Supporting Information

Light-assisted Green and efficient Construction of Thiadiazole/Selenadiazole Derivatives

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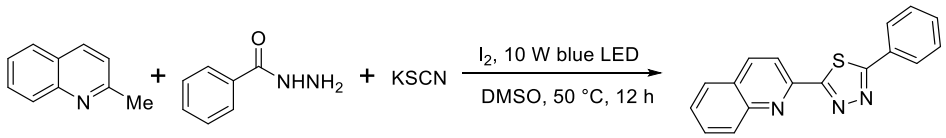
1. General information

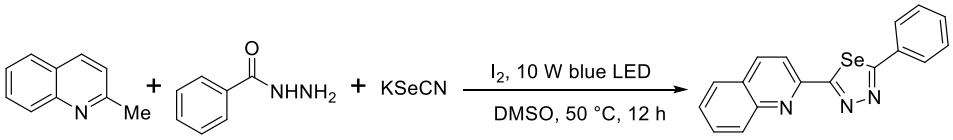
All starting materials and reagents were purchased from commercial sources and used as received unless otherwise noted. ^{1}H, ^{13}C, and ^{19}F NMR are given by 400 MHz, 100 MHz, and 376 MHz spectrometer, respectively. Chemical shift values are given in ppm (parts per million) with tetramethyl silane (TMS) as an internal standard. The peak patterns are reported as follows: s, singlet; d, doublet; t, triplet; q, quartet; quint, quintet; sext, sextet; hept, heptet; m, multiplet; dd, doublet of doublets; dt, doublet of triplets; td, triplet of doublets. The coupling constants (*J*) are recorded in Hertz (Hz). Photochemical experiments have been performed in a parallel photoreactor (designed by WATTCAS: WP-TEC-1020HSL, 10 W, λ= 425 nm). Melting points were measured with a micro melting point apparatus, without correction. Infrared spectra were recorded on a TENSOR 27 FT-IR spectrophotometer and reported in wave numbers (cm-1). High-resolution mass spectra (HRMS) were obtained on a Bruker Daltonics MicroTof-Q II mass spectrometer with an electrospray ion source (ESI). Single crystal X-ray diffraction measurements were carried out on a Rigaku XtaLAB Synergy fourcircle diffractometer under Mo-Kα radiation (λ = 0.71073 Å); Fluorescence was measured with F-4600 fluorescence spectrophotometer. Chemiluminescence imaging of the cells was recorded on Leica DMi8 inverted microscope. Flash column chromatography was operated over silica gel 200-300 mesh. DMSO used for the synthesis of products was analytical reagent grade and used without any pretreatment.

2. Typical procedure 1



The reactants, including 36 mg (1.0 eq, 0.25 mmol) 2-methylquinoline, 51 mg (2.0 eq, 0.5 mmol) benzoylhydrazine, 51 mg (2.0 eq, 0.5 mmol) KSCN, and 63 mg (1.0 eq., 0.25 mmol) iodine monomer, were accurately weighed and transferred to a 25 mL quartz light reaction tube. Next, 2.0 mL of dimethylsulfoxide was added to the reaction tube, which was then placed in a photocatalytic parallel reactor and adjusted to 50 °C using a 10 W blue LED lamp. The reaction mixture was stirred magnetically for 12 h. After completion of the reaction, the resulting solution was poured into a 250 mL partition funnel and extracted three times with saturated sodium chloride solution and dichloromethane. The organic layer was collected and dried with anhydrous sodium sulfate in a 50 mL conical flask. The reaction mixture was then concentrated by reduced-pressure distillation using a rotary evaporator and purified by column chromatography on silica gel (generally PE/EA=8/1-10/1) to obtain the desired product **m1**. Other derivatives were synthesized similarly to **m1**.

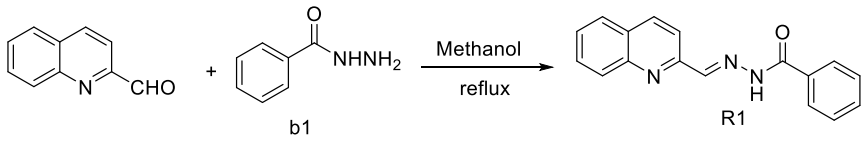
3. Typical procedure 2



A 25 mL quartz light reaction tube was charged with 0.25 mmol (1.0 eq., 36.0 mg) 2-methylquinoline, 0.5 mmol (2.0 eq., 51.0 mg) benzoylhydrazine, 0.5 mmol (2.0 eq., 72.0 mg) KSeCN, and 0.25 mmol (1.0 eq., 63.0 mg) I_2. The mixture was dissolved in 2.0 mL of dimethylsulfoxide and placed in a photocatalytic parallel reactor. The reaction was stirred magnetically at a constant temperature of 50 °C for 12 h using a 10 W blue LED lamp. After completion of the reaction, the reaction stock solution was transferred into a 250 mL partition funnel and subjected to extraction with saturated sodium chloride solution and dichloromethane three times. The organic phase was dried with anhydrous sodium sulfate in a 50 mL conical flask. The dried reaction mixture was concentrated under reduced pressure distillation using a rotary evaporator and purified by silica gel column chromatography (typically PE: EA=8:1-10:1) to obtain the desired product **n1**. Similarly, other selenodiazole derivatives were synthesized.

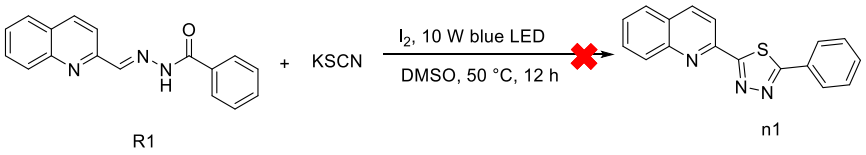
4. Mechanism studies

4.1 Synthesis of R1



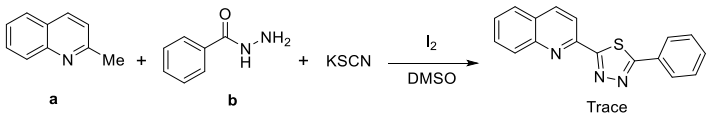
Quinoline-2-carboxaldehyde (0.2 mmol, 1.0 equiv) and **b1** (0.2 mmol, 1.0 equiv) in EtOH (5.0 mL) were added in 50 mL round-bottomed flask under reflux for 3 h. After cooling to room temperature, the resulting precipitate was filtered, washed with methanol, and dried to afford **R1**. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.19 (s, 1H), 8.61 (s, 1H), 8.38 (d, J = 8.7 Hz, 1H), 8.11 (d, J = 8.6 Hz, 1H), 8.02 (d, J = 8.4 Hz, 1H), 7.95 (t, J = 9.0 Hz, 3H), 7.75 (ddd, J = 8.3, 6.8, 1.5 Hz, 1H), 7.59 (t, J = 7.4 Hz, 2H), 7.53 (dd, J = 8.2, 6.4 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.1, 154.4, 148.5, 147.9, 137.3, 133.8, 132.6, 130.6, 129.5, 129.1, 128.6, 128.5, 128.3, 127.9, 118.1.

4.2 Controlled Experiments



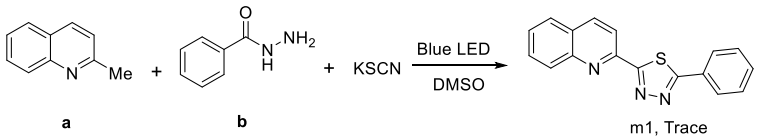
R1 (0.25 mmol, 1.0 equiv), KSCN(0.5 mmol, 2.0 equiv) were added in 25 mL round-bottomed flask, and the reaction mixture was performed under standard conditions. This reaction did not afford desired product **n1**.

4.3 Controlled Experiments (a)



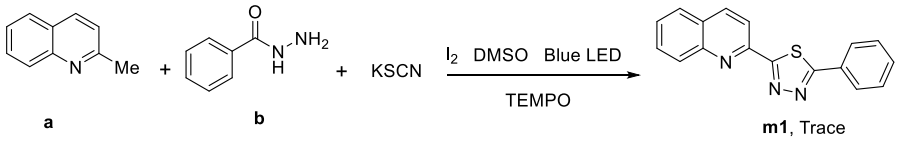
A 25 mL round-bottom flask was prepared, containing 0.25 mmol (1.0 eq., 36.0 mg) of 2-methylquinoline, 0.5 mmol (2.0 eq., 51.0 mg) of benzoylhydrazine, 0.5 mmol (2.0 eq., 51.0 mg) of KSCN, and 0.25 mmol (1.0 eq., 63.0 mg) of I_2. 2.0 mL of dimethylsulfoxide (DMSO) was added to this flask. Then, the reaction mixture was covered with tinfoil to protect it from light and transferred to a 50 °C sand bath. Continuous magnetic stirring was applied for a duration of 12 h.

4.4 Controlled Experiments (b)



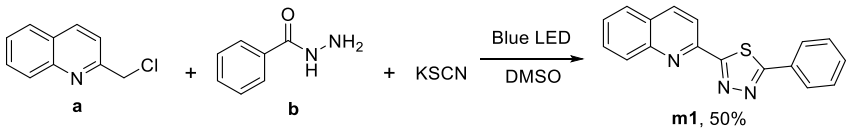
A 25 mL quartz photoreaction tube was utilized for the experiment. It contained 0.25 mmol (1.0 eq., 36.0 mg) of 2-methylquinoline, 0.5 mmol (2.0 eq., 51.0 mg) of benzoylhydrazine, and 0.5 mmol (2.0 eq., 51.0 mg) of KSCN. To this tube, 2.0 mL of dimethyl sulfoxide (DMSO) was added. The photoreaction tube was then placed inside a photocatalytic parallel reactor and adjusted to 50 °C. The reaction mixture was subjected to magnetic stirring for 12 h with a 10 W blue LED lamp.

4.5 Controlled Experiments (c)



A 25 mL quartz light reaction tube was prepared, containing 0.25 mmol (1.0 eq., 36.0 mg) of 2-methylquinoline, 0.5 mmol (2.0 eq., 51.0 mg) of benzoylhydrazine, 0.5 mmol (2.0 eq., 51.0 mg) of KSCN, and 0.25 mmol (1.0 eq., 63.0 mg) of iodine monomer. To this tube, 0.5 mmol (2.0 eq., 79.0 mg) of TEMPO and 2.0 mL of DMSO were added. The light reaction tube was then placed inside a photocatalytic parallel reactor and adjusted to 50 °C. The reaction mixture was subjected to magnetic stirring at room temperature for a duration of 12 h using a 10 W blue LED lamp.

4.6 Controlled Experiments (d)



A 25 mL quartz photoreaction tube was utilized for the experiment. It contained 0.25 mmol (1.0 eq., 45.0 mg) of 2-(chloromethyl)quinoline, 0.5 mmol (2.0 eq., 51.0 mg) of benzoylhydrazine, and 0.5 mmol (2.0 eq., 51.0 mg) of KSCN. To this tube, 2.0 mL of dimethyl sulfoxide (DMSO) was added. The photoreaction tube was then placed inside a photocatalytic parallel reactor and adjusted to 50 °C. The reaction mixture was subjected to magnetic stirring at 50 °C for a duration of 12 h with a 10 W blue LED lamp.

5. Detecting the residual concentration of cyanide in the solution

To detect the residual concentration of cyanide in the solution after the reaction, a commercial test reagent (LOHAND BIOLOGICAL) was employed. The reaction solution was extracted with dichloromethane and water, and the aqueous phase was tested according to the method shown in the kit. At the same time, 0.5 mmol of KSCN was weighed as the control group, and the CN^- concentration was determined by standard colorimetric card. By comparison with the standard colorimetric card, the color of the solution suggested that there was almost no cyanide in the system after the reaction (Figure **S1**).

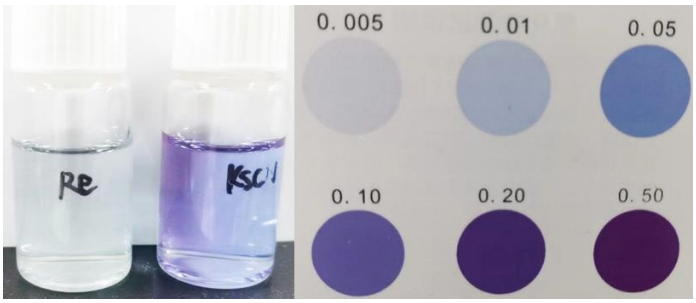


Figure S1. Detecting the residual concentration of cyanide in the solution and the comparison with the standard colorimetric card.

6. Photophysical properties

Fluorescence was measured with F-4600 fluorescence spectrophotometer under the optimal excitation wavelength at room temperature.

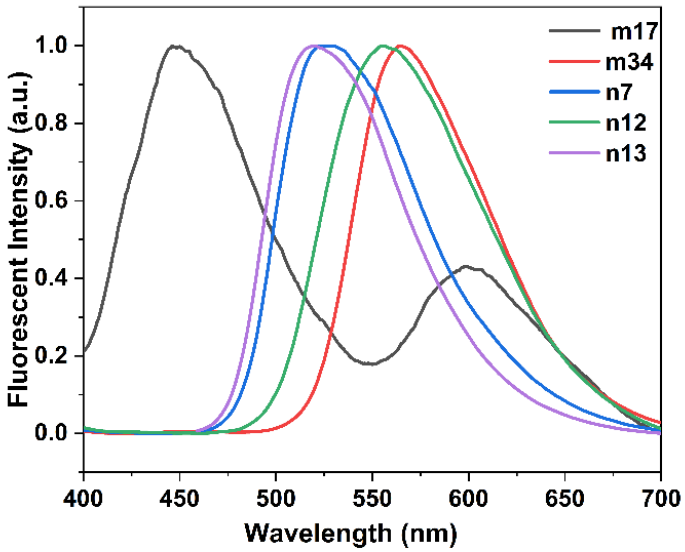


Figure S2. Emission spectra of partial compounds.

The UV absorption spectra of solid substances were measured at room temperature using a UV-3600 UV absorption spectrometer.

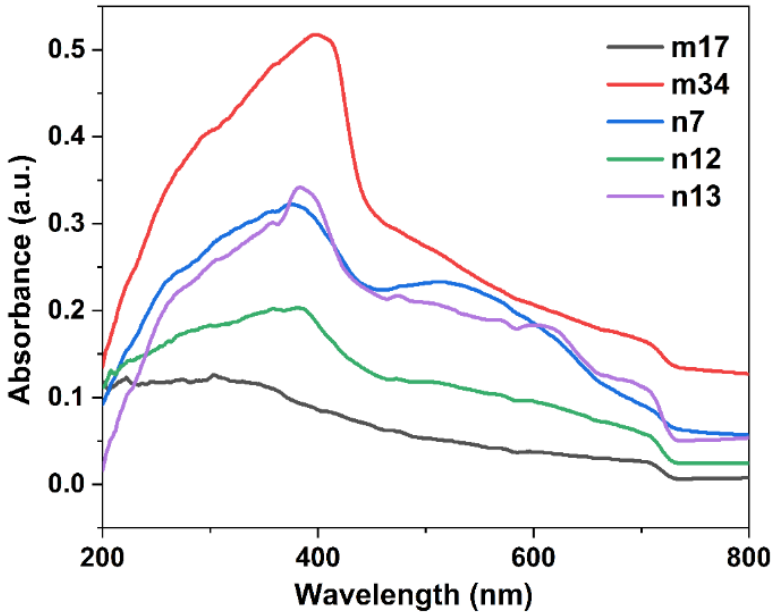


Figure S3. UV absorption of some compounds.

The solid-state fluorescence lifetime of substances was determined at room temperature using the FLSP920 transient fluorescence spectrometer.

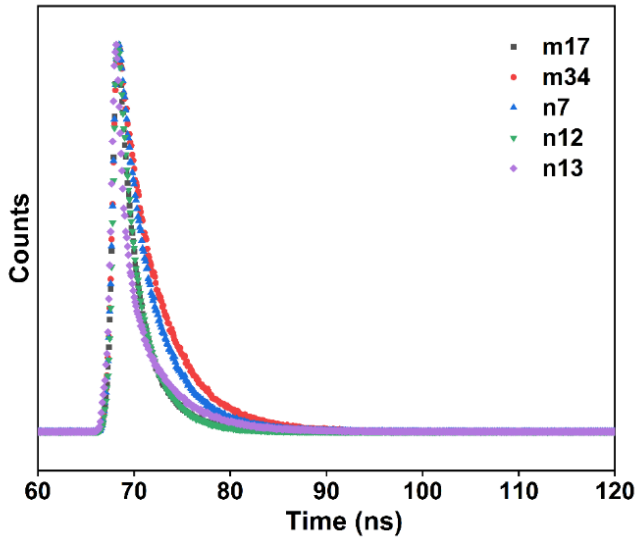


Figure S4. Solid-state steady-state fluorescence test of some compounds

Table S1. Solid-state steady-state fluorescence test of some compounds

Compounds	τ_1 (ns)	B_1/%	τ_2 (ns)	B_2/%	τ_{AVE} (ns)
m17	1.8792	72.28	4.4896	27.72	3.127
m34	4.1172	100	-	-	4.117
n7	2.5039	30.13	3.923	69.87	3.617
n12	2.3064	82.72	4.819	17.28	3.069
n13	0.8149	18.65	4.1829	81.35	4.038

7. Comparisons of this work and previously reported synthesis

We compared the reaction conditions and reagents of this reaction with other reported methods for the construction of 1,3,4-thiadiazole and 1,3,4-selenothiazoles. According to the existing methods, encounter challenges have been found related to the choice of sulfur source, since some of the methods may include unpleasant odors or high toxicity. As shown in Table R1, compared with some related reports for the synthesis of 1,3,4-thiadiazole derivatives, our reaction was taken place without the use of base but under photocatalytic synthesis in low temperature and resulted in relatively high yields, which is clean, efficient, green and as a consequence in line with the requirements of green chemistry in modern organic synthesis.

Table S2. Comparision the reaction conditions and reagents for synthesis of 1,3,4-thiadiazole derivatives.[a]

Entry	Reactants	Cat.	Sovlents	Time (h)	Temp (ºC)	Yield (%)
1	benzoyl hydrazine + CS_2	KOH/H_2SO_4	Ethanol	substep, long	0-5	60-80
2	thiocarbonyl pyridine formyl hydrazide (need pre-synthesis)	$Zn(NO_3)_2·4H_2O$	Ethanol	3	60	/
3	nitro-paraffin + ureas aryl-compound	PPA	/	2.5	120	38-75
4	thioacylhydrazine + DMA derivatives	$TiCl_4$	/	1.5	110	70-80
5	Isothiocyanates + hydrazones	DDQ，electrocatalysis (10 mA)	CH_3CN/H_2O	2.7	35	40-60
6	Benzene sulfonyl hydrazone + KSCN	NCS $BF_3·OEt_2$	tertiary butanol	0.5-4	85	45-80
7	benzaldehyde + p-toluene sulfonyl hydrazine + KSCN	I_2	DMSO	12	100	60-80
This work	2-methylquinoline + benzoylhydrazine + KSCN	/	DMSO	12	50	70

8. Cell cytotoxicity and imaging

HepG2 cells in the normal growth state were subjected to digestion using 0.25% trypsin and suspended in individual cell suspensions using DMEM (Dulbecco's modified Eagle's medium) containing 10% fetal bovine serum and 1% penicillin-streptomycin. These cell suspensions were then inoculated into 96-well cell culture plates, with 103 - 104 cells per well. The plates were subsequently placed in an incubator and incubated until the cells adhered to the bottom of the wells. To assess the cytotoxicity of **m34**, it was diluted with the medium to obtain different concentrations ranging from 0, 5, 10, 15, 20, 25, 30, 35, to 40 μM. The medium in the 96-well plate was aspirated, and the corresponding concentration of the m33 solution was added to each well. For each concentration, six replicate wells were prepared, and blank control wells were also included. The plate was incubated for 10 minutes to allow for crystal dissolution. Subsequently, the OD (optical density) value of each well was measured using an enzyme marker at a wavelength of 380 nm. The obtained results were recorded, and the cell survival rate was calculated using the following formula: Cell survival rate = (OD value of the drug addition group / OD value of the control group) × 100%

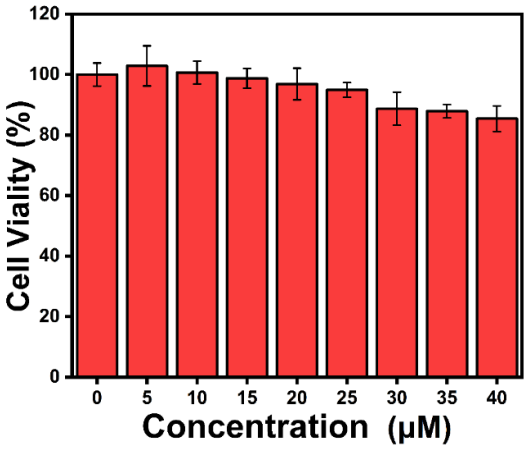


Figure S5. MTT assay of compound **m34** in HepG2 cells.

The compound **m34** was initially fully dissolved in a DMSO solution to prepare a master mix with a concentration of 1.0×10^{-3} mol/L. Subsequently, 10 μL of the prepared master mix was added to a culture dish, resulting in a final concentration of **m34** of 1.0×10^{-5} mol/L. The dish was then co-incubated with HepG2 cells in a CO_2 incubator for a duration of 30 minutes. After co-incubation, the cells were subjected to three washes using PBS-buffered solvent. Finally, focused fluorescence microscopy was employed to observe the cells. Fluorescence field, bright field, and superimposed field images were acquired at an excitation wavelength of 380 nm.

9. X-ray Crystallographic Data

The single crystal for compound **m2** and **m3** were prepared from a mixture solvent of dichloromethane and Petroleum ether (v/v = 1:1). The data were collected on a Bruker Smart APEXIICCD instrument using Mo-Kα radiation (λ = 0.71073 Å) at 296 K. The crystal structures were solved and refined using the SHELXTL software package. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were added to the riding model and refined with isotropic thermal parameters. The data can be obtained free from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_ request/cif. CCDC numbers: 1991748 (for **m2**) and 2268163 (for **m3**). The thermal ellipsoid plots of crystal structures were recorded in Figure **S6-7**. Further details of structural analyses of **m2** and **m3** were recorded in Table **S2**.

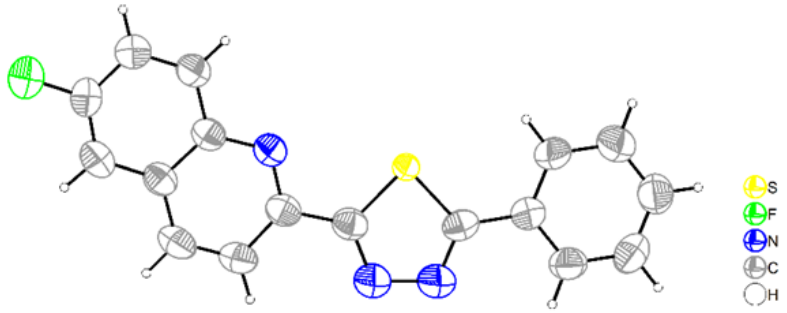


Figure S6. ORTEP views and atomic numbering of compound **m2** with thermal ellipsoids at 50% probability level.

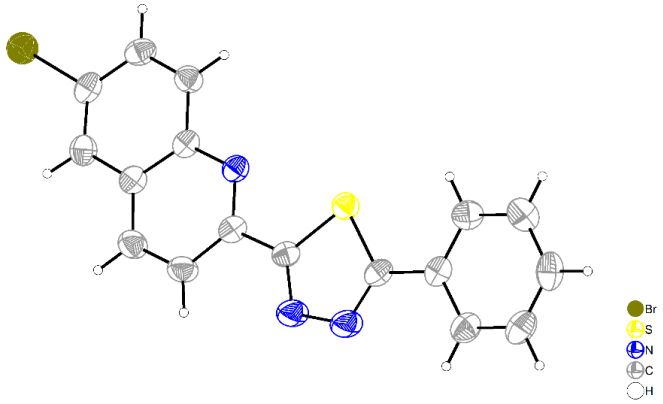
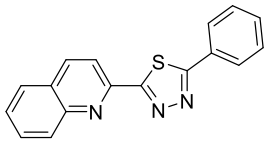


Figure S7. ORTEP views and atomic numbering of compound **m3** with thermal ellipsoids at 50% probability level.

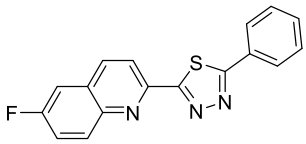
Table S3. X-ray data of **m2**

compound	**m2**	**m3**
formula	$C_{17}H_{10}FN_3S$	$C_{17}H_{10}BrN_3S$
formula weight	307.34	404.06
temperature (K)	296.15	220.00
crystal system	monoclinic	monoclinic
space group	*P*121/*n*1	*C*12/c*1*
a, Å	9.140(2)	27.47(2)
b, Å	15.767(4)	3.862(3)
c, Å	9.982(2)	32.65(3)
α, deg	90	90
β, deg	101.097(5)	111.657(7)
γ, deg	90	90
Volume (Å3)	1411.6(6)	3220(4)
Z	4	8
density ($mg \cdot cm^{-3}$)	1.446	1.667
μ (mm^{-1})	0.239	4.026
F(000)	632	1611
reflections collected / unique	7527 / 2789	24073 / 3068
R_{int}	0.0639	0.0459
completeness to θ_{full} (%)	99.8	100.0
max. and min. transmission	0.7453 / 0.6560	0.7508 / 0.5236
Goodness-of-fit on F^2	0.951	1.037
Final R indices [I>2σ(I)]	0.0520, 0.1032	0.0309, 0.0778
R indices (all data)	0.1314, 0.1336	0.0426, 0.0825
Largest diff. peak and hole hole (e. $Å^{-3}$)	0.227, -0.216	0.635 / -0.579

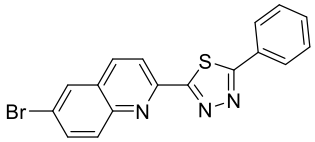
10. Spectral data of the synthesized compounds



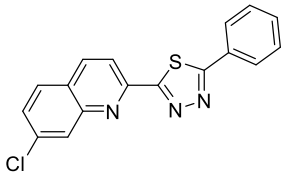
2-phenyl-5-(quinolin-2-yl)-1,3,4-thiadiazole (m1); Eluant: 8: 1; 15.5 mg, 70% yield; white solid; m.p. = 249 – 250 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.51 (d, *J* = 8.4 Hz, 1H), 8.33 (d, *J* = 8.4 Hz, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 8.11 – 8.09 (m, 2H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.81 – 7.77 (m, 1H), 7.64 – 7.60 (m, 1H), 7.54 (d, *J* = 2.8 Hz, 2H), 7.53 – 7.52 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS,) δ 170.5, 170.5, 149.3, 148.1, 137.3, 131.4, 130.4, 130.3, 129.6, 129.3, 128.9, 128.1, 127.9, 127.8, 118.5; IR (KBr): 2923, 1460, 828, 759, 680 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{12}N_3S$: $[M+H]^+$ 290.0746, Found: 290.0756.



2-(6-fluoroquinolin-2-yl)-5-phenyl-1,3,4-thiadiazole (m2); Eluant: 8: 1; 13.8 mg, 63% yield; white solid; m.p. = 199 – 200 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.52 (d, *J* = 8.5 Hz, 1H), 8.27 (d, *J* = 8.6 Hz, 1H), 8.16 (dd, *J* = 9.2, 5.3 Hz, 1H), 8.10 (dt, *J* = 7.3, 3.6 Hz, 2H), 7.61 – 7.47 (m, 5H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.5, 170.2, 161.2 (d, *J* = 250.6 Hz), 148.8, 145.1, 136.6 (d, *J* = 5.6 Hz), 132.2 (d, *J* = 8.9 Hz), 131.4, 130.3, 129.6 (d, *J* = 10.3 Hz), 129.3, 128.1, 120.7 (d, *J* = 25.9 Hz), 119.2, 111.1 (d, *J* = 21.9 Hz); ^{19}F-NMR (376 MHz, Chloroform-*d*) δ -108.4 – -112.9 (m, 1F); IR (KBr): 2923, 1450, 1218, 823, 754, 675 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{11}N_3SF$: $[M+H]^+$ 308.0652, Found: 308.0660.

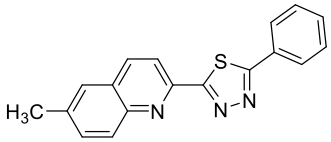


2-(6-bromoquinolin-2-yl)-5-phenyl-1,3,4-thiadiazole (m3); Eluant: 8: 1; 14.5 mg, 62% yield; white solid; m.p. = 196 – 197 ℃;^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.51 (d, *J* = 8.6 Hz, 1H), 8.22 (d, *J* = 8.6 Hz, 1H), 8.09 (dd, *J* = 6.5, 2.8 Hz, 2H), 8.05 (d, *J* = 2.3 Hz, 1H), 8.01 (d, *J* = 9.1 Hz, 1H), 7.84 (dd, *J* = 8.9, 2.1 Hz, 1H), 7.55 – 7.52 (m, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.7, 170.0, 149.6, 146.6, 136.3, 133.9, 131.5, 131.2, 130.3, 130.0, 129.8, 129.3, 128.1, 121.9, 119.4; IR (KBr): 2924, 1420, 828, 759, 540 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{11}N_3SBr$: $[M+H]^+$ 367.9852, Found: 367.9840.

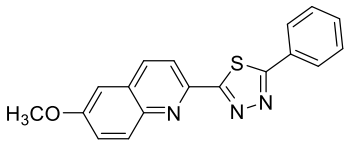


2-(7-chloroquinolin-2-yl)-5-phenyl-1,3,4-thiadiazole (m4); Eluant: 8: 1; 14.5 mg, 65% yield; white solid; m.p. = 201 – 202 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.50 (d, *J* = 8.5 Hz, 1H), 8.30 (d, *J* = 8.6 Hz, 1H), 8.17 (d, *J* = 2.2 Hz, 1H), 8.10 (dd, *J* = 6.6, 3.2 Hz, 2H), 7.83 (d, *J* =

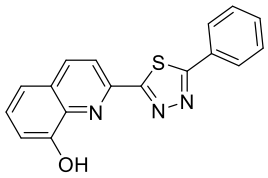
8.8 Hz, 1H), 7.59 – 7.50 (m, 4H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.8, 170.1, 150.2, 148.3, 137.2, 136.3, 131.5, 130.3, 129.4, 129.1, 128.8, 128.6, 128.2, 127.2, 118.7; IR (KBr): 2923, 1454, 843, 759, 683 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{11}N_3SCl$: $[M+H]^+$ 324.0357, Found: 324.0358.



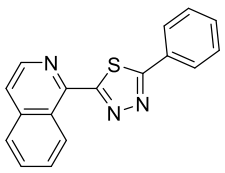
2-(6-methylquinolin-2-yl)-5-phenyl-1,3,4-thiadiazole (m5); Eluant: 8: 1; 15.7 mg, 75% yield; white solid; m.p. = 249 – 250 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.42 (dd, *J* = 8.5, 3.2 Hz, 1H), 8.18 (dd, *J* = 8.6, 3.9 Hz, 1H), 8.07 (dq, *J* = 5.6, 2.2 Hz, 2H), 8.01 (dd, *J* = 8.5, 2.8 Hz, 1H), 7.64 – 7.54 (m, 2H), 7.51 (dt, *J* = 3.6, 1.7 Hz, 3H), 2.54 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.6, 170.2, 148.3, 146.6, 138.0, 136.5, 132.6, 131.3, 130.4, 129.3, 129.2, 128.9, 128.1, 126.8, 118.4, 21.8; IR (KBr): 2914, 1518, 1365, 828, 754, 685 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{14}N_3S$: $[M+H]^+$ 304.0903 Found: 304.0892.



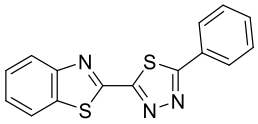
2-(6-methoxyquinolin-2-yl)-5-phenyl-1,3,4-thiadiazole (m6); Eluant: 8: 1; 16.5 mg, 74% yield ; white solid; m.p. = 207 – 208 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.45 (d, *J* = 8.6 Hz, 1H), 8.20 (dd, *J* = 8.7, 0.7 Hz, 1H), 8.11 – 8.07 (m, 2H), 8.06 – 8.01 (m, 1H), 7.55 – 7.50 (m, 3H), 7.43 (dd, *J* = 9.2, 2.8 Hz, 1H), 7.14 (d, *J* = 2.8 Hz, 1H), 3.98 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.7, 170.1, 158.9, 146.9, 144.2, 135.8, 131.3, 131.1, 130.5, 130.2, 129.3, 128.1, 123.3, 118.8, 105.3, 55.8; IR (KBr): 2923, 1450, 1233. 1031, 828, 759, 680 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{14}N_3OS$: $[M+H]^+$ 320.0852, Found: 320.0867.



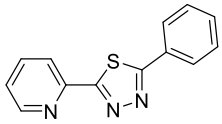
2-(5-phenyl-1,3,4-thiadiazol-2-yl)quinolin-8-ol (m7); Eluant: 8: 1; 16.2 mg, 74% yield; white solid; m.p. = 200 – 201 ℃; ^{1}H NMR (400 MHz, DMSO-*d6*) δ 10.05 (s, 1H), 8.50 (d, *J* = 8.6 Hz, 1H), 8.34 (d, *J* = 8.5 Hz, 1H), 8.06 (dd, *J* = 6.7, 3.0 Hz, 2H), 7.59 (p, *J* = 3.7 Hz, 3H), 7.54 – 7.44 (m, 2H), 7.18 (dd, *J* = 7.2, 1.6 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.5, 169.4, 152.1, 147.1, 137.8, 137.6, 131.6, 130.2, 129.4, 129.3, 129.2, 128.2, 119.2, 118.3, 111.3; IR (KBr): 3401, 3061, 1415, 1016, 838, 764, 690 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{12}N_3OS$: $[M+H]^+$ 306.0696, Found: 306.0686.



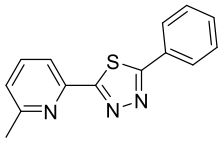
2-(isoquinolin-1-yl)-5-phenyl-1,3,4-thiadiazole (m8); Eluant: 8: 1; 14.8 mg, 69% yield; white solid; m.p. = 163 – 164 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 9.94 – 9.80 (m, 1H), 8.61 (d, *J* = 5.5 Hz, 1H), 8.11 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.92 (dd, *J* = 6.6, 3.2 Hz, 1H), 7.85 – 7.74 (m, 3H), 7.64 – 7.43 (m, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*, TMS) δ 172.2, 170.0, 147.6, 147.5, 141.9, 137.2, 131.3, 130.8, 130.3, 129.3, 128.1, 127.8, 127.0, 126.0, 123.1; IR (KBr): 2919, 1415, 833, 740,675 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{12}N_3S$: $[M+H]^+$ 290.0746, Found: 290.0735.



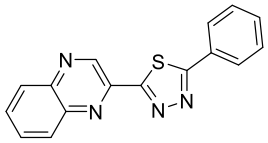
2-(5-phenyl-1,3,4-thiadiazol-2-yl)benzo[d]thiazole (m9); Eluant: 8: 1; 15.1 mg, 70% yield; white solid; m.p. = 156 - 157 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.14 (d, *J* = 7.6 Hz, 1H), 8.06 (dd, *J* = 7.6, 2.1 Hz, 2H), 8.02 – 7.94 (m, 1H), 7.61 – 7.48 (m, 5H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.5, 162.9, 157.9, 153.4, 135.5, 131.9, 129.7, 129.5, 128.3, 127.0, 124.3, 124.1, 122.2; IR (KBr): 2925, 1400, 936, 759, 685 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{15}H_{10}N_3S_2$: $[M+H]^+$ 296.0311, Found: 296.0300.



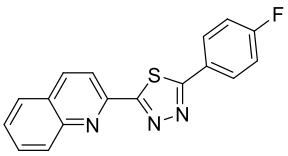
2-phenyl-5-(pyridin-2-yl)-1,3,4-thiadiazole (m10); Eluant: 8: 1; 10.7 mg, 53% yield; white solid; m.p. = 131 – 132 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.67 (d, *J* = 4.8 Hz, 1H), 8.40 (d, *J* = 7.7 Hz, 1H), 8.13 – 7.99 (m, 2H), 7.87 (t, *J* = 7.9 Hz, 1H), 7.51 (d, *J* = 5.3 Hz, 3H), 7.40 (t, *J* = 6.2 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.0, 169.9, 149.9, 149.2, 137.2, 131.3, 130.3, 129.2, 128.0, 125.3, 121.0; IR (KBr): 2928, 1435, 784, 685,600 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{13}H_{10}N_3S$: $[M+H]^+$ 240.0590, Found: 240.0589.



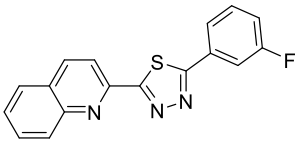
2-(6-methylpyridin-2-yl)-5-phenyl-1,3,4-thiadiazole (m11); Eluant: 8: 1; 12.4 mg, 60% yield; white solid; m.p. = 140 – 141 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.18 (d, *J* = 7.7 Hz, 1H), 8.04 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.72 (t, *J* = 7.7 Hz, 1H), 7.54 – 7.45 (m, 3H), 7.23 (d, *J* = 7.8 Hz, 1H), 2.61 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.5, 169.9, 159.1, 148.6, 137.4, 131.2, 130.5, 129.3, 128.0, 125.1, 118.1, 24.4; IR (KBr): 2923, 1454, 1420, 808, 754, 685 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{14}H_{12}N_3S$: $[M+H]^+$ 254.0746, Found: 254.0745.



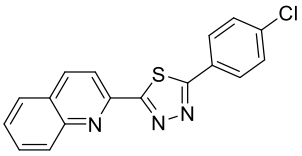
2-phenyl-5-(quinoxalin-2-yl)-1,3,4-thiadiazole (m12); Eluant: 8: 1; 10.7 mg, 50% yield; white solid; m.p. = 179 – 180 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 9.90 (s, 1H), 8.23 (dq, *J* = 6.9, 3.6 Hz, 1H), 8.18 (dd, *J* = 6.4, 3.5 Hz, 1H), 8.13 – 8.09 (m, 2H), 7.88 (dt, *J* = 6.6, 3.6 Hz, 2H), 7.56 (dd, *J* = 5.3, 2.0 Hz, 3H).^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.9, 168.1, 144.1, 143.1, 142.8, 142.0, 131.8, 131.3, 131.0, 130.0, 129.7, 129.5, 129.4, 128.3; IR (KBr): 2923, 1415, 1021, 760,685 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{16}H_{11}N_4S$: $[M+H]^+$ 291.0699, Found: 291.0698.



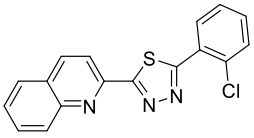
2-(4-fluorophenyl)-5-(naphthalen-2-yl)-1,3,4-thiadiazole (m13); Eluant: 8: 1; 13.3 mg, 65% yield; white solid; m.p. = 201 – 202 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.49 (d, *J* = 8.6 Hz, 1H), 8.33 (d, *J* = 8.6 Hz, 1H), 8.16 (d, *J* = 8.6 Hz, 1H), 8.13 – 8.06 (m, 2H), 7.93 – 7.87 (m, 1H), 7.82 – 7.75 (m, 1H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.25 – 7.14 (m, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.6, 169.3, 164.6 (d, *J* = 252.6 Hz), 149.1, 148.0, 137.3, 130.4, 130.1 (d, *J* = 8.7 Hz), 129.6, 128.9, 127.9, 127.9, 126.7 (d, *J* = 3.5 Hz), 118.4, 116.5 (d, *J* = 22.2 Hz); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -107.8 – -107.9 (m, 1F); IR (KBr): 2923, 1425, 1159, 838 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{11}N_3SF$: $[M+H]^+$ 308.0652, Found: 308.0658.



2-(3-fluorophenyl)-5-(quinolin-2-yl)-1,3,4-thiadiazole (m14); Eluant: 8: 1; 13.3 mg, 65% yield; white solid; m.p. = 249 – 250 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.49 (d, *J* = 8.6 Hz, 1H), 8.33 (d, *J* = 8.4 Hz, 1H), 8.16 (d, *J* = 8.6 Hz, 1H), 7.94 – 7.88 (m, 1H), 7.86 – 7.82 (m, 2H), 7.79 (ddd, *J* = 8.3, 6.9, 1.5 Hz, 1H), 7.62 (ddd, *J* = 8.2, 6.9, 1.3 Hz, 1H), 7.50 (td, *J* = 8.2, 5.7 Hz, 1H), 7.25 – 7.16 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.9, 169.1, 163.0 (d, *J* = 248.1 Hz), 148.9, 148.0, 137.3, 132.3 (d, *J* = 7.0 Hz), 130.9 (d, *J* = 8.1 Hz), 130.4, 129.5, 128.9, 127.9, 127.9, 123.9 (d, *J* = 2.4 Hz), 118.3, 118.2 (d, *J* = 23.9 Hz), 114.74 (d, *J* = 23.7 Hz); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -106.2 – -109.7 (m, 1F); IR (KBr): 2835, 1592, 1366, 828, 750 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{11}N_3SF$: $[M+H]^+$ 308.0652, Found: 308.0658.

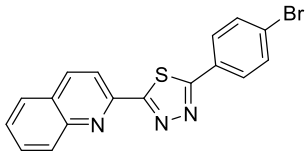


2-(4-chlorophenyl)-5-(quinolin-2-yl)-1,3,4-thiadiazole (m15) Eluant: 8: 1; 14.4 mg, 68% yield; white solid; m.p. = 232 – 233 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.49 (d, *J* = 8.4 Hz, 1H), 8.32 (d, *J* = 8.6 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 8.06 – 8.00 (m, 2H), 7.89 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.79 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.62 (ddd, *J* = 8.2, 6.8, 1.3 Hz, 1H), 7.58 – 7.45 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.8, 169.3, 149.1, 148.0, 146.3, 137.5, 137.4, 130.5, 129.6, 129.6, 129.3, 129.0, 128.9, 128.0, 118.5; IR (KBr): 2923, 1459, 1090, 828 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{11}ClN_3S$: $[M+H]^+$ 324.0357, Found: 324.0360.

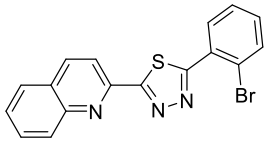


2-(2-chlorophenyl)-5-(quinolin-2-yl)-1,3,4-thiadiazole (m16); Eluant: 8: 1; 13.9 mg, 66% yield; white solid; m.p. = 180 – 181 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.52 (d, *J* = 8.6 Hz, 1H), 8.44 – 8.39 (m, 1H), 8.32 (d, *J* = 8.6 Hz, 1H), 8.18 (d, *J* = 8.6 Hz, 1H), 7.88 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.78 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.65 – 7.61 (m, 1H), 7.60 – 7.54 (m, 1H), 7.52 – 7.42

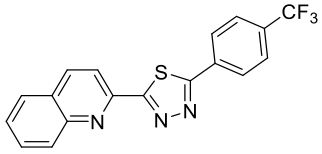
(m, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 171.7, 165.9, 149.4, 148.1, 137.3, 133.0, 131.8, 131.2, 130.8, 130.4, 129.7, 129.3, 128.9, 127.9, 127.9, 127.4, 118.6; IR (KBr): 2923, 1405, 760, 680 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{11}N_3SCl$: $[M+H]^+$ 324.0357, Found: 324.0358.



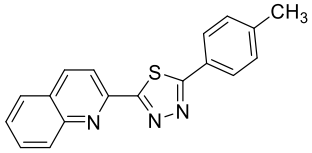
2-(4-bromophenyl)-5-(quinolin-2-yl)-1,3,4-thiadiazole (m17); Eluant: 8: 1; 15.3 mg, 67% yield; white solid; m.p. = 180 – 181 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.47 (d, *J* = 8.6 Hz, 1H), 8.31 (d, *J* = 8.6 Hz, 1H), 8.13 (d, *J* = 8.5 Hz, 1H), 7.99 – 7.91 (m, 2H), 7.88 (d, *J* = 8.3 Hz, 1H), 7.77 (t, *J* = 7.5 Hz, 1H), 7.68 – 7.64 (m, 2H), 7.61 (t, *J* = 7.5 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.7, 170.0, 149.6, 146.6, 136.3, 133.9, 131.5, 131.2, 130.3, 130.0, 129.8, 129.4, 128.1, 121.9, 119.4; IR (KBr): 2928, 1459, 818, 750, 675 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{10}BrN_3SK$: $[M+K]^+$ 407.9391, Found: 407.9390.



2-(2-bromophenyl)-5-(quinolin-2-yl)-1,3,4-thiadiazole (m18) Eluant: 8: 1; 14.8 mg, 65% yield; white solid; m.p. = 186–187 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.50 (d, *J* = 8.5 Hz, 1H), 8.31 (d, *J* = 8.6 Hz, 1H), 8.24 (dd, *J* = 7.9, 1.8 Hz, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 7.92 – 7.84 (m, 1H), 7.77 (dd, *J* = 7.5, 6.0 Hz, 2H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.41 – 7.33 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ171.7, 167.4, 149.3, 148.1, 137.4, 134.2, 132.0, 131.9, 131.3, 130.4, 129.7, 128.9, 127.9, 127.9, 127.9, 122.8, 118.6; IR (KBr): 2923, 1425, 828, 754, 700 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{10}BrN_3SK$: $[M+K]^+$ 407.9391, Found: 407.9390.

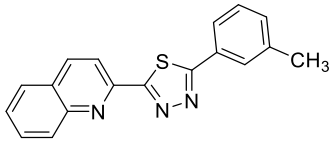


2-(quinolin-2-yl)-5-(4-(trifluoromethyl)phenyl)-1,3,4-thiadiazole (m19) Eluant: 10: 1; 11.2 mg, 50% yield; white solid; m.p. = 212 – 213 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 (d, *J* = 8.4 Hz, 1H), 8.29 (d, *J* = 8.6 Hz, 1H), 8.17 (d, *J* = 8.0 Hz, 2H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 8.2 Hz, 1H), 7.76 (d, *J* = 7.8 Hz, 3H), 7.60 (t, *J* = 7.5 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.44, 168.83, 148.89, 148.04, 137.45, 133.59, 132.91 (q, *J* = 32.6 Hz), 130.51, 129.62, 128.99, 128.35, 128.04, 127.95, 126.32 (q, *J* = 4.0 Hz), 123.78 (d, *J* = 272.6 Hz), 118.42; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.85; IR (KBr): 2835, 1592, 1321, 828, 750 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{11}F_3N_3S$: $[M+H]^+$ 358.0620, Found: 358.0622.

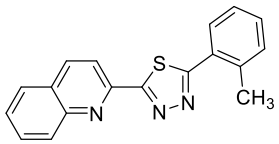


2-(quinolin-2-yl)-5-(p-tolyl)-1,3,4-thiadiazole (m20) Eluant: 8: 1; 14.6 mg, 72% yield; white solid; m.p. = 153 – 154 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.50 (dd, *J* = 8.6, 1.7 Hz, 1H), 8.32 (d, *J* = 8.7 Hz, 1H), 8.17 (d, *J* = 8.7 Hz, 1H), 7.98 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.89 (d, *J* = 8.2

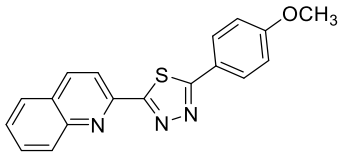
Hz, 1H), 7.78 (t, *J* = 7.7 Hz, 1H), 7.62 (t, *J* = 7.7 Hz, 1H), 7.33 (d, *J* = 7.7 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.6, 170.0, 149.3, 147.9, 141.8, 137.3, 130.3, 130.3, 129.5, 128.8, 128.0, 127.8, 127.7, 127.6, 118.4, 21.6; IR (KBr): 2923, 1592, 1361, 823, 750 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{14}N_3S$: $[M+H]^+$ 304.0903, Found: 304.0901.



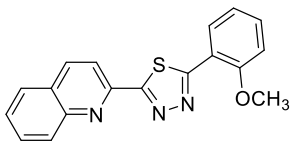
2-(quinolin-2-yl)-5-(m-tolyl)-1,3,4-thiadiazole (m21); Eluant: 8: 1; 13.8 mg, 68% yield; white solid; m.p. = 148 – 149 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.48 (d, *J* = 8.6 Hz, 1H), 8.29 (d, *J* = 8.6 Hz, 1H), 8.13 (d, *J* = 8.5 Hz, 1H), 7.92 (s, 1H), 7.86 (d, *J* = 8.1 Hz, 2H), 7.79 – 7.74 (m, 1H), 7.63 – 7.56 (m, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 7.8 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.8, 170.4, 149.3, 148.0, 139.2, 137.3, 132.2, 130.4, 130.2, 129.6, 129.2, 128.9, 128.6, 127.9, 127.8, 125.4, 118.5, 21.5; IR (KBr): 2830, 1592, 1361, 754, 690 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{14}N_3S$: $[M+H]^+$ 304.0903, Found: 304.0895.



2-(quinolin-2-yl)-5-(o-tolyl)-1,3,4-thiadiazole (m22); Eluant: 8: 1; 14.2 mg, 70% yield; white solid; m.p. = 130 – 131 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.51 (d, *J* = 8.7 Hz, 1H), 8.32 (d, *J* = 8.7 Hz, 1H), 8.21 – 8.11 (m, 1H), 7.89 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.84 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.80 – 7.75 (m, 1H), 7.66 – 7.57 (m, 1H), 7.45 – 7.31 (m, 3H), 2.69(s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.9, 170.0, 149.4, 148.0, 137.5, 137.4, 131.8, 130.9, 130.7, 130.4, 129.6, 129.5, 128.9, 127.9, 127.9, 126.5, 118.5, 21.9; IR (KBr): 2830, 1592, 1366, 770 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{14}N_3S$: $[M+H]^+$ 304.0903, Found: 304.0899.

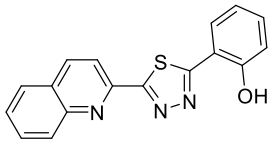


2-(4-methoxyphenyl)-5-(quinolin-2-yl)-1,3,4-thiadiazole (m23); Eluant: 8: 1; 15.5 mg, 74% yield; white solid; m.p. = 172 – 173 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.48 (d, *J* = 8.5 Hz, 1H), 8.29 (d, *J* = 8.6 Hz, 1H), 8.13 (d, *J* = 8.5 Hz, 1H), 8.03 (d, *J* = 8.2 Hz, 2H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.02 (d, *J* = 8.3 Hz, 2H), 3.89 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.3, 169.7, 162.2, 149.4, 148.0, 137.2, 130.3, 129.7, 129.6, 128.8, 127.9, 127.7, 123.1, 118.5, 114.7, 55.6; IR (KBr): 2923, 1592, 1257, 833 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{14}N_3OS$: $[M+H]^+$ 320.0852, Found: 320.0855.

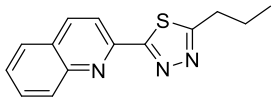


2-(2-methoxyphenyl)-5-(quinolin-2-yl)-1,3,4-thiadiazole (m24); Eluant: 8: 1; 16.8 mg, 80% yield; white solid; m.p. = 185 – 186 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.58 (dd, *J* = 7.9, 1.8 Hz, 1H), 8.48 (d, *J* = 8.6 Hz, 1H), 8.22 (d, *J* = 8.6 Hz, 1H), 8.13 (d, *J* = 8.5 Hz, 1H), 7.80 (dd, *J* =

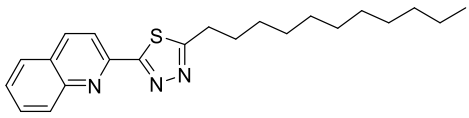
8.3, 1.4 Hz, 1H), 7.71 (ddd, *J* = 8.4, 6.8, 1.6 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.45 (td, *J* = 8.1, 7.7, 1.7 Hz, 1H), 7.15 – 7.07 (m, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 4.03 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.7, 164.2, 156.3, 150.1, 148.1, 137.1, 132.4, 130.2, 129.6, 128.8, 128.7, 127.9, 127.5, 121.3, 119.4, 118.6, 111.4, 55.9; IR (KBr): 2840, 1587, 1361, 744 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{14}N_3OS$: $[M+H]^+$ 320.0852, Found: 320,0855.



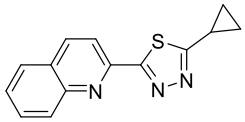
2-(5-(quinolin-2-yl)-1,3,4-thiadiazol-2-yl)phenol (m25); Eluant: 8: 1; 14.9 mg, 71% yield; white solid; m.p. = 123 – 124 ℃; ^{1}H NMR (400 MHz, DMSO-*d6*) δ 11.42 (s, 1H), 8.57 (d, *J* = 8.5 Hz, 1H), 8.40 (d, *J* = 8.6 Hz, 1H), 8.34 – 8.28 (m, 1H), 8.08 (dd, *J* = 17.8, 8.2 Hz, 2H), 7.88 – 7.80 (m, 1H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.42 (td, *J* = 8.4, 1.6 Hz, 1H), 7.11 (d, *J* = 8.1 Hz, 1H), 7.01 (t, *J* = 7.7 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-*d6*) δ 170.1, 164.7, 155.7, 149.8, 147.9, 138.5, 133.2, 131.3, 129.4, 129.0, 128.8, 128.4, 128.1, 120.3, 118.5, 117.1, 117.1; IR (KBr): 3436, 2830, 1602, 1026, 823, 750 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{12}N_3OS$: $[M+H]^+$ 306.0696, Found: 306.0695.



2-propyl-5-(quinolin-2-yl)-1,3,4-thiadiazole (m26); Eluant: 8: 1; 13.9 mg, 73% yield; white solid; m.p. = 114 – 115 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.42 (d, *J* = 8.6 Hz, 1H), 8.27 (d, *J* = 8.6 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.85 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.78 – 7.69 (m, 1H), 7.61 – 7.54 (m, 1H), 3.15 (t, *J* = 7.6 Hz, 2H), 1.91 (dt, *J* = 14.9, 7.4 Hz, 2H), 1.07 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 173.0, 170.7, 149.5, 148.0, 137.3, 130.3, 129.6, 128.8, 127.9, 127.7, 118.4, 32.4, 23.6, 13.7; IR (KBr): 2953, 2830, 1587, 1361, 848, 754 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{14}H_{14}N_3S$: $[M+H]^+$ 256.0903, Found:256.0906.

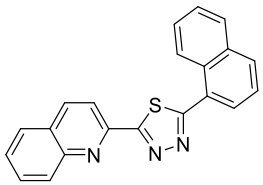


2-(quinolin-2-yl)-5-undecyl-1,3,4-thiadiazole (m27); Eluant: 8: 1; 16.2 mg, 68% yield; white solid; m.p. = 74 – 75 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.45 (d, *J* = 8.6 Hz, 1H), 8.30 (d, *J* = 8.5 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.81 – 7.73 (m, 1H), 7.60 (t, *J* = 7.5 Hz, 1H), 3.27 – 3.06 (m, 2H), 1.97 – 1.76 (m, 2H), 1.51 – 1.41 (m, 2H), 1.28 (dd, *J* = 11.2, 4.9 Hz, 14H), 0.92 – 0.80 (m, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 173.2, 170.7, 149.4, 148.0, 137.2, 130.2, 129.6, 128.8, 127.8, 127.6, 118.4, 31.9, 30.4, 30.2, 29.6(2C), 29.5, 29.3, 29.3, 29.0, 22.7, 14.1; IR (KBr): 2923, 2854, 1597, 1361, 838, 740 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{22}H_{30}N_3S$: $[M+H]^+$ 368.2155, Found: 368.2150.

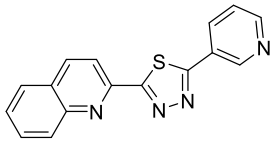


2-cyclopropyl-5-(quinolin-2-yl)-1,3,4-thiadiazole (m28); Eluant: 8: 1; 12.9 mg, 70% yield; white solid; m.p. = 121 – 122 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.37 (d, *J* = 8.5 Hz, 1H), 8.23 (d, *J* = 8.6 Hz, 1H), 8.07 (d, *J* = 8.5 Hz, 1H), 7.82 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.75 – 7.68 (m, 1H), 7.58 – 7.52 (m, 1H), 2.47 (tt, *J* = 8.4, 5.1 Hz, 1H), 1.36 – 1.26 (m, 2H), 1.25 – 1.16 (m, 3H).

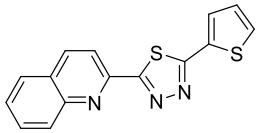
^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 176.3, 169.1, 149.4, 147.9, 137.2, 130.3, 129.5, 128.7, 127.9, 127.7, 118.3, 12.3, 12.2; IR (KBr): 2923, 2830, 1582, 1361, 770 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{14}H_{11}N_3SK$: $[M+K]^+$ 292.0305, Found: 292.0303.



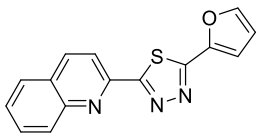
2-(naphthalen-1-yl)-5-(quinolin-2-yl)-1,3,4-thiadiazole (m29); Eluant: 8: 1; 15.6 mg, 72% yield; white solid; m.p. = 182 – 183 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.85 (d, *J* = 8.3 Hz, 1H), 8.57 (d, *J* = 8.5 Hz, 1H), 8.36 (d, *J* = 8.4 Hz, 1H), 8.19 (d, *J* = 8.4 Hz, 1H), 8.03 (d, *J* = 8.3 Hz, 1H), 7.99 – 7.93 (m, 2H), 7.91 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.82 – 7.75 (m, 1H), 7.67 – 7.62 (m, 2H), 7.59 (t, *J* = 7.7 Hz, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.1, 170.0, 149.3, 148.1, 137.5, 134.1, 131.7, 130.7, 130.5, 130.0, 129.7, 129.0, 128.7, 127.99, 128.96(2C), 127.2, 126.8, 125.9, 125.2, 118.5; IR (KBr): 2919, 1597, 1356, 803 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{21}H_{14}N_3S$: $[M+H]^+$ 340.0903, Found: 340.0909.



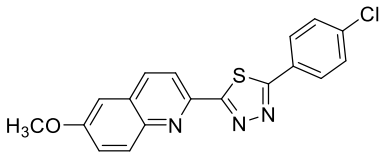
2-(pyridin-3-yl)-5-(quinolin-2-yl)-1,3,4-thiadiazole (m30) Eluant: 8: 1; 11.9 mg, 60% yield; white solid; m.p. = 173 – 174 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 9.25 (d, *J* = 2.4 Hz, 1H), 8.75 (dd, *J* = 4.9, 1.8 Hz, 1H), 8.46 (d, *J* = 8.8 Hz, 1H), 8.43 – 8.37 (m, 1H), 8.30 (d, *J* = 8.6 Hz, 1H), 8.12 (d, *J* = 8.5 Hz, 1H), 7.87 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.81 – 7.73 (m, 1H), 7.66 – 7.56 (m, 1H), 7.47 (dd, *J* = 8.0, 4.9 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ171.3, 167.2, 152.1, 149.0, 148.8, 148.0, 137.4, 134.9, 130.5, 129.6, 129.0, 128.0, 127.9, 126.8, 124.1, 118.4; IR (KBr): 2820, 1592, 1356, 774 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{16}H_{11}N_4S$: $[M+H]^+$ 291.0699, Found: 291.0689.



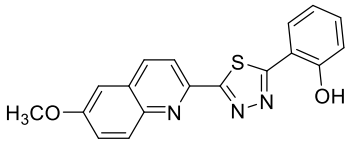
2-(quinolin-2-yl)-5-(thiophen-2-yl)-1,3,4-thiadiazole (m31); Eluant: 8: 1; 13.6 mg, 68% yield; white solid; m.p. = 208 – 209 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.46 (d, *J* = 8.5 Hz, 1H), 8.30 (dd, *J* = 8.7, 0.9 Hz, 1H), 8.18 – 8.07 (m, 1H), 7.88 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.77 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.67 (dd, *J* = 3.7, 1.2 Hz, 1H), 7.61 (ddd, *J* = 8.1, 7.0, 1.3 Hz, 1H), 7.54 (dd, *J* = 5.0, 1.1 Hz, 1H), 7.17 (dd, *J* = 5.0, 3.7 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 169.8, 164.3, 149.1, 148.0, 137.3, 132.8, 130.4, 130.1, 129.8, 129.5, 128.9, 128.3, 127.9, 127.9, 118.5; IR (KBr): 2835, 1582, 1361, 710 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{15}H_{10}N_3S_2$: $[M+H]^+$ 296.0311, Found: 296.0320.



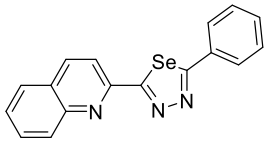
2-(furan-2-yl)-5-(quinolin-2-yl)-1,3,4-thiadiazole (m32); Eluant: 8: 1; 13.0 mg, 67% yield; white solid; m.p. = 225 – 226 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.48 (d, *J* = 8.4 Hz, 1H), 8.30 (d, *J* = 8.6 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 7.88 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.80 – 7.75 (m, 1H), 7.66 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.64 – 7.58 (m, 1H), 7.30 – 7.27 (m, 1H), 6.63 (dd, *J* = 3.4, 1.6 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 169.8, 160.6, 149.1, 148.0, 146.1, 145.3, 137.3, 130.4, 129.6, 128.9, 127.9, 127.8, 118.5, 112.7, 112.2; IR (KBr): 2831, 1592, 1361, 769 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{15}H_9N_3OSNa$: $[M+Na]^+$ 302.0359, Found: 302.0358.



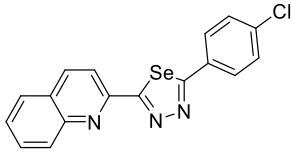
2-(4-chlorophenyl)-5-(6-methoxyquinolin-2-yl)-1,3,4-thiadiazole (m33); Eluant: 8: 1; 14.2 mg, 65% yield; white solid; m.p. = 233 – 234 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.40 (d, *J* = 8.5 Hz, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 7.99 (dd, *J* = 8.8, 5.2 Hz, 3H), 7.51 – 7.44 (m, 2H), 7.40 (dd, *J* = 9.2, 2.9 Hz, 1H), 7.10 (d, *J* = 2.8 Hz, 1H), 3.95 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 171.0, 168.8, 159.0, 146.7, 144.1, 137.4, 135.8, 131.1, 130.3, 129.6, 129.2, 129.0, 123.4, 118.8, 105.3, 55.8; IR (KBr): 2919, 2820, 1587, 1356, 818, 769 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{13}ClN_3OS$: $[M+H]^+$ 354.0462, Found: 354.0460.



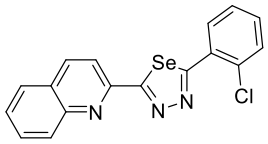
2-(5-(6-methoxyquinolin-2-yl)-1,3,4-thiadiazol-2-yl)phenol (m34); Eluant: 8: 1; 12.7 mg, 60% yield; white solid; m.p. = 227 – 228 ℃; ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.42 (s, 1H), 8.48 (d, *J* = 8.6 Hz, 1H), 8.38 (d, *J* = 8.5 Hz, 1H), 8.34 (d, *J* = 7.6 Hz, 1H), 8.09 – 8.01 (m, 1H), 7.53 – 7.48 (m, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 8.2 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 3.95 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 170.3, 164.3, 158.8, 155.6, 147.3, 143.8, 137.0, 133.1, 130.9, 130.4, 128.1, 123.8, 120.3, 118.8, 117.2, 117.1, 106.5, 56.2. IR (KBr): 3436, 2825, 1587, 1356, 1031, 754 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{14}N_3O_2S$: $[M+H^+]$ 336.0801, Found: 336.0800.



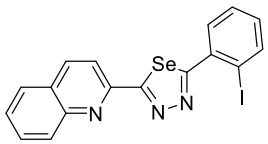
2-phenyl-5-(quinolin-2-yl)-1,3,4-selenadiazole (n1) Eluant: 8: 1; 16.4 mg, 65% yield; white solid; m.p. = 150 - 151 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.41 (d, *J* = 8.6 Hz, 1H), 8.36 (d, *J* = 8.6 Hz, 1H), 8.30 (ddd, *J* = 6.4, 3.5, 1.8 Hz, 3H), 7.92 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.83 (ddd, *J* = 8.6, 6.9, 1.5 Hz, 1H), 7.72 – 7.61 (m, 1H), 7.63 – 7.51 (m, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ166.0, 164.3, 148.1, 143.5, 137.6, 132.2, 130.7, 130.2, 129.2, 128.8, 128.4, 127.9, 127.6, 123.7, 120.0; IR (KBr): 2923, 1597, 1361, 780, 690 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{12}N_3Se$: $[M+H]^+$ 338.0192, Found: 338.0193.



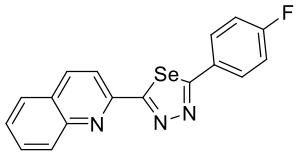
2-(4-chlorophenyl)-5-(quinolin-2-yl)-1,3,4-selenadiazole (n2) Eluant: 8: 1; 14.0 mg, 60% yield; white solid; m.p. = 178 – 179 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.43 – 8.33 (m, 2H), 8.29 (d, *J* = 8.6 Hz, 1H), 8.27 – 8.18 (m, 2H), 7.92 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.83 (ddd, *J* = 8.5, 6.8, 1.6 Hz, 1H), 7.67 (dd, *J* = 8.1, 6.9 Hz, 1H), 7.57 – 7.52 (m, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ165.2, 164.4, 148.0, 143.3, 138.5, 137.6, 130.7, 130.2, 129.6, 128.8 (2C), 128.5, 127.9, 122.2, 120.0; IR (KBr): 2928, 1602, 1361, 833, 750 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{10}ClN_3SeK$: $[M+K]^+$ 409.9358, Found: 409.9555.



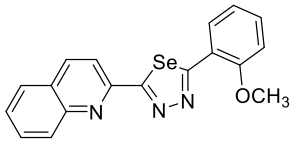
2-(2-chlorophenyl)-5-(quinolin-2-yl)-1,3,4-selenadiazole (n3) Eluant: 8: 1; 11.7 mg, 50% yield; white solid; m.p. = 133 – 134 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.42 – 8.33 (m, 2H), 8.28 (d, *J* = 8.5 Hz, 1H), 8.14 (dd, *J* = 7.6, 2.1 Hz, 1H), 7.90 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.81 (ddd, *J* = 8.5, 6.8, 1.7 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.59 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.51 (td, *J* = 7.9, 2.0 Hz, 1H), 7.47 – 7.42 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 164.6, 164.2, 148.1, 143.3, 137.6, 133.7, 132.8, 131.7, 131.3, 130.7, 130.4, 128.9, 128.5, 127.9, 127.2, 123.2, 120.0; IR (KBr): 2830, 1592, 1361, 774 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{10}ClN_3SeK$: $[M+K]^+$ 409.9358, Found: 409.9360.



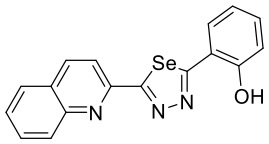
2-(2-iodophenyl)-5-(quinolin-2-yl)-1,3,4-selenadiazole (n4) Eluant: 8: 1; 14.8 mg, 55% yield; white solid; m.p. = 152–153 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.44 – 8.35 (m, 2H), 8.29 (d, *J* = 8.8 Hz, 1H), 8.10 (d, *J* = 7.4 Hz, 1H), 8.00 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.92 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.82 (ddd, *J* = 8.6, 6.8, 1.8 Hz, 1H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.60 – 7.51 (m, 1H), 7.26 (td, *J* = 7.8, 1.8 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 165.5, 164.6, 148.1, 143.3, 141.4, 137.6, 132.7, 131.8, 130.7, 130.4, 129.2, 128.9, 128.5, 128.3, 127.9, 127.6, 120.0; IR (KBr): 2830, 1587, 1356, 828, 759, 734 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{11}IN_3Se$: $[M+H]^+$ 463.9158, Found: 463.9160.



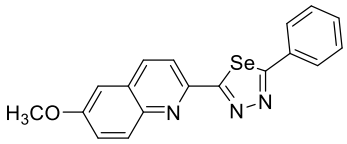
2-(4-fluorophenyl)-5-(quinolin-2-yl)-1,3,4-selenadiazole (n5) Eluant: 8: 1; 13.2 mg, 58% yield; white solid; m.p. = 158 – 159 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.42 – 8.30 (m, 2H), 8.30 – 8.24 (m, 3H), 7.88 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.83 – 7.77 (m, 1H), 7.67 – 7.61 (m, 1H), 7.23 (t, *J* = 8.5 Hz, 2H).^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 165.1, 165.1 (d, *J* = 253.8 Hz), 164.3, 148.0, 143.4, 137.6, 130.7, 130.2, 129.9 (d, J = 8.9 Hz), 128.8, 128.4, 127.9, 120.0 (d, *J* = 3.0 Hz), 119.9, 116.5 (d, *J* = 22.4 Hz); ^{19}F NMR (376 MHz, Chloroform-*d*) δ -106.0 – -106.1 (m, 1F); IR (KBr): 2825, 1597, 1489, 1361, 1228, 833, 754 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{11}FN_3Se$: $[M+H]^+$ 356.0097, Found: 356.0010.



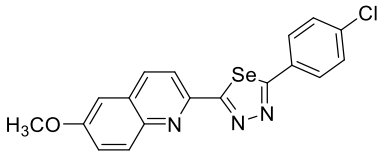
2-(2-methoxyphenyl)-5-(quinolin-2-yl)-1,3,4-selenadiazole (n6) Eluant: 8: 1; 15.8 mg, 68% yield; white solid; m.p. = 205 – 206 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.33 (d, *J* = 8.5 Hz, 1H), 8.31 – 8.25 (m, 2H), 8.22 (d, *J* = 8.6 Hz, 1H), 8.17 (d, *J* = 9.1 Hz, 1H), 7.47 (dd, *J* = 9.2, 2.9 Hz, 1H), 7.28 – 7.22 (m, 2H), 7.14 (d, *J* = 2.9 Hz, 1H), 3.98 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.7, 164.2, 156.3, 150.1, 148.1, 137.1, 132.4, 130.2, 129.6, 128.8, 128.7, 127.9, 127.5, 121.3, 119.4, 118.6, 111.4, 55.9; IR (KBr): 2835, 1597, 1361, 774 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{13}N_3OSe$: $[M+H]^+$ 368.0297, Found: 368.0295.



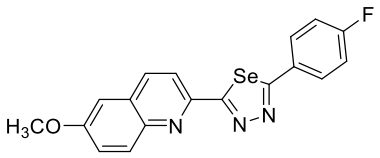
2-(5-(quinolin-2-yl)-1,3,4-selenadiazol-2-yl)phenol (n7) Eluant: 8: 1; 15.4 mg, 68% yield; white solid; m.p. = 211 – 212 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 10.18 (s, 1H), 8.33 (s, 2H), 8.26 (d, *J* = 8.4 Hz, 1H), 8.09 – 8.02 (m, 1H), 7.92 – 7.85 (m, 1H), 7.84 – 7.77 (m, 1H), 7.64 (dd, *J* = 8.2, 6.9 Hz, 1H), 7.52 – 7.40 (m, 1H), 7.14 (d, *J* = 8.8 Hz, 1H), 7.05 (t, *J* = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 165.6, 162.8, 158.0, 148.0, 142.9, 137.7, 134.2, 130.8, 130.2, 128.9, 128.6, 127.9, 127.4, 120.1, 119.9, 117.7, 107.9; IR (KBr): 3431, 2835, 1587, 1356, 1070, 754 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{12}N_3OSe$: $[M+H]^+$ 354.0141, Found: 354.0139.



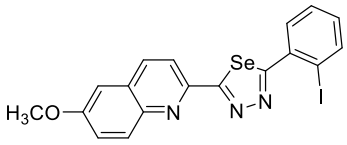
2-(6-methoxyquinolin-2-yl)-5-phenyl-1,3,4-selenadiazole (n8) Eluant: 8: 1; 17.7 mg, 68% yield; white solid; m.p. = 168 – 169 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.32 (d, *J* = 8.6 Hz, 1H), 8.29 – 8.24 (m, 2H), 8.19 (dd, *J* = 16.9, 8.9 Hz, 2H), 7.58 – 7.51 (m, 3H), 7.45 (dd, *J* = 9.2, 2.5 Hz, 1H), 7.13 (d, *J* = 3.0 Hz, 1H), 3.96 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 165.7, 164.4, 159.3, 144.2, 141.0, 136.0, 132.1, 131.7, 130.2, 129.1, 127.5, 123.8, 123.7, 120.4, 105.1, 55.8; IR (KBr): 2835, 1617, 1356, 1238, 823, 725, 680 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{13}N_3OSek$: $[M+k]^+$ 405.9856, Found: 405.9857.



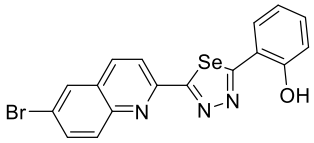
2-(2-iodophenyl)-5-(6-methoxyquinolin-2-yl)-1,3,4-selenadiazole (n9) Eluant: 8: 1; 15.9 mg, 66% yield; white solid; m.p. = 202 – 203 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.32 (d, *J* = 8.5 Hz, 1H), 8.25 – 8.18 (m, 3H), 8.15 (d, *J* = 9.2 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.45 (dd, *J* = 9.1, 2.6 Hz, 1H), 7.13 (d, *J* = 2.9 Hz, 1H), 3.97 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 164.9, 164.5, 159.4, 144.2, 140.9, 138.4, 136.0, 131.6, 130.3, 129.5, 128.8, 123.8, 122.3, 120.4, 105.2, 55.8; IR (KBr): 2928, 1597, 1361, 769 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{12}ClN_3OSeK$: $[M+K]^+$ 439.9464, Found: 439.9463.



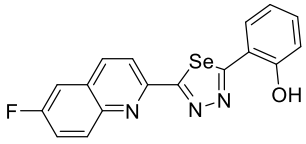
2-(4-fluorophenyl)-5-(6-methoxyquinolin-2-yl)-1,3,4-selenadiazole (n10) Eluant: 8: 1; 15.9 mg, 67% yield; white solid; m.p. = 178–179 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.31 (d, *J* = 8.5 Hz, 1H), 8.29 – 8.24 (m, 2H), 8.21 (d, *J* = 8.6 Hz, 1H), 8.15 (d, *J* = 9.1 Hz, 1H), 7.45 (dd, *J* = 9.3, 2.9 Hz, 1H), 7.26 – 7.20 (m, 2H), 7.13 (d, *J* = 2.9 Hz, 1H), 3.96 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 165.1 (d, *J* = 253.4 Hz), 164.9, 164.4, 159.3, 144.1, 140.9, 136.0, 131.6, 130.2, 129.8 (d, *J* = 9.3 Hz), 123.7, 120.3, 120.1 (d, *J* = 3.1 Hz), 116.5 (d, *J* = 22.2 Hz), 105.2, 55.8; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -99.2 – -112.1 (m, 1F); IR (KBr): 2825, 1612, 1341, 764 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{12}FN_3OSeK$: $[M+K]^+$ 423.9762, Found: 423.9766.



2-(2-iodophenyl)-5-(6-methoxyquinolin-2-yl)-1,3,4-selenadiazole (n11); Eluant: 8: 1; 17.8 mg, 64% yield; white solid; m.p. = 152 – 153 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.33 (d, *J* = 8.6 Hz, 1H), 8.22 (d, *J* = 8.6 Hz, 1H), 8.16 (d, *J* = 9.2 Hz, 1H), 8.08 (d, *J* = 7.5 Hz, 1H), 7.99 – 7.94 (m, 1H), 7.53 – 7.48 (m, 1H), 7.44 (dd, *J* = 9.2, 3.0 Hz, 1H), 7.26 – 7.20 (m, 1H), 7.13 (d, *J* = 3.0 Hz, 1H), 3.96 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 165.2, 164.7, 159.4, 144.2, 141.8, 141.3, 140.8, 136.1, 132.7, 131.8, 130.3, 129.2, 128.3, 123.8, 120.4, 105.1, 94.8, 55.8; IR (KBr): 2825, 1597, 1356, 770 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{18}H_{13}IN_3OSe$: $[M+H]^+$ 493.9264, Found: 493.9260.

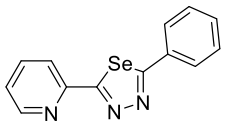


2-(5-(6-bromoquinolin-2-yl)-1,3,4-selenadiazol-2-yl)phenol (n12) Eluant: 8: 1; 14.6 mg, 59% yield; white solid; m.p. = 219 – 220 ℃; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.47 (s, 1H), 8.64 (d, *J* = 8.8 Hz, 1H), 8.46 (d, *J* = 2.3 Hz, 1H), 8.40 (d, *J* = 8.6 Hz, 1H), 8.15 (d, *J* = 9.1 Hz, 1H), 8.02 (dd, *J* = 8.9, 2.3 Hz, 1H), 7.93 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.56 – 7.49 (m, 1H), 7.15 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.08 (td, *J* = 7.6, 1.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.1, 163.6, 157.1, 146.4, 144.0, 137.9, 134.6, 134.4, 132.0, 130.9, 130.1, 129.8, 122.1, 121.2, 120.3, 117.7, 110.1; IR (KBr): 3445, 2928, 1592, 1361, 1060, 774 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{10}BrN_3OSe$ Na: $[M+Na]^+$ 453.9062, Found: 453.9061.



2-(5-(6-fluoroquinolin-2-yl)-1,3,4-selenadiazol-2-yl)phenol (n13) Eluant: 8: 1; 13.9 mg, 60% yield; white solid; m.p. = 210 – 211 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 10.17 (s, 1H), 8.38 (d, J = 8.6 Hz, 1H), 8.32 (d, *J* = 4.9 Hz, 1H), 8.30 – 8.26 (m, 1H), 8.06 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.64 – 7.56 (m, 1H), 7.55 – 7.50 (m, 1H), 7.50 – 7.45 (m, 1H), 7.16 (dd, *J* = 8.5, 1.1 Hz, 1H),

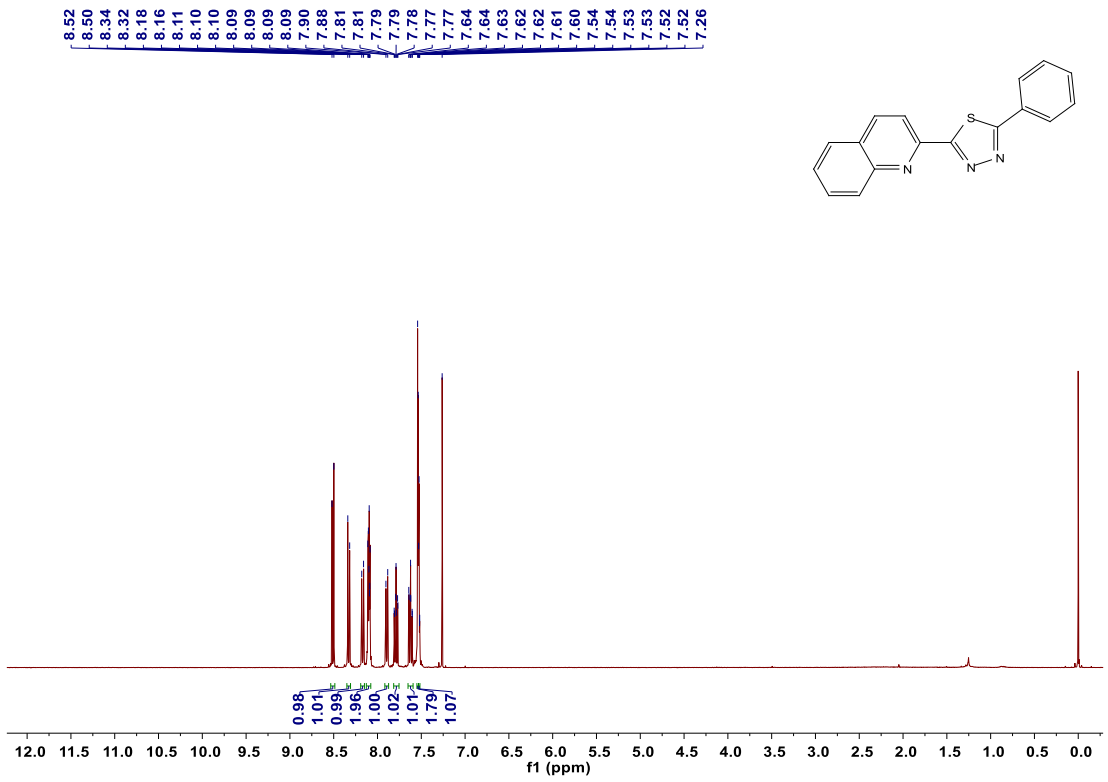
7.10 – 7.03 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 165.6, 162.6, 161.7 (d, *J* = 252.1 Hz), 158.0, 145.2, 142.4, 137.0 (d, *J* = 5.8 Hz), 134.3, 132.9 (d, *J* = 9.2 Hz), 129.8 (d, *J* = 10.2 Hz), 127.4, 121.3 (d, *J* = 26.0 Hz), 120.7, 120.1, 117.7, 111.1 (d, *J* = 22.0 Hz), 107.9; IR (KBr): 3431, 2835, 1597, 1361, 1065, 774 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{17}H_{10}FN_3OSeK$: $[M+K]^+$ 409.9605, Found: 409.9601.

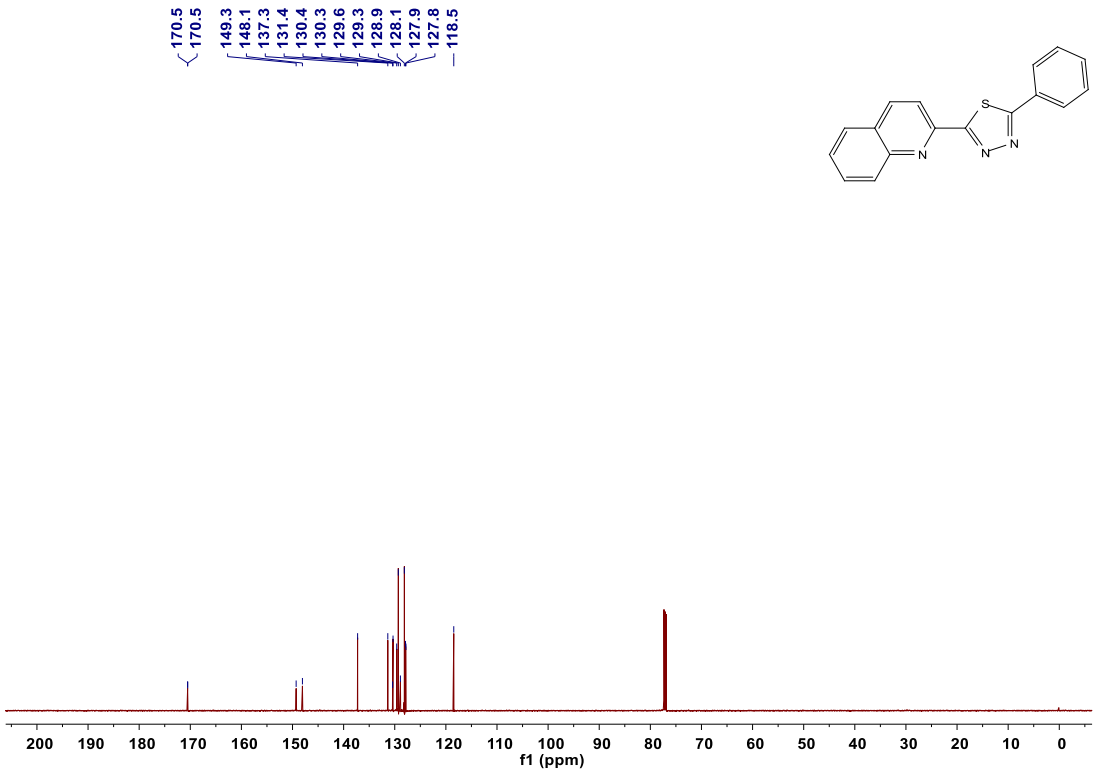


2-phenyl-5-(pyridin-2-yl)-1,3,4-selenadiazole (n14) Eluant: 8: 1; 7.7 mg, 37% yield; white solid; m.p. = 166 – 167 ℃; ^{1}H NMR (400 MHz, Chloroform-*d*, TMS) δ 8.67 (d, *J* = 4.7 Hz, 1H), 8.40 (d, *J* = 8.1 Hz, 1H), 8.05 (d, *J* = 3.7 Hz, 2H), 7.87 (t, *J* = 7.5 Hz, 1H), 7.52 (q, *J* = 3.4 Hz, 3H), 7.40 (dd, *J* = 7.8, 4.5 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*, TMS) δ 170.0, 170.0, 149.9, 149.2, 137.2, 131.3, 130.2, 129.2, 128.0, 125.3, 121.0; IR (KBr): 2825, 1592, 764, 685, 610 cm^{-1}; HRMS Calcd(ESI) m/z for $C_{13}H_9N_3SeNa$: $[M+Na]^+$ 309.9854, Found: 309.9855.

11. Appendix (copies of ^{1}H and ^{13}C NMR spectra)

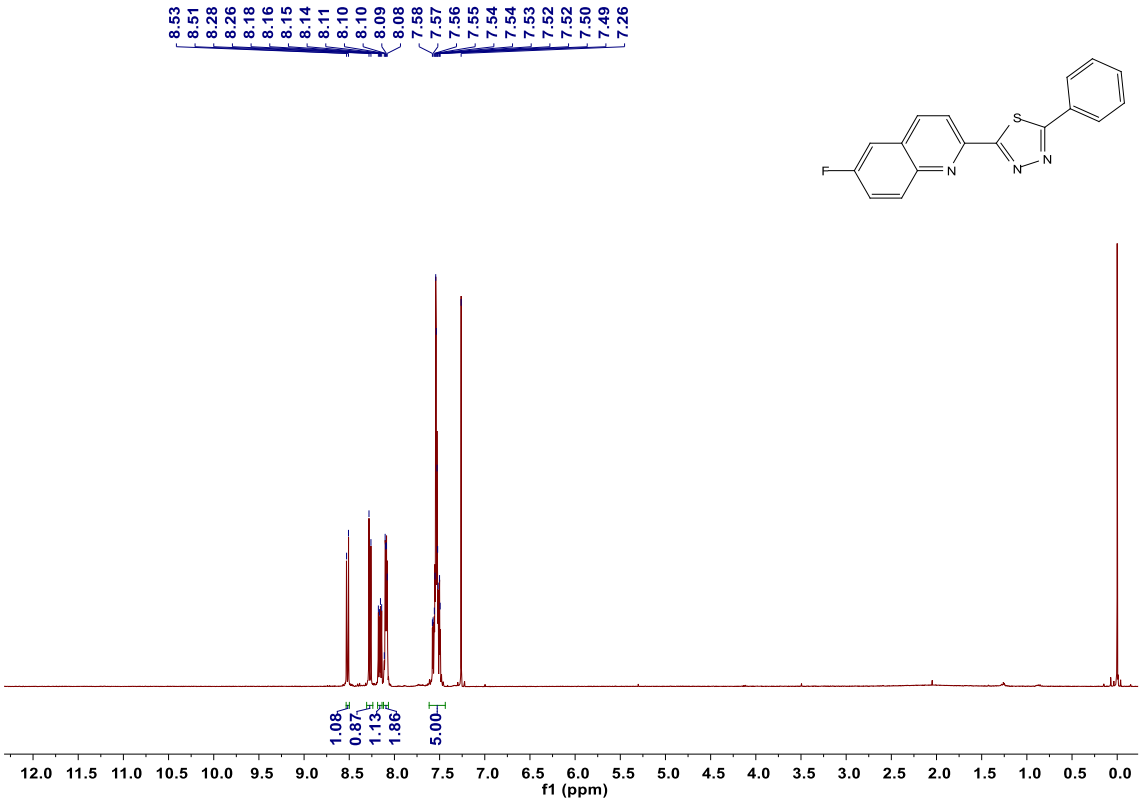
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m1**

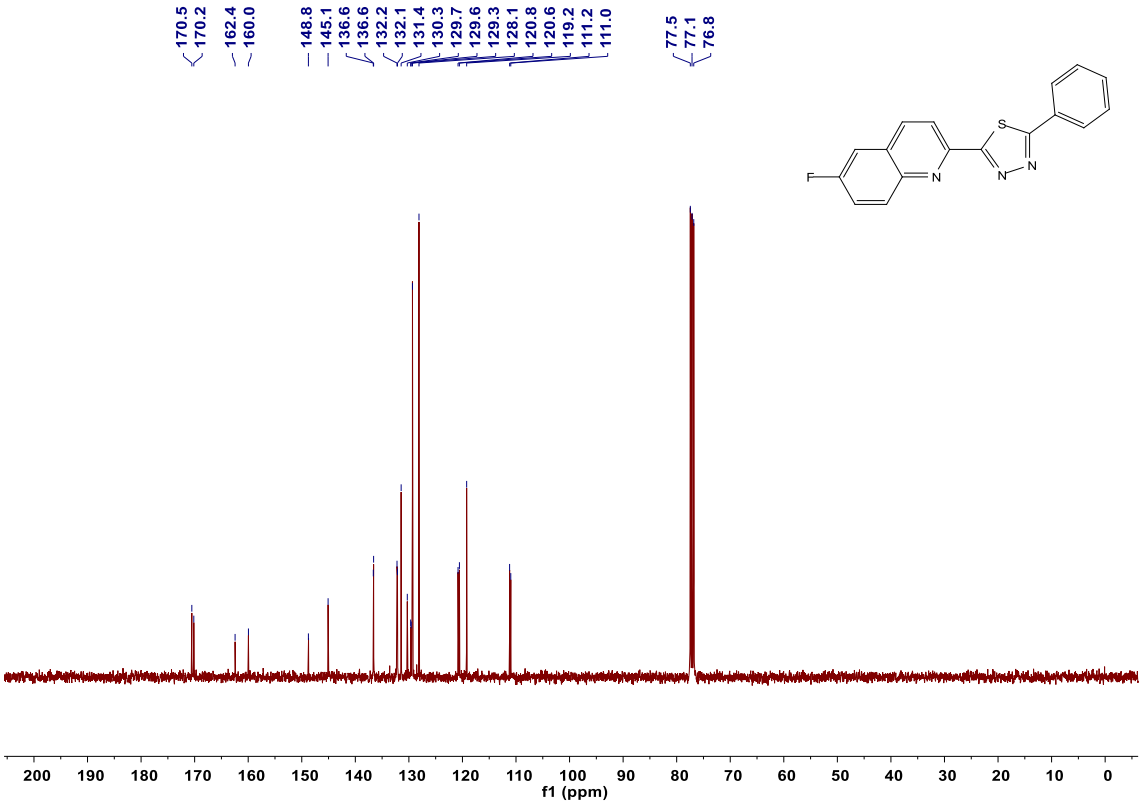


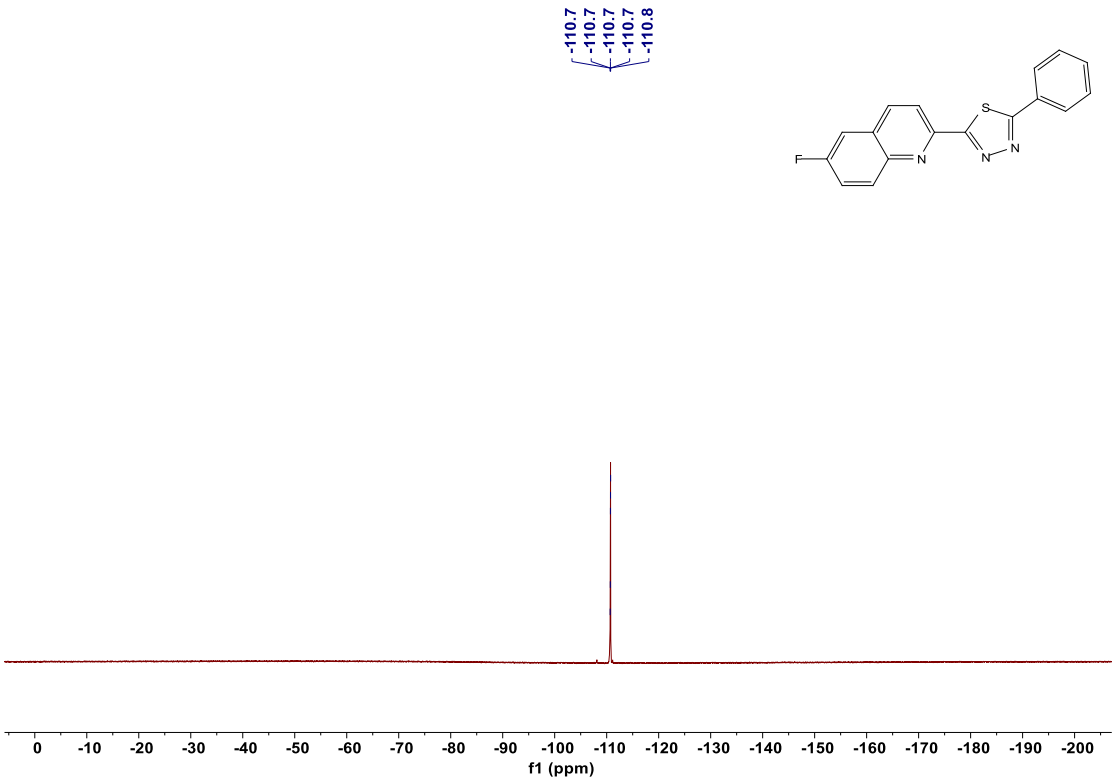


^{1}H NMR (400 MHz, Chloroform-*d*), ^{13}C NMR (100 MHz, Chloroform-*d*), and

^{19}F NMR (376 MHz, Chloroform-*d*) of **m2**






-110.7
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-110.7
-110.7
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F
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-10
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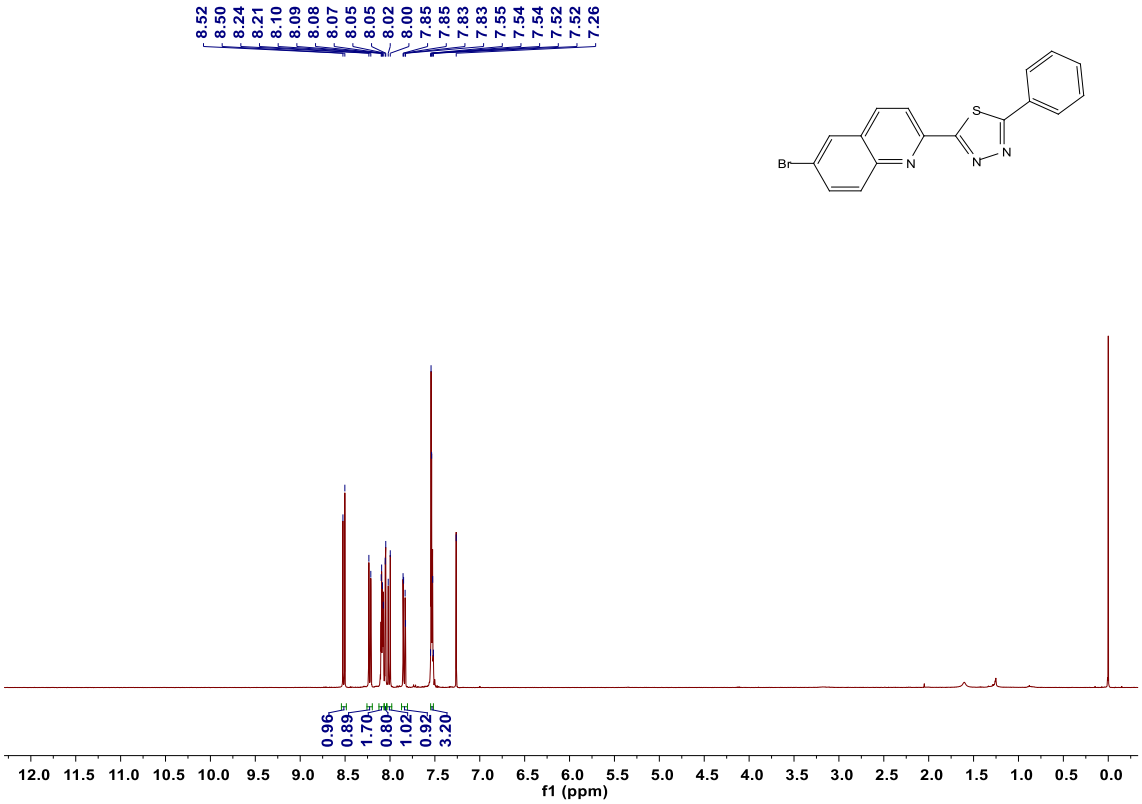
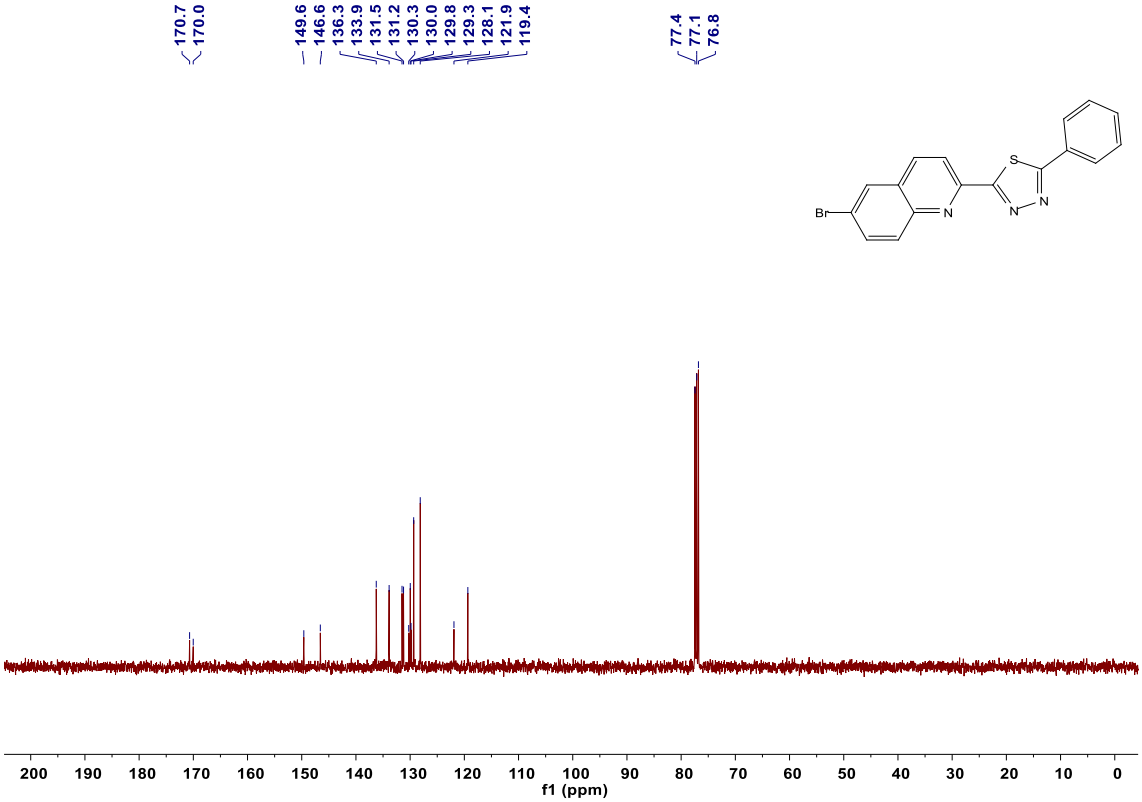
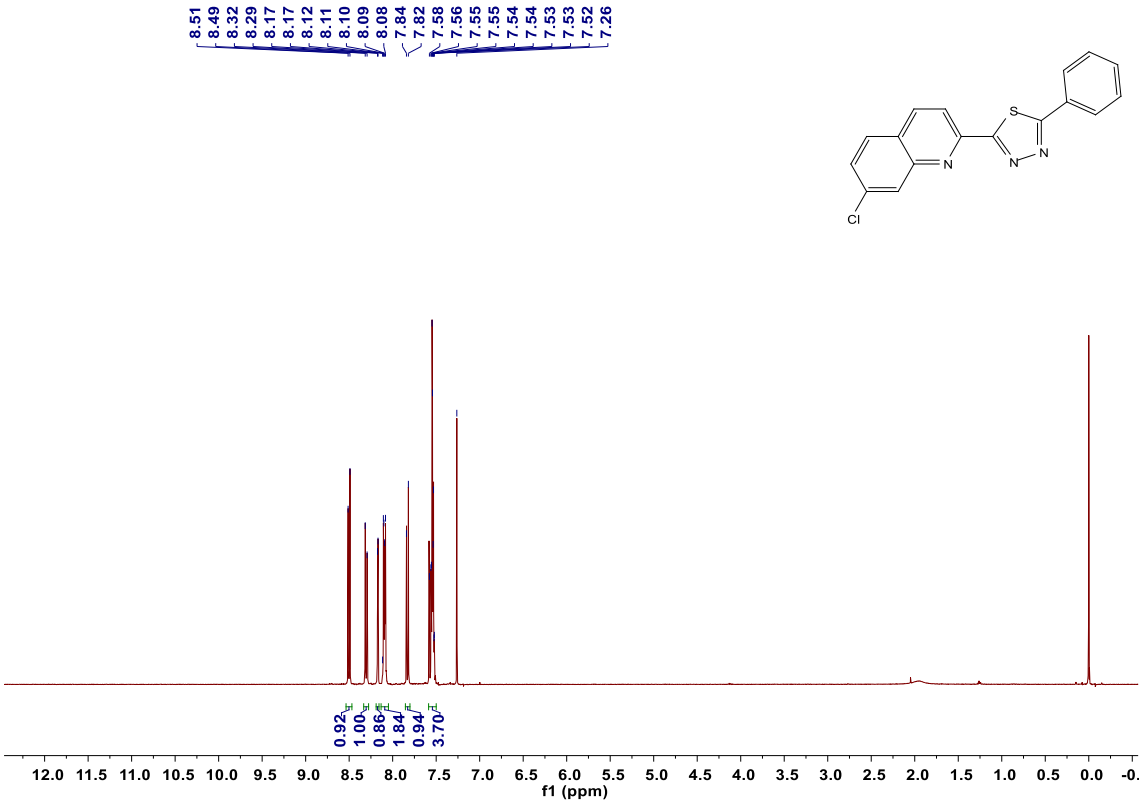
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

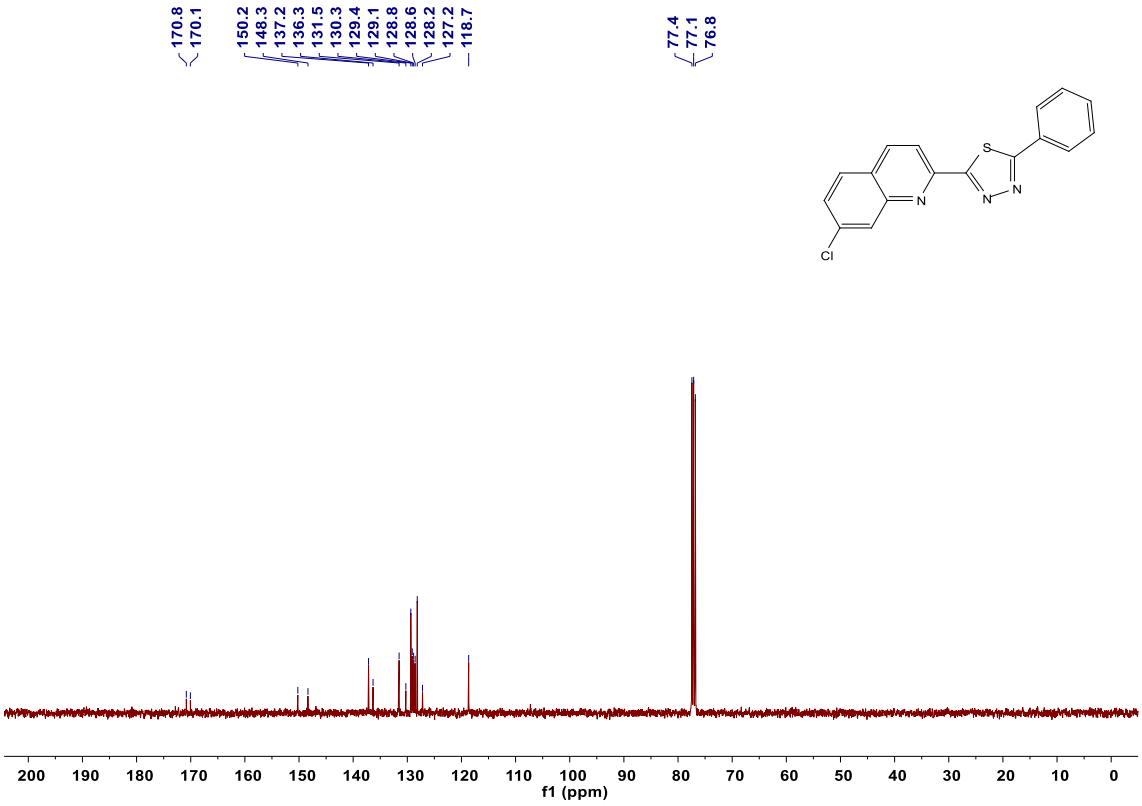
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m3**



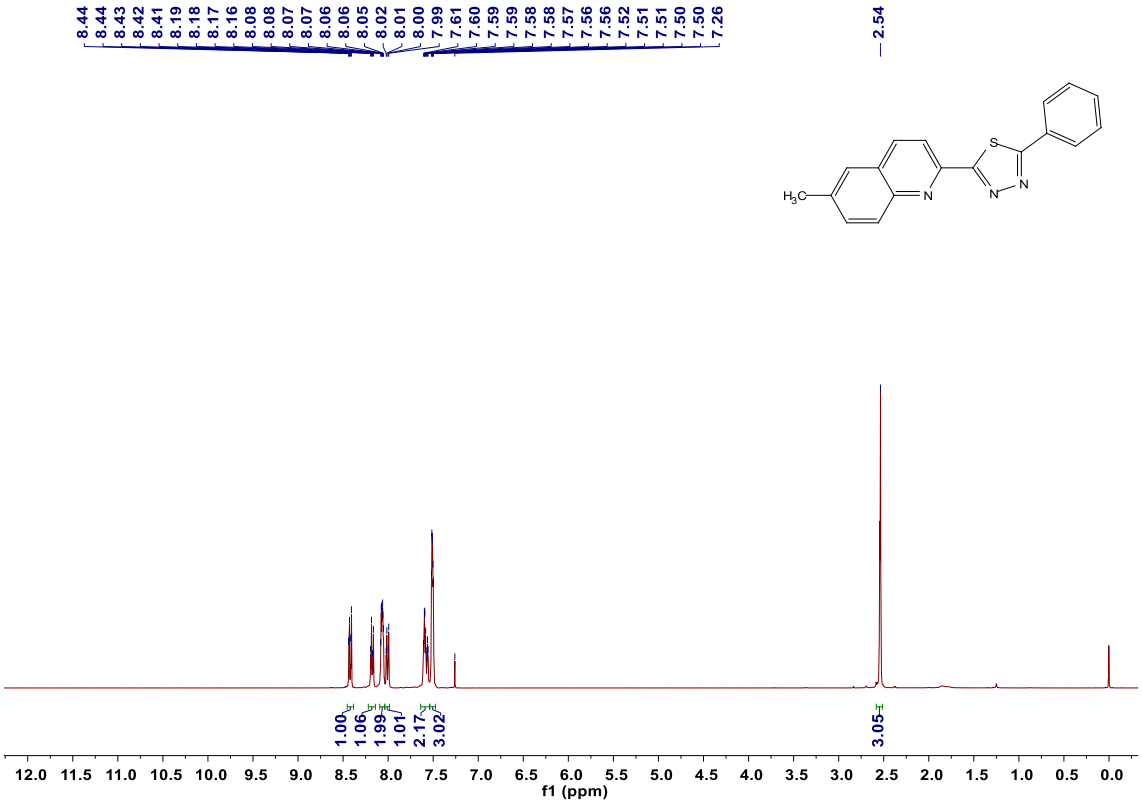


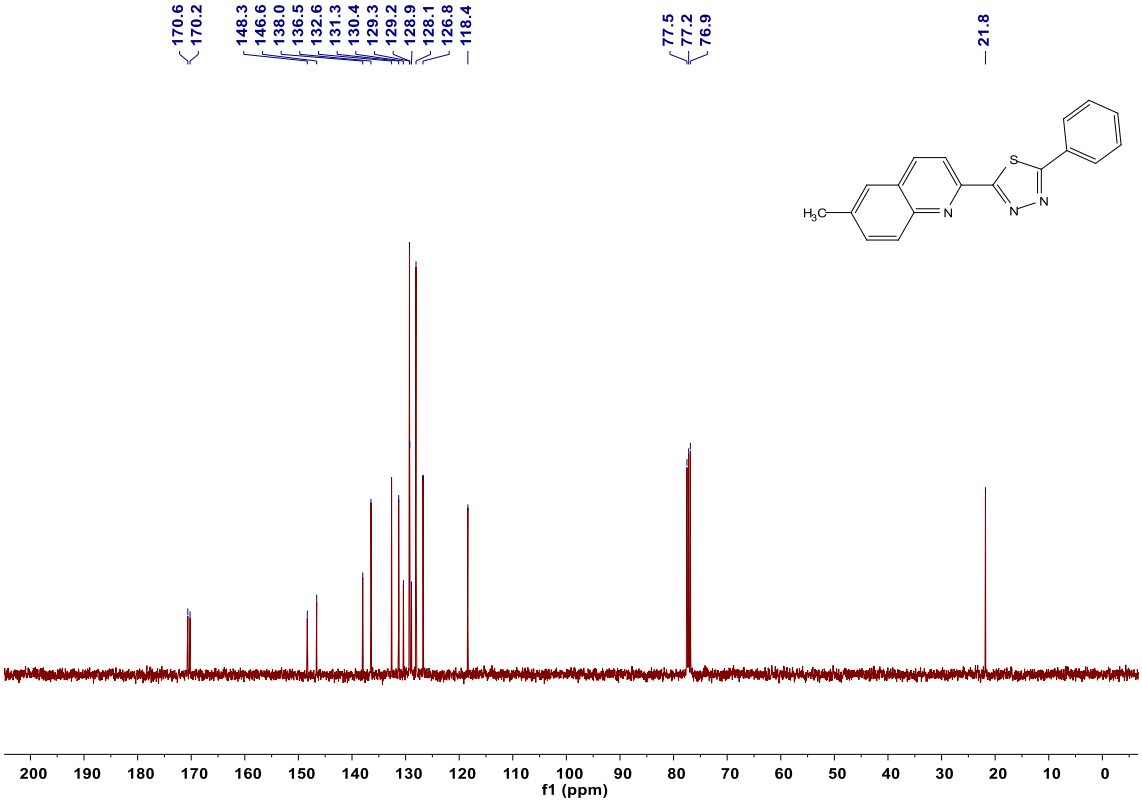
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m4**



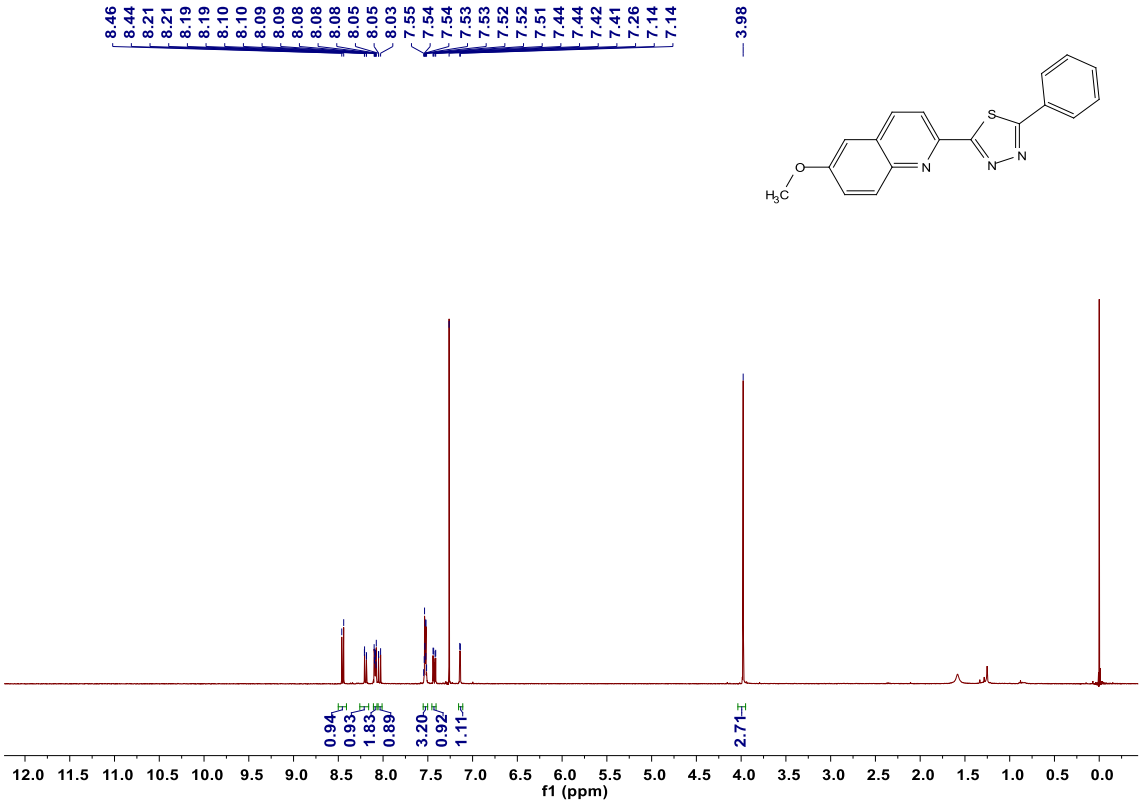


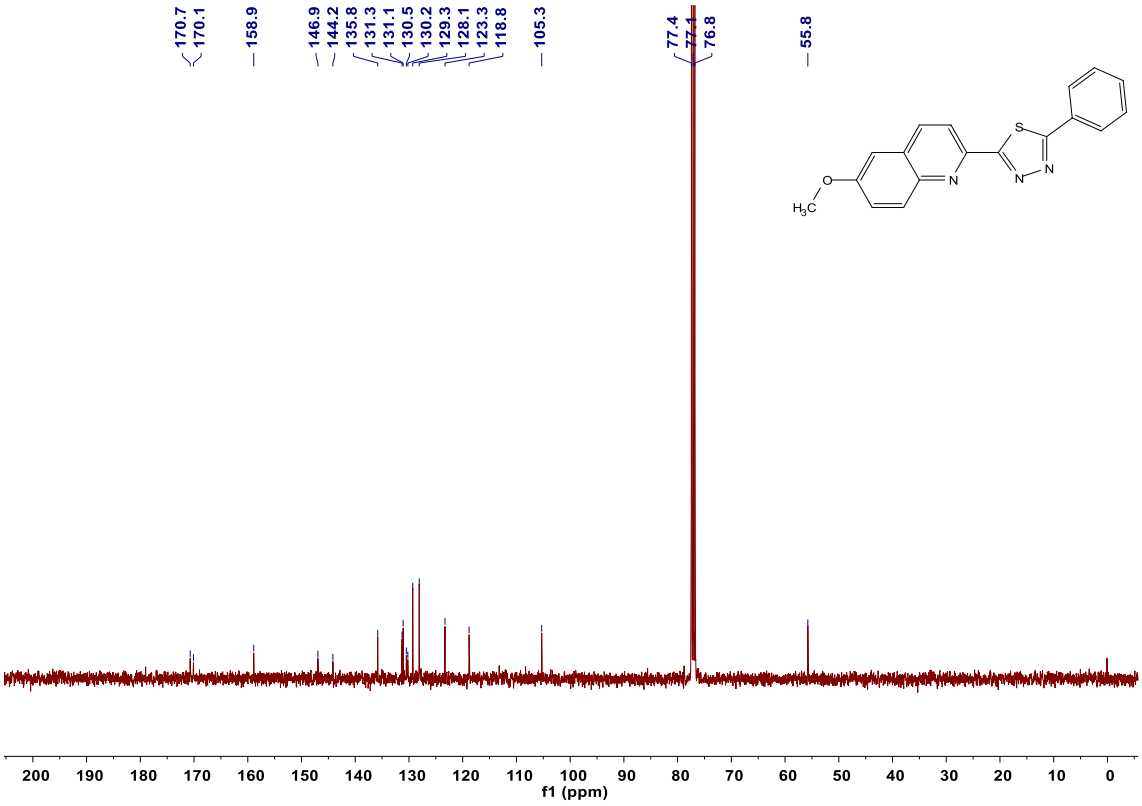
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m5**



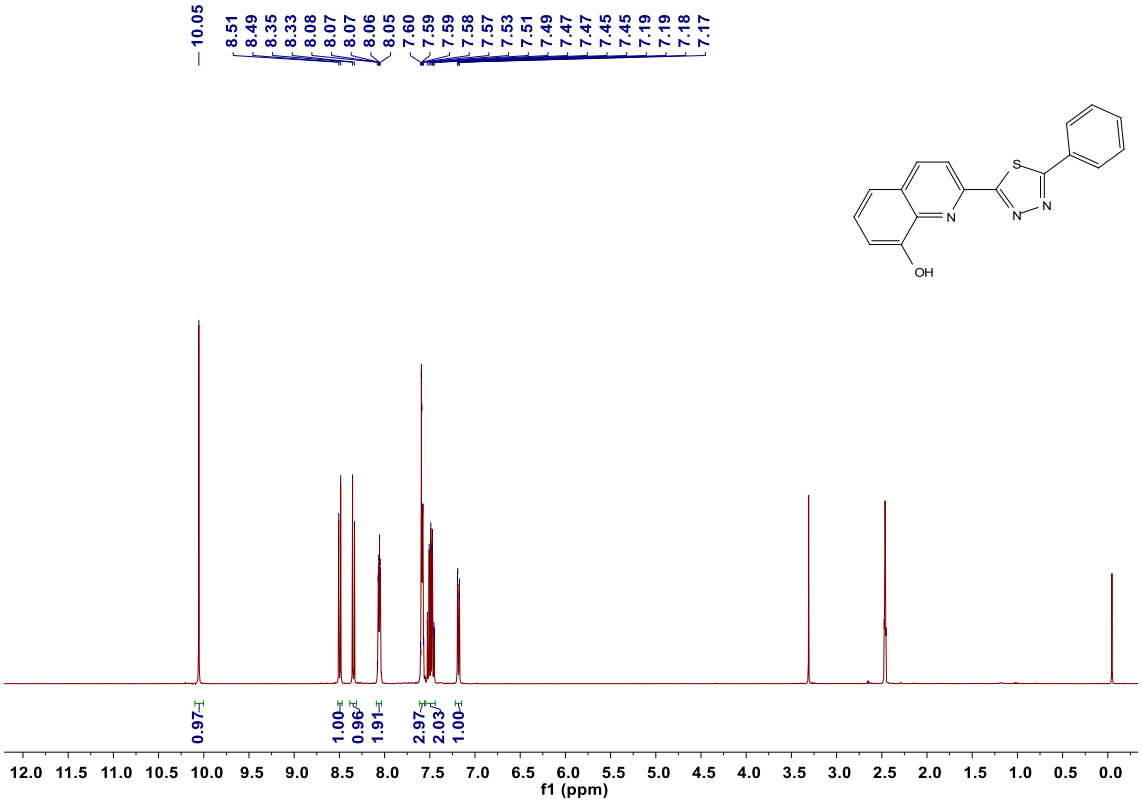


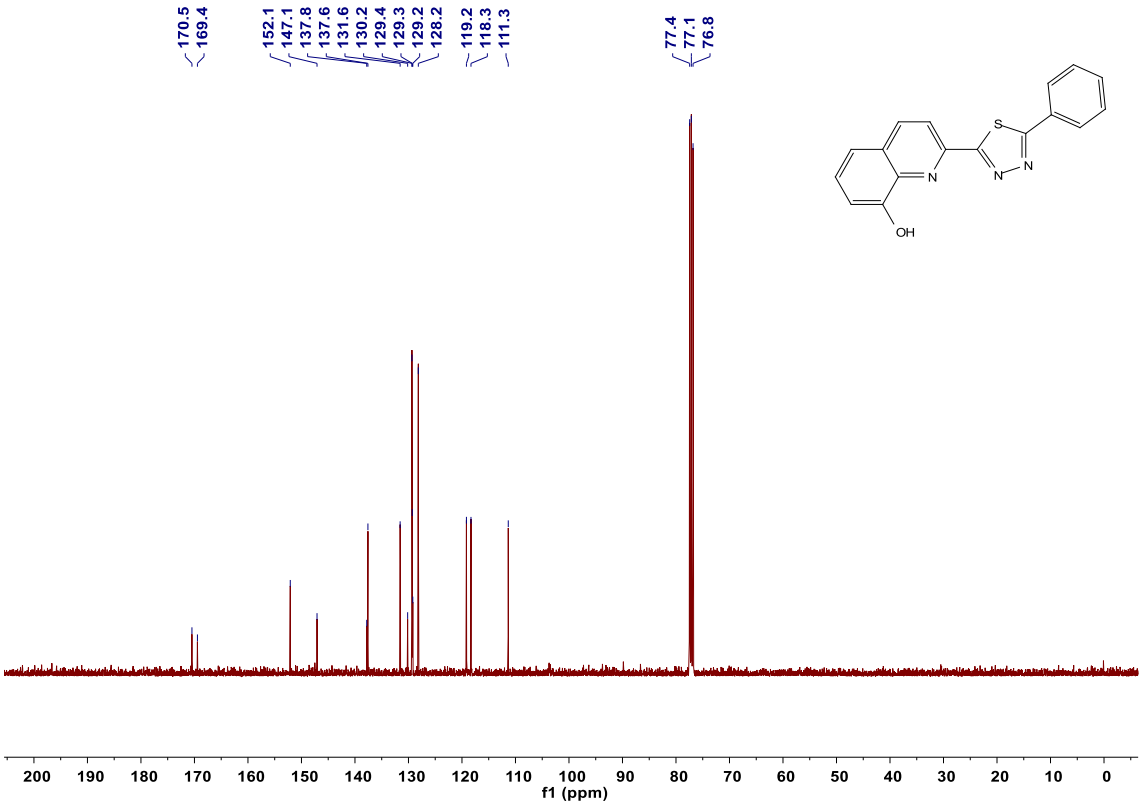
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m6**



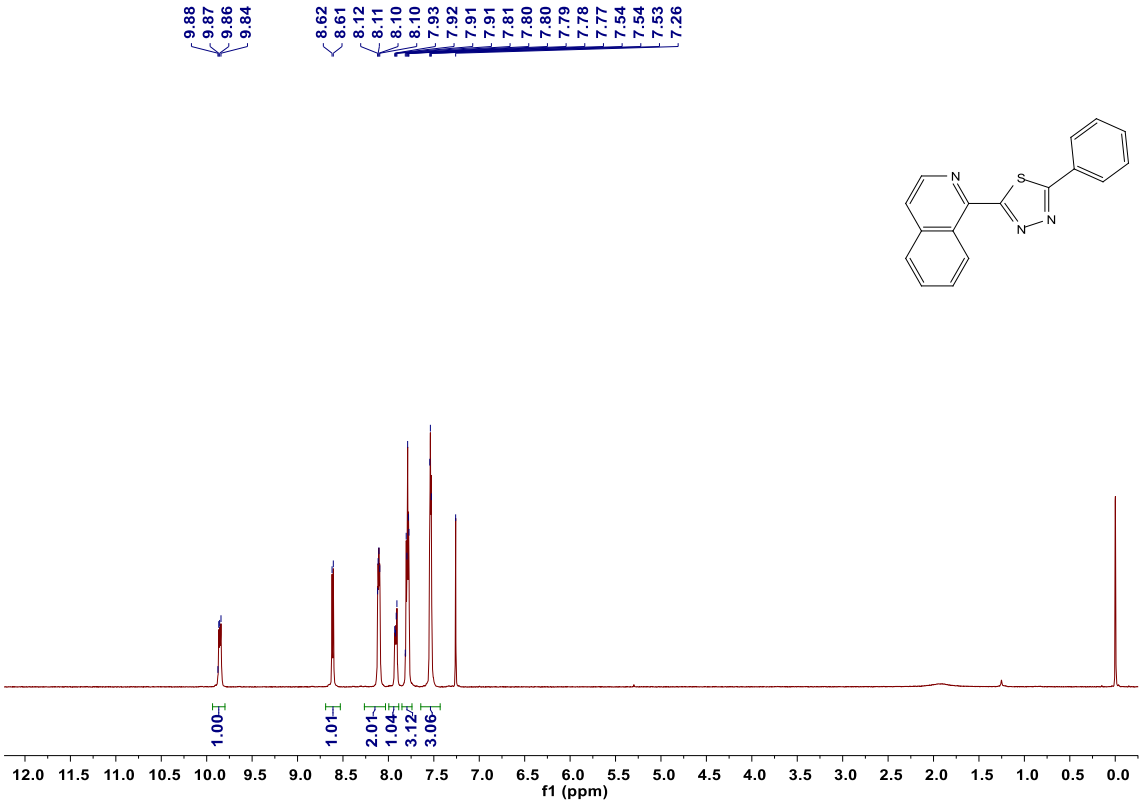


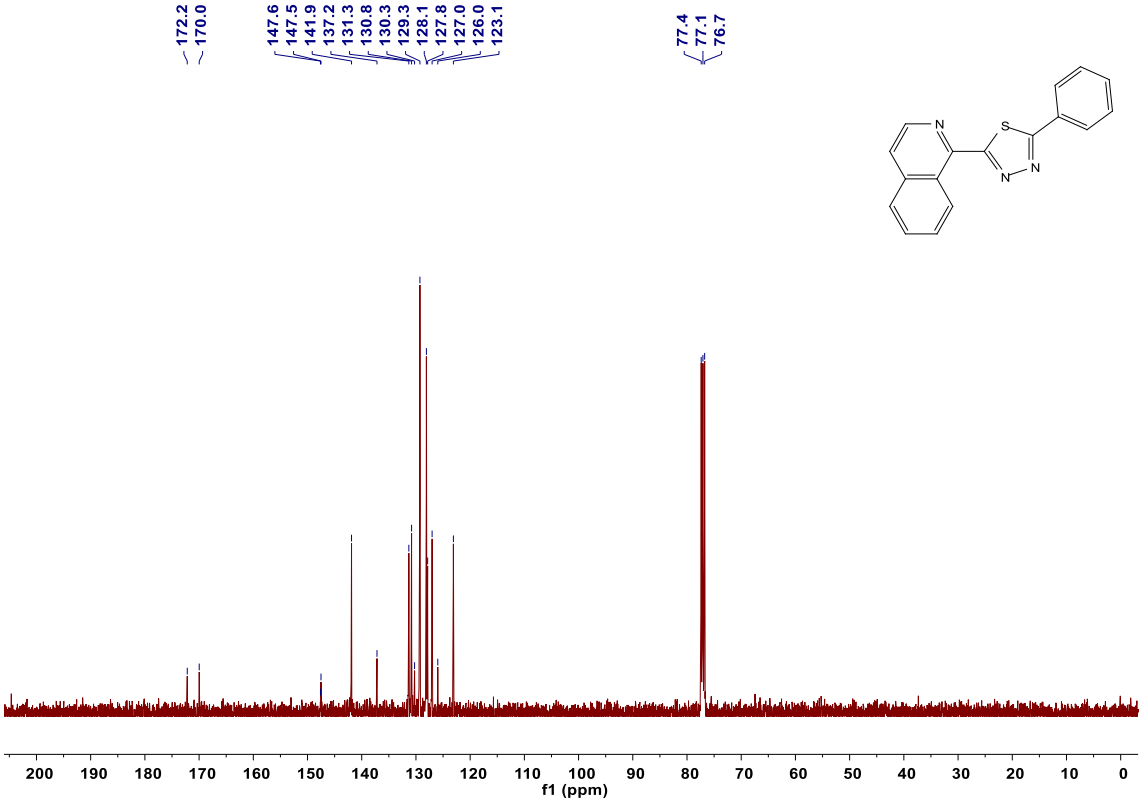
^{1}H NMR (400 MHz, DMSO-*d6)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m7**



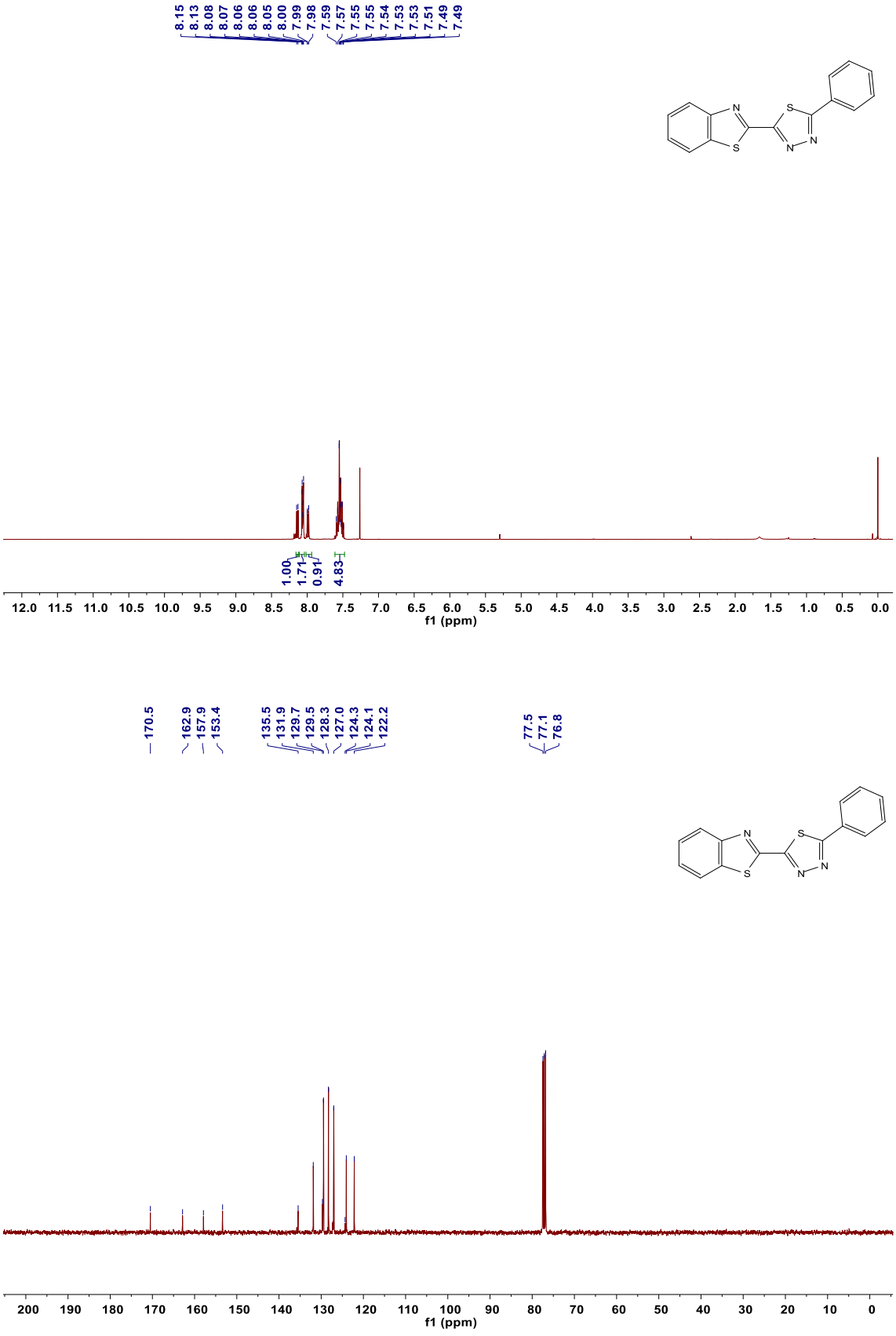


^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m8**

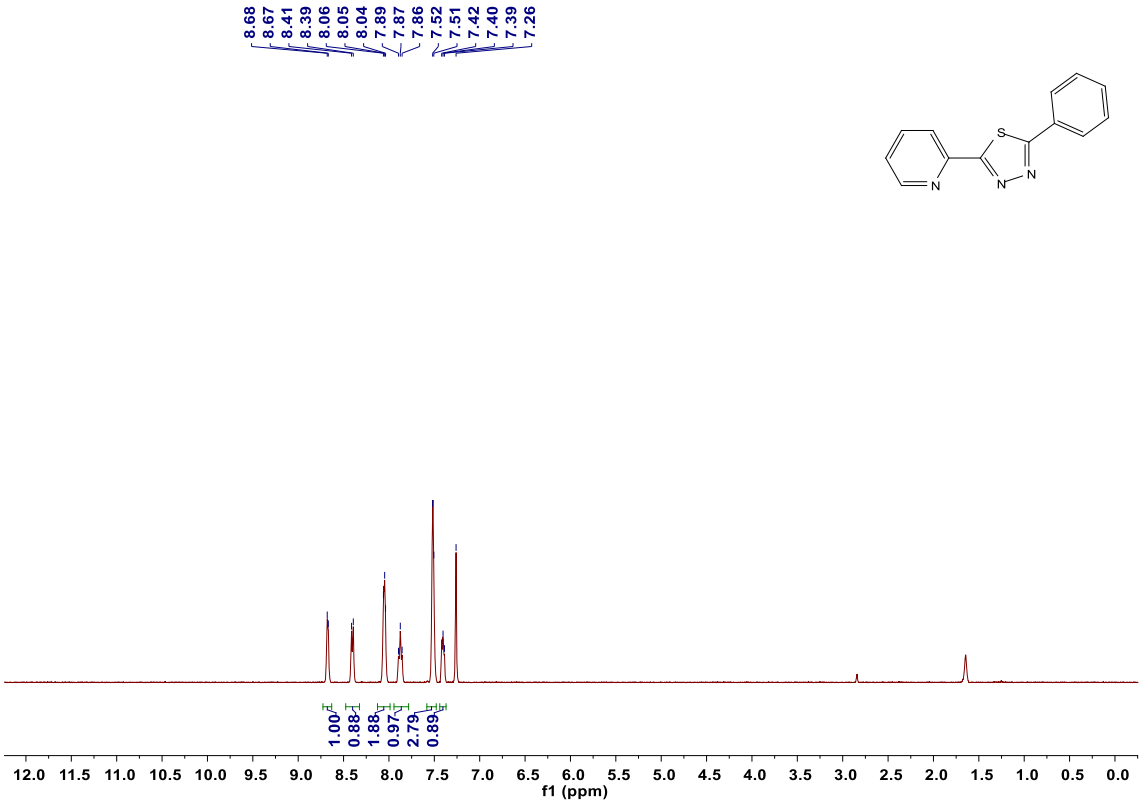


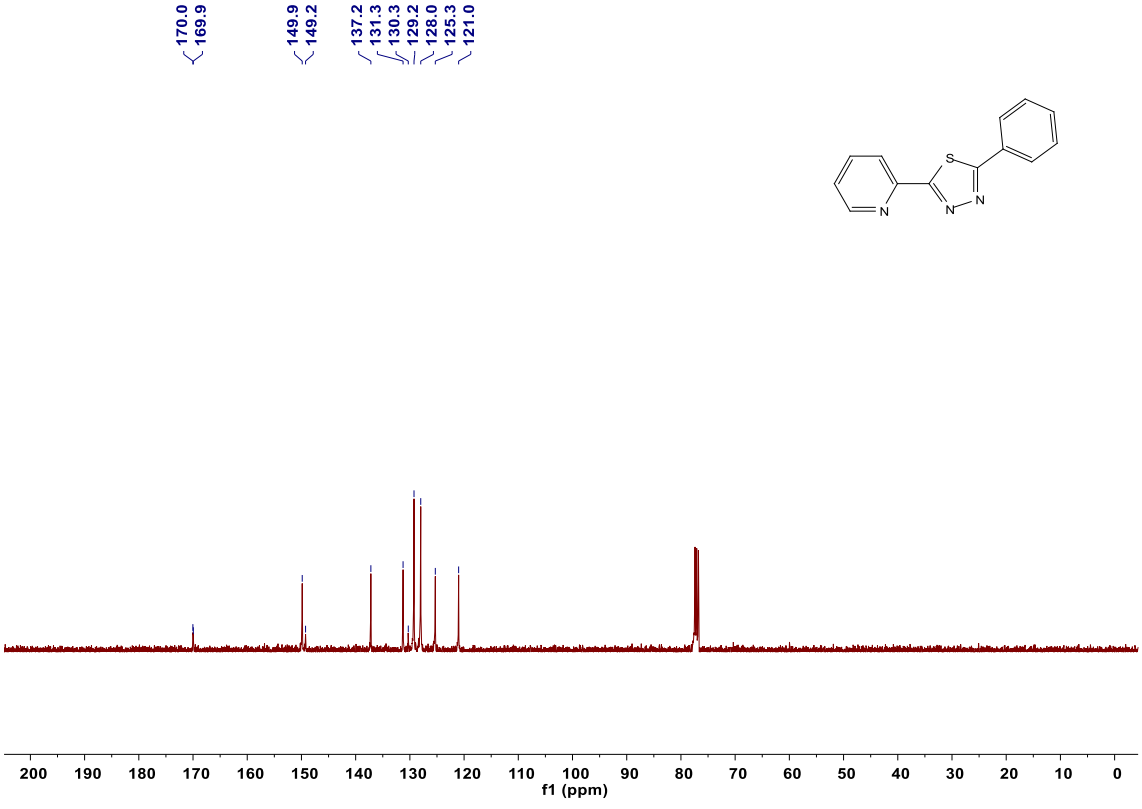


^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m9**

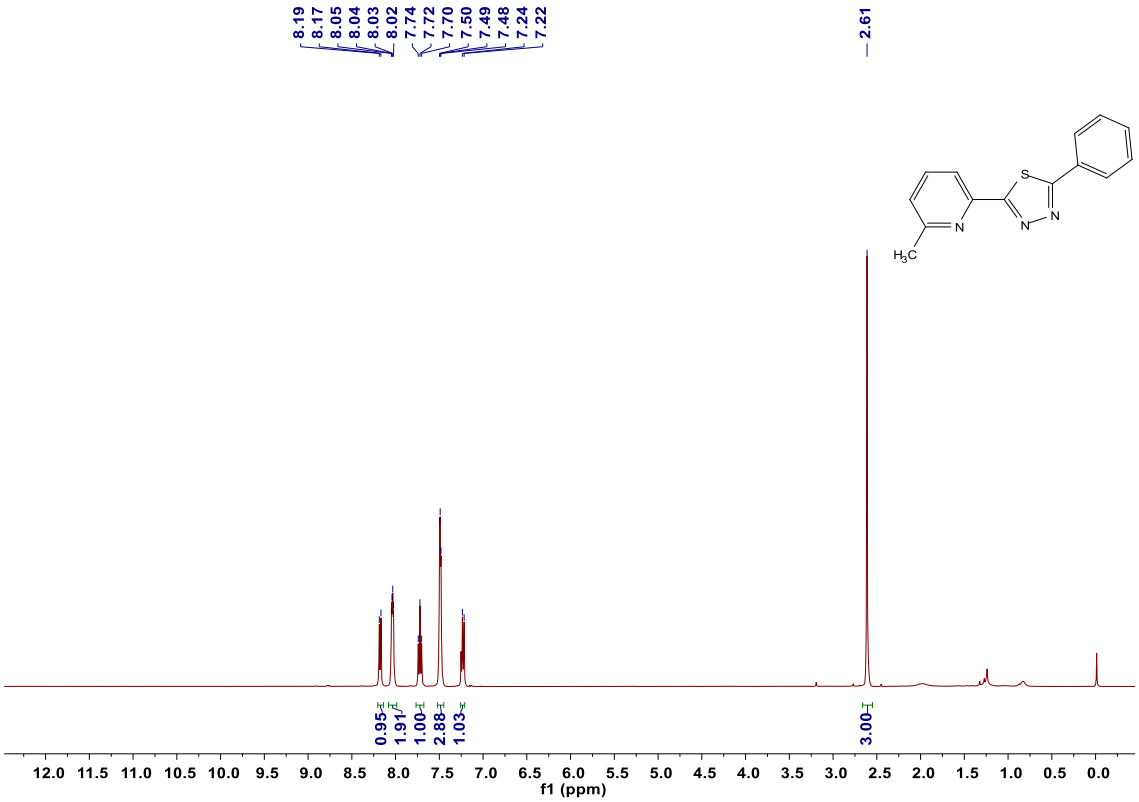


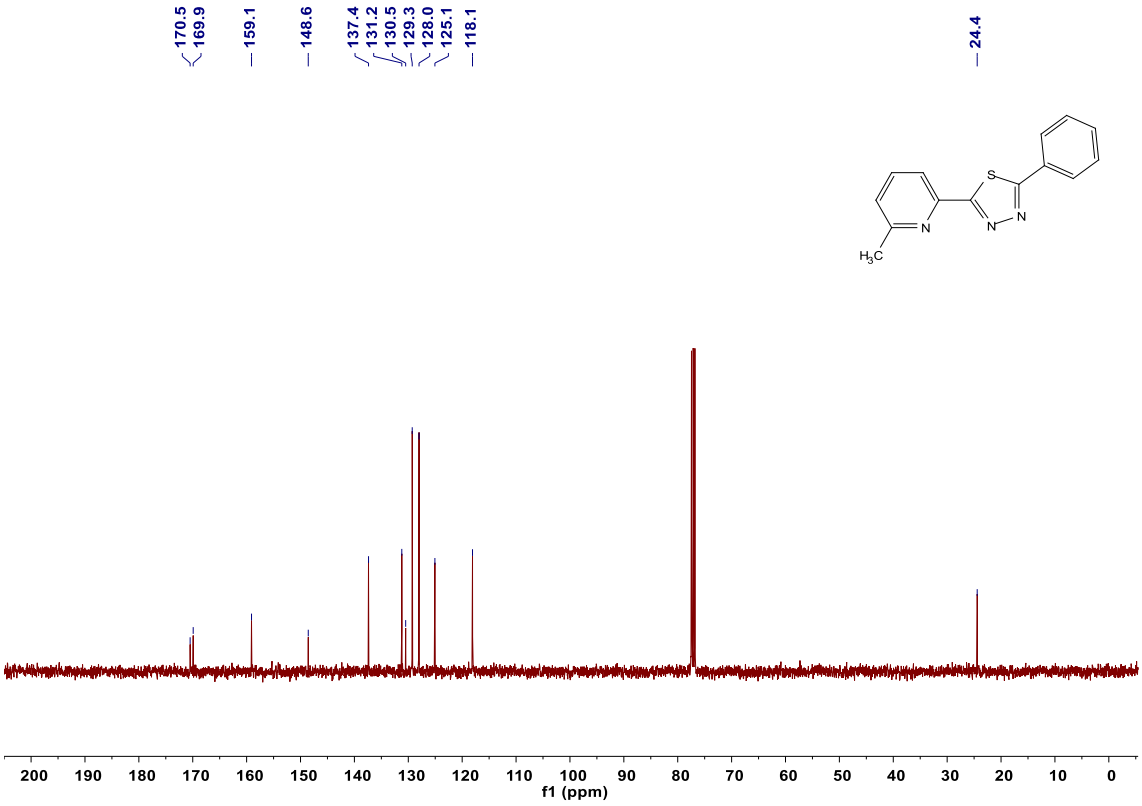
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m10**



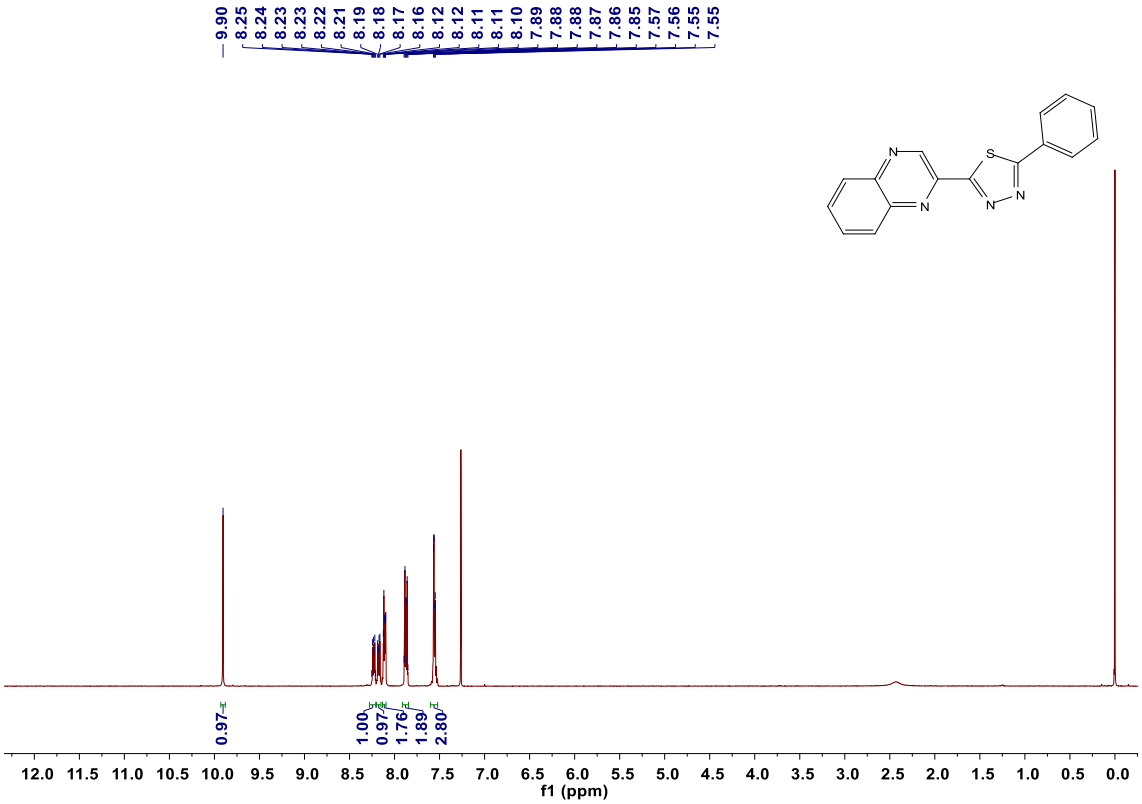


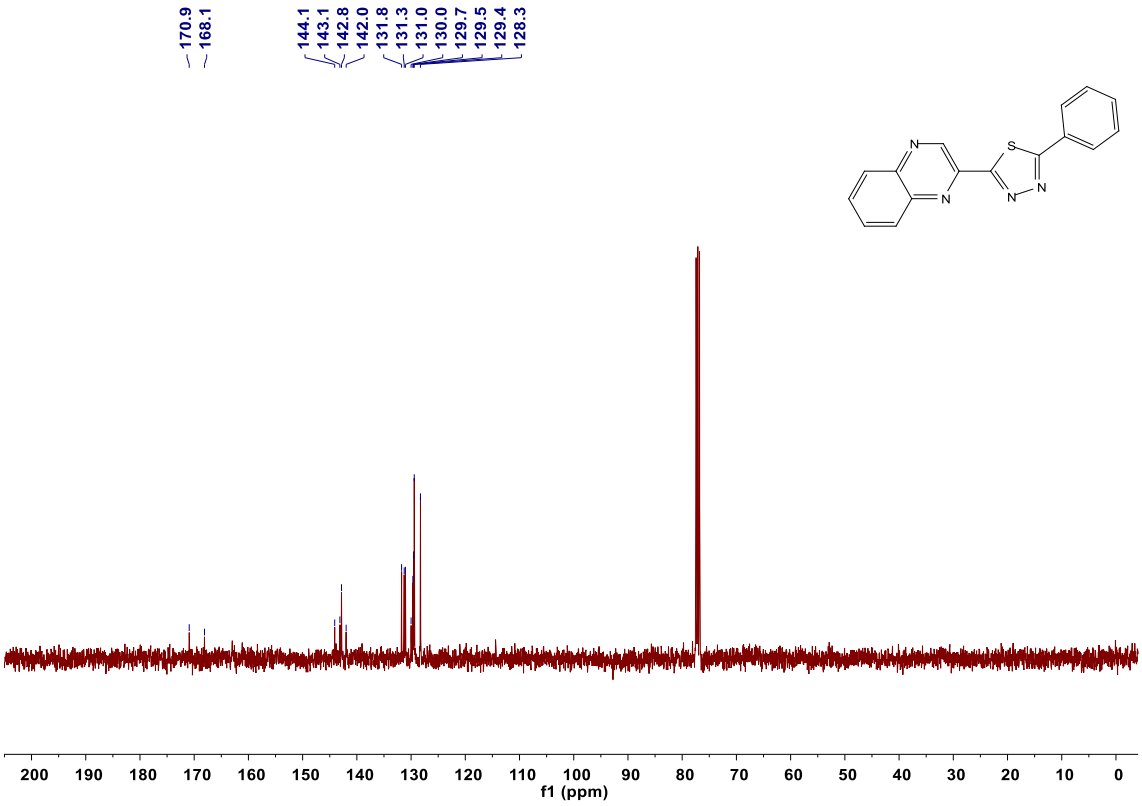
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m11**





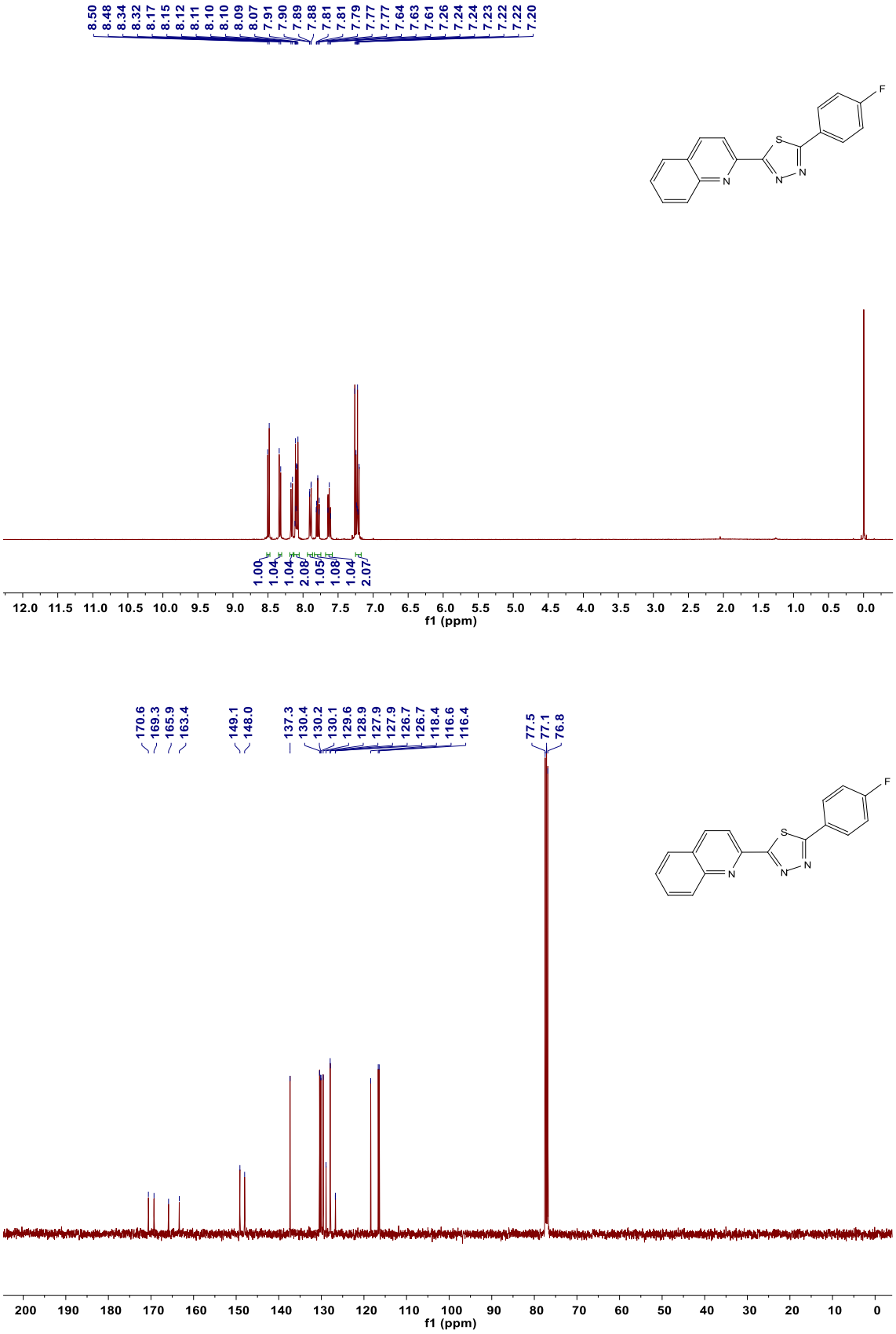
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m12**

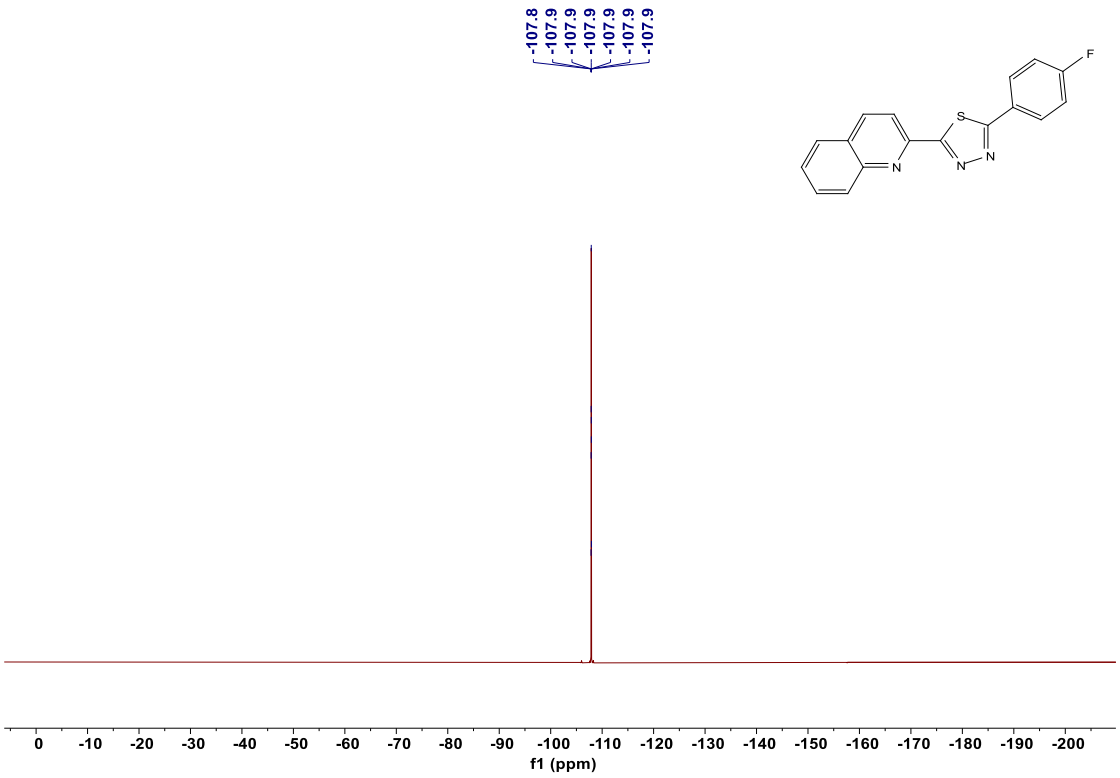




^{1}H NMR (400 MHz, Chloroform-*d*), ^{13}C NMR (100 MHz, Chloroform-*d*), and

^{19}F NMR (376 MHz, Chloroform-*d*) of **m13**

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-107.9
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-30
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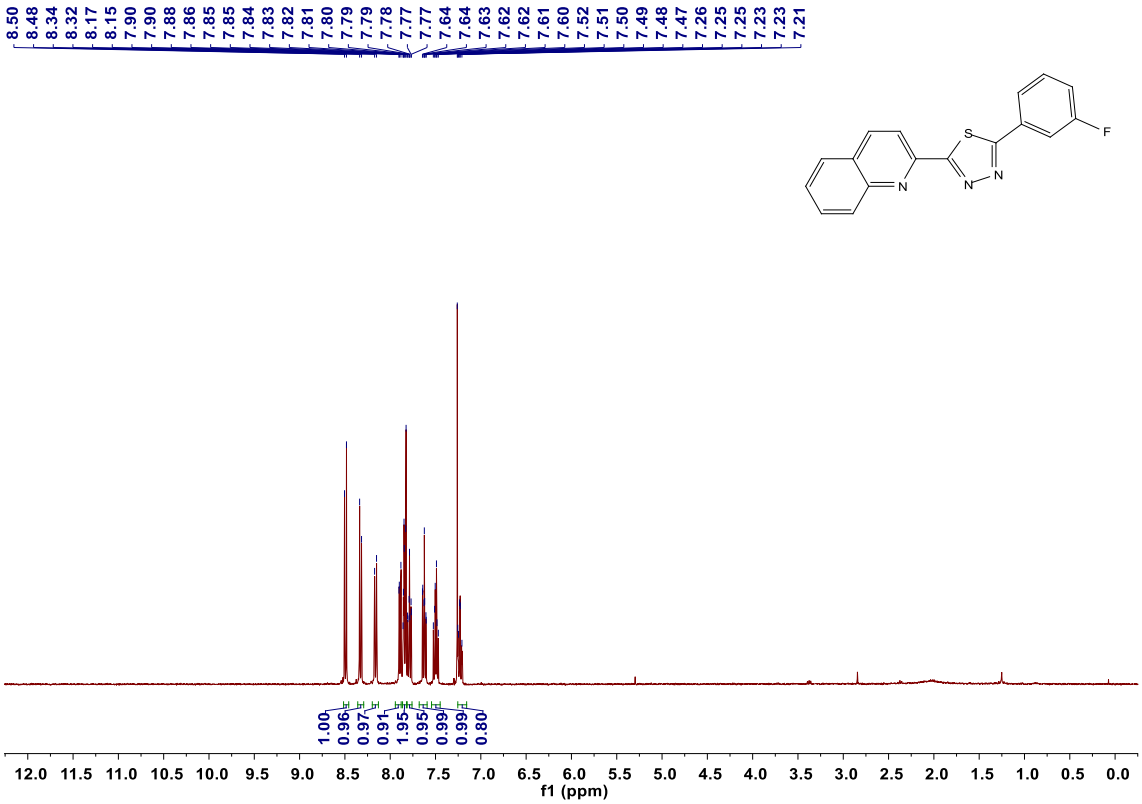
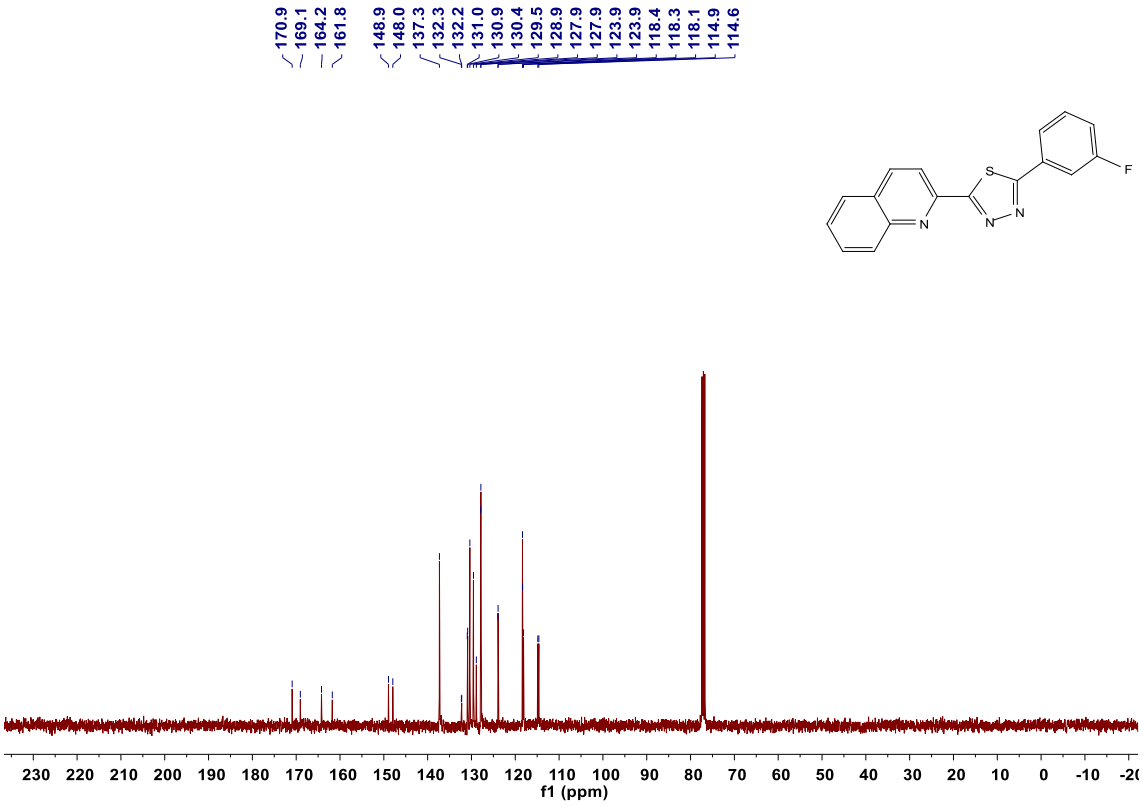
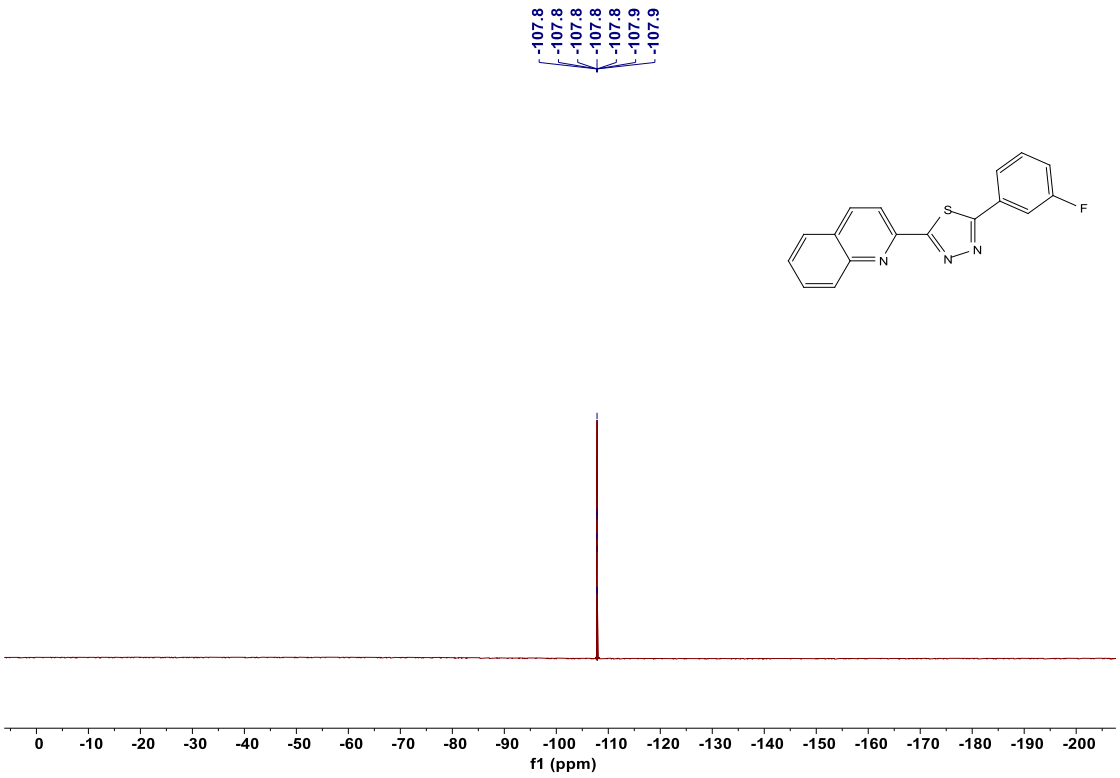
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

^{1}H NMR (400 MHz, Chloroform-*d*), ^{13}C NMR (100 MHz, Chloroform-*d*), and

^{19}F NMR (376 MHz, Chloroform-*d*) of **m14**






-107.8
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-107.9
-107.9
S
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N
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-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
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-180
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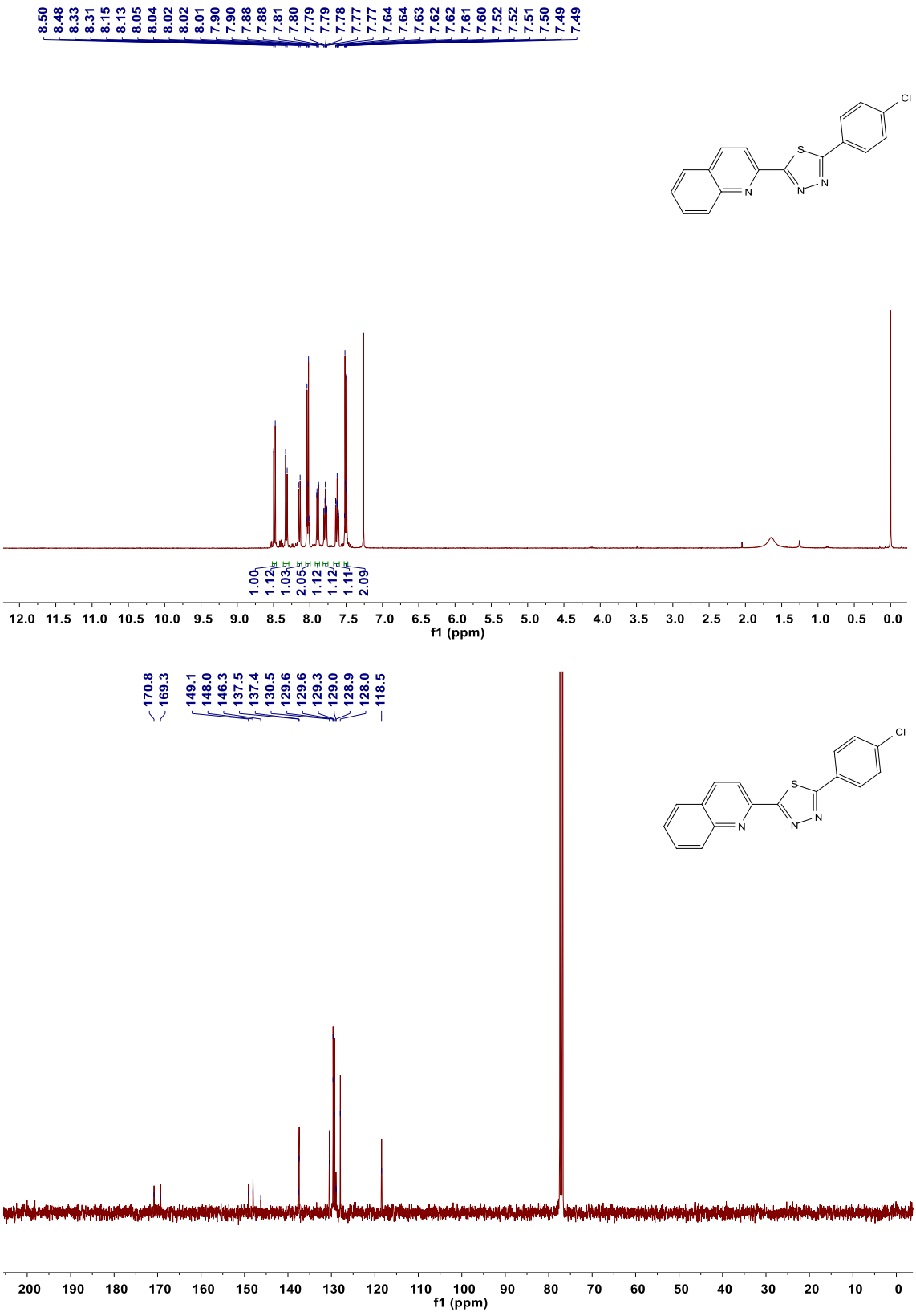
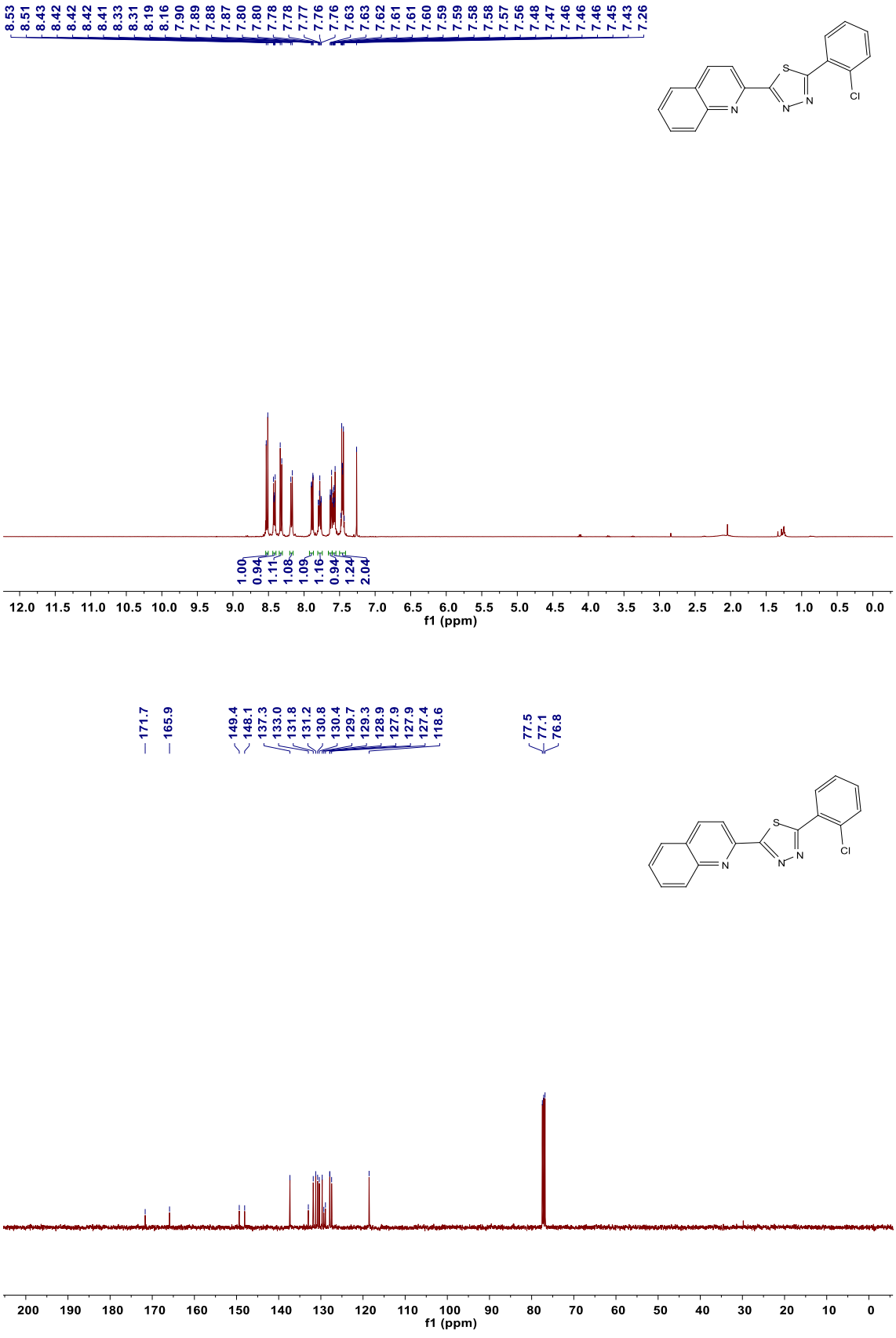
-200
f1 (ppm)

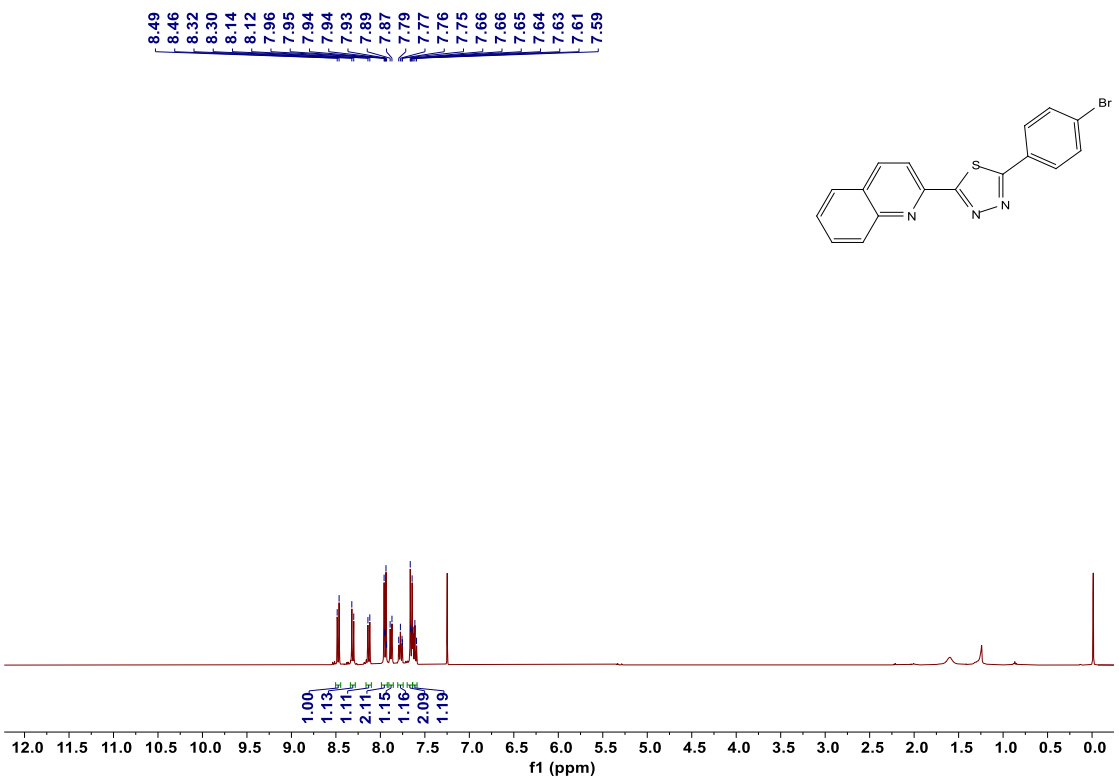
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m15**

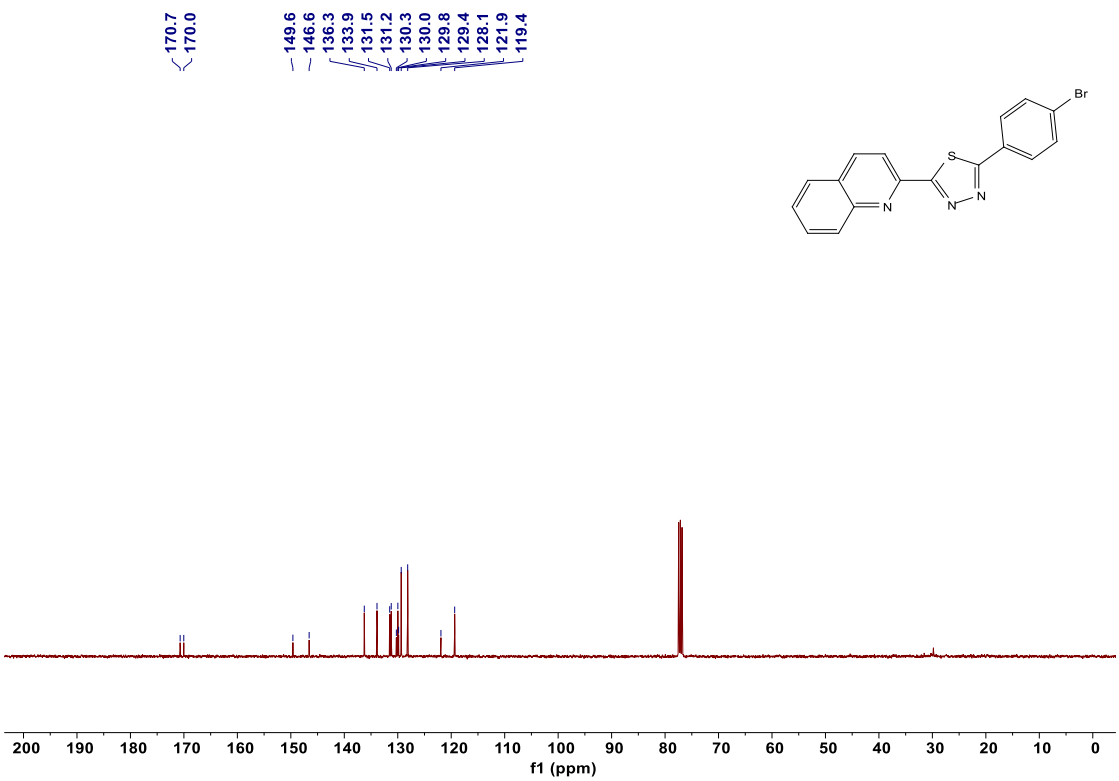


^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m16**

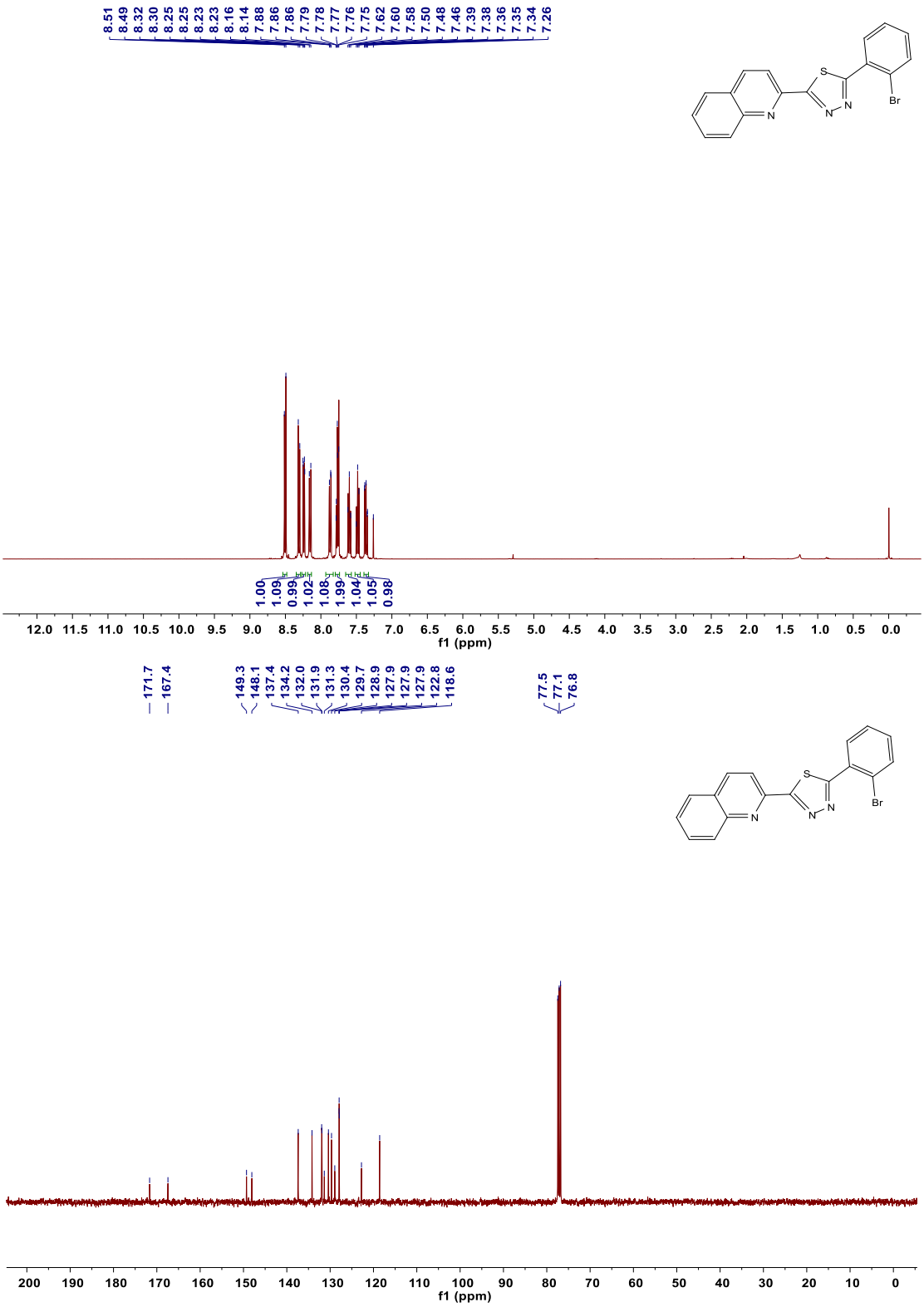


^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m17**

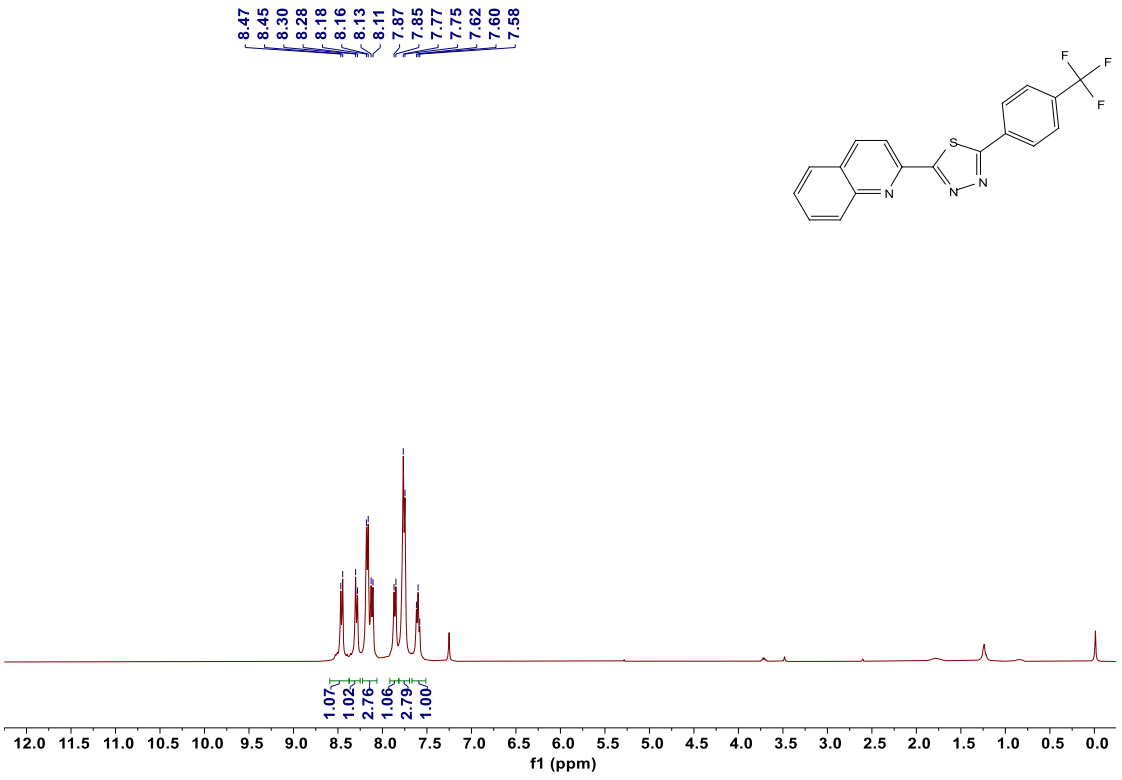


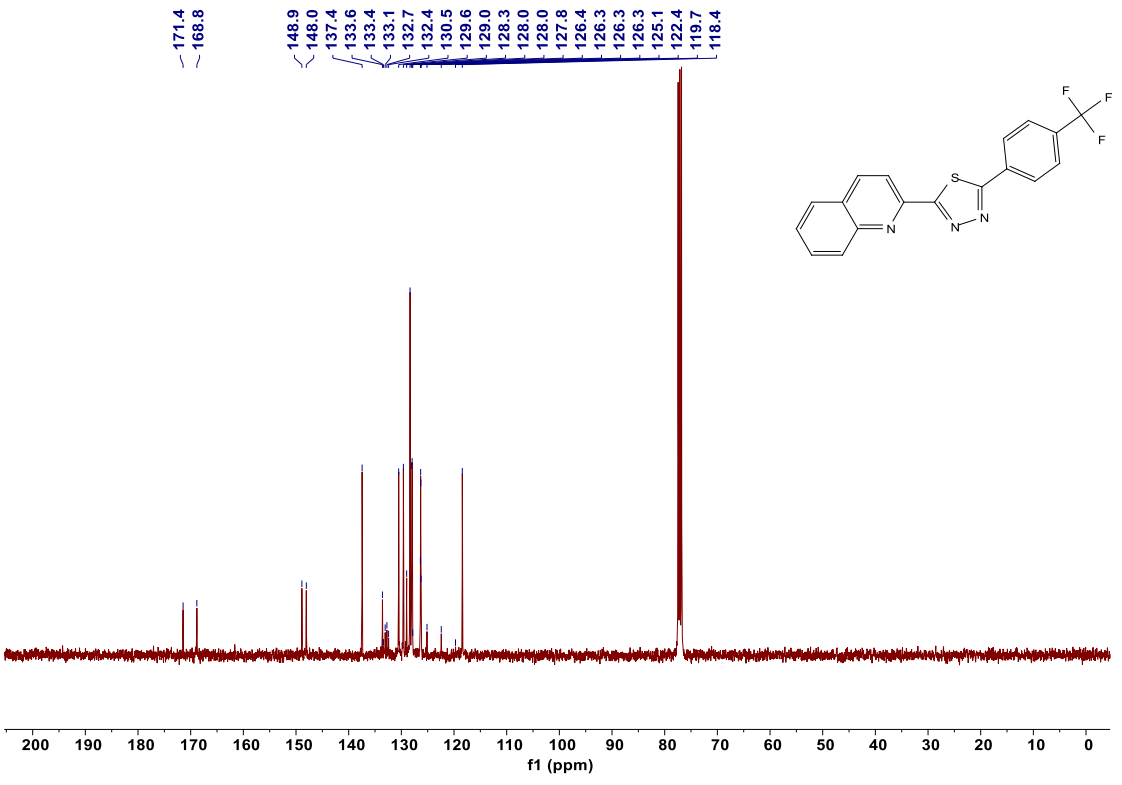


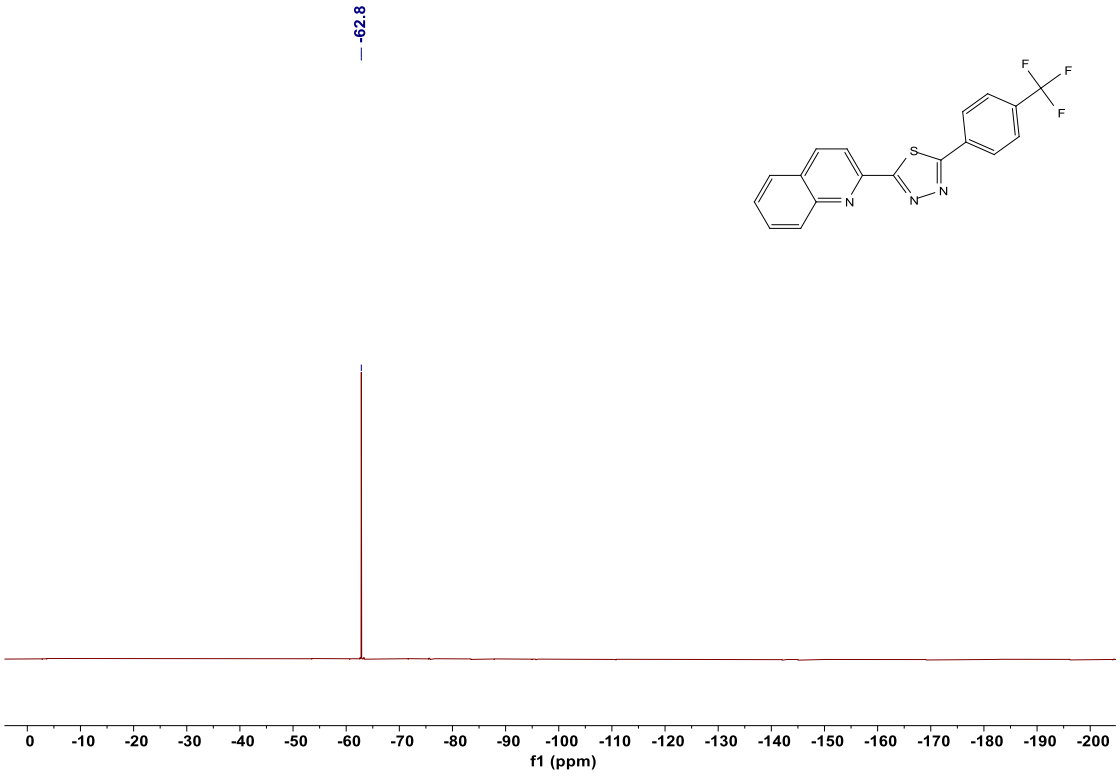
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m18**



^{1}H NMR (400 MHz, Chloroform-*d*), ^{13}C NMR (100 MHz, Chloroform-*d*), and ^{19}F NMR (376 MHz, Chloroform-*d*) of **m19**






-62.8
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-110
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-130
-140
-150
-160
-170
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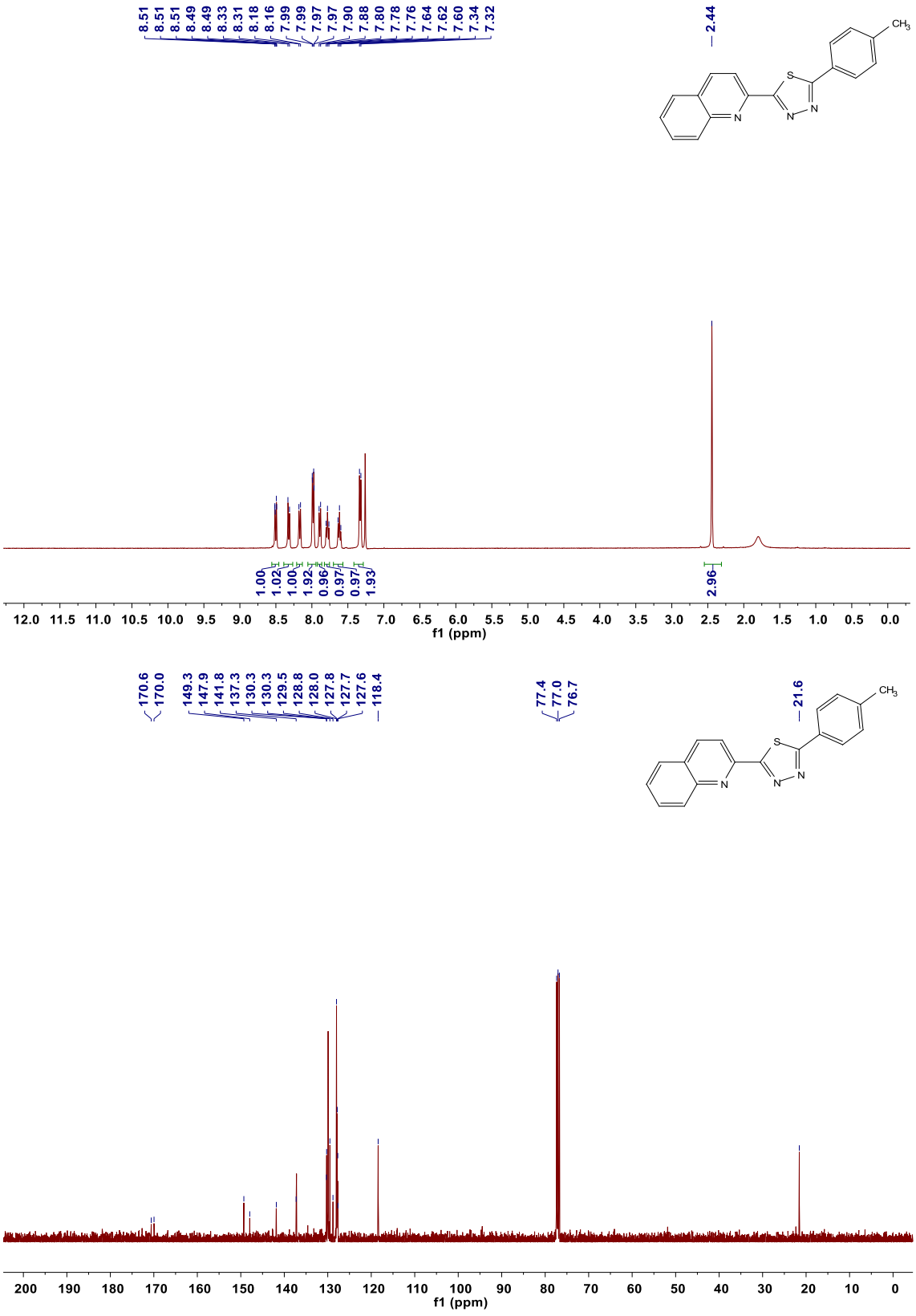
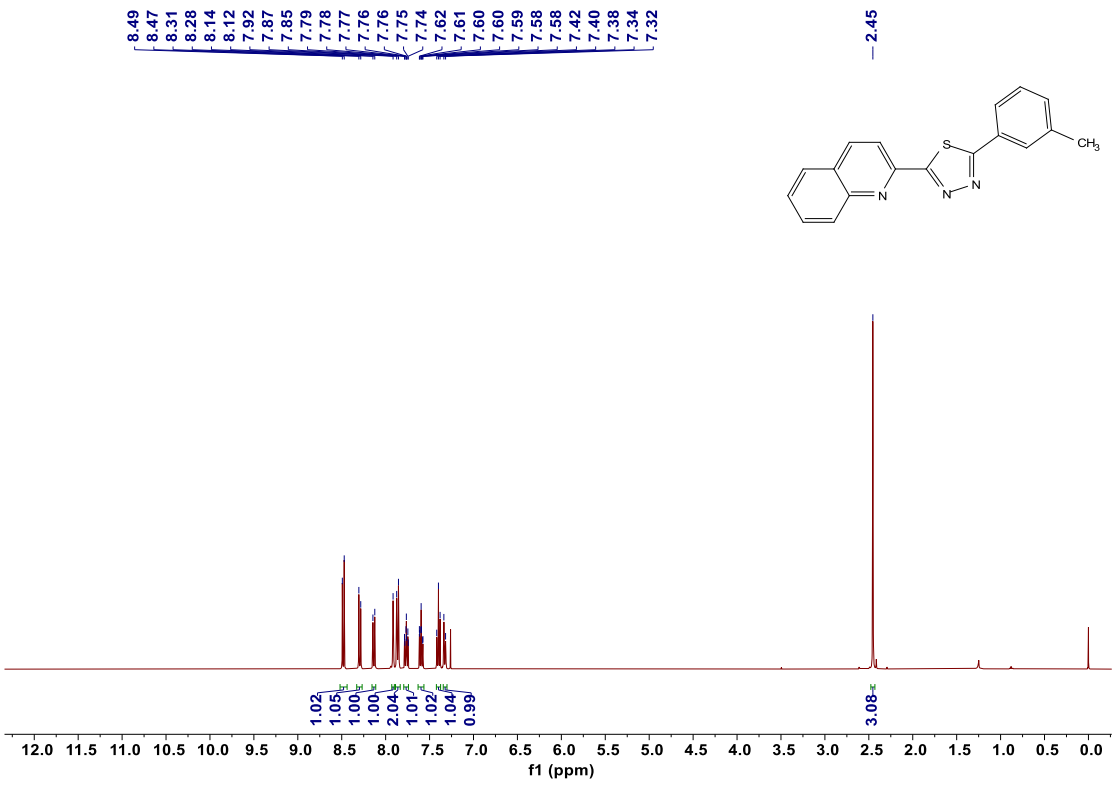
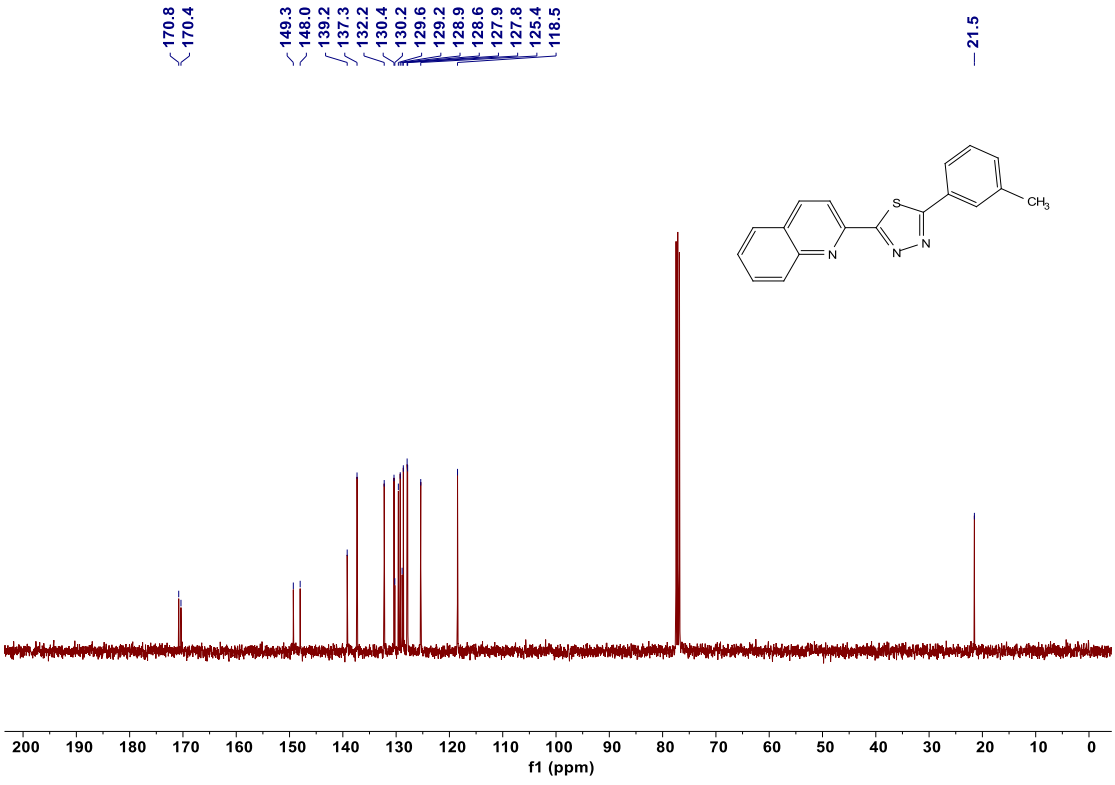
-200
f1 (ppm)

^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m20**

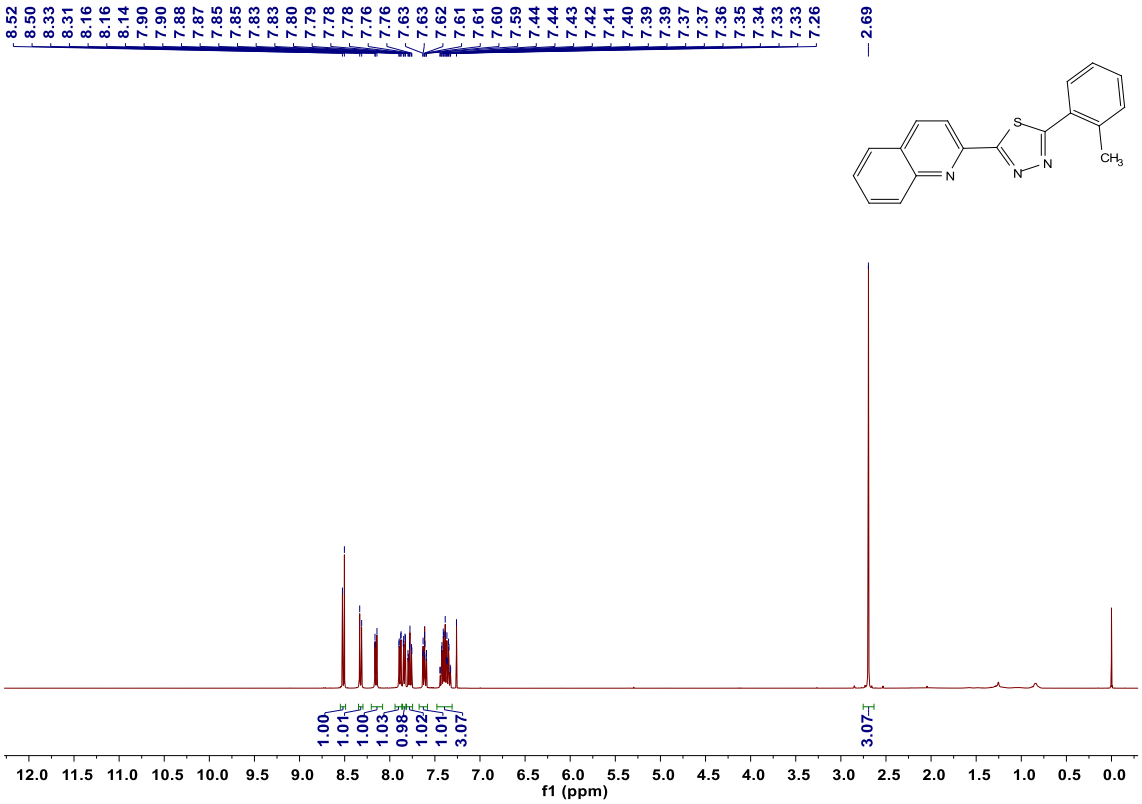


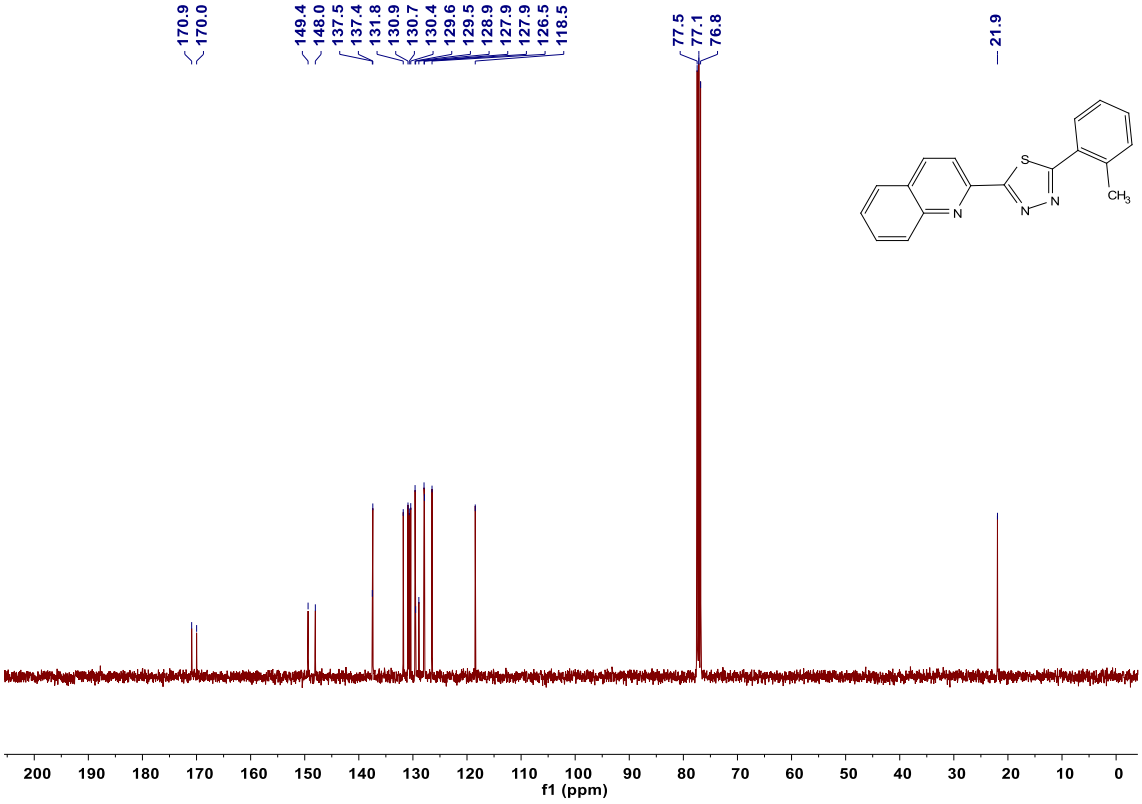
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m21**



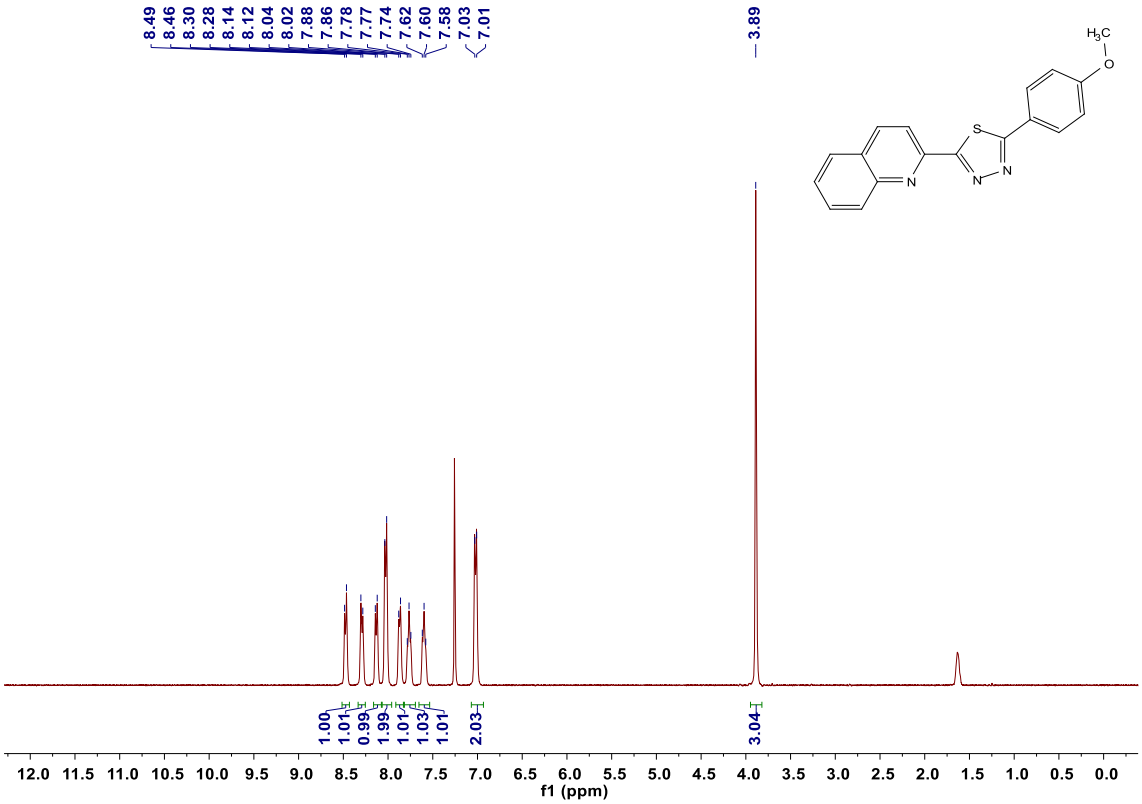


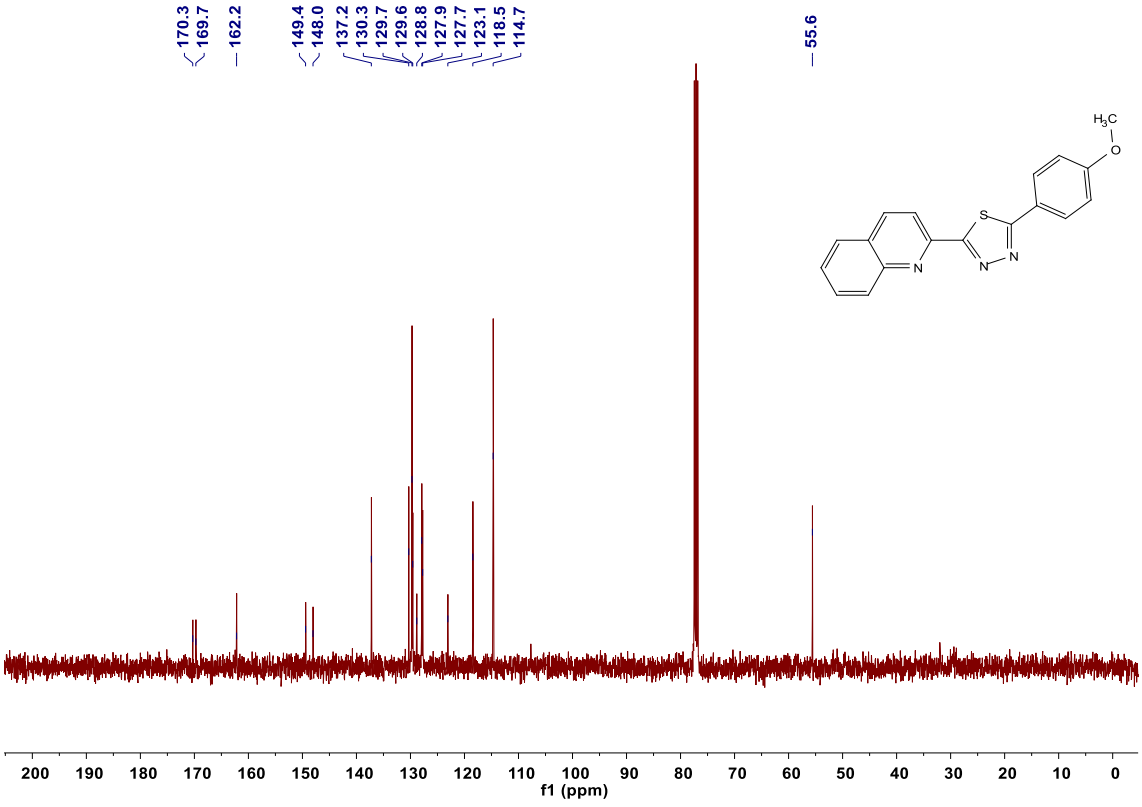
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m22**



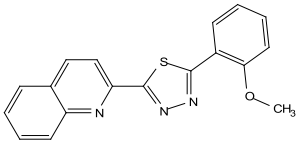


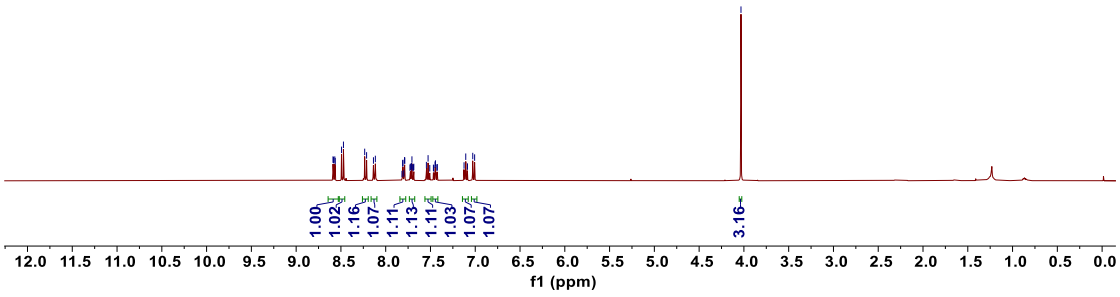
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m23**

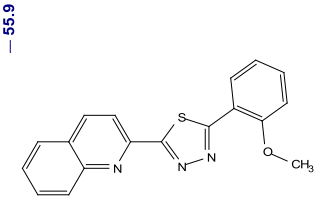


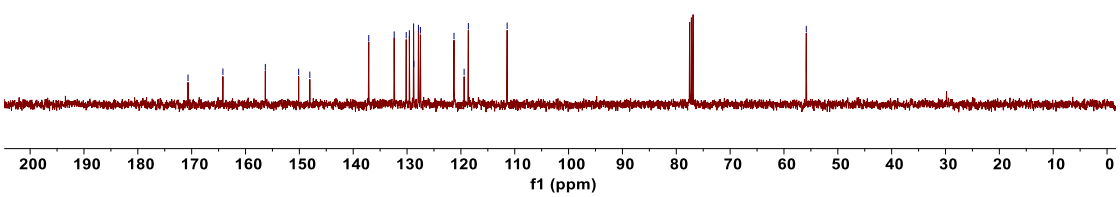


^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m24**

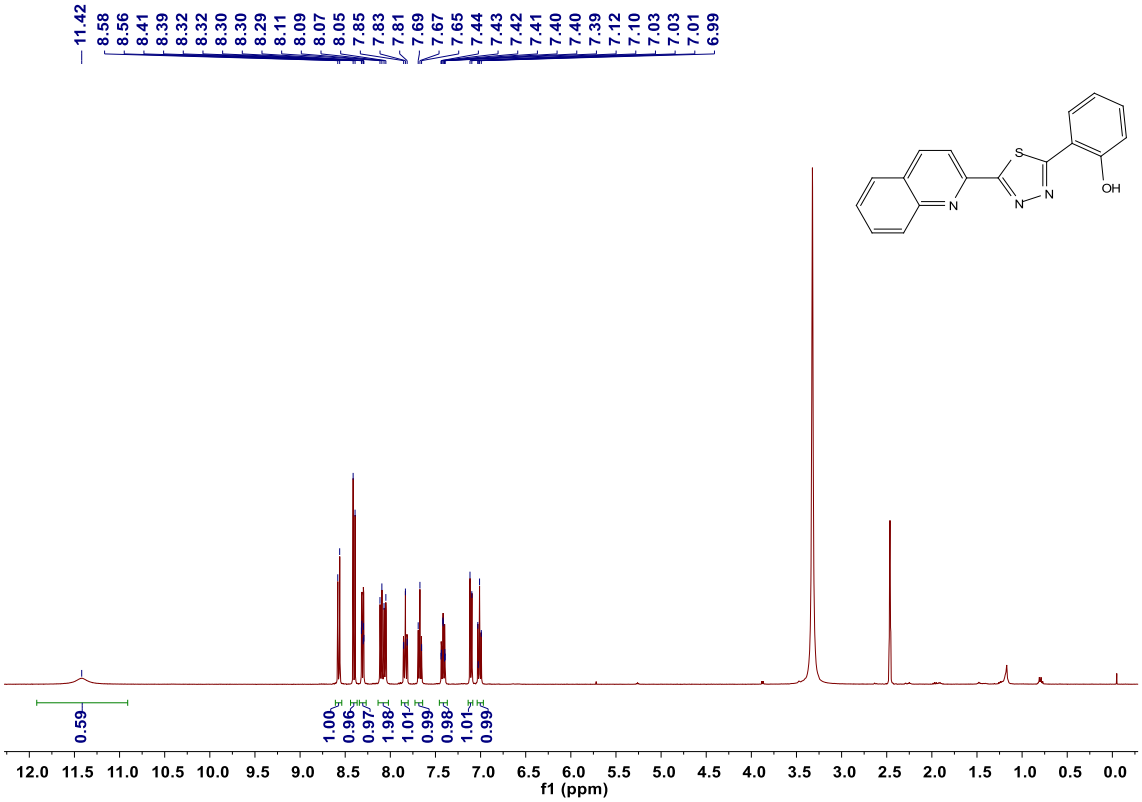


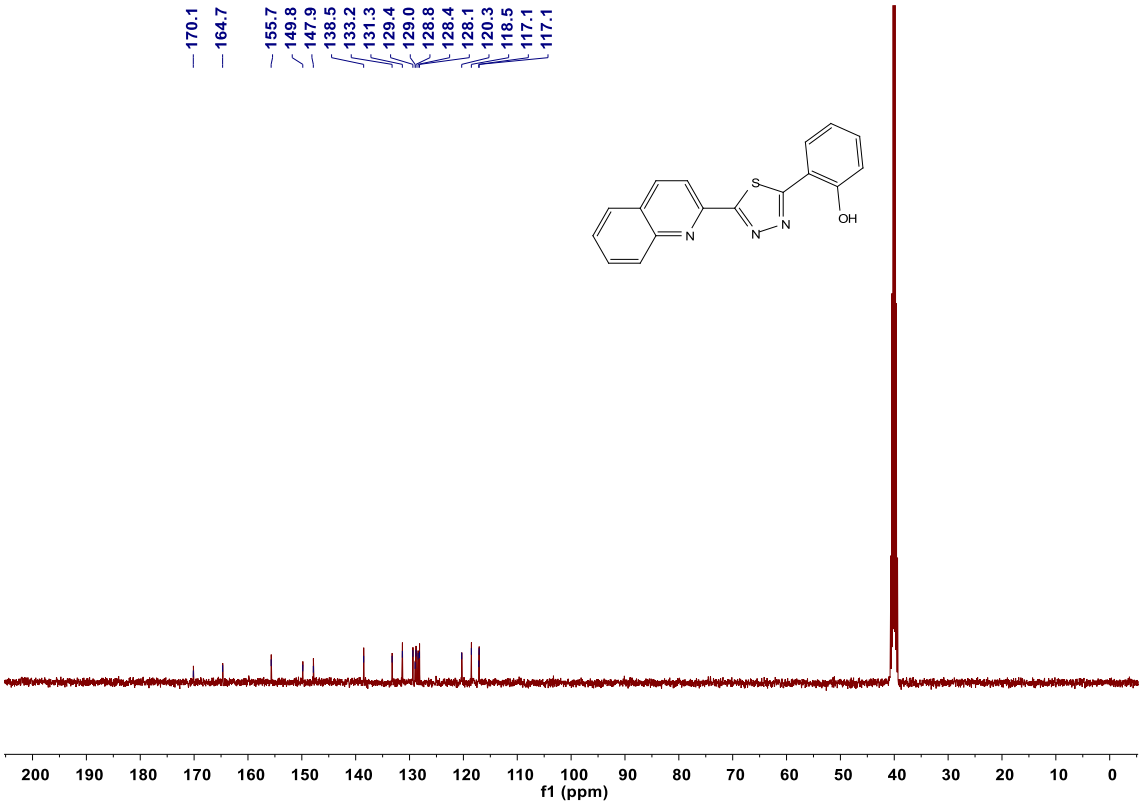




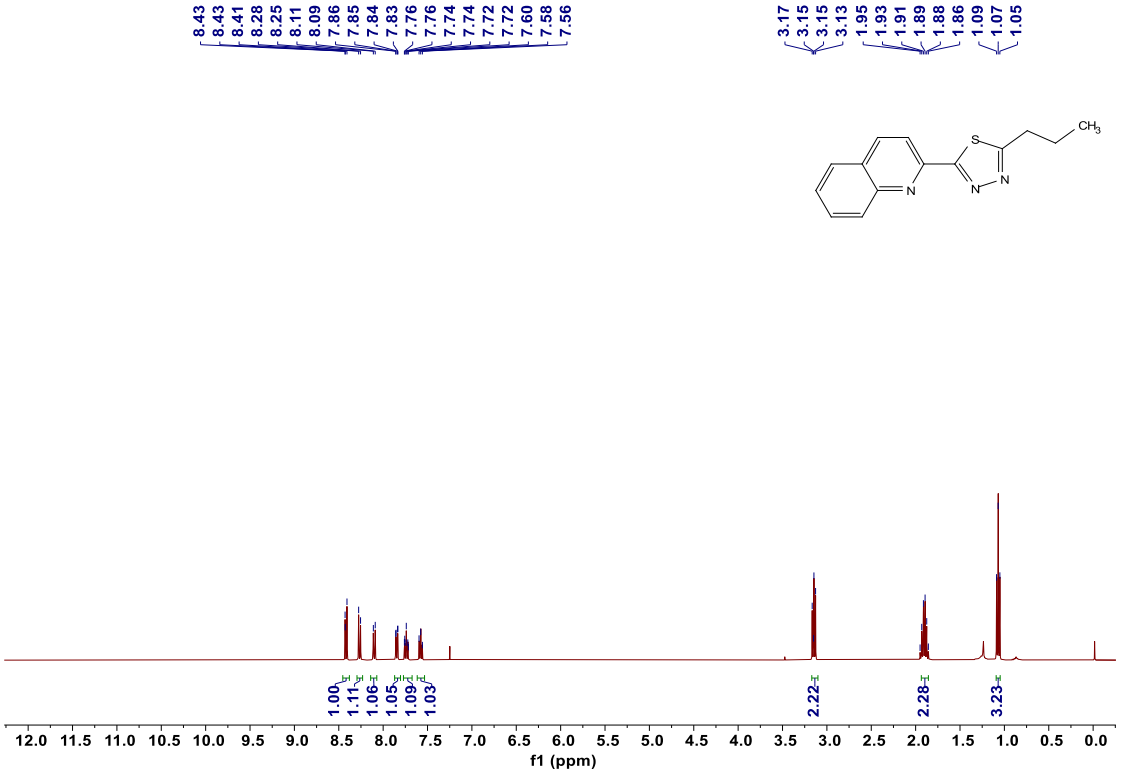


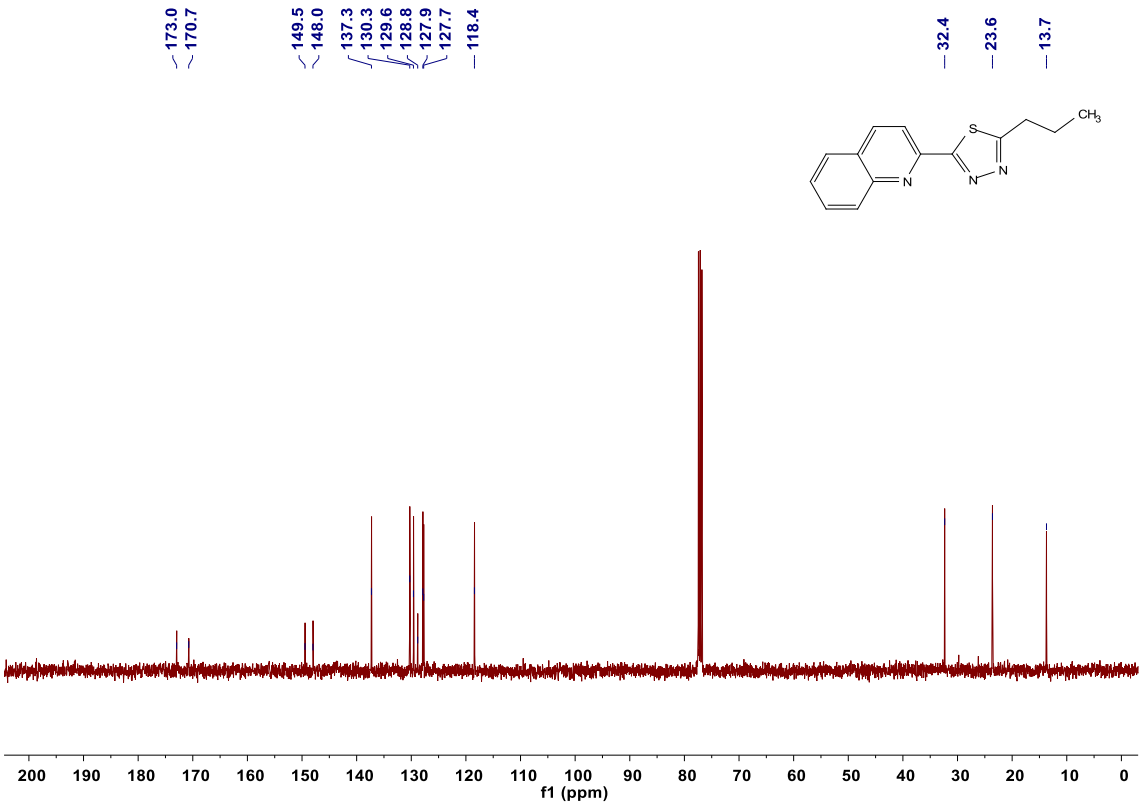
^{1}H NMR (400 MHz, DMSO-*d6)* and ^{13}C NMR (100 MHz, DMSO-*d6*) of **m25**



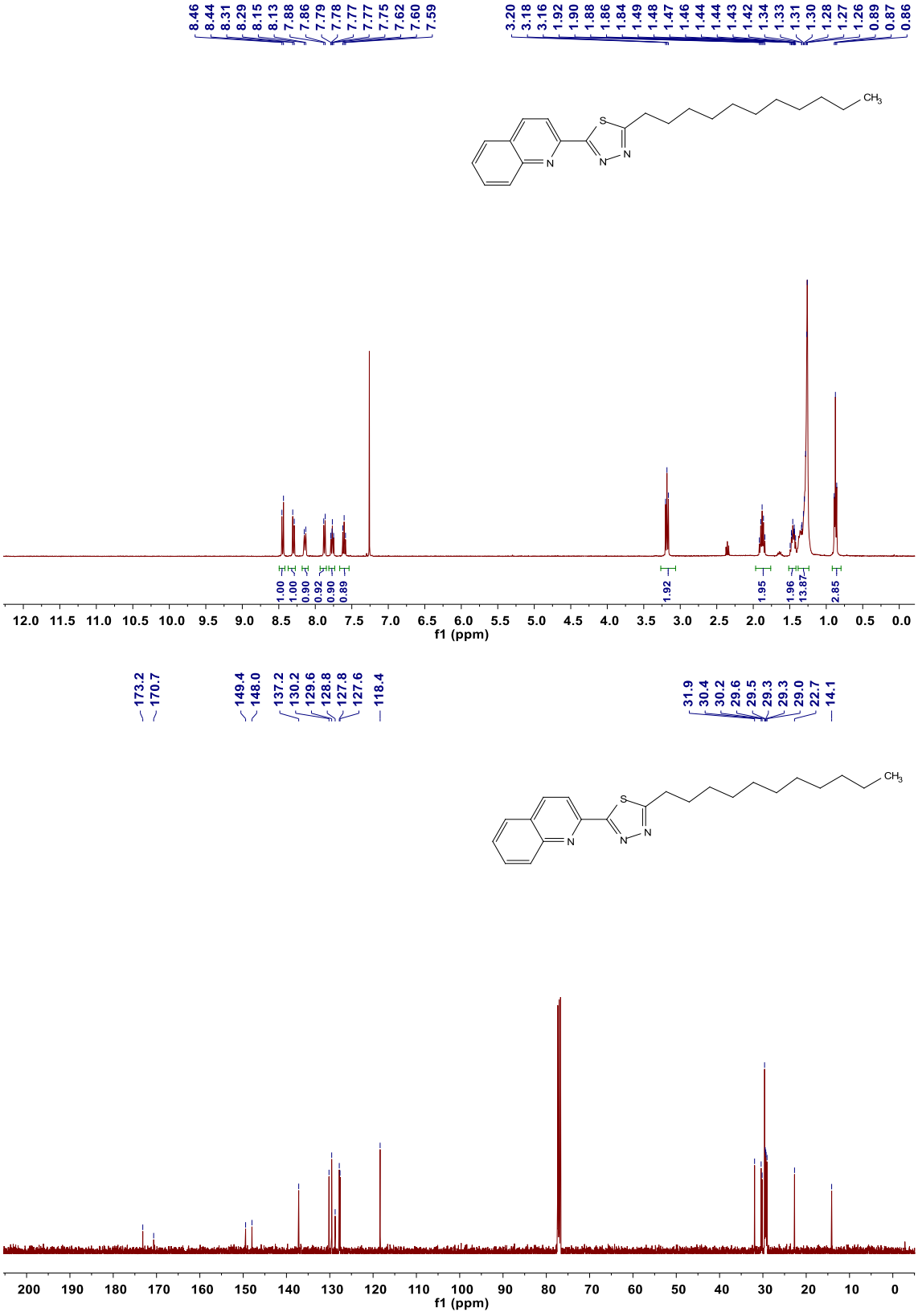


^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m26**

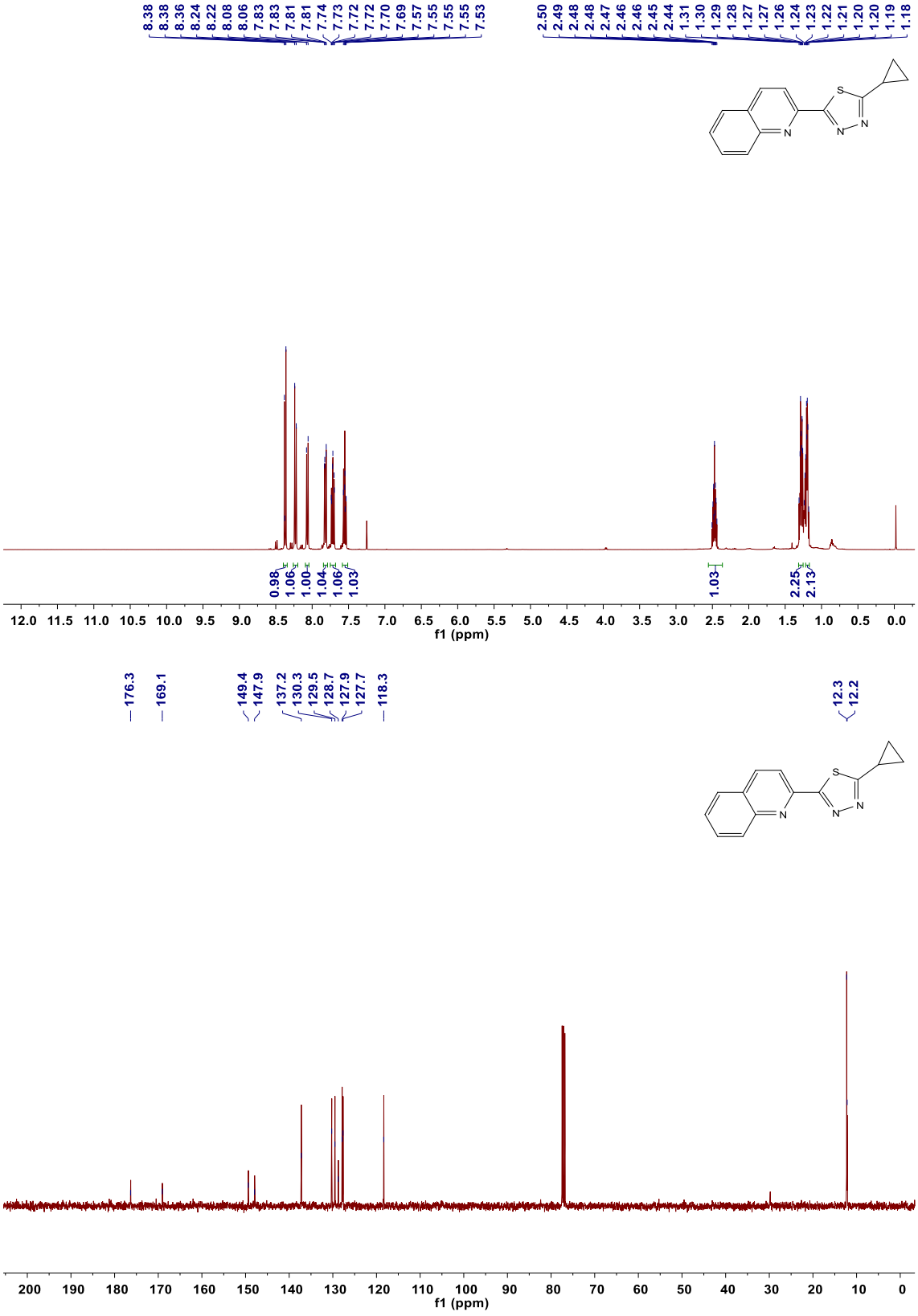




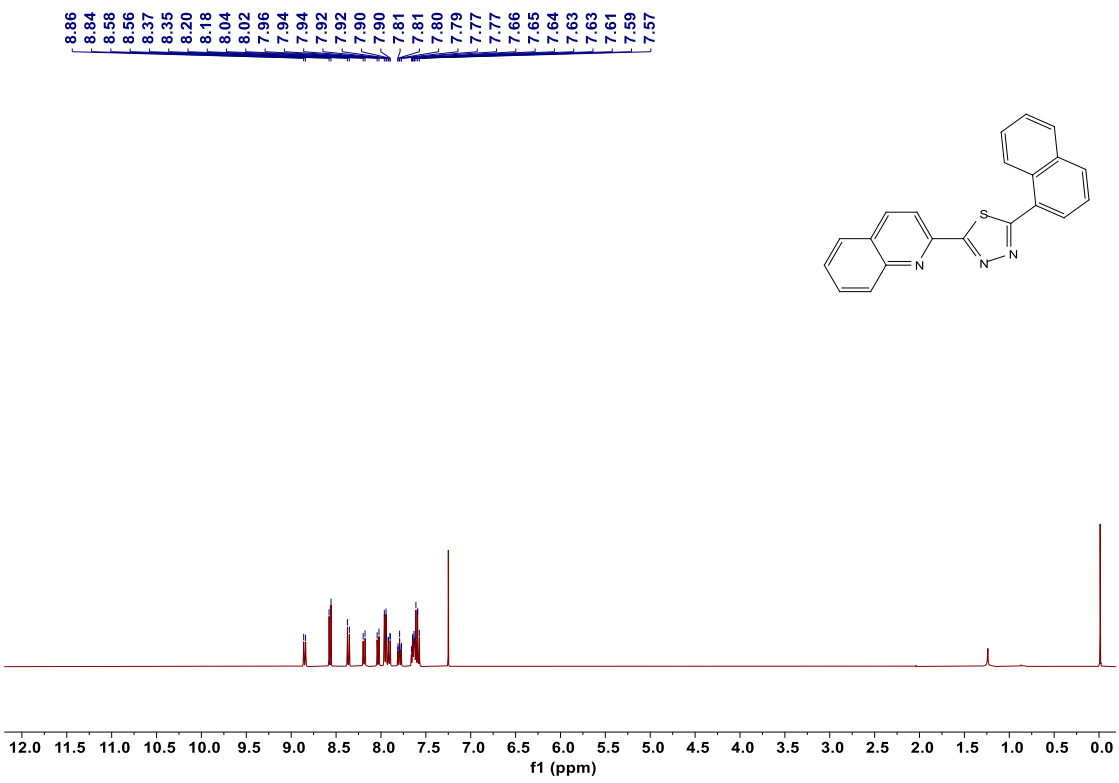
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m27**

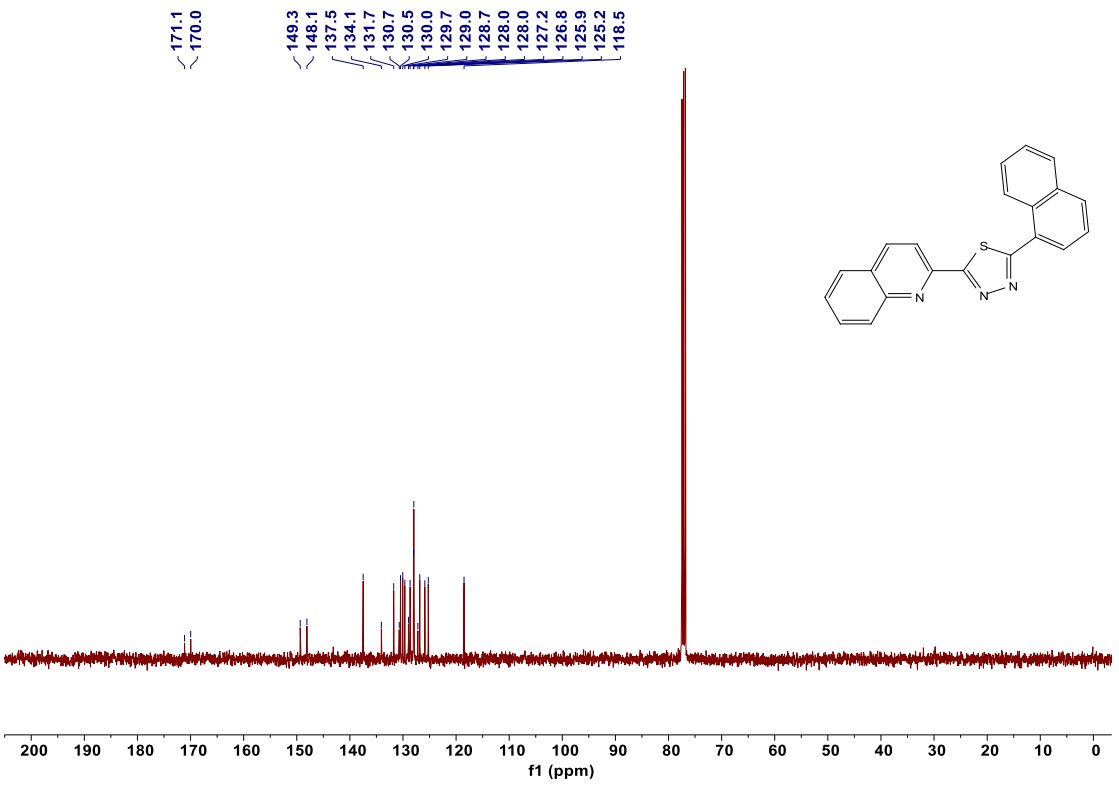


^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m28**

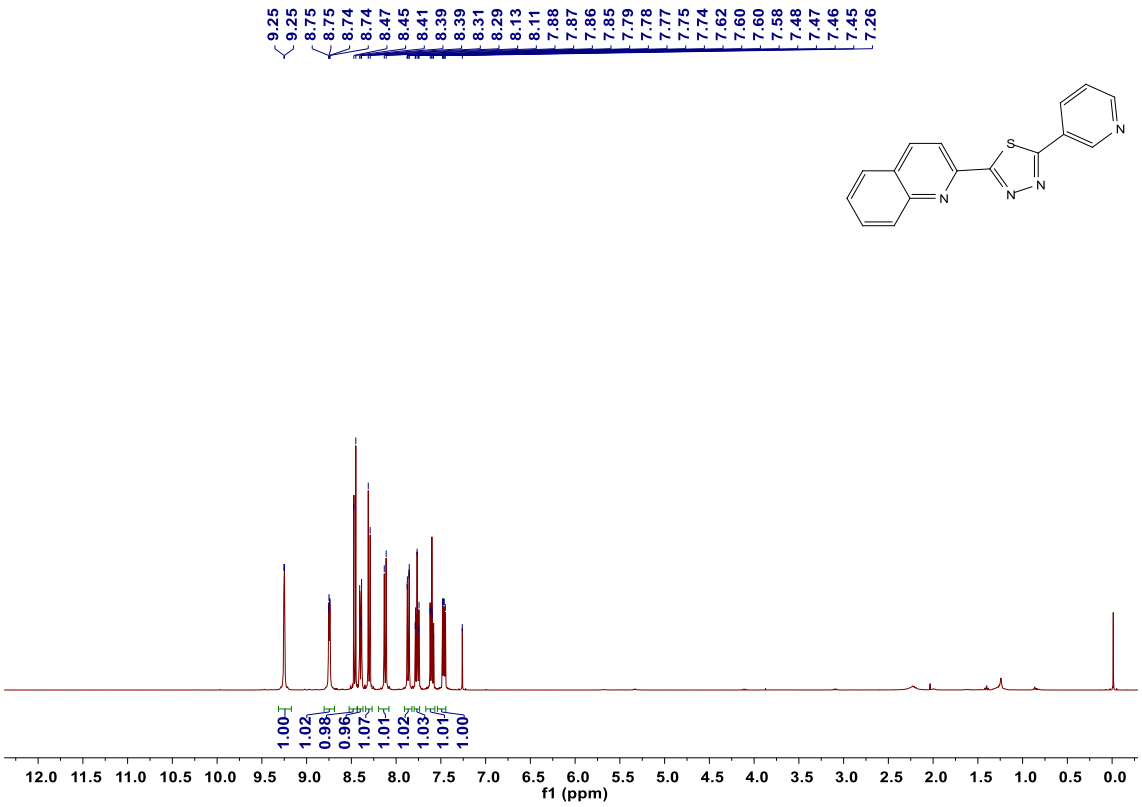


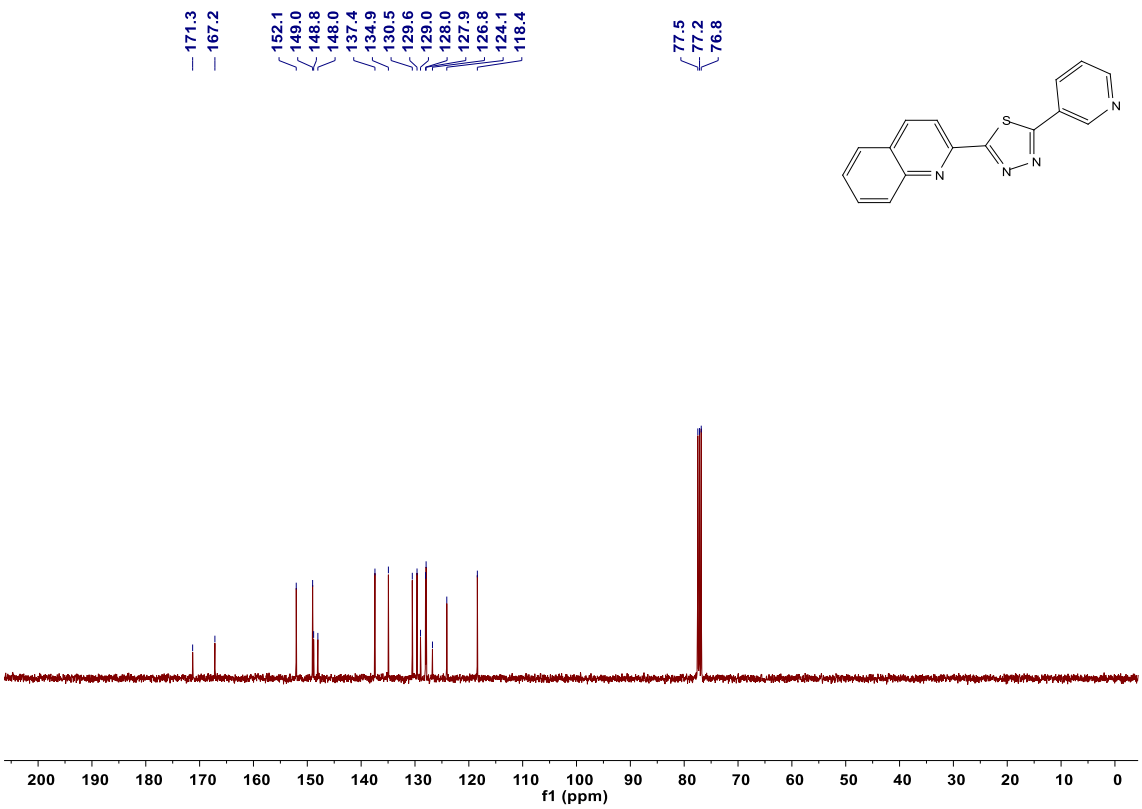
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m29**



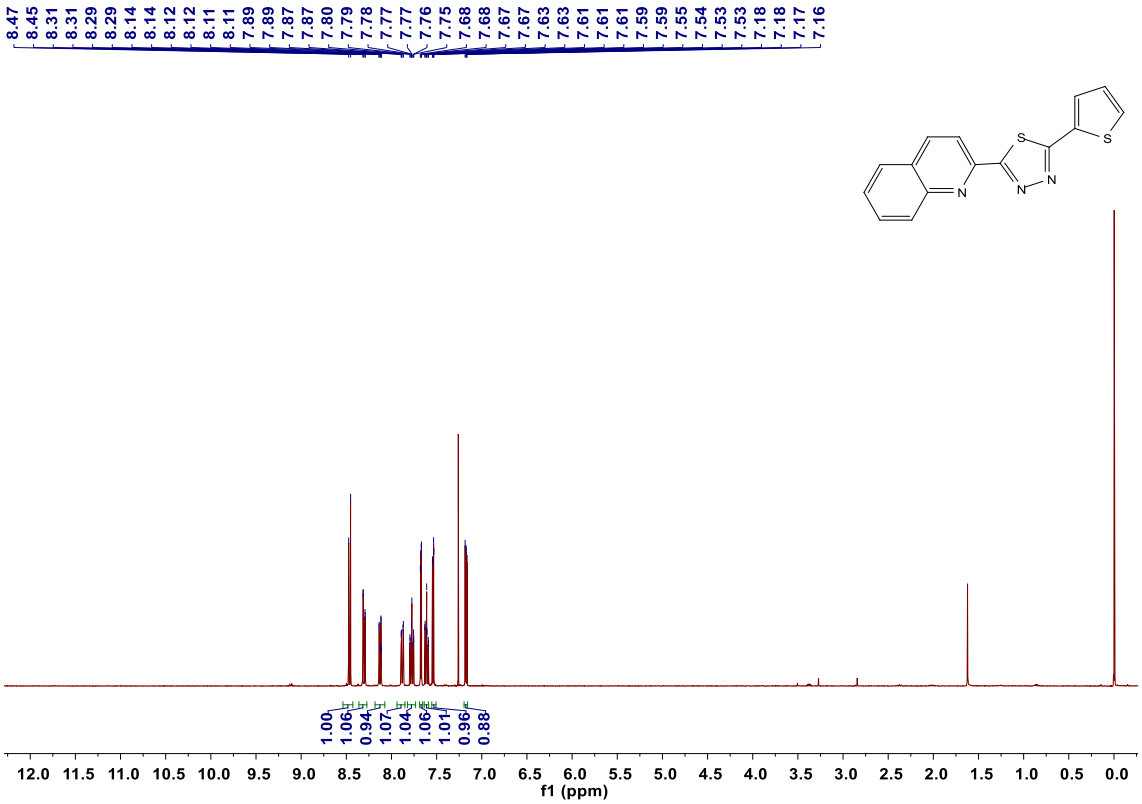


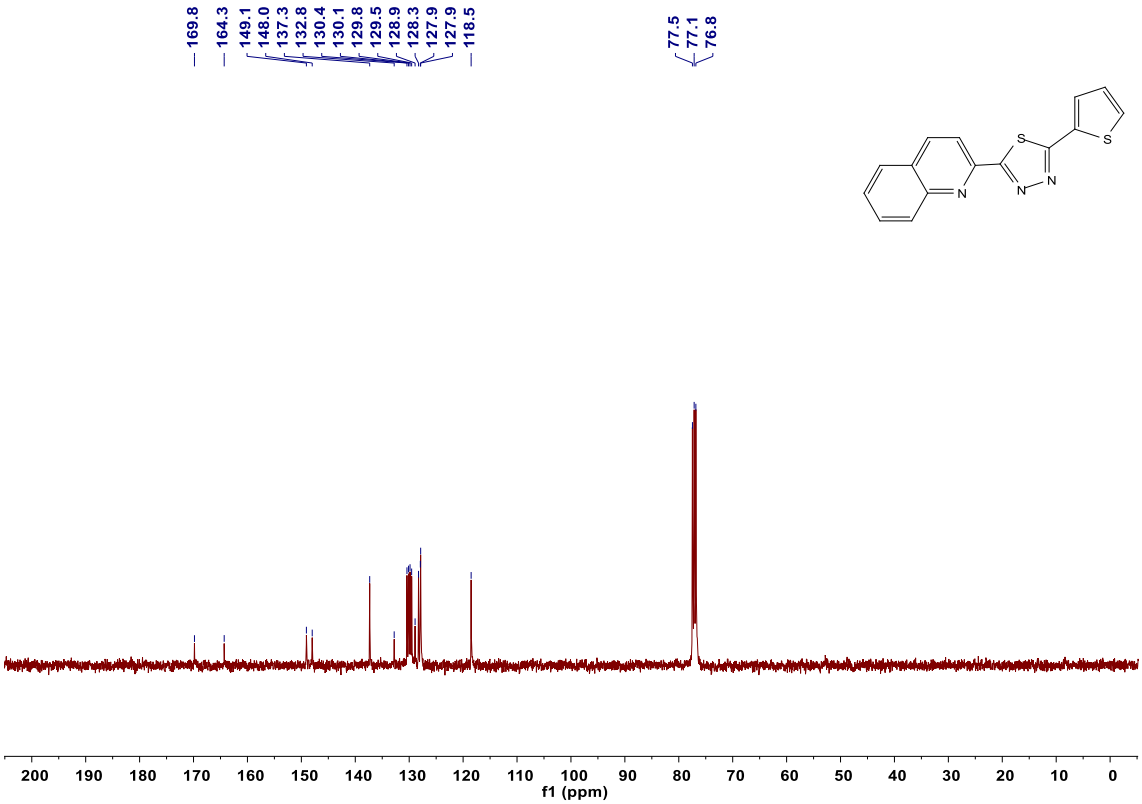
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m30**



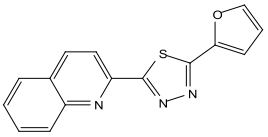


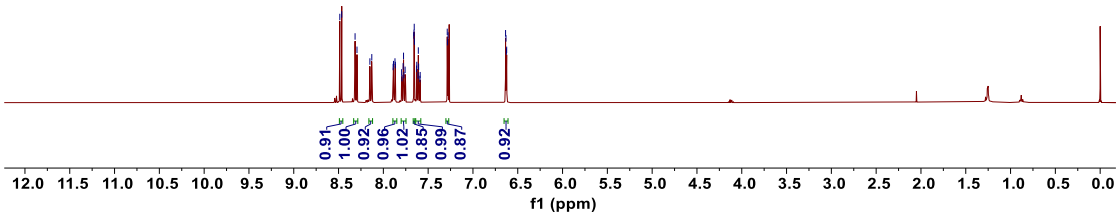
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m31**

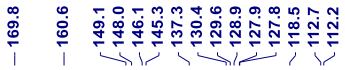


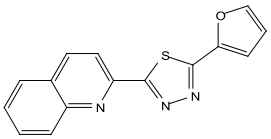


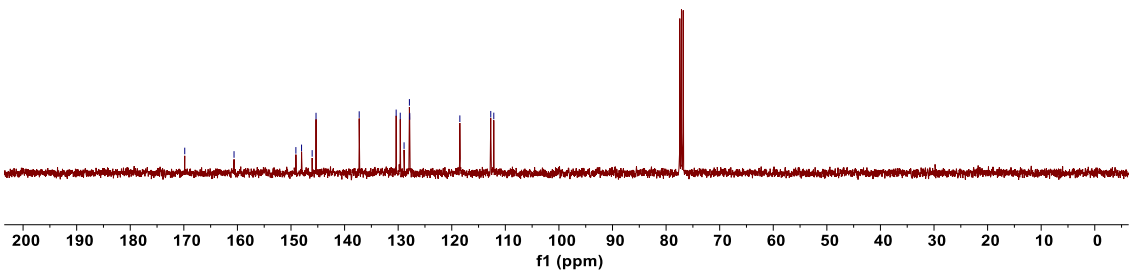
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m32**



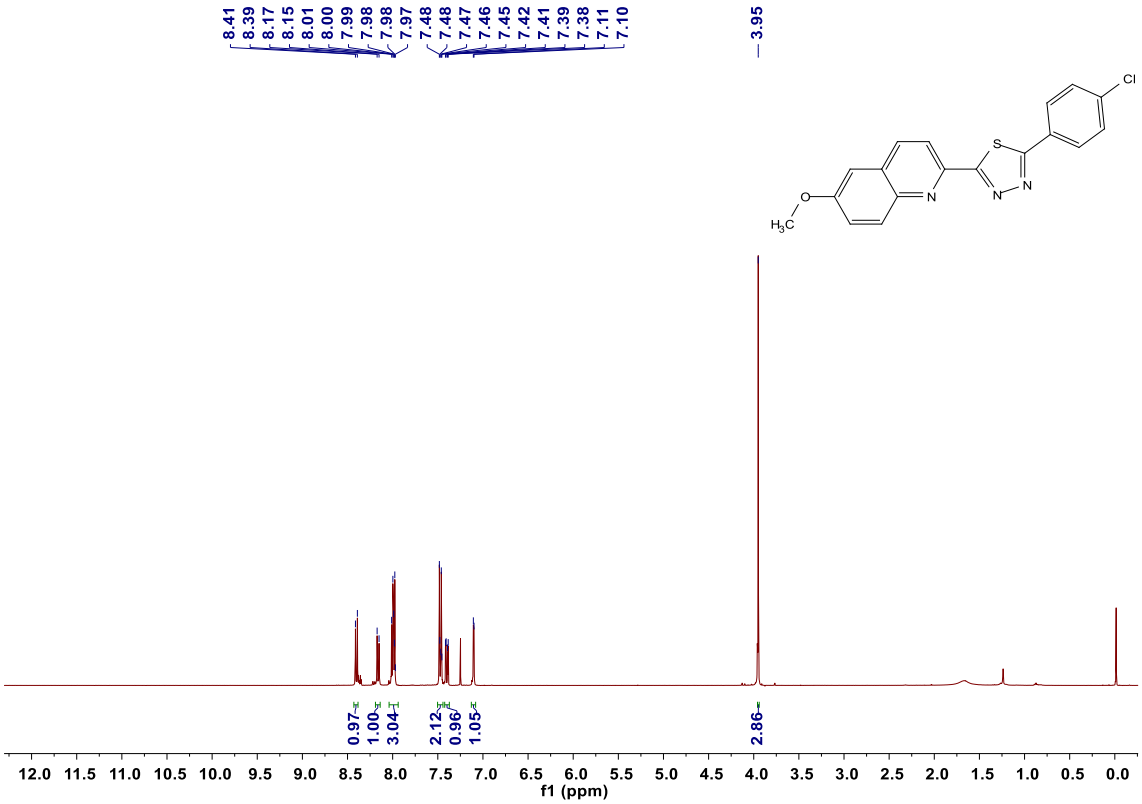


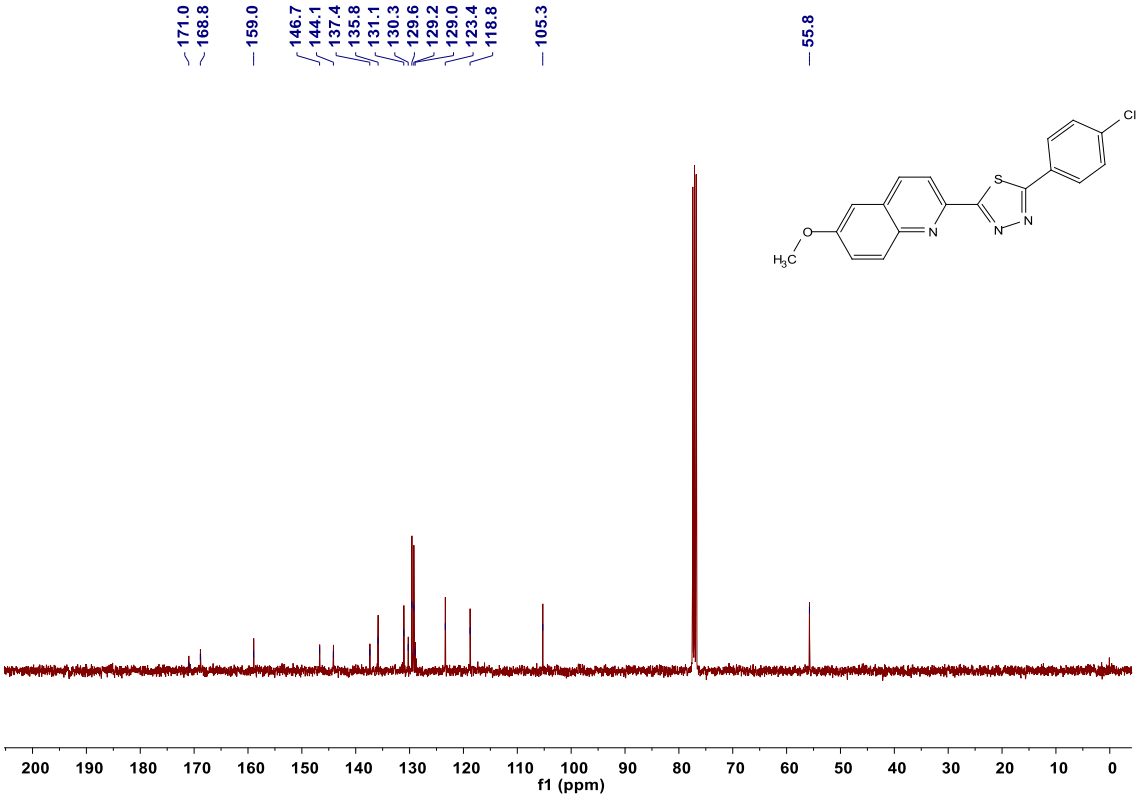




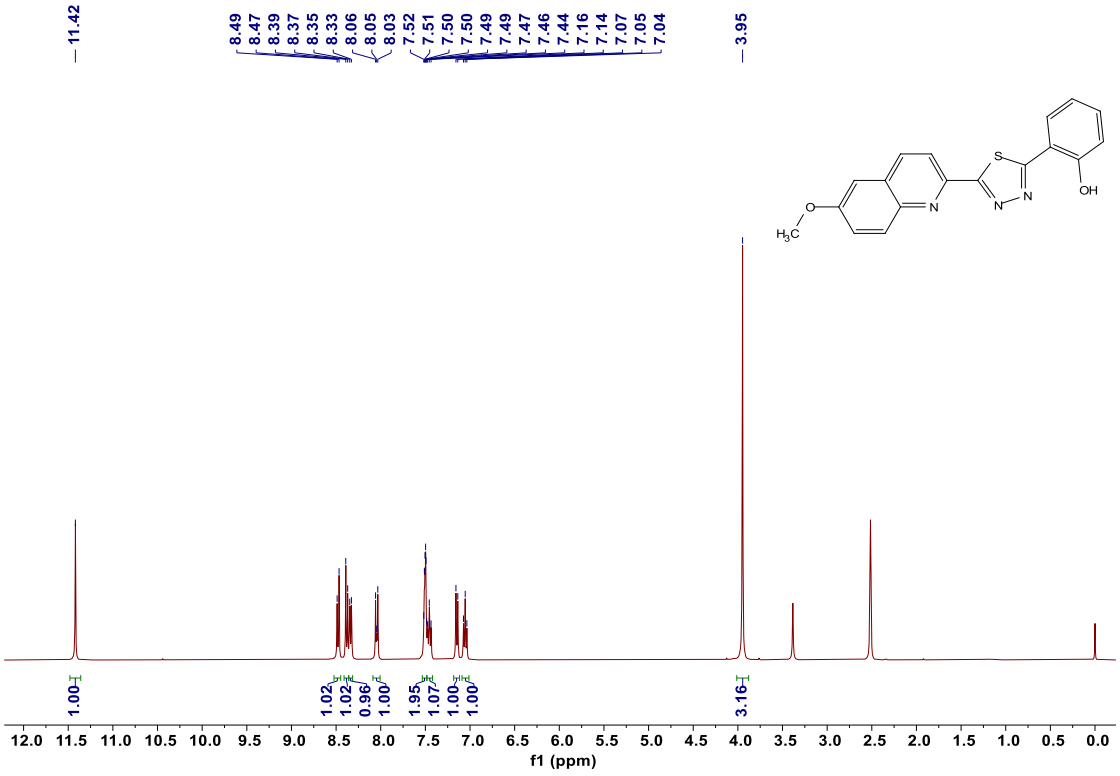


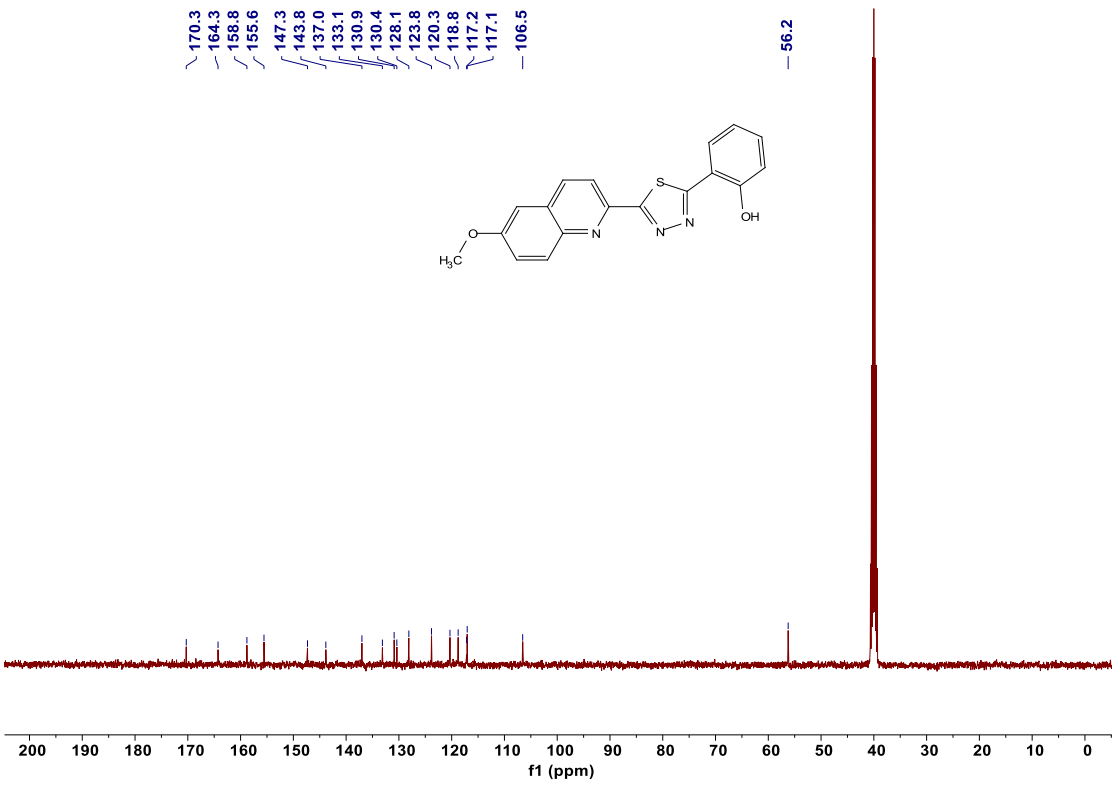
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **m33**



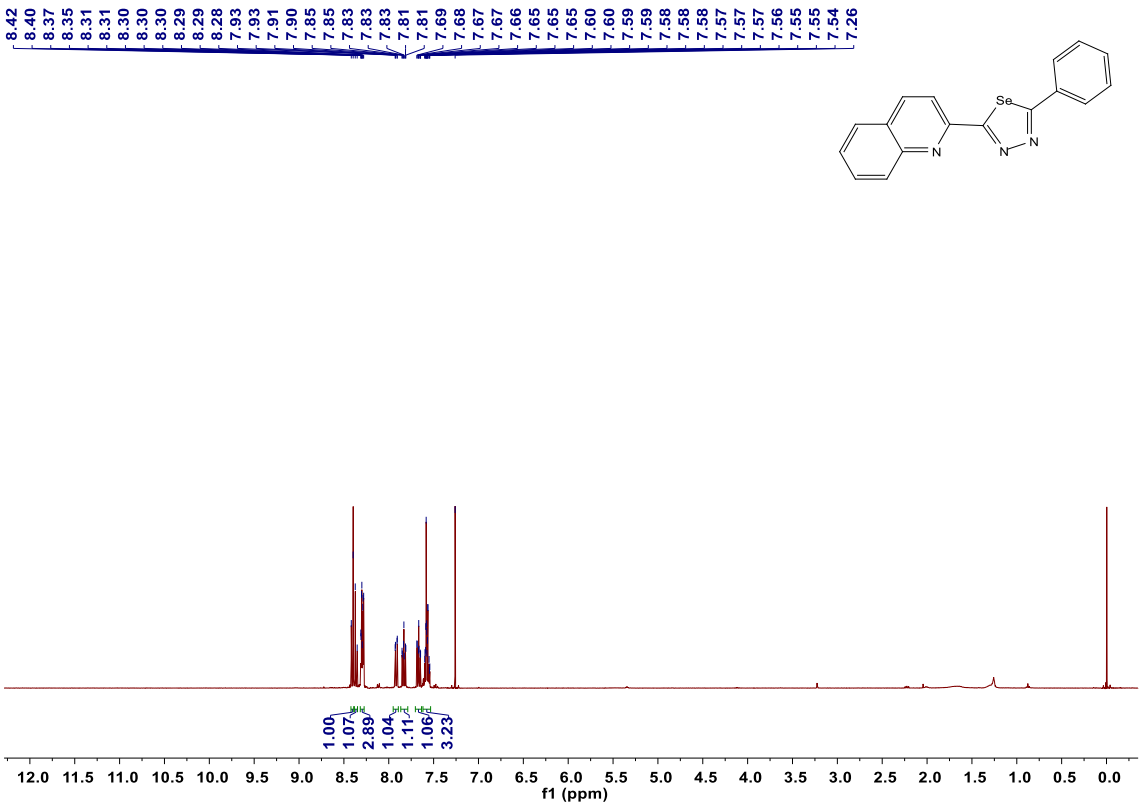


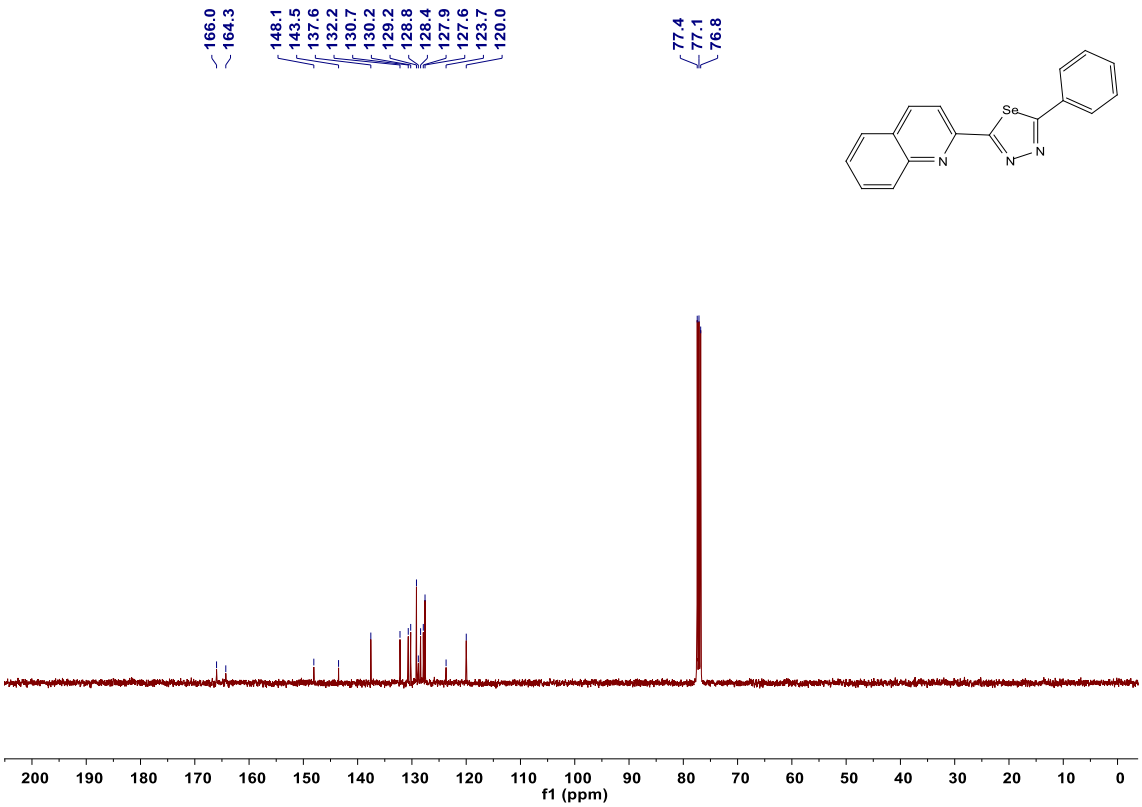
^{1}H NMR (400 MHz, DMSO-d_6) and ^{13}C NMR (100 MHz, DMSO-d_6) of **m34**



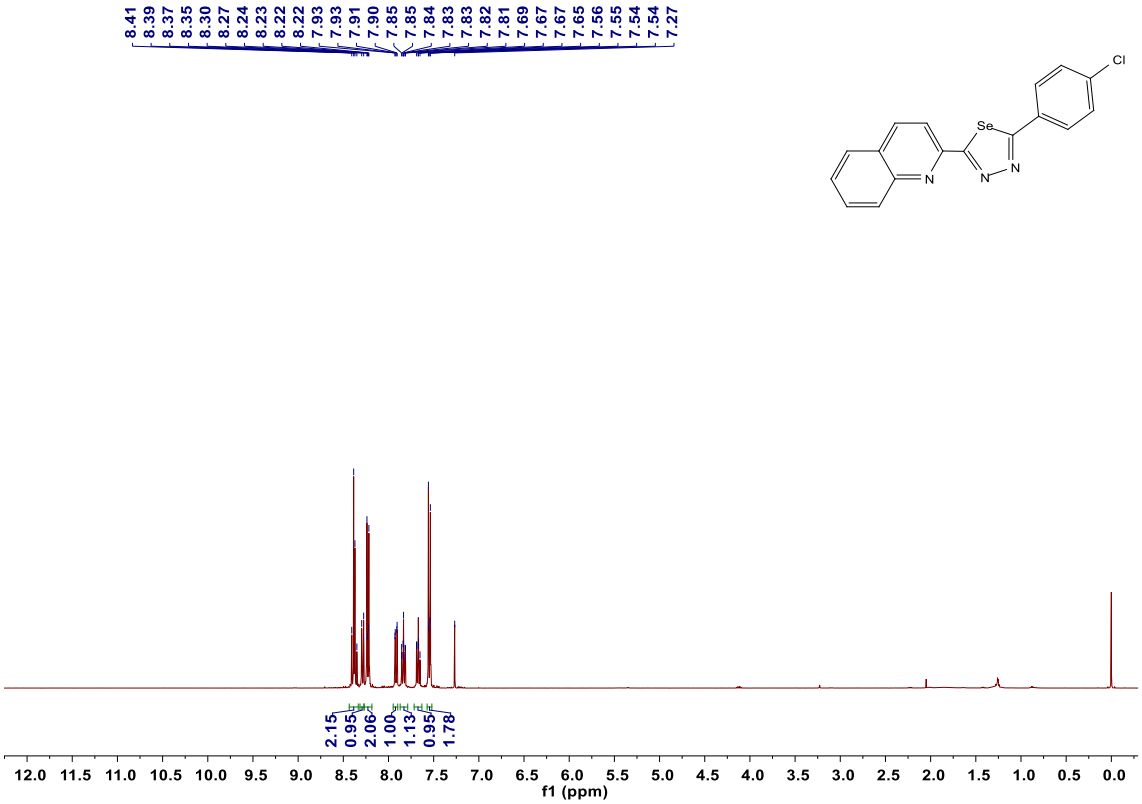


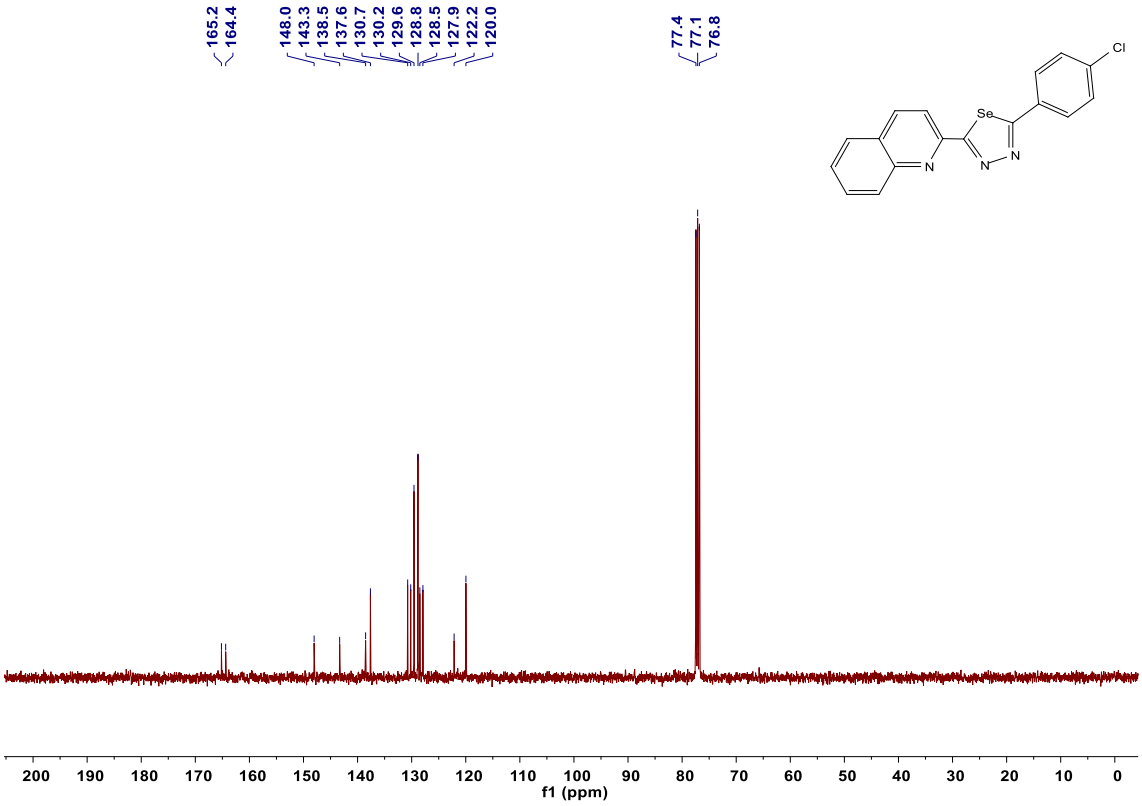
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **n1**



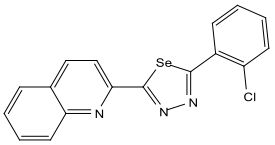


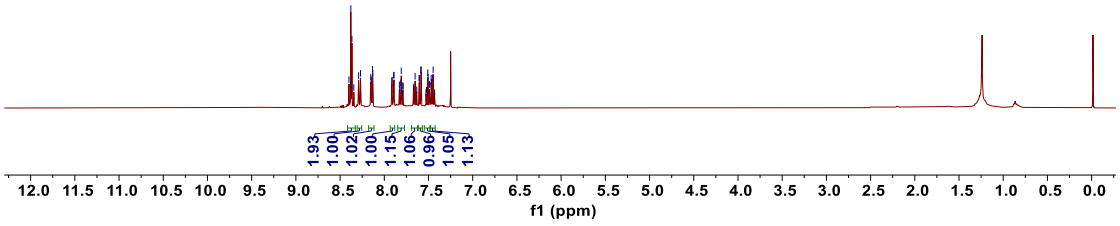
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **n2**

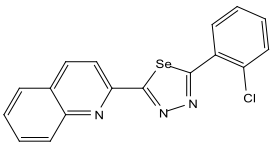


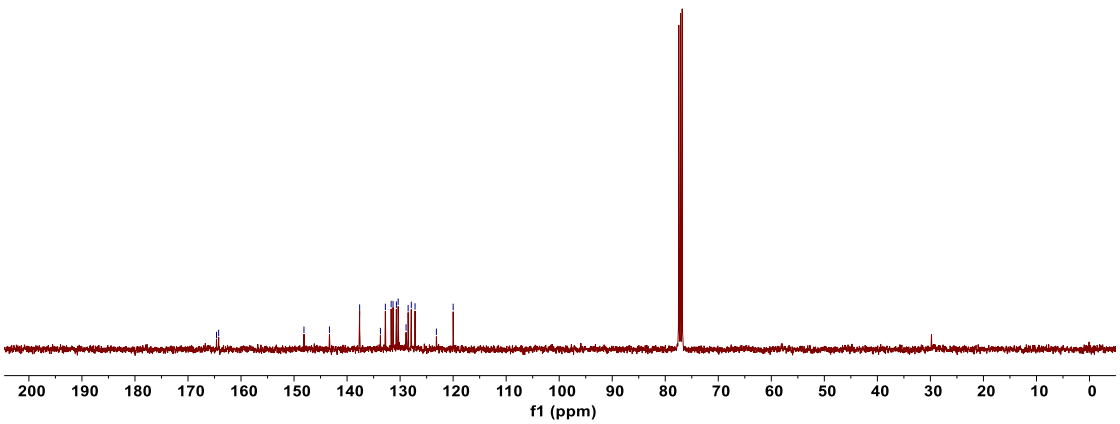


^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **n3**

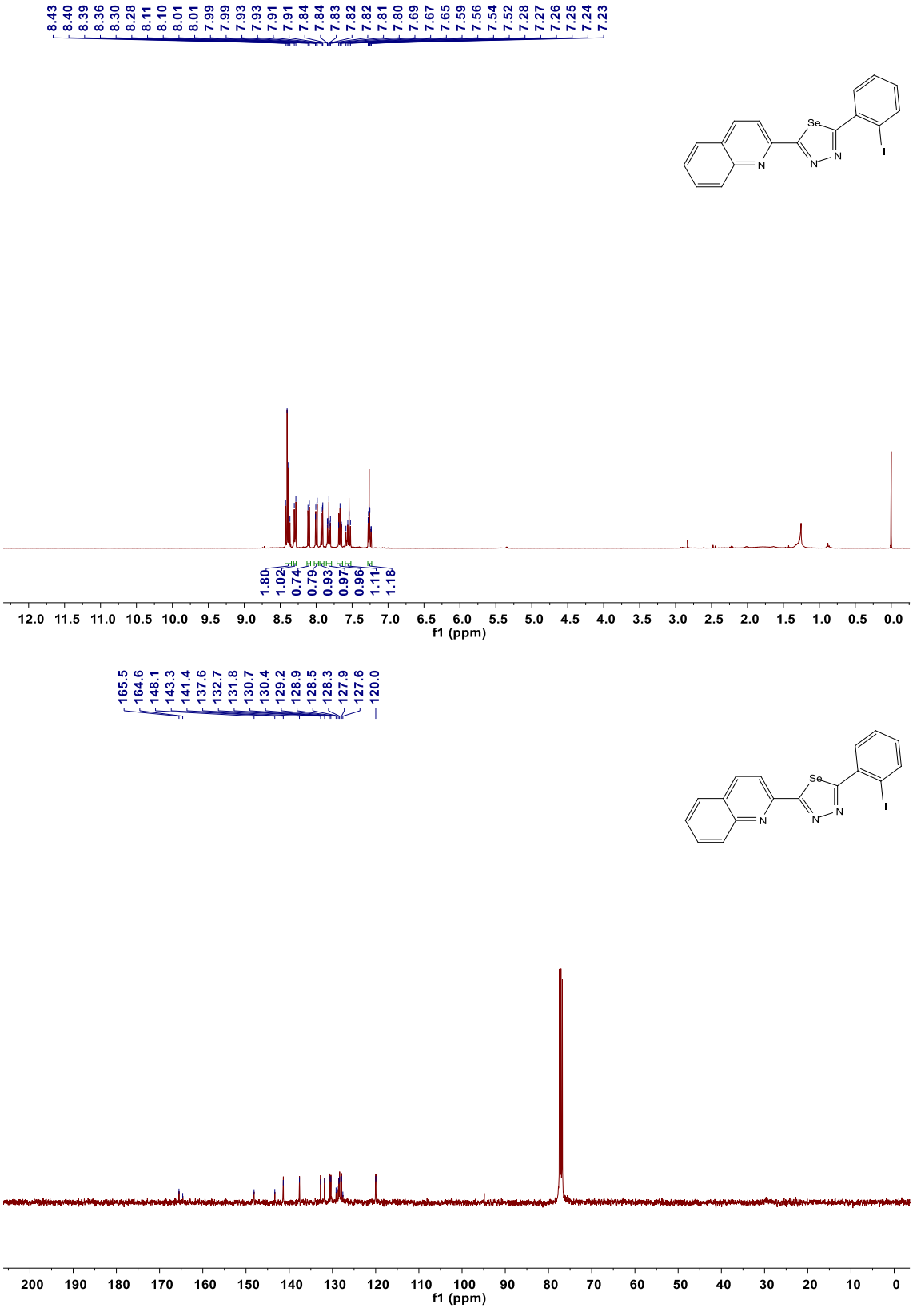






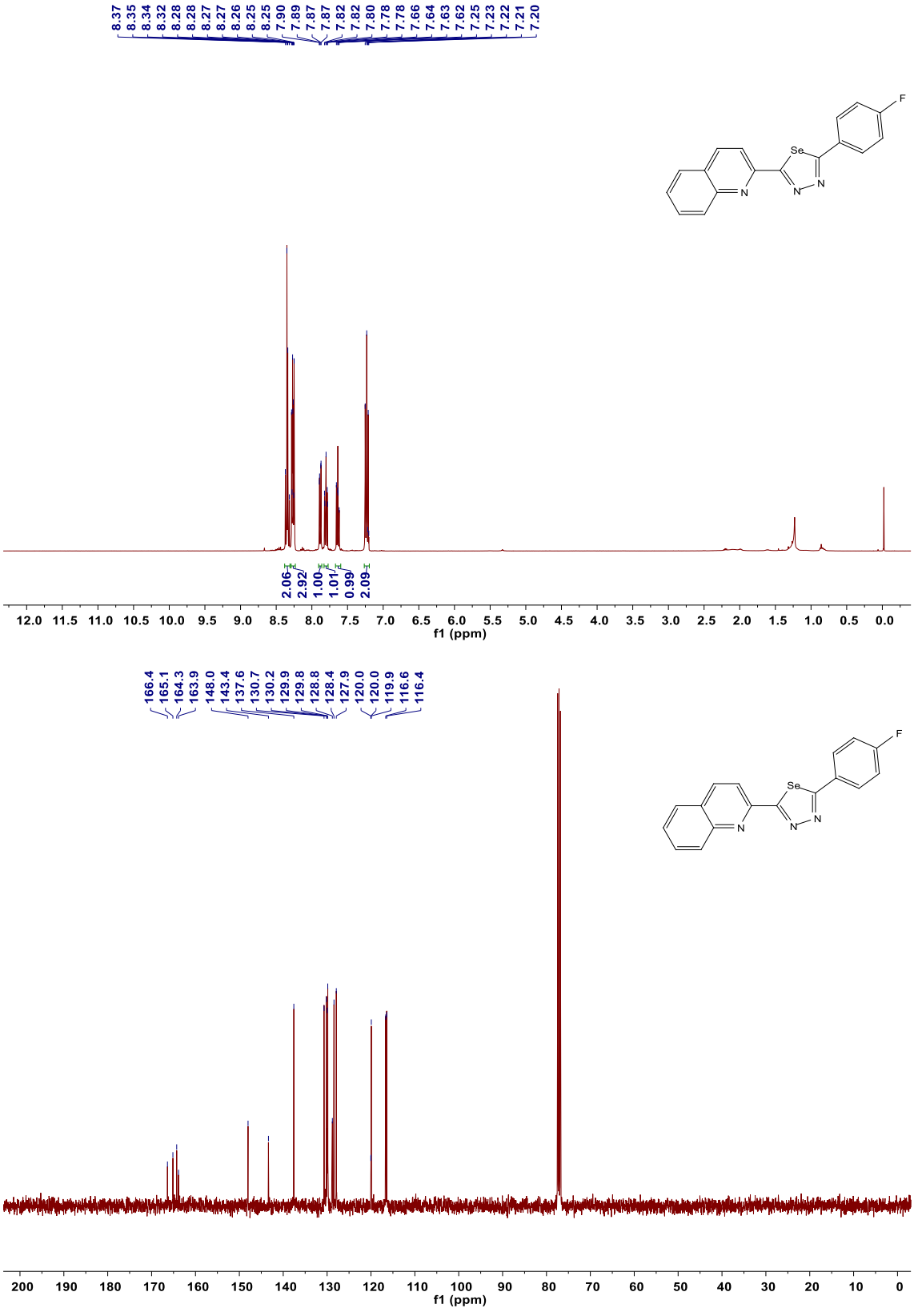


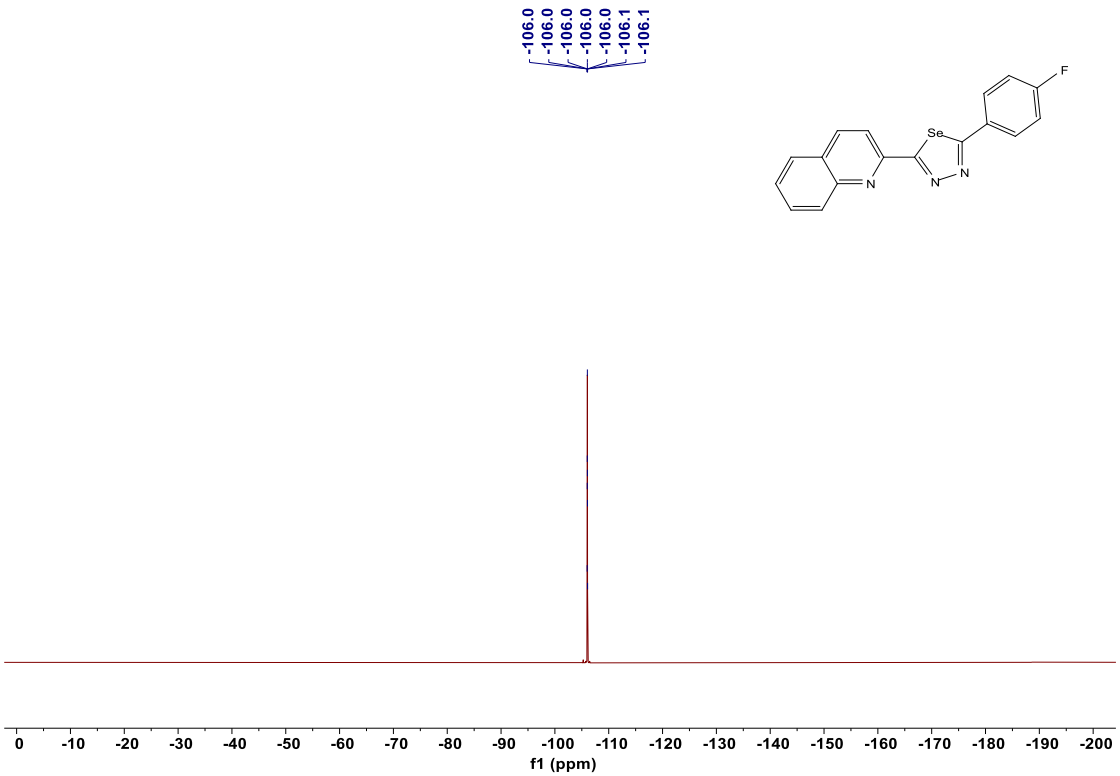
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **n4**



^{1}H NMR (400 MHz, Chloroform-*d*), ^{13}C NMR (100 MHz, Chloroform-*d*), and

^{19}F NMR (376 MHz, Chloroform-*d*)of **n5**

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-90
-100
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-120
-130
-140
-150
-160
-170
-180
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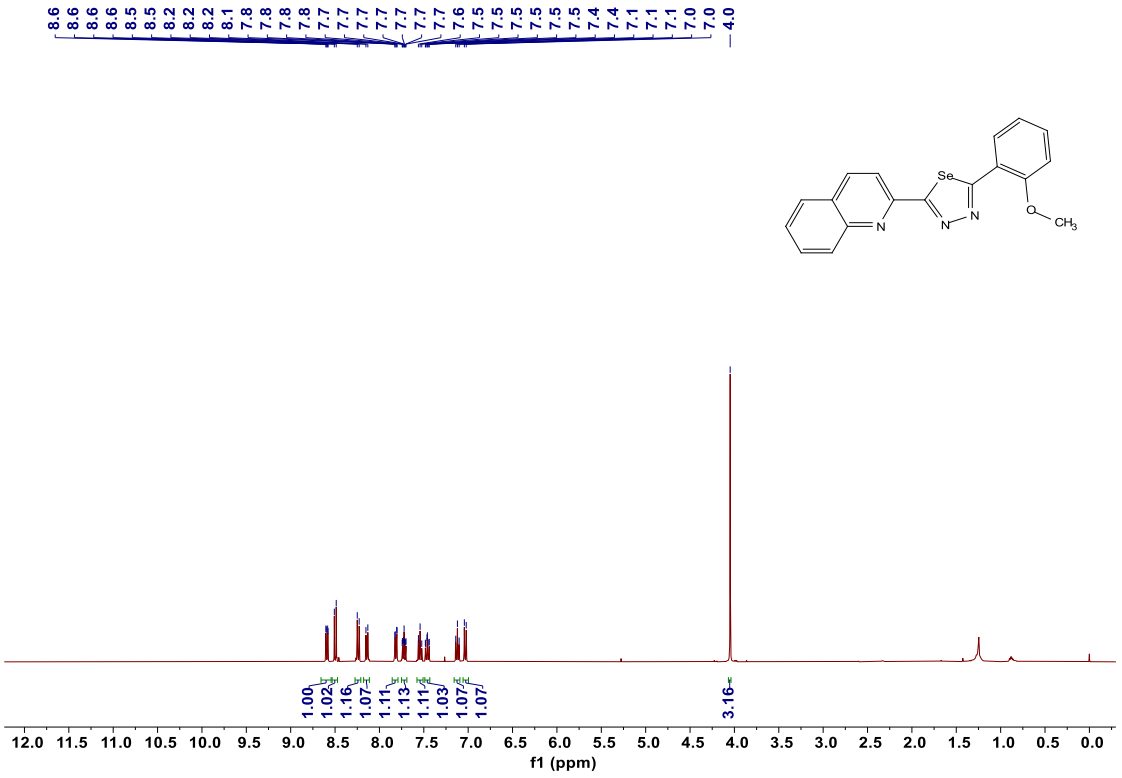
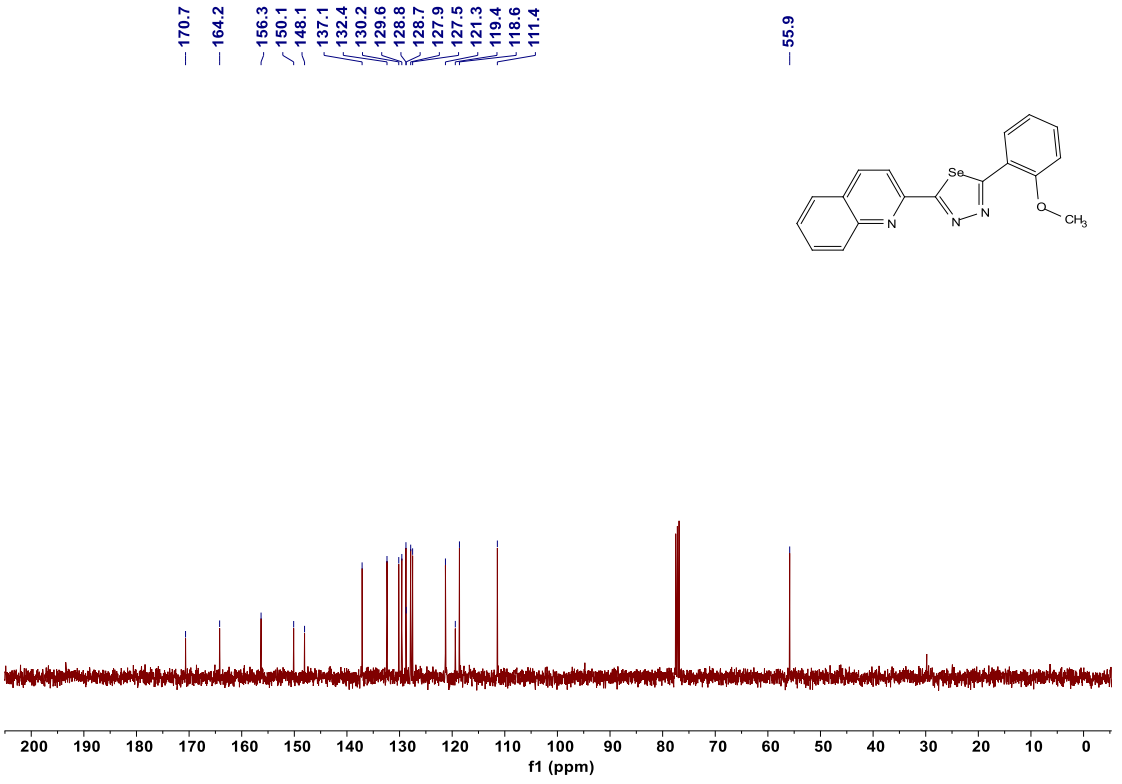
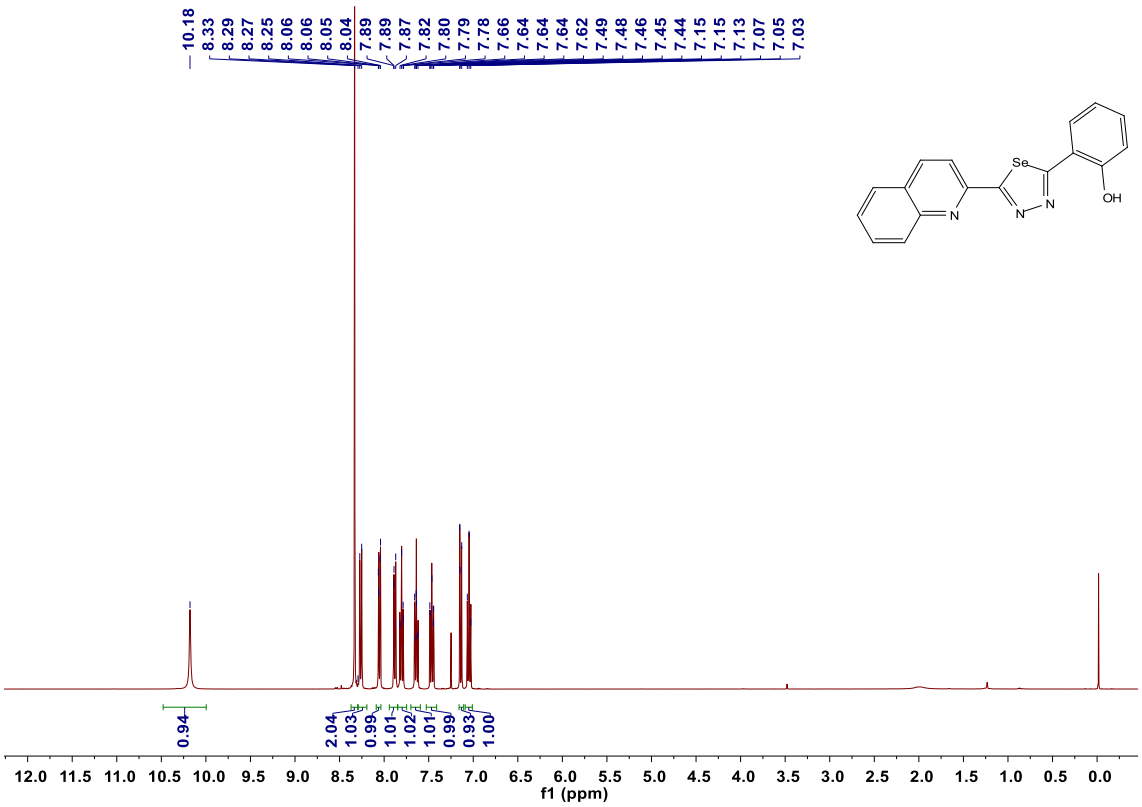
-200
f1 (ppm)

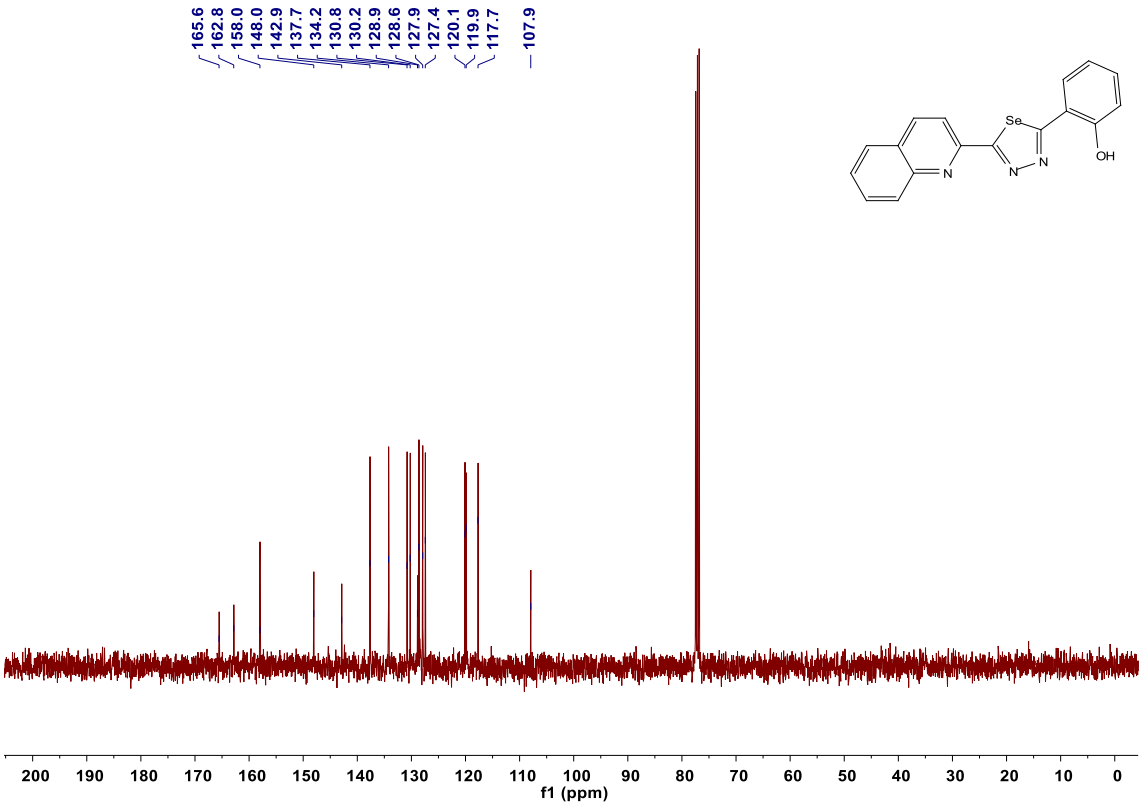
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **n6**



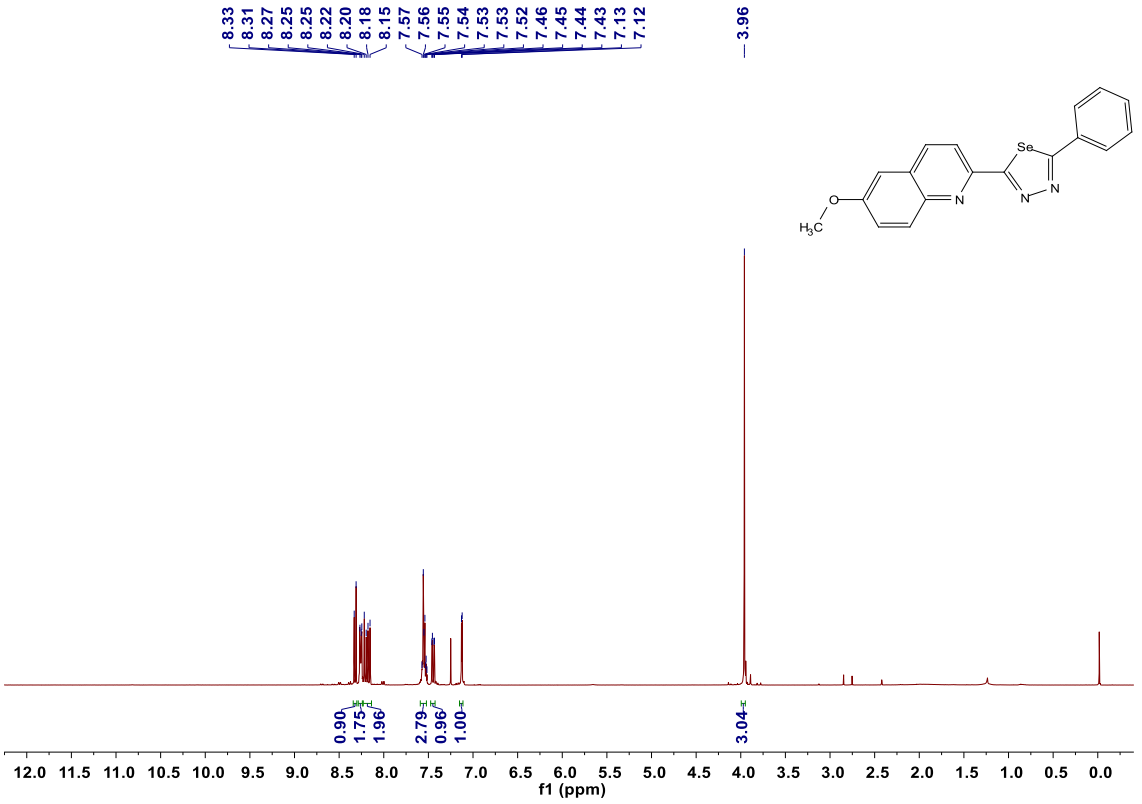


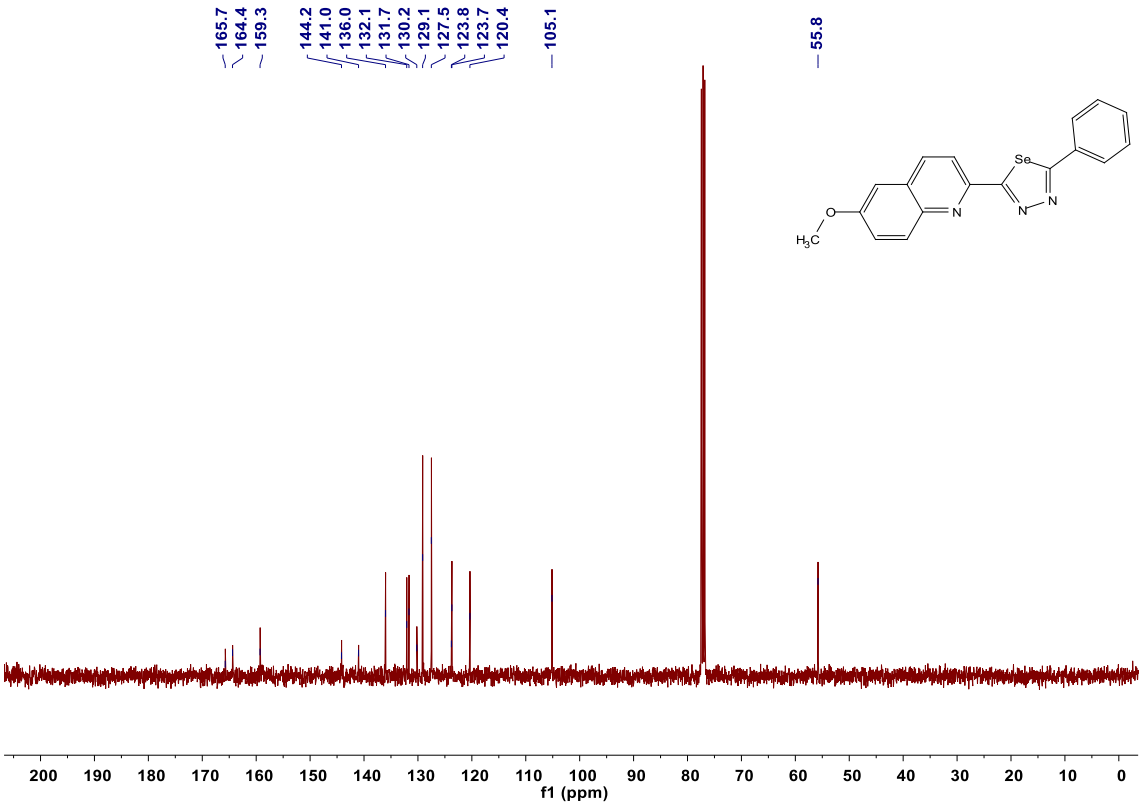
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **n7**



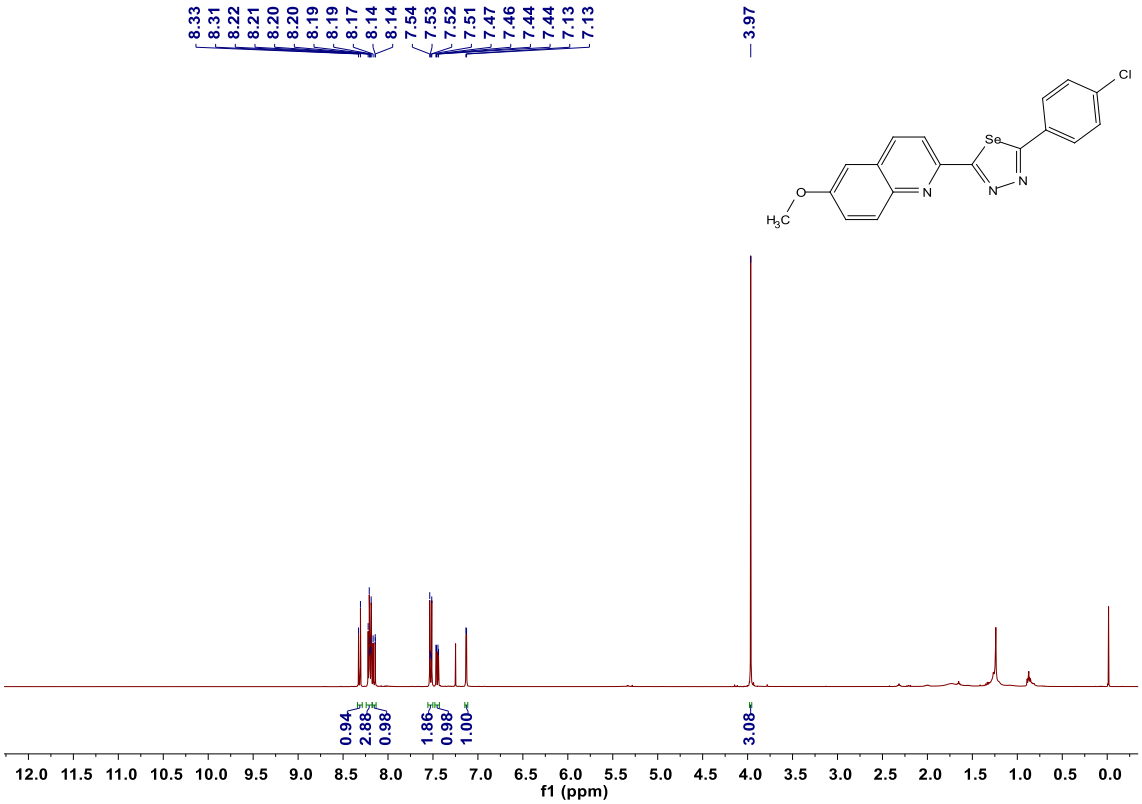


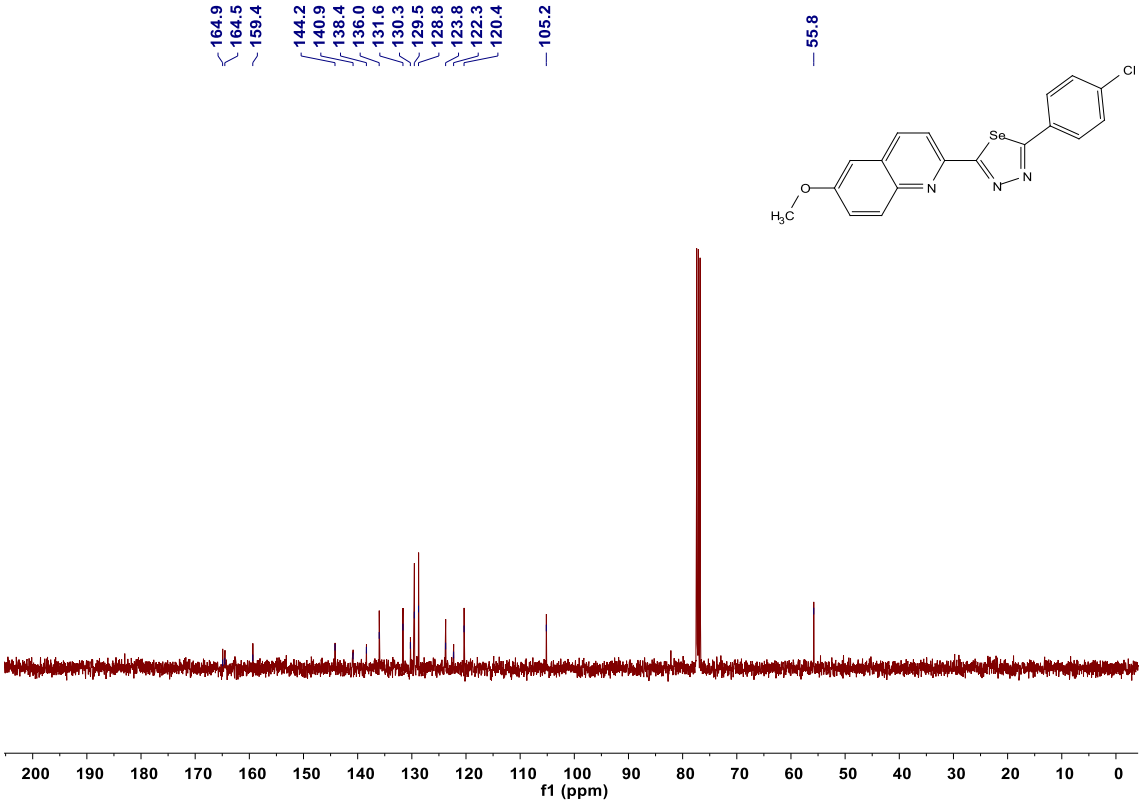
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **n8**





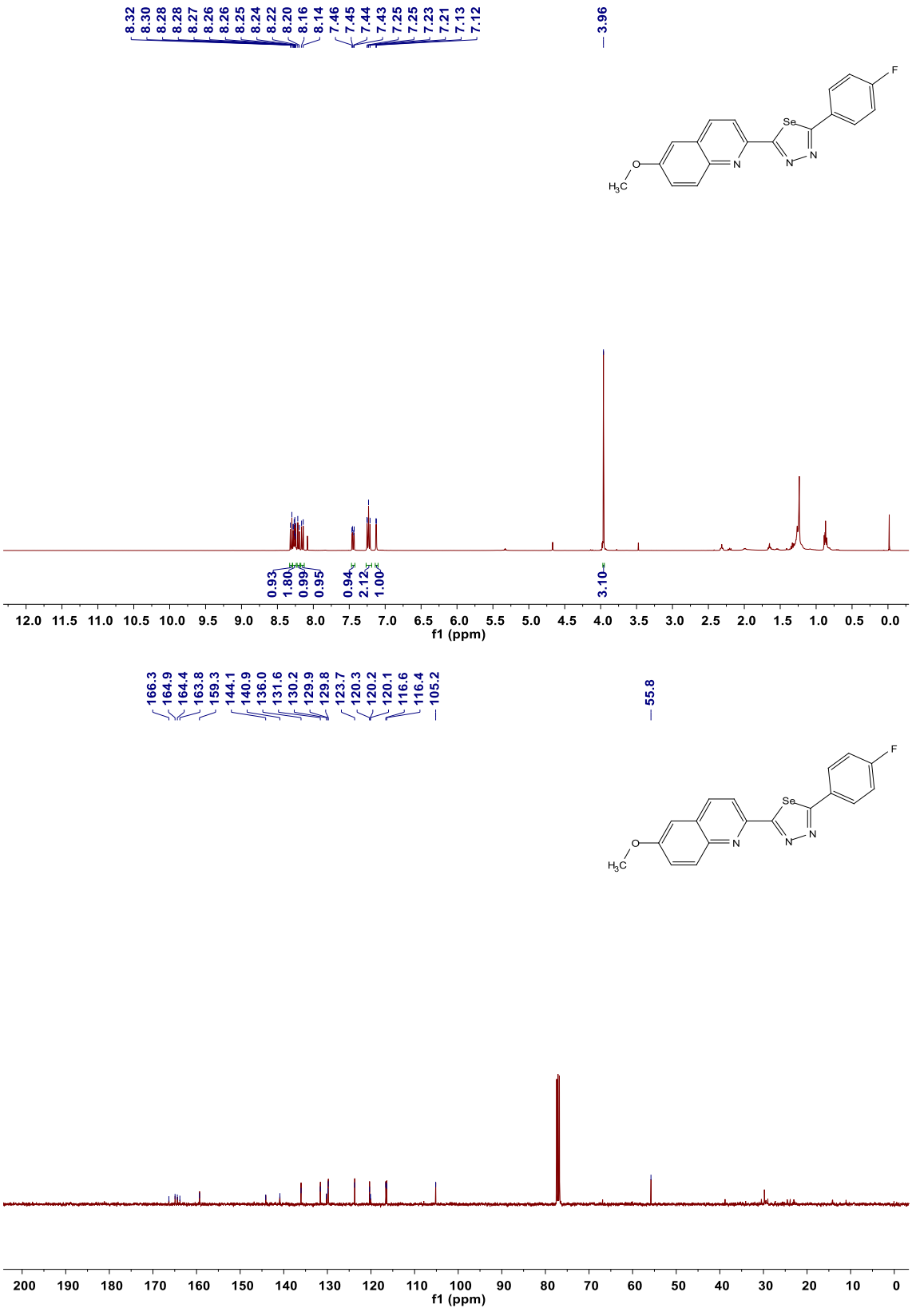
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **n9**

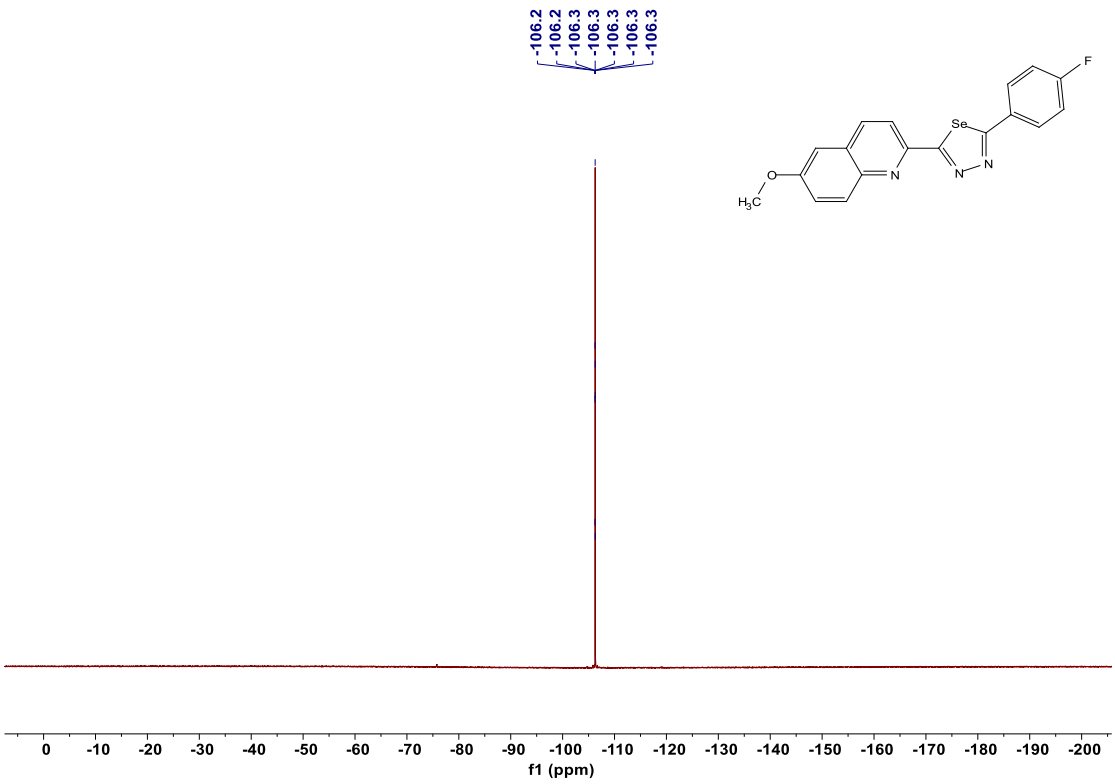




^{1}H NMR (400 MHz, Chloroform-*d*), ^{13}C NMR (100 MHz, Chloroform-*d*), and

^{19}F NMR (376 MHz, Chloroform-*d*) of **n1**0

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-80
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-110
-120
-130
-140
-150
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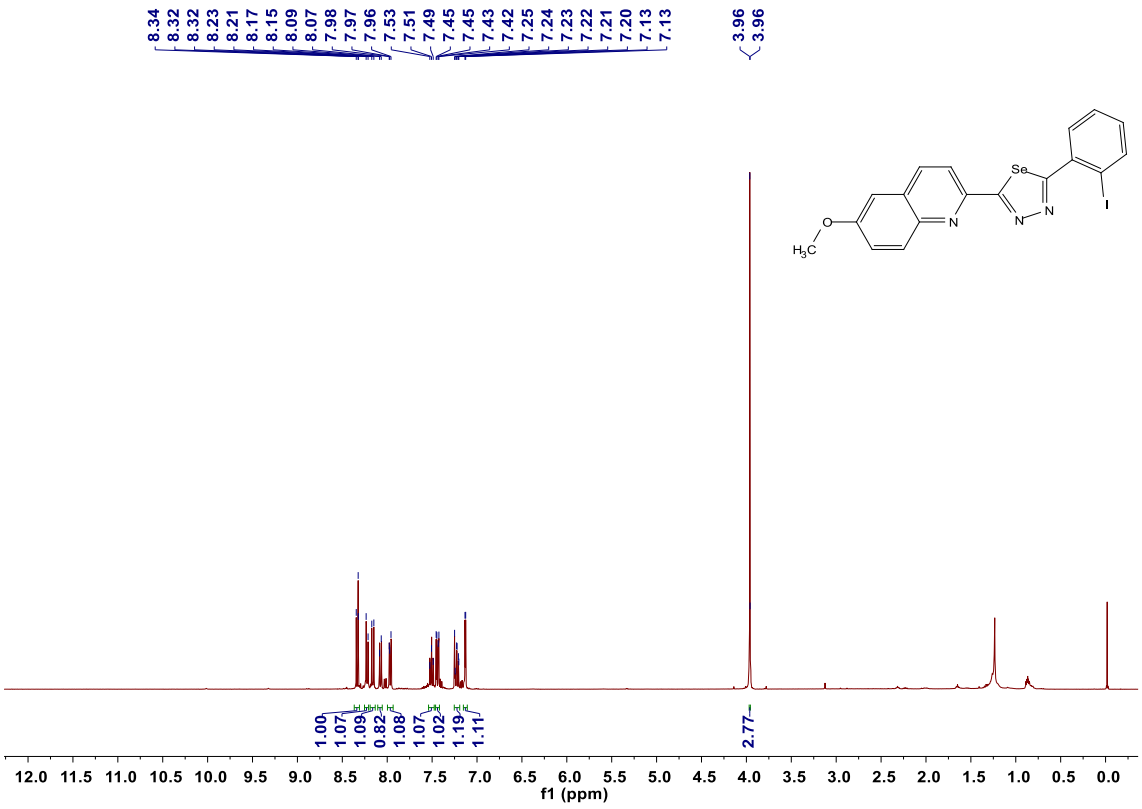
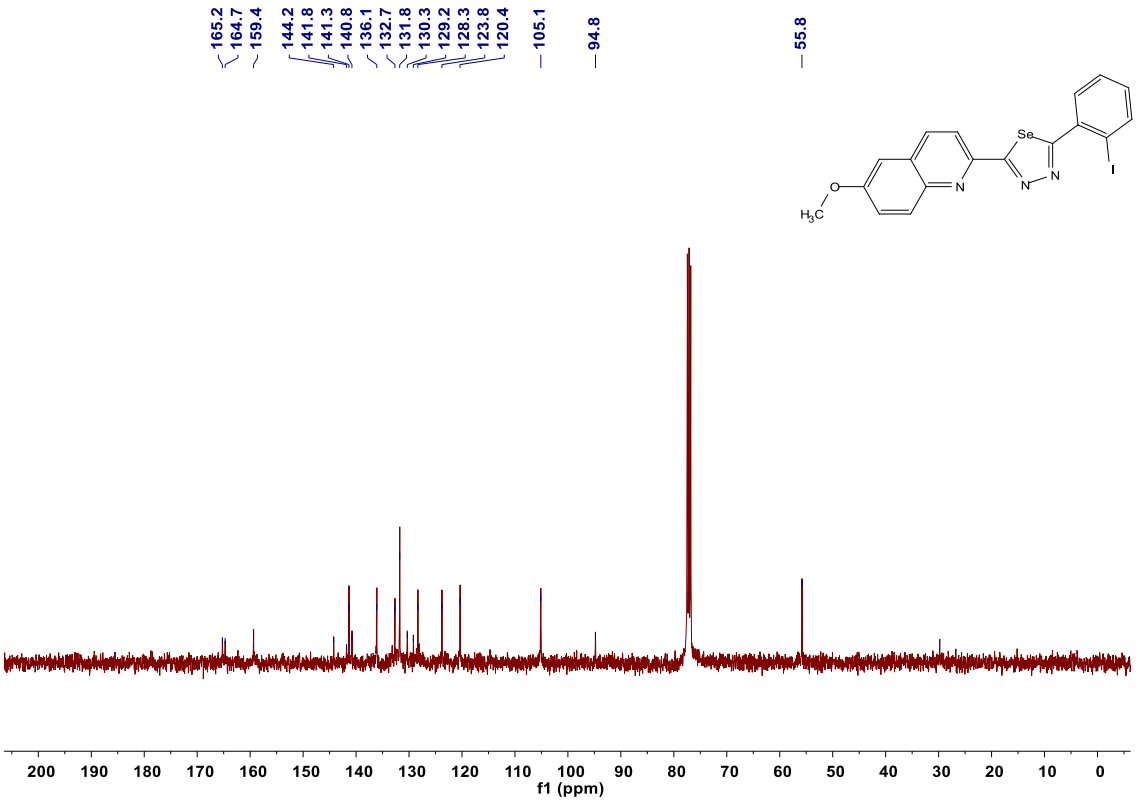
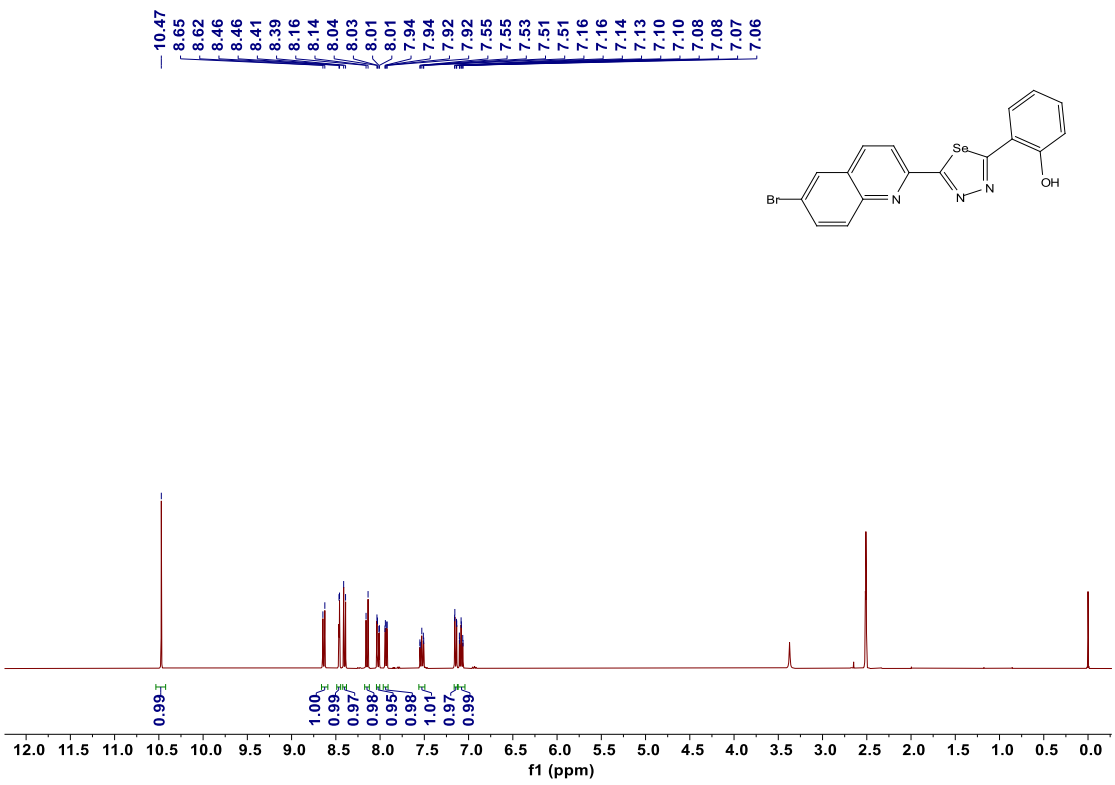
f1 (ppm)

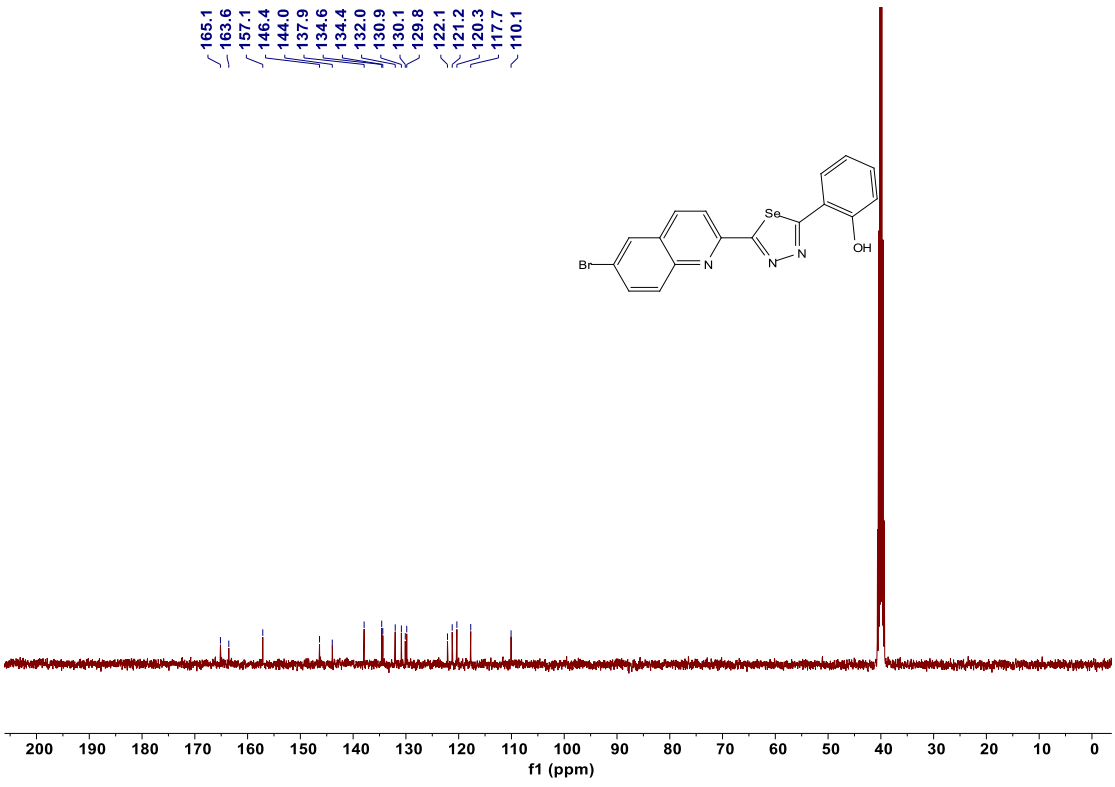
^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **n11**



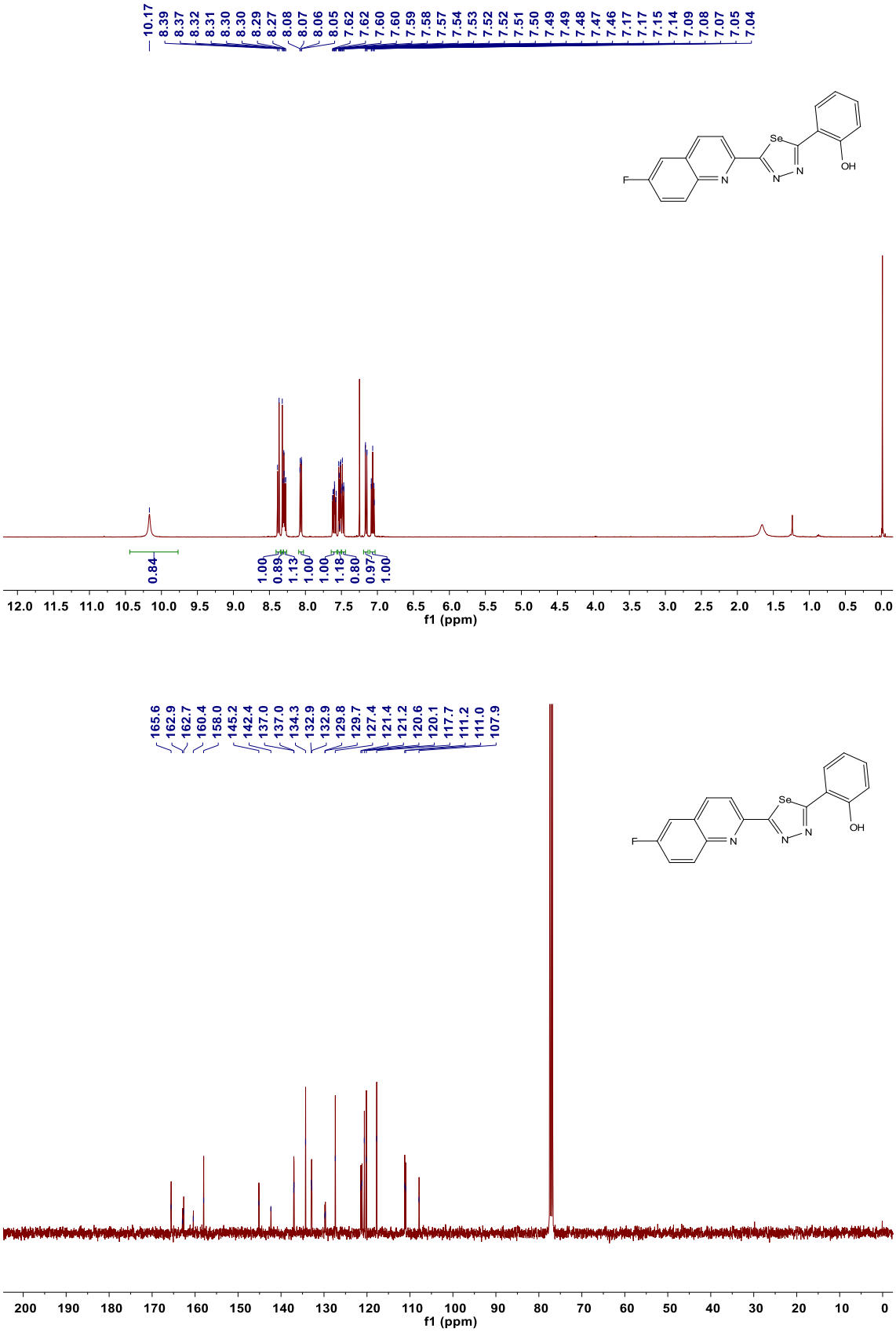


^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, DMSO-d_6) of **n12**





^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **n13**



^{1}H NMR (400 MHz, Chloroform-*d)* and ^{13}C NMR (100 MHz, Chloroform-*d*) of **n14**