0.91
0.97
0.91
2.01
9
8
7
6
5
4
3
2
1
0

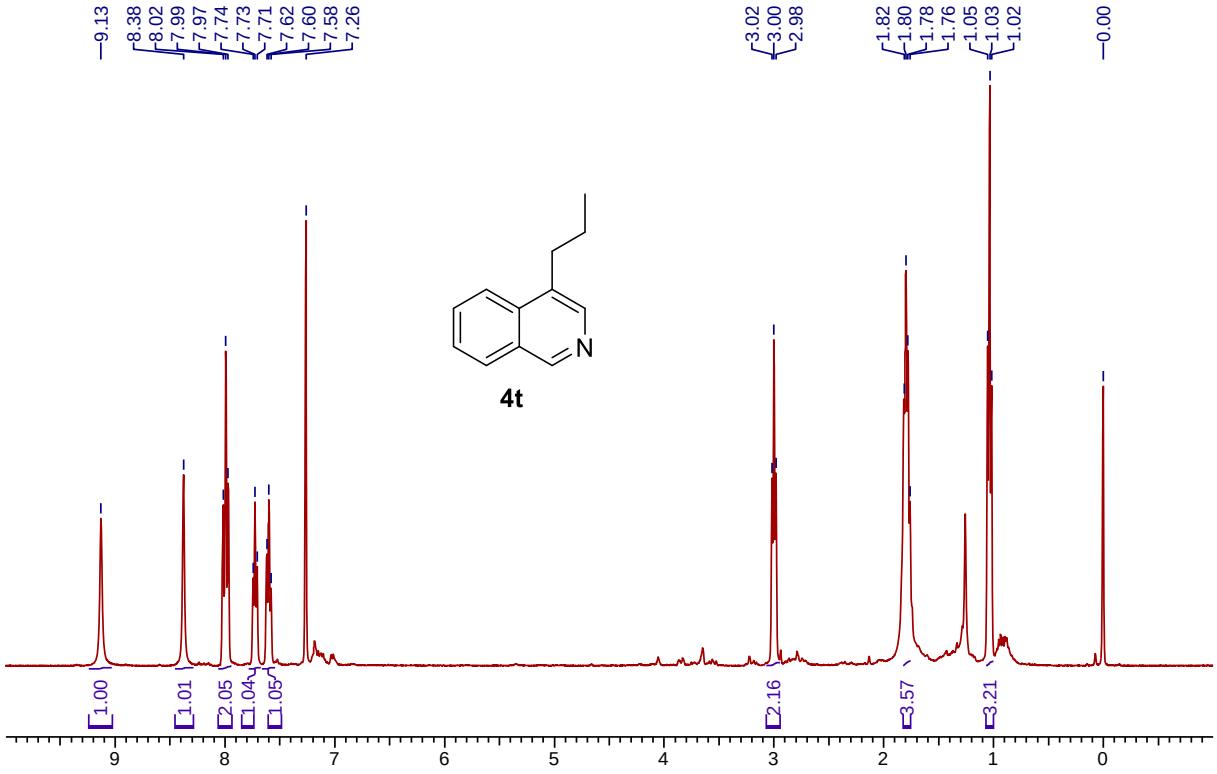

153.10
151.97
143.04
141.52
134.81
130.69
128.47
128.32
127.57
127.15
123.15
110.43
106.76
77.32
77.00
76.68
29.20
O
N
4q
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

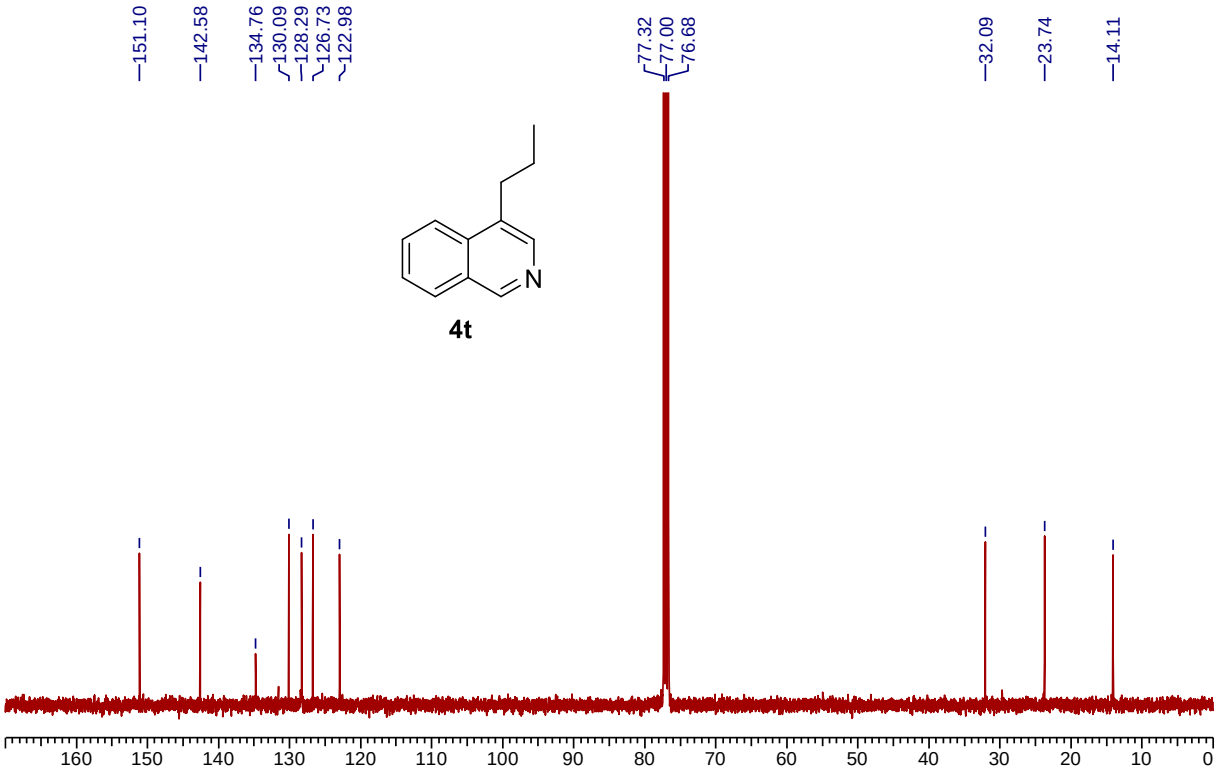

9.20
8.43
7.94
7.71
7.71
7.69
7.61
7.26
7.26
7.25
7.25
6.95
6.95
6.94
6.87
4.38
0.00
S
N
4r
1.00
1.07
1.12
1.09
1.09
1.14
0.90
1.03
1.00
2.05
9
8
7
6
5
4
3
2
1
0

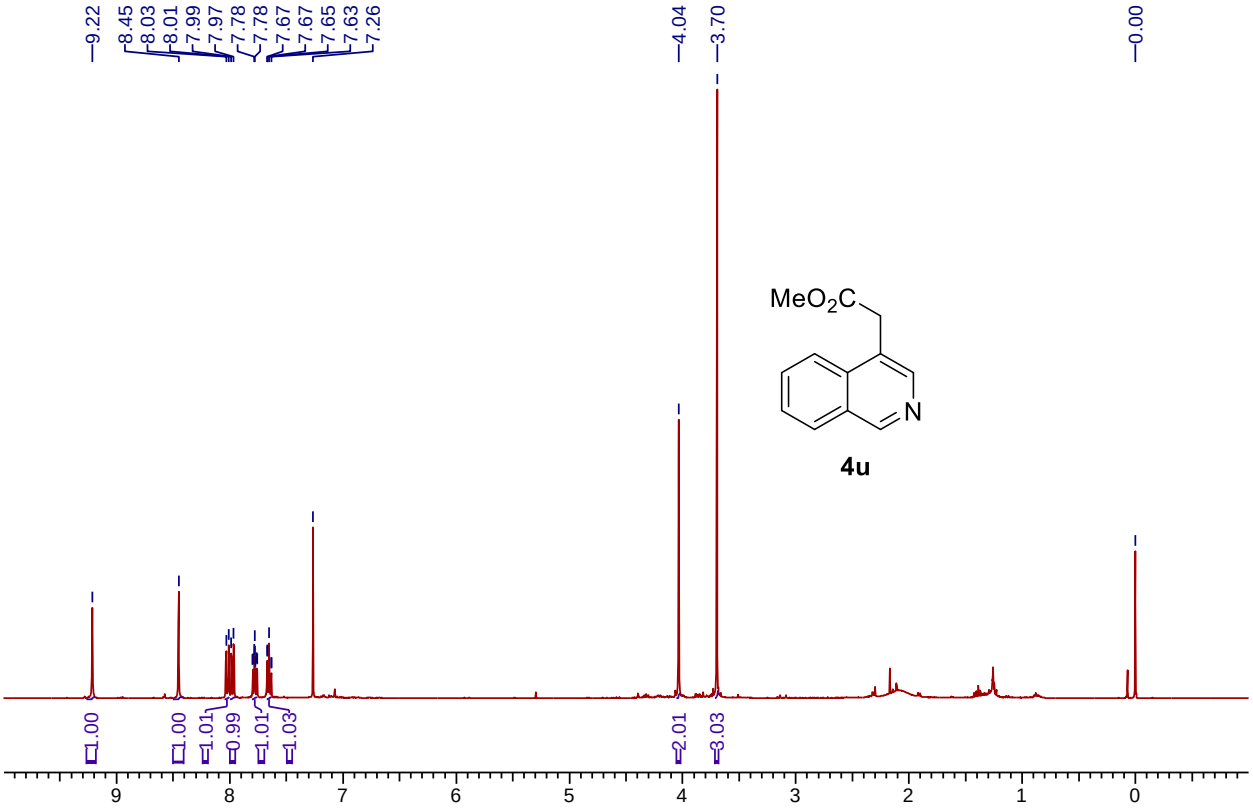

151.90
143.18
140.11
134.76
130.47
129.62
128.54
128.27
128.07
127.02
125.82
123.32
121.50
77.32
77.00
76.68
31.14
S
N
4r
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

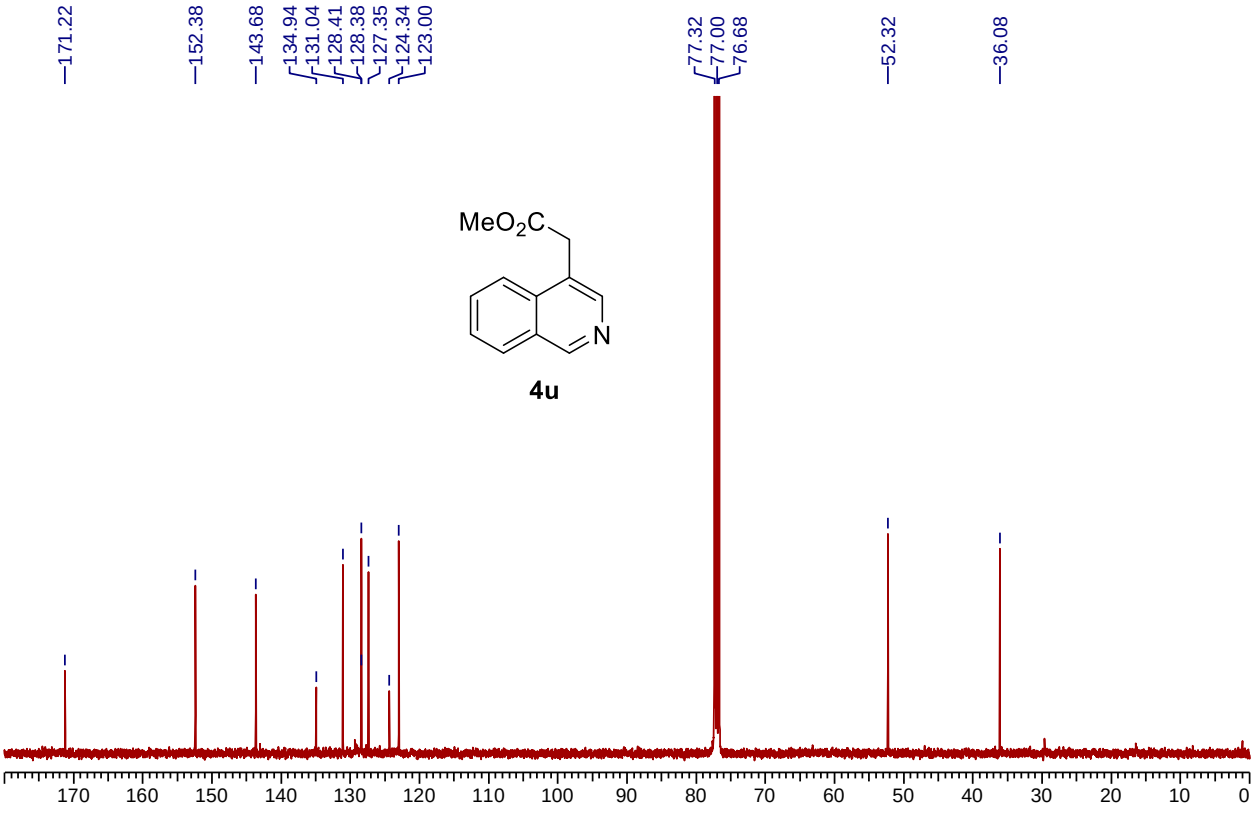

9.16
8.39
8.00
7.98
7.74
7.72
7.72
7.70
7.63
7.63
7.61
7.59
7.26
6.12
6.10
6.08
6.05
5.15
5.15
5.12
5.12
5.12
5.08
5.07
3.80
3.78
0.00
1.00
0.99
1.99
1.00
1.00
0.98
2.01
2.03
N
4s

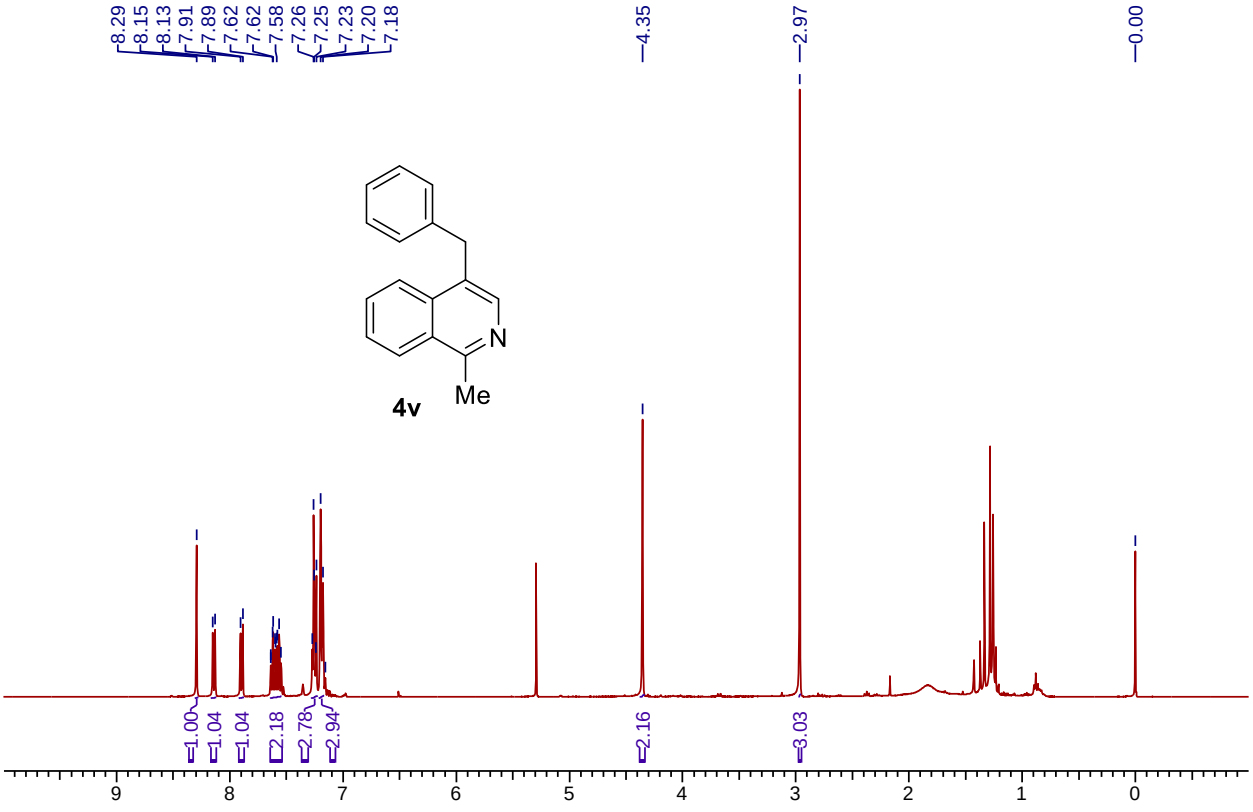

151.62
142.85
136.00
134.78
130.25
129.12
128.42
128.22
126.90
123.20
116.78
77.32
77.00
76.68
34.33
N
4s

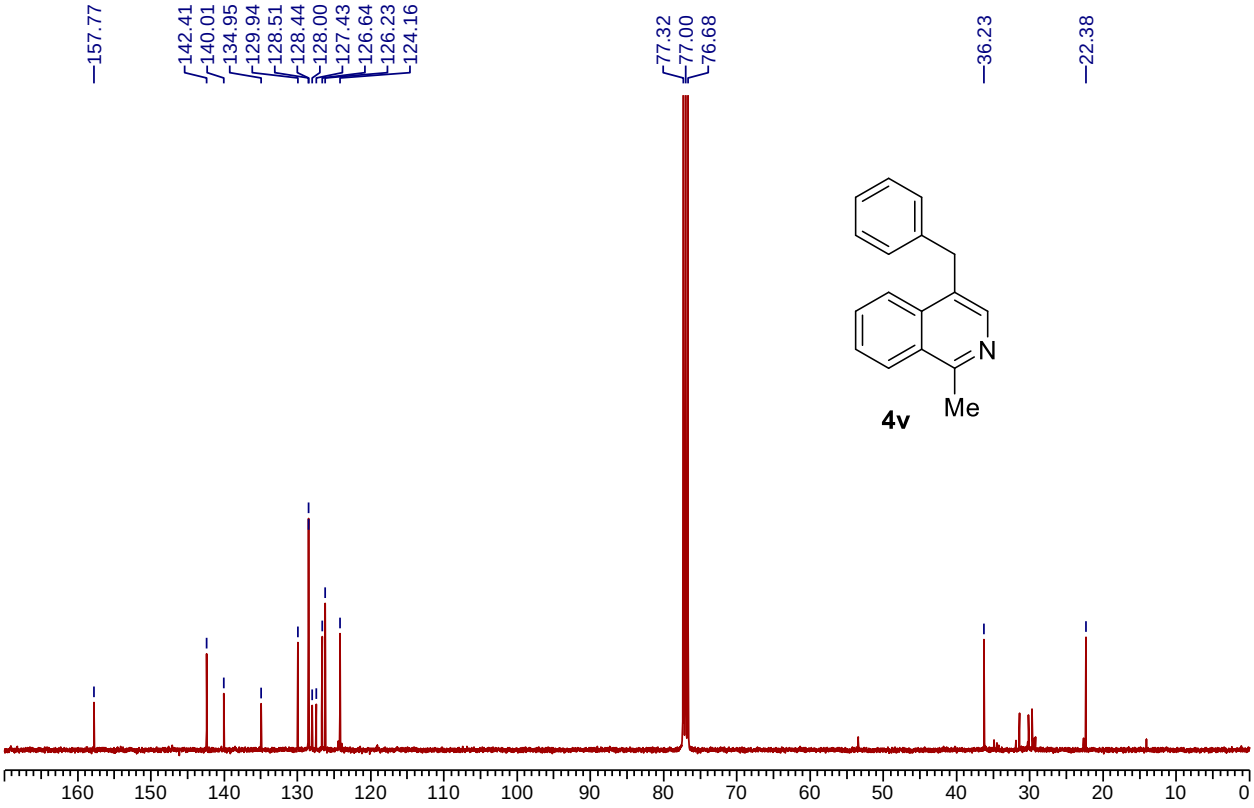

9.13
8.38
8.02
7.99
7.97
7.74
7.73
7.71
7.62
7.60
7.58
7.26
3.02
3.00
2.98
1.82
1.80
1.78
1.76
1.05
1.03
1.02
0.00
N
4t
1.00
1.01
2.05
1.04
1.05
2.16
3.57
3.21

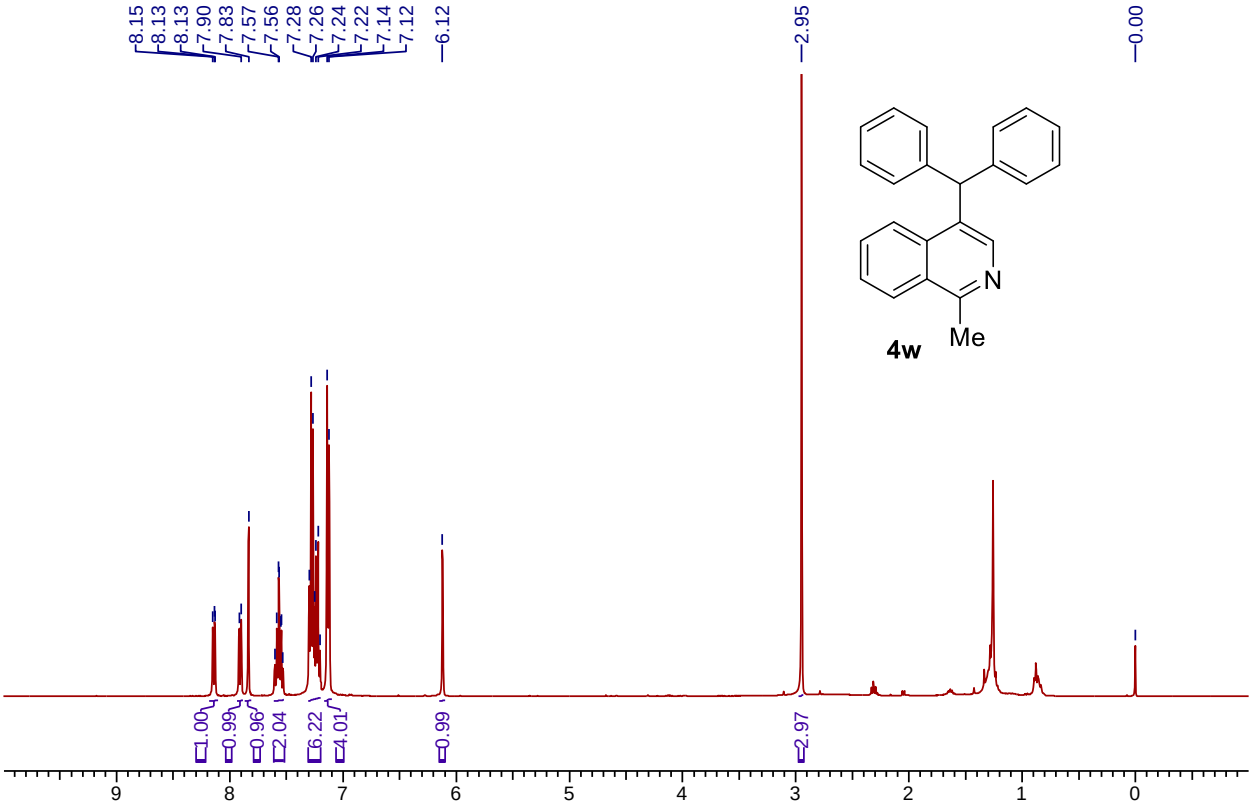

151.10
142.58
134.76
130.09
128.29
126.73
122.98
77.32
77.00
76.68
32.09
23.74
14.11
N
4t

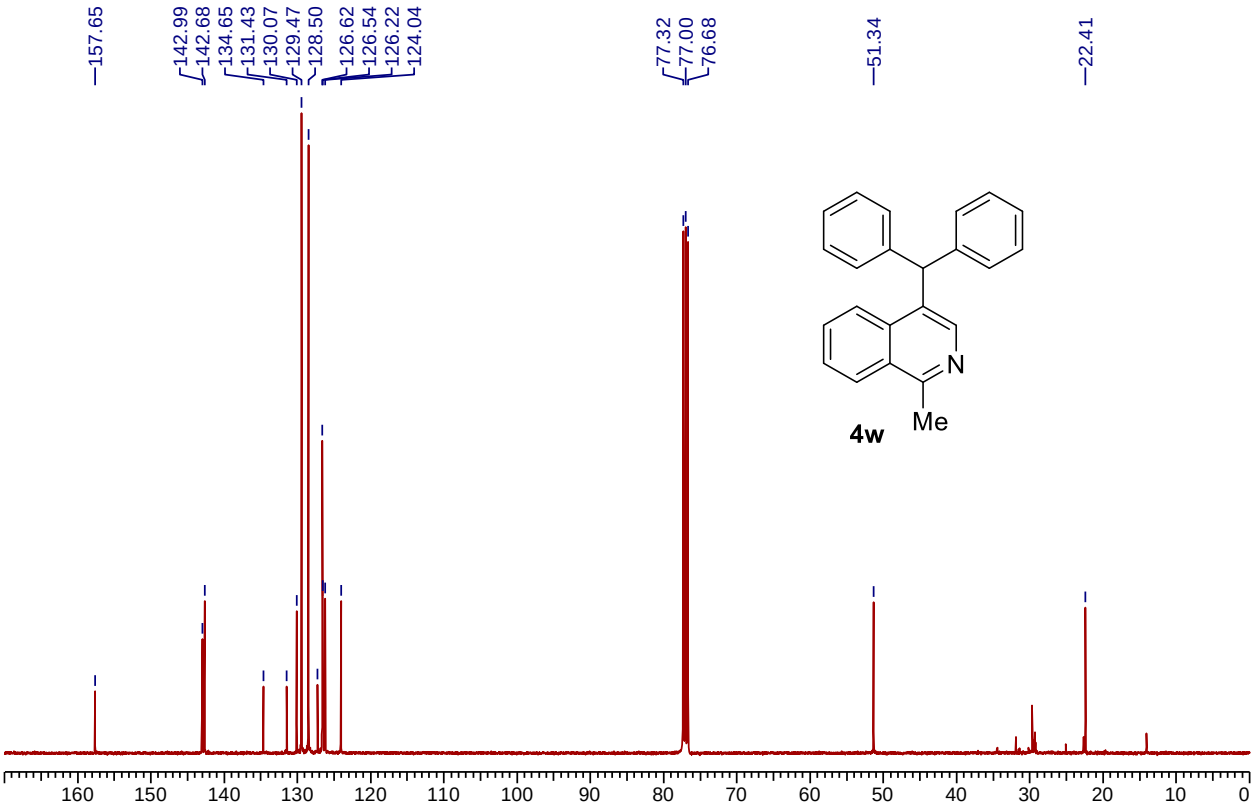

9.22
8.45
8.03
8.01
7.99
7.97
7.78
7.78
7.67
7.67
7.65
7.63
7.26
4.04
3.70
0.00
MeO2C
N
4u
1.00
1.00
1.01
0.99
1.01
1.03
2.01
3.03
9
8
7
6
5
4
3
2
1
0

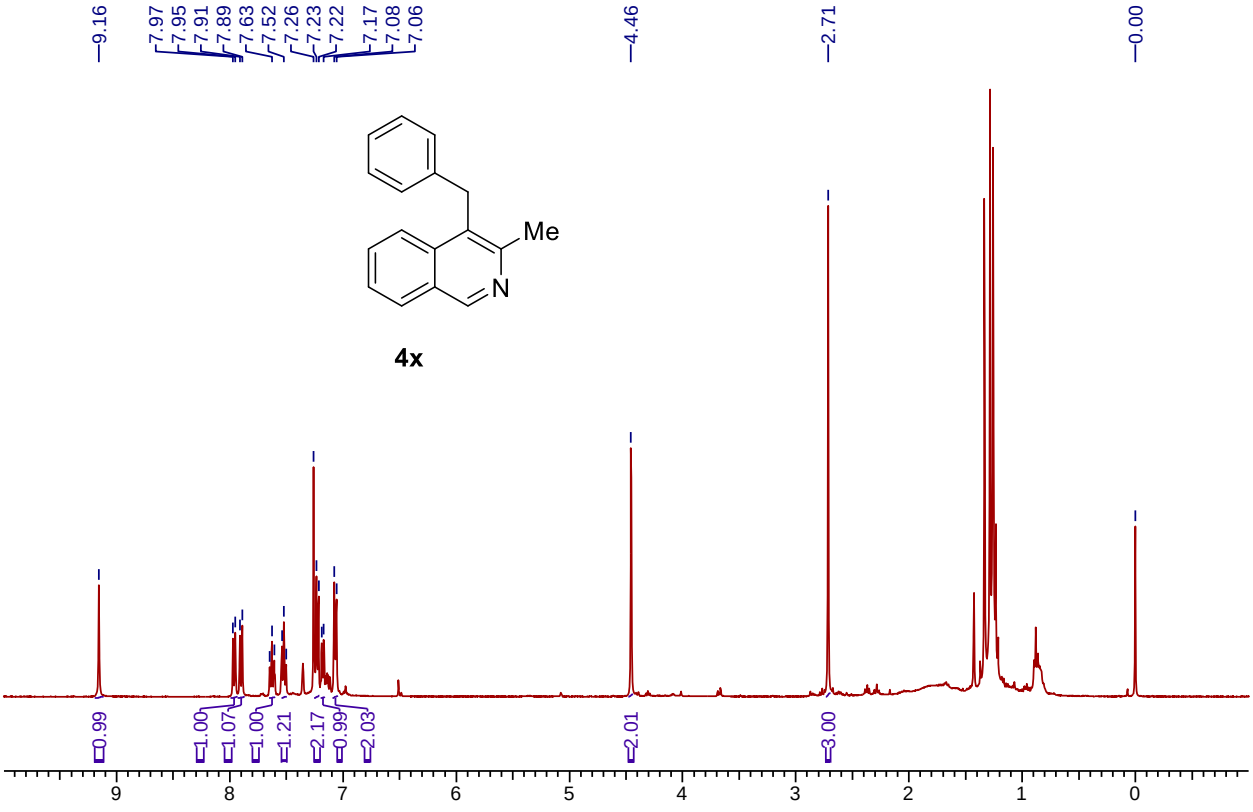

171.22
152.38
143.68
134.94
131.04
128.41
128.38
127.35
124.34
123.00
77.32
77.00
76.68
52.32
36.08
MeO2C
N
4u
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

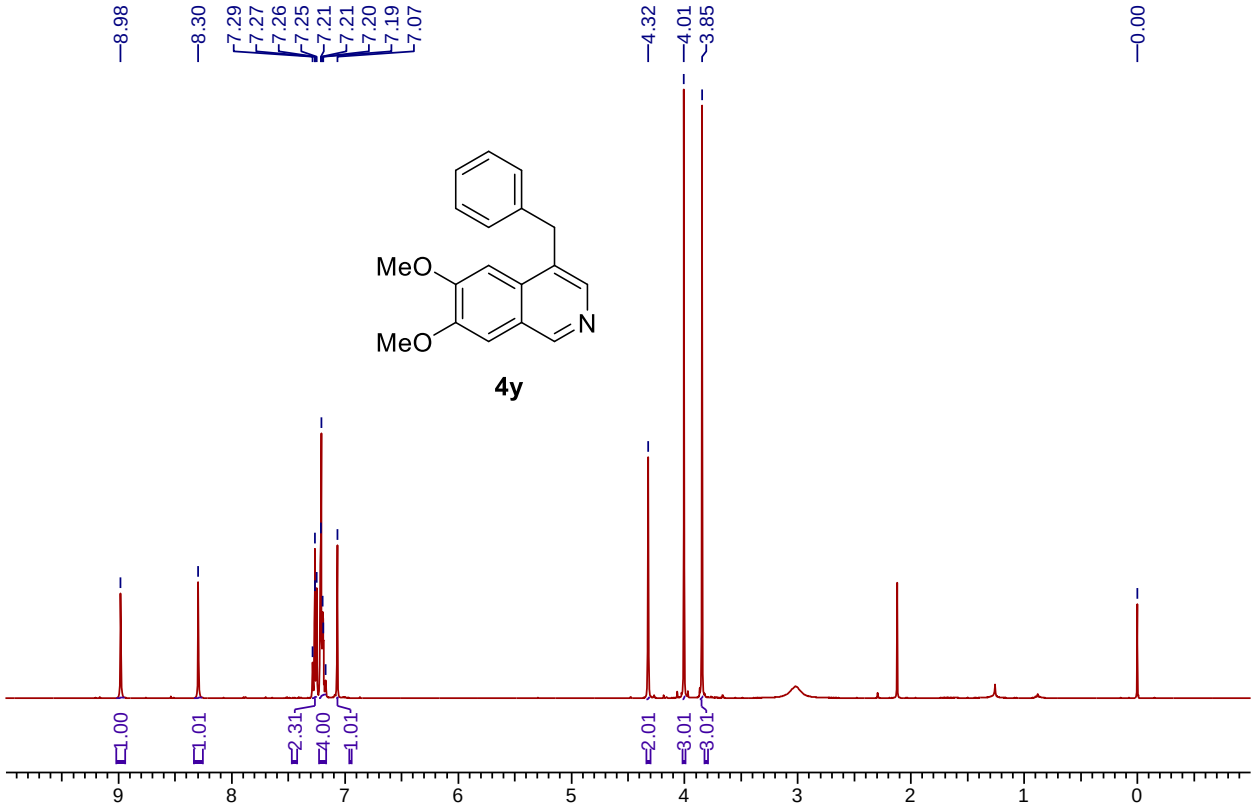

8.29
8.15
8.13
7.91
7.89
7.62
7.62
7.58
7.26
7.25
7.23
7.20
7.18
4.35
2.97
0.00
N
Me
4v
1.00
1.04
1.04
2.18
2.78
2.94
2.16
3.03
9
8
7
6
5
4
3
2
1
0

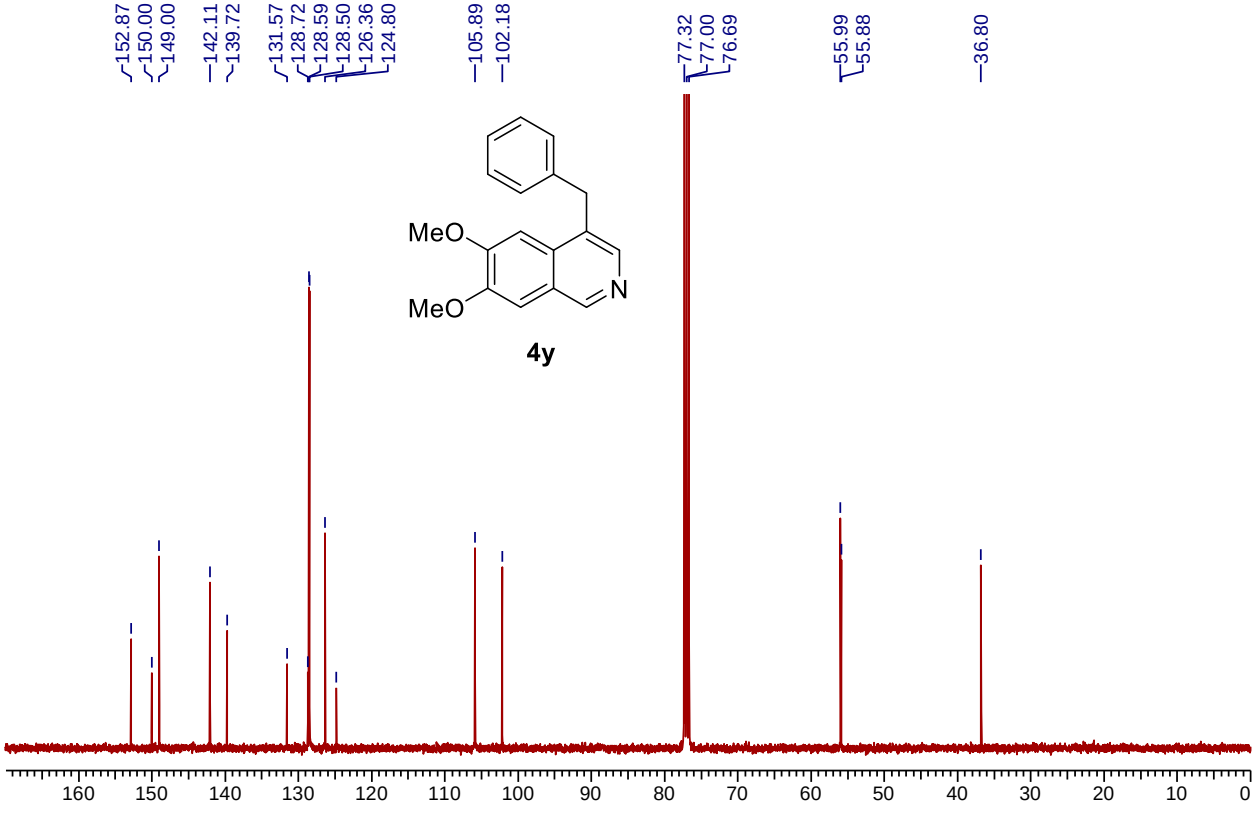

157.77
142.41
140.01
134.95
129.94
128.51
128.44
128.00
127.43
126.64
126.23
124.16
77.32
77.00
76.68
36.23
22.38
N
Me
4v
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

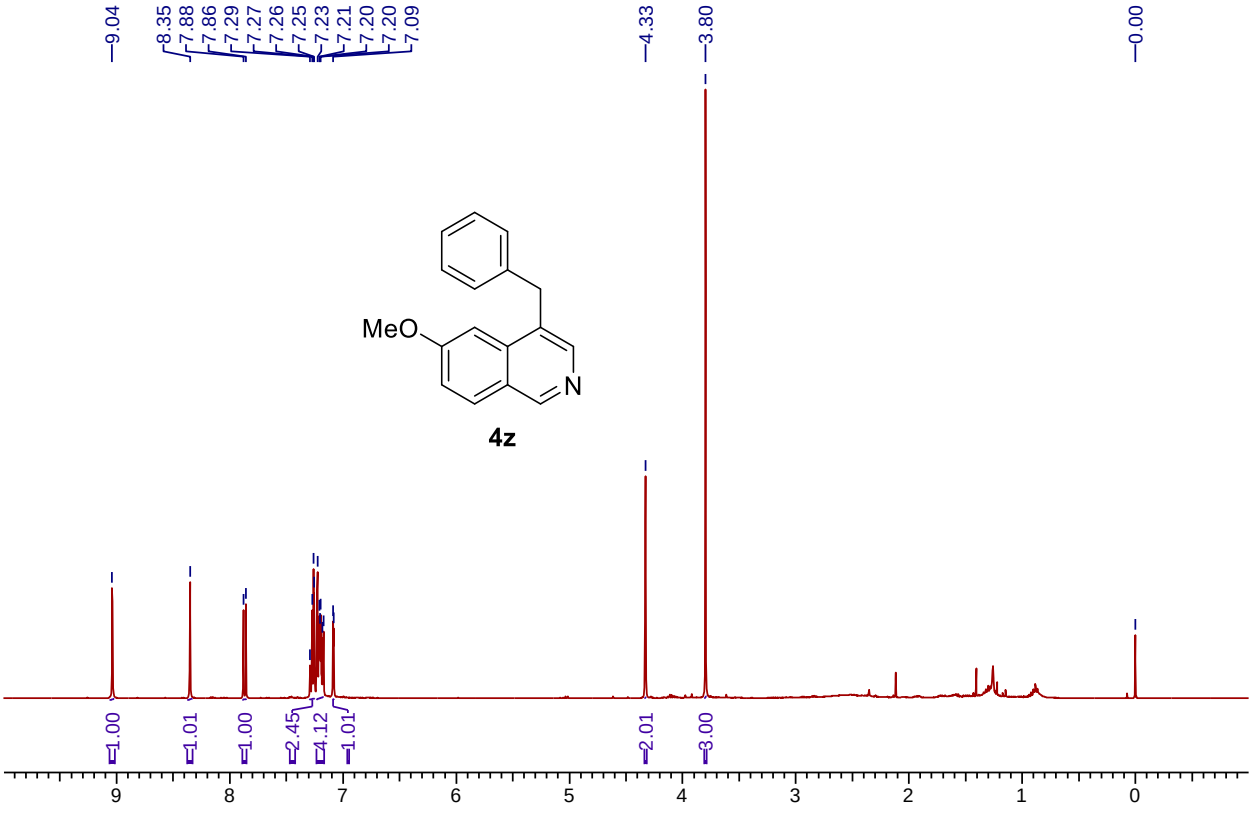

8.15
8.13
8.13
7.90
7.83
7.57
7.56
7.28
7.26
7.24
7.22
7.14
7.12
6.12
2.95
0.00
N
Me
4w
1.00
0.99
0.96
2.04
6.22
4.01
0.99
2.97
9
8
7
6
5
4
3
2
1
0

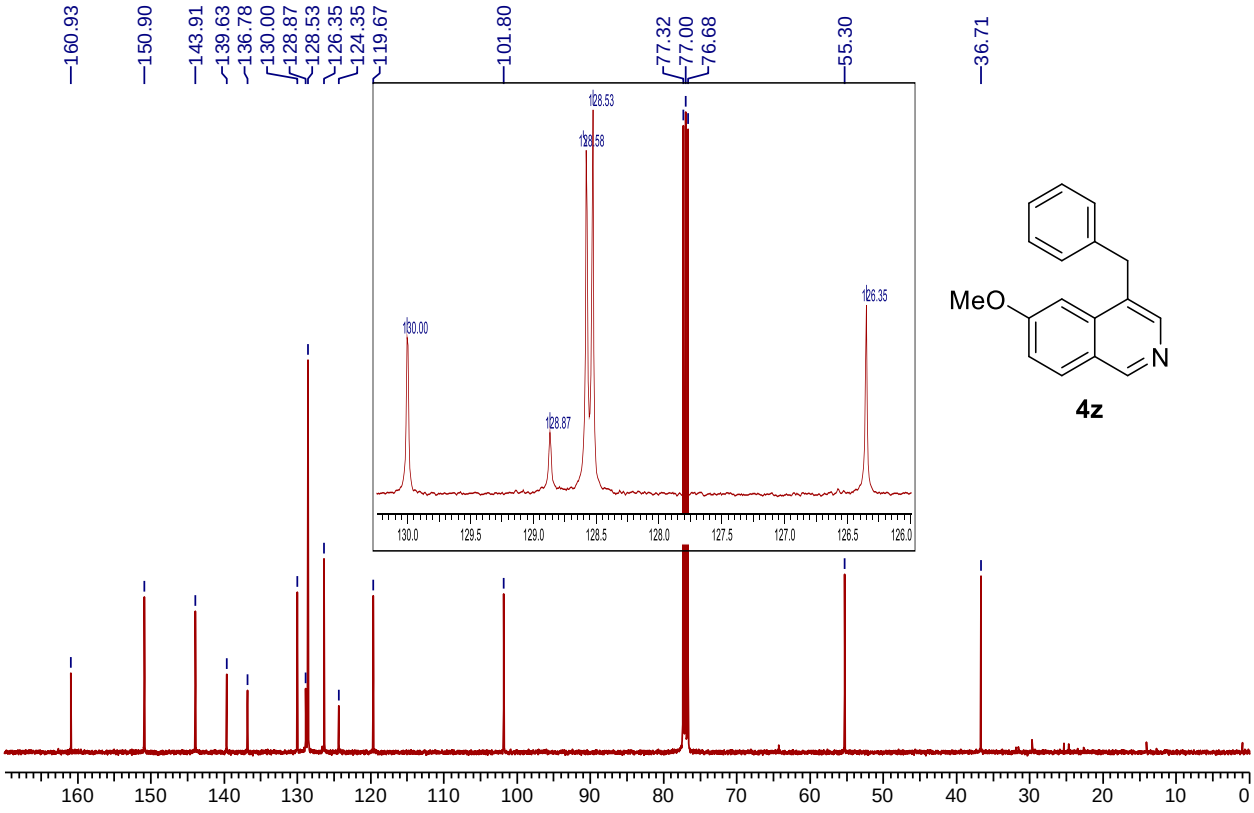

157.65
142.99
142.68
134.65
131.43
130.07
129.47
128.50
126.62
126.54
126.22
124.04
77.32
77.00
76.68
51.34
22.41
N
Me
4w
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

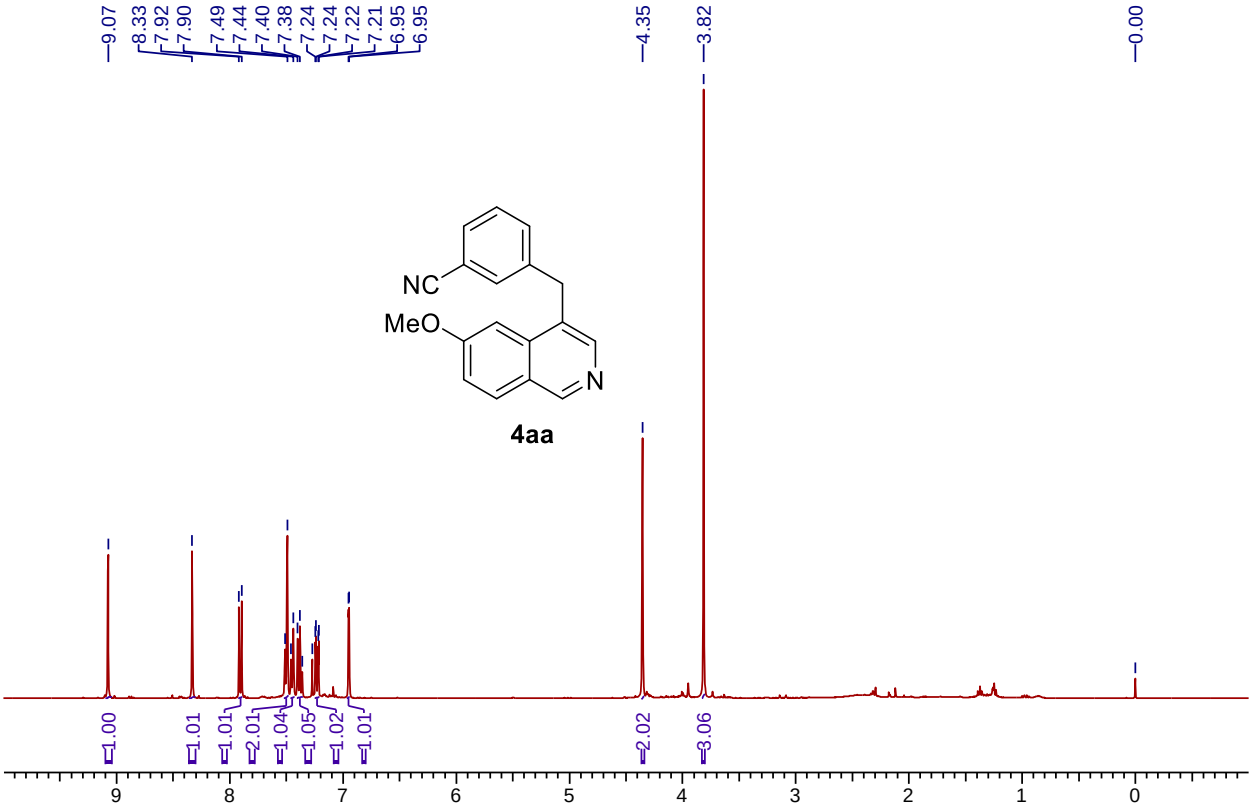

9.16
7.97
7.95
7.91
7.89
7.63
7.52
7.26
7.23
7.22
7.17
7.08
7.06
4.46
2.71
0.00
Me
N
4x
0.99
1.00
1.07
1.00
1.21
2.17
0.99
2.03
2.01
3.00
9
8
7
6
5
4
3
2
1
0

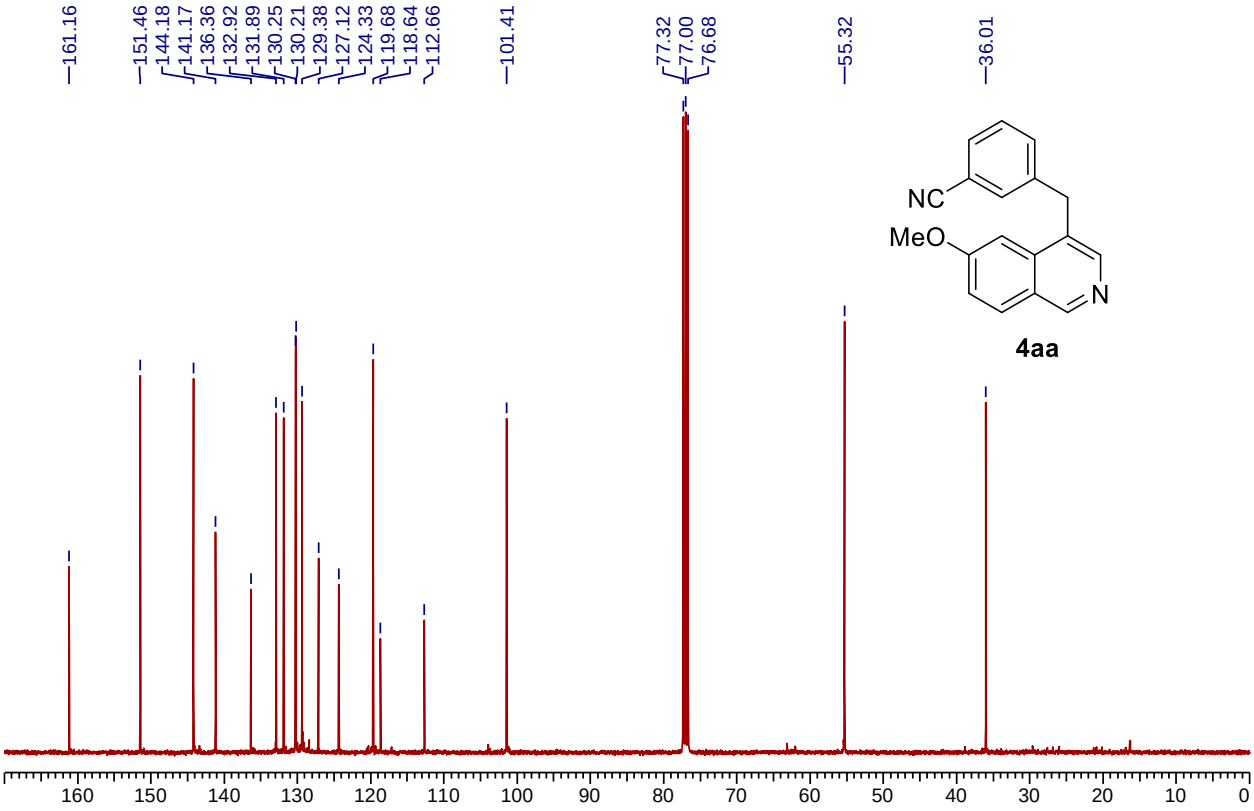

8.98
8.30
7.29
7.27
7.26
7.25
7.21
7.21
7.20
7.19
7.07
4.32
4.01
3.85
0.00
MeO
MeO
N
4y
1.00
1.01
2.31
4.00
1.01
2.01
3.01
3.01

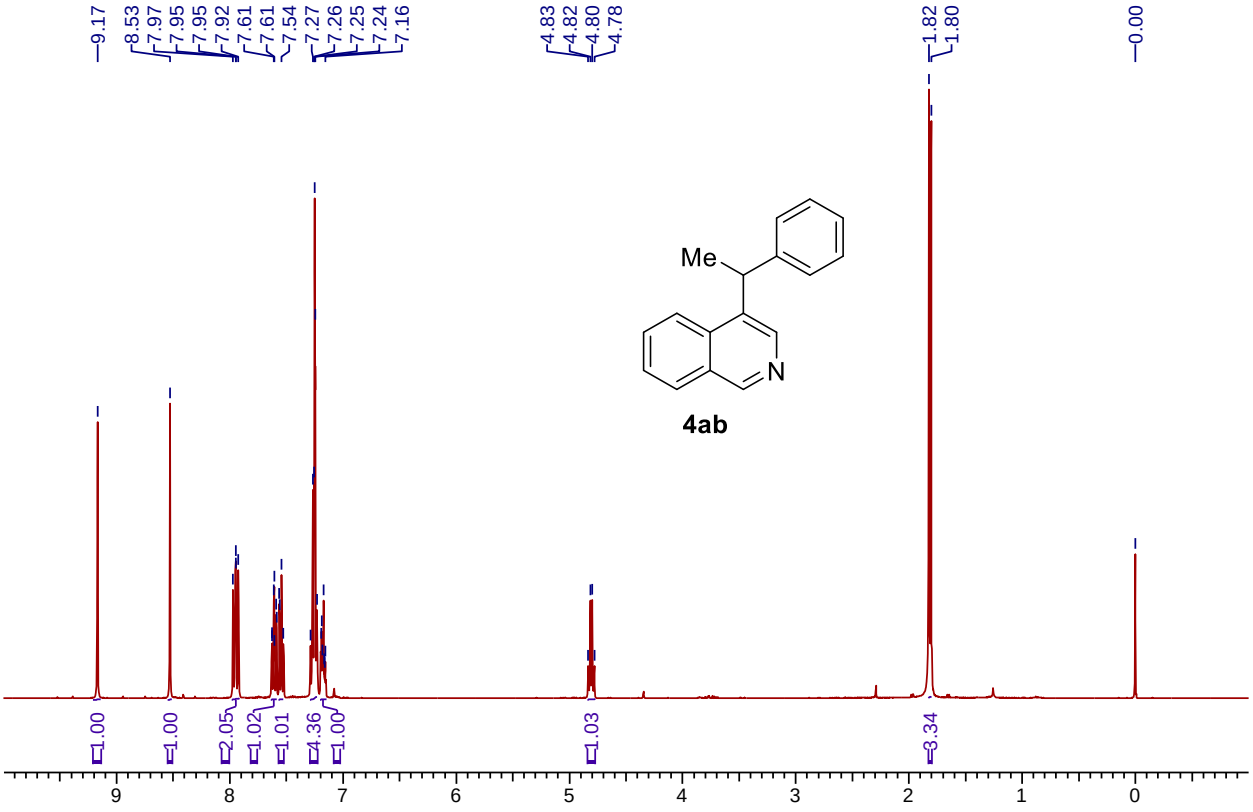

152.87
150.00
149.00
142.11
139.72
131.57
128.72
128.59
128.50
126.36
124.80
105.89
102.18
77.32
77.00
76.69
55.99
55.88
36.80
MeO
MeO
N
4y

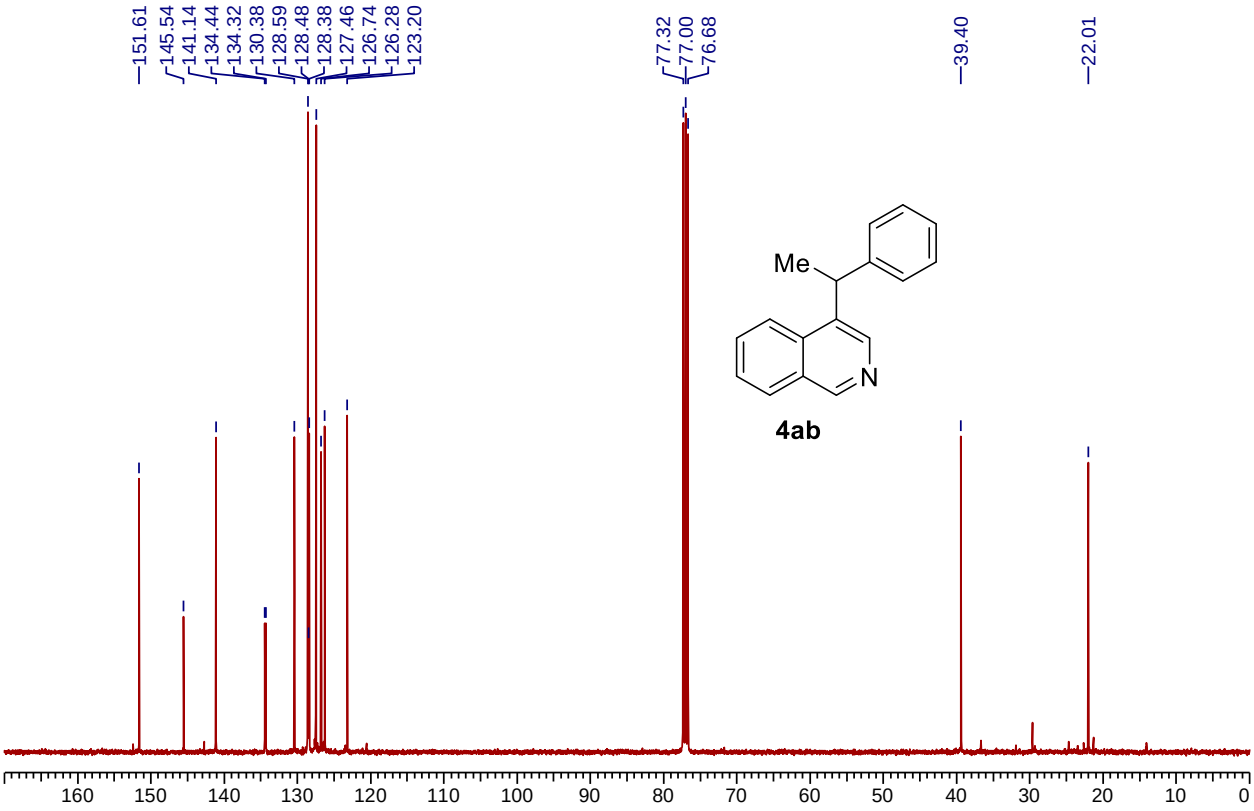

9.04
8.35
7.88
7.86
7.29
7.27
7.26
7.25
7.23
7.21
7.20
7.20
7.09
4.33
3.80
0.00
MeO
N
4z
1.00
1.01
1.00
2.45
4.12
1.01
2.01
3.00

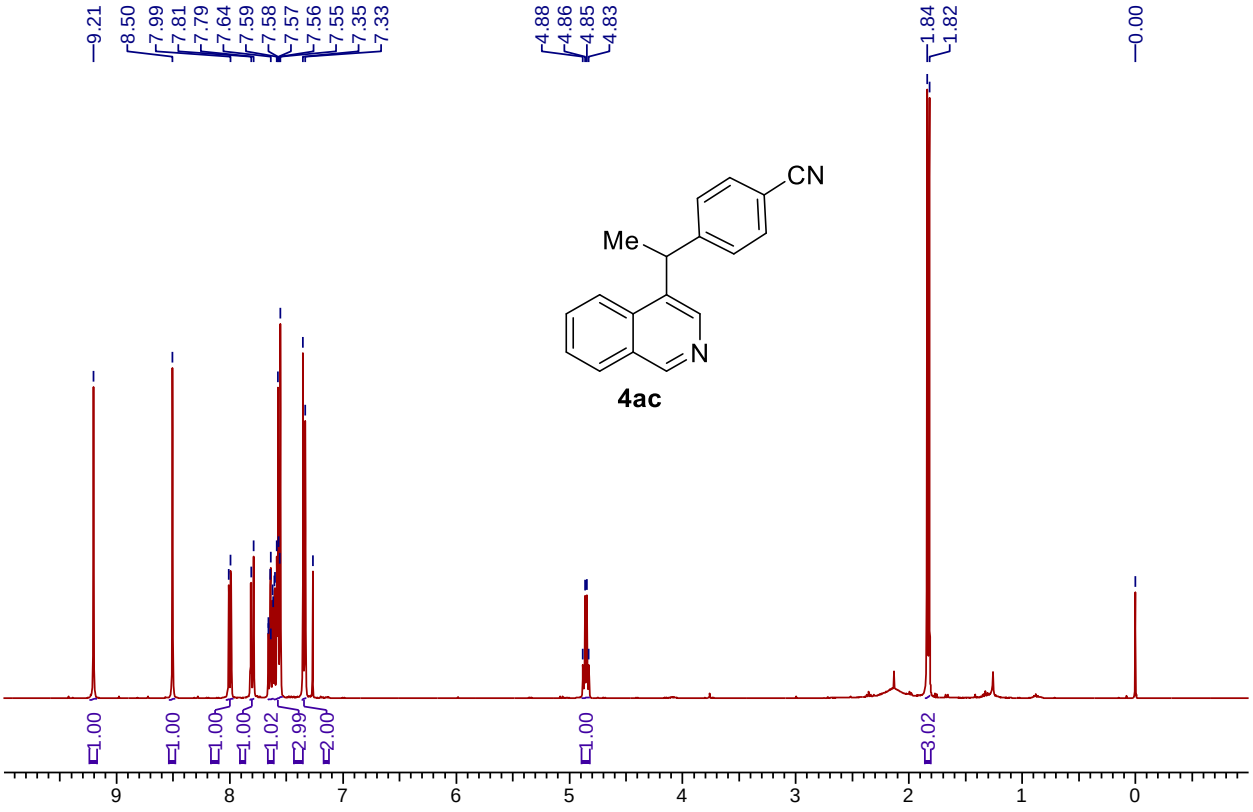

160.93
150.90
143.91
139.63
136.78
130.00
128.87
128.53
126.35
124.35
119.67
101.80
77.32
77.00
76.68
55.30
36.71
128.53
128.58
130.00
128.87
126.35
MeO
N
4z

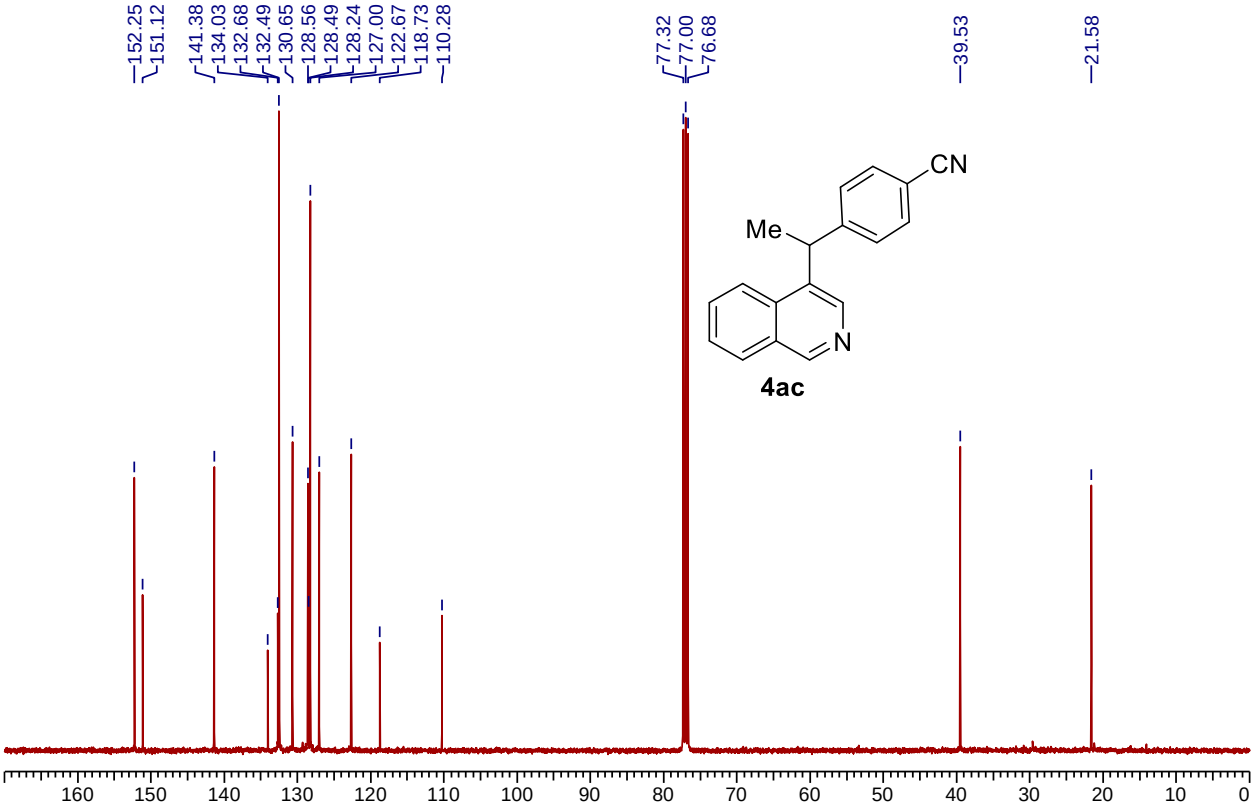

9.07
8.33
7.92
7.90
7.49
7.44
7.40
7.38
7.24
7.24
7.22
7.21
6.95
6.95
4.35
3.82
0.00
NC
MeO
N
4aa
1.00
1.01
1.01
2.01
1.04
1.05
1.02
1.01
2.02
3.06

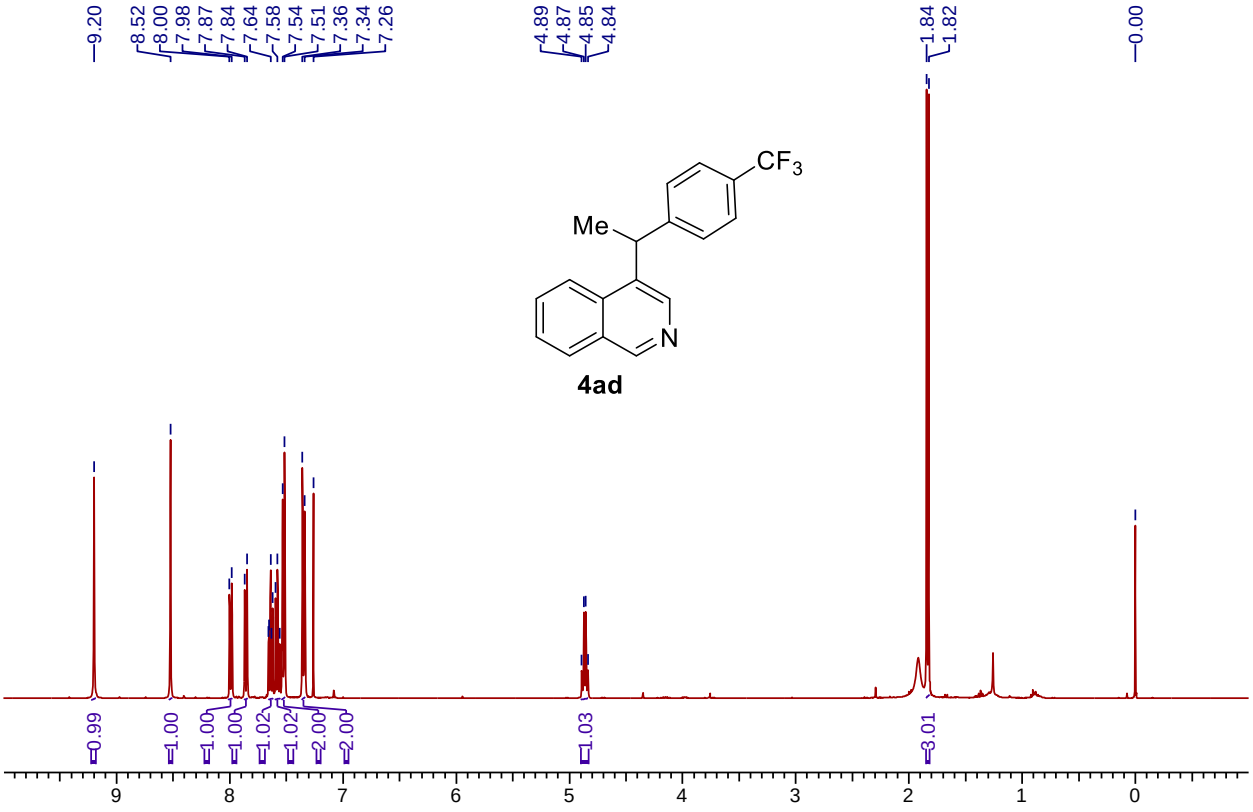

161.16
151.46
144.18
141.17
136.36
132.92
131.89
130.25
130.21
129.38
127.12
124.33
119.68
118.64
112.66
101.41
77.32
77.00
76.68
55.32
36.01
NC
MeO
N
4aa

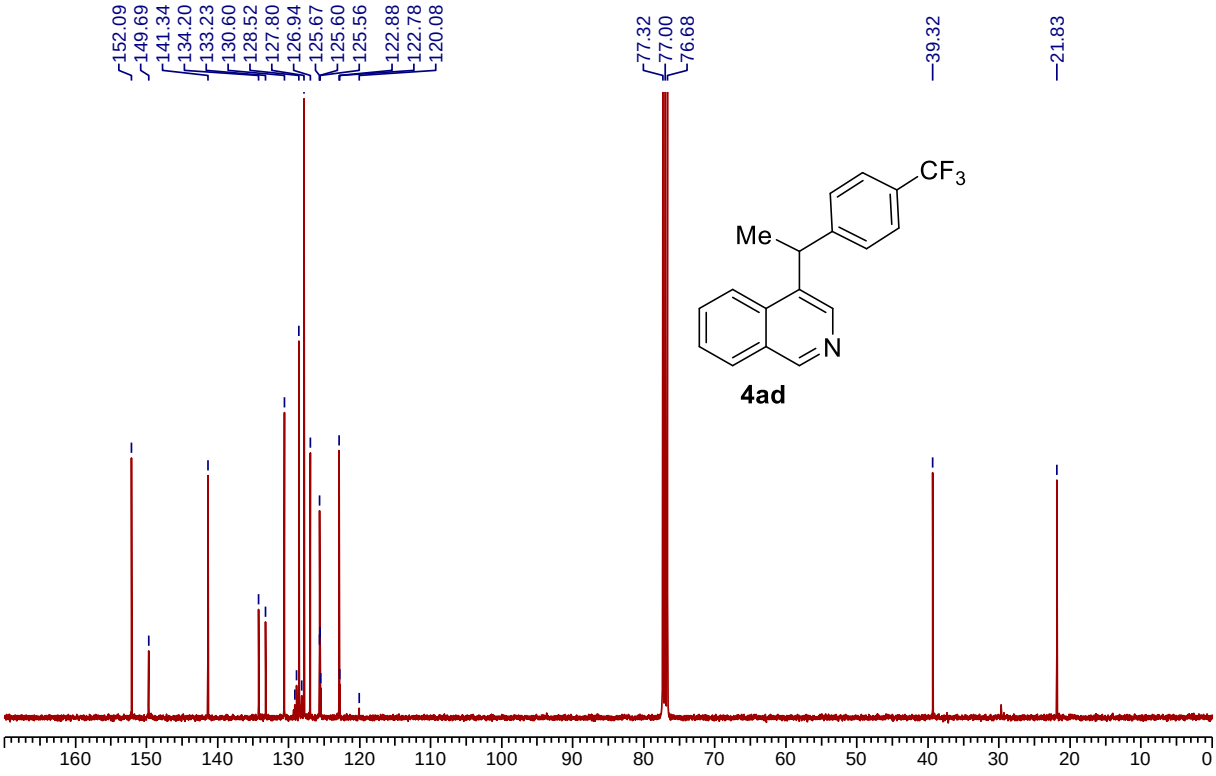

9.17
8.53
7.97
7.95
7.95
7.92
7.61
7.61
7.54
7.27
7.26
7.25
7.24
7.16
4.83
4.82
4.80
4.78
1.82
1.80
0.00
Me
N
4ab
1.00
1.00
2.05
1.02
1.01
4.36
1.00
1.03
3.34
9
8
7
6
5
4
3
2
1
0

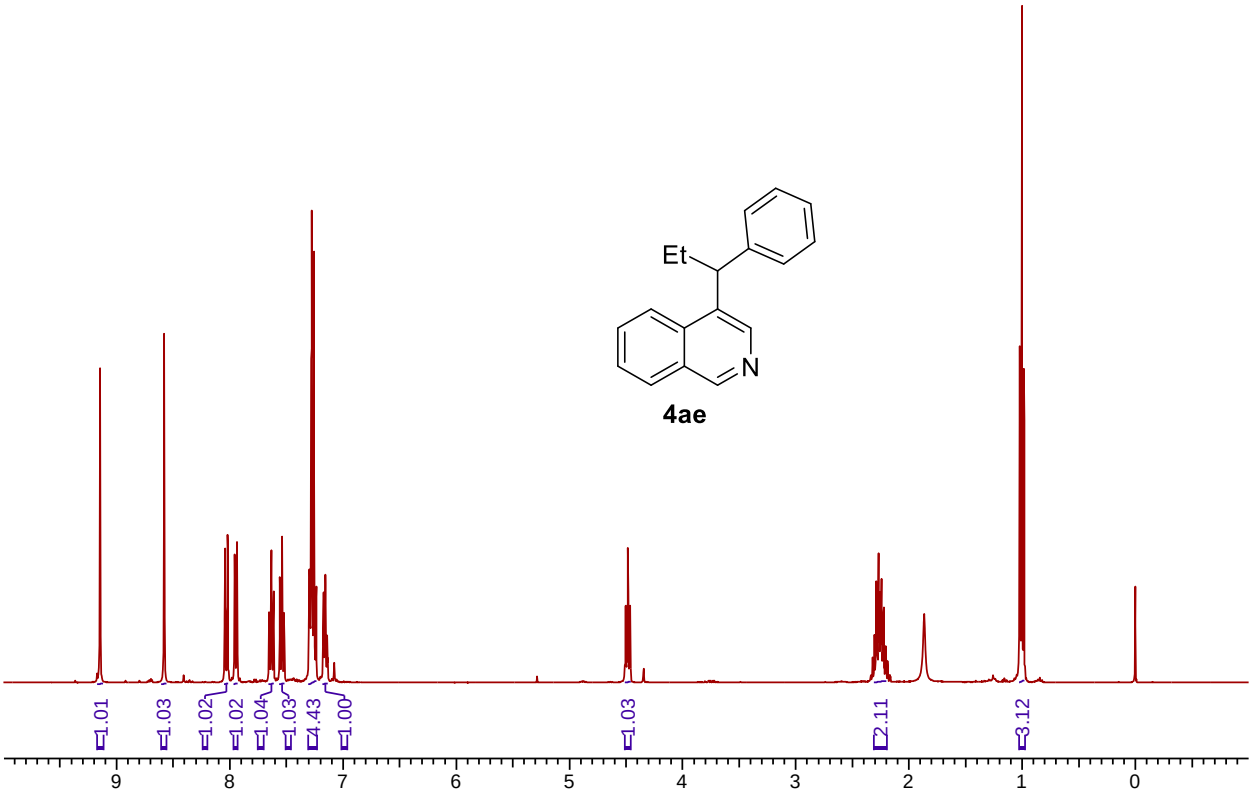

151.61
145.54
141.14
134.44
134.32
130.38
128.59
128.48
128.38
127.46
126.74
126.28
123.20
77.32
77.00
76.68
39.40
22.01
Me
N
4ab
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

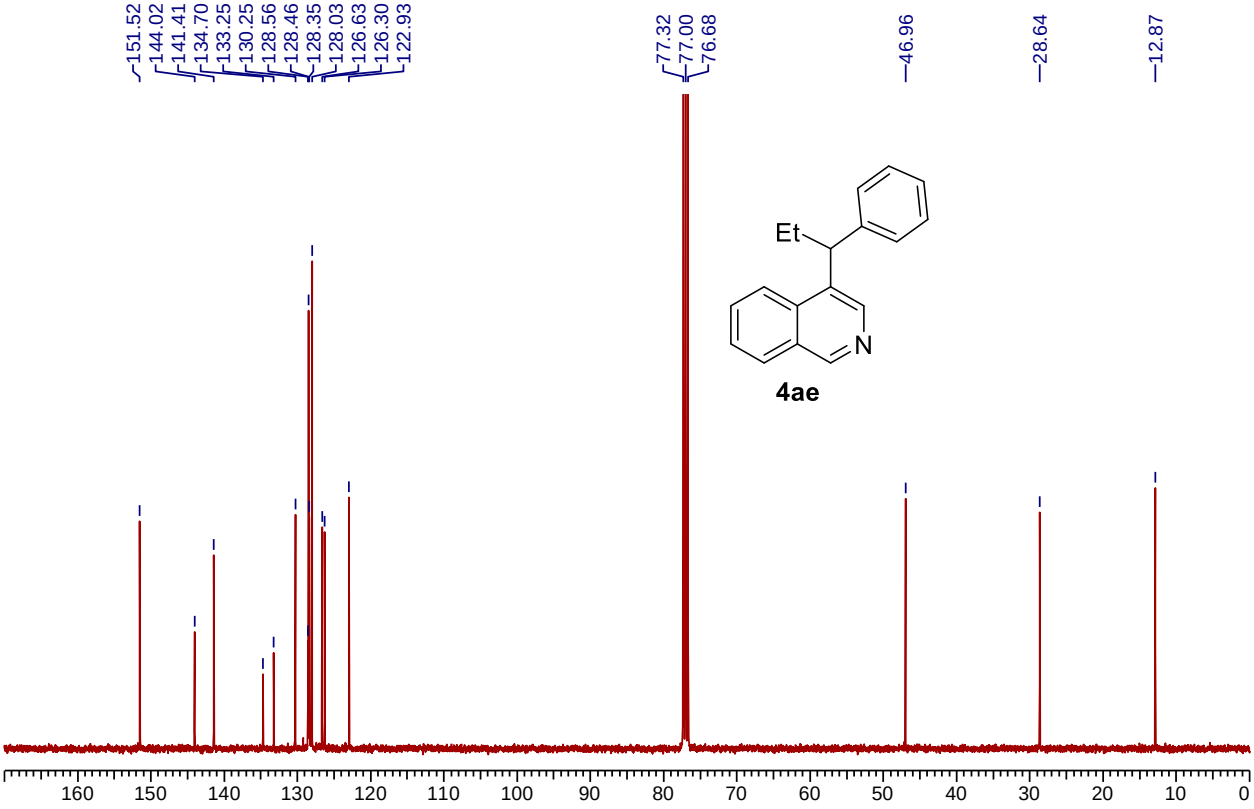

9.21
8.50
7.99
7.81
7.79
7.64
7.59
7.58
7.57
7.56
7.55
7.35
7.33
4.88
4.86
4.85
4.83
1.84
1.82
0.00
CN
Me
N
4ac
1.00
1.00
1.00
1.00
1.02
2.99
2.00
1.00
3.02

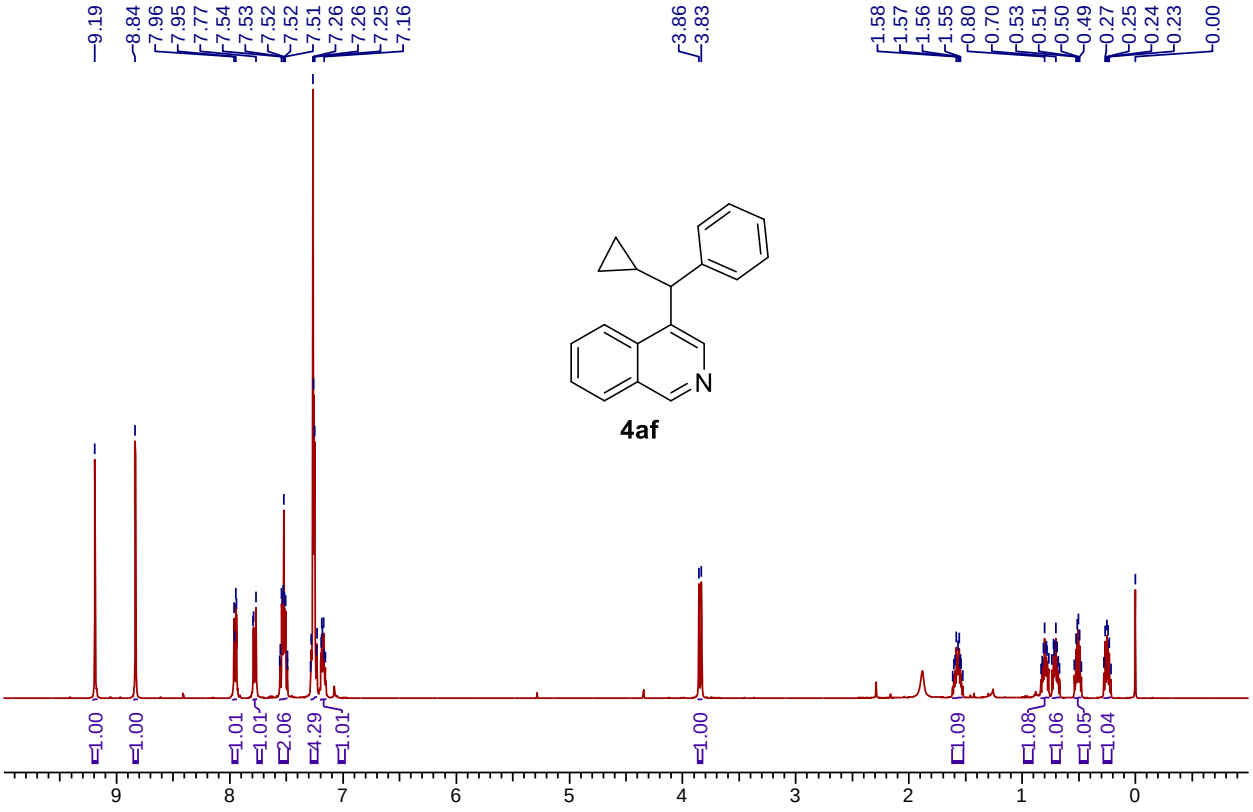

152.25
151.12
141.38
134.03
132.68
132.49
130.65
128.56
128.49
128.24
127.00
122.67
118.73
110.28
77.32
77.00
76.68
39.53
21.58
CN
Me
N
4ac

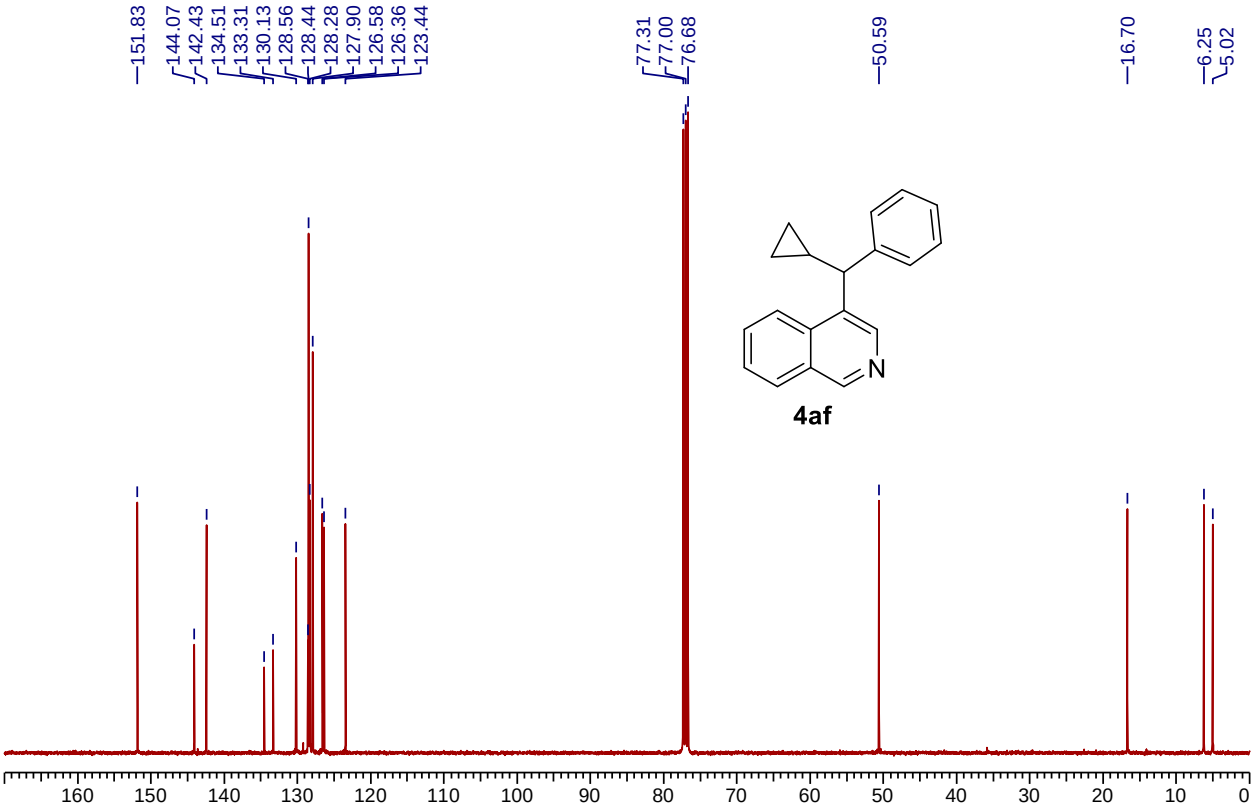

9.20
8.52
8.00
7.98
7.87
7.84
7.64
7.58
7.54
7.51
7.36
7.34
7.26
4.89
4.87
4.85
4.84
1.84
1.82
0.00
CF3
Me
N
4ad
0.99
1.00
1.00
1.00
1.02
1.02
2.00
2.00
1.03
3.01

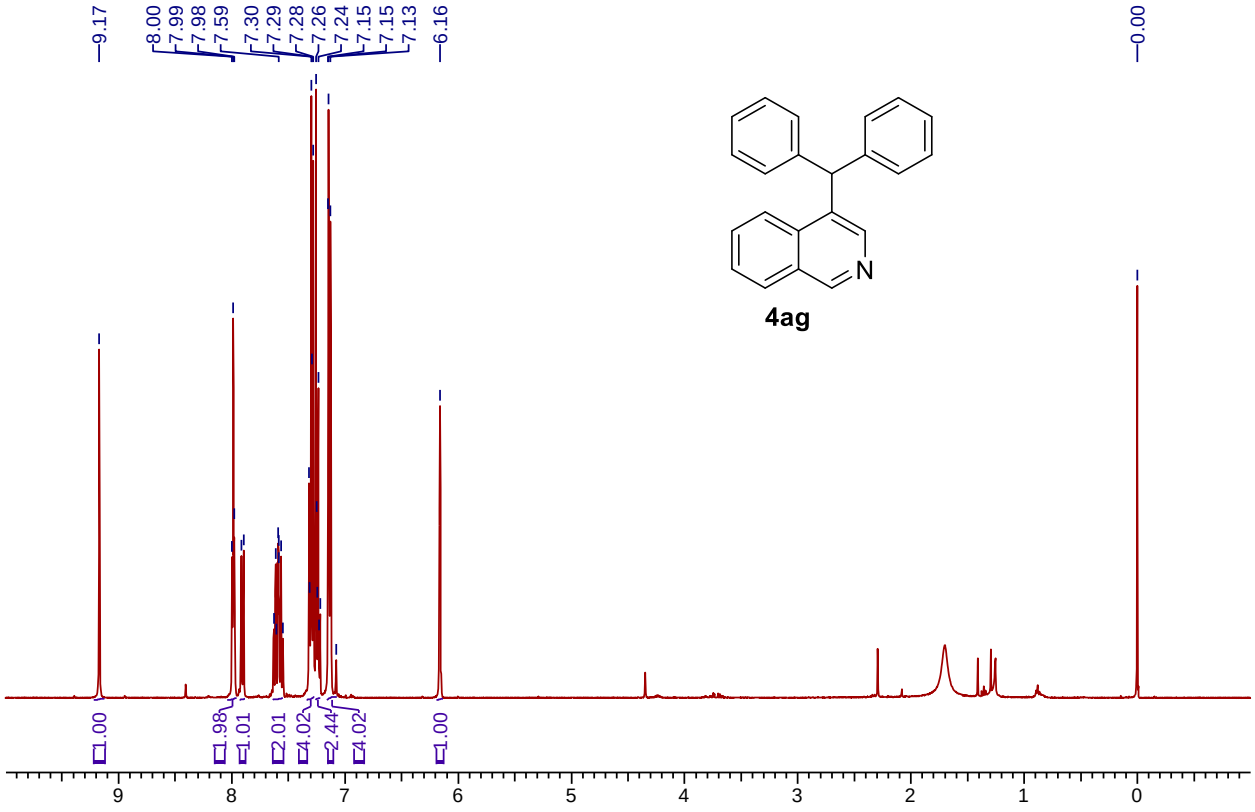

152.09
149.69
141.34
134.20
133.23
130.60
128.52
127.80
126.94
125.67
125.60
125.56
122.88
122.78
120.08
77.32
77.00
76.68
39.32
21.83
CF3
Me
N
4ad

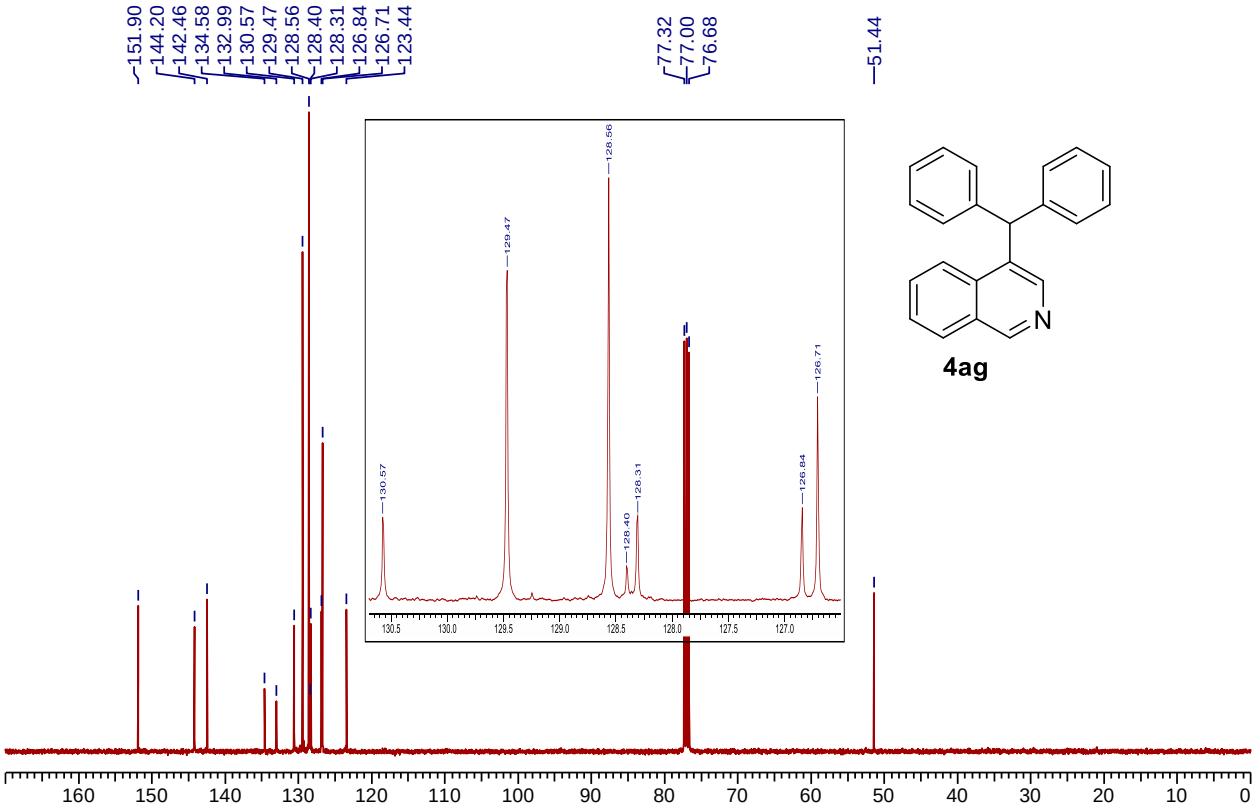

Et
N
4ae
1.01
1.03
1.02
1.02
1.04
1.03
4.43
1.00
1.03
2.11
3.12
9
8
7
6
5
4
3
2
1
0

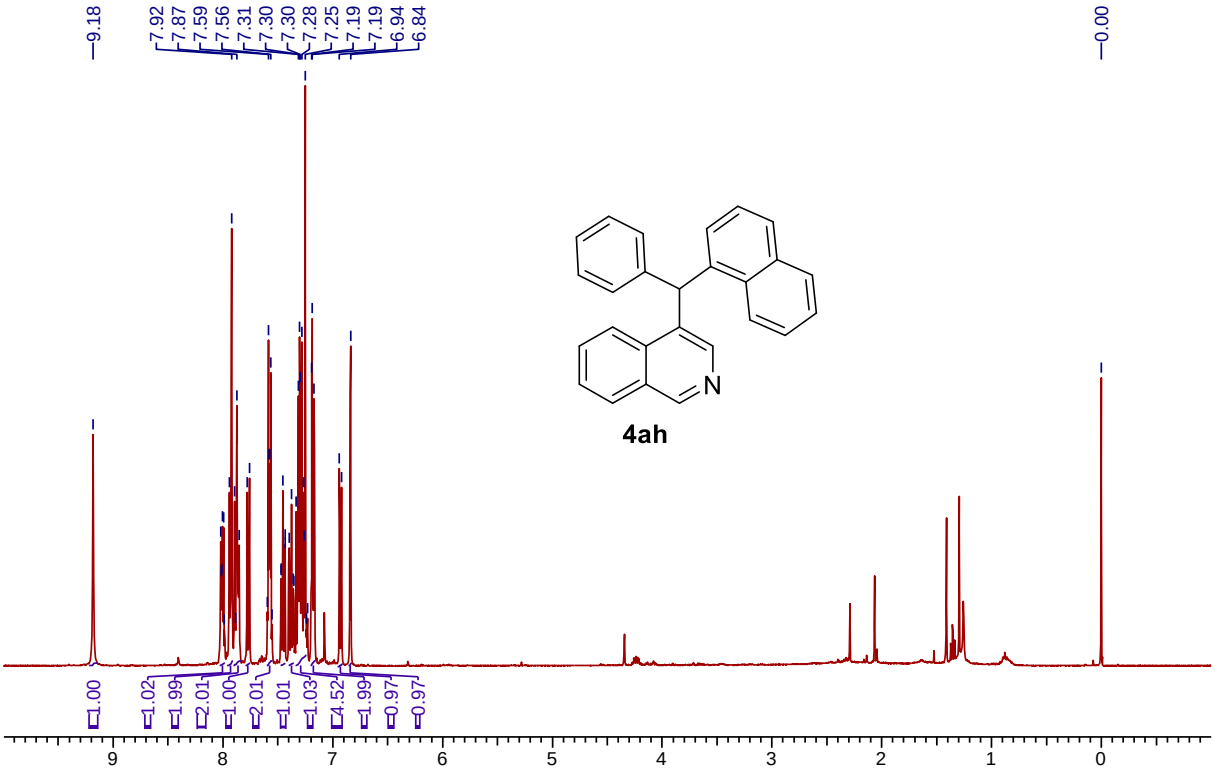

151.52
144.02
141.41
134.70
133.25
130.25
128.56
128.46
128.35
128.03
126.63
126.30
122.93
77.32
77.00
76.68
46.96
28.64
12.87
Et
N
4ae
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

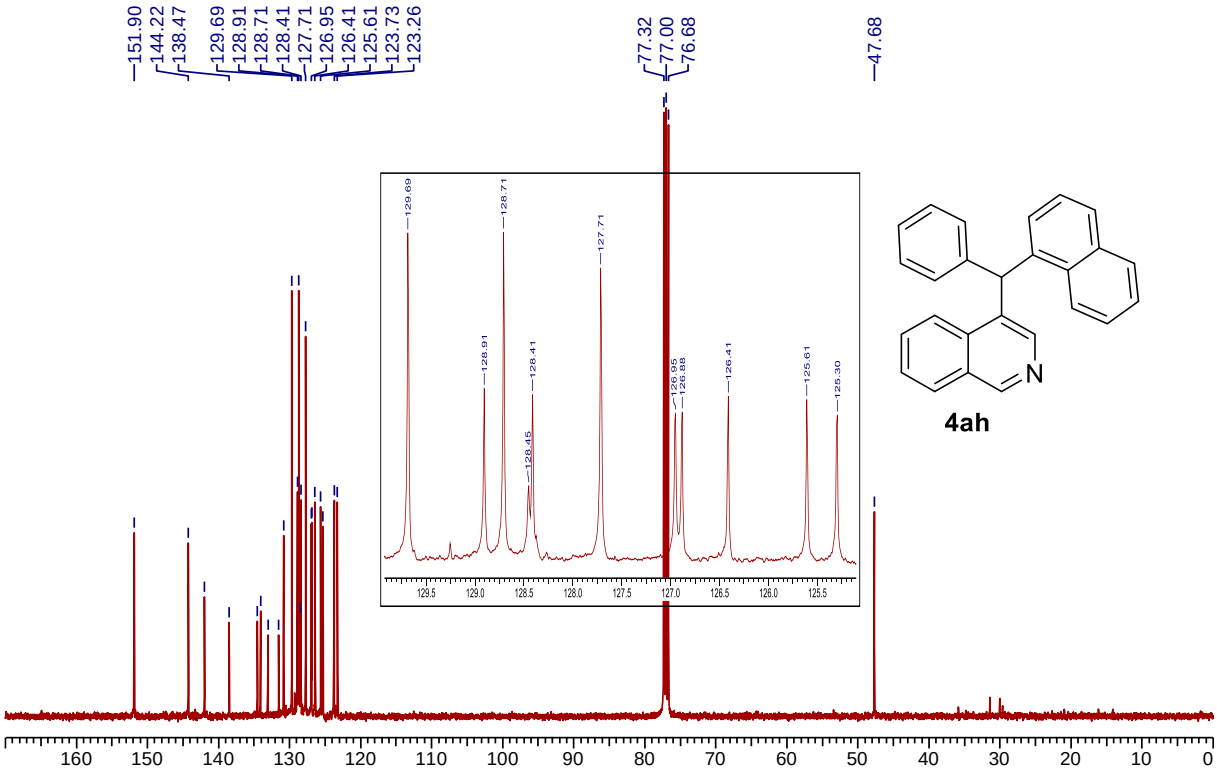

9.19
8.84
7.96
7.95
7.77
7.54
7.53
7.52
7.52
7.51
7.26
7.26
7.25
7.16
3.86
3.83
1.58
1.57
1.56
1.55
0.80
0.70
0.53
0.51
0.50
0.49
0.27
0.25
0.24
0.23
0.00
1.00
1.00
1.01
1.01
2.06
4.29
1.01
1.00
1.09
1.08
1.06
1.05
1.04
N
4af

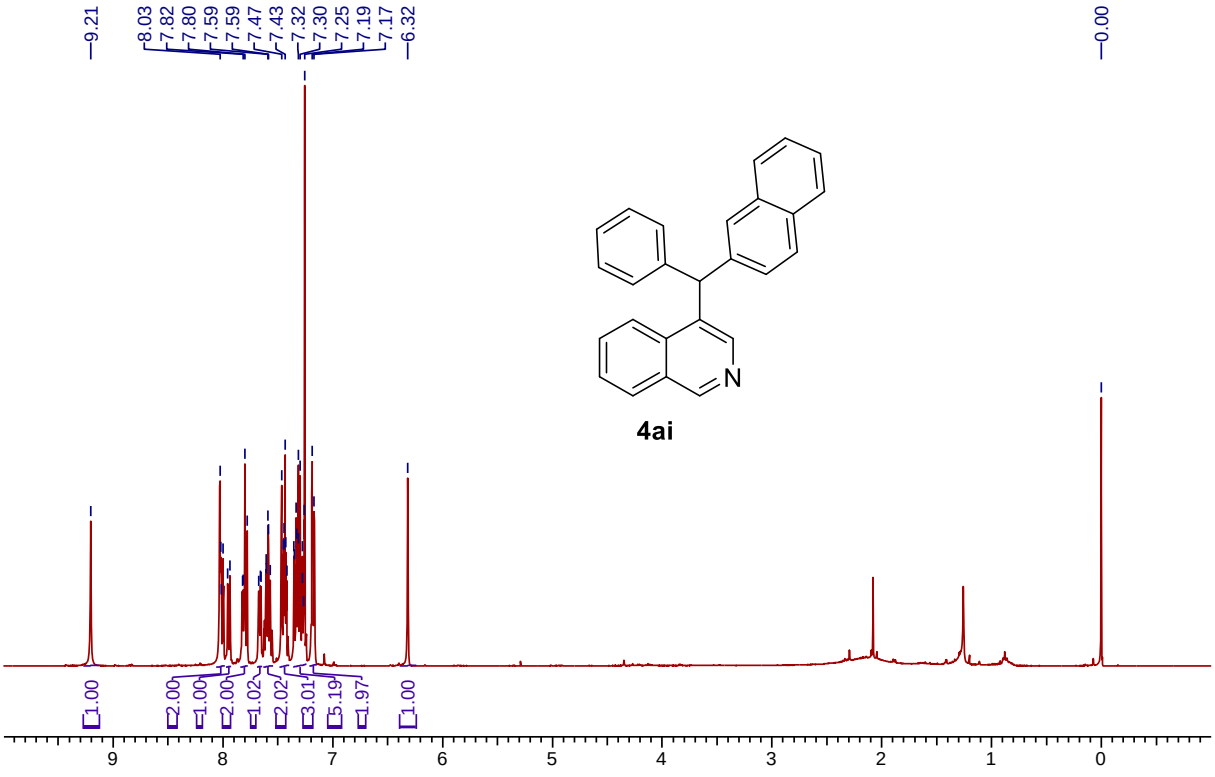

151.83
144.07
142.43
134.51
133.31
130.13
128.56
128.44
128.28
127.90
126.58
126.36
123.44
77.31
77.00
76.68
50.59
16.70
6.25
5.02
N
4af

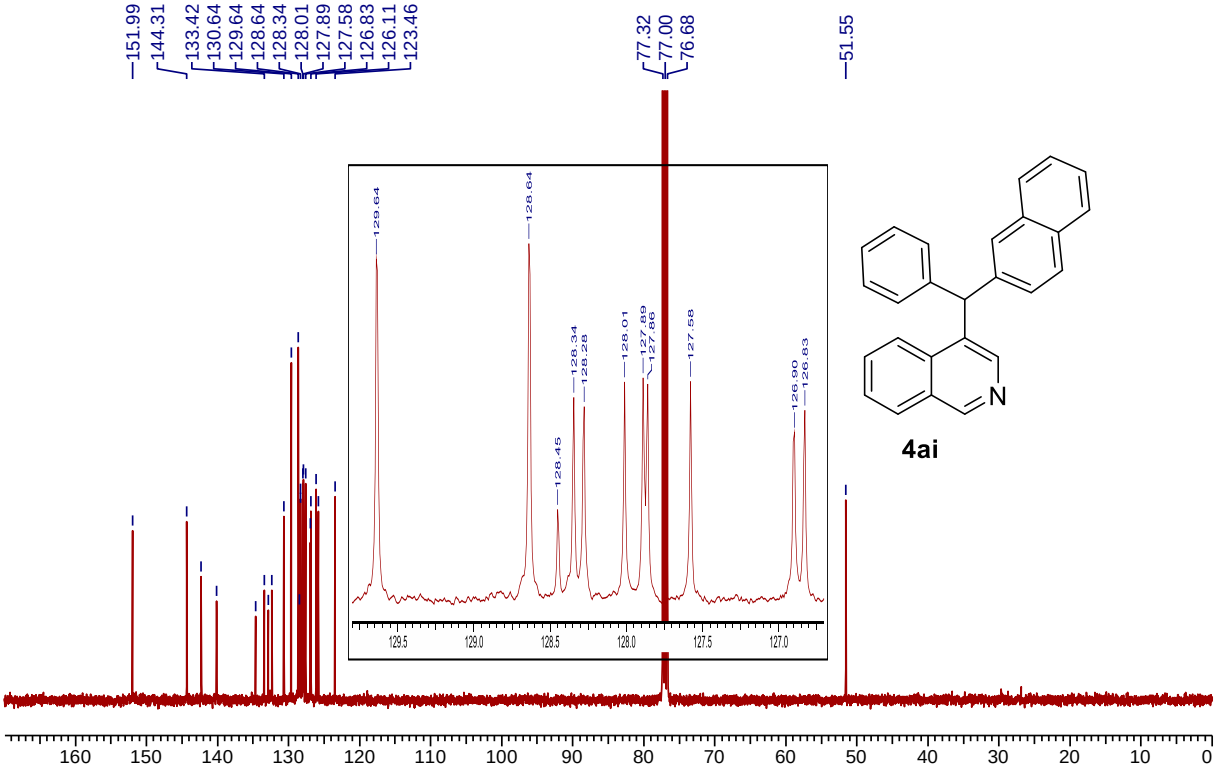

9.17
8.00
7.99
7.98
7.59
7.30
7.29
7.28
7.26
7.24
7.15
7.15
7.13
6.16
0.00
1.00
1.98
1.01
2.01
4.02
2.44
4.02
1.00
N
4ag

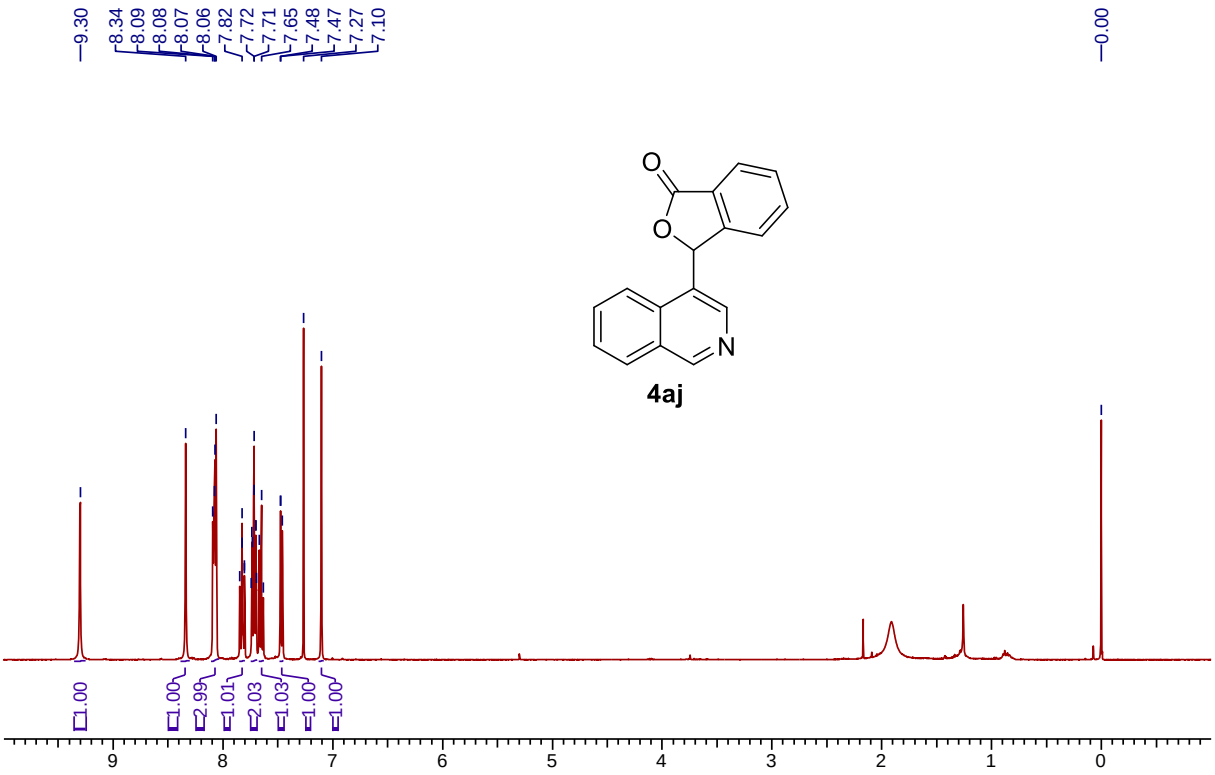

151.90
144.20
142.46
134.58
132.99
130.57
129.47
128.56
128.40
128.31
126.84
126.71
123.44
77.32
77.00
76.68
51.44
130.57
129.47
128.56
128.40
128.31
126.84
126.71
N
4ag

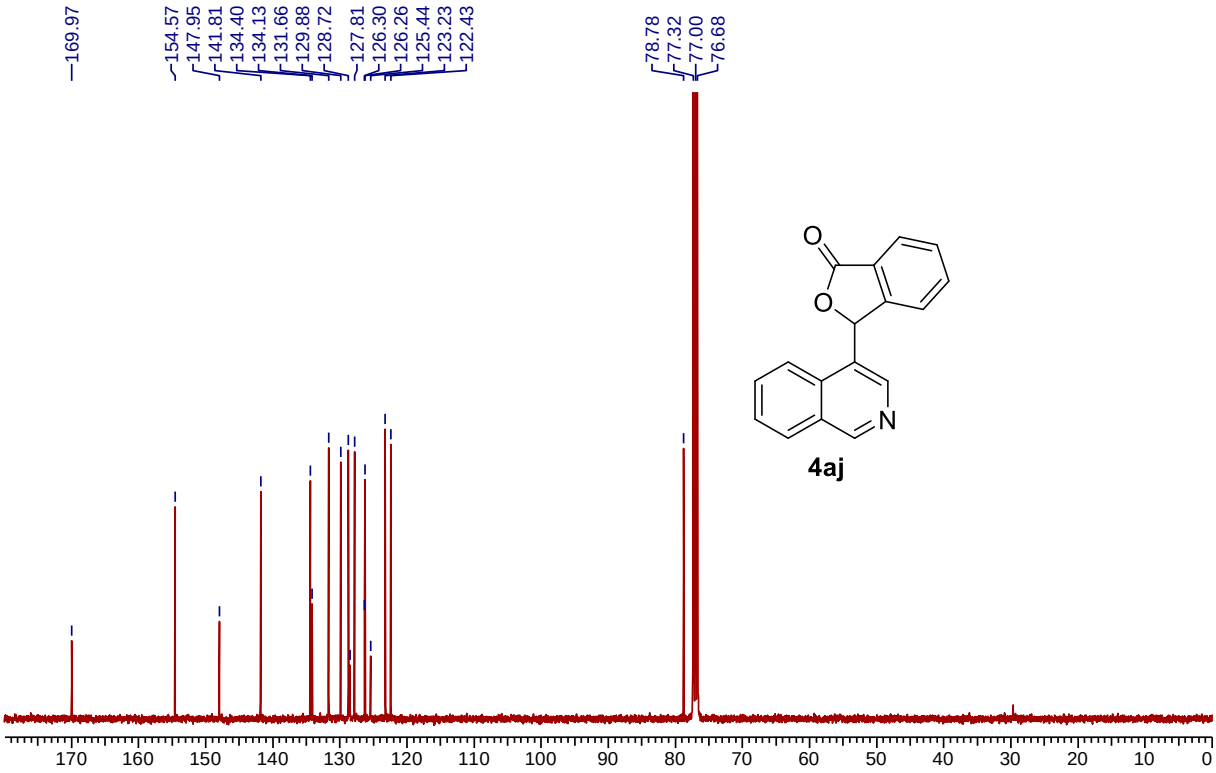

9.18
7.92
7.87
7.59
7.56
7.31
7.30
7.30
7.28
7.25
7.19
7.19
6.94
6.84
0.00
1.00
1.02
1.99
2.01
1.00
2.01
1.01
1.03
4.52
1.99
0.97
0.97
N
4ah

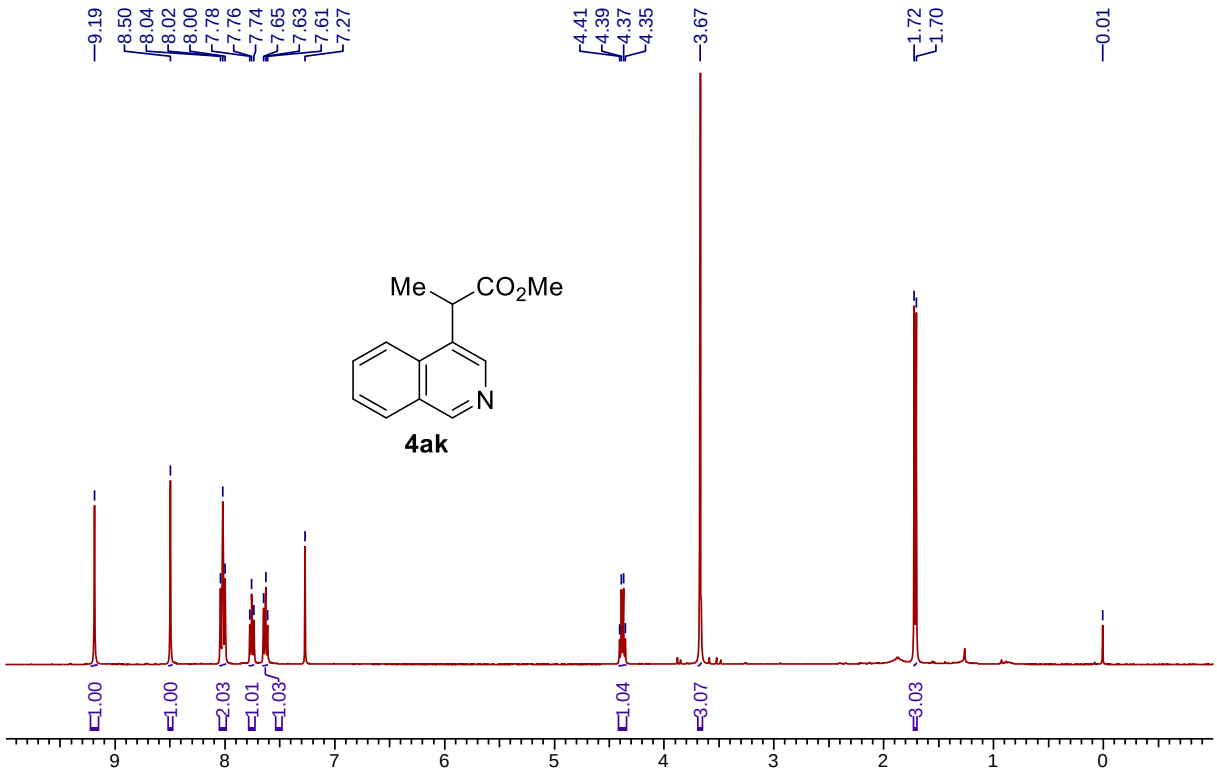

151.90
144.22
138.47
129.69
128.91
128.71
128.41
127.71
126.95
126.41
125.61
123.73
123.26
77.32
77.00
76.68
47.68
129.69
128.91
128.71
128.45
128.41
127.71
126.95
126.88
126.41
125.61
125.30
N
4ah

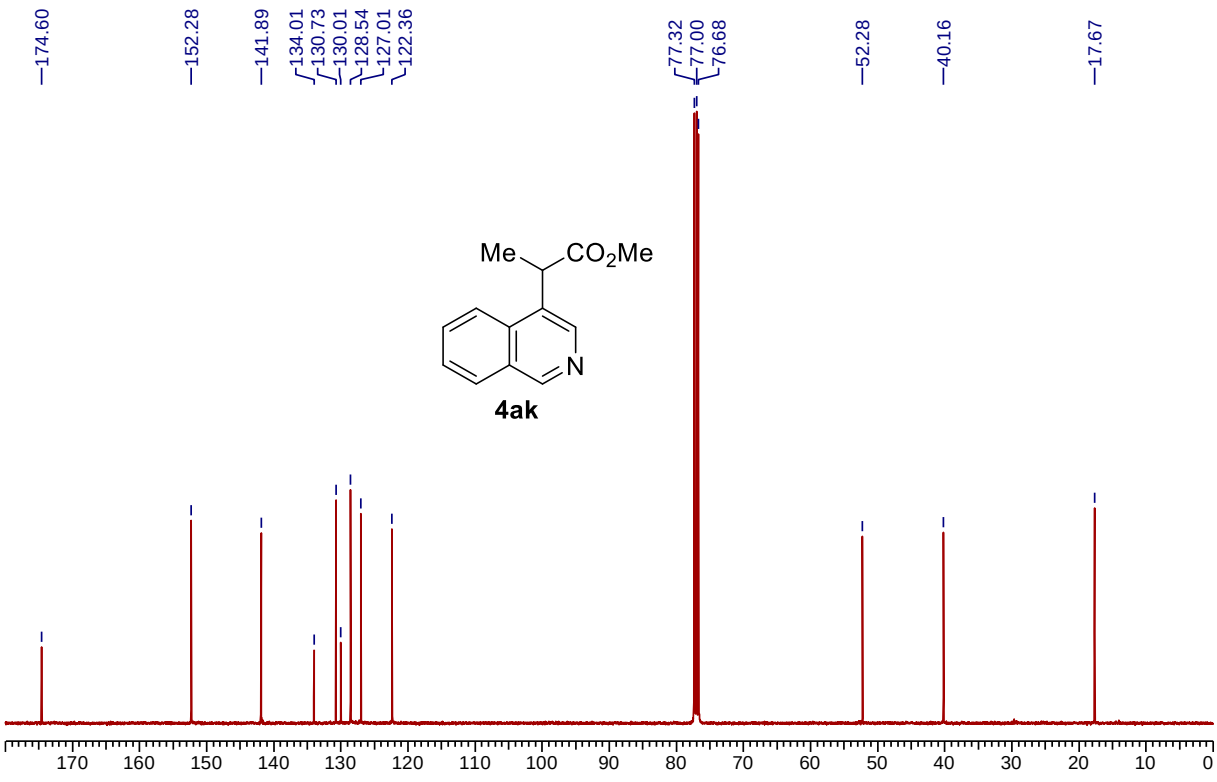

9.21
8.03
7.82
7.80
7.59
7.59
7.47
7.43
7.32
7.30
7.25
7.19
7.17
6.32
0.00
N
4ai
1.00
2.00
1.00
2.00
1.02
2.02
3.01
5.19
1.97
1.00

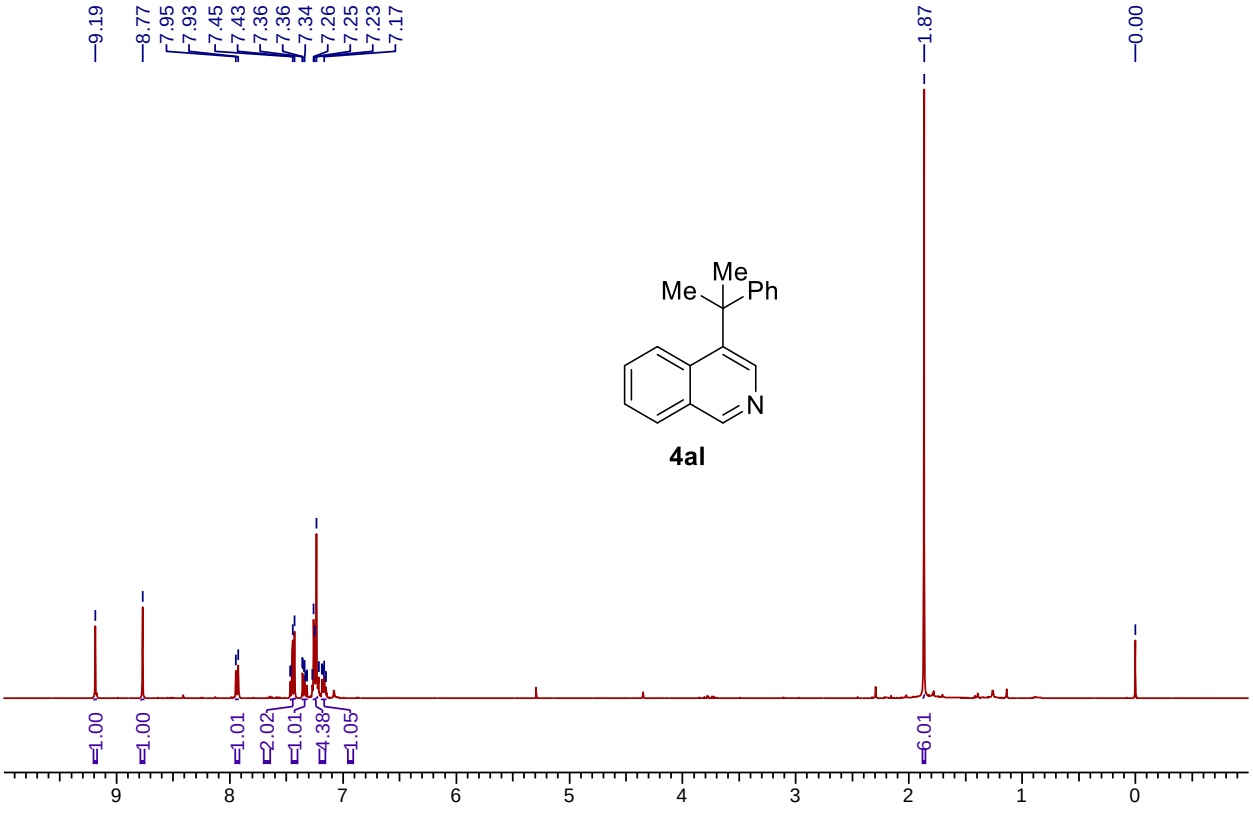

151.99
144.31
133.42
130.64
129.64
128.64
128.34
128.01
127.89
127.58
126.83
126.11
123.46
77.32
77.00
76.68
51.55
129.64
128.64
128.45
128.34
128.28
128.01
127.89
127.68
127.68
126.90
126.83
N
4ai

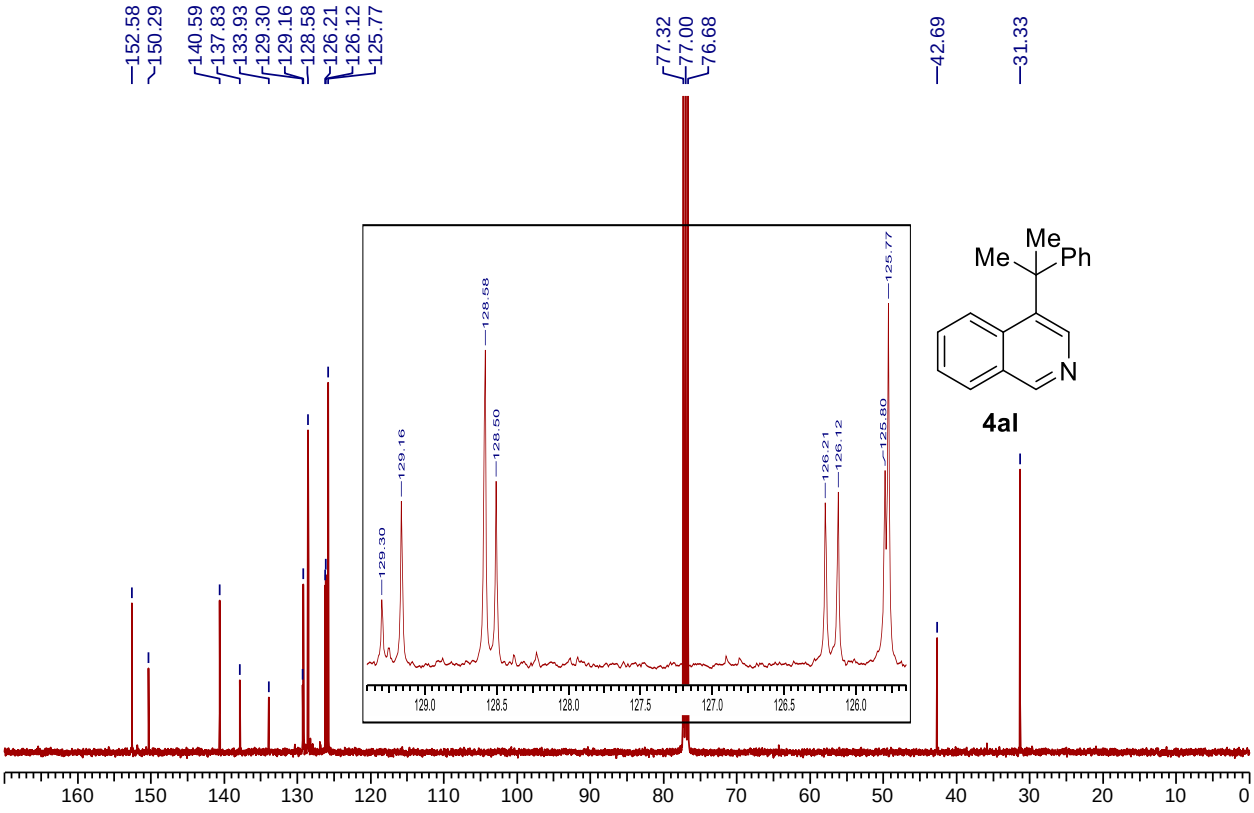

9.30
8.34
8.09
8.08
8.07
8.06
7.82
7.72
7.71
7.65
7.48
7.47
7.27
7.10
0.00
O
O
N
4aj
1.00
1.00
2.99
1.01
2.03
1.03
1.00
1.00
9
8
7
6
5
4
3
2
1
0


169.97
154.57
147.95
141.81
134.40
134.13
131.66
129.88
128.72
127.81
126.30
126.26
125.44
123.23
122.43
78.78
77.32
77.00
76.68
O
O
N
4aj
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

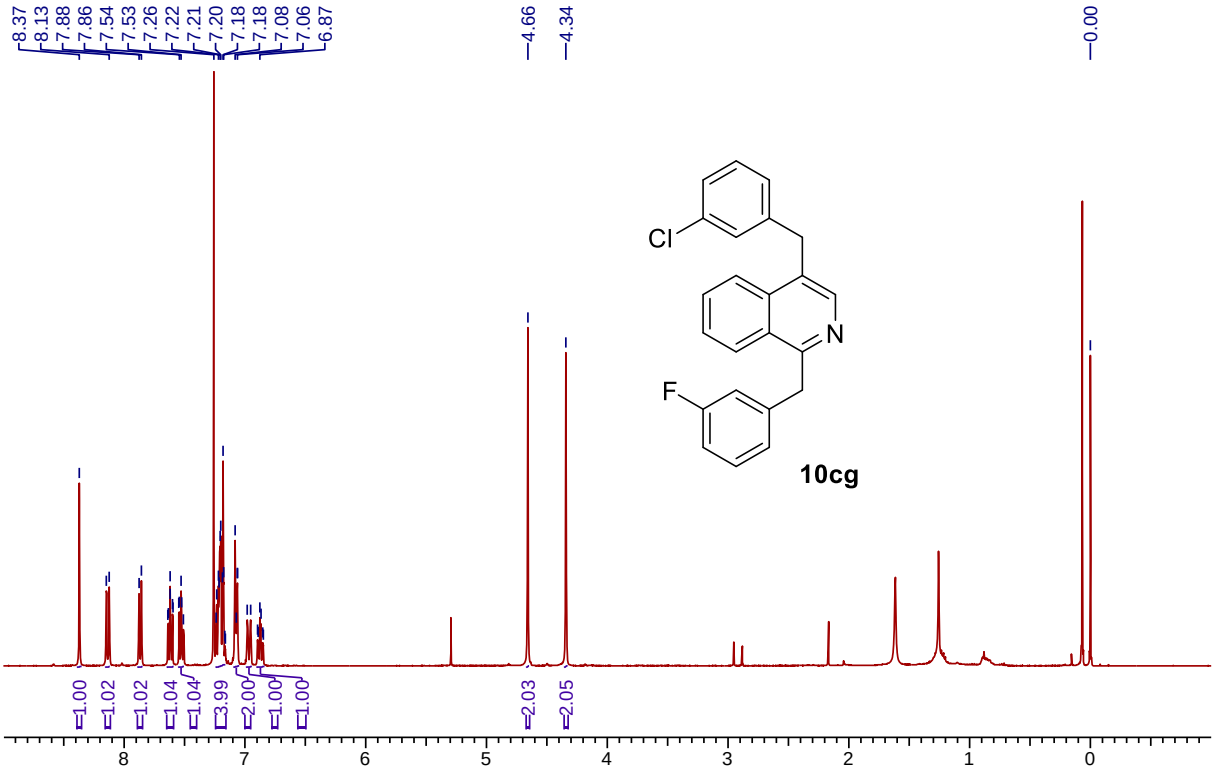

9.19
8.50
8.04
8.02
8.00
7.78
7.76
7.74
7.65
7.63
7.61
7.27
4.41
4.39
4.37
4.35
3.67
1.72
1.70
0.01
Me
CO2Me
N
4ak
1.00
1.00
2.03
1.01
1.03
1.04
3.07
3.03

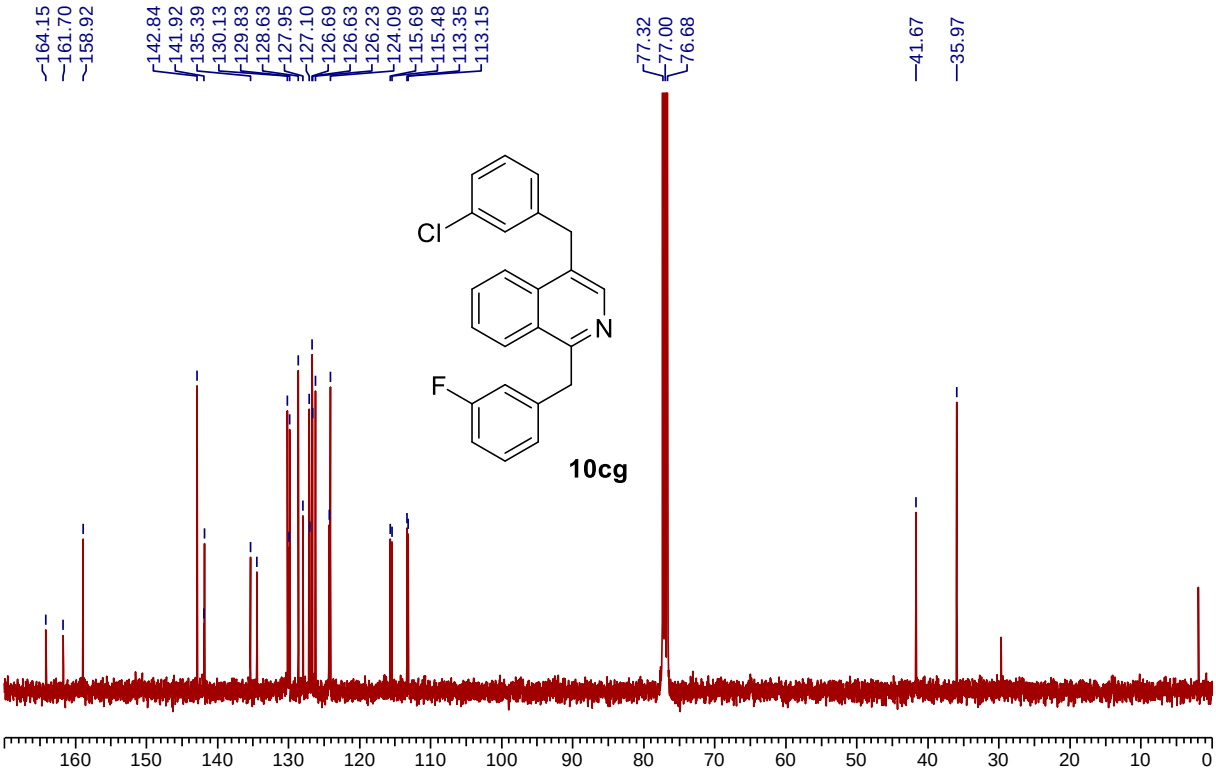

174.60
152.28
141.89
134.01
130.73
130.01
128.54
127.01
122.36
77.32
77.00
76.68
52.28
40.16
17.67
Me
CO2Me
N
4ak

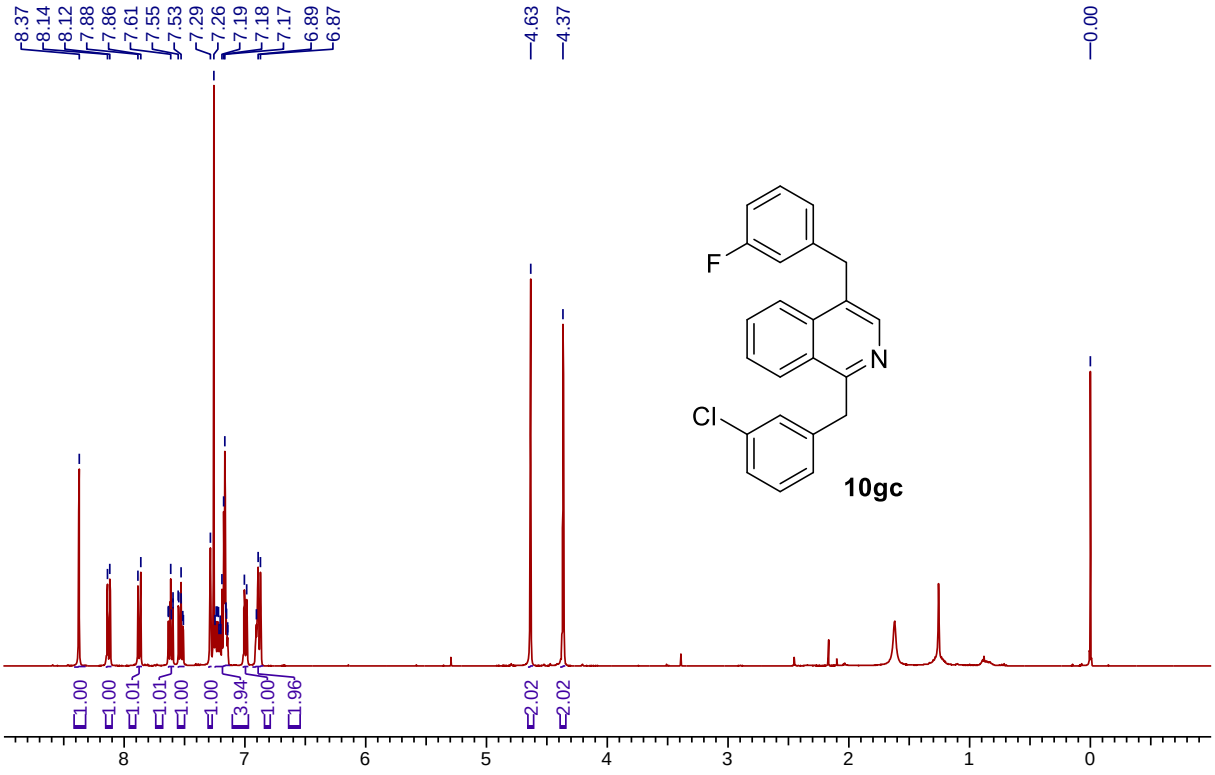

9.19
8.77
7.95
7.93
7.45
7.43
7.36
7.36
7.34
7.26
7.25
7.23
7.17
1.87
0.00
Me
Me
Ph
N
4al
1.00
1.00
1.01
2.02
1.01
4.38
1.05
6.01
9
8
7
6
5
4
3
2
1
0

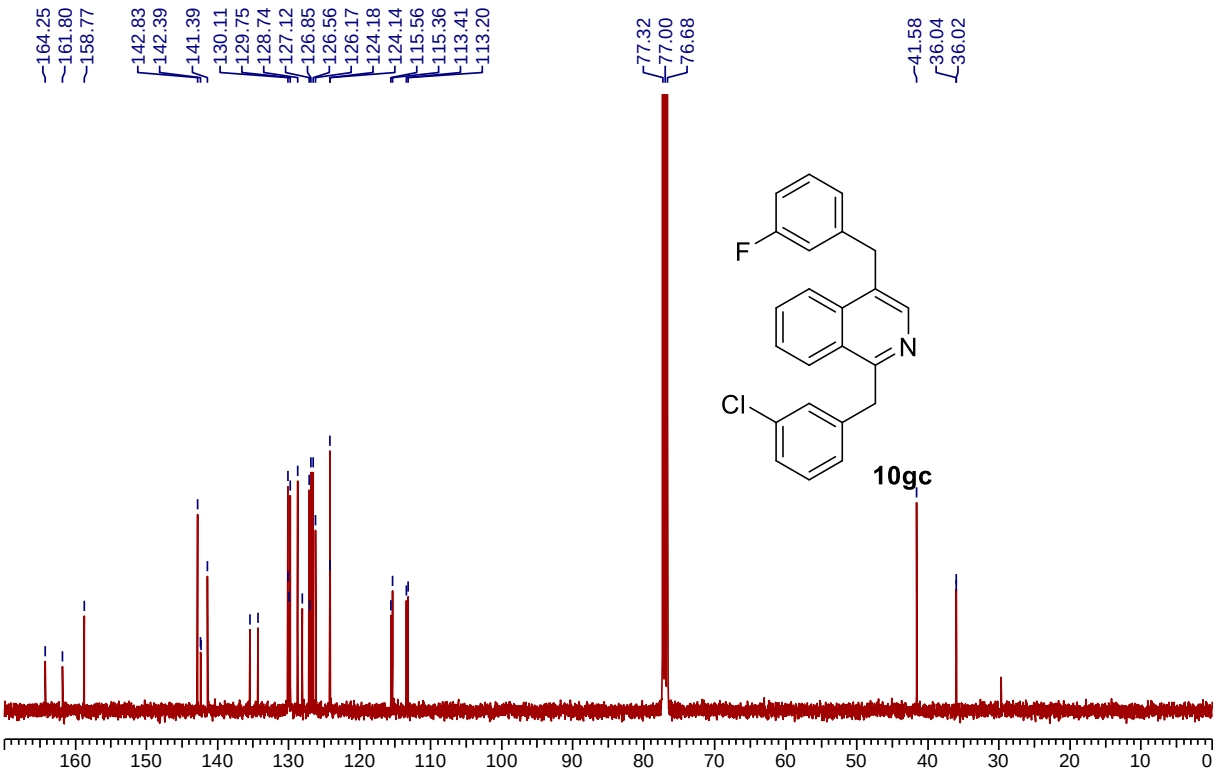

152.58
150.29
140.59
137.83
133.93
129.30
129.16
128.58
126.21
126.12
125.77
77.32
77.00
76.68
42.69
31.33
129.30
129.16
128.58
128.50
126.21
126.12
125.80
125.77
129.0
128.5
128.0
127.5
127.0
126.5
126.0
Me
Me
Ph
N
4al
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

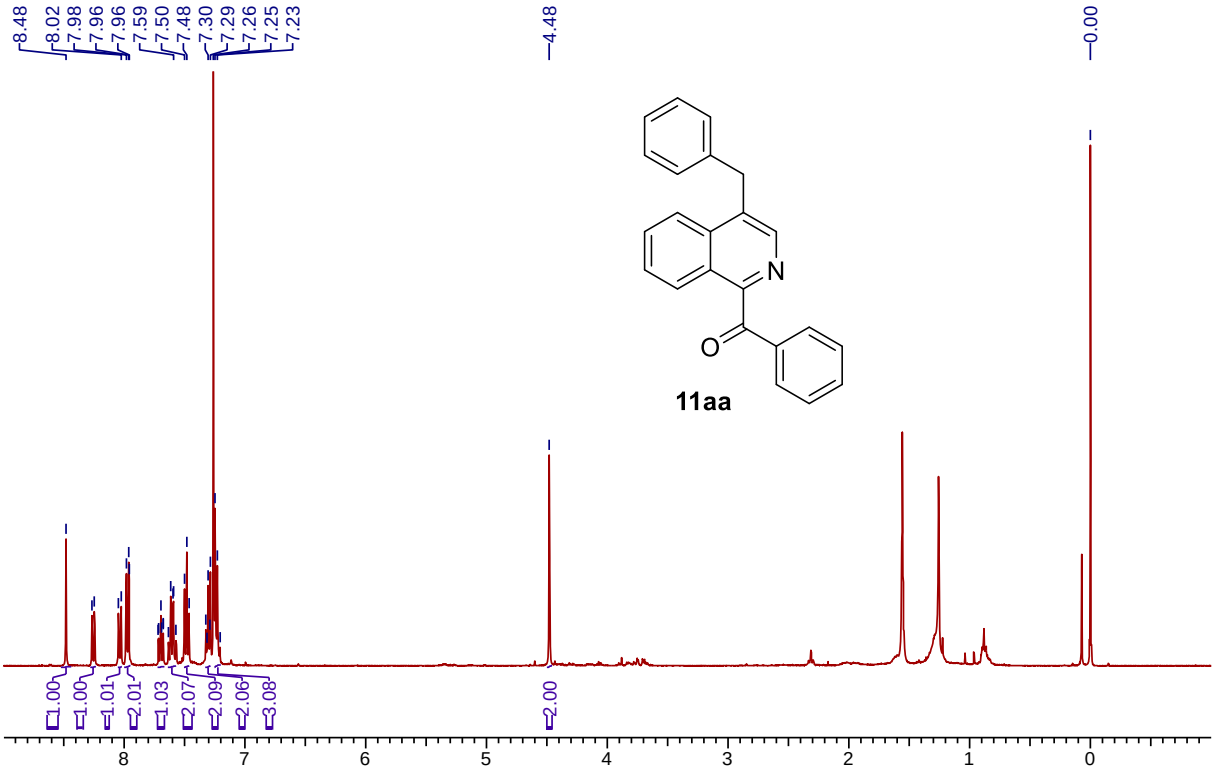
14c. NMR Spectra for Phosphite Mediate Sequential Functionalization of Isoquinolines:

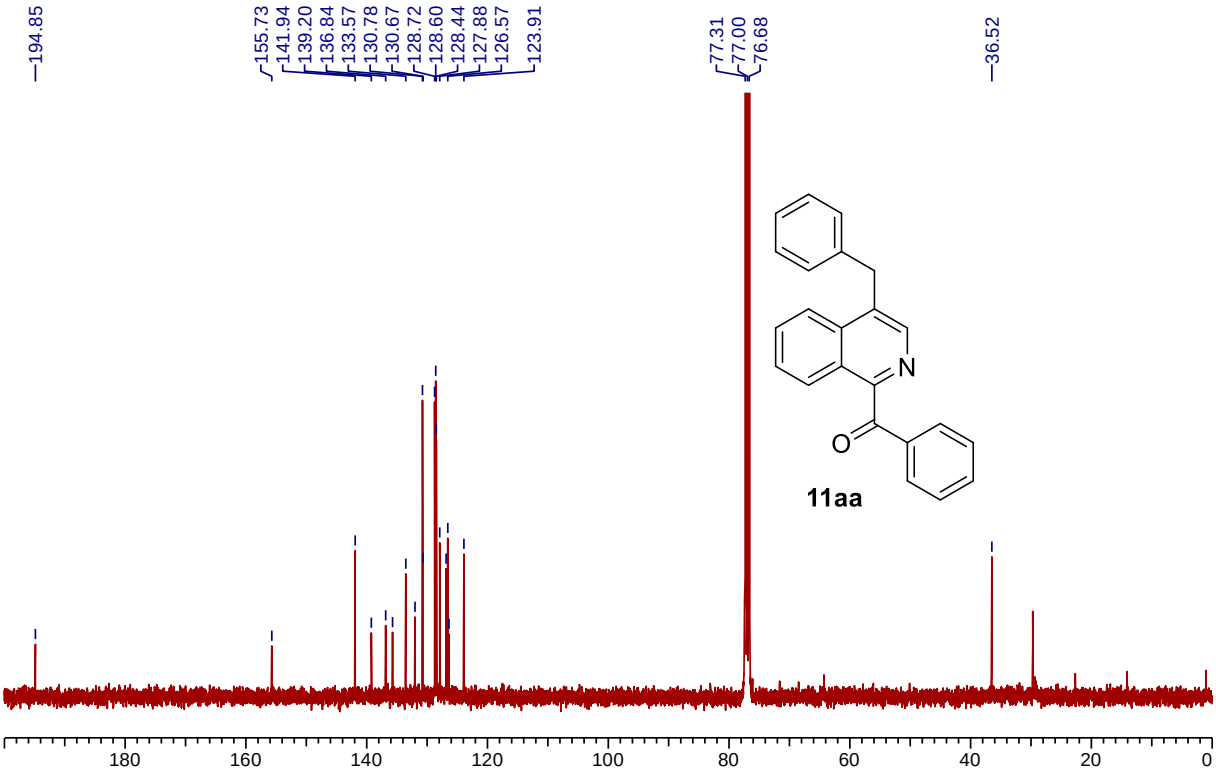


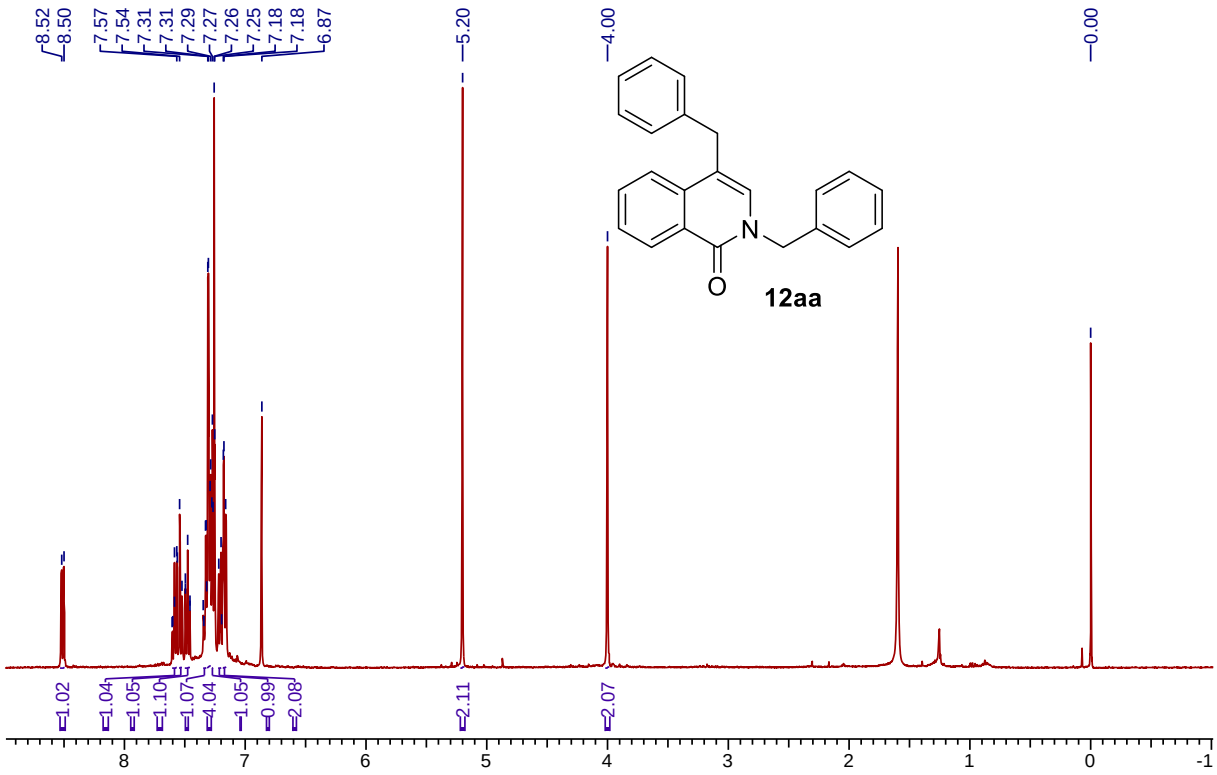


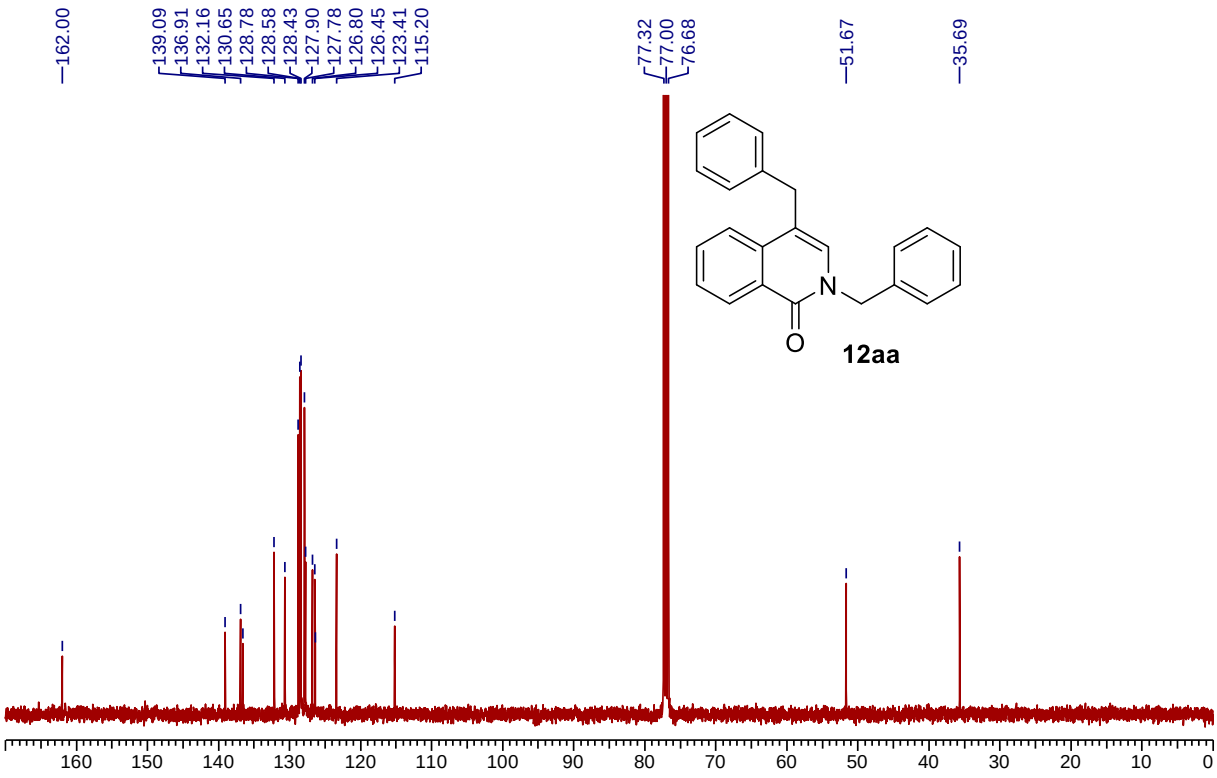

8.37
8.14
8.12
7.88
7.86
7.61
7.55
7.53
7.29
7.26
7.19
7.18
7.17
6.89
6.87
4.63
4.37
0.00
1.00
1.00
1.01
1.01
1.00
1.00
3.94
1.00
1.96
2.02
2.02
F
N
Cl
10gc


164.25
161.80
158.77
142.83
142.39
141.39
130.11
129.75
128.74
127.12
126.85
126.56
126.17
124.18
124.14
115.56
115.36
113.41
113.20
77.32
77.00
76.68
41.58
36.04
36.02
F
N
Cl
10gc


8.48
8.02
7.98
7.96
7.96
7.59
7.50
7.48
7.30
7.29
7.26
7.25
7.23
4.48
0.00
1.00
1.00
1.01
2.01
1.03
2.07
2.09
2.06
3.08
2.00
N
O
11aa


194.85
155.73
141.94
139.20
136.84
133.57
130.78
130.67
128.72
128.60
128.44
127.88
126.57
123.91
77.31
77.00
76.68
36.52
N
O
11aa


8.52
8.50
7.57
7.54
7.31
7.31
7.29
7.27
7.26
7.25
7.18
7.18
6.87
5.20
4.00
0.00
1.02
1.04
1.05
1.10
1.07
4.04
1.05
0.99
2.08
2.11
2.07
8
7
6
5
4
3
2
1
0
-1
N
O
12aa


162.00
139.09
136.91
132.16
130.65
128.78
128.58
128.43
127.90
127.78
126.80
126.45
123.41
115.20
77.32
77.00
76.68
51.67
35.69
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
N
O
12aa