Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Base-Promoted Thioannulation of *o*-Alkynyl Oxime Ethers with Sodium Sulfide for the General Synthesis of Isothiocoumarins

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Supporting Information

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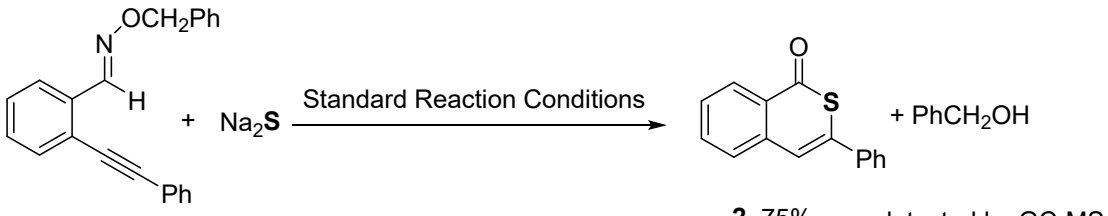
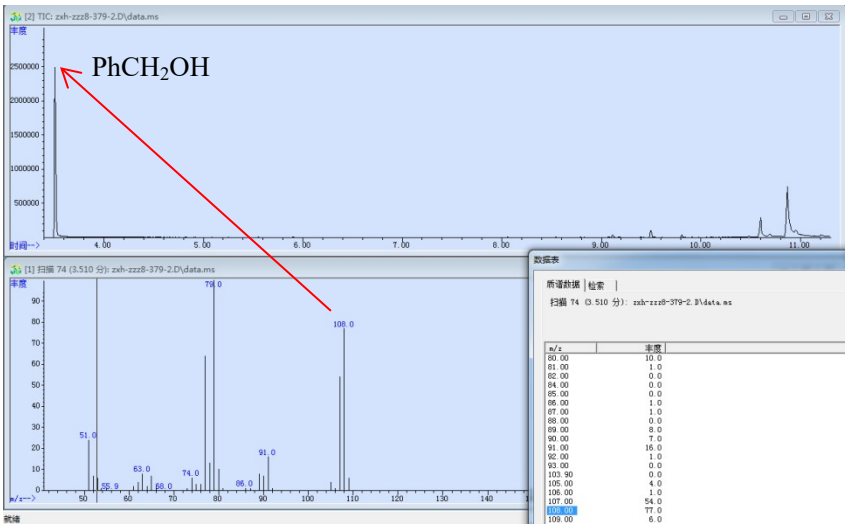
1. The GC-MS analysis of control experiments

eq. 1:

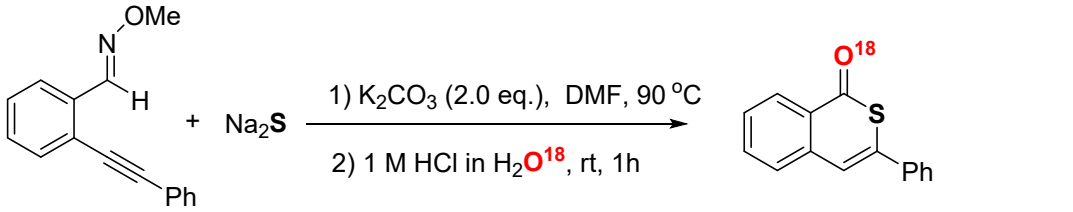


1bb

2, 75% detected by GC-MS

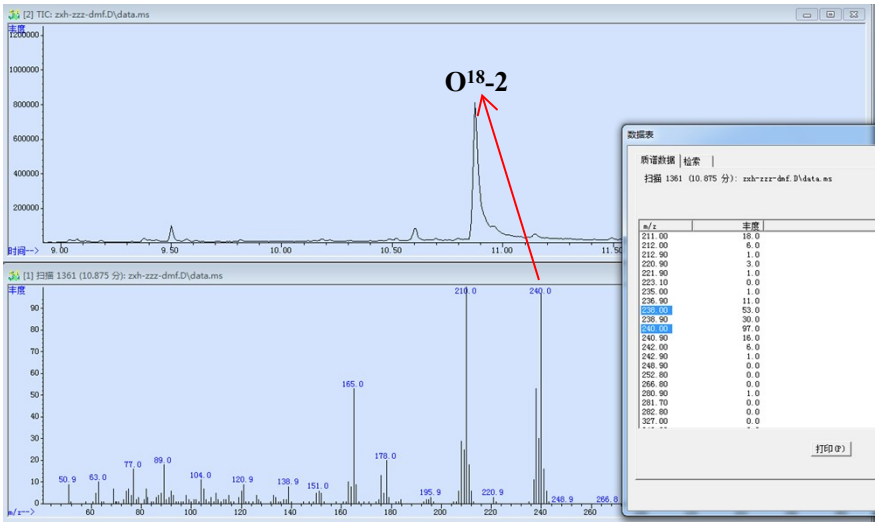


eq. 4: O^{18}-2 GC analysis

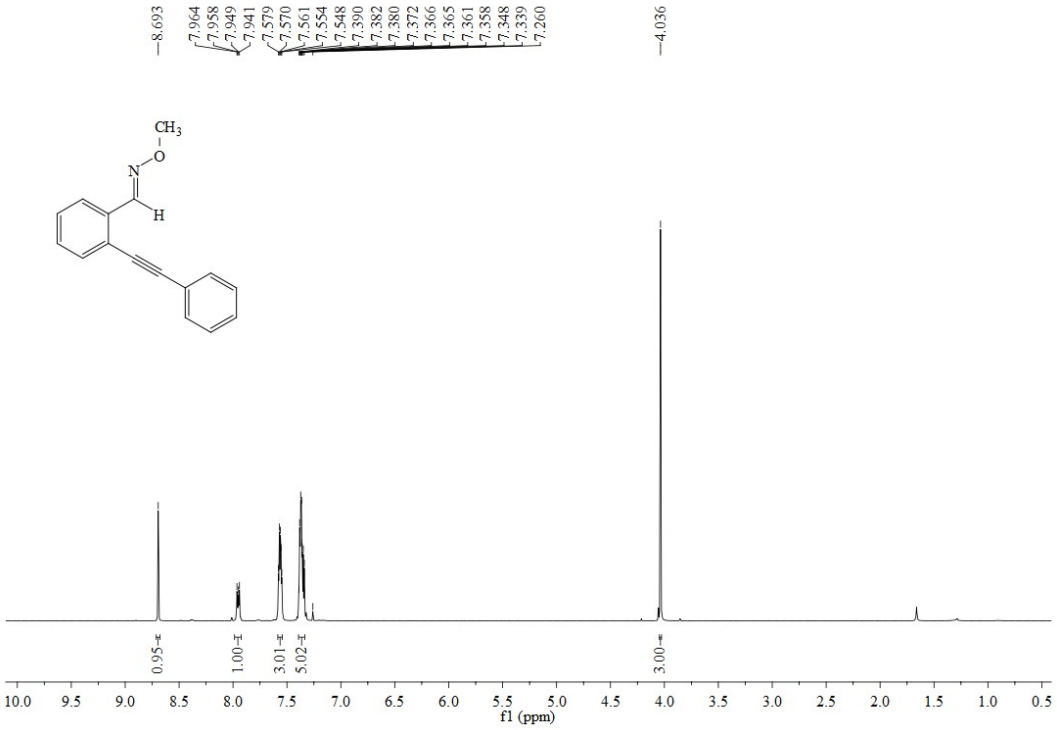


1aa

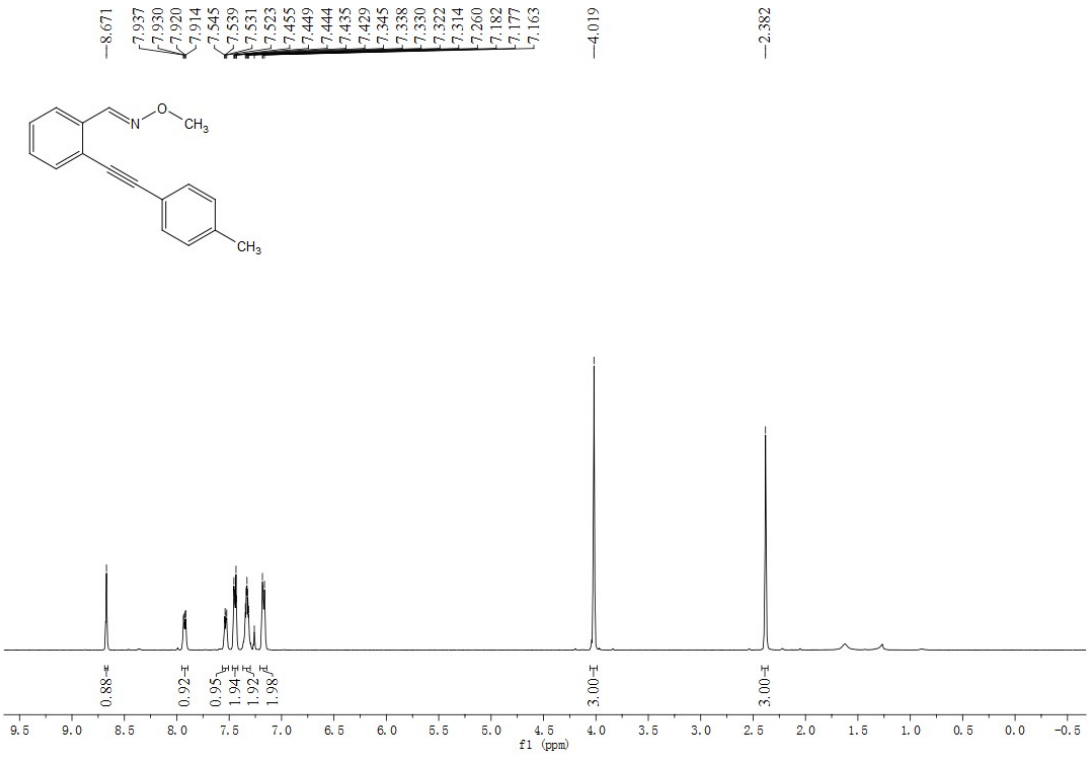
O^{18}-2, ^{18}O:^{16}O = 65:35, 80%



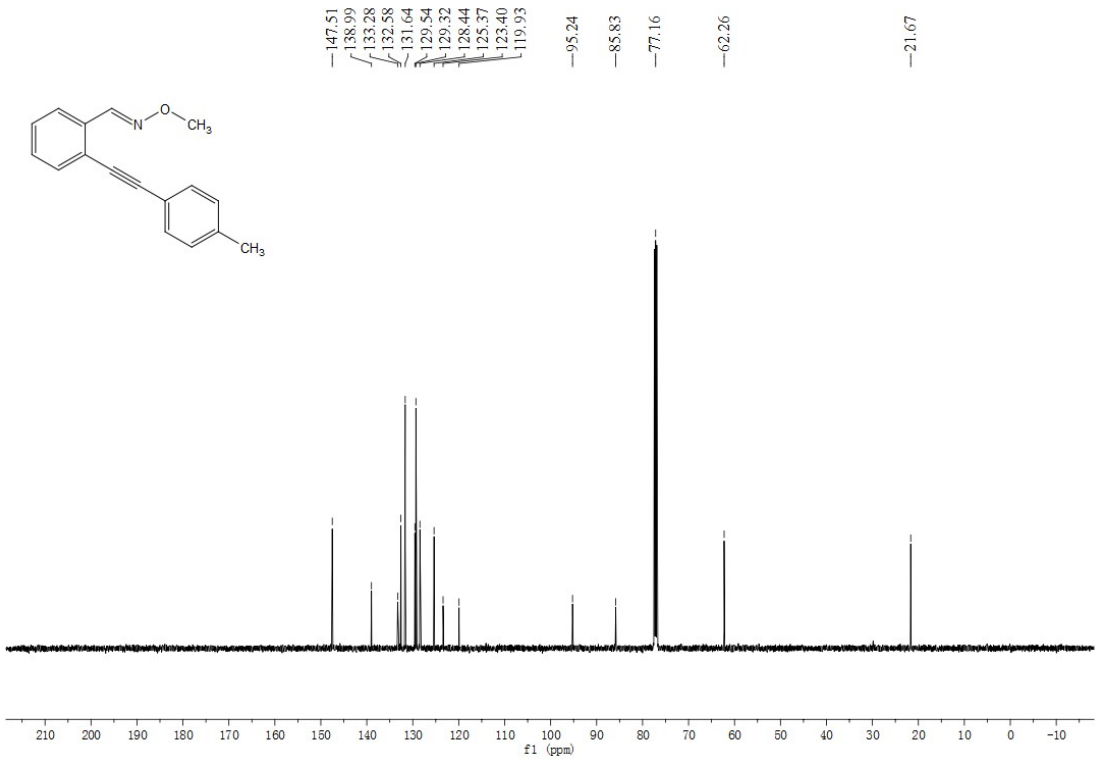
2. NMR spectra for all compounds 1aa-1bb, 2-32 and D-2



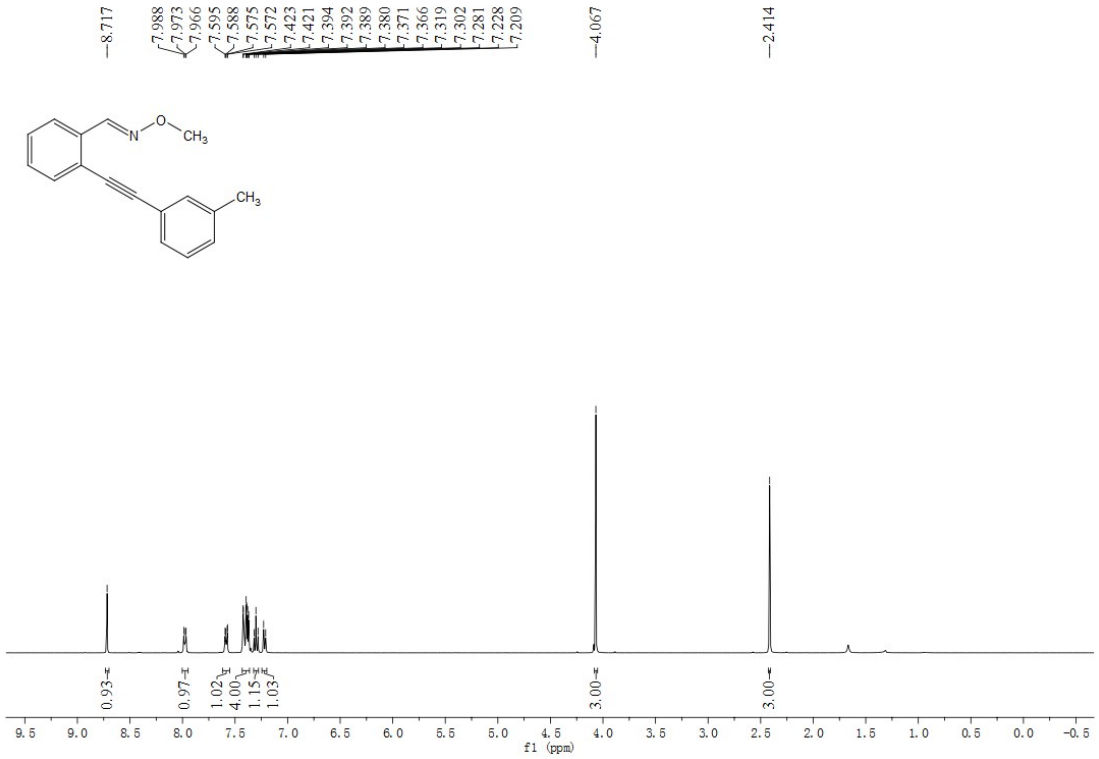
^{1}H NMR 400 MHz, in $CDCl_3$: 2-(phenylethynyl)benzaldehyde O-methyl oxime (1aa)



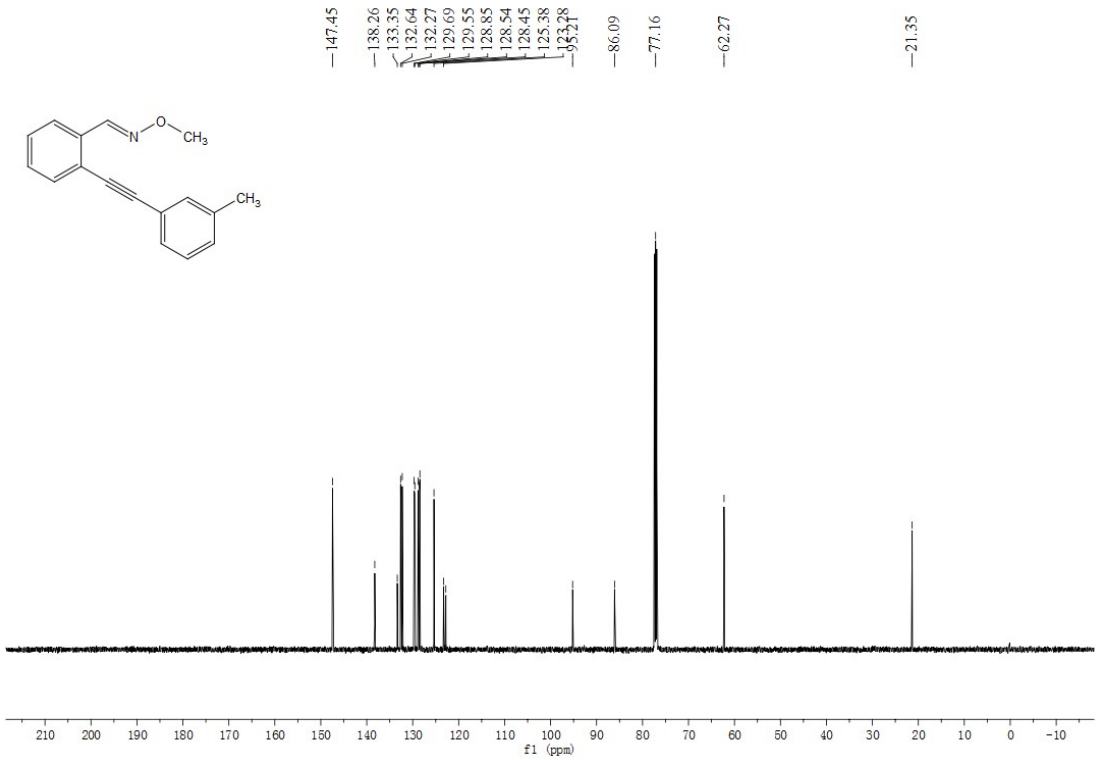
^{1}H NMR 400 MHz, in $CDCl_3$: 2-(p-tolylethynyl)benzaldehyde O-methyl oxime (1ab)



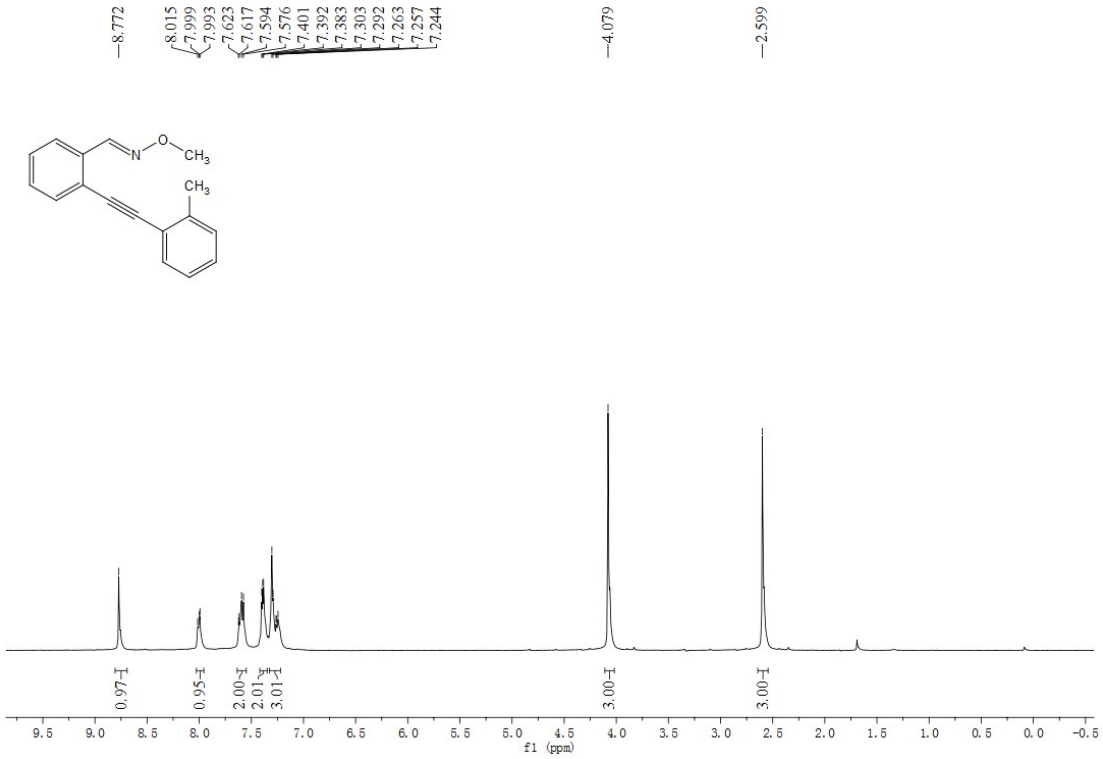
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 2-(p-tolylethynyl)benzaldehyde O-methyl oxime (1ab)



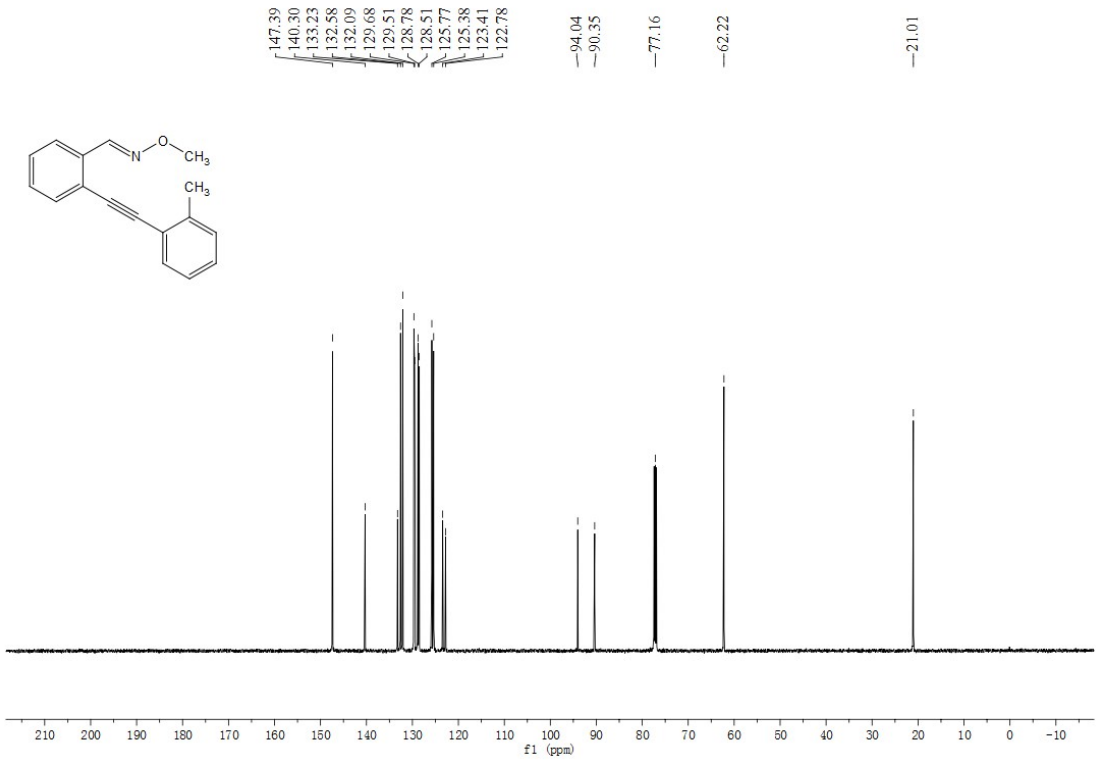
^{1}H NMR 400 MHz, in $CDCl_3$: 2-(m-tolylethynyl)benzaldehyde O-methyl oxime (1ac)



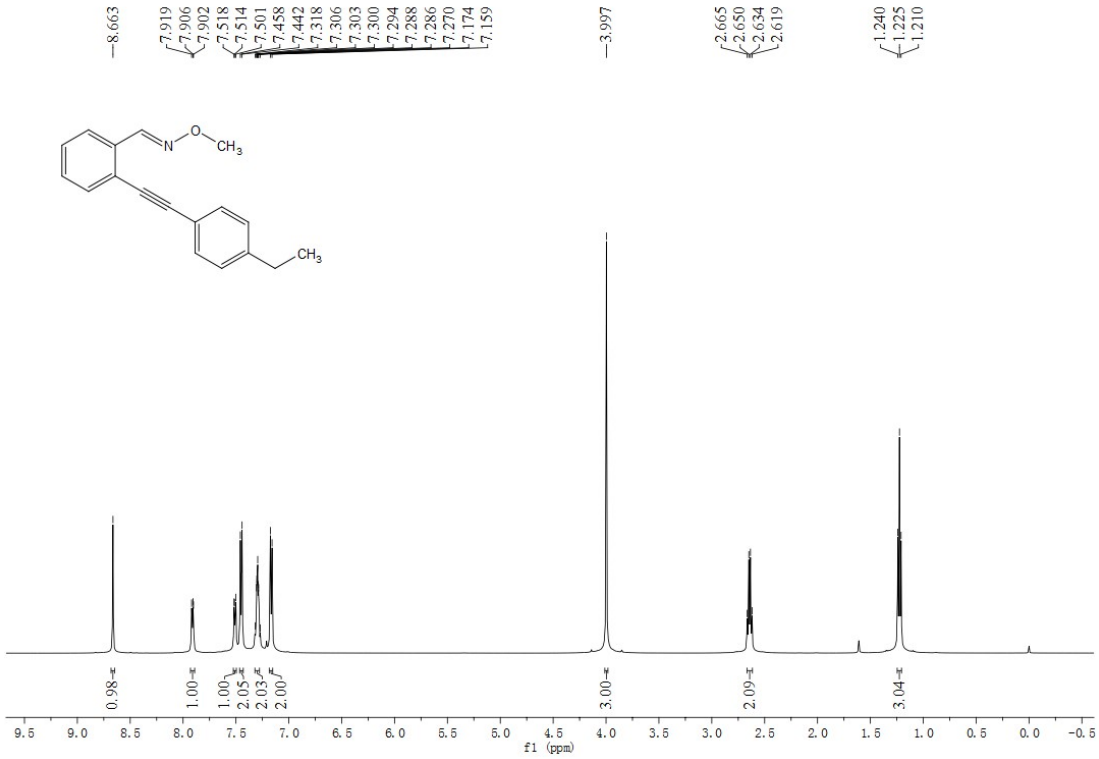
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 2-(m-tolylethynyl)benzaldehyde O-methyl oxime (1ac)



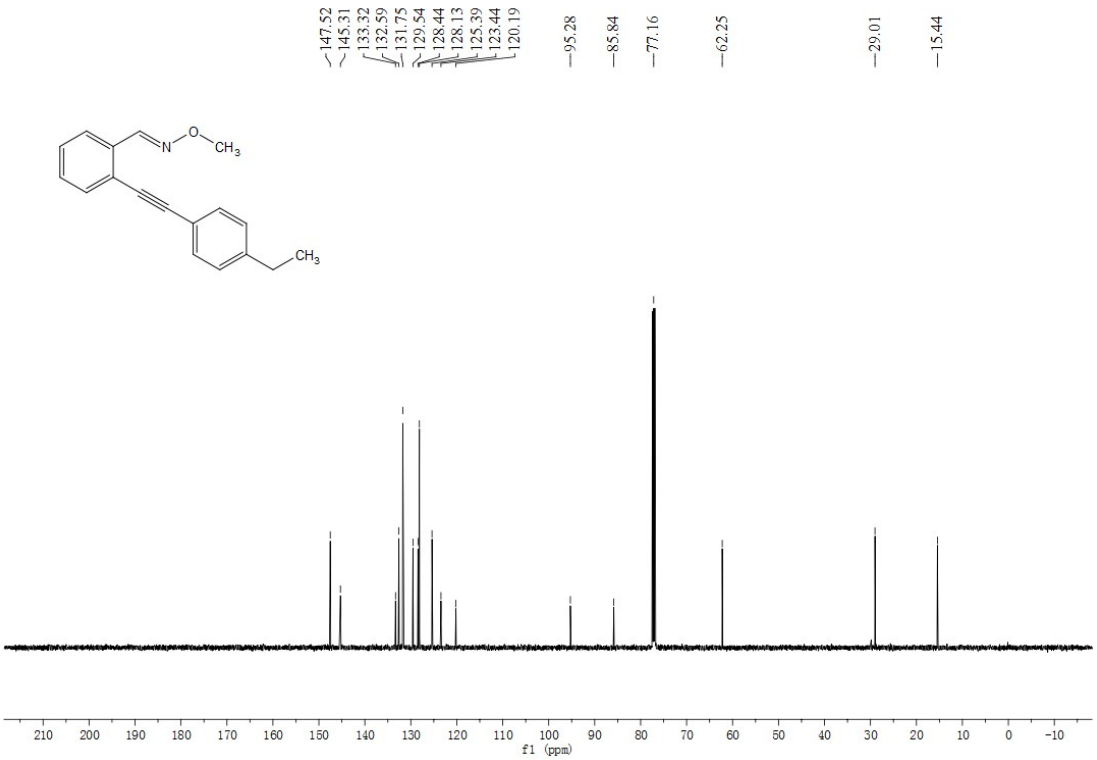
^{1}H NMR 400 MHz, in $CDCl_3$: 2-(o-tolylethynyl)benzaldehyde O-methyl oxime (1ad)



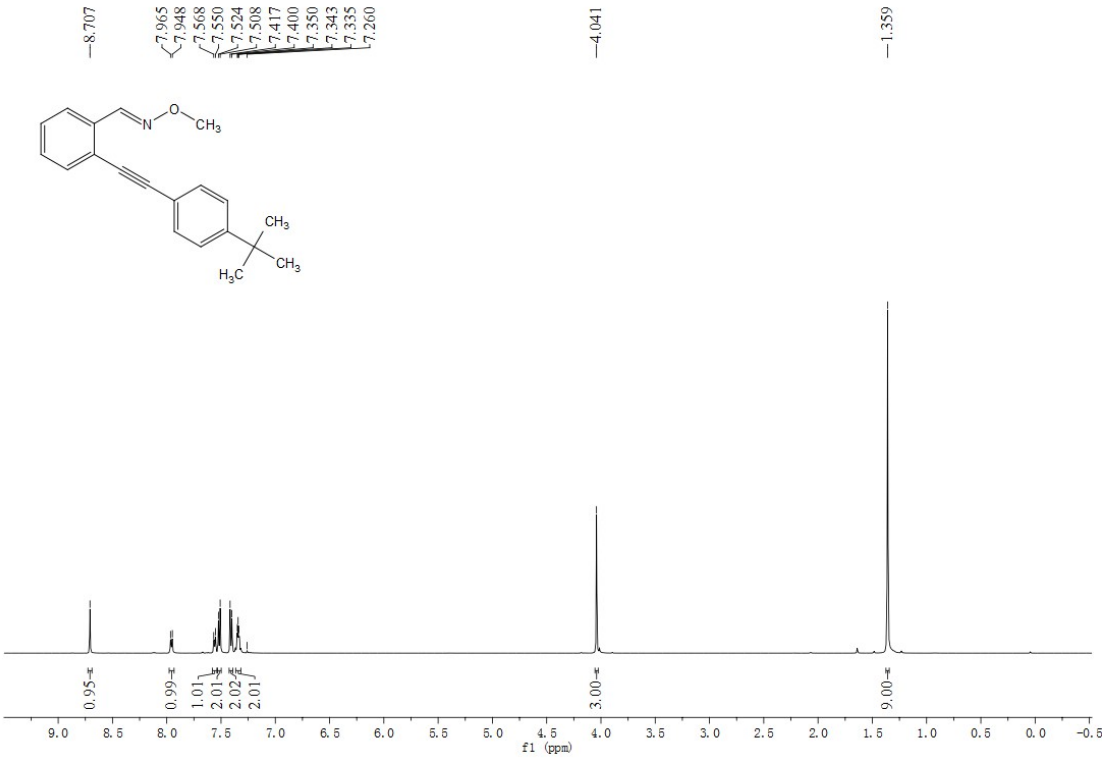
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 2-(o-tolylethynyl)benzaldehyde O-methyl oxime (1ad)



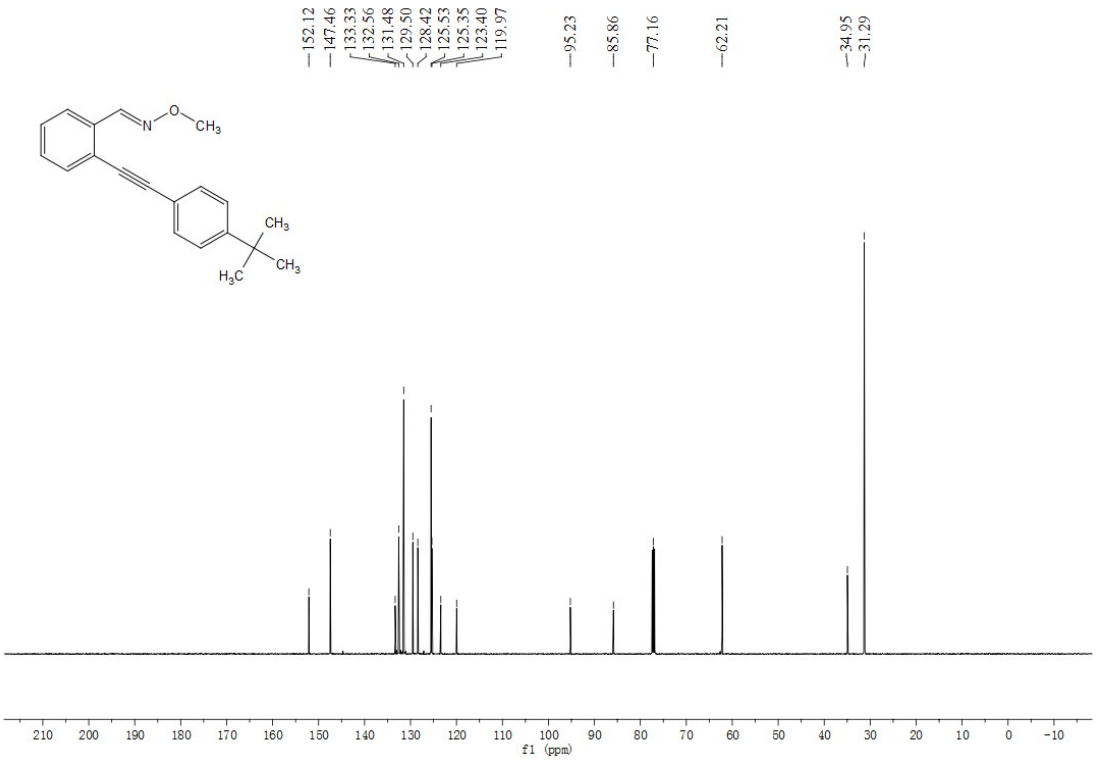
^{1}H NMR 500 MHz, in $CDCl_3$: 2-((4-ethylphenyl)ethynyl)benzaldehyde O-methyl oxime (1ae)



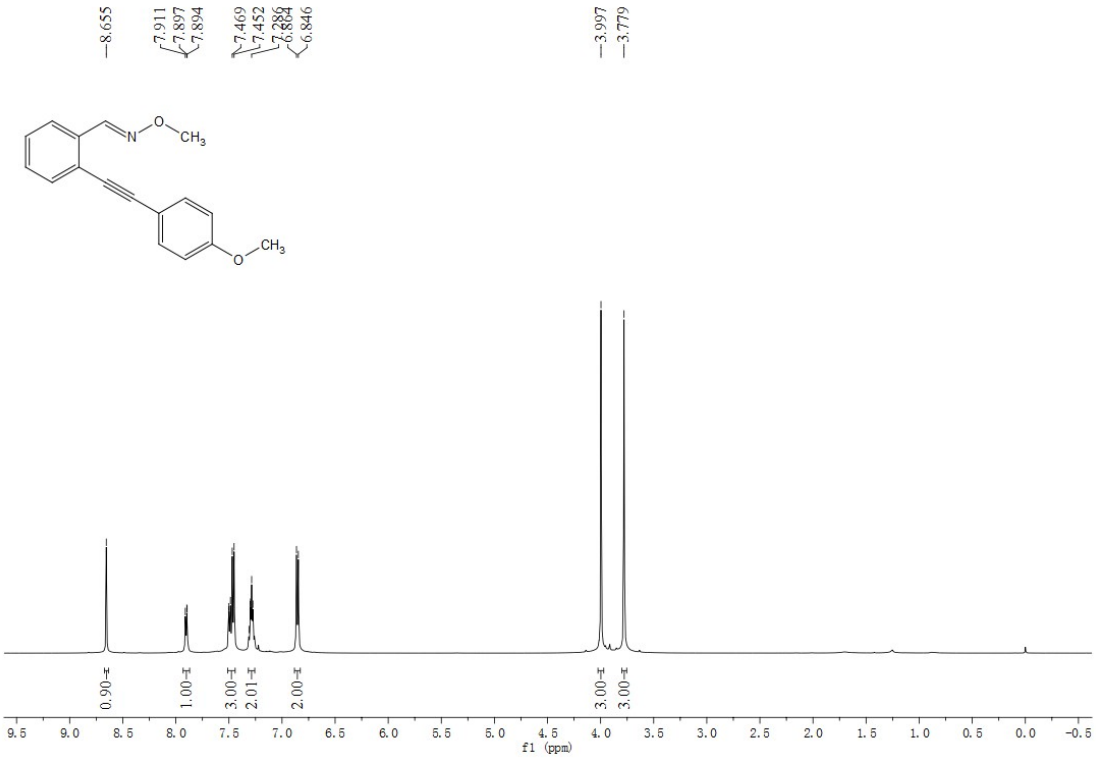
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 2-((4-ethylphenyl)ethynyl)benzaldehyde O-methyl oxime (1ae)



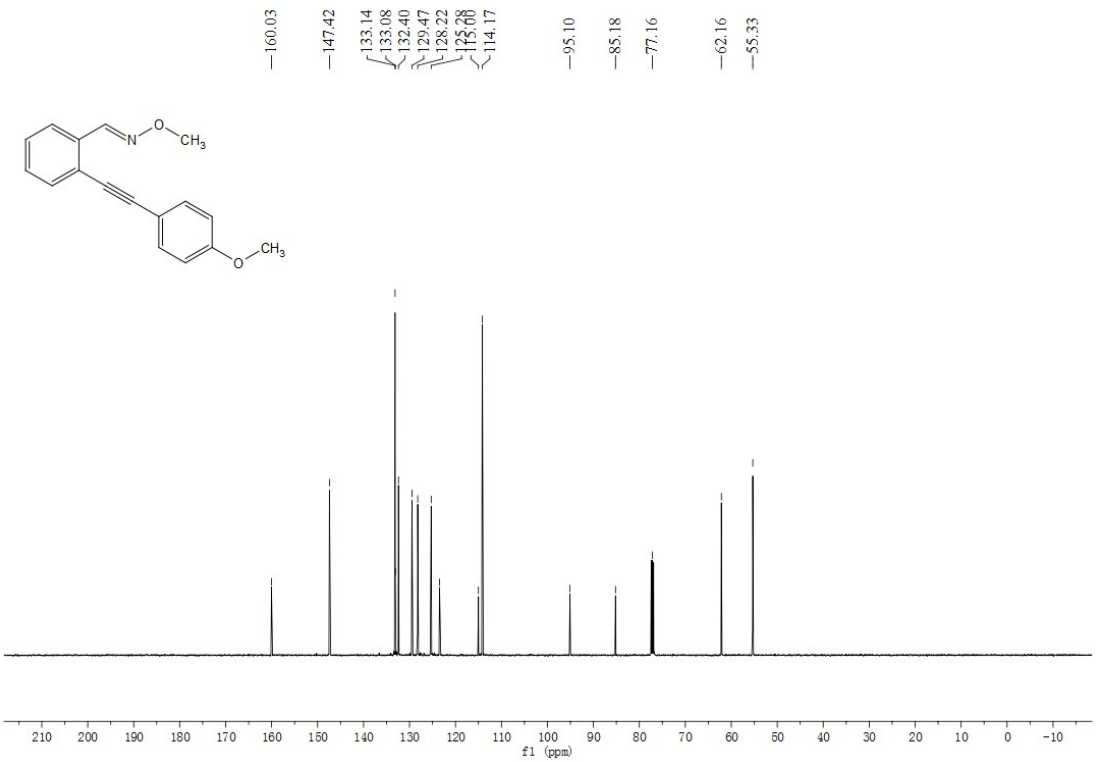
^{1}H NMR 500 MHz, in $CDCl_3$: 2-((4-(tert-butyl)phenyl)ethynyl)benzaldehyde O-methyl oxime (1af)



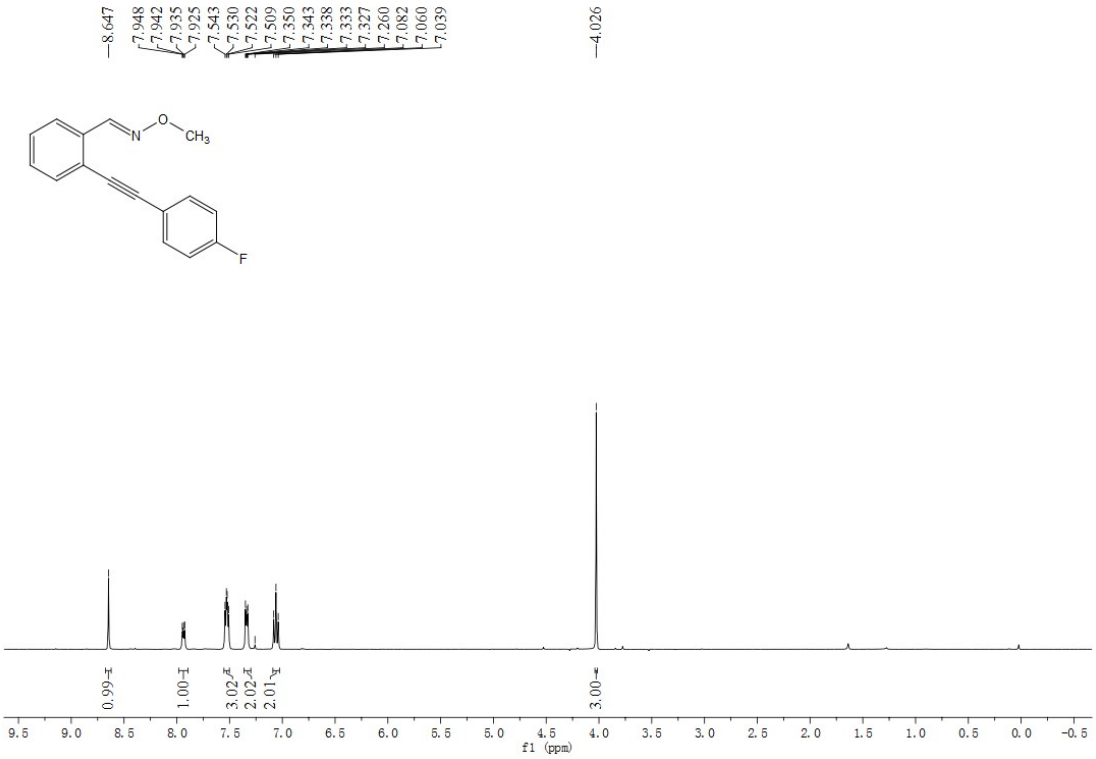
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 2-((4-(tert-butyl)phenyl)ethynyl)benzaldehyde O-methyl oxime (1af)



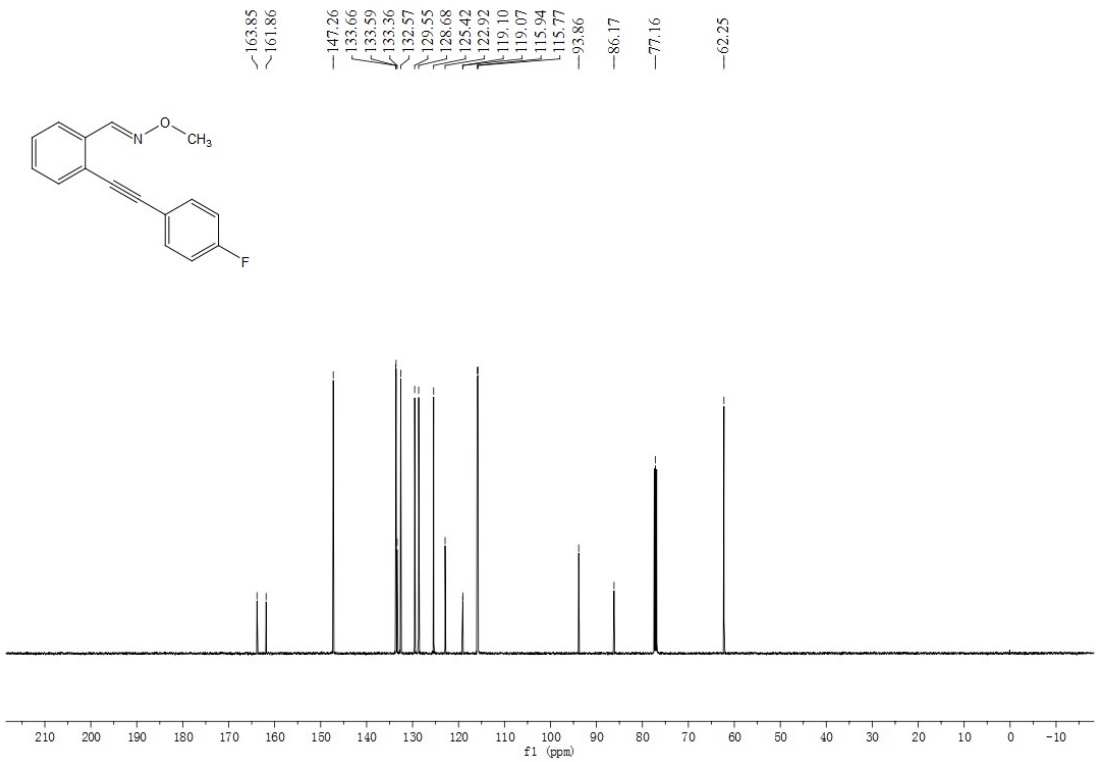
^{1}H NMR 500 MHz, in $CDCl_3$: 2-((4-methoxyphenyl)ethynyl)benzaldehyde O-methyl oxime (1ag)



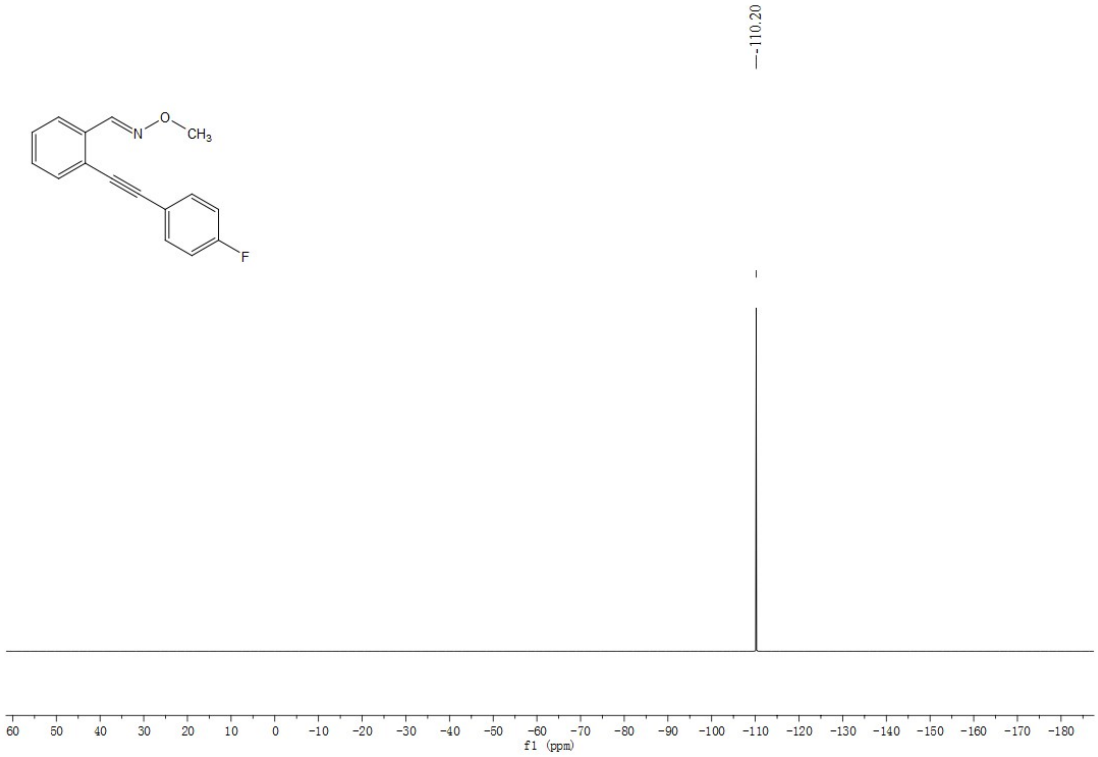
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 2-((4-methoxyphenyl)ethynyl)benzaldehyde O-methyl oxime (1ag)



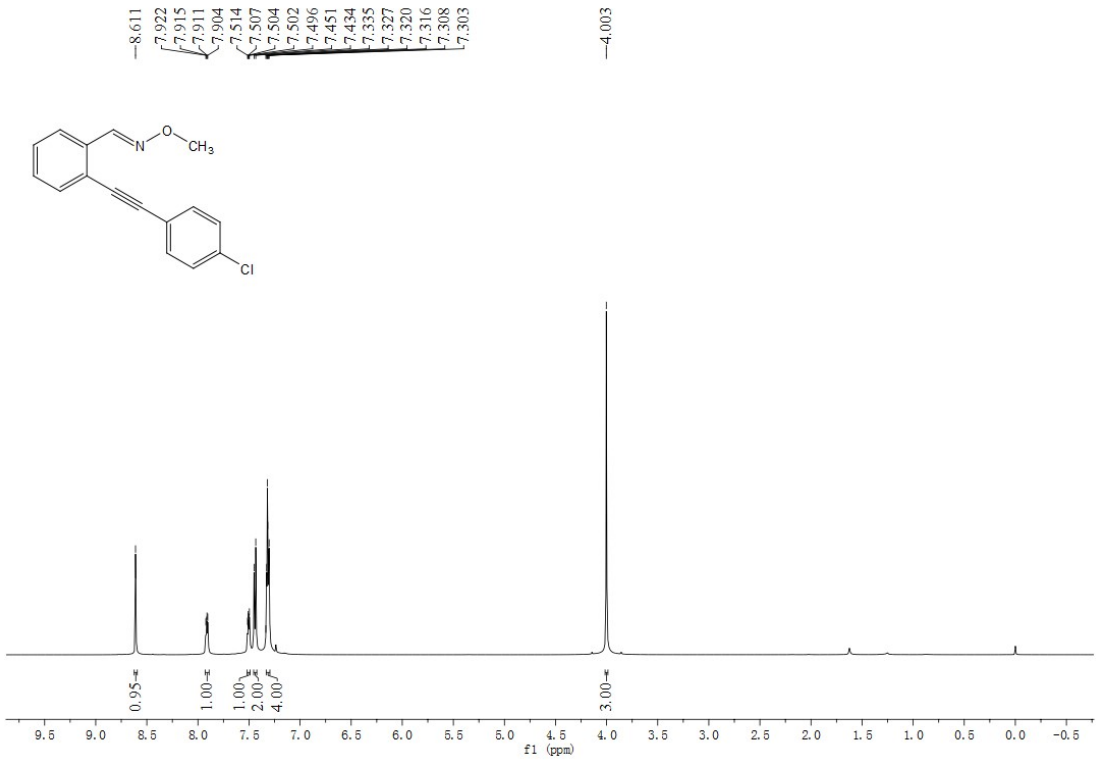
^{1}H NMR 500 MHz, in $CDCl_3$: 2-((4-fluorophenyl)ethynyl)benzaldehyde O-methyl oxime (1ah)



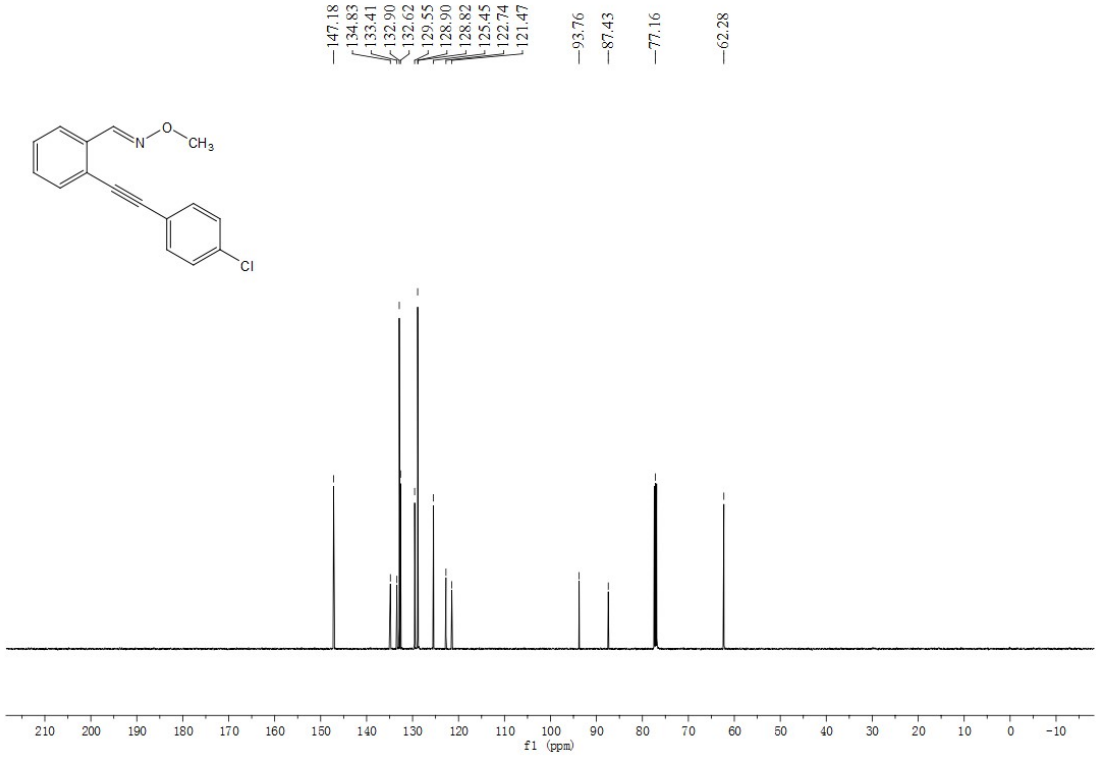
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 2-((4-fluorophenyl)ethynyl)benzaldehyde O-methyl oxime (1ah)



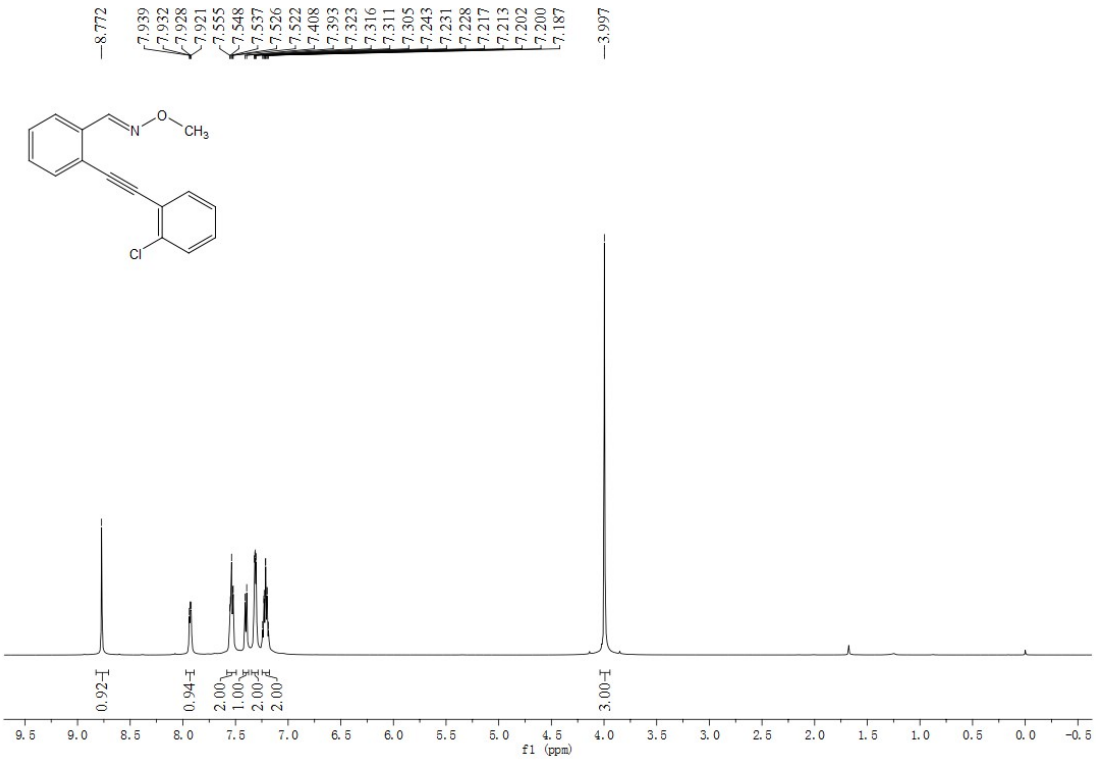
^{19}F NMR 470 MHz, in $CDCl_3$: 2-((4-fluorophenyl)ethynyl)benzaldehyde O-methyl oxime (1ah)



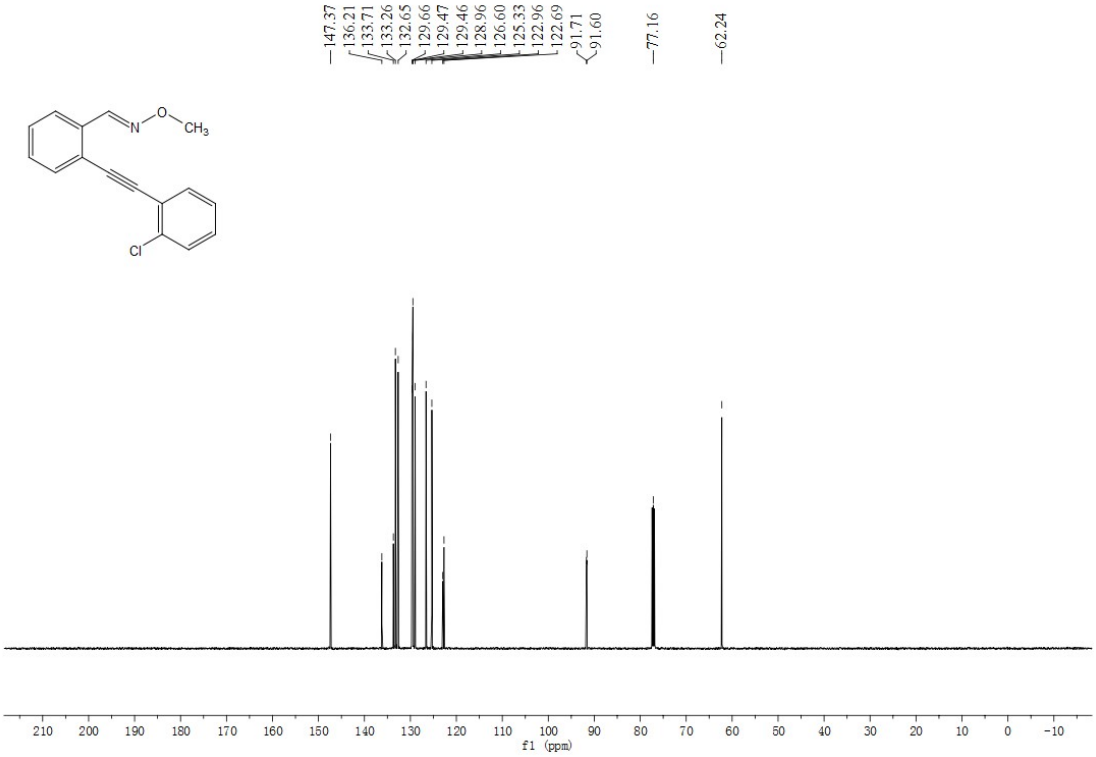
^{1}H NMR 500 MHz, in $CDCl_3$: 2-((4-chlorophenyl)ethynyl)benzaldehyde O-methyl oxime (1ai)



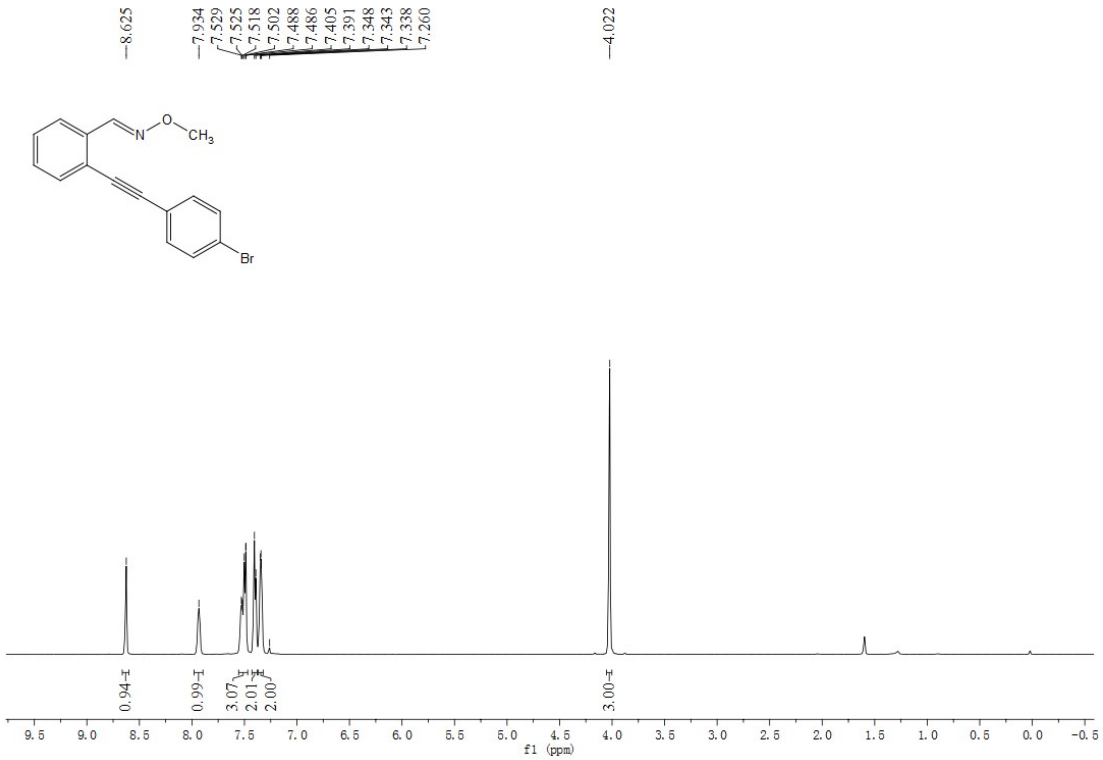
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 2-((4-chlorophenyl)ethynyl)benzaldehyde O-methyl oxime (1ai)



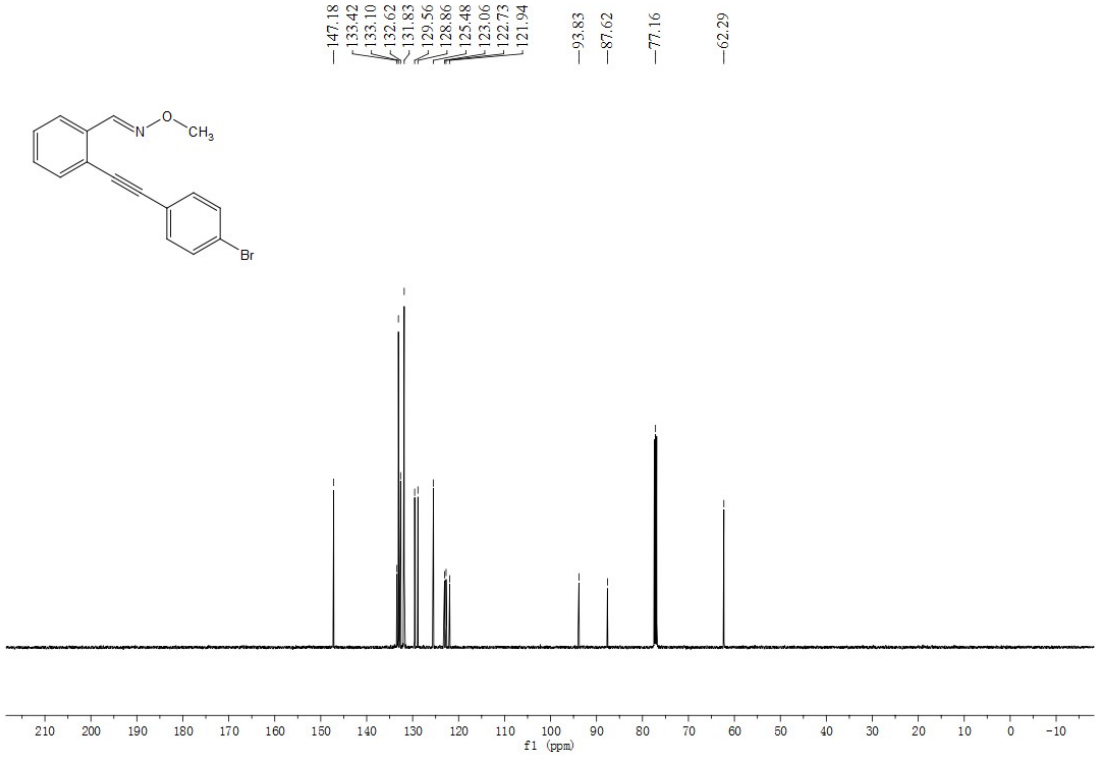
^{1}H NMR 500 MHz, in $CDCl_3$: 2-((2-chlorophenyl)ethynyl)benzaldehyde O-methyl oxime (1aj)



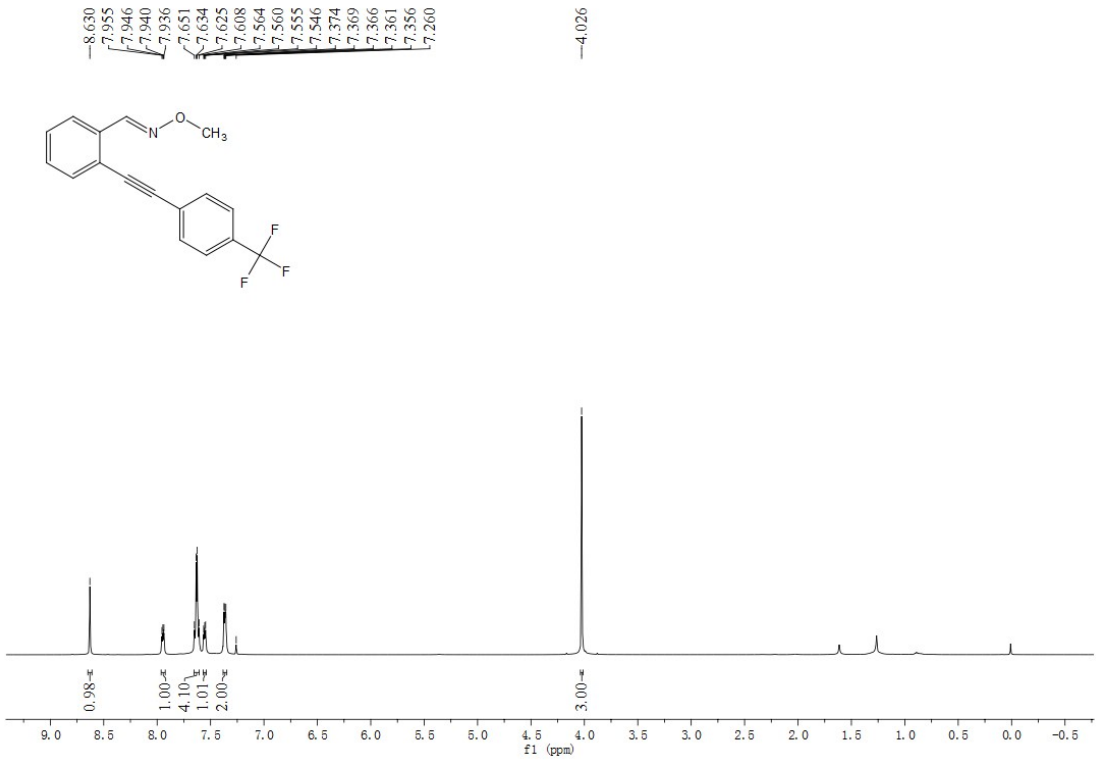
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 2-((2-chlorophenyl)ethynyl)benzaldehyde O-methyl oxime (1aj)



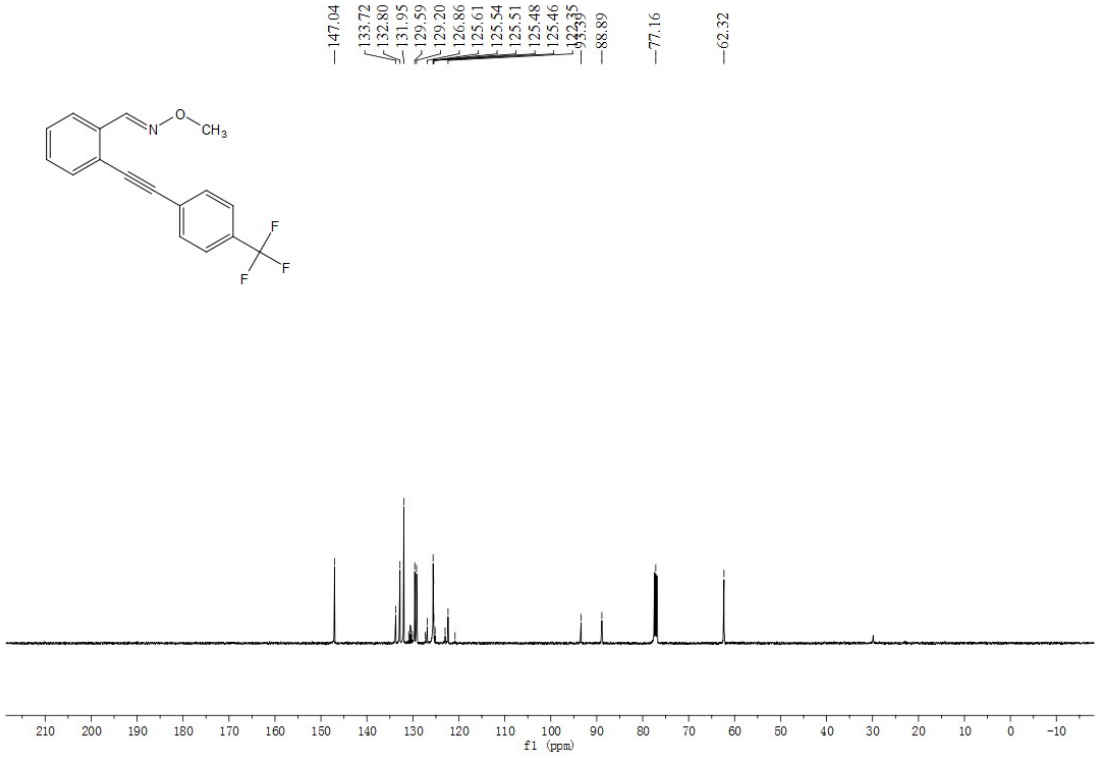
^{1}H NMR 500 MHz, in $CDCl_3$: 2-((4-bromophenyl)ethynyl)benzaldehyde O-methyl oxime (1ak)



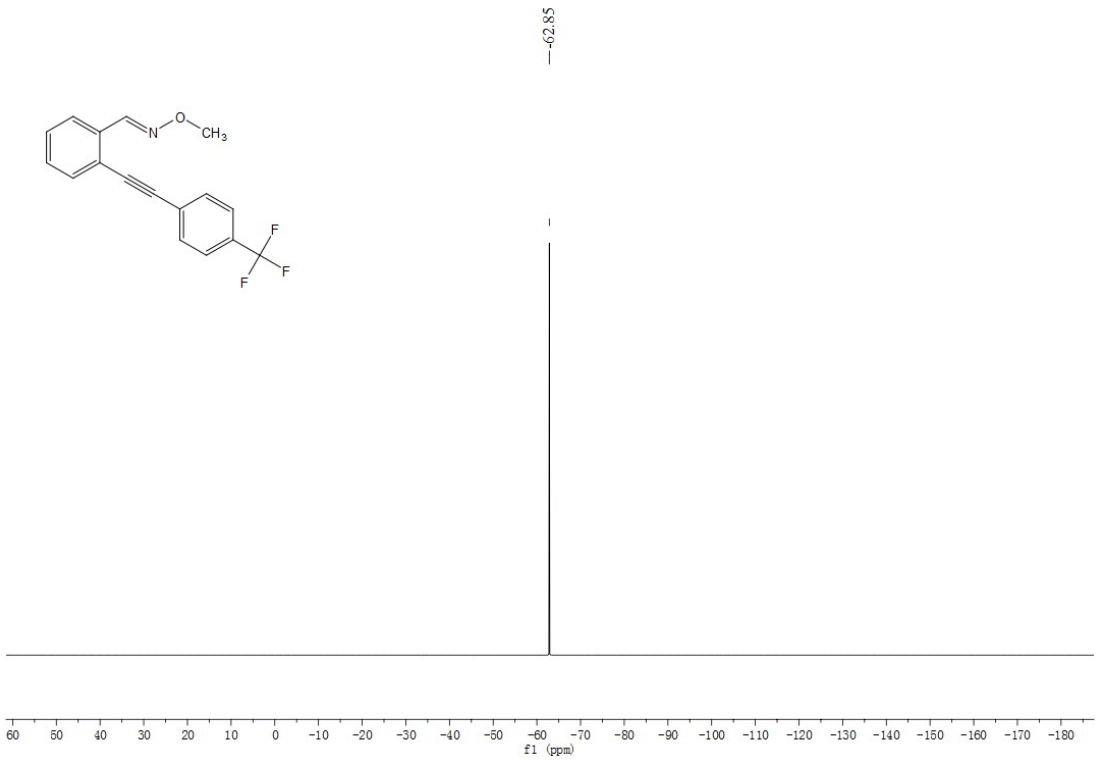
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 2-((4-bromophenyl)ethynyl)benzaldehyde O-methyl oxime (1ak)



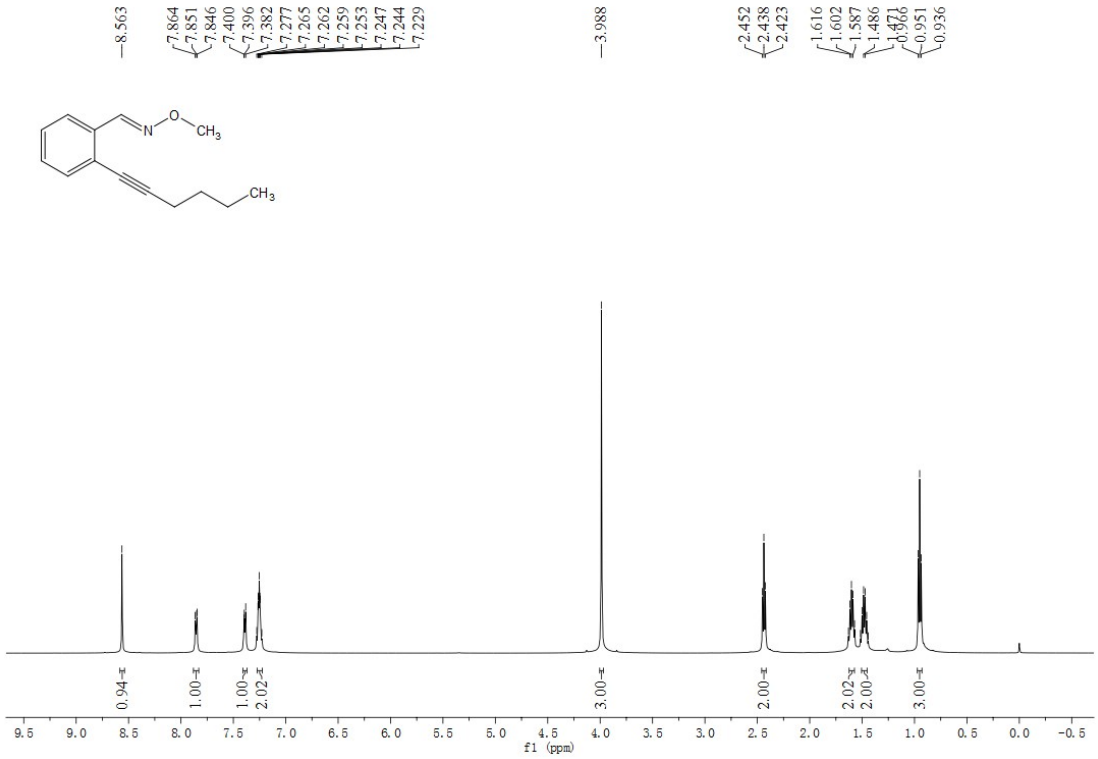
^{1}H NMR 500 MHz, in $CDCl_3$: 2-((4-(trifluoromethyl)phenyl)ethynyl)benzaldehyde O-methyl oxime (1al)



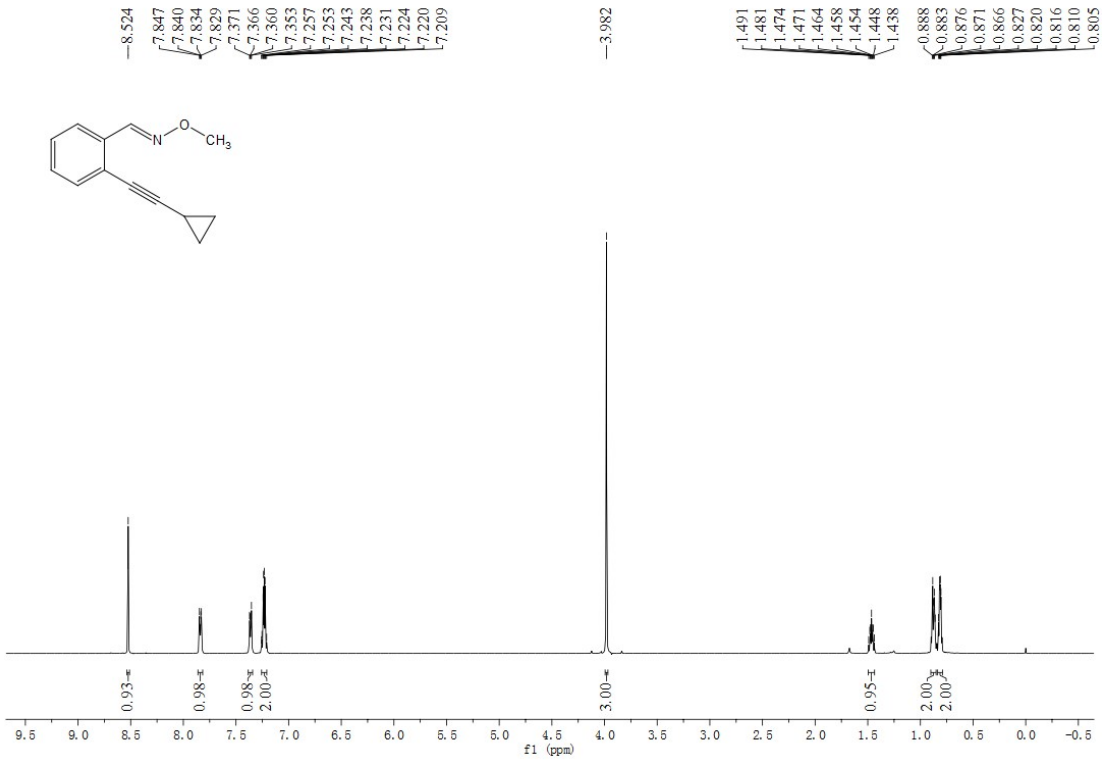
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 2-((4-(trifluoromethyl)phenyl)ethynyl)benzaldehyde O-methyl oxime (1al)



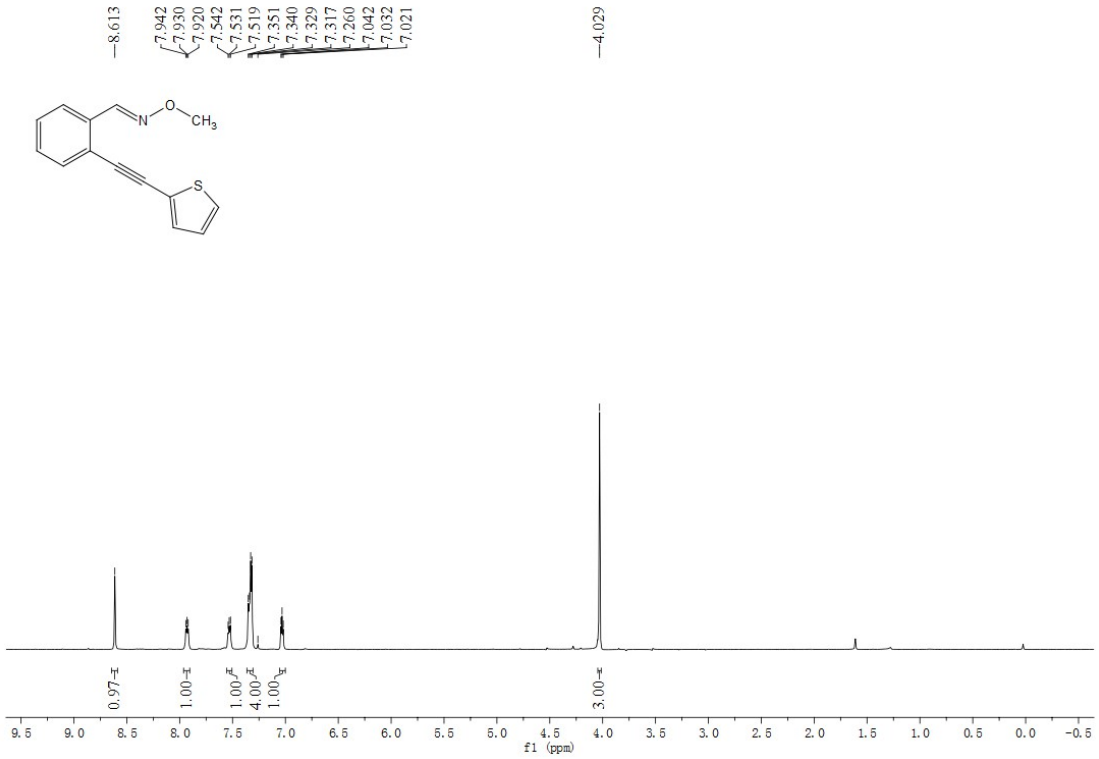
^{19}F NMR 470 MHz, in $CDCl_3$: 2-((4-(trifluoromethyl)phenyl)ethynyl)benzaldehyde O-methyl oxime (1al)



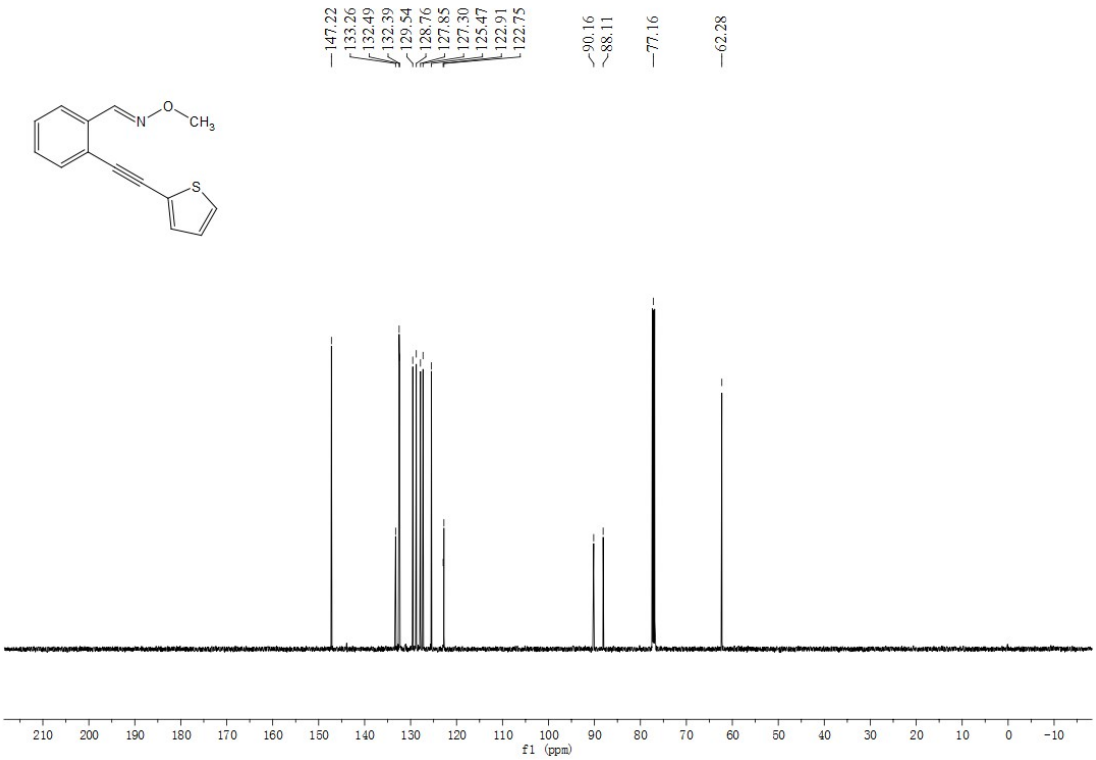
^{1}H NMR 500 MHz, in $CDCl_3$: 2-(hex-1-yn-1-yl)benzaldehyde O-methyl oxime (1am)



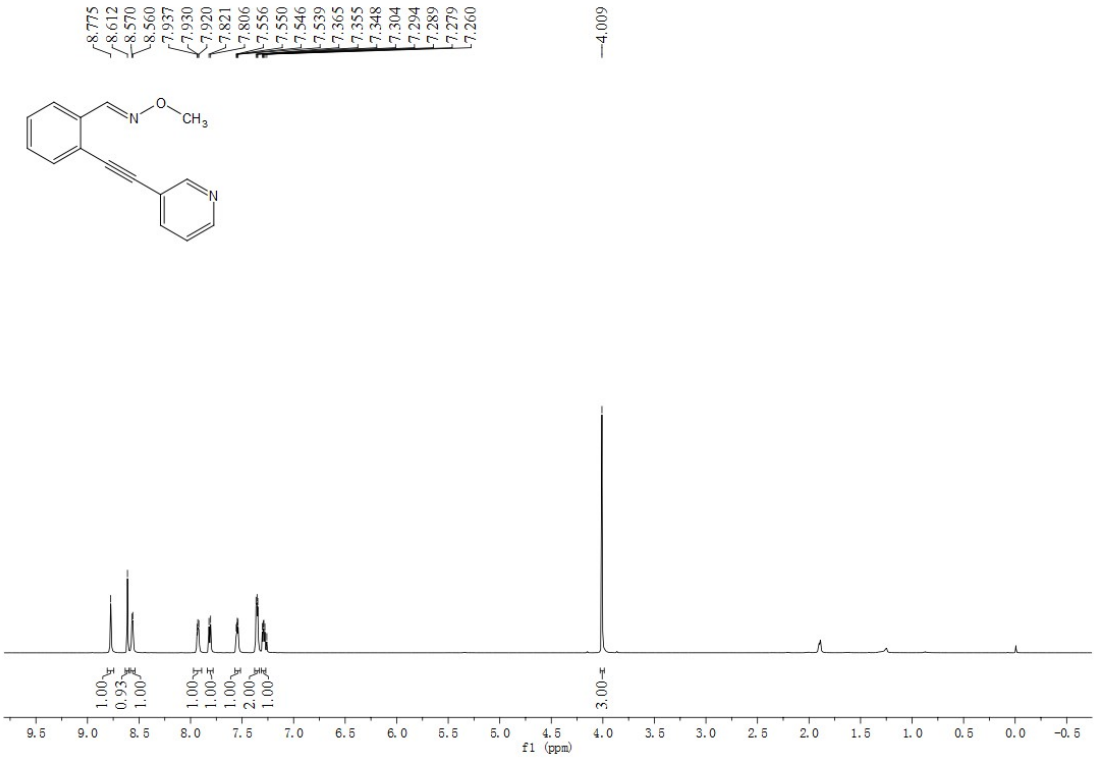
^{1}H NMR 500 MHz, in $CDCl_3$: 2-(cyclopropylethynyl)benzaldehyde O-methyl oxime (1an)



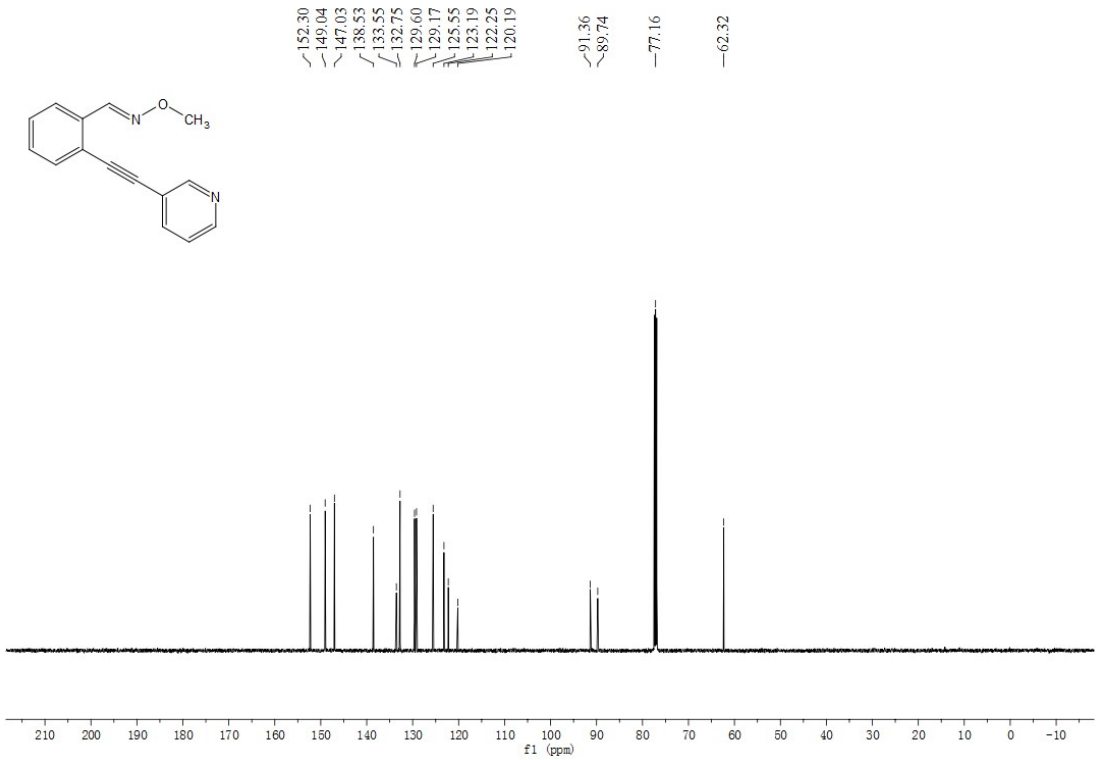
^{1}H NMR 400 MHz, in $CDCl_3$: 2-(thiophen-2-ylethynyl)benzaldehyde O-methyl oxime (1ao)



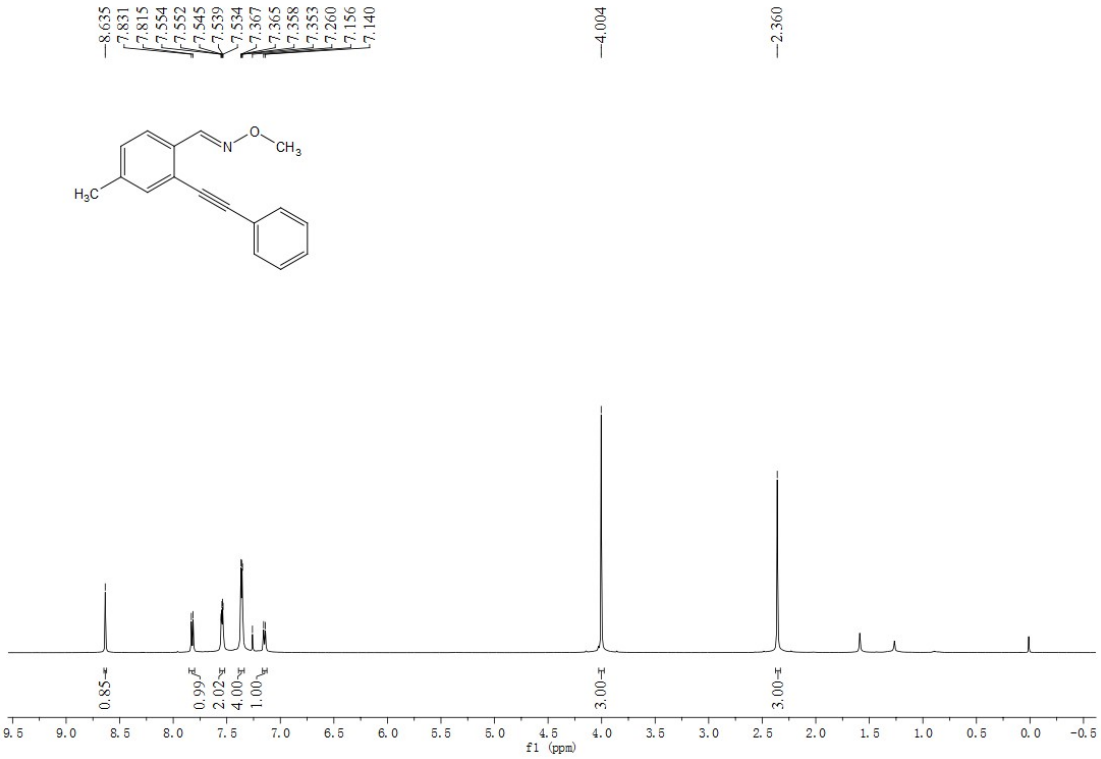
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 2-(thiophen-2-ylethynyl)benzaldehyde O-methyl oxime (1ao)



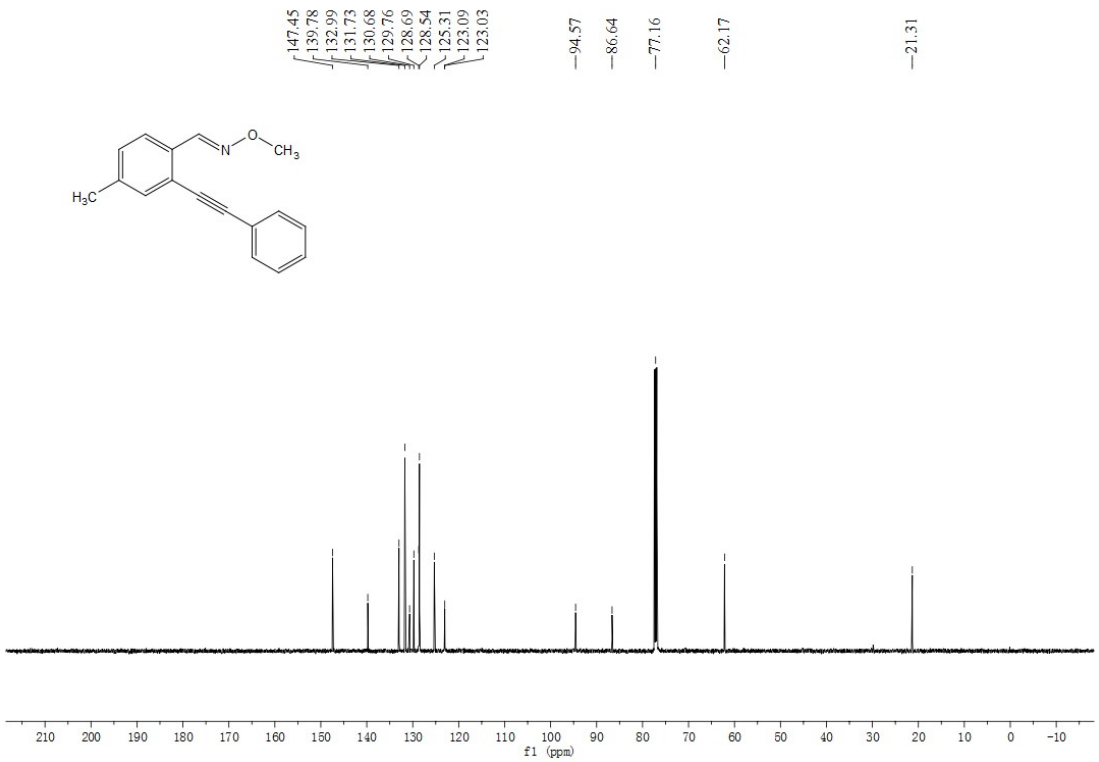
^{1}H NMR 500 MHz, in $CDCl_3$: 2-(pyridin-3-ylethynyl)benzaldehyde O-methyl oxime (1ap)



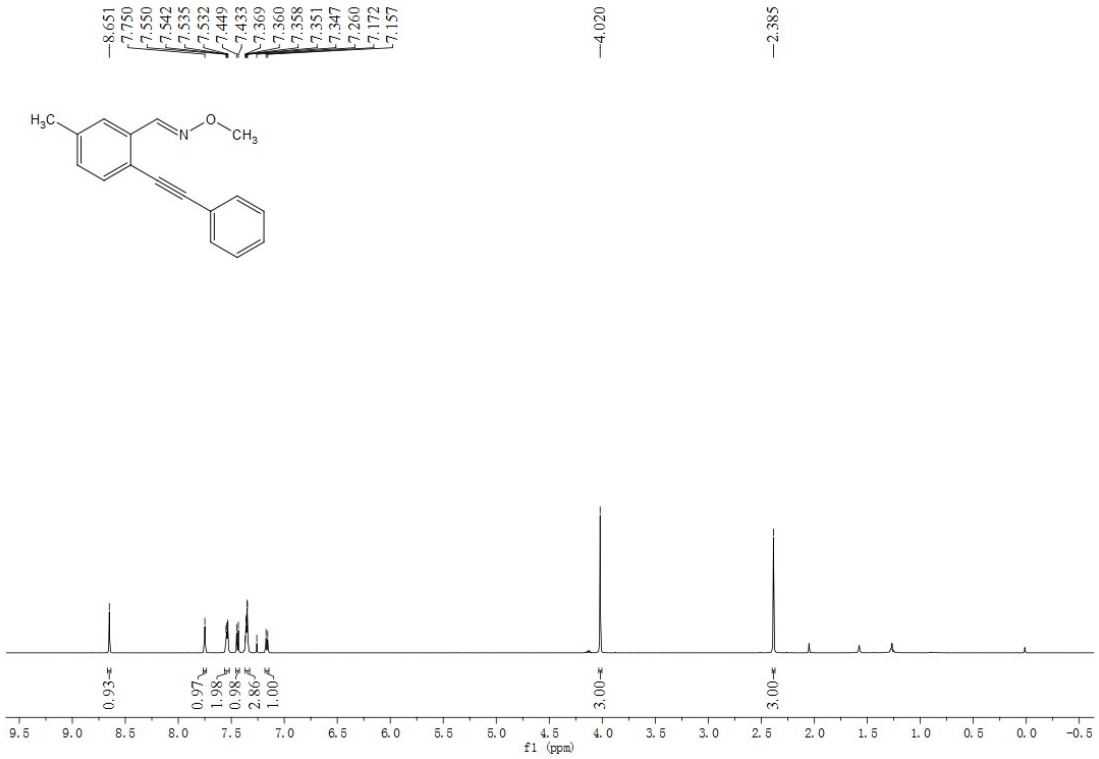
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 2-(pyridin-3-ylethynyl)benzaldehyde O-methyl oxime (1ap)



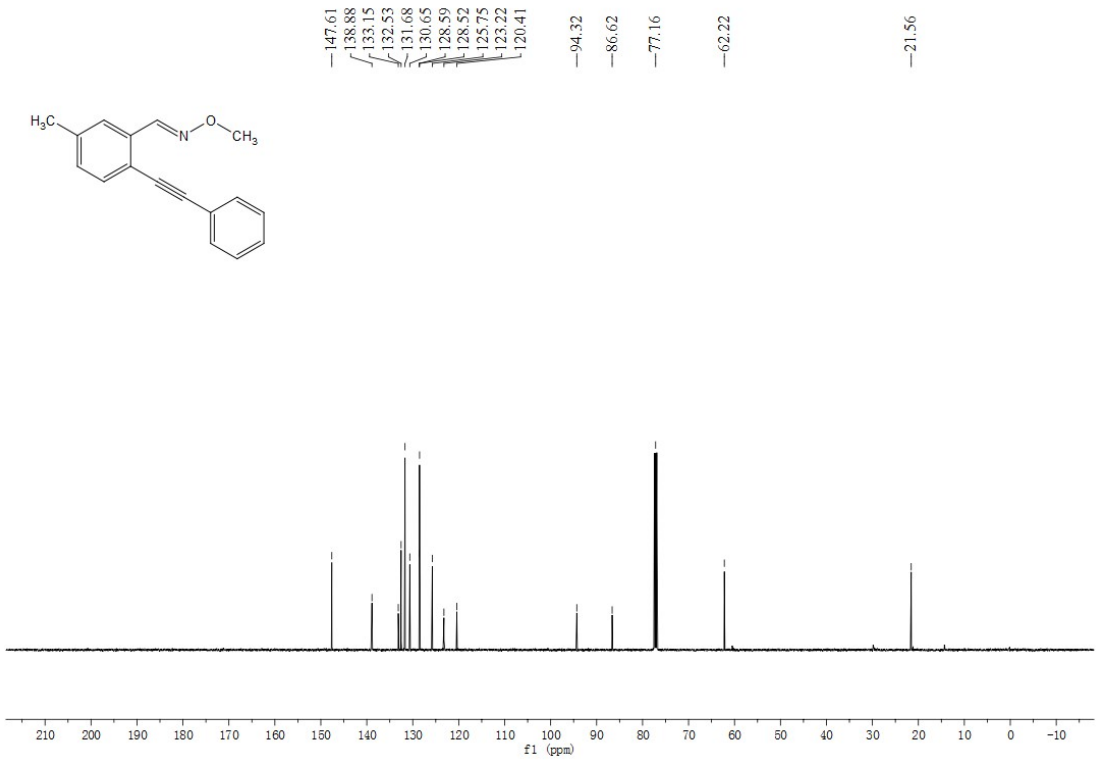
^{1}H NMR 500 MHz, in $CDCl_3$: 4-methyl-2-(phenylethynyl)benzaldehyde O-methyl oxime (1aq)



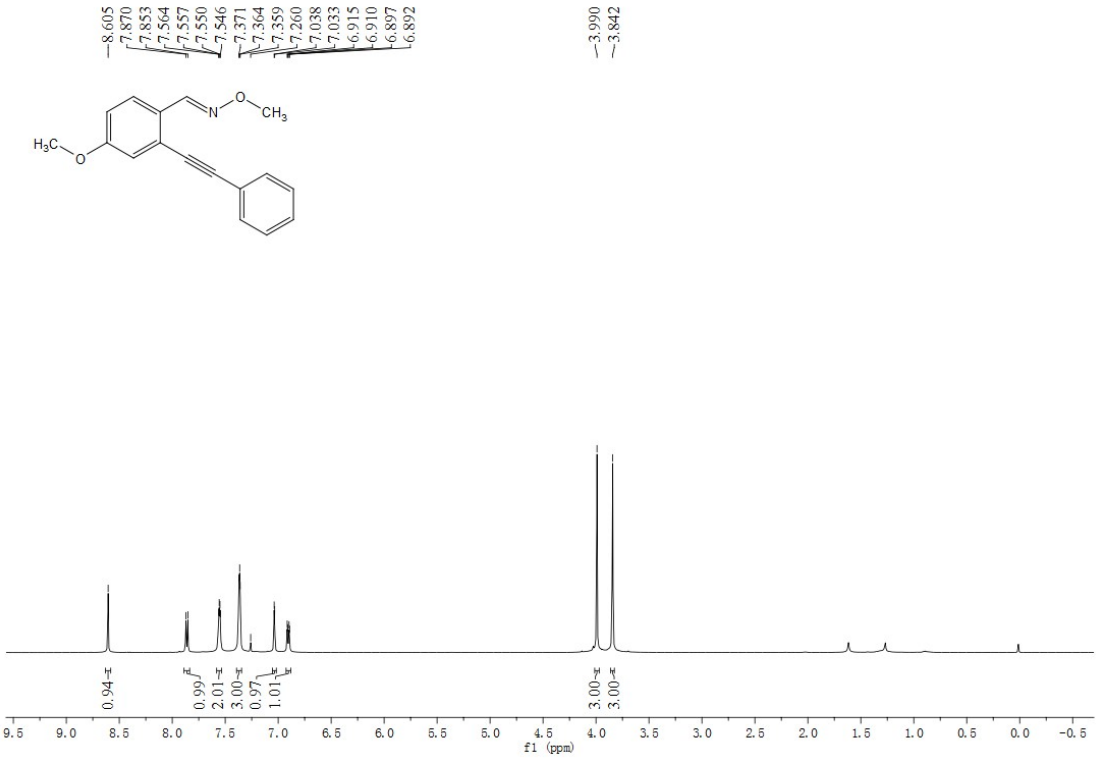
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 4-methyl-2-(phenylethynyl)benzaldehyde O-methyl oxime (1aq)



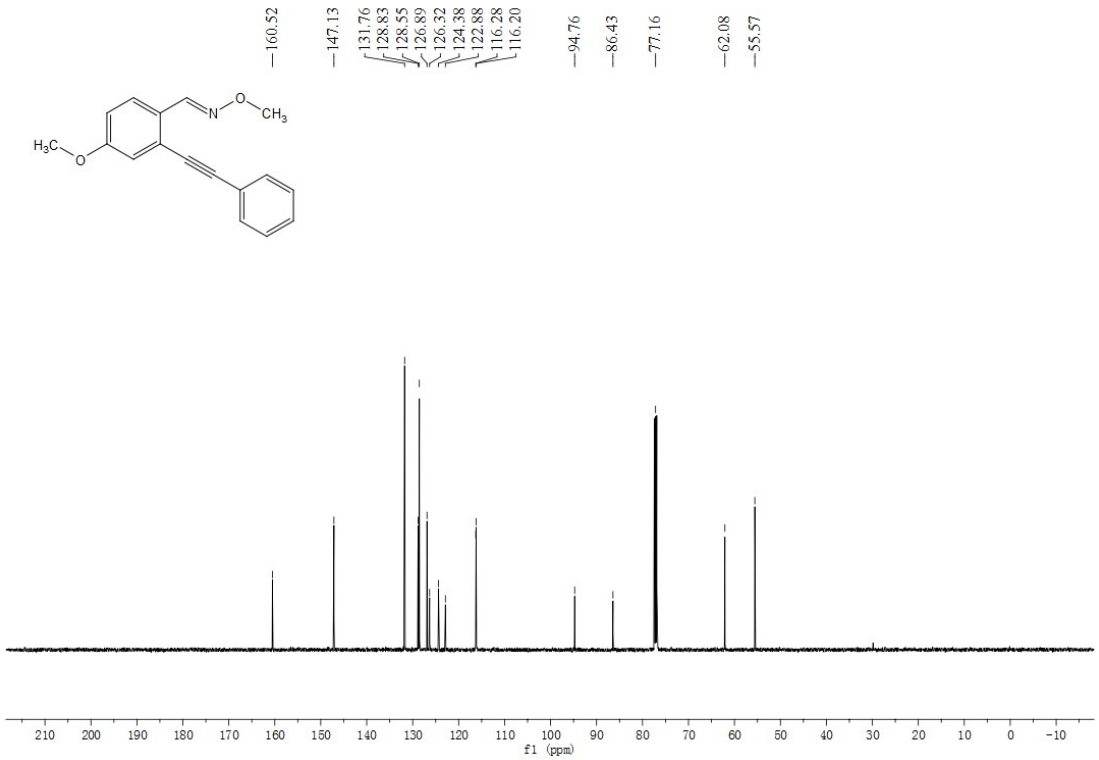
^{1}H NMR 500 MHz, in $CDCl_3$: 5-methyl-2-(phenylethynyl)benzaldehyde O-methyl oxime (1ar)



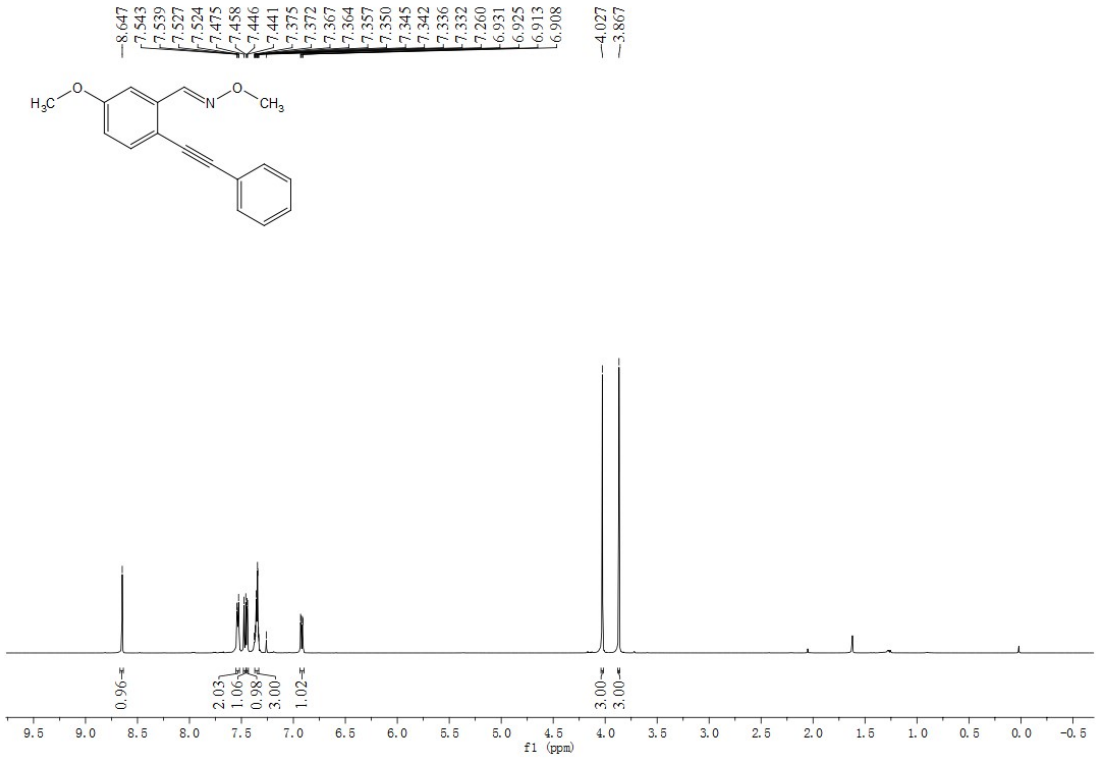
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 5-methyl-2-(phenylethynyl)benzaldehyde O-methyl oxime (1ar)



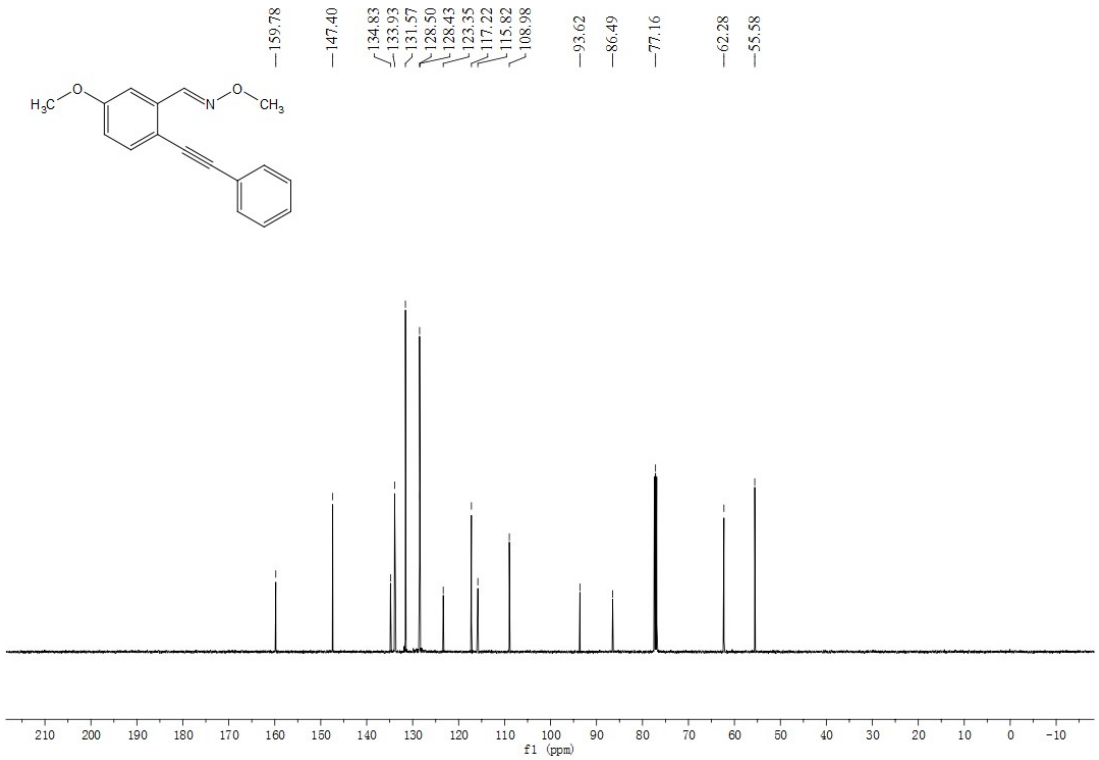
^{1}H NMR 500 MHz, in $CDCl_3$: 4-methoxy-2-(phenylethynyl)benzaldehyde O-methyl oxime (1as)



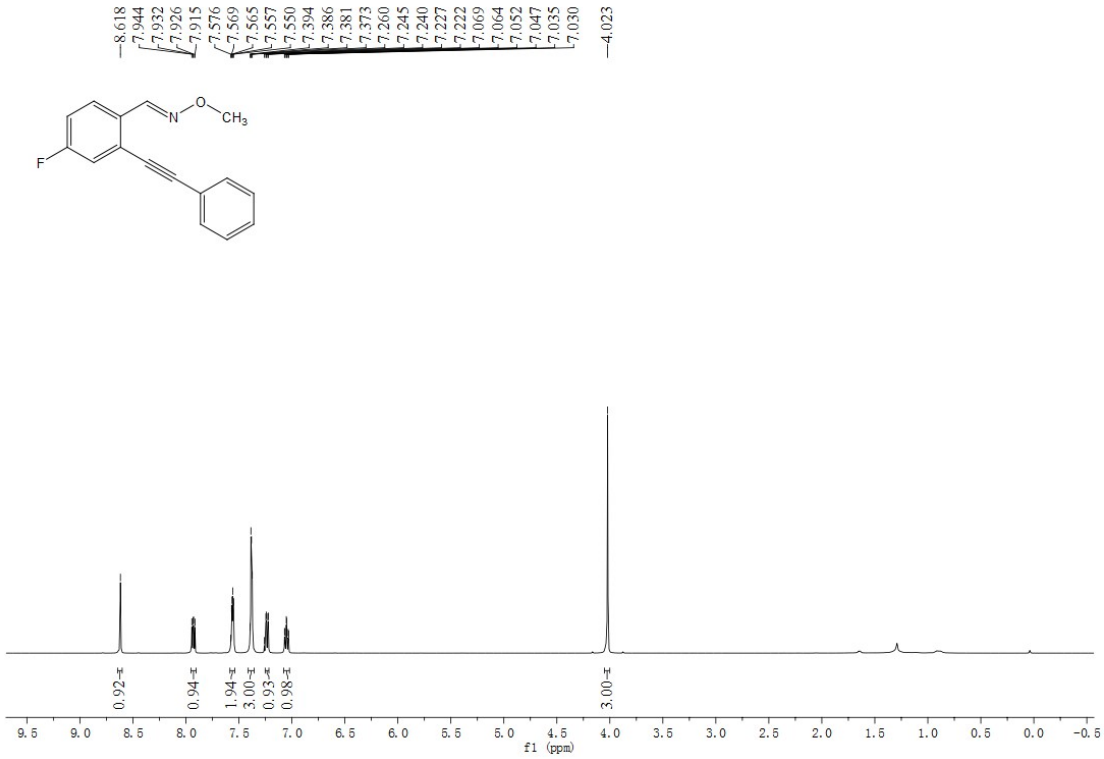
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 4-methoxy-2-(phenylethynyl)benzaldehyde O-methyl oxime (1as)



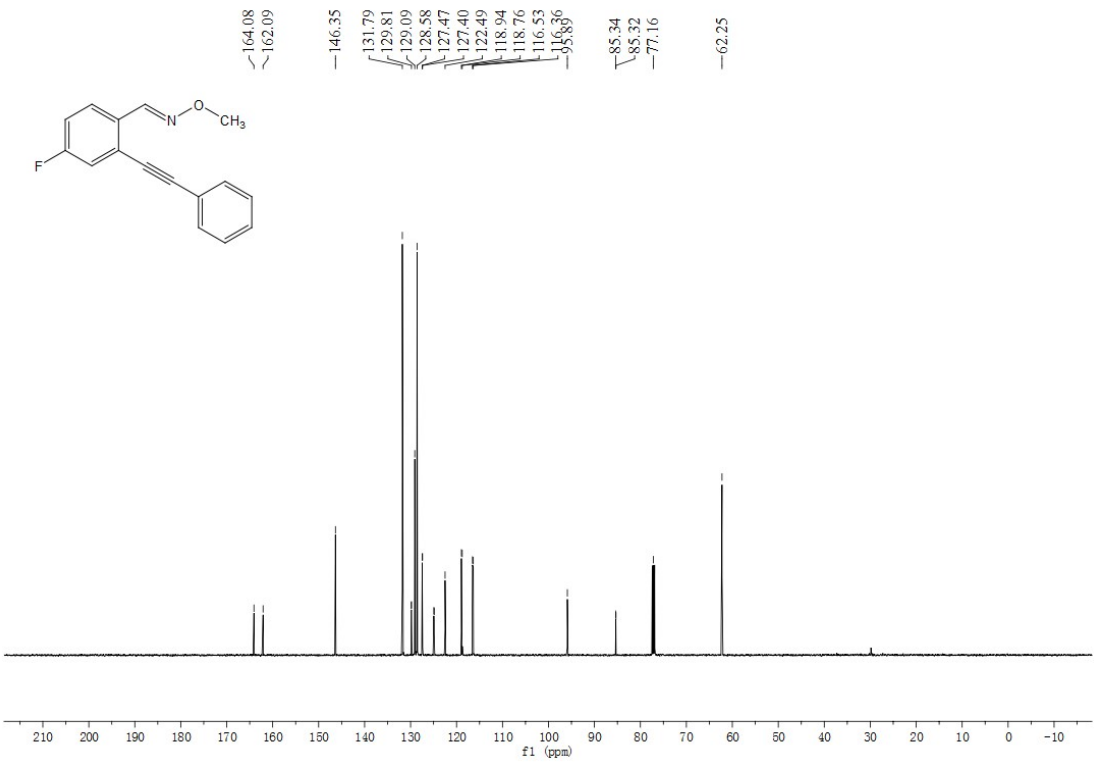
^{1}H NMR 500 MHz, in $CDCl_3$: 5-methoxy-2-(phenylethynyl)benzaldehyde O-methyl oxime (1at)



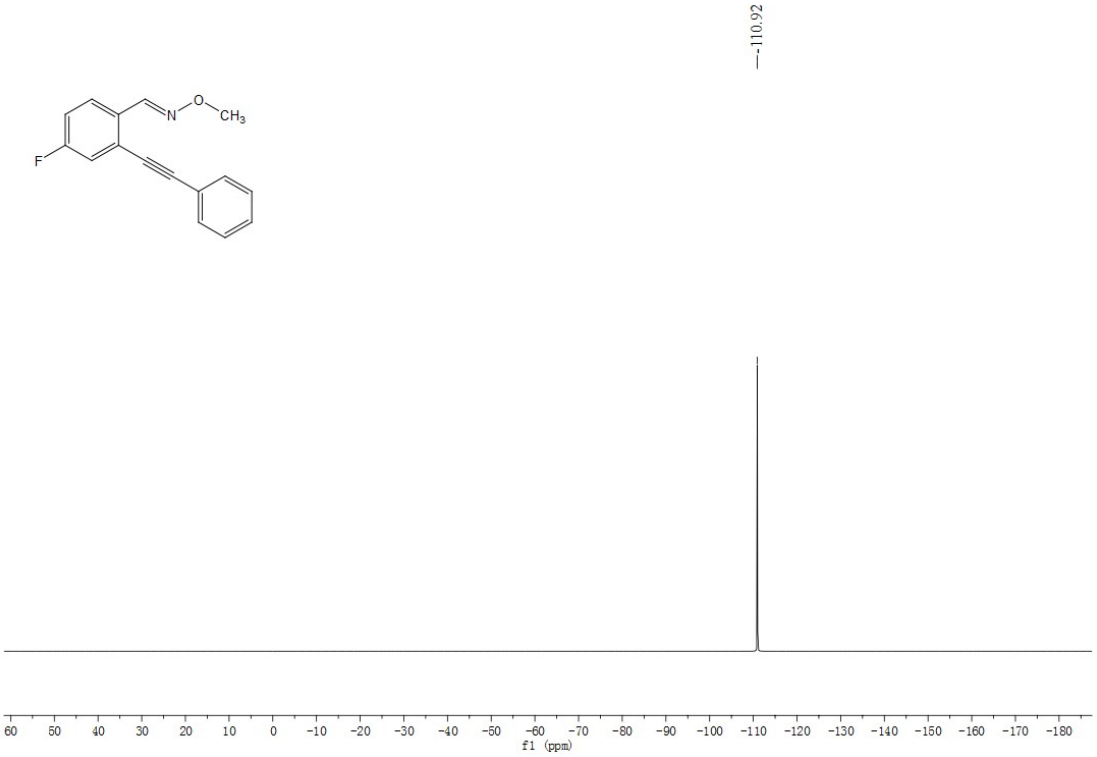
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 5-methoxy-2-(phenylethynyl)benzaldehyde O-methyl oxime (1at)



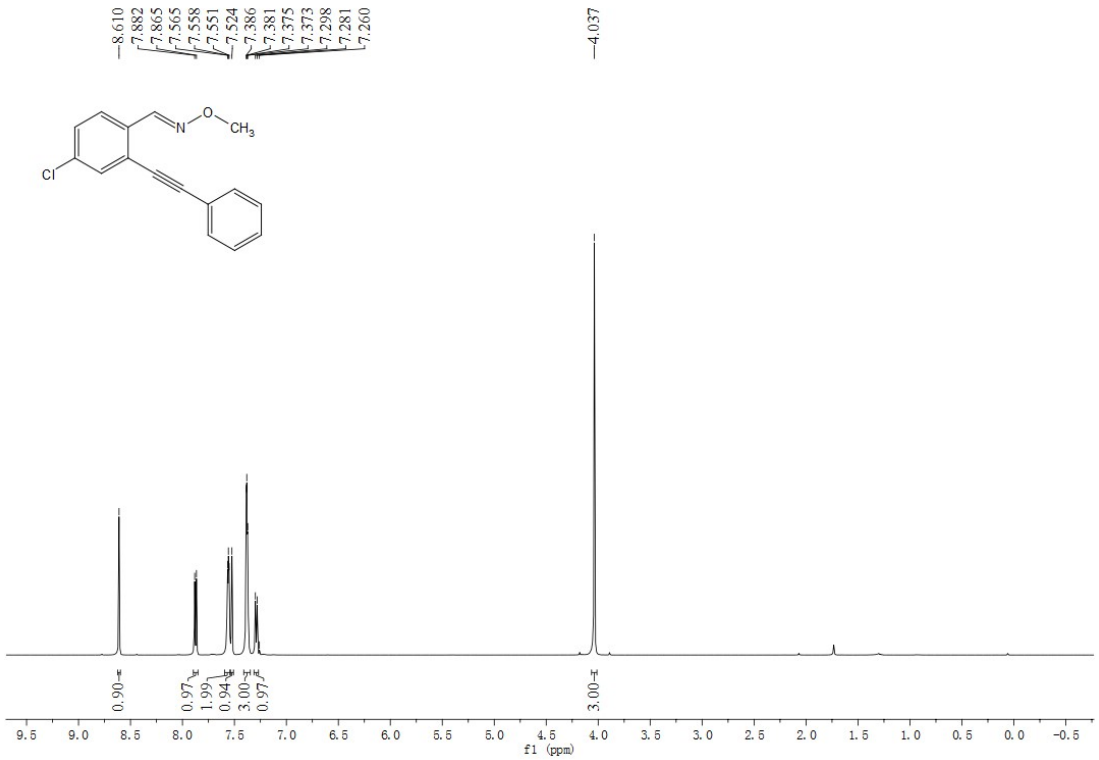
^{1}H NMR 500 MHz, in $CDCl_3$: 4-fluoro-2-(phenylethynyl)benzaldehyde O-methyl oxime (1au)



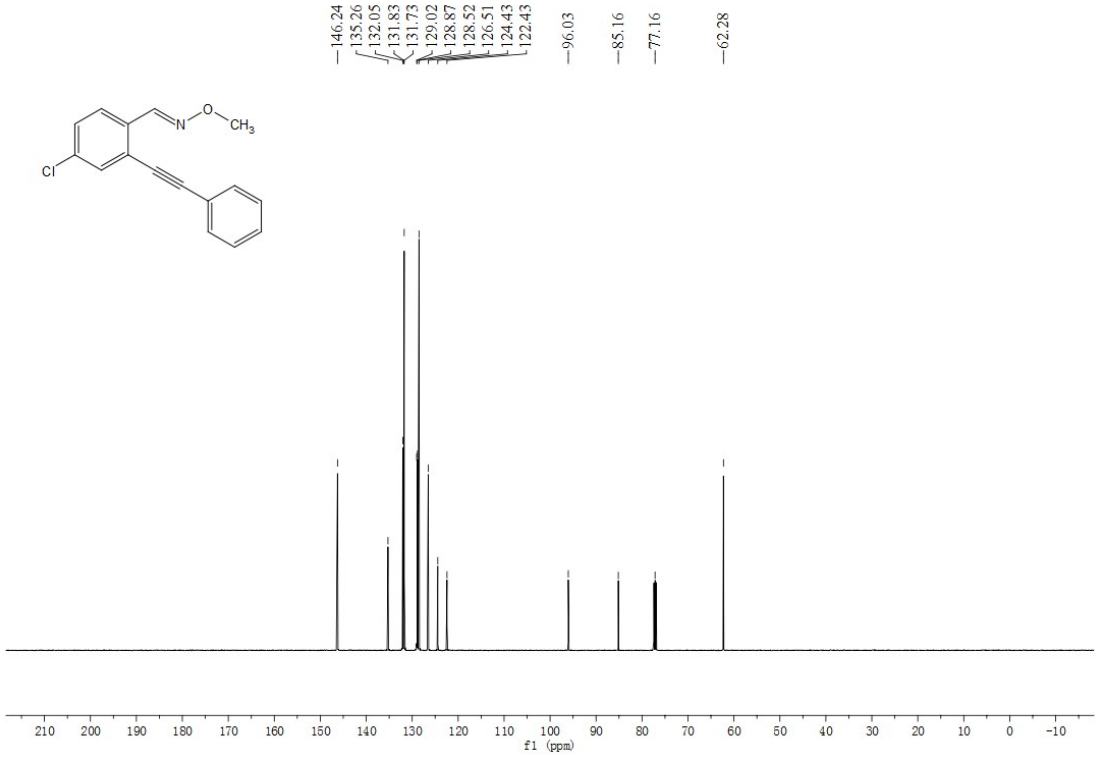
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 4-fluoro-2-(phenylethynyl)benzaldehyde O-methyl oxime (1au)



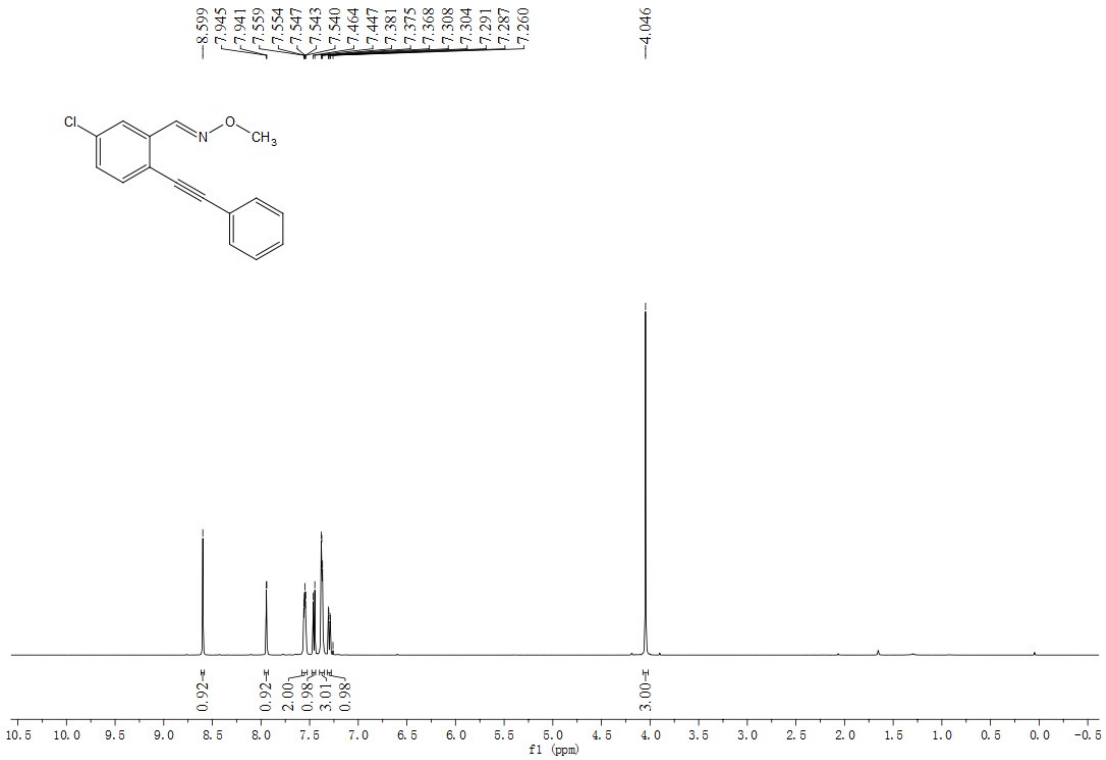
^{19}F NMR 470 MHz, in $CDCl_3$: 4-fluoro-2-(phenylethynyl)benzaldehyde O-methyl oxime (1au)



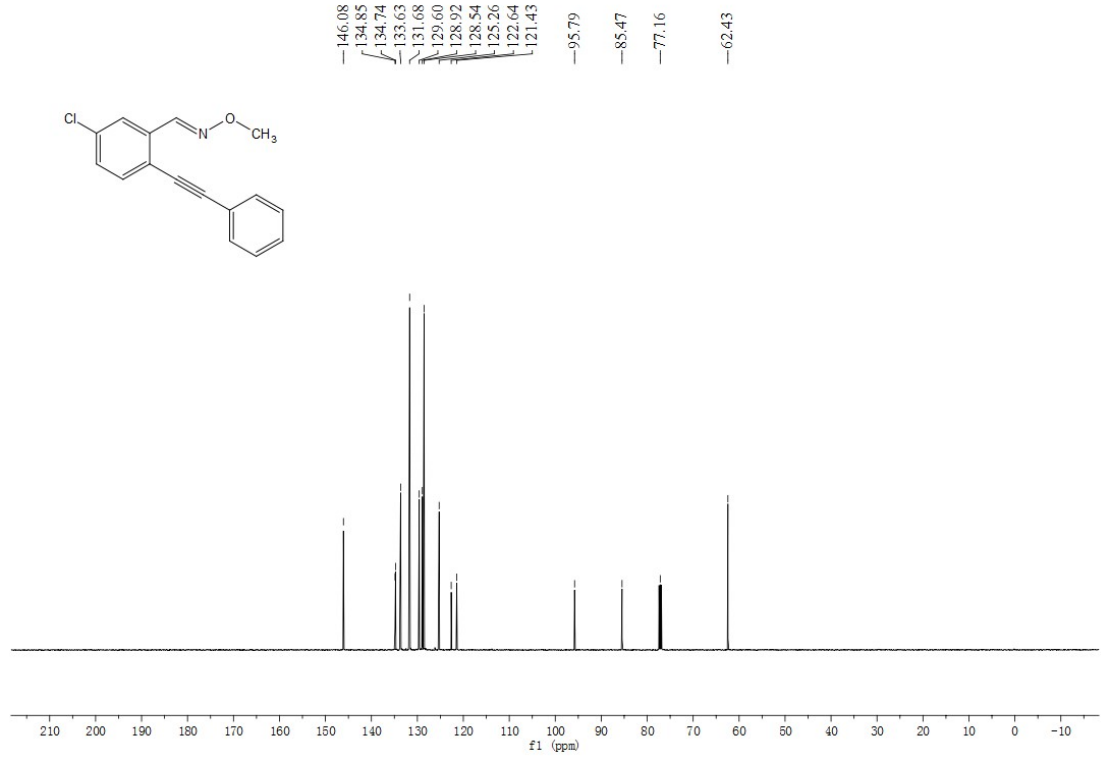
^{1}H NMR 500 MHz, in $CDCl_3$: 4-chloro-2-(phenylethynyl)benzaldehyde O-methyl oxime (1av)



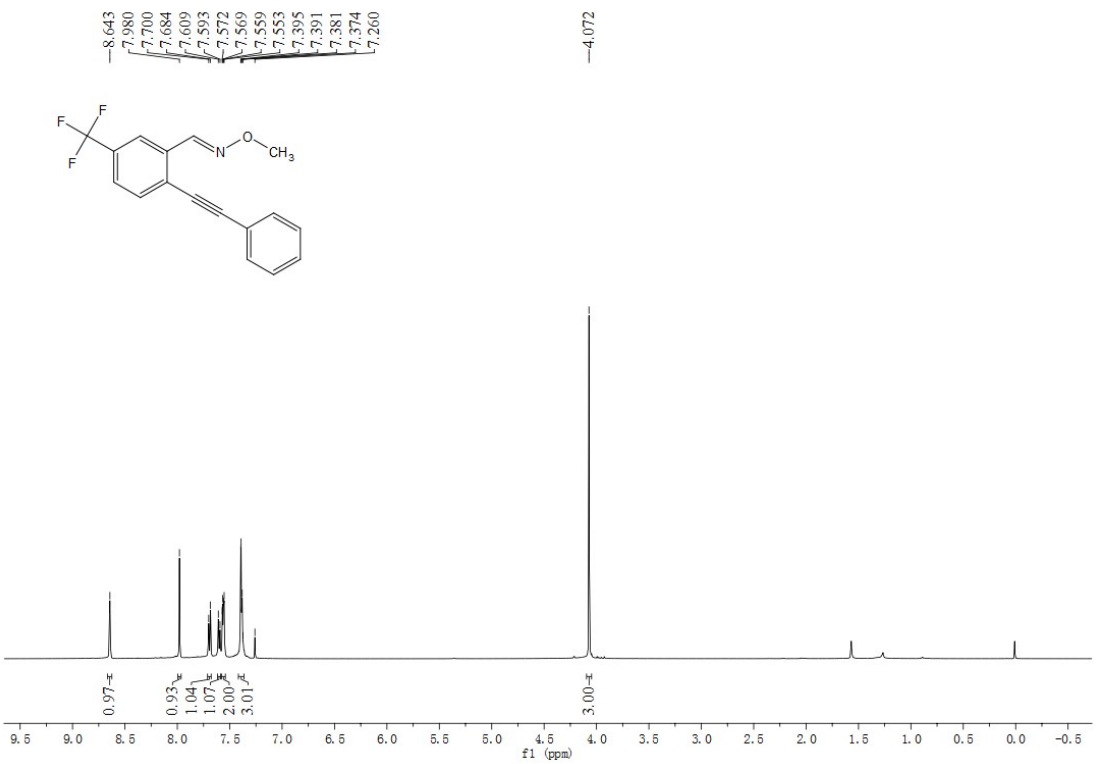
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 4-chloro-2-(phenylethynyl)benzaldehyde O-methyl oxime (1av)



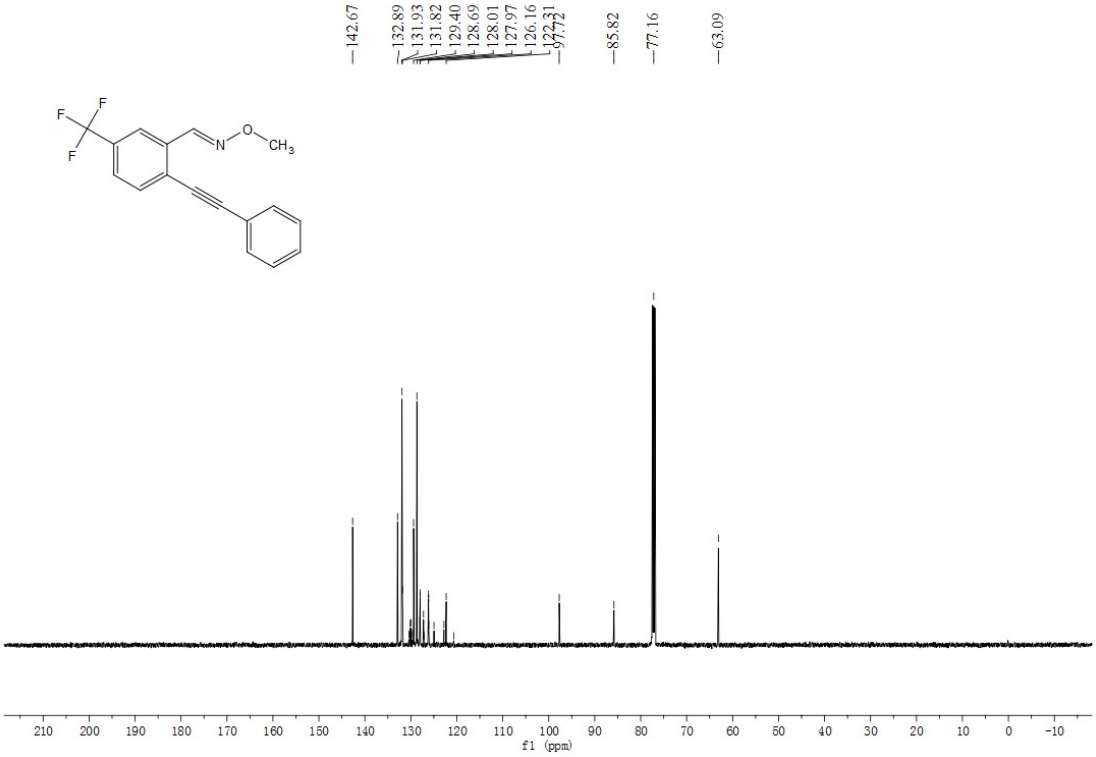
^{1}H NMR 500 MHz, in $CDCl_3$: 5-chloro-2-(phenylethynyl)benzaldehyde O-methyl oxime (1aw)



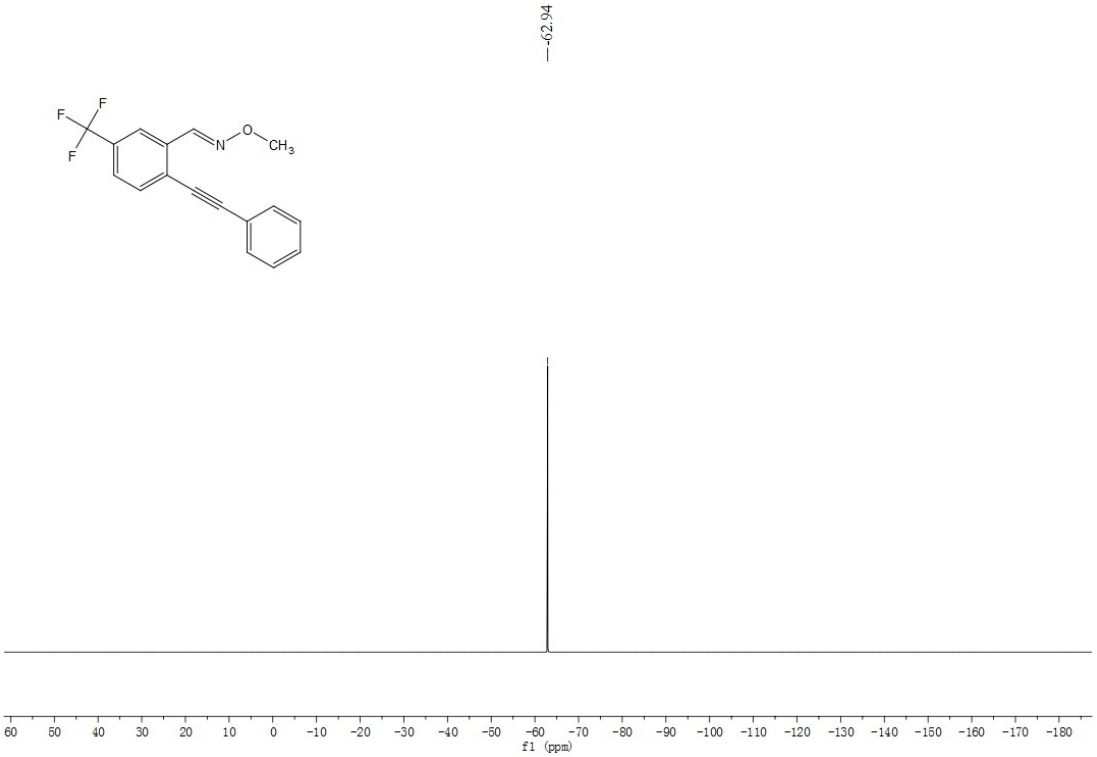
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 5-chloro-2-(phenylethynyl)benzaldehyde O-methyl oxime (1aw)



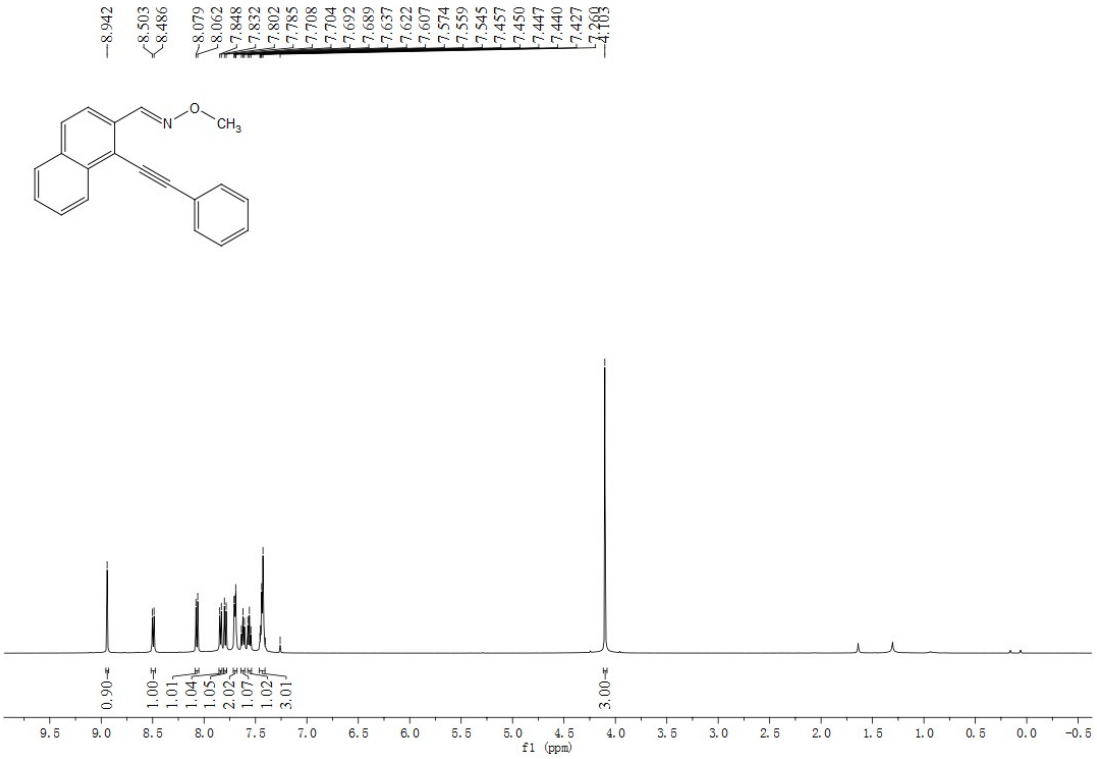
^{1}H NMR 500 MHz, in $CDCl_3$: 2-(phenylethynyl)-5-(trifluoromethyl)benzaldehyde O-methyl oxime (1ax)



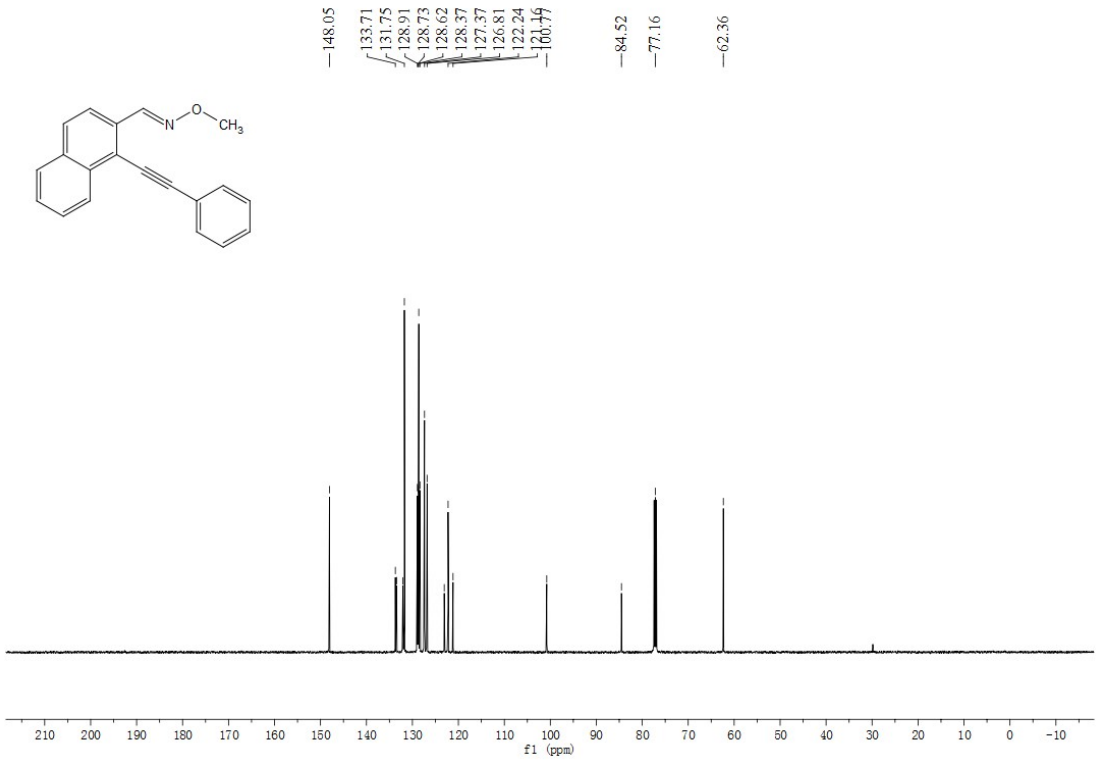
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 2-(phenylethynyl)-5-(trifluoromethyl)benzaldehyde O-methyl oxime (1ax)



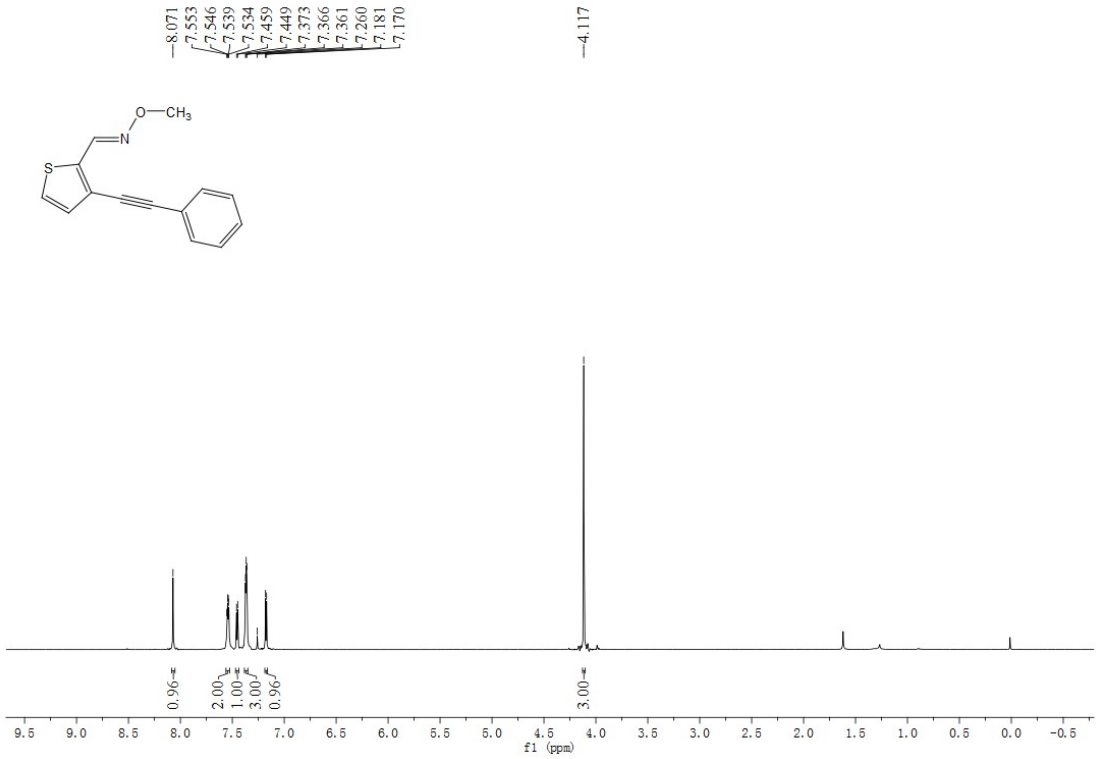
^{19}F NMR 470 MHz, in $CDCl_3$: 2-(phenylethynyl)-5-(trifluoromethyl)benzaldehyde O-methyl oxime (1ax)



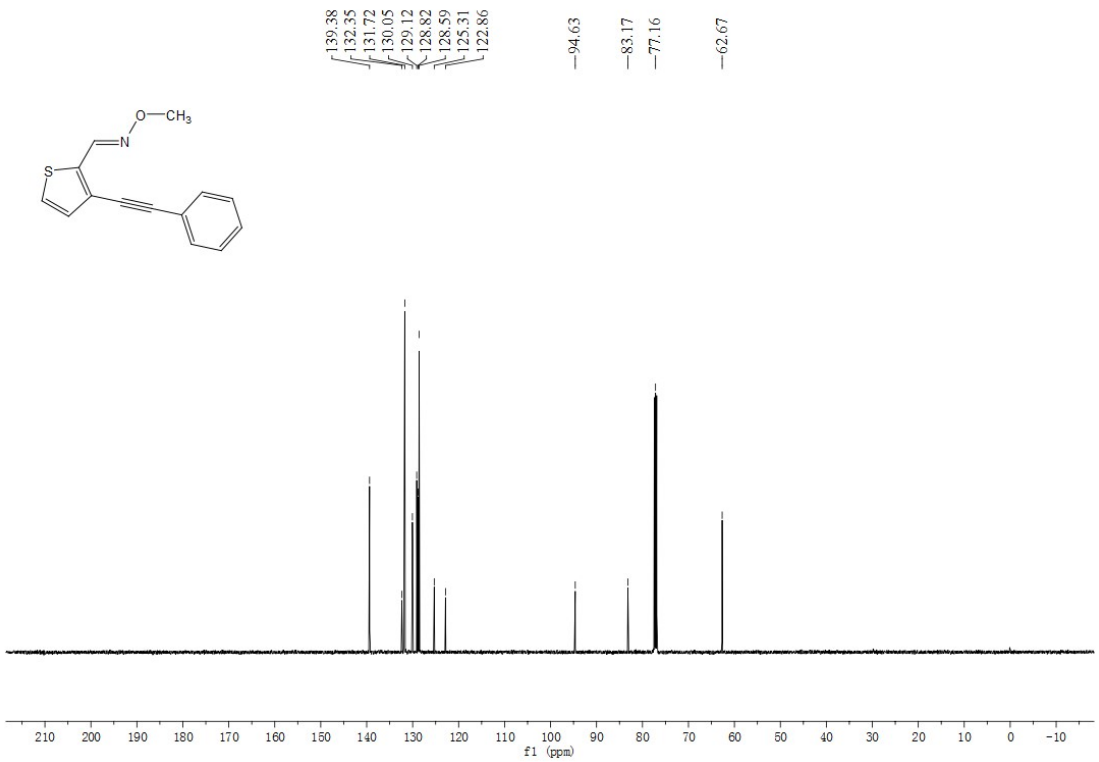
^{1}H NMR 500 MHz, in $CDCl_3$: 1-(phenylethynyl)-2-naphthaldehyde O-methyl oxime (1ay)



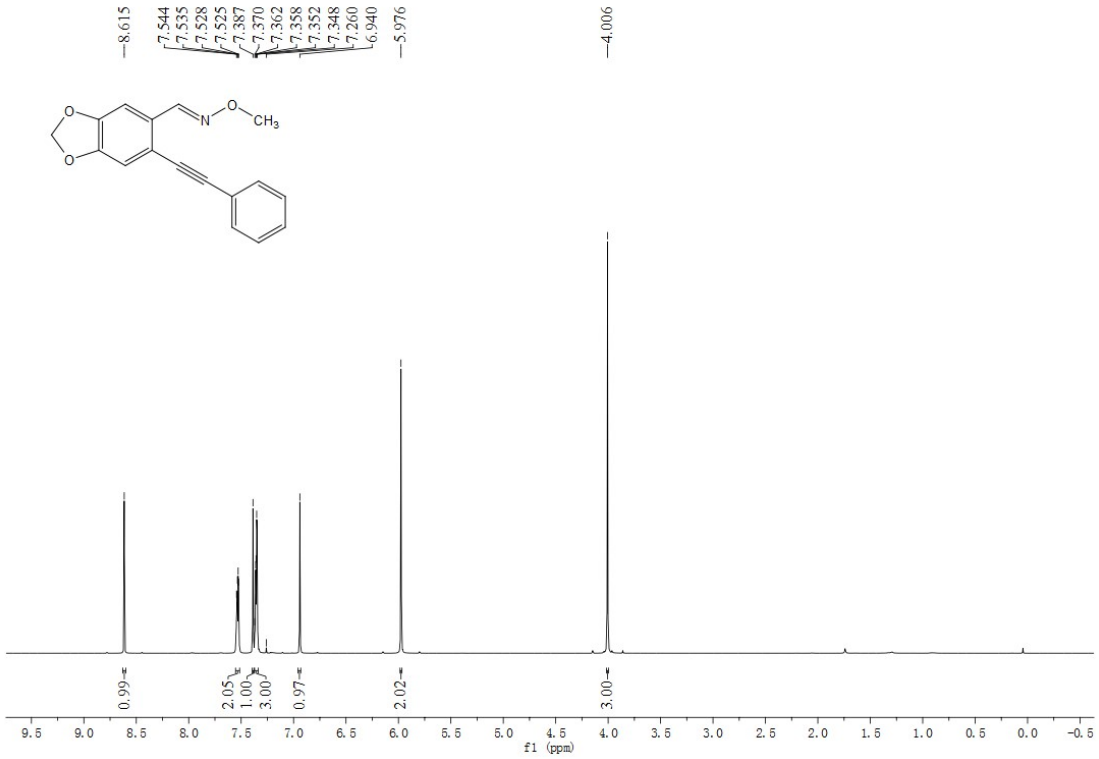
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 1-(phenylethynyl)-2-naphthaldehyde O-methyl oxime (1ay)



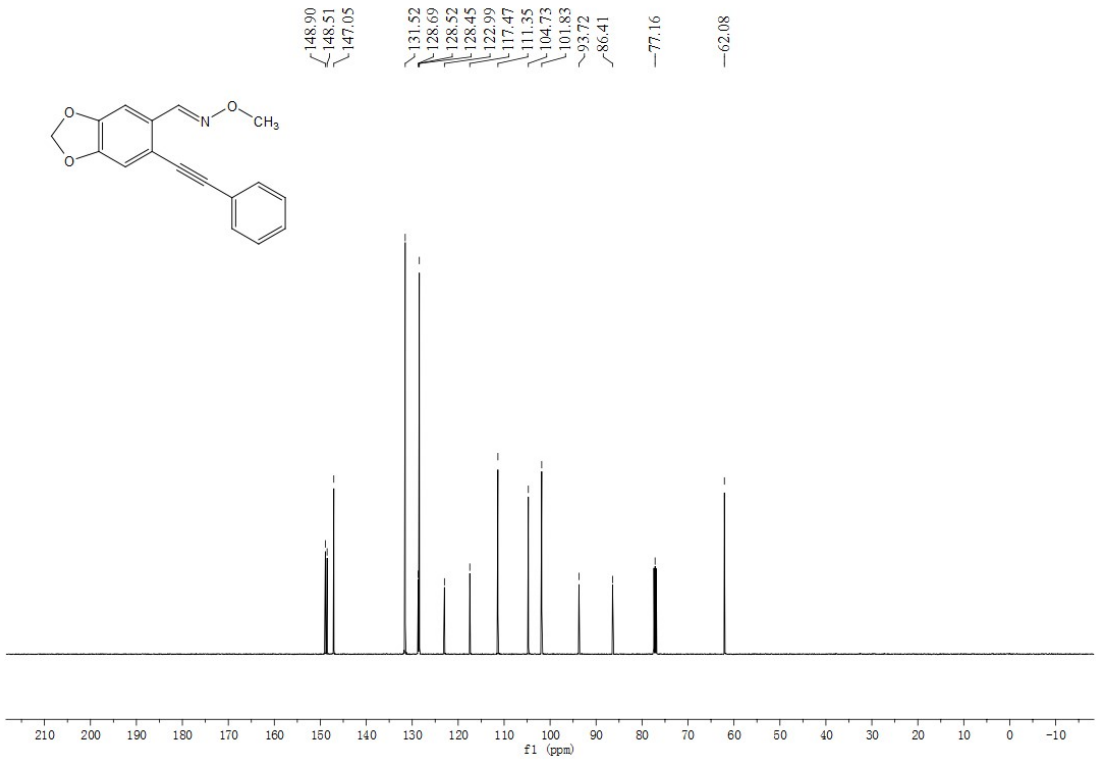
^{1}H NMR 500 MHz, in $CDCl_3$: 3-(phenylethynyl)thiophene-2-carbaldehyde O-methyl oxime (1az)



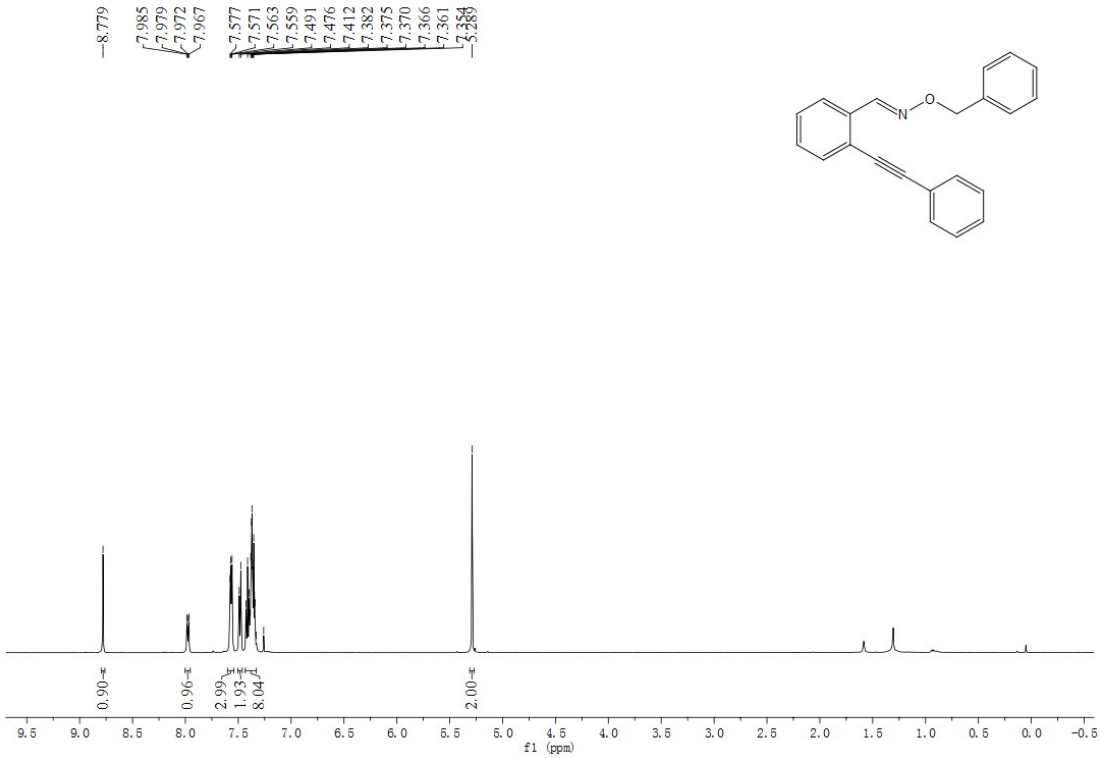
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 3-(phenylethynyl)thiophene-2-carbaldehyde O-methyl oxime (1az)



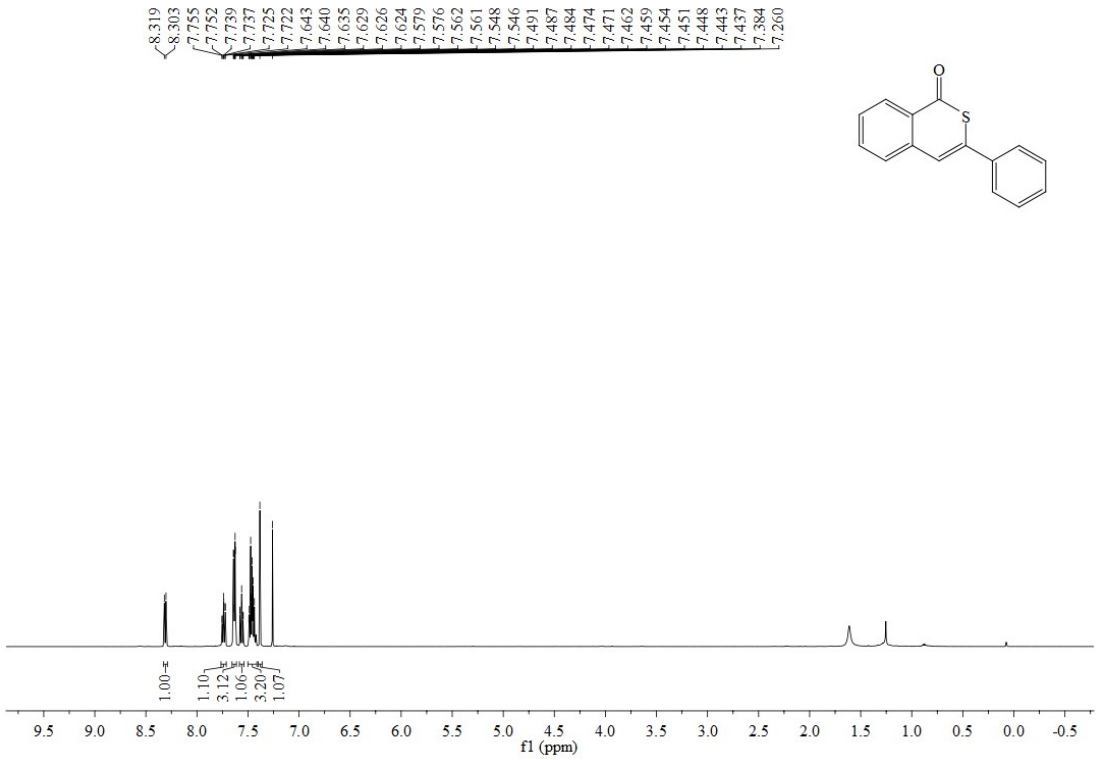
^{1}H NMR 500 MHz, in $CDCl_3$: 6-(phenylethynyl)benzo[*d*][1,3]dioxole-5-carbaldehyde O-methyl oxime (1ba)



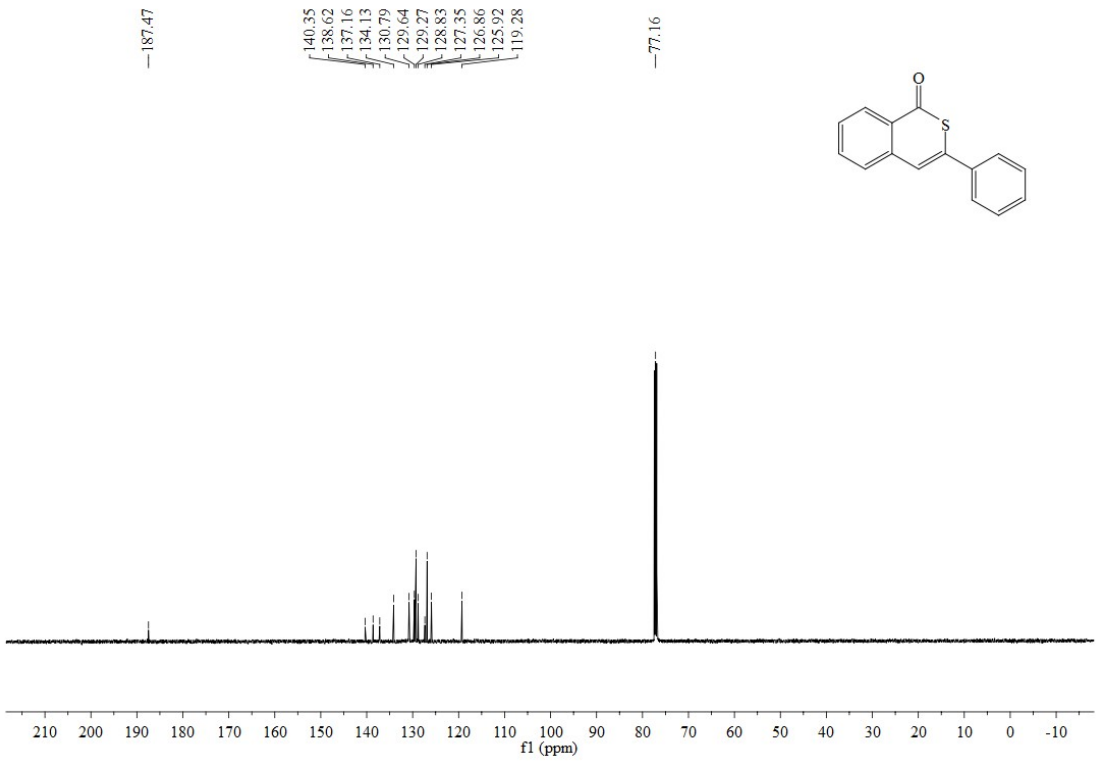
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 6-(phenylethynyl)benzo[*d*][1,3]dioxole-5-carbaldehyde O-methyl oxime (1ba)



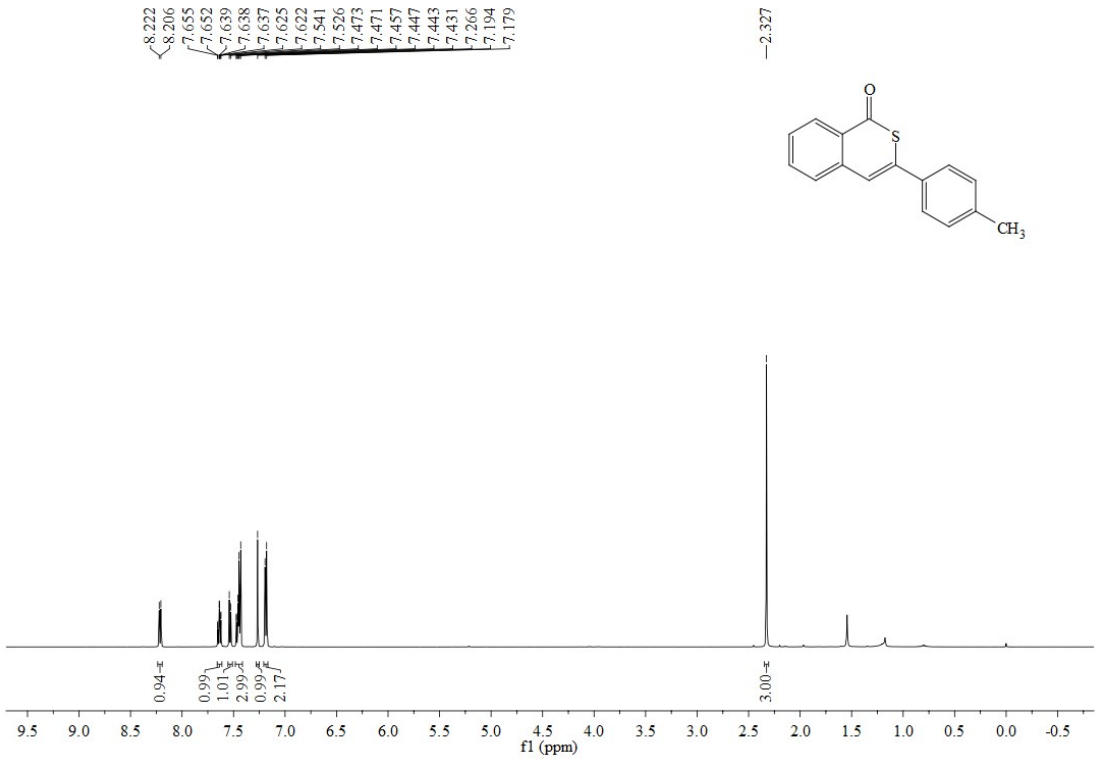
^{1}H NMR 500 MHz, in $CDCl_3$: 2-(phenylethynyl)benzaldehyde O-benzyl oxime (1bb)



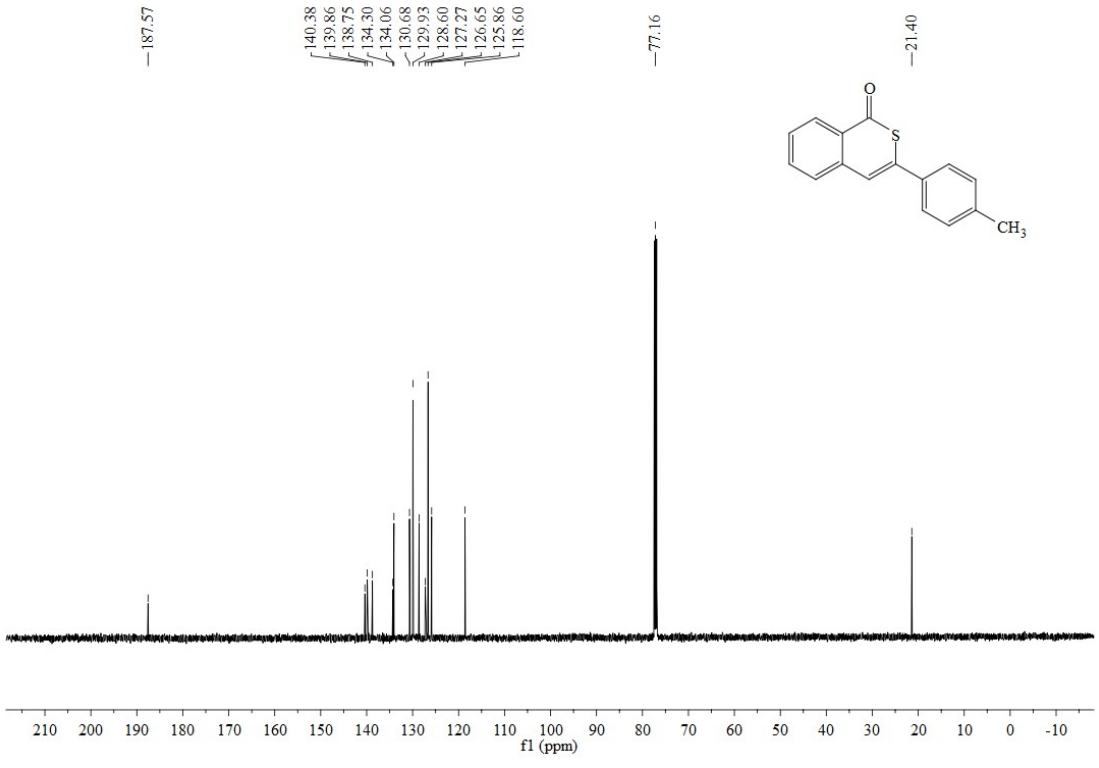
^{1}H NMR 500 MHz, in $CDCl_3$: 3-phenyl-1*H*-isothiochromen-1-one (2)



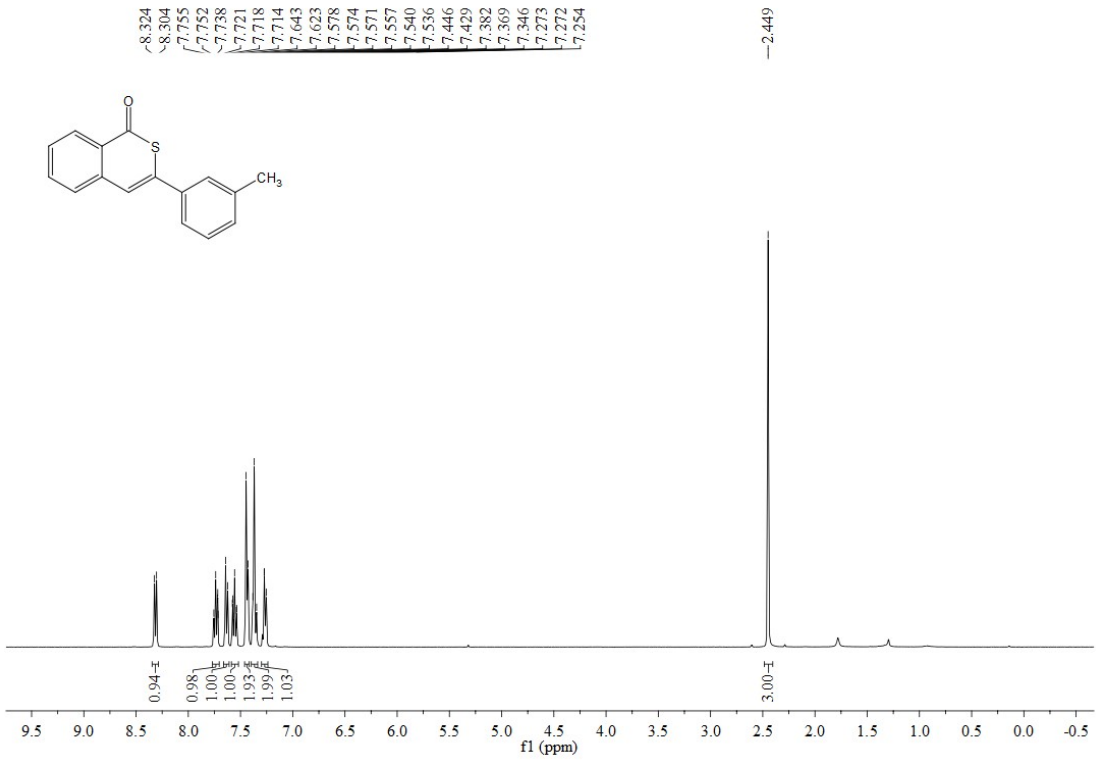
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 3-phenyl-1*H*-isothiochromen-1-one (2)



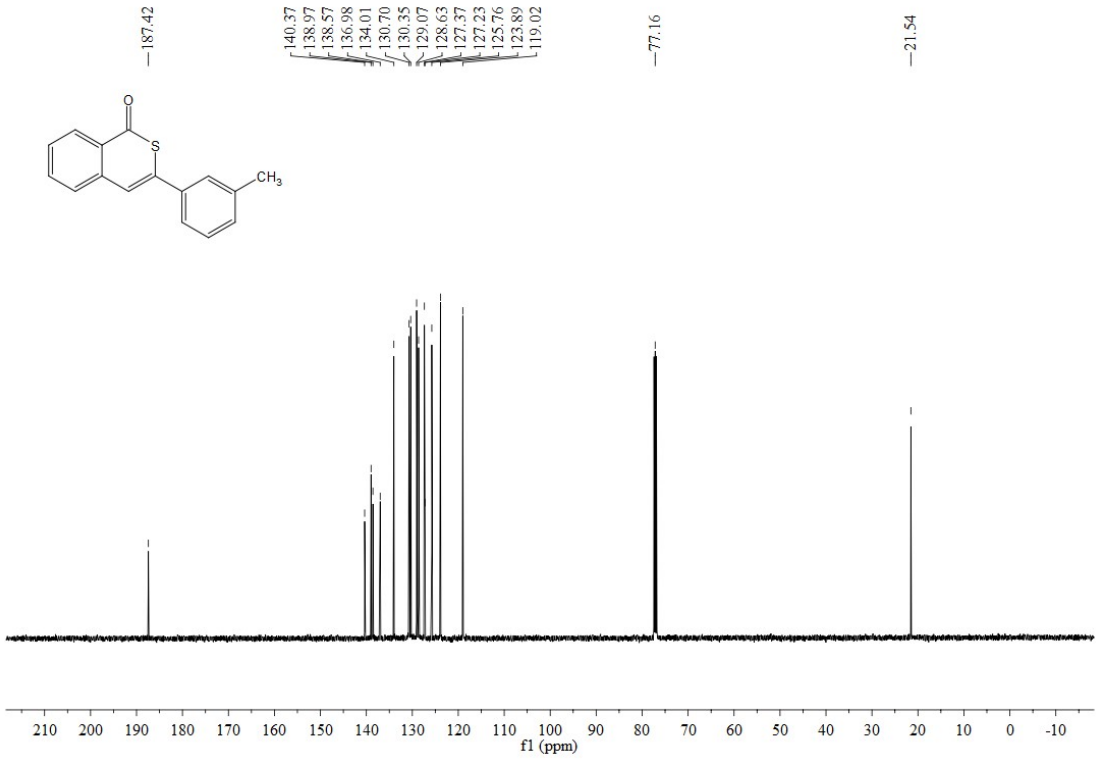
^{1}H NMR 500 MHz, in $CDCl_3$: 3-(p-tolyl)-1*H*-isothiochromen-1-one (3)



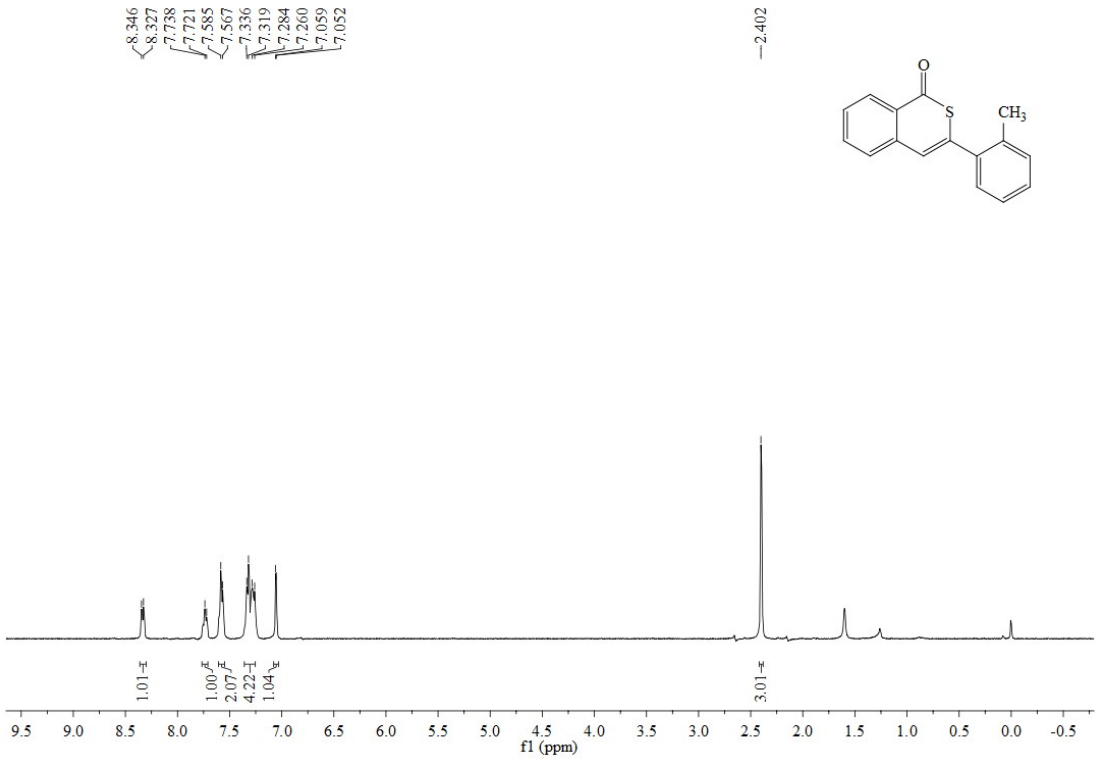
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 3-(p-tolyl)-1*H*-isothiochromen-1-one (3)



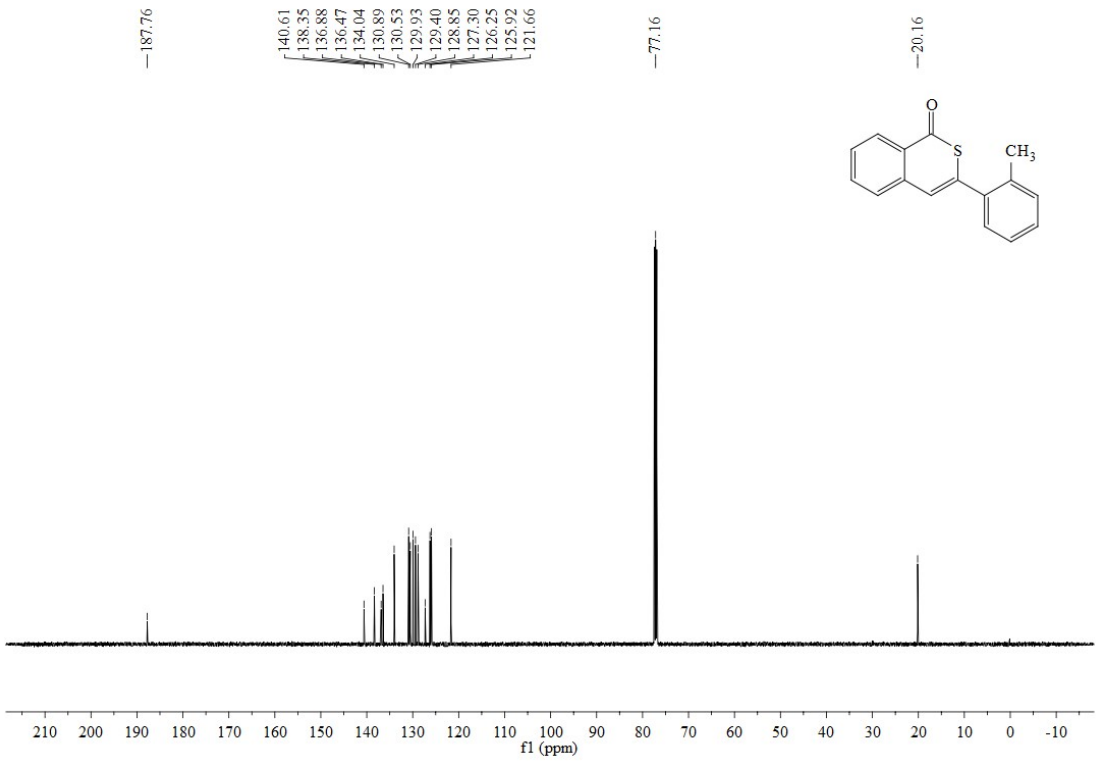
^{1}H NMR 400 MHz, in $CDCl_3$: 3-(m-tolyl)-1*H*-isothiochromen-1-one (4)



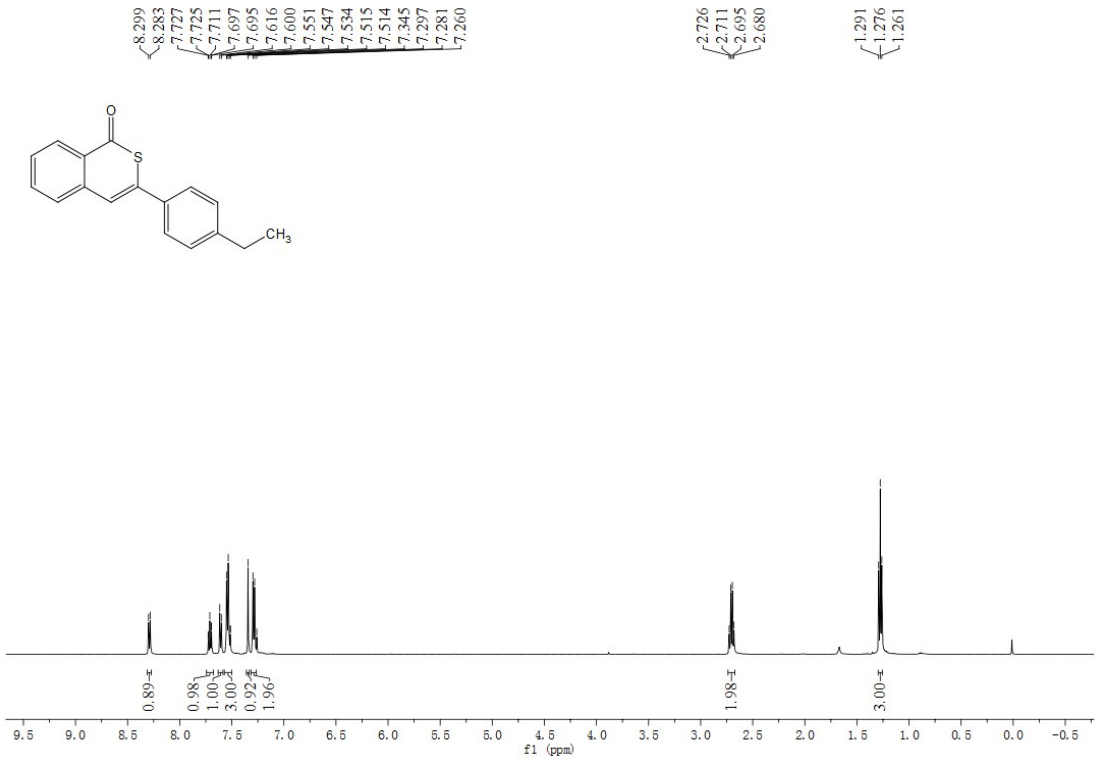
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 3-(m-tolyl)-1*H*-isothiochromen-1-one (4)



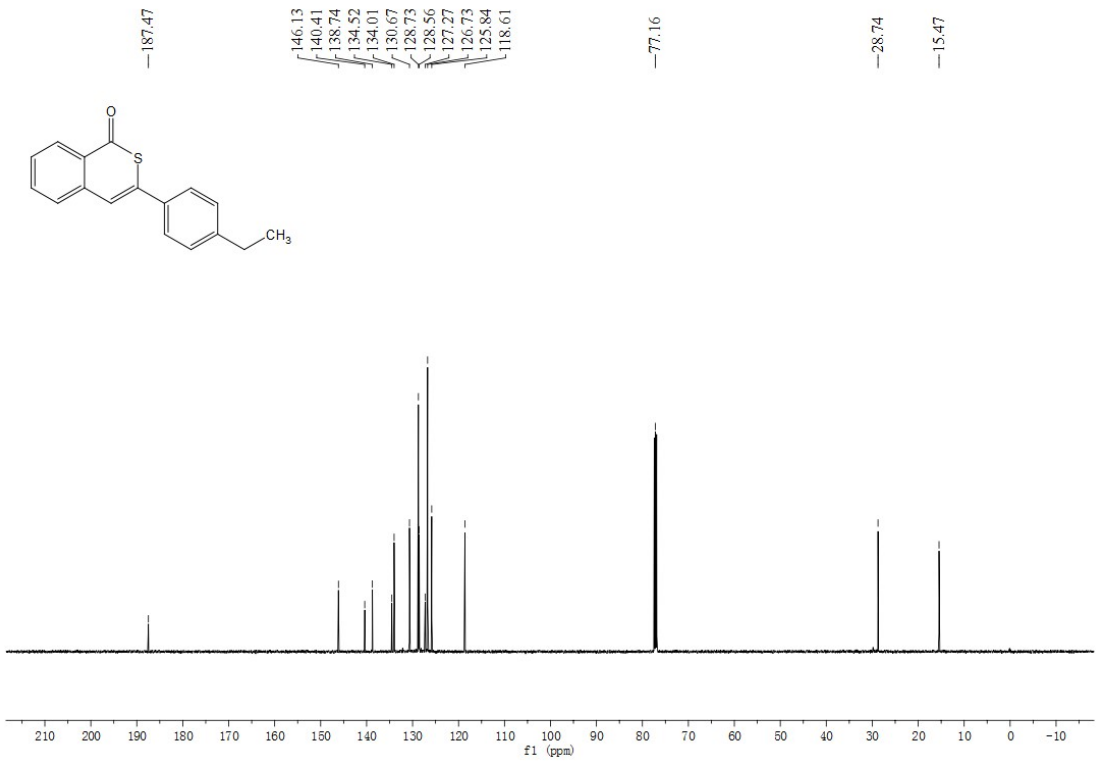
^{1}H NMR 400 MHz, in $CDCl_3$: 3-(o-tolyl)-1*H*-isothiochromen-1-one (5)



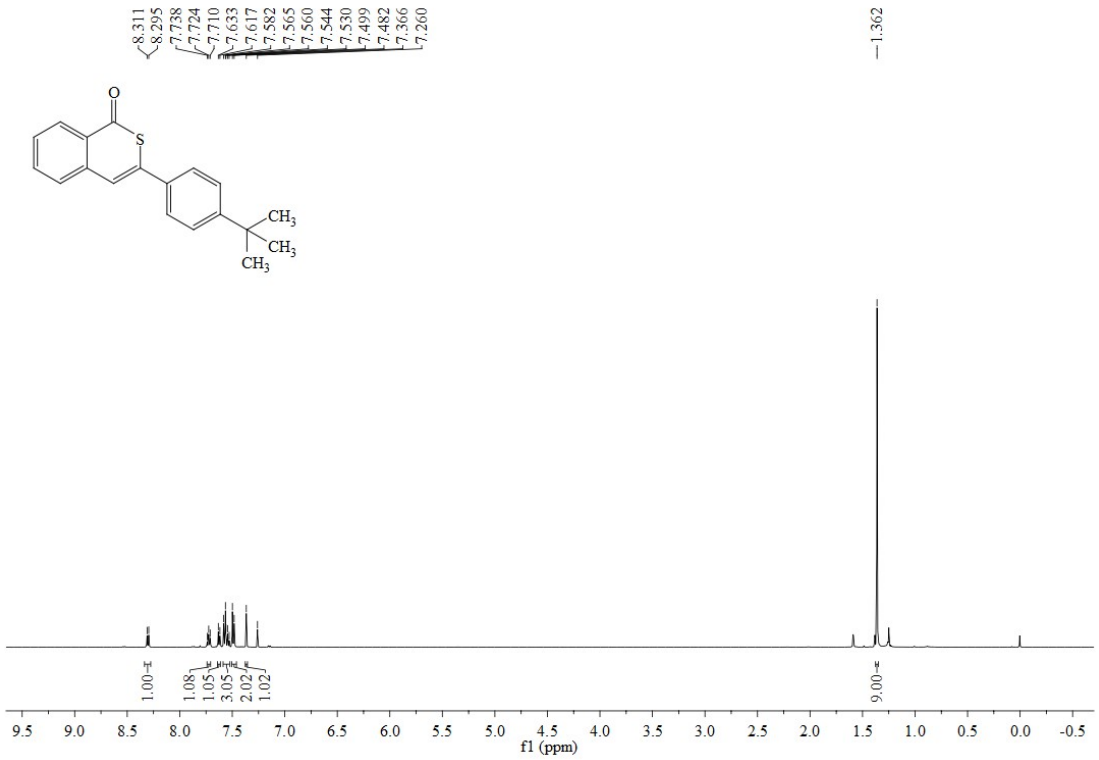
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 3-(o-tolyl)-1*H*-isothiochromen-1-one (5)



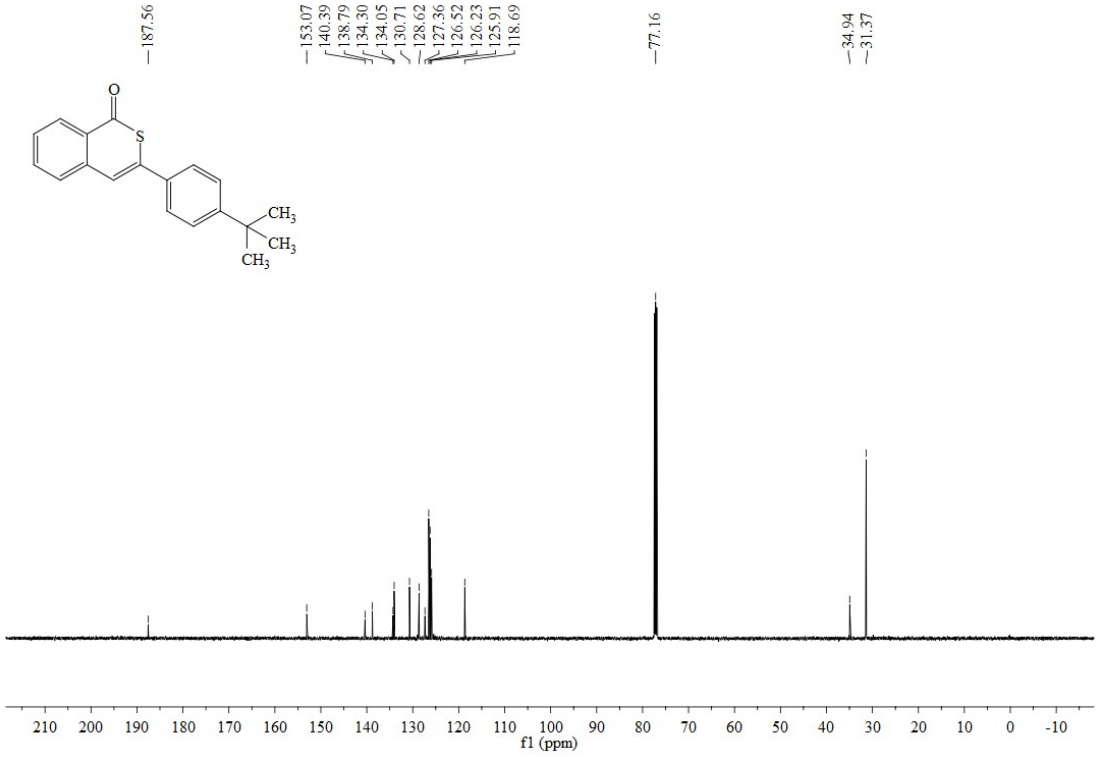
^{1}H NMR 500 MHz, in $CDCl_3$: 3-(4-ethylphenyl)-1*H*-isothiochromen-1-one (6)



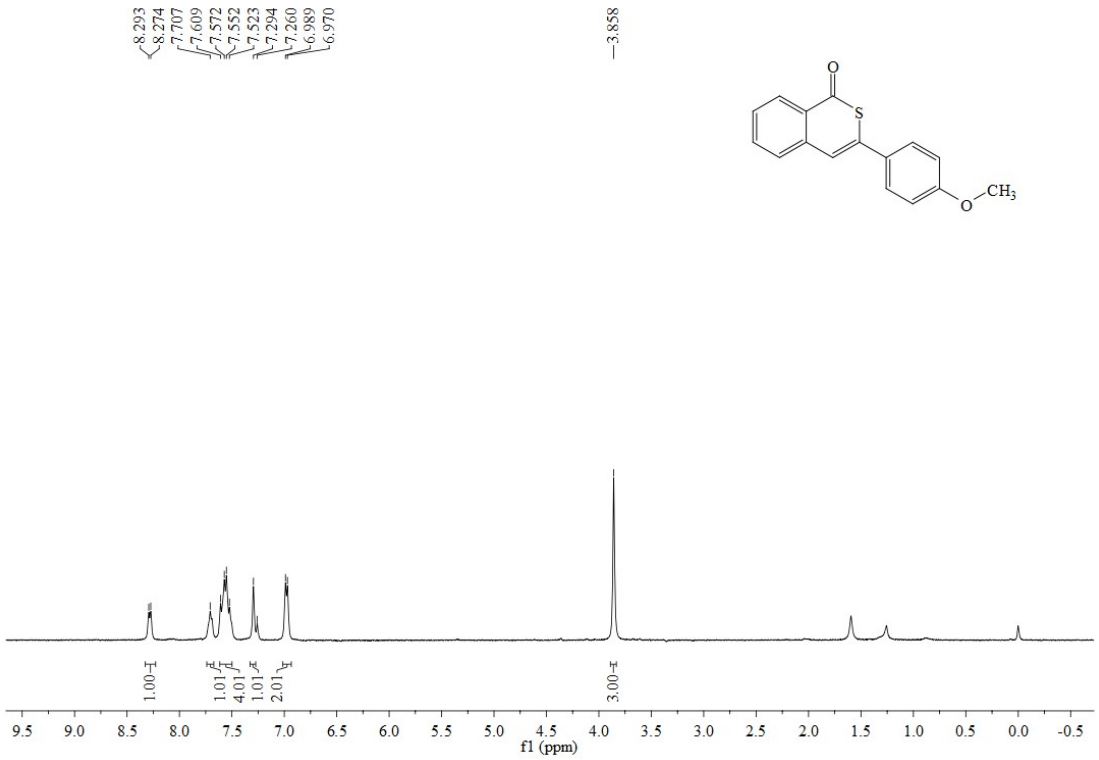
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 3-(4-ethylphenyl)-1*H*-isothiochromen-1-one (6)



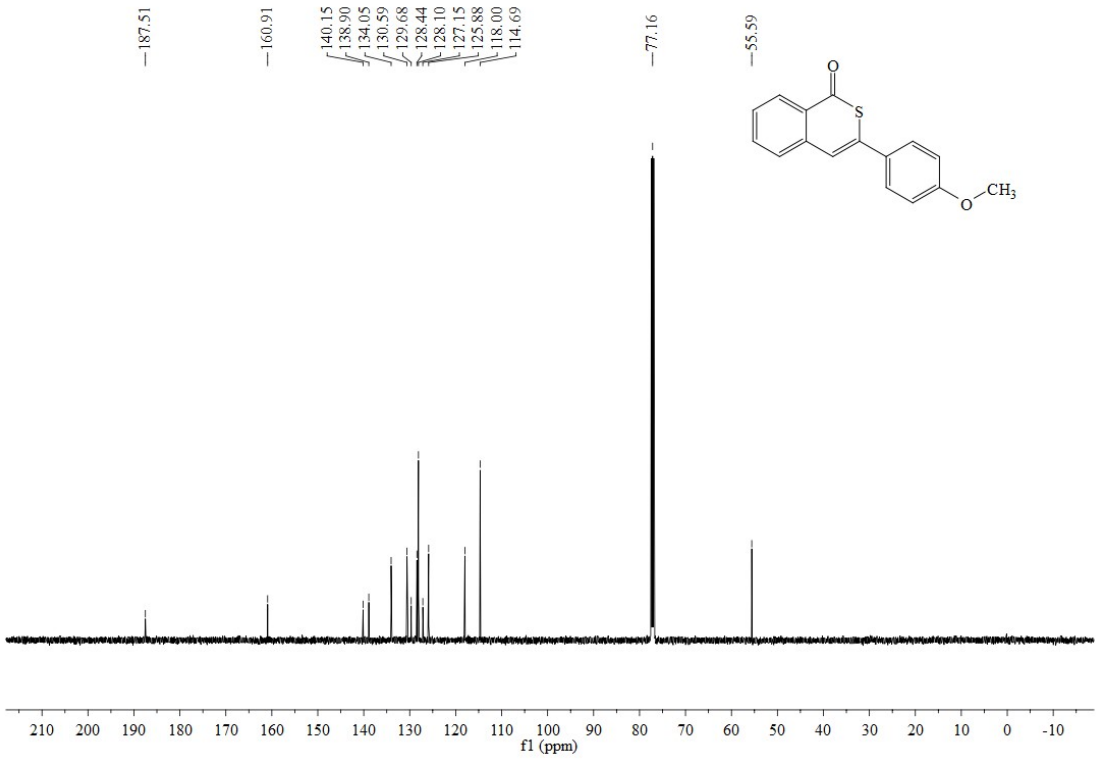
^{1}H NMR 500 MHz, in $CDCl_3$: 3-(4-(tert-butyl)phenyl)-1*H*-isothiochromen-1-one (7)



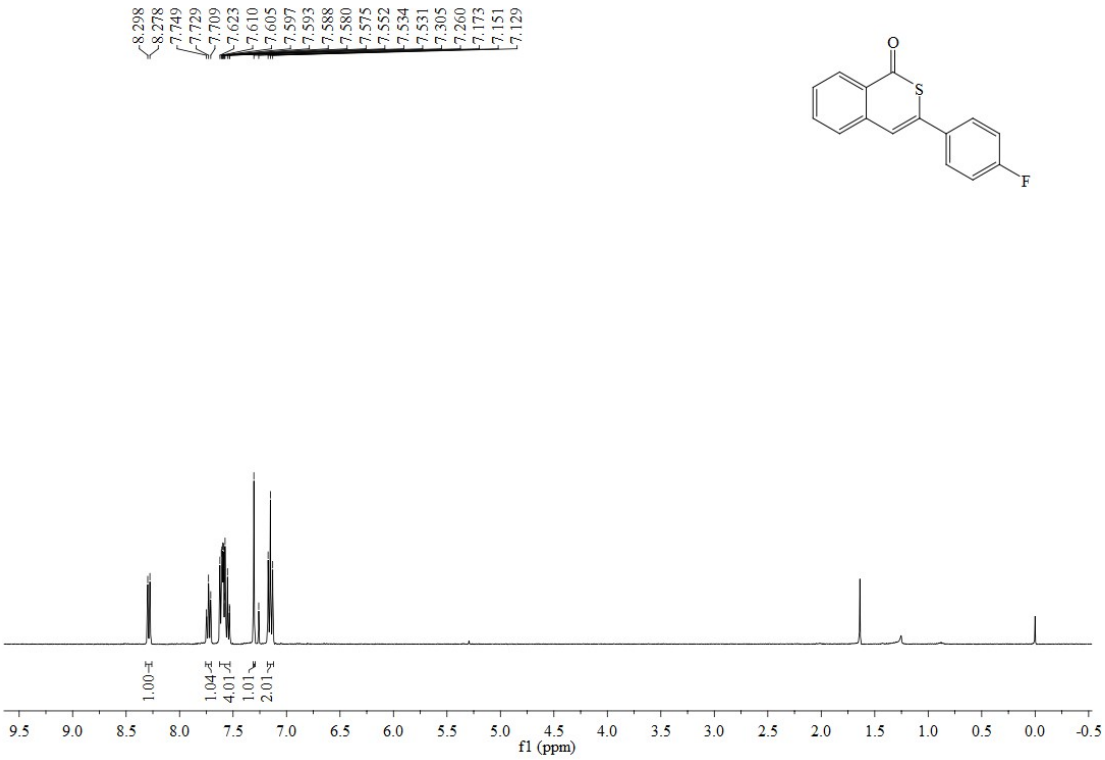
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 3-(4-(tert-butyl)phenyl)-1*H*-isothiochromen-1-one (7)



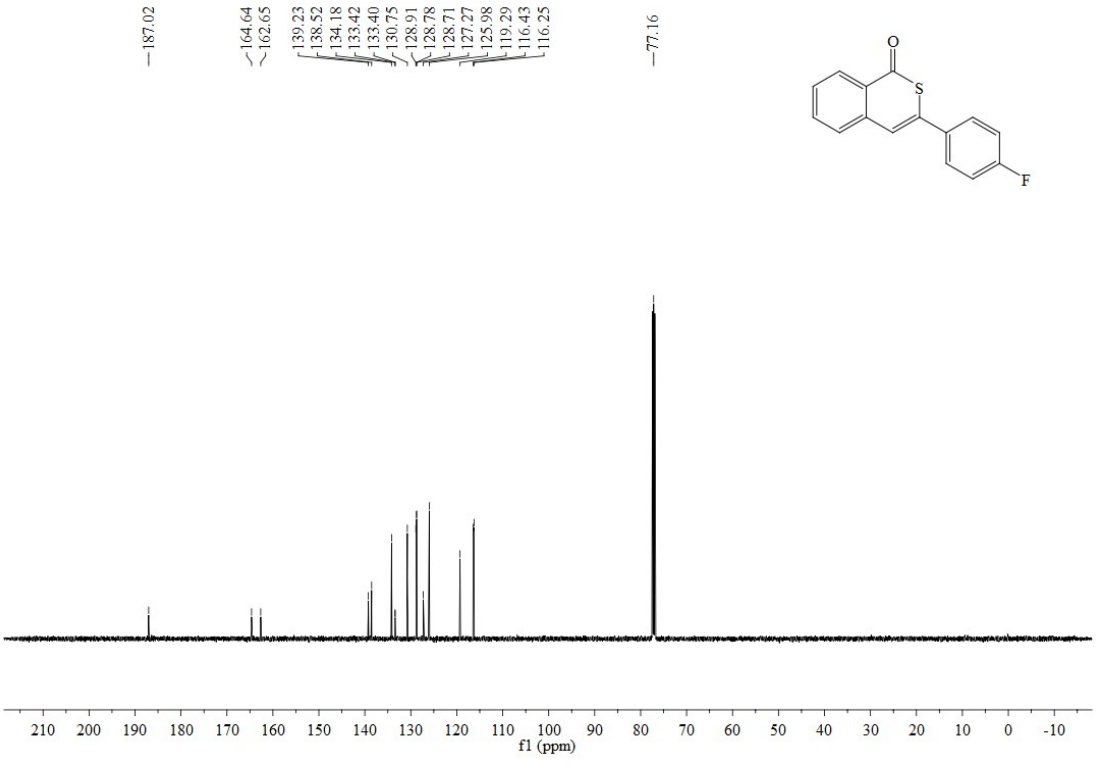
^{1}H NMR 400 MHz, in $CDCl_3$: 3-(4-methoxyphenyl)-1*H*-isothiochromen-1-one (8)



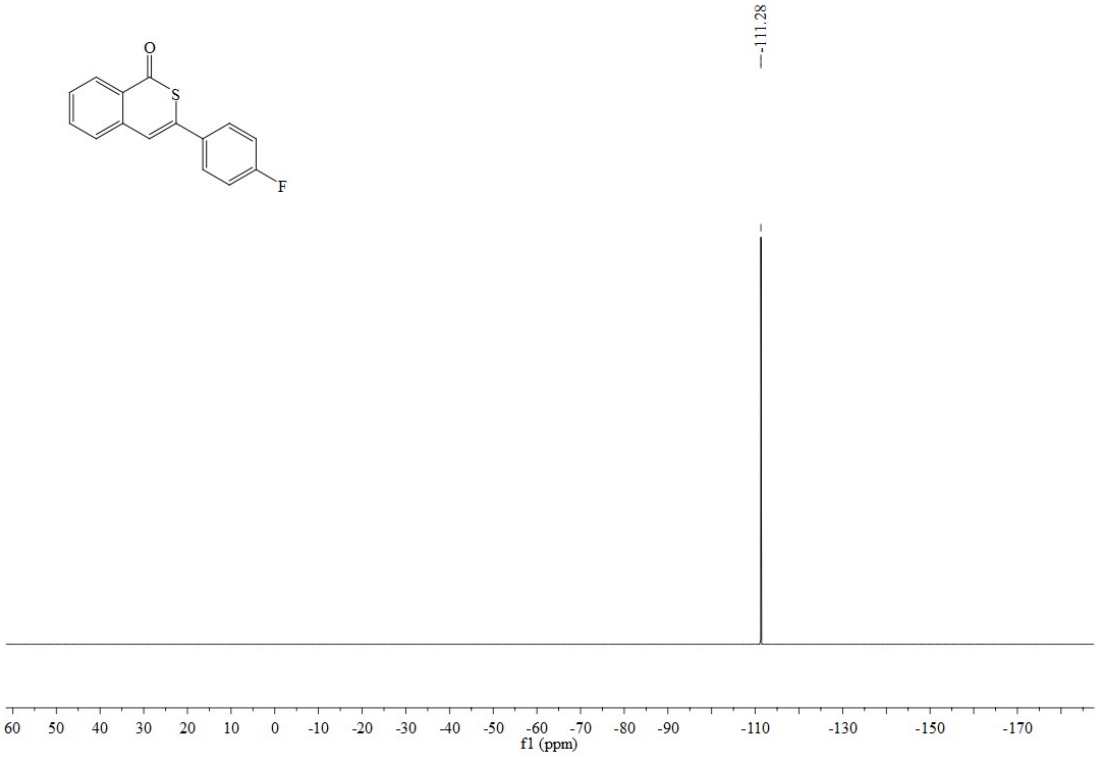
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 3-(4-methoxyphenyl)-1*H*-isothiochromen-1-one (8)



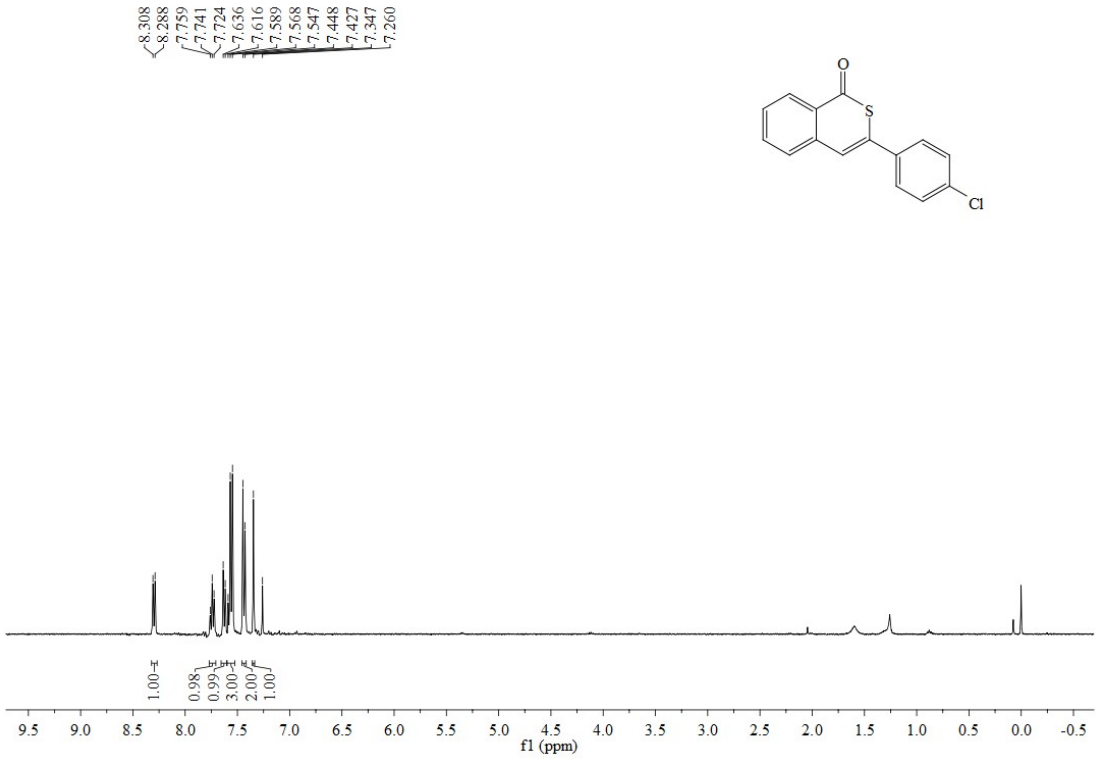
^{1}H NMR 400 MHz, in $CDCl_3$: 3-(4-fluorophenyl)-1*H*-isothiochromen-1-one (9)



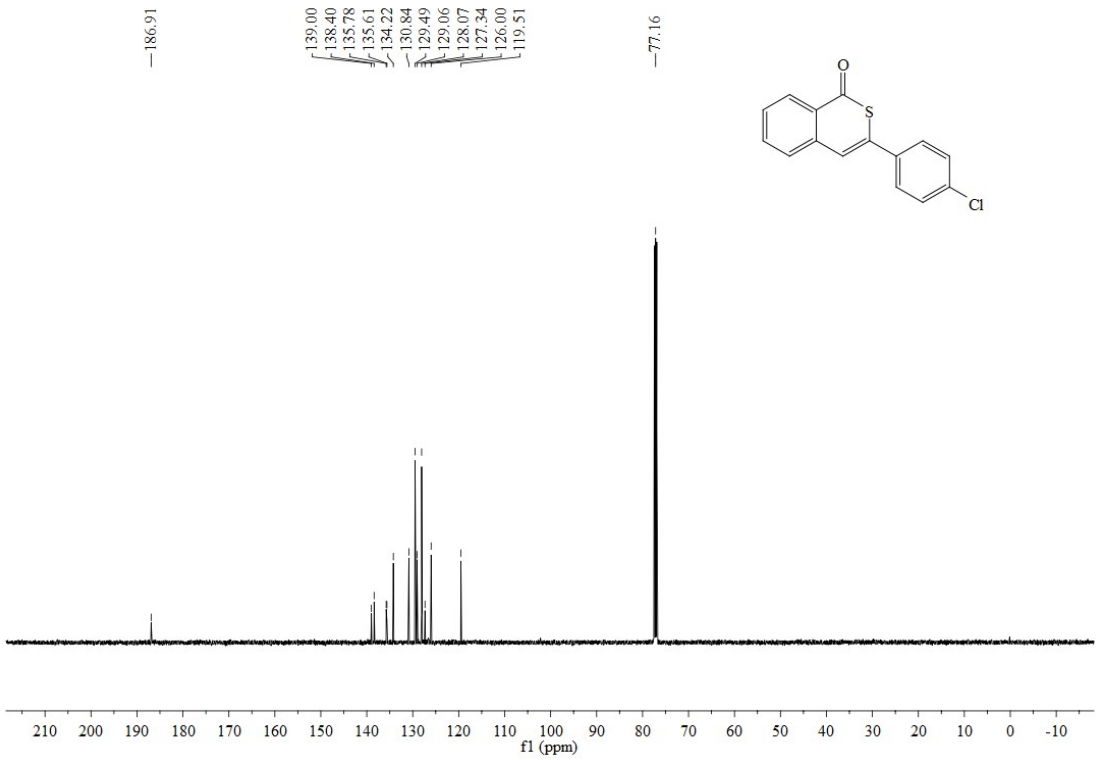
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 3-(4-fluorophenyl)-1*H*-isothiochromen-1-one (9)



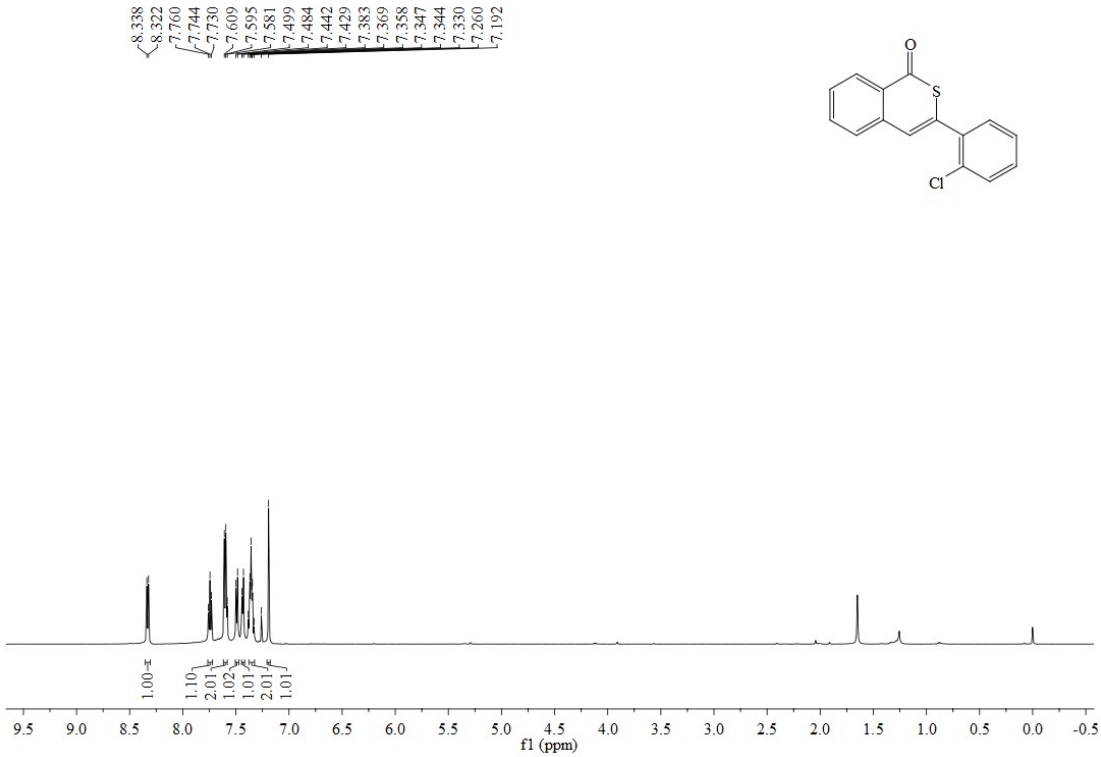
^{19}F NMR 470 MHz, in $CDCl_3$: 3-(4-fluorophenyl)-1*H*-isothiochromen-1-one (9)



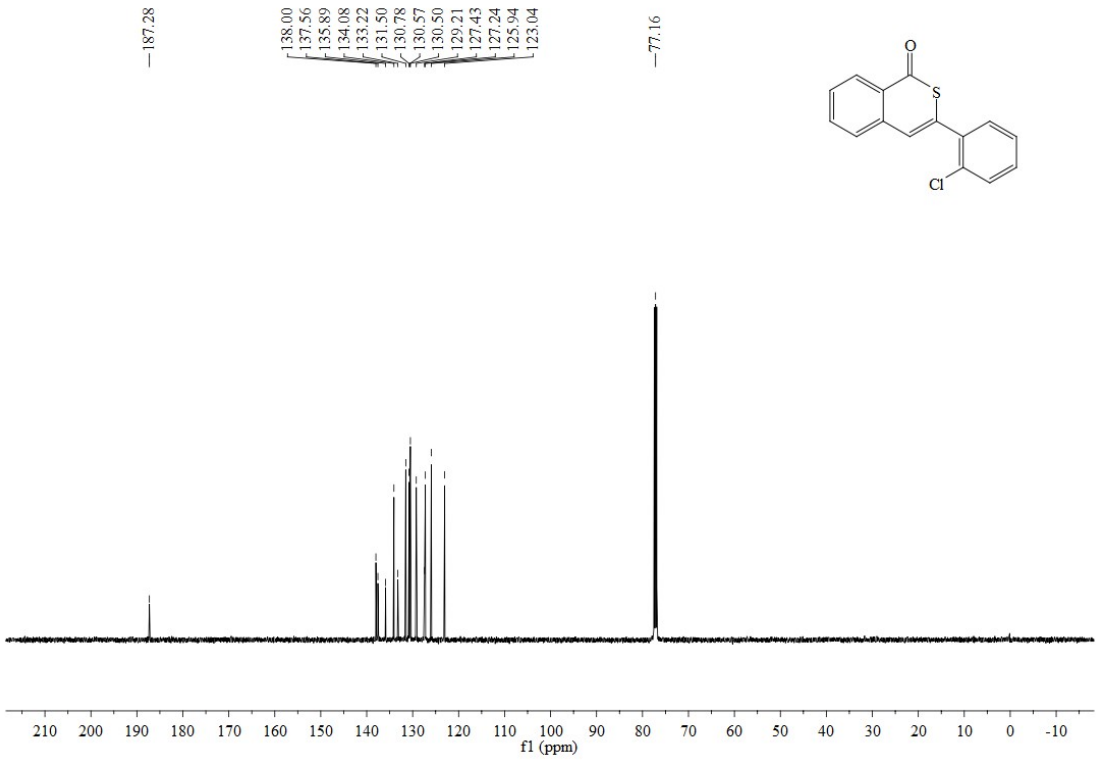
^{1}H NMR 400 MHz, in $CDCl_3$: 3-(4-chlorophenyl)-1*H*-isothiochromen-1-one (10)



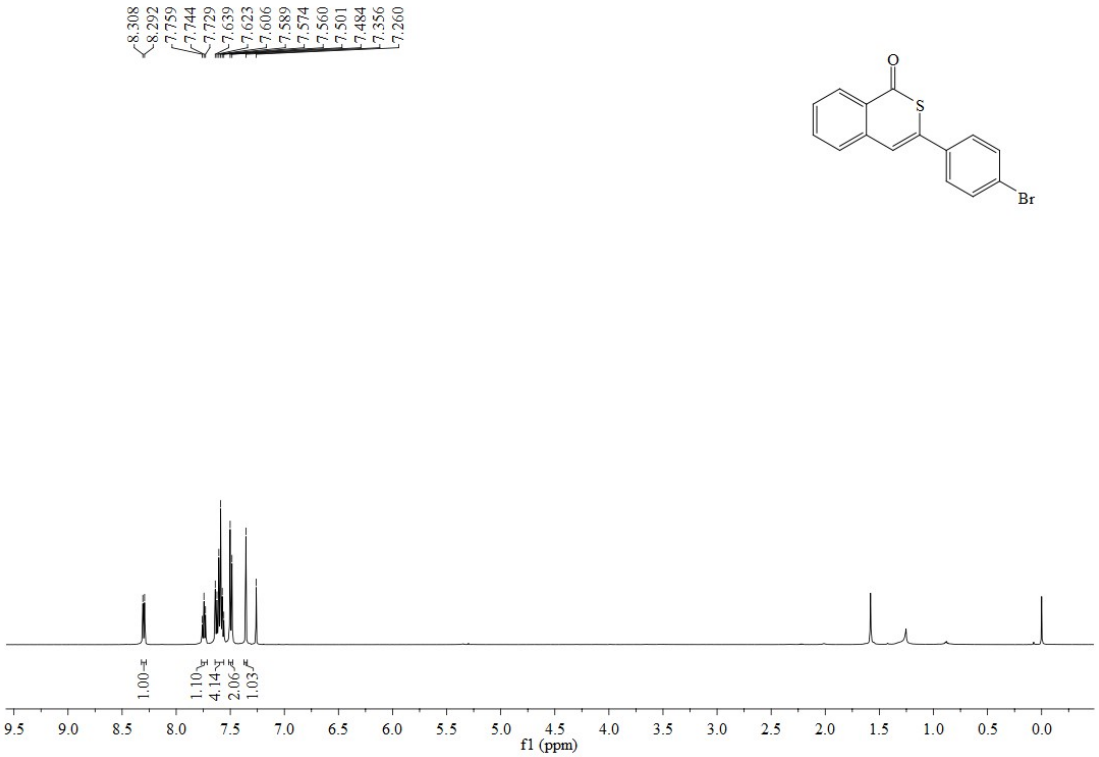
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 3-(4-chlorophenyl)-1*H*-isothiochromen-1-one (10)



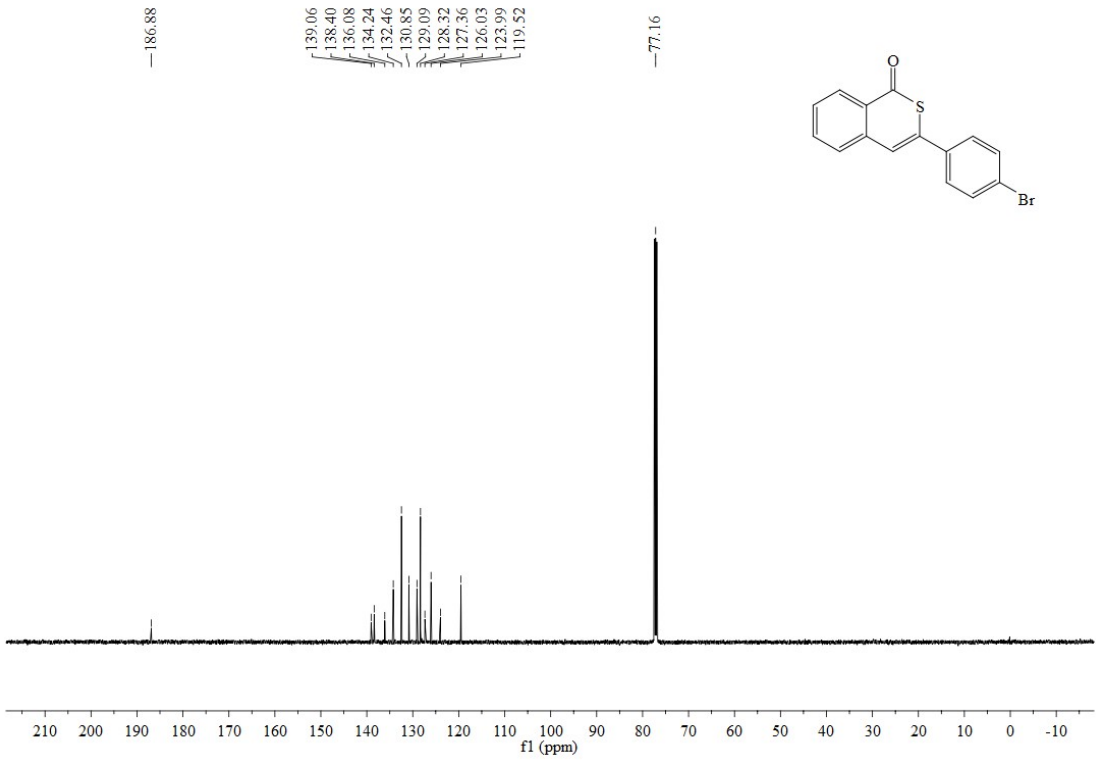
^{1}H NMR 500 MHz, in $CDCl_3$: 3-(2-chlorophenyl)-1*H*-isothiochromen-1-one (11)



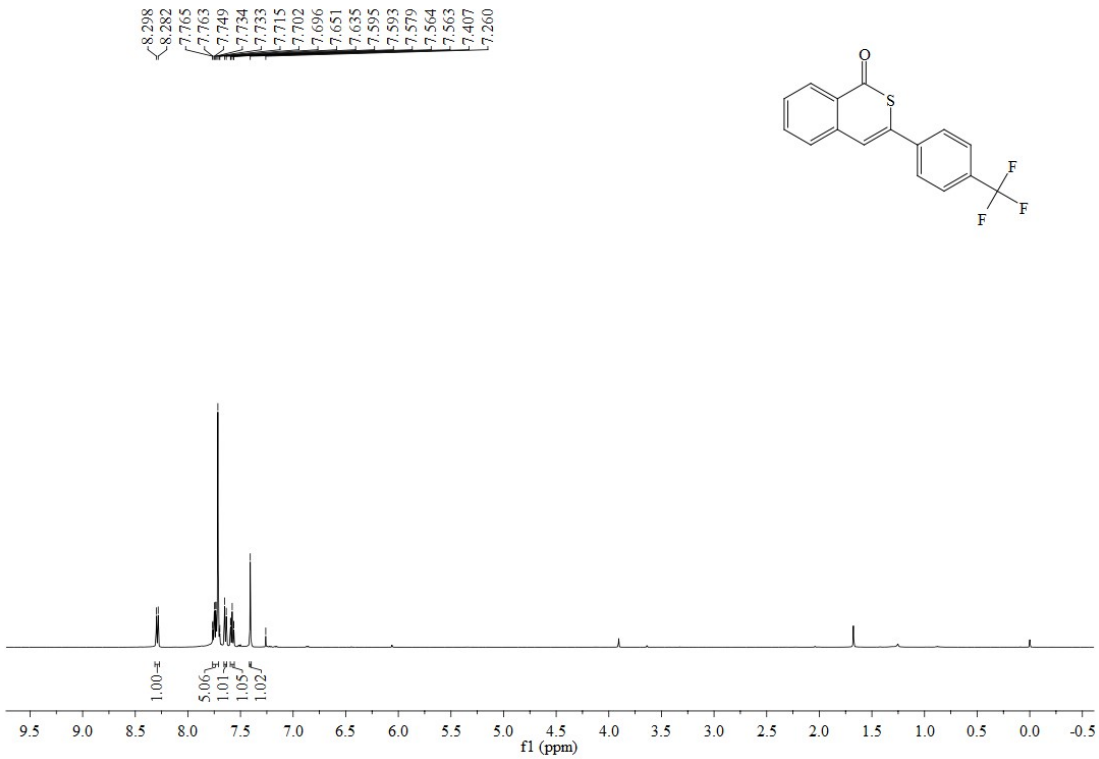
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 3-(2-chlorophenyl)-1*H*-isothiochromen-1-one (11)



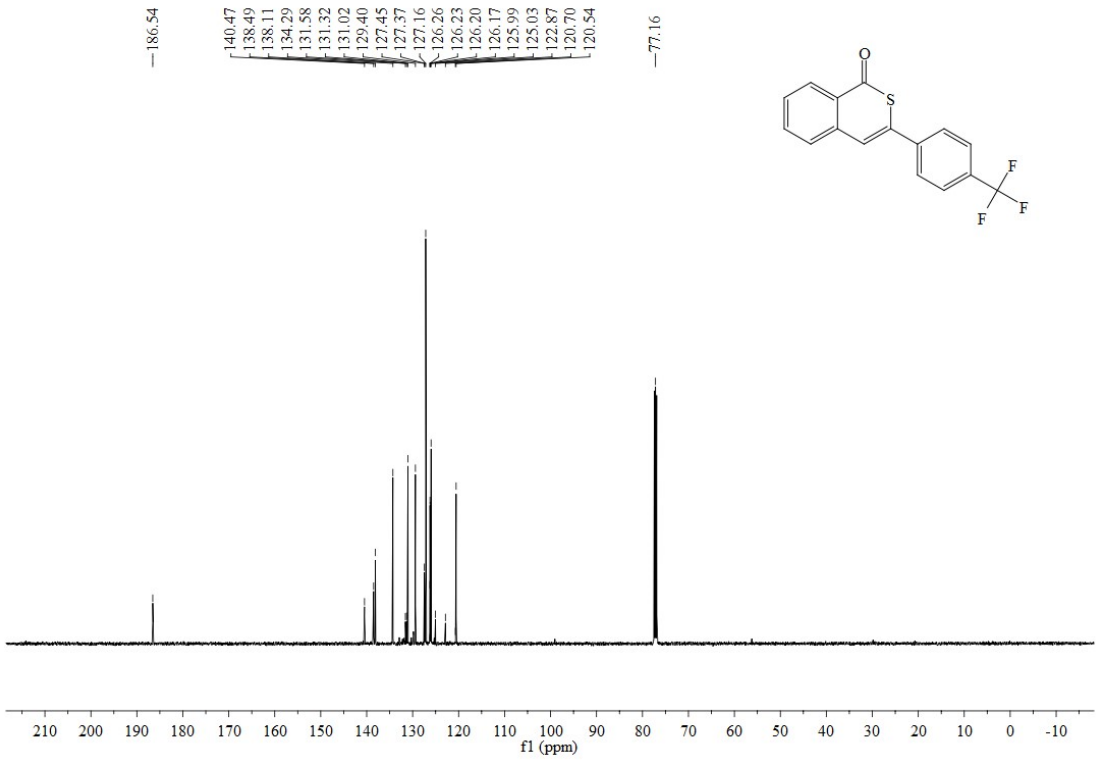
^{1}H NMR 500 MHz, in $CDCl_3$: 3-(4-bromophenyl)-1*H*-isothiochromen-1-one (12)



$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 3-(4-bromophenyl)-1*H*-isothiochromen-1-one (12)

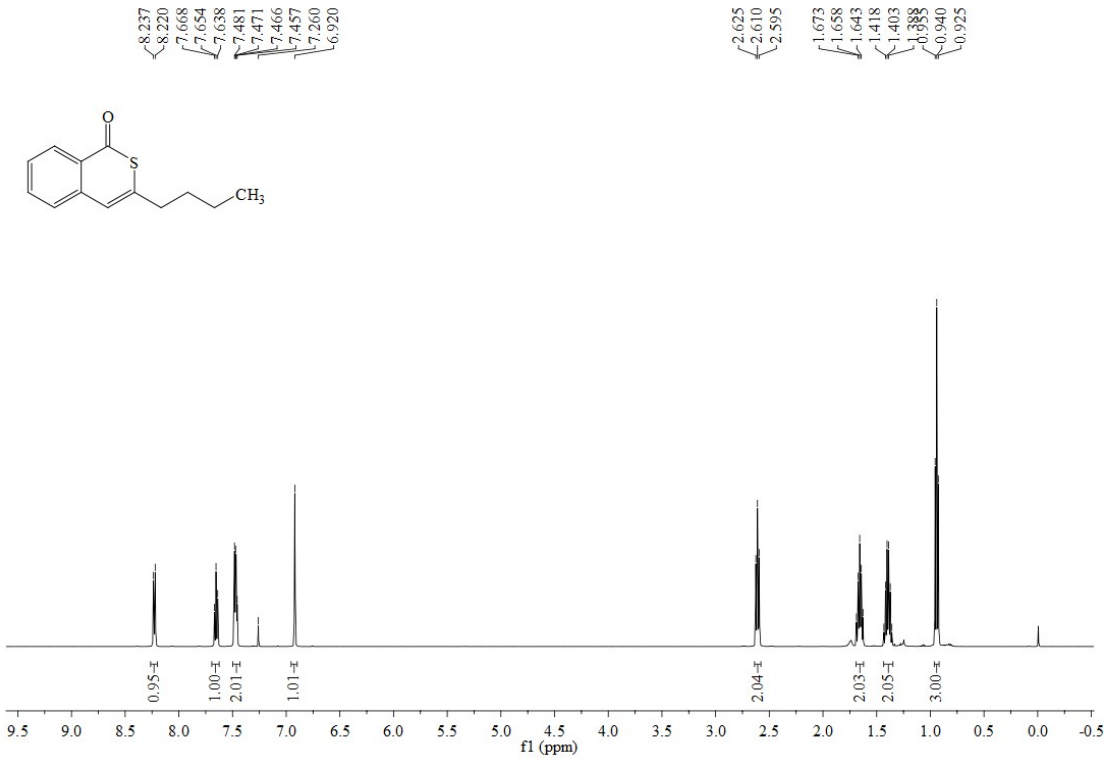


^{1}H NMR 500 MHz, in $CDCl_3$: 3-(4-(trifluoromethyl)phenyl)-1*H*-isothiochromen-1-one (13)

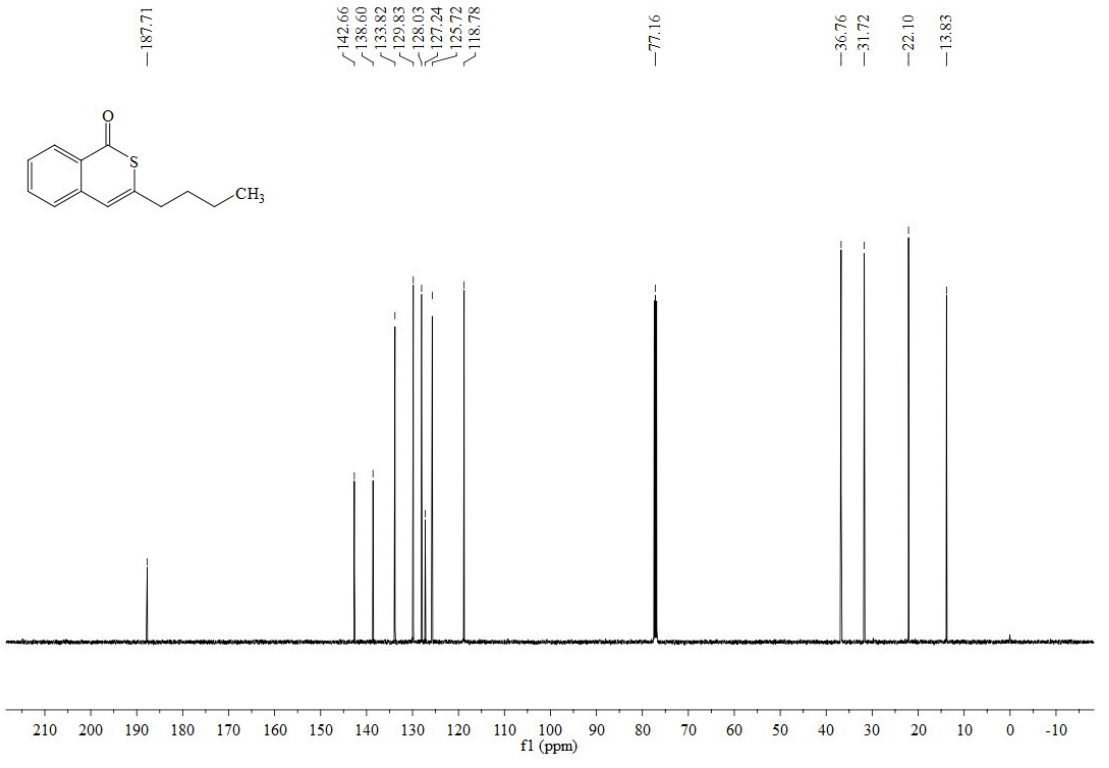


$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 3-(4-(trifluoromethyl)phenyl)-1*H*-isothiochromen-1-one (13)

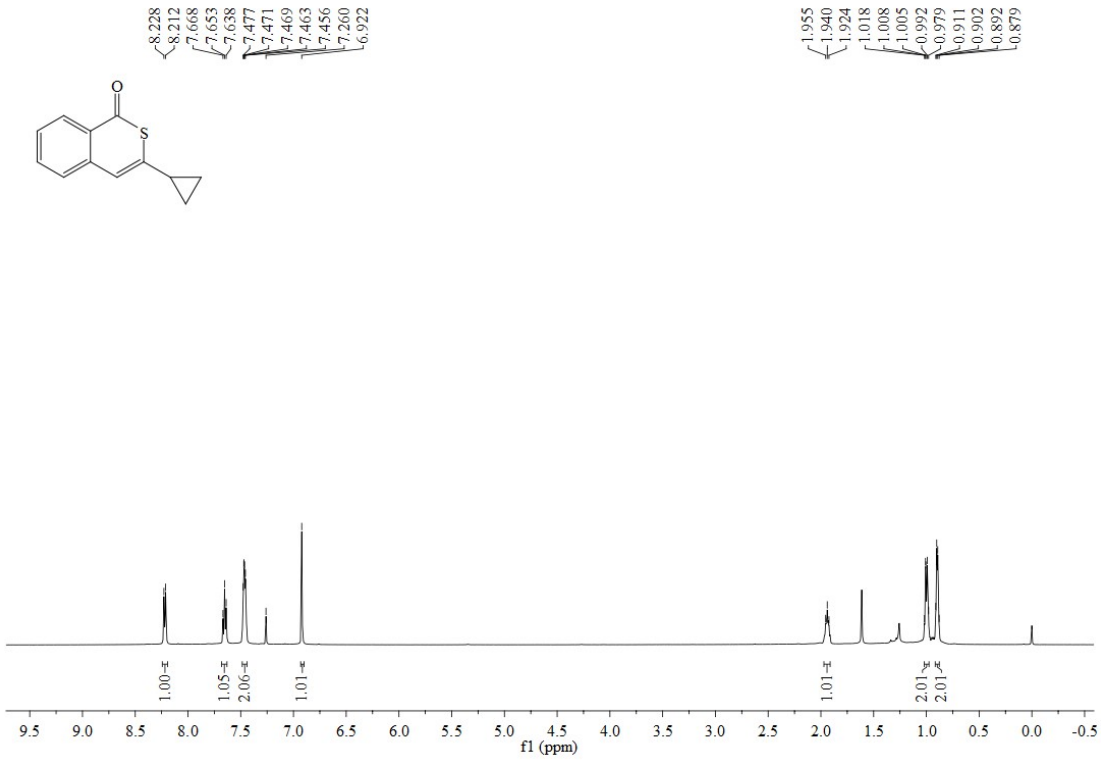
^{19}F NMR 470 MHz, in $CDCl_3$: 3-(4-(trifluoromethyl)phenyl)-1*H*-isothiochromen-1-one (13)



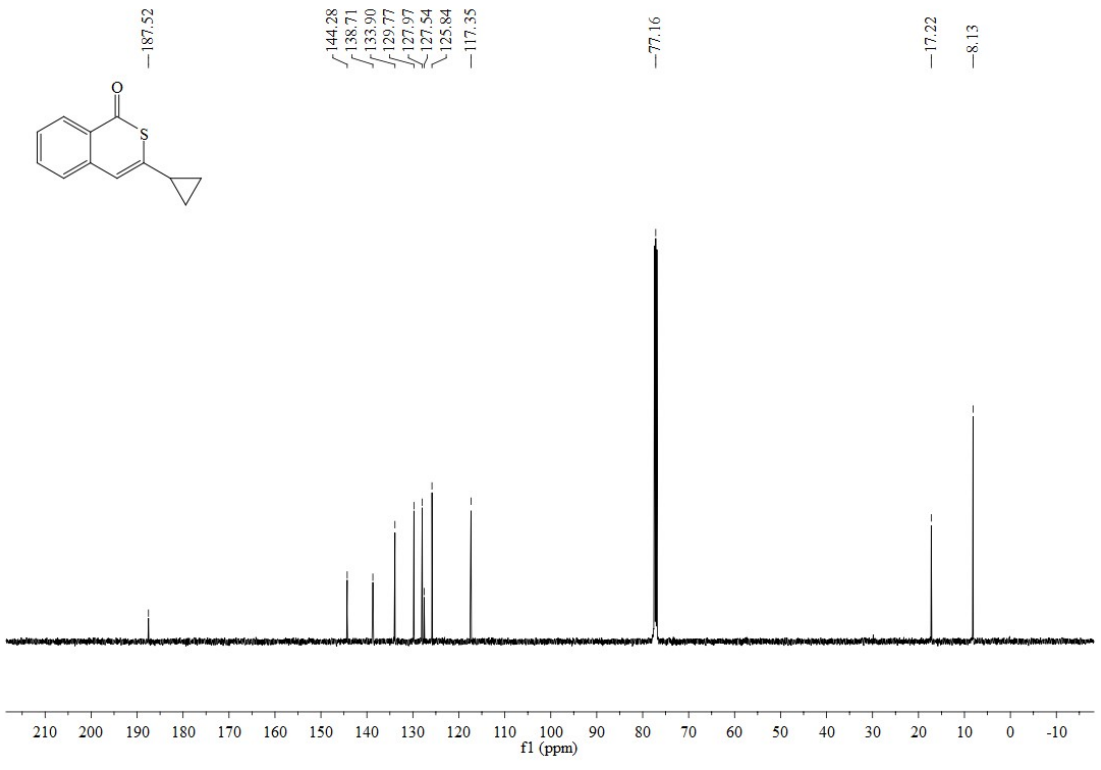
^{1}H NMR 500 MHz, in $CDCl_3$: 3-butyl-1*H*-isothiochromen-1-one (14)



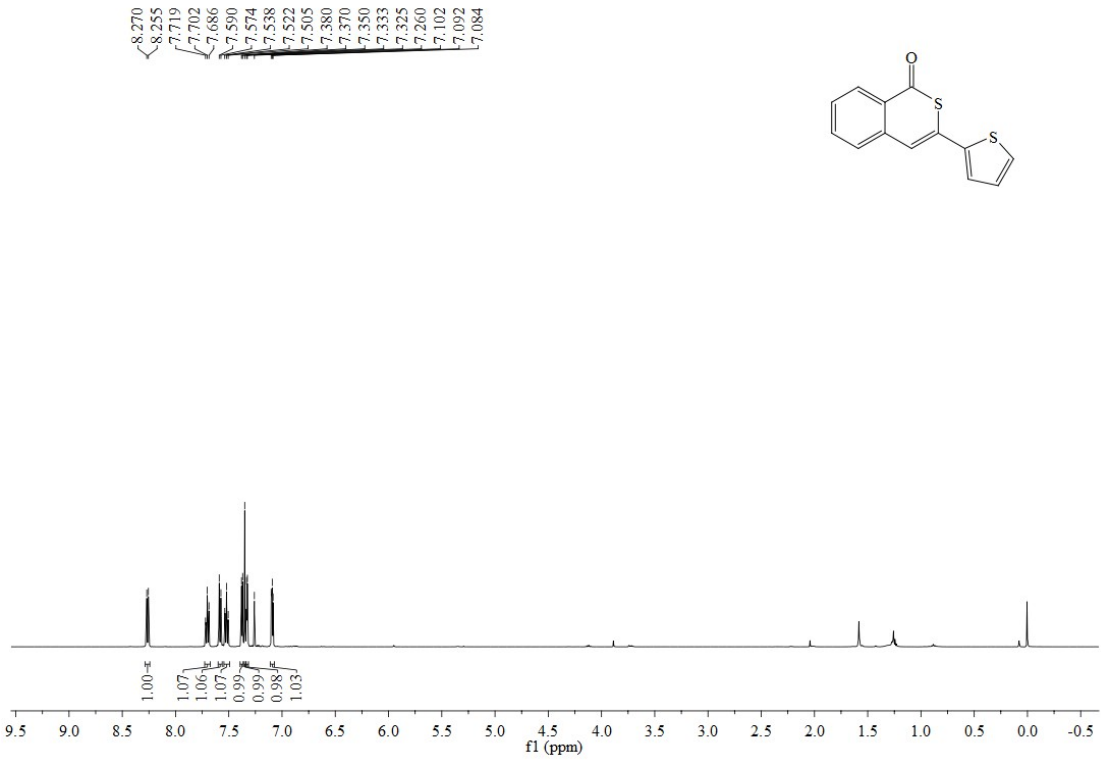
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 3-butyl-1*H*-isothiochromen-1-one (14)



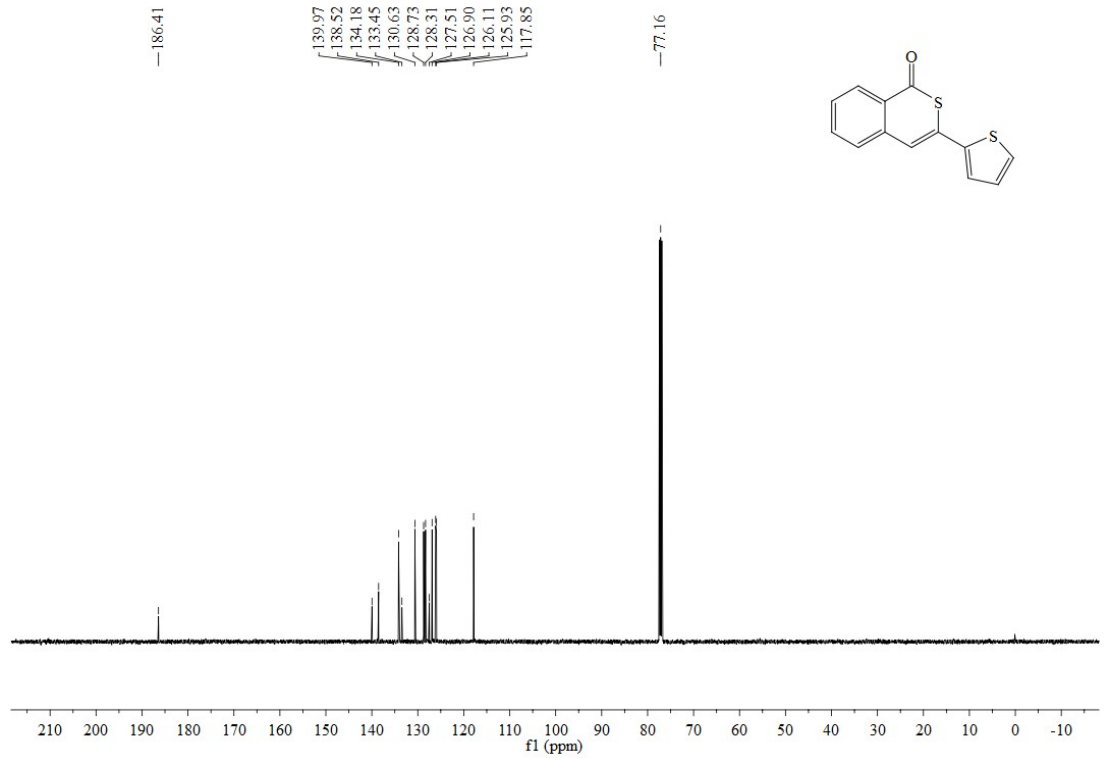
^{1}H NMR 500 MHz, in $CDCl_3$: 3-cyclopropyl-1*H*-isothiochromen-1-one (15)



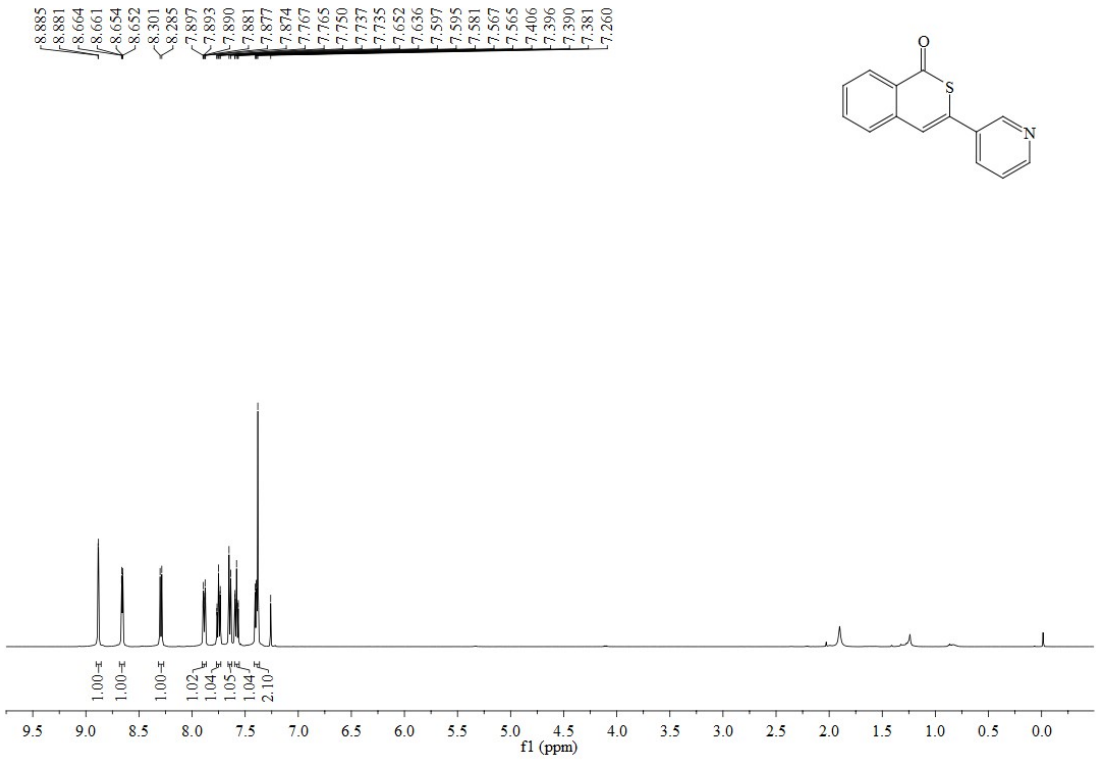
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 3-cyclopropyl-*1H*-isothiochromen-1-one (15)



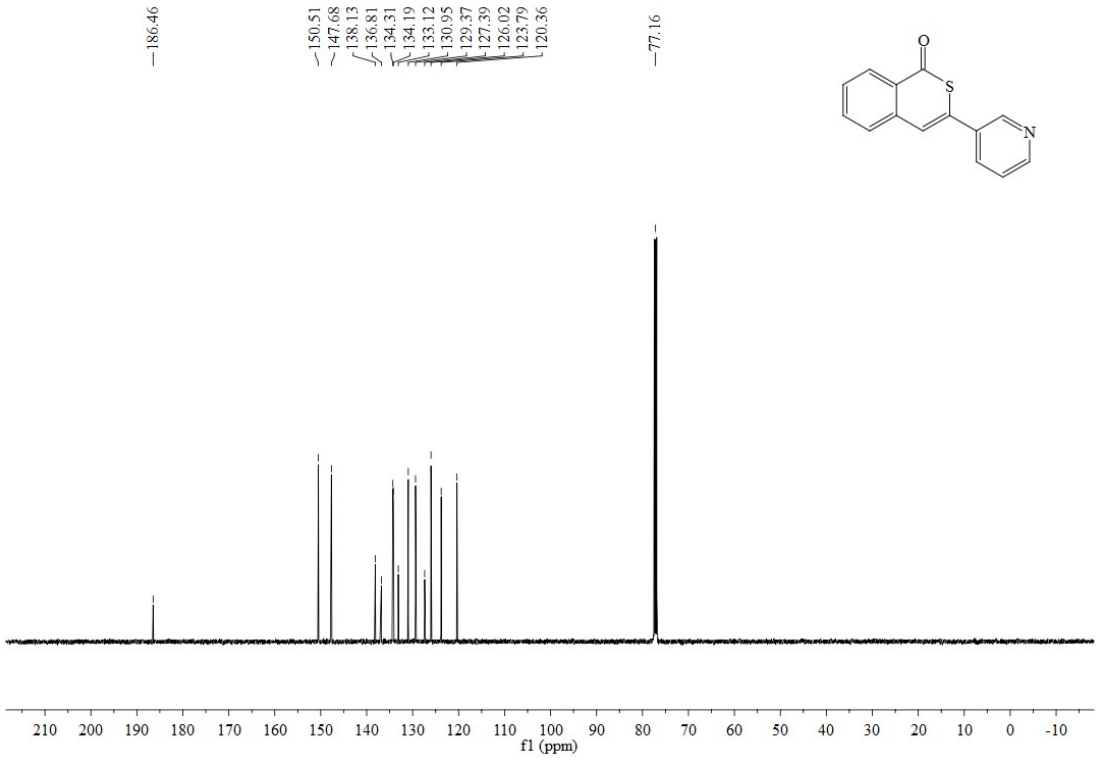
^{1}H NMR 500 MHz, in $CDCl_3$: 3-(thiophen-2-yl)-1*H*-isothiochromen-1-one (16)



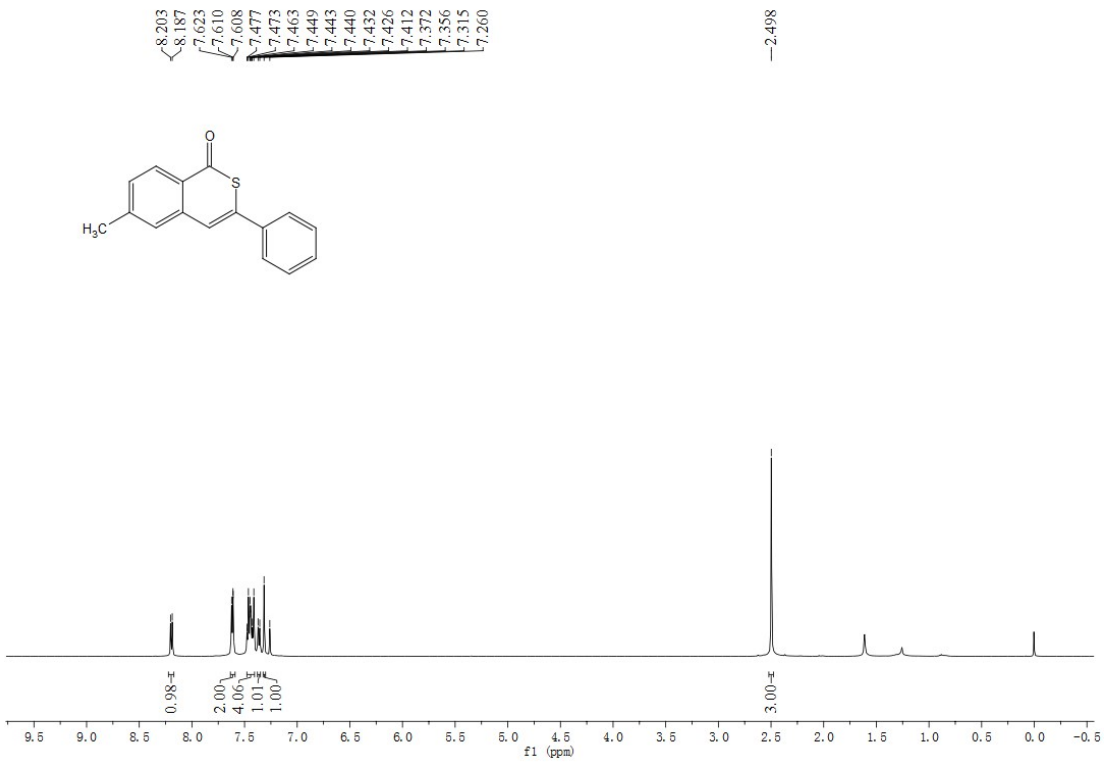
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 3-(thiophen-2-yl)-1*H*-isothiochromen-1-one (16)



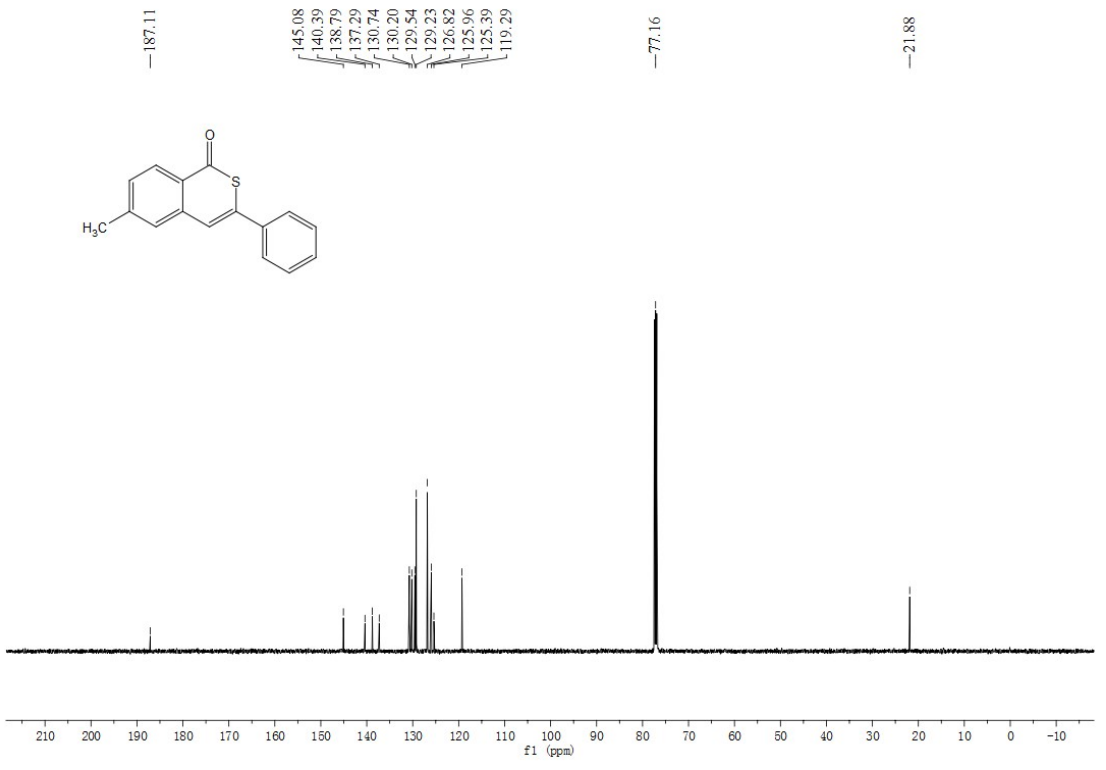
^{1}H NMR 500 MHz, in $CDCl_3$: 3-(pyridin-3-yl)-1*H*-isothiochromen-1-one (17)



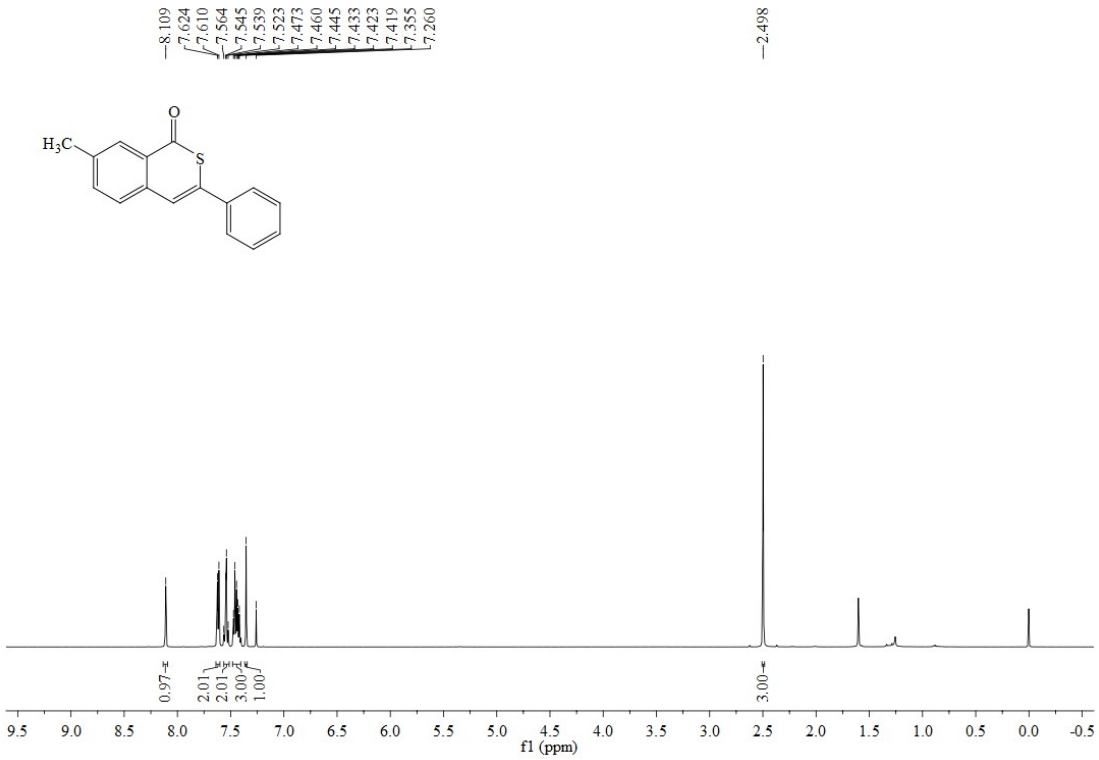
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 3-(pyridin-3-yl)-1*H*-isothiochromen-1-one (17)



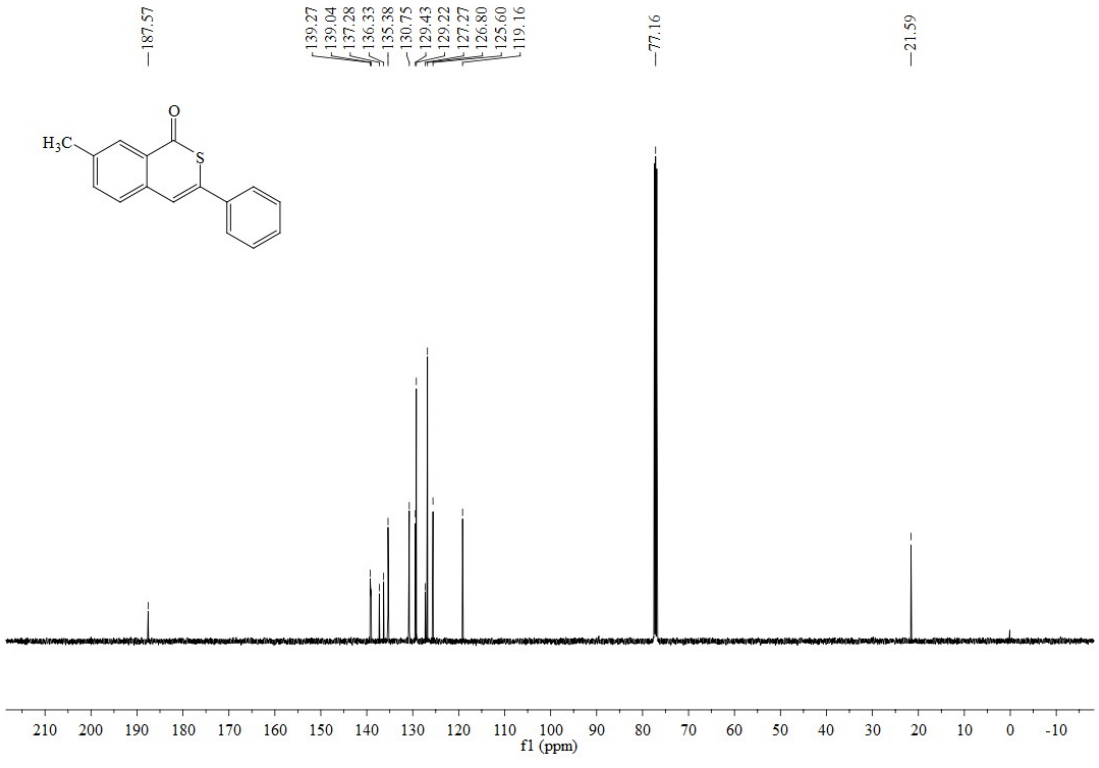
^{1}H NMR 500 MHz, in $CDCl_3$: 6-methyl-3-phenyl-1*H*-isothiochromen-1-one (18)



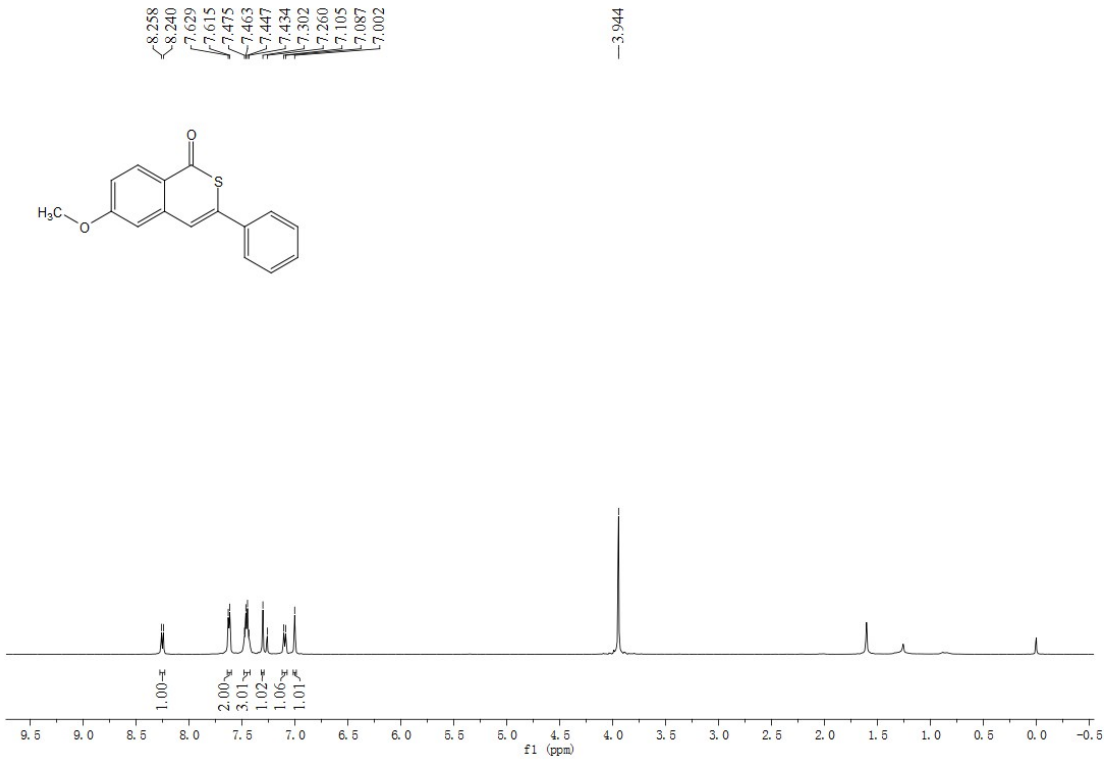
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 6-methyl-3-phenyl-1*H*-isothiochromen-1-one (18)



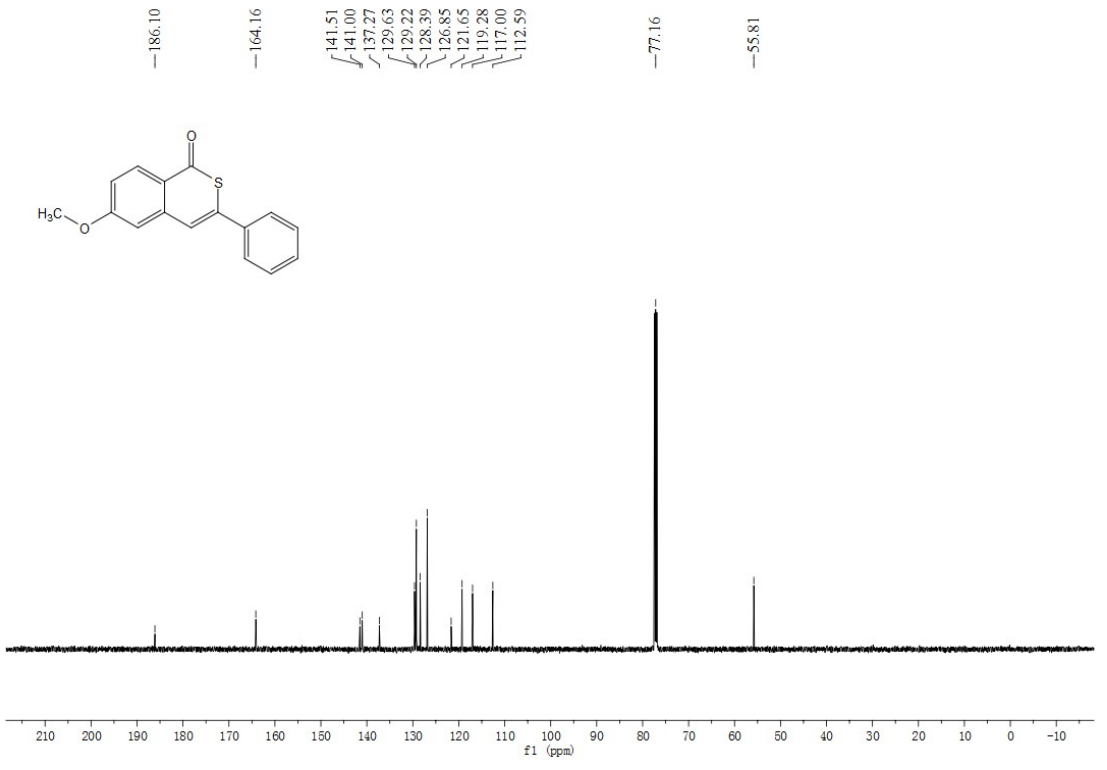
^{1}H NMR 500 MHz, in $CDCl_3$: 7-methyl-3-phenyl-1*H*-isothiochromen-1-one (19)



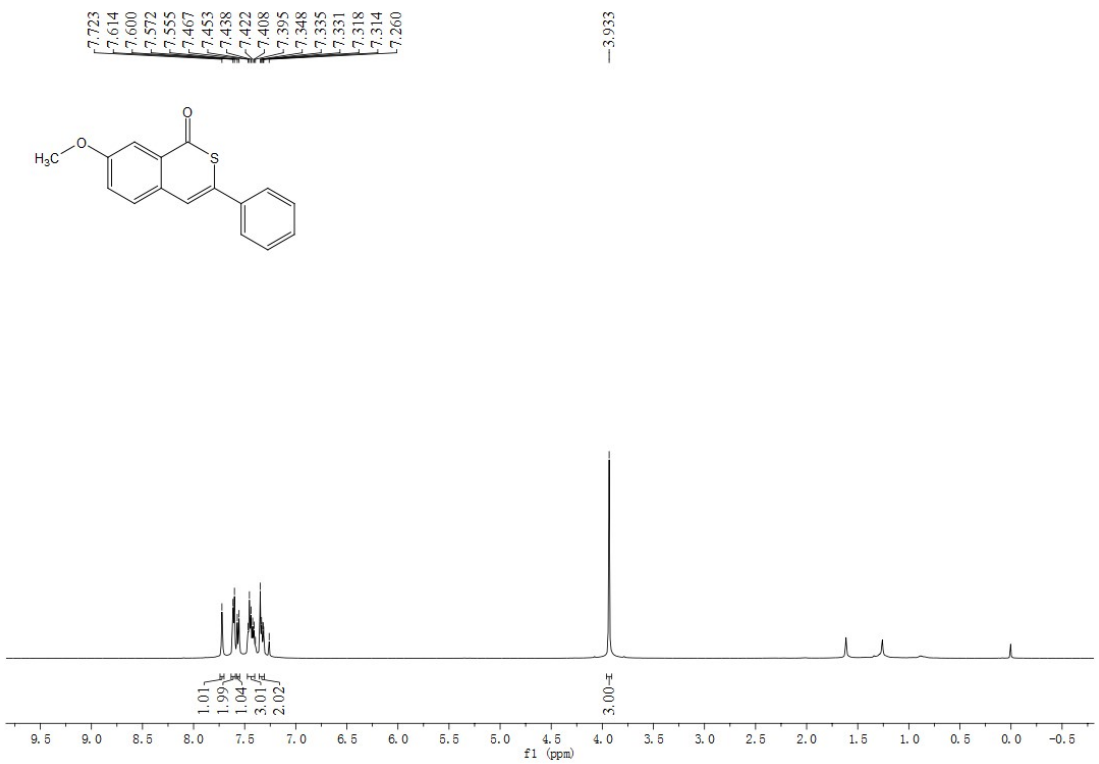
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 7-methyl-3-phenyl-1*H*-isothiochromen-1-one (19)



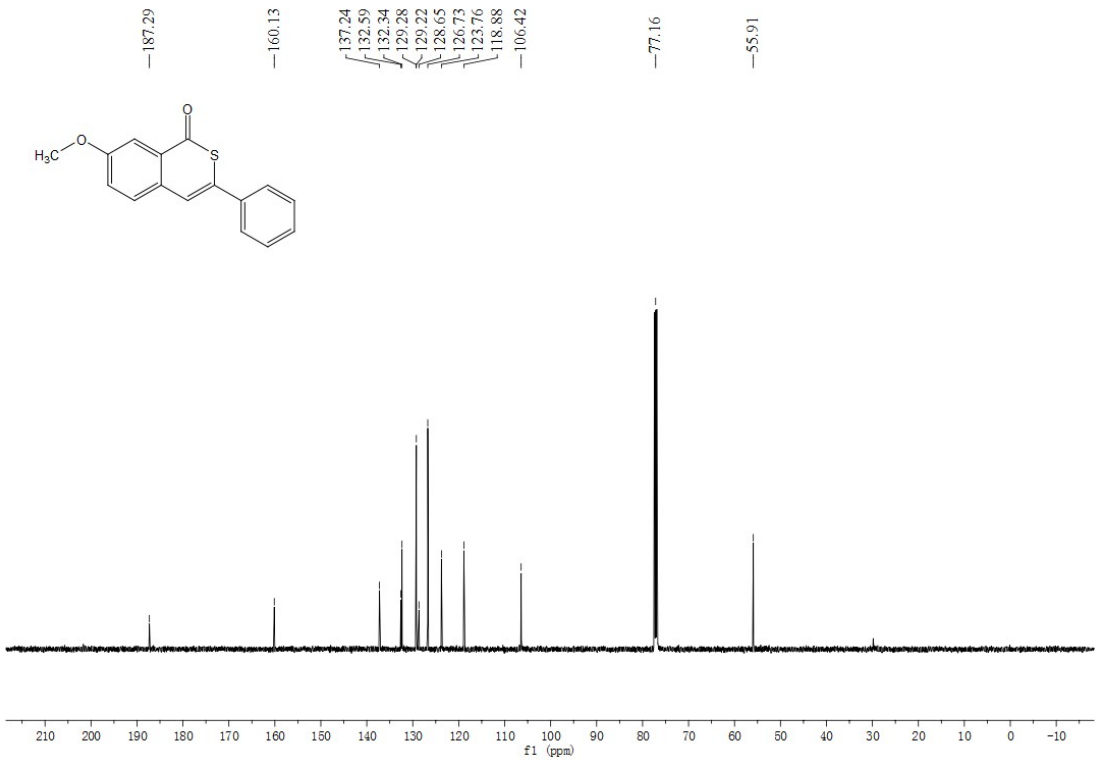
^{1}H NMR 500 MHz, in $CDCl_3$: 6-methoxy-3-phenyl-1*H*-isothiochromen-1-one (20)



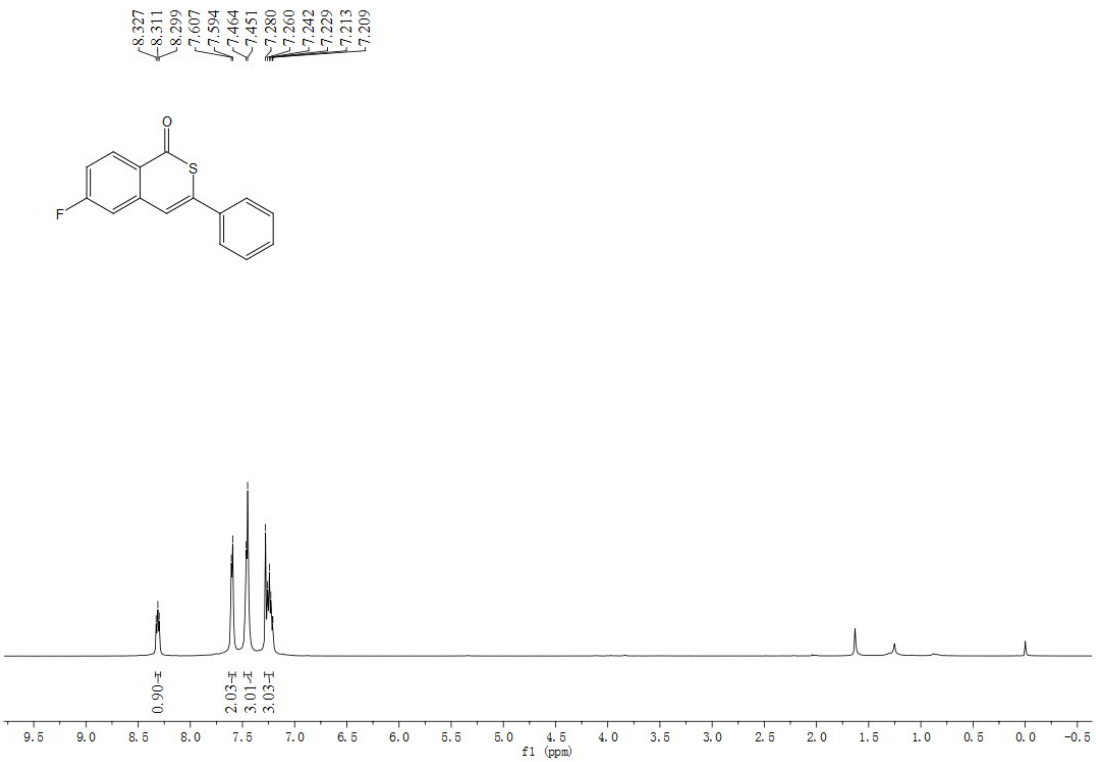
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 6-methoxy-3-phenyl-1*H*-isothiochromen-1-one (20)



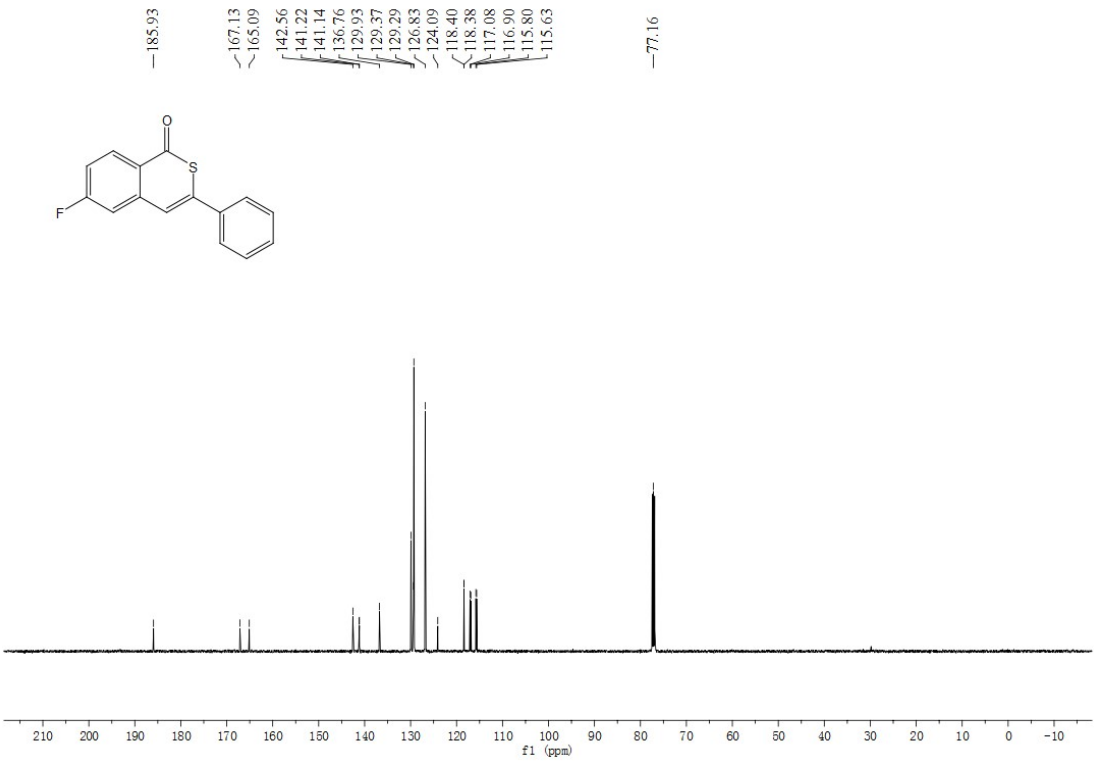
^{1}H NMR 500 MHz, in $CDCl_3$: 7-methoxy-3-phenyl-1*H*-isothiochromen-1-one (21)



^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 7-methoxy-3-phenyl-1*H*-isothiochromen-1-one (21)

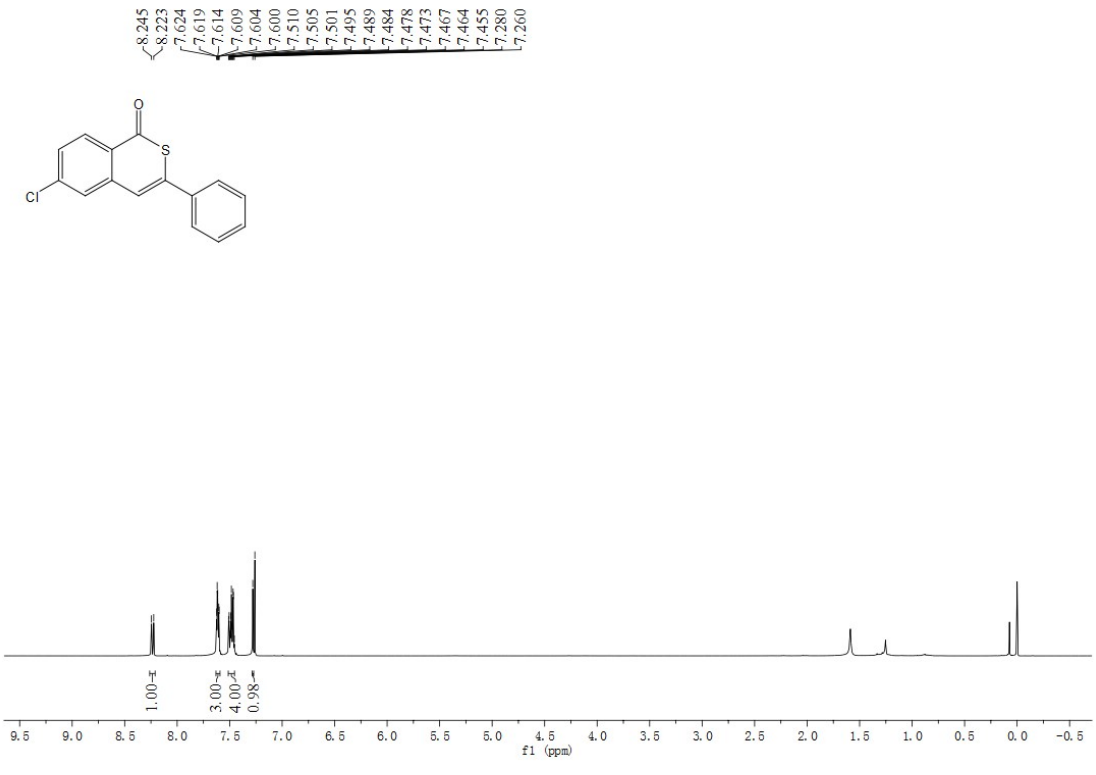


^{1}H NMR 500 MHz, in $CDCl_3$: 6-fluoro-3-phenyl-1*H*-isothiochromen-1-one (22)

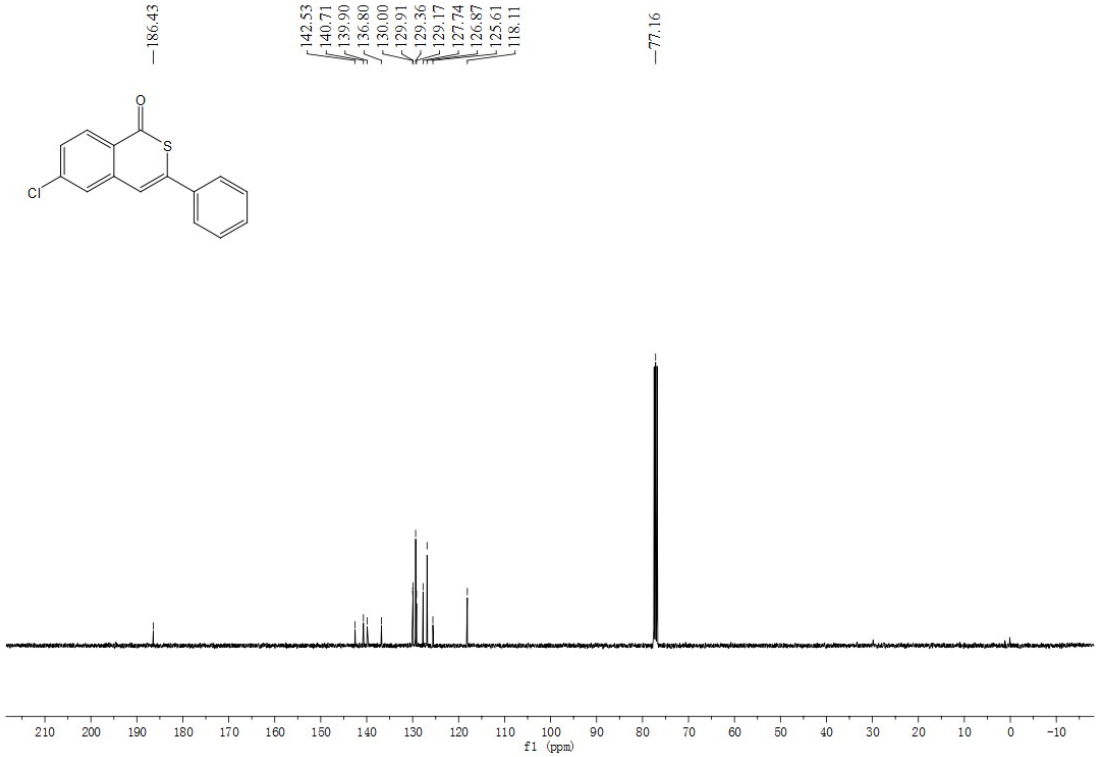


^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 6-fluoro-3-phenyl-1*H*-isothiochromen-1-one (22)

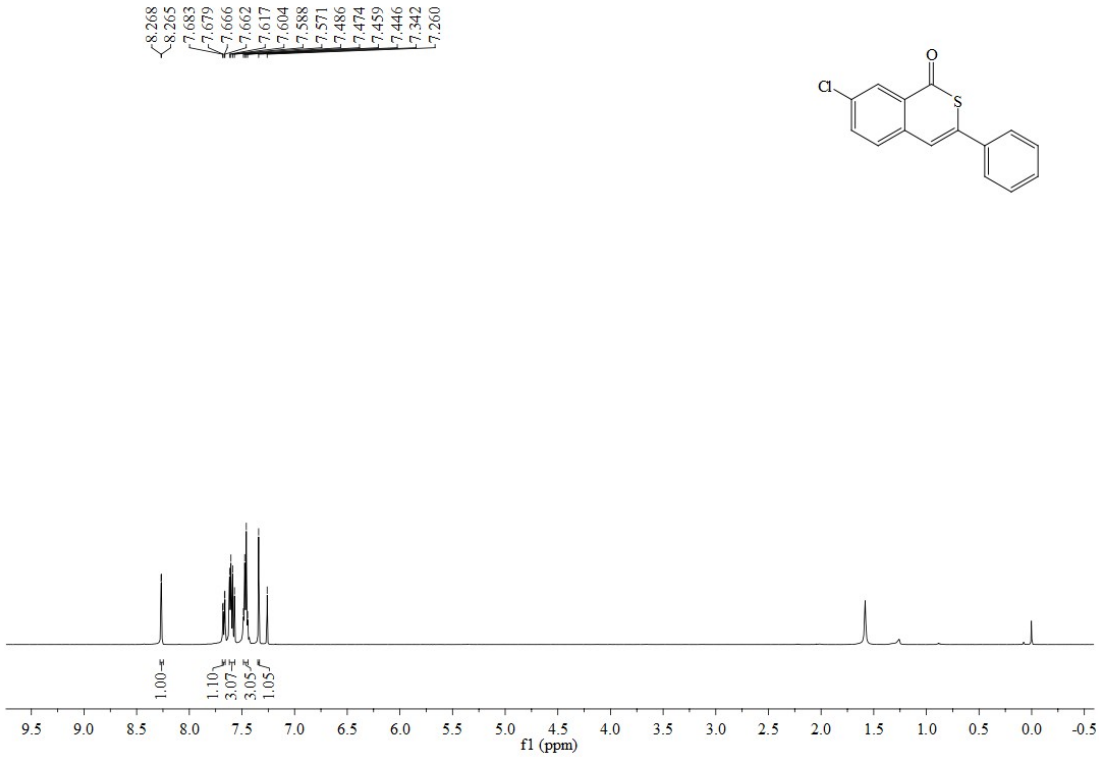
^{19}F NMR 470 MHz, in $CDCl_3$: 6-fluoro-3-phenyl-1*H*-isothiochromen-1-one (22)



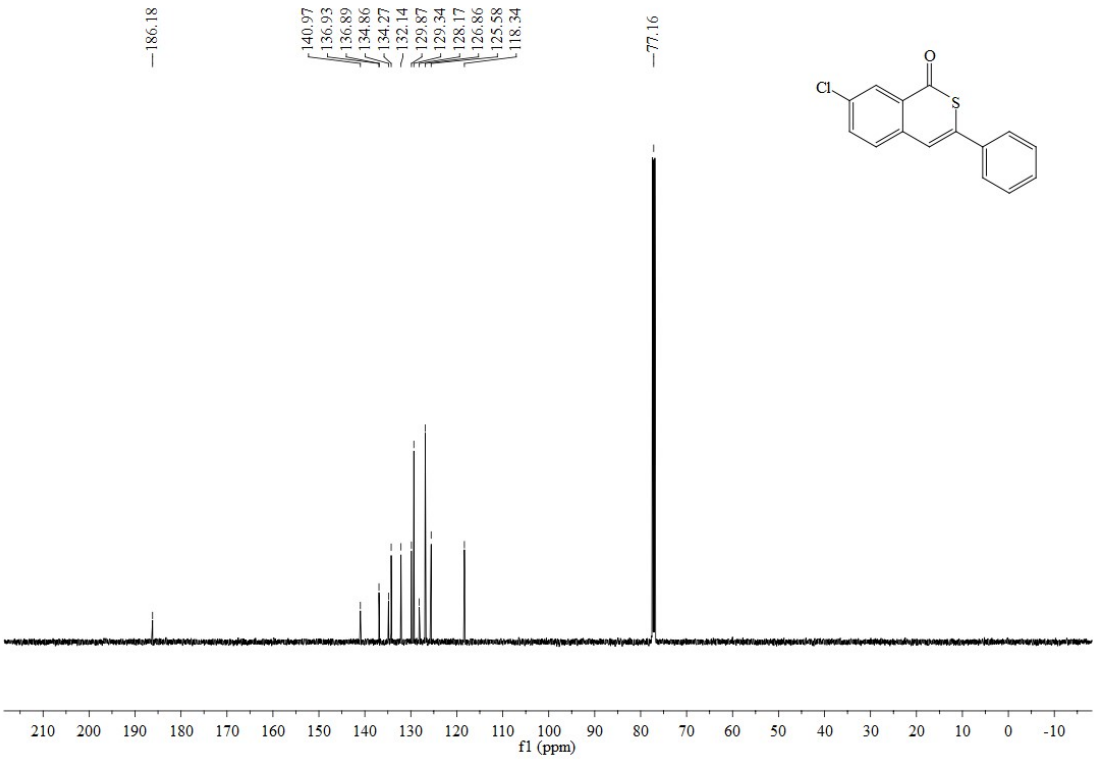
^{1}H NMR 400 MHz, in $CDCl_3$: 6-chloro-3-phenyl-1*H*-isothiochromen-1-one (23)



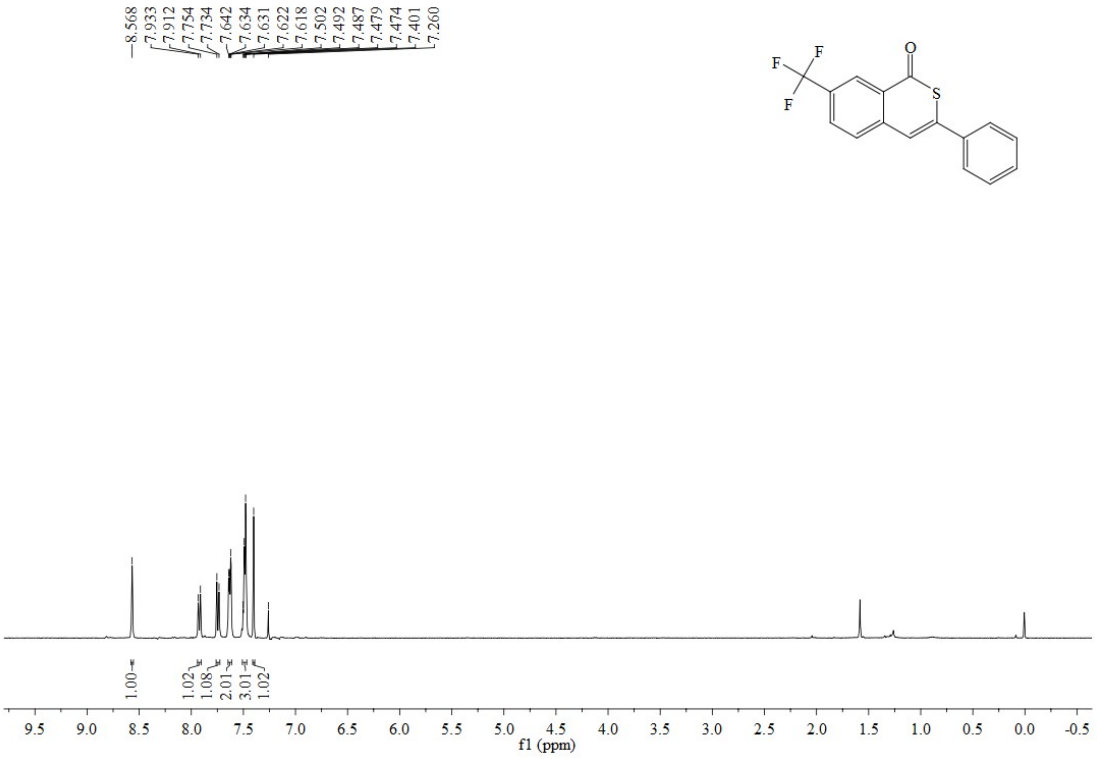
$^{13}C\{^{1}H\}$ NMR 100 MHz, in $CDCl_3$: 6-chloro-3-phenyl-1*H*-isothiochromen-1-one (23)



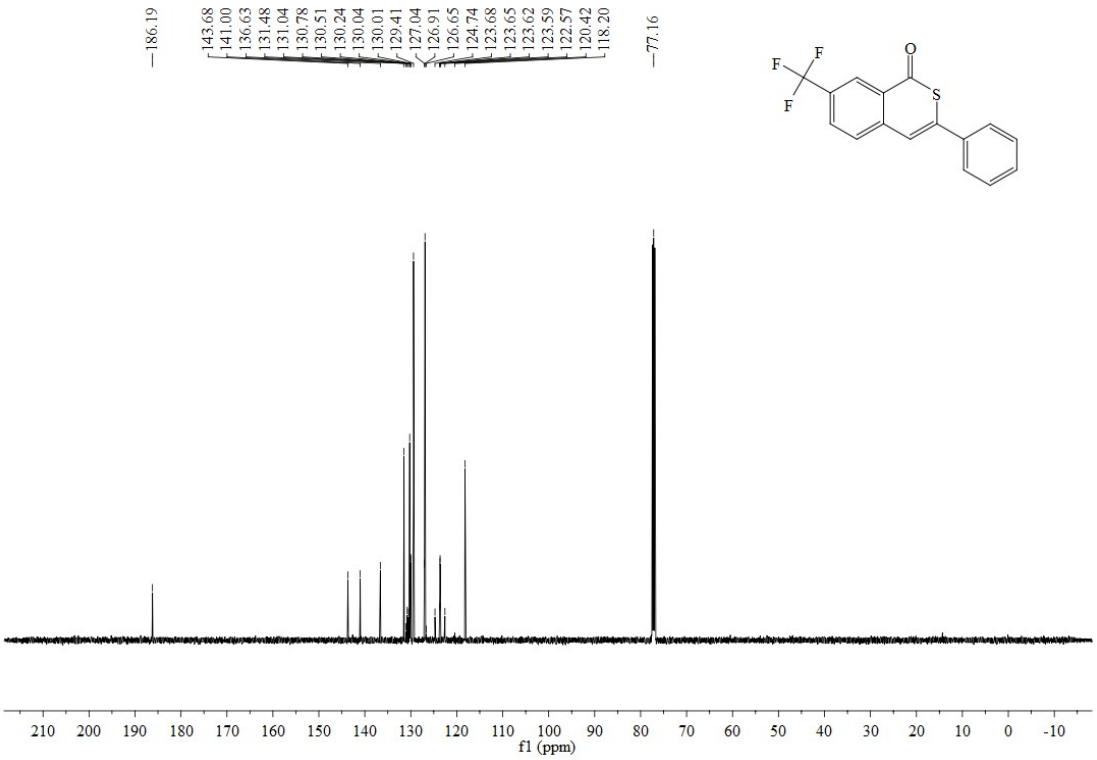
^{1}H NMR 500 MHz, in $CDCl_3$: 7-chloro-3-phenyl-1*H*-isothiochromen-1-one (24)



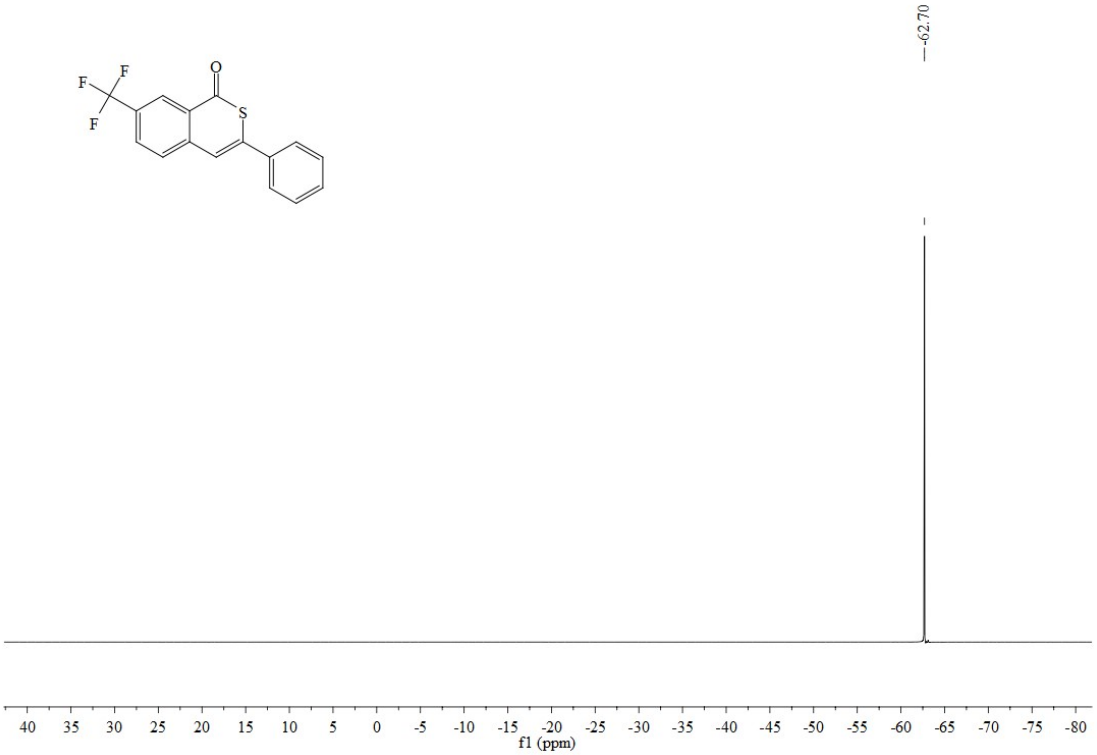
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 7-chloro-3-phenyl-1*H*-isothiochromen-1-one (24)



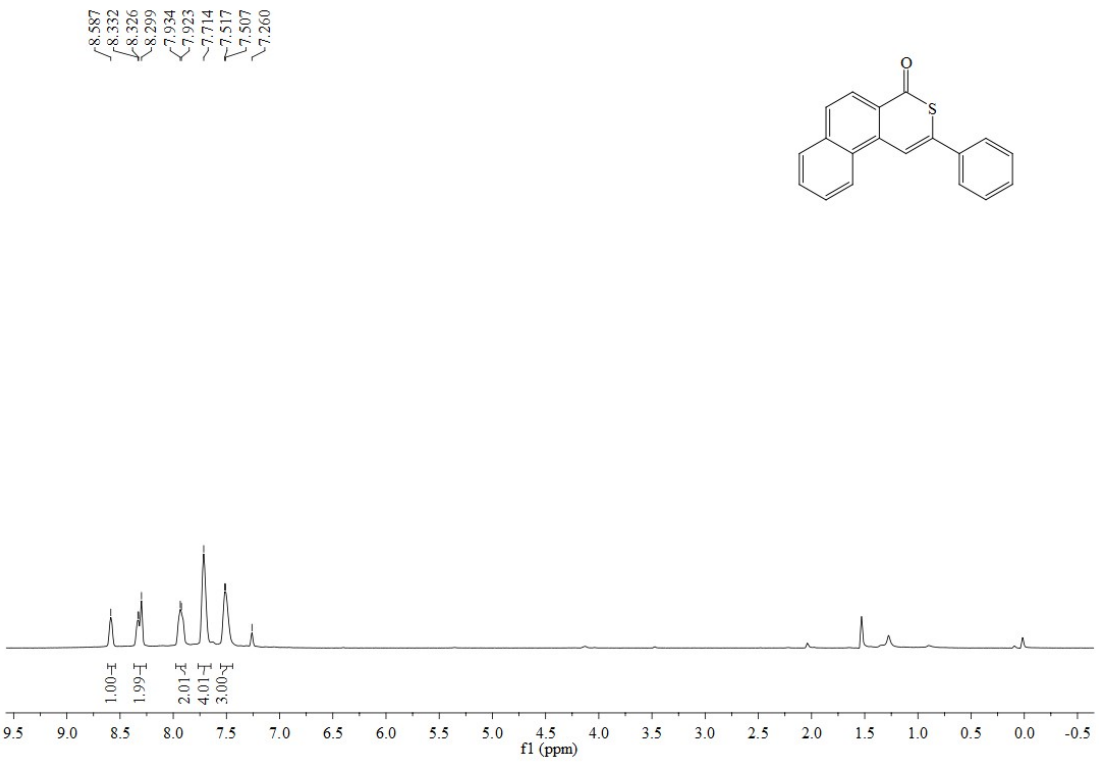
^{1}H NMR 500 MHz, in $CDCl_3$: 3-phenyl-7-(trifluoromethyl)-1*H*-isothiochromen-1-one (25)



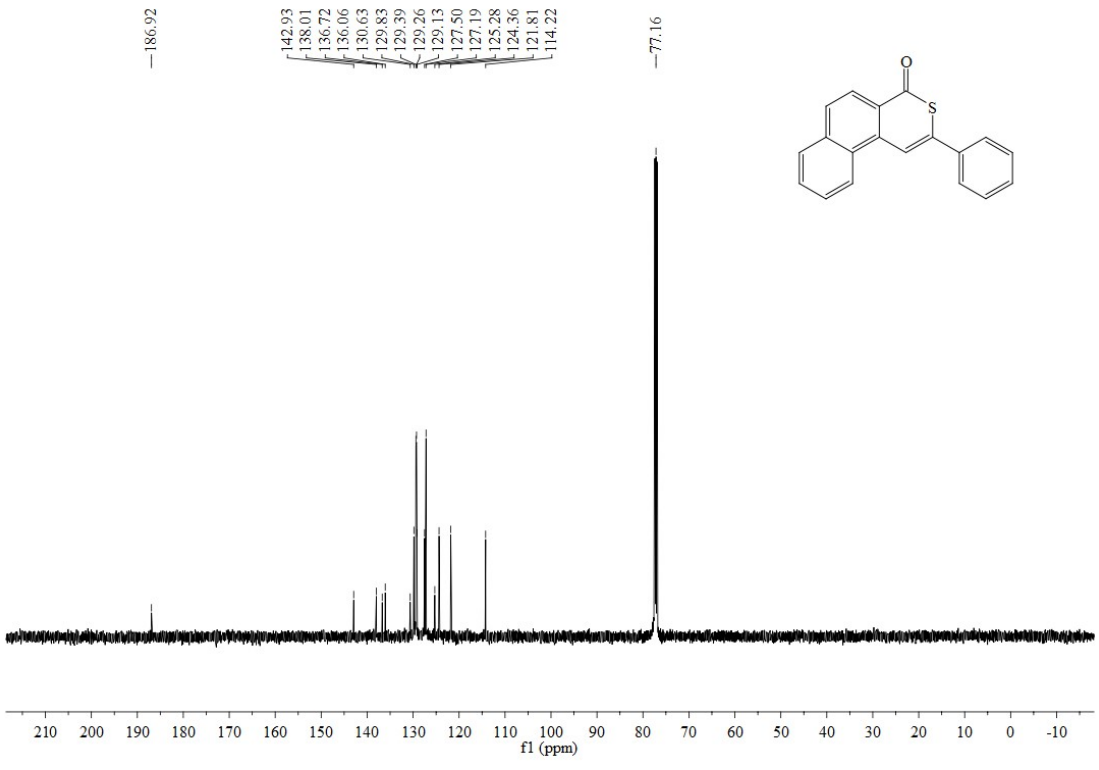
$^{13}C\{^{1}H\}$ NMR 125 MHz, in $CDCl_3$: 3-phenyl-7-(trifluoromethyl)-1*H*-isothiochromen-1-one (25)



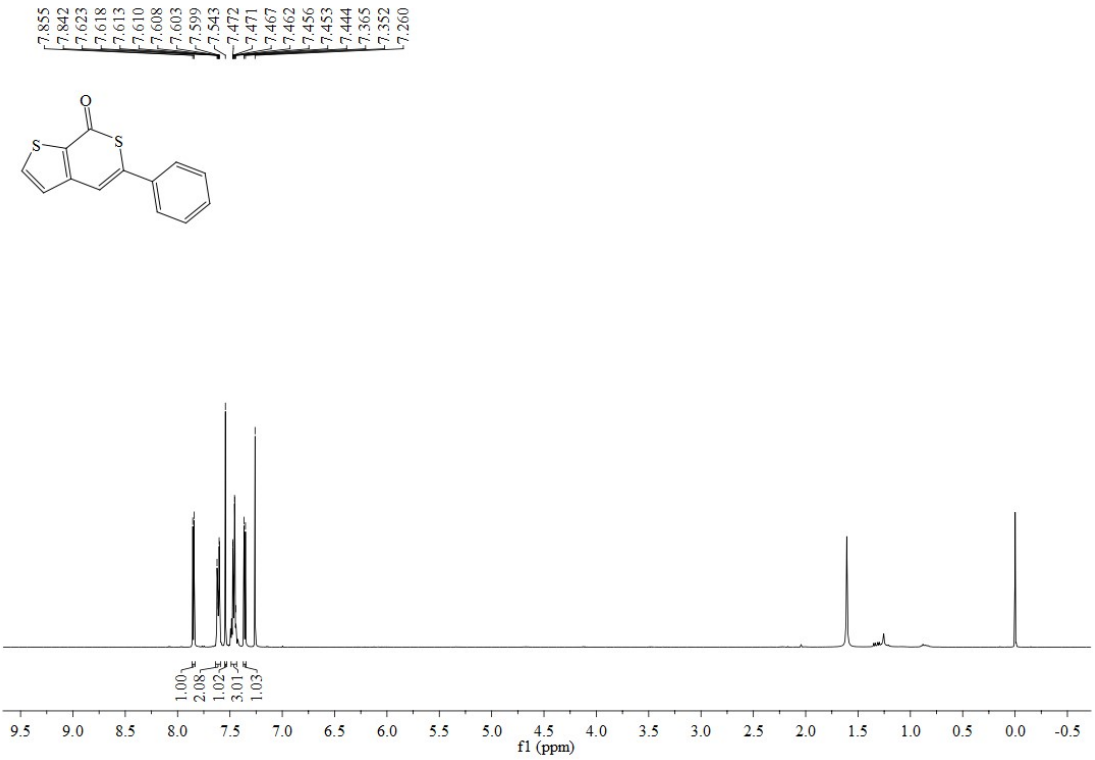
^{19}F NMR 470 MHz, in $CDCl_3$: 3-phenyl-7-(trifluoromethyl)-1*H*-isothiochromen-1-one (25)



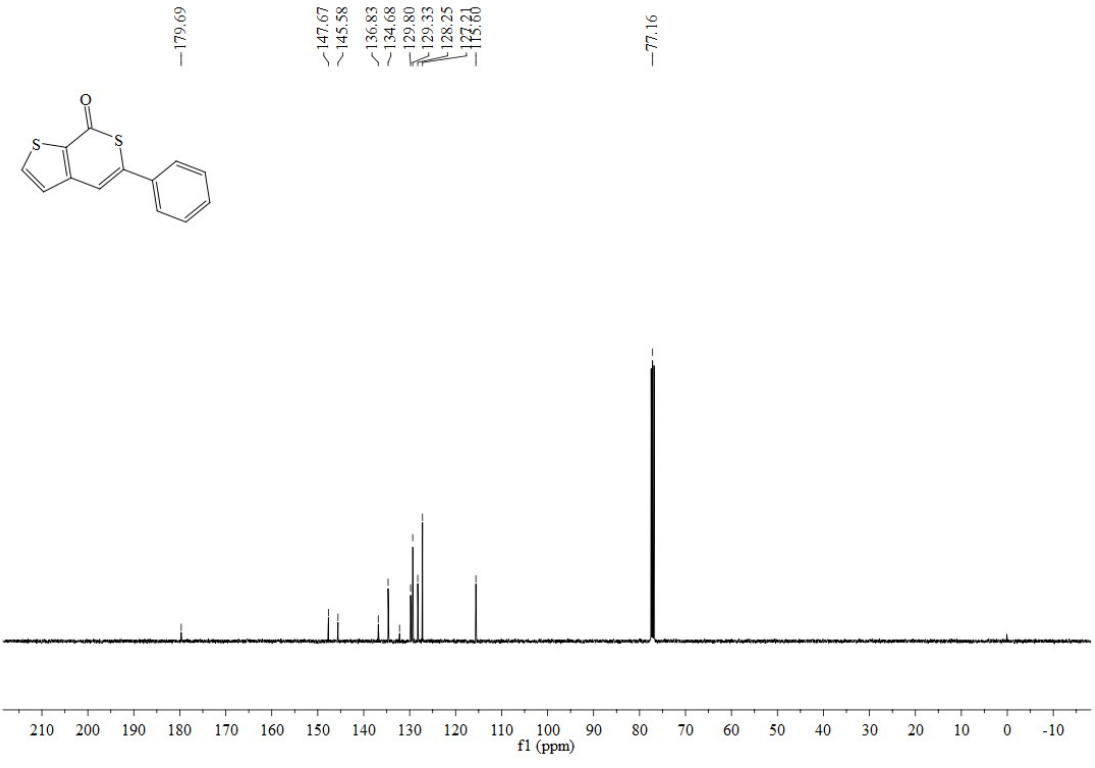
^{1}H NMR 500 MHz, in $CDCl_3$: 2-phenyl-4*H*-benzo[*f*]isothiochromen-4-one (26)



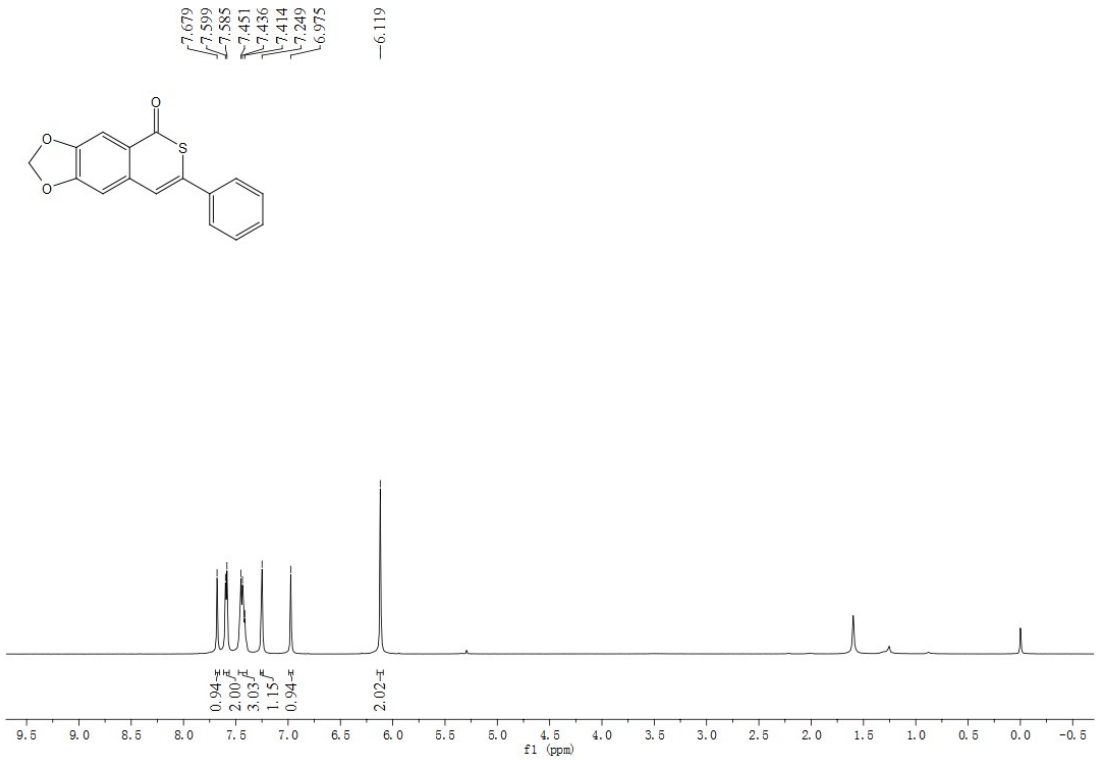
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 2-phenyl-4*H*-benzo[*f*]isothiochromen-4-one (26)



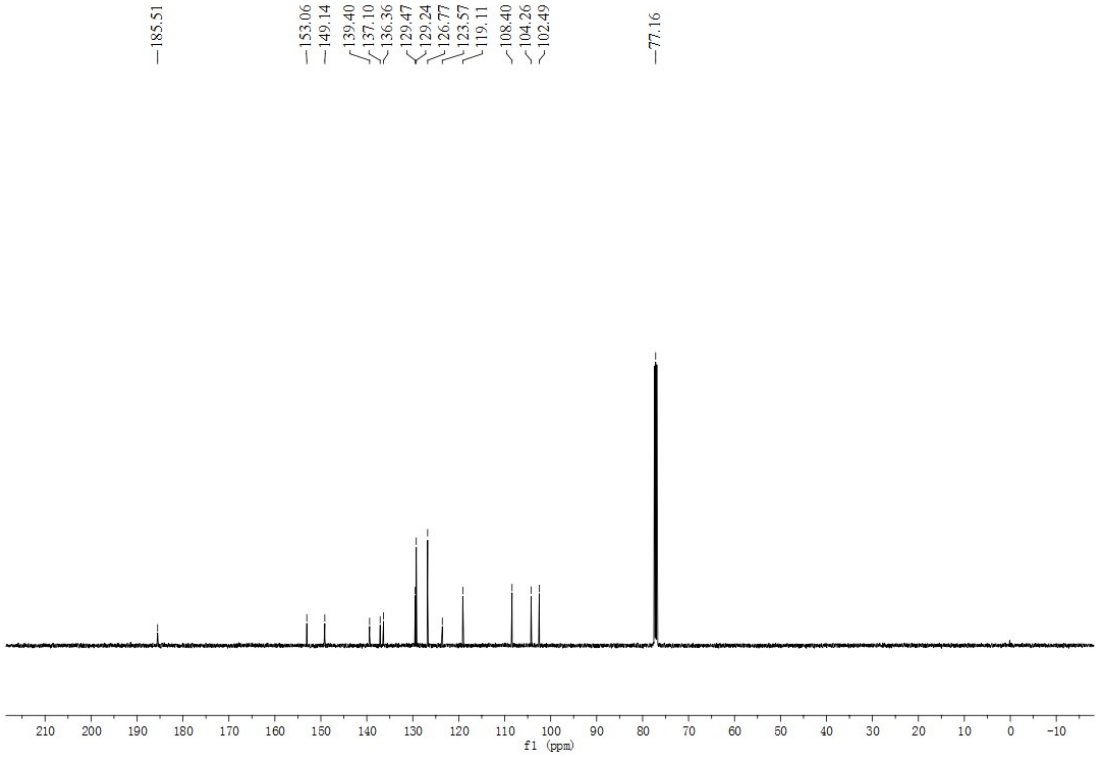
^{1}H NMR 400 MHz, in $CDCl_3$: 5-phenyl-7*H*-thieno[2,3-*c*]thiopyran-7-one (27)



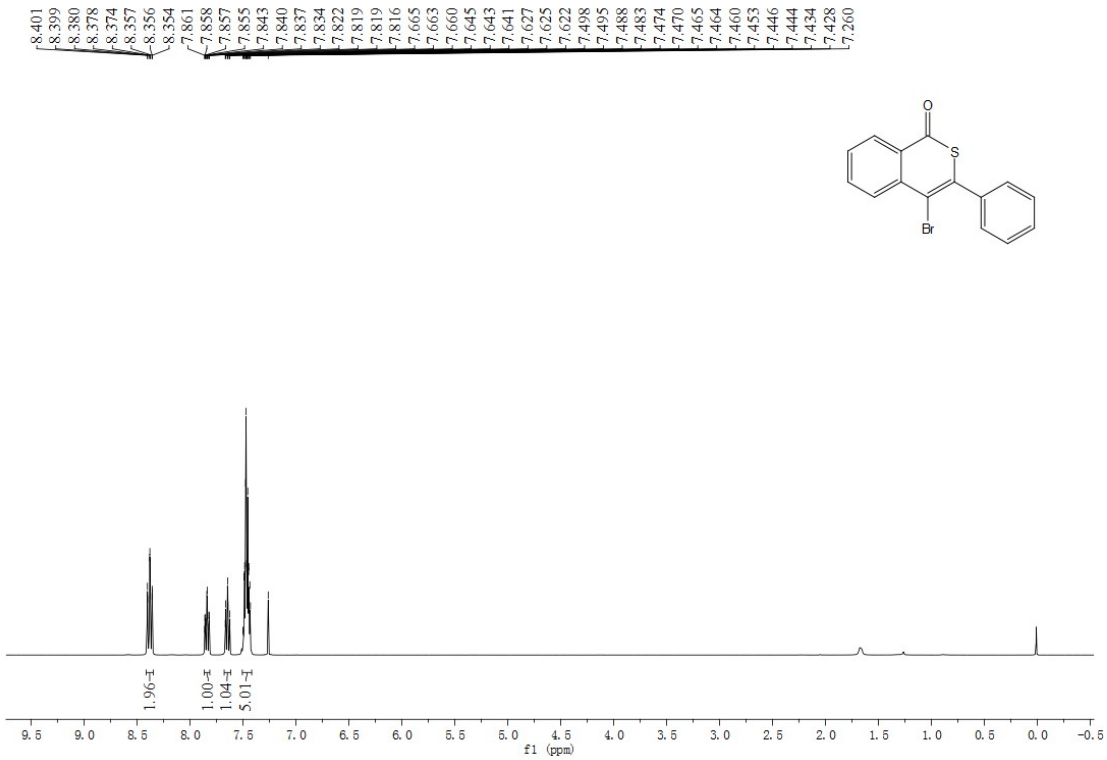
^{13}C{^{1}H} NMR 100 MHz, in $CDCl_3$: 5-phenyl-7*H*-thieno[2,3-*c*]thiopyran-7-one (27)



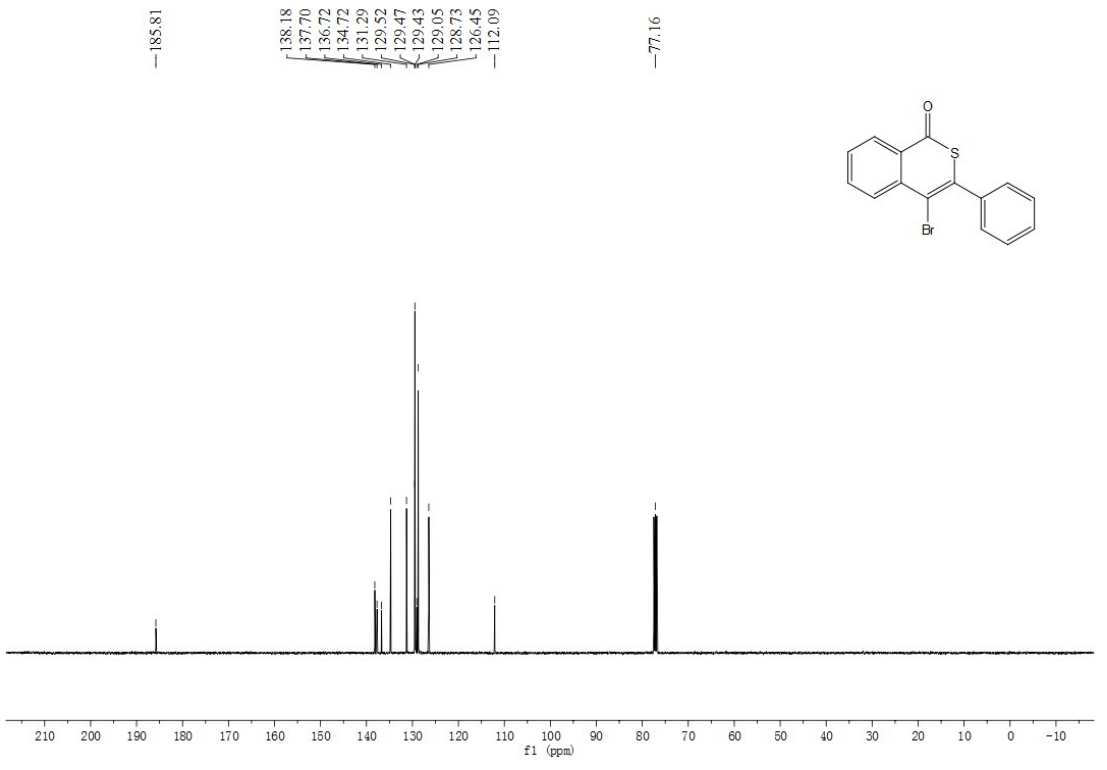
^{1}H NMR 500 MHz, in $CDCl_3$: 7-phenyl-5*H*-isothiochromeno[6,7-d][1,3]dioxol-5-one (28)



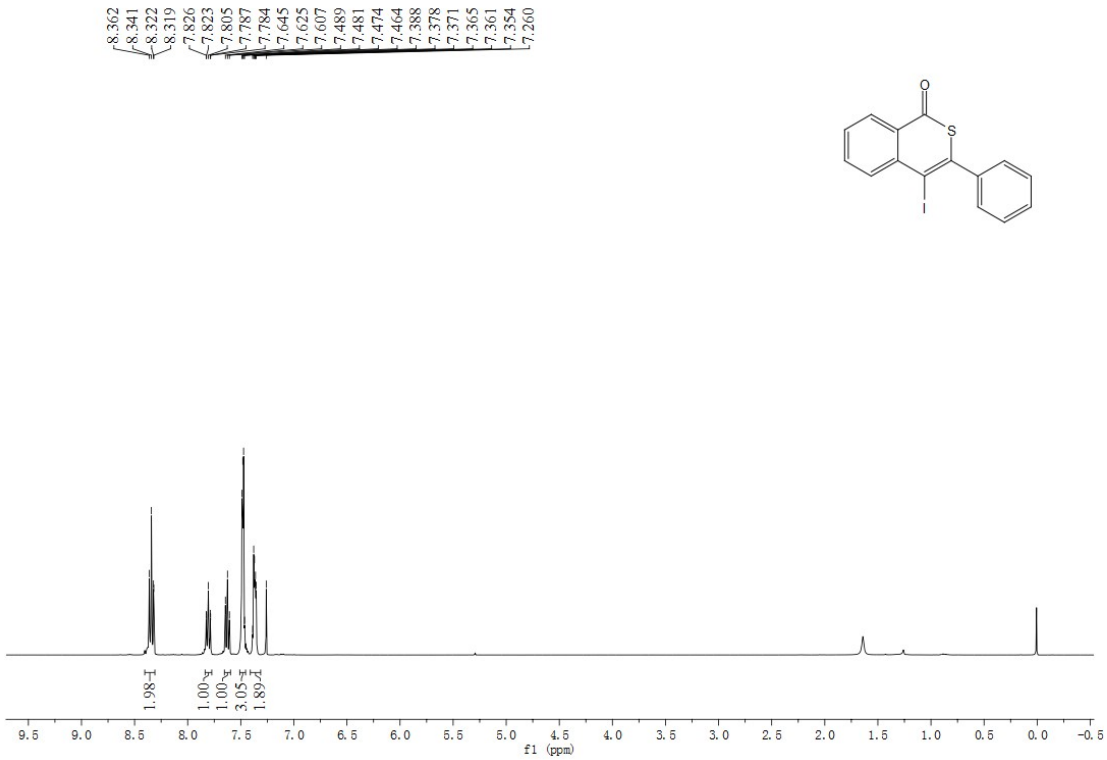
^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 7-phenyl-5*H*-isothiochromeno[6,7-d][1,3]dioxol-5-one (28)



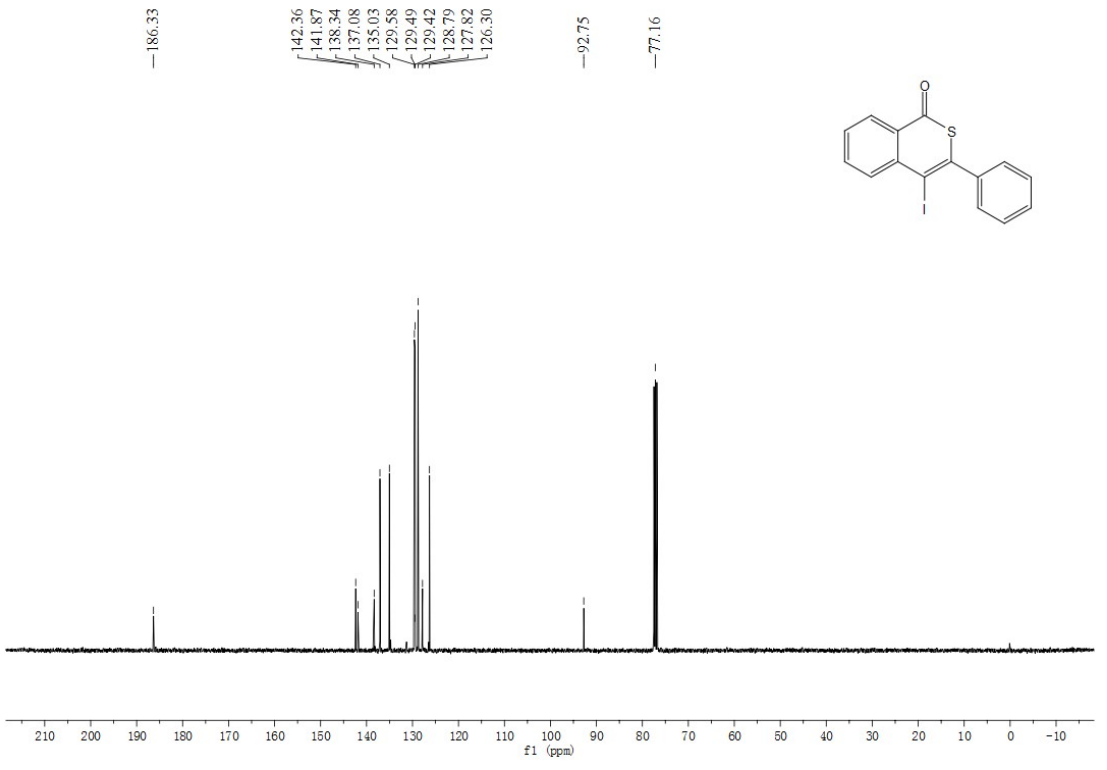
^{1}H NMR 400 MHz, in $CDCl_3$: 4-bromo-3-phenyl-1*H*-isothiochromen-1-one (29)



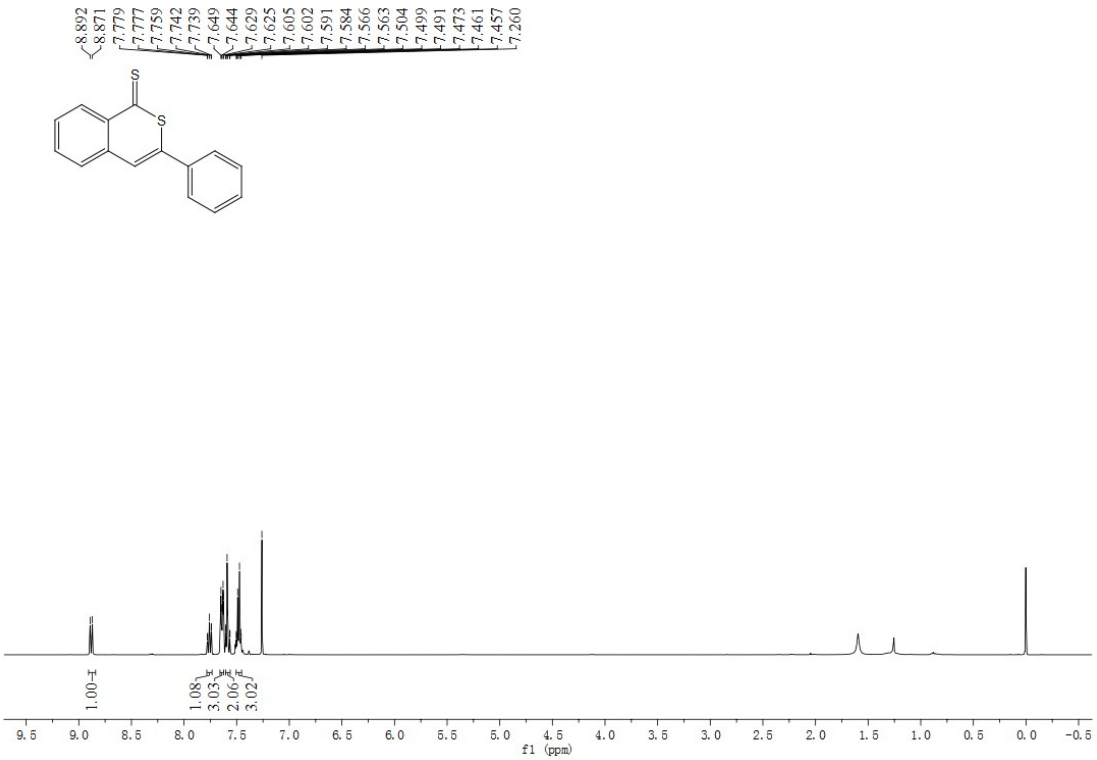
^{13}C{^{1}H} NMR 100 MHz, in $CDCl_3$: 4-bromo-3-phenyl-1*H*-isothiochromen-1-one (29)



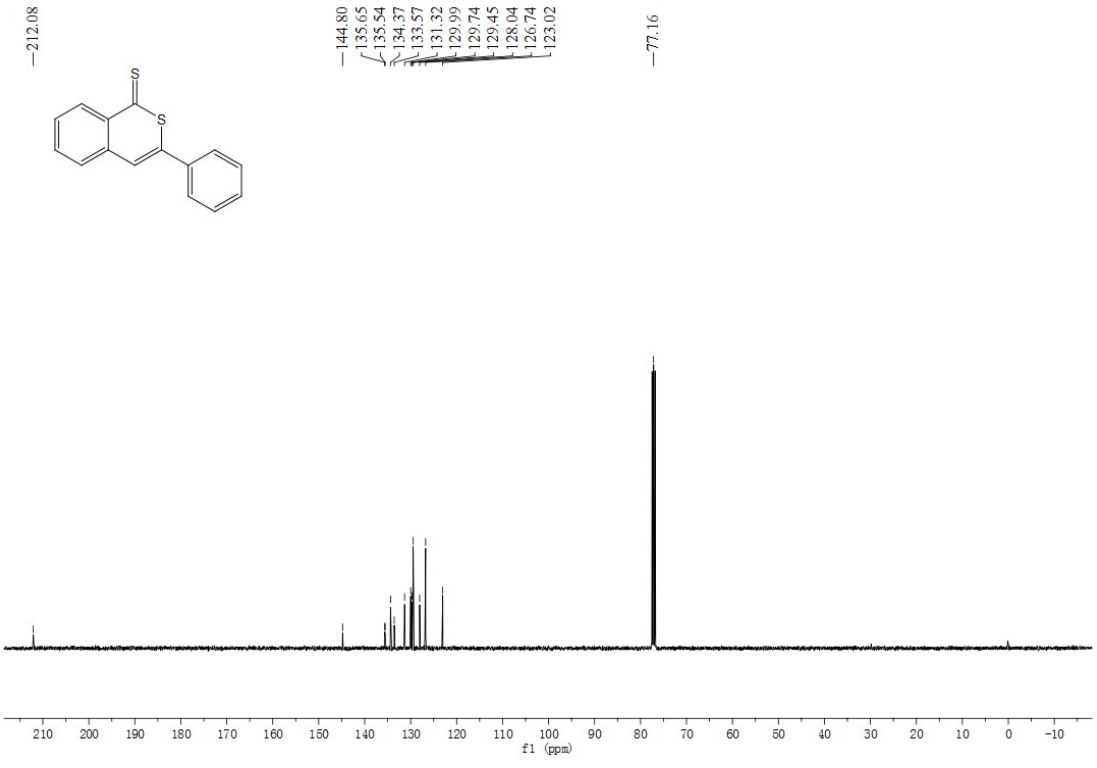
^{1}H NMR 400 MHz, in $CDCl_3$: 4-iodo-3-phenyl-1*H*-isothiochromen-1-one (30)



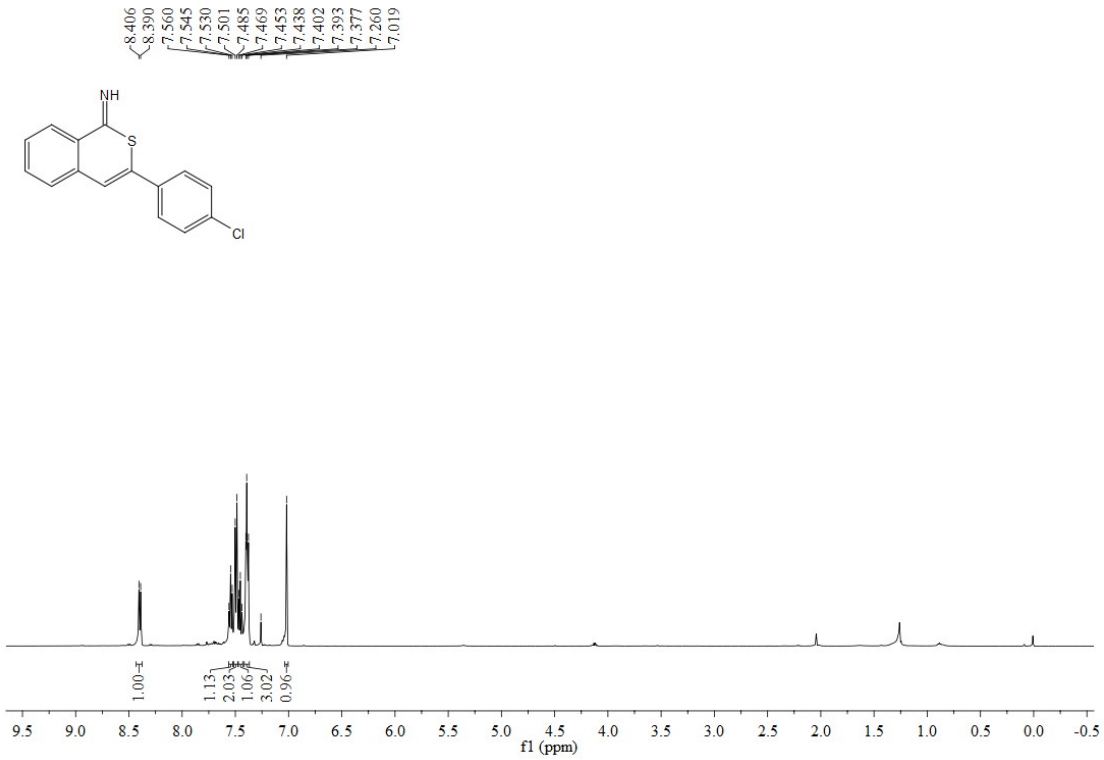
^{13}C{^{1}H} NMR 100 MHz, in $CDCl_3$: 4-iodo-3-phenyl-1*H*-isothiochromen-1-one (30)



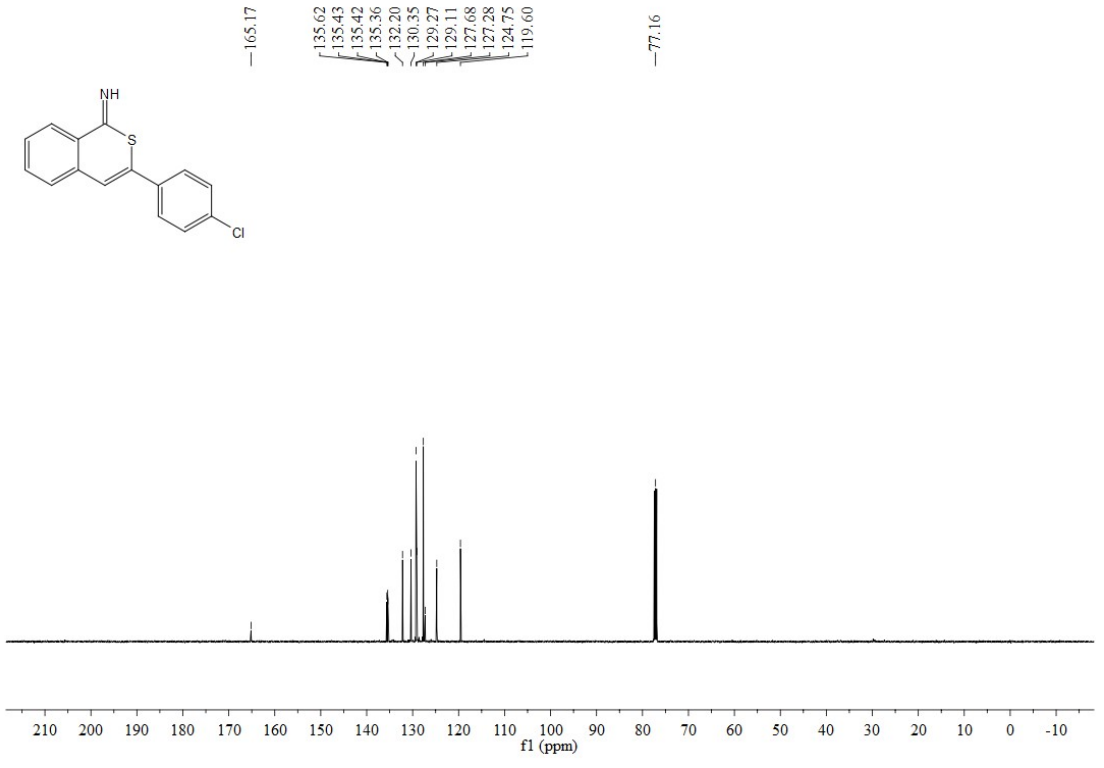
^{1}H NMR 400 MHz, in $CDCl_3$: 3-phenyl-1*H*-isothiochromene-1-thione (31)



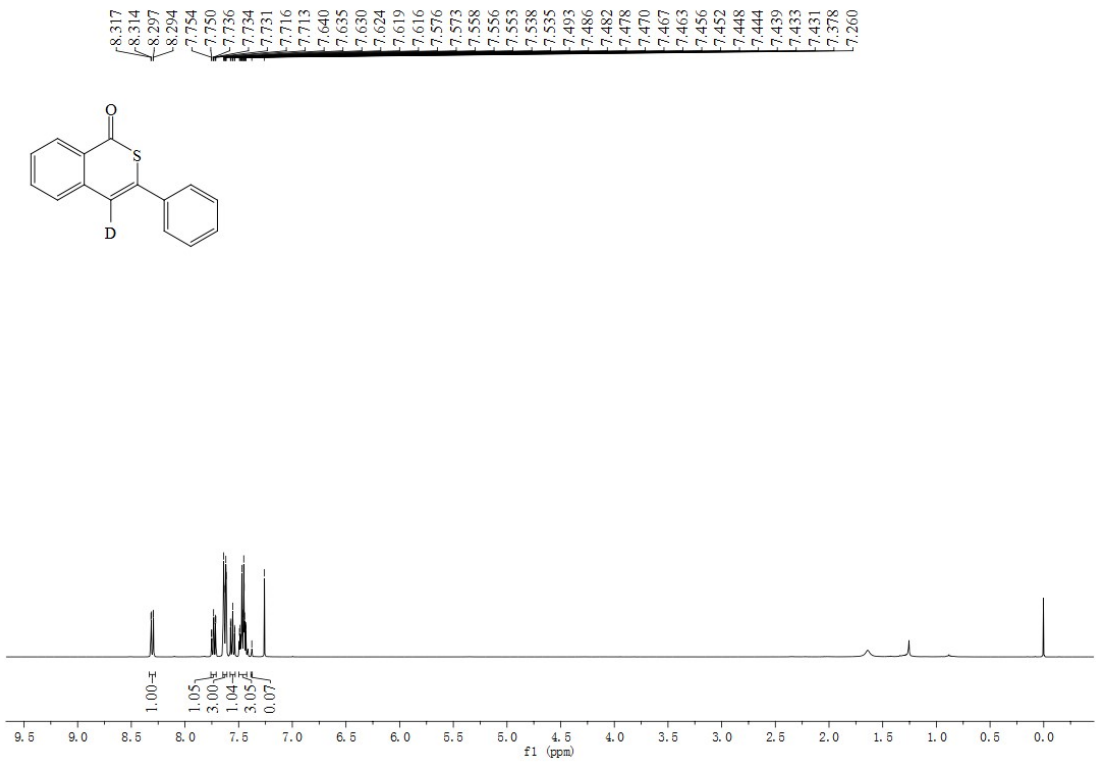
^{13}C{^{1}H} NMR 100 MHz, in $CDCl_3$: 3-phenyl-1*H*-isothiochromene-1-thione (31)



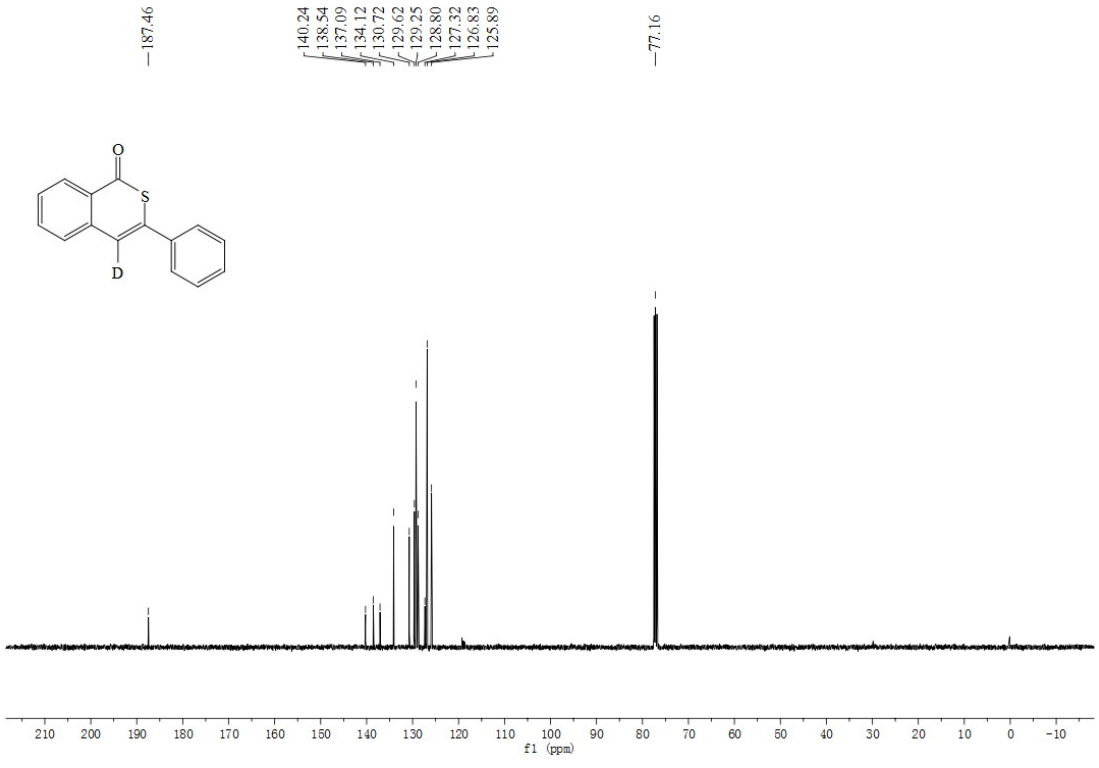
^{1}H NMR 500 MHz, in $CDCl_3$: 3-(4-chlorophenyl)-1*H*-isothiochromen-1-imine (32)



^{13}C{^{1}H} NMR 125 MHz, in $CDCl_3$: 3-(4-chlorophenyl)-1*H*-isothiochromen-1-imine (32)

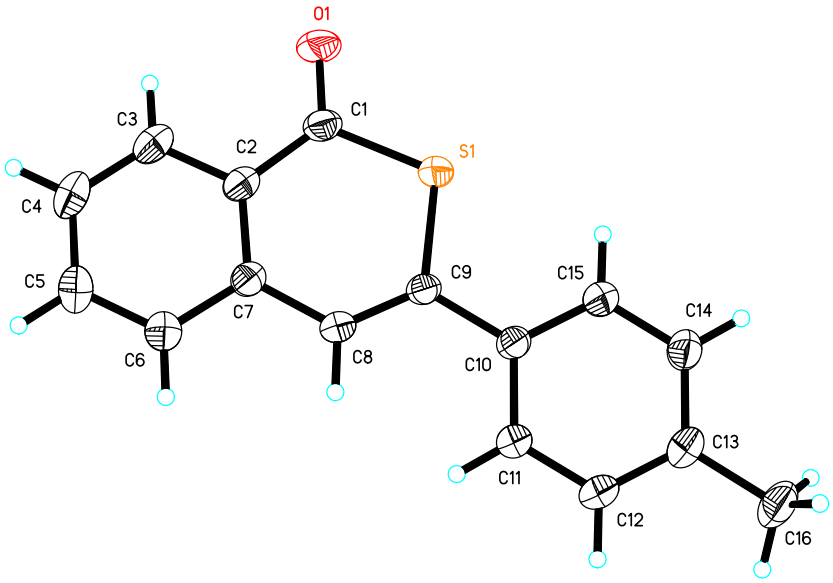


^{1}H NMR 400 MHz, in $CDCl_3$: 3-phenyl-1*H*-isothiochromen-1-one-4-*d* (D-2)



^{13}C{^{1}H} NMR 100 MHz, in $CDCl_3$: 3-phenyl-1*H*-isothiochromen-1-one-4-*d* (D-2)

3. X-ray crystal structure and data of compound 3



The figure of compound 3

The displacement ellipsoids are drawn at the 30% probability level

Single crystals suitable for X-ray analysis were obtained by slow evaporation of mixed petroleum ether: ethyl acetate (5:1, v:v).

Sheldrick, G. M.; SHELXL-97, Program for X-ray Crystal Structure Solution and Refinement, University of Göttingen: Germany, 1997.

Sheldrick, G.M. SHELXTL. *Structure Determination Software Programs. Version 6.14. Bruker AXS. Madison, Wisconsin, USA 2000.*

Supplementary crystallographic data was deposited at the Cambridge Crystallographic Data Centre (CCDC) under the number CCDC- 2084840 (**3**) and can be obtained free of charge *via* www.ccdc.cam.ac.uk/data_request.cif.

Table S1: Crystal Structure and Data Refinement Parameters of compound 3

Compound	**3**
Empirical Formula	C16 H12 O S
Formula Weight	252.32
Crystal System / Space Group	Triclinic, P -1
a / Å	7.2215(3)
b / Å	8.8635(4)
c / Å	9.7122(4)
α / °	91.3540(10)
β / °	92.0140(10)
γ / °	92.341(2)
V / $Å^3$	620.56(5)
Z	2
D_{calc} (Mg/m^3)	1.350
μ (mm^{-1})	0.244
Crystal size (mm)	0.200 x 0.150 x 0.110
Color / Shape	yellow
Temp (K)	293(2)
Theta range for collection	3.076 to 26.000°
Reflections collected	8960
Independent reflections	2401
Data/restraints/parameters	2401 / 0 / 164
Goodness of fit on F^2	1.066
Final R indices [I > 2σ(I)]	R1 = 0.0375, wR2 = 0.1070
R indices (all data)	R1 = 0.0416, wR2 = 0.1117
Largest difference peak/hole	0.238 and -0.168