Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Iron-Catalyzed Hydrogen Atom Transfer Induced Cyclization of 1,6-Enynes for the Synthesis of Ketoximes: a Combined Experimental and Computational Study

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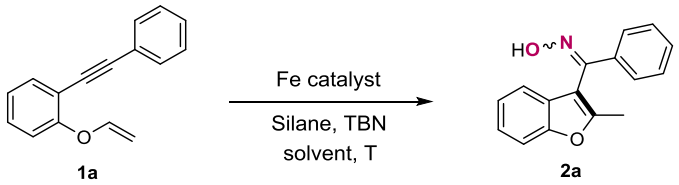
I. General Remarks.

Column chromatography was carried out on silica gel. Unless noted ^{1}H NMR spectra were recorded on 400 MHz in $CDCl_3$ or *d*-DMSO, ^{13}C NMR spectra were recorded on 100 MHz in $CDCl_3$ or *d*-DMSO, ^{19}F NMR spectra were recorded on 376 MHz in $CDCl_3$ or *d*-DMSO. IR spectra were recorded on an FT-IR spectrometer and only major peaks are reported in cm^{-1}. Melting points were determined on a microscopic apparatus and were uncorrected. All new products were further characterized by HRMS (high resolution mass spectra), high resolution mass spectrometry (HRMS) spectra was obtained on a micrOTOF instrument equipped with an ESI source; copies of their ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra are provided. $Fe(acac)_3$, $Fe(dmp)_3$, $Fe(OTf)_3$, PMHS, TBN, and **THF (super dry)** were purchased from Sigma-Aldrich. All reagents or catalysts were directly used from purchased without further purification.

II. Optimization conditions for the synthesis of product 2, 6, 8, 9.

Table S1. Screening of the reaction conditions [a]



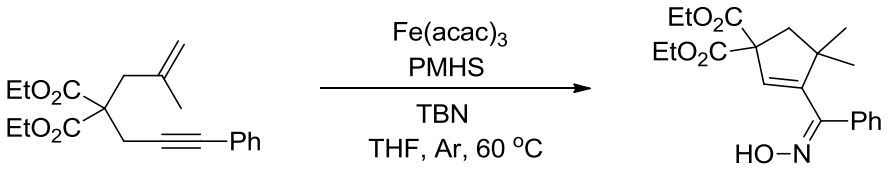
1a 2a

Entry	Silane (equiv.)	Solvent (mL)	Temp. (^{o}C)	Time (h)	Yield (%)[b]
1	PMHS (2.0)	THF (2.0)	60	24	60 (8:1)
2	Et_3SiH (2.0)	THF (2.0)	60	24	0
3	Ph_3SiH (2.0)	THF (2.0)	60	24	0
4	$(EtO)_3SiH$ (2.0)	THF (2.0)	60	24	0
5	$PhSiH_3$ (2.0)	THF (2.0)	60	24	68 (8:1)
6	PMHS (2.0)	CH_3CN (2.0)	60	24	0
7	PMHS (2.0)	DCE (2.0)	60	24	<5
8	PMHS (2.0)	*i*PrOH (2.0)	60	24	40 (8:1)
9	PMHS (2.0)	Toluene (2.0)	60	24	10 (8:1)
10	PMHS (3.0)	THF (2.0)	60	24	66 (8:1)
11	**PMHS (3.0)**	**THF (2.0)**	**60**	**36**	**73 (8:1)**
12	PMHS (3.0)	THF (2.0)	RT	36	<5
13	PMHS (3.0)	THF (2.0)	40	36	60 (8:1)
14	PMHS (3.0)	THF (2.0)	80	36	48 (8:1)
15[c]	PMHS (3.0)	THF (2.0)	60	36	24 (8:1)

16 [d]	PMHS (3.0)	THF (2.0)	60	36	47 (8:1)
17 [e]	PMHS (3.0)	THF (2.0)	60	36	40 (7:1)
18 [f]	PMHS (3.0)	THF (2.0)	60	36	0
19 [g]	PMHS (3.0)	THF (2.0)	60	36	0

[a] Reaction conditions: **1a** (0.2 mmol), $Fe(acac)_3$ (0.04 mmol, 20 mmol%), silane (0.6 mmol), TBN (0.4 mmol), solvent (2.0 mL, super dry), 60 °C, 36h, under Ar atmosphere. [b] Isolated yield; Ratio of Z/E was determined by crude ^1H NMR. [c] In air. [d] 10 mmol% $Fe(acac)_3$ was used. [e] 20 mmol% $Fe(dmp)_3$ was used. [f] 20 mmol% $Fe(OTf)_3$ was used. [g] 20 mmol% $FeCl_3$ was used.

Table S2. Screening of the reaction conditions for oximation

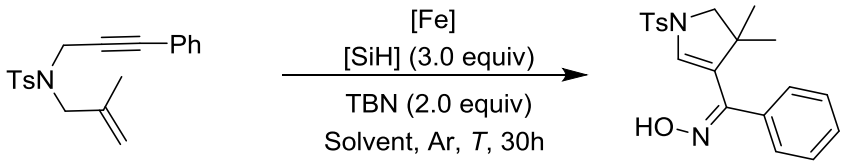


5 **6a**

Entry	Oxidant (equiv)	Catalyst (20%)	Hydrogen Source (equiv.)	Solvent (mL)	Atmosphere	Temp (℃)	Yield (%)
1	TBN (2.0)	$Fe(acac)_3$	$PhSiH_3$ (3.0)	THF (2.0)	Ar	60	50
2	TBN (3.0)	$Fe(acac)_3$	PMHS (3.0)	THF (2.0)	Ar	60	42
3	TBN (2.0)	$Fe(acac)_3$	PMHS (2.0) + *i*PrOH (3.0)	THF (2.0)	Ar	60	44
4	TBN (2.0)	$Fe(acac)_3$ + Dppe (30%)	PMHS (3.0)	THF (2.0)	Ar	60	10
5	TBN (2.0)	$Fe(acac)_3$	PMHS (3.0)	2-MeTHF (2.0)	Ar	60	52
6	TBN (2.0)	$Fe(acac)_3$	PMHS (3.0)	2-MeTHF (2.0)	Ar	80	51
7	TBN (2.0)	$Fe(acac)_3$ (30%)	PMHS (3.0)	THF (2.0)	Ar	60	49
8	TBN (2.0)	$Fe(acac)_3$	PMHS (3.0)	THF (2.0) 4A MS	Ar	60	13
9	TBN (2.0)	$Fe(acac)_3$	$NaBH_4$ (3.0)	THF (2.0)	Ar	60	0
10	**TBN (2.0)**	**$Fe(acac)_3$**	**PMHS (3.0)**	**THF (2.0)**	**Ar**	**60**	**56 (Z/E>98: 2)**
11	TBN (2.0)	$Fe(acac)_3$	PMHS (3.0)	THF (1.0)	Ar	60	44

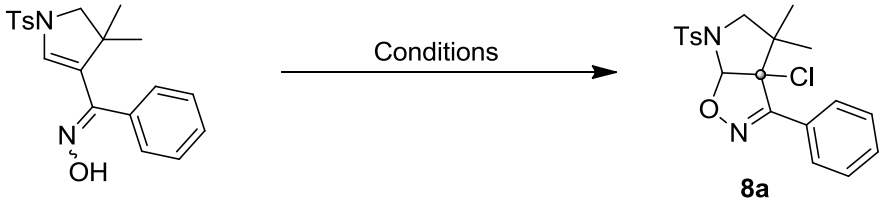
[a] Reaction conditions: **1a** (0.1 mmol), $Fe(acac)_3$ (0.02 mmol, 20 mmol%), silane (0.3 mmol), TBN (0.2 mmol), solvent (2.0 mL, **super dry**), 60 ℃, 24 h, under Ar atmosphere.

Table S3. Screening of the reaction conditions for oximation



Entry	Oxidant (equiv.)	Catalyst (20%)	Addition (equiv.)	Solvent (ml)	Temp. (℃)	Yield (%)
1	TBN(2.0)	$Fe(acac)_3$	$PhSiH_3$(2.0)	THF (1.0)	40	46
2	TBN(2.0)	$Fe(acac)_3$	$PhSiH_3$(2.0)	THF (1.0)	60	60
3	TBN(2.0)	$Fe(acac)_3$	$PhSiH_3$(2.0)	CH_3CN (1.0)	60	_
4	TBN(2.0)	$Fe(acac)_3$	$PhSiH_3$(2.0)	DCE (1.0)	60	<5
5	TBN(2.0)	$Fe(acac)_3$	$PhSiH_3$(2.0)	Toluene (1.0)	60	10
6	TBN(2.0)	$Fe(acac)_3$	$PhSiH_3$(2.0)	DMF (1.0)	60	_
7	TBN(2.5)	$Fe(acac)_3$	$PhSiH_3$(3.0)	THF (1.0)	60	52
8	TBN(2.0)	$Fe(OTf)_3$	$PhSiH_3$(2.0)	THF (1.0)	60	_
9	TBN(2.0)	$FeCl_3$	$PhSiH_3$(2.0)	THF (1.0)	60	_
10	TBN(2.0)	$Fe(OTf)_2$	$PhSiH_3$(2.0)	THF (1.0)	60	_
11	TBN(2.0)	$Fe(acac)_3$	$PhSiH_3$(2.0)	THF (1.0)	50	56
12	TBN(2.0)	$Fe(acac)_3$	$PhSiH_3$(2.0)	THF (1.0)	40	51
13	TBN(3.0)	$Fe(acac)_3$	$PhSiH_3$(2.0)	THF (2.0)	60	41
14	TBN(4.0)	$Fe(acac)_3$	$PhSiH_3$(2.0)	THF (2.0)	60	<5
15	TBN(2.0)	$Fe(acac)_3$	Et_3SiH(2.0)	THF (2.0)	60	_
16	TBN(2.0)	$Fe(acac)_3$	Ph_3SiH (2.0)	THF (2.0)	60	_
17	TBN(2.0)	$Fe(acac)_3$	$PhSiH_3$(2.0)	THF (2.0)	rt	40
18	TBN(2.0)	$Fe(acac)_3$	$(EtO)_3SiH$ (2.0)	THF (2.0)	60	33
19	TBN(1.5)	$Fe(acac)_3$	$PhSiH_3$(2.0)	THF (2.0)	60	60
20	TBN(2.0)	$Fe(acac)_3$	PMHS(2.0)	THF (2.0)	40	64
21	**TBN(2.0)**	**$Fe(acac)_3$**	**PMHS(3.0)**	**THF (2.0)**	**60**	**72**
22	TBN(2.0)	$Fe(acac)_3$	PMHS(3.0)	EtOH (2.0)	60	44
23	TBN(2.0)	$Fe(acac)_3$	PMHS(3.0)	iPrOH (2.0)	60	48
24	TBN(2.0)	$Fe(acac)_3$	PMHS(3.0)	DCM (2.0)	60	<10
25	TBN(2.0)	$Fe(acac)_3$	PMHS(3.0)	EtOAc (2.0)	60	<5
26	TBN(2.0)	$Fe(acac)_3$	PMHS(3.0)	EtOH/THF (1:1)	60	32
27	TBN(2.0)	$Fe(acac)_3$	PMHS(3.0)	THF (3.0)	60	50
28	TBN(2.0)	$Fe(acac)_3$	PMHS(3.0)	CF_3CH_2OH (2.0)	60	_
29	TBN(2.0)	$Fe(acac)_3$	PMHS(3.0)	Dioxane (2.0)	60	_
30	TBN(2.0)	$Fe(acac)_3$ (10%)	PMHS(3.0)	THF (2.0)	60	58
31	TBN(2.0)	$Fe(acac)_3$	$PhSiH_3$(2.0)	THF (2.0)	60	70

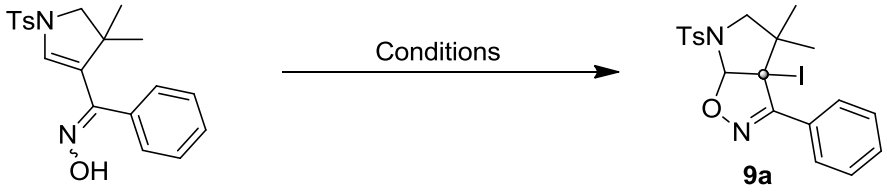
Table S4. Screening of the reaction conditions for oxychlorination



Entry	Catalyst	Solvent (ml)	Atmosphere	Temp (℃)	Time (h)	Yield (%)

1	**$CuCl_2$ $2H_2O$ (2 eq.)**	**MeCN:H_2O (4:1)**	**air**	**75**	**2h**	**70**
2	$CuCl_2$ $2H_2O$ (2 eq.)	DMSO:H_2O (4:1)	air	80	2h	40
3	$CuCl_2$ $2H_2O$ (2 eq.)	EtOH:H_2O (4:1)	air	80	2h	58
4	$CuCl_2$ $2H_2O$ (1 eq.)	MeCN:H_2O (4:1)	air	75	2h	64
5	$CuBr_2$ (2 eq.)	MeCN:H_2O (4:1)	air	75	2h	_
6	$CuSO_4$ $5H_2O$ (2 eq.)	MeCN:H_2O (4:1)	air	75	2h	_

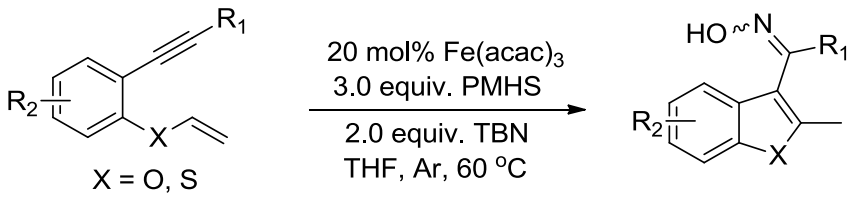
Table S5. Screening of the reaction conditions for oxyiodination



Entry	Catalyst	Solvent (ml)	Oxidant	Temp (℃)	Time (h)	Yield (%)
1	I_2 (10%)	CH_3CN/H_2O (9:1)	H_2O_2 (2.0)	r.t.	12	10
2	I_2 (20%)	CH_3CN/H_2O (9:1)	H_2O_2 (2.0)	r.t.	12	31
3	I_2 (50%)	CH_3CN/H_2O (9:1)	H_2O_2 (2.0)	r.t.	12	64
4	**I_2 (60%)**	**CH_3CN/H_2O (9:1)**	**H_2O_2 (2.0)**	**r.t.**	**12**	**77**
5	I_2 (60%)	CH_3CN/H_2O (9:1)	O_2 (1 atm)	r.t.	12	50
6	I_2 (60%)	CH_3CN/H_2O (9:1)	Ar (1 atm)	r.t.	12	43
7	I_2 (60%)	CH_3CN/H_2O (9:1)	H_2O_2 (2.0)	r.t.	12	24[a]

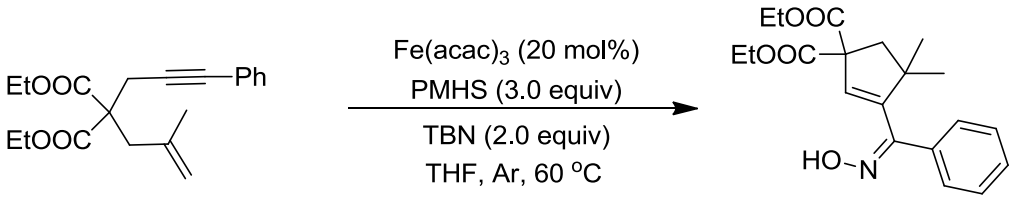
[a] 2 equivalent of TEMPO was added.

III. General Procedure for the synthesis of products 2, 4, 6, 8, 9

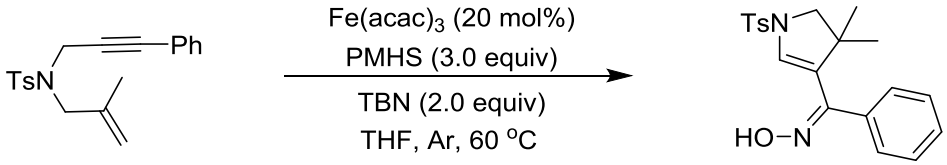


The mixture of 1,6-enynes **1** or **3** (0.20 mmol) and PMHS (0.60 mmol), TBN (0.40 mmol), $Fe(acac)_3$ (0.040 mmol) were combined in THF (2.0 mL, **super dry**) at 60 ℃

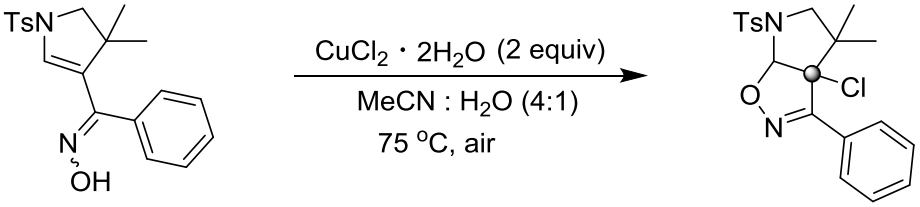
for 36 h under Ar atmosphere. After the reaction, 6 mL water was added to quench the reaction, and the resulting mixture was extracted twice with DCM. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. Purification of the crude product by flash column chromatography afforded the products **2** or **4** (petroleum ether/ethyl acetate as eluent (25:1-15:1)).



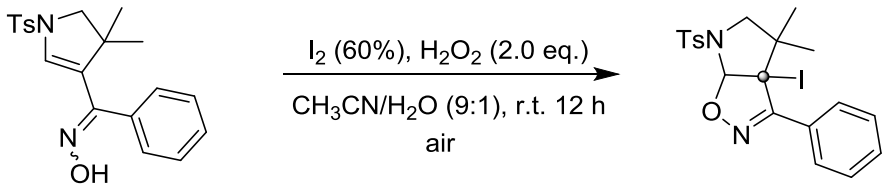
The mixture of 1,6-enynes (0.10 mmol) and PMHS (0.30 mmol), $Fe(acac)_3$ (0.020 mmol), TBN (0.20 mol) were combined in THF (2.0 mL, **super dry**) at 60 ℃ for 24 h under 1 atm Ar atmosphere. After the reaction, 6 mL water was added to quench the reaction, and the resulting mixture was extracted twice with DCM. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. Purification of the crude product by flash column chromatography afforded the product (petroleum ether/ethyl acetate as eluent (12:1-6:1)).



The mixture of 1,6-enynes (0.20 mmol) and PMHS (0.60 mmol), $Fe(acac)_3$ (0.040 mmol), TBN (0.40 mol) were combined in THF (2.0 mL, **super dry**) at 60 ℃ for 30 h under 1 atm Ar atmosphere. After the reaction, 6 mL water was added to quench the reaction, and the resulting mixture was extracted twice with DCM. The combined organic extracts were washed with brine, dried over Na_2SO_4 and concentrated. Purification of the crude product by flash column chromatography afforded the product (petroleum ether/ethyl acetate as eluent (12:1-6:1)).



(4,4-dimethyl-1-tosyl-4,5-dihydro-1H-pyrrol-3-yl)(phenyl)methanone oxime was dissolved in MeCN (2.0 mL), $CuCl_2$·$2H_2O$ (2.0 equiv.) and H_2O (0.50 mL) were added. When the suspension was heated to reflux, the mixture became a bluish clear solution. The resulting reaction solution was then stirred at reflux (75 ℃) for around 2 h and monitored by TLC. After the reaction was complete, the solvents were removed by vacuum distillation. The residue was partitioned between EtOAc (10.0 mL) and H_2O (3.0 mL), the organic and aqueous phases were separated. Organic phase was washed with brine (5.0 mL) and dried over anhyd. $MgSO_4$. Concentration of the organic solution gave crude product, which was purified by flash chromatography (PE/EA = 6:1) to afford the cyclization product **6**.



(4,4-dimethyl-1-tosyl-4,5-dihydro-1H-pyrrol-3-yl)(phenyl)methanone oxime was dissolved in MeCN (2.0 mL), I_2 (60% mmol), H_2O_2 (2.0 equiv.) and H_2O (0.20 mL) were added. The resulting reaction solution was then stirred in air at room temperature for around 12 h and monitored by TLC. After the reaction was complete, the solvents were removed by vacuum distillation. The residue was partitioned between EtOAc (10.0 mL) and H_2O (3.0 mL), the organic and aqueous phases were separated. Organic phase was washed with brine (5.0 mL) and dried over anhyd. $MgSO_4$. Concentration of the organic solution gave crude product, which was purified by flash chromatography (PE/EA = 6:1) to afford the cyclization product.

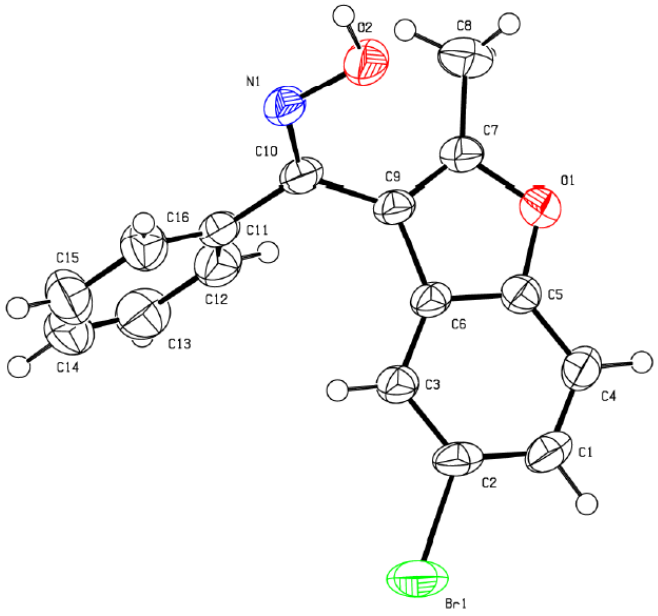
IV. X-ray Crystal Diffraction Data for 2q, 2u, 2x, 4i, 6e and 8g

Datablock: CCDC 1973197 (2x)

Bond precision: C-C = 0.0048 A Wavelength=1.54178
Cell: a=6.8906(3) b=10.6824(5) c=10.8082(5)
alpha=67.251(2) beta=75.267(2) gamma=84.165(2)
Temperature: 273 K

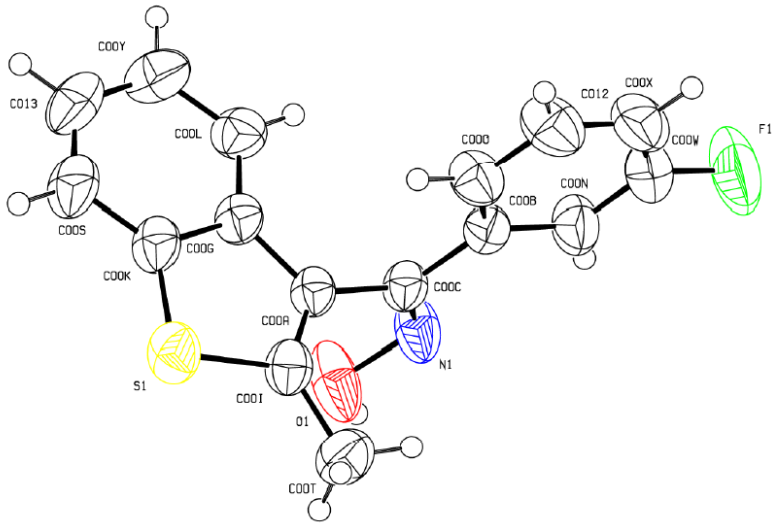
	Calculated	Reported
Volume	709.56(6)	709.56(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H12 Br N O2	?
Sum formula	C16 H12 Br N O2	C16 H12 Br N O2
Mr	330.17	330.18
Dx,g cm-3	1.545	1.545
Z	2	2
Mu (mm-1)	3.954	3.954
F000	332.0	332.0
F000’	331.45	
h,k,lmax	8,12,12	8,12,12
Nref	2505	2480
Tmin,Tmax		0.436, 0.753
Tmin’		

Correction method= # Reported T Limits: Tmin=0.436 Tmax=0.753
AbsCorr = MULTI-SCAN
Data completeness= 0.990 Theta(max)= 66.563
R(reflections)= 0.0355(2237) wR2(reflections)= 0.1063(2480)
S = 1.137 Npar= 186



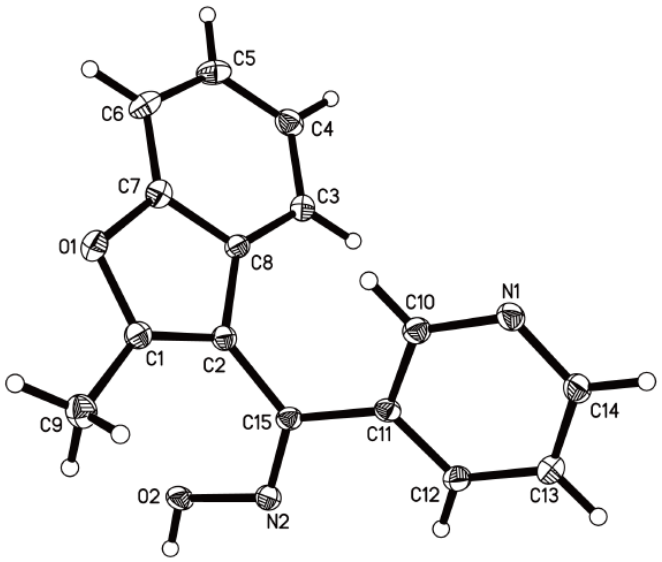
Crystal data and structure refinement for **4i** (**CCDC 1974019)**

Identification code	cu_hh2_0m_a	
Empirical formula	C16 H12 Cl0 F N O S	
Formula weight	285.33	
Temperature	273(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pccn	
Unit cell dimensions	a = 11.6155(3) Å	a= 90 °.
	b = 28.9732(8) Å	b= 90 °.
	c = 8.2494(2) Å	g = 90 °.
Volume	2776.24(12) $Å^3$	
Z	8	
Density (calculated)	1.365 Mg/m^3	
Absorption coefficient	2.130 mm^{-1}	
F(000)	1184	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	3.050 to 67.021 °.	
Index ranges	-13<=h<=13, -34<=k<=34, -9<=l<=9	
Reflections collected	105558	
Independent reflections	2460 [R(int) = 0.0835]	
Completeness to theta = 67.021 °	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7528 and 0.6185	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2460 / 0 / 185	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.1010	
R indices (all data)	R1 = 0.0457, wR2 = 0.1057	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.162 and -0.278 e.$Å^{-3}$	



Crystal data and structure refinement for **2u** (**CCDC 1970736)**

Identification code	M2579a	
Empirical formula	C15 H12 N2 O2	
Formula weight	252.27	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 12.7787(5) Å	= 90°.
	b = 13.1791(6) Å	= 90°.
	c = 14.9158(7) Å	= 90°.
Volume	2512.00(19) $Å^3$	
Z	8	
Density (calculated)	1.334 Mg/m^3	
Absorption coefficient	0.091 mm^{-1}	
F(000)	1056	
Crystal size	0.12 x 0.16 x 0.20 mm^3	
Theta range for data collection	2.606 to 25.092 °.	
Index ranges	-15<=h<=15, -13<=k<=15, -17<=l<=17	
Reflections collected	12410	
Independent reflections	2235 [R(int) = 0.0542]	
Completeness to theta = 25.092 °	100.0 %	
Absorption correction	multi-scan	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2235 / 0 / 172	
Goodness-of-fit on F^2	1.120	
Final R indices [I>2sigma(I)]	R1 = 0.0531, wR2 = 0.1775	
R indices (all data)	R1 = 0.0719, wR2 = 0.2053	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.553 and -0.503 e.$Å^{-3}$	

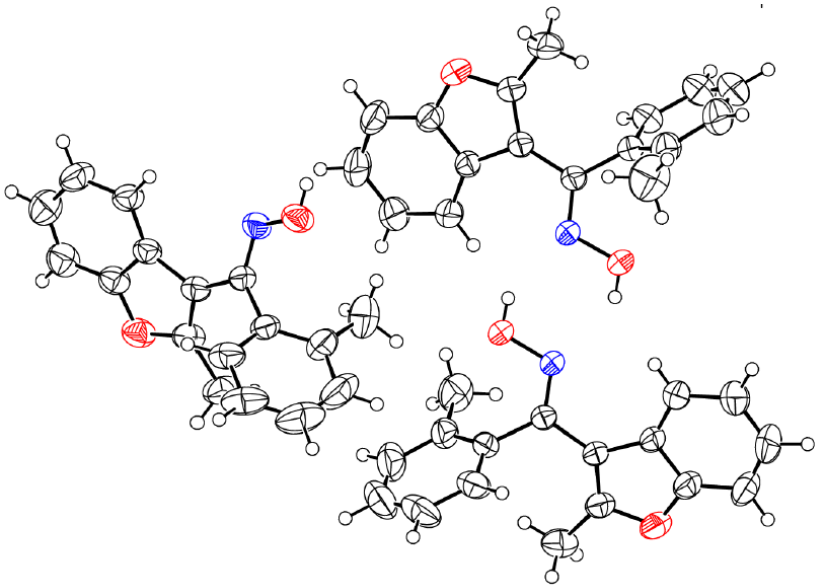


Datablock: CCDC 1970737 (2q)

Bond precision: C-C = 0.0041 A Wavelength=1.54184
Cell: a=11.9534(6) b=14.3176(7) c=14.6657(11)
alpha=61.766(6) beta=75.556(5) gamma=87.984(4)
Temperature: 293 K

	Calculated	Reported
Volume	2131.3(3)	2131.3(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C17 H15 N O2	3(C17 H15 N O2)
Sum formula	C17 H15 N O2	C51 H45 N3 O6
Mr	265.30	795.90
Dx,g cm-3	1.240	1.240
Z 6 2		
Mu (mm-1)	0.653	0.653
F000	840.0	840.0
F000’	842.50	
h,k,lmax	14,17,17	14,17,17
Nref 7543 7412		
Tmin,Tmax	0.889,0.925	0.240,1.000
Tmin’ 0.883		

Correction method= # Reported T Limits: Tmin=0.240 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 0.983 Theta(max)= 66.597
R(reflections)= 0.0516(5273) wR2(reflections)= 0.1516(7412)
S = 1.015 Npar= 550

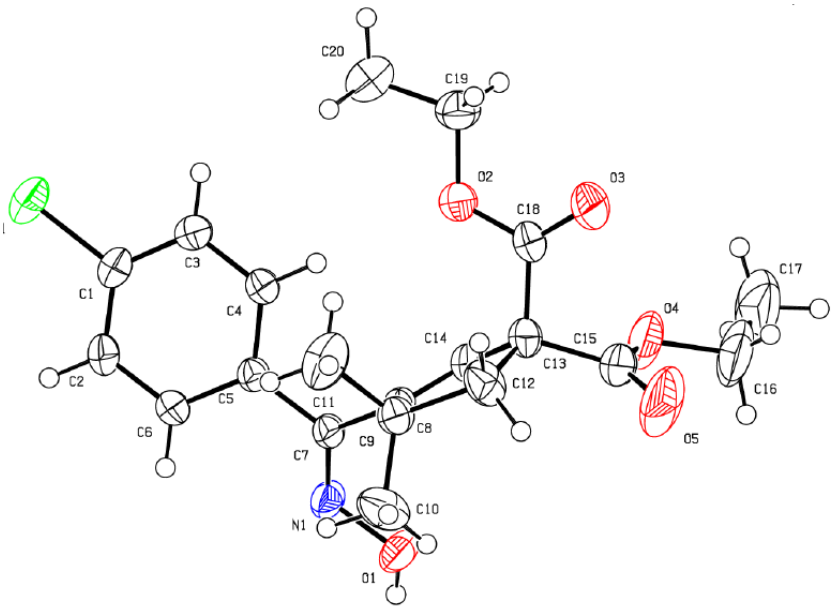


Crystal data and structure refinement for **6e** (CCDC 2031399)

Datablock: 20200910_x1_0m_a
Bond precision: C-C = 0.0032 A Wavelength=0.71073
Cell: a=7.207(7) b=11.693(11) c=12.233(9)
Alpha = 78.96(3) beta=84.63(3) gamma=87.16(3)
Temperature: 169 K

	Calculated	Reported
Volume	1006.9(16)	1006.9(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C20 H24 Cl N O5	C20 H24 Cl N O5
Sum formula	C20 H24 Cl N O5	C20 H24 Cl N O5
Mr	393.85	393.85
Dx,g cm^{-3}	1.299	1.299
Z	2	2
Mu (mm-1)	0.220	0.220
F000	416.0	416.0
F000’ 416.50		
h,k,lmax	9,15,15	9,15,15
Nref	4634	4618
Tmin,Tmax		0.128,0.488
Tmin’		

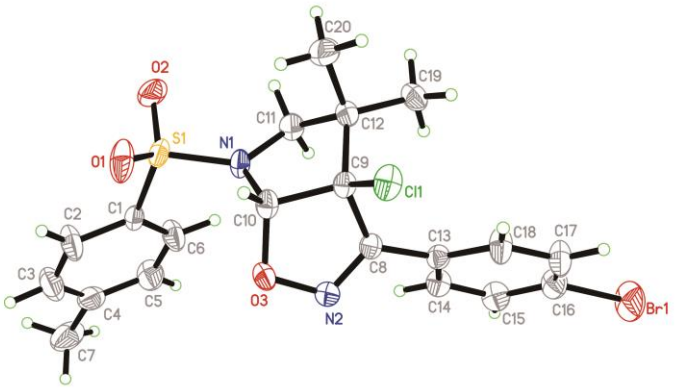
Correction method= # Reported T Limits: Tmin=0.128 Tmax=0.488
AbsCorr = MULTI-SCAN
Data completeness= 0.997 Theta(max)= 27.499
R(reflections)= 0.0535(3633) wR2(reflections)= 0.1627(4618)
S = 1.063 Npar= 249



Datablock: CCDC 2008347 (8g)

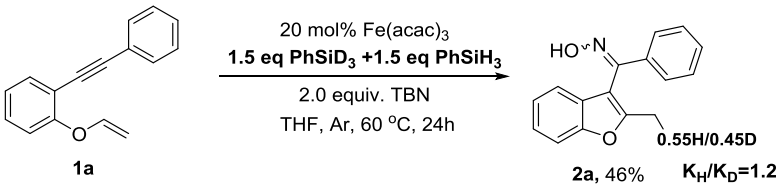
Crystal data and structure refinement for C200605a_a.

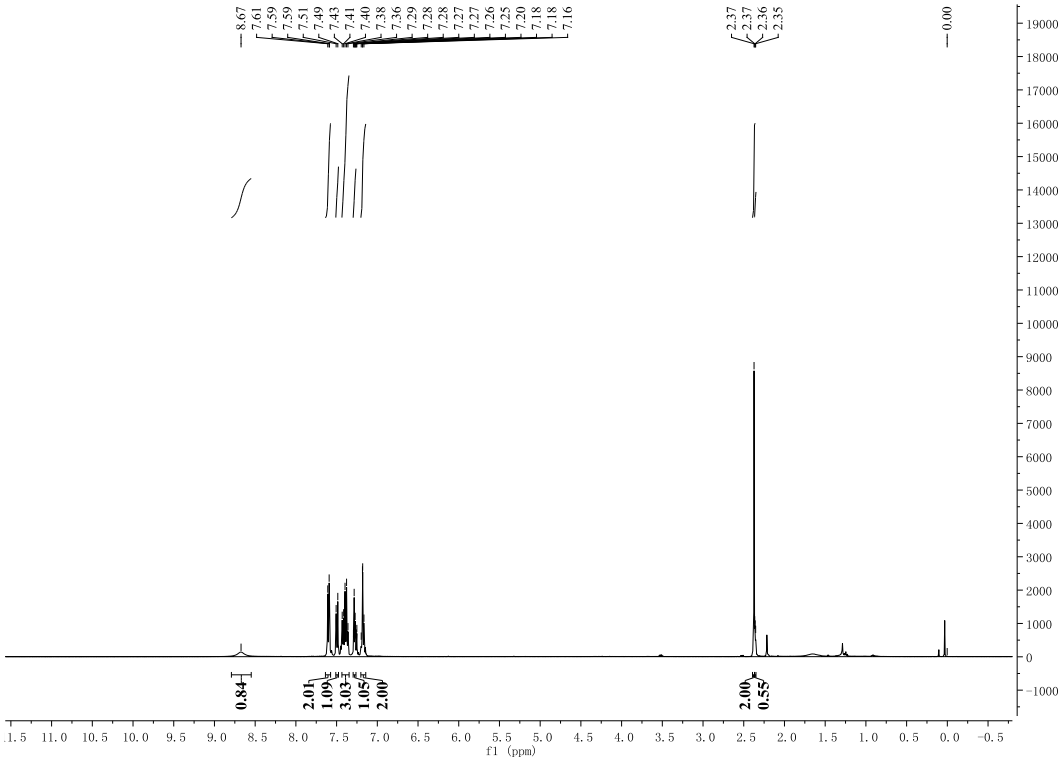
Identification code	C200605a_a
Empirical formula	C40 H40 Br2 Cl2 N4 O6 S2
Formula weight	967.60
Temperature	273(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	$Pca2_1$
Unit cell dimensions	a = 7.9608(3) Å α= 90 °. b = 23.8872(9) Å β= 90 °. c = 21.8984(8) Å γ = 90 °.
Volume	4164.2(3) $Å^3$
Z	4
Density (calculated)	1.543 Mg/m^3
Absorption coefficient	5.010 mm^{-1}
F(000)	1968
Crystal size	0.20 x 0.18 x 0.16 mm^3
Theta range for data collection	3.701 to 66.710 °.
Index ranges	-9<=h<=9, -28<=k<=28, -26<=l<=26
Reflections collected	25004
Independent reflections	7334 [R(int) = 0.0460]
Completeness to theta = 66.710 °	99.7 %
Absorption correction	multi-scan
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7334 / 1 / 511
Goodness-of-fit on F^2	1.001
Final R indices [I>2sigma(I)]	R1 = 0.0358, wR2 = 0.1058
R indices (all data)	R1 = 0.0406, wR2 = 0.1114
Absolute structure parameter	0.071(5)
Extinction coefficient	n/a
Largest diff. peak and hole	0.453 and -0.622 e.$Å^{-3}$



V. Deuterium labeling experiments:

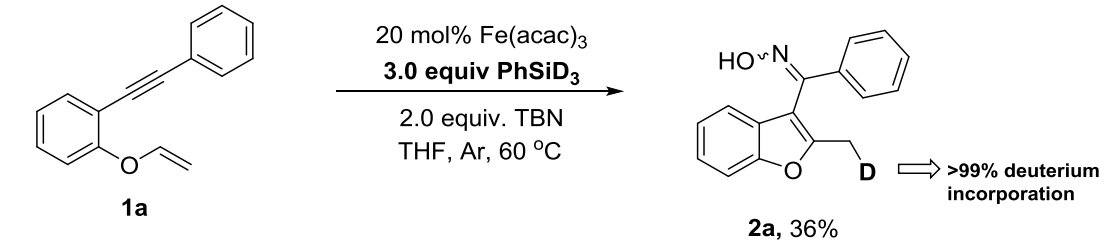
1.5 eq. $PhSiD_3$ and 1.5 eq. $PhSiH_3$ was added in the standard conditions. (K_H/K_D=1.2)





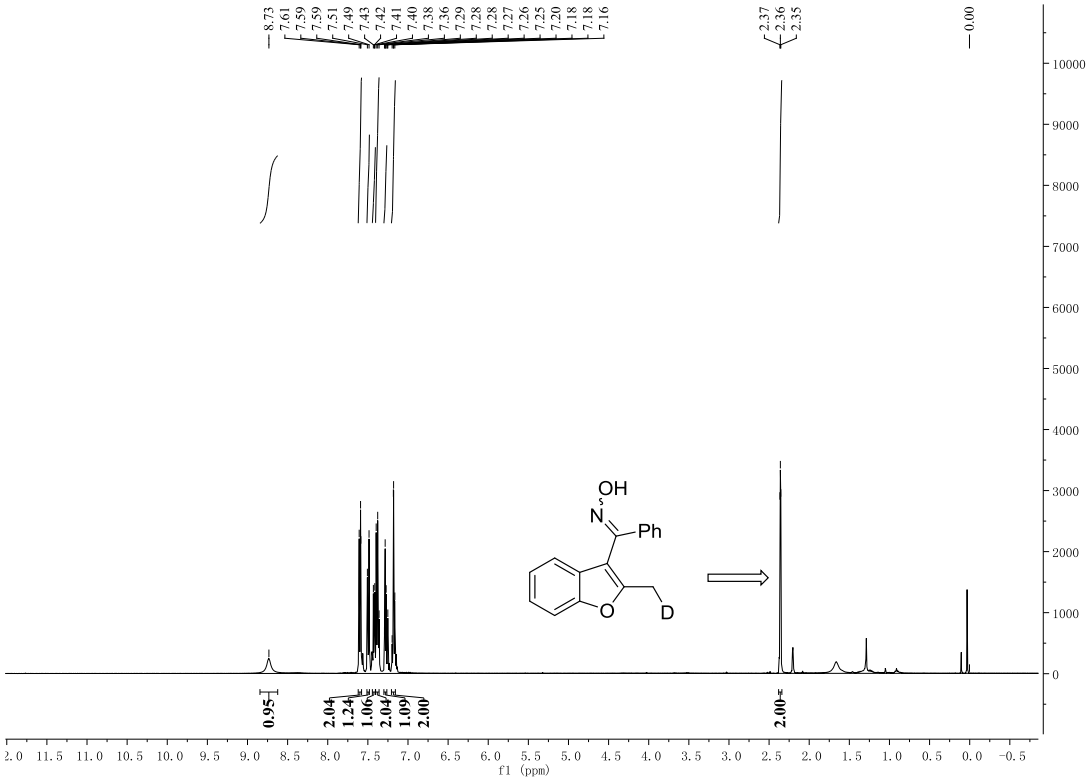
3.0 eq. $PhSiD_3$ was added in the standard conditions.

Isotope labeling experiments:

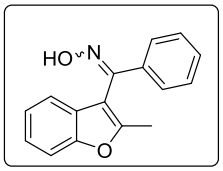


1a

2a, 36%

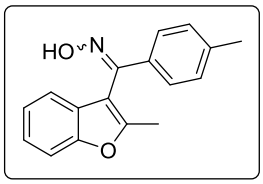


VI. Data of products 2, 4, 6, 8, 9, 10, 11, 12, 13



(2-methylbenzofuran-3-yl)(phenyl)methanone oxime **2a**, 73%, oil. Z/E = 8:1

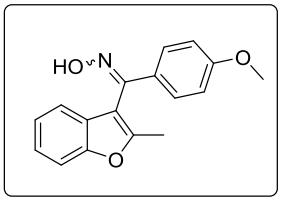
^{1}H NMR (400 MHz, $CDCl_3$): 8.83 (s, 1H), 7.61 – 7.58 (m, 2H), 7.49 (d, *J* = 8.2 Hz, 1H), 7.43 – 7.36 (m, 3H), 7.30 – 7.26 (m, 1H), 7.20 – 7.15 (m, 2H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 156.0, 155.5, 154.1, 153.7, 152.7, 151.3, 135.1, 132.6, 129.7, 129.4, 129.2, 128.6, 128.3, 127.9, 127.4, 123.7 (d, *J* = 17.6 Hz), 122.9, 122.7, 120.9 (d, *J* = 18.4 Hz), 112.7, 110.8, 110.5, 108.5, 14.3, 13.7. IR (cm^{-1}): 3275, 3043, 1592, 1473, 1454, 1429, 1410, 1393, 1324, 1249, 1179, 1127, 1091, 1012, 976, 930, 917, 831, 741, 701. HRMS (ESI) m/z calcd for $C_{16}H_{14}NO_2^+$ $(M+H)^+$: 252.1019, found 252.1024.



(2-methylbenzofuran-3-yl)(p-tolyl)methanone oxime **2b**, 68%, oil, Z/E = 5.0:1

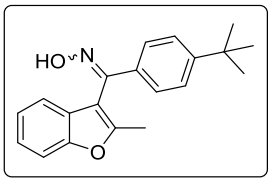
^{1}H NMR (400 MHz, $CDCl_3$): 9.11 (s, 1H), 7.49 (dd, *J* = 8.2, 2.8 Hz, 3H), 7.28 (d, *J* = 6.0 Hz, 1H), 7.18 (d, *J* = 8.6 Hz, 4H), 2.39 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 155.9, 155.5, 154.1, 153.7, 151.2, 139.8, 139.5, 132.3, 129.4-128.9, 127.9,

127.3, 123.6 (d, *J* = 16.7 Hz), 122.9, 122.6, 121.0 (d, *J* = 11.5 Hz), 110.7, 110.5, 108.6, 21.4 (d, *J* = 17.6 Hz), 14.2, 13.7. IR (cm^{-1}): 3254, 3032, 2919, 2363, 1683, 1606, 1508, 1474, 1455, 1389, 1288, 1264, 1248, 1178, 1128, 1012, 975, 929, 914, 820, 743, 702, 593. HRMS (ESI) m/z calcd for $C_{17}H_{16}NO_2^+$ $(M+H)^+$: 266.1176, found 266.1188.



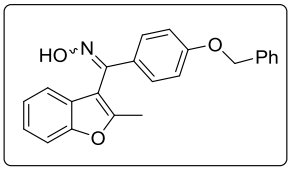
(4-methoxyphenyl)(2-methylbenzofuran-3-yl)methanone oxime **2c**, 78%, oil, Z/E = 15.0:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.95 (s, 1H), 7.55 – 7.47 (m, 3H), 7.28 (dd, *J* = 6.5, 1.9 Hz, 1H), 7.22 – 7.16 (m, 2H), 6.91 – 6.87 (m, 2H), 3.84 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 160.9, 160.3, 155.8, 155.5, 154.1, 153.8, 151.5, 150.8, 133.9, 131.7 (d, *J* = 6.4 Hz), 131.2, 128.9, 128.5, 128.0-127.5, 124.6, 123.6 (d, *J* = 14.2 Hz), 122.8 (d, *J* = 17.6 Hz), 120.8 (d, *J* = 12.7 Hz), 114.7, 114.2, 113.9, 113.6, 113.0, 110.6 (d, *J* = 19.1 Hz), 108.7, 55.2, 14.2, 13.6. IR (cm^{-1}): 3275, 3055, 2934, 2838, 2359, 1604, 1509, 1455, 1393, 1302, 1265, 1174, 1127, 1072, 1029, 973, 913, 834, 746, 699, 597. HRMS (ESI) m/z calcd for $C_{17}H_{16}NO_3^+$$(M+H)^+$: 282.1125, found 282.1128.



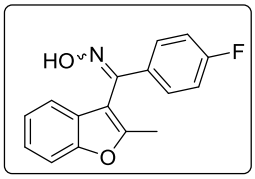
(4-(tert-butyl)phenyl)(2-methylbenzofuran-3-yl)methanone oxime **2d**, 73%, oil, Z/E = 6.0:1

^{1}H NMR (400 MHz, $CDCl_3$): 9.40 (s, 1H), 7.52 (dd, *J* = 12.7, 8.4 Hz, 3H), 7.39 (d, *J* = 8.6 Hz, 2H), 7.31 – 7.26 (m, 1H), 7.20 (dd, *J* = 10.0, 9.1 Hz, 2H), 2.39 (s, 3H), 1.35 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): 155.9, 155.4, 154.1, 153.8, 153.0, 152.6, 151.1, 132.1, 129.7-128.9, 128.0, 127.7, 127.1, 126.1, 125.6-125.1, 124.2, 123.8-123.2, 122.8, 122.6, 121.3, 120.9 (d, *J* = 5.5 Hz), 112.9, 110.7, 110.5, 108.6, 34.7 (d, *J* = 10.1 Hz), 31.2 (d, *J* = 5.5 Hz), 29.6, 14.2, 13.6. IR(cm^{-1}): 3275, 3961, 2868, 2364, 1605, 1558, 1541, 1455, 1394, 1363, 1267, 1249, 1179, 1106, 1014, 975, 931, 914, 836, 741, 702, 570. HRMS (ESI) m/z calcd for $C_{20}H_{22}NO_2^+$ $(M+H)^+$: 308.1645, found 308.1651.



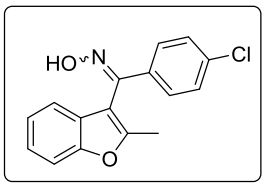
(4-(benzyloxy)phenyl)(2-methylbenzofuran-3-yl)methanone oxime **2e**, 56%, oil, Z/E = 15.0:1

^{1}H NMR (400 MHz, $CDCl_3$): 9.48 (s, 1H), 7.56 (d, *J* = 8.9 Hz, 2H), 7.52 (d, *J* = 8.2 Hz, 1H), 7.46 (dd, *J* = 12.9, 6.8 Hz, 4H), 7.42 – 7.37 (m, 1H), 7.32 – 7.27 (m, 1H), 7.21 (dt, *J* = 13.9, 6.8 Hz, 2H), 6.99 (d, *J* = 8.9 Hz, 2H), 5.11 (s, 2H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 160.1, 159.5, 155.8, 155.4, 154.1, 153.8, 151.6, 150.7, 136.5, 131.2, 128.8, 128.5, 128.1-127.7, 127.4 (d, *J* = 5.4 Hz), 123.6 (d, *J* = 13.5 Hz), 122.7 (d, *J* = 17.1 Hz), 120.9 (d, *J* = 7.5 Hz), 114.9, 114.5, 110.7, 110.7 (d, *J* = 20.2 Hz), 108.7, 70.0, 14.2, 13.7. IR(cm^{-1}): 3274, 3034, 2364, 1602, 1508, 1473, 1454, 1387, 1297, 1245, 1174, 1150, 1127, 1009, 974, 913, 832, 724, 697. HRMS (ESI) m/z calcd for $C_{23}H_{20}N_1O_3^+$ $(M+H)^+$: 358.1438, found 358.1438.



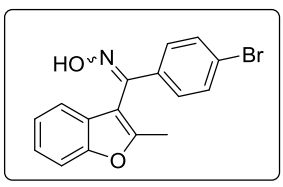
(4-fluorophenyl)(2-methylbenzofuran-3-yl)methanone oxime **2f**, 72%, oil, Z/E = 8:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.77 (s, 1H), 7.60 – 7.56 (m, 2H), 7.50 (d, *J* = 8.2 Hz, 1H), 7.30 – 7.27 (m, 1H), 7.16 (dd, *J* = 6.6, 1.0 Hz, 2H), 7.09 – 7.04 (m, 2H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 168.6, 165.0, 162.5, 155.9, 155.6, 154.0 (d, *J* = 30.5 Hz), 150.5, 131.9-131.3, 131.2 (d, *J* = 3.2 Hz), 130.3, 129.4 (dd, *J* = 17.6, 8.4 Hz), 123.8 (d, *J* = 16.3 Hz), 122.9 (d, *J* = 18.3 Hz), 120.8 (d, *J* = 10.4 Hz), 116.1-115.2, 110.9, 110.6, 108.3, 14.3, 13.7. ^{19}F NMR (376 MHz, $CDCl_3$): -110.37 (s, 1F), -110.86 (s, 1F). IR (cm^{-1}): 3280, 3064, 2921, 1601, 1508, 1474, 1455, 1322, 1225, 1179, 1158, 1127, 1066, 1014, 976, 929, 916, 838, 745, 702, 590. HRMS (ESI) m/z calcd for $C_{16}H_{13}FNO_2^+$ $(M+H)^+$: 270.0925, found 270.0926.



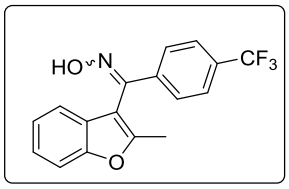
(4-chlorophenyl)(2-methylbenzofuran-3-yl)methanone oxime **2g**, 66%, oil, Z/E = 8:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.96 (s, 1H), 7.56 – 7.50 (m, 3H), 7.37 – 7.33 (m, 2H), 7.28 (td, *J* = 6.8, 3.3 Hz, 1H), 7.20 – 7.13 (m, 2H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 155.7, 154.1, 150.5, 135.8, 135.4, 133.5, 131.6, 130.7, 129.1-128.5, 128.1, 127.6, 123.9 (d, *J* = 16.7 Hz), 122.9 (d, *J* = 19.6 Hz), 120.7 (d, *J* = 16.0 Hz), 110.9, 108.0, 14.3, 13.8. IR (cm^{-1}): 3291, 3058, 1594, 1490, 1474, 1454, 1430, 1395, 1322, 1248, 1179, 1128, 1091, 1013, 976, 930, 915, 831, 742, 701. HRMS (ESI) m/z calcd for $C_{16}H_{13}ClN_1O_2^+$ $(M+H)^+$: 286.0629, found 286.0638.



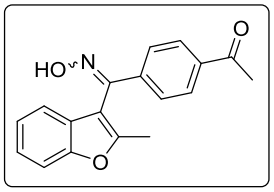
(4-bromophenyl)(2-methylbenzofuran-3-yl)methanone oxime **2h**, 67%, oil, Z/E = 10.0:1

^{1}H NMR (400 MHz, $CDCl_3$): 9.08 (s, 1H), 7.52 – 7.46 (m, 5H), 7.30 – 7.25 (m, 1H), 7.20 – 7.14 (m, 2H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 155.7, 154.1, 153.8, 150.6, 149.2, 134.0, 132.1-131.4, 131.1 (d, *J* = 17.2 Hz), 128.9, 128.4, 127.6, 127.3, 124.3-123.7 (m), 123.0, 122.8, 120.7 (d, *J* = 11.7 Hz), 116.1, 110.9, 110.7, 108.0, 14.3, 13.8. IR(cm^{-1}): 3275, 3055, 2919, 1616, 1588, 1487, 1455, 1395, 1263, 1249, 1178, 1128, 1079, 1010, 977, 914, 827, 721, 702. HRMS (ESI) m/z calcd for $C_{16}H_{13}BrN_1O_2^+$ $(M+H)^+$: 330.0124, found 330.0112.



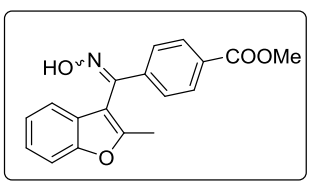
(2-methylbenzofuran-3-yl)(4-(trifluoromethyl)phenyl)methanone oxime **2i**, 68%, oil, Z/E = 12.0:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.97 (s, 1H), 7.68 (dd, *J* = 34.7, 8.2 Hz, 4H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.29 (ddd, *J* = 8.4, 5.7, 1.4 Hz, 1H), 7.16 (dtd, *J* = 8.6, 7.8, 0.9 Hz, 2H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 156.1, 155.8, 154.2, 153.8, 150.4, 138.5, 132.0, 131.7, 131.3, 131.0, 129.7, 127.7, 127.5, 127.1, 125.9-125.0, 124.0 (d, *J* = 19.8 Hz), 123.1, 122.9, 122.5, 120.8, 120.6, 111.0, 110.7, 107.9, 14.3, 13.8. ^{19}F NMR (376 MHz, $CDCl_3$): -62.75 (s, 3F), -63.80 (s, 3F). IR (cm^{-1}): 3291, 3058, 1614, 1474, 1455, 1407, 1315, 1249, 1167, 1124, 1066, 1015, 932, 842, 745, 597. HRMS (ESI) m/z calcd for $C_{17}H_{13}F_3N_1O_2^+$ $(M+H)^+$: 320.0893, found 320.0899.



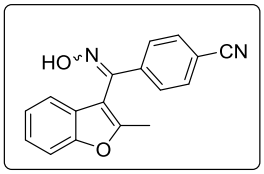
1-(4-((hydroxyimino)(2-methylbenzofuran-3-yl)methyl)phenyl)ethan-1-one **2j**, 72%, oil, Z/E = 18:1

^{1}H NMR (400 MHz, $CDCl_3$): 9.22 (s, 1H), 7.96 (d, *J* = 8.6 Hz, 2H), 7.69 (d, *J* = 8.6 Hz, 2H), 7.50 (d, *J* = 8.2 Hz, 1H), 7.30 – 7.25 (m, 1H), 7.15 (d, *J* = 9.0, 7.8, 1.1 Hz, 2H), 2.64 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 197.8, 155.7, 154.1, 150.5, 139.5, 137.6, 129.5, 128.5, 128.3, 127.7 (d, *J* = 22.3 Hz), 127.5-127.4, 123.9 (d, *J* = 19.6 Hz), 123.0, 122.8, 120.8, 120.6, 110.9, 108.0, 26.6, 14.3. IR(cm^{-1}): 3308, 2917, 2363, 1689, 1602, 1455, 1429, 1400, 1359, 1266, 1180, 1151, 1128, 1014, 978, 932, 839, 741, 701, 592. HRMS (ESI) m/z calcd for $C_{18}H_{16}N_1O_3^+$ $(M+H)^+$: 294.1125, found 294.1128.



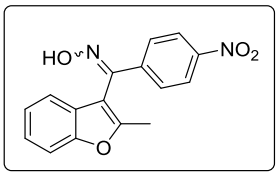
methyl-4-((hydroxyimino)(2-methylbenzofuran-3-yl)methyl)benzoate **2k**, 74%, oil, Z/E = 10.0:1

^{1}H NMR (400 MHz, $CDCl_3$): 9.13 (s, 1H), 8.05 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.2 Hz, 1H), 7.28 (t, *J* = 6.7 Hz, 1H), 7.15 (q, *J* = 8.0 Hz, 2H), 3.95 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 168.7, 166.7 (d, *J* = 6.7 Hz), 155.7, 154.2, 153.9, 150.7, 139.5, 132.2, 131.6, 130.3, 130.1, 129.9-129.5 (m), 129.3, 127.7-127.3 (m), 126.8, 123.9 (d, *J* = 19.1 Hz), 123.1, 122.8, 116.2, 110.9, 110.7, 108.1, 52.3 (d, *J* = 6.3 Hz), 14.3, 13.8. IR (cm^{-1}): 3392, 2952, 2363, 1717, 1700, 1606, 1455, 1435, 1404, 1287, 1248, 1179, 1105, 1017, 976, 931, 915, 861, 825, 775, 735, 703. HRMS (ESI) m/z calcd for $C_{18}H_{16}N_1O_4^+$ $(M+H)^+$: 310.1074, found 310.1078.



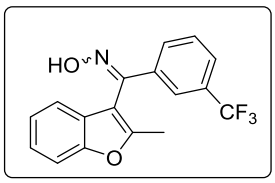
4-((hydroxyimino)(2-methylbenzofuran-3-yl)methyl)benzonitrile **2l**, 80%, M.P.= 123-125 ℃, yellow solid, Z/E = 8:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.88 (s, 1H), 7.69 (dd, *J* = 21.5, 8.6 Hz, 4H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.29 (t, *J* = 8.3 Hz, 1H), 7.17 (t, *J* = 7.5 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.1, 155.8, 154.2, 153.8, 151.0, 150.1, 139.4, 137.0, 132.7, 132.3, 132.1, 130.0, 127.9, 127.4, 124.2, 124.0, 123.1, 122.9, 120.6, 120.3, 118.4, 118.3, 113.1, 111.8, 111.0, 110.8, 107.4, 14.3, 13.8. IR (cm^{-1}): 3356, 3055, 2364, 2229, 1717, 1603, 1506, 1474, 1455, 1394, 1265, 1248, 1179, 1127, 1014, 979, 932, 840, 735, 702. HRMS (ESI) m/z calcd for $C_{17}H_{13}N_2O_2^+$ $(M+H)^+$: 277.0972, found 277.0986.



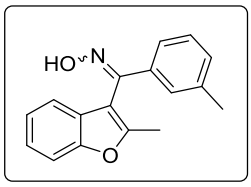
(2-methylbenzofuran-3-yl)(4-nitrophenyl)methanone oxime **2m**, 45%, M.P.=139-141 ℃, yellow solid, Z/E = 9:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.75 (s, 1H), 8.26 – 8.20 (m, 2H), 7.80 – 7.76 (m, 2H), 7.52 (d, *J* = 8.2 Hz, 1H), 7.32 – 7.27 (m, 1H), 7.20 – 7.15 (m, 1H), 7.09 (d, *J* = 7.7 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 156.1, 155.9, 154.2, 153.8, 150.9, 149.9, 148.4, 148.0, 141.1, 133.4, 130.6, 130.4, 128.3 (d, *J* = 18.5 Hz), 127.3, 126.9, 124.1 (d, *J* = 19.0 Hz), 123.9-123.5, 123.2, 123.0, 120.6, 120.3, 111.1, 110.8, 107.4, 14.3, 13.9. IR (cm^{-1}): 3309, 3045, 2365, 1716, 1683, 1598, 1518, 1489, 1474, 1455, 1435, 1345, 1288, 1263, 1249, 1179, 1129, 1106, 1013, 979, 933, 916, 850, 750, 736, 700. HRMS (ESI) m/z calcd for $C_{16}H_{13}N_2O_4^+$ $(M+H)^+$: 297.0870, found 297.0877.



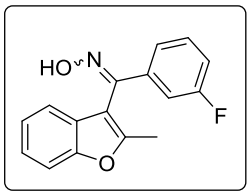
(2-methylbenzofuran-3-yl)(3-(trifluoromethyl)phenyl)methanone oxime **2n**, 60%, oil, Z/E = 13.0:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.86 (s, 1H), 7.94 (s, 1H), 7.72 (dd, *J* = 21.4, 7.8 Hz, 2H), 7.54 – 7.48 (m, 2H), 7.29 (ddd, *J* = 8.3, 5.6, 1.7 Hz, 1H), 7.16 (ddd, *J* = 8.8, 7.4, 1.0 Hz, 2H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 156.1, 155.8, 154.2, 153.8, 151.3, 150.3, 136.0, 133.2, 132.7, 131.6, 131.3, 130.9 (d, *J* = 18.0 Hz), 129.1, 128.9, 127.9, 127.6-127.5, 127.5-127.0, 126.3 (dd, *J* = 7.4, 3.7 Hz), 125.2, 124.4-123.8, 123.2, 122.9, 122.5, 120.7 (d, *J* = 16.6 Hz), 112.2, 110.9, 110.7, 107.8, 15.1, 14.3, 13.8. ^{19}F NMR (376 MHz, $CDCl_3$): -62.69 (d, 3F), -62.64 (d, 3F). IR (cm^{-1}): 3274, 3064, 2364, 1616, 1473, 1455, 1436, 1327, 1284, 1245, 1167, 1125, 1072, 1014, 978, 954, 906, 850, 805, 790, 743, 695, 657. HRMS (ESI) m/z calcd for $C_{17}H_{13}F_3N_1O_2^+$ $(M+H)^+$: 320.0893, found 320.0899.



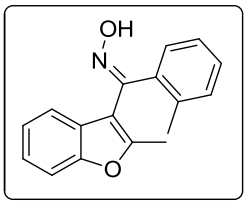
(2-methylbenzofuran-3-yl)(m-tolyl)methanone oxime **2o**, 57%, oil, Z/E = 10.0:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.90 (s, 1H), 7.50 (d, *J* = 8.2 Hz, 1H), 7.43 (s, 1H), 7.37 (d, *J* = 6.4 Hz, 1H), 7.27 (dd, *J* = 9.3, 5.3 Hz, 3H), 7.18 (dd, *J* = 13.9, 6.9 Hz, 2H), 2.37 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 156.0, 155.4, 154.1, 153.7, 151.5, 138.2 (d, *J* = 14.1 Hz), 135.1, 130.5, 130.1, 129.4, 128.3, 127.9 (d, *J* = 7.4 Hz), 126.1, 124.7, 123.7 (d, *J* = 18.4 Hz), 122.9, 122.7, 120.9, 110.7, 108.6, 21.3, 14.2, 13.8. IR (cm^{-1}): 3275, 3036, 2919, 2363, 1716, 1603, 1558, 1540, 1474, 1455, 1436, 1387, 1270, 1250, 1177, 1124, 976, 957, 910, 850, 817, 788, 746, 704. HRMS (ESI) m/z calcd for $C_{17}H_{16}N_1O_2^+$ $(M+H)^+$: 266.1176, found 266.1187.



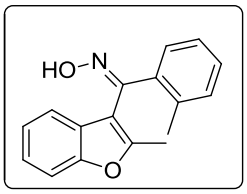
(3-fluorophenyl)(2-methylbenzofuran-3-yl)methanone oxime **2p**, 65%, oil, Z/E = 13.0:1

^{1}H NMR (400 MHz, $CDCl_3$): 9.21 (s, 1H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.38 – 7.32 (m, 3H), 7.32 – 7.27 (m, 1H), 7.19 (dd, *J* = 4.8, 0.9 Hz, 2H), 7.13 (ddd, *J* = 5.2, 4.0, 2.1 Hz, 1H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 164.1, 161.6, 156.0, 155.6, 154.1, 153.8, 150.5 (d, *J* = 2.8 Hz), 137.4 (d, *J* = 7.7 Hz), 130.0 (d, *J* = 10.0 Hz), 127.6, 127.3, 125.0, 123.9 (d, *J* = 18.3 Hz), 123.2 (d, *J* = 10.6 Hz), 122.8, 120.7 (d, *J* = 13.5 Hz), 116.8, 116.7-116.2, 114.4, 114.1, 110.9, 110.6, 108.1, 14.2, 13.7. ^{19}F NMR (376 MHz, $CDCl_3$): -112.23 (s, 1F), -112.44 (s, 1F). IR (cm^{-1}): 3273, 2921, 1608, 1581, 1486, 1454, 1389, 1267, 1250, 1200, 1177, 1100, 1013, 971, 909, 830, 788, 741, 704. HRMS (ESI) m/z calcd for $C_{16}H_{13}FNO_2^+$ $(M+H)^+$: 270.0925, found 270.0926.



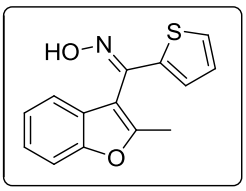
(E-)-(2-methylbenzofuran-3-yl)(o-tolyl)methanone oxime (minor) **2q**, 27%, pale yellow solid, M.P.= 100-102 ℃.

^{1}H NMR (400 MHz, $CDCl_3$): 7.73 (d, *J* = 7.8 Hz, 1H), 7.44 – 7.36 (m, 3H), 7.34 – 7.27 (m, 2H), 7.23 (qd, *J* = 7.6, 1.3 Hz, 2H), 2.32 (s, 3H), 2.01 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 156.1, 155.7, 154.1, 153.8 (d, *J* = 18.5 Hz), 151.9, 137.0, 136.0, 135.4, 133.5, 130.9, 130.1, 129.8, 129.1 (d, *J* = 8.7 Hz), 127.8, 127.2 (d, *J* = 62.4 Hz), 126.0 (d, *J* = 8.8 Hz), 124.0, 123.6, 123.1, 122.7, 121.8, 121.2, 112.0, 110.6 (d, *J* = 19.6 Hz), 110.1, 20.2, 19.5, 14.3, 13.5. IR(cm^{-1}): 3274, 2927, 2359, 1601, 1474, 1454, 1387, 1280, 1246, 1178, 1025, 975, 909, 892, 742, 727, 669. HRMS (ESI) m/z calcd for $C_{17}H_{16}N_1O_2^+$ $(M+H)^+$: 266.1176, found 266.1186.



(Z)-(2-methylbenzofuran-3-yl)(o-tolyl)methanone oxime (major) **2q'**, 43%, oil.

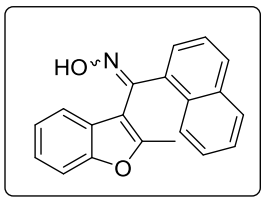
^{1}H NMR (400 MHz, $CDCl_3$): 9.41 (s, 1H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.33 (td, *J* = 7.5, 1.4 Hz, 1H), 7.29 – 7.22 (m, 3H), 7.20 (d, *J* = 3.7 Hz, 1H), 7.17 – 7.12 (m, 1H), 2.30 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 156.2, 155.7, 154.1, 153.8 (d, *J* = 18.5 Hz), 151.9, 137.0, 136.0, 135.4, 133.5, 130.9, 130.1, 129.8, 129.1 (d, *J* = 8.7 Hz), 127.8, 127.2 (d, *J* = 62.4 Hz), 126.0 (d, *J* = 8.8 Hz), 124.0, 123.6, 123.1, 122.7, 121.8, 121.2, 112.0, 110.5 (d, *J* = 19.6 Hz), 110.1, 20.2, 19.5, 14.3, 13.5. IR(cm^{-1}): 3274, 2919, 2363, 1603, 1474, 1455, 1436, 1388, 1270, 1248, 1178, 1124, 1025, 975, 909, 892, 742, 704. HRMS (ESI) m/z calcd for $C_{17}H_{16}N_1O_2^+$ $(M+H)^+$: 266.1176, found 266.1187.



(E)-(2-methylbenzofuran-3-yl)(thiophen-2-yl)methanone oxime (**minor**) **E-2r** (isolated), 21%, oil.

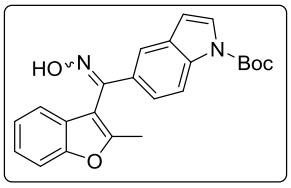
^{1}H NMR (400 MHz, $CDCl_3$): 8.52 (s, 1H), 7.50 (d, *J* = 8.1 Hz, 1H), 7.36 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.29 (ddd, *J* = 8.2, 7.1, 1.4 Hz, 1H), 7.22 (dd, *J* = 10.8, 4.2 Hz, 1H), 7.02 (ddd, *J* = 8.7, 4.3, 2.5 Hz, 2H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 155.3 (d, *J* = 6.2 Hz), 154.1, 153.8, 147.1, 144.7, 138.6, 132.6, 131.5, 129.2, 128.6, 127.7-127.2, 125.8, 123.7 (d, *J* = 2.9 Hz), 122.8 (d, *J* = 4.6 Hz), 120.7, 120.0, 112.1, 110.8 (d, *J* = 4.7 Hz), 108.1, 14.2. IR(cm^{-1}): 3273, 2920, 2359, 1609,

1474, 1454, 1418, 1389, 1263, 1247, 1179, 1119, 1100, 1054, 975, 919, 878, 840, 729, 708. HRMS (ESI) m/z calcd for $C_{14}H_{12}N_1O_2S^+$ $(M+H)^+$: 258.0583, found 258.0598.



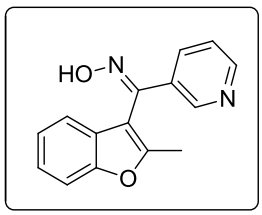
(2-methylbenzofuran-3-yl)(naphthalen-1-yl)methanone oxime **2s**, 63%, M.P.= 146-148 ℃ white solid, Z/E = 4:1

^{1}H NMR (400 MHz, DMSO): 11.90 (s, 1H), 8.14 (d, *J* = 8.3 Hz, 1H), 7.99 (t, *J* = 7.3 Hz, 2H), 7.52 (dd, *J* = 14.7, 5.8 Hz, 4H), 7.49 – 7.43 (m, 1H), 7.21 (t, *J* = 7.3 Hz, 1H), 7.08 (t, *J* = 7.4 Hz, 1H), 7.01 (d, *J* = 7.5 Hz, 1H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, DMSO): 155.1, 153.8, 148.8, 134.3, 133.9, 131.5, 129.8, 129.0, 128.4, 128.0, 127.1, 126.5, 125.8, 125.4, 124.1, 123.3, 121.0, 111.7, 111.2, 14.6. IR (cm^{-1}): 3275, 3049, 2364, 1615, 1455, 1266, 1052, 1026, 1007, 969, 914, 724, 700. HRMS (ESI) m/z calcd for $C_{20}H_{15}N_1O_2^+$ $(M+H)^+$: 302.1176, found 302.1180.



tert-butyl-5-((hydroxyimino)(2-methylbenzofuran-3-yl)methyl)-1H-indole-1-carboxylate, **2t**, 45%, oil, Z/E = 17:1

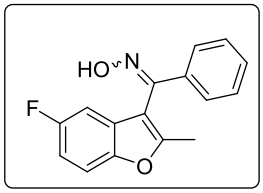
^{1}H NMR (400 MHz, $CDCl_3$): 9.37 (s, 1H), 8.15 (d, *J* = 8.7 Hz, 1H), 7.77 (d, *J* = 1.4 Hz, 1H), 7.67 – 7.60 (m, 2H), 7.52 (d, *J* = 8.2 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.22 (d, *J* = 6.8 Hz, 1H), 7.18 – 7.13 (m, 1H), 6.56 (d, *J* = 3.7 Hz, 1H), 2.40 (s, 3H), 1.71 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): 155.9, 155.6, 154.1, 153.7, 151.5, 149.5, 135.9, 131.7, 130.7, 130.3, 130.0, 129.8, 128.0, 127.7, 126.7 (d, *J* = 19.2 Hz), 125.4, 123.6 (d, *J* = 6.6 Hz), 122.8 (d, *J* = 19.4 Hz), 122.2, 121.0, 120.5, 115.2, 115.0, 113.1, 110.7, 110.5, 109.0, 107.6, 84.0, 65.8, 28.1, 15.2, 14.3, 13.7. IR(cm^{-1}): 3273, 2980, 2363, 1733, 1608, 1540, 1471, 1455, 1374, 1328, 1323, 1264, 1236, 1174, 1137, 1081, 1023, 965, 849, 823, 785, 731, 703, 611. HRMS (ESI) m/z calcd for $C_{23}H_{23}N_2O_4^+$ $(M+H)^+$: 391.1652, found 391.1640.



(Z)-(2-methylbenzofuran-3-yl)(pyridin-3-yl)methanone oxime **2u**, 44%, M.P.= 152-154 ℃, white solid

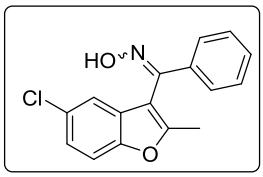
^{1}H NMR (400 MHz, DMSO): 12.00 (s, 1H), 8.71 (s, 1H), 8.60 (d, *J* = 3.8 Hz, 1H), 7.86 – 7.80 (m, 1H), 7.59 (d, *J* = 8.2 Hz, 1H), 7.42 (dd, *J* = 8.0, 4.8 Hz, 1H), 7.27 (t, *J*

= 8.2 Hz, 1H), 7.15 (t, *J* = 7.2 Hz, 1H), 7.01 (d, *J* = 7.6 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, DMSO): 155.3, 154.0, 150.4, 147.9, 146.5, 134.5, 131.8, 127.9, 124.1 (d, *J* = 3.2 Hz), 123.3, 120.6, 111.3, 108.4, 14.4. IR (cm^{-1}): 3397, 2363, 1635, 1475, 1455, 1417, 1179, 1021, 1003, 937, 915, 821, 751, 708, 624. HRMS (ESI) m/z calcd for $C_{15}H_{13}N_2O_2^+$ $(M+H)^+$: 253.0972, found 253.0980.



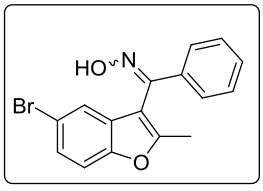
(5-fluoro-2-methylbenzofuran-3-yl)(phenyl)methanone oxime **2v**, 74%, M.P.=118-120 ℃, brown solid, Z/E = 15.0:1

^{1}H NMR (400 MHz, $CDCl_3$): 9.47 (s, 1H), 7.60 – 7.56 (m, 2H), 7.41 (ddd, *J* = 14.4, 10.2, 7.1 Hz, 4H), 6.99 (td, *J* = 9.1, 2.6 Hz, 1H), 6.88 (dd, *J* = 8.7, 2.6 Hz, 1H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 160.4 (d, *J* = 19.1 Hz), 158.3-157.7, 157.6, 152.4, 150.9, 150.3, 149.9, 134.8, 132.2, 129.9, 129.6, 129.1, 128.8 (d, *J* = 13.3 Hz), 128.5, 127.5, 111.4 (q, *J* = 16.9 Hz), 109.0 (d, *J* = 3.7 Hz), 107.1, 106.9, 106.7, 14.4, 13.9. ^{19}F NMR (376 MHz, $CDCl_3$): -120.29 (s, 1F), -120.55 (s, 1F). IR (cm^{-1}): 3274, 3057, 2921, 2364, 1623, 1595, 1558, 1469, 1389, 1363, 1265, 1250, 1168, 1117, 1096, 980, 952, 921, 855, 797, 766, 737, 696, 647, 594. HRMS (ESI) m/z calcd for $C_{16}H_{13}F_1N_1O_2^+$ $(M+H)^+$: 270.0925, found 270.0936.



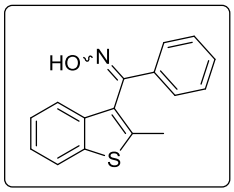
(5-chloro-2-methylbenzofuran-3-yl)(phenyl)methanone oxime **2w**, 76%, M.P.= 147-149 ℃, brown solid, Z/E = 43:1

^{1}H NMR (400 MHz, $CDCl_3$): 9.55 (s, 1H), 7.60 – 7.56 (m, 2H), 7.46 – 7.38 (m, 4H), 7.26 – 7.21 (m, 2H), 2.35 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$): 157.5, 157.1, 152.5, 152.1, 150.8, 134.7, 129.9, 129.6, 129.2, 129.0, 128.9-128.3, 127.3, 124.0 (d, *J* = 19.1 Hz), 120.9, 120.6, 111.7, 111.5, 108.5, 14.2, 13.8. IR (cm^{-1}): 3226, 3057, 2922, 2364, 1604, 1577, 1456, 1388, 1259, 1186, 1134, 1059, 1008, 980, 944, 916, 893, 860, 800, 760, 734, 693, 583. HRMS (ESI) m/z calcd for $C_{16}H_{13}ClN_1O_2^+$ $(M+H)^+$: 286.0629, found 286.0632.



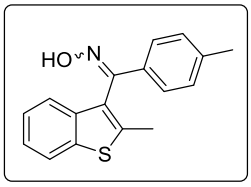
(5-bromo-2-methylbenzofuran-3-yl)(phenyl)methanone oxime **2x**, 58%, M.P.=158-160 ℃, brown solid, Z/E = 30.0:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.82 (s, 1H), 7.58 – 7.54 (m, 2H), 7.47 – 7.38 (m, 3H), 7.37 – 7.35 (m, 3H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 157.4, 156.9, 152.9, 152.5 (d, *J* = 7.3 Hz), 150.8, 134.7, 132.9, 132.2, 130.5, 129.9 (d, *J* = 14.6 Hz), 129.6, 129.3, 129.0, 128.7, 128.5, 127.3, 126.8, 126.6, 124.1, 123.6, 116.2, 115.9, 112.3 (d, *J* = 15.9 Hz), 112.0, 108.3, 14.2, 13.8. IR (cm^{-1}): 3274, 3056, 2364, 1714, 1603, 1576, 1489, 1455, 1388, 1260, 1185, 1133, 1049, 978, 939, 916, 892, 860, 798, 767, 737, 694, 680, 637, 579. HRMS (ESI) m/z calcd for $C_{16}H_{13}BrN_1O_2^+$ $(M+H)^+$: 330.0124, found 330.0120.



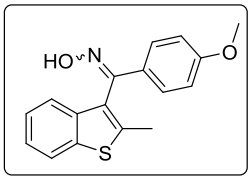
(2-methylbenzo[b]thiophen-3-yl)(phenyl)methanone oxime **4a**, 71%, M.P.=153-155 ℃, white solid, Z/E = 25.0:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.59 (s, 1H), 7.83 (d, *J* = 7.2 Hz, 1H), 7.58 – 7.52 (m, 2H), 7.40 – 7.27 (m, 6H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 153.4, 140.0, 138.4, 134.8, 129.7, 128.6, 128.2, 126.8, 125.1, 124.3, 123.9, 122.5, 122.0, 15.1. IR (cm^{-1}): 3247, 3063, 2918, 2363, 1607, 1580, 1541, 1485, 1434, 1353, 1285, 1259, 1190, 1170, 1154, 1086, 1065, 1024, 1001, 977, 870, 839, 782, 731, 680, 634, 616. HRMS (ESI) m/z calcd for $C_{16}H_{14}N_1O_1S^+$ $(M+H)^+$: 268.0791, found 268.0799.



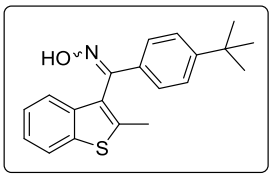
(2-methylbenzo[b]thiophen-3-yl)(p-tolyl)methanone oxime **4b**, 68%, oil, Z/E = 19:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.84 (s, 1H), 7.83 (d, *J* = 7.3 Hz, 1H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.38 – 7.26 (m, 3H), 7.15 (d, *J* = 8.0 Hz, 2H), 2.46 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 153.3, 144.2, 139.8 (d, *J* = 6.8 Hz), 138.5 (d, *J* = 5.7 Hz), 137.9, 136.0, 132.1, 129.8 (d, *J* = 11.9 Hz), 129.3, 128.9, 126.8, 125.3, 124.6, 124.2 (d, *J* = 11.9 Hz), 123.9, 123.2, 122.6, 121.9, 121.7, 21.7, 21.3, 15.6, 15.1. IR (cm^{-1}): 3274, 3055, 2918, 2361, 1652, 1603, 1558, 1508, 1457, 1434, 1308, 1264, 1179, 1154, 955, 910, 824, 731, 702, 608, 583. HRMS (ESI) m/z calcd for $C_{17}H_{16}NOS^+$ $(M+H)^+$: 282.0947, found 282.0955.



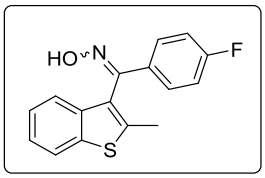
(4-methoxyphenyl)(2-methylbenzo[b]thiophen-3-yl)methanone oxime **4c**, 71%, oil, Z/E = 15:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.86 (s, 1H), 7.83 (dd, *J* = 6.7, 1.3 Hz, 1H), 7.49 – 7.44 (m, 2H), 7.38 – 7.27 (m, 3H), 6.88 – 6.83 (m, 2H), 3.82 (s, 3H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 160.8, 152.8, 139.8, 138.5 (d, *J* = 3.7 Hz), 131.7, 128.3, 127.7, 127.3, 125.3 (d, *J* = 16.8 Hz), 124.3, 123.8 (d, *J* = 13.0 Hz), 122.6, 121.9 (d, *J* = 19.6 Hz), 114.0, 113.5, 55.2, 15.1, 14.7. IR (cm^{-1}): 3275, 3055, 2930, 2363, 1716, 1647, 1597, 1558, 1508, 1457, 1350, 1308, 1249, 1240, 1165, 1111, 1023, 909, 879, 842, 802, 780, 731, 637, 604, 558. HRMS (ESI) m/z calcd for $C_{17}H_{16}N_1O_2S^+$ $(M+H)^+$: 298.0896, found 298.0890.



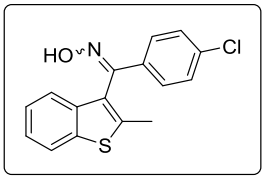
(4-(tert-butyl)phenyl)(2-methylbenzo[b]thiophen-3-yl)methanone oxime **4d**, 71%, oil, Z/E = 15.0:1

^{1}H NMR (400 MHz, $CDCl_3$): 9.15 (s, 1H), 7.84 (dd, *J* = 6.9, 1.6 Hz, 1H), 7.48 (d, *J* = 8.6 Hz, 2H), 7.41 – 7.34 (m, 3H), 7.33 – 7.27 (m, 2H), 2.48 (s, 3H), 1.34 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): 153.2, 152.9, 139.7, 138.5 (d, *J* = 6.4 Hz), 131.9, 129.6, 127.9, 126.5, 125.5 (d, *J* = 13.8 Hz), 125.1, 124.5, 124.3, 123.9, 122.6, 121.9, 34.6, 31.1, 15.1. IR (cm^{-1}): 3275, 2962, 2363, 1603, 1558, 1456, 1434, 1362, 1265, 1250, 1176, 1154, 1088, 957, 913, 840, 764, 732, 703, 605. HRMS (ESI) m/z calcd for $C_{20}H_{22}N_1O_1S^+$ $(M+H)^+$: 324.1417, found 324.1410.



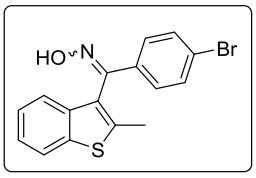
(4-fluorophenyl)(2-methylbenzo[b]thiophen-3-yl)methanone oxime **4e**, 86%, M.P.= 148-150 ℃, yellow solid, Z/E = 100:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.89 (s, 1H), 7.90 – 7.79 (m, 1H), 7.36 – 7.26 (m, 6H), 7.10 (tdd, *J* = 7.4, 4.9, 2.6 Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 164.1, 161.7, 152.5 (d, *J* = 2.9 Hz), 140.3, 138.5, 138.2, 137.1 (d, *J* = 7.7 Hz), 130.1 (d, *J* = 8.2 Hz), 124.5 (d, *J* = 12.7 Hz), 124.0, 122.6 (d, *J* = 2.9 Hz), 122.3, 122.1, 116.8, 116.6, 113.7, 113.5, 15.1. ^{19}F NMR (376 MHz, $CDCl_3$): -112.35 (s). IR (cm^{-1}): 3400, 3057, 1613, 1489, 1434, 1266, 1213, 1073, 1023, 1002, 960, 816, 758, 732, 625. HRMS (ESI) m/z calcd for $C_{16}H_{13}F_1N_1O_1S^+$ $(M+H)^+$: 286.0696, found 286.0697.



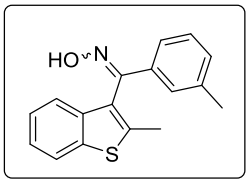
(4-chlorophenyl)(2-methylbenzo[b]thiophen-3-yl)methanone oxime **4f**, 83%, oil, Z/E = 23:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.90 (s, 1H), 7.84 (d, *J* = 7.4 Hz, 1H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.32 (d, *J* = 8.3 Hz, 5H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 152.5, 140.3, 138.5, 138.2, 137.9, 135.8, 133.3, 131.3, 128.9, 128.5, 128.1, 124.5 (d, *J* = 17.0 Hz), 124.0, 122.4, 122.0 (d, *J* = 18.8 Hz), 15.3, 14.9. IR(cm^{-1}): 3269, 3058, 2917, 2358, 1590, 1560, 1489, 1458, 1434, 1280, 1250, 1176, 1088, 1012, 957, 905, 833, 759, 727, 648. HRMS (ESI) m/z calcd for $C_{16}H_{13}ClN_1O_1S^+$ $(M+H)^+$: 302.0401, found 302.0407.



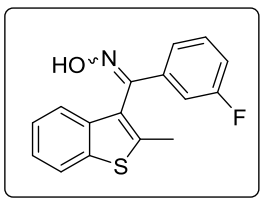
(4-bromophenyl)(2-methylbenzo[b]thiophen-3-yl)methanone oxime **4g**, 78%, oil, Z/E = 19:1

^{1}H NMR (400 MHz, $CDCl_3$): 8.72 (s, 1H), 7.83 (d, *J* = 7.5 Hz, 1H), 7.47 (d, *J* = 8.6 Hz, 2H), 7.40 (d, *J* = 8.7 Hz, 2H), 7.33 – 7.27 (m, 3H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 152.6, 140.3, 138.5, 138.2, 133.8, 131.8, 131.5 (d, *J* = 4.4 Hz), 128.3, 124.4 (d, *J* = 5.7 Hz), 124.0 (t, *J* = 8.9 Hz), 122.3, 122.0 (d, *J* = 18.7 Hz), 15.1, 14.8. IR (cm^{-1}): 3273, 2918, 2247, 1586, 1486, 1434, 1249, 1176, 1070, 1009, 957, 904, 831, 784, 769, 727, 648. HRMS (ESI) m/z calcd for $C_{16}H_{13}BrN_1O_1S^+$ $(M+H)^+$: 345.9896, found 345.9885.



(2-methylbenzo[b]thiophen-3-yl)(m-tolyl)methanone oxime **4h**, 71%, oil, Z/E = 38:1

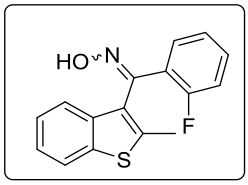
^{1}H NMR (400 MHz, $CDCl_3$): 8.96 (s, 1H), 7.88 – 7.80 (m, 1H), 7.38 (dd, *J* = 10.1, 2.4 Hz, 2H), 7.35 – 7.28 (m, 3H), 7.23 (d, *J* = 5.8 Hz, 2H), 2.47 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 152.0, 141.5, 138.3, 138.0, 134.6, 133.2, 131.2, 130.6, 130.3, 129.8, 126.7 (d, *J* = 26.0 Hz), 125.3, 124.5, 124.2, 123.7, 122.8, 121.8, 15.6, 15.1. IR (cm^{-1}): 3245, 3049, 2916, 2636, 1457, 1434, 1283, 1258, 1187, 1132, 1095, 1065, 993, 959, 909, 883, 825, 796, 778, 750, 724, 694, 674, 629, 610. HRMS (ESI) m/z calcd for $C_{17}H_{16}N_1O_1S^+$ $(M+H)^+$: 282.0947, found 282.0954.



(3-fluorophenyl)(2-methylbenzo[b]thiophen-3-yl)methanone oxime **4i**, 83%, M.P.= 168-170 ℃, brown solid, Z/E = 75.0:1

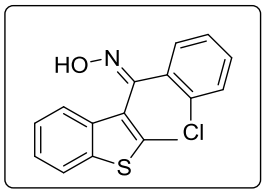
^{1}H NMR (400 MHz, $CDCl_3$): 8.79 (s, 1H), 7.89 – 7.81 (m, 1H), 7.36 – 7.28 (m, 6H), 7.10 (ddd, *J* = 11.8, 7.2, 3.6 Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$):

164.1, 161.7, 152.6 (d, *J* = 2.9 Hz), 140.3, 138.5, 138.2, 137.1 (d, *J* = 7.6 Hz), 130.1 (d, *J* = 8.2 Hz), 124.5 (d, *J* = 14.7 Hz), 124.0, 122.7 (d, *J* = 2.9 Hz), 122.3, 122.1, 116.8, 116.6, 113.7, 113.5, 15.0. ^{19}F NMR (376 MHz, $CDCl_3$): -112.37 (s). IR (cm^{-1}): 3245, 3064, 2917, 2363, 1607, 1580, 1541, 1485, 1434, 1285, 1259, 1190, 1170, 1154, 1086, 1024, 1001, 977, 870, 839, 794, 756, 731, 691, 680, 670, 634, 616. HRMS (ESI) m/z calcd for $C_{16}H_{13}F_1N_1O_1S^+$ $(M+H)^+$: 286.0696, found 286.0699.



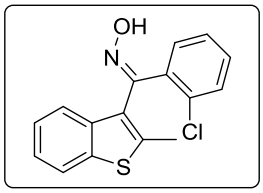
(2-fluorophenyl)(2-methylbenzo[b]thiophen-3-yl)methanone oxime **4j**, 79%, oil, Z/E = 23.0:1

^{1}H NMR (400 MHz, DMSO): 11.84 (s, 1H), 7.89 (s, 1H), 7.47 – 7.40 (m, 2H), 7.30 – 7.19 (m, 5H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, DMSO): 161.4, 159.0, 147.4 (d, *J* = 2.3 Hz), 139.1, 138.5, 138.0, 131.3 (d, *J* = 8.4 Hz), 130.5 (d, *J* = 2.6 Hz), 127.0, 125.0 (d, *J* = 3.5 Hz), 124.8-124.4, 124.2, 122.6, 122.3, 116.9, 116.6, 55.3, 40.6, 40.4, 40.2, 40.0, 39.7, 39.5, 39.3, 15.2. ^{19}F NMR (376 MHz, DMSO): -109.93 (s, 1F), -114.49 (s, 1F). IR (cm^{-1}): 3275, 3054, 1609, 1488, 1434, 1266, 1211, 1074, 1023, 1001, 960, 817, 758, 732, 704, 625. HRMS (ESI) m/z calcd for $C_{16}H_{13}F_1N_1O_1S^+$ $(M+H)^+$: 286.0696, found 286.0699.



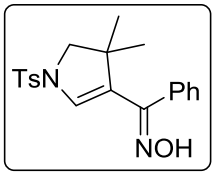
(E)-(2-chlorophenyl)(2-methylbenzo[b]thiophen-3-yl)methanone oxime **4k**, 52%, M.P.= 139 - 141 ℃, brown solid.

^{1}H NMR (400 MHz, $CDCl_3$): 9.44 (s, 1H), 7.82 – 7.74 (m, 1H), 7.51 (dd, *J* = 7.4, 1.9 Hz, 1H), 7.45 – 7.38 (m, 2H), 7.35 – 7.26 (m, 4H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 152.0, 141.5, 138.3, 138.0, 134.6, 133.2, 131.2, 130.6, 130.3, 129.8, 126.7 (d, *J* = 26.0 Hz), 125.3, 124.5, 124.2, 123.7, 122.8, 121.8, 15.6, 15.1. IR (cm^{-1}): 3258, 3058, 1473, 1423, 1289, 1263, 1154, 1129, 1055, 1001, 957, 927, 904, 760, 732, 715, 704, 638. HRMS (ESI) m/z calcd for $C_{16}H_{13}ClN_1O_1S^+$ $(M+H)^+$: 302.0401, found 302.0407.



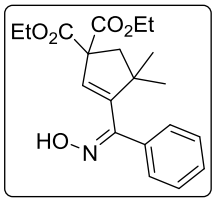
(Z)-(2-chlorophenyl)(2-methylbenzo[b]thiophen-3-yl)methanone oxime **4k'**, 20%, oil.

^{1}H NMR (400 MHz, $CDCl_3$): 8.63 (s, 1H), 7.81 – 7.73 (m, 2H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.39 – 7.33 (m, 3H), 7.31 – 7.28 (m, 2H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 151.7, 142.4, 139.2, 137.6, 133.0 (d, *J* = 5.5 Hz), 130.3 (t, *J* = 13.8 Hz), 129.8, 127.2, 126.6 (d, *J* = 14.6 Hz), 124.6 (d, *J* = 17.4 Hz), 124.1, 123.9, 122.8, 121.7, 15.1. IR (cm^{-1}): 3261, 3055, 1474, 1433, 1361, 1287, 1264, 1239, 1176, 1155, 1128, 1066, 1053, 1027, 1001, 956, 928, 904, 787, 756, 733, 715, 704, 677, 650, 635.



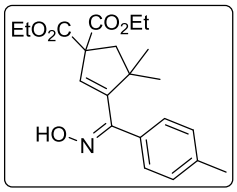
(4,4-dimethyl-1-tosyl-4,5-dihydro-1H-pyrrol-3-yl)(phenyl)methanone oxime, 72%

^{1}H NMR (400 MHz, $CDCl_3$): 7.73 (d, *J* = 8.3 Hz, 2H), 7.37 (dd, *J* = 7.1, 4.7 Hz, 5H), 7.32 (d, *J* = 6.9 Hz, 2H), 6.61 (s, 1H), 3.31 (s, 2H), 2.48 (s, 3H), 0.92 (s, 6H).



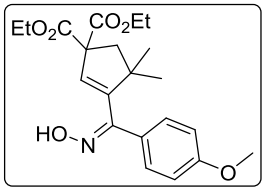
diethyl (Z)-3-((hydroxyimino)(phenyl)methyl)-4,4-dimethylcyclopent-2-ene-1,1-dicarboxylate, **6a**, oil, 56%, Z:E >98:2.

^{1}H NMR (400 MHz, $CDCl_3$): 8.16 (s, 1H, OH), 7.67 (dd, *J* = 6.5, 3.2 Hz, 2H), 7.38 (dd, *J* = 5.2, 1.8 Hz, 3H), 5.86 (s, 1H), 4.28 (q, *J* = 7.1 Hz, 4H), 2.51 (s, 2H), 1.32 (t, *J* = 7.1 Hz, 6H), 1.05 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 171.1, 154.9, 146.9, 135.1, 129.5, 128.3, 127.3, 126.9, 65.5, 61.7, 49.0, 46.6, 28.9. IR (cm^{-1}): 3445, 2978, 2870, 1958, 1932, 1731, 1553, 1494, 1463, 1445, 1388, 1366, 1256, 1208, 1137, 1099, 1076, 1061, 1039, 1015, 978, 955, 922, 853, 772, 697. HRMS (ESI) m/z calcd for $C_{20}H_{25}N_1O_5^+$ $(M+H)^+$: 360.1805, found 360.1818.



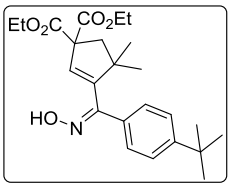
Diethyl-(Z)-3-((hydroxyimino)(p-tolyl)methyl)-4,4-dimethylcyclopent-2-ene-1,1-dicarboxylate, **6b**, M.P. = 119 -121 ℃, 60%, Z:E >98:2.

^{1}H NMR (400 MHz, $CDCl_3$): 8.31 (s, 1H, OH), 7.55 (d, *J* = 8.2 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 5.83 (s, 1H), 4.28 (q, *J* = 7.1 Hz, 4H), 2.51 (s, 2H), 2.37 (s, 3H), 1.32 (t, *J* = 7.1 Hz, 6H), 1.05 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 171.2, 154.8, 147.1, 139.5, 132.3, 129.0, 127.0, 126.8, 65.5, 61.7, 49.0, 46.6, 28.9, 21.3, 14.0. IR (cm^{-1}): 3450, 2978, 2931, 2869, 1959, 1933, 1731, 1605, 1533, 1511, 1463, 1387, 1366, 1257, 1213, 1136, 1098, 1062, 1040, 1015, 978, 955, 922, 852, 824, 790, 729, 628. HRMS (ESI) m/z calcd for $C_{21}H_{27}N_1O_5^+$ $(M+H)^+$: 374.1962, found 374.1969.



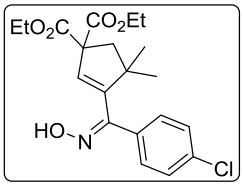
diethyl (Z)-3-((hydroxyimino)(4-methoxyphenyl)methyl)-4,4-dimethylcyclopent-2-ene-1,1-dicarboxylate, **6c**, oil, 50%, Z:E >98:2.

^{1}H NMR (400 MHz, $CDCl_3$): 7.60 (d, *J* = 8.9 Hz, 2H), 6.89 (d, *J* = 8.9 Hz, 2H), 5.82 (s, 1H), 4.30 – 4.25 (m, 4H), 3.84 (s, 3H), 2.50 (s, 2H), 1.32 (t, *J* = 7.1 Hz, 6H), 1.05 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 171.2, 160.7, 154.5, 147.2, 128.3, 127.6, 127.0, 113.7, 65.4, 61.7, 55.2, 49.0, 46.6, 28.9, 14.0. IR (cm^{-1}): 3449, 2977, 2931, 1958, 1933, 1730, 1607, 1511, 1463, 1387, 1366, 1298, 1252, 1212, 1176, 1136, 1098, 1062, 1034, 978, 954, 922, 837, 785, 625. HRMS (ESI) m/z calcd for $C_{21}H_{27}N_1O_6^+$ $(M+H)^+$: 390.1911, found 390.1919.



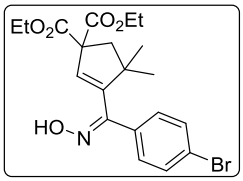
diethyl (Z)-3-((4-(tert-butyl)phenyl)(hydroxyimino)methyl)-4,4-dimethylcyclopent-2-ene-1,1-dicarboxylate, **6d**, oil, 53%, Z:E >98:2.

^{1}H NMR (400 MHz, $CDCl_3$): 8.31 (s, 1H, OH), 7.57 (s, 2H), 7.37 (d, *J* = 8.5 Hz, 2H), 5.80 (s, 1H), 4.26 (q, *J* = 7.1 Hz, 4H), 2.50 (s, 2H), 1.32 (s, 9H), 1.31 (t, *J* = 7.1 Hz, 6 H), 1.05 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 171.2, 154.7, 152.7, 147.2, 132.2, 127.1, 126.6, 65.5, 61.7, 49.0, 46.6, 34.7, 31.2, 28.9, 14.0. IR (cm^{-1}): 3449, 2962, 2904, 2858, 1958, 1932, 1731, 1604, 1554, 1508, 1463, 1389, 1365, 1256, 1206, 1139, 1095, 1062, 1039, 1016, 978, 955, 924, 842, 728, 626. HRMS (ESI) m/z calcd for $C_{24}H_{33}N_1O_5^+$ $(M+H)^+$: 416.2431, found 416.2446.



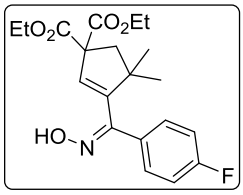
diethyl (Z)-3-((4-chlorophenyl)(hydroxyimino)methyl)-4,4-dimethylcyclopent-2-ene-1,1-dicarboxylate, **6e**, M.P. = 109 -111 ℃, 51%, Z:E >98:2.

^{1}H NMR (400 MHz, $CDCl_3$): 8.06 (s, 1H, OH), 7.61 (d, *J* = 8.7 Hz, 2H), 7.34 (d, *J* = 8.7 Hz, 2H), 5.83 (s, 1H), 4.28 (q, *J* = 7.1 Hz, 4H), 2.51 (s, 2H), 1.31 (t, *J* = 7.1 Hz, 6H), 1.04 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 171.1, 154.0, 146.7, 135.5, 133.6, 128.6, 128.2, 127.7, 61.8, 49.1, 46.5, 28.9, 14.0. IR (cm^{-1}): 3435, 2978, 1958, 1932, 1730, 1591, 1553, 1490, 1463, 1389, 1366, 1256, 1211, 1179, 1136, 1091, 1061, 1040, 1013, 979, 957, 923, 836, 730, 630. HRMS (ESI) m/z calcd for $C_{20}H_{24}C_lN_1O_5^+$ $(M+H)^+$: 394.1416, found 394.1424.



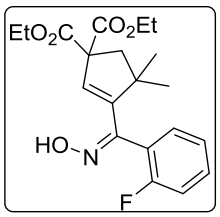
diethyl (Z)-3-((4-bromophenyl)(hydroxyimino)methyl)-4,4-dimethylcyclopent-2-ene-1,1-dicarboxylate, **6f**, M.P. = 131 -133 ℃, 49%, Z:E >98:2.

^{1}H NMR (400 MHz, $CDCl_3$): 7.97 (s, 1H, OH), 7.57 – 7.49 (m, 4H), 5.83 (s, 1H), 4.28 (q, *J* = 7.1 Hz, 4H), 2.51 (s, 2H), 1.31 (t, *J* = 7.1 Hz, 6H), 1.04 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 171.1, 154.1, 146.6, 134.1, 131.5, 128.4, 123.9, 65.5, 61.8, 49.1, 46.5, 28.9, 14.0. IR (cm^{-1}): 3432, 2960, 2917, 2848, 1958, 1932, 1730, 1586, 1486, 1463, 1390, 1366, 1256, 1206, 1180, 1134, 1098, 1073, 1009, 980, 957, 922, 851, 832, 730, 636. HRMS (ESI) m/z calcd for $C_{20}H_{24}BrN_1O_5^+(M+H)^+$: 438.0911, found 438.0911.



diethyl (Z)-3-((4-fluorophenyl)(hydroxyimino)methyl)-4,4-dimethylcyclopent-2-ene-1,1-dicarboxylate, **6g**, M.P. = 97-99 ℃, 56%, Z:E >98:2.

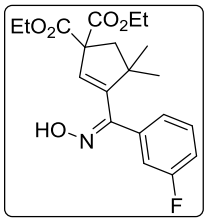
^{1}H NMR (400 MHz, $CDCl_3$): 8.30 (s, 1H, OH), 7.66 (dd, *J* = 8.8, 5.4 Hz, 2H), 7.06 (t, *J* = 8.7 Hz, 2H), 5.84 (s, 1H), 4.27 (q, *J* = 7.1 Hz, 4H), 2.51 (s, 2H), 1.31 (t, *J* = 7.1 Hz, 6H), 1.04 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 171.1, 164.8 (d, *J* = 249.0 Hz), 162.4, 153.9, 146.9, 131.3, 128.8 (d, *J* = 9.0 Hz), 128.7, 127.5, 115.5 (d, *J* = 22.0 Hz), 115.2, 65.4, 61.8, 49.0, 46.5, 28.9, 14.0. ^{19}F NMR (376 MHz, $CDCl_3$): -111.71. IR (cm^{-1}): 3440, 2979, 2934, 1958, 1932, 1730, 1600, 1553, 1508, 1464, 1446, 1388, 1366, 1257, 1223, 1167, 1137, 1097, 1061, 1039, 1014, 979, 956, 923, 842, 732, 658. HRMS (ESI) m/z calcd for $C_{20}H_{24}F_1N_1O_5^+$ $(M+H)^+$: 378.1711, found 378.1718.



diethyl-3-((2-fluorophenyl)(hydroxyimino)methyl)-4,4-dimethylcyclopent-2-ene-1,1-dicarboxylate, **6h**, oil, 57%, E:Z = 4:1.

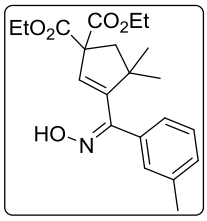
^{1}H NMR (400 MHz, $CDCl_3$): 8.67 (s, 1H, OH), 7.46 (t, *J* = 8.4 Hz, 1H), 7.37 – 7.31 (m, 1H), 7.13 (d, *J* = 7.6 Hz, 1H), 7.10 – 7.05 (m, 1H), 5.97 (s, 1H), 4.27 – 4.21 (m, 4H), 2.45 (s, 2H), 1.27 (t, *J* = 7.1 Hz, 6H), 0.99 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 170.9, 161.5 (d, *J* = 250.0 Hz), 158.9, 146.1, 130.9 (d, *J* = 8.0 Hz), 130.8, 130.5 (d, *J* = 2.0 Hz), 130.4, 128.5, 124.0, 123.9, 123.6 (d, *J* = 11.0 Hz), 123.5, 116.4 (d, *J* = 22.0 Hz), 116.2, 65.3, 61.7, 61.4, 48.5, 46.7, 28.3, 14.0. ^{19}F NMR (376 MHz, $CDCl_3$): -113.52. IR (cm^{-1}): 3433, 2979, 1958, 1933, 1731, 1612, 1491, 1448, 1387, 1366, 1253,

1216, 1139, 1094, 1061, 1038, 1015, 980, 956, 928, 854, 813, 763, 664. HRMS (ESI) m/z calcd for $C_{20}H_{24}F_1N_1O_5^+$ $(M+H)^+$: 378.1711, found 378.1727.



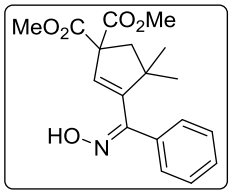
diethyl (Z)-3-((3-fluorophenyl)(hydroxyimino)methyl)-4,4-dimethylcyclopent-2-ene-1,1-dicarboxylate, **6i**, oil, 51%, Z:E >98:2.

^{1}H NMR (400 MHz, $CDCl_3$): 8.09 (s, 1H, OH), 7.44 (d, *J* = 7.9 Hz, 1H), 7.38 (d, *J* = 10.1 Hz, 1H), 7.35 – 7.30 (m, 1H), 7.06 (td, *J* = 8.0, 1.8 Hz, 1H), 5.83 (s, 1H), 4.29 – 4.24 (m, 4H), 2.50 (s, 2H), 1.30 (t, *J* = 7.1 Hz, 6H), 1.04 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 171.1, 163.9 (d, *J* = 244.0 Hz), 161.5, 153.9, 146.6, 137.5 (d, *J* = 8.0 Hz), 137.4, 129.9 (d, *J* = 8.0 Hz), 129.8, 127.7, 122.7, 122.6, 116.4 (d, *J* = 21.0 Hz), 116.2, 113.9 (d, *J* = 23.0 Hz), 113.6, 65.5, 61.8, 49.1, 46.6, 28.8, 14.0. ^{19}F NMR (376 MHz, $CDCl_3$): -112.74. IR (cm^{-1}): 3433, 2978, 1959, 1932, 1730, 1612, 1579, 1485, 1464, 1441, 1388, 1366, 1260, 1213, 1133, 1096, 1075, 1060, 1015, 971, 877, 826, 791, 696, 653. HRMS (ESI) m/z calcd for $C_{20}H_{24}F_1N_1O_5^+$ $(M+H)^+$: 378.1711, found 378.1725.



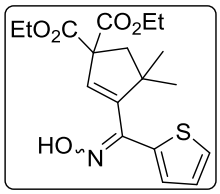
diethyl-3-((hydroxyimino)(m-tolyl)methyl)-4,4-dimethylcyclopent-2-ene-1,1-dicarboxylate, **6j**, oil, 61%, Z:E = 7:1.

^{1}H NMR (400 MHz, $CDCl_3$): 8.15 (s, 1H, OH), 7.48 (s, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.27 – 7.22 (m, 1H), 7.18 (d, *J* = 7.5 Hz, 1H), 5.83 (s, 1H), 4.26 (q, *J* = 7.1 Hz, 4H), 2.49 (s, 2H), 2.36 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 6H), 1.03 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 171.1, 155.0, 146.9, 137.9, 135.0, 130.2, 128.1, 127.2, 124.3, 65.5, 61.7, 48.9, 46.6, 28.8, 21.4, 14.0. IR (cm^{-1}): 3444, 2978, 1958, 1933, 1731, 1580, 1554, 1463, 1387, 1259, 1213, 1135, 1096, 1064, 1039, 1016, 957, 856, 793, 702, 642. HRMS (ESI) m/z calcd for $C_{21}H_{27}N_1O_5^+$ $(M+H)^+$: 374.1962, found 374.1976.



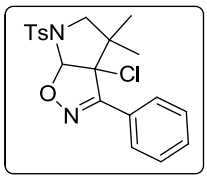
Dimethyl-3-((hydroxyimino)(phenyl)methyl)-4,4-dimethylcyclopent-2-ene-1,1-dicarboxylate, **6k**, M.P. = 119.5 -121.5 ℃, 55%, Z:E = 12:1.

^{1}H NMR (400 MHz, $CDCl_3$): 8.42 (s, 1H, OH), 7.65 – 7.61 (m, 2H), 7.36 (dd, *J* = 5.0, 1.8 Hz, 3H), 5.83 (s, 1H), 3.80 (s, 6H), 2.50 (s, 2H), 1.02 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 171.6, 154.8, 147.3, 135.0, 129.5, 128.3, 126.9, 126.8, 65.2, 52.9, 49.0, 46.72, 28.8, 14.0. IR (cm^{-1}): 3449, 2955, 1958, 1932, 1734, 1553, 1494, 1434, 1387, 1365, 1261, 1218, 1140, 1102, 1062, 1007, 980, 920, 843, 772, 697, 642. HRMS (ESI) m/z calcd for $C_{18}H_{21}N_1O_5^+$ $(M+H)^+$: 332.1492, found 332.1499.



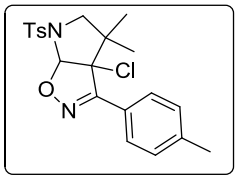
Diethyl-3-((hydroxyimino)(thiophen-2-yl)methyl)-4,4-dimethylcyclopent-2-ene-1,1-dicarboxylate, **6l**, oil, 65%, E:Z = 5:1.

^{1}H NMR (400 MHz, $CDCl_3$): 8.26 (s, 1H, OH), 7.27 (dd, *J* = 12.7, 4.4 Hz, 2H), 7.01 – 6.97 (m, 1H), 5.82 (s, 1H), 4.25 (t, *J* = 7.1 Hz, 4H), 2.52 (s, 2H), 1.28 (t, *J* = 7.1 Hz, 6H), 1.17 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): 171.0, 150.5, 147.7, 139.4, 132.4, 130.9, 130.5, 129.3, 127.6, 127.2, 127.1, 125.6, 65.3, 62.2, 61.7, 49.2, 47.7, 47.1, 46.7, 29.1, 28.4, 28.3, 27.7, 14.0. IR (cm^{-1}): 3432, 2979, 2934, 2869, 1958, 1932, 1730, 1555, 1463, 1388, 1366, 1347, 1255, 1214, 1135, 1095, 1039, 1014, 977, 956, 855, 830, 710, 643. HRMS (ESI) m/z calcd for $C_{18}H_{23}N_1O_5S^+$ $(M+H)^+$: 366.1370, found 366.1377.



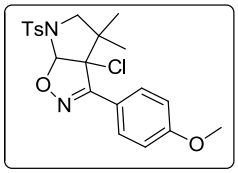
3a-chloro-4,4-dimethyl-3-phenyl-6-tosyl-4,5,6,6a-tetrahydro-3aH-pyrrolo[3,2-d]isoxazole, **8a**, oil, 56%.

^{1}H NMR (400 MHz, $CDCl_3$): 7.86 (d, *J* = 8.3 Hz, 2H), 7.70 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.46 – 7.34 (m, 5H), 6.34 (s, 1H), 3.54 (d, *J* = 9.7 Hz, 1H), 3.01 (d, *J* = 9.7 Hz, 1H), 2.47 (s, 3H), 1.37 (s, 3H), 0.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 156.8, 143.9, 136.1, 130.4, 129.7, 128.6, 128.5, 128.0, 127.5, 101.3, 85.4, 59.1, 46.7, 26.0, 21.8, 21.5. IR (cm^{-1}): 3416, 2974, 2878, 1597, 1494, 1465, 1443, 1396, 1351, 1289, 1256, 1230, 1164, 1092, 1062, 1043, 1016, 977, 926, 885, 815, 787, 763, 734, 696, 682, 664. HRMS (ESI) m/z calcd for $C_{20}H_{21}ClN_2O_3SNa^+$ $(M+Na)^+$: 427.08536, found 427.08545.



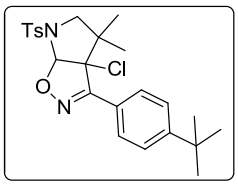
3a-chloro-4,4-dimethyl-3-(p-tolyl)-6-tosyl-4,5,6,6a-tetrahydro-3aH-pyrrolo[3,2-d]isoxazole, **8b**, M.P. = 151-153 ℃, 54%.

^{1}H NMR (400 MHz, $CDCl_3$): 7.86 (d, *J* = 8.3 Hz, 2H), 7.59 (d, *J* = 8.3 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 6.33 (s, 1H), 3.54 (d, *J* = 9.7 Hz, 1H), 3.01 (d, *J* = 9.7 Hz, 1H), 2.48 (s, 3H), 2.38 (s, 3H), 1.38 (s, 3H), 0.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 156.8, 140.7, 136.2, 129.7, 129.2, 127.9, 127.6, 125.6, 101.3, 85.5, 59.2, 46.7, 26.1, 21.9, 21.6, 21.3. IR (cm^{-1}): 3418, 2922, 1958, 1597, 1511, 1466, 1396, 1352, 1289, 1257, 1230, 1162, 1094, 1062, 1043, 978, 919, 885, 817, 783, 732, 705, 665, 624. HRMS (ESI) m/z calcd for $C_{21}H_{23}ClN_2O_3SNa^+$ $(M+Na)^+$: 441.10101, found 441.10123.



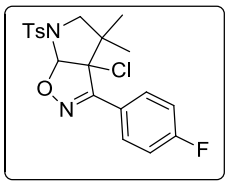
3a-chloro-3-(4-methoxyphenyl)-4,4-dimethyl-6-tosyl-4,5,6,6a-tetrahydro-3aH-pyrrolo[3,2-d]isoxazole, **8c**, M.P. = 154-156 ℃, 52%.

^{1}H NMR (400 MHz, $CDCl_3$): 7.86 (d, *J* = 8.3 Hz, 2H), 7.69 – 7.62 (m, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 6.92 – 6.85 (m, 2H), 6.32 (s, 1H), 3.84 (s, 3H), 3.53 (d, *J* = 9.7 Hz, 1H), 3.01 (d, *J* = 9.7 Hz, 1H), 2.47 (s, 3H), 1.38 (s, 3H), 0.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 161.2, 156.3, 143.9, 136.0, 129.7, 129.5, 127.6, 120.6, 113.9, 101.4, 85.5, 59.2, 55.3, 46.7, 26.0, 21.9, 21.6. IR (cm^{-1}): 3423, 2971, 1607, 1512, 1465, 1396, 1351, 1306, 1256, 1179, 1162, 1092, 1063, 1041, 978, 939, 918, 884, 833, 815, 784, 728, 705, 667, 625. HRMS (ESI) m/z calcd for $C_{21}H_{23}ClN_2O_4SNa^+$ $(M+Na)^+$: 457.09593, found 457.09601.



3-(4-(tert-butyl)phenyl)-3a-chloro-4,4-dimethyl-6-tosyl-4,5,6,6a-tetrahydro-3aH-pyrrolo[3,2-d]isoxazole, **8d**, M.P. = 115-117 ℃, 58%.

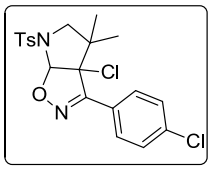
^{1}H NMR (400 MHz, $CDCl_3$): 7.86 (d, *J* = 8.3 Hz, 2H), 7.67 – 7.61 (m, 2H), 7.41 – 7.35 (m, 4H), 6.33 (s, 1H), 3.54 (d, *J* = 9.7 Hz, 1H), 3.02 (d, *J* = 9.7 Hz, 1H), 2.48 (s, 3H), 1.38 (s, 3H), 1.32 (s, 9H), 0.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 156.7, 153.8, 143.9, 136.0, 129.7, 127.7, 127.6, 125.5, 125.4, 101.4, 85.5, 59.2, 46.7, 34.8, 31.1, 26.0, 22.1, 21.6. IR (cm^{-1}): 3439, 2964, 1597, 1465, 1396, 1352, 1289, 1231, 1164, 1095, 1062, 1044, 979, 918, 887, 840, 729, 705, 665. HRMS (ESI) m/z calcd for $C_{24}H_{29}ClN_2O_3SNa^+$ $(M+Na)^+$: 483.14796, found 483.14807.



3a-chloro-3-(4-fluorophenyl)-4,4-dimethyl-6-tosyl-4,5,6,6a-tetrahydro-3aH-pyrrolo[3,2-d]isoxazole, **8e**, M.P. = 141-143 ℃, 55%.

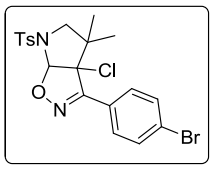
^{1}H NMR (400 MHz, $CDCl_3$): 7.86 (d, *J* = 8.3 Hz, 2H), 7.76 – 7.68 (m, 2H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.07 (t, *J* = 8.6 Hz, 2H), 6.35 (s, 1H), 3.55 (d, *J* = 9.8 Hz, 1H), 3.01 (s,

1H), 2.47 (s, 3H), 1.37 (s, 3H), 0.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.2, (d, *J* = 251.0 Hz), 162.6, 155.8, 144.0, 136.0, 130.1 (d, *J* = 5.0 Hz), 130.0, 129.7, 127.5, 124.8, (d, *J* = 4.0 Hz) 124.7, 115.9 (d, *J* = 22.0 Hz), 115.7, 101.5, 85.3, 59.1, 46.8, 26.0, 21.9, 21.6. ^{19}F NMR (376 MHz, $CDCL_3$): -109.18. IR (cm^{-1}): 3431, 2982, 1598, 1509, 1466, 1396, 1351, 1304, 1235, 1160, 1043, 1016, 979, 919, 889, 842, 815, 86, 732, 705, 669, 623. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClFN_2O_3SNa^+$ $(M+Na)^+$: 445.07594, found 445.07620.



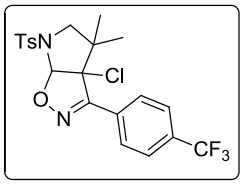
3a-chloro-3-(4-chlorophenyl)-4,4-dimethyl-6-tosyl-4,5,6,6a-tetrahydro-3aH-pyrrolo[3,2-d]isoxazole, **8f**, M.P. = 148-150 ℃, 53%.

^{1}H NMR (400 MHz, $CDCl_3$): 7.85 (d, *J* = 8.3 Hz, 2H), 7.70 – 7.64 (m, 2H), 7.40 – 7.33 (m, 4H), 6.36 (s, 1H), 3.55 (d, *J* = 9.8 Hz, 1H), 2.99 (d, *J* = 9.8 Hz, 1H), 2.48 (s, 3H), 1.38 (s, 3H), 0.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 155.8, 144.1, 136.7, 136.0, 129.7, 129.3, 128.9, 127.6, 127.1, 101.7, 85.3, 59.1, 46.9, 26.0, 22.1, 21.6. IR (cm^{-1}): 3424, 2981, 1596, 1492, 1466, 1398, 1353, 1305, 1289, 1256, 1230, 1163, 1100, 1062, 1043, 1015, 979, 920, 889, 829, 788, 732, 705, 665, 607. HRMS (ESI) m/z calcd for $C_{20}H_{20}Cl_2N_2O_3SNa^+$ $(M+Na)^+$: 461.04639, found 461.04675.



3-(4-bromophenyl)-3a-chloro-4,4-dimethyl-6-tosyl-4,5,6,6a-tetrahydro-3aH-pyrrolo[3,2-d]isoxazole, **8g**, M.P. = 169-171 ℃, 52%.

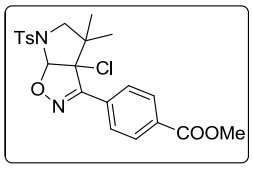
^{1}H NMR (400 MHz, $CDCl_3$): 7.85 (d, *J* = 8.3 Hz, 2H), 7.64 – 7.57 (m, 2H), 7.55 – 7.49 (m, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 6.36 (s, 1H), 3.55 (d, *J* = 9.8 Hz, 1H), 2.99 (d, *J* = 9.8 Hz, 1H), 2.48 (s, 3H), 1.38 (s, 3H), 0.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 155.9, 144.1, 131.8, 129.7, 129.5, 127.6, 125.0, 101.7, 85.3, 59.1, 46.9, 26.0, 22.1, 21.6. IR (cm^{-1}): 3422, 2981, 1590, 1487, 1466, 1396, 1352, 1304, 1288, 1256, 1230, 1163, 1097, 1061, 1043, 1010, 978, 919, 889, 827, 787, 732, 713, 665. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClBrN_2O_3SNa^+$ $(M+Na)^+$: 504.99587, found 504.99600.



3a-chloro-4,4-dimethyl-6-tosyl-3-(4-(trifluoromethyl)phenyl)-4,5,6,6a-tetrahydro-3aH-pyrrolo[3,2-d]isoxazole, **8h**, M.P. = 128-130 ℃, 50%.

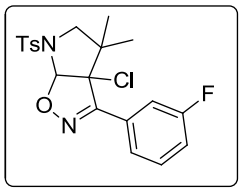
^{1}H NMR (400 MHz, $CDCl_3$): 7.87 (dd, *J* = 8.2, 6.4 Hz, 4H), 7.64 (d, *J* = 8.3 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 6.40 (s, 1H), 3.57 (d, *J* = 9.8 Hz, 1H), 3.01 (d, *J* = 9.9 Hz, 1H), 2.48 (s, 3H), 1.39 (s, 3H), 0.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 155.7, 144.2, 135.9, 129.8, 128.3 (q, *J* = 79.0 Hz), 127.6 (q, *J* = 4.0 Hz), 125.5, 125.5, 125.4, 124.9

(q, *J* = 270.0 Hz), 122.2, 85.2, 59.1, 47.0, 26.0, 22.2, 21.6. ^{19}F NMR (376 MHz, $CDCl_3$): -63.04. IR (cm^{-1}): 2982, 1618, 1597, 1467, 1408, 1353, 1323, 1231, 1164, 1130, 1099, 1061, 1043, 1016, 979, 921, 893, 848, 773, 734, 705, 693, 664. HRMS (ESI) m/z calcd for $C_{21}H_{20}ClF_3N_2O_3SNa^+$ $(M+Na)^+$: 495.07275, found 495.07291.



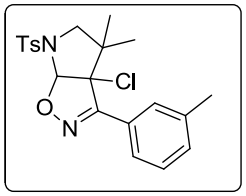
Methyl-4-(3a-chloro-4,4-dimethyl-6-tosyl-4,5,6,6a-tetrahydro-3aH-pyrrolo[3,2-d]isoxazol-3-yl)benzoate, **8i**, M.P. > 200 ℃, 54%.

^{1}H NMR (400 MHz, $CDCl_3$): 8.06 – 8.02 (m, 2H), 7.88 – 7.78 (m, 4H), 7.38 (d, *J* = 8.1 Hz, 2H), 6.38 (s, 1H), 3.94 (s, 3H), 3.56 (d, *J* = 9.8 Hz, 1H), 2.99 (d, *J* = 9.8 Hz, 1H), 2.48 (s, 3H), 1.38 (s, 3H), 0.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 166.2, 156.1, 144.1, 136.0, 132.9, 131.7, 129.7, 129.6, 127.6, 101.8, 85.3, 59.1, 52.3, 46.9, 26.0, 22.1, 21.6. IR (cm^{-1}): 3427, 2951, 1724, 1597, 1466, 1436, 1405, 1353, 1279, 1185, 1163, 1113, 1092, 1062, 1043, 1017, 978, 919, 892, 861, 820, 787, 772, 732, 702, 664. HRMS (ESI) m/z calcd for $C_{22}H_{23}ClN_2O_5SNa^+$ $(M+Na)^+$: 485.09084, found 485.09113 .



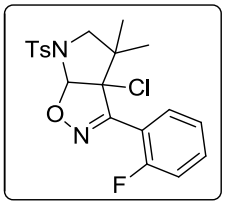
3a-chloro-3-(3-fluorophenyl)-4,4-dimethyl-6-tosyl-4,5,6,6a-tetrahydro-3aH-pyrrolo[3,2-d]isoxazole, **8j**, oil, 53%.

^{1}H NMR (400 MHz, $CDCl_3$): 7.86 (d, *J* = 8.3 Hz, 2H), 7.51 (dt, *J* = 7.8, 1.2 Hz, 1H), 7.45 (dt, *J* = 9.8, 2.3 Hz, 1H), 7.40 – 7.34 (m, 3H), 7.18 – 7.11 (m, 1H), 6.37 (s, 1H), 3.56 (d, *J* = 9.8 Hz, 1H), 3.00 (d, *J* = 9.8 Hz, 1H), 2.48 (s, 3H), 1.39 (s, 3H), 0.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 163.3 (d, *J* = 246.0 Hz), 161.1, 135.9, 130.6, (d, *J* = 8.0 Hz), 130.5, 130.3 (d, *J* = 8.0 Hz), 130.2, 129.7, 127.6, 123.8 (d, *J* = 3.0 Hz), 117.5 (d, *J* = 21.0 Hz), 117.3, 115.2 (d, *J* = 23.0 Hz), 115.0, 101.6, 85.2, 59.1, 46.9, 26.0, 21.9, 21.6. ^{19}F NMR (376 MHz, $CDCL_3$): -111.36. IR (cm^{-1}): 3425, 2981, 1958, 1590, 1485, 1466, 1441, 1396, 1352, 1289, 1203, 1161, 1133, 1093, 1075, 1062, 1043, 922, 847, 819, 786, 732, 692, 663. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClFN_2O_3SNa^+$ $(M+Na)^+$: 445.07594, found 445.07599.



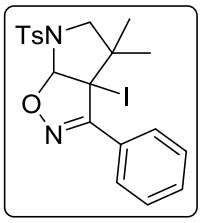
3a-chloro-4,4-dimethyl-3-(m-tolyl)-6-tosyl-4,5,6,6a-tetrahydro-3aH-pyrrolo[3,2-d]isoxazole, **8k**, M.P. = 130-132 ℃, 43%.

^{1}H NMR (400 MHz, $CDCl_3$): 7.87 (d, *J* = 8.3 Hz, 2H), 7.54 – 7.45 (m, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.30 – 7.23 (m, 2H), 6.33 (s, 1H), 3.54 (d, *J* = 9.7 Hz, 1H), 3.01 (d, *J* = 9.7 Hz, 1H), 2.48 (s, 3H), 2.36 (s, 3H), 1.38 (s, 3H), 0.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 156.9, 143.9, 138.4, 136.1, 131.2, 129.7, 128.5, 128.5, 128.4, 127.6, 125.2, 101.2, 85.5, 59.1, 46.7, 26.1, 21.8, 21.6, 21.3. IR (cm^{-1}): 3426, 2921, 1597, 1465, 1351, 1162, 1094, 1043, 923, 814, 784, 700, 676, 664. HRMS (ESI) m/z calcd for $C_{21}H_{23}ClN_2O_3SNa^+$ $(M+Na)^+$: 441.10101, found 441.10117.



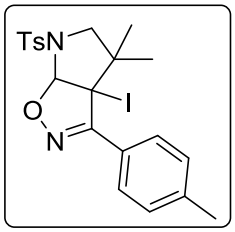
3a-chloro-3-(2-fluorophenyl)-4,4-dimethyl-6-tosyl-4,5,6,6a-tetrahydro-3aH-pyrrolo[3,2-d]isoxazole, **8l**, M.P. = 127-129 ℃, 47%.

^{1}H NMR (400 MHz, $CDCl_3$): 7.86 (d, *J* = 8.3 Hz, 2H), 7.73 (td, *J* = 7.6, 1.7 Hz, 1H), 7.47 – 7.40 (m, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 1.0 Hz, 1H), 7.10 (d, *J* = 9.0 Hz, 1H), 6.34 (s, 1H), 3.60 (d, *J* = 9.6 Hz, 1H), 3.13 (d, *J* = 9.6 Hz, 1H), 2.46 (s, 3H), 1.35 (s, 3H), 0.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 160.86 (d, *J* = 249.0 Hz), 158.4, 152.0 (d, *J* = 2.0 Hz), 143.9, 136.3, 132.1 (d, *J* = 9.0 Hz), 131.9, 130.5, 129.6, 127.4, 124.2 (d, *J* = 4.0 Hz), 124.1, 116.9 (d, *J* = 13.0 Hz), 116.7, 116.4 (d, *J* = 22.0 Hz), 116.2, 99.4, 86.5, 58.9, 46.2, 26.5, 21.6, 19.5. ^{19}F NMR (376 MHz, $CDCl_3$): -111.78. IR (cm^{-1}): 3425, 2981, 1597, 1493, 1466, 1449, 1396, 1349, 1289, 1256, 1231, 1164, 1119, 1094, 1074, 1016, 939, 918, 884, 814, 785, 763, 732, 705, 671. HRMS (ESI) m/z calcd for $C_{20}H_{20}ClFN_2O_3SNa^+$ $(M+Na)^+$: 445.07594, found 445.07593.



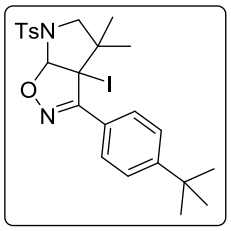
3a-iodo-4,4-dimethyl-3-phenyl-6-tosyl-3a,5,6,6a-tetrahydro-4H-pyrrolo[3,2-d] isoxazole, **9a**, 60%, oil

^{1}H NMR (400 MHz, $CDCl_3$): 7.87 (d, *J* = 8.3 Hz, 2H), 7.77 – 7.72 (m, 2H), 7.45 (t, *J* = 7.4 Hz, 1H), 7.40 – 7.33 (m, 4H), 6.53 (s, 1H), 3.52 (d, *J* = 9.4 Hz, 1H), 2.97 (d, *J* = 9.4 Hz, 1H), 2.48 (s, 3H), 1.39 (s, 3H), 0.79 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 159.6, 143.8, 136.3, 130.5, 129.6, 129.1, 128.9, 128.4, 127.5, 104.0, 55.7, 54.5, 46.7, 32.5, 21.6. IR (cm^{-1}): 3424, 3061, 2925, 1726, 1596, 1493, 1465, 1443, 1395, 1348, 1308, 1289, 1253, 1160, 1093, 1059, 1034, 1016, 976, 937, 880, 837, 814, 763, 697, 682, 664. HRMS (ESI) m/z calcd for $C_{20}H_{22}IN_2O_3S^+$ $(M+H)^+$: 497.0390, found 497.0389.



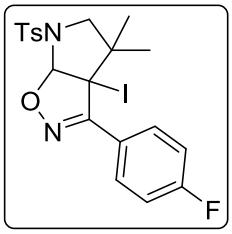
3a-iodo-4,4-dimethyl-3-(p-tolyl)-6-tosyl-3a,5,6,6a-tetrahydro-4H-pyrrolo[3,2-d] isoxazole, **9b**, 55%, M.P. = 141-143 ℃

^{1}H NMR (400 MHz, $CDCl_3$): 7.86 (d, *J* = 8.3 Hz, 2H), 7.62 (d, *J* = 8.2 Hz, 2H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.15 (d, *J* = 8.1 Hz, 2H), 6.51 (s, 1H), 3.50 (d, *J* = 9.4 Hz, 1H), 2.96 (d, *J* = 9.4 Hz, 1H), 2.47 (s, 3H), 2.37 (s, 3H), 1.38 (s, 3H), 0.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 159.5, 143.8, 140.8, 136.3, 129.6, 129.1, 128.8, 127.4, 126.0, 103.9, 55.7, 54.6, 46.7, 32.5, 21.6, 21.5, 21.3. IR (cm^{-1}): 3387, 2973, 2923, 2875, 2258, 1597, 1510, 1494, 1464, 1395, 1348, 1308, 1288, 1253, 1227, 1184, 1162, 1118, 1093, 1058, 1036, 1016, 978, 938, 885, 838, 816, 775, 732, 705, 621. HRMS (ESI) m/z calcd for $C_{21}H_{24}IN_2O_3S^+$ $(M+H)^+$: 511.0547, found 511.0542.



3-(4-(tert-butyl)phenyl)-3a-iodo-4,4-dimethyl-6-tosyl-3a,5,6,6a-tetrahydro-4H pyrrolo [3,2-d]isoxazole, **9c**, 53%, M.P. = 118-120 ℃

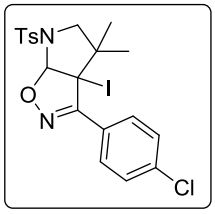
^{1}H NMR (400 MHz, $CDCl_3$): 7.86 (d, *J* = 8.3 Hz, 2H), 7.67 (d, *J* = 8.5 Hz, 2H), 7.37 (dd, *J* = 8.3, 5.0 Hz, 4H), 6.51 (s, 1H), 3.51 (d, *J* = 9.4 Hz, 1H), 2.97 (d, *J* = 9.4 Hz, 1H), 2.48 (s, 3H), 1.39 (s, 3H), 1.32 (s, 9H), 0.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 159.5, 153.9, 143.7, 136.3, 129.6, 128.6, 127.5, 125.8, 125.3, 103.9, 55.8, 54.6, 46.7, 34.8, 32.5, 31.1, 21.8, 21.6. IR (cm^{-1}): 3404, 2964, 2868, 1597, 1507, 1494, 1464, 1395, 1349, 1269, 1252, 1228, 1163, 1117, 1093, 1058, 1036, 1016, 979, 938, 886, 840, 814, 779, 729, 705, 664, 609. HRMS (ESI) m/z calcd for $C_{24}H_{30}IN_2O_3S^+$ $(M+H)^+$: 553.1016, found 553.1016.



3-(4-fluorophenyl)-3a-iodo-4,4-dimethyl-6-tosyl-3a,5,6,6a-tetrahydro-4H-pyrrolo [3,2-d]isoxazole, **9d**, 54%, M.P. = 125-127 ℃

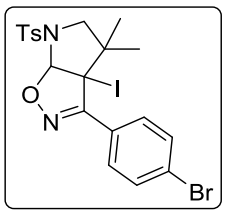
^{1}H NMR (400 MHz, $CDCl_3$): 7.85 (d, *J* = 8.3 Hz, 2H), 7.75 (dd, *J* = 8.9, 5.3 Hz, 2H), 7.37 (d, *J* = 8.1 Hz, 2H), 7.05 (t, *J* = 8.6 Hz, 2H), 6.52 (s, 1H), 3.52 (d, *J* = 9.5 Hz, 1H), 2.95 (d, *J* = 9.5 Hz, 1H), 2.47 (s, 3H), 1.37 (s, 3H), 0.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 165.3 (d, *J* = 250.0 Hz), 162.8, 158.6, 143.9, 136.2, 131.0 (d, *J* = 9.0

Hz), 130.9, 129.6, 127.4, 125.1 (d, *J* = 4.0 Hz), 115.7 (d, *J* = 22.0 Hz), 115.5, 104.1, 55.7, 54.3, 46.8, 32.5, 21.7. ^{19}F NMR (376 MHz, $CDCl_3$): -109.14. IR (cm^{-1}): 3067, 2974, 2928, 2877, 2258, 1913, 1760, 1597, 1508, 1465, 1395, 1348, 1319, 1289, 1236, 1160, 1119, 1093, 1057, 1035, 1016, 979, 937, 886, 842, 815, 777, 733, 705, 665, 621. HRMS (ESI) m/z calcd for $C_{20}H_{21}FIN_2O_3S^+$ $(M+H)^+$: 515.0296, found 515.0294.



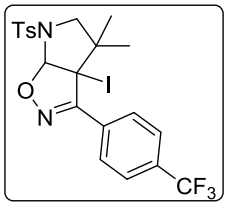
3-(4-chlorophenyl)-3a-iodo-4,4-dimethyl-6-tosyl-3a,5,6,6a-tetrahydro-4H-pyrrolo [3,2-d]isoxazole, **9e**, 52%, M.P. = 134-136 ℃

^{1}H NMR (400 MHz, $CDCl_3$): 7.85 (d, *J* = 8.3 Hz, 2H), 7.71 (d, *J* = 8.6 Hz, 2H), 7.35 (dd, *J* = 13.6, 8.4 Hz, 4H), 6.53 (s, 1H), 3.52 (d, *J* = 9.5 Hz, 1H), 2.94 (d, *J* = 9.5 Hz, 1H), 2.47 (s, 3H), 1.38 (s, 3H), 0.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 158.6, 143.9, 136.8, 136.2, 130.2, 129.7, 128.7, 127.5, 127.4, 104.3, 55.7, 54.1, 46.9, 32.5, 21.8, 21.6. IR (cm^{-1}): 3405, 2971, 2876, 1595, 1491, 1465, 1396, 1349, 1285, 1252, 1227, 1162, 1095, 1057, 1035, 1016, 979, 936, 987, 887, 830, 814, 779, 731, 704, 664, 617, 603. HRMS (ESI) m/z calcd for $C_{20}H_{21}ClIN_2O_3S^+$ $(M+H)^+$: 531.0001, found 531.0012.



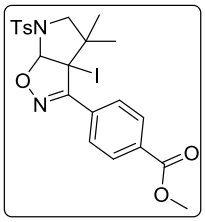
3-(4-bromophenyl)-3a-iodo-4,4-dimethyl-6-tosyl-3a,5,6,6a-tetrahydro-4H-pyrrolo [3,2-d]isoxazole, **9f**, 55%, M.P. = 131-133 ℃

^{1}H NMR (400 MHz, $CDCl_3$): 7.85 (d, *J* = 8.3 Hz, 2H), 7.64 (d, *J* = 8.6 Hz, 2H), 7.49 (d, *J* = 8.6 Hz, 2H), 7.37 (d, *J* = 8.2 Hz, 2H), 6.53 (s, 1H), 3.52 (d, *J* = 9.5 Hz, 1H), 2.94 (d, *J* = 9.5 Hz, 1H), 2.47 (s, 3H), 1.38 (s, 3H), 0.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 158.6, 143.9, 136.2, 131.7, 130.4, 129.7, 127.9, 127.4, 125.2, 104.3, 55.7, 54.1, 46.9, 32.5, 21.9, 21.6. IR (cm^{-1}): 3386, 2973, 2876, 2257, 1916, 1724, 1589, 1486, 1464, 1395, 1349, 1285, 1252, 1227, 1161, 1093, 1057, 1035, 1010, 979, 937, 887, 826, 779, 732, 713, 664, 617. HRMS (ESI) m/z calcd for $C_{20}H_{21}BrIN_2O_3S^+$ $(M+H)^+$: 574.9495, found 574.9498.



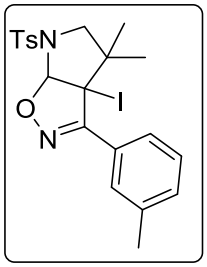
3a-iodo-4,4-dimethyl-6-tosyl-3-(4-(trifluoromethyl)phenyl)-3a,5,6,6a-tetrahydro-4H-pyrrolo[3,2-d]isoxazole, **9g**, M.P. = 130-132 ℃, 56%.

^{1}H NMR (400 MHz,$CDCl_3$): 7.92 (d, *J* = 8.2 Hz, 2H), 7.86 (d, *J* = 8.1 Hz, 2H), 7.62 (d, *J* = 8.2 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 6.57 (s, 1H), 3.54 (d, *J* = 9.6 Hz, 1H), 2.96 (d, *J* = 9.6 Hz, 1H), 2.48 (s, 3H), 1.39 (s, 3H), 0.81 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 158.5, 144.0, 136.1, 132.7, 132.5 (q, *J* = 33.0 Hz), 132.1, 129.7, 129.3, 127.6 (q, *J* = 271.0 Hz), 127.4, 125.4 (q, *J* = 4.0 Hz), 125.3, 125.3, 125.3, 104.5, 55.8, 53.9, 46.9, 32.4, 22.0, 21.5. ^{19}F NMR (376 MHz, $CDCl_3$): -63.01. IR (cm^{-1}): 3064, 2975, 2982, 2877, 1928, 1724, 1617, 1596, 1494, 1465, 1406, 1323, 1252, 1228, 1163, 1129, 1094, 1067, 1058, 1035, 1016, 979, 937, 889, 846, 814, 783, 770, 737, 705, 693, 664, 622. HRMS (ESI) m/z calcd for $C_{21}H_{20}F_3IN_2O_3S^+$ $(M+H)^+$: 565.0264, found 565.0274.



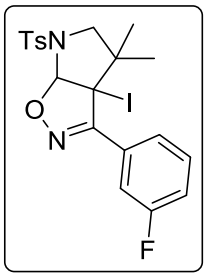
Methyl 4-(3a-iodo-4,4-dimethyl-6-tosyl-3a,5,6,6a-tetrahydro-4H-pyrrolo[3,2-d] isoxazol-3-yl)benzoate, **9h**, M.P. = 126-128 ℃, 57%.

^{1}H NMR (400 MHz, $CDCl_3$): 8.01 (d, *J* = 8.5 Hz, 2H), 7.85 (dd, *J* = 8.3, 3.8 Hz, 4H), 7.37 (d, *J* = 8.2 Hz, 2H), 6.55 (s, 1H), 3.93 (s, 3H), 3.52 (d, *J* = 9.5 Hz, 1H), 2.95 (d, *J* = 9.6 Hz, 1H), 2.47 (s, 3H), 1.38 (s, 3H), 0.78 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 166.1, 158.9, 143.9, 136.1, 133.4, 131.8, 129.7, 129.5, 128.9, 127.4, 104.4, 55.8, 54.0, 52.3, 46.9, 32.4, 21.9, 21.5. IR (cm^{-1}): 2974, 2951, 2877, 1932, 1723, 1609, 1597, 1574, 1494, 1464, 1435, 1403, 1350, 1309, 1279, 1184, 1162, 1113, 1093, 1058, 1035, 1018, 979, 937, 889, 859, 815, 771, 735, 710, 702, 664, 618, 603. HRMS (ESI) m/z calcd for $C_{22}H_{23}IN_2O_5S^+$ $(M+H)^+$: 555.0445, found 555.0439.



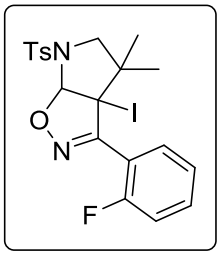
3a-iodo-4,4-dimethyl-3-(m-tolyl)-6-tosyl-3a,5,6,6a-tetrahydro-4H-pyrrolo[3,2-d] isoxazole, **9i**, 50%, oil

^{1}H NMR (400 MHz, $CDCl_3$): 7.87 (d, *J* = 8.3 Hz, 2H), 7.59 (d, *J* = 8.5 Hz, 1H), 7.44 (s, 1H), 7.38 (d, *J* = 8.1 Hz, 2H), 7.29 – 7.21 (m, 2H), 6.50 (s, 1H), 3.51 (d, *J* = 9.4 Hz, 1H), 2.97 (d, *J* = 9.4 Hz, 1H), 2.47 (s, 3H), 2.34 (s, 3H), 1.37 (s, 3H), 0.79 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 159.8, 143.9, 138.3, 136.3, 131.4, 129.7, 129.5, 128.9, 128.3, 127.5, 126.2, 103.9, 55.9, 54.7, 46.7, 32.5, 21.6, 21.4. IR (cm^{-1}): 2973, 2923, 2876, 1597, 1464, 1395, 1374, 1349, 1286, 1252, 1228, 1161, 1119, 1093, 1060, 1036, 1016, 938, 884, 814, 775, 733, 700, 676, 663, 635. HRMS (ESI) m/z calcd for $C_{21}H_{24}IN_2O_3S^+$ $(M+H)^+$: 511.0547, found 511.0554.



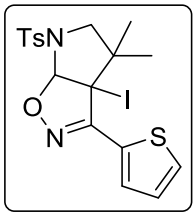
3-(3-fluorophenyl)-3a-iodo-4,4-dimethyl-6-tosyl-3a,5,6,6a-tetrahydro-4H-pyrrolo [3,2-d]isoxazole, **9j**, oil , 53%.

^{1}H NMR (400 MHz, $CDCl_3$): 7.85 (d, *J* = 8.3 Hz, 2H), 7.55 (d, *J* = 7.9 Hz, 1H), 7.46 (d, *J* = 9.8 Hz, 1H), 7.40 – 7.30 (m, 3H), 7.14 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.53 (s, 1H), 3.53 (d, *J* = 9.5 Hz, 1H), 2.95 (d, *J* = 9.5 Hz, 1H), 2.47 (s, 3H), 1.39 (s, 3H), 0.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 163.3 (d, *J* = 245.0 Hz), 160.9, 158.6, 143.9, 136.1, 131.1 (d, *J* = 8.0 Hz), 131.0, 130.1 (d, *J* = 9.0 Hz), 130.0, 129.7, 127.5, 124.8 (d, *J* = 3.0 Hz), 124.8, 117.6 (d, *J* = 21.0 Hz), 117.4, 116.2 (d, *J* = 23.0 Hz), 115.9, 104.3, 55.7, 54.1, 46.8, 32.5, 21.8, 21.5. ^{19}F NMR (376 MHz, $CDCl_3$): -111.32. IR (cm^{-1}): 3069, 2974, 2877, 1611, 1587, 1543, 1486, 1464, 1436, 1395, 1374, 1349, 1284, 1252, 1229, 1201, 1161, 1094, 1074, 1057, 1035, 1016, 990, 967, 937, 912, 887, 834, 776, 705, 692, 673, 662. HRMS (ESI) m/z calcd for $C_{20}H_{20}FIN_2O_3S^+$ $(M+H)^+$: 537.0116, found 537.0115.



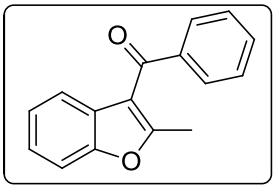
3-(2-fluorophenyl)-3a-iodo-4,4-dimethyl-6-tosyl-3a,5,6,6a-tetrahydro-4H-pyrrolo [3,2-d]isoxazole, **9k**, 50%, oil

^{1}H NMR (400 MHz, $CDCl_3$): 8.00 (t, *J* = 8.3 Hz, 1H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.47 – 7.39 (m, 1H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.18 (t, *J* = 8.1 Hz, 1H), 7.08 (d, *J* = 8.7 Hz, 1H), 6.51 (s, 1H), 3.58 (d, *J* = 9.3 Hz, 1H), 3.20 (d, *J* = 9.3 Hz, 1H), 2.45 (s, 3H), 1.36 (s, 3H), 0.72 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 160.9 (d, *J* = 249.0 Hz), 158.4, 154.3, 143.7, 136.4, 132.0 (d, *J* = 8.0 Hz), 131.9, 131.2 (d, *J* = 2.0 Hz), 129.7, 127.3, 124.1 (d, *J* = 4.0 Hz), 124.1, 117.3 (d, *J* = 13.0 Hz), 117.2, 116.4 (d, *J* = 22.0 Hz), 116.2, 102.6, 57.7, 55.5, 46.4, 32.7, 21.5, 19.8. ^{19}F NMR (376 MHz, $CDCl_3$): -111.14. IR (cm^{-1}): 3066, 2974, 2932, 2878, 2256, 1924, 1723, 1614, 1597, 1580, 1492, 1464, 1448, 1395, 1374, 1347, 1316, 1287, 1252, 1228, 1183, 1162, 1118, 1093, 1057, 1039, 1016, 980, 936, 912, 881, 837, 813, 776, 762, 731, 705, 670, 659, 604. HRMS (ESI) m/z calcd for $C_{20}H_{21}FIN_2O_3S^+$ $(M+H)^+$: 515.0296, found 515.0294.



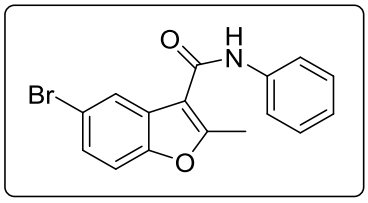
3a-iodo-4,4-dimethyl-3-(thiophen-2-yl)-6-tosyl-3a,5,6,6a-tetrahydro-4H-pyrrolo[3,2-d]isoxazole, **9l**, oil, 43%.

^{1}H NMR (400 MHz, $CDCl_3$): 7.84 (d, *J* = 8.3 Hz, 2H), 7.59 (d, *J* = 4.8 Hz, 1H), 7.39 – 7.34 (m, 3H), 7.06 (dd, *J* = 5.1, 3.8 Hz, 1H), 6.59 (s, 1H), 3.51 (d, *J* = 9.6 Hz, 1H), 3.02 (d, *J* = 9.6 Hz, 1H), 2.46 (s, 3H), 1.42 (s, 3H), 0.95 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 155.3, 143.9, 136.1, 130.2, 129.6, 128.9, 128.5, 127.4, 127.1, 104.5, 55.6, 54.2, 47.3, 32.6, 21.8, 21.5. IR (cm^{-1}): 3106, 2975, 2936, 2875, 2256, 1734, 1654, 1596, 1553, 1493, 1464, 1431, 1395, 1349, 1289, 1252, 1226, 1184, 1161, 1119, 1092, 1072, 1057, 1041, 1016, 971, 934, 881, 845, 814, 777, 734, 705, 665, 624. HRMS (ESI) m/z calcd for $C_{18}H_{19}IN_2O_3S_2^+$ $(M+H)^+$: 502.9955, found 502.9953.



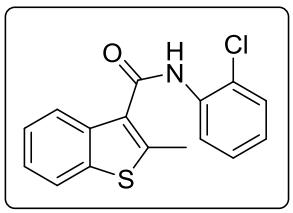
(2-methylbenzofuran-3-yl)(phenyl)methanone, **10**, 60%, oil.

^{1}H NMR (400 MHz, $CDCl_3$): 7.88 – 7.81 (m, 2H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.54 – 7.48 (m, 3H), 7.44 (d, *J* = 7.3 Hz, 1H), 7.33 – 7.28 (m, 1H), 7.23 (dd, *J* = 11.6, 4.4 Hz, 1H), 2.57 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 192.0, 161.9, 153.6, 139.3, 132.6, 129.0, 128.4, 126.8, 124.3, 123.5, 121.3, 116.9, 110.8, 14.6. IR (cm^{-1}): 3065, 2961, 2921, 2850, 1648, 1638, 1579, 1474, 1456, 1386, 1267, 1174, 1124, 1066, 939, 877, 846, 792, 745, 719, 696.



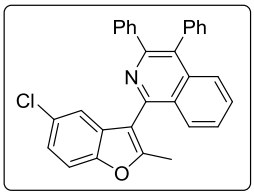
5-bromo-2-methyl-N-phenylbenzofuran-3-carboxamide, **11**, 65%, M.P. = 145-147 ℃, white solid.

^{1}H NMR (400 MHz, $CDCl_3$): 7.86 (d, *J* = 1.9 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.60 (s, 1H), 7.45 – 7.39 (m, 3H), 7.36 (d, *J* = 8.7 Hz, 1H), 7.21 (t, *J* = 7.4 Hz, 1H), 2.76 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 161.6, 161.4, 152.3, 137.4, 129.2, 127.4 (d, *J* = 3.5 Hz), 124.8, 122.0, 120.4, 116.9, 112.8, 112.1, 14.0. IR (cm^{-1}): 3278, 3065, 2359, 1647, 1598, 1532, 1498, 1441, 1385, 1361, 1346, 1310, 1251, 1177, 1118, 1091, 1073, 1048, 938, 880, 752, 690, 580. HRMS (ESI) m/z calcd for $C_{16}H_{13}BrN_1O_2^+$ $(M+H)^+$: 330.0124, found 330.0126.



N-(2-chlorophenyl)-2-methylbenzo[b]thiophene-3-carboxamide, **12**, 70%, M.P. = 103-105 ℃, white solid.

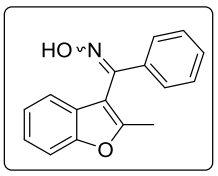
^{1}H NMR (400 MHz, $CDCl_3$): 8.66 (d, *J* = 8.1 Hz, 1H), 8.18 (s, 1H), 8.10 (d, *J* = 8.1 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.48 – 7.42 (m, 2H), 7.38 (tdd, *J* = 4.5, 3.6, 1.2 Hz, 2H), 7.13 (td, *J* = 7.9, 1.5 Hz, 1H), 2.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 162.6, 145.1, 137.9, 137.6, 134.6, 129.1, 128.4, 127.8, 125.1, 124.8, 124.5, 122.8, 122.2 (d, *J* = 18.8 Hz), 121.5, 15.4. IR (cm^{-1}): 3403, 3259, 3059, 1670, 1589, 1583, 1508, 1457, 1433, 1349, 1297, 1255, 1201, 1069, 1034, 939, 878, 779, 749, 688, 651, 565. HRMS (ESI) m/z calcd for $C_{16}H_{13}ClN_1O_1S^+$ $(M+H)^+$: 302.0401, found 302.0406.



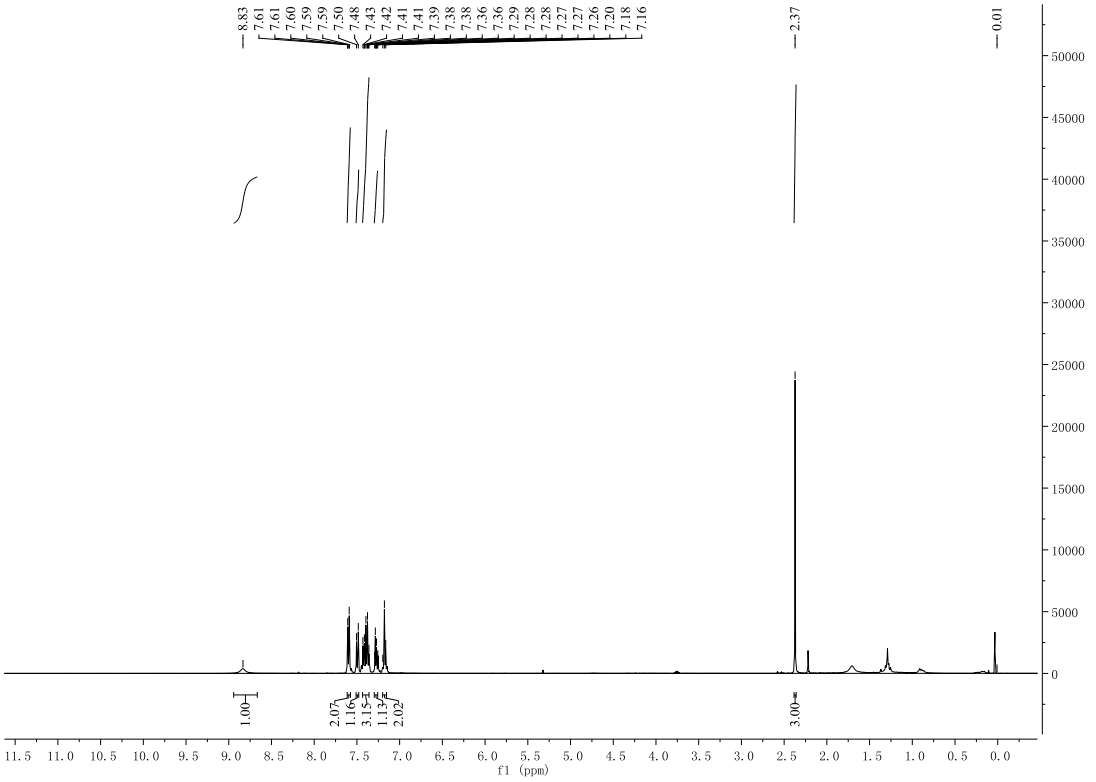
1-(5-chloro-2-methylbenzofuran-3-yl)-3,4-diphenylisoquinoline, **13**, 81%, M.P. = 101-103 ℃, white solid.

^{1}H NMR (400 MHz, $CDCl_3$): 8.05 (d, *J* = 8.3 Hz, 1H), 7.81 (d, *J* = 8.5 Hz, 1H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.50 – 7.40 (m, 7H), 7.37 (d, *J* = 5.7 Hz, 2H), 7.30 – 7.21 (m, 4H), 2.63 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): 156.4, 152.4, 152.0, 150.2, 140.7, 137.3, 136.9, 131.3 (d, *J* = 11.5 Hz), 130.9, 130.3 (t, *J* = 6.7 Hz), 128.4 (d, *J* = 8.5 Hz), 127.6, 127.4, 127.0 (d, *J* = 18.9 Hz), 126.7-126.2, 125.1, 123.9, 119.9, 115.7, 111.8, 13.7. IR (cm^{-1}): 3056, 1614, 1541, 1501, 1455, 1442, 1406, 1363, 1335, 1260, 1178, 1109, 1030, 973, 935, 896, 802, 771, 736, 701, 688, 635, 611, 572. HRMS (ESI) m/z calcd for $C_{30}H_{21}Cl_1N_1O^+$ $(M+H)^+$: 446.1306, found 446.1310.

VII. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra of compound 2, 4, 6, 8, 9, 10, 11, 12, 13


HO
N
O

2a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7.61
7.60
7.59
7.59
7.50
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7.41
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7.38
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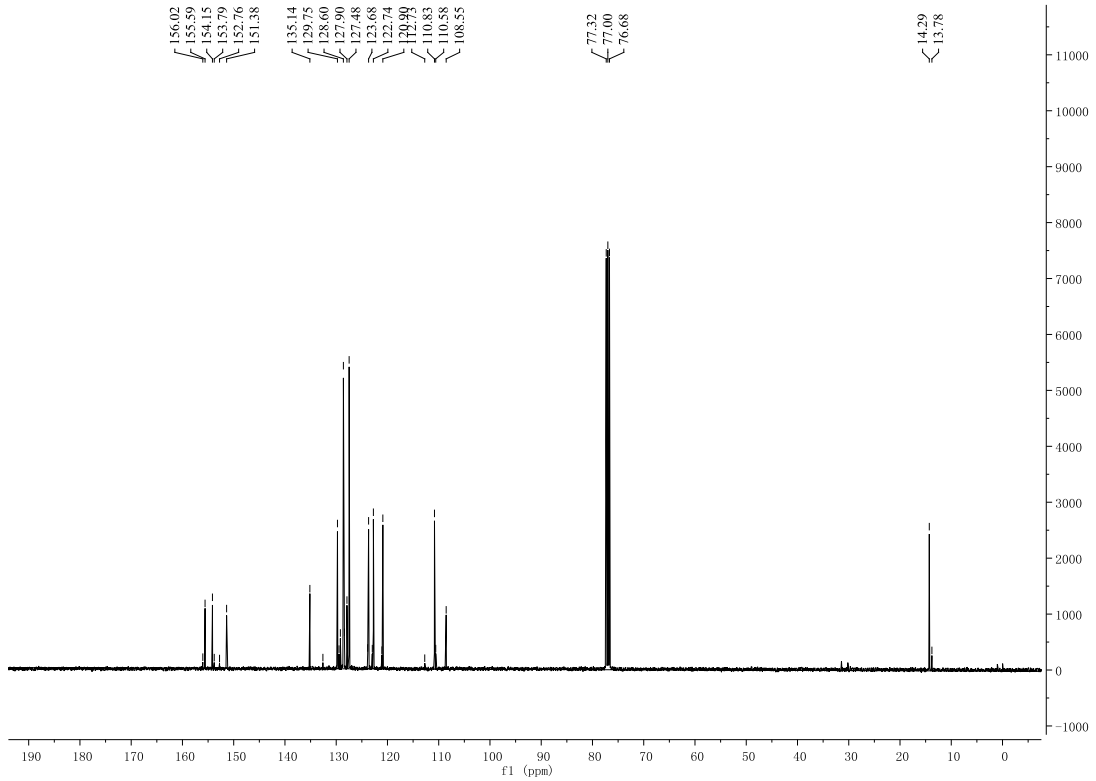
7.20
7.18
7.16
2.37
0.01
1.00
2.07
1.16
3.15
1.13
2.02
3.00
f1 (ppm)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151.38
135.14
129.75
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127.90
127.48
123.68
122.74
120.99
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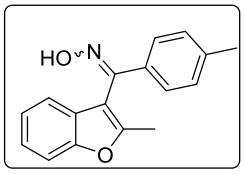
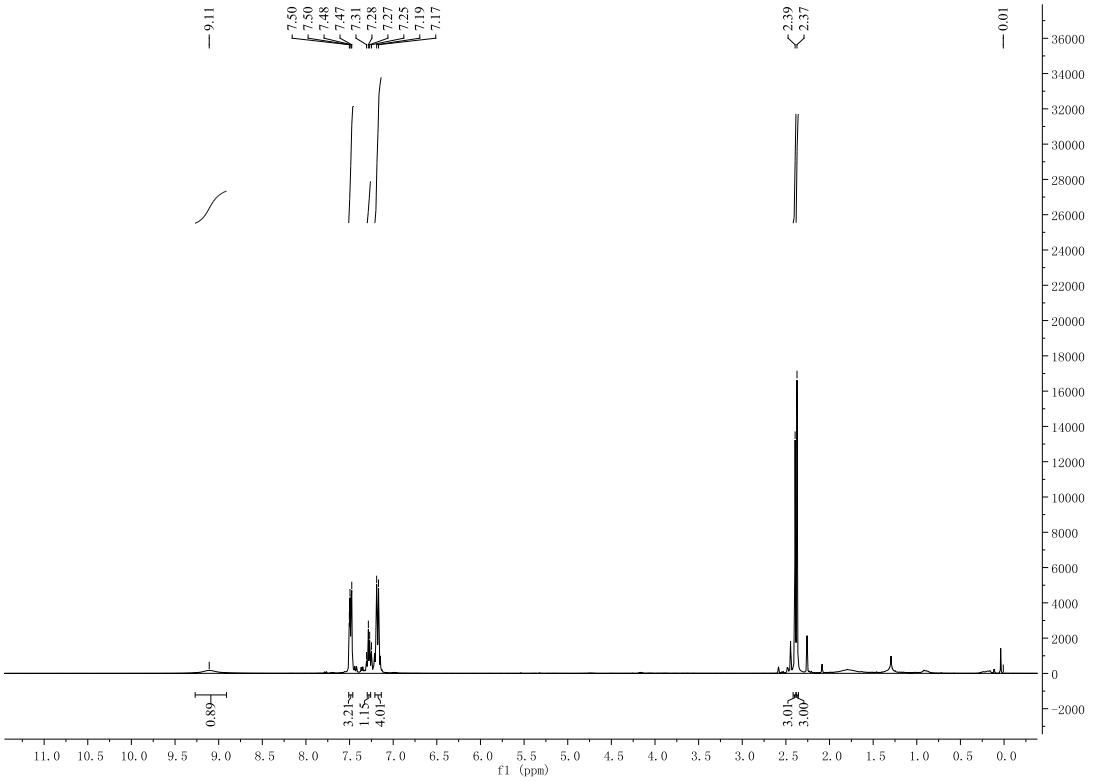
110.83
110.58
108.55
77.32
77.00
76.68
14.29
13.78
f1 (ppm)


HO
N
O

2b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7.28
7.27
7.25
7.19
7.17
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2.37
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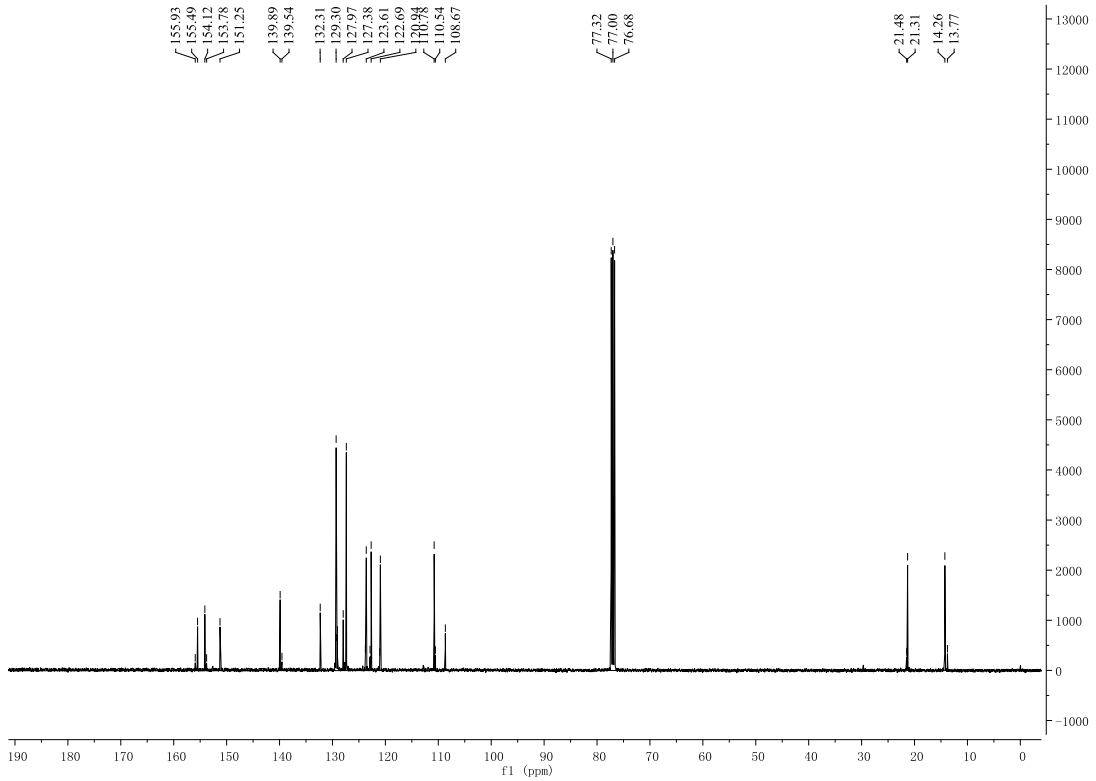
0.89
3.21
1.15
4.01
3.01
3.00
f1 (ppm)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132.31
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127.97
127.38
123.61
122.69
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120.78
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77.00
76.68
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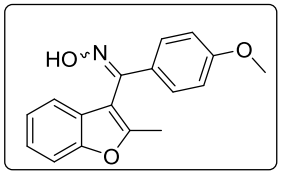
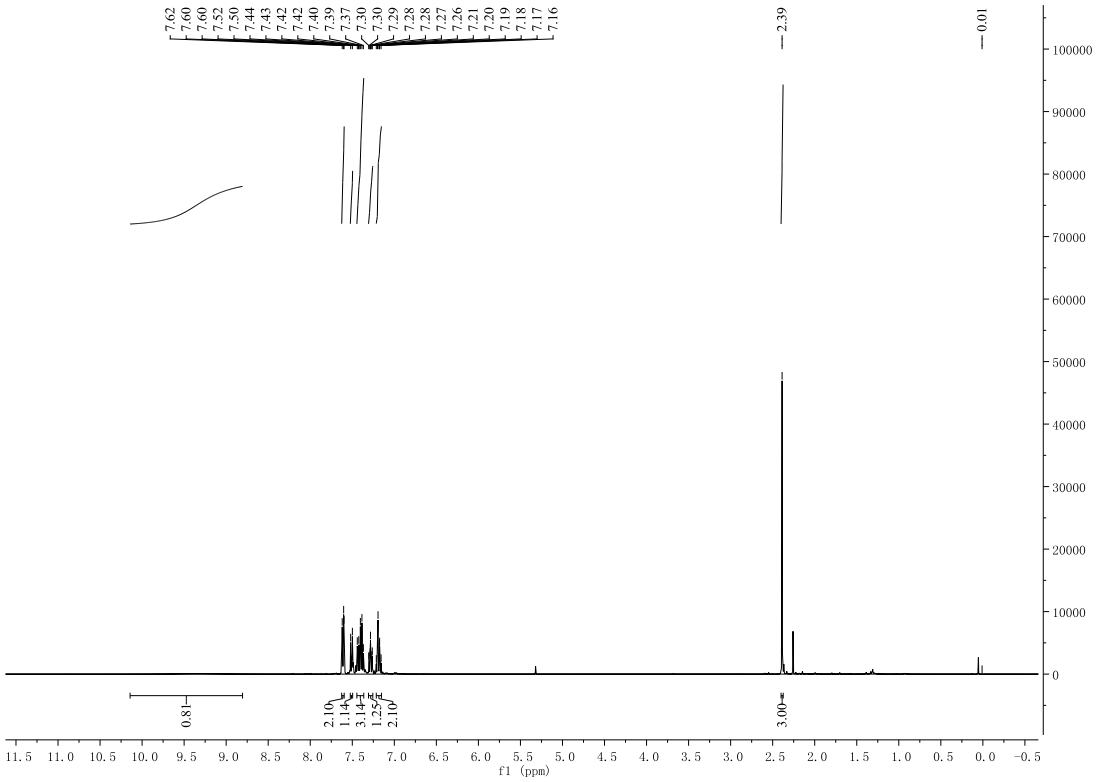
21.31
14.26
13.77
f1 (ppm)


HO
N
O
O

2c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7.60
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7.43
7.42
7.42
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7.39
7.37
7.30
7.30
7.29
7.28
7.28
7.27
7.26
7.21
7.20
7.19
7.18
7.17
7.16
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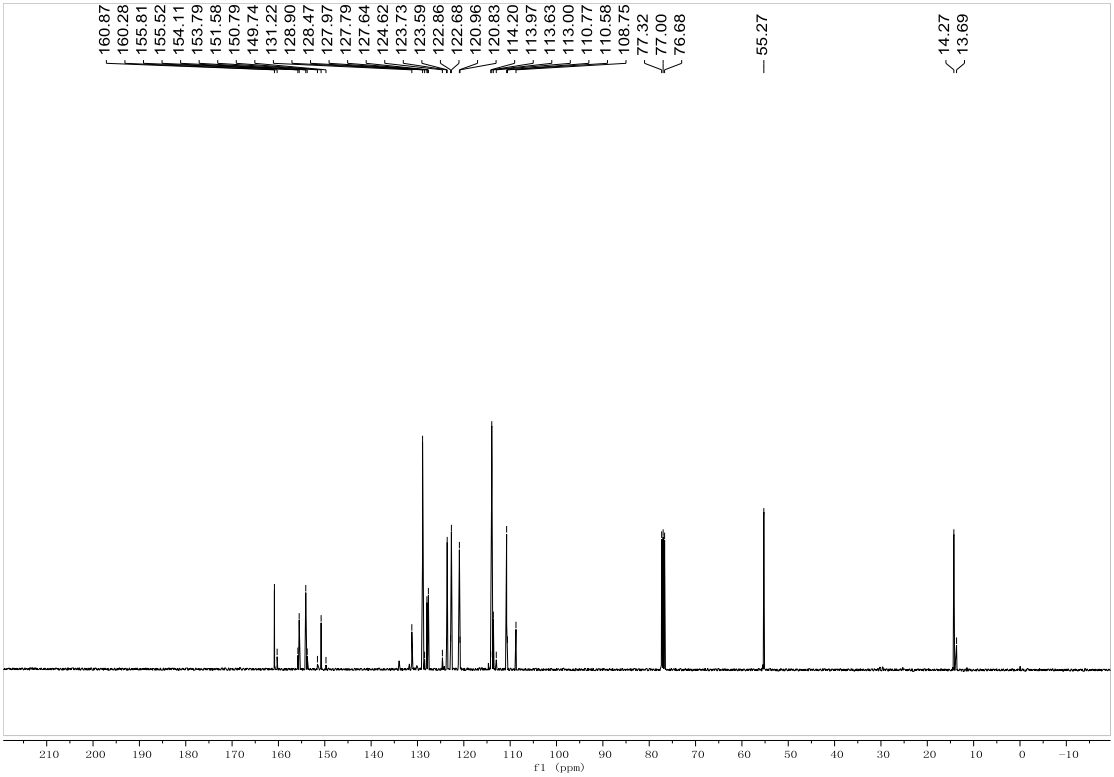
0.81
2.10
1.14
3.14
1.25
2.10
3.00
f1 (ppm)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153.79
151.58
150.79
149.74
131.22
128.90
128.47
127.97
127.79
127.64
124.62
123.73
123.59
122.86
122.68
120.96
120.83
114.20
113.97
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76.68
55.27
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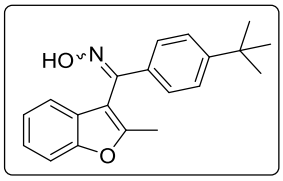
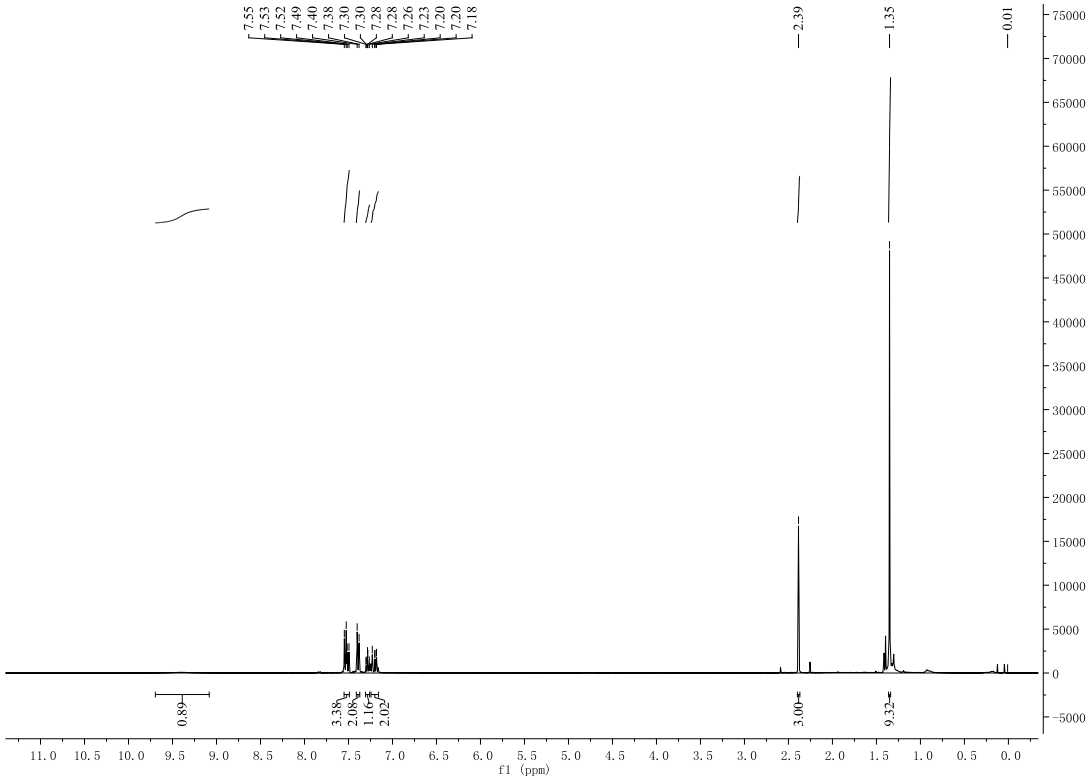
13.69
f1 (ppm)


HO
N
O

2d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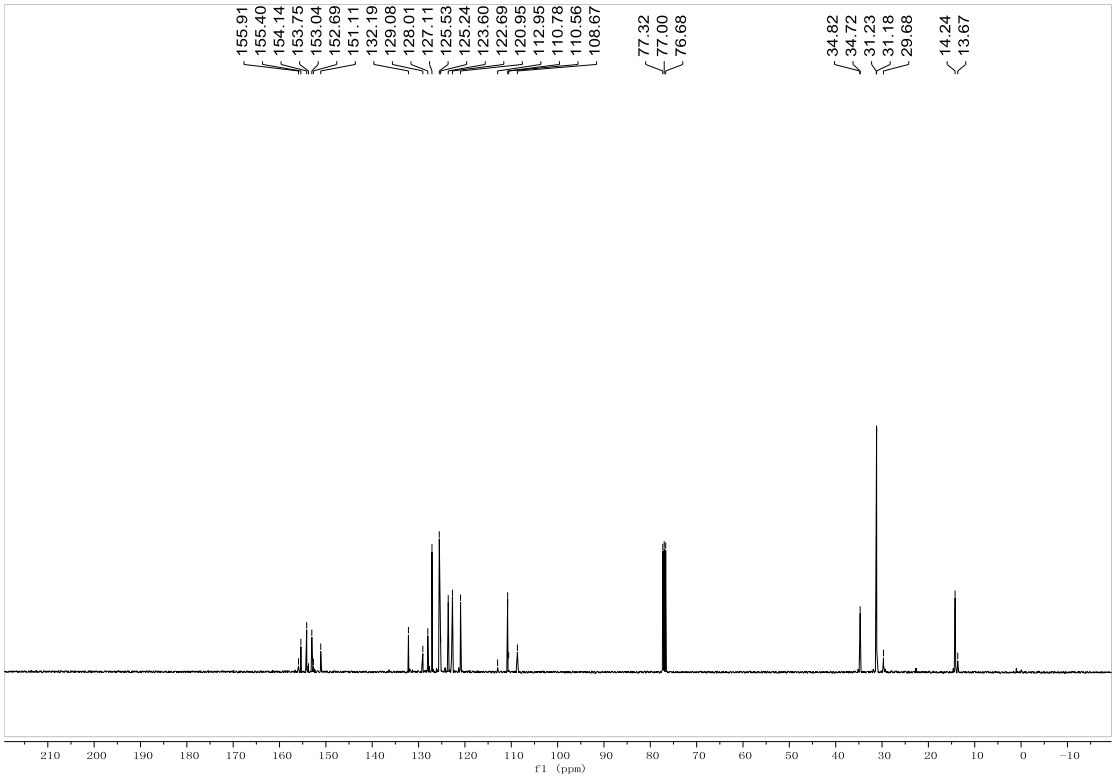
7.49
7.40
7.38
7.30
7.30
7.28
7.28
7.26
7.23
7.20
7.20
7.18
2.39
1.35
0.01
0.89
3.38
2.08
1.16
2.02
3.00
9.32
f1 (ppm)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153.75
153.04
152.69
151.11
132.19
129.08
128.01
127.11
125.53
125.24
123.60
122.69
120.95
112.95
110.78
110.56
108.67
77.32
77.00
76.68
34.82
34.72
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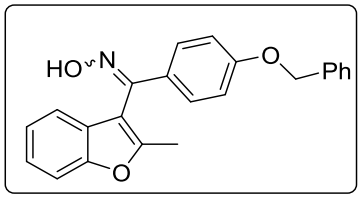
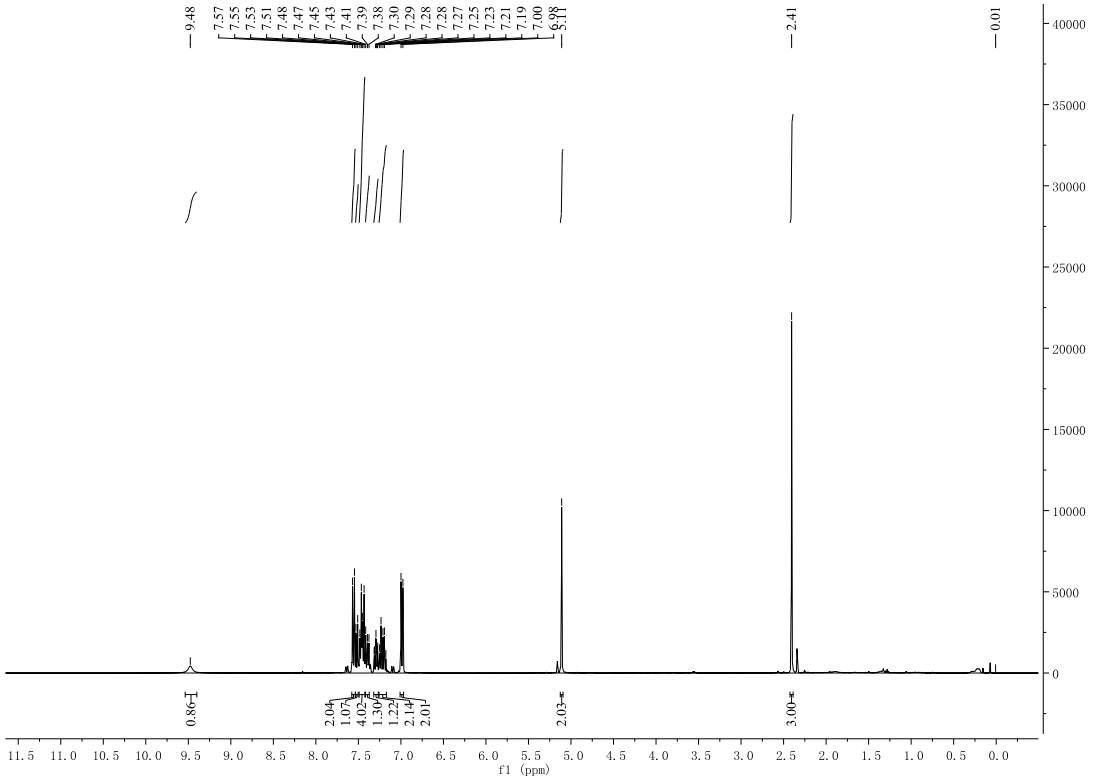
31.18
29.68
14.24
13.67
f1 (ppm)


HO
N
O
Ph
O

2e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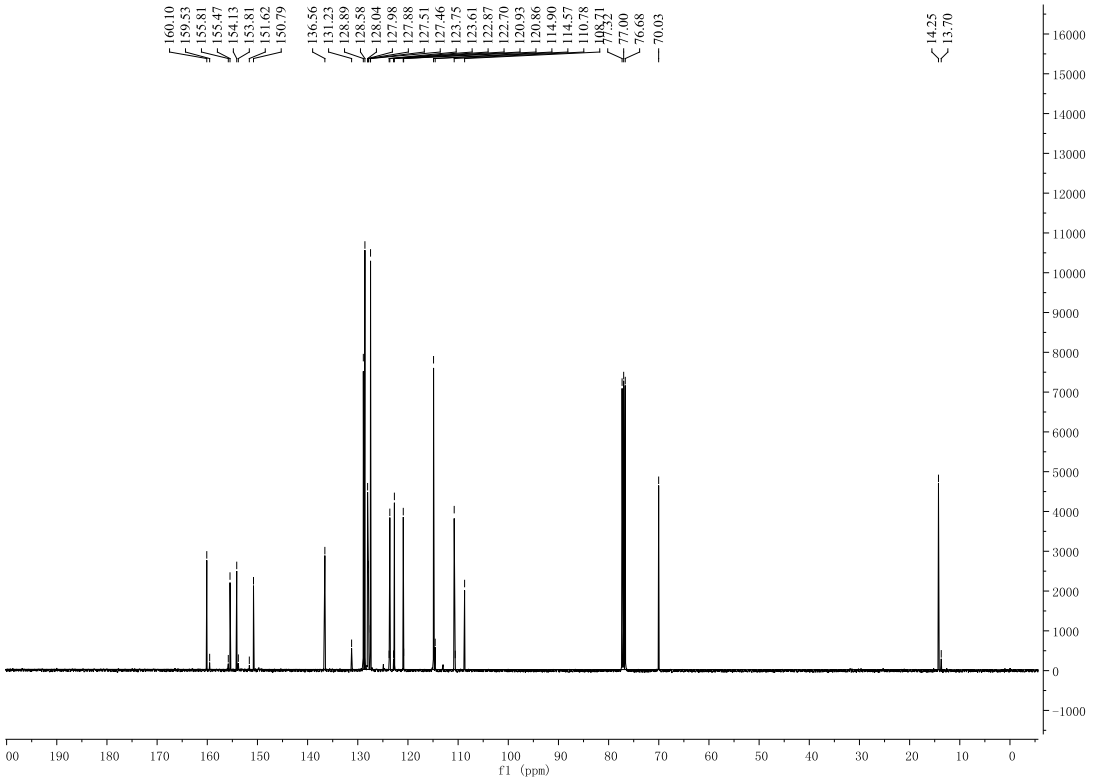
7.48
7.47
7.45
7.43
7.41
7.39
7.38
7.30
7.29
7.28
7.28
7.27
7.25
7.23
7.21
7.19
7.00
6.98
5.11
2.41
0.01
0.86
2.04
1.07
4.02
1.30
1.22
2.14
2.01
2.03
3.00
f1 (ppm)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150.79
136.56
131.23
128.89
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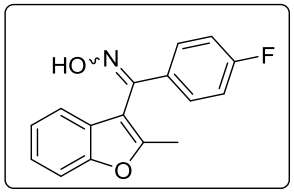
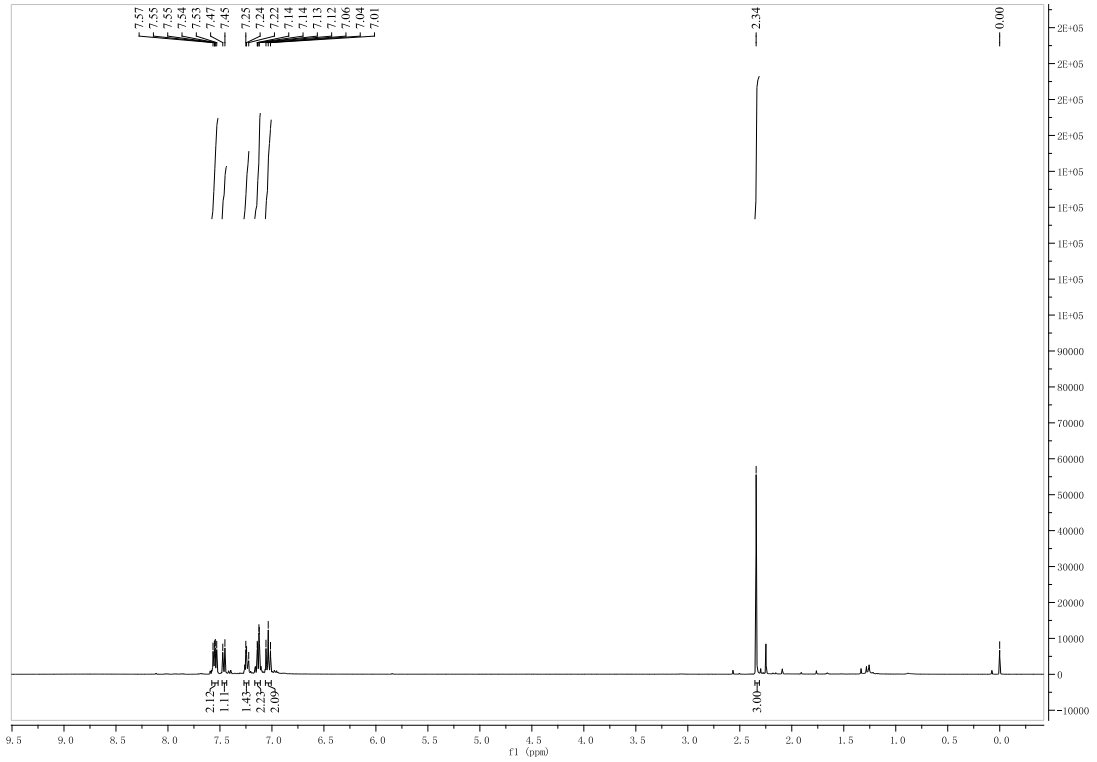
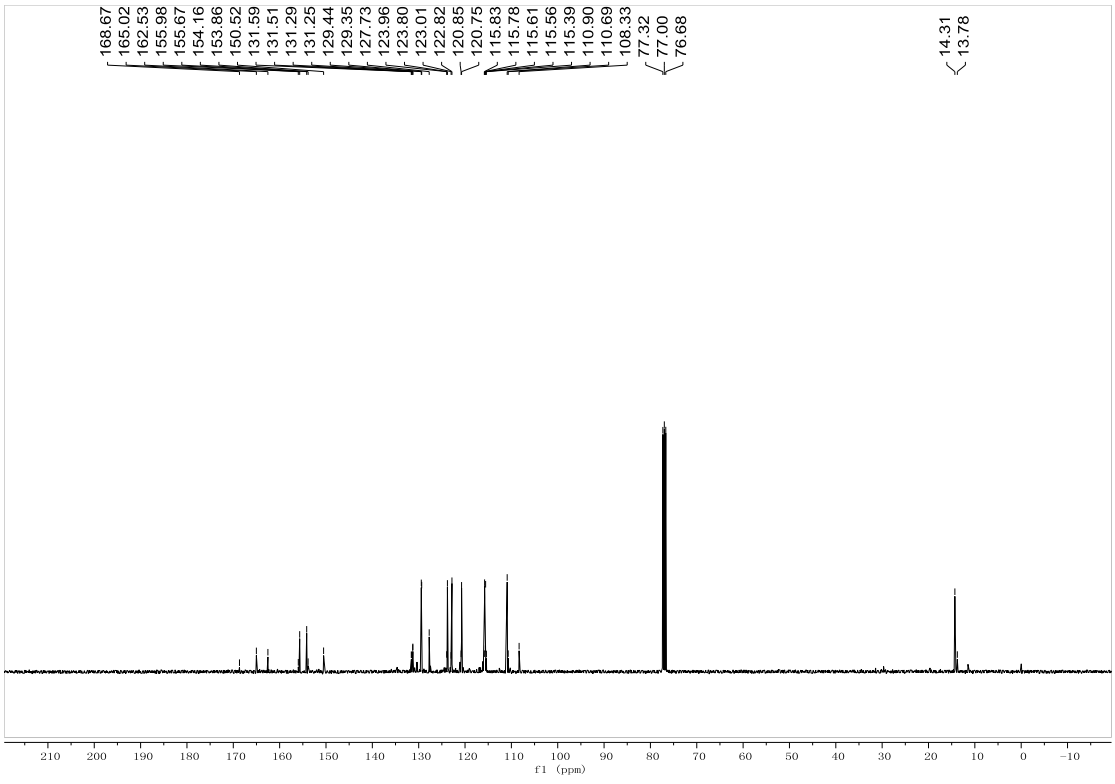
128.04
127.98
127.88
127.51
127.46
123.75
123.61
122.87
122.70
120.93
120.86
114.90
114.57
110.78
108.71
77.32
77.00
76.68
70.03
14.25
13.70
f1 (ppm)


HO
N
F
O

2f


7.57
7.55
7.55
7.54
7.53
7.47
7.45
7.25
7.24
7.22
7.14
7.13
7.12
7.06
7.04
7.01
2.34
0.00
2.12
1.11
1.43
2.23
2.09
3.00
f1 (ppm)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150.52
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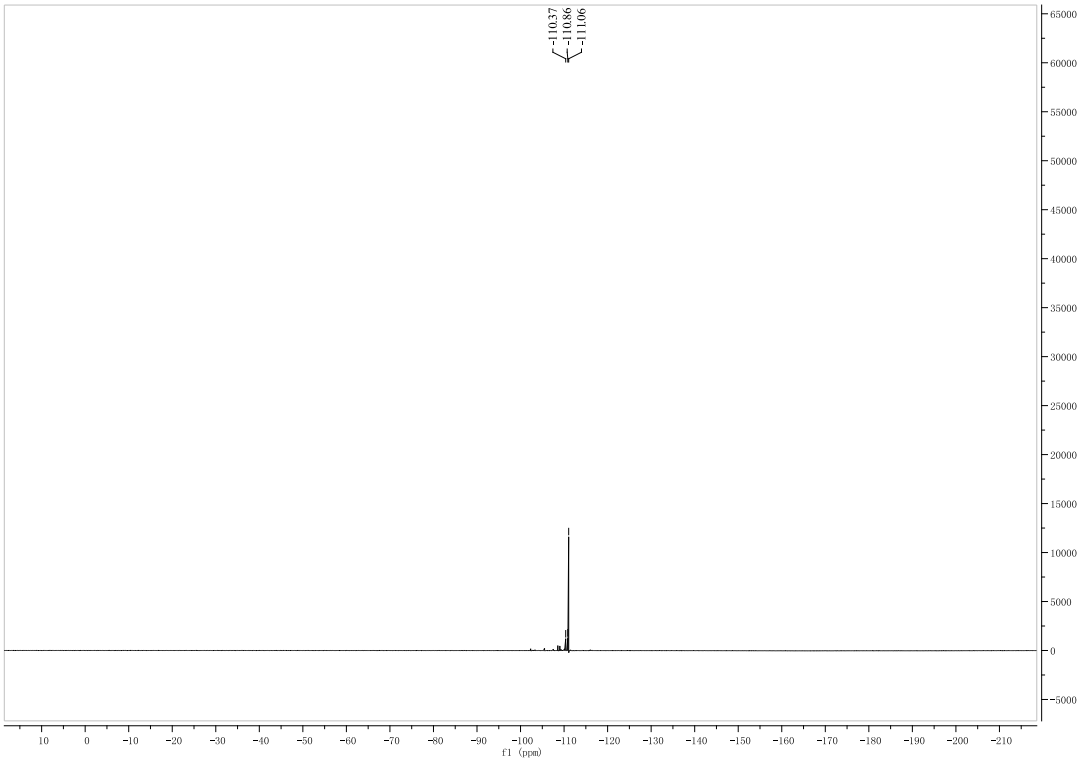
131.51
131.29
131.25
129.44
129.35
127.73
123.96
123.80
123.01
122.82
120.85
120.75
115.83
115.78
115.61
115.56
115.39
110.90
110.69
108.33
77.32
77.00
76.68
14.31
13.78
f1 (ppm)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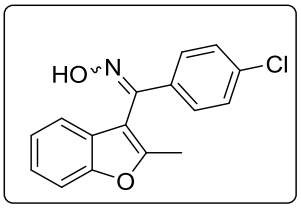
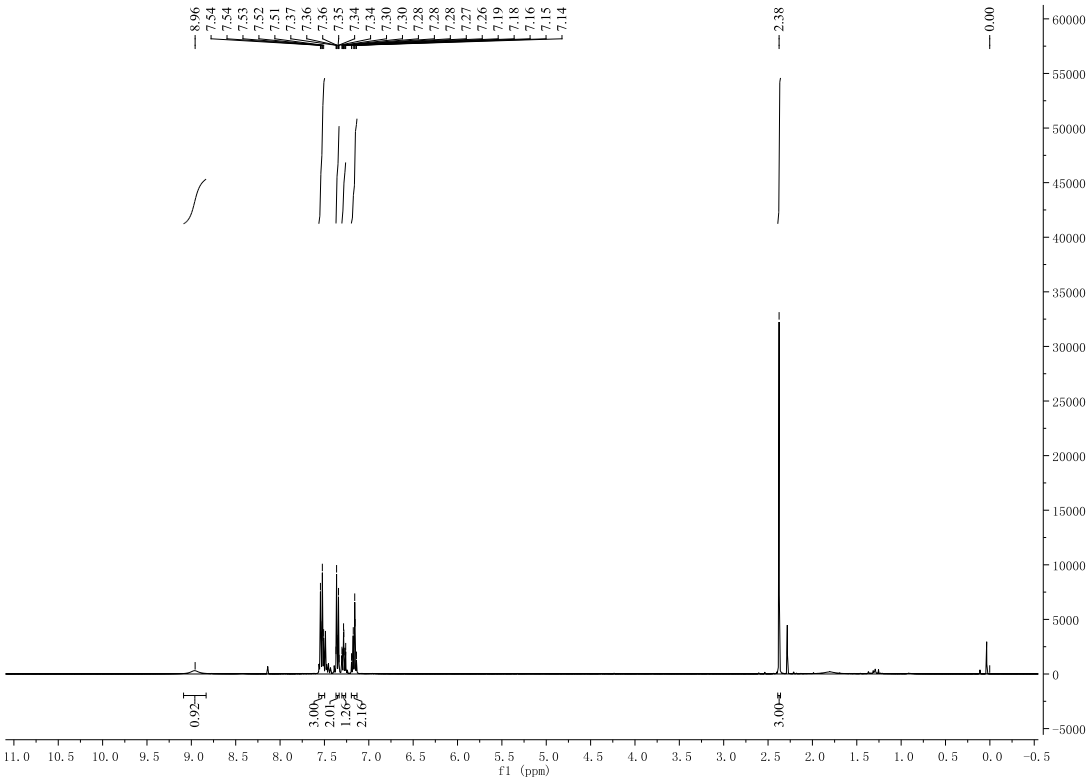
-111.06
f1 (ppm)


HO
N
Cl
O

2g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7.51
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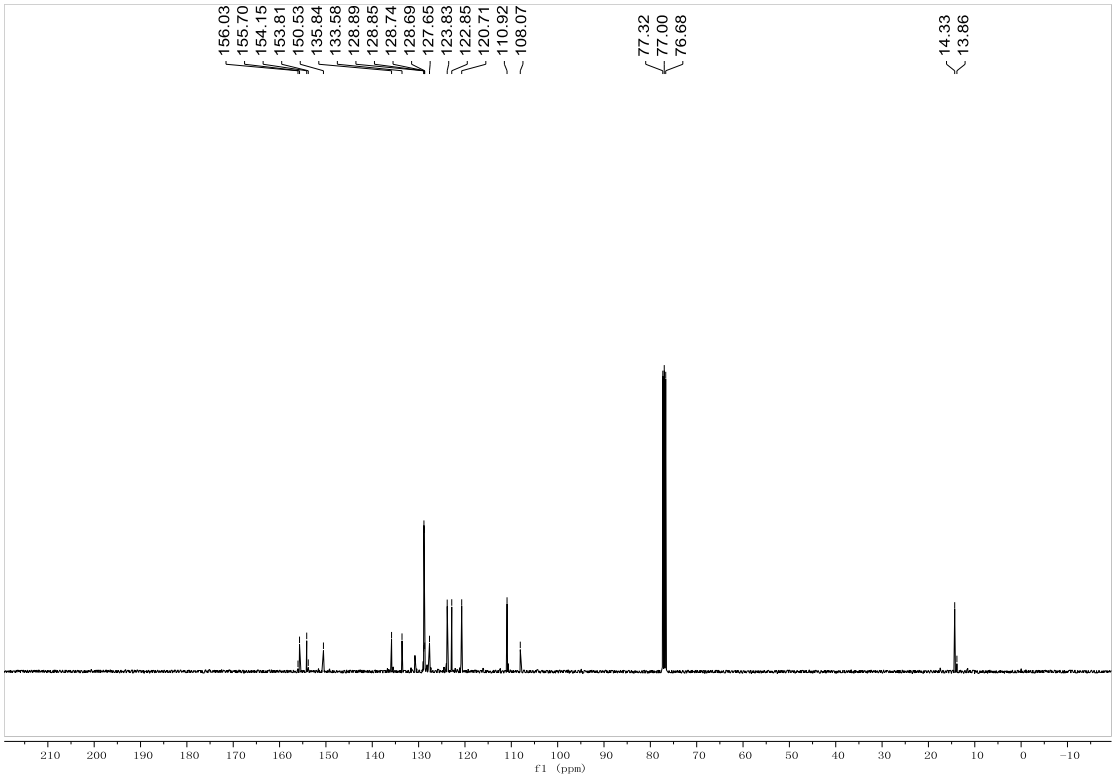
7.36
7.36
7.35
7.34
7.34
7.30
7.30
7.28
7.28
7.28
7.27
7.26
7.19
7.18
7.16
7.15
7.14
2.38
0.00
0.92
3.00
2.01
1.26
2.16
3.00
f1 (ppm)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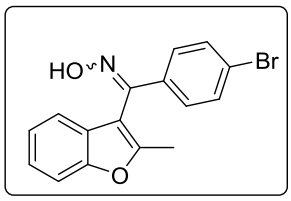
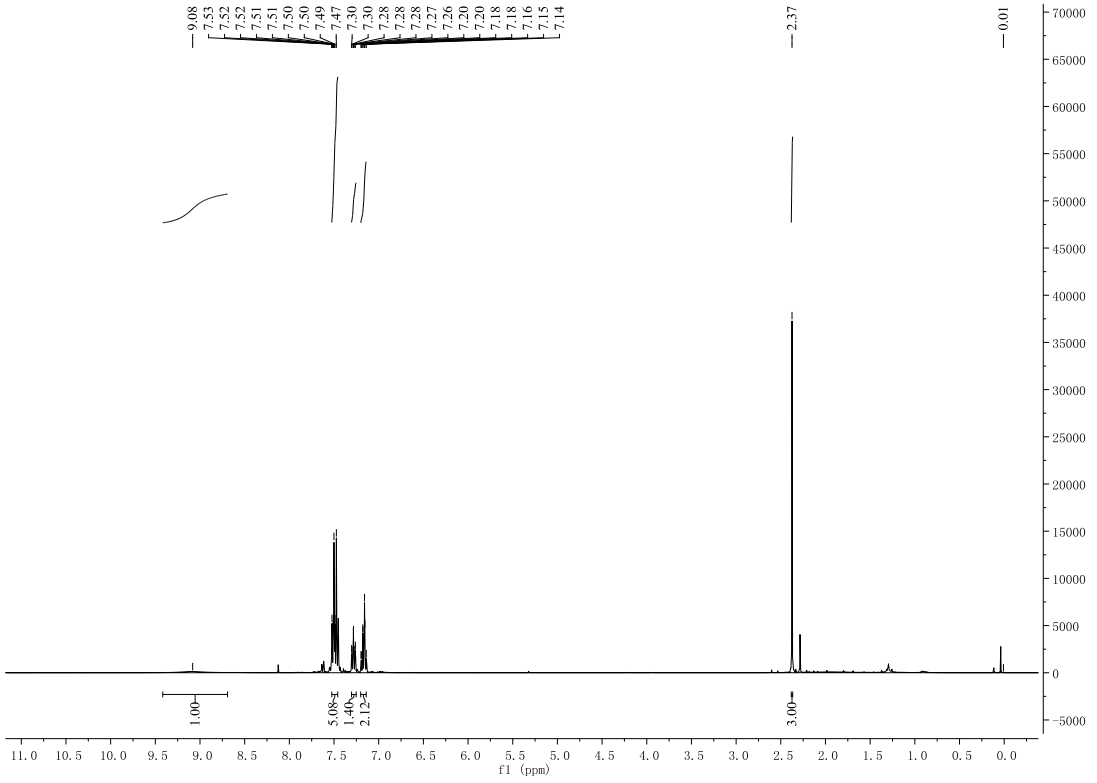
133.58
128.89
128.85
128.74
128.69
127.65
123.83
122.85
120.71
110.92
108.07
77.32
77.00
76.68
14.33
13.86
f1 (ppm)


HO
N
Br
O

2h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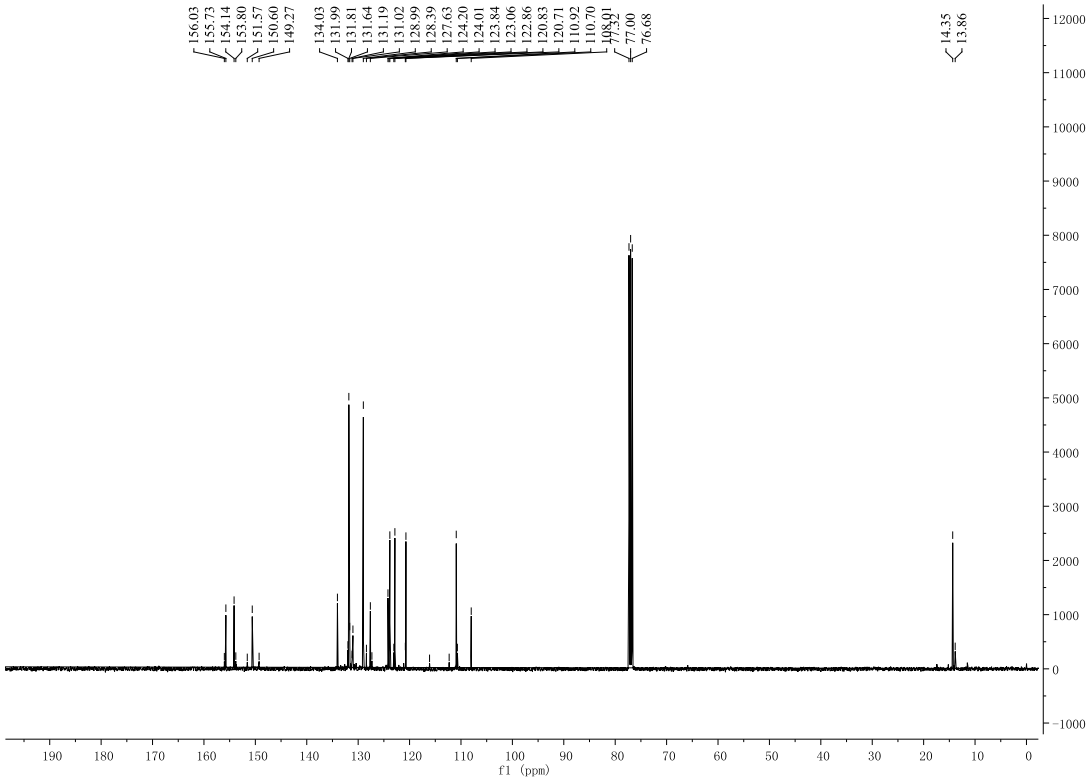
7.50
7.50
7.49
7.47
7.30
7.30
7.28
7.28
7.28
7.27
7.26
7.20
7.20
7.18
7.18
7.16
7.15
7.14
2.37
0.01
1.00
5.08
1.40
2.12
3.00
f1 (ppm)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134.03
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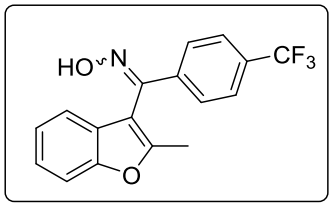
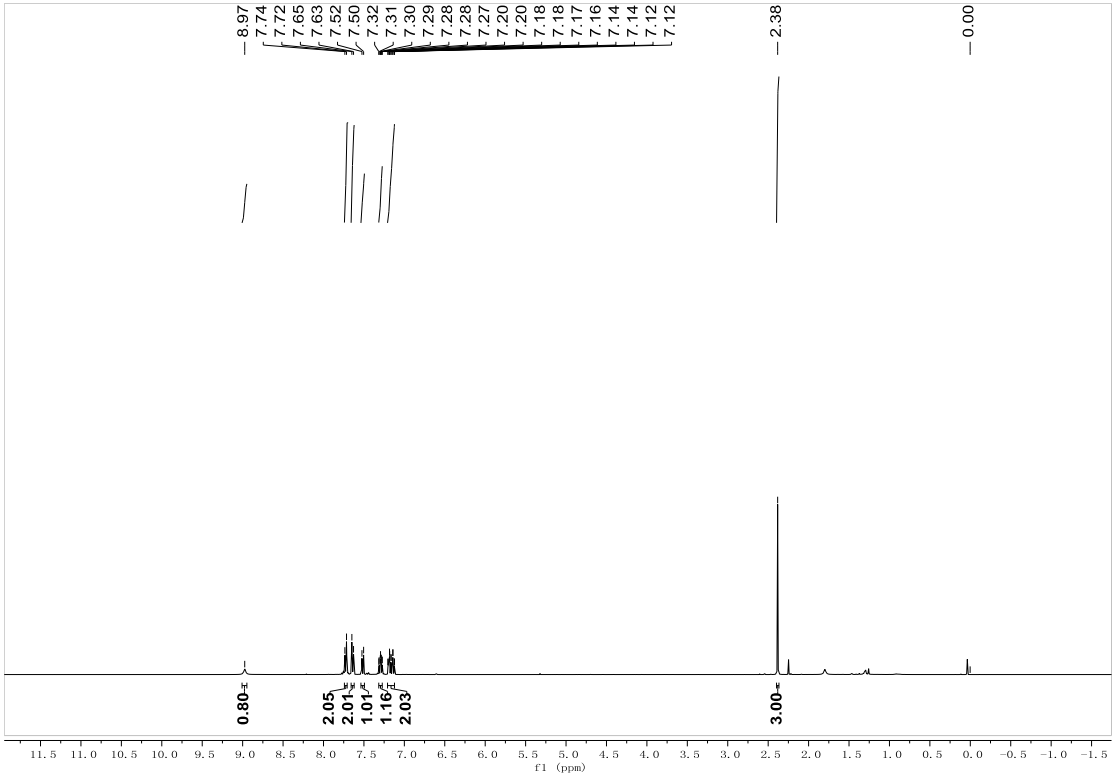
131.81
131.64
131.19
131.02
128.99
128.39
127.63
124.20
124.01
123.84
123.06
122.86
120.83
120.71
110.92
110.70
108.01
77.32
77.00
76.68
14.35
13.86
f1 (ppm)


HO
N
CF3
O

2i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7.32
7.31
7.30
7.29
7.28
7.28
7.27
7.20
7.20
7.18
7.18
7.17
7.16
7.14
7.14
7.12
7.12
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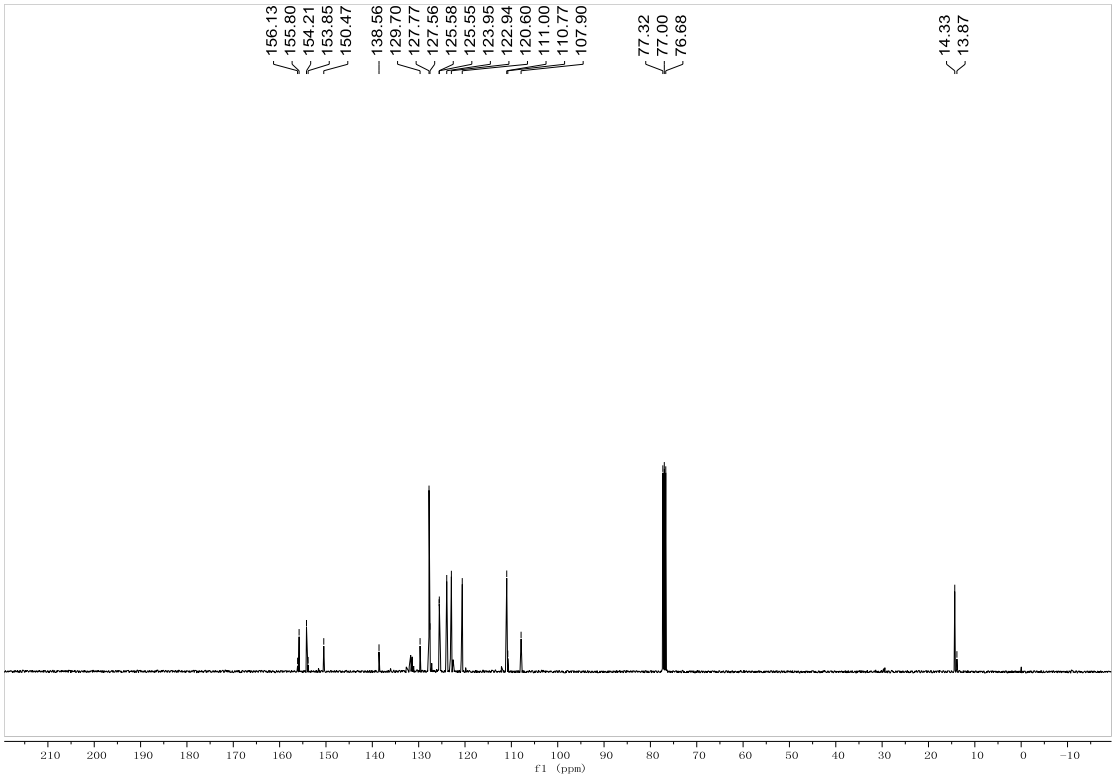
0.80
2.05
2.01
1.01
1.16
2.03
3.00
f1 (ppm)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125.55
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111.00
110.77
107.90
77.32
77.00
76.68
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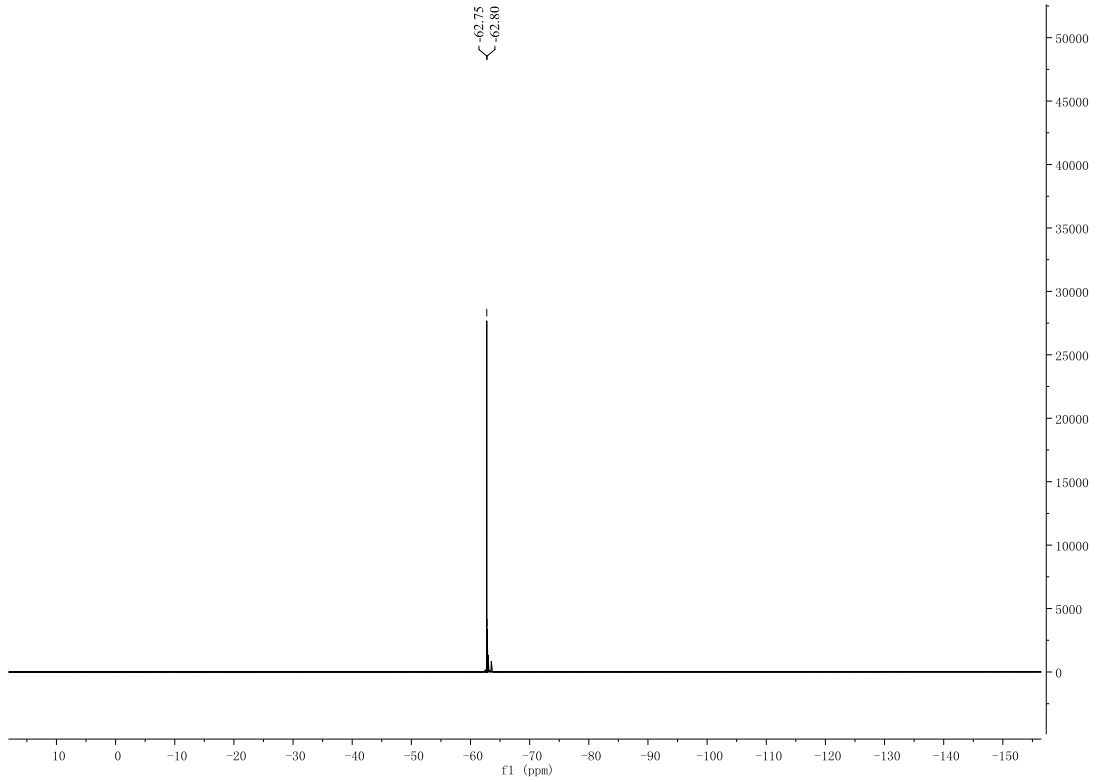
13.87
f1 (ppm)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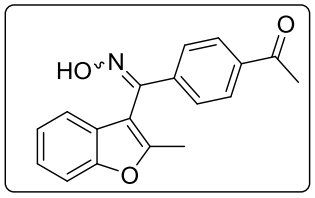
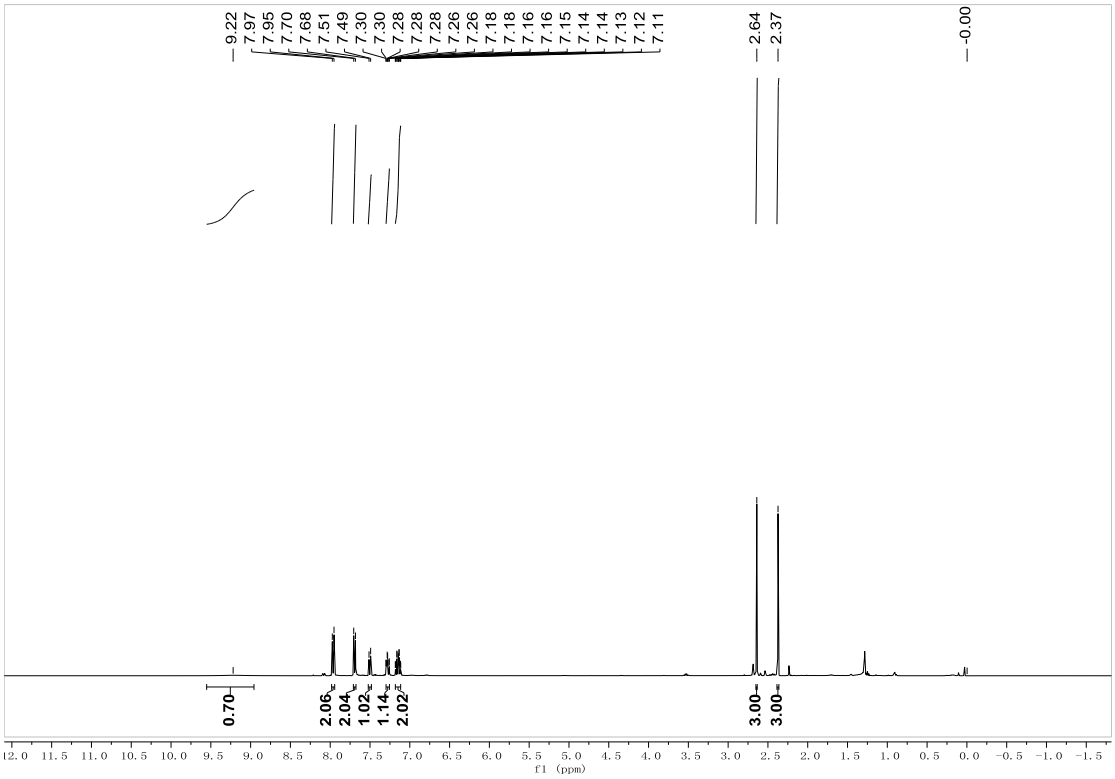

HO
N
O
O

2j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7.28
7.28
7.28
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7.26
7.18
7.18
7.16
7.16
7.15
7.14
7.14
7.13
7.12
7.11
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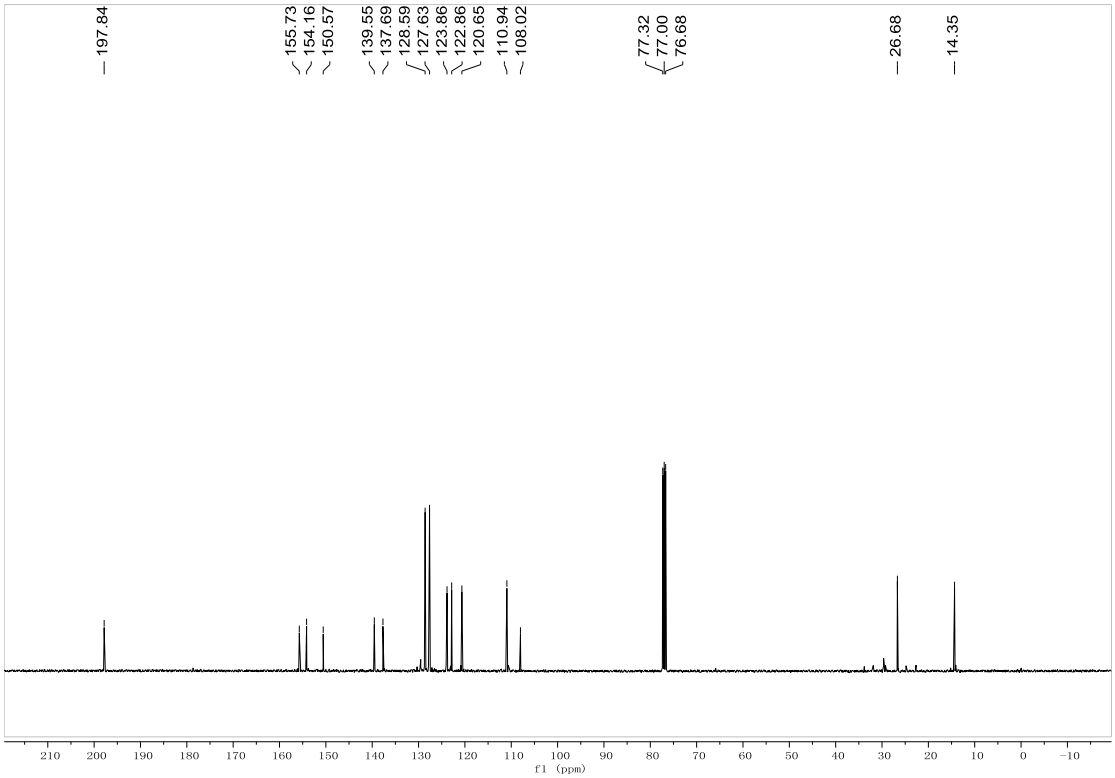
0.70
2.06
2.04
1.02
1.14
2.02
3.00
3.00
f1 (ppm)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120.65
110.94
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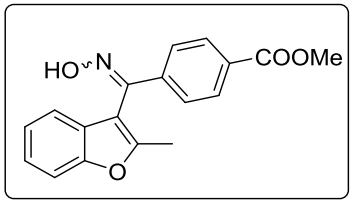
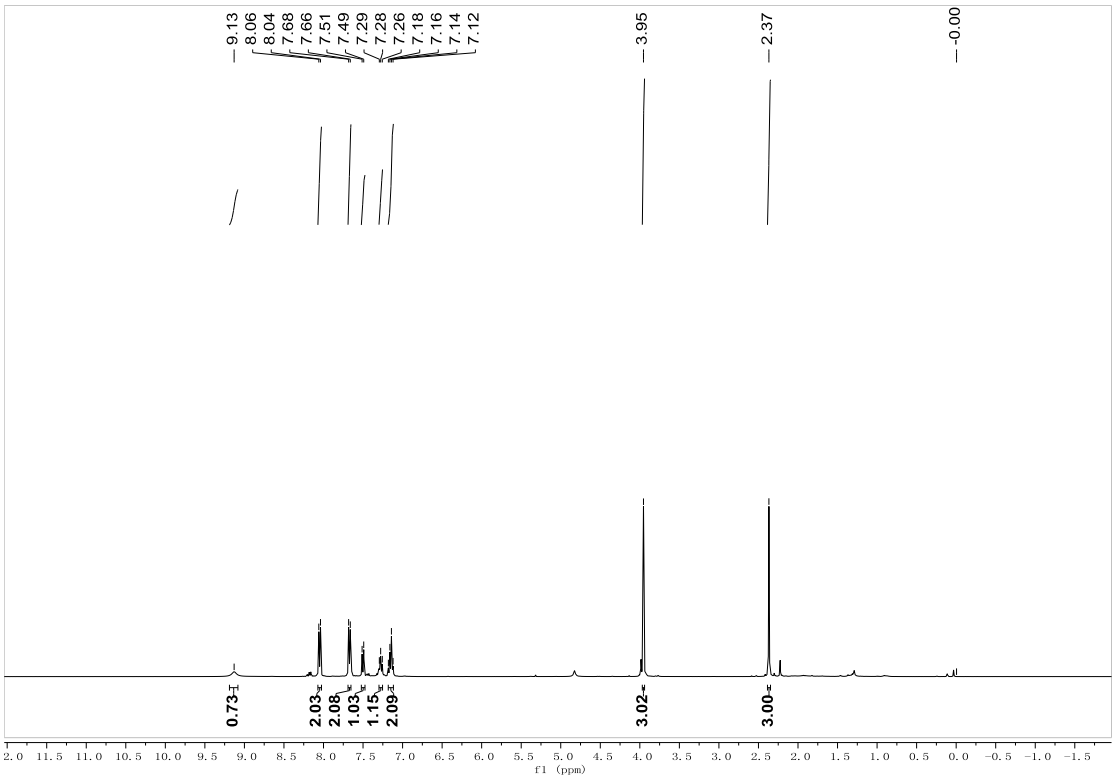
77.00
76.68
26.68
14.35
f1 (ppm)


HO
N
COOMe
O

2k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7.68
7.66
7.51
7.49
7.29
7.28
7.26
7.18
7.16
7.14
7.12
3.95
2.37
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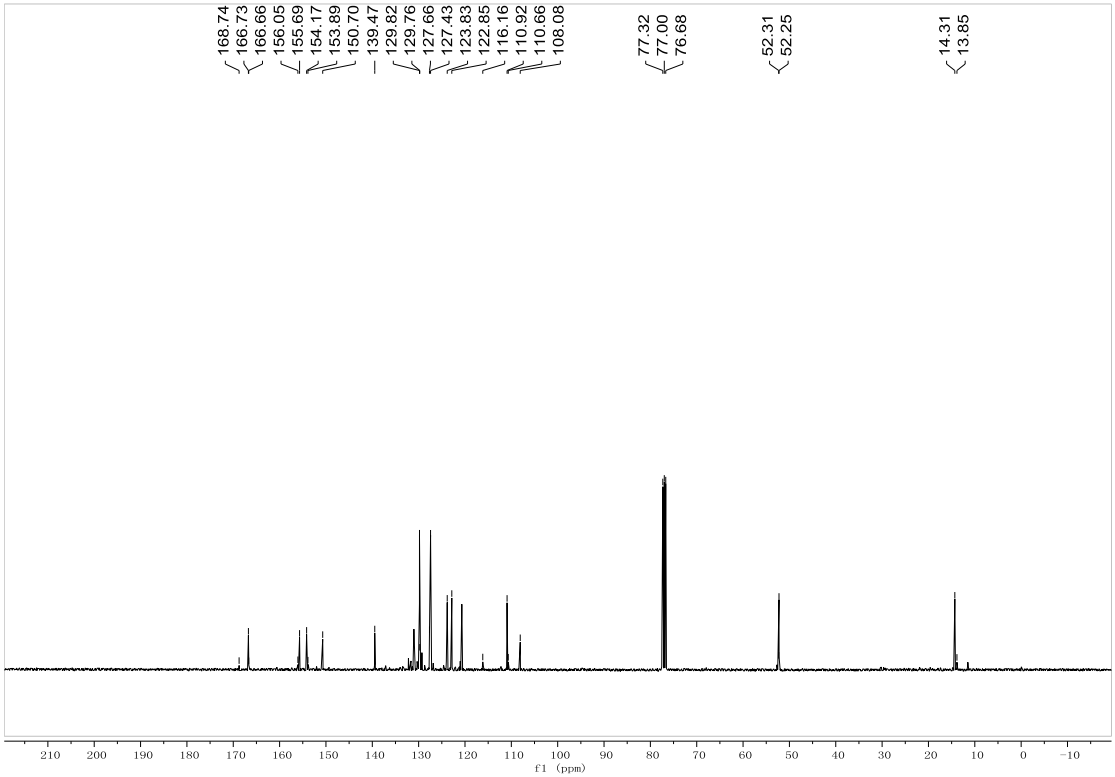
0.73
2.03
2.08
1.03
1.15
2.09
3.02
3.00
f1 (ppm)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150.70
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127.43
123.83
122.85
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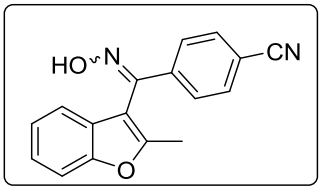
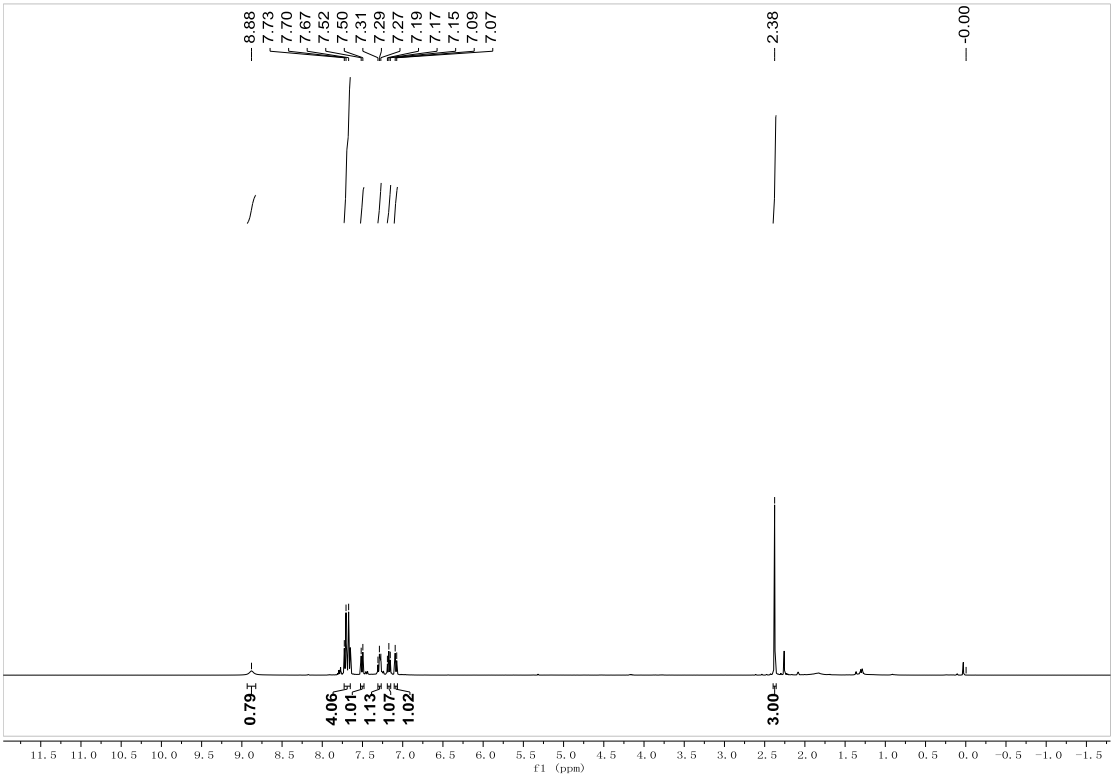
77.00
76.68
52.31
52.25
14.31
13.85
f1 (ppm)


HO
N
CN
O

2l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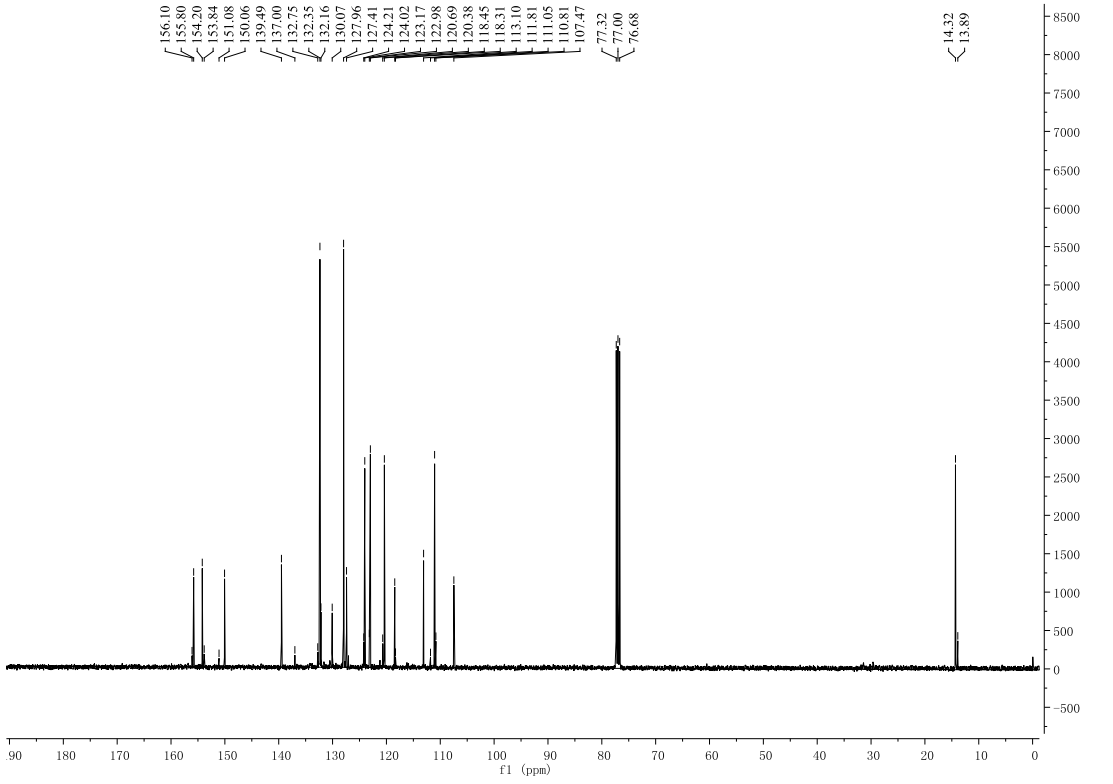
7.19
7.17
7.15
7.09
7.07
2.38
-0.00
0.79
4.06
1.01
1.13
1.07
1.02
3.00
f1 (ppm)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150.06
139.49
137.00
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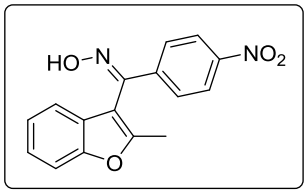
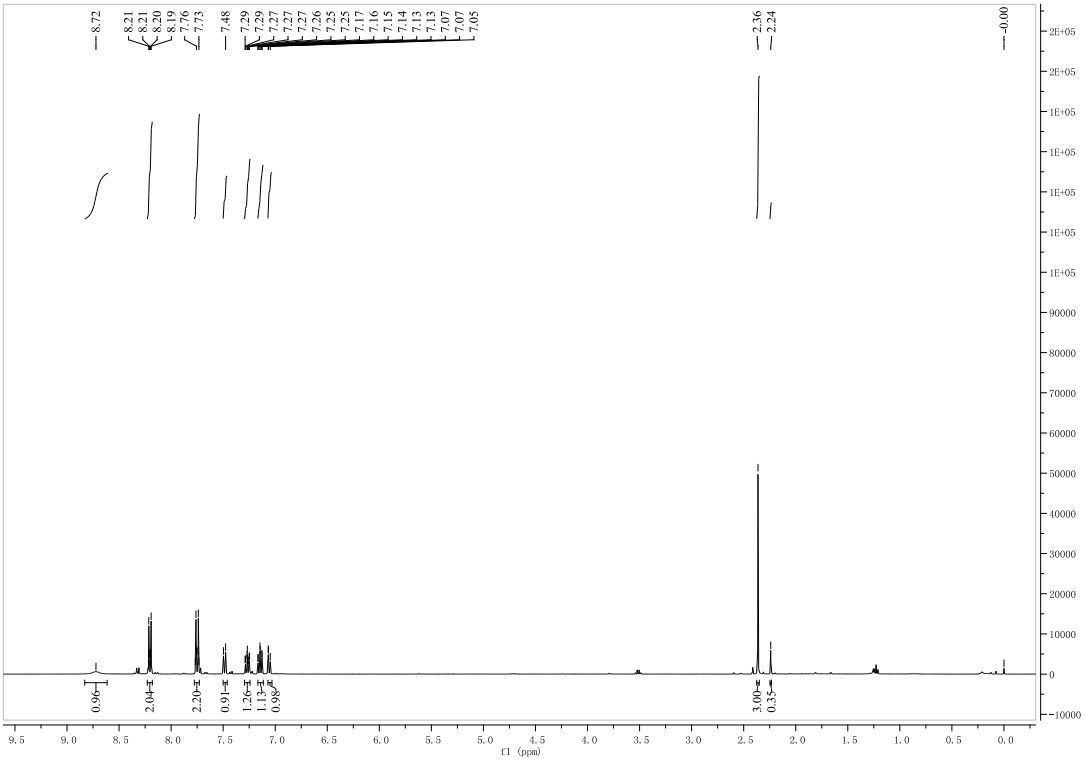
132.35
132.16
130.07
127.96
127.41
124.21
124.02
123.17
122.98
120.69
120.38
118.45
118.31
113.10
111.81
111.05
110.81
107.47
77.32
77.00
76.68
14.32
13.89
f1 (ppm)


HO-N
NO2
O

2m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8.21
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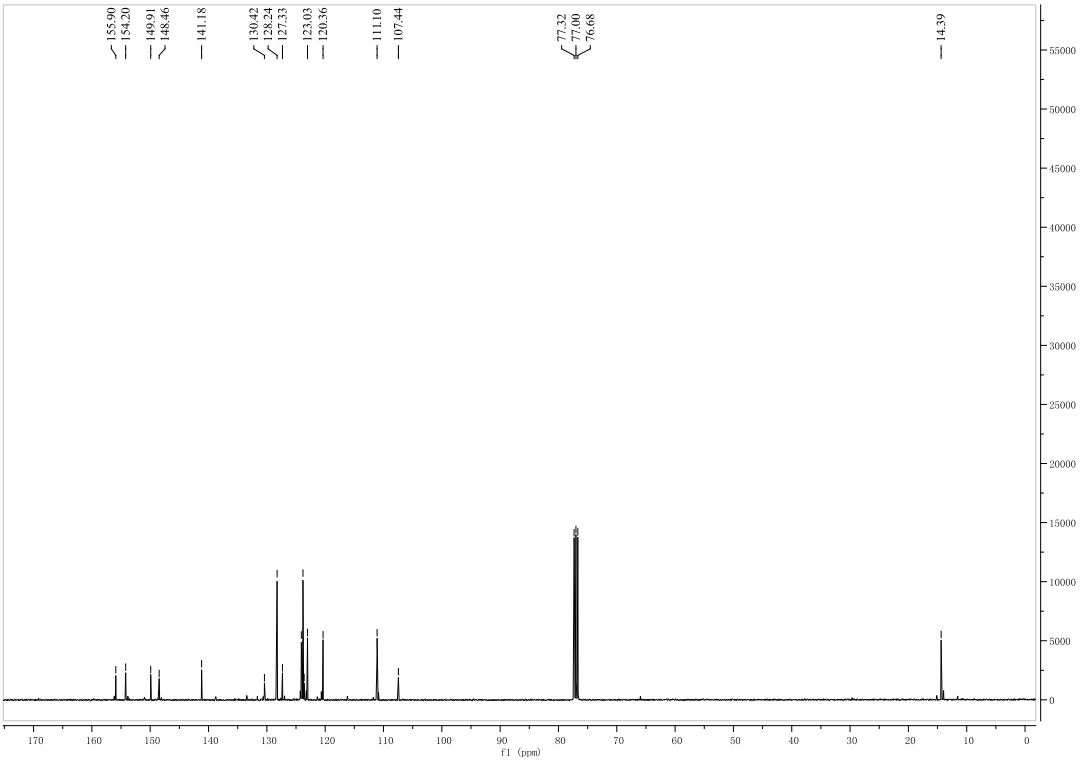
7.73
7.48
7.29
7.29
7.27
7.27
7.27
7.26
7.25
7.25
7.17
7.16
7.15
7.14
7.13
7.13
7.07
7.07
7.05
2.36
2.24
0.00
0.96
2.04
2.20
0.91
1.26
1.13
0.98
3.00
0.35
f1 (ppm)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127.33
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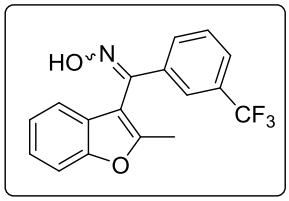
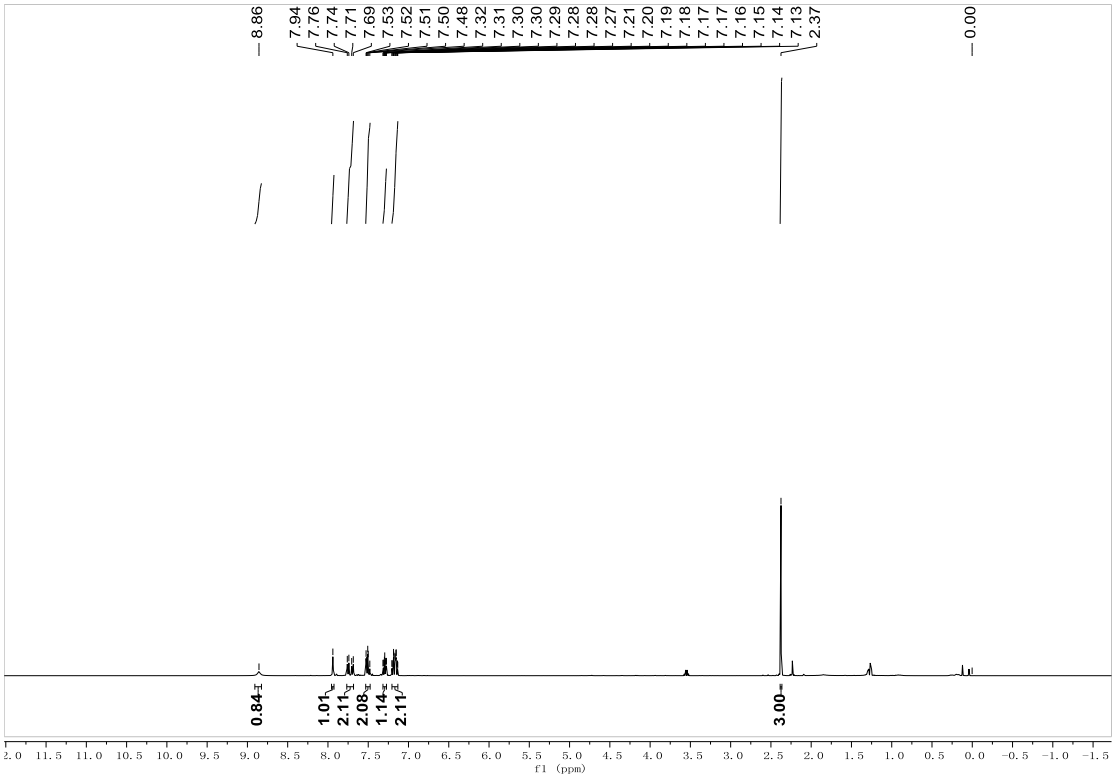
120.36
111.10
107.44
77.32
77.00
76.68
14.39
f1 (ppm)


HO
N
CF3
O

2n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7.76
7.74
7.71
7.69
7.53
7.52
7.51
7.50
7.48
7.32
7.31
7.30
7.30
7.29
7.28
7.28
7.27
7.21
7.20
7.19
7.18
7.17
7.17
7.16
7.15
7.14
7.13
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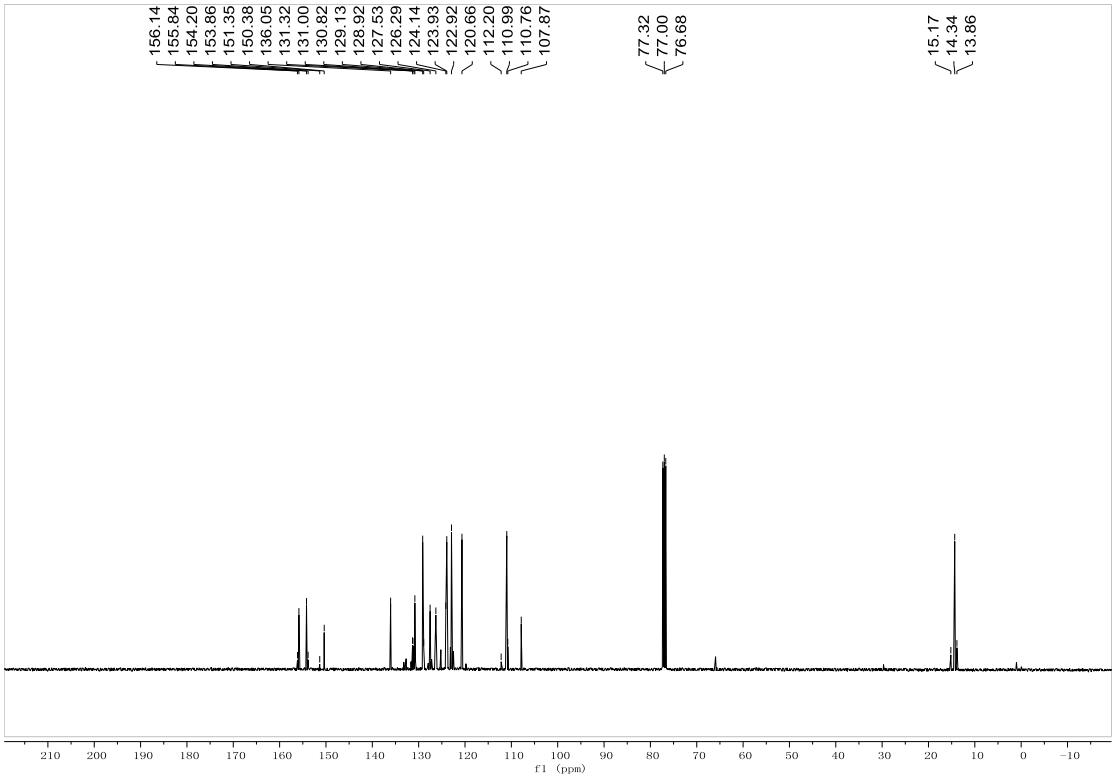
1.01
2.11
2.08
1.14
2.11
3.00
f1 (ppm)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131.32
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130.82
129.13
128.92
127.53
126.29
124.14
123.93
122.92
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112.20
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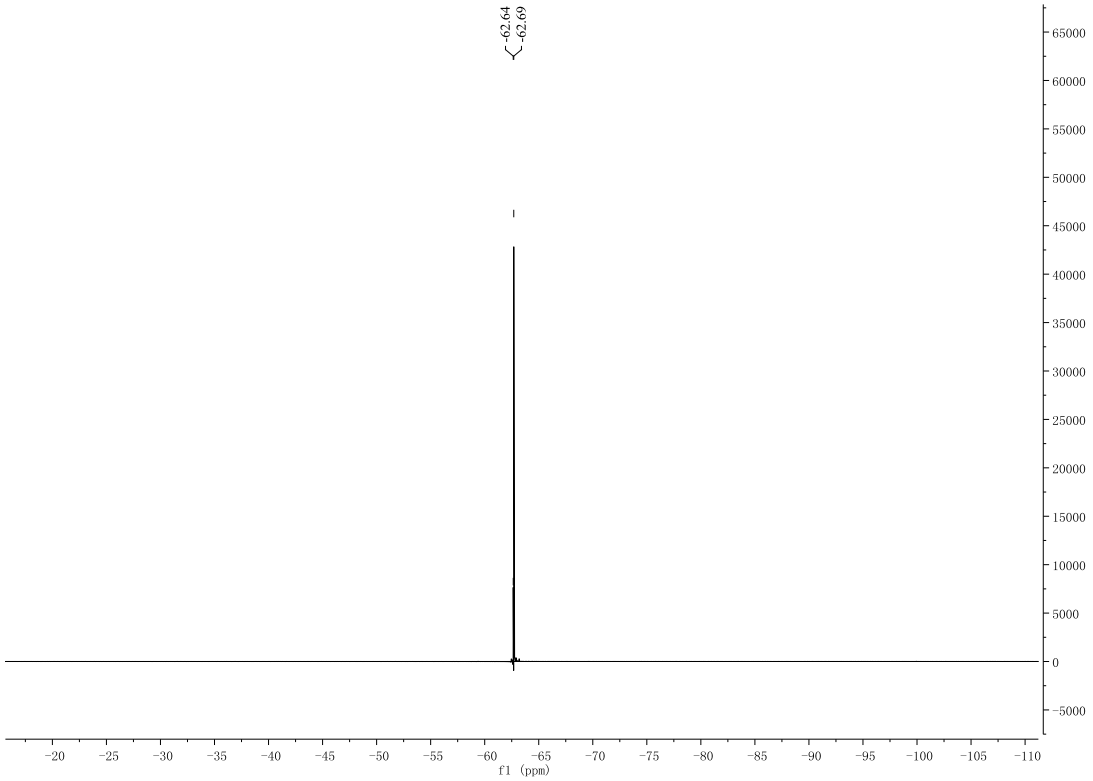
110.76
107.87
77.32
77.00
76.68
15.17
14.34
13.86
f1 (ppm)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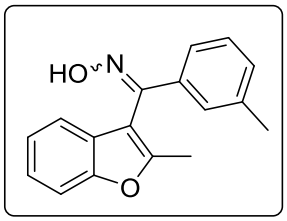
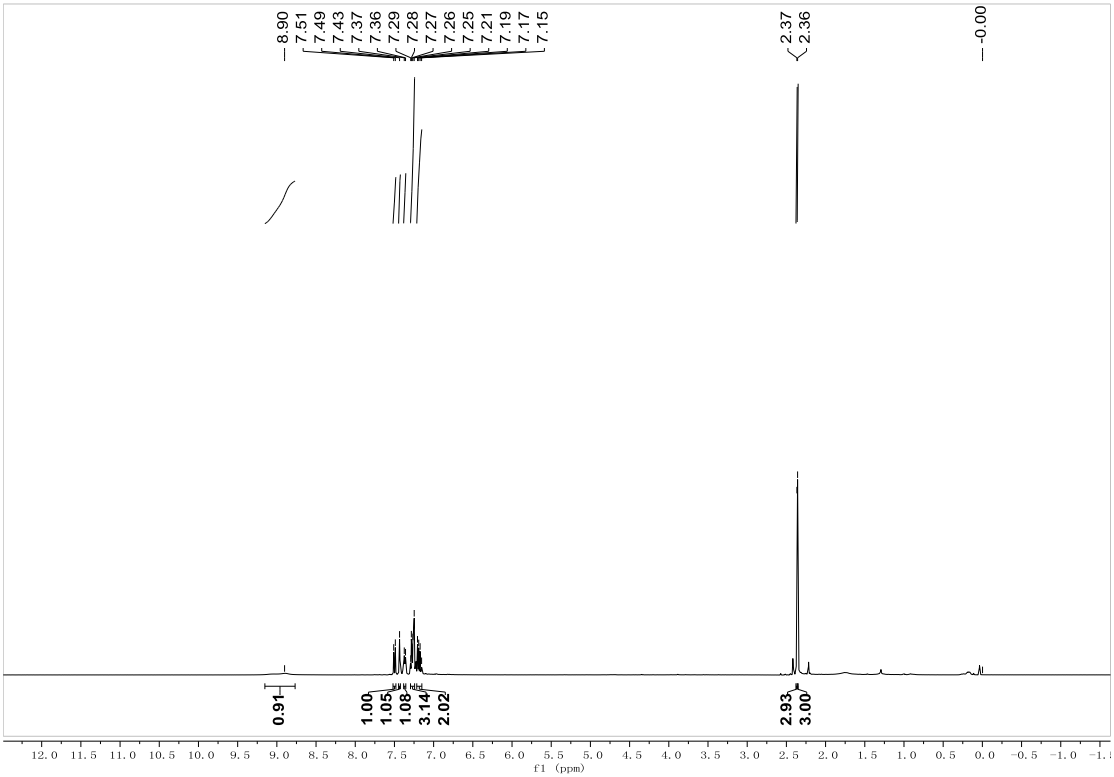
f1 (ppm)


HO
N
O

2o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7.36
7.29
7.28
7.27
7.26
7.25
7.21
7.19
7.17
7.15
2.37
2.36
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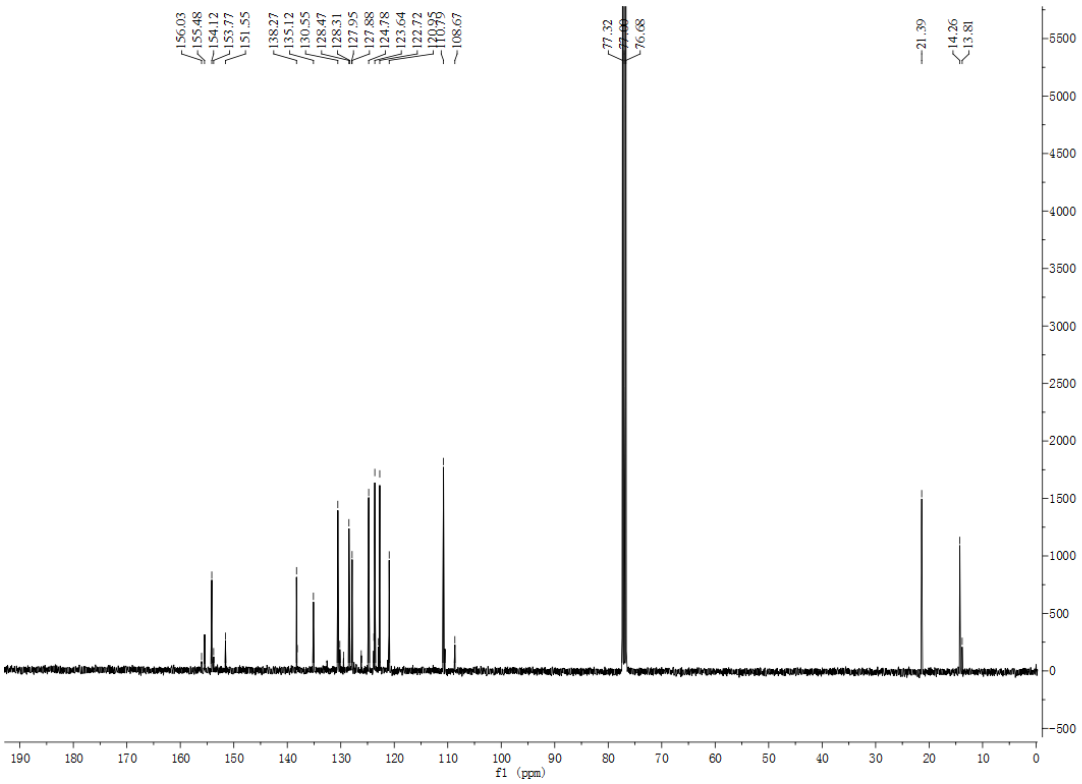
0.91
1.00
1.05
1.08
3.14
2.02
2.93
3.00
f1 (ppm)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128.31
127.95
127.88
124.78
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122.72
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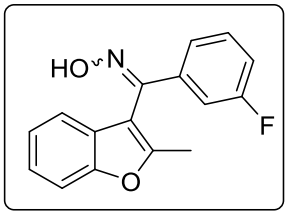
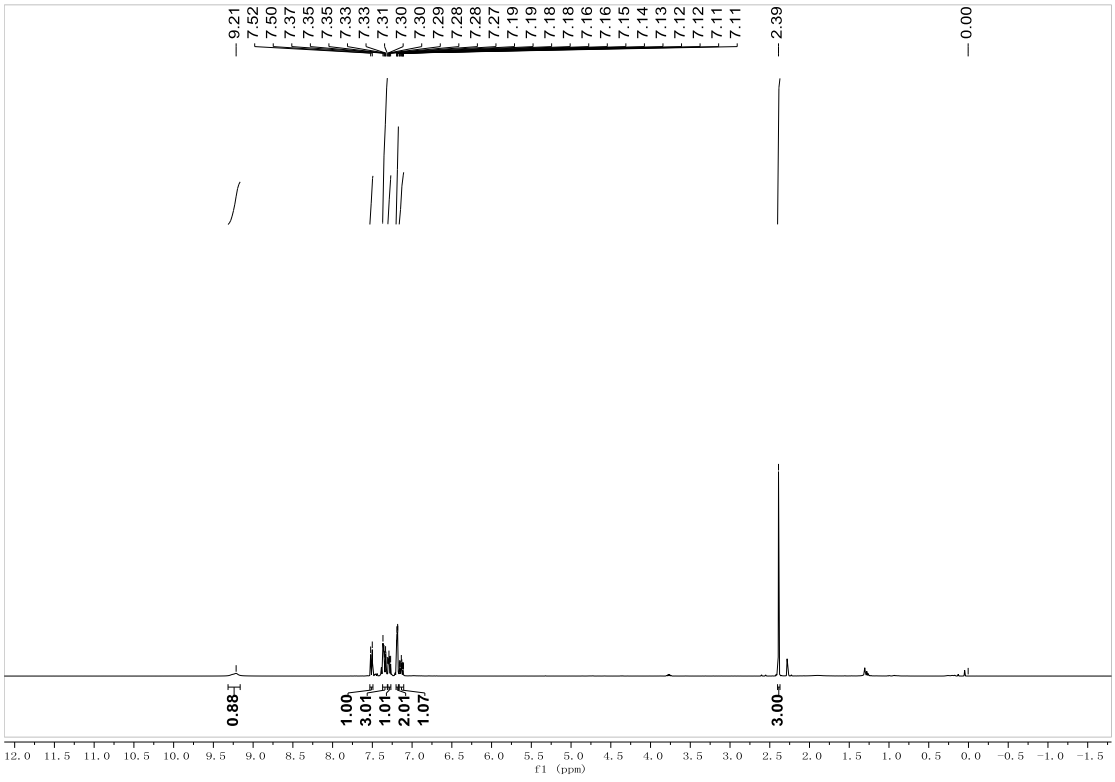
110.79
108.67
77.32
77.00
76.68
21.39
14.26
13.81
f1 (ppm)


HO
N
F
O

2p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7.33
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7.30
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7.29
7.28
7.28
7.27
7.19
7.19
7.18
7.18
7.16
7.16
7.15
7.14
7.13
7.12
7.12
7.11
7.11
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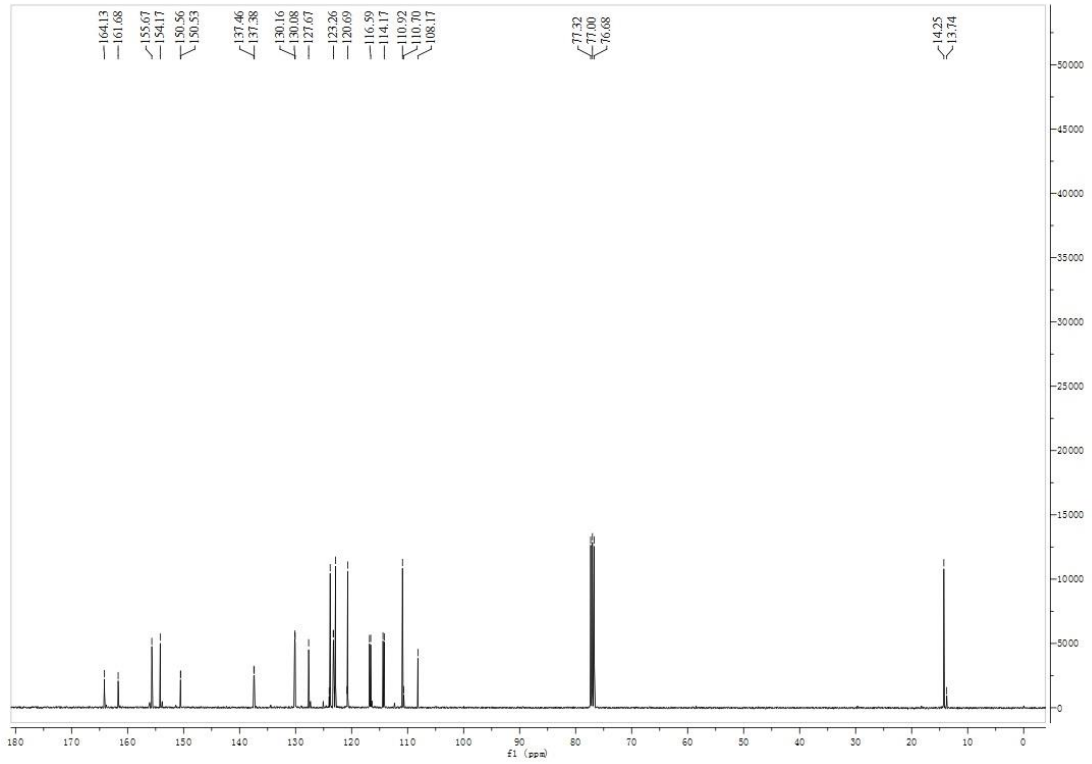
0.88
1.00
3.01
1.01
2.01
1.07
3.00
f1 (ppm)


164.13
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154.17
150.56
150.53
137.46
137.38
130.16
130.08
127.67
123.26
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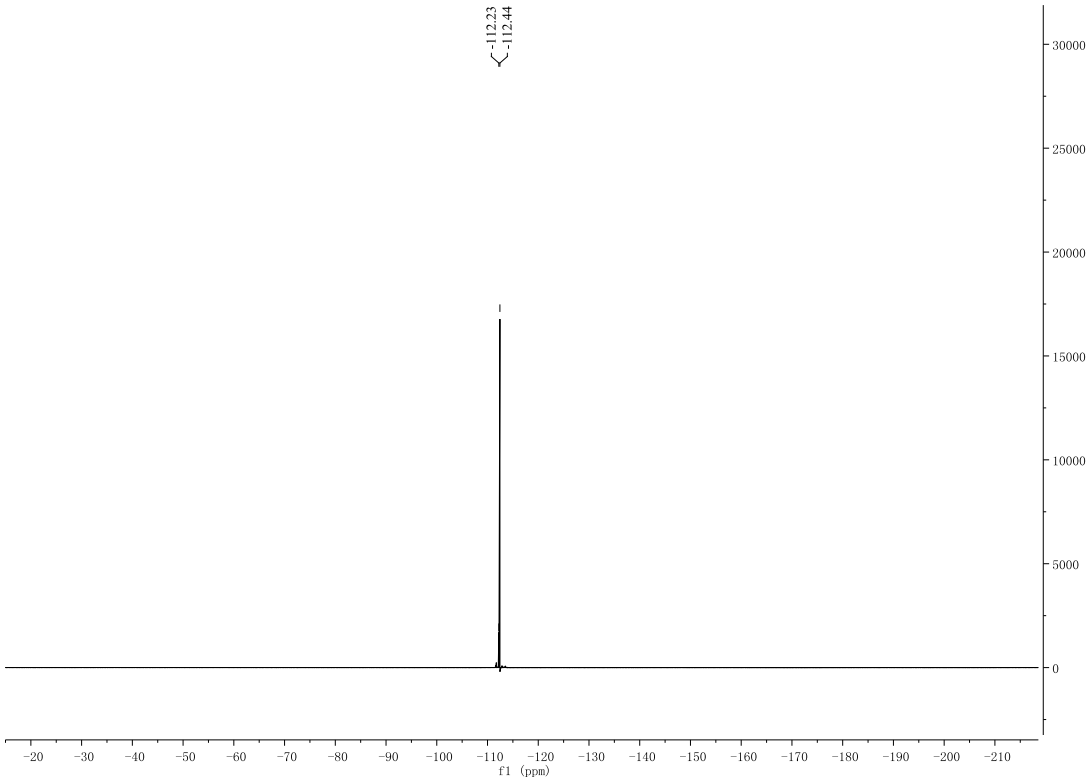
77.00
76.68
14.25
13.74
f1 (ppm)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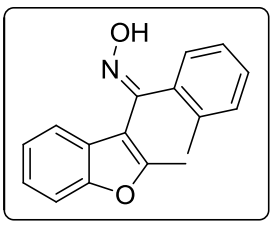
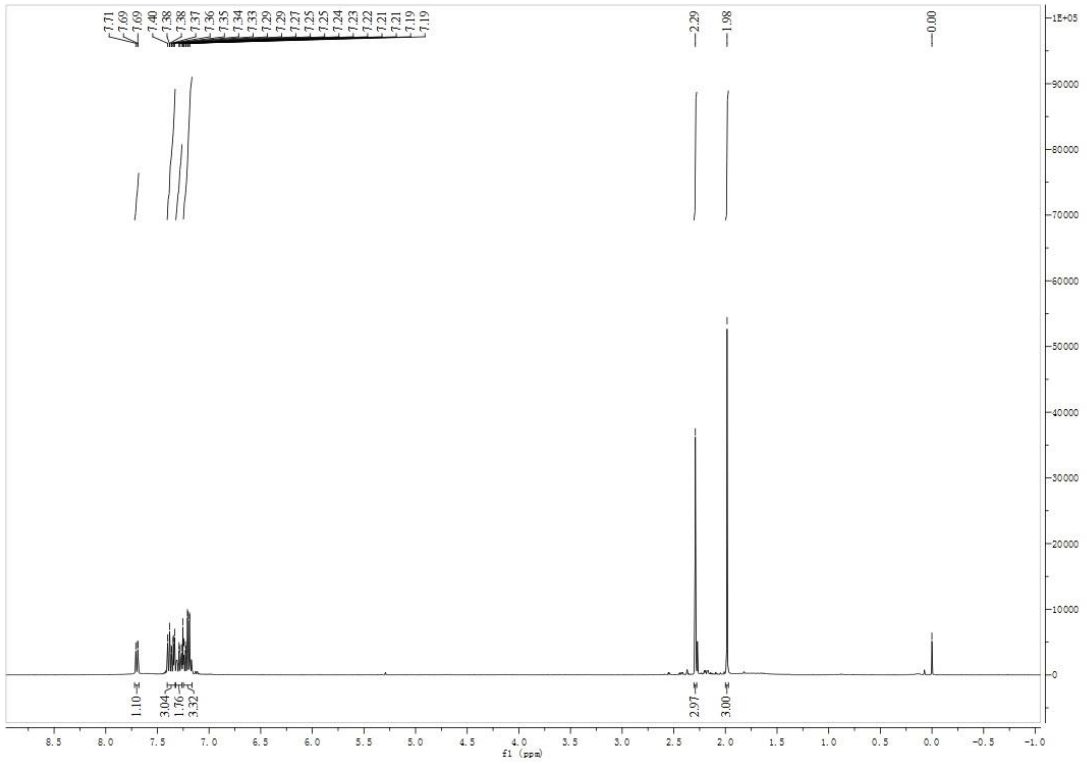
-112.44
f1 (ppm)


OH
N
O

2q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7.69
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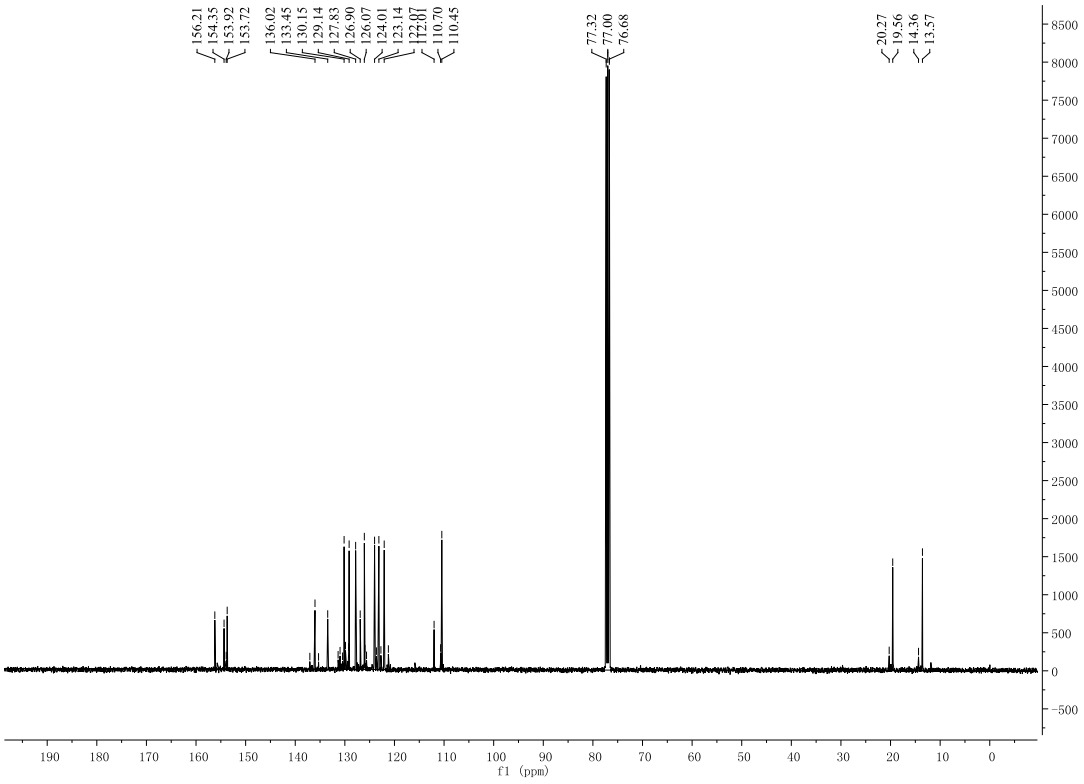
7.38
7.37
7.36
7.35
7.34
7.33
7.29
7.29
7.27
7.25
7.25
7.24
7.23
7.22
7.21
7.21
7.19
7.19
2.29
1.98
0.00
1.10
3.04
1.76
3.32
2.97
3.00
f1 (ppm)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136.02
133.45
130.15
129.14
127.83
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126.07
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123.14
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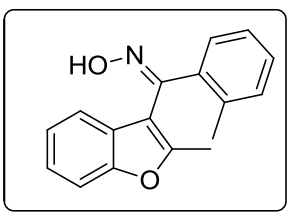
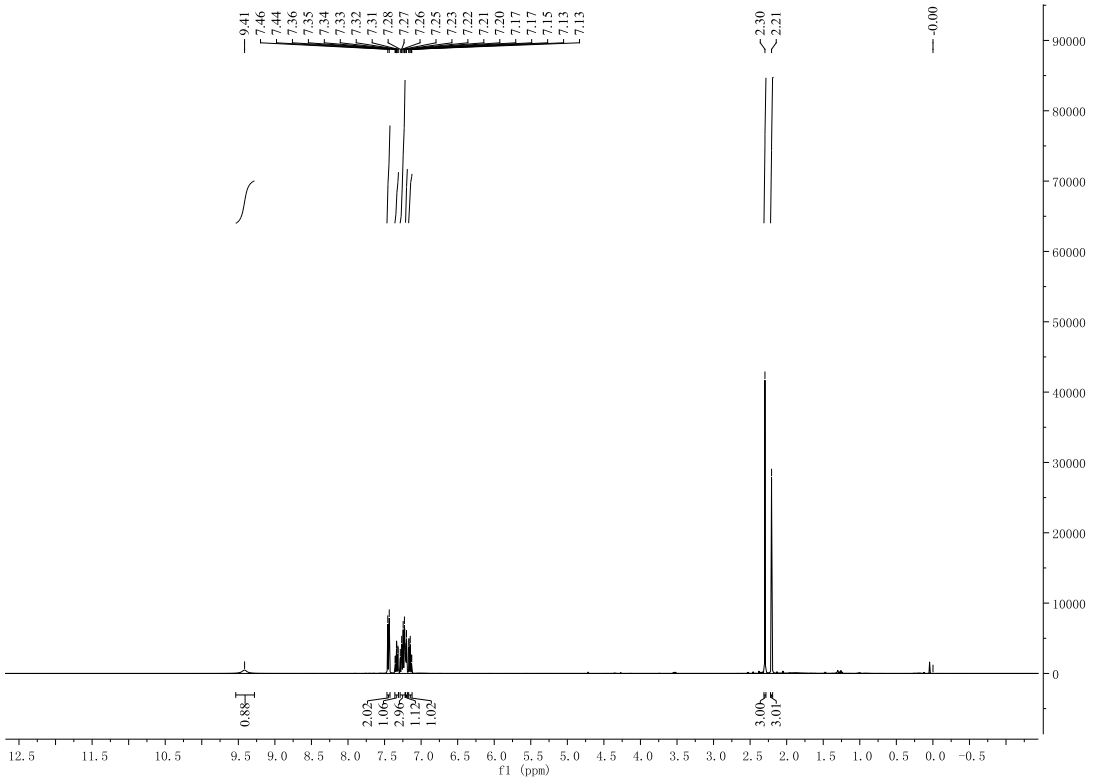
77.00
76.68
20.27
19.56
14.36
13.57
f1 (ppm)


HO-N
O

2q'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7.34
7.33
7.32
7.31
7.28
7.27
7.26
7.25
7.23
7.22
7.21
7.20
7.17
7.17
7.15
7.13
7.13
2.30
2.21
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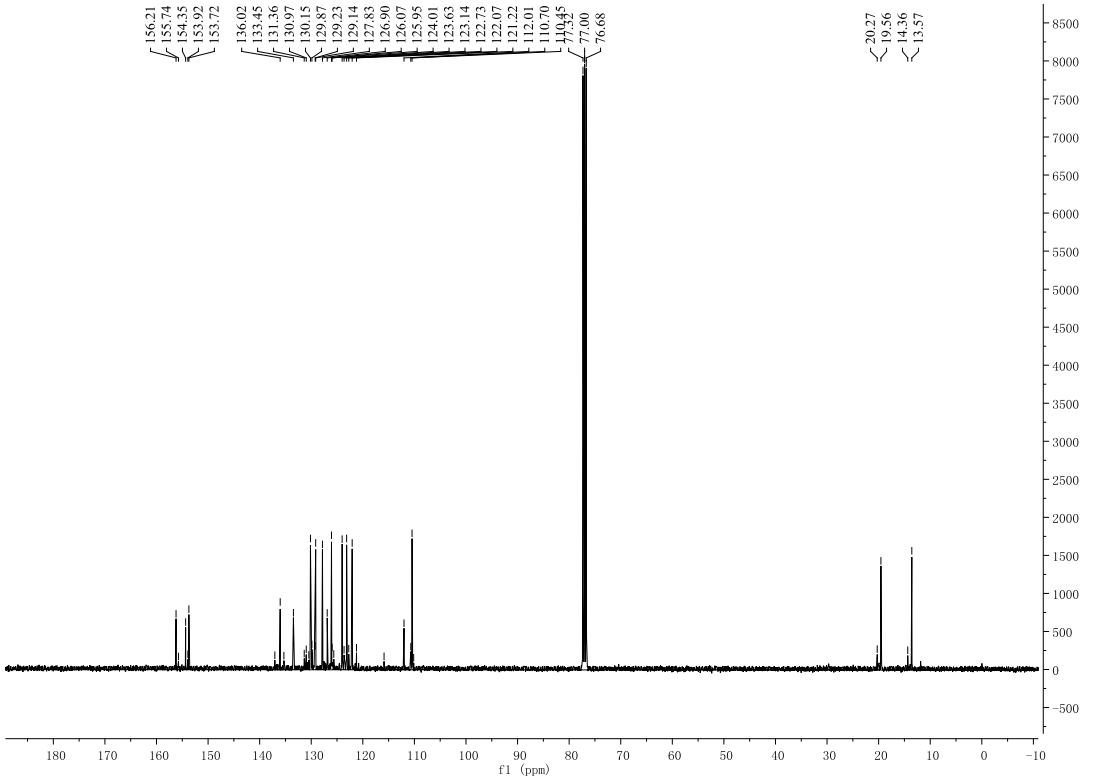
0.88
2.02
1.06
2.96
1.12
1.02
3.00
3.01
f1 (ppm)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153.72
136.02
133.45
131.36
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130.15
129.87
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129.14
127.83
126.90
126.07
125.95
124.01
123.63
123.14
122.73
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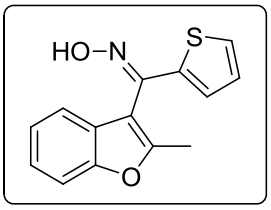
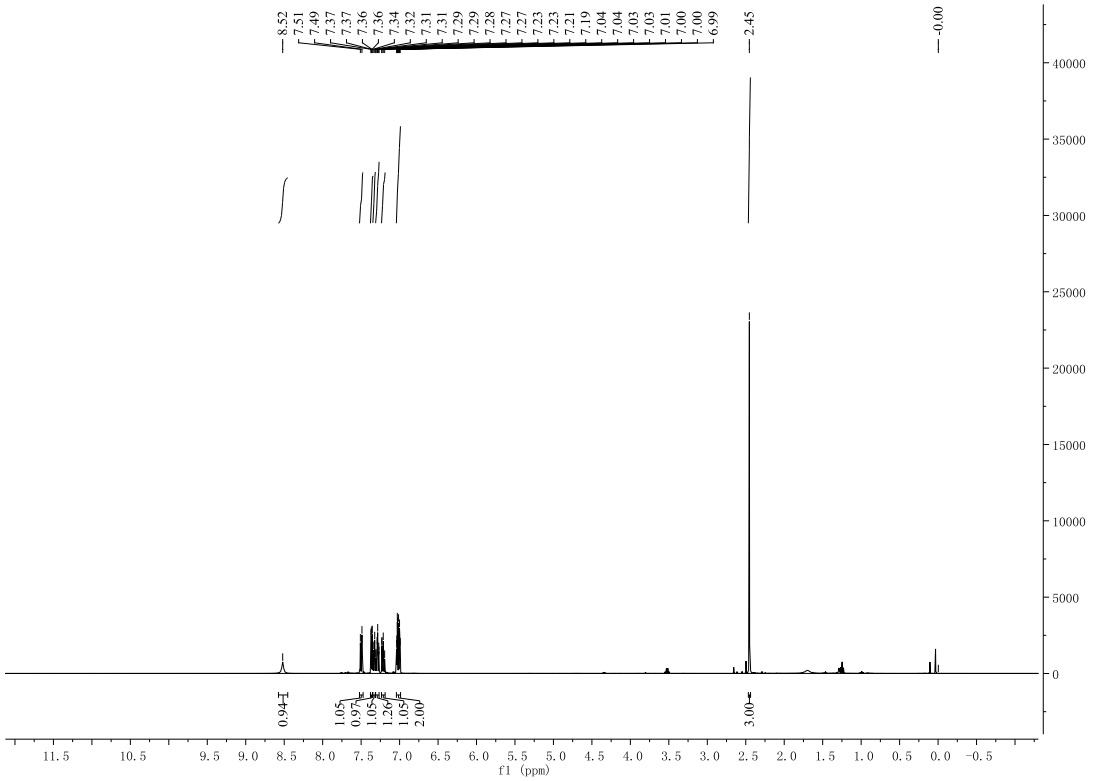
77.00
76.68
20.27
19.56
14.36
13.57
f1 (ppm)


HO–N
S
O

2r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7.29
7.28
7.27
7.27
7.23
7.23
7.21
7.19
7.04
7.04
7.03
7.03
7.01
7.00
7.00
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0.94
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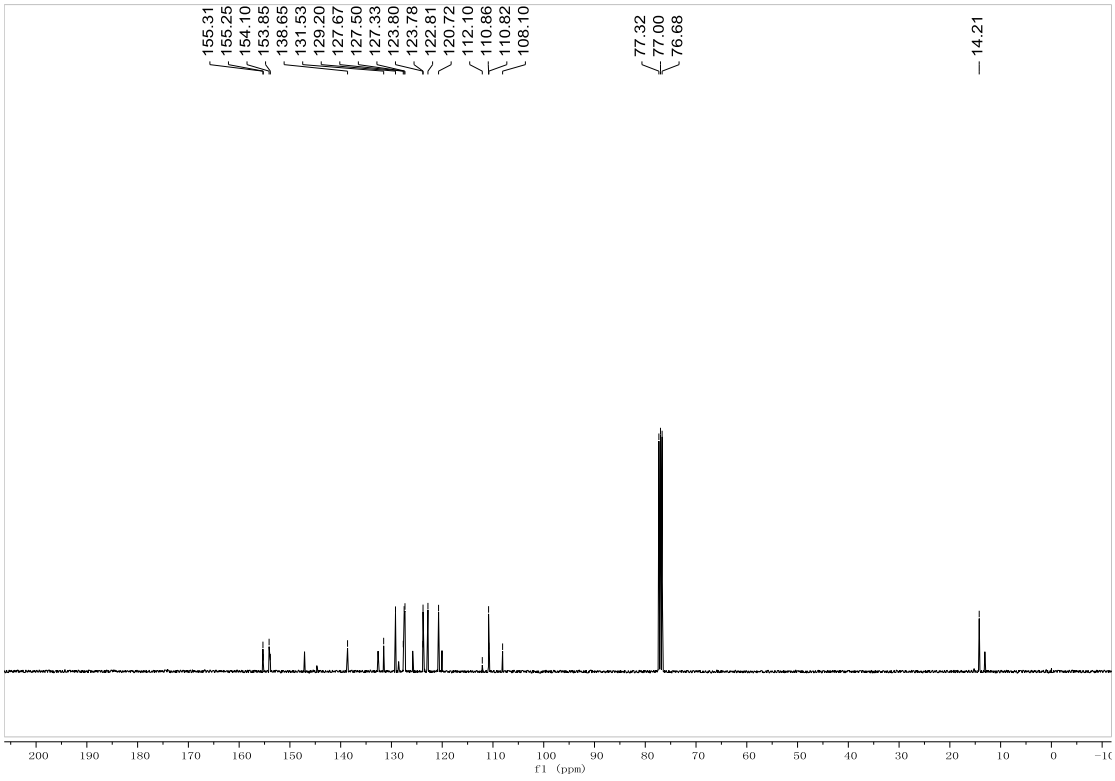
0.97
1.05
1.20
1.05
2.00
3.00
f1 (ppm)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131.53
129.20
127.67
127.50
127.33
123.80
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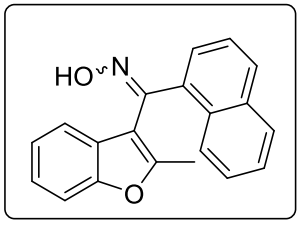
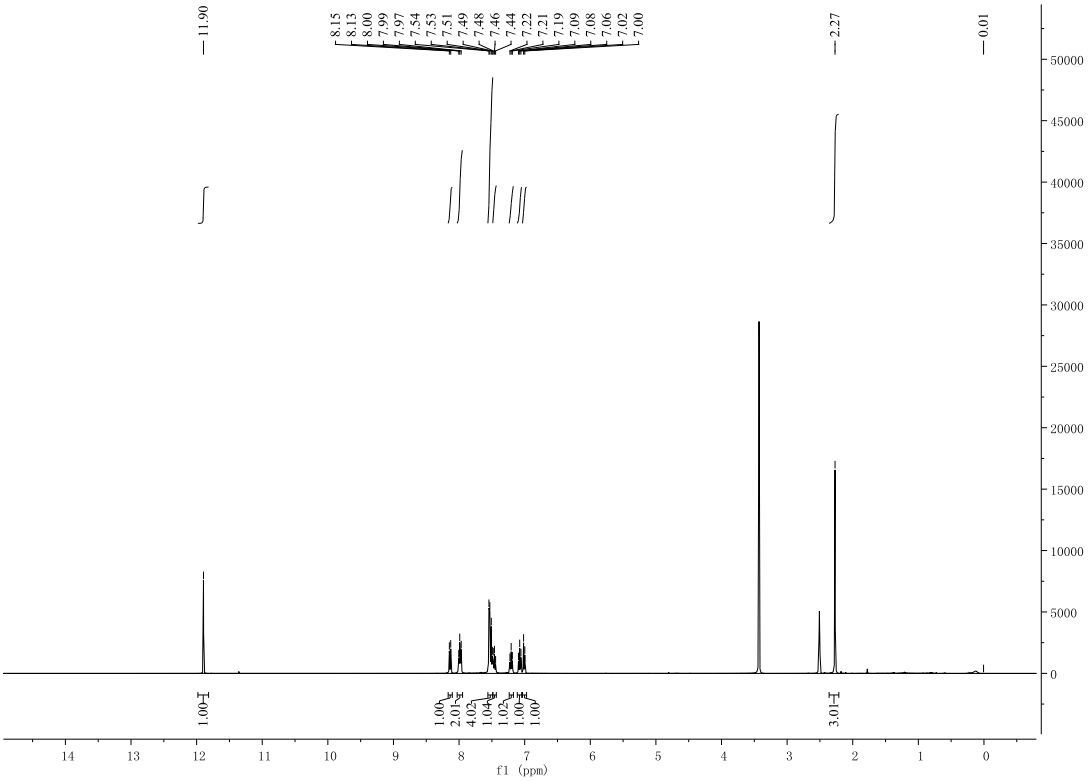
120.72
112.10
110.86
110.82
108.10
77.32
77.00
76.68
14.21
f1 (ppm)


HO
N
O

2s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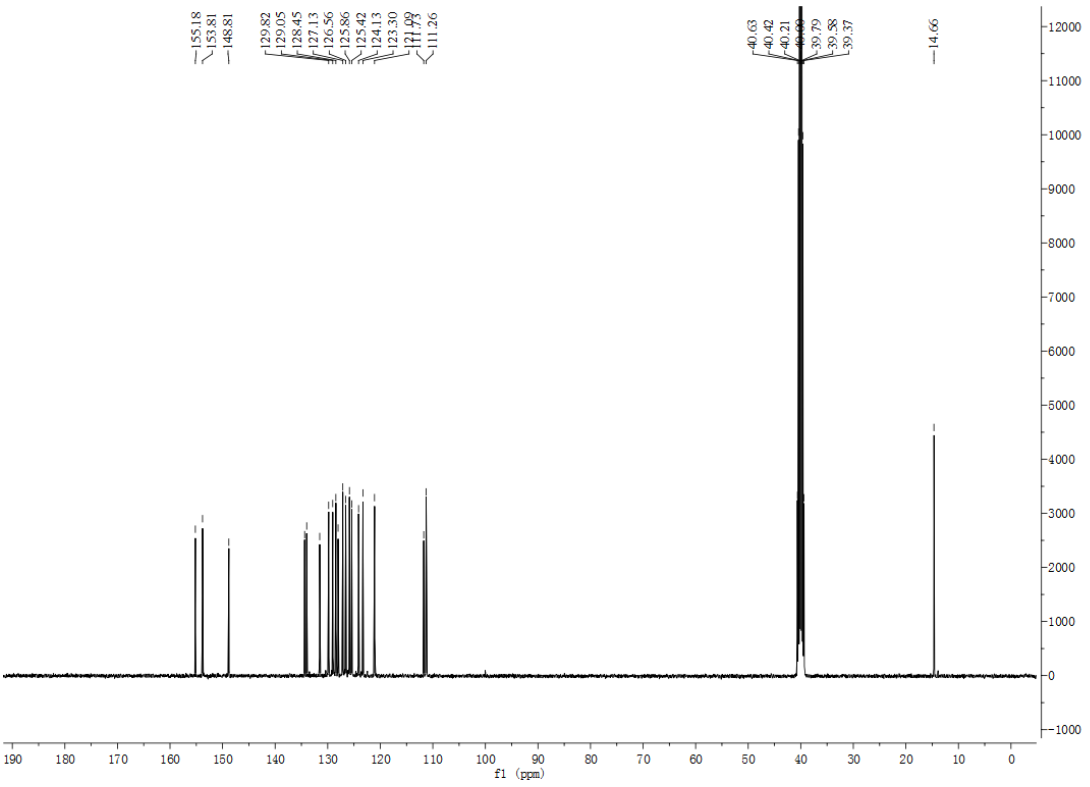
7.53
7.51
7.49
7.48
7.46
7.44
7.22
7.21
7.19
7.09
7.08
7.06
7.02
7.00
2.27
0.01
1.00
2.01
4.03
1.04
1.02
1.00
1.00
3.01
f1 (ppm)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127.13
126.56
125.86
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124.13
123.30
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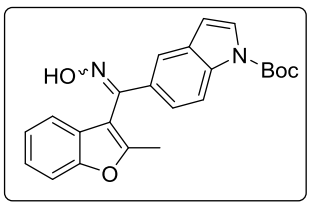
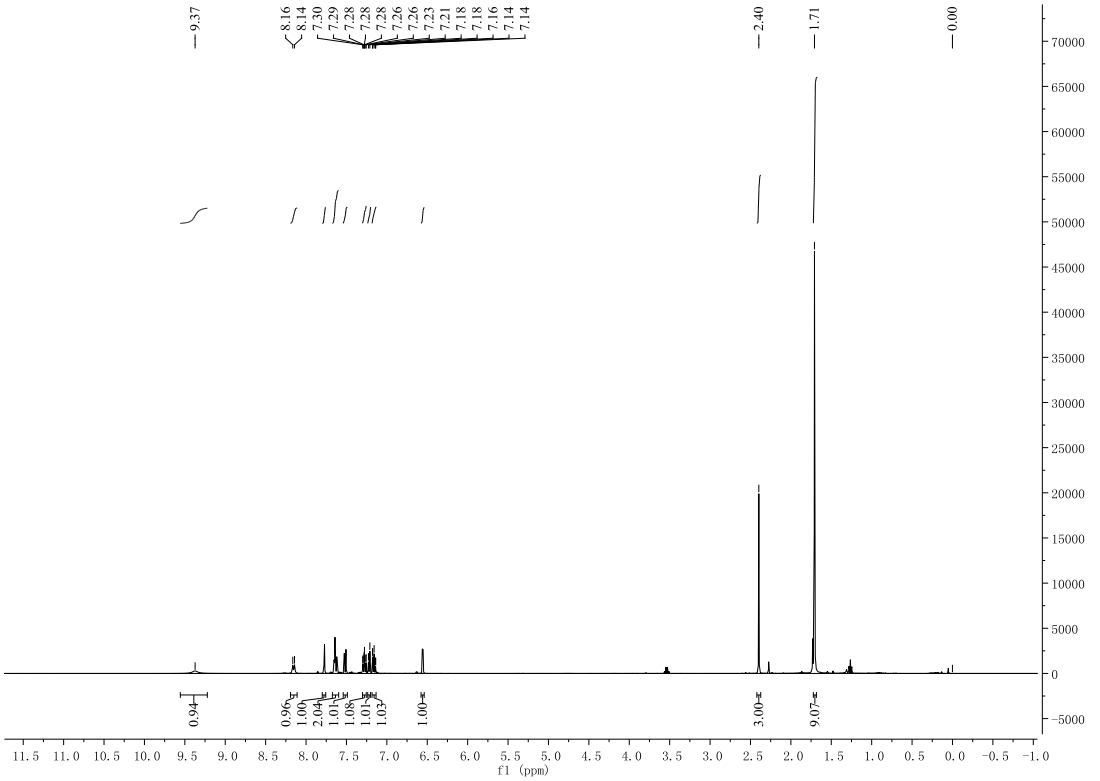
39.79
39.58
39.37
14.66
f1 (ppm)


HO
N
N
Boc
O

2t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7.26
7.26
7.23
7.21
7.18
7.18
7.16
7.14
7.14
2.40
1.71
0.00
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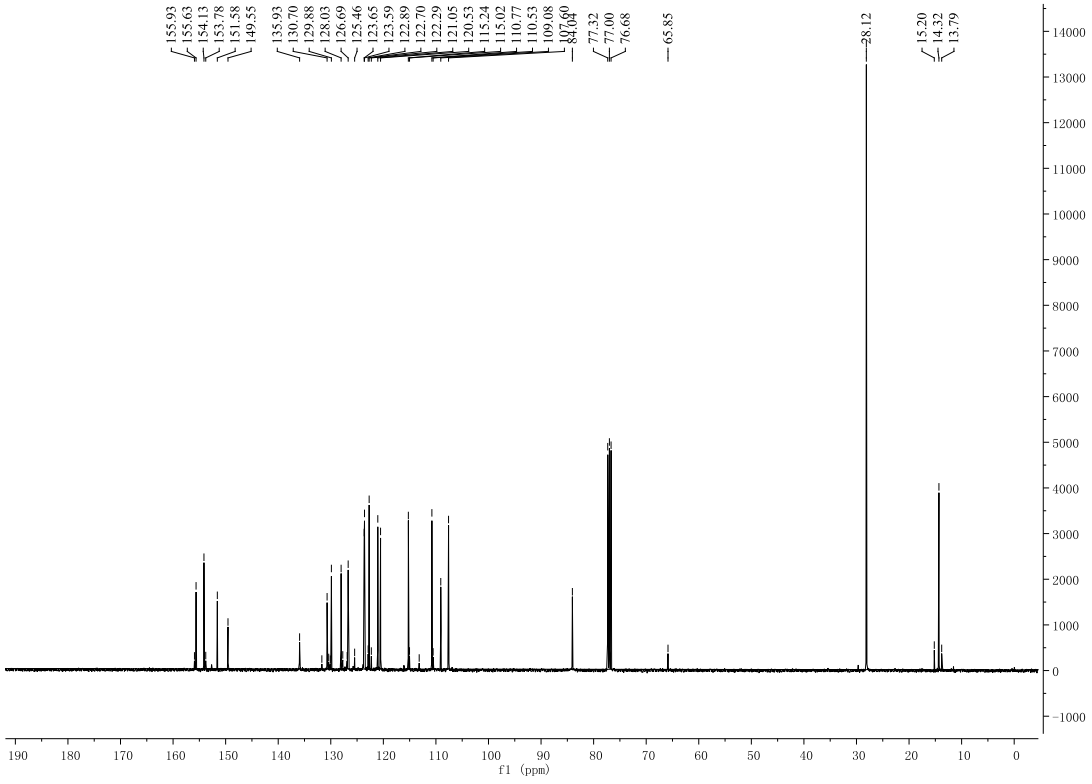
0.96
1.00
2.04
1.01
1.08
1.01
1.03
1.00
3.00
9.07
f1 (ppm)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123.65
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122.89
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122.29
121.05
120.53
115.24
115.02
110.77
110.53
109.08
107.60
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77.00
76.68
65.85
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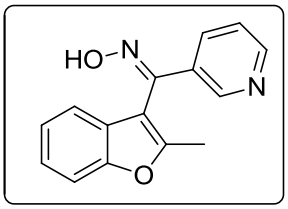
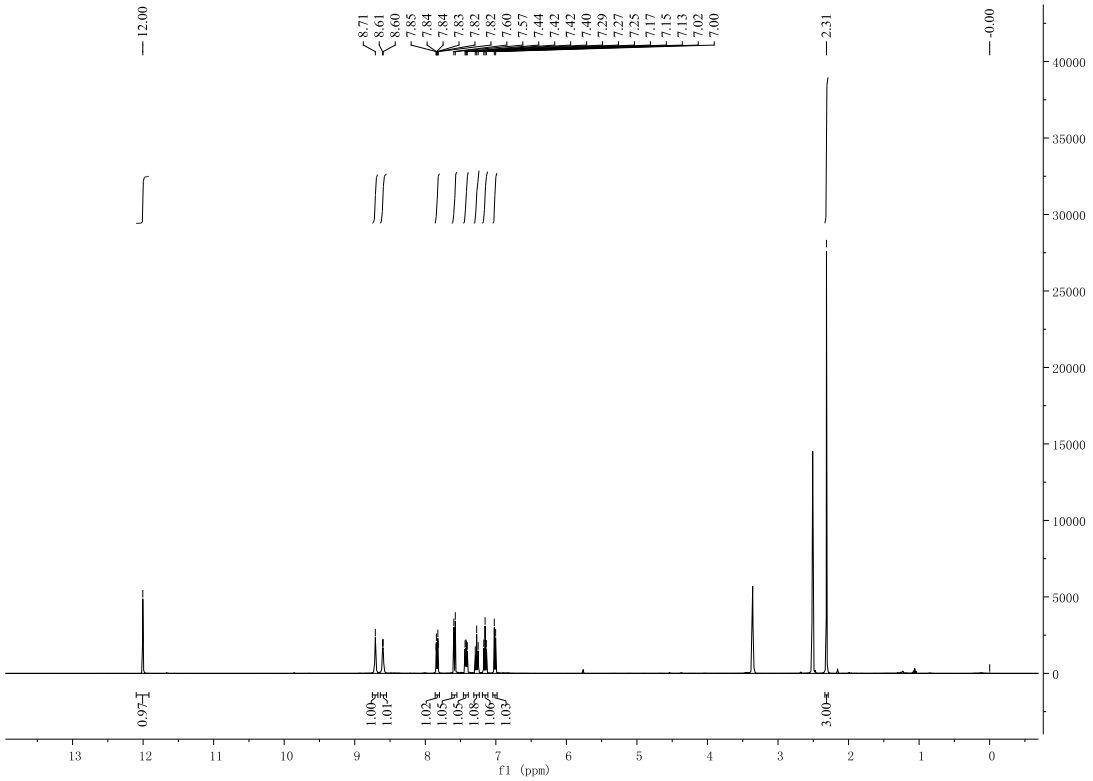
15.20
14.32
13.79
f1 (ppm)


HO
N
N
O

2u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7.84
7.84
7.83
7.82
7.82
7.60
7.57
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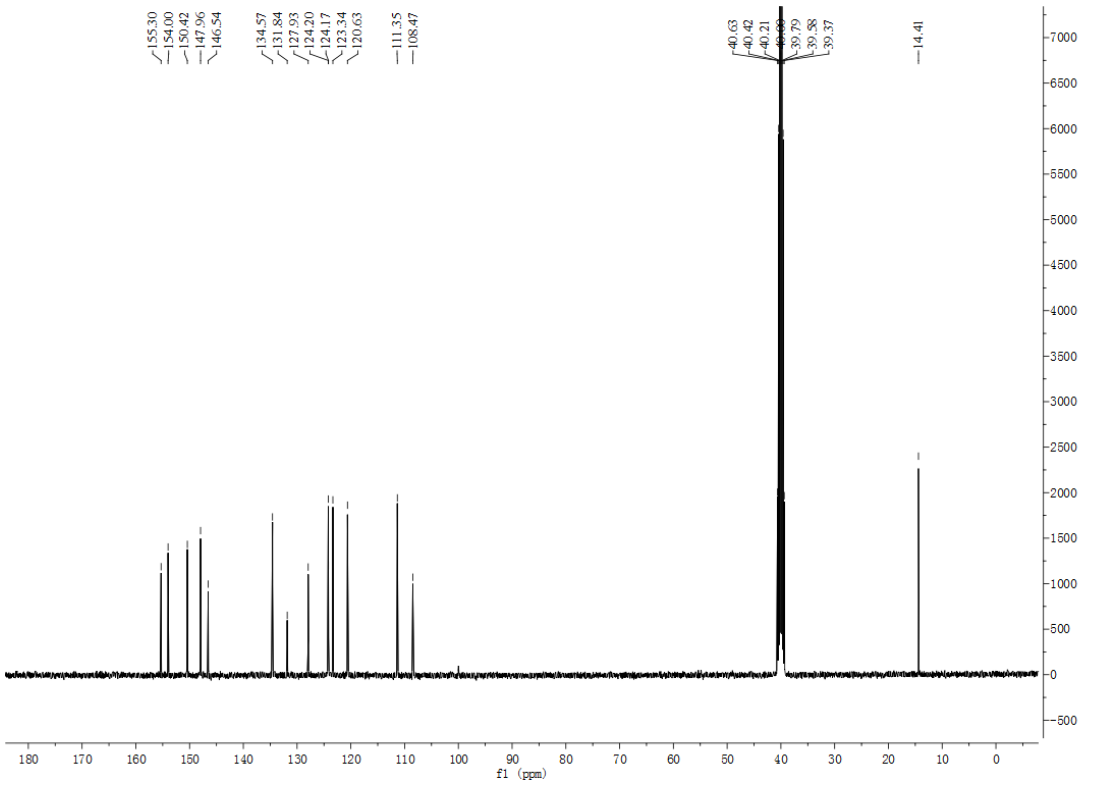
7.42
7.42
7.40
7.29
7.27
7.25
7.17
7.15
7.13
7.02
7.00
2.31
-0.00
0.97
1.00
1.01
1.02
1.05
1.05
1.08
1.06
1.03
3.00
f1 (ppm)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131.84
127.93
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124.17
123.34
120.63
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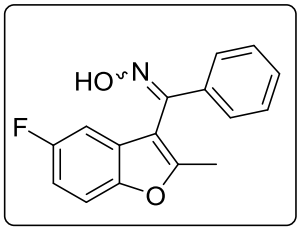
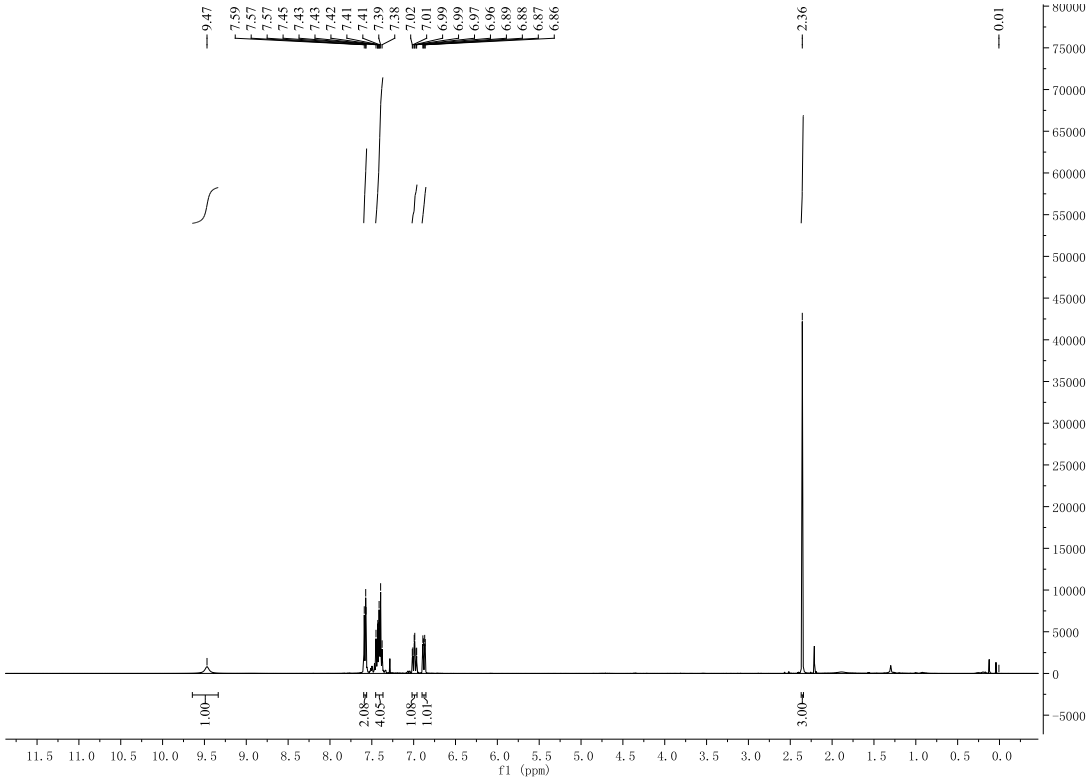
39.79
39.58
39.37
14.41
f1 (ppm)


HO
N
F
O

2v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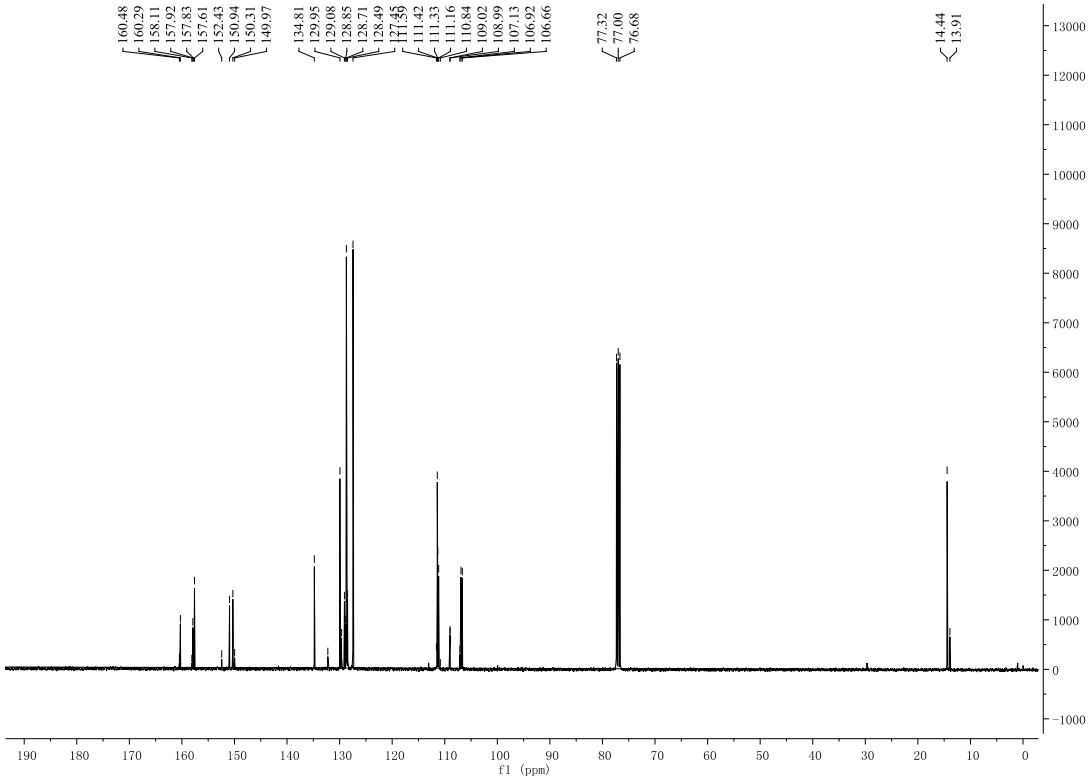
7.43
7.42
7.41
7.41
7.39
7.38
7.02
7.01
6.99
6.99
6.97
6.96
6.89
6.88
6.87
6.86
2.36
0.01
1.00
2.08
4.05
1.08
1.01
3.00
f1 (ppm)


160.48
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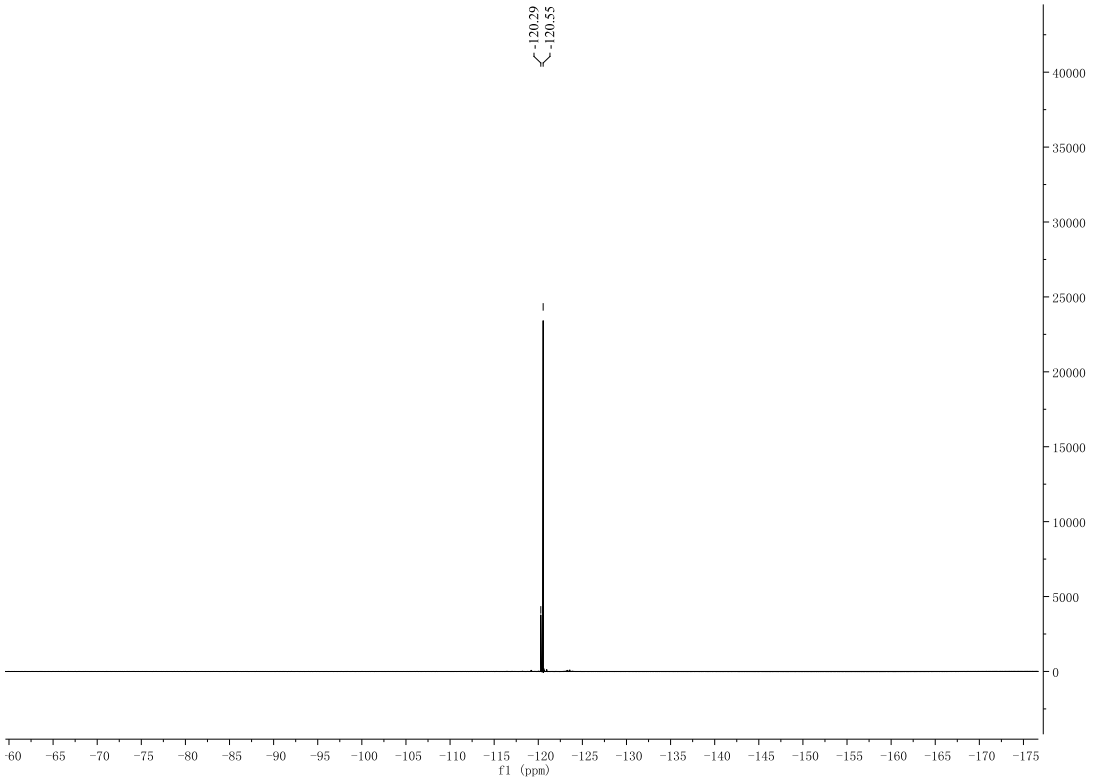
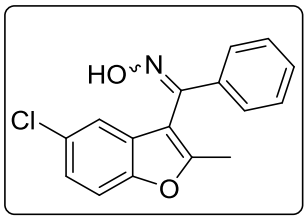
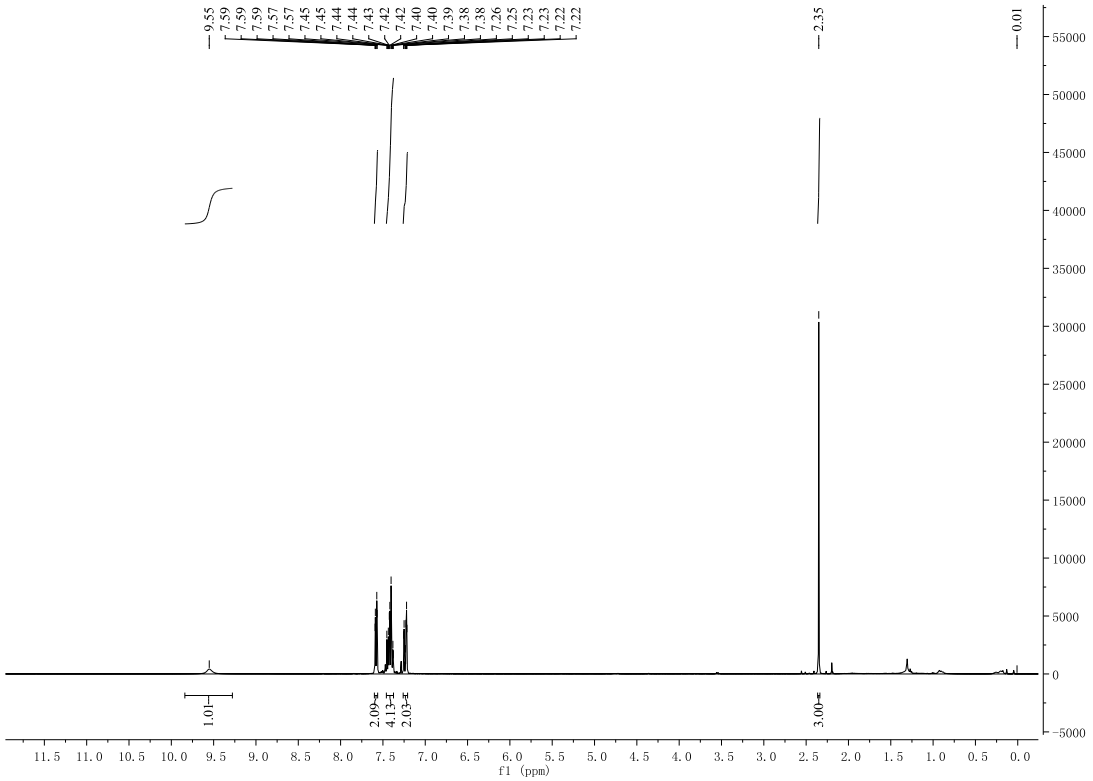
158.11
157.92
157.83
157.61
152.43
150.94
150.31
149.97
134.81
129.95
129.08
128.85
128.71
128.49
111.42
111.33
111.16
110.84
109.02
108.99
107.13
106.92
106.66
77.32
77.00
76.68
14.44
13.91
f1 (ppm)


-120.29
-120.55
f1 (ppm)


HO
N
Cl
O

2w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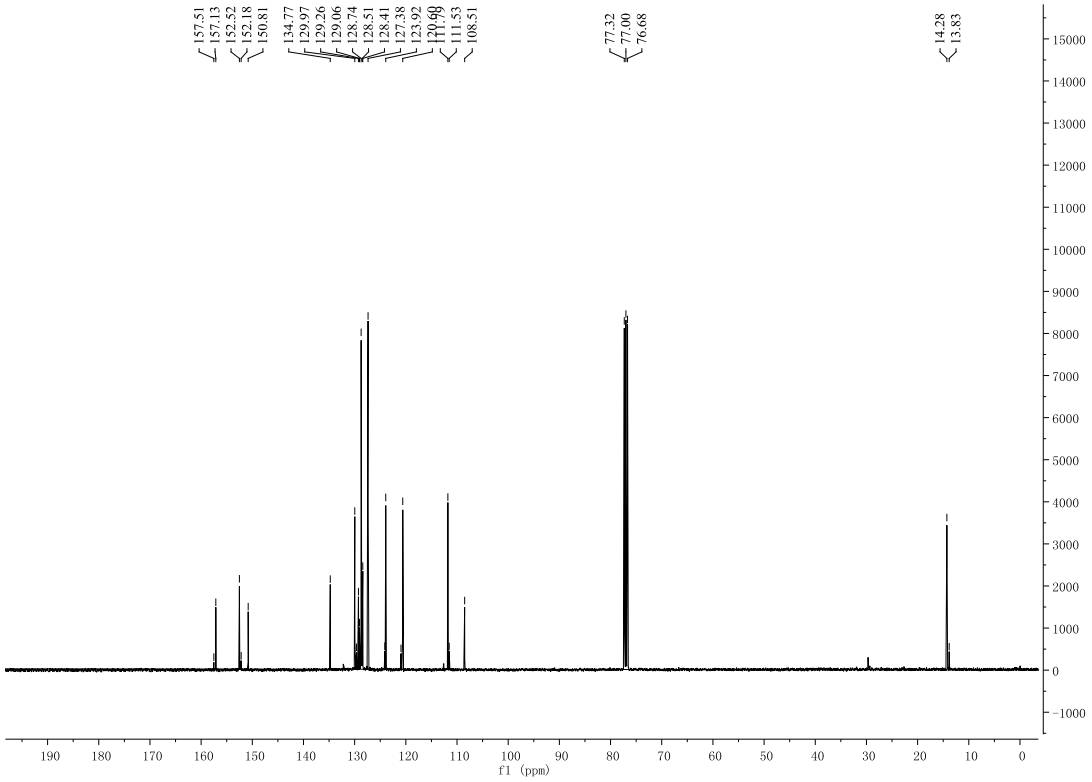
7.59
7.59
7.57
7.57
7.57
7.45
7.45
7.44
7.44
7.43
7.42
7.42
7.42
7.40
7.40
7.39
7.38
7.38
7.26
7.25
7.23
7.23
7.22
7.22
2.35
0.01
1.01
2.09
4.13
2.03
3.00
f1 (ppm)


157.51
157.13
152.52
152.18
150.81
134.77
129.97
129.26
129.06
128.74
128.51
128.41
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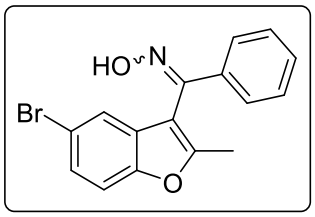
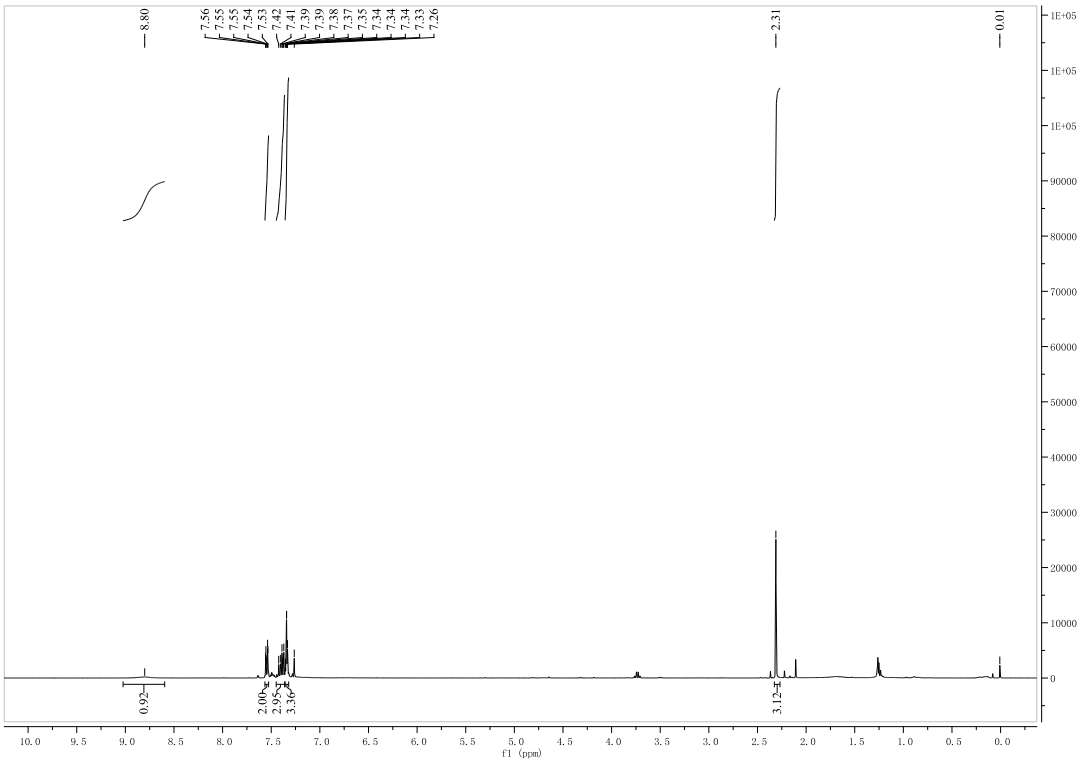
77.00
76.68
14.28
13.83
f1 (ppm)


HO
N
Br
O

2x


8.80
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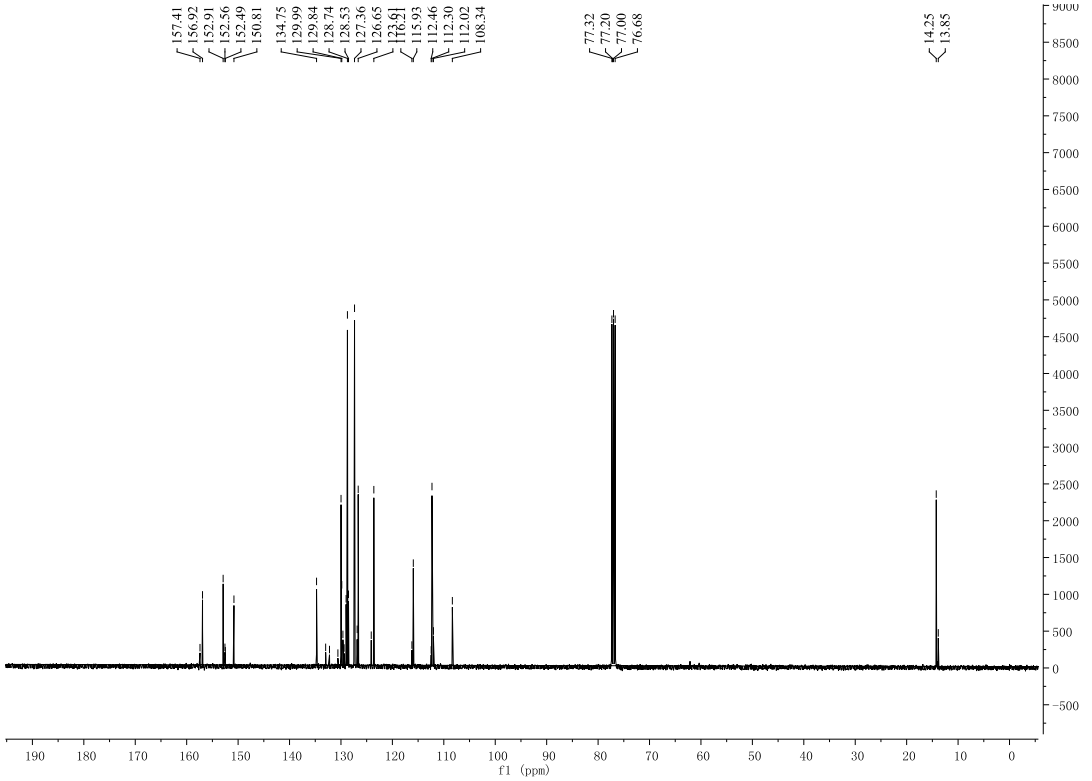
7.55
7.55
7.54
7.53
7.42
7.41
7.39
7.39
7.38
7.37
7.35
7.34
7.34
7.34
7.33
7.26
2.31
0.01
0.92
2.06
2.95
3.36
3.12
f1 (ppm)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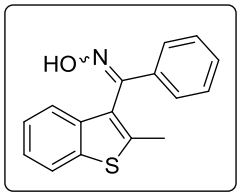
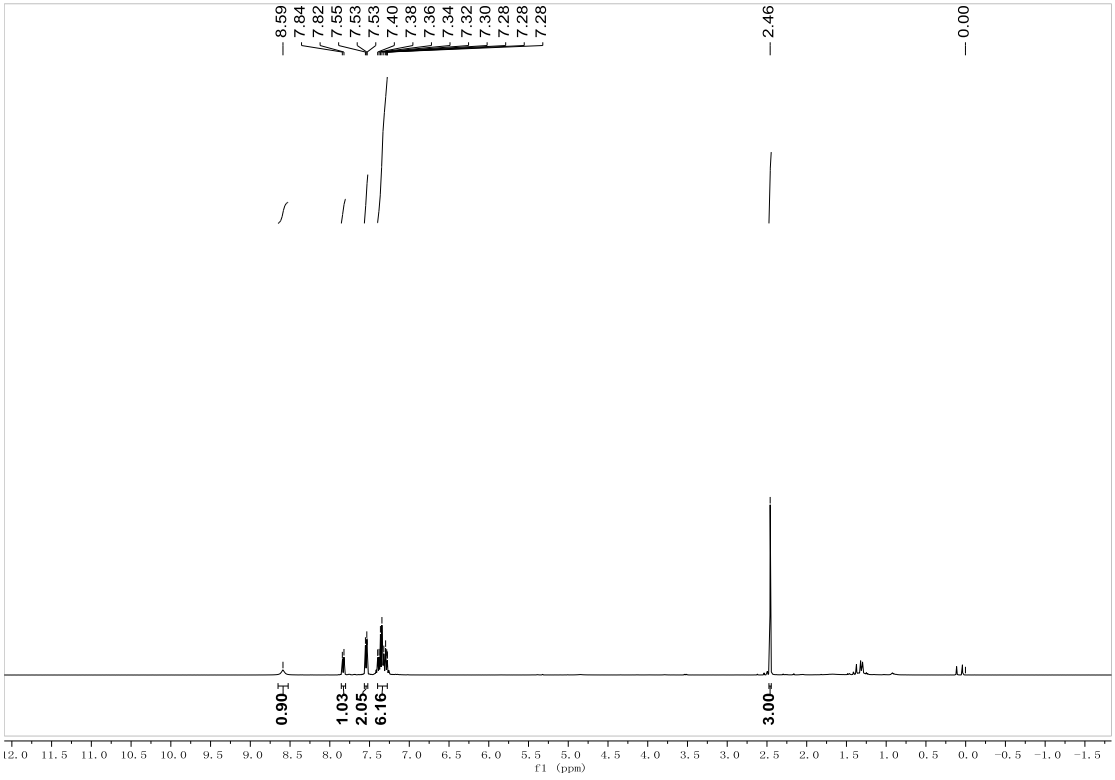
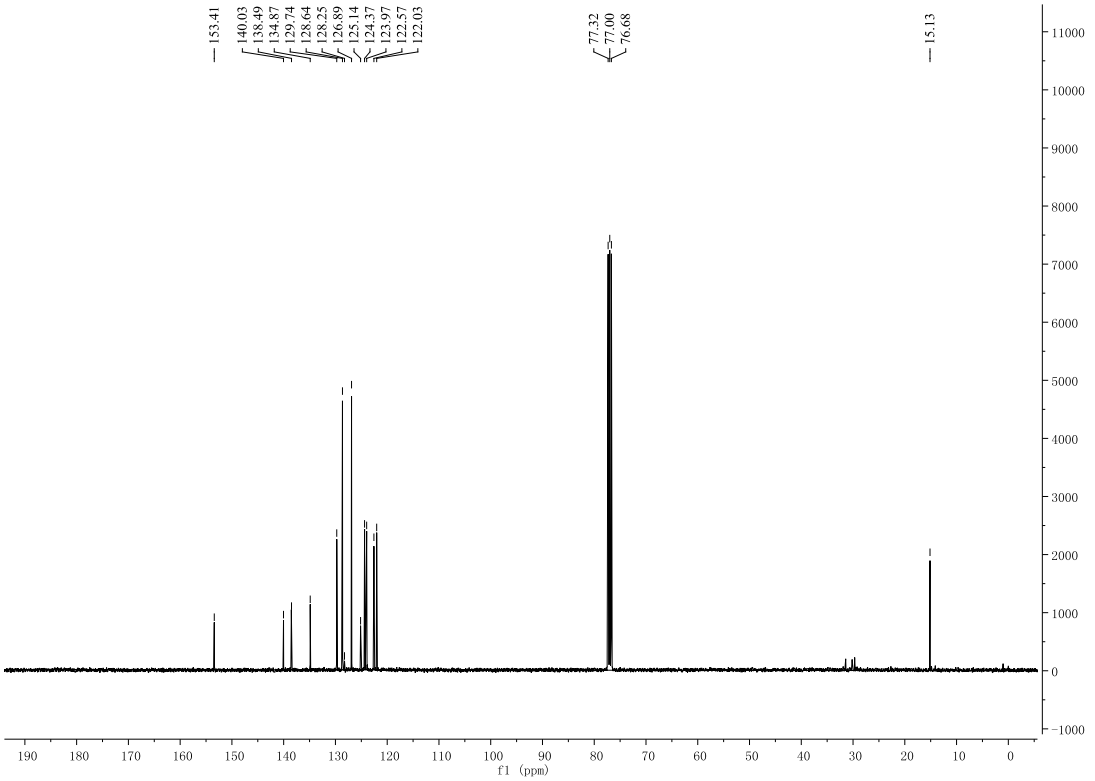
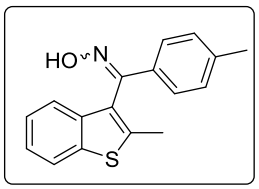
156.92
152.91
152.56
152.49
150.81
134.75
129.99
129.84
128.74
128.53
127.36
126.65
123.91
115.93
112.46
112.30
112.02
108.34
77.32
77.20
77.00
76.68
14.25
13.85
f1 (ppm)


HO
N
S

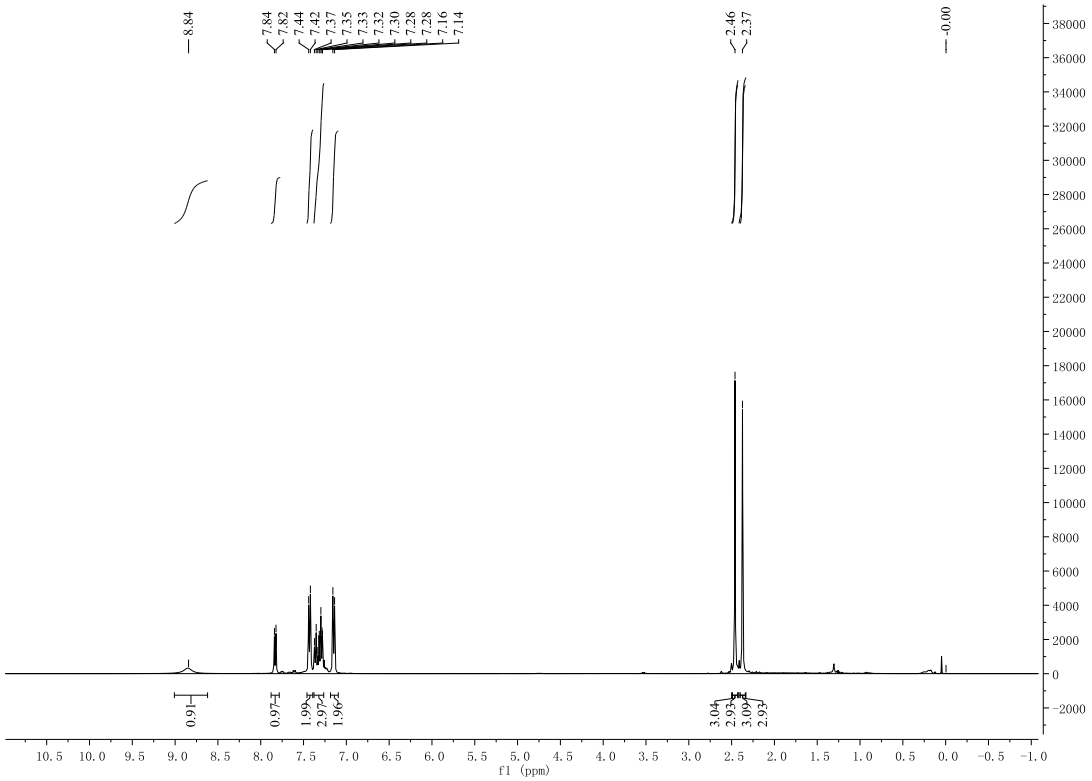
4a


8.59
7.84
7.82
7.55
7.53
7.53
7.40
7.38
7.36
7.34
7.32
7.30
7.28
7.28
7.28
2.46
0.00
0.90
1.03
2.05
6.16
3.00
f1 (ppm)


153.41
140.03
138.49
134.87
129.74
128.64
128.25
126.89
125.14
124.37
123.97
122.57
122.03
77.32
77.00
76.68
15.13
f1 (ppm)


HO
N
S

4b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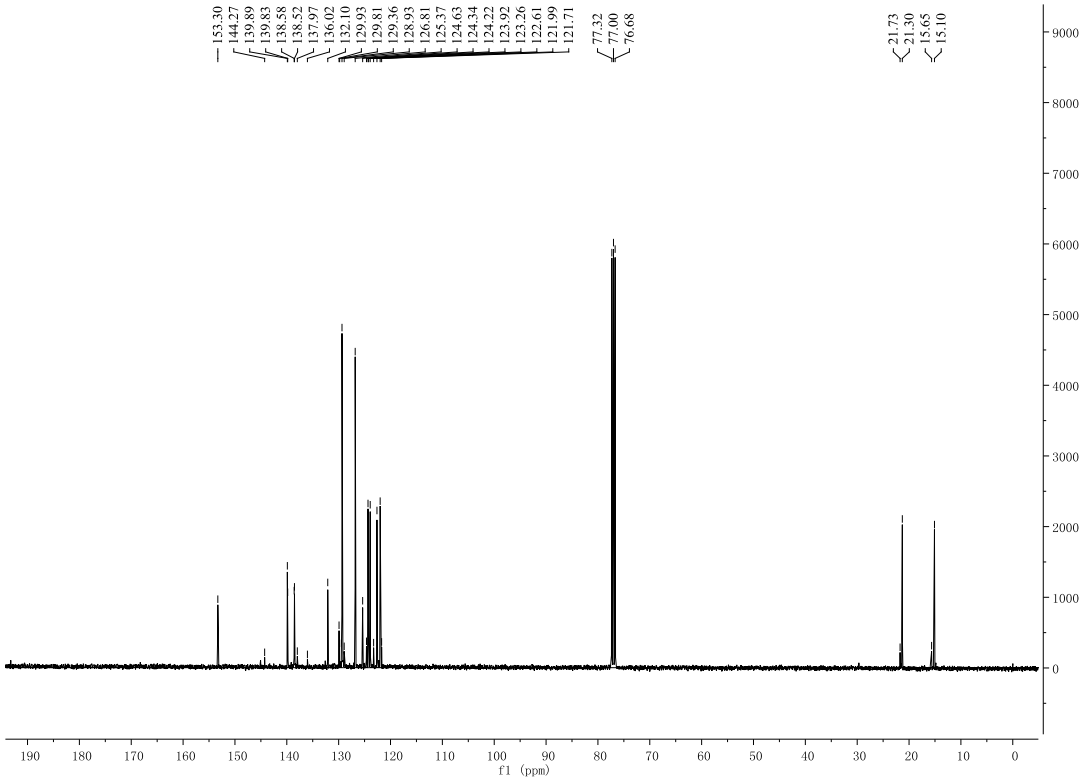
7.84
7.82
7.44
7.42
7.37
7.35
7.33
7.32
7.30
7.28
7.28
7.16
7.14
2.46
2.37
0.00
0.91
0.97
1.99
2.97
1.96
3.04
2.95
3.09
2.93
f1 (ppm)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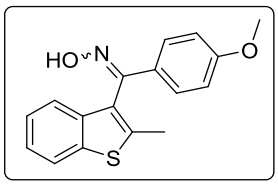
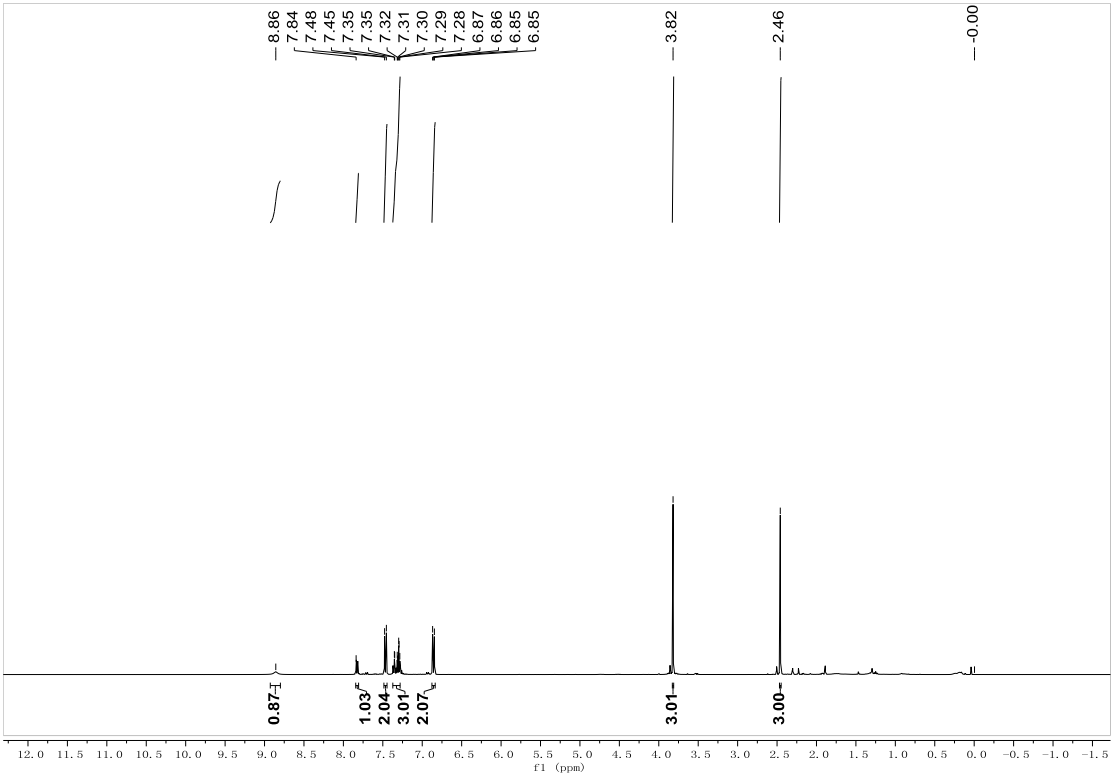
144.27
139.89
139.83
138.58
138.52
137.97
136.02
132.10
129.93
129.81
129.36
128.93
126.81
125.37
124.63
124.34
124.22
123.92
123.26
122.61
121.99
121.71
77.32
77.00
76.68
21.73
21.30
15.65
15.10
f1 (ppm)


HO
N
O
S

4c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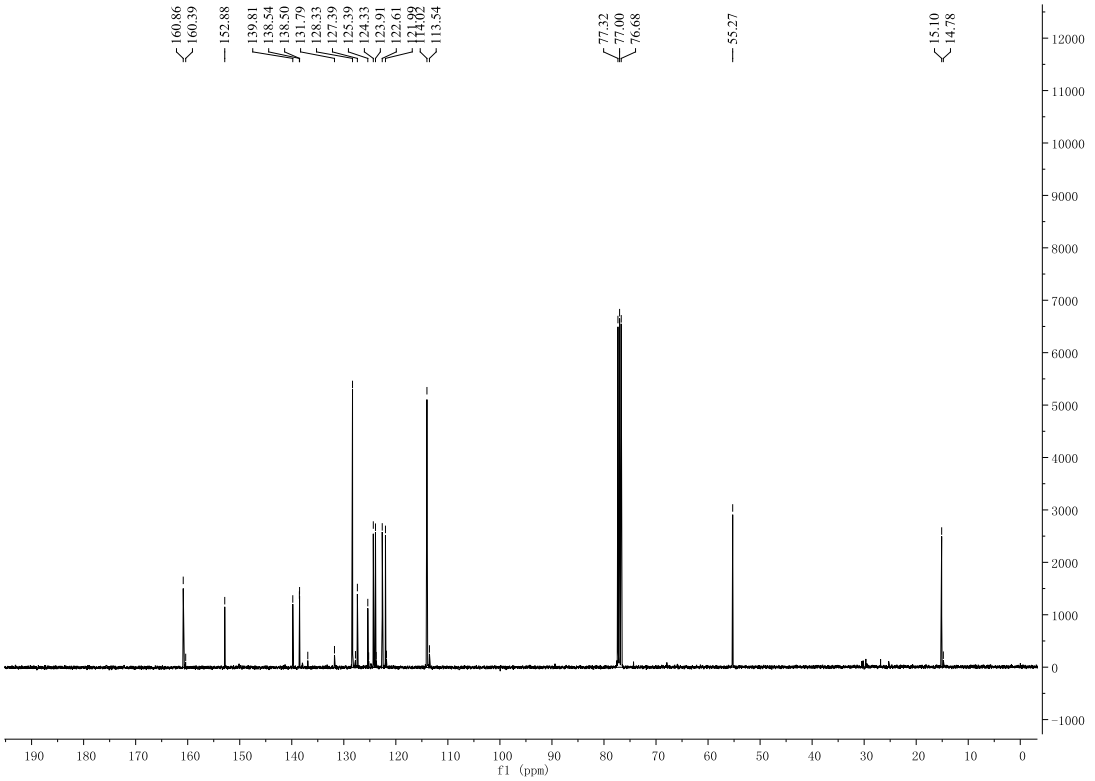
7.84
7.48
7.45
7.35
7.35
7.32
7.31
7.30
7.29
7.28
6.87
6.86
6.85
6.85
3.82
2.46
-0.00
0.87
1.03
2.04
3.01
2.07
3.01
3.00
f1 (ppm)


160.86
160.39
152.88
139.81
138.54
138.50
131.79
128.33
127.39
125.39
124.33
123.91
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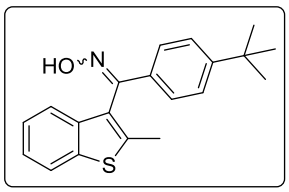
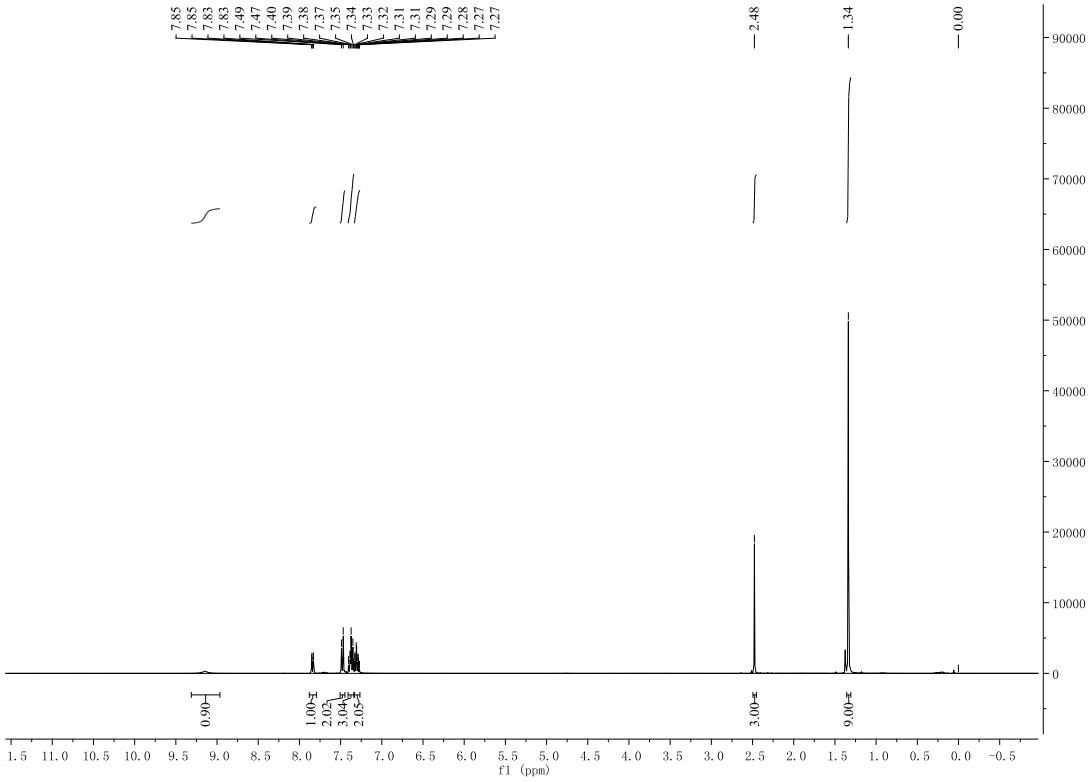
76.68
55.27
15.10
14.78
f1 (ppm)


HO
N
S

4d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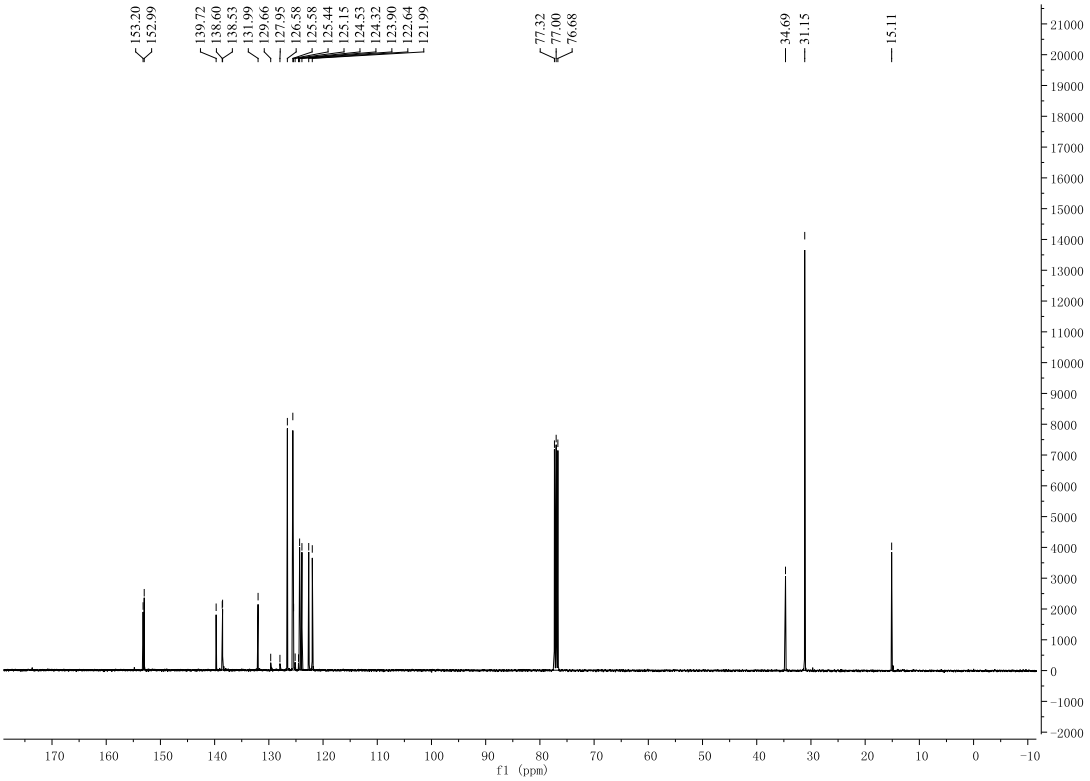
7.85
7.83
7.83
7.49
7.47
7.40
7.39
7.38
7.37
7.35
7.34
7.33
7.32
7.31
7.31
7.29
7.29
7.28
7.27
7.27
2.48
1.34
0.00
0.90
1.00
2.02
3.04
2.05
3.00
9.00
f1 (ppm)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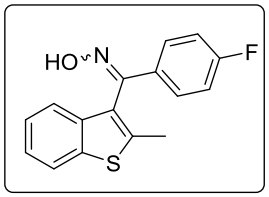
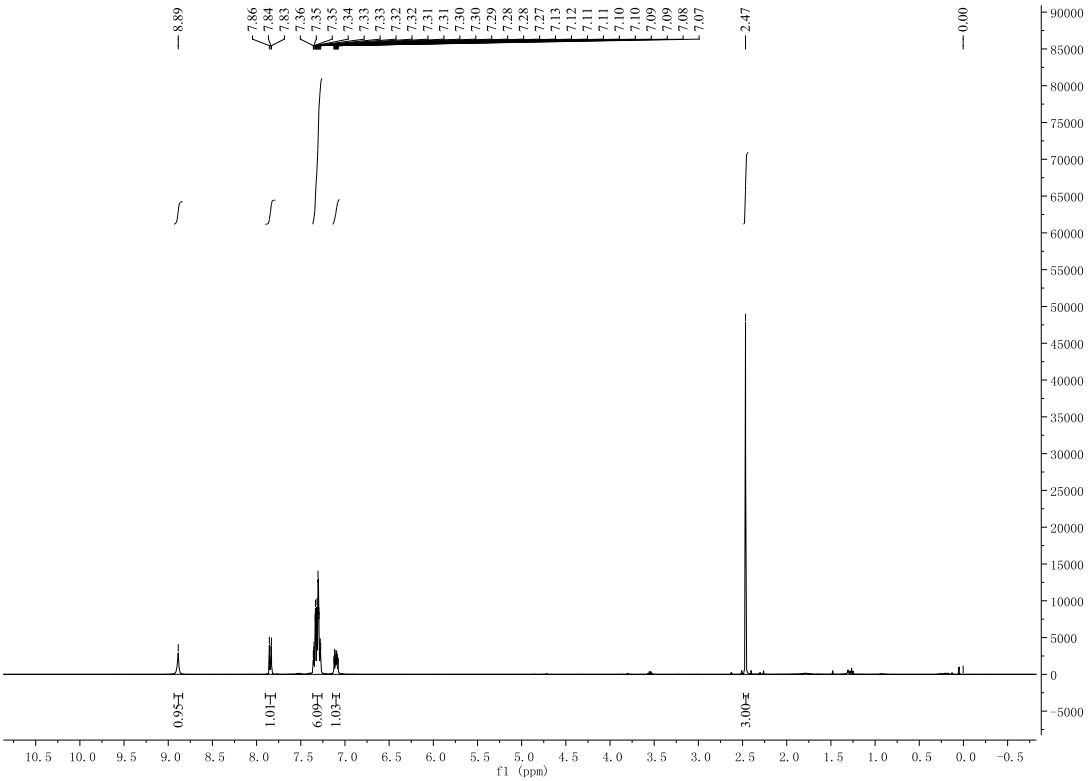
129.66
127.95
126.58
125.58
125.44
125.15
124.53
124.32
123.90
122.64
121.99
77.32
77.00
76.68
34.69
31.15
15.11
f1 (ppm)


HO
N
F
S

4e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7.83
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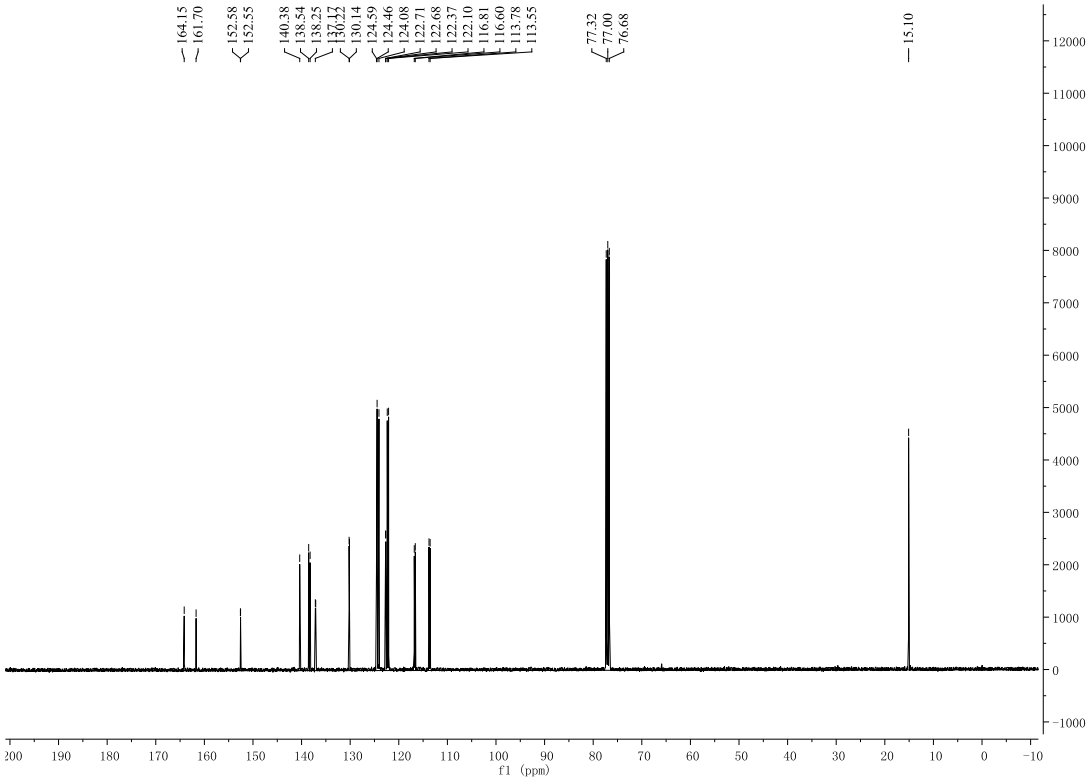
7.35
7.35
7.34
7.33
7.33
7.32
7.32
7.31
7.31
7.30
7.30
7.30
7.29
7.28
7.28
7.27
7.13
7.12
7.11
7.11
7.10
7.10
7.09
7.09
7.09
7.08
7.07
2.47
0.00
0.95
1.01
6.09
1.03
3.00
f1 (ppm)


164.15
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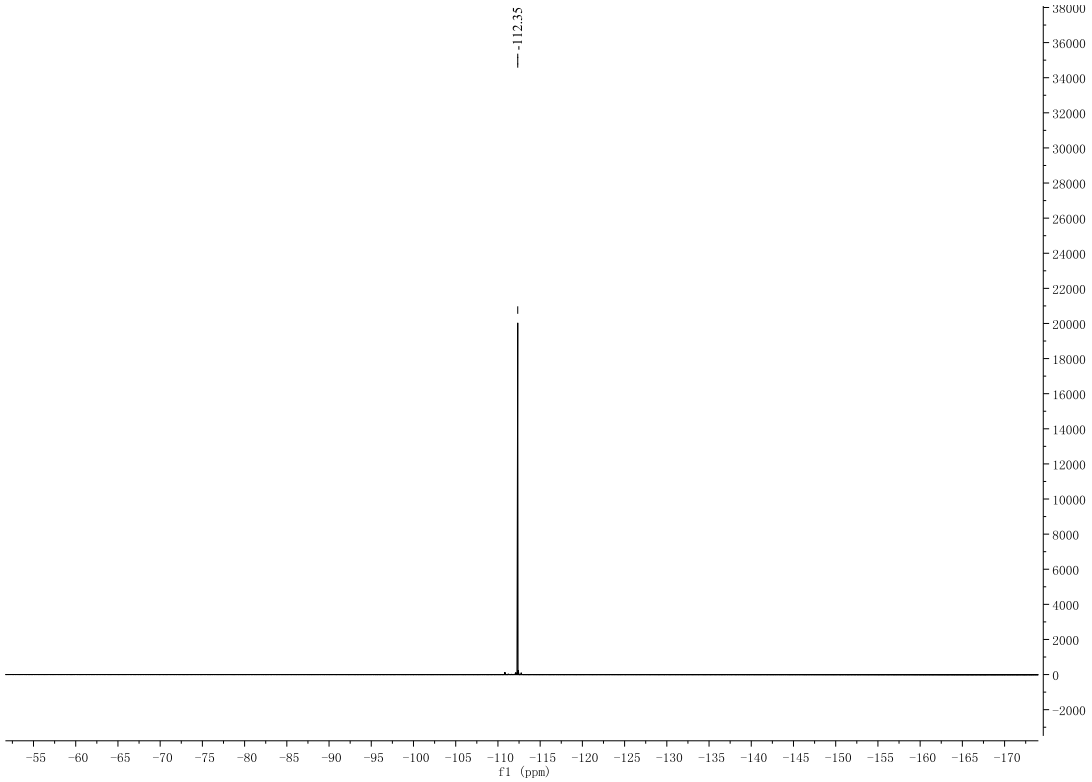
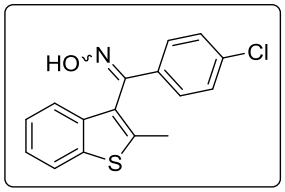
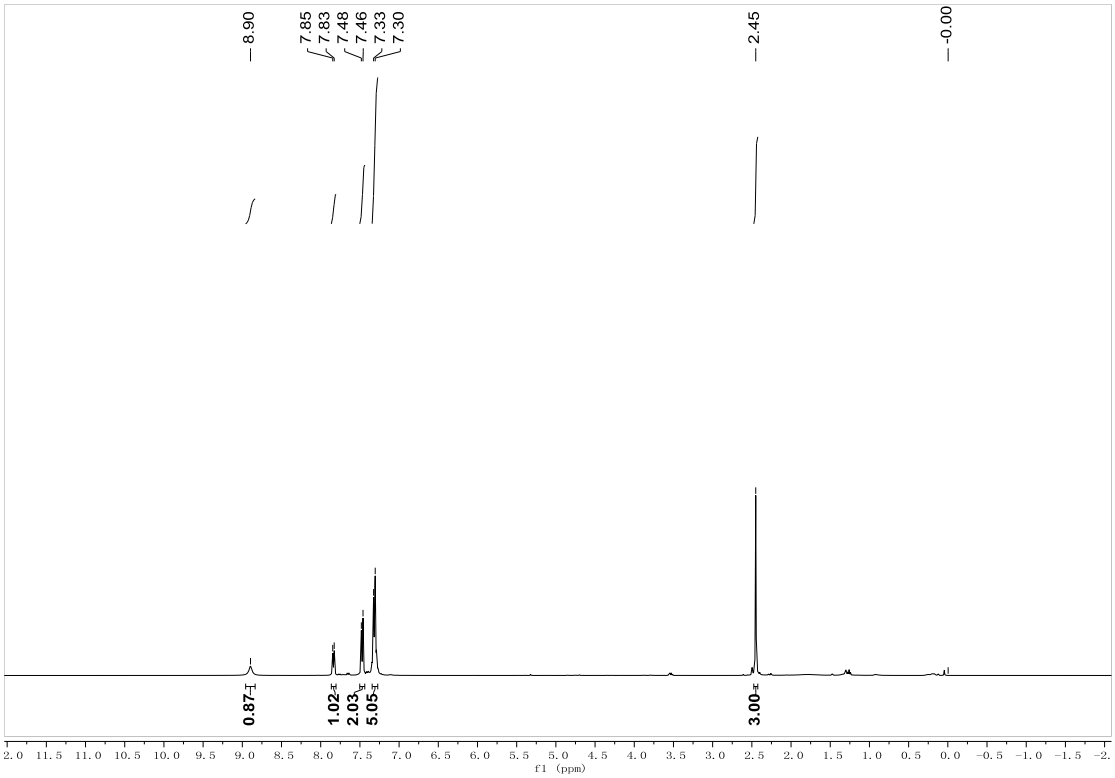
138.54
138.25
137.17
130.22
130.14
124.59
124.46
124.08
122.71
122.68
122.37
122.10
116.81
116.60
113.78
113.55
77.32
77.00
76.68
15.10
f1 (ppm)


-112.35
f1 (ppm)


HO
N
Cl
S

4f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7.85
7.83
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7.46
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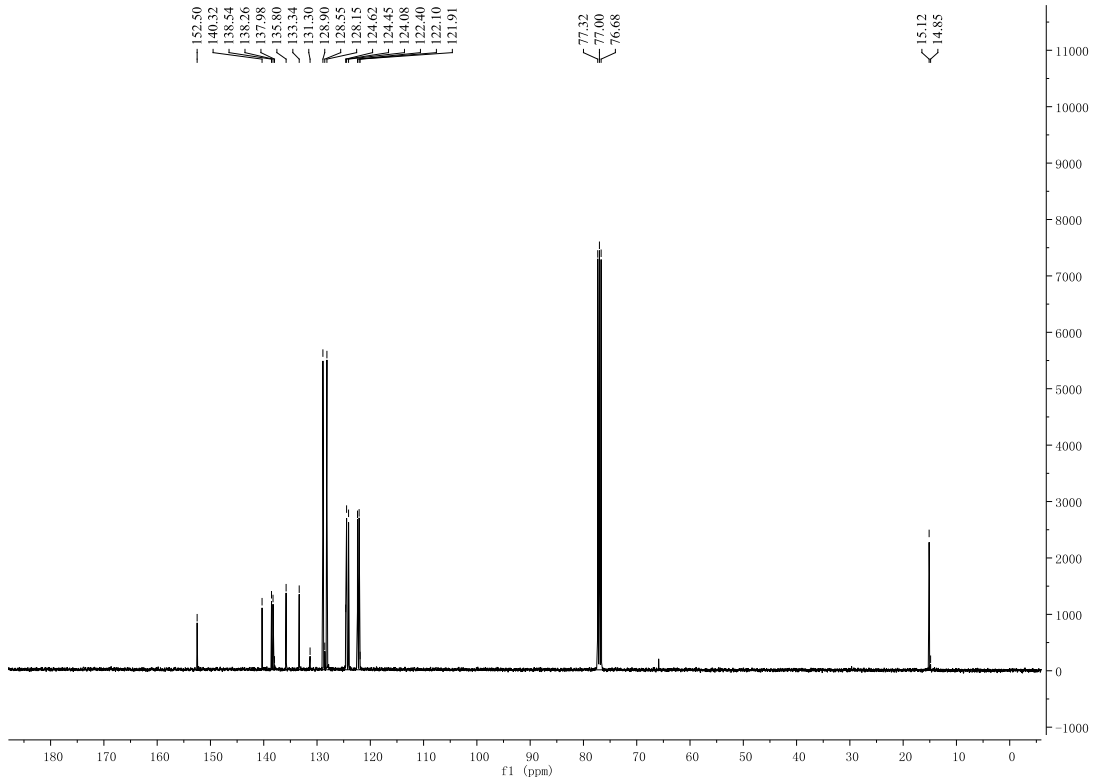
7.30
2.45
0.00
0.87
1.02
2.03
5.05
3.00
f1 (ppm)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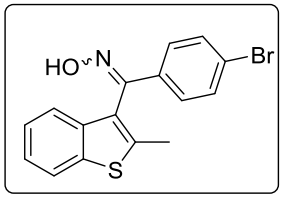
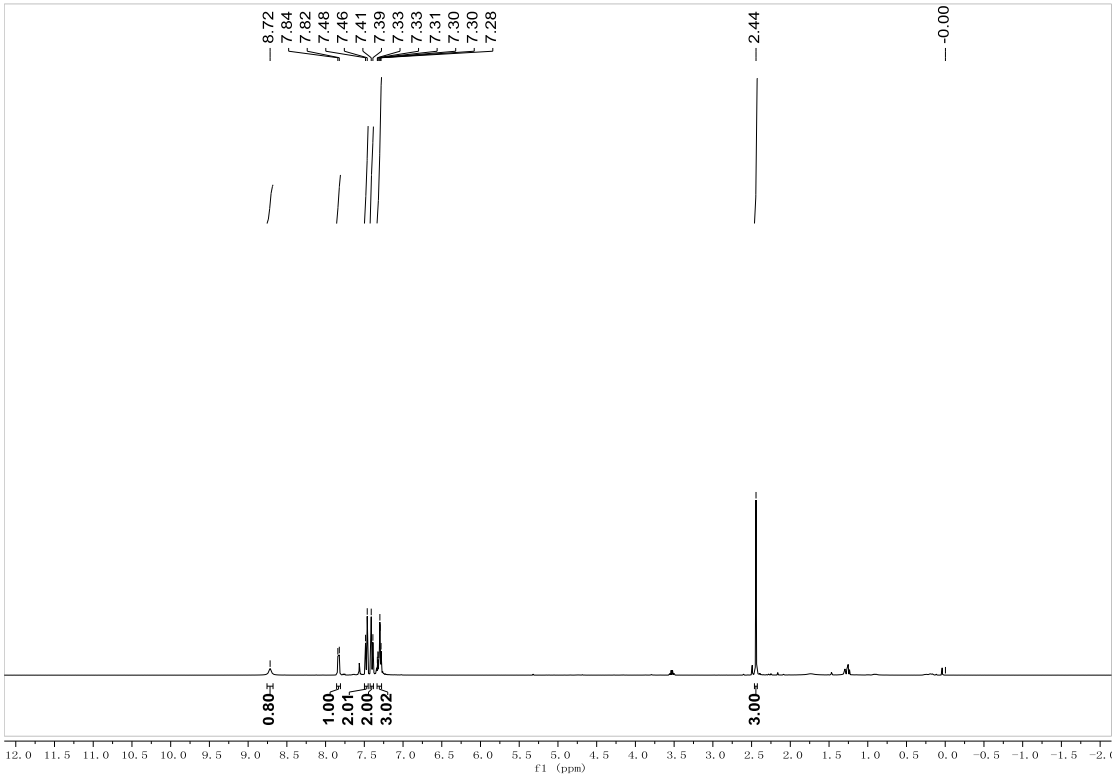
138.26
137.98
135.80
133.34
131.30
128.90
128.55
128.15
124.62
124.45
124.08
122.40
122.10
121.91
77.32
77.00
76.68
15.12
14.85
f1 (ppm)


HO
N
Br
S

4g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7.46
7.41
7.39
7.33
7.31
7.30
7.30
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2.44
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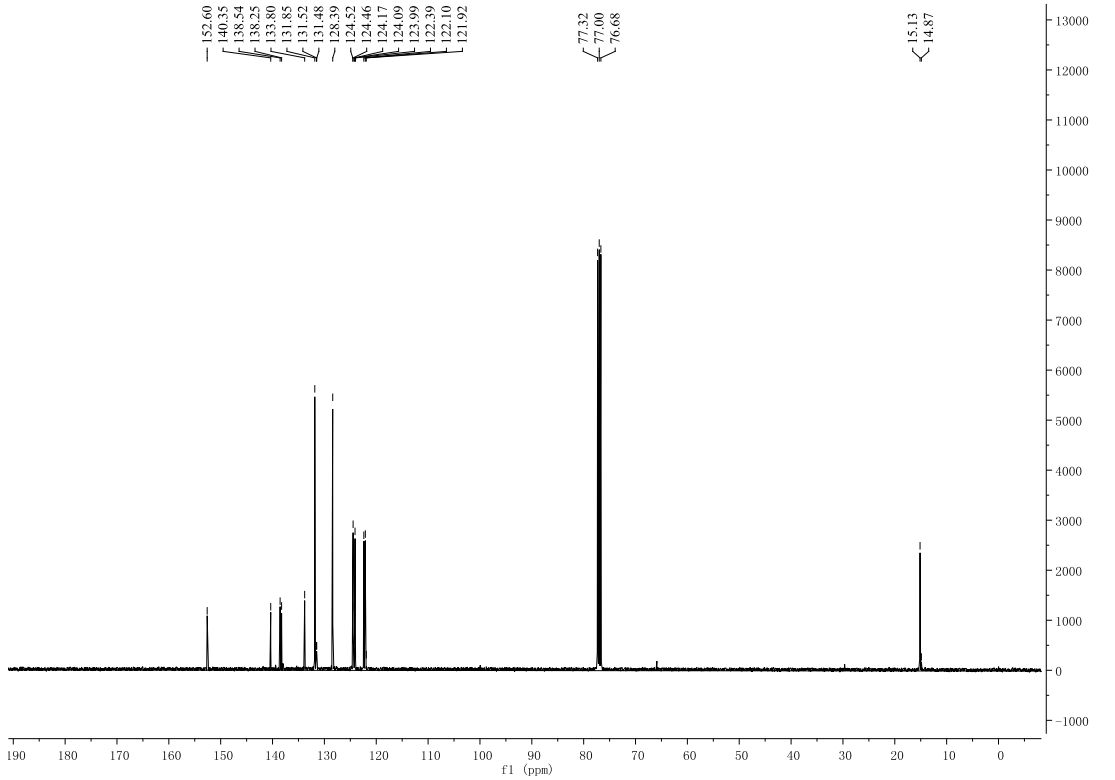
0.80
1.00
2.01
2.00
3.02
3.00
f1 (ppm)


152.60
140.35
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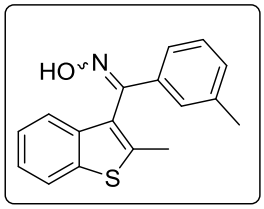
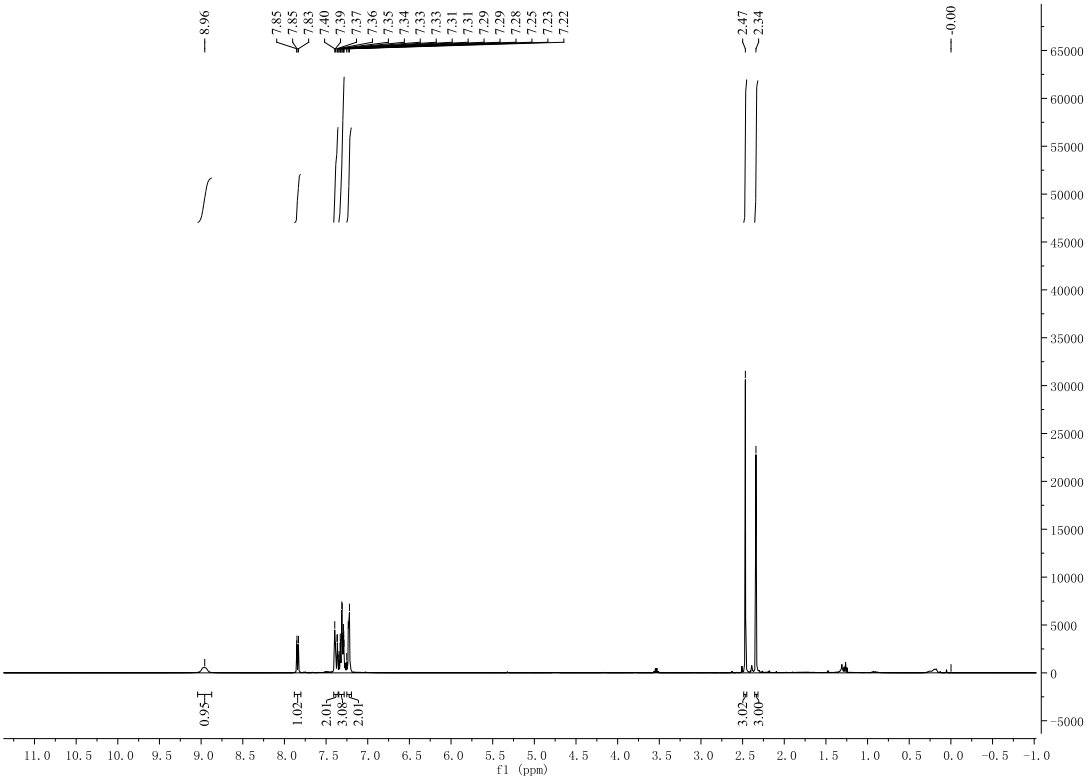
138.25
133.80
131.85
131.52
131.48
128.39
124.52
124.46
124.17
124.09
123.99
122.39
122.10
121.92
77.32
77.00
76.68
15.13
14.87
f1 (ppm)


HO
N
S

4h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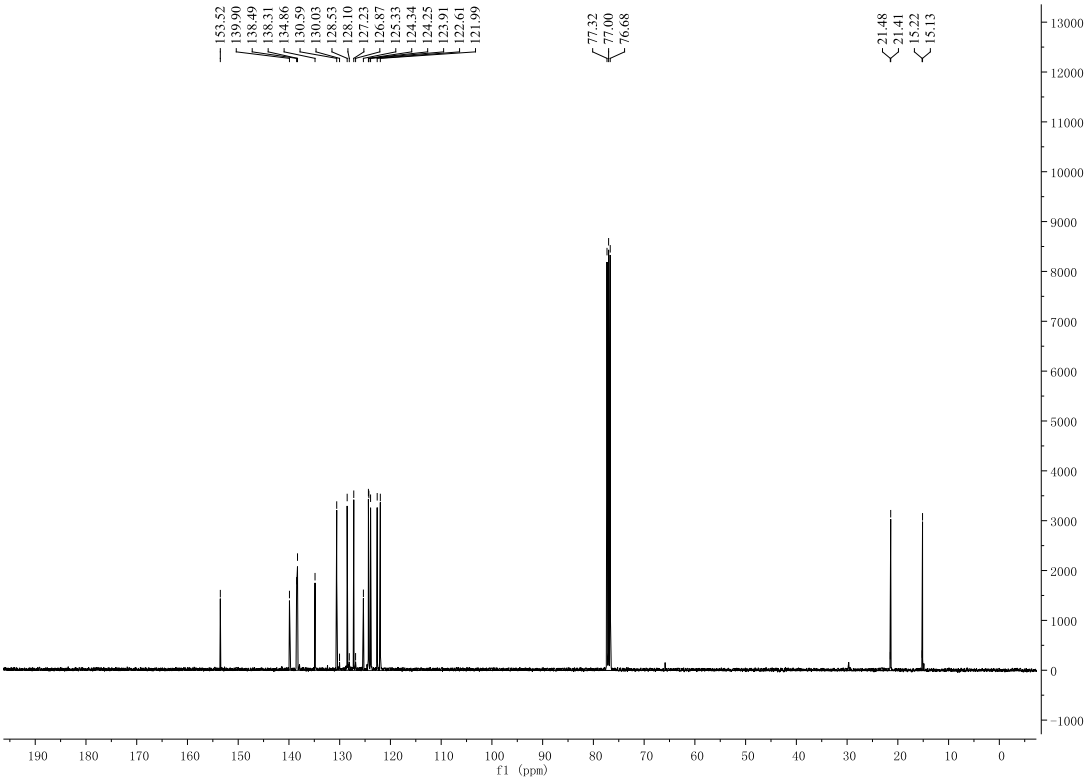
7.37
7.36
7.35
7.34
7.33
7.33
7.31
7.31
7.29
7.29
7.28
7.25
7.23
7.22
2.47
2.34
-0.00
0.95
1.02
2.01
3.08
2.01
3.02
3.00
f1 (ppm)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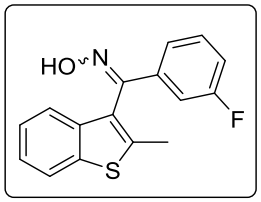
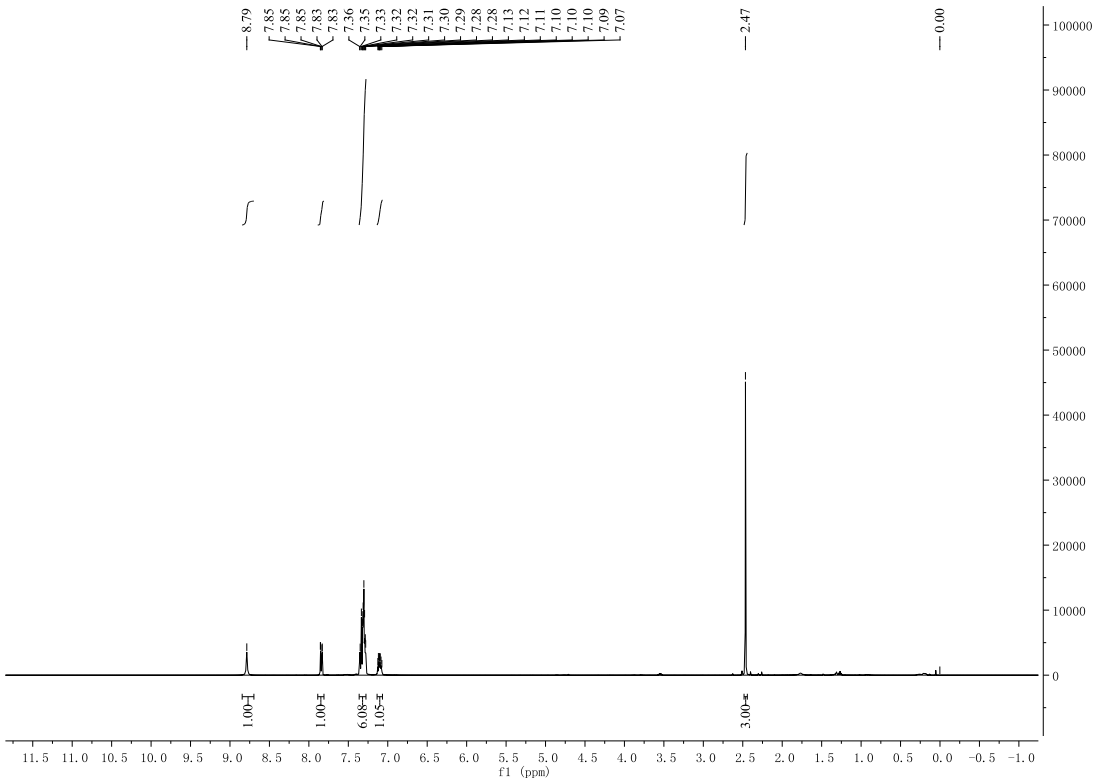
134.86
130.59
130.03
128.53
128.10
127.23
126.87
125.33
124.34
124.25
123.91
122.61
121.99
77.32
77.00
76.68
21.48
21.41
15.22
15.13
f1 (ppm)


HO
N
F
S

4i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7.85
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7.83
7.36
7.35
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7.32
7.32
7.31
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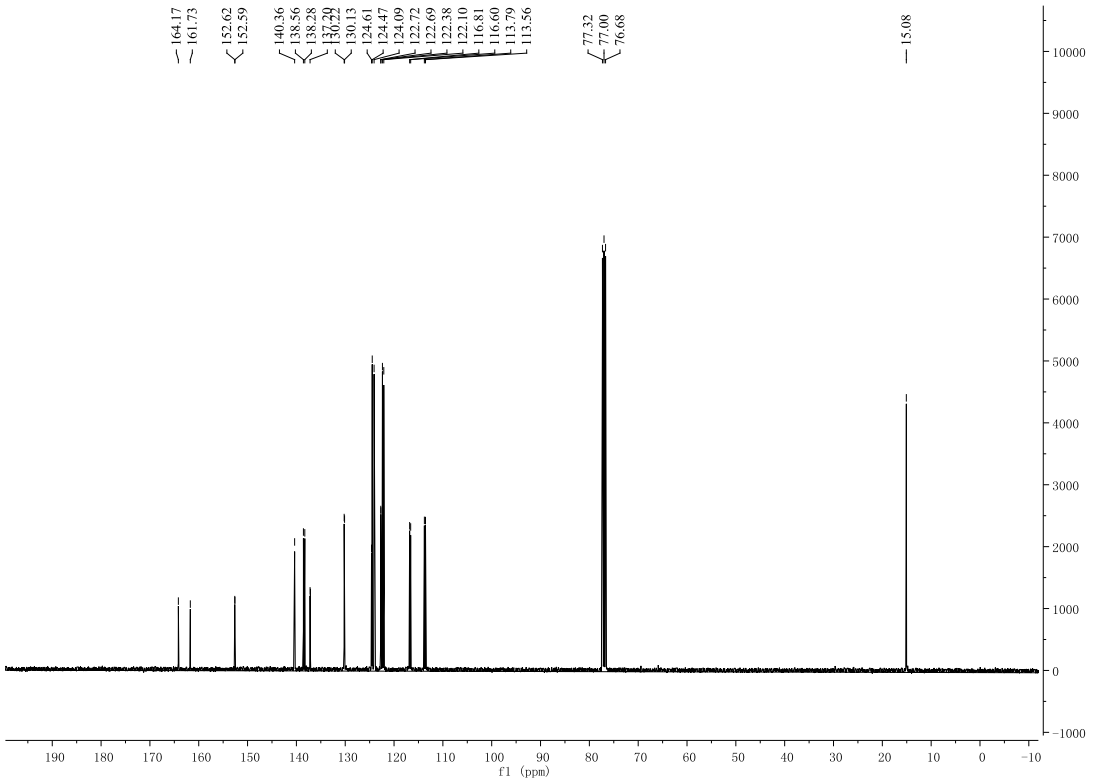
7.29
7.28
7.28
7.13
7.12
7.11
7.10
7.10
7.10
7.09
7.07
2.47
0.00
1.00
1.00
6.08
1.05
3.00
f1 (ppm)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137.20
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130.13
124.61
124.47
124.09
122.72
122.69
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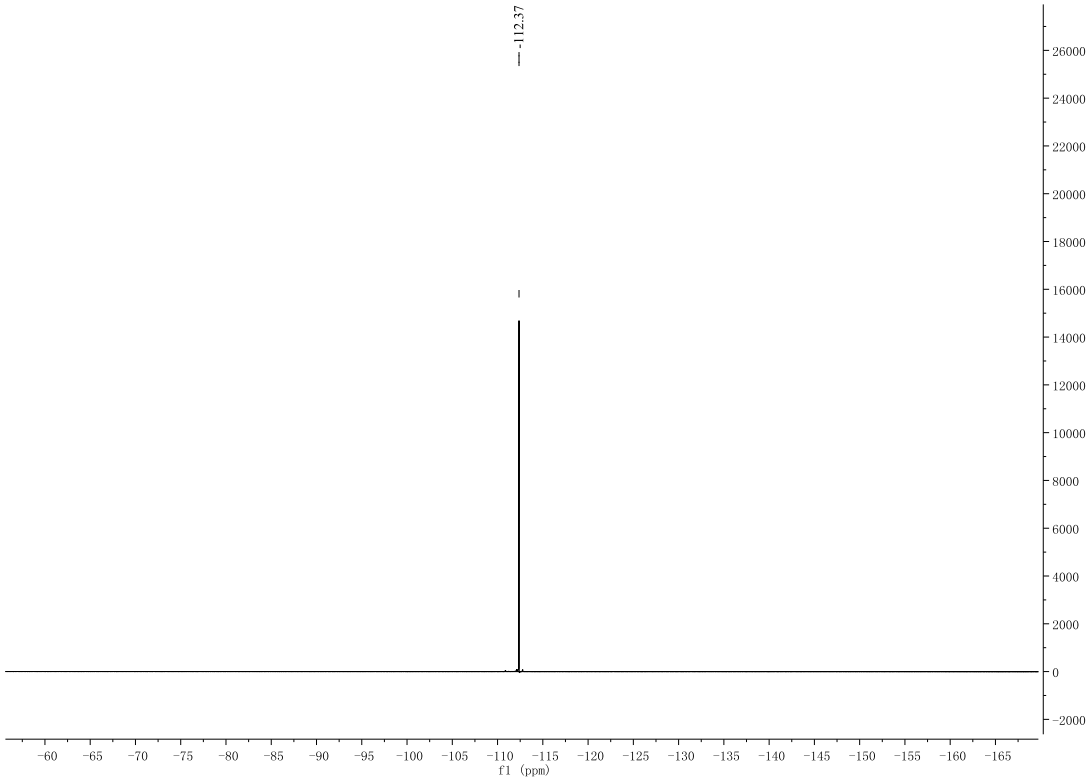
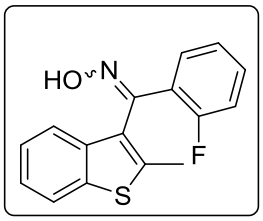
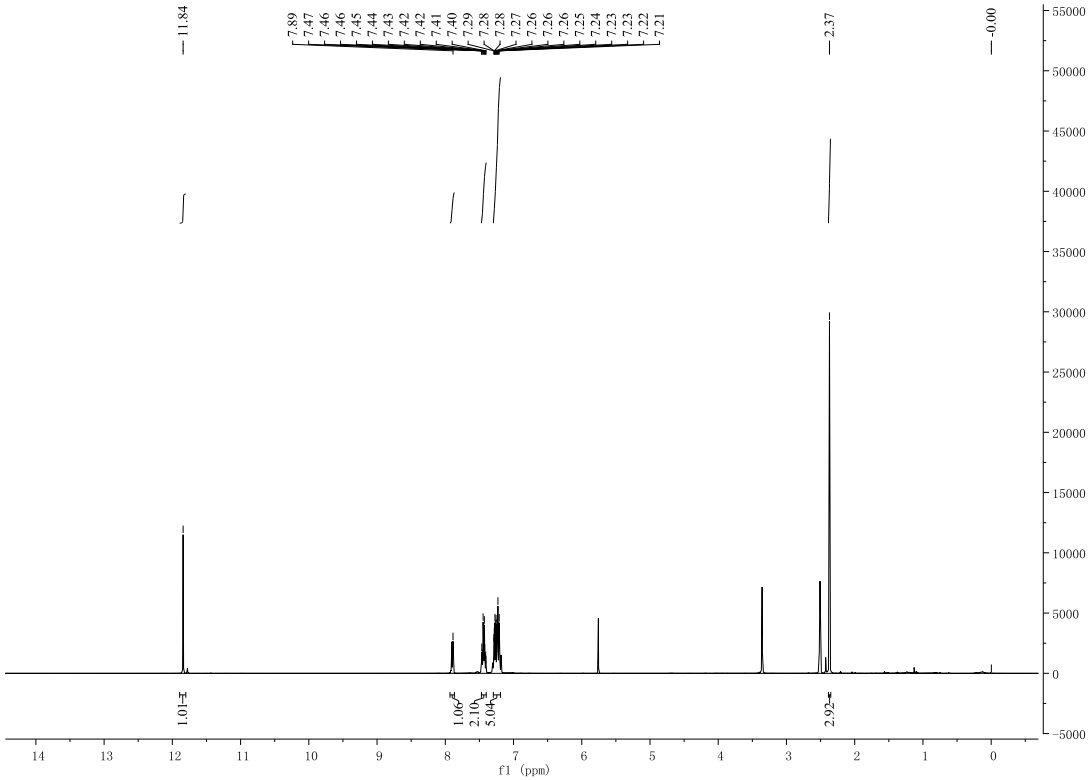
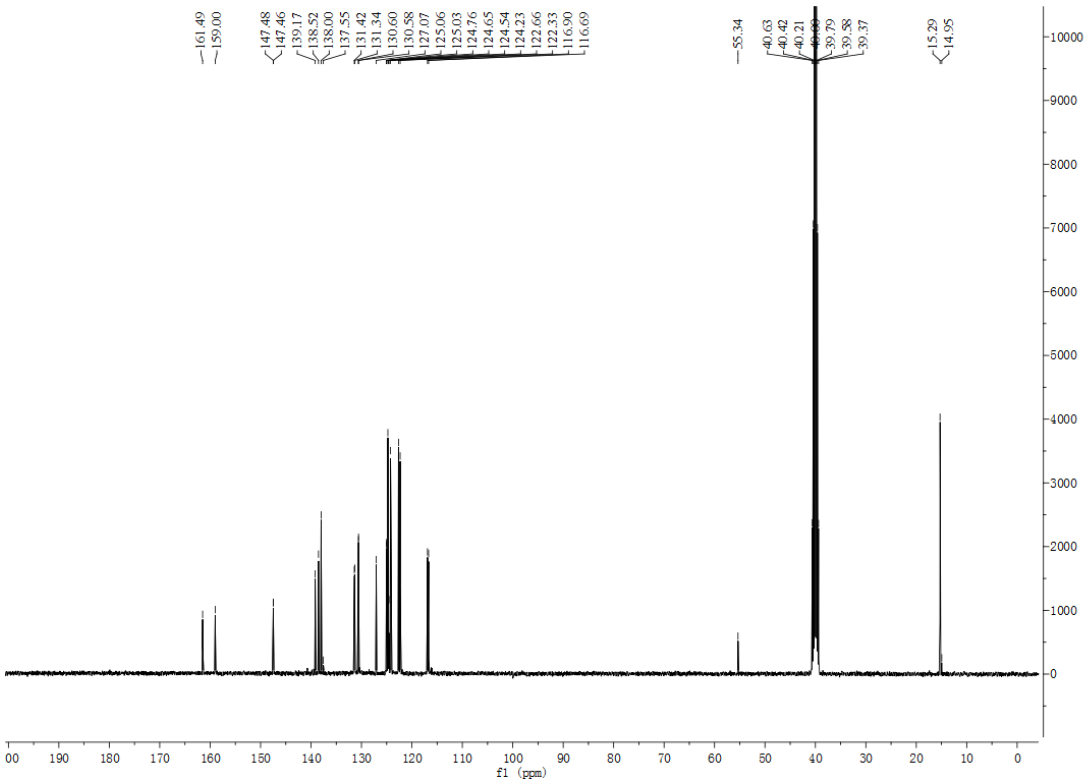
116.81
116.60
113.79
113.56
77.32
77.00
76.68
15.08
f1 (ppm)


-112.37
f1 (ppm)


HO
N
F
S

4j


11.84
7.89
7.47
7.46
7.46
7.45
7.44
7.43
7.42
7.42
7.41
7.40
7.29
7.28
7.28
7.27
7.26
7.26
7.25
7.24
7.23
7.23
7.22
7.21
2.37
-0.00
1.01
1.06
2.10
5.04
2.92
f1 (ppm)


161.49
159.00
147.48
147.46
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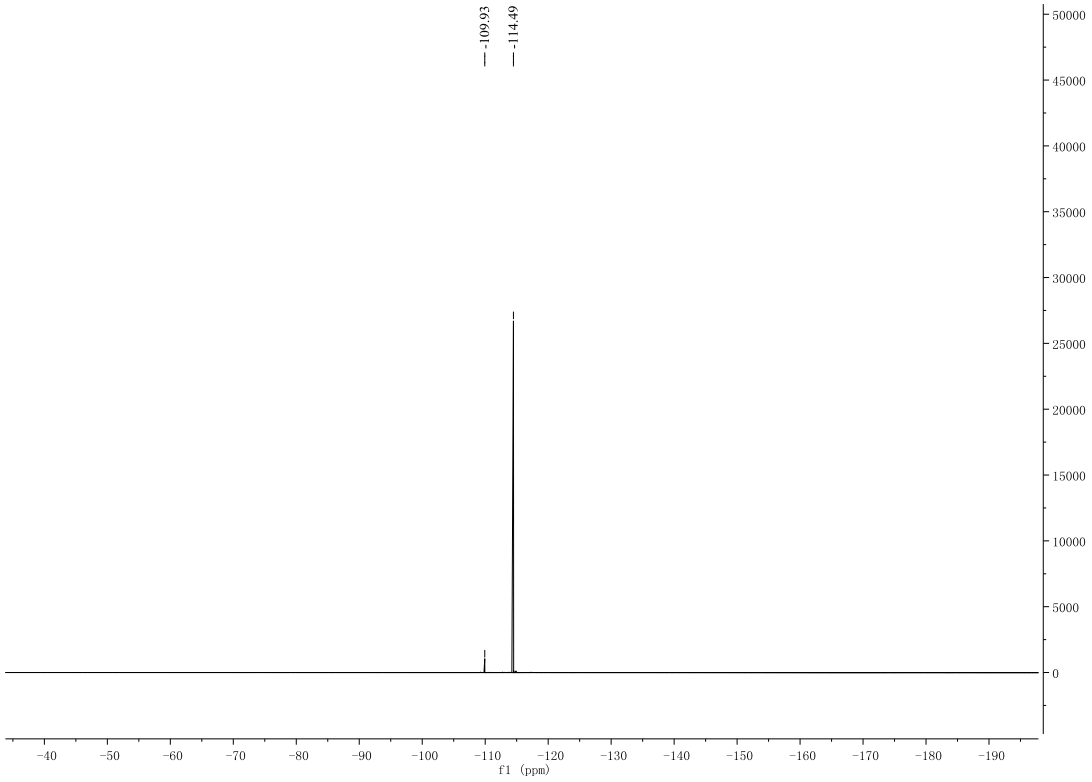
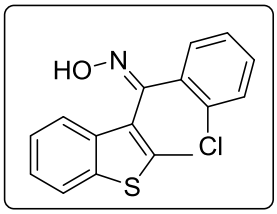
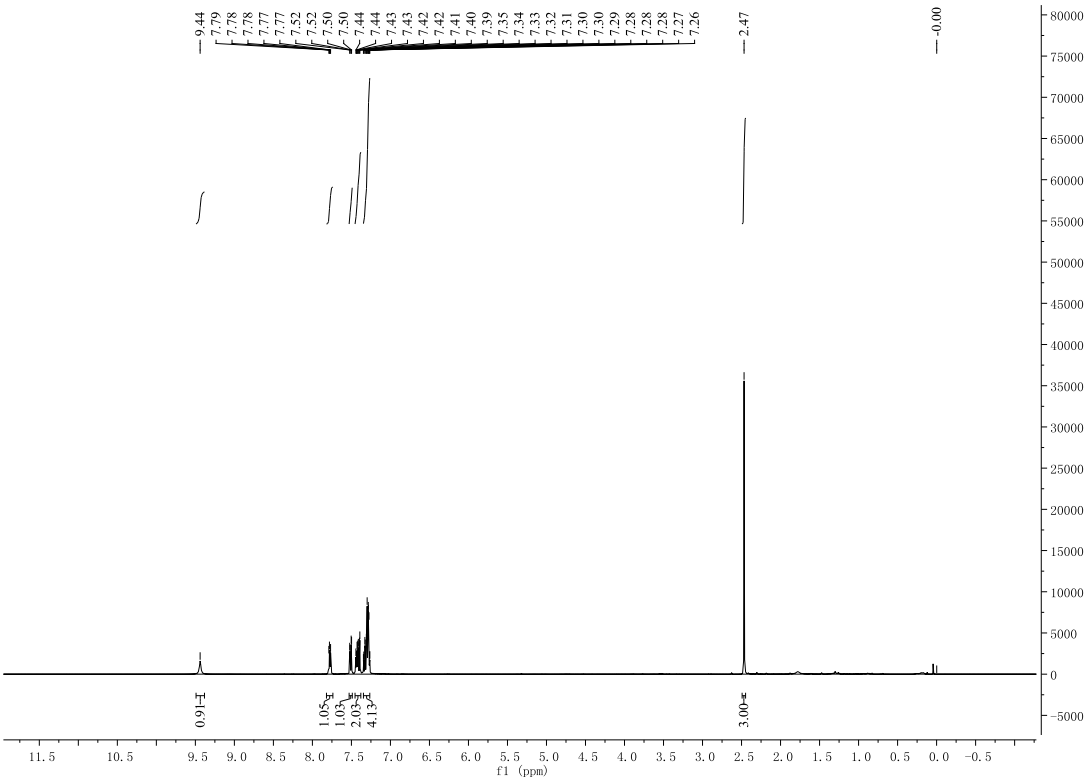
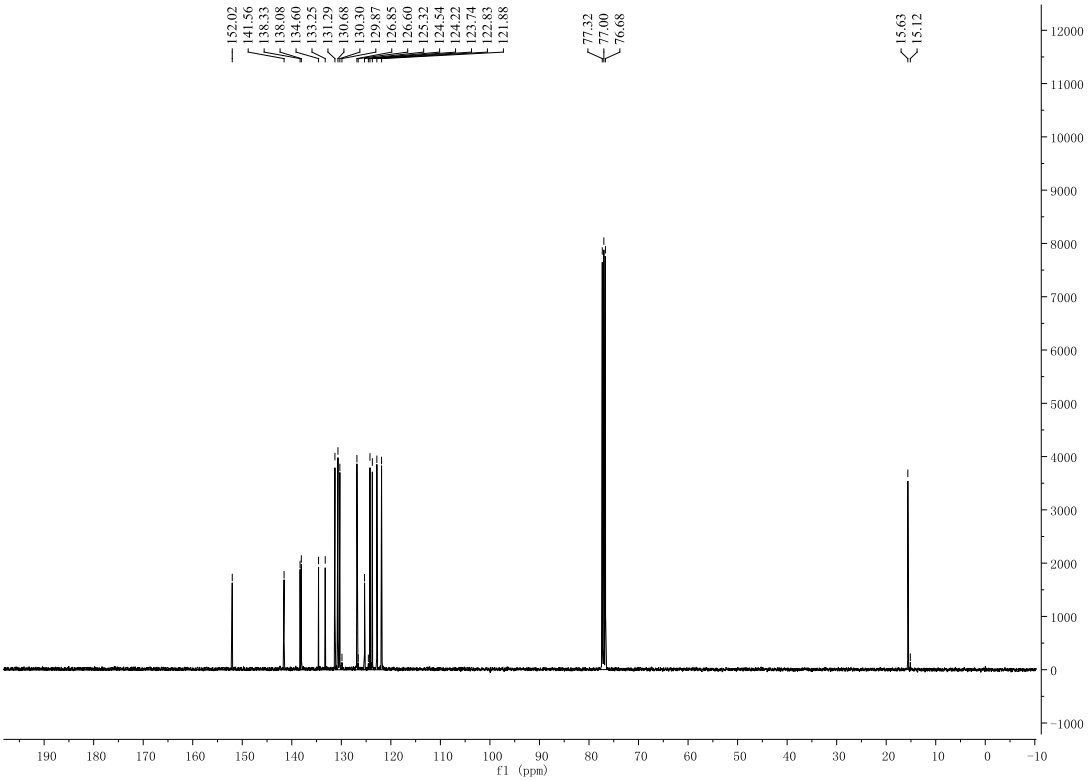
138.52
138.00
137.55
131.42
131.34
130.60
130.58
127.07
125.06
125.03
124.76
124.65
124.54
124.23
122.66
122.33
116.90
116.69
55.34
40.63
40.42
40.21
39.79
39.58
39.37
15.29
14.95
f1 (ppm)

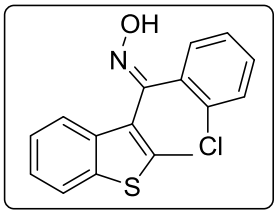

-109.93
-114.49
f1 (ppm)


HO
N
Cl
S

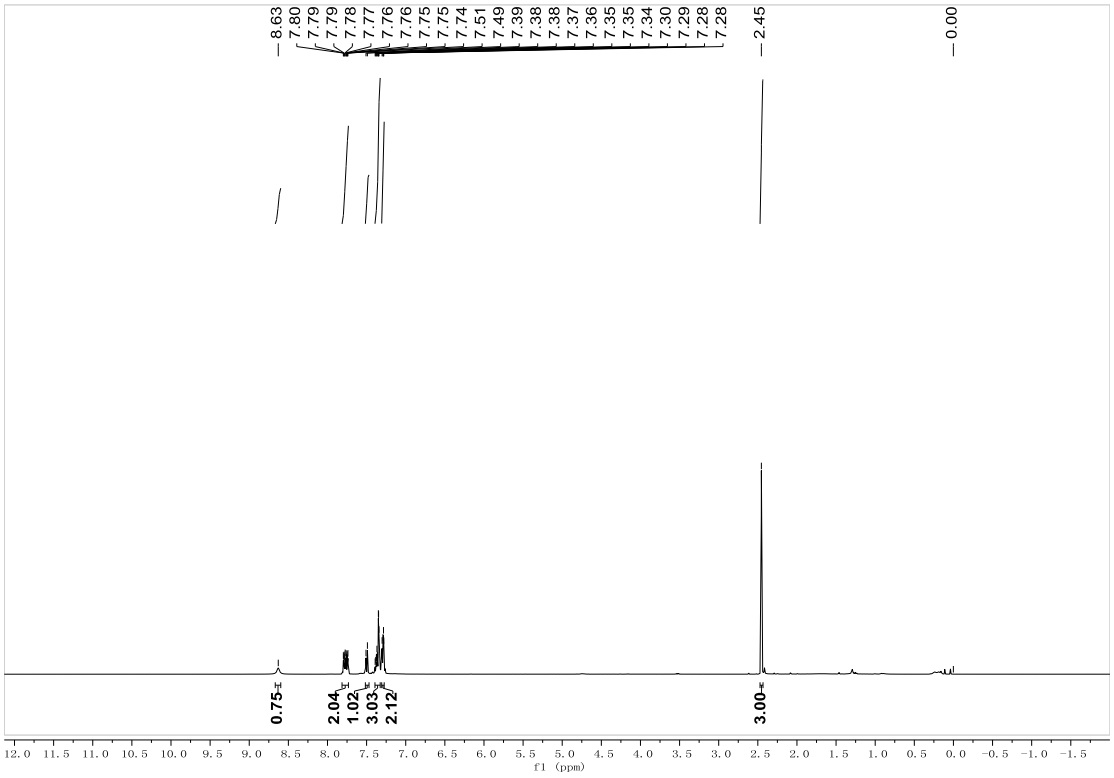
4k

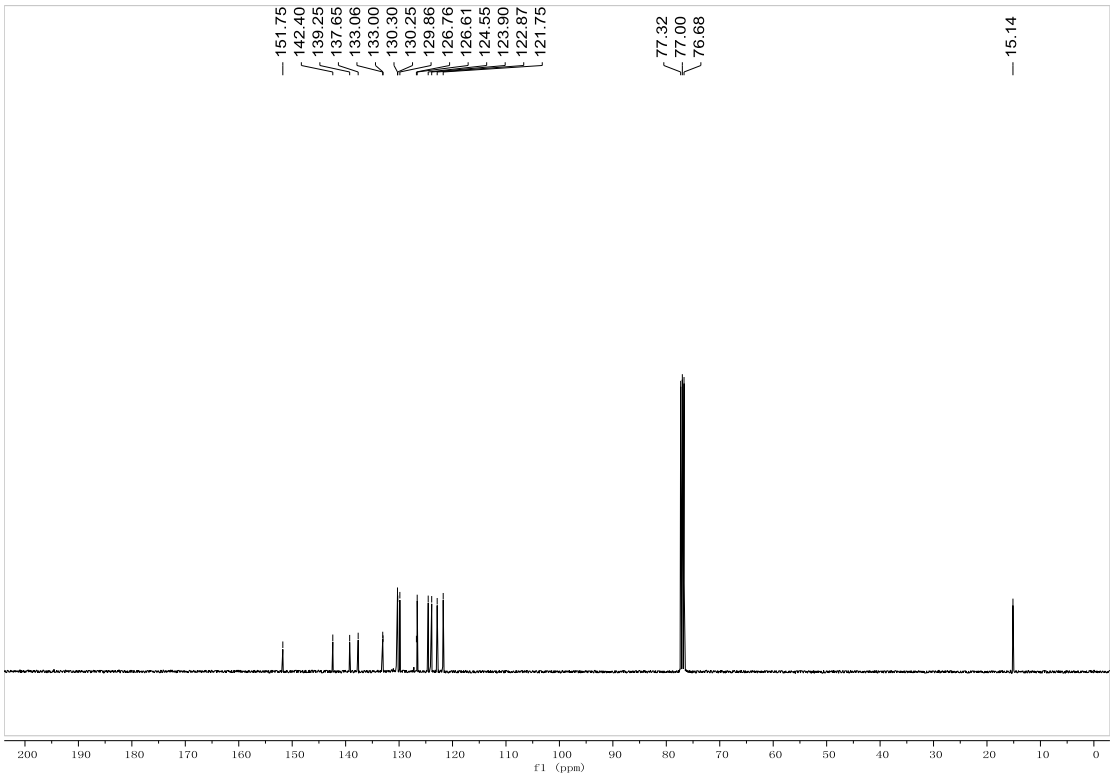

9.44
7.79
7.78
7.78
7.78
7.77
7.77
7.52
7.52
7.50
7.50
7.44
7.44
7.43
7.43
7.42
7.42
7.41
7.40
7.39
7.35
7.34
7.33
7.32
7.31
7.30
7.30
7.29
7.28
7.28
7.28
7.27
7.26
2.47
-0.00
0.91
1.05
1.03
2.03
4.13
3.00
f1 (ppm)


152.02
141.56
138.33
138.08
134.60
133.25
131.29
130.68
130.30
129.87
126.85
126.60
125.32
124.54
124.22
123.74
122.83
121.88
77.32
77.00
76.68
15.63
15.12
f1 (ppm)


OH
N
Cl
S

4k’


8.63
7.80
7.79
7.79
7.78
7.77
7.76
7.76
7.75
7.75
7.74
7.51
7.49
7.39
7.38
7.38
7.37
7.36
7.35
7.35
7.34
7.30
7.29
7.28
7.28
2.45
0.00
0.75
2.04
1.02
3.03
2.12
3.00
f1 (ppm)


151.75
142.40
139.25
137.65
133.06
133.00
130.30
130.25
129.86
126.76
126.61
124.55
123.90
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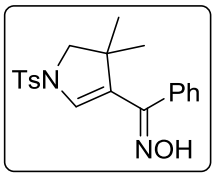
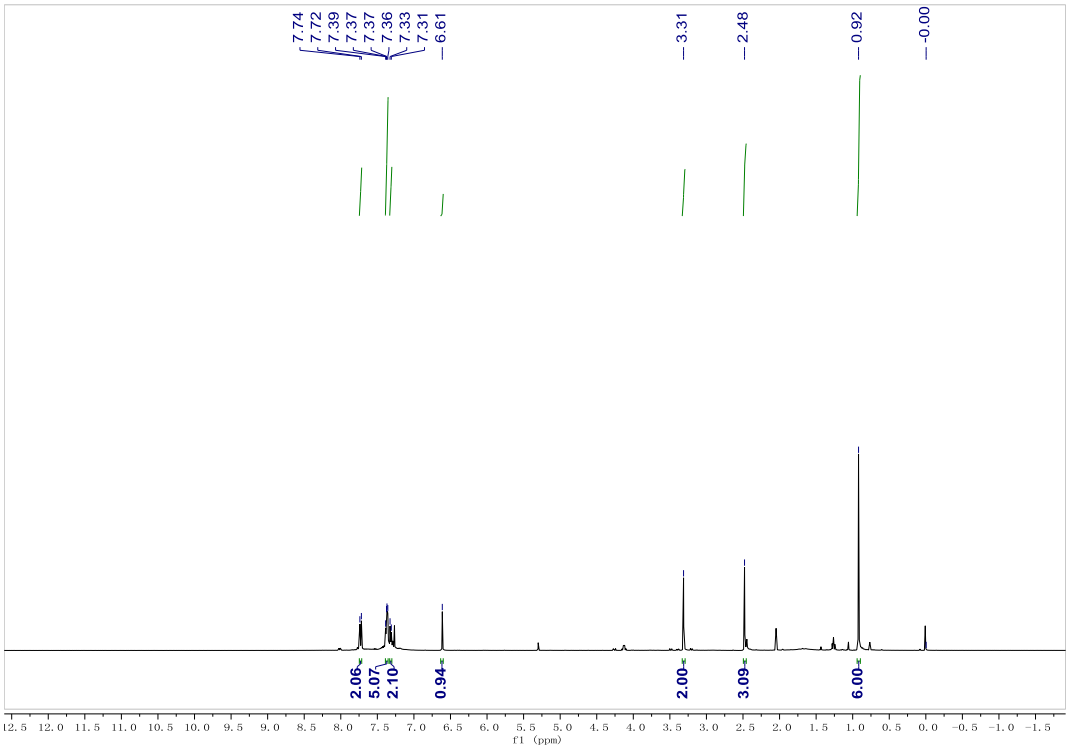
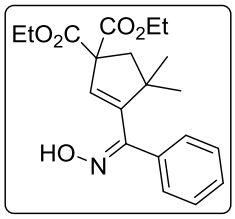
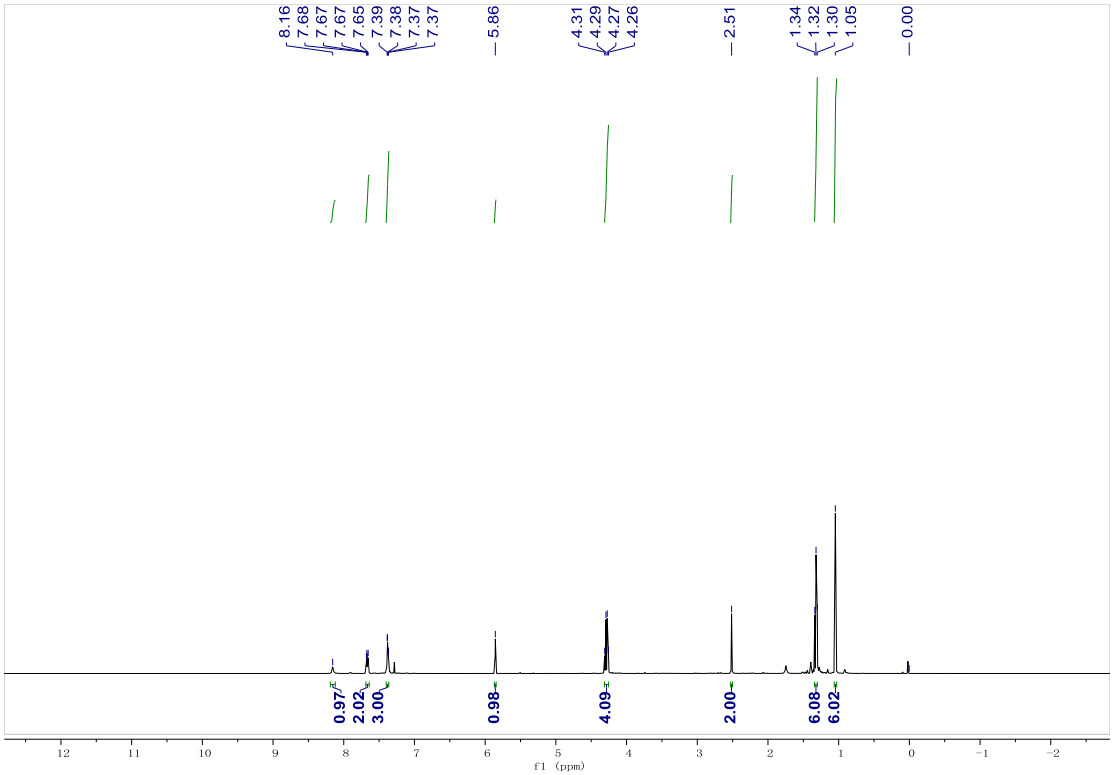
121.75
77.32
77.00
76.68
15.14
f1 (ppm)

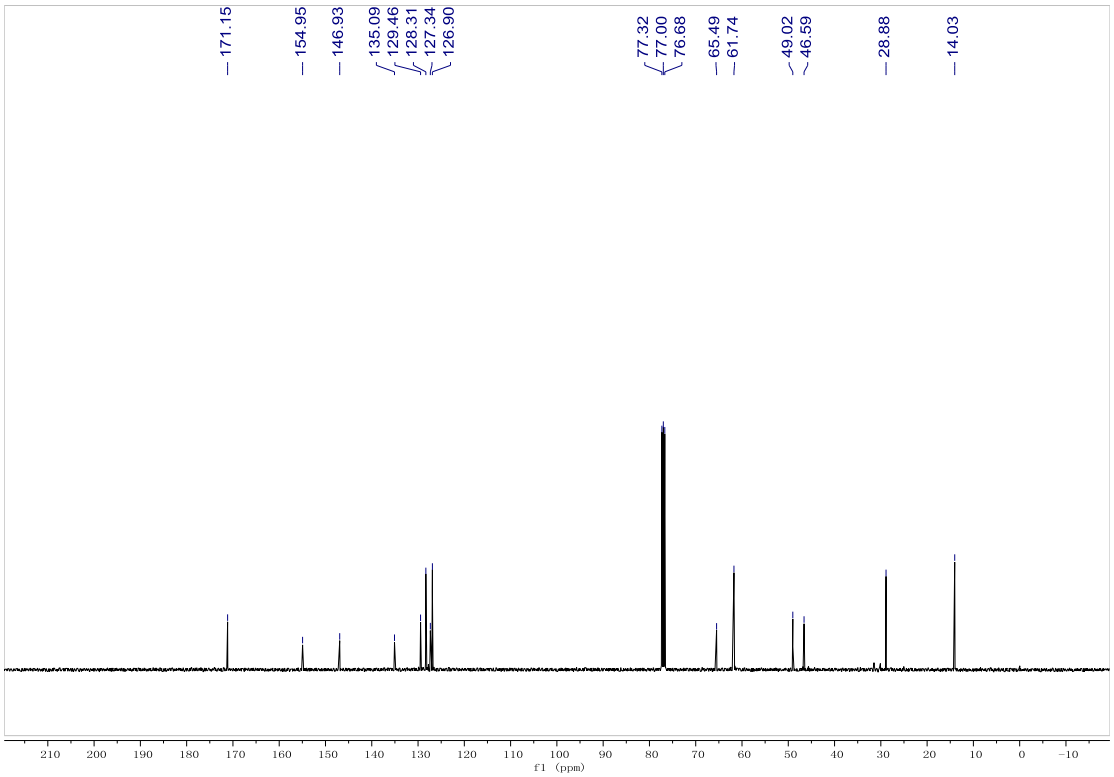

TsN
Ph
NOH


7.74
7.72
7.39
7.37
7.37
7.36
7.33
7.31
6.61
3.31
2.48
0.92
-0.00
2.06
5.07
2.10
0.94
2.00
3.09
6.00
f1 (ppm)


EtO2C
CO2Et
HO
N

6a


8.16
7.68
7.67
7.67
7.65
7.39
7.38
7.37
7.37
5.86
4.31
4.29
4.27
4.26
2.51
1.34
1.32
1.30
1.05
0.00
0.97
2.02
3.00
0.98
4.09
2.00
6.08
6.02
f1 (ppm)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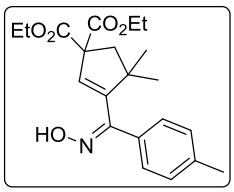
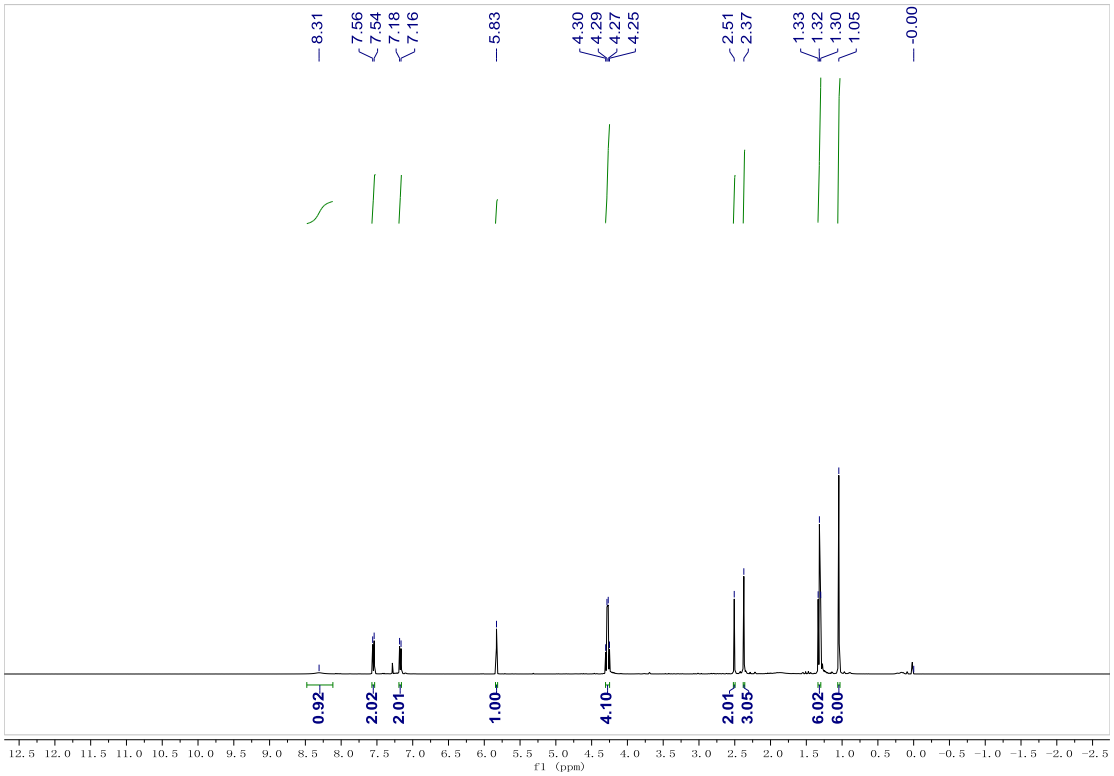
154.95
146.93
135.09
129.46
128.31
127.34
126.90
77.32
77.00
76.68
65.49
61.74
49.02
46.59
28.88
14.03
f1 (ppm)


EtO2C
CO2Et
HO
N

6b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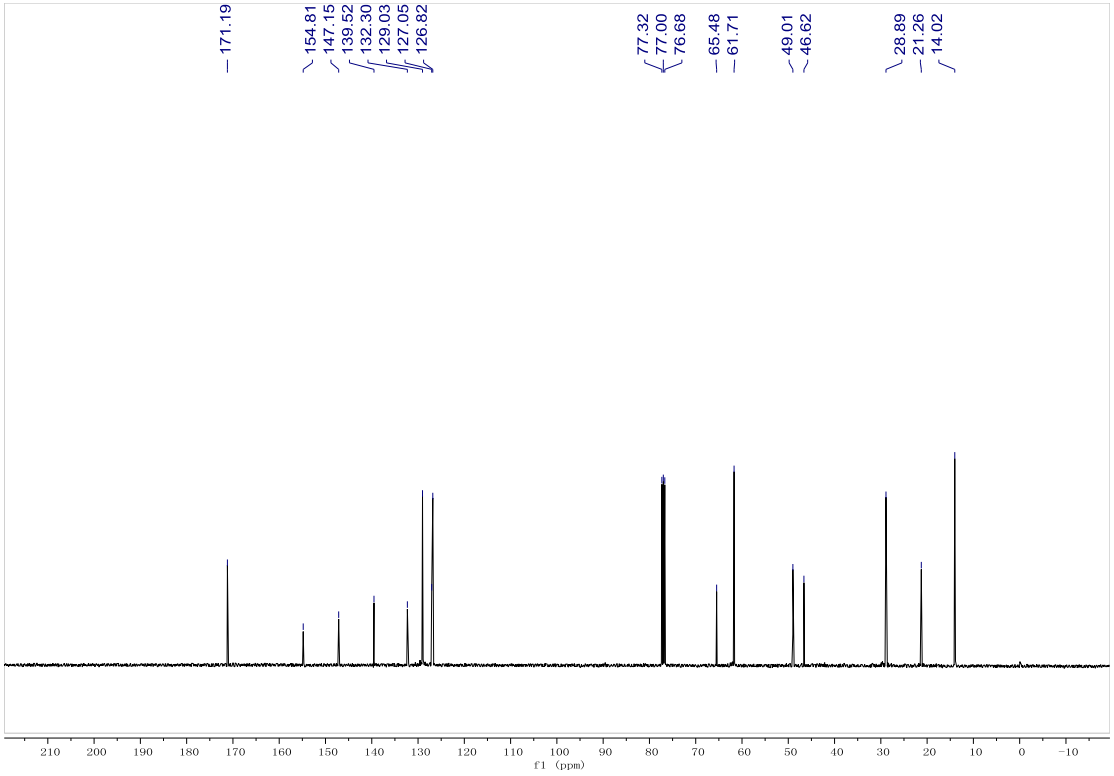
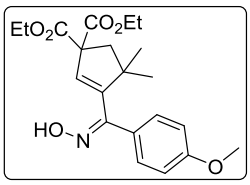
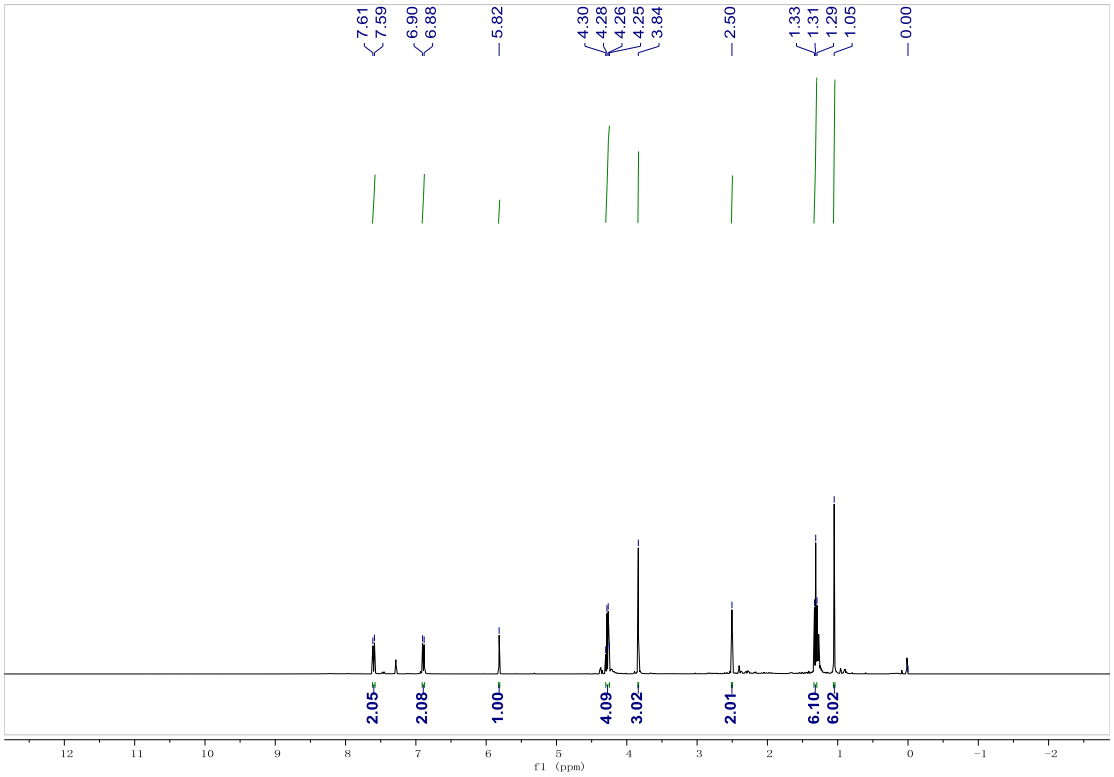
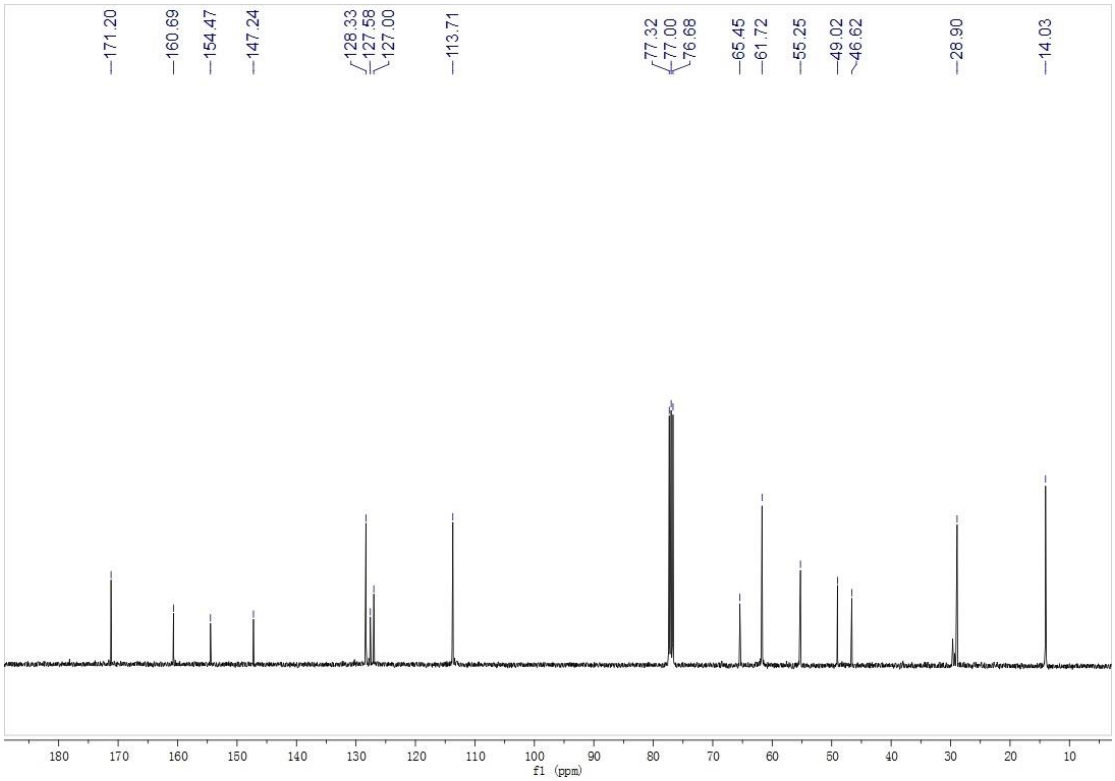
7.56
7.54
7.18
7.16
5.83
4.30
4.29
4.27
4.25
2.51
2.37
1.33
1.32
1.30
1.05
-0.00
0.92
2.02
2.01
1.00
4.10
2.01
3.05
6.02
6.00
f1 (ppm)


171.19
154.81
147.15
139.52
132.30
129.03
127.05
126.82
77.32
77.00
76.68
65.48
61.71
49.01
46.62
28.89
21.26
14.02
f1 (ppm)


EtO2C
CO2Et
HO
N
O

6c


7.61
7.59
6.90
6.88
5.82
4.30
4.28
4.26
4.25
3.84
2.50
1.33
1.31
1.29
1.05
0.00
2.05
2.08
1.00
4.09
3.02
2.01
6.10
6.02
f1 (ppm)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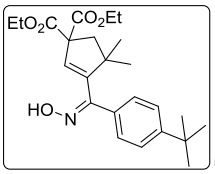
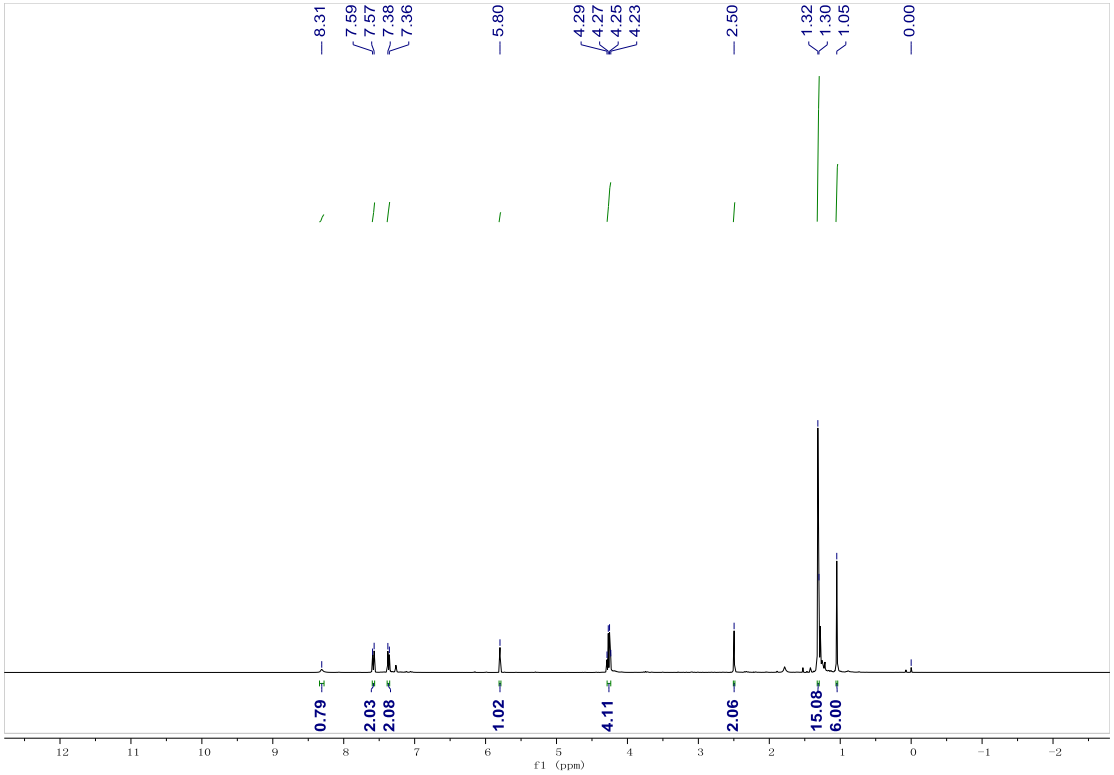
160.69
154.47
147.24
128.33
127.58
127.00
113.71
77.32
77.00
76.68
65.45
61.72
55.25
49.02
46.62
28.90
14.03
f1 (ppm)


EtO2C
CO2Et
HO
N

6d


8.31
7.59
7.57
7.38
7.36
5.80
4.29
4.27
4.25
4.23
2.50
1.32
1.30
1.05
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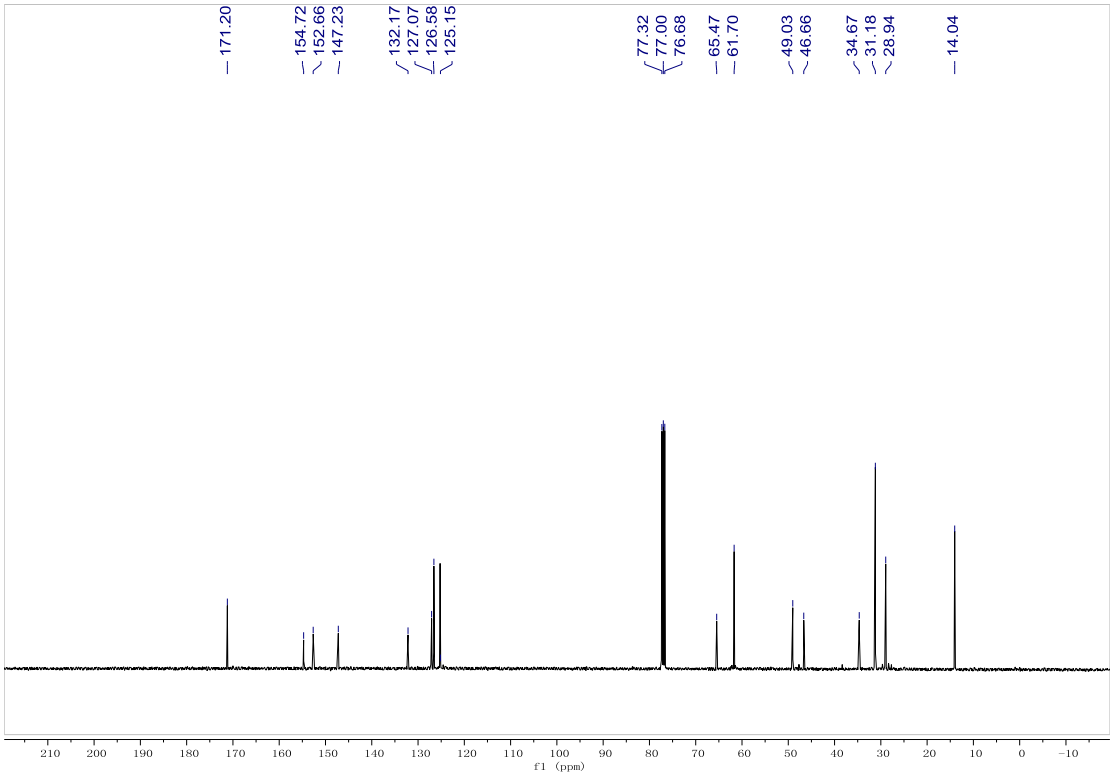
0.79
2.03
2.08
1.02
4.11
2.06
15.08
6.00
f1 (ppm)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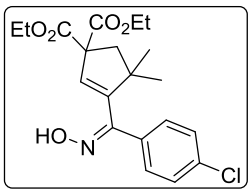
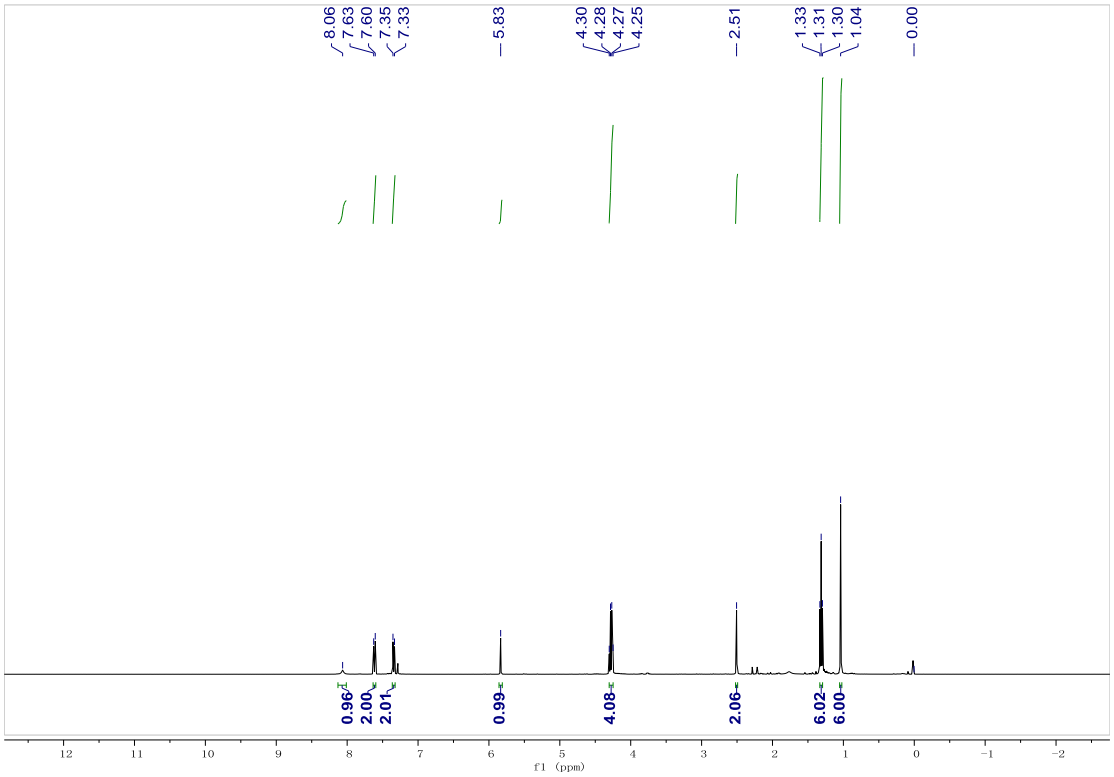
154.72
152.66
147.23
132.17
127.07
126.58
125.15
77.32
77.00
76.68
65.47
61.70
49.03
46.66
34.67
31.18
28.94
14.04
f1 (ppm)


EtO2C
CO2Et
HO
N
Cl

6e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7.33
5.83
4.30
4.28
4.27
4.25
2.51
1.33
1.31
1.30
1.04
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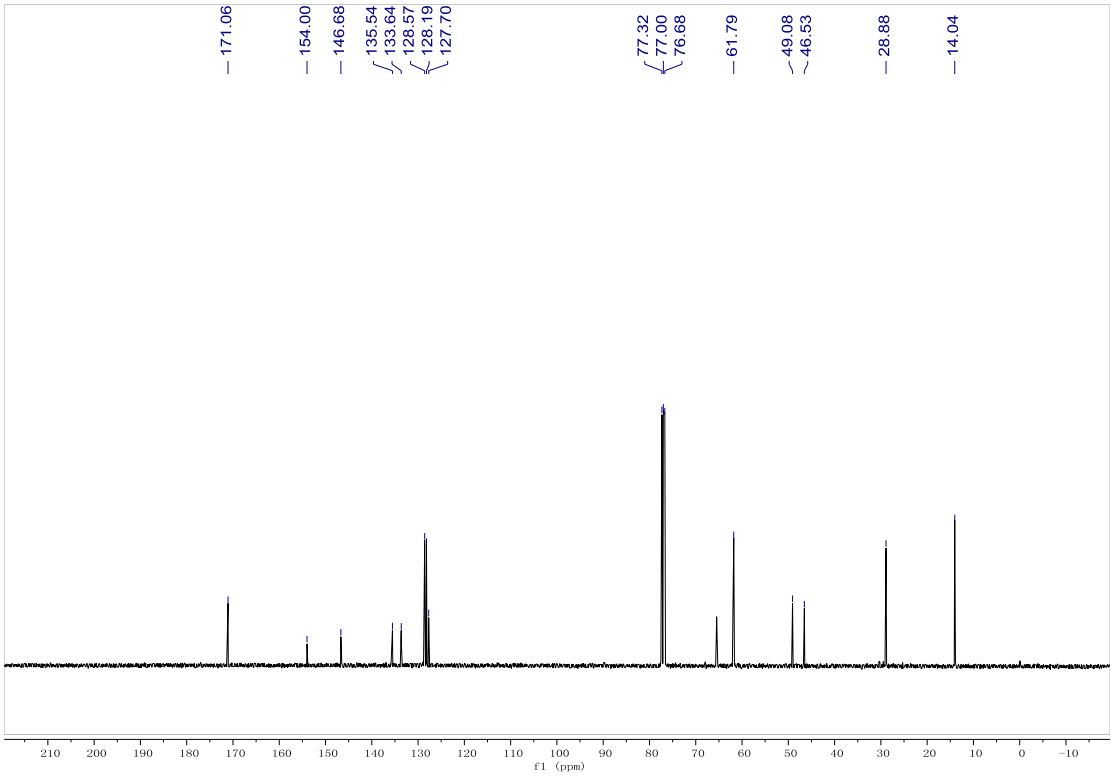
0.96
2.00
2.01
0.99
4.08
2.06
6.02
6.00
f1 (ppm)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135.54
133.64
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128.19
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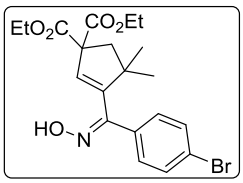
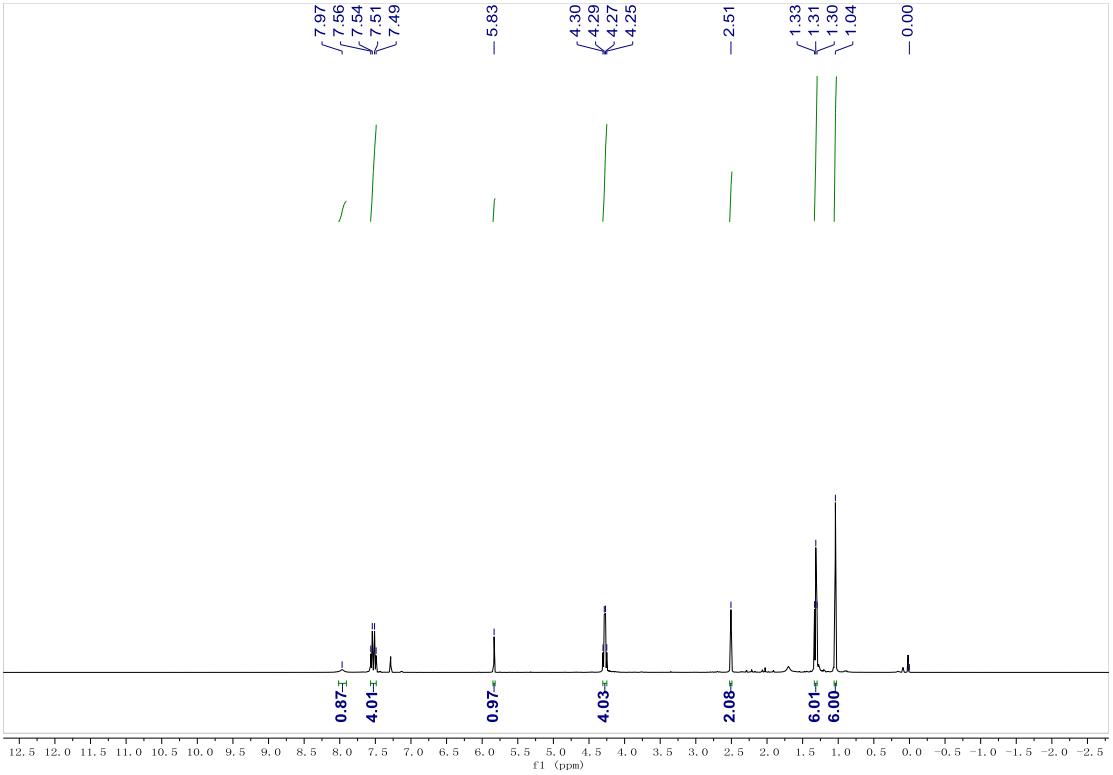
77.32
77.00
76.68
61.79
49.08
46.53
28.88
14.04
f1 (ppm)


EtO2C
CO2Et
HO
N
Br
6f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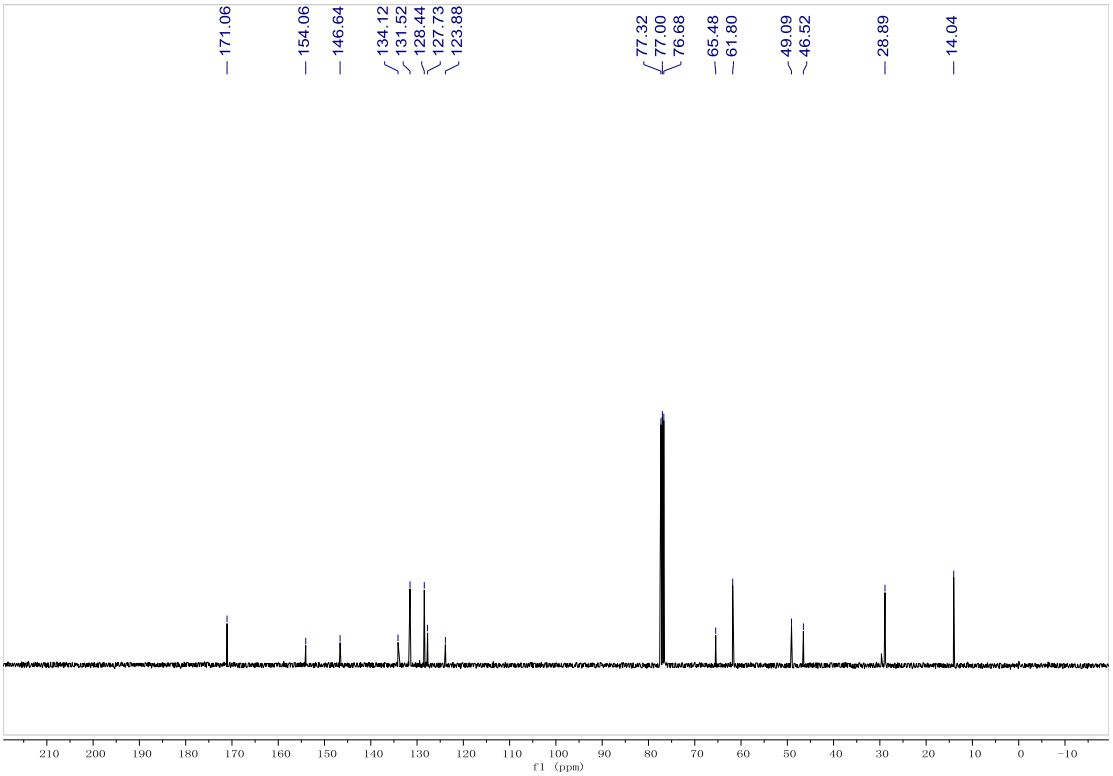
7.54
7.51
7.49
5.83
4.30
4.29
4.27
4.25
2.51
1.33
1.31
1.30
1.04
0.00
0.87
4.01
0.97
4.03
2.08
6.01
6.00
f1 (ppm)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131.52
128.44
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123.88
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77.00
76.68
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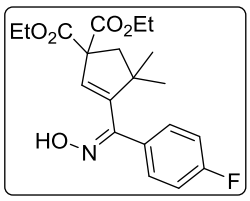
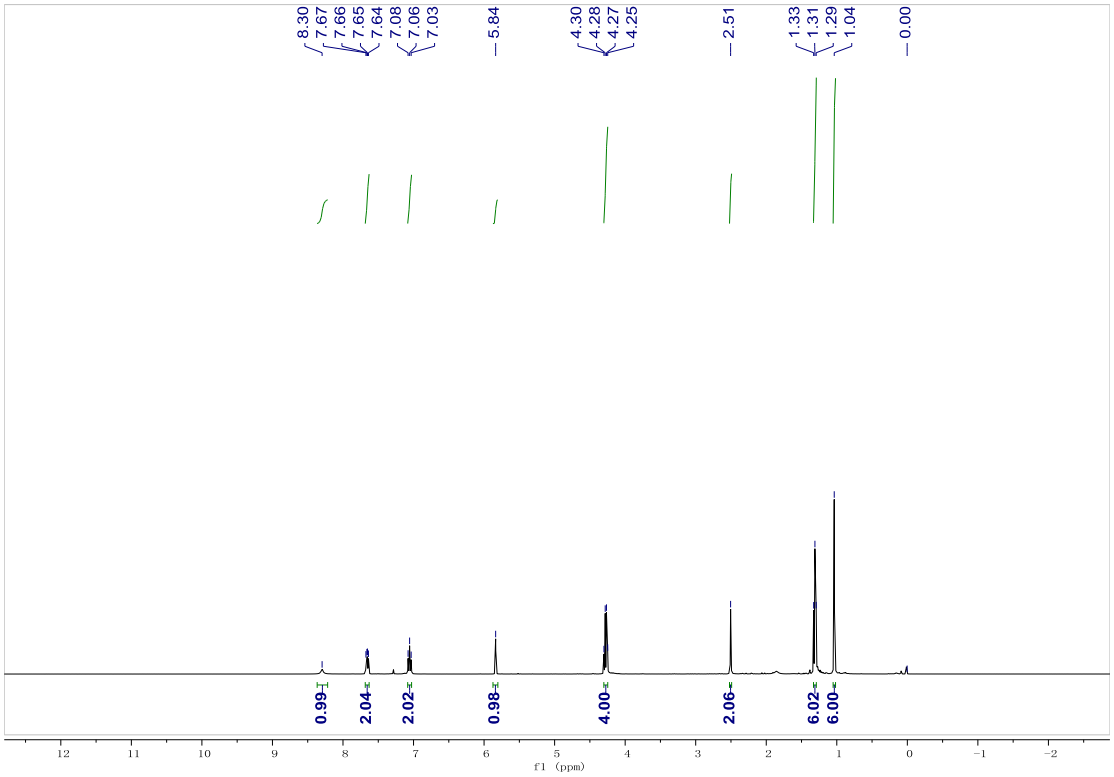
49.09
46.52
28.89
14.04
f1 (ppm)


EtO2C
CO2Et
HO
N
F

6g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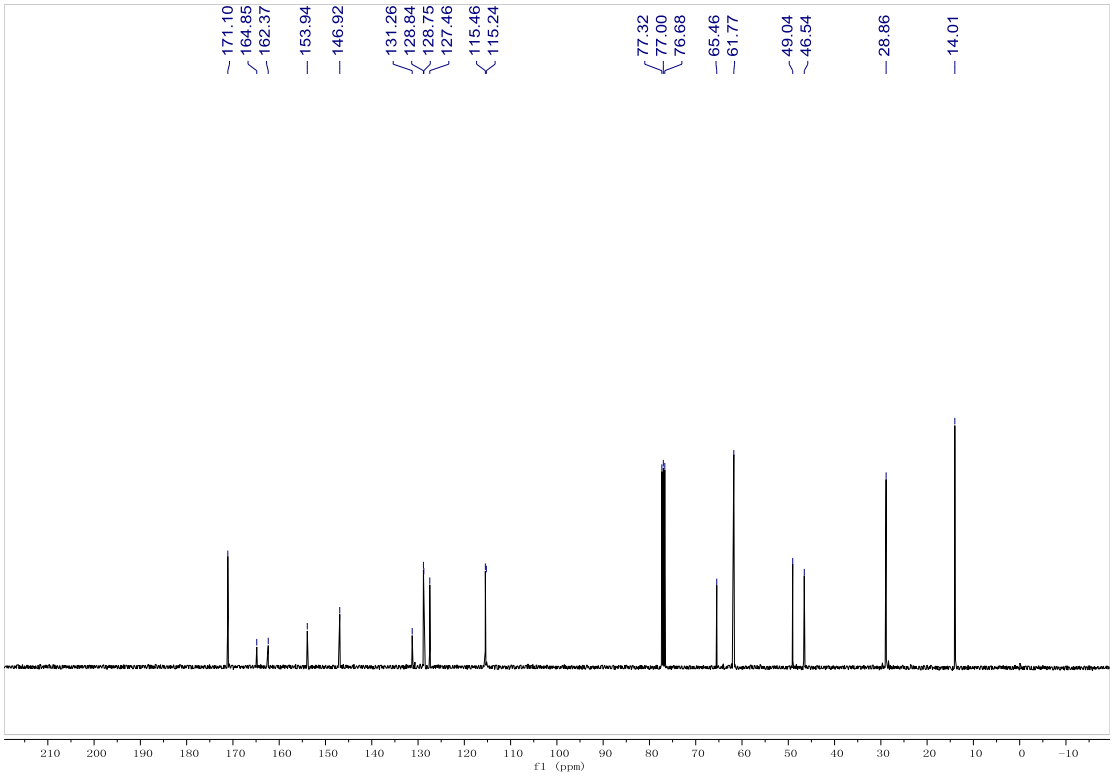
7.08
7.06
7.03
5.84
4.30
4.28
4.27
4.25
2.51
1.33
1.31
1.29
1.04
0.00
0.99
2.04
2.02
0.98
4.00
2.06
6.02
6.00
f1 (ppm)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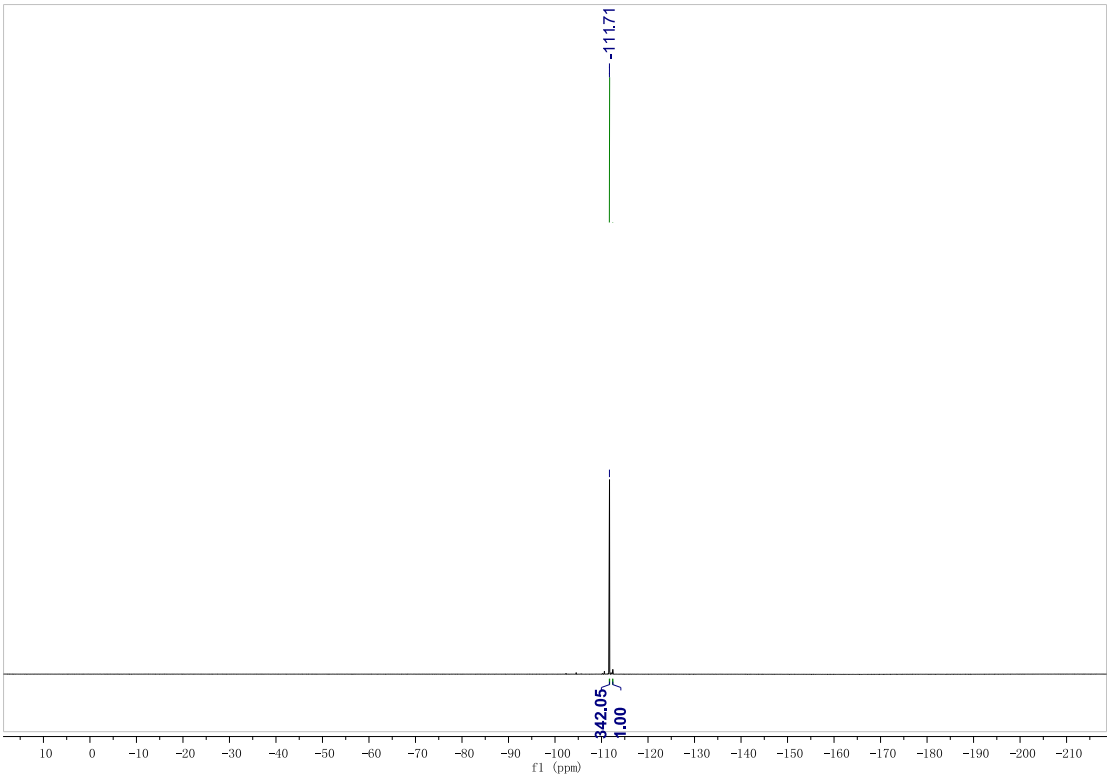
162.37
153.94
146.92
131.26
128.84
128.75
127.46
115.46
115.24
77.32
77.00
76.68
65.46
61.77
49.04
46.54
28.86
14.01
f1 (ppm)


-111.71
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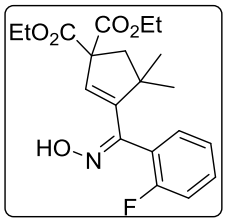
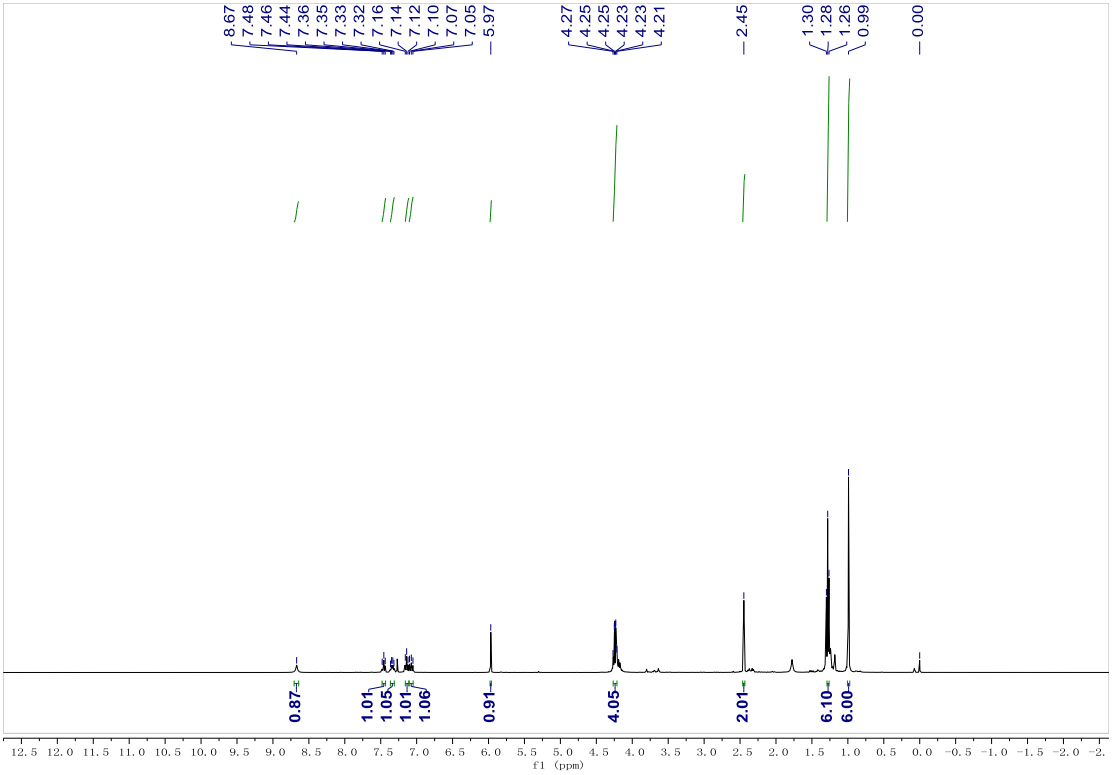
1.00
f1 (ppm)


EtO2C
CO2Et
HO
N
F

6h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7.46
7.44
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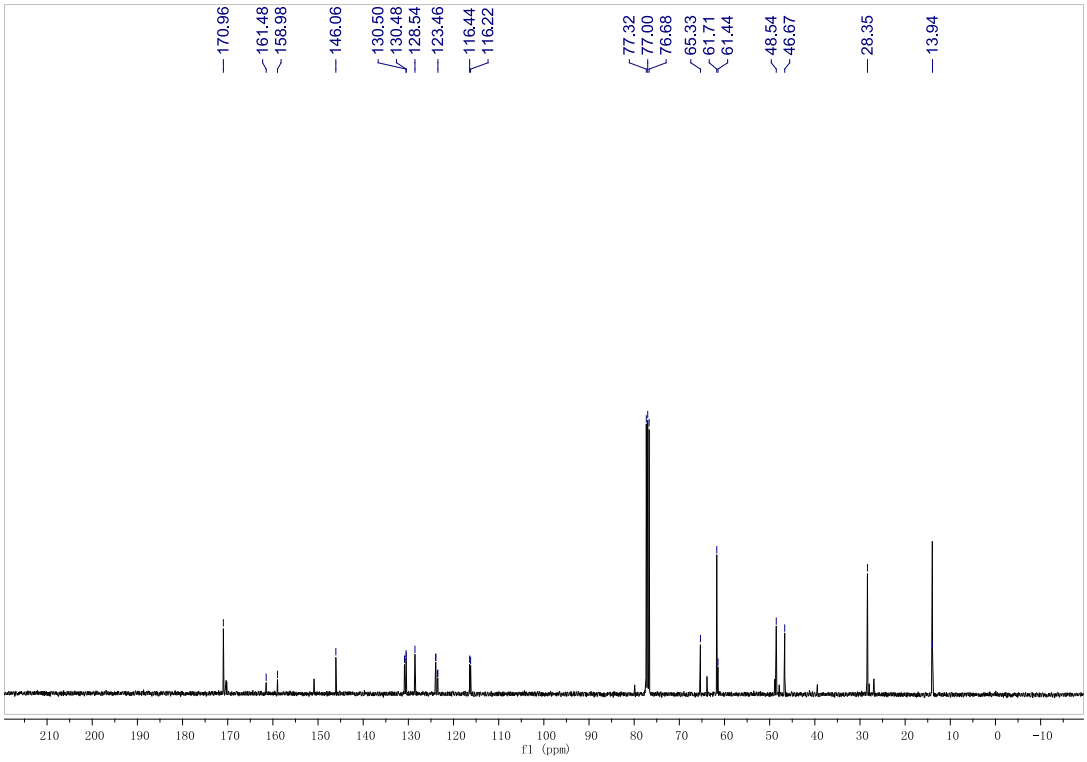
7.35
7.33
7.32
7.16
7.14
7.12
7.10
7.07
7.05
5.97
4.27
4.25
4.23
4.23
4.21
2.45
1.30
1.28
1.26
0.99
0.00
0.87
1.01
1.05
1.01
1.06
0.91
4.05
2.01
6.10
6.00
f1 (ppm)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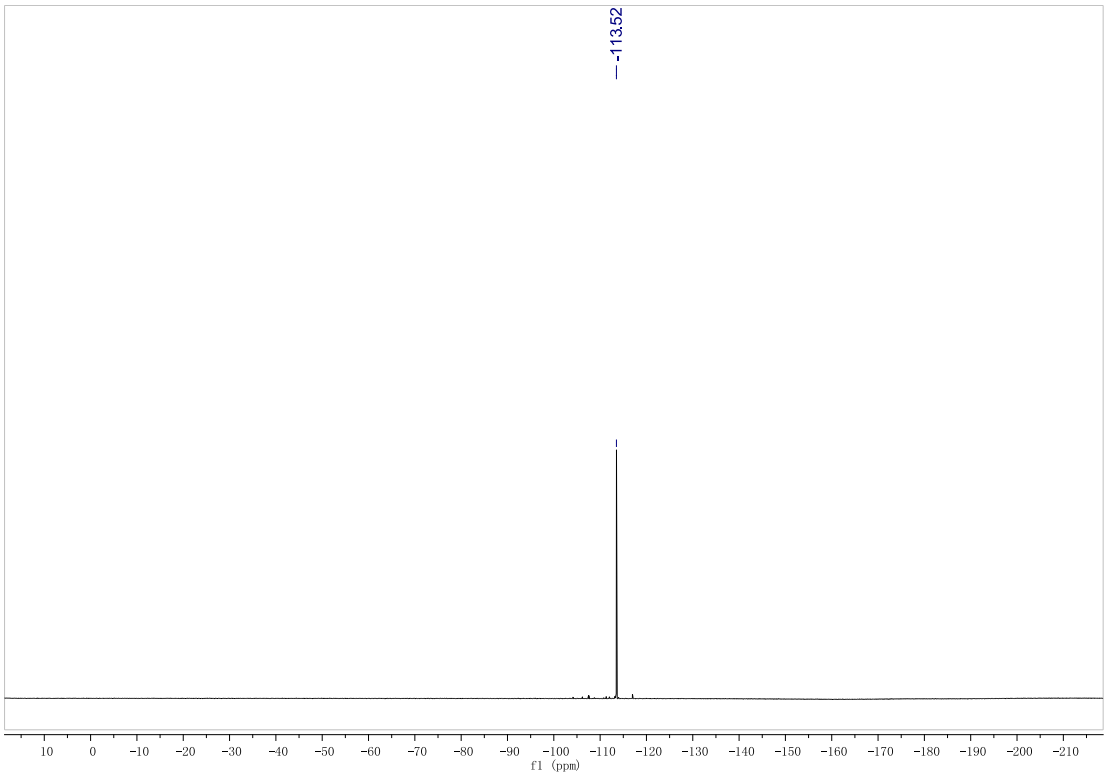
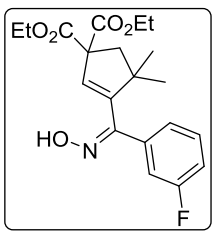
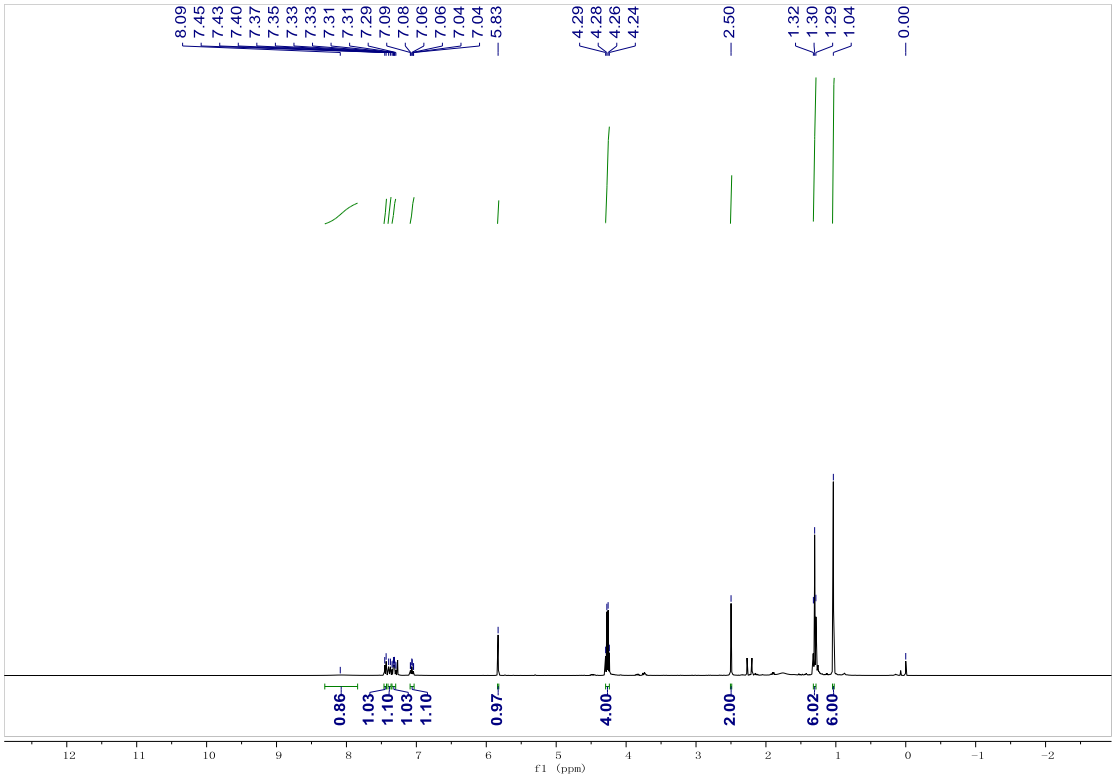
128.54
123.46
116.44
116.22
77.32
77.00
76.68
65.33
61.71
61.44
48.54
46.67
28.35
13.94
f1 (ppm)


-113.52
f1 (ppm)


EtO2C
CO2Et
HO
N
F

6i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7.45
7.43
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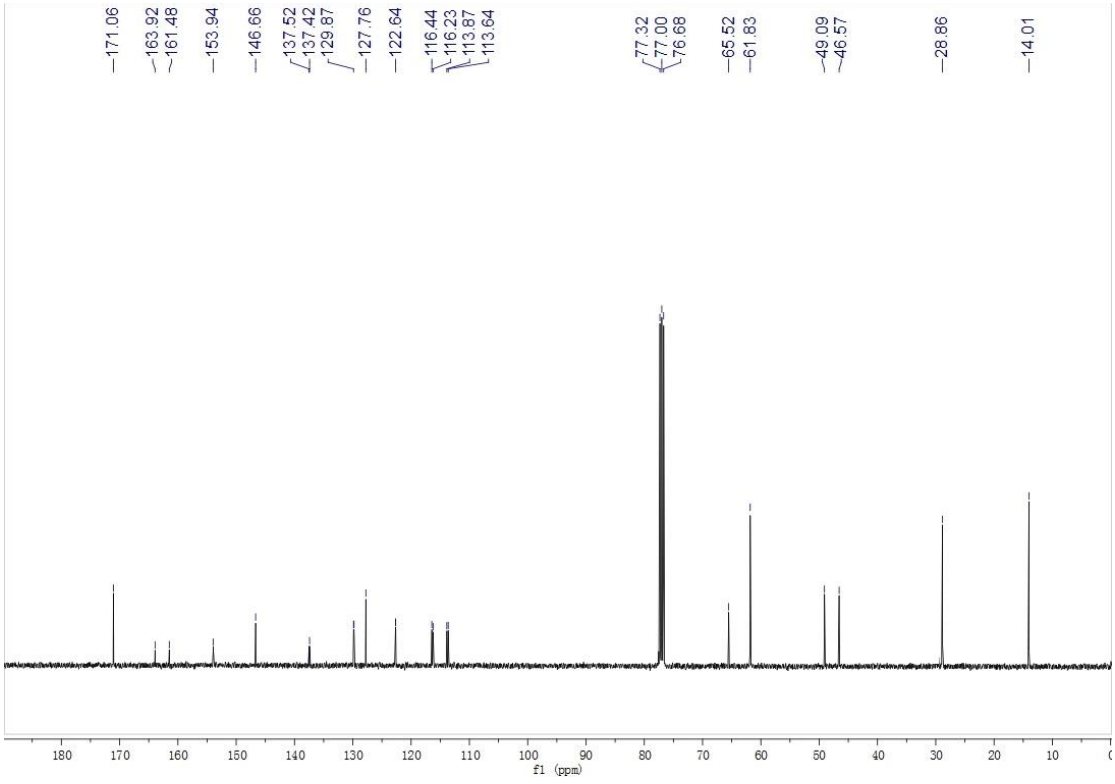
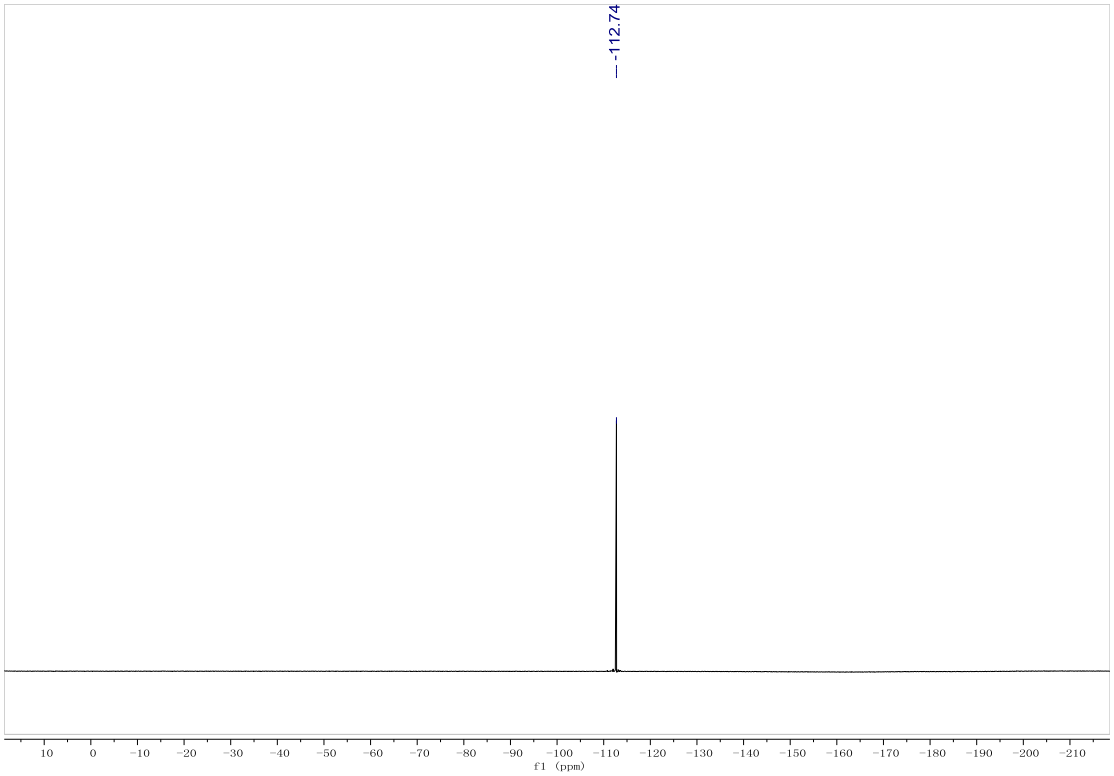
7.35
7.33
7.33
7.31
7.31
7.29
7.09
7.08
7.06
7.06
7.04
7.04
5.83
4.29
4.28
4.26
4.24
2.50
1.32
1.30
1.29
1.04
0.00
0.86
1.03
1.10
1.03
1.10
0.97
4.00
2.00
6.02
6.00
f1 (ppm)


171.06
163.92
161.48
153.94
146.66
137.52
137.42
129.87
127.76
122.64
116.44
116.23
113.87
113.64
77.32
77.00
76.68
65.52
61.83
49.09
46.57
28.86
14.01
f1 (ppm)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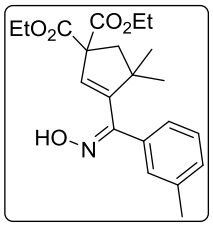
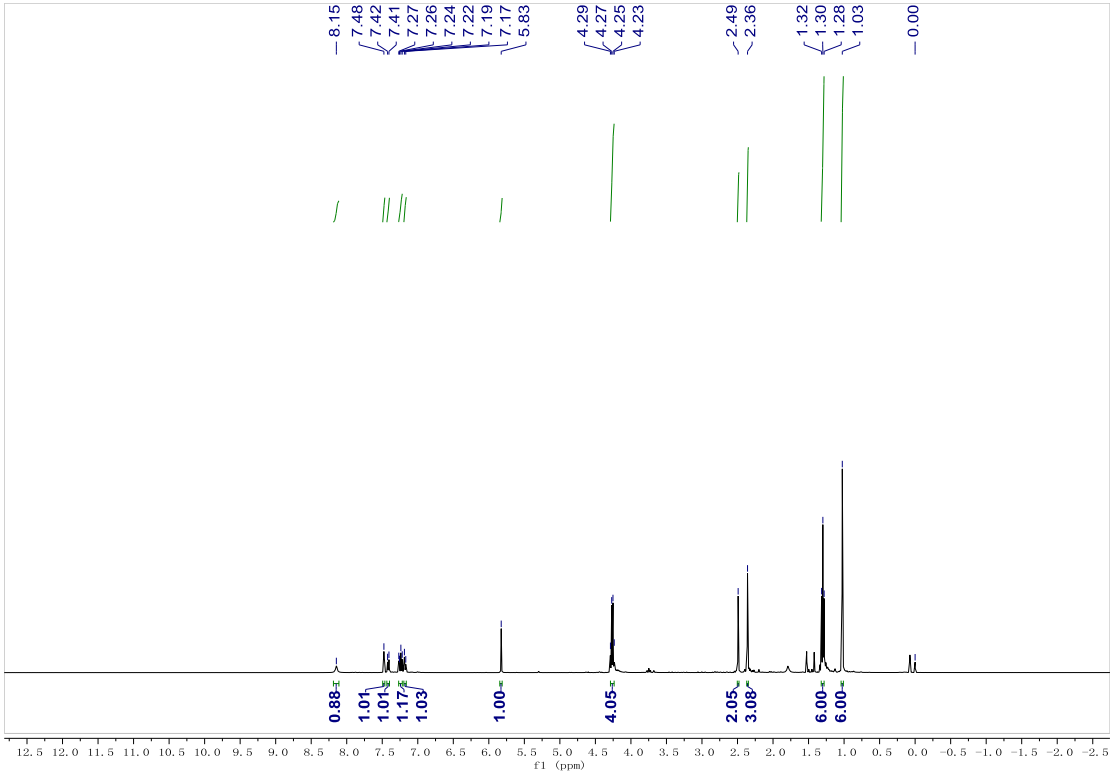
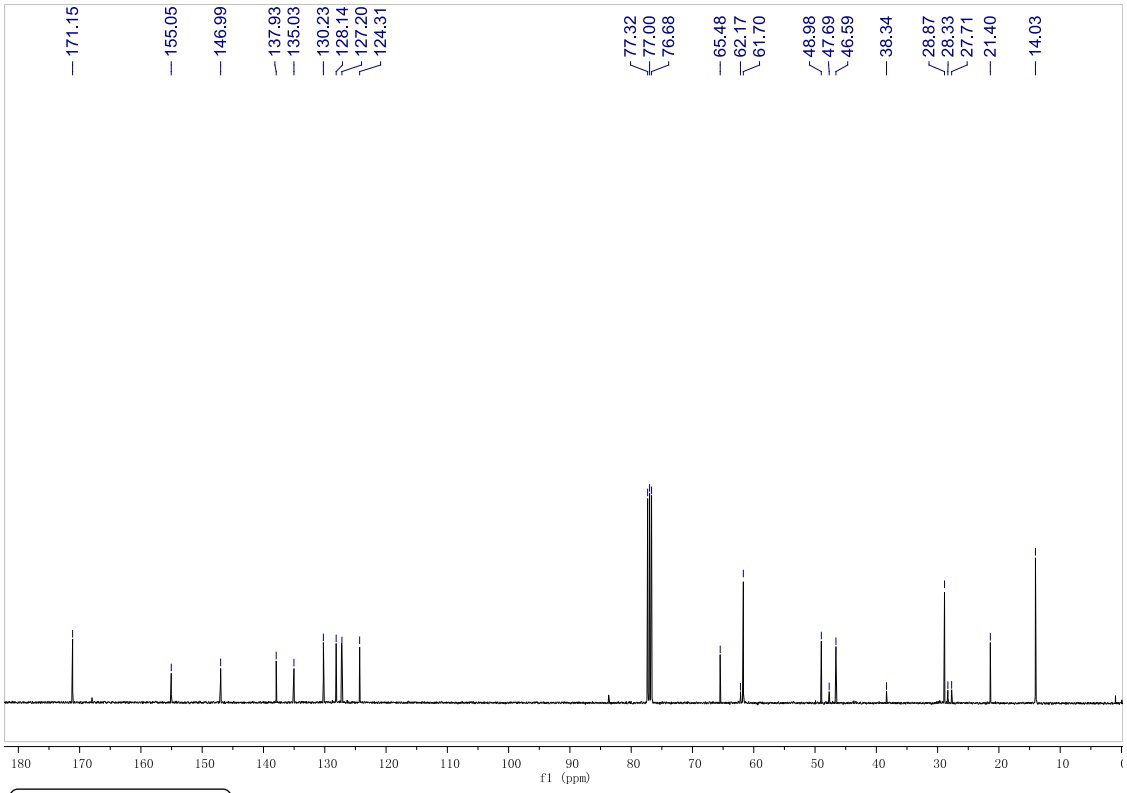
f1 (ppm)


EtO2C
CO2Et
HO
N

6j


8.15
7.48
7.42
7.41
7.27
7.26
7.24
7.22
7.19
7.17
5.83
4.29
4.27
4.25
4.23
2.49
2.36
1.32
1.30
1.28
1.03
0.00
0.88
1.01
1.01
1.17
1.03
1.00
4.05
2.05
3.08
6.00
6.00
f1 (ppm)


171.15
155.05
146.99
137.93
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130.23
128.14
127.20
124.31
77.32
77.00
76.68
65.48
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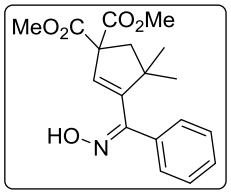
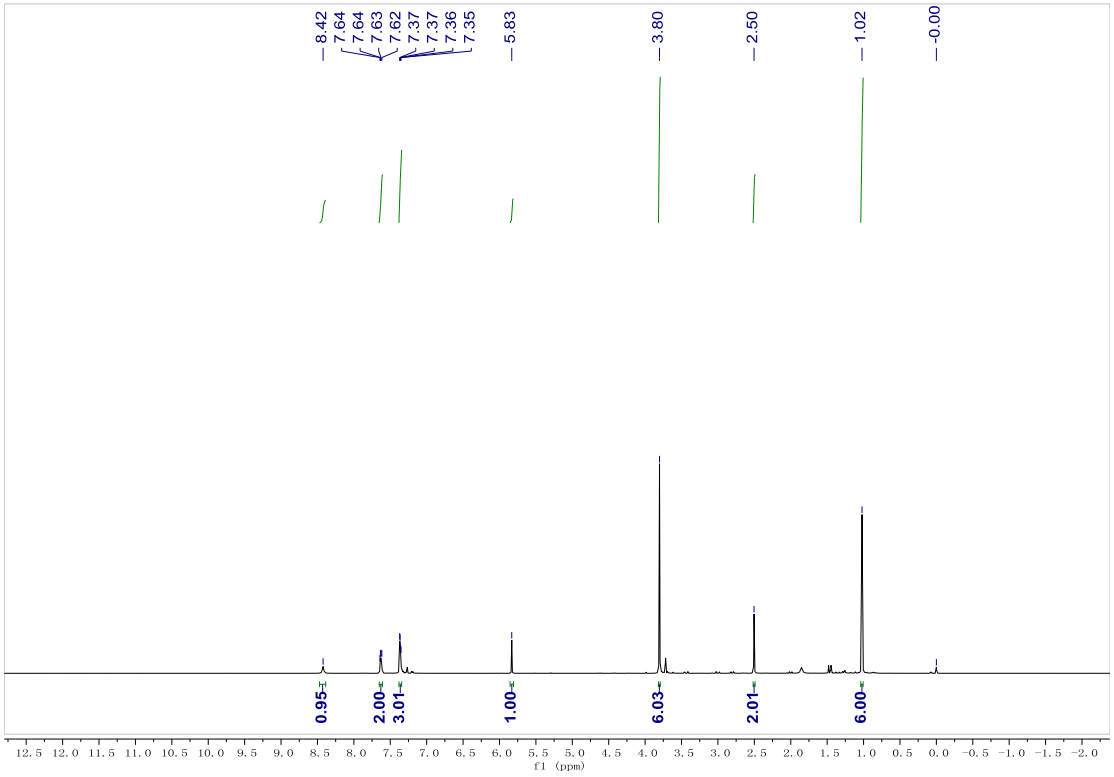
47.69
46.59
38.34
28.87
28.33
27.71
21.40
14.03
f1 (ppm)


MeO2C
CO2Me
HO
N

6k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7.62
7.37
7.37
7.36
7.35
5.83
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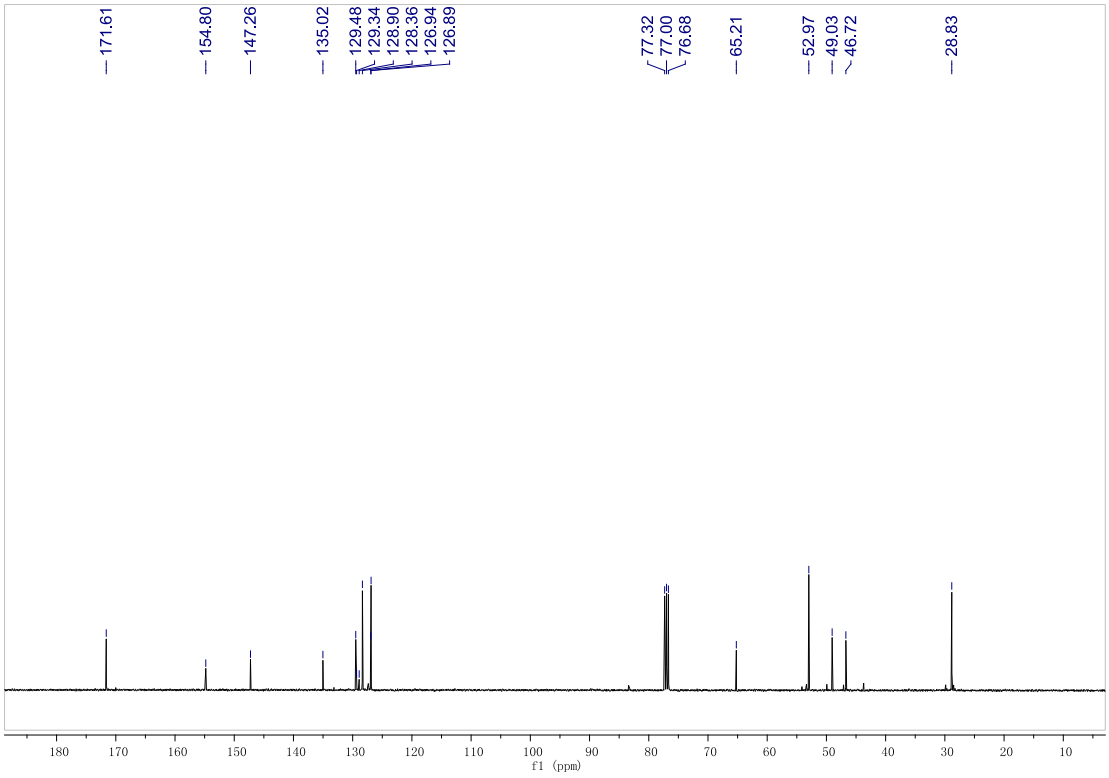
0.95
2.00
3.01
1.00
6.03
2.01
6.00
f1 (ppm)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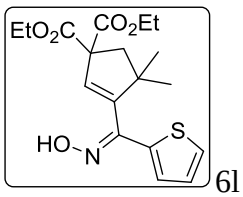
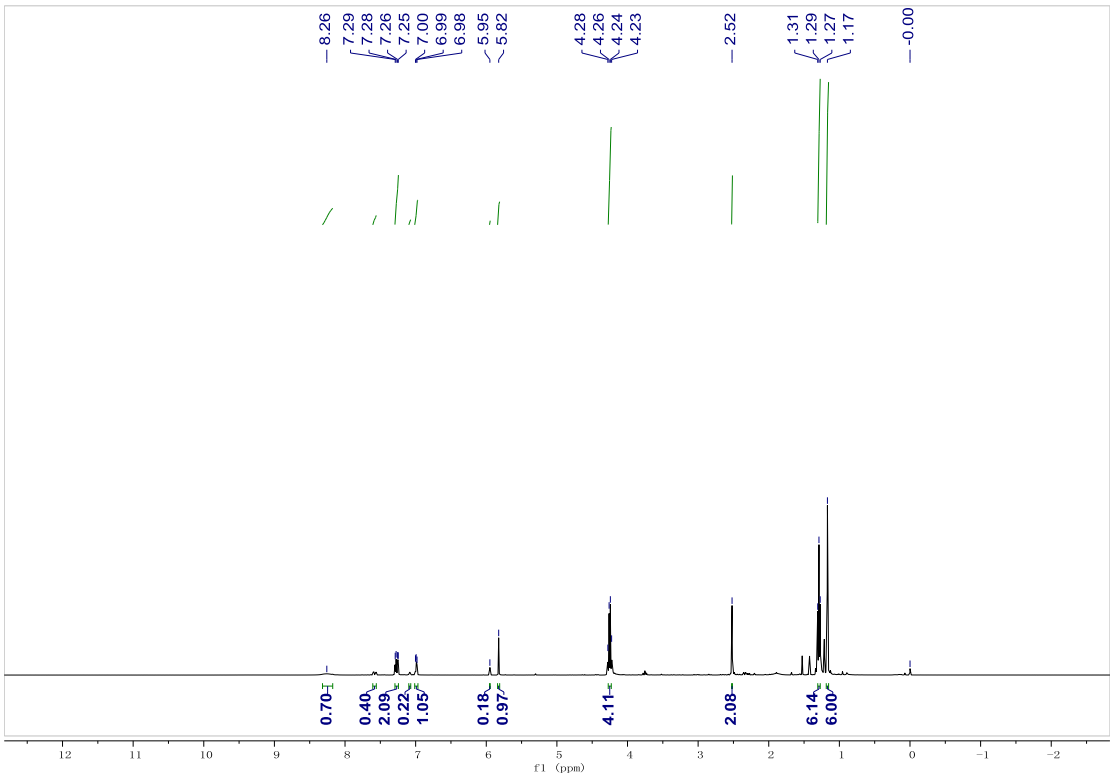
154.80
147.26
135.02
129.48
129.34
128.90
128.36
126.94
126.89
77.32
77.00
76.68
65.21
52.97
49.03
46.72
28.83
f1 (ppm)


EtO2C
CO2Et
HO
N
S

6l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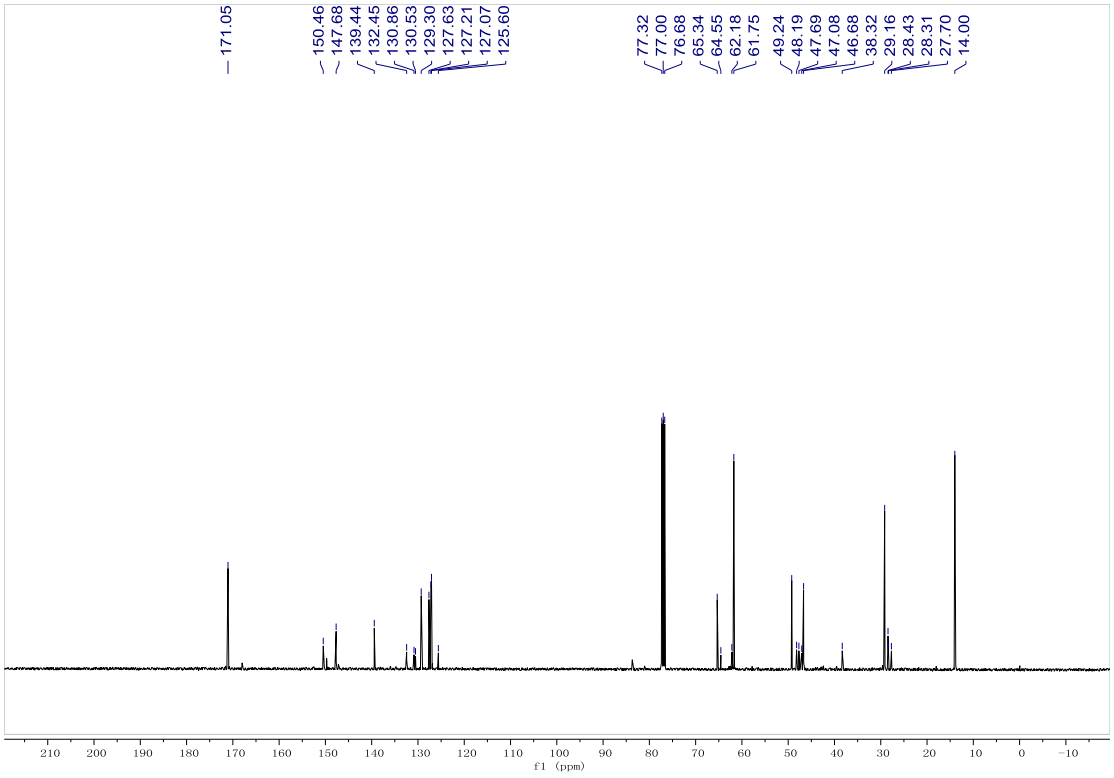
7.25
7.00
6.99
6.98
5.95
5.82
4.28
4.26
4.24
4.23
2.52
1.31
1.29
1.27
1.17
-0.00
0.70
0.40
2.09
0.22
1.05
0.18
0.97
4.11
2.08
6.14
6.00
f1 (ppm)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132.45
130.86
130.53
129.30
127.63
127.21
127.07
125.60
77.32
77.00
76.68
65.34
64.55
62.18
61.75
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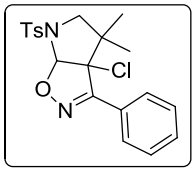
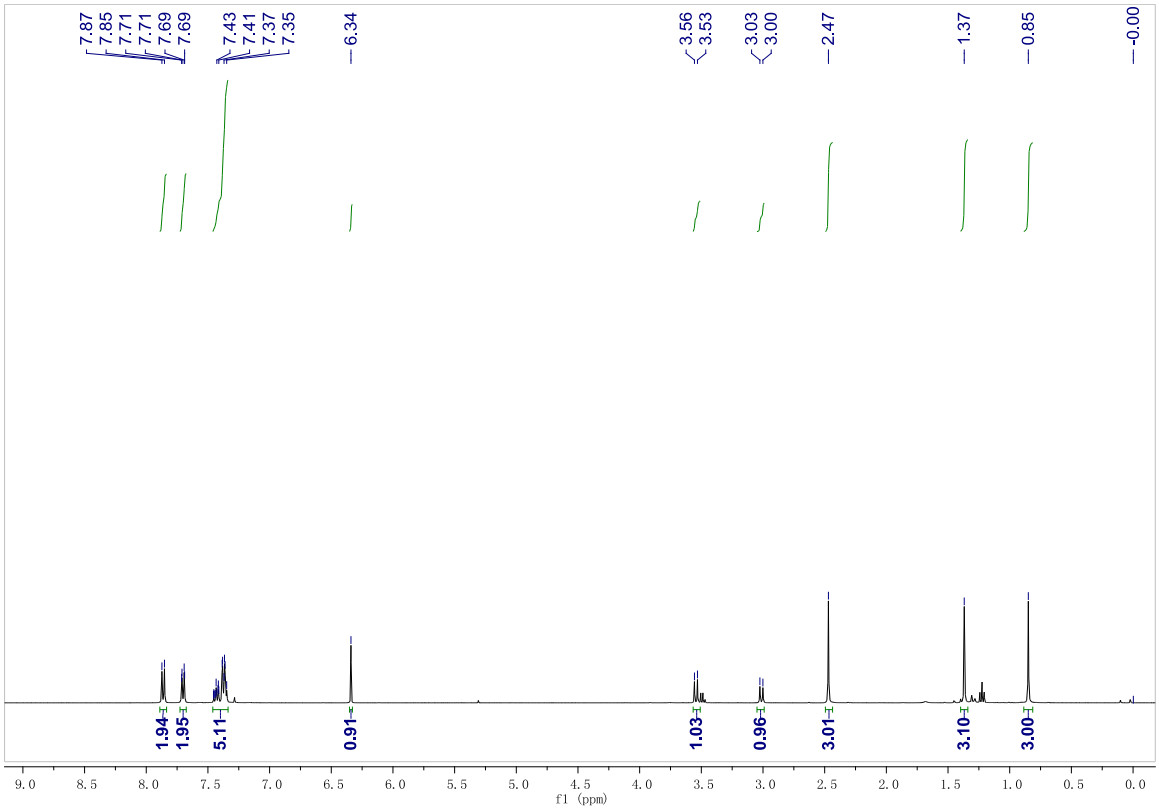
28.43
28.31
27.70
14.00
f1 (ppm)


TsN
Cl
O
N

8a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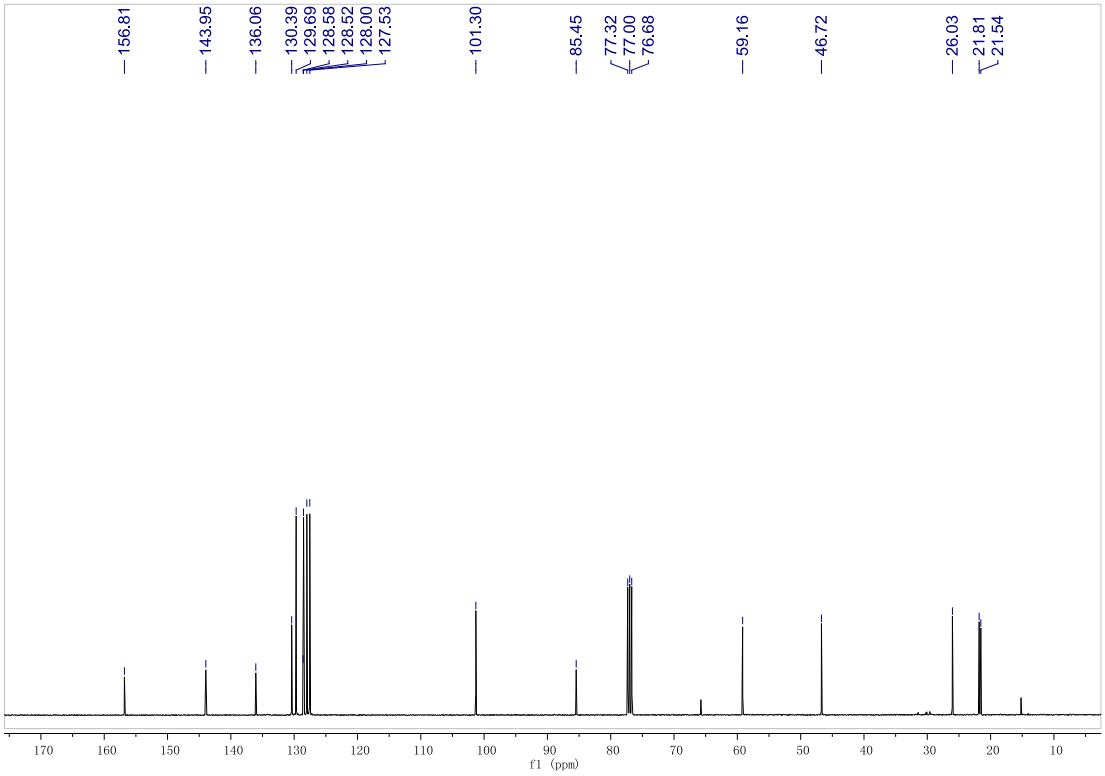
7.69
7.69
7.43
7.41
7.37
7.35
6.34
3.56
3.53
3.03
3.00
2.47
1.37
0.85
-0.00
1.94
1.95
5.11
0.91
1.03
0.96
3.01
3.10
3.00
f1 (ppm)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129.69
128.58
128.52
128.00
127.53
101.30
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77.32
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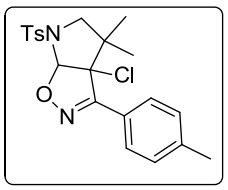
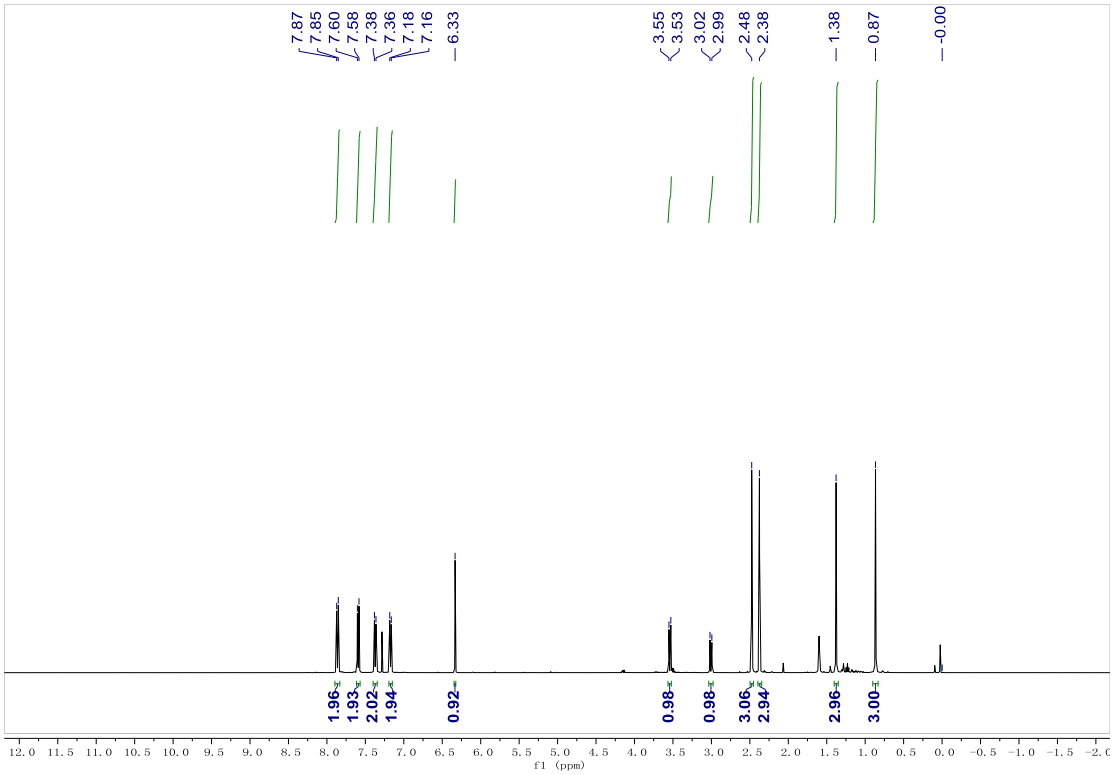
46.72
26.03
21.81
21.54
f1 (ppm)


TsN
Cl
O
N

8b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7.85
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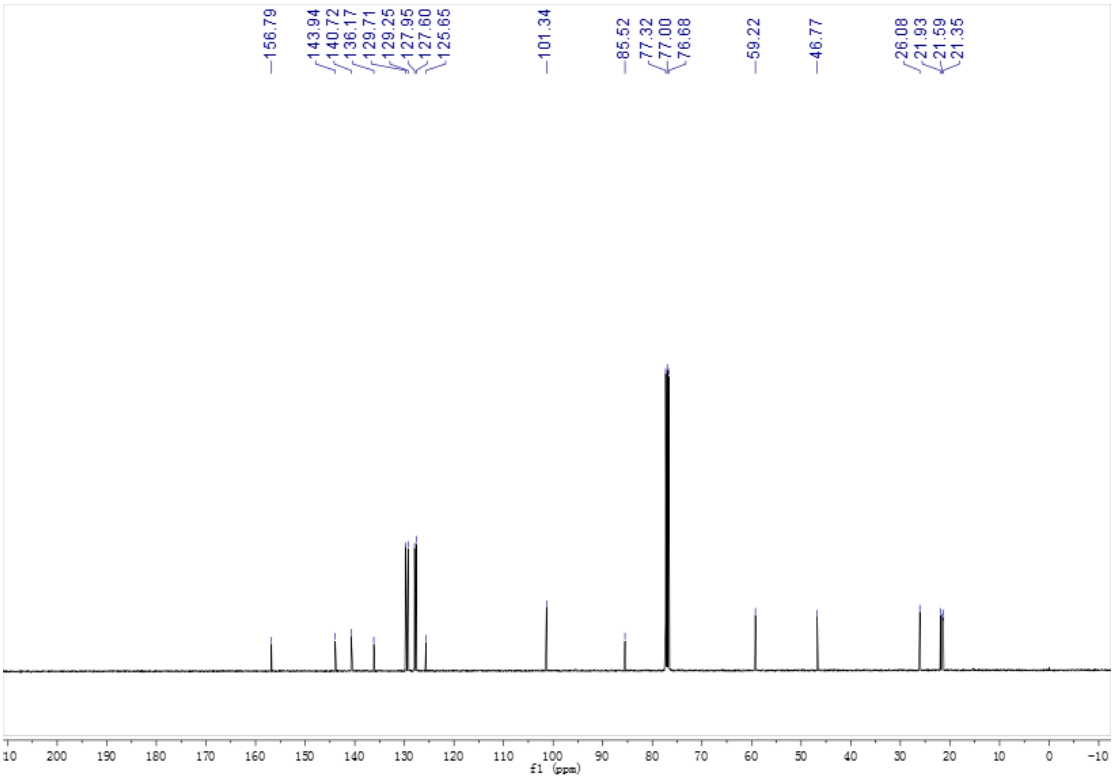
7.58
7.38
7.36
7.18
7.16
6.33
3.55
3.53
3.02
2.99
2.48
2.38
1.38
0.87
-0.00
1.96
1.93
2.02
1.94
0.92
0.98
0.98
3.06
2.94
2.96
3.00
f1 (ppm)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129.25
127.95
127.60
125.65
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85.52
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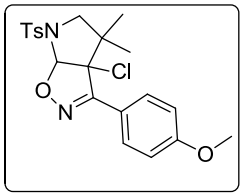
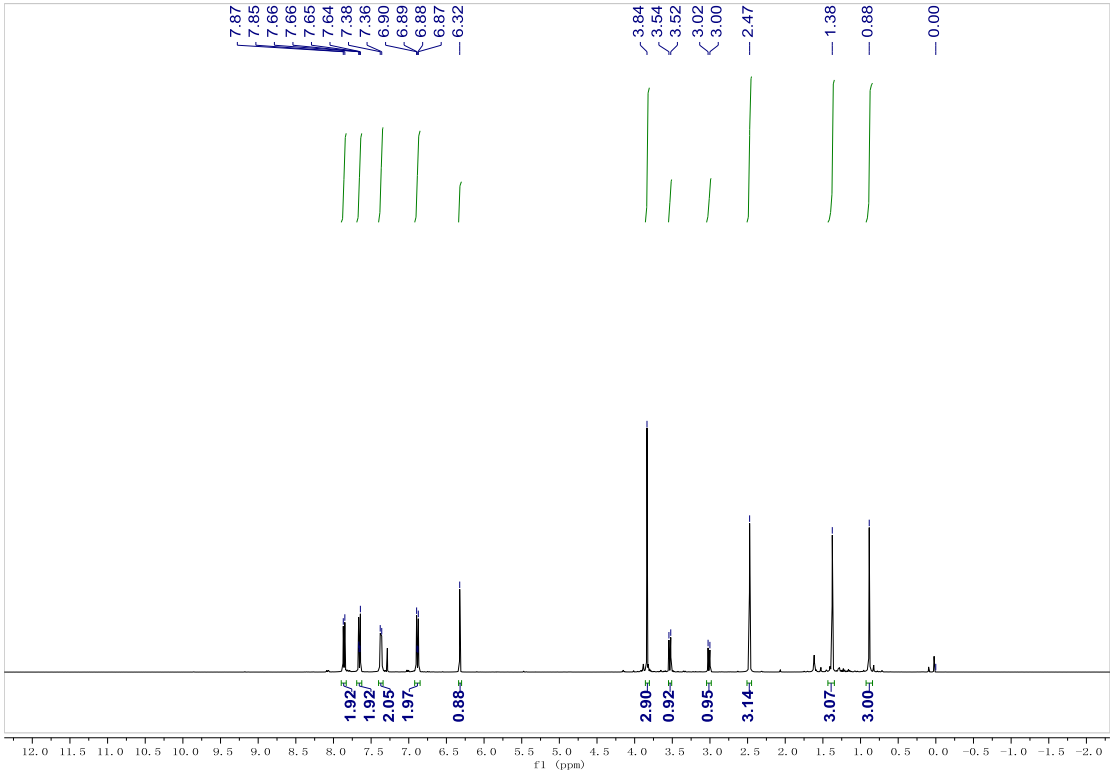
26.08
21.93
21.59
21.35
f1 (ppm)


TsN
Cl
O
N
O

8c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7.36
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6.89
6.88
6.87
6.32
3.84
3.54
3.52
3.02
3.00
2.47
1.38
0.88
0.00
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1.92
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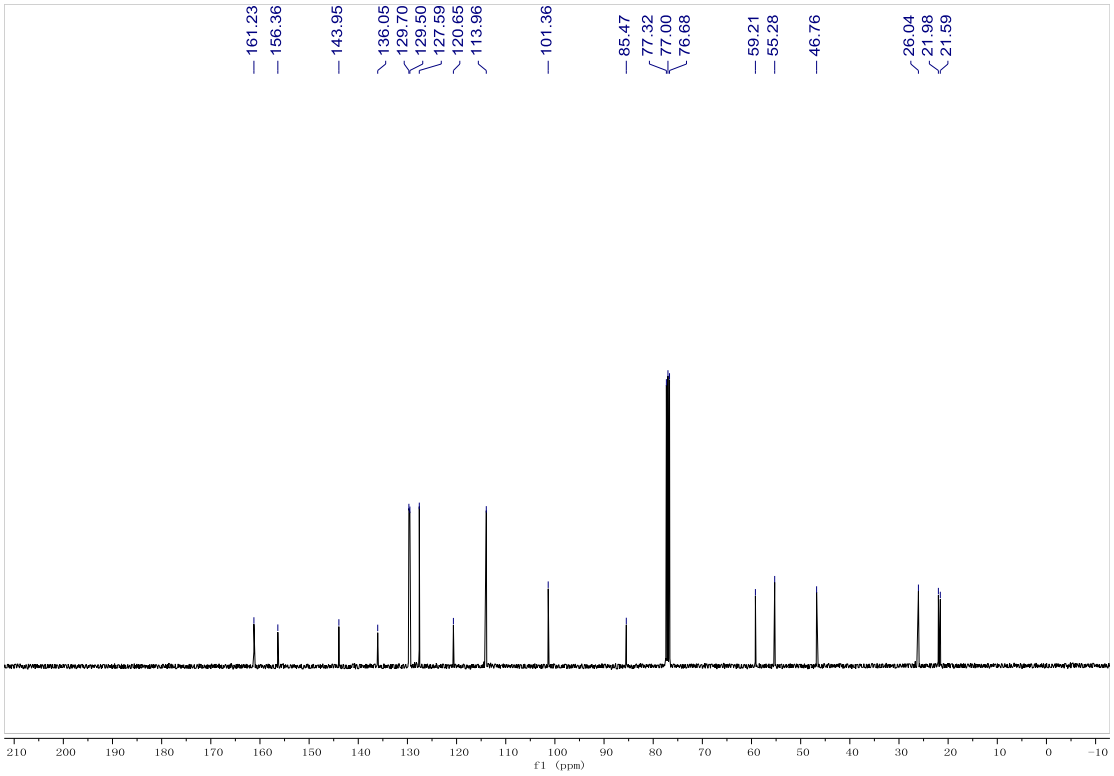
1.97
0.88
2.90
0.92
0.95
3.14
3.07
3.00
f1 (ppm)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127.59
120.65
113.96
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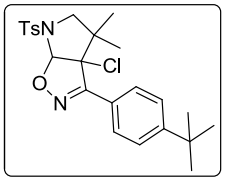
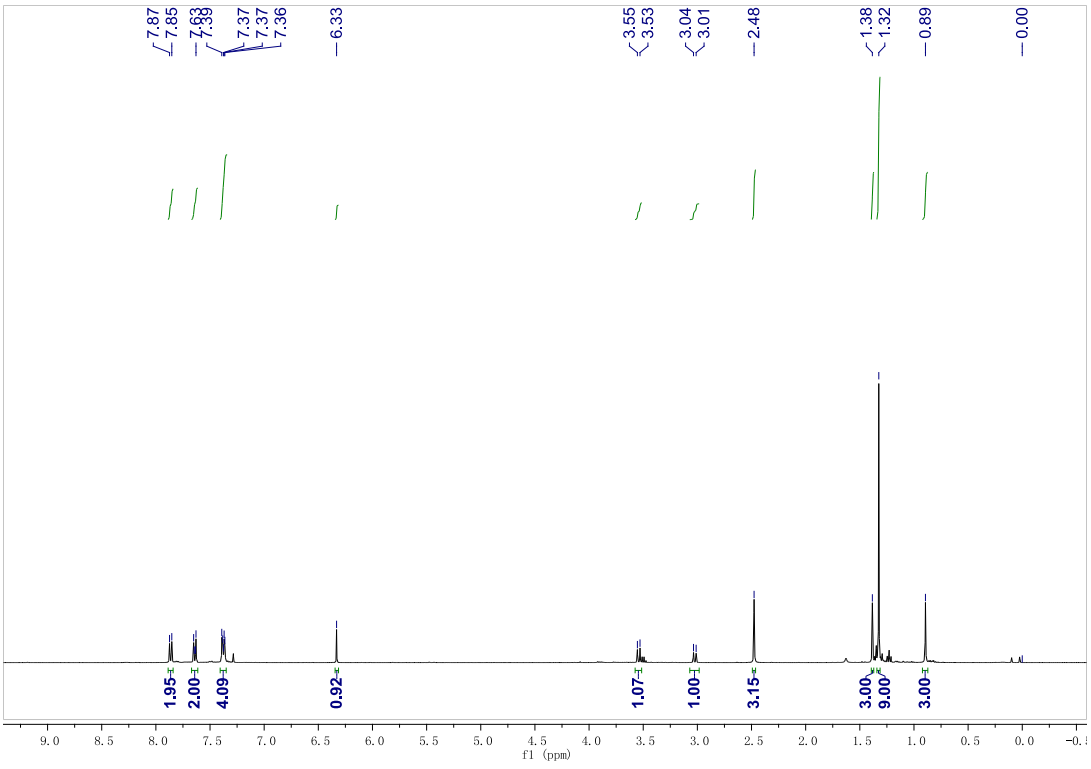
21.59
f1 (ppm)


TsN
Cl
O
N

8d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3.53
3.04
3.01
2.48
1.38
1.32
0.89
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1.95
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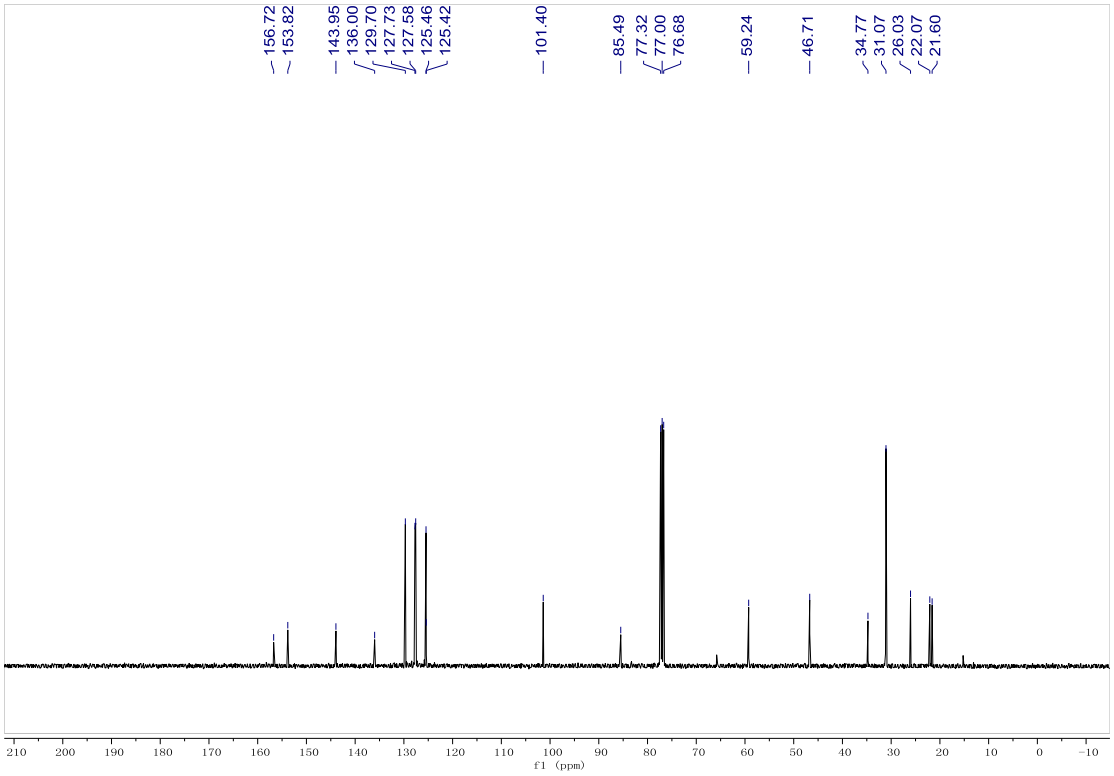
4.09
0.92
1.07
1.00
3.15
3.00
9.00
3.00
f1 (ppm)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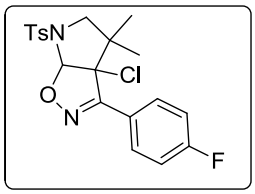
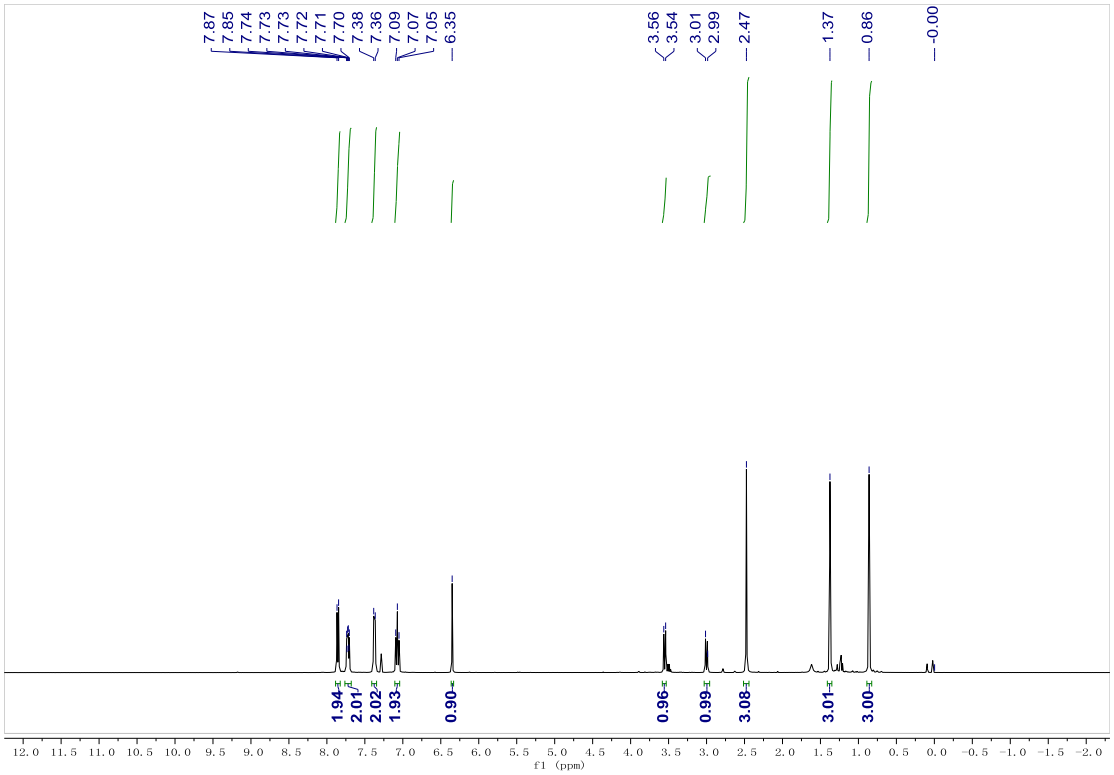
31.07
26.03
22.07
21.60
f1 (ppm)


TsN
Cl
O
N
F

8e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3.56
3.54
3.01
2.99
2.47
1.37
0.86
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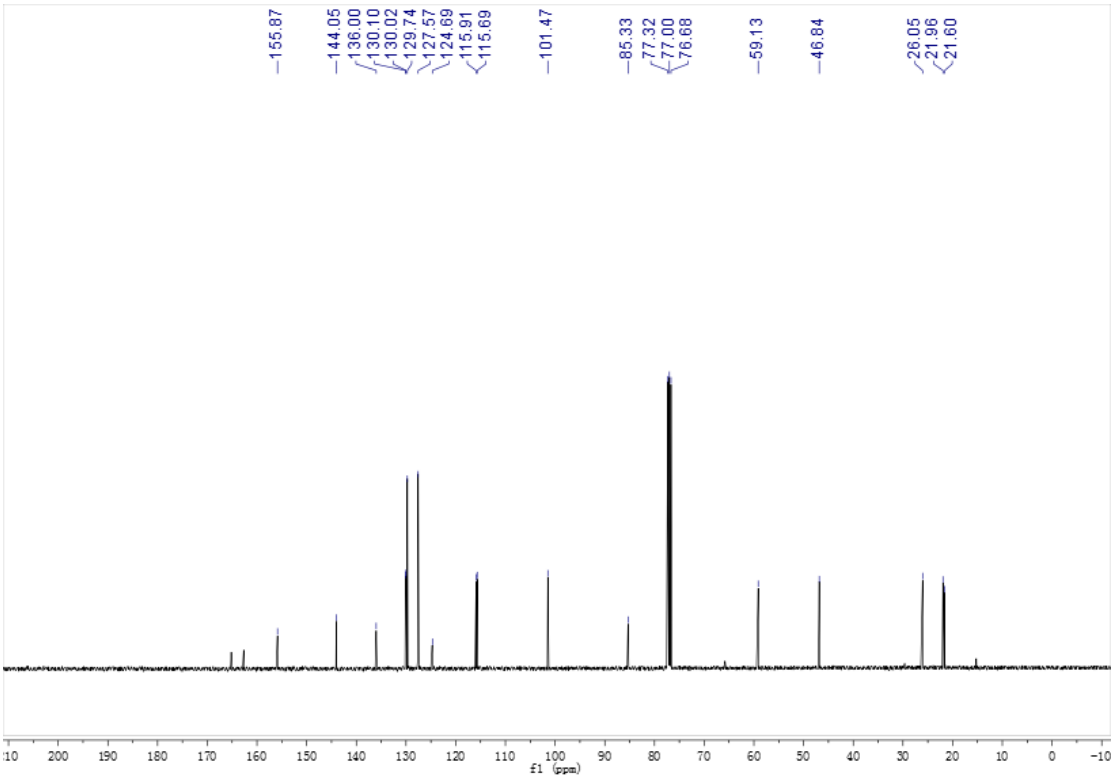
2.02
1.93
0.90
0.96
0.99
3.08
3.01
3.00
f1 (ppm)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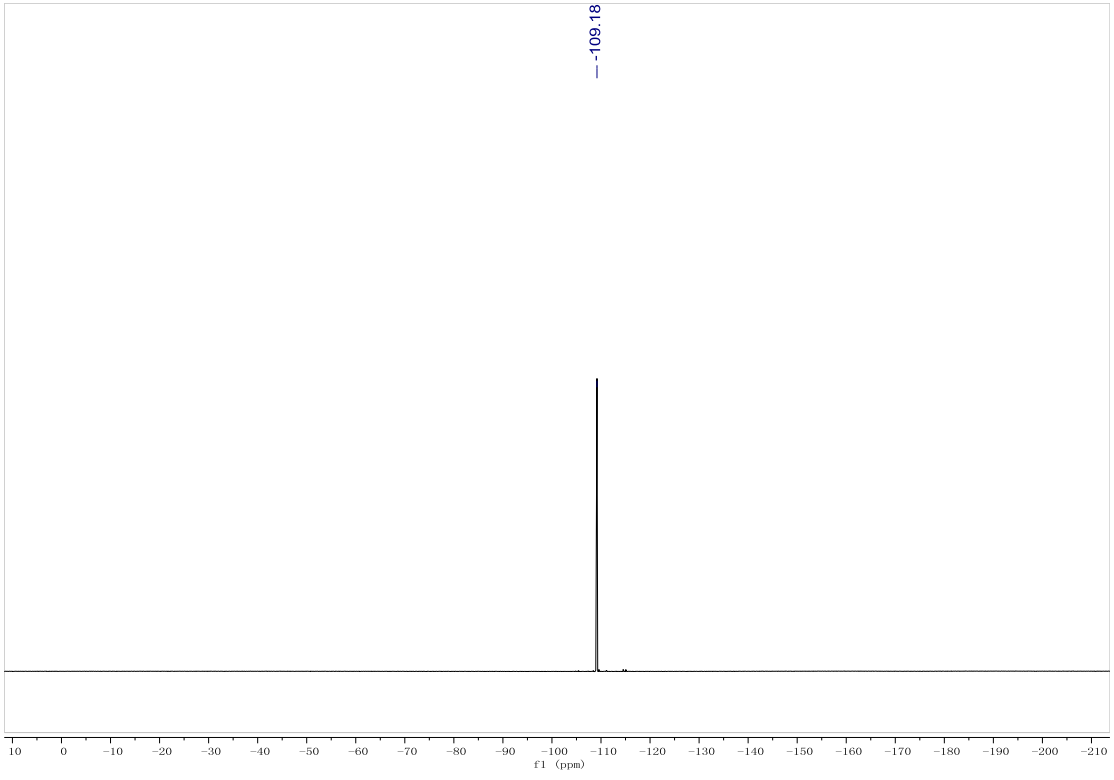
46.84
26.05
21.96
21.60
f1 (ppm)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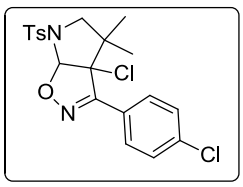
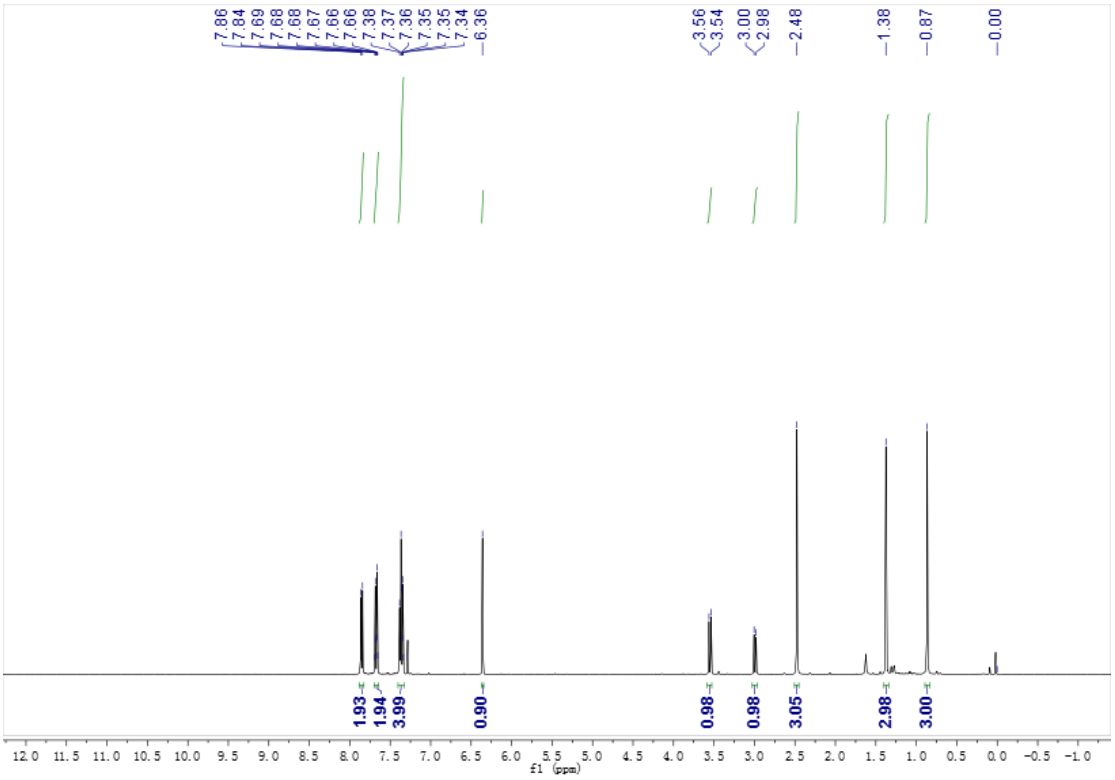

TsN
Cl
O
N
Cl

8f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6.36
3.56
3.54
3.00
2.98
2.48
1.38
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0.90
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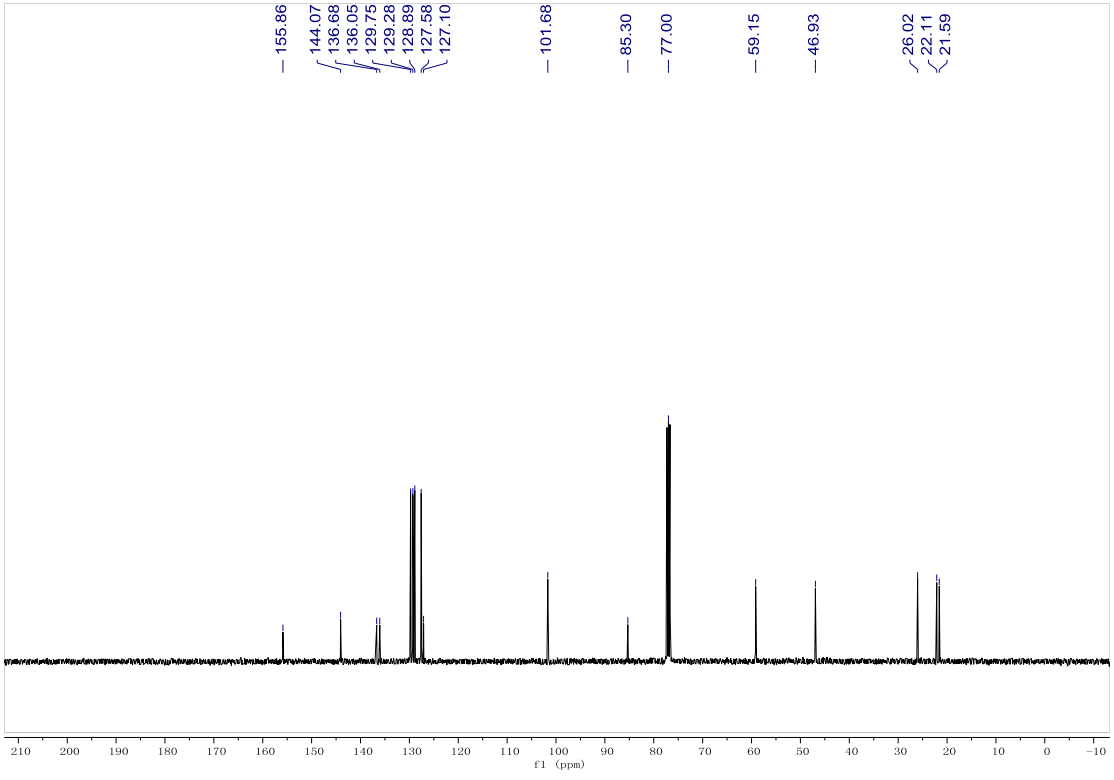
0.98
3.05
2.98
3.00
f1 (ppm)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77.00
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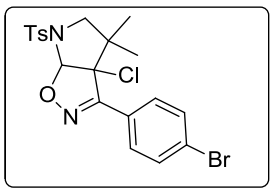
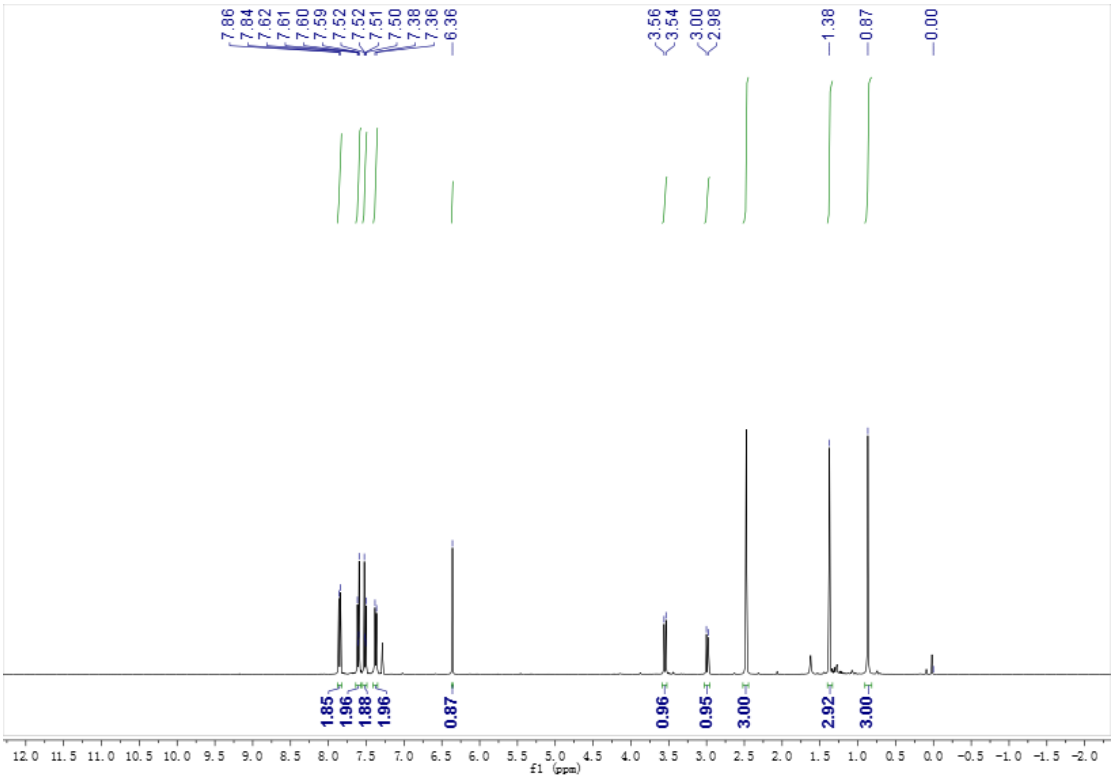
46.93
26.02
22.11
21.59
f1 (ppm)


TsN
Cl
O
N
Br

8g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3.56
3.54
3.00
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1.38
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1.85
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1.96
0.87
0.96
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3.00
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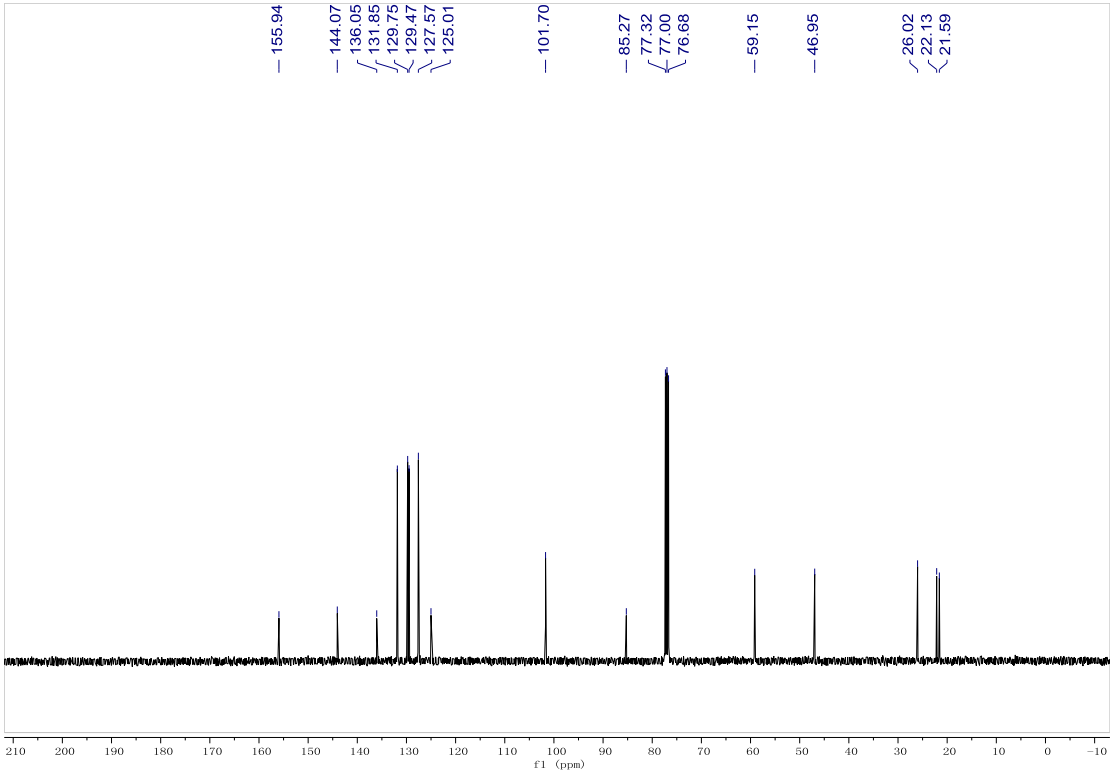
3.00
f1 (ppm)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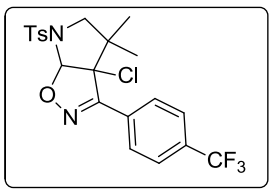
26.02
22.13
21.59
f1 (ppm)


TsN
Cl
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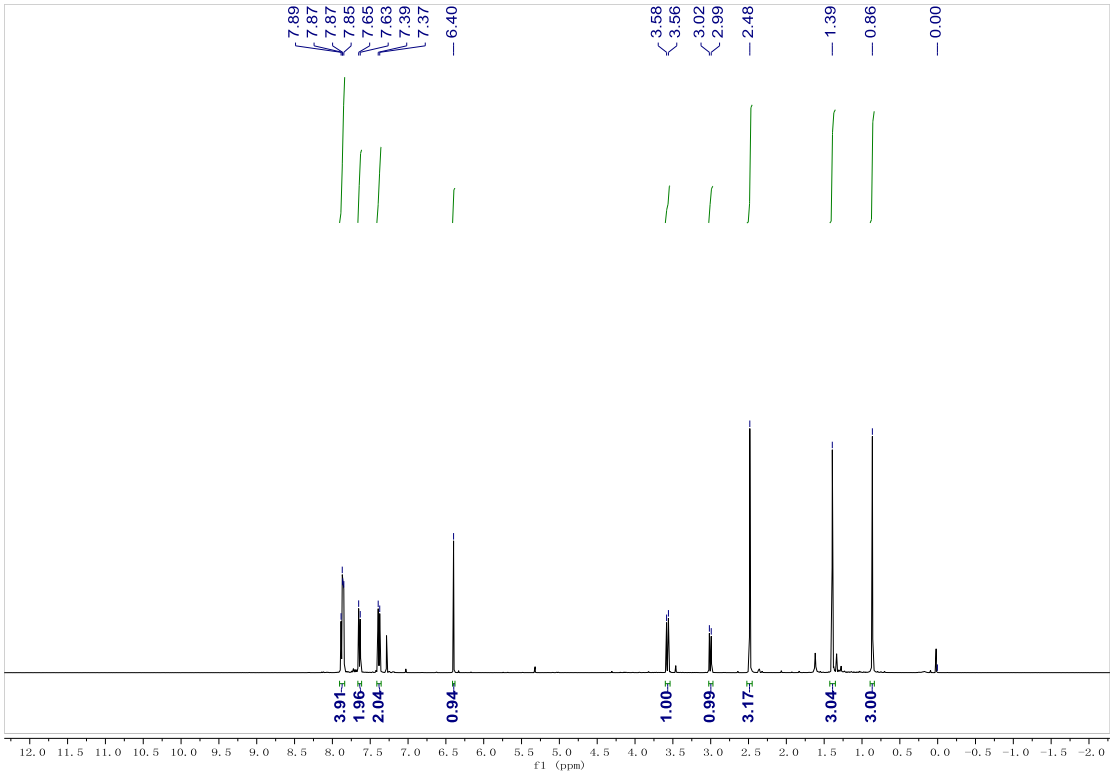
N
CF3

8h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7.37
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3.58
3.56
3.02
2.99
2.48
1.39
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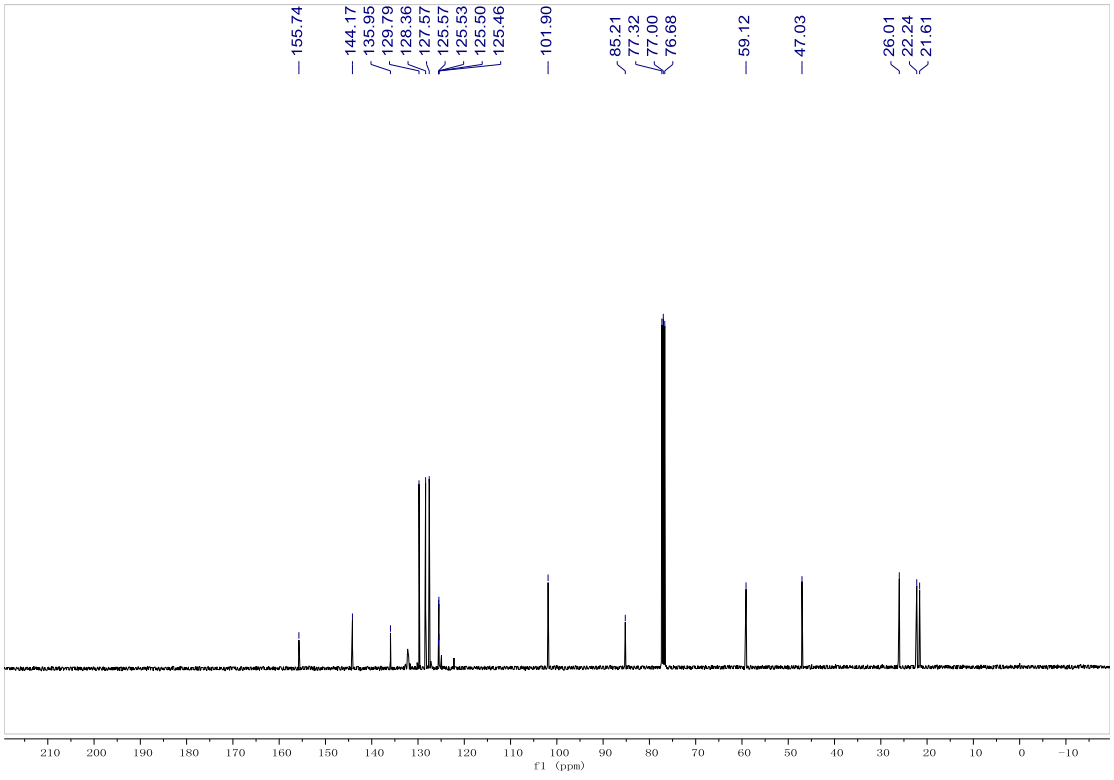
2.04
0.94
1.00
0.99
3.17
3.04
3.00
f1 (ppm)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125.57
125.53
125.50
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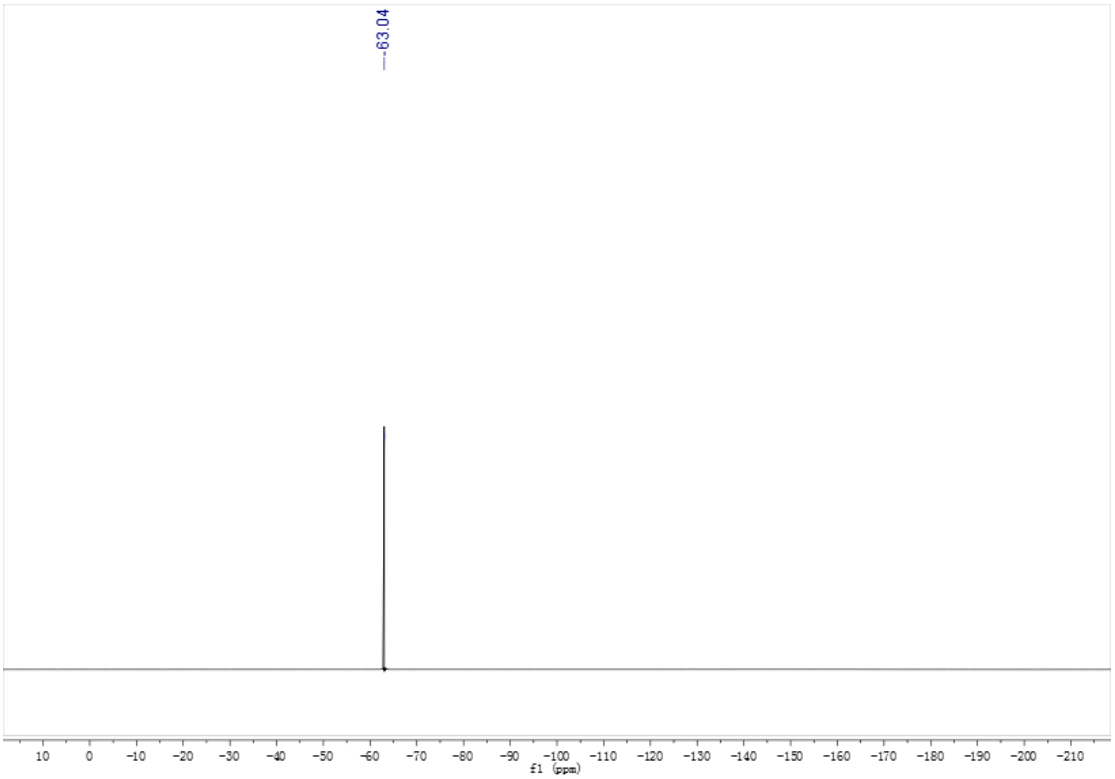
77.00
76.68
59.12
47.03
26.01
22.24
21.61
f1 (ppm)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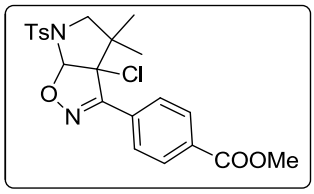
f1 (ppm)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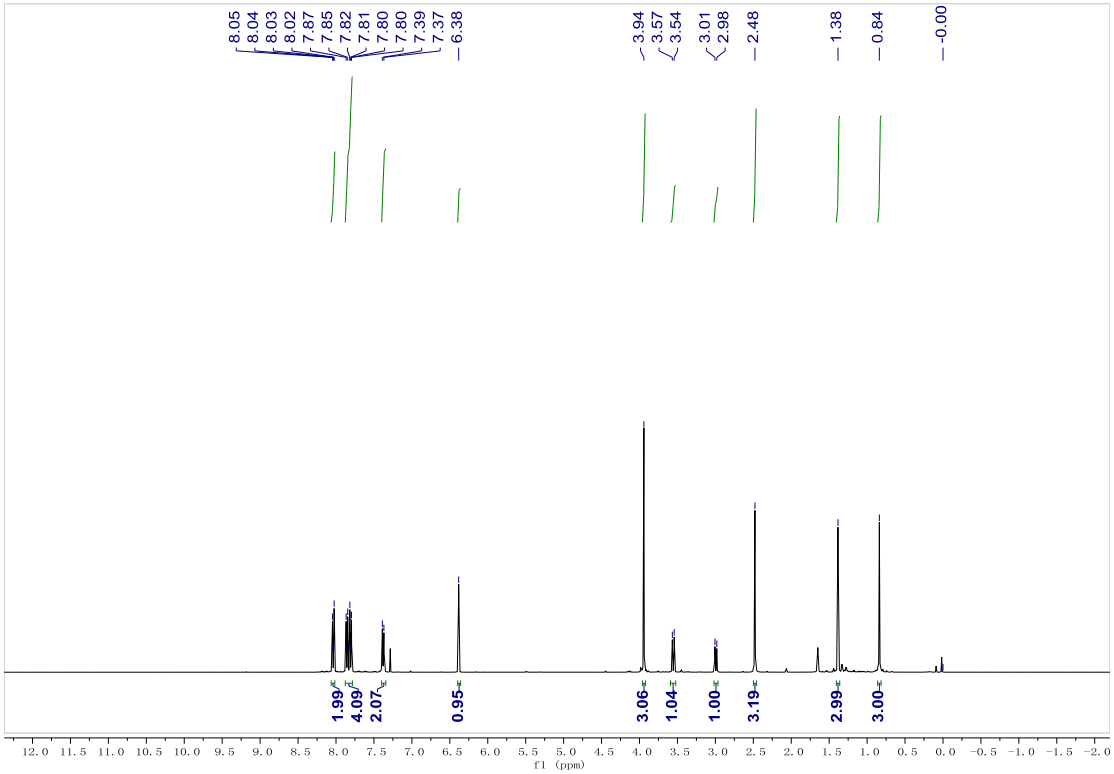
Cl
O
N
COOMe

8i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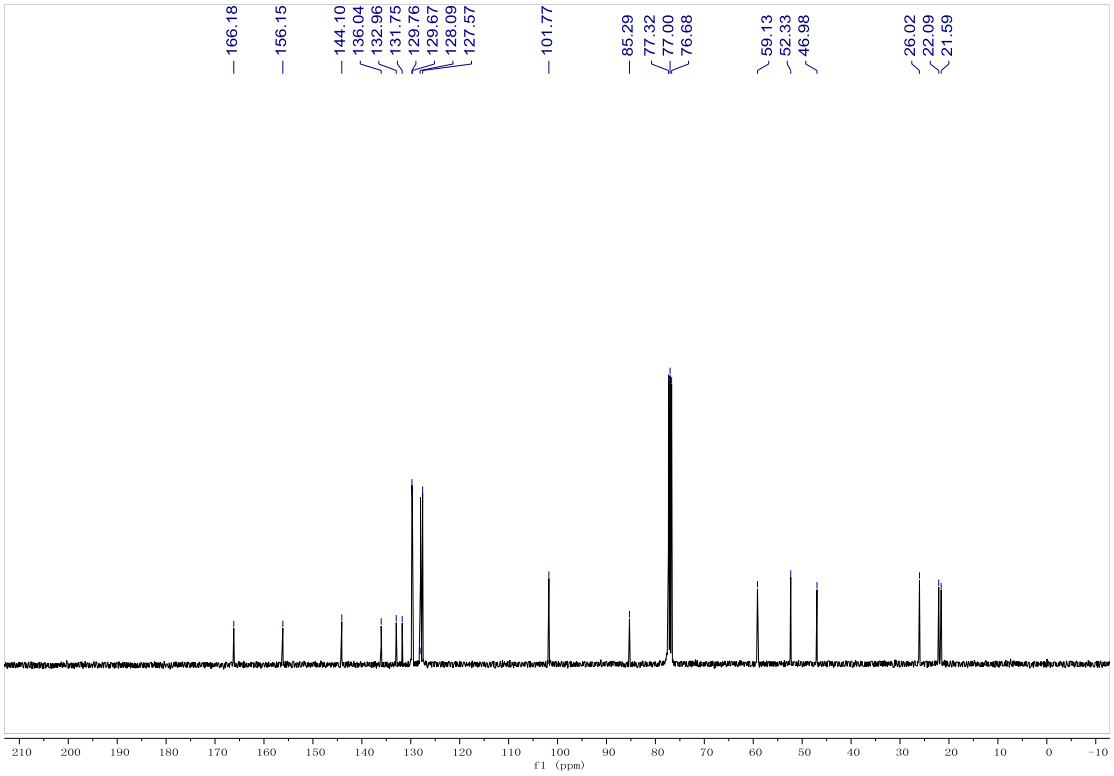
7.80
7.39
7.37
6.38
3.94
3.57
3.54
3.01
2.98
2.48
1.38
0.84
-0.00
1.99
4.09
2.07
0.95
3.06
1.04
1.00
3.19
2.99
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)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129.67
128.09
127.57
101.77
85.29
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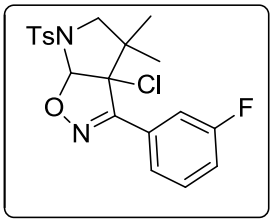
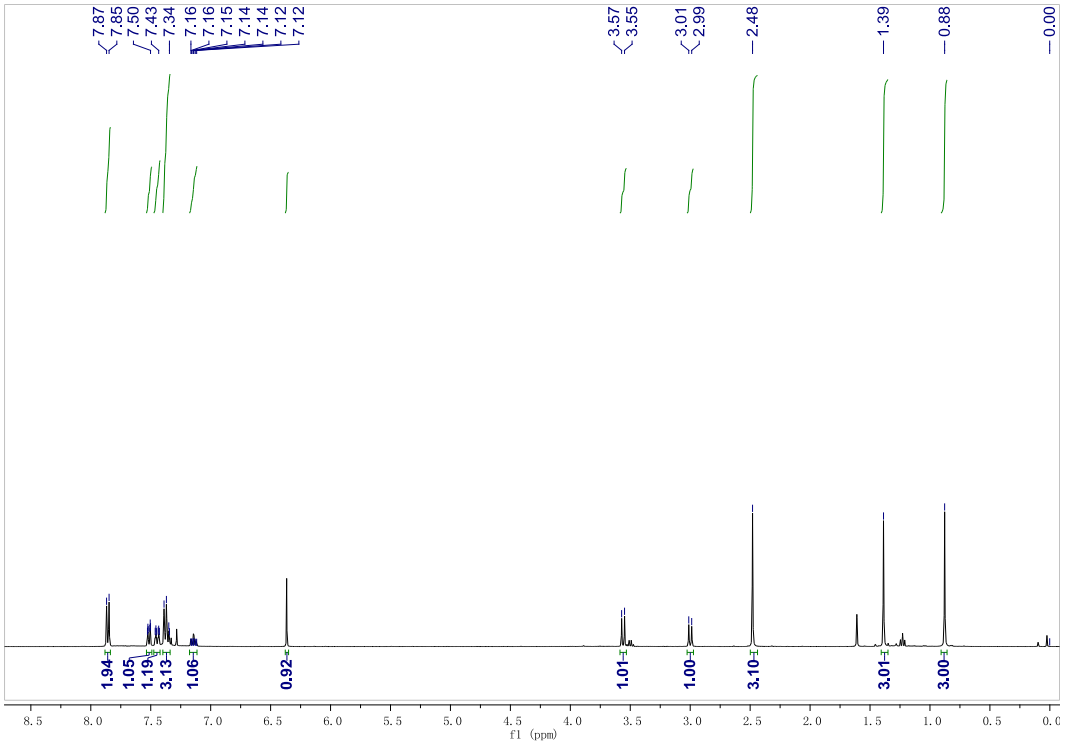
77.00
76.68
59.13
52.33
46.98
26.02
22.09
21.59
f1 (ppm)


TsN
Cl
O
N
F

8j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7.14
7.12
7.12
3.57
3.55
3.01
2.99
2.48
1.39
0.88
0.00
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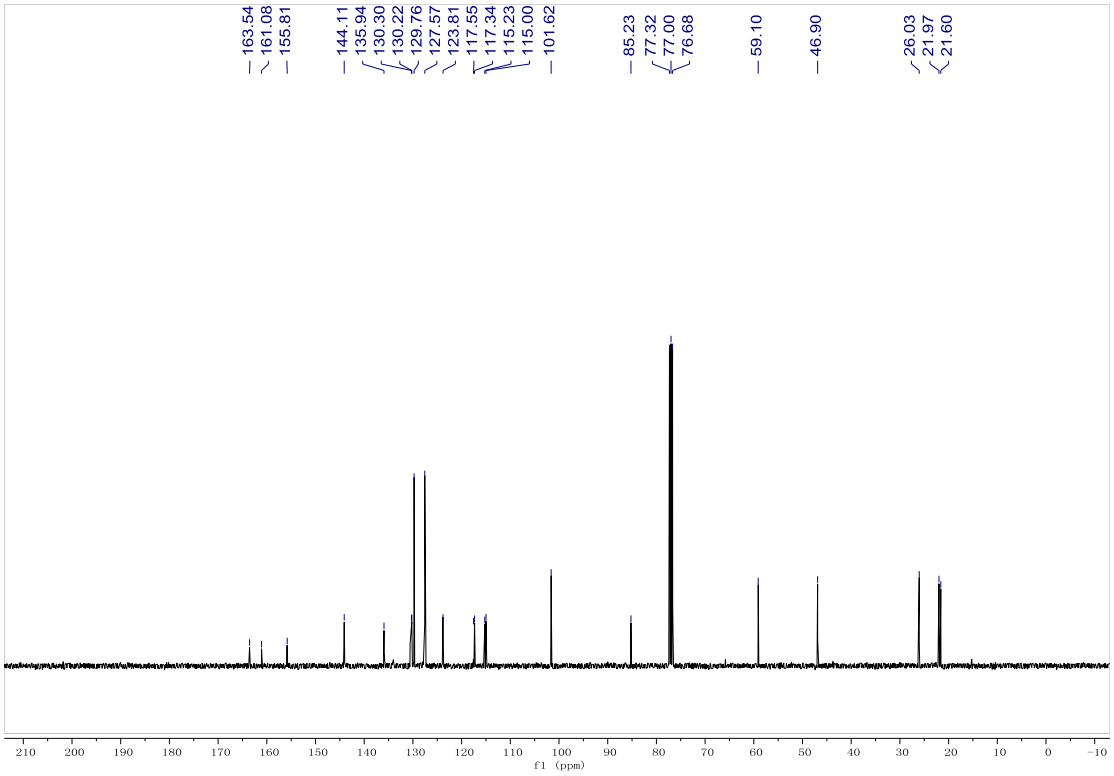
1.05
1.19
3.13
1.06
0.92
1.01
1.00
3.10
3.01
3.00
f1 (ppm)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130.22
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123.81
117.55
117.34
115.23
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101.62
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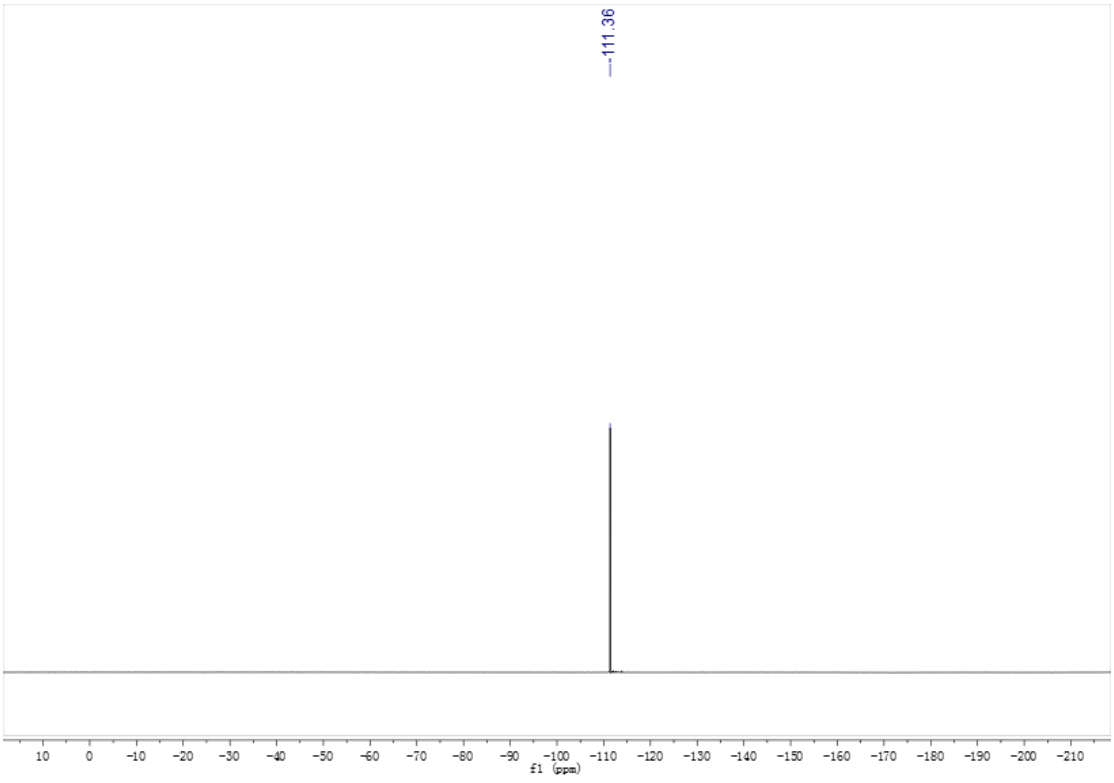
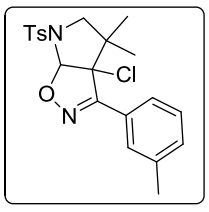
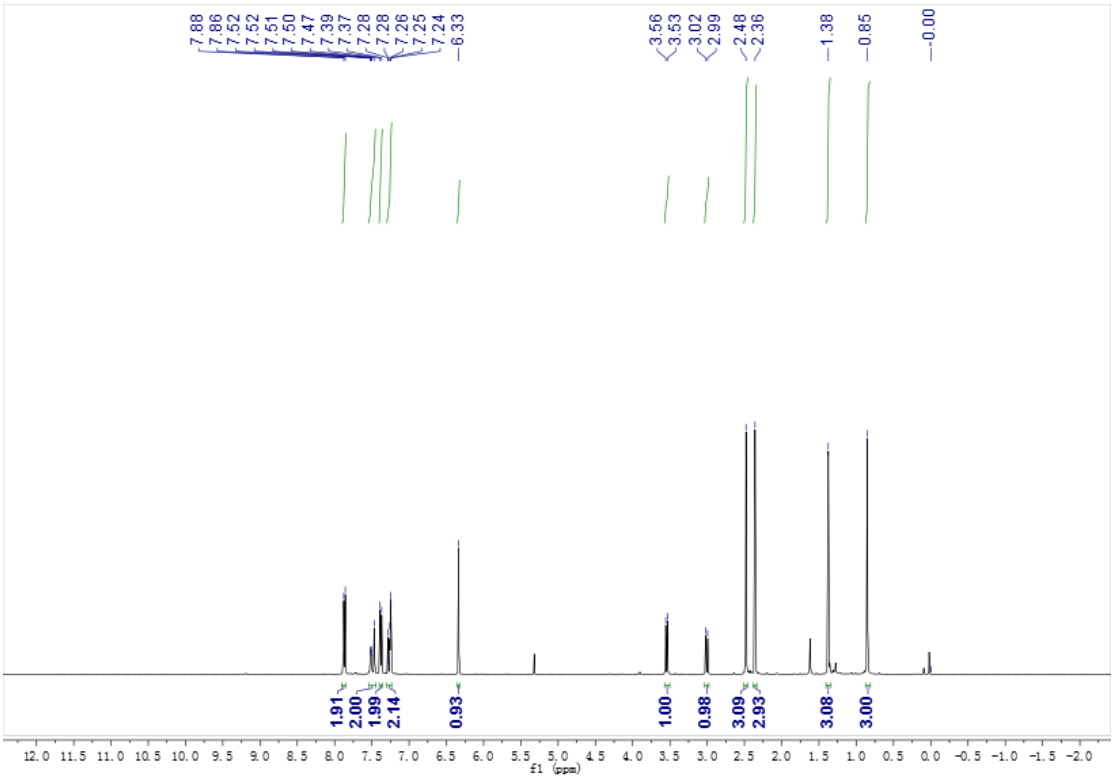
77.32
77.00
76.68
59.10
46.90
26.03
21.97
21.60
f1 (ppm)


111.36
f1 (ppm)


TsN
Cl
O
N

8k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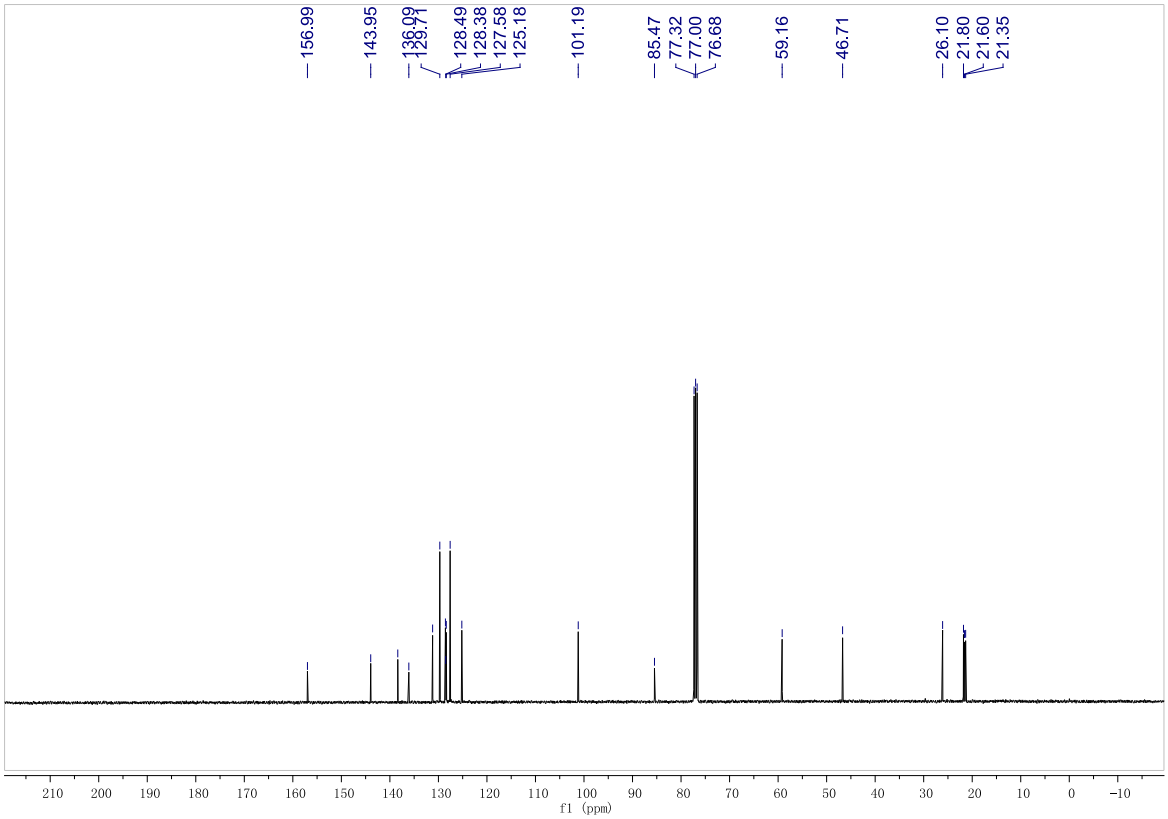
7.28
7.26
7.25
7.24
6.33
3.56
3.53
3.02
2.99
2.48
2.36
1.38
0.85
0.00
1.91
2.00
1.99
2.14
0.93
1.00
0.98
3.09
2.93
3.08
3.00
f1 (ppm)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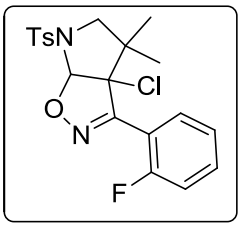
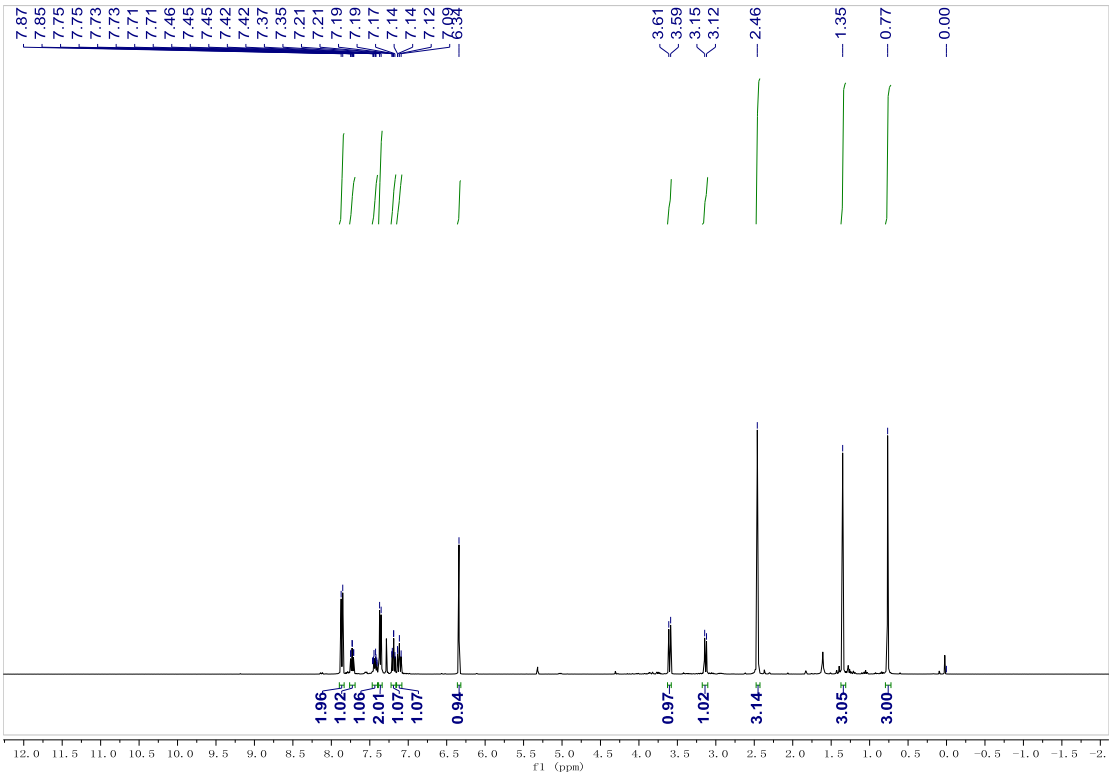
26.10
21.80
21.60
21.35
f1 (ppm)


TsN
Cl
O
N
F

8l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7.21
7.21
7.19
7.19
7.17
7.14
7.14
7.12
7.09
6.94
3.61
3.59
3.15
3.12
2.46
1.35
0.77
0.00
1.96
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1.06
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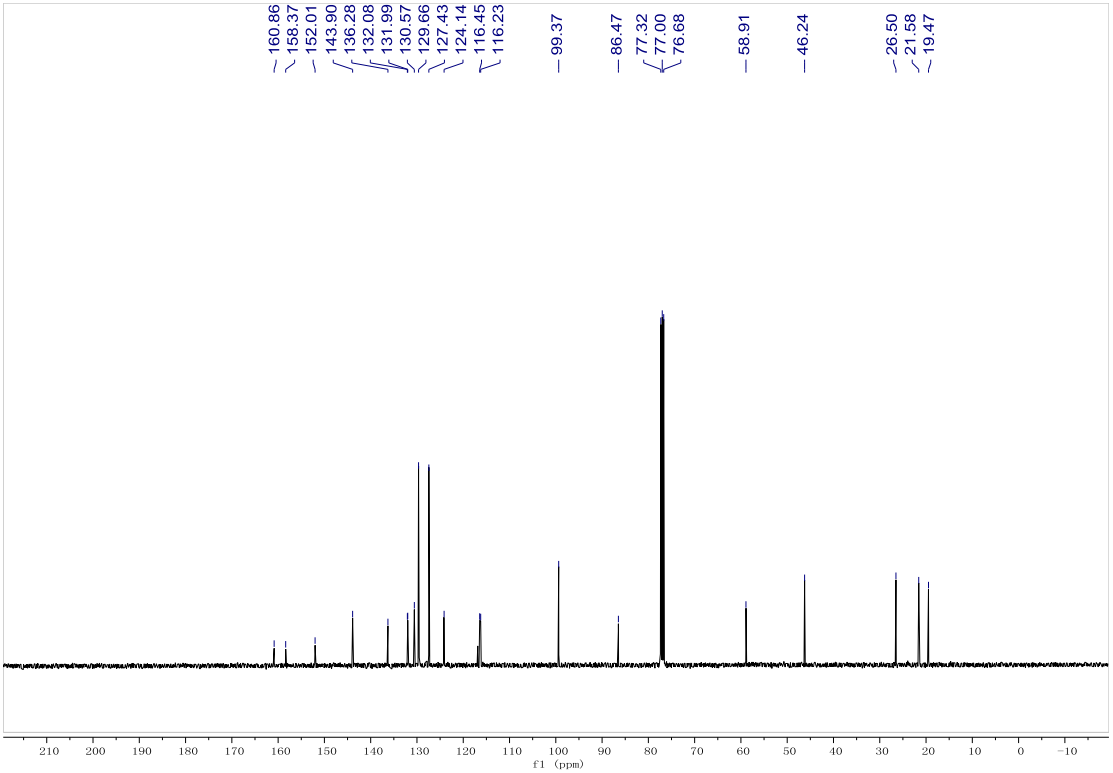
1.07
1.07
0.94
0.97
1.02
3.14
3.05
3.00
f1 (ppm)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132.08
131.99
130.57
129.66
127.43
124.14
116.45
116.23
99.37
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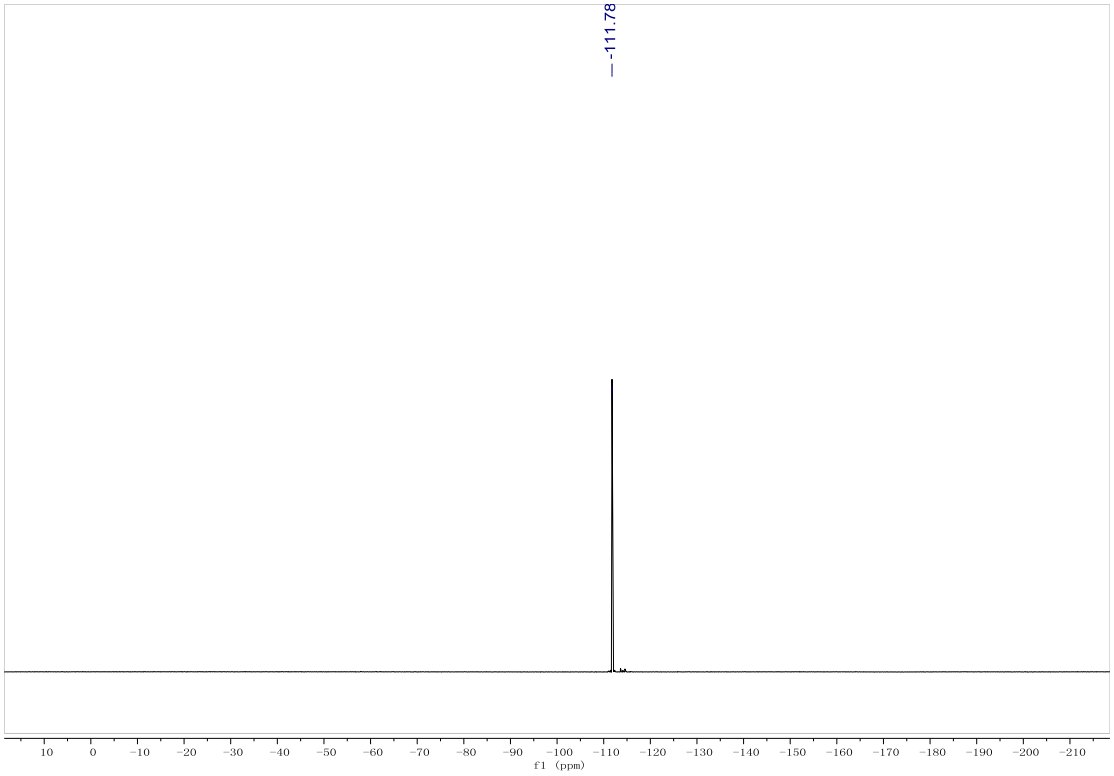
77.32
77.00
76.68
58.91
46.24
26.50
21.58
19.47
f1 (ppm)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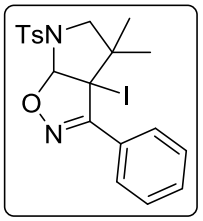
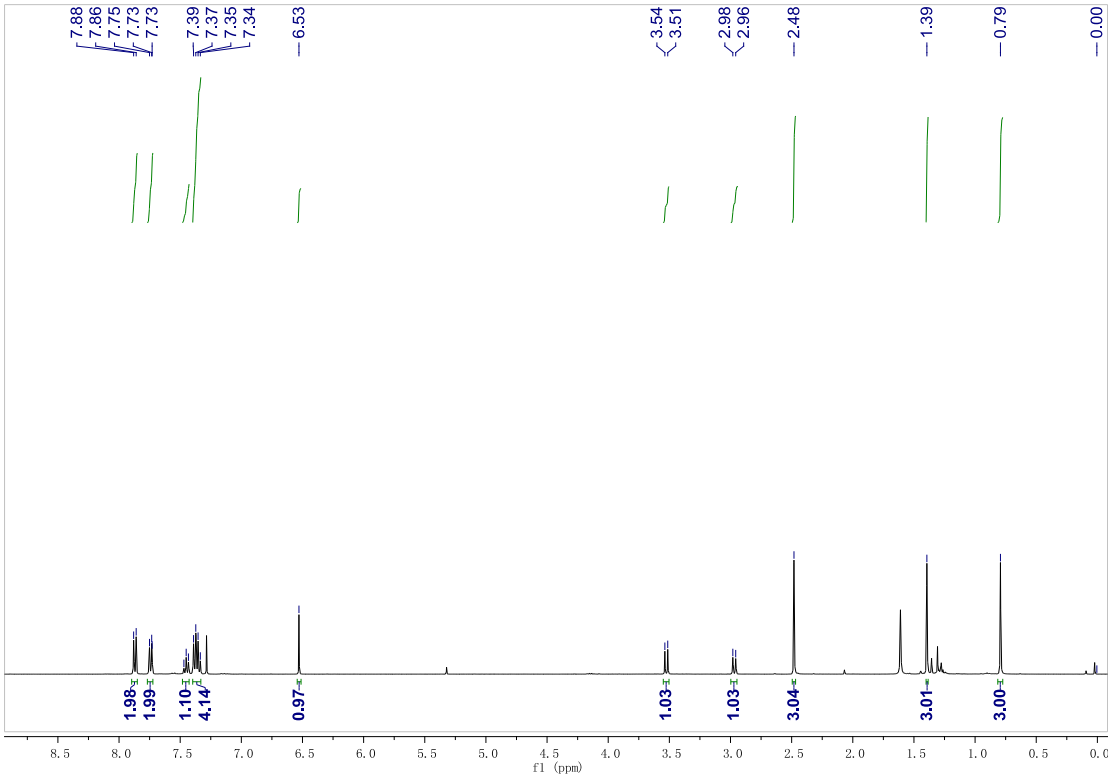
f1 (ppm)


TsN
O
N
I

9a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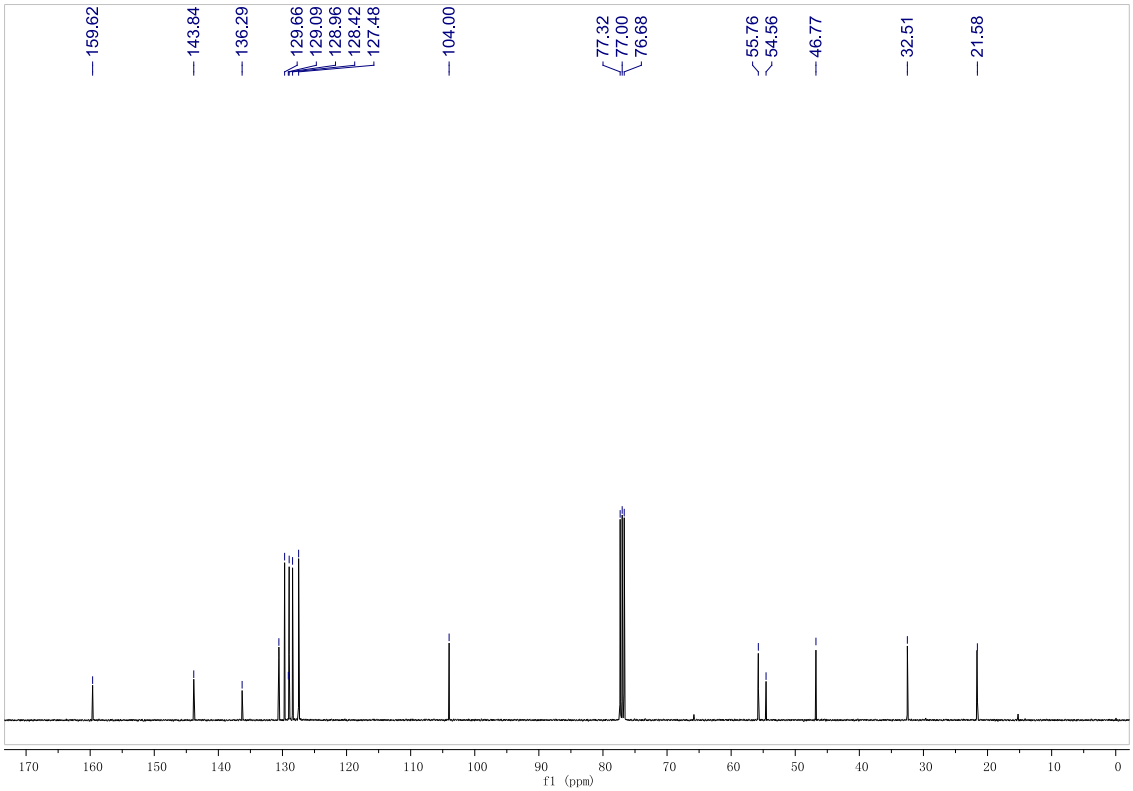
3.51
2.98
2.96
2.48
1.39
0.79
0.00
1.98
1.99
1.10
4.14
0.97
1.03
1.03
3.04
3.01
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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77.32
77.00
76.68
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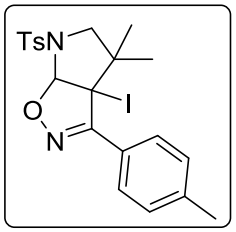
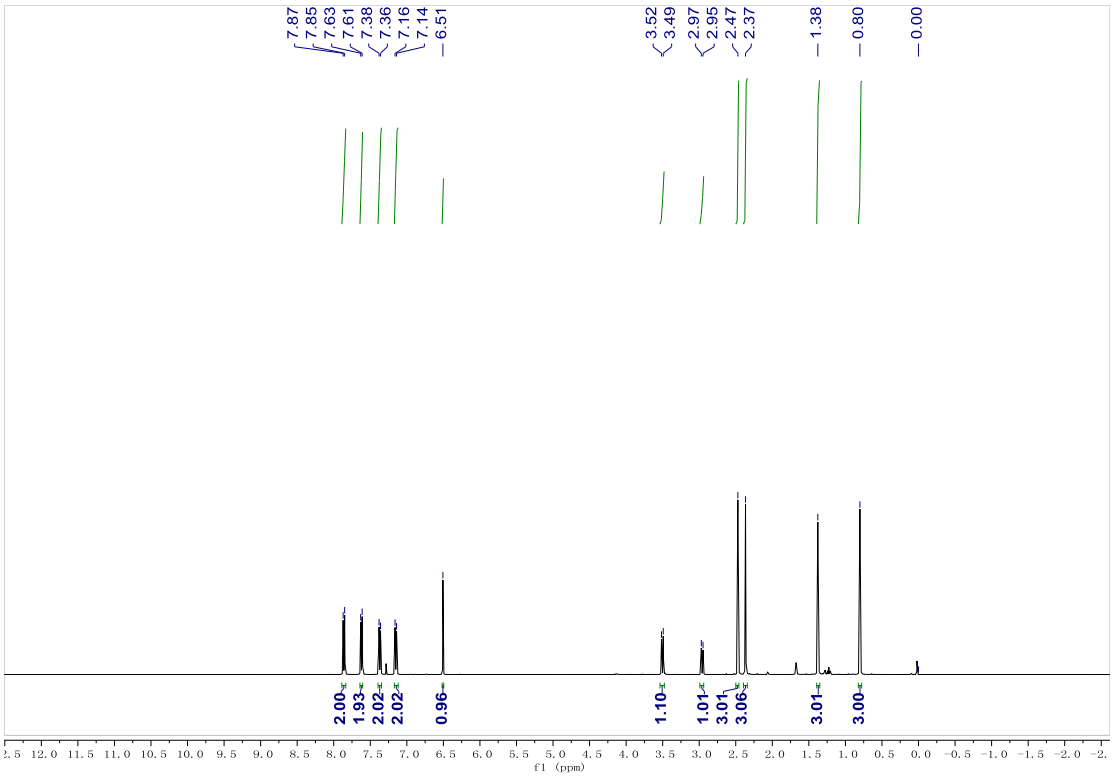
46.77
32.51
21.58
f1 (ppm)


TsN
O
N
I

9b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3.49
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2.95
2.47
2.37
1.38
0.80
0.00
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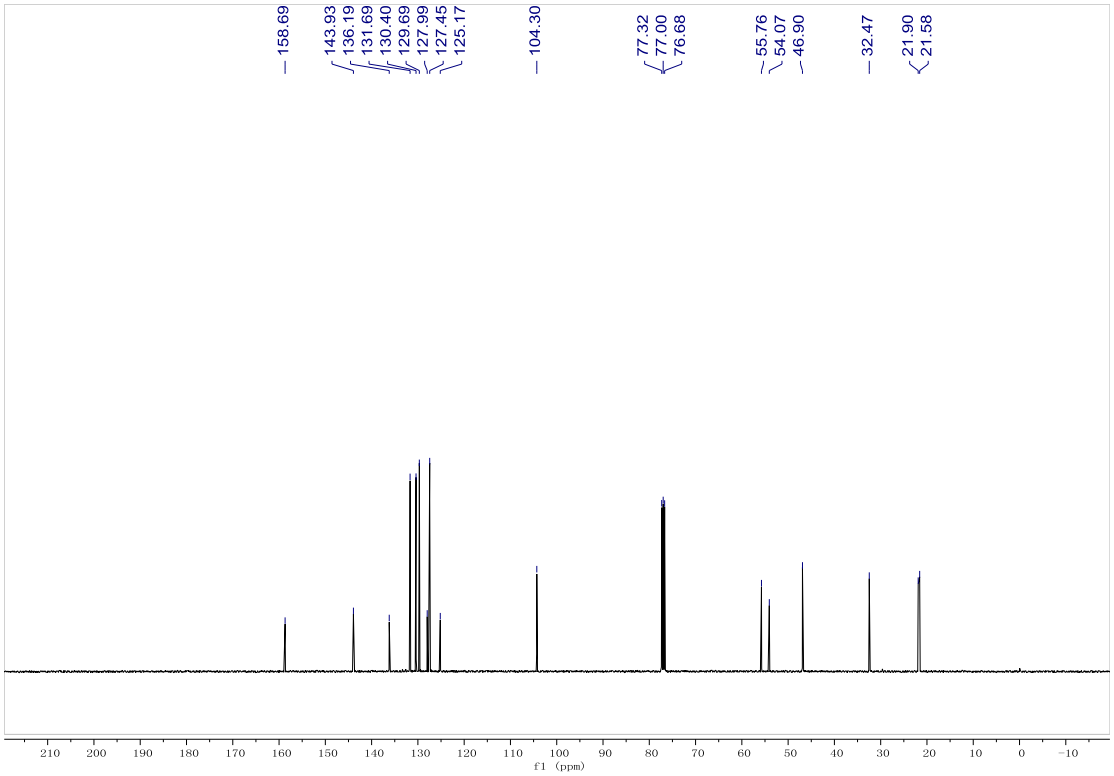
2.02
0.96
1.10
1.01
3.01
3.06
3.01
3.00
f1 (ppm)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129.69
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127.45
125.17
104.30
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77.00
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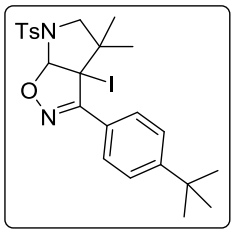
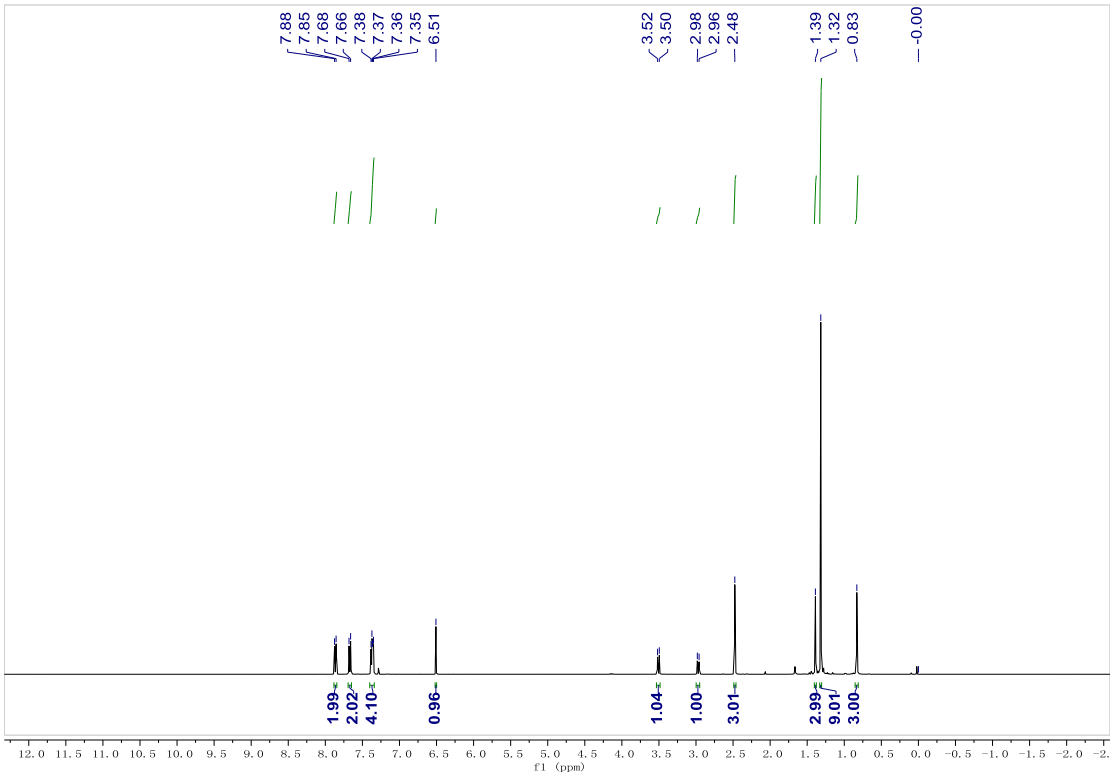
54.07
46.90
32.47
21.90
21.58
f1 (ppm)


TsN
O
N
I

9c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7.35
6.51
3.52
3.50
2.98
2.96
2.48
1.39
1.32
0.83
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1.99
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4.10
0.96
1.04
1.00
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2.99
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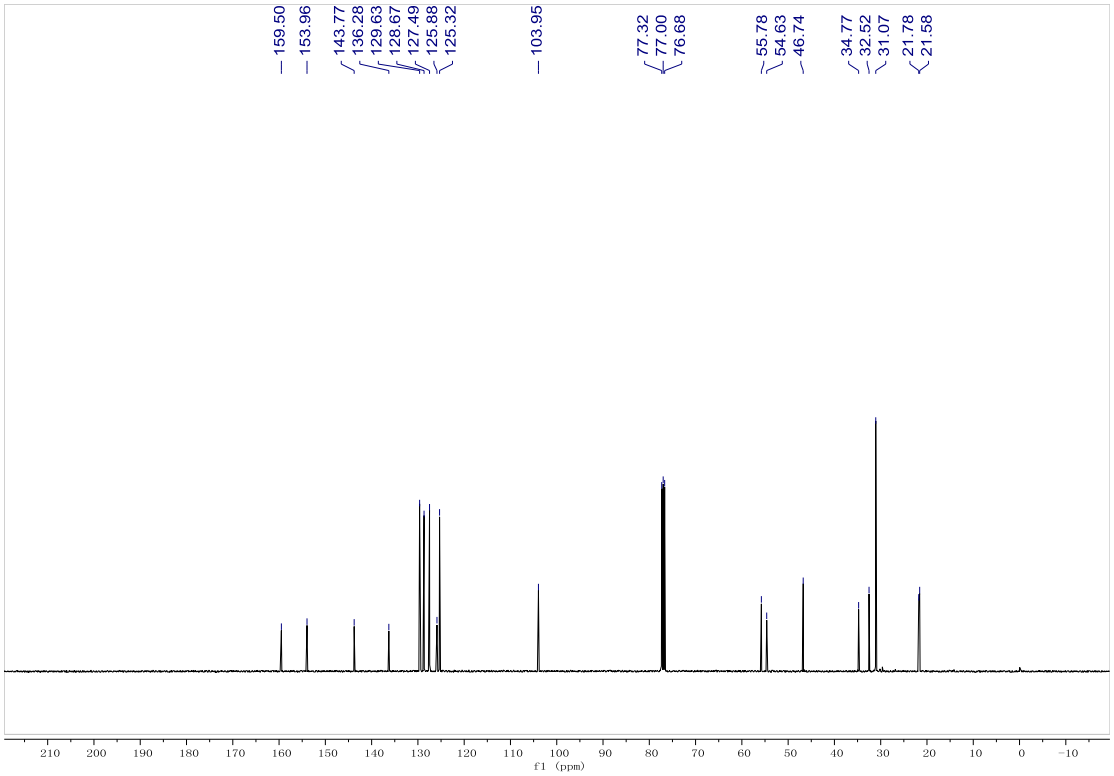
3.00
f1 (ppm)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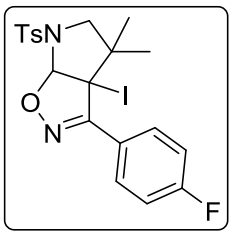
32.52
31.07
21.78
21.58
f1 (ppm)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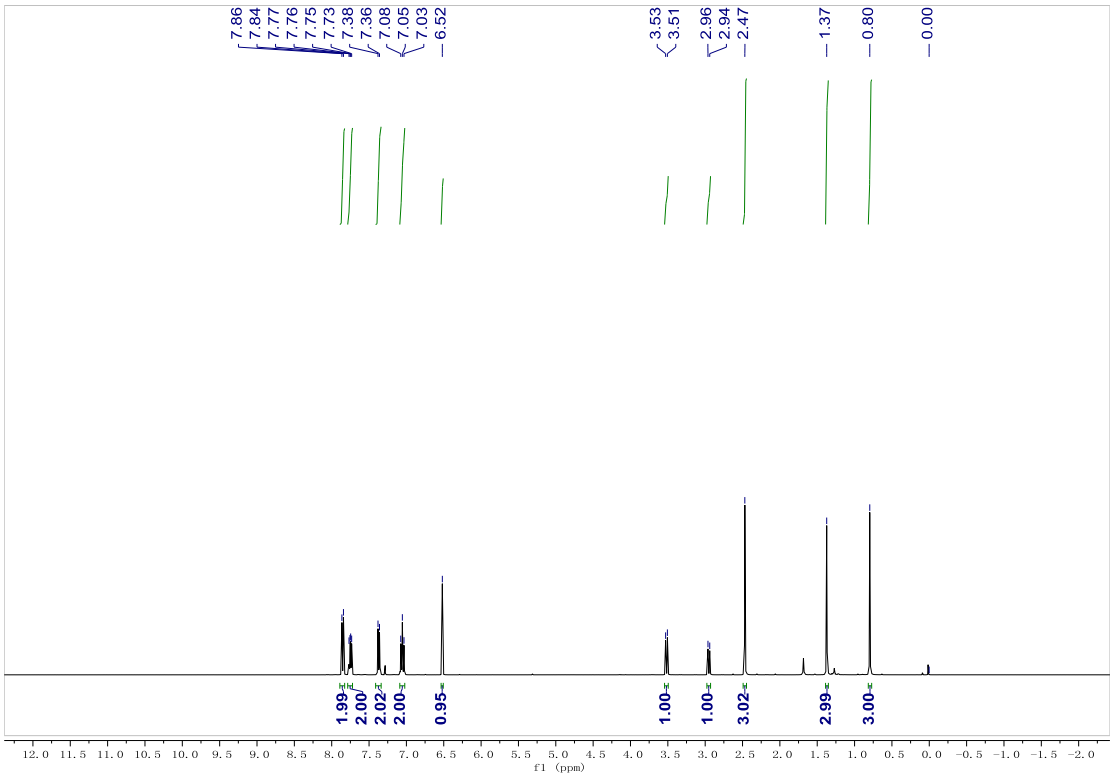
O
N
I
F

9d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6.52
3.53
3.51
2.96
2.94
2.47
1.37
0.80
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0.95
1.00
1.00
3.02
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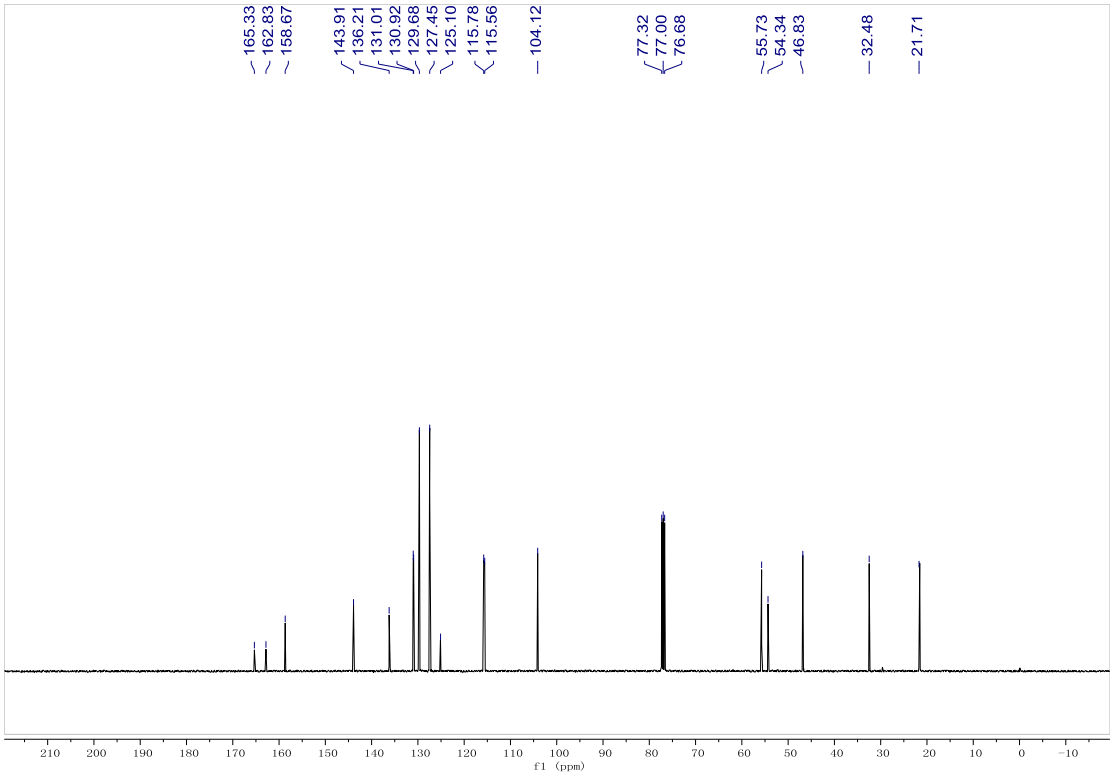
3.00
f1 (ppm)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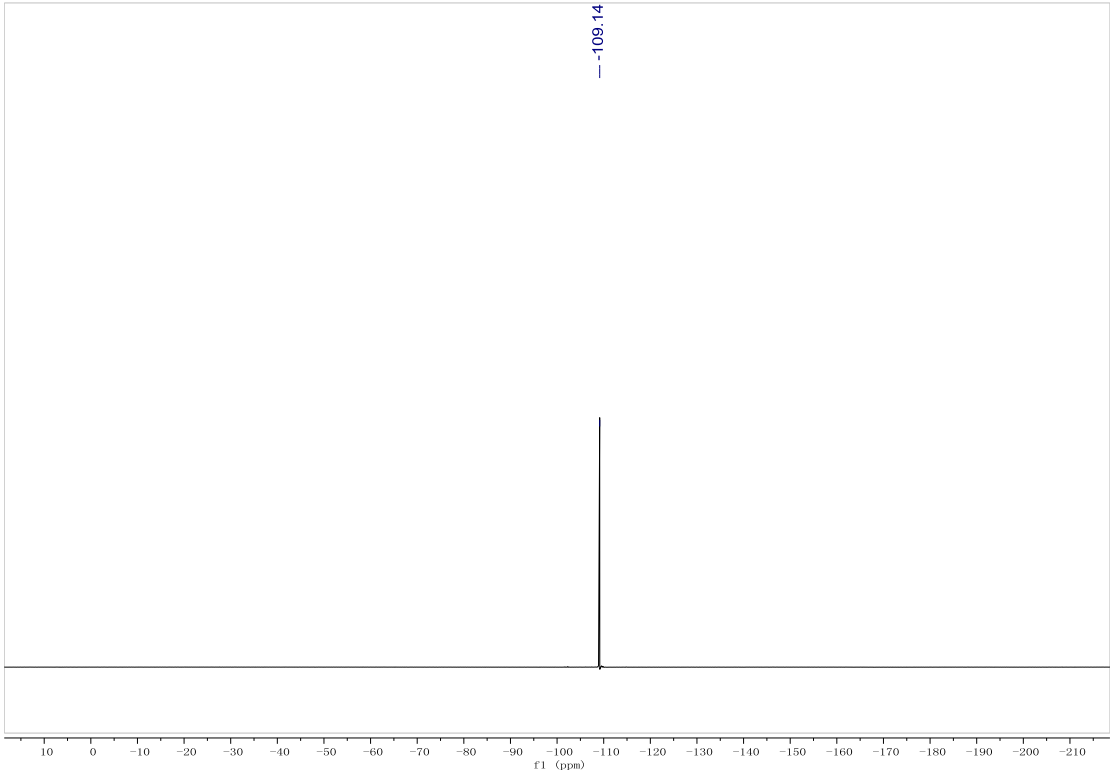
32.48
21.71
f1 (ppm)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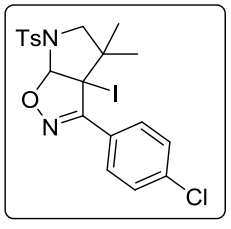
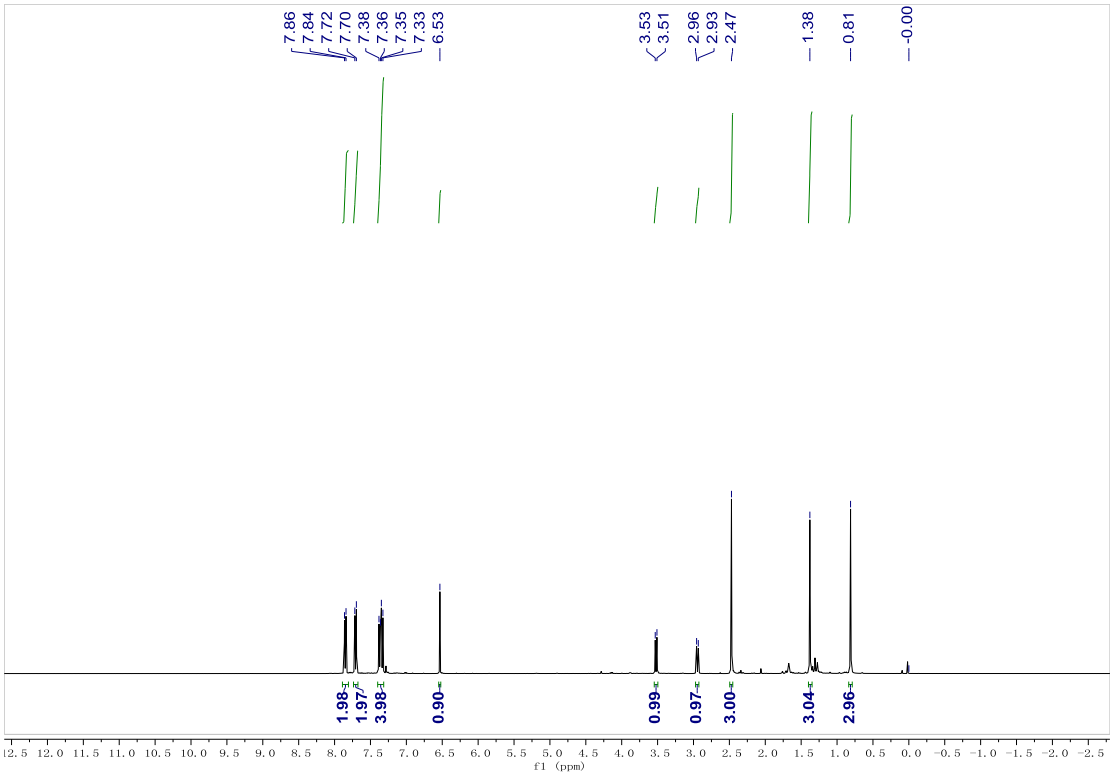

TsN
O
N
I
Cl

9e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3.51
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2.93
2.47
1.38
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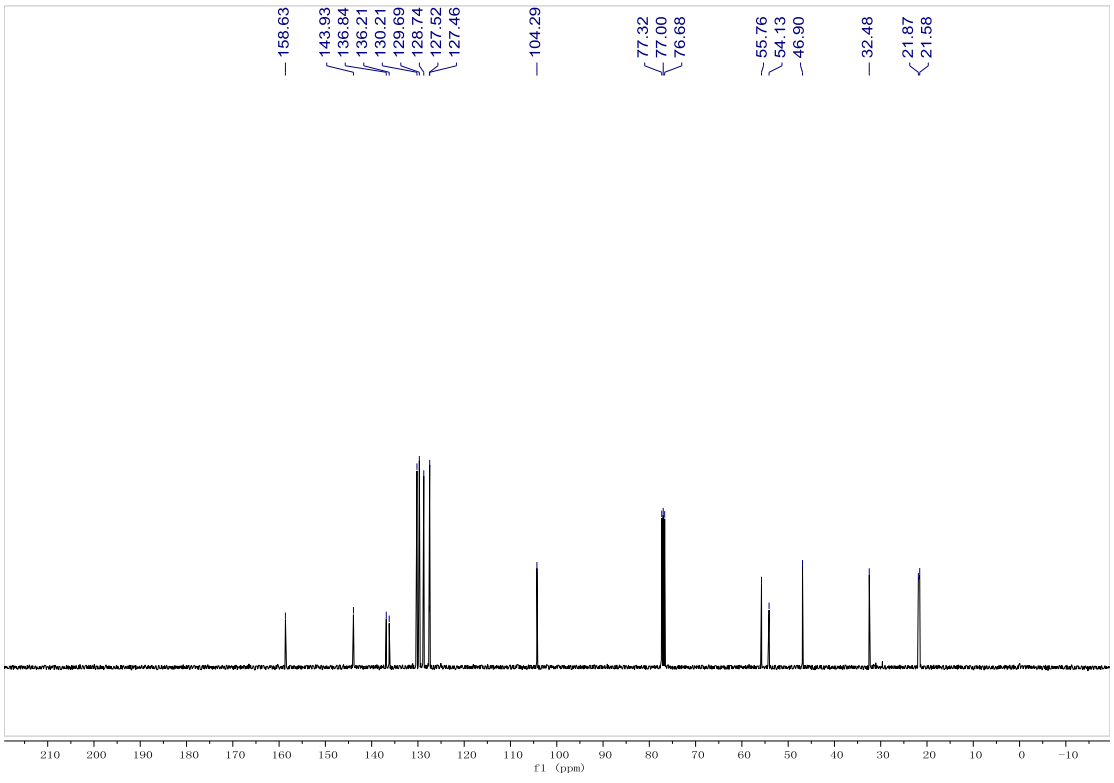
1.97
3.98
0.90
0.99
0.97
3.00
3.04
2.96
f1 (ppm)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104.29
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77.00
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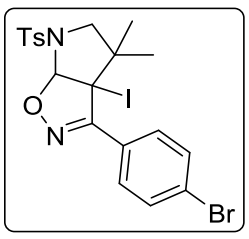
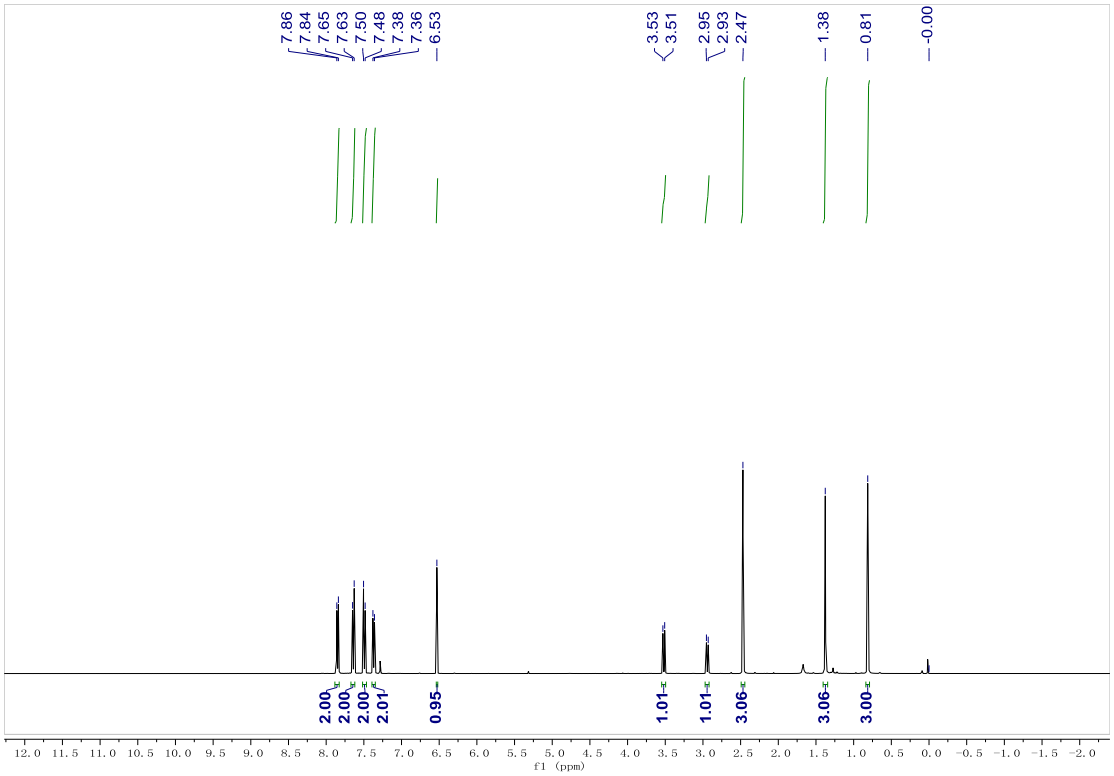
46.90
32.48
21.87
21.58
f1 (ppm)


TsN
O
N
I
Br

9f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6.53
3.53
3.51
2.95
2.93
2.47
1.38
0.81
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1.01
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3.06
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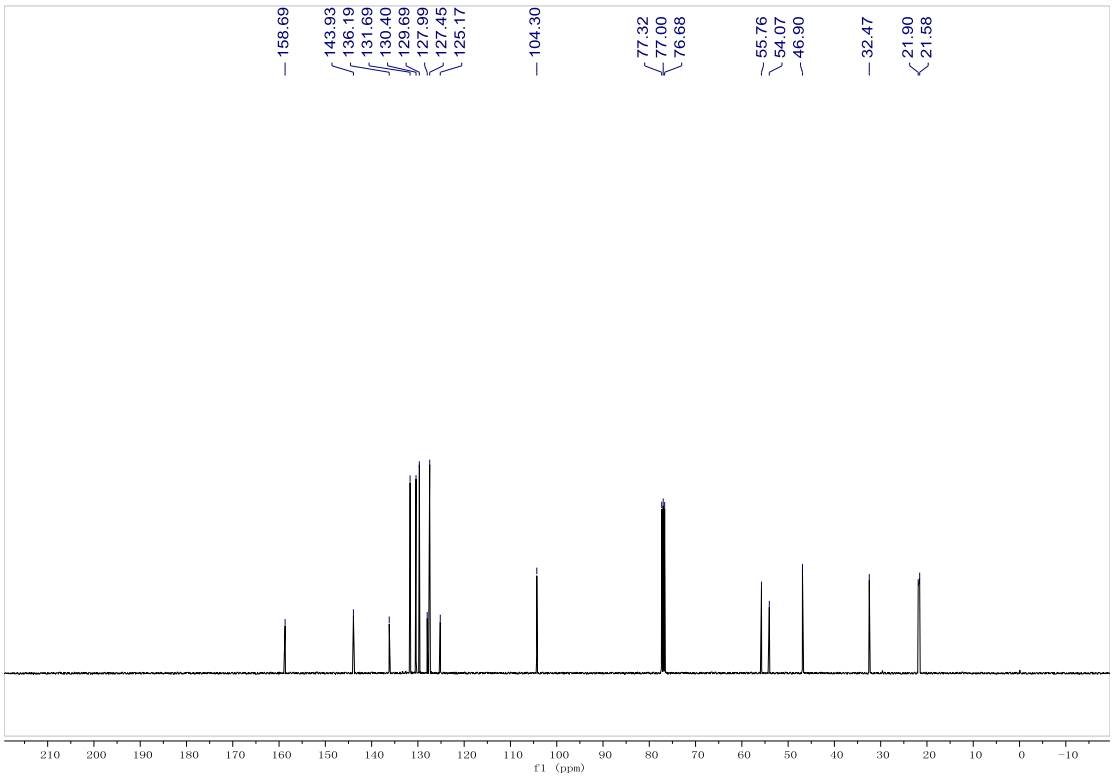
3.00
f1 (ppm)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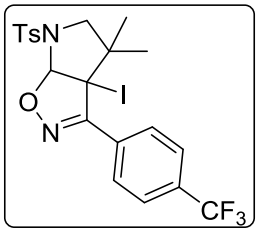
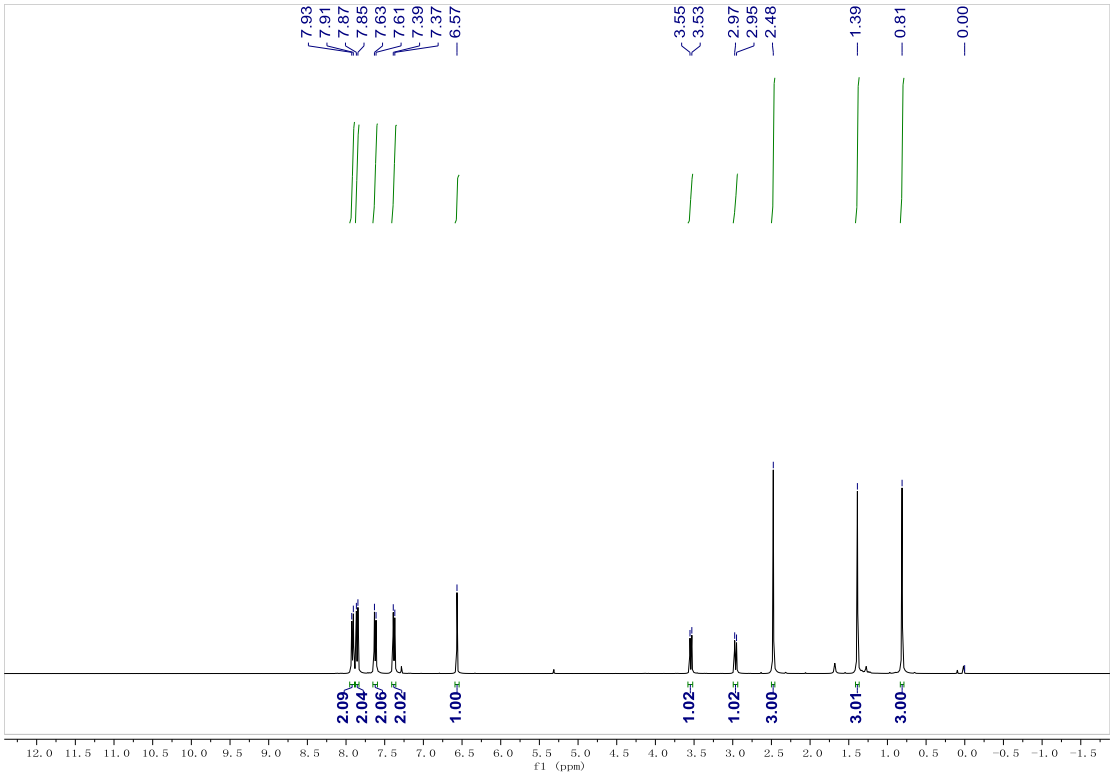
77.00
76.68
55.76
54.07
46.90
32.47
21.90
21.58
f1 (ppm)


TsN
O
N
I
CF3

9g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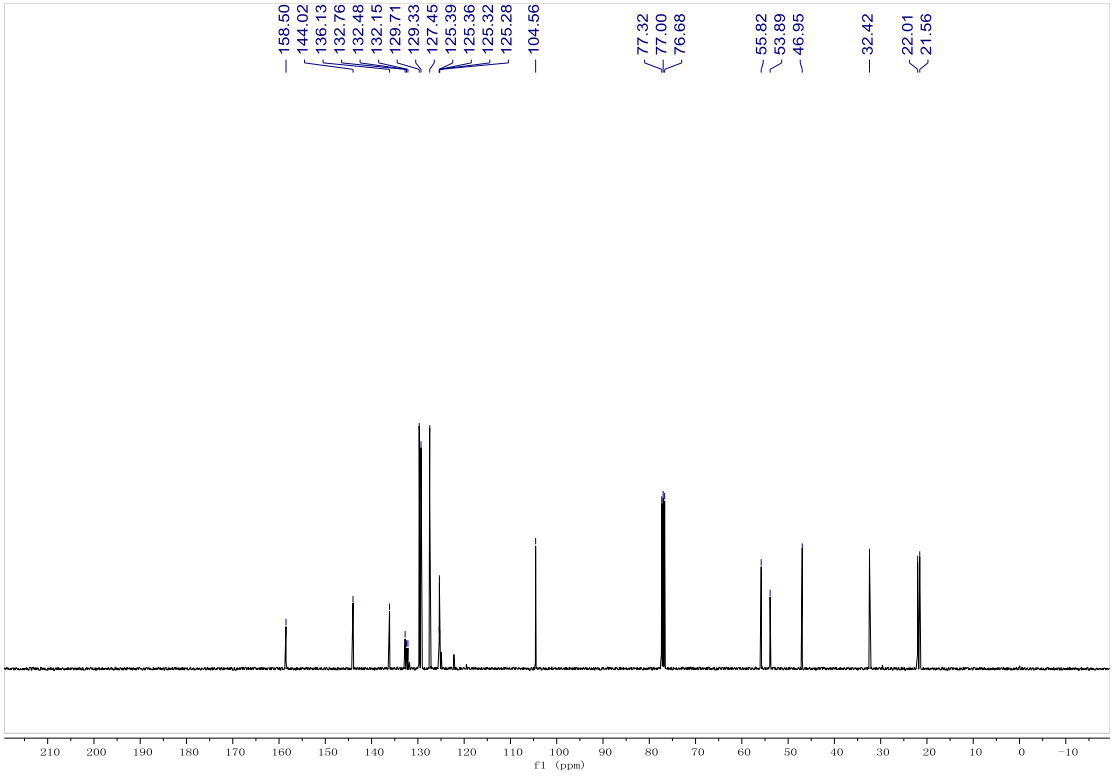
7.87
7.85
7.63
7.61
7.39
7.37
6.57
3.55
3.53
2.97
2.95
2.48
1.39
0.81
0.00
2.09
2.04
2.06
2.02
1.00
1.02
1.02
3.00
3.01
3.00
f1 (ppm)


158.50
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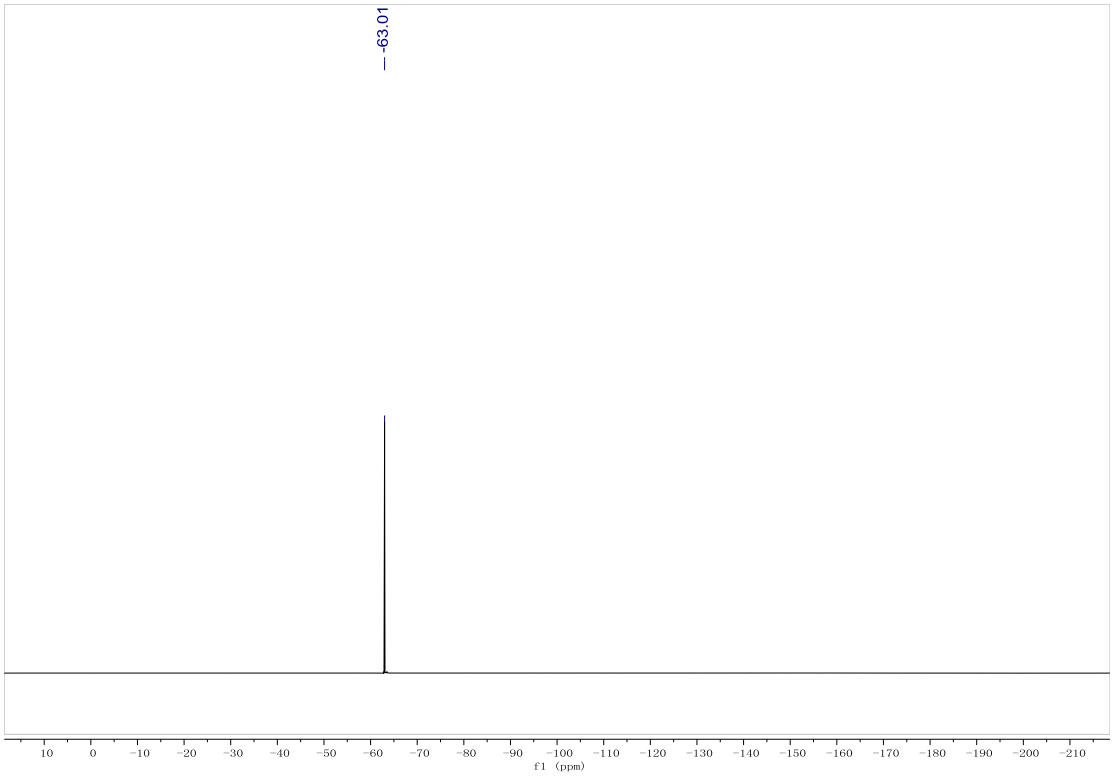
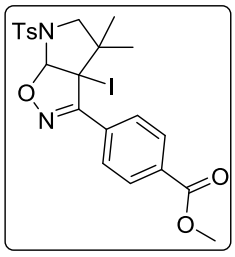
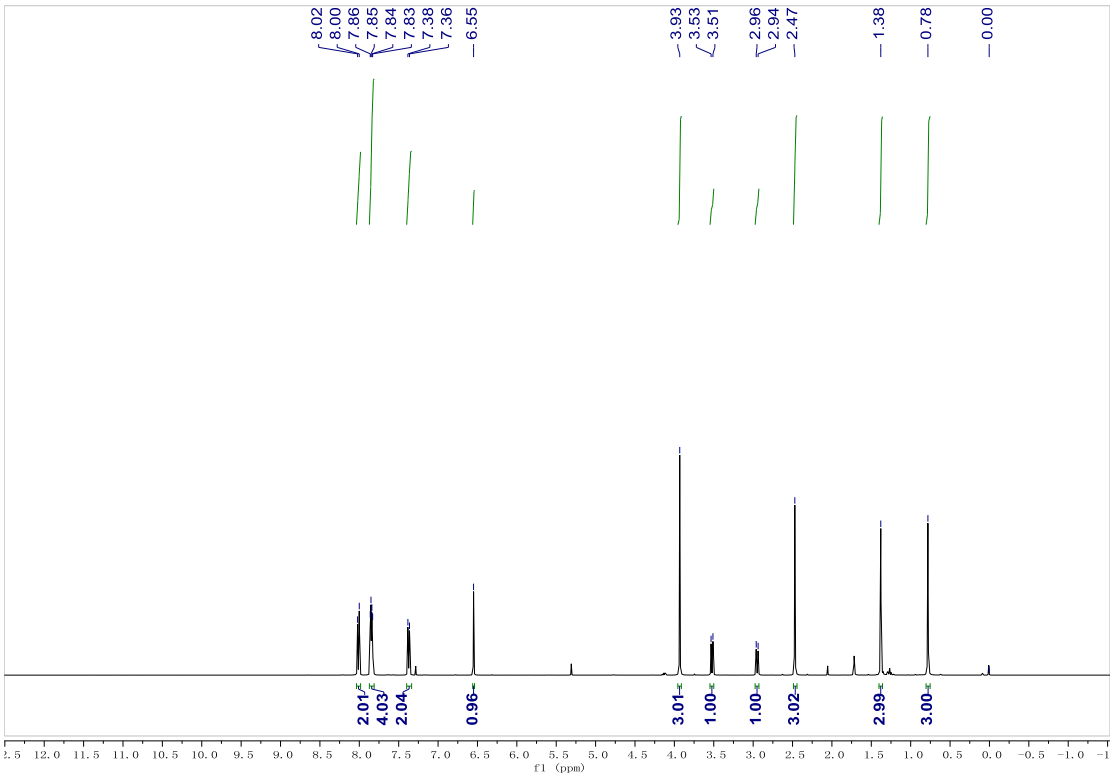
136.13
132.76
132.48
132.15
129.71
129.33
127.45
125.39
125.36
125.32
125.28
104.56
77.32
77.00
76.68
55.82
53.89
46.95
32.42
22.01
21.56
f1 (ppm)


-63.01
f1 (ppm)


TsN
O
N
I
O
O

9h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8.00
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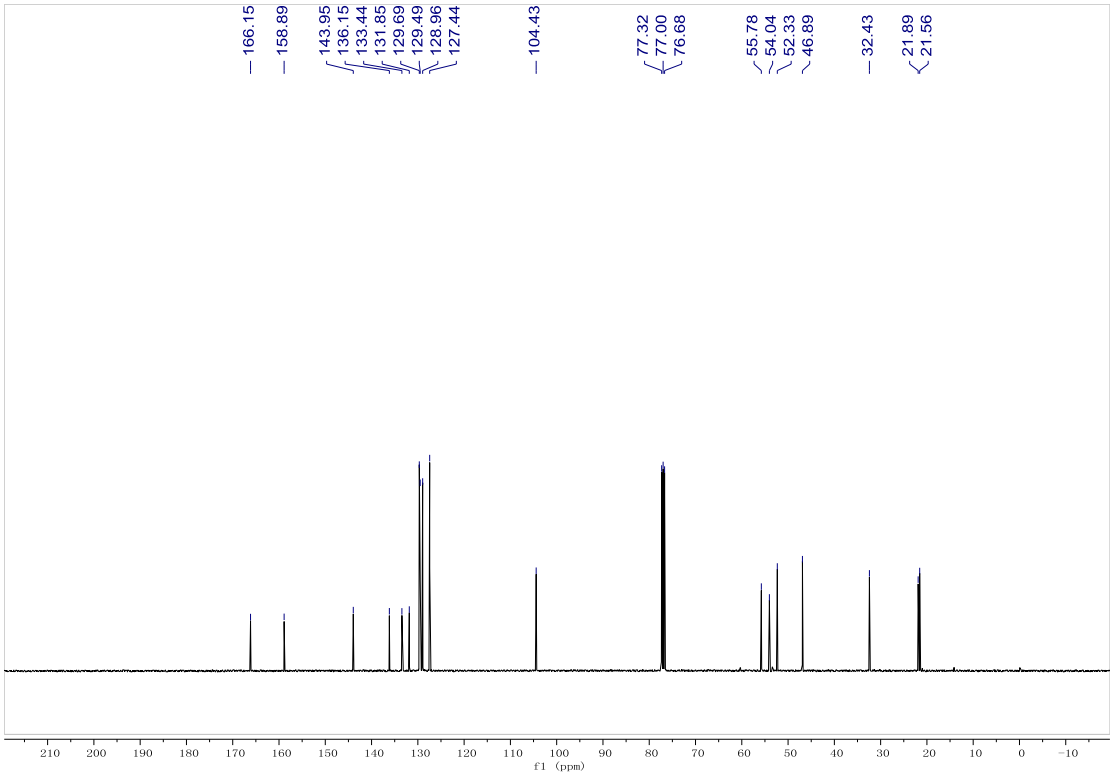
7.84
7.83
7.38
7.36
6.55
3.93
3.53
3.51
2.96
2.94
2.47
1.38
0.78
0.00
2.01
4.03
2.04
0.96
3.01
1.00
1.00
3.02
2.99
3.00
f1 (ppm)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133.44
131.85
129.69
129.49
128.96
127.44
104.43
77.32
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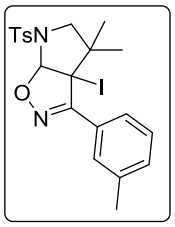
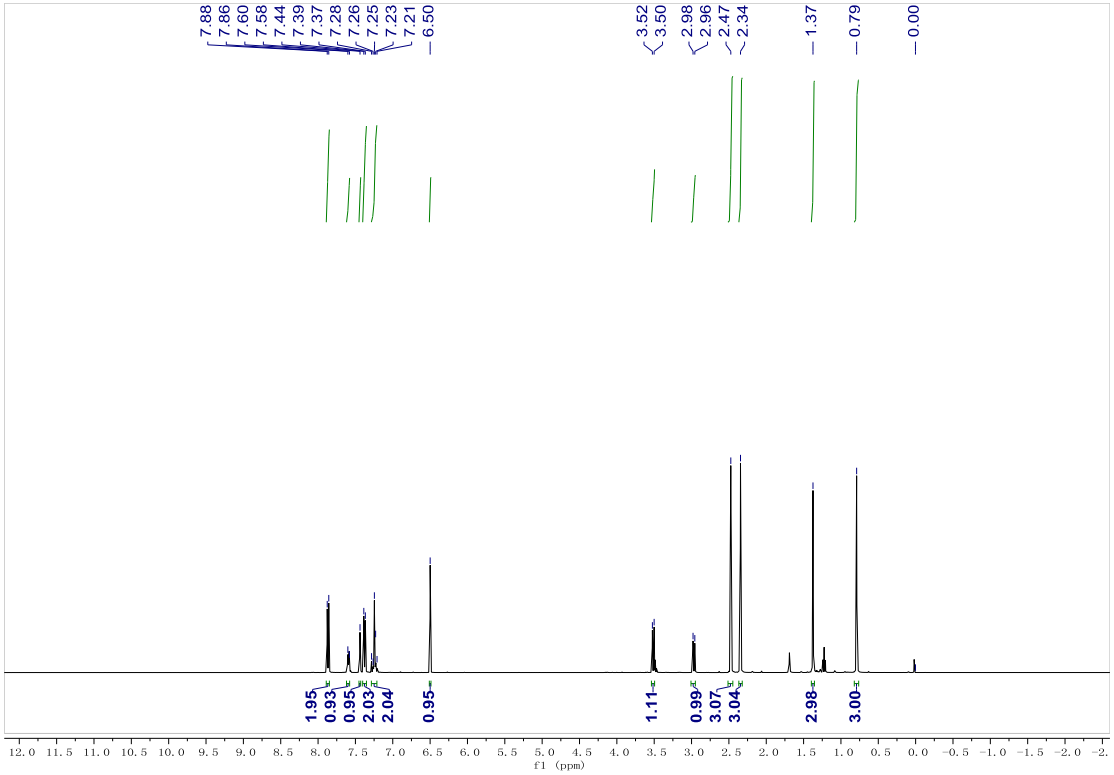
76.68
55.78
54.04
52.33
46.89
32.43
21.89
21.56
f1 (ppm)


TsN
O
N
I

9i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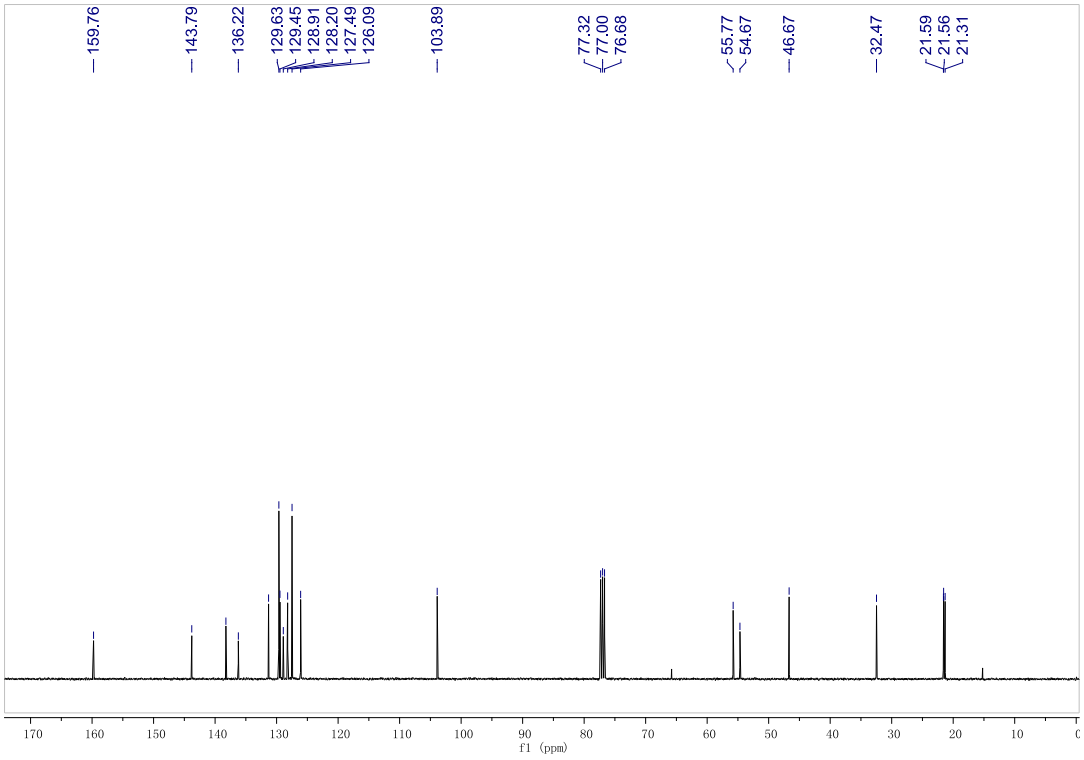
7.44
7.39
7.37
7.28
7.26
7.25
7.23
7.21
6.50
3.52
3.50
2.98
2.96
2.47
2.34
1.37
0.79
0.00
1.95
0.93
0.95
2.03
2.04
0.95
1.11
0.99
3.07
3.04
2.98
3.00
f1 (ppm)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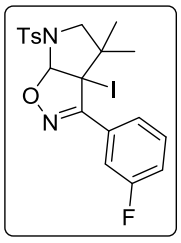
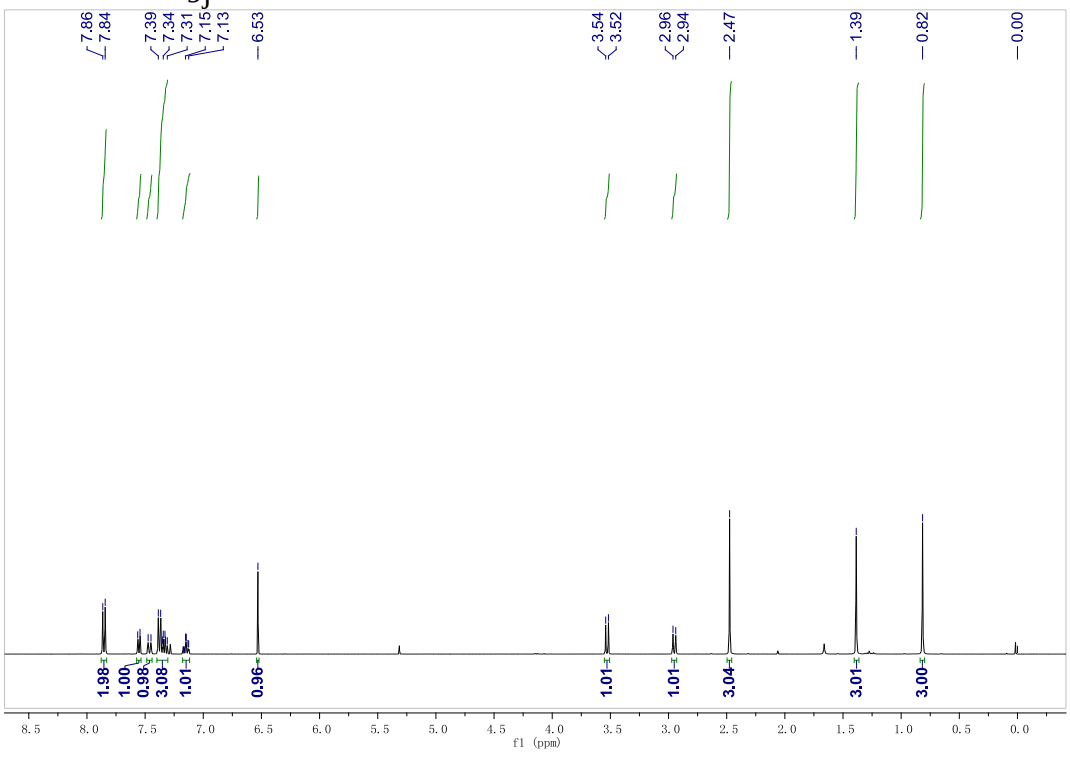
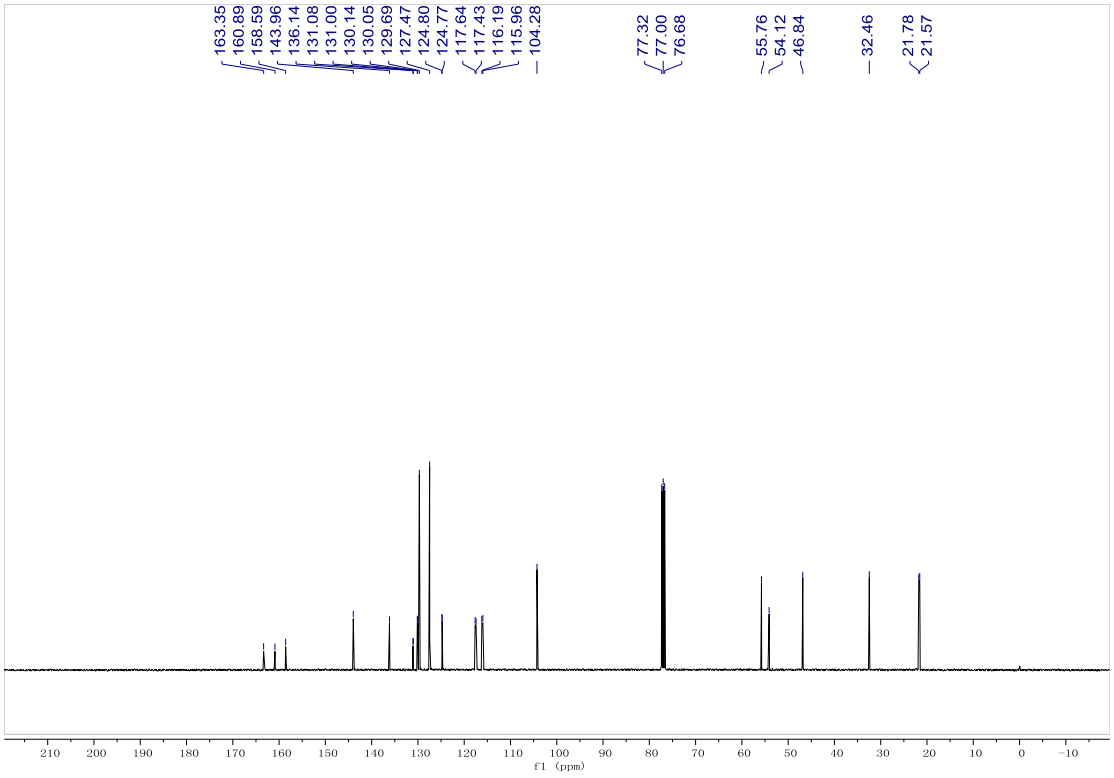
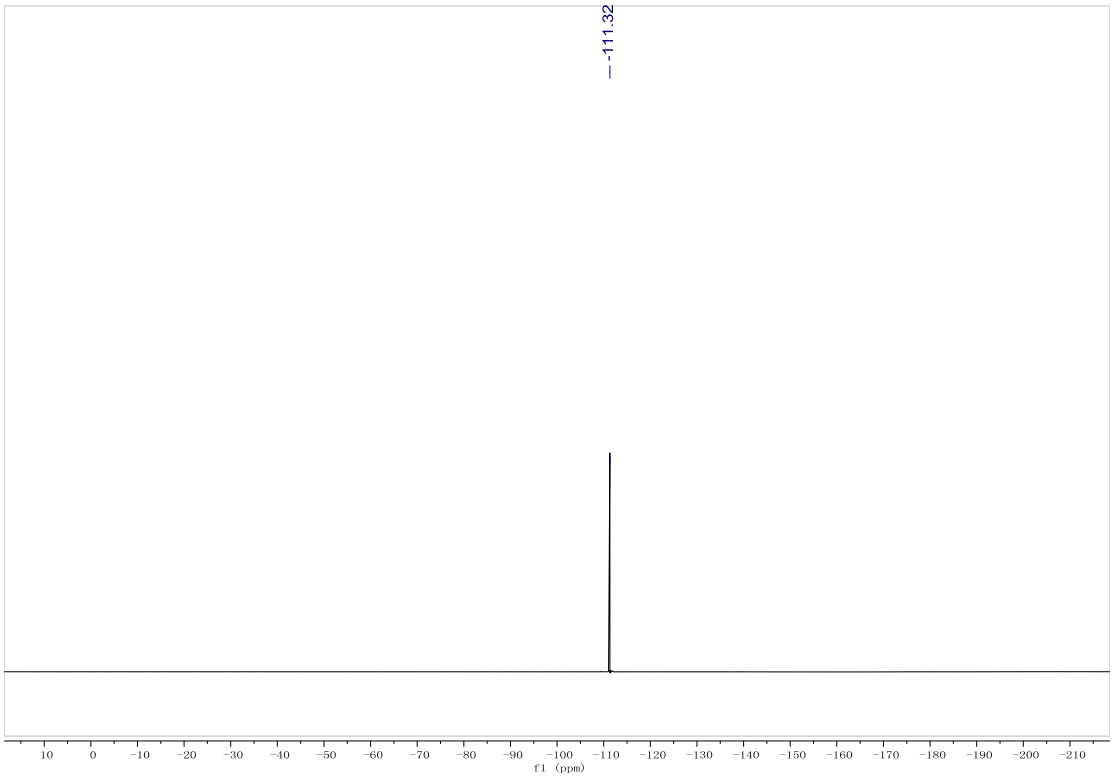
143.79
136.22
129.63
129.45
128.91
128.20
127.49
126.09
103.89
77.32
77.00
76.68
55.77
54.67
46.67
32.47
21.59
21.56
21.31
f1 (ppm)

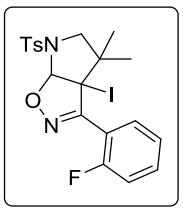

TsN
O
N
I
F

9j

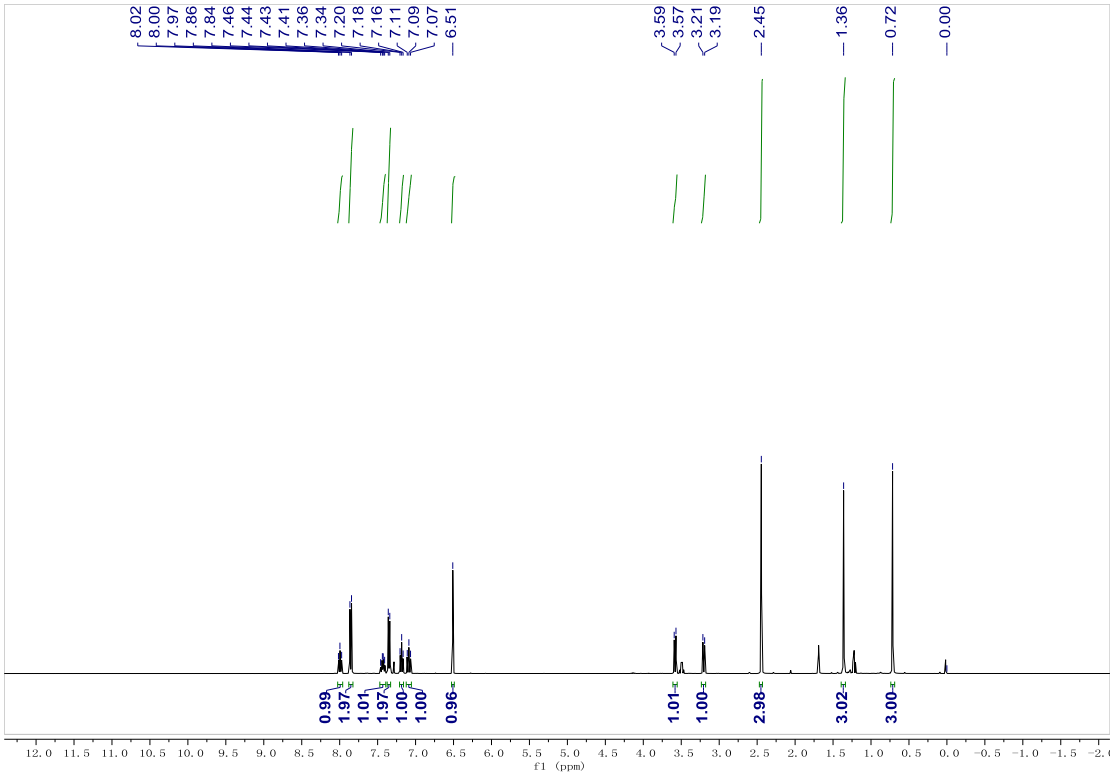

7.86
7.84
7.39
7.34
7.31
7.15
7.13
6.53
3.54
3.52
2.96
2.94
2.47
1.39
0.82
0.00
1.98
1.00
0.98
3.08
1.01
0.96
1.01
1.01
3.04
3.01
3.00
f1 (ppm)

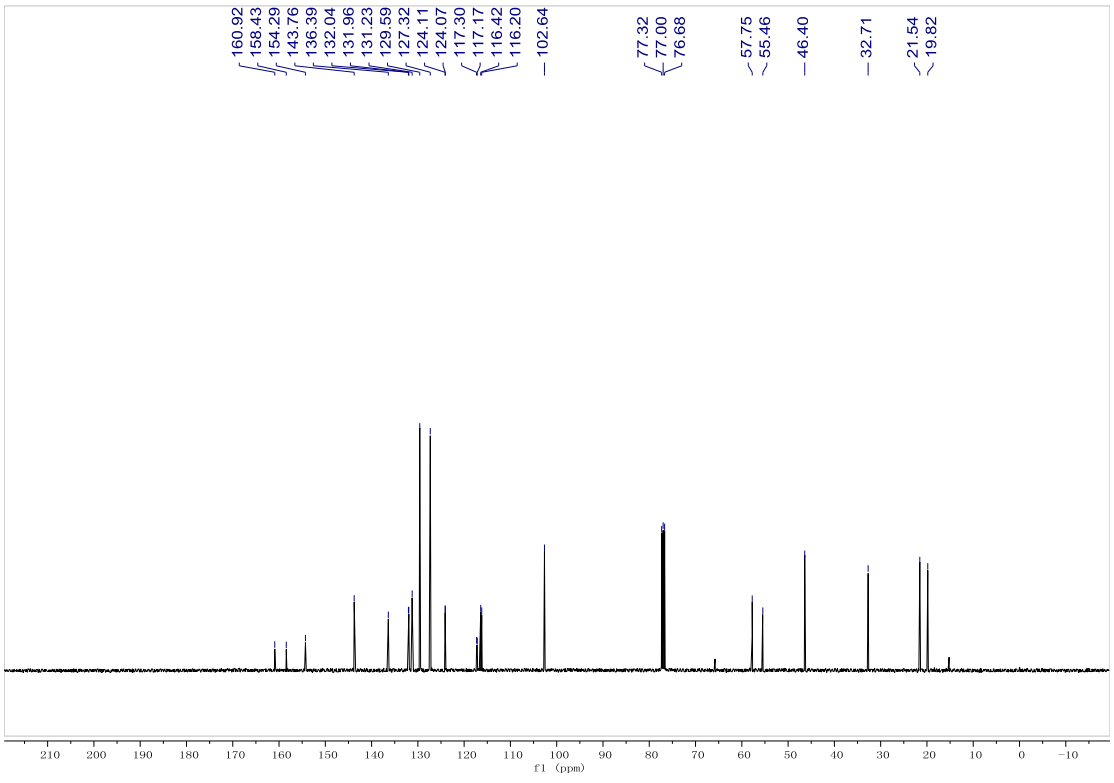

163.35
160.89
158.59
143.96
136.14
131.08
131.00
130.14
130.05
129.69
127.47
124.80
124.77
117.64
117.43
116.19
115.96
104.28
77.32
77.00
76.68
55.76
54.12
46.84
32.46
21.78
21.57
f1 (ppm)


-111.32
f1 (ppm)


TsN
O
N
I
F

9k


8.02
8.00
7.97
7.86
7.84
7.46
7.44
7.43
7.41
7.36
7.34
7.20
7.18
7.16
7.11
7.09
7.07
6.51
3.59
3.57
3.21
3.19
2.45
1.36
0.72
0.00
0.99
1.97
1.01
1.97
1.00
1.00
0.96
1.01
1.00
2.98
3.02
3.00
f1 (ppm)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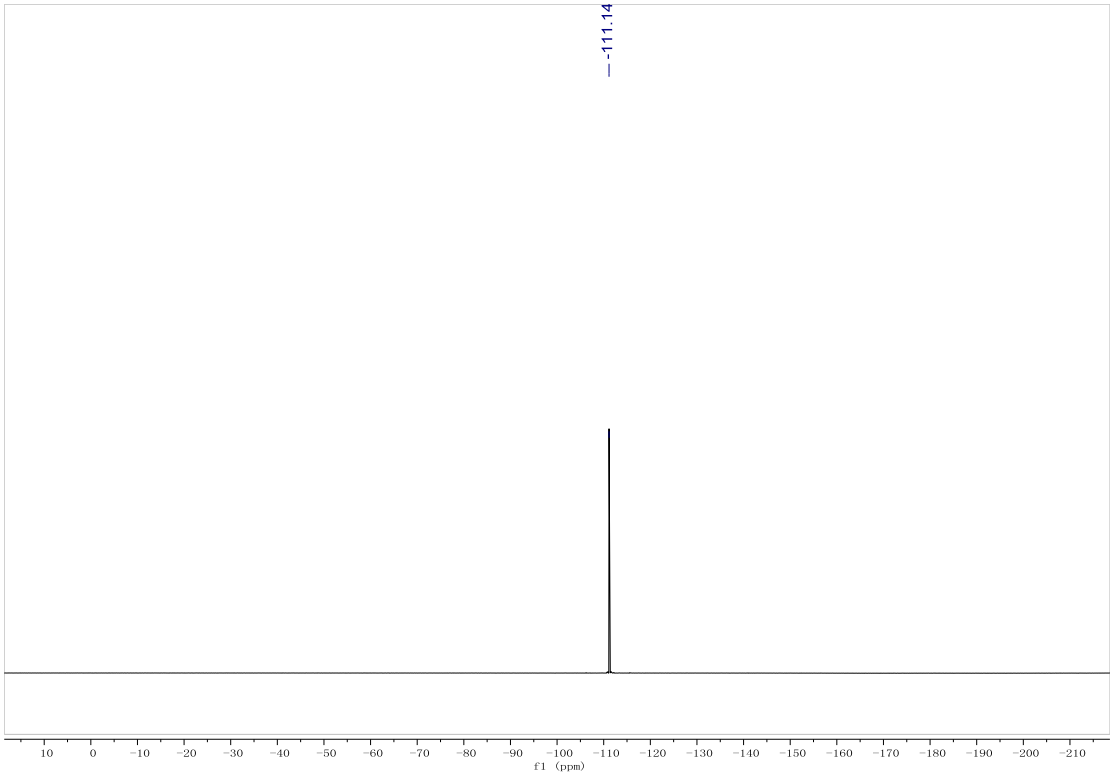
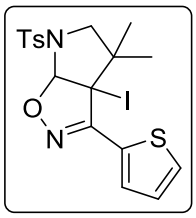
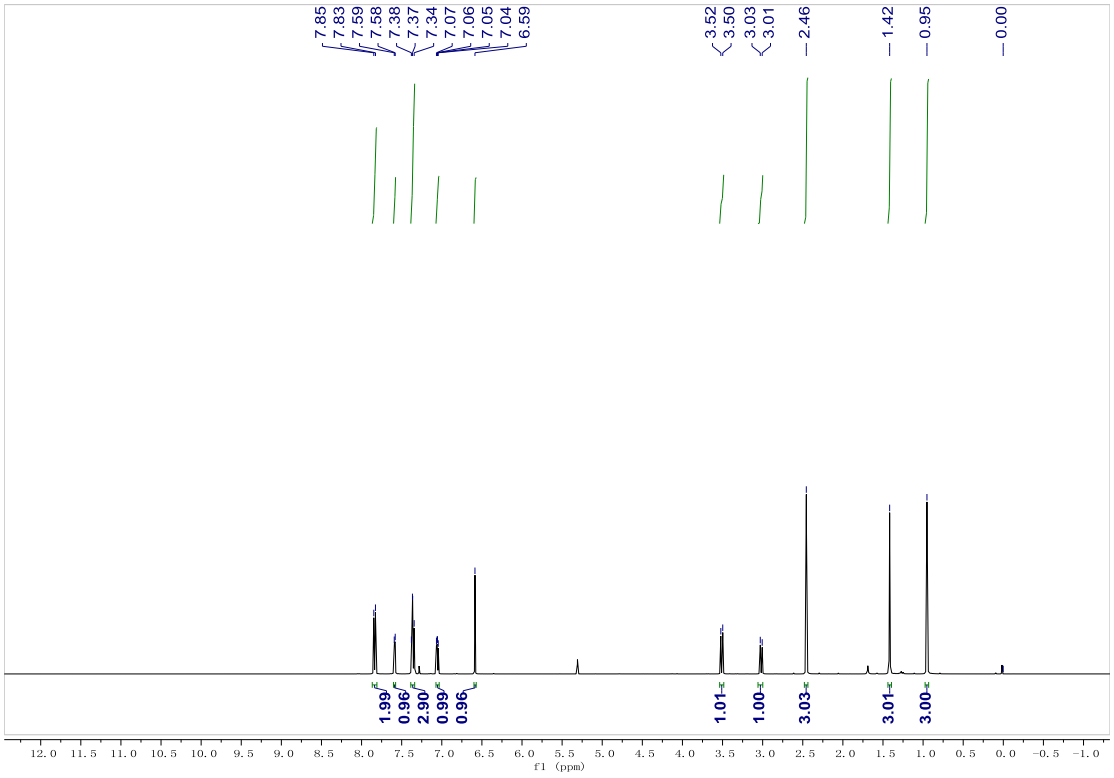
158.43
154.29
143.76
136.39
132.04
131.96
131.23
129.59
127.32
124.11
124.07
117.30
117.17
116.42
116.20
102.64
77.32
77.00
76.68
57.75
55.46
46.40
32.71
21.54
19.82
f1 (ppm)


-111.14
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


TsN
O
N
I
S

9l


7.85
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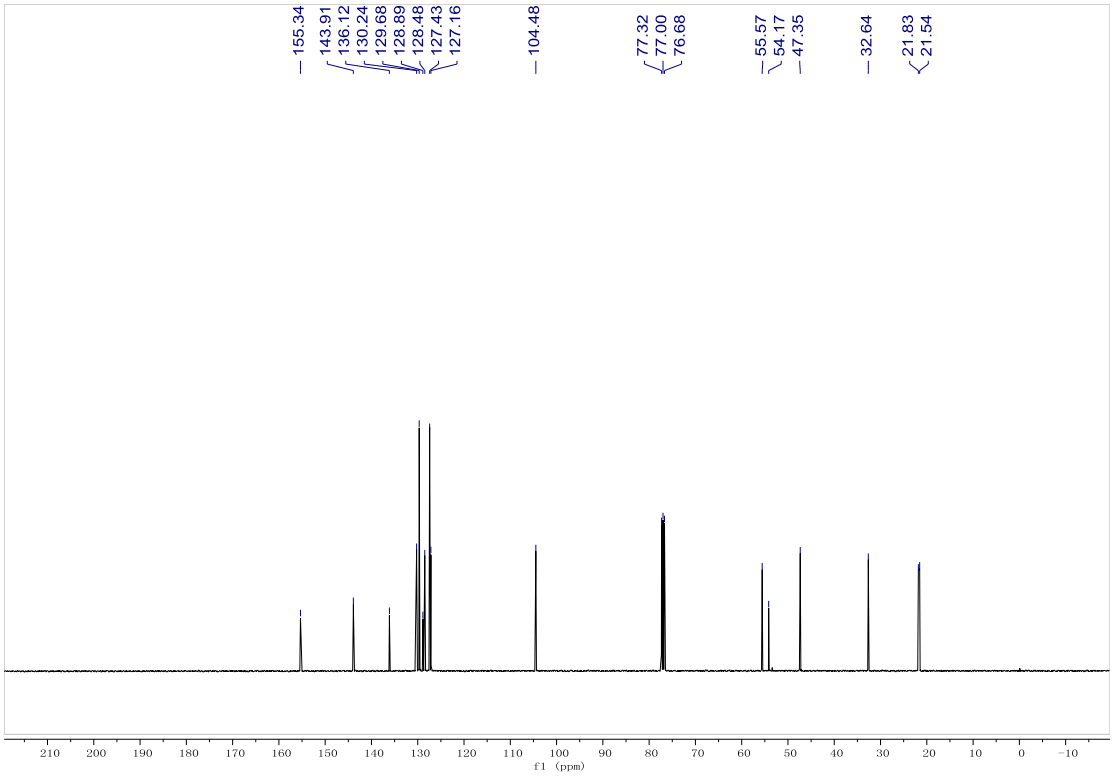
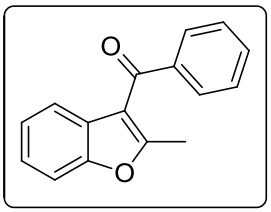
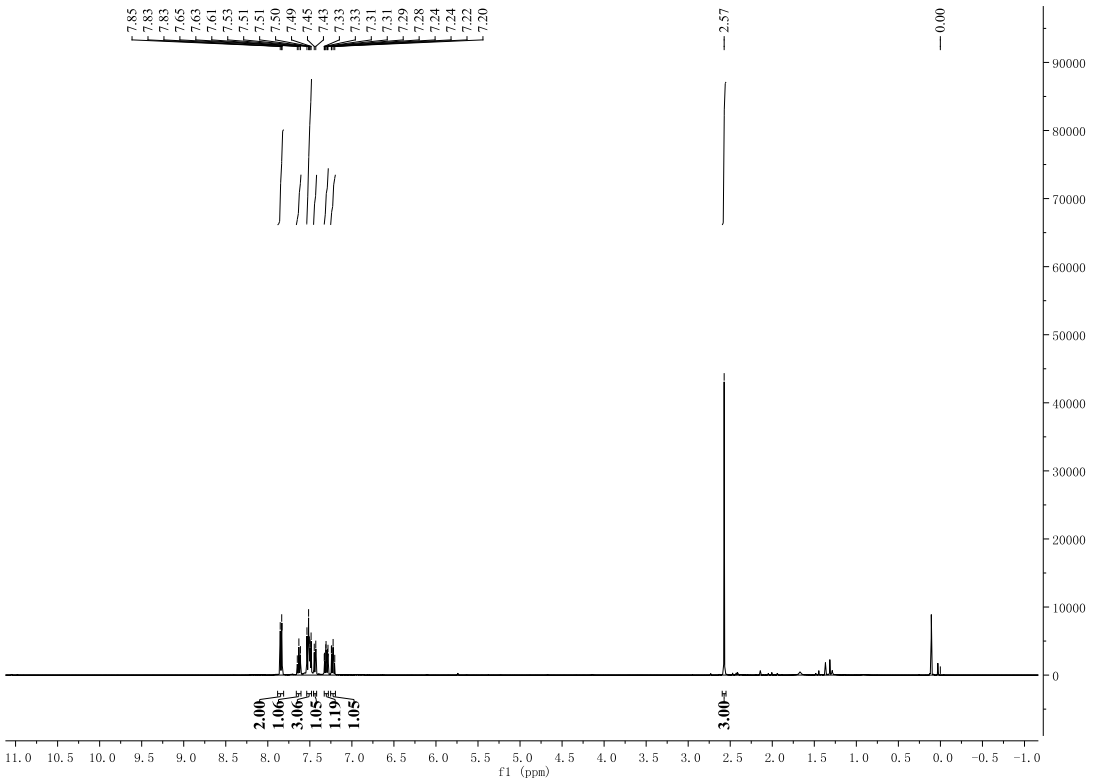
7.59
7.58
7.38
7.37
7.34
7.07
7.06
7.05
7.04
6.59
3.52
3.50
3.03
3.01
2.46
1.42
0.95
0.00
1.99
0.96
2.90
0.99
0.96
1.01
1.00
3.03
3.01
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


155.34
143.91
136.12
130.24
129.68
128.89
128.48
127.43
127.16
104.48
77.32
77.00
76.68
55.57
54.17
47.35
32.64
21.83
21.54
f1 (ppm)



10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7.83
7.83
7.65
7.63
7.61
7.53
7.51
7.51
7.50
7.49
7.45
7.43
7.33
7.33
7.31
7.31
7.29
7.28
7.24
7.24
7.22
7.20
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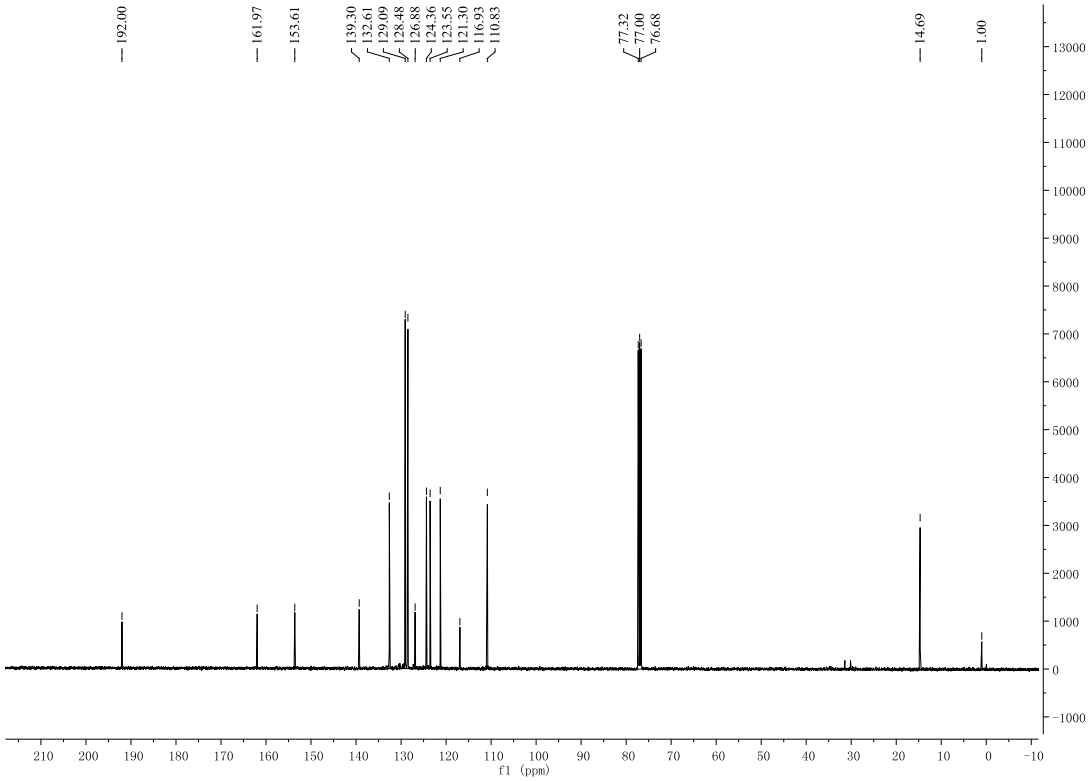
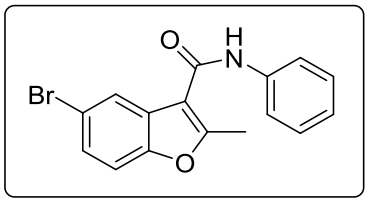
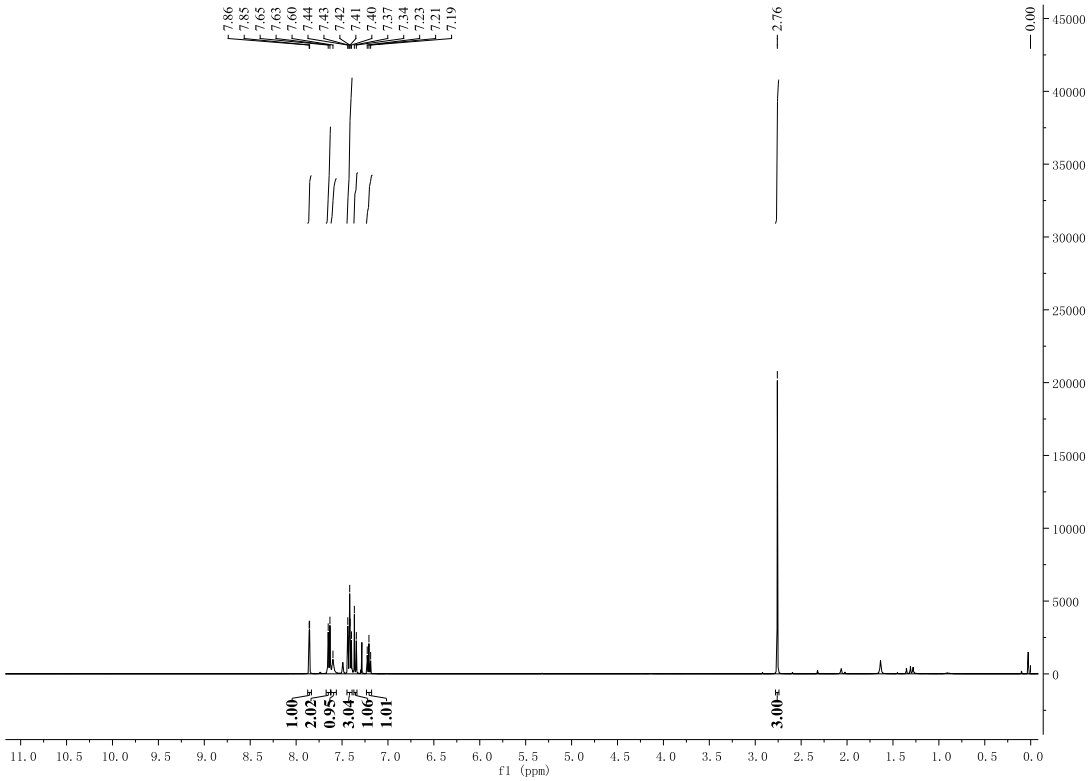
0.00
2.00
1.06
3.06
1.05
1.19
1.05
3.00
f1 (ppm)


192.00
161.97
153.61
139.30
132.61
129.09
128.48
126.88
124.36
123.55
121.30
116.93
110.83
77.32
77.00
76.68
14.69
1.00
f1 (ppm)


O
H
N
Br
O

11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7.63
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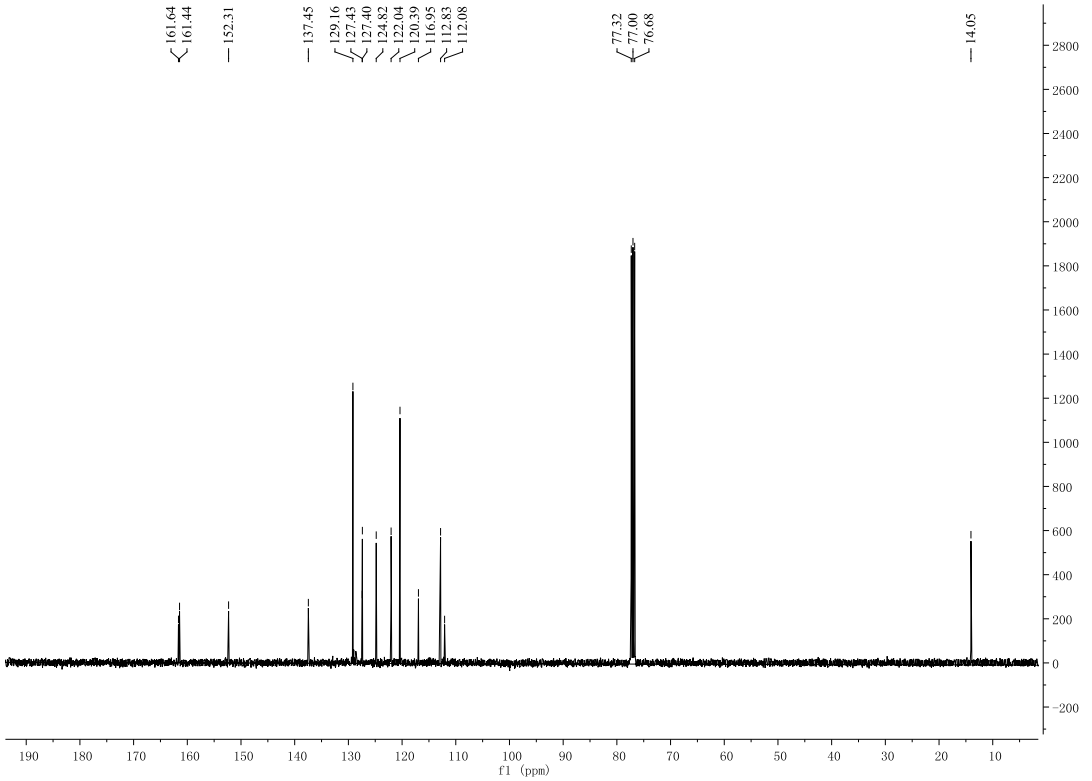
7.44
7.43
7.42
7.41
7.40
7.37
7.34
7.23
7.21
7.19
2.76
0.00
1.00
2.02
0.95
3.04
1.06
1.01
3.00
f1 (ppm)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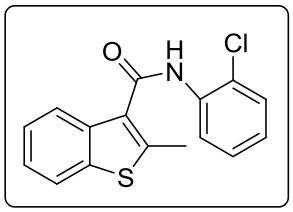
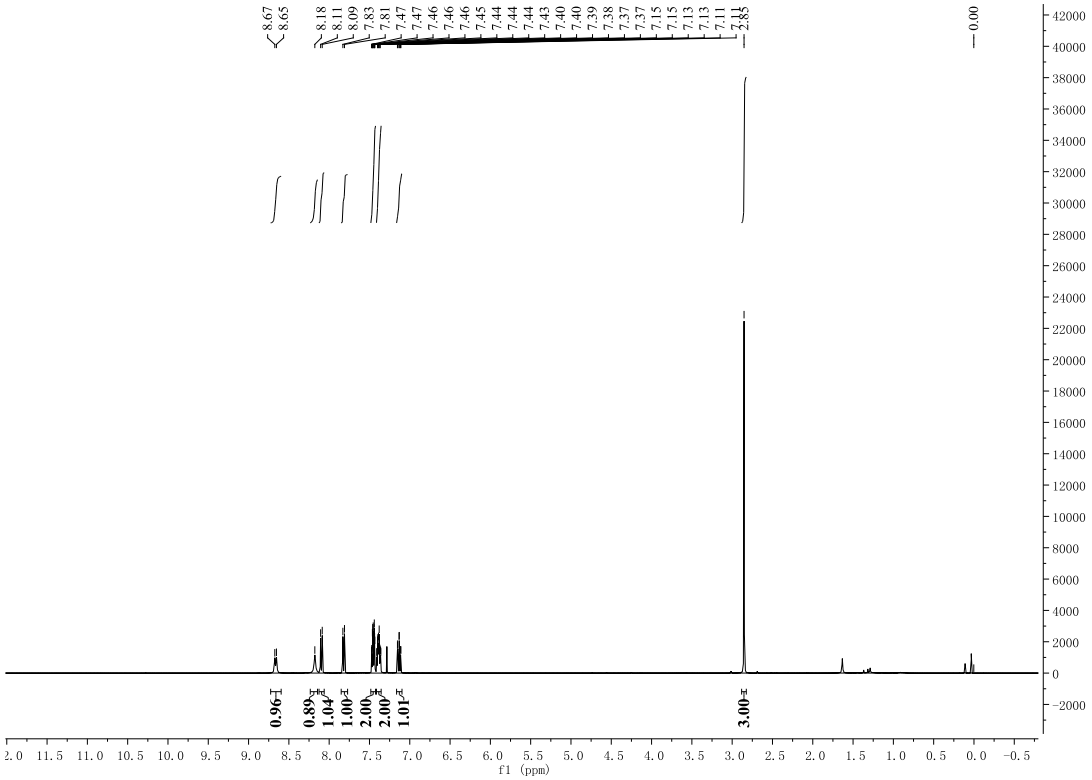
161.44
152.31
137.45
129.16
127.43
127.40
124.82
122.04
120.39
116.95
112.83
112.08
77.32
77.00
76.68
14.05
f1 (ppm)


O
H
N
Cl
S

12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7.46
7.45
7.44
7.44
7.44
7.43
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7.40
7.39
7.38
7.37
7.37
7.15
7.15
7.13
7.13
7.11
7.11
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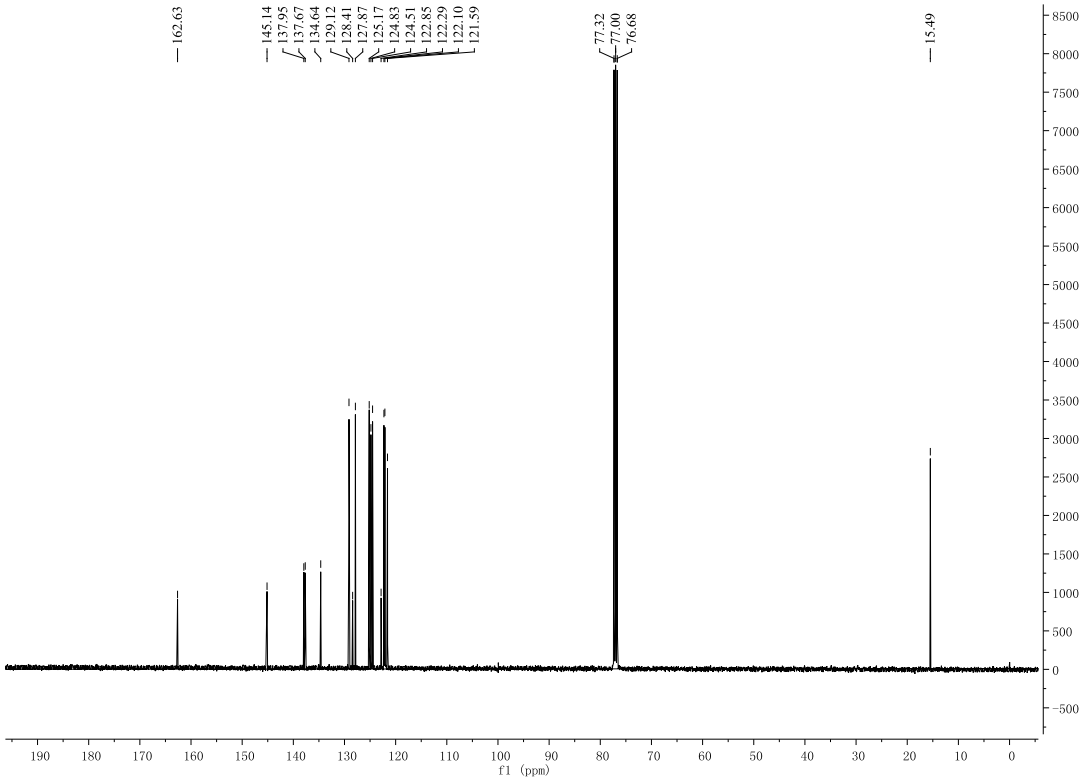
0.96
0.89
1.04
1.00
2.00
2.00
1.01
3.00
f1 (ppm)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137.95
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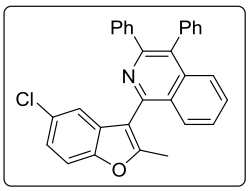
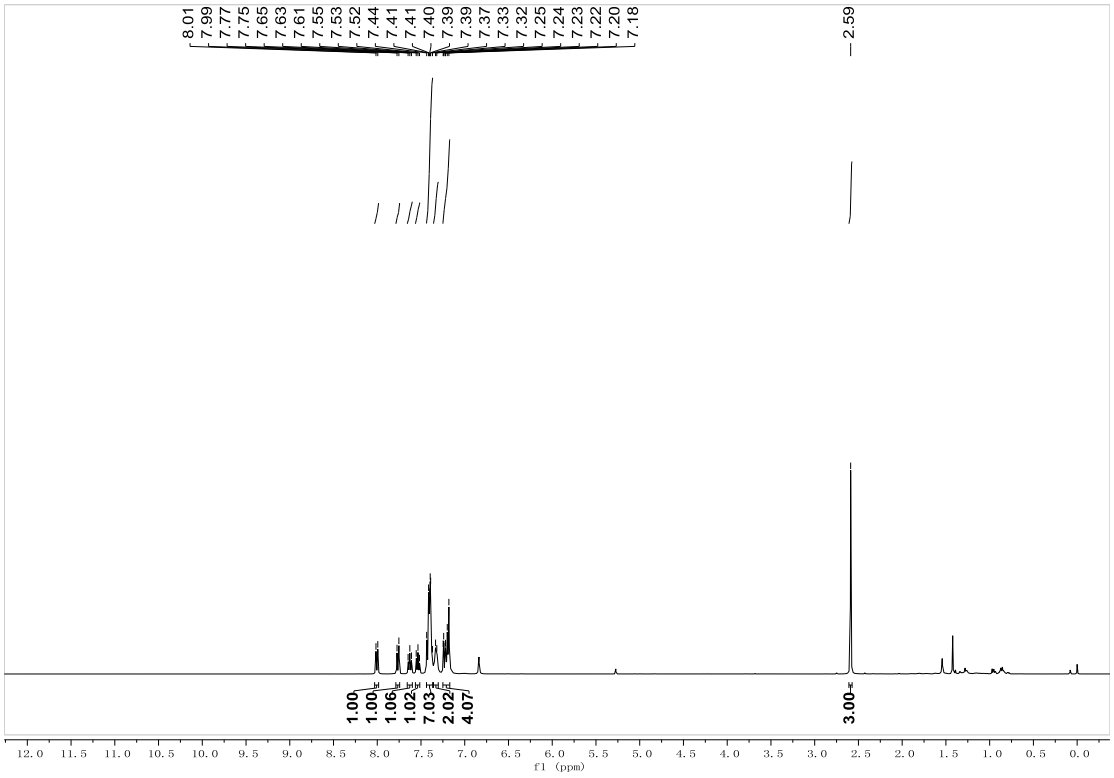
134.64
129.12
128.41
127.87
125.17
124.83
124.51
122.85
122.29
122.10
121.59
77.32
77.00
76.68
15.49
f1 (ppm)


Ph
Ph
N
Cl
O

13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7.99
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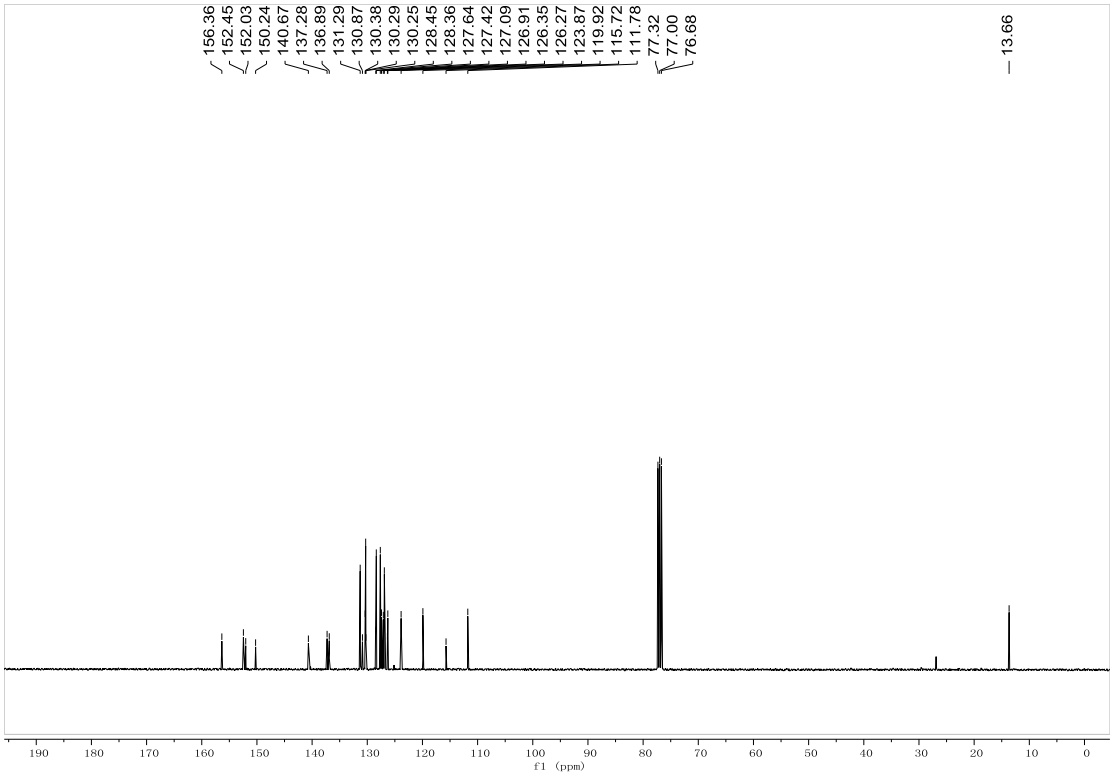
7.75
7.65
7.63
7.61
7.55
7.53
7.52
7.44
7.41
7.41
7.40
7.39
7.39
7.37
7.33
7.32
7.25
7.24
7.23
7.22
7.20
7.18
2.59
1.00
1.00
1.06
1.02
7.03
2.02
4.07
3.00
f1 (ppm)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152.03
150.24
140.67
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131.29
130.87
130.38
130.29
130.25
128.45
128.36
127.64
127.42
127.09
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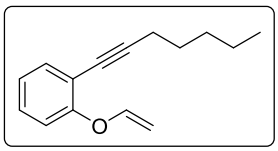
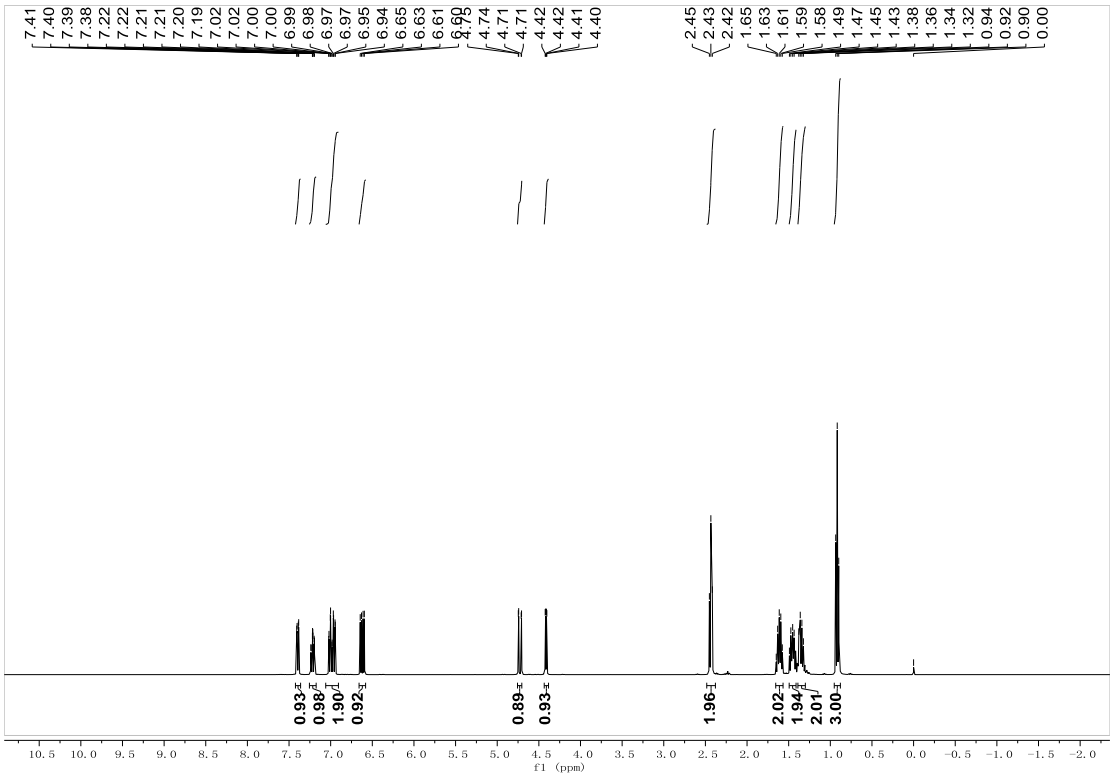
126.35
126.27
123.87
119.92
115.72
111.78
77.32
77.00
76.68
13.66
f1 (ppm)

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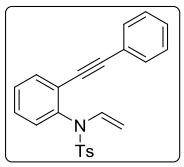
7.21
7.20
7.19
7.02
7.02
7.00
7.00
6.99
6.98
6.97
6.97
6.95
6.94
6.65
6.63
6.61
6.60
4.75
4.74
4.71
4.71
4.42
4.42
4.41
4.40
2.45
2.43
2.42
1.65
1.63
1.61
1.59
1.58
1.49
1.47
1.45
1.43
1.38
1.36
1.34
1.32
0.94
0.92
0.90
0.00
0.93
0.98
1.90
0.92
0.89
0.93
1.96
2.02
1.94
2.01
3.00
f1 (ppm)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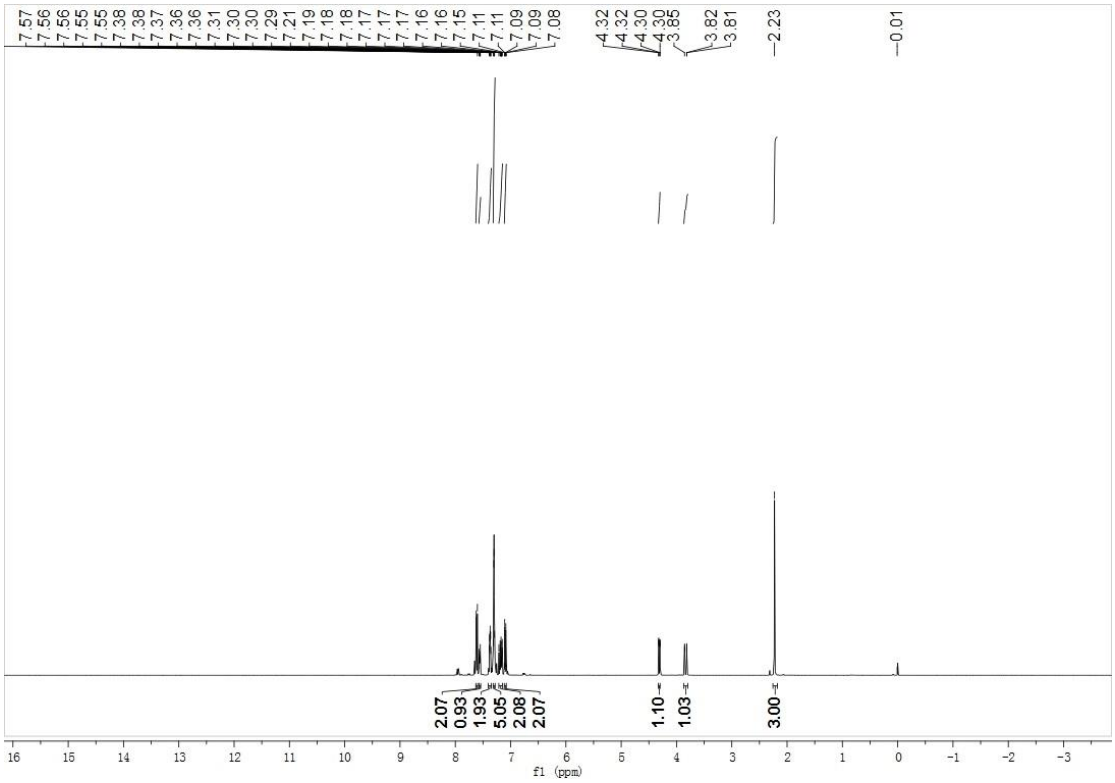
Ts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7.09
7.09
7.08
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4.32
4.30
4.30
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3.82
3.81
2.23
0.01
2.07
0.93
1.93
5.05
2.08
2.07
1.10
1.03
3.00
f1 (ppm)