Supporting Information

An efficient and facile strategy for trifluoromethylation and perfluoroalkylation of isoquinolines and heteroarenes

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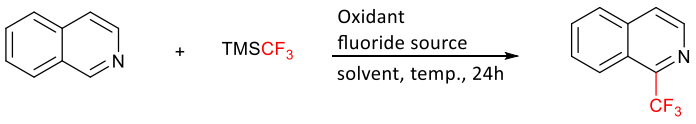
1. General information

All commercially sourced reagents were used as supplied unless otherwise stated. The ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a Bruker Avance 400 spectrometer (400 MHz, 101 MHz or 376 MHz, respectively). ^{1}H NMR chemical shifts are reported in ppm (δ) relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard ($CDCl_3$, δ 7.26 ppm). ^{13}C NMR chemical shifts were determined relative to the solvent: $CDCl_3$ at δ 77.16 ppm. High resolution mass spectroscopy data of the products were collected on a BioTOF Q instrument. Visualization on TLC was achieved by UV light (254 nm). Flash chromatography was performed on silica gel 90, 200-300 mesh.

2. Optimization of the reaction conditions

Table S1. Screening reaction conditions for trifluoromethylation of isoquinoline.[a]



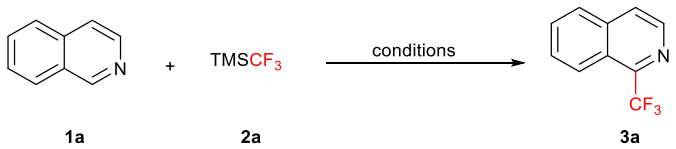
1a 2a 3a

Entry	Oxidant	F$^-$	Temp. (°C)	Solvent	Yield[b] (%)
1	PIFA	KF	r.t.	CH_3CN	trace
2	PIFA	KF	r.t.	dioxane	n.r.
3	PIFA	KF	r.t.	MeOH	n.r.
4	PIFA	KF	r.t.	toluene	n.r.
5	PIFA	KF	r.t.	THF	trace
6	PIFA	KF	r.t.	DMF	10
7	PIFA	KF	r.t.	NMP	57
8	PIDA	KF	r.t.	NMP	6
9	TBHP	KF	r.t.	NMP	n.r.
10	$K_2S_2O_8$	KF	r.t.	NMP	n.r.

11	PIFA	CsF	r.t.	NMP	52
12	PIFA	TBAF	r.t.	NMP	trace
13	PIFA	AgF	r.t.	NMP	n.r.
14	PIFA	KF	0	NMP	73
15	PIFA	KF	-10	NMP	66
16[c]	PIFA	KF	0	NMP	42
17[d]	PIFA	KF	0	NMP	65

[a] Reaction conditions: **1a** (0.2 mmol), $TMSCF_3$ (3.0 equiv.), oxidant (3.0 equiv.), fluoride source (4.0 equiv.) in 2.0 mL anhydrous solvent for 24 h under Ar. [b] Isolated yield. n.r. = no reaction. [c] $TMSCF_3$ (2.0 equiv.), PIFA (2.0 equiv.), KF (2.0 equiv.). [d]$TMSCF_3$ (4.0 equiv.), PIFA (4.0 equiv.), KF (4.0 equiv.).

Table S2. Screening of hypervalent iodine reagents (HIRs) under optimized condition.



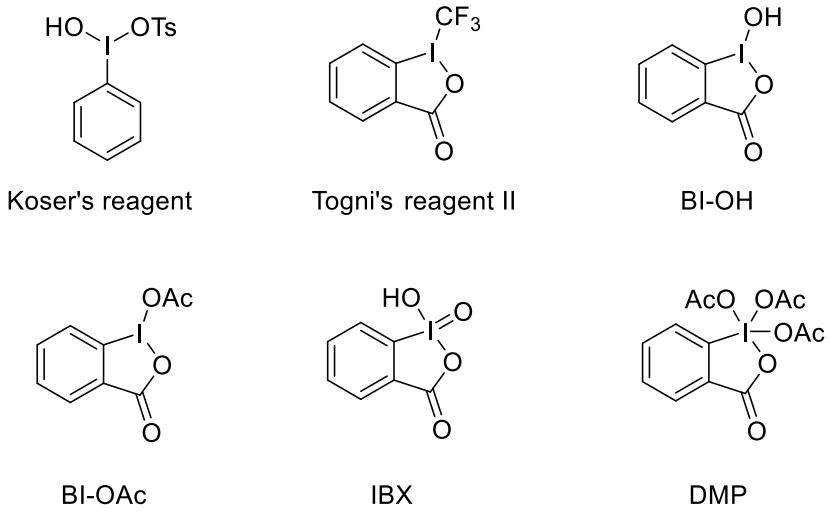
1a 2a 3a

Entry	HIRs	Temp. (°C)	Solvent	Yield (%)[a]
1	Koser's reagent	0	NMP	4
2	Togni's reagent II	0	NMP	n.r.
3	BI-OH	0	NMP	n.r.
4	BI-OAc	0	NMP	n.r.
5	PhIO	0	NMP	7
6	$PhIO_2$	0	NMP	n.r.
7	IBX	0	NMP	n.r.
8	DMP	0	NMP	n.r.
9	Koser's reagent	r.t.	NMP	3

10	PhIO	r.t.	NMP	5
11	PhIO	0	CH_3CN	n.r.
12	PhIO	0	DMF	n.r.
13	PhIO	0	MeOH	n.r.
14	PhIO	0	DCM	n.r.

[a] Reaction conditions: **1a** (0.2 mmol), $TMSCF_3$ (3.0 equiv.), HIRs (3.0 equiv.), KF (4.0 equiv.) in 2.0 mL anhydrous solvent for 24 h under Ar. [b] Isolated yield. n.r. = no reaction.

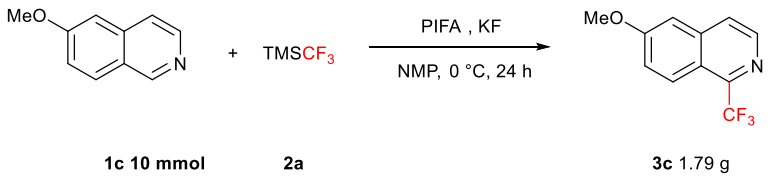
HIRs:



3. General procedure for the trifluoromethylation of isoquinolines

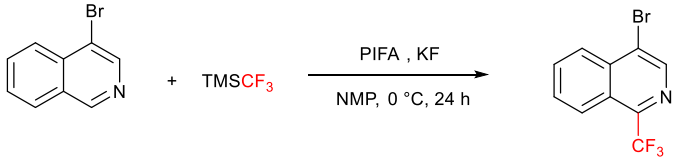
In an argon glovebox, isoquinoline **1a** (0.2 mmol, 23.5 μL), PIFA (3.0 equiv., 258 mg), and KF (4.0 equiv., 46.5 mg) weighed into an oven-dried glass vial equipped with a stir bar. The vial was sealed with a septum and brought outside of the glovebox. Under Ar, anhydrous NMP (2.0 mL) and $TMSCF_3$ (3.0 equiv, 90 μL) were added in quick succession to the glass vial by syringe. The mixture was then allowed to stir at 0 ^oC for 24 hours. After complete consumption of substrates (monitored by TLC), the resulting mixture was diluted with EtOAc and washed by saturated $NaHCO_3$ solution (×2). The organic layer was dried over Na_2SO_4 and concentrated under vacuum. The crude product was purified by silica gel column chromatography using 5% EtOAc/petroleum ether as the eluent (The reaction of **1a** as an example).

4. Gram-scale synthesis of 3c and 3k



Scheme S1. Gram-scale synthesis of **3c**

In an argon glovebox, 6-methoxyisoquinoline **1c** (10 mmol, 1.59 g), PIFA (3.0 equiv., 12.9 g), and KF (4.0 equiv., 3.4 g) weighed into an oven-dried glass vial equipped with a stir bar. The vial was sealed with a septum and brought outside of the glovebox. Under Ar, anhydrous NMP (200 mL) and $TMSCF_3$ (3.0 equiv., 4.4 mL) were added in quick succession to the round-bottomed flask by syringe. The mixture was then allowed to stir at 0 °C for 24 hours. After complete consumption of substrates (monitored by TLC), the resulting mixture was diluted with EtOAc and washed by saturated $NaHCO_3$ solution (×2). The organic layer was dried over Na_2SO_4 and concentrated under vacuum. The crude product was purified by silica gel column chromatography using 5% EtOAc/petroleum ether as the eluent to give the product **3c** (1.79 g, 79%).



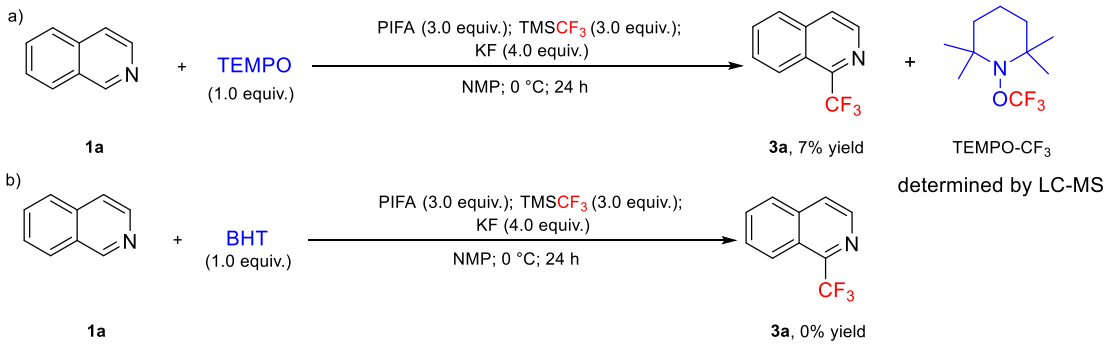
Scheme S2. Gram-scale synthesis of **3k**

In an argon glovebox, 4-bromoisoquinoline **1k** (10 mmol, 2.07 g), PIFA (3.0 equiv., 12.9 g), and KF (4.0 equiv., 3.4 g) weighed into an oven-dried glass vial equipped with a stir bar. The vial was sealed with a septum and brought outside of the glovebox. Under Ar, anhydrous NMP (200 mL) and $TMSCF_3$ (3.0 equiv., 4.4 mL) were added in quick succession to the round-bottomed flask by syringe. The mixture was then allowed to stir at 0 °C for 24 hours. After complete consumption of substrates (monitored by TLC), the resulting mixture was diluted with EtOAc and washed by saturated $NaHCO_3$ solution (×2). The organic layer was dried over Na_2SO_4

and concentrated under vacuum. The crude product was purified by silica gel column chromatography using 5% EtOAc/petroleum ether as the eluent to give the product **3k** (1.34 g, 49%).

5. The study on the mechanism

5.1 The control experiments of mechanism study (Scheme S3):



Scheme S3 The control experiments of mechanism study

In order to gain preliminary mechanism information about this reaction, several control experiments were conducted using **1a** as a substrate.

a) In an argon glovebox, isoquinoline **1a** (0.2 mmol, 23.5 µL), PIFA (3.0 equiv, 258 mg), KF (4.0 equiv, 46.5 mg) and 2,2,6,6-tetramethyl-1-piperidinyloxyl (TEMPO) (0.2 mmol, 31.2 mg) weighed into an oven-dried glass vial equipped with a stir bar. Under Ar, NMP (2.0 mL) and $TMSCF_3$ (3.0 equiv, 90 µL) were added in quick succession to the glass vial by syringe. The vial was sealed with a septum and brought outside of the glovebox. The mixture was then allowed to stir at 0 °C for 24 hours. After the reaction, the mixture was then analyzed directly by LC-MS, and TEMPO-CF_3 adduct was detected. Finally, the product **3a** was isolated in 7% yield.

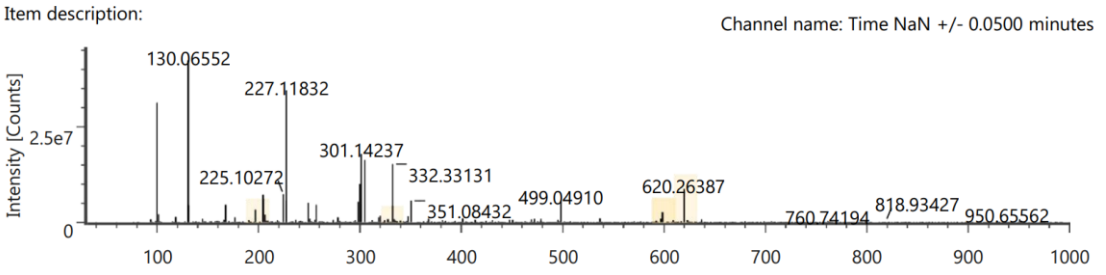
b) In an argon glovebox, isoquinoline **1a** (0.2 mmol, 23.5 µL), PIFA (3.0 equiv., 258 mg), KF (4.0 equiv., 46.5 mg) and 2,6-di-*tert*-butyl-4-methylphenol (BHT) (0.2 mmol, 44 mg) weighed into an oven-dried glass vial. Under Ar, NMP (2.0 mL) and $TMSCF_3$ (3.0 equiv., 90 µL) were added in quick succession to the glass vial by syringe equipped with a stir bar. The vial was sealed with a septum and brought

outside of the glovebox. The mixture was then allowed to stir at 0 °C for 24 hours. After the reaction, no **3a** was detected.

We then used high resolution electrospray ionization mass spectra (HRMS-ESI) to detect the possibility of active intermediate $[Ph–I–CF_3]^+$ in the reaction process.[1] Samples were taken at 5 minutes, 30 minutes and 60 minutes respectively after the beginning of the reaction and diluted with MeCN prior to the injection into the mass spectrometer. However, the possible intermediate $[Ph–I–CF_3]^+$ don't be detected. The results are as follows: the intermediate $[Ph–I–CF_3]^+$ ($C_7H_5F_3I$) did not be observed.

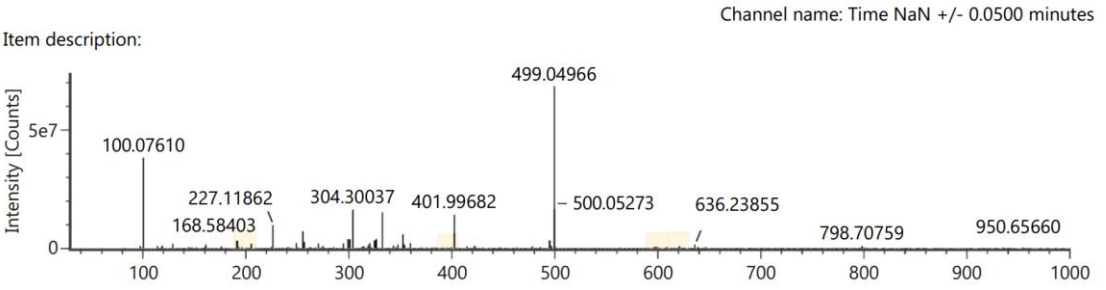
5 mins

.	Formula	Neutral mass (Da)	Observed m/z	Mass error (mDa)	Mass error (ppm)	Response	Adducts	Identification status
1	$C_7H_5F_3I$	272.93880						Not Observed



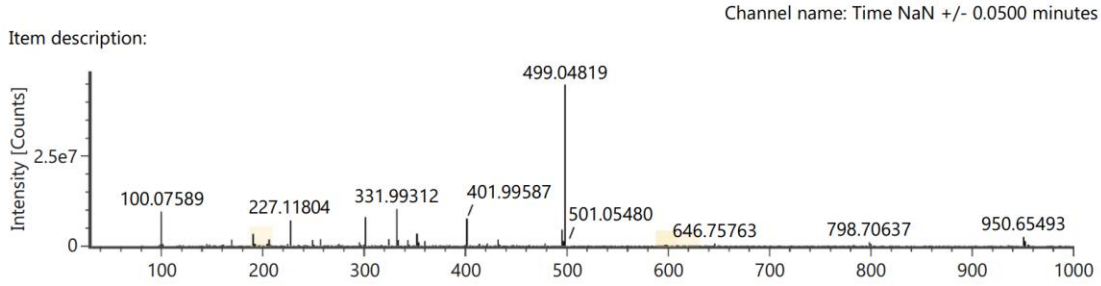
30 mins

.	Formula	Neutral mass (Da)	Observed m/z	Mass error (mDa)	Mass error (ppm)	Response	Adducts	Identification status
1	$C_7H_5F_3I$	272.93880						Not Observed



60 mins

.	Formula	Neutral mass (Da)	Observed m/z	Mass error (mDa)	Mass error (ppm)	Response	Adducts	Identification status
1	$C_7H_5F_3I$	272.93880						Not Observed



In conclusion, based on the radical trap experiments and detected results of HRMS-ESI, the CF_3 radical addition process was probably involved in our system.

5.2 Density functional theory (DFT) calculations

All geometries were fully optimized at the B3LYP[2] functional level of density functional theory and 6-31G(d) basis set,[3] using the SDD pseudopotential[4] for the iodine, considering Grimme's DFT empirical dispersion correction with Becke-Johnson damping scheme (D3BJ).[5] Solvation effects were accounted for polarisable continuum model (PCM)[6] with solvent parameters of NMP including static dielectric constant (298 K) and dynamic dielectric constant. Vibrational frequencies were calculated at the same level to identify stationary points as local minima (no imaginary frequency) or transition states (only one imaginary frequency) which were checked by the calculations of intrinsic reaction coordinate (IRC).[7] The wave function stability of broken-symmetry singlet states was verified. The single-point energy calculations were performed based on optimized structures, employing the 6-311+G (d, p) basis set for all atoms in combination with the SDD pseudopotential for iodine, considering also DFT-D3BJ empirical dispersion correction and PCM solvation model. The Gibbs free energy was determined according to the single-point energy and the thermal correction to the Gibbs free energy obtained from the vibrational frequency analysis at the experimental reaction temperature (0 °C), together with DFT-D3BJ empirical dispersion correction. All DFT calculations were carried out with Gaussian 16 program.[8]

The polarization parameter function (ζ)[9] was calculated by Multiwfn[10] and then

plotted on the electron density isosurface.

$$\zeta(\boldsymbol{r}) = \left(\rho^{\alpha}(\boldsymbol{r}) - \rho^{\beta}(\boldsymbol{r})\right) / \left(\rho^{\alpha}(\boldsymbol{r}) + \rho^{\beta}(\boldsymbol{r})\right)$$

ρ^{α}: α electron density

ρ^{β}: β electron density

This function shows the ratio of unpaired electrons to total electrons on the molecule.

5.2.1 The Description for DFT Calculations

The most preferred reaction pathway was presented in Figure S1. From the energy profile, the trifluoromethylation process and the whole SET (single electron transfer) step was shown (Figure S1). Theoretical calculations indicated that the net reaction leading to **3a** had a large thermodynamic driving force of ca. 120.3 kcal/mol. The N atom of isoquinoline **1a** firstly formed a stable complex with PIFA and caused little energy increase (0.7 kcal/mol). The structure of complex was predicted by the potential energy scanning and conformer search. Further, the decarboxylation and participation of CF_3^- happened to get the stable **INT1**. The subsequent homolysis resulted in the broken-symmetry singlet state **INT2** with the rise of energy (19.3 kcal/mol). The broken-symmetry singlet state **TS** with 7-membered ring generated to produce the final 1a, PhI and TFA. The energy barrier was 3.5 kcal/mol from **INT2** to **TS**. The detailed transformation process of transient state **TS** was shown in the IRC plot (Figure S2).

As seen in the intrinsic reaction coordinate (IRC) plot, the process of the **INT2** to go over the energy barrier was displayed clearly. There were two main parts for this transformation, the first one was the single electron transfer (SET) (the curve colored with red) and dehydrogenation (the curve colored with blue). After homolysis of **INT2**, the single electron was distributed on the iodine of $PhICOOCF_3$ named α electron and on the trifluoromethyl radical named β electron with the opposite spin direction. At the transition state on the top of energy barrier, the β electron "flowed" to the $PhICOOCF_3$ gradually, which reflected by the shrink of the isosurface for the polarization parameter function (ζ) on iodine. Meantime, the energy also declined

dramatically. When the bond formed between the C-1 and CF_3 group, the β single electron was localized on C-3 mainly and finally transferred to $PhICOOCF_3$. Then the CF_3COO^- left form $PhICOOCF_3$ and captured the hydrogen at C-1 to end up the charge transfer with the energy down.

We also tried to find the transition states on the C-3 position, but no reasonable result was obtained for the trifluoromethyl radical. Thus, it is believed that trifluoromethylation of C-3 in current reaction condition is not favorable. Furthermore, for explaining the selectivity and providing the prediction profile, the electron localization function (ELF), average Local ionization energy (ALIE), total electrostatic potential (ESP) and atomic charge (NPA charge) were evaluated for **1a-1π** and **3a-3π**, and showed as graphical representation for distinguishing the differences easily (only the figures of **1a-1π** and **3a** was attached for the space limitations in this article). There were significant features at C-1 comparing to other position in the isoquinolines. For C-1, the values showed the weak localization of electron in the ELF map, difficult to participate in the electrophilic reaction comparing to other position in the ALIE map, and relative low electronegativity on the Van der Waals surface in ESP map. From these different four aspects, they suggested that relative deficiency for electron at C-1 and unbalance of electron distribution on the aromatic ring. This should be the driving force for the SET mechanism. From the representative product **3a**, the whole *N*-system was electron deficient due to the electron withdrawing of CF_3 group, but the electron distribution is not be changed. This is a main reason for the stop of trifluoromethylation of C-3 in the SET mechanism. In the different methods, readily available NPA charge is recommended for developing to prediction of this kind of reaction.

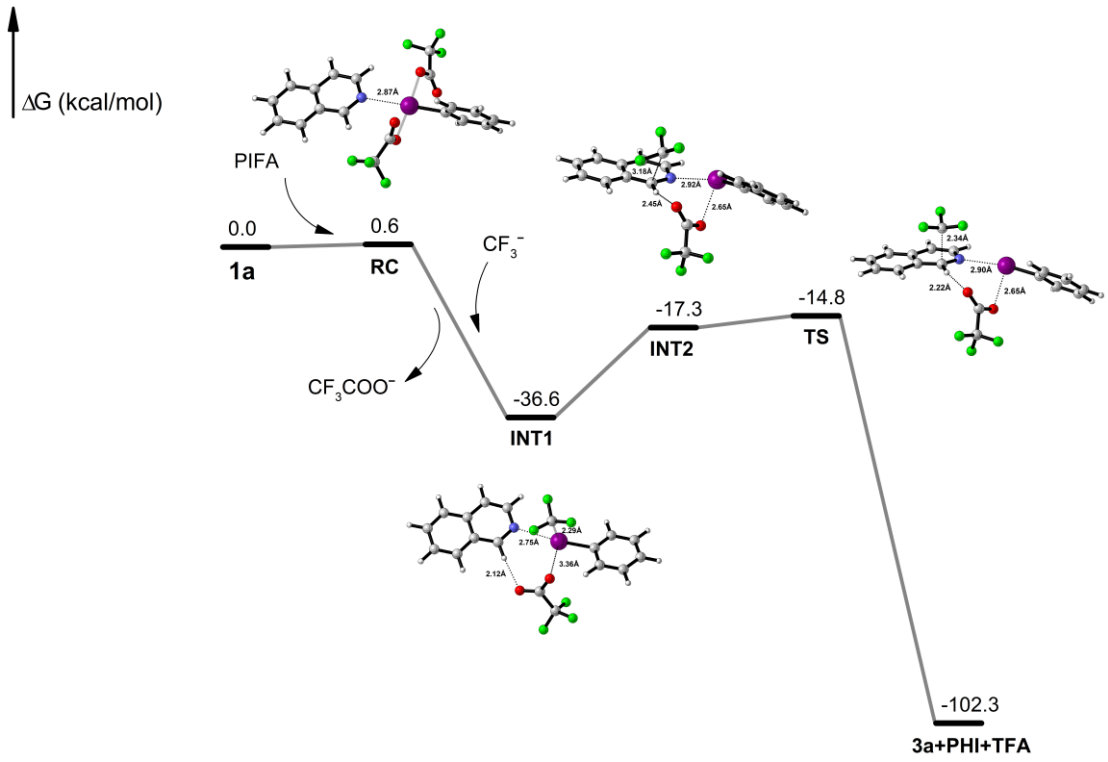


Figure S1. DFT-calculated energy profile of the trifluoromethylation of **1a**

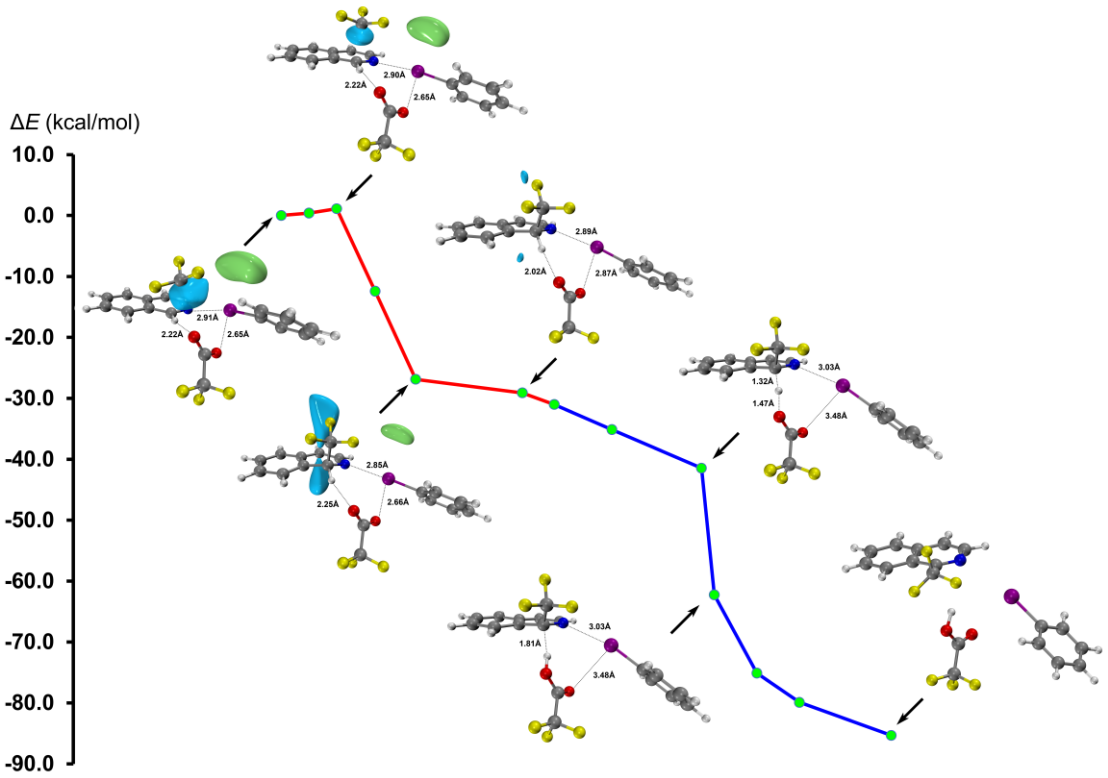


Figure S2. IRC plot of the key transition state TS with representative structures; carbon: gray, hydrogen: white, oxygen: red, nitrogen: blue, fluorine: yellow and iodine: purple. The single electron transfer showed by isosurface maps of polarization

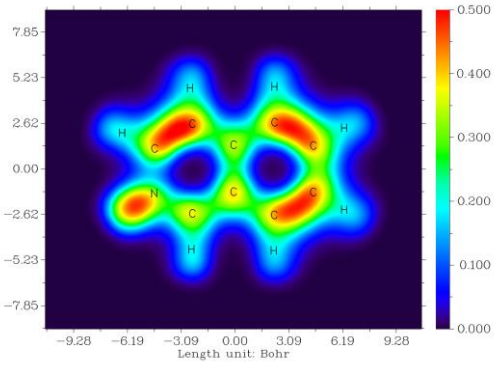
parameter function on the structures (isovalue 0.3): green: α electron, blue: β electron. The red curve is the process of the electron transfer, and the blue curve is dehydrogenation process.

5.2.2. Characteristics related with the wave function of 1a-1 π

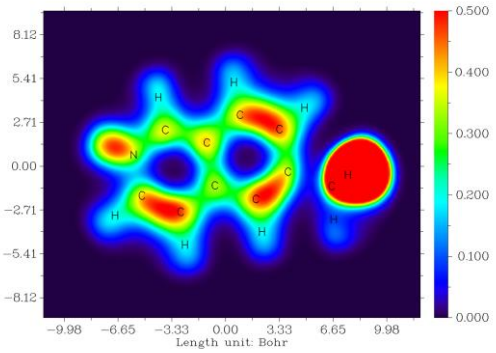
All geometry optimizations and single-point energy calculations for the *N* electron systems were performed at the B3LYP/6-311+G (d,p) theoretical levels. All the optimizations met the "very tight" convergence criteria setting in the Gaussian 16 software. Characteristics related with the wave function were calculated using Multiwfn.

1) Color-filled map of ELF (Electron Localization Function) of 1a-1 π at 1.4 Å above the *N* ring plane[11]

The ELF function can be represented in three-dimensional real space to show electron localization at different positions. The Large ELF value means that electrons are greatly localized.



1a



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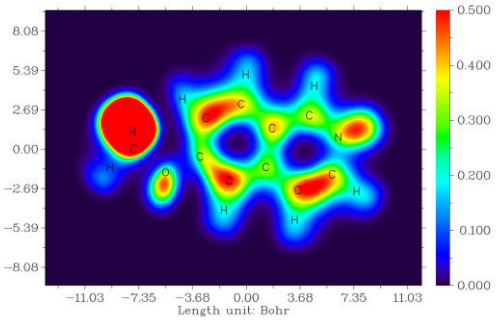

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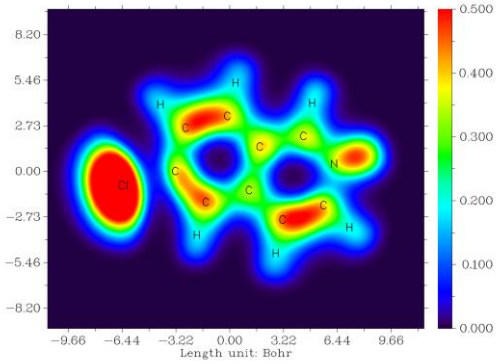

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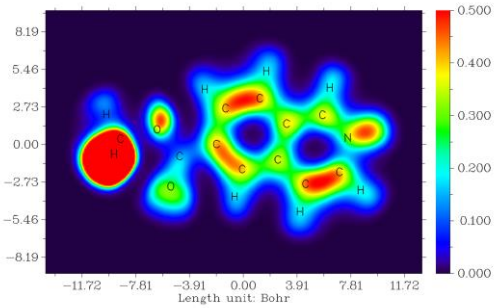

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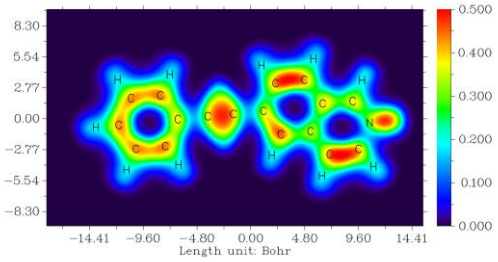

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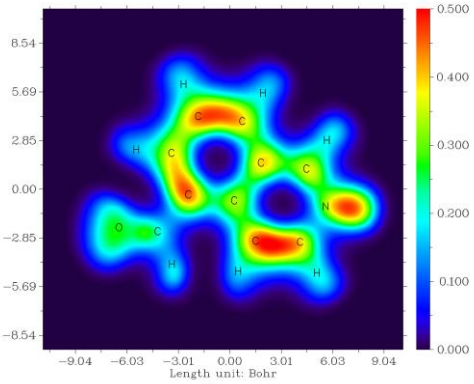

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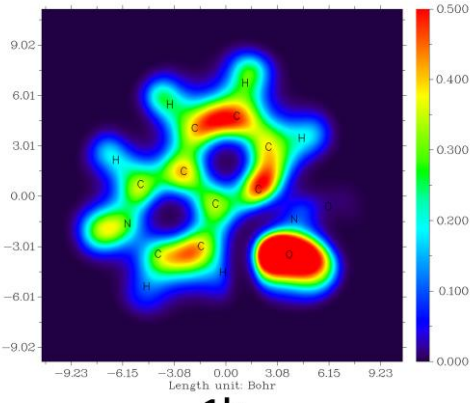

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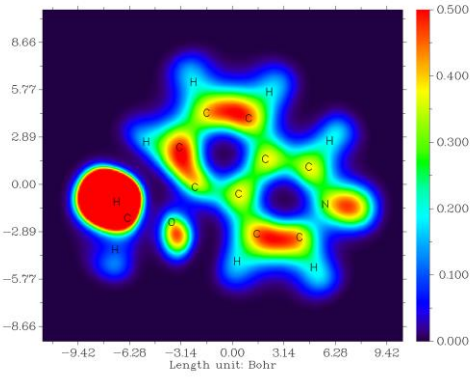

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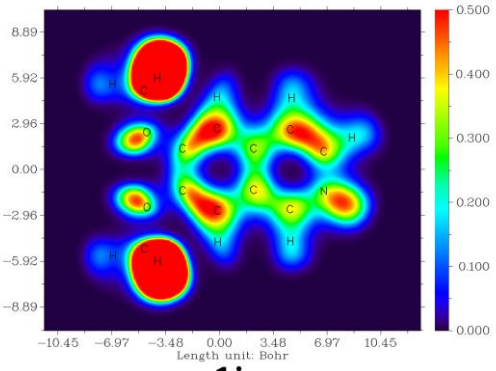

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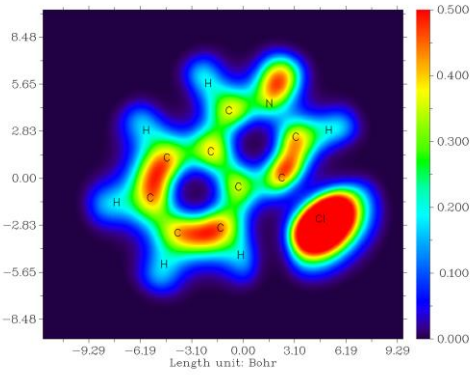

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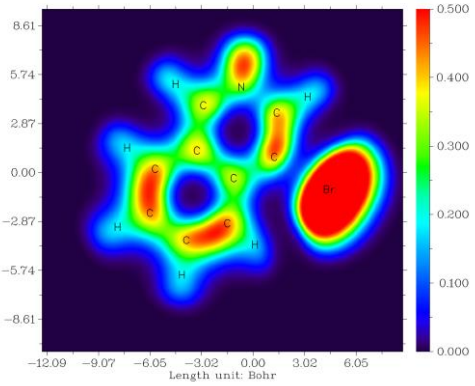

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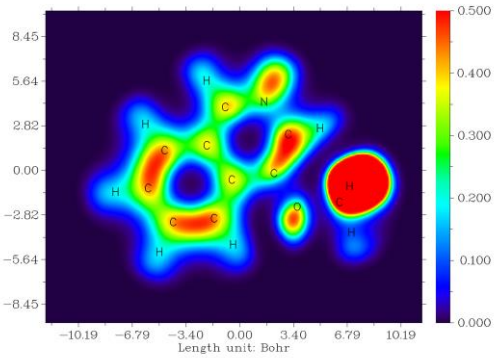

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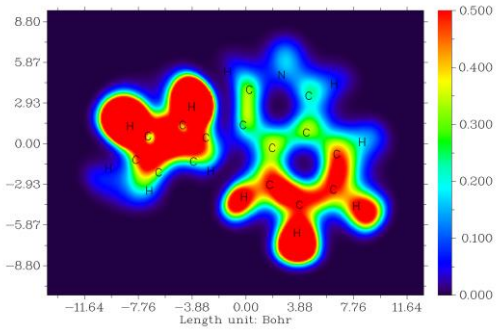

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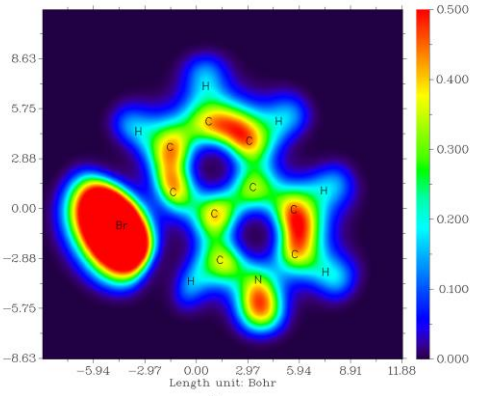
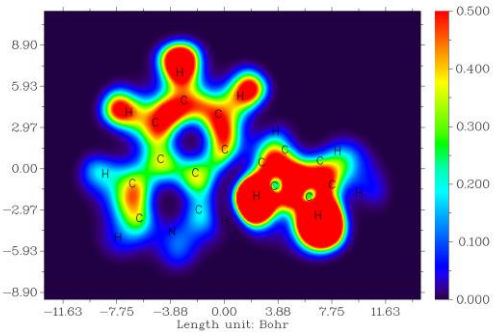
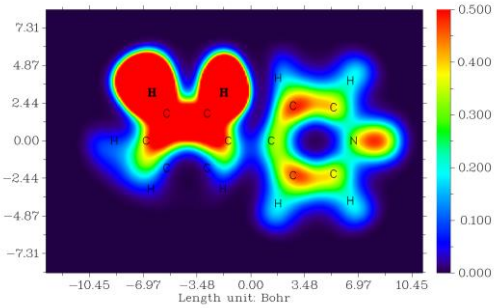


1o



1p



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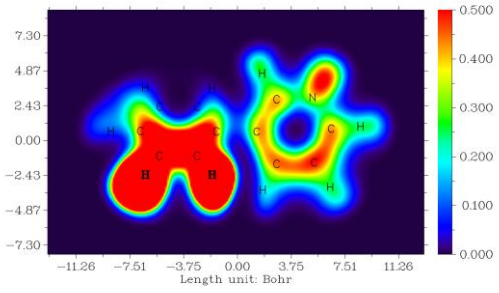

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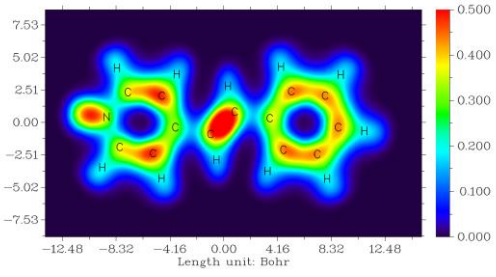

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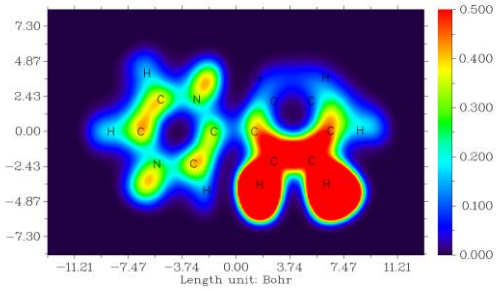
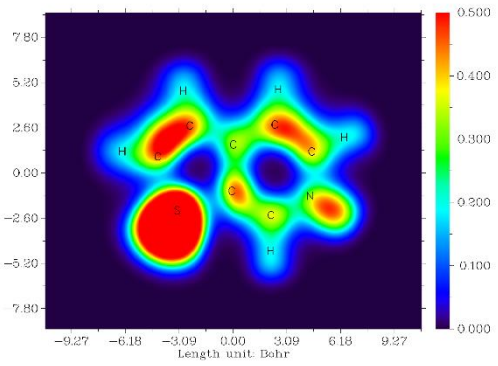
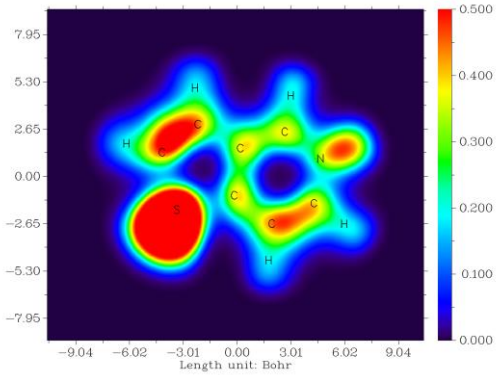


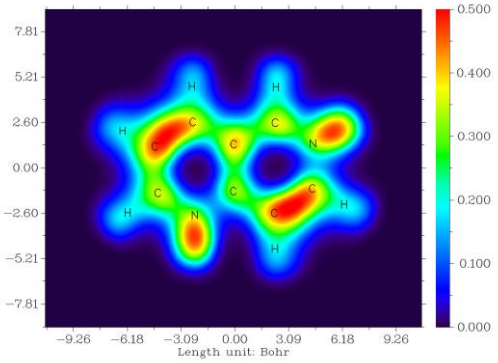
1t



1u



1v



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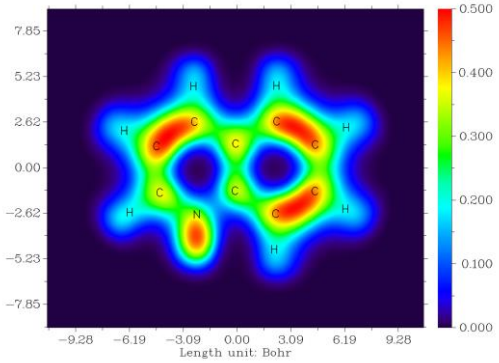
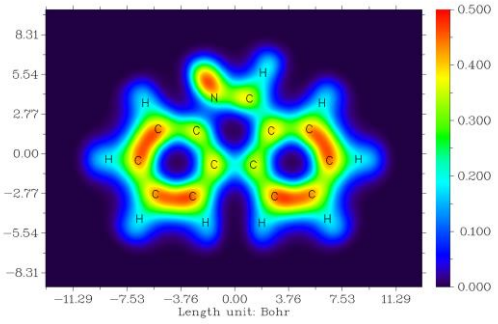
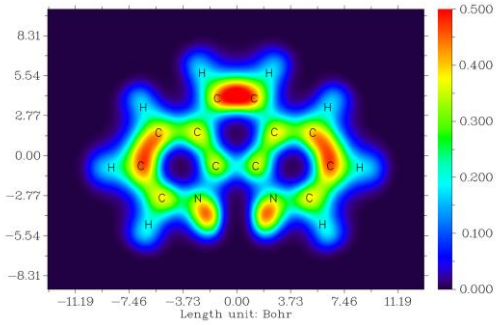


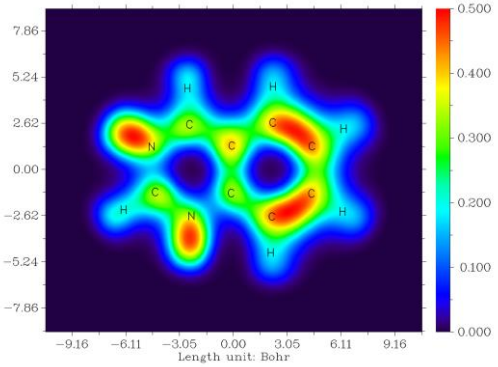
1x



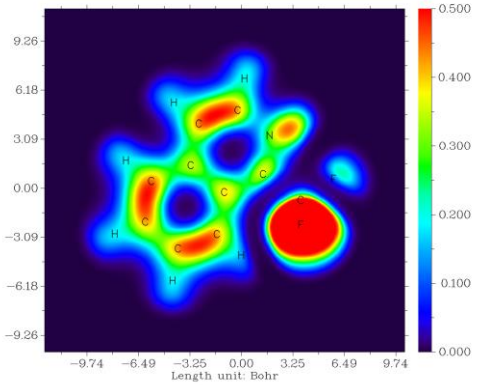
3y



1z



1π



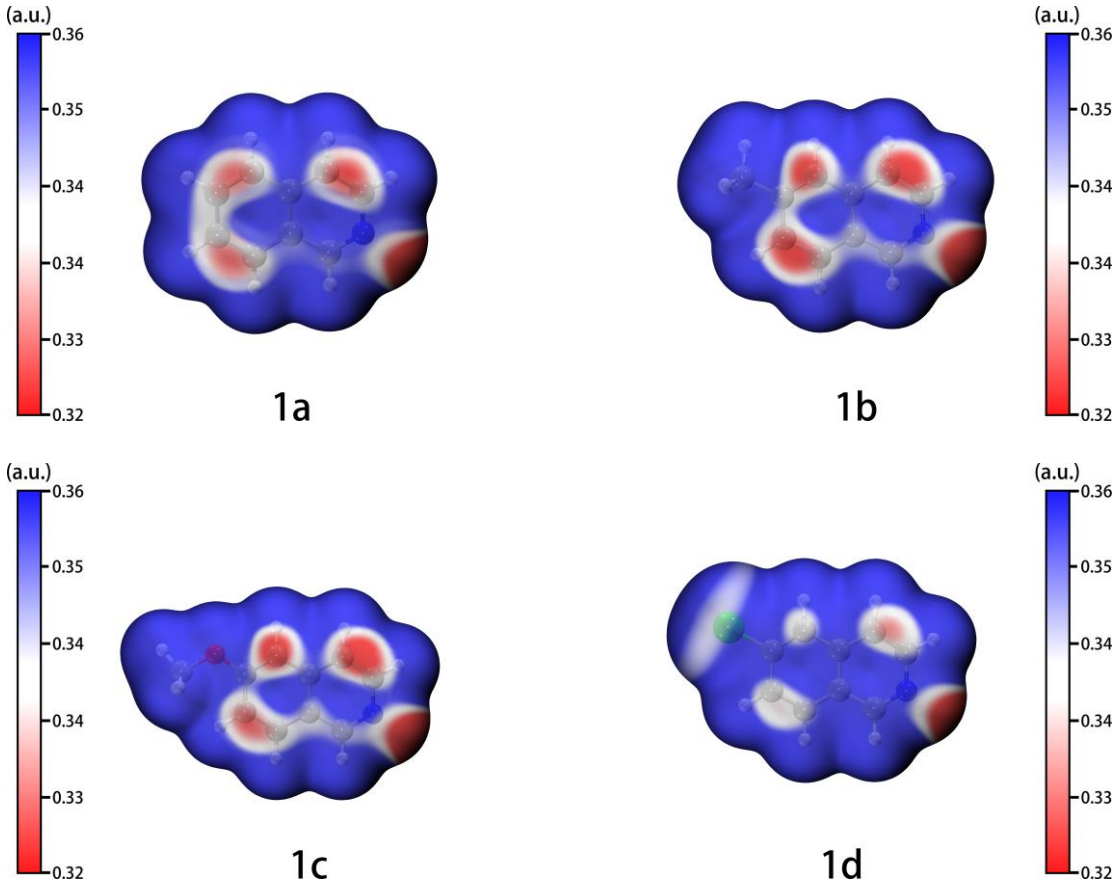
3a

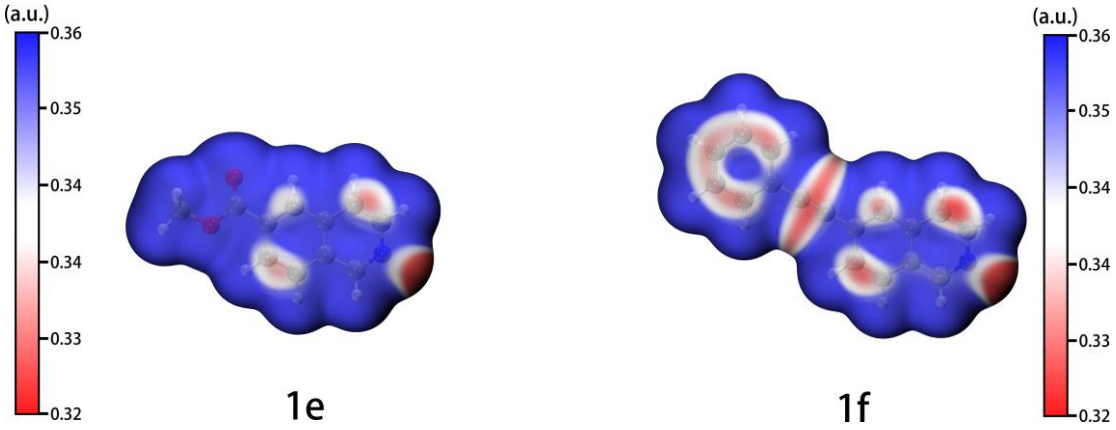
2) Isosurface maps of ALIE (Average Local Ionization Energy) of 1a-1π (isovalue 0.001)[12]

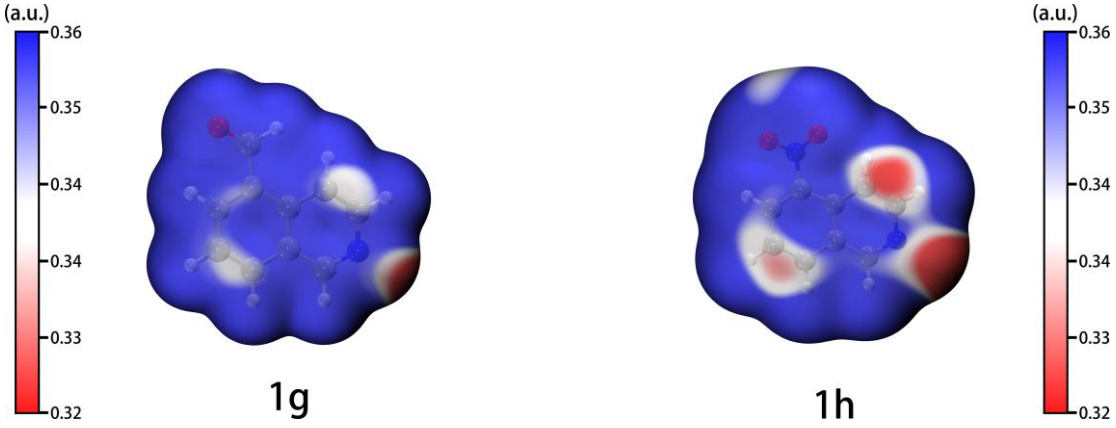
Average local ionization energy is written as

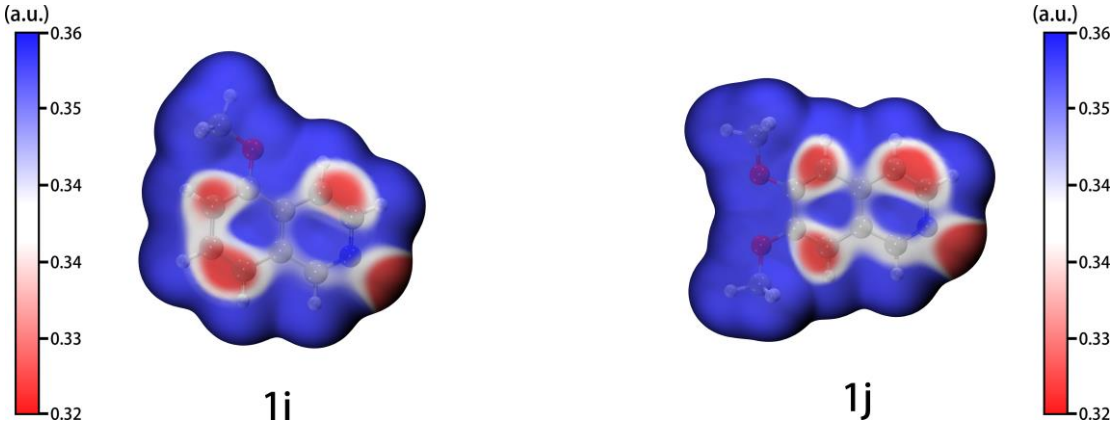
$$\bar{I}(r) = \frac{\sum_i \rho_i(\boldsymbol{r})|\varepsilon_i|}{\rho(\boldsymbol{r})}$$

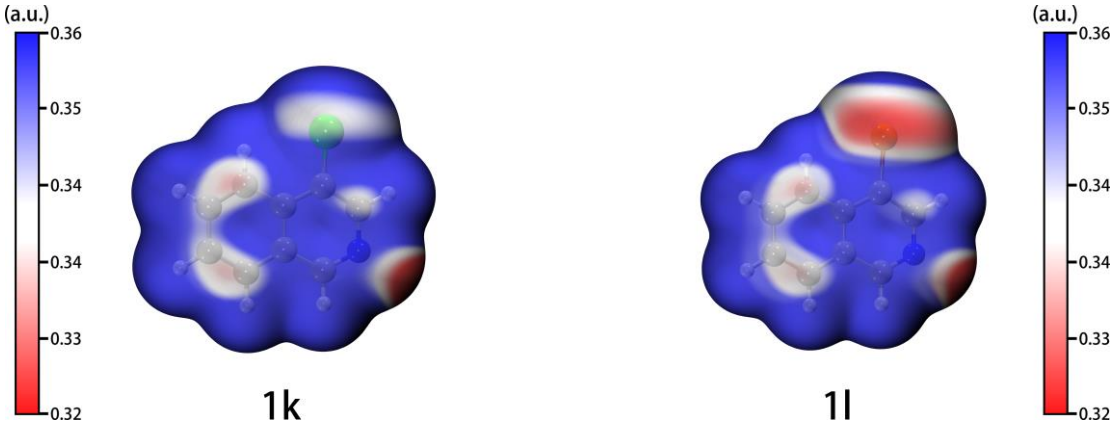
Where ρ_i (**r**) and ε_i are the electron density function and orbital energy of the molecular orbital, respectively. Lower value of $\bar{I}(r)$ indicates that the favored sites for reaction with electrophiles.

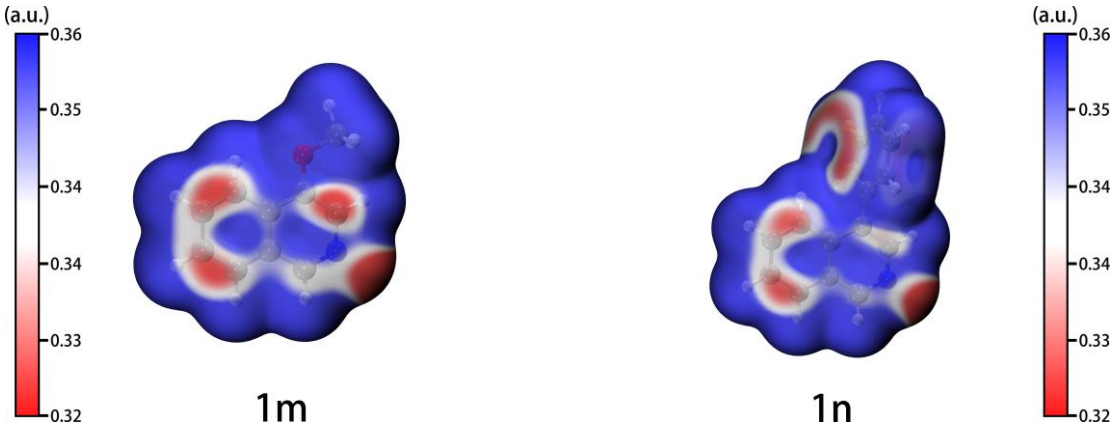


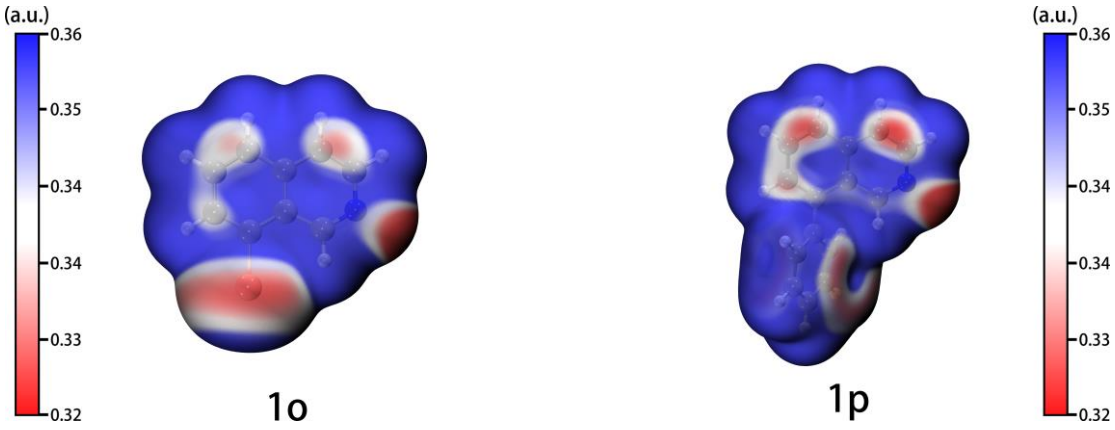

(a.u.)
0.36
0.35
0.34
0.34
0.33
0.32
1e
1f

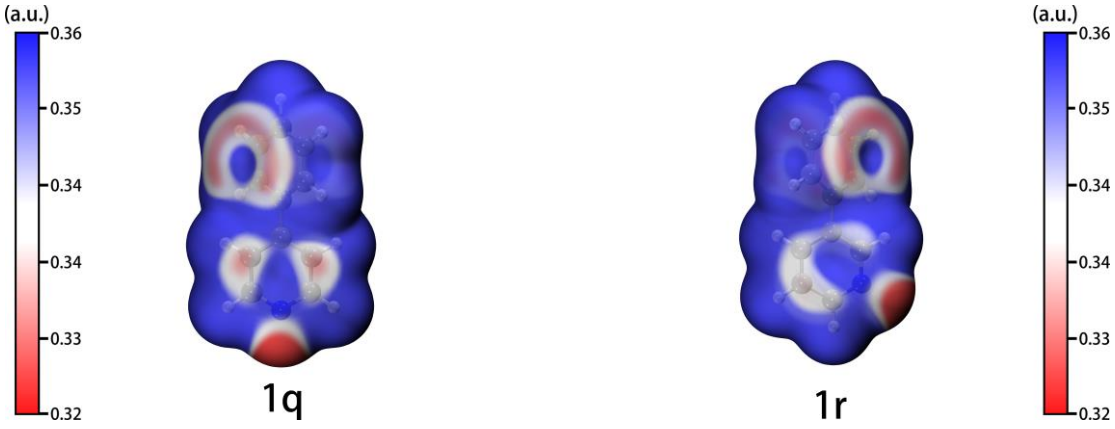

(a.u.)
0.36
0.35
0.34
0.34
0.33
0.32
1g
1h

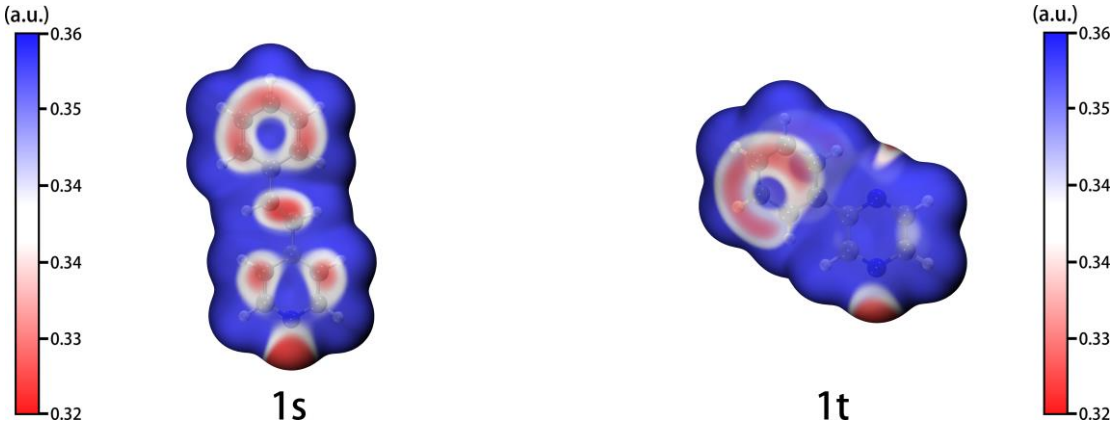

(a.u.)
0.36
0.35
0.34
0.34
0.33
0.32
1i
1j

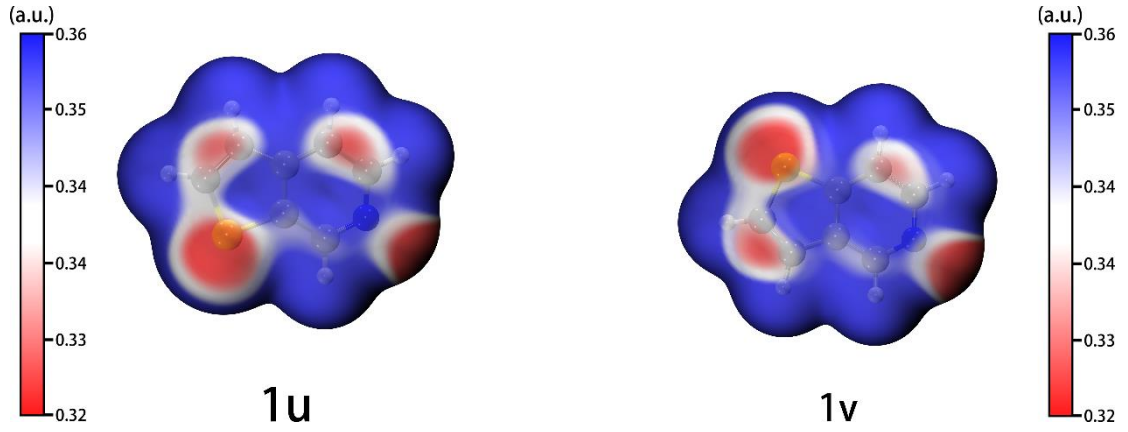

(a.u.)
0.36
0.35
0.34
0.34
0.33
0.32
1k
1l

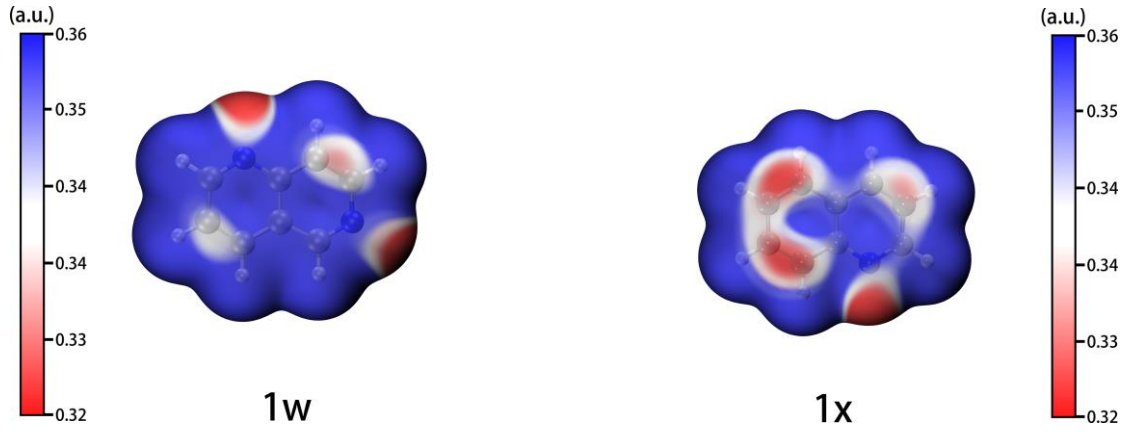

(a.u.)
0.36
0.35
0.34
0.34
0.33
0.32
1m
1n

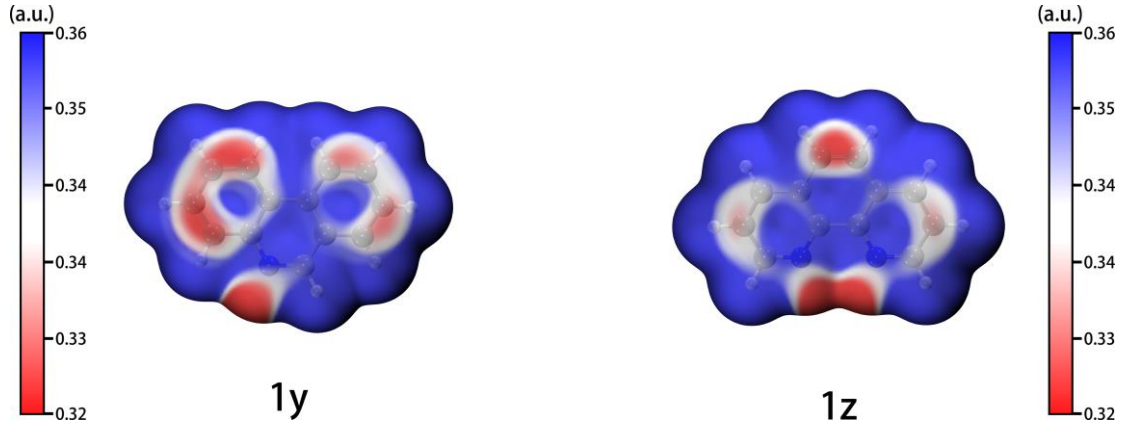

(a.u.)
0.36
0.35
0.34
0.34
0.33
0.32
1o
1p

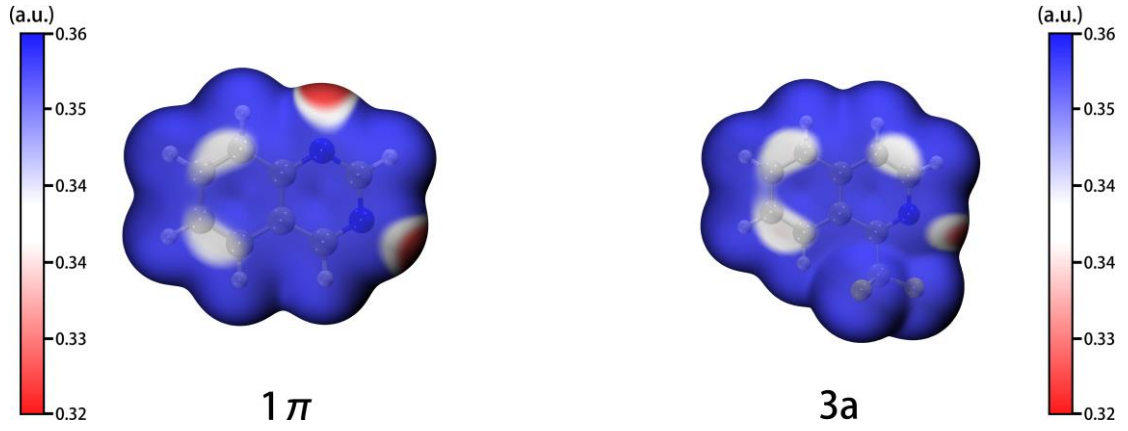

(a.u.)
0.36
0.35
0.34
0.34
0.33
0.32
1q
1r


(a.u.)
0.36
0.35
0.34
0.34
0.33
0.32
1s
1t


(a.u.)
0.36
0.35
0.34
0.34
0.33
0.32
1u
1v

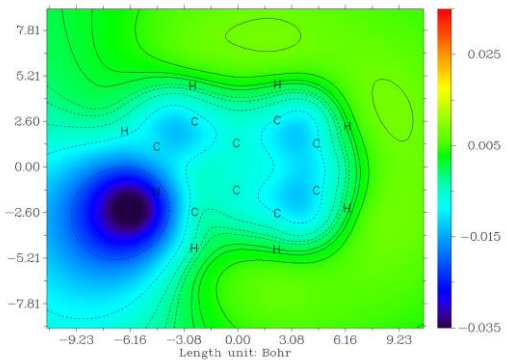

(a.u.)
0.36
0.35
0.34
0.34
0.33
0.32
1w
1x


(a.u.)
0.36
0.35
0.34
0.34
0.33
0.32
1y
1z

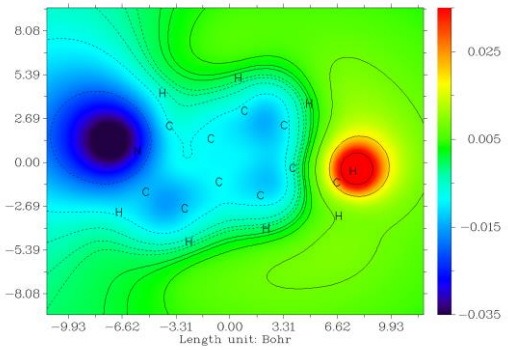

(a.u.)
0.36
0.35
0.34
0.34
0.33
0.32
1π
3a

3) Color-filled map with contour lines of total ESP (Electrostatic Potential) at 1.8 Å below the *N* ring plane[13]

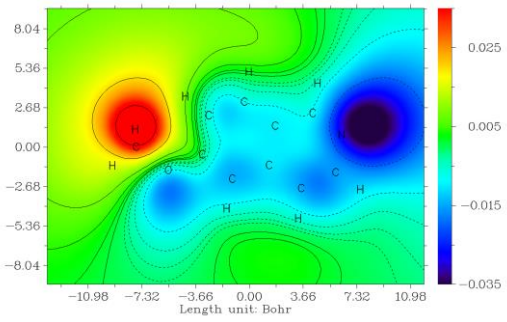
The molecule electrostatic potential V(***r***) is defined by the electronic density $\rho(\boldsymbol{r})$ and the charges and positions of nuclei, which are assumed by be fixed in space. This function measures the electrostatic interaction between a unit point charge placed at *r* and a positive (negative) value implies that current position is dominated by nuclear (electronic) charges.



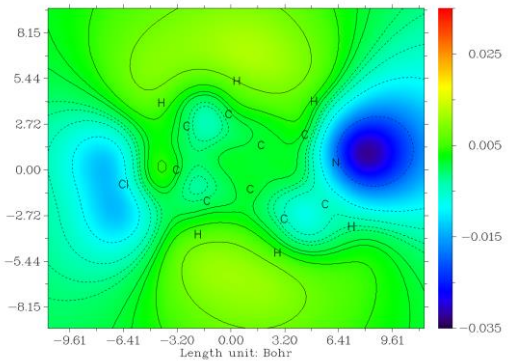
1a



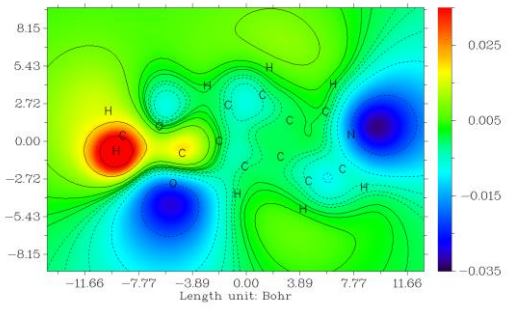
1b



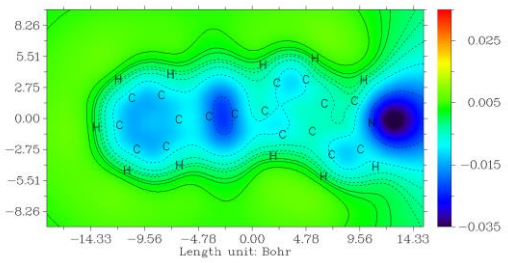
1c



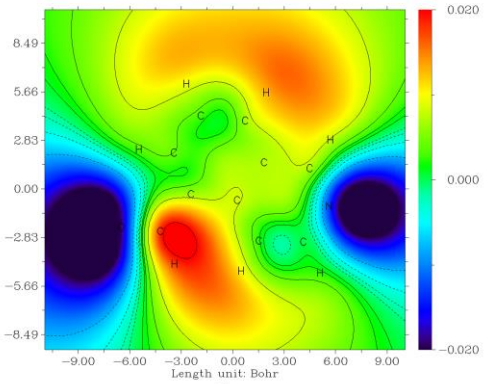
1d



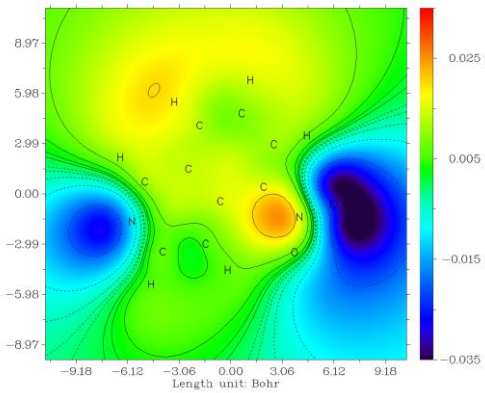
1e



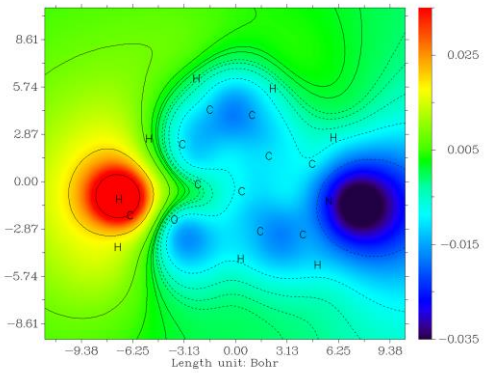
1f



1g



1h



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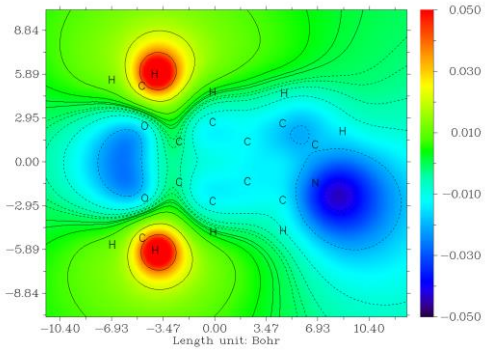
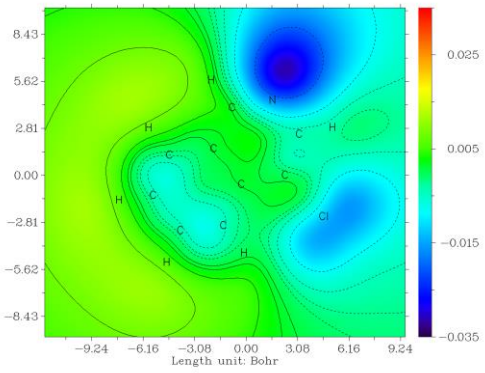


1j



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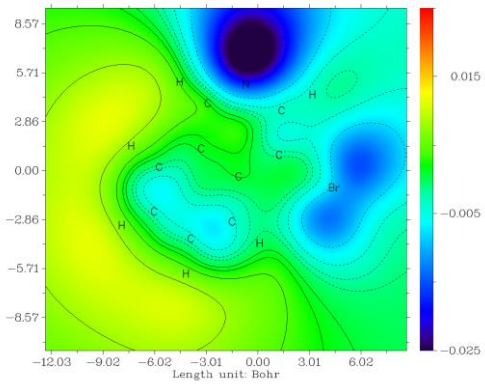
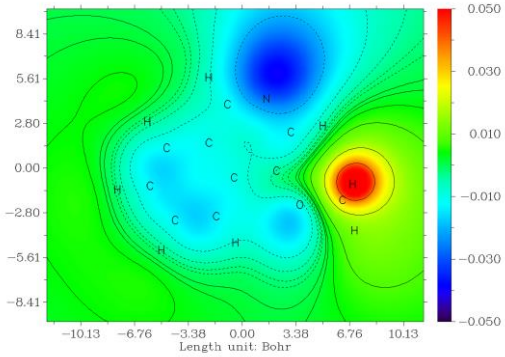


1l



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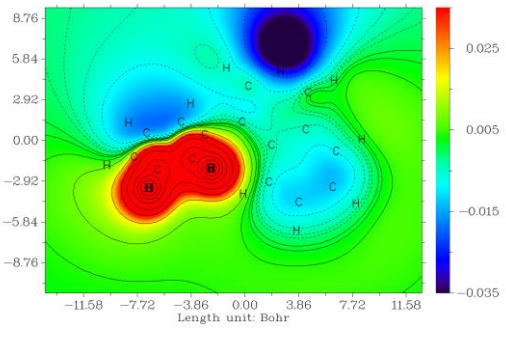

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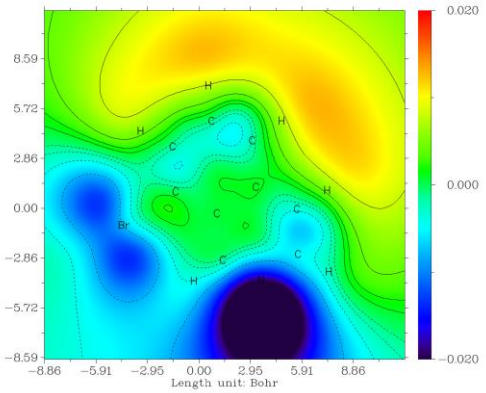
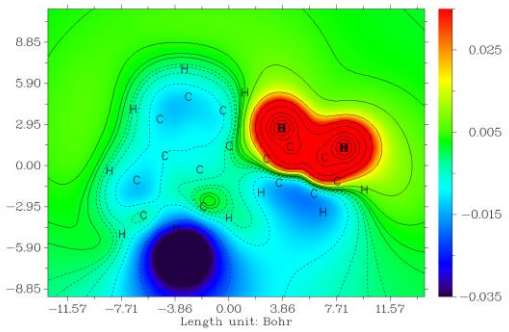
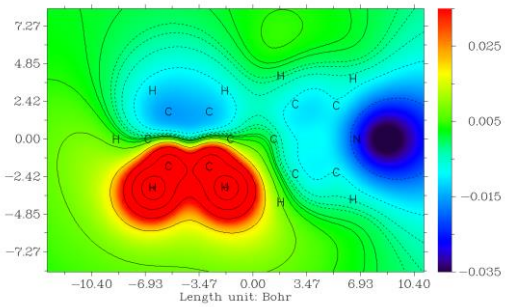


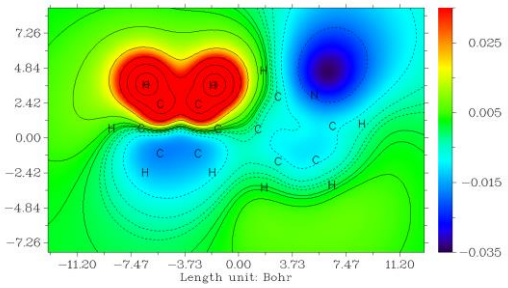
1o



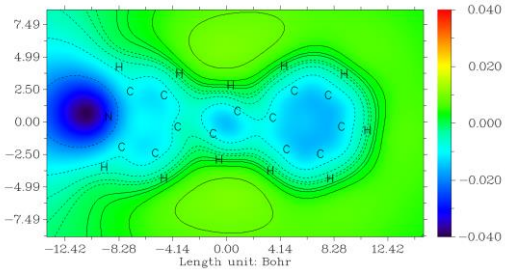
1p



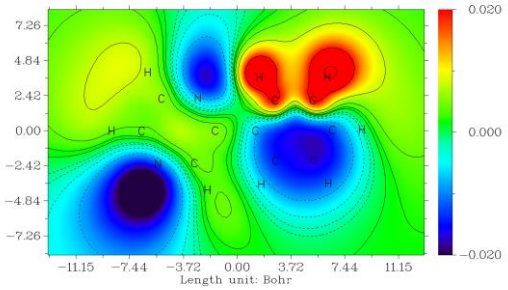
1q



1r



1s



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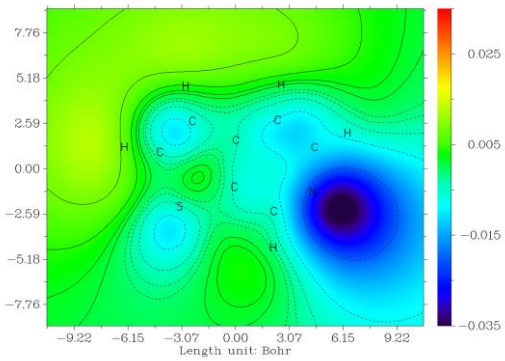
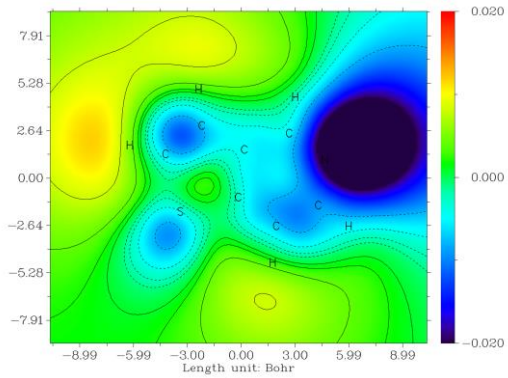
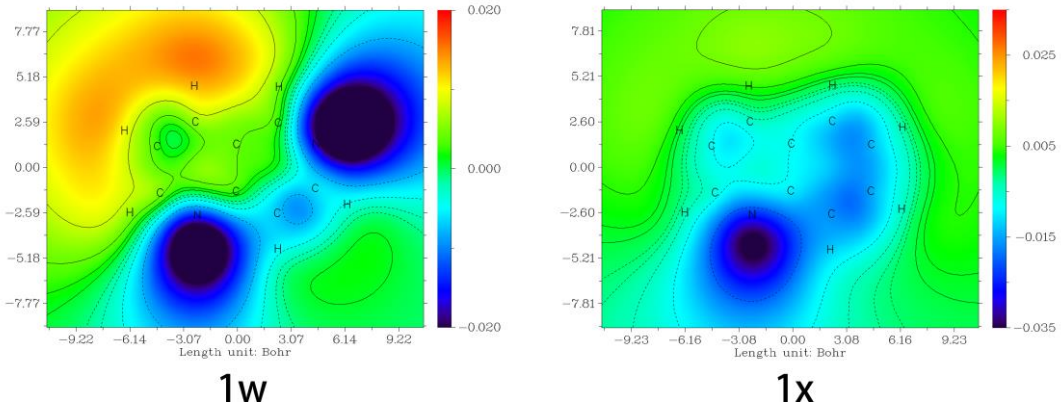


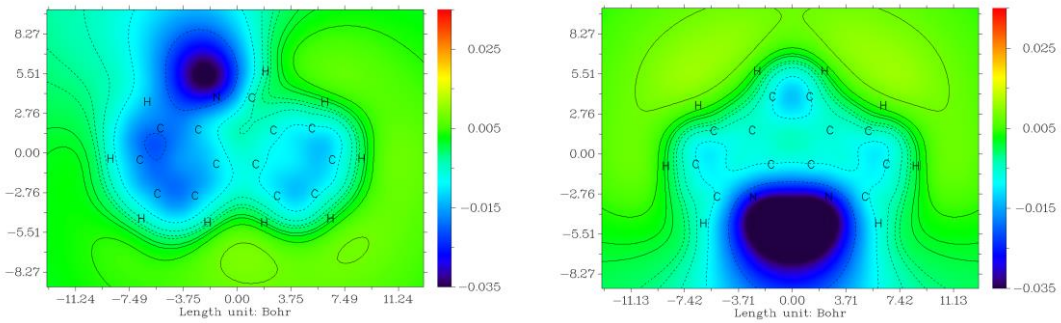
1u



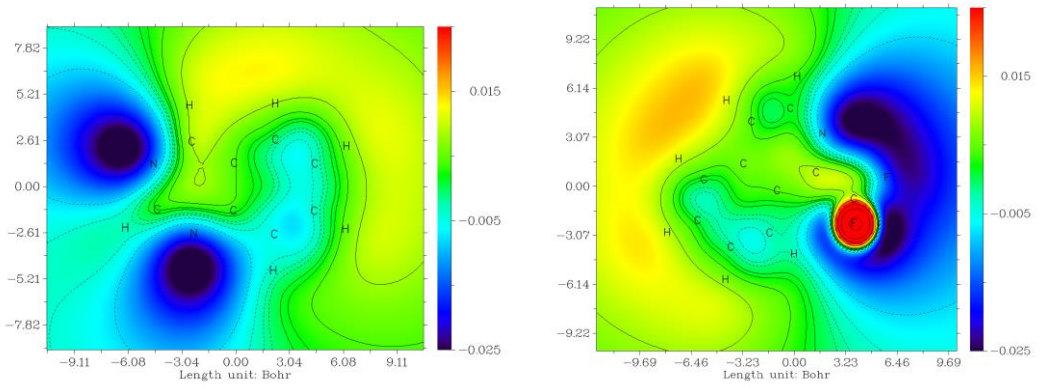
1v



1w 1x



1y 1z



1π 3a

4) NPA charges for prediction of products[14]

Population analysis was carried out on the basis of optimized structure with NBO 3.1 in Gaussian 16 program. The population analysis was performed on the *N* electron system, which values are per atom charge density. And these population values equivalent to their atomic partial charges. For example, the value of +0.10 in isoquinoline indicates a partial positive charge of 10% of a proton's charge, whereas the value of -0.22 indicates a partial negative charge of 22% of an electron's charge.

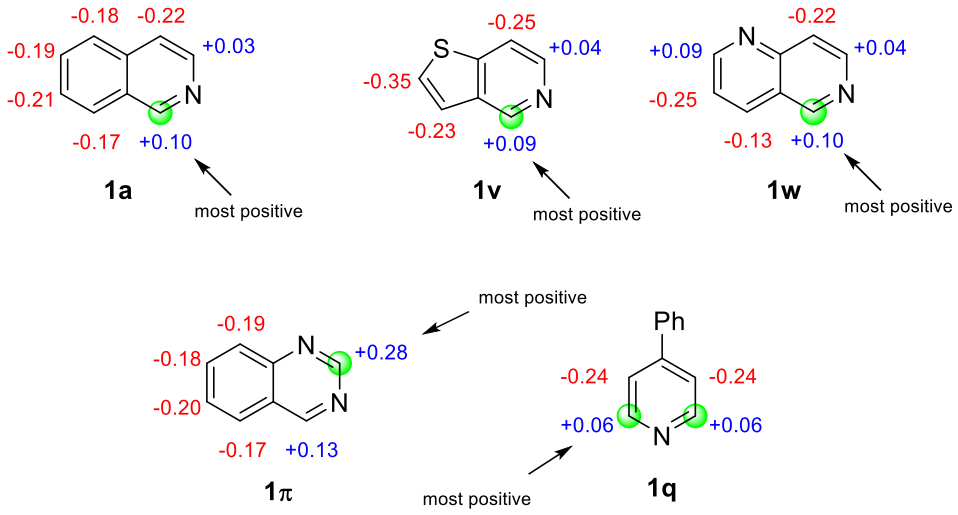


Figure S3. Partial charges distribution of *N*-heteroarenes.

We tried to conduct density functional theory (DFT) calculations to support our hypothesis for the high selective C-H trifluoromethylation of these electron-deficient substrates. The population analysis was performed on the N electron system, which values are per atom charge density. And these population values equivalent to their atomic partial charges. For example, the value of +0.10 in isoquinoline indicates a partial positive charge of 10% of a proton's charge, whereas the value of -0.22 indicates a partial negative charge of 22% of an electron's charge (Figure S1).

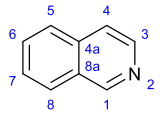
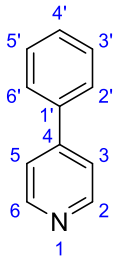
As with our calculated results in these electron-deficient heteroarenes, the most positive site of isoquinolines and pyridines are consistent with the regioselectivity observed in reaction. Therefore, the positive site identified on less electron rich N-heteroarenes via the partial charge analysis that are most reactive position toward attack by nucleophilic CF_3 radicals. All substrates (**1a-1π**) were computed and the regioselectivity of experimental observations that closely fits with partial charges distribution.

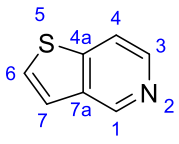
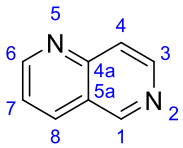
Population Analysis for 1a-1π

Atom: the corresponding atom in the numbering molecule;

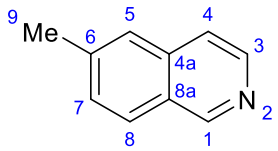
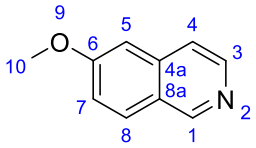
***ρ*(*N*):** the natural population for the *N* electron system calculated by NBO;

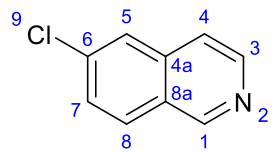
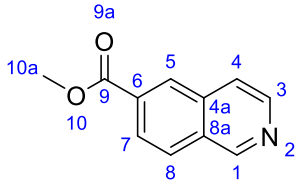
***δ*(*N*):** the partial charge $\delta(N)$ of every atom in the molecule with *N* electrons was calculated by subtracting $\rho(N)$ from the normal electron count of corresponding atom.

 1a			 1q		
Atom	***ρ*(*N*)**	***δ*(*N*)**	**Atom**	***ρ*(*N*)**	***δ*(*N*)**
1	5.90030	0.09970	1	7.45518	-0.45518
2	7.45351	-0.45351	2	5.94341	0.05659
3	5.96847	0.03153	3	6.23510	-0.23510
4	6.21894	-0.21894	4	6.01326	-0.01326
4a	6.04109	-0.04109	5	6.23510	-0.23510
5	6.18410	-0.18410	6	5.94341	0.05659
6	6.18522	-0.18522	1′	6.06307	-0.06307
7	6.10248	-0.20535	2′	6.18524	-0.18524
8	6.16572	-0.16572	3′	6.19666	-0.19666
8a	6.10248	-0.10248	4′	6.19877	-0.19877
			5′	-0.19666	-0.19666
			6′	-0.18524	-0.18524

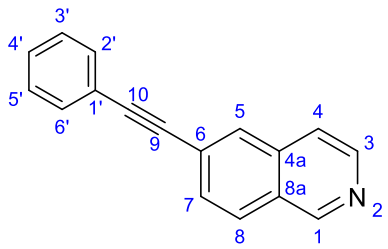
 1v			 1w		
Atom	***ρ*(*N*)**	***δ*(*N*)**	**Atom**	***ρ*(*N*)**	***δ*(*N*)**
1	5.91404	0.08596	1	5.90158	0.09842
2	7.45763	-0.45763	2	7.44892	-0.44892
3	5.95712	0.04288	3	5.96157	0.03843
4	6.25227	-0.25227	4	5.81700	-0.22321
4a	6.16230	-0.16230	4a	6.13661	0.18300

5	15.59713	0.40287	5	7.44564	-0.18410
6	6.35064	-0.35064	6	5.91260	0.08740
7	6.23483	-0.23483	7	6.25004	-0.25004
7a	6.13339	-0.13339	8	6.12837	-0.12837
			8a	6.13661	-0.13661

 **1b**			 **1c**		
Atom	***ρ*(*N*)**	***δ*(*N*)**	**Atom**	***ρ*(*N*)**	***δ*(*N*)**
1	5.90100	0.09900	1	5.89622	0.10378
2	7.45763	-0.45763	2	7.46509	-0.46509
3	5.96767	0.03233	3	5.96605	0.03395
4	6.22109	-0.22109	4	6.22683	-0.22683
4a	6.03135	-0.03135	4a	6.23590	-0.23590
5	6.19188	-0.19188	5	6.02489	-0.02489
6	6.01148	-0.01148	6	6.23590	-0.23590
7	6.20263	-0.20263	7	5.66000	0.34000
8	6.15842	-0.15842	8	6.27812	-0.27812
8a	6.10735	-0.10735	8a	6.14472	-0.14472
9	6.59051	-0.59051	4a	6.12285	-0.12285
			9	8.53697	-0.53697
			10	6.20893	-0.20893

 **1d**	 **1e**

Atom	$\rho(N)$	$\delta(N)$	Atom	$\rho(N)$	$\delta(N)$
1	5.89773	0.10227	1	5.90278	0.09722
2	7.45165	-0.45165	2	7.44422	-0.44422
3	5.96206	0.03794	3	5.96866	0.03134
4	6.22006	-0.22006	4	6.20905	-0.20905
4a	6.02689	-0.02689	4a	6.05200	-0.05200
5	6.21255	-0.21255	5	6.11456	-0.11456
6	6.02219	-0.02219	6	6.14769	-0.14769
7	6.22586	-0.22586	7	6.17500	-0.17500
8	6.14827	-0.14827	8	6.16661	-0.16661
8a	6.10619	-0.10619	8a	6.08882	-0.08882
9	16.98845	0.01155	9	5.20246	0.79754
			9a	8.59691	-0.59691
			10	6.21341	-0.21341



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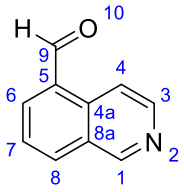
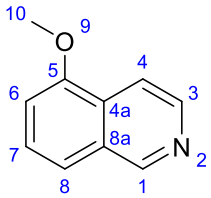


1g

Atom	$\rho(N)$	$\delta(N)$	Atom	$\rho(N)$	$\delta(N)$
1	5.90236	0.09764	1	5.89748	0.10252
2	7.45236	-0.45236	2	7.44830	-0.44830
3	5.96714	0.03286	3	5.95397	0.04603
4	6.21723	-0.21723	4	6.22953	-0.22953
4a	6.04632	-0.04632	4a	6.01377	-0.01377
5	6.13425	-0.13425	5	6.15538	-0.15538
6	6.13654	-0.13654	6	6.11801	-0.11801

7	6.16953	-0.16953	7	6.20911	-0.20911
8	6.16408	-0.16408	8	6.13667	-0.13667
8a	6.09918	-0.09918	8a	6.09248	-0.09248
9	5.91376	0.08624	9	5.58486	0.41514
10	6.01913	-0.01913	10	8.52986	-0.52986
1’	6.14697	-0.14697			
2’	6.14715	-0.14715			
3’	6.21068	-0.21068			
4’	6.19365	-0.19365			
5’	6.21067	-0.21067			
6’	6.14724	-0.14724			



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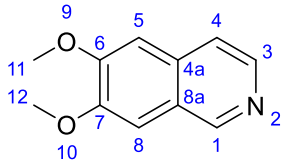
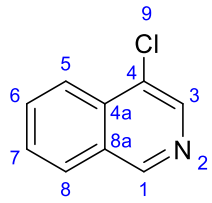
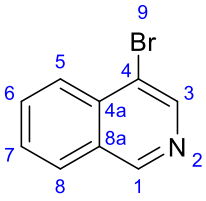
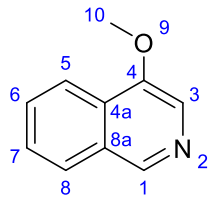
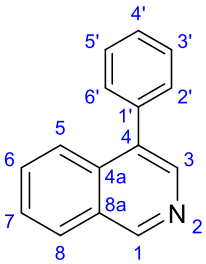


1j

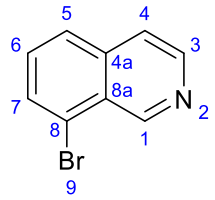
Atom	***ρ*(*N*)**	***δ*(*N*)**	**Atom**	***ρ*(*N*)**	***δ*(*N*)**
1	5.90419	0.09581	1	5.91354	0.08646
2	7.45184	-0.45184	2	7.46205	-0.46205
3	5.96996	0.03004	3	5.97447	0.02553
4	6.21466	-0.21466	4	6.22715	-0.22715
4a	6.06937	-0.06937	4a	6.03557	-0.03557
5	5.65258	0.34742	5	6.28203	-0.28203
6	6.28912	-0.28912	6	5.67573	0.32427
7	6.18433	-0.18433	7	5.69692	0.30308
8	6.20031	-0.20031	8	6.25641	-0.25641
8a	6.08972	-0.08972	8a	6.10277	-0.10277
9	8.53922	-0.53922	9	8.51829	-0.51829
10	6.20722	-0.20722	10	8.52201	-0.52201

			11	6.20892	-0.20892
			12	6.20851	-0.20851

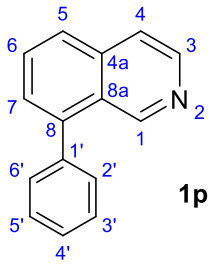
 1k			 1l		
Atom	***ρ*(*N*)**	***δ*(*N*)**	**Atom**	***ρ*(*N*)**	***δ*(*N*)**
1	5.90321	0.09679	1	5.90151	0.09849
2	7.43854	-0.43854	2	7.43825	-1.43825
3	5.98866	0.01134	3	5.98953	0.01047
4	6.04988	-0.04988	4	6.11318	-0.11318
4a	6.06780	-0.06780	4a	6.07168	-0.07168
5	6.18510	-0.18510	5	6.18429	-0.18429
6	6.17651	-0.17651	6	6.17594	-0.17594
7	6.20048	-0.20048	7	6.20027	-0.20027
8	6.16370	-0.16370	8	6.16378	-0.16378
8a	6.09013	-0.09013	8a	6.08944	-0.08944
9	16.99133	0.00867	9	34.92886	0.07114

 1m			 1n		
Atom	***ρ*(*N*)**	***δ*(*N*)**	**Atom**	***ρ*(*N*)**	***δ*(*N*)**
1	5.92859	0.07141	1	5.90690	0.09310
2	7.43851	-0.43851	2	7.44797	-0.44797
3	6.06732	-0.06732	3	5.95229	0.04771

4	5.68477	0.31523	4	6.06670	-0.06670
4a	6.07128	-0.07128	4a	6.02412	-0.02412
5	6.17994	-0.17994	5	6.19263	-0.19263
6	6.18809	-0.18809	6	6.18347	-0.18347
7	6.20284	-0.20284	7	6.20450	-0.20450
8	6.16867	-0.16867	8	6.17132	-0.17132
8a	6.09095	-0.09095	8a	6.08567	-0.08567
9	8.54047	-0.54047	1′	6.05553	-0.05553
10	6.20708	-0.20708	2′	6.18947	-0.18947
			3′	6.19725	-0.19725
			4′	6.20341	-0.20341
			5′	6.19929	-0.19929
			6′	6.19342	-0.19342



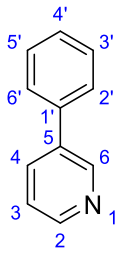
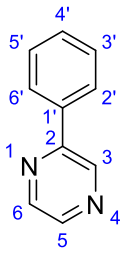
1m

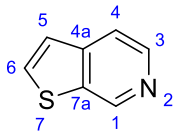


1p

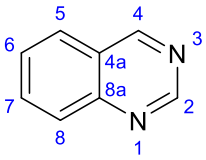
Atom	***ρ*(*N*)**	***δ*(*N*)**	**Atom**	***ρ*(*N*)**	***δ*(*N*)**
1	5.89955	0.10045	1	5.90442	0.09558
2	7.44503	-0.44503	2	7.45340	-0.45340
3	5.96303	0.03697	3	5.96712	0.03288
4	6.21682	-0.21682	4	6.21899	-0.21899
4a	6.02777	-0.02777	4a	6.03676	-0.03676
5	6.18334	-0.18334	5	6.18595	-0.18595
6	6.17404	-0.17404	6	6.18001	-0.18001
7	6.22894	-0.22894	7	6.19303	-0.19303
8	6.06253	-0.06253	8	5.96712	0.03288

8a	6.13469	-0.13469	8a	6.09241	-0.09241
9	34.92659	0.07341	1′	6.05781	-0.05781
			2′	6.19200	-0.19200
			3′	6.19760	-0.19760
			4′	6.20224	-0.20224
			5′	6.19717	-0.19717
			6′	6.19069	-0.19069

 **1r**			 **1t**		
Atom	***ρ*(*N*)**	***δ*(*N*)**	**Atom**	***ρ*(*N*)**	***δ*(*N*)**
1	7.44753	-0.44753	1	7.42834	-0.42834
2	5.95271	0.04729	2	5.83179	0.16821
3	6.23845	-0.23845	3	5.96692	0.03308
4	6.15731	-0.15731	4	7.41172	-0.41172
5	6.08656	-0.08656	5	5.99717	0.00283
6	5.93186	0.06814	6	5.97618	0.02382
1′	6.05731	-0.05731	1′	6.08274	-0.08274
2′	6.18884	-0.18884	2′	6.18373	-0.18373
3′	6.19621	-0.19621	3′	6.20116	-0.20116
4′	6.20255	-0.20255	4′	6.19351	-0.19351
5′	6.19682	-0.19682	5′	6.19890	-0.19890
6′	6.19033	-0.19033	6′	6.16847	-0.16847

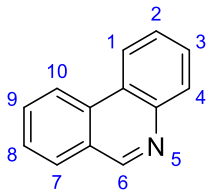


1u

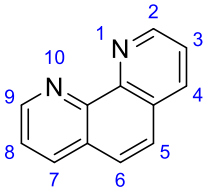


1π

Atom	$\rho(N)$	$\delta(N)$	Atom	$\rho(N)$	$\delta(N)$
1	5.94691	0.05309	1	7.46438	-0.46438
2	7.45208	-0.45208	2	5.72317	0.27683
3	5.96452	0.03548	3	7.47978	-0.47978
4	6.22198	-0.22198	4	5.86913	0.13087
4a	6.06851	-0.06851	4a	6.13608	-0.13608
5	6.24644	-0.24644	5	6.16783	-0.16783
6	6.33960	-0.33960	6	6.20043	-0.20043
7	15.59343	0.40657	7	6.17785	-0.17785
7a	6.22406	-0.22406	8	6.18928	-0.18928
			8a	5.81890	0.18110



3y



3z

Atom	$\rho(N)$	$\delta(N)$	Atom	$\rho(N)$	$\delta(N)$
1	6.18638	-0.18638	1	7.41513	-0.41513
2	6.19371	-0.19371	2	5.93152	0.06848
3	6.20018	-0.20018	3	6.24004	-0.24004
4	6.17897	-0.17897	4	6.14608	-0.14608
5	7.44619	-0.44619	5	6.17525	-0.17525
6	5.87413	0.12587	6	6.17462	-0.17462
7	6.15246	-0.15246	7	6.14602	-0.14602
8	6.21332	-0.21332	8	6.24003	-0.24003

9	6.18033	-0.18033	9	5.93160	0.06840
10	6.18463	-0.18463	10	7.41651	-0.41651

Cartesian coordinates for the optimized structures

1a

C	-1.26737808	-1.35866773	-0.00000015
C	-0.00843699	-0.69843430	-0.00000005
C	-0.00995714	0.72728619	0.00000005
C	-1.27146137	1.37378550	0.00000007
C	-2.41774306	0.61788459	0.00000000
H	1.21573165	-2.48276411	-0.00000013
H	-1.29020911	-2.44725695	-0.00000019
C	1.22451463	-1.39775057	-0.00000005
C	1.23197216	1.41347333	0.00000012
H	-1.32810763	2.45688295	0.00000014
H	-3.39397250	1.09198532	0.00000000
C	2.41305176	0.70980910	0.00000011
C	2.41236002	-0.70649343	0.00000002
H	1.23638025	2.49822341	0.00000019
H	3.35520889	-1.24125709	0.00000000
N	-2.42786576	-0.74312417	-0.00000011
H	3.35849720	1.24069942	0.00000016

1b

C	-1.93435052	1.18965880	0.00000006
C	-0.57782009	0.77114701	-0.00000011
C	-0.31405162	-0.62830138	-0.00000022
C	-1.43470082	-1.49578778	-0.00000015
C	-2.70129981	-0.96360565	0.00000010
H	0.31203035	2.74494950	-0.00000027
H	-2.15672677	2.25558561	0.00000063
C	0.51196087	1.67834006	-0.00000012
C	1.03278771	-1.07522959	0.00000003
H	-1.29176899	-2.57097252	-0.00000008
H	-3.57282793	-1.61054415	0.00000031
C	2.08361819	-0.18413577	0.00000029
C	1.80198283	1.21188781	0.00000000
H	1.22756719	-2.14327617	-0.00000000
H	2.62979700	1.91379555	-0.00000015
N	-2.96335250	0.37117622	0.00000003
C	3.51704783	-0.65166731	0.00000001
H	4.05085965	-0.28028653	-0.88054185
H	4.05085953	-0.28028701	0.88054218
H	3.58263016	-1.74103499	-0.00000033

1c

C	2.31005743	1.22871681	-0.00000011
C	0.96710153	0.76675689	-0.00000000
C	0.74347381	-0.64319562	0.00000005
C	1.89657112	-1.47321196	0.00000011
C	3.14232397	-0.89900502	0.00000012
H	0.01875329	2.70899220	-0.00000014

H	2.49620037	2.30181376	0.00000008
C	-0.14674035	1.63661641	0.00000000
C	-0.57812696	-1.13417574	-0.00000012
H	1.79009439	-2.55237237	0.00000025
H	4.03420032	-1.51760688	0.00000018
C	-1.64910517	-0.25999995	-0.00000001
C	-1.43073823	1.14323161	0.00000006
H	-0.77048092	-2.20064205	-0.00000052
H	-2.26671979	1.82924831	-0.00000000
N	3.36464322	0.44585691	-0.00000005
O	-2.88864312	-0.82464277	-0.00000026
C	-4.03834731	0.01416959	0.00000011
H	-4.07561847	0.64365446	-0.89510293
H	-4.89298855	-0.66001735	0.00000167
H	-4.07561718	0.64365552	0.89510269

1d

C	2.36452497	1.11963956	-0.00020374
C	0.98451131	0.78302075	-0.00014588
C	0.63954527	-0.59957956	0.00011924
C	1.70545704	-1.53384640	0.00030614
C	3.00044653	-1.07660736	0.00022570
H	0.22079449	2.80932909	-0.00054126
H	2.65022950	2.17011599	-0.00040381
C	-0.04427323	1.75746806	-0.00033951
C	-0.72881938	-0.97255317	0.00018353
H	1.49838654	-2.59813392	0.00051068
H	3.83218993	-1.77361949	0.00036500
C	-1.69138400	0.00515216	-0.00001069
C	-1.36473278	1.38156889	-0.00027451
H	-1.00570694	-2.01948031	0.00038438
H	-2.15796897	2.11776877	-0.00042107
N	3.34091839	0.24064736	-0.00002744
Cl	-3.38917692	-0.44565231	0.00006686

1e

C	3.08371454	1.14632587	0.00000005
C	1.70326963	0.80703091	0.00000020
C	1.36446620	-0.57725583	-0.00000008
C	2.43202263	-1.51030971	-0.00000049
C	3.72595735	-1.05116901	-0.00000055
H	0.93632991	2.83055592	0.00000077
H	3.36857754	2.19697581	0.00000035
C	0.67109559	1.77864270	0.00000058
C	-0.00133808	-0.94791516	0.00000004
H	2.22460426	-2.57453332	-0.00000075
H	4.56061097	-1.74447892	-0.00000089
C	-0.98841328	0.01555049	0.00000040
C	-0.64660808	1.39538558	0.00000065
H	-0.28377099	-1.99415750	-0.00000021
H	-1.43692466	2.13354420	0.00000090
N	4.06056808	0.26818143	-0.00000027
C	-2.40942933	-0.44627982	0.00000040
O	-2.75356359	-1.60573903	0.00000162
O	-3.28213799	0.58278592	-0.00000117
C	-4.67675378	0.22464346	-0.00000100
H	-5.21768500	1.16823187	-0.00000263
H	-4.91900285	-0.35884133	-0.88905527

H	-4.91900339	-0.35883857	0.88905493

1f

C	4.86135235	0.82981806	0.00000000
C	3.44639325	0.71644905	0.00000000
C	2.88539321	-0.59405804	0.00000000
C	3.79162927	-1.68541012	0.00000000
C	5.14264737	-1.43996710	0.00000000
H	3.01214322	2.83752020	-0.00000100
H	5.31004239	1.82178113	0.00000000
C	2.58237719	1.84130013	0.00000000
C	1.47919411	-0.74302006	0.00000000
H	3.41814025	-2.70348419	0.00000100
H	5.85365644	-2.25987116	0.00000100
C	0.64670705	0.36708503	0.00000000
C	1.22266409	1.67609512	0.00000000
H	1.04822608	-1.73741213	0.00000000
H	0.56176004	2.53403218	-0.00000100
N	5.68732740	-0.19301601	0.00000000
C	-0.76752505	0.22051002	0.00000000
C	-1.97341414	0.10899401	0.00000000
C	-3.38976625	-0.02770000	0.00000000
C	-4.21888430	1.10935508	0.00000000
C	-3.98579529	-1.30250010	-0.00000100
H	-3.76628127	2.09357515	0.00000100
C	-5.60200440	0.97090707	0.00000000
C	-5.36984937	-1.43144210	-0.00000100
H	-6.22923645	1.85514013	0.00000100
C	-6.18262244	-0.29760302	0.00000000
H	-7.26155754	-0.40187203	0.00000000
H	-5.81615344	-2.41942217	-0.00000100
H	-3.35300124	-2.18175216	-0.00000100

1g

C	2.40770852	0.63997664	0.00000025
C	0.99733309	0.81979755	0.00000006
C	0.16658358	-0.34282406	-0.00000022
C	0.83830795	-1.59365788	-0.00000037
C	2.21195265	-1.62981388	-0.00000012
H	1.06771611	2.97766165	0.00000034
H	3.04725156	1.52095229	0.00000058
C	0.41616407	2.10996263	0.00000009
C	-1.25452127	-0.15862611	-0.00000039
H	0.29292178	-2.52752732	-0.00000068
H	2.73351634	-2.58147339	-0.00000005
C	-0.95202057	2.26043492	-0.00000018
H	-1.39585655	3.24888747	-0.00000015
N	3.00669347	-0.52743390	0.00000045
C	-1.77928724	1.12347601	-0.00000039
H	-2.85813321	1.22881166	-0.00000057
C	-2.20259055	-1.30015749	-0.00000030
O	-3.40946215	-1.17947501	0.00000104
H	-1.75635448	-2.31088497	-0.00000162

1h

C	0.37368884	2.53911098	0.07633228
C	-0.94623144	2.15718558	0.06789978
C	-1.30042845	0.78807387	0.02120761

C	-0.29619093	-0.23103708	0.00315539
C	1.05806590	0.22133289	0.01714223
C	1.38254669	1.55886867	0.03859455
H	-3.43413722	1.15405131	-0.00012013
H	0.64883563	3.58586944	0.11070622
H	-1.73631865	2.90000764	0.09287860
C	-2.66380626	0.38530945	-0.01672323
C	-0.75407760	-1.57176694	-0.06524118
H	2.42681849	1.84058761	0.03091745
C	-2.10570616	-1.81974260	-0.10354868
H	-0.05526457	-2.39312926	-0.07396424
H	-2.46710399	-2.84140806	-0.15616867
N	2.19532712	-0.72302128	0.00964078
O	3.25503757	-0.32730293	-0.46023489
O	2.02430568	-1.83828017	0.48869066
N	-3.06743272	-0.86059628	-0.07604191

1i

C	2.49384824	0.56503646	0.00000058
C	1.09582710	0.82020190	0.00000016
C	0.22958819	-0.30814581	-0.00000042
C	0.82025495	-1.59331048	-0.00000061
C	2.19088959	-1.69995438	-0.00000026
H	1.23106879	2.98446331	0.00000079
H	3.17946025	1.41064727	0.00000122
C	0.55899148	2.13382221	0.00000028
C	-1.18403213	-0.08872875	-0.00000082
H	0.19574877	-2.47665128	-0.00000098
H	2.66882167	-2.67429972	-0.00000008
C	-0.80105681	2.30731084	-0.00000024
H	-1.22417109	3.30540082	-0.00000024
N	3.03319405	-0.63358940	0.00000075
C	-1.68219085	1.19750340	-0.00000082
H	-2.74859053	1.37800794	-0.00000143
O	-1.94288267	-1.21800859	-0.00000145
C	-3.35925543	-1.08743122	0.00000193
H	-3.75105564	-2.10297573	0.00000412
H	-3.70888029	-0.56161039	0.89465293
H	-3.70888486	-0.56161267	-0.89464867

1j

C	2.45823864	-1.35340373	0.00000015
C	1.20384450	-0.69512500	0.00000055
C	1.20351003	0.72567926	0.00000038
C	2.46098900	1.37350652	-0.00000019
C	3.61174030	0.61894395	-0.00000059
H	-0.01075175	-2.48035033	0.00000124
H	2.48240818	-2.44212376	0.00000027
C	-0.03166946	-1.39830538	0.00000107
C	-0.03925530	1.41431985	0.00000062
H	2.51700612	2.45685307	-0.00000036
H	4.58604929	1.09746910	-0.00000108
C	-1.22496670	-0.71975704	0.00000129
N	3.62325240	-0.73778376	-0.00000043
C	-1.22735472	0.72203917	0.00000098
O	-2.45819622	1.28415739	0.00000105
O	-2.45525080	-1.28923317	0.00000178
H	-0.03238299	2.49618646	0.00000043

C	-2.55402927	2.70326683	0.00000045
H	-3.61931872	2.92614678	0.00000035
H	-2.09056232	3.13223842	0.89465376
H	-2.09056230	3.13223764	-0.89465322
C	-2.53733437	-2.70845434	0.00000144
H	-2.06953577	-3.13361093	-0.89452197
H	-2.06953491	-3.13361147	0.89452415
H	-3.60027915	-2.94260145	0.00000189

1k

C	-0.41962186	2.15632804	-0.00000455
C	-0.99828612	0.85978086	-0.00000130
C	-0.12592634	-0.27176266	-0.00000037
C	1.26437564	0.01888209	0.00000011
C	1.70943401	1.31843252	0.00000223
H	-3.05433052	1.52397717	0.00000032
H	-1.07316286	3.02616852	0.00000307
C	-2.40112569	0.65796432	0.00000049
C	-0.68981849	-1.57209131	-0.00000009
H	2.77173979	1.53424590	0.00000177
C	-2.92090850	-0.61350520	0.00000084
N	0.87305934	2.38634603	0.00000200
C	-2.05560426	-1.73257415	0.00000049
H	-0.03522636	-2.43359139	0.00000009
H	-2.47741998	-2.73125883	0.00000104
H	-3.99399642	-0.76534713	0.00000125
Cl	2.44563945	-1.28160844	-0.00000050

1l

C	-1.51344826	2.08646029	0.00000100
C	-1.71945529	0.68197345	0.00000026
C	-0.57266283	-0.17231809	0.00000009
C	0.68695427	0.48529399	0.00000004
C	0.76331078	1.85703571	-0.00000037
H	-3.87790006	0.77033252	-0.00000010
H	-2.37835132	2.74663683	-0.00000069
C	-3.01656826	0.11090978	-0.00000015
C	-0.76974643	-1.57600580	0.00000005
H	1.72479502	2.35703864	-0.00000041
C	-3.17650672	-1.25318047	-0.00000018
N	-0.33189210	2.65841705	-0.00000048
C	-2.04204078	-2.09779706	-0.00000010
H	0.09189085	-2.23044360	0.00000006
H	-2.17913076	-3.17321251	-0.00000017
H	-4.16936724	-1.68765374	-0.00000027
Br	2.32206541	-0.51788138	0.00000003

1m

C	-0.23241638	-0.31288042	0.00000023
C	-0.82151366	-1.60066234	0.00000032
C	-1.06821779	0.83836678	0.00000008
C	-2.19184519	-1.73027771	0.00000025
H	-0.18029075	-2.47221770	0.00000044
C	1.17826706	-0.09261555	0.00000035
C	-2.47510909	0.67103654	0.00000001
C	-0.44772727	2.11889307	0.00000002
C	-3.02645442	-0.58867847	0.00000011
H	-2.63961987	-2.71776884	0.00000033

C	1.65743042	1.20161380	0.00000026	C	-1.48357991	0.23072402	-0.03463054
O	1.95083087	-1.21218633	0.00000049	C	-2.37330067	0.71353884	0.93440700
H	-3.10837567	1.55192706	-0.00000010	C	-1.96214646	-0.68178244	-0.98613017
N	0.85036307	2.29697635	0.00000010	C	-3.70208428	0.29374819	0.95507995
H	-1.07004395	3.01129089	-0.00000011	H	-2.01562373	1.41303500	1.68171706
H	-4.10346654	-0.71225176	0.00000009	C	-3.29045466	-1.09932293	-0.96681140
H	2.72003415	1.40937522	0.00000030	H	-1.29344868	-1.04936493	-1.75646645
C	3.36665215	-1.05937474	0.00000214	C	-4.16486213	-0.61448005	0.00530457
H	3.70722648	-0.52765979	-0.89431932	H	-4.37409688	0.67506019	1.71584300
H	3.70722425	-0.52765866	0.89432376	H	-3.64474109	-1.79831190	-1.71633974
H	3.77374422	-2.06890457	0.00000327	H	-5.19865124	-0.94059285	0.02023664

1n

C	2.44115601	1.82987616	-0.20590587
C	2.34755205	0.42201463	-0.05031244
C	1.04755546	-0.16260459	0.03080775
C	-0.07721126	0.71619329	-0.07230899
C	0.17083518	2.06854711	-0.21354170
H	4.47889936	0.06275863	-0.02444941
H	3.42584341	2.29022605	-0.26613622
C	3.49940461	-0.39895579	0.04456049
C	0.95381295	-1.56475739	0.23972918
H	-0.66182630	2.75955957	-0.30009254
C	3.37438076	-1.75435036	0.22816212
N	1.40411345	2.63133618	-0.27790130
C	2.08909034	-2.33561521	0.33414621
H	-0.02176613	-2.02352373	0.33522991
H	2.00002026	-3.40382508	0.49817035
H	4.25570892	-2.38101506	0.30225943

1o

C	0.75471263	-1.56843604	-0.00000034
C	0.57981120	-0.15617469	-0.00000000
C	1.76042193	0.65124532	0.00000005
C	3.00715309	-0.02196700	0.00000008
C	3.03831670	-1.39336827	0.00000025
H	-0.12136573	-2.20839338	0.00000024
C	-0.67831943	0.50592814	0.00000012
C	1.64801804	2.06455856	-0.00000002
H	3.98246394	-1.92831469	-0.00000024
C	-0.76812247	1.87593062	0.00000000
N	1.92325326	-2.16960183	-0.00000009
C	0.41037514	2.65770587	-0.00000007
H	2.55041351	2.66547125	-0.00000007
H	0.32087846	3.73796851	-0.00000019
H	-1.73695741	2.35802916	-0.00000008
H	3.92815977	0.55030995	-0.00000011

Br	-2.31144475	-0.50515409	0.00000002	H	5.18565339	-0.91775199	0.00014790

1p

C	-0.92802438	-1.55217782	-0.25379323	C	2.87256893	1.13762076	0.00569721
C	-1.05622394	-0.15065377	-0.03335302	C	1.48184802	1.19171077	0.00602602
C	-2.38367833	0.37134530	0.04765074	C	0.74587625	-0.00000011	0.00000003
C	-3.45781548	-0.54857376	-0.04813684	C	1.48184799	-1.19171102	-0.00602610
C	-3.19379488	-1.88192668	-0.23258241	C	2.87256889	-1.13762105	-0.00569758
H	0.06193373	-1.98229330	-0.36607496	N	3.57442224	-0.00000015	-0.00000024
C	0.06232101	0.73941199	0.06456358	C	-0.73775617	-0.00000009	0.00000018
C	-2.57895755	1.76664038	0.20329976	C	-1.45587840	-0.93207738	-0.76311031
H	-4.00080216	-2.60395738	-0.30680333	C	-1.45587819	0.93207722	0.76311084
C	-0.18105994	2.09374251	0.19725497	C	-2.84803449	-0.93046774	-0.76498214
N	-1.93849771	-2.38910898	-0.34960552	C	-2.84803429	0.93046764	0.76498299
C	-1.49524232	2.60707895	0.26565451	C	-3.54959388	-0.00000004	0.00000049
H	-3.58927580	2.15582328	0.26708332	H	3.45217335	2.05671348	0.00345495
H	-1.64046002	3.67541387	0.38144699	H	0.98091647	2.15238226	-0.01375261
H	0.65836985	2.77501187	0.27809946	H	0.98091641	-2.15238250	0.01375267
H	-4.48057812	-0.19363314	0.01768042	H	3.45217329	-2.05671378	-0.00345537
C	1.47010922	0.25077852	0.03412738	H	-0.92035437	-1.64624584	-1.37821983
C	2.36284395	0.72868145	-0.93450507	H	-0.92035401	1.64624566	1.37822024
C	1.94533657	-0.65536088	0.99281299	H	-3.38517873	-1.65226682	-1.36998210
C	3.69163333	0.30938498	-0.94827138	H	-3.38517837	1.65226674	1.36998306
H	2.00689875	1.42157174	-1.68885483	H	-4.63361525	-0.00000002	0.00000061
C	3.27450848	-1.07063479	0.98178731				
H	1.27355989	-1.02191540	1.76081585	**1r**			
C	4.15188750	-0.59147323	0.00991874	C	1.48655174	1.52292495	0.05958294
H	4.36543276	0.68395502	-1.71080471	C	0.75239987	0.32609139	0.05841169
H	3.62569233	-1.76604071	1.73593424	C	1.48945072	-0.86390227	0.06878197

C	2.87836046	-0.80840254	0.07355225
C	-0.73041620	0.33392840	0.05143175
C	-1.45768216	-0.56518406	0.84539164
C	-1.44119385	1.24141742	-0.74789874
C	-2.84985544	-0.55782747	0.83988900
C	-2.83360547	1.24912844	-0.75257559
C	-3.54367932	0.34977169	0.04098162
C	3.49775449	0.43937759	0.06277544
N	2.81858637	1.59032335	0.05848690
H	0.96344954	2.47491927	0.08081711
H	0.97861765	-1.82028245	0.05117613
H	3.47312388	-1.71438831	0.07327525
H	-0.92871615	-1.25880192	1.48952278
H	-0.89979339	1.92920833	-1.38747638
H	-3.39319033	-1.25579582	1.46707222
H	-3.36413897	1.95343969	-1.38354694
H	-4.62767222	0.35597678	0.03697832
H	4.58090655	0.52009393	0.05749874

1s

C	-4.21781230	-1.00668707	0.00000000
C	-3.87906928	1.24285309	0.00000000
C	-2.49836618	1.09572508	0.00000000
C	-1.93966414	-0.19347601	0.00000000
C	-2.84976020	-1.26145809	0.00000000
H	-4.92497235	-1.83171413	0.00000100
H	-4.31755631	2.23698016	0.00000000
H	-1.87411913	1.98085214	0.00000000
H	-2.49208818	-2.28551716	0.00000000
C	-0.50215304	-0.47248603	0.00000000
C	0.48852003	0.43768303	0.00000000
H	-0.25061202	-1.52934211	0.00000000
H	0.22565502	1.49229611	0.00000000
C	1.93059514	0.17934401	0.00000000
C	2.48923018	-1.11192108	0.00000000
C	2.81030520	1.27519609	0.00000000
C	3.86611828	-1.29279809	0.00000000
H	1.84463013	-1.98281414	-0.00000100
C	4.19043230	1.09463908	0.00000000
H	2.40109317	2.28028817	0.00000000
C	4.72523634	-0.19134201	0.00000000
H	4.27462831	-2.29721317	-0.00000100
H	4.84671335	1.95760814	0.00000000
H	5.79928644	-0.33743702	0.00000000
N	-4.74490534	0.22062602	0.00000000

1t

C	-1.52334435	-1.19223029	-0.02440123
C	-0.77052480	-0.00358756	-0.00013511
N	-1.39708833	1.18334622	-0.02221310
C	-2.72854601	1.17351393	-0.03435822
C	-3.46024042	-0.01166181	-0.02118886
N	-2.85406091	-1.20161439	-0.02659013
C	0.71239348	-0.00443471	0.02373558
C	1.43811647	-1.09265912	0.52973467
C	1.41727152	1.10578525	-0.46346231
C	2.83025948	-1.07576153	0.53649550
C	2.80784455	1.11864589	-0.46007105

C	3.52026591	0.02774444	0.03811622
H	-1.03521597	-2.16013081	-0.06190156
H	-3.22840170	2.13785559	-0.05186598
H	-4.54562039	-0.00419995	-0.01508091
H	0.91981116	-1.94897859	0.94473373
H	0.85881721	1.95216914	-0.84225640
H	3.37534190	-1.92189194	0.93931486
H	3.33781829	1.98184483	-0.84689388
H	4.60432023	0.03976143	0.04253120

1u

C	0.04044349	0.86567312	-0.00000000
C	0.00000000	-0.54631685	0.00000000
C	1.18759780	-1.28306802	0.00000000
C	2.42409672	0.65338677	-0.00000000
C	1.30691962	1.47199372	-0.00000000
C	-2.25510118	0.50120639	-0.00000000
H	1.17612979	-2.36949481	0.00000000
H	3.41893827	1.08762148	-0.00000000
H	1.41288001	2.55078331	-0.00000000
N	2.37810360	-0.69451097	0.00000000
S	-1.65160301	-1.13781740	0.00000000
C	-1.27654405	1.44189521	-0.00000000
H	-3.32302255	0.66280101	-0.00000000
H	-1.47047698	2.50632219	-0.00000000

1v

C	1.43874932	1.32487652	0.00000005
C	0.12016687	0.83839939	0.00000018
C	-0.05536202	-0.56302229	0.00000010
C	1.05719675	-1.40525828	-0.00000003
C	2.30572426	-0.79877666	-0.00000008
N	2.50360718	0.53436381	-0.00000006
H	1.62550410	2.39613107	0.00000009
H	0.96527886	-2.48446182	-0.00000014
H	3.20320673	-1.40943251	-0.00000019
C	-1.13272209	1.54579124	0.00000005
C	-2.19996774	0.71092441	-0.00000024
S	-1.75358991	-0.98487591	0.00000007
H	-1.21710924	2.62454802	-0.00000009
H	-3.24740429	0.97307724	-0.00000043

1w

C	2.38331514	-0.62699035	-0.00000041
C	1.23178938	-1.37609799	0.00000005
C	-0.01899234	-0.71401659	0.00000062
C	-0.00582850	0.71009985	0.00000024
C	1.25552246	1.36357290	0.00000027
H	3.35541359	-1.10921056	-0.00000060
H	1.25611213	-2.45880287	-0.00000003
C	-1.24663182	1.38937356	-0.00000007
H	1.28753412	2.45196971	-0.00000033
C	-2.40258811	0.65027164	-0.00000021
C	-2.30697608	-0.76471110	-0.00000037
H	-1.26871287	2.47442170	-0.00000002
H	-3.37778626	1.12201002	-0.00000014
H	-3.21753986	-1.35936960	0.00000028
N	2.40818199	0.73443836	-0.00000009

N	-1.17570792	-1.43587121	0.00000009

1x

C	2.39510764	-0.71618403	0.00000000
C	1.20508459	-1.40346767	0.00000000
C	-0.02900557	-0.70398503	-0.00000000
C	-0.01417236	0.72606275	0.00000000
C	1.23114107	1.40589110	0.00000000
C	2.40995354	0.69974593	0.00000000
H	3.33387747	-1.25867231	0.00000000
H	1.17101216	-2.48632799	0.00000000
C	-1.26451192	1.39201303	0.00000000
H	1.23755531	2.49112978	0.00000000
H	3.35829434	1.22499447	0.00000000
C	-2.42009684	0.65242258	0.00000000
C	-2.32394437	-0.76094746	-0.00000000
H	-1.29270786	2.47703952	-0.00000000
H	-3.39481382	1.12573654	-0.00000000
H	-3.23181538	-1.35977373	0.00000002
N	-1.18839099	-1.42334763	0.00000000

1y

C	3.54856197	-0.24399572	-0.00000022
C	2.79837796	0.91293408	-0.00000029
C	1.38903736	0.85052510	-0.00000024
C	0.72818702	-0.40425077	-0.00000012
C	1.52044079	-1.57321009	-0.00000004
C	2.89947969	-1.49269891	-0.00000009
C	0.58995515	2.04457605	-0.00000033
C	-0.72227000	-0.39683711	-0.00000008
C	-1.38242221	0.86357929	-0.00000018
C	-2.79273461	0.91433934	-0.00000015
H	-3.25862202	1.89240399	-0.00000022
C	-3.53911004	-0.24493840	-0.00000004
C	-2.89238401	-1.49408583	0.00000006
C	-1.51338830	-1.56645318	0.00000004
H	1.10253306	3.00623868	-0.00000043
H	4.63130310	-0.19637538	-0.00000026
H	3.28164352	1.88452253	-0.00000039
H	1.05043021	-2.54836751	0.00000006
H	3.48890760	-2.40279670	-0.00000003
H	-4.62206657	-0.19632175	-0.00000002
H	-3.47895358	-2.40583664	0.00000015
H	-1.03852891	-2.53976500	0.00000011
N	-0.70671808	2.06991170	-0.00000030

1z

C	-3.47866384	-0.37074430	0.00000086
C	-2.82512734	0.84058711	0.00000011
C	-1.41472491	0.86794173	-0.00000070
C	-0.72934258	-0.37934865	-0.00000283
C	-2.70356555	-1.54653288	0.00000101
C	-0.67895774	2.09833742	-0.00000013
C	0.72934251	-0.37934862	0.00000204
C	1.41472466	0.86794186	0.00000053
C	2.82512711	0.84058734	0.00000049
H	3.37697418	1.77505224	0.00000033
C	3.47866396	-0.37074400	-0.00000006

C	2.70356602	-1.54653272	-0.00000088
H	-1.23145399	3.03221219	0.00000001
H	-4.56058213	-0.43079435	0.00000186
H	-3.37697447	1.77505200	0.00000066
H	-3.19306902	-2.51759551	0.00000033
H	4.56058225	-0.43079392	-0.00000013
H	3.19306966	-2.51759530	-0.00000042
C	0.67895736	2.09833750	-0.00000029
H	1.23145325	3.03221260	-0.00000060
N	-1.38361316	-1.56004584	-0.00000154
N	1.38361348	-1.56004569	0.00000111

1π

C	2.39366628	0.69556877	0.00000027
C	1.21626934	1.40424223	-0.00000009
C	-0.02005456	0.71303109	-0.00000031
C	-0.03990263	-0.71056620	-0.00000039
C	1.18857365	-1.41606433	0.00000002
C	2.37538602	-0.72148107	0.00000026
C	-1.28675236	1.34753432	-0.00000041
C	-2.31827691	-0.67614258	0.00000063
H	-1.34800663	2.43487135	0.00000083
H	3.34398565	1.21667173	0.00000056
H	1.21888890	2.48933888	-0.00000009
H	1.15805619	-2.49883241	0.00000001
H	3.31540802	-1.26188571	0.00000046
H	-3.26124736	-1.21476490	0.00000221
N	-2.41972127	0.68206366	0.00000013
N	-1.22035556	-1.39379686	-0.00000068

3a

C	0.75685075	0.46931296	-0.00000308
C	-0.54064166	-0.13334251	-0.00000042
C	-1.65350140	0.76380810	0.00000025
C	-1.38970474	2.15530106	-0.00000151
C	-0.09227759	2.59736206	-0.00000322
H	0.03895232	-2.22841040	0.00000052
C	-0.78802701	-1.53237703	0.00000113
C	-2.97095509	0.23766661	0.00000220
H	-2.21218522	2.86187437	-0.00000123
H	0.14316594	3.65601341	-0.00000503
C	-3.17710308	-1.11955754	0.00000317
C	-2.07708432	-2.00838328	0.00000252
H	-3.80951655	0.92527971	0.00000281
H	-2.25435705	-3.07758846	0.00000297
N	0.97472643	1.76003150	-0.00000378
H	-4.18582692	-1.51651172	0.00000471
C	2.00975506	-0.40097803	-0.00000007
F	2.04173667	-1.21535897	1.08852714
F	2.04173715	-1.21536294	-1.08852415
F	3.13795029	0.30697172	-0.00000123

TS (broken-symmetry singlet)

C	2.14596280	-0.01156764	-0.16762987
C	3.53749871	0.28932504	-0.32833915
C	4.31252126	-0.56666243	-1.16648093
C	3.63720552	-1.62939300	-1.82269438
C	2.27624836	-1.78196621	-1.64989456

H	3.55616379	2.00883626	0.98173916
H	1.49978326	0.68521785	0.36307021
C	4.15623516	1.36997515	0.34031690
C	5.69921669	-0.30881063	-1.31560487
H	4.18672042	-2.30662585	-2.46896716
H	1.73578513	-2.57285681	-2.16317794
C	6.28001471	0.75402871	-0.65628325
C	5.50654627	1.60030487	0.17550733
H	6.29171318	-0.95761209	-1.95402419
H	5.98360697	2.43185215	0.68473230
N	1.52905461	-0.97454624	-0.86143284
H	7.34191099	0.94823862	-0.77330388
I	-1.31573967	-1.25822645	-0.40088344
C	-3.42564018	-1.18951002	-0.10123093
C	-3.92253301	-0.94324147	1.18213368
C	-4.28030568	-1.36678848	-1.19305834
C	-5.30359875	-0.88249023	1.37104294
H	-3.24779369	-0.80070968	2.01907421
C	-5.65917263	-1.30439712	-0.98802357
H	-3.88107166	-1.54976923	-2.18467185
C	-6.17055799	-1.06226355	0.28974617
H	-5.70011323	-0.69279745	2.36376117
H	-6.33190583	-1.44250383	-1.82887735
H	-7.24415803	-1.01285468	0.44269312
C	2.33576690	-1.16775865	1.86282394
F	3.07214101	-0.46086702	2.71768208
F	2.93989664	-2.31593430	1.56632820
F	1.12677442	-1.39742617	2.37010917
O	-1.58665299	1.33372080	-0.88457765
C	-1.06496781	2.03818869	0.04679979
O	-0.32330937	1.74277753	0.97652899
C	-1.52853797	3.52901638	-0.09026419
F	-1.29045336	4.00398100	-1.32721037
F	-2.85269876	3.62581087	0.14492680
F	-0.89248225	4.31767836	0.78652929

1a for mechanism calculation

C	-1.25013643	1.37505753	0.00000000
C	0.00000000	0.69981134	0.00000000
C	-0.01779171	-0.72828603	-0.00000000
C	-1.28683208	-1.36172487	0.00000000
C	-2.42625380	-0.59207312	0.00000000
H	1.24207279	2.47408766	-0.00000000
H	-1.25581041	2.46545173	0.00000000
C	1.24053217	1.38738268	0.00000000
C	1.21549889	-1.43076823	-0.00000000
H	-1.35301106	-2.44576596	0.00000000
H	-3.40795857	-1.05952626	0.00000000
C	2.40616908	-0.73825432	-0.00000000
C	2.42162150	0.68008895	-0.00000000
H	1.20479118	-2.51712343	-0.00000000
H	3.37246116	1.20419988	-0.00000000
N	-2.42382487	0.77305211	0.00000000
H	3.34738325	-1.28009198	-0.00000000

INT1

C	-2.10546215	-2.95447821	-1.54542011

C	-1.14012108	-2.91361821	-0.50091704
C	-1.58215512	-2.50818018	0.79628806
C	-2.95453221	-2.17944515	0.94155207
C	-3.78550427	-2.25297216	-0.15179601
H	0.55886604	-3.52651026	-1.70165712
H	-1.78606313	-3.26058624	-2.54169918
C	0.23023202	-3.22482423	-0.71097505
C	-0.63469404	-2.42154718	1.84974113
H	-3.33511824	-1.84890013	1.90223413
H	-4.83506035	-1.98707014	-0.06392700
C	0.68955905	-2.72174620	1.61819812
C	1.12829608	-3.12588223	0.33089902
H	-0.96723707	-2.09863815	2.83143820
H	2.17988816	-3.33597124	0.16606601
N	-3.37642124	-2.63938619	-1.39515910
H	1.41450010	-2.63148519	2.42016818
I	0.29721602	0.20062801	-0.71656605
C	0.72806905	2.25064316	-0.29308802
C	0.85378106	3.13403223	-1.36079910
C	0.85519106	2.61976119	1.04212108
C	1.12474908	4.47103532	-1.06005208
H	0.74582706	2.80539120	-2.38758617
C	1.12671008	3.96198829	1.31281709
H	0.74905405	1.89387813	1.83660313
C	1.26010009	4.88045535	0.26836202
H	1.22874909	5.18658037	-1.86918214
H	1.23213209	4.28444331	2.34363217
H	1.47044611	5.92157840	0.49116704
O	2.46871918	-0.19797101	-0.82180806
C	3.06850522	-0.30025502	0.33383202
O	2.63208619	-0.06968000	1.44453010
C	4.50953332	-0.83768906	0.14369301
F	5.19828538	-0.78067005	1.28880609
F	4.46045932	-2.12836915	-0.25430202
F	5.17784037	-0.14114601	-0.79044806
O	-1.85132513	0.88703006	1.51668811
C	-2.38732717	0.89673107	0.42476103
O	-1.84868313	0.72856205	-0.75191105
C	-3.90512628	1.19806809	0.32629202
F	-4.45977232	0.74851005	-0.80900906
F	-4.55636433	0.63941705	1.36046010
F	-4.09363429	2.53156118	0.38491403

INT2 (broken-symmetry singlet)

C	2.24452839	-0.05747258	-0.56821884
C	3.60657504	0.23111720	-0.29796566
C	4.58986125	-0.69063484	-0.77239990
C	4.12862284	-1.83197513	-1.47838982
C	2.77889778	-2.01048736	-1.67101868
H	3.24746312	2.06418972	0.79647115
H	1.47285606	0.62216434	-0.21324954
C	4.00751605	1.38115790	0.42957763
C	5.95951655	-0.42597574	-0.51136891
H	4.83866865	-2.56024059	-1.85824648
H	2.39717840	-2.87827231	-2.20121123
C	6.32316001	0.70071445	0.19350392
C	5.34351751	1.60988378	0.67002413
H	6.71086304	-1.12266465	-0.87164964

H	5.65571600	2.48747344	1.22755654	C	0.88065497	1.74129459	-0.85606075
N	1.83962383	-1.13092277	-1.22035150	C	0.00009293	1.09936286	-0.00000381
H	7.37228211	0.89855208	0.39212340	C	-0.88040895	1.74133711	0.85608326
I	-0.98382423	-1.54844494	-0.60261539	C	-0.87139420	3.13975516	0.84057764
C	-2.99563042	-1.22915066	0.02144704	C	0.00022391	3.83406234	0.00006289
C	-3.21287379	-0.62994324	1.26554220	H	1.54764655	3.67662499	-1.49814227
C	-4.05107561	-1.57422031	-0.82620184	H	1.55958147	1.19619620	-1.49902917
C	-4.52573405	-0.38191416	1.66751973	H	-1.55938910	1.19627271	1.49902398
H	-2.37825634	-0.35782521	1.90026711	H	-1.54721490	3.67670008	1.49825920
C	-5.35780090	-1.32292443	-0.40526681	H	0.00027628	4.91910501	0.00009000
H	-3.86218124	-2.02808044	-1.79278670	I	-0.00000706	-1.08484558	-0.00005366
C	-5.59520516	-0.72739967	0.83655935	O	-2.14370046	-0.96013814	0.44973194
H	-4.71069886	0.08330642	2.63087075	C	-2.91554989	-0.53180755	-0.52003730
H	-6.18825770	-1.58894124	-1.05192739	O	-2.61701000	-0.24767273	-1.66016266
H	-6.61394698	-0.53082328	1.15589036	C	-4.36231462	-0.35604828	0.00577009
C	0.92438200	-0.26608827	2.31627698	F	-5.19469848	-0.02077647	-0.98570874
F	1.61008437	0.82764231	2.62588200	F	-4.81501498	-1.48344157	0.57976352
F	1.67817840	-1.35350060	2.45290913	F	-4.38631311	0.62520776	0.93096482
F	-0.17850084	-0.36021984	3.05347424	O	2.61707986	-0.24799759	1.66009271
O	-1.19434662	0.95549907	-1.44954703	C	2.91558819	-0.53209496	0.51994974
C	-1.06186509	1.75793491	-0.46239967	O	2.14369701	-0.96031056	-0.44983704
O	-0.59230348	1.59751732	0.65888132	C	4.36236249	-0.35642087	-0.00585965
C	-1.68075435	3.15373910	-0.80658012	F	4.81496877	-1.48381577	-0.57992375
F	-1.36233173	3.55853831	-2.04871239	F	5.19478155	-0.02127295	0.98563149
F	-3.02581352	3.07486465	-0.72610895	F	4.38643014	0.62488806	-0.93099679
F	-1.26801727	4.09356846	0.05527870				

3a for mechanism calculation

PIFA

C	0.87177463	3.13971275	-0.84048668	C	0.08878649	2.60159014	-0.00004918
				C	1.38891240	2.15770429	-0.00002549

C	1.65185190	0.76573433	0.00000452
C	0.53610502	-0.13089454	0.00000877
C	-0.75970935	0.46948596	-0.00001792
H	3.80886310	0.92774187	0.00002676
H	-0.14143817	3.66313536	-0.00007233
H	2.21396419	2.86334258	-0.00002960
C	2.96954725	0.23868241	0.00003017
C	0.77793657	-1.53175712	0.00003857
C	2.06841296	-2.00994488	0.00006280
C	3.17209486	-1.12163447	0.00005865
H	-0.05208067	-2.22638465	0.00004223
H	2.24507021	-3.08097269	0.00008538
H	4.18112109	-1.52216149	0.00007814
N	-0.98350672	1.76582372	-0.00004553
C	-2.00003407	-0.40623903	-0.00001547
F	-2.02852296	-1.21739394	1.08752151
F	-2.02849729	-1.21743638	-1.08752148
F	-3.13568830	0.30351591	-0.00004273

TFA

C	-0.59596095	-0.00158469	0.00004557
F	-1.18341300	1.19774286	0.00019296
F	-0.99797736	-0.67931954	1.08945269
F	-0.99813576	-0.67912885	-1.08942371
C	0.93956669	0.15618662	-0.00006392
O	1.49299391	1.22629371	-0.00014017
O	1.51554294	-1.04594620	-0.00007562
H	2.48580577	-0.92404200	-0.00016108

CF_3COO^-

C	-0.52148069	0.01333416	-0.00374451
F	-1.07363246	1.24003292	-0.15762868
F	-1.00645440	-0.48325575	1.16818357
F	-1.03612786	-0.76652916	-0.99134956
C	1.04410546	0.01062852	-0.01179147
O	1.58537011	1.13535186	-0.00488628
O	1.52840288	-1.14235288	-0.00506775

CF_3^-

C	-0.25814077	0.02911071	0.10013556
F	0.42782128	0.66220678	-0.99898193
F	0.42782128	0.66220678	1.19925305
F	0.42371553	-1.24144184	0.10013556

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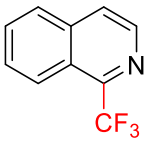
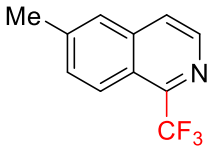
7. Characterization data for the products



3a

1-(Trifluoromethyl)isoquinoline (3a)

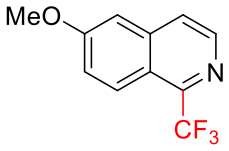
Yield: 73%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 5.6 Hz, 1H), 8.28 (d, *J* = 9.3 Hz, 1H), 7.90 (d, *J* = 8.1 Hz, 1H), 7.82 (d, *J* = 5.6 Hz, 1H), 7.78 – 7.73 (m, 1H), 7.69 (ddd, *J* = 8.2, 6.9, 1.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.41 (q, *J* = 33.2 Hz), 140.86, 137.26, 131.00, 128.94, 127.63, 124.81 – 124.71 (m), 124.70, 124.66, 122.23 (q, *J* = 276.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.99. ESI-HRMS: m/z calcd for $C_{10}H_7F_3N[M+H]^+$: 198.0525, found: 198.0523.



3b

6-Methyl-1-(trifluoromethyl)isoquinoline (3b)

Yield: 78%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 5.6 Hz, 1H), 8.17 (d, *J* = 8.7 Hz, 1H), 7.73 (d, *J* = 5.6 Hz, 1H), 7.66 (s, 1H), 7.52 (dd, *J* = 8.8, 1.7 Hz, 1H), 2.55 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.17 (q, *J* = 33.2 Hz), 141.66, 140.85, 137.62, 131.26, 126.41, 124.44 (q, *J* = 2.9 Hz), 124.11, 123.14, 122.39 (q, *J* = 276.3 Hz), 22.00. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.04. ESI-HRMS: m/z calcd for $C_{11}H_9F_3N[M+H]^+$: 212.0681, found: 212.0682.

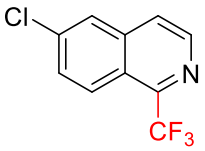


3c

6-Methoxy-1-(trifluoromethyl)isoquinoline (3c)

Yield: 82%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 5.6 Hz, 1H), 8.12 (d, *J* = 11.1 Hz, 1H), 7.65 (d, *J* = 5.6 Hz, 1H), 7.26 (dd, *J* = 9.4, 2.6 Hz, 1H), 7.07 (s, 1H), 3.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.12, 145.75 (q, *J* = 33.1 Hz),

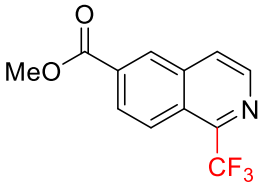
141.15, 139.57, 126.30 (q, J = 3.2 Hz), 123.72, 122.16, 126.69 – 118.02 (m), 120.33, 104.78, 55.59. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.83. ESI-HRMS: m/z calcd for $C_{11}H_9F_3NO[M+H]^+$: 228.0631, found: 228.0632.



3d

6-Chloro-1-(trifluoromethyl)isoquinoline (3d)

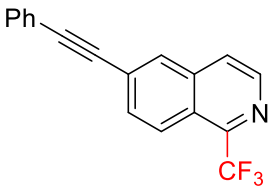
Yield: 64%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, J = 5.6 Hz, 1H), 8.19 (d, J = 7.5 Hz, 1H), 7.86 (s, 1H), 7.72 (d, J = 5.6 Hz, 1H), 7.60 (dd, J = 9.2, 2.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.63 (q, J = 33.6 Hz), 141.94, 137.97, 137.47, 130.00, 126.43 (q, J = 3.1 Hz), 126.31, 123.61, 122.90, 122.06 (q, J = 276.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.02. ESI-HRMS: m/z calcd for $C_{10}H_6ClF_3N[M+H]^+$: 232.0135, found: 232.0140.



3e

1-(Trifluoromethyl)isoquinoline-6-carboxymethylate (3e)

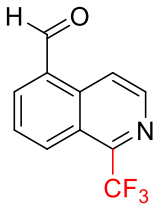
Yield: 61%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, J = 5.6 Hz, 1H), 8.64 (s, 1H), 8.34 (d, J = 9.0 Hz, 1H), 8.25 (dd, J = 9.0, 1.6 Hz, 1H), 7.95 (d, J = 5.6 Hz, 1H), 4.01 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.88, 146.72 (q, J = 33.6 Hz), 141.75, 136.65, 132.14, 130.14, 128.28, 126.22, 125.53, 125.18 (q, J = 3.1 Hz), 123.97 – 117.54 (m), 52.91. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.46. ESI-HRMS: m/z calcd for $C_{12}H_9F_3NO_2[M+H]^+$: 256.0580, found: 256.0579.



3f

6-(Phenylethynyl)-1-(trifluoromethyl)isoquinoline (3f)

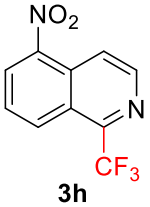
Yield: 72%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, *J* = 5.6 Hz, 1H), 8.26 (d, *J* = 7.2 Hz, 1H), 8.08 (s, 1H), 7.87 – 7.71 (m, 2H), 7.64 – 7.55 (m, 2H), 7.44 – 7.35 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.54 (q, *J* = 33.4 Hz), 141.65, 137.04, 131.98, 131.51, 130.40, 129.24, 128.65, 126.38, 124.80 (q, *J* = 3.1 Hz), 124.15, 123.74, 123.61, 126.23 – 117.81 (m), 93.30, 88.24. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.96. ESI-HRMS: m/z calcd for $C_{18}H_{11}F_3N[M+H]^+$: 298.0838, found: 298.0841.



3g

1-(Trifluoromethyl)isoquinoline-5-carbaldehyde (3g)

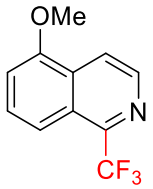
Yield: 36%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.39 (s, 1H), 9.30 (d, *J* = 5.9 Hz, 1H), 8.77 (d, *J* = 5.9 Hz, 1H), 8.57 (d, *J* = 9.4 Hz, 1H), 8.29 (d, *J* = 7.9 Hz, 1H), 7.91 (dd, *J* = 8.7, 7.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.32, 146.86 (q, *J* = 33.4 Hz), 144.00, 140.31, 134.70, 131.21 (q, *J* = 3.3 Hz), 131.07, 128.06, 124.80, 122.12 (q, *J* = 276.5 Hz), 121.63. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.34. ESI-HRMS: m/z calcd for $C_{11}H_7F_3NO[M+H]^+$: 226.0474, found: 226.0475.



3h

5-Nitro-1-(trifluoromethyl)isoquinoline (3h)

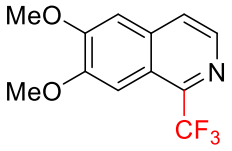
Yield: 64%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, *J* = 6.0 Hz, 1H), 8.66 (t, *J* = 7.4 Hz, 2H), 8.58 (d, *J* = 7.7 Hz, 1H), 7.87 (t, *J* = 8.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ147.32 (q, *J* = 33.8 Hz), 145.81, 144.08, 131.30 (q, *J* = 3.4 Hz), 129.69, 128.66, 127.54, 125.18, 121.89 (q, *J* = 276.6 Hz), 119.63. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.36. ESI-HRMS: m/z calcd for $C_{10}H_6F_3N_2O_2[M+H]^+$: 243.0376, found: 243.0376.



3i

5-Methoxy-1-(trifluoromethyl)isoquinoline (3i)

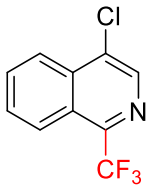
Yield: 68%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, *J* = 8.7 Hz, 1H), 7.78 (d, *J* = 8.6 Hz, 1H), 7.72 – 7.65 (m, 2H), 6.93 (d, *J* = 7.7 Hz, 1H), 4.01 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.08, 148.88 – 147.65 (m), 148.10, 133.27, 130.99, 122.02, 121.76 (q, *J* = 275.3 Hz), 121.73, 115.89 (q, *J* = 2.2 Hz), 105.93, 56.01. ^{19}F NMR (376 MHz, CDCl3) δ -67.60. ESI-HRMS: m/z calcd for $C_{11}H_9F_3NO[M+H]^+$: 228.0630, found: 228.0631.



3j

6,7-Dimethoxy-1-(trifluoromethyl)isoquinoline (3j)

Yield: 76%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 5.5 Hz, 1H), 7.61 (d, *J* = 5.5 Hz, 1H), 7.39 (s, 1H), 7.06 (s, 1H), 3.98 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.39, 151.33, 143.62 (q, *J* = 32.7 Hz), 139.60, 134.56, 123.13, 122.57 (q, *J* = 276.0 Hz), 120.99, 105.13, 102.32 (q, *J* = 3.3 Hz), 56.16, 56.05. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.49. ESI-HRMS: m/z calcd for $C_{12}H_{11}F_3NO_2[M+H]^+$: 258.0736, found: 258.0734.

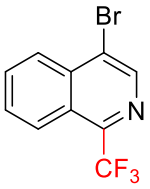


3k

4-Chloro-1-(trifluoromethyl)isoquinoline (3k)

Yield: 52%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (s, 1H), 8.34 (dd, *J* = 8.4, 4.6 Hz, 2H), 7.92 (t, *J* = 7.7 Hz, 1H), 7.81 (t, *J* = 7.9 Hz, 1H). ^{13}C NMR (101

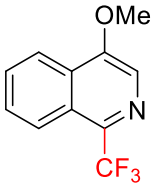
MHz, $CDCl_3$) δ 145.19 (q, *J* = 33.7 Hz), 139.87, 134.77, 132.42, 132.06, 129.80, 125.62, 125.11 (q, *J* = 3.1 Hz), 124.43, 122.07 (q, *J* = 276.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.68. ESI-HRMS: m/z calcd for $C_{10}H_6ClF_3N[M+H]^+$: 232.0135, found: 232.0134.



3l

4-Bromo-1-(trifluoromethyl)isoquinoline (3l)

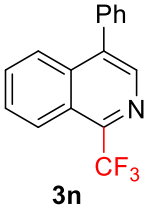
Yield: 56%, white solid. ^1H NMR (400 MHz, $CDCl_3$) δ 8.77 (s, 1H), 8.29 (dd, *J* = 8.3, 4.6 Hz, 2H), 7.88 (t, *J* = 7.8 Hz, 1H), 7.82 – 7.73 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.85 (q, *J* = 33.7 Hz), 142.75, 135.96, 132.28, 129.84, 127.08, 125.84, 125.12 (q, *J* = 3.2 Hz), 123.96, 122.10 (q, *J* = 276.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.68. ESI-HRMS: m/z calcd for $C_{10}H_6BrF_3N[M+H]^+$: 275.9630, found: 275.9632.



3m

4-Methoxy-1-(trifluoromethyl)isoquinoline (3m)

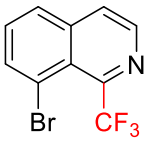
Yield: 63%, white solid. ^1H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.6 Hz, 1H), 8.21 (d, *J* = 7.8 Hz, 1H), 8.08 (s, 1H), 7.76 – 7.65 (m, 2H), 4.10 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.86, 138.87 (q, *J* = 33.3 Hz), 129.96, 129.06, 129.01, 125.38, 124.17 (q, *J* = 3.1 Hz), 122.53 (q, *J* = 275.1 Hz), 122.01, 120.83, 56.43. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.44. ESI-HRMS: m/z calcd for $C_{11}H_9F_3NO[M+H]^+$: 228.0631, found: 228.0617.



3n

4-Phenyl-1-(trifluoromethyl)isoquinoline (3n)

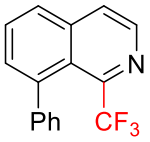
Yield: 65%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 8.42 – 8.33 (m, 1H), 8.01 (dq, *J* = 6.9, 3.4 Hz, 1H), 7.74 (dt, *J* = 6.6, 3.4 Hz, 2H), 7.61 – 7.45 (m, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.71 (q, *J* = 33.1 Hz), 140.72, 137.38, 136.15, 135.74, 131.03, 130.18, 128.89, 128.70, 128.69, 126.05, 124.86 (q, *J* = 3.2 Hz), 124.68, 122.48 (q, *J* = 276.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.68. ESI-HRMS: m/z calcd for $C_{16}H_{11}F_3N[M+H]^+$: 274.0838, found: 274.0839.



3o

8-Bromo-1-(trifluoromethyl)isoquinoline (3o)

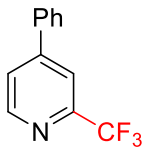
Yield: 54%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, *J* = 5.4 Hz, 1H), 8.08 (d, *J* = 7.5 Hz, 1H), 7.86 (d, *J* = 8.2 Hz, 1H), 7.81 (d, *J* = 5.4 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.81 (q, *J* = 34.5 Hz), 140.27, 140.12, 137.23, 130.74, 128.16, 125.36, 125.27, 121.69 (q, *J* = 275.0 Hz), 117.47. ^{19}F NMR (376 MHz, $CDCl_3$) δ -55.97. ESI-HRMS: m/z calcd for $C_{10}H_6BrF_3N[M+H]^+$: 275.9630, found: 275.9630.



3p

8-Phenyl-1-(trifluoromethyl)isoquinoline (3p)

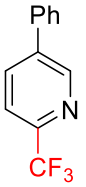
Yield: 40%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 5.3 Hz, 1H), 7.96 – 7.86 (m, 2H), 7.78 – 7.70 (m, 1H), 7.57 (dd, *J* = 7.1, 1.3 Hz, 1H), 7.42 (dp, *J* = 3.8, 2.1 Hz, 3H), 7.36 (dd, *J* = 6.7, 3.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.29 (q, *J* = 34.3 Hz), 142.11 (q, *J* = 2.7 Hz), 140.16, 138.76, 133.37, 129.84, 129.68 (q, *J* = 1.9 Hz), 127.73, 127.43, 124.51, 123.94, 121.37 (q, *J* = 275.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -58.86. ESI-HRMS: m/z calcd for $C_{16}H_{11}F_3N[M+H]^+$: 274.0838, found: 274.0840.



3q

4-Phenyl-2-(trifluoromethyl)pyridine (3q)

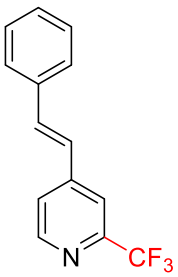
Yield: 68%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 5.1 Hz, 1H), 7.90 (s, 1H), 7.70 (d, *J* = 5.1 Hz, 1H), 7.70 – 7.63 (m, 2H), 7.56 – 7.48 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.58, 150.41, 148.98 (q, *J* = 34.3 Hz), 136.99, 130.01, 129.52, 127.23, 124.29, 121.77 (q, *J* = 274.4 Hz), 118.60 (q, *J* = 2.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -67.98. ESI-HRMS: m/z calcd for $C_{12}H_9F_3N[M+H]^+$: 224.0682, found: 224.0672.



3r

5-Phenyl-2-(trifluoromethyl)pyridine (3r)

Yield: 52%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.94 (s, 1H), 8.04 (d, *J* = 9.8 Hz, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.61 (d, *J* = 6.9 Hz, 2H), 7.50 (dt, *J* = 14.0, 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.59, 146.90 (q, *J* = 34.8 Hz), 139.61, 136.48, 135.62, 129.46, 129.14, 127.46, 121.83 (q, *J* = 273.8 Hz), 120.57 (q, *J* = 2.7 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -67.69. ESI-HRMS: m/z calcd for $C_{12}H_9F_3N[M+H]^+$: 224.0682, found: 224.0682.

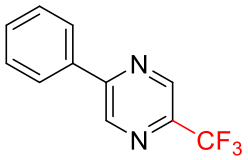


3s

(*E*)-4-Styryl-2-(trifluoromethyl)pyridine (3s)

Yield: 61%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 5.1 Hz, 1H), 7.76

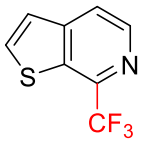
(s, 1H), 7.56 (d, *J* = 7.1 Hz, 2H), 7.53 (d, *J* = 4.4 Hz, 1H), 7.45 – 7.37 (m, 3H), 7.36 (d, *J* = 3.5 Hz, 1H), 7.07 (d, *J* = 16.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.50, 148.84 (q, *J* = 34.1 Hz), 146.62, 135.63, 135.11, 129.45, 129.08, 127.35, 124.73, 123.44, 121.76 (q, *J* = 272.6 Hz), 117.68, 117.49 (q, *J* = 2.7 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -68.05. ESI-HRMS: m/z calcd for $C_{14}H_{11}F_3N[M+H]^+$: 250.0838, found: 250.0852.



3t

2-Phenyl-5-(trifluoromethyl)pyrazine (3t)

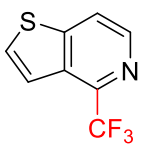
Yield: 42%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (s, 1H), 8.99 (s, 1H), 8.08 (dd, *J* = 6.7, 2.9 Hz, 2H), 7.60 – 7.53 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.64, 141.78 (q, *J* = 35.7 Hz), 141.55, 141.17 (q, *J* = 3.2 Hz), 135.13, 131.21, 129.44, 127.57, 121.56 (q, *J* = 274.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -67.39. ESI-HRMS: m/z calcd for $C_{11}H_8F_3N_2[M+H]^+$: 225.0634, found: 225.0632.



3u

7-(Trifluoromethyl)thieno[2,3-c]pyridine (3u)

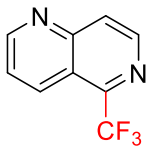
Yield: 43%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, *J* = 5.3 Hz, 1H), 7.88 (d, *J* = 5.3 Hz, 1H), 7.83 (d, *J* = 5.5 Hz, 1H), 7.47 (d, *J* = 5.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.59, 142.85 (q, *J* = 36.1 Hz), 142.31, 133.89, 132.59, 121.91 (q, *J* = 274.9 Hz), 123.07, 120.75. ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.27. ESI-HRMS: m/z calcd for $C_8H_5F_3NS[M+H]^+$: 204.0089, found: 204.0088.



3v

4-(Trifluoromethyl)thieno[3,2-c]pyridine (3v)

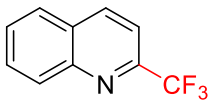
Yield: 55%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, *J* = 5.5 Hz, 1H), 7.98 (d, *J* = 5.5 Hz, 1H), 7.66 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.61, 142.90 (q, *J* = 35.1 Hz), 141.27, 132.15, 129.97, 122.19 (q, *J* = 275.0 Hz), 121.42 (q, *J* = 2.7 Hz), 120.46. ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.18. ESI-HRMS: m/z calcd for $C_8H_5F_3NS[M+H]^+$: 204.0089, found: 204.0092.



3w

5-(Trifluoromethyl)-1,6-naphthyridine (3w)

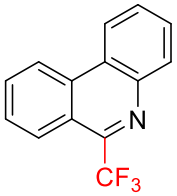
Yield: 41%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.16 (d, *J* = 4.2 Hz, 1H), 8.79 (d, *J* = 5.8 Hz, 1H), 8.60 (d, *J* = 9.4 Hz, 1H), 8.12 (d, *J* = 5.8 Hz, 1H), 7.63 (dd, *J* = 8.7, 4.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.41, 151.18, 147.24 (q, *J* = 33.8 Hz), 144.77, 133.00 (q, *J* = 3.0 Hz), 126.15, 123.69, 121.81 (q, *J* = 276.6 Hz), 120.50. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.56. ESI-HRMS: m/z calcd for $C_9H_6F_3N_2[M+H]^+$: 199.0478, found: 199.0477.



3x

2-(Trifluoromethyl)quinoline (3x)

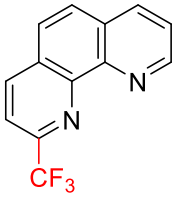
Yield: 47%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.5 Hz, 1H), 8.23 (d, *J* = 8.5 Hz, 1H), 7.90 (d, *J* = 8.2 Hz, 1H), 7.82 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.73 (d, *J* = 8.5 Hz, 1H), 7.67 (t, *J* = 7.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.96 (q, *J* = 34.6 Hz), 147.22, 138.24, 130.92, 130.14, 128.93, 128.70, 127.79, 121.69 (q, *J* = 275.1 Hz), 116.84 (q, *J* = 2.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -67.45. ESI-HRMS: m/z calcd for $C_{10}H_6F_3N[M+H]^+$: 198.0525, found: 198.0523.



3y

6-(Trifluoromethyl)phenanthridine (3y)

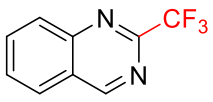
Yield: 32%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 8.4 Hz, 1H), 8.55 (d, *J* = 9.5 Hz, 1H), 8.36 (d, *J* = 8.4 Hz, 1H), 8.27 (d, *J* = 7.5 Hz, 1H), 7.88 (t, *J* = 8.3 Hz, 1H), 7.83 – 7.68 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.56 (q, *J* = 32.7 Hz), 141.79, 134.00, 131.44, 131.17, 129.41, 129.29, 128.13, 125.97 (q, *J* = 3.1 Hz), 125.16, 122.59, 122.13, 122.05 (q, *J* = 277.2 Hz), 121.81. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.46. ESI-HRMS: m/z calcd for $C_{14}H_9F_3N[M+H]^+$: 248.0682, found: 248.0678.



3z

2-(Trifluoromethyl)-1,10-phenanthroline (3z)

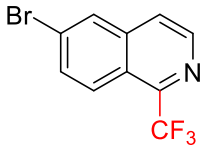
Yield: 35%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.25 (dd, *J* = 4.4, 1.7 Hz, 1H), 8.41 (d, *J* = 8.3 Hz, 1H), 8.27 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.96 (d, *J* = 8.3 Hz, 1H), 7.88 (d, *J* = 8.9 Hz, 1H), 7.82 (d, *J* = 8.8 Hz, 1H), 7.68 (dd, *J* = 8.1, 4.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.17, 147.91 (q, *J* = 35.1 Hz), 145.82, 145.69, 138.05, 136.38, 129.97, 129.30, 128.99, 125.93, 123.84, 121.77 (q, *J* = 275.3 Hz), 119.22 (q, *J* = 2.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.53. ESI-HRMS: m/z calcd for $C_{13}H_8F_3N_2[M+H]^+$: 249.0634, found: 249.0679.



3π

2-(Trifluoromethyl)quinazoline (3π)

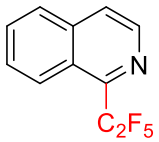
Yield: 25%, white solid. Yield: 25%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.54 (s, 1H), 8.20 (d, *J* = 8.9 Hz, 1H), 8.09 – 8.02 (m, 2H), 7.83 (t, *J* = 7.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.77, 152.95 (q, *J* = 36.4 Hz), 149.73, 135.66, 130.14, 129.22, 127.46, 125.27, 120.08 (q, *J* = 275.5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -69.87. ESI-HRMS: m/z calcd for $C_9H_6F_3N_2[M+H]^+$: 199.0478, found: 199.0452.



3λ

6-Bromo-1-(trifluoromethyl)isoquinoline (3λ)

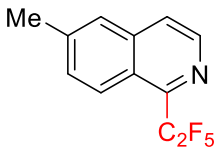
Yield: 66%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, *J* = 5.6 Hz, 1H), 8.13 (d, *J* = 9.1 Hz, 1H), 8.07 (d, *J* = 1.9 Hz, 1H), 7.80 – 7.65 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.78 (q, *J* = 33.4 Hz), 141.95, 138.24, 132.55, 129.72, 126.34 (q, *J* = 3.1 Hz), 126.04, 123.47, 123.14, 122.05 (q, *J* = 276.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.00. ESI-HRMS: m/z calcd for $C_{10}H_6BrF_3N[M+H]^+$: 275.9630, found: 275.9632.



4a

1-(Perfluoroethyl)isoquinoline (4a)

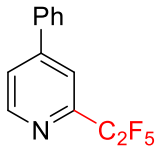
Yield: 69%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, *J* = 5.6 Hz, 1H), 8.39 (d, *J* = 8.6 Hz, 1H), 7.92 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 5.5 Hz, 1H), 7.79 – 7.74 (m, 1H), 7.70 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.39 (t, J = 25.3 Hz), 140.84, 137.37, 130.87, 128.92, 127.87, 125.97, 124.92 (t, J = 6.2 Hz), 124.60, 119.37 (qt, J = 286.7, 35.9 Hz), 113.65 (tq, J = 255.4, 36.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -81.18 (s, 3F), -107.63 (s, 2F). ESI-HRMS: m/z calcd for $C_{11}H_7F_5N[M+H]^+$: 248.0493, found: 248.0491.



4b

6-Methyl-1-(perfluoroethyl)isoquinoline (4b)

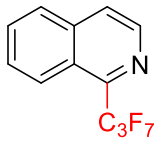
Yield: 74%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (d, *J* = 5.6 Hz, 1H), 8.26 (d, *J* = 8.9 Hz, 1H), 7.72 (d, *J* = 5.5 Hz, 1H), 7.66 (s, 1H), 7.51 (dd, *J* = 8.9, 1.7 Hz, 1H), 2.55 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.98 (t, *J* = 25.3 Hz), 141.54, 140.86, 137.76, 131.27, 126.63, 124.64 (t, *J* = 6.1 Hz), 124.36, 124.08, 119.37 (qt, *J* = 286.8, 36.1 Hz), 113.62 (tq, *J* = 255.6, 37.1 Hz), 21.93. ^{19}F NMR (376 MHz, $CDCl_3$) δ -81.30 (s, 3F), -107.92 (s, 2F). ESI-HRMS: m/z calcd for $C_{12}H_9F_5N[M+H]^+$: 262.0650, found: 262.0647.



4c

4-Phenyl-2-(perfluoroethyl)pyridine (4c)

Yield: 72%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, *J* = 5.1 Hz, 1H), 7.91 (s, 1H), 7.69 (dd, *J* = 5.1, 1.5 Hz, 1H), 7.65 (dt, *J* = 8.5, 2.3 Hz, 2H), 7.57 – 7.44 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.52, 150.31, 148.43 (t, *J* = 25.2 Hz), 136.90, 129.99, 129.48, 127.19, 124.22, 120.00 (t, *J* = 4.4 Hz), 119.10 (qt, *J* = 286.6, 37.7 Hz), 111.48 (tq, *J* = 254.8, 37.9 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -83.10 (s, 3F), -117.29 (s, 2F). ESI-HRMS: m/z calcd for $C_{13}H_9F_5N[M+H]^+$: 274.0650, found: 274.0647.

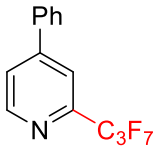


4d

1-(Perfluoropropyl)isoquinoline (4d)

Yield: 67%, colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 5.5 Hz, 1H), 8.36 (d, *J* = 8.5 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.84 (d, *J* = 5.5 Hz, 1H), 7.75 (t, *J* = 7.1 Hz, 1H), 7.69 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ

146.11 (t, *J* = 23.8 Hz), 141.10, 137.45, 130.80, 128.96, 127.86, 126.46, 125.05 (tt, *J* = 6.9, 2.4 Hz), 124.73, 118.20 (qt, *J* = 287.6, 34.2 Hz), 114.97 (tt, *J* = 255.8, 31.1 Hz), 109.67 (tq, *J* = 267.4, 37.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -79.85 (t, *J* = 9.6 Hz, 3F), -107.05 (qd, *J* = 9.6, 4.7 Hz, 2F), -124.80 – -124.88 (m, 2F). ESI-HRMS: m/z calcd for $C_{12}H_7F_7N[M+H]^+$: 298.0461, found: 298.0458.



4e

4-Phenyl-2-(perfluoropropyl)pyridine (4e)

Yield: 71%, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 5.1 Hz, 1H), 7.90 (s, 1H), 7.70 (d, *J* = 5.0 Hz, 1H), 7.66 (dt, *J* = 8.6, 2.3 Hz, 2H), 7.56 – 7.48 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.53, 150.26, 148.43 (t, *J* = 25.2 Hz), 136.93, 130.02, 129.51, 127.23, 124.26, 120.38 (t, *J* = 4.8 Hz), 119.95 – 110.98 (m), 113.09 (tt, *J* = 256.6, 30.3 Hz), 109.74 – 106.16 (m). ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.27 (t, *J* = 9.4 Hz, 3F), -114.91 (q, *J* = 9.3 Hz, 2F), -126.35 (s, 2F). ESI-HRMS: m/z calcd for $C_{14}H_9F_7N[M+H]^+$: 324.0618, found: 324.0619.

8. ^{1}H, ^{13}C NMR and ^{19}F NMR spectra of the products


8.58
8.56
8.30
8.27
7.91
7.89
7.83
7.82
7.77
7.77
7.75
7.74
7.73
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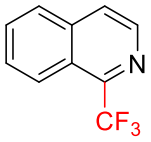
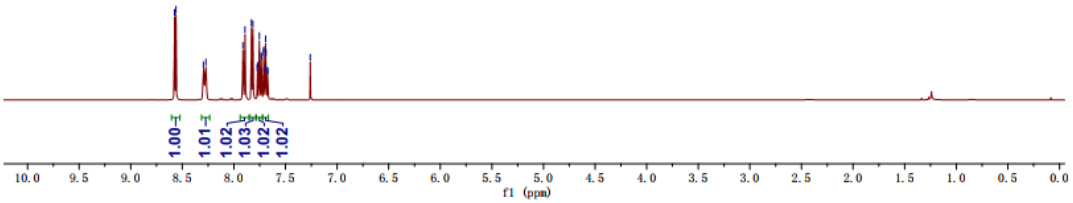
7.70
7.69
7.69
7.68
7.67
7.26


N
CF3

3a


1.00
1.01
1.02
1.03
1.02
1.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


147.02
146.70
146.37
146.04
140.86
137.26
131.00
128.94
127.63
126.47
125.00
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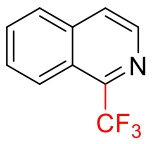
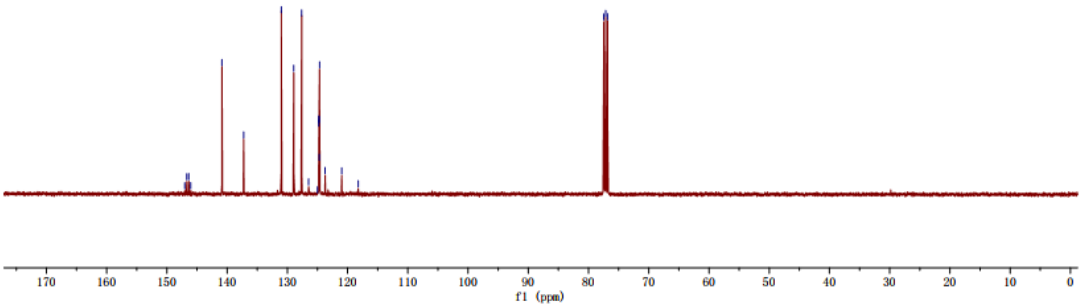
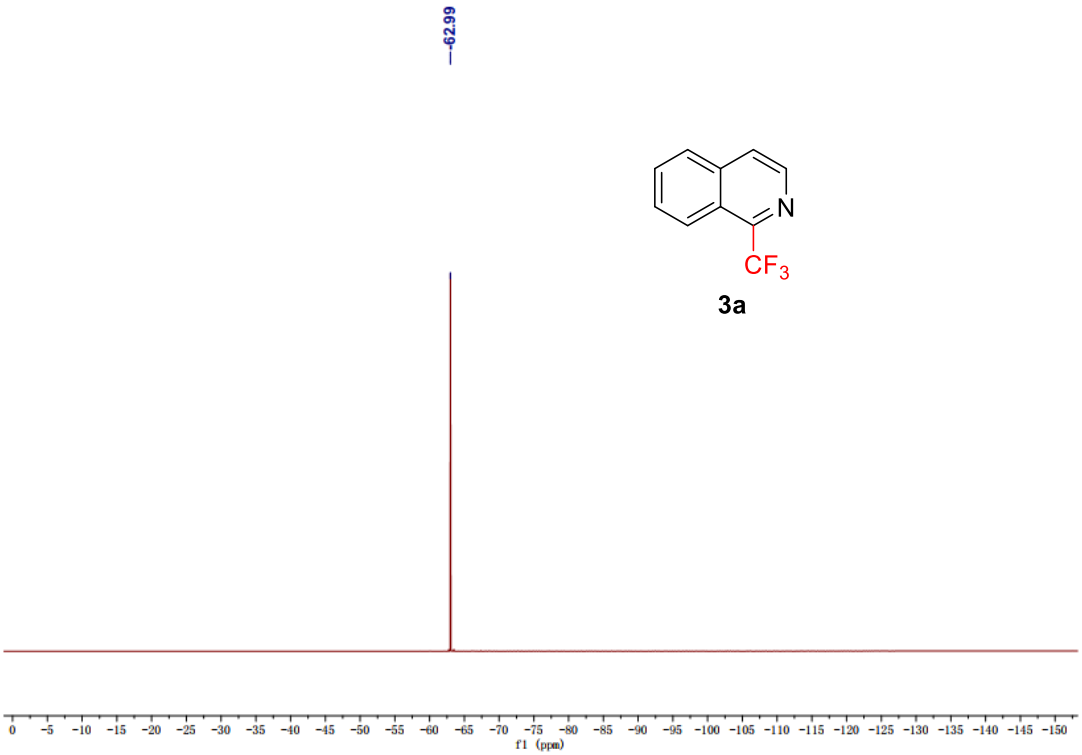
123.73
120.98
118.24


77.48
77.16
76.84

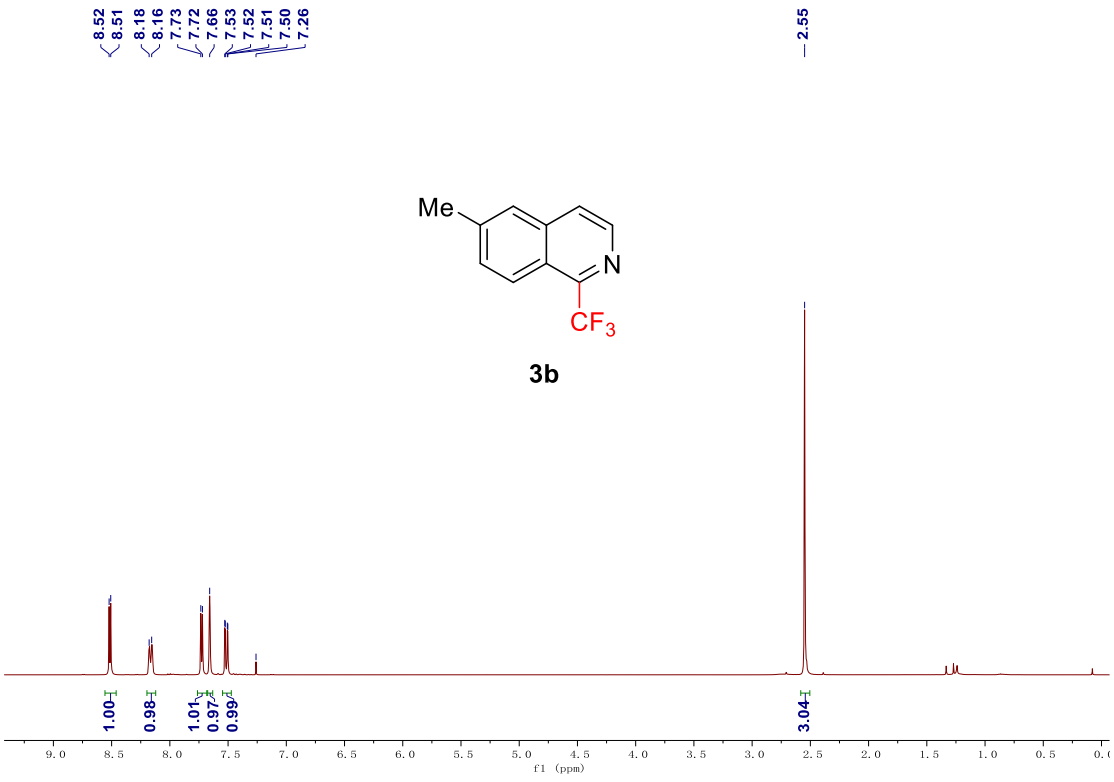

N
CF3

3a

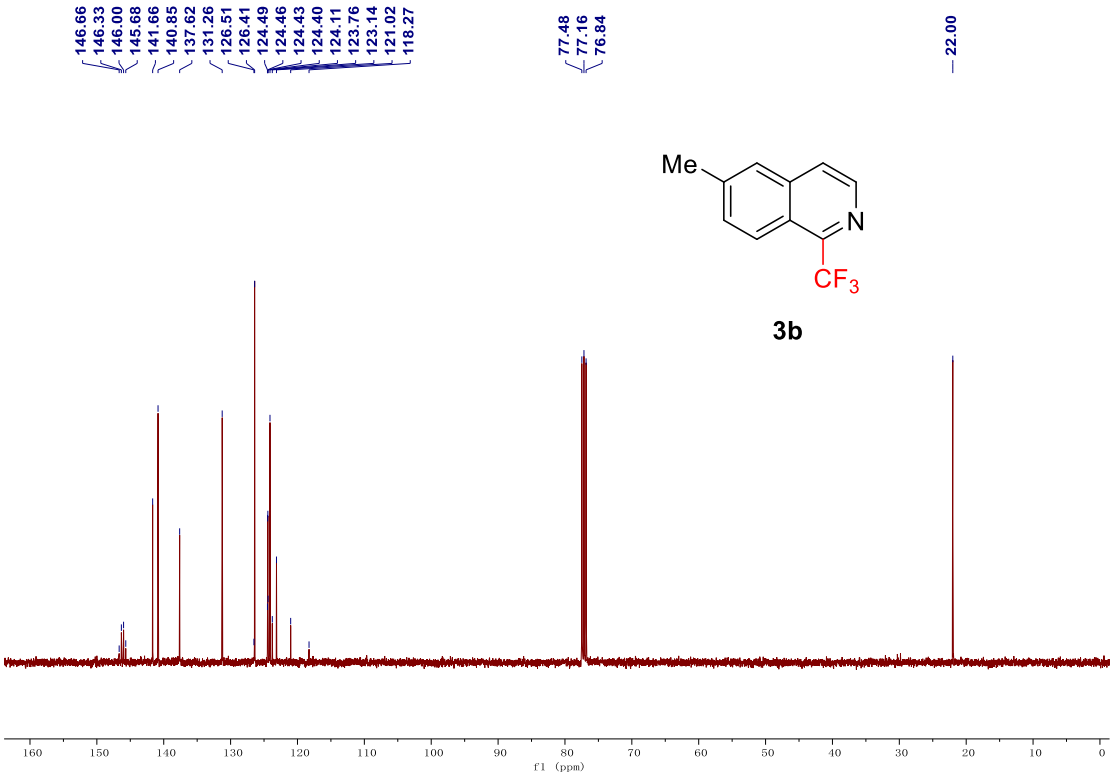

170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-62.99
N
CF3
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150
f1 (ppm)

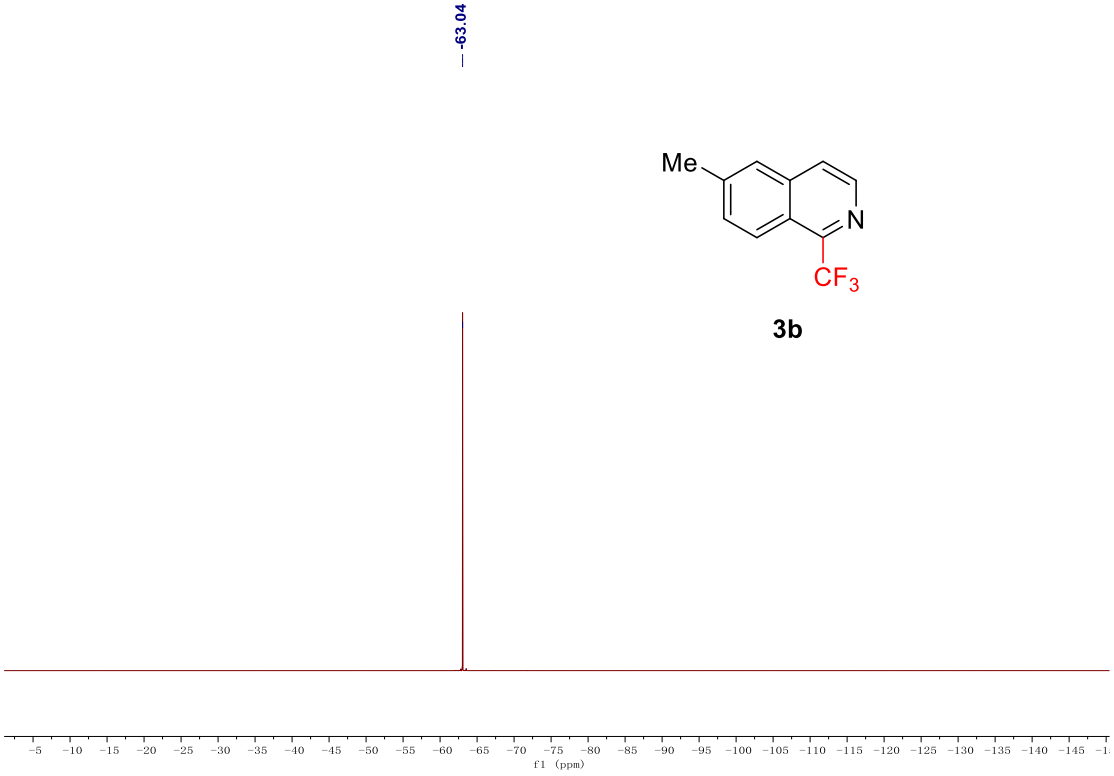
3a


8.52
8.51
8.18
8.16
7.73
7.72
7.66
7.53
7.52
7.51
7.50
7.26
2.55
Me
N
CF3
1.00
0.98
1.01
0.97
0.99
3.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

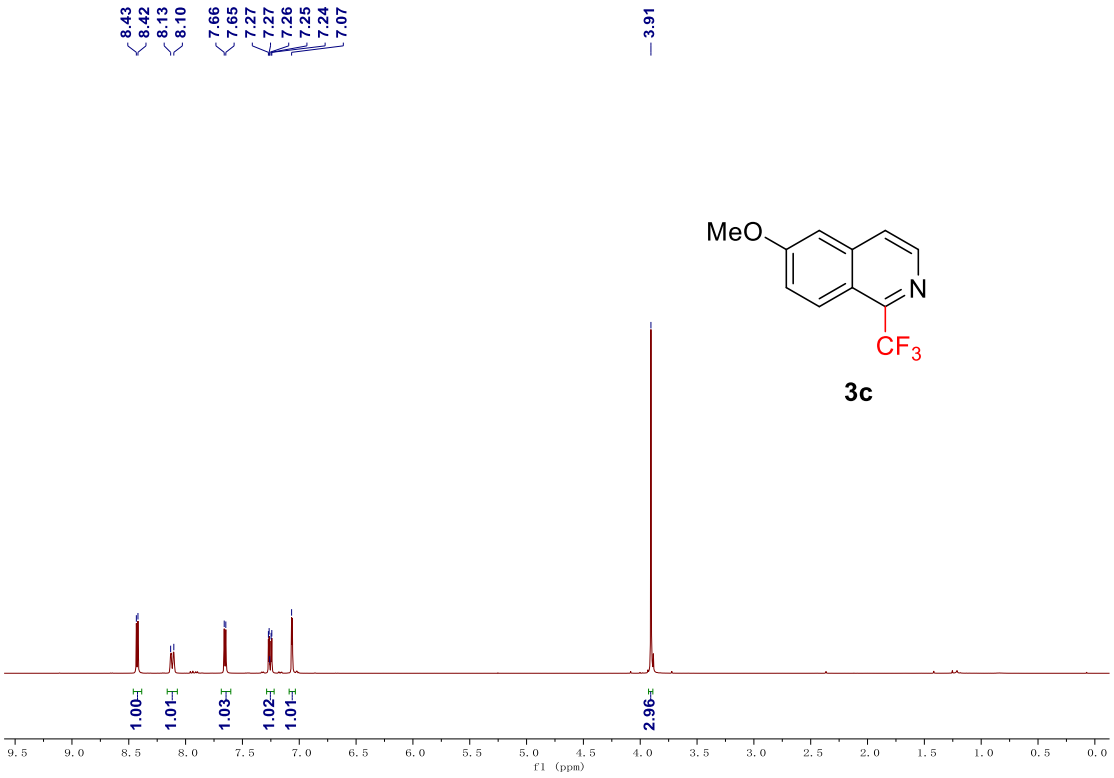
3b


146.66
146.33
146.00
145.68
141.66
140.85
137.62
131.26
126.51
126.41
124.49
124.46
124.43
124.40
124.11
123.76
123.14
121.02
118.27
77.48
77.16
76.84
22.00
Me
N
CF3
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

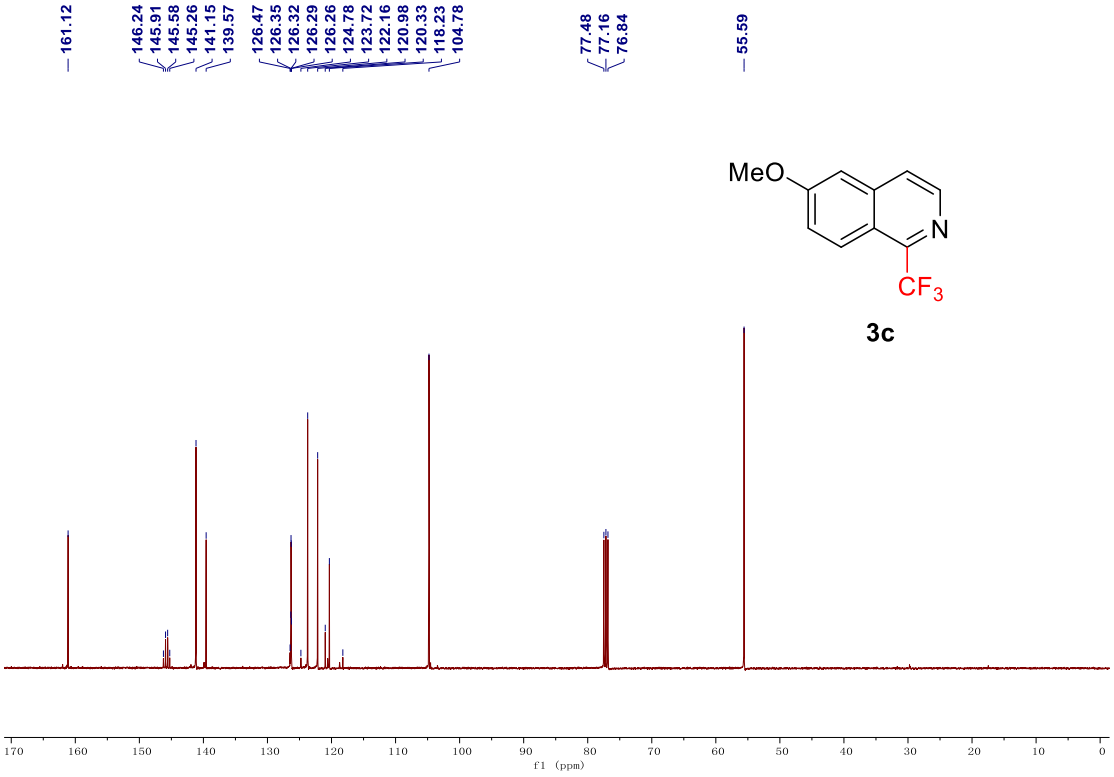
3b


-63.04
Me
N
CF3
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
f1 (ppm)

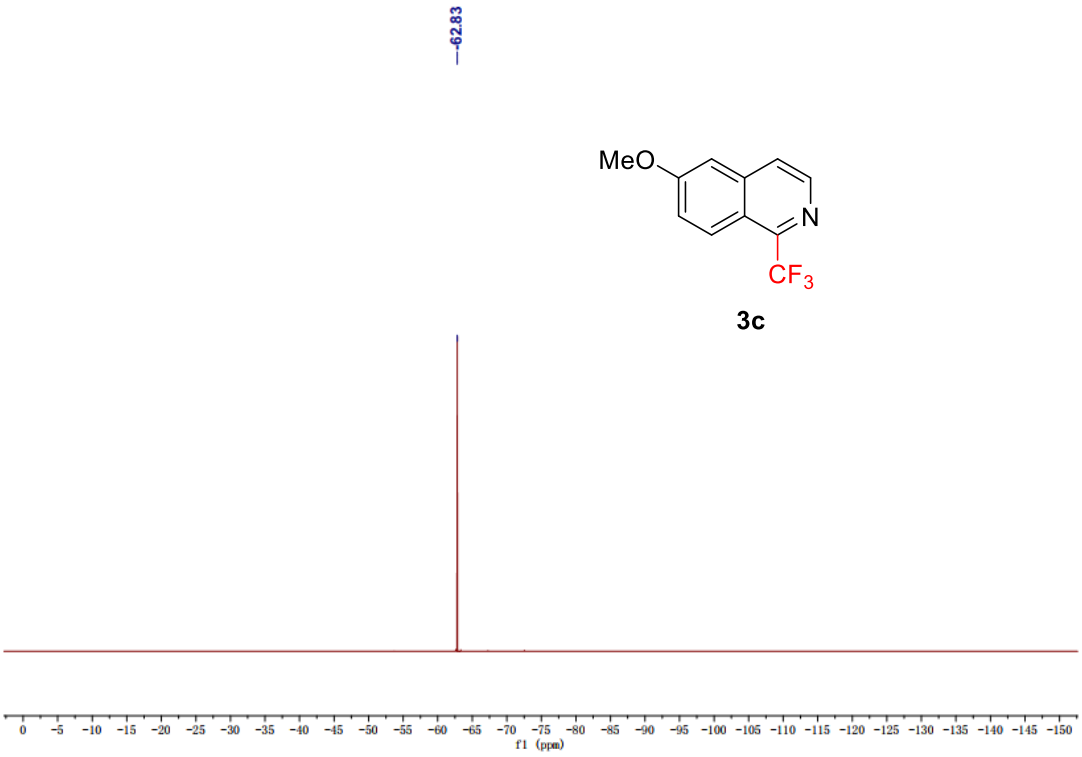
3b


8.43
8.42
8.13
8.10
7.66
7.65
7.27
7.27
7.26
7.25
7.24
7.07
3.91
MeO
N
CF3
1.00
1.01
1.03
1.02
1.01
2.96
f1 (ppm)

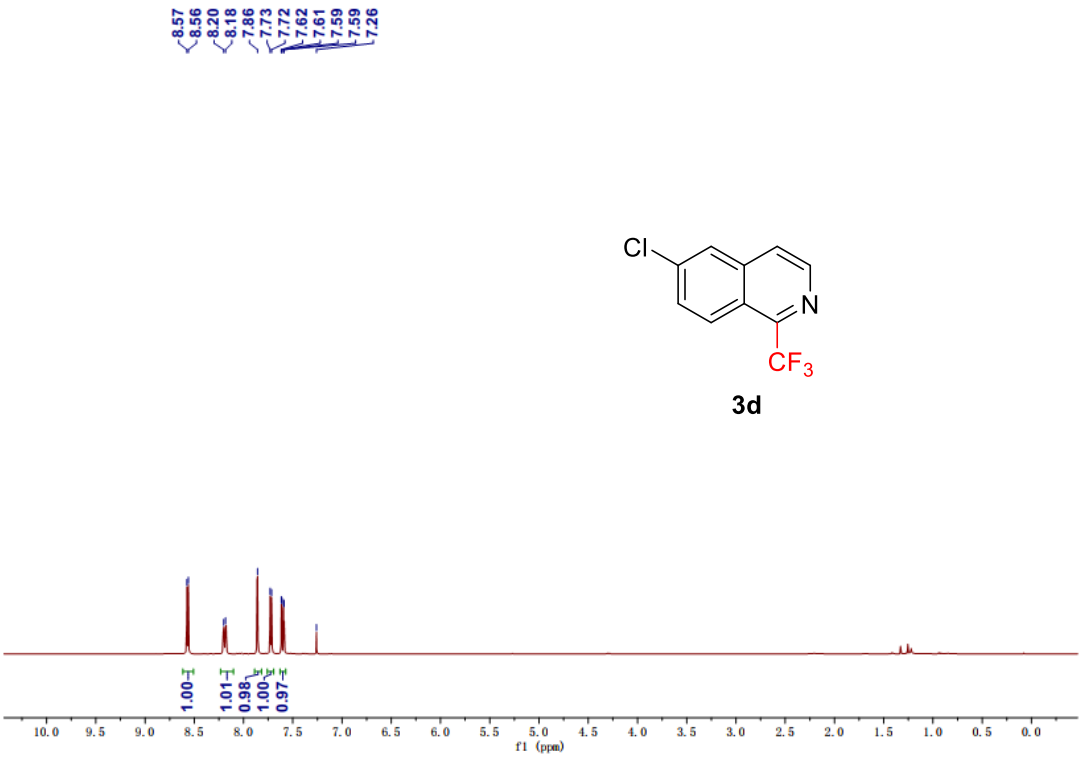
3c


161.12
146.24
145.91
145.58
145.26
141.15
139.57
126.47
126.35
126.32
126.29
126.26
124.78
123.72
122.16
120.98
120.33
118.23
104.78
77.48
77.16
76.84
55.59
MeO
N
CF3
f1 (ppm)

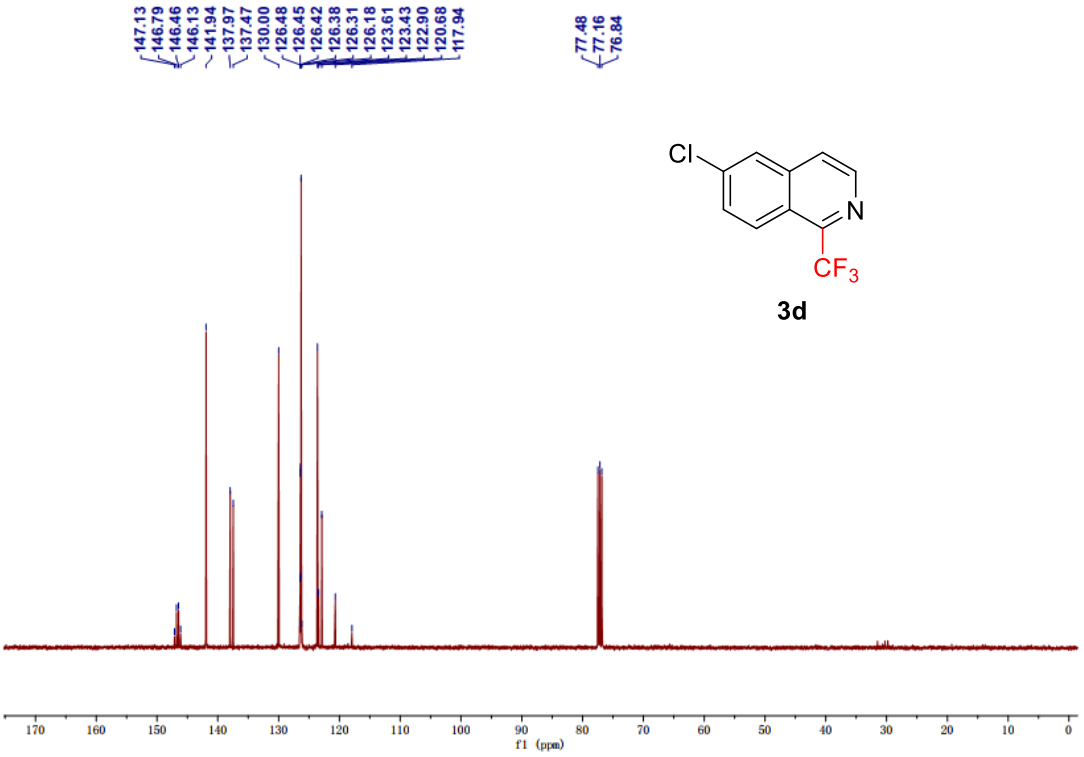
3c

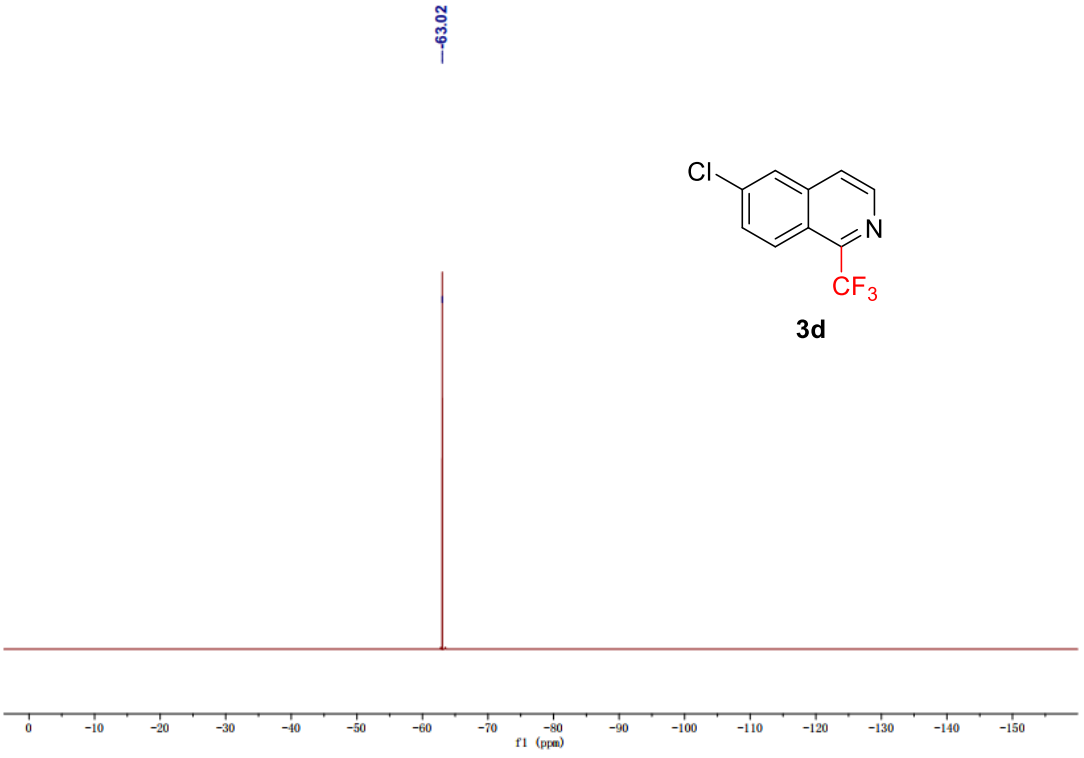

-62.83
MeO
N
CF3
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150
f1 (ppm)

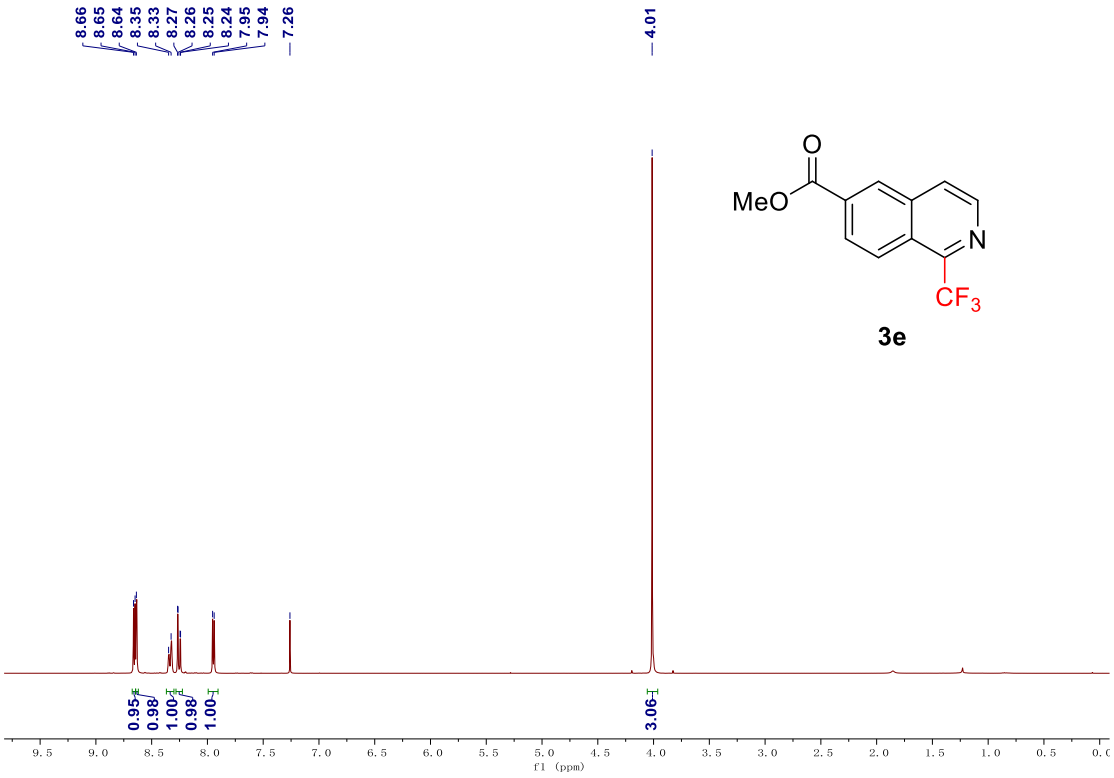
3c


8.57
8.56
8.20
8.18
7.86
7.73
7.72
7.62
7.61
7.59
7.59
7.26
Cl
N
CF3
1.00
1.01
0.98
1.00
0.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

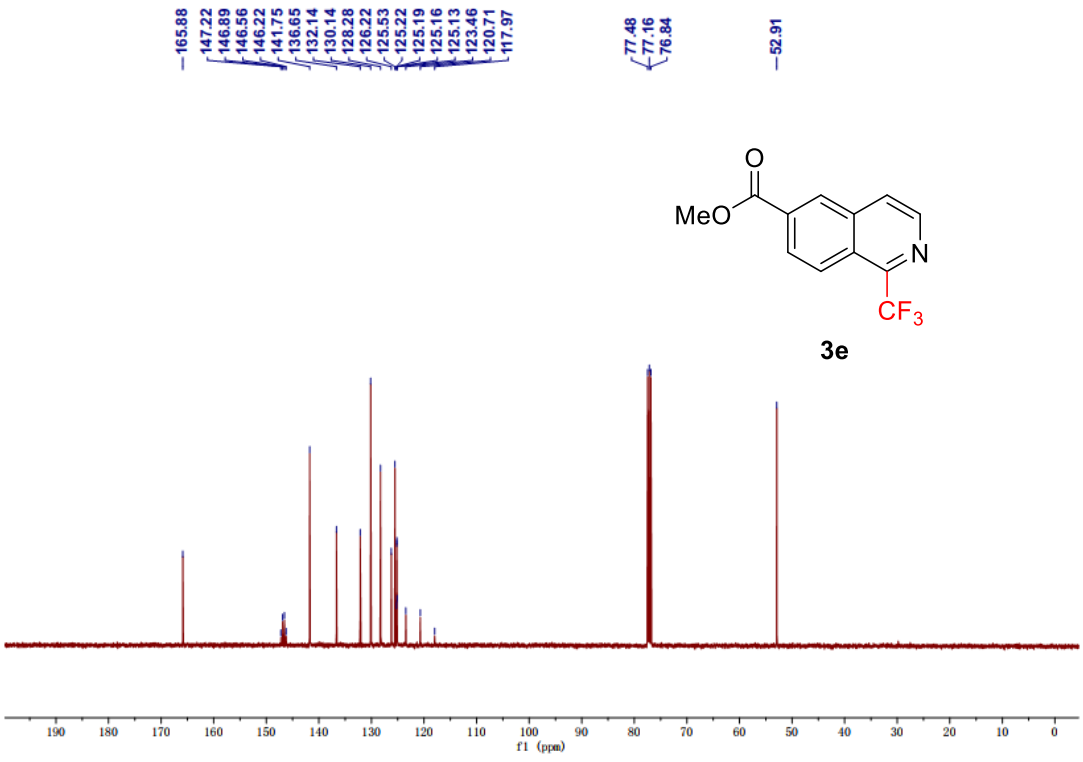
3d


147.13
146.79
146.46
146.13
141.94
137.97
137.47
130.00
126.48
126.45
126.42
126.38
126.31
126.18
123.61
123.43
122.90
120.68
117.94
77.48
77.16
76.84
Cl
N
CF3
3d
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

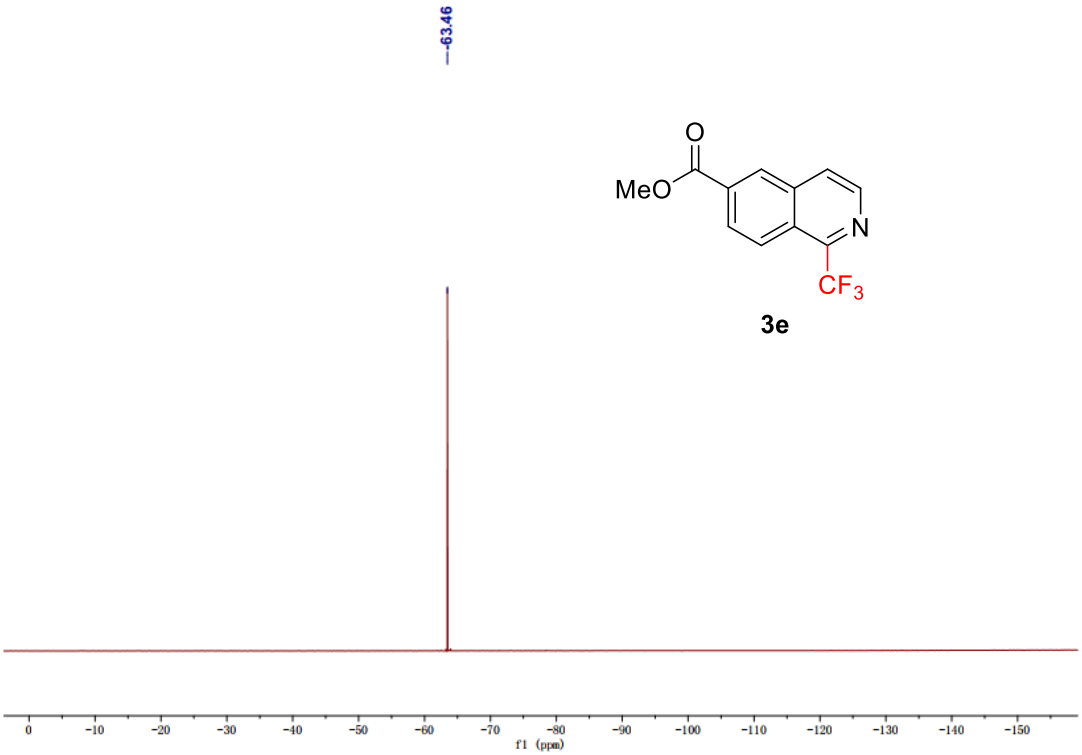

-63.02
Cl
N
CF3
3d
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)


8.66
8.65
8.64
8.35
8.33
8.27
8.26
8.25
8.24
7.95
7.94
7.26
4.01
O
MeO
N
CF3
0.95
0.98
1.00
0.98
1.00
3.06
f1 (ppm)

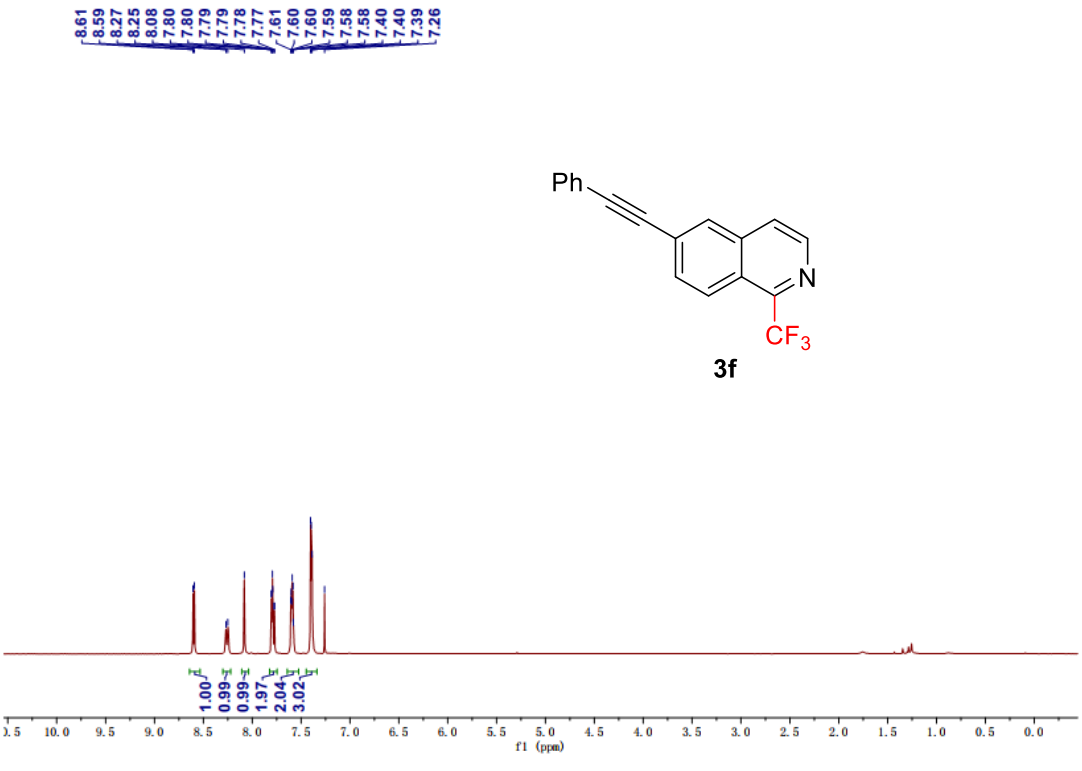
3e


165.88
147.22
146.89
146.56
146.22
141.75
136.65
132.14
130.14
128.28
126.22
125.53
125.22
125.19
125.16
125.13
123.46
120.71
117.97
77.48
77.16
76.84
52.91
O
MeO
N
CF3
f1 (ppm)

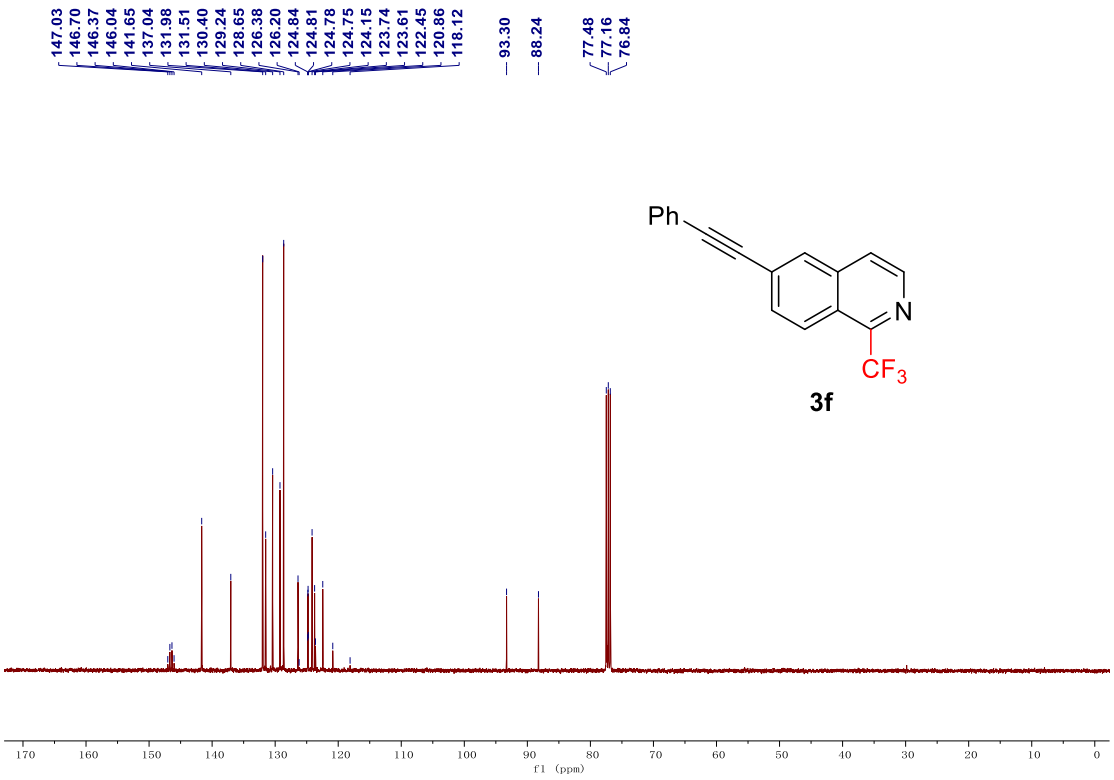
3e


-63.46
O
MeO
N
CF3
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

3e


8.61
8.59
8.27
8.25
8.08
7.80
7.80
7.79
7.79
7.78
7.77
7.61
7.60
7.60
7.59
7.58
7.58
7.40
7.40
7.39
7.26
Ph
N
CF3
1.00
0.99
0.99
1.97
2.04
3.02
f1 (ppm)

3f


147.03
146.70
146.37
146.04
141.65
137.04
131.98
131.51
130.40
129.24
128.65
126.38
126.20
124.84
124.81
124.78
124.75
124.15
123.74
123.61
122.45
120.86
118.12
93.30
88.24
77.48
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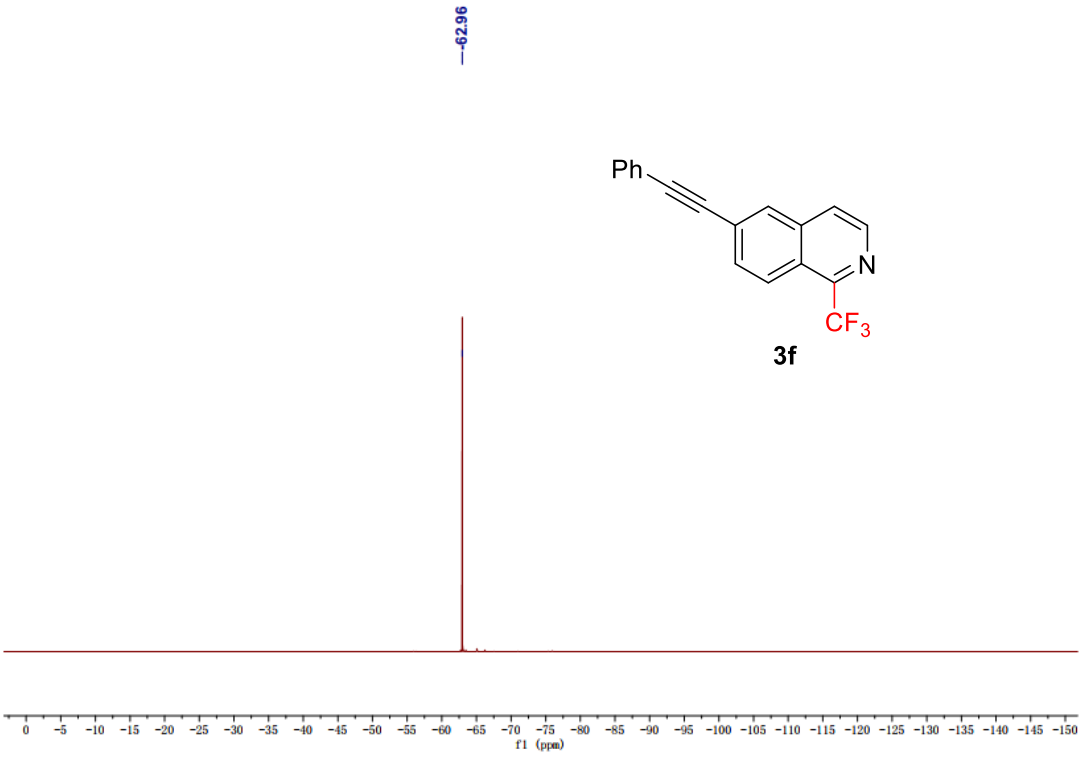
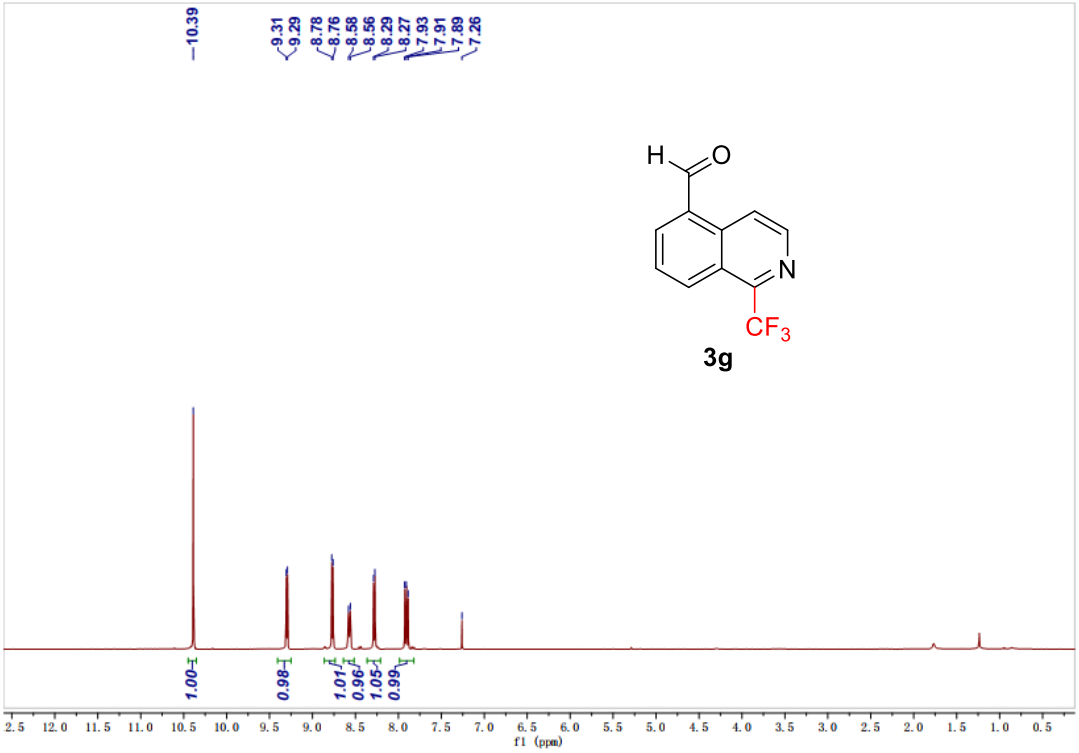
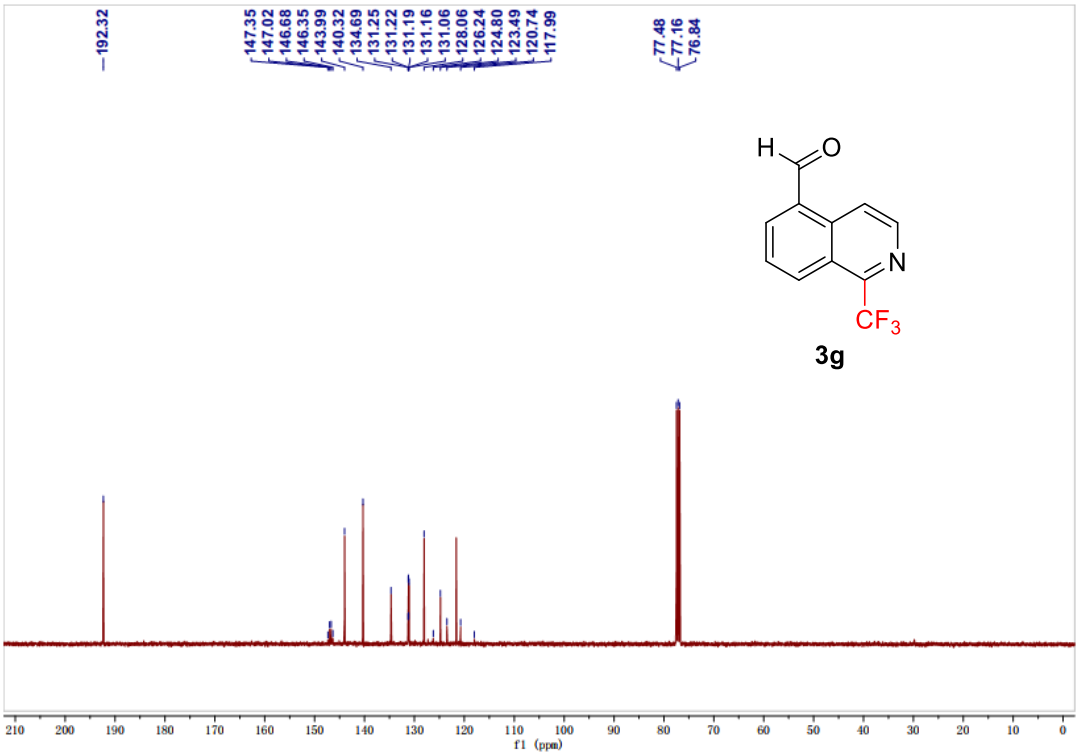
76.84
Ph
N
CF3
3f
f1 (ppm)


-62.96
Ph
N
CF3
3f
f1 (ppm)


10.39
9.31
9.29
8.78
8.76
8.58
8.56
8.29
8.27
7.93
7.91
7.89
7.26
H
O
N
CF3
3g
1.00
0.98
1.01
0.96
1.05
0.99
f1 (ppm)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146.68
146.35
143.99
140.32
134.69
131.25
131.22
131.19
131.16
131.06
128.06
126.24
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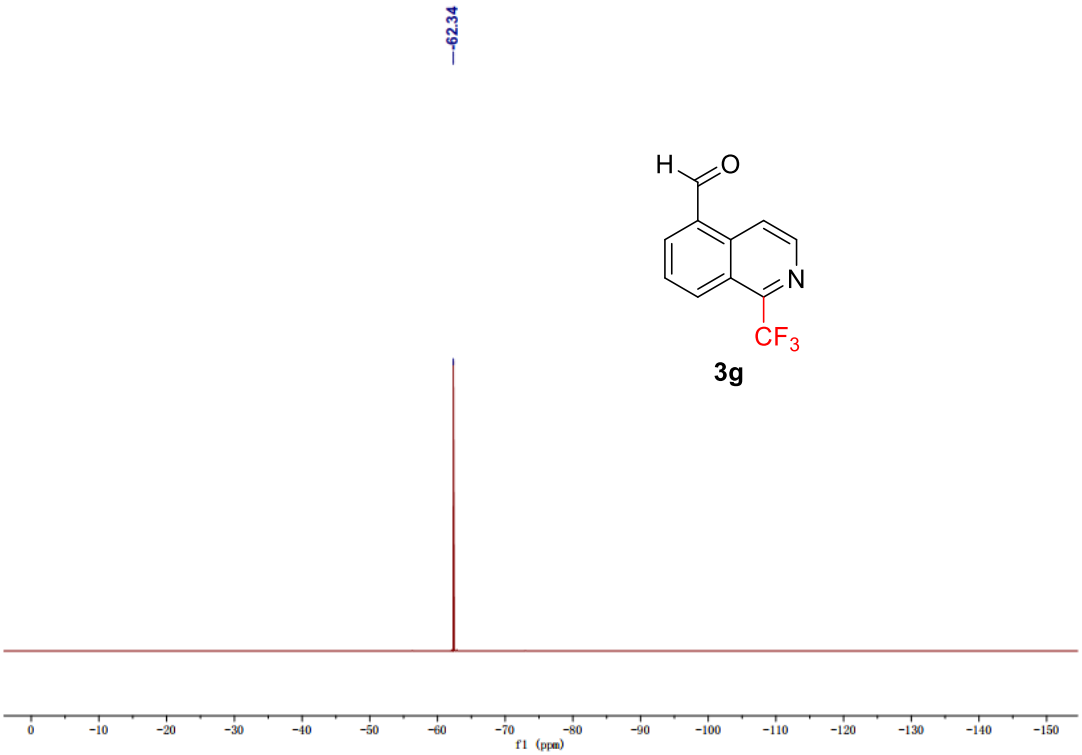
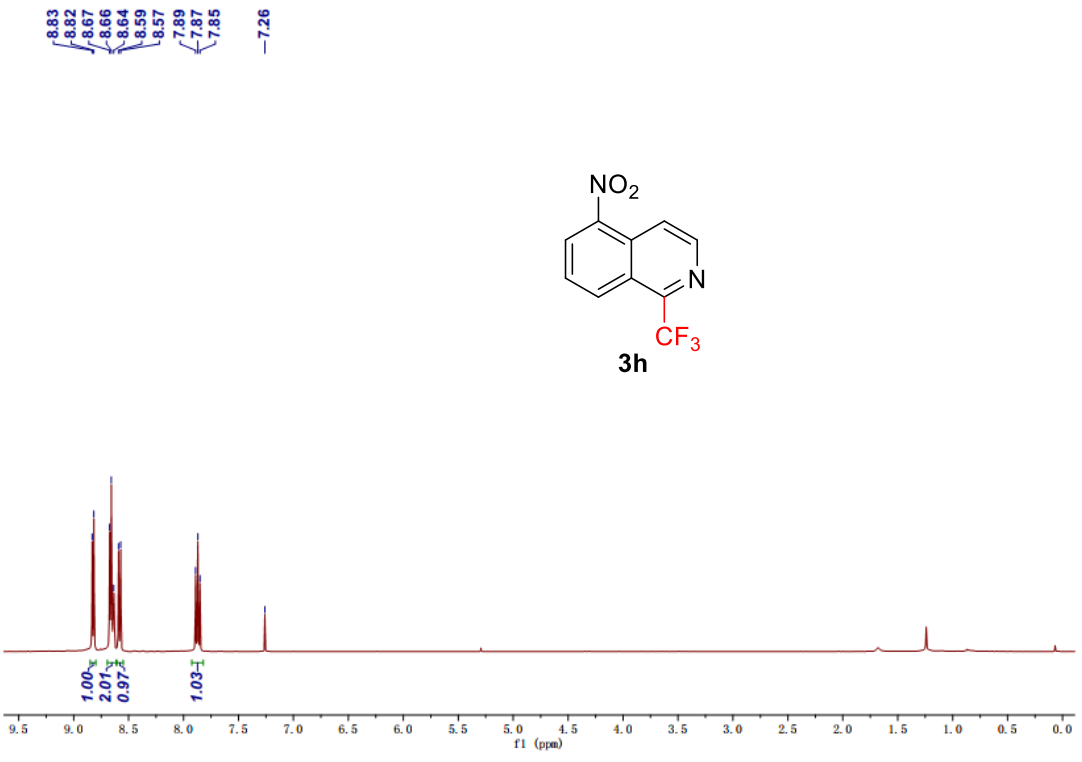
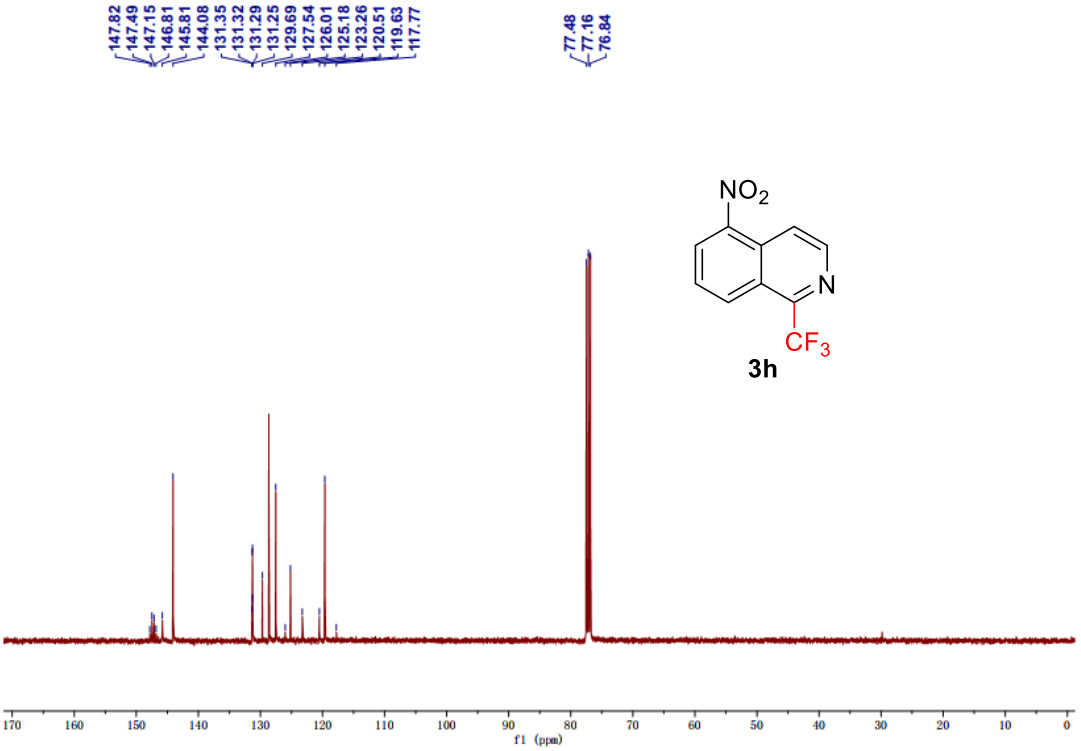
76.84
H
O
N
CF3
3g
f1 (ppm)


-62.34
H
O
N
CF3
f1 (ppm)

3g


8.83
8.82
8.67
8.66
8.64
8.59
8.57
7.89
7.87
7.85
7.26
NO2
N
CF3
1.00
2.01
0.97
1.03
f1 (ppm)

3h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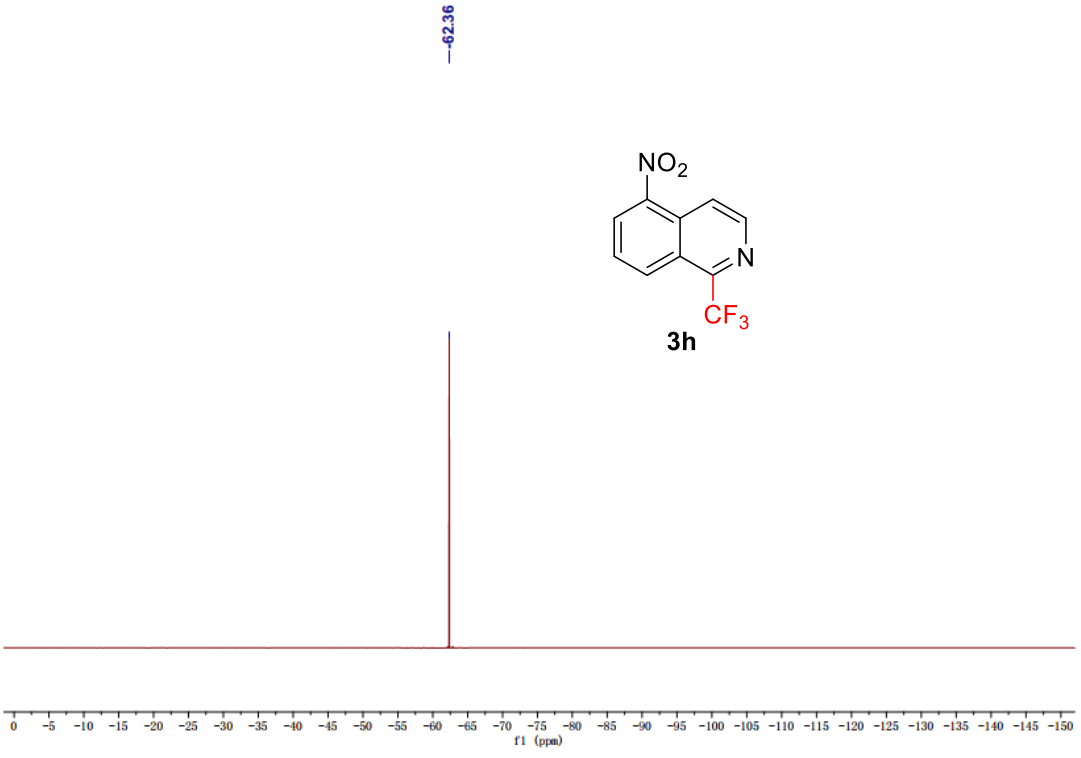
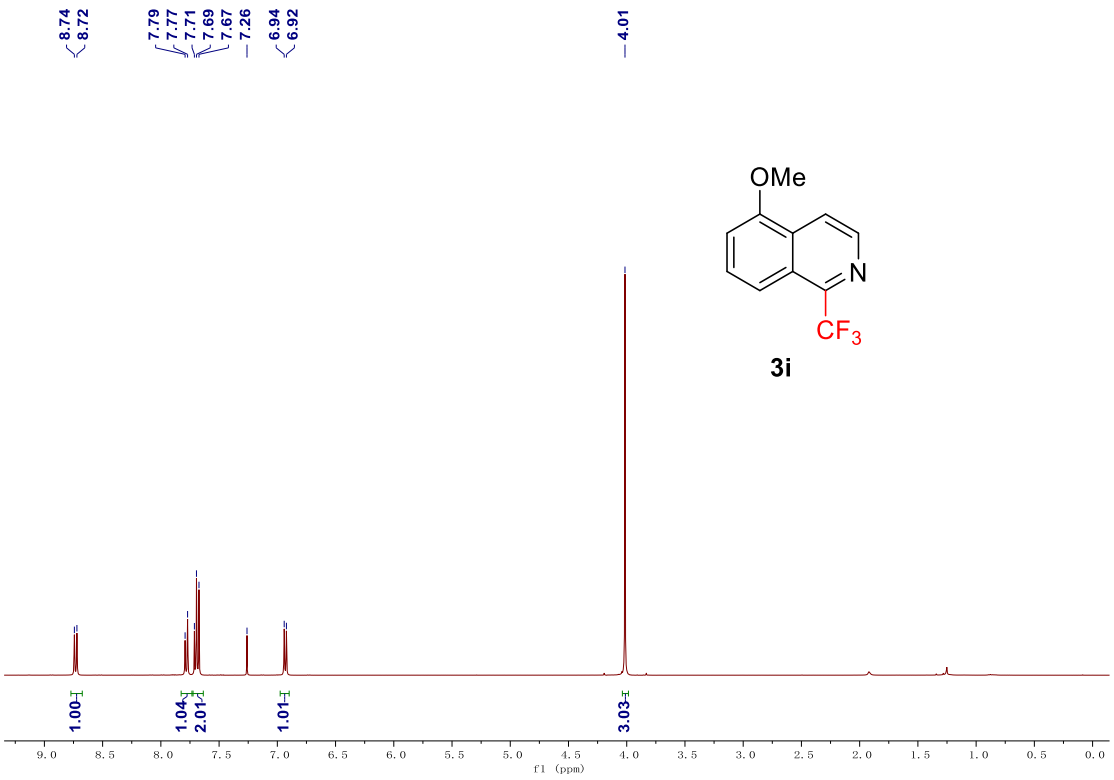
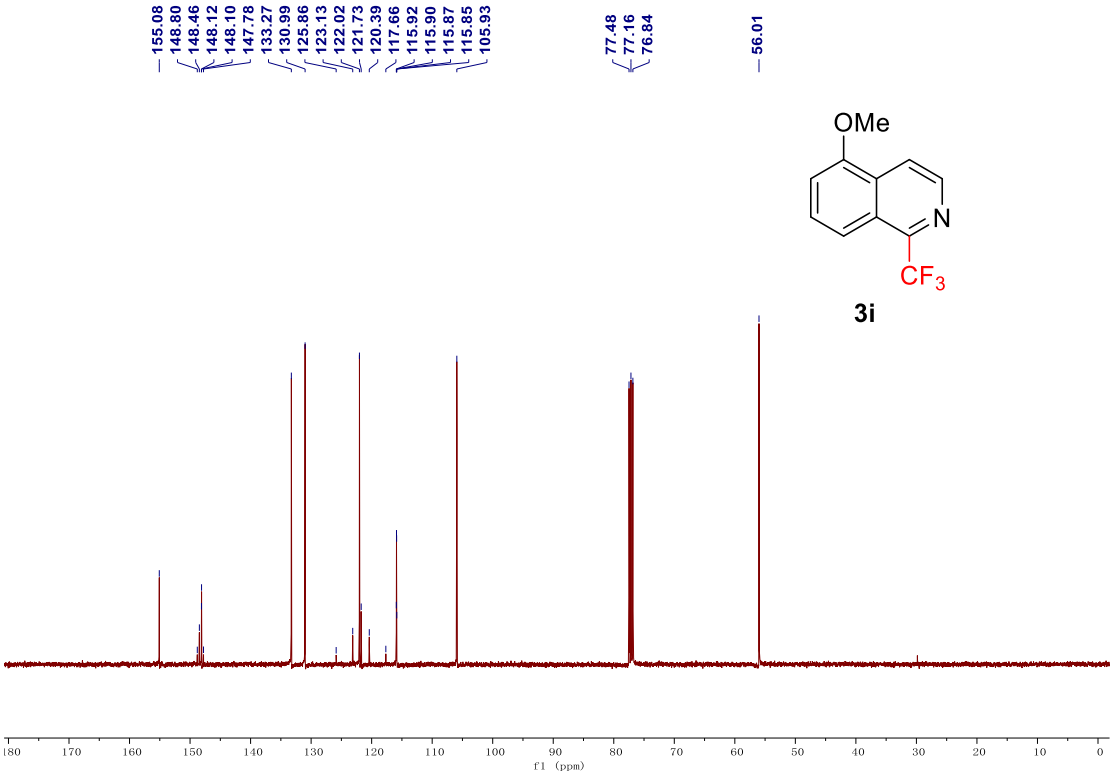
145.81
144.08
131.35
131.32
131.29
131.25
129.69
127.54
126.01
125.18
123.26
120.51
119.63
117.77
77.48
77.16
76.84
NO2
N
CF3
3h
f1 (ppm)


-62.36
NO2
N
CF3
3h
f1 (ppm)


8.74
8.72
7.79
7.77
7.71
7.69
7.67
7.26
6.94
6.92
4.01
OMe
N
CF3
3i
1.00
1.04
2.01
1.01
3.03
f1 (ppm)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148.10
147.78
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130.99
125.86
123.13
122.02
121.73
120.39
117.66
115.92
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115.87
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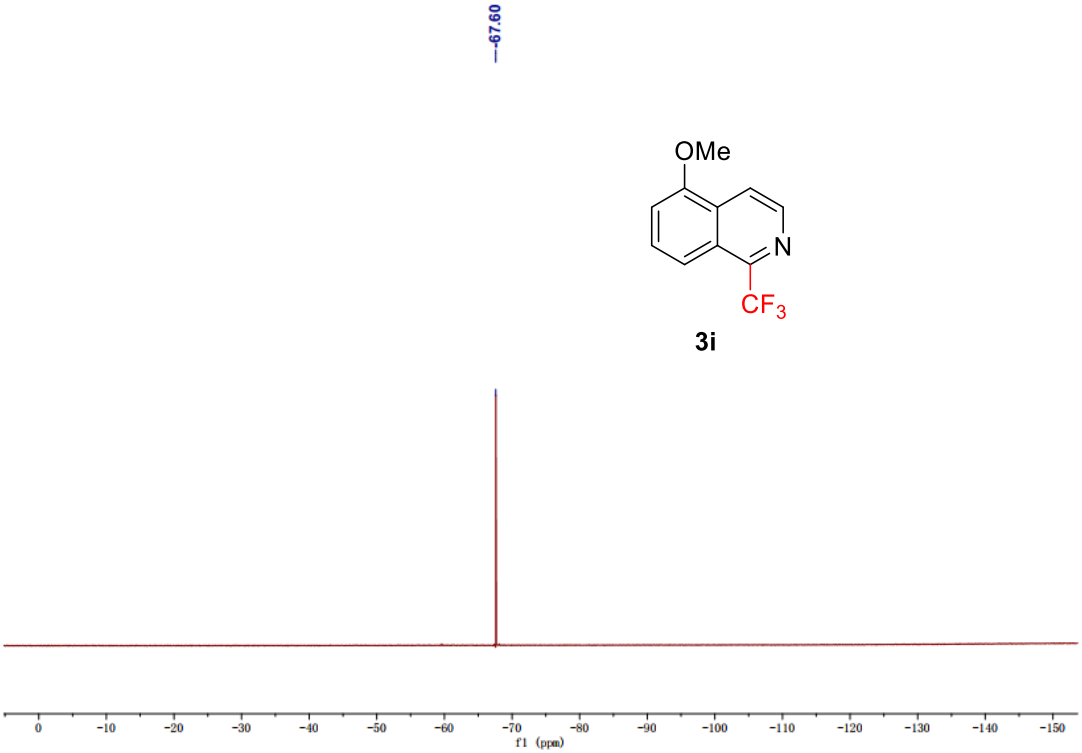
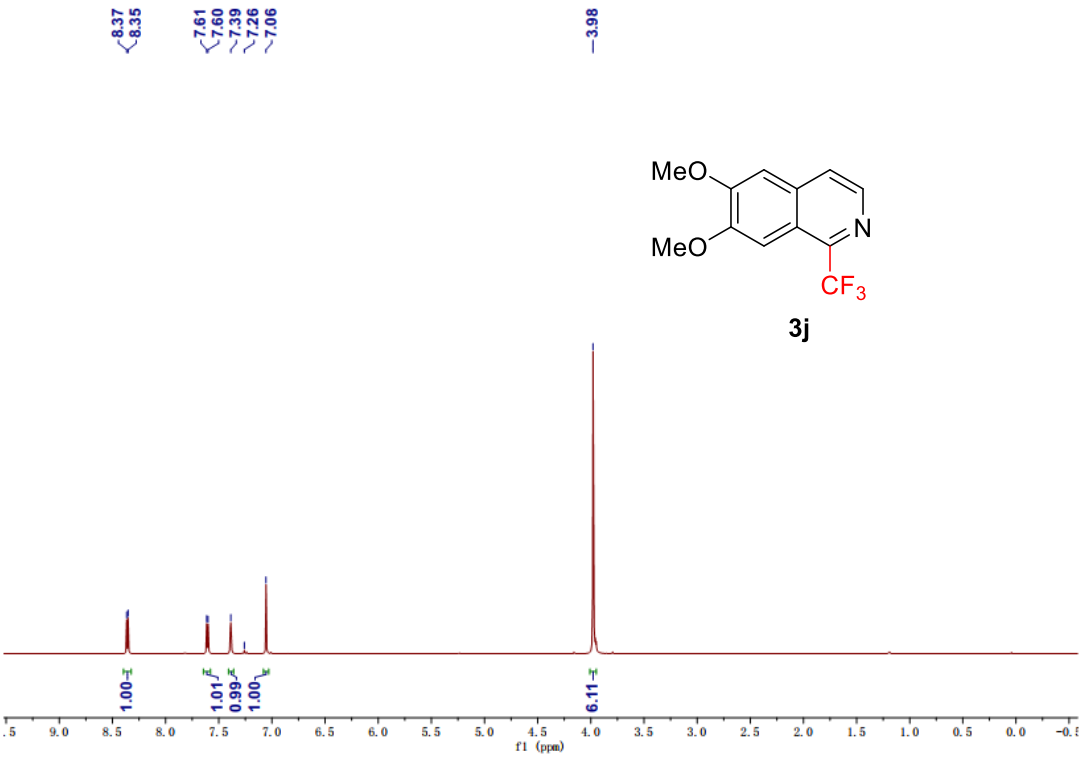
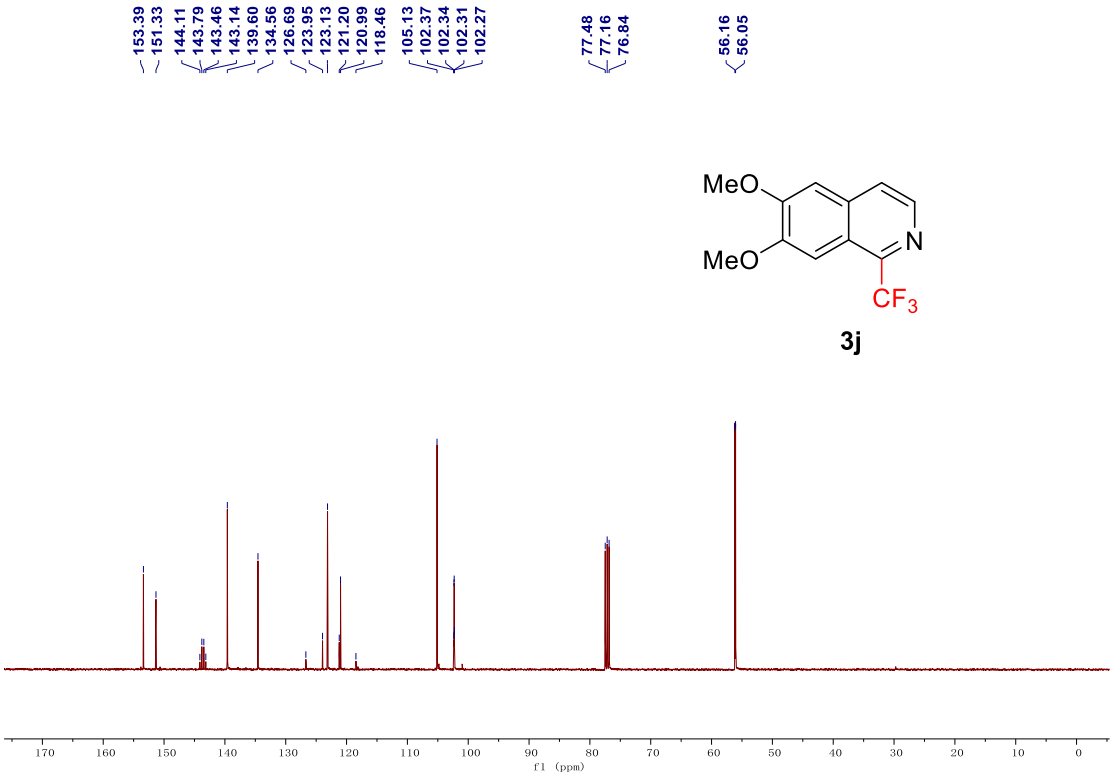
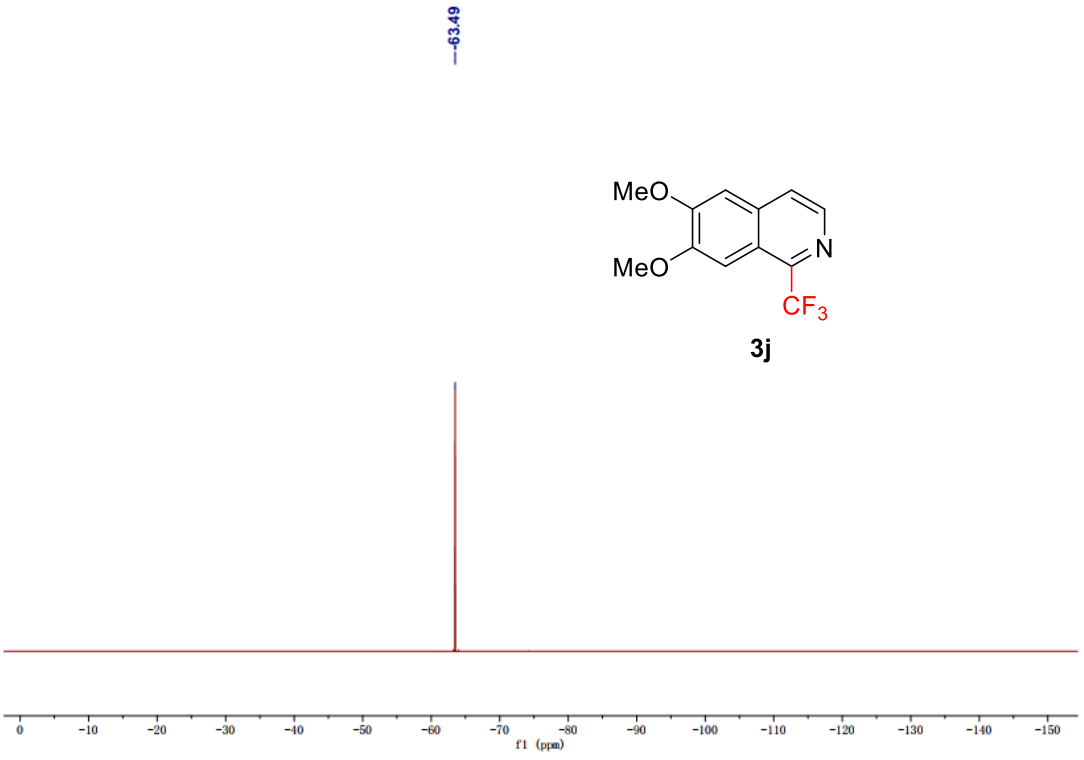
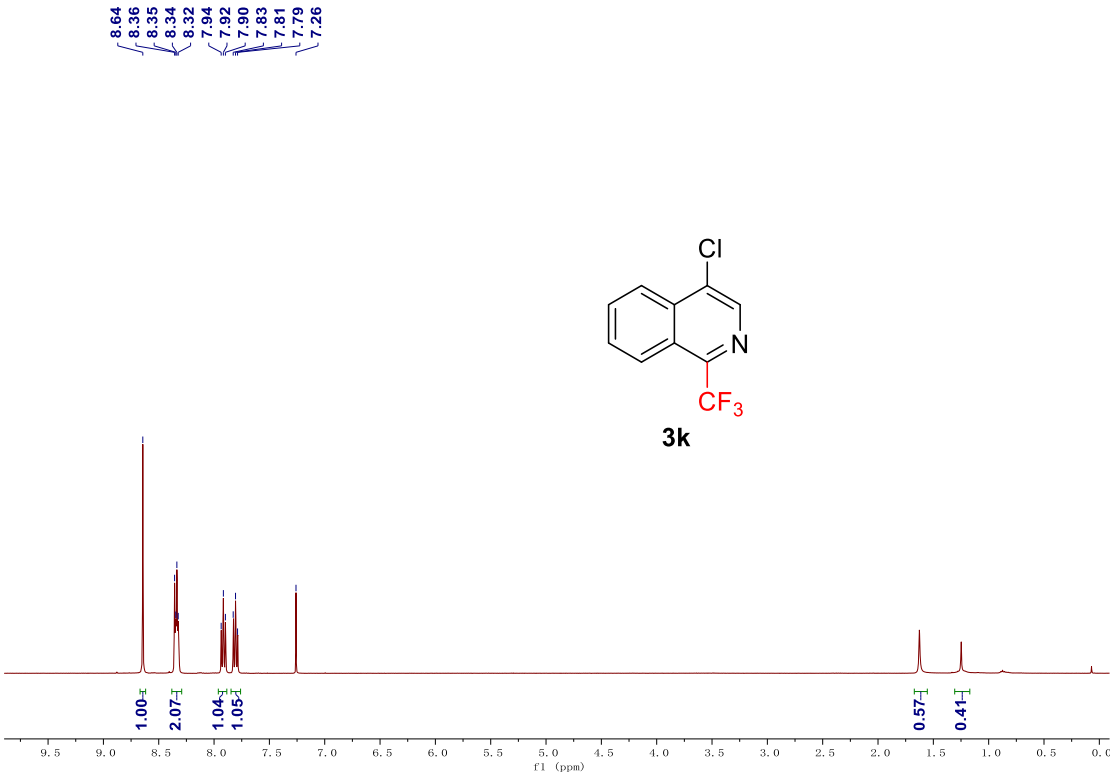
105.93
77.48
77.16
76.84
56.01
OMe
N
CF3
3i
f1 (ppm)

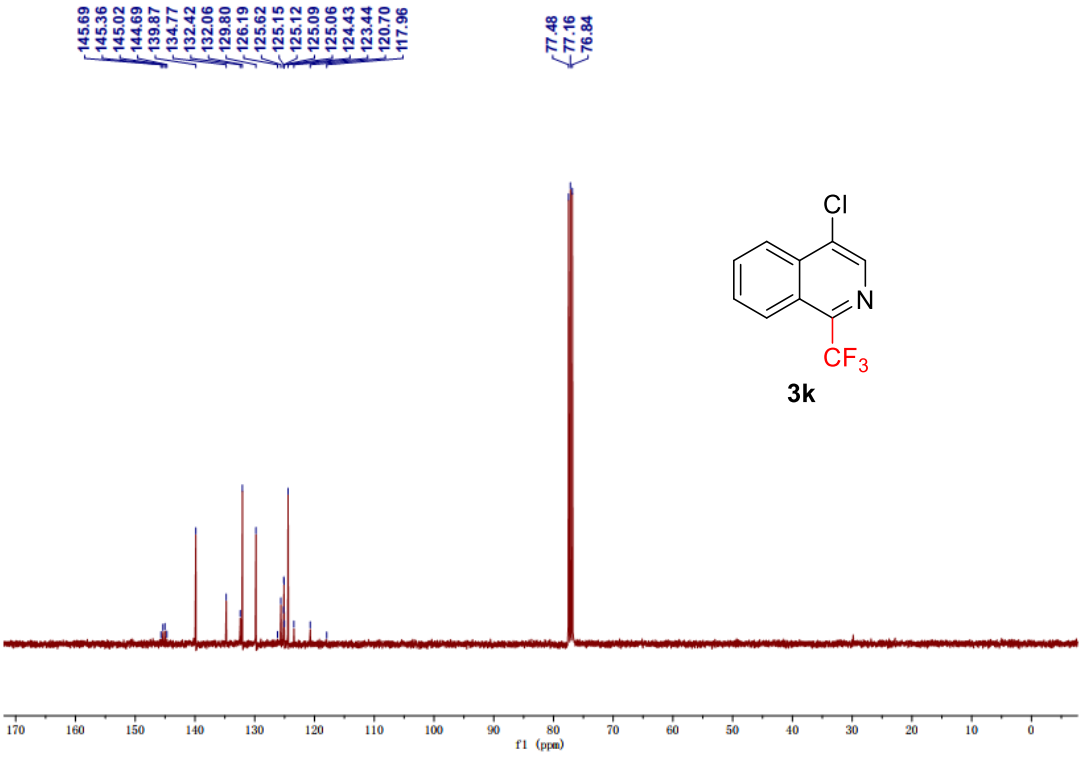

-67.60
OMe
N
CF3
3i
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

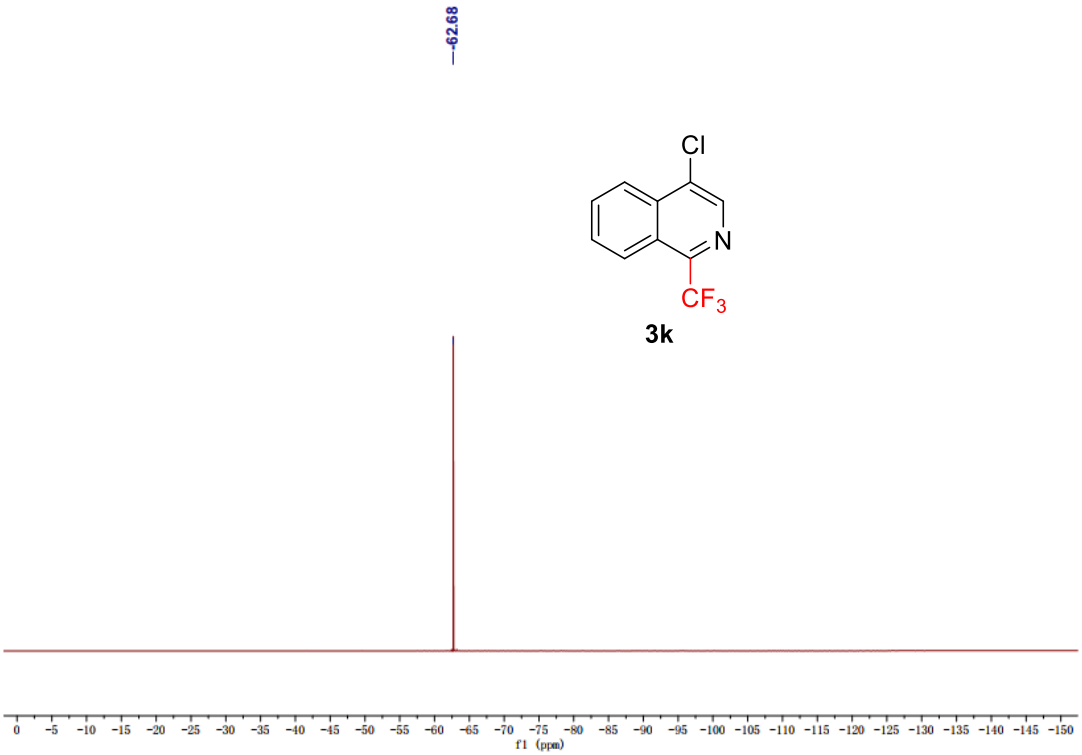

8.37
8.35
7.61
7.60
7.39
7.26
7.06
3.98
MeO
MeO
N
CF3
3j
1.00
1.01
0.99
1.00
6.11
f1 (ppm)


153.39
151.33
144.11
143.79
143.46
143.14
139.60
134.56
126.69
123.95
123.13
121.20
120.99
118.46
105.13
102.37
102.34
102.31
102.27
77.48
77.16
76.84
56.16
56.05
MeO
MeO
N
CF3
3j
f1 (ppm)

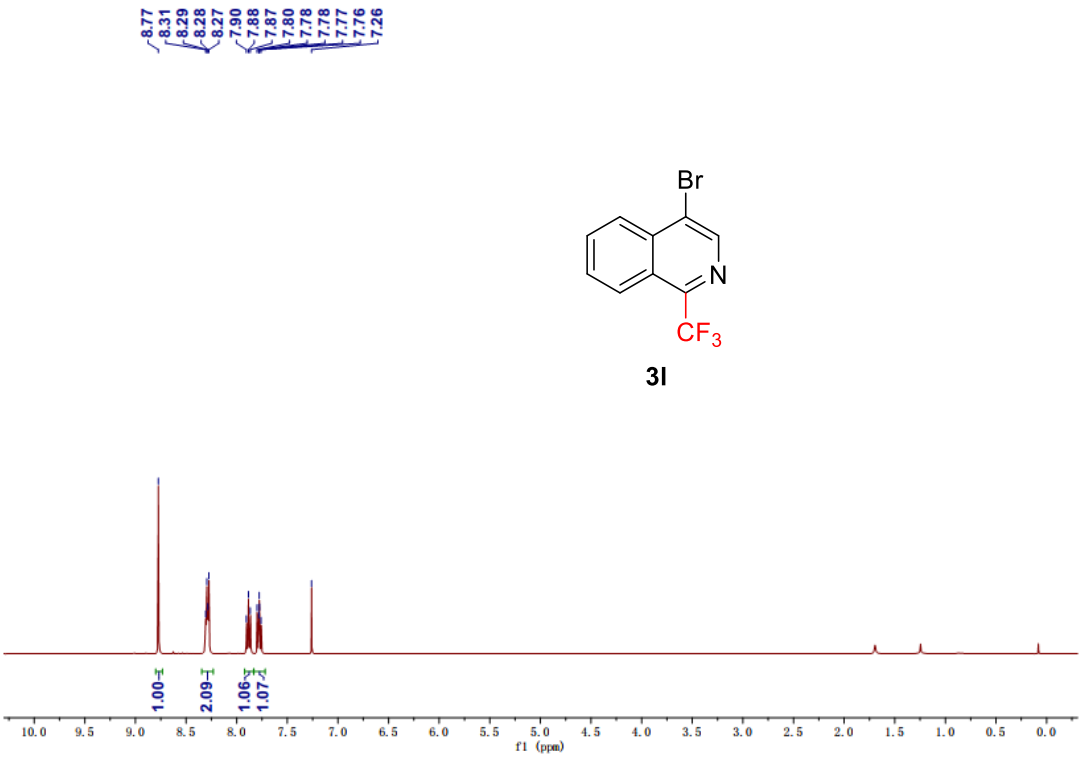

-63.49
MeO
MeO
N
CF3
3j
f1 (ppm)


8.64
8.36
8.35
8.34
8.32
7.94
7.92
7.90
7.83
7.81
7.79
7.26
Cl
N
CF3
3k
1.00
2.07
1.04
1.05
0.57
0.41
f1 (ppm)


145.69
145.36
145.02
144.69
139.87
134.77
132.42
132.06
129.80
126.19
125.62
125.15
125.12
125.09
125.06
124.43
123.44
120.70
117.96
77.48
77.16
76.84
Cl
N
CF3
3k
f1 (ppm)

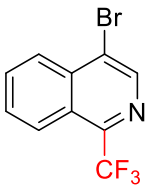

-62.68
Cl
N
CF3
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150
f1 (ppm)

3k

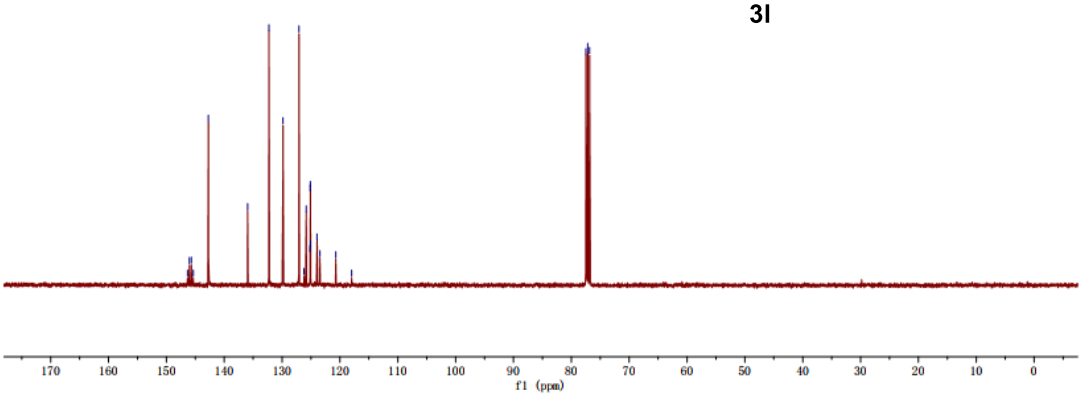

8.77
8.31
8.29
8.28
8.27
7.90
7.88
7.87
7.80
7.78
7.78
7.77
7.76
7.26
Br
N
CF3
1.00
2.09
1.06
1.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3l

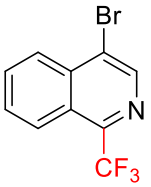

146.35
146.02
145.68
145.35
142.75
135.96
132.28
129.84
127.08
126.21
125.84
125.17
125.14
125.11
125.08
123.96
123.47
120.72
117.98
77.48
77.16
76.84


Br
N
CF3

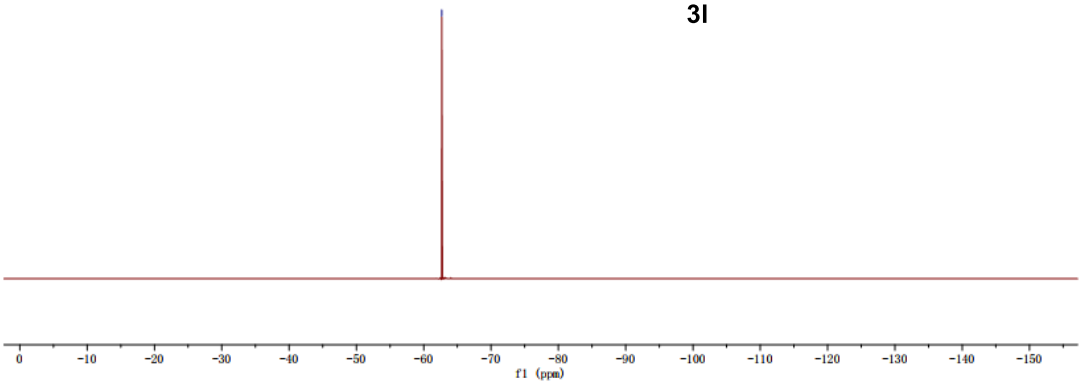
3l

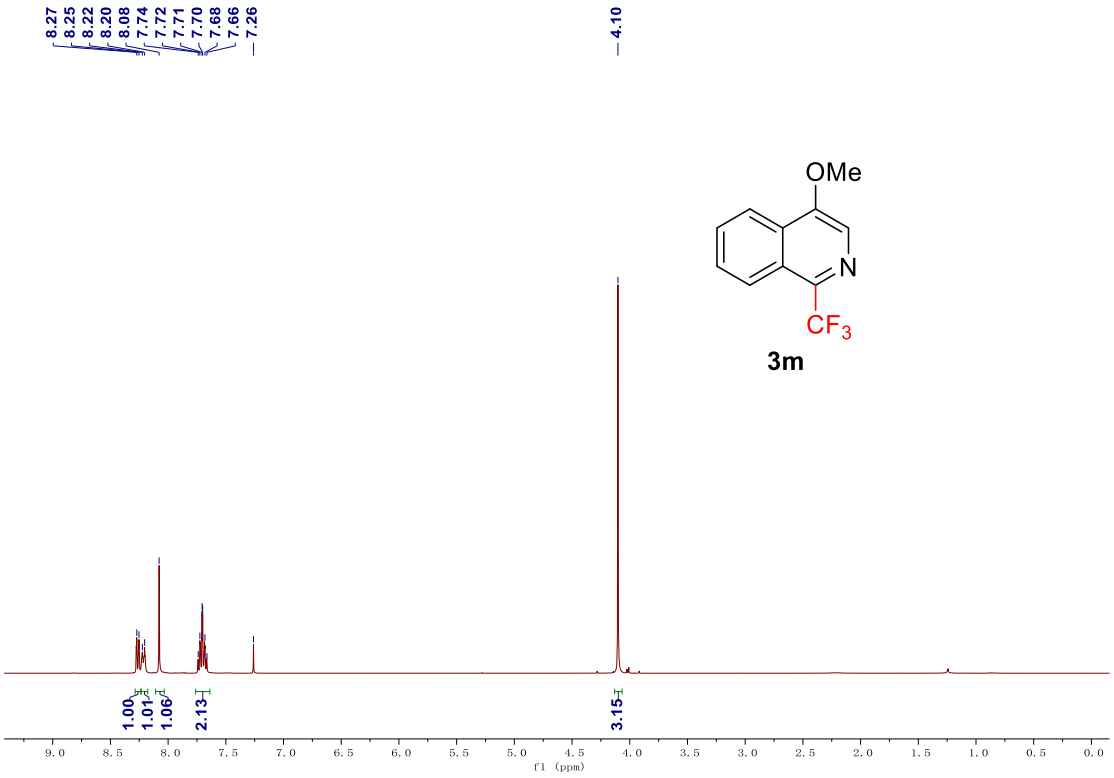

170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

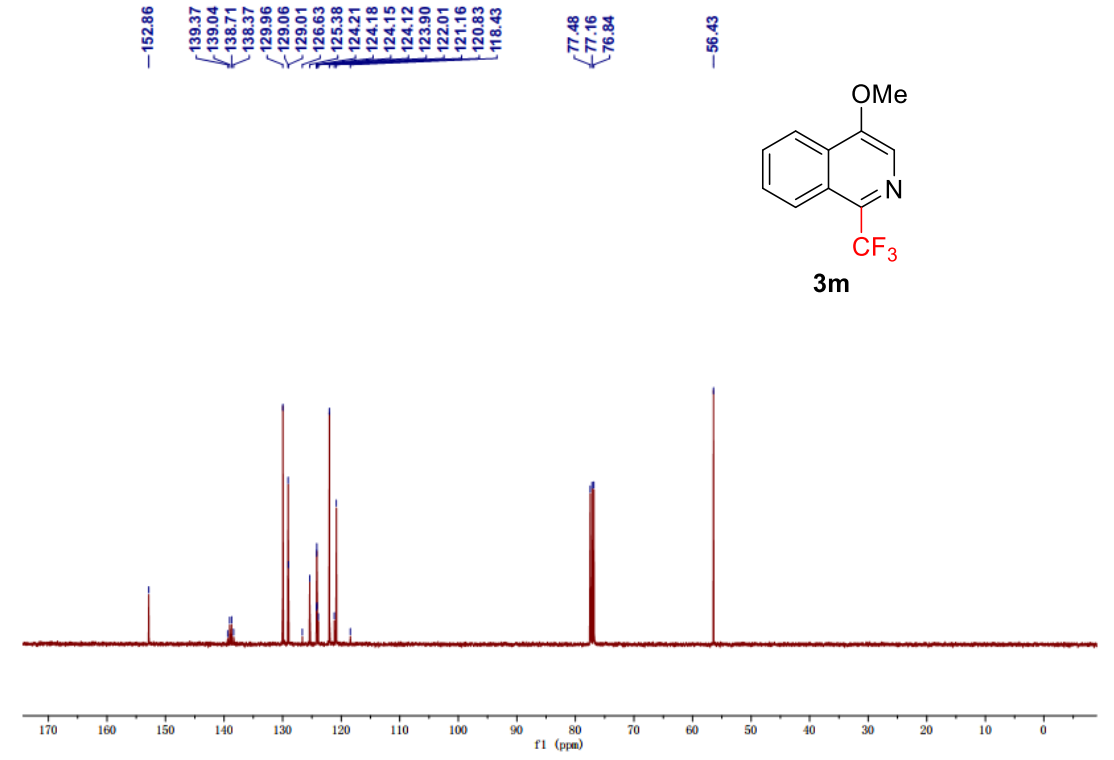

-62.68

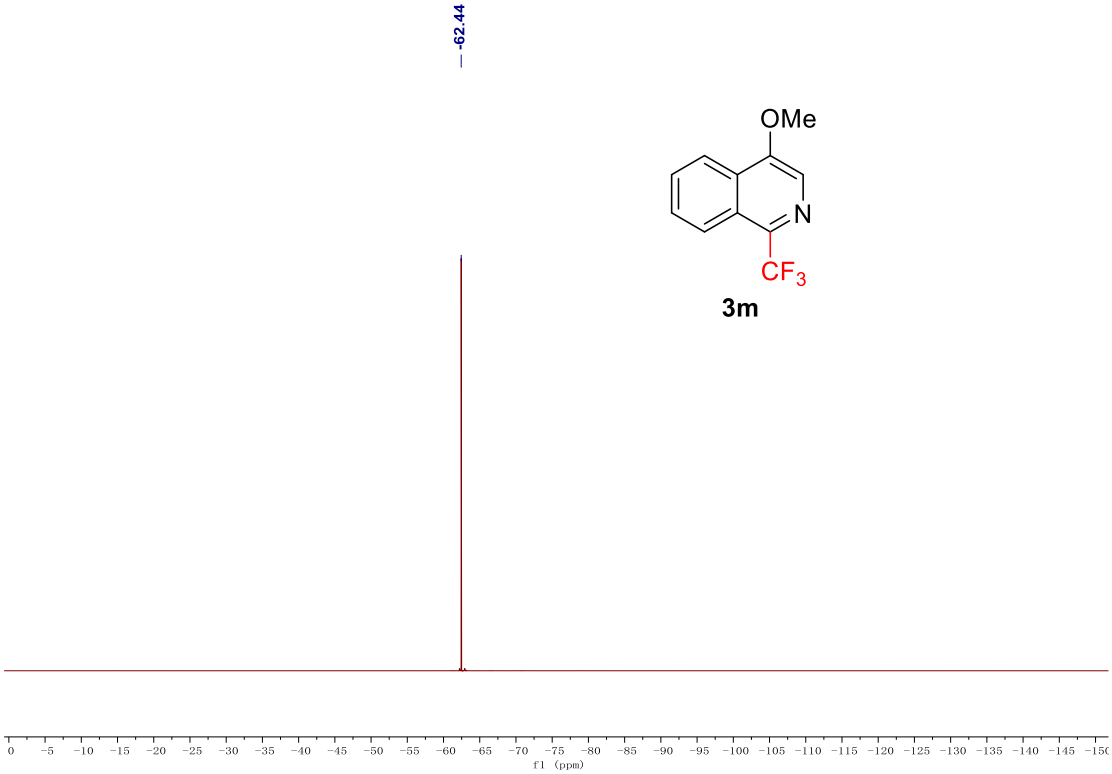

Br
N
CF3

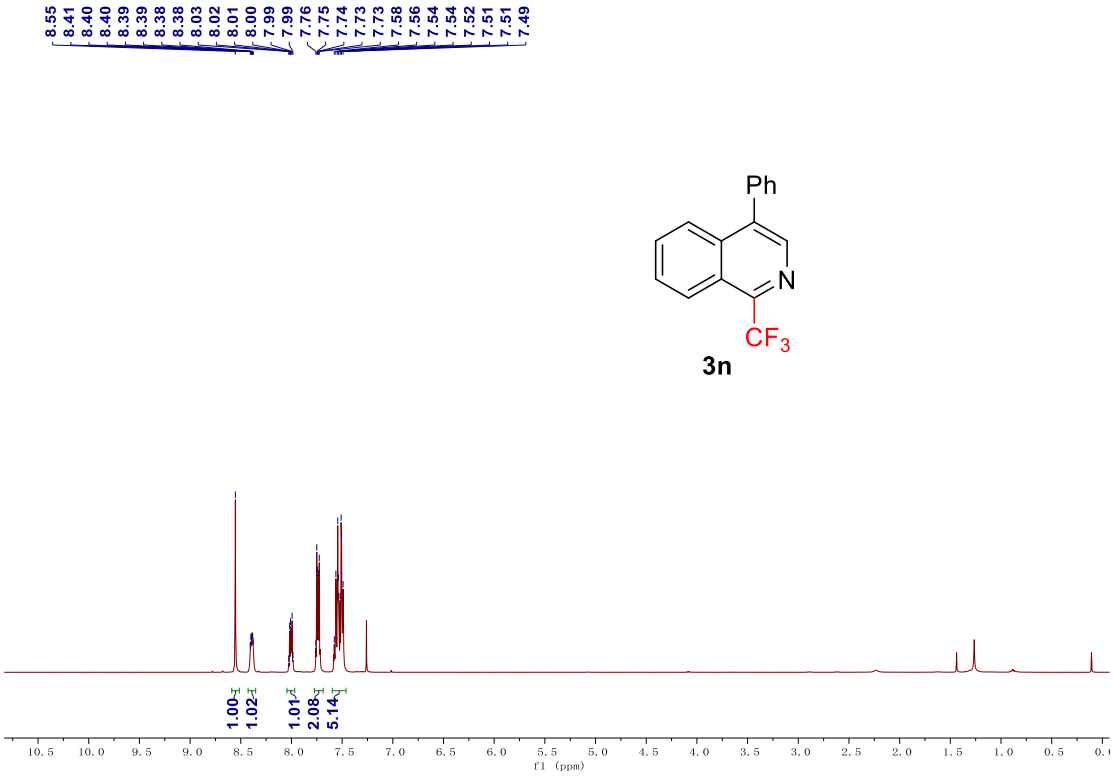
3l

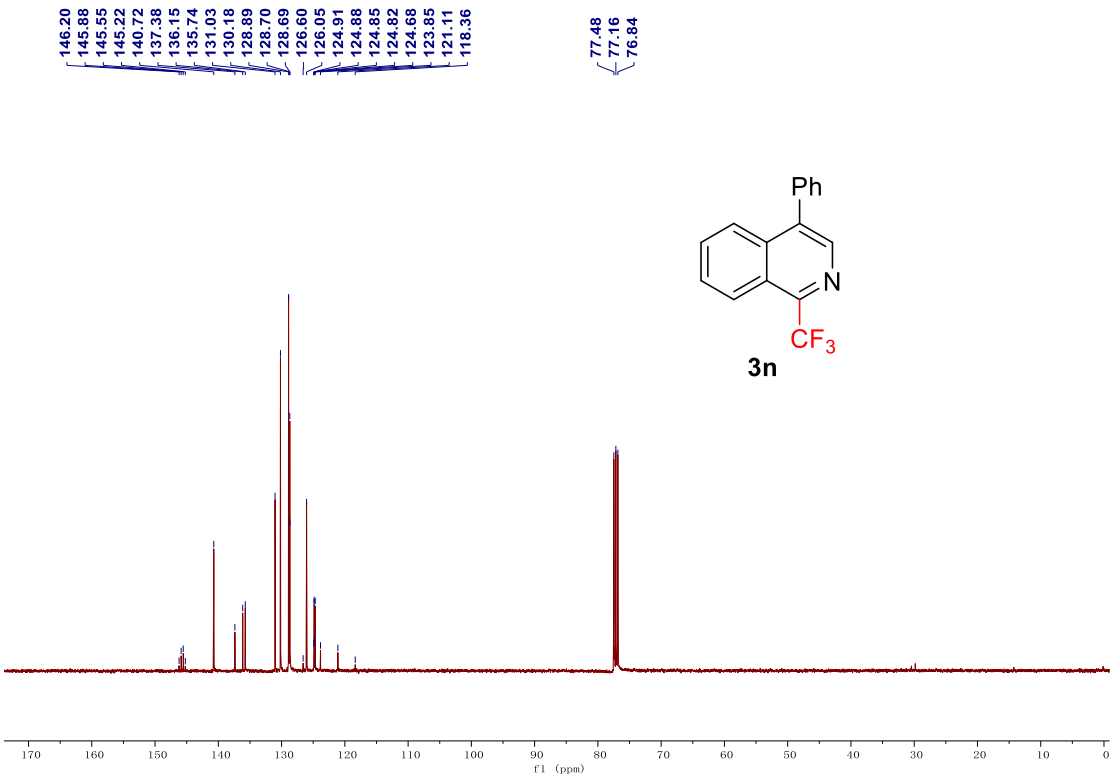

0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

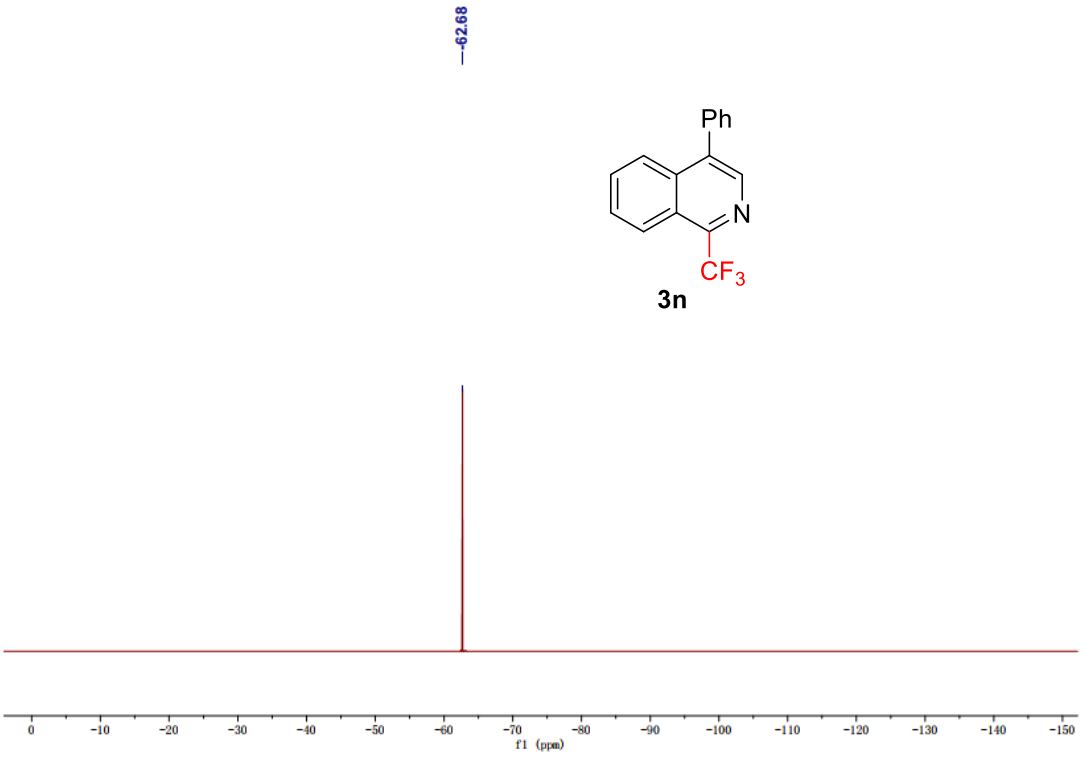

8.27
8.25
8.22
8.20
8.08
7.74
7.72
7.71
7.70
7.68
7.66
7.26
4.10
OMe
N
CF3
3m
1.00
1.01
1.06
2.13
3.15
f1 (ppm)


152.86
139.37
139.04
138.71
138.37
129.96
129.06
129.01
126.63
125.38
124.21
124.18
124.15
124.12
123.90
122.01
121.16
120.83
118.43
77.48
77.16
76.84
56.43
OMe
N
CF3
3m
f1 (ppm)

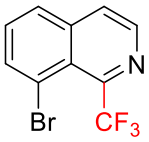

-62.44
OMe
N
CF3
3m
f1 (ppm)


8.55
8.41
8.40
8.40
8.39
8.39
8.38
8.38
8.03
8.02
8.01
8.00
7.99
7.99
7.76
7.75
7.74
7.73
7.73
7.58
7.56
7.54
7.54
7.52
7.51
7.51
7.49
Ph
N
CF3
3n
1.00
1.02
1.01
2.08
5.14
f1 (ppm)

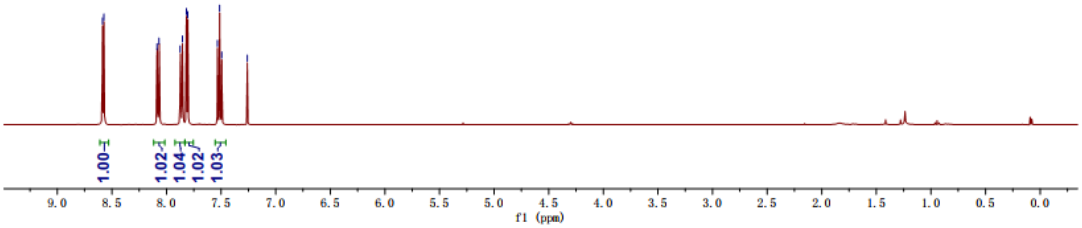

146.20
145.88
145.55
145.22
140.72
137.38
136.15
135.74
131.03
130.18
128.89
128.70
128.69
126.60
126.05
124.91
124.88
124.85
124.82
124.68
123.85
121.11
118.36
77.48
77.16
76.84
Ph
N
CF3
3n
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-62.68
Ph
N
CF3
3n
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)


8.59
8.57
8.09
8.07
7.87
7.85
7.82
7.81
7.53
7.51
7.49
7.26

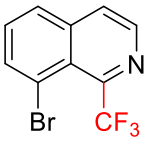

N
Br
CF3

3o

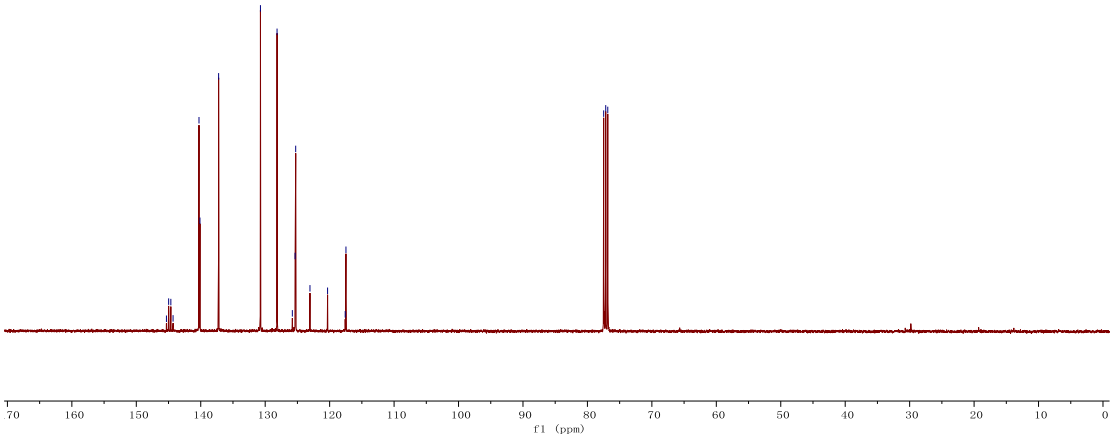

1.00
1.02
1.04
1.02
1.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

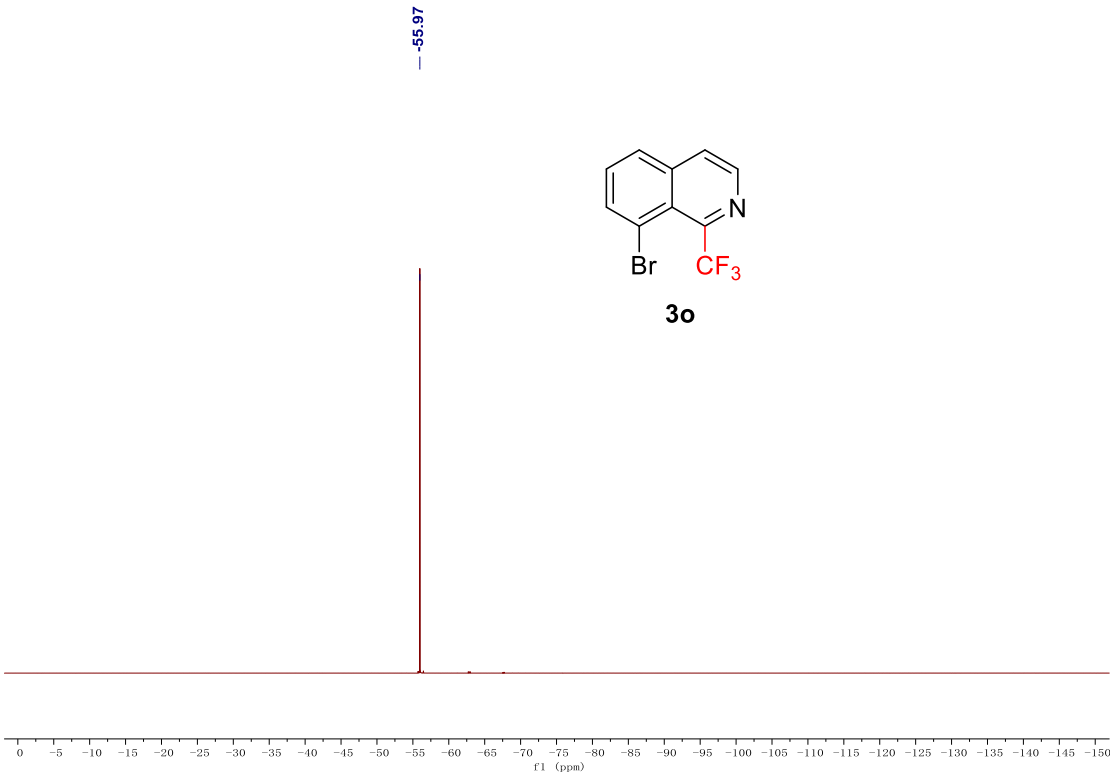

145.32
144.98
144.64
144.30
140.27
140.12
137.23
130.74
128.16
125.79
125.36
125.27
123.05
120.32
117.59
117.47


77.48
77.16
76.84


N
Br
CF3

3o

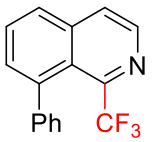

70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-55.97
f1 (ppm)

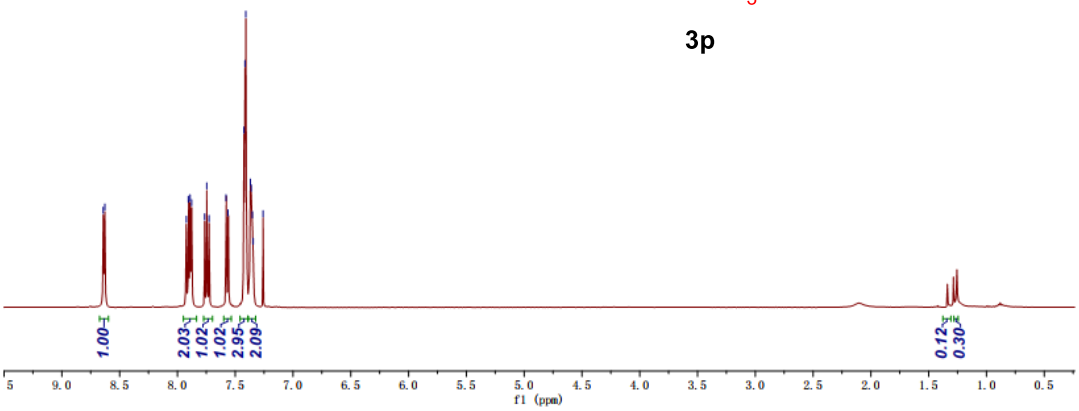
N
Br
CF3

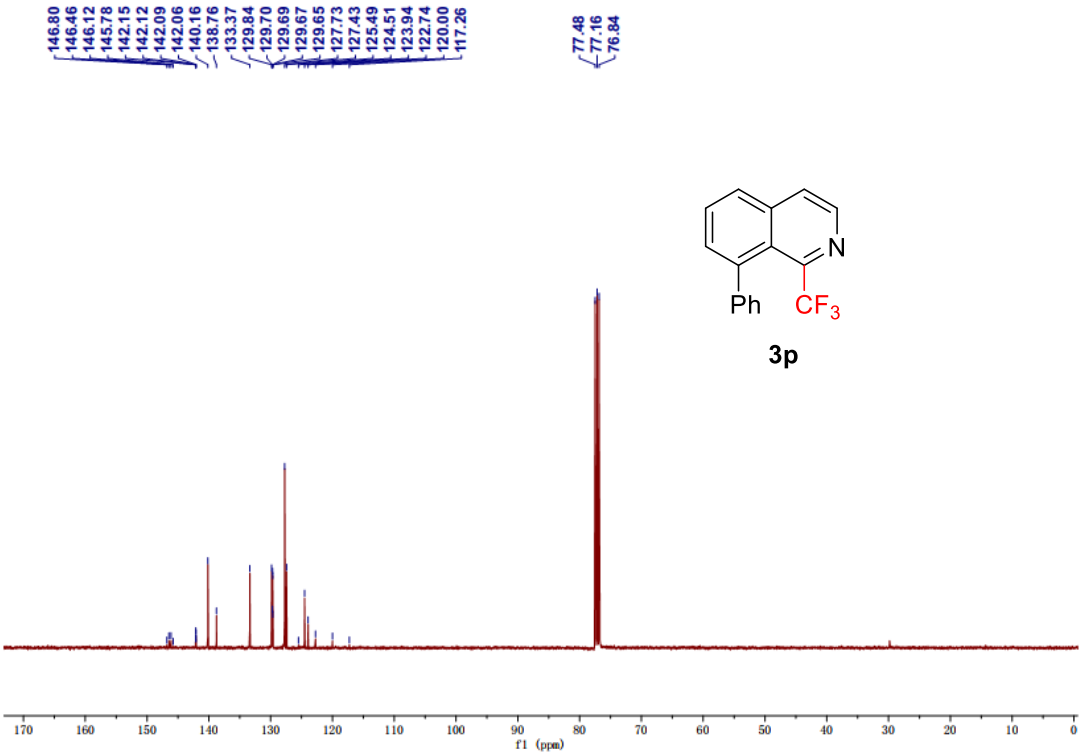
3o


8.64
8.63
7.92
7.91
7.89
7.88
7.76
7.75
7.73
7.58
7.56
7.42
7.42
7.41
7.37
7.36
7.35
7.34
7.26

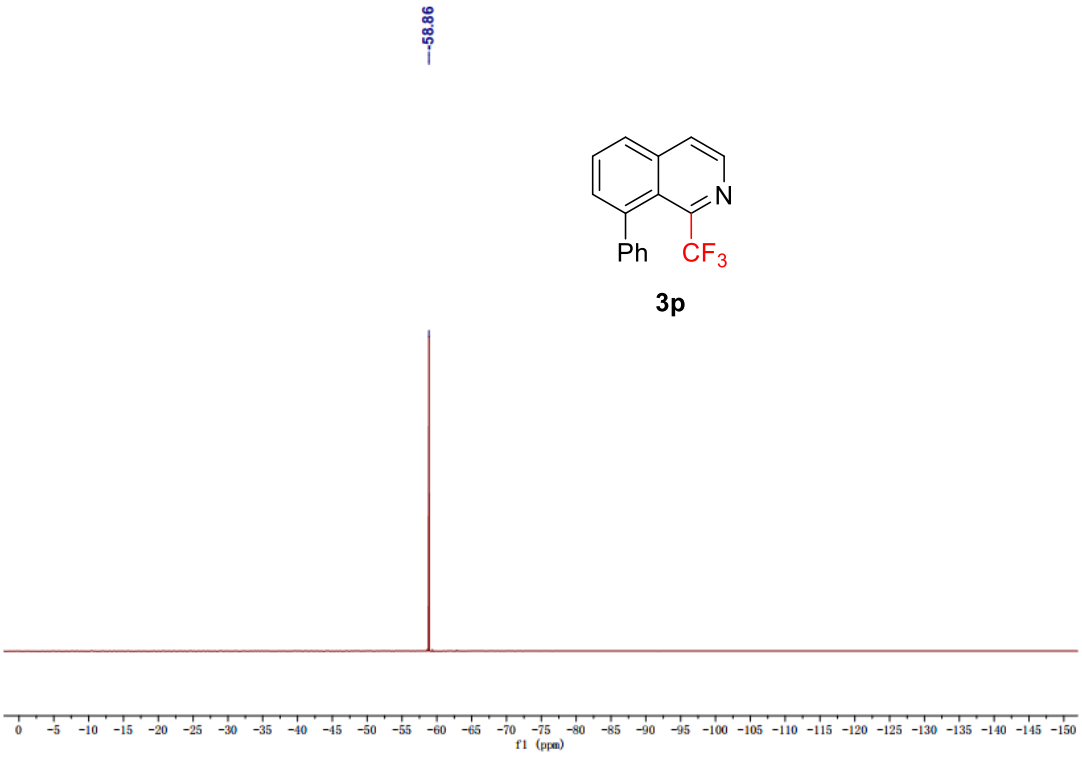

N
Ph
CF3

3p


1.00
2.03
1.02
1.02
2.95
2.09
0.12
0.30
f1 (ppm)

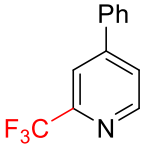

146.80
146.46
146.12
145.78
142.15
142.12
142.09
142.06
140.16
138.76
133.37
129.84
129.70
129.69
129.67
129.65
127.73
127.43
125.49
124.51
123.94
122.74
120.00
117.26
77.48
77.16
76.84
N
Ph
CF3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3p

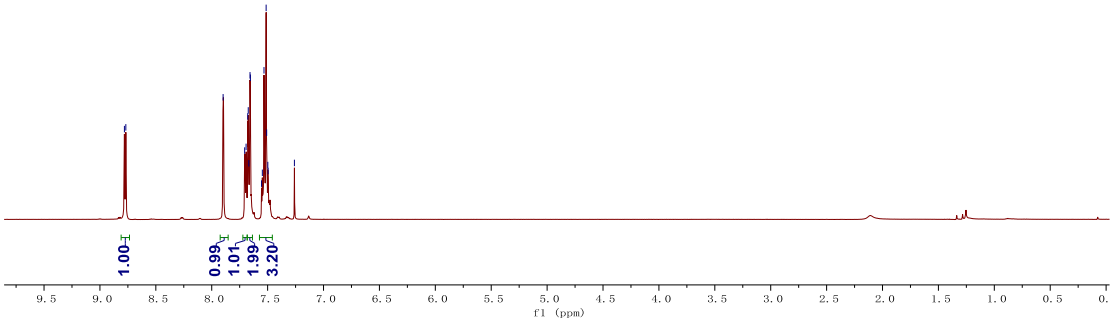

-58.86
N
Ph
CF3
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
f1 (ppm)

3p


8.78
8.77
7.90
7.71
7.69
7.68
7.67
7.67
7.66
7.65
7.55
7.55
7.53
7.51
7.51
7.50
7.50
7.26

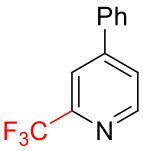

Ph
F3C
N

3q


1.00
0.99
1.01
1.99
3.20
f1 (ppm)

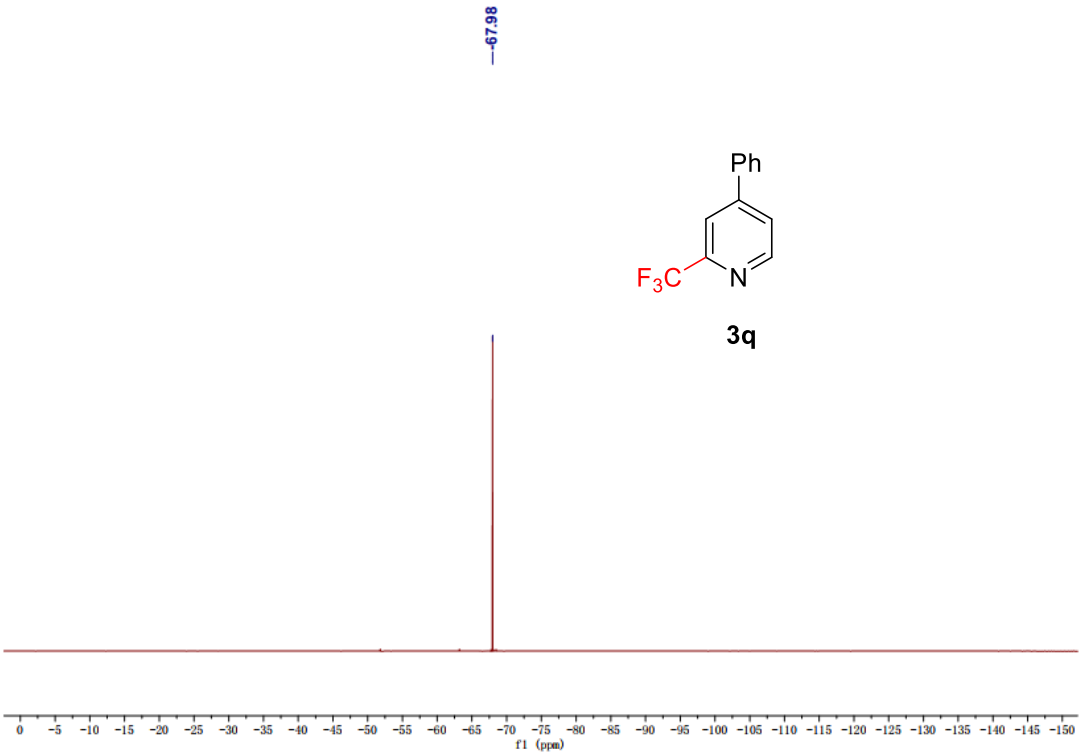

150.58
150.41
149.49
149.15
148.81
148.47
136.99
130.01
129.52
127.23
125.86
124.29
123.14
120.41
118.64
118.61
118.58
118.56
117.68


77.48
77.16
76.84

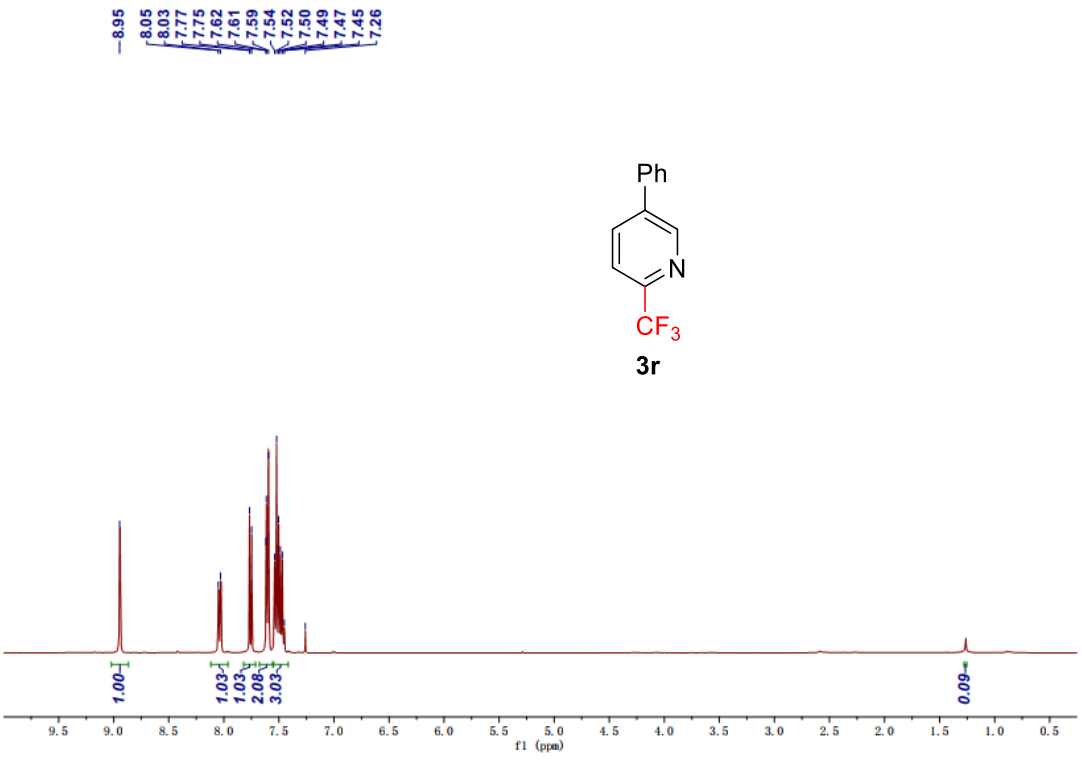

Ph
F3C
N

3q

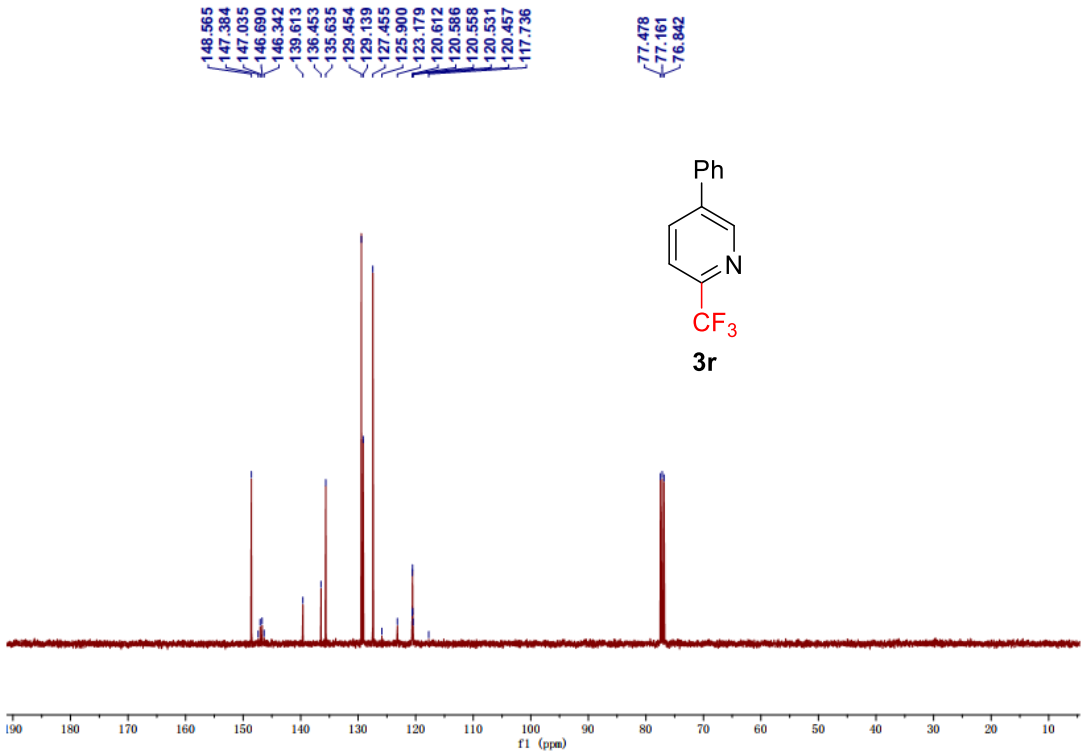
f1 (ppm)

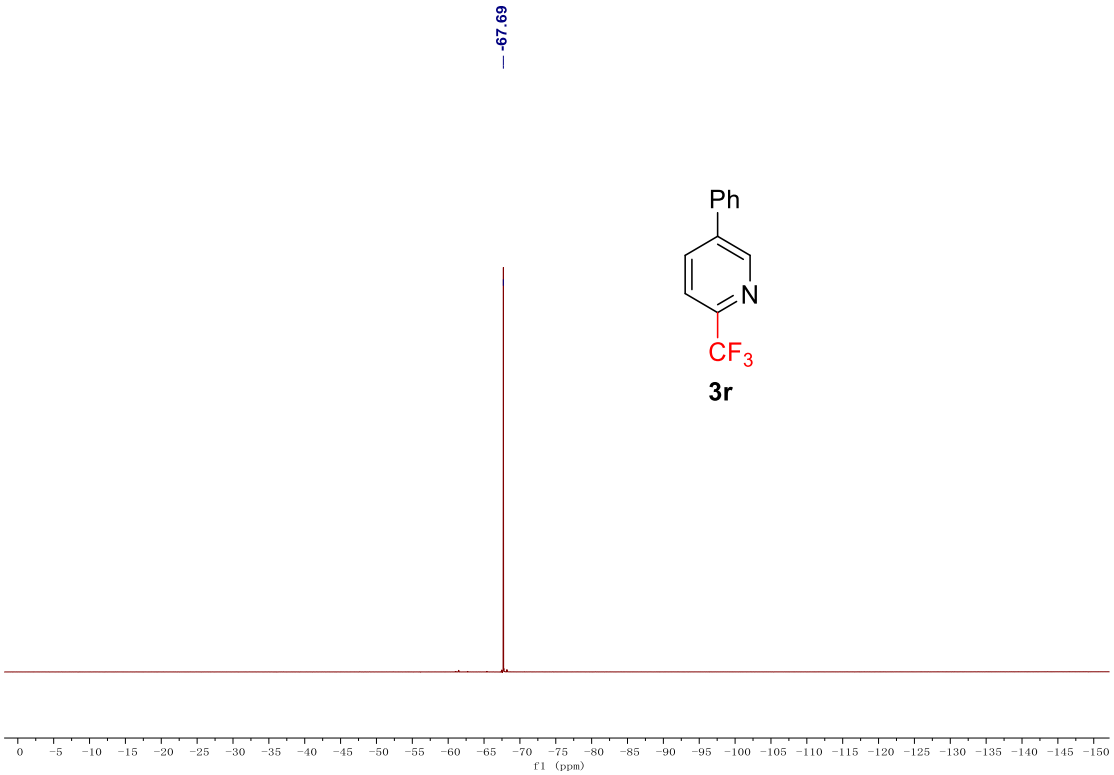

-67.98
Ph
F3C
N
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150
f1 (ppm)

3q

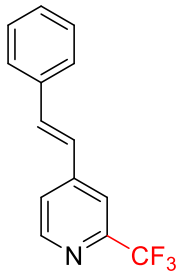

8.95
8.05
8.03
7.77
7.75
7.62
7.61
7.59
7.54
7.52
7.50
7.49
7.47
7.45
7.26
Ph
N
CF3
1.00
1.03
1.03
2.08
3.03
0.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

3r

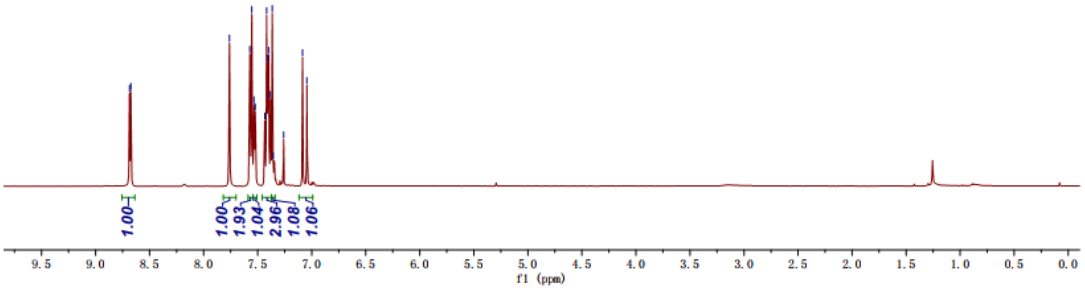

148.565
147.384
147.035
146.690
146.342
139.613
136.453
135.635
129.454
129.139
127.455
125.900
123.179
120.612
120.586
120.558
120.531
120.457
117.736
77.478
77.161
76.842
Ph
N
CF3
3r
f1 (ppm)


-67.69
Ph
N
CF3
3r
f1 (ppm)

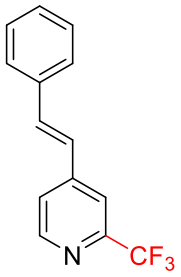

8.69
8.67
7.76
7.57
7.55
7.53
7.52
7.43
7.42
7.41
7.40
7.38
7.37
7.36
7.26
7.09
7.04


N
CF3

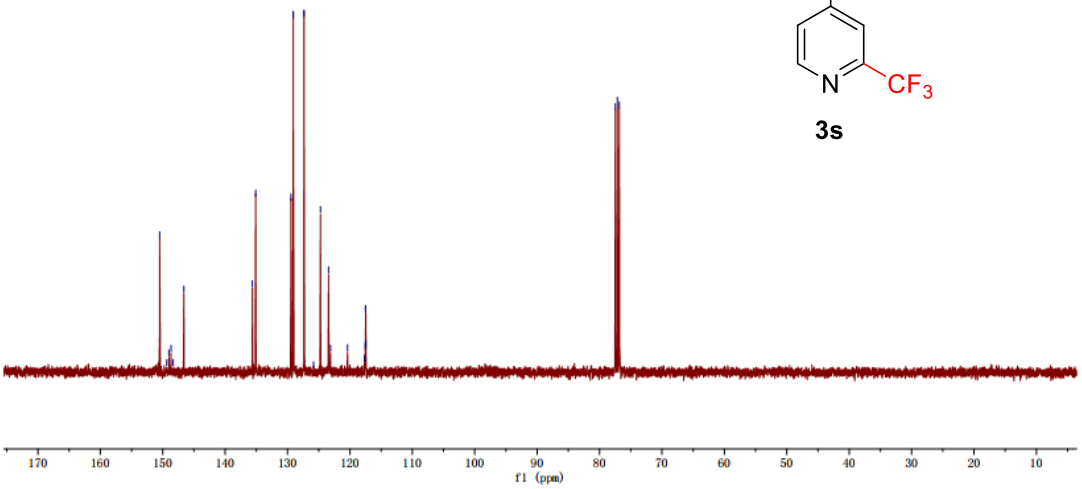
3s

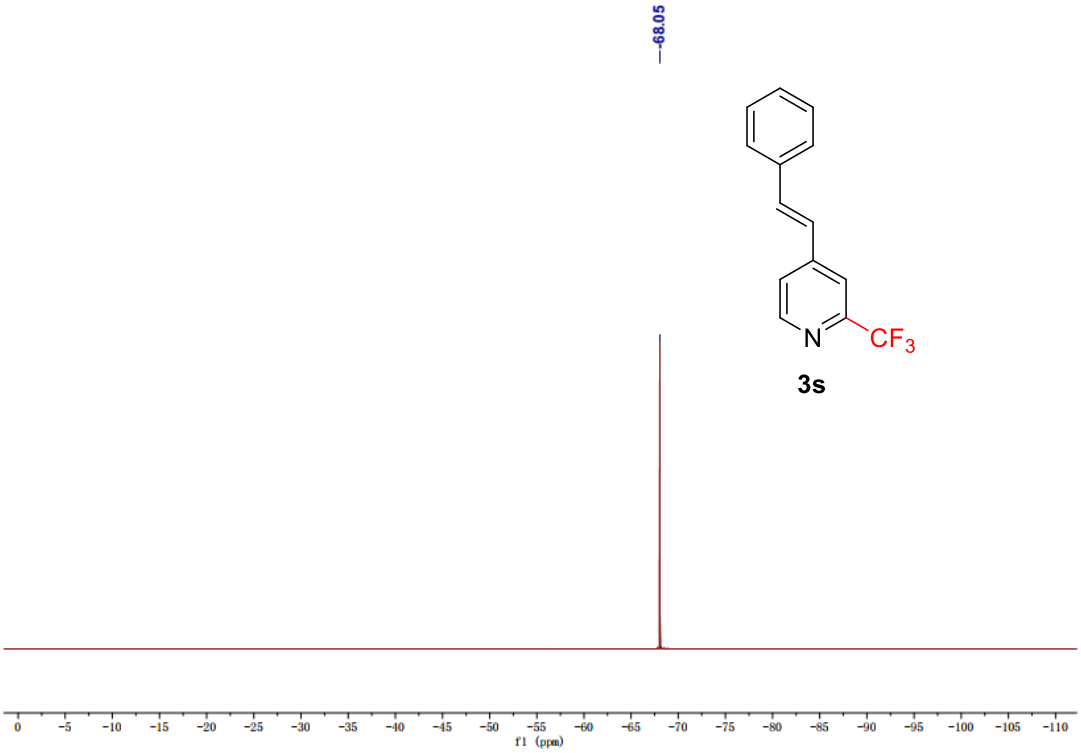

1.00
1.00
1.93
1.04
2.96
1.08
1.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


150.50
149.35
149.01
148.67
148.33
146.62
135.63
135.11
129.45
129.08
127.35
125.84
124.73
123.44
123.12
120.40
117.68
117.54
117.51
117.48
117.45
77.48
77.16
76.84

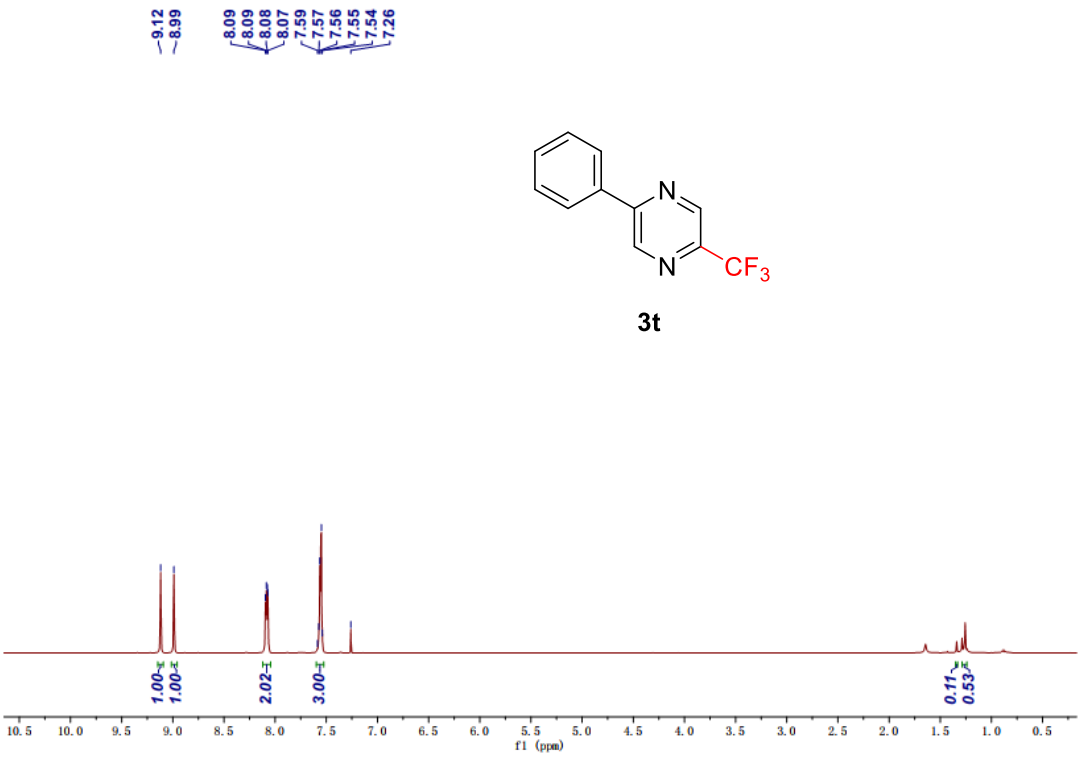

N
CF3

3s

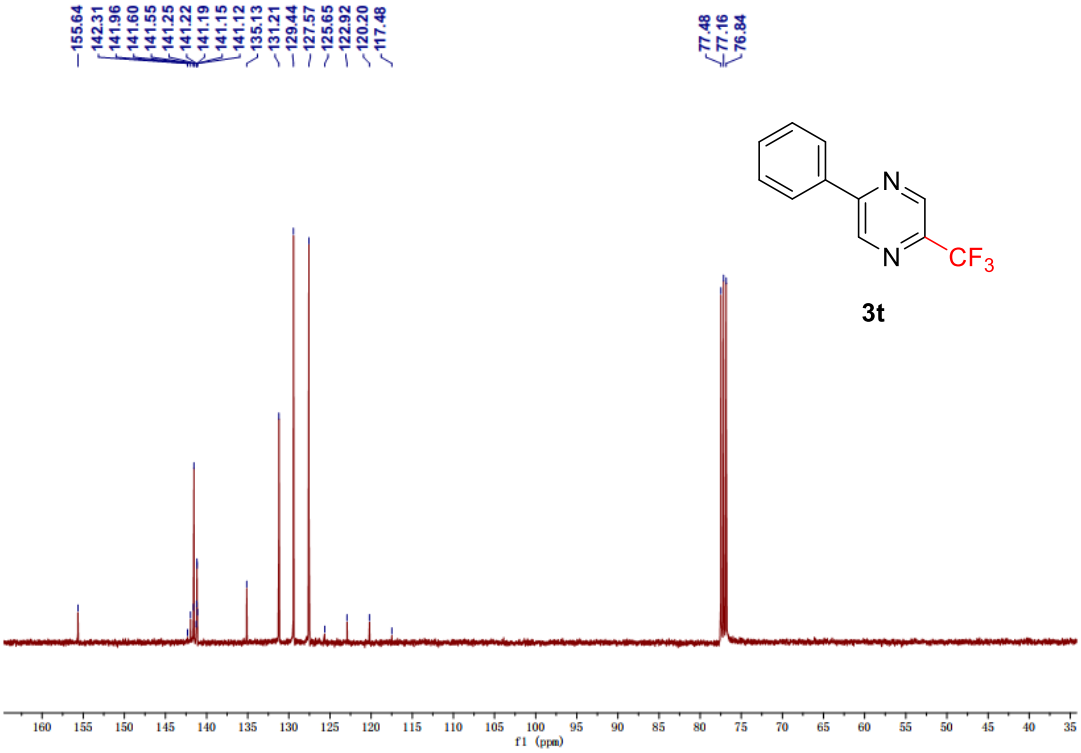

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

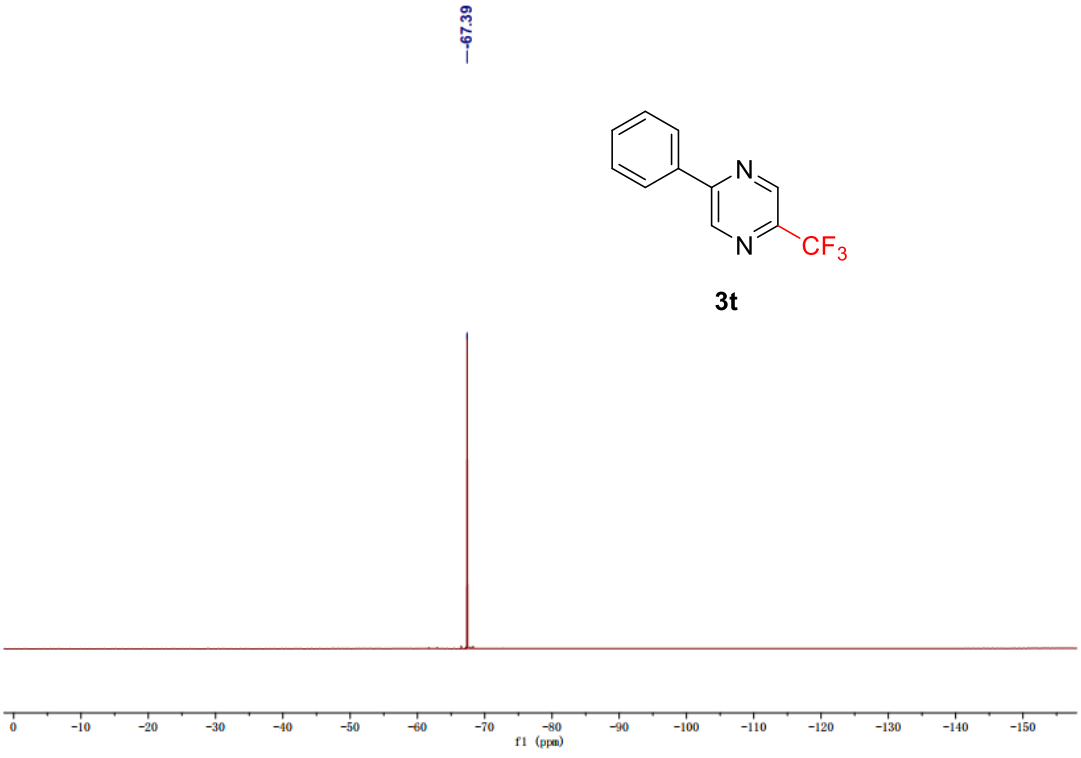

-68.05
N
CF3
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110
f1 (ppm)

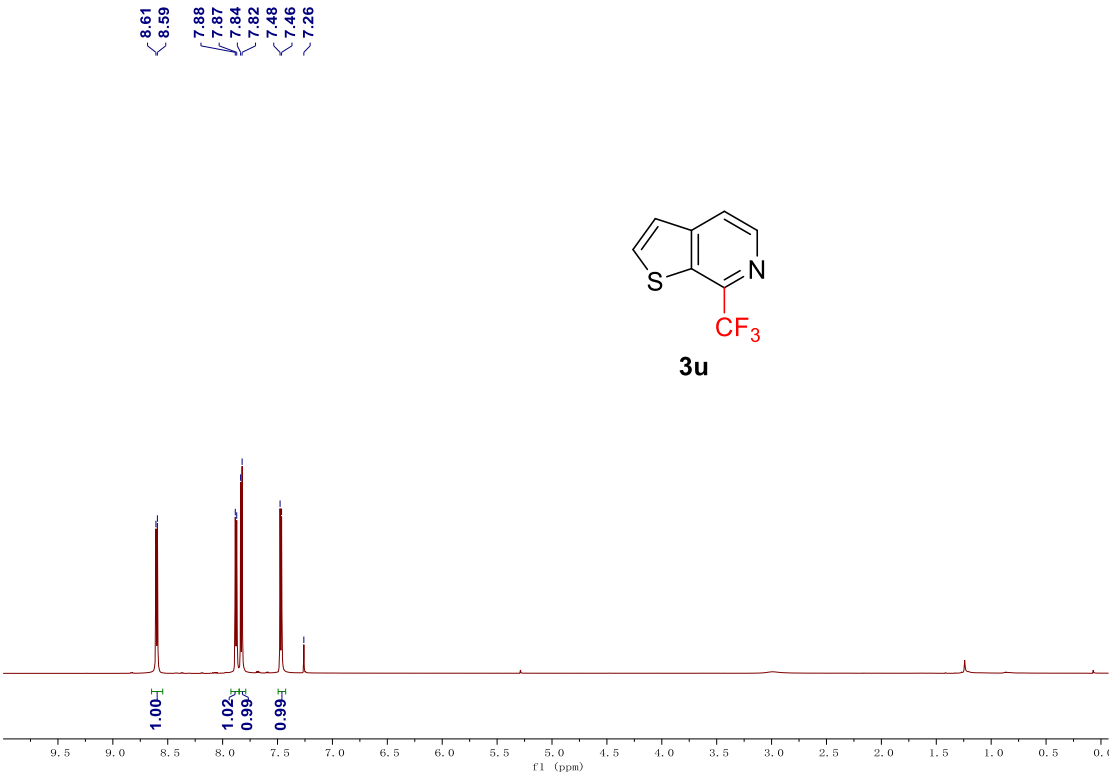
3s


9.12
8.99
8.09
8.09
8.08
8.07
7.59
7.57
7.56
7.55
7.54
7.26
N
N
CF3
1.00
1.00
2.02
3.00
0.11
0.53
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

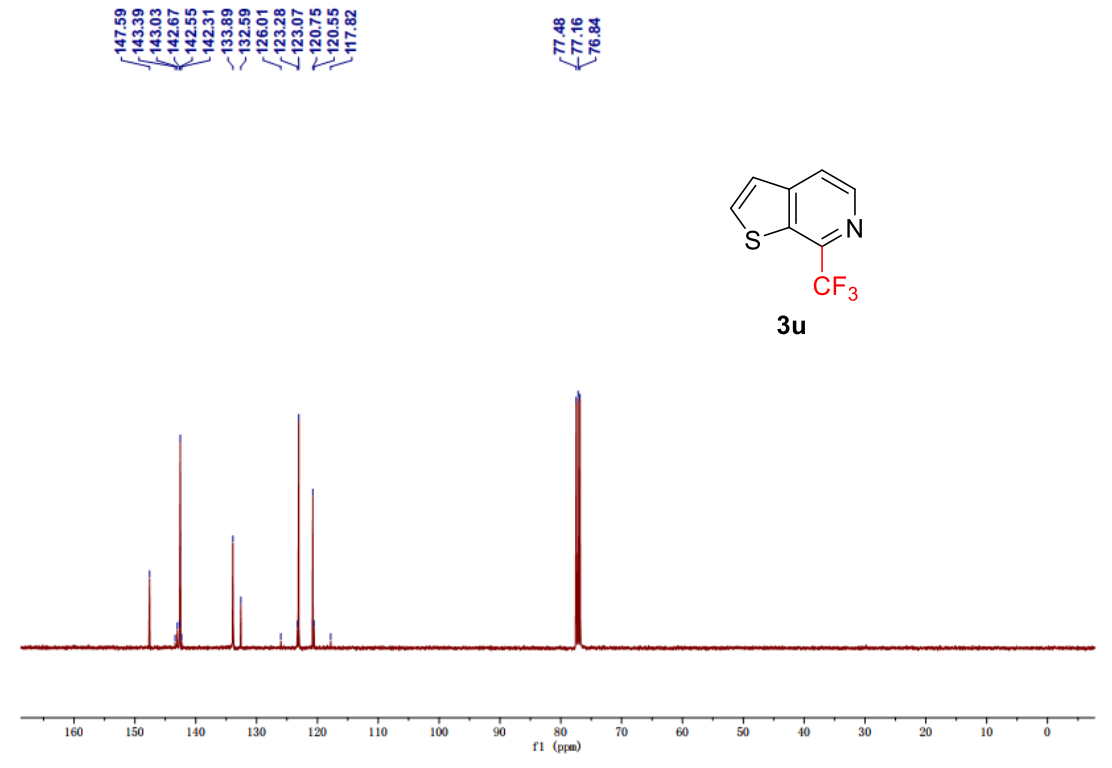
3t


155.64
142.31
141.96
141.60
141.55
141.25
141.22
141.19
141.15
141.12
135.13
131.21
129.44
127.57
125.65
122.92
120.20
117.48
77.48
77.16
76.84
N
N
CF3
3t
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
f1 (ppm)

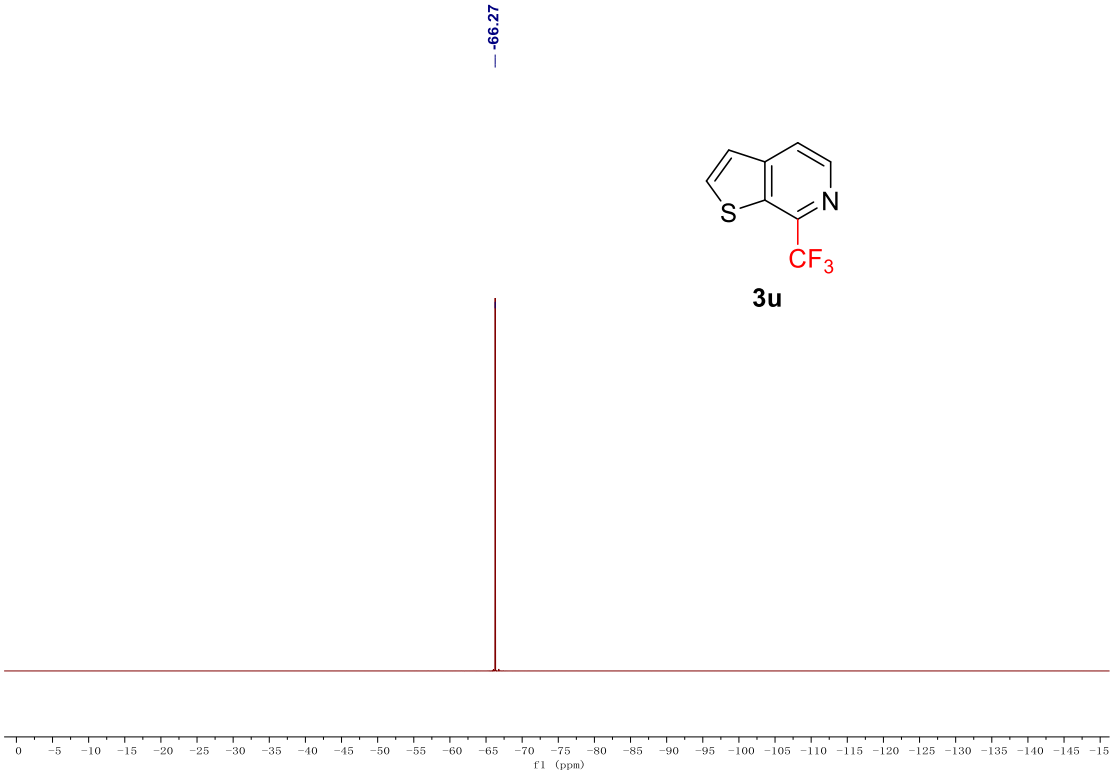

-67.39
N
N
CF3
3t
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
f1 (ppm)


8.61
8.59
7.88
7.87
7.84
7.82
7.48
7.46
7.26
S
N
CF3
1.00
1.02
0.99
0.99
f1 (ppm)

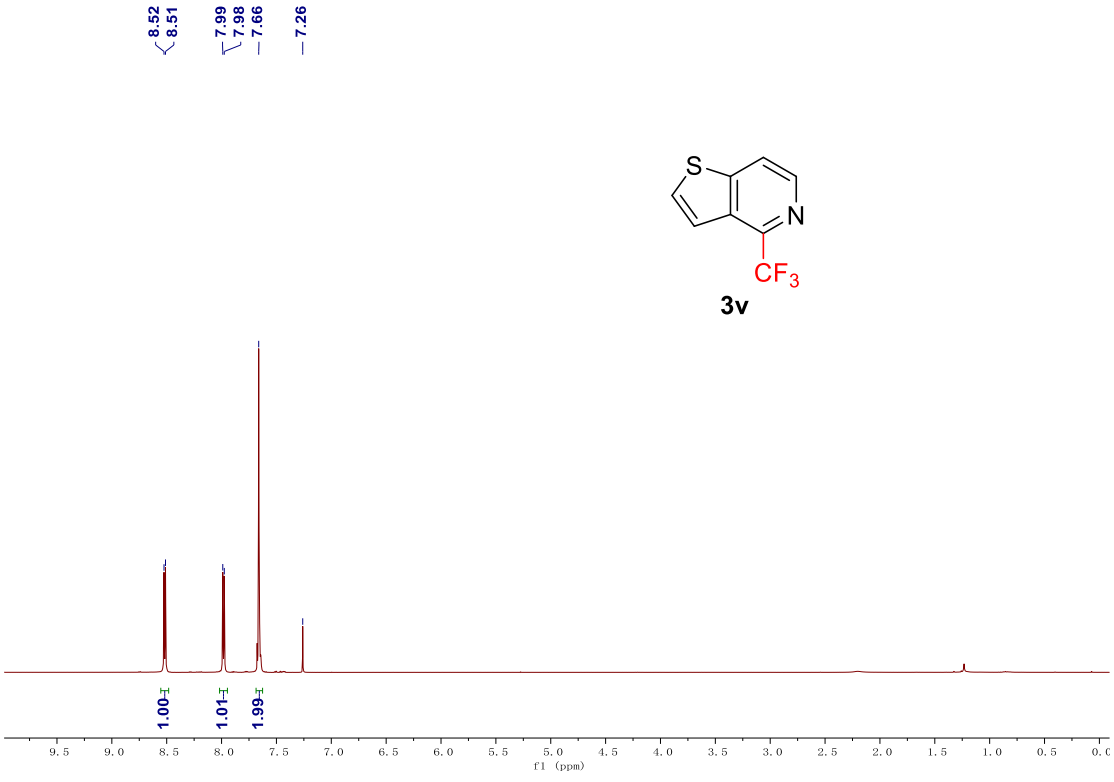
3u


147.59
143.39
143.03
142.67
142.55
142.31
133.89
132.59
126.01
123.28
123.07
120.75
120.55
117.82
77.48
77.16
76.84
S
N
CF3
f1 (ppm)

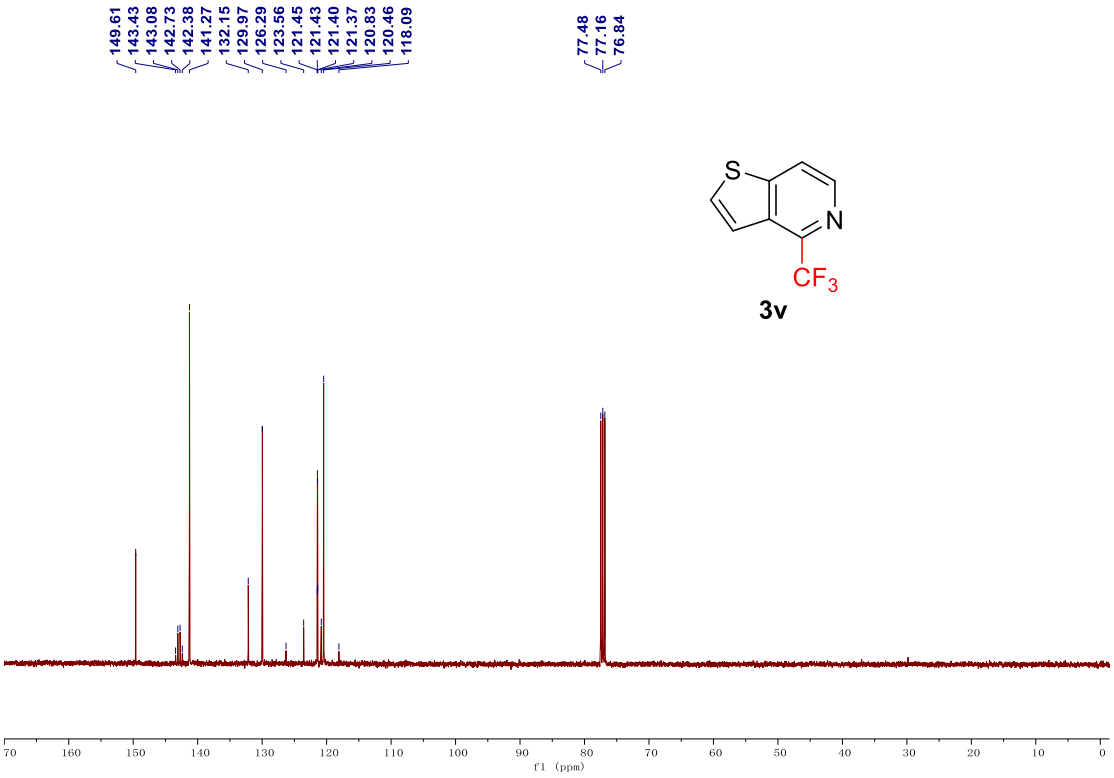
3u

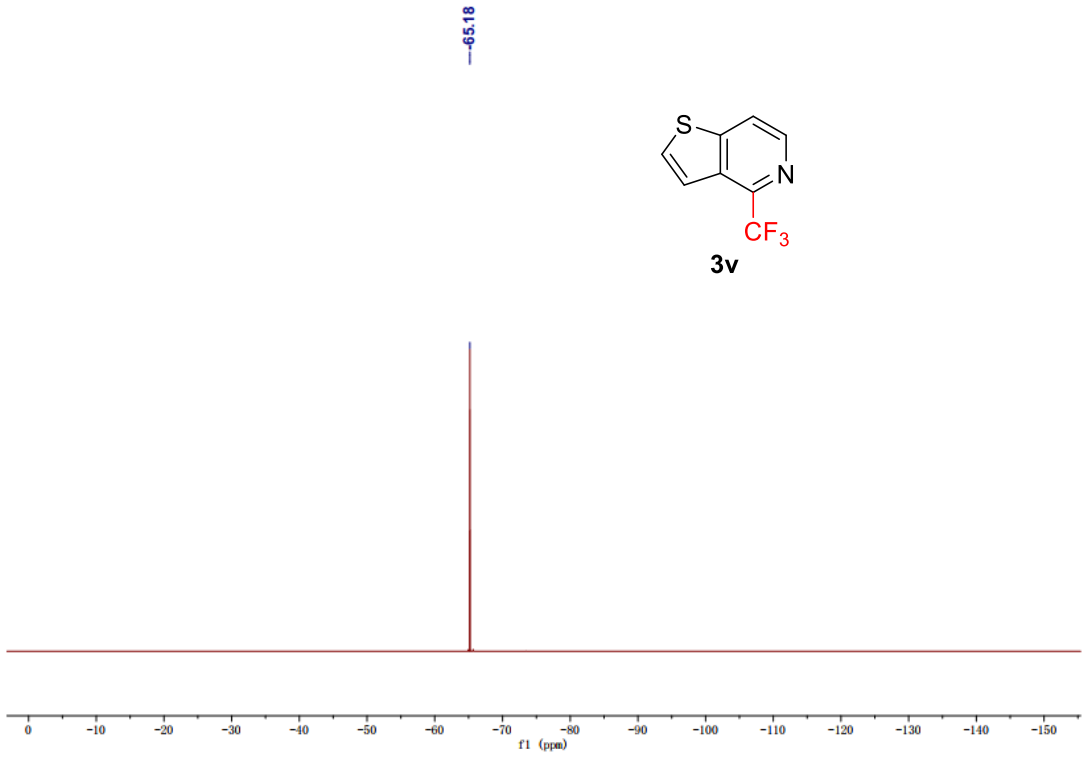

-66.27
S
N
CF3
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -15
f1 (ppm)

3u

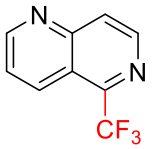

8.52
8.51
7.99
7.98
7.66
7.26
S
N
CF3
1.00
1.01
1.99
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3v

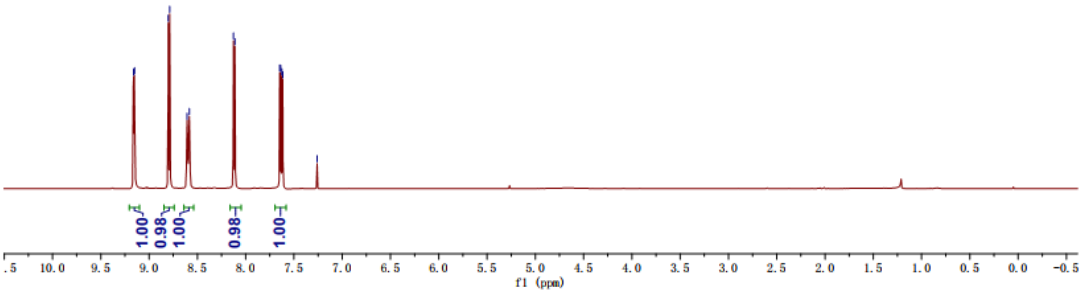

149.61
143.43
143.08
142.73
142.38
141.27
132.15
129.97
126.29
123.56
121.45
121.43
121.40
121.37
120.83
120.46
118.09
77.48
77.16
76.84
S
N
CF3
3v
f1 (ppm)

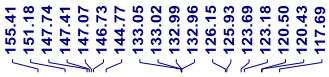

-65.18
S
N
CF3
3v
f1 (ppm)


9.16
9.15
8.80
8.79
8.61
8.58
8.13
8.11
7.65
7.64
7.63
7.62
7.26

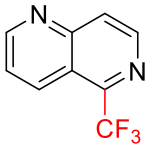

N
N
CF3

3w

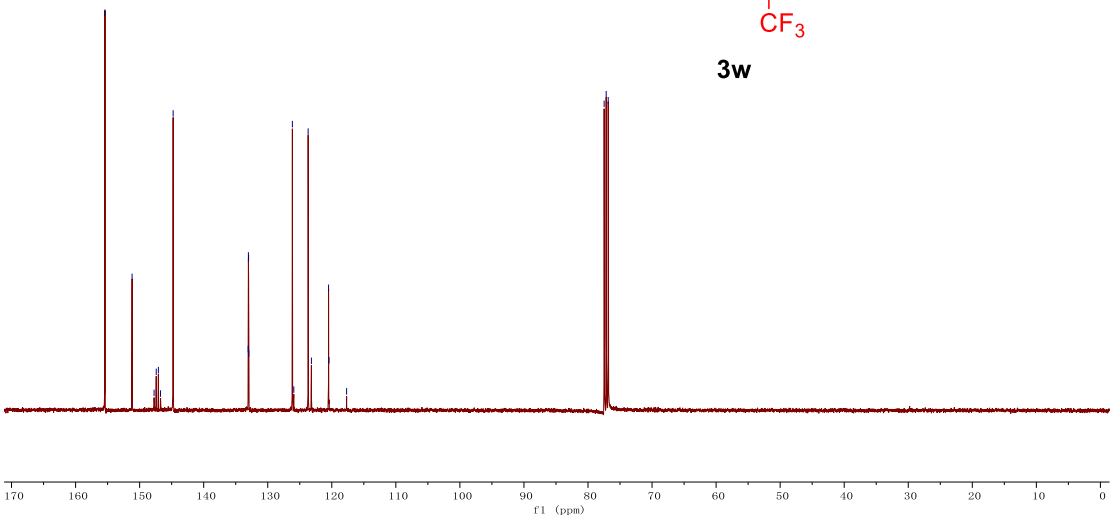

1.00
0.98
1.00
0.98
1.00
f1 (ppm)

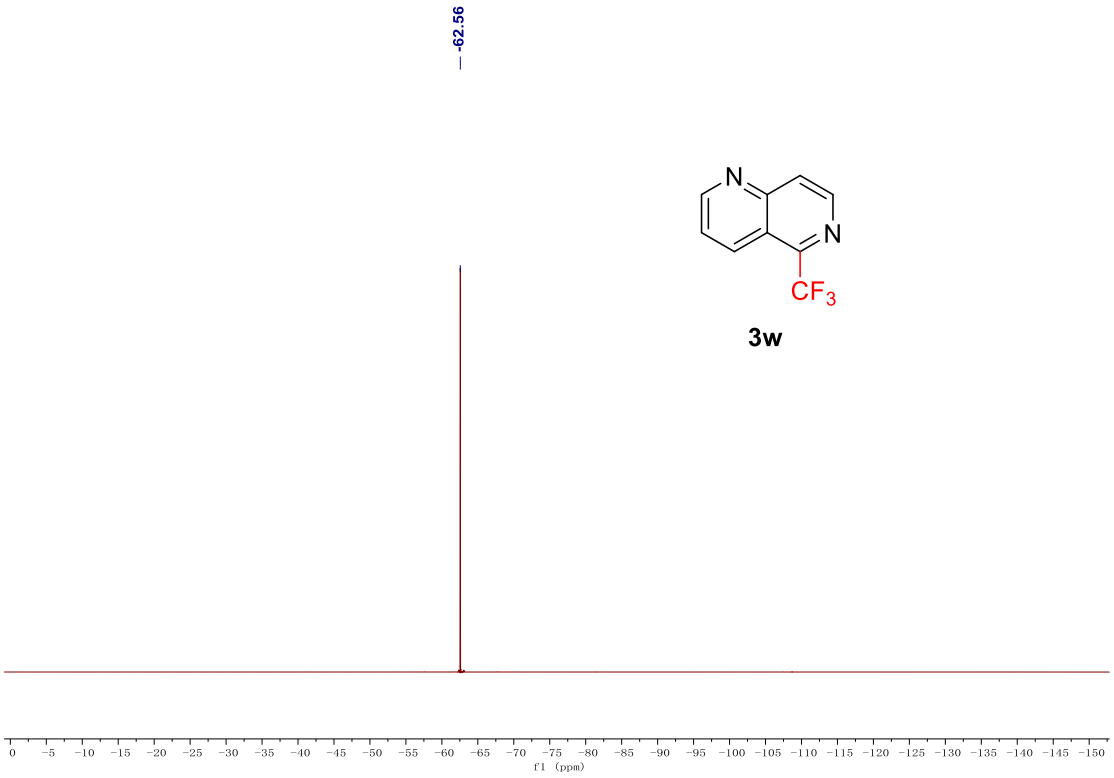

155.41
151.18
147.74
147.41
147.07
146.73
144.77
133.05
133.02
132.99
132.96
126.15
125.93
123.69
123.18
120.50
120.43
117.69


77.48
77.16
76.84

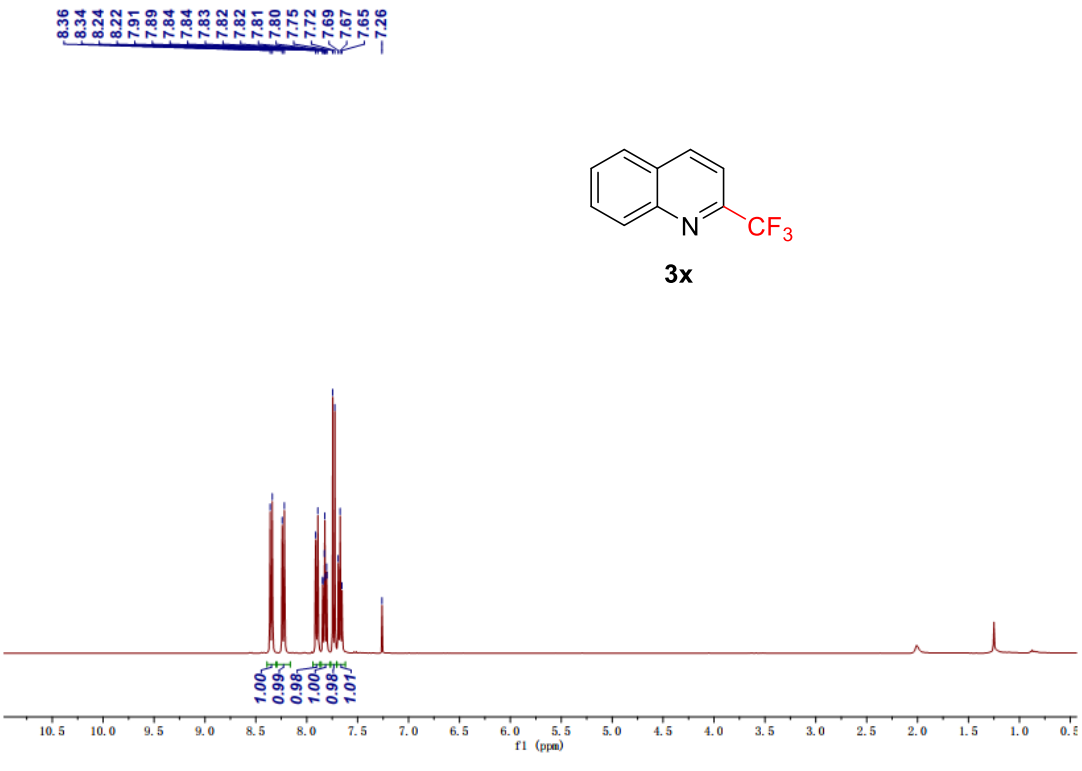

N
N
CF3

3w


f1 (ppm)

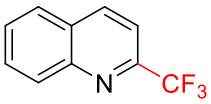

-62.56
N
N
CF3
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150
f1 (ppm)

3w

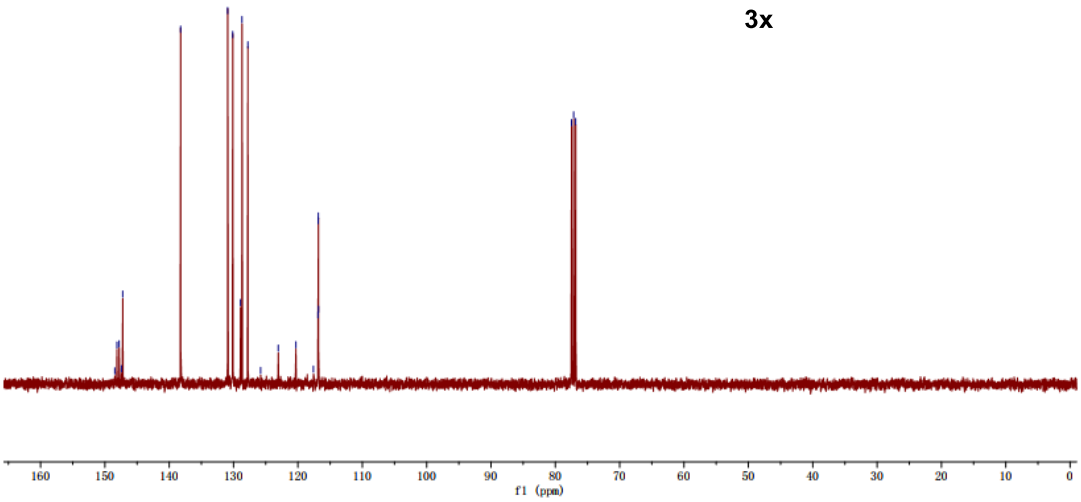

8.36
8.34
8.24
8.22
7.91
7.89
7.84
7.84
7.83
7.82
7.82
7.81
7.80
7.75
7.72
7.69
7.67
7.65
7.26
N
CF3
1.00
0.99
0.98
1.00
0.98
1.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)

3x

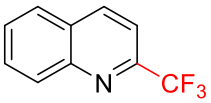

148.47
148.13
147.79
147.44
147.22
138.24
130.92
130.14
128.93
128.70
127.79
125.79
123.06
120.32
117.59
116.87
116.85
116.83
116.81
77.48
77.16
76.84


N
CF3

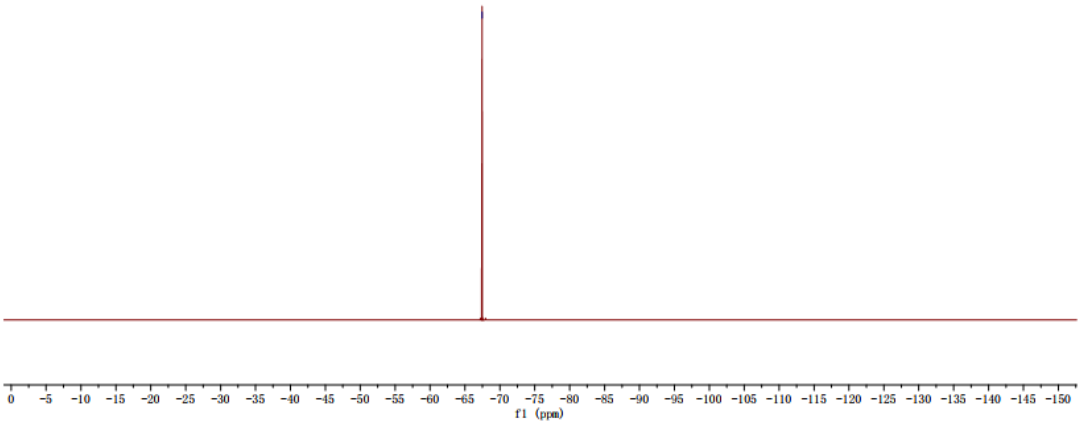
3x


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

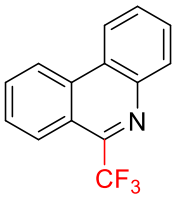

-67.45


N
CF3

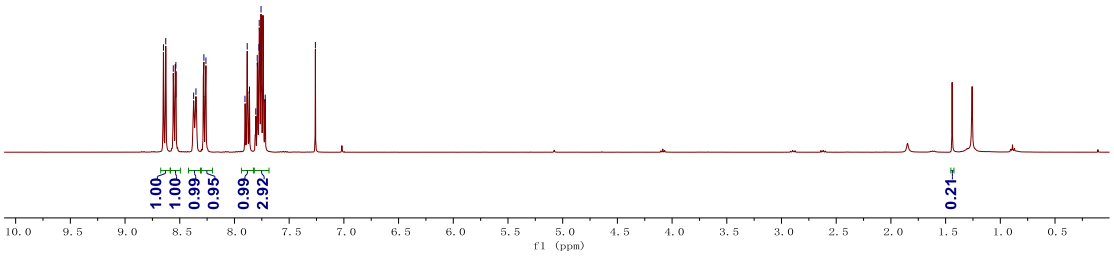
3x


0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
f1 (ppm)


8.65
8.63
8.56
8.54
8.37
8.35
8.28
8.26
7.90
7.88
7.86
7.81
7.79
7.79
7.78
7.77
7.76
7.75
7.72
7.26

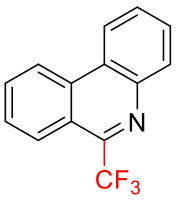

N
CF3

3y

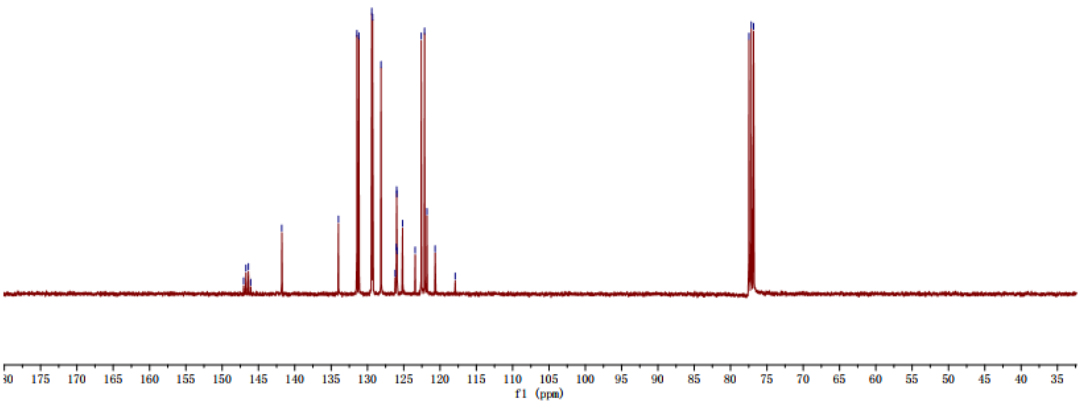

1.00
1.00
0.99
0.95
0.99
2.92
0.21
f1 (ppm)

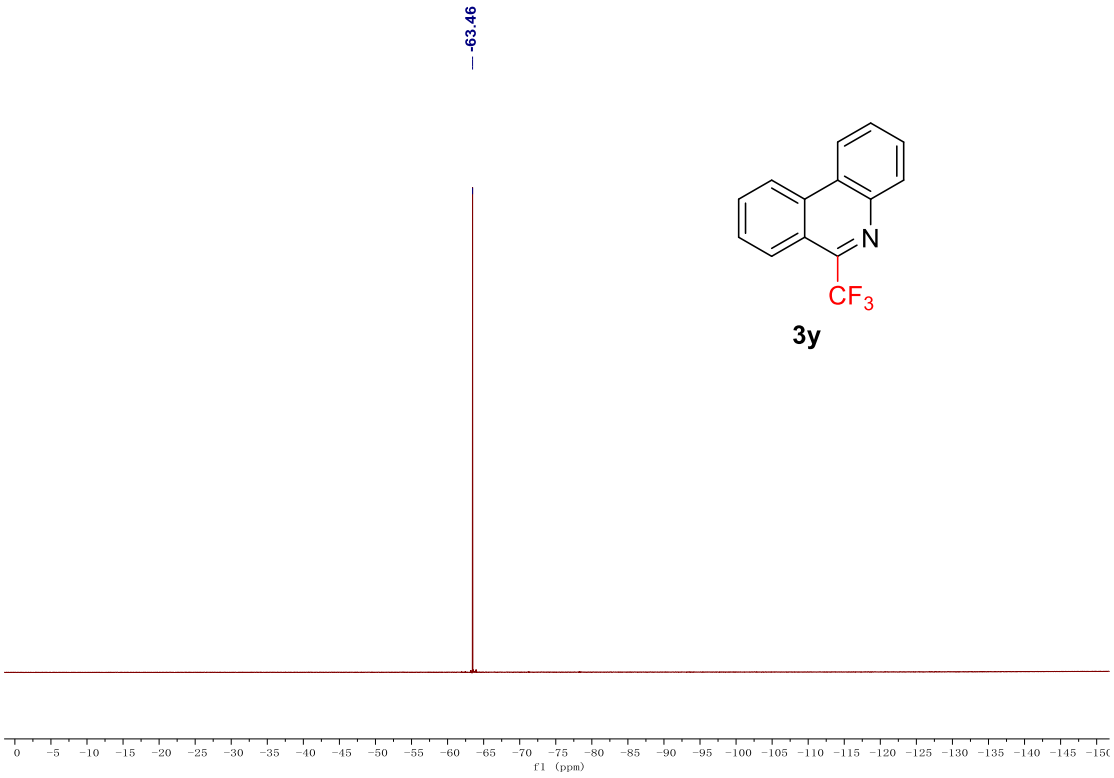

147.05
146.72
146.39
146.07
141.79
134.00
131.44
131.17
129.41
129.29
128.13
126.18
126.01
125.98
125.95
125.92
125.16
123.43
122.59
122.13
121.81
120.67
117.92


77.48
77.16
76.84

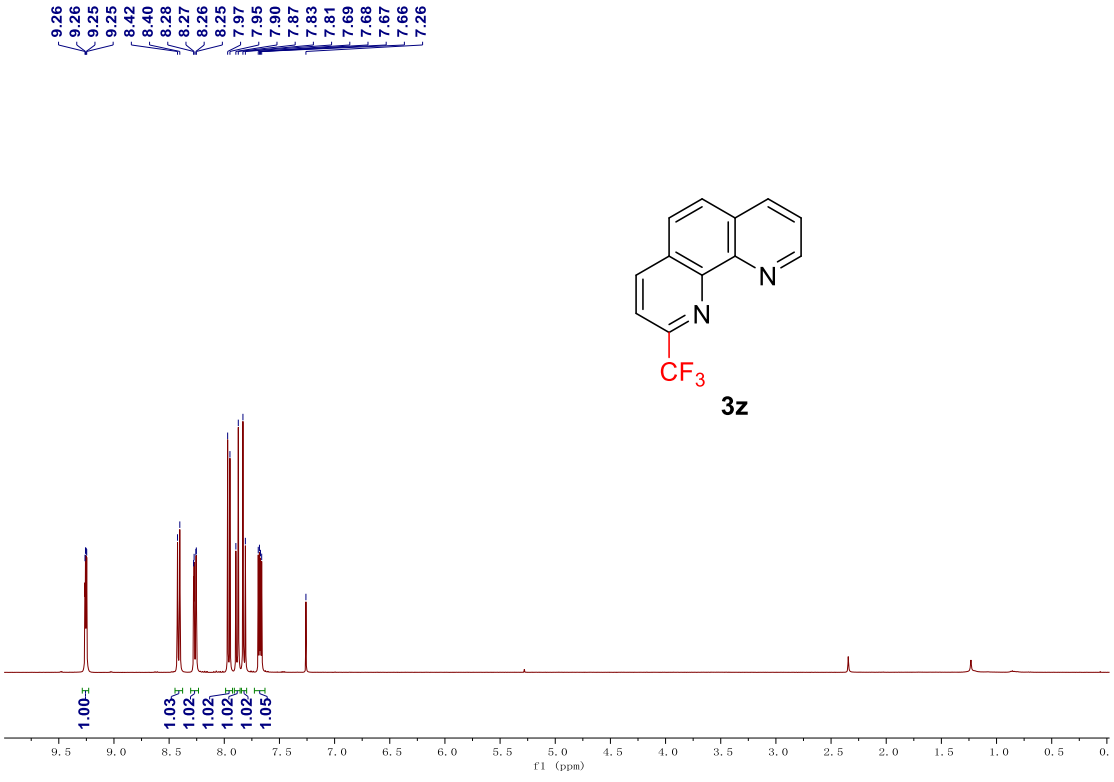

N
CF3

3y

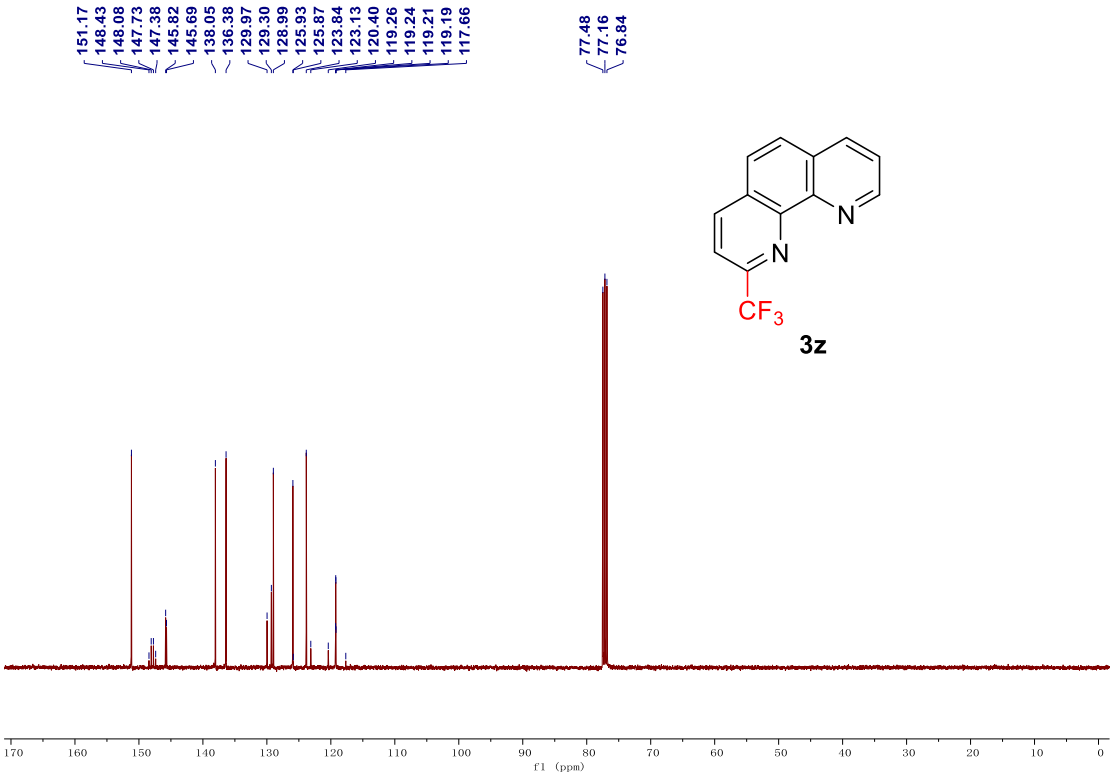

f1 (ppm)

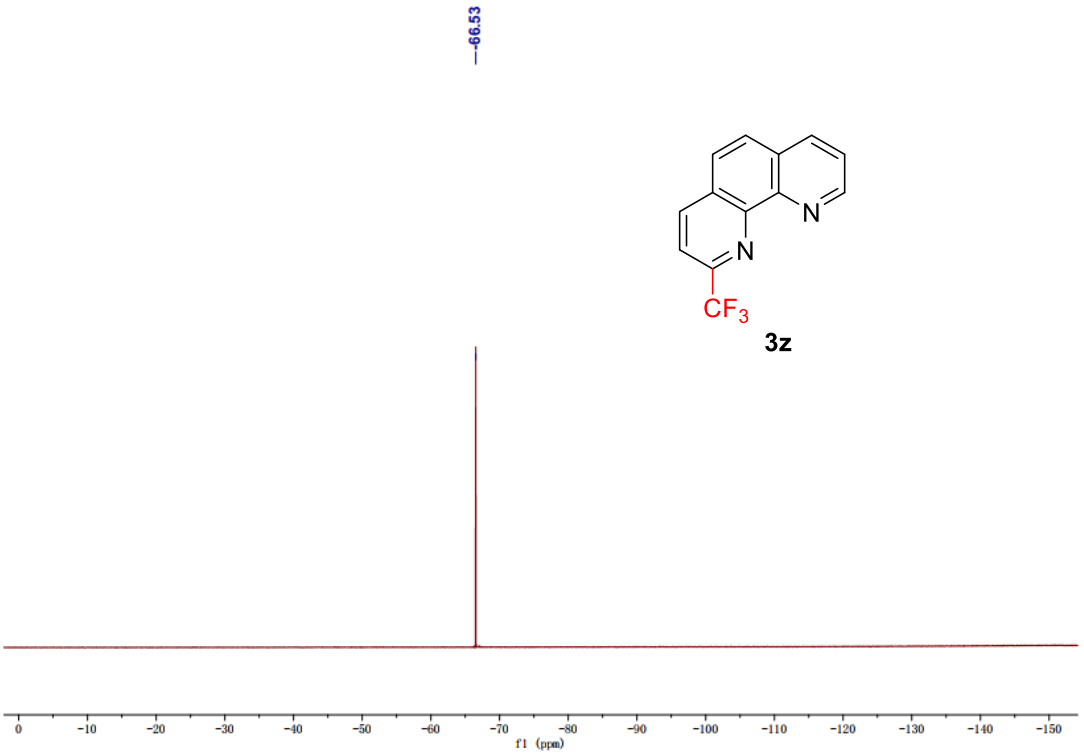

-63.46
N
CF3
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150
f1 (ppm)

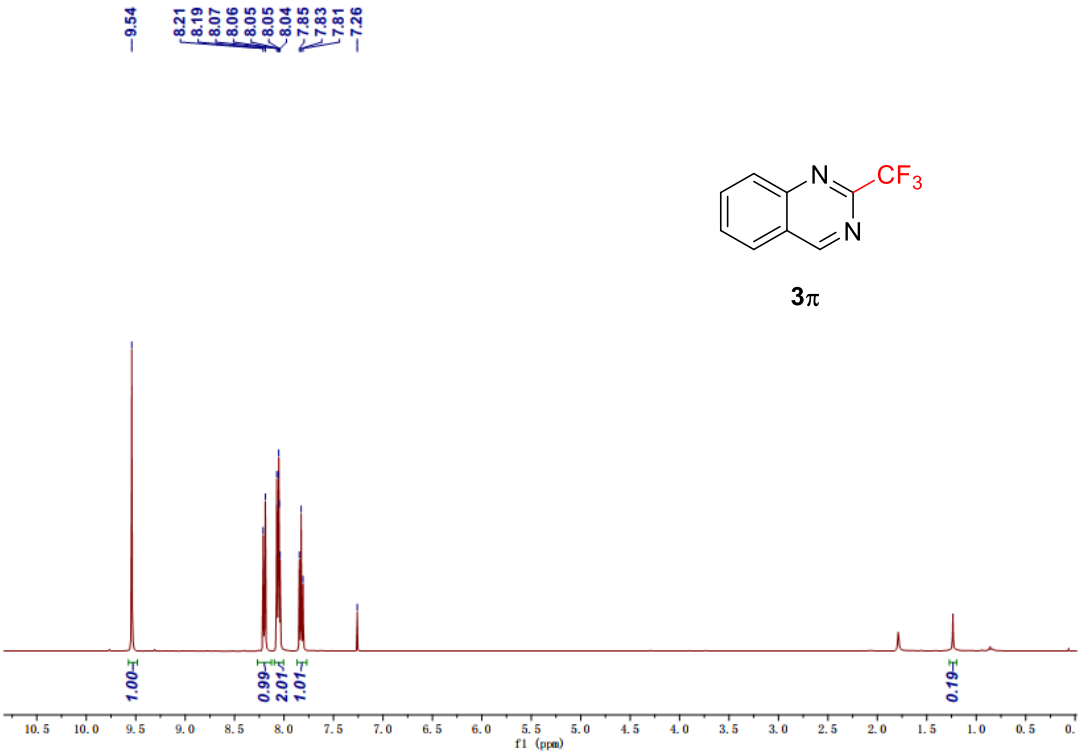
3y


9.26
9.26
9.25
9.25
8.42
8.40
8.28
8.27
8.26
8.25
7.97
7.95
7.90
7.87
7.83
7.81
7.69
7.68
7.67
7.66
7.26
N
N
CF3
1.00
1.03
1.02
1.02
1.02
1.02
1.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)

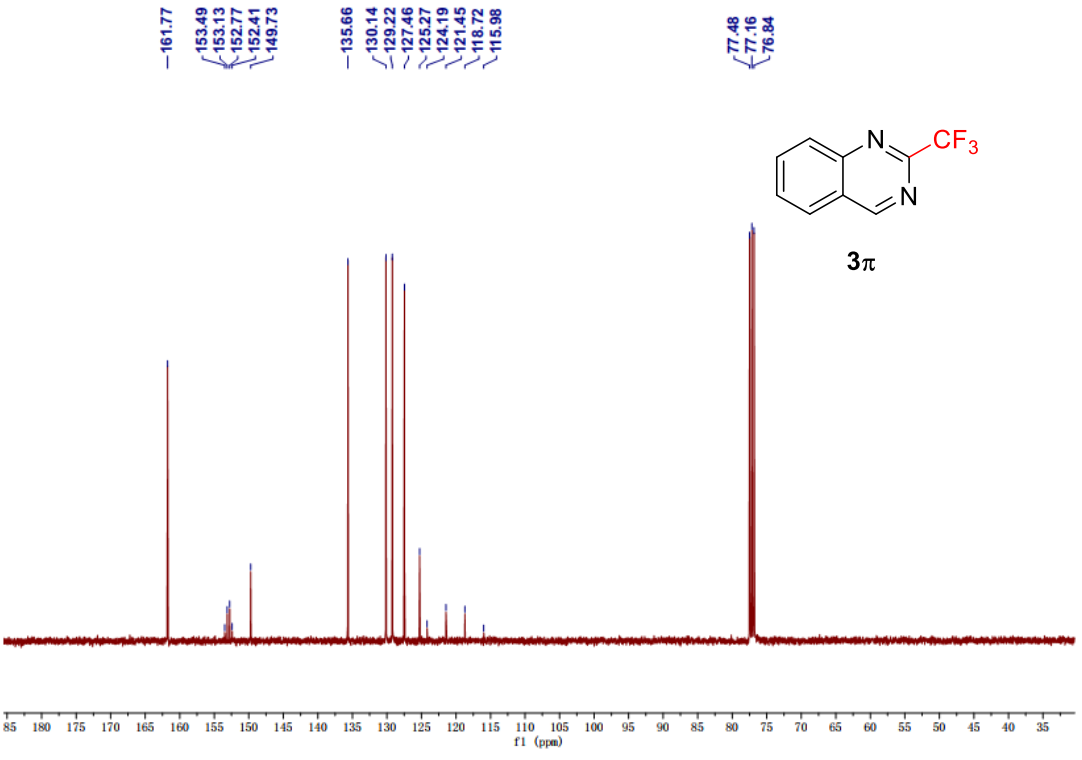
3z


151.17
148.43
148.08
147.73
147.38
145.82
145.69
138.05
136.38
129.97
129.30
128.99
125.93
125.87
123.84
123.13
120.40
119.26
119.24
119.21
119.19
117.66
77.48
77.16
76.84
N
N
CF3
3z
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

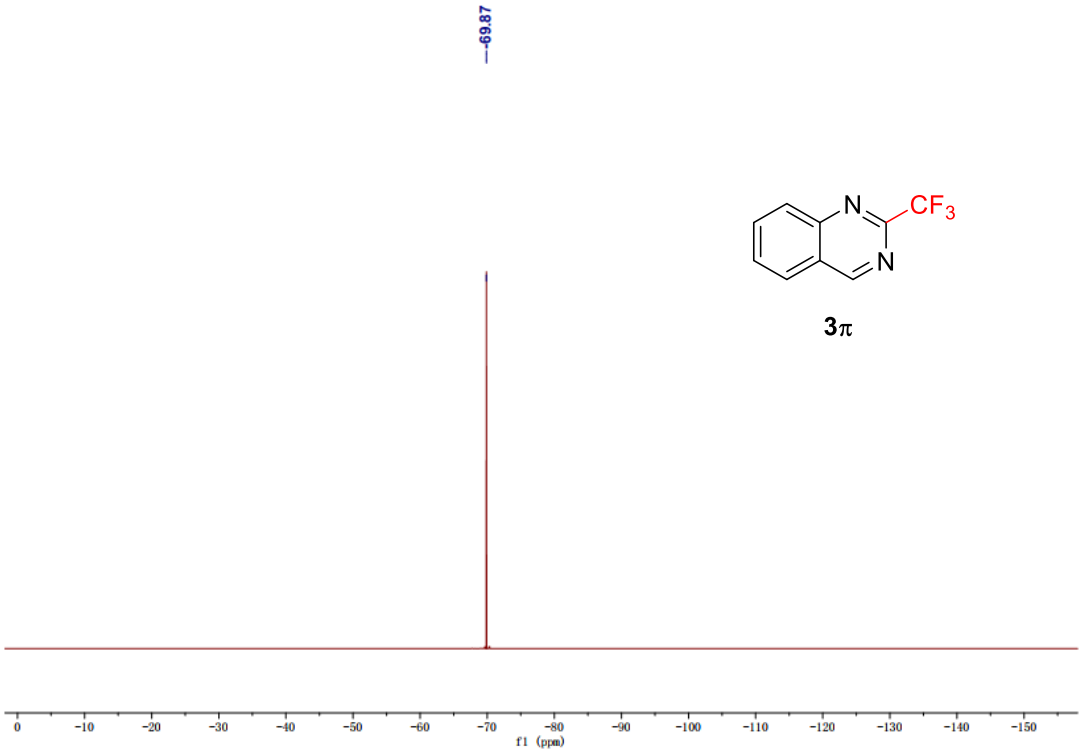

-66.53
N
N
CF3
3z
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)


9.54
8.21
8.19
8.07
8.06
8.05
8.05
8.04
7.85
7.83
7.81
7.26
N
CF3
N
1.00
0.99
2.01
1.01
0.19
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.
f1 (ppm)

3π

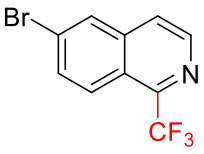

161.77
153.49
153.13
152.77
152.41
149.73
135.66
130.14
129.22
127.46
125.27
124.19
121.45
118.72
115.98
77.48
77.16
76.84
N
CF3
N
85 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35
f1 (ppm)

3π

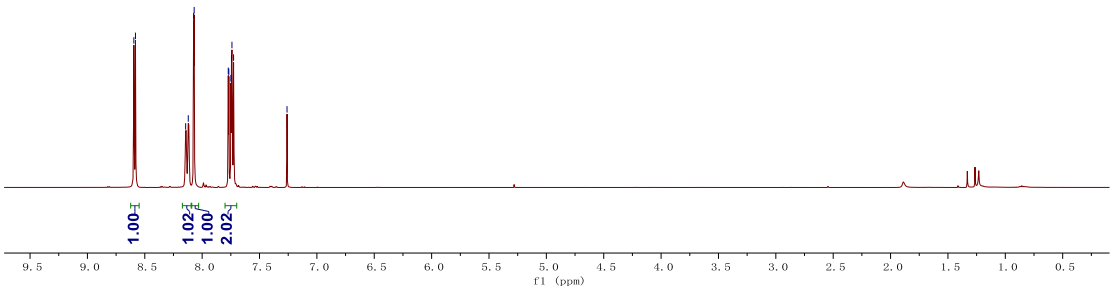

-69.87
N
CF3
N
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

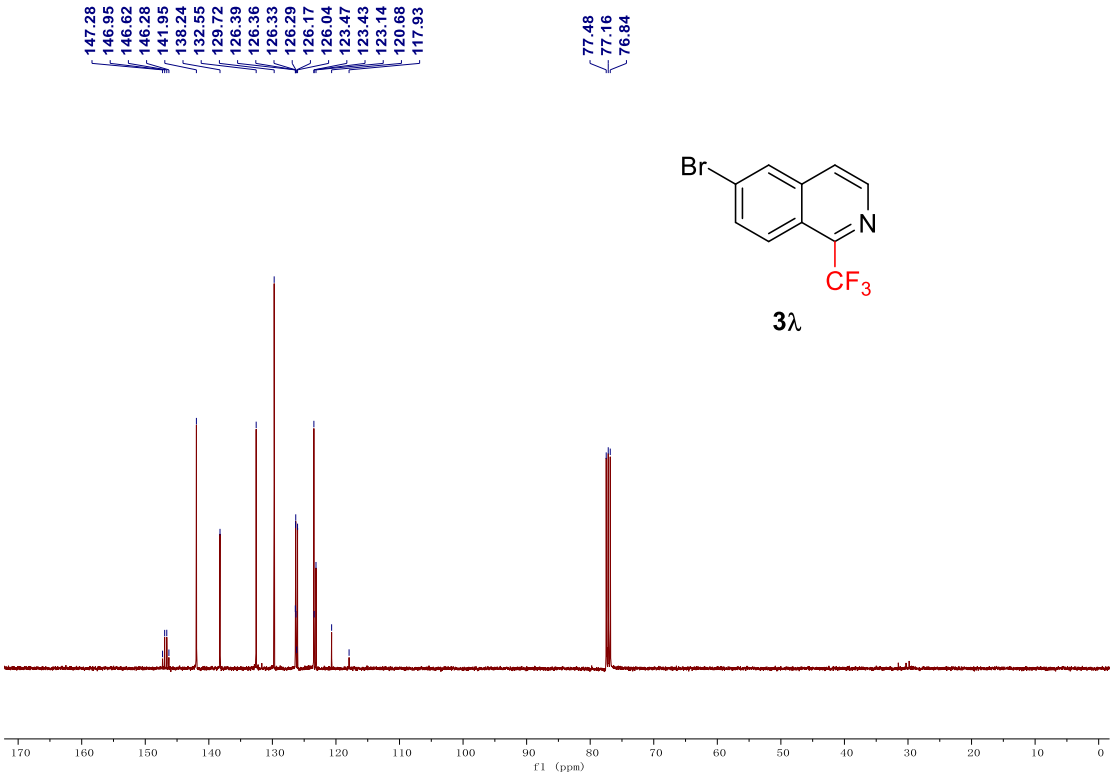
3π

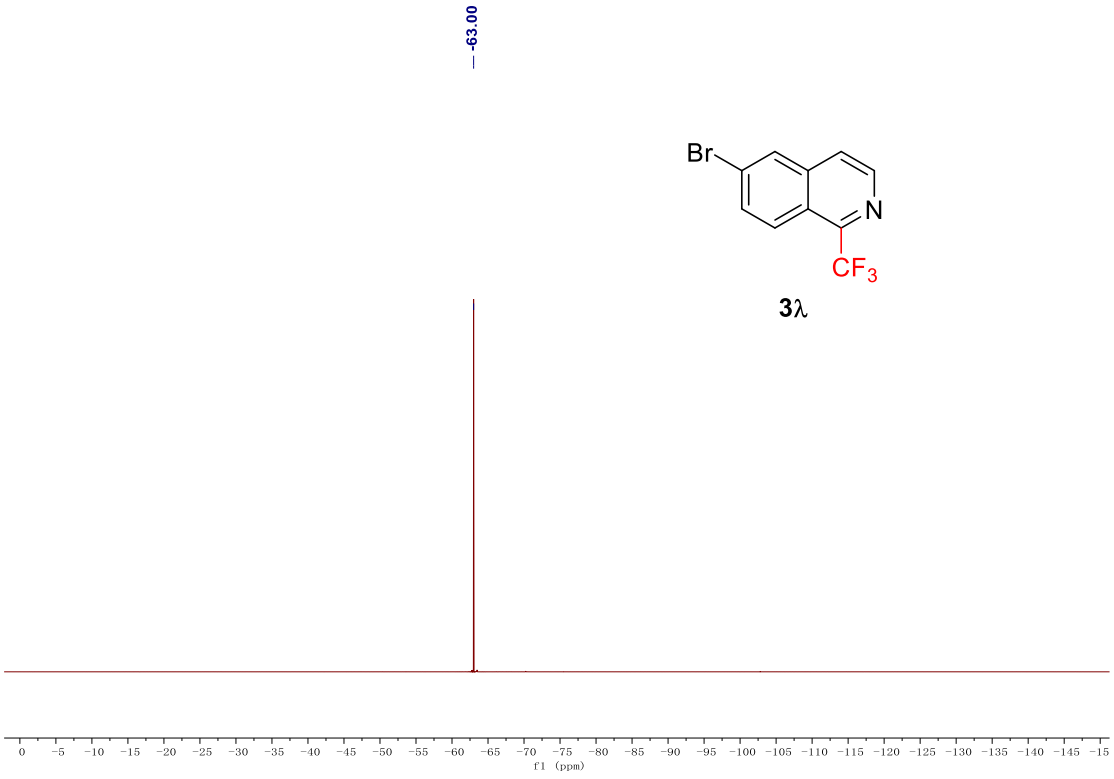

8.60
8.58
8.14
8.12
8.07
8.07
7.77
7.77
7.75
7.74
7.74
7.73
7.26


Br
N
CF3

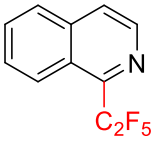
3λ


1.00
1.02
1.00
2.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

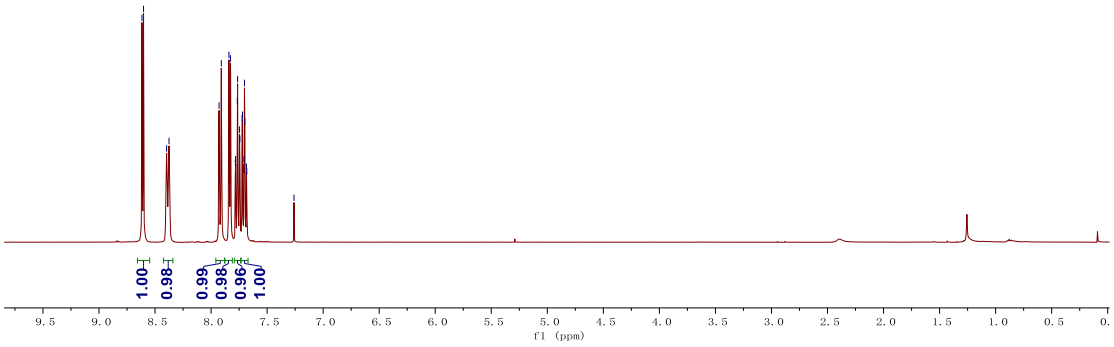

147.28
146.95
146.62
146.28
141.95
138.24
132.55
129.72
126.39
126.36
126.33
126.29
126.17
126.04
123.47
123.43
123.14
120.68
117.93
77.48
77.16
76.84
Br
N
CF3
3λ
f1 (ppm)


-63.00
Br
N
CF3
3λ
f1 (ppm)

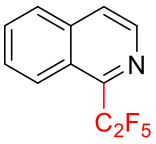

8.62
8.60
8.40
8.38
7.93
7.91
7.84
7.83
7.78
7.78
7.77
7.76
7.75
7.74
7.72
7.72
7.71
7.70
7.70
7.68
7.68
7.26


N
C2F5

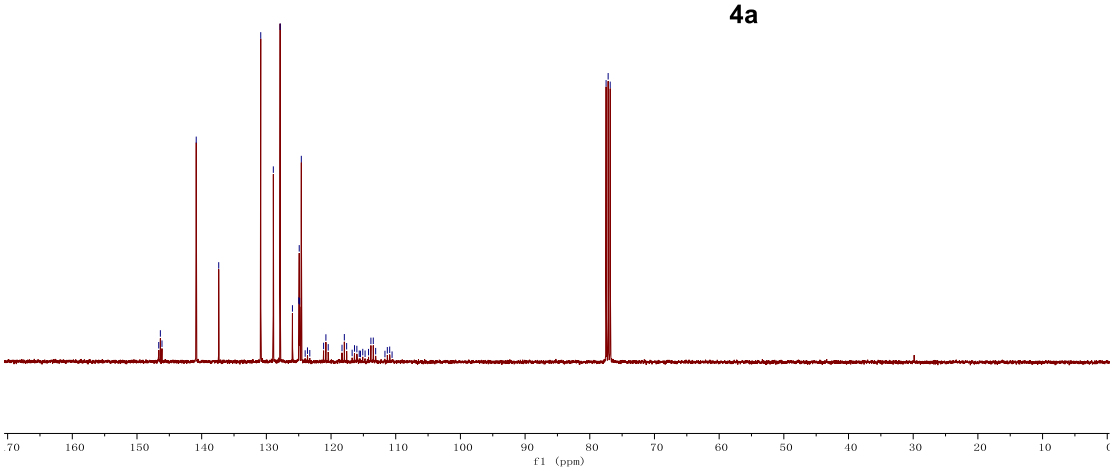
4a

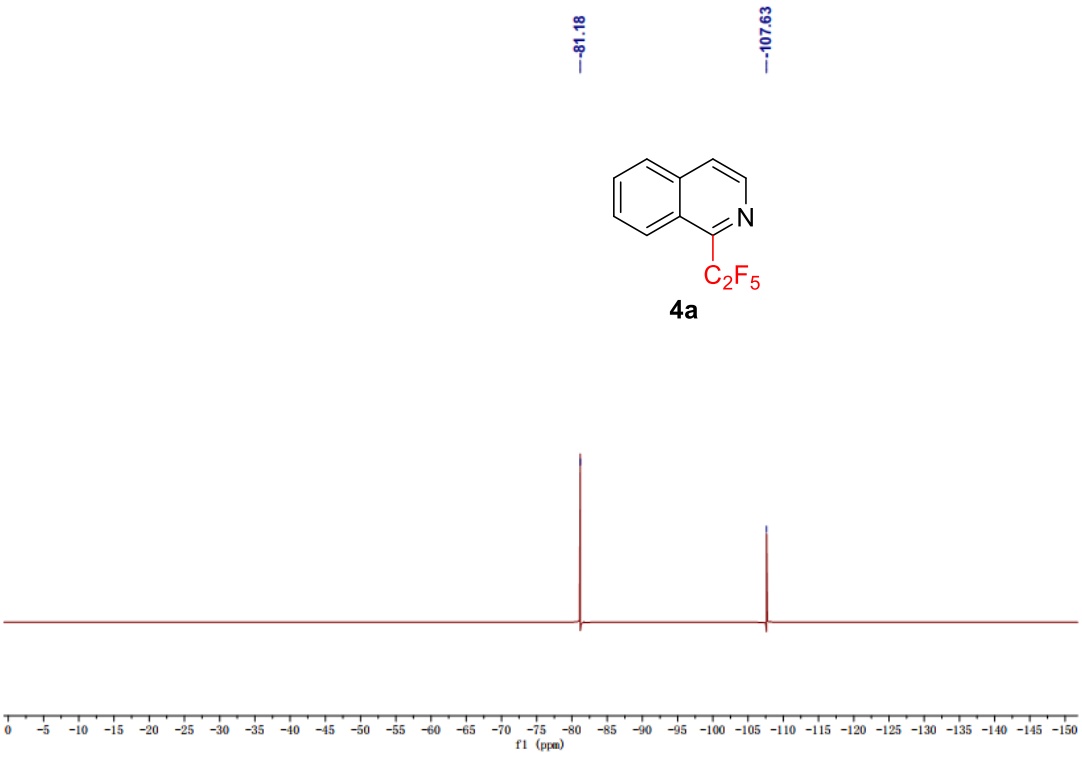

1.00
0.98
0.99
0.98
0.96
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

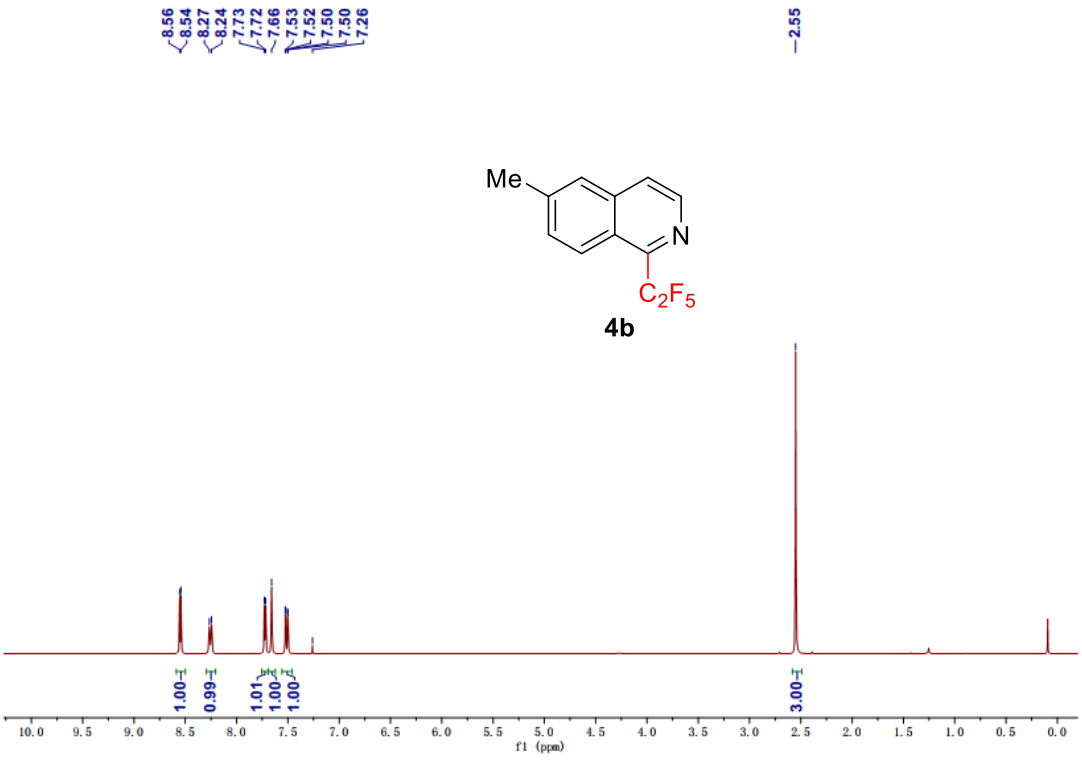

146.64
146.39
146.14
140.84
137.37
130.87
128.92
127.87
125.97
124.98
124.92
124.86
124.60
124.00
123.64
123.29
121.15
120.79
120.44
118.30
117.95
117.59
116.74
116.37
116.01
115.64
115.45
115.10
114.74
114.20
113.84
113.47
113.10
111.67
111.30
110.93
110.57
77.48
77.16
76.84


N
C2F5

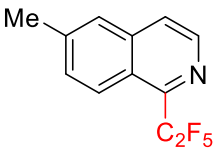
4a


70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

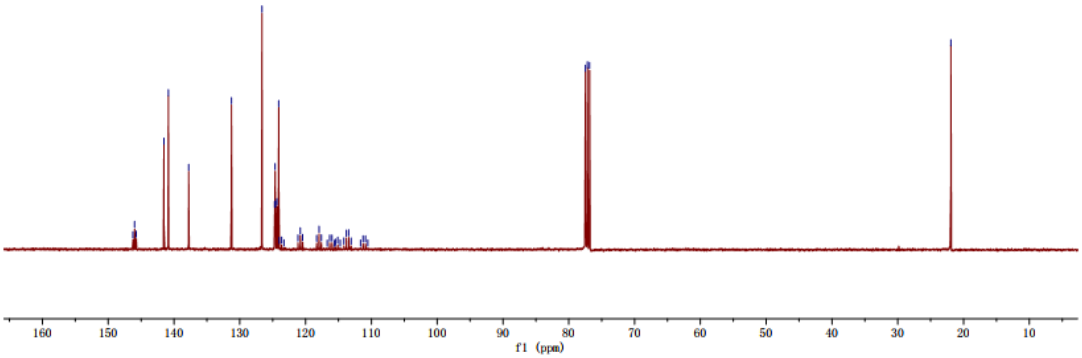

-81.18
-107.63
N
C_2F_5
4a
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150
f1 (ppm)


8.56
8.54
8.27
8.24
7.73
7.72
7.66
7.53
7.52
7.50
7.50
7.26
2.55
Me
N
C_2F_5
4b
1.00
0.99
1.01
1.00
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

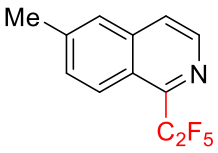

146.23
145.98
145.73
141.54
140.86
137.76
131.27
126.63
124.70
124.64
124.58
124.36
124.08
124.01
123.65
123.29
121.16
120.80
120.44
118.31
117.95
117.59
116.71
116.35
115.98
115.61
115.46
115.10
114.74
114.17
113.81
113.44
113.07
111.63
111.27
110.90
110.53
77.48
77.16
76.84
21.93


Me
N
C2F5

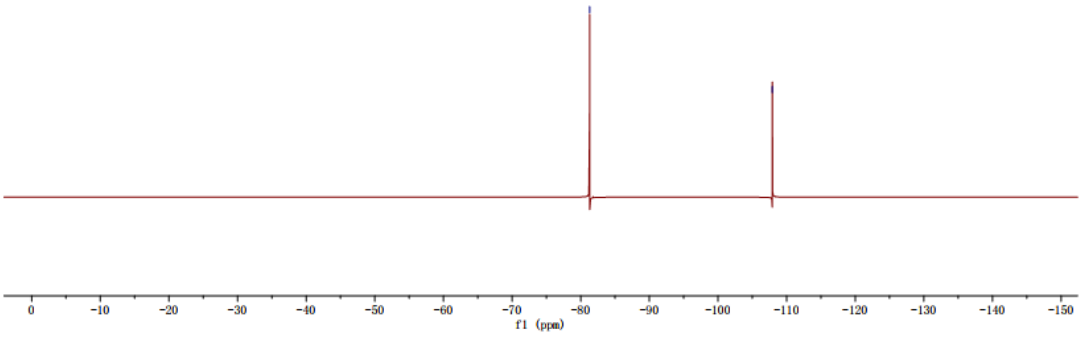
4b


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

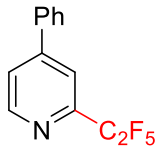

-81.30
-107.92


Me
N
C2F5

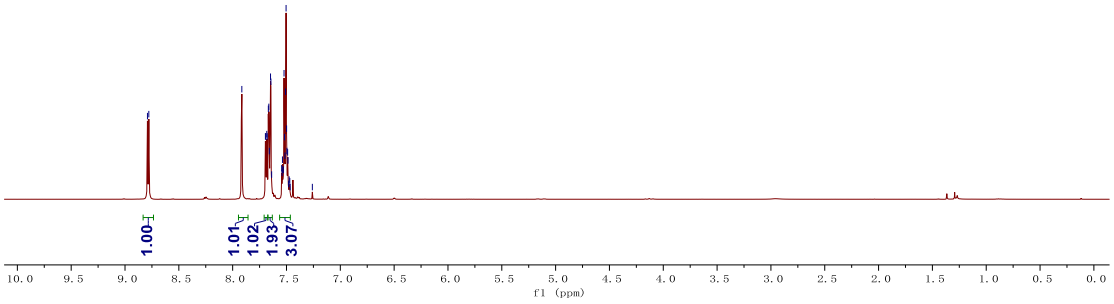
4b


0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

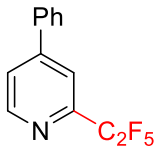

8.79
8.78
7.91
7.70
7.69
7.68
7.68
7.67
7.66
7.66
7.65
7.64
7.64
7.54
7.54
7.54
7.53
7.53
7.52
7.52
7.51
7.51
7.50
7.50
7.50
7.49
7.49
7.48
7.47
7.47
7.47
7.26


Ph
N
C_2F_5

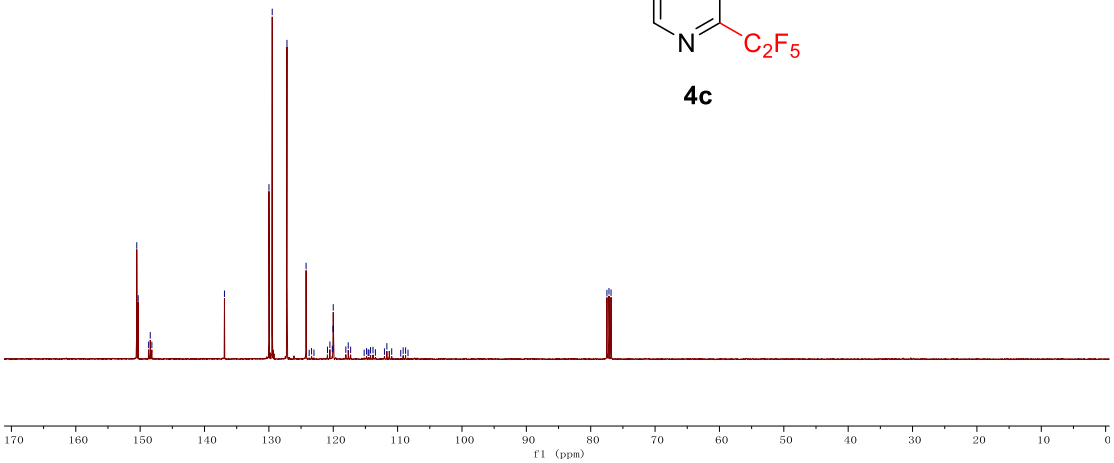
4c

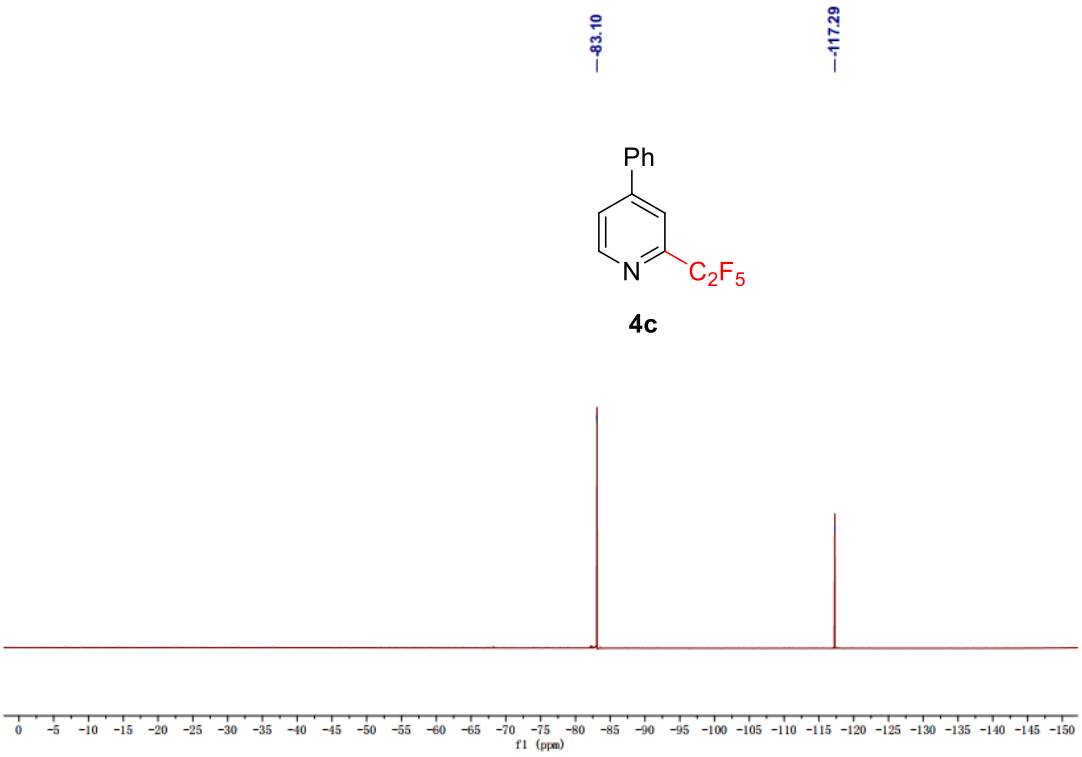

1.00
1.01
1.02
1.93
3.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

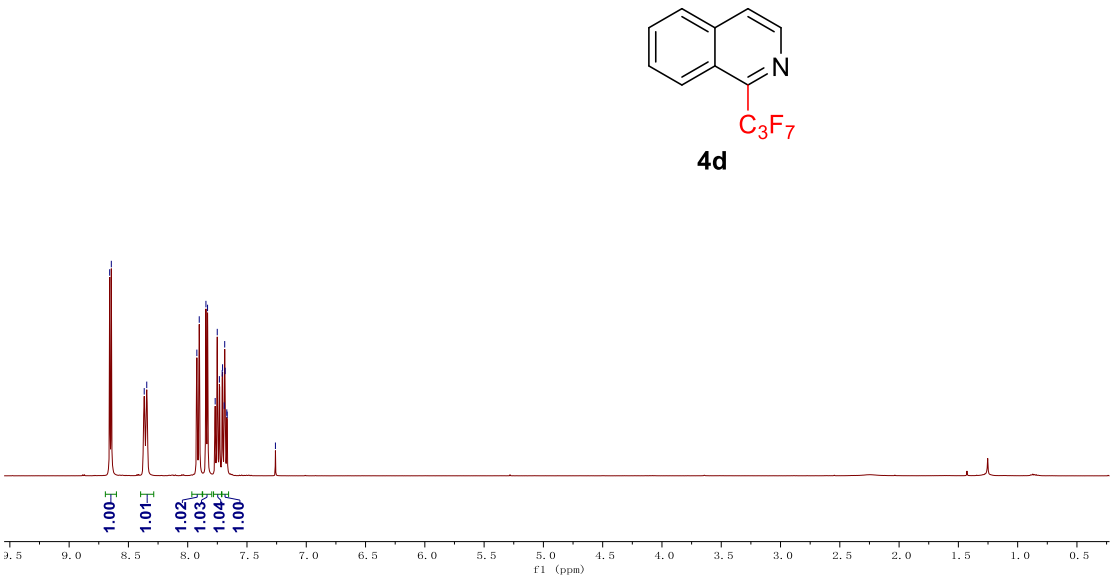

150.52
150.31
148.68
148.43
148.18
136.90
129.99
129.48
127.19
124.22
123.74
123.37
122.99
120.89
120.52
120.15
120.04
120.00
119.96
118.05
117.67
117.30
115.20
114.82
114.58
114.45
114.20
113.82
113.45
112.05
111.67
110.92
109.51
109.14
108.76
108.38
77.48
77.16
76.84


Ph
N
C_2F_5

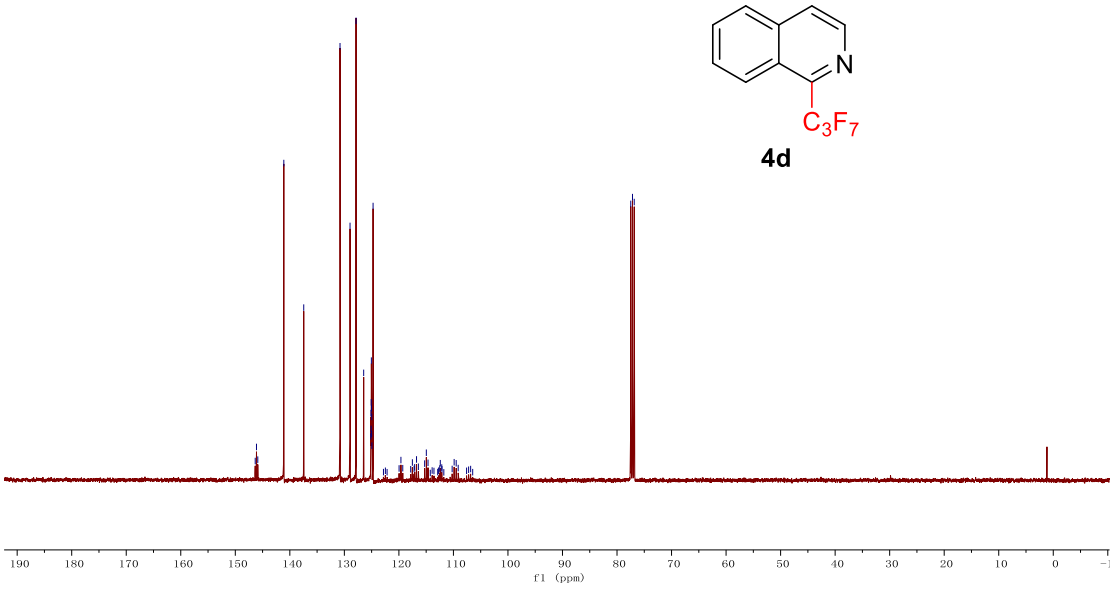
4c


170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

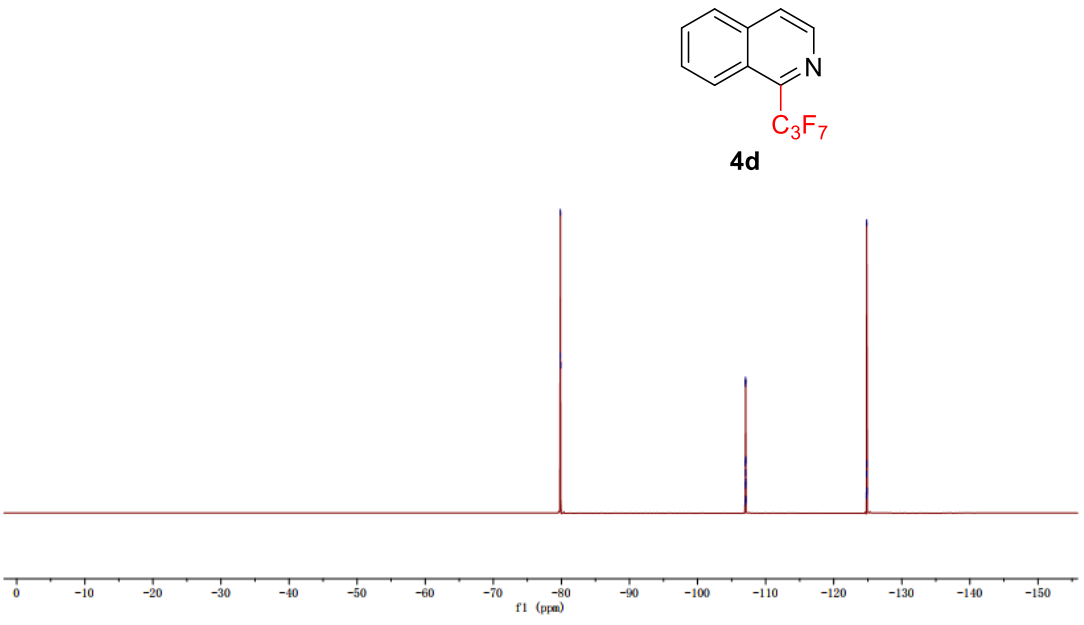

-83.10
-117.29
Ph
N
C_2F_5
4c
f1 (ppm)
8.66
8.64
8.37
8.35
7.92
7.90
7.85
7.83
7.77
7.75
7.73
7.71
7.71
7.69
7.69
7.68
7.67
7.67
7.26


N
C_3F_7
4d
1.00
1.01
1.02
1.03
1.04
1.00
f1 (ppm)

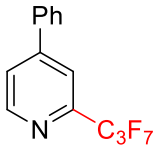

146.35
146.11
145.88
141.10
137.45
130.80
128.96
127.86
126.46
125.14
125.12
125.09
125.07
125.05
125.02
125.00
124.98
124.95
124.73
122.83
122.48
122.17
119.96
119.63
119.29
117.83
117.53
117.21
117.10
116.77
116.43
115.28
114.97
114.66
114.24
113.90
113.57
112.89
112.72
112.51
112.41
112.14
112.10
111.76
110.23
109.87
109.49
109.12
107.59
107.22
106.84
106.47
77.48
77.16
76.84


N
C3F7
4d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

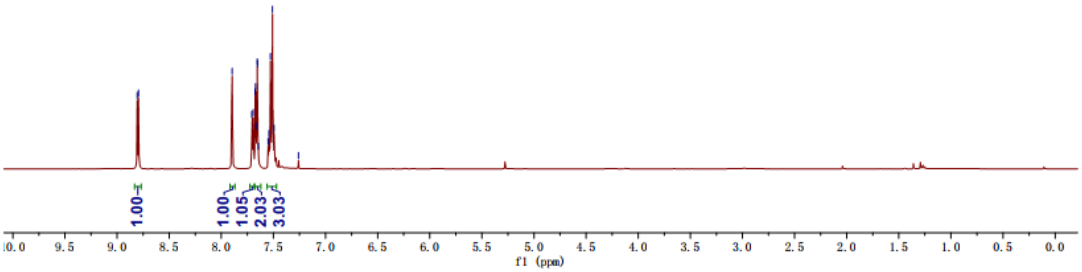

-79.83
-79.85
-79.88
-106.99
-107.00
-107.02
-107.03
-107.04
-107.05
-107.07
-107.08
-107.09
-124.81
-124.82
-124.84
-124.85
-124.87


N
C3F7
4d
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

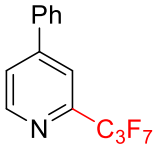

8.81
8.79
7.90
7.71
7.69
7.68
7.67
7.67
7.66
7.65
7.65
7.55
7.54
7.53
7.51
7.49
7.26


Ph
N
C3F7

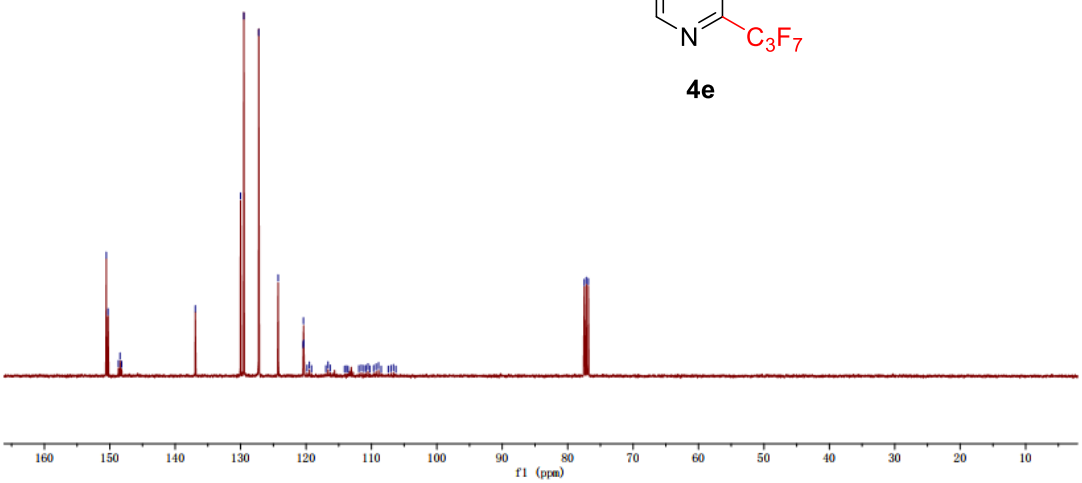
4e

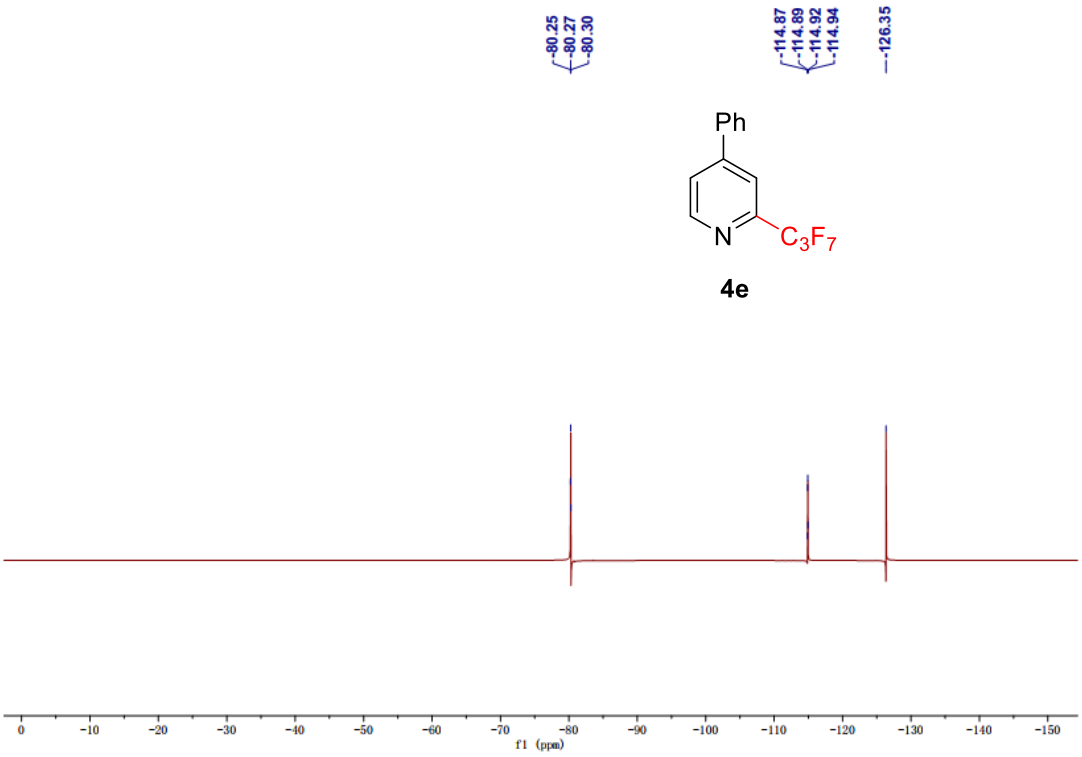

1.00
1.00
1.05
2.03
3.03
f1 (ppm)


150.53
150.26
148.68
148.43
148.18
136.93
130.02
129.51
127.23
124.26
120.43
120.38
120.34
119.83
119.49
119.16
116.96
116.63
116.30
114.10
113.78
113.57
111.92
111.54
111.17
110.84
110.54
110.24
109.66
109.28
108.90
108.52
107.42
107.01
106.64
106.26
77.48
77.16
76.84


Ph
N
C3F7

4e


f1 (ppm)


-80.25
-80.27
-80.30
-114.87
-114.89
-114.92
-114.94
-126.35
Ph
N
C_3F_7
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

4e