Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

2,11-Dimethoxyldipyridopurinone as an Efficient Reducing Visible-Light Photocatalyst for Organic Transformations

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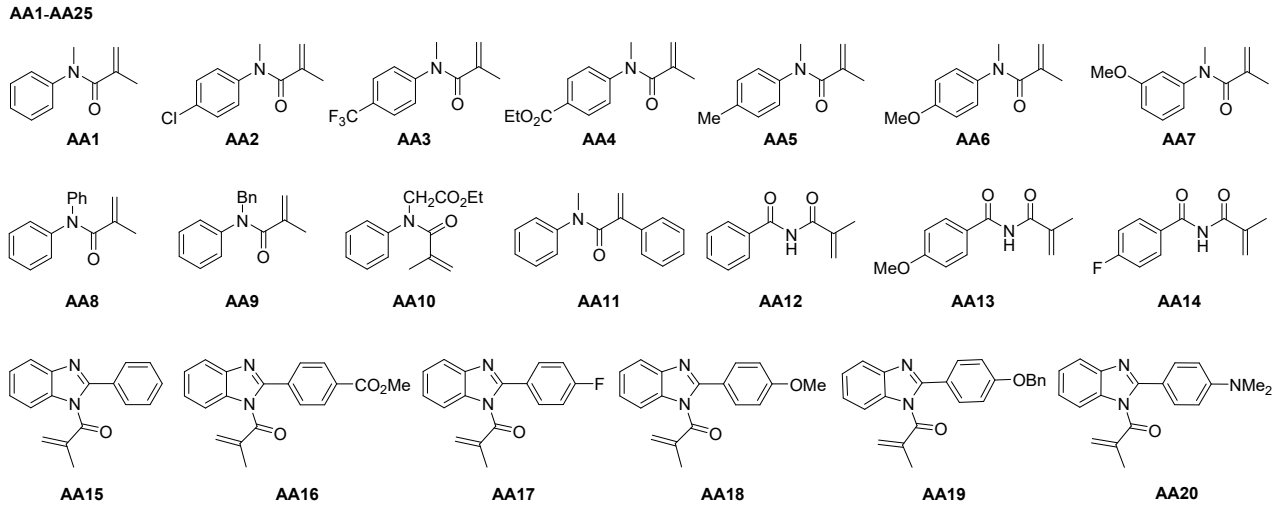
1. General Information

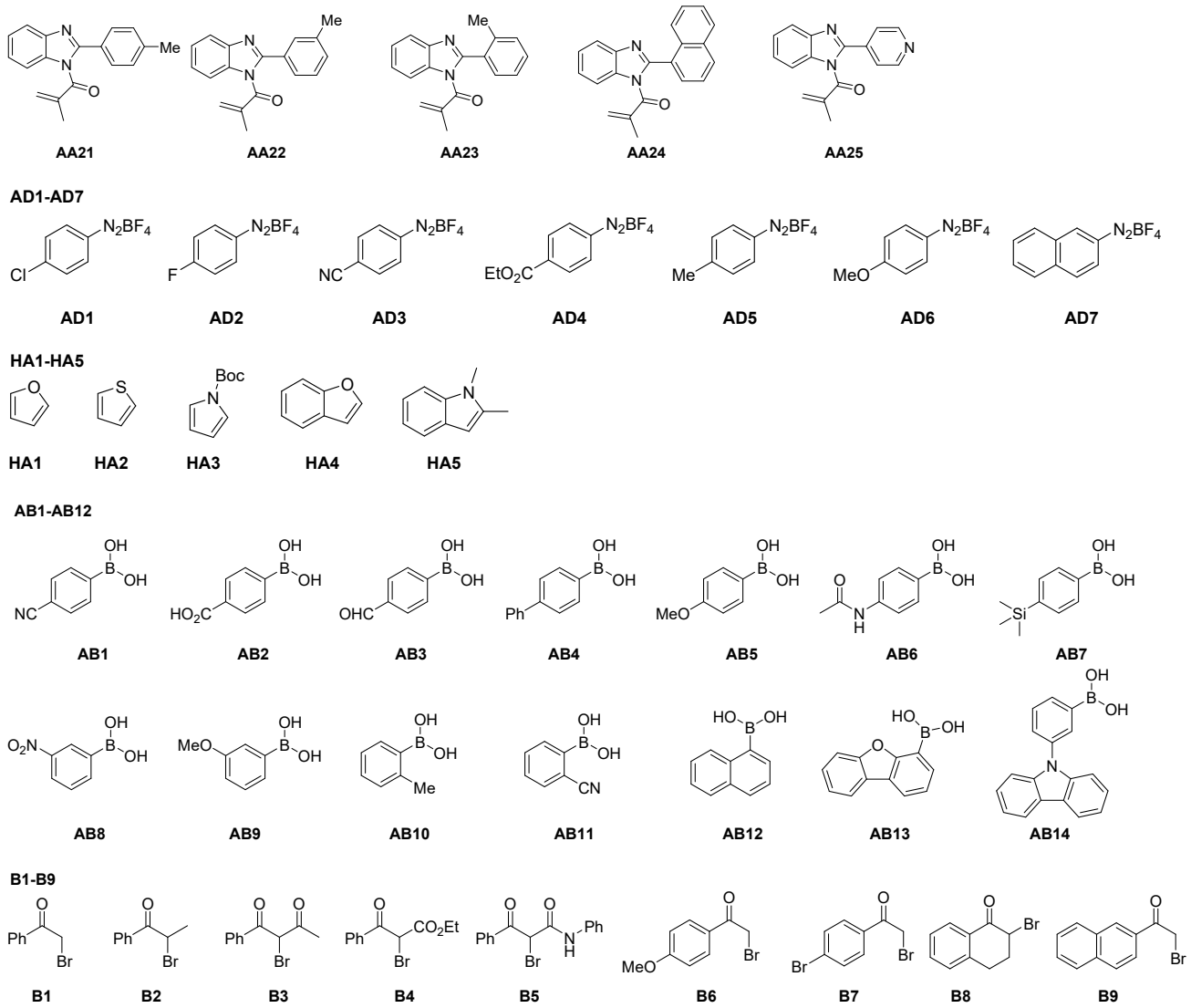
Petroleum ether used here refers to the 60–90 °C boiling point fraction of petroleum.^{1}H NMR and ^{13}C NMR spectra were recorded on a 400/600 MHz NMR spectrometer (^{1}H NMR, 400/600 MHz; ^{13}C NMR, 100/150 MHz at 25 °C). Coupling constants are reported in Hz. Multiplicities were given as: singlet (s), doublet (d), triplet (t), quartet (q), dd (doublet of doublet), quintet (quint.), septet (sept.), multiplet (m) etc. All high-resolution mass spectra (HRMS) were measured on a mass spectrometer (ESI-oa-TOF), and the purity of all samples used for HRMS (>95%) was confirmed by ^{1}H NMR and ^{13}C NMR spectroscopic analysis. All reagents were purchased from commercial sources and used without further treatment. All reactions were monitored by thin layer chromatography (TLC) with GF254 silica gel-coated plates. Flash chromatography was carried out on SiO_2 (silica gel 200–300 mesh).

Materials and Methods

The synthesis of **DP4** and HE-D^{3} were following the previously reported procedure.[1] All compounds of acrylamides (Figure S1, **AA1-AA25**), aryl diazonium salts (Figure S1, **AD1-AD7**) and α-bromo carbonyl compounds (Figure S1, **B2-B5**, **B8)** were synthesized following the procedure described in literatures.[2] Starting materials such as heteroarenes (Figure S1, **HA1-HA5**), arylboronic acids (Figure S1, **AB1-AB14**), α-bromoaryl ketone (Figure S1, **B1**, **B6, B7, B9**), Umemoto Reagent, CF_3SO_2Cl, and $C_4F_9SO_2Cl$ used in the article were purchased commercially. All reactions were irradiated with blue LEDs (435-440 nm, 20 W).

Figure S1. Series of materials used in text.





Characterization of DP4

Figure S2. UV-vis absorption spectra of **DP4**

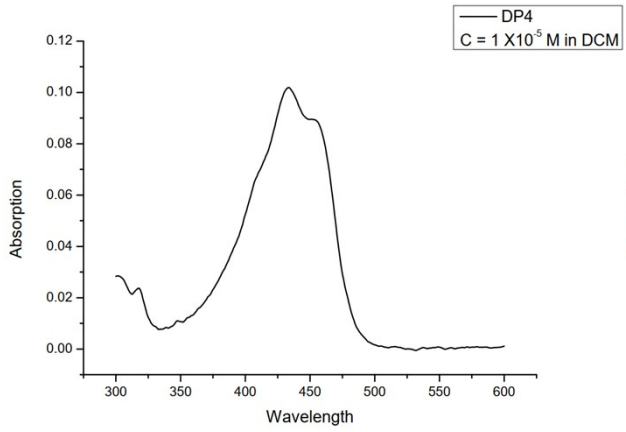


Figure S3. Excitation and emission spectra of **DP4**

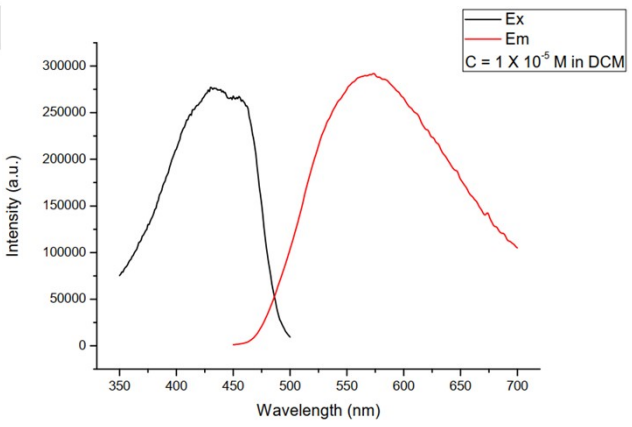


Figure S4. CV of **DP4** (1 mM) in DCM (SCE)

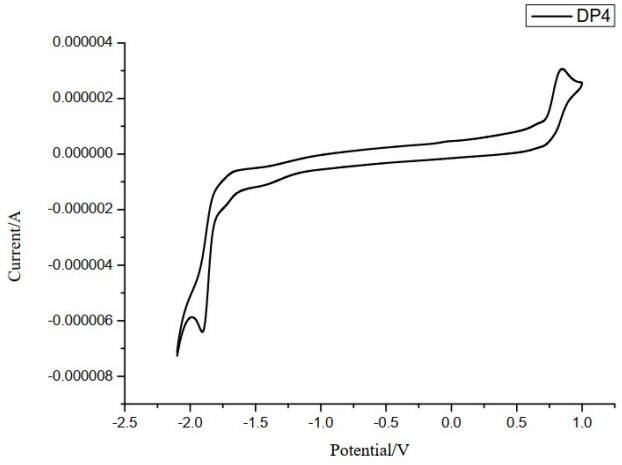


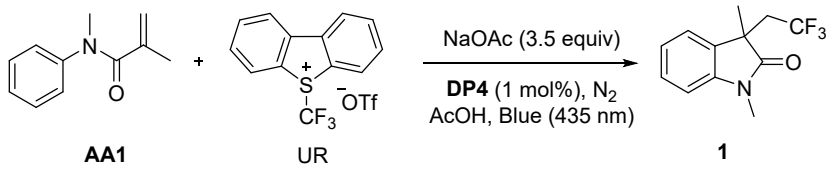
Table S1. The absorption, excitation, emission wavelength and redox potentials of **DP4**

	$\lambda_{abs(max)}$	λ_{Ex}	λ_{Em}	$E_{1/2}$red	E*red	$E_{1/2}$ox	E*ox
DP4	433 nm	432 nm	568 nm	-1.86 V	0.69 V	0.78 V	-1.77 V

Experimental setup for the photocatalytic reactions

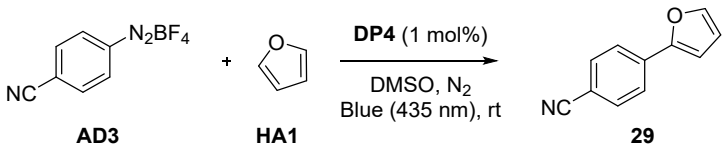
2. General Procedures

Intramolecular aryltrifluoromethylations of acrylamides (1 as an example)



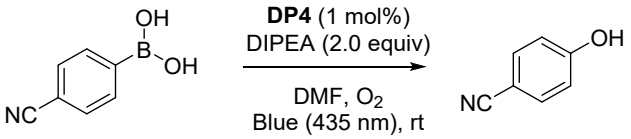
In a 10 mL shrek tube with magnetic stirring bar, the **AA1** (52.5 mg, 0.3 mmol), **DP4** (0.9 mg, 1 mol%), NaOAc (86.1 mg, 1.05 mmol) and UR (241.2 mg, 0.6 mmol) were successively added. The mixture was degased by bubbling N_2 for 5 min, and followed by addition of AcOH (3 mL) via syringe. The vial was sealed and protected by parafilm. The reaction mixture was stirred for 1 h under blue LED (distance app. 2.5 cm). The substrate was completely consumed (monitored by TLC analysis). Then the AcOH was removed by rotary evaporation. The residue was purified by flash column chromatography on silica gel using petroleum ether/ethyl acetate (20:1) as the eluent. The product **1** was obtained as a white solid (62 mg, 85%).

C−H Arylation of heteroarenes (29 as an example)



In a 10 mL shrek tube with magnetic stirring bar, the **AD3** (65.1 mg, 0.3 mmol), **HA1** (204.2 mg, 3 mmol) and **DP4** (0.9 mg, 1 mol%) were dissolved in dry DMSO (3 mL) and the resulting mixture was degassed by "pump-freeze-thaw". The reaction mixture was stirred for 3.5 h under blue LED (distance app. 2.5 cm). The substrate was completely consumed (monitored by TLC analysis). The reaction mixture was diluted with diethyl ether and washed with water (15 mL). The aqueous layer was washed three times with diethyl ether. The combined organic layers were dried over $NaSO_4$, filtered and concentrated in vacuum. The residue was purified by flash column chromatography on silica gel using petrol ether/ethyl acetate (10:1) as the eluent. The product **29** was obtained as a white solid (36.5 mg, 72%).

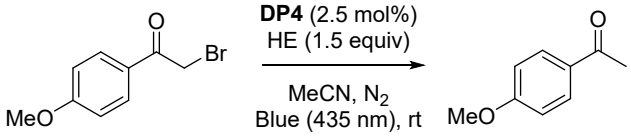
Hydroxylations of arylboronic acids (40 as an example)



AB1 **40**

In a 10 mL shrek tube with magnetic stirring bar, the **AB1** (44.1 mg, 0.3 mmol), **DP4** (0.9 mg, 1 mol%) and DIPEA (77.5 mg, 0.6 mmol) were dissolved in DMF (2 mL) and the resulting mixture were filled with oxygen. The reaction mixture was stirred for 27 h under blue LED (distance app. 2.5 cm). The substrate was completely consumed (monitored by TLC analysis), the reaction mixture was cooled to 0 ℃ and quenched carefully by aqueous solution of HCl (10%, 5 mL). The resultant mixture was extracted with Et_2O (3 x 20 mL). The combined organic layers were washed with brine (10 mL) and dried over Na_2SO_4. After removal of the solvent in vacuum, the residue was purified by flash column chromatography on silica gel using petrol ether/ethyl ether (5:1) as the eluent. The product **40** was obtained as a white solid (34.6 mg, 97%).

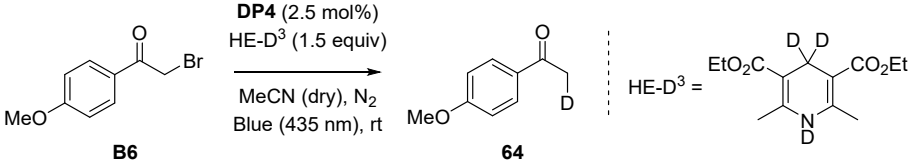
Dehalodeuteration of α-bromocarbonyl (59 as an example)



B6 **59**

In a 10 mL shrek tube with magnetic stirring bar, **DP4** (1.5 mg, 2.5 mol %), **B6** (45.6 mg, 0.20 mmol), and Hantzsch ester (75.3 mg, 0.3 mmol) were dissolved in MeCN (2 mL). The mixture was degased by bubbling N_2 for 5 min, and then stirred for 10 min under blue LED (distance app. 2.5 cm). The substrate was completely consumed (monitored by TLC analysis). After removal of the solvent in vacuum, the residue was purified by flash column chromatography on silica gel using petrol ether/ethyl ether (50:1) as the eluent. The product **59** was obtained as a white solid (29.4 mg, 98%).

Deuteration of α-bromocarbonyl (64 as an example)



B6 **64**

In a nitrogen-filled glovebox, **DP4** (1.5 mg, 2.5 mol %), **B6** (45.6 mg, 0.20 mmol), HE-D^3 (76.8

mg, 0.3 mmol), MeCN (dry, 2 mL) were successively added to an oven-dried sealable tube (10.0 mL). Then the tube was securely sealed and taken outside the glovebox. The mixture was stirred for 10 min under blue LED (distance app. 2.5 cm). The substrate was completely consumed (monitored by TLC analysis). After removal of the solvent in vacuum, the residue was purified by flash column chromatography on silica gel using petrol ether/ethyl ether (50:1) as the eluent. The product **64** was obtained as a white solid (28.7 mg, 95%).

3. Control experiments

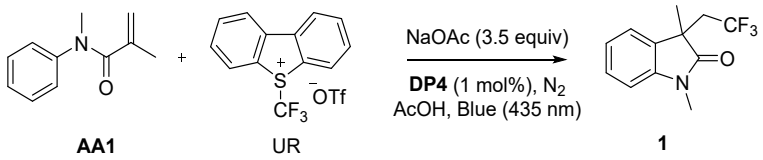


Table S2. Control experiments: intramolecular aryltrifluoromethylations of acrylamides

Entry	Cat.	Visible light	Yield of **1**/%
1	DP4	\	trace
2	\	Blue LED	14
3	DP4	Blue LED	85

[a]Unless otherwise noted, the reaction was conducted with **AA1** (0.3 mmol), UR (0.6 mmol), NaOAc (1.05 mmol), **DP4** (1 mol%), in AcOH (3 mL), N_2 atomosphere, r.t., Blue LED, 1 h. Isolated yields.

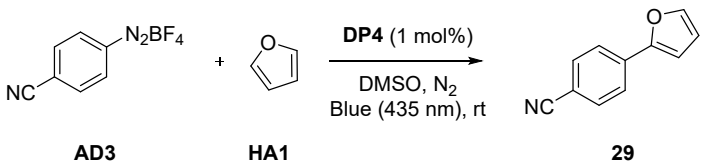
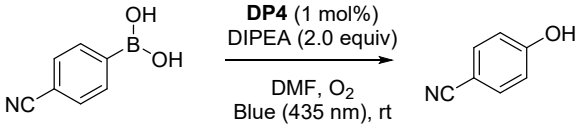


Table S3. Control experiments: the direct C−H arylation of heteroarenes.

Entry	Cat.	Visible light	Yield of **29**/%

1	DP4	\	0
2	\	Blue LED	23
3	DP4	Blue LED	72

[a]Unless otherwise noted, the reaction was conducted with **AD3** (0.3 mmol), HA1 (3 mmol), **DP4** (1 mol%), in DMSO (3 mL), N_2 atomosphere, r.t., Blue LED, 3.5 h. Isolated yields.



AB1 **40**

Table S4. Control experiments: hydroxylations of arylboronic acids.

Entry	Cat.	Atmosphere	Solvent	Base	Yield of **40**/%[a]
1	**DP_4**	O_2	MeCN	\	trace
2	**DP_4**	N_2	MeCN	DIPEA	0
3	\	O_2	MeCN	DIPEA	trace
4	**DP_4**	O_2	MeCN	DIPEA	0[b]
5	**DP_4**	O_2	MeCN	DIPEA	73
6	**DP_4**	O_2	DMF	DIPEA	97
7	\	O_2	DMF	DIPEA	trace

[a]Unless otherwise noted, the reaction was conducted with **AB1** (0.3 mmol), DIPEA (0.6 mmol), **DP4** (1 mol%), in solvent (2 mL), O_2 atomosphere, r.t., Blue LED, 27 h. Isolated yields. [b]Without visible light.

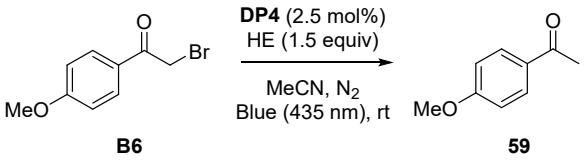


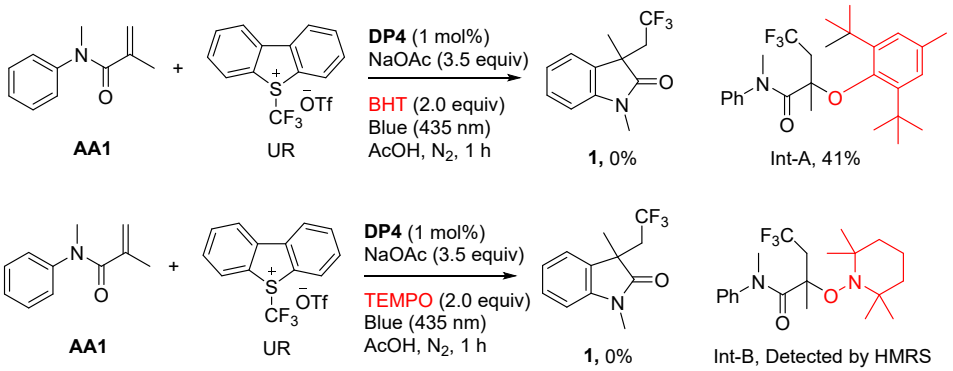
Table S5. Control experiments: dehalodeuteration of α-bromocarbonyl.

Entry	Cat.	Additive	Visible light	Yield of **59**/%
1	DP4	\	Blue LED	0
2	DP4	HE	\	0
3	\	HE	Blue LED	37
4	DP4	HE	Blue LED	95

[a]Unless otherwise noted, the reaction was conducted with **B6** (0.2 mmol), HE (0.3 mmol), **DP4** (2.5 mol%), in MeCN (2 mL), N_2 atomosphere, r.t., Blue LED, 10 min. Isolated yields.

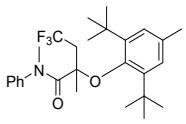
4. Mechanistic studies

Scheme S1. Mechanistic investigations for intramolecular aryltrifluoromethylations of acrylamides.



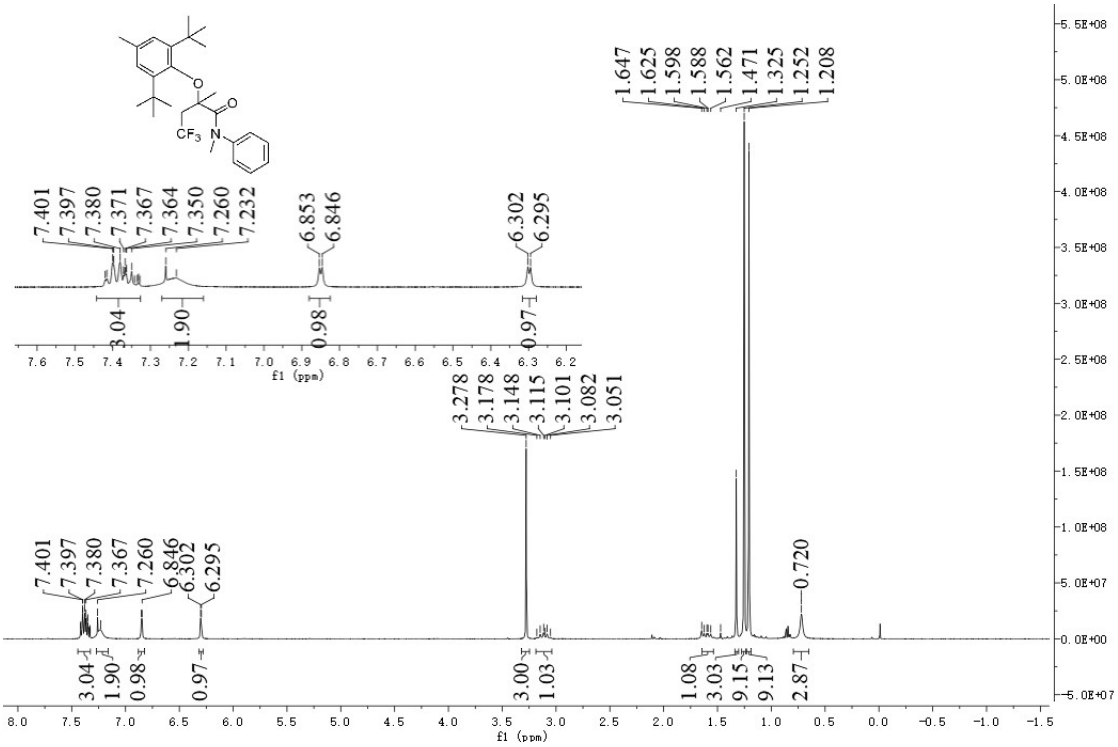
In a 10 mL shrek tube with magnetic stirring bar, the **AA1** (0.3 mmol), **DP4** (1 mol%), NaOAc (1.05 mmol), BHT/TEMPO (0.6 mmol), and UR (0.6 mmol) were successively added. The mixture was degased by bubbling N_2 for 5 min, and followed by addition of AcOH (3 mL) via syringe. The vial was sealed and protected by parafilm. The reaction mixture was stirred for 1 h under blue LED (distance app. 2.5 cm). The substrate was completely consumed (monitored by TLC analysis). Then the AcOH was removed by rotary evaporation. After removal of the solvent in vacuum, the product **1**

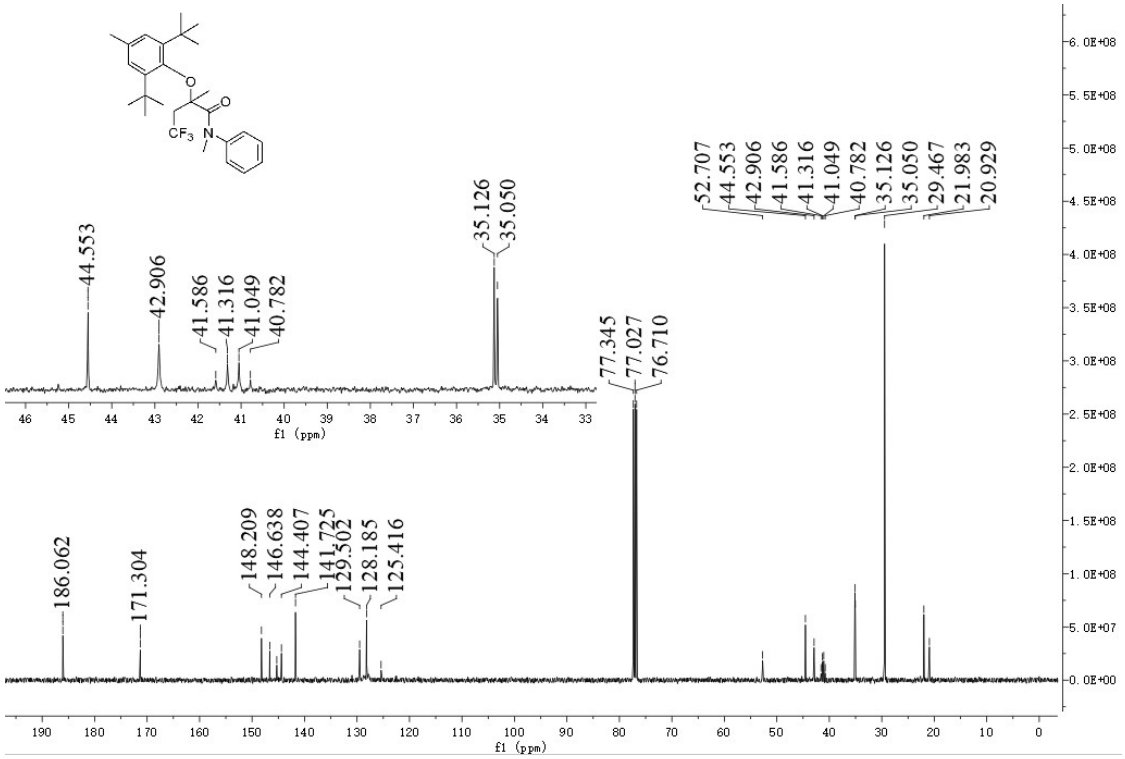
was not observed by TLC from the residues respectively. The BHT-trapped intermediate Int-A was separated in 41% yield by flash column chromatography on silica gel using petrol ether/ethyl ether (50:1) as the eluent. The TEMPO-trapped intermediate Int-B was not seperated, but detected by HMRS from the residue.



2-(2,6-Di-tert-butyl-4-methylphenoxy)-4,4,4-trifluoro-*N*,2-dimethyl-*N*-phenylbutanamide (Int-A)

White solid. Mp: 167-169 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.33 (m, 3H), 7.23 (s, 2H), 6.85 (d, J = 2.8 Hz, 1H), 6.30 (d, J = 2.8 Hz, 1H), 3.28 (s, 3H), 3.19-3.04 (m, 1H), 1.68-1.54 (m, 1H), 1.33 (s, 3H), 1.25 (s, 9H), 1.21 (s, 9H), 0.72 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 186.1, 171.3, 148.2, 146.6, 145.3, 144.4, 141.7, 129.5, 128.2, 125.4, 52.7, 44.6, 42.9, 41.18 (q, J = 27.0 Hz), 35.13, 35.05, 29.5, 22.0, 21.0. HRMS (ESI), m/z calcd. for $C_{27}H_{37}F_3NO_2$ ([M+H]$^+$) 464.2771, found: 464.2760.





Mass Spectrum SmartFormula Report

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Comment

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Operator Demo User
Instrumen compact 8255754.2017 6

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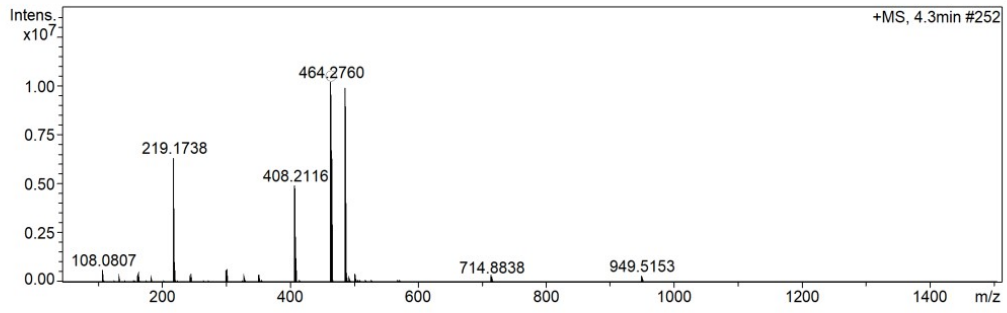

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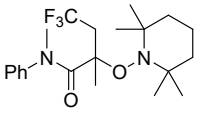

4,4,4-Trifluoro-*N*,2-dimethyl-*N*-phenyl-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)butanamide (Int-B)

HRMS (ESI), m/z calcd. for $C_{21}H_{32}F_3N_2O_2$ ($[M+H]^+$) 401.2410, found: 401.2403.

Mass Spectrum SmartFormula Report

Analysis Info

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Comment

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Instrumen compact 8255754.2017 6

Acquisition Paramet

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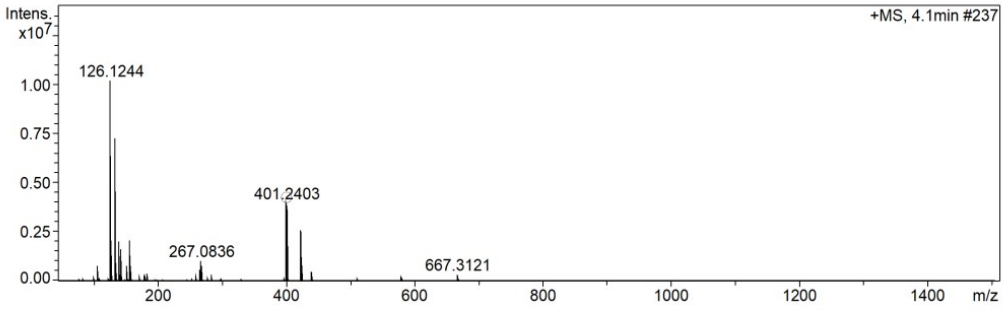
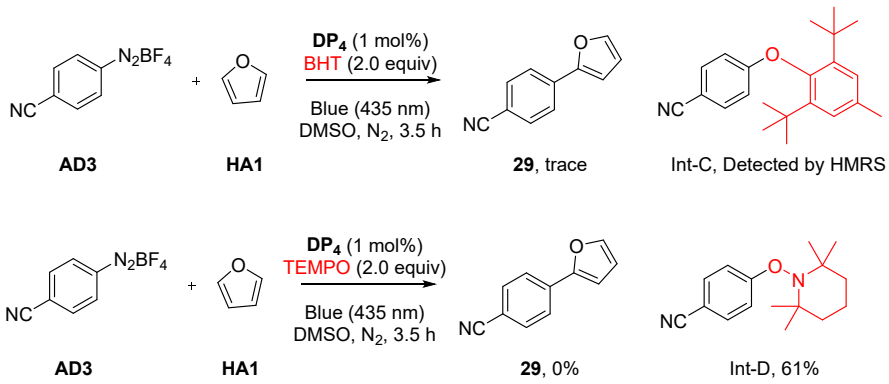


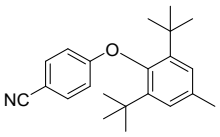
Meas. m/z # Ion Formula m/z err [ppm] mSigma # mSigma Score rdb e¡¥ Conf N-Rule
401.2403 1 C21H32F3N2O2 401.2410 1.8 2.8 1 100.00 6.0 even ok

Scheme S2. Mechanistic investigations for the direct C−H arylation of heteroarenes.



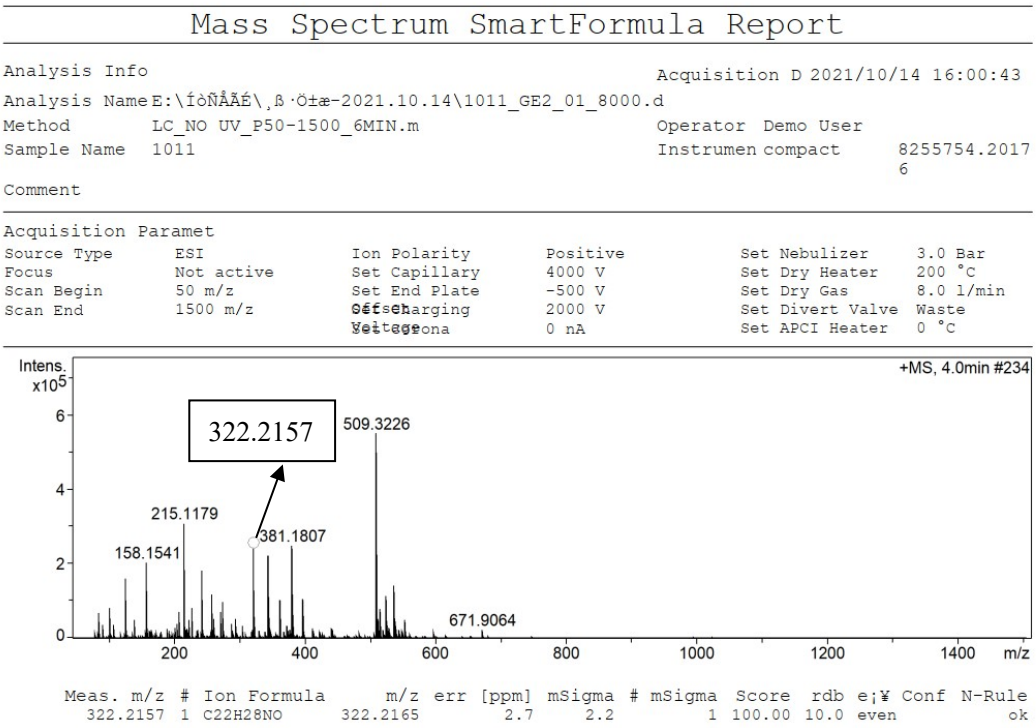
In a 10 mL shrek tube with magnetic stirring bar, the **AD3** (0.3 mmol), **HA1** (3 mmol), BHT/TEMPO (0.6 mmol) and **DP4** (1 mol%) were dissolved in dry DMSO (3 mL) and the resulting mixture was degassed by "pump-freeze-thaw". The reaction mixture was stirred for 3.5 h under blue LED (distance app. 2.5 cm). The substrate was completely consumed (monitored by TLC analysis). The reaction mixture was diluted with diethyl ether and washed with water (15 mL). The aqueous layer was washed three times with diethyl ether. The combined organic layers were dried over $NaSO_4$, filtered and concentrated in vacuum. For the BHT experiment, trace amount of the product **29** was observed by TLC and the BHT-trapped intermediate Int-C was not seperated, but detected by HMRS from the residue. For the TEMPO experiment, the product **29** was not observed by TLC and

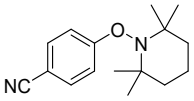
the TEMPO-trapped intermediate Int-D was seperated in 61% yield by flash column chromatography on silica gel using petrol ether/ethyl ether (200:1) as the eluent from the residue.



4-(2,6-Di-*tert*-butyl-4-methylphenoxy)benzonitrile (Int-C)

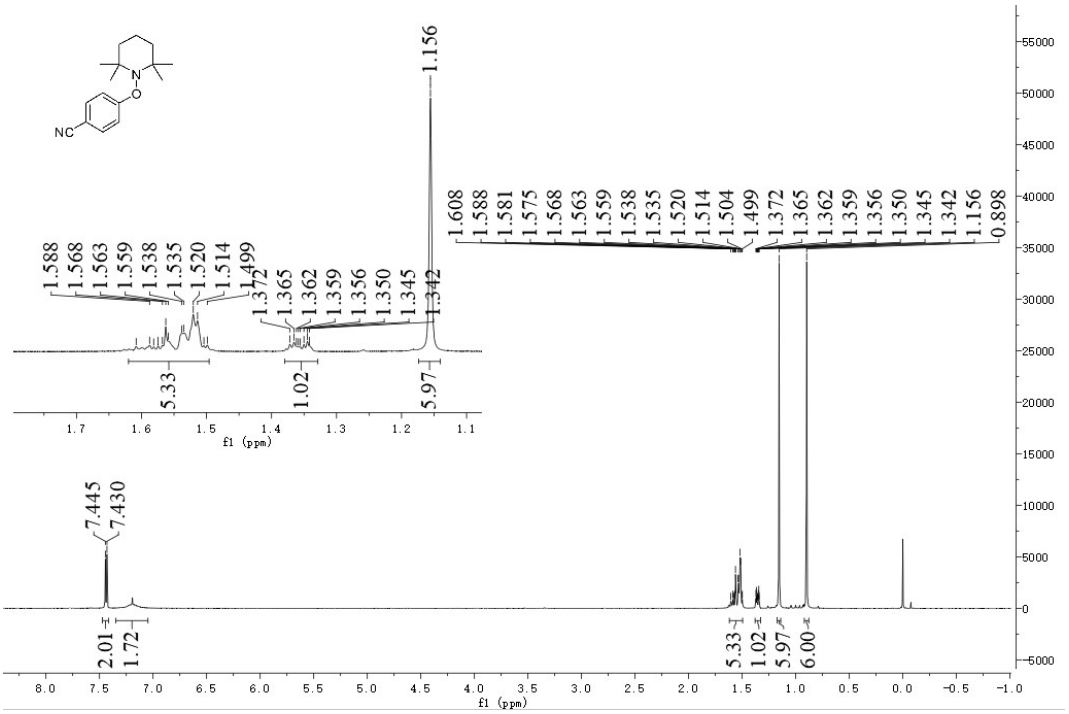
HRMS (ESI), m/z calcd. for $C_{22}H_{28}NO$ ([M+H]$^+$) 322.2165, found: 322.2157.





4-((2,2,6,6-Tetramethylpiperidin-1-yl)oxy)benzonitrile (Int-D)[3]

White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.44 (d, J = 9.0 Hz, 2H), 7.35-7.05 (m, 2H), 1.62-1.50 (m, 5H), 1.39-1.33 (m, 1H), 1.16 (s, 6H), 0.90 (s, 6H). HRMS (ESI), m/z calcd. for $C_{16}H_{22}N_2NaO$ ([M+Na]$^+$) 281.1624, found: 281.1622.



Mass Spectrum SmartFormula Report

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Comment

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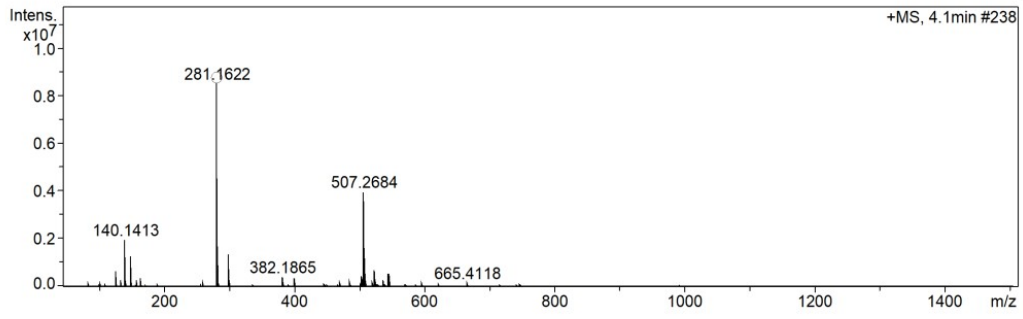
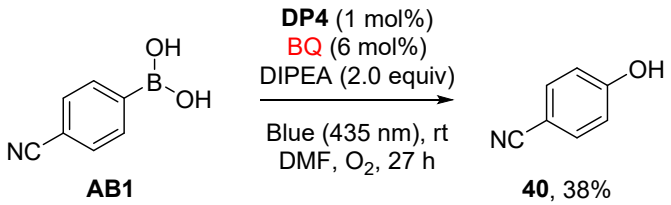
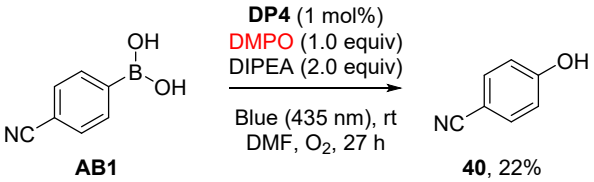
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
281.1622	1	C16H22N2NaO	281.1624	0.8	6.9	1	100.00	7.0	even		ok

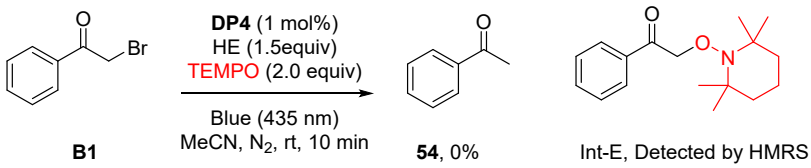
Scheme S3. Mechanistic investigations for hydroxylations of arylboronic acids.



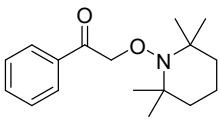


In a 10 mL shrek tube with magnetic stirring bar, the **AB1** (0.3 mmol), **DP4** (1 mol%), 1,4-benzoquinone (BQ, 6 mol%)/5,5-dimethyl-1-pyrroline *N*-oxide (DMPO, 1.0 equiv) and DIPEA (0.6 mmol) were dissolved in DMF (2 mL) and the resulting mixture filled with oxygen. The reaction mixture was stirred for 27 h under blue LED (distance app. 2.5 cm). The substrate was completely consumed (monitored by TLC analysis), the reaction mixture was cooled to 0 ℃ and quenched carefully by aqueous solution of HCl (10%, 5 mL). The resultant mixture was extracted with Et_2O (3 x 20 mL). The combined organic layers were washed with brine (10 mL) and dried over Na_2SO_4. After removal of the solvent in vacuum, the residue was purified to afford **40** by flash column chromatography on silica gel using petrol ether/ethyl ether (5:1) as the eluent.

Scheme S4. Mechanistic investigations for dehalodeuteration of α-bromocarbonyl.



In a 10 mL shrek tube with magnetic stirring bar, **DP4** (2.5 mol %), **B6** (0.20 mmol), TMPEO (0.6 mmol) and Hantzsch ester (0.3 mmol) were dissolved in MeCN (2 mL). The mixture was degased by bubbling N_2 for 5 min, and then stirred for 10 min under blue LED (distance app. 2.5 cm). The substrate was completely consumed (monitored by TLC analysis). After removal of the solvent in vacuum, the product **54** was not observed by TLC and the TEMPO-trapped intermediates Int-E was detected by HMRS from the residue.



1-Phenyl-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)ethan-1-one (Int-E)

HRMS (ESI), m/z calcd. for $C_{17}H_{25}NNaO_2$ ($[M+Na]^+$) 298.1777, found: 298.1746.

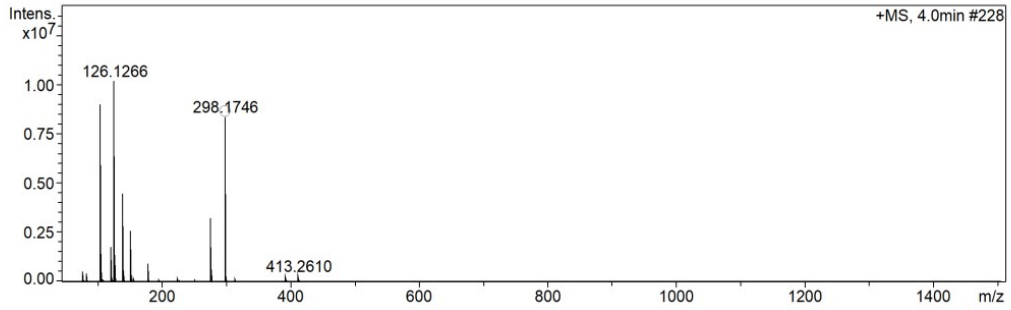
Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2021/12/13 16:01:30

Analysis Name E:\ÍòÑÅÃÉ\¸ß·Ö±æ-2021.12.13\1213_RA3_01_9348.d
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User
Sample Name 1213 — Instrumen compact 8255754.2017 6
Comment

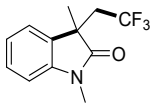
Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
298.1746	1	C17H25NNaO2	298.1777	10.7	1.2	1	100.00	6.0	even		ok

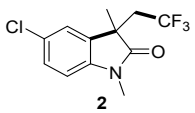
5. Characterization of compounds



1

1,3-Dimethyl-3-(2,2,2-trifluoroethyl)indolin-2-one (1)[4]

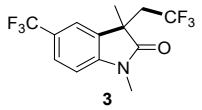
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (td, J = 7.6, 1.2 Hz, 1H), 7.27 (d, J = 7.2 Hz, 1H), 7.09 (t, J = 7.4 Hz, 1H), 6.88 (d, J = 8.0 Hz, 1H), 3.24 (s, 3H), 2.88-2.57 (m, 2H), 1.41 (s, 3H). ^{19}F NMR δ -62.0.



2

5-Chloro-1,3-dimethyl-3-(2,2,2-trifluoroethyl)indolin-2-one (2)[5]

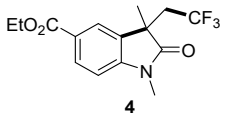
Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.28 (dd, J = 8.1, 2.1 Hz, 1H), 7.23 (d, J = 1.8 Hz, 1H), 6.80 (d, J = 7.8 Hz, 1H), 3.21 (s, 3H), 2.88-2.76 (m, 1H), 2.68-2.56 (m, 1H), 1.40 (s, 3H). ^{19}F NMR δ -62.0.



3

1,3-Dimethyl-3-(2,2,2-trifluoroethyl)-5-(trifluoromethyl)indolin-2-one (3)[5]

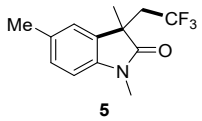
Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.60 (d, J = 8.4 Hz, 1H), 7.49 (s, 1H), 6.96 (d, J = 8.4 Hz, 1H), 3.27 (s, 3H), 2.92-2.80 (m, 1H), 2.74-2.62 (m, 1H), 1.43 (s, 3H). ^{19}F NMR δ -61.5, -62.1.



4

Ethyl-1,3-dimethyl-2-oxo-3-(2,2,2-trifluoroethyl)indoline-5-carboxylate (4)[6]

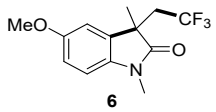
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 8.0 Hz, 1H), 7.92 (s, 1H), 6.90 (d, J = 8.0 Hz, 1H), 4.36 (q, J = 7.2 Hz, 2H), 3.25 (s, 3H), 2.96-2.60 (m, 2H), 1.46-1.34 (m, 6H). ^{19}F NMR δ -62.0.



5

1,3,5-Trimethyl-3-(2,2,2-trifluoroethyl)indolin-2-one (5)[5]

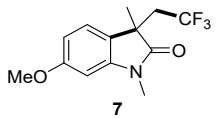
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13-7.09 (m, 1H), 7.07 (s, 1H), 6.76 (d, J = 8.0 Hz, 1H), 3.21 (s, 3H), 2.89-2.71 (m, 10.8 Hz, 1H), 2.68-2.55 (m, 1H), 2.35 (s, 3H), 1.39 (s, 3H). ^{19}F NMR δ -61.9.



6

5-Methoxy-1,3-dimethyl-3-(2,2,2-trifluoroethyl)indolin-2-one (6)[4]

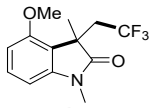
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.94-6.71 (m, 3H), 3.79 (s, 3H), 3.20 (s, 3H), 2.89-2.72 (m, 1H), 2.71-2.54 (m, 1H), 1.39 (s, 3H). ^{19}F NMR δ -61.9.



7

6-Methoxy-1,3-dimethyl-3-(2,2,2-trifluoroethyl)indolin-2-one (7)[7]

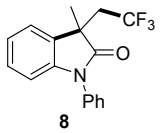
Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.15 (d, J = 8.4 Hz, 1H), 6.59 (dd, J = 8.4, 2.4 Hz, 1H), 6.46 (d, J = 2.4 Hz, 1H), 3.84 (s, 3H), 3.21 (s, 3H), 2.85-2.72 (m, 1H), 2.67-2.56 (m, 1H), 1.38 (s, 3H). ^{19}F NMR δ -61.9.



7'

4-Methoxy-1,3-dimethyl-3-(2,2,2-trifluoroethyl)indolin-2-one (7')[8]

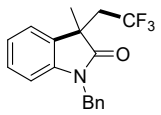
Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.26 (t, J = 8.1 Hz, 1H), 6.63 (d, J = 8.4 Hz, 1H), 6.53 (d, J = 7.8 Hz, 1H), 3.86 (s, 3H), 3.21 (s, 3H), 3.02-2.92 (m, 1H), 2.86-2.74 (m, 1H), 1.43 (s, 3H). ^{19}F NMR δ -64.0.



8

3-Methyl-1-phenyl-3-(2,2,2-trifluoroethyl)indolin-2-one (8)[4]

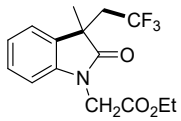
Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (t, J = 7.8 Hz, 2H), 7.44-7.38 (m, 3H), 7.32 (d, J = 7.2 Hz, 1H), 7.24 (td, J = 7.8, 1.2 Hz, 1H), 7.13 (td, J = 7.5, 0.8 Hz, 1H), 6.84 (d, J = 7.8 Hz, 1H), 3.04-2.90 (m, 1H), 2.79-2.66 (m, 1H), 1.54 (s, 3H). ^{19}F NMR δ -61.9.



9

1-Benzyl-3-methyl-3-(2,2,2-trifluoroethyl)indolin-2-one (9)[4]

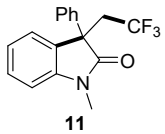
Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35-7.22 (m, 6H), 7.18 (td, J = 7.8, 1.2 Hz, 1H), 7.05 (td, J = 7.5, 0.9 Hz, 1H), 6.75 (d, J = 7.8 Hz, 1H), 4.98 (d, J = 16.2 Hz, 1H), 4.89 (d, J = 16.2, 1H), 2.98-2.94 (m, 1H), 2.75-2.65 (m, 1H), 1.46 (s, 3H). ^{19}F NMR δ -61.7.



10

Ethyl-2-(3-methyl-2-oxo-3-(2,2,2-trifluoroethyl)indolin-1-yl)acetate (10)[4]

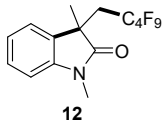
Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.30-7.26 (m, 2H), 7.10 (td, J = 7.5, 0.9 Hz, 1H), 6.76 (d, J = 8.4 Hz, 1H), 4.52 (d, J = 17.4 Hz, 1H), 4.43 (d, J = 17.4 Hz, 1H), 4.20 (q, J = 7.2 Hz, 2H), 2.91-2.79 (m, 1H), 2.72-2.61 (m, 1H), 1.45 (s, 3H), 1.23 (t, J = 6.9 Hz, 3H). ^{19}F NMR δ -61.7.



11

1-Methyl-3-phenyl-3-(2,2,2-trifluoroethyl)indolin-2-one (11)[4]

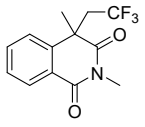
Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.41-7.36 (m, 1H), 7.35-7.25 (m, 6H), 7.16 (td, J = 7.5, 0.9 Hz, 1H), 6.94 (d, J = 7.8 Hz, 1H), 3.49-3.37 (m, 1H), 3.22 (s, 3H), 3.13-2.98 (m, 1H). ^{19}F NMR δ -61.1.



12

1,3-Dimethyl-3-(2,2,3,3,4,4,5,5,5-nonafluoropentyl)indolin-2-one (12)[4]

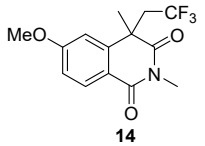
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.26 (m, 2H), 7.13 (td, J = 7.4, 1.0 Hz, 1H), 6.93 (d, J = 7.6 Hz, 1H), 3.29 (s, 3H), 2.98-2.85 (m, 1H), 2.74-2.55 (m, 1H), 1.48 (s, 3H). ^{19}F NMR δ -81.01 – -81.21 (m, 3F), -108.53 – -109.39 (m, 1F), -114.22 – -115.11 (m, 1F), -124.54 – -124.61 (m, 2F), -125.75 – -126.10 (m, 2F).



13

2,4-Dimethyl-4-(2,2,2-trifluoroethyl)isoquinoline-1,3(2*H*,4*H*)-dione (13)[9]

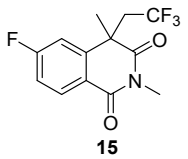
White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.29 (dd, J = 8.1, 0.9 Hz, 1H), 7.66 (td, J = 7.8, 1.5 Hz, 1H), 7.50 (t, J = 7.8 Hz, 1H), 7.42 (d, J = 7.8 Hz, 1H), 3.41 (s, 3H), 3.39-3.30 (m, 1H), 2.85-2.75 (m, 1H), 1.66 (s, 3H). ^{19}F NMR δ -61.7.



14

6-Methoxy-2,4-dimethyl-4-(2,2,2-trifluoroethyl)isoquinoline-1,3(2*H*,4*H*)-dione (14)[9]

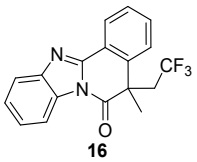
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, J = 8.8 Hz, 1H), 7.00 (dd, J = 8.8, 2.4 Hz, 1H), 6.85 (d, J = 2.4 Hz, 1H), 3.90 (s, 3H), 3.41-3.26 (m, 4H), 2.84-2.69 (m, 1H), 1.65 (s, 3H). ^{19}F NMR δ -61.6.



15

6-Fluoro-2,4-dimethyl-4-(2,2,2-trifluoroethyl)isoquinoline-1,3(2*H*,4*H*)-dione (15)[9]

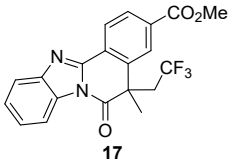
White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.32 (dd, J = 9.0, 6.0 Hz, 1H), 7.22-7.16 (m, 1H), 7.10 (dd, J = 9.0, 2.4 Hz, 1H), 3.44-3.30 (m, 4H), 2.80-2.68 (m, 1H), 1.66 (s, 3H). ^{19}F NMR δ -61.7, 103.1.



16

5-Methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (16)[9]

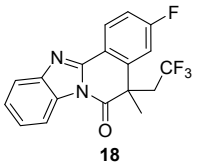
White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.52 (dd, J = 7.8, 1.2 Hz, 1H), 8.38-8.34 (m, 1H), 7.85-7.81 (m, 1H), 7.60 (td, J = 7.8, 1.5 Hz, 1H), 7.53 (td, J = 7.5, 0.9 Hz, 1H), 7.49-7.42 (m, 3H), 3.53-3.42 (m, 1H), 3.01-2.86 (m, 1H), 1.76 (s, 3H). ^{19}F NMR δ -61.4.



17

Methyl-5-methyl-6-oxo-5-(2,2,2-trifluoroethyl)-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-3-carboxylate (17)[10]

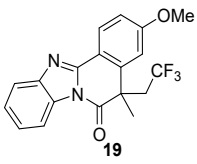
White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.59 (d, J = 8.4 Hz, 1H), 8.38-8.34 (m, 1H), 8.19-8.14 (m, 2H), 7.88-7.83 (m, 1H), 7.51-7.45 (m, 2H), 3.99 (s, 3H), 3.56-3.45 (m, 1H), 3.08-3.97 (m, 1H), 1.80 (s, 3H). ^{19}F NMR δ -61.4.



18

3-Fluoro-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (18)[10]

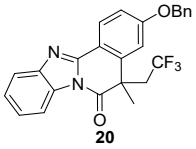
White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.53 (dd, J = 8.7, 5.7 Hz, 1H), 8.38-8.31 (m, 1H), 7.81 (dd, J = 6.9, 1.5 Hz, 1H), 7.48-7.42 (m, 2H), 7.28-7.22 (m, 1H), 7.16 (dd, J = 9.6, 2.4 Hz, 1H), 3.57-3.47 (m, 1H), 2.92-3.82 (m, 1H), 1.76 (s, 3H). ^{19}F NMR δ -61.4, -106.2.



19

3-Methoxy-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (19)[10]

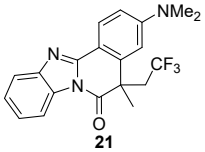
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (d, J = 9.0 Hz, 1H), 8.36-8.26 (m, 1H), 7.78 (d, J = 7.2 Hz, 1H), 7.46-7.36 (m, 2H), 7.07 (dd, J = 9.0, 2.4 Hz, 1H), 6.93 (d, J = 2.4 Hz, 1H), 3.91 (s, 3H), 3.52-3.38 (m, 1H), 2.95-2.83 (m, 1H), 1.74 (s, 3H). ^{19}F NMR δ -61.3.



20

3-(Benzyloxy)-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (20)[10]

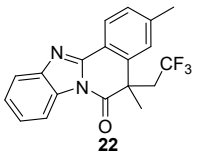
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, J = 8.8 Hz, 1H), 8.33 (dd, J = 7.0, 1.7 Hz, 1H), 7.79 (dd, J = 7.0, 1.4 Hz, 1H), 7.54-7.33 (m, 7H), 7.16 (dd, J = 8.6, 2.2 Hz, 1H), 7.01 (d, J = 2.4 Hz, 1H), 5.26-5.00 (m, 2H), 3.53-3.34 (m, 1H), 2.92-2.77 (m, 1H), 1.72 (s, 3H). ^{19}F NMR δ -61.3.



21

3-(Dimethylamino)-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (21)[10]

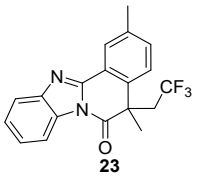
Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 (d, J = 9.0 Hz, 1H), 8.29 (d, J = 7.8 Hz, 1H), 7.73 (d, J = 7.8 Hz, 1H), 7.39 (td, J = 7.5, 0.9 Hz, 1H), 7.34 (td, J = 7.8, 0.9 Hz, 1H), 6.84 (dd, J = 9.0, 2.4 Hz, 1H), 6.57 (d, J = 1.8 Hz, 1H), 3.53-3.42 (m, 1H), 3.09 (s, 6H), 2.99-2.87 (m, 1H), 1.74 (s, 3H). ^{19}F NMR δ -61.0.



22

3,5-Dimethyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (22)[10]

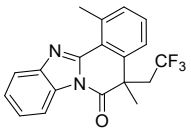
White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.39 (d, J = 8.4 Hz, 1H), 8.34 (dd, J = 7.5, 1.5 Hz, 1H), 7.81 (dd, J = 7.2, 1.2 Hz, 1H), 7.47-7.39 (m, 2H), 7.33 (d, J = 7.8 Hz, 1H), 7.25 (s, 1H), 3.51-3.39 (m, 1H), 2.99-2.87 (m, 1H), 2.47 (s, 3H), 1.74 (s, 3H). ^{19}F NMR δ -61.3.



23

2,5-Dimethyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (23)[10]

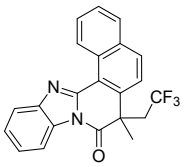
Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.37-8.32 (m, 2H), 7.83 (dd, J = 6.9, 1.5 Hz, 1H), 7.48-7.38 (m, 3H), 7.35 (d, J = 7.8 Hz, 1H), 3.51-3.39 (m, 1H), 2.97-2.87 (m, 1H), 2.47 (s, 3H), 1.73 (s, 3H). ^{19}F NMR δ -61.3.



24

1,5-Dimethyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (24)[10]

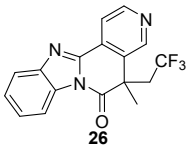
Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.42-8.37 (m, 1H), 7.88-7.83 (m, 1H), 7.48-7.42 (m, 3H), 7.35 (d, J = 8.7, 2H), 3.53-3.43 (m, 1H), 3.07 (s, 3H), 2.99-2.88 (m, 1H), 1.76 (s, 3H). ^{19}F NMR δ -61.2.



25

7-Methyl-7-(2,2,2-trifluoroethyl)benzo[h]benzo[4,5]imidazo[2,1-*a*]isoquinolin-8(7*H*)-one (25)[10]

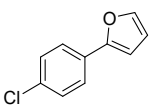
Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.54 (d, J = 8.8 Hz, 1H), 8.46-8.40 (m, 1H), 8.05 (d, J = 8.4 Hz, 1H), 7.97-7.90 (m, 2H), 7.86-7.78 (m, 1H), 7.69-7.61 (m, 1H), 7.56-7.45 (m, 3H), 3.64-3.45 (m, 1H), 3.19-2.96 (m, 1H), 1.82 (s, 3H). ^{19}F NMR δ -61.6.



26

5-Methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*][2,6]naphthyridin-6(5*H*)-one (26)[10]

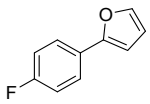
Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.84 (s, 1H), 8.77 (d, J = 5.4 Hz, 1H), 8.40-8.36 (m, 1H), 8.30 (d, J = 4.8 1H), 7.91-7.87 (m, 1H), 7.55-7.48 (m, 2H), 3.58-2.46 (m, 1H), 3.08-3.01 (m, 1H), 1.84 (s, 3H). ^{19}F NMR δ -61.3.



27

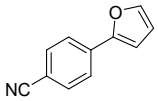
2-(4-Chlorophenyl)furan (27)[11]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 8.4 Hz, 2H), 7.47 (d, J = 1.6 Hz, 1H), 7.35 (d, J = 8.4 Hz, 2H), 6.64 (d, J = 3.6 Hz, 1H), 6.47 (dd, J = 3.4, 1.8 Hz, 1H).



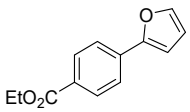
2-(4-Fluorophenyl)furan (28)[12]

White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66-7.61 (m, 2H), 7.46 (d, J = 1.2 Hz, 1H), 7.11-7.04 (m, 2H), 6.58 (d, J = 2.4 Hz, 1H), 6.47 (dd, J = 2.0, 1.2 Hz, 1H).



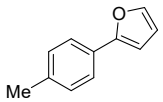
4-(Furan-2-yl)benzonitrile (29)[11]

White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, J = 9.0 Hz, 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.54 (d, J = 1.8 Hz, 1H), 6.81 (d, J = 4.2 Hz, 1H), 6.53 (dd, J = 3.0, 1.8 Hz, 1H).



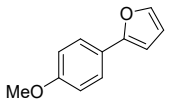
Ethyl 4-(furan-2-yl)benzoate (30)[11]

White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, J = 9.0 Hz, 2H), 7.72 (d, J = 9.0 Hz, 2H), 7.51 (d, J = 1.8 Hz, 1H), 6.78 (d, J = 3.0 Hz, 1H), 6.50 (dd, J = 3.0, 1.8 Hz, 1H), 4.38 (q, J = 7.2 Hz, 2H), 1.40 (t, J = 7.2 Hz, 3H).



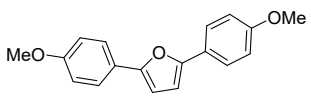
2-(*p*-Tolyl)furan (31)[11]

White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57 (d, J = 8.4 Hz, 2H), 7.45 (d, J = 1.2 Hz, 1H), 7.20 (d, J = 7.8 Hz, 2H), 6.60 (d, J = 3.0 Hz, 1H), 6.46 (dd, J = 3.0, 1.8 Hz, 1H), 2.37 (s, 3H).



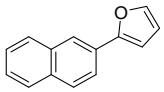
2-(4-Methoxyphenyl)furan (32)[11]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 9.2 Hz, 2H), 7.43 (dd, J = 1.8, 0.6 Hz, 1H), 6.92 (d, J = 9.2 Hz, 2H), 6.51 (dd, J = 3.4, 0.6 Hz, 1H), 6.44 (dd, J = 3.4, 1.8 Hz, 1H), 3.83 (s, 3H).



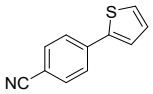
2,5-Bis(4-methoxyphenyl)furan (32')[13]

Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.8 Hz, 2H), 7.78 (d, J = 8.8 Hz, 2H), 7.05 (d, J = 3.6 Hz, 1H), 7.00 (d, J = 9.2 Hz, 2H), 6.96 (d, J = 8.8 Hz, 2H), 6.79 (d, J = 3.6 Hz, 1H), 3.89 (s, 3H), 3.86 (s, 3H).



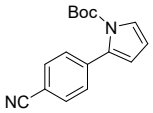
2-(Naphthalen-2-yl)furan (33)[14]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.90-7.74 (m, 4H), 7.53 (d, J = 1.6 Hz, 1H), 7.51-7.42 (m, 2H), 6.78 (d, J = 3.6 Hz, 1H), 6.53 (dd, J = 3.4, 1.8 Hz, 1H).



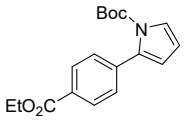
4-(Thiophen-2-yl)benzonitrile (34)[11]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.63 (m, 4H), 7.42 (dd, J = 3.6, 1.2 Hz, 1H), 7.40 (dd, J = 5.0, 1.0 Hz, 1H), 7.13 (dd, J = 4.8, 3.6 Hz, 1H).



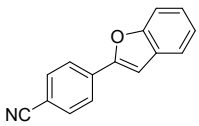
2-(4-Cyano-phenyl)-pyrrole-1-carboxylic acid tert-butyl ester (35)[11]

White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 7.8 Hz, 2H), 7.39 (dd, J = 3.0, 1.8 Hz, 1H), 6.29-6.24 (m, 2H), 1.42 (s, 9H).



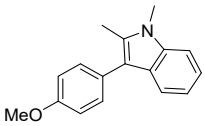
2-(4-Ethoxycarbonyl -phenyl)-pyrrole-1-carboxylic acid tert-butyl ester (36)[11]

Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, J = 8.4 Hz, 2H), 7.42 (d, J = 8.4 Hz, 2H), 7.38 (dd, J = 3.3, 2.1 Hz, 1H), 6.27-6.22 (m, 2H), 4.39 (q, J = 7.2 Hz, 2H), 1.40 (t, J = 7.2 Hz, 3H), 1.38 (s, 9H).



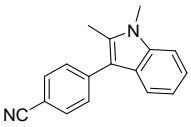
4-(Benzofuran-2-yl)benzonitrile (37)[15]

White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (d, J = 8.4 Hz, 2H), 7.70 (d, J = 8.4 Hz, 2H), 7.62 (d, J = 7.2 Hz, 1H), 7.53 (d, J = 7.8 Hz, 1H), 7.35 (t, J = 7.8 Hz, 1H), 7.27 (*t*, J = 7.8 Hz, 1H), 7.16 (s, 1H).



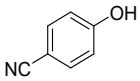
4-(1,2-Dimethyl-1*H*-indol-3-yl)benzonitrile (38)[16]

Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57-8.51 (m, 1H), 7.85 (d, J = 8.8 Hz, 2H), 7.27-7.22 (m, 3H), 6.98 (d, J = 8.8 Hz, 2H), 3.85 (s, 3H), 3.66 (s, 3H), 2.74 (s, 3H).



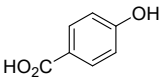
3-(4-Methoxyphenyl)-1,2-dimethyl-1*H*-indole (39)[17]

Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51-8.44 (m, 1H), 7.83 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.32-7.18 (m, 3H), 3.59 (s, 3H), 2.66 (s, 3H).



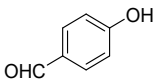
4-Hydroxybenzonitrile (40)[18]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, J = 8.8 Hz, 2H), 6.93 (d, J = 8.8 Hz, 2H), 6.18 (s, 1H).



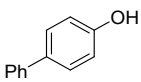
4-Hydroxybenzoic acid (41)[18]

White solid. ^{1}H NMR (400 MHz, DMSO) δ 12.40 (s, 1H), 10.20 (s, 1H), 7.79 (d, J = 8.8 Hz, 2H), 6.82 (d, J = 8.8 Hz, 2H).



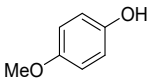
4-Hydroxybenzaldehyde (42)[18]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.87 (s, 1H), 7.82 (d, J = 8.8 Hz, 2H), 6.98 (d, J = 8.4 Hz, 2H), 6.21 (s, 1H).



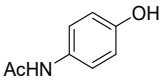
[1,1'-Biphenyl]-4-ol (43)[18]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58-7.51 (m, 2H), 7.49 (d, J = 8.8 Hz, 2H), 7.42 (t, J = 7.8 Hz, 2H), 7.31 (t, J = 7.4 Hz, 1H), 6.91 (d, J = 8.8 Hz, 2H), 4.82 (s, 1H).



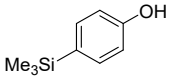
4-Methoxyphenol (44)[18]

Brown solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 6.75-6.65 (m, 4H), 3.69 (s, 3H).



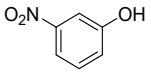
***N*-(4-Hydroxyphenyl)acetamide (45)**[19]

Brown solid. ^{1}H NMR (400 MHz, MeOD) δ 7.30 (d, J = 8.8 Hz, 2H), 6.73 (d, J = 8.8 Hz, 2H), 2.07 (s, 3H).



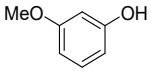
4-(Trimethylsilyl)phenol (46)[20]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, J = 8.8 Hz, 2H), 6.84 (d, J = 8.8 Hz, 2H), 4.82 (s, 1H), 0.25 (s, 9H).



3-Nitrophenol (47)[18]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.78 (m, 1H), 7.71 (t, J = 2.3 Hz, 1H), 7.41 (t, J = 8.2 Hz, 1H), 7.22-7.15 (m, 1H), 5.66 (s, 1H).



3-Methoxyphenol (48)[19]

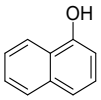
Brown liqiud. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.05 (t, J = 8.1 Hz, 1H), 6.42 (dd, J = 8.1, 1.5 Hz, 1H), 6.38-6.32 (m, 2H), 4.58 (s, 1H), 3.70 (s, 3H).

2-Hydroxybenzonitrile (49)[21]

Brown solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.51 (dd, J = 7.8, 1.8 Hz, 1H), 7.49-7.43 (m, 1H), 7.02 (d, J = 8.4 Hz, 1H), 6.98 (t, J = 7.5 Hz, 1H), 6.68 (s, 1H).

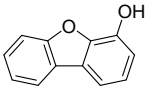
***o*-Cresol (50)**[18]

White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.14 (d, J = 7.2 Hz, 1H), 7.10 (t, J = 7.8 Hz, 1H), 6.87 (t, J = 7.2 Hz, 1H), 6.78 (d, J = 7.8 Hz, 1H), 4.71 (s, 1H), 2.27 (s, 3H).



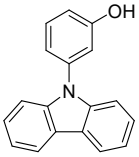
Naphthalen-1-ol (51)[18]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27-8.17 (m, 1H), 7.88-7.80 (m, 1H), 7.57-7.43 (m, 3H), 7.33 (t, J = 7.4, 1H), 6.82 (dd, J = 7.2, 0.8 Hz, 1H), 5.35 (s, 1H).



Dibenzo[*b*,*d*]furan-4-ol (52)[22]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.92 (m, 1H), 7.59 (d, J = 8.4 Hz, 1H), 7.52 (dd, J = 7.8, 1.0 Hz, 1H), 7.50-7.42 (m, 1H), 7.37 (td, J = 7.6, 0.8 Hz, 1H), 7.23 (t, J = 7.8 Hz, 1H), 7.03 (dd, J = 8.0, 0.8 Hz, 1H), 5.39 (s, 1H).

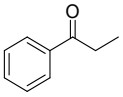


3-(9*H*-Carbazol-9-yl)phenol (53)[23]

White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.18 (d, J = 7.2 Hz, 2H), 7.49-7.40 (m, 5H), 7.32 (t, J = 7.5 Hz, 2H), 7.16 (d, J = 7.8 Hz, 1H), 7.01 (s, 1H), 6.92 (dd, J = 8.1, 2.1 Hz, 1H), 5.24 (s, 1H).

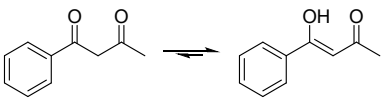
Acetophenone (54)[24]

Colorless liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (d, J = 7.2 Hz, 2H), 7.54 (t, J = 7.5 Hz, 1H), 7.44 (t, J = 7.8 Hz, 2H), 2.59 (s, 3H).



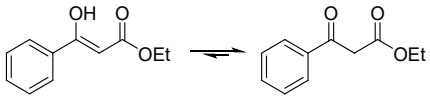
Propiophenone (55)[24]

Colorless liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (d, J = 7.2 Hz, 2H), 7.54 (t, J = 7.2 Hz, 1H), 7.45 (t, J = 7.8 Hz, 2H), 3.00 (q, J = 7.2 Hz, 2H), 1.22 (t, J = 7.2 Hz, 3H).



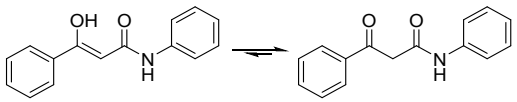
1-Phenylbutane-1,3-dione (56)[25]

White solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 16.16 (s, 1H), 7.88 (d, J = 7.2 Hz, 2H), 7.52 (t, J = 7.5 Hz, 1H), 7.45 (t, J = 7.8 Hz, 2H), 6.18 (s, 1H), 2.20 (s, 3H).



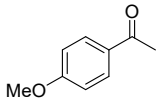
Ethyl-3-oxo-3-phenylpropanoate (57)[26]

Yellow liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 (d, J = 7.2 Hz, 2H), 7.60 (t, J = 7.5 Hz, 1H), 7.49 (t, J = 7.8 Hz, 2H), 4.22 (q, J = 7.2 Hz, 2H), 3.99 (s, 2H), 1.26 (t, J = 7.2 Hz, 3H).



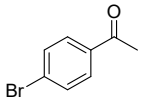
3-Oxo-*N*,3-diphenylpropanamide (58)[27]

Yellow solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.29 (s, 1H), 8.04 (d, J = 7.2 Hz, 2H), 7.65 (t, J = 7.5 Hz, 1H), 7.59 (d, J = 7.8 Hz, 2H), 7.52 (t, J = 7.8 Hz, 2H), 7.34 (t, J = 7.8 Hz, 2H), 7.13 (t, J = 7.5 Hz, 1H), 4.12 (s, 2H).



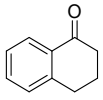
1-(4-Methoxyphenyl)ethan-1-one (59)[28]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, J = 9.2 Hz, 2H), 6.93 (d, J = 8.8 Hz, 2H), 3.86 (s, 3H), 2.55 (s, 3H).



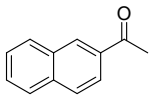
1-(4-Bromophenyl)ethan-1-one (60)[24]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 8.8 Hz, 2H), 7.60 (d, J = 8.8Hz, 2H), 2.58 (s, 3H).



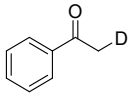
3,4-Dihydronaphthalen-1(2*H*)-one (61)[29]

Brown liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02 (d, J = 7.8 Hz, 1H), 7.45 (t, J = 7.5 Hz, 1H), 7.29 (t, J = 7.8 Hz, 1H), 7.24 (d, J = 7.8 Hz, 1H), 2.95 (t, J = 6.0 Hz, 2H), 2.66-2.61 (m, 2H), 2.16-2.09 (m, 2H).



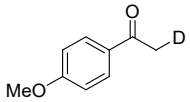
1-(Naphthalen-2-yl)ethan-1-one (62)[24]

White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.03 (dd, J = 8.8, 1.6 Hz, 1H), 7.96 (d, J = 8.0 Hz, 1H), 7.91-7.85 (m, 2H), 7.64-7.51 (m, 2H), 2.72 (s, 3H).



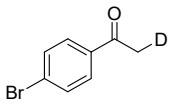
2-Deutero-1-phenylethanone (63)

Colorless liquid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (d, J = 7.2 Hz, 2H), 7.57 (t, J = 7.5 Hz, 1H), 7.47 (t, J = 7.8 Hz, 2H), 2.60 (t, J = 2.1 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.2, 137.2, 133.1, 128.6, 128.3, 28.39 (t, J = 19.5 Hz, 1H). HRMS (ESI), m/z calcd. for C_8H_8DO ($[M+H]^+$) 122.0711 found: 122.0711.



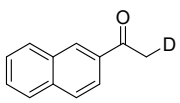
2-Deuterio-1-(4-methoxy-phenyl)-ethanone (64)

White solid. Mp: 35 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, J = 9.2 Hz, 2H), 6.86 (d, J = 8.8 Hz, 2H), 3.80 (s, 3H), 2.47 (t, J = 2.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.9, 163.5, 130.6, 130.4, 113.7, 55.5, 26.11 (t, J = 19.5 Hz, 1H). HRMS (ESI), m/z calcd. for $C_9H_{10}DO_2$ ($[M+H]^+$) 152.0816, found: 152.0816.



1-(4-Bromo-phenyl)-2-deuterio-ethanone (65)

White solid. Mp: 103 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 8.8 Hz, 2H), 7.61 (d, J = 8.3 Hz, 2H), 2.57 (t, J = 2.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.1, 135.9, 131.9, 129.9, 128.3, 26.31 (t, J = 19.5 Hz, 1H). HRMS (ESI), m/z calcd. for $C_8H_7BrDO_2$ ($[M+H]^+$) 199.9816, found: 199.9812.



2-Deuterio-ethanone-1-(2-naphthalenyl) (66)

White solid. Mp: 58 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.03 (dd, J = 8.4, 1.8 Hz, 1H), 7.96 (d, J = 7.8 Hz, 1H), 7.88 (t, J = 8.4 Hz, 2H), 7.64-7.58 (m, 1H), 7.57-7.53 (m, 1H), 2.71 (t, J = 2.1 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.2, 135.6, 134.5, 132.5, 130.2, 129.6, 128.5, 128.4, 127.8, 126.8, 123.9, 26.46 (t, J = 19.5 Hz, 1H). HRMS (ESI), m/z calcd. for $C_{12}H_{10}DO$ ($[M+H]^+$) 172.0867, found: 172.0867.

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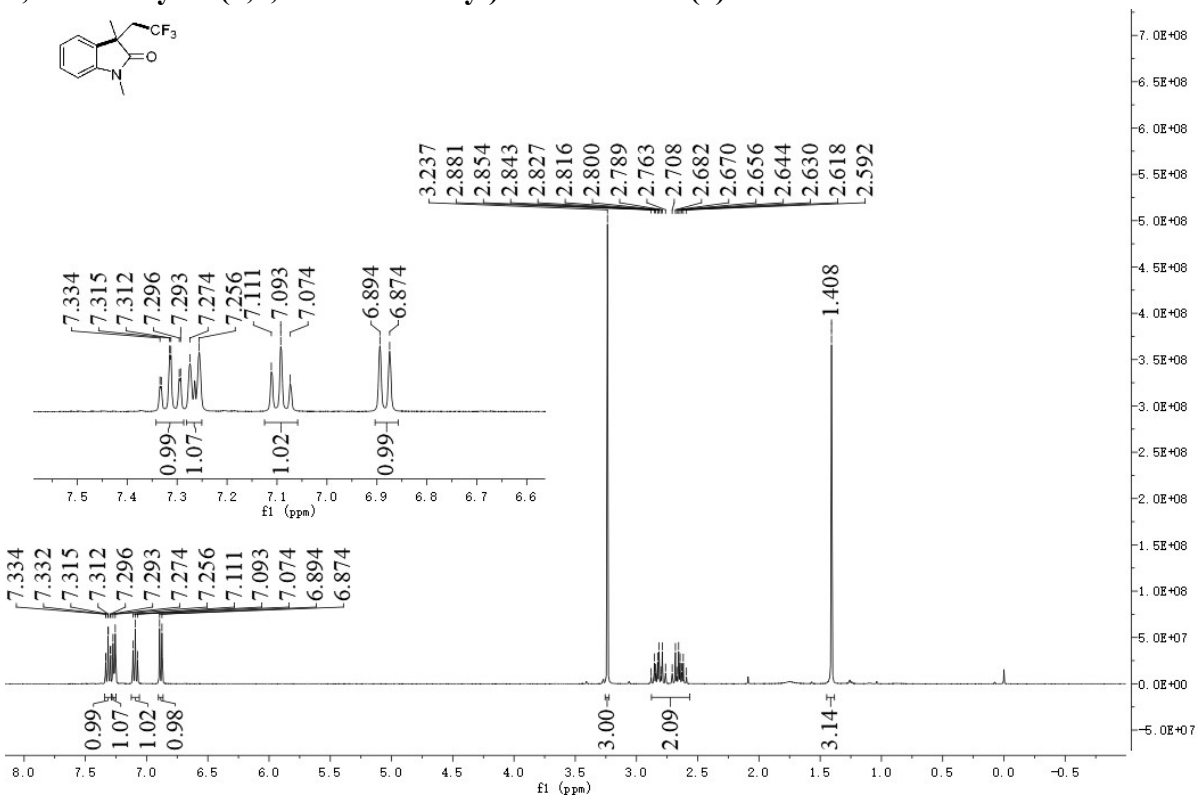
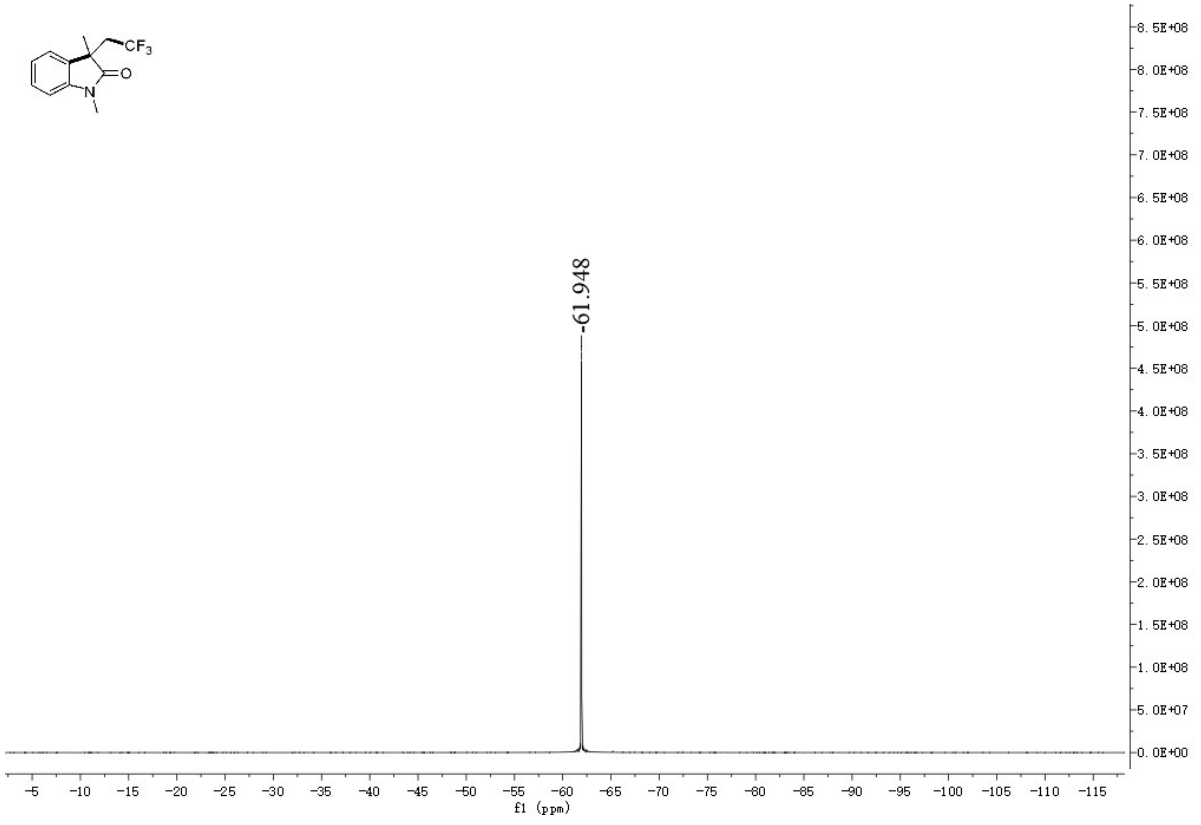
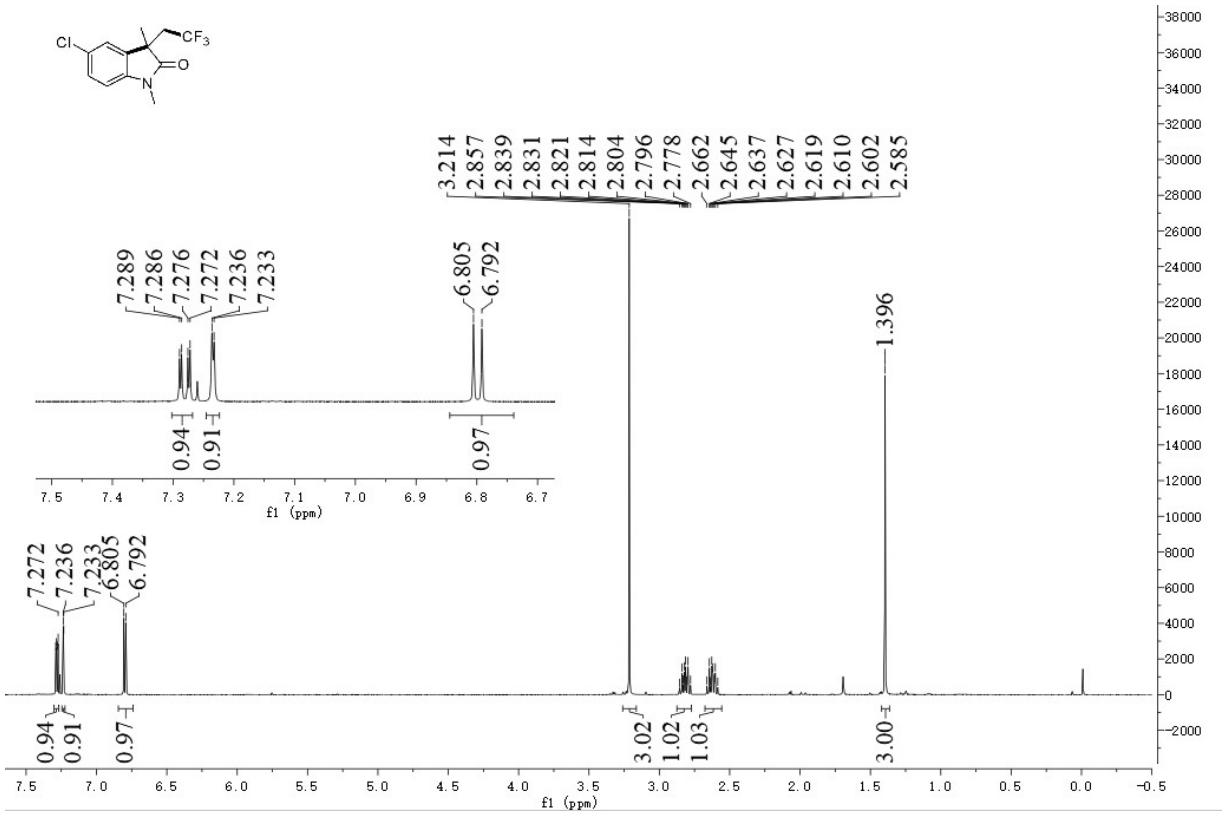
7. NMR spectra of products

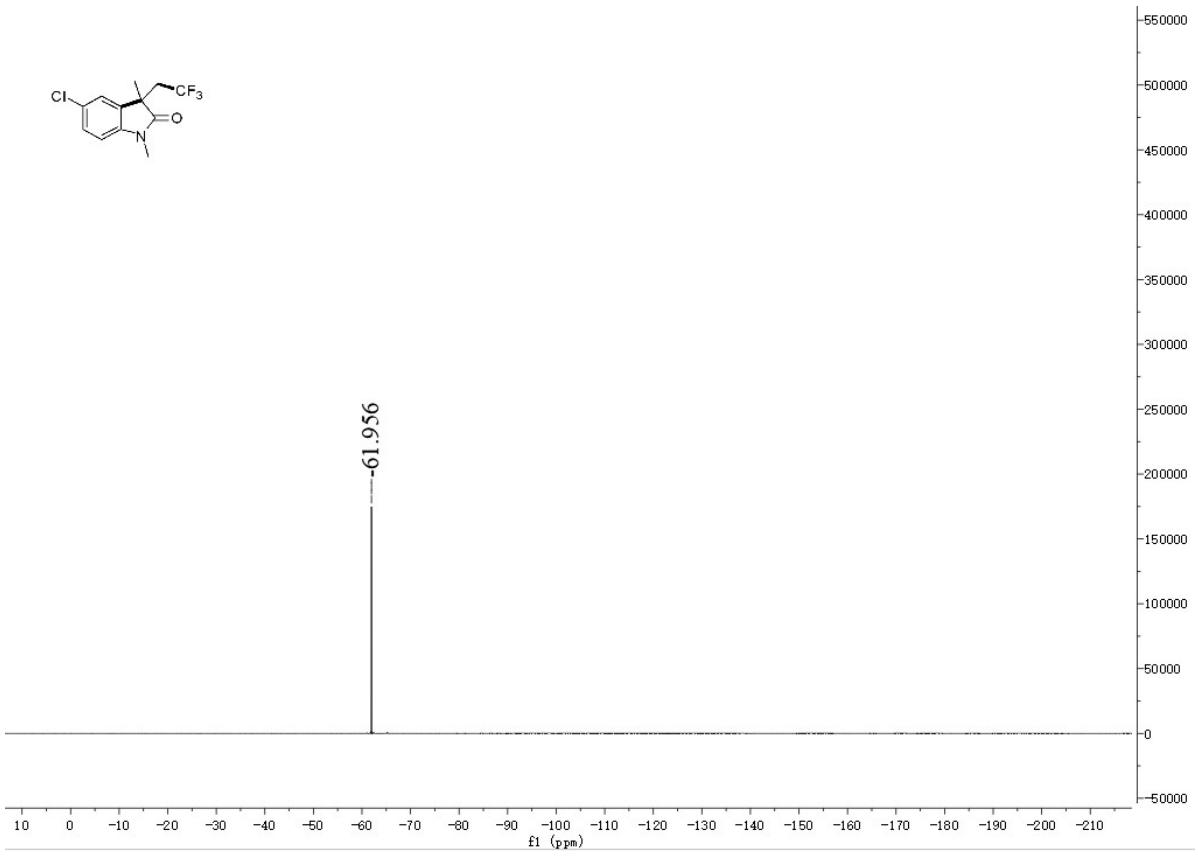
1,3-Dimethyl-3-(2,2,2-trifluoroethyl)indolin-2-one (1)



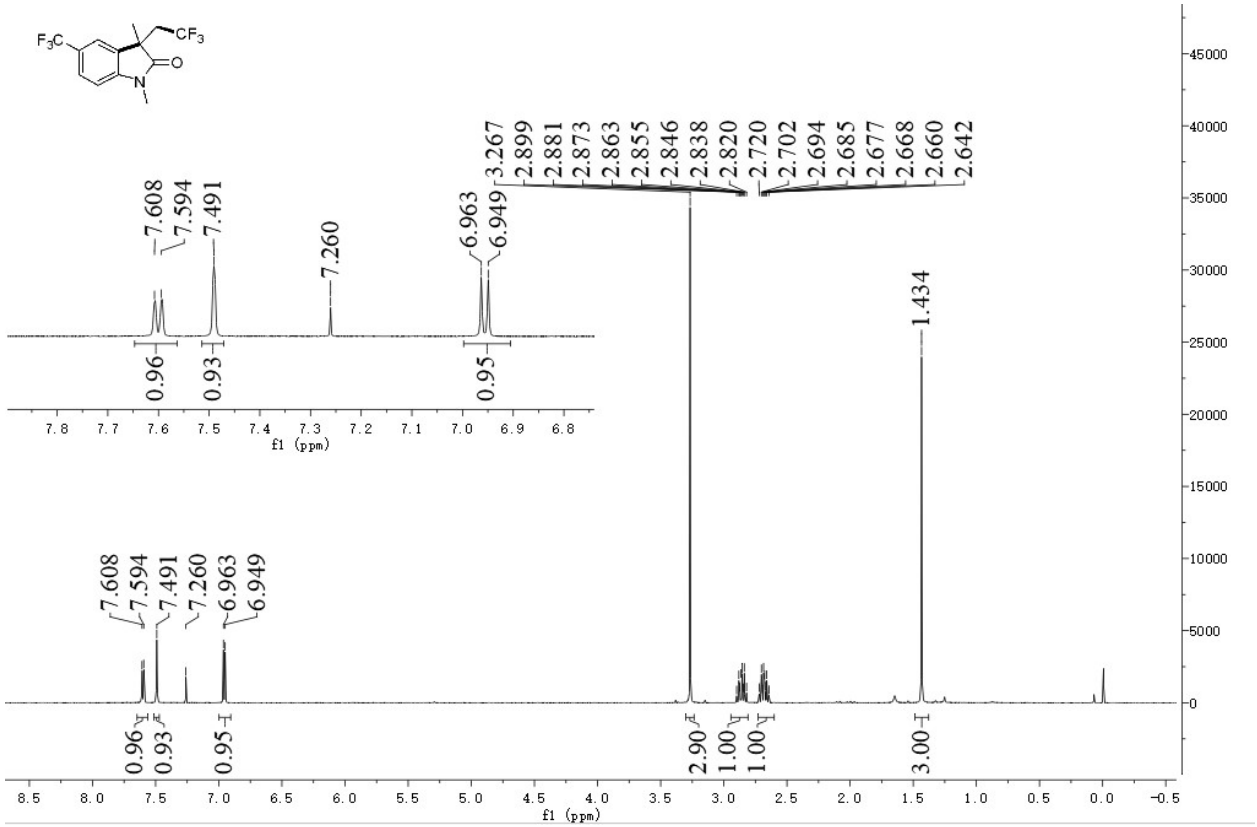


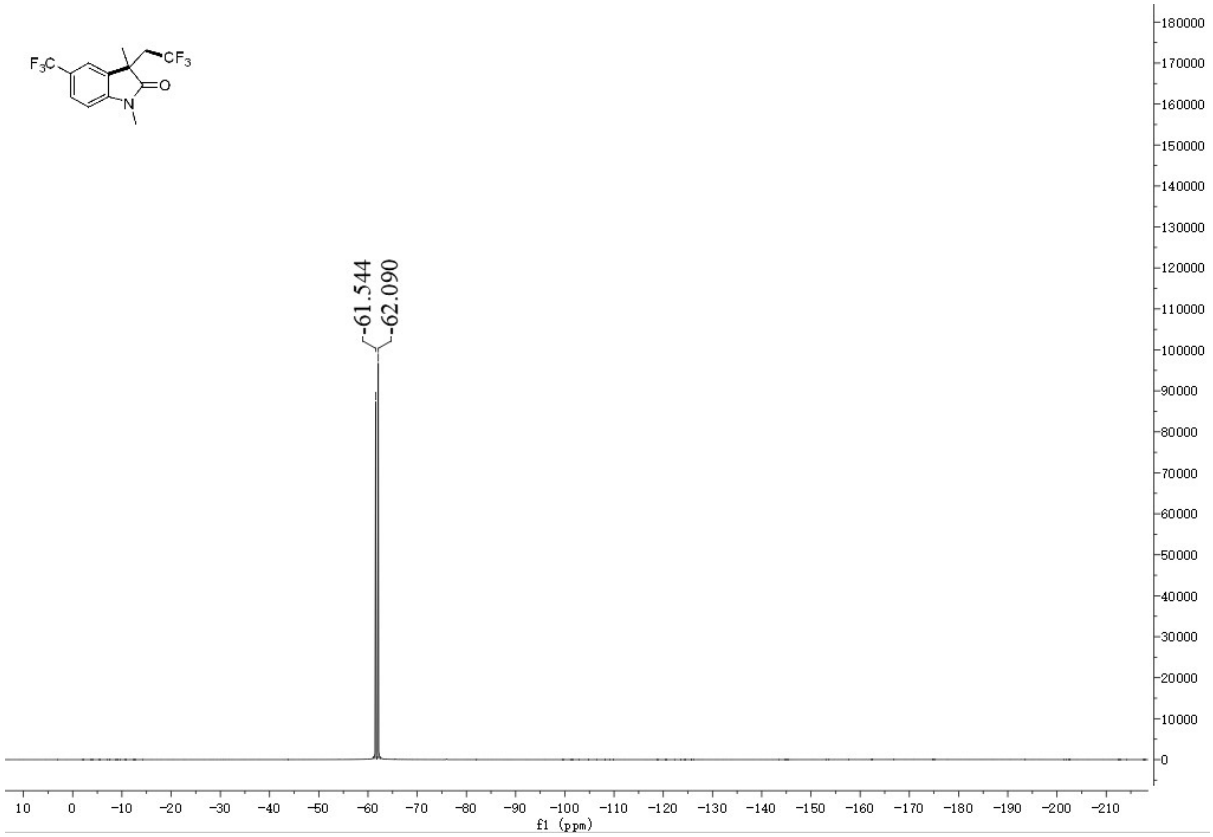
5-Chloro-1,3-dimethyl-3-(2,2,2-trifluoroethyl)indolin-2-one (2)



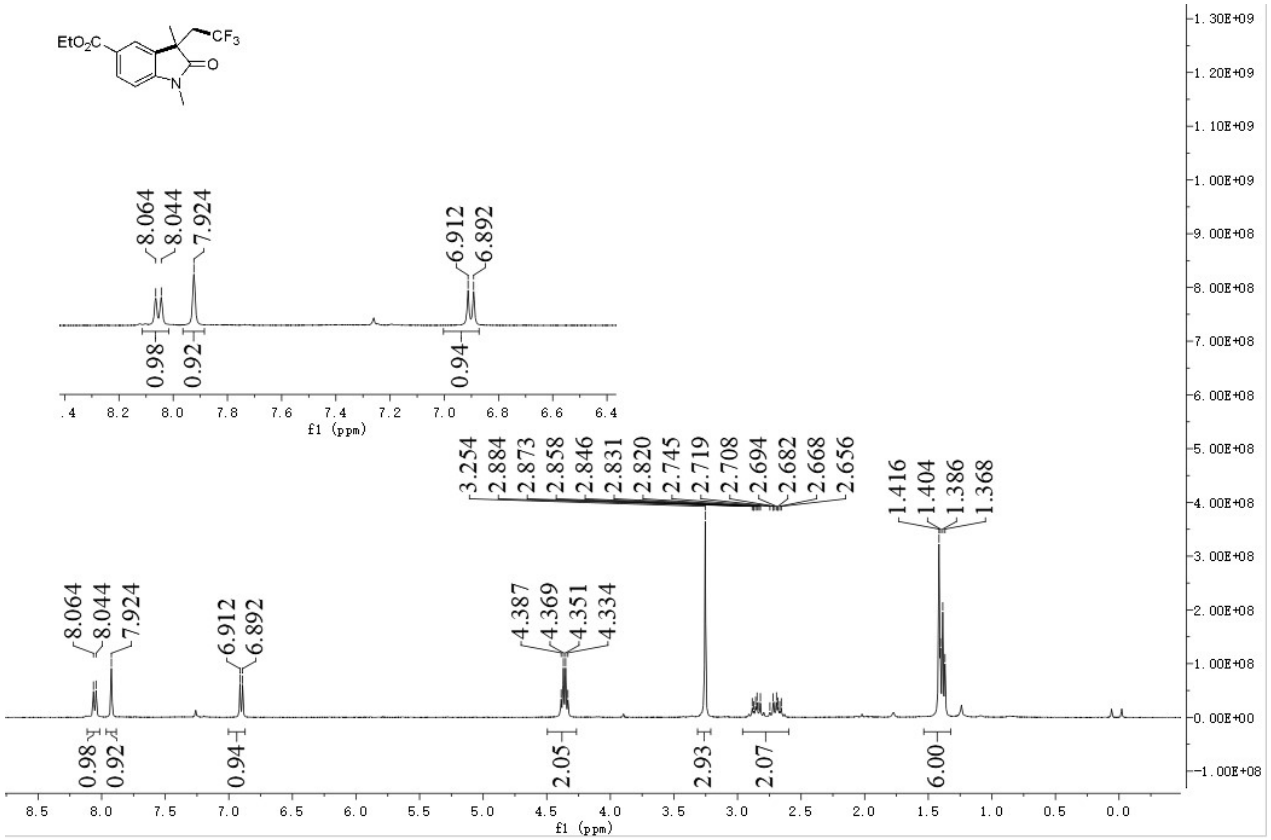


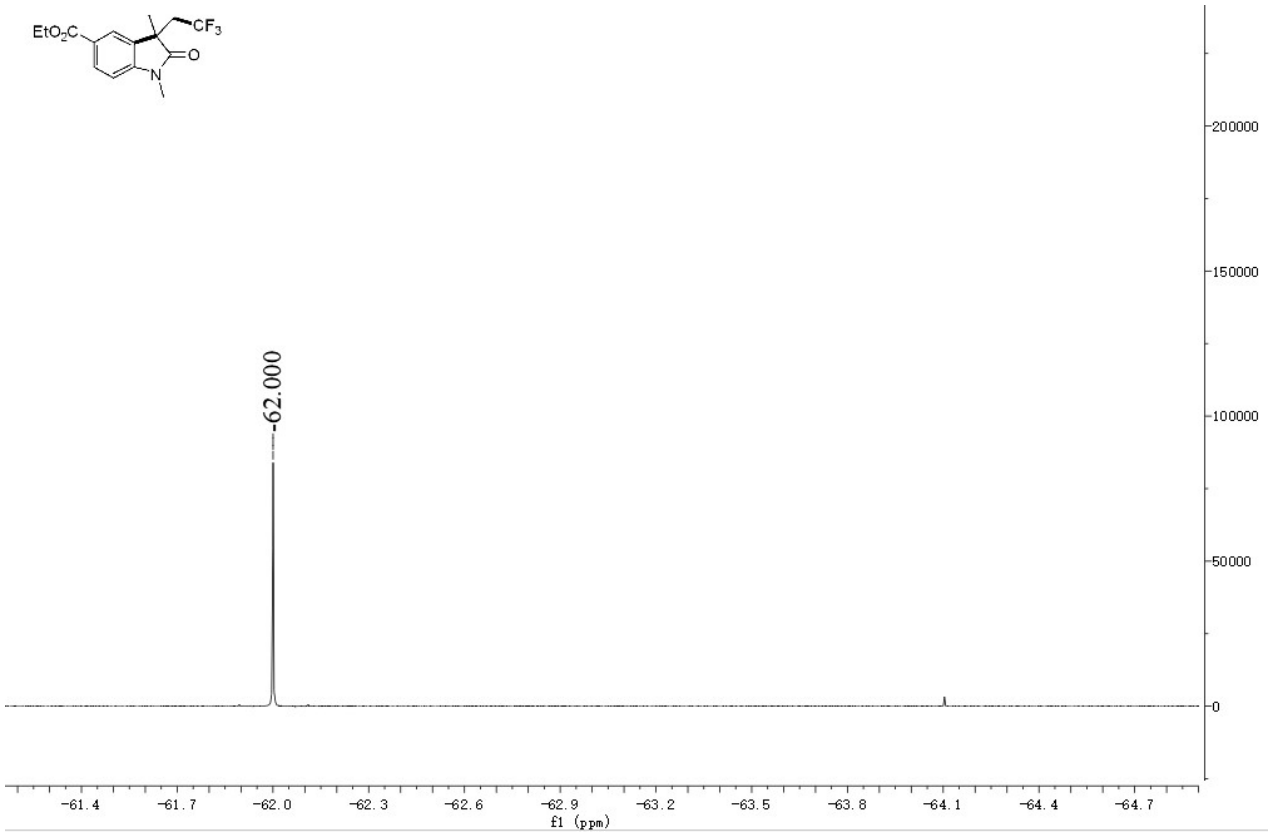
1,3-Dimethyl-3-(2,2,2-trifluoroethyl)-5-(trifluoromethyl)indolin-2-one (3)



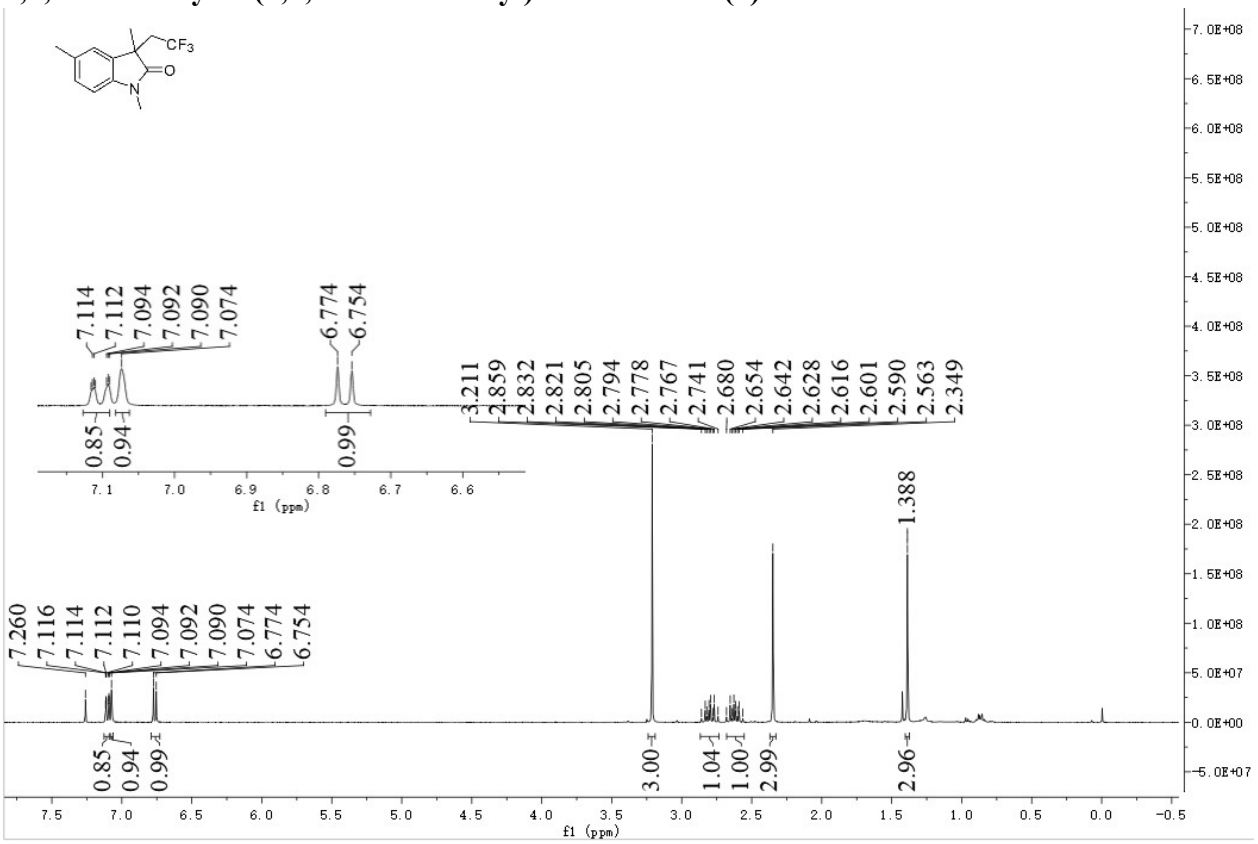


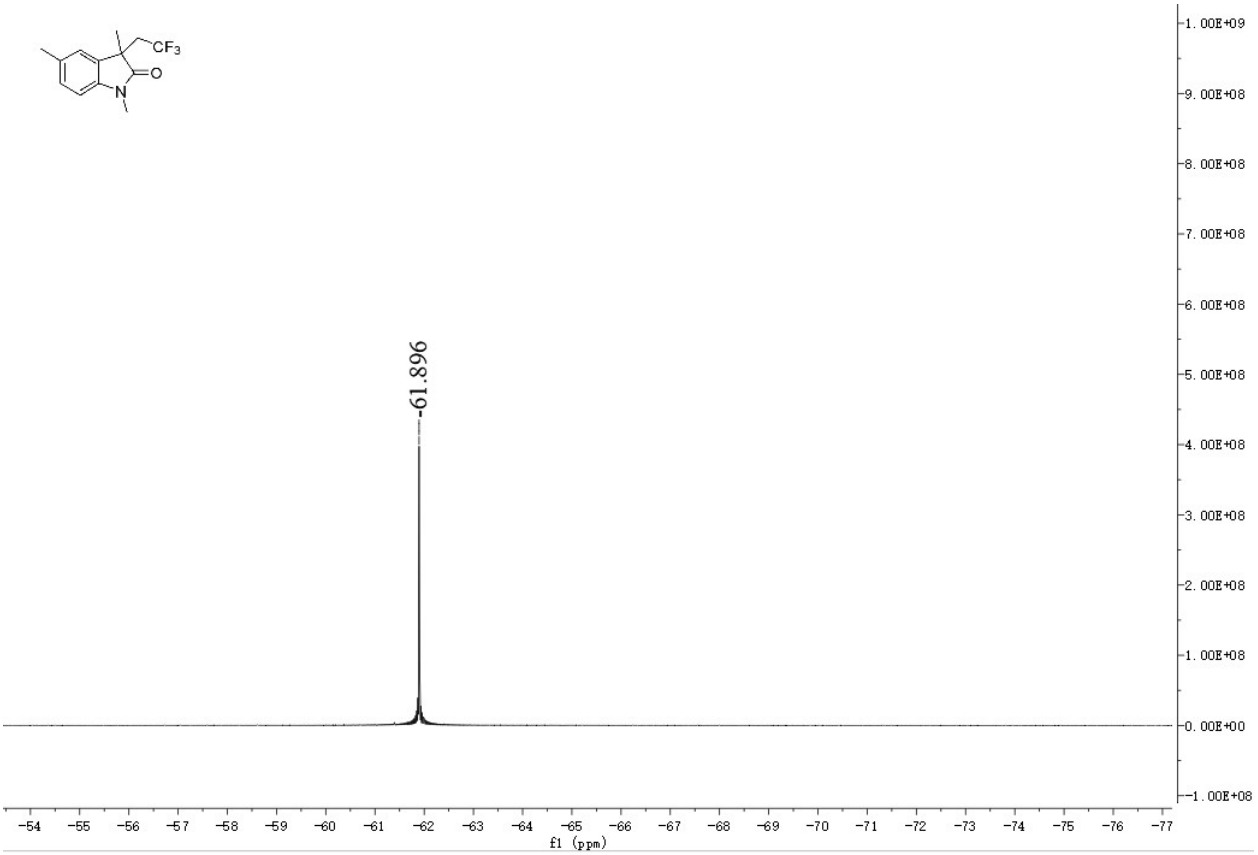
Ethyl-1,3-dimethyl-2-oxo-3-(2,2,2-trifluoroethyl)indoline-5-carboxylate (4)



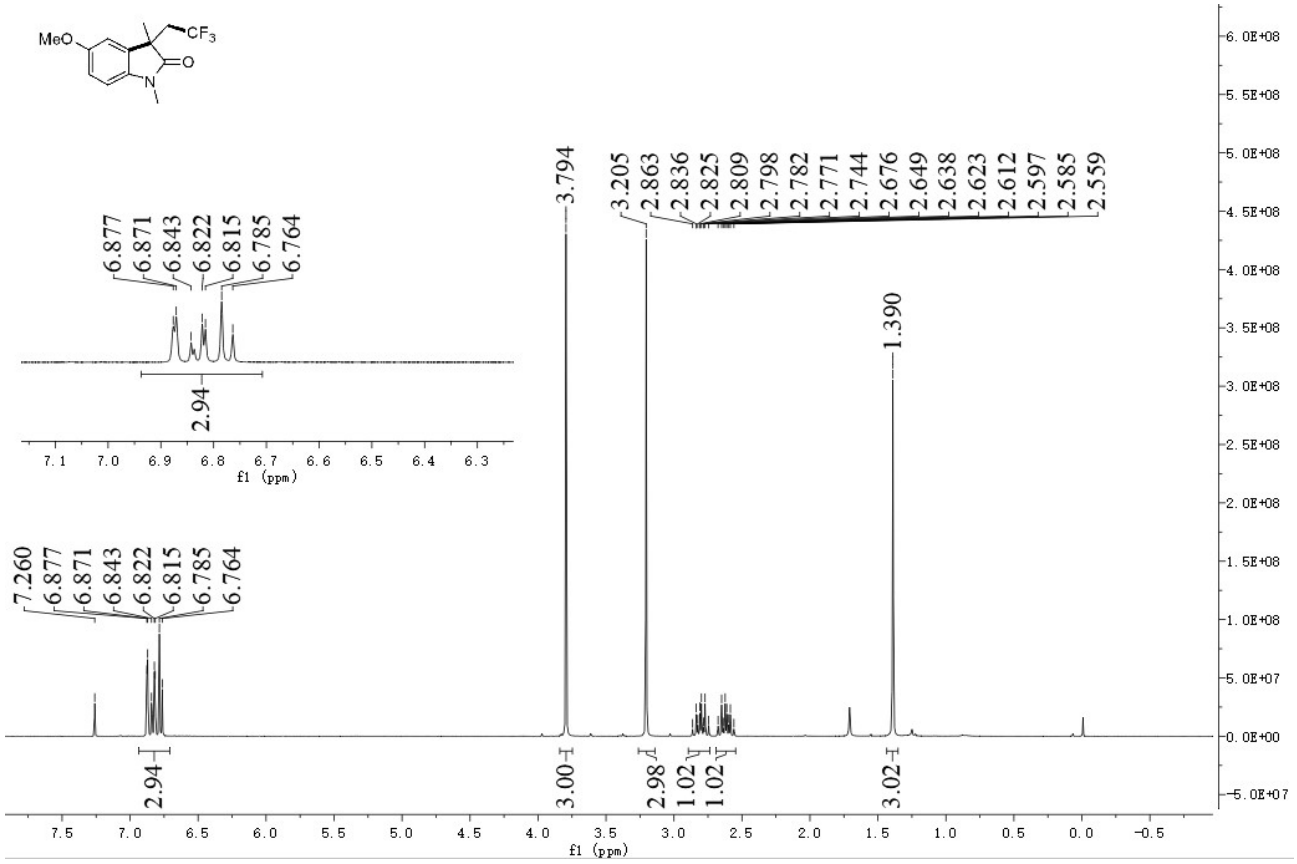


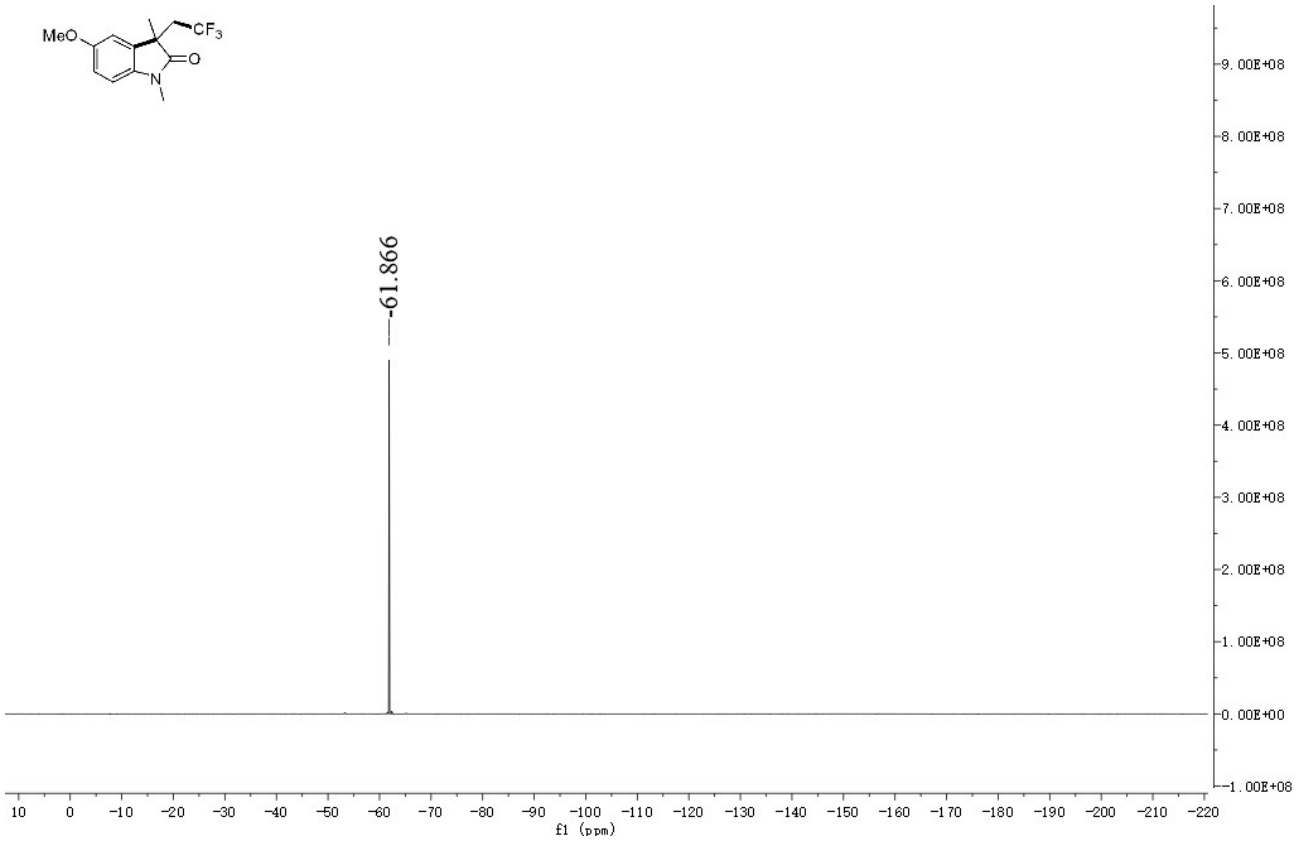
1,3,5-Trimethyl-3-(2,2,2-trifluoroethyl)indolin-2-one (5)



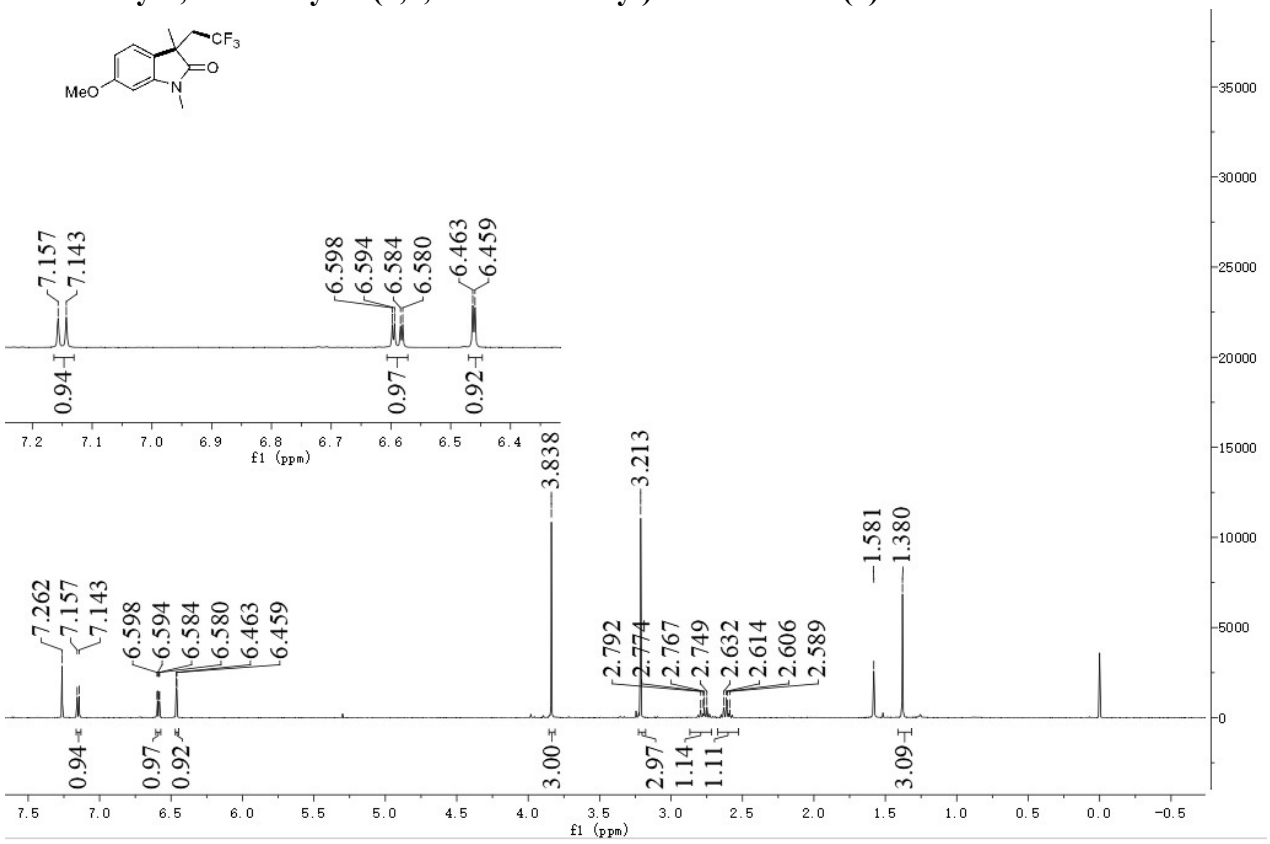


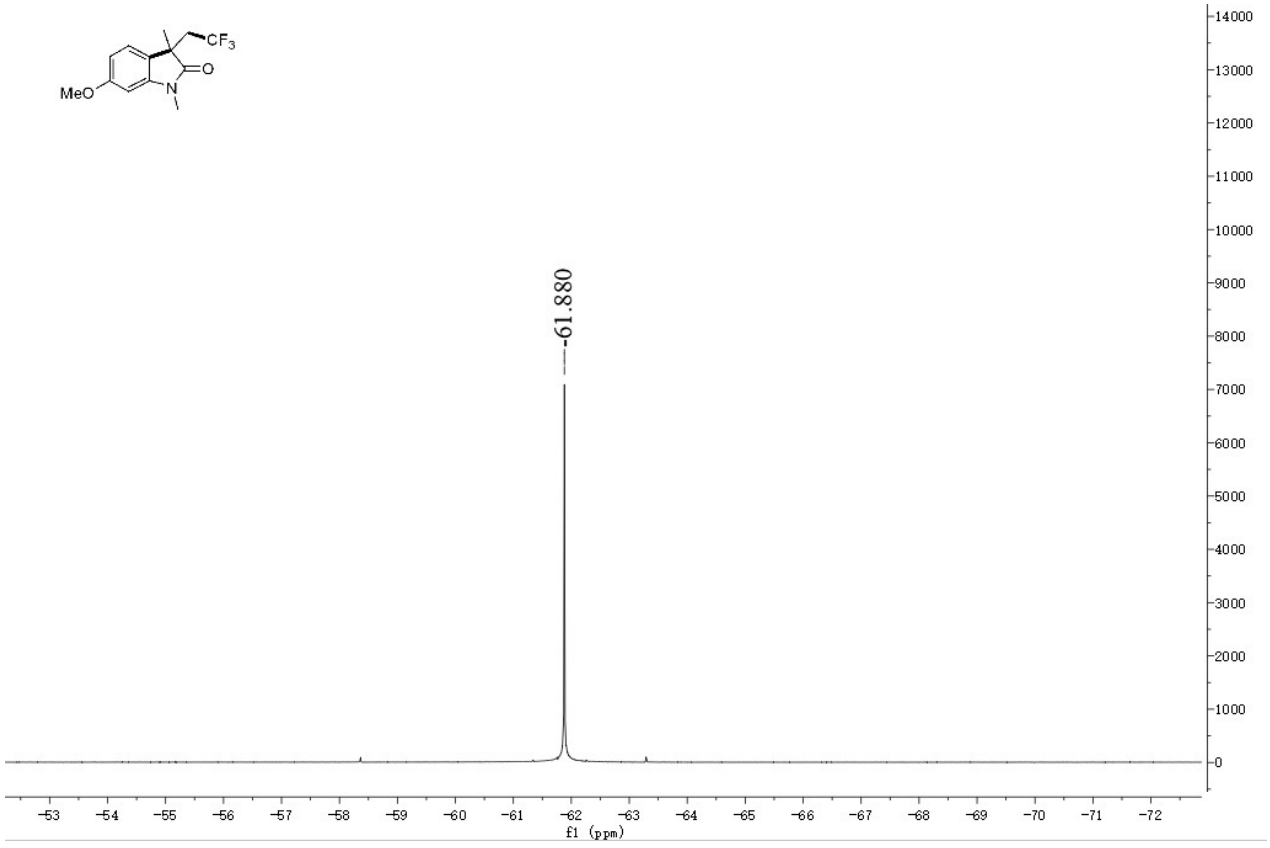
5-Methoxy-1,3-dimethyl-3-(2,2,2-trifluoroethyl)indolin-2-one (6)



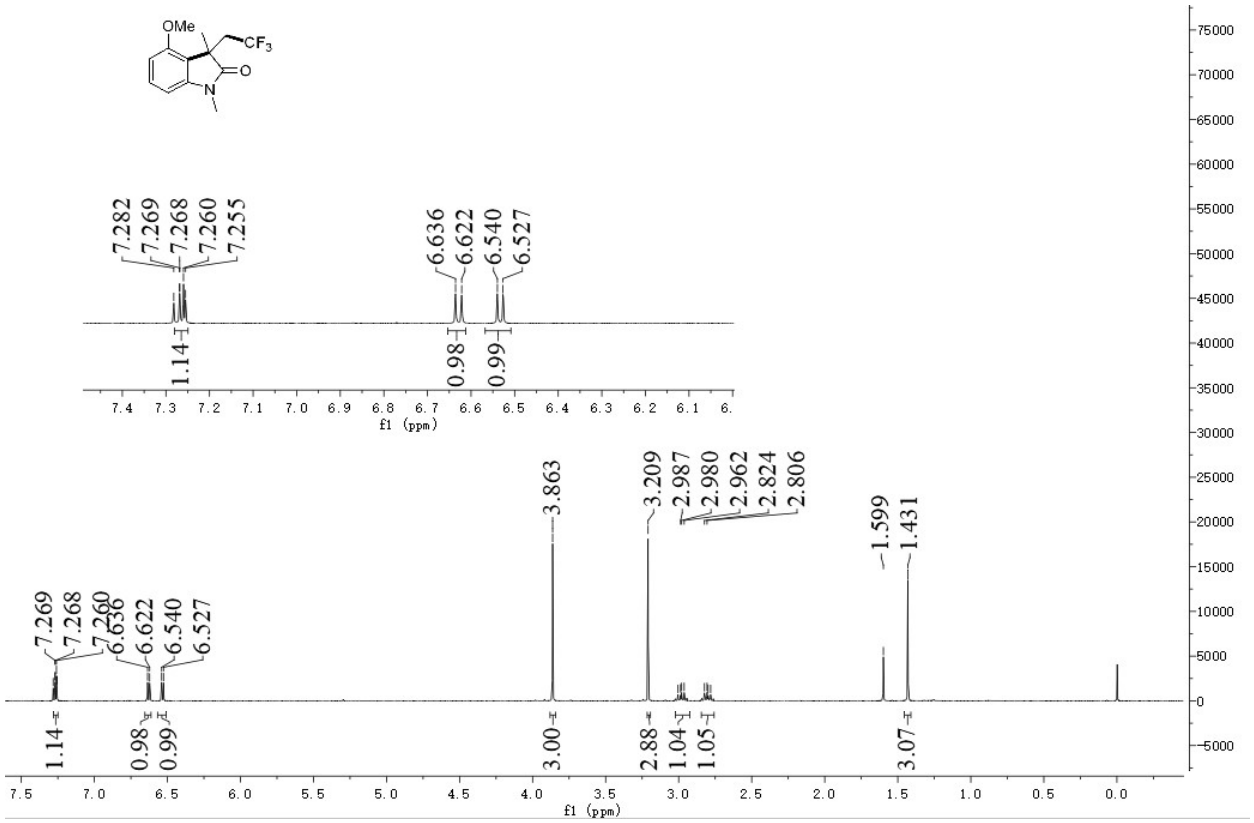


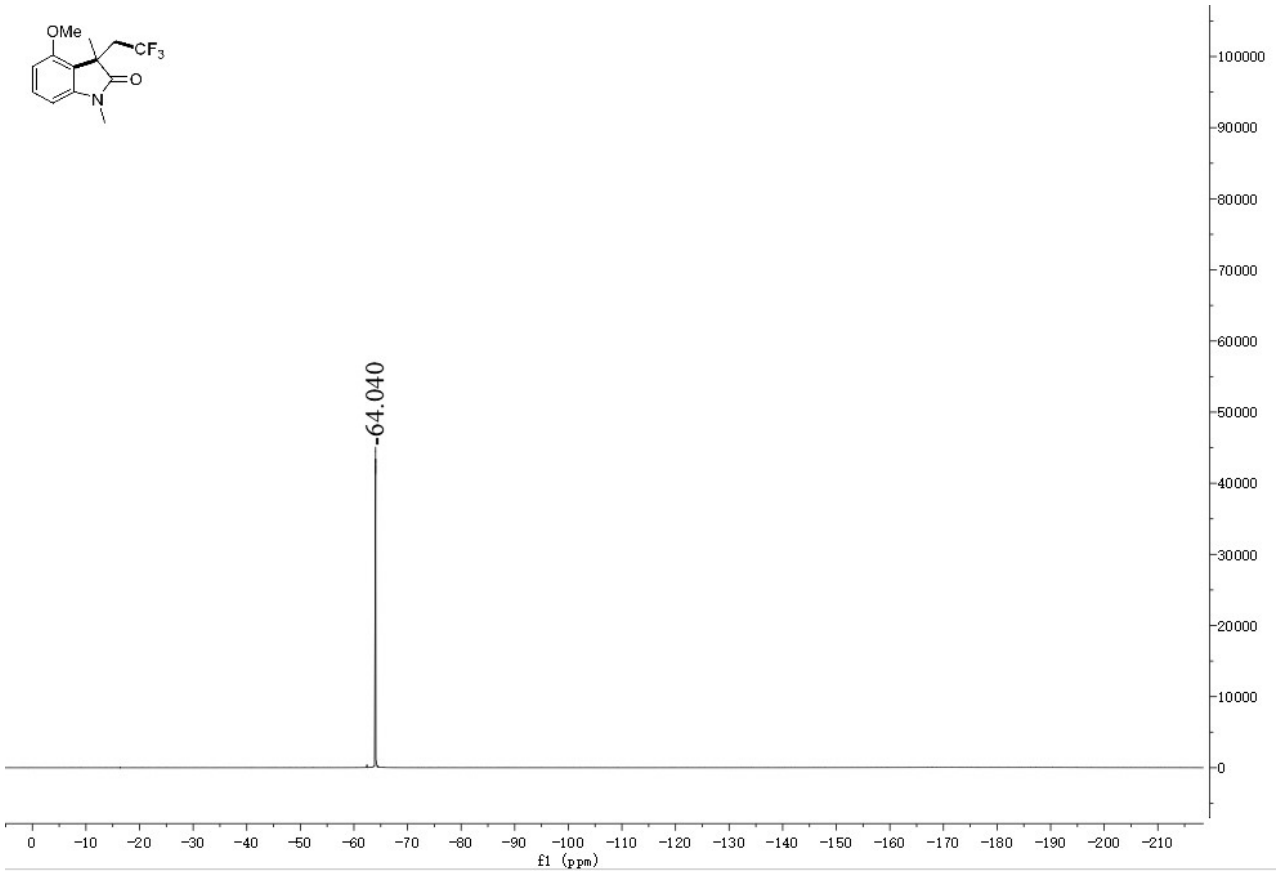
6-Methoxy-1,3-dimethyl-3-(2,2,2-trifluoroethyl)indolin-2-one (7)



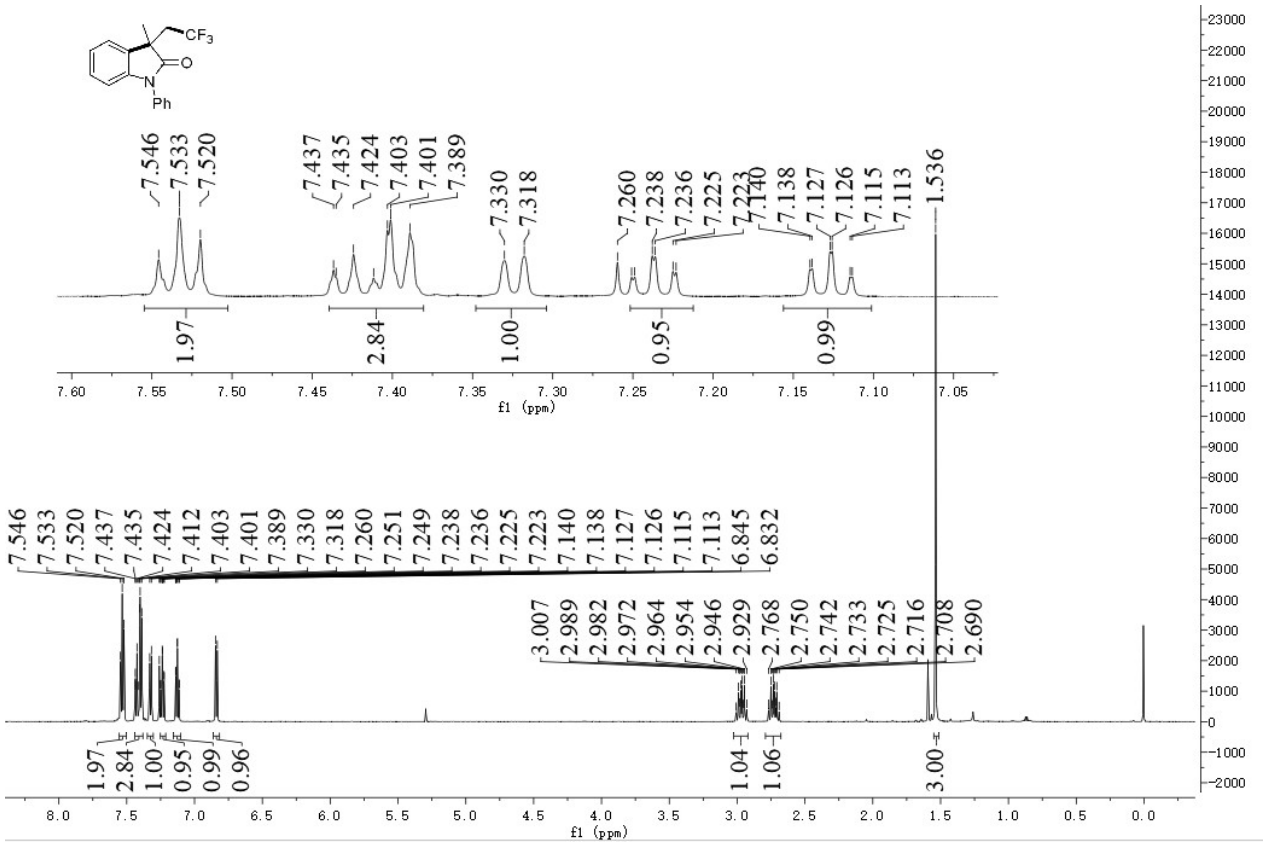


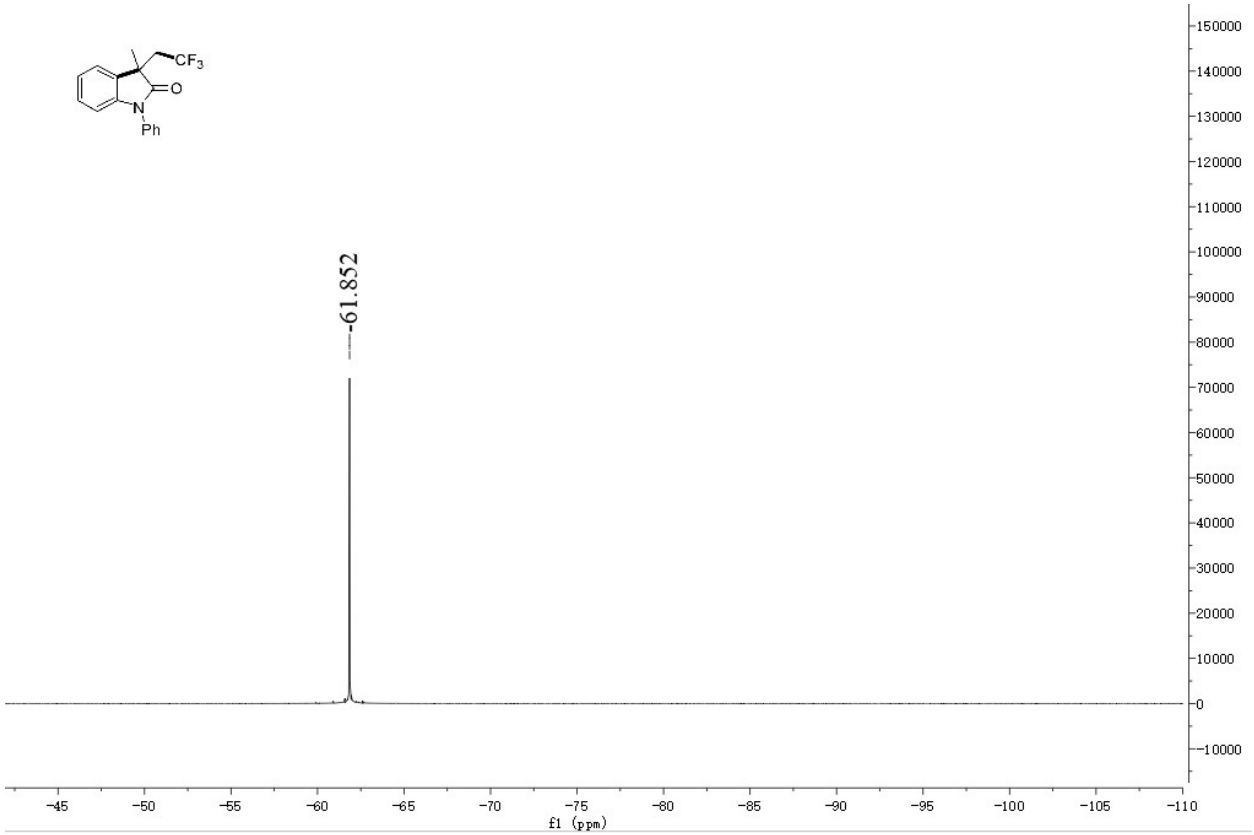
4-Methoxy-1,3-dimethyl-3-(2,2,2-trifluoroethyl)indolin-2-one (7')



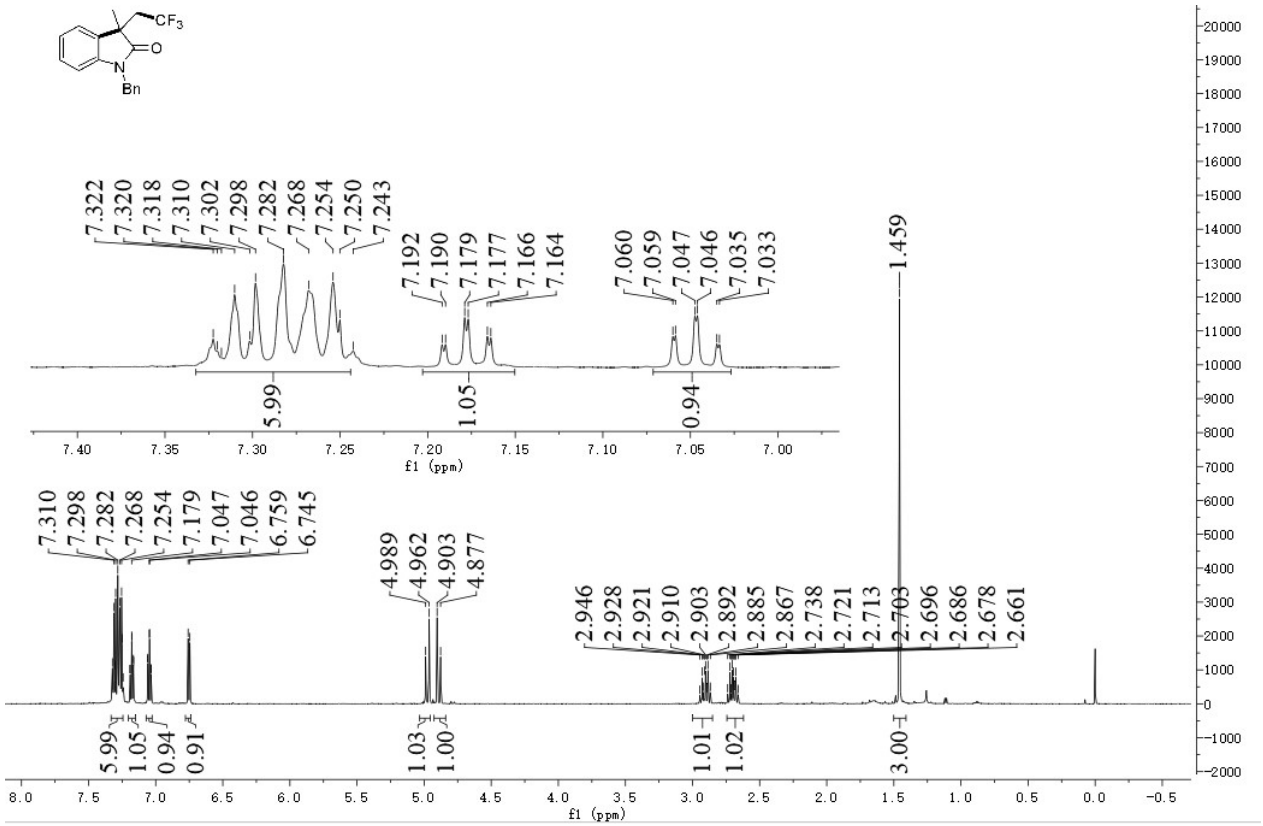


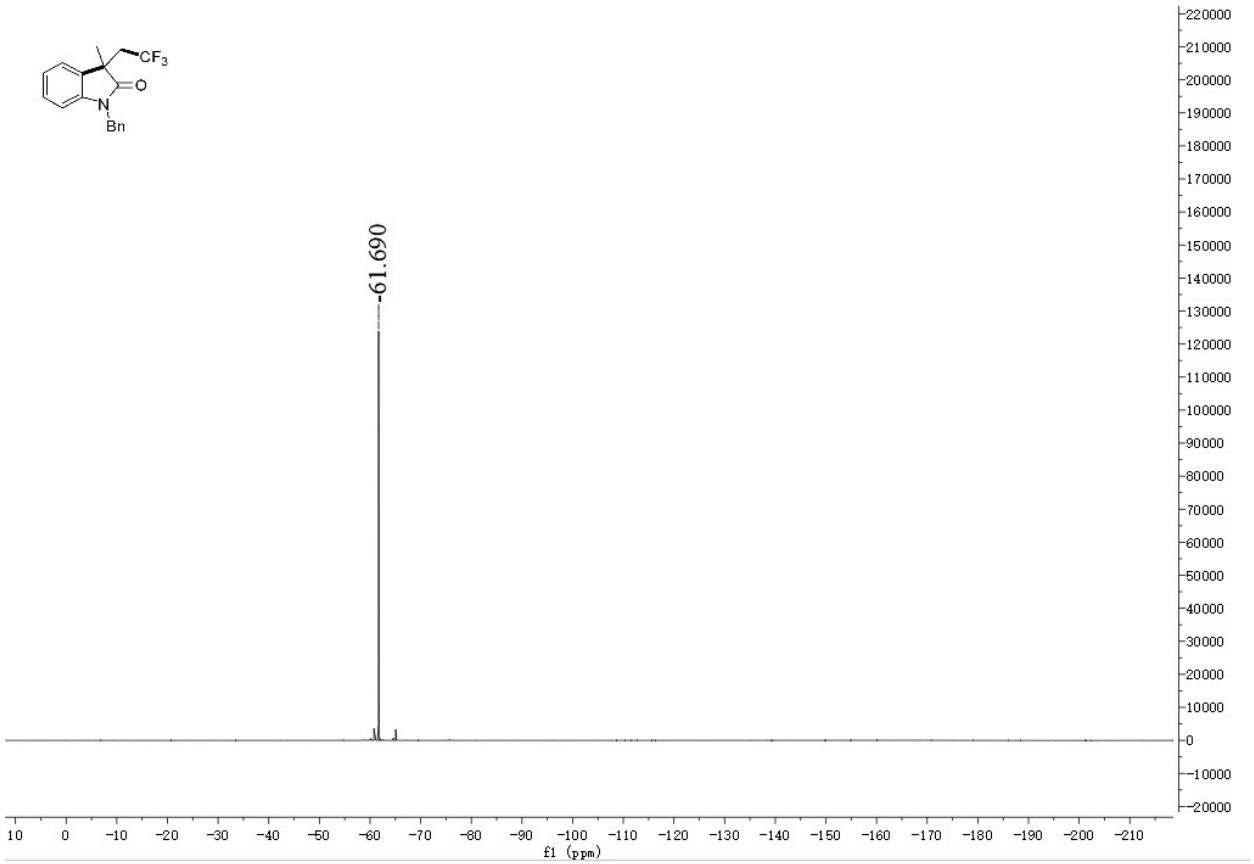
3-Methyl-1-phenyl-3-(2,2,2-trifluoroethyl)indolin-2-one (8)



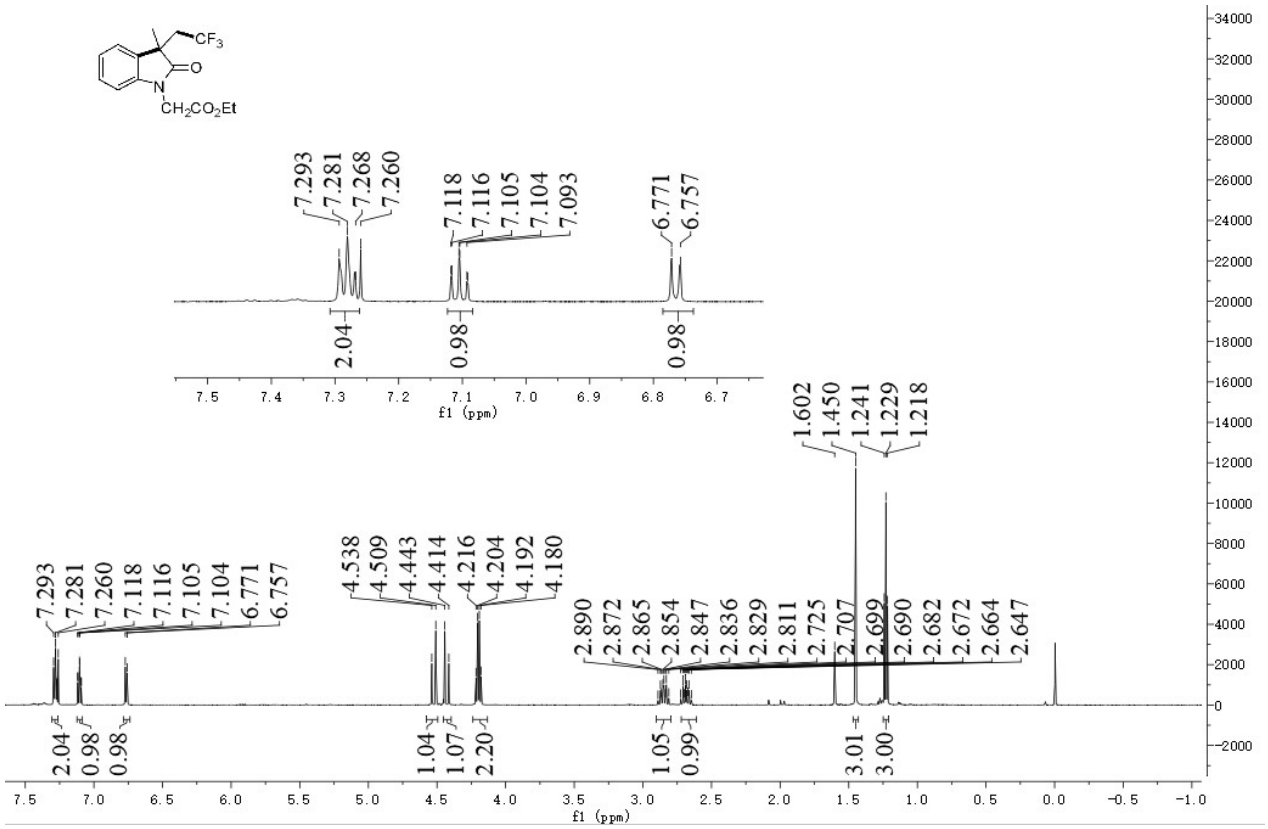


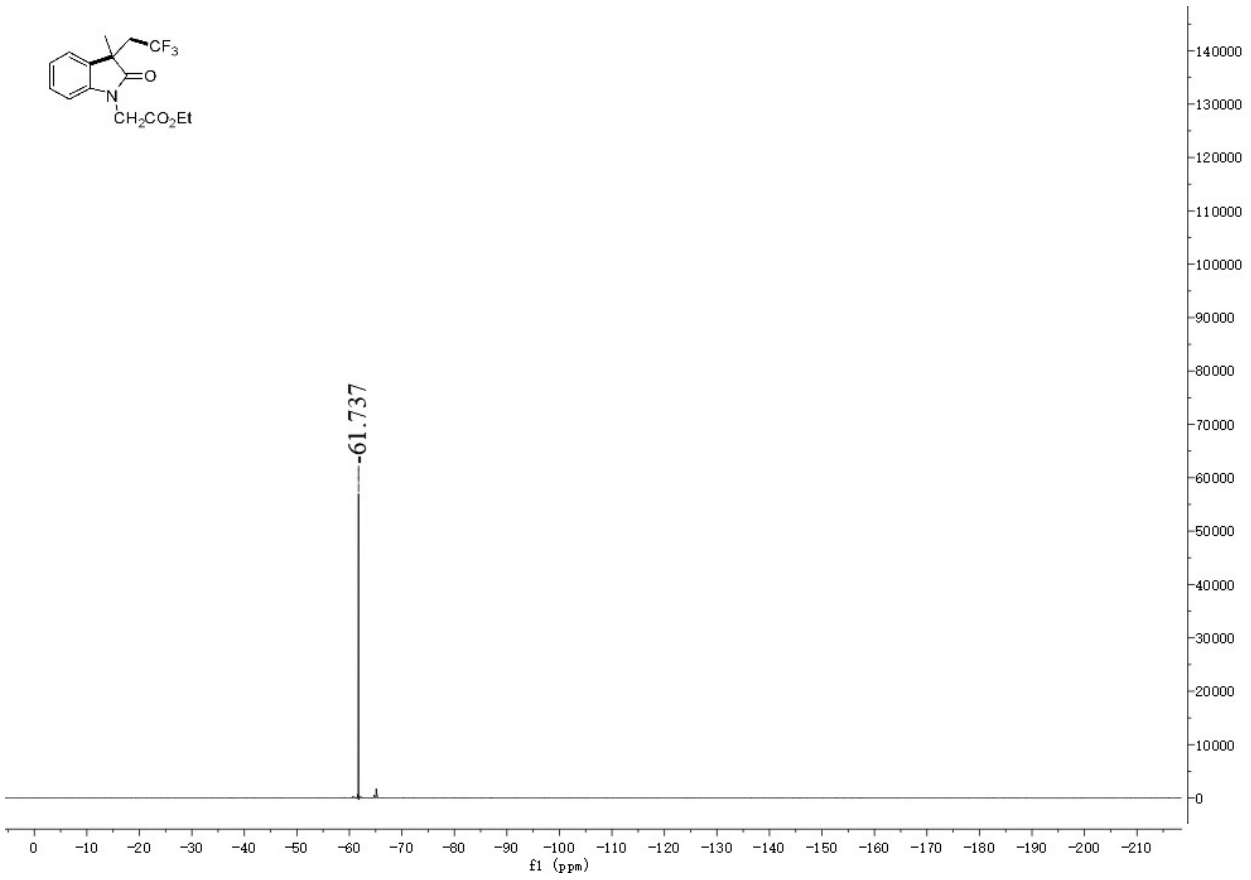
1-Benzyl-3-methyl-3-(2,2,2-trifluoroethyl)indolin-2-one (9)



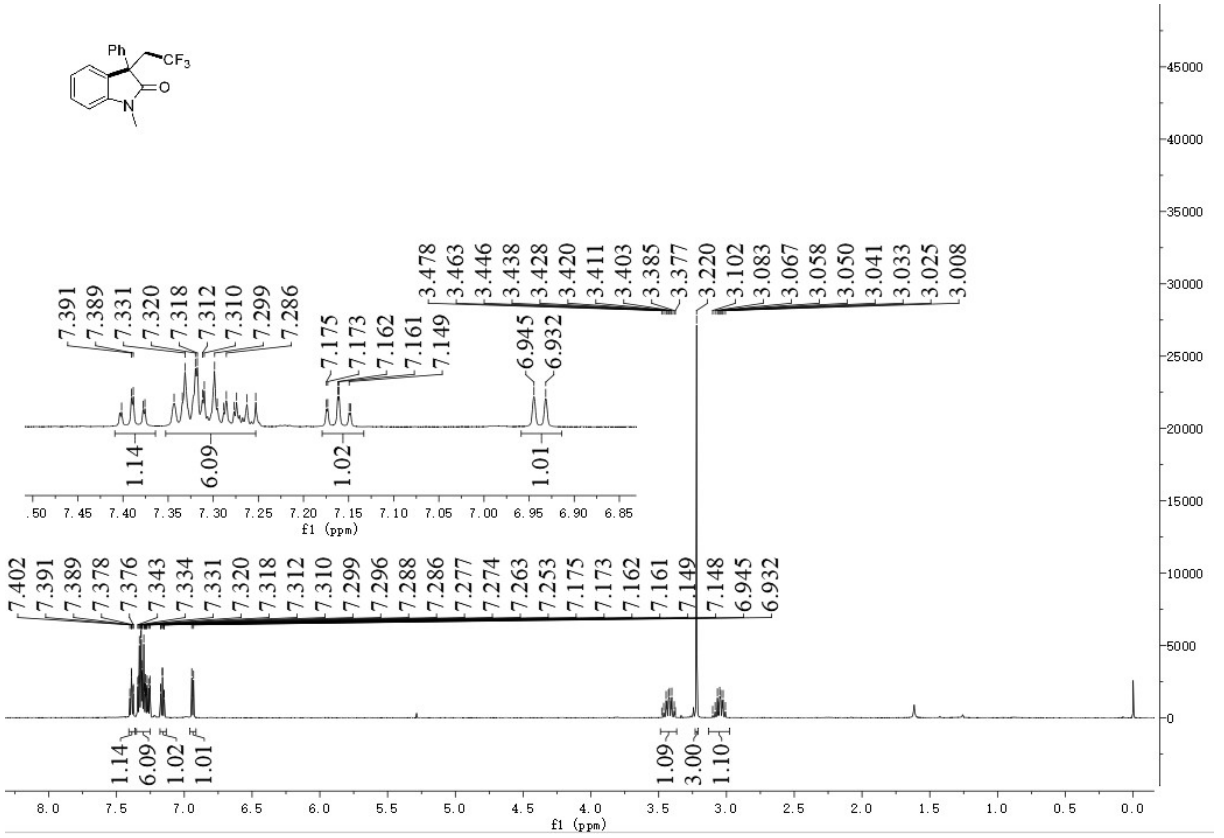


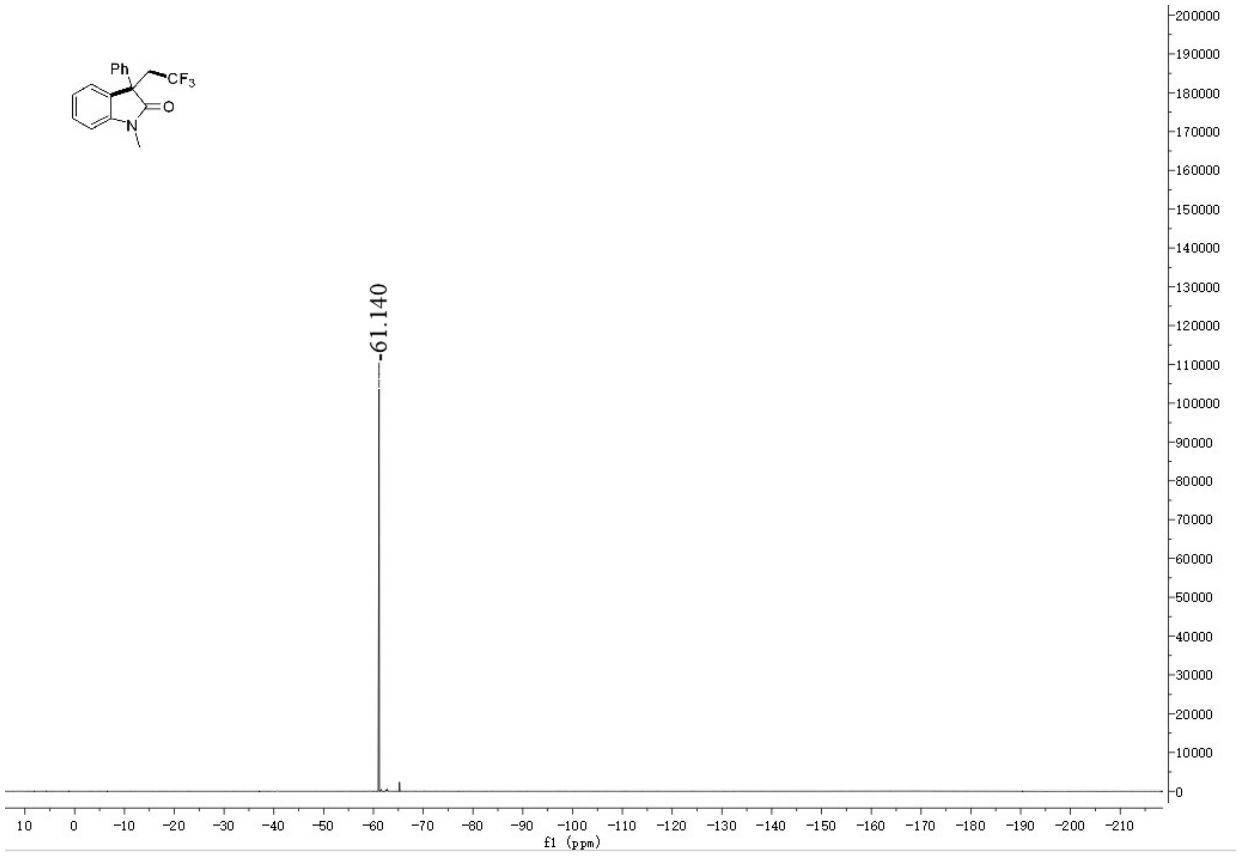
Ethyl-2-(3-methyl-2-oxo-3-(2,2,2-trifluoroethyl)indolin-1-yl)acetate (10)



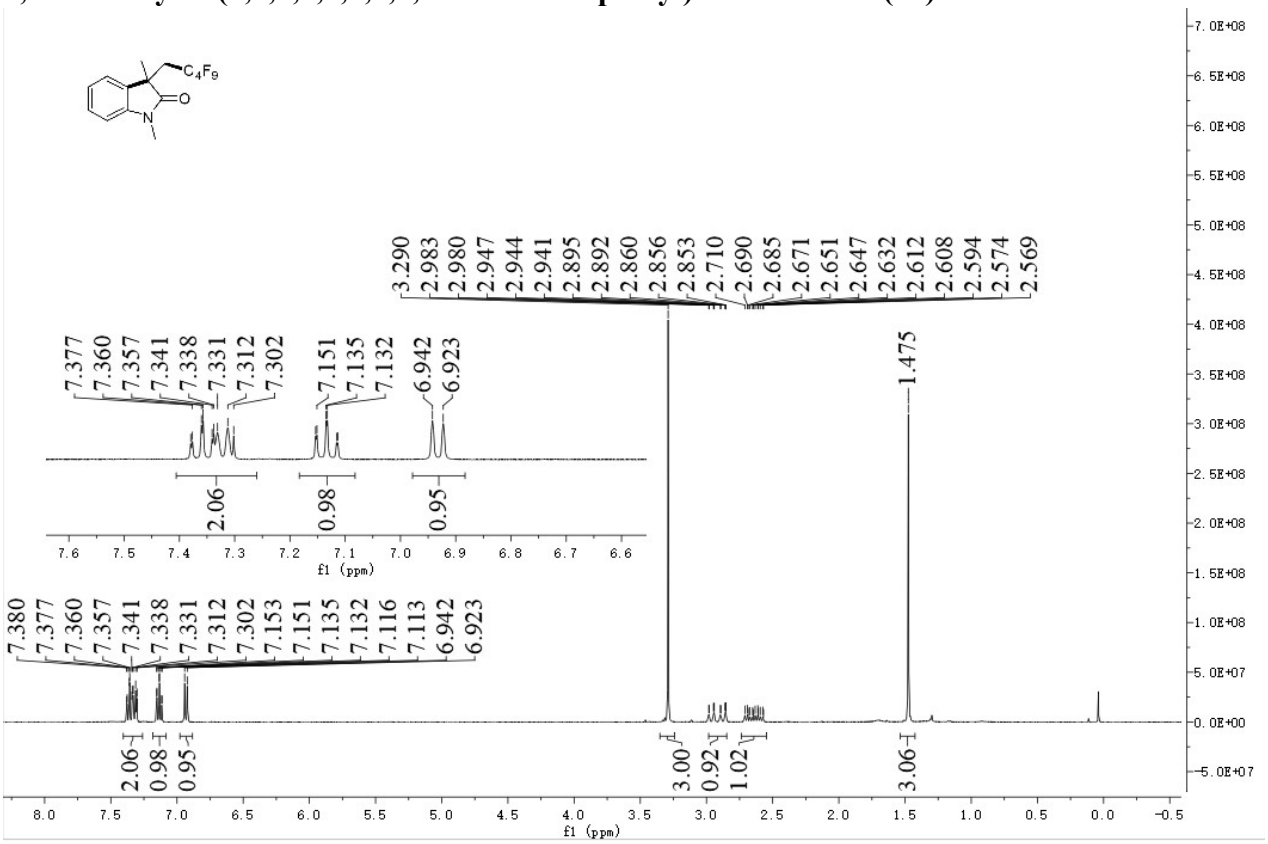


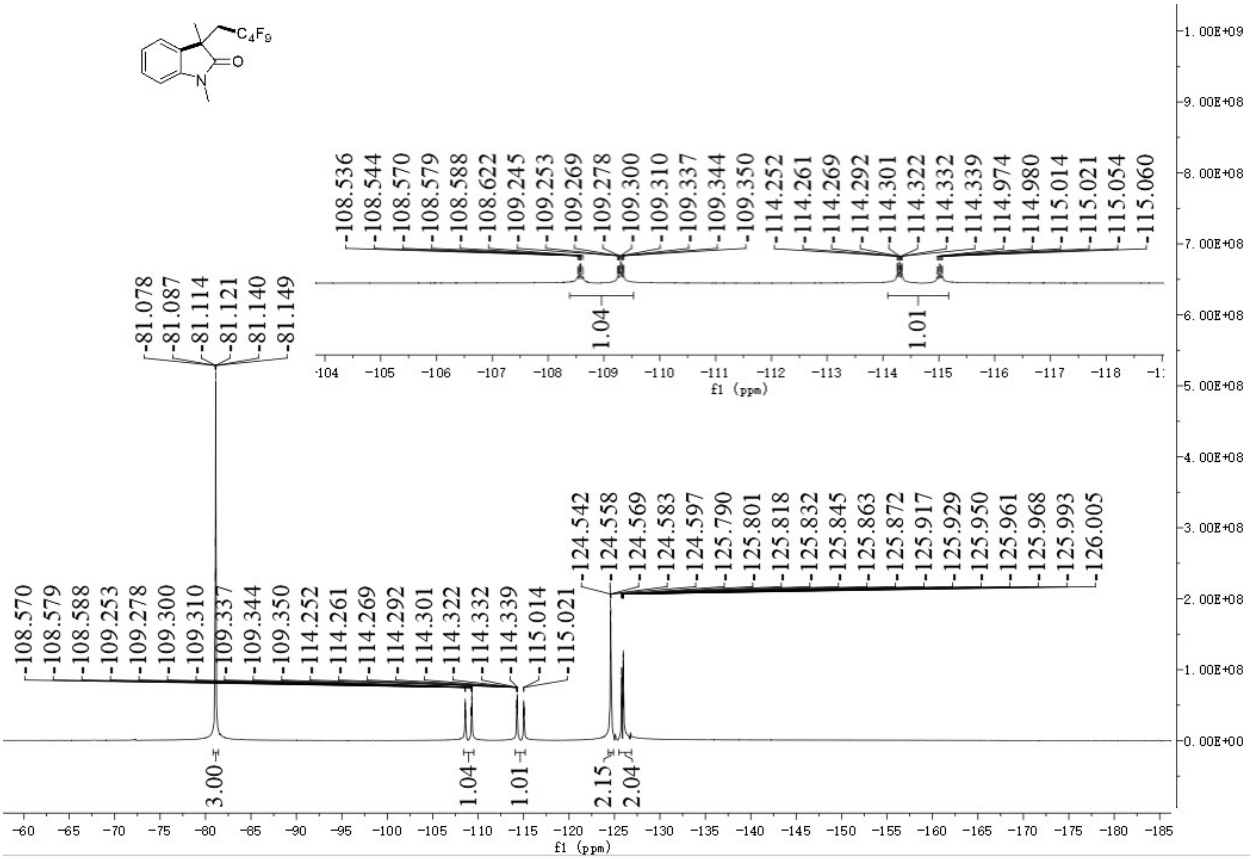
1-Methyl-3-phenyl-3-(2,2,2-trifluoroethyl)indolin-2-one (11)



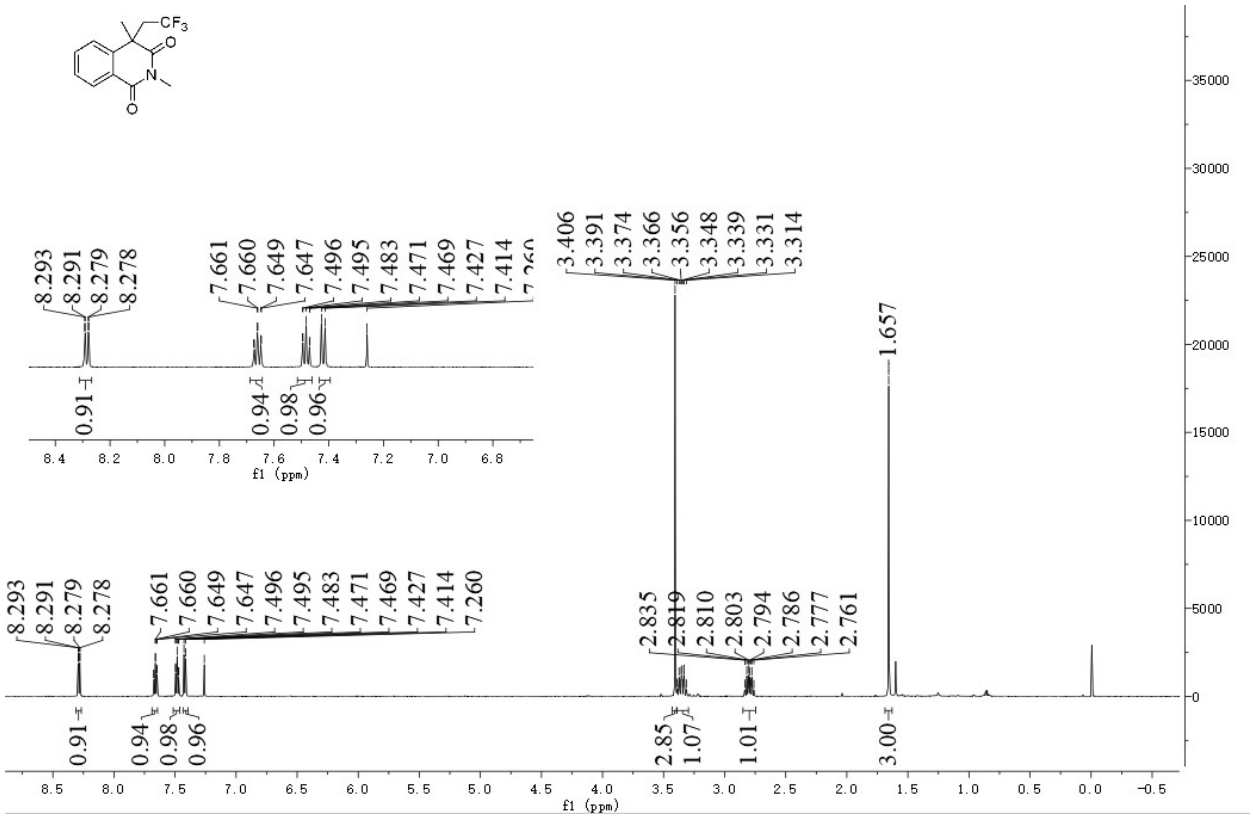


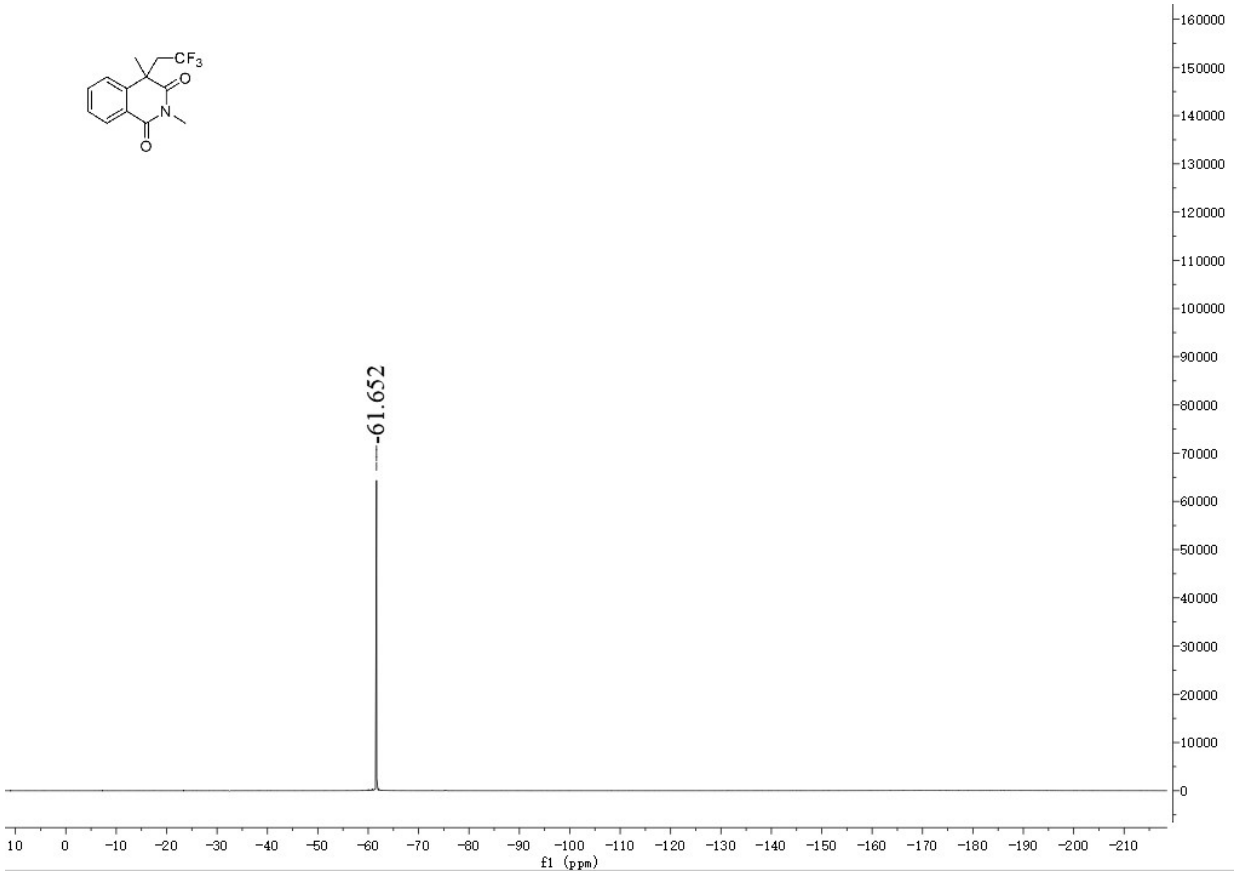
1,3-Dimethyl-3-(2,2,3,3,4,4,5,5,5-nonafluoropentyl)indolin-2-one (12)



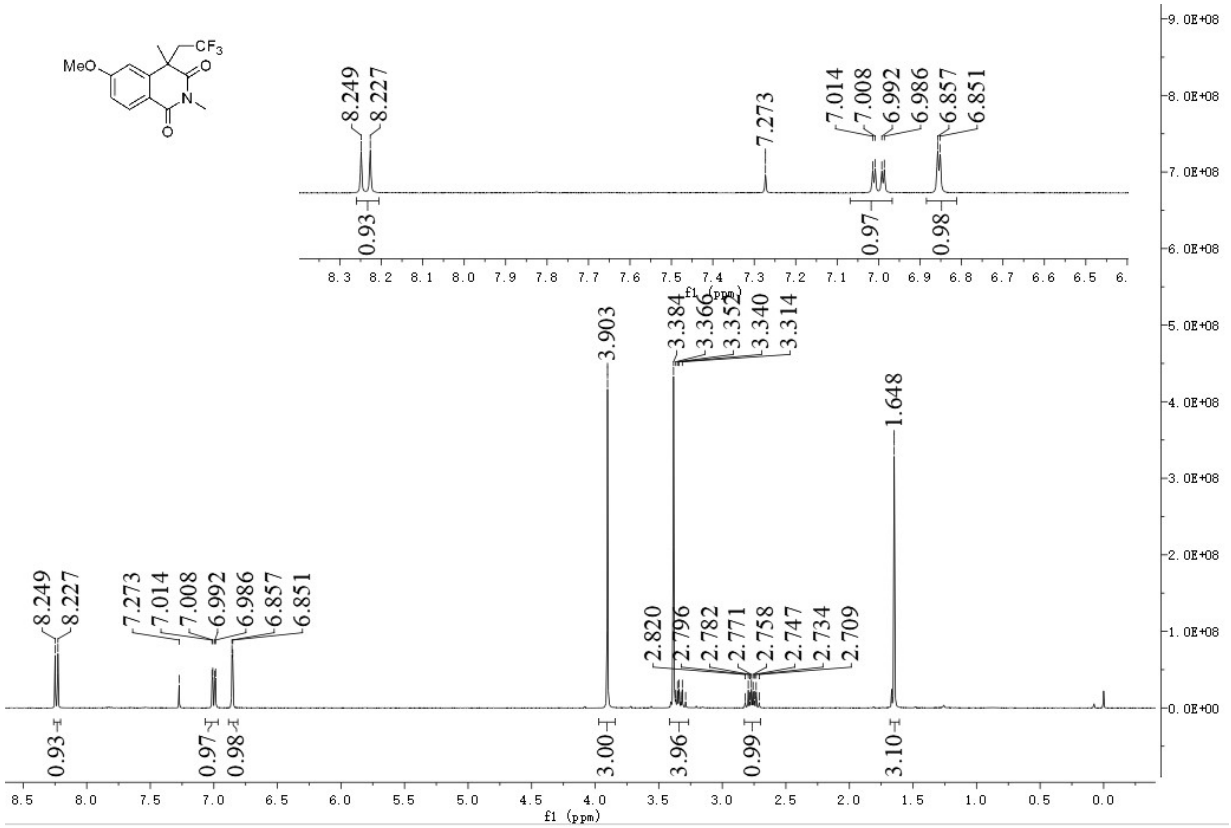


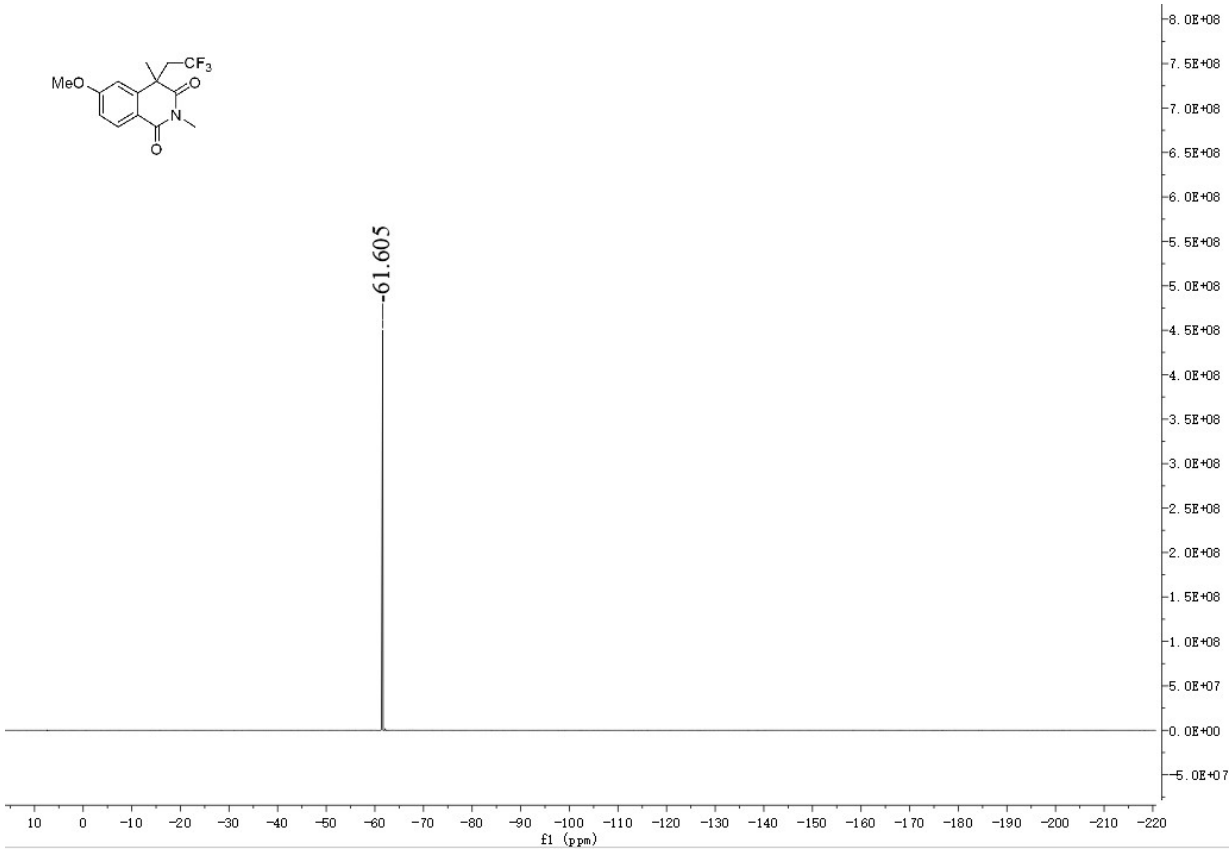
2,4-Dimethyl-4-(2,2,2-trifluoroethyl)isoquinoline-1,3(2*H*,4*H*)-dione (13)



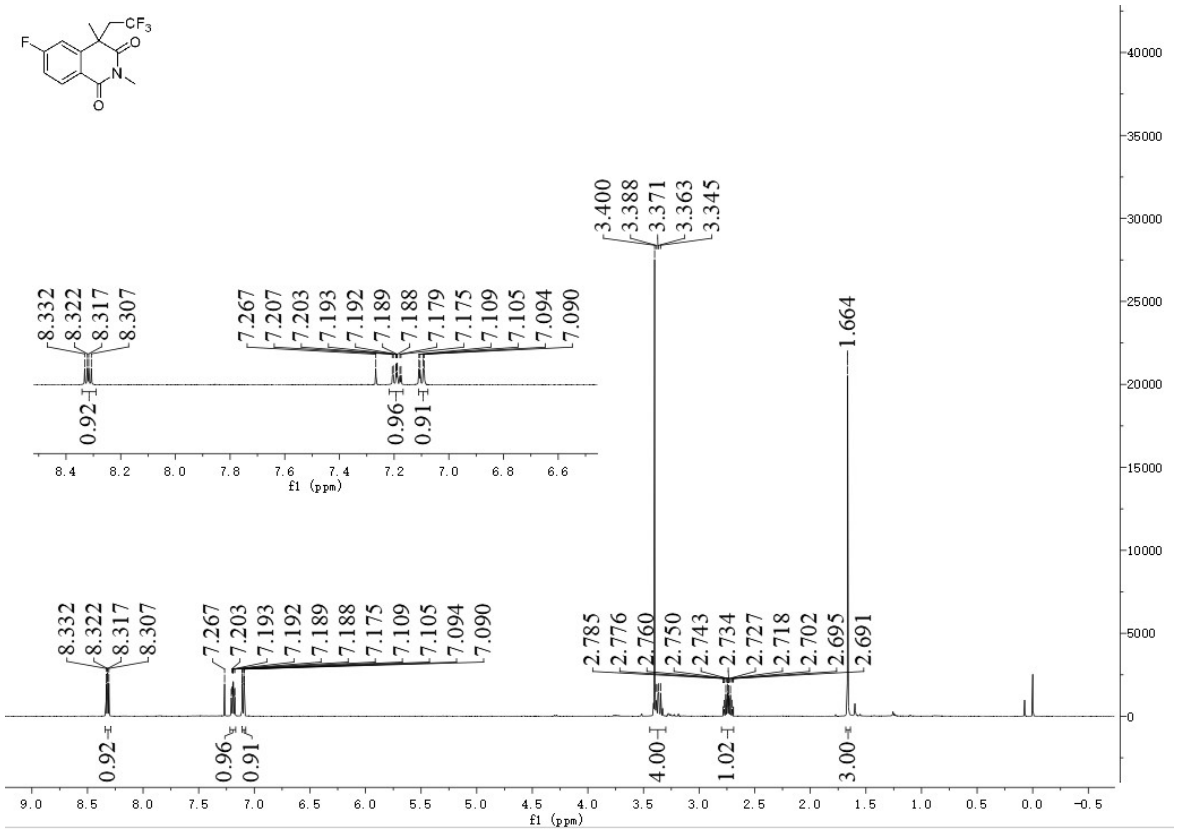


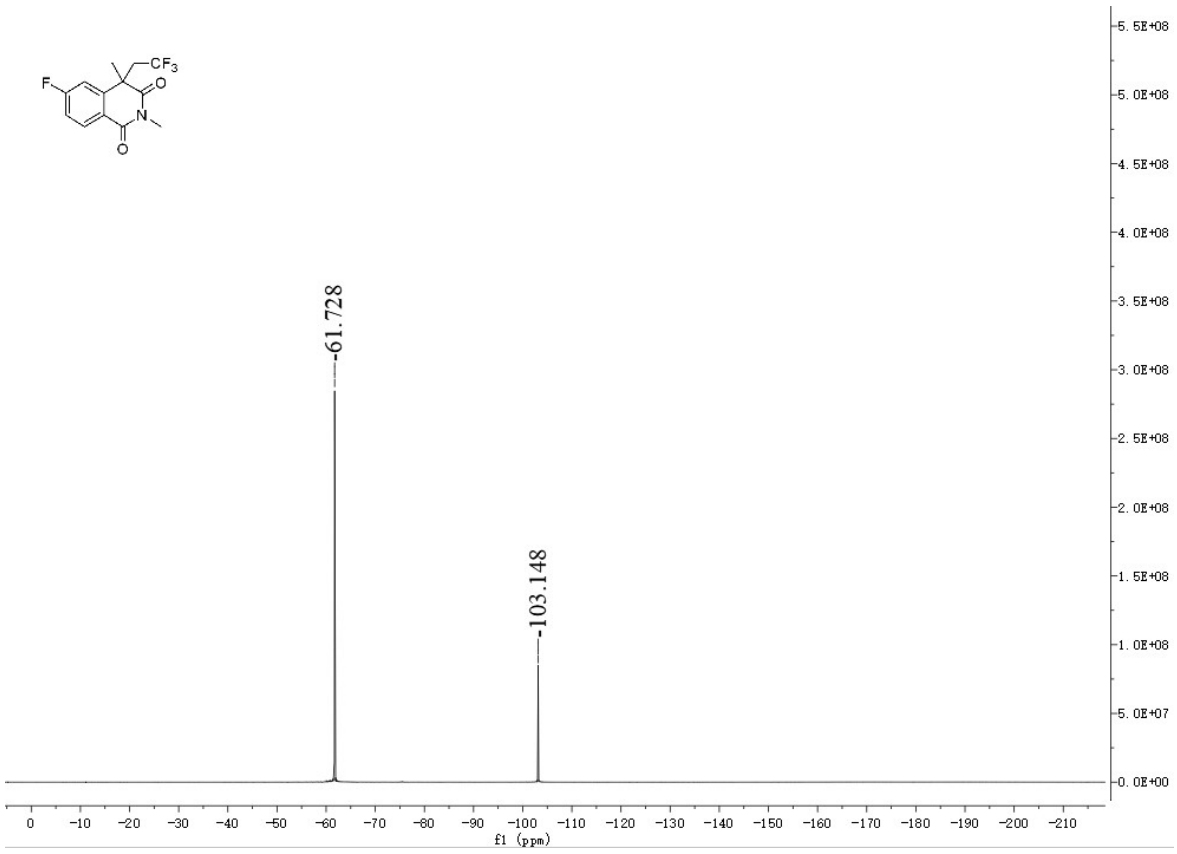
6-Methoxy-2,4-dimethyl-4-(2,2,2-trifluoroethyl)isoquinoline-1,3(2*H*,4*H*)-dione (14)



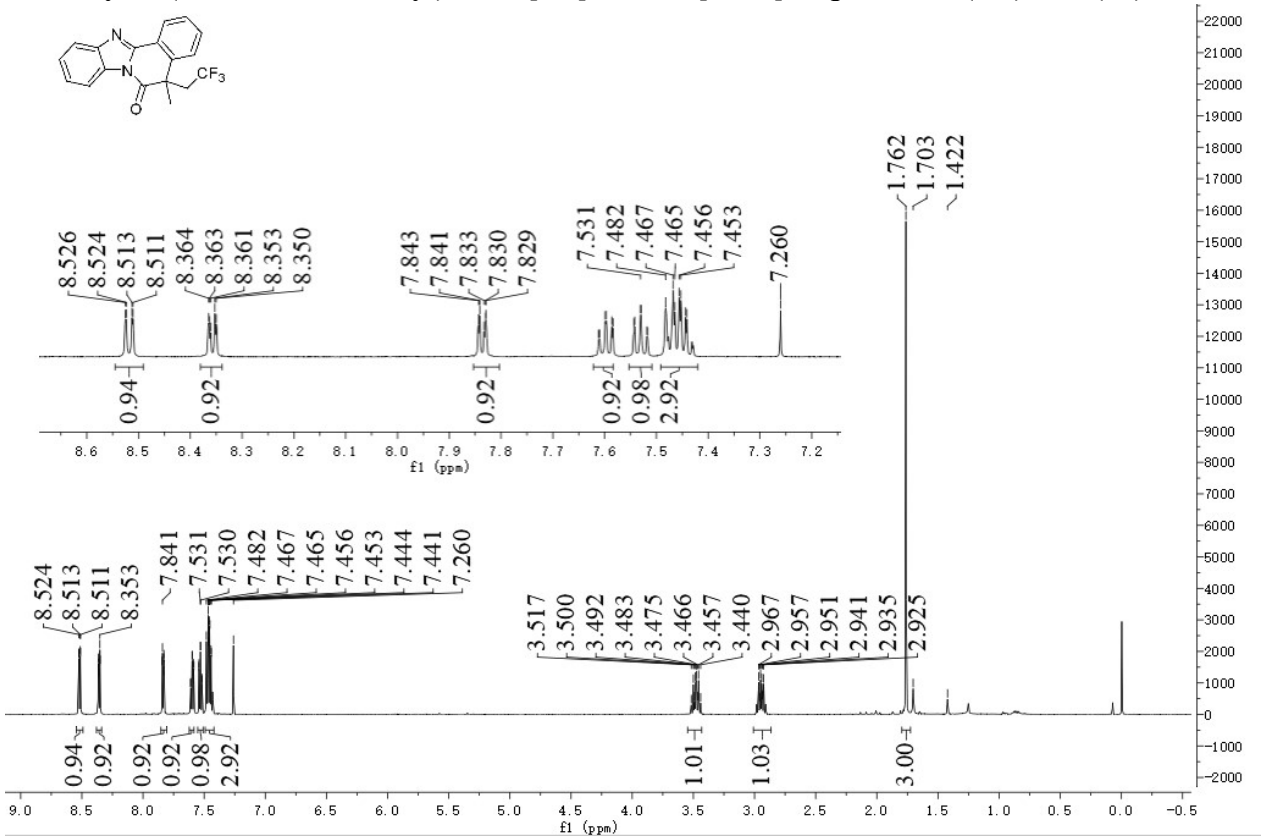


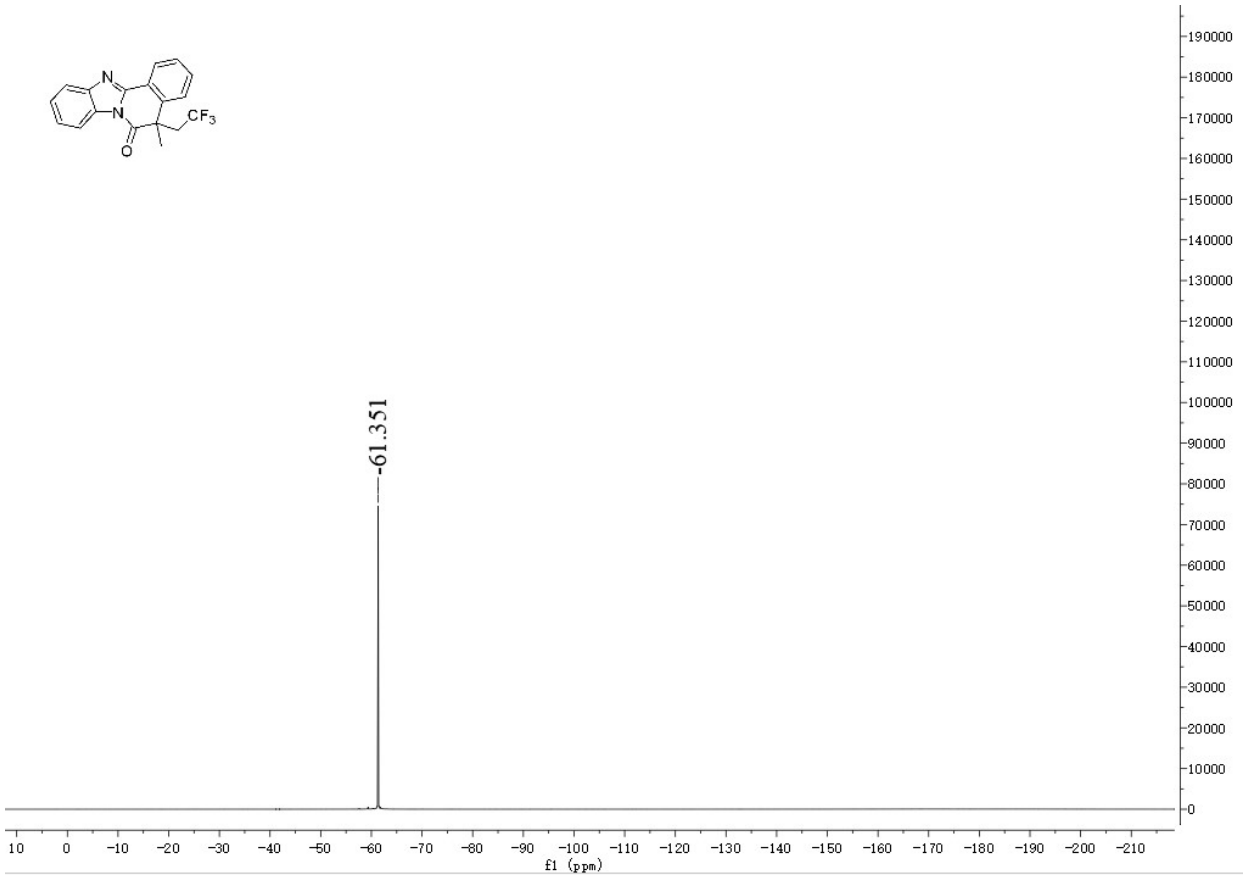
6-Fluoro-2,4-dimethyl-4-(2,2,2-trifluoroethyl)isoquinoline-1,3(2*H*,4*H*)-dione (15)



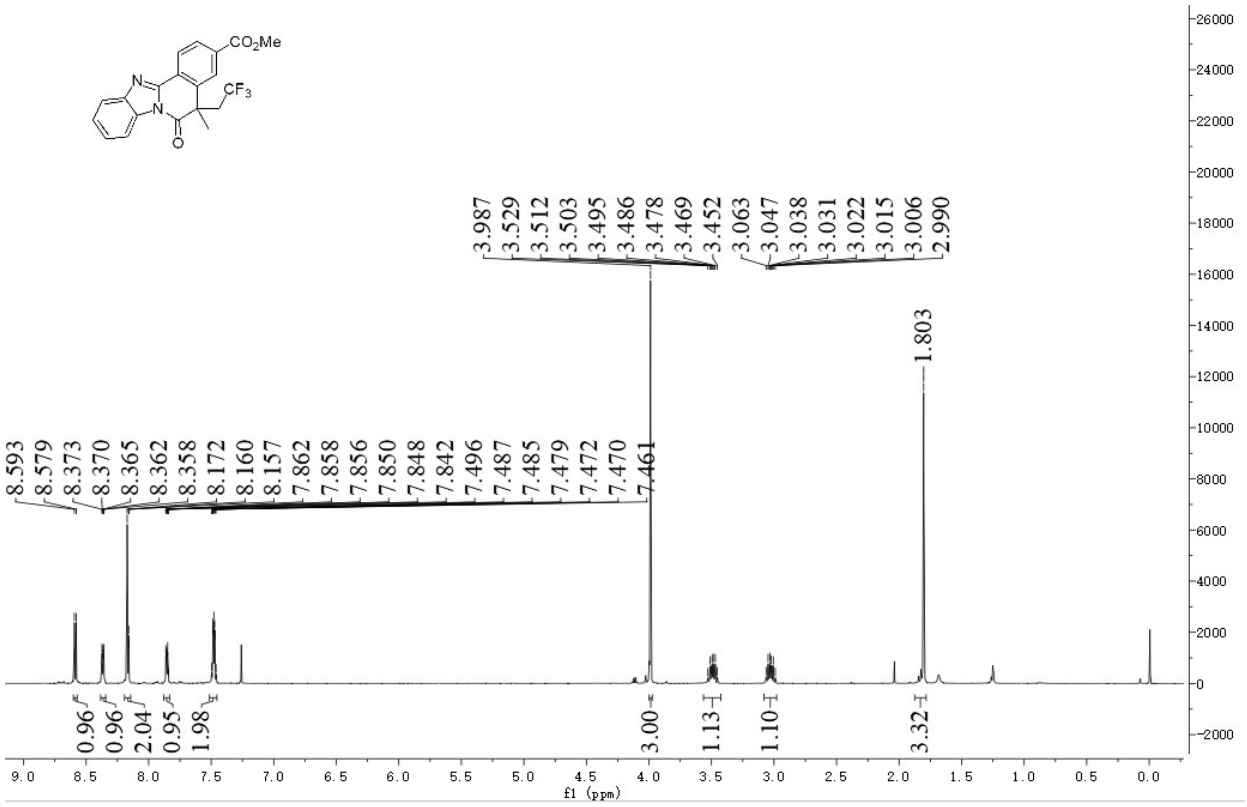


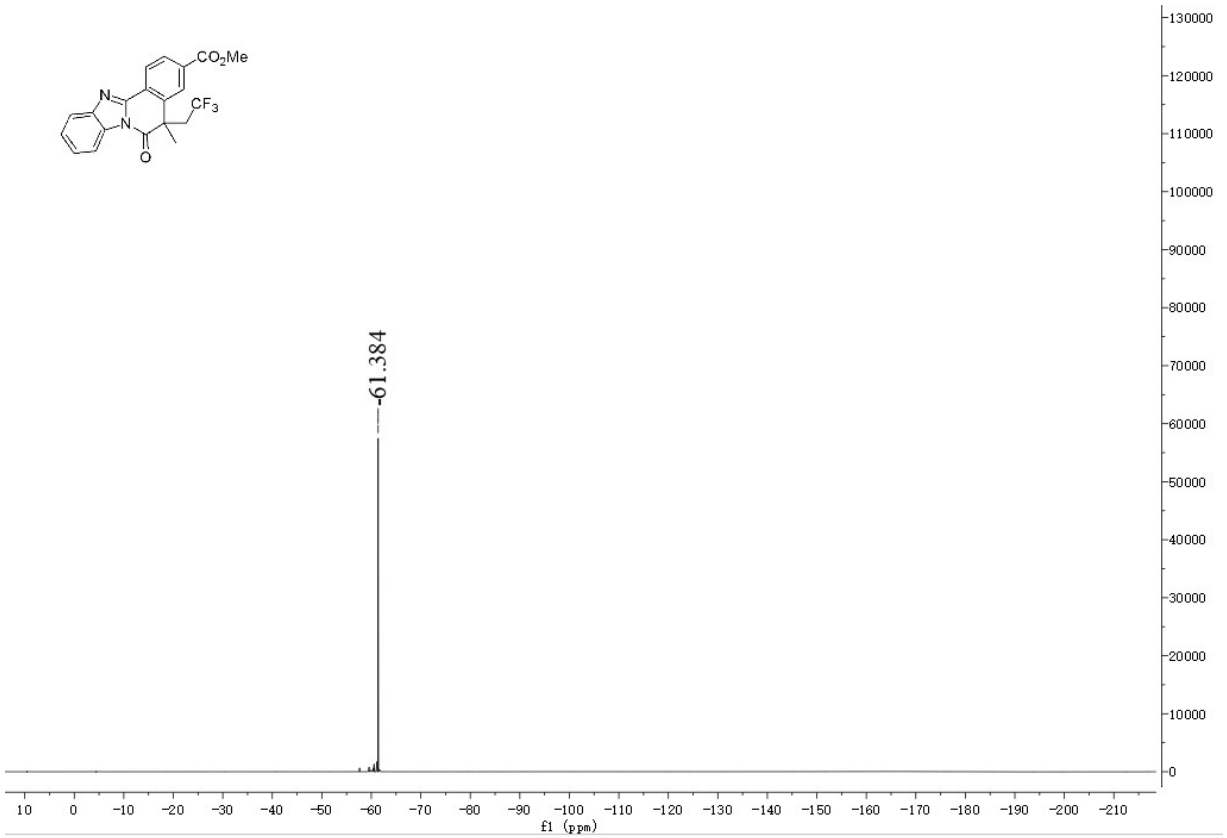
5-Methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (16)



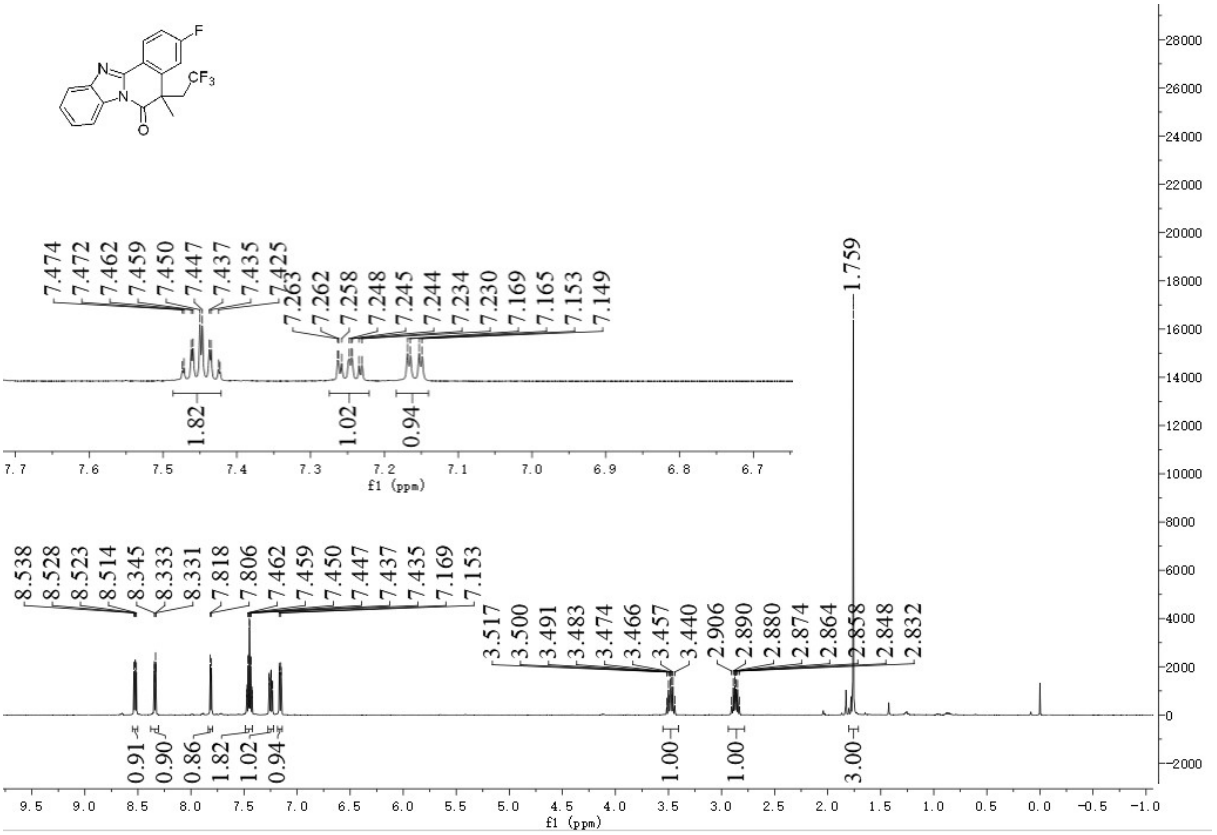


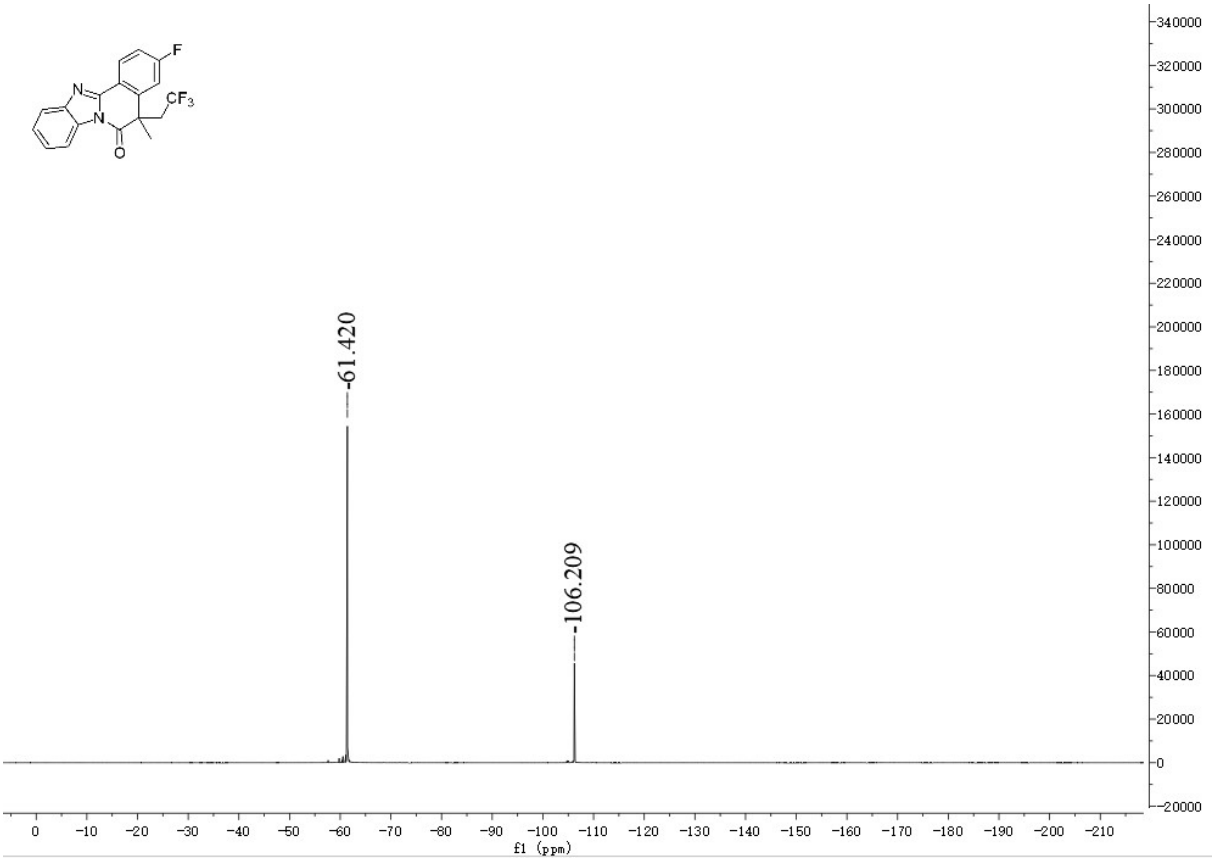
Methyl-5-methyl-6-oxo-5-(2,2,2-trifluoroethyl)-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-3-carboxylate (17)



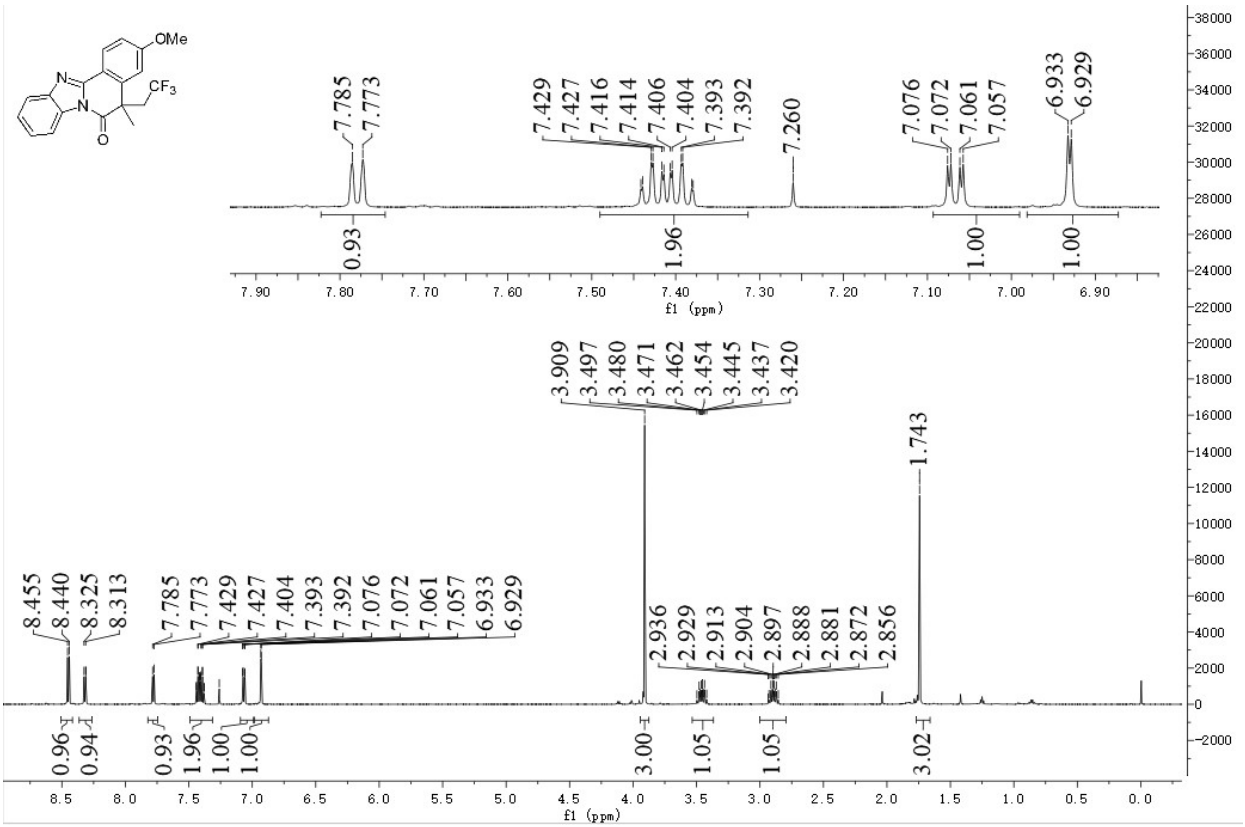


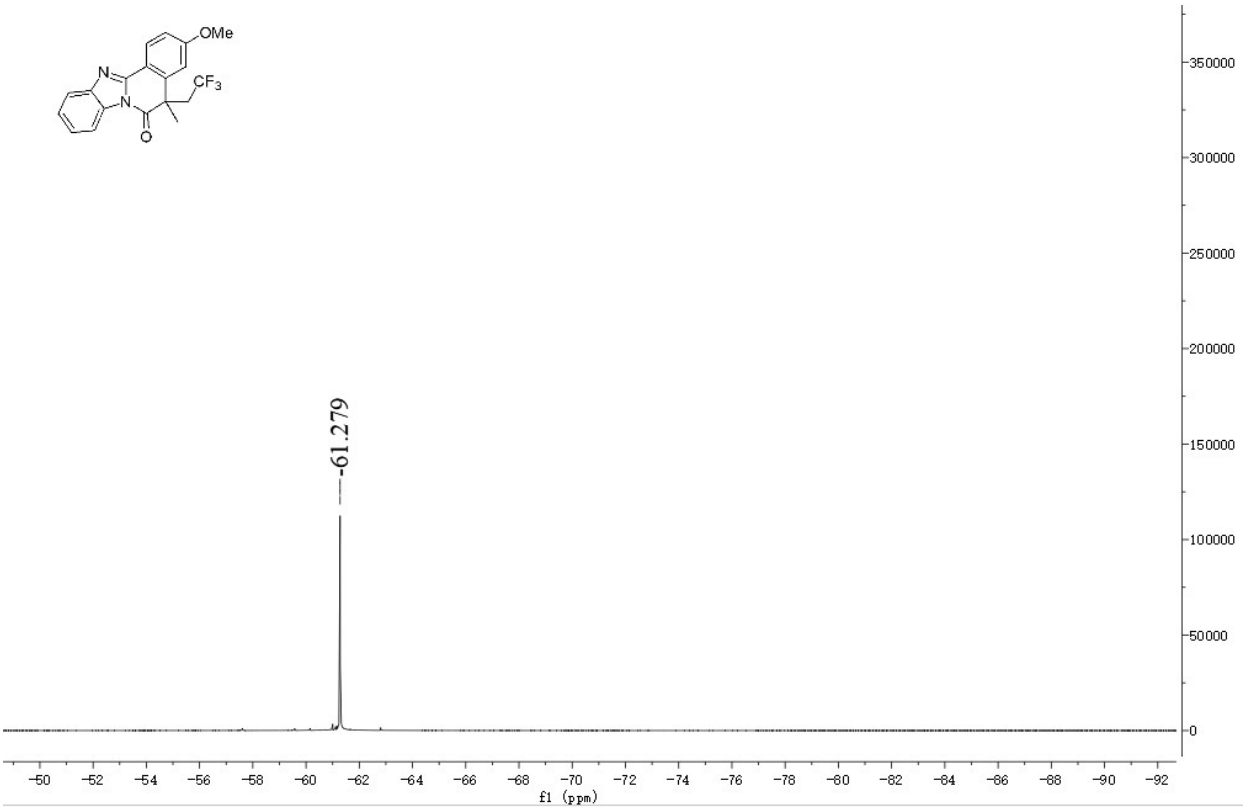
3-Fluoro-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (18)



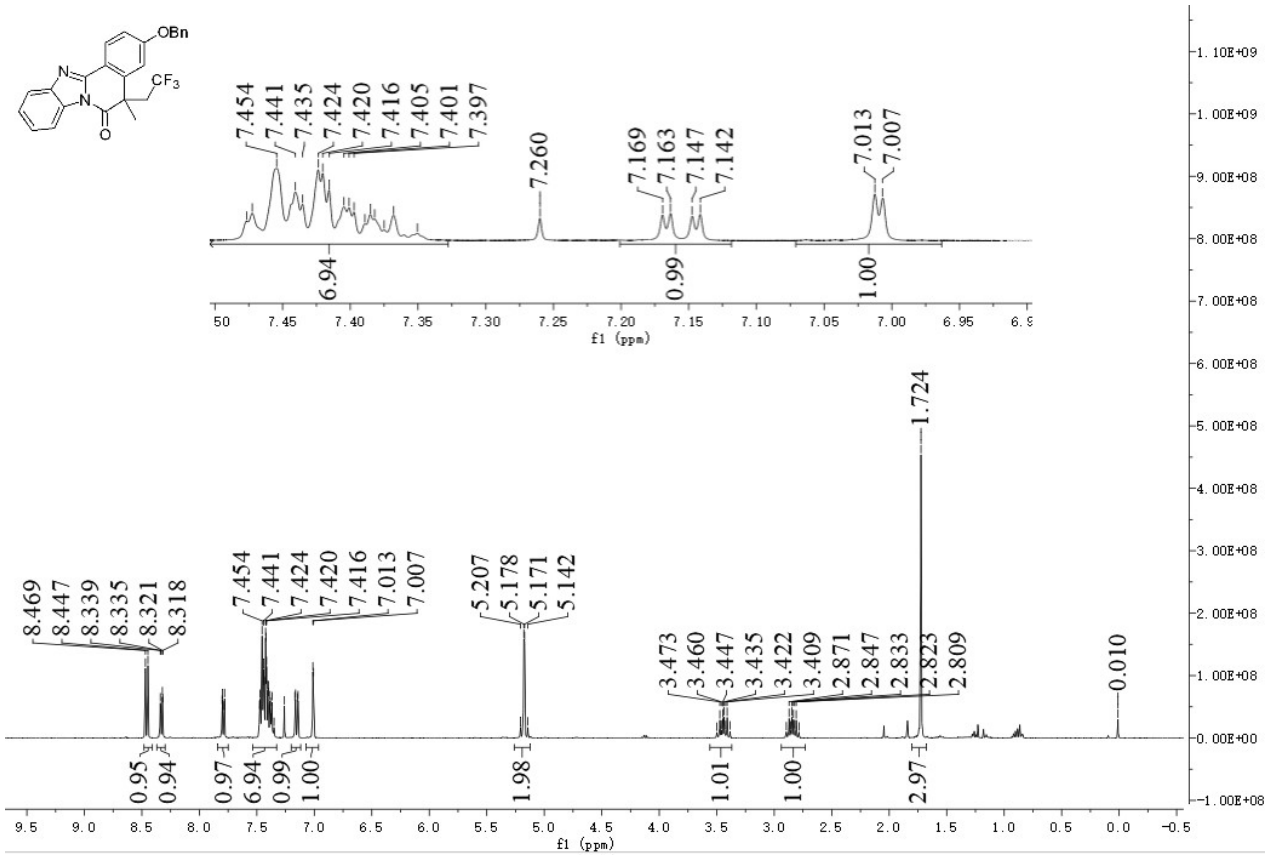


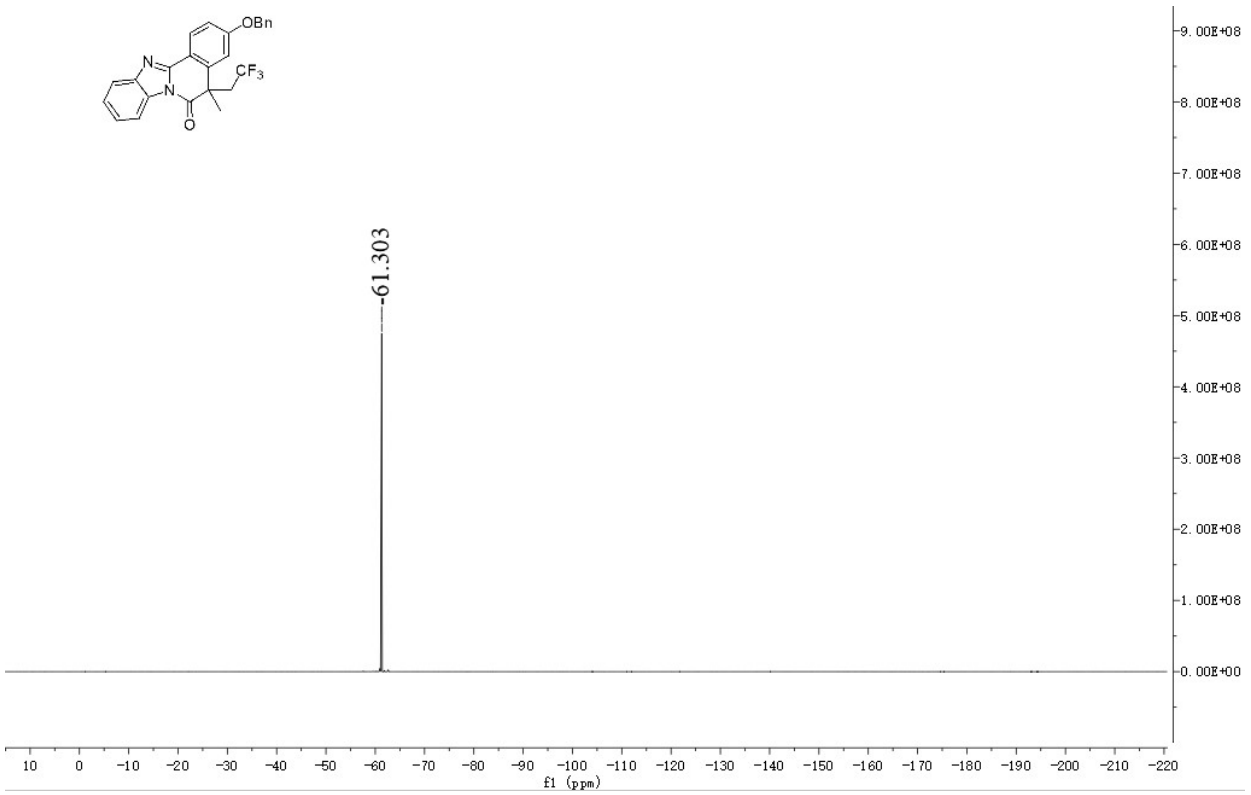
3-Methoxy-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (19)



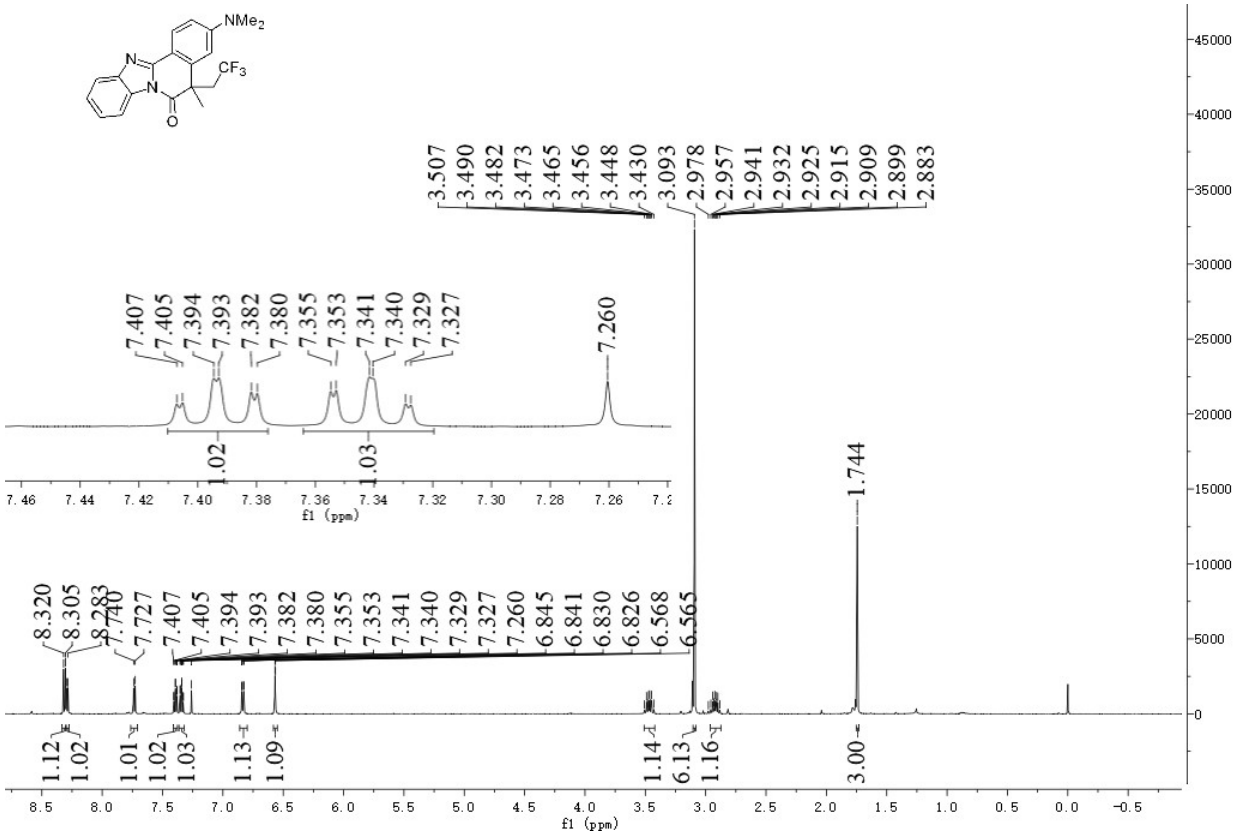


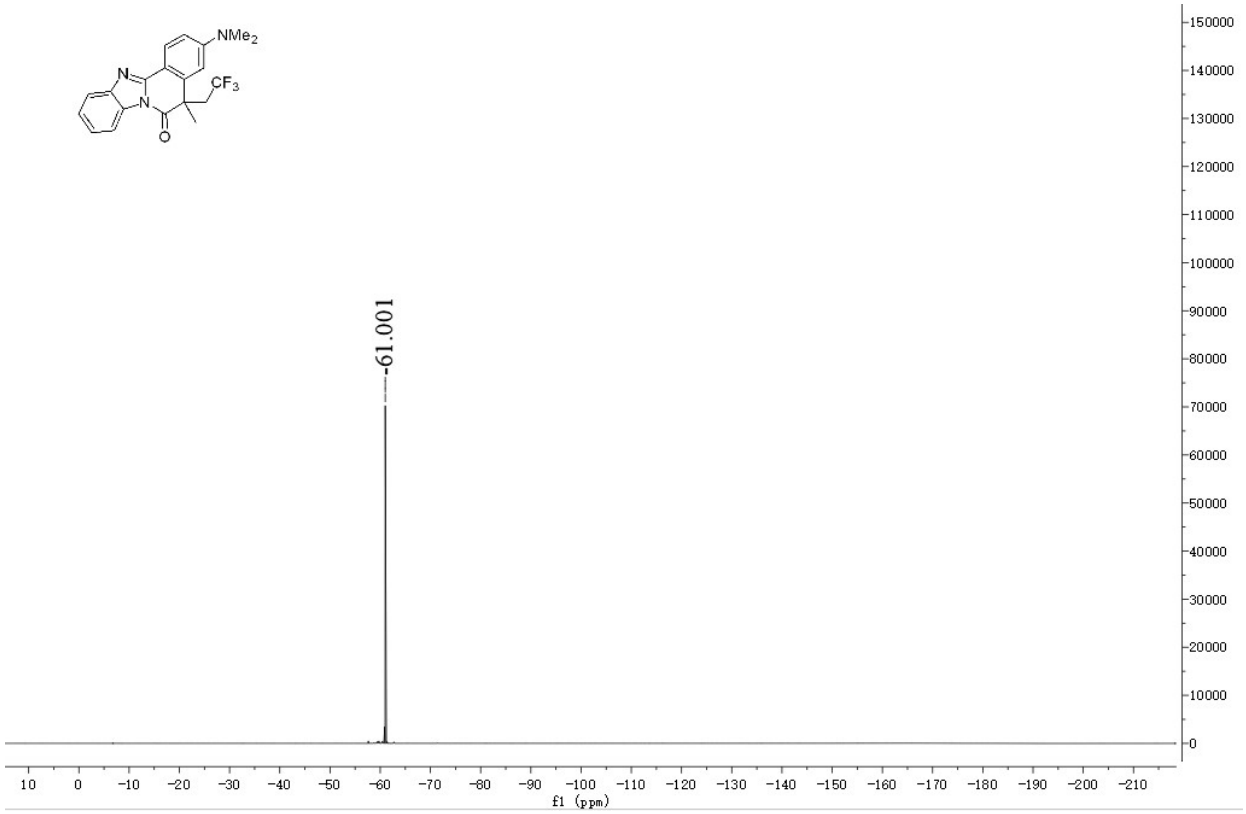
3-(Benzyloxy)-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (20)



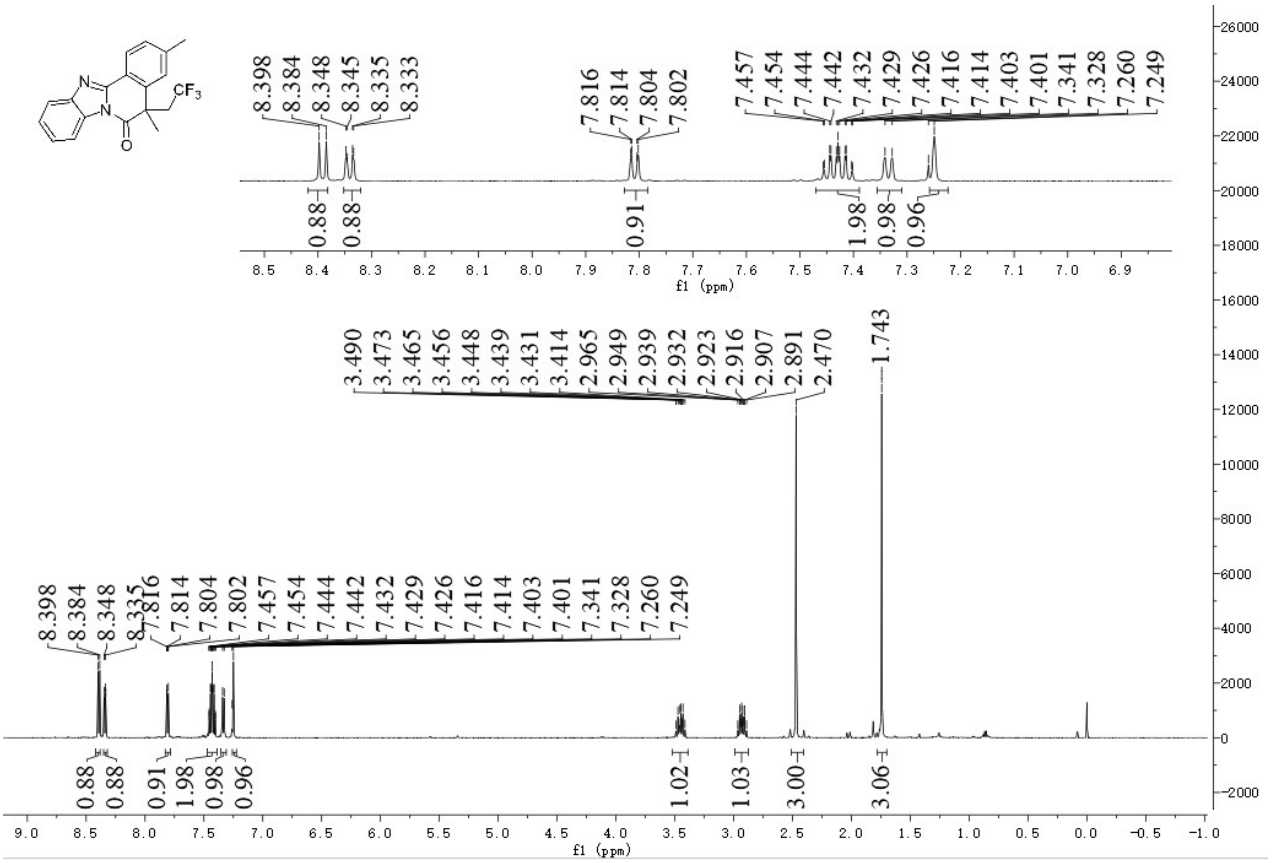


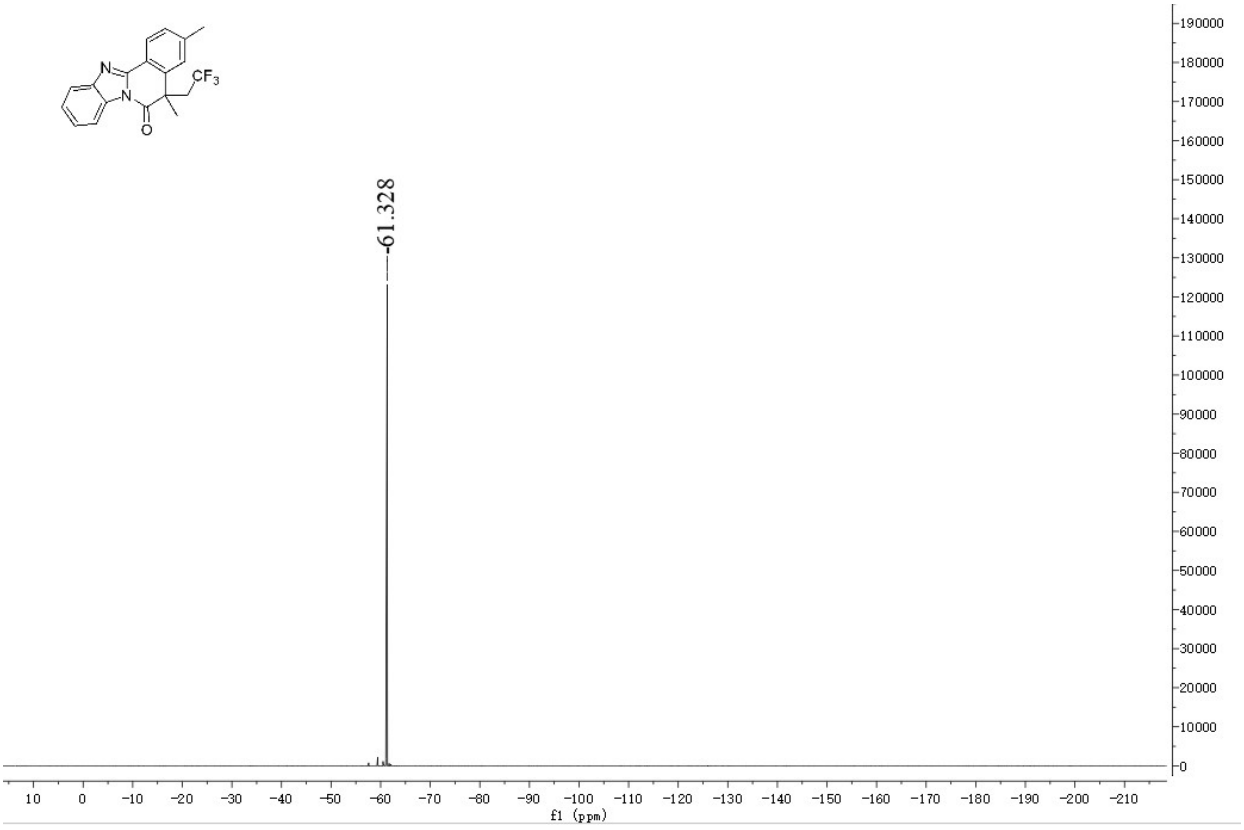
3-(Dimethylamino)-5-methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (21)



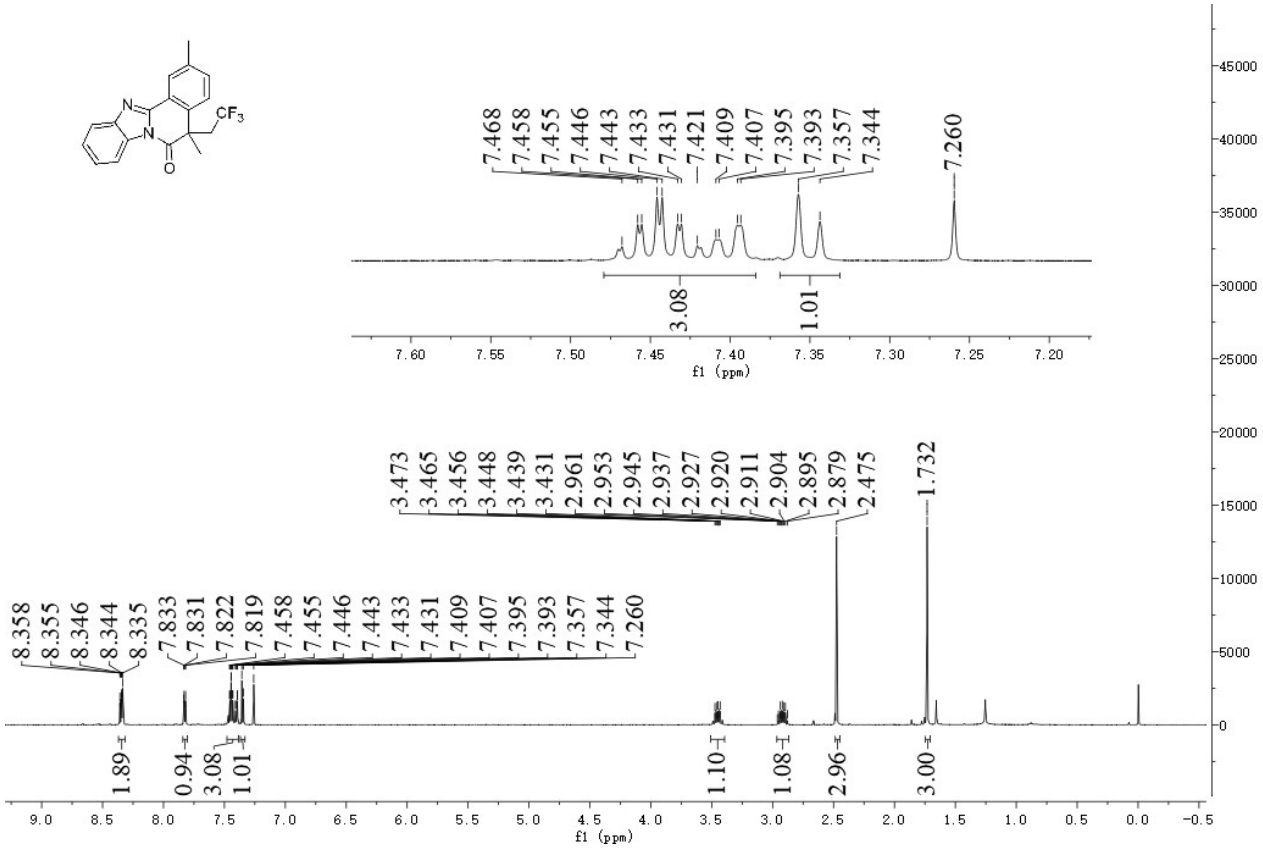


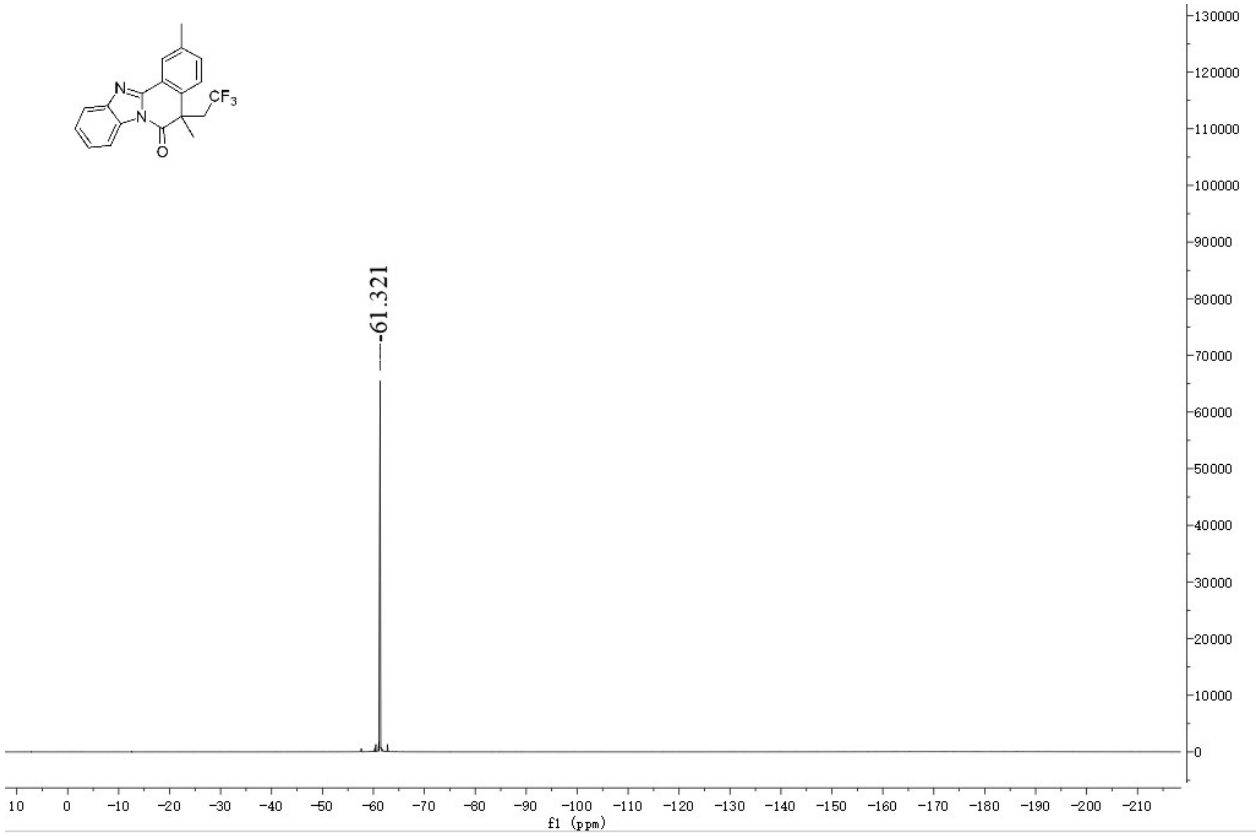
3,5-Dimethyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (22)



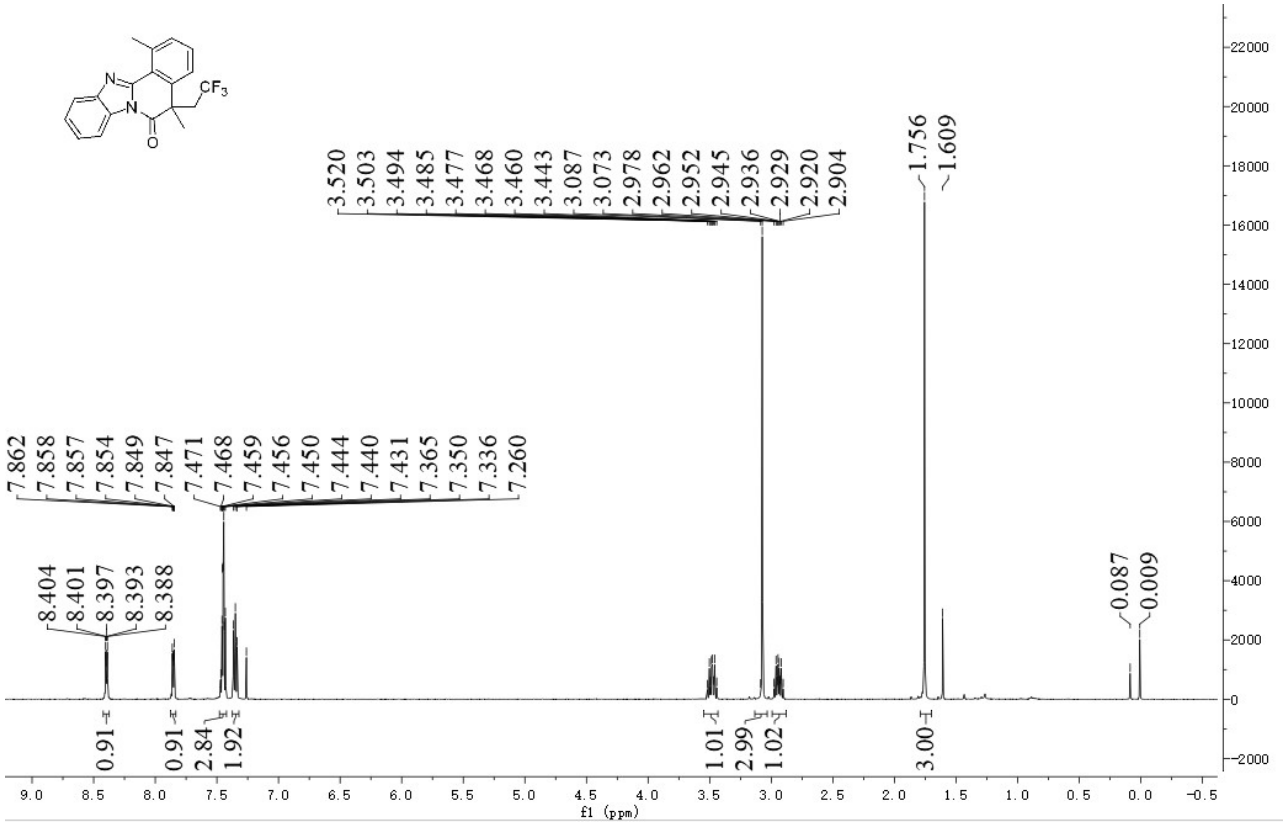


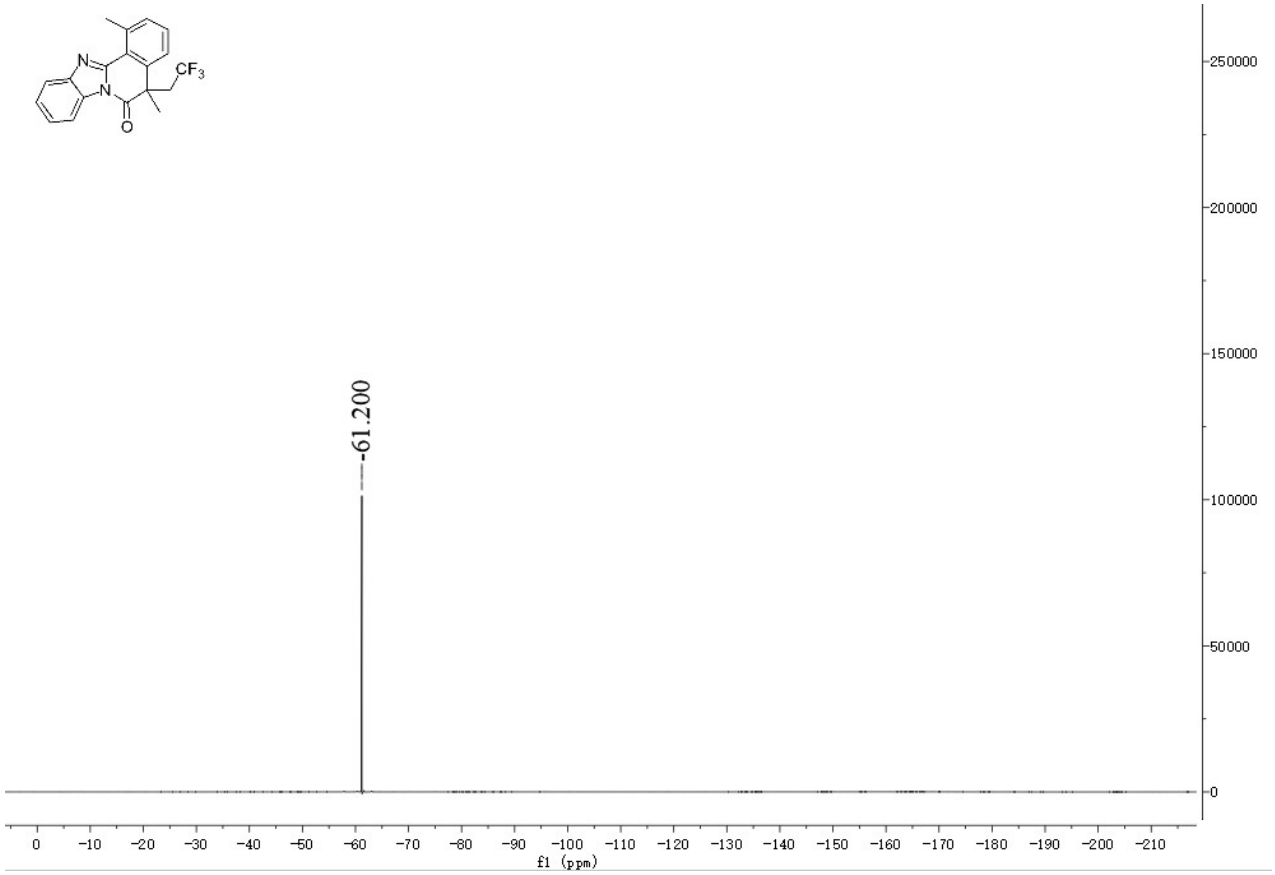
2,5-Dimethyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (23)



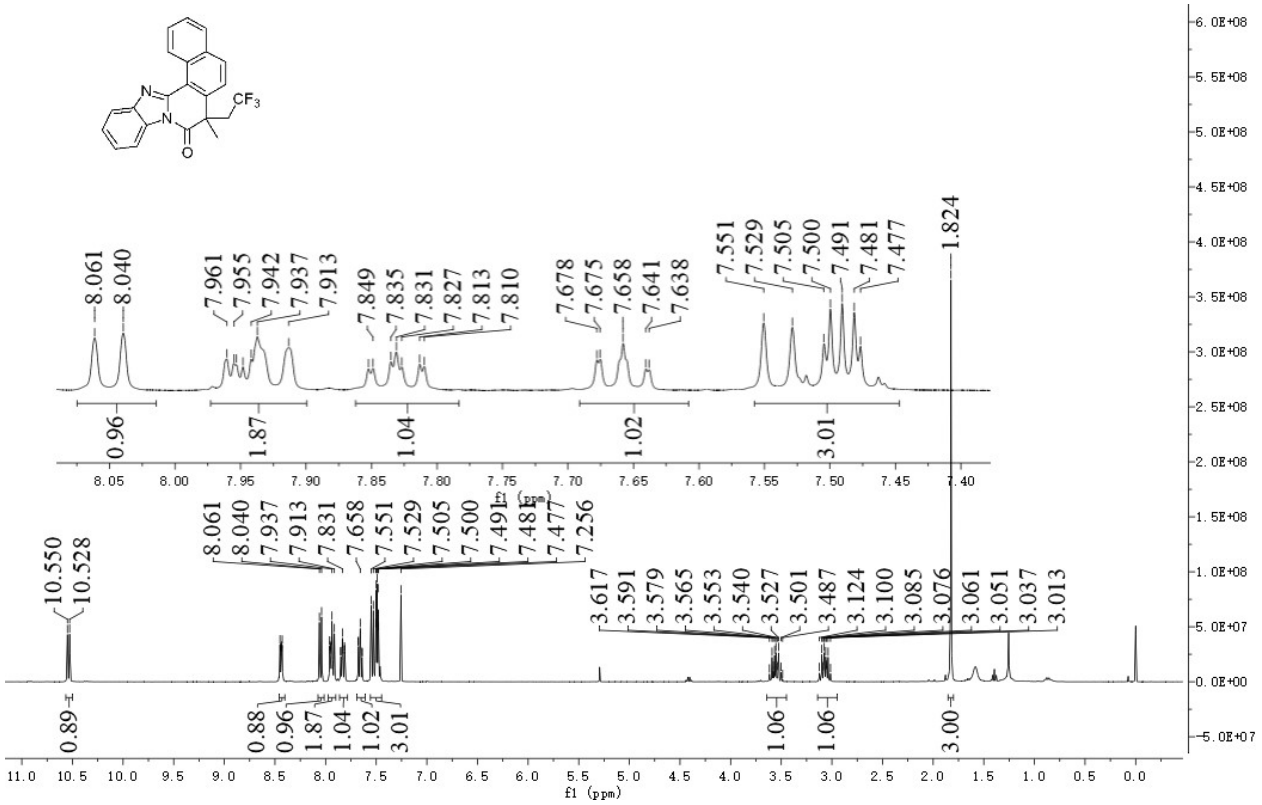


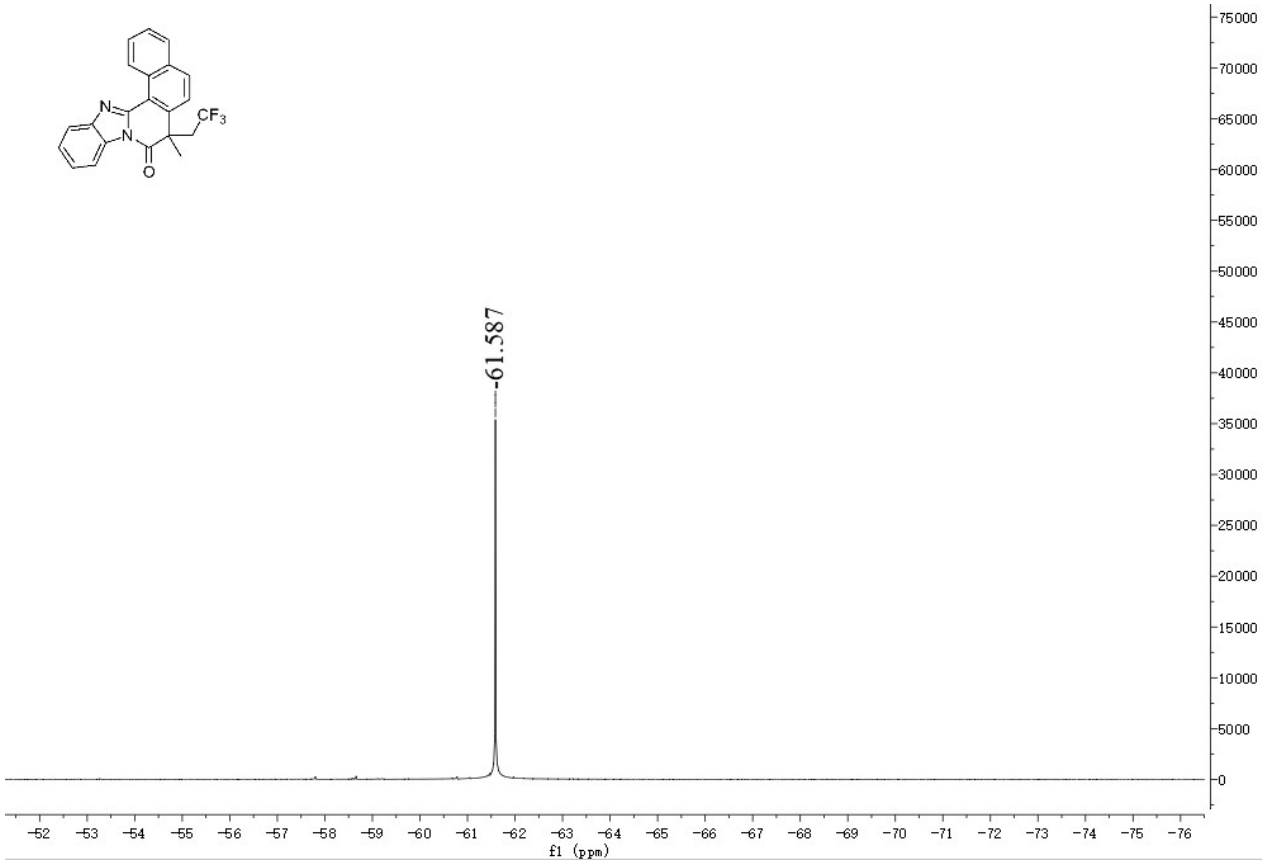
1,5-Dimethyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (24)



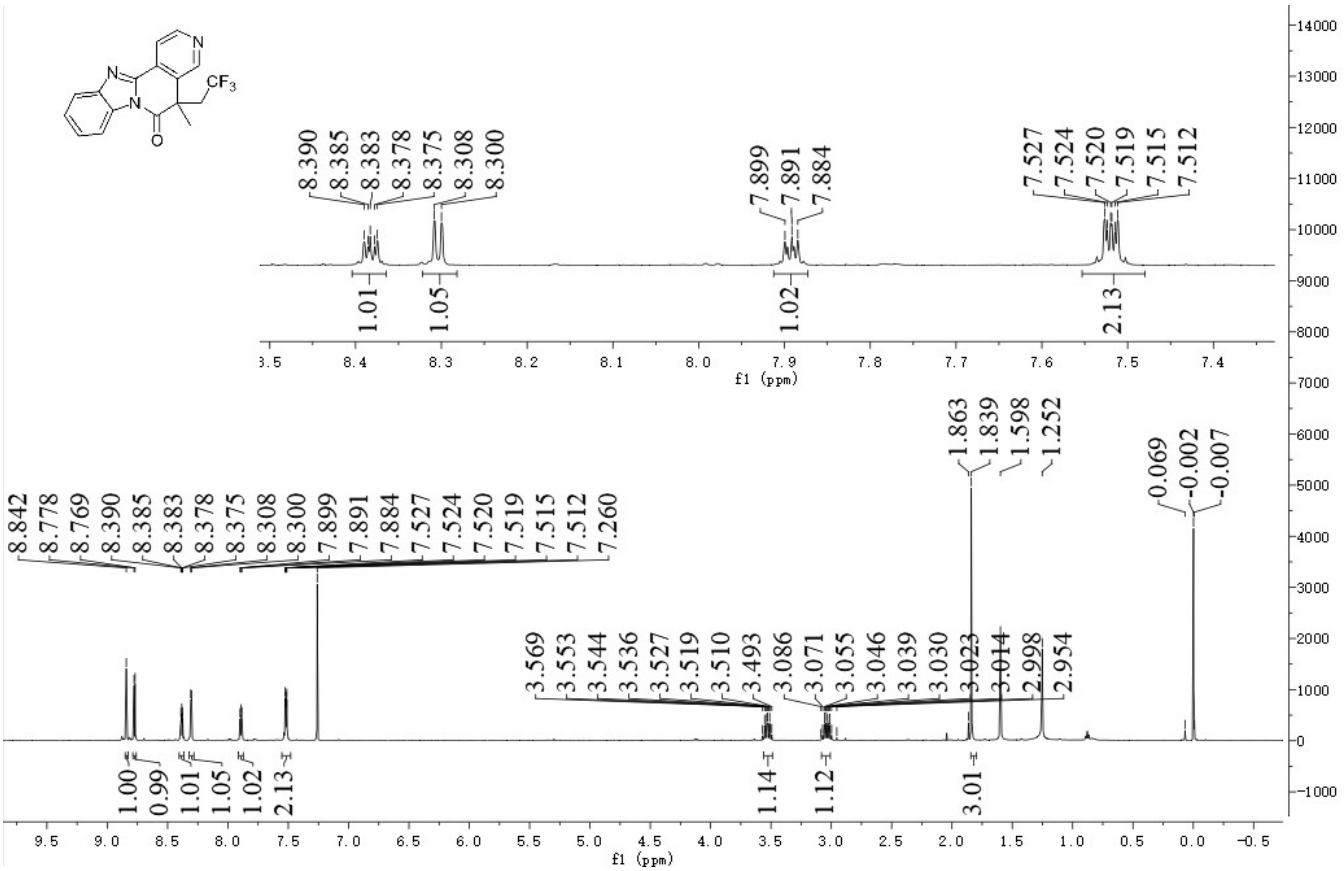


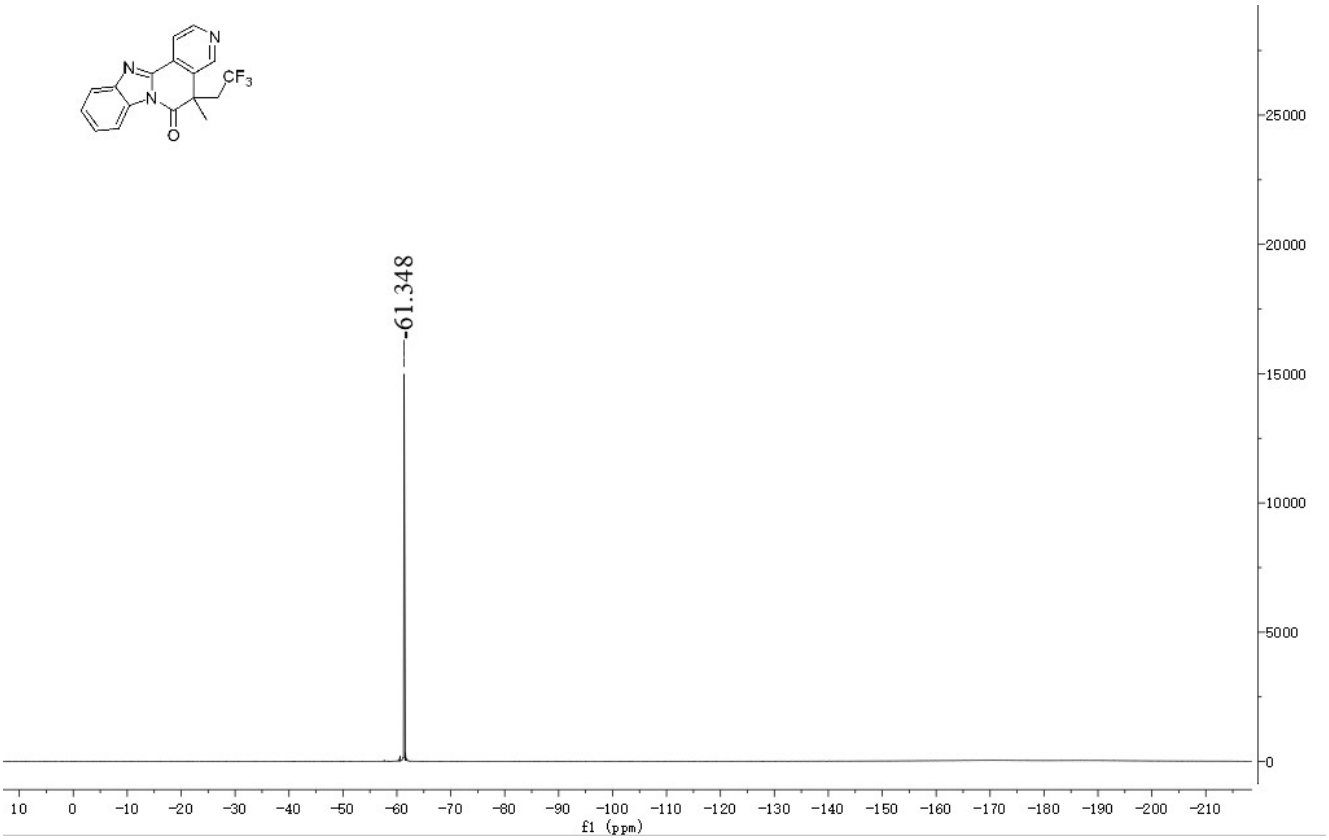
7-Methyl-7-(2,2,2-trifluoroethyl)benzo[h]benzo[4,5]imidazo[2,1-*a*]isoquinolin-8(7*H*)-one (25)



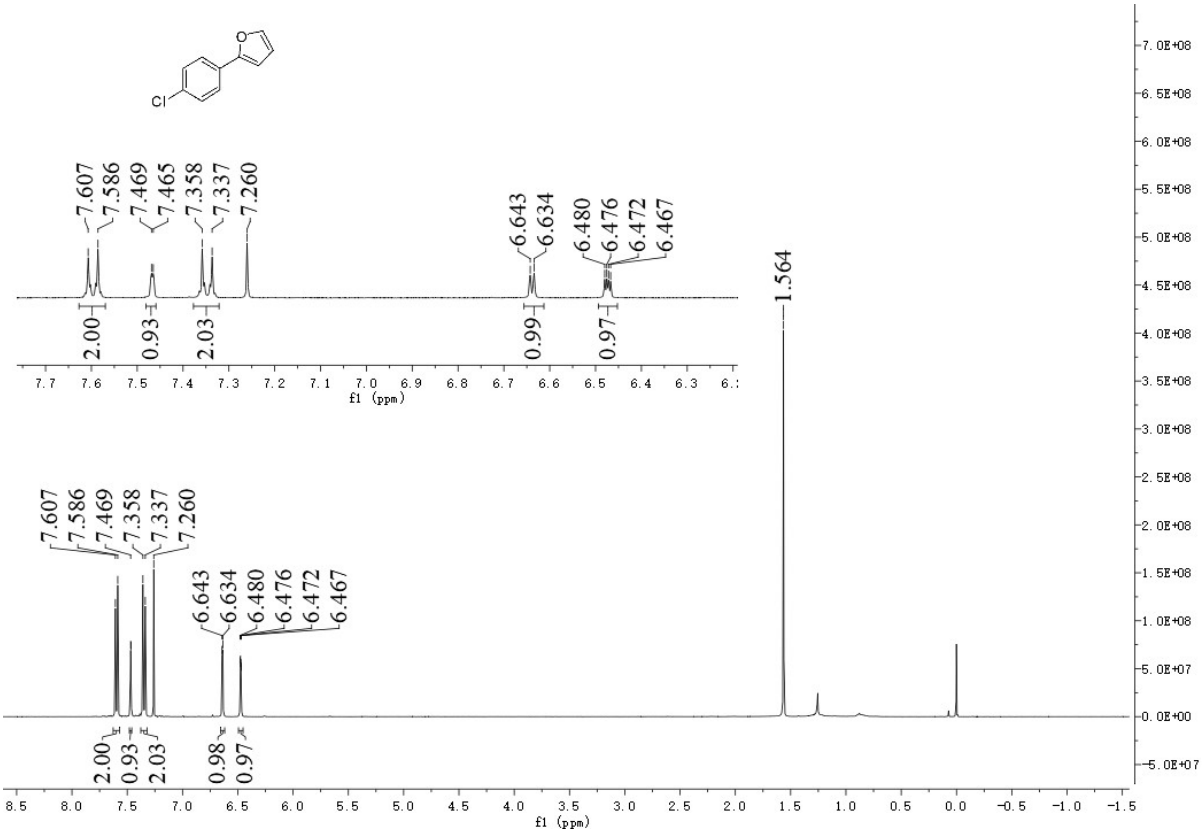


5-Methyl-5-(2,2,2-trifluoroethyl)benzo[4,5]imidazo[2,1-*a*][2,6]naphthyridin-6(5*H*)-one (26)

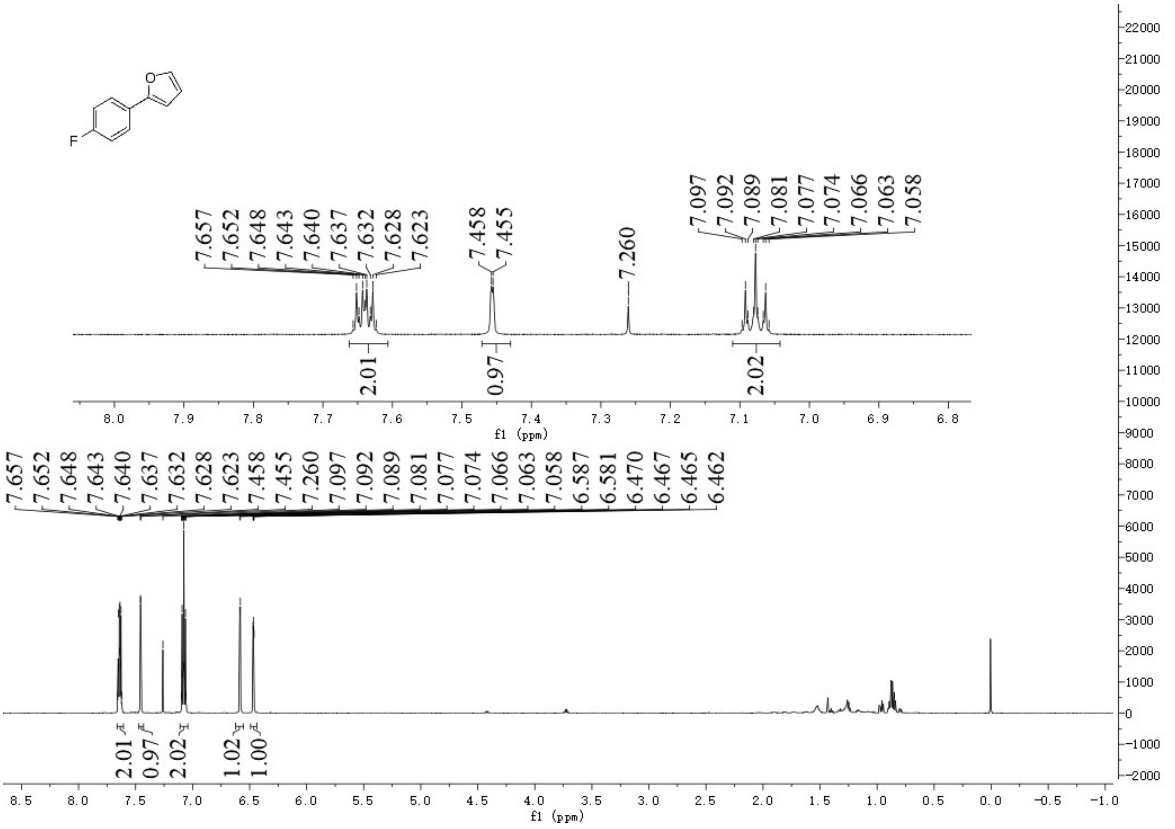




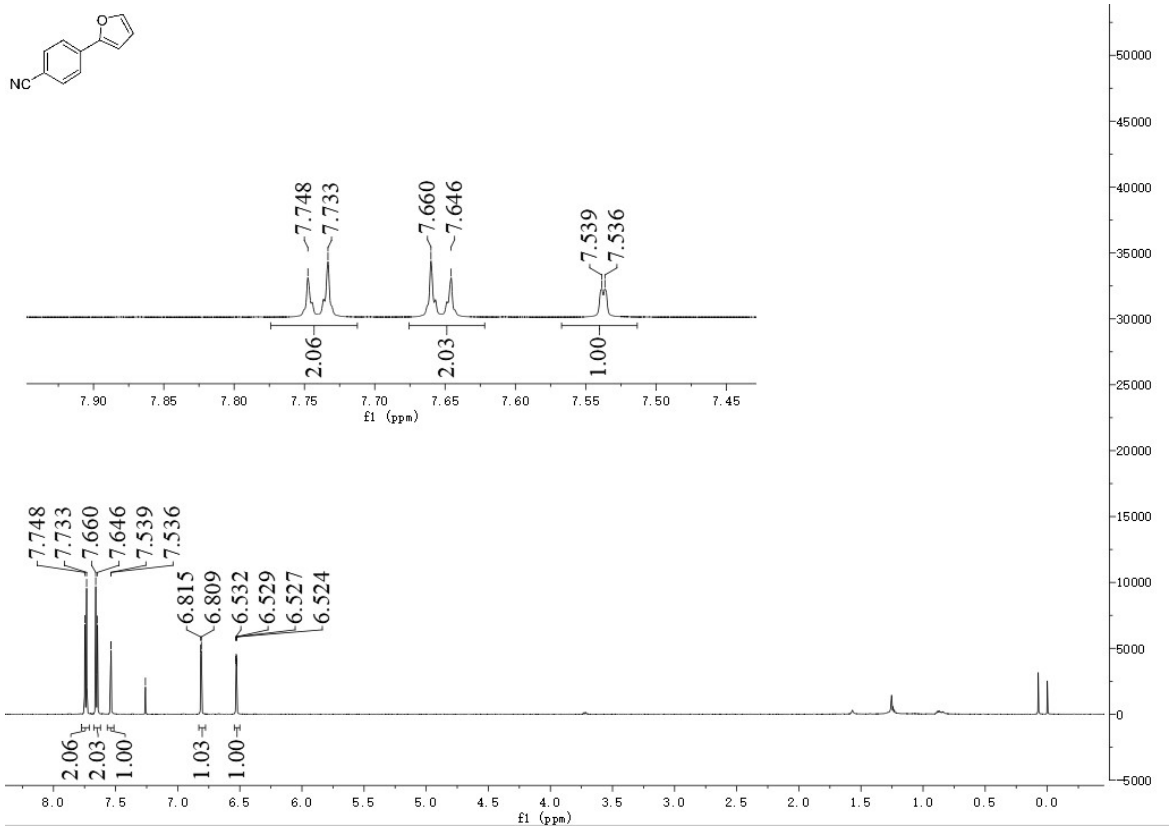
2-(4-Chlorophenyl)furan (27)



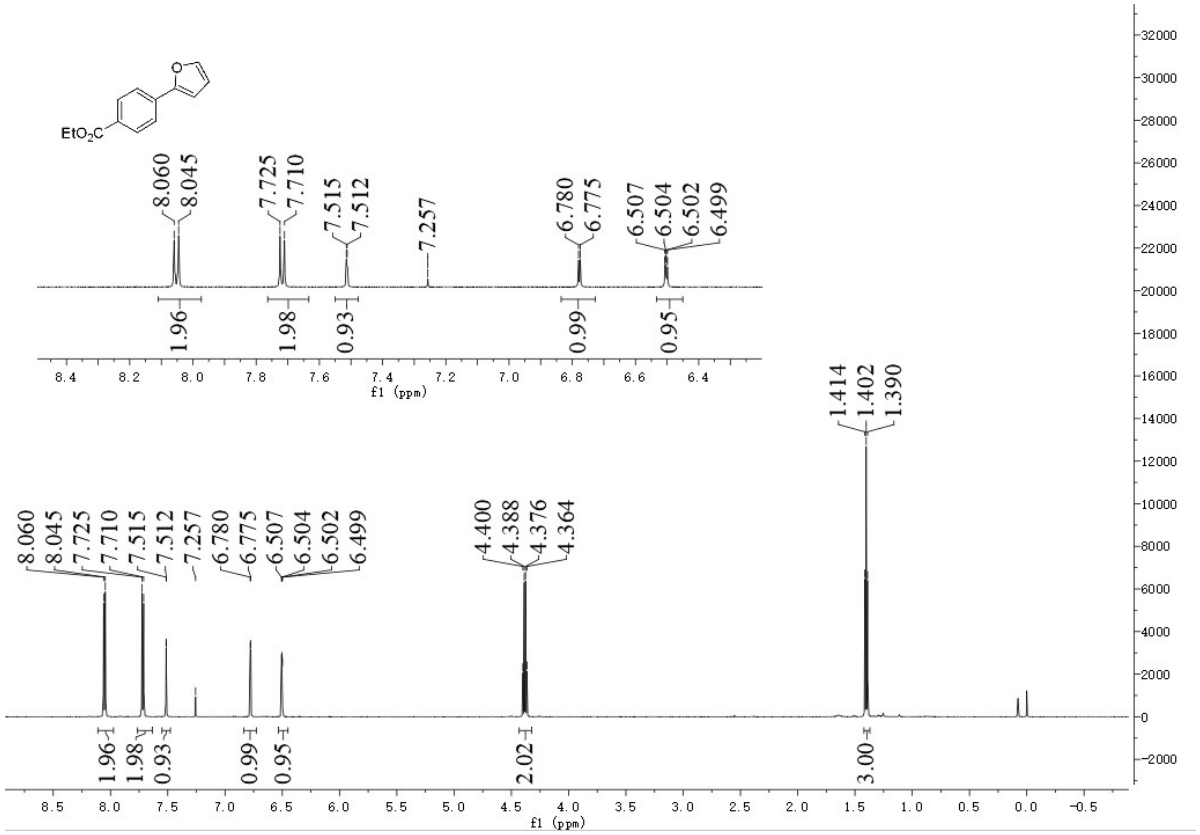
2-(4-Fluorophenyl)furan (28)



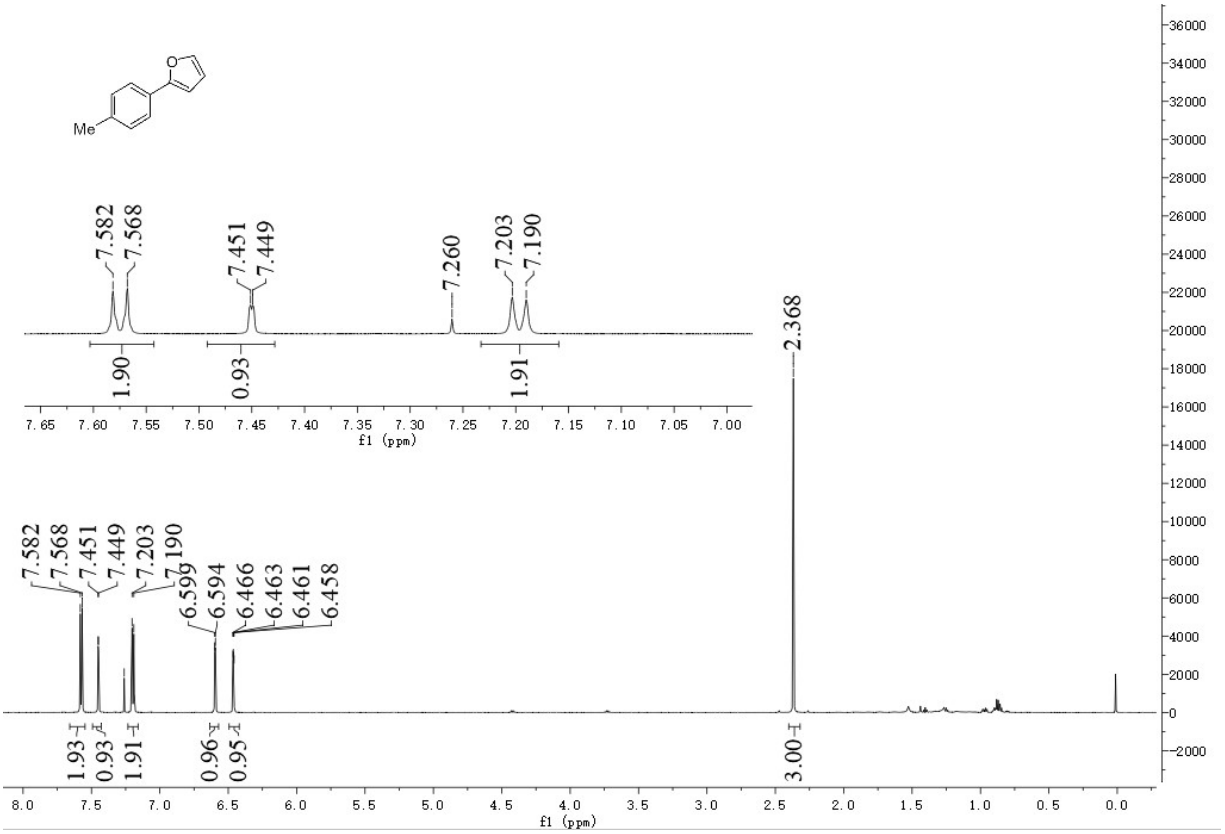
4-(Furan-2-yl)benzonitrile (29)



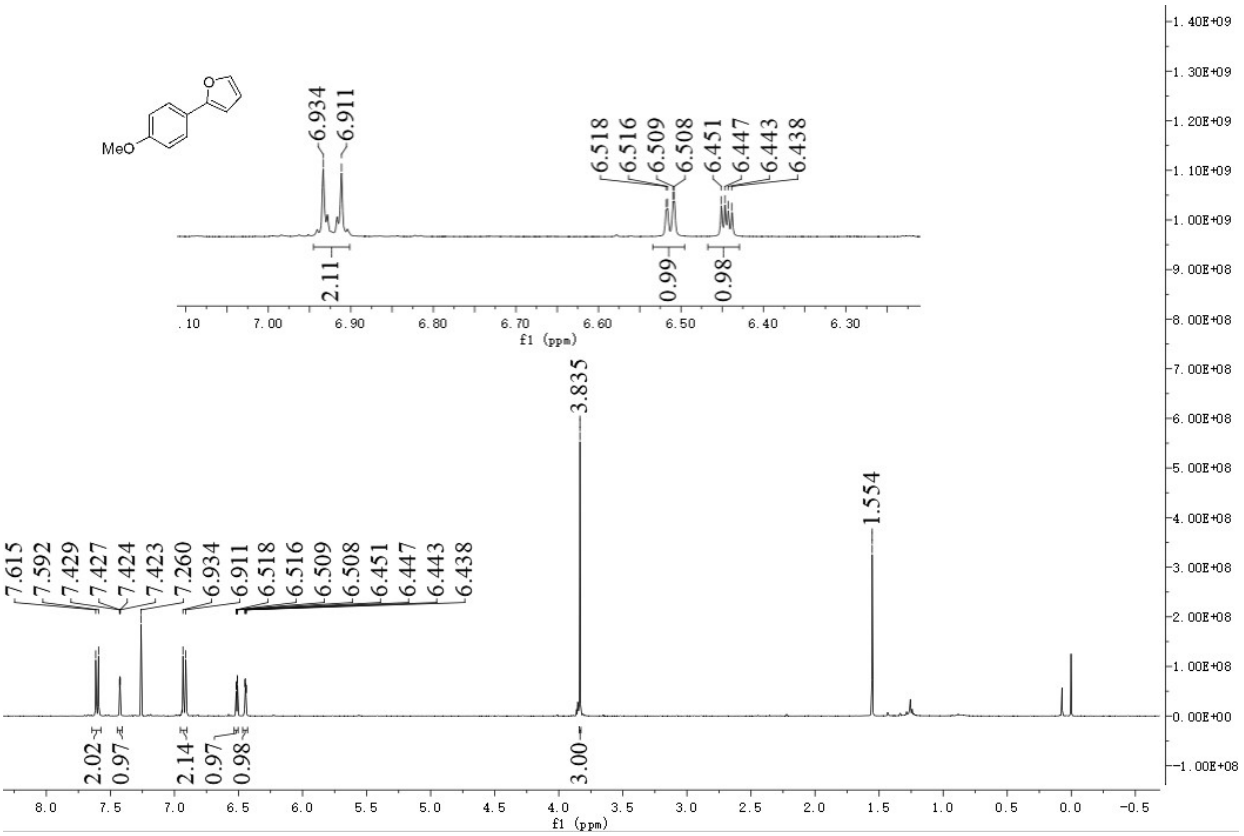
Ethyl 4-(furan-2-yl)benzoate (30)



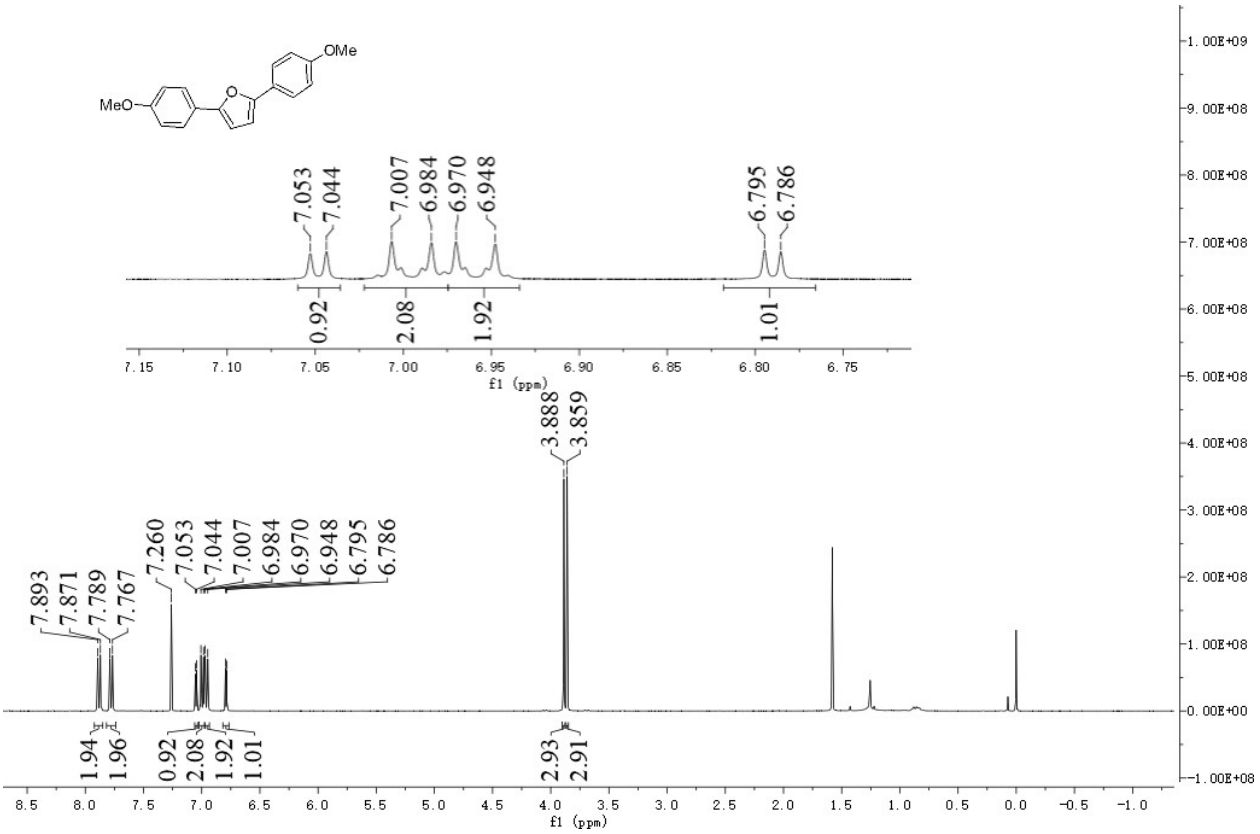
2-(*p*-Tolyl)furan (31)



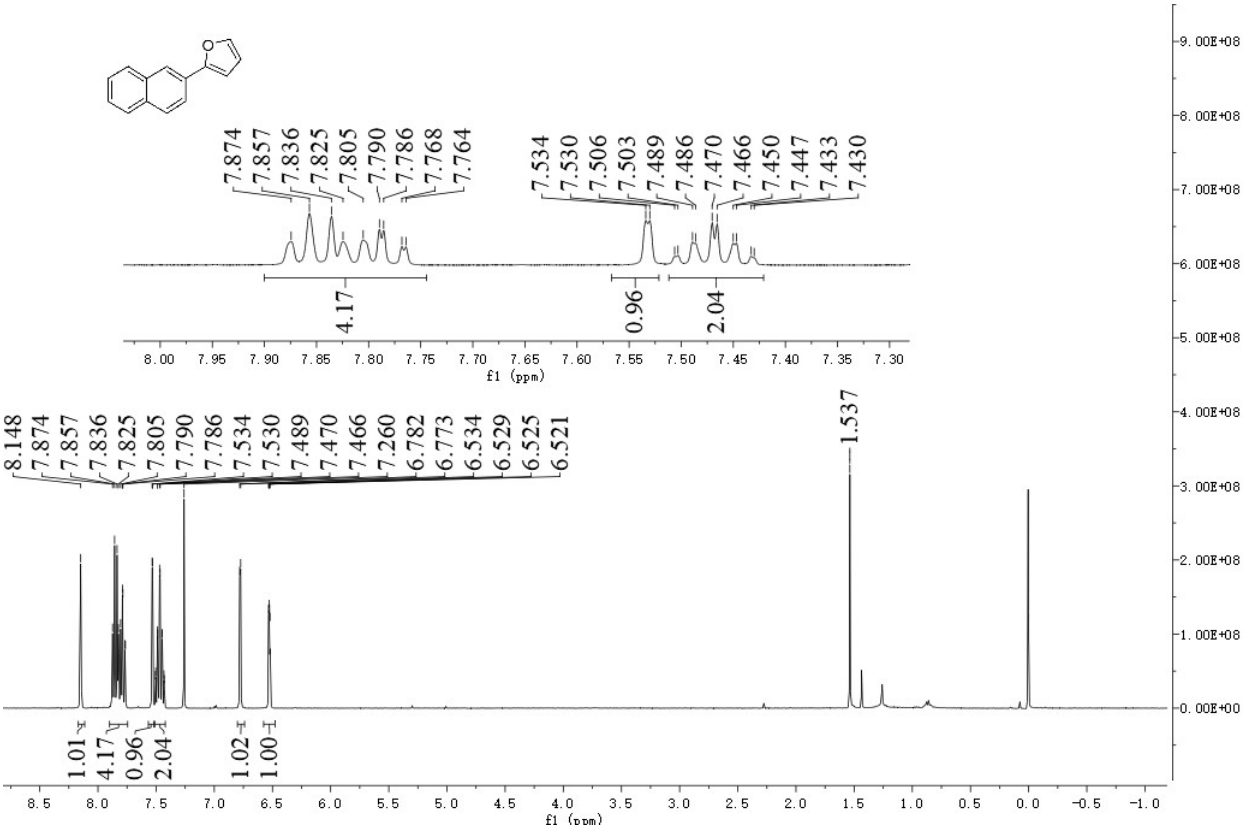
2-(4-Methoxyphenyl)furan (32)



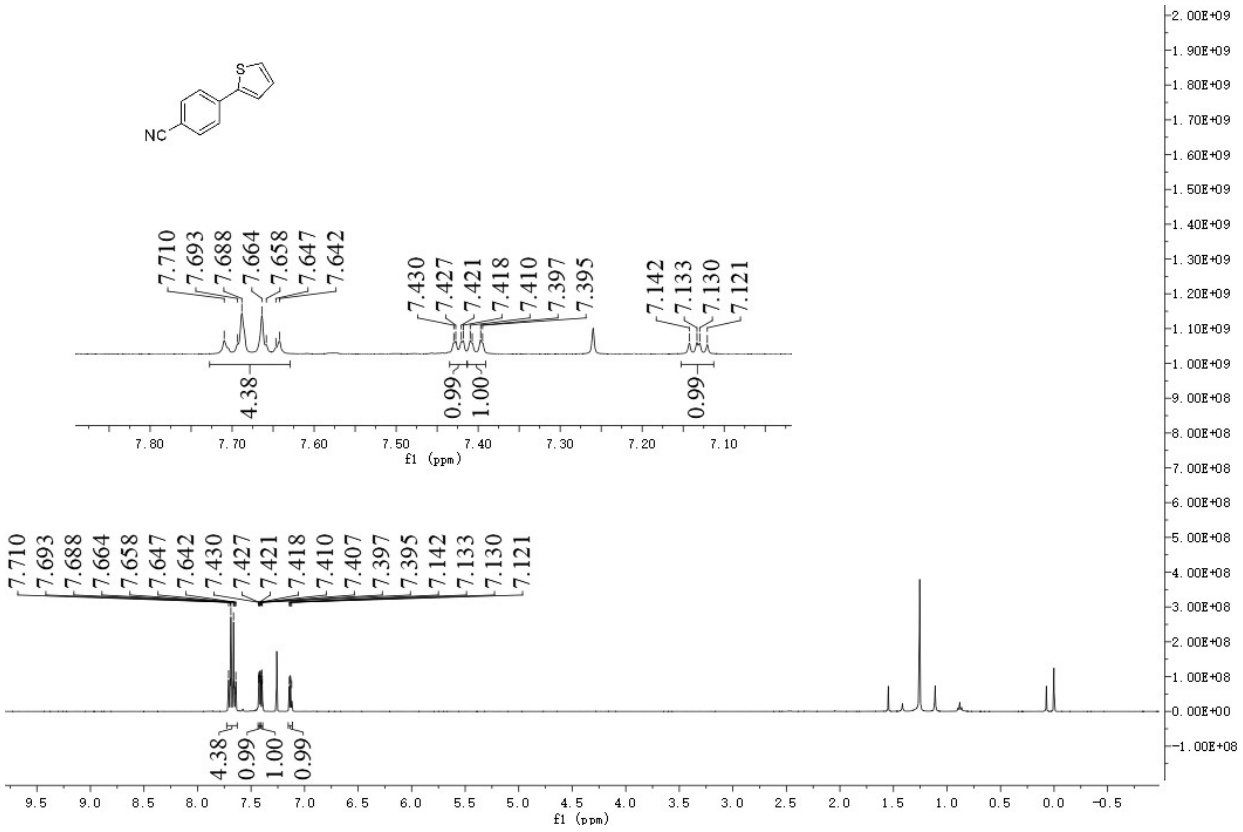
2,5-Bis(4-methoxyphenyl)furan (32')



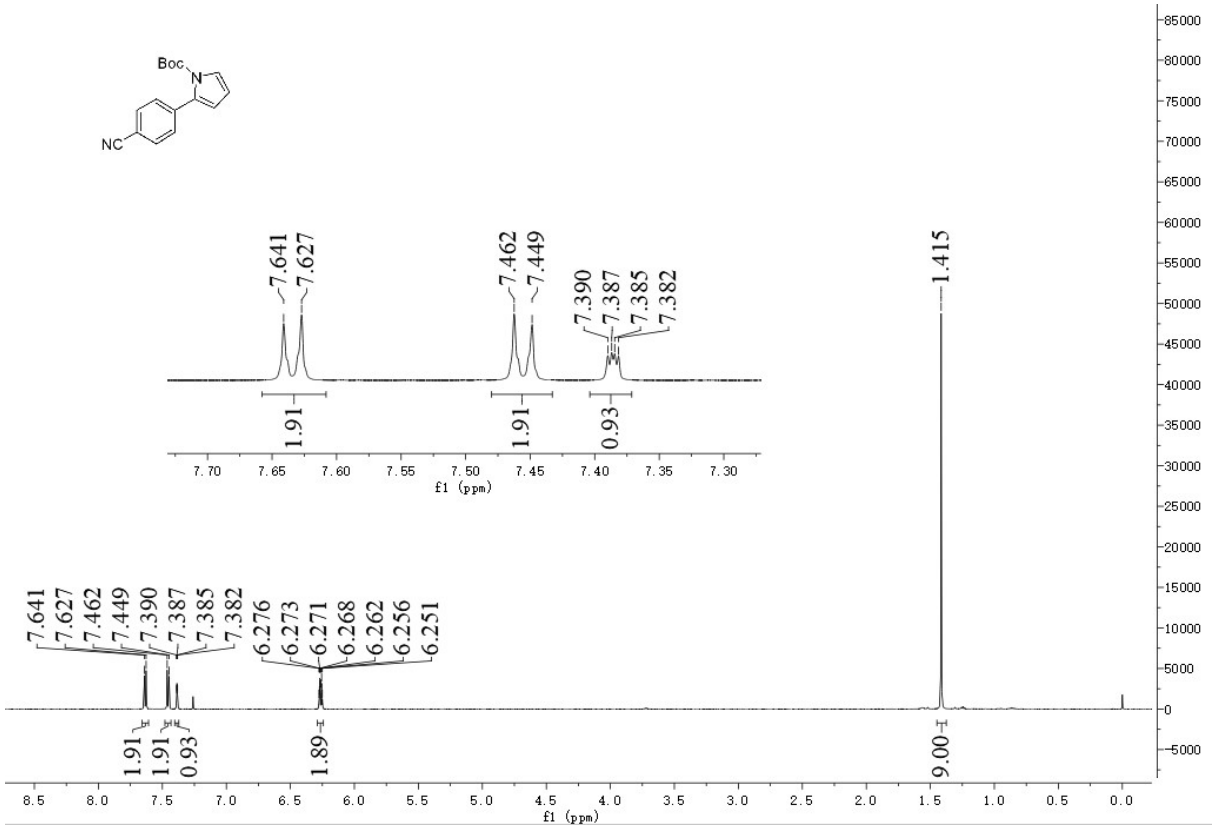
2-(Naphthalen-2-yl)furan (33)



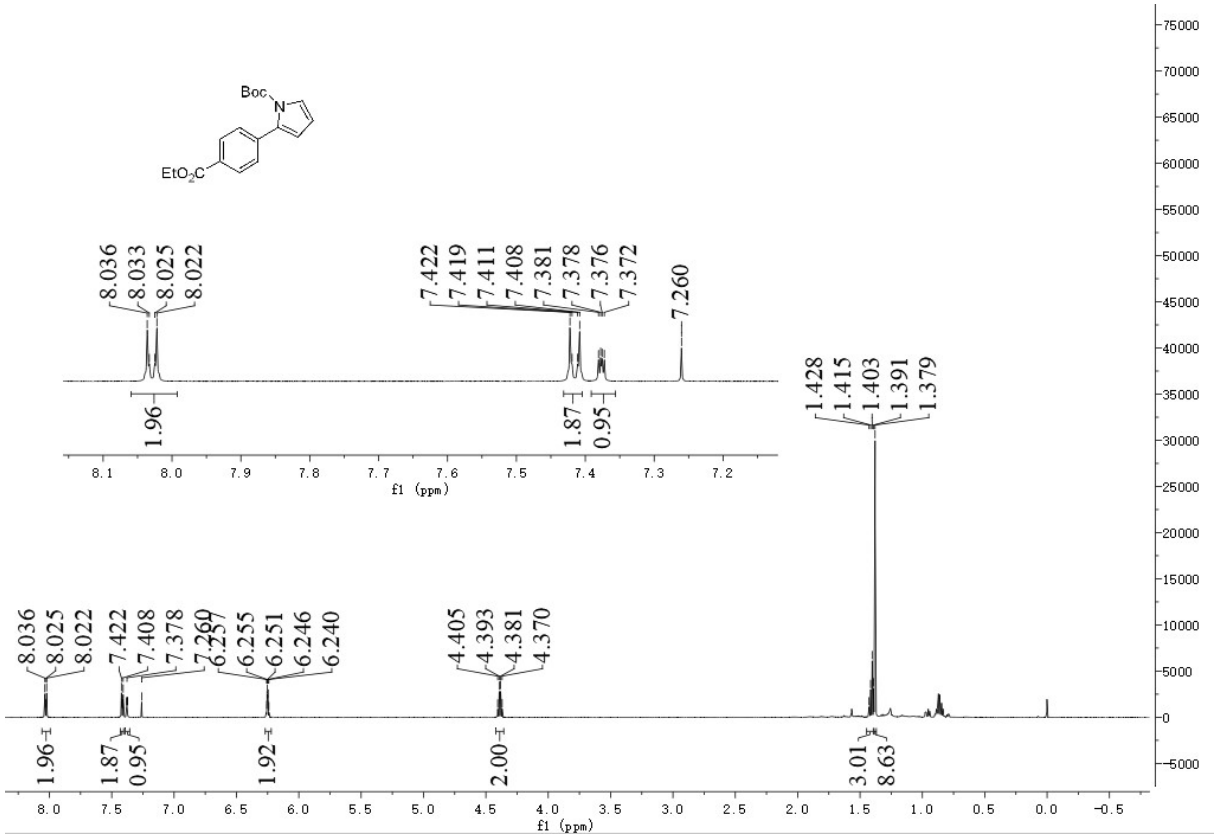
4-(Thiophen-2-yl)benzonitrile (34)



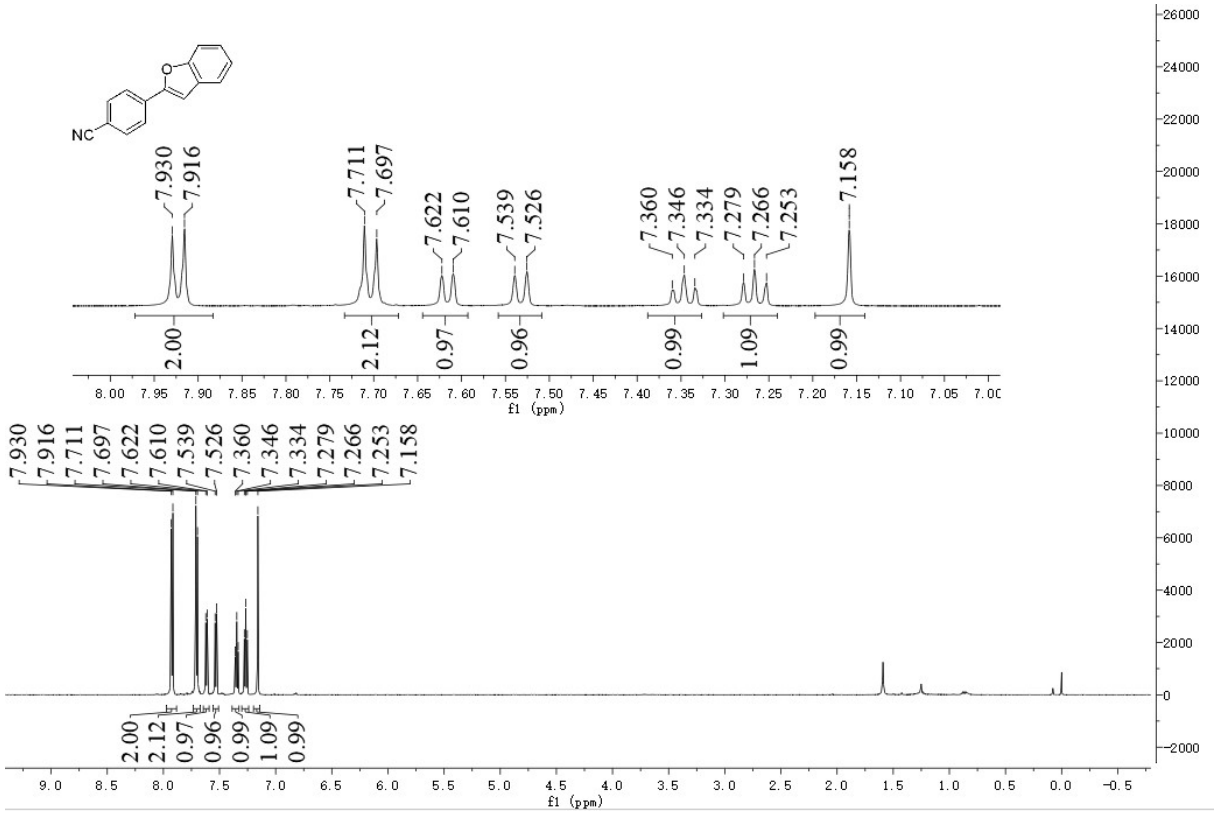
2-(4-Cyano-phenyl)-pyrrole-1-carboxylic acid tert-butyl ester (35)



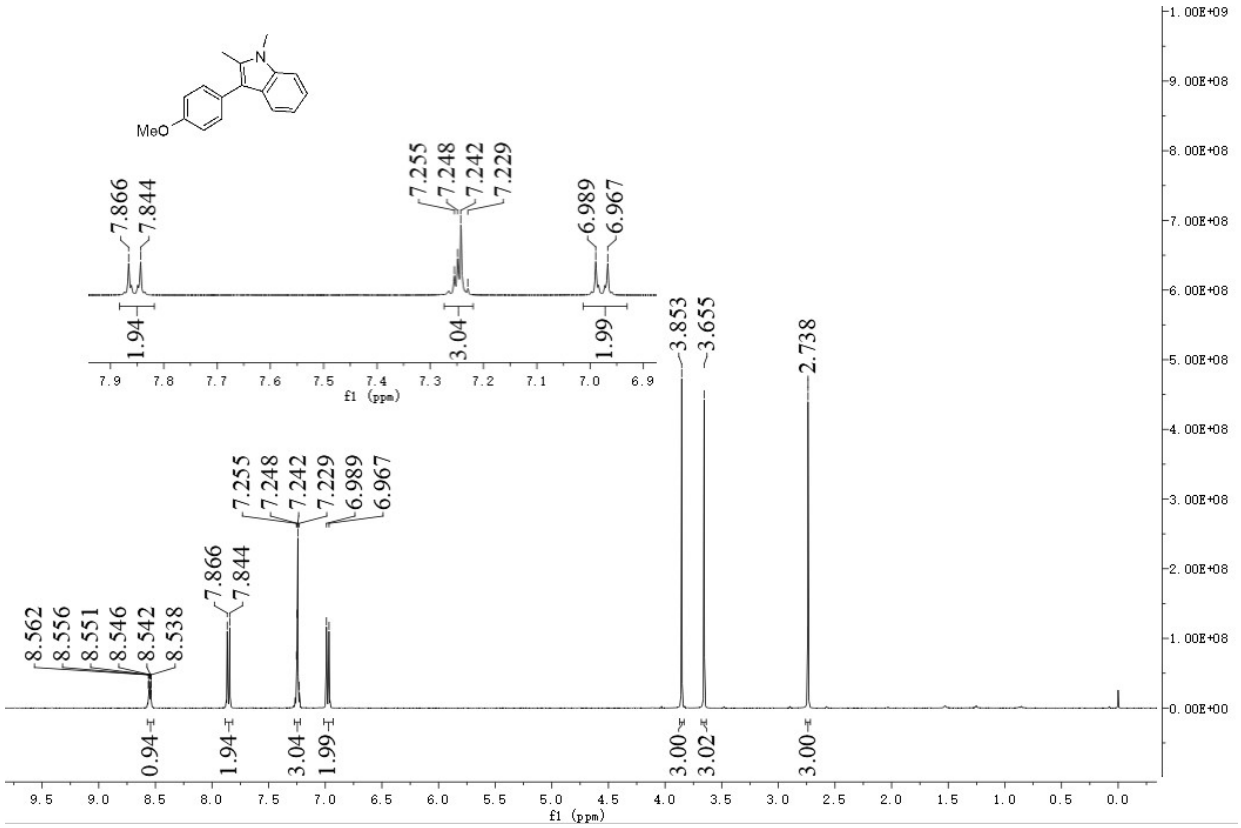
2-(4- Ethoxycarbonyl -phenyl)-pyrrole-1-carboxylic acid tert-butyl ester (36)



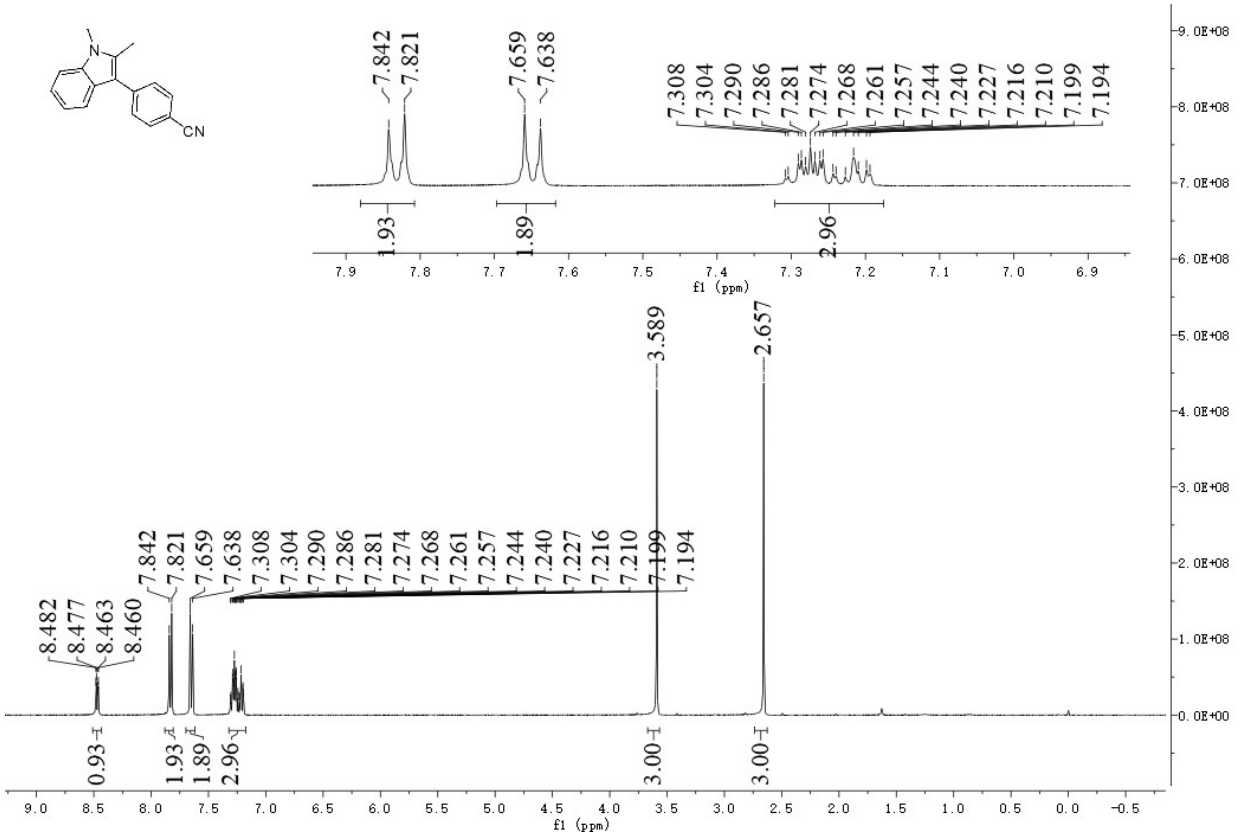
4-(Benzofuran-2-yl)benzonitrile (37)



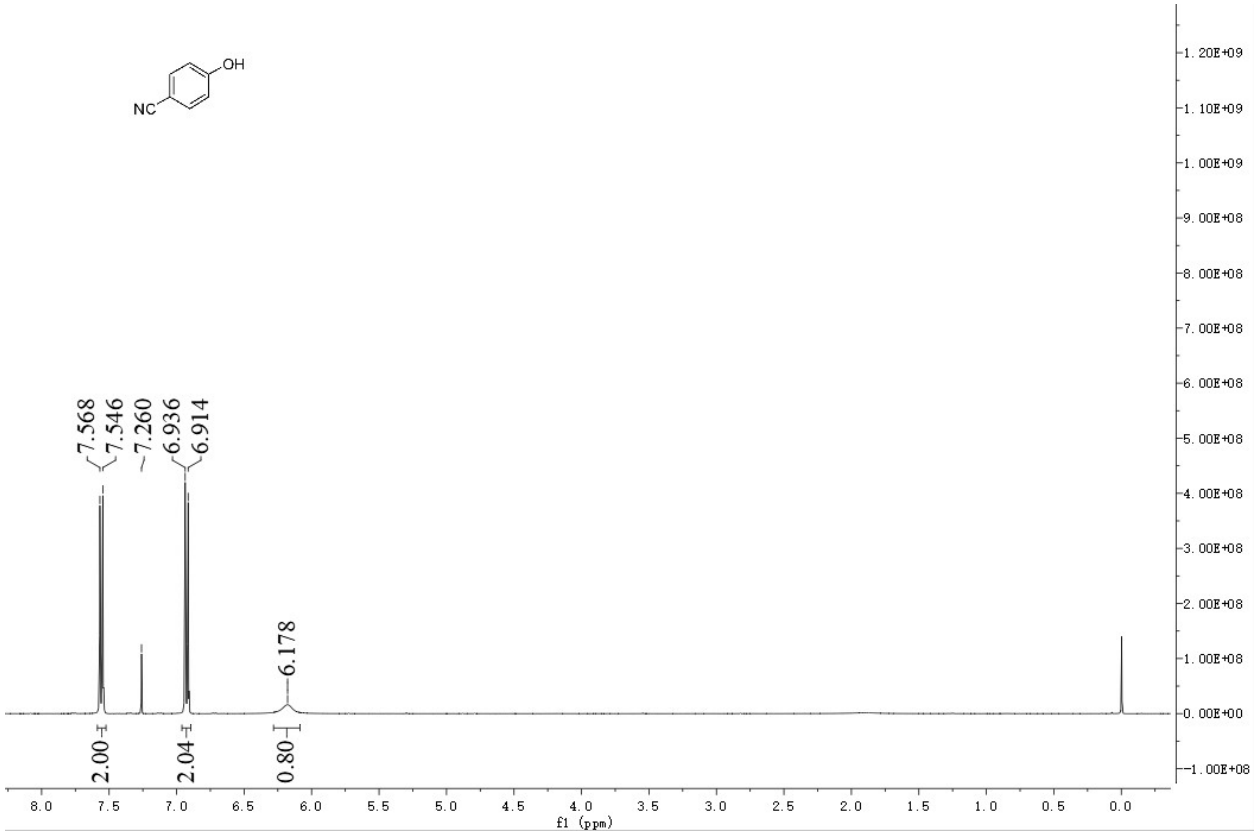
4-(1,2-Dimethyl-1*H*-indol-3-yl)benzonitrile (38)



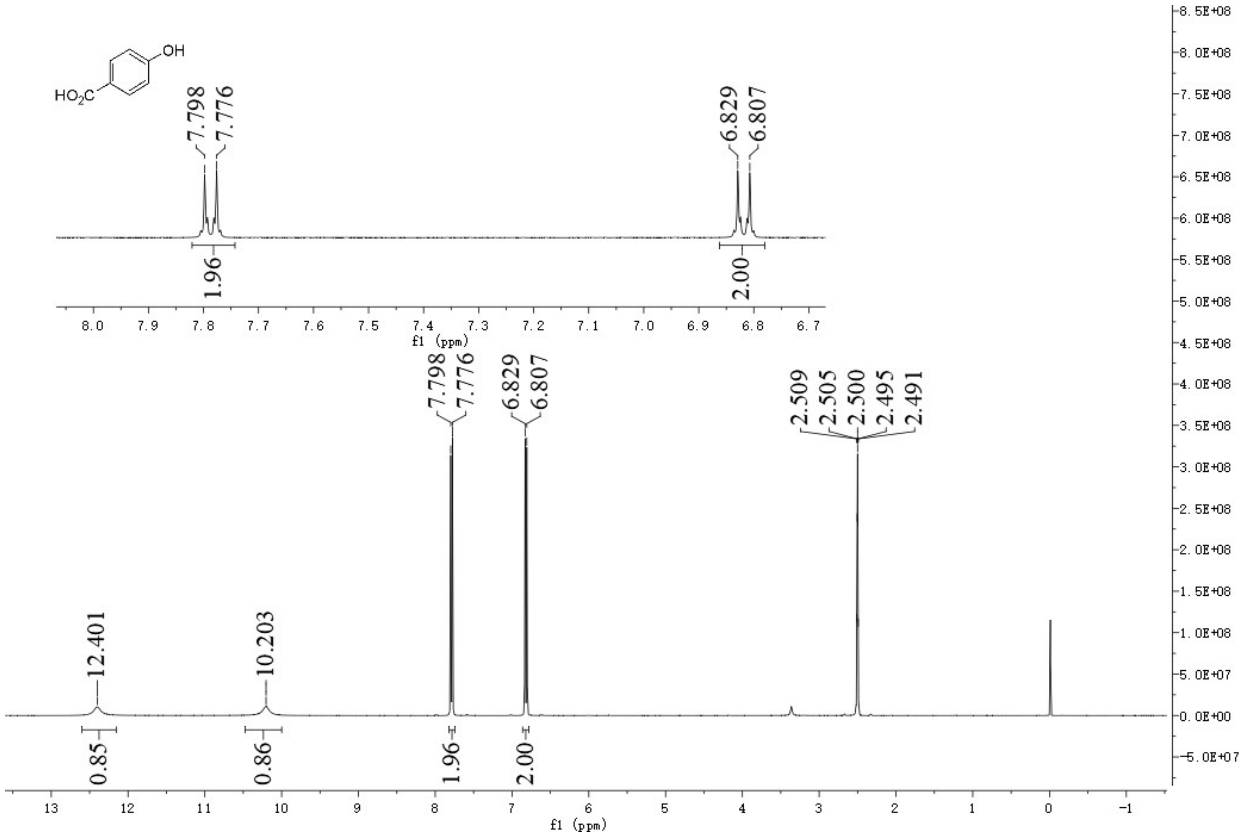
3-(4-Methoxyphenyl)-1,2-dimethyl-1*H*-indole (39)



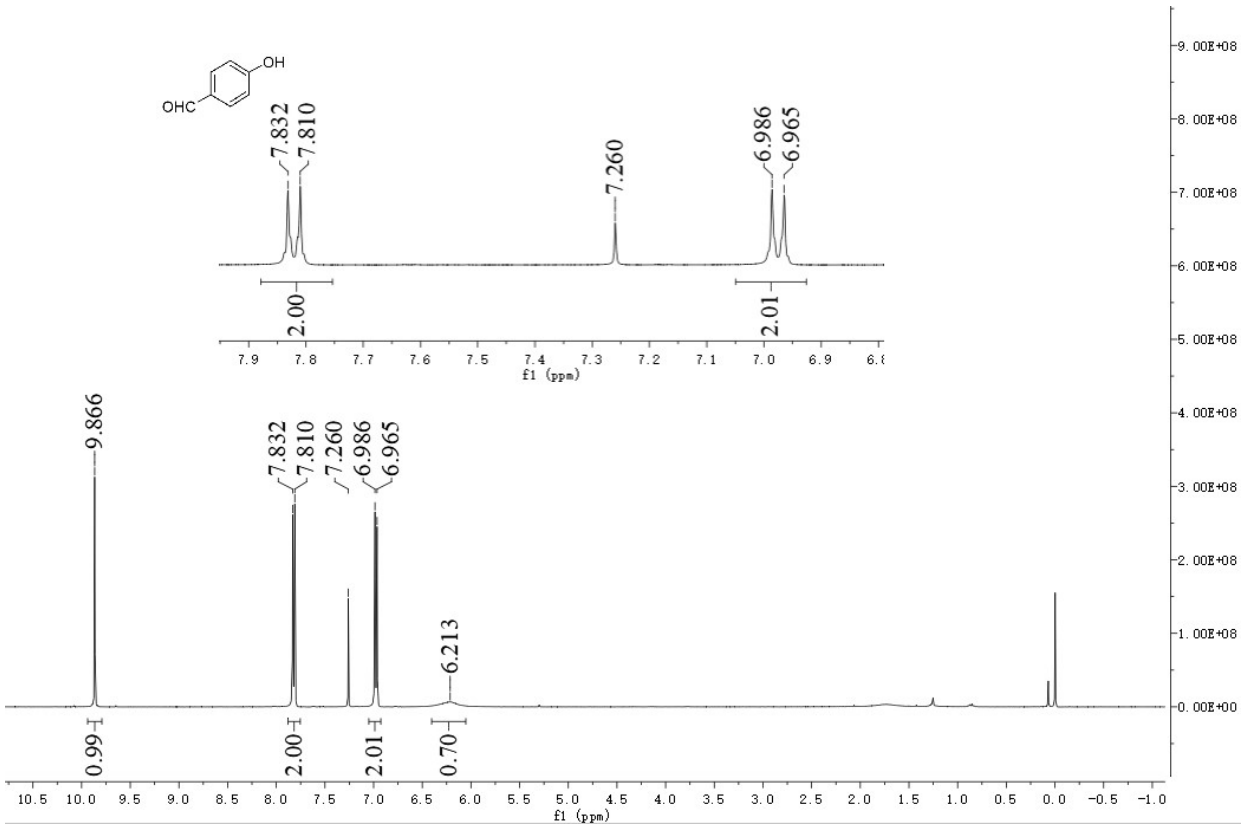
4-Hydroxybenzonitrile (40)



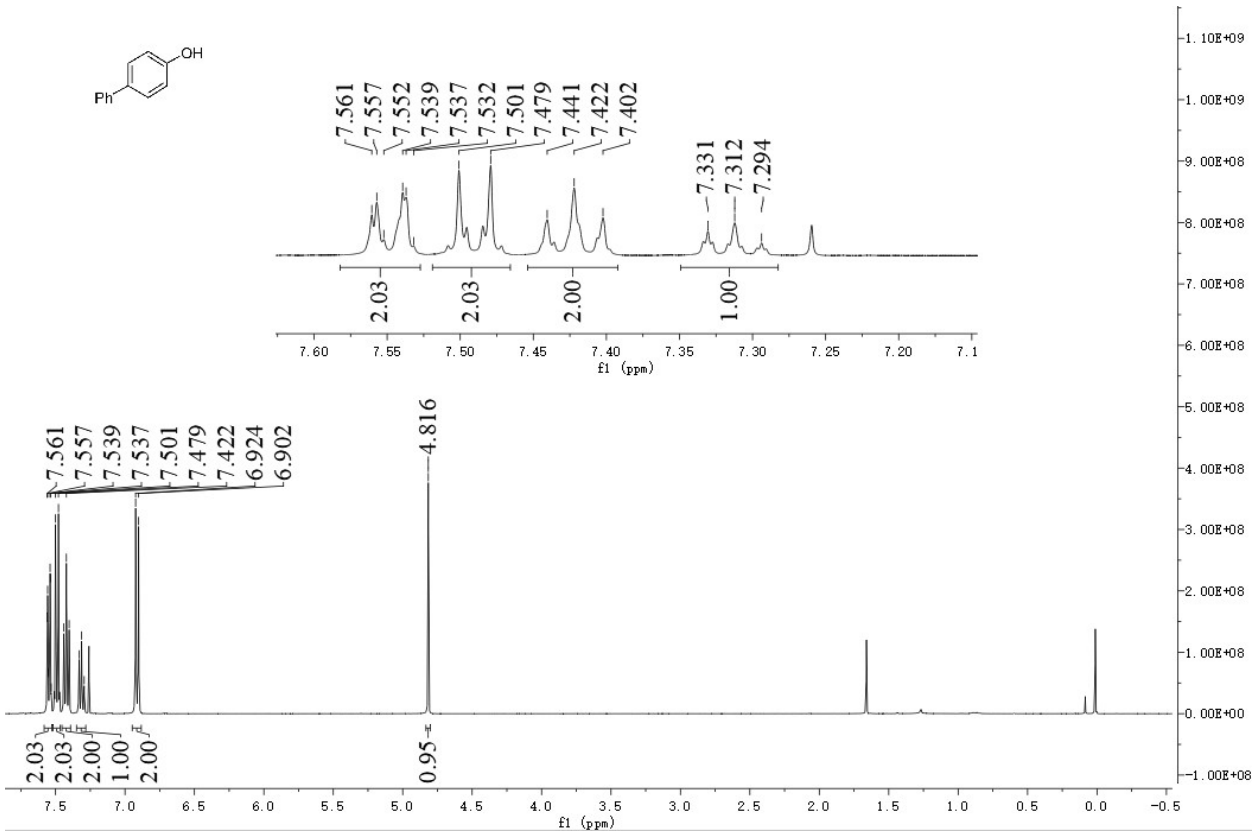
4-Hydroxybenzoic acid (41)



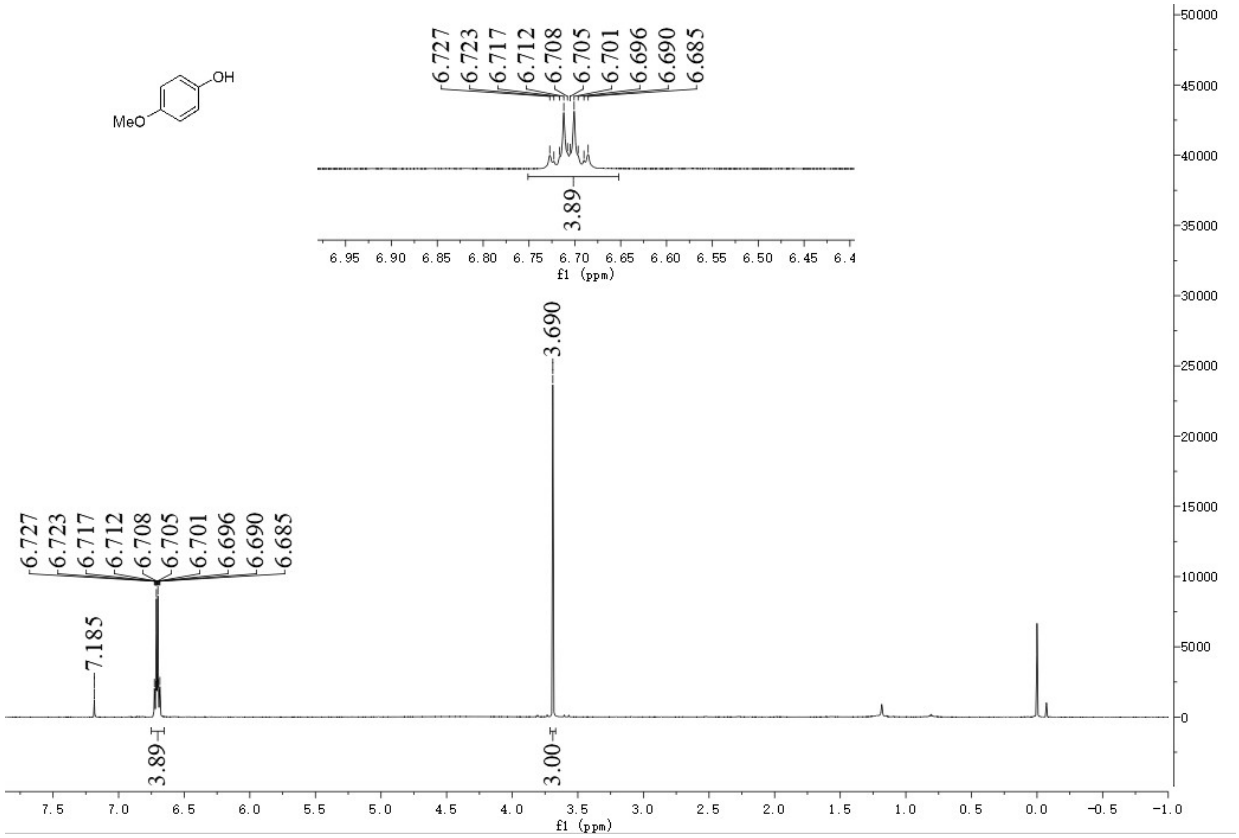
4-Hydroxybenzaldehyde (42)



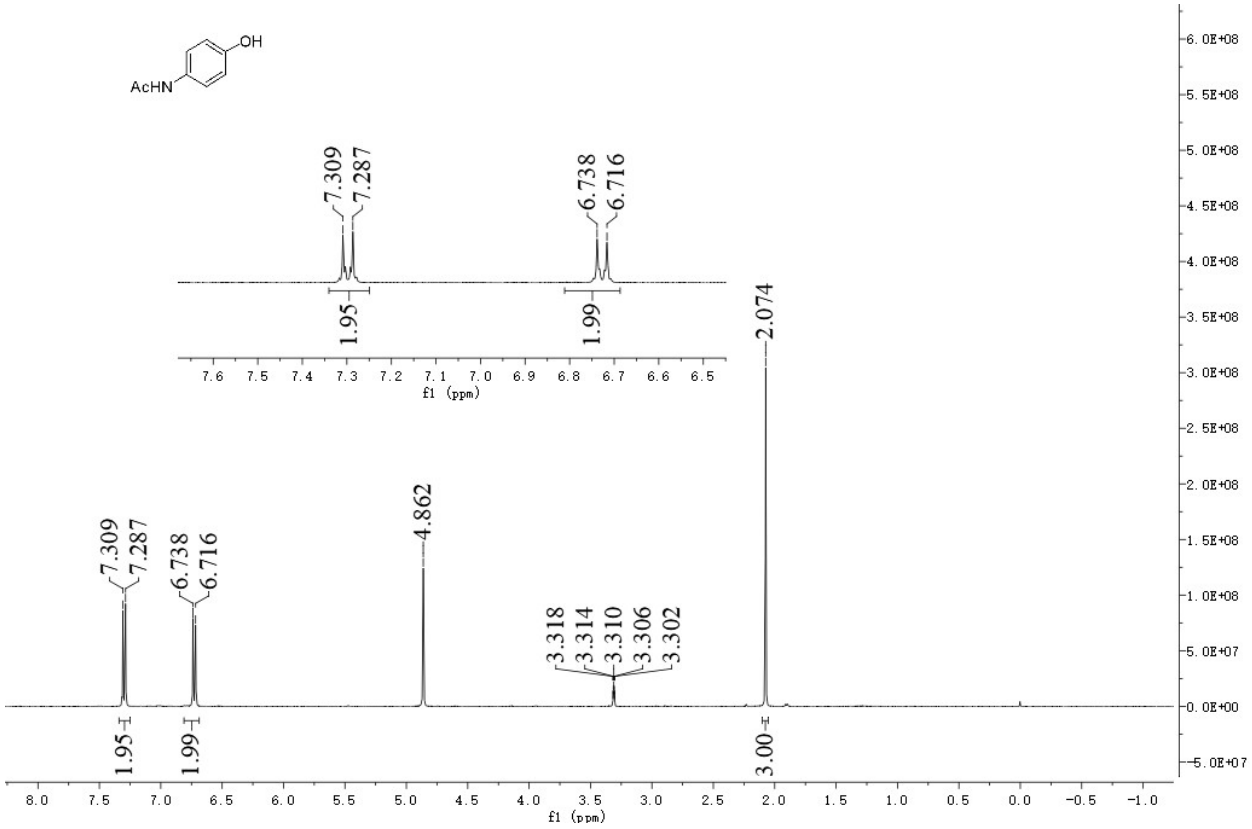
[1,1'-Biphenyl]-4-ol (43)



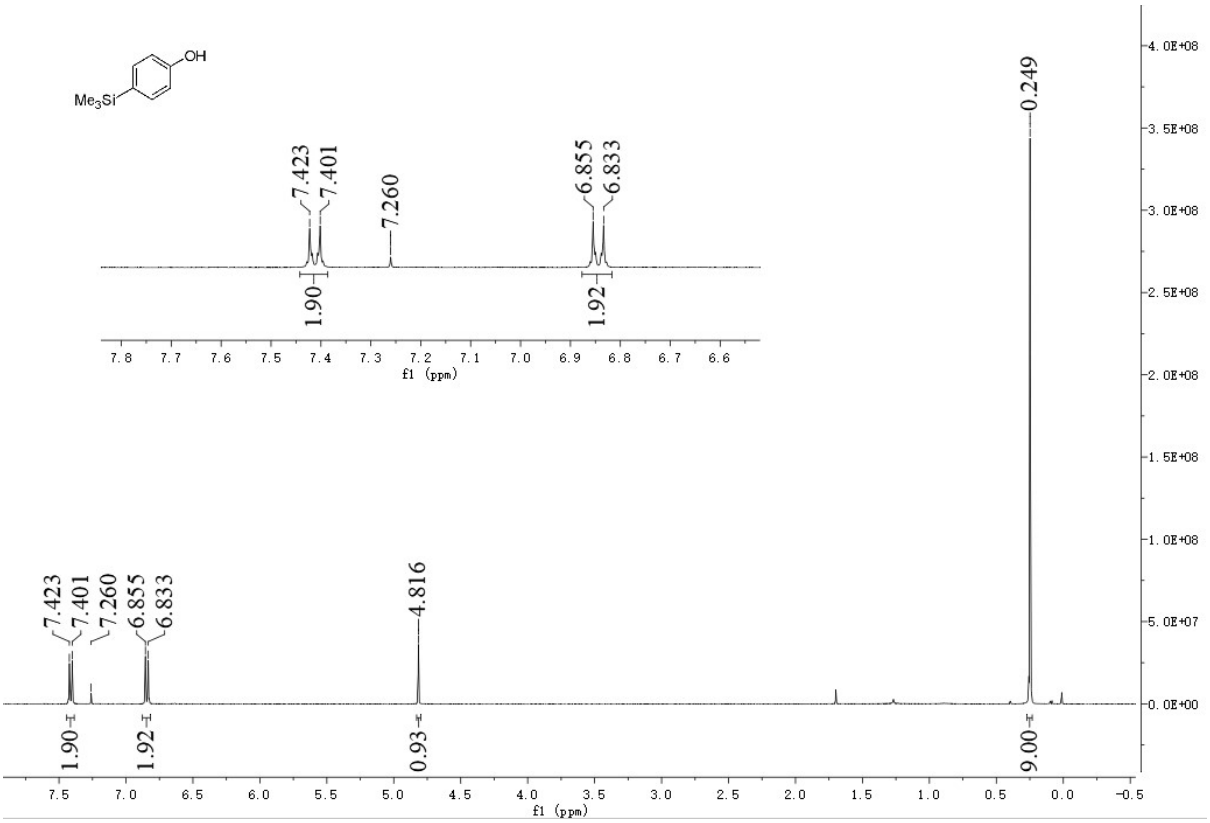
4-Methoxyphenol (44)



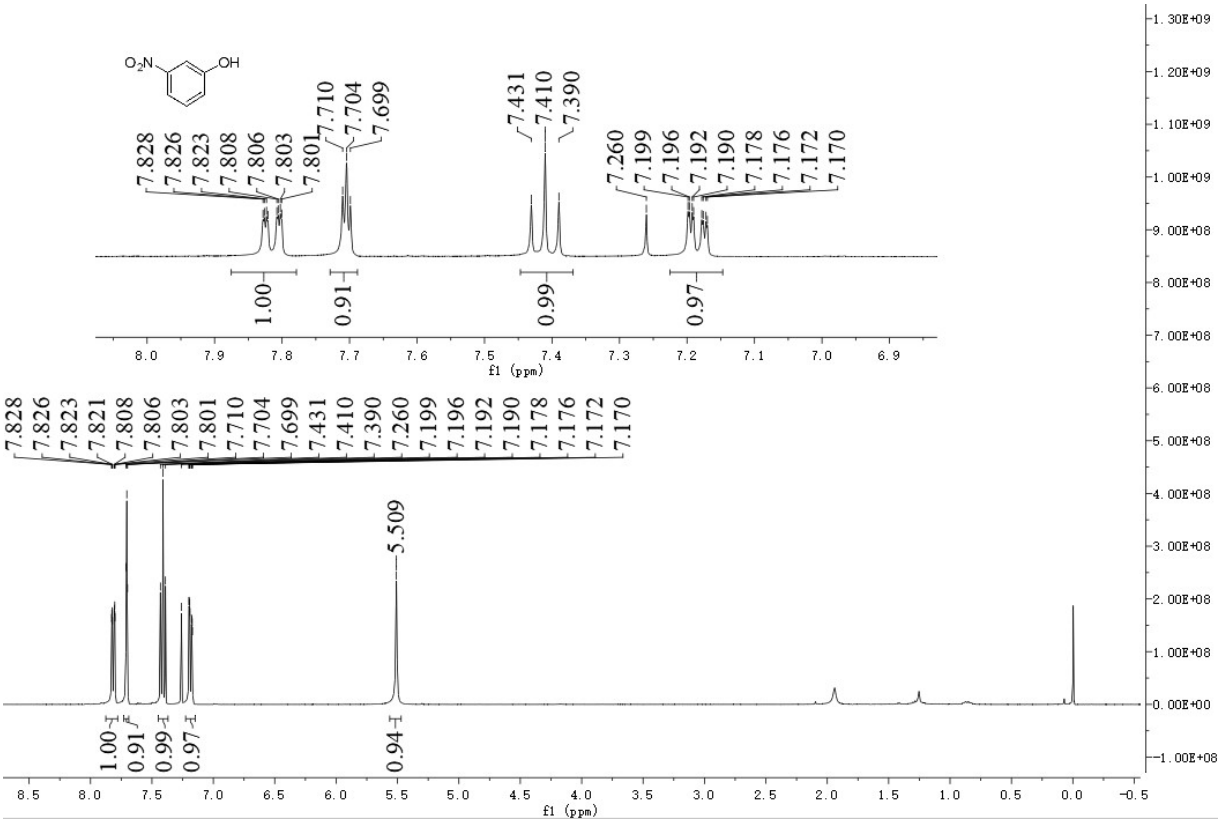
N-(4-Hydroxyphenyl)acetamide (45)



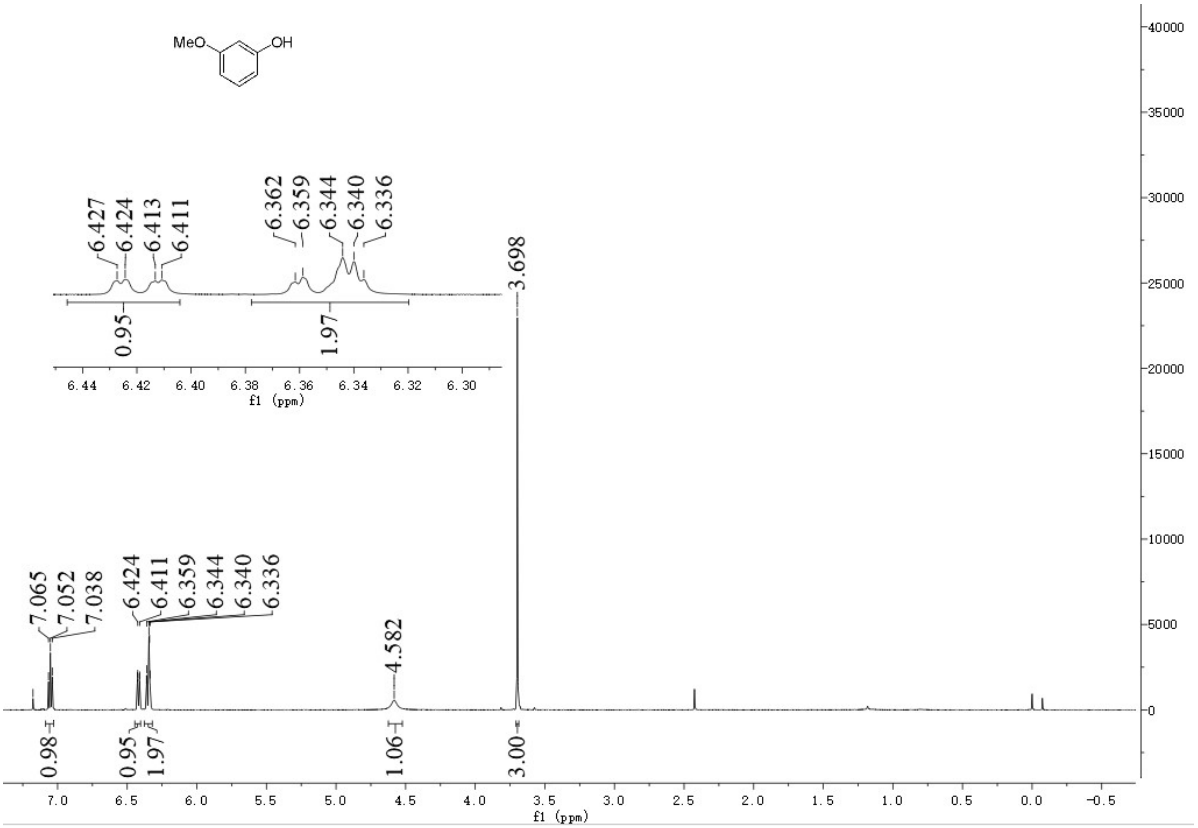
4-(Trimethylsilyl)phenol (46)



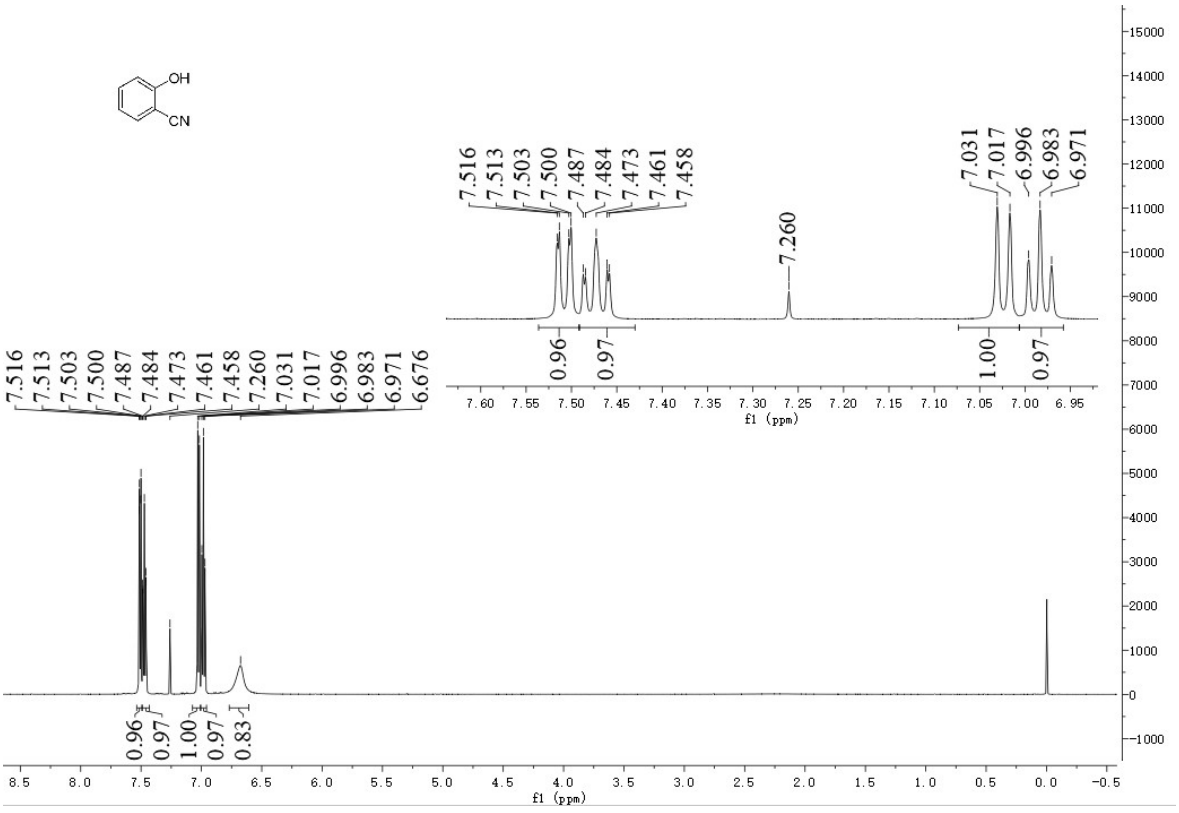
3-Nitrophenol (47)



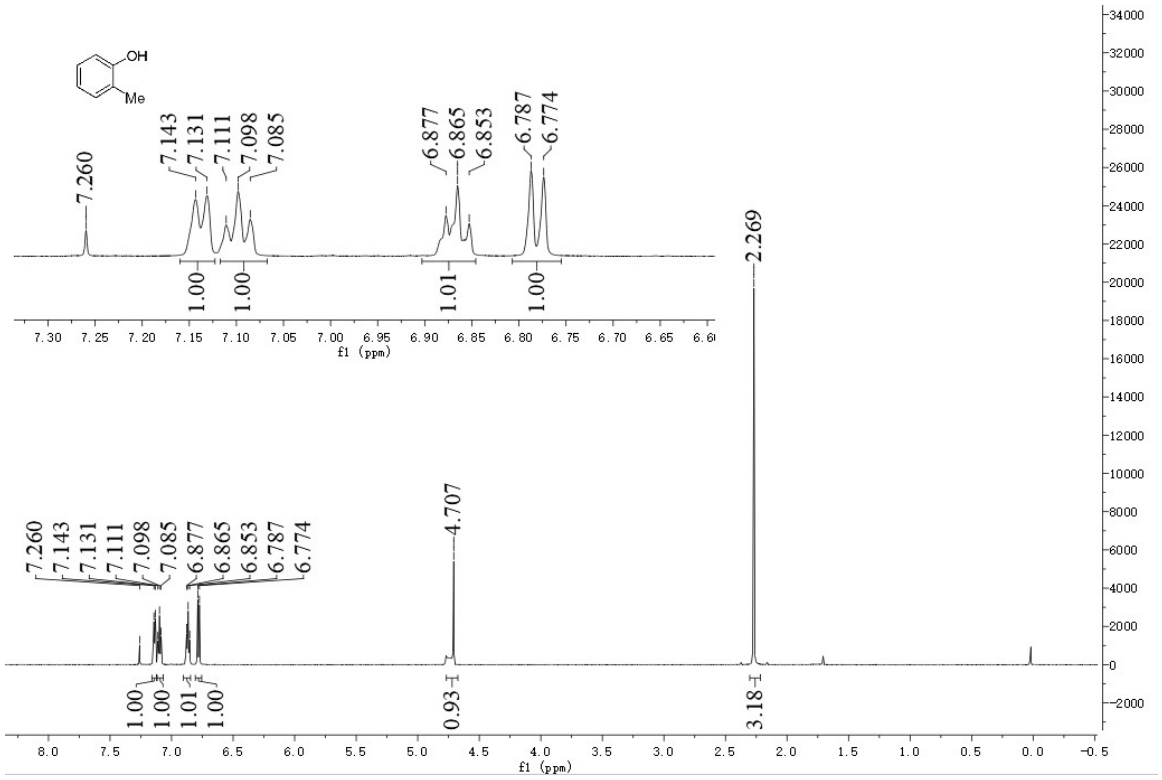
3-Methoxyphenol (48)



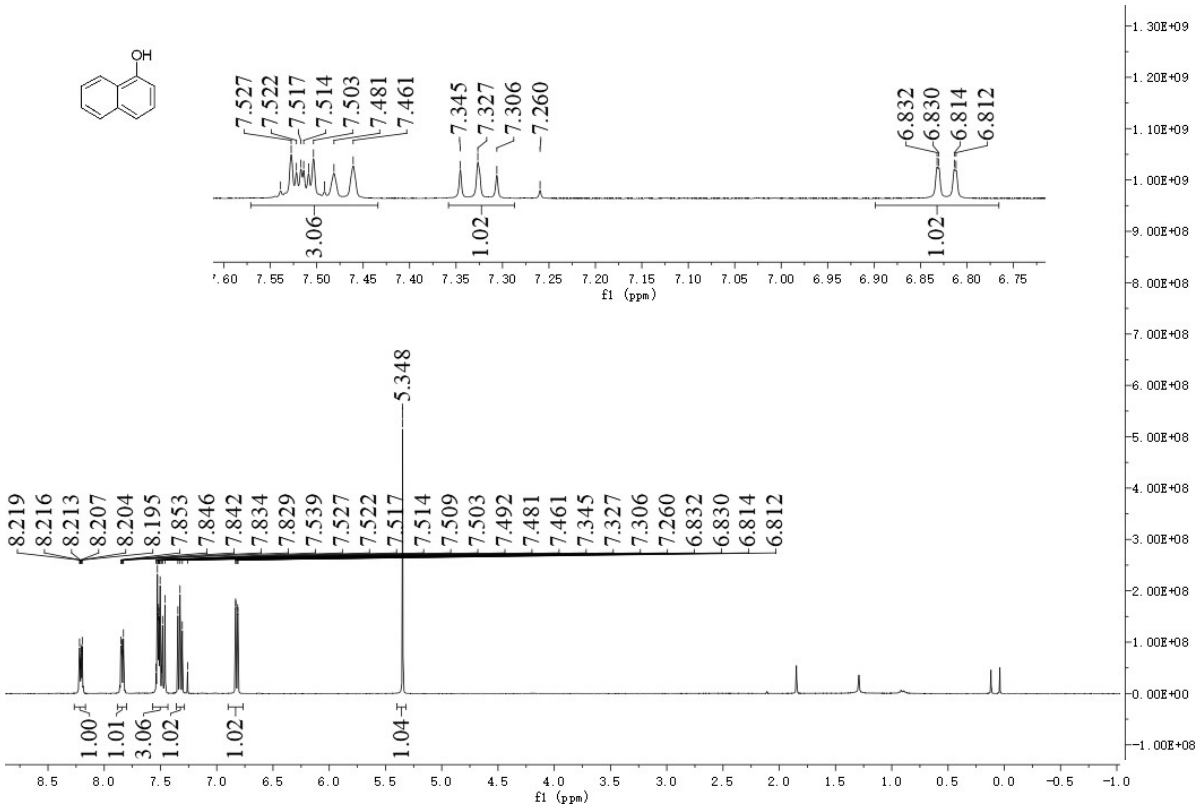
2-Hydroxybenzonitrile (49)



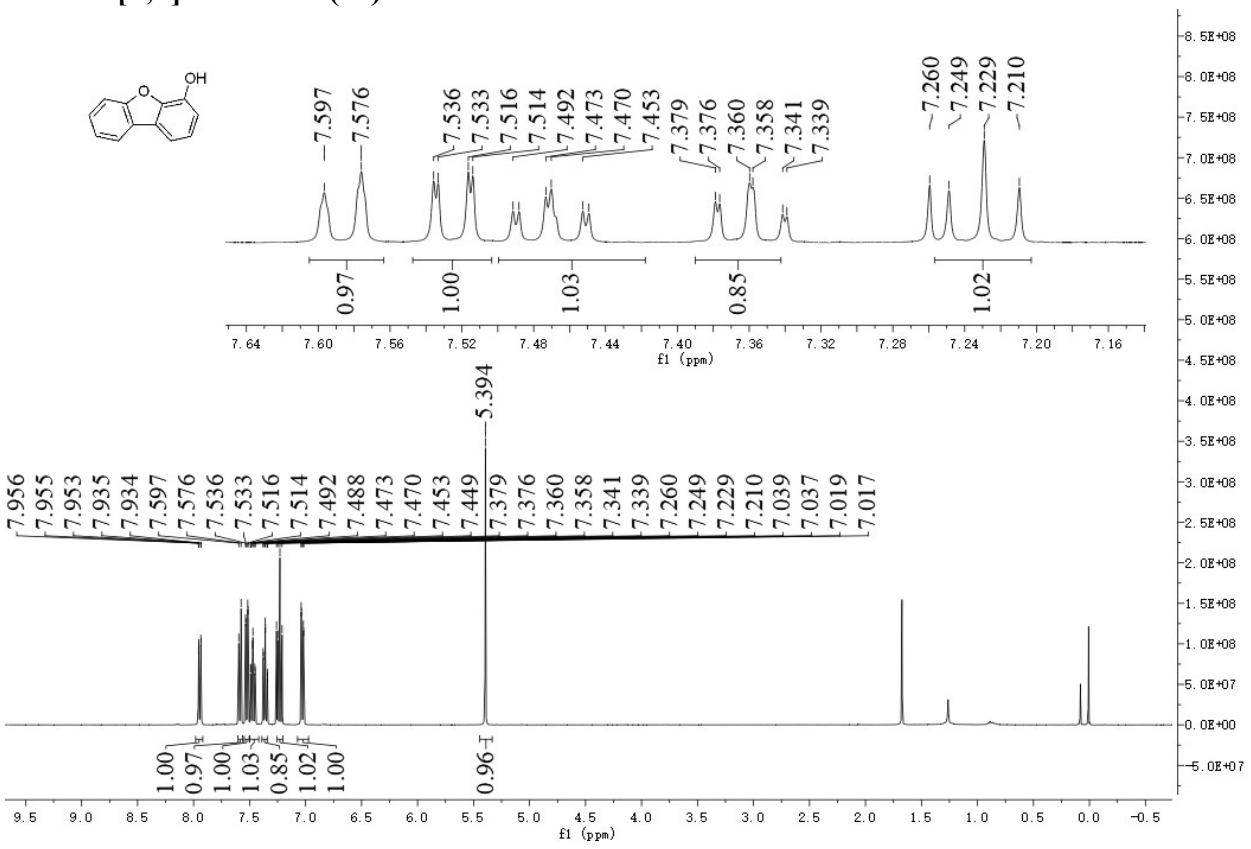
o-Cresol (50)



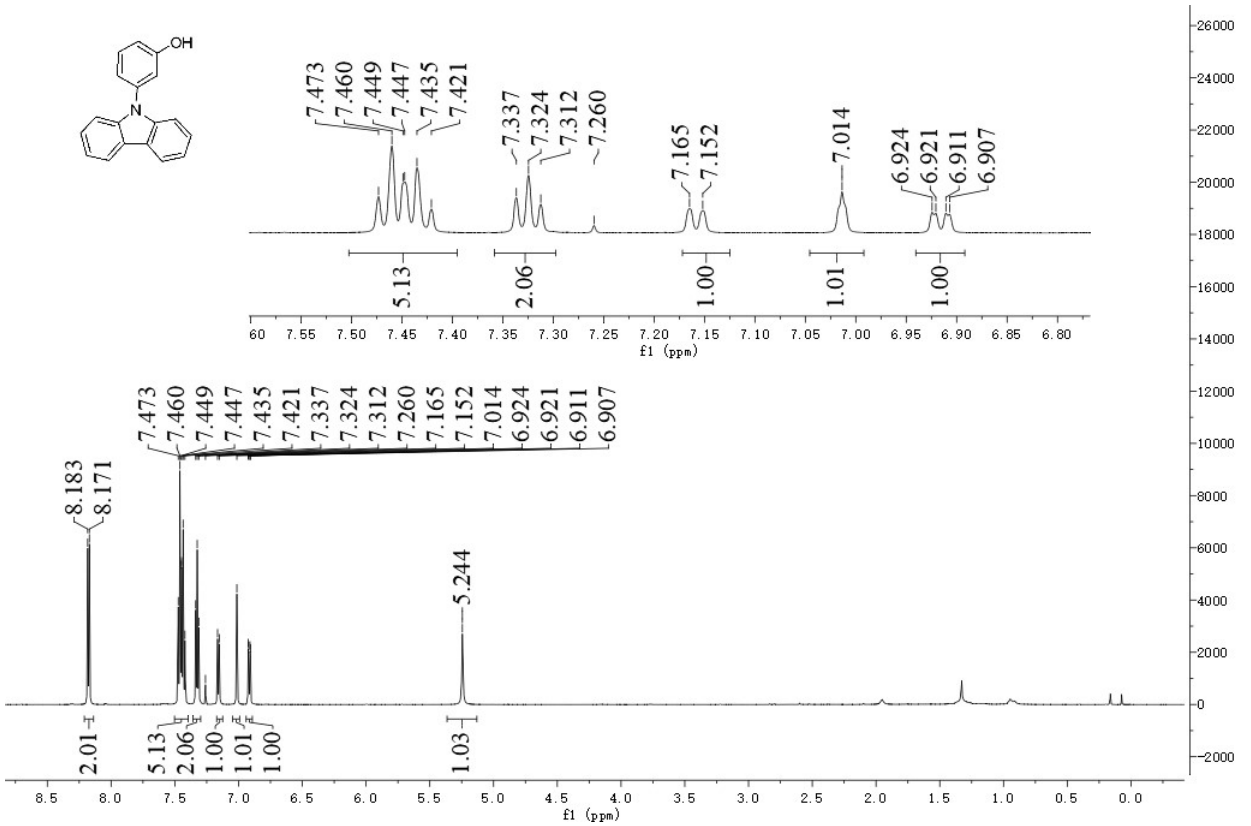
Naphthalen-1-ol (51)



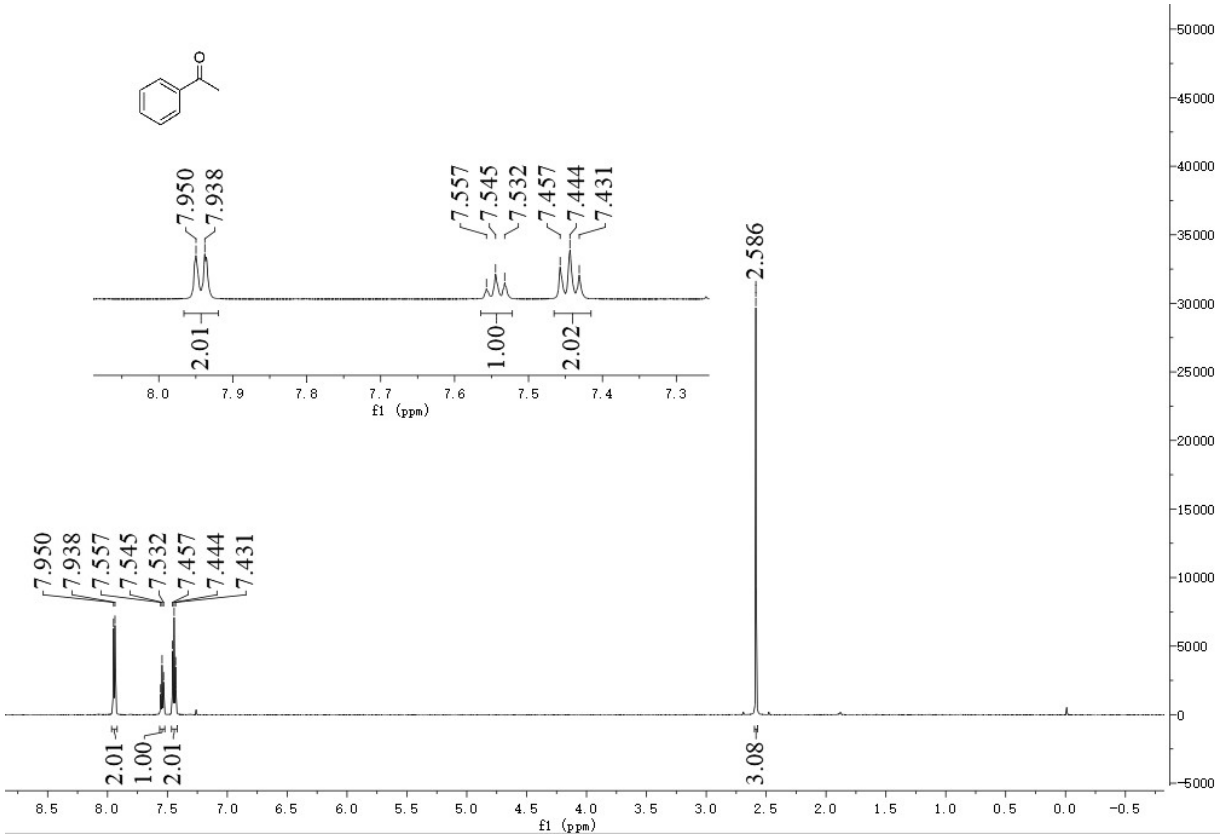
Dibenzo[b,d]furan-4-ol (52)



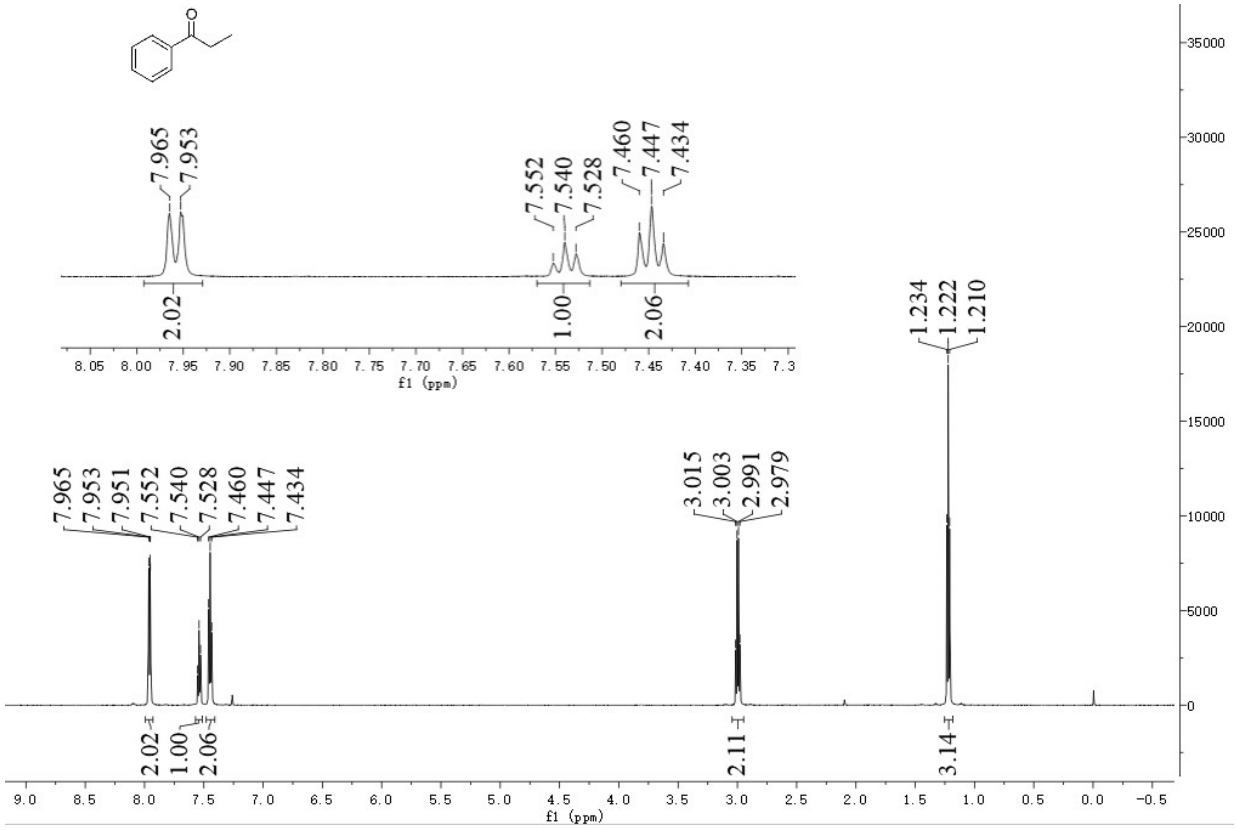
3-(9*H*-Carbazol-9-yl)phenol (53)



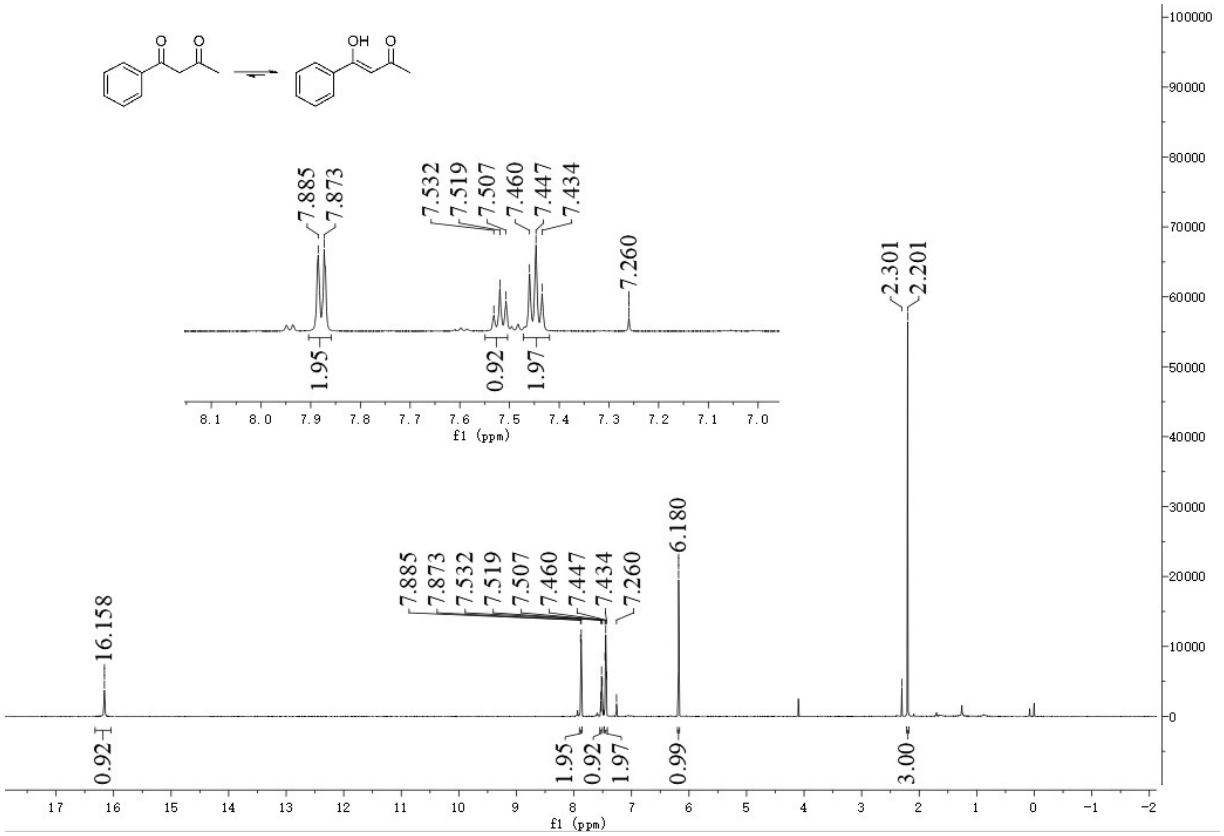
Acetophenone (54)



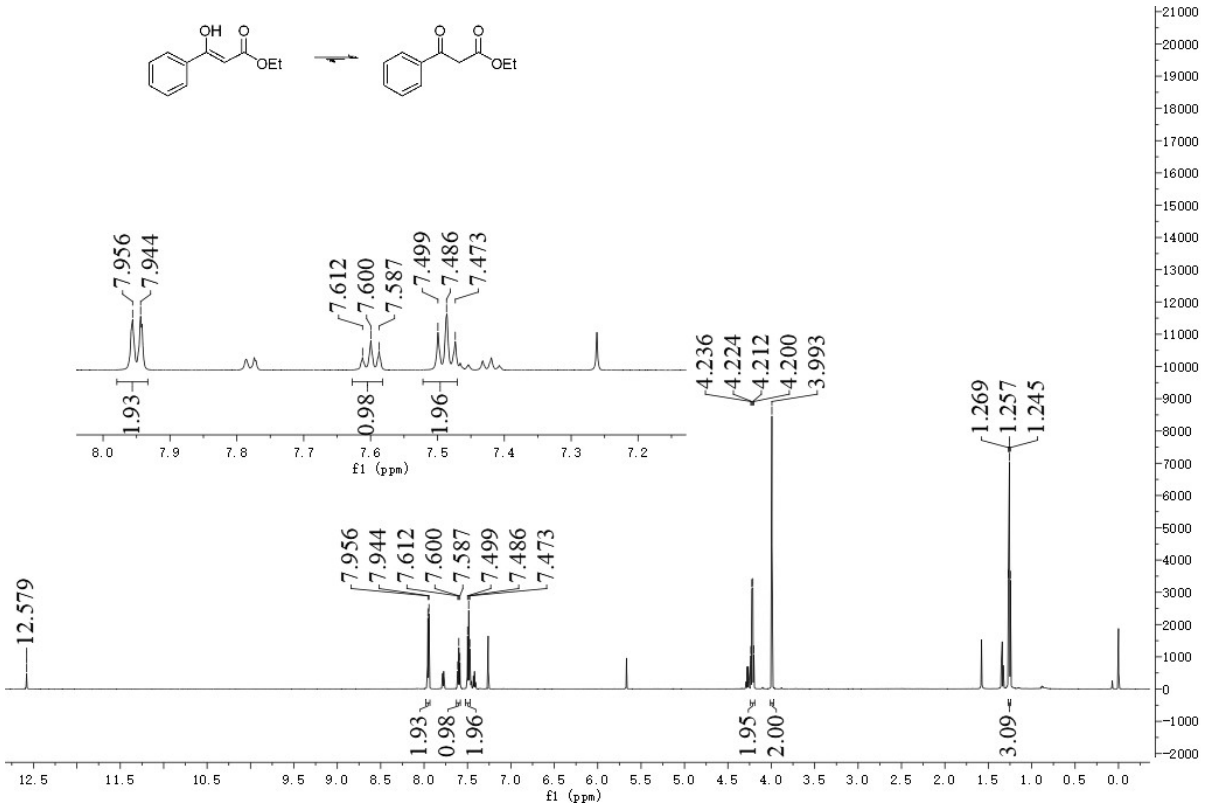
Propiophenone (55)



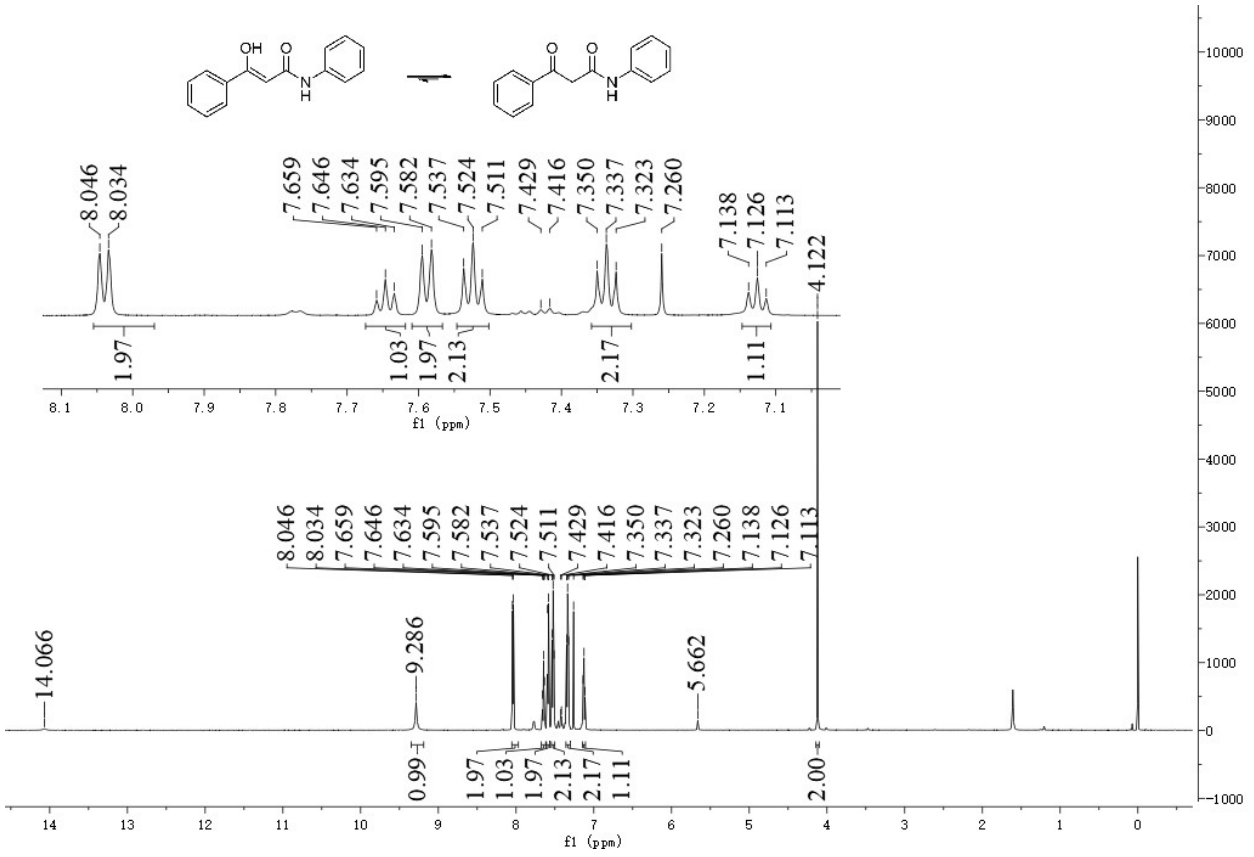
1-Phenylbutane-1,3-dione (56)



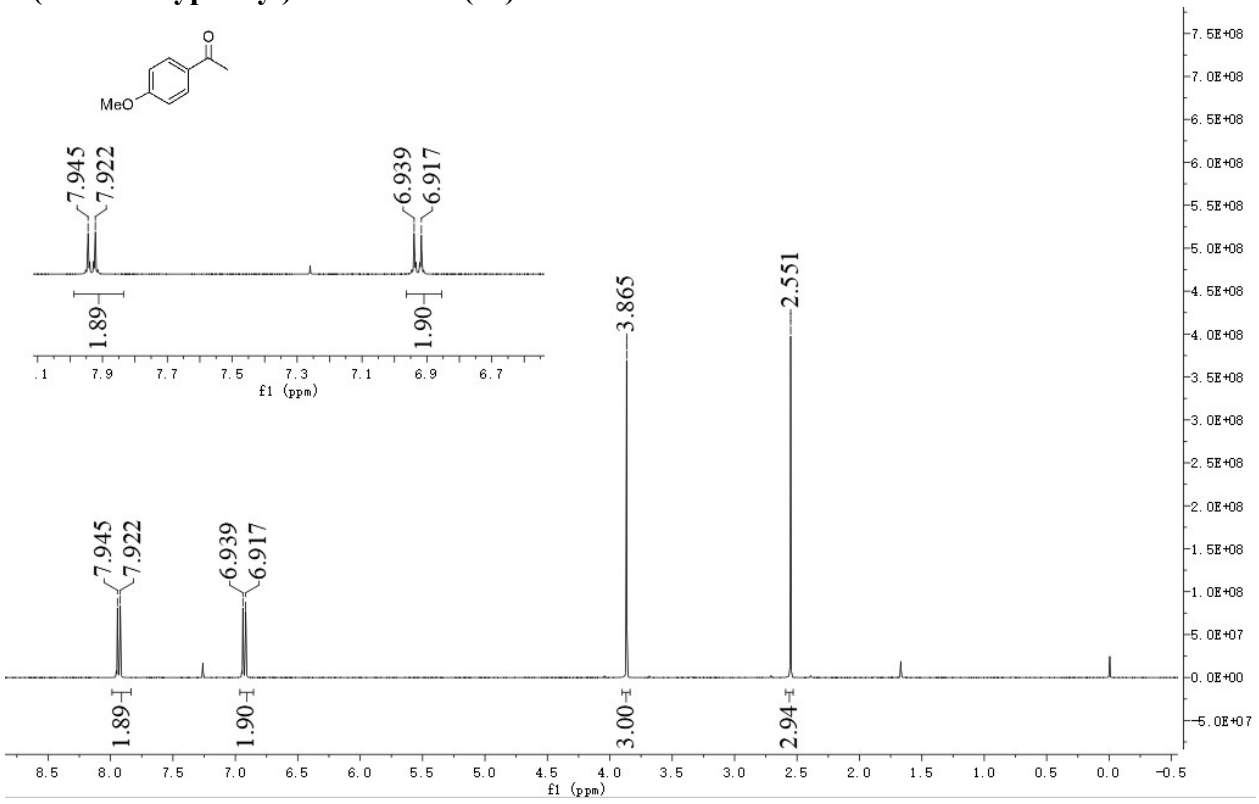
Ethyl-3-oxo-3-phenylpropanoate (57)



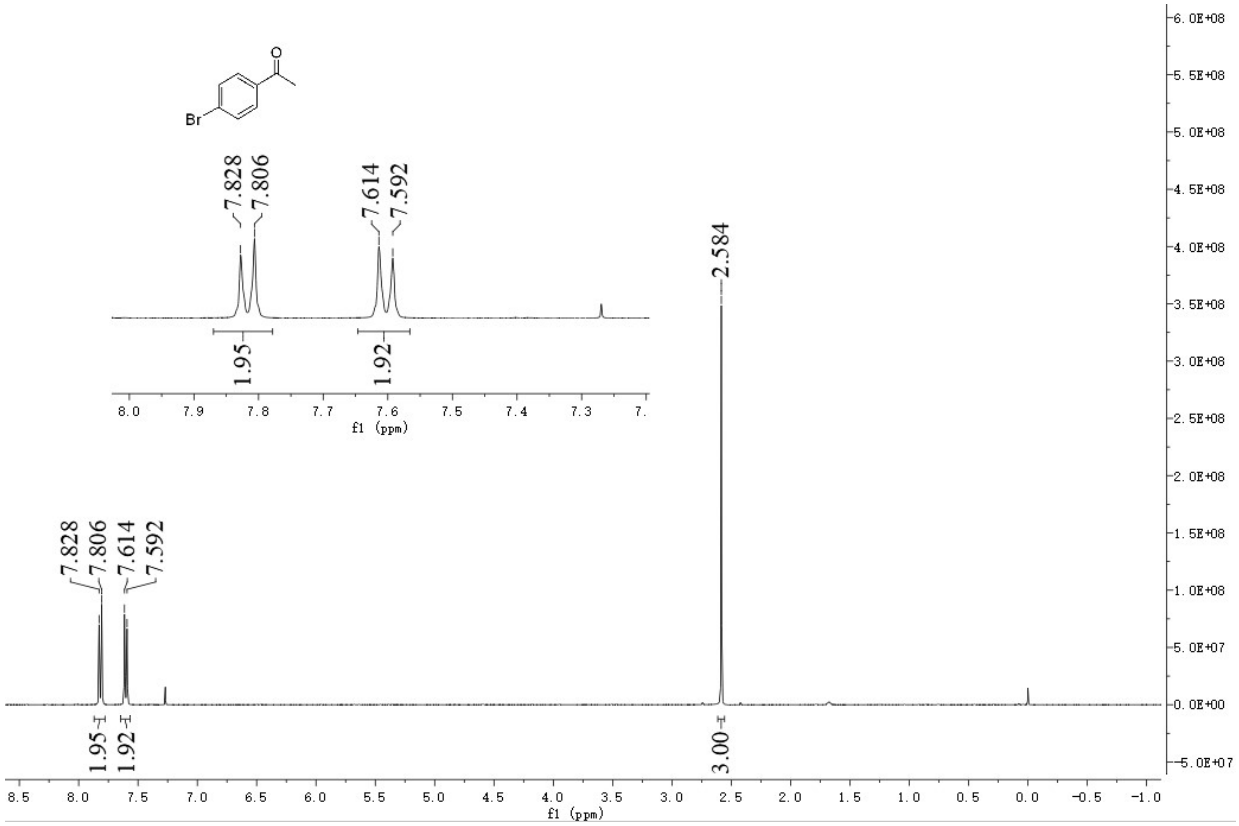
3-Oxo-*N*,3-diphenylpropanamide (58)



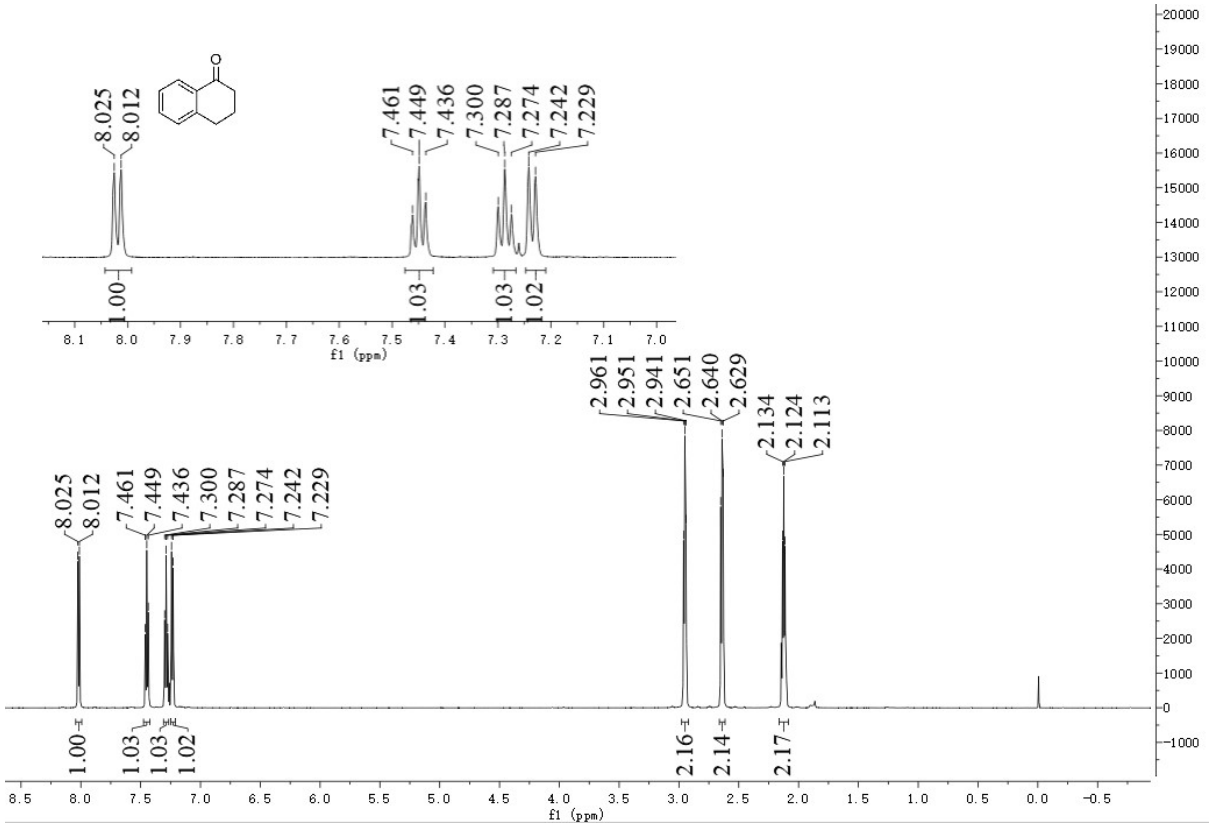
1-(4-Methoxyphenyl)ethan-1-one (59)



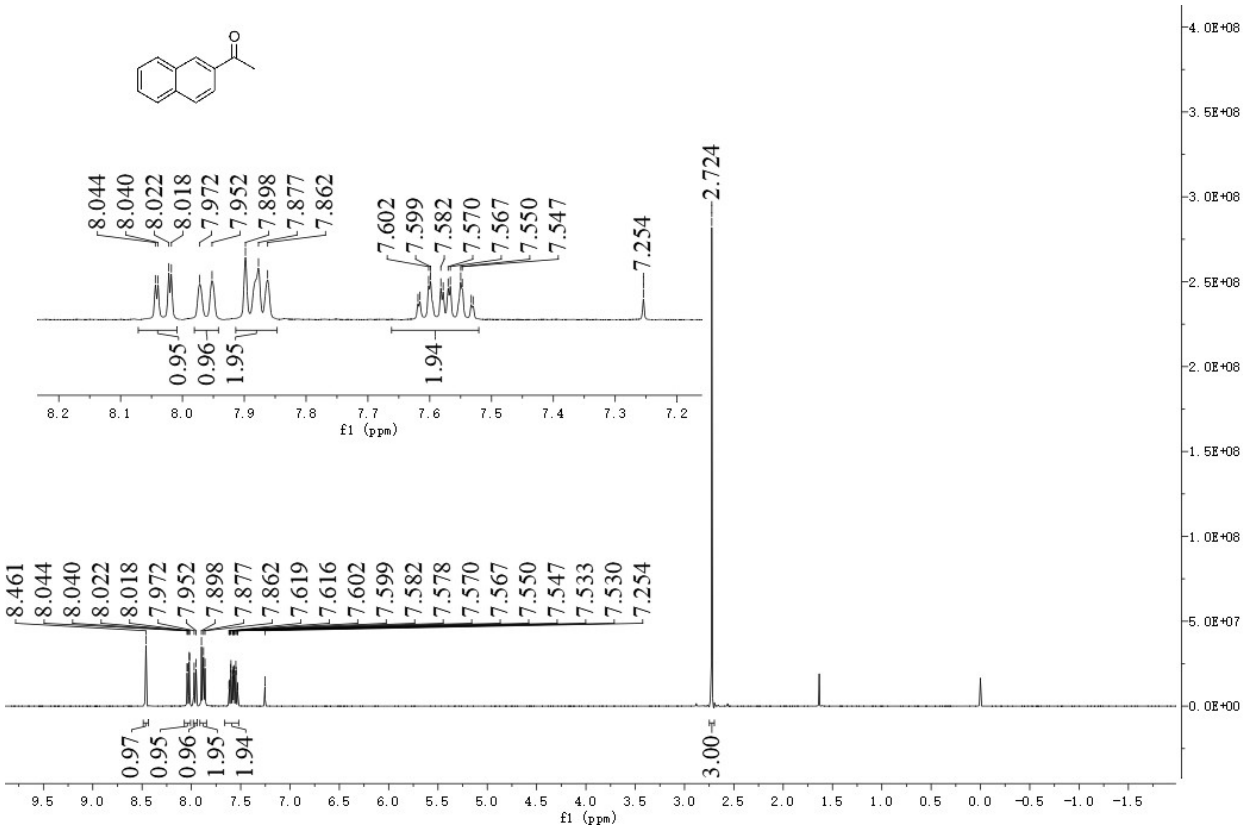
1-(4-Bromophenyl)ethan-1-one (60)



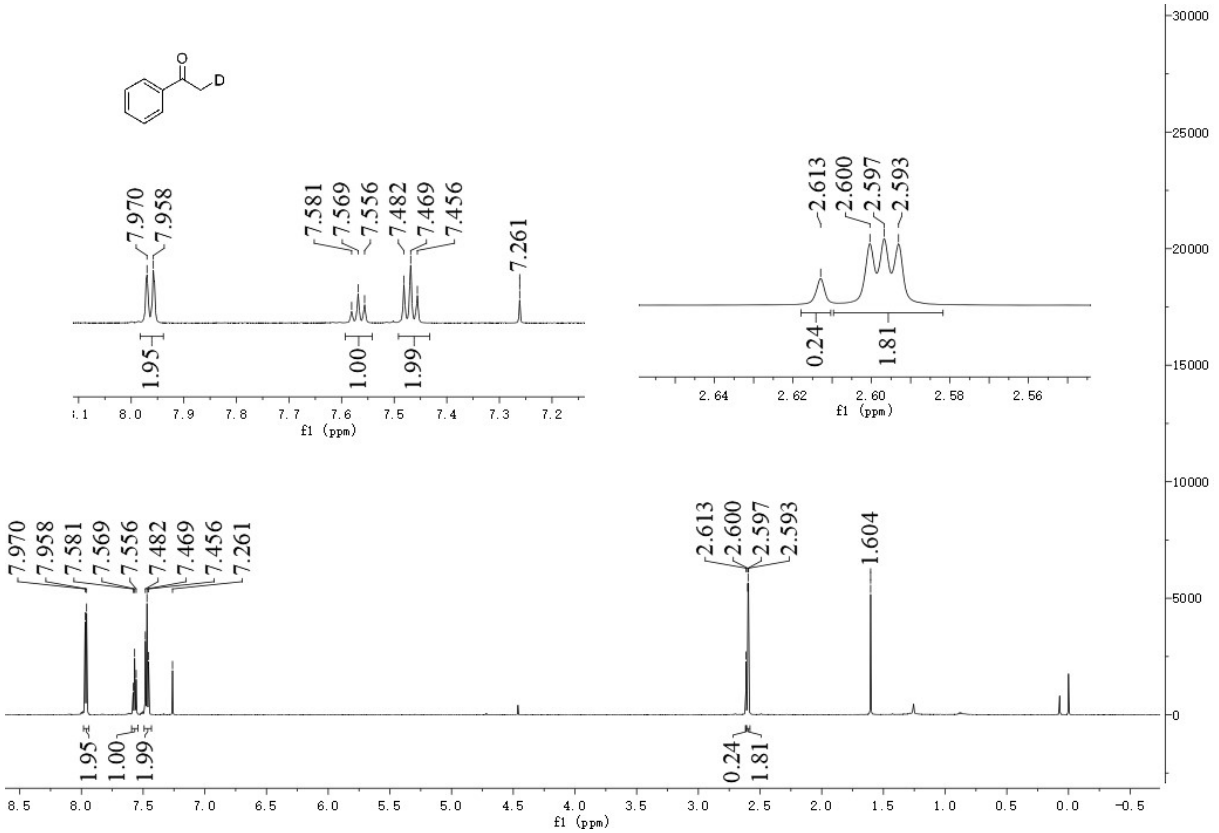
3,4-Dihydronaphthalen-1(2*H*)-one (61)

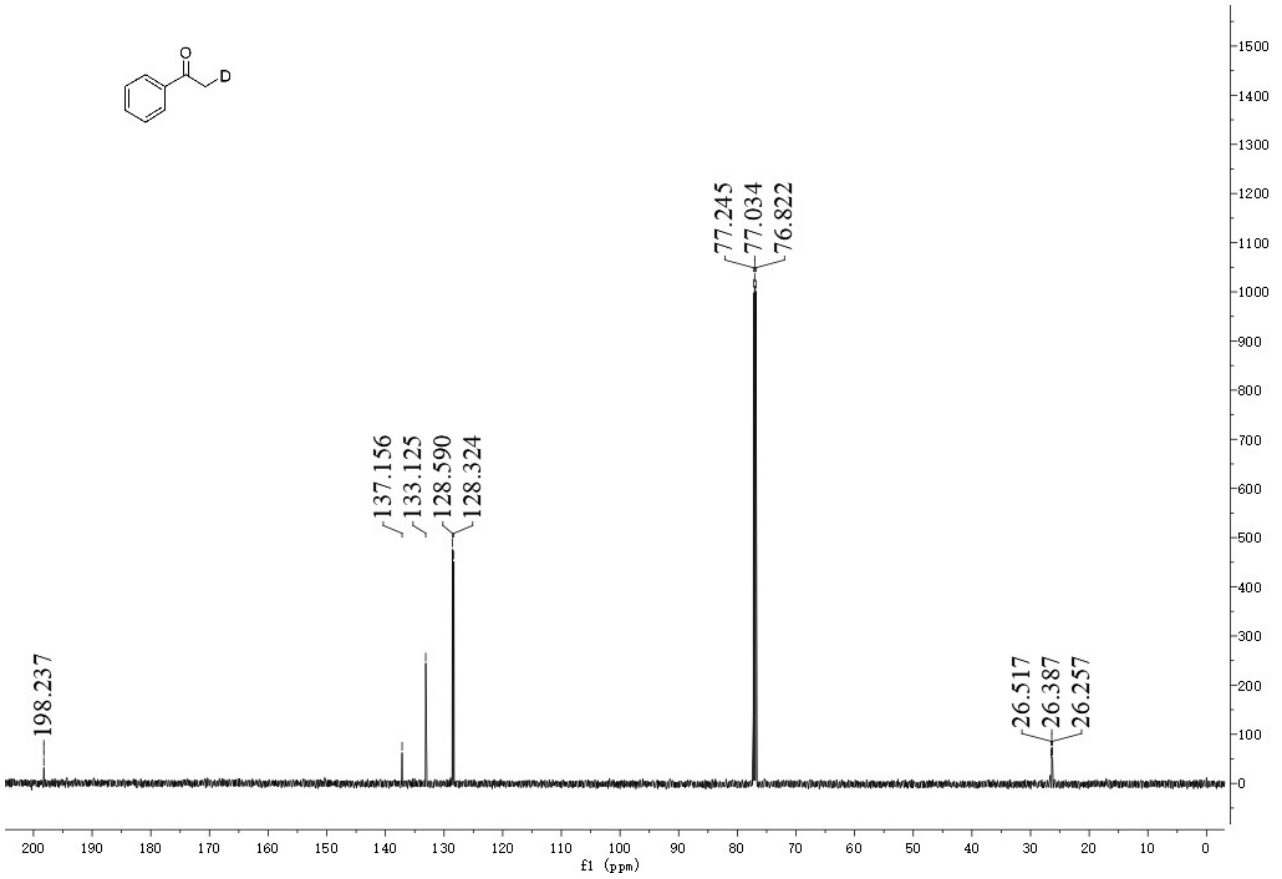


1-(Naphthalen-2-yl)ethan-1-one (62)

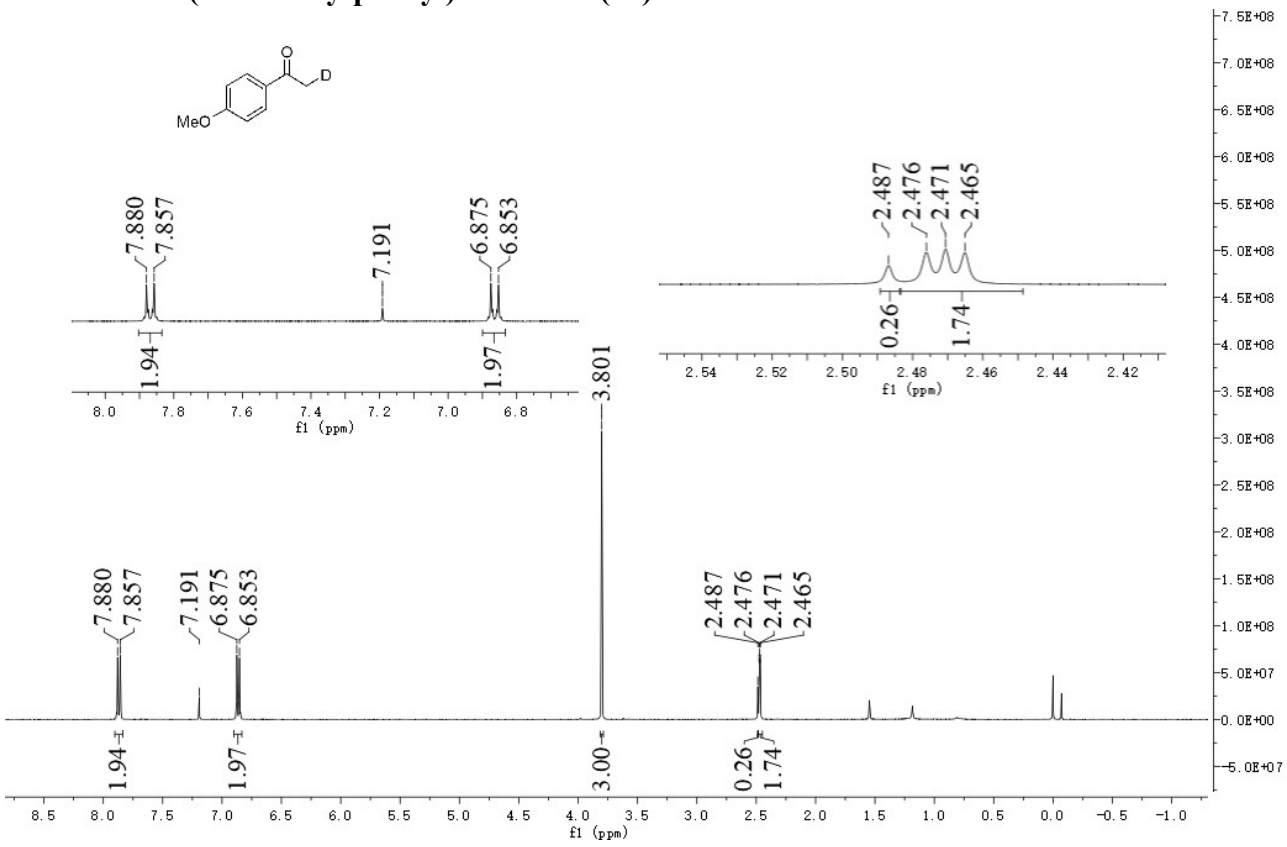


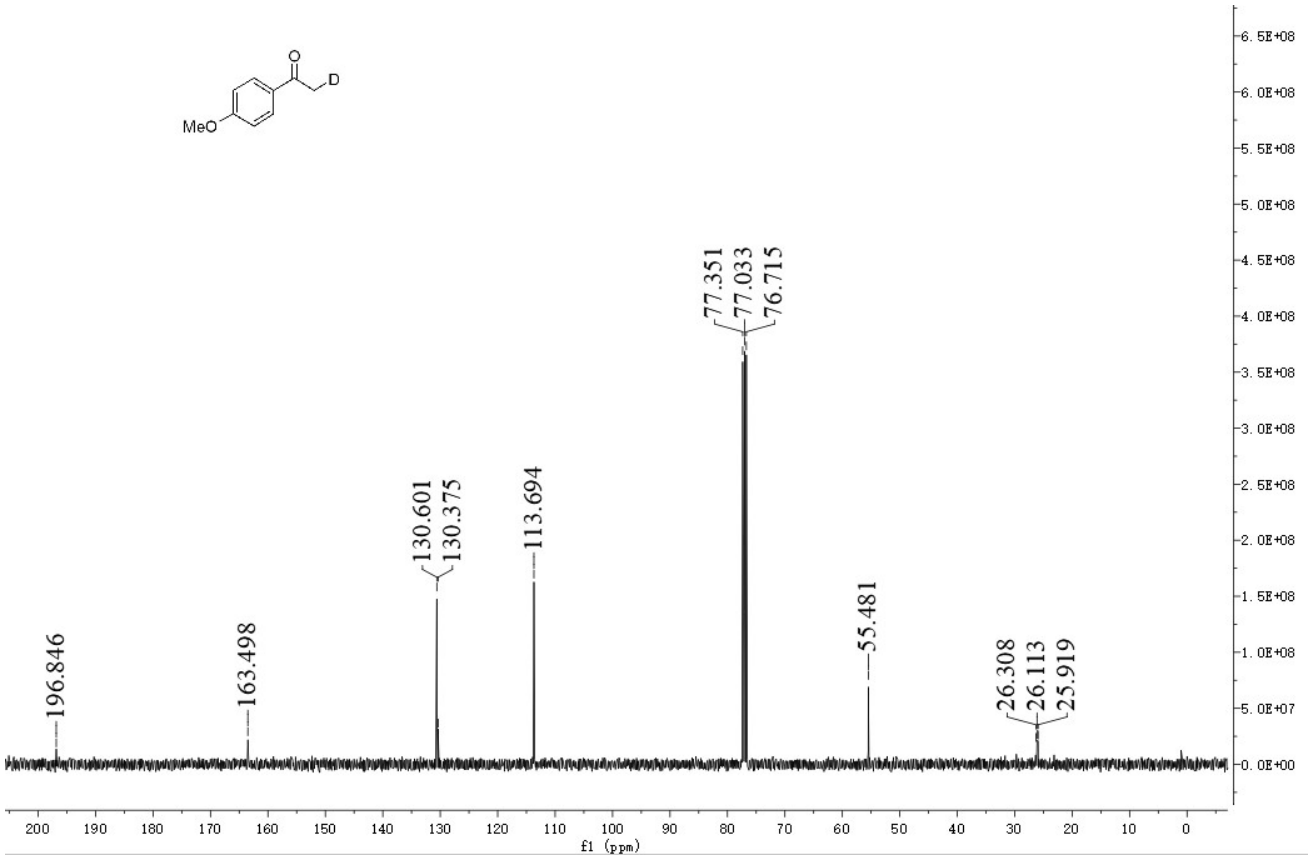
2-Deutero-1-phenylethanone (63)



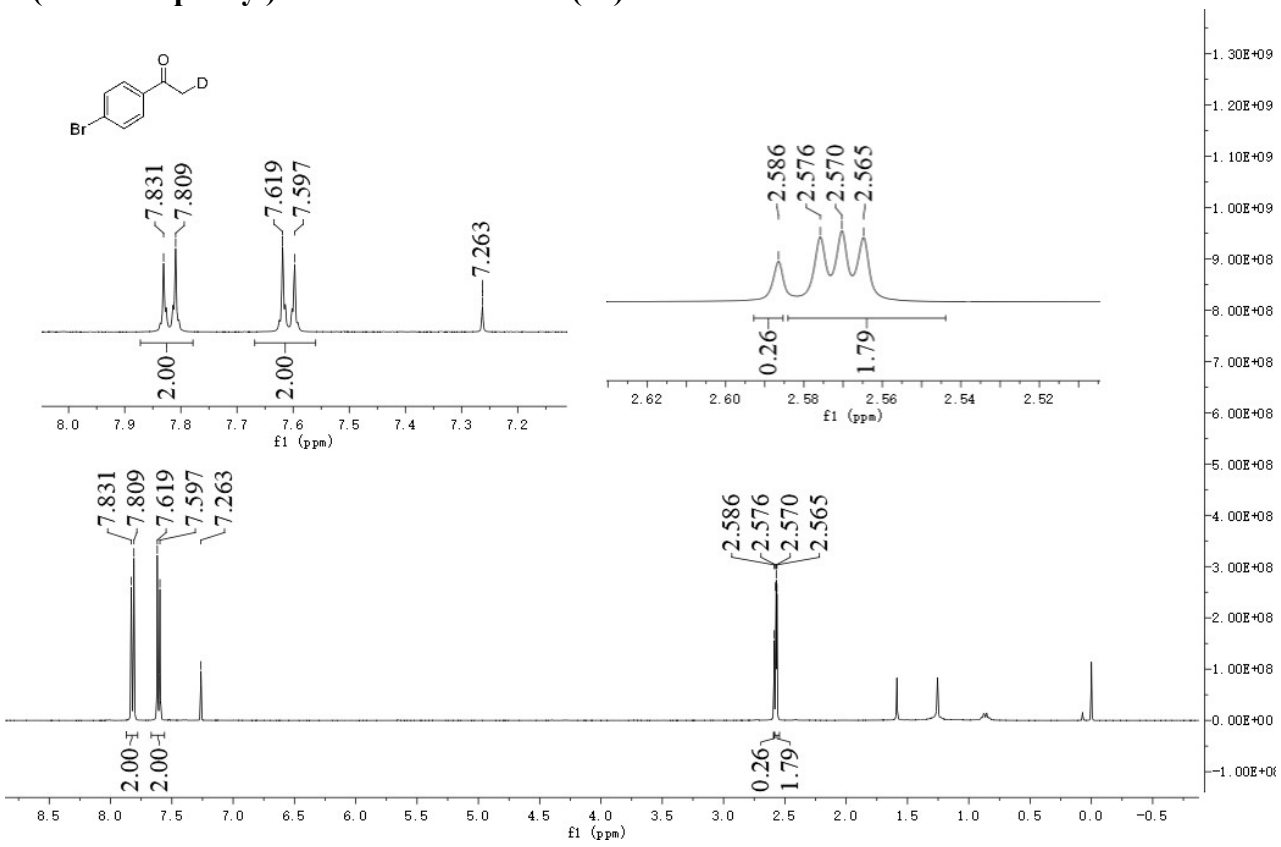


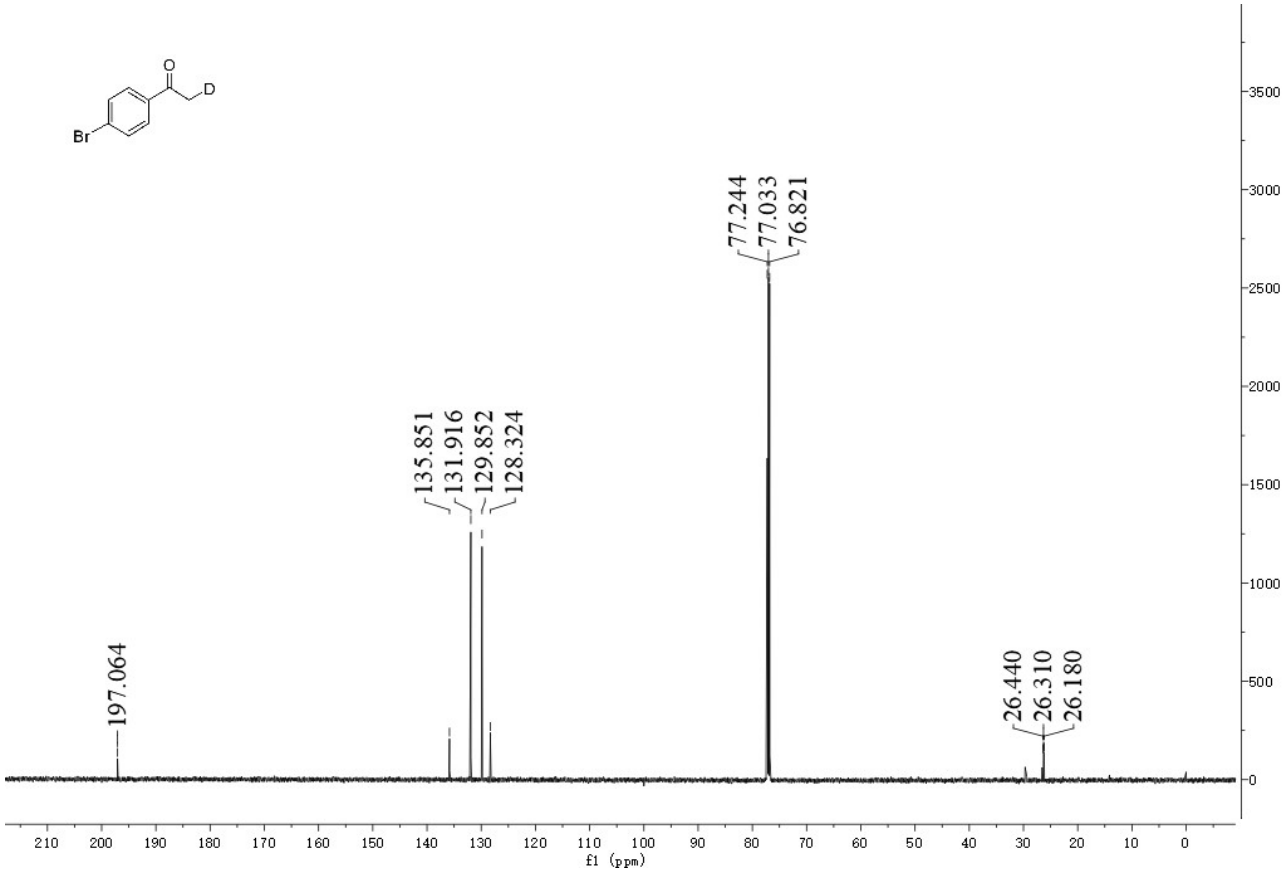
2-Deuterio-1-(4-methoxy-phenyl)-ethanone (64)



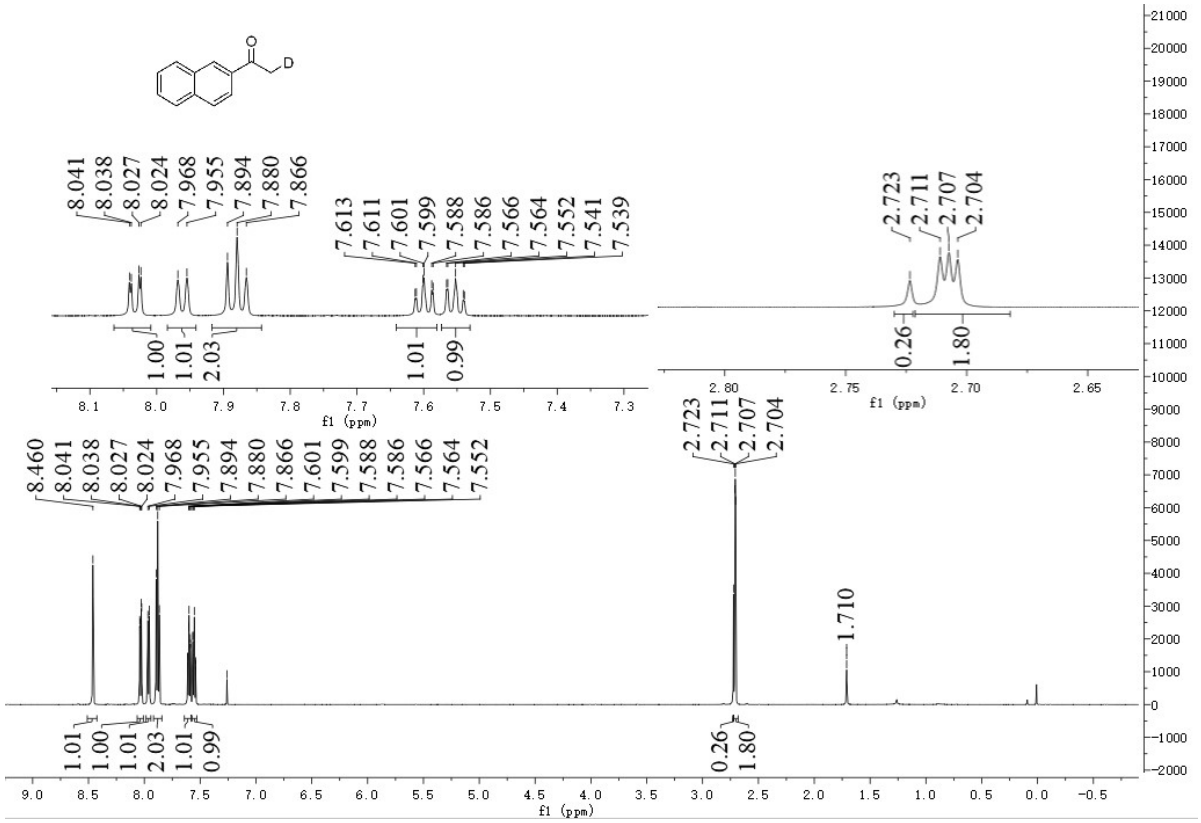


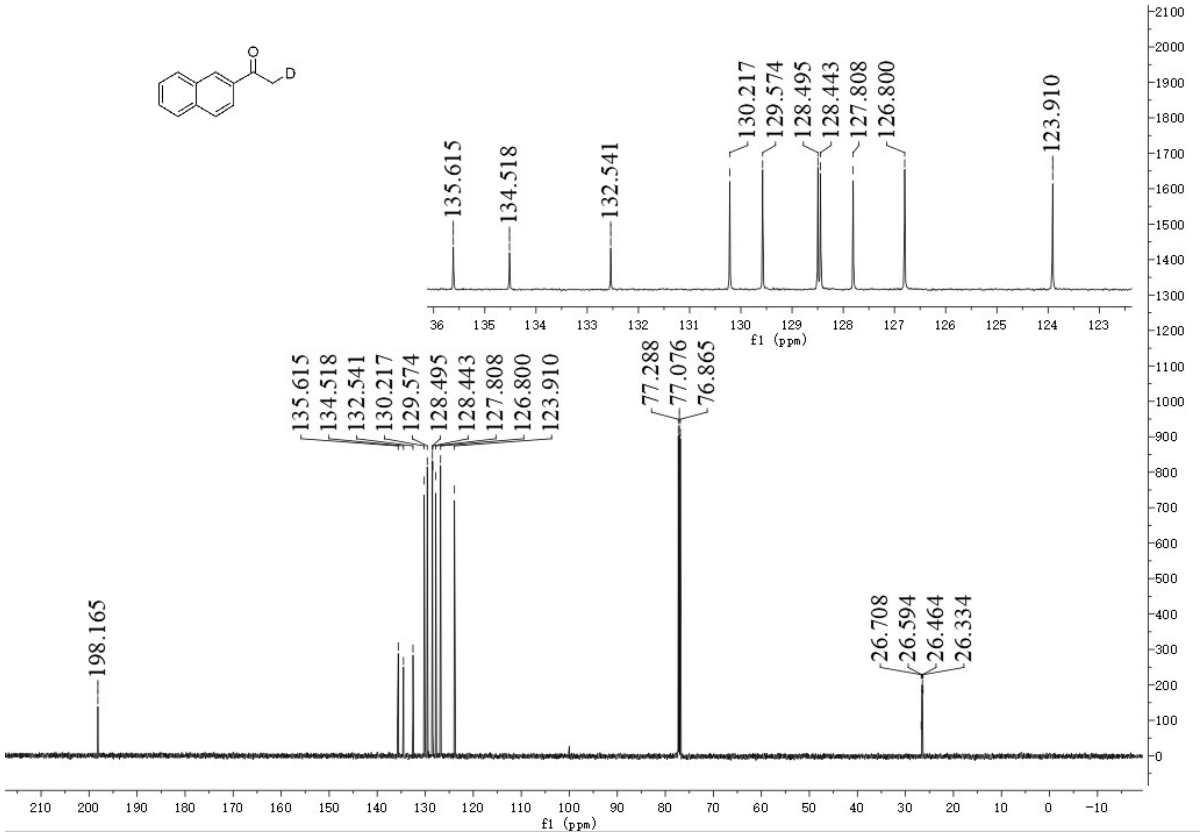
1-(4-Bromo-phenyl)-2-deuterio-ethanone (65)





2-Deuterio-ethanone-1-(2-naphthalenyl) (66)

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