

Supporting Information

Electro-oxidative [3+2] cycloaddition for the synthesis of 5-selenyltetrazoles

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General information

All glassware was oven dried at 110 °C for hours and cooled down under vacuum. All reagents and solvents were purchased from commercial sources and used as received without further purification unless otherwise indicated. The instrument for electrolysis is a DC-regulated power supply (HY3005B) (made in China). Electrolysis was conducted at constant current mode employing a C plate (100 mm×10 mm×2 mm, about 15 mm immersion depth in solution) as the anode and a C plate (100 mm×10 mm×2 mm, about 15 mm immersion depth in solution) as the cathode under an inter-electrode distance of 10 mm. Cyclic voltammetry was performed on CHI760E Electrochemical Analyzer. Thin-layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (bp. 60-90 °C). GC-MS spectra were recorded on SHIMADZU GCMS-QP2020NX. ¹H NMR, ¹⁹F NMR and ¹³C NMR spectra were recorded in CDCl₃ or DMSO on a Bruker DRX-400 spectrometer operating at 400 MHz, 376 MHz and 100 MHz, respectively. All chemical shifts (δ) are reported in ppm and coupling constants (*J*) in Hz. All chemical shifts are reported relative to tetramethylsilane and d-solvent peaks (77.16 ppm, chloroform), respectively. High-resolution mass spectra (HRMS) were obtained on an Agilent mass spectrometer using ESI-TOF (electrospray ionization-time of flight).

Experimental procedure

Caution!

Trimethylsilyl azide (TMSN₃) and tetrazole substrates are highly reactive and potentially explosive compounds. Handle with appropriate personal protective equipment, including gloves and eye protection, under adequate ventilation. Avoid exposure to heat, sparks, or open flames.

Selenium-containing compounds and electrochemically generated bromine are highly toxic and corrosive substances. Handle with appropriate personal protective equipment, including chemical-resistant gloves and eye protection, under adequate ventilation (preferably in a fume hood). Avoid inhalation, skin contact, or eye exposure. All waste materials must be properly collected and disposed of as hazardous chemicals.

General Procedure for the Synthesis of Substrates: Isocyanides **1a-1j**^[1] and diselenides **2a-2l**^[2] were synthesized according to the known methods.

Procedure and experimental setup for the electrolysis: In an oven-dried undivided three-necked bottle (25 mL) equipped with a stir bar, 1-isocyano-4-methylbenzene **1a** (35.1 mg, 0.30 mmol), 1,2-diphenyldiselenane **2a** (62.4 mg, 0.20 mmol) and TMSN₃ **3a** (92.0 mg, 0.80 mmol), ⁿBu₄NBr (32.2 mg, 0.10 mmol) and MeCN : HFIP = 5 : 1 (3 mL) were combined and added. The bottle was equipped with a C plate (100 mm×10 mm×2 mm, about 15 mm immersion depth in solution) as the anode and a C plate (100 mm×10 mm×2 mm, about 15 mm immersion depth in solution) as the cathode, which was then charged with argon. The reaction mixture was stirred at 360 rpm and electrolyzed at a constant current of 12 mA ($j = 4 \text{ mA/cm}^2$) at room temperature for 1.5 h (2.2 F/mol). When the reaction finished, the solvent was removed with a rotary evaporator. The pure product was obtained by flash chromatography on silica gel using petroleum ether and ethyl acetate as the eluent.

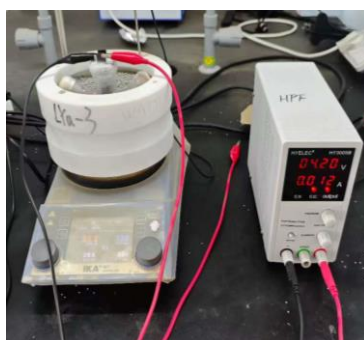


Figure S1: Images of the electrolysis setup.

General procedure for cyclic voltammetry (CV): Cyclic voltammetry was performed on a “computer-controlled CH Instrument Electrochemical Analyzer [CHI760E]” in a three-electrode cell connected to a schlenk line under argon at room temperature. The working electrode was a glassy carbon electrode (length: 80 mm, diameter: 3 mm, about 10 mm immersion depth in solution), the counter electrode was a platinum wire (length: 37 mm, diameter: 0.5 mm, surface area: 0.59 cm²). The electrode was polished with figure-eightS34motions on a cloth polishing pad in a water-alumina slurry. The reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution, and separated from the reaction by a salt bridge. 6 mL MeCN/HFIP (5 : 1) containing 0.1 M ⁿBu₄NBF₄ were poured into the electrochemical cell in all experiments. For the cyclic voltammetric measurement, the IUPAC convention was followed. The starting point for the CV curve was at 0.0 volt and measured in the positive direction. For the CV experiments, the initial potential was 0.0 V, the switching potential was +2.0 V or +2.7 V and the scan rate was 100 mV/s. All solutions used for the voltametric experiments were deoxygenated by purging with high purity argon gas up to 5 mins and measurements were performed in an argon atmosphere at room temperature (25 ± 2 °C).

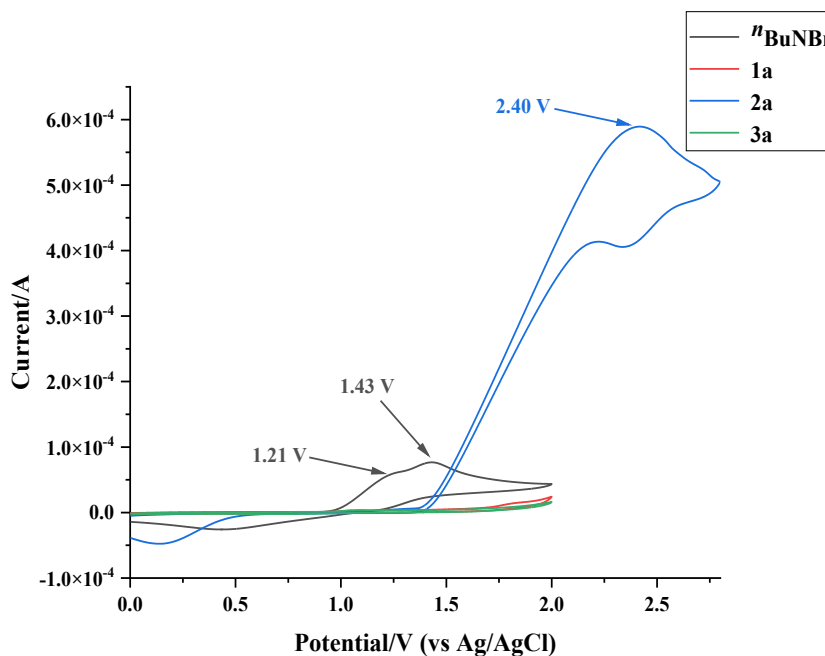


Figure S2: Cyclic voltammograms of **1a** (1-isocyano-4-methylbenzene), **2a** (1,2-diphenyldisilane), **3a** (TMSN₃) or ⁿBu₄NBr following IUPAC convention. A three-electrode configuration having a glassy carbon as a working electrode, platinum wire as a counter electrode, and Ag/AgCl as a reference electrode in 0.1 M ⁿBu₄NBF₄ in MeCN : HFIP = 5 : 1 (6 mL) was used. Scan rate: 0.1 V/s.

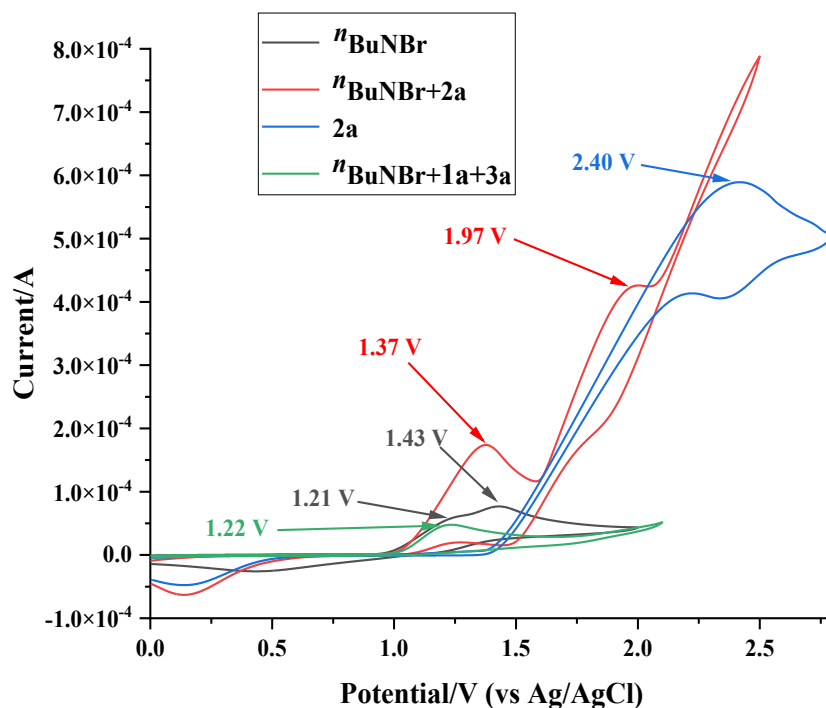


Figure S3: Cyclic voltammograms following IUPAC convention. A three-electrode configuration having a glassy carbon as a working electrode, platinum wire as a counter electrode, and Ag/AgCl as a reference electrode in 0.1 M $n\text{Bu}_4\text{NBF}_4$ in MeCN : HFIP = 5 : 1 (6 mL) was used. Scan rate: 0.1 V/s.

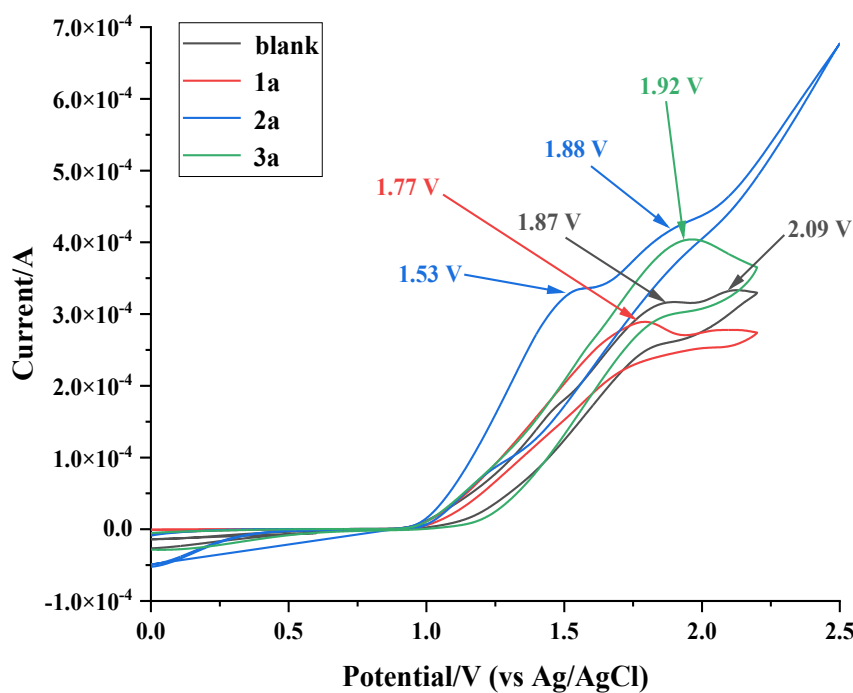
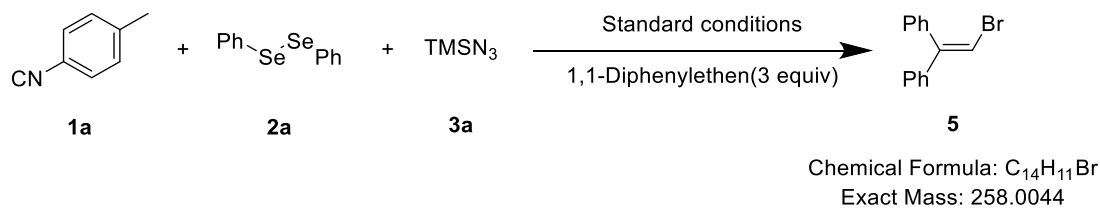


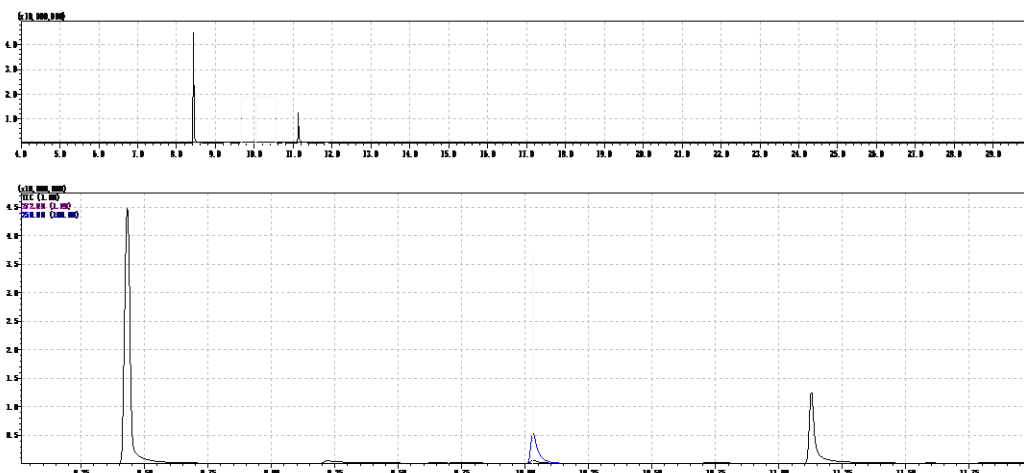
Figure S4: Cyclic voltammograms of **1a** (1-isocyano-4-methylbenzene), **2a** (1,2-diphenyldisilane), **3a** (TMSN_3) following IUPAC convention. A three-electrode configuration having a glassy carbon as a working electrode, platinum wire as a counter electrode, and Ag/AgCl as a reference electrode in 0.1 M $n\text{Bu}_4\text{NBr}$ in MeCN : HFIP = 5 : 1 (6 mL) was used. Scan rate: 0.1 V/s.

Control Experiments

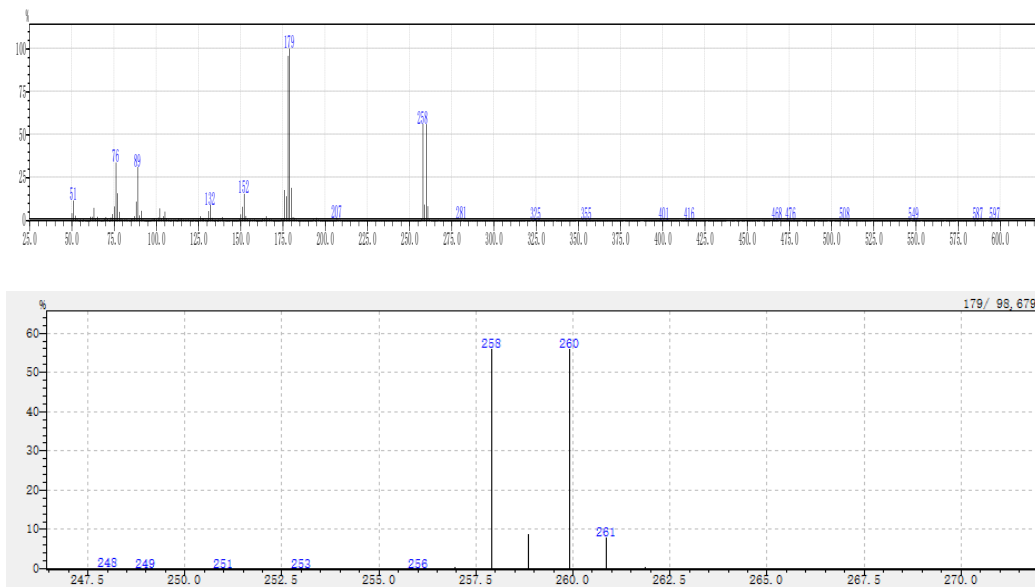
GC-MS analysis of raw reaction mixture by using 1,1-diphenylethen as radical inhibitor



Spectra of GC-MS



MS spectra of the peak at 10.030 min



[MS Spectrum]	Base Peak	m/z	179.00	51.00	11348	11.50
# of Peaks	517	(Inten : 98,679)		51.95	2678	2.71
Raw Spectrum 10.030 (scan :	Event#	1		53.00	708	0.72
1207)	m/z Absolute	Intensity		54.00	111	0.11
Background	No	Relative Intensity		55.00	497	0.50
Background Spectrum	50.00	4106	4.16	56.00	198	0.20

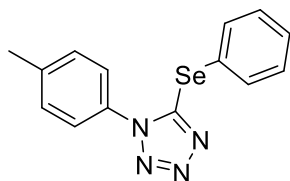
57.00	650	0.66	101.05	1578	1.60	146.00	124	0.13
58.00	95	0.10	102.05	6871	6.96	147.00	220	0.22
59.00	212	0.21	103.05	963	0.98	148.00	73	0.07
60.00	223	0.23	104.05	2329	2.36	149.05	612	0.62
61.00	2007	2.03	105.05	5018	5.09	150.00	3455	3.50
61.95	1983	2.01	106.05	11091.12		151.00	7786	7.89
63.00	7102	7.20	107.05	448	0.45	152.00	15146	15.35
63.95	840	0.85	108.00	166	0.17	153.00	2508	2.54
65.00	2015	2.04	109.00	258	0.26	154.00	559	0.57
66.00	511	0.52	110.00	343	0.35	155.00	254	0.26
67.00	137	0.14	111.05	525	0.53	155.90	450	0.46
68.00	106	0.11	112.00	218	0.22	156.90	289	0.29
69.05	733	0.74	113.00	11301.15		157.95	650	0.66
70.05	1891	1.92	113.95	552	0.56	159.00	84	0.09
71.00	726	0.74	115.00	1318	1.34	160.00	130	0.13
72.00	137	0.14	116.10	508	0.51	161.00	129	0.13
73.05	1595	1.62	117.10	294	0.30	162.00	212	0.21
74.00	3561	3.61	118.10	377	0.38	162.95	970	0.98
75.05	7965	8.07	119.10	410	0.42	164.05	641	0.65
76.05	33275	33.72	120.10	103	0.10	165.00	2308	2.34
77.00	15486	15.69	121.10	185	0.19	166.00	540	0.55
78.05	4769	4.83	122.10	302	0.31	167.00	649	0.66
79.00	1084	1.10	123.10	170	0.17	167.95	574	0.58
79.95	468	0.47	124.10	132	0.13	169.00	172	0.17
81.05	388	0.39	125.05	499	0.51	170.00	38	0.04
82.00	607	0.62	126.00	2342	2.37	171.00	41	0.04
82.95	331	0.34	127.10	1238	1.25	172.00	33	0.03
84.00	166	0.17	128.05	11361.15		172.90	22	0.02
85.10	732	0.74	129.10	298	0.30	173.90	790	0.80
86.10	988	1.00	130.00	217	0.22	175.05	1290	1.31
87.10	2255	2.29	131.05	5302	5.37	176.00	17324	17.56
88.05	10713	10.86	132.05	8781	8.90	177.05	13739	13.92
89.05	30525	30.93	133.05	1367	1.39	178.00	94420	95.68
90.05	2818	2.86	134.10	223	0.23	179.00	98679	100.00
91.05	5505	5.58	135.10	249	0.25	180.00	18633	18.88
92.05	642	0.65	136.10	86	0.09	180.95	1893	1.92
93.00	170	0.17	137.00	495	0.50	182.00	1455	1.47
94.00	94	0.10	137.95	324	0.33	183.00	514	0.52
95.00	207	0.21	139.00	1796	1.82	184.00	100	0.10
96.00	210	0.21	140.00	361	0.37	185.00	63	0.06
97.05	329	0.33	141.00	180	0.18	186.00	55	0.06
98.00	11351.15		142.00	81	0.08	187.00	76	0.08
99.00	11051.12		143.00	26	0.03	188.00	34	0.03
100.00	566	0.57	145.00	31	0.03	189.00	42	0.04

190.00	57	0.06	234.00	30	0.03	277.90	36	0.04
191.00	215	0.22	235.00	65	0.07	278.90	57	0.06
191.90	58	0.06	236.00	63	0.06	279.90	47	0.05
192.90	590	0.60	237.00	34	0.03	280.90	295	0.30
194.00	230	0.23	238.00	55	0.06	281.90	126	0.13
195.00	1466	1.49	239.00	57	0.06	282.90	46	0.05
196.00	444	0.45	240.00	55	0.06	283.90	73	0.07
197.00	113	0.11	241.00	68	0.07	284.90	54	0.05
198.00	47	0.05	242.00	36	0.04	285.90	27	0.03
199.00	63	0.06	243.00	84	0.09	286.90	16	0.02
200.00	19	0.02	244.00	70	0.07	287.90	30	0.03
201.00	92	0.09	245.00	164	0.17	288.90	34	0.03
202.00	52	0.05	246.00	190	0.19	289.90	13	0.01
203.00	50	0.05	247.00	52	0.05	290.90	10	0.01
204.00	44	0.04	248.00	201	0.20	291.90	2	0.00
205.00	66	0.07	249.00	110	0.11	292.90	13	0.01
206.00	27	0.03	250.00	52	0.05	293.90	10	0.01
206.95	1331	1.35	251.00	135	0.14	294.90	33	0.03
208.00	308	0.31	252.00	63	0.06	295.90	21	0.02
209.00	254	0.26	253.00	87	0.09	296.90	13	0.01
210.00	71	0.07	254.00	46	0.05	297.90	24	0.02
211.00	58	0.06	255.00	33	0.03	298.90	18	0.02
212.00	14	0.01	256.00	84	0.09	299.90	11	0.01
213.00	38	0.04	256.95	699	0.71	300.90	21	0.02
214.00	16	0.02	257.90	55430	56.17	301.90	3	0.00
215.00	38	0.04	258.85	8968	9.09	302.90	27	0.03
216.00	54	0.05	259.90	55303	56.04	303.90	27	0.03
217.00	63	0.06	260.85	8106	8.21	304.90	10	0.01
218.00	24	0.02	261.85	628	0.64	305.90	11	0.01
219.00	86	0.09	262.90	73	0.07	306.90	33	0.03
220.00	34	0.03	263.90	54	0.05	307.90	24	0.02
221.00	114	0.12	264.90	108	0.11	308.90	6	0.01
222.00	98	0.10	265.90	60	0.06	309.90	18	0.02
223.00	76	0.08	266.90	250	0.25	310.90	24	0.02
224.00	54	0.05	267.90	116	0.12	311.90	18	0.02
225.00	74	0.07	268.90	50	0.05	312.90	29	0.03
226.00	33	0.03	269.90	54	0.05	313.90	60	0.06
227.00	39	0.04	270.90	50	0.05	314.90	16	0.02
228.00	41	0.04	271.90	34	0.03	315.90	16	0.02
229.00	44	0.04	272.90	8	0.01	316.90	24	0.02
230.00	86	0.09	273.90	29	0.03	317.90	13	0.01
231.00	10	0.01	274.90	33	0.03	319.90	22	0.02
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233.00	38	0.04	276.90	36	0.04	322.90	13	0.01

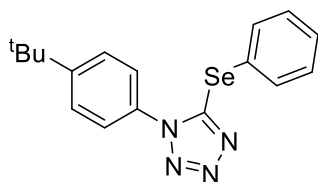
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326.90	62	0.06	373.90	21	0.02	421.90	34	0.03
327.90	27	0.03	374.90	27	0.03	422.90	8	0.01
328.90	46	0.05	375.90	18	0.02	423.90	24	0.02
329.90	19	0.02	377.90	21	0.02	424.90	21	0.02
330.90	18	0.02	378.90	13	0.01	426.90	13	0.01
331.90	26	0.03	379.90	27	0.03	427.90	10	0.01
332.90	13	0.01	380.90	24	0.02	428.90	44	0.04
333.90	16	0.02	381.90	31	0.03	429.90	42	0.04
334.90	14	0.01	382.90	27	0.03	430.90	14	0.01
336.90	8	0.01	383.90	14	0.01	431.90	58	0.06
337.90	34	0.03	384.90	3	0.00	432.90	14	0.01
338.90	42	0.04	385.90	36	0.04	433.90	33	0.03
339.90	3	0.00	388.90	6	0.01	434.90	30	0.03
340.90	142	0.14	389.90	26	0.03	435.90	33	0.03
341.90	63	0.06	390.90	10	0.01	436.90	19	0.02
342.90	86	0.09	391.90	31	0.03	440.90	30	0.03
343.90	38	0.04	392.90	16	0.02	441.90	3	0.00
344.90	44	0.04	393.90	26	0.03	443.90	14	0.01
345.90	42	0.04	394.90	2	0.00	444.90	13	0.01
346.90	38	0.04	395.90	2	0.00	446.90	13	0.01
347.90	3	0.00	396.90	10	0.01	447.90	21	0.02
349.90	6	0.01	397.90	29	0.03	449.90	16	0.02
350.90	6	0.01	398.90	14	0.01	450.90	18	0.02
351.90	8	0.01	399.90	31	0.03	451.90	11	0.01
352.90	52	0.05	400.90	129	0.13	452.90	19	0.02
353.90	18	0.02	401.90	14	0.01	453.90	24	0.02
354.90	185	0.19	402.90	41	0.04	455.90	34	0.03
355.90	62	0.06	403.90	10	0.01	456.90	36	0.04
356.90	38	0.04	404.90	44	0.04	458.90	5	0.01
357.90	31	0.03	405.90	14	0.01	459.90	30	0.03
358.90	60	0.06	406.90	18	0.02	460.90	31	0.03
360.90	34	0.03	407.90	2	0.00	461.90	19	0.02
361.90	19	0.02	408.90	26	0.03	462.90	39	0.04
362.90	30	0.03	410.90	8	0.01	464.90	18	0.02
363.90	14	0.01	411.90	5	0.01	465.90	13	0.01
364.90	50	0.05	412.90	57	0.06	466.90	18	0.02
365.90	36	0.04	413.90	22	0.02	467.90	46	0.05
366.90	24	0.02	414.90	71	0.07	469.90	3	0.00
367.90	21	0.02	415.90	62	0.06	470.90	33	0.03
368.90	49	0.05	416.90	57	0.06	471.90	5	0.01
369.90	5	0.01	417.90	33	0.03	472.90	21	0.02
370.90	30	0.03	418.90	27	0.03	473.90	46	0.05

474.90	46	0.05	517.90	21	0.02	558.90	3	0.00
475.90	49	0.05	518.90	13	0.01	559.90	14	0.01
476.90	38	0.04	519.90	27	0.03	560.90	14	0.01
477.90	5	0.01	520.90	30	0.03	561.90	27	0.03
478.90	34	0.03	521.90	33	0.03	562.90	26	0.03
479.90	19	0.02	522.90	22	0.02	563.90	38	0.04
480.90	34	0.03	524.90	24	0.02	564.90	54	0.05
482.90	6	0.01	525.90	19	0.02	565.90	22	0.02
483.90	41	0.04	526.90	29	0.03	567.90	10	0.01
484.90	14	0.01	527.90	26	0.03	568.90	11	0.01
485.90	6	0.01	528.90	27	0.03	569.90	13	0.01
486.90	18	0.02	529.90	14	0.01	570.90	3	0.00
487.90	2	0.00	530.90	30	0.03	571.90	16	0.02
488.90	44	0.04	531.90	24	0.02	572.90	2	0.00
489.90	22	0.02	532.90	38	0.04	574.90	18	0.02
491.90	22	0.02	533.90	24	0.02	575.90	24	0.02
492.90	42	0.04	534.90	39	0.04	576.90	14	0.01
493.90	10	0.01	535.90	3	0.00	577.90	26	0.03
494.90	33	0.03	536.90	3	0.00	578.90	10	0.01
495.90	5	0.01	537.90	29	0.03	579.90	21	0.02
496.90	14	0.01	538.90	24	0.02	580.90	5	0.01
498.90	11	0.01	539.90	13	0.01	581.90	31	0.03
499.90	22	0.02	540.90	19	0.02	582.90	19	0.02
501.90	3	0.00	541.90	10	0.01	583.90	38	0.04
502.90	11	0.01	542.90	26	0.03	584.90	34	0.03
503.90	8	0.01	543.90	24	0.02	585.90	26	0.03
504.90	2	0.00	544.90	11	0.01	586.90	44	0.04
506.90	30	0.03	545.90	26	0.03	587.90	10	0.01
507.90	44	0.04	547.90	18	0.02	588.90	19	0.02
508.90	14	0.01	548.90	71	0.07	589.90	33	0.03
509.90	3	0.00	549.90	39	0.04	590.90	27	0.03
510.90	36	0.04	550.90	18	0.02	592.90	14	0.01
511.90	41	0.04	551.90	10	0.01	593.90	21	0.02
512.90	13	0.01	553.90	22	0.02	594.90	29	0.03
513.90	5	0.01	554.90	41	0.04	595.90	3	0.00
514.90	16	0.02	555.90	21	0.02	596.90	24	0.02
515.90	13	0.01	556.90	24	0.02	597.90	10	0.01
516.90	19	0.02	557.90	8	0.01	598.90	18	0.02

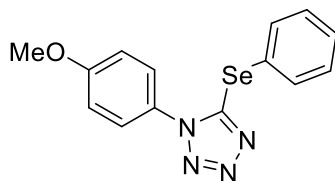
Detail descriptions for products



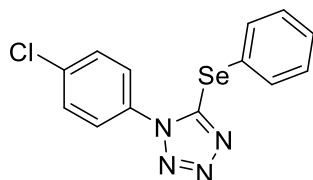
5-(phenylselanyl)-1-(p-tolyl)-1H-tetrazole (4aa): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 77%, 73.0 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.63-7.58 (m, 2H), 7.41-7.36 (m, 1H), 7.36-7.32 (m, 5H), 7.32-7.29 (m, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 147.1, 141.0, 135.2, 131.5, 130.4, 129.9, 129.8, 124.6, 124.4, 21.4. HRMS (ESI-TOF) calculated for $\text{C}_{14}\text{H}_{13}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 317.0300; found: 317.0305.



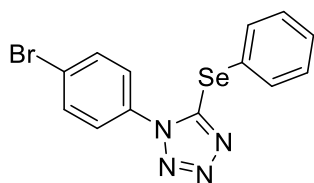
1-(4-(tert-butyl)phenyl)-5-(phenylselanyl)-1H-tetrazole (4ba): by silica gel column chromatography (petroleum ether /ethyl acetate = 20:1), yield: 70%, 75.2 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, J = 7.6 Hz, 2H), 7.53 (d, J = 8.3 Hz, 2H), 7.38 (d, J = 8.7 Hz, 3H), 7.31 (t, J = 7.4 Hz, 2H), 1.37 (s, 9H). ^{13}C NMR (100 MHz, CDCl_3) δ 154.0, 147.1, 135.3, 131.4, 129.9, 129.8, 126.8, 124.4, 124.3, 35.1, 31.3. HRMS (ESI-TOF) calculated for $\text{C}_{17}\text{H}_{19}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 359.0769; found: 359.0772.



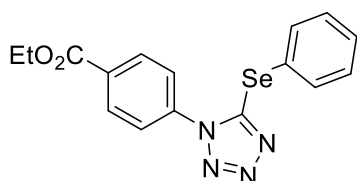
1-(4-methoxyphenyl)-5-(phenylselanyl)-1H-tetrazole (4ca): by silica gel column chromatography (petroleum ether /ethyl acetate = 5:1), yield: 81%, 80.7 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.50 (d, J = 7.3 Hz, 2H), 7.32-7.18 (m, 5H), 6.92 (d, J = 8.9 Hz, 2H), 3.78 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 161.0, 147.3, 135.1, 129.8, 129.7, 126.6, 126.3, 124.3, 114.8, 55.7. HRMS (ESI-TOF) calculated for $\text{C}_{14}\text{H}_{13}\text{N}_4\text{OSe}$ $[\text{M}+\text{H}]^+$: 333.0249; found: 333.0246.



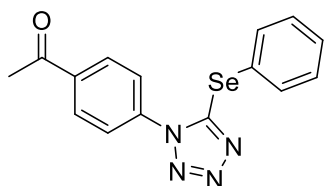
1-(4-chlorophenyl)-5-(phenylselanyl)-1H-tetrazole (4da): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 70%, 70.6 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.57 (d, J = 7.8 Hz, 2H), 7.50 (d, J = 7.7 Hz, 2H), 7.42-7.35 (m, 3H), 7.31 (t, J = 7.3 Hz, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 147.1, 136.6, 135.2, 132.5, 130.0, 129.96, 129.93, 126.1, 124.1. HRMS (ESI-TOF) calculated for $\text{C}_{13}\text{H}_{10}\text{ClN}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 336.9754; found: 336.9758.



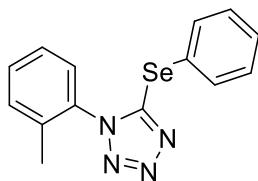
1-(4-bromophenyl)-5-(phenylselanyl)-1H-tetrazole (4ea): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 65%, 74.1 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.69-7.63 (m, 2H), 7.57 (d, J = 7.4 Hz, 2H), 7.42-7.29 (m, 5H). ^{13}C NMR (100 MHz, CDCl_3) δ 147.0, 135.2, 133.0, 132.9, 130.0, 129.9, 126.3, 124.7, 124.1. HRMS (ESI-TOF) calculated for $\text{C}_{13}\text{H}_{10}\text{BrN}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 380.9249; found: 380.9252.



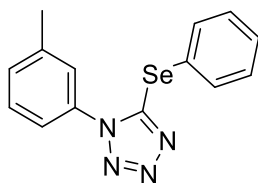
ethyl 4-(5-(phenylselanyl)-1H-tetrazol-1-yl)benzoate (4fa): by silica gel column chromatography (petroleum ether /ethyl acetate = 3:1), yield: 84%, 94.2 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 8.23-8.16 (m, 2H), 7.61-7.53 (m, 4H), 7.40-7.34 (m, 1H), 7.33-7.26 (m, 2H), 4.41 (q, J = 7.1 Hz, 2H), 1.41 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 165.1, 147.0, 137.3, 135.2, 132.2, 131.1, 129.9, 124.4, 124.1, 61.7, 14.3. HRMS (ESI-TOF) calculated for $\text{C}_{16}\text{H}_{15}\text{N}_4\text{O}_2\text{Se}$ $[\text{M}+\text{H}]^+$: 375.0355; found: 375.0351.



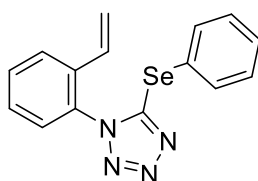
1-(4-(5-(phenylselanyl)-1H-tetrazol-1-yl)phenyl)ethan-1-one (4ga): by silica gel column chromatography (petroleum ether /ethyl acetate = 3:1), yield: 82%, 84.6 mg; brown solid. ^1H NMR (400 MHz, CDCl_3) δ 8.13-8.08 (m, 2H), 7.66-7.56 (m, 4H), 7.41-7.35 (m, 1H), 7.33-7.28 (m, 2H), 2.67-2.63 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 196.5, 147.1, 138.2, 137.4, 135.2, 130.0, 129.9, 129.8, 124.6, 124.0, 26.9. HRMS (ESI-TOF) calculated for $\text{C}_{15}\text{H}_{13}\text{N}_4\text{OSe}$ $[\text{M}+\text{H}]^+$: 345.0249; found: 345.0255.



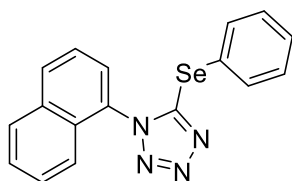
5-(phenylselanyl)-1-(o-tolyl)-1H-tetrazole (4ha): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 54%, 51.2 mg; yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.54-7.49 (m, 2H), 7.47 (td, J = 7.6, 1.3 Hz, 1H), 7.40-7.31 (m, 3H), 7.31-7.26 (m, 2H), 7.14 (d, J = 7.8 Hz, 1H), 1.95 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 148.0, 135.5, 135.4, 135.3, 132.9, 131.6, 131.2, 129.8, 127.1, 127.0, 123.9, 17.4. HRMS (ESI-TOF) calculated for $\text{C}_{14}\text{H}_{13}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 317.0300; found: 317.0302.



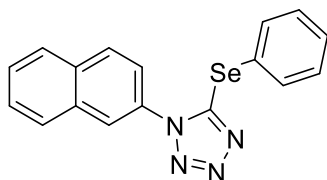
5-(phenylselanyl)-1-(*m*-tolyl)-1*H*-tetrazole (4ia): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 66%, 62.6 mg; yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.54-7.49 (m, 2H), 7.36-7.21 (m, 5H), 7.19-7.14 (m, 2H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 147.1, 140.2, 135.3, 133.9, 131.3, 129.9, 129.8, 129.5, 125.3, 124.3, 121.7, 21.4. HRMS (ESI-TOF) calculated for $\text{C}_{14}\text{H}_{13}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 317.0300; found: 317.0304.



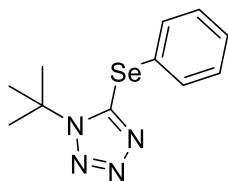
5-(phenylselanyl)-1-(2-vinylphenyl)-1*H*-tetrazole (4ja): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 58%, 57.0 mg; transparent oil. ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, $J = 7.9$ Hz, 1H), 7.50-7.41 (m, 3H), 7.33-7.25 (m, 2H), 7.22-7.16 (m, 2H), 7.08 (d, $J = 7.9$ Hz, 1H), 5.99 (dd, $J = 17.4, 11.0$ Hz, 1H), 5.59 (d, $J = 17.3$ Hz, 1H), 5.20 (d, $J = 10.9$ Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 147.6, 134.4, 134.1, 130.4, 130.2, 128.9, 128.8, 128.7, 127.7, 126.4, 125.8, 123.0, 118.1. HRMS (ESI-TOF) calculated for $\text{C}_{15}\text{H}_{13}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 329.0300; found: 329.0303.



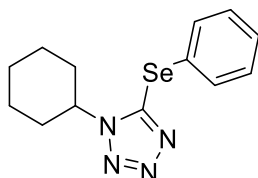
1-(naphthalen-1-yl)-5-(phenylselanyl)-1*H*-tetrazole (4ka): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 68%, 71.8 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.95 (d, $J = 8.3$ Hz, 1H), 7.84 (d, $J = 8.2$ Hz, 1H), 7.46 (q, $J = 8.2$ Hz, 2H), 7.41-7.28 (m, 4H), 7.18-7.11 (m, 1H), 7.09-6.98 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 149.1, 135.3, 134.1, 131.7, 130.0, 129.6, 128.8, 128.4, 128.2, 127.4, 125.3, 124.9, 123.7, 121.8. HRMS (ESI-TOF) calculated for $\text{C}_{17}\text{H}_{13}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 353.0300; found: 353.0298.



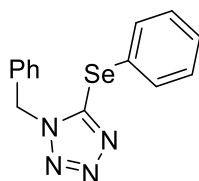
1-(naphthalen-2-yl)-5-(phenylselanyl)-1*H*-tetrazole (4la): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 66%, 69.7 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.90 (d, $J = 8.7$ Hz, 1H), 7.86-7.77 (m, 3H), 7.56-7.48 (m, 4H), 7.45 (d, $J = 8.7$ Hz, 1H), 7.26 (t, $J = 7.3$ Hz, 1H), 7.19 (t, $J = 7.5$ Hz, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 147.4, 135.3, 133.5, 132.8, 131.3, 130.1, 129.9, 129.8, 128.5, 128.1, 128.0, 127.8, 124.3, 123.9, 121.9. HRMS (ESI-TOF) calculated for $\text{C}_{17}\text{H}_{13}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 353.0300; found: 353.0304.



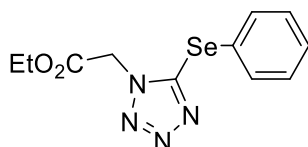
1-(tert-butyl)-5-(phenylselanyl)-1H-tetrazole (4ma): by silica gel column chromatography (petroleum ether /ethyl acetate = 8:1), yield: 66%, 55.8 mg; yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.72-7.67 (m, 2H), 7.44-7.34 (m, 3H), 1.79 (s, 9H). ^{13}C NMR (100 MHz, CDCl_3) δ 144.4, 135.0, 129.9, 129.7, 125.7, 61.7, 29.6. HRMS (ESI-TOF) calculated for $\text{C}_{11}\text{H}_{15}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 283.0456; found: 283.0459.



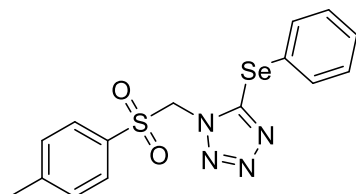
1-cyclohexyl-5-(phenylselanyl)-1H-tetrazole (4na): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 65%, 60.1 mg; transparent oil. ^1H NMR (400 MHz, CDCl_3) δ 7.64-7.55 (m, 2H), 7.41-7.27 (m, 3H), 4.35 (tt, J = 11.6, 4.1 Hz, 1H), 1.95-1.73 (m, 7H), 1.38-1.25 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 144.6, 134.1, 130.0, 129.5, 125.5, 59.2, 32.7, 25.3, 24.8. HRMS (ESI-TOF) calculated for $\text{C}_{13}\text{H}_{17}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 309.0613; found: 309.0617.



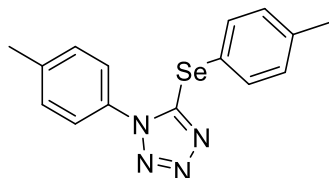
1-benzyl-5-(phenylselanyl)-1H-tetrazole (4oa): by silica gel column chromatography (petroleum ether /ethyl acetate = 3:1), yield: 68%, 64.5 mg; yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.47-7.40 (m, 2H), 7.30-7.16 (m, 6H), 7.13-7.05 (m, 2H), 5.44 (s, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 145.9, 134.0, 133.2, 130.0, 129.5, 129.1, 129.0, 128.0, 125.1, 52.0. HRMS (ESI-TOF) calculated for $\text{C}_{14}\text{H}_{13}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 317.0300; found: 317.0295.



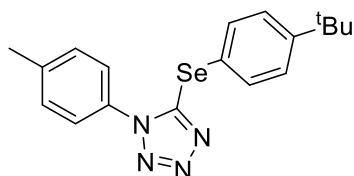
ethyl 2-(5-(phenylselanyl)-1H-tetrazol-1-yl)acetate (4pa):^[3] by silica gel column chromatography (petroleum ether /ethyl acetate = 3:1), yield: 82%, 76.8 mg; yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.65-7.58 (m, 2H), 7.41-7.29 (m, 3H), 5.13 (s, 2H), 4.17 (q, J = 7.1 Hz, 2H), 1.23 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 164.9, 146.8, 134.2, 130.1, 129.6, 124.9, 63.0, 49.0, 14.1.



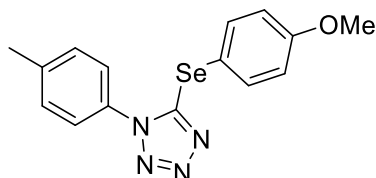
5-(phenylselanyl)-1-(tosylmethyl)-1H-tetrazole (4qa): by silica gel column chromatography (petroleum ether /ethyl acetate = 3:1), yield: 77%, 91.0 mg; yellow oil. ¹H NMR (400 MHz, CDCl₃) δ 7.70-7.63 (m, 2H), 7.50 (d, *J* = 8.3 Hz, 2H), 7.40-7.30 (m, 5H), 5.63 (s, 2H), 2.43 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 149.0, 147.1, 134.6, 131.9, 130.6, 130.0, 129.8, 129.0, 124.9, 65.8, 21.9. HRMS (ESI-TOF) calculated for C₁₅H₁₅N₄O₂SSe [M+H]⁺: 395.0075; found: 395.0078.



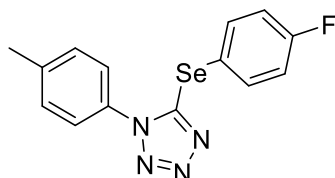
1-(p-tolyl)-5-(p-tolylselanyl)-1H-tetrazole (4ab): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 71%, 70.3 mg; yellow solid. ¹H NMR (400 MHz, CDCl₃) δ 7.54-7.49 (m, 2H), 7.38-7.32 (m, 4H), 7.15 (d, *J* = 7.9 Hz, 2H), 2.46 (s, 3H), 2.36 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 147.6, 140.9, 140.4, 135.6, 131.6, 130.8, 130.4, 124.6, 120.6, 21.44, 21.43. HRMS (ESI-TOF) calculated for C₁₅H₁₅N₄Se [M+H]⁺: 331.0456; found: 331.0459.



5-((4-(tert-butyl)phenyl)selanyl)-1-(p-tolyl)-1H-tetrazole (4ac): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 70%, 78.1 mg; yellow oil. ¹H NMR (400 MHz, CDCl₃) δ 7.55-7.51 (m, 2H), 7.37-7.34 (m, 2H), 7.34-7.31 (m, 4H), 2.45 (s, 3H), 1.30 (s, 9H). ¹³C NMR (100 MHz, CDCl₃) δ 153.2, 147.5, 140.9, 135.2, 131.6, 130.3, 127.1, 124.6, 120.7, 34.9, 31.2, 21.4. HRMS (ESI-TOF) calculated for C₁₈H₂₁N₄Se [M+H]⁺: 373.0926; found: 373.0922.

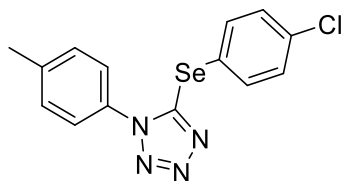


5-((4-methoxyphenyl)selanyl)-1-(p-tolyl)-1H-tetrazole (4ad): by silica gel column chromatography (petroleum ether /ethyl acetate = 20:1), yield: 68%, 70.6 mg; yellow oil. ¹H NMR (400 MHz, CDCl₃) δ 7.60-7.53 (m, 2H), 7.40-7.32 (m, 4H), 6.91-6.85 (m, 2H), 3.82 (s, 3H), 2.47 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 161.2, 148.1, 140.9, 137.7, 131.7, 130.4, 124.6, 115.7, 114.1, 55.5, 21.5. HRMS (ESI-TOF) calculated for C₁₅H₁₅N₄OSe [M+H]⁺: 347.0406; found: 347.0409.

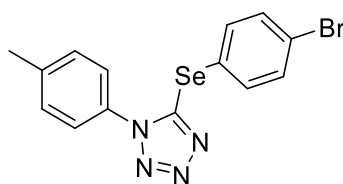


5-((4-fluorophenyl)selanyl)-1-(p-tolyl)-1H-tetrazole (4ae): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 69%, 69.2 mg; yellow oil. ¹H NMR (400 MHz, CDCl₃) δ 7.66-7.58 (m, 2H), 7.35 (s, 4H), 7.08-6.99 (m, 2H), 2.46 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 163.9 (d, *J* = 251.1 Hz), 147.3 (d, *J* = 1.5 Hz), 141.1, 137.9 (d, *J* = 8.5 Hz), 131.5, 130.5, 124.5,

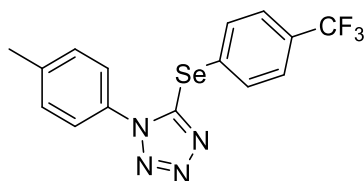
123.7, 117.3 (d, $J = 21.9$ Hz), 21.4. ^{19}F NMR (376 MHz, CDCl_3) δ -109.96. HRMS (ESI-TOF) calculated for $\text{C}_{14}\text{H}_{12}\text{FN}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 335.0206; found: 335.0207.



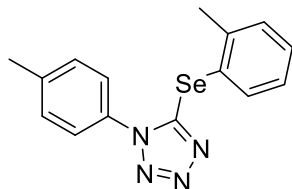
5-((4-chlorophenyl)selenanyl)-1-(p-tolyl)-1H-tetrazole (4af): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 66%, 69.3 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.59-7.54 (m, 2H), 7.35 (s, 4H), 7.33-7.29 (m, 2H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 146.9, 141.2, 136.7, 136.6, 131.5, 130.5, 130.2, 124.5, 122.3, 21.5. HRMS (ESI-TOF) calculated for $\text{C}_{14}\text{H}_{12}\text{ClN}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 350.9910; found: 350.9912.



5-((4-bromophenyl)selenanyl)-1-(p-tolyl)-1H-tetrazole (4ag): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 64%, 75.6 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.52-7.41 (m, 4H), 7.39-7.31 (m, 4H), 2.48-2.44 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 146.8, 141.2, 136.9, 133.1, 131.5, 130.5, 124.6, 123.7, 123.0, 21.5. HRMS (ESI-TOF) calculated for $\text{C}_{14}\text{H}_{12}\text{BrN}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 394.9405; found: 394.9408.

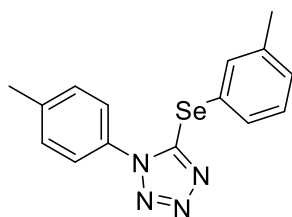


1-(p-tolyl)-5-((4-(trifluoromethyl)phenyl)selenanyl)-1H-tetrazole (4ah): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 56%, 64.5 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.75 (d, $J = 8.1$ Hz, 2H), 7.57 (d, $J = 8.2$ Hz, 2H), 7.34 (s, 4H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 146.3, 141.3, 135.0, 131.8 (q, $J = 32.9$ Hz), 130.5, 129.1 (q, $J = 1.6$ Hz), 126.6 (q, $J = 3.7$ Hz), 124.6, 123.73, 123.72 (q, $J = 270.9$ Hz), 21.4. ^{19}F NMR (376 MHz, CDCl_3) δ -63.00. HRMS (ESI-TOF) calculated for $\text{C}_{15}\text{H}_{12}\text{F}_3\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 385.0174; found: 385.0177.

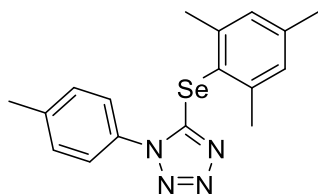


1-(p-tolyl)-5-(o-tolylselenanyl)-1H-tetrazole (4ai): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 69%, 68.3 mg; yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.50 (d, $J = 7.9$ Hz, 1H), 7.31-7.24 (m, 4H), 7.24-7.18 (m, 2H), 7.04 (td, $J = 7.4, 2.1$ Hz, 1H), 2.38 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 147.0, 142.1, 140.9, 136.7, 131.6, 131.0, 130.6, 130.4, 127.3, 125.5, 124.5, 23.0, 21.4. (ESI-TOF) calculated for $\text{C}_{15}\text{H}_{15}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 331.0456; found:

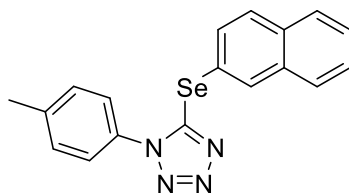
331.0457.



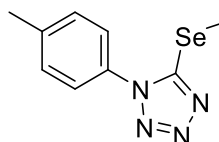
1-(p-tolyl)-5-(m-tolylselanyl)-1H-tetrazole (4aj): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 66%, 65.3 mg; yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.42-7.37 (m, 2H), 7.33 (s, 4H), 7.24-7.18 (m, 2H), 2.46 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 147.3, 140.9, 139.9, 135.9, 132.3, 131.6, 130.7, 130.3, 129.7, 124.7, 124.0, 21.44, 21.37. (ESI-TOF) calculated for $\text{C}_{15}\text{H}_{15}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 331.0456; found: 331.0452.



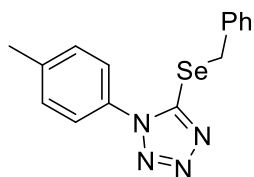
5-(mesitylselanyl)-1-(p-tolyl)-1H-tetrazole (4ak): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 70%, 75.2 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.41 (d, J = 8.4 Hz, 2H), 7.35 (d, J = 8.2 Hz, 2H), 6.97 (s, 2H), 2.46 (s, 3H), 2.40 (s, 6H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 147.5, 143.3, 140.8, 140.7, 131.7, 130.4, 129.4, 124.2, 123.0, 24.3, 21.4, 21.2. HRMS (ESI-TOF) calculated for $\text{C}_{17}\text{H}_{19}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 359.0769; found: 359.0772.



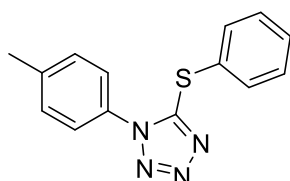
5-(naphthalen-2-ylselanyl)-1-(p-tolyl)-1H-tetrazole (4al): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 67%, 73.6 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 8.02 (s, 1H), 7.78-7.73 (m, 1H), 7.71 (d, J = 8.6 Hz, 1H), 7.69-7.65 (m, 1H), 7.55 (dd, J = 8.6, 1.7 Hz, 1H), 7.49-7.41 (m, 2H), 7.28-7.18 (m, 4H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 147.1, 141.0, 135.3, 133.9, 133.4, 131.6, 131.4, 130.4, 129.7, 128.0, 127.9, 127.6, 127.0, 124.7, 121.5, 21.4. HRMS (ESI-TOF) calculated for $\text{C}_{18}\text{H}_{15}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 367.0456; found: 367.0455.



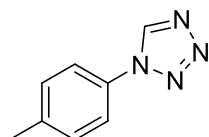
5-(methylselanyl)-1-(p-tolyl)-1H-tetrazole (4am): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 56%, 42.7 mg; white solid. ^1H NMR (400 MHz, CDCl_3) δ 7.43-7.39 (m, 2H), 7.35 (d, J = 8.4 Hz, 2H), 2.72 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 147.4, 140.8, 131.6, 130.5, 123.8, 21.4, 8.2. HRMS (ESI-TOF) calculated for $\text{C}_9\text{H}_{11}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 255.0143; found: 255.0147.



5-(benzylselanyl)-1-(p-tolyl)-1H-tetrazole (4an): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 66%, 65.3 mg; yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.32-7.28 (m, 2H), 7.26-7.21 (m, 4H), 7.21-7.18 (m, 2H), 7.18-7.14 (m, 1H), 4.57 (s, 2H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 147.3, 140.7, 136.5, 131.5, 130.4, 129.2, 128.9, 128.0, 123.9, 32.6, 21.4. (ESI-TOF) calculated for $\text{C}_{15}\text{H}_{15}\text{N}_4\text{Se}$ $[\text{M}+\text{H}]^+$: 331.0456; found: 331.0457.



5-(phenylthio)-1-(p-tolyl)-1H-tetrazole (4ao): by silica gel column chromatography (petroleum ether /ethyl acetate = 10:1), yield: 40%, 32.1 mg; brown solid. ^1H NMR (400 MHz, CDCl_3) δ 7.59-7.54 (m, 2H), 7.44-7.39 (m, 5H), 7.38-7.34 (m, 2H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 153.8, 140.9, 134.1, 131.1, 130.4, 130.1, 129.9, 125.0, 124.4, 21.5. (ESI-TOF) calculated for $\text{C}_{14}\text{H}_{13}\text{N}_4\text{S}$ $[\text{M}+\text{H}]^+$: 269.0855; found: 269.0859.



1-(p-tolyl)-1H-tetrazole (6):⁴ by silica gel column chromatography (petroleum ether /ethyl acetate = 3:1), yield: 25%, 12.0 mg; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 8.97 (s, 1H), 7.57 (d, J = 8.3 Hz, 2H), 7.37 (d, J = 8.2 Hz, 2H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 140.6, 140.5, 131.5, 130.8, 121.2, 21.3.

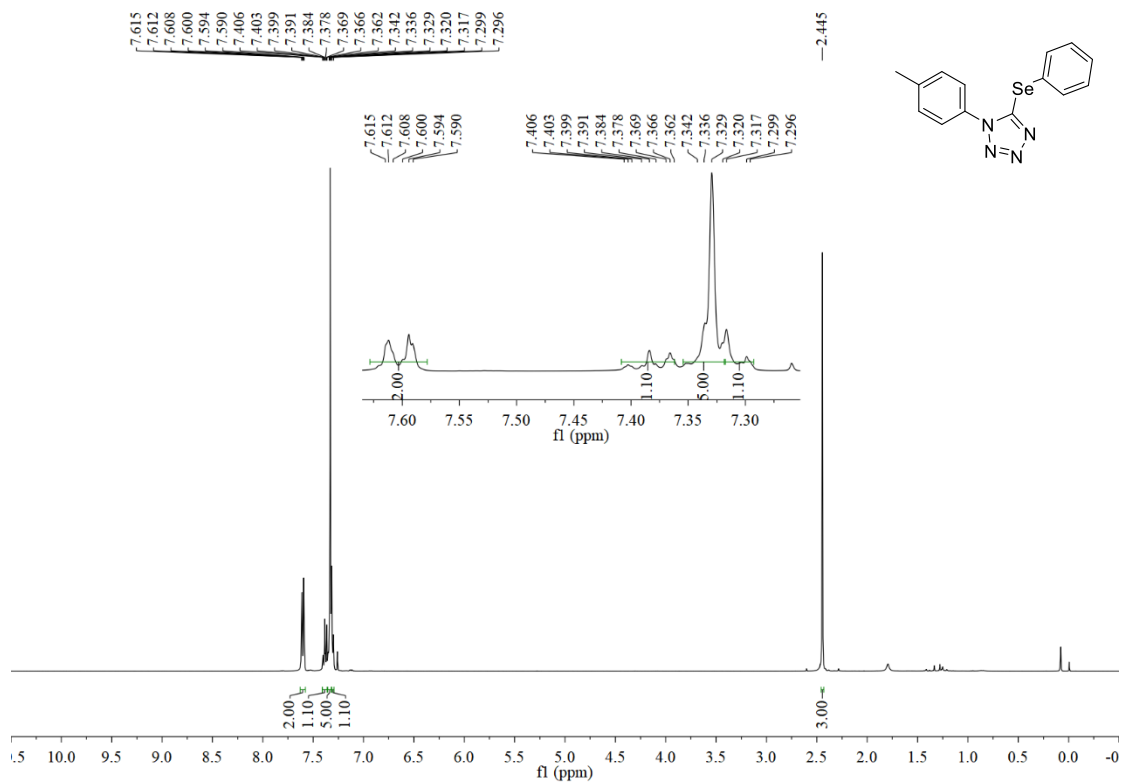
Reference

- (1) Škoch, K.; Císařová, I.; Štěpnička, P. Selective Gold-Catalysed Synthesis of Cyanamides and 1-Substituted 1H-Tetrazol-5-Amines from Isocyanides. *Chem. - Eur. J.*, **2018**, *24*, 13788-13791.
- (2) Dapkekar, A. B.; Satyanarayana, G. An electrochemical cascade process: synthesis of 3-selenylindoles from 2-alkynylanilines with diselenides. *Chem. Commun.*, **2023**, *59*, 8719-8722.
- (3) Fan, Y.; Wu, W.; Wu, M.; Liu, P.; Sun, P. Electrochemical [3+2] Cycloaddition to Access 5-Aryl(alkyl)thiotetrazoles. *Adv. Synth. Catal.*, **2025**, *367*, e70003
- (4) Zhang, G.; Guan, C.; Han, L.; Zhao, Y.; Ding, C. A late-stage functionalization tool: sulfonyl fluoride mediated deoxymethylation of phenols. *Org. Biomol. Chem.*, **2022**, *20*, 7640-7644.

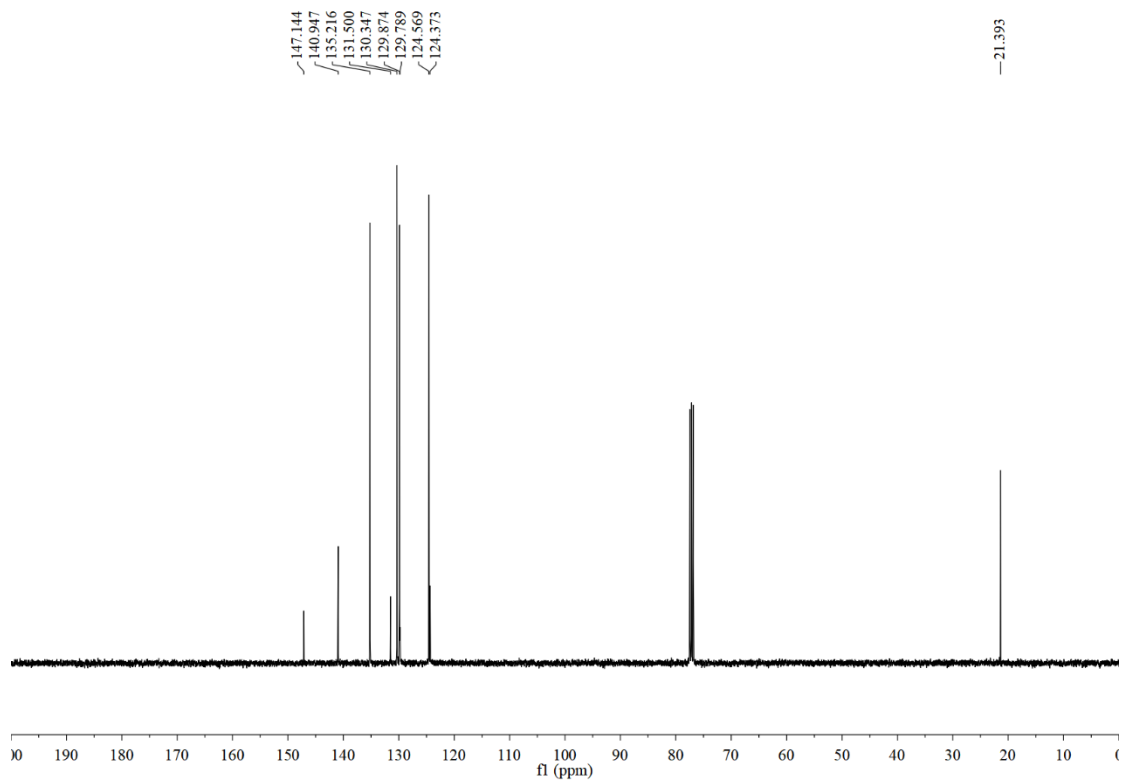
Copies of product NMR Spectra

4aa

^1H NMR (400MHz, CDCl_3) of compound 4aa

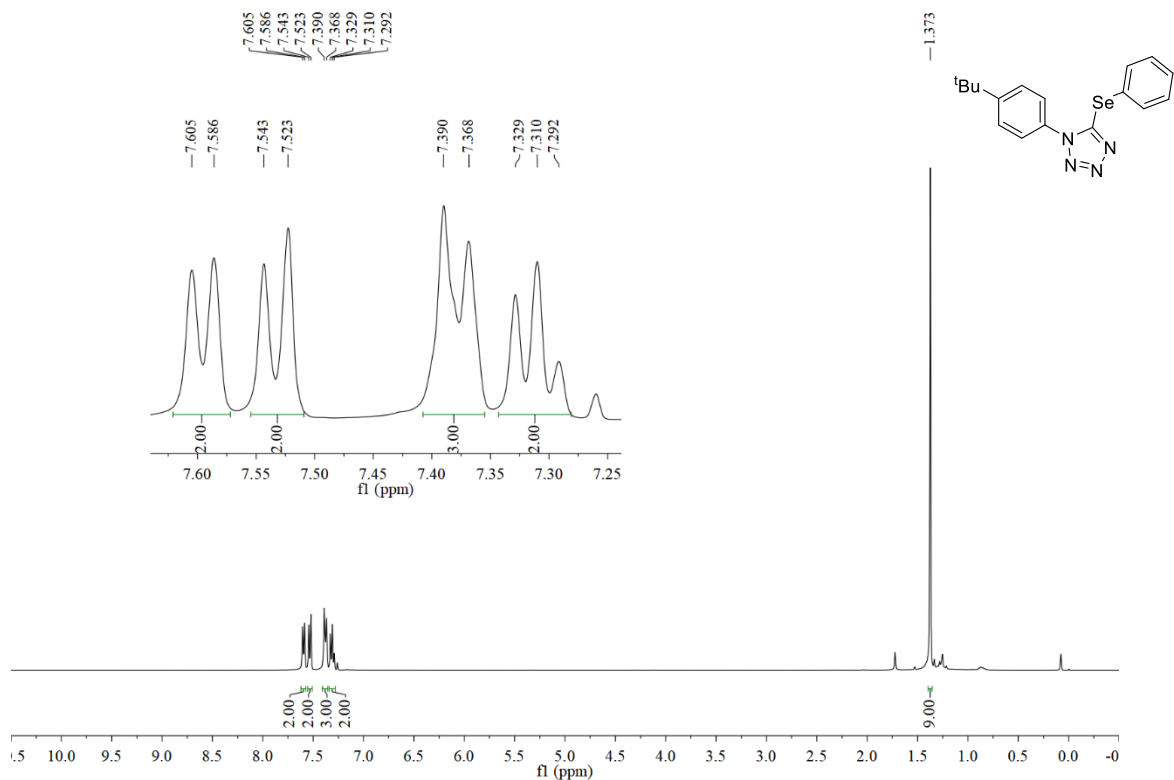


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4aa

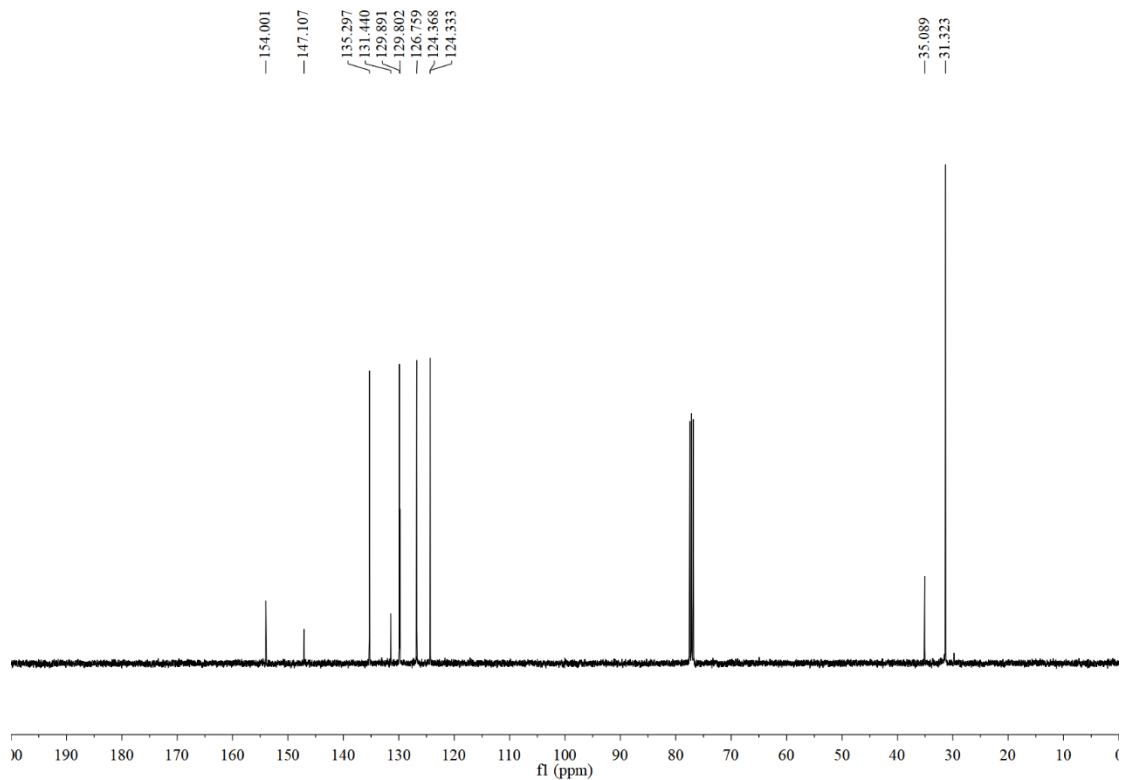


4ba

^1H NMR (400MHz, CDCl_3) of compound 4ba

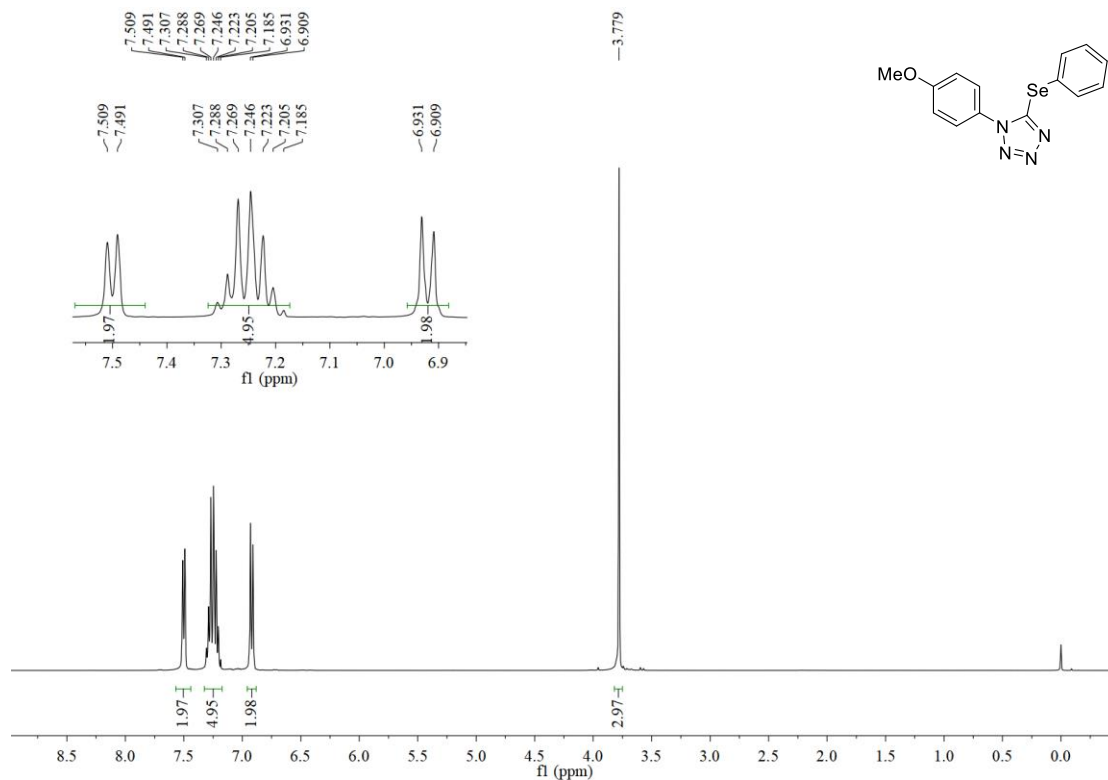


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4ba

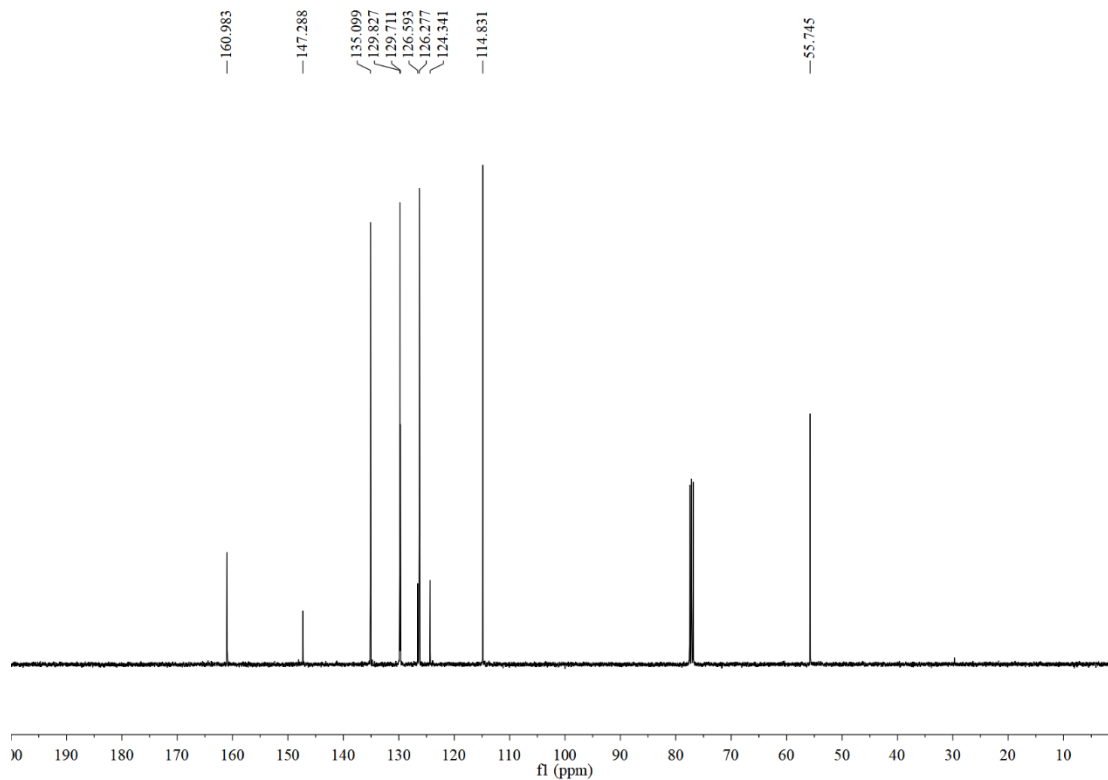


4ca

^1H NMR (400MHz, CDCl_3) of compound 4ca

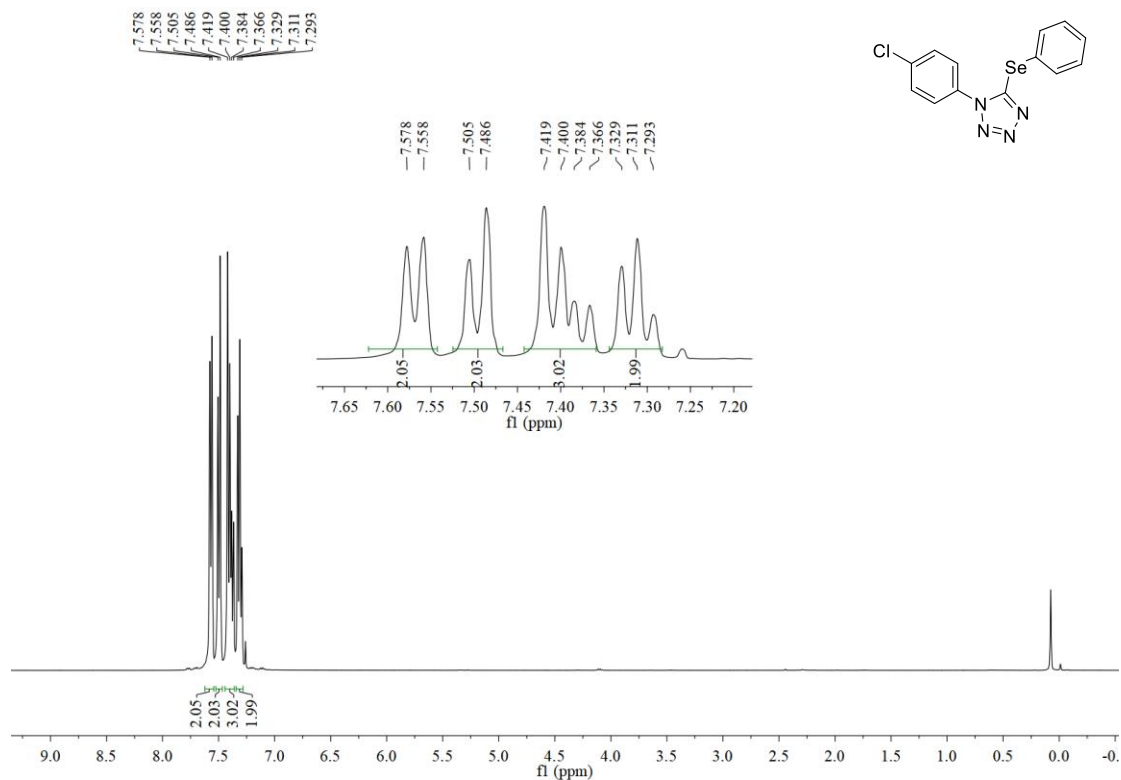


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4ca

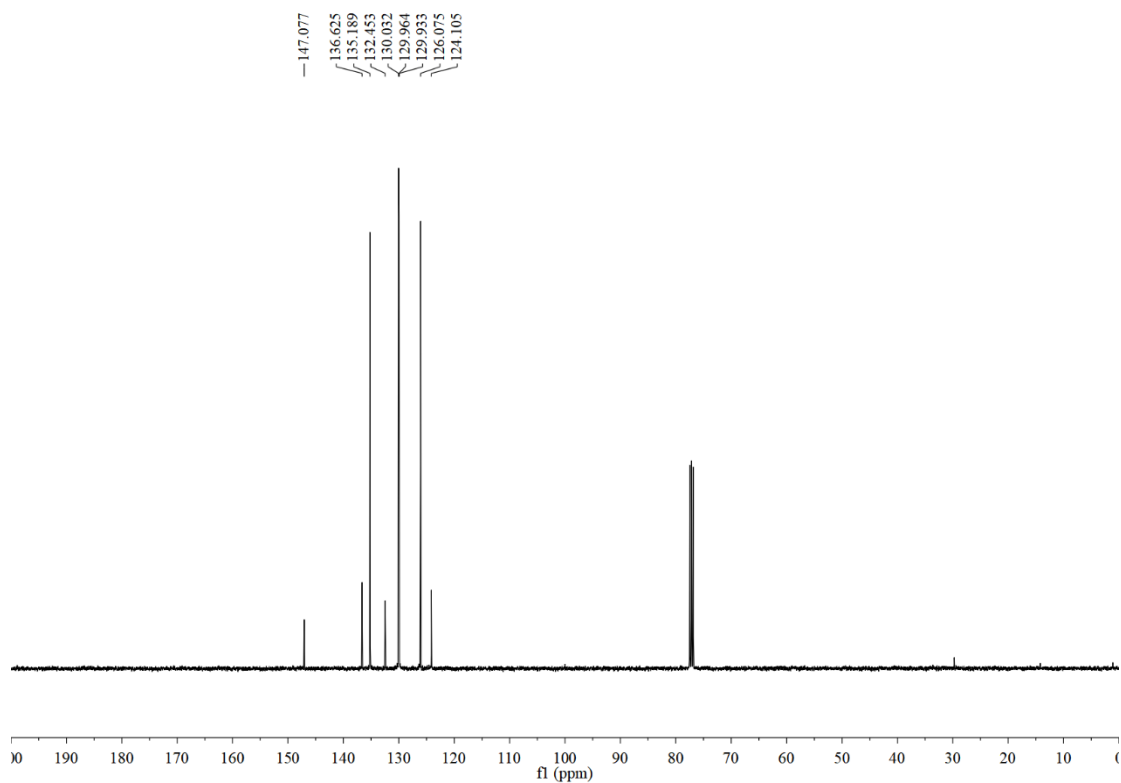


4da

^1H NMR (400MHz, CDCl_3) of compound 4da

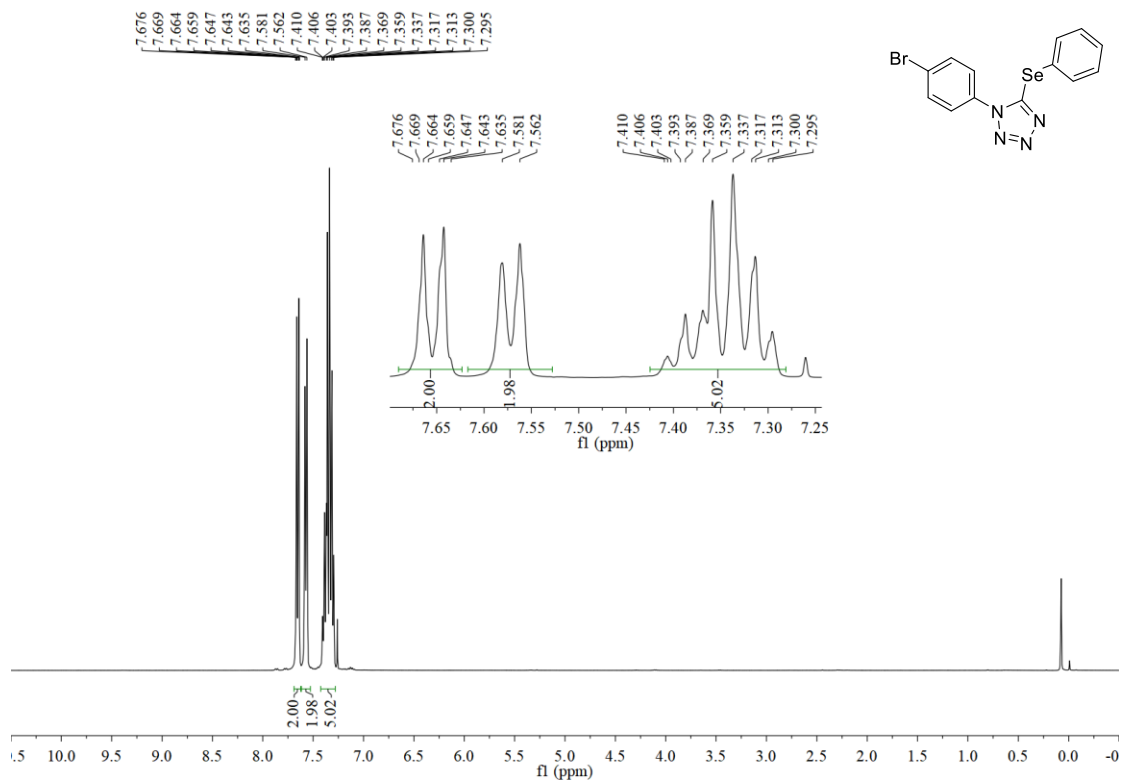


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4da

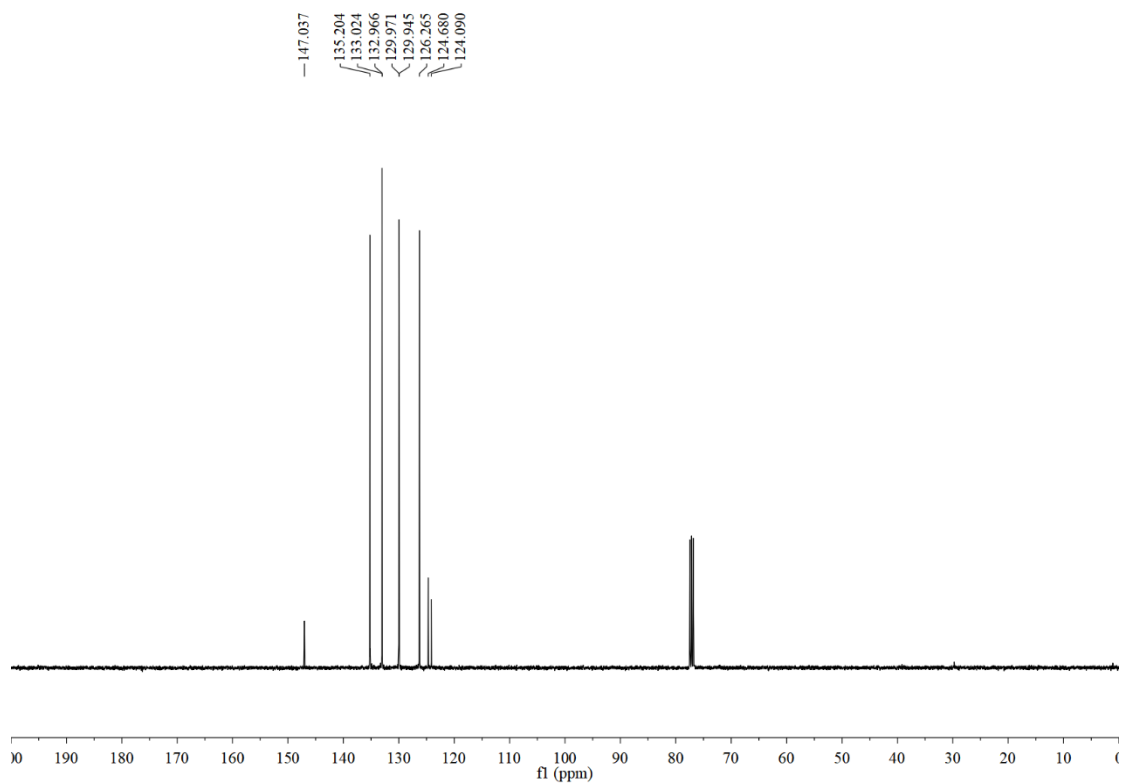


4ea

^1H NMR (400MHz, CDCl_3) of compound 4ea

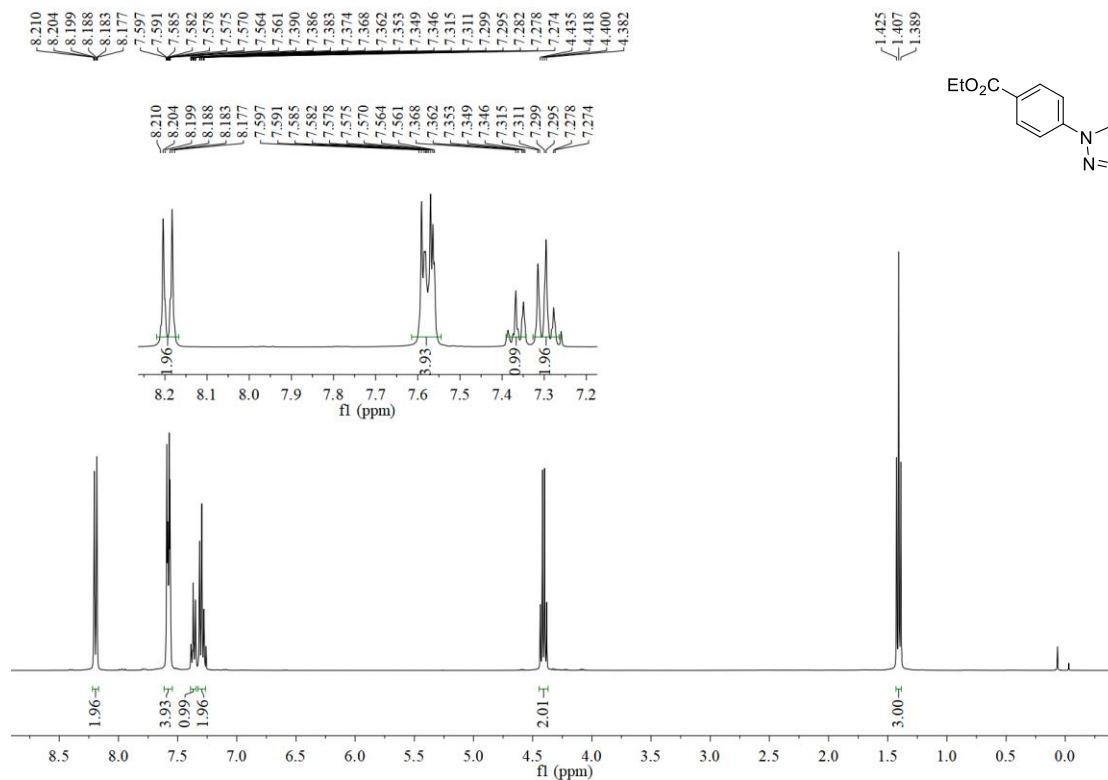


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4ea

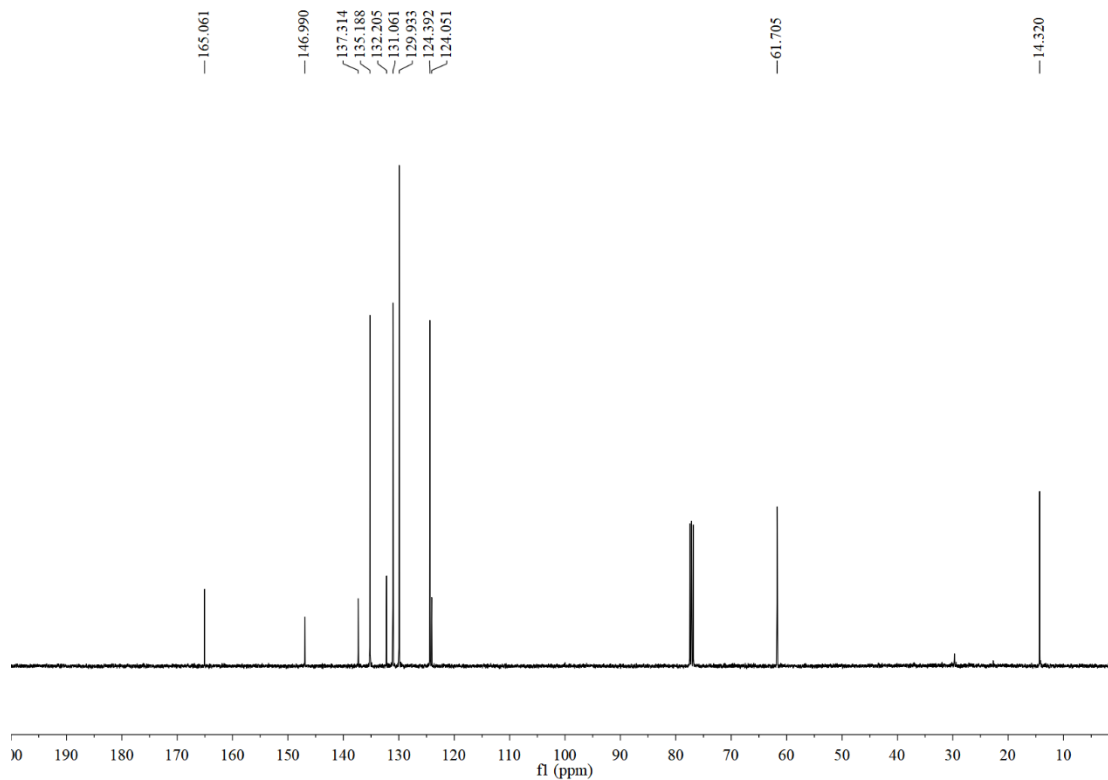


4fa

¹H NMR (400MHz, CDCl₃) of compound 4fa

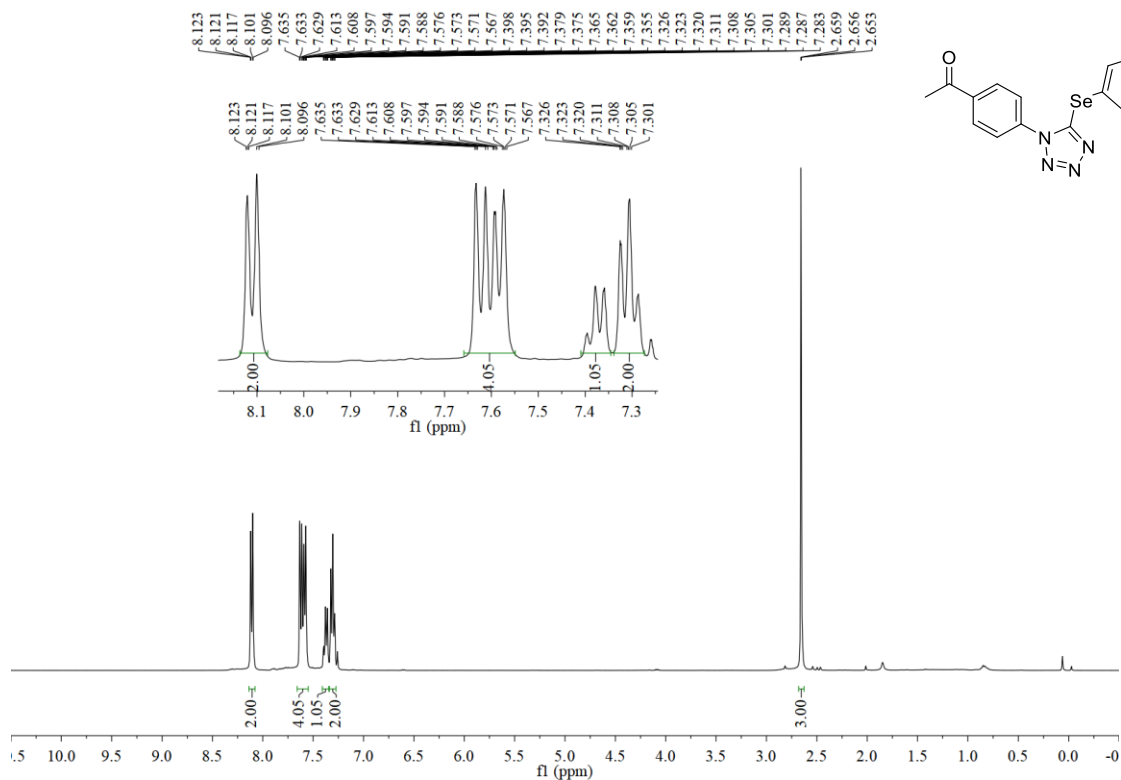


¹³C{¹H} NMR (100MHz, CDCl₃) of compound 4fa

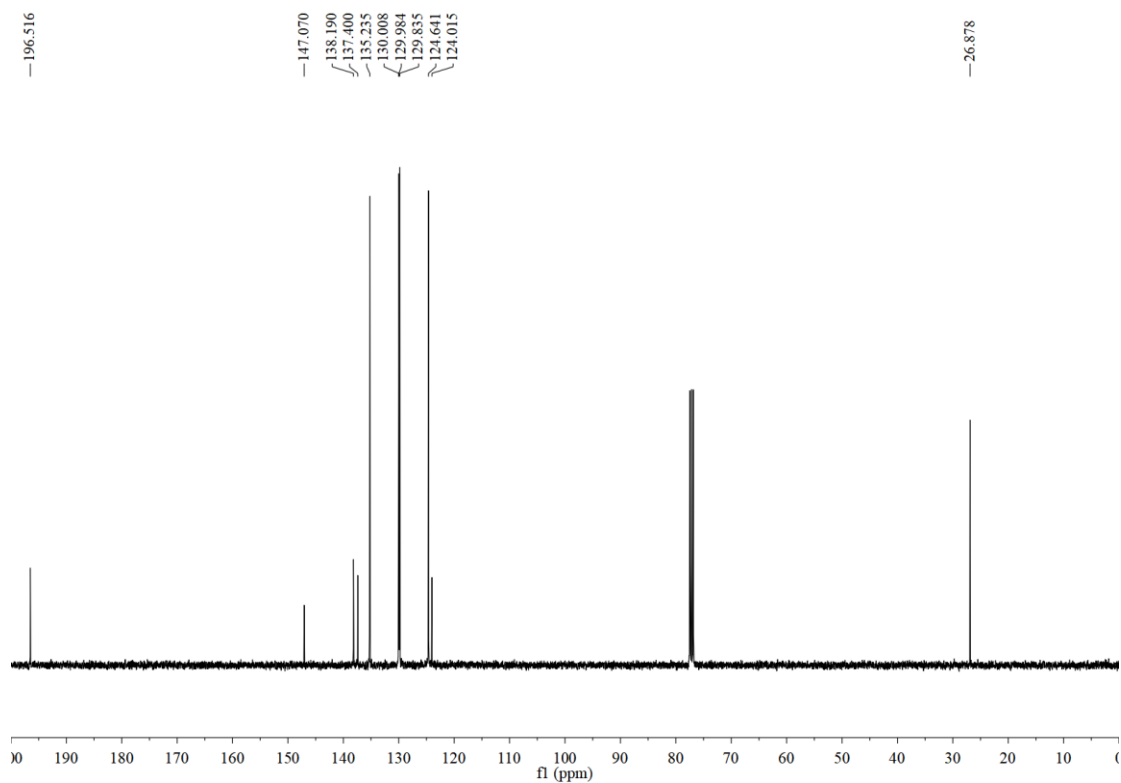


4ga

¹H NMR (400MHz, CDCl₃) of compound 4ga

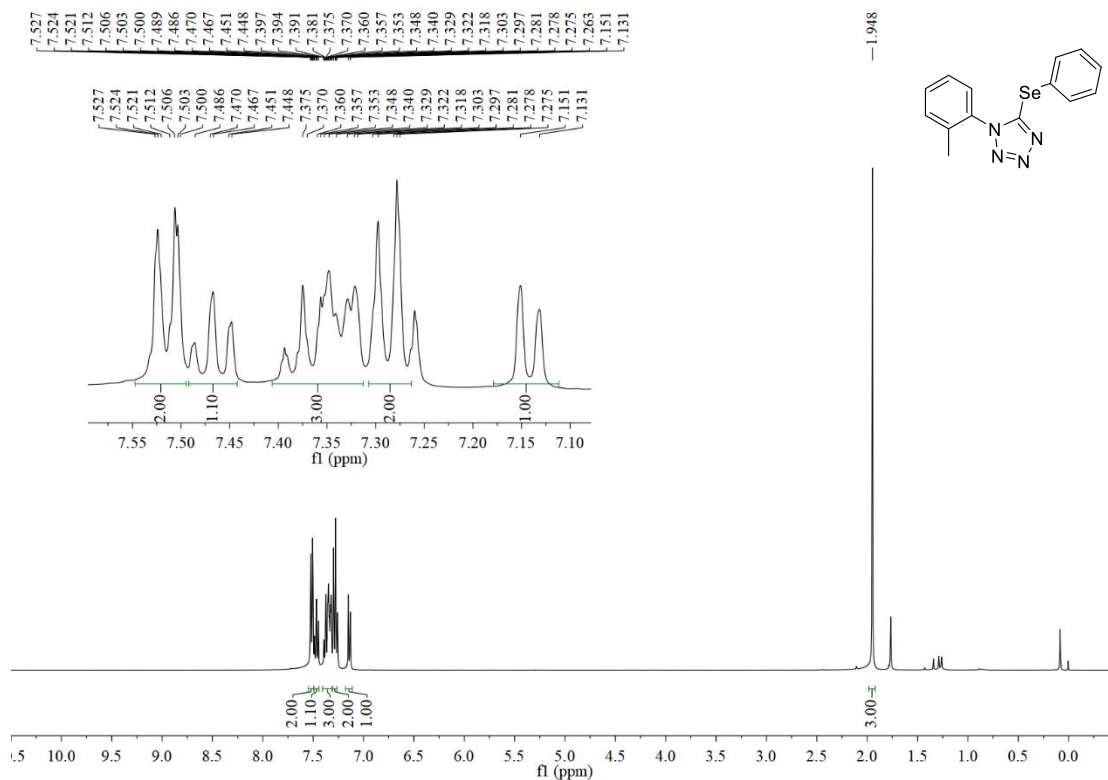


¹³C{¹H} NMR (100MHz, CDCl₃) of compound 4ga

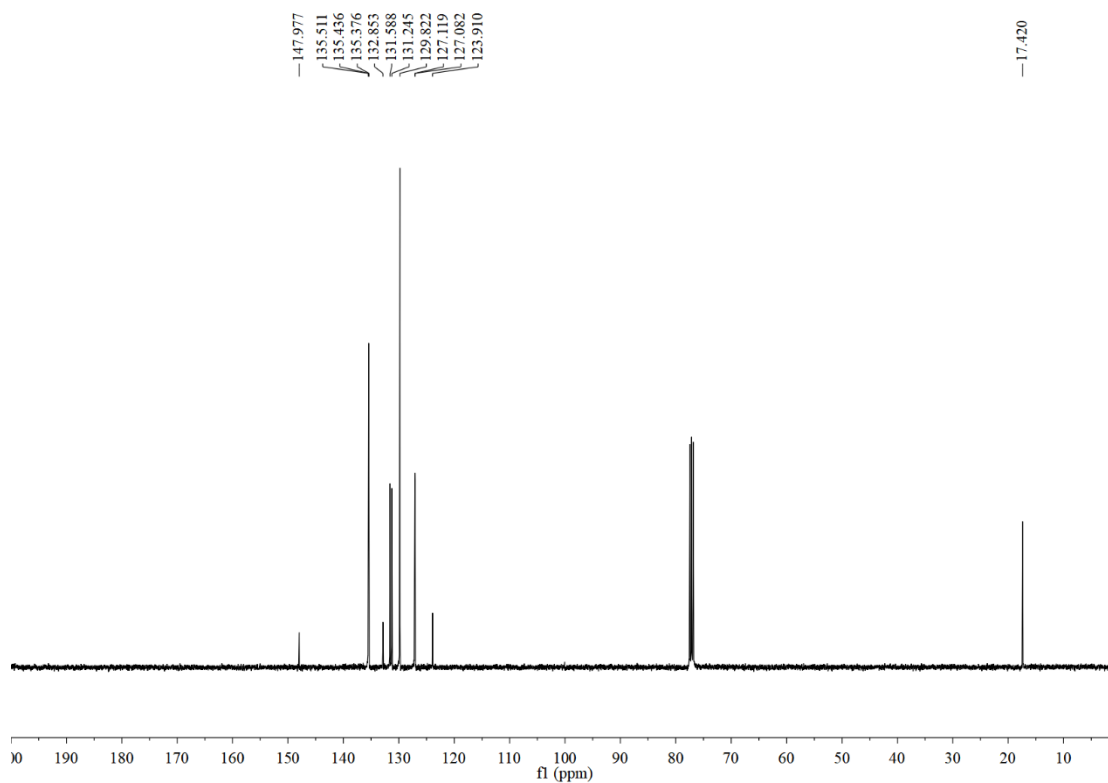


4ha

^1H NMR (400MHz, CDCl_3) of compound 4ha

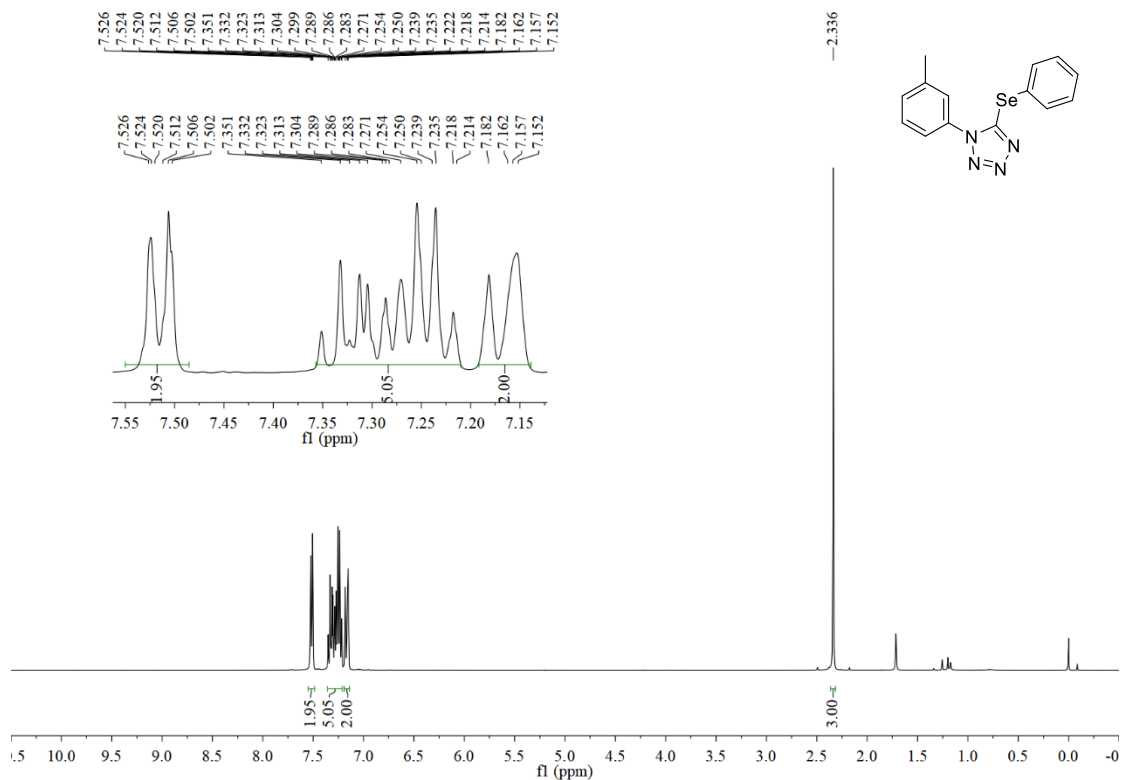


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4ha

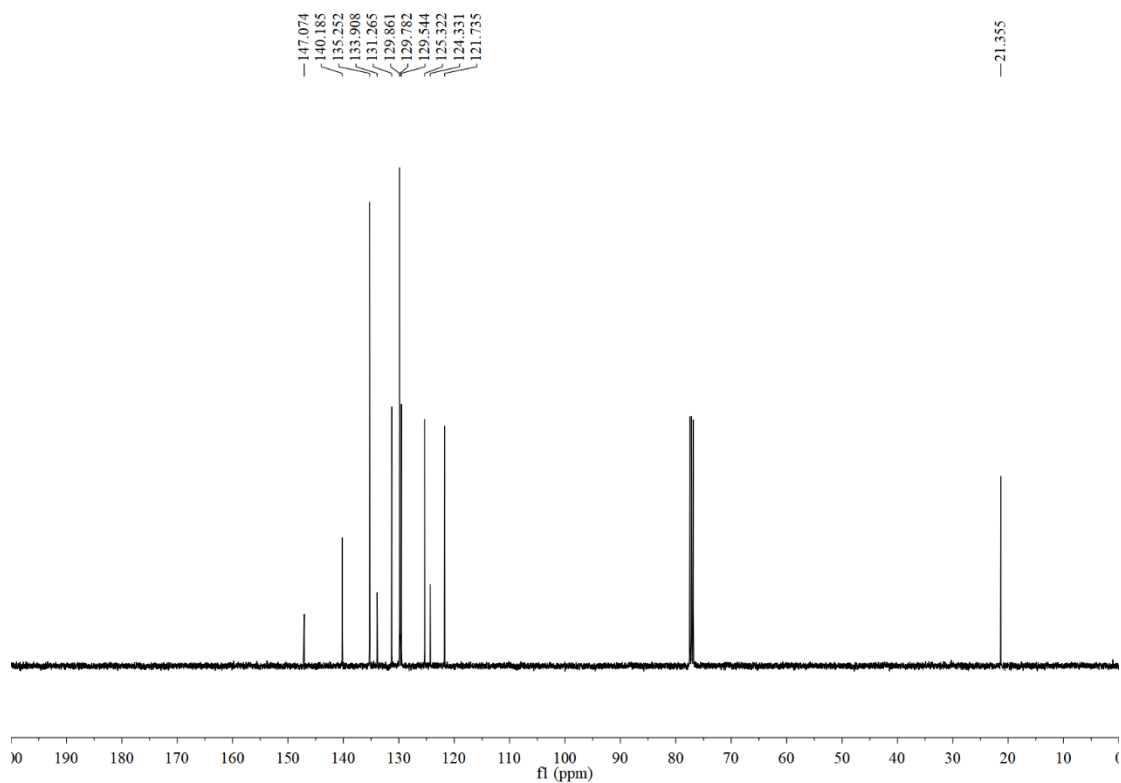


4ia

¹H NMR (400MHz, CDCl₃) of compound 4ia

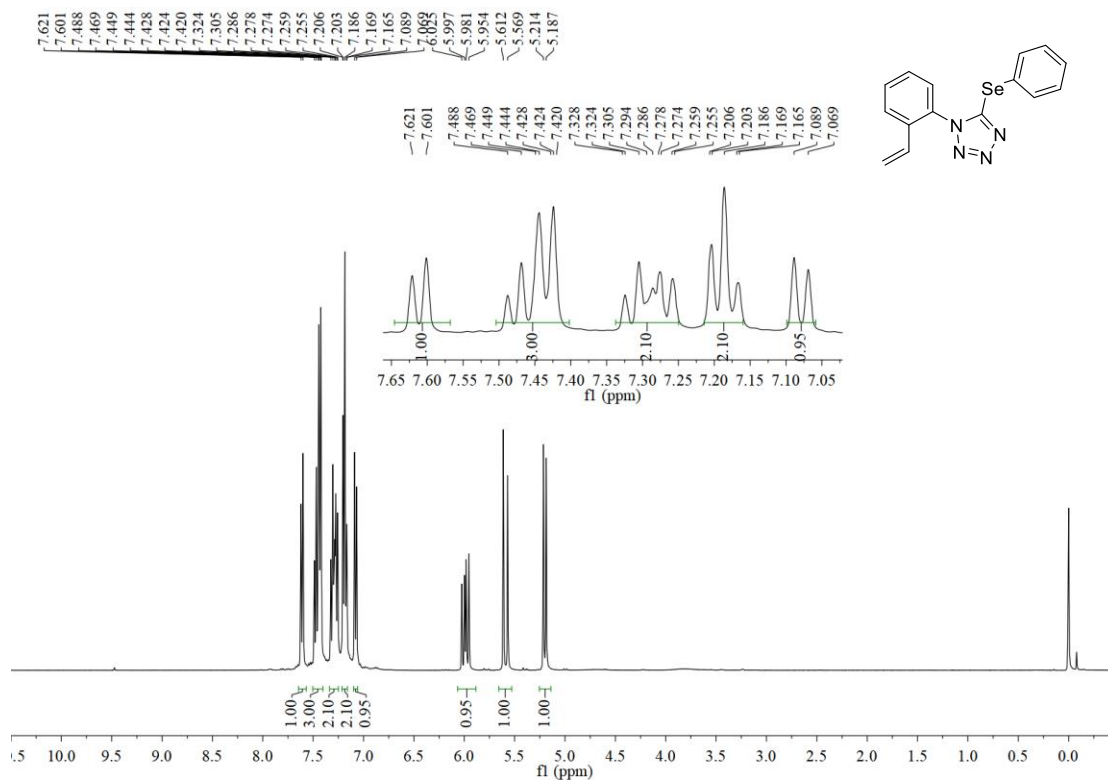


¹³C{¹H} NMR (100MHz, CDCl₃) of compound 4ia

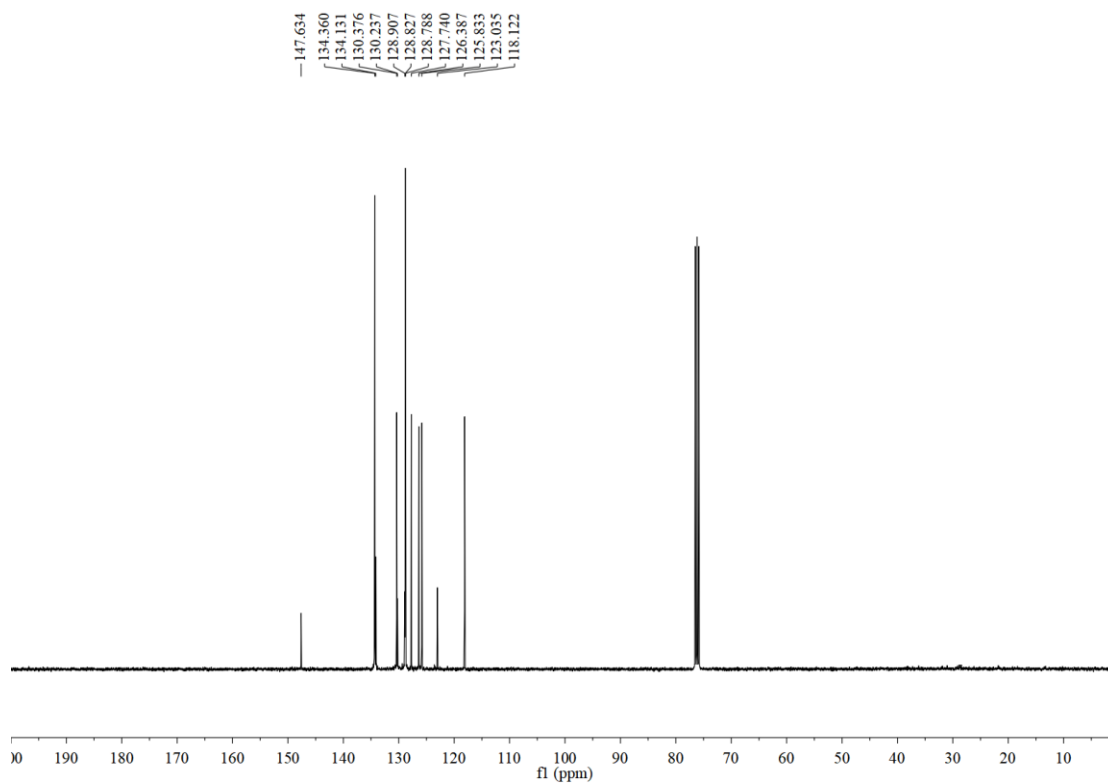


4ja

¹H NMR (400MHz, CDCl₃) of compound 4ja

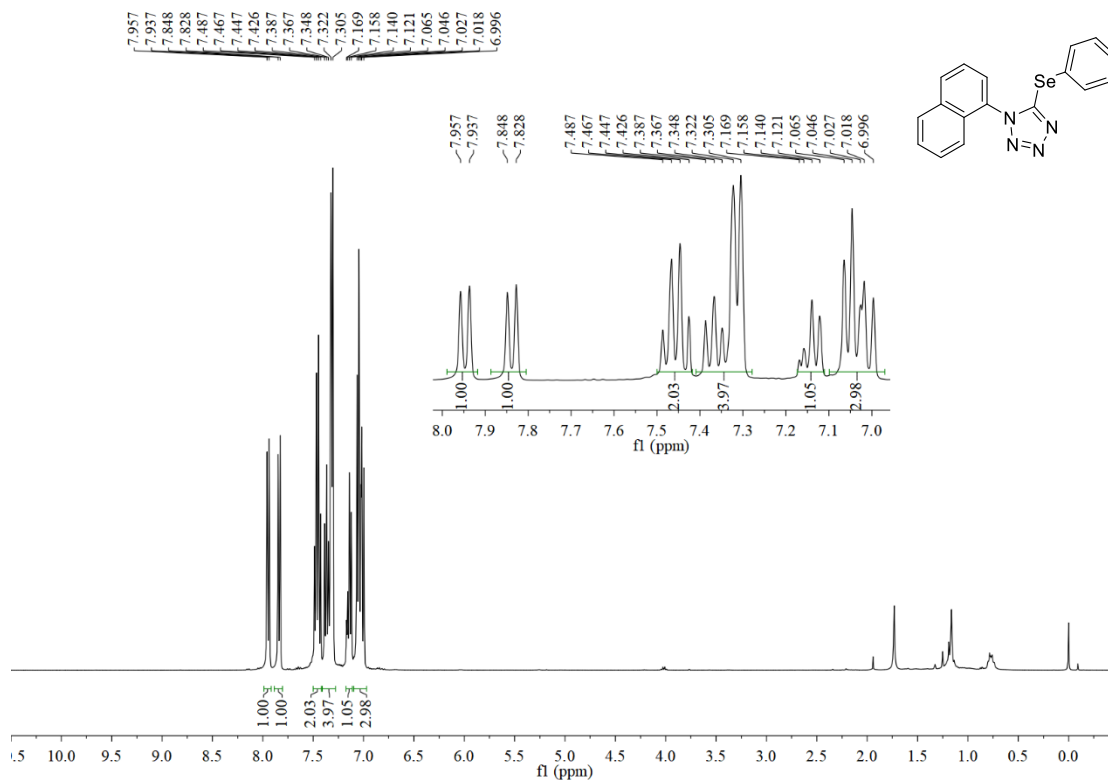


¹³C{¹H} NMR (100MHz, CDCl₃) of compound 4ja

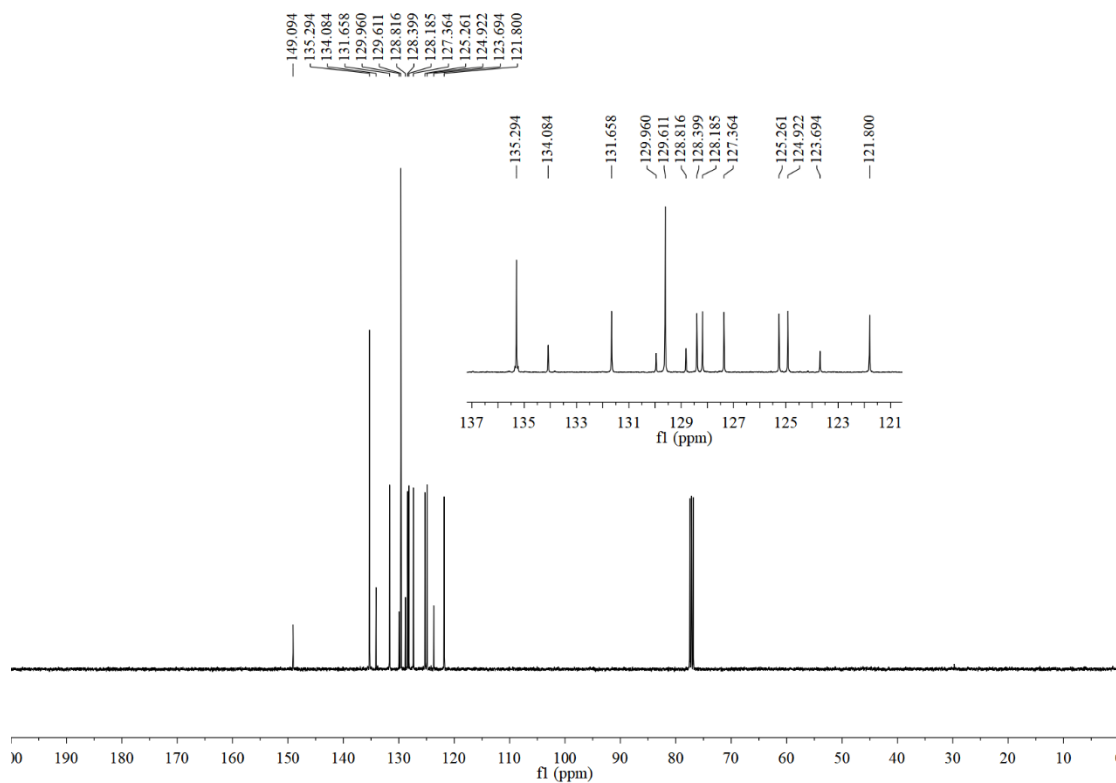


4ka

^1H NMR (400MHz, CDCl_3) of compound 4ka

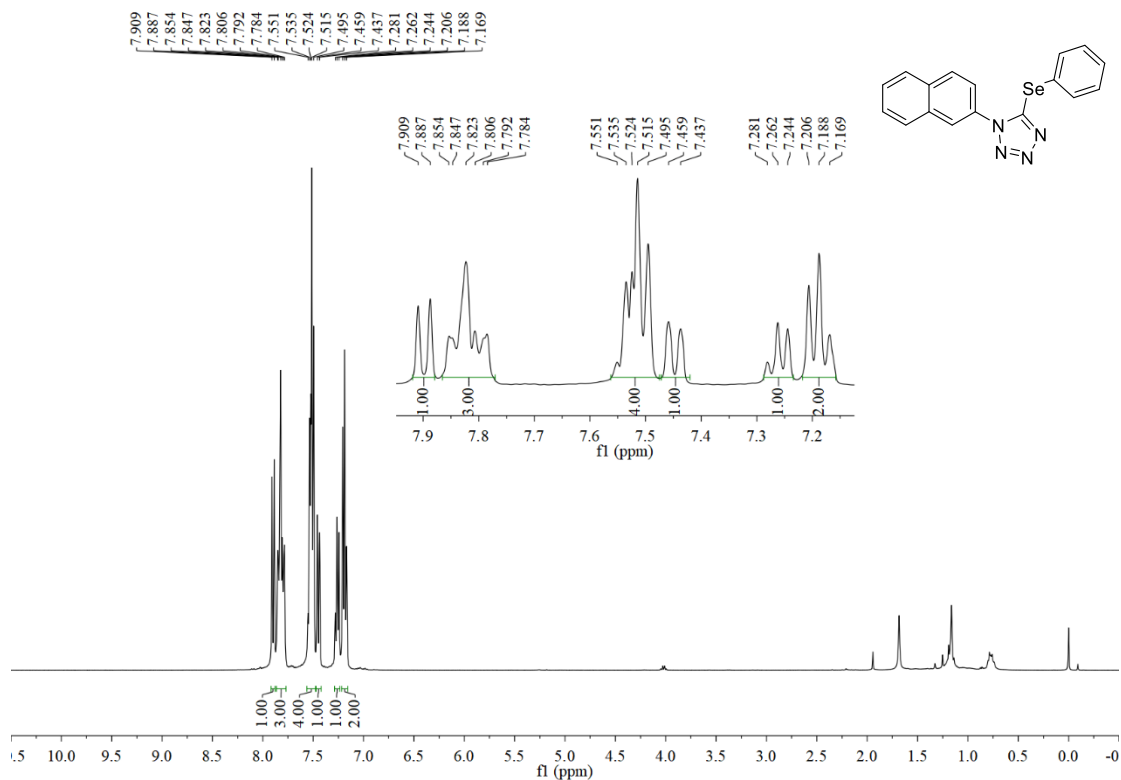


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4ka

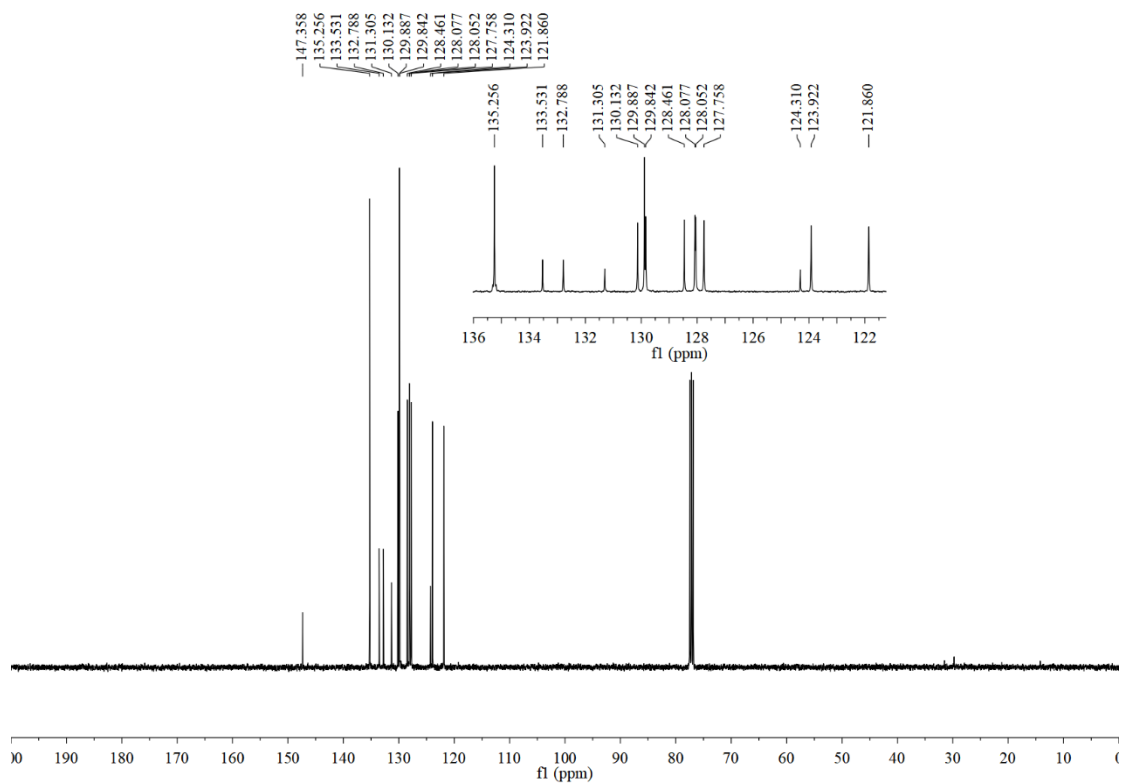


4la

^1H NMR (400MHz, CDCl_3) of compound 4la

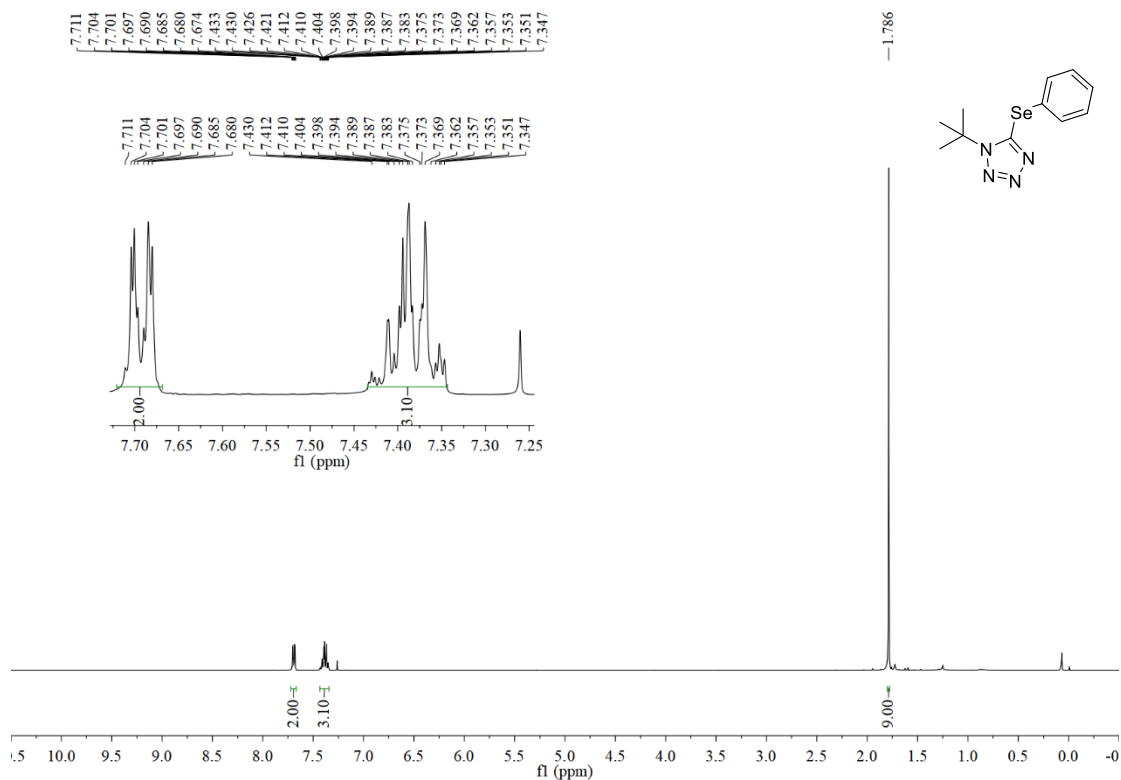


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4la

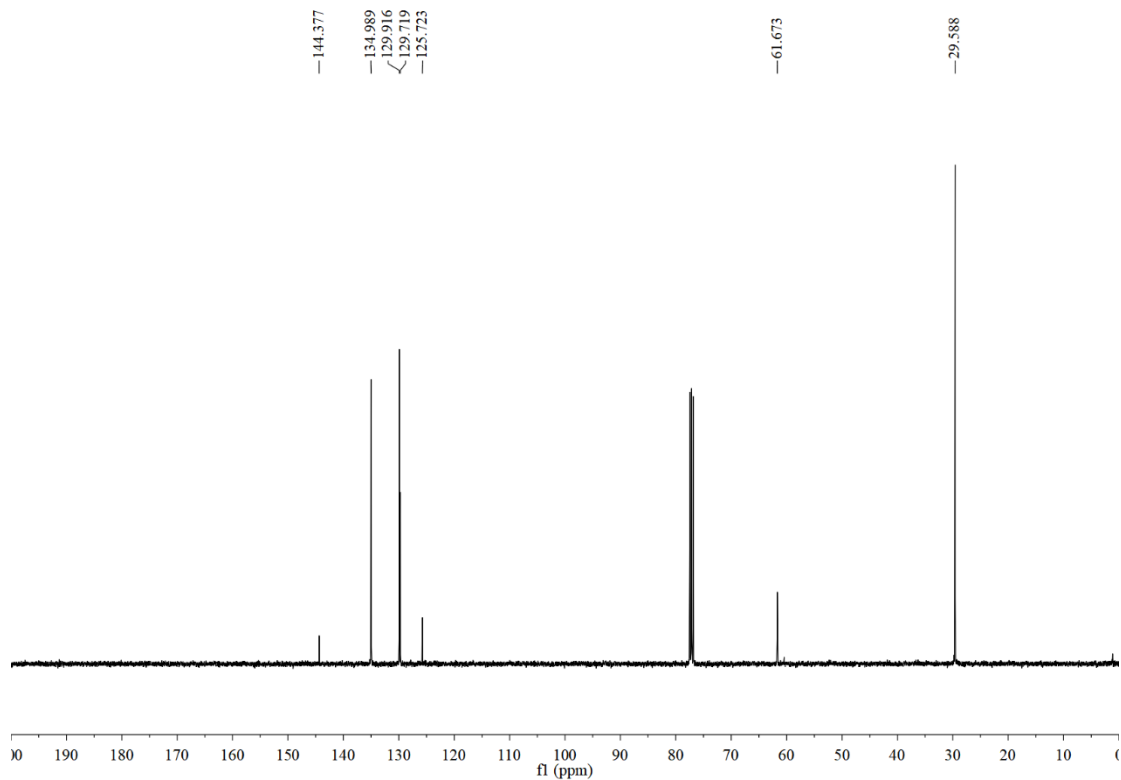


4ma

¹H NMR (400MHz, CDCl₃) of compound 4ma

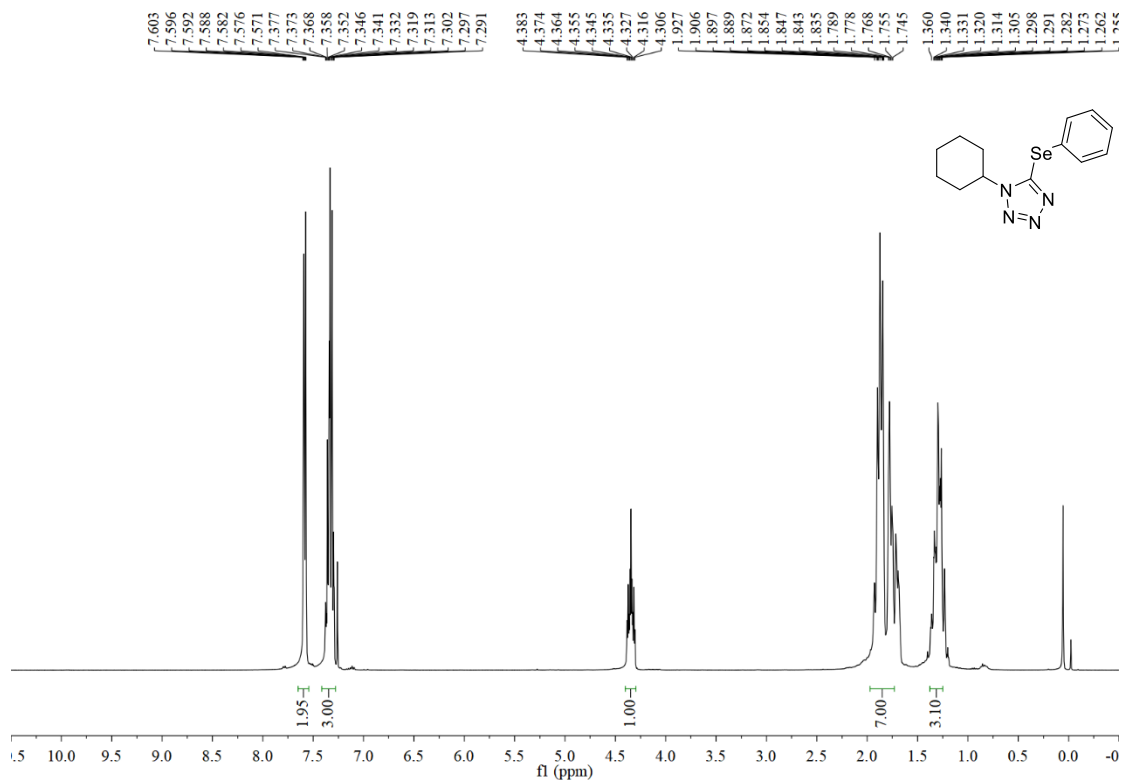


¹³C{¹H} NMR (100MHz, CDCl₃) of compound 4ma

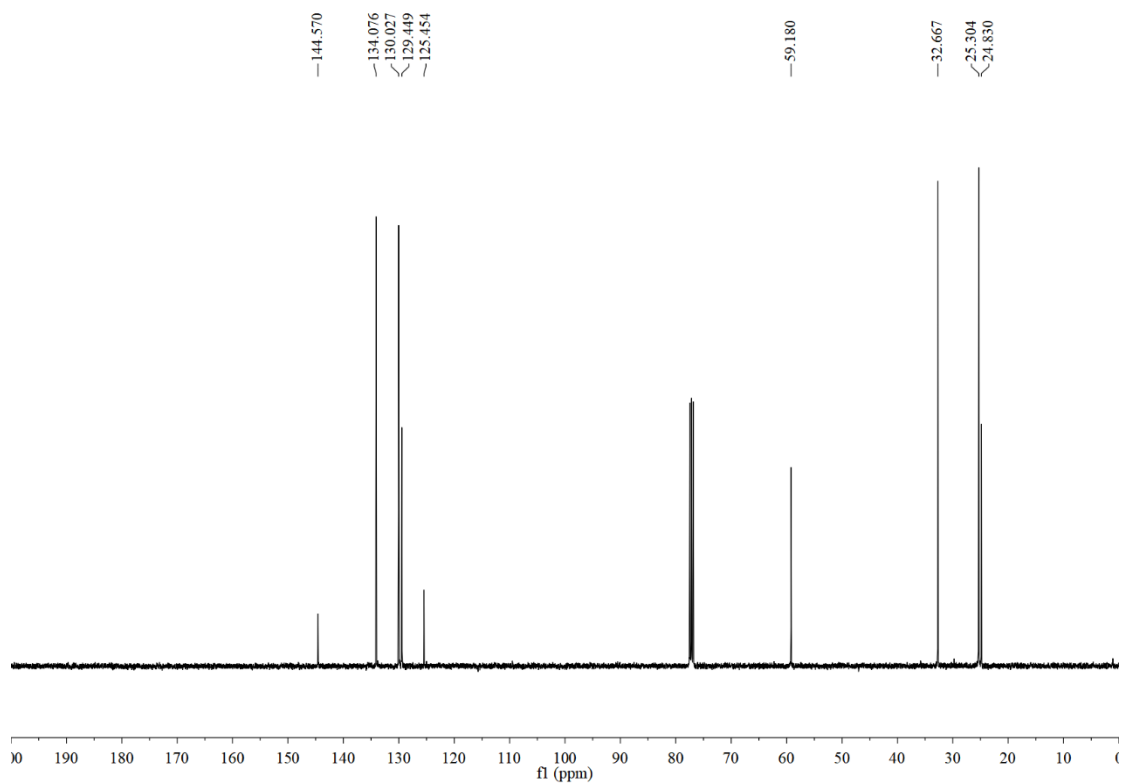


4na

^1H NMR (400MHz, CDCl_3) of compound 4na

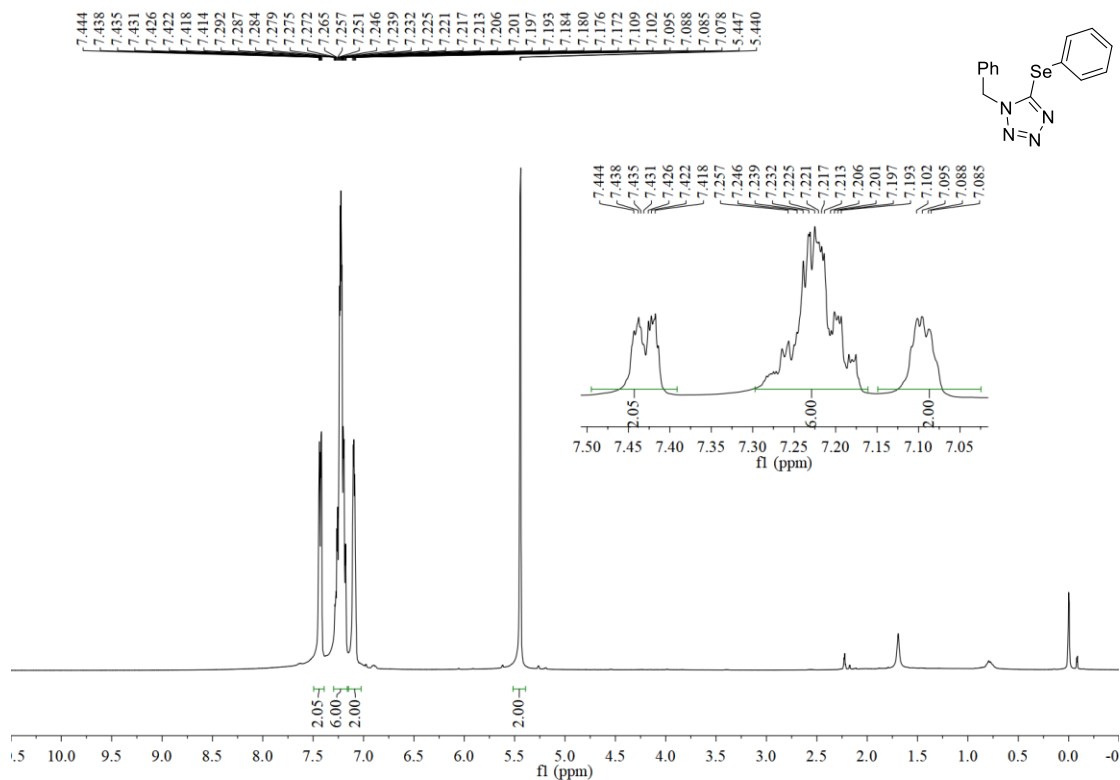


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4na

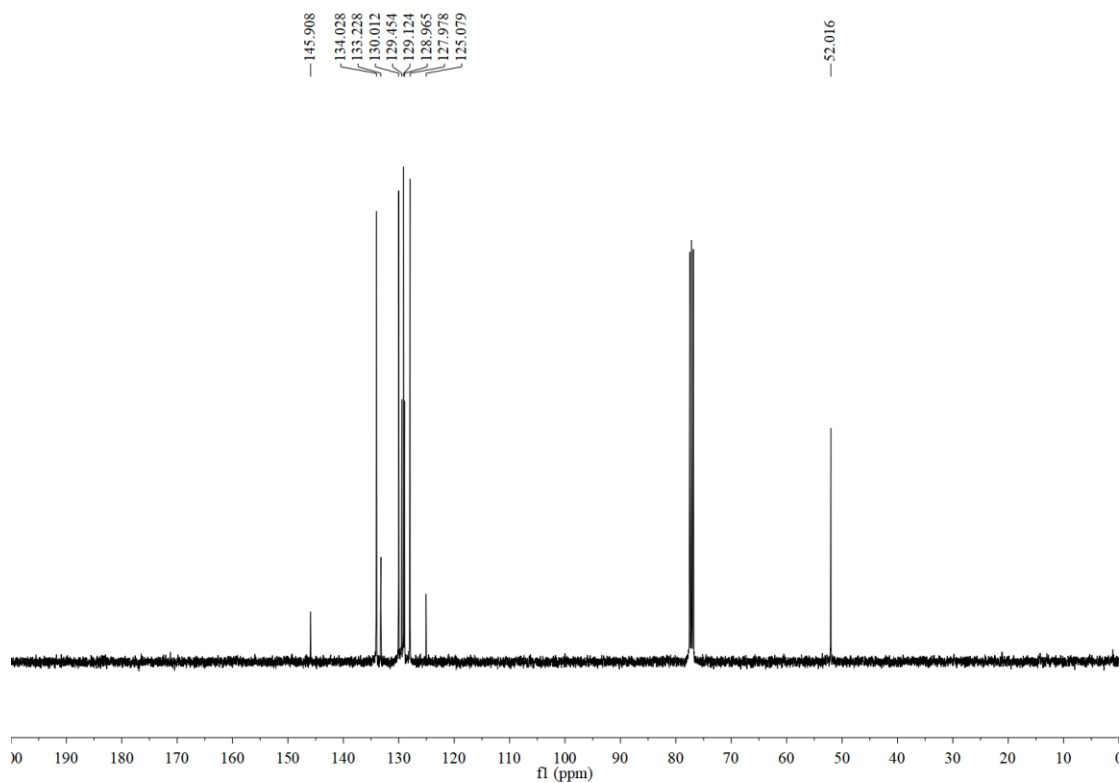


40a

¹H NMR (400MHz, CDCl₃) of compound 40a

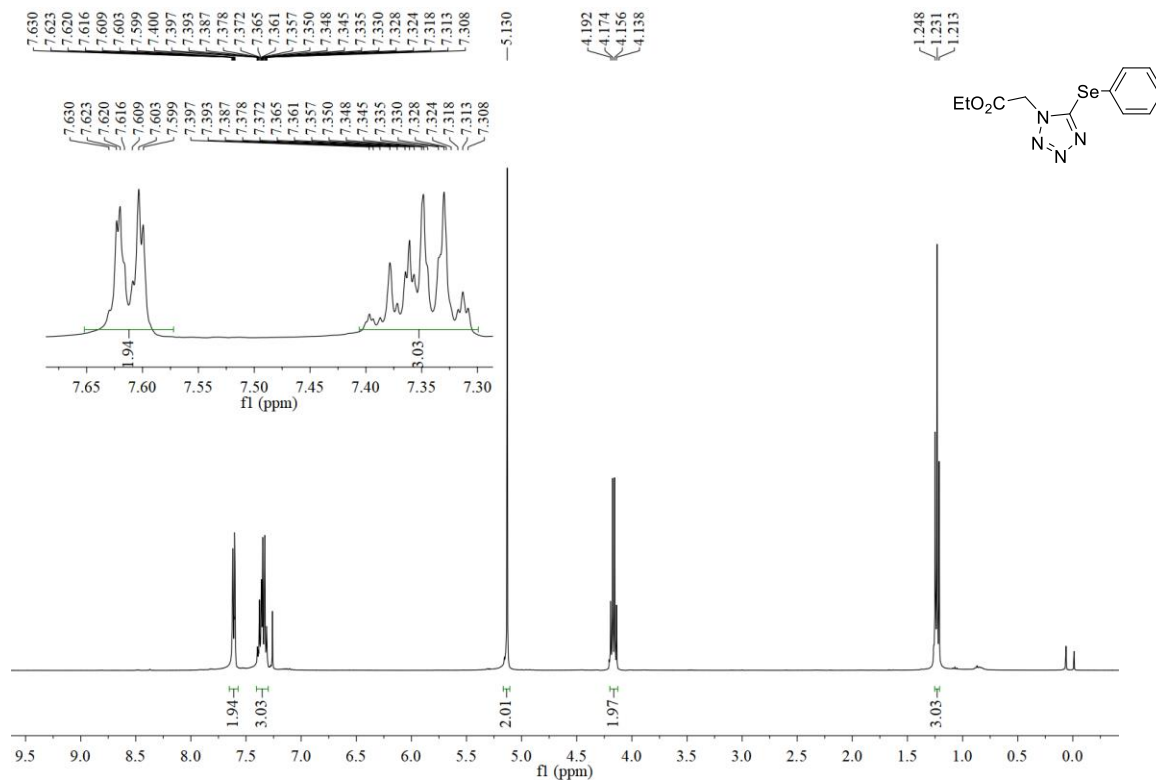


¹³C{¹H} NMR (100MHz, CDCl₃) of compound 40a

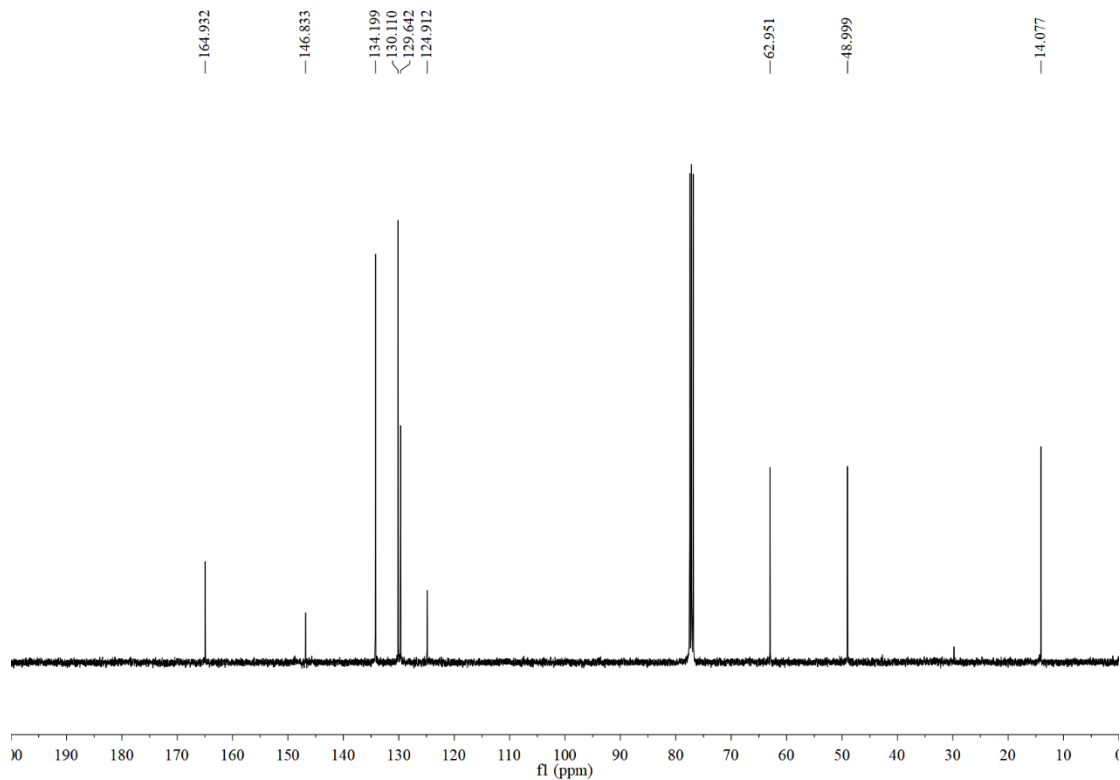


4pa

¹H NMR (400MHz, CDCl₃) of compound 4pa

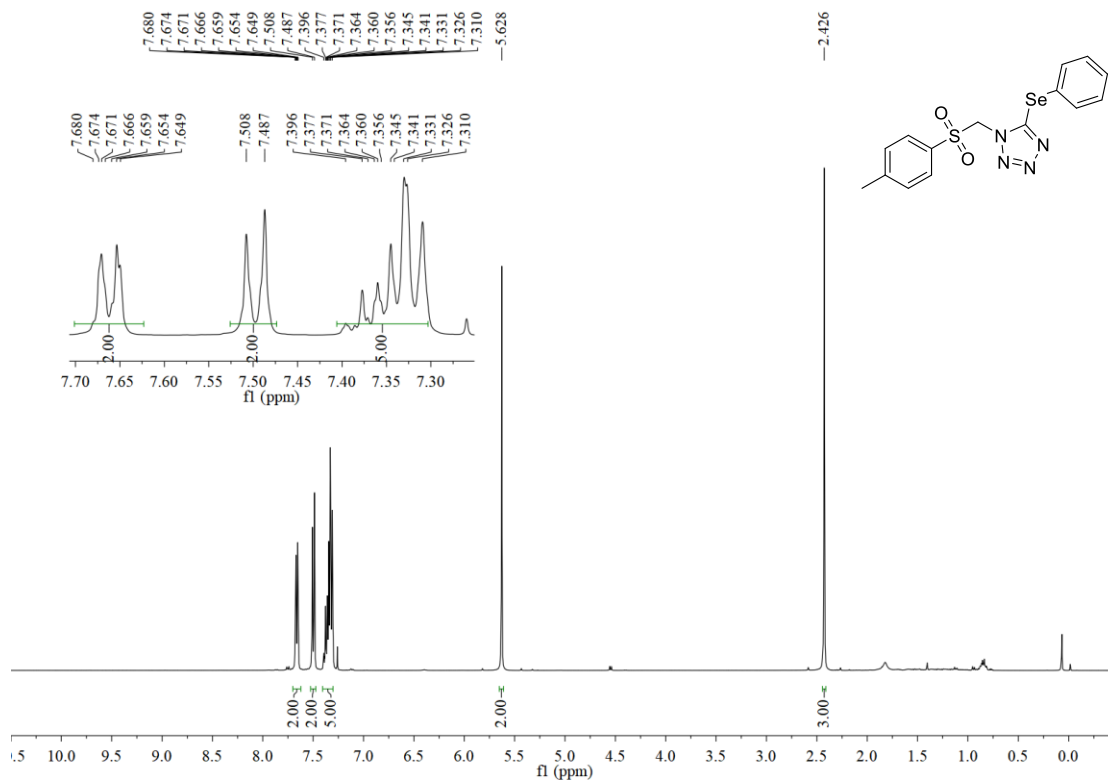


¹³C{¹H} NMR (100MHz, CDCl₃) of compound 4pa

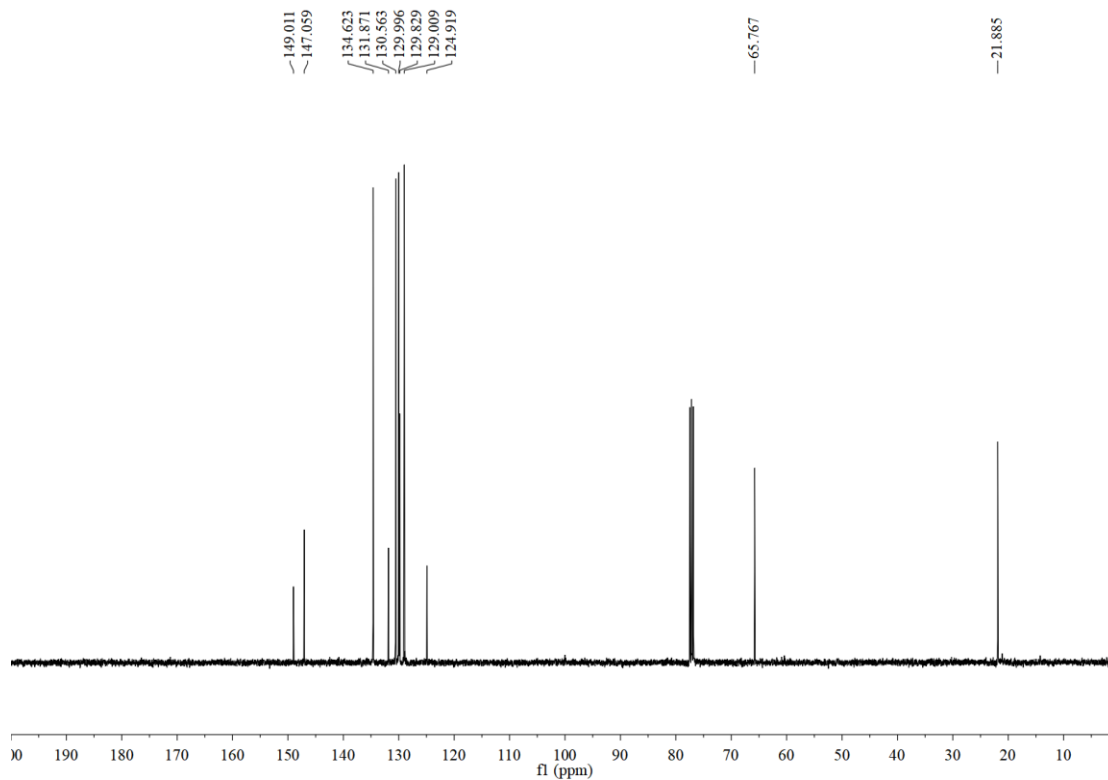


4qa

^1H NMR (400MHz, CDCl_3) of compound 4qa

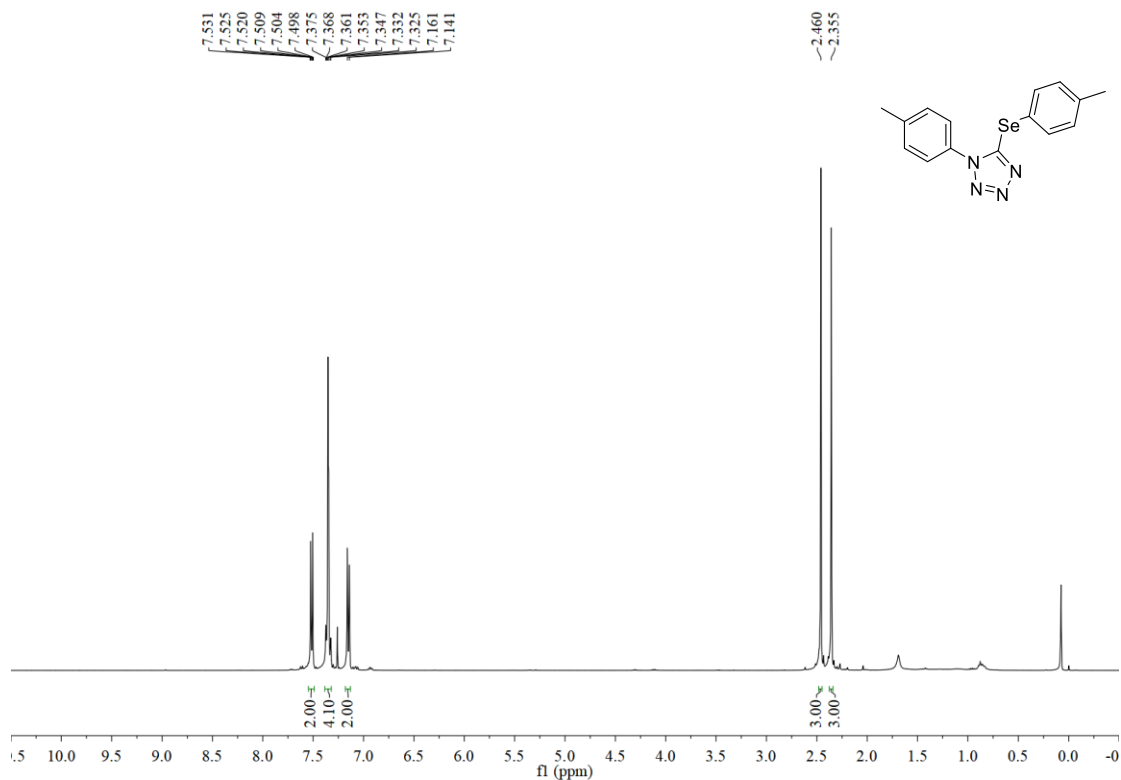


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4qa

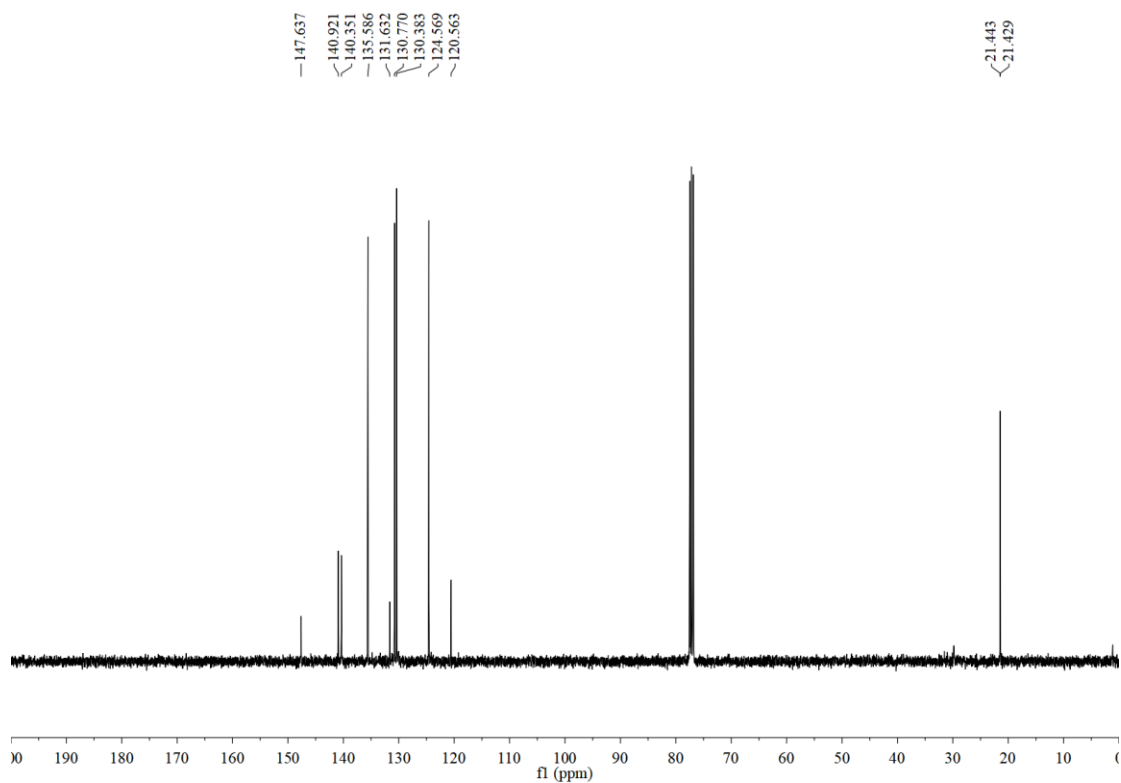


4ab

^1H NMR (400MHz, CDCl_3) of compound 4ab

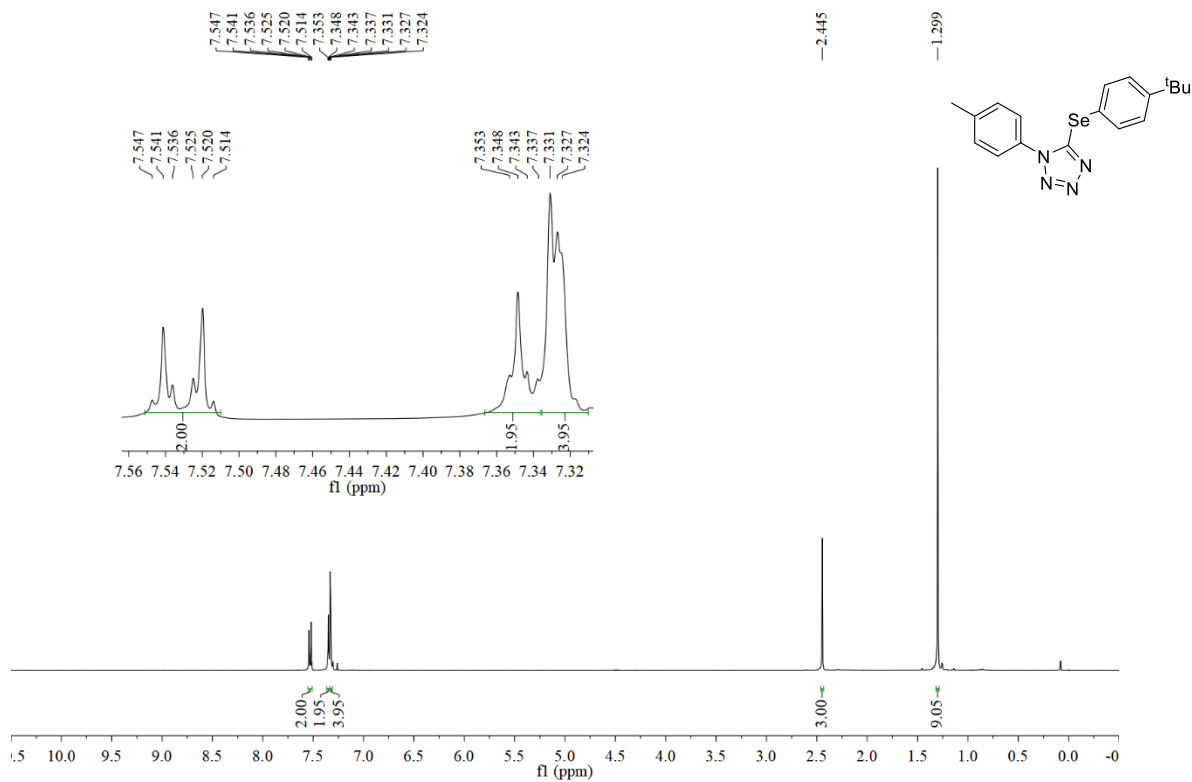


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4ab

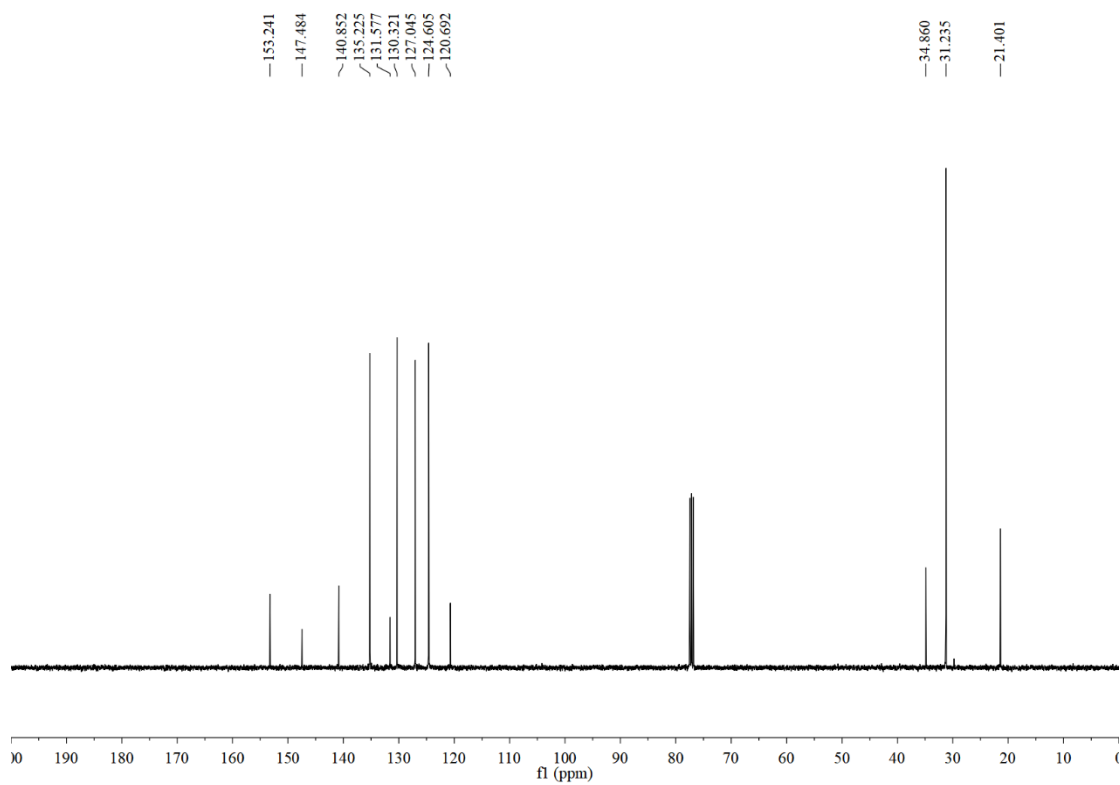


4ac

^1H NMR (400MHz, CDCl_3) of compound 4ac

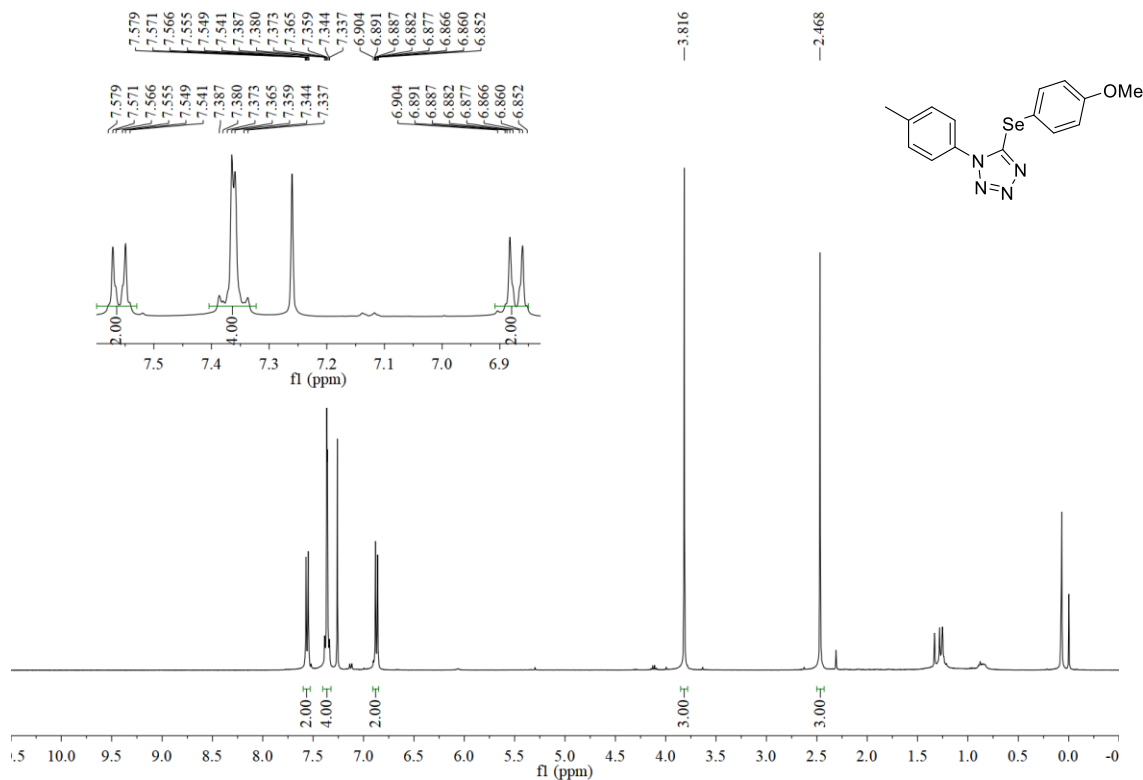


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4ac

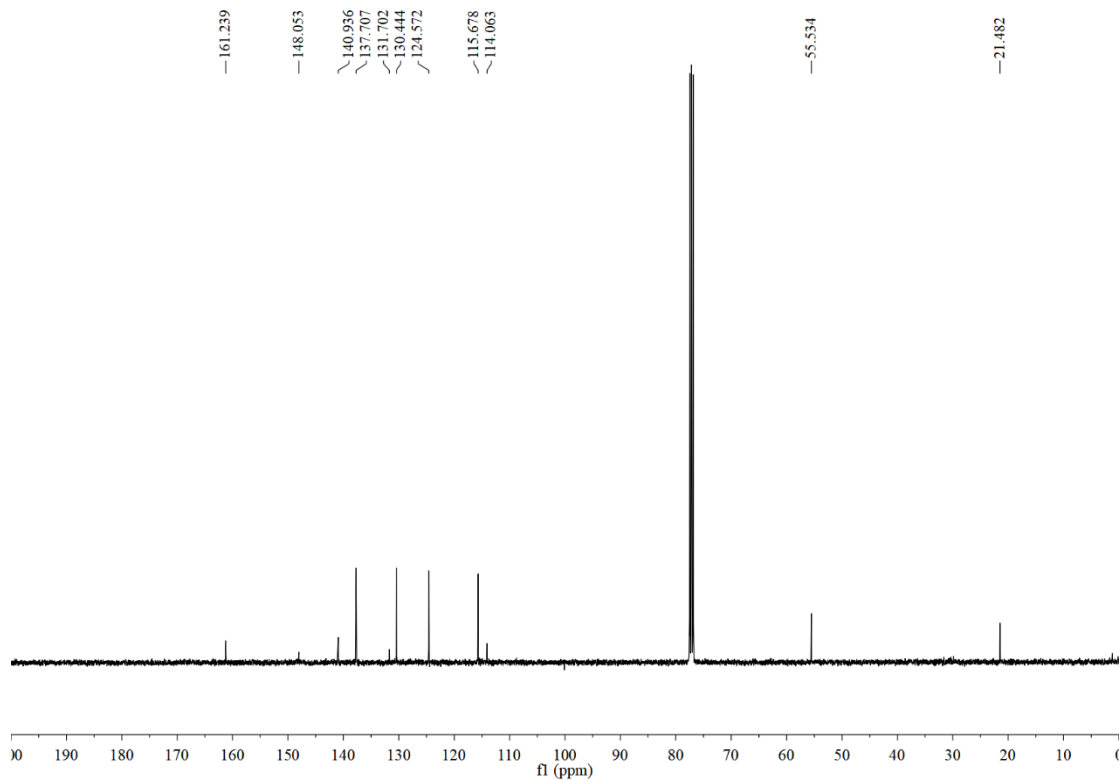


4ad

¹H NMR (400MHz, CDCl₃) of compound 4ad

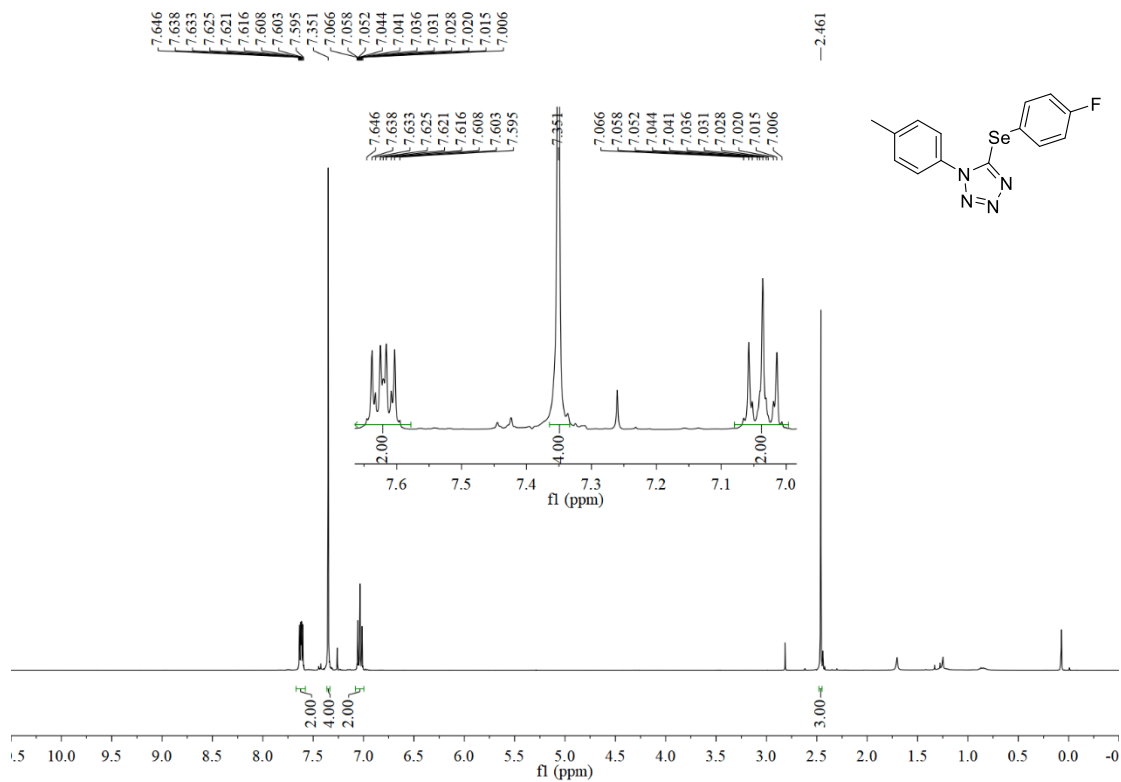


¹³C{¹H} NMR (100MHz, CDCl₃) of compound 4ad

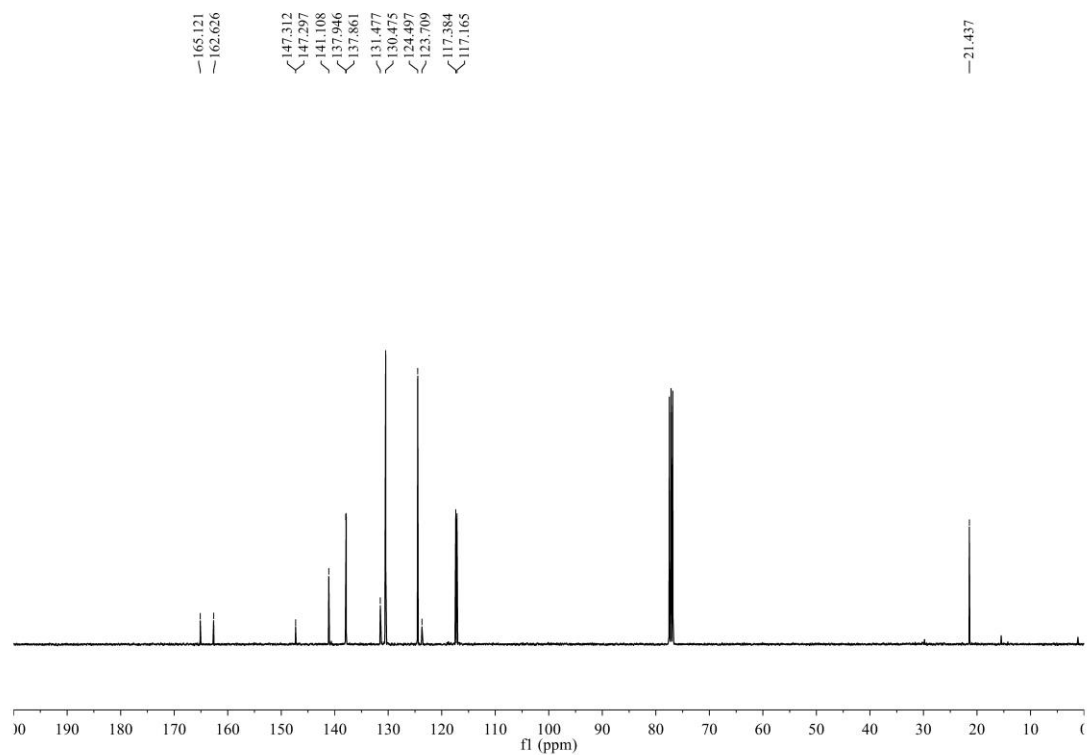


4ae

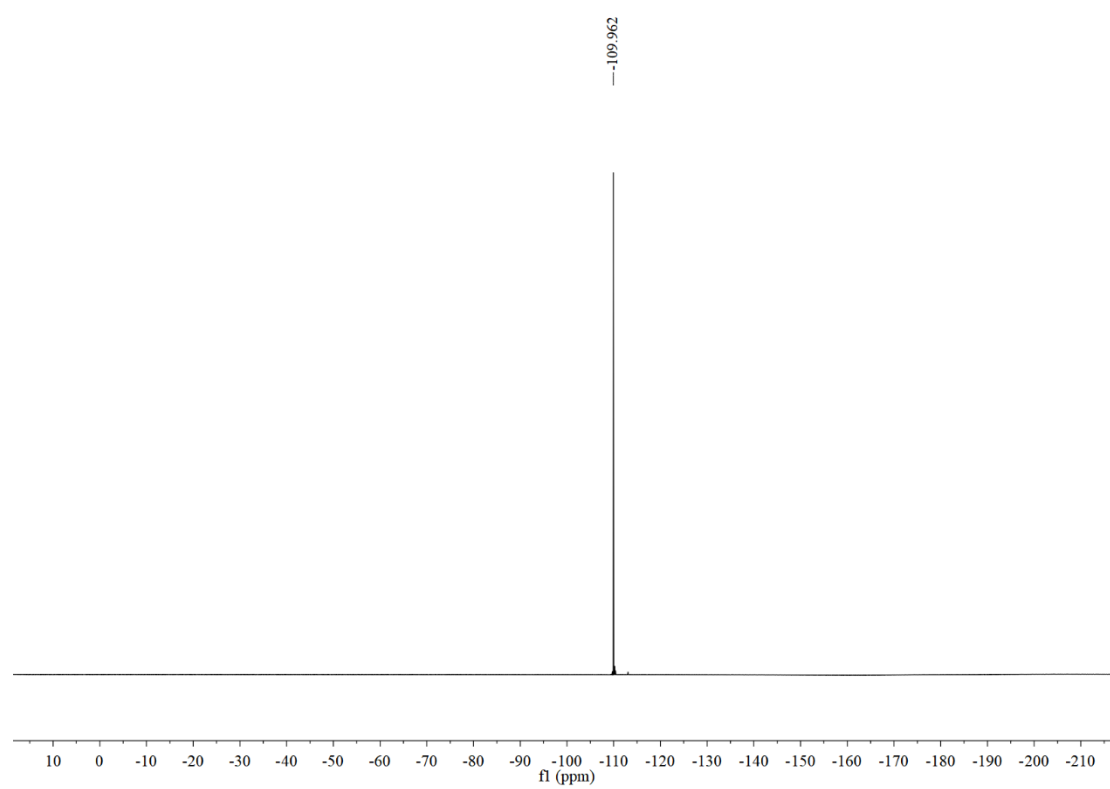
^1H NMR (400MHz, CDCl_3) of compound 4ae



$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4ae

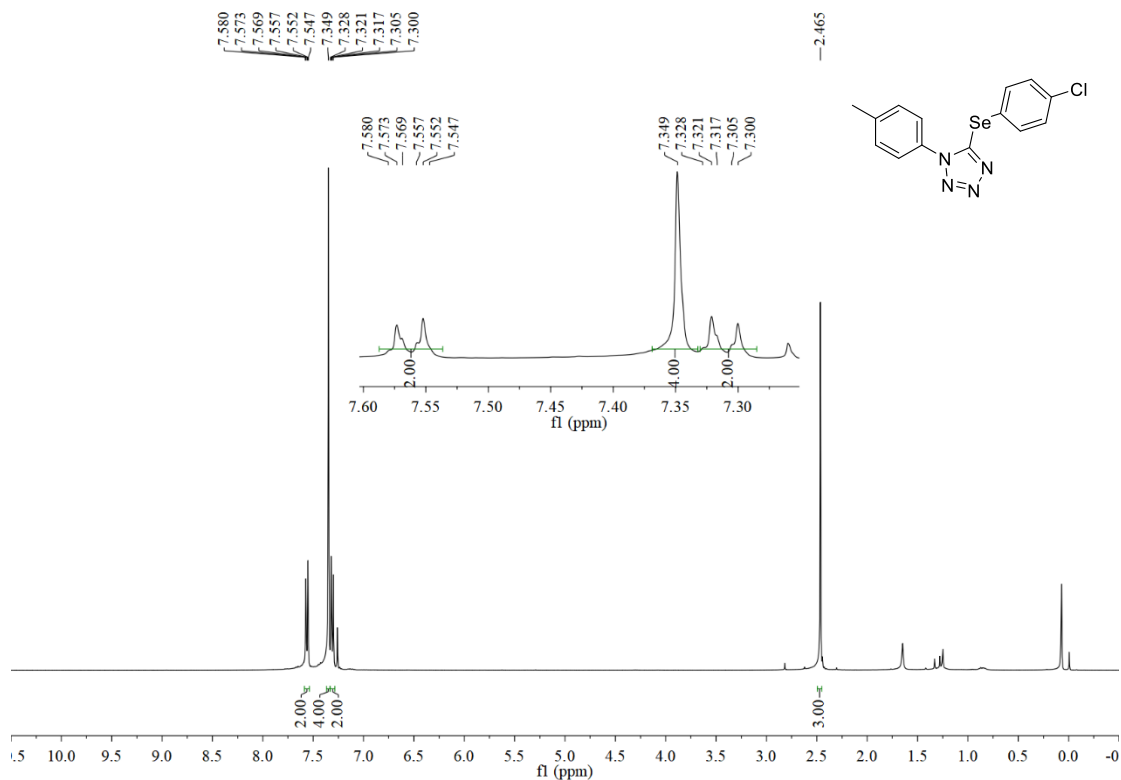


^{19}F NMR (376MHz, CDCl_3) of compound 4ae

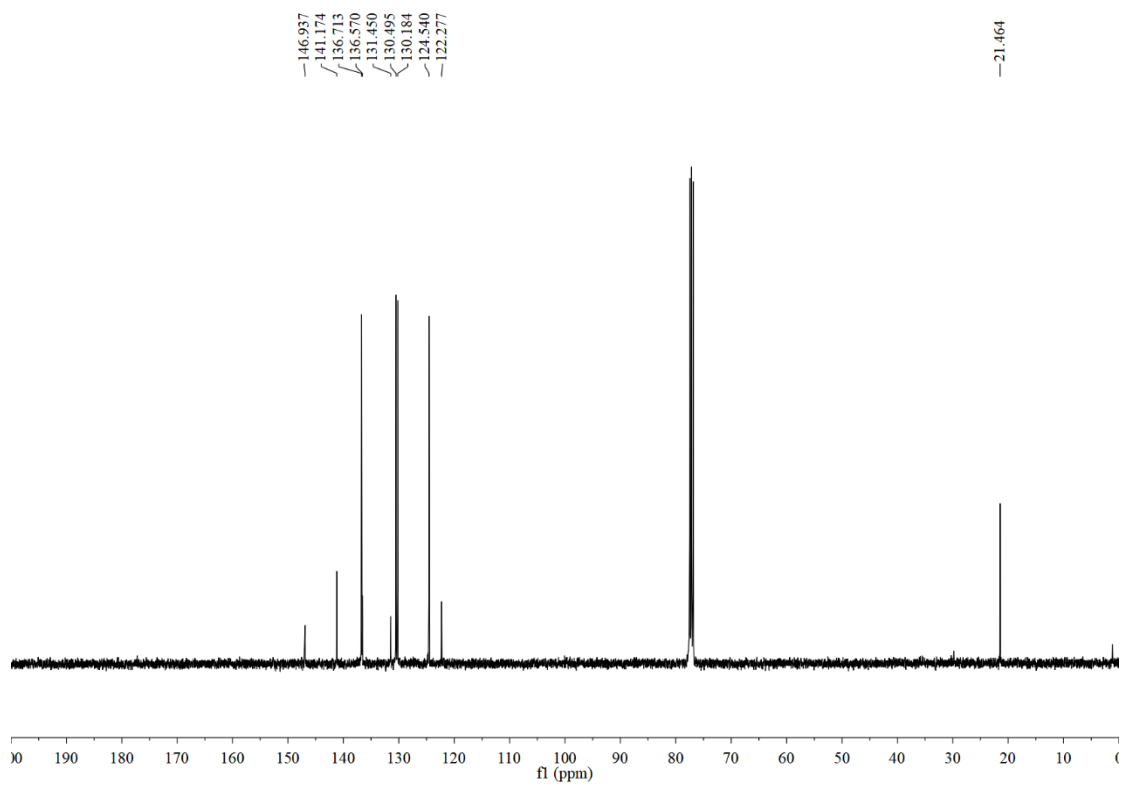


4af

¹H NMR (400MHz, CDCl₃) of compound 4af

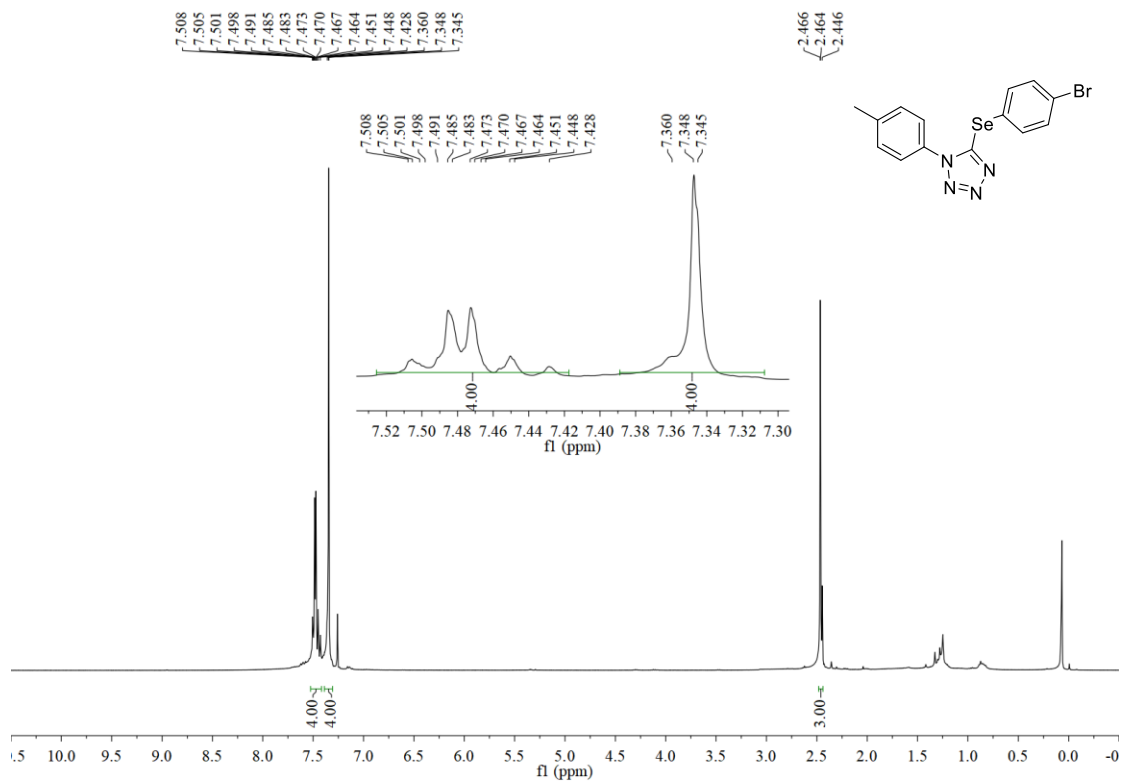


¹³C{¹H} NMR (100MHz, CDCl₃) of compound 4af

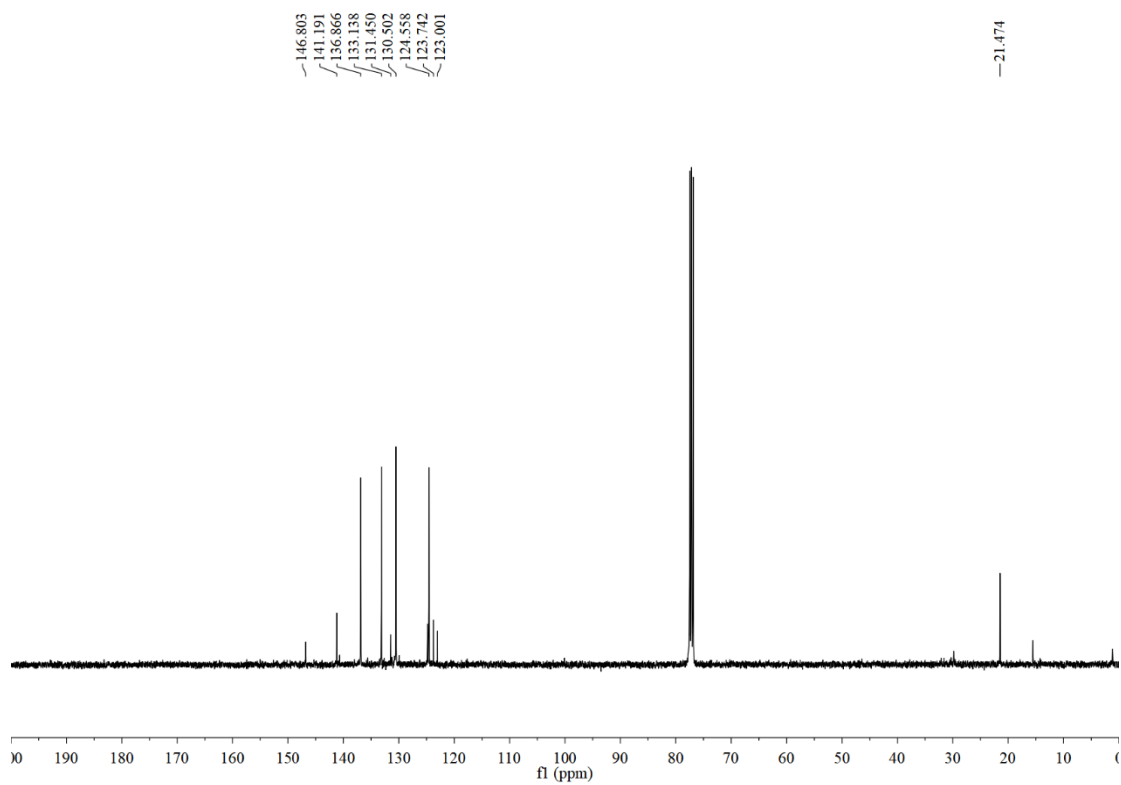


4ag

^1H NMR (400MHz, CDCl_3) of compound 4ag

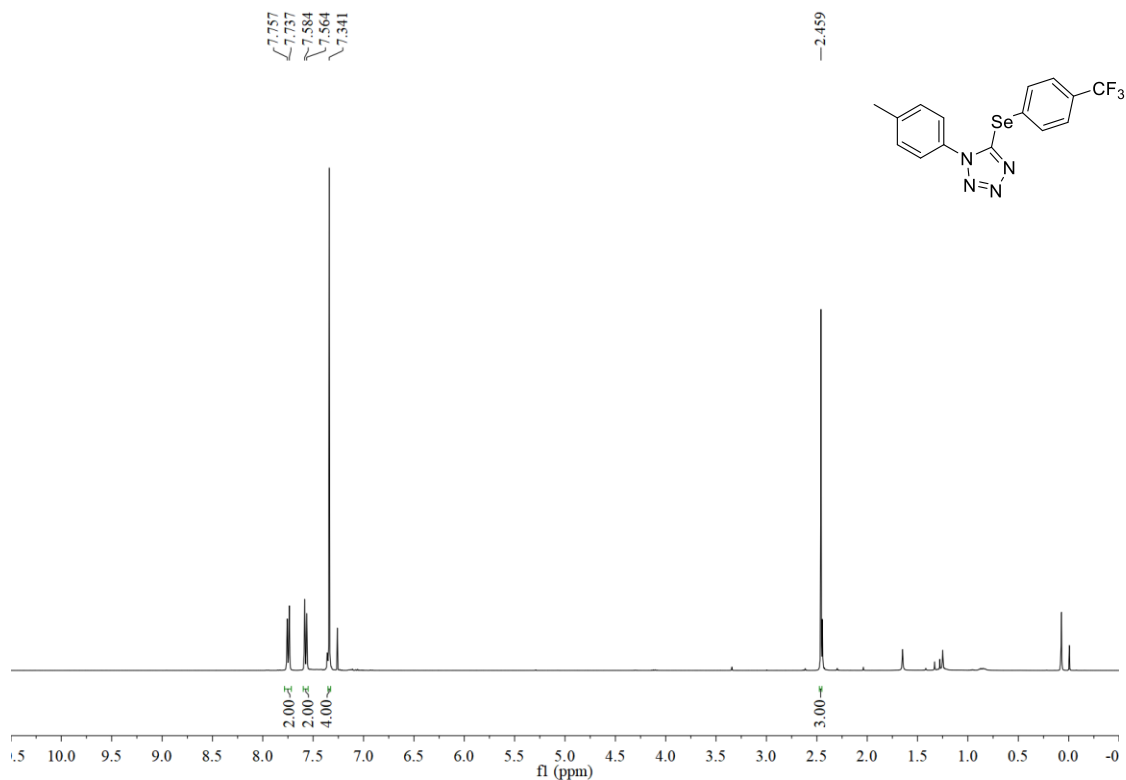


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4ag

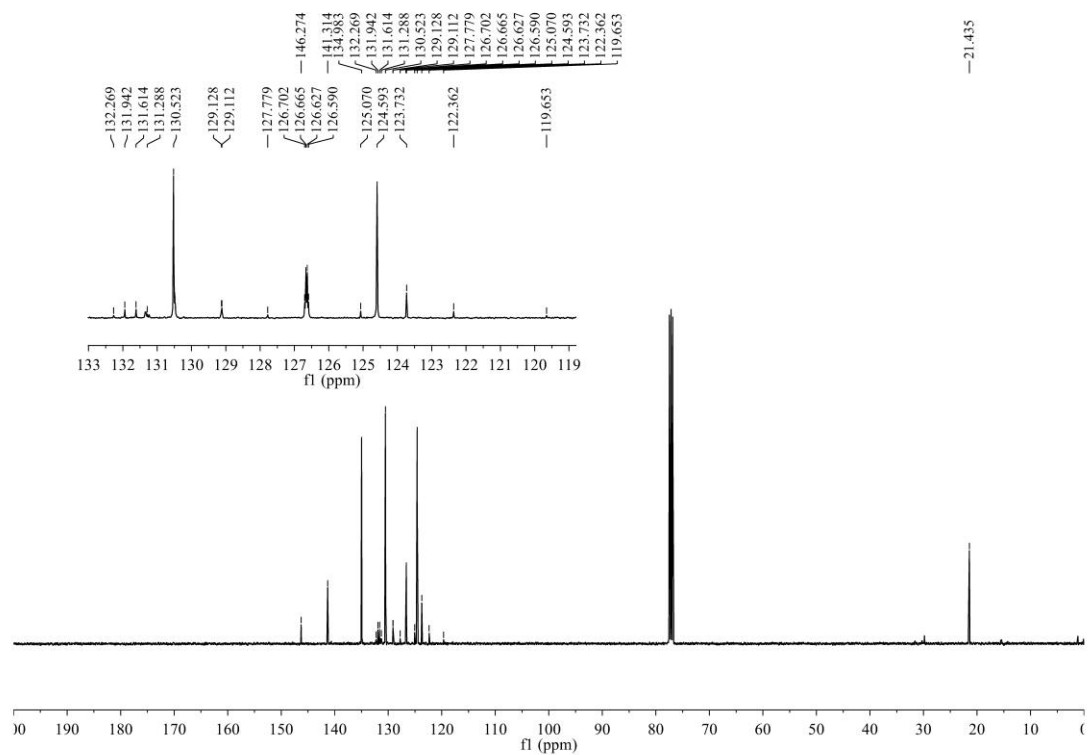


4ah

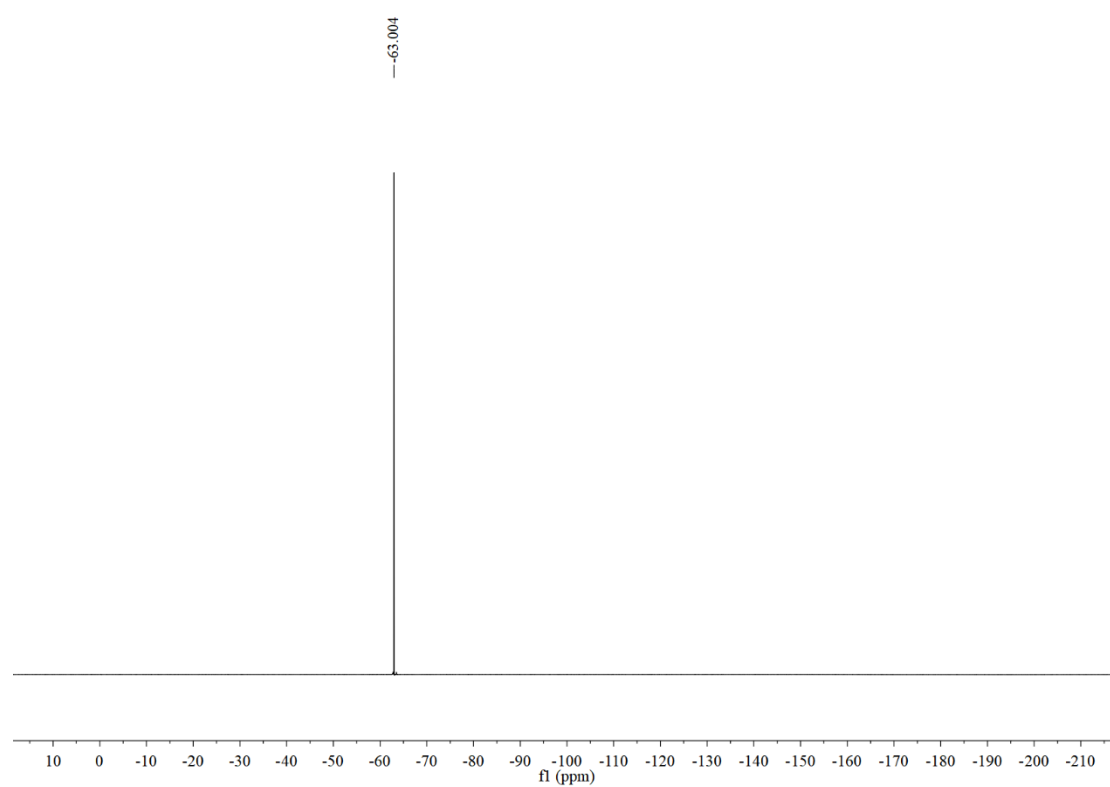
¹H NMR (400MHz, CDCl₃) of compound 4ah



¹³C{¹H} NMR (100MHz, CDCl₃) of compound 4ah

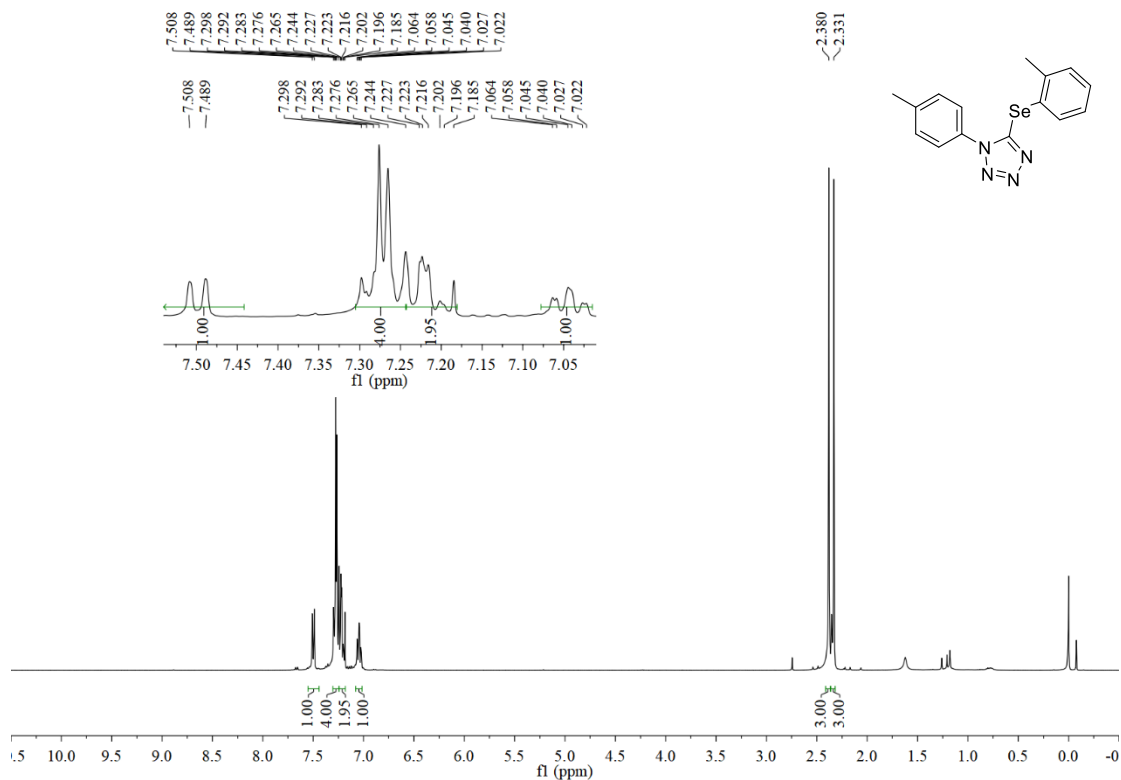


^{19}F NMR (376MHz, CDCl_3) of compound 4ah

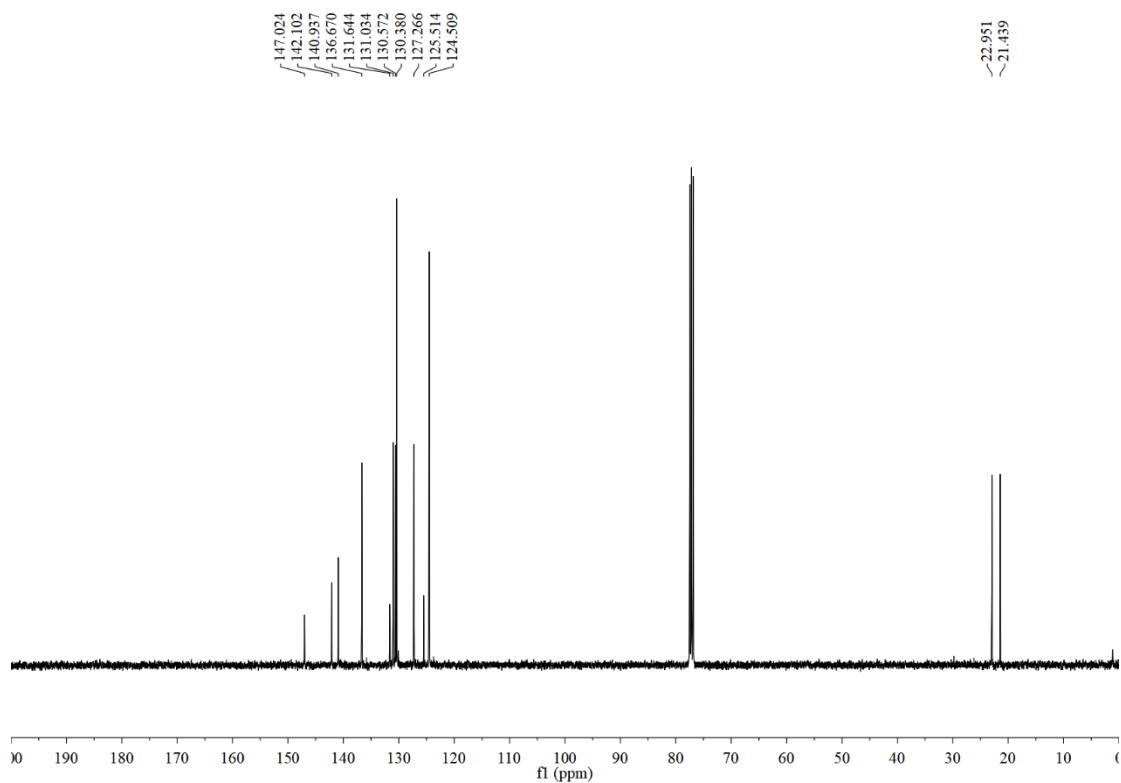


4ai

¹H NMR (400MHz, CDCl₃) of compound 4ai

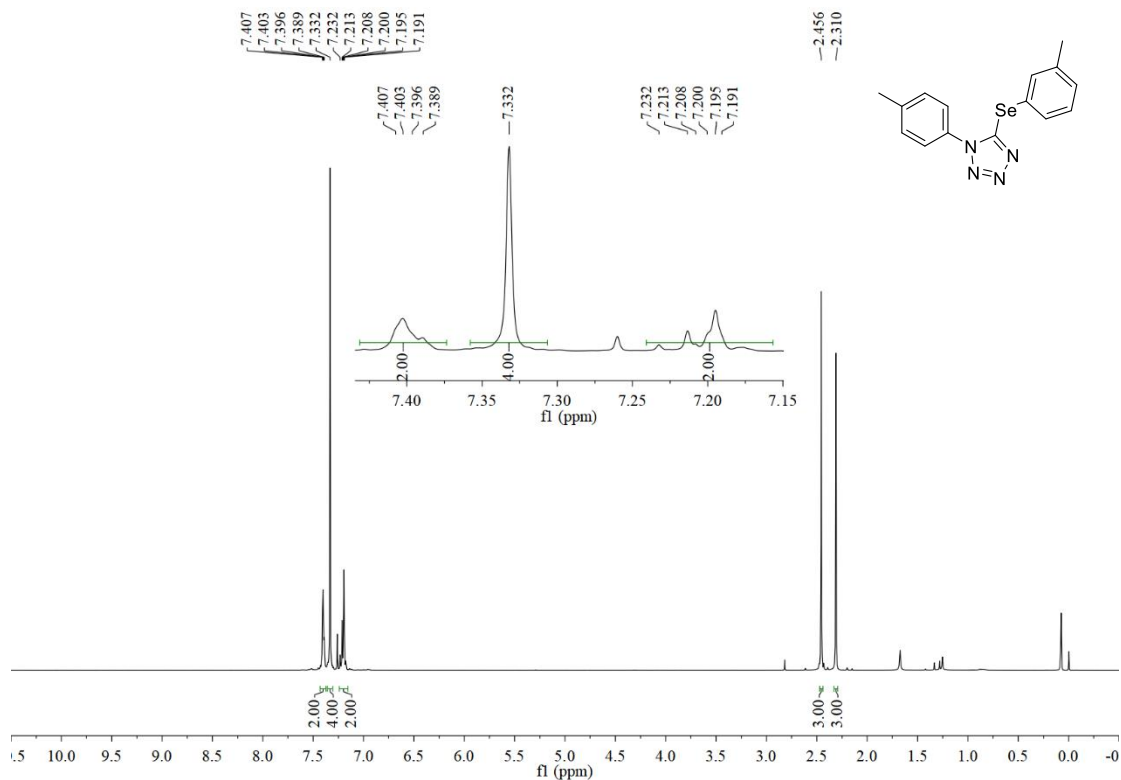


¹³C{¹H} NMR (100MHz, CDCl₃) of compound 4ai

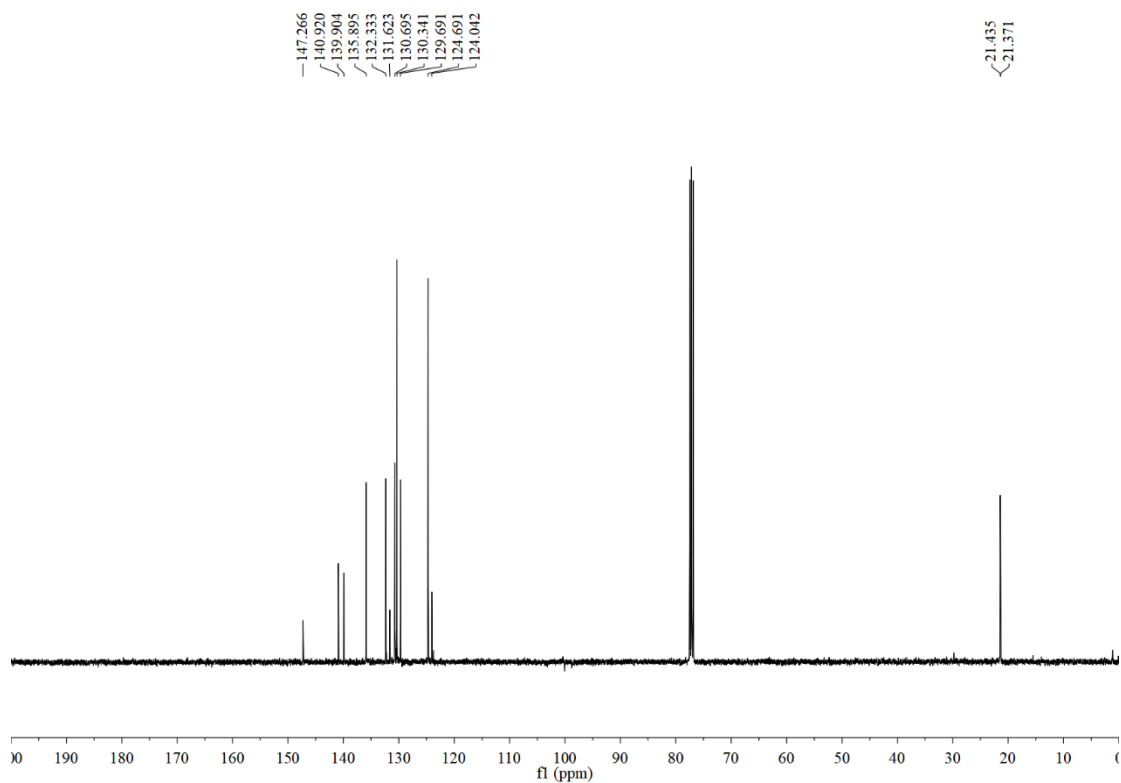


4aj

^1H NMR (400MHz, CDCl_3) of compound 4aj

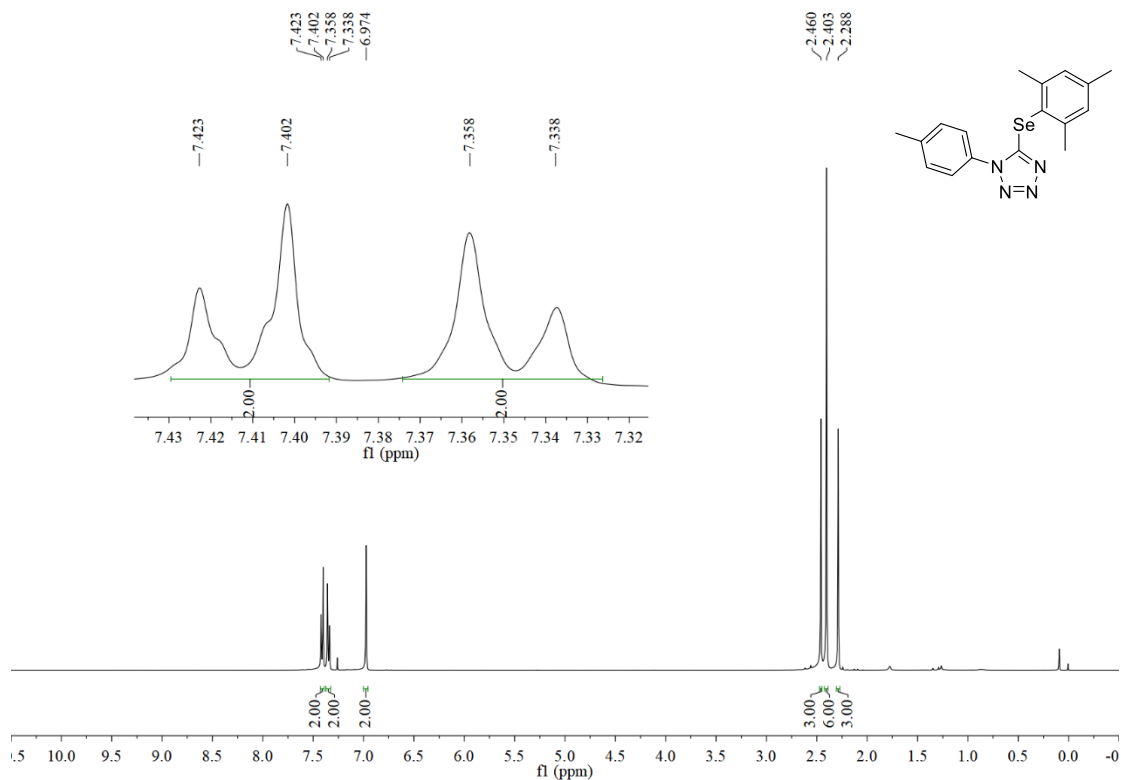


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4aj

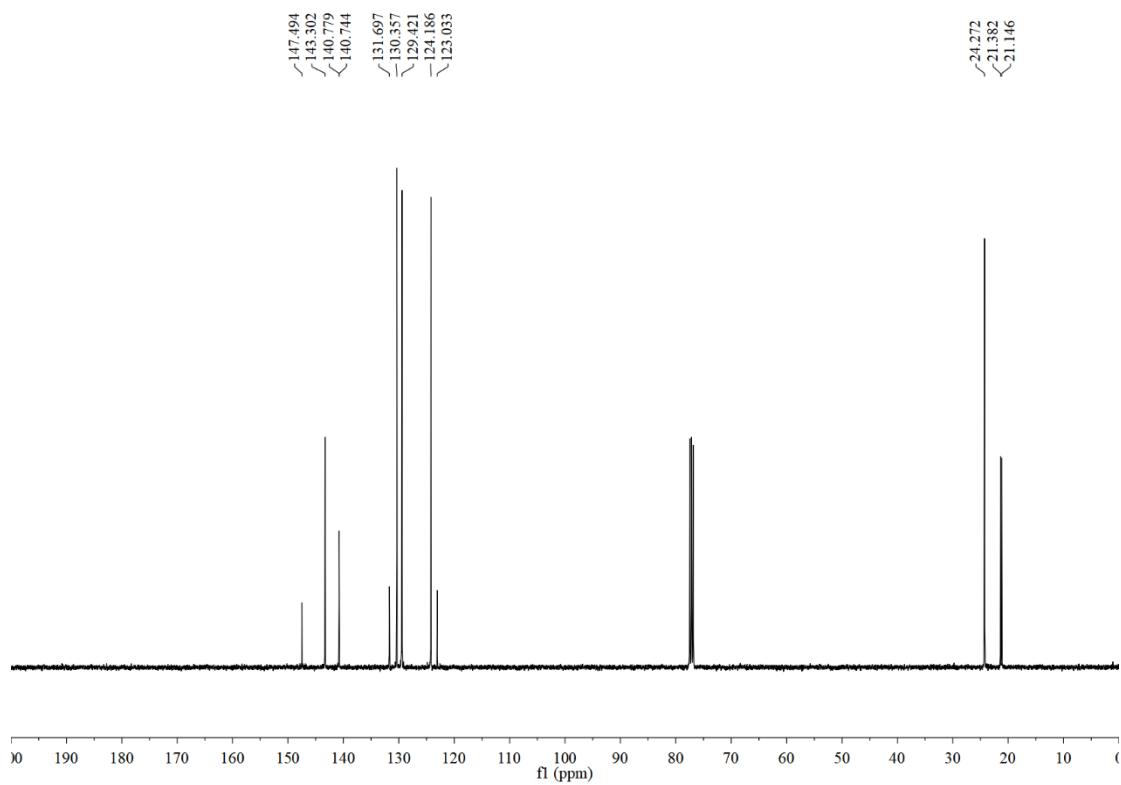


4ak

^1H NMR (400MHz, CDCl_3) of compound 4ak

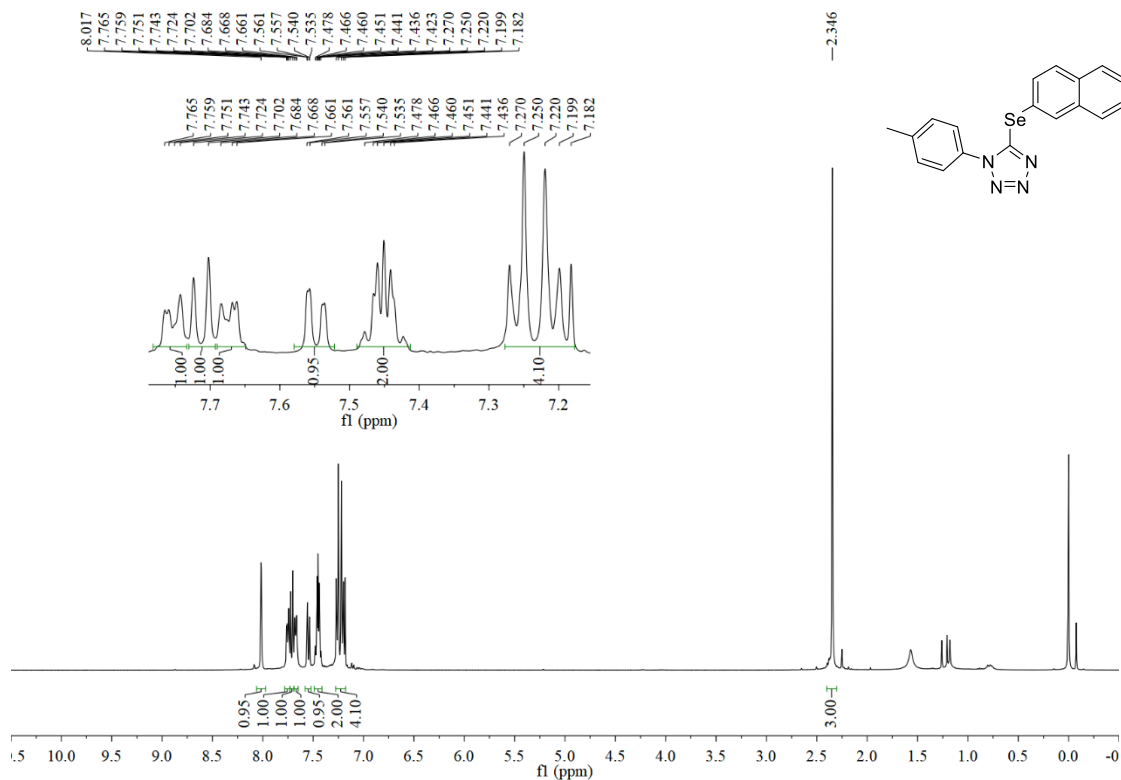


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4ak

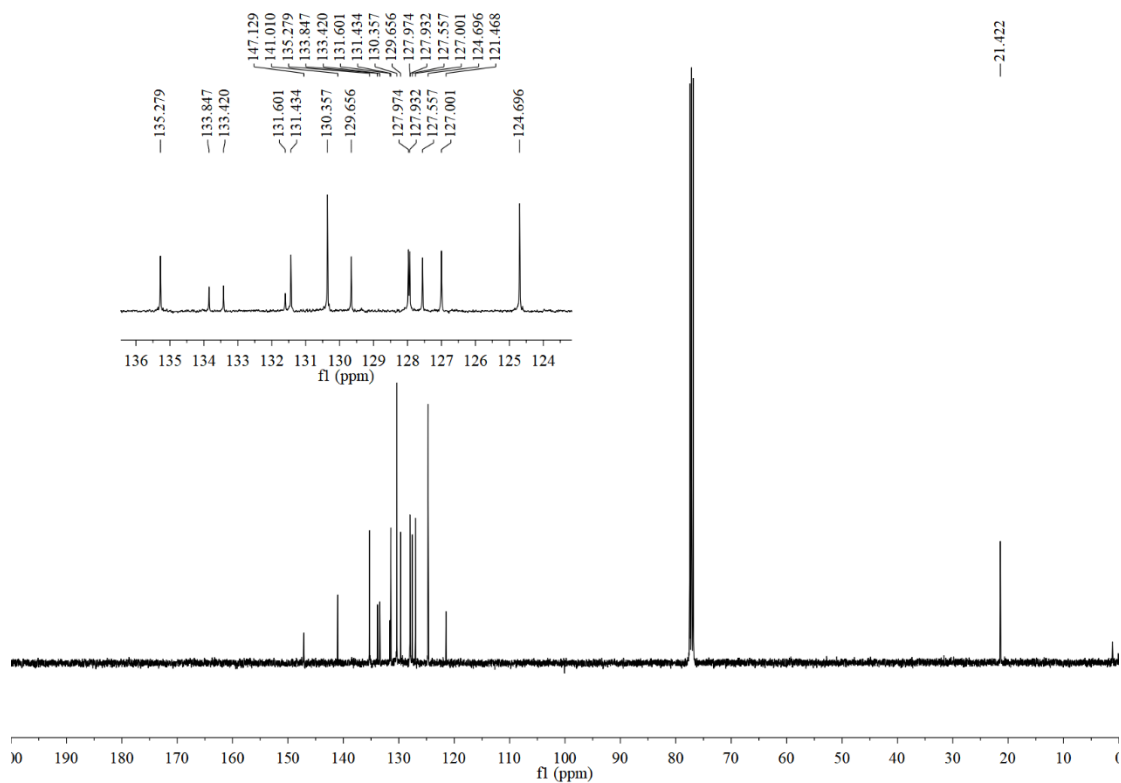


4al

^1H NMR (400MHz, CDCl_3) of compound 4al

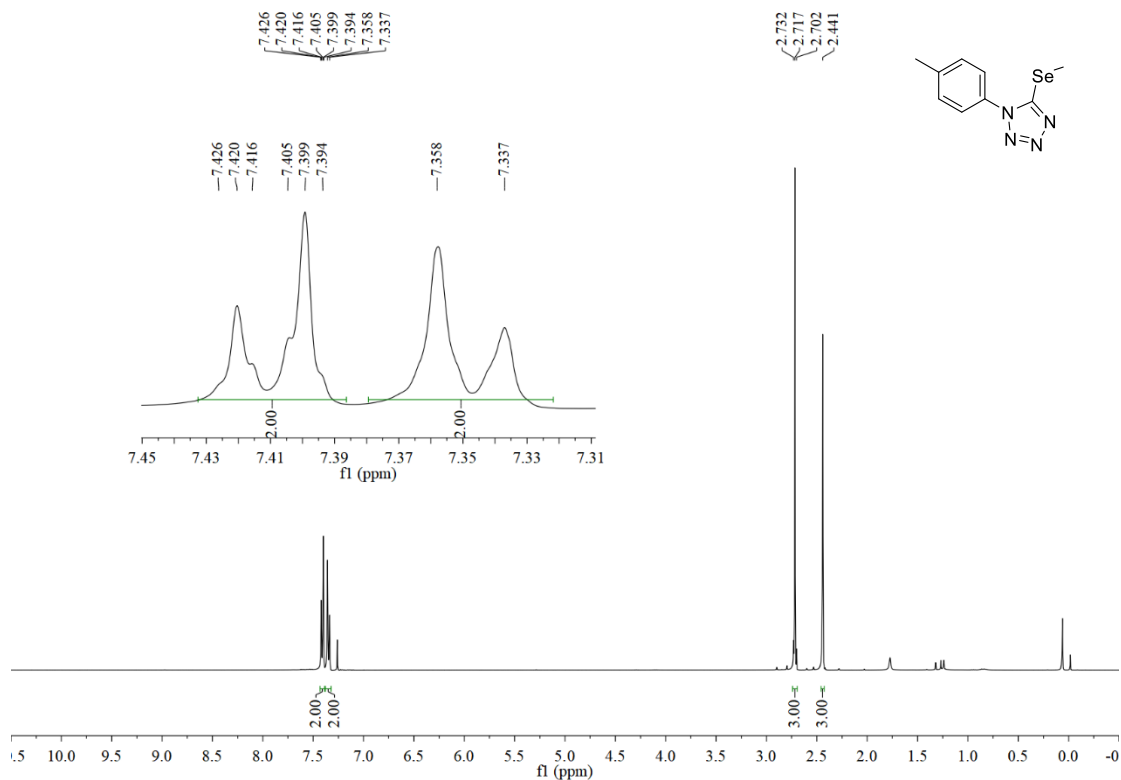


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4al

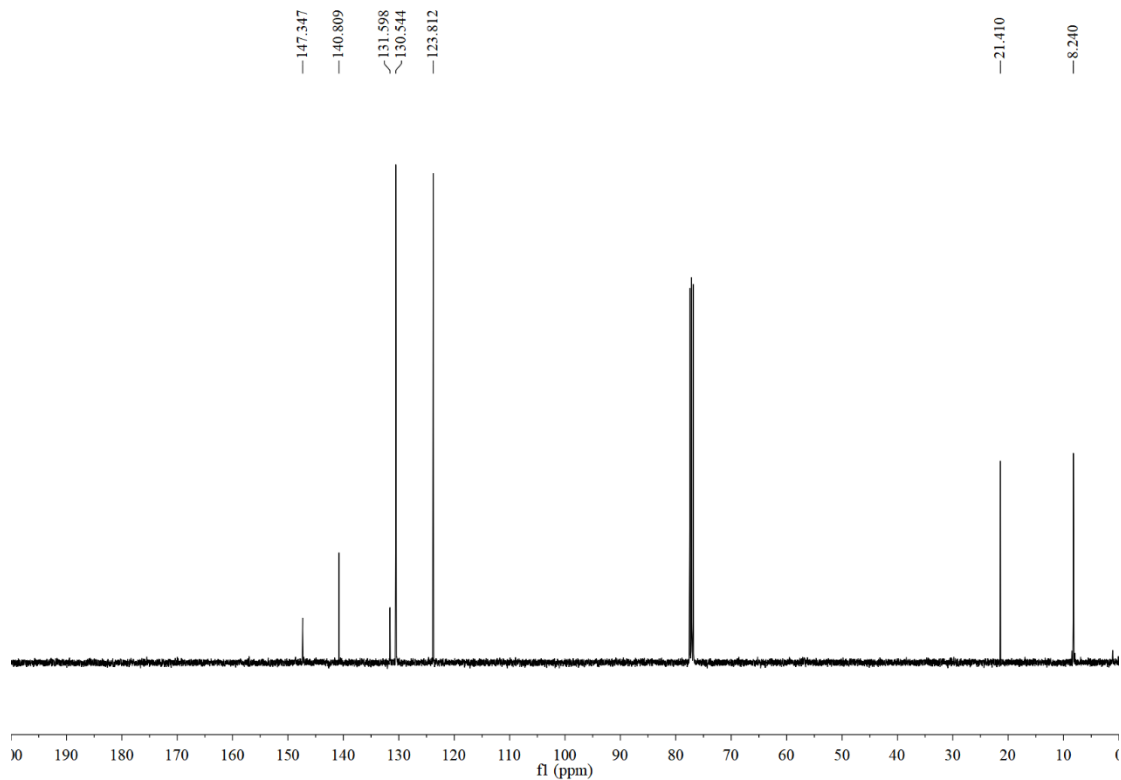


4am

^1H NMR (400MHz, CDCl_3) of compound 4am

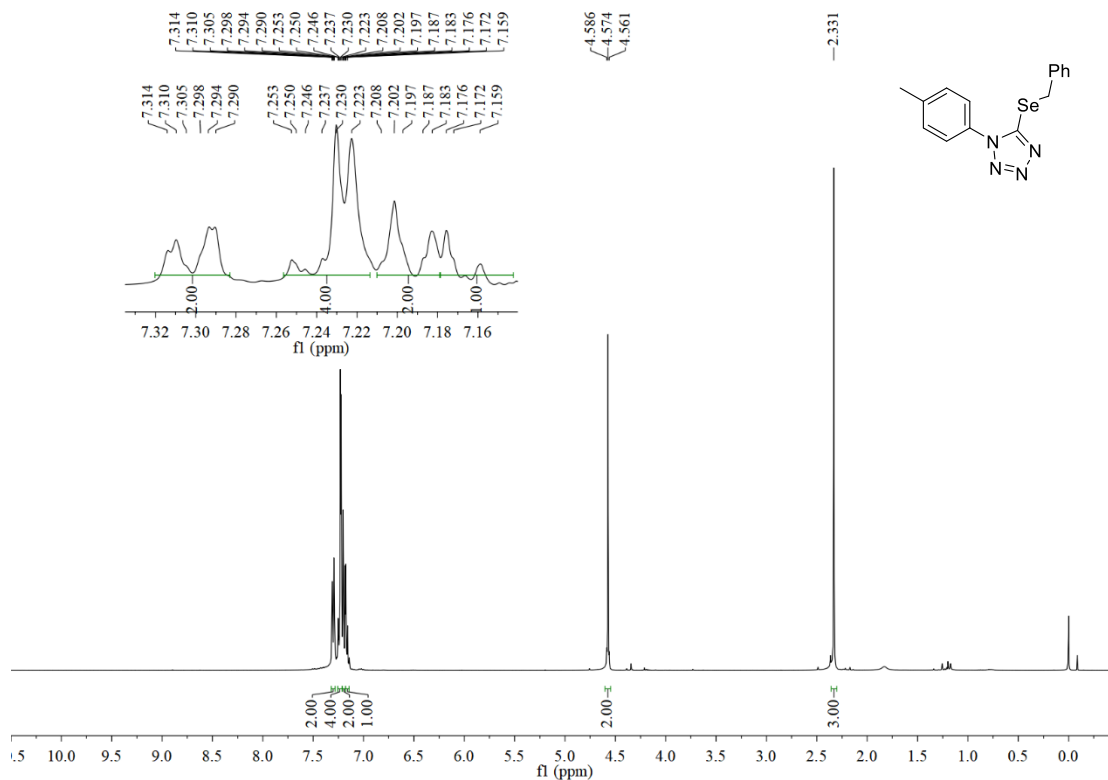


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4am

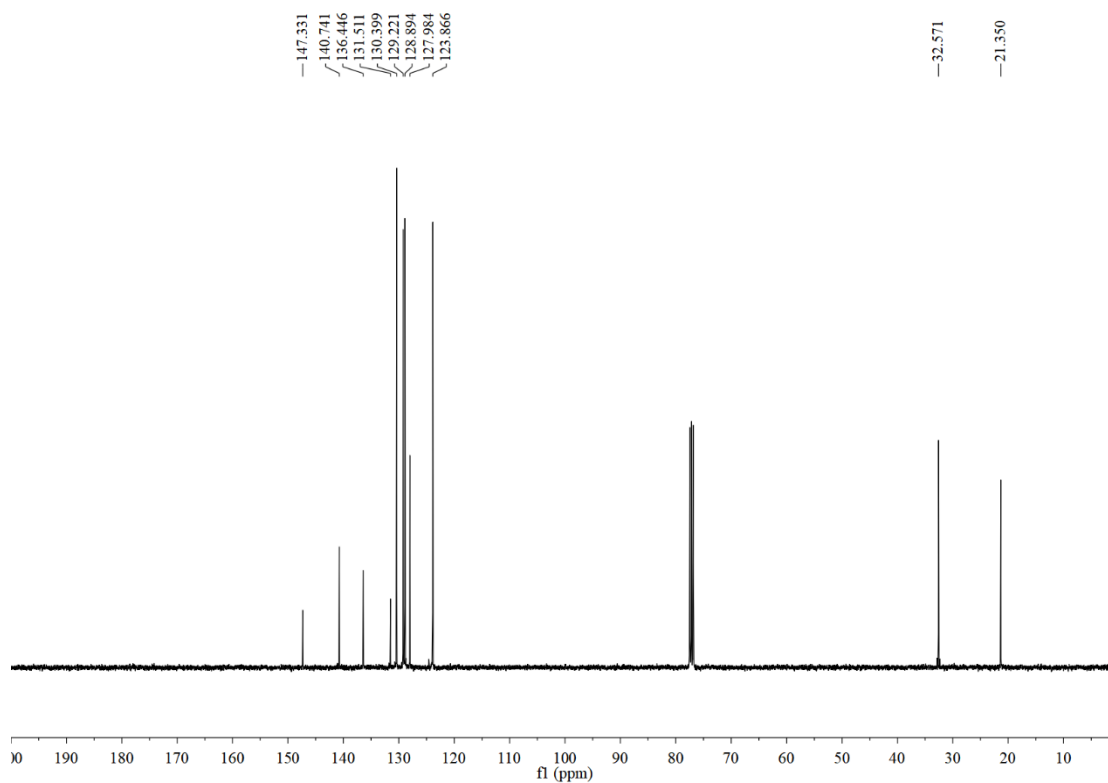


4an

^1H NMR (400MHz, CDCl_3) of compound 4an

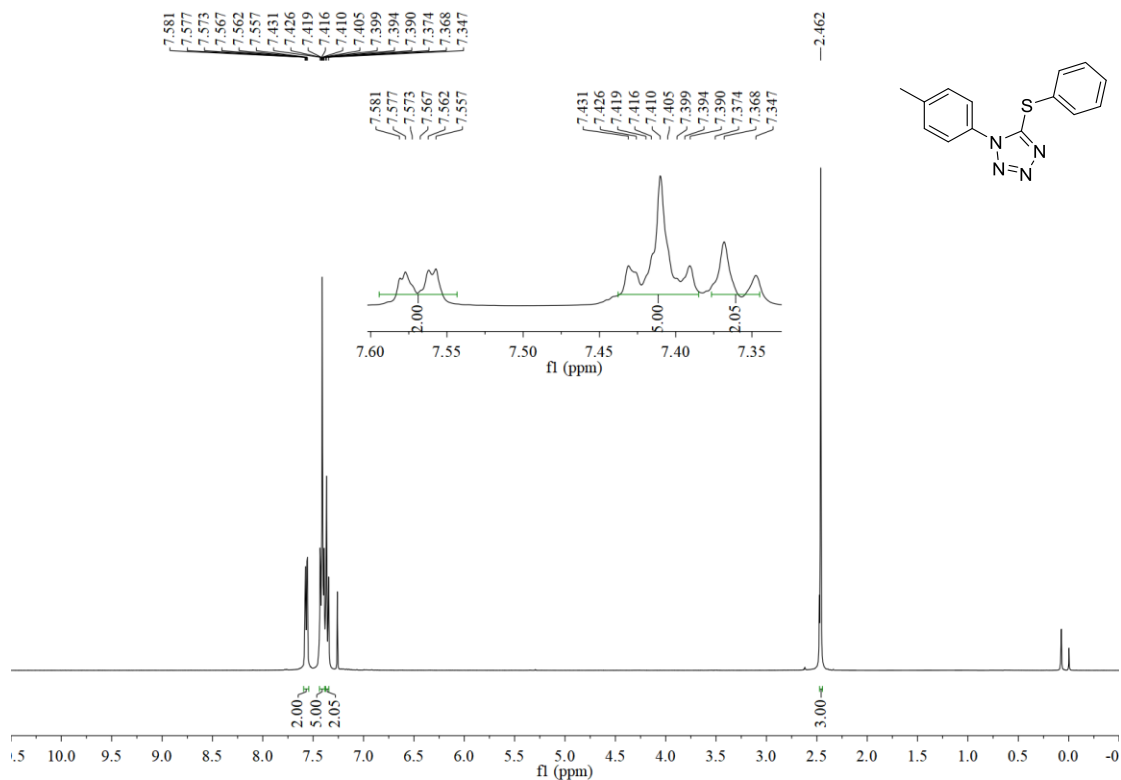


$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 4an

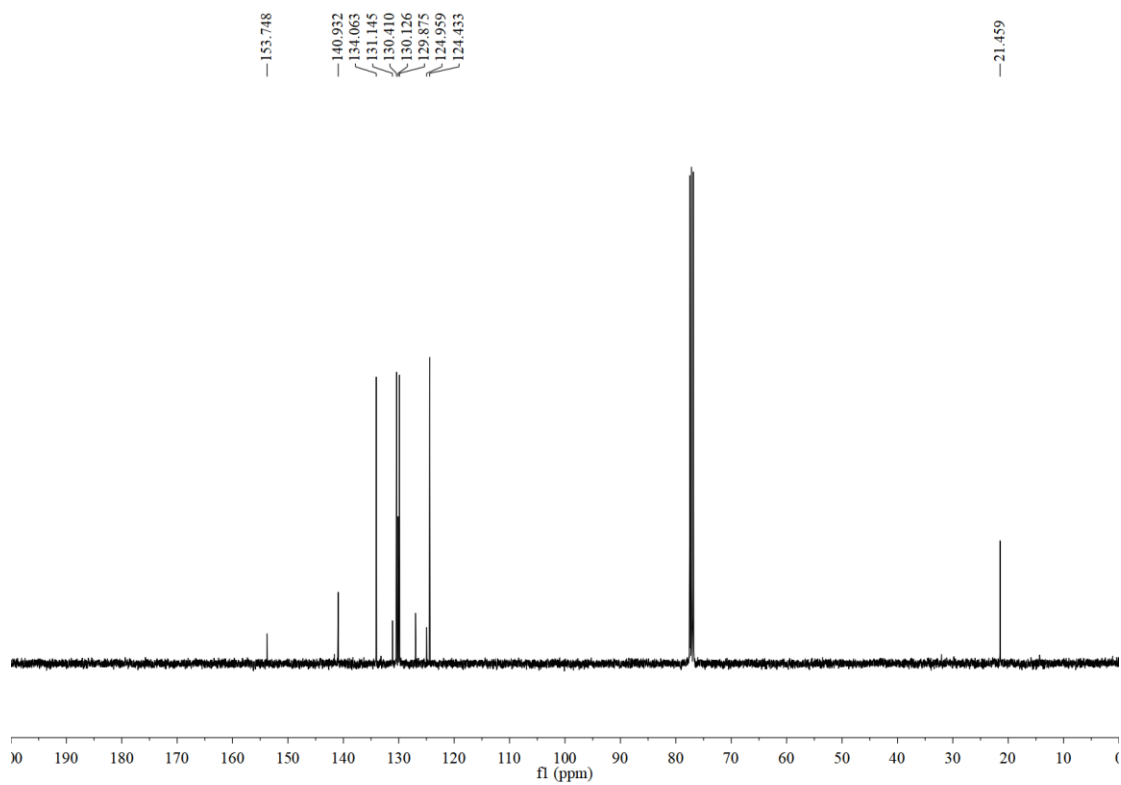


4ao

¹H NMR (400MHz, CDCl₃) of compound 4ao

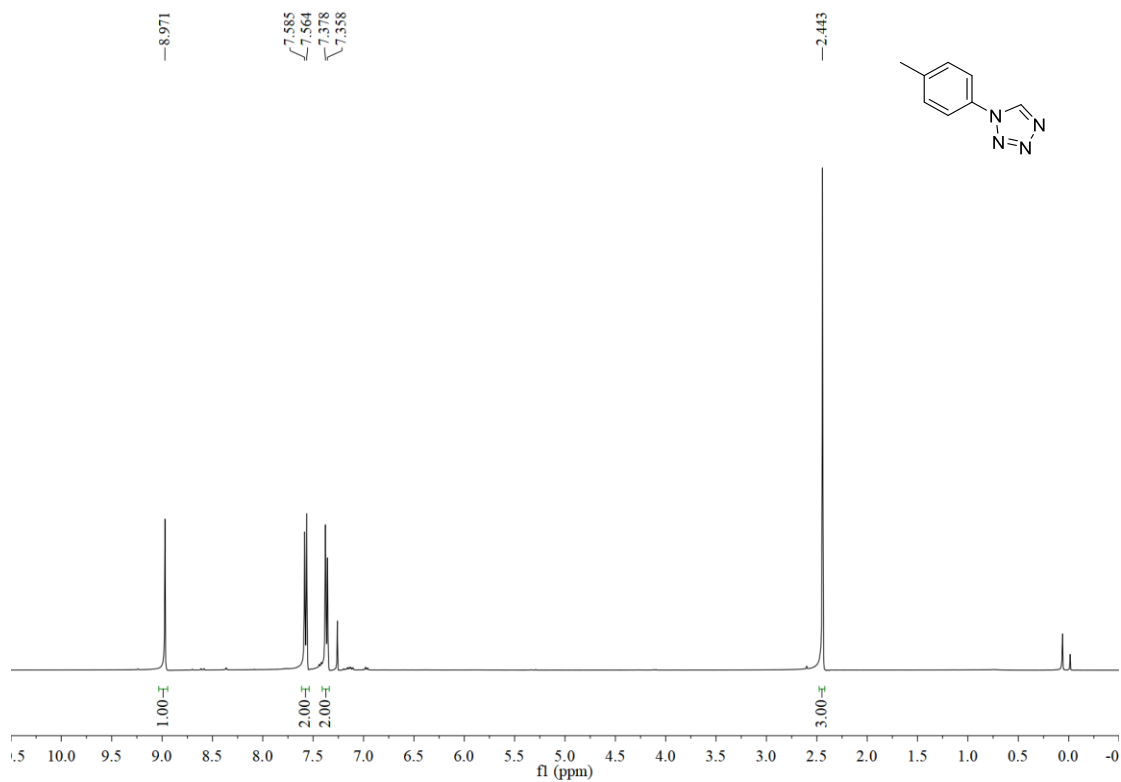


¹³C{¹H} NMR (100MHz, CDCl₃) of compound 4ao



6

^1H NMR (400MHz, CDCl_3) of compound 6



$^{13}\text{C}\{^1\text{H}\}$ NMR (100MHz, CDCl_3) of compound 6

