Supporting Information

for

Skeletal Editing of Benzodithiol-3-ones for the Assembly of Benzo[d][1,3]oxathiin-4-ones

Wenxin Lv,[#] Xuan Kong,[#] Yushang Qing, Jing Zheng, Yuan Yin, Yao Zhou*, Dun-jia Wang

Hubei Key Laboratory of Pollutant Analysis & Reuse Technology, College of Chemistry and Chemical Engineering, Hubei Normal University, Huangshi 435002, China

[#] Wenxin Lv and Xuan Kong contributed equally to the experimental work.

*E-mail: yaozhou@hbnu.edu.cn

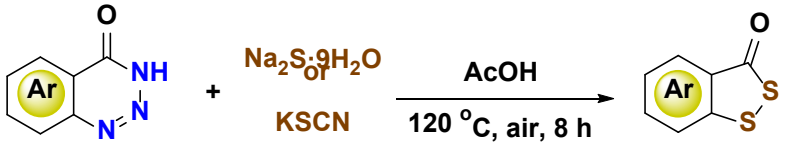
Table of Contents

1. General information

All reagents and solvents were obtained from commercial suppliers and used without further purification. The 3*H*-benzo[c][1,2]dithiol-3-one (**1a**) was purchased from Bide Pharmatech Ltd and paraformaldehyde was purchased from Energy Chemical. Unless otherwise stated, all experiments were conducted in a seal tube under air atmosphere. Reactions were monitored by TLC or GC-MS analysis. Flash column chromatography was performed over silica gel (200-300 mesh).

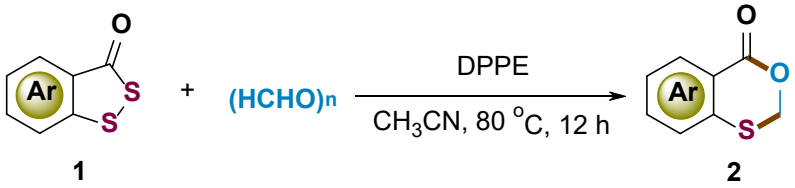
^{1}H-NMR and ^{13}C-NMR spectra were recorded in $CDCl_3$ on a Bruker Avance 300 spectrometer (300 MHz ^{1}H, 75 MHz ^{13}C) at room temperature. Chemical shifts were reported in ppm on the scale relative to $CDCl_3$ (δ = 7.26 for ^{1}H-NMR , δ = 77.00 for ^{13}C-NMR) or DMSO-d_6 (δ = 2.50 for ^{1}H-NMR, δ = 39.96 for ^{13}C-NMR) as an internal reference. High resolution mass spectra were recorded using Q-TOF time-of-flight mass spectrometer. Coupling constants (*J*) were reported in Hertz (Hz).

2. General procedure for the synthesis of starting materials 1



1,2-Benzodithiol-3-ones **1** were prepared according to our previous work which are known compounds. AcOH (15 mL) was added to a mixture of benzo[d][1,2,3]triazin-4(3H)-one (3 mmol) and $Na_2S·9H_2O$ or KSCN (12 mmol) in a 150 mL sealed tube. Then the reaction mixture was stirred at 120 °C in an oil bath for 8 h. Upon completion of the reaction, ethyl acetate was added to the mixture, and then washed with saturated brine with thrice. The combined water layers were extracted with ethyl acetate twice. The combined organic layers were dried over anhydrous Na_2SO_4. The solvents were removed via rotary evaporator and the residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 30:1, v/v) to give the desired product as yellow solid.

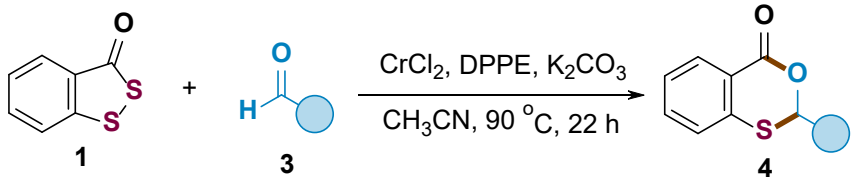
3. General procedure to synthesize products 2



CH_3CN (2 mL) was added to a mixture of 1,2-benzodithiol-3-ones **1** (0.3 mmol), paraformaldehyde (1.2 mmol, 36 mg) and DPPE (0.2 mmol, 79.4 mg) in a sealed tube. Then the reaction mixture was stirred at 80 °C for 12 h. Upon completion of the reaction, the solvents were removed via rotary evaporator and the residue was purified by flash column chromatograph (silica gel, petroleum ether: EtOAc as the eluent) to give the desired product benzo[d][1,3]oxathiin-4-ones **2**.

[*Scale-up for larger synthesis of* ***2a***]: CH_3CN (30 mL) was added to a mixture of 1,2-benzodithiol-3-ones **1a** (0.84 g, 5 mmol), paraformaldehyde (0.45 g, 15 mmol) and DPPE (1.31 g, 3.3 mmol) in a 150 mL sealed tube. Then the reaction mixture was stirred at 80 °C for 18 h. Upon completion of the reaction, the solvents were removed via rotary evaporator and the residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the desired productbenzo[d][1,3]oxathiin-4-ones **2a** as colourless oil (0.67 g, 81%).

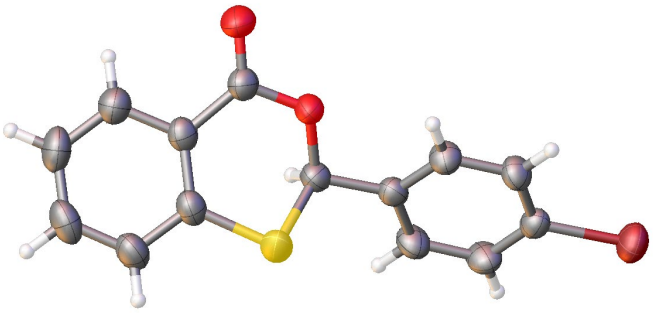
4. General procedure to synthesize products 4



CH_3CN (2 mL) was added to a mixture of 1,2-benzodithiol-3-ones **1** (0.3 mmol), aldehydes (0.2 mmol), $CrCl_2$ (20 mol%, 5 mg), K_2CO_3 (0.4 mmol, 55.2 mg) and DPPE (0.2 mmol, 79.4 mg) in a sealed tube. Then the reaction mixture was stirred at 90 °C for 22 h. Upon completion of the reaction, the solvents were removed via rotary evaporator and the residue was purified by flash column chromatograph (silica gel, petroleum ether: EtOAc as the eluent) to give the desired product benzo[d][1,3]oxathiin-4-ones **4**.

5. Crystal data of 4h

Crystallographic data for compound **4h** (CCDC-2353212) has already been deposited with the Cambridge Crystallographic Data Centre, Copies of the data can be obtained, free of charge, on application to CCDC (Email: deposit@ccdc.cam.ac.uk)



Displacement ellipsoids are drawn at 50% probability leve

Bond precision: C-C = 0.0044 A Wavelength=0.71073

Cell: a=9.4078(8) b=13.1508(11) c=10.7940(9)
alpha=90 beta=107.573(9) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	1273.1(2)	1273.11(19)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C14 H9 Br O2 S	C14 H9 Br O2 S
Sum formula	C14 H9 Br O2 S	C14 H9 Br O2 S
Mr	321.17	321.18
Dx,g cm-3	1.676	1.676
Z	4	4
Mu (mm-1)	3.382	3.382
F000	640.0	640.0
F000'	639.61	
h,k,lmax	12,18,14	12,17,14
Nref	3453	2933
Tmin,Tmax	0.608,0.666	0.847,1.000
Tmin'	0.596	

Correction method= # Reported T Limits: Tmin=0.847
Tmax=1.000 AbsCorr = MULTI-SCAN

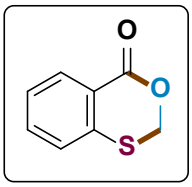
Data completeness= 0.849 Theta(max)= 29.214

R(reflections)= 0.0406(2037) wR2(reflections)= 0.0912(2933)

S = 1.022 Npar= 163

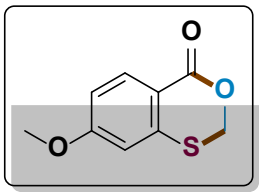
6. Characterization data for the products

4H-benzo[d][1,3]oxathiin-4-one (2a) (CAS Number: 5651-33-2)



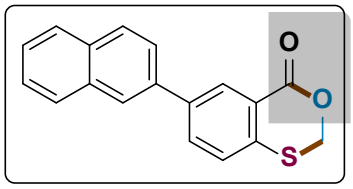
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a colourless oil (44.3 mg, 89%). ^{1}H NMR (300 MHz, $CDCl_3$) ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.16 (d, *J* = 7.9 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 1H), 7.38 – 7.28 (m, 2H), 5.41 (s, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 163.2, 138.7, 133.4, 132.7, 127.6, 126.8, 124.5, 68.8.

7-methoxy-4H-benzo[d][1,3]oxathiin-4-one (2b)



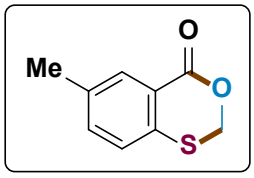
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 15:1, v/v) to give the product as a white solid (54.6 mg, 93%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (d, *J* = 2.8 Hz, 1H), 7.25 (d, *J* = 8.6 Hz, 1H), 7.07 (dd, *J* = 8.6, 2.8 Hz, 1H), 5.39 (s, 2H), 3.84 (s, 3H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 163.3, 158.5, 129.6, 128.7, 125.3, 121.8, 115.6, 69.1, 55.7. HRMS (ESI, m/z) calcd for $C_9H_9O_3S$ $[M+H]^+$: 197.0267; found: 197.0270.

6-(naphthalen-2-yl)-4H-benzo[d][1,3]oxathiin-4-one (2c)



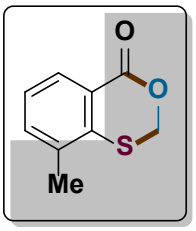
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (74.5 mg, 85%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.56 (d, *J* = 1.9 Hz, 1H), 8.06 (s, 1H), 7.93 (d, *J* = 8.6 Hz, 2H), 7.89 – 7.81 (m, 2H), 7.72 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.56 – 7.49 (m, 2H), 7.46 (d, *J* = 8.2 Hz, 1H), 5.47 (s, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 163.4, 139.9, 137.4, 136.0, 133.5, 132.8 132.1, 131.2, 128.8, 128.2, 128.1, 127.6, 126.6, 126.4, 125.8, 124.8, 124.7, 68.8. HRMS (ESI, m/z) calcd for $C_{18}H_{13}O_2S$ $[M+H]^+$: 293.0631; found: 293.0631.

6-methyl-4H-benzo[d][1,3]oxathiin-4-one (2d)



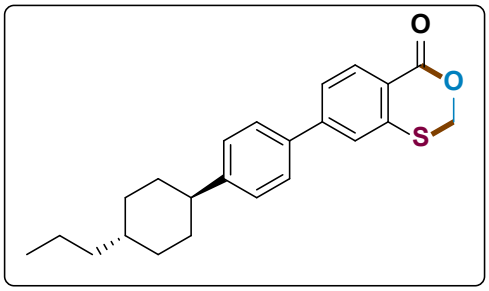
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a colourless oil (47.5 mg, 88%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.38 – 7.21 (m, 2H), 5.40 (s, 2H), 2.38 (s, 3H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 163.5, 137.0, 135.2, 134.5, 132.9, 127.4, 124.2, 68.8, 20.9. HRMS (ESI, m/z) calcd for $C_9H_9O_2S$ $[M+H]^+$: 181.0318; found: 181.0323.

8-methyl-4H-benzo[d][1,3]oxathiin-4-one (2e)



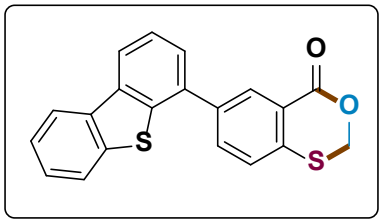
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (48.6 mg, 90%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (d, J = 7.8 Hz, 1H), 7.37 (d, J = 7.4 Hz, 1H), 7.22 (d, J = 7.7 Hz, 1H), 5.39 (s, 2H), 2.35 (s, 3H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 163.7, 138.6, 135.6, 134.5, 130.3, 126.0, 124.4, 68.0, 19.8. HRMS (ESI, m/z) calcd for $C_9H_9O_2S$ $[M+H]^+$: 181.0318; found: 181.0319.

7-(4-((1s,4r)-4-propylcyclohexyl)phenyl)-4H-benzo[d][1,3]oxathiin-4-one (2f)



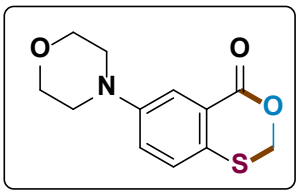
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (101.0 mg, 92%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.41 (d, J = 2.0 Hz, 1H), 7.71 (dd, J = 8.2, 2.1 Hz, 1H), 7.53 (d, J = 8.2 Hz, 2H), 7.41 (d, J = 8.2 Hz, 1H), 7.31 (d, J = 8.2 Hz, 2H), 5.45 (s, 2H), 2.51 (ddd, J = 12.2, 7.7, 3.0 Hz, 1H), 1.91 (t, J = 11.0 Hz, 4H), 1.59 – 1.43 (m, 2H), 1.42 – 1.28 (m, 3H), 1.28 – 1.18 (m, 2H), 1.15 – 0.99 (m, 2H), 0.91 (t, J = 7.1 Hz, 3H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 163.3, 148.0, 140.0, 136.9, 136.3, 131.8, 130.8, 128.3, 127.5, 126.7, 124.7, 68.8, 44.3, 39.7, 37.0, 34.2, 33.5, 20.0, 14.4. HRMS (ESI, m/z) calcd for $C_{23}H_{27}O_2S$ $[M+H]^+$: 367.1726; found: 367.1727.

6-(dibenzo[b,d]thiophen-4-yl)-4H-benzo[d][1,3]oxathiin-4-one (2g)



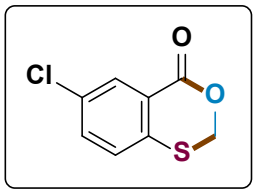
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 10:1, v/v) to give the product as a white solid (80.4 mg, 77%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.57 (d, *J* = 1.9 Hz, 1H), 8.20 (d, *J* = 6.7 Hz, 2H), 7.92 (dd, *J* = 8.1, 2.0 Hz, 1H), 7.88 – 7.82 (m, 1H), 7.60 – 7.54 (m, 1H), 7.49 (dd, *J* = 6.0, 4.5 Hz, 4H), 7.33 (s, 1H), 5.52 (s, 2H).^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 163.1, 139.5, 139.2, 138.3, 136.5, 135.6, 134.6, 133.1, 132.4, 128.4, 128.1, 127.0, 126.8, 125.3, 124.9, 124.6, 122.7, 121.8, 121.2, 68.8. HRMS (ESI, m/z) calcd for $C_{20}H_{13}O_2S_2[M+H]^+$: 349.0351; found: 349.0354.

6-morpholino-4H-benzo[d][1,3]oxathiin-4-one (2h)



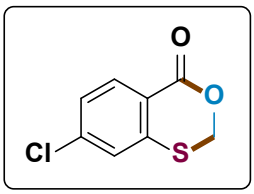
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 5:1, v/v) to give the product as a yellow oil (68.5 mg, 91%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 2.8 Hz, 1H), 7.30 – 7.25 (m, 1H), 7.10 (dd, *J* = 8.7, 2.8 Hz, 1H), 5.42 (s, 2H), 4.01 – 3.78 (m, 4H), 3.30 – 3.13 (m, 4H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 163.81 (s), 150.1, 128.4, 127.8, 125.1, 121.3, 118.5, 69.1, 66.6, 48.7. HRMS (ESI, m/z) calcd for $C_{20}H_{13}O_2S_2[M+H]^+$: 252.0689; found: 252.0693.

6-chloro-4H-benzo[d][1,3]oxathiin-4-one (2i)



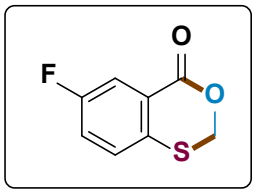
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (48.6 mg, 81%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (d, *J* = 2.1 Hz, 1H), 7.43 (dd, *J* = 8.4, 2.2 Hz, 1H), 7.29 (d, *J* = 8.4 Hz, 1H), 5.40 (s, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 162.0, 137.0, 133.5, 132.7, 132.2, 128.8, 125.5, 68.7. HRMS (ESI, m/z) calcd for $C_8H_6ClO_2S$ $[M+H]^+$: 200.9772; found: 200.9774.

7-chloro-4H-benzo[d][1,3]oxathiin-4-one (2j)



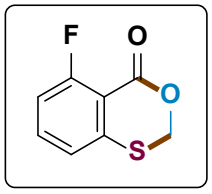
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (50.4 mg, 84%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.5 Hz, 1H), 7.31 (d, *J* = 1.5 Hz, 1H), 7.28 – 7.20 (m, 1H), 5.37 (s, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 162.5, 140.4, 140.1, 134.0, 127.4, 127.3, 122.6, 68.6. HRMS (ESI, m/z) calcd for $C_8H_6ClO_2S$ $[M+H]^+$: 200.9772; found: 200.9777.

6-fluoro-4H-benzo[d][1,3]oxathiin-4-one (2k)



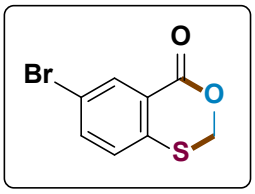
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (47.4 mg, 86%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 8.7, 2.8 Hz, 1H), 7.34 (dd, *J* = 8.7, 4.9 Hz, 1H), 7.26 – 7.18 (m, 1H), 5.41 (s, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 161.1 (d, *J* = 246.8 Hz), 162.2 (d, *J* = 2.6 Hz), 134.0 (d, *J* = 3.3 Hz), 129.3 (d, *J* = 7.4 Hz), 126.0 (d, *J* = 7.4 Hz), 121.4 (d, *J* = 22.5 Hz), 119.1 (d, *J* = 24.0 Hz), 69.0. HRMS (ESI, m/z) calcd for $C_8H_6FO_2S$ $[M+H]^+$: 185.0067; found: 185.0070.

5-fluoro-4H-benzo[d][1,3]oxathiin-4-one (2l)



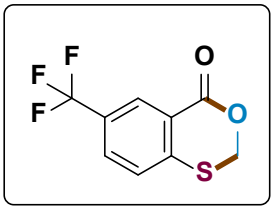
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (41.4 mg, 75%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 (td, *J* = 8.1, 5.1 Hz, 1H), 7.18 (d, *J* = 7.9 Hz, 1H), 7.11 – 6.98 (m, 1H), 5.38 (s, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 164.1 (d, *J* = 265.5 Hz), 158.8 (d, *J* = 4.9 Hz), 141.3, 134.4 (d, *J* = 10.5 Hz), 123.6 (d, *J* = 4.1 Hz), 115.5 (d, *J* = 21.8 Hz), 113.7 (d, *J* = 8.7 Hz), 68.8. HRMS (ESI, m/z) calcd for $C_8H_6FO_2S$ $[M+H]^+$: 185.0067; found: 185.0069.

6-bromo-4H-benzo[d][1,3]oxathiin-4-one (2m)



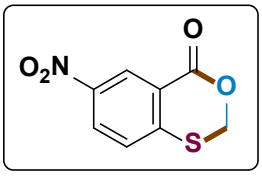
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (50.3 mg, 69%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.33 (d, J = 2.1 Hz, 1H), 7.63 (dd, J = 8.4, 2.2 Hz, 1H), 7.29 (d, J = 1.2 Hz, 1H), 5.45 (s, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 162.0, 137.7, 136.4, 135.3, 129.0, 125.8, 120.3, 68.7. HRMS (ESI, m/z) calcd for $C_8H_6BrO_2S$ $[M+H]^+$: 244.9266; found: 244.9272.

6-(trifluoromethyl)-4H-benzo[d][1,3]oxathiin-4-one (2n)



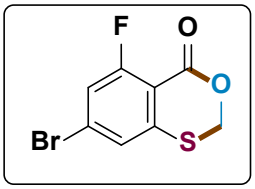
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (56.1 mg, 80%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.31 (d, J = 8.2 Hz, 1H), 7.64 (s, 1H), 7.58 (d, J = 8.2 Hz, 1H), 5.47 (s, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 162.0, 140.0, 134.9 (q, J = 33.0 Hz), 129.8 (q, J = 273.4 Hz), 124.7 (q, J = 3.9 Hz), 123.4 (q, J = 3.6 Hz), 121.0, 68.8. HRMS (ESI, m/z) calcd for $C_9H_6F_3O_2S$ $[M+H]^+$: 235.0035; found: 235.0038.

6-nitro-4H-benzo[d][1,3]oxathiin-4-one (2o)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 5:1, v/v) to give the product as a yellow solid (46.8 mg, 74%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.38 (d, J = 8.6 Hz, 1H), 8.24 (d, J = 2.1 Hz, 1H), 8.13 (dd, J = 8.6, 2.1 Hz, 1H), 5.50 (s, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 161.4, 141.0, 134.2, 131.1, 129.0, 122.7, 121.2, 68.9. HRMS (ESI, m/z) calcd for $C_8H_6NO_4S$ $[M+H]^+$: 212.0012; found: 212.0016.

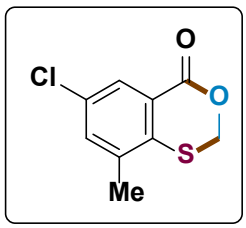
7-bromo-6-fluoro-4H-benzo[d][1,3]oxathiin-4-one (2p)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (54.8 mg, 70%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.39 (d, J = 7.0 Hz, 1H), 7.13 (d, J = 7.9 Hz, 1H), 5.43 (s, 2H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 161.4 (d, J = 258.0 Hz), 161.3, 140.4

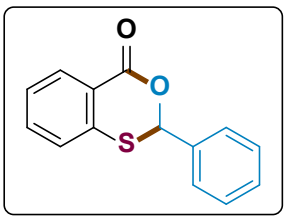
(d, J = 9.1 Hz), 138.3 (d, J = 2.6 Hz), 121.7 (d, J = 3.5 Hz), 115.3 (d, J = 25.5 Hz), 107.9 (d, J = 25.5 Hz), 68.7. HRMS (ESI, m/z) calcd for $C_8H_5BrFO_2S$ $[M+H]^+$: 262.9172; found: 262.9177.

6-chloro-8-methyl-4H-benzo[d][1,3]oxathiin-4-one (2q)



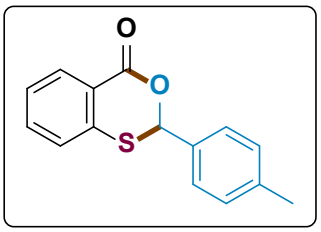
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (53.2 mg, 83%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 (d, J = 2.0 Hz, 1H), 7.35 (d, J = 1.6 Hz, 1H), 5.38 (s, 2H), 2.33 (s, 3H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$) δ 162.6, 137.5, 137.1, 134.3, 132.0, 129.8, 125.5, 68.0, 19.6. HRMS (ESI, m/z) calcd for $C_9H_8ClO_2S$ $[M+H]^+$: 214.9928; found: 214.9929.

2-phenyl-4H-benzo[d][1,3]oxathiin-4-one (4a) (CAS Number: 5651-35-4)



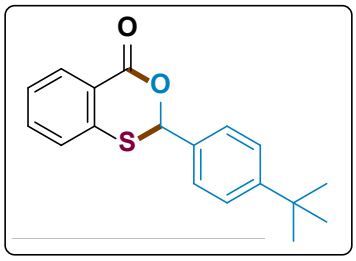
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a colourless oil (21.8 mg, 45%).^{1}H NMR (300 MHz, $CDCl_3$) δ 8.23 (d, J = 7.9 Hz, 1H), 7.60 (dd, J = 6.6, 2.8 Hz, 2H), 7.56 – 7.50 (m, 1H), 7.47 – 7.42 (m, 3H), 7.36 (t, J = 7.5 Hz, 2H), 6.58 (s, 1H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$) δ 164.0, 138.7, 134.6, 133.7, 132.7, 129.9, 128.8, 127.4, 126.8, 126.7, 124.2, 83.6.

2-(p-tolyl)-4H-benzo[d][1,3]oxathiin-4-one (4b) (CAS Number: 146853-01-2)



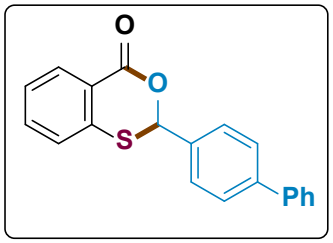
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a pink solid (20.5 mg, 40%).^{1}H NMR (300 MHz, $CDCl_3$) δ 8.22 (d, J = 7.9 Hz, 1H), 7.51 (dd, J = 13.3, 7.5 Hz, 3H), 7.35 (t, J = 7.4 Hz, 2H), 7.24 (d, J = 9.0 Hz, 2H), 6.54 (s, 1H), 2.39 (s, 3H). $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$) δ 164.1, 140.0, 138.8, 133.7, 132.7, 131.7, 129.4, 127.4, 126.8, 126.7, 124.3, 83.6, 21.4.

2-(4-(tert-butyl)phenyl)-4H-benzo[d][1,3]oxathiin-4-one (4c)



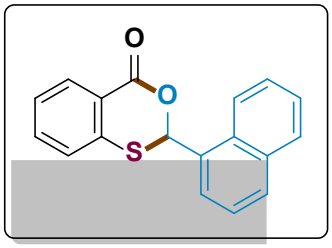
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a colourless oil (27.4 mg, 46%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.30 – 8.14 (m, 1H), 7.51 (dd, *J* = 11.2, 4.9 Hz, 3H), 7.46 (d, *J* = 8.5 Hz, 2H), 7.41 – 7.31 (m, 2H), 6.55 (s, 1H), 1.34 (s, 9H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 164.1, 153.1, 138.8, 133.7, 132.7, 131.7, 127.4, 126.8, 126.5, 125.7, 124.2, 83.6, 34.8, 31.2. HRMS (ESI, m/z) calcd for $C_{18}H_{19}O_2S$ $[M+H]^+$: 299.1100; found: 299.1105.

2-([1,1'-biphenyl]-4-yl)-4H-benzo[d][1,3]oxathiin-4-one (4d)



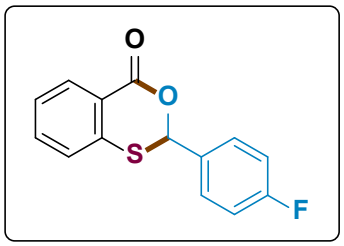
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (31.8 mg, 50%).^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 – 8.19 (m, 1H), 7.67 (s, 4H), 7.64 – 7.59 (m, 2H), 7.58 – 7.51 (m, 1H), 7.47 (t, *J* = 7.3 Hz, 2H), 7.42 – 7.35 (m, 3H), 6.63 (s, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 164.0, 142.8, 140.2, 138.7, 133.8, 133.5, 132.8, 128.9, 127.8, 127.5, 127.4, 127.3, 127.2, 126.9, 124.2, 83.5. HRMS (ESI, m/z) calcd for $C_{20}H_{15}O_2S$ $[M+H]^+$: 319.0787; found: 319.0789.

2-(naphthalen-1-yl)-4H-benzo[d][1,3]oxathiin-4-one (4e)



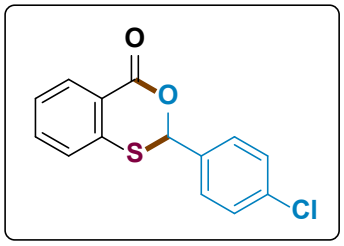
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a yellow oil (33.2 mg, 57%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.30 (dd, *J* = 8.2, 1.3 Hz, 1H), 8.19 – 8.08 (m, 1H), 7.99 (d, *J* = 7.2 Hz, 1H), 7.96 – 7.87 (m, 2H), 7.62 – 7.50 (m, 4H), 7.46 – 7.35 (m, 2H), 7.24 (s, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 164.3, 139.1, 133.9, 133.7, 133.0, 130.6, 129.9, 129.5, 129.1, 127.5, 127.0, 126.8, 126.2, 125.9, 125.3, 124.2, 123.0, 81.6. HRMS (ESI, m/z) calcd for $C_{18}H_{13}O_2S$ $[M+H]^+$: 293.0631; found: 293.0632.

2-(4-fluorophenyl)-4H-benzo[d][1,3]oxathiin-4-one (4f)



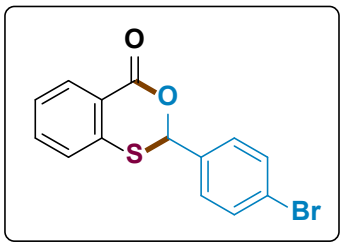
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (28.6 mg, 55%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.22 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.65 – 7.48 (m, 3H), 7.41 – 7.32 (m, 2H), 7.12 (t, *J* = 8.6 Hz, 2H), 6.54 (s, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 163.4 (d, *J* = 247.5 Hz), 163.8, 138.4, 133.8, 132.7, 130.6 (d, *J* = 3.2 Hz), 128.7 (d, *J* = 8.6 Hz), 127.4, 126.9, 124.1, 115.8 (d, *J* = 8.6 Hz), 82.9. HRMS (ESI, m/z) calcd for $C_{14}H_{10}FO_2S$ $[M+H]^+$: 261.0380; found: 261.0385.

2-(4-chlorophenyl)-4H-benzo[d][1,3]oxathiin-4-one (4g) (CAS Number: 38058-00-3)



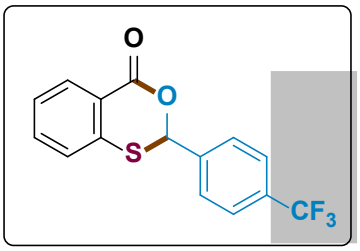
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (29.2 mg, 53%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.28 – 8.18 (m, 1H), 7.53 (dd, *J* = 11.0, 4.9 Hz, 3H), 7.43 (s, 1H), 7.42 – 7.33 (m, 3H), 6.55 (s, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 163.7, 138.3, 135.8, 133.9, 133.2, 132.8, 129.0, 128.1, 127.4, 127.0, 124.1, 82.8.

2-(4-bromophenyl)-4H-benzo[d][1,3]oxathiin-4-one (4h)



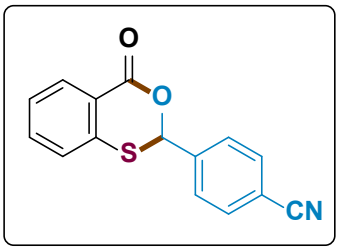
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (37.8 mg, 59%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.22 (d, *J* = 7.9 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.49 (t, *J* = 10.2 Hz, 3H), 7.40 – 7.33 (m, 2H), 6.53 (s, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 163.6, 138.2, 133.9, 133.7, 132.8, 132.0, 128.3, 127.4, 127.0, 124.1, 124.0, 82.8. $C_{14}H_{10}BrO_2S$ $[M+H]^+$: 320.9579; found: 320.9582.

2-(4-(trifluoromethyl)phenyl)-4H-benzo[d][1,3]oxathiin-4-one (4i)



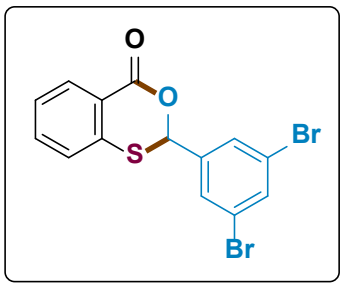
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 15:1, v/v) to give the product as a white solid (32.2 mg, 52%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.24 (dd, J = 8.2, 1.4 Hz, 1H), 7.72 (t, J = 5.9 Hz, 4H), 7.61 – 7.50 (m, 1H), 7.46 – 7.34 (m, 2H), 6.64 (s, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 163.5, 138.4 (q, J = 1.3 Hz), 138.0, 134.0, 132.8, 132.0 (q, J = 32.3 Hz), 127.5, 127.2, 127.1, 125.8 (q, J = 3.8 Hz), 124.1, 123.7 (q, J = 271.5 Hz), 82.5. HRMS (ESI, m/z) calcd for $C_{15}H_{10}F_3O_2S$ $[M+H]^+$: 311.0348; found: 311.0349.

4-(4-oxo-4H-benzo[d][1,3]oxathiin-2-yl)benzonitrile (4j)



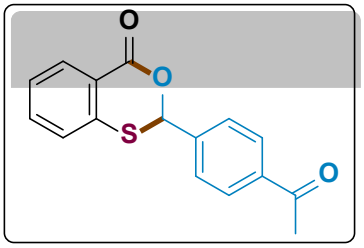
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 10:1, v/v) to give the product as a white solid (32.0 mg, 60%).^{1}H NMR (300 MHz, $CDCl_3$) δ 8.22 (dd, J = 8.1, 1.2 Hz, 1H), 7.74 (s, 4H), 7.55 (t, J = 8.3 Hz, 1H), 7.39 (t, J = 7.1 Hz, 2H), 6.63 (s, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 163.2, 139.4, 137.6, 134.1, 132.8, 132.6, 127.5, 127.3, 127.2, 124.0, 118.0, 113.6, 82.2. HRMS (ESI, m/z) calcd for $C_{15}H_{10}NO_2S$ $[M+H]^+$: 268.0427; found: 268.0427.

2-(3,5-dibromophenyl)-4H-benzo[d][1,3]oxathiin-4-one (4k)



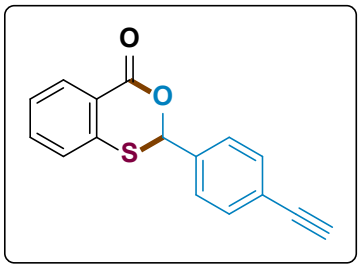
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (30.1 mg, 38%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.22 (dd, J = 8.1, 1.3 Hz, 1H), 7.77 – 7.63 (m, 3H), 7.55 (t, J = 6.9 Hz, 1H), 7.39 (t, J = 7.0 Hz, 2H), 6.50 (s, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 163.2, 138.1, 137.7, 135.4, 134.1, 132.9, 128.4, 127.5, 127.4, 123.9, 123.3, 81.5. HRMS (ESI, m/z) calcd for $C_{14}H_9Br_2O_2S$ $[M+H]^+$: 398.8685; found: 398.8688.

2-(4-acetylphenyl)-4H-benzo[d][1,3]oxathiin-4-one (4l)



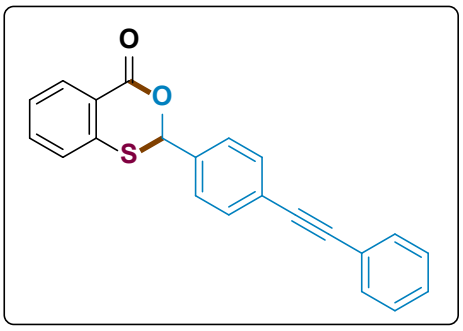
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 15:1, v/v) to give the product as a white solid (28.8 mg, 51%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.24 (dd, *J* = 8.1, 1.2 Hz, 1H), 8.04 (d, *J* = 8.3 Hz, 2H), 7.72 (d, *J* = 8.3 Hz, 2H), 7.61 – 7.52 (m, 1H), 7.44 – 7.35 (m, 2H), 6.65 (s, 1H), 2.64 (s, 3H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 197.4, 163.6, 139.3, 138.1, 138.0, 134.0, 132.8, 128.7, 127.5, 127.1, 126.9, 124.1, 82.8, 26.8. HRMS (ESI, m/z) calcd for $C_{16}H_{13}O_3S$ $[M+H]^+$: 285.0580; found: 285.0585.

2-(4-ethynylphenyl)-4H-benzo[d][1,3]oxathiin-4-one (4m)



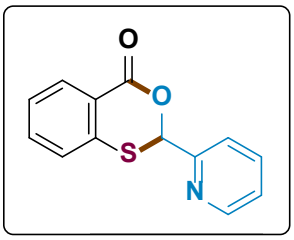
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (24.5 mg, 46%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.23 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.56 (s, 3H), 7.55 – 7.50 (m, 1H), 7.42 – 7.33 (m, 2H), 7.26 (s, 1H), 6.57 (s, 1H), 3.15 (s, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 163.8, 138.3, 135.0, 133.9, 132.8, 132.5, 127.4, 127.0, 126.7, 124.1, 123.8, 83.1, 82.8, 78.6. HRMS (ESI, m/z) calcd for $C_{16}H_{11}O_2S$ $[M+H]^+$: 267.0474; found: 267.0476.

2-(4-(phenylethynyl)phenyl)-4H-benzo[d][1,3]oxathiin-4-one (4n)



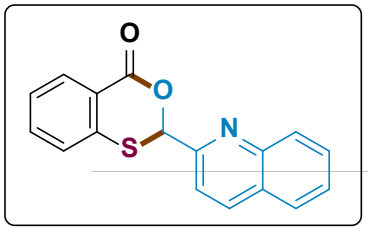
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 20:1, v/v) to give the product as a white solid (36.4 mg, 53%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.24 (d, *J* = 7.7 Hz, 1H), 7.60 (s, 4H), 7.58 – 7.51 (m, 3H), 7.37 (dd, *J* = 8.4, 5.1 Hz, 5H), 6.59 (s, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 163.9, 138.4, 134.4, 133.9, 132.8, 131.9, 131.7, 128.6, 128.4, 127.4, 127.0, 126.7, 125.0, 124.2, 122.8, 90.7, 88.5, 83.2. HRMS (ESI, m/z) calcd for $C_{22}H_{15}O_2S$ $[M+H]^+$: 343.0787; found: 343.0790.

2-(pyridin-2-yl)-4H-benzo[d][1,3]oxathiin-4-one (4o)



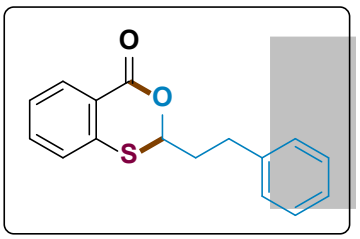
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 2:1, v/v) to give the product as a white solid (39.3 mg, 81%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.60 (d, *J* = 4.7 Hz, 1H), 8.20 (d, *J* = 7.0 Hz, 1H), 7.80 (ddd, *J* = 12.7, 9.6, 4.5 Hz, 2H), 7.57 – 7.46 (m, 1H), 7.42 – 7.30 (m, 3H), 6.72 (s, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 163.5, 153.6, 149.2, 138.2, 137.3, 133.8, 132.6, 127.7, 126.8, 124.3, 124.0, 121.5, 83.9. HRMS (ESI, m/z) calcd for $C_{13}H_{10}NO_2S$ $[M+H]^+$: 244.0427; found: 244.0427.

2-(quinolin-2-yl)-4H-benzo[d][1,3]oxathiin-4-one (4p)



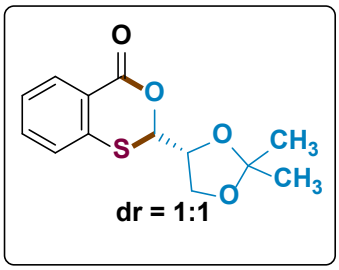
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 2:1, v/v) to give the product as a white solid (27.5 mg, 47%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.6 Hz, 1H), 8.27 (d, *J* = 7.7 Hz, 1H), 8.18 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 8.8 Hz, 1H), 7.80 (t, *J* = 7.0 Hz, 2H), 7.64 (t, *J* = 7.7 Hz, 1H), 7.57 – 7.50 (m, 1H), 7.47 – 7.36 (m, 2H), 6.98 (s, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 163.6, 153.5, 138.1, 133.9, 132.7, 131.8, 131.1, 131.0, 130.5, 129.1, 128.8, 128.7, 128.2, 127.8, 127.7, 126.9, 124.2, 118.6, 84.2. HRMS (ESI, m/z) calcd for $C_{17}H_{12}NO_2S$ $[M+H]^+$: 294.0583; found: 294.0588.

2-phenethyl-4H-benzo[d][1,3]oxathiin-4-one (4q)



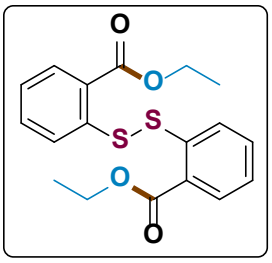
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 10:1, v/v) to give the product as a colourless oil (39.4 mg, 73%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.0 Hz, 1H), 7.57 – 7.42 (m, 1H), 7.36 – 7.27 (m, 4H), 7.25 – 7.19 (m, 3H), 5.54 (t, *J* = 5.5 Hz, 1H), 2.94 (t, *J* = 7.8 Hz, 2H), 2.56 – 2.42 (m, 1H), 2.40 – 2.23 (m, 1H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 164.1, 139.8, 138.3, 133.6, 132.6, 128.6, 128.5, 127.6, 126.6, 126.4, 124.1, 81.9, 35.7, 30.9. HRMS (ESI, m/z) calcd for $C_{16}H_{15}O_2S$ $[M+H]^+$: 271.0787; found: 271.0787.

2-(2,2-dimethyl-1,3-dioxolan-4-yl)-4H-benzo[d][1,3]oxathiin-4-one (4r)



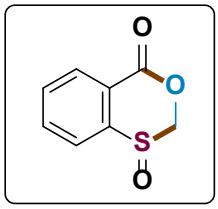
The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 2:1, v/v) to give the product as a yellow oil (34.0 mg, 64%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.8 Hz, 1H), 7.48 – 7.39 (m, 1H), 7.29 (s, 1H), 7.21 – 7.16 (m, 1H), 5.67 (d, *J* = 4.8 Hz, 0.5 H), 5.47 (d, *J* = 7.4 Hz, 0.5 H), 4.57 – 4.50 (d, *J* = 6.4, 0.5 H), 4.47 – 4.39 (m, 0.5 H), 4.25 – 4.18 (m, 0.5 H), 4.15 – 4.09 (m, 1.5 H), 1.48 (s, 1.5 H), 1.42 (s, 1.5 H), 1.33 (s, 3H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 197.4, 163.1, 162.9, 142.4, 137.6, 137.5, 135.5, 133.8, 133.7, 132.5, 132.4, 131.2, 131.0, 128.0, 127.9, 126.7, 126.5, 125.1, 123.9, 123.8, 110.9, 110.9, 83.2, 82.9, 75.3, 74.9, 66.5, 65.6, 26.6, 26.1, 24.9, 24.7. HRMS (ESI, m/z) calcd for $C_{13}H_{15}O_4S$ $[M+H]^+$: 267.0686; found: 267.0689.

Diethyl 2,2'-disulfanediyldibenzoate (5)



EtOH (2 mL) was added to a mixture of **2a** (51 mg, 0.3 mmol), DMAP (7.3 mg, 0.06 mmol) and Et_3N (61.2 mg, 0.6 mmol) in a sealed tube. Then, the mixture was stirred at 80 °C under O_2 atmosphere for 12 h. Upon completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 15:1, v/v) to give the desired **5** as white solid (33 mg, 61%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 7.7, 0.9 Hz, 2H), 7.71 (d, *J* = 8.1 Hz, 2H), 7.36 (t, *J* = 7.1 Hz, 2H), 7.20 (dd, *J* = 12.4, 4.5 Hz, 2H), 4.42 (q, *J* = 7.1 Hz, 4H), 1.41 (t, *J* = 7.1 Hz, 6H). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 166.5, 140.3, 132.9, 131.4, 127.6, 125.8, 125.4, 61.5, 14.3. HRMS (ESI, m/z) calcd for $C_{18}H_{19}O_4S_2$ $[M+H]^+$: 363.0720; found: 363.0723.

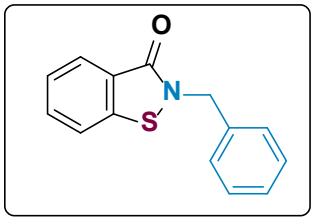
2H,4H-benzo[d][1,3]oxathiin-4-one 1-oxide (6) (CAS Number: 36665-23-3)



CH_2Cl_2 (2 mL) was added to a mixture of **2a** (51 mg, 0.3 mmol), *m*-CPBA (69.0 mg, 0.4 mmol) in a sealed tube. Then, the mixture was stirred at RT for about 2 h. Upon completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 10:1, v/v) to give the desired **6** as white solid (42.5 mg, 78%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.20 (d, *J* = 7.5 Hz, 1H), 7.96 (d, *J* = 7.3 Hz,

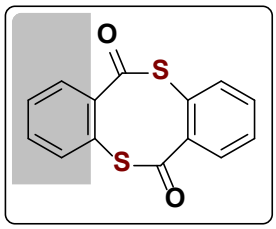
1H), 7.86 (dt, J = 15.3, 7.3 Hz, 2H), 5.34 (s, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 159.2, 138.6, 135.2, 134.2, 132.7, 123.4, 122.6, 79.5.

2-benzylbenzo[d]isothiazol-3(2H)-one (7) (CAS Number: 2514-36-5)



PhMe (2 mL) was added to a mixture of 2H,4H-benzo[d][1,3]oxathiin-4-one 1-oxide **6** (0.2 mmol, 36.4 mg,), $BnNH_2$ (0.3 mmol, 32.1 mg) in a sealed tube. Then, the mixture was stirred at 50 ºC for about 5 h. Upon completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 5:1, v/v) to give the desired **7** as yellow oil (44.3 mg, 92%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (d, J = 7.9 Hz, 1H), 7.59 (t, J = 7.6 Hz, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.42 (d, J = 7.6 Hz, 1H), 7.35 (s, 5H), 5.06 (s, 2H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 165.3, 140.4, 136.1, 131.8, 128.8, 128.4, 128.3, 126.8, 125.5, 124.5, 120.4, 47.6. HRMS (ESI, m/z) calcd for $C_{14}H_{12}NOS$ $[M+H]^+$: 242.0634; found: 242.0637.

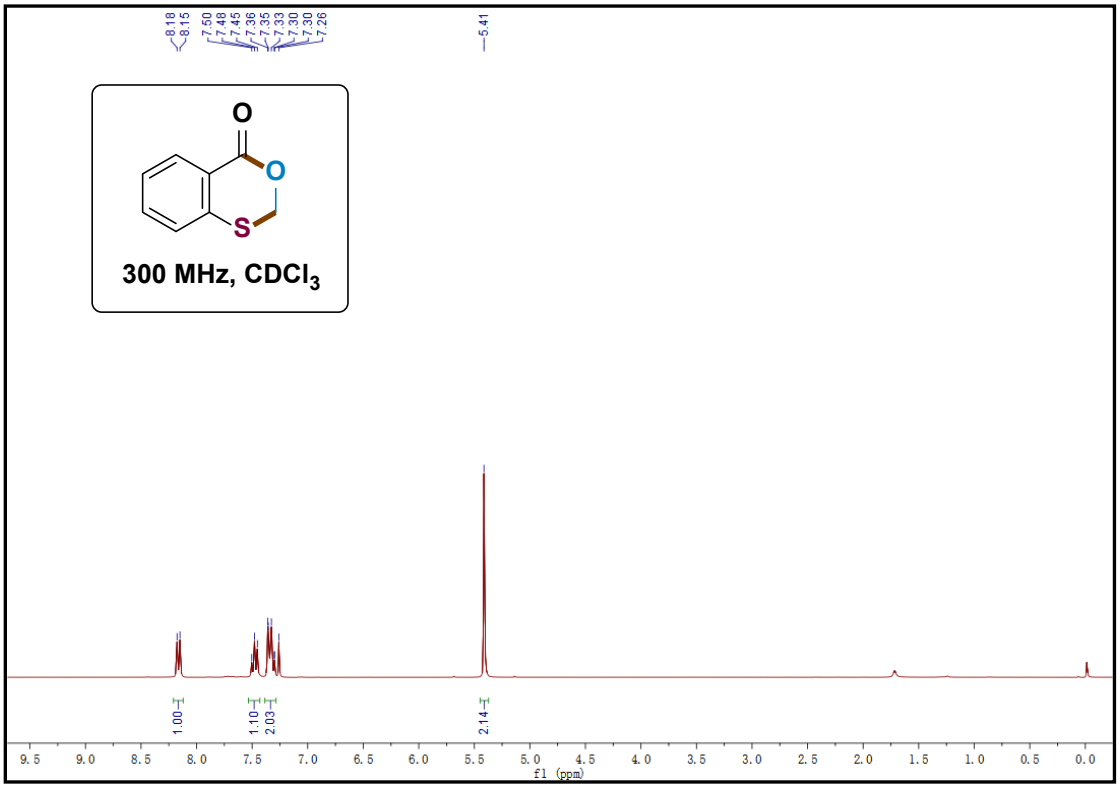
6H,12H-dibenzo[b,f][1,5]dithiocine-6,12-dione (8) (CAS Number: 21083-38-5)

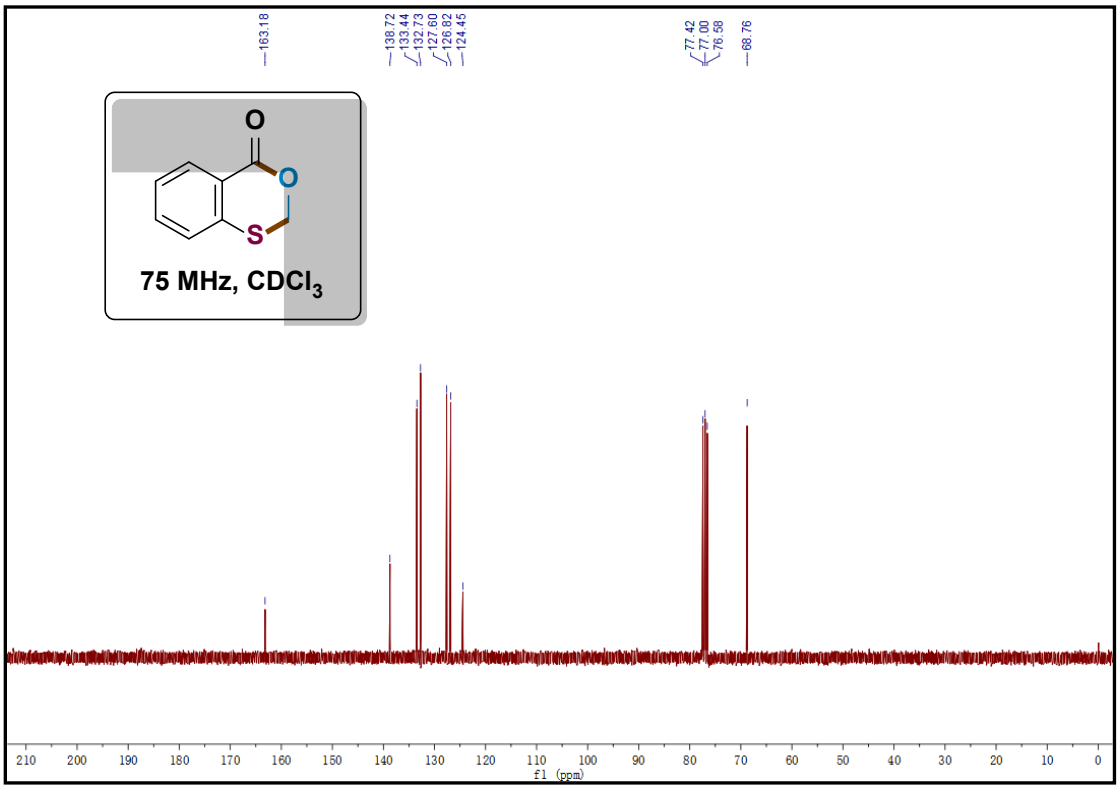


CH_3CN (2 mL) was added to a mixture of benzo[c][1,2]dithiol-3-one **1a** (0.3 mmol, 50.4 mg), DPPE (0.2 mmol, 79.4 mg) in a sealed tube. Then, the mixture was stirred at 80 ºC for about 12 h. Upon completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatograph (silica gel, petroleum ether:EtOAc = 5:1, v/v) to give the desired **8** as white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 – 7.31 (m, 4H), 7.29 – 7.22 (m, 4H). $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 197.4, 142.5, 135.6, 131.2, 131.0, 126.5, 125.2. HRMS (ESI, m/z) calcd for $C_{14}H_9O_2S_2$ $[M+H]^+$: 273.0038; found: 273.0039.

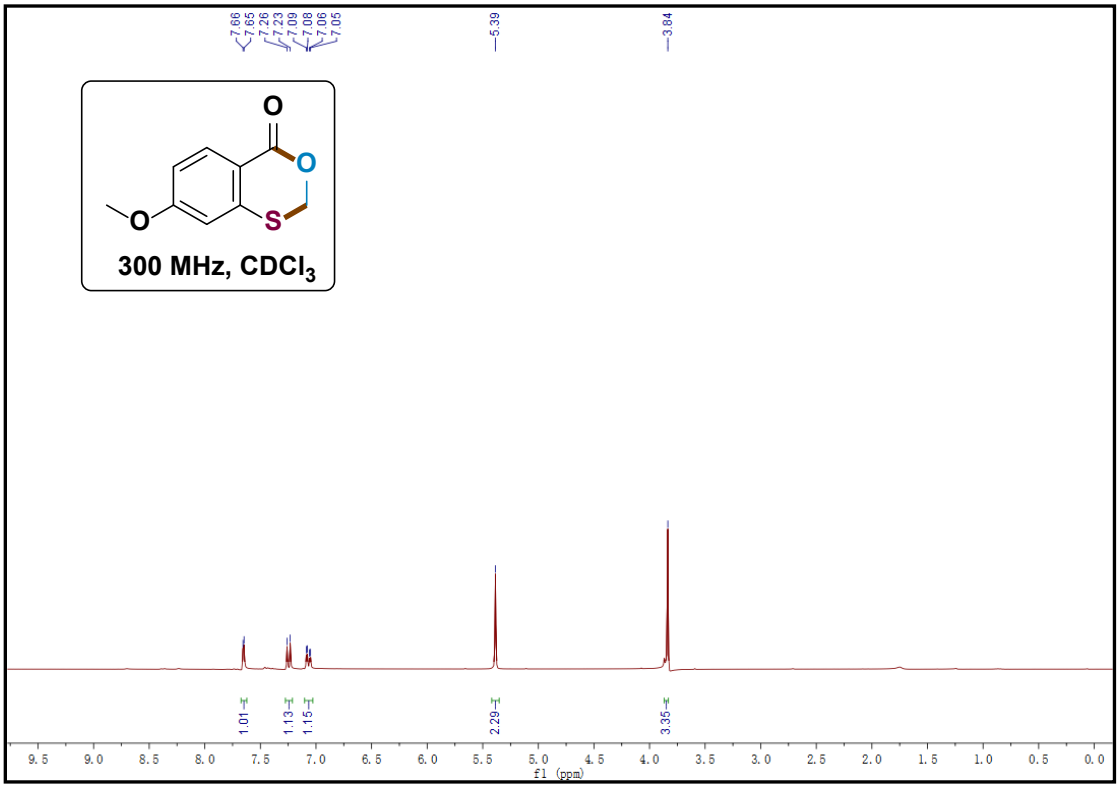
7. NMR spectroscopic data for the products

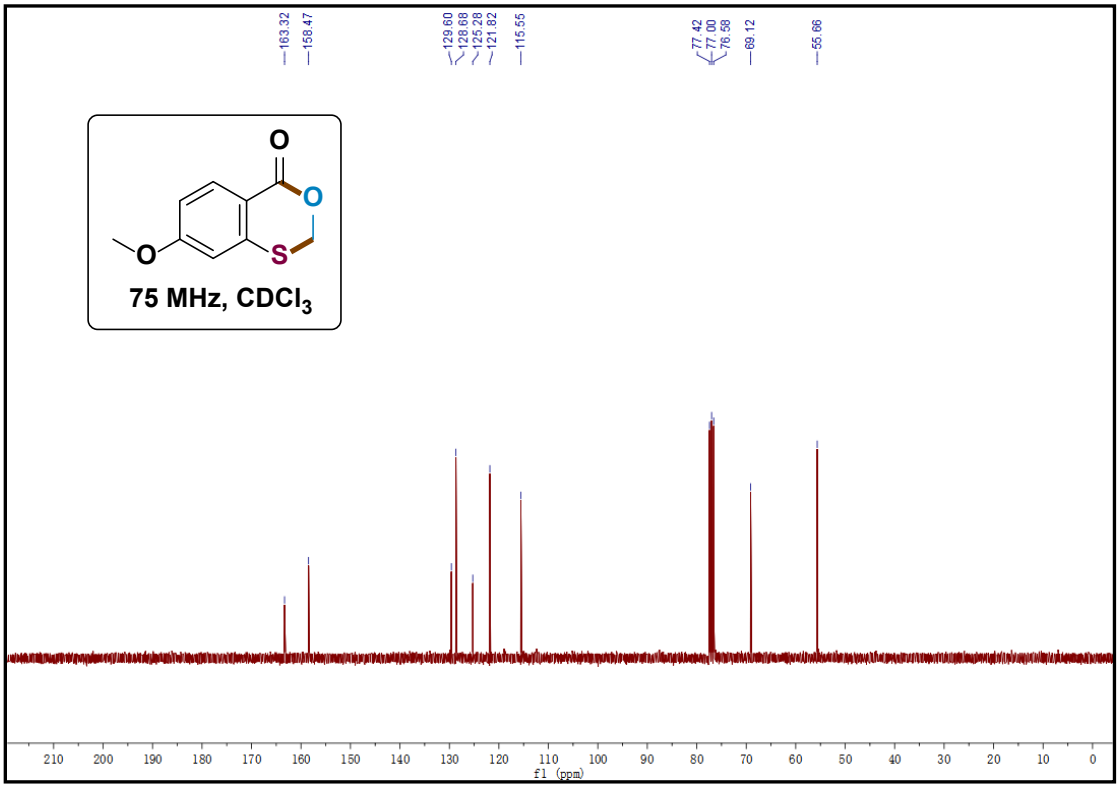
4H-benzo[d][1,3]oxathiin-4-one (2a)



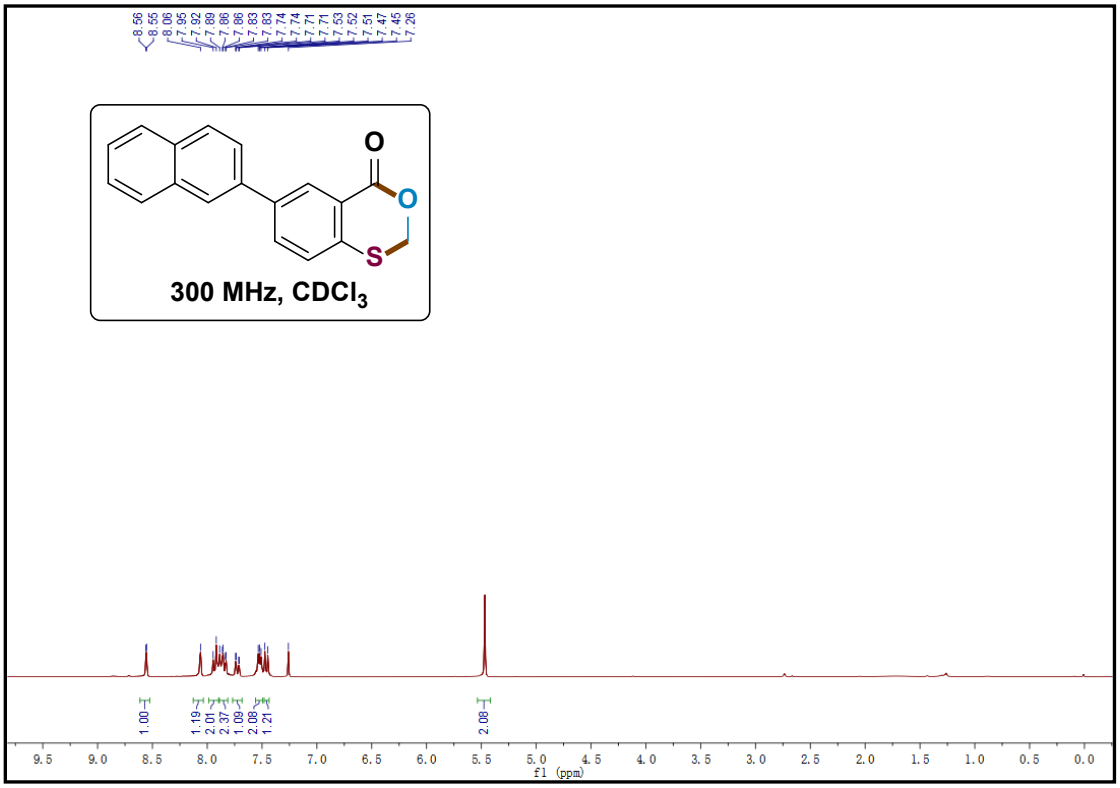


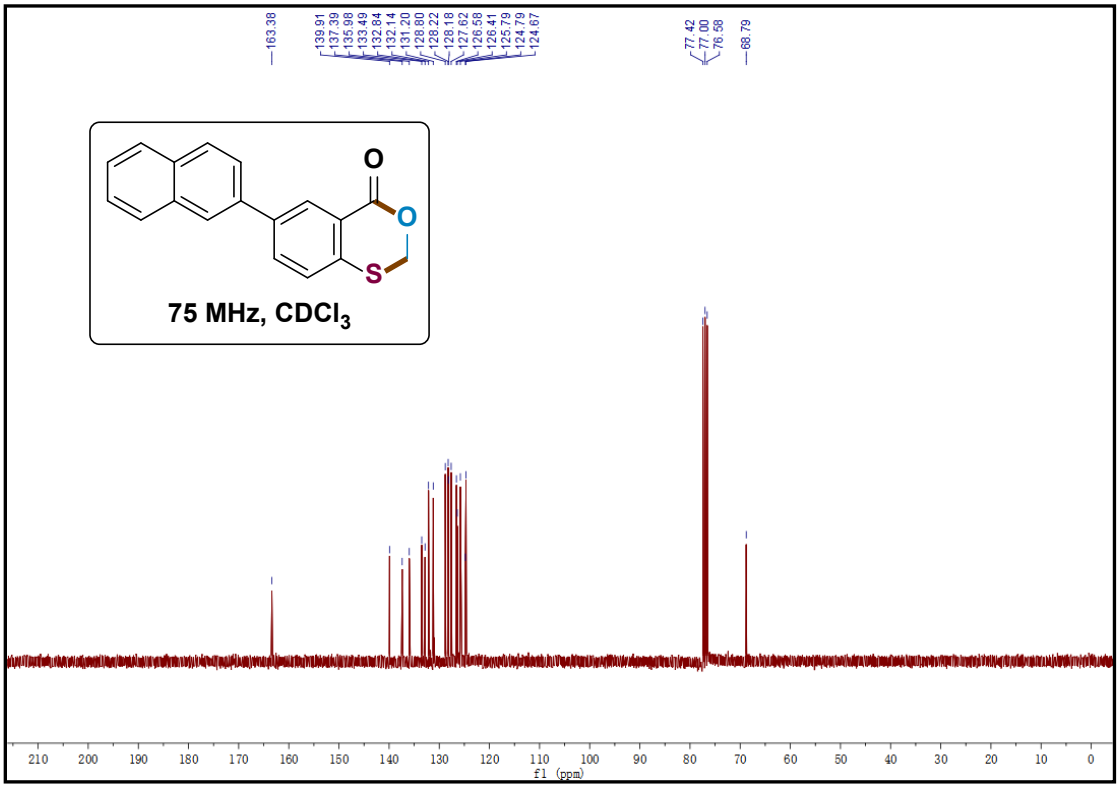
6-methoxy-4H-benzo[d][1,3]oxathiin-4-one (2b)



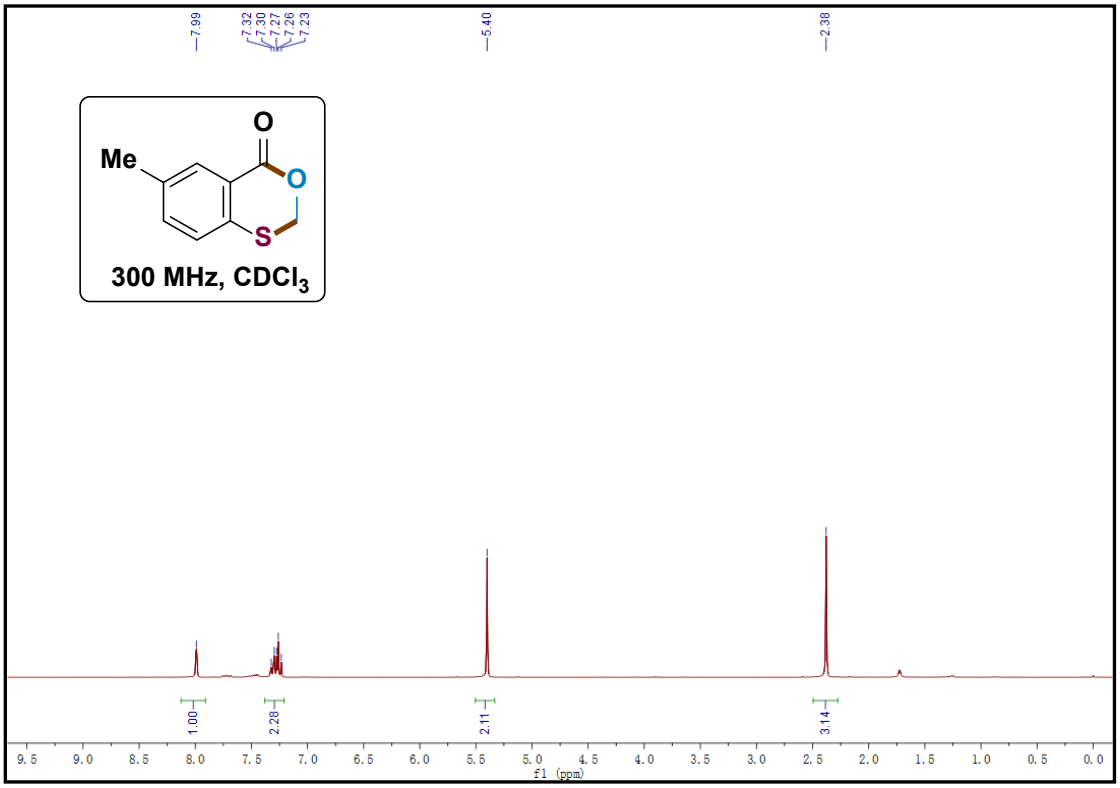


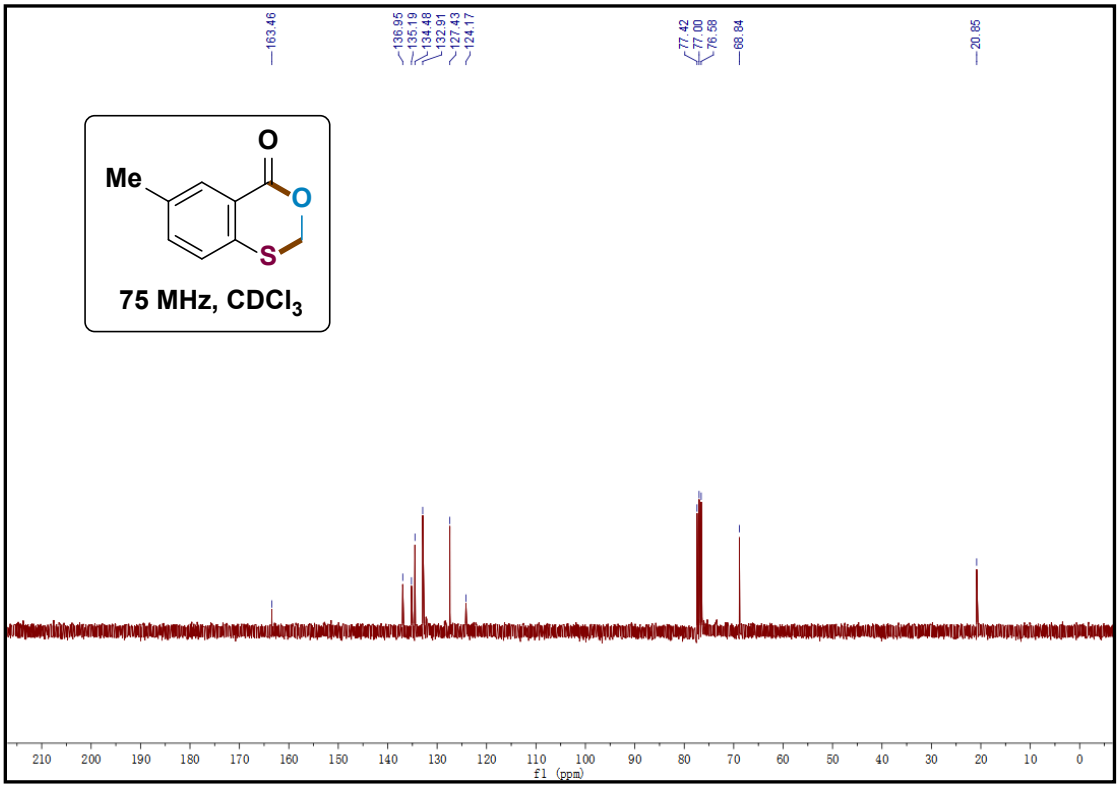
6-(naphthalen-2-yl)-4H-benzo[d][1,3]oxathiin-4-one (2c)



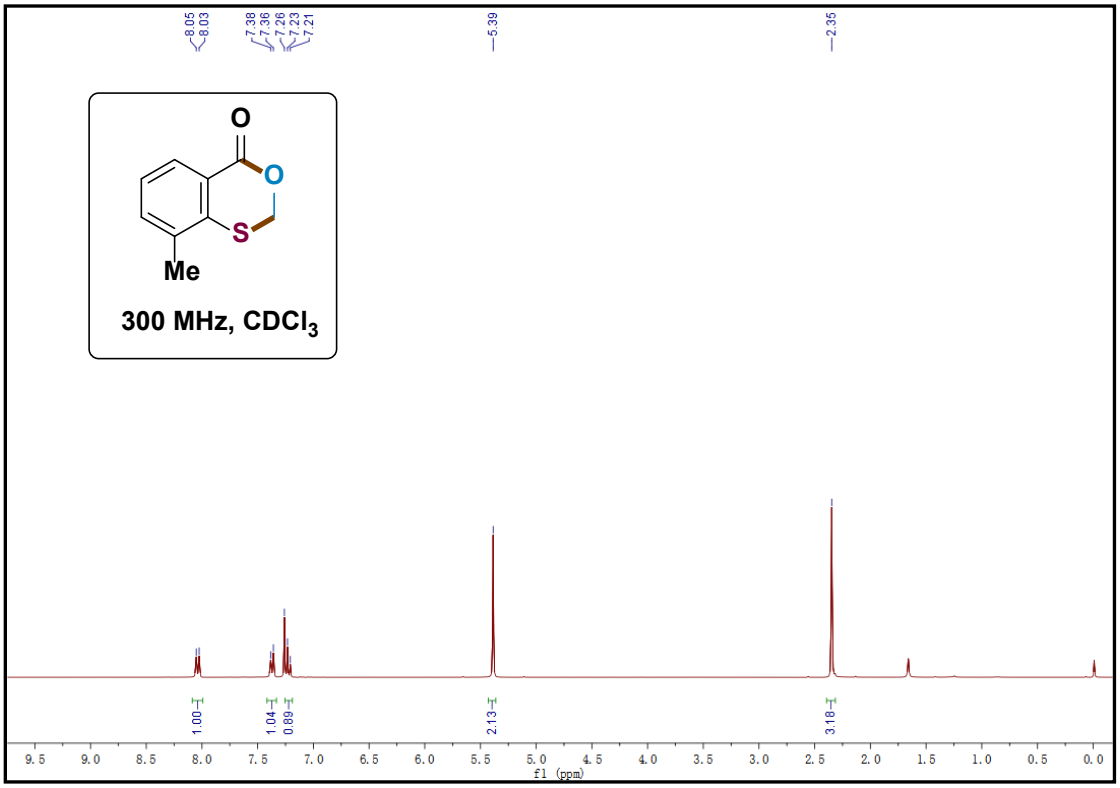


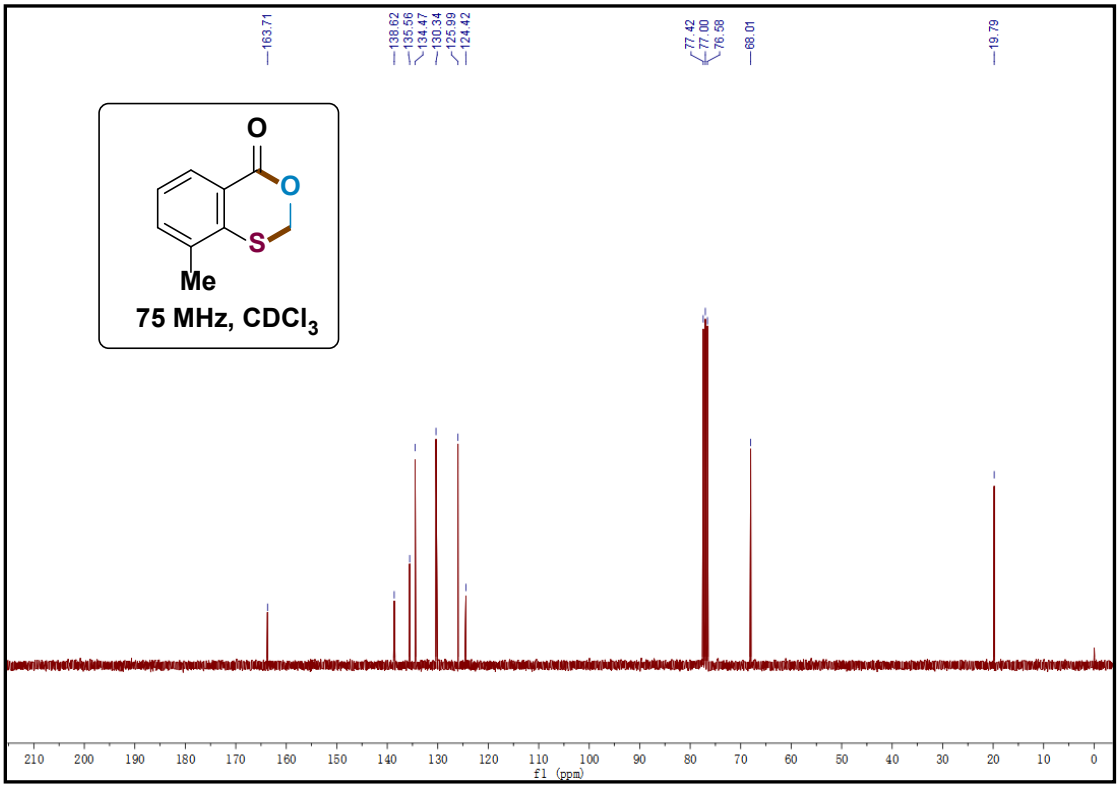
6-methyl-4H-benzo[d][1,3]oxathiin-4-one (2d)



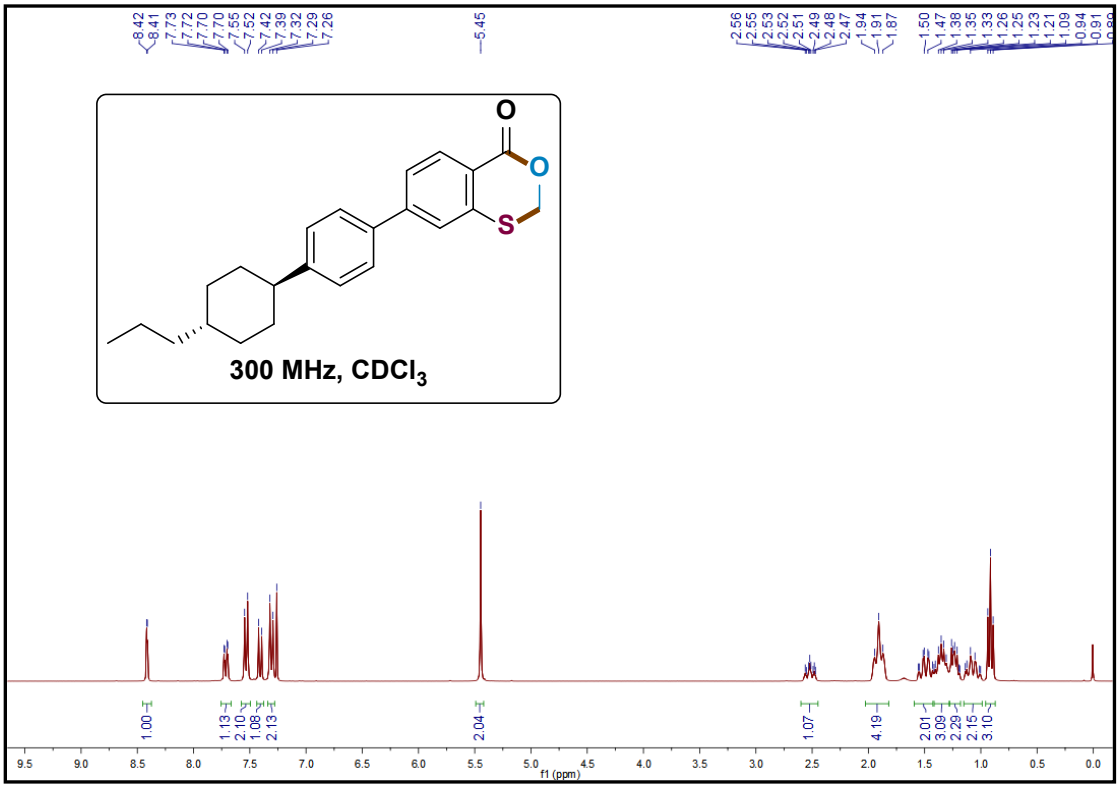


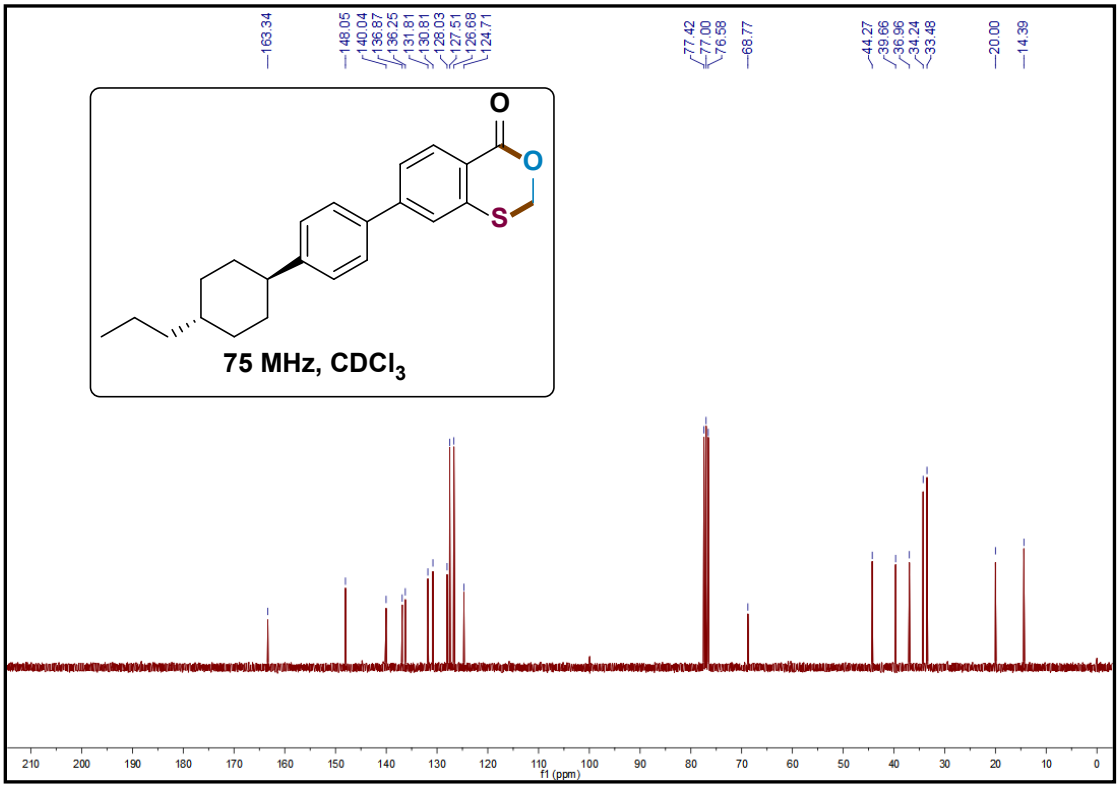
8-methyl-4H-benzo[d][1,3]oxathiin-4-one (2e)



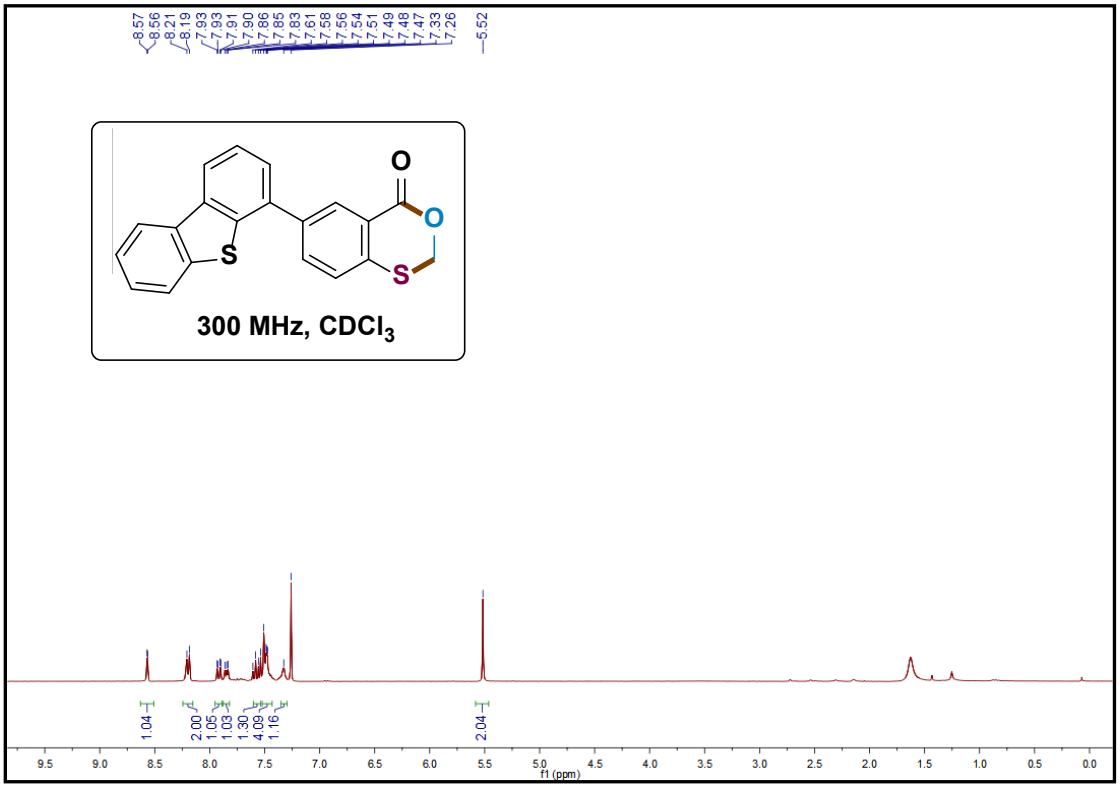


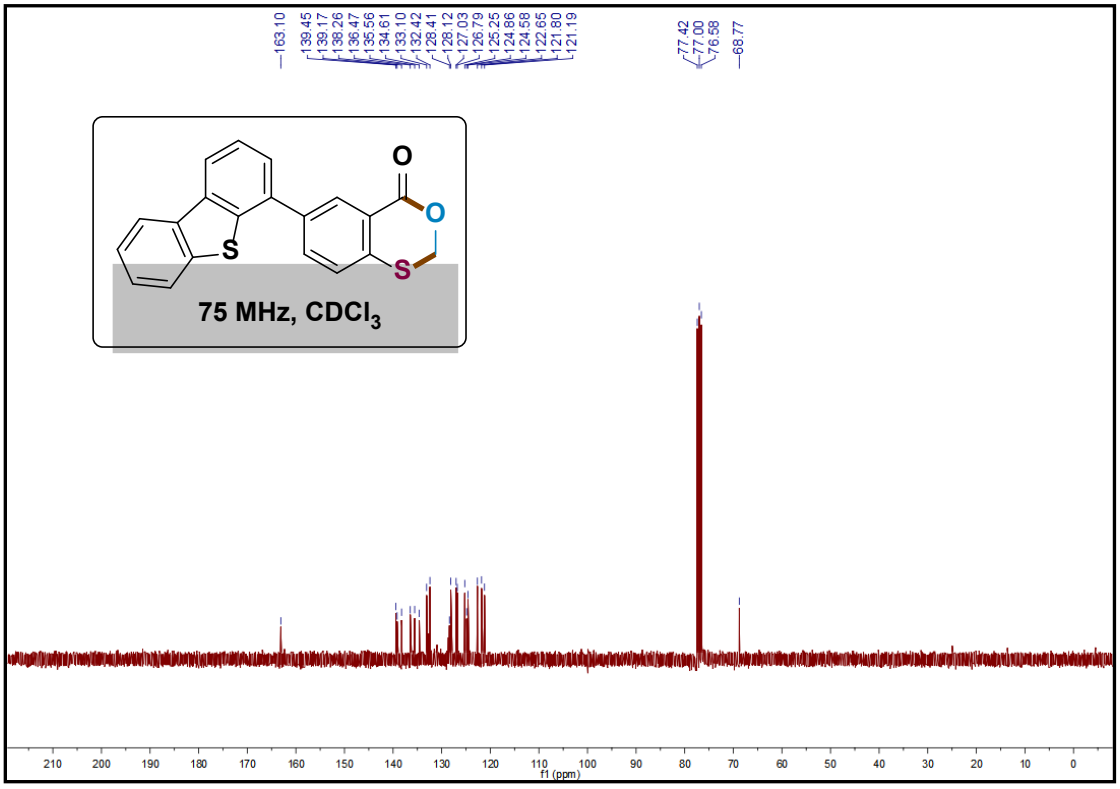
7-(4-((1s,4r)-4-propylcyclohexyl)phenyl)-4H-benzo[d][1,3]oxathiin-4-one (2f)



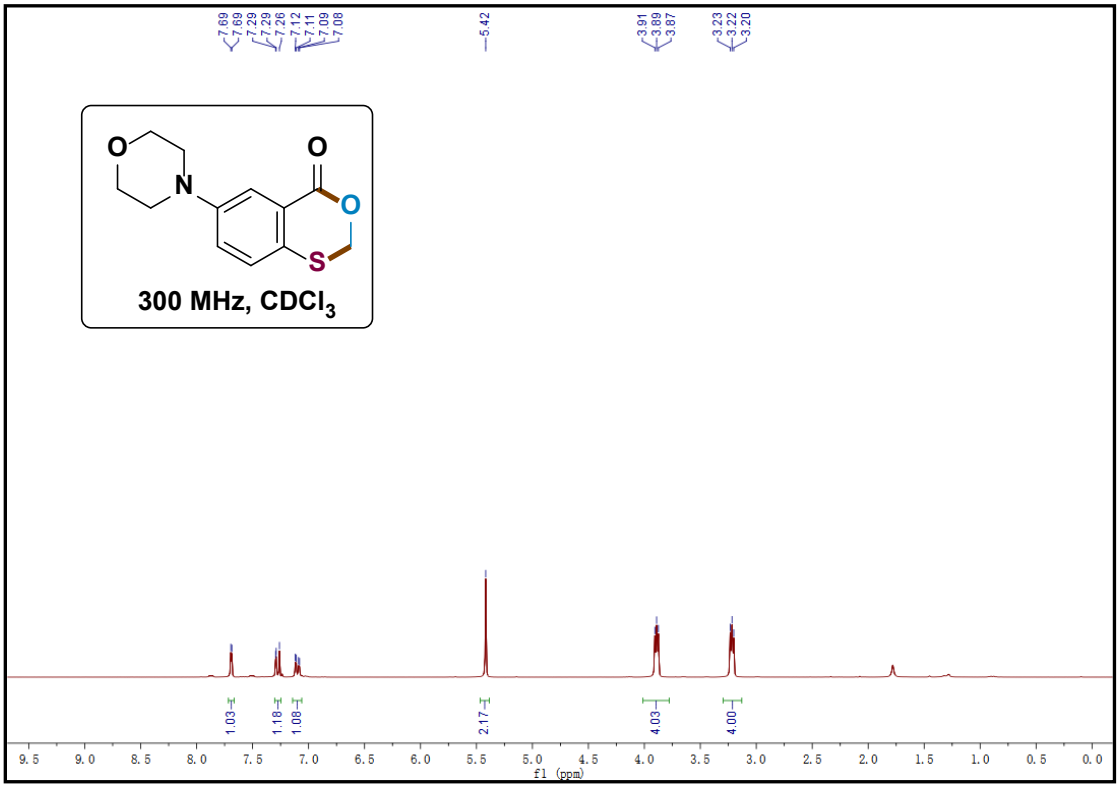


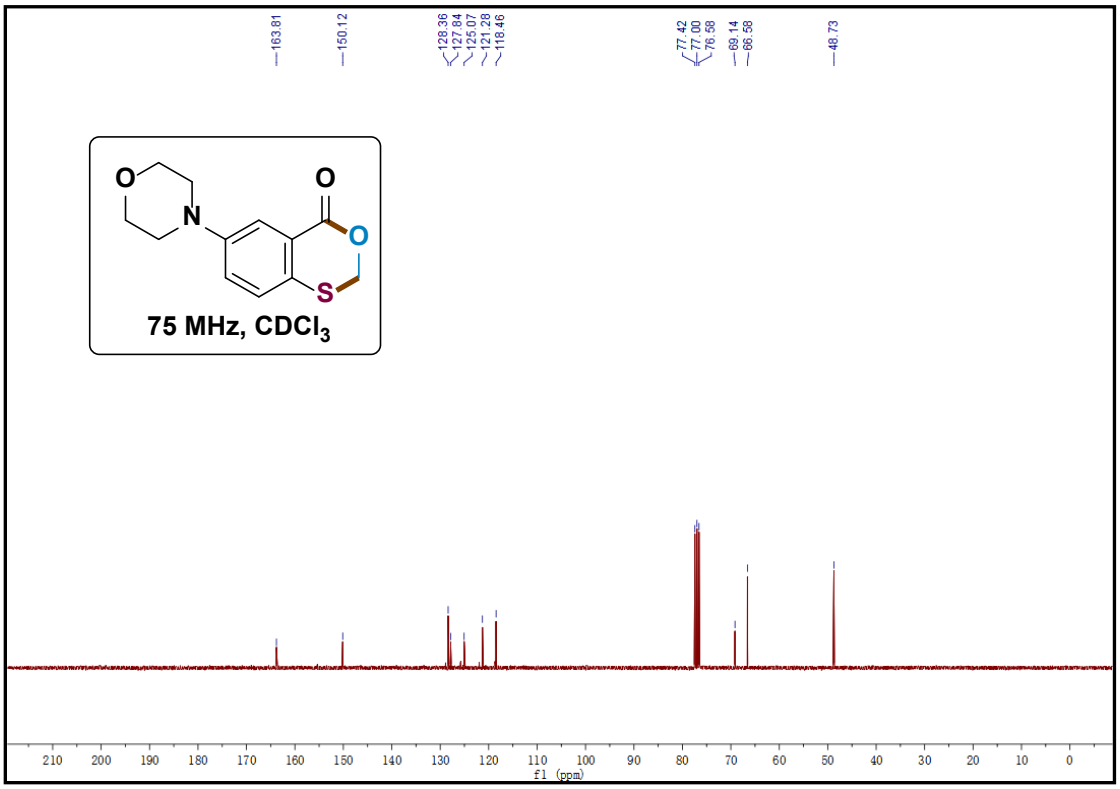
6-(dibenzo[b,d]thiophen-4-yl)-4H-benzo[d][1,3]oxathiin-4-one (2g)



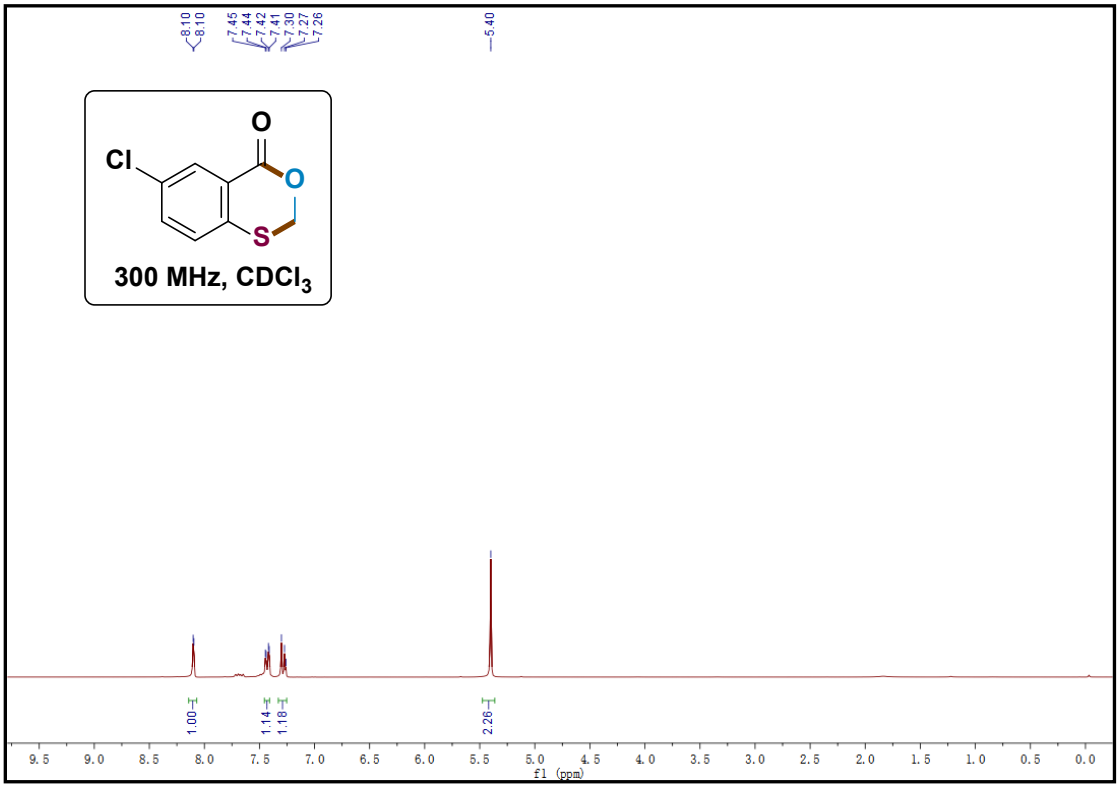


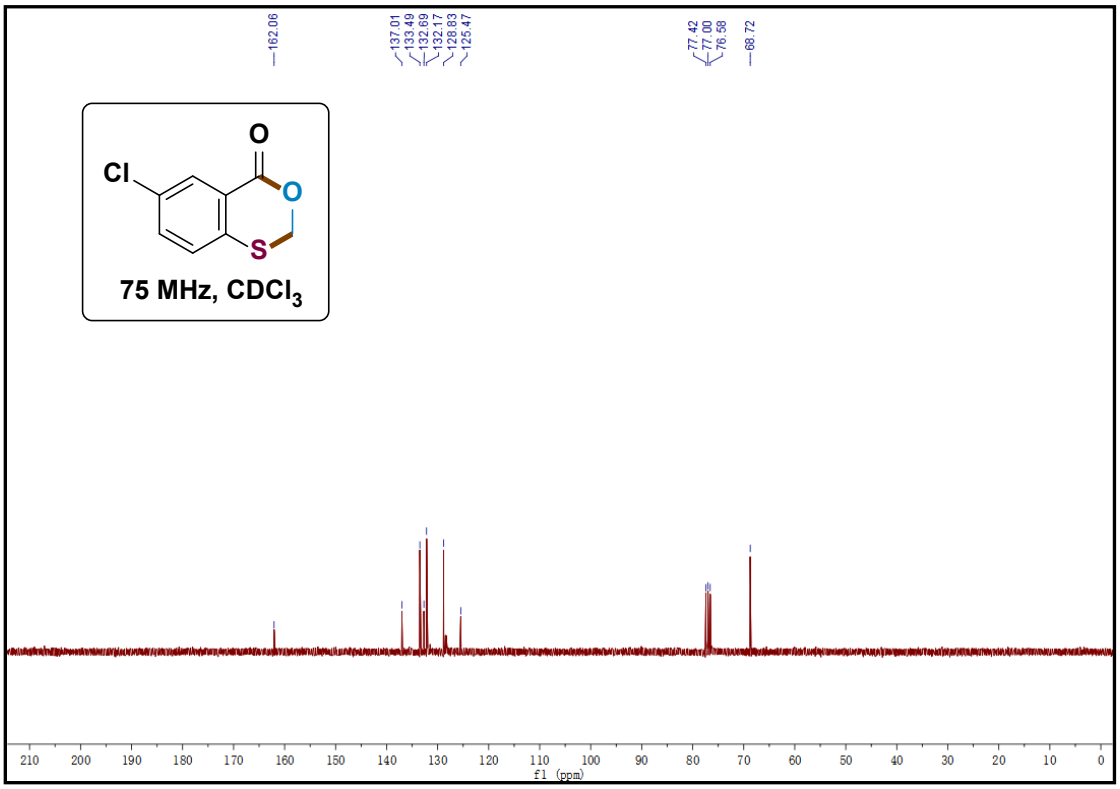
6-morpholino-4H-benzo[d][1,3]oxathiin-4-one (2h)



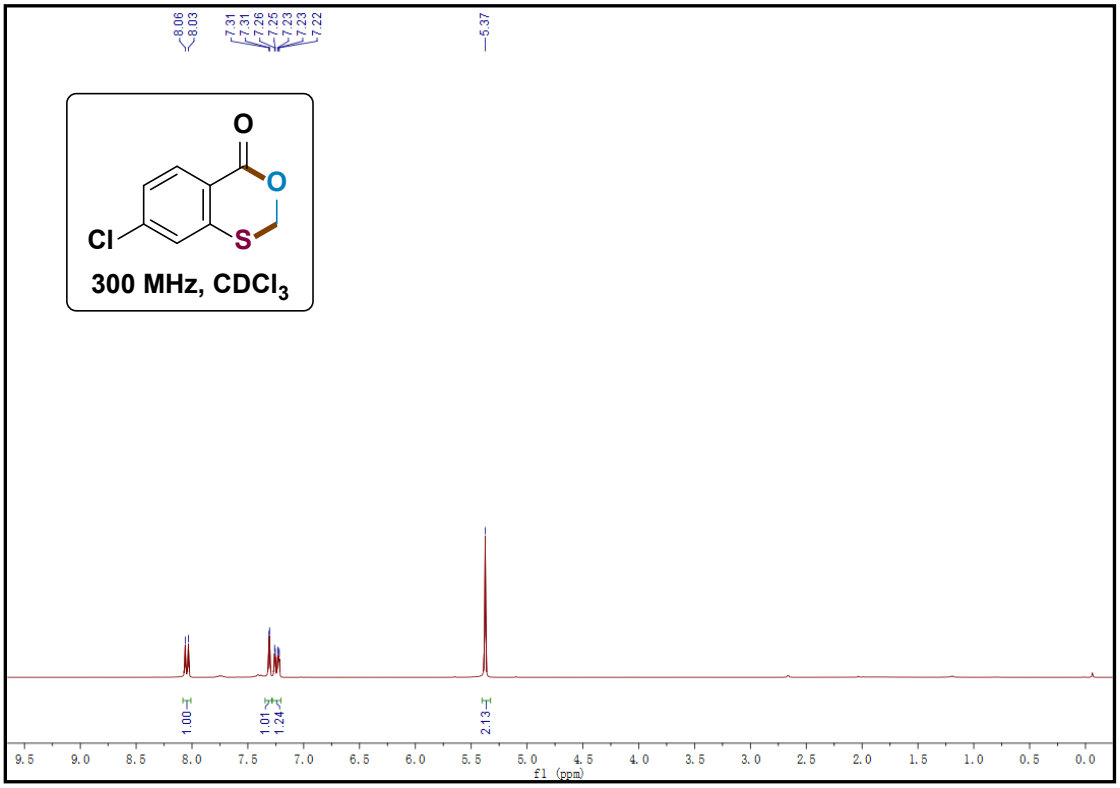


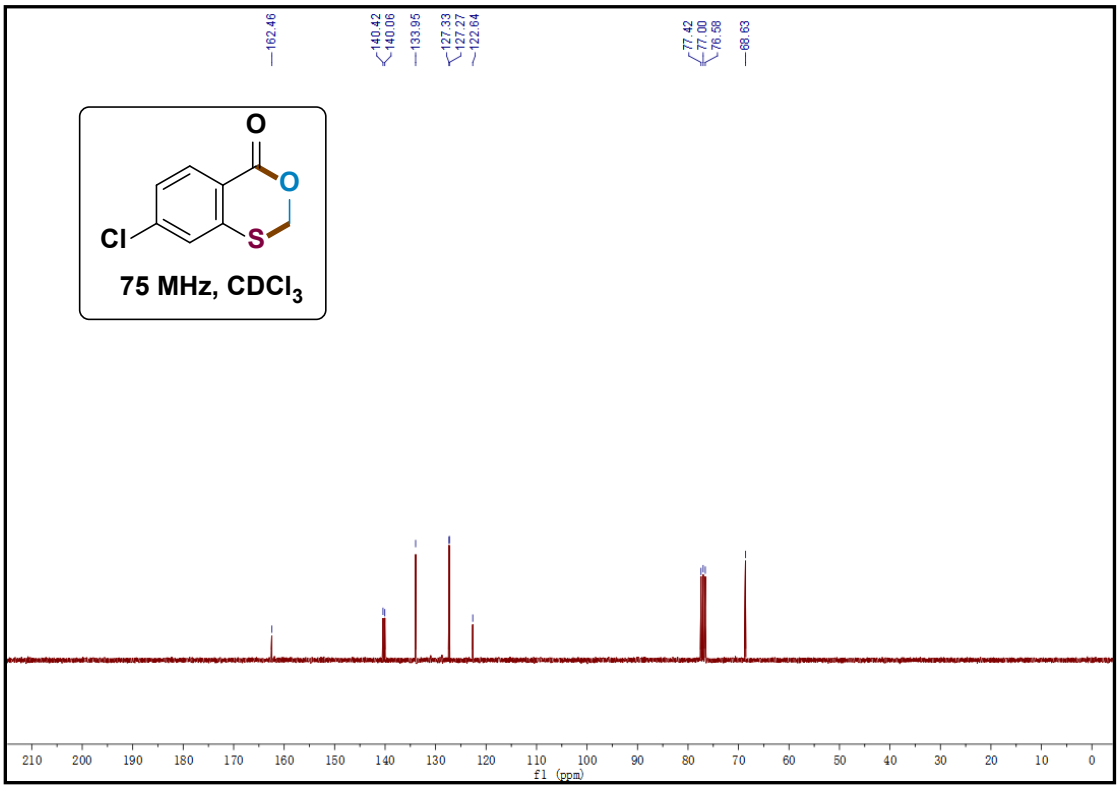
6-chloro-4H-benzo[d][1,3]oxathiin-4-one (2i)



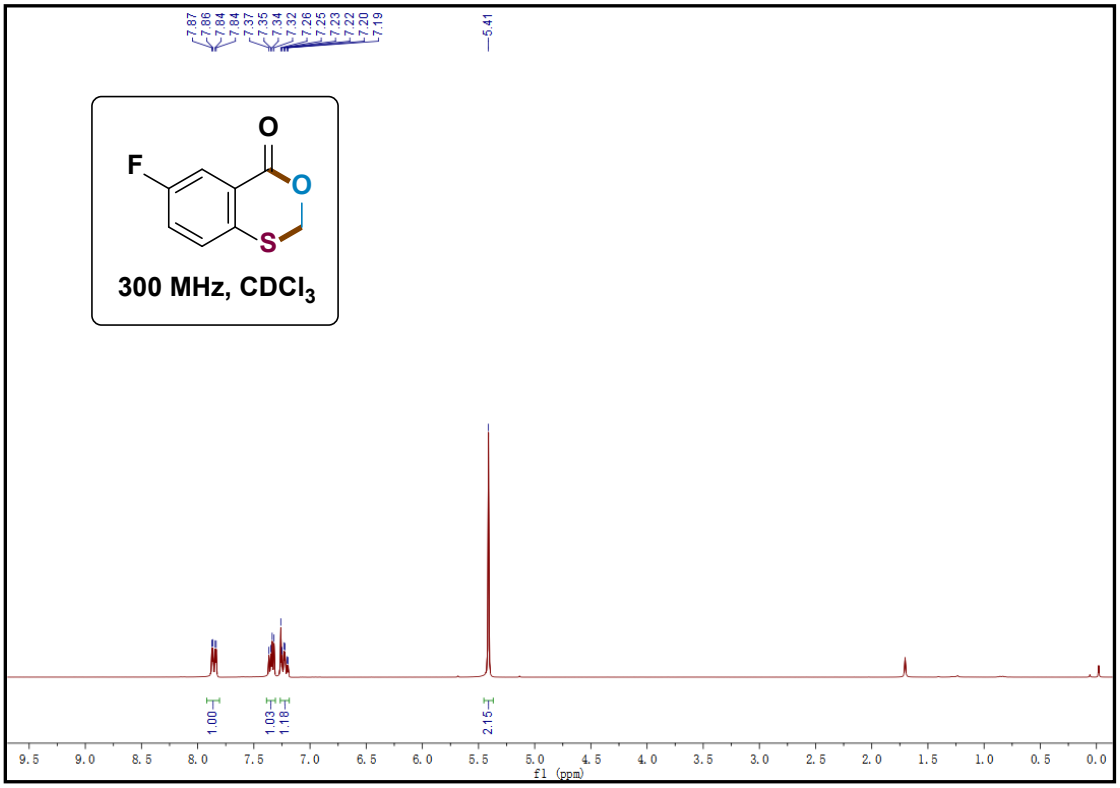


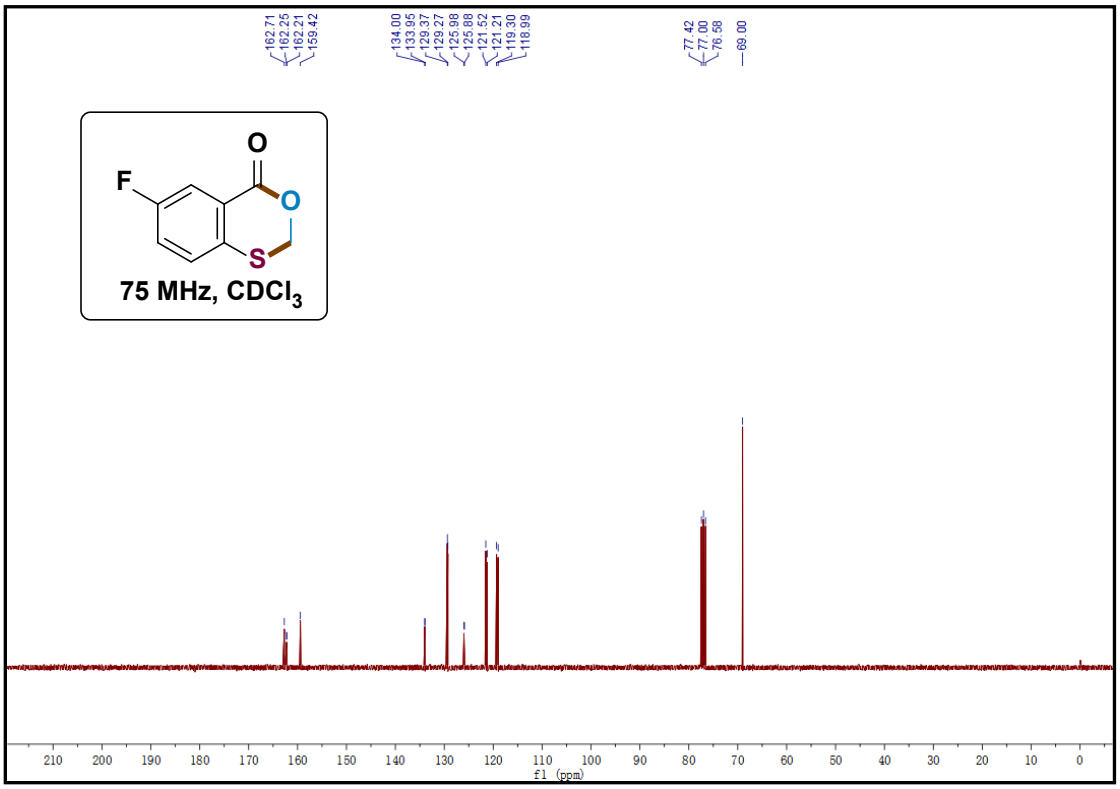
7-chloro-4H-benzo[d][1,3]oxathiin-4-one (2j)



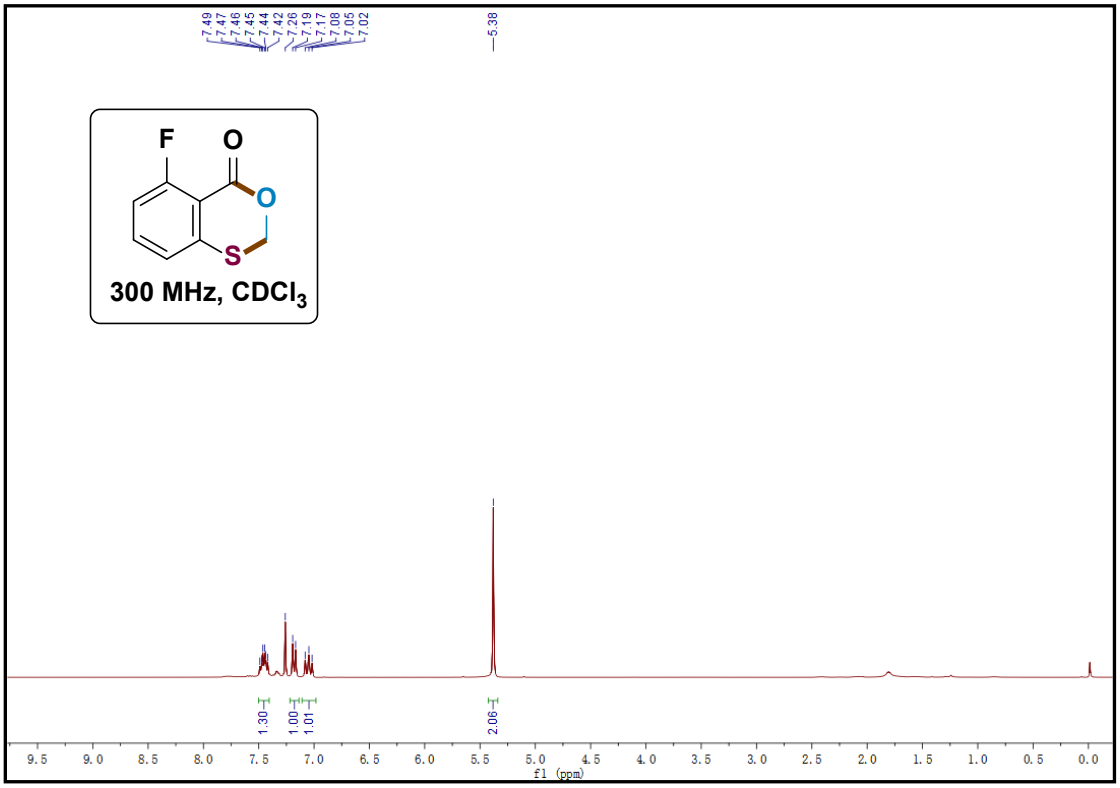


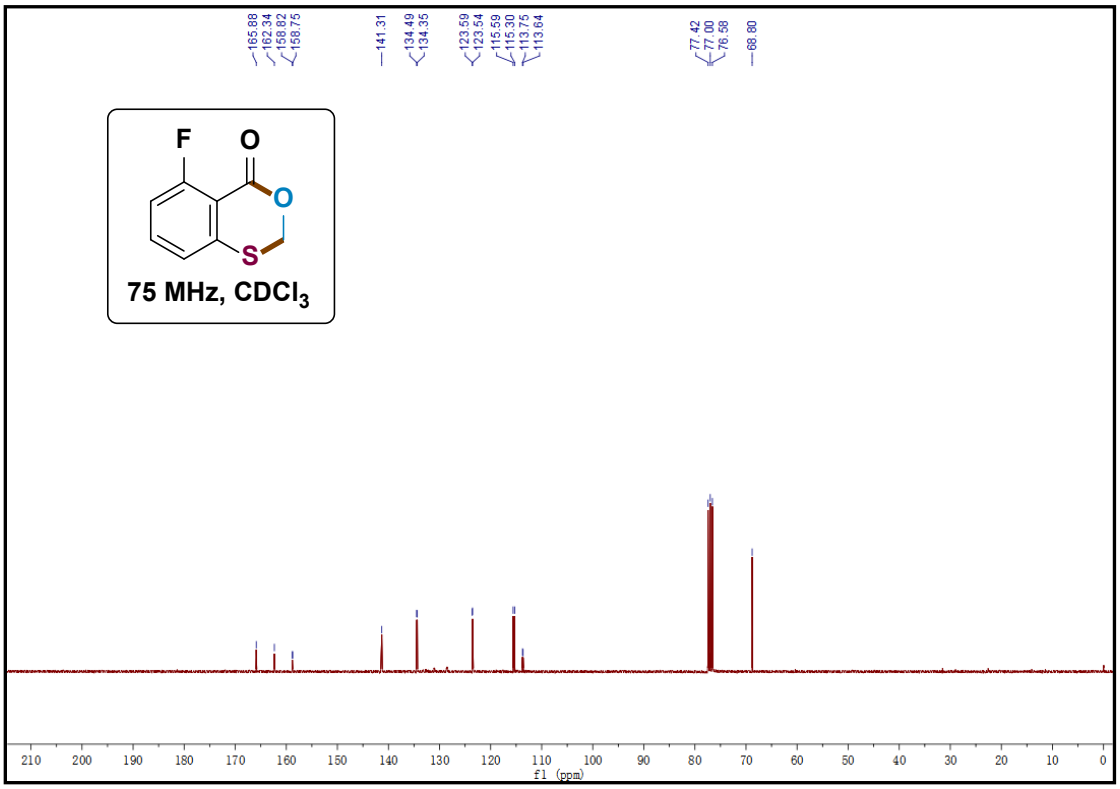
6-fluoro-4H-benzo[d][1,3]oxathiin-4-one (2k)



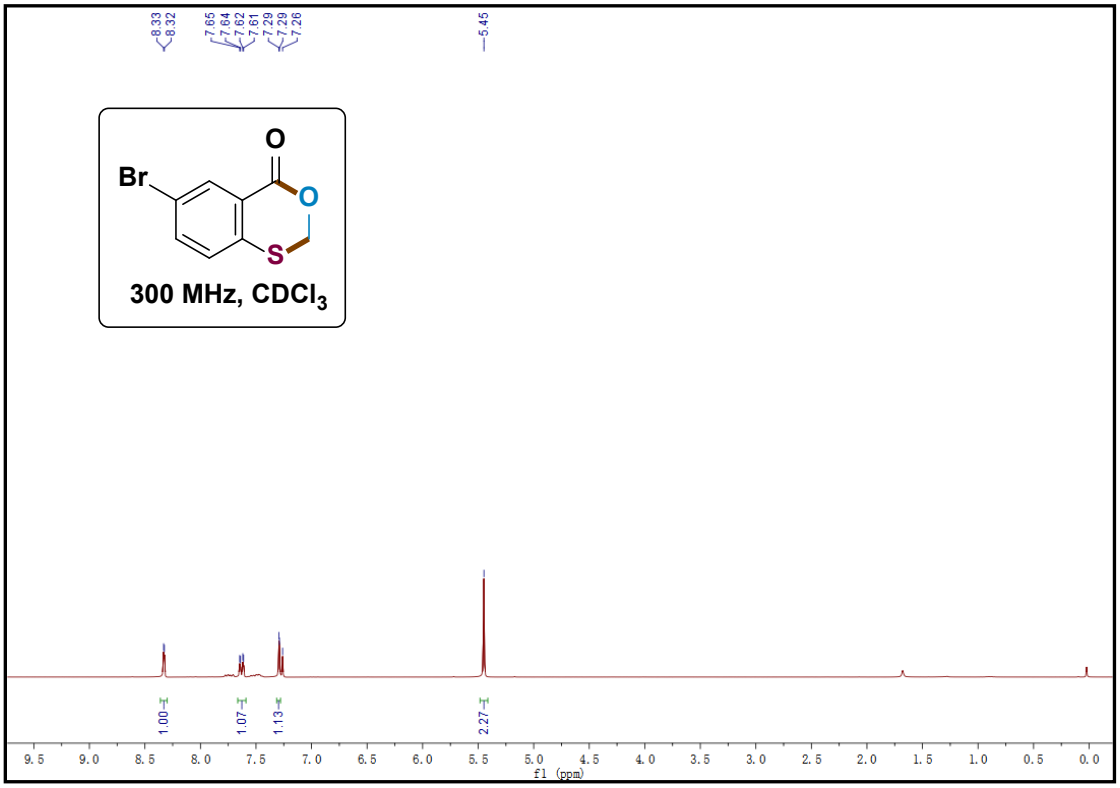


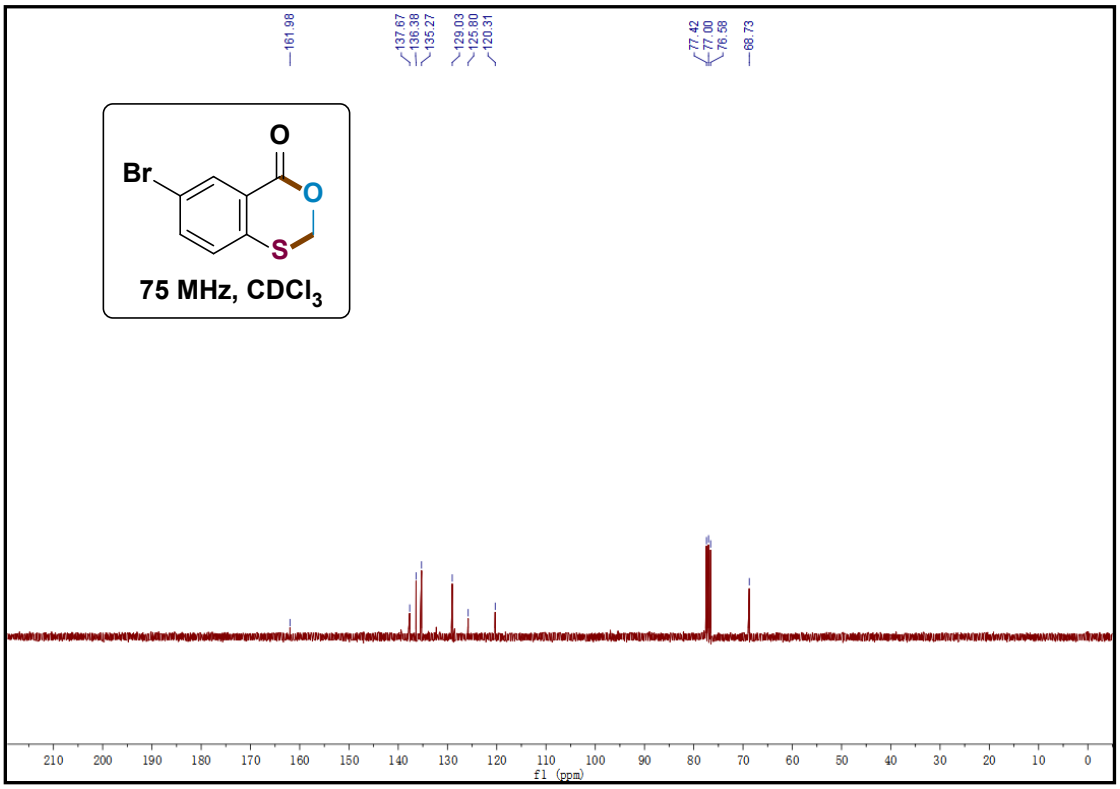
5-fluoro-4H-benzo[d][1,3]oxathiin-4-one (2l)



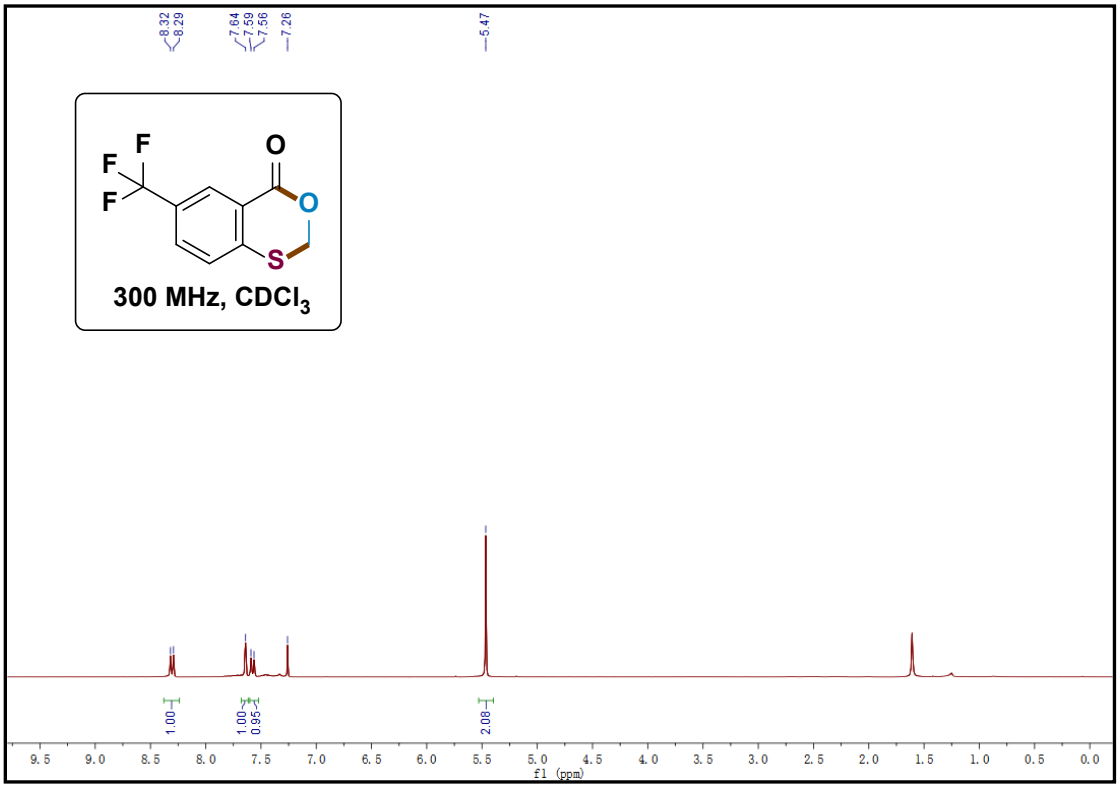


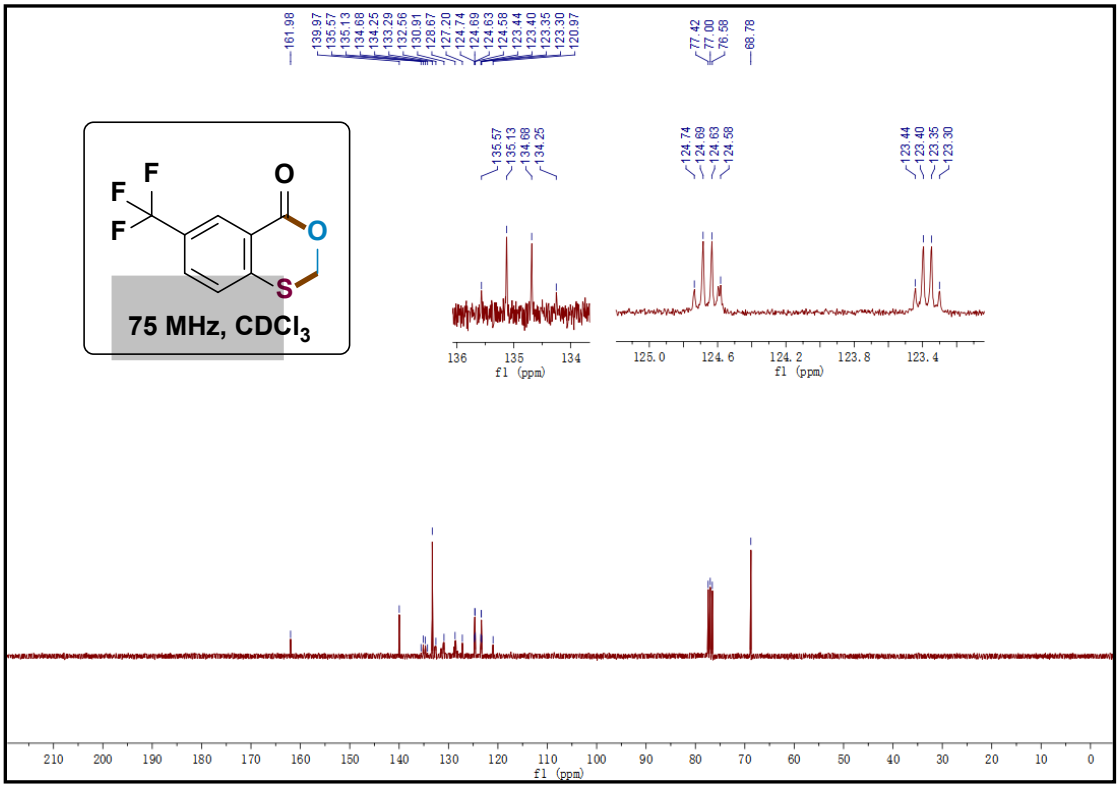
6-bromo-4H-benzo[d][1,3]oxathiin-4-one (2m)



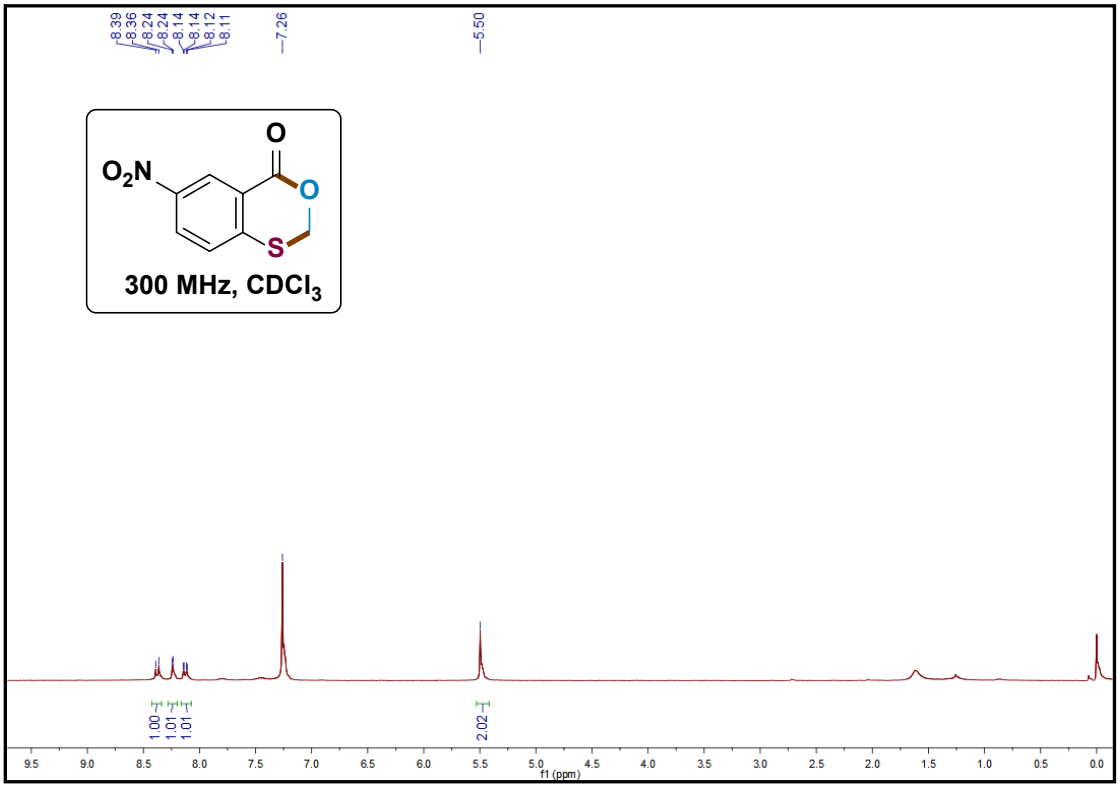


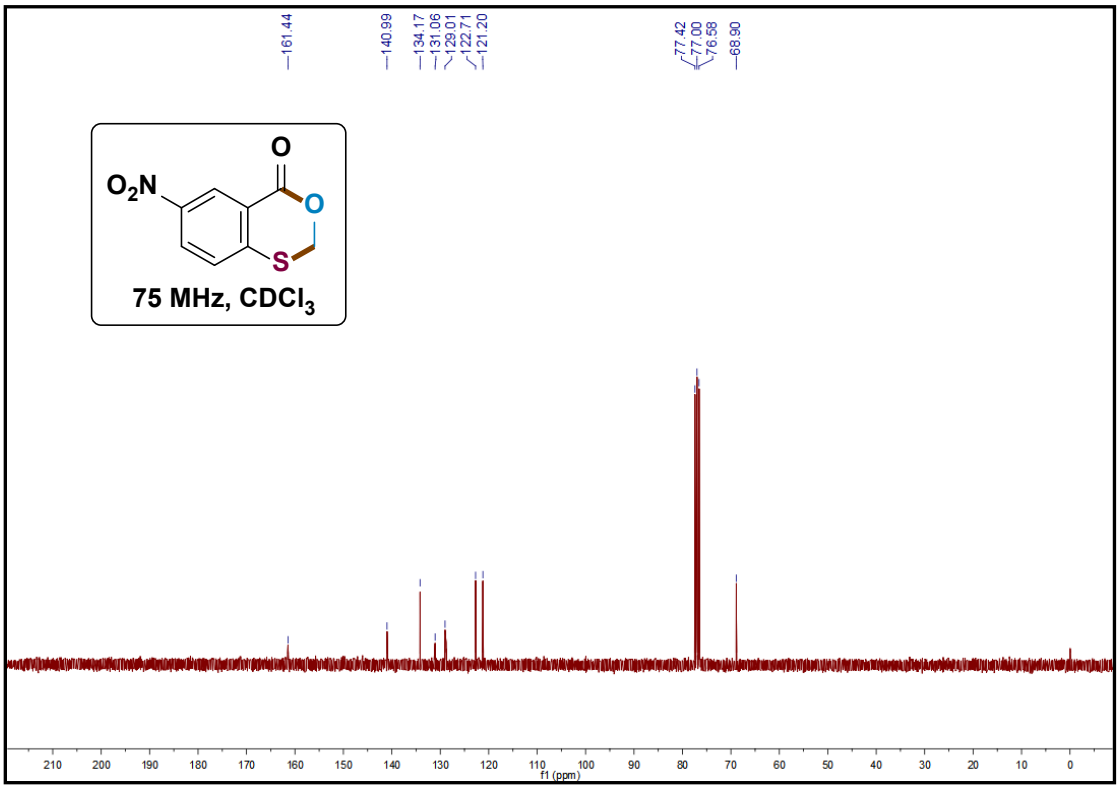
6-(trifluoromethyl)-4H-benzo[d][1,3]oxathiin-4-one (2n)



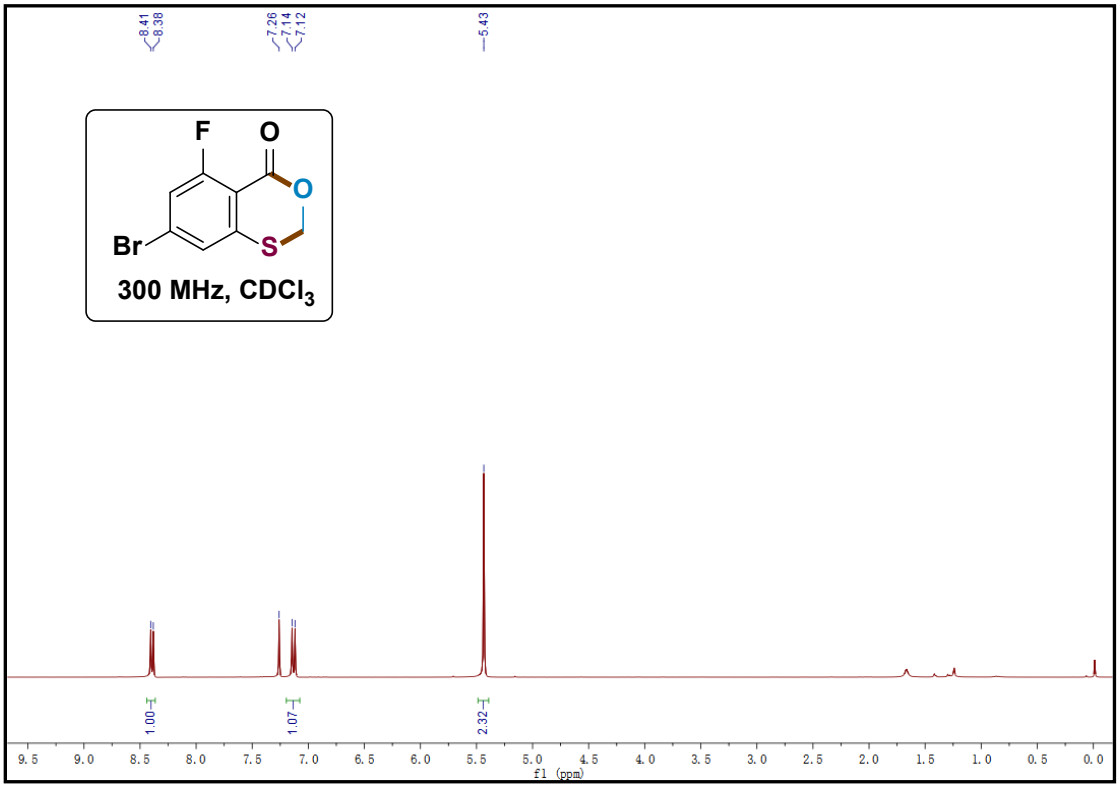


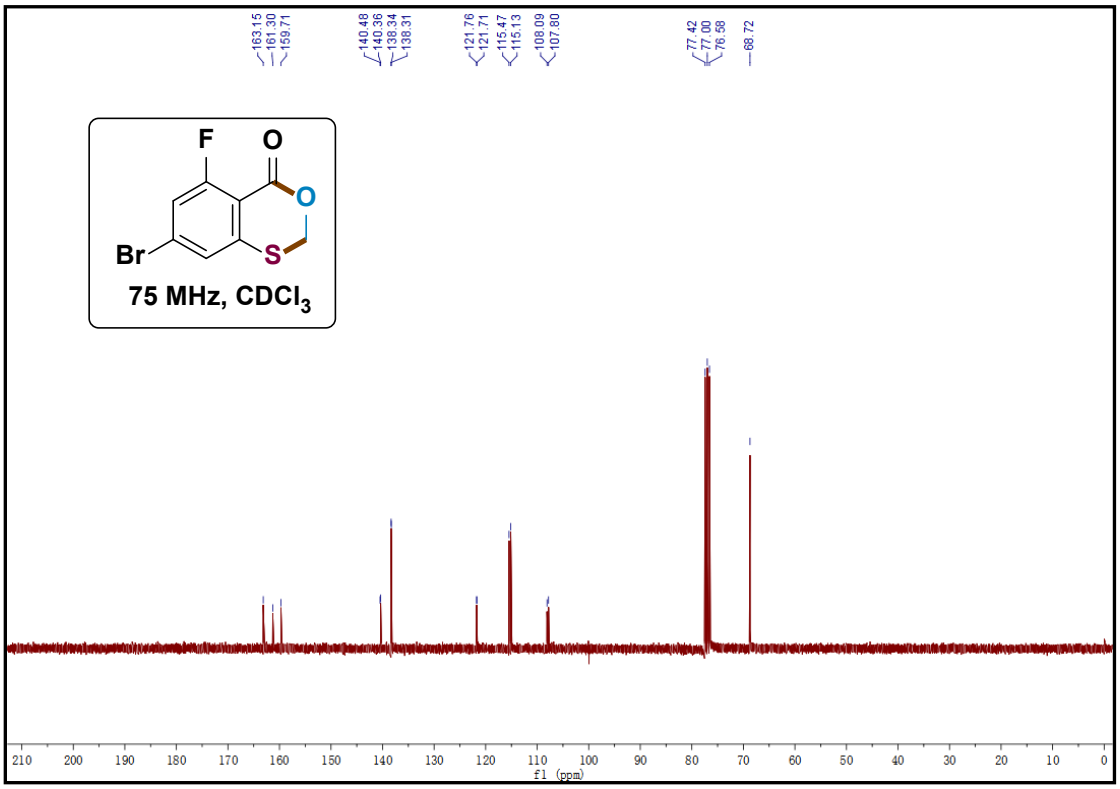
6-nitro-4H-benzo[d][1,3]oxathiin-4-one (2o)



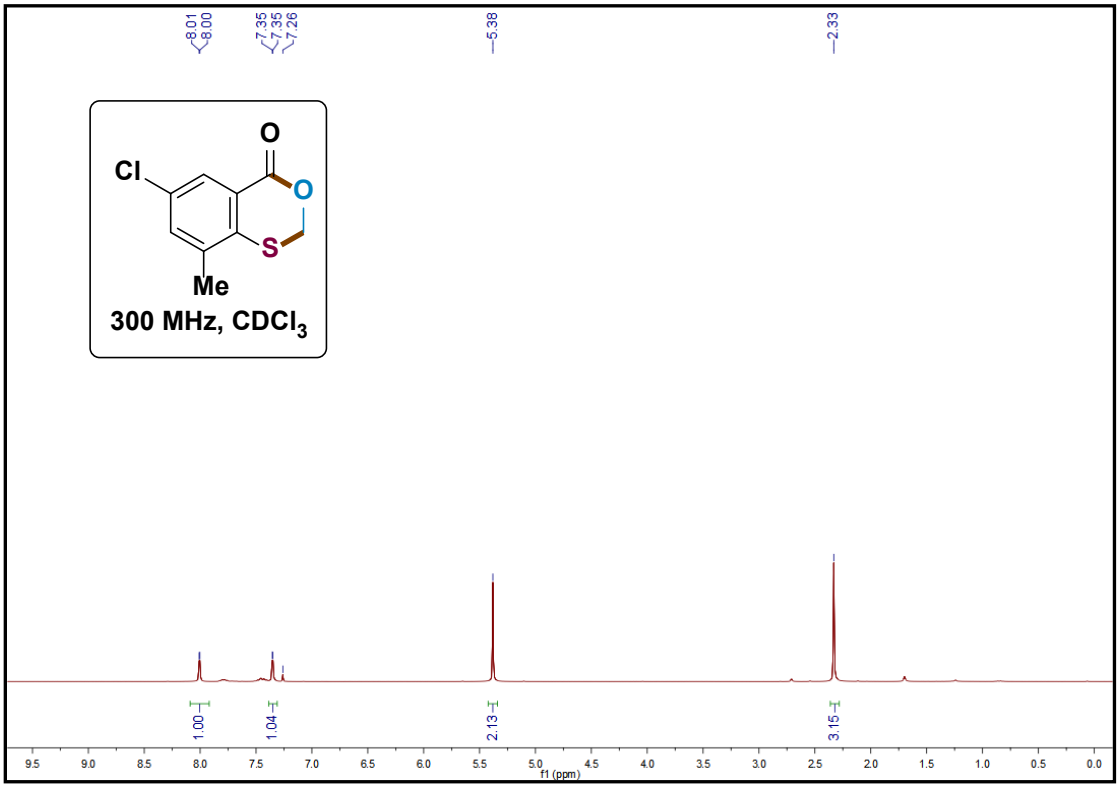


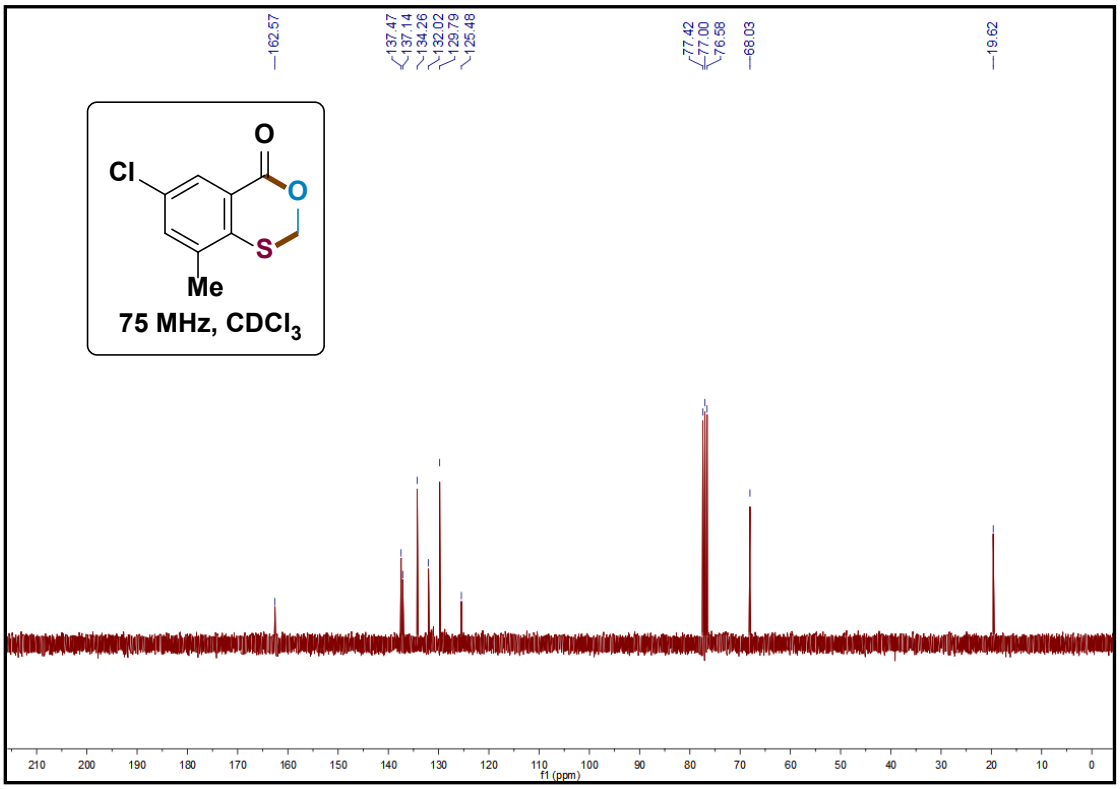
7-bromo-6-fluoro-4H-benzo[d][1,3]oxathiin-4-one (2p)



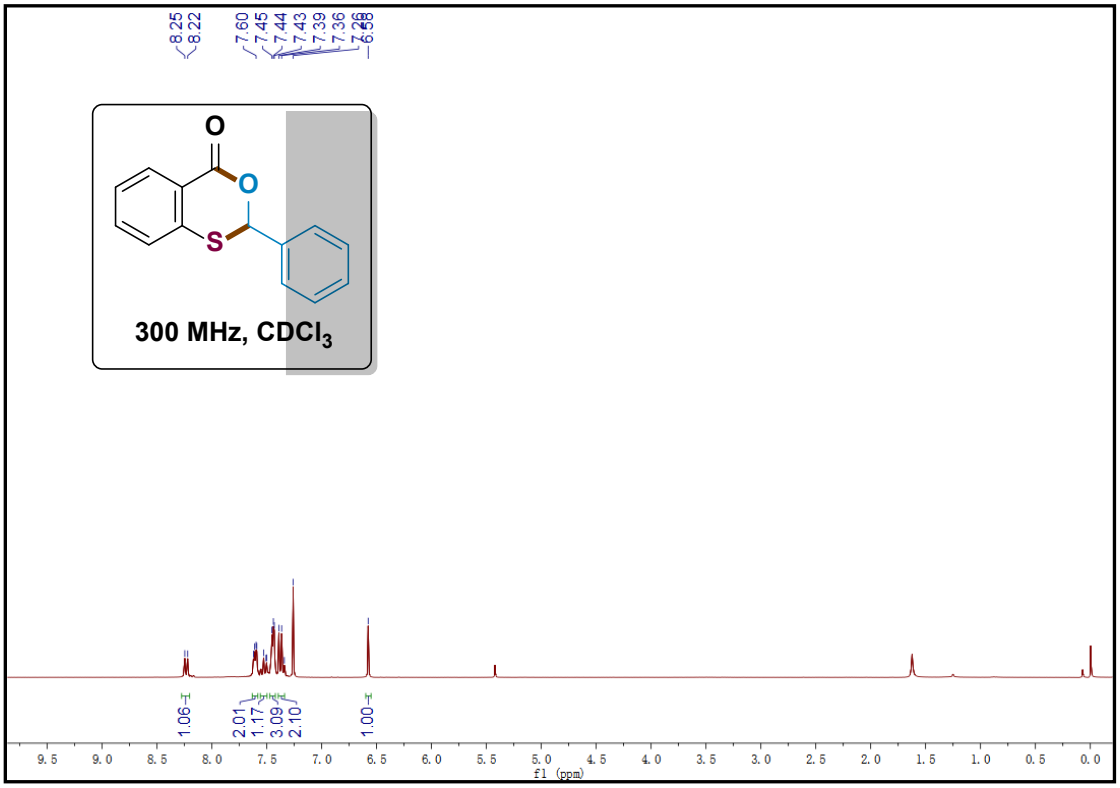


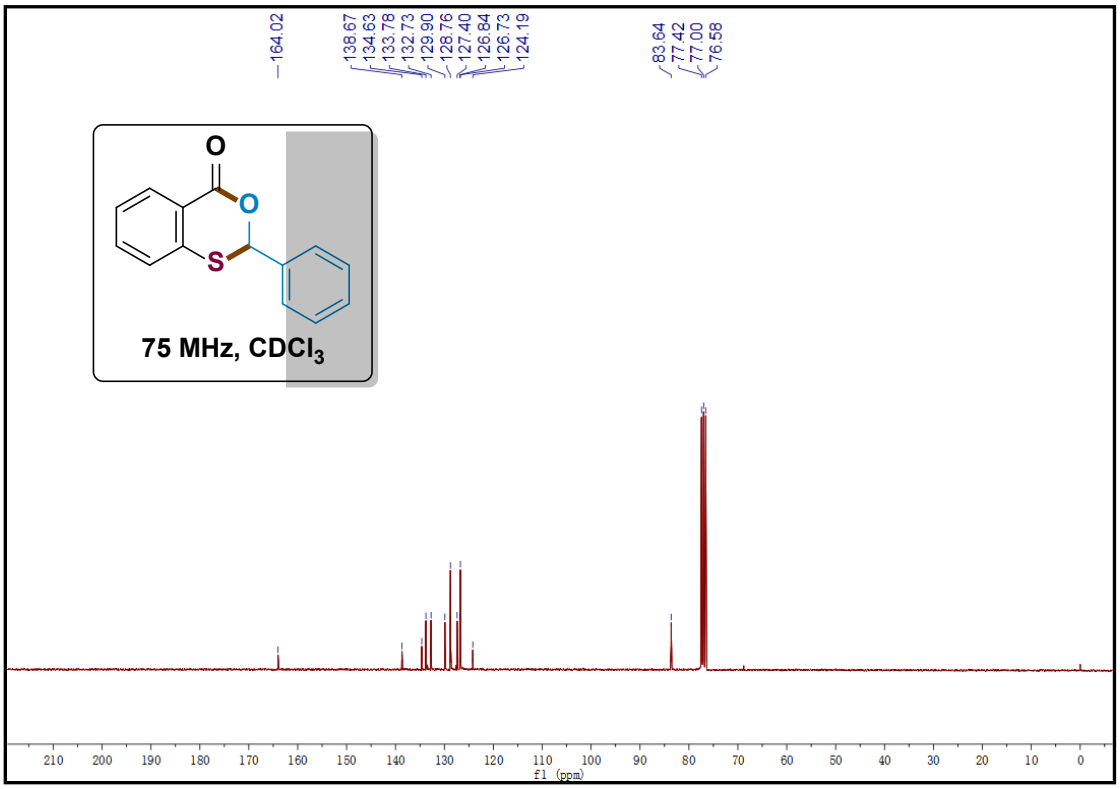
6-chloro-8-methyl-4H-benzo[d][1,3]oxathiin-4-one (2q)



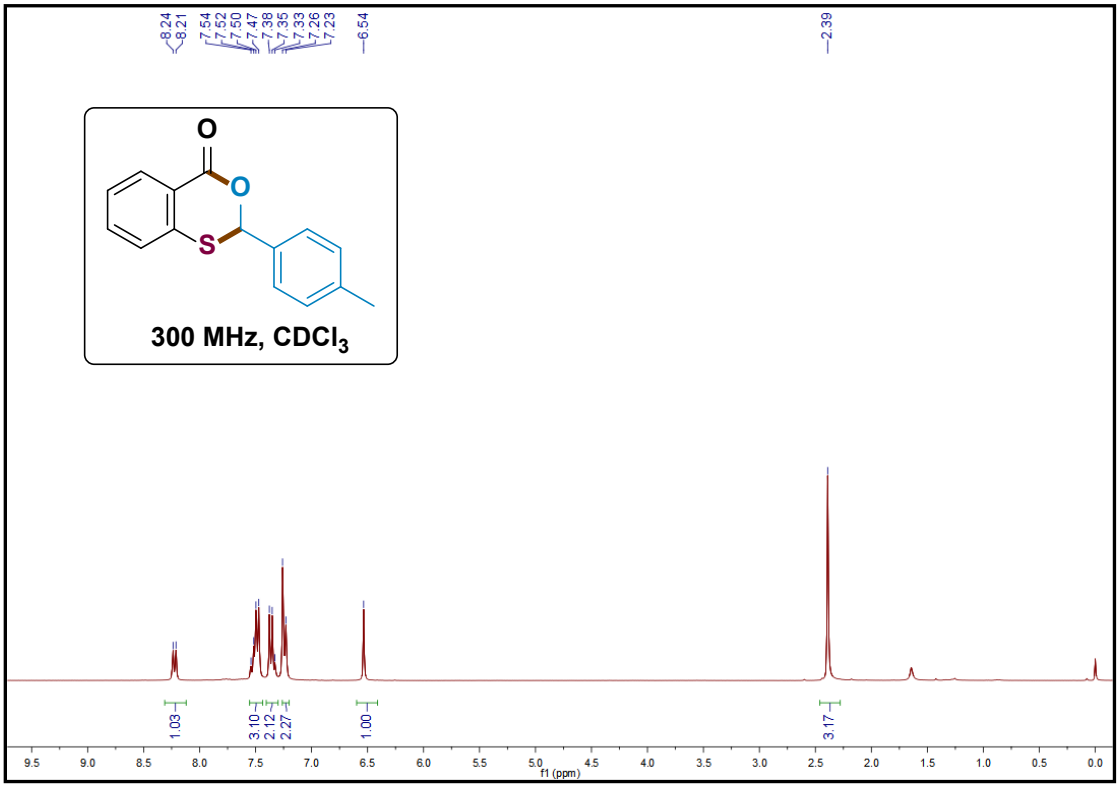


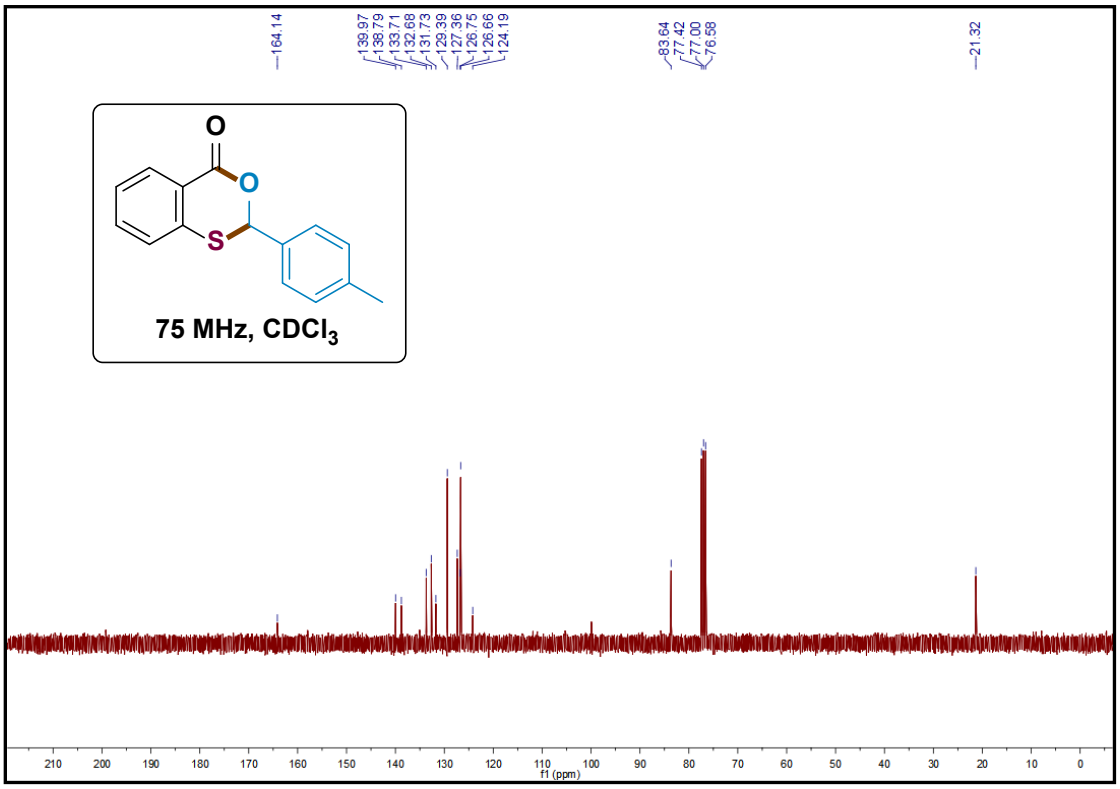
phenyl-4H-benzo[d][1,3]oxathiin-4-one (4a)



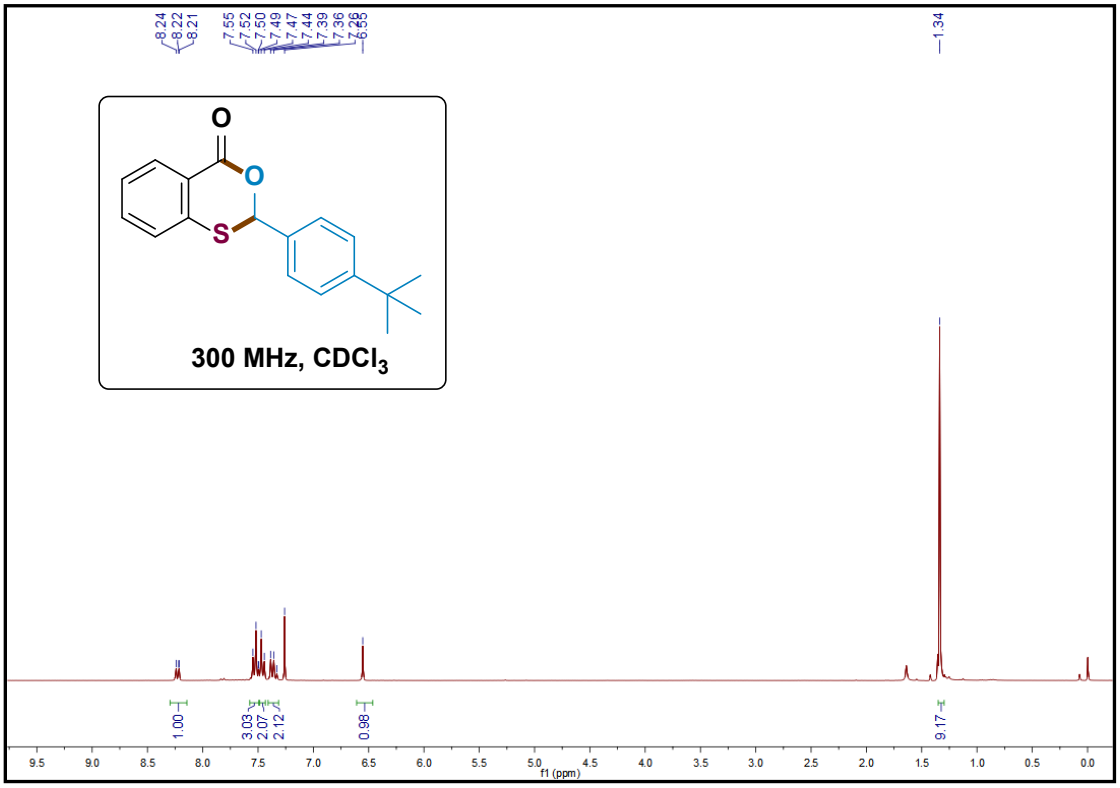


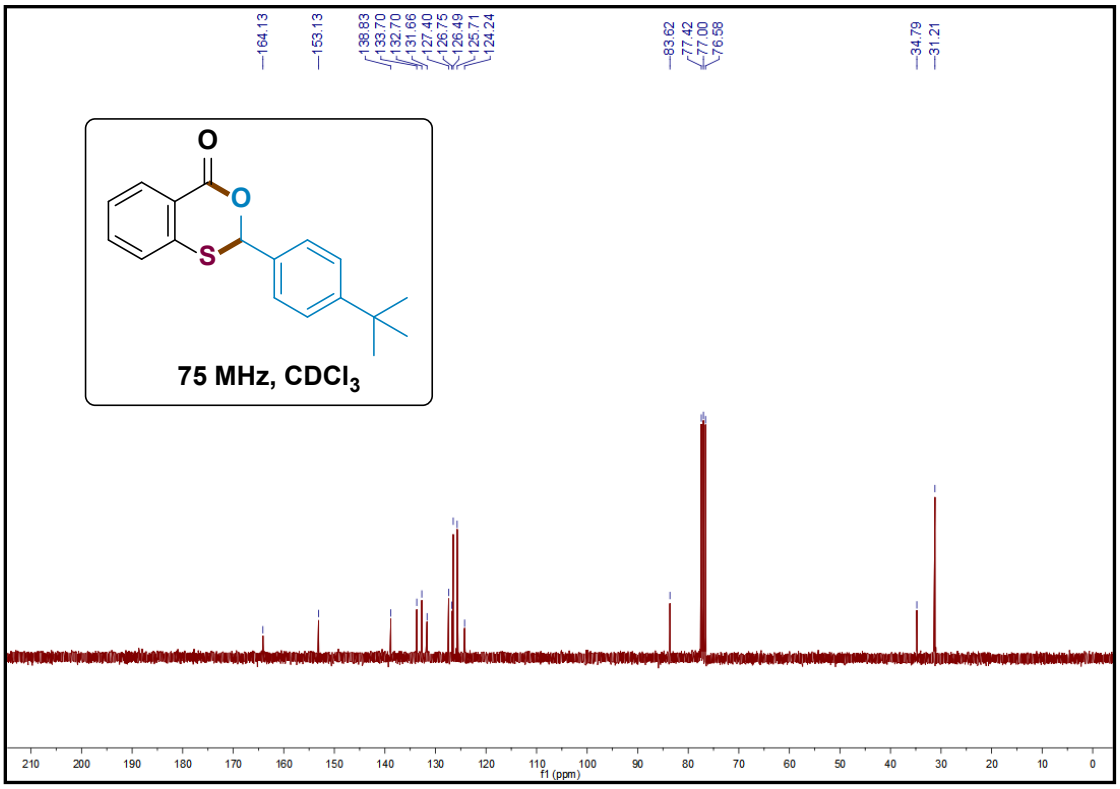
2-(p-tolyl)-4H-benzo[d][1,3]oxathiin-4-one (4b)



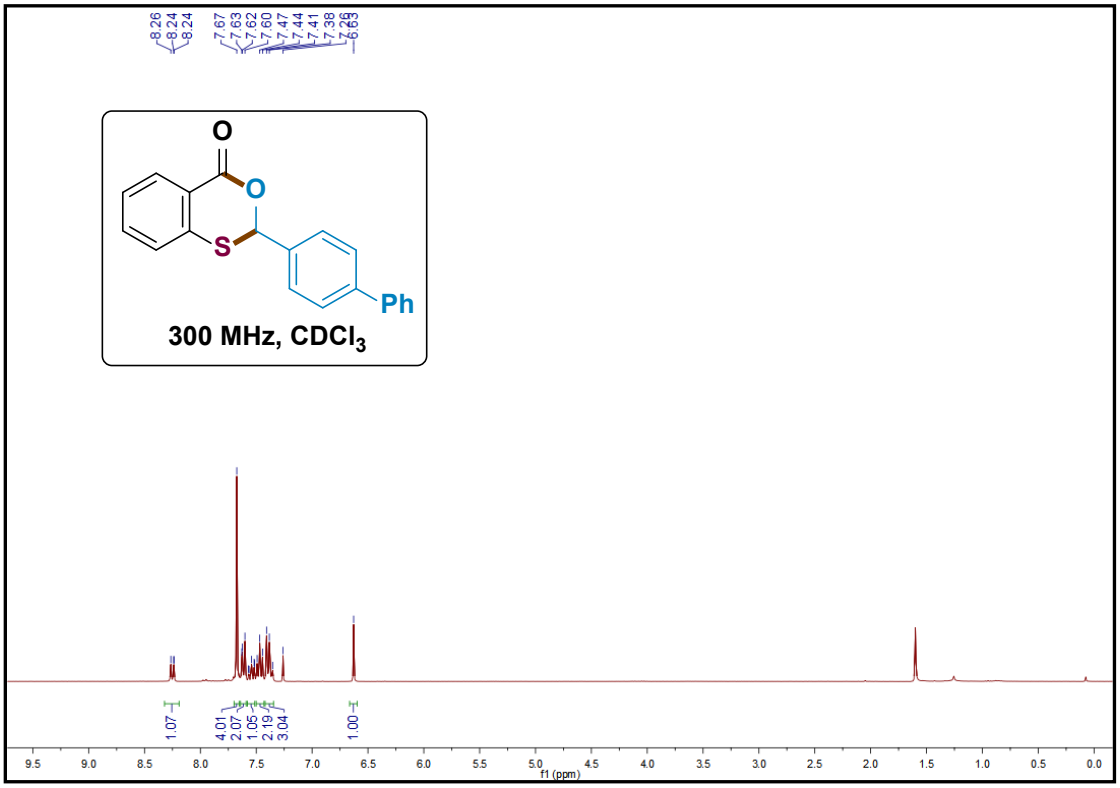


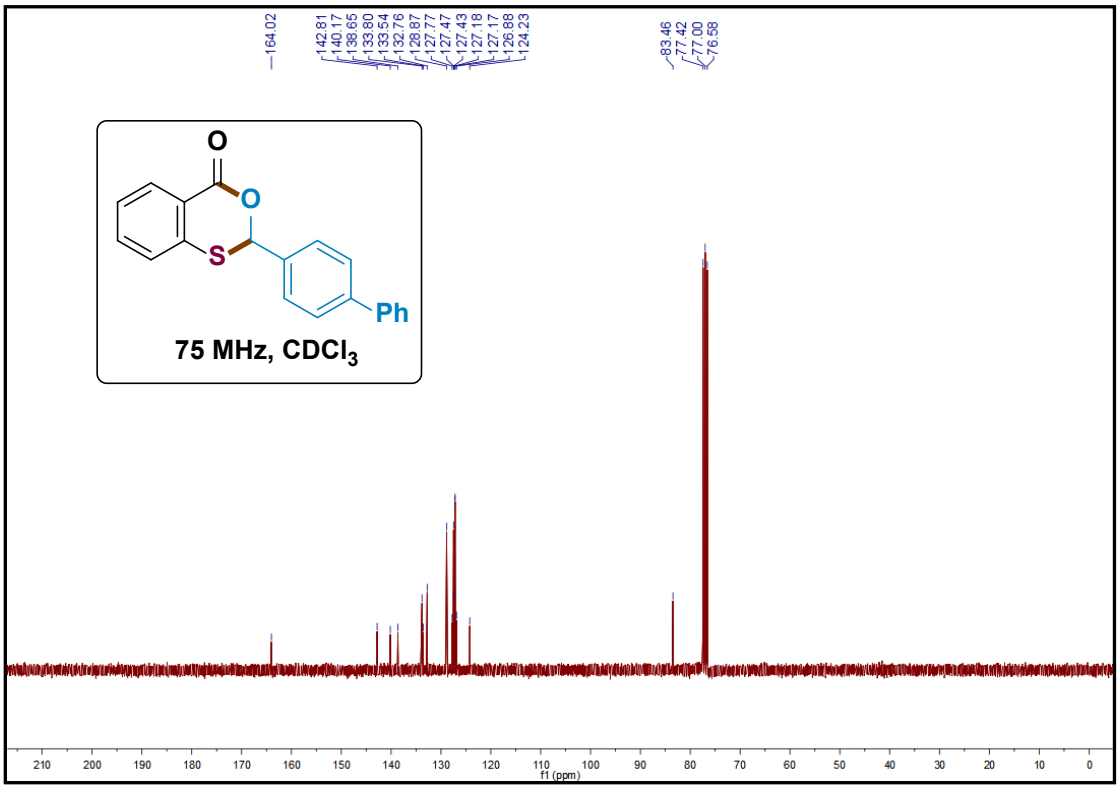
2-(4-(tert-butyl)phenyl)-4H-benzo[d][1,3]oxathiin-4-one (4c)



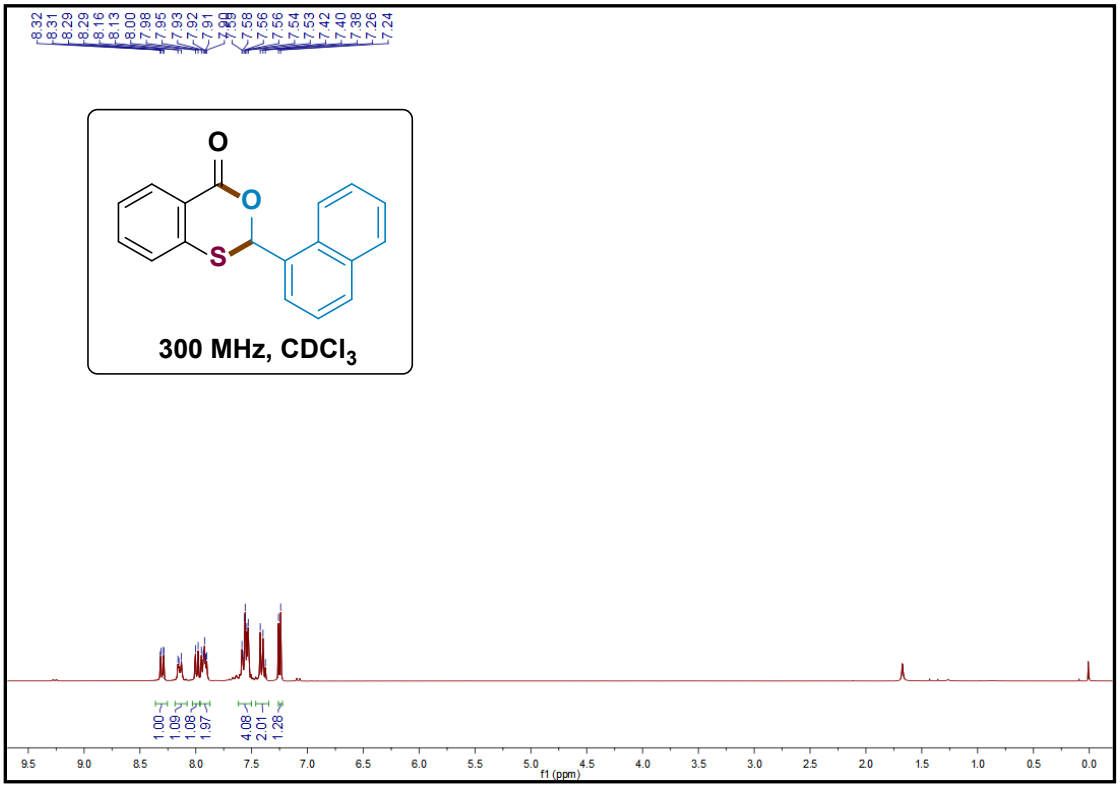


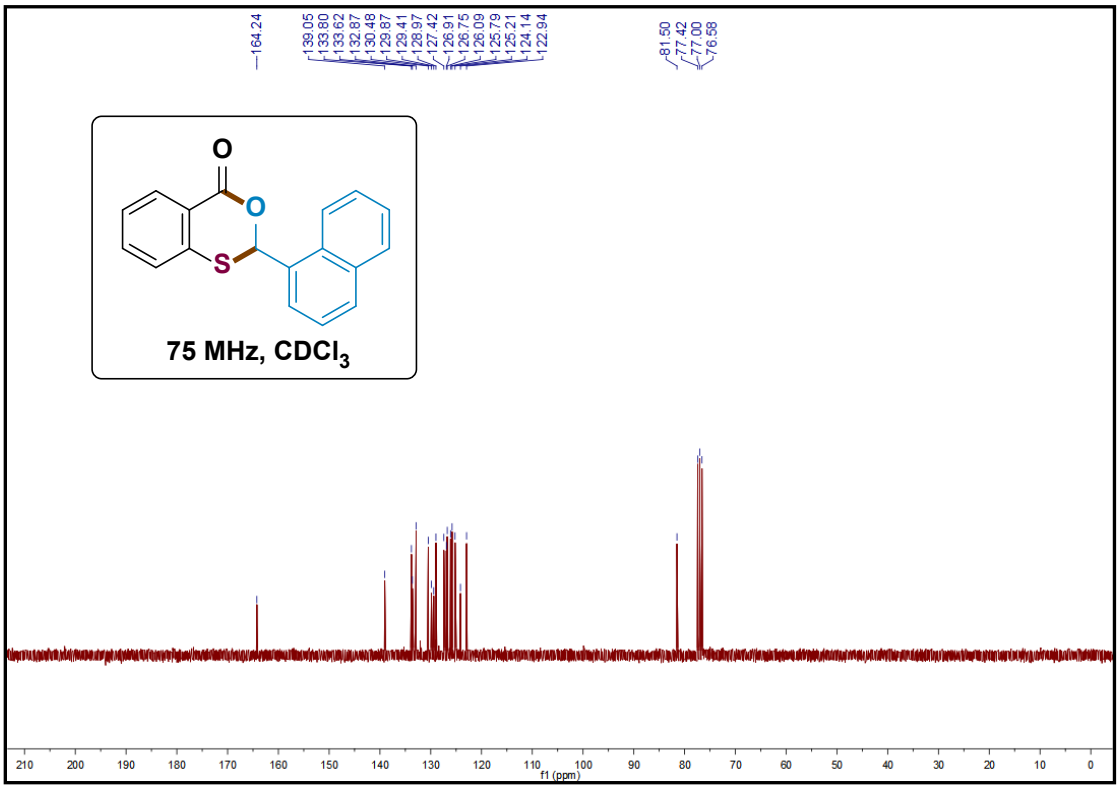
2-([1,1'-biphenyl]-4-yl)-4H-benzo[d][1,3]oxathiin-4-one (4d)



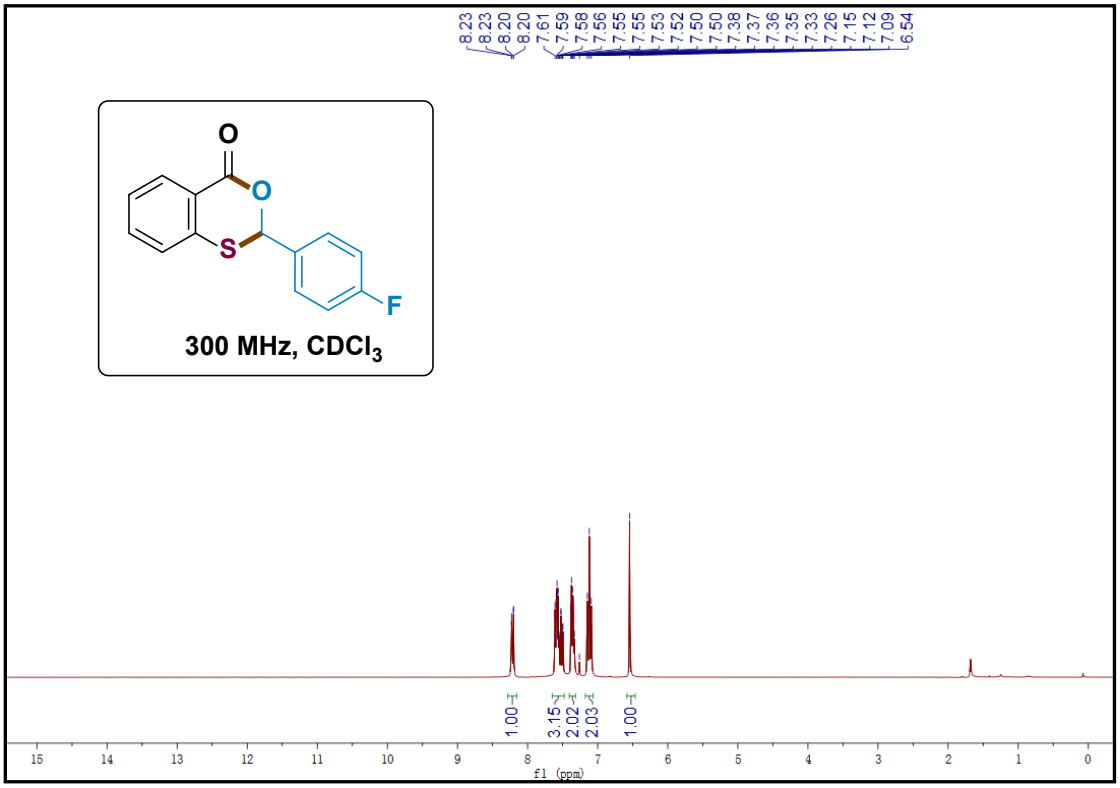


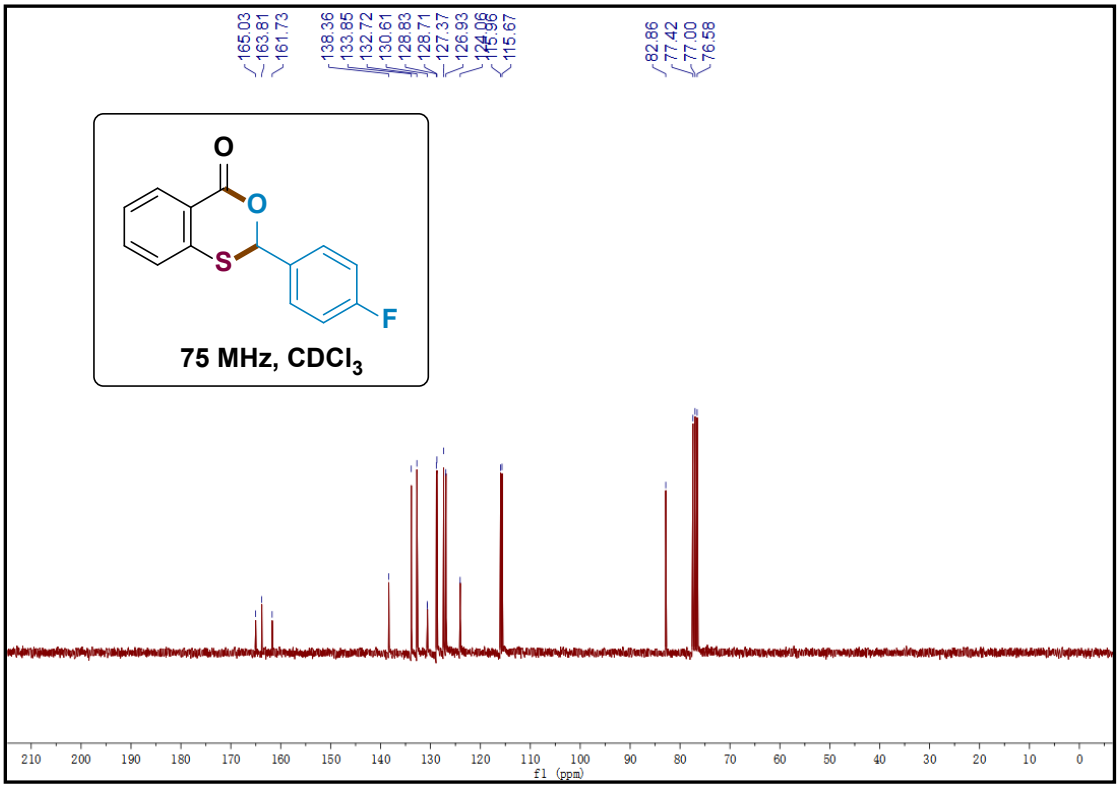
2-(naphthalen-1-yl)-4H-benzo[d][1,3]oxathiin-4-one (4e)



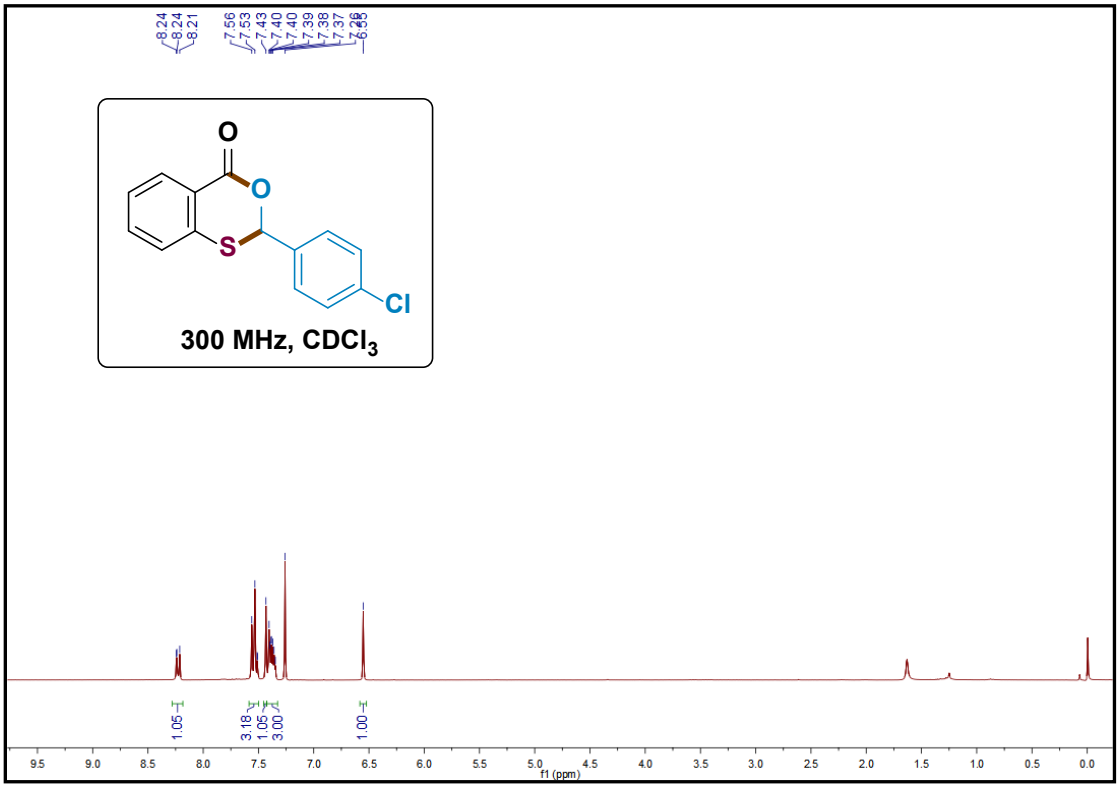


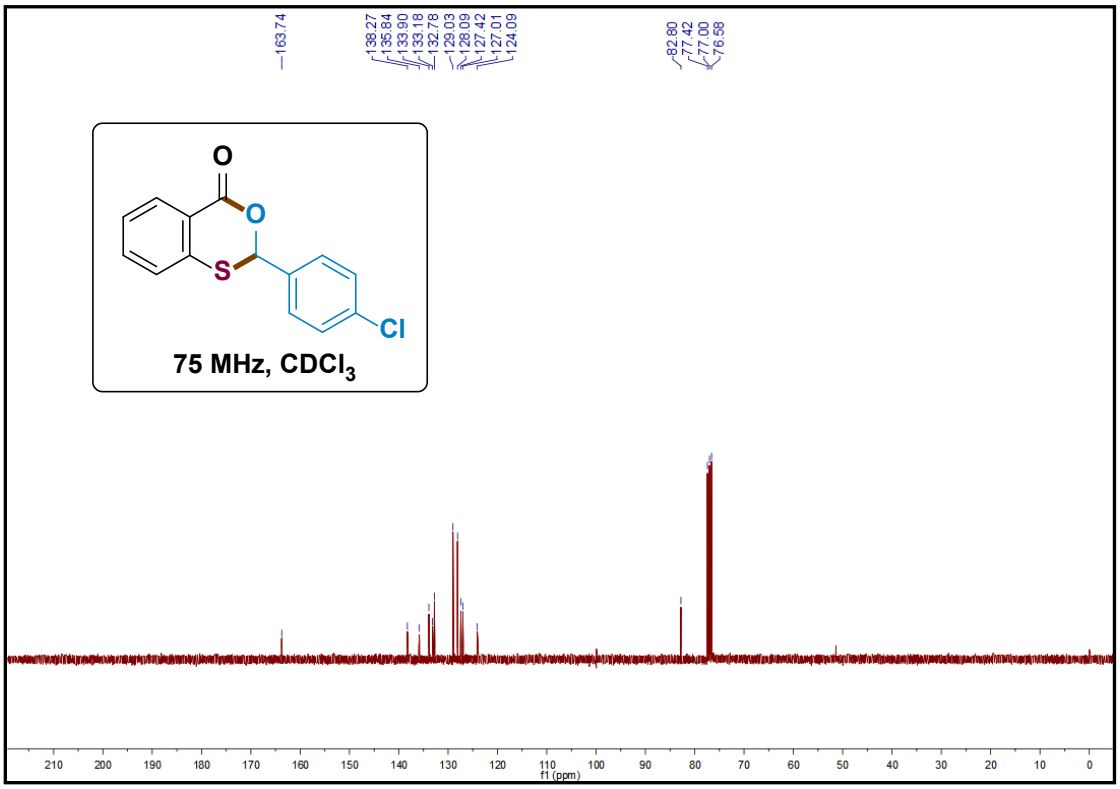
2-(4-fluorophenyl)-4H-benzo[d][1,3]oxathiin-4-one (4f)



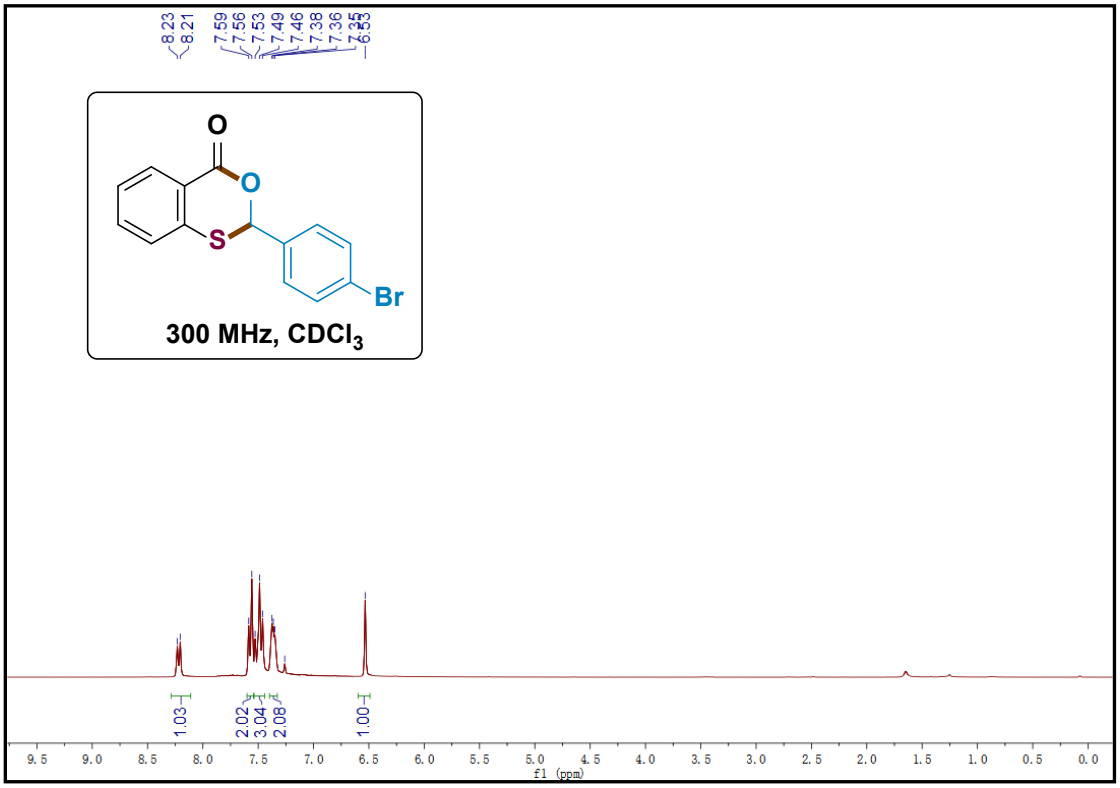


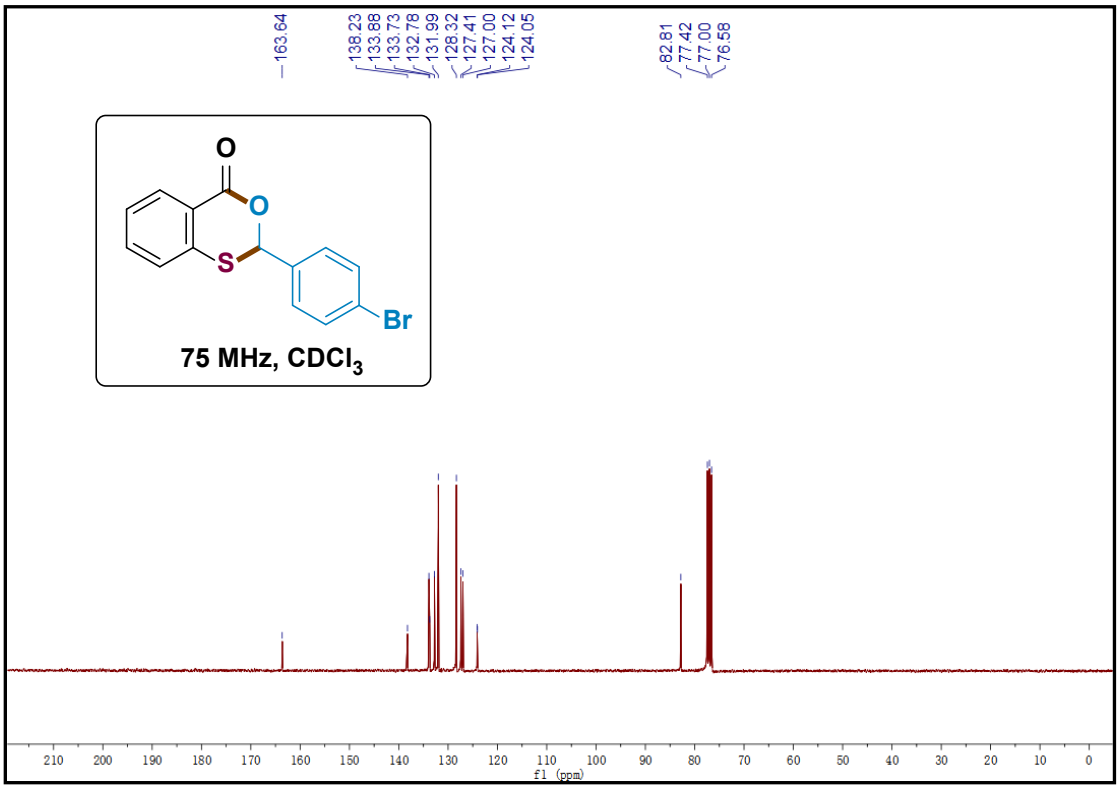
2-(4-chlorophenyl)-4H-benzo[d][1,3]oxathiin-4-one (4g)



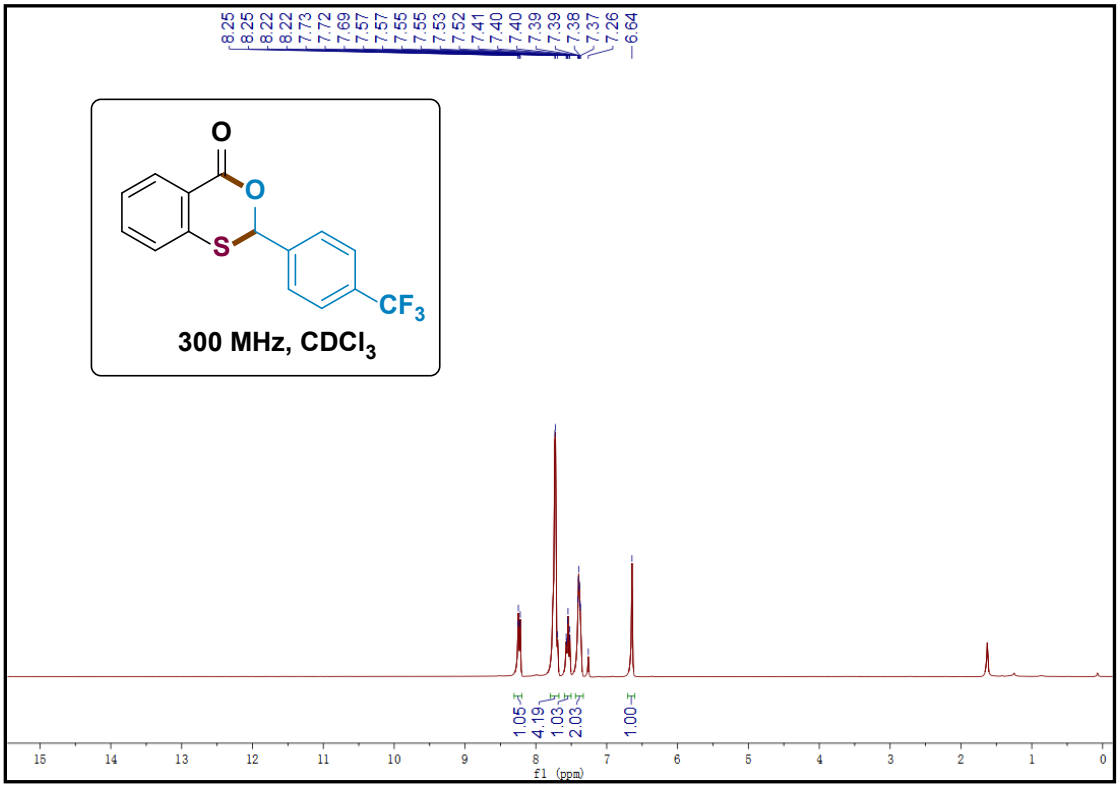


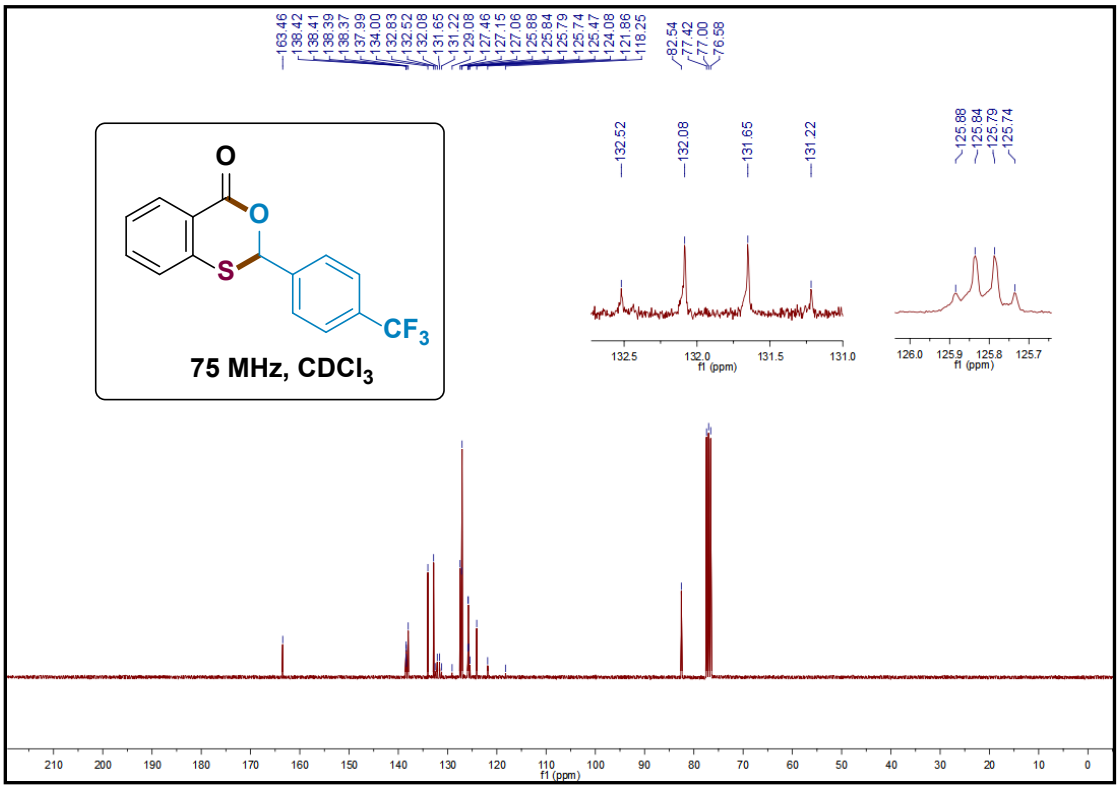
2-(4-bromophenyl)-4H-benzo[d][1,3]oxathiin-4-one (4h)



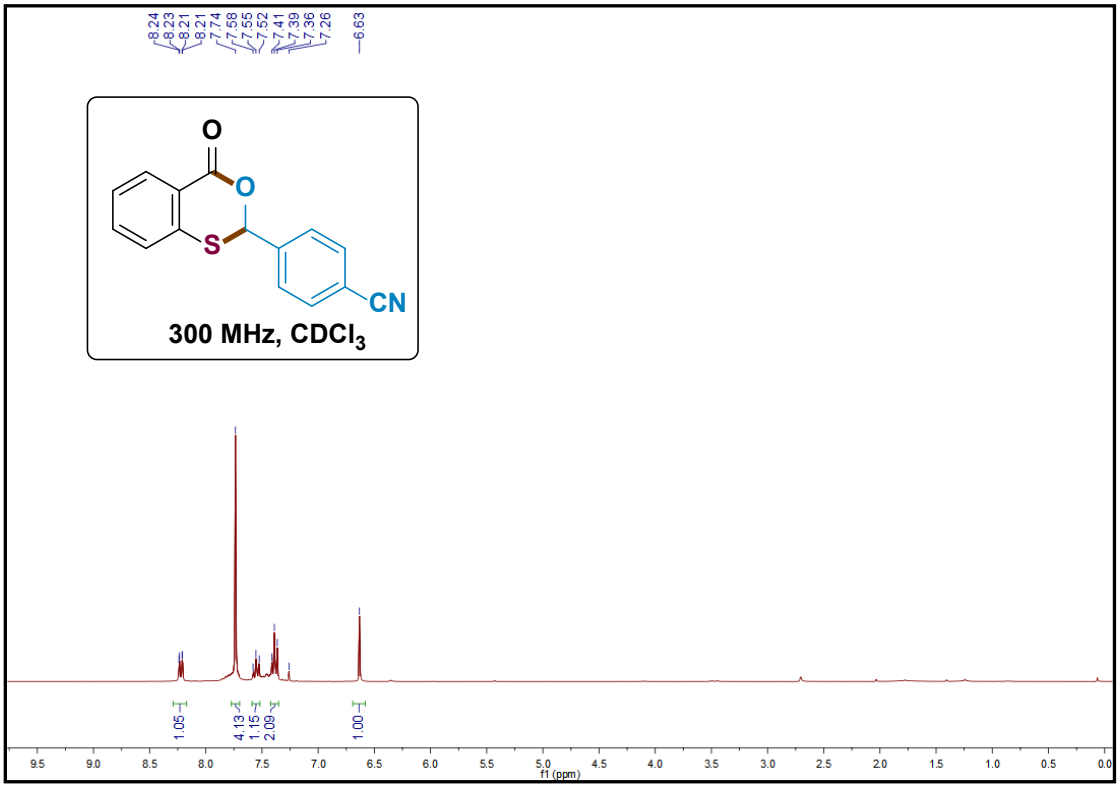


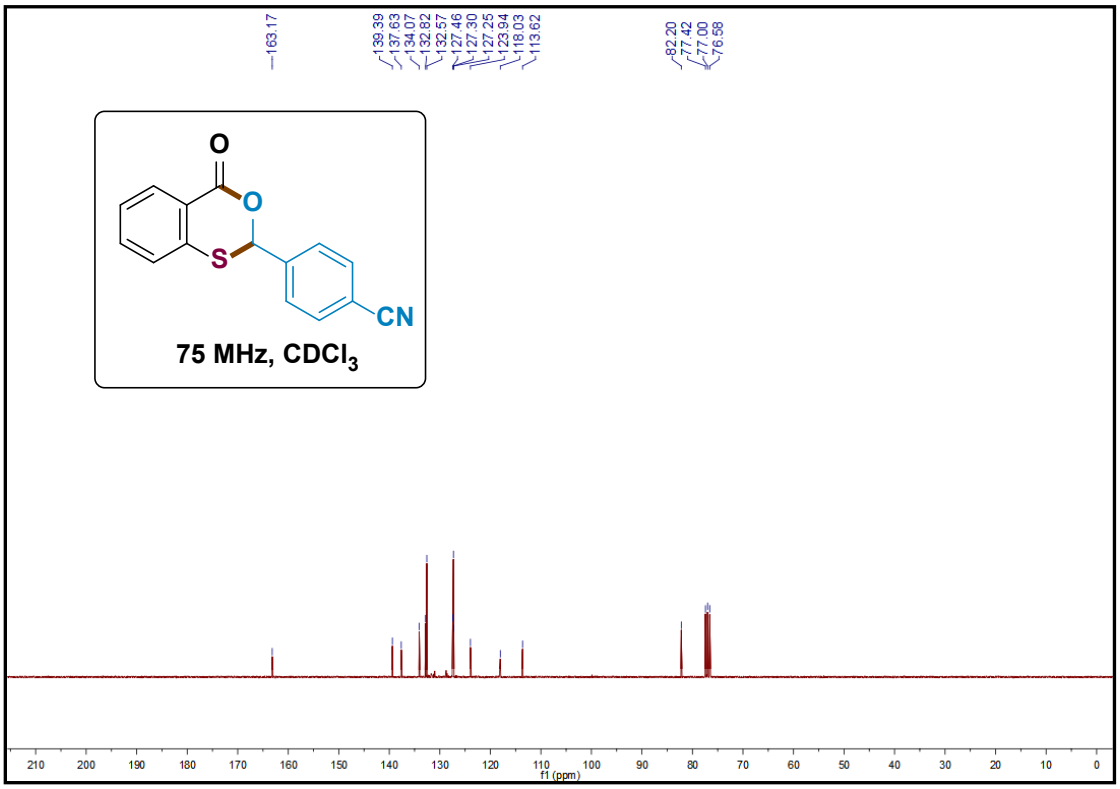
2-(4-(trifluoromethyl)phenyl)-4H-benzo[d][1,3]oxathiin-4-one (4i)



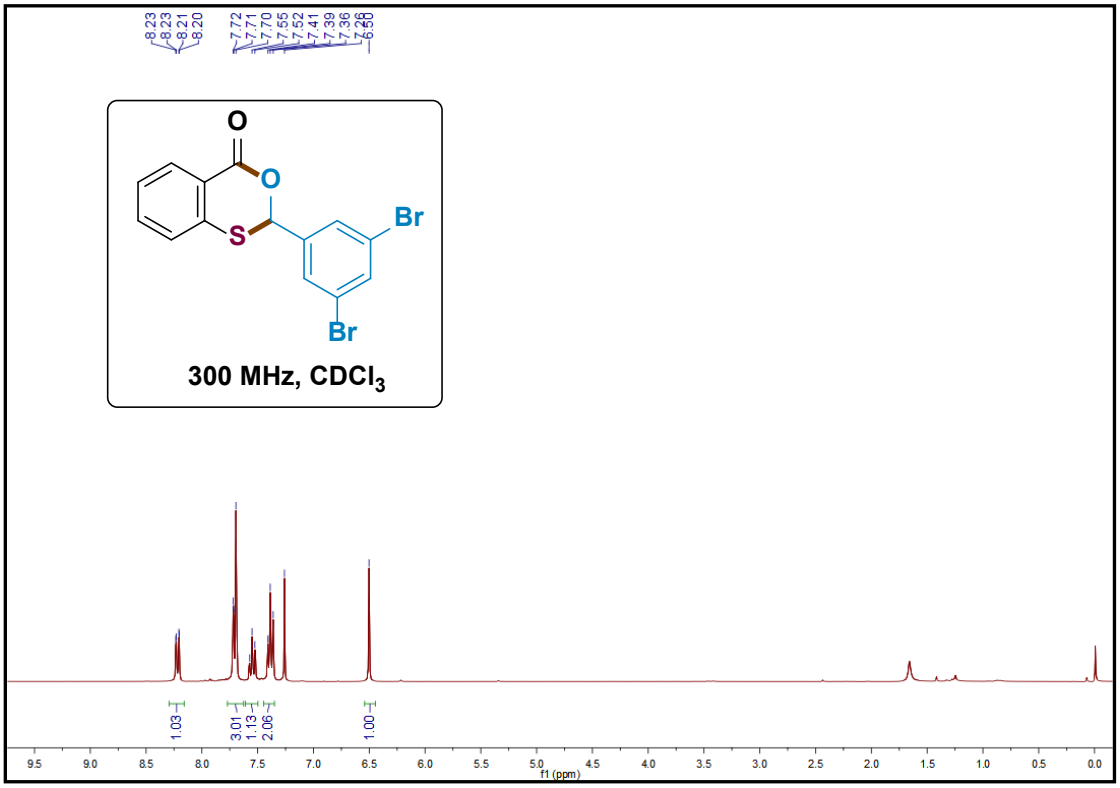


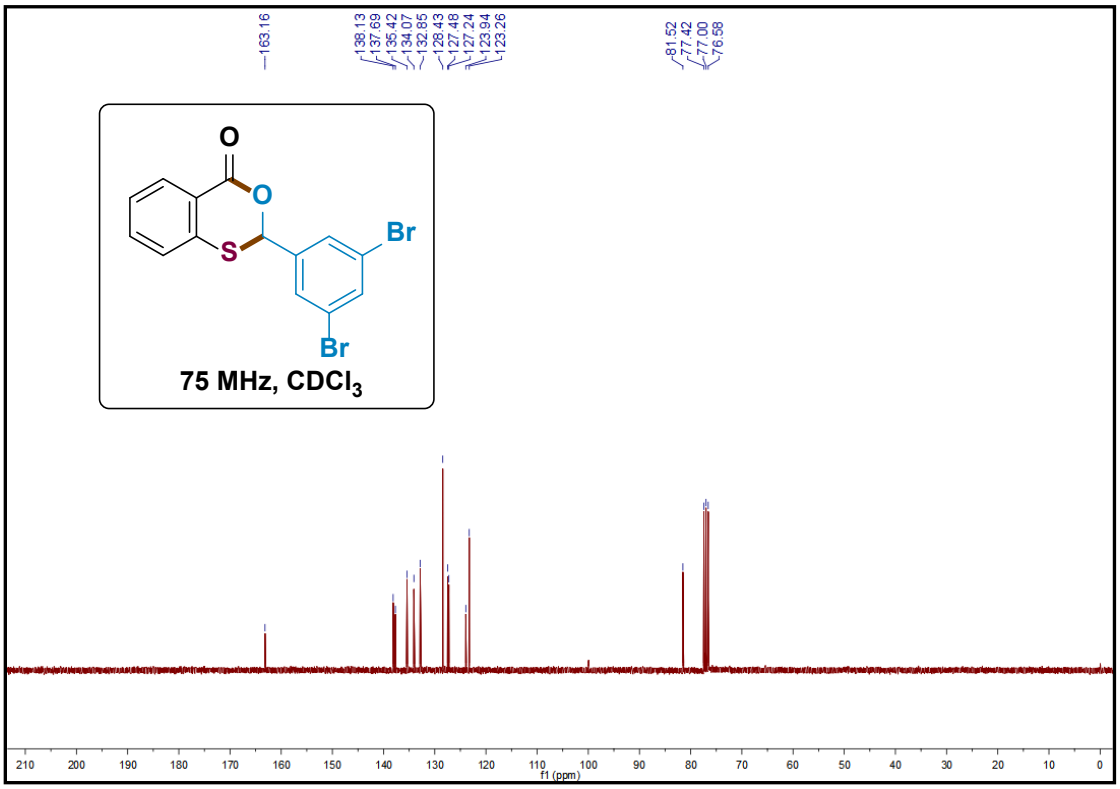
4-(4-oxo-4H-benzo[d][1,3]oxathiin-2-yl)benzonitrile (4j)



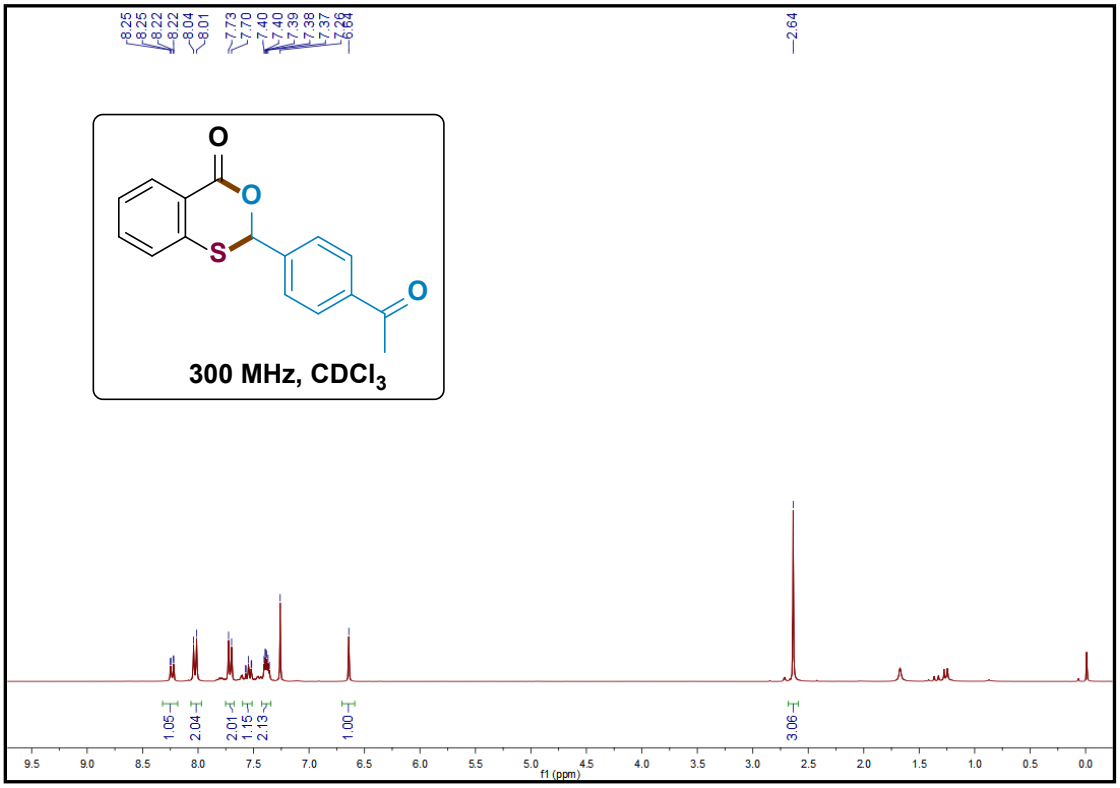


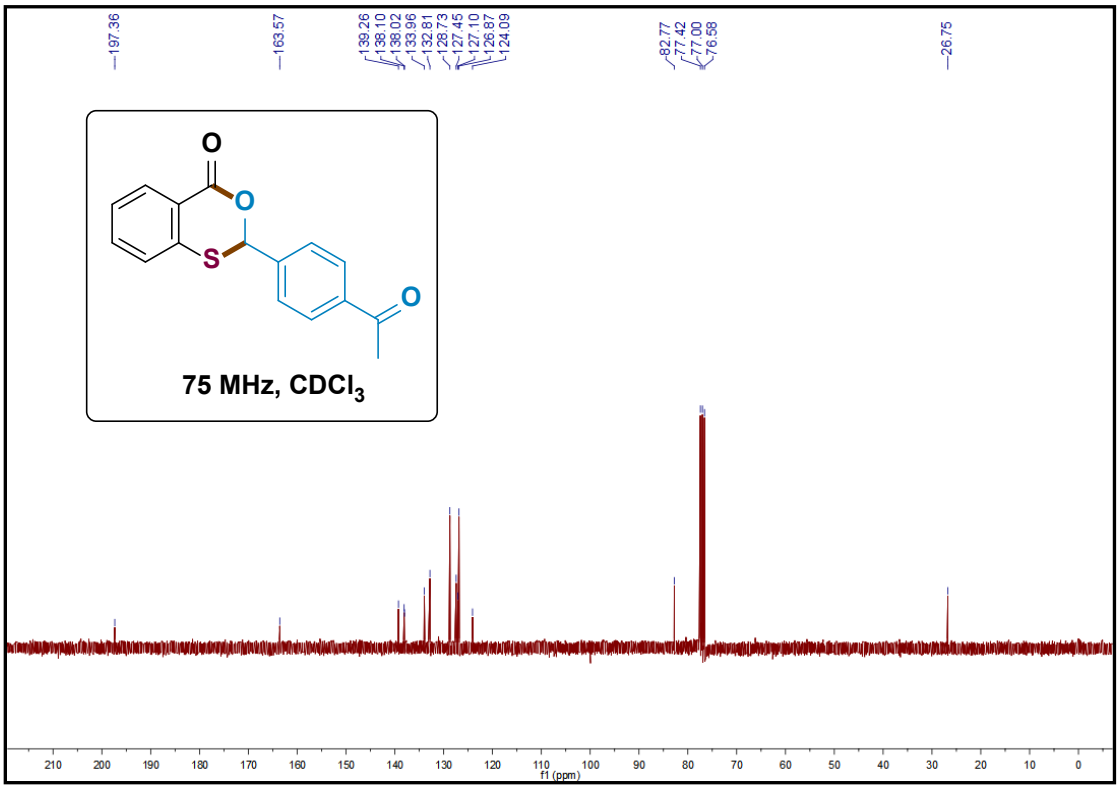
2-(3,5-dibromophenyl)-4H-benzo[d][1,3]oxathiin-4-one (4k)



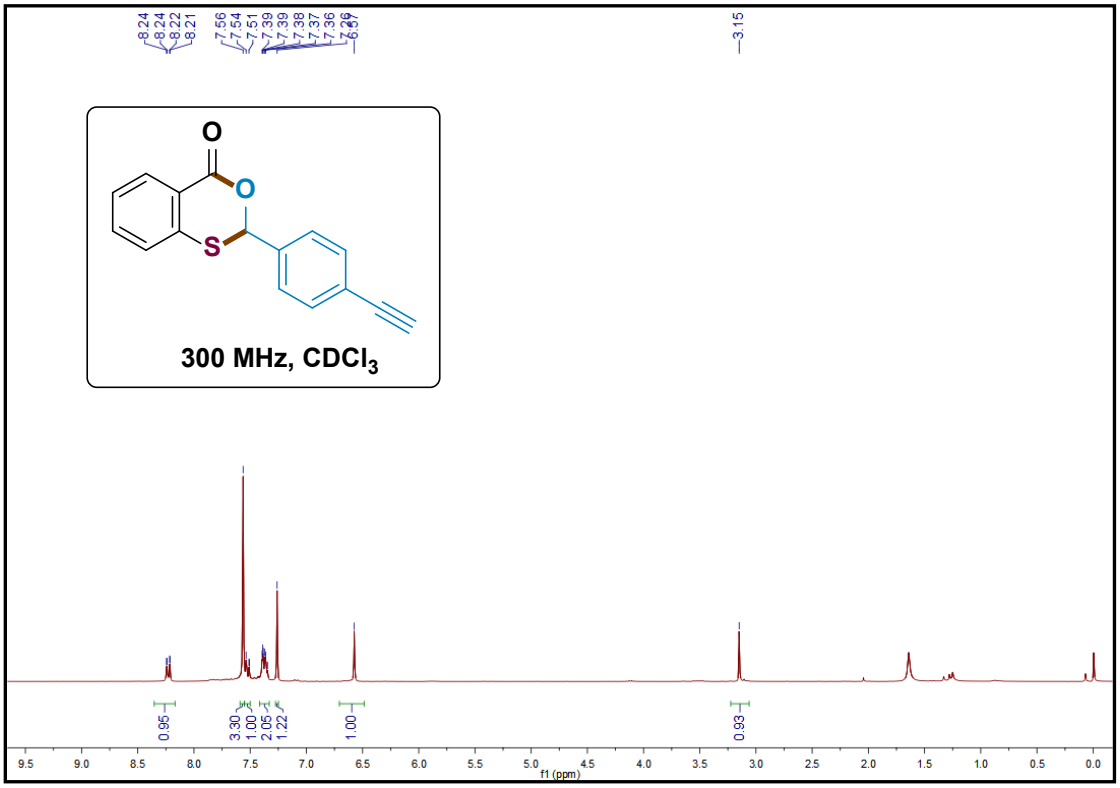


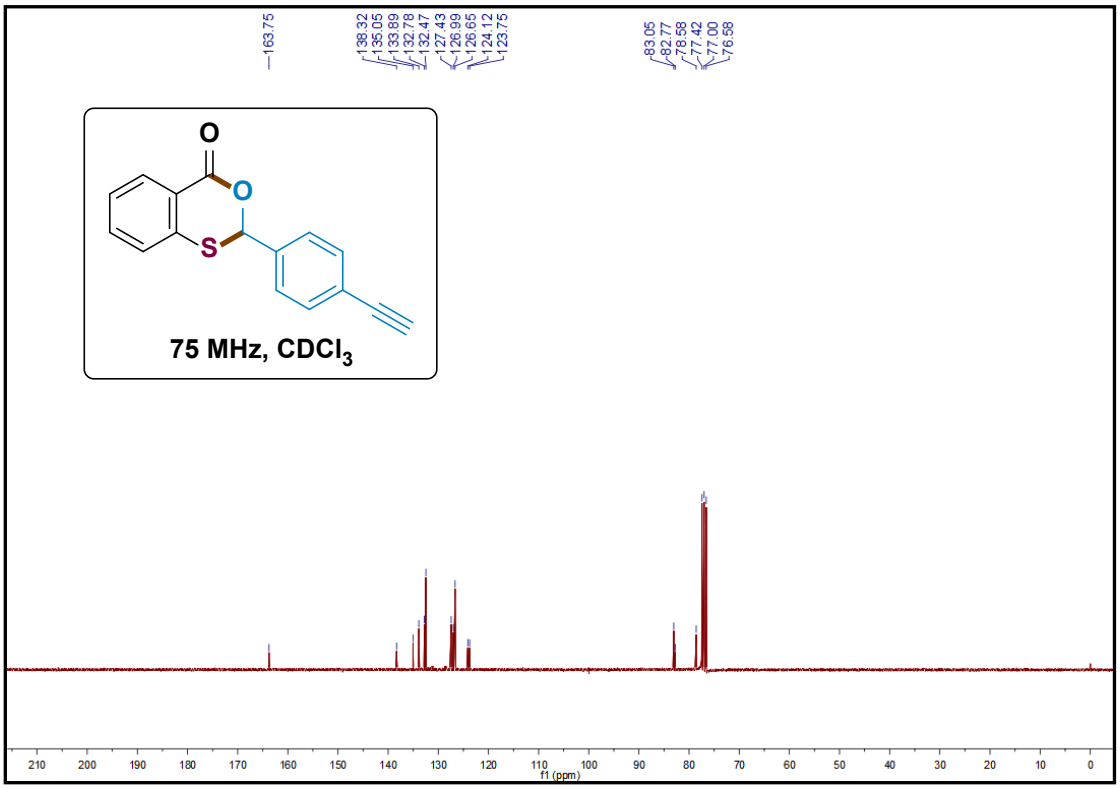
2-(4-acetylphenyl)-4H-benzo[d][1,3]oxathiin-4-one (4l)



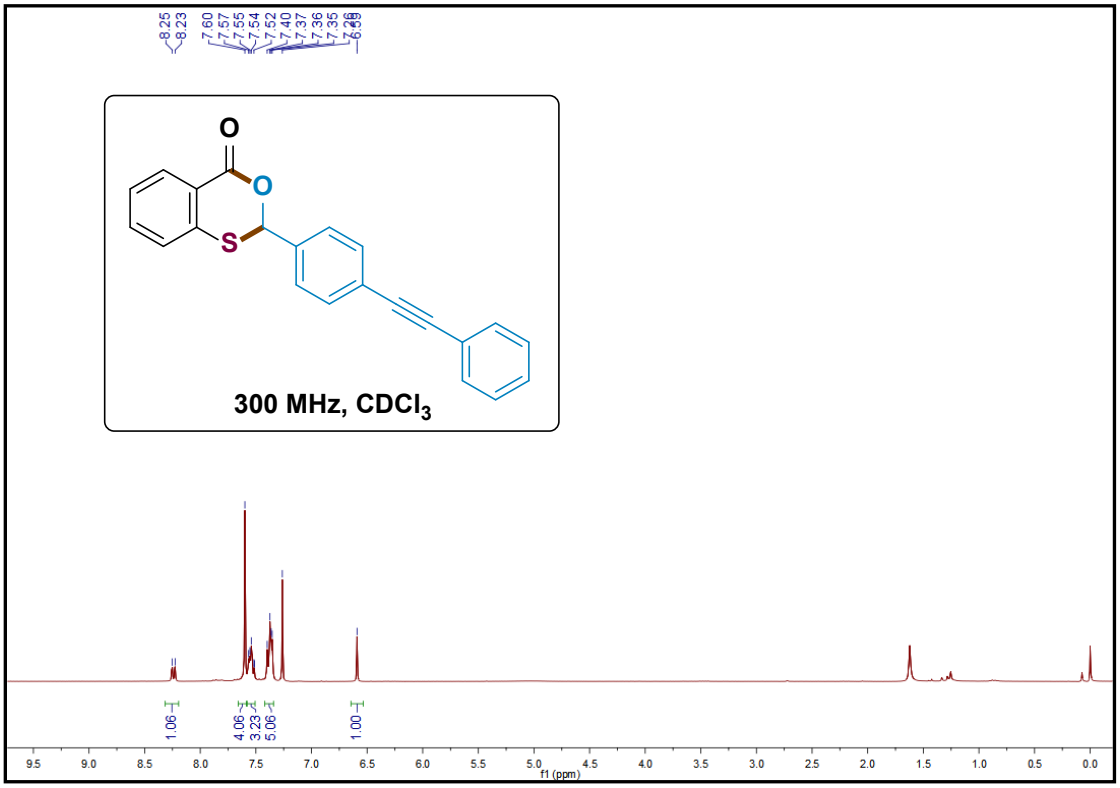


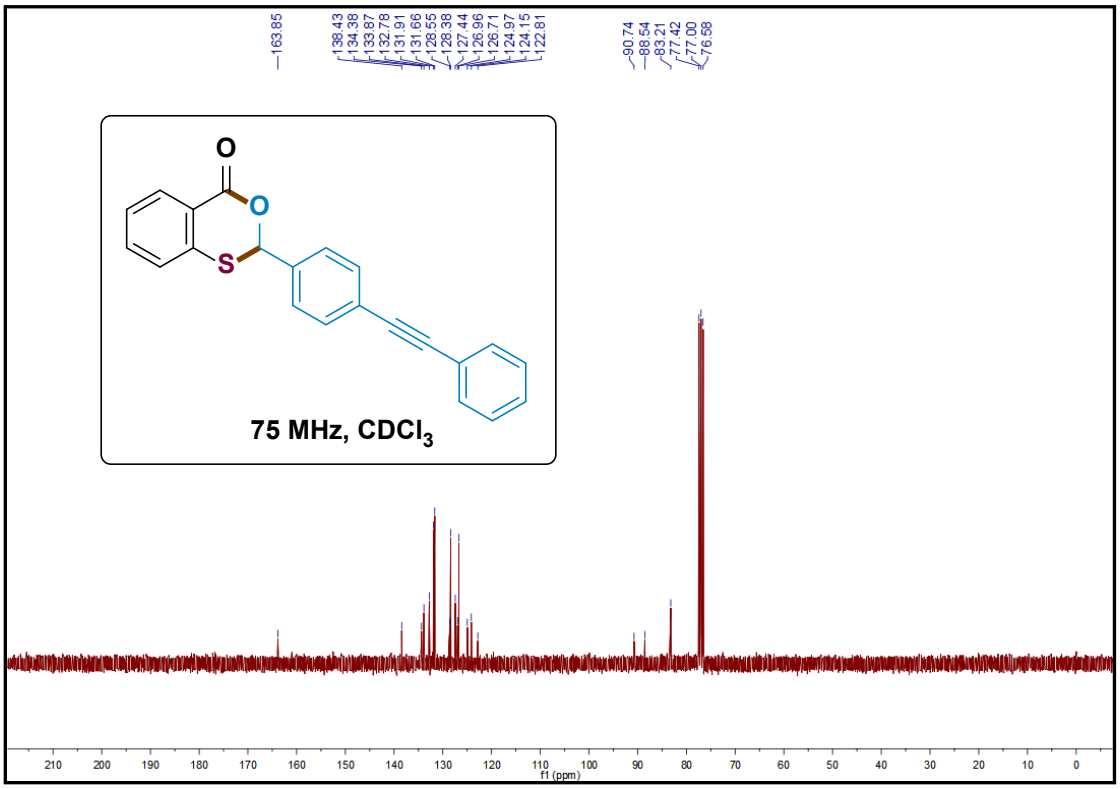
2-(4-ethynylphenyl)-4H-benzo[d][1,3]oxathiin-4-one (4m)



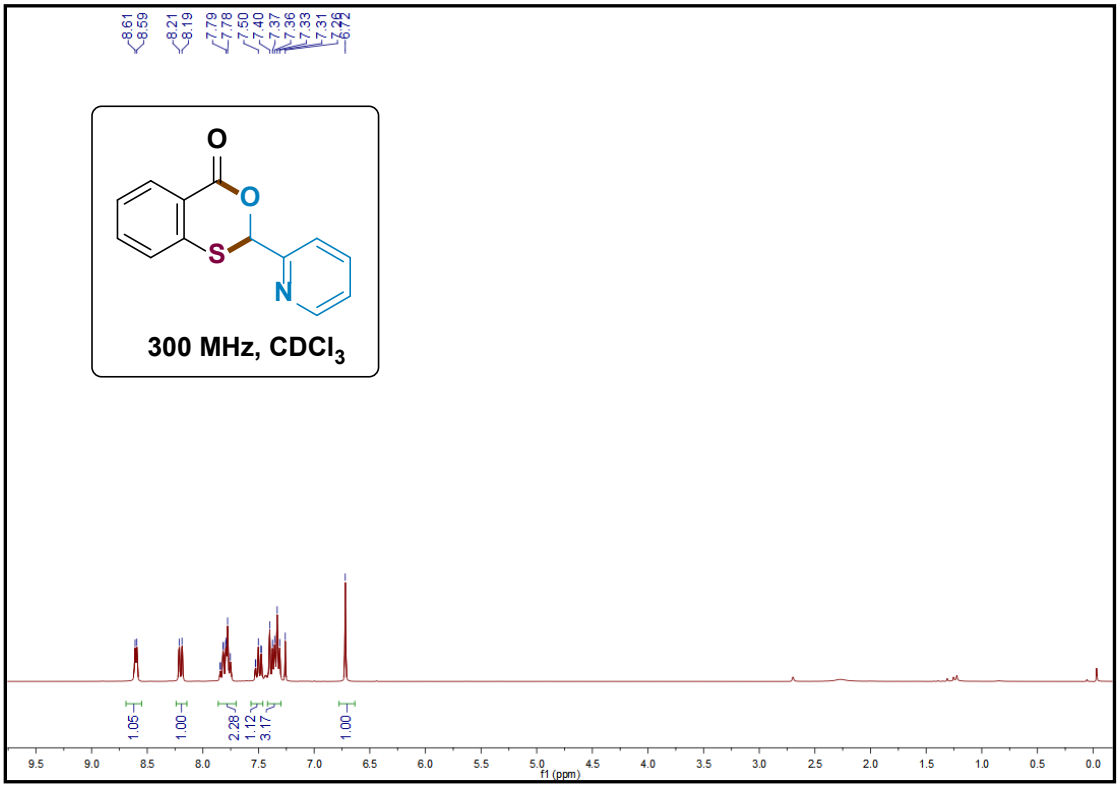


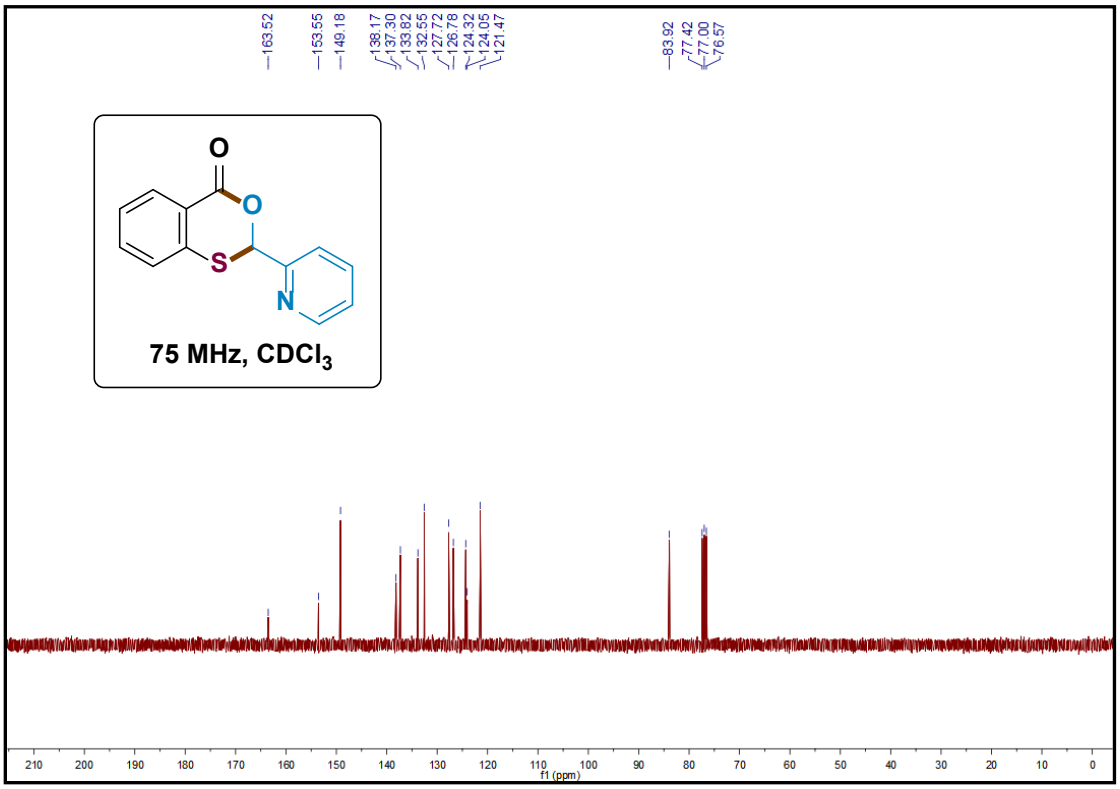
2-(4-(phenylethynyl)phenyl)-4H-benzo[d][1,3]oxathiin-4-one (4n)



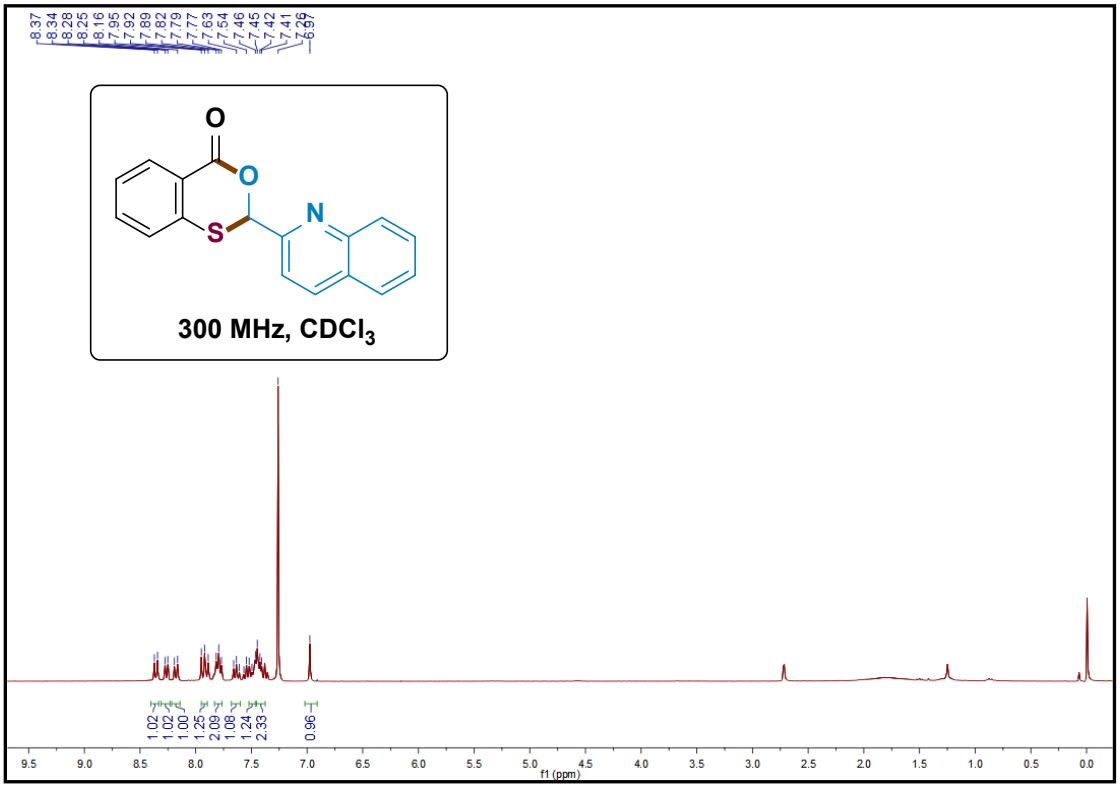


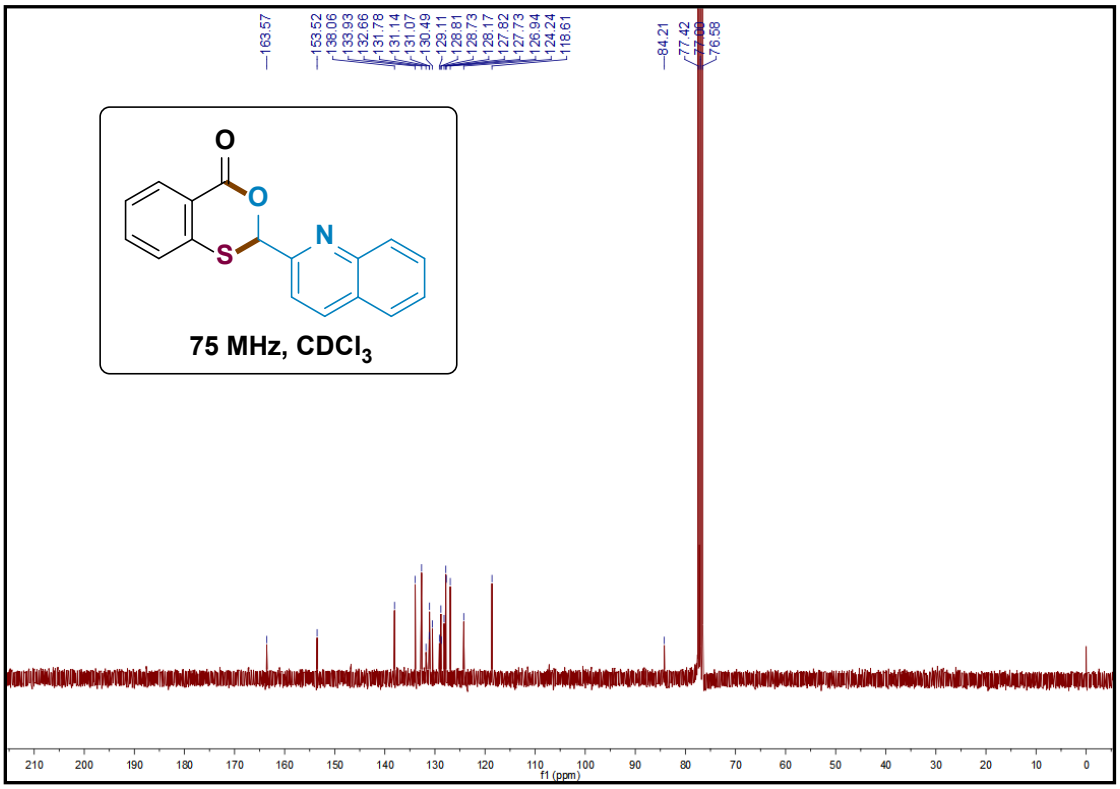
2-(pyridin-2-yl)-4H-benzo[d][1,3]oxathiin-4-one (4o)



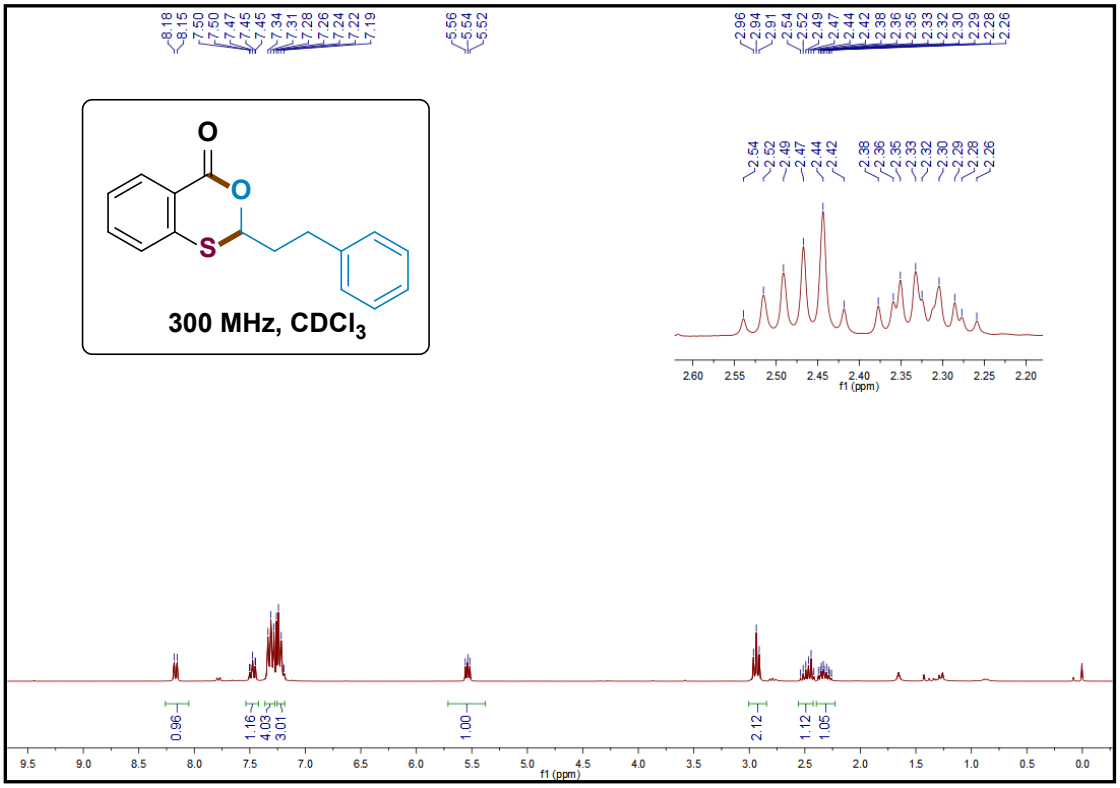


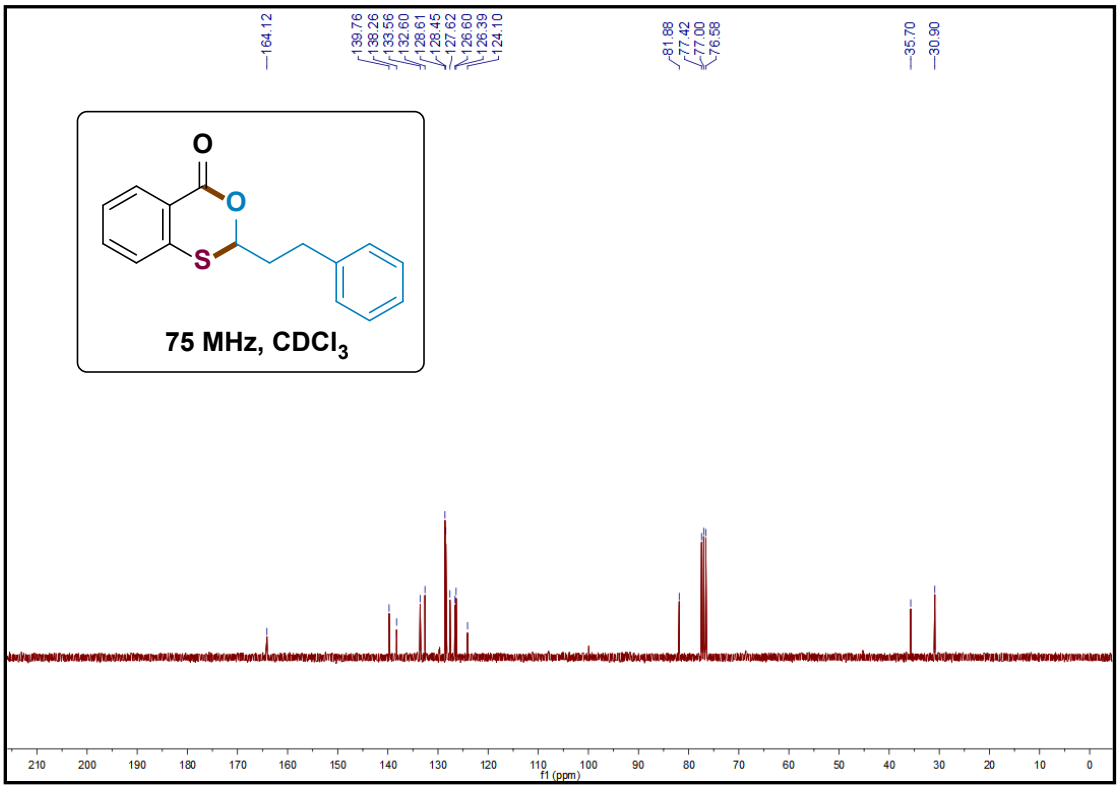
2-(quinolin-2-yl)-4H-benzo[d][1,3]oxathiin-4-one (4p)



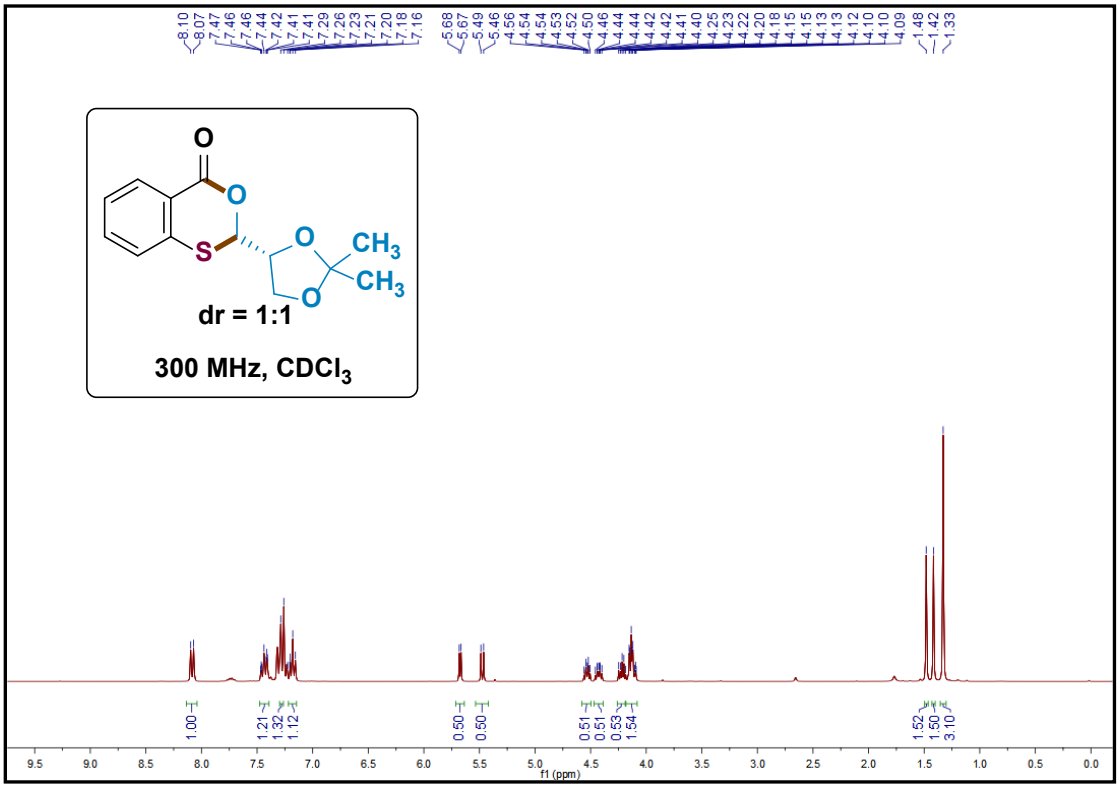


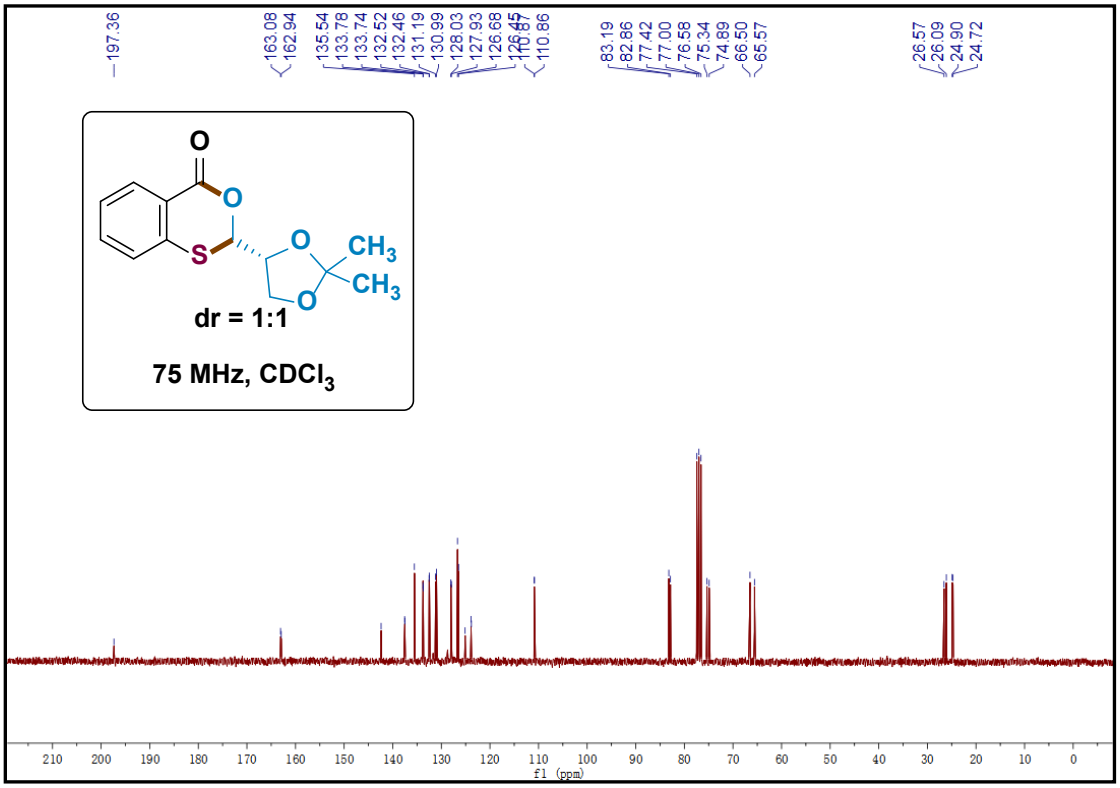
2-phenethyl-4H-benzo[d][1,3]oxathiin-4-one (4q)



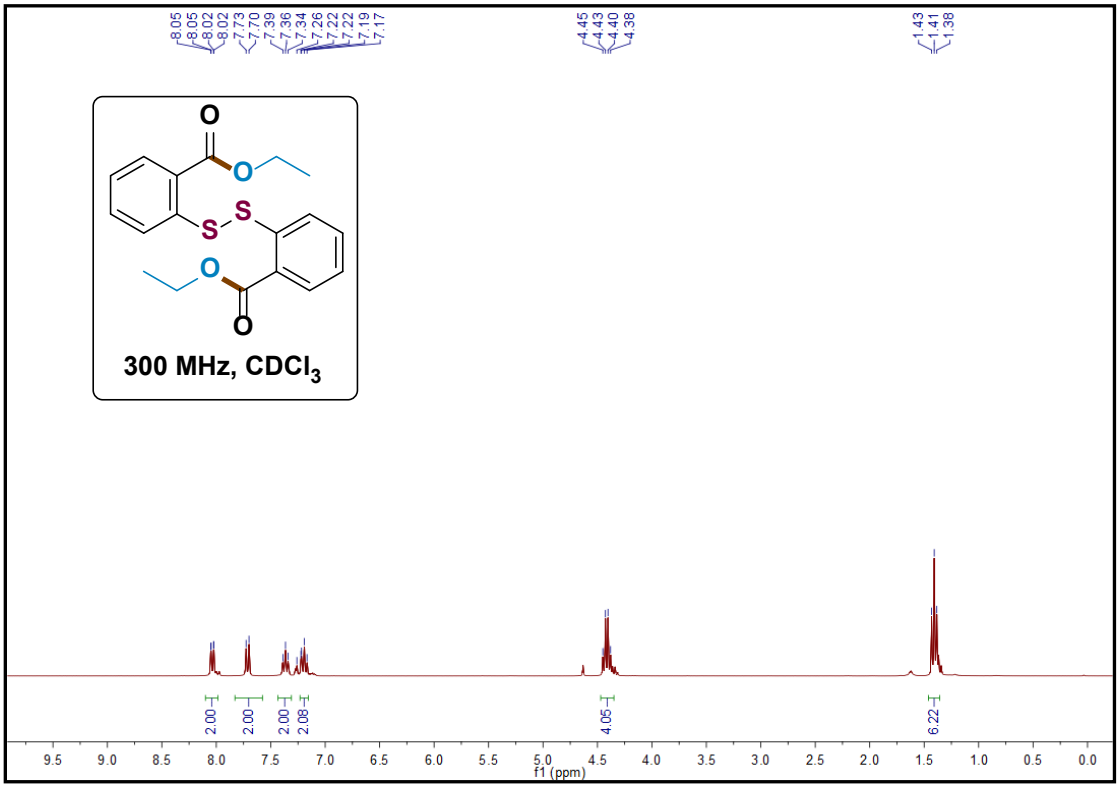


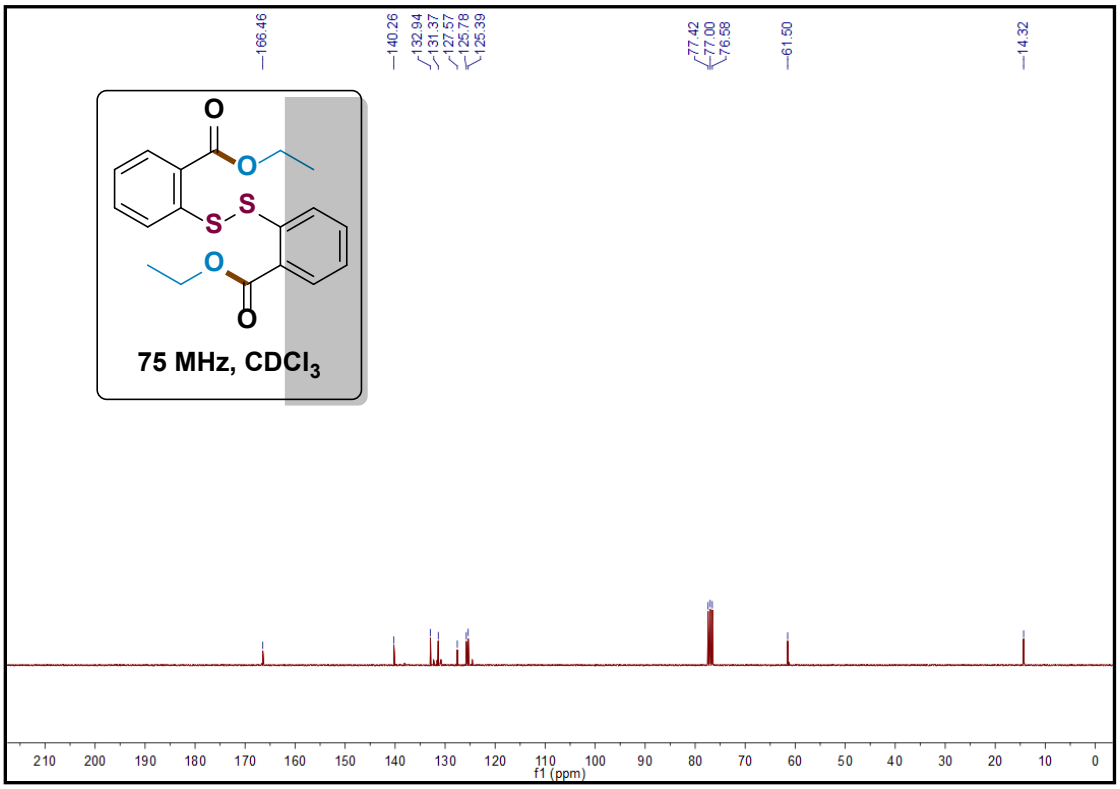
2-(2,2-dimethyl-1,3-dioxolan-4-yl)-4H-benzo[d][1,3]oxathiin-4-one (4r)



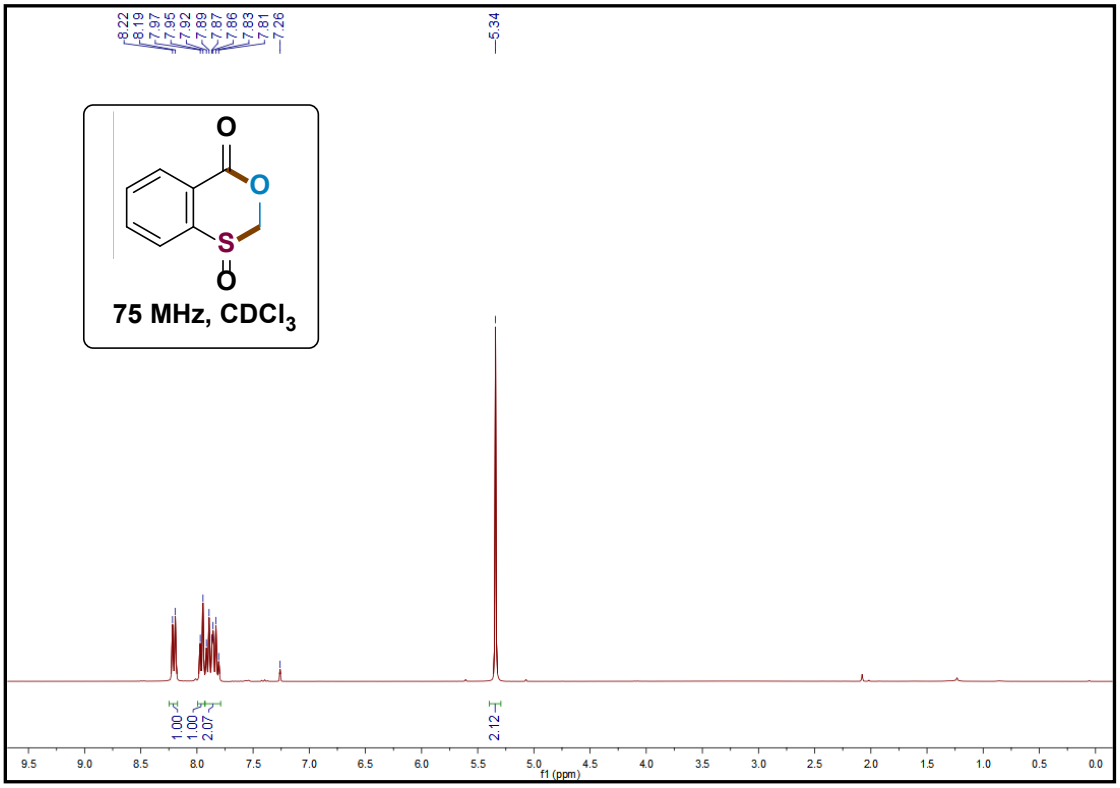


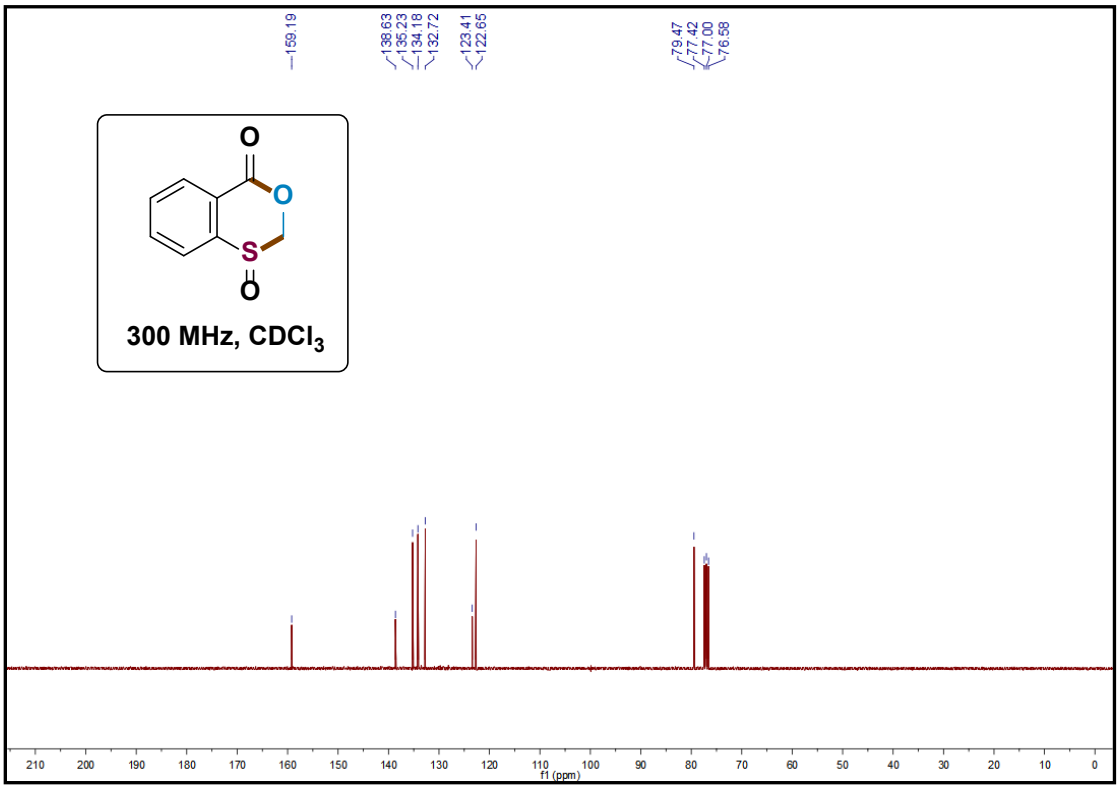
Diethyl 2,2'-disulfanediyldibenzoate (5)



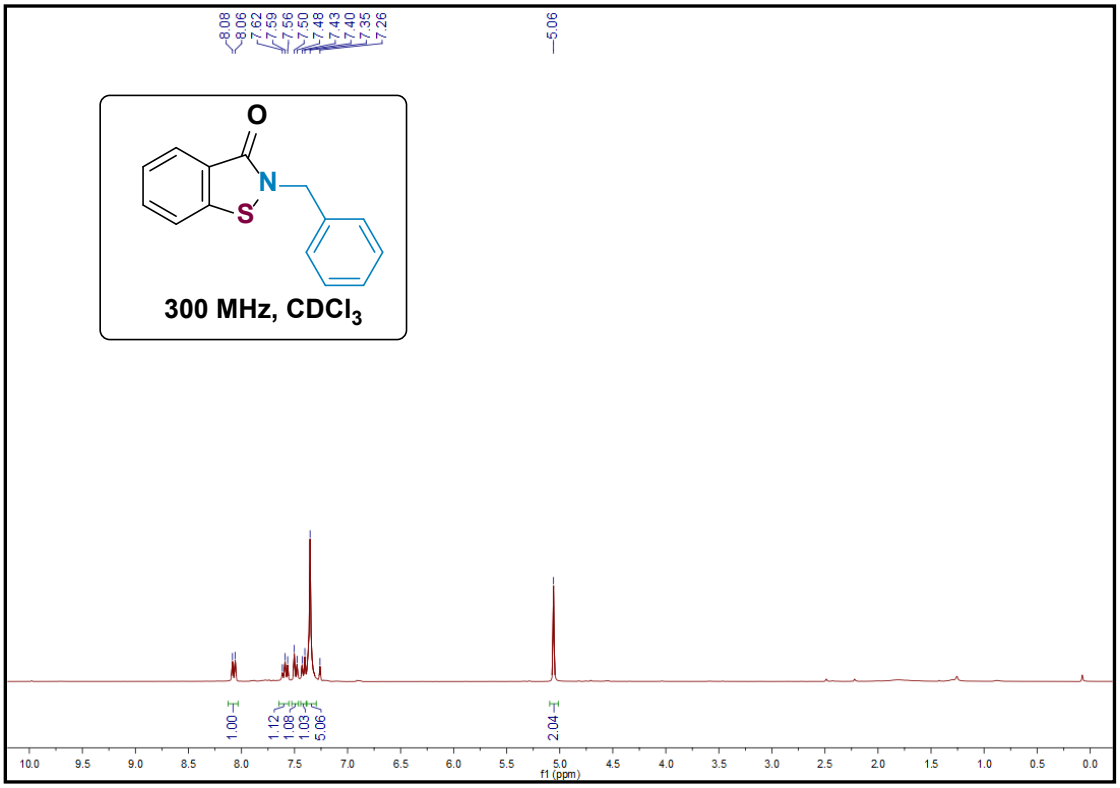


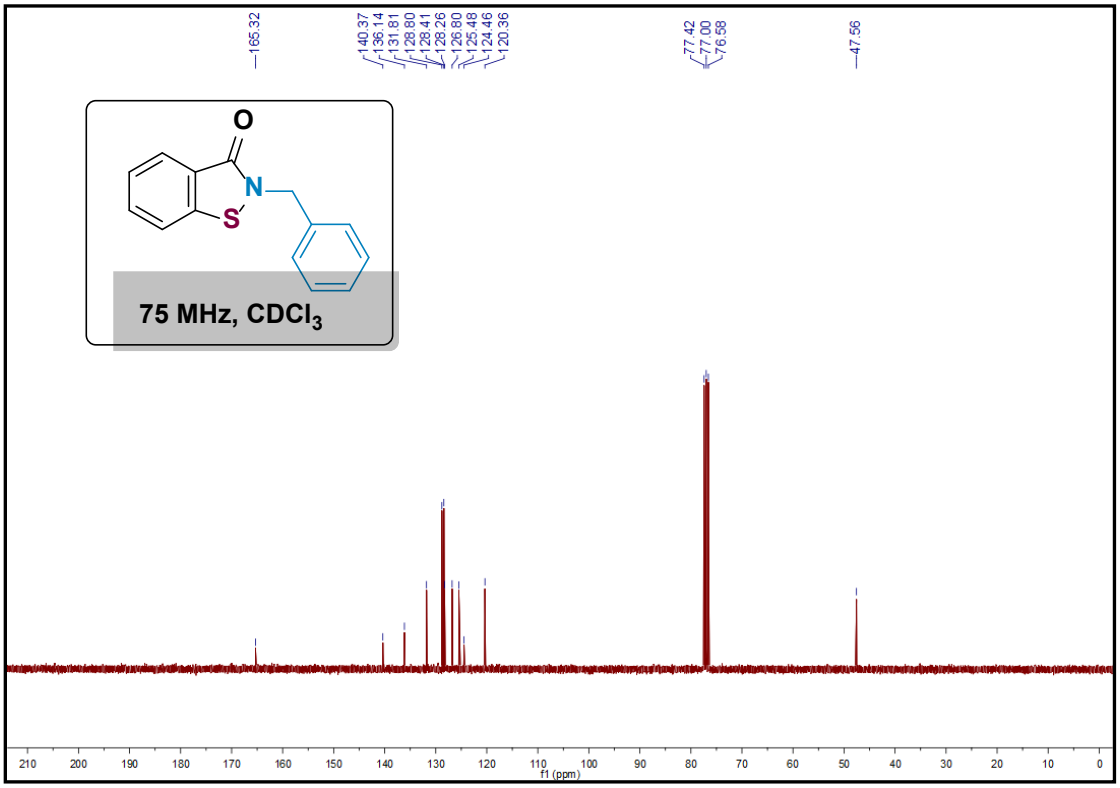
2H,4H-benzo[d][1,3]oxathiin-4-one 1-oxide (6)





2-benzylbenzo[d]isothiazol-3(2H)-one (7)





6H,12H-dibenzo[b,f][1,5]dithiocine-6,12-dione (8)