Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Copper(I)-Catalyzed Multicomponent Interrupted Click Reaction: Modular Synthesis of Triazole Sulfides from Element Sulfur

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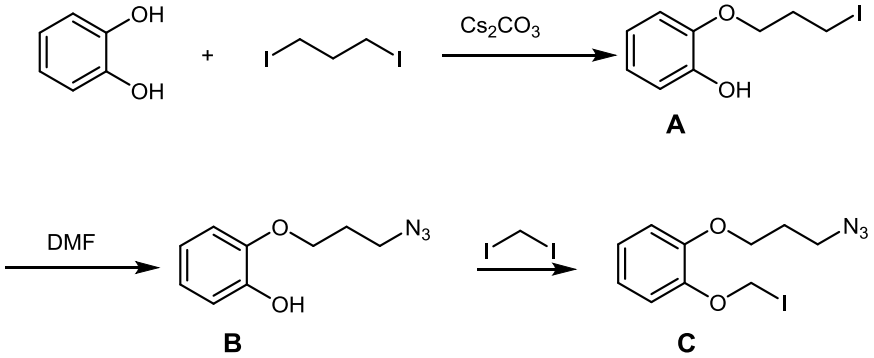
General information

Unless otherwise noted, analytic grade solvents were used for the chromatography, and all the reagents were obtained commercially and used without further purification. All reactions were performed under nitrogen atmosphere and in a flame-dried or oven-dried glassware with magnetic stirring. Column chromatography was performed with silica gel (200 – 300 mesh) as the stationary phase. Reactions were monitored by TLC. Solvent compositions are given in (v/v). All NMR spectra were recorded on Bruker-500 MHz spectrometer in DMSO-d_6 or $CDCl_3$. HRMS were measured on the Q-TOF6510 instruments. The chemical shifts (δ) were expressed in ppm and *J* values were given in Hz. The following abbreviations are used to indicate the multiplicity: singlet (s), doublet (d), triplet (t) and multiplet (m). All first order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted were designated as multiplet (m). Mass analyses and HRMS were obtained by ESI on a TOF mass analyzer.

Synthesis of the starting materials

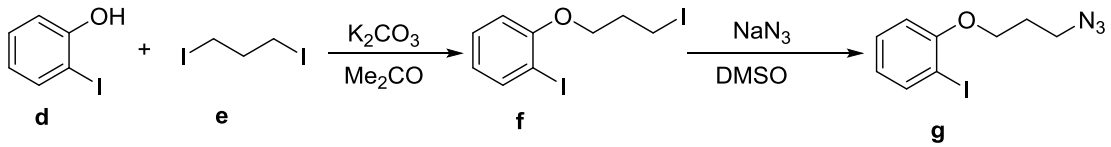
1) Typical procedure for the preparation of 1-(3-azidopropoxy)-2-(iodomethoxy)benzene.



A mixture of 1,2-benzenediol (2.2 g, 20 mmol) and Cs_2CO_3 (6.5 g, 20 mmol) in DMF (30 mL) was stirred at 60 ^oC for 1 h. To the solution was added 1,3-Dllodopropane (8.9 g, 30 mmol) and the reaction mixture was stirred at 60℃ for 24 h. The reaction mixture was quenched with water, diluted with EtOAc, dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purifed by silica column chromatography (petroleum ether: EtOAc = 50:1) to afford compound **A** (2.2 g, 8 mmol)**.**

To a solution of **A** (3.6 g, 8 mmol) in DMF (30 mL) was added NaN_3 (4.14 g, 30 mmol). The resulting mixture was stirred at 100 ^oC for 24 h. After cooling, the mixture was filtered. The filtrate was diluted with water, extracted with CH_2Cl_2 and dried over Na_2SO_4. Removal of the solvent under reduced pressure and purification on silica gel afforded the target compound **B** the reaction stopped by filtration and evaporation under vacuum. The crude product was purified by silica column chromatography (petroleum ether: EtOAc = 50:1) to afford compound **B** (0.96 g, 5 mmol)**.**

A mixture of **B** (5 mmol), Cs_2CO_3 (1.6 g, 5 mmol) and diiodomethane (2.7 g, 10 mmol) in DMF (30 ml) wasstirred at 60 ^oC for 24 h. After cooling, the mixture was filtered. The filtrate was diluted with water, extracted with CH_2Cl_2 and dried over Na_2SO_4. Removal of the solvent under reduced pressure and purification on silica gel afforded the target compound **C** (1.0 g, 3 mmol).

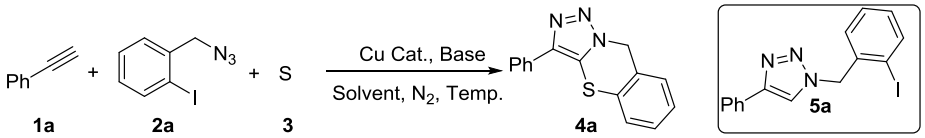


To a stirred solution of **d** 2-iodophenol (5 mmol) and **e** 1,3-Dllodopropane (7.5 mmol) in acetone (15 mL) was added K_2CO_3 (10 mmol). The resulting mixture was refluxed at 70 ^oC for 12 h. Upon completion, the reaction mixture was filtered with a pad of Celite. The filtrate was then concentrated under vacuum. The residue was purified by silica gel column chromatography using a petroleum ether/AcOEt as the eluent to give the product **f** (1.16 g, 3mmol).

To a solution of **f** (3 mmol) in DMSO (10 mL) was added NaN_3 (4.14 g, 30 mmol) .

The resulting mixture was stirred at 100 ^{o}C for 24 h. After cooling, the mixture was filtered. The filtrate was diluted with water, extracted with CH_2Cl_2 and dried over Na_2SO_4. Removal of the solvent under reduced pressure and purification on silica gel afforded the target compound **g** (0.6 g, 2mmol).

Optimization of reaction conditions



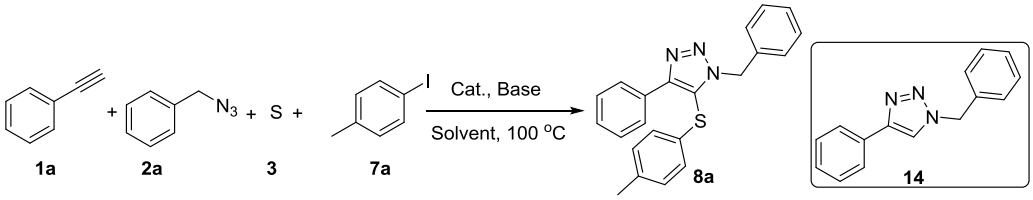
1a 2a 3 4a

Entry	Cat. (10 mol%)	Base (2 equiv)	Solvent	Yield(%)[b] **5a:6a**
1	CuI	$NaHCO_3$	DMSO	70:21
2	CuBr	$NaHCO_3$	DMSO	61:33
3	CuCl	$NaHCO_3$	DMSO	54:18
4	**CuSCN**	**$NaHCO_3$**	**DMSO**	**88:3**
5	CuCN	$NaHCO_3$	DMSO	45:50
6	CuF_2	$NaHCO_3$	DMSO	35:48
7	$CuCl_2$	$NaHCO_3$	DMSO	52:56
8	$CuBr_2$	$NaHCO_3$	DMSO	60:15
9	$CuSO_4$	$NaHCO_3$	DMSO	33:56
10	$Cu(OAc)_2$	$NaHCO_3$	DMSO	30:50
11	CuSCN	Cs_2CO_3	DMSO	68:25
12	CuSCN	Na_2CO_3	DMSO	55:21
13	CuSCN	K_2CO_3	DMSO	60:23
14	CuSCN	$KHCO_3$	DMSO	82:12
15	CuSCN	Et_3N	DMSO	38:49
16	CuSCN	^{t}BuOLi	DMSO	30:50
17	CuSCN	CH_3OLi	DMSO	25:58
18	CuSCN	CaH	DMSO	40:40
19	CuSCN	$NaHCO_3$	DMF	60:30
20	CuSCN	$NaHCO_3$	DCE	59:15
21	CuSCN	$NaHCO_3$	THF	48:45
22	CuSCN	$NaHCO_3$	CH_3CN	66:21
23[cde]	CuSCN	$NaHCO_3$	DMSO	0:90

[a]

Reaction conditions: 1a (0.2 mmol), 2a (0.3 mmol), 3 (0.4 mmol), Cu catalyst (10 mol%), base (0.4 mmol), DMSO (2 mL) was stirred at 50 ^{o}C under N_2 atmosphere for 24 h. [b][b] aIsolated yield. [c] reaction at 70 ^{o}C. [d] reaction at 90 ^{o}C. [c] reaction at 110 ^{o}C.

Optimization of four-component interrupted click reaction

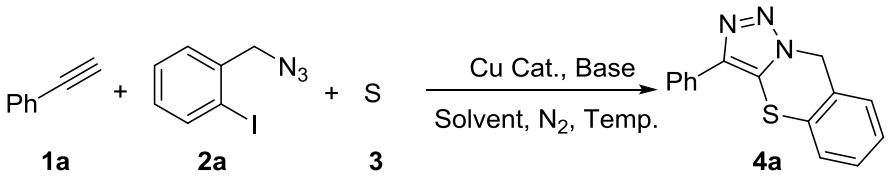


Entry	Cat. (10 mol%)	Base (2 equiv)	Solvent	Yield(%)[b] **8a:14**
1	CuI	K_2CO_3	DMF	35:50
2	CuBr	K_2CO_3	DMF	33:56
3	CuCl	K_2CO_3	DMF	30:46
4	CuSCN	K_2CO_3	DMF	44:32
5	CuCN	K_2CO_3	DMF	5:71
6	CuF_2	K_2CO_3	DMF	2:82
7	$CuCl_2$	K_2CO_3	DMF	3:79
8	$CuBr_2$	K_2CO_3	DMF	0:80
9	$CuSO_4$	K_2CO_3	DMF	10:65
10	$Cu(OAc)_2$	K_2CO_3	DMF	4:68
11	CuSCN	Cs_2CO_3	DMF	30:52
12	CuSCN	Na_2CO_3	DMF	15:60
13	CuSCN	$KHCO_3$	DMF	25:46
14	CuSCN	$NaHCO_3$	DMF	60:23
15	CuSCN	Et_3N	DMF	40:32
16	CuSCN	^{t}BuOLi	DMF	36:38
17	CuSCN	CH_3OLi	DMF	10:68
18	CuSCN	CaH	DMF	45:30
19	CuSCN	$NaHCO_3$	DMSO	63:0
20	CuSCN	$NaHCO_3$	DCE	5:85
21	CuSCN	$NaHCO_3$	THF	45:35
22	CuSCN	$NaHCO_3$	CH_3CN	48:39
23[c]	**CuSCN**	**$NaHCO_3$**	**DMSO**	**70:0**

f

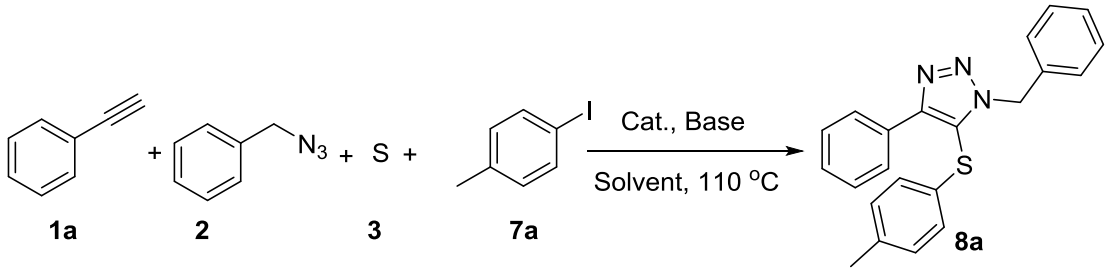
[a] Reaction conditions: 1a (0.2 mmol), 2a (0.3 mmol), 3 (0.4 mmol), 4a (0.4 mmol), CuI (10 mol%), base (0.4 mmol), DMSO (2 mL) was stirred at 100°C under N_2 atmosphere for 24 h. [b][aIsolated yield. [c] reaction at 110 °C

General procedure for thee-component interrupted click reaction



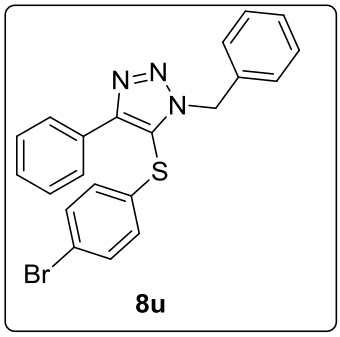
To a mixture of CuSCN (0.02 mmol), $NaHCO_3$(0.4 mmol) in DMSO (1 mL) under N_2 atmosphere, **1a** benzyl azide (0.3 mmol), **2a** phenylacetylene (0.2 mmol) and **3** S (0.4 mmol) were added. The system was stirred at 50 ^oC for 24 h. The reaction mixture was filtered and evaporated under reduced pressure and purified by column chromatography (petroleum ether: EtOAc = 5:1 to 10:1) to give **4a** (50 mg, 88% yield) as a yellow soild.

General procedure for the four-component interrupted click reaction

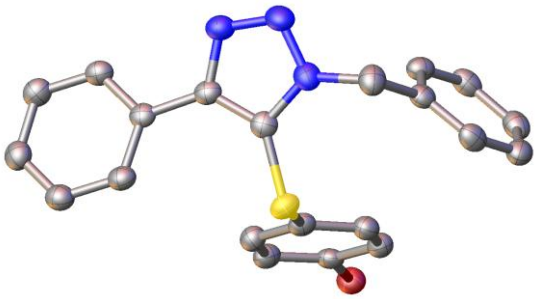


A 25 ml Schlenk tube equipped with a magnetic stirring bar was charged with **1a** benzyl azide (0.3 mmol), **2a** phenylacetylene (0.2 mmol), **3** S (0.4 mmol), **7a** (0.4 mmol) CuSCN (0.02 mmol), $NaHCO_3$(0.4 mmol) and DMSO (2 mL). The tube was sealed, and then the mixture was stirred under a nitrogen atmosphere at 110 ^oC for 24 h. After completion of the reaction, the resulting solution was cooled down to room temperature, and the solvent was removed with the aid of a rotary evaporator. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to provide the desired product **8a** (50 mg,70%) as a yellow soild.

X-ray Crystallography Data for 8u



8u



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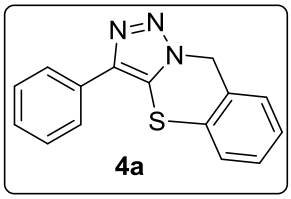
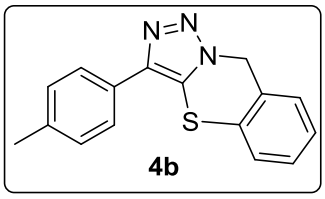
Characterization Data



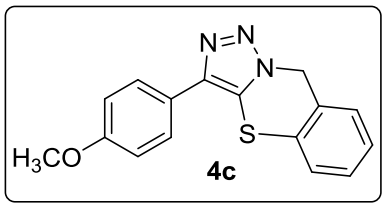
4a

3-(p-tolyl)-9H-benzo[e][1,2,3]triazolo[5,1-b][1,3]thiazine. Yellow soild. 50 mg, 88% yield. 86-87^{o}C, PE : EA = 7 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 – 7.87 (m, 2H), 7.51 – 7.42 (m, 3H), 7.41 – 7.30 (m, 4H), 5.55 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.50, 130.36, 130.32, 129.00, 128.98, 128.83, 128.28, 128.06, 127.76, 127.37, 126.35, 123.79, 50.32. HRMS exact mass calcd for $C_{15}H_{11}N_3S$ $[M+H]^+$ requires m/z 266.0746, found m/z 266.0749.



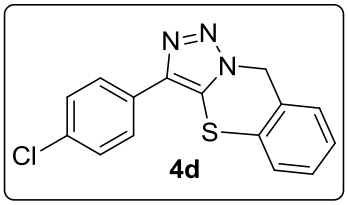
4b

3-(p-tolyl)-9H-benzo[e][1,2,3]triazolo[5,1-b][1,3]thiazine. Yellow soild. 46 mg, 82% yield. 90-91^{o}C, PE : EA = 7 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.2 Hz, 2H), 7.47 – 7.44 (m, 1H), 7.41 – 7.38 (m, 1H), 7.36 – 7.32 (m, 2H), 7.31 – 7.27 (m, 2H), 5.55 (s, 2H), 2.40 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.63, 137.95, 130.43, 129.51, 129.13, 128.97, 128.26, 127.71, 127.47, 127.37, 126.28, 123.32, 50.33, 21.36. HRMS exact mass calcd for $C_{16}H_{13}N_3S$ $[M+H]^+$ requires m/z 280.0903, found m/z 280.0910.



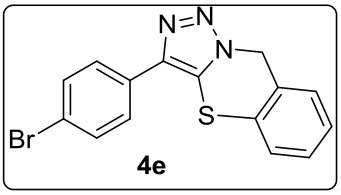
4c

3-(4-methoxyphenyl)-9H-benzo[e][1,2,3]triazolo[5,1-b][1,3]thiazine. Yellow soild. 49 mg, 83% yield. 80-81^{o}C, PE : EA = 6 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 – 7.80 (m, 2H), 7.47 – 7.43 (m, 1H), 7.42 – 7.38 (m, 1H), 7.36 – 7.32 (m, 2H), 7.04 – 6.99 (m, 2H), 5.55 (s, 2H), 3.86 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.48, 153.54, 142.44, 130.49, 129.19, 128.95, 128.26, 127.70, 127.37, 123.01, 122.71, 114.27, 55.36, 50.34. HRMS exact mass calcd for $C_{16}H_{13}N_3OS$ $[M+H]^+$ requires m/z 296.0852, found m/z 296.0853.



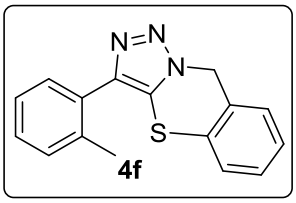
4d

3-(4-chlorophenyl)-9H-benzo[e][1,2,3]triazolo[5,1-b][1,3]thiazine. Yellow soild. 50 mg, 80% yield. 76-77°C, PE : EA = 6 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 – 7.79 (m, 2H), 7.44 (m, 3H), 7.41 – 7.37 (m, 1H), 7.37 – 7.32 (m, 2H), 5.54 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.36, 132.74, 129.20, 128.03, 127.97, 127.78, 127.61, 127.27, 126.84, 126.45, 126.34, 122.92, 49.27. HRMS exact mass calcd for $C_{15}H_{10}ClN_3S$ $[M+H]^+$ requires m/z 300.0357, found m/z 300.0358.



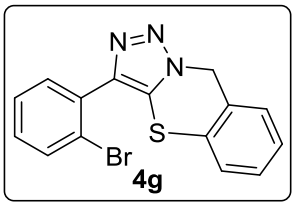
4e

3-(4-bromophenyl)-9H-benzo[e][1,2,3]triazolo[5,1-b][1,3]thiazine Yellow soild. 50 mg, 73% yield. 85-86°C, PE : EA = 6 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 – 7.75 (m, 2H), 7.62 – 7.57 (m, 2H), 7.49 – 7.44 (m, 1H), 7.43 – 7.39 (m, 1H), 7.38 – 7.33 (m, 2H), 5.55 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.46, 131.97, 130.27, 129.31, 129.09, 128.69, 128.31, 127.90, 127.79, 127.41, 124.02, 121.99, 50.33. HRMS exact mass calcd for $C_{15}H_{10}BrN_3S$ $[M+H]^+$ requires m/z 343.9852, found m/z 343.9857.



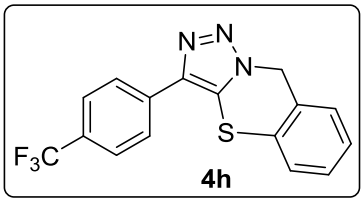
4f

3-(o-tolyl)-9H-benzo[e][1,2,3]triazolo[5,1-b][1,3]thiazine Yellow soild. 33 mg, 60% yield. 87-88°C, PE : EA = 6 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (m, 2H), 7.39 – 7.36 (m, 1H), 7.36 – 7.31 (m, 4H), 7.31 – 7.27 (m, 1H), 5.59 (s, 2H), 2.45 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.21, 136.25, 129.90, 129.47, 128.72, 128.20, 128.13, 127.90, 127.62, 127.25, 126.58, 126.35, 124.77, 124.10, 49.42, 19.55. HRMS exact mass calcd for $C_{16}H_{13}N_3S$ $[M+H]^+$ requires m/z 280.0903, found m/z 280.0908.



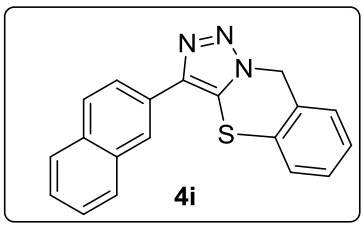
4g

3-(2-bromophenyl)-9H-benzo[e][1,2,3]triazolo[5,1-b][1,3]thiazine. Yellow soild. 43 mg, 62% yield. 75-76°C, PE : EA = 7 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.57 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.40 (dtd, *J* = 7.4, 3.9, 1.7 Hz, 3H), 7.35 – 7.27 (m, 3H), 5.58 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.96, 133.12, 132.04, 131.30, 130.93, 130.28, 129.83, 128.97, 128.15, 127.64, 127.51, 127.42, 126.61, 122.86, 50.74. HRMS exact mass calcd for $C_{15}H_{10}BrN_3S$ $[M+H]^+$ requires m/z 343.9852, found m/z 343.9858.



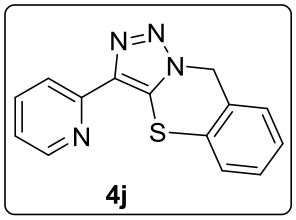
4h

3-(4-(trifluoromethyl)phenyl)-9H-benzo[e][1,2,3]triazolo[5,1-b][1,3]thiazine. Yellow soild. 49 mg, 73% yield. 79-80°C, PE : EA = 5 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.1 Hz, 2H), 7.72 (d, *J* = 8.1 Hz, 2H), 7.55 – 7.33 (m, 4H), 5.57 (s, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.57. ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.04, 133.82, 130.16, 129.86, 129.60, 129.15, 128.41, 128.35, 128.00, 127.41, 126.34, 125.79, 125.76, 125.21, 124.97, 123.04, 53.45, 50.32. HRMS exact mass calcd for $C_{16}H_{10}F_3N_3S$ $[M+H]^+$ requires m/z 334.0620, found m/z 334.0622.



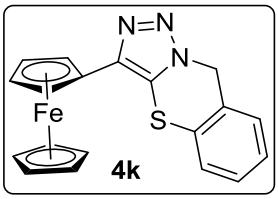
4i

3-(naphthalen-2-yl)-9H-benzo[e][1,2,3]triazolo[5,1-b][1,3]thiazine. Brown soild. 46 mg, 74% yield. 86-87°C, PE : EA = 8 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (d, *J* = 1.8 Hz, 1H), 8.10 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.86 (dd, *J* = 7.4, 1.8 Hz, 1H), 7.55 – 7.47 (m, 3H), 7.42 (dd, *J* = 6.2, 2.9 Hz, 1H), 7.39 – 7.33 (m, 2H), 5.59 (s, 2H).^{13}C NMR (126 MHz, $CDCl_3$) δ 141.49, 132.42, 131.93, 129.32, 128.00, 127.94, 127.54, 127.26, 127.24, 126.77, 126.37, 125.42, 125.25, 124.26, 124.23, 123.21, 123.03, 119.80, 49.32. HRMS exact mass calcd for $C_{19}H_{13}N_3S$ $[M+H]^+$ requires m/z 316.0903, found m/z 316.0902.



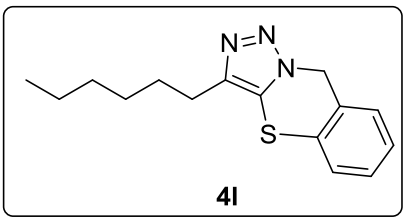
4j

3-(pyridin-2-yl)-9H-benzo[e][1,2,3]triazolo[5,1-b][1,3]thiazine. Brown soild. 27 mg, 50% yield. 56-57°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.16 – 9.08 (m, 1H), 8.60 (d, *J* = 4.9 Hz, 1H), 8.24 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.48 – 7.33 (m, 5H), 5.57 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.98, 146.34, 138.54, 132.45, 129.24, 128.14, 127.52, 127.33, 126.98, 126.45, 125.59, 123.73, 122.68, 52.43. HRMS exact mass calcd for $C_{14}H_{10}N_4S$ $[M+H]^+$ requires m/z 267.0699, found m/z 267.0701.



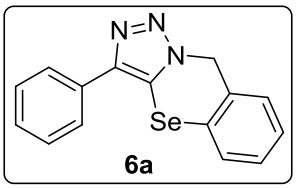
4k

Black soild. 53 mg, 71% yield. 65-66°C, PE : EA = 7 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 – 7.46 (m, 1H), 7.40 – 7.31 (m, 3H), 5.53 (s, 2H), 4.86 (t, *J* = 1.9 Hz, 2H), 4.33 (t, *J* = 1.8 Hz, 2H), 4.12 (s, 5H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.79, 130.10, 128.95, 128.90, 128.29, 127.58, 127.27, 122.15, 69.39, 68.70, 66.65, 50.15. HRMS exact mass calcd for $C_{19}H_{15}FeN_3S$ $[M+H]^+$ requires m/z 374.0409, found m/z 374.0414.



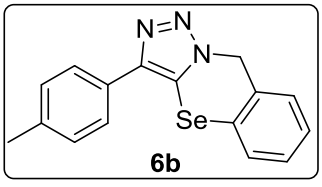
4l

3-hexyl-9H-benzo[e][1,2,3]triazolo[5,1-b][1,3]thiazine. Brown soild. 33 mg, 60% yield. 46-47°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (m, 1H), 7.38 – 7.28 (m, 3H), 5.47 (s, 2H), 2.77 – 2.61 (m, 2H), 1.78 – 1.67 (m, 2H), 1.40 – 1.28 (m, 6H), 0.88 (td, *J* = 5.9, 3.0 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.53, 130.59, 129.34, 128.79, 128.23, 127.40, 127.35, 123.61, 50.23, 31.51, 29.68, 28.89, 25.29, 22.54, 14.01. HRMS exact mass calcd for $C_{15}H_{19}N_3S$ $[M+H]^+$ requires m/z 274.1372, found m/z 274.1375.



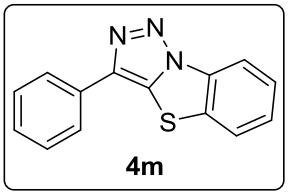
6a

3-phenyl-9H-benzo[e][1,2,3]triazolo[5,1-b][1,3]selenazine. Brown soild. 44 mg, 71% yield. 124-125°C, PE : EA = 7 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 – 7.83 (m, 2H), 7.57 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.50 – 7.42 (m, 3H), 7.39 – 7.29 (m, 3H), 5.51 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.99, 133.06, 130.67, 129.50, 129.14, 128.92, 128.81, 128.08, 128.05, 127.25, 126.39, 118.04, 52.40. HRMS exact mass calcd for $C_{15}H_{11}N_3Se$ $[M+H]^+$ requires m/z 314.0191, found m/z 314.0192.



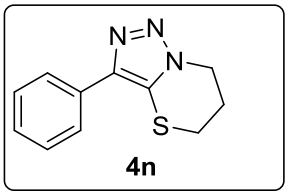
6b

(p-tolyl)-9H-benzo[e][1,2,3]triazolo[5,1-b][1,3]selenazine. Yellow soild. 50 mg, 76% yield. 120-121°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 – 7.71 (m, 2H), 7.57 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.43 (m, 1H), 7.36 – 7.27 (m, 4H), 5.50 (s, 2H), 2.40 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 145.10, 137.96, 133.10, 129.51, 129.49, 129.11, 128.92, 128.04, 127.80, 127.34, 126.31, 117.64, 52.40, 21.33. HRMS exact mass calcd for $C_{16}H_{13}N_3Se$ $[M+H]^+$ requires m/z 328.0347, found m/z 328.0350.



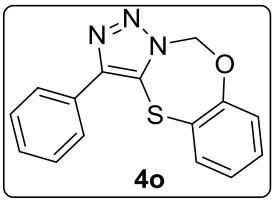
4m

3-phenylbenzo[4,5]thiazolo[3,2-c][1,2,3]triazole. Yellow soild. 33 mg, 65% yield. 99-100°C, PE : EA = 6 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (dt, *J* = 8.2, 1.4 Hz, 1H), 7.90 (ddt, *J* = 8.1, 3.0, 1.6 Hz, 2H), 7.81 (ddd, *J* = 8.1, 2.0, 1.2 Hz, 1H), 7.62 (ddt, *J* = 8.2, 7.3, 1.4 Hz, 1H), 7.56 – 7.50 (m, 3H), 7.37 (ddt, *J* = 7.5, 5.9, 1.3 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.51, 137.85, 133.15, 131.18, 130.05, 129.07, 127.91, 127.28, 127.21, 125.43, 124.73, 114.75. HRMS exact mass calcd for $C_{14}H_9N_3S$ $[M+H]^+$ requires m/z 252.0590, found m/z 252.0590.



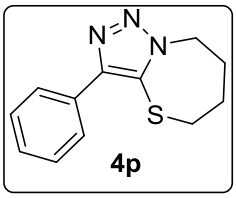
4n

3-phenyl-6,7-dihydro-5H-[1,2,3]triazolo[5,1-b][1,3]thiazine. Yellow soild. 50 mg, 95% yield. 79-80°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 – 7.65 (m, 2H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.31 – 7.27 (m, 1H), 3.90 (s, 2H), 3.70 (t, *J* = 6.8 Hz, 2H), 3.12 (t, *J* = 6.8 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.74, 140.89, 134.56, 128.81, 127.23, 126.93, 50.45, 33.04, 29.68. HRMS exact mass calcd for $C_{11}H_{11}N_3S$ $[M+H]^+$ requires m/z 218.0746, found m/z 218.0748.



4o

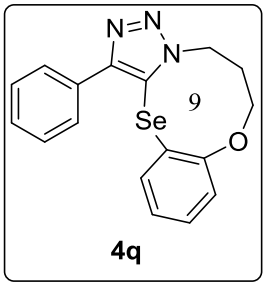
3-phenyl-10,10a-dihydrobenzo[2,3][1,4]oxathiepino[6,5-c]pyrazole. Yellow soild. 38 mg, 68% yield. 66-67°C, PE : EA = 7 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 – 7.78 (m, 2H), 7.59 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.46 – 7.42 (m, 3H), 7.41 – 7.27 (m, 3H), 5.51 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 133.30, 133.13, 132.86, 129.85, 128.82, 128.58, 128.00, 127.81, 127.23, 126.52, 126.40, 125.90, 55.06. HRMS exact mass calcd for $C_{15}H_{11}N_3OS$ $[M+H]^+$ requires m/z 282.0696, found m/z 282.0699.



4p

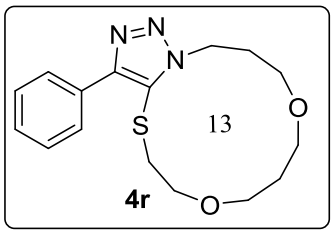
3-phenyl-5,6,7,8-tetrahydro-[1,2,3]triazolo[5,1-b][1,3]thiazepine. Yellow soild. 40 mg, 86% yield. 83-84°C, PE : EA = 5 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 – 7.70 (m, 2H), 7.48 – 7.45 (m, 1H), 7.41 – 7.38 (m, 2H), 3.89 (td, *J* = 7.2, 5.5 Hz, 2H), 3.40 (t, *J* = 6.6 Hz, 2H), 1.93 – 1.83 (m, 2H), 1.77 – 1.70 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.98, 131.08, 128.57, 128.55, 127.16, 126.56, 51.06, 46.06, 26.45, 25.49.

HRMS exact mass calcd for $C_{12}H_{13}N_3S$ $[M+H]^+$ requires m/z 232.0903, found m/z 232.0906.



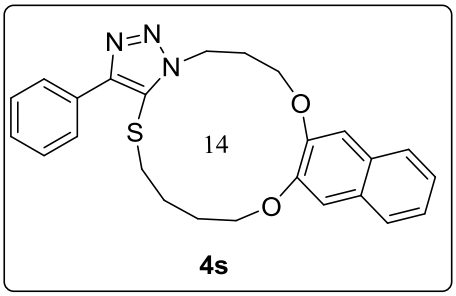
4q

1-phenyl-3a,4,5,6-tetrahydrobenzo[2,3][1,4]oxaselenonino[6,5-c]pyrazole. Yellow soild. 43 mg, 60% yield. 188-189°C, PE : EA = 4 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 – 7.77 (m, 3H), 7.40 (td, *J* = 7.6, 1.9 Hz, 2H), 7.33 – 7.26 (m, 2H), 6.81 – 6.70 (m, 2H), 4.75 (td, *J* = 6.7, 2.1 Hz, 2H), 4.02 (td, *J* = 5.6, 2.0 Hz, 2H), 2.50 (dq, *J* = 8.7, 5.6 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.81, 147.64, 139.51, 130.60, 129.70, 128.81, 128.12, 125.75, 123.11, 120.55, 112.27, 86.51, 64.98, 46.99, 29.72. HRMS exact mass calcd for $C_{17}H_{15}N_3OSe$ $[M+K]^+$ requires m/z 396.0012, found m/z 396.0018.



4r

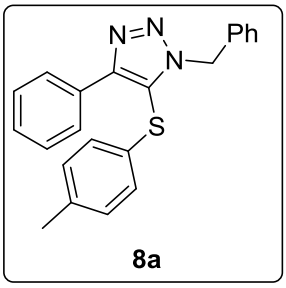
3-phenyl-5,6,9,10,13,14-hexahydro-8H,12H-[1,2,3]triazolo[5,1-e][1,10]dioxa[4]thia[6]azacyclotridecine. Yellow soild. 34 mg, 54% yield. 96-97°C, PE : EA = 1 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.72 (dd, *J* = 5.6, 3.0 Hz, 2H), 7.53 (dd, *J* = 5.7, 3.3 Hz, 1H), 4.30 (t, *J* = 6.7 Hz, 2H), 3.72 (t, *J* = 7.0 Hz, 2H), 3.33 (t, *J* = 6.8 Hz, 2H), 1.82 – 1.76 (m, 2H), 1.75 – 1.69 (m, 2H), 1.67 – 1.63 (m, 2H), 1.48 – 1.40 (m, 2H), 0.97 (d, *J* = 7.4 Hz, 2H).^{13}C NMR (126 MHz, $CDCl_3$) δ 168.42, 134.02, 132.06, 130.93, 128.85, 123.30, 65.59, 50.91, 37.30, 30.58, 26.26, 25.86, 19.20, 13.75. HRMS exact mass calcd for $C_{16}H_{21}N_3O_2S$ $[M+H]^+$ requires m/z 320.1427, found m/z 320.1435.



4s

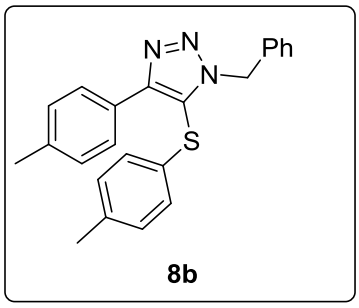
phenyl-6,7,17,18-tetrahydro-5H,16H-naphtho[2,3-b][1,2,3]triazolo[5,1-i][1,4]dioxa[8]thia[10]azacyclotridecine. Yellow soild. 35 mg, 40% yield. 90-91°C, PE : EA = 1 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 – 7.77 (m, 3H), 7.71 (dd, *J* = 5.7, 3.3 Hz, 1H), 7.53 (dd, *J* = 5.7, 3.3 Hz, 1H), 7.40 (dd, *J* = 8.4, 7.0 Hz, 2H), 7.34 – 7.26 (m, 2H),

6.75 (m, 2H), 4.76 (t, *J* = 6.7 Hz, 2H), 4.31 (t, *J* = 6.7 Hz, 2H), 4.02 (t, *J* = 5.7 Hz, 2H), 2.55 – 2.46 (m, 2H), 1.80 – 1.67 (m, 2H), 1.48 – 1.41 (m, 2H), 0.96 (d, *J* = 7.4 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.52, 130.87, 129.69, 128.84, 128.80, 128.11, 125.74, 123.11, 120.52, 112.26, 86.50, 65.54, 64.97, 46.97, 30.59, 29.72, 19.18, 13.69. HRMS exact mass calcd for $C_{25}H_{25}N_3O_2S$ $[M+H]^+$ requires m/z 432.1740, found m/z 432.1750.



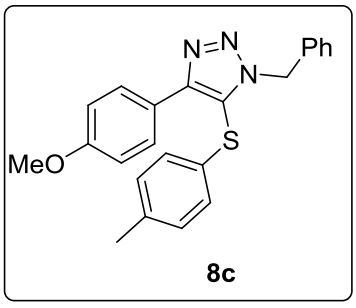
8a

1-benzyl-4-phenyl-5-(p-tolylthio)-1H-1,2,3-triazole.[1,2] Yellow soild. 50 mg, 70% yield. 140-141°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 – 8.06 (m, 2H), 7.42 – 7.38 (m, 2H), 7.36 – 7.33 (m, 1H), 7.23 (s, 5H), 6.95 (d, *J* = 8.1 Hz, 2H), 6.83 – 6.77 (m, 2H), 5.58 (s, 2H), 2.25 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.49, 135.76, 133.62, 129.21, 129.19, 128.87, 127.62, 127.59, 127.50, 127.11, 126.97, 126.04, 125.94, 122.05, 51.20, 19.84. HRMS exact mass calcd for $C_{22}H_{19}N_3S$ $[M+H]^+$ requires m/z 358.1372, found m/z 358.1385.



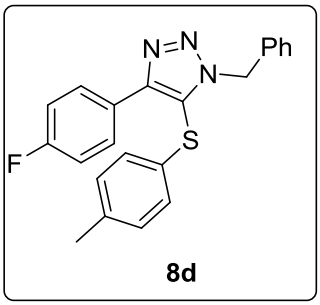
8b

1-benzyl-4-(p-tolyl)-5-(p-tolylthio)-1H-1,2,3-triazole.[1,2] Yellow soild. 53 mg, 72% yield. 149-150°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.2 Hz, 2H), 7.23 (s, 5H), 7.20 (d, *J* = 8.2 Hz, 2H), 6.95 (d, *J* = 8.1 Hz, 2H), 6.79 (d, *J* = 8.3 Hz, 2H), 5.56 (s, 2H), 2.36 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.57, 136.70, 134.69, 130.20, 130.04, 129.28, 128.65, 128.13, 128.10, 128.02, 127.36, 126.93, 126.86, 122.58, 52.22, 21.35, 20.91. HRMS exact mass calcd for $C_{23}H_{21}N_3S$ $[M+H]^+$ requires m/z 372.1529, found m/z 372.1530.



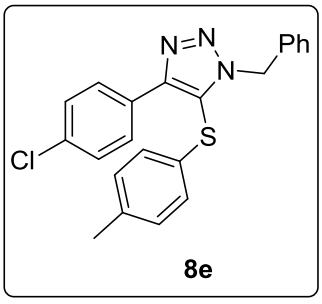
8c

1-benzyl-4-(4-methoxyphenyl)-5-(p-tolylthio)-1H-1,2,3-triazole.[1,2] Yellow soild. 56 mg, 73% yield. 176-177°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.9 Hz, 2H), 7.22 (s, 5H), 6.97 – 6.91 (m, 4H), 6.81 – 6.77 (m, 2H), 5.56 (s, 2H), 3.82 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.98, 150.49, 136.68, 134.75, 130.19, 130.11, 128.63, 128.40, 128.10, 128.00, 126.83, 122.90, 122.01, 114.00, 55.25, 52.20, 20.86. HRMS exact mass calcd for $C_{23}H_{21}N_3OS$ $[M+H]^+$ requires m/z 388.1478, found m/z 388.1472.



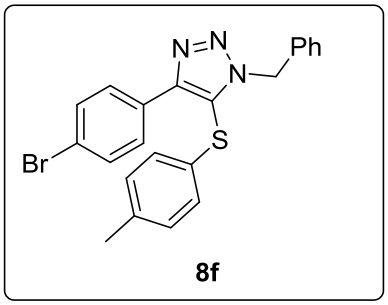
8d

1-benzyl-4-(4-fluorophenyl)-5-(p-tolylthio)-1H-1,2,3-triazole. Yellow soild. 37 mg, 60% yield. 170-171°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 – 8.03 (m, 2H), 7.23 (s, 5H), 7.10 – 7.05 (m, 2H), 6.98 – 6.93 (m, 2H), 6.82 – 6.72 (m, 2H), 5.57 (s, 2H), 2.25 (s, 3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -112.69. ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.98, 162.01, 149.69, 136.93, 134.54, 130.28, 129.64, 128.94, 128.88, 128.70, 128.23, 128.04, 126.88, 126.39, 126.37, 122.86, 115.66, 115.49, 52.31, 20.91. HRMS exact mass calcd for $C_{22}H_{18}FN_3S$ $[M+H]^+$ requires m/z 376.1278, found m/z 376.1289.



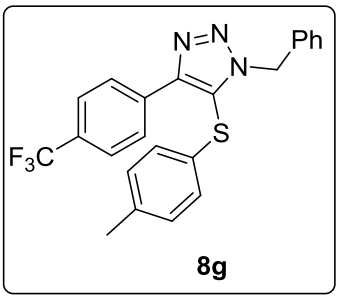
8e

1-benzyl-4-(4-chlorophenyl)-5-(p-tolylthio)-1H-1,2,3-triazole.[1] Yellow soild. 51 mg, 65% yield. 134-135°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 – 8.01 (m, 2H), 7.38 – 7.34 (m, 2H), 7.24 (s, 5H), 6.95 (d, *J* = 8.1 Hz, 2H), 6.81 – 6.73 (m, 2H), 5.57 (s, 2H), 2.25 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.03, 149.38, 137.02, 134.60, 134.49, 130.31, 129.49, 128.80, 128.72, 128.26, 128.13, 128.06, 126.96, 123.30, 52.32, 20.92. HRMS exact mass calcd for $C_{22}H_{18}ClN_3S$ $[M+H]^+$ requires m/z 392.0983, found m/z 392.0988.



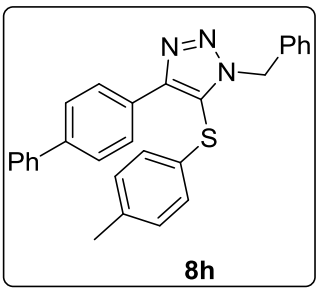
8f

1-benzyl-4-(4-bromophenyl)-5-(p-tolylthio)-1H-1,2,3-triazole.[2] Yellow soild. 59 mg, 68% yield. 145-146°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 – 7.94 (m, 2H), 7.54 – 7.49 (m, 2H), 7.26 – 7.21 (m, 5H), 6.95 (d, *J* = 8.0 Hz, 2H), 6.81 – 6.73 (m, 2H), 5.57 (s, 2H), 2.25 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.39, 137.04, 134.47, 131.75, 130.32, 129.45, 129.16, 128.72, 128.52, 128.26, 128.06, 126.97, 123.35, 122.91, 52.32, 20.92. HRMS exact mass calcd for $C_{22}H_{18}BrN_3S$ $[M+H]^+$ requires m/z 436.0478, found m/z 436.0467.



8g

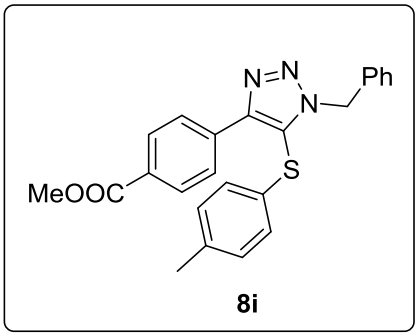
1-benzyl-5-(p-tolylthio)-4-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazole. Yellow soild. 56 mg, 66% yield. 207-208°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.2 Hz, 2H), 7.64 (d, *J* = 8.3 Hz, 2H), 7.25 (s, 5H), 6.96 (d, *J* = 8.1 Hz, 2H), 6.83 – 6.72 (m, 2H), 5.59 (s, 2H), 2.25 (s, 3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.69. ^{13}C NMR (126 MHz, $CDCl_3$) δ 148.93, 137.19, 134.37, 133.66, 130.49, 130.37, 129.25, 128.75, 128.32, 128.08, 127.16, 127.02, 125.56, 125.53, 125.50, 125.47, 124.21, 52.38, 29.72, 20.91. HRMS exact mass calcd for $C_{23}H_{18}F_3N_3S$ $[M+H]^+$ requires m/z 426.1246, found m/z 426.1248.



8h

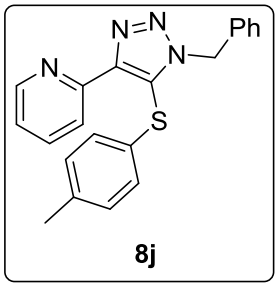
4-([1,1'-biphenyl]-4-yl)-1-benzyl-5-(p-tolylthio)-1H-1,2,3-triazole. Yellow soild. 61 mg, 71% yield. 140-141°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 – 8.16 (m, 2H), 7.68 – 7.60 (m, 4H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.25 (d, *J* = 8.1 Hz, 5H), 6.97 (d, *J* = 8.0 Hz, 2H), 6.85 – 6.81 (m, 2H), 5.59 (s, 2H), 2.26 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.20, 141.27, 140.56, 136.84, 134.63,

130.28, 129.87, 129.18, 128.82, 128.70, 128.19, 128.04, 127.49, 127.37, 127.24, 127.04, 126.94, 123.05, 52.28, 20.93. HRMS exact mass calcd for $C_{28}H_{23}N_3S$ $[M+H]^+$ requires m/z 434.1685, found m/z 434.1680.



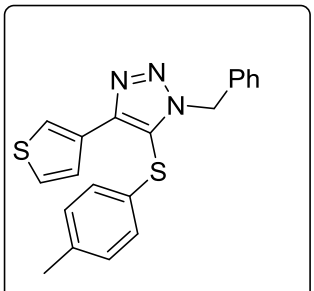
8i

methyl 4-(1-benzyl-5-(p-tolylthio)-1H-1,2,3-triazol-4-yl)benzoate. Yellow soild. 55 mg, 66% yield. 189-190°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 – 8.16 (m, 2H), 8.08 – 8.03 (m, 2H), 7.24 (s, 5H), 6.95 (d, *J* = 8.0 Hz, 2H), 6.83 – 6.76 (m, 2H), 5.59 (s, 2H), 3.91 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.79, 148.17, 136.11, 133.51, 133.41, 129.30, 128.87, 128.81, 128.28, 127.71, 127.25, 127.01, 126.11, 125.75, 123.29, 51.31, 51.13, 19.88. HRMS exact mass calcd for $C_{24}H_{21}N_3O_2S$ $[M+H]^+$ requires m/z 416.1427, found m/z 416.1422.



8j

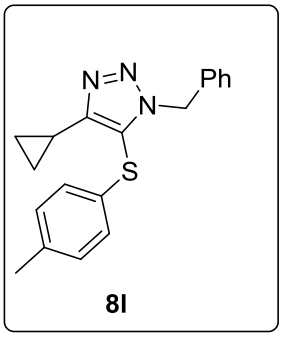
2-(1-benzyl-5-(p-tolylthio)-1H-1,2,3-triazol-4-yl)pyridine. White soild. 44 mg, 61% yield. 135-136°C, PE : EA = 5 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (m, 1H), 8.10 (m, 1H), 7.73 (m, 1H), 7.26 – 7.15 (m, 6H), 7.02 – 6.80 (m, 4H), 5.58 (s, 2H), 2.24 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.85, 149.75, 149.68, 137.11, 136.45, 134.59, 130.05, 129.70, 128.68, 128.33, 128.17, 127.93, 126.13, 123.03, 122.22, 52.28, 20.95. HRMS exact mass calcd for $C_{21}H_{18}N_4S$ $[M+H]^+$ requires m/z 359.1325, found m/z 359.1335.



8k

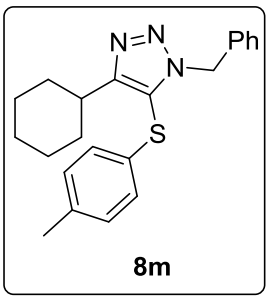
1-benzyl-4-(thiophen-3-yl)-5-(p-tolylthio)-1H-1,2,3-triazole. Yellow soild. 44 mg, 61% yield. 105-106°C, PE : EA = 15 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (dd, *J* =

3.0, 1.2 Hz, 1H), 7.82 (dd, *J* = 5.1, 1.2 Hz, 1H), 7.34 (dd, *J* = 5.1, 3.0 Hz, 1H), 7.22 (p, *J* = 1.7 Hz, 5H), 6.97 – 6.94 (m, 2H), 6.83 – 6.77 (m, 2H), 5.57 (s, 2H), 2.25 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.57, 136.87, 134.63, 131.12, 130.27, 129.62, 128.68, 128.18, 127.96, 126.90, 126.43, 125.78, 123.09, 122.41, 52.24, 20.92. HRMS exact mass calcd for $C_{20}H_{17}N_3S_2$ $[M+H]^+$ requires m/z 364.0937, found m/z 364.0936.



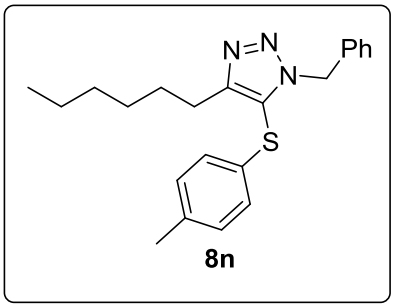
8l

1-benzyl-4-cyclopropyl-5-(p-tolylthio)-1H-1,2,3-triazole. Yellow oil. 57 mg, 58% yield. PE : EA = 15 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 – 7.14 (m, 5H), 6.97 (d, *J* = 8.0 Hz, 2H), 6.85 – 6.80 (m, 2H), 5.47 (s, 2H), 2.26 (s, 3H), 1.99 – 1.90 (m, 1H), 1.13 – 1.06 (m, 2H), 0.94 – 0.89 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.31, 136.74, 134.88, 130.06, 128.61, 128.05, 127.96, 127.45, 127.44, 123.78, 52.12, 20.91, 8.01, 7.98, 6.69. HRMS exact mass calcd for $C_{19}H_{19}N_3S$ $[M+H]^+$ requires m/z 322.1372, found m/z 322.1370.



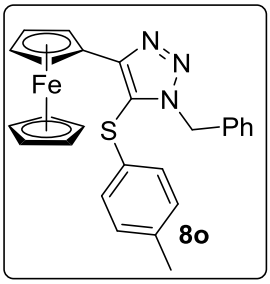
8m

1-benzyl-4-cyclohexyl-5-(p-tolylthio)-1H-1,2,3-triazole. Yellow soild. 46 mg, 63% yield. 76-77^{o}C, PE : EA = 15 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25 – 7.17 (m, 5H), 6.99 – 6.93 (m, 2H), 6.76 (d, *J* = 8.2 Hz, 2H), 5.49 (s, 2H), 2.71 – 2.65 (m, 2H), 2.27 (s, 3H), 1.66 – 1.60 (m, 3H), 1.37 – 1.24 (m, 3H), 0.87 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.35, 136.77, 134.85, 130.26, 130.04, 128.63, 128.07, 127.98, 127.38, 124.02, 52.23, 31.19, 25.14, 22.43, 20.90, 13.77. HRMS exact mass calcd for $C_{22}H_{25}N_3S$ $[M+H]^+$ requires m/z 364.1842, found m/z 364.1844.



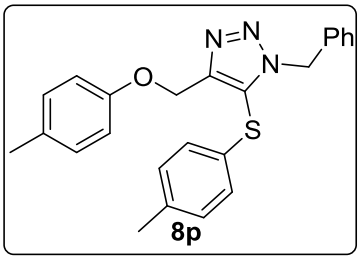
8n

1-benzyl-4-hexyl-5-(p-tolylthio)-1H-1,2,3-triazole. Yellow oil. 60 mg, 63% yield. PE : EA = 15 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25 – 7.16 (m, 5H), 6.96 (d, *J* = 7.9 Hz, 2H), 6.78 – 6.73 (m, 2H), 5.49 (s, 2H), 2.73 – 2.60 (m, 2H), 2.26 (s, 3H), 1.68 – 1.59 (m, 3H), 1.28 – 1.20 (m, 6H), 0.84 (d, *J* = 3.8 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.33, 136.78, 134.89, 133.23, 130.03, 128.62, 128.06, 127.96, 127.44, 124.07, 52.22, 31.48, 29.00, 28.98, 25.45, 22.49, 20.87, 14.00. HRMS exact mass calcd for $C_{22}H_{27}N_3S$ $[M+H]^+$ requires m/z 366.1998, found m/z 366.1993.



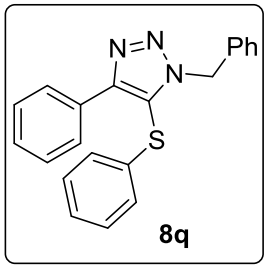
8o

Colorless soild. 65 mg, 70% yield. 66-67°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 (td, *J* = 4.3, 2.1 Hz, 3H), 7.01 (dd, *J* = 14.9, 8.1 Hz, 3H), 6.86 – 6.82 (m, 2H), 6.76 (s, 1H), 5.54 (s, 2H), 5.01 (t, *J* = 1.9 Hz, 2H), 4.28 (t, *J* = 1.9 Hz, 2H), 3.98 (s, 5H), 2.27 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.34, 136.65, 134.81, 130.19, 130.01, 128.65, 128.10, 127.88, 126.72, 115.20, 69.49, 69.02, 67.23, 52.11, 20.87. HRMS exact mass calcd for $C_{26}H_{23}FeN_3S$ $[M+H]^+$ requires m/z 466.1035, found m/z 466.1025



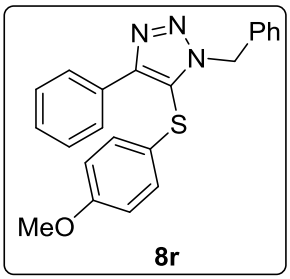
8p

1-benzyl-4-((p-tolyloxy)methyl)-5-(p-tolylthio)-1H-1,2,3-triazole. Yellow soild. 57 mg, 71% yield. 155-156°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27 – 7.23 (m, 3H), 7.20 (d, *J* = 1.9 Hz, 2H), 7.06 (d, *J* = 8.3 Hz, 2H), 6.97 (d, *J* = 8.2 Hz, 2H), 6.91 (d, *J* = 8.3 Hz, 2H), 6.86 (d, *J* = 8.6 Hz, 2H), 5.53 (s, 2H), 5.11 (s, 2H), 2.29 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.21, 146.94, 136.47, 133.34, 129.37, 129.08, 128.97, 128.78, 127.65, 127.18, 126.98, 126.94, 114.11, 113.82, 60.00, 51.31, 19.92, 19.46. HRMS exact mass calcd for $C_{24}H_{23}N_3OS$ $[M+H]^+$ requires m/z 402.1635, found m/z 402.1652.



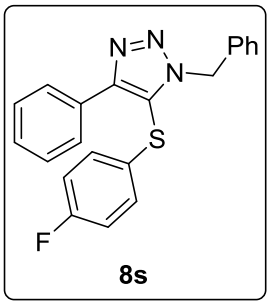
8q

1-benzyl-4-phenyl-5-(phenylthio)-1H-1,2,3-triazole.[1,2] Yellow soild. 47mg, 69% yield. 102-103°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 – 8.03 (m, 2H), 7.40 – 7.31 (m, 3H), 7.25 – 7.18 (m, 5H), 7.18 – 7.06 (m, 3H), 6.90 – 6.84 (m, 2H), 5.57 (s, 2H).^{13}C NMR (126 MHz, $CDCl_3$) δ 150.81, 134.52, 133.57, 130.14, 129.47, 128.71, 128.68, 128.58, 128.26, 128.06, 127.06, 126.63, 126.54, 122.44, 52.34. HRMS exact mass calcd for $C_{21}H_{17}N_3S$ $[M+H]^+$ requires m/z 344.1216, found m/z 344.1218.



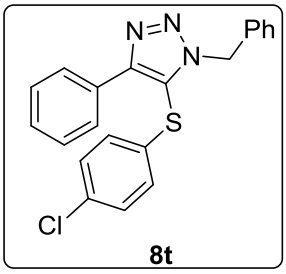
8r

1-benzyl-5-((4-methoxyphenyl)thio)-4-phenyl-1H-1,2,3-triazole. Yellow soild. 54 mg, 72% yield. 100-101°C, PE : EA = 15 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 – 7.99 (m, 2H), 7.36 – 7.32 (m, 2H), 7.30 – 7.27 (m, 1H), 7.15 (m, 5H), 6.82 – 6.77 (m, 2H), 6.61 – 6.57 (m, 2H), 5.52 (s, 2H), 3.65 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.97, 149.14, 133.69, 129.25, 128.43, 127.65, 127.57, 127.51, 127.13, 126.87, 126.10, 123.04, 122.69, 114.10, 54.33, 51.17. HRMS exact mass calcd for $C_{22}H_{19}N_3OS$ $[M+H]^+$ requires m/z 374.1322, found m/z 374.1324.



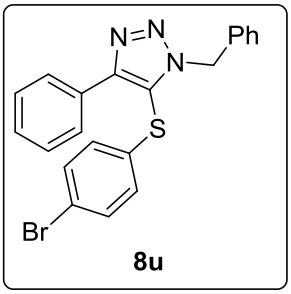
8s

1-benzyl-5-((4-fluorophenyl)thio)-4-phenyl-1H-1,2,3-triazole. Yellow soild. 43 mg, 60% yield. 136-137°C, PE : EA = 15 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 – 8.02 (m, 2H), 7.42 – 7.38 (m, 2H), 7.37 – 7.34 (m, 1H), 7.21 (qd, *J* = 4.5, 2.8 Hz, 5H), 6.83 – 6.75 (m, 4H), 5.61 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.73, 160.77, 150.68, 134.43, 130.03, 128.84, 128.80, 128.78, 128.71, 128.61, 128.38, 128.28, 127.94, 127.04, 122.78, 116.66, 116.48, 52.39. HRMS exact mass calcd for $C_{21}H_{16}FN_3S$ $[M+H]^+$ requires m/z 362.1122, found m/z 362.1133.



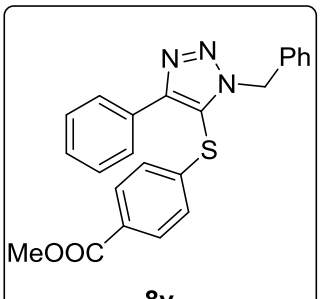
8t

1-benzyl-5-((4-chlorophenyl)thio)-4-phenyl-1H-1,2,3-triazole. Yellow soild. 51 mg, 68% yield. 179-180°C, PE : EA = 15 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 – 8.00 (m, 2H), 7.41 – 7.34 (m, 3H), 7.24 – 7.18 (m, 5H), 7.08 – 7.03 (m, 2H), 6.81 – 6.70 (m, 2H), 5.60 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.97, 134.29, 132.69, 131.96, 129.93, 129.50, 128.87, 128.72, 128.65, 128.29, 128.00, 127.70, 126.99, 121.88, 52.47. HRMS exact mass calcd for $C_{21}H_{16}ClN_3S$ $[M+H]^+$ requires m/z 378.0826, found m/z 378.0824.



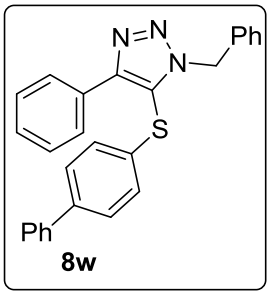
8u

1-benzyl-5-((4-bromophenyl)thio)-4-phenyl-1H-1,2,3-triazole Yellow soild. 55 mg, 65% yield. 215-216°C, PE : EA = 15 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 – 8.01 (m, 2H), 7.42 – 7.34 (m, 3H), 7.26 – 7.15 (m, 7H), 6.71 – 6.61 (m, 2H), 5.60 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.01, 134.28, 132.68, 132.40, 129.93, 128.87, 128.72, 128.64, 128.28, 127.99, 127.91, 126.99, 121.70, 120.51, 52.47. HRMS exact mass calcd for $C_{21}H_{16}BrN_3S$ $[M+H]^+$ requires m/z 422.0321, found m/z 422.0333.



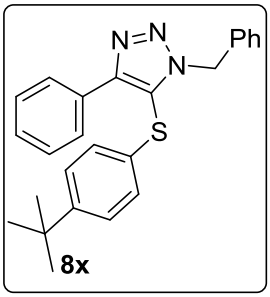
8v

methyl 4-((1-benzyl-4-phenyl-1H-1,2,3-triazol-5-yl)thio)benzoate. Yellow soild. 57 mg, 72% yield. 152-153°C, PE : EA = 15 : 1. Colorless oil. 51.5 mg, 83% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 – 7.97 (m, 2H), 7.78 – 7.72 (m, 2H), 7.39 – 7.33 (m, 3H), 7.24 – 7.15 (m, 5H), 6.86 – 6.78 (m, 2H), 5.60 (s, 2H), 3.88 (s, 3H).^{13}C NMR (126 MHz, $CDCl_3$) δ 165.25, 150.29, 138.71, 133.08, 129.41, 128.73, 127.92, 127.68, 127.64, 127.36, 127.07, 125.90, 124.27, 119.69, 114.59, 51.58, 51.19. HRMS exact mass calcd for $C_{23}H_{19}N_3O_2S$ $[M+H]^+$ requires m/z 402.1271, found m/z 402.1277.



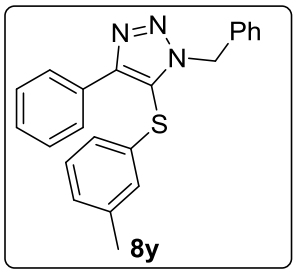
8w

5-([1,1'-biphenyl]-4-ylthio)-1-benzyl-4-phenyl-1H-1,2,3-triazole. Brown soild. 52 mg, 62% yield. 126-127°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 – 8.06 (m, 2H), 7.47 – 7.43 (m, 2H), 7.38 (ddd, *J* = 7.9, 6.8, 1.9 Hz, 4H), 7.35 – 7.28 (m, 4H), 7.24 – 7.12 (m, 5H), 6.93 – 6.84 (m, 2H), 5.59 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.91, 139.96, 139.73, 134.53, 132.48, 130.22, 128.91, 128.78, 128.69, 128.65, 128.21, 128.10, 127.64, 127.11, 126.99, 126.97, 126.86, 122.41, 52.41. HRMS exact mass calcd for $C_{27}H_{21}N_3S$ $[M+H]^+$ requires m/z 420.1529, found m/z 420.1548.



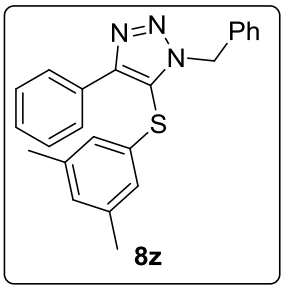
8x

1-benzyl-5-((4-(tert-butyl)phenyl)thio)-4-phenyl-1H-1,2,3-triazole. Brown soild. 52 mg, 65% yield. 156-157°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 – 8.06 (m, 2H), 7.39 (dd, *J* = 8.3, 6.6 Hz, 2H), 7.33 (t, *J* = 7.3 Hz, 1H), 7.18 (s, 5H), 7.15 – 7.10 (m, 2H), 6.82 – 6.78 (m, 2H), 5.57 (s, 2H), 1.23 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.72, 150.00, 134.58, 130.27, 129.93, 128.66, 128.60, 128.58, 128.16, 128.03, 127.12, 126.66, 126.53, 114.97, 52.27, 34.45, 31.20. HRMS exact mass calcd for $C_{25}H_{25}N_3S$ $[M+H]^+$ requires m/z 400.1842, found m/z 400.1845.



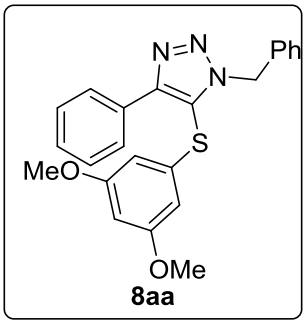
8y

1-benzyl-4-phenyl-5-(m-tolylthio)-1H-1,2,3-triazole. Brown soild. 44 mg, 61% yield. 120-121°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 – 8.03 (m, 2H), 7.41 – 7.37 (m, 2H), 7.36 – 7.34 (m, 1H), 7.23 (q, *J* = 3.1 Hz, 5H), 7.04 (t, *J* = 7.7 Hz, 1H), 6.94 – 6.89 (m, 1H), 6.73 – 6.69 (m, 1H), 6.59 (d, *J* = 1.9 Hz, 1H), 5.58 (s, 2H), 2.14 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.79, 139.51, 134.53, 133.29, 130.17, 129.27, 128.68, 128.62, 128.57, 128.24, 128.08, 127.52, 127.07, 126.93, 123.59, 122.52, 52.32, 21.31. HRMS exact mass calcd for $C_{22}H_{19}N_3S$ $[M+H]^+$ requires m/z 358.1372, found m/z 358.1375.



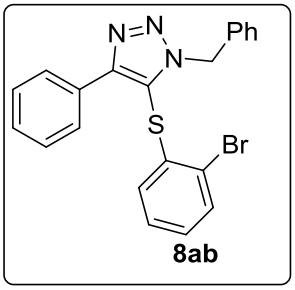
8z

1-benzyl-5-((3,5-dimethylphenyl)thio)-4-phenyl-1H-1,2,3-triazole. Yellow soild. 45 mg, 60% yield. 143-144°C, PE : EA = 15 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 – 8.04 (m, 2H), 7.44 – 7.39 (m, 2H), 7.39 – 7.34 (m, 1H), 7.25 (m, 5H), 6.78 – 6.72 (m, 1H), 6.48 (d, *J* = 1.5 Hz, 2H), 5.60 (s, 2H), 2.14 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.75, 139.26, 134.58, 134.51, 133.06, 130.24, 128.64, 128.56, 128.54, 128.23, 128.12, 127.12, 124.09, 122.66, 52.29, 21.19. HRMS exact mass calcd for $C_{23}H_{21}N_3S$ $[M+H]^+$ requires m/z 372.1529, found m/z 372.1530.



8aa

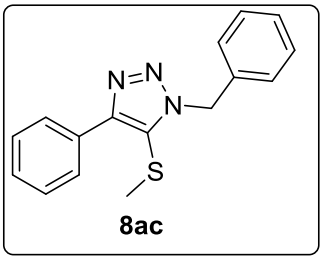
1-benzyl-5-((3,5-dimethoxyphenyl)thio)-4-phenyl-1H-1,2,3-triazole. Yellow soild. 50 mg, 62% yield. 230-231°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 – 8.02 (m, 2H), 7.41 – 7.35 (m, 3H), 7.27 – 7.22 (m, 5H), 6.19 (t, *J* = 2.2 Hz, 1H), 6.00 (d, *J* = 2.2 Hz, 2H), 5.59 (s, 2H), 3.59 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.33, 151.00, 135.48, 134.55, 130.14, 128.72, 128.62, 128.59, 128.24, 128.08, 127.13, 122.13, 104.45, 99.06, 55.29, 52.34. HRMS exact mass calcd for $C_{23}H_{21}N_3O_2S$ $[M+H]^+$ requires m/z 404.1427, found m/z 404.1425.



8ab

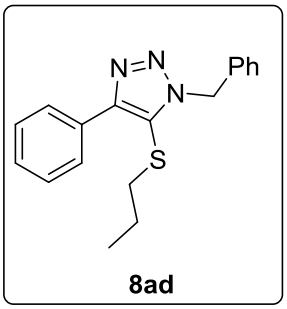
1-benzyl-5-((2-bromophenyl)thio)-4-phenyl-1H-1,2,3-triazole. Yellow soild. 52 mg, 62% yield. 130-131°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 – 7.91 (m, 2H), 7.41 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.33 – 7.25 (m, 3H), 7.19 – 7.17 (m, 2H), 7.10 – 7.05 (m, 3H), 6.84 (dd, *J* = 7.7, 1.6 Hz, 1H), 6.76 (dd, *J* = 7.8, 1.4 Hz, 1H), 6.06 (dd, *J* = 8.0, 1.5 Hz, 1H), 5.52 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.38, 138.56, 133.77, 132.94, 132.01, 128.75, 127.86, 127.64, 127.57, 127.27, 127.08, 126.26,

125.82, 125.23, 120.38, 119.22, 51.58. HRMS exact mass calcd for $C_{21}H_{16}BrN_3S$ $[M+H]^+$ requires m/z 422.0321, found m/z 422.0323.



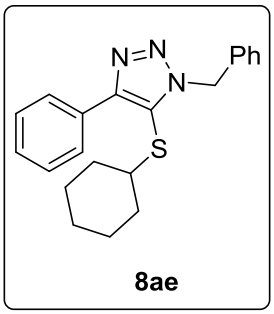
8ac

1-benzyl-5-(methylthio)-4-phenyl-1H-1,2,3-triazole. Yellow soild. 34 mg, 60% yield. 50-51°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 – 7.98 (m, 2H), 7.39 – 7.35 (m, 2H), 7.31 – 7.26 (m, 6H), 5.62 (s, 2H), 1.87 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 148.75, 135.40, 130.69, 128.90, 128.62, 128.52, 128.43, 128.32, 127.81, 126.74, 52.12, 18.47. HRMS exact mass calcd for $C_{16}H_{15}N_3S$ $[M+H]^+$ requires m/z 282.1059, found m/z 282.1063.



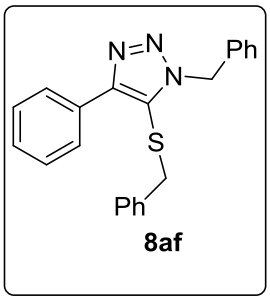
8ad

1-benzyl-4-phenyl-5-(propylthio)-1H-1,2,3-triazole. Yellow oil. 48 mg, 77% yield. PE : EA = 20 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 – 8.10 (m, 2H), 7.47 – 7.42 (m, 2H), 7.40 – 7.28 (m, 6H), 5.70 (s, 2H), 2.38 – 2.28 (m, 2H), 1.34 – 1.30 (m, 2H), 0.76 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 134.38, 129.73, 127.82, 127.55, 127.50, 127.34, 127.26, 126.73, 125.86, 124.70, 50.98, 36.81, 21.54, 11.99. HRMS exact mass calcd for $C_{18}H_{19}N_3S$ $[M+H]^+$ requires m/z 310.1372, found m/z 310.1374.



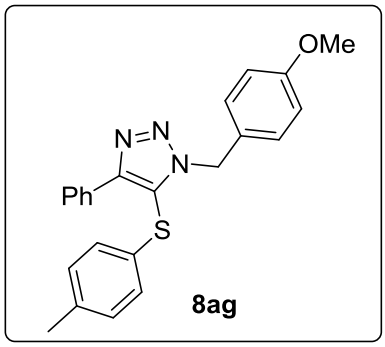
8ae

1-benzyl-5-(cyclohexylthio)-4-phenyl-1H-1,2,3-triazole. Yellow soild. 38 mg, 65% yield. 115-116°C, PE : EA = 20 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 – 8.16 (m, 2H), 7.43 (dd, *J* = 8.3, 6.8 Hz, 2H), 7.38 – 7.30 (m, 6H), 5.70 (s, 2H), 1.57 (s, 10H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.59, 135.53, 130.95, 128.82, 128.43, 128.29, 128.27, 127.78, 127.04, 124.95, 51.97, 49.04, 33.07, 25.73, 25.26. HRMS exact mass calcd for $C_{21}H_{23}N_3S$ $[M+H]^+$ requires m/z 350.1685, found m/z 350.1682.



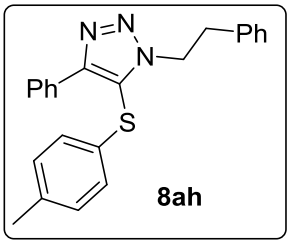
8af

1-**benzyl-5-(benzylthio)-4-phenyl-1H-1,2,3-triazole.** Brown soild. 42 mg, 59% yield. 75-76°C, PE : EA = 7 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 – 8.08 (m, 2H), 7.46 – 7.41 (m, 2H), 7.38 – 7.28 (m, 4H), 7.26 – 7.23 (m, 2H), 7.20 – 7.14 (m, 3H), 6.86 (dd, *J* = 7.6, 2.0 Hz, 2H), 5.24 (s, 2H), 3.55 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.57, 136.05, 135.33, 130.66, 128.84, 128.76, 128.69, 128.56, 128.44, 128.28, 127.85, 127.82, 126.83, 124.53, 51.64, 40.13. HRMS exact mass calcd for $C_{22}H_{19}N_3S$ $[M+H]^+$ requires m/z 358.1372, found m/z 358.1372.



8ag

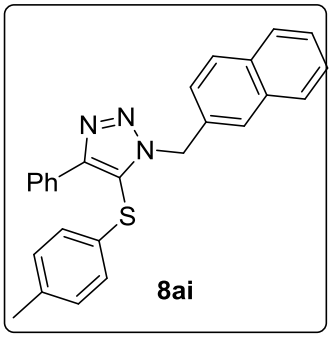
1-(4-methoxybenzyl)-4-phenyl-5-(p-tolylthio)-1H-1,2,3-triazole. Brown soild. 42 mg, 63% yield. 75-76°C, PE : EA = 7 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 – 7.97 (m, 2H), 7.23 (s, 5H), 6.99 – 6.88 (m, 4H), 6.84 – 6.73 (m, 2H), 5.57 (s, 2H), 3.82 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.98, 150.49, 136.68, 134.75, 130.19, 130.11, 128.63, 128.40, 128.10, 128.00, 126.83, 122.90, 122.01, 114.00, 55.25, 52.20, 20.86. HRMS exact mass calcd for $C_{23}H_{21}N_3OS$ $[M+H]^+$ requires m/z 388.1478, found m/z 388.1477.



8ah

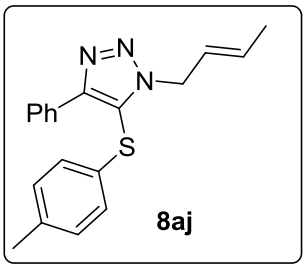
phenethyl-4-phenyl-5-(p-tolylthio)-1H-1,2,3-triazole. Brown soild. 49 mg, 66% yield. 75-76°C, PE : EA = 7 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 – 8.02 (m, 2H), 7.44 – 7.37 (m, 2H), 7.37 – 7.32 (m, 1H), 7.27 – 7.22 (m, 2H), 7.13 – 7.07 (m, 2H), 7.02 (s, 2H), 6.93 – 6.87 (m, 2H), 6.76 – 6.74 (m, 1H), 4.64 – 4.56 (m, 2H), 3.17 – 3.08 (m, 2H), 2.26 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.63, 150.21, 137.12, 137.03, 130.44, 130.01, 128.81, 128.73, 128.67, 128.60, 127.18, 126.99, 123.35,

115.20, 49.73, 36.45, 20.92. HRMS exact mass calcd for $C_{23}H_{21}N_3S$ $[M+H]^+$ requires m/z 372.1529, found m/z 372.1528.



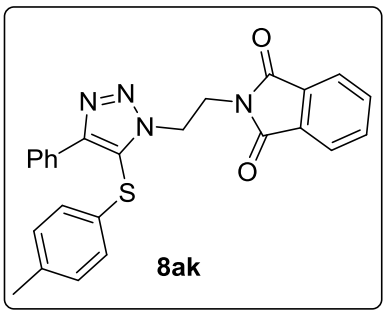
8ai

1-(naphthalen-2-ylmethyl)-4-phenyl-5-(p-tolylthio)-1H-1,2,3-triazole. Brown soild. 59 mg,73% yield. 261-262°C, PE : EA = 6 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (dt, *J* = 6.7, 1.4 Hz, 2H), 7.78 – 7.73 (m, 1H), 7.69 (d, *J* = 8.5 Hz, 1H), 7.65 – 7.60 (m, 1H), 7.51 (d, *J* = 1.7 Hz, 1H), 7.46 – 7.34 (m, 6H), 6.80 – 6.66 (m, 4H), 5.75 (s, 2H), 2.07 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.83, 136.63, 133.04, 132.94, 131.80, 130.26, 130.00, 129.73, 128.67, 128.57, 128.52, 127.95, 127.57, 127.42, 127.08, 126.73, 126.27, 126.20, 125.37, 123.09, 52.54, 20.70. HRMS exact mass calcd for $C_{26}H_{21}N_3S$ $[M+H]^+$ requires m/z 408.1529, found m/z 408.1524.



8aj

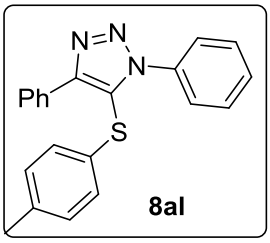
(E)-1-(but-2-en-1-yl)-4-phenyl-5-(p-tolylthio)-1H-1,2,3-triazole Brown soild. 38 mg, 59% yield. 49-50°C, PE : EA = 8 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 8.4, 1.4 Hz, 2H), 7.69 – 7.57 (m, 2H), 7.54 – 7.46 (m, 3H), 7.42 – 7.33 (m, 2H), 3.56 (s, 3H), 3.23 (s, 3H), 1.26 (s, 2H), 0.99 – 0.86 (m, 2H).^{13}C NMR (126 MHz, $CDCl_3$) δ 147.72, 134.35, 129.88, 129.64, 127.88, 127.60, 127.41, 127.30, 126.79, 125.68, 64.54, 51.10, 29.56, 17.45, 12.71. HRMS exact mass calcd for $C_{19}H_{19}N_3S$ $[M+H]^+$ requires m/z 322.1372, found m/z 322.1377.



8ak

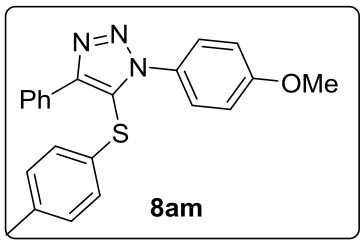
2-(2-(4-phenyl-5-(p-tolylthio)-1H-1,2,3-triazol-1-yl)ethyl)isoindoline-1,3-dione. Brown soild. 42 mg, 68% yield. 172-173°C, PE : EA = 6 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 – 8.07 (m, 2H), 7.44 – 7.40 (m, 2H), 7.39 – 7.34 (m, 1H), 7.30 – 7.24

(m, 3H), 7.14 – 7.09 (m, 2H), 7.04 (d, *J* = 8.1 Hz, 2H), 6.95 – 6.87 (m, 2H), 4.63 – 4.55 (m, 2H), 3.17 – 3.09 (m, 2H), 2.27 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.01, 150.21, 137.05, 130.43, 130.28, 130.17, 128.82, 128.73, 128.63, 128.59, 127.11, 127.08, 126.99, 123.14, 49.69, 36.49, 20.95. HRMS exact mass calcd for $C_{25}H_{20}N_4O_2S$ $[M+H]^+$ requires m/z 441.1380, found m/z 441.1385.



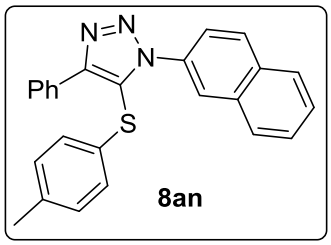
8al

1,4-diphenyl-5-(p-tolylthio)-1H-1,2,3-triazole. Yellow soild. 48 mg, 70% yield. 111-112°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 – 8.13 (m, 2H), 7.51 – 7.36 (m, 8H), 6.96 (d, *J* = 8.0 Hz, 2H), 6.86 – 6.77 (m, 2H), 2.24 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.41, 137.11, 136.15, 130.24, 130.14, 129.65, 129.01, 128.72, 128.58, 127.95, 127.39, 125.82, 124.63, 121.48, 20.90. HRMS exact mass calcd for $C_{21}H_{17}N_3S$ $[M+H]^+$ requires m/z 344.1216, found m/z 344.1205.



8am

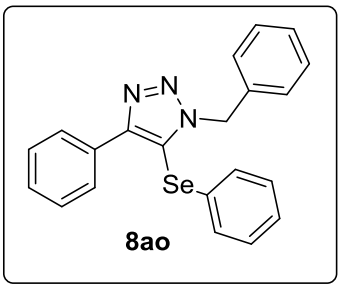
(4-methoxyphenyl)-4-phenyl-5-(p-tolylthio)-1H-1,2,3-triazole. Brown soild. 45mg, 60% yield. 172-173°C, PE : EA = 6 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 – 8.11 (m, 2H), 7.45 (dd, *J* = 8.3, 6.6 Hz, 2H), 7.40 – 7.37 (m, 1H), 7.35 – 7.32 (m, 2H), 7.03 (d, *J* = 8.0 Hz, 1H), 6.99 – 6.94 (m, 3H), 6.84 – 6.82 (m, 1H), 6.78 – 6.70 (m, 1H), 3.86 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.48, 152.38, 149.25, 136.02, 129.15, 129.02, 127.67, 127.57, 126.81, 126.33, 126.13, 123.70, 114.10, 113.17, 54.57, 19.91. HRMS exact mass calcd for $C_{22}H_{19}N_3OS$ $[M+H]^+$ requires m/z 374.1322, found m/z 374.1314.



8an

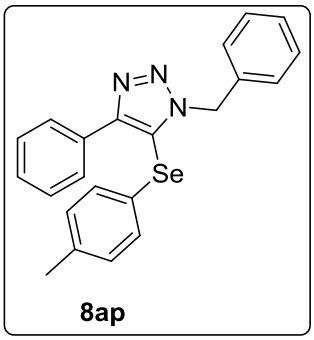
1-(naphthalen-2-yl)-4-phenyl-5-(p-tolylthio)-1H-1,2,3-triazole. Brown soild. 42 mg, 53% yield. 142-143°C, PE : EA = 6 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.27 – 8.15 (m, 2H), 7.98 – 7.87 (m, 3H), 7.86 – 7.75 (m, 1H), 7.64 – 7.53 (m, 3H), 7.51 – 7.43 (m, 2H), 7.44 – 7.36 (m, 1H), 7.00 – 6.90 (m, 2H), 6.90 – 6.79 (m, 2H), 2.23 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.91, 150.52, 137.17, 133.50, 133.32, 132.79, 130.32, 130.17, 129.04, 128.77, 128.63, 128.47, 128.04, 127.86, 127.42, 127.40, 127.07,

124.93, 124.89, 123.24, 20.90. HRMS exact mass calcd for $C_{25}H_{19}N_3S$ $[M+H]^+$ requires m/z 394.1372, found m/z 394.1374.



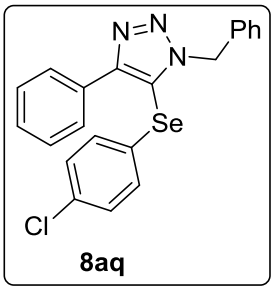
8ao

1-benzyl-4-phenyl-5-(phenylselanyl)-1H-1,2,3-triazoleRed oil.[3] Red soild. 58 mg, 74% yield. 210-211°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 – 8.00 (m, 2H), 7.41 – 7.35 (m, 3H), 7.22 (s, 5H), 7.16 – 7.09 (m, 3H), 7.00 – 6.96 (m, 2H), 5.66 (s, 2H).^{13}C NMR (126 MHz, $CDCl_3$) δ 134.85, 130.48, 129.75, 129.70, 129.25, 128.68, 128.56, 128.47, 128.44, 127.93, 127.87, 127.52, 127.48, 127.25, 53.16. HRMS exact mass calcd for $C_{21}H_{17}N_3Se$ $[M+H]^+$ requires m/z 392.0660, found m/z 392.0661.



8ap

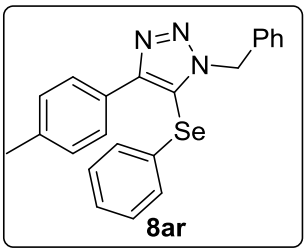
1-**benzyl-4-phenyl-5-(p-tolylselanyl)-1H-1,2,3-triazole.**[3] Yellow soild. 62 mg, 76% yield. 232-233°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (dt, *J* = 6.3, 1.3 Hz, 2H), 7.42 – 7.38 (m, 2H), 7.37 – 7.33 (m, 1H), 7.30 – 7.19 (m, 5H), 6.97 – 6.86 (m, 4H), 5.65 (s, 2H), 2.25 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.36, 137.48, 135.00, 130.66, 130.48, 129.77, 128.68, 128.49, 128.45, 128.10, 127.88, 127.52, 125.73, 118.34, 53.07, 20.96. HRMS exact mass calcd for $C_{22}H_{19}N_3Se$ $[M+H]^+$ requires m/z 406.0817, found m/z 406.0819.



8aq

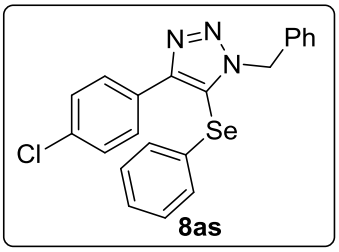
benzyl-5-((4-chlorophenyl)selanyl)-4-phenyl-1H-1,2,3-triazole.[3] Brown soild. 59 mg, 70% yield. 198-199°C, PE : EA = 10 : 1. ^{1}H NMR (400 MHz, $CDCl_3$) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 – 7.97 (m, 2H), 7.42 – 7.35 (m, 3H), 7.24 – 7.17 (m, 5H), 7.07 – 6.99 (m, 2H), 6.86 – 6.79 (m, 2H), 5.67 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ

151.73, 134.65, 133.50, 130.52, 130.46, 130.35, 129.73, 128.73, 128.55, 128.22, 127.85, 127.64, 127.44, 117.43, 53.27. HRMS exact mass calcd for $C_{21}H_{16}ClN_3Se$ $[M+H]^+$ requires m/z 426.0271, found m/z 426.0270.



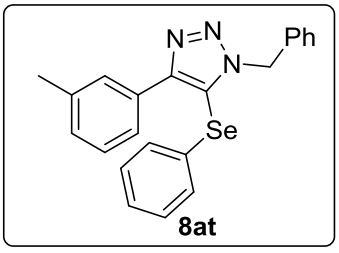
8ar

benzyl-5-(phenylselanyl)-4-(p-tolyl)-1H-1,2,3-triazole. Brown soild. 61 mg, 75% yield. 201-202°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (dd, *J* = 7.7, 1.8 Hz, 1H), 8.18 – 8.05 (m, 2H), 8.01 – 7.88 (m, 2H), 7.69 (d, *J* = 9.1 Hz, 1H), 7.64 – 7.60 (m, 1H), 7.56 – 7.46 (m, 4H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.07 (d, *J* = 7.8 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.31, 148.89, 135.74, 135.24, 132.53, 130.38, 129.89, 129.35, 128.30, 128.13, 127.40, 125.14, 123.80, 112.84, 30.94, 21.03. HRMS exact mass calcd for $C_{22}H_{19}N_3Se$ $[M+H]^+$ requires m/z 406.0817, found m/z 406.0833.



8as

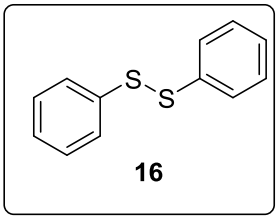
benzyl-4-(4-chlorophenyl)-5-(phenylthio)-1H-1,2,3-triazole Brown soild. 53 mg, 62% yield. 186-187°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 – 8.16 (m, 1H), 8.15 – 8.09 (m, 2H), 7.99 – 7.90 (m, 2H), 7.69 (d, *J* = 9.0 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.54 – 7.50 (m, 3H), 7.23 (q, *J* = 8.5 Hz, 4H), 4.94 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.29, 136.84, 135.82, 131.64, 129.52, 128.86, 128.54, 128.46, 127.73, 127.31, 126.46, 124.22, 122.40, 111.80, 29.76. HRMS exact mass calcd for $C_{21}H_{16}ClN_3Se$ $[M+H]^+$ requires m/z 426.0271, found m/z 426.0277.



8at

benzyl-5-(phenylselanyl)-4-(m-tolyl)-1H-1,2,3-triazole Yellow soild. 48 mg, 59% yield. 155-156°C, PE : EA = 10 : 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 – 8.13 (m, 1H), 7.99 – 7.91 (m, 2H), 7.89 – 7.83 (m, 1H), 7.81 (d, *J* = 9.1 Hz, 1H), 7.60 (d, *J* = 9.0 Hz, 1H), 7.43 – 7.36 (m, 2H), 7.25 – 7.22 (m, 3H), 7.19 – 7.13 (m, 2H), 7.12 – 7.04 (m, 1H), 4.89 (s, 2H), 2.37 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.13,

148.11, 142.36, 137.39, 134.39, 129.16, 129.03, 128.29, 127.99, 127.57, 127.20, 126.27, 125.20, 124.04, 122.69, 111.78, 30.28, 20.70. HRMS exact mass calcd for $C_{22}H_{19}N_3Se$ $[M+H]^+$ requires m/z 406.0817, found m/z 406.0821.



16

1,2-diphenyldisulfane[4] White soild. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 – 7.46 (m, 4H), 7.32 – 7.27 (m, 4H), 7.24 – 7.19 (m, 2H).

References

1. Ding, S., Jia, G. & Sun, J. Iridium-Catalyzed Intermolecular Azide–Alkyne Cycloaddition of Internal Thioalkynes under Mild Conditions. *Angew. Chem. Int. Ed.* **53**, 1877 –1880 (2014)

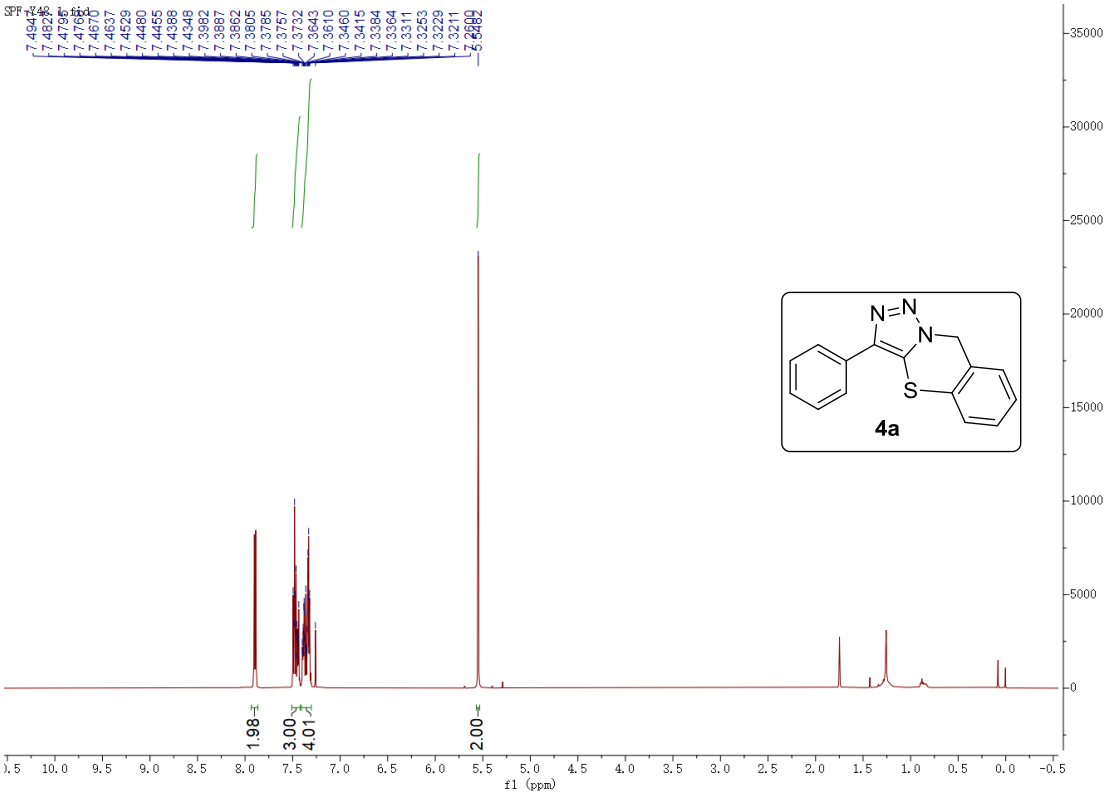
2. Song, W., Zheng, N., Li, M., He, J., Li, J., Dong, K., Ullah, K. & Zheng, Y. Rhodium(I)-Catalyzed Regioselective Azide-internal Alkynyl Trifluoromethyl Sulfide Cycloaddition and Azide-internal Thioalkyne Cycloaddition under Mild Conditions. *Adv. Synth. Catal.* **361**, 469 – 475 (2019)

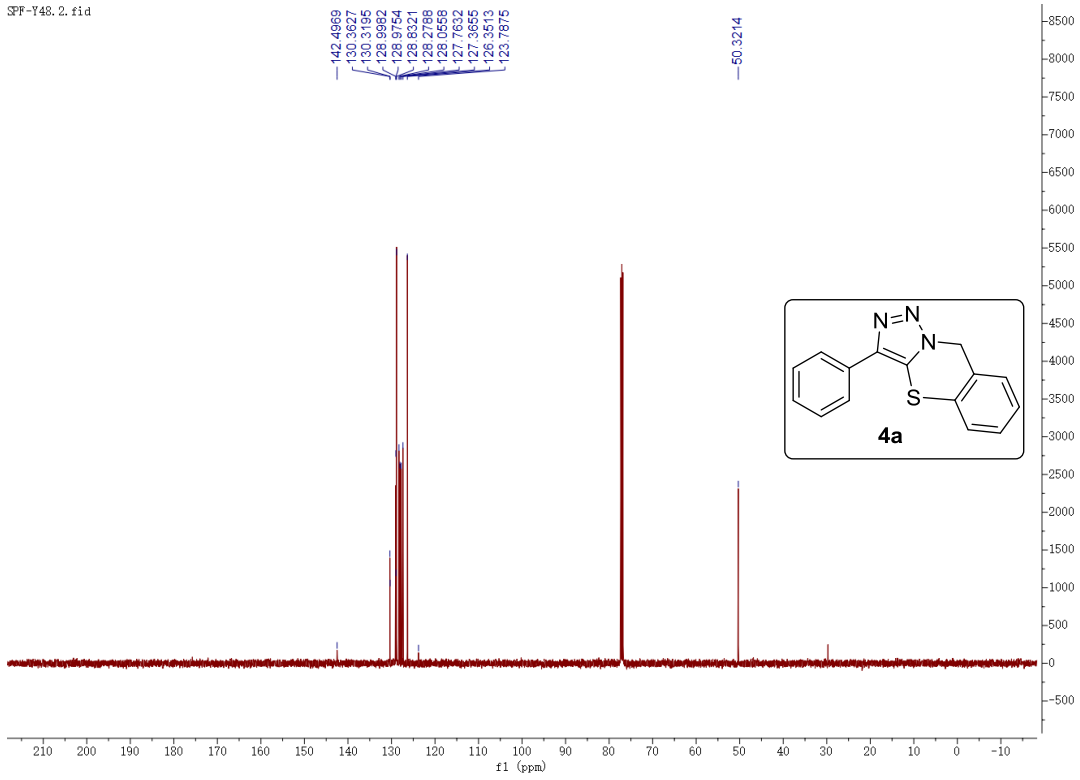
3. Cui, F. et al. Copper-Catalyzed Decarboxylative/Click Cascade Reaction: Regioselective Assembly of 5-Selenotriazole Anticancer Agents. *Org. Lett.* **20**, 925−929 (2018)

4. Ge, X., Cheng, L., Sun, F., Liu, X., Chen, X., Qian, C. & Zhou, S. Mechanistic and experimental study on copper-catalyzed C3-sulfenylation of indoles with sulfur powder and aryl iodides. *Catal. Commun.* **123**, 32–37 (2019)

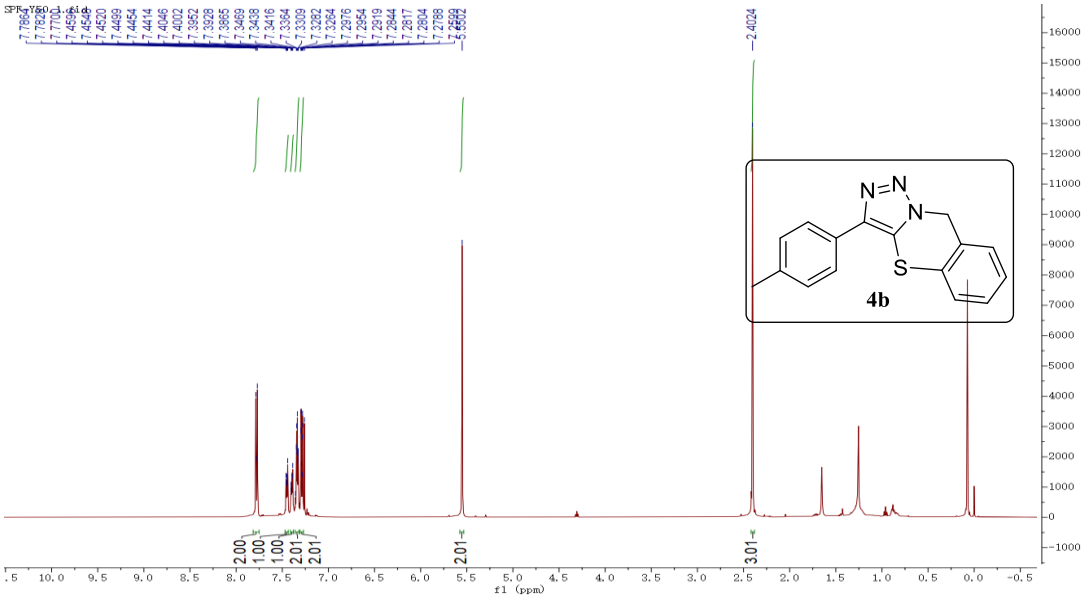
NMR spectra for the products

Compound 4a





Compound 4b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3.01
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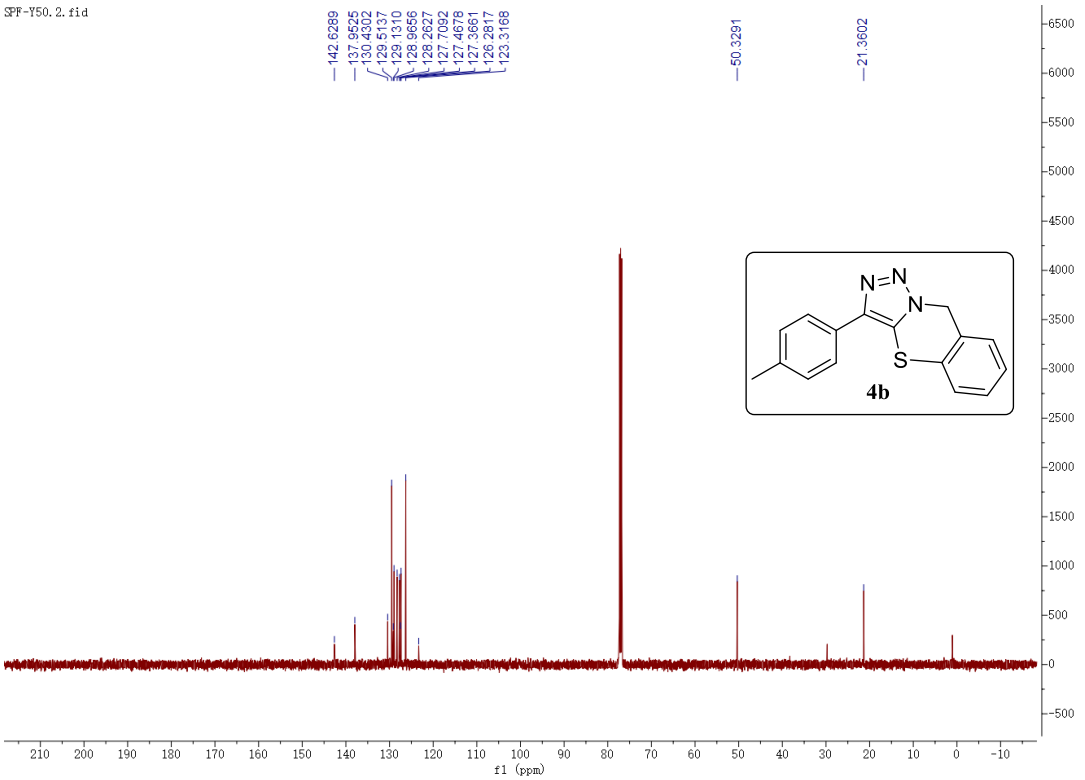
4b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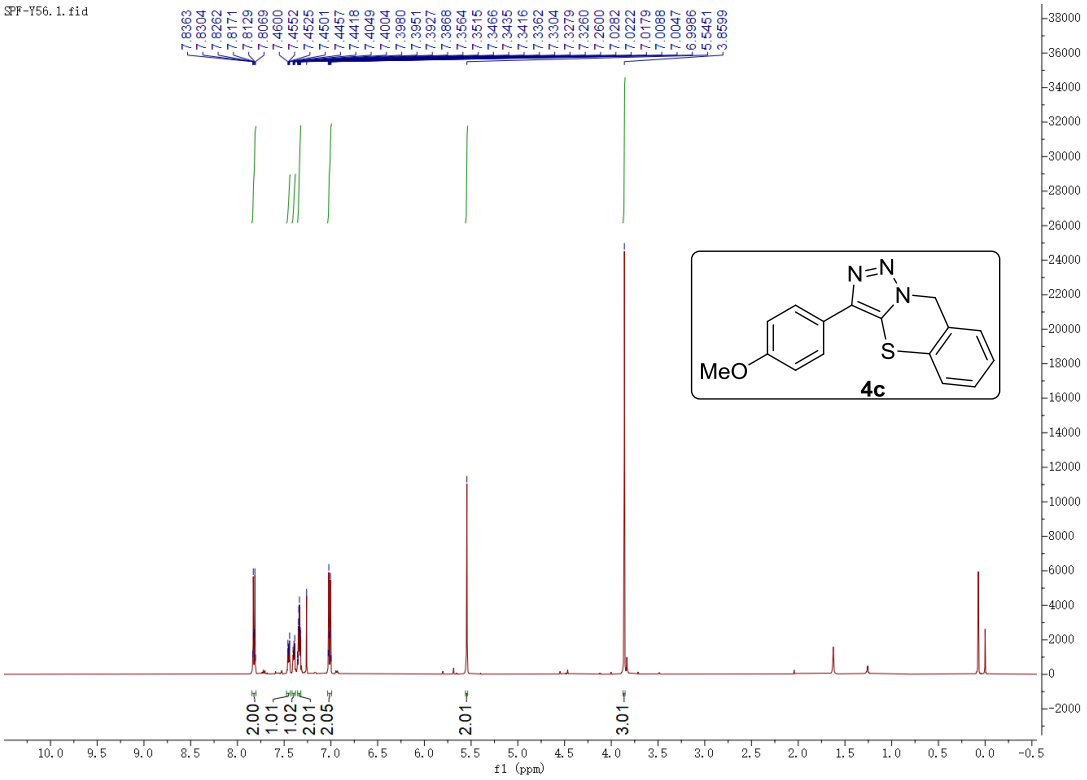
4b

Compound 4c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7.4004
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7.2600
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7.0222
7.0179
7.0088
7.0047
6.9986
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2.01
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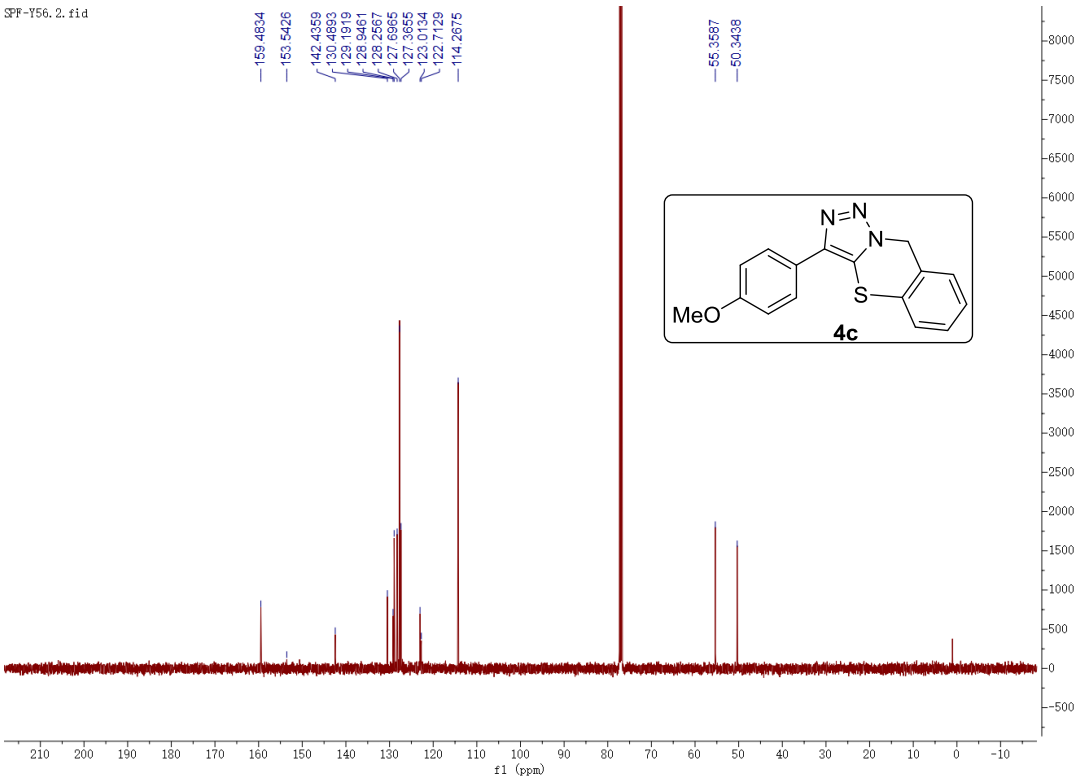
3.01
f1 (ppm)
MeO
4c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123.0134
122.7129
114.2675
55.3587
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f1 (ppm)
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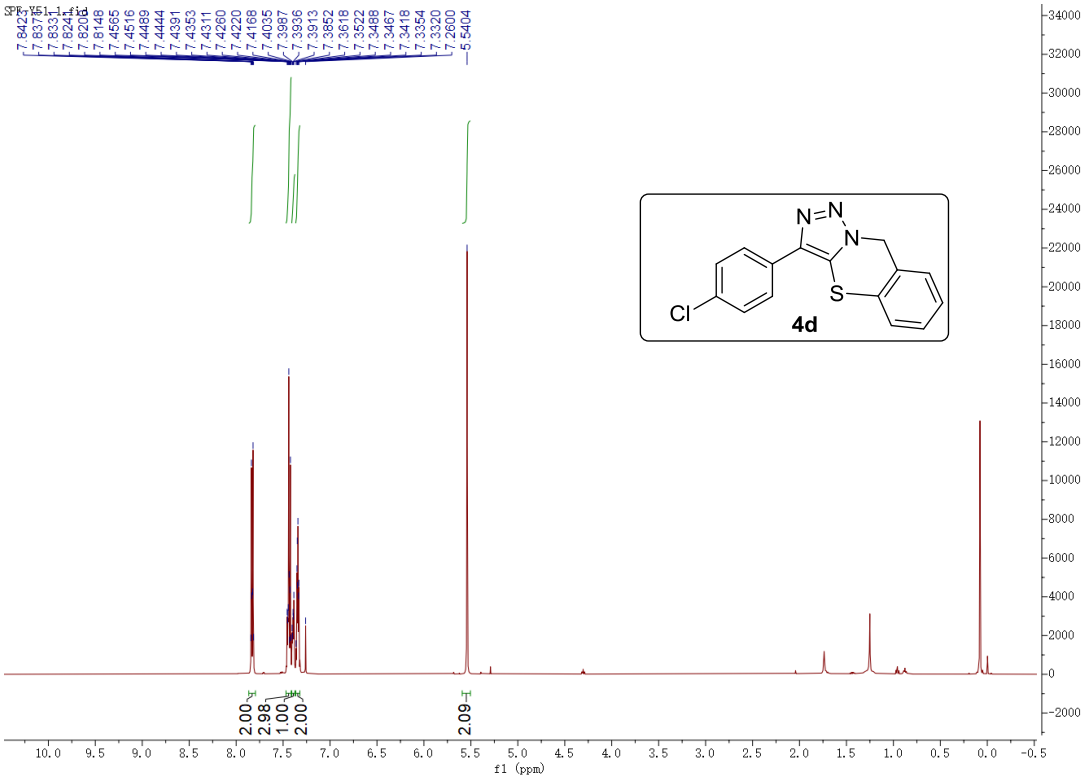
4c

Compound 4d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7.4353
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7.3522
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7.3418
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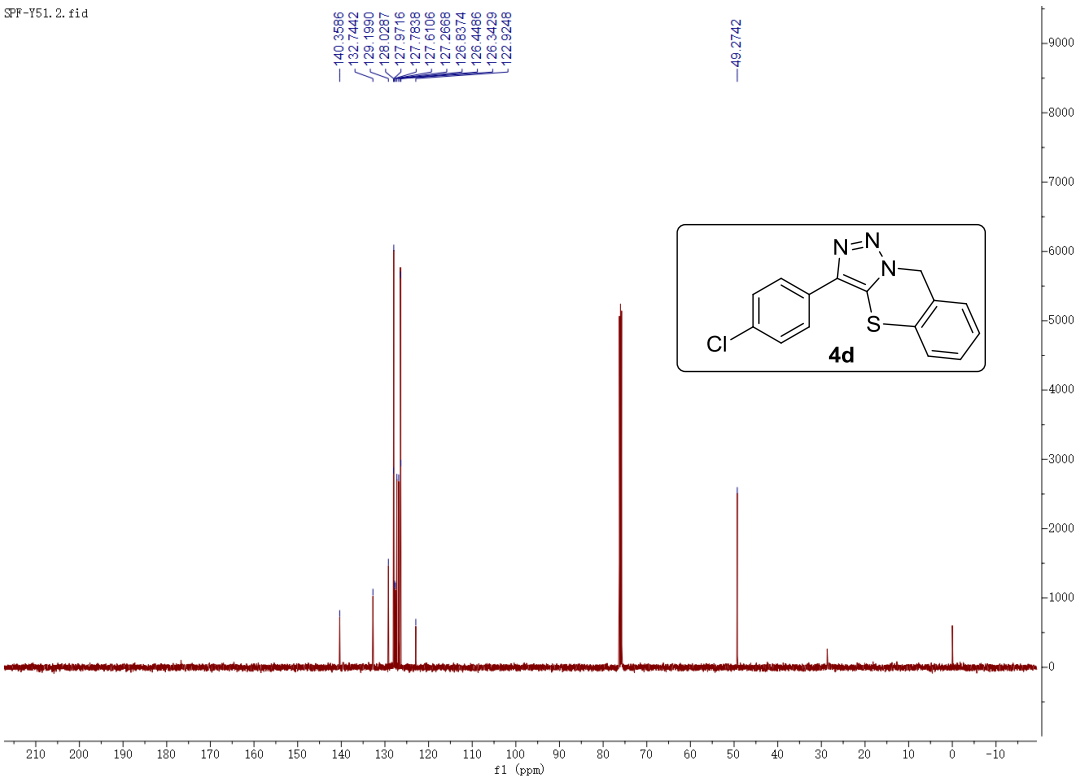
Cl
4d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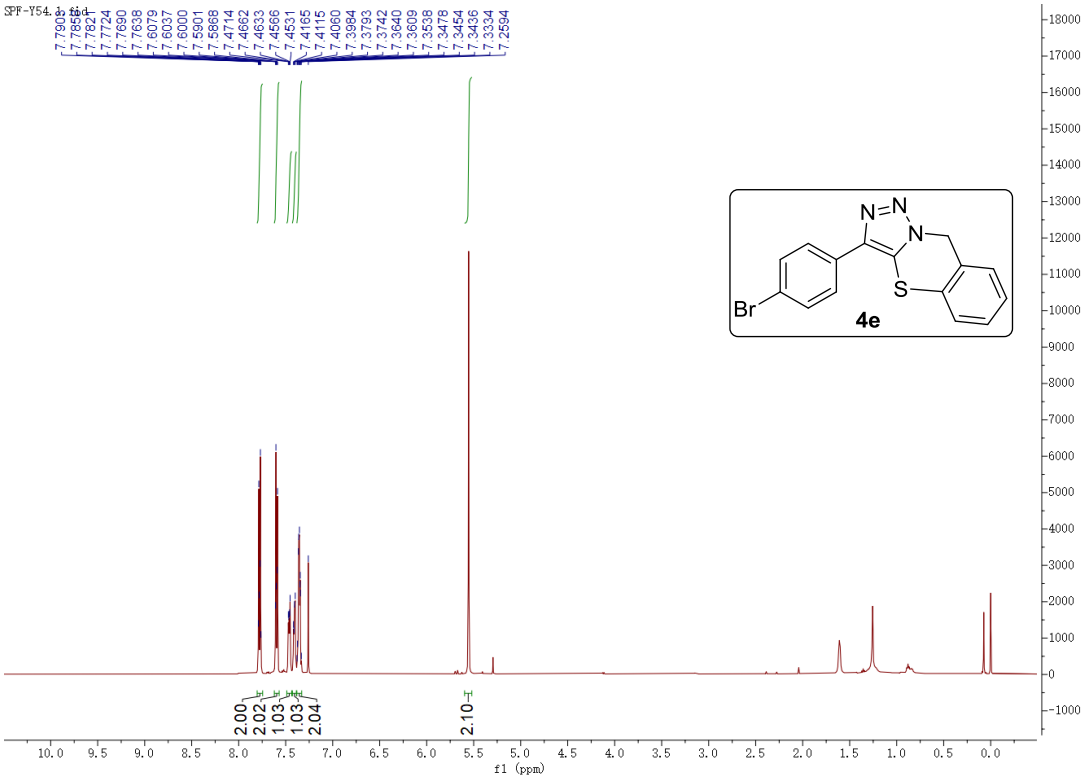
f1 (ppm)
Cl
4d

Compound 4e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7.4115
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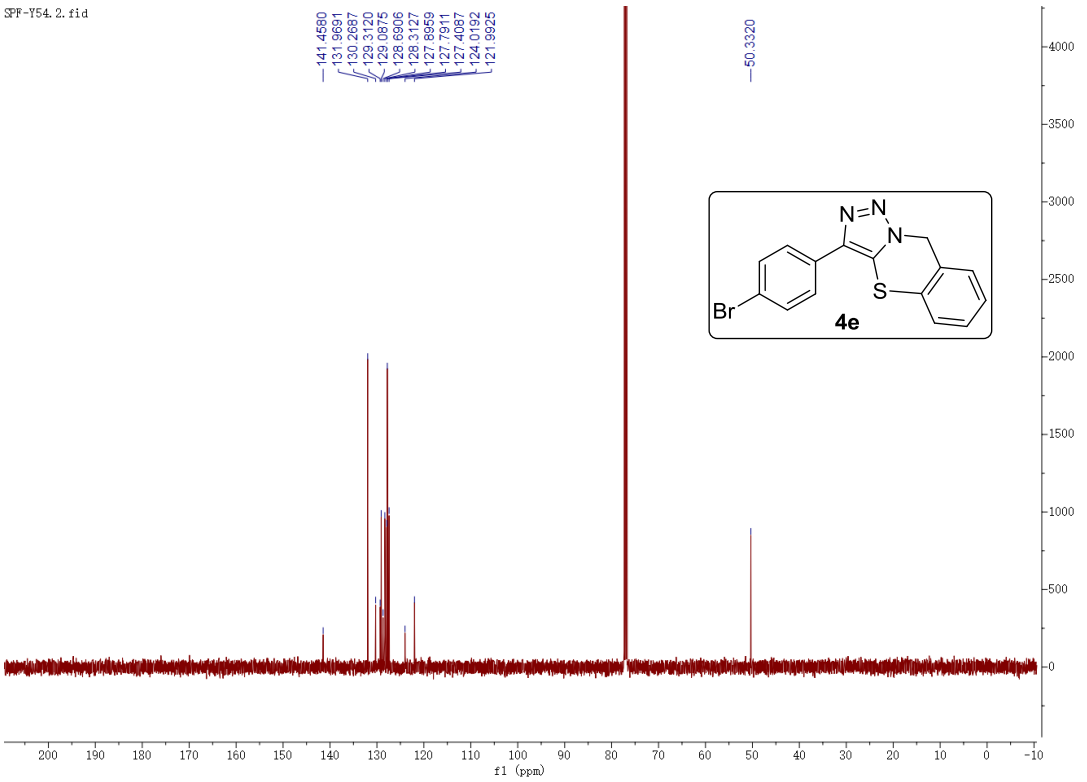
Br
4e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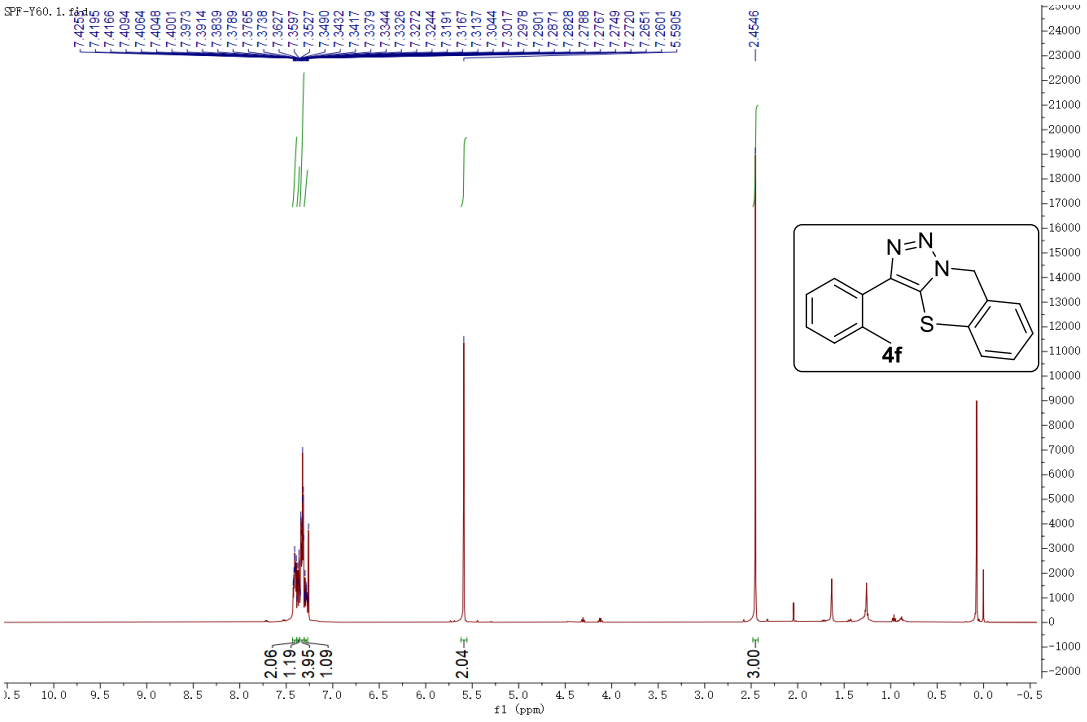
f1 (ppm)
Br
4e

Compound 4f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7.3527
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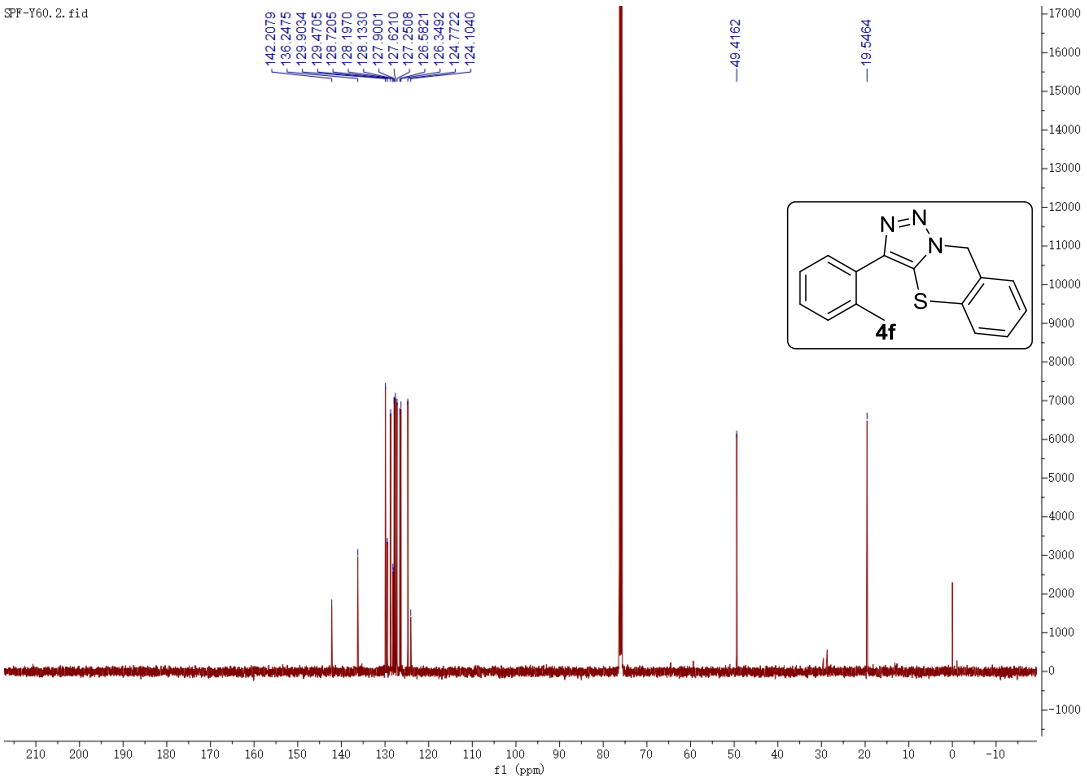
4f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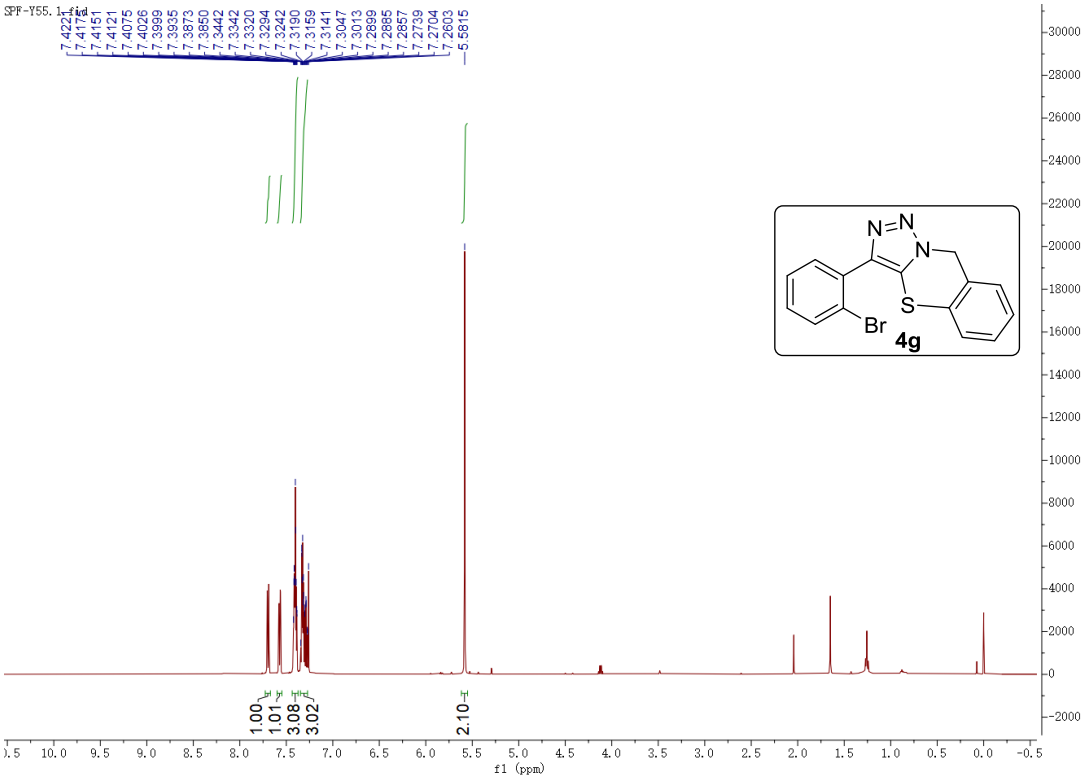
Compound 4g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f1 (ppm)
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N
S
Br
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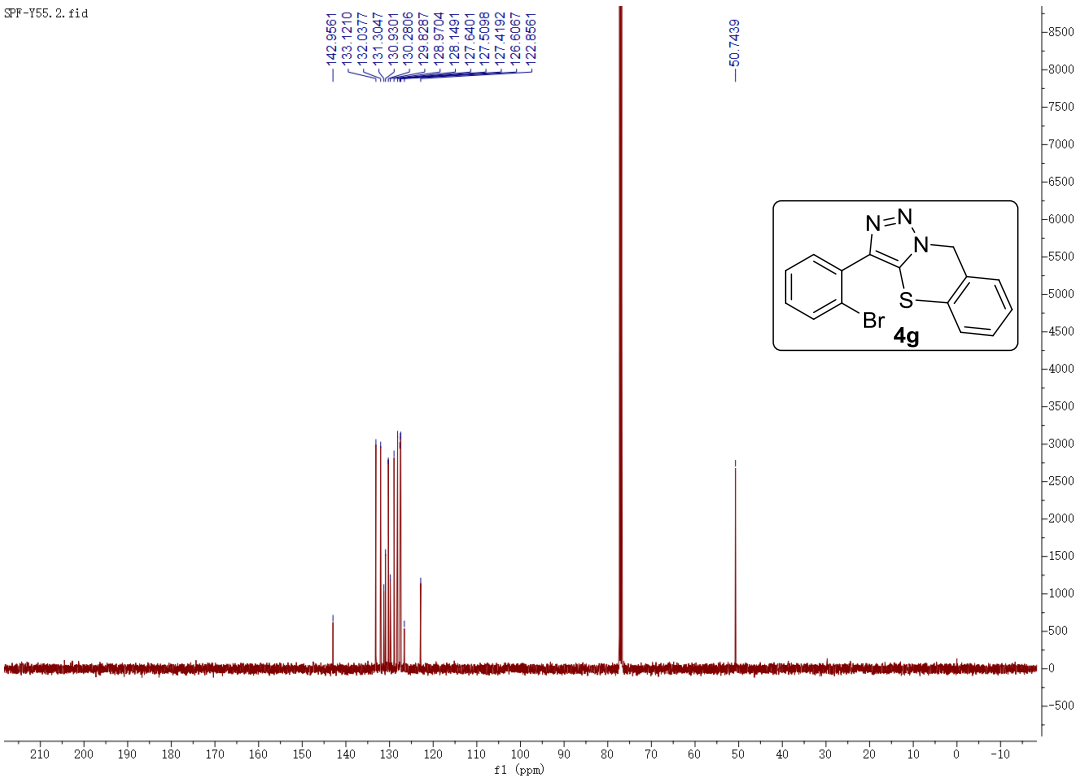
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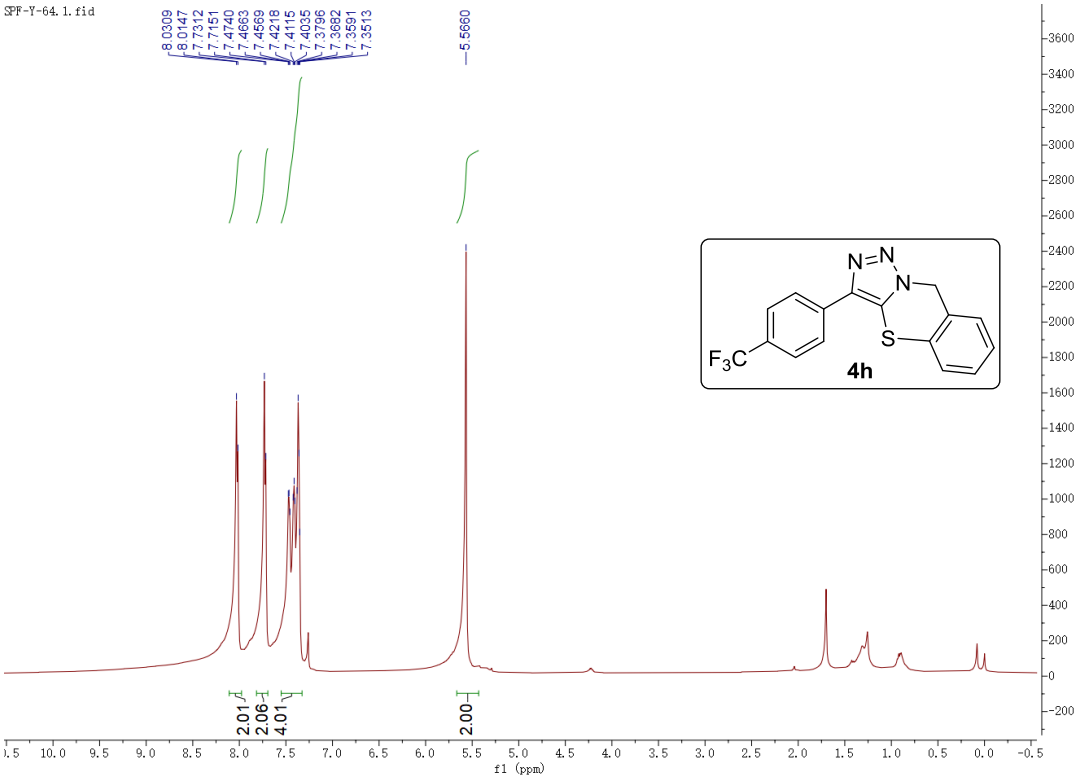
N
N
S
Br
4g

Compound 4h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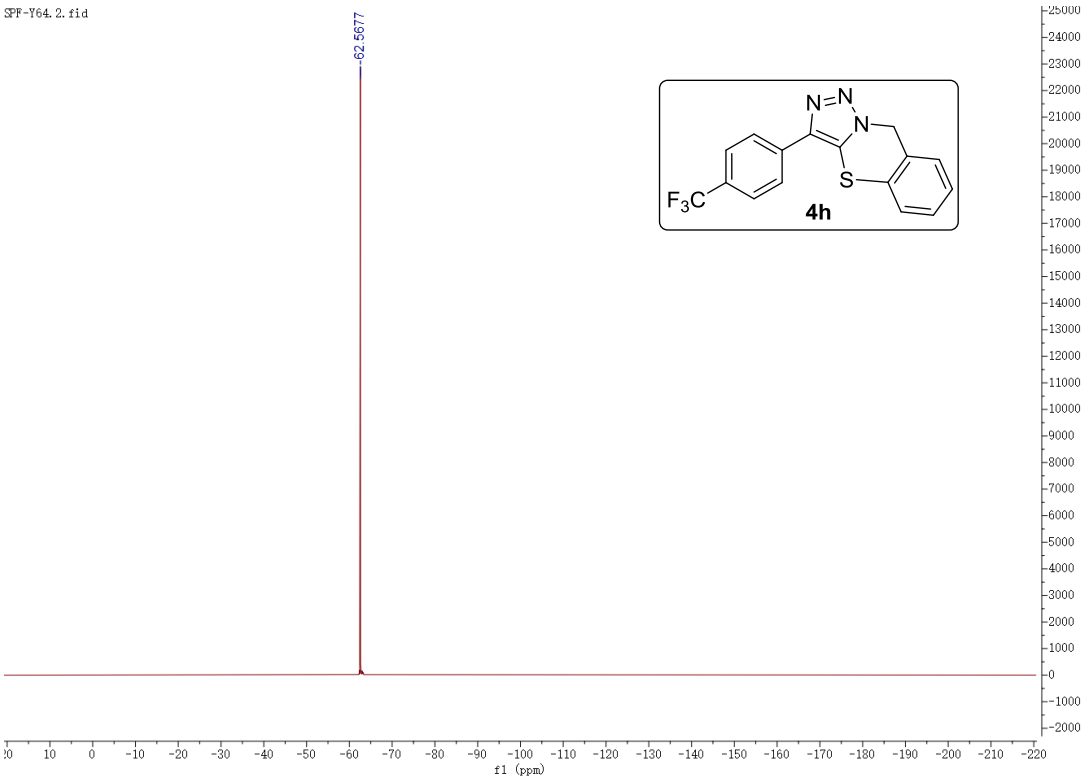
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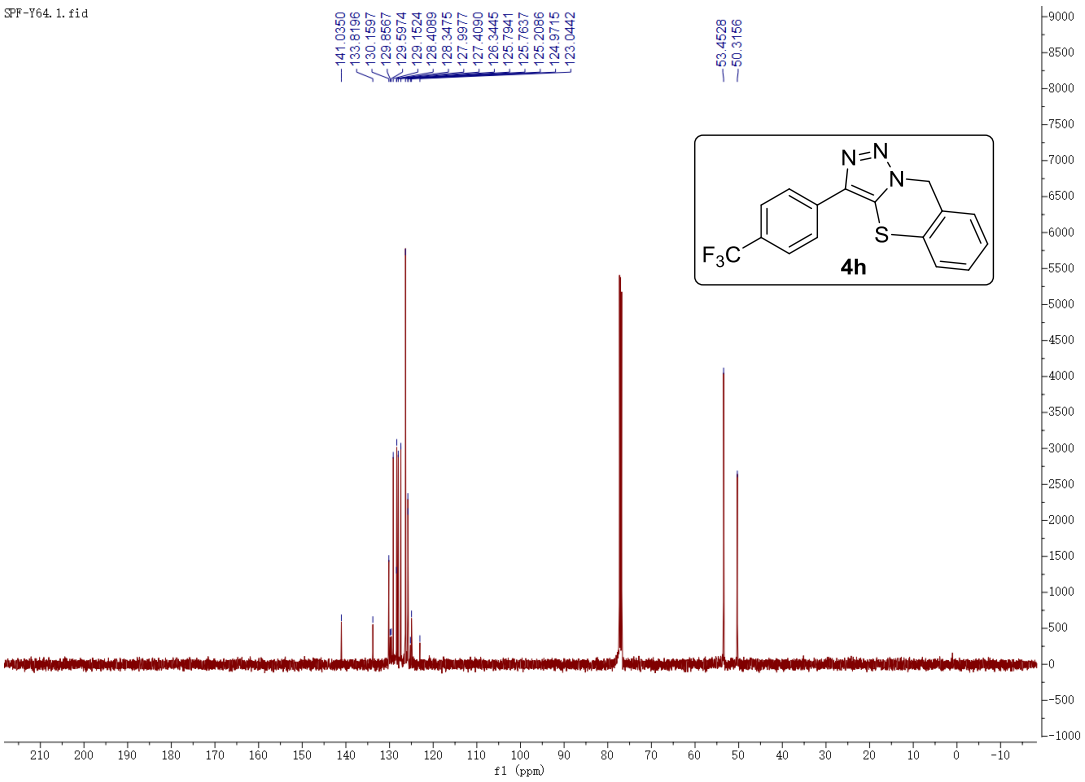
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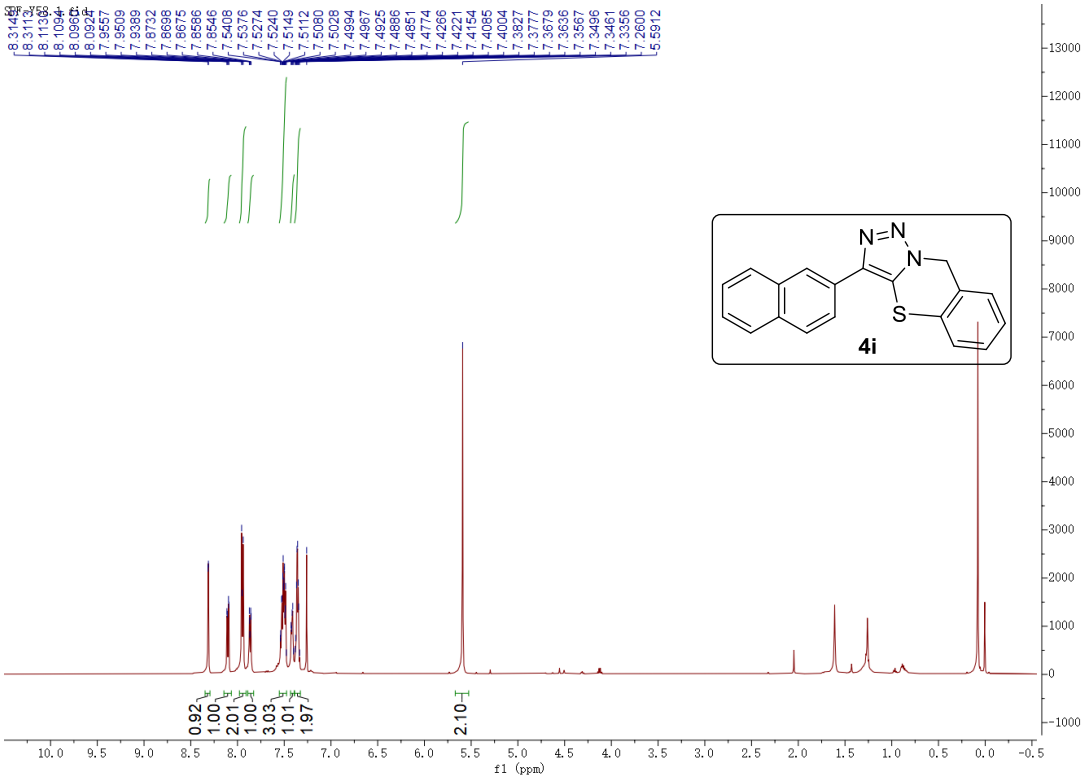
f1 (ppm)

Compound 4i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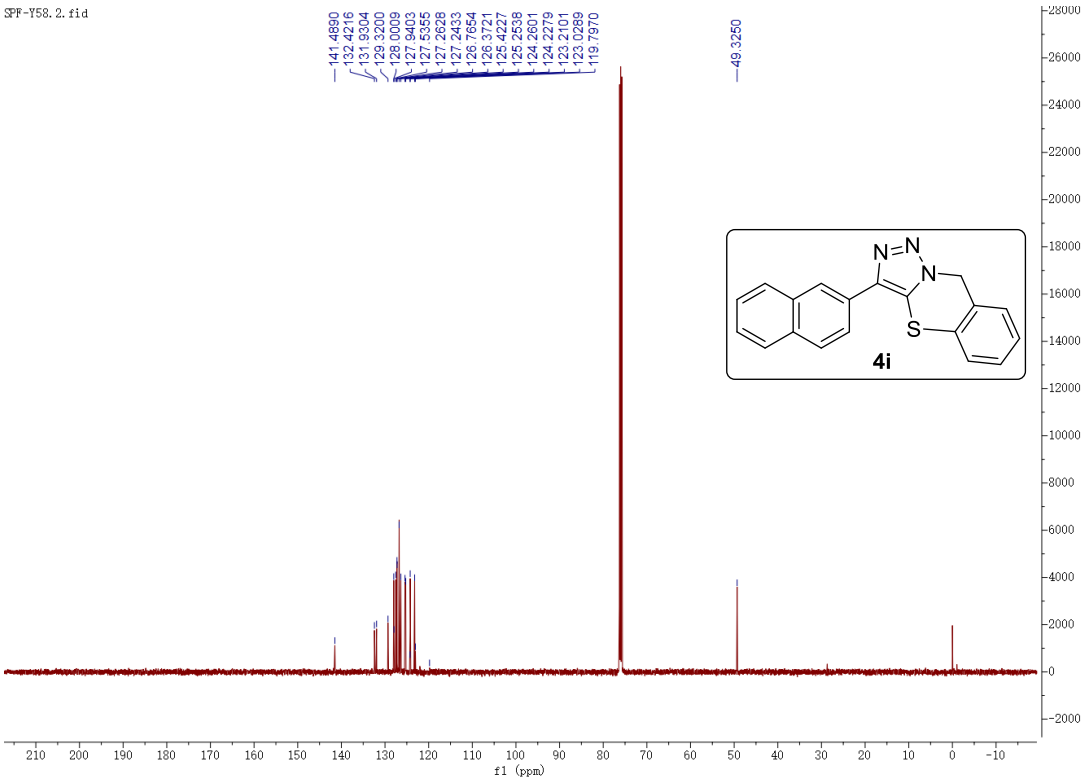
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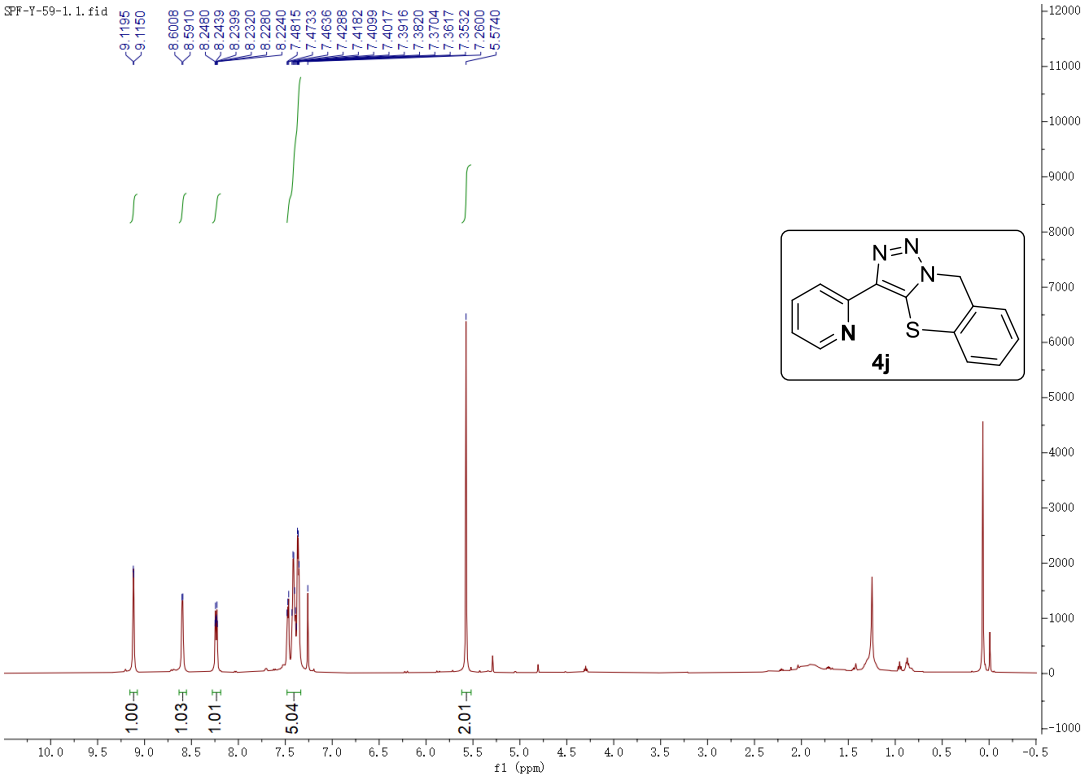
f1 (ppm)

Compound 4j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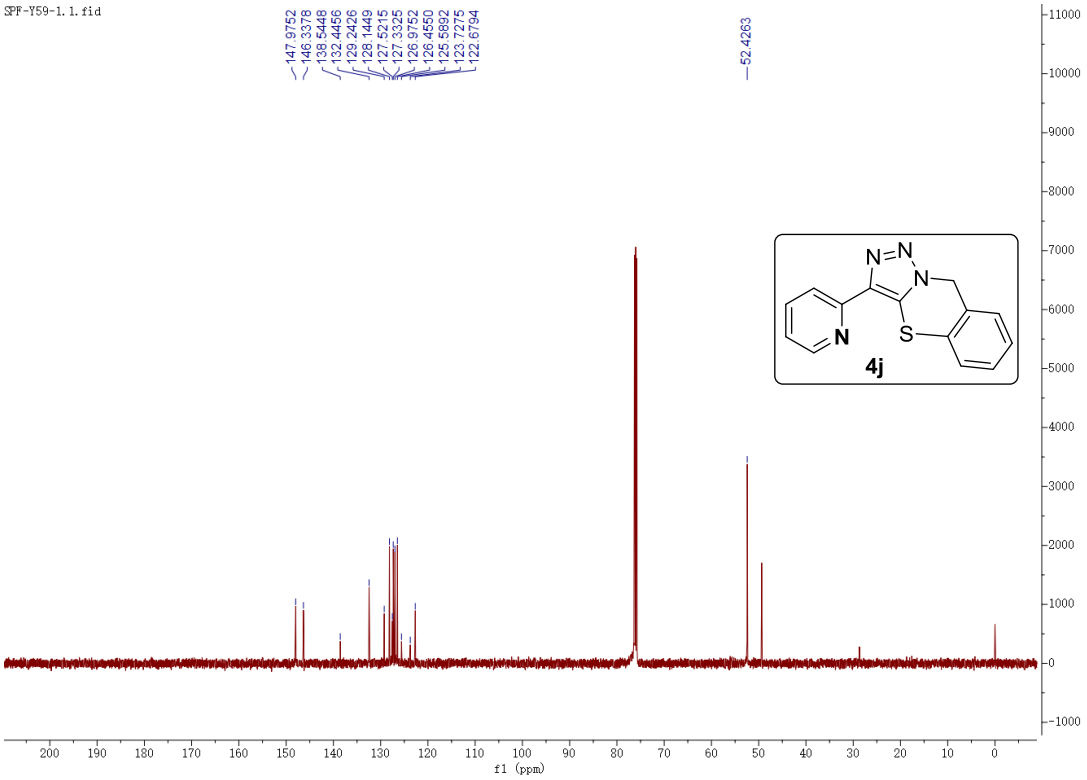
f1 (ppm)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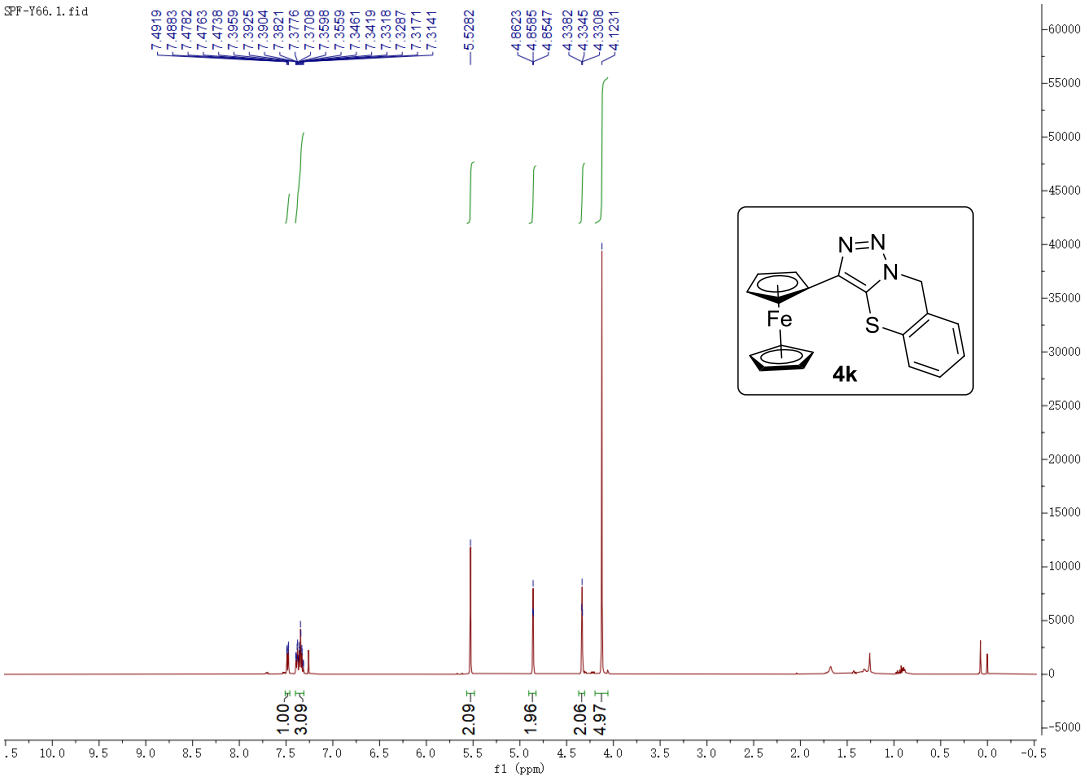
N
S
4j
f1 (ppm)

Compound 4k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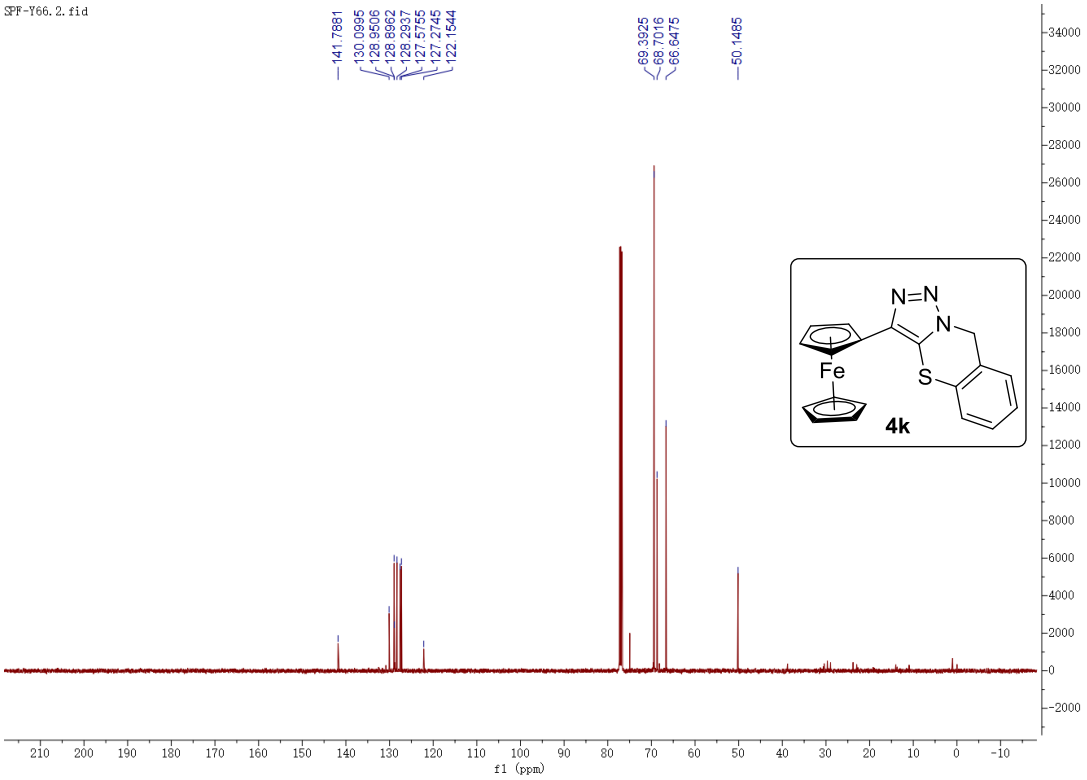
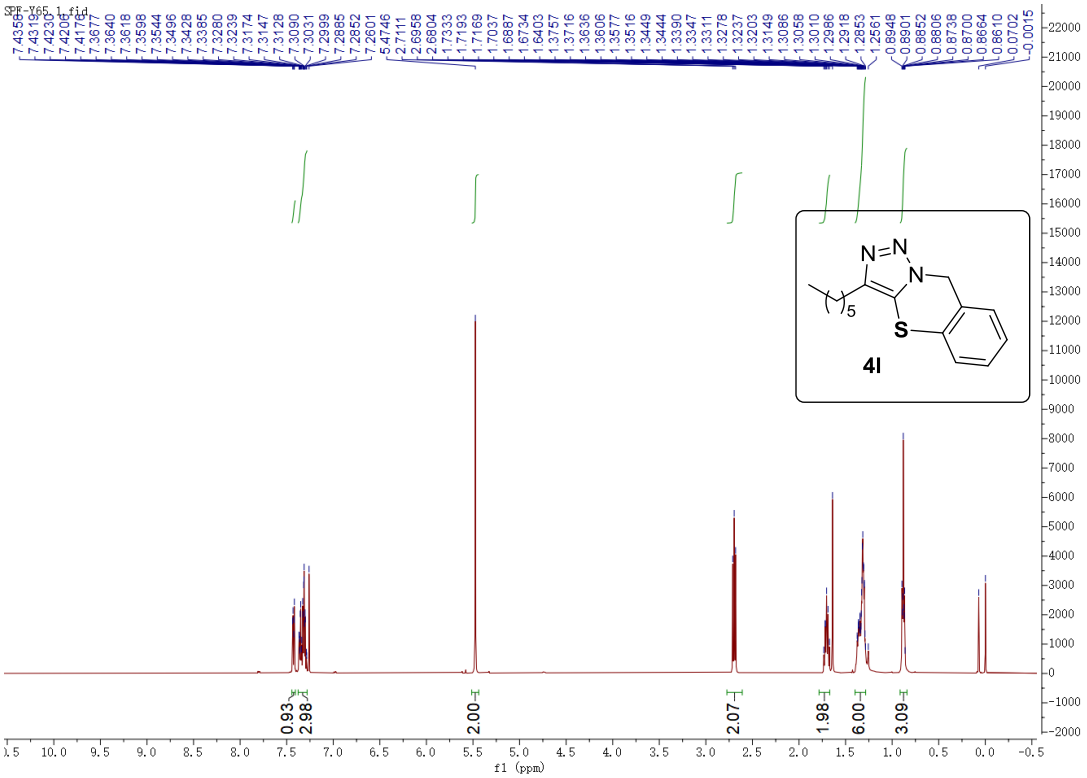
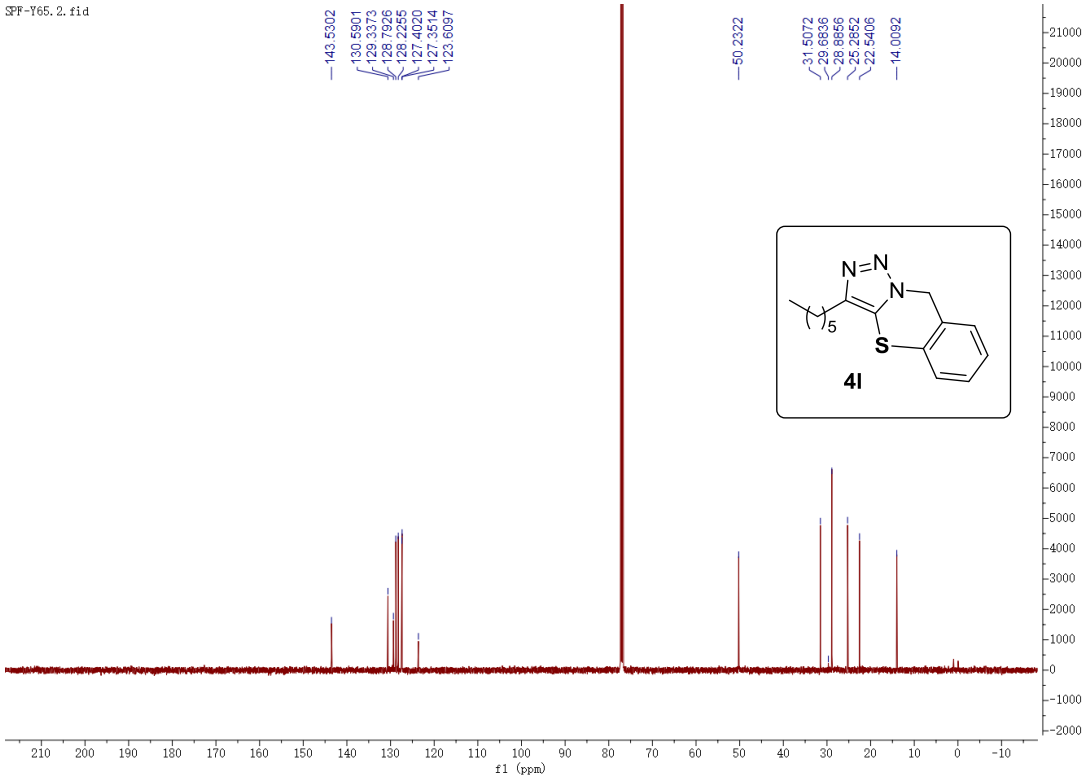
N=N
N
Fe
S
4k
f1 (ppm)

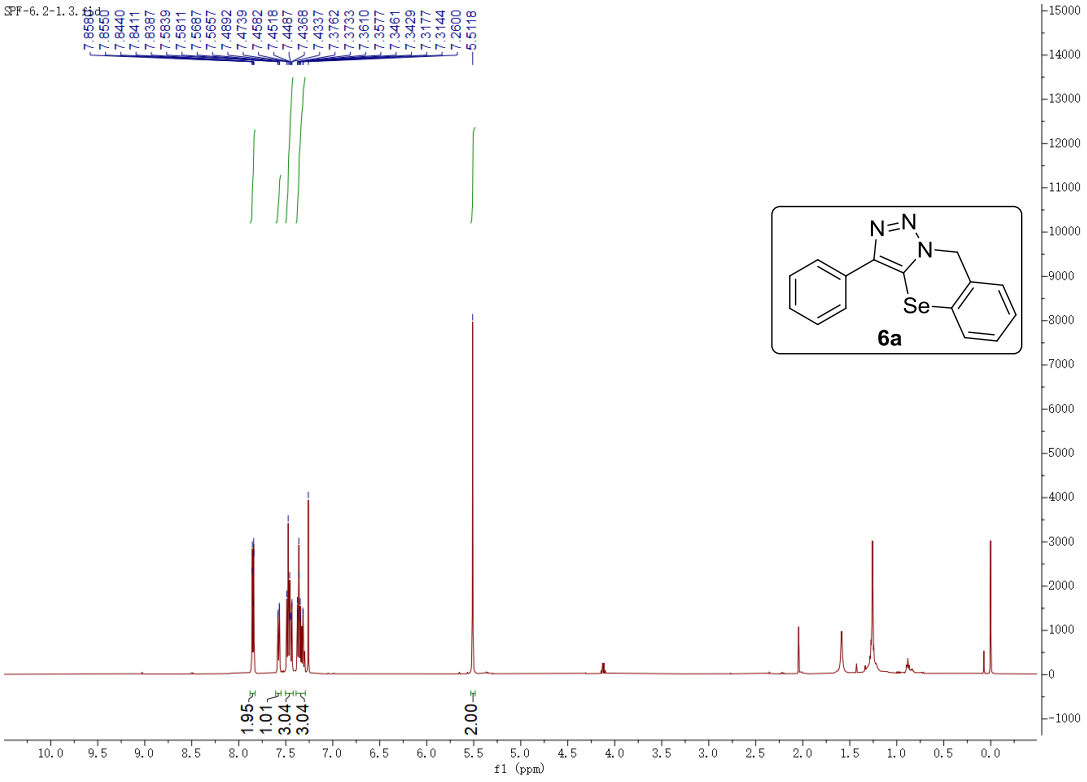

SPF-Y66.2.fid
141.7881
130.0995
128.9506
128.8962
128.2937
127.5755
127.2745
122.1544
69.3925
68.7016
66.6475
50.1485
N=N
N
Fe
S
4k
f1 (ppm)

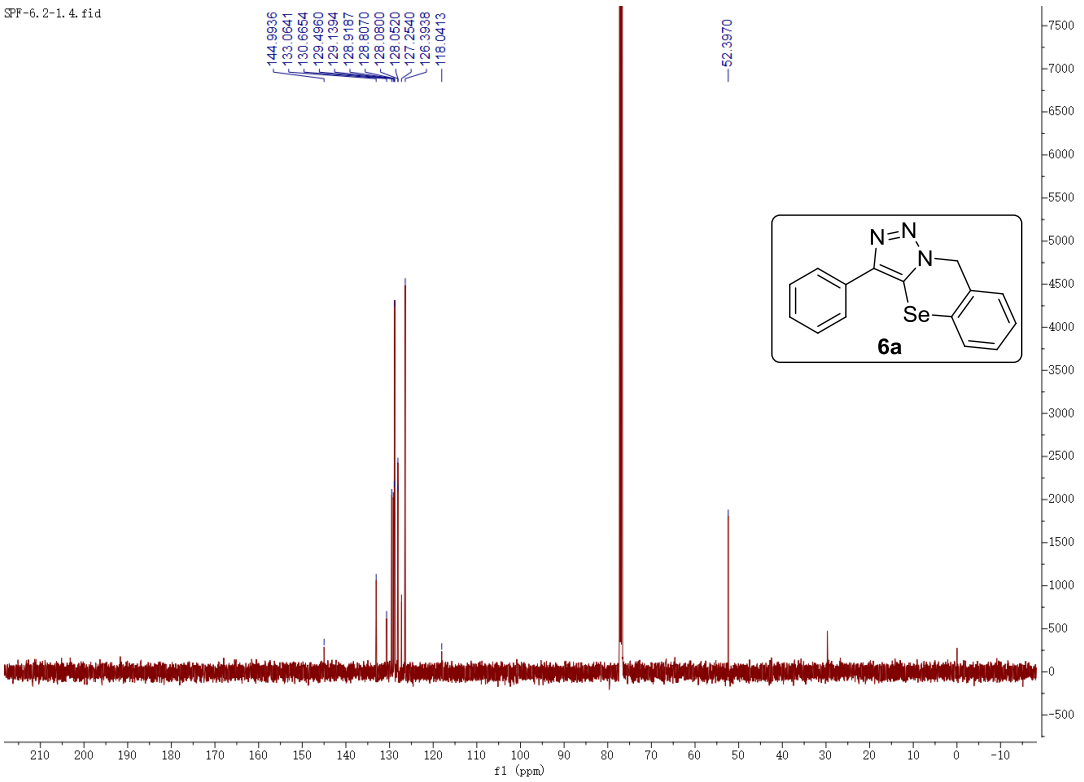
Compound 4l


SPF-Y65.1.fid
N=N
N
5
S
4l
0.93
2.98
2.00
2.07
1.98
6.00
3.09
f1 (ppm)

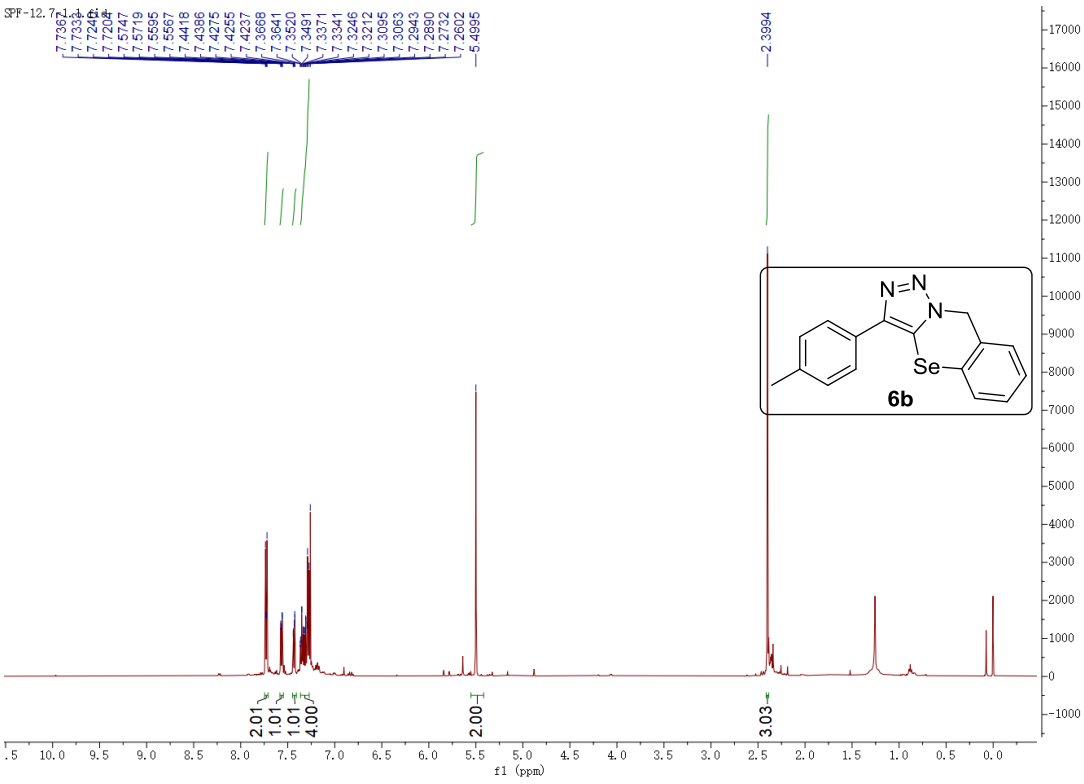

SPF-Y65.2.fid
143.5302
130.5901
129.3373
128.7926
128.2255
127.4020
127.3514
123.6097
50.2322
31.5072
29.6836
28.8656
25.2852
22.5406
14.0092
N=N
N
S
5
4l
f1 (ppm)

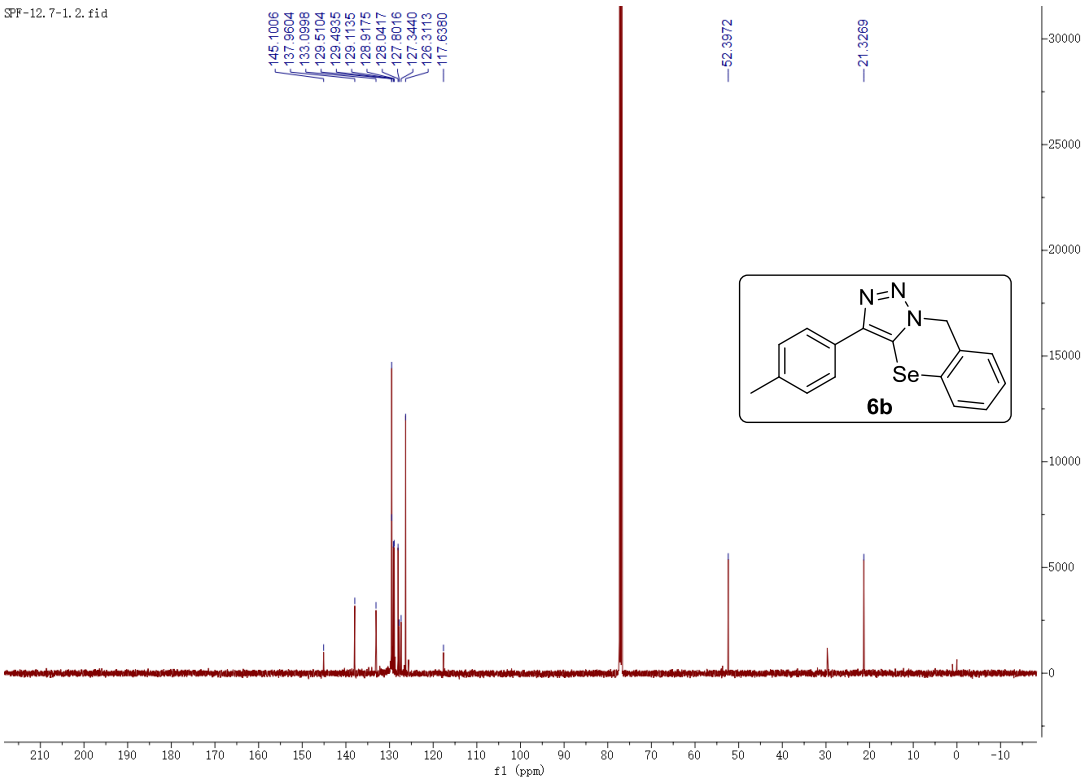
Compound 6a


SPF-6.2-1.3.fid
7.8584
7.8550
7.8440
7.8411
7.8387
7.5839
7.5811
7.5687
7.5657
7.4892
7.4739
7.4562
7.4518
7.4487
7.4368
7.4337
7.3762
7.3733
7.3610
7.3577
7.3461
7.3429
7.3177
7.3144
7.2600
5.5118
1.95
1.01
3.04
3.04
2.00
N=N
N
Se
6a
f1 (ppm)

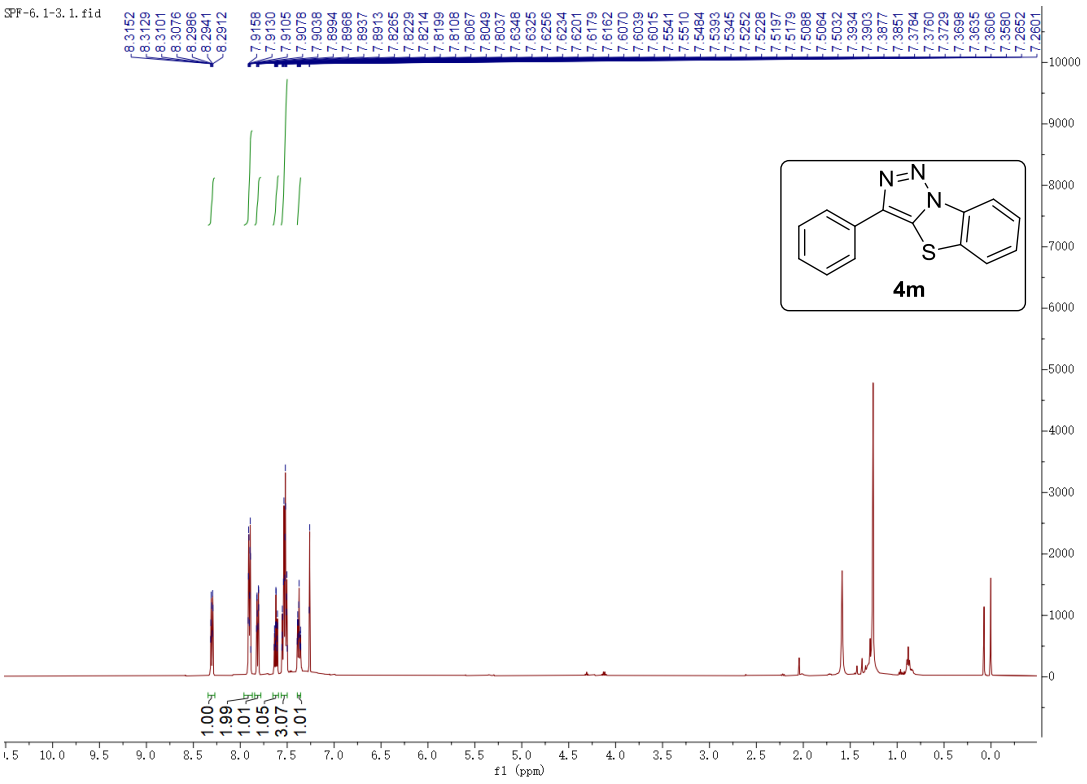

SPF-6.2-1.4.fid
144.9936
133.0641
130.6654
129.4960
129.1394
128.9187
128.8070
128.0800
128.0520
127.2540
126.3938
118.0413
52.3970
N=N
N
Se
6a
f1 (ppm)

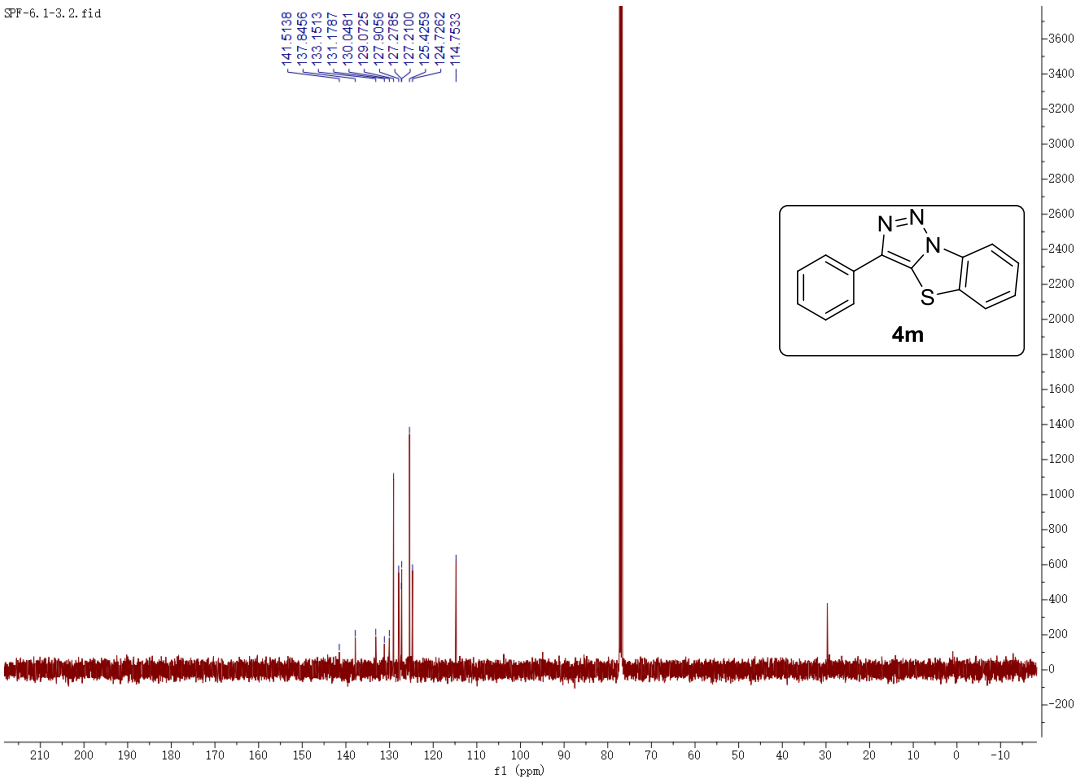
Compound 6b


7.7367
7.7333
7.7244
7.7204
7.5747
7.5719
7.5595
7.5567
7.4418
7.4386
7.4275
7.4255
7.4237
7.3668
7.3641
7.3520
7.3491
7.3371
7.3341
7.3246
7.3212
7.3095
7.3063
7.2943
7.2890
7.2732
7.2602
5.4985
2.3984
2.01
1.01
1.01
4.00
2.00
3.03
N=N
N
Se
6b
f1 (ppm)

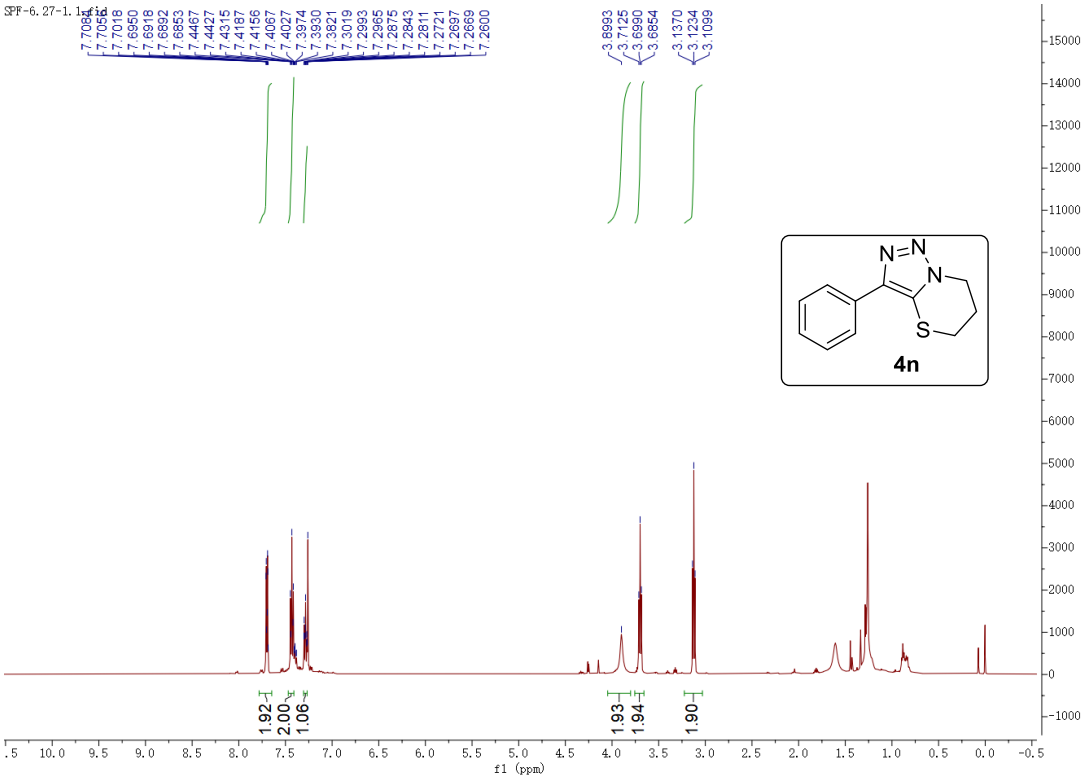

SPF-12.7-1.2.fid
145.1006
137.9604
133.0998
129.5104
129.4935
129.1135
128.9175
128.0417
127.8016
127.3440
126.3113
117.6380
52.3972
21.3269
6b
f1 (ppm)

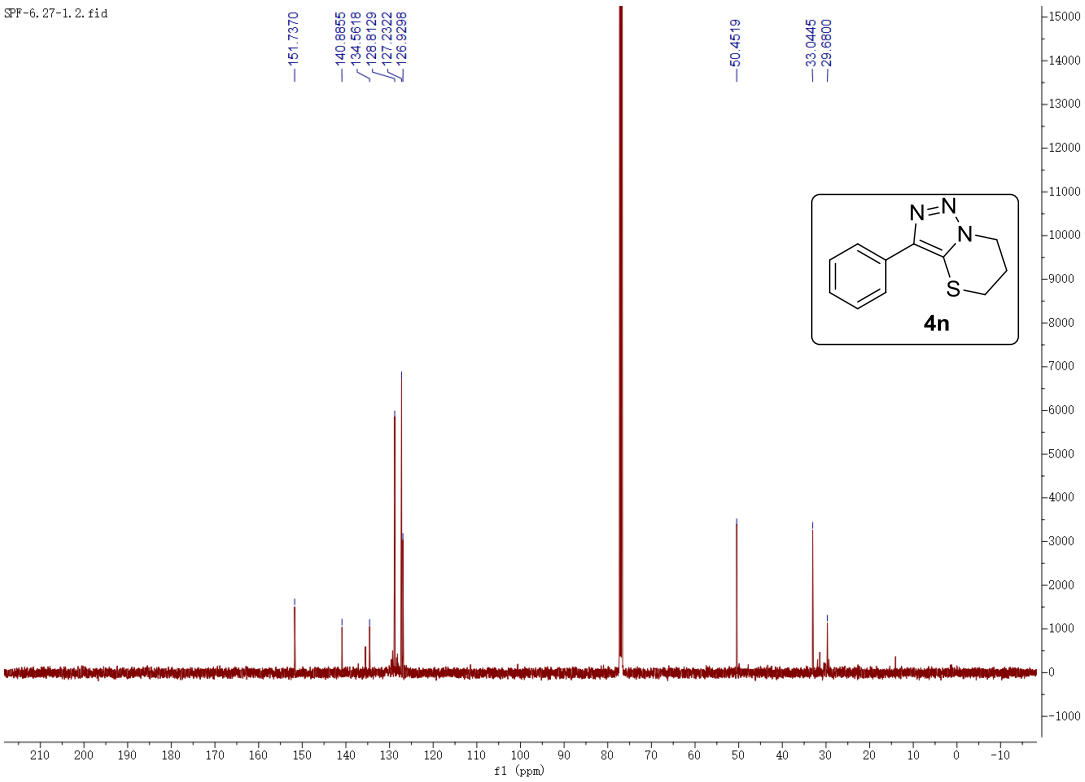
Compound 4m


SPF-6.1-3.1.fid
8.3152
8.3129
8.3101
8.3076
8.2986
8.2941
8.2912
7.9158
7.9130
7.9105
7.9078
7.9038
7.8994
7.8968
7.8937
7.8913
7.8265
7.8229
7.8214
7.8199
7.8108
7.8067
7.8049
7.8037
7.6348
7.6325
7.6256
7.6234
7.6201
7.6179
7.6162
7.6070
7.6039
7.6015
7.5541
7.5510
7.5484
7.5393
7.5345
7.5252
7.5228
7.5197
7.5179
7.5088
7.5064
7.5032
7.3934
7.3903
7.3877
7.3851
7.3784
7.3760
7.3729
7.3698
7.3635
7.3606
7.3580
7.2652
7.2601
4m
1.00
1.99
1.01
1.05
3.07
1.01
f1 (ppm)

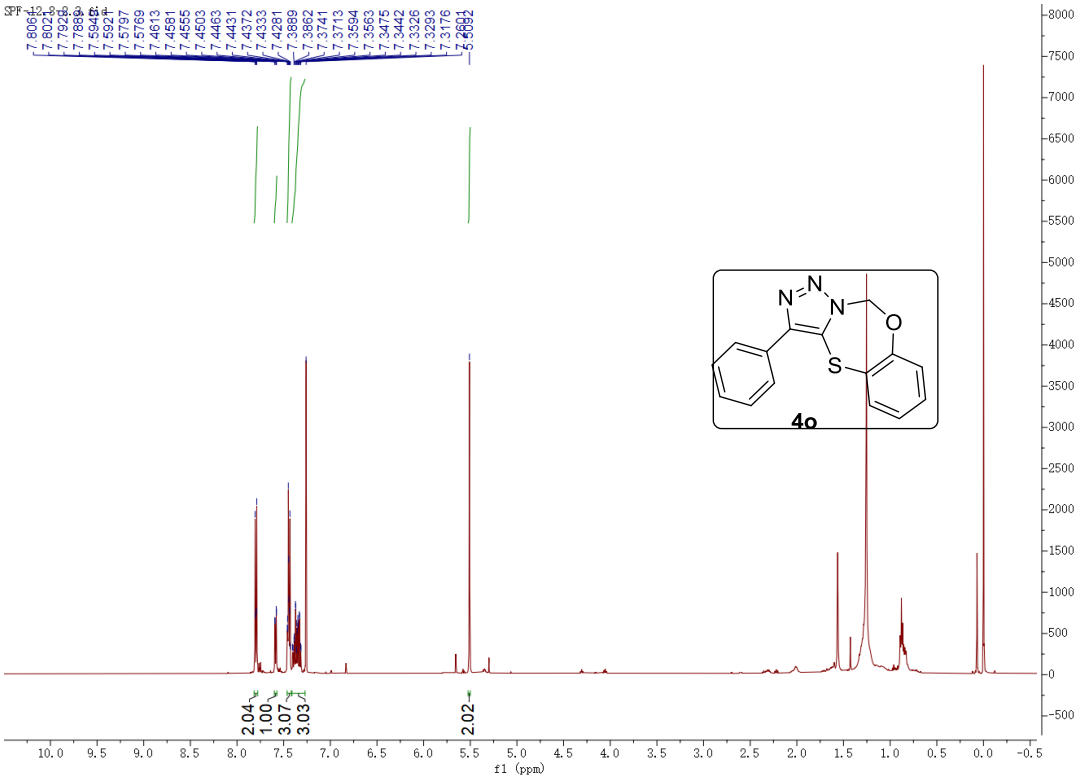

SPF-6.1-3.2.fid
141.5138
137.8456
133.1513
131.1787
130.0481
129.0725
127.9056
127.2785
127.2100
125.4259
124.7262
114.7533
4m
f1 (ppm)

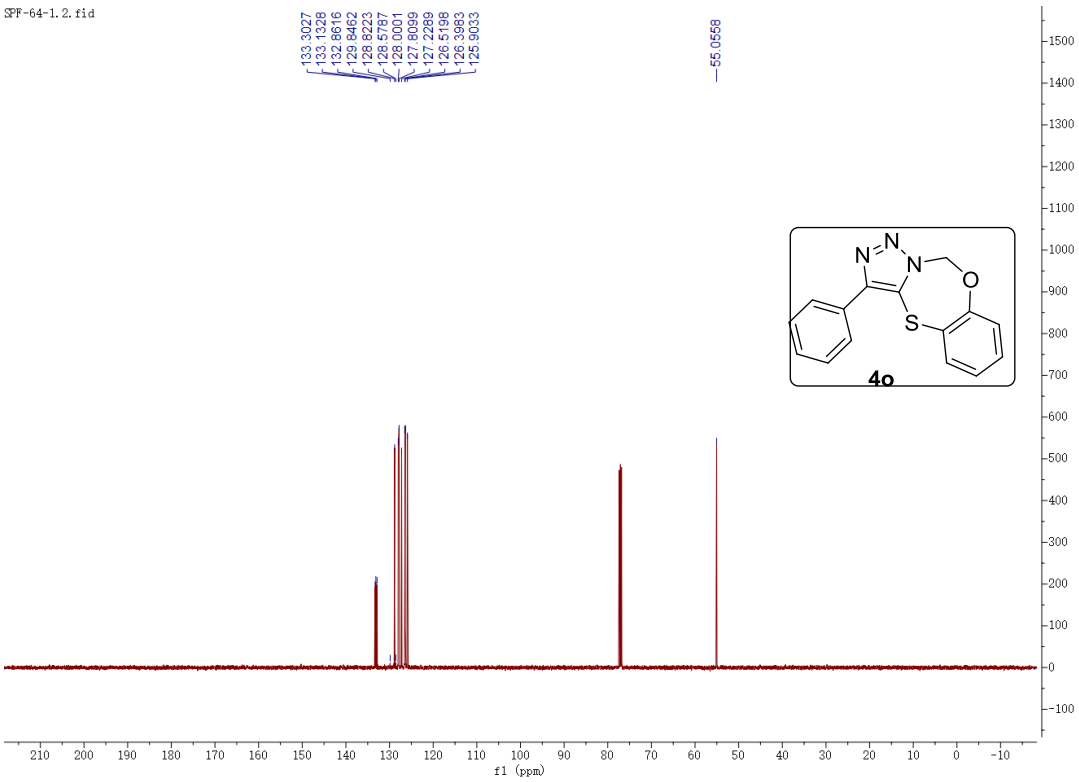
Compound 4n


SPF-6.27-1.1.fid
7.7084
7.7056
7.7018
7.6950
7.6918
7.6892
7.6853
7.4467
7.4427
7.4315
7.4197
7.4156
7.4067
7.4027
7.3974
7.3930
7.3821
7.3019
7.2993
7.2965
7.2875
7.2843
7.2811
7.2721
7.2697
7.2669
7.2600
3.8993
3.7125
3.6990
3.6854
3.1370
3.1234
3.1099
4n
1.92
2.00
1.06
1.93
1.94
1.90
f1 (ppm)

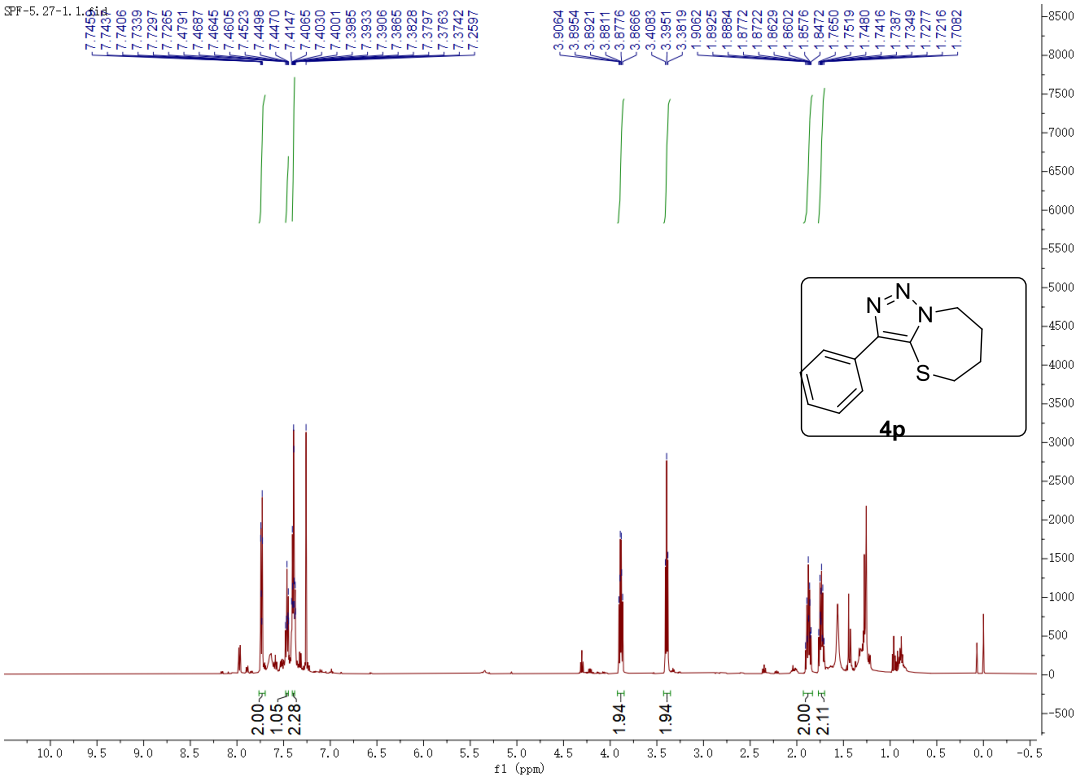

SPF-6.27-1.2.fid
151.7370
140.8855
134.5618
128.8129
127.2322
126.9298
50.4519
33.0445
29.6800
4n
f1 (ppm)

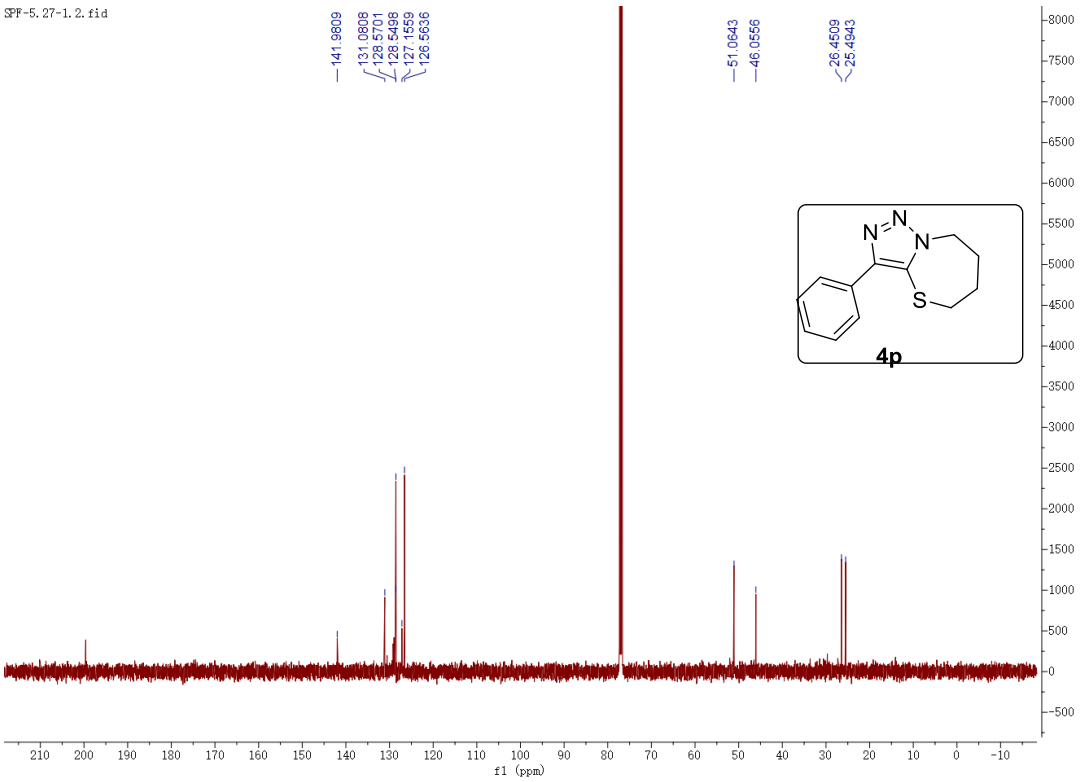
Compound 4o


7.8061
7.8025
7.7928
7.7889
7.5948
7.5924
7.5797
7.5769
7.4613
7.4581
7.4555
7.4503
7.4463
7.4431
7.4372
7.4333
7.4281
7.3889
7.3862
7.3741
7.3713
7.3594
7.3563
7.3475
7.3442
7.3326
7.3293
7.3176
7.2601
5.8092
2.04
1.00
3.07
3.03
2.02
4o
f1 (ppm)

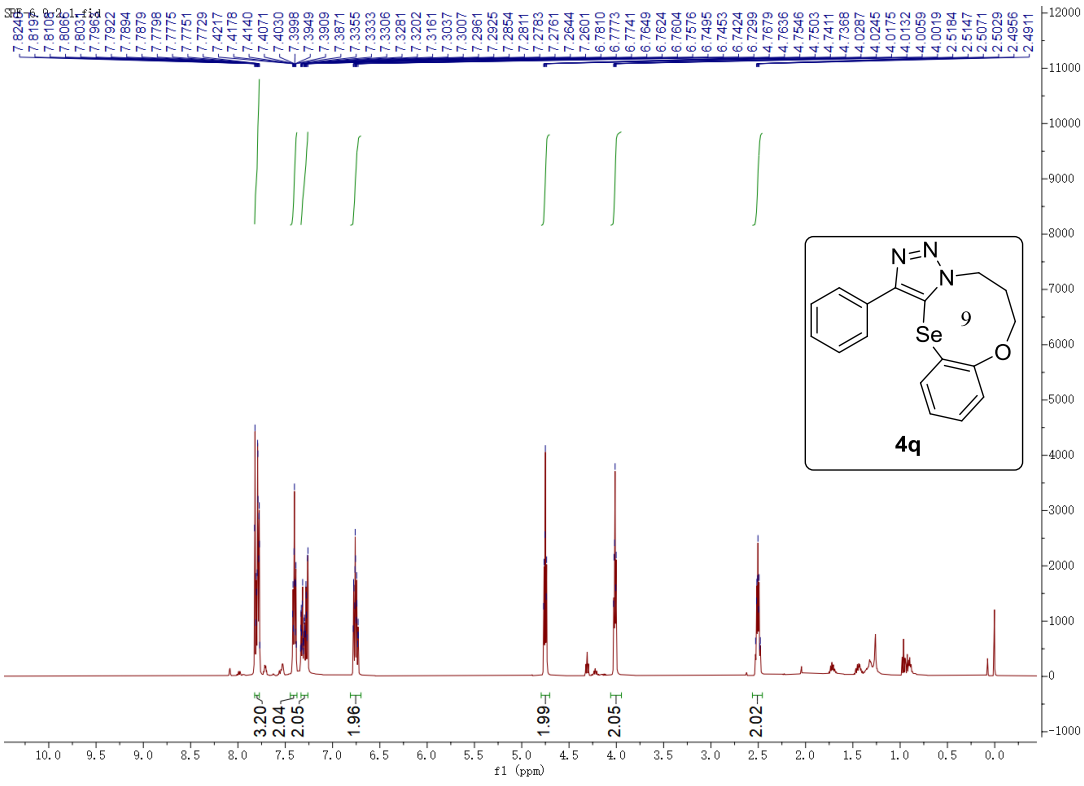

SPF-64-1.2.fid
133.3027
133.1328
132.8616
129.8462
128.8223
128.5787
128.0001
127.8099
127.2289
126.5198
126.3983
125.9033
55.0558
4o
f1 (ppm)

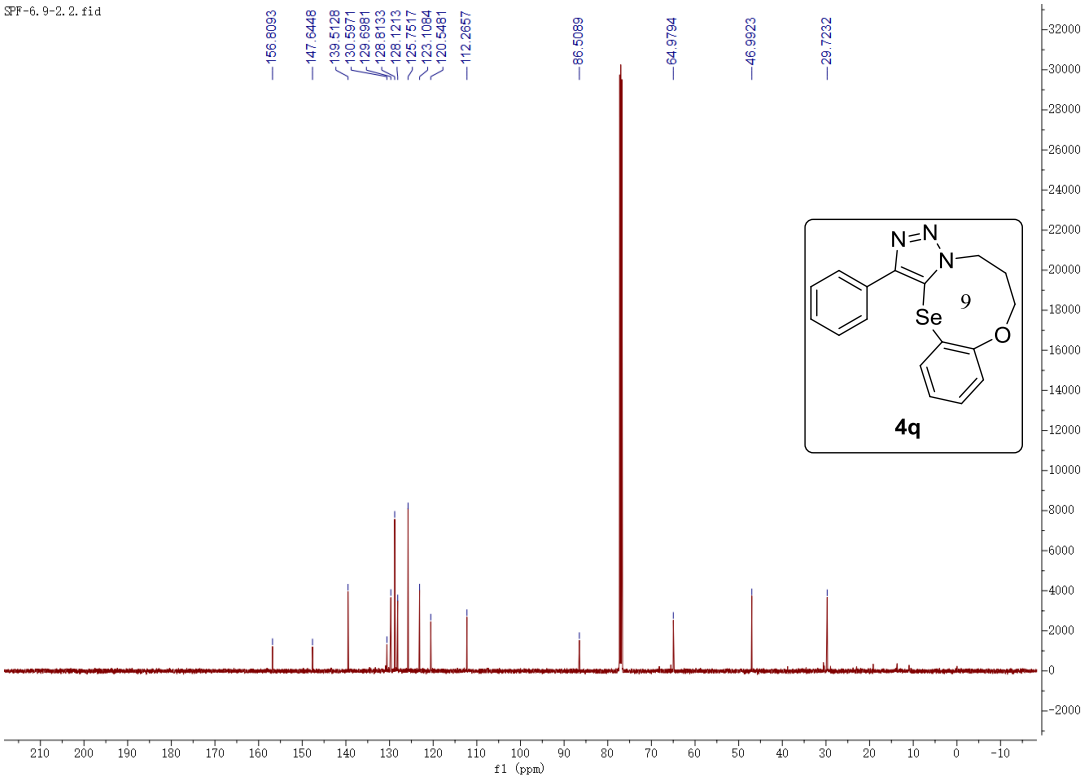
Compound 4p


SPF-5.27-1.1.fid
7.7456
7.7437
7.7406
7.7339
7.7297
7.7265
7.4791
7.4687
7.4645
7.4605
7.4523
7.4498
7.4470
7.4147
7.4065
7.4030
7.4001
7.3985
7.3933
7.3906
7.3865
7.3828
7.3797
7.3763
7.3742
7.2597
3.9064
3.8954
3.8921
3.8811
3.8776
3.8666
3.4083
3.3951
3.3819
1.9062
1.8925
1.8884
1.8772
1.8722
1.8629
1.8602
1.8576
1.8472
1.7650
1.7519
1.7480
1.7416
1.7387
1.7349
1.7277
1.7216
1.7082
4p
2.00
1.05
2.28
1.94
1.94
2.00
2.11
f1 (ppm)

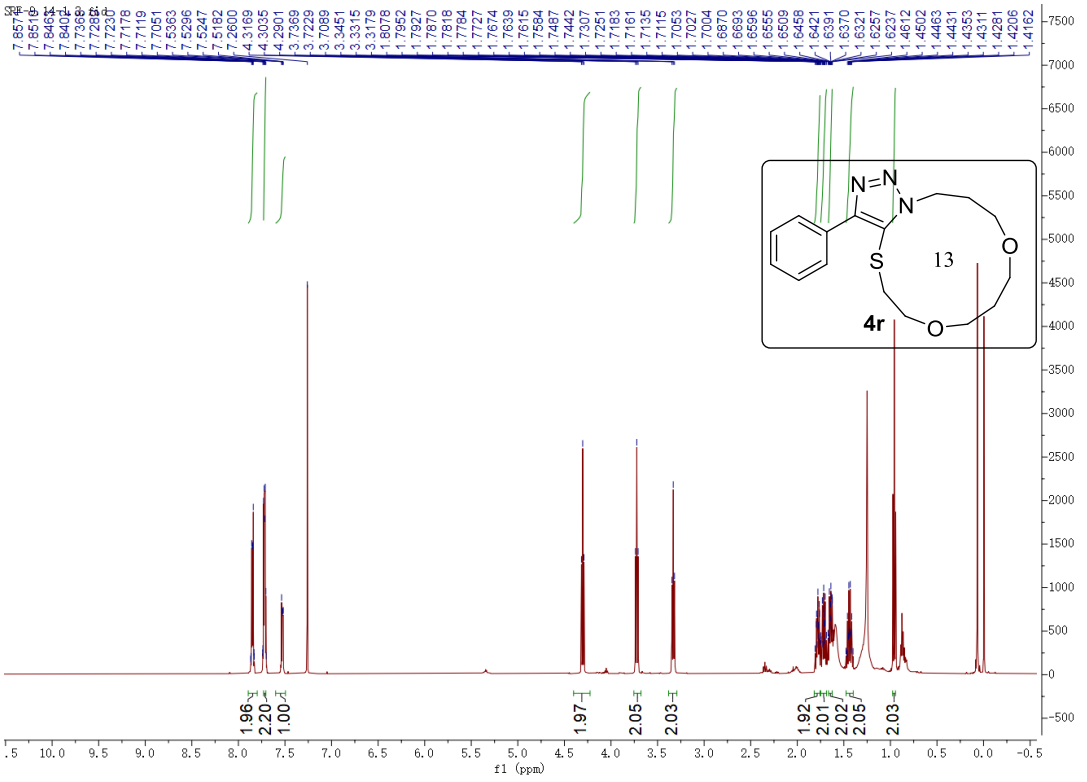

SPF-5.27-1.2.fid
141.9809
131.0808
128.5701
128.5498
127.1559
126.5636
51.0643
46.0556
26.4509
25.4943
4p
f1 (ppm)

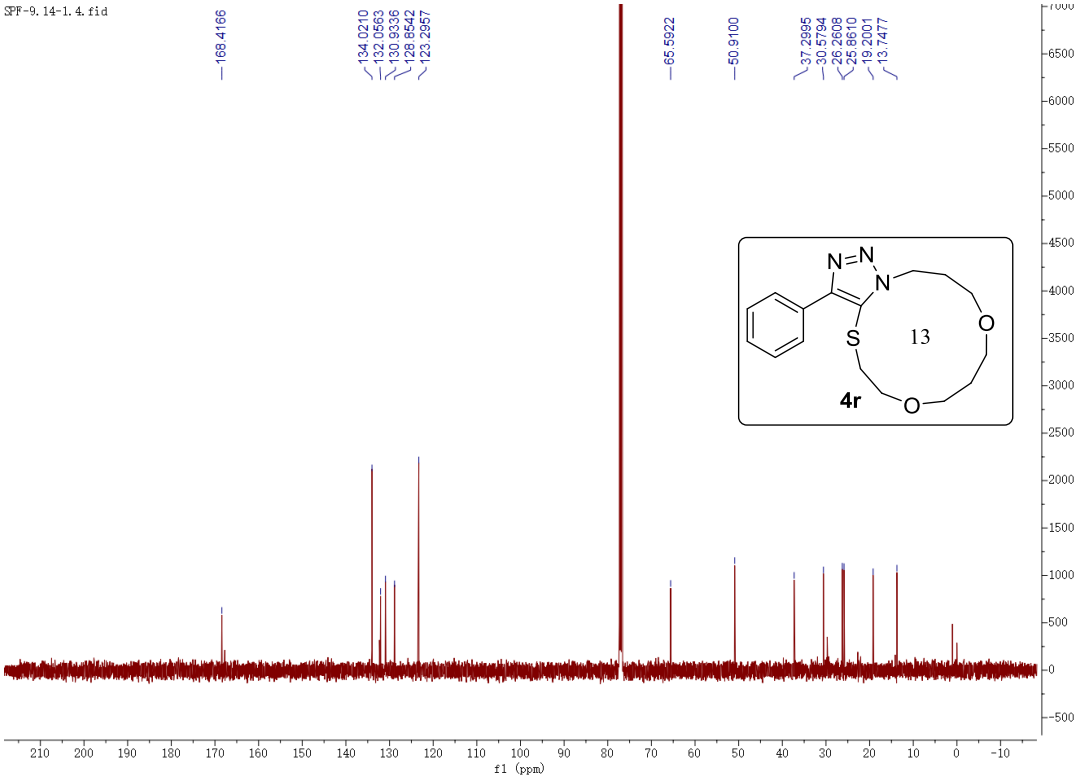
Compound 4q


4q
3.20
2.04
2.05
1.96
1.99
2.05
2.02
f1 (ppm)

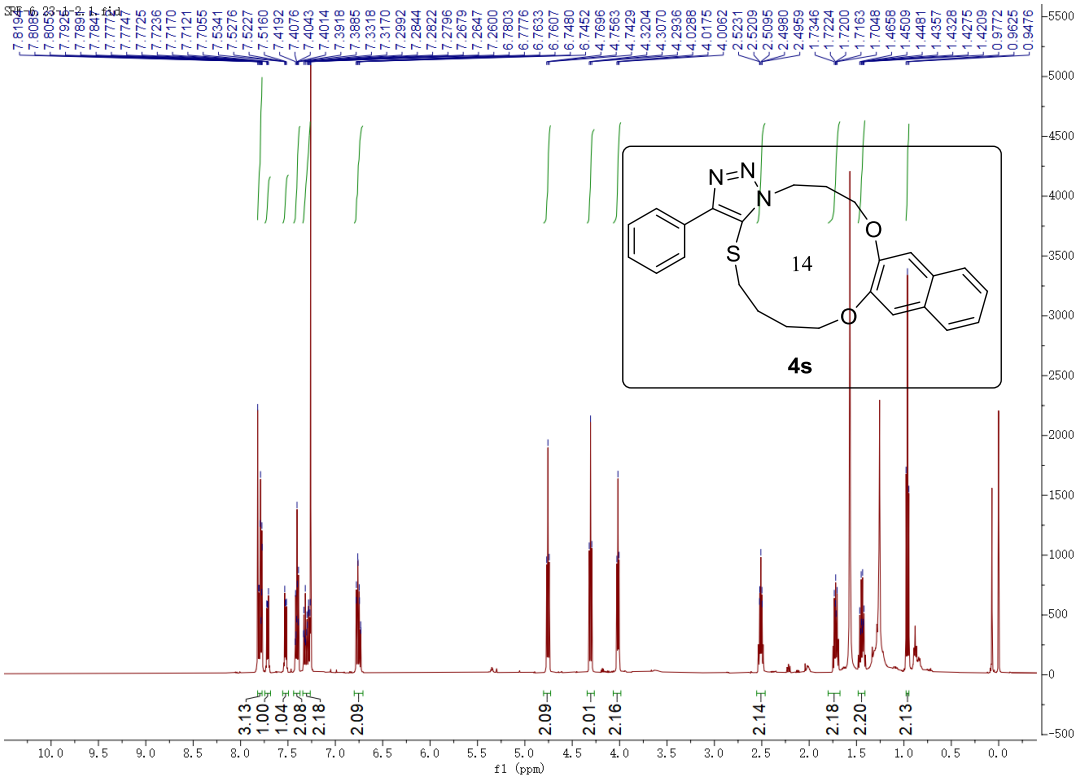

SPF-6.9-2.2.fid
156.8093
147.6448
139.5126
130.5971
129.6981
128.8133
128.1213
125.7517
123.1084
120.5481
112.2657
86.5089
64.9794
46.9923
29.7232
N=N
N
9
Se
O
4q
f1 (ppm)

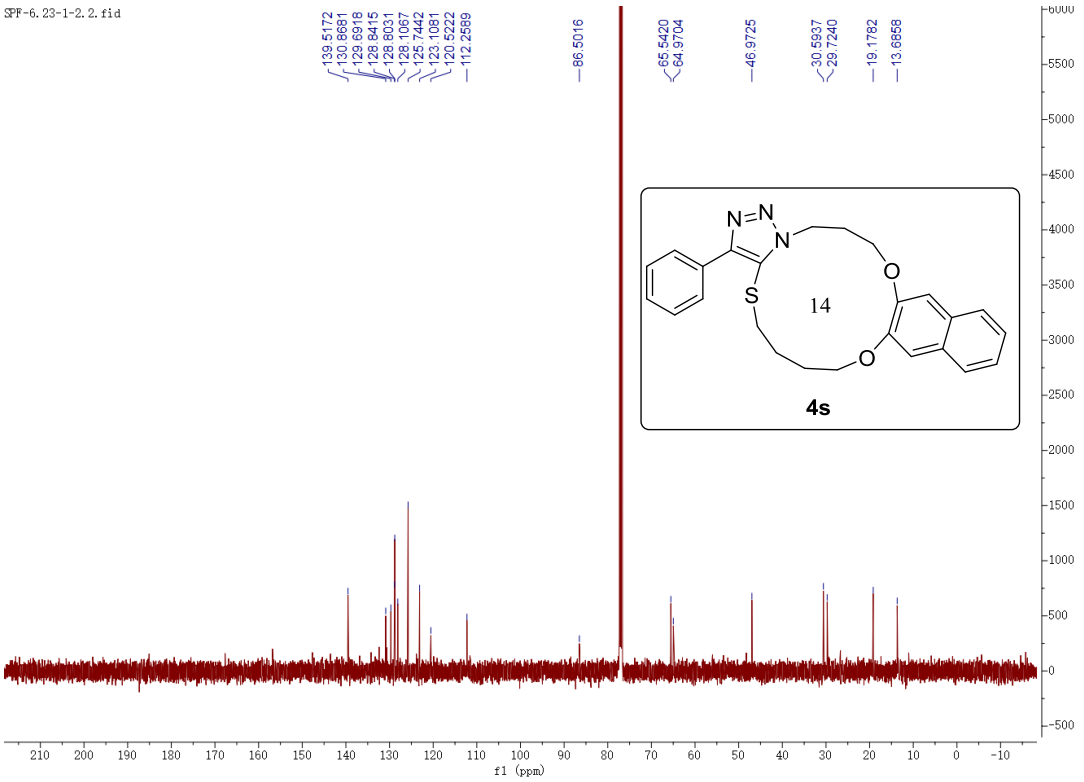
Compound 4r


N=N
N
S
13
O
O
4r
1.96
2.20
1.00
1.97
2.05
2.03
1.92
2.01
2.02
2.05
2.03
f1 (ppm)

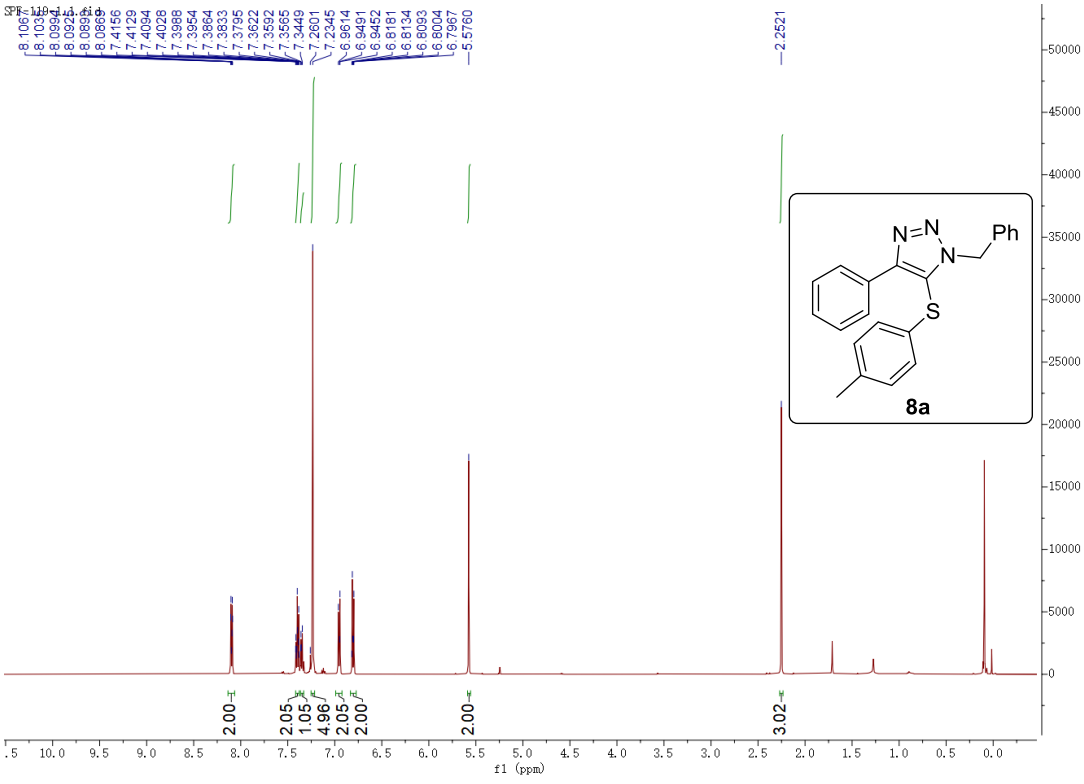

SPF-9.14-1.4.fid
168.4166
134.0210
132.0563
130.9336
128.6542
123.2957
65.5922
50.9100
37.2995
30.5794
26.2608
25.8610
19.2001
13.7477
N=N
N
S
O
O
13
4r
f1 (ppm)

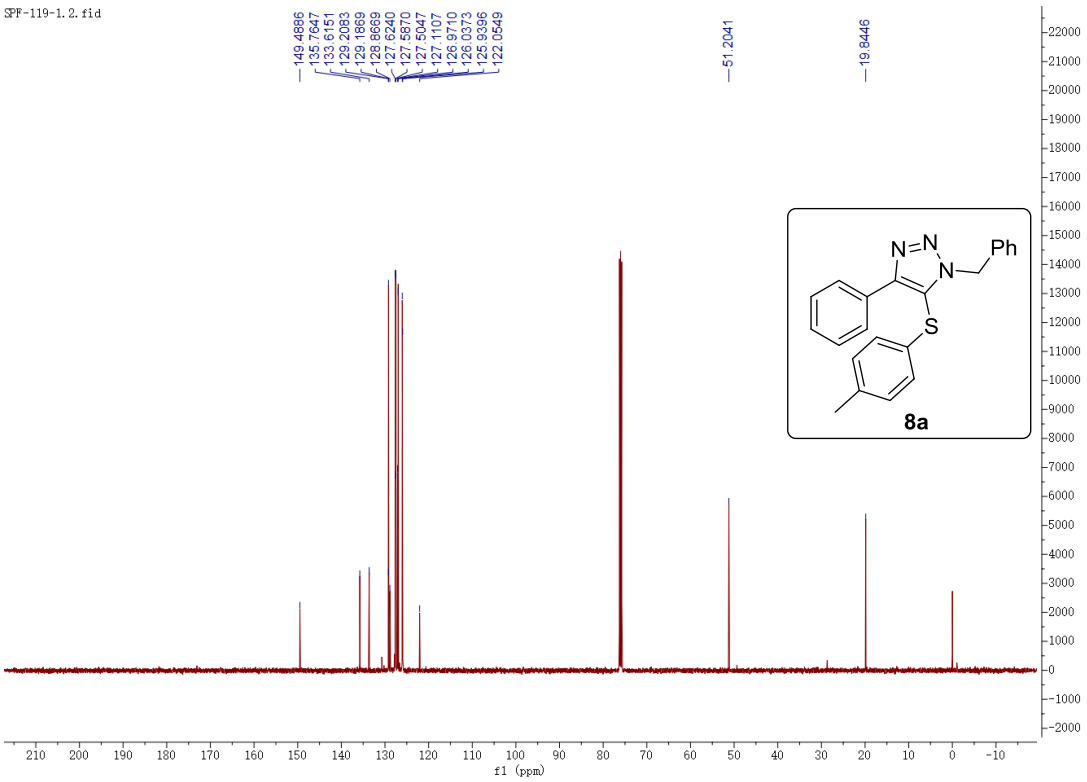
Compound 4t


N=N
N
S
O
O
14
4s
3.13
1.00
1.04
2.08
2.18
2.09
2.09
2.01
2.16
2.14
2.18
2.20
2.13
f1 (ppm)

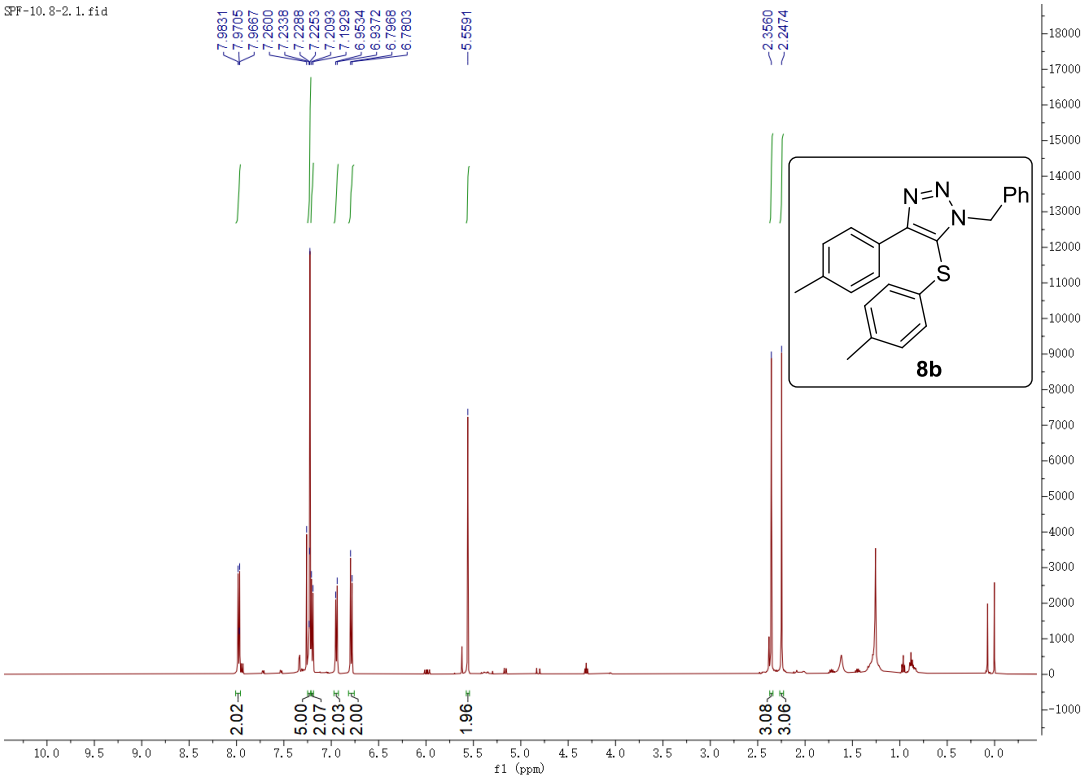

SPF-6.23-1-2.2.fid
139.5172
130.8681
129.6918
128.8415
128.8031
128.1067
125.7442
123.1081
120.5222
112.2589
86.5016
65.5420
64.9704
46.9725
30.5937
29.7240
19.1782
13.6858
14
4s
f1 (ppm)

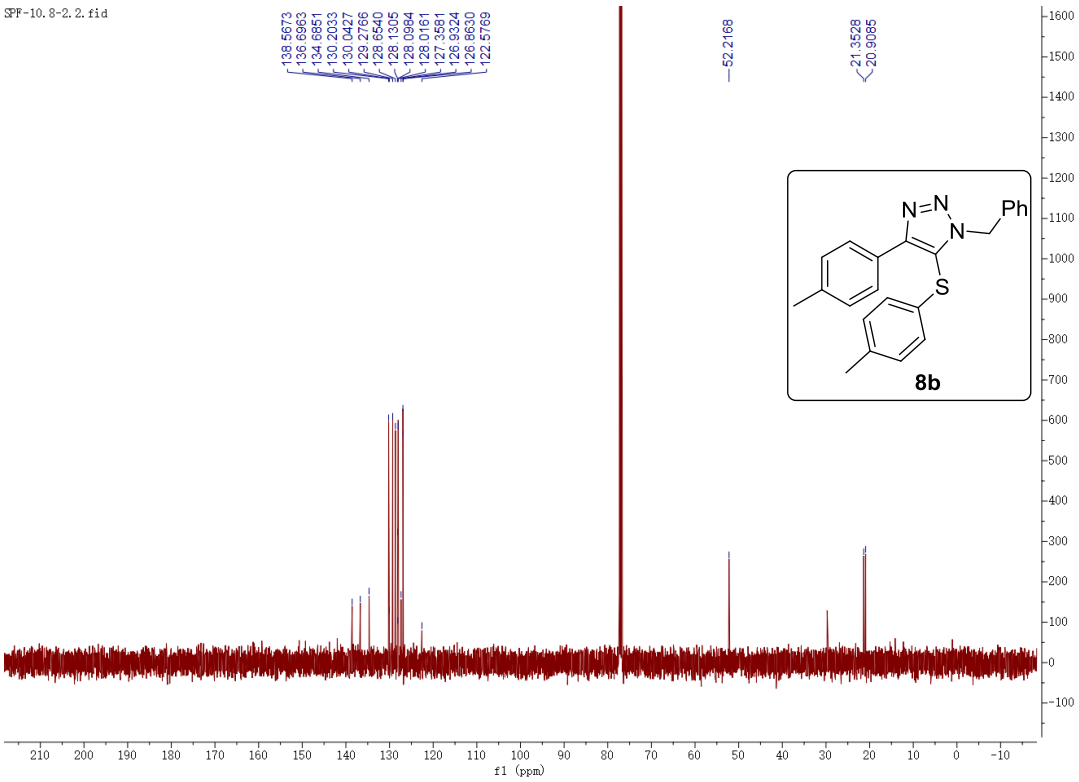
Compound 8a


8.1067
8.1035
8.0994
8.0925
8.0869
8.0818
7.4156
7.4129
7.4094
7.4028
7.3988
7.3954
7.3864
7.3833
7.3795
7.3622
7.3592
7.3565
7.3449
7.2601
7.2345
6.9614
6.9491
6.9452
6.8181
6.8134
6.8093
6.8004
6.7967
5.5760
2.2521
Ph
8a
2.00
2.05
1.05
4.96
2.05
2.00
2.00
3.02
f1 (ppm)

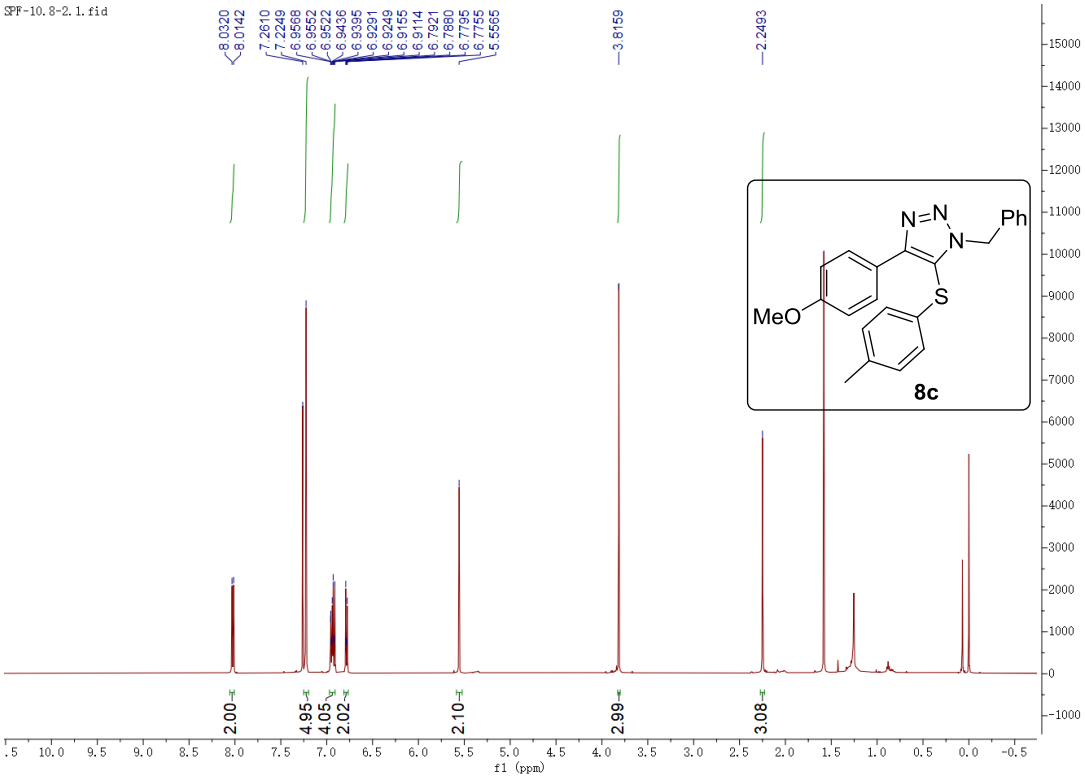

SPF-119-1.2.fid
149.4886
135.7647
133.6151
129.2083
129.1869
128.8669
127.6240
127.5870
127.5047
127.1107
126.9710
126.0373
125.9396
122.0549
51.2041
19.8446
N=N
N
Ph
S
8a
f1 (ppm)

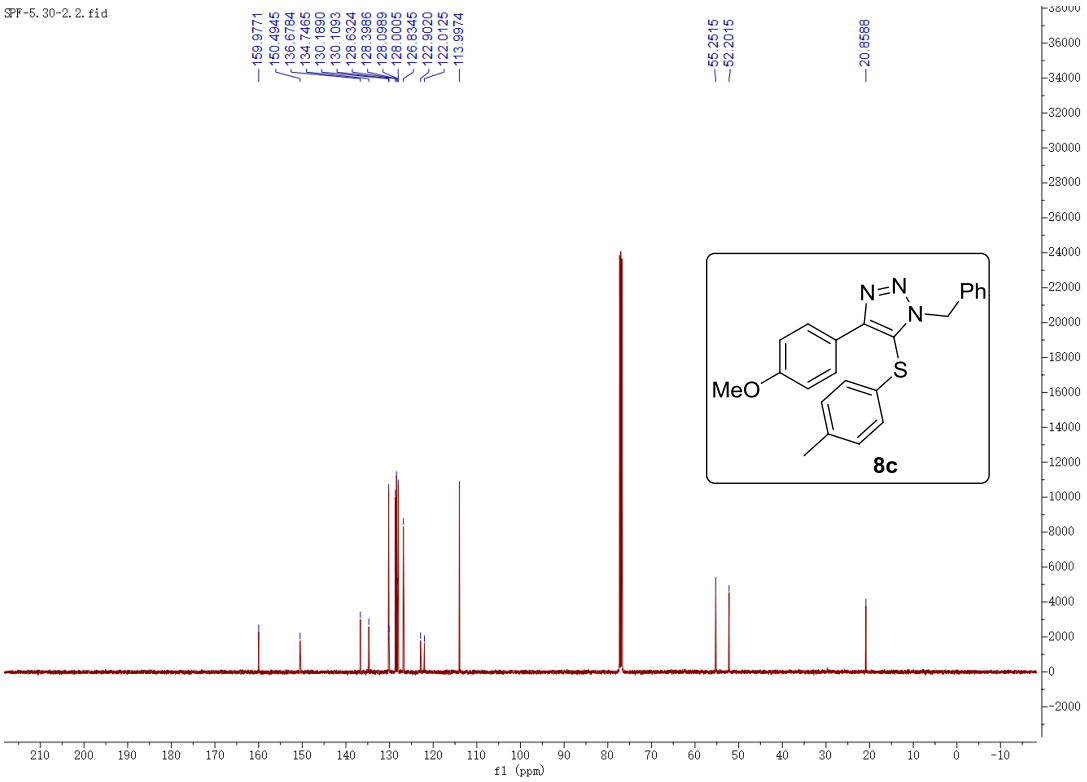
Compound 8b


SPF-10.8-2.1.fid
7.9831
7.9705
7.9667
7.2600
7.2338
7.2288
7.2253
7.2093
7.1929
6.9534
6.9372
6.7968
6.7803
5.5591
2.3560
2.2474
2.02
5.00
2.07
2.03
2.00
1.96
3.08
3.06
N=N
N
Ph
S
8b
f1 (ppm)

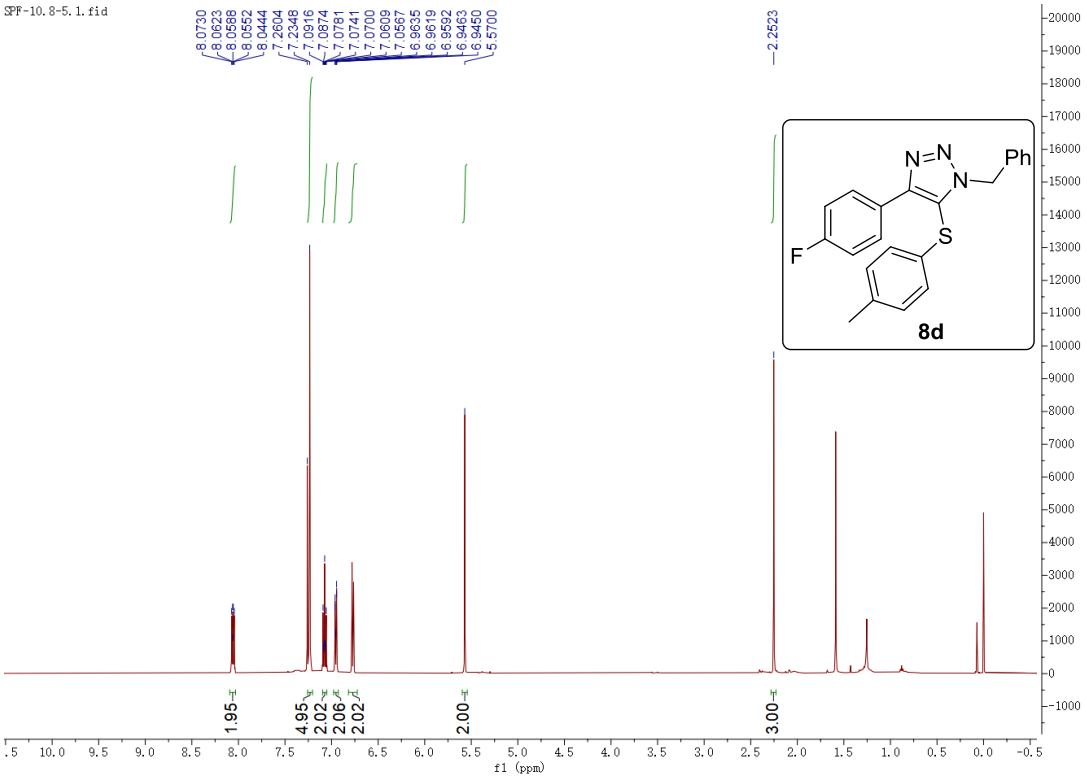

SPF-10.8-2.2.fid
138.5673
136.6963
134.6851
130.2033
130.0427
129.2766
128.6540
128.1305
128.0984
128.0161
127.3581
126.9324
126.8630
122.5769
52.2168
21.3528
20.9085
N=N
N
Ph
S
8b
f1 (ppm)

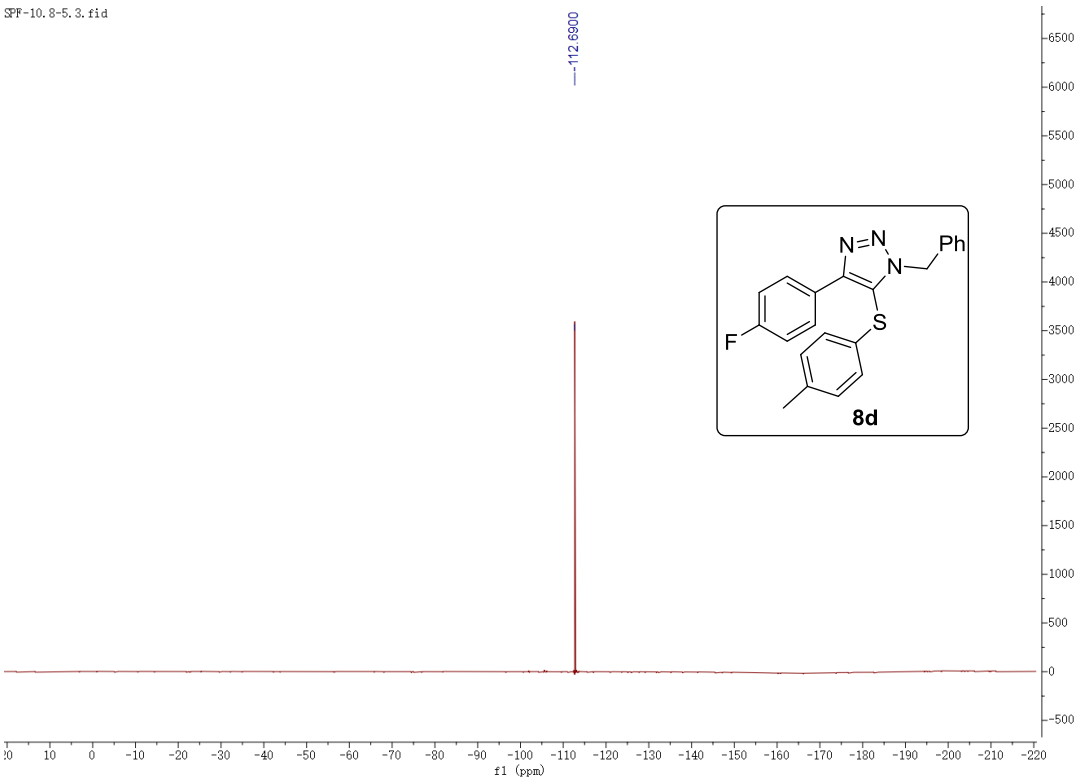
Compound 8c

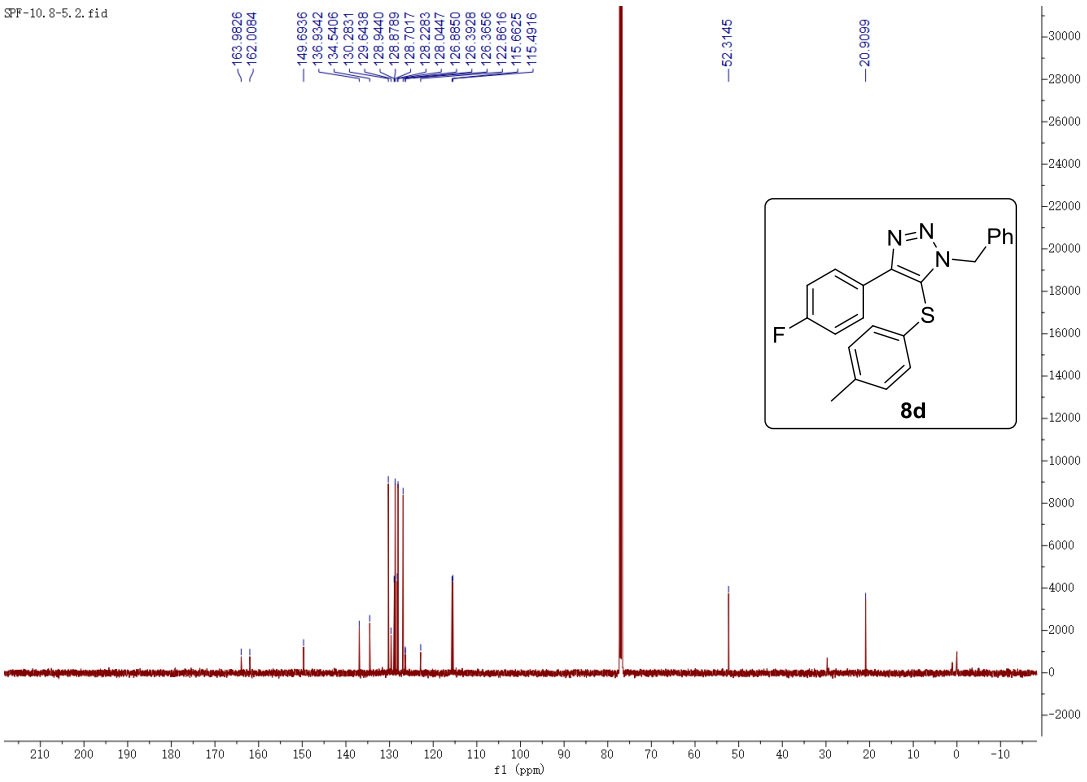

SPF-10.8-2.1.fid
8.0320
8.0142
7.2610
7.2249
6.9568
6.9552
6.9522
6.9436
6.9395
6.9291
6.9249
6.9155
6.9114
6.7921
6.7880
5.7795
5.7755
5.5565
3.8159
2.2493
2.00
4.95
4.05
2.02
2.10
2.99
3.08
N=N
N
Ph
S
MeO
8c
f1 (ppm)


SPF-5.30-2.2.fid
159.9771
150.4945
136.6784
134.7465
130.1890
130.1093
128.8324
128.3986
128.0989
128.0005
126.8345
122.9020
122.0125
113.9974
55.2515
52.2015
20.8588
N=N
N
Ph
S
MeO
8c
f1 (ppm)

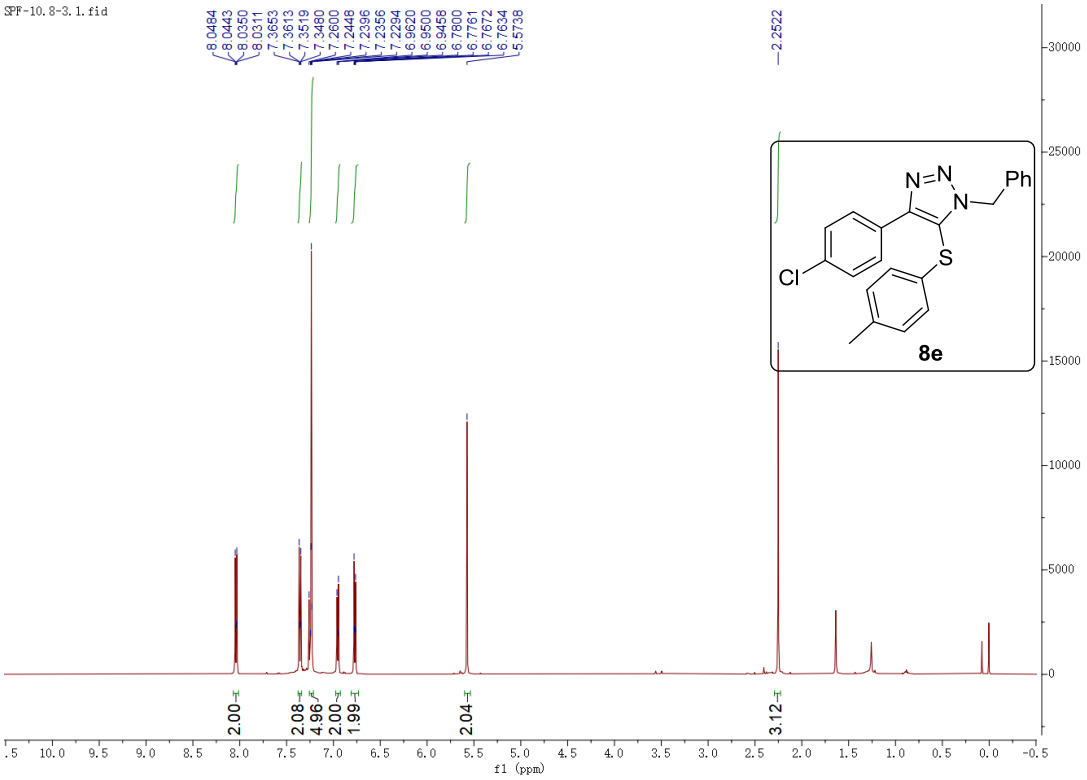
Compound 8d

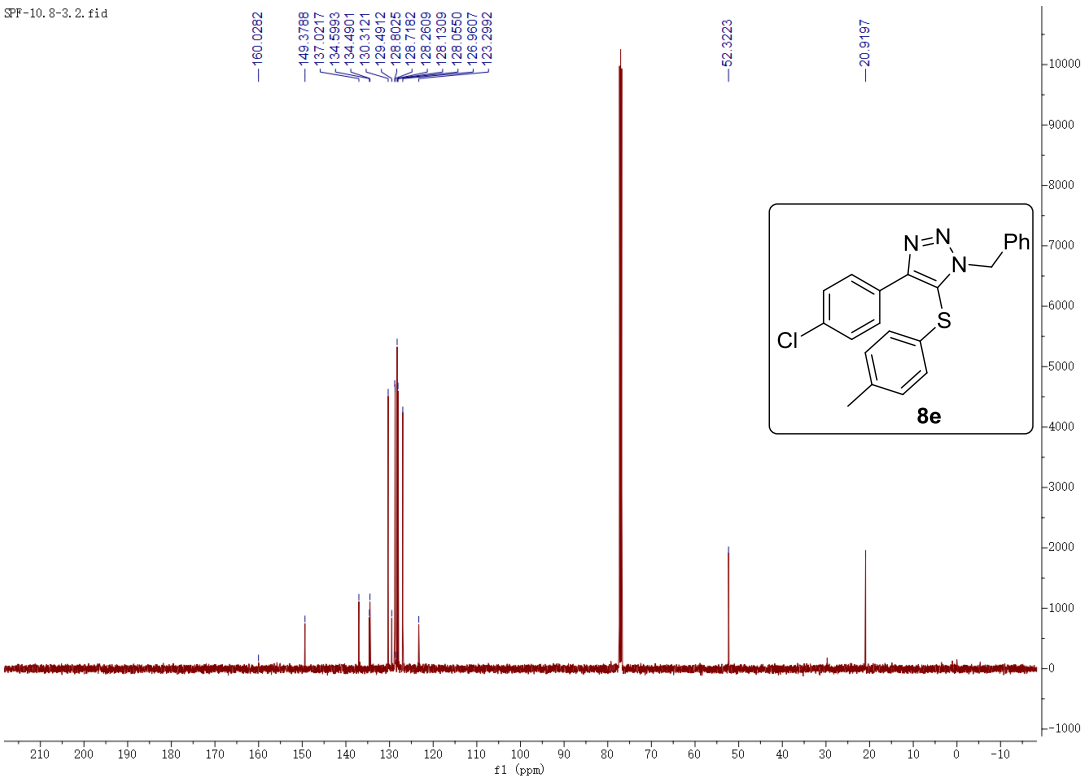

SPF-10.8-5.1.fid
8.0730
8.0623
8.0588
8.0552
8.0444
7.2604
7.2348
7.0916
7.0874
7.0781
7.0741
7.0700
7.0609
7.0567
6.9635
6.9619
6.9592
6.9463
6.9450
5.5700
2.2523
N=N
N
Ph
S
F
8d
1.95
4.95
2.02
2.06
2.02
2.00
3.00
f1 (ppm)


SPF-10.8-5.3.fid
-112.6900
N=N
Ph
N
S
F
8d
f1 (ppm)

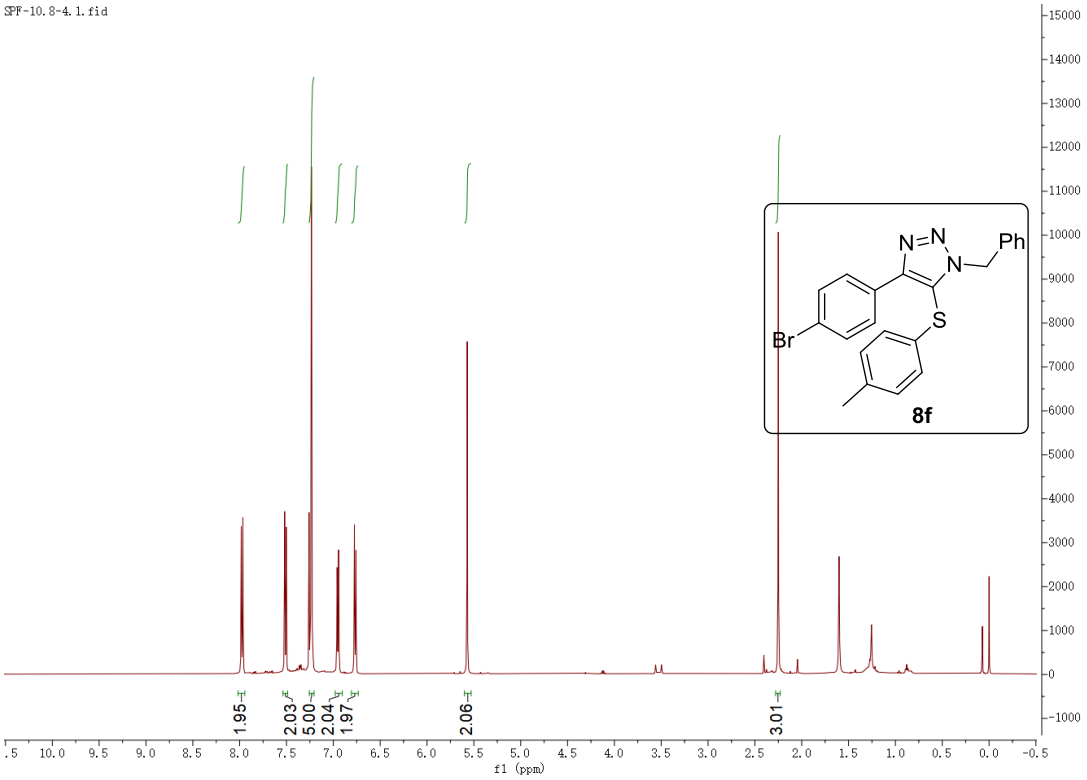

SPF-10.8-5.2.fid
163.9826
162.0084
149.6936
136.9342
134.5406
130.2831
129.6438
128.9440
128.8789
128.7017
128.2283
128.0447
126.8850
126.3928
126.3656
122.8616
115.6625
115.4916
52.3145
20.9099
N=N
Ph
N
S
F
8d
f1 (ppm)

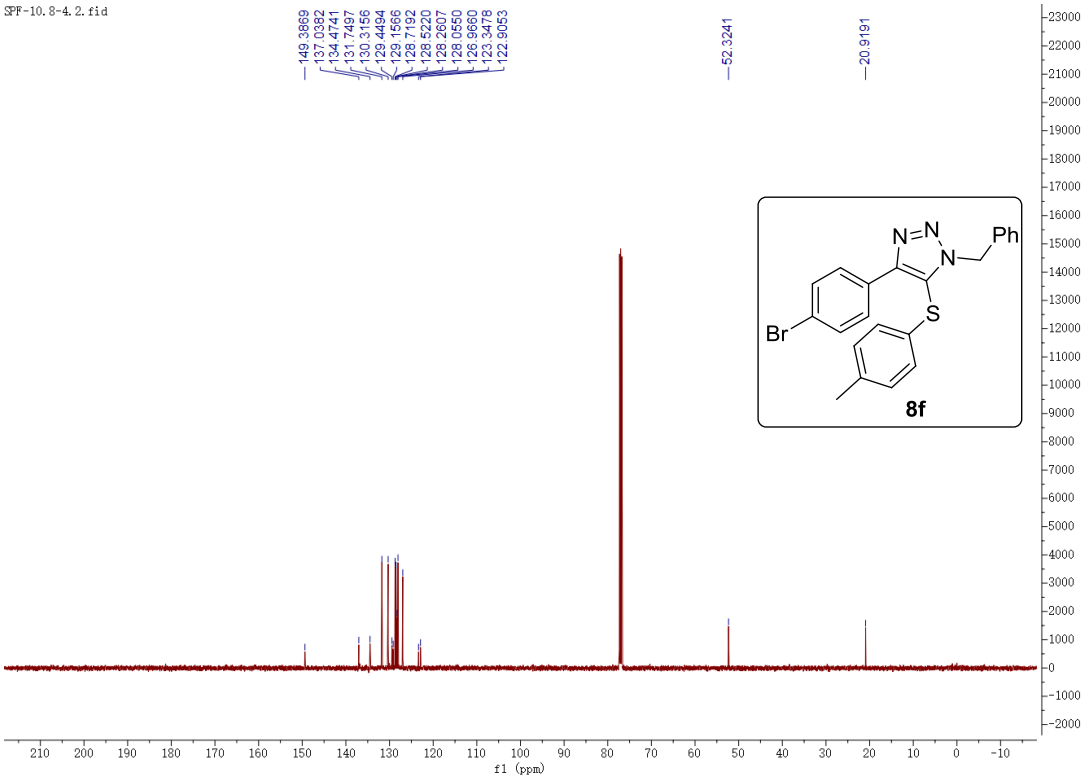
Compound 8e


SPF-10.8-3.1.fid
8.0484
8.0443
8.0350
8.0311
7.3653
7.3613
7.3519
7.3480
7.2600
7.2448
7.2396
7.2356
7.2294
6.9620
6.9500
6.9458
6.7800
6.7761
6.7672
6.7634
5.5738
2.2522
2.00
2.08
4.96
2.00
1.99
2.04
3.12
f1 (ppm)
N
N
Ph
S
Cl
8e

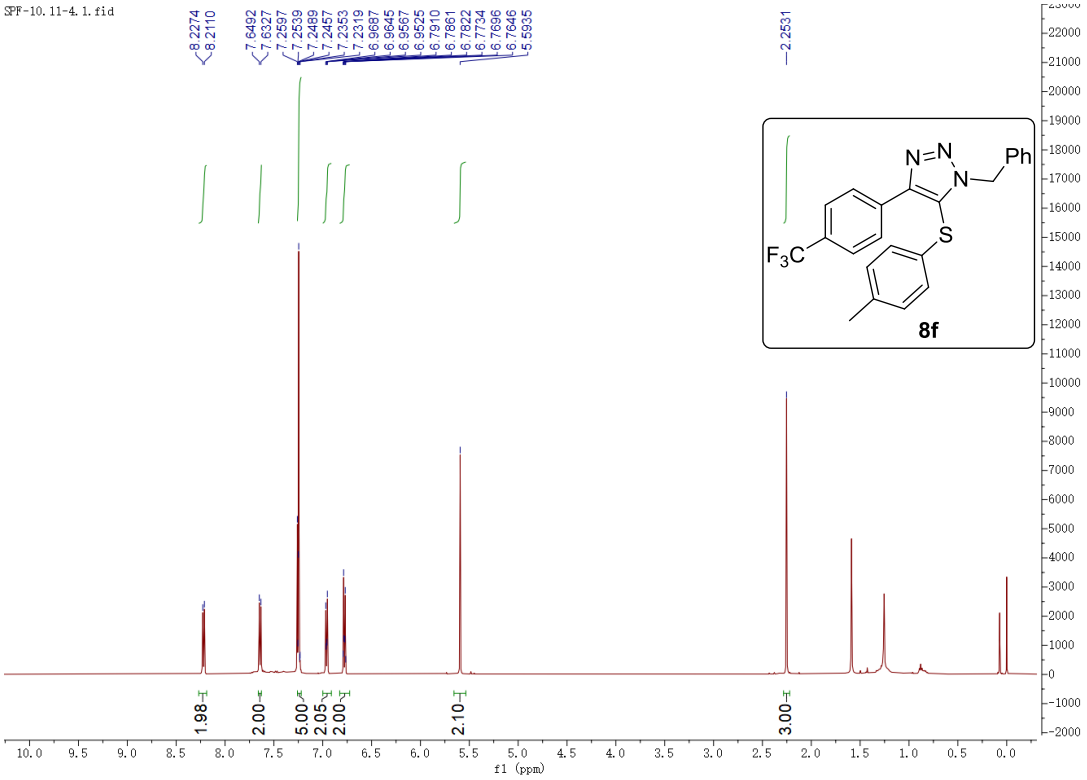

SPF-10.8-3.2.fid
160.0282
149.3788
137.0217
134.5993
134.4901
130.3121
129.4912
128.8025
128.7182
128.2609
128.1309
128.0550
126.9607
123.2992
52.3223
20.9197
f1 (ppm)
N
N
Ph
S
Cl
8e

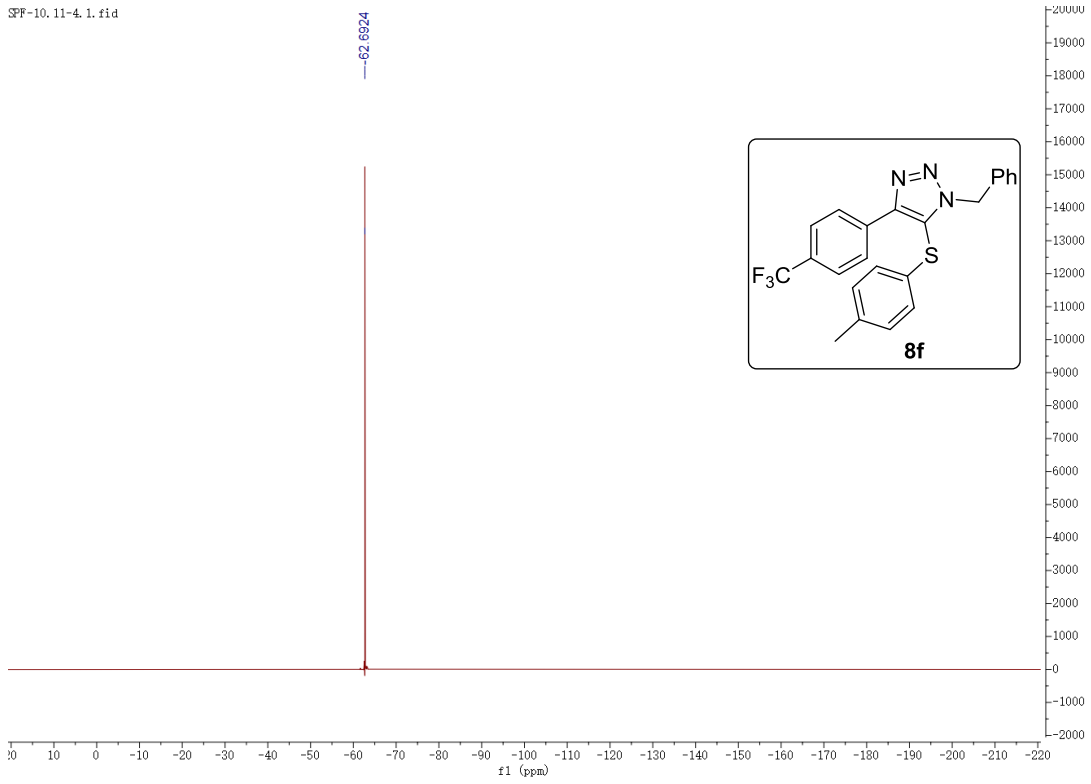
Compound 8f

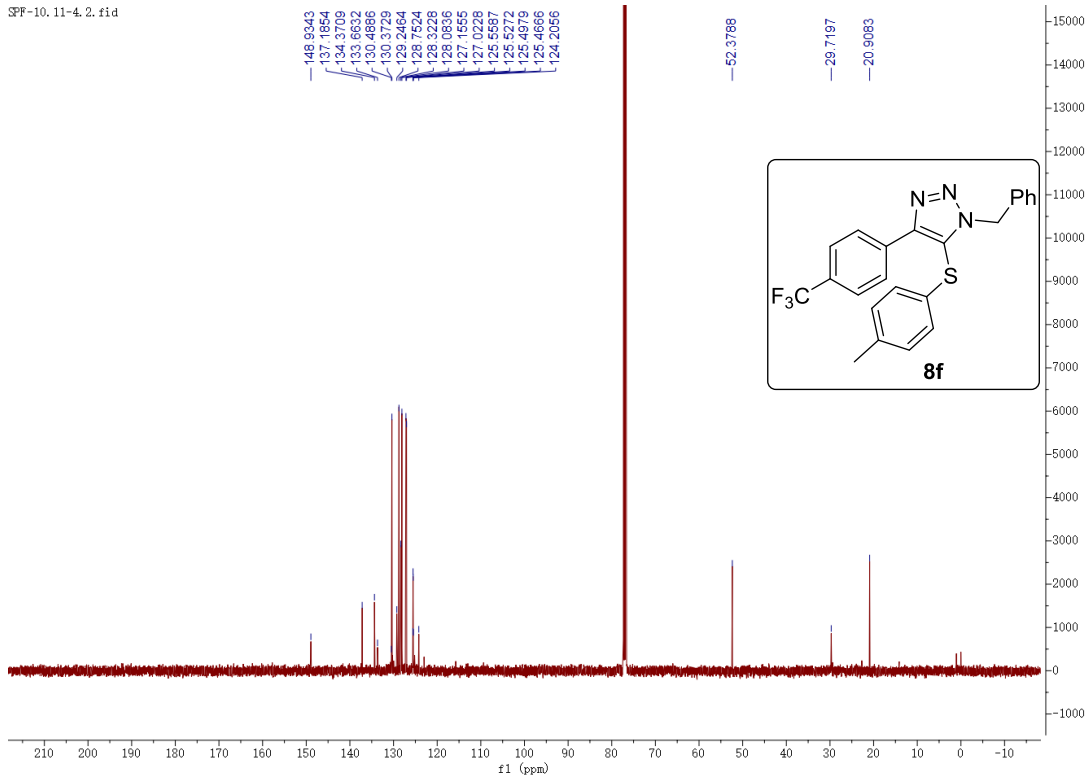

SPF-10.8-4.1.fid
1.95
2.03
5.00
2.04
1.97
2.06
3.01
f1 (ppm)
N=N
Ph
N
S
Br
8f


SPF-10.8-4.2.fid
149.3869
137.0382
134.4741
131.7497
130.3156
129.4494
129.1566
128.7192
128.5220
128.2607
128.0550
126.9660
123.3478
122.9053
52.3241
20.9191
f1 (ppm)
N=N
Ph
N
S
Br
8f

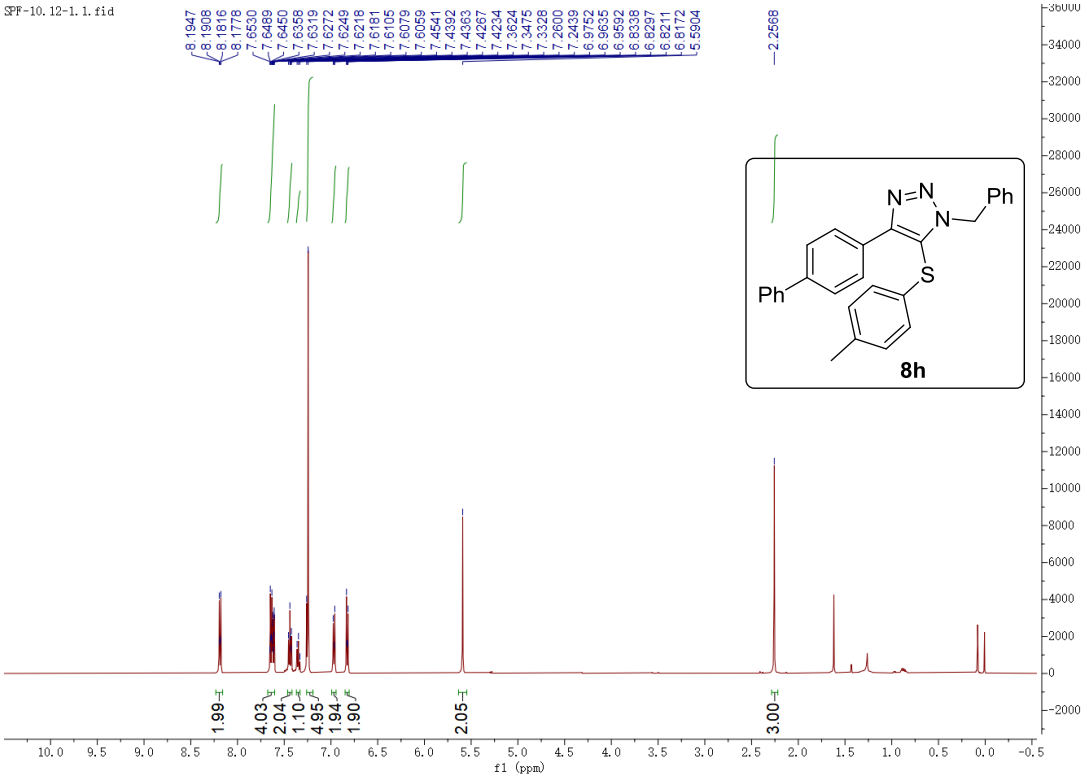
Compound 8g

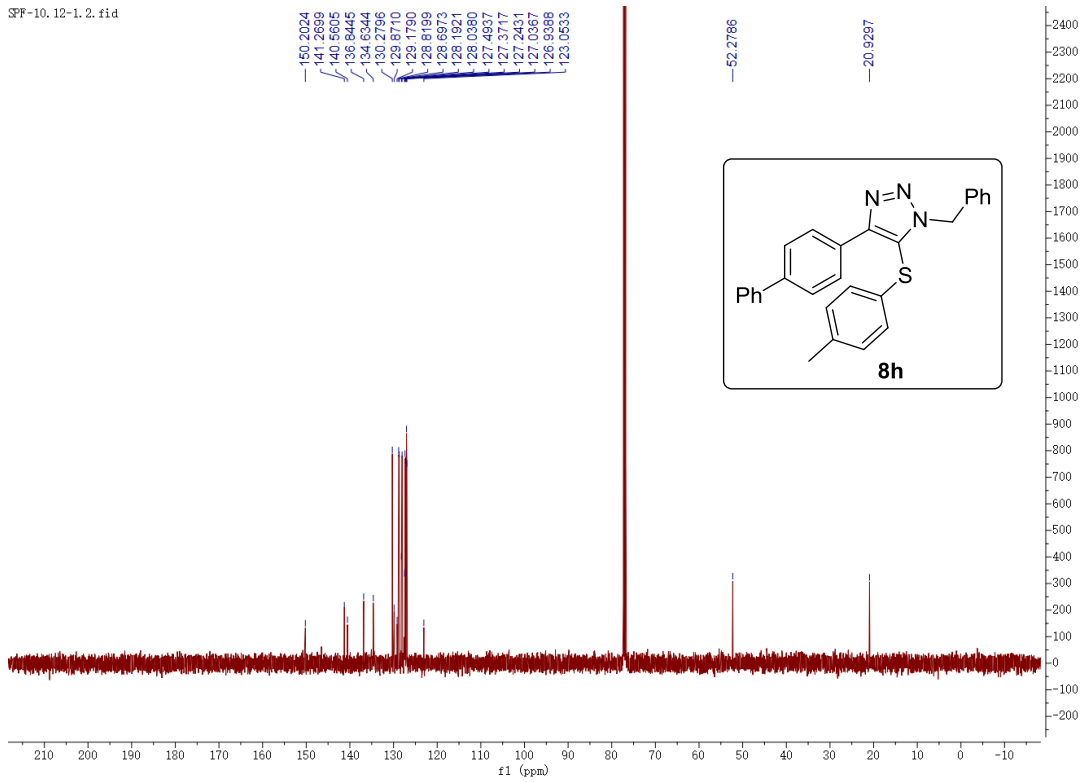

SPF-10.11-4.1.fid
8.2274
8.2110
7.6492
7.6327
7.2597
7.2539
7.2489
7.2457
7.2353
7.2319
6.9687
6.9645
6.9567
6.9525
6.7910
6.7861
6.7822
6.7734
6.7696
6.7646
5.5935
2.2531
1.98
2.00
5.00
2.05
2.00
2.10
3.00
f1 (ppm)
8f


SPF-10.11-4.1.fid
-62.6924
f1 (ppm)
8f

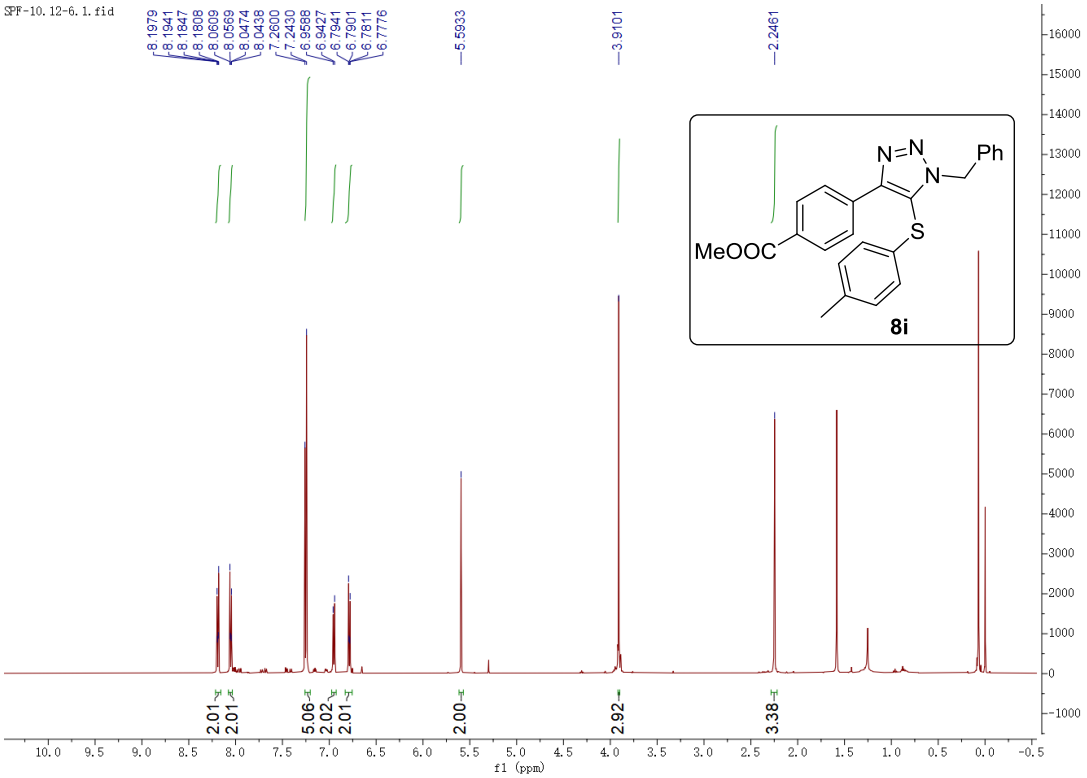

SPF-10.11-4.2.fid
148.9343
137.1854
134.3709
133.6632
130.4686
130.3729
129.2464
128.7524
128.3228
128.0836
127.1555
127.0228
125.5587
125.5272
125.4979
125.4666
124.2056
52.3788
29.7197
20.9083
N=N
Ph
N
S
F3C
8f
f1 (ppm)

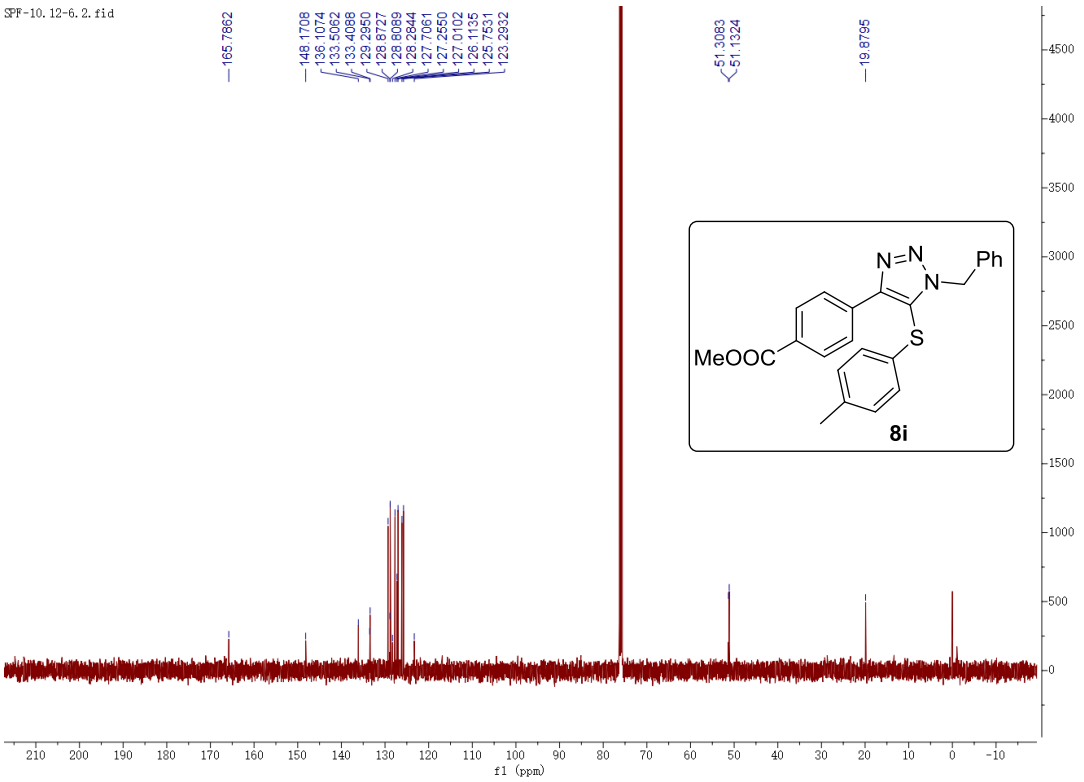
Compound 8h


SPF-10.12-1.1.fid
8.1947
8.1908
8.1816
8.1778
7.6530
7.6489
7.6450
7.6358
7.6319
7.6272
7.6249
7.6218
7.6181
7.6105
7.6079
7.6059
7.4541
7.4392
7.4363
7.4267
7.4234
7.3624
7.3475
7.3328
7.2600
7.2439
6.9752
6.9635
6.9592
6.8338
6.8297
6.8211
6.8172
5.5904
2.2568
N=N
Ph
N
S
Ph
8h
1.99
4.03
2.04
1.10
4.95
1.94
1.90
2.05
3.00
f1 (ppm)

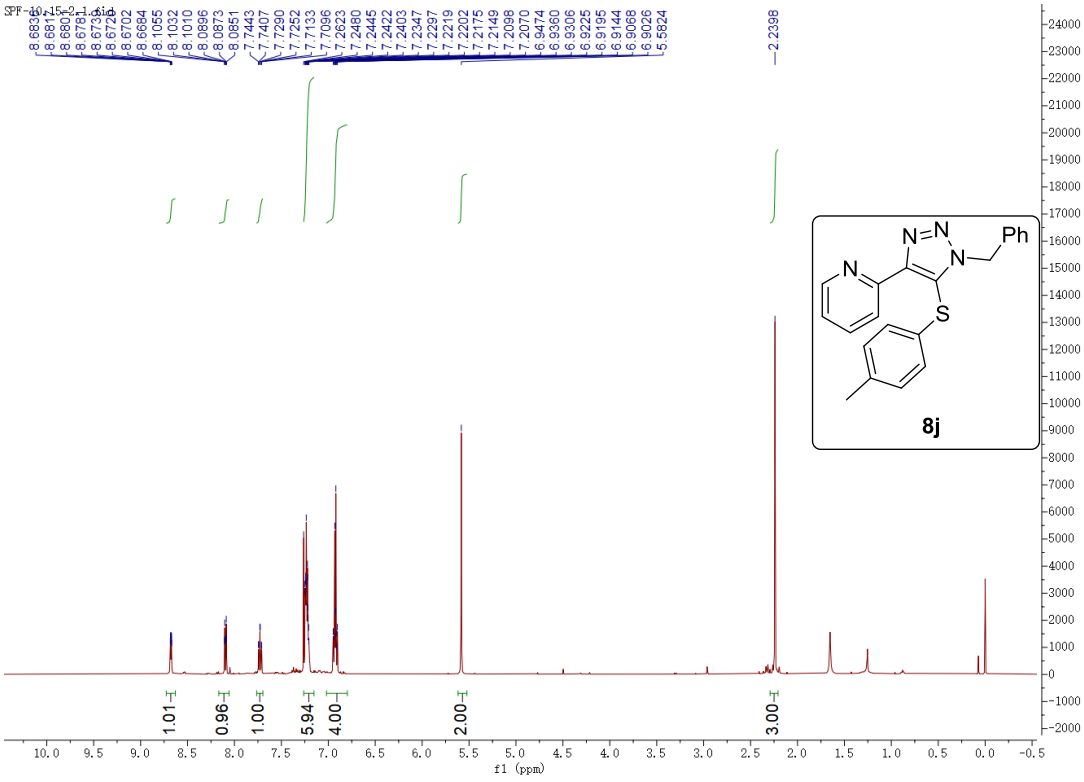

SPF-10.12-1.2.fid
150.2024
141.2699
140.5605
136.8445
134.6344
130.2796
129.8710
129.1790
128.8199
128.6973
128.1921
128.0380
127.4937
127.3717
127.2431
127.0367
126.9388
123.0533
52.2786
20.9297
N=N
N
Ph
S
Ph
8h
f1 (ppm)

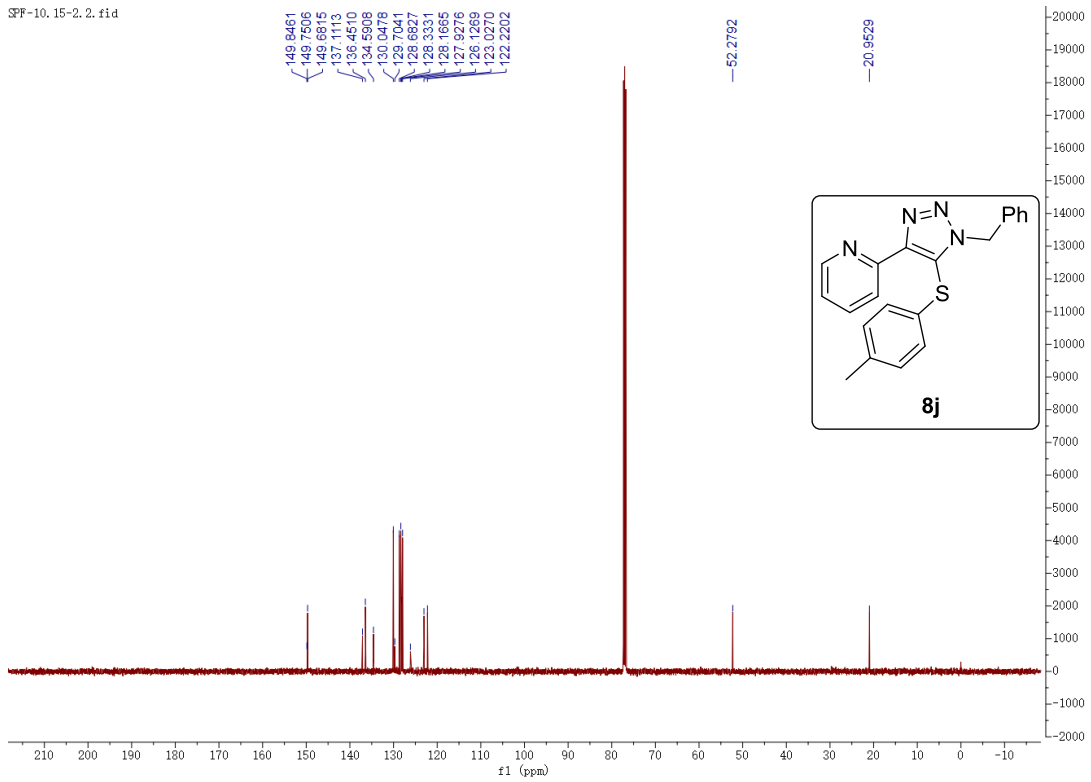
Compound 8i


SPF-10.12-6.1.fid
8.1979
8.1941
8.1847
8.1808
8.0609
8.0569
8.0474
8.0438
7.2600
7.2430
6.9588
6.9427
6.7941
6.7901
6.7811
6.7776
5.5933
3.9101
2.2461
N=N
N
Ph
S
MeOOC
8i
2.01
2.01
5.06
2.02
2.01
2.00
2.92
3.38
f1 (ppm)

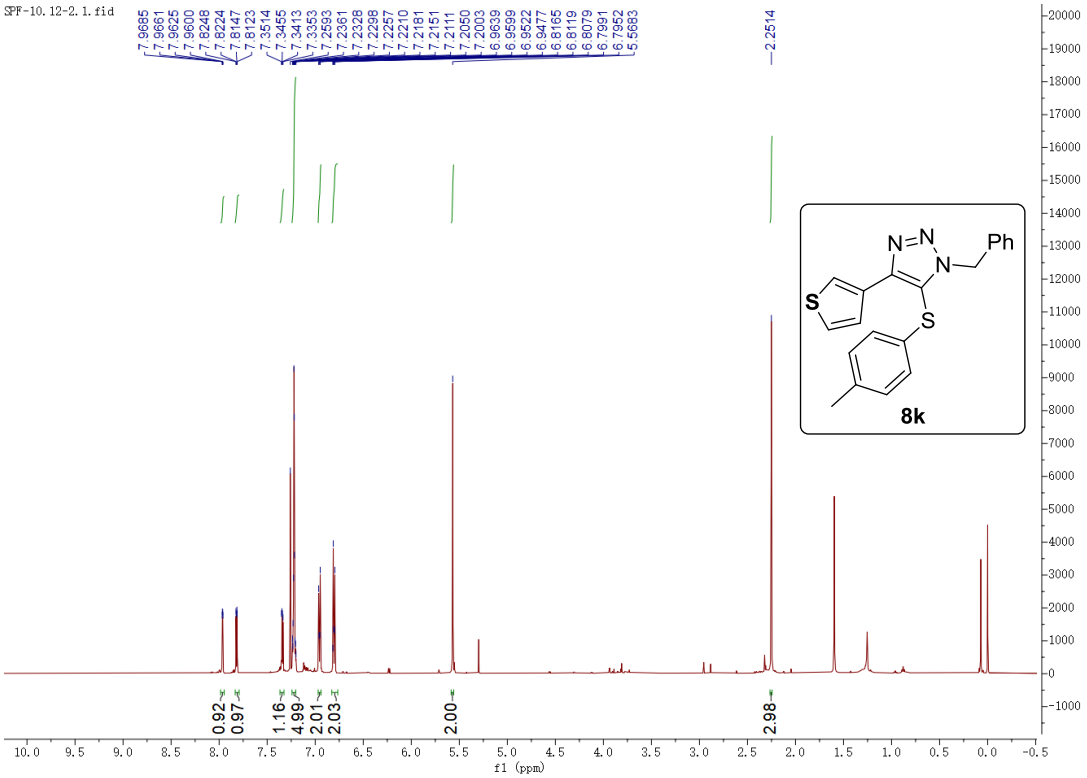

SPF-10.12-6.2.fid
165.7862
148.1708
136.1074
133.5062
133.4088
129.2950
128.8727
128.8089
128.2844
127.7061
127.2550
127.0102
126.1135
125.7531
123.2932
51.3083
51.1324
19.8795
MeOOC
N=N
N
Ph
S
8i
f1 (ppm)

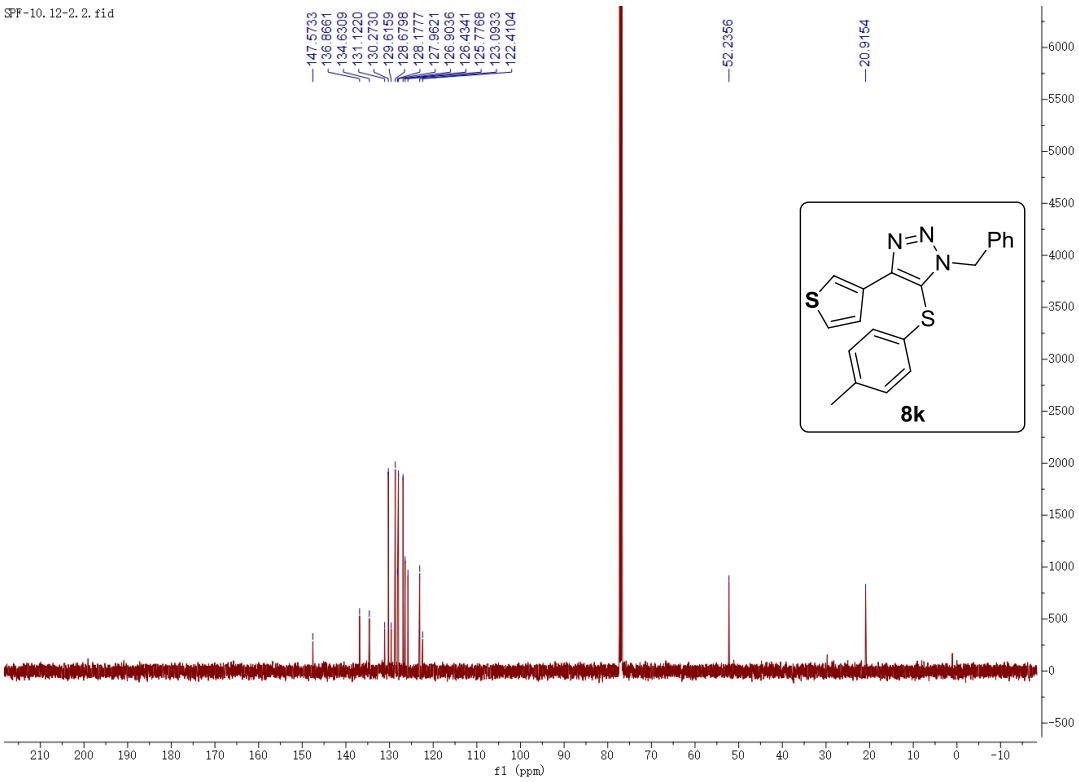
Compound 8j


2.2398
N=N
N
Ph
N
S
8j
1.01
0.96
1.00
5.94
4.00
2.00
3.00
f1 (ppm)

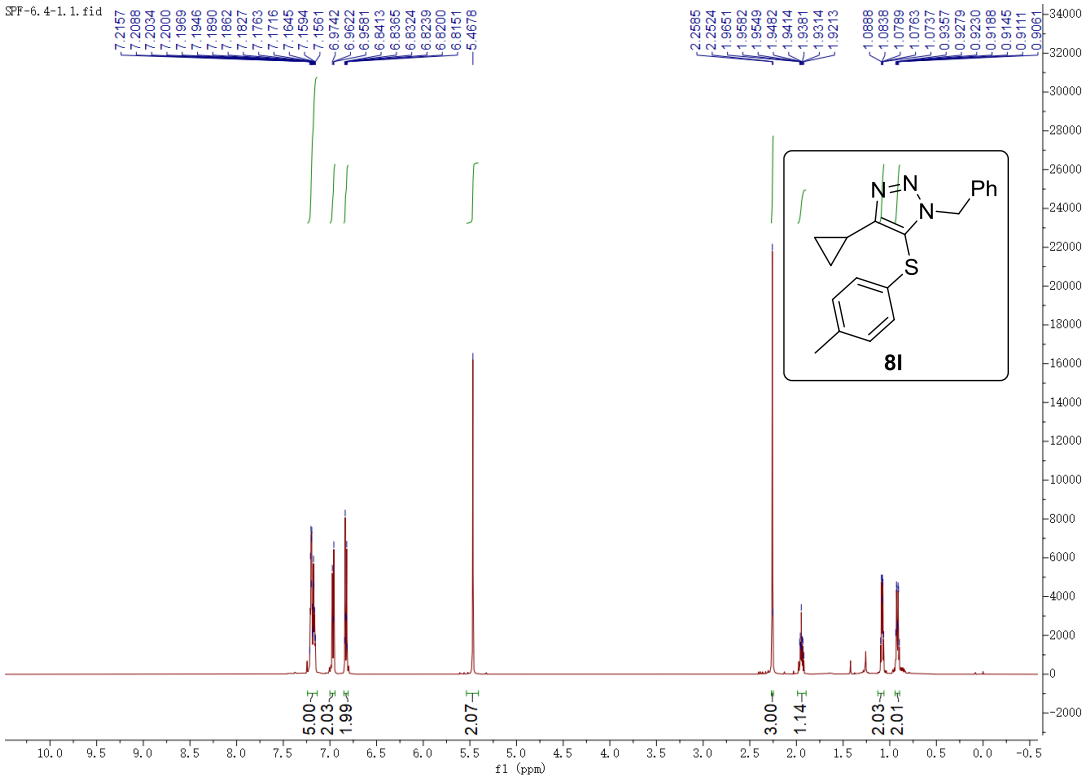

SPF-10.15-2.2.fid
149.8461
149.7506
149.6815
137.1113
136.4510
134.5908
130.0478
129.7041
128.6827
128.3331
128.1665
127.9276
126.1269
123.0270
122.2202
52.2792
20.9529
N
N
N
Ph
S
8j
f1 (ppm)

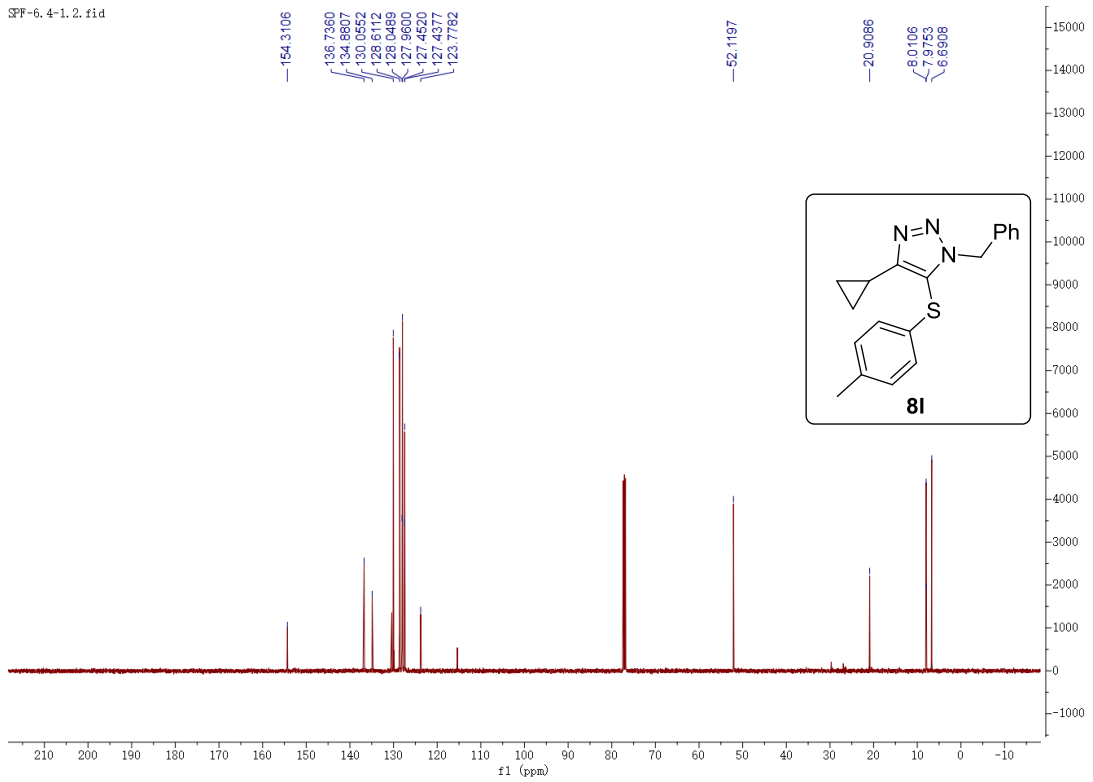
Compound 8k


SPF-10.12-2.1.fid
7.9685
7.9661
7.9625
7.9600
7.8248
7.8224
7.8147
7.8123
7.3514
7.3455
7.3413
7.3353
7.2593
7.2361
7.2328
7.2298
7.2257
7.2210
7.2181
7.2151
7.2111
7.2050
7.2003
6.9639
6.9599
6.9522
6.9477
6.8165
6.8119
6.8079
6.7991
5.7952
5.5683
2.2514
0.92
0.97
1.16
4.99
2.01
2.03
2.00
2.98
N
N
N
Ph
S
S
8k
f1 (ppm)

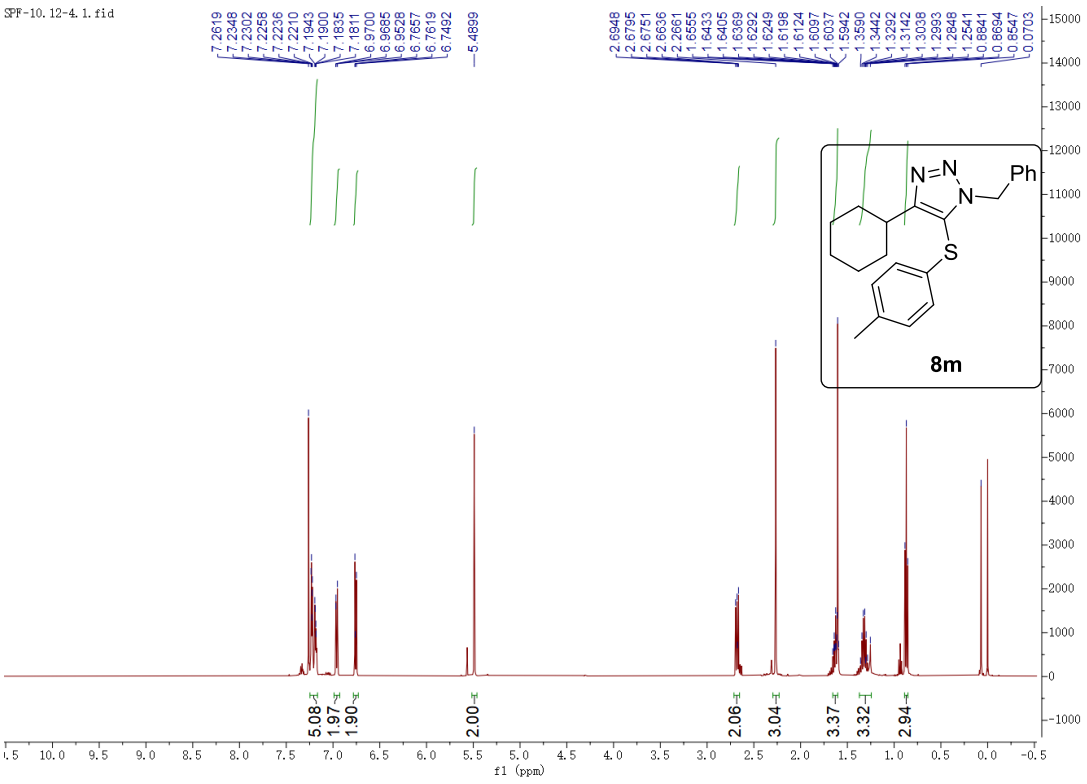

SPF-10.12-2.2.fid
147.5733
136.8661
134.6309
131.1220
130.2730
129.6159
128.6798
128.1777
127.9621
126.9036
126.4341
125.7768
123.0933
122.4104
52.2356
20.9154
N
N
Ph
S
S
8k
f1 (ppm)

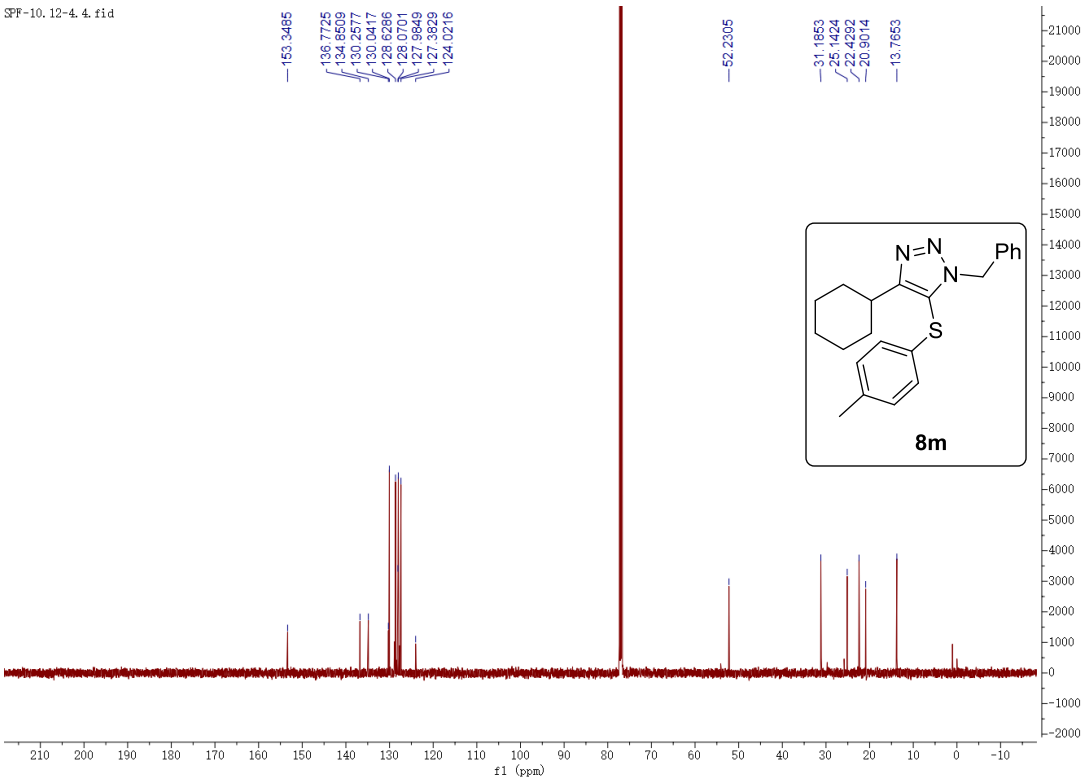
Compound 8l


SPF-6.4-1.1.fid
7.2157
7.2088
7.2034
7.2000
7.1969
7.1946
7.1890
7.1862
7.1827
7.1763
7.1716
7.1645
7.1594
7.1561
6.9742
6.9622
6.9581
6.8413
6.8365
6.8324
6.8239
6.8200
6.8151
5.4678
2.2585
2.2524
1.9651
1.9582
1.9549
1.9482
1.9414
1.9381
1.9314
1.9213
1.0888
1.0838
1.0789
1.0763
1.0737
0.9357
0.9279
0.9230
0.9188
0.9145
0.9111
0.9061
5.00
2.03
1.99
2.07
3.00
1.14
2.03
2.01
N
N
Ph
S
8l
f1 (ppm)

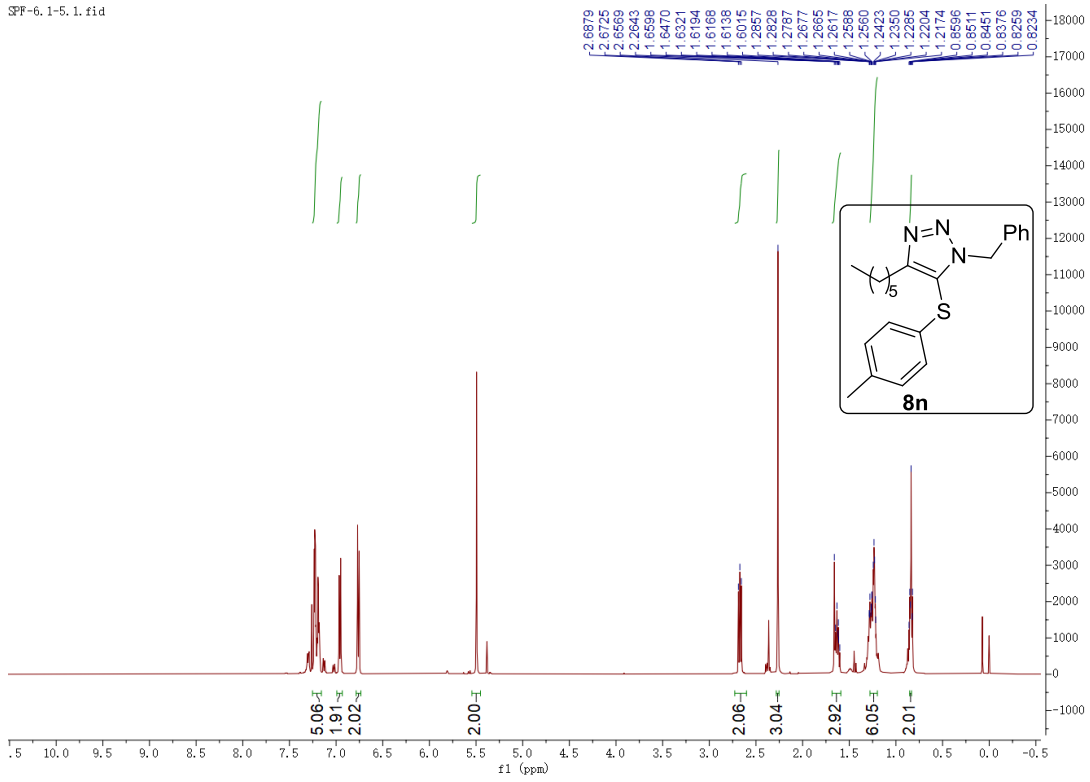

SPF-6.4-1.2.fid
154.3106
136.7360
134.8807
130.0552
128.6112
128.0489
127.9600
127.4520
127.4377
123.7782
52.1197
20.9086
8.0106
7.9753
6.6908
N=N
N
Ph
S
8l
f1 (ppm)

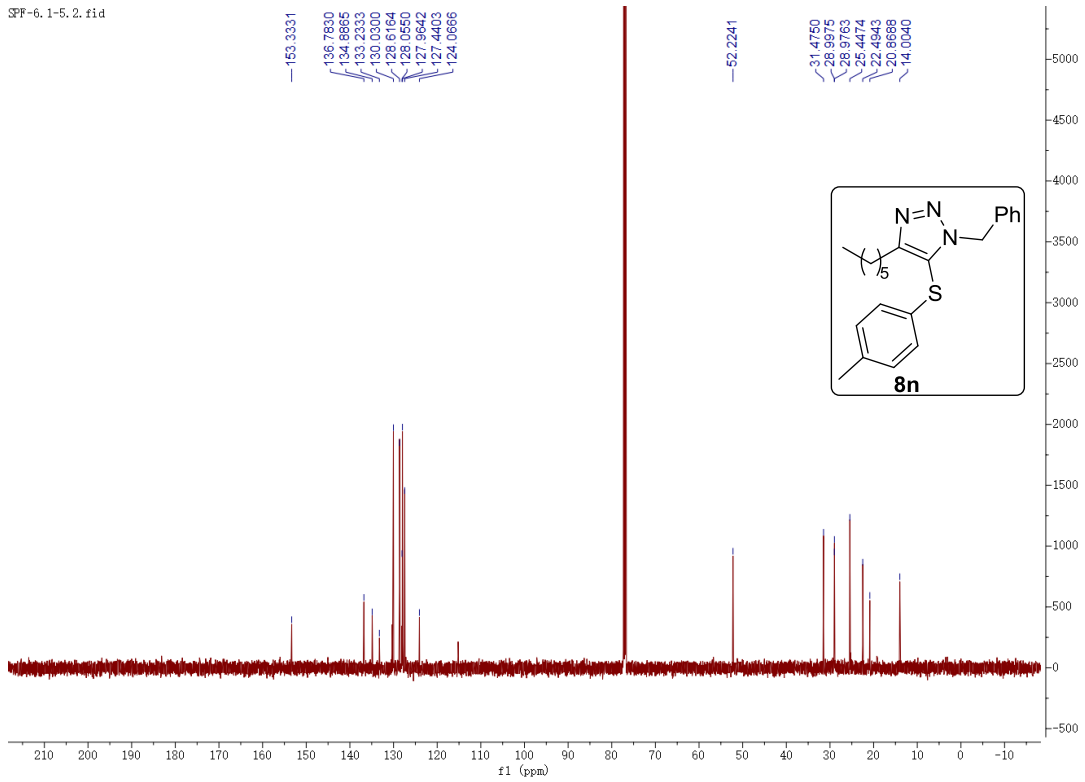
Compound 8m


SPF-10.12-4.1.fid
7.2619
7.2348
7.2302
7.2258
7.2236
7.2210
7.1943
7.1900
7.1835
7.1811
6.9700
6.9685
6.9528
6.7657
6.7619
6.7492
5.4899
2.6948
2.6795
2.6751
2.6636
2.2661
1.6555
1.6433
1.6405
1.6369
1.6292
1.6249
1.6198
1.6124
1.6097
1.6037
1.5942
1.3590
1.3442
1.3292
1.3142
1.3038
1.2993
1.2848
1.2541
0.8841
0.8694
0.8547
0.0703
N=N
N
Ph
S
8m
5.08
1.97
1.90
2.00
2.06
3.04
3.37
3.32
2.94
f1 (ppm)

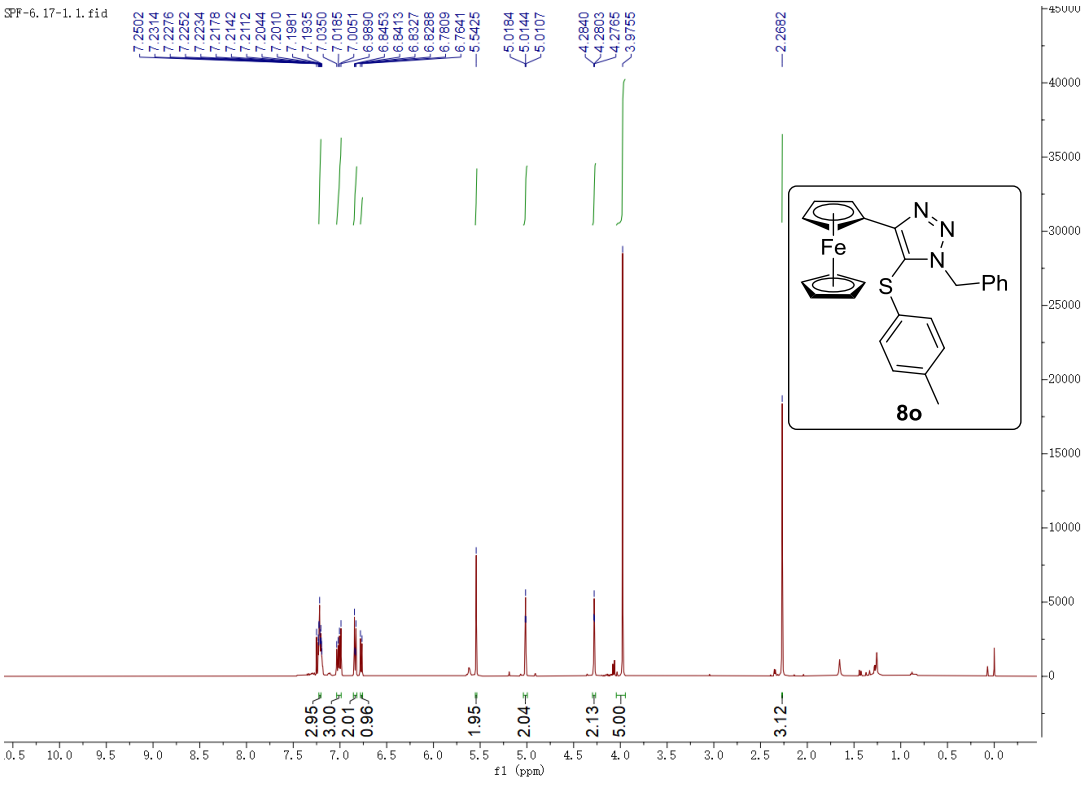

SPF-10.12-4.4.fid
153.3485
136.7725
134.6509
130.2577
130.0417
128.6286
128.0701
127.9849
127.3829
124.0216
52.2305
31.1653
25.1424
22.4292
20.9014
13.7653
N=N
N
Ph
S
8m
f1 (ppm)

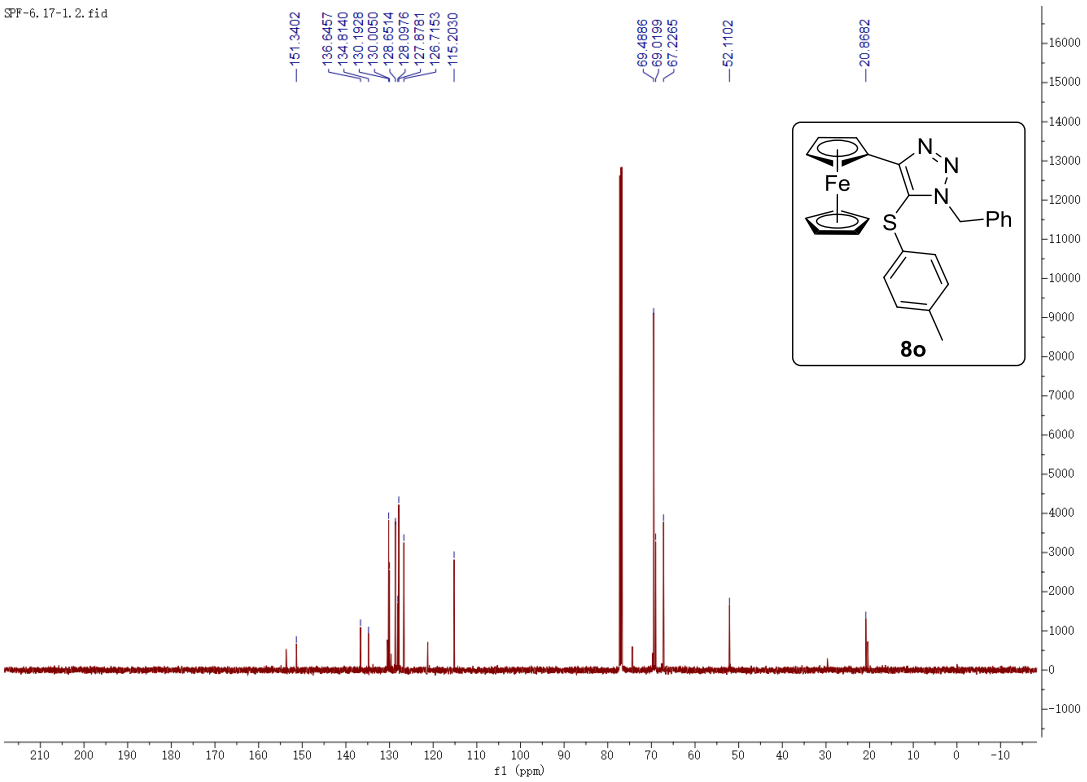
Compound 8n


SPF-6.1-5.1.fid
2.6879
2.6725
2.6569
2.2643
1.6598
1.6470
1.6321
1.6194
1.6168
1.6138
1.6015
1.2857
1.2828
1.2787
1.2677
1.2665
1.2617
1.2588
1.2560
1.2423
1.2350
1.2285
1.2204
1.2174
0.8596
0.8511
0.8451
0.8376
0.8259
0.8234
N=N
N
Ph
5
S
8n
5.06
1.91
2.02
2.00
2.06
3.04
2.92
6.05
2.01
f1 (ppm)

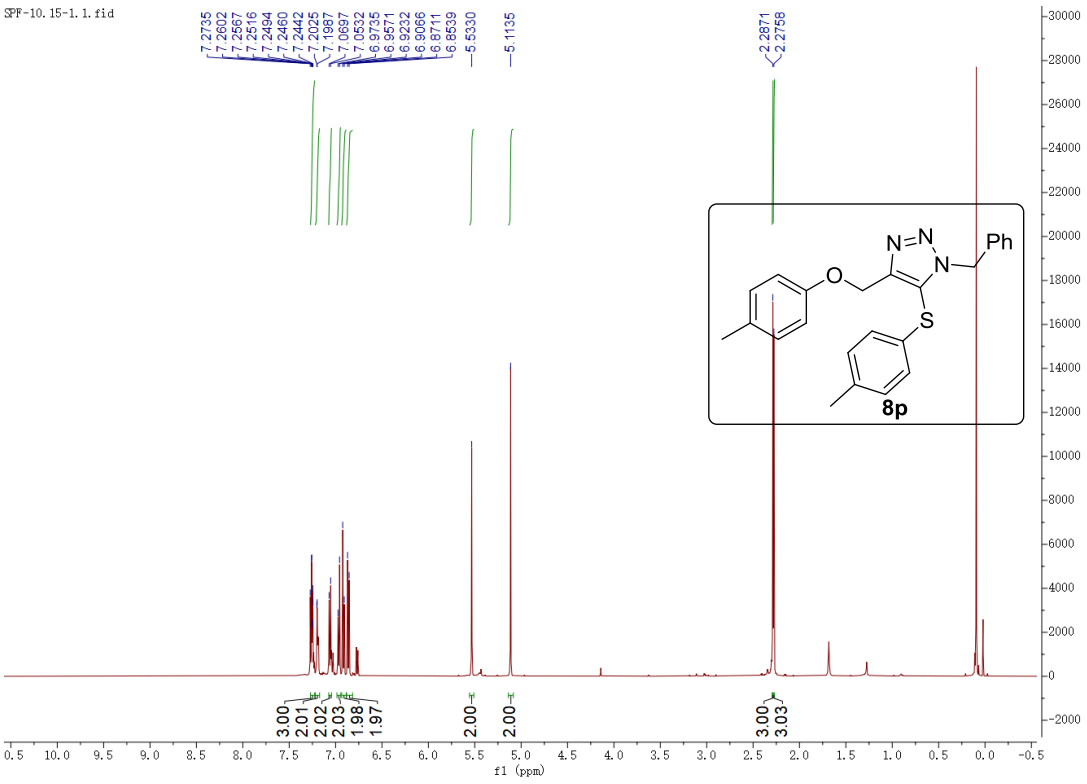

SPF-6.1-5.2.fid
153.3331
136.7830
134.8865
133.2333
130.0300
128.6164
128.0550
127.9642
127.4403
124.0666
52.2241
31.4750
28.9975
28.9763
25.4474
22.4943
20.8688
14.0040
N=N
N
Ph
5
S
8n
f1 (ppm)

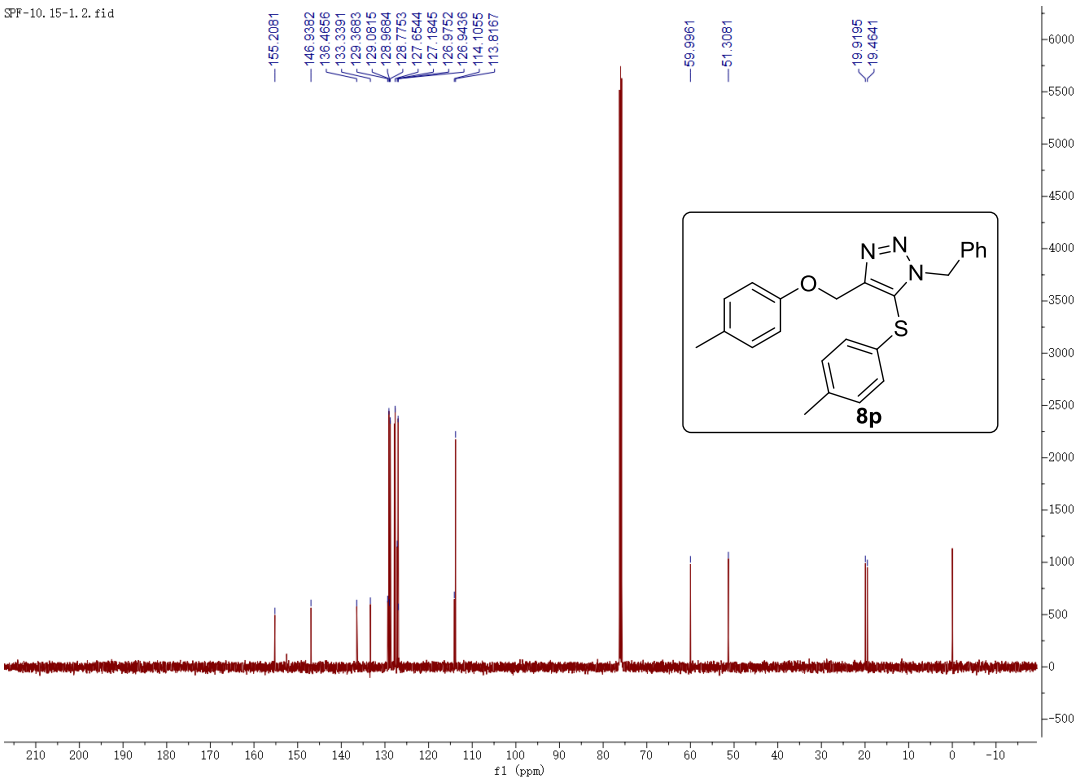
Compound 8o


SPF-6.17-1.1.fid
7.2502
7.2314
7.2276
7.2252
7.2234
7.2178
7.2142
7.2112
7.2044
7.2010
7.1981
7.1935
7.0350
7.0185
7.0051
6.9890
6.8453
6.8413
6.8327
6.8288
6.7809
6.7641
5.5425
5.0184
5.0144
5.0107
4.2840
4.2803
4.2765
3.9755
2.6682
Fe
N=N
N
Ph
S
8o
2.95
3.00
2.01
0.96
1.95
2.04
2.13
5.00
3.12
f1 (ppm)

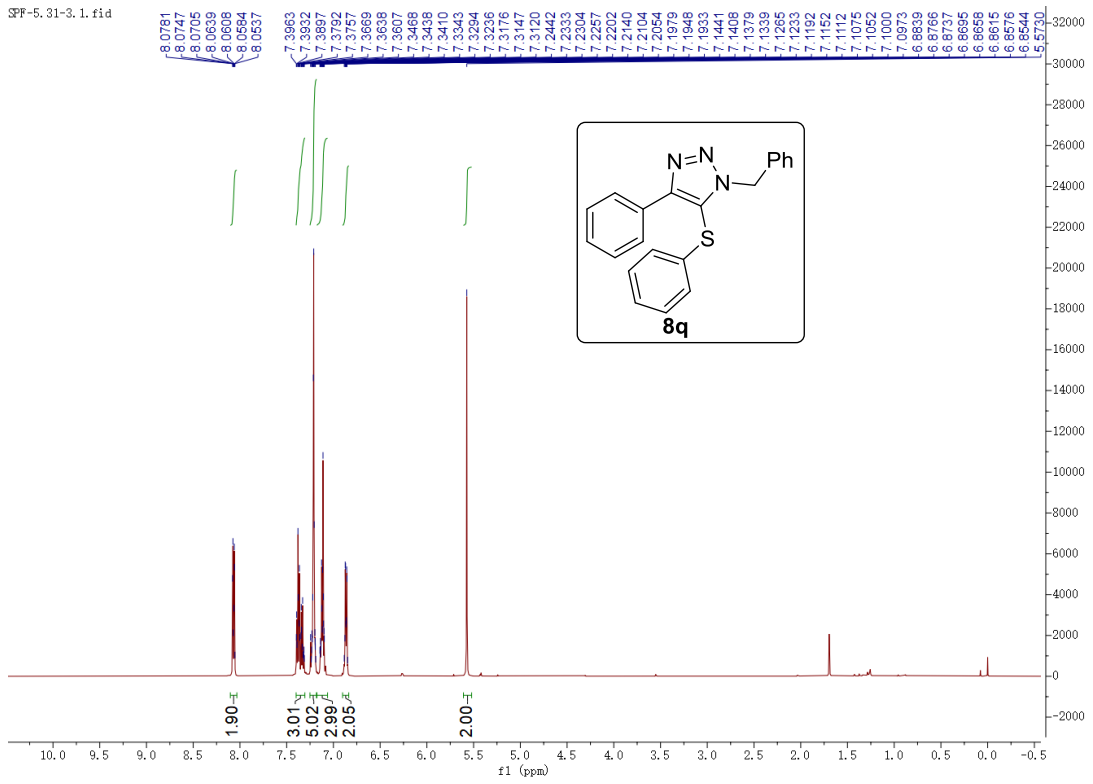

SPF-6.17-1.2.fid
151.3402
136.6457
134.8140
130.1928
130.0050
128.6514
128.0976
127.8781
126.7153
115.2030
69.4886
69.0199
67.2265
52.1102
20.8682
Fe
N
N
N
S
Ph
8o
f1 (ppm)

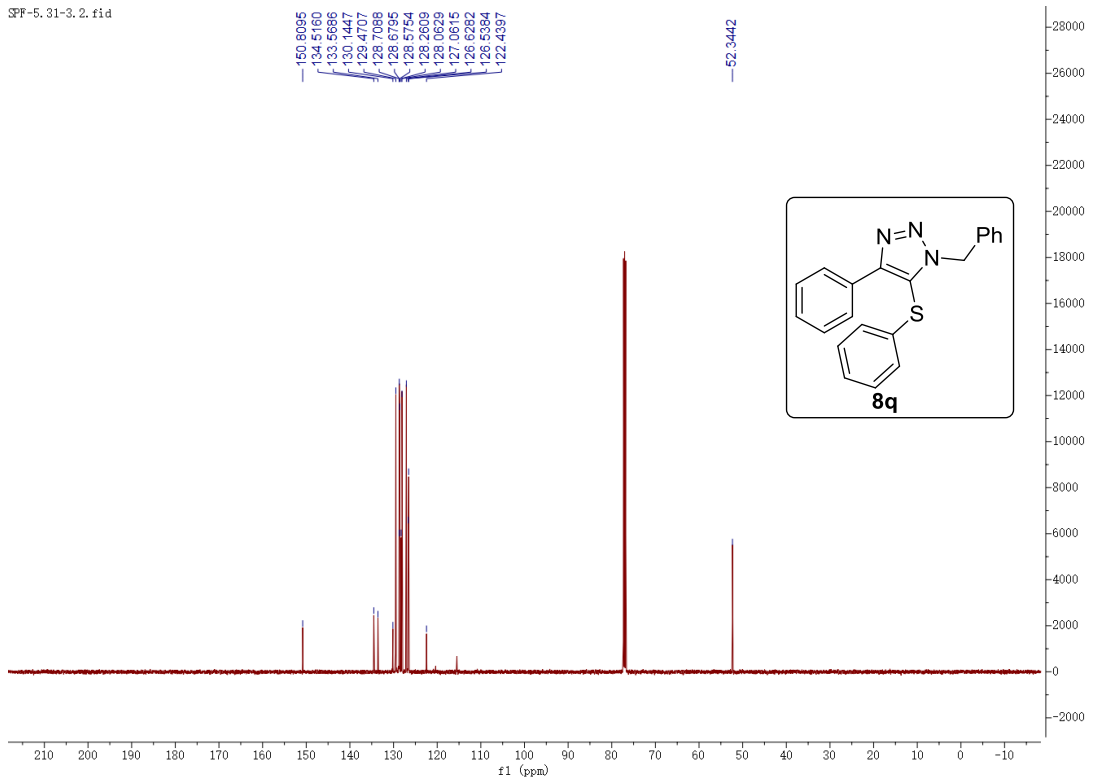
Compound 8p


SPF-10.15-1.1.fid
7.2735
7.2602
7.2567
7.2516
7.2494
7.2460
7.2442
7.2025
7.1987
7.0697
7.0532
6.9735
6.9571
6.9232
6.9066
6.8711
6.8539
5.5330
5.1135
2.2871
2.2758
3.00
2.01
2.02
2.03
1.98
1.97
2.00
2.00
3.00
3.03
N=N
N
Ph
O
S
8p
f1 (ppm)

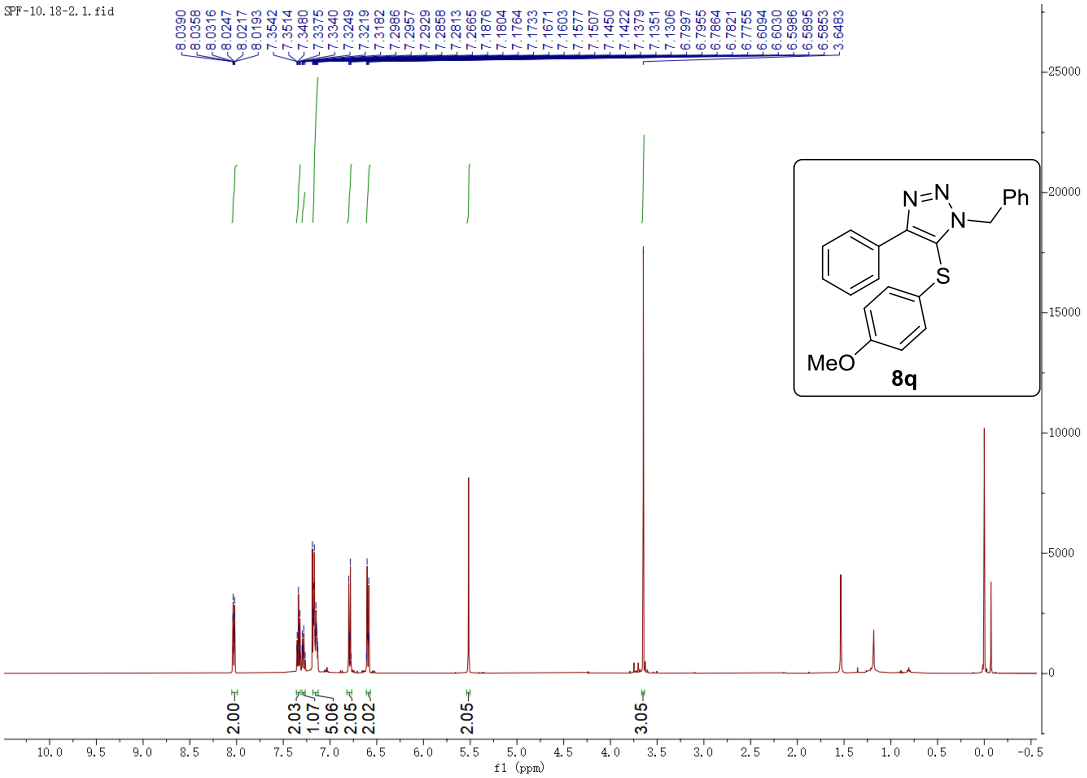

SPF-10.15-1.2.fid
155.2081
146.9382
136.4656
133.3391
129.3683
129.0815
128.9684
128.7753
127.6544
127.1845
126.9752
126.9436
114.1055
113.8167
59.9961
51.3081
19.9195
19.4641
N=N
Ph
N
O
S
8p
f1 (ppm)

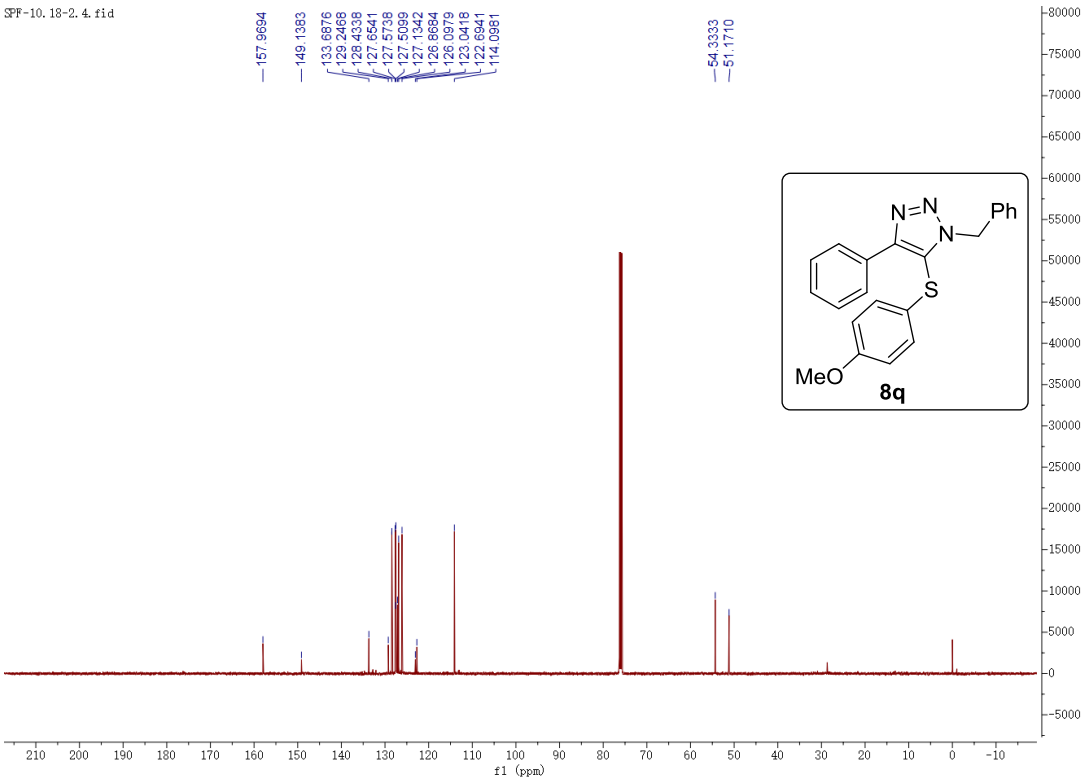
Compound 8q


SPF-5.31-3.1.fid
8.0781
8.0747
8.0705
8.0639
8.0608
8.0584
8.0537
7.3963
7.3932
7.3897
7.3792
7.3757
7.3669
7.3638
7.3607
7.3468
7.3438
7.3410
7.3343
7.3294
7.3236
7.3176
7.3147
7.3120
7.2442
7.2333
7.2304
7.2257
7.2202
7.2140
7.2104
7.2054
7.1979
7.1948
7.1933
7.1441
7.1408
7.1379
7.1339
7.1265
7.1233
7.1192
7.1152
7.1112
7.1075
7.1052
7.1000
7.0973
6.8839
6.8766
6.8737
6.8695
6.8658
6.8615
6.8576
6.8544
5.5730
1.90
3.01
5.02
2.99
2.05
2.00
N=N
Ph
N
S
8q
f1 (ppm)

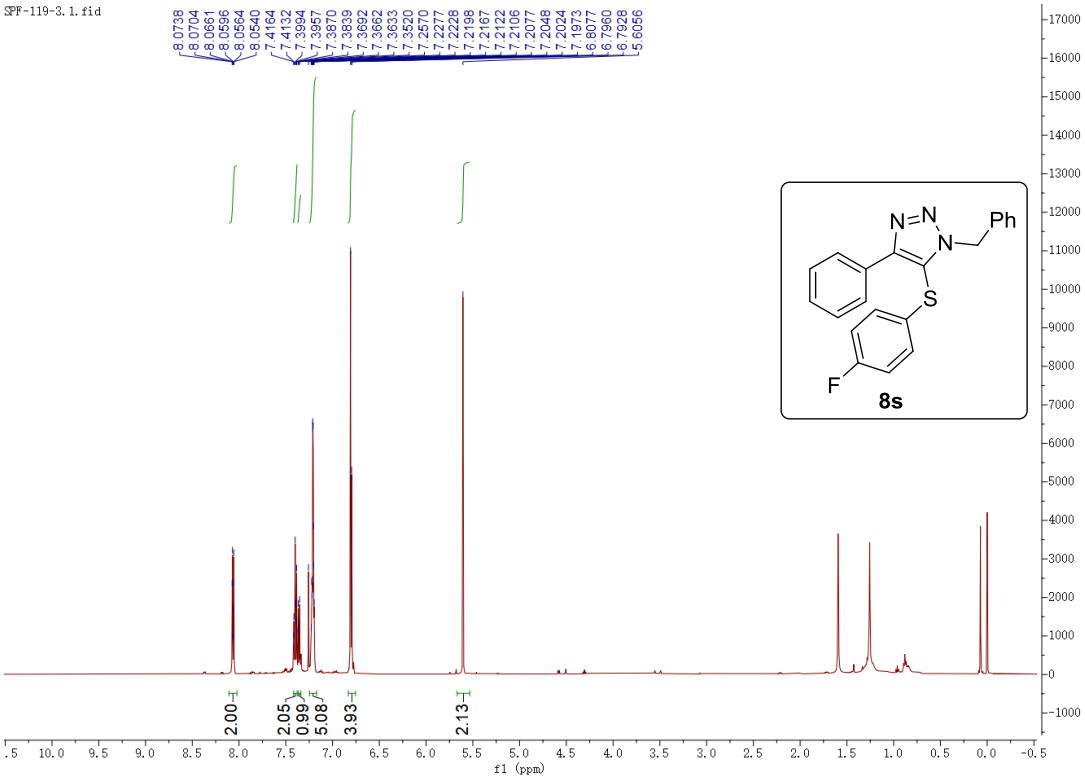

SPF-5.31-3.2.fid
150.8095
134.5160
133.5686
130.1447
129.4707
128.7088
128.6795
128.5754
128.2609
128.0629
127.0615
126.6282
126.5384
122.4397
52.3442
N=N
N
Ph
S
8q
f1 (ppm)

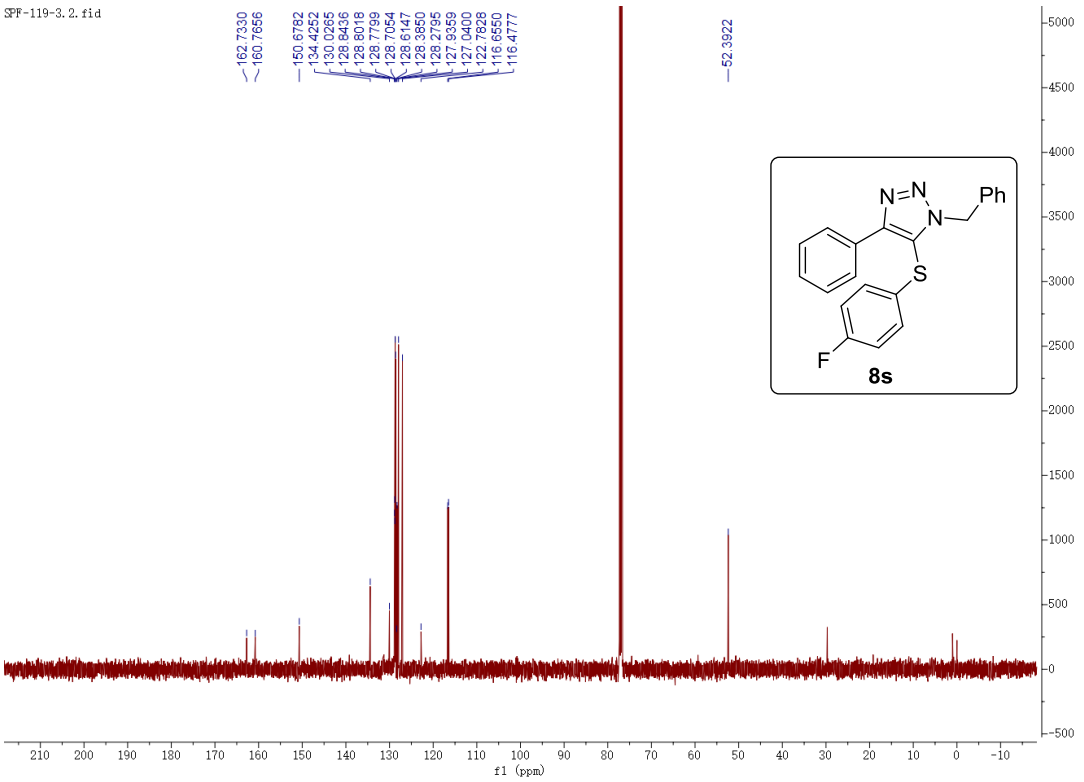
Compound 8r


SPF-10.18-2.1.fid
8.0390
8.0358
8.0316
8.0247
8.0217
8.0193
7.3542
7.3514
7.3480
7.3375
7.3340
7.3249
7.3219
7.3182
7.2986
7.2957
7.2929
7.2858
7.2813
7.2665
7.1876
7.1804
7.1764
7.1733
7.1671
7.1603
7.1577
7.1507
7.1450
7.1422
7.1379
7.1351
7.1306
6.7997
6.7955
6.7864
6.7821
6.7755
6.6094
6.6030
6.5986
6.5895
6.5853
6.5483
2.00
2.03
1.07
5.06
2.05
2.02
2.05
3.05
N=N
N
Ph
S
MeO
8q
f1 (ppm)

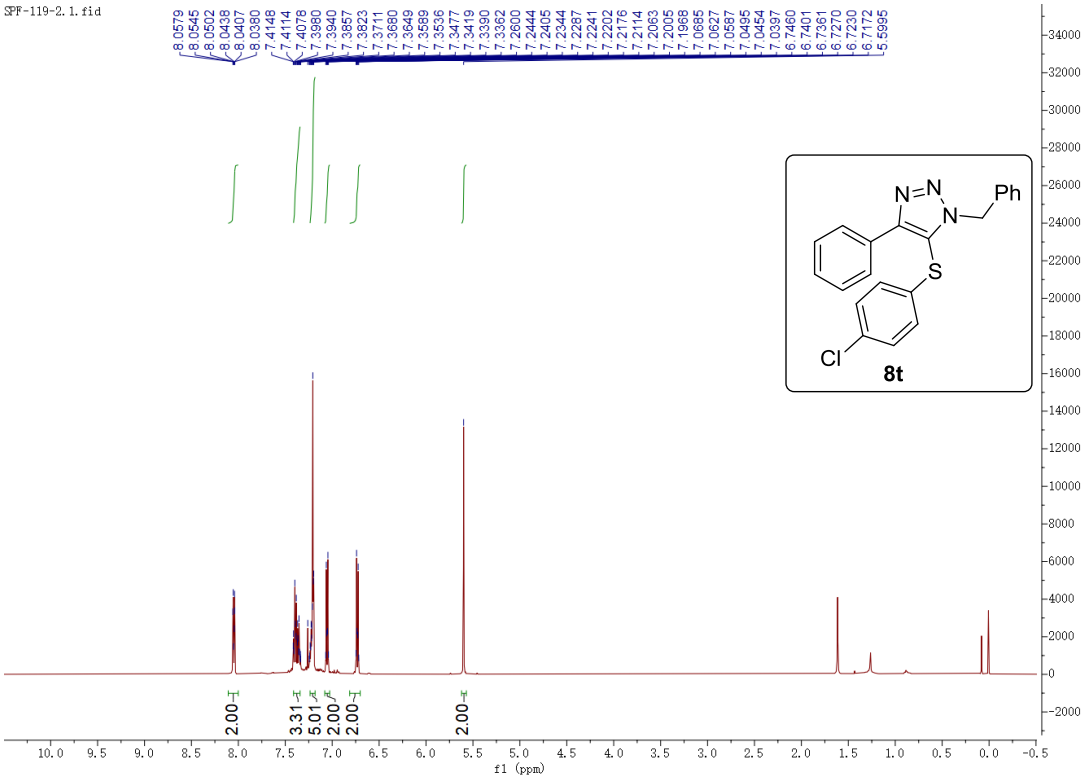

SPF-10.18-2.4.fid
157.9694
149.1383
133.6876
129.2468
128.4338
127.6541
127.5738
127.5099
127.1342
126.8684
126.0979
123.0418
122.6941
114.0981
54.3333
51.1710
N=N
N
Ph
S
MeO
8q
f1 (ppm)

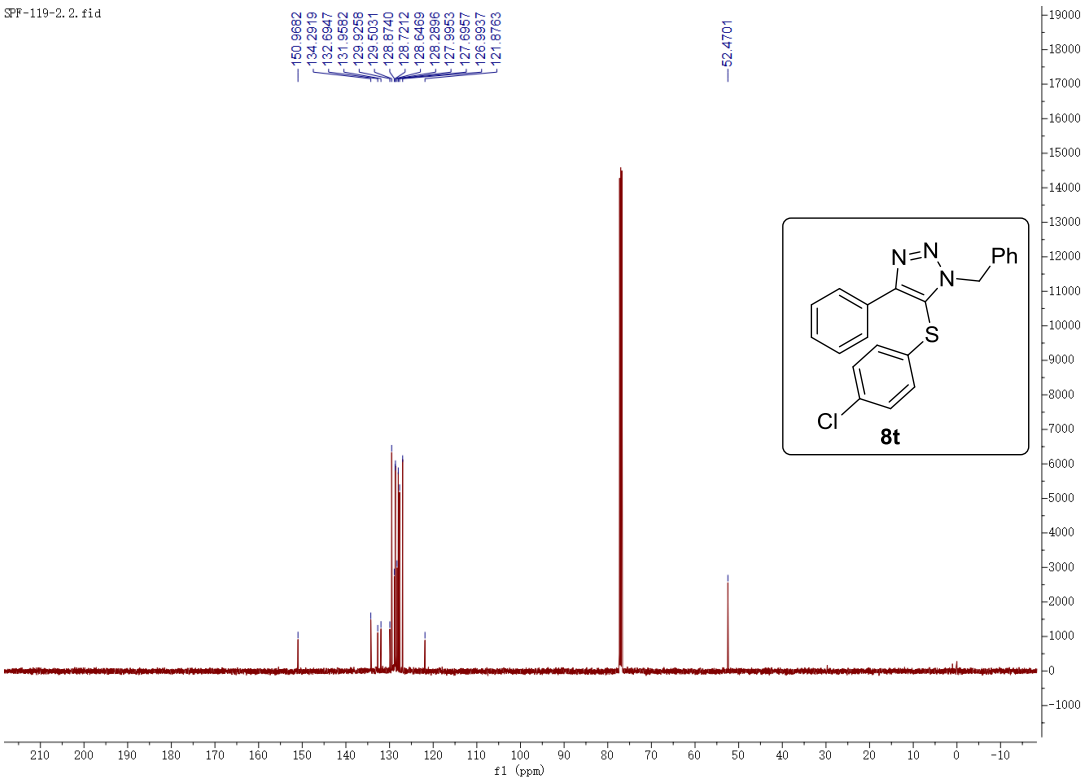
Compound 8s


SPF-119-3.1.fid
8.0738
8.0704
8.0661
8.0596
8.0564
8.0540
7.4164
7.4132
7.3994
7.3957
7.3870
7.3839
7.3692
7.3662
7.3633
7.3520
7.2570
7.2277
7.2228
7.2198
7.2167
7.2122
7.2106
7.2077
7.2048
7.2024
7.1973
6.8077
6.7960
6.7928
5.6056
2.00
2.05
0.99
5.08
3.93
2.13
N=N
N
Ph
S
F
8s
f1 (ppm)

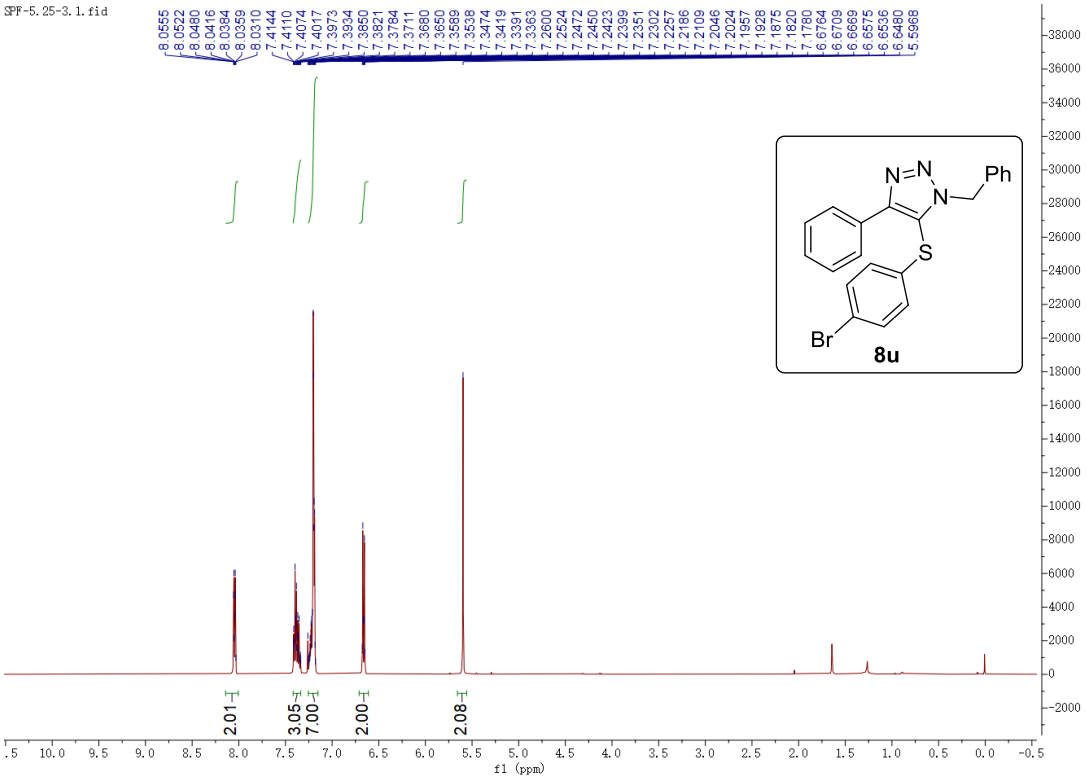

SPF-119-3.2.fid
162.7330
160.7656
150.6782
134.4252
130.0265
128.8436
128.8018
128.7799
128.7054
128.6147
128.3850
128.2795
127.9359
127.0400
122.7828
116.6550
116.4777
52.3922
N=N
Ph
N
S
F
8s
f1 (ppm)

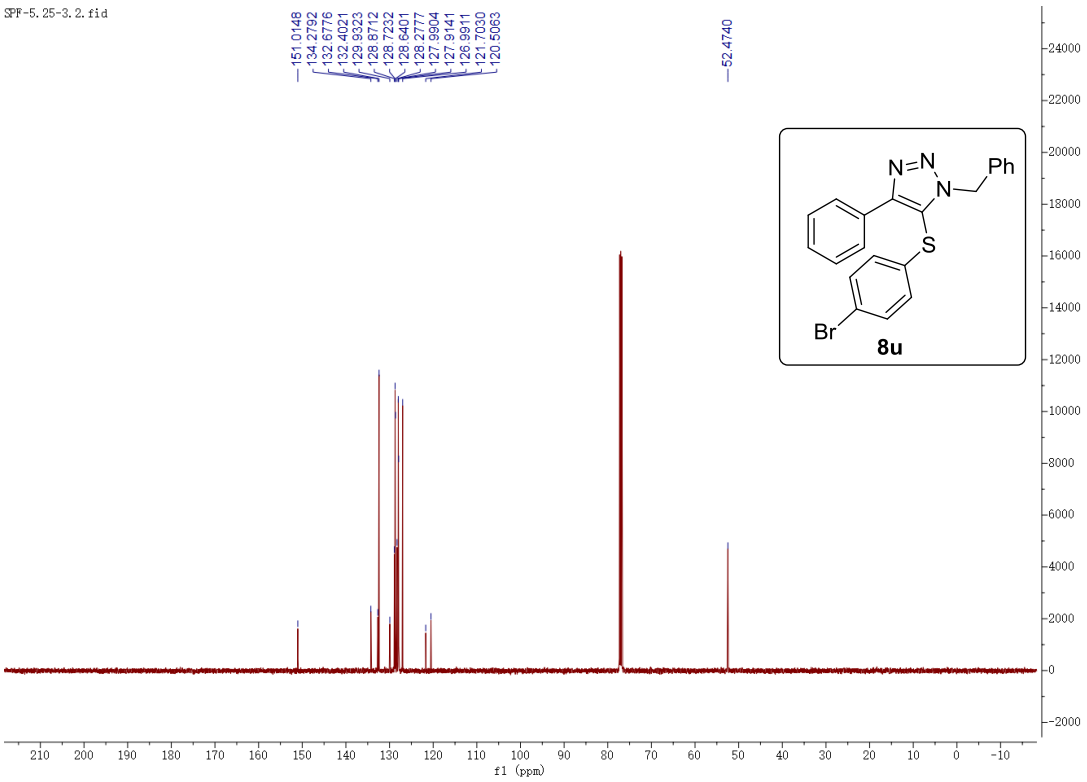
Compound 8t


SPF-119-2.1.fid
8.0579
8.0545
8.0502
8.0438
8.0407
8.0380
7.4148
7.4114
7.4078
7.3980
7.3940
7.3857
7.3823
7.3711
7.3680
7.3649
7.3569
7.3536
7.3477
7.3419
7.3390
7.3362
7.2600
7.2444
7.2405
7.2344
7.2287
7.2241
7.2202
7.2176
7.2114
7.2063
7.2005
7.1968
7.0685
7.0627
7.0587
7.0495
7.0454
7.0397
6.7460
6.7401
6.7361
6.7270
6.7230
6.7172
5.5995
2.00
3.31
5.01
2.00
2.00
2.00
N=N
Ph
N
S
Cl
8t
f1 (ppm)

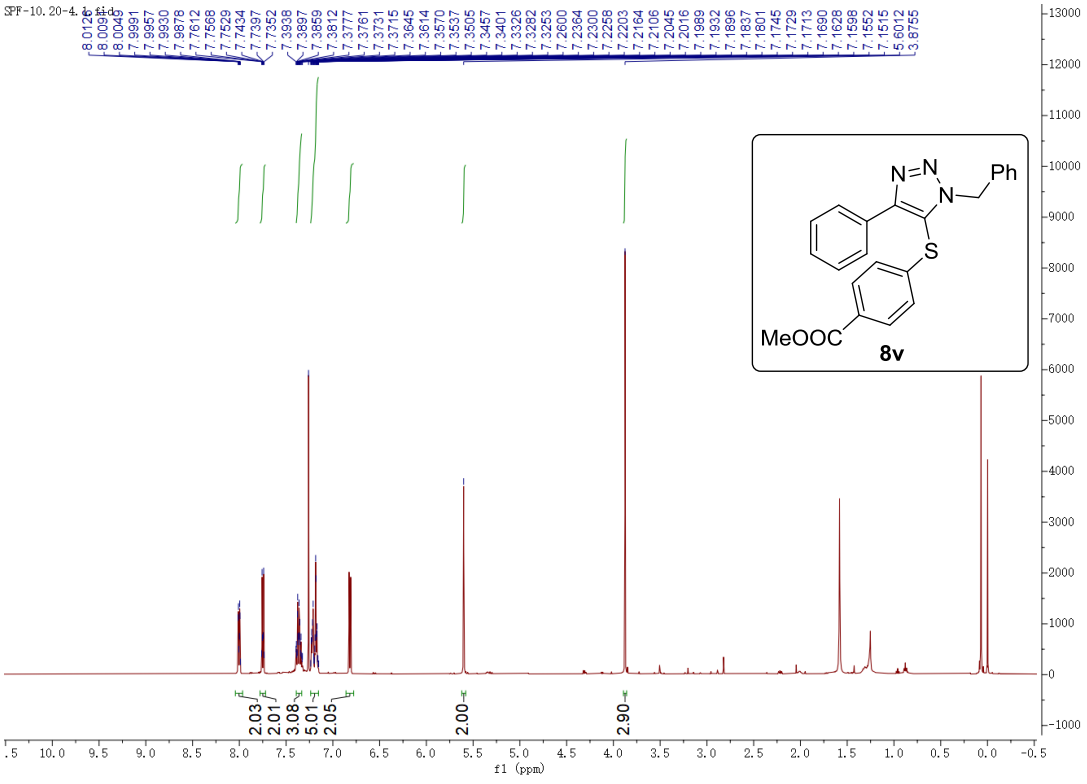

SPF-119-2.2.fid
150.9682
134.2919
132.6947
131.9582
129.9258
129.5031
128.8740
128.7212
128.6469
128.2896
127.9953
127.6957
126.9937
121.8763
52.4701
N=N
Ph
N
S
Cl
8t
f1 (ppm)

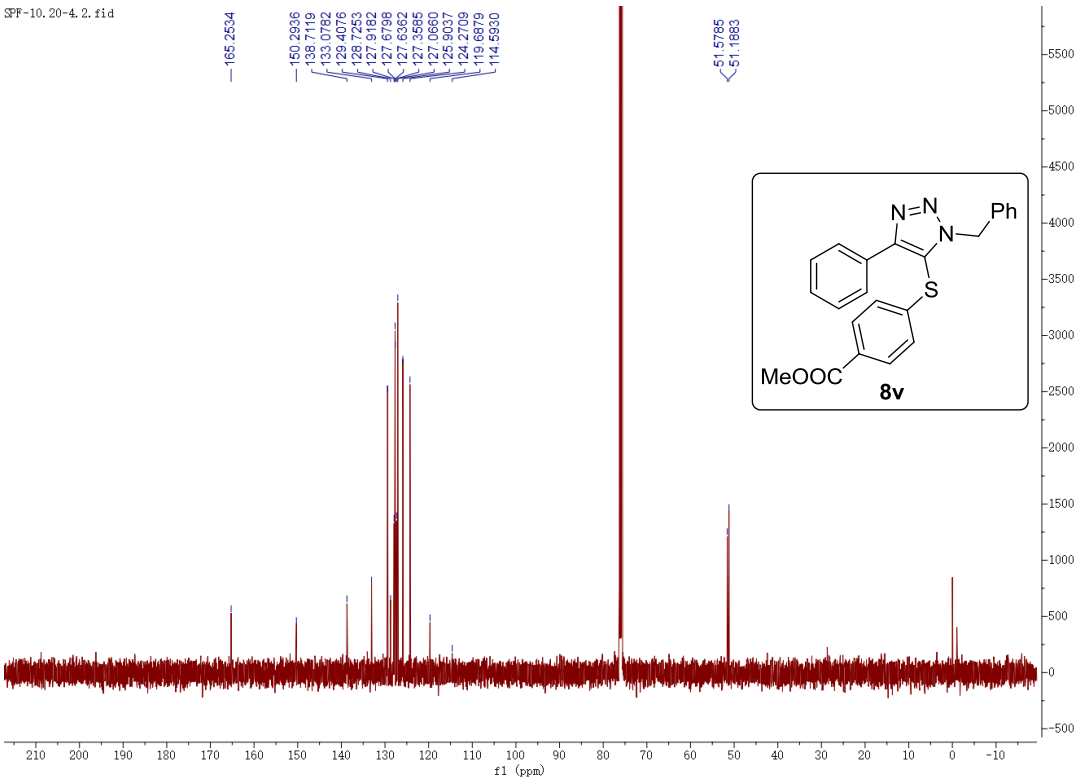
Compound 8u


SPF-5.25-3.1.fid
8.0555
8.0522
8.0480
8.0416
8.0384
8.0359
8.0310
7.4144
7.4110
7.4074
7.4017
7.3973
7.3934
7.3850
7.3821
7.3784
7.3711
7.3680
7.3650
7.3589
7.3538
7.3474
7.3419
7.3391
7.3363
7.2600
7.2524
7.2472
7.2450
7.2423
7.2399
7.2351
7.2302
7.2257
7.2186
7.2109
7.2046
7.2024
7.1957
7.1928
7.1875
7.1820
7.1780
6.6764
6.6709
6.6669
6.6575
6.6536
6.6480
5.5968
2.01
3.05
7.00
2.00
2.08
N=N
Ph
N
S
Br
8u
f1 (ppm)

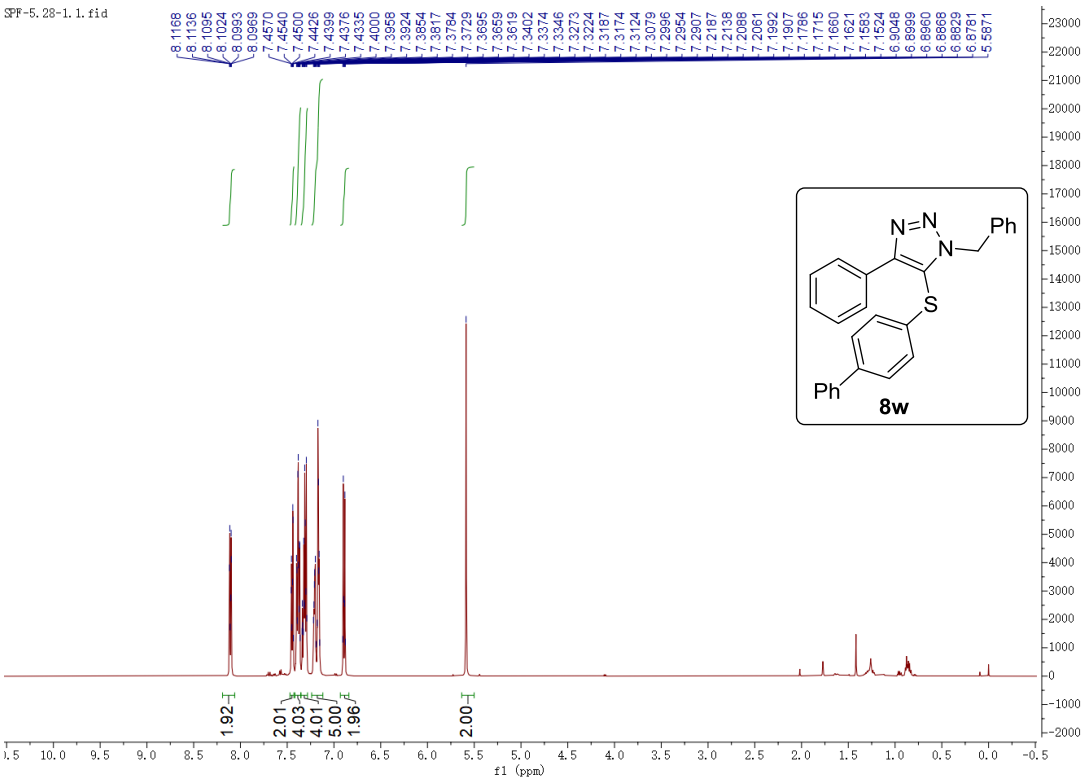

SPF-5.25-3.2.fid
151.0148
134.2792
132.6776
132.4021
129.9323
128.8712
128.7232
128.6401
128.2777
127.9904
127.9141
126.9911
121.7030
120.5063
52.4740
N=N
Ph
N
S
Br
8u
f1 (ppm)

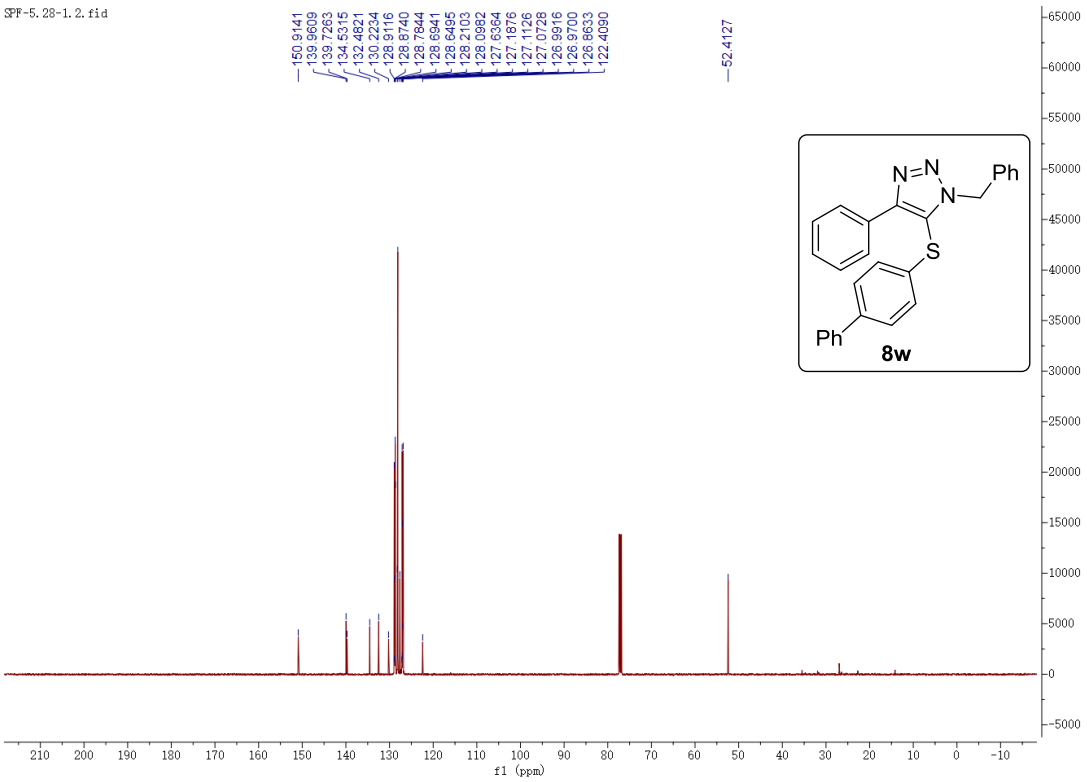
Compound 8v


SPF-10.20-4.1.fid
N=N
Ph
N
S
MeOOC
8v
2.03
2.01
3.08
5.01
2.05
2.00
2.90
f1 (ppm)

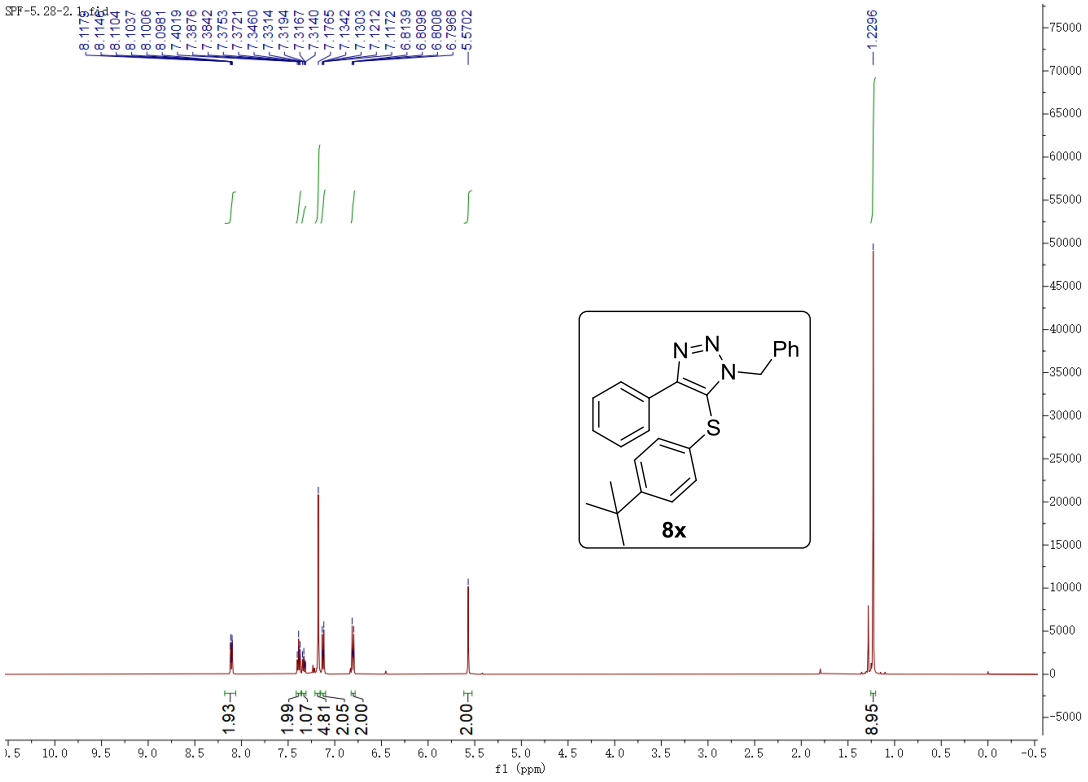

SPF-10.20-4.2.fid
165.2534
150.2936
138.7719
133.0782
129.4076
128.7253
127.9182
127.6798
127.6362
127.3585
127.0660
125.9037
124.2709
119.6879
114.5930
51.5785
51.1883
N=N
N
Ph
S
MeOOC
8v
f1 (ppm)

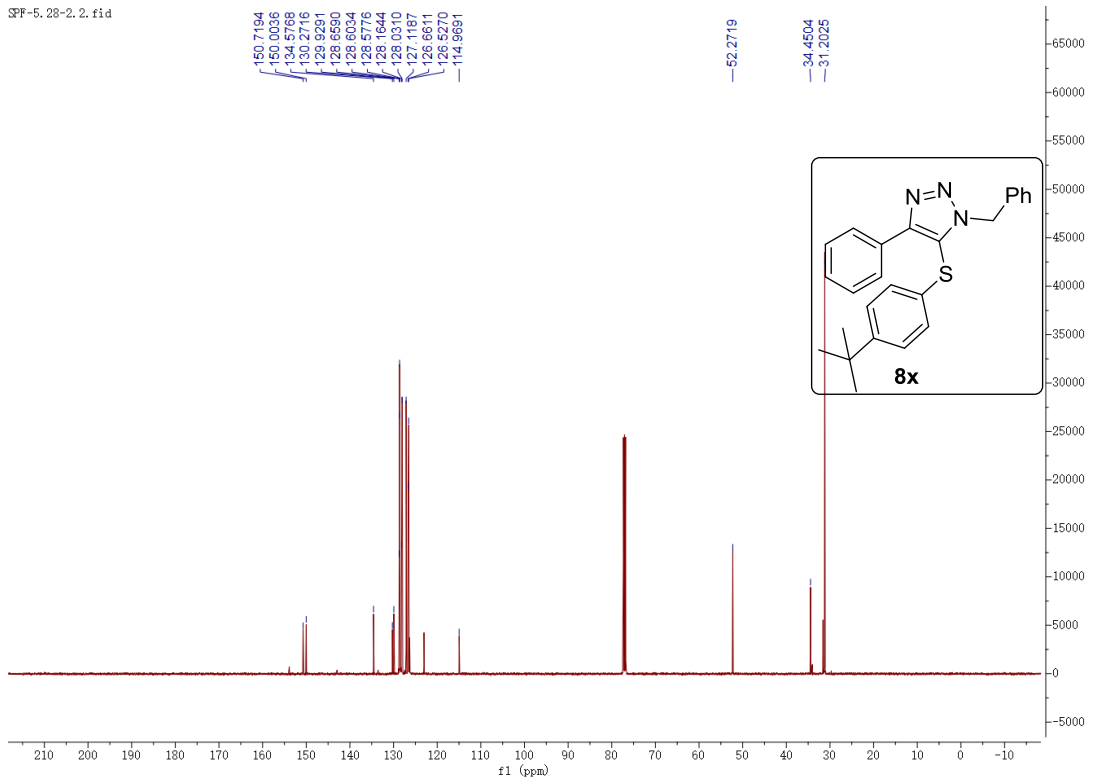
Compound 8w


SPF-5.28-1.1.fid
8.1168
8.1136
8.1095
8.1024
8.0993
8.0969
7.4570
7.4540
7.4500
7.4426
7.4399
7.4376
7.4335
7.4000
7.3958
7.3924
7.3854
7.3817
7.3784
7.3729
7.3695
7.3659
7.3619
7.3402
7.3374
7.3346
7.3273
7.3224
7.3167
7.3174
7.3124
7.3079
7.2996
7.2954
7.2907
7.2187
7.2138
7.2088
7.2061
7.1992
7.1907
7.1786
7.1715
7.1660
7.1621
7.1583
7.1524
6.9048
6.8999
6.8960
6.8868
6.8829
6.8781
5.5871
1.92
2.01
4.03
4.01
5.00
1.96
2.00
N=N
N
Ph
S
Ph
8w
f1 (ppm)

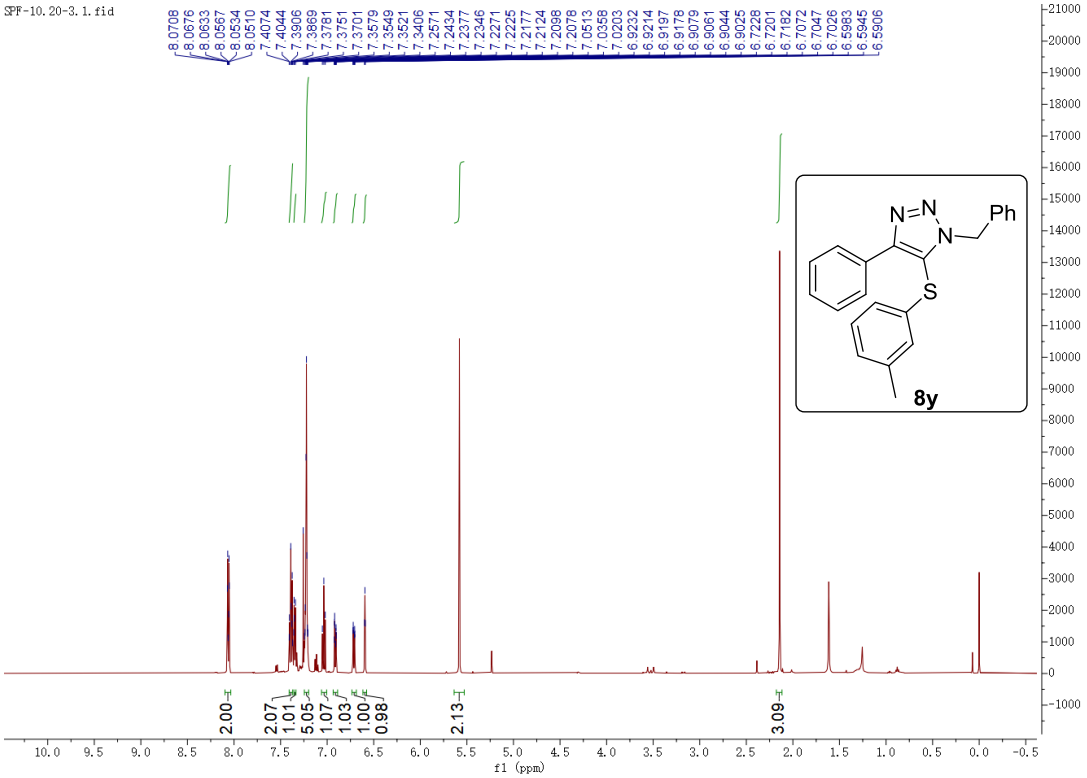

SPF-5.28-1.2.fid
150.9141
139.9609
139.7263
134.5315
132.4821
130.2234
128.9116
128.8740
128.7844
128.6941
128.6495
128.2103
128.0982
127.6364
127.1876
127.1126
127.0728
126.9916
126.9700
126.8633
122.4090
52.4127
N=N
N
Ph
S
Ph
8w
f1 (ppm)

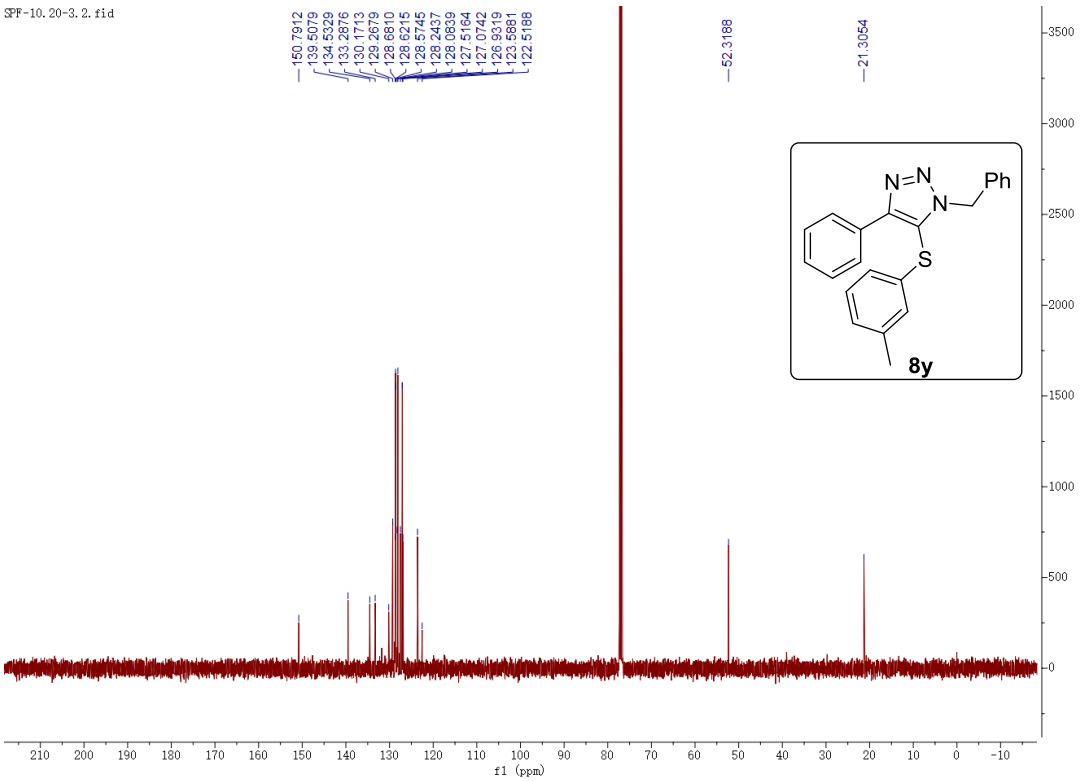
Compound 8x


SPF-5.28-2.1.fid
8.1175
8.1144
8.1104
8.1037
8.1006
8.0981
7.4019
7.3876
7.3842
7.3753
7.3721
7.3460
7.3314
7.3194
7.3167
7.3140
7.1765
7.1342
7.1303
7.1212
7.1172
6.8139
6.8098
6.8008
6.7968
5.5702
1.2296
N=N
N
Ph
S
8x
1.93
1.99
1.07
4.81
2.05
2.00
2.00
8.95
f1 (ppm)

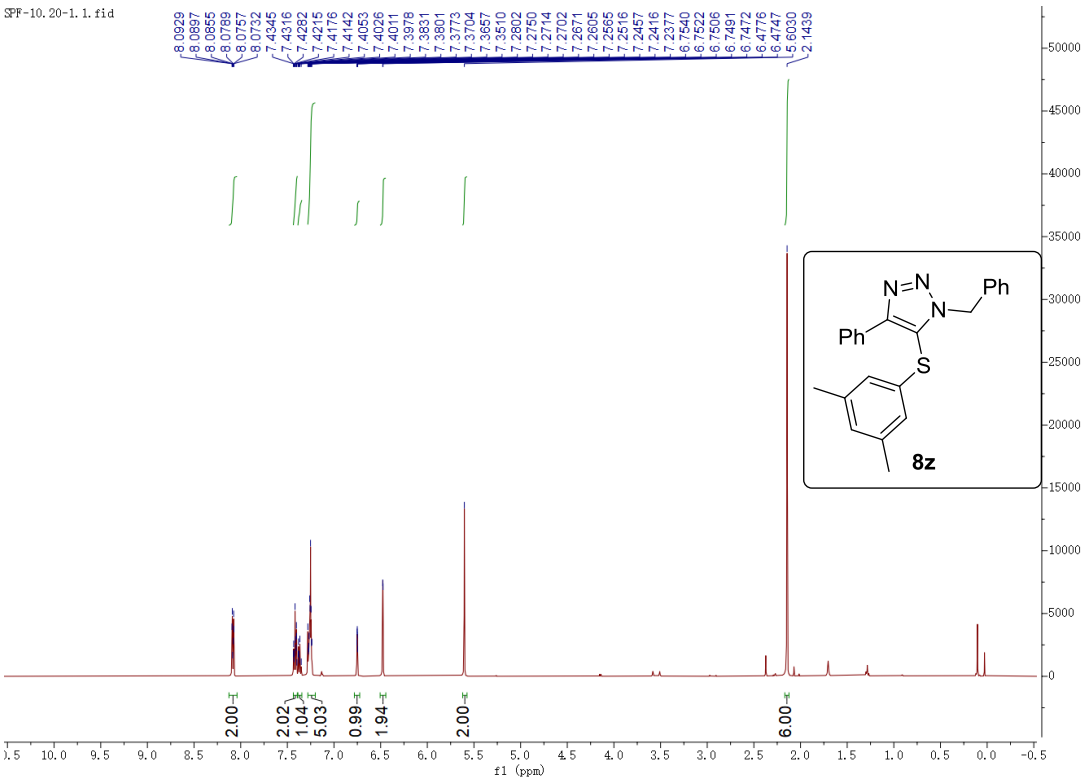

SPF-5.28-2.2.fid
150.7194
150.0036
134.5768
130.2716
129.9291
128.6590
128.6034
128.5776
128.1644
128.0310
127.1187
126.6611
126.5270
114.9691
52.2719
34.4504
31.2025
N=N
N
Ph
S
8x
f1 (ppm)

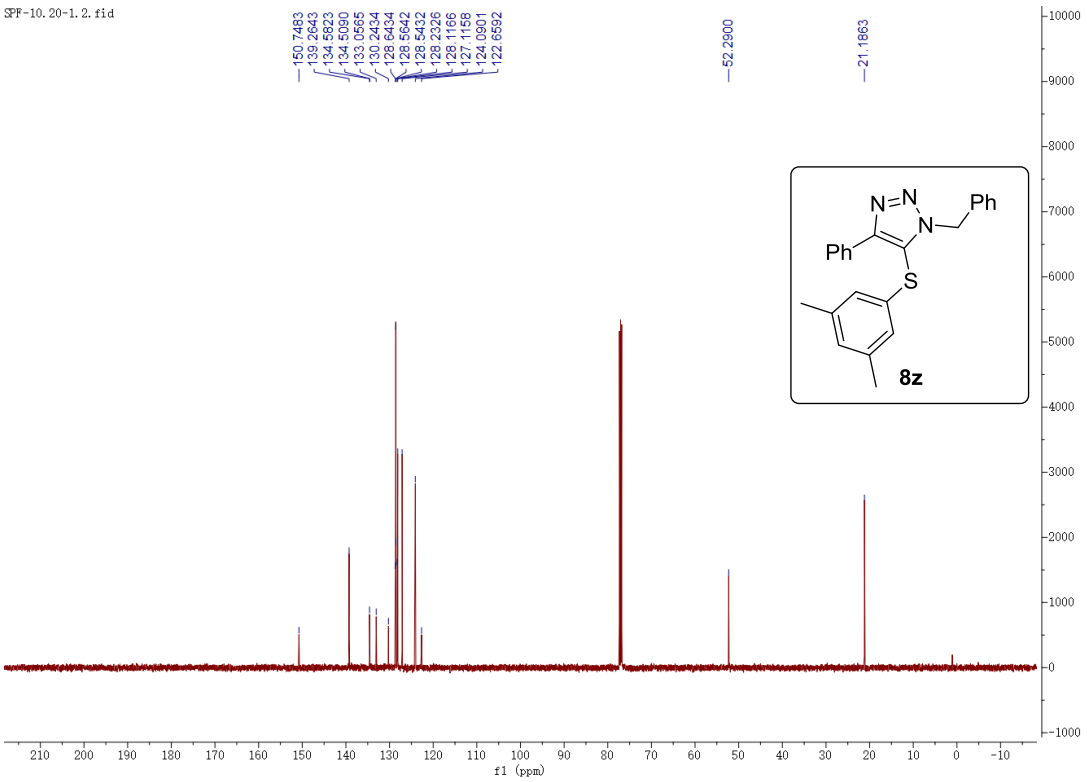
Compound 8y


SPF-10.20-3.1.fid
8.0708
8.0676
8.0633
8.0567
8.0534
8.0510
7.4074
7.4044
7.3906
7.3869
7.3781
7.3751
7.3701
7.3579
7.3549
7.3521
7.3406
7.2571
7.2434
7.2377
7.2346
7.2271
7.2225
7.2177
7.2124
7.2098
7.2078
7.0513
7.0358
7.0203
6.9232
6.9214
6.9197
6.9178
6.9079
6.9061
6.9044
6.9025
6.7228
6.7201
6.7182
6.7072
6.7047
6.7026
6.5983
6.5945
6.5906
2.00
2.07
1.01
5.05
1.07
1.03
1.00
0.98
2.13
3.09
N=N
N
Ph
S
8y
f1 (ppm)

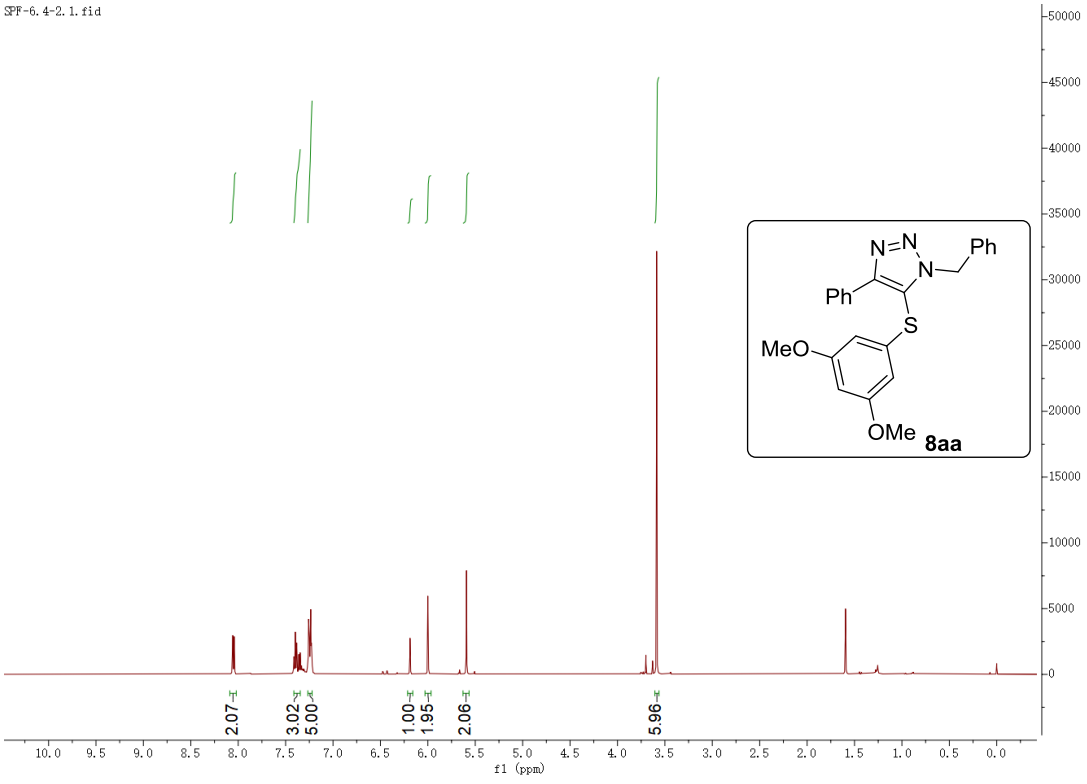

SPF-10.20-3.2.fid
150.7912
139.5079
134.5329
133.2876
130.1713
129.2679
128.6810
128.6215
128.5745
128.2437
128.0839
127.5164
127.0742
126.9319
123.5881
122.5188
52.3188
21.3054
N=N
N
Ph
S
8y
f1 (ppm)

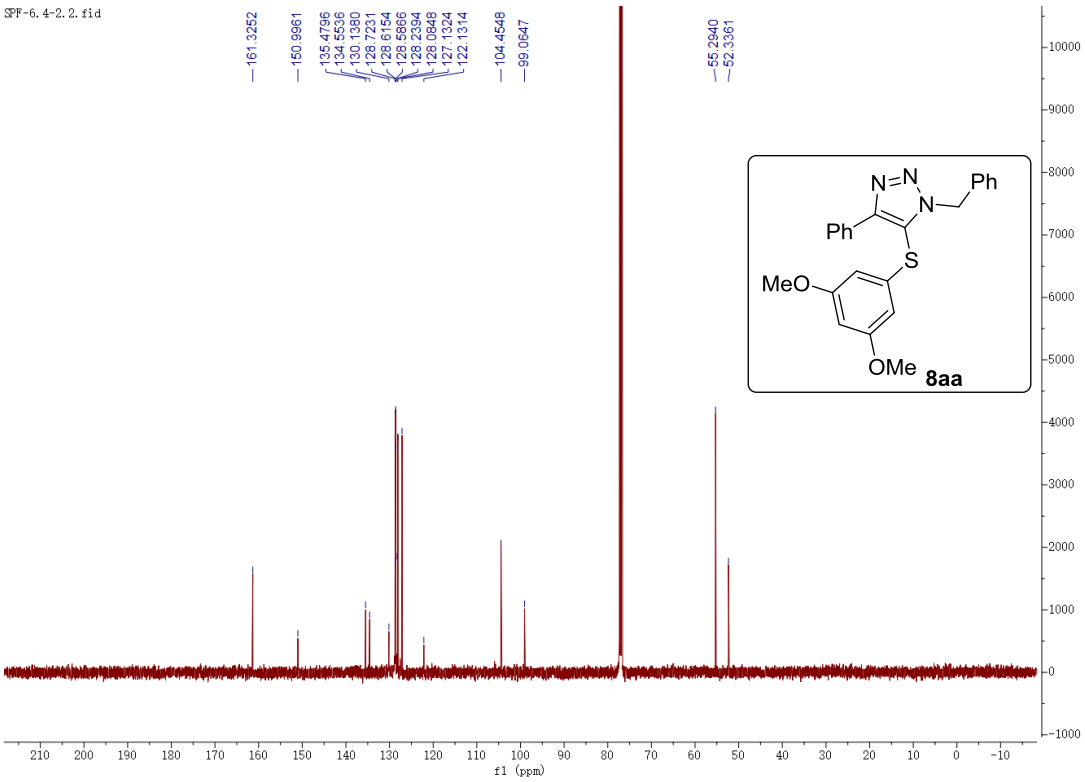
Compound 8z


SPF-10.20-1.1.fid
8.0929
8.0897
8.0855
8.0789
8.0757
8.0732
7.4345
7.4316
7.4282
7.4215
7.4176
7.4142
7.4053
7.4026
7.4011
7.3978
7.3831
7.3801
7.3773
7.3704
7.3657
7.3510
7.2802
7.2750
7.2714
7.2702
7.2671
7.2605
7.2565
7.2516
7.2457
7.2416
7.2377
6.7540
6.7522
6.7506
6.7491
6.7472
6.4776
6.4747
5.6030
2.1439
2.00
2.02
1.04
5.03
0.99
1.94
2.00
6.00
N=N
N
Ph
Ph
S
8z
f1 (ppm)

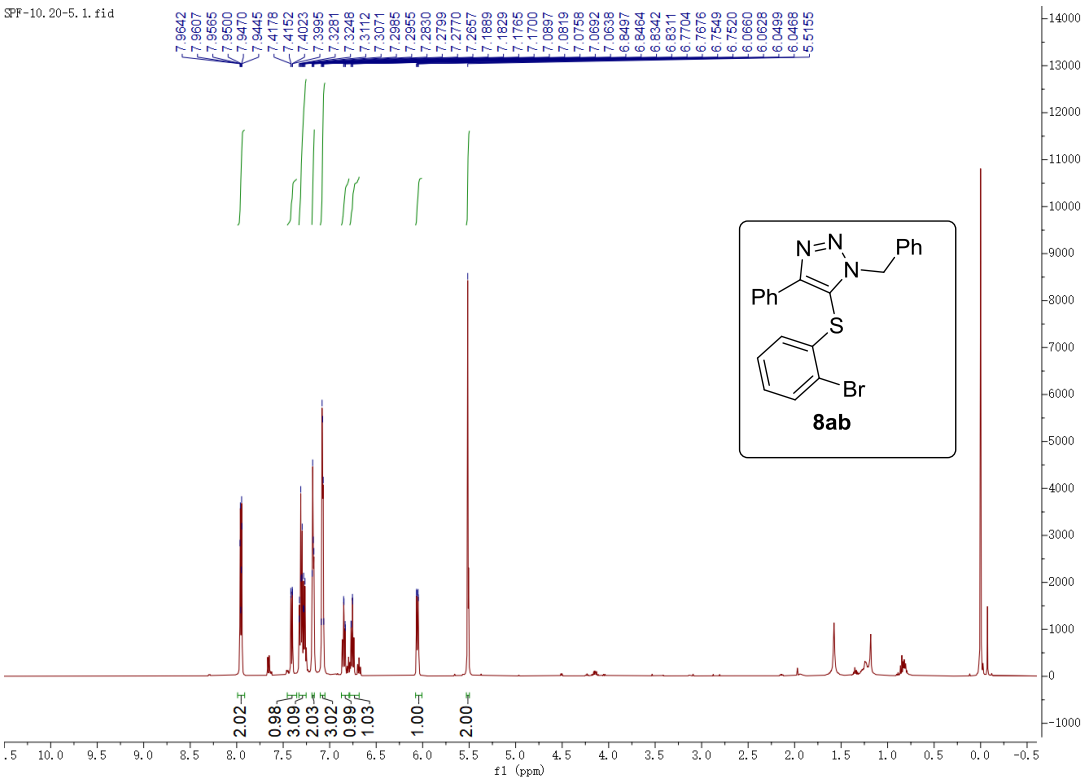


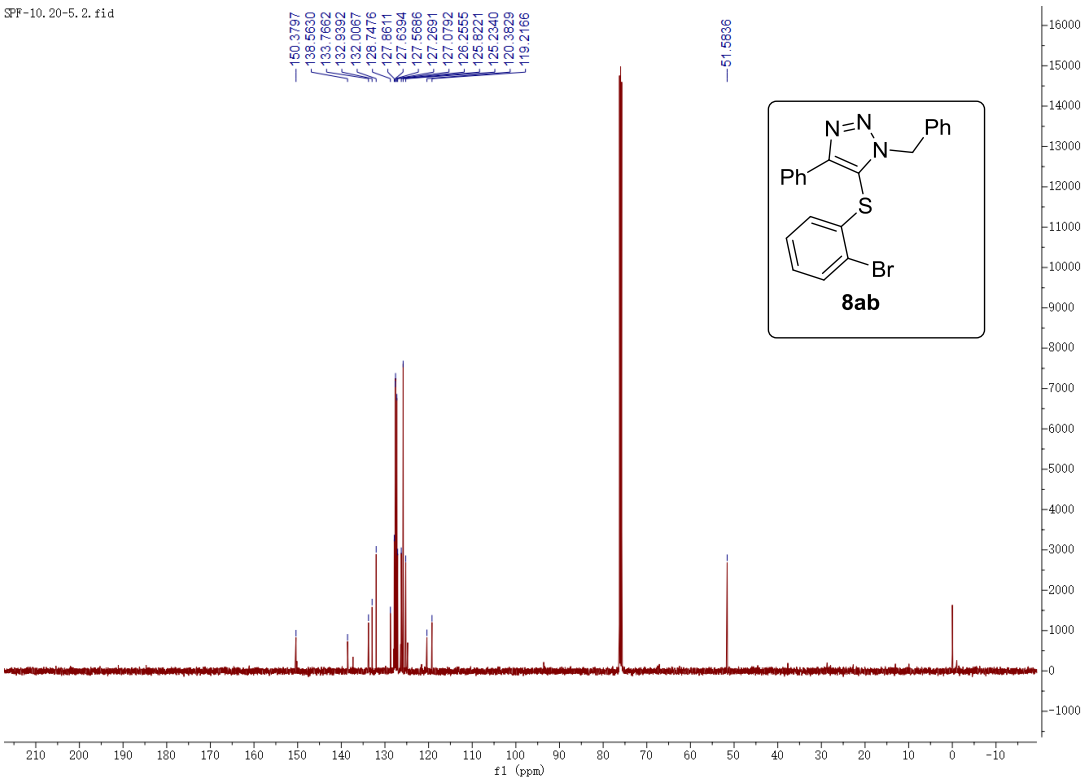
Compound 8aa



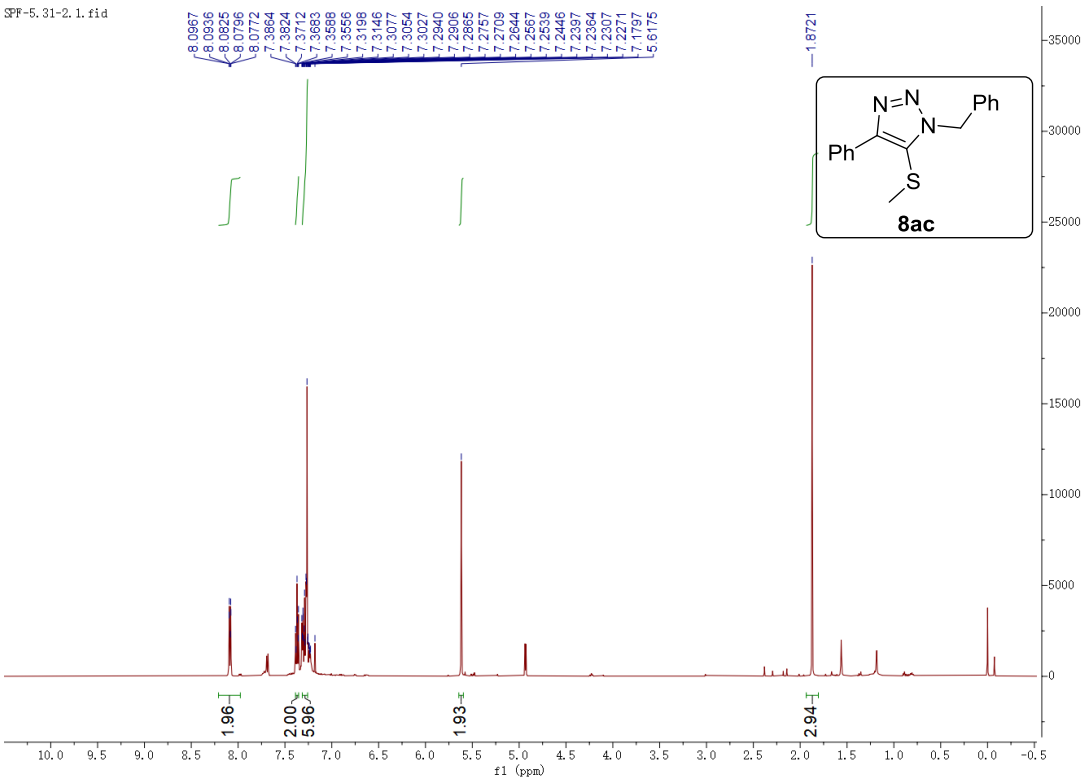


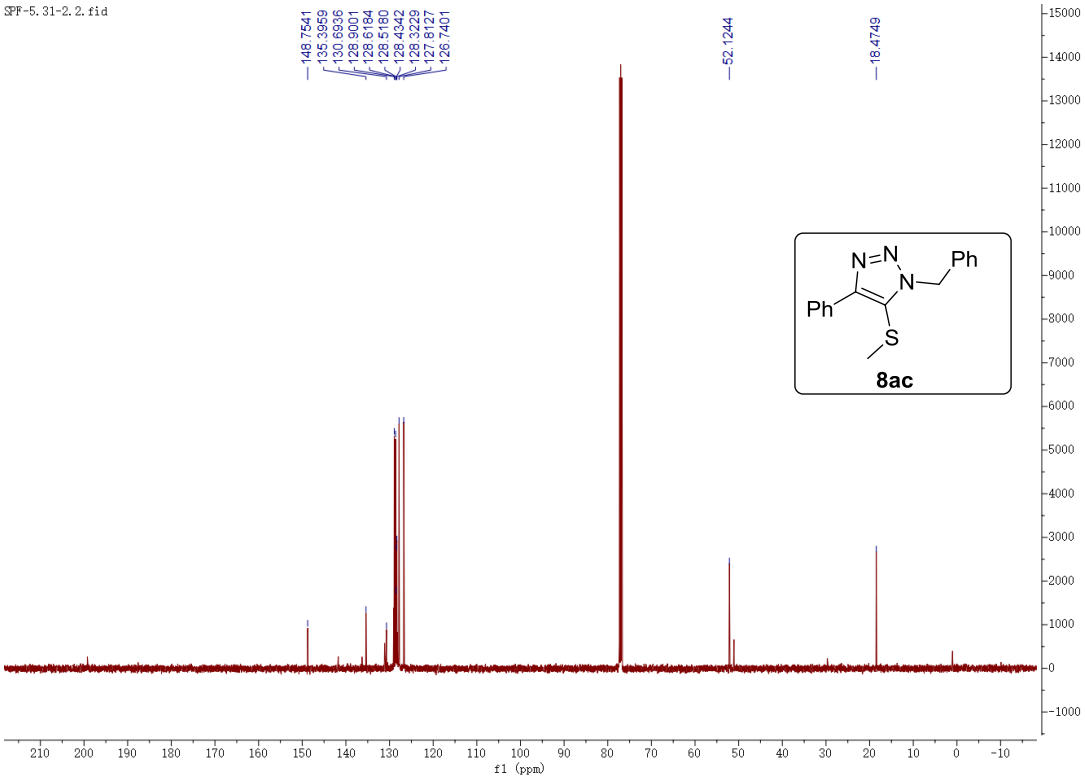
Compound 8ab



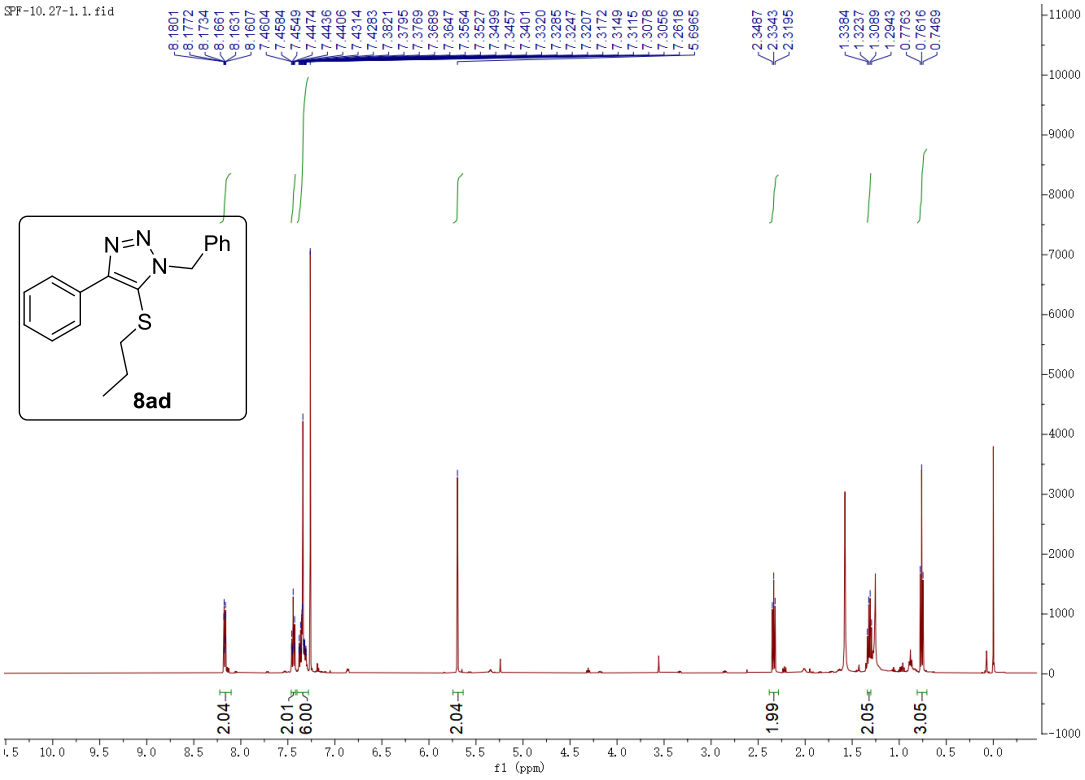


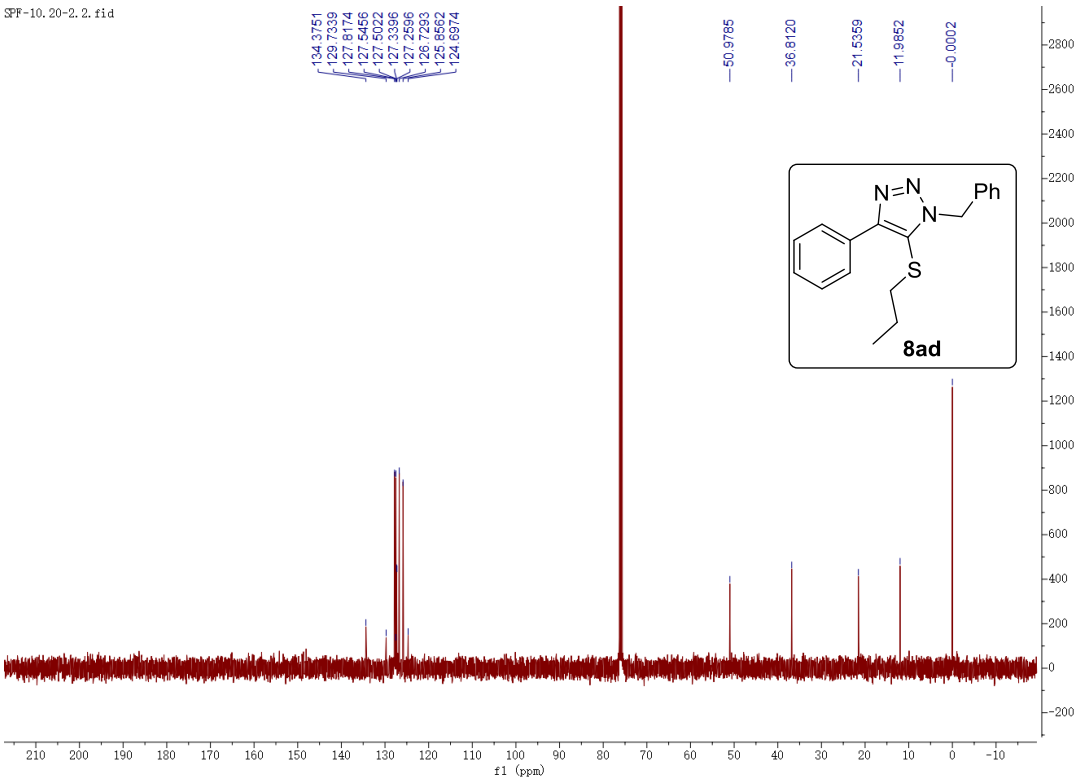
Compound 8ac





Compound 8ad





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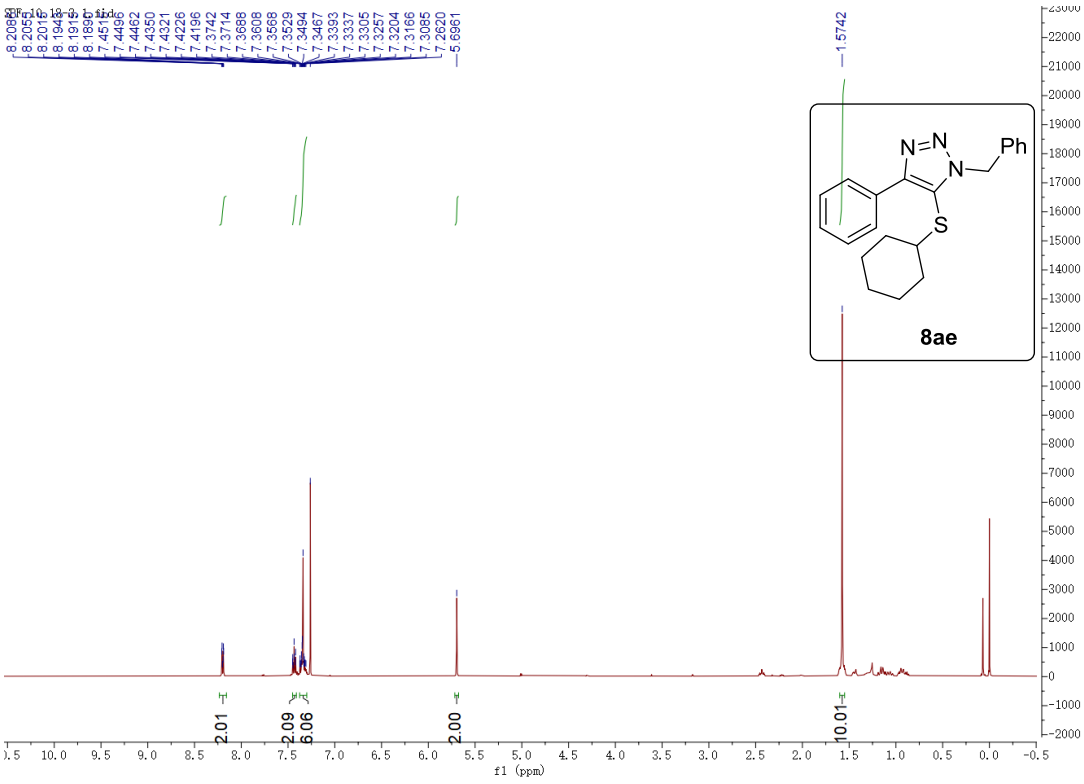

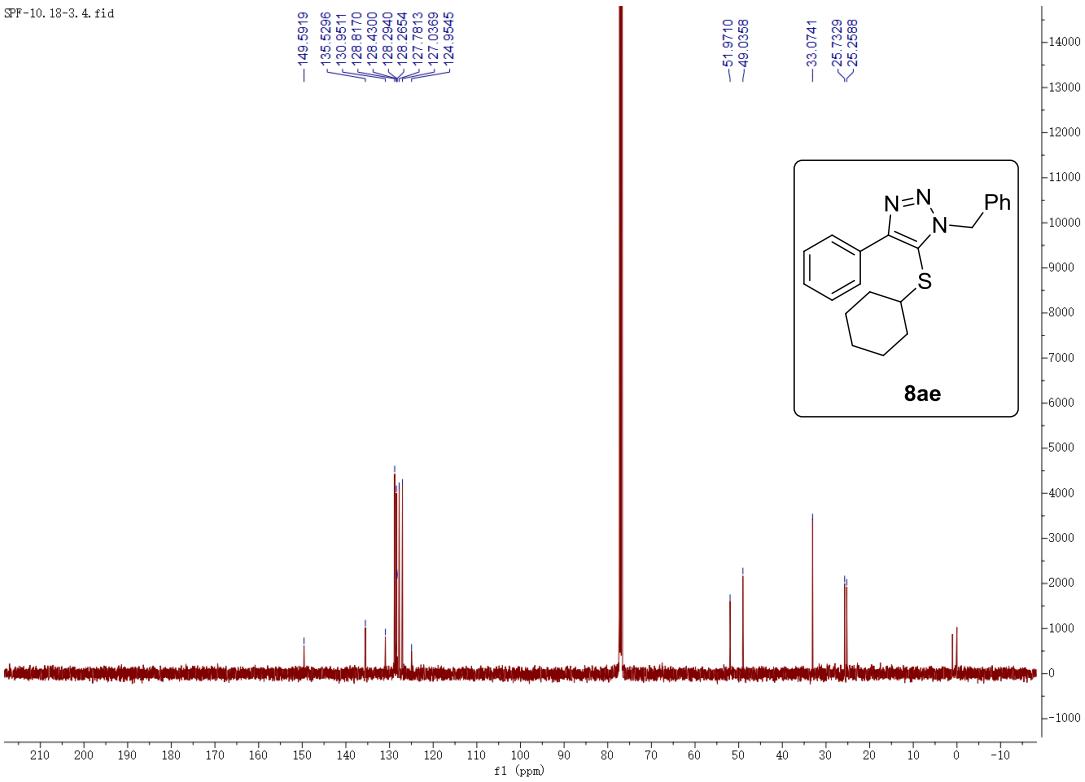

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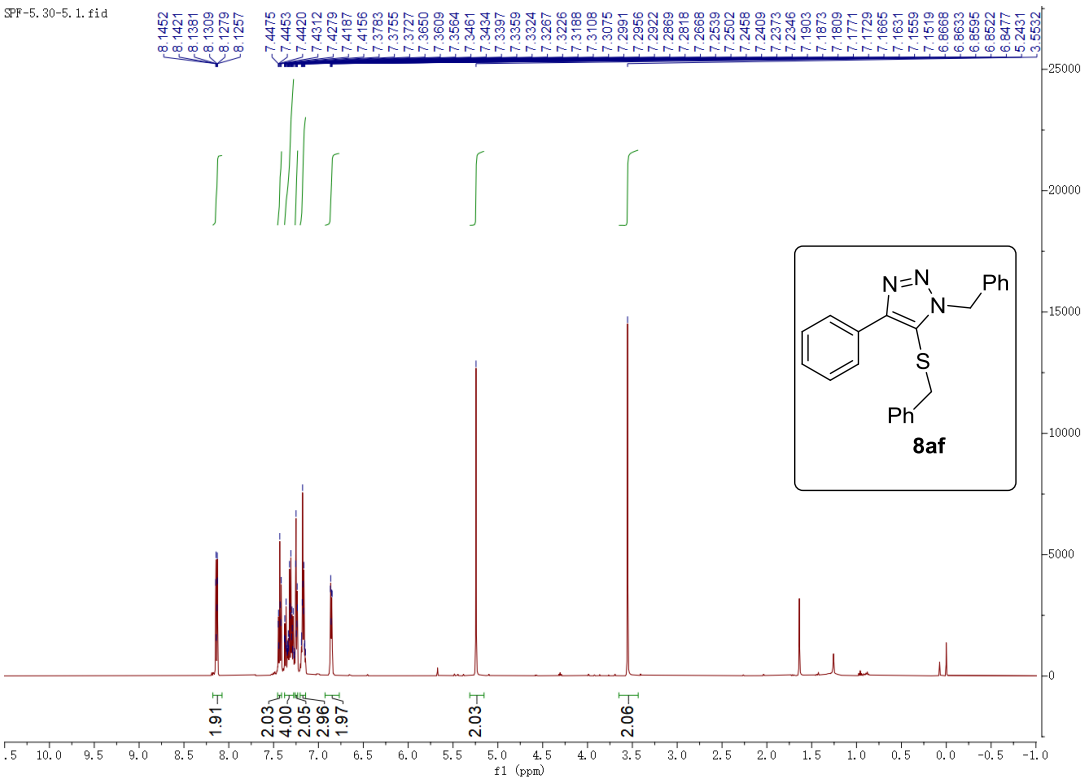

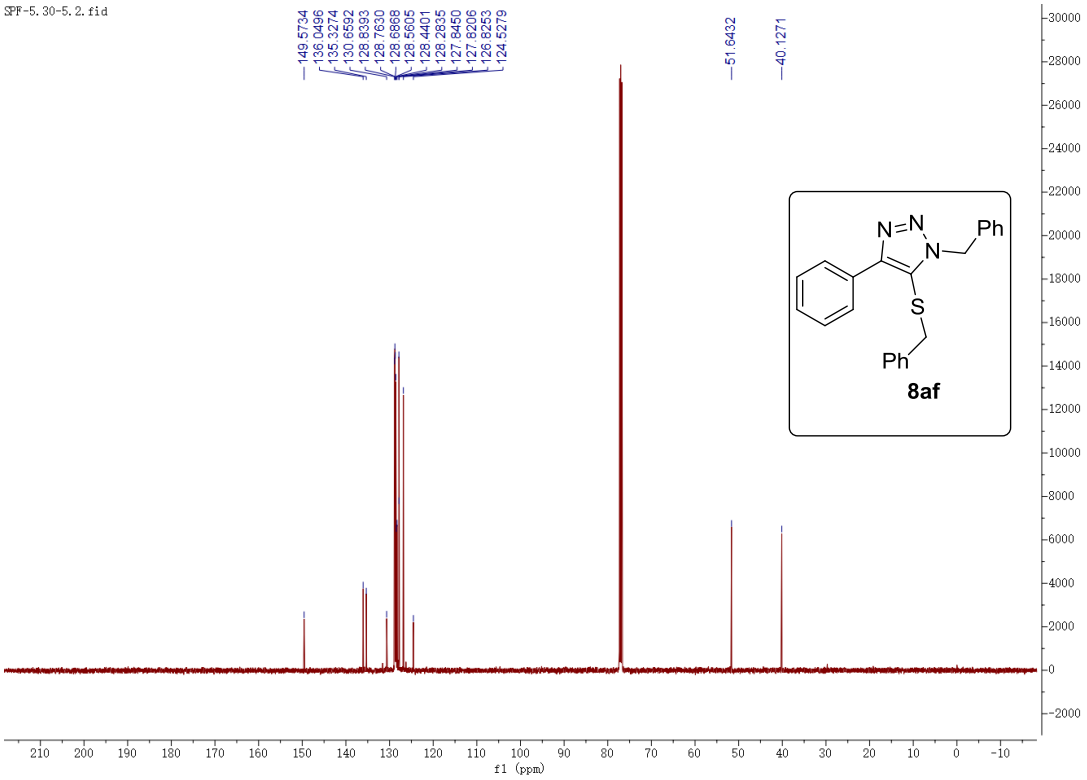

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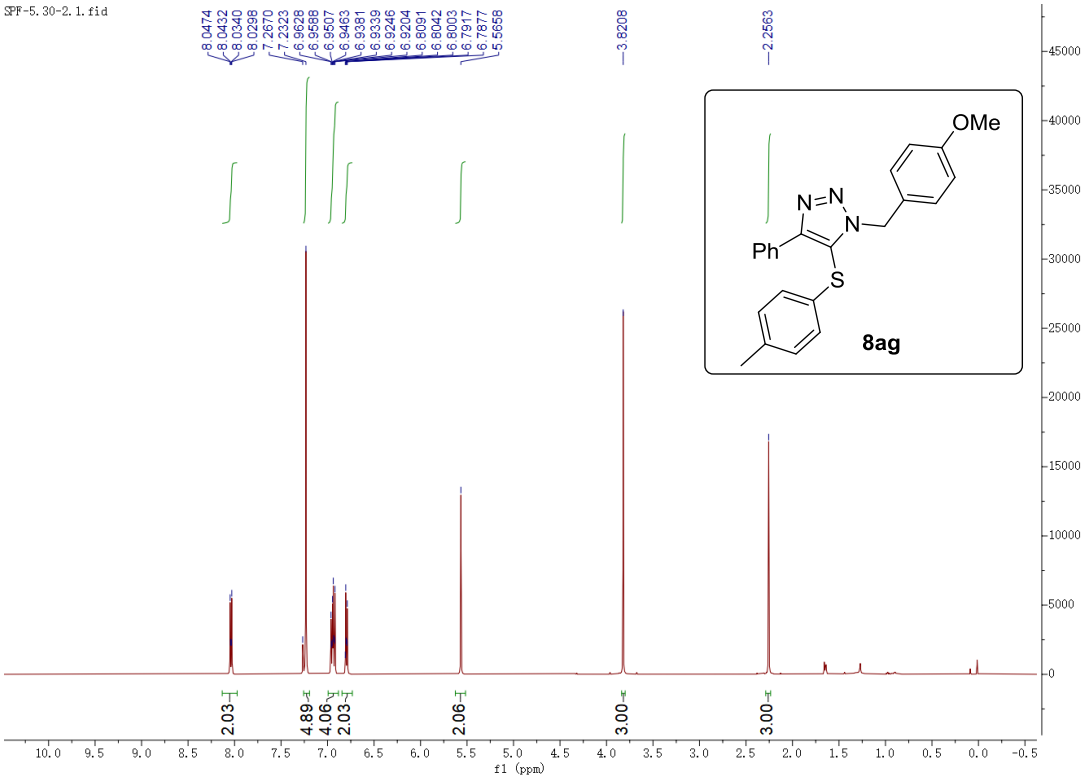

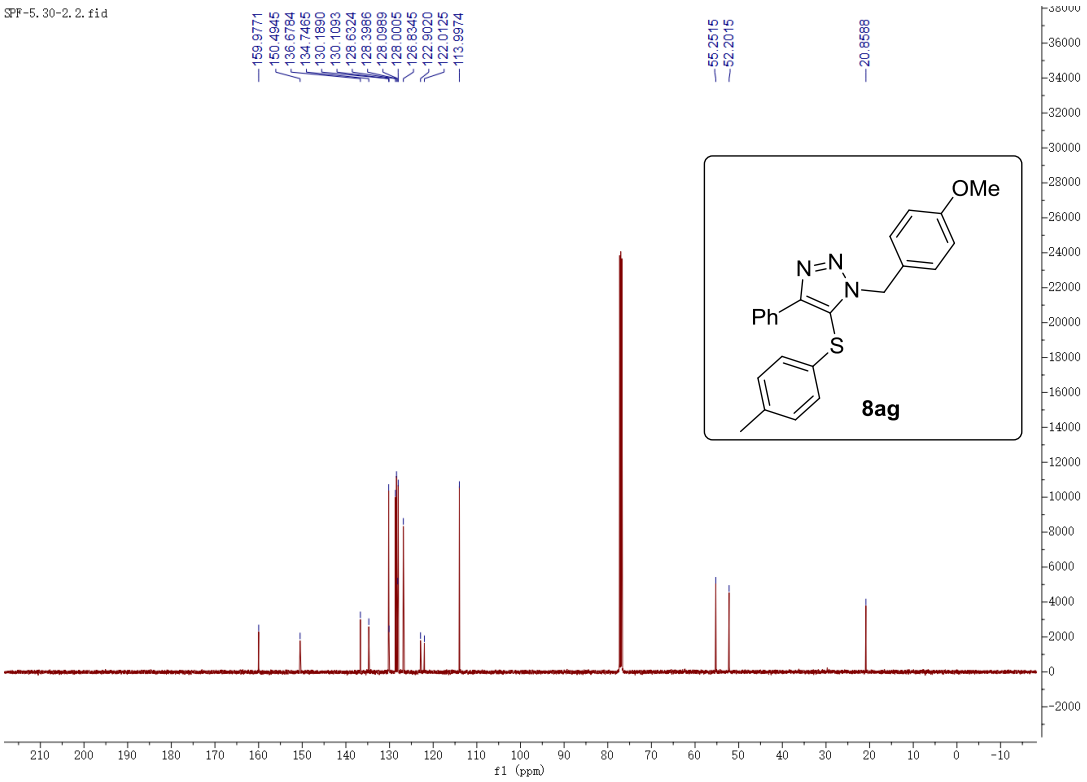

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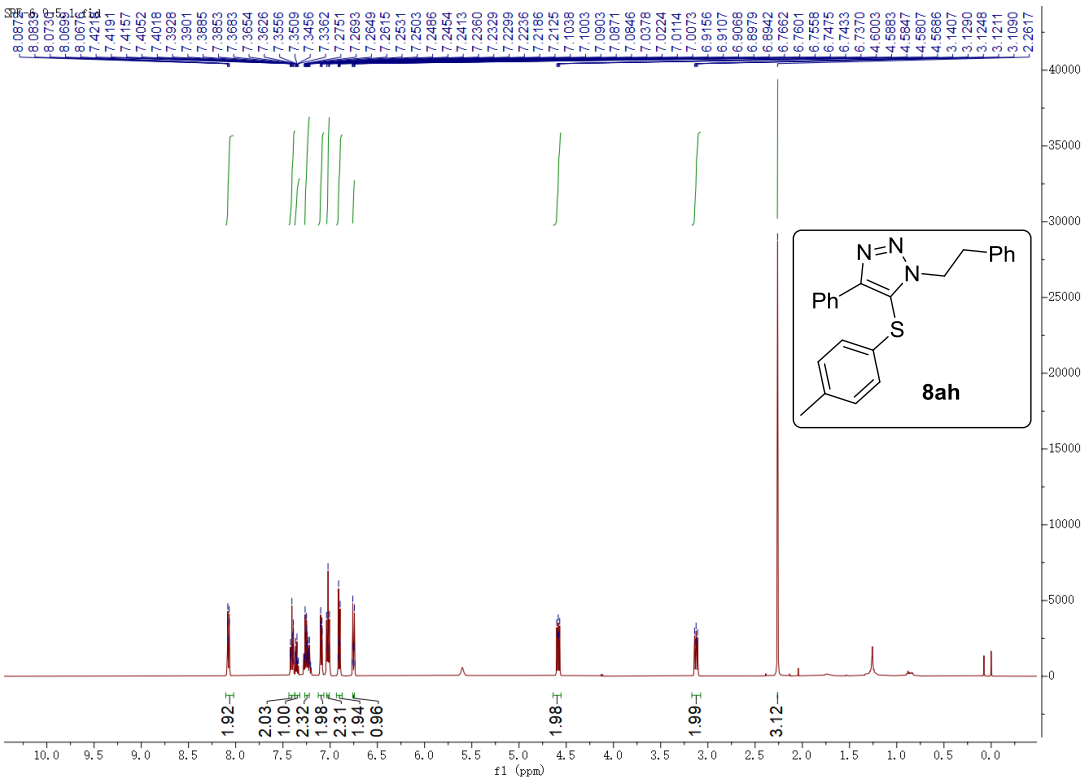

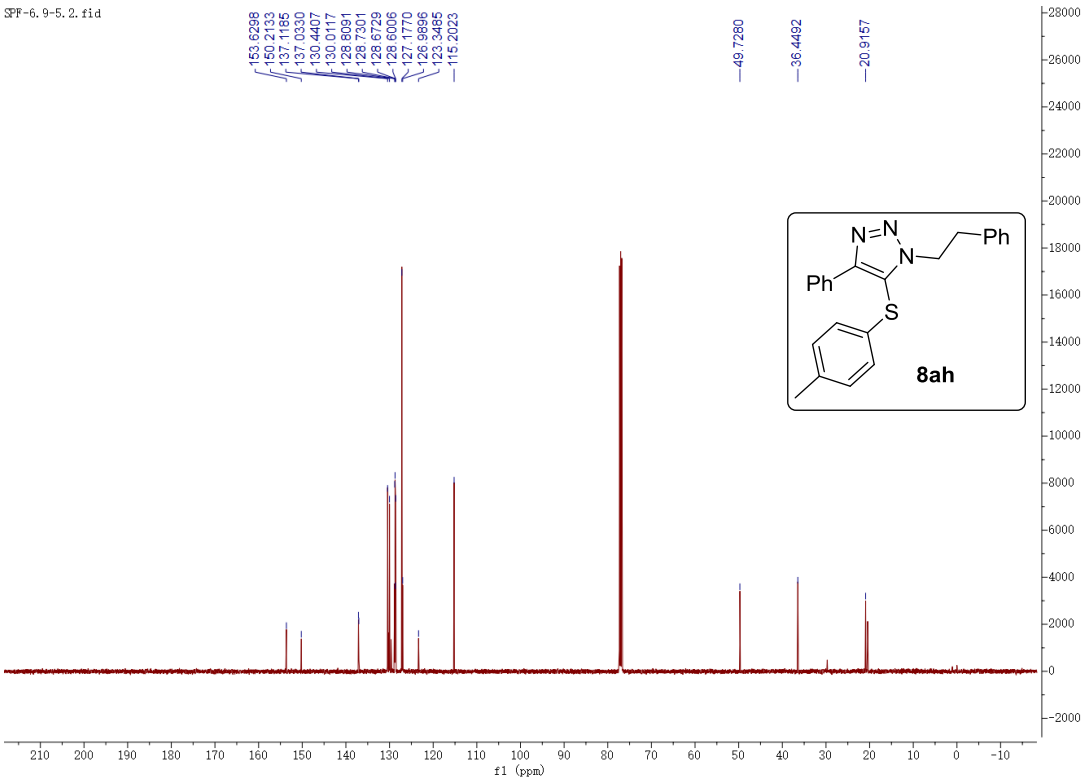

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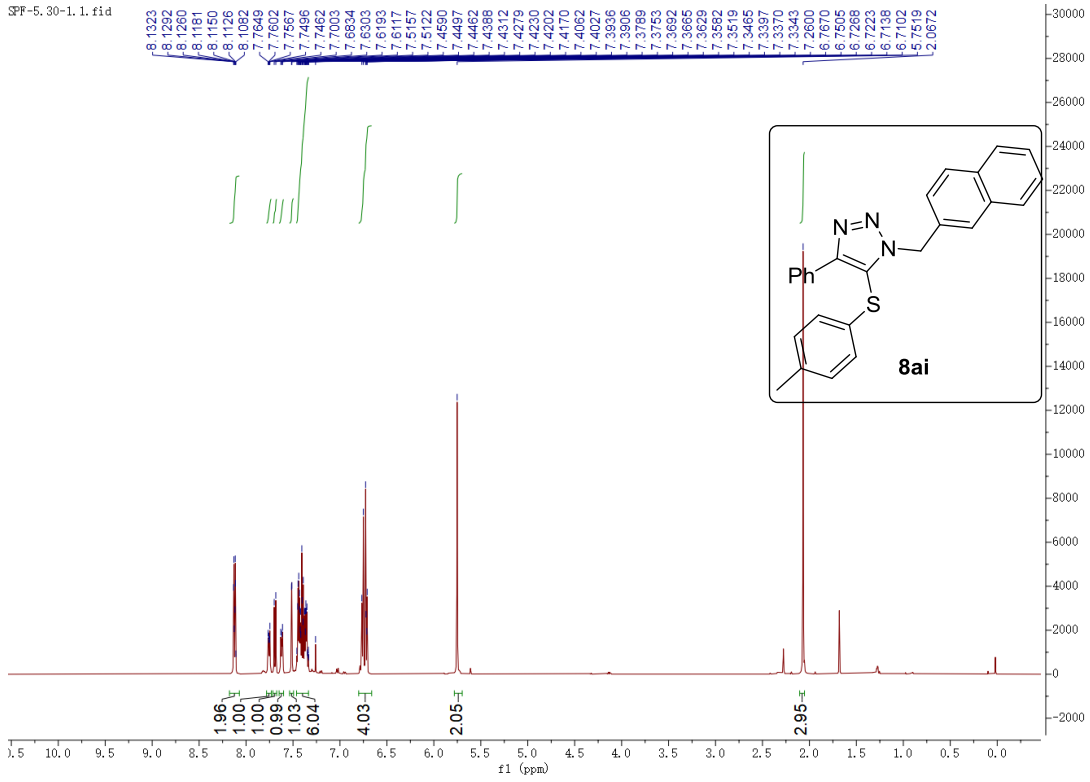

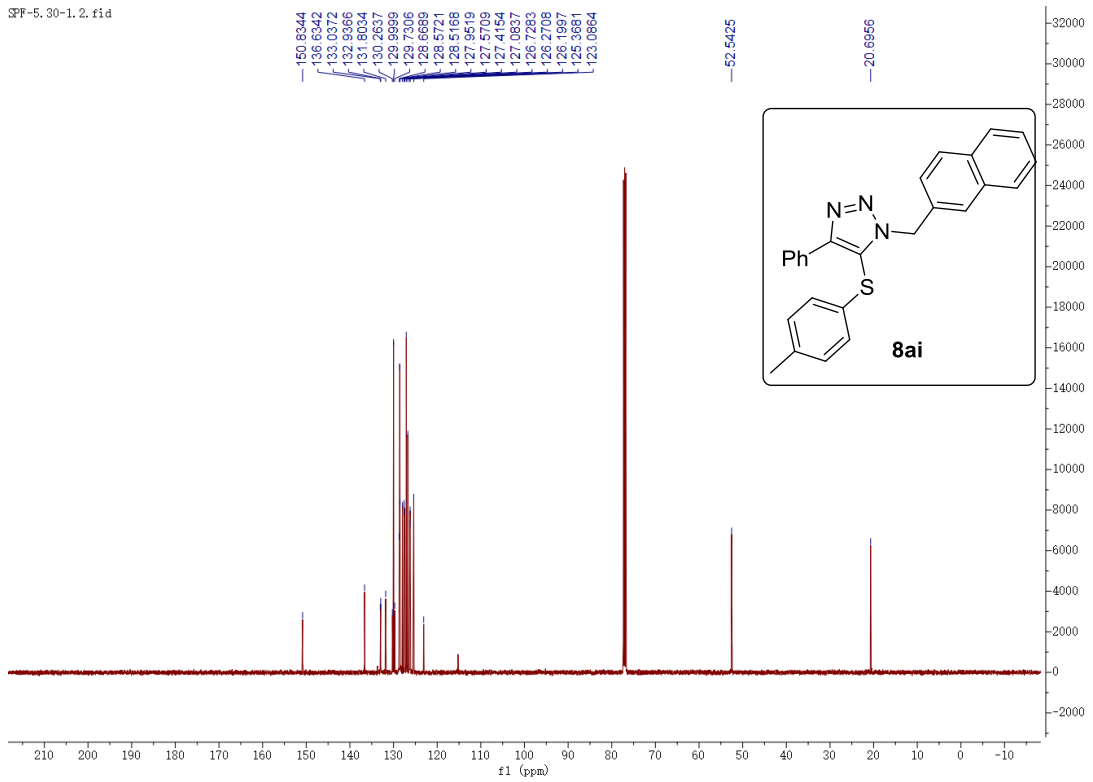

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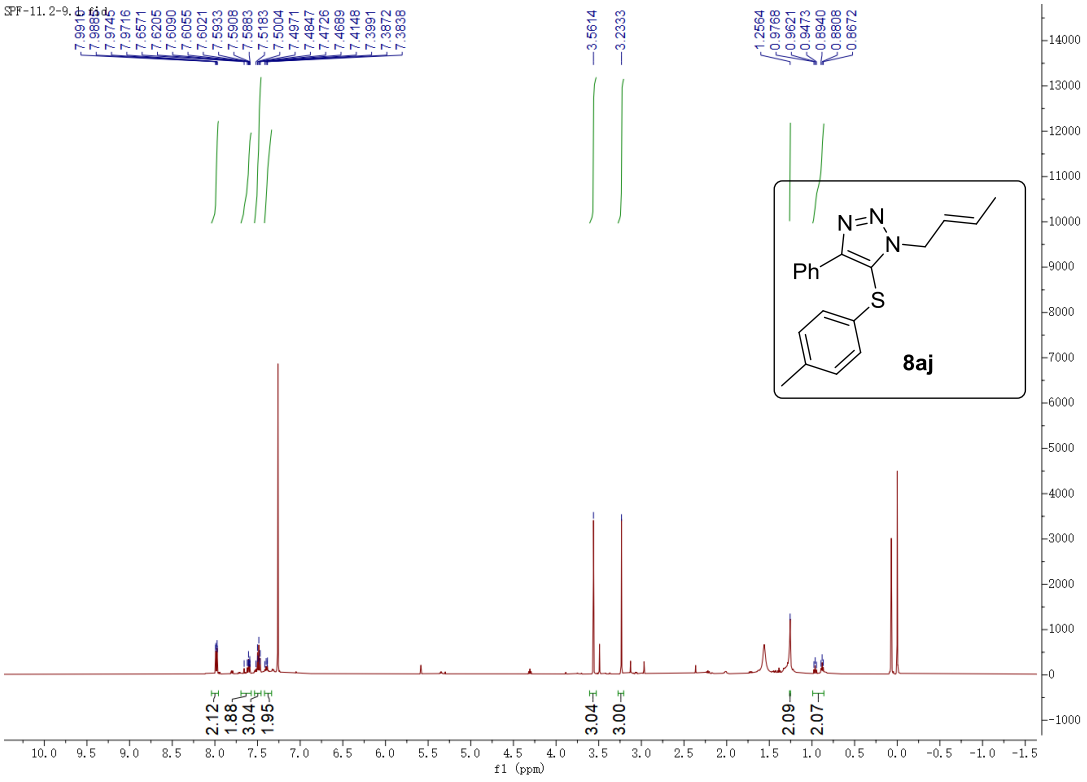

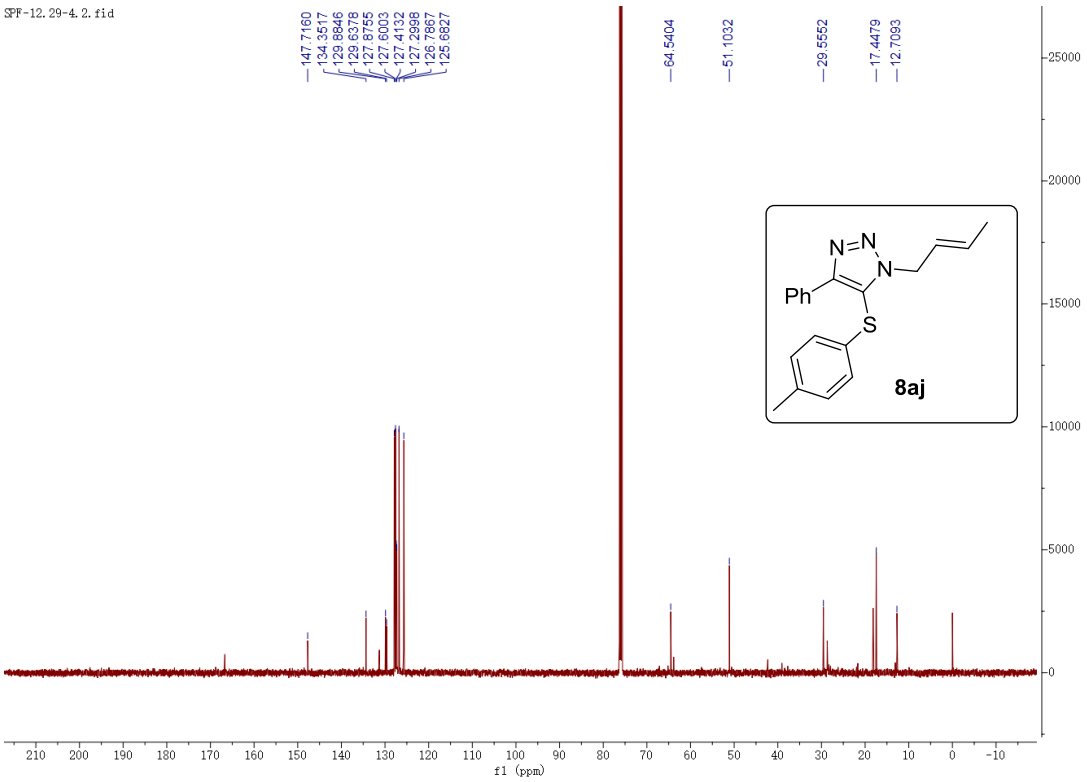

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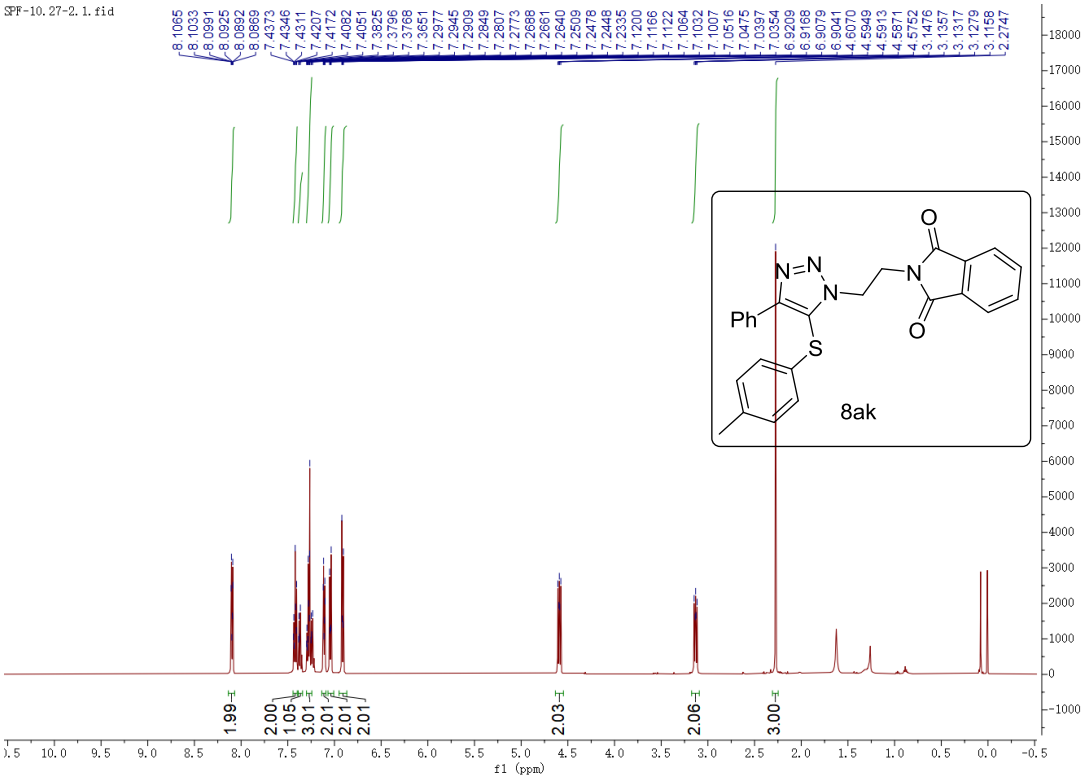

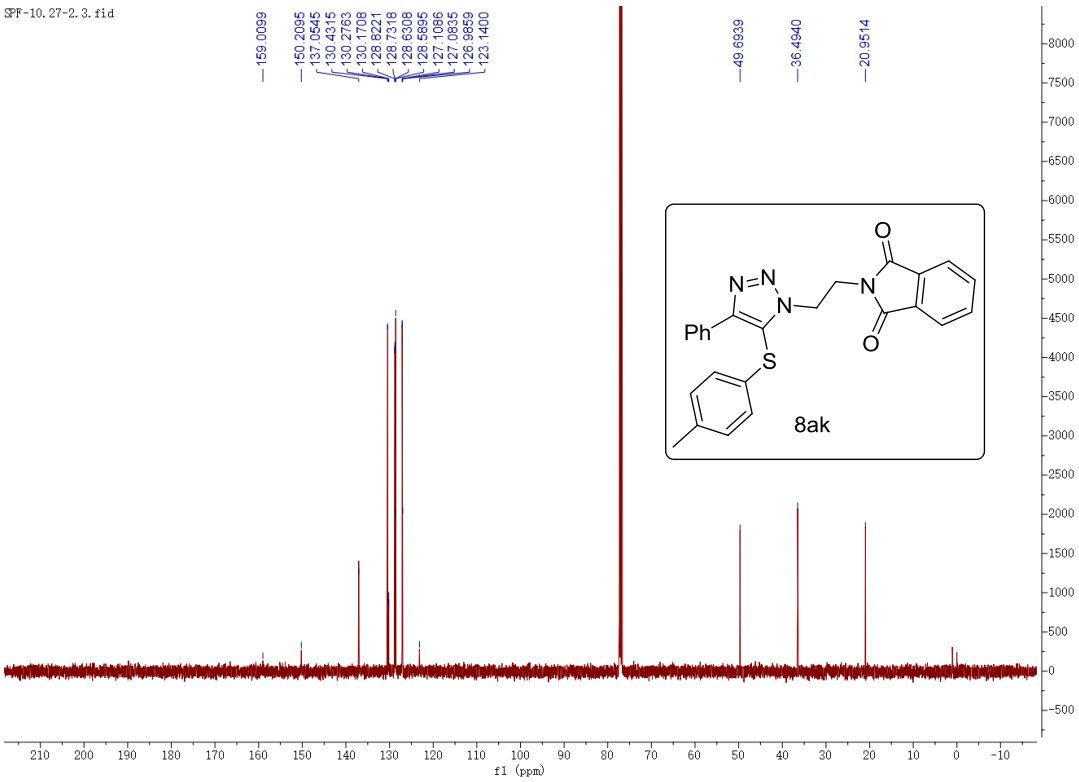

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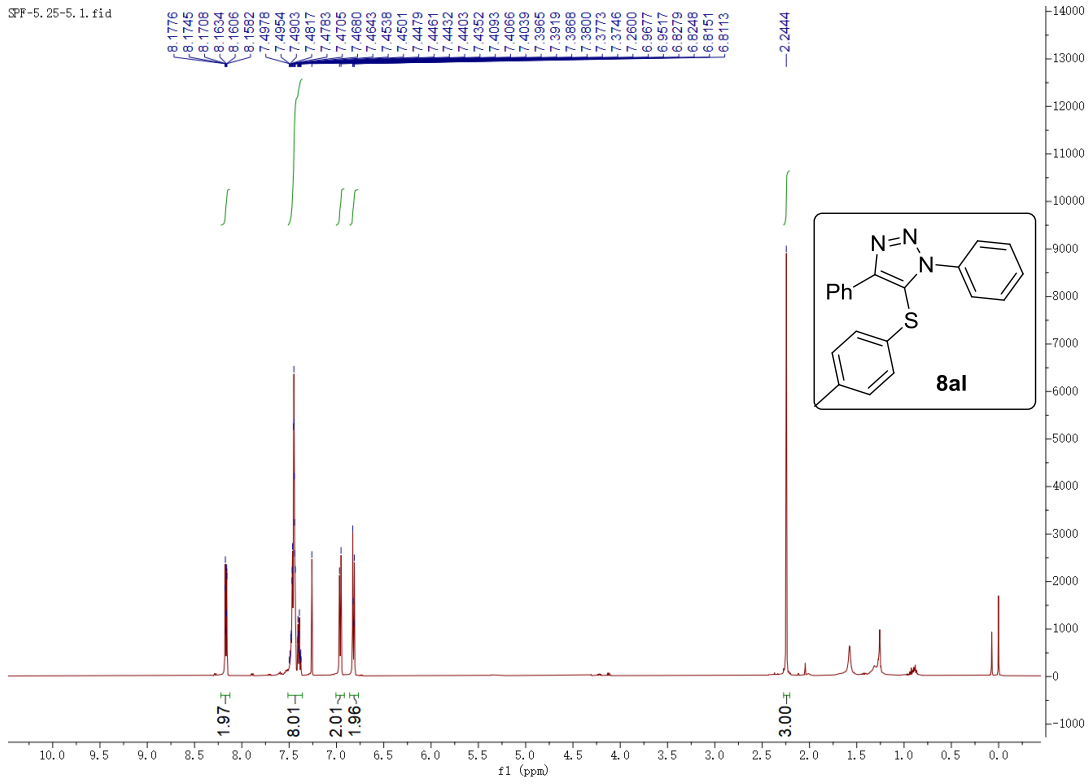

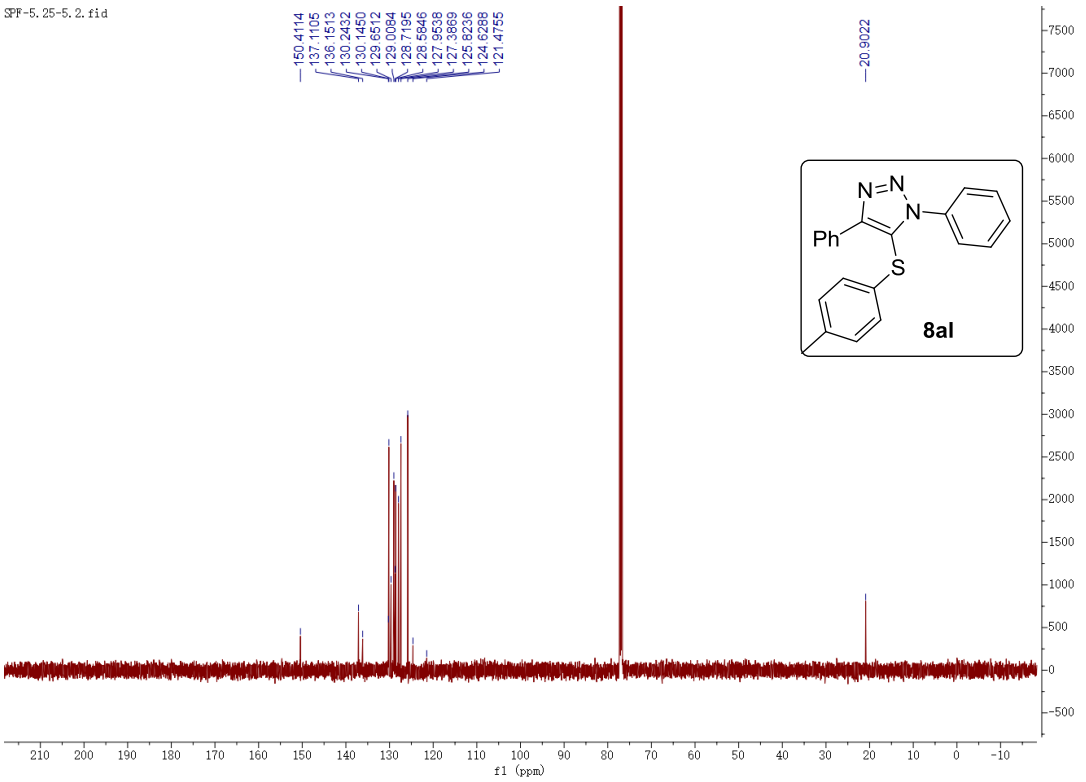

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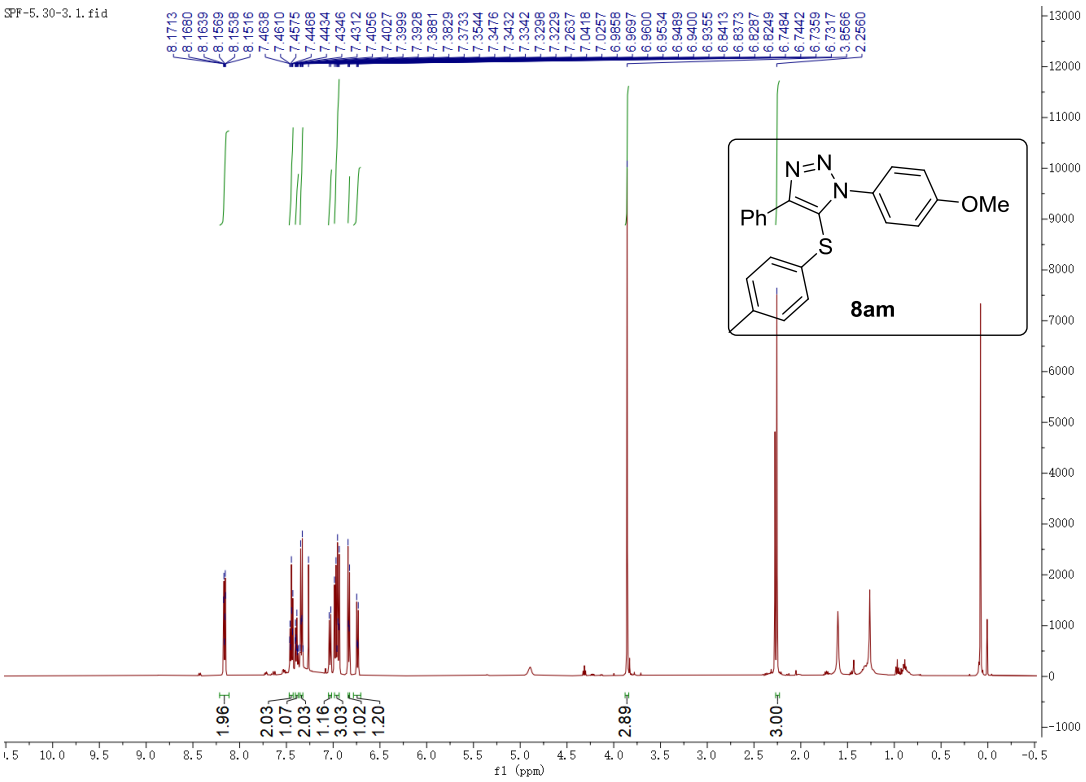

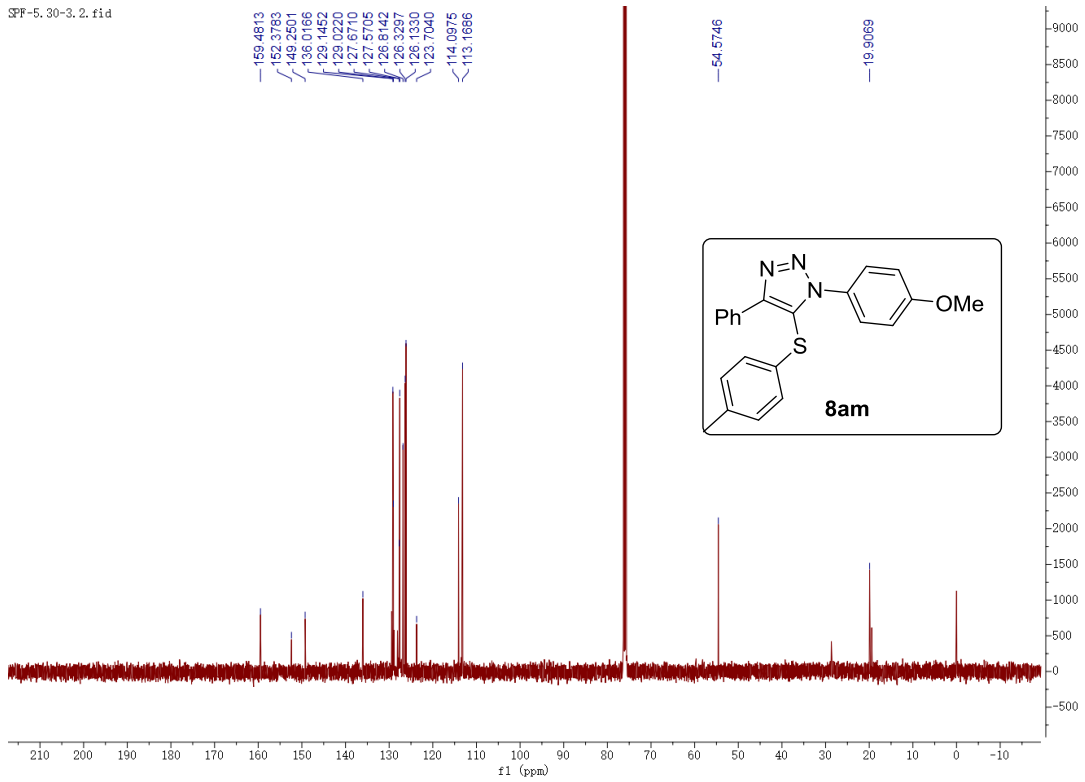

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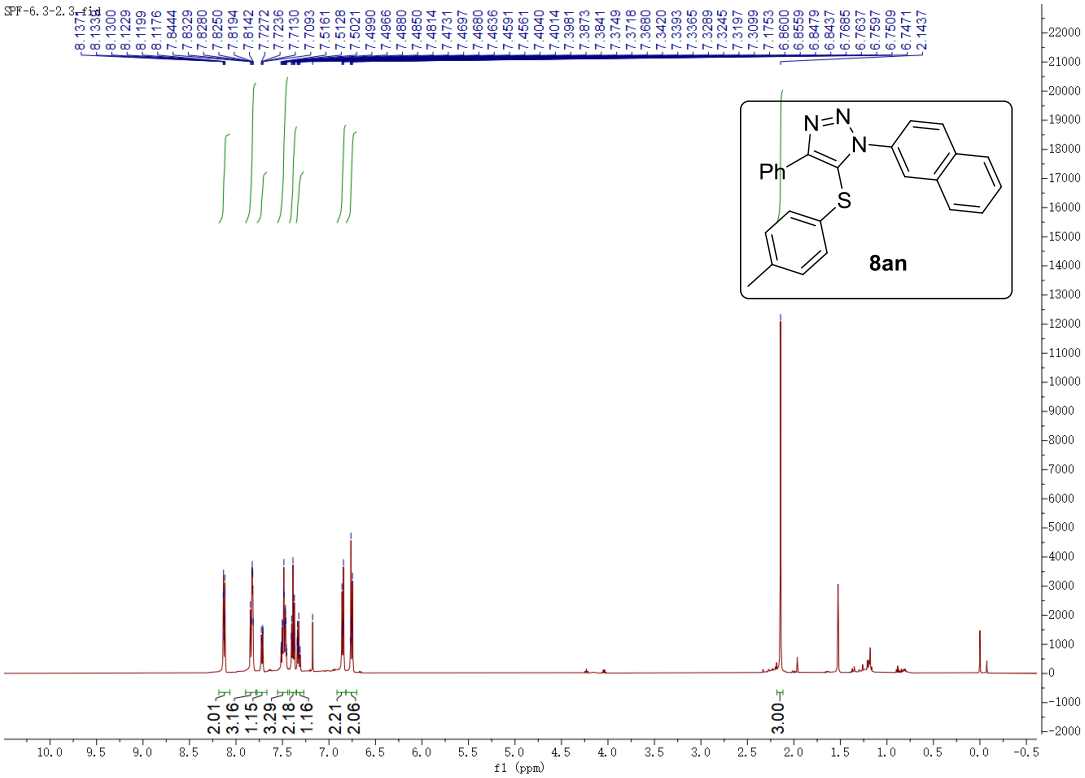

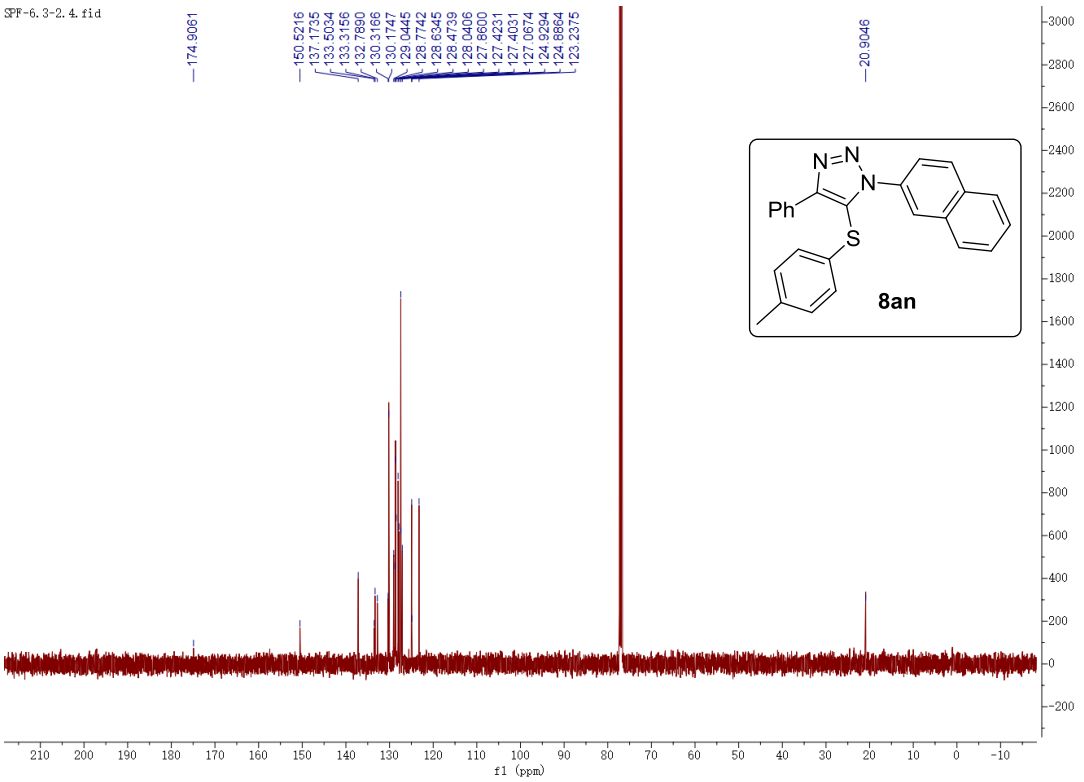

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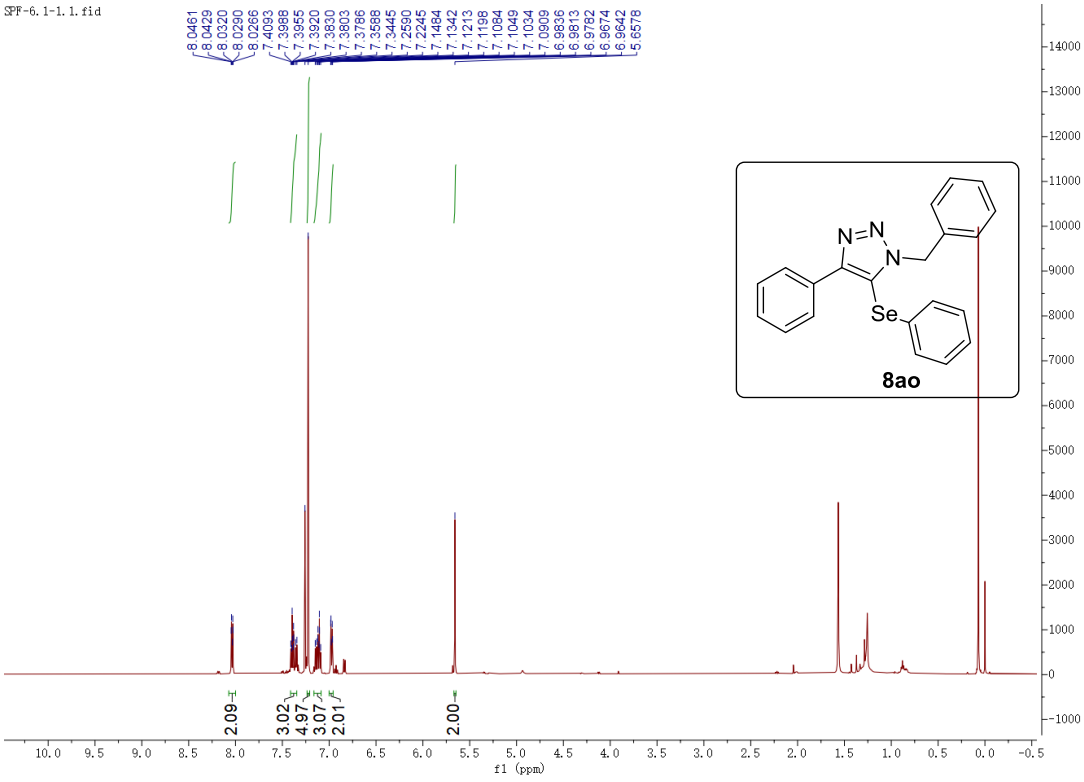

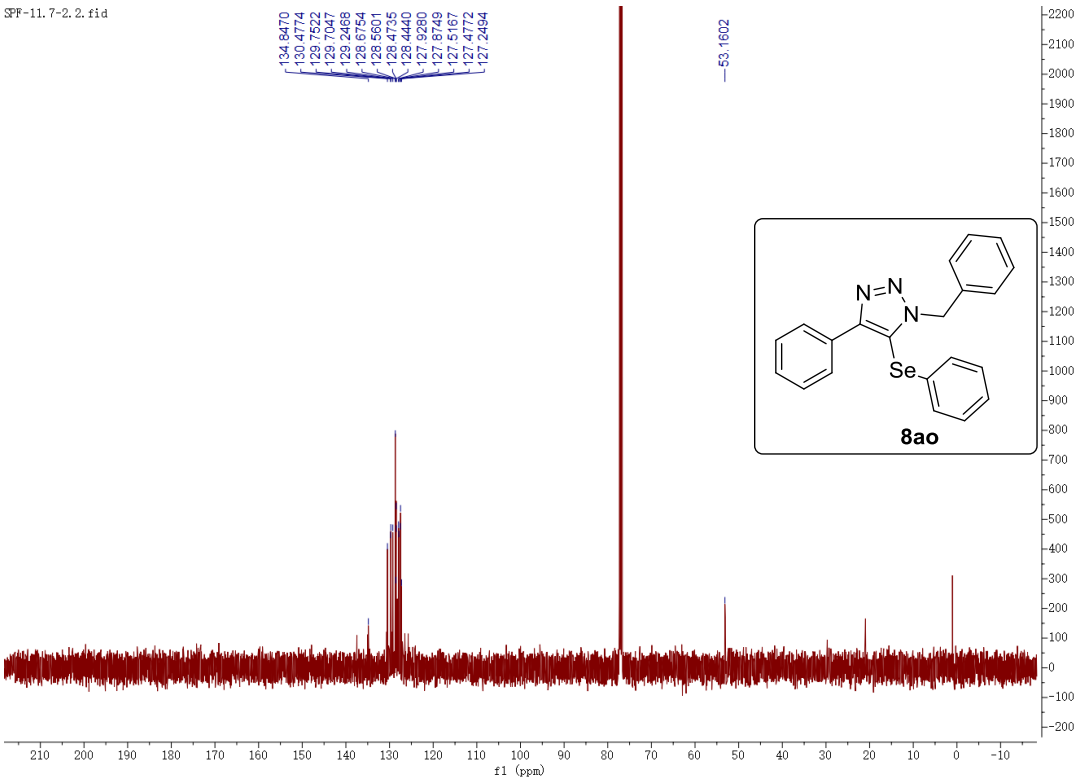

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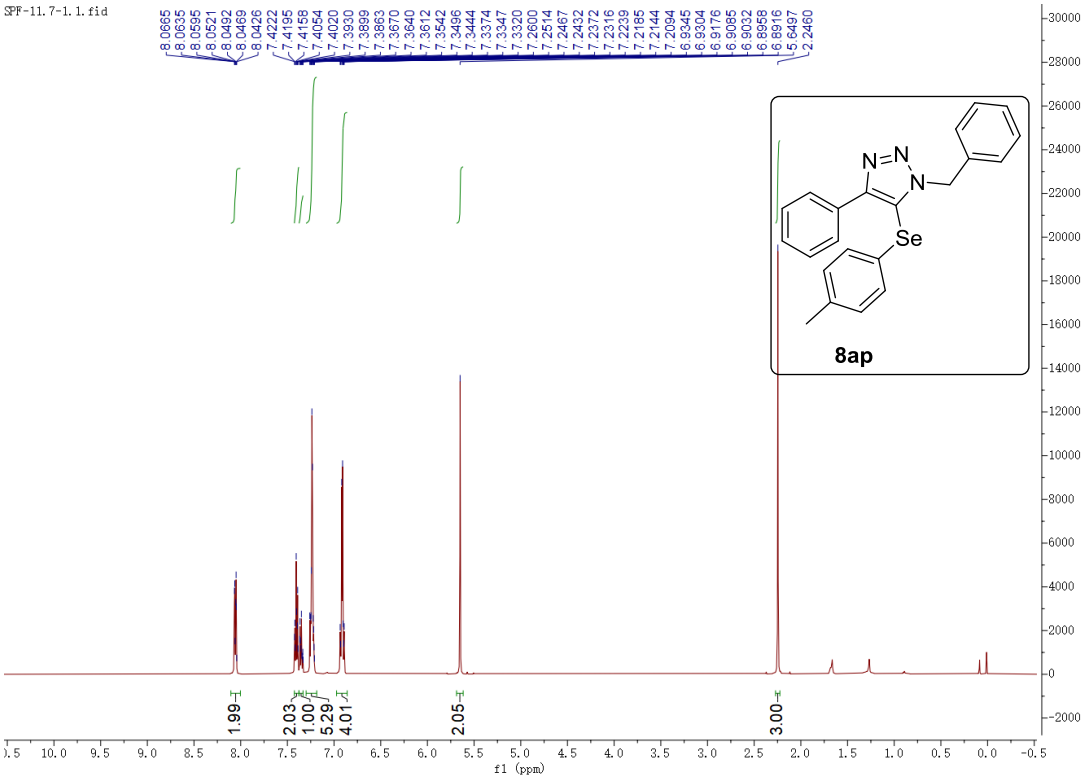

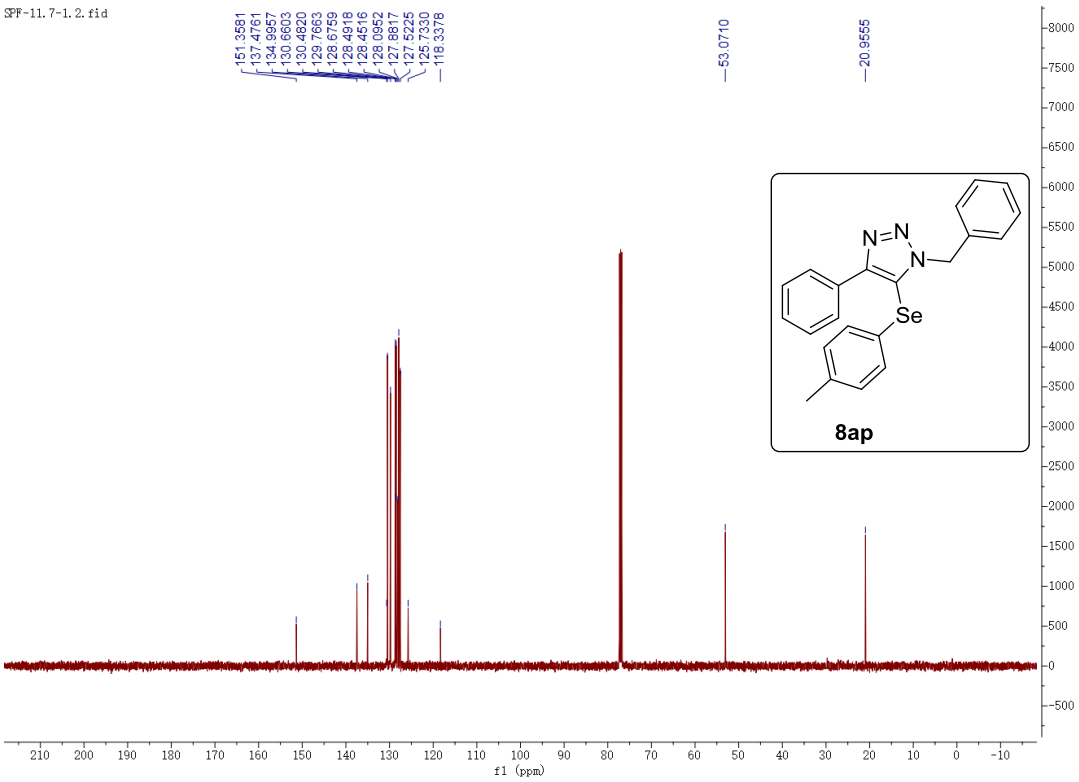

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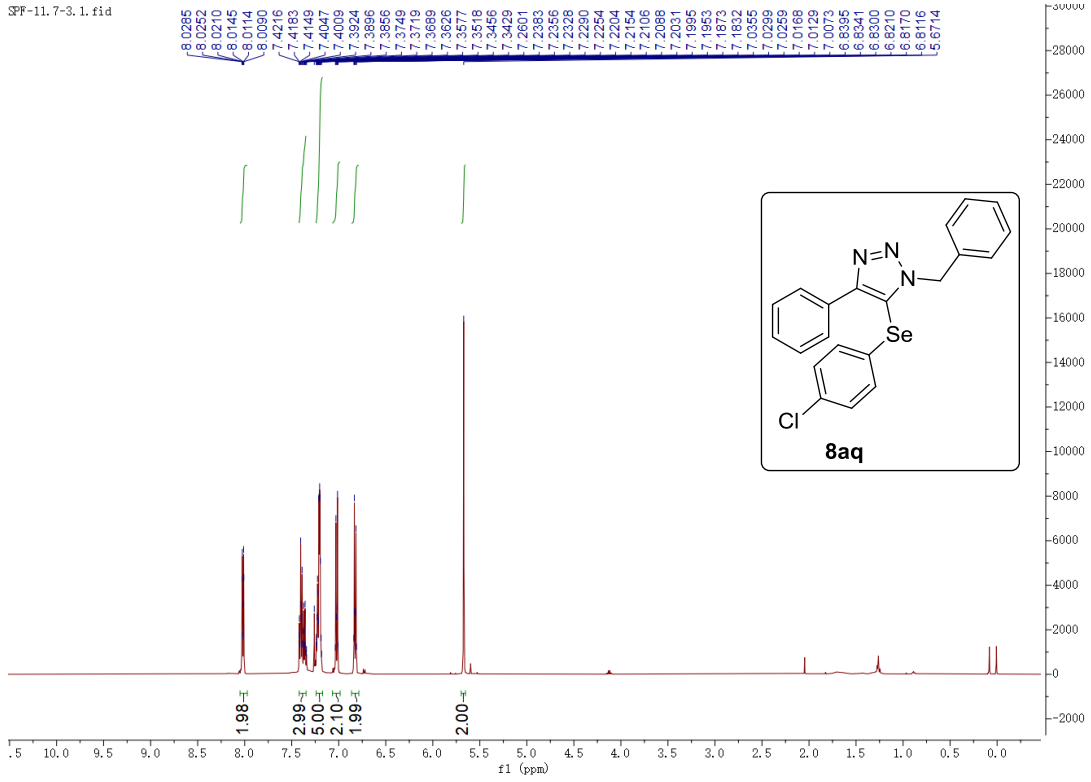

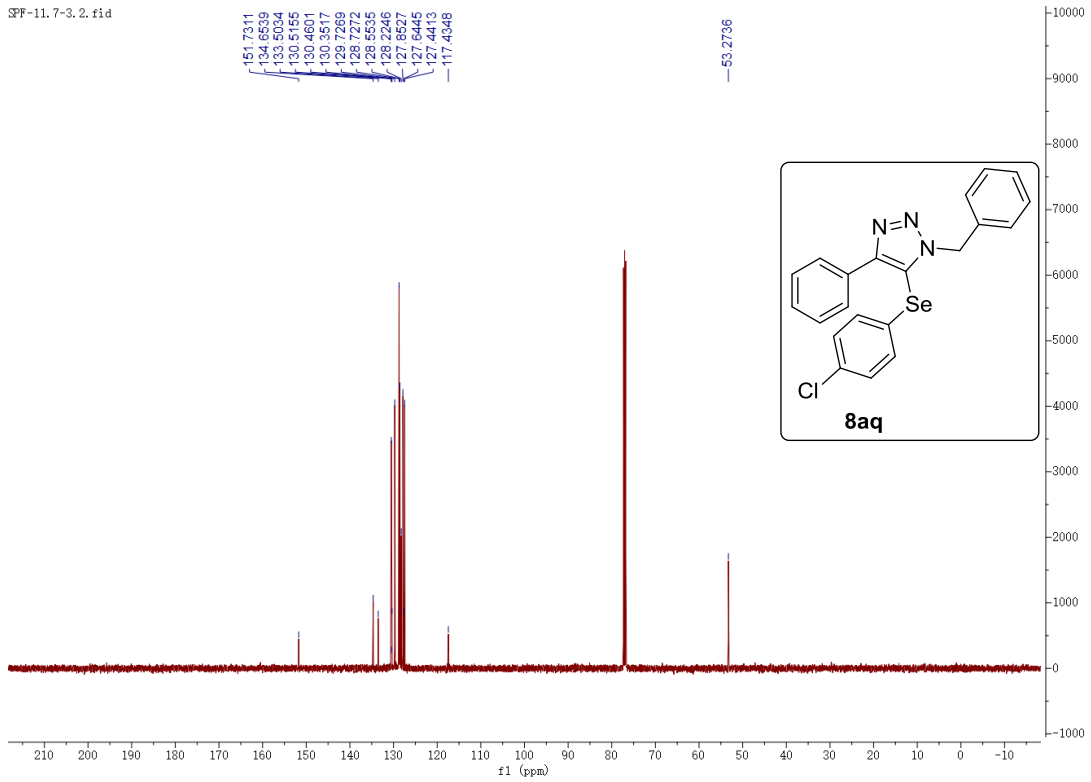

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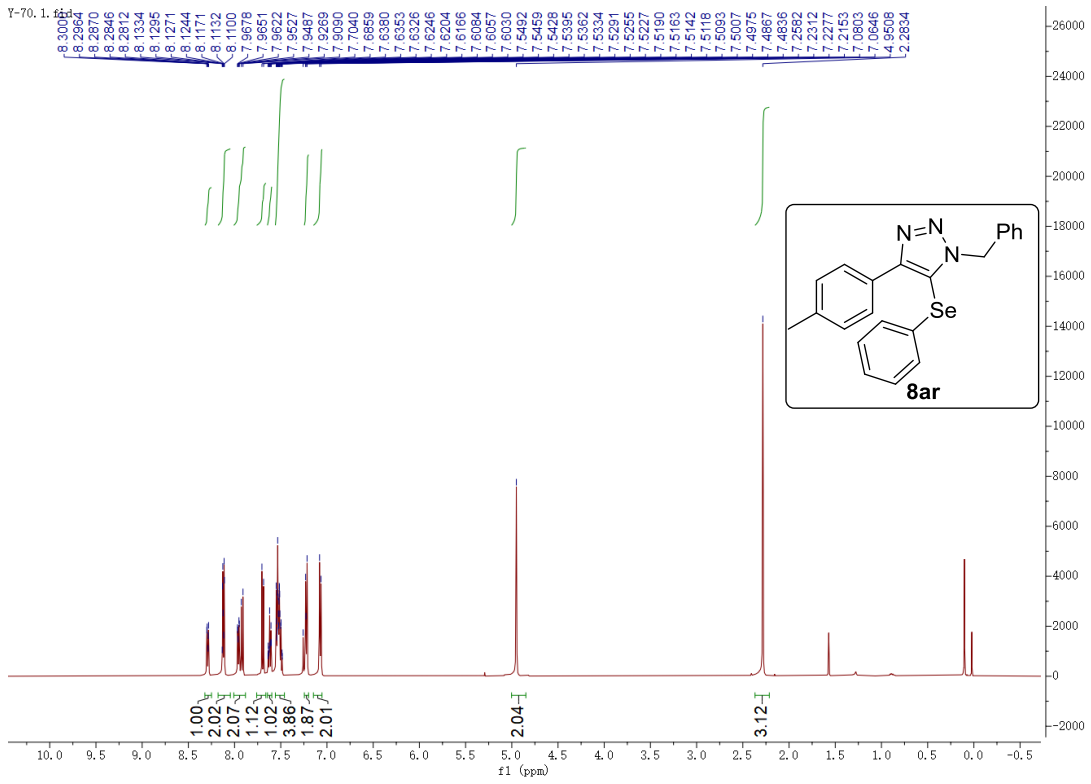

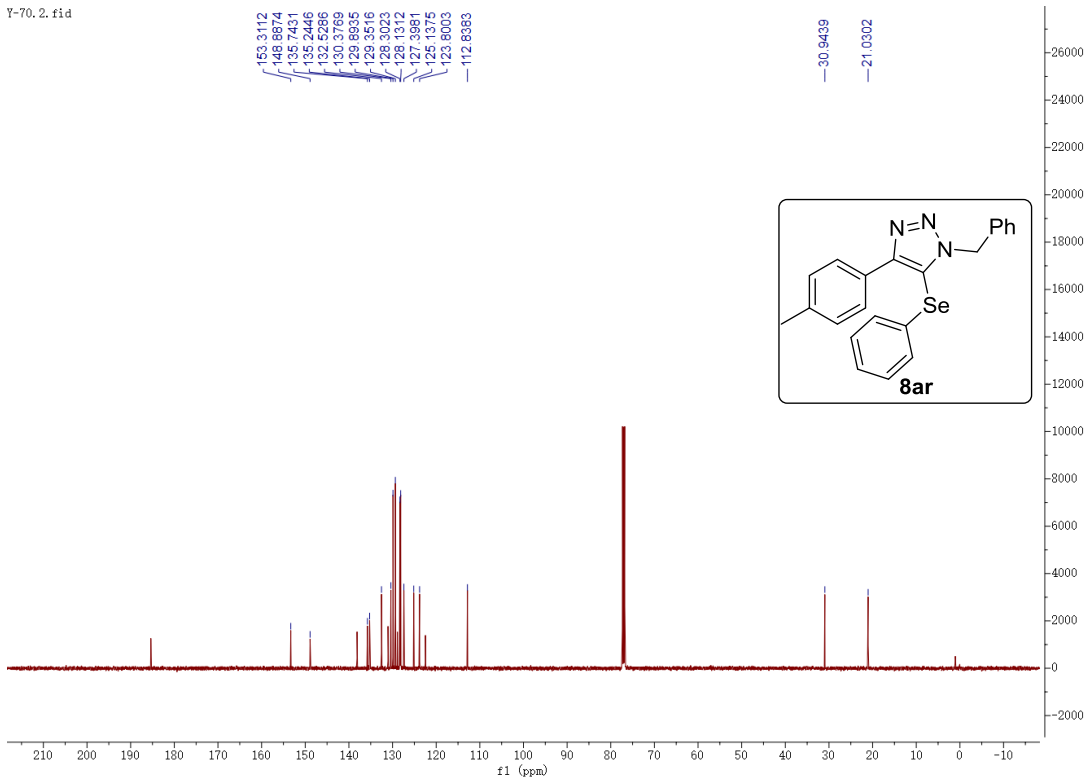

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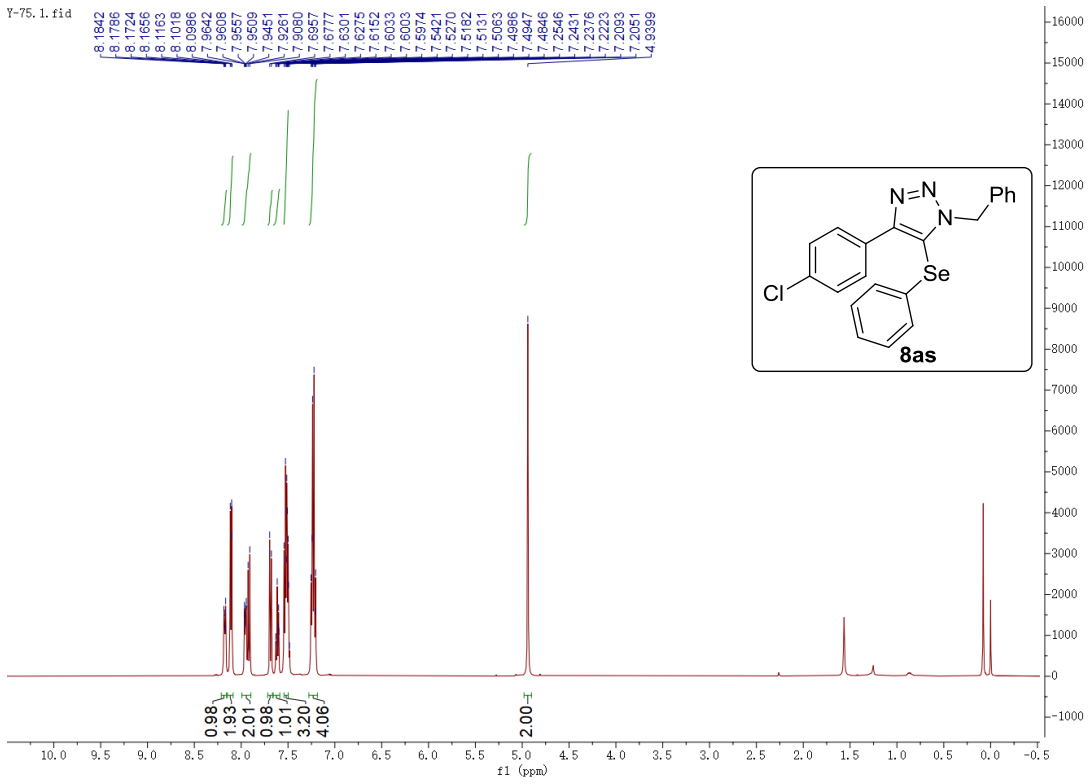

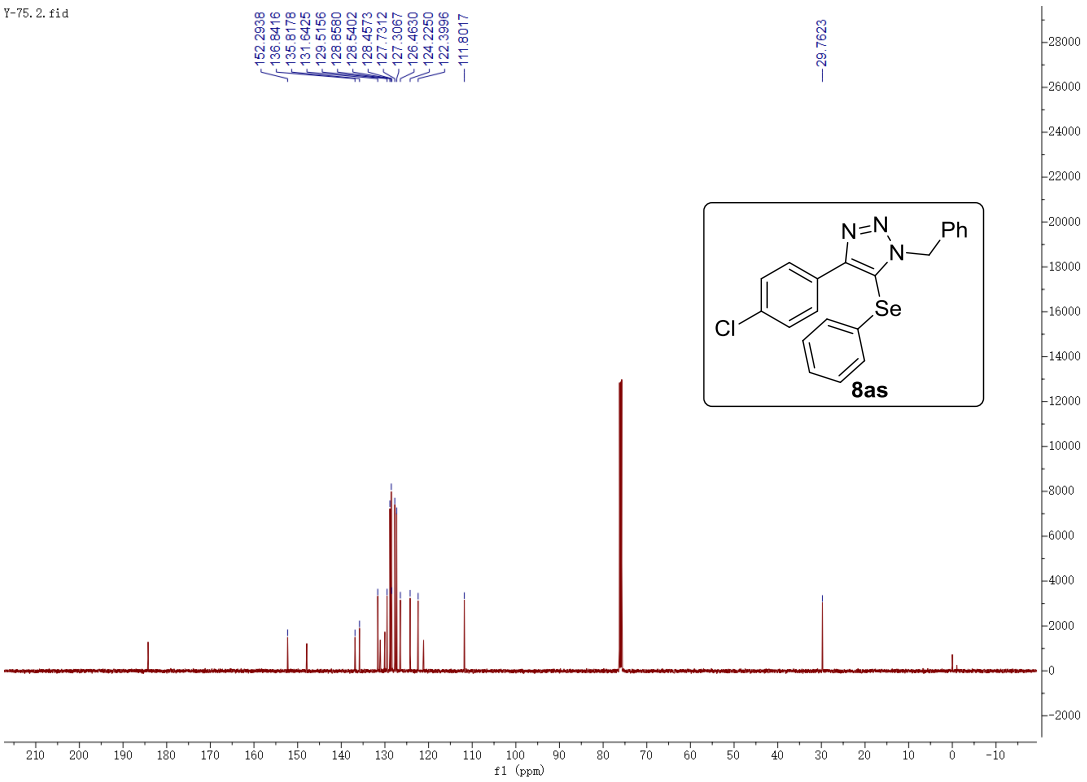

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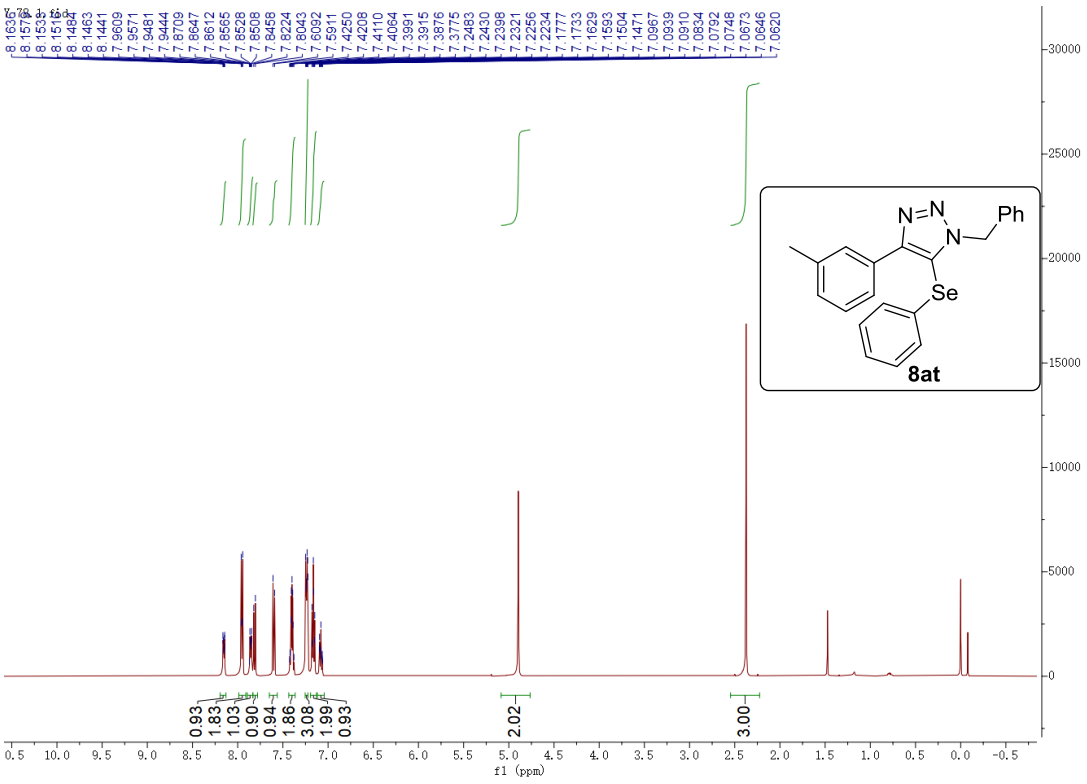

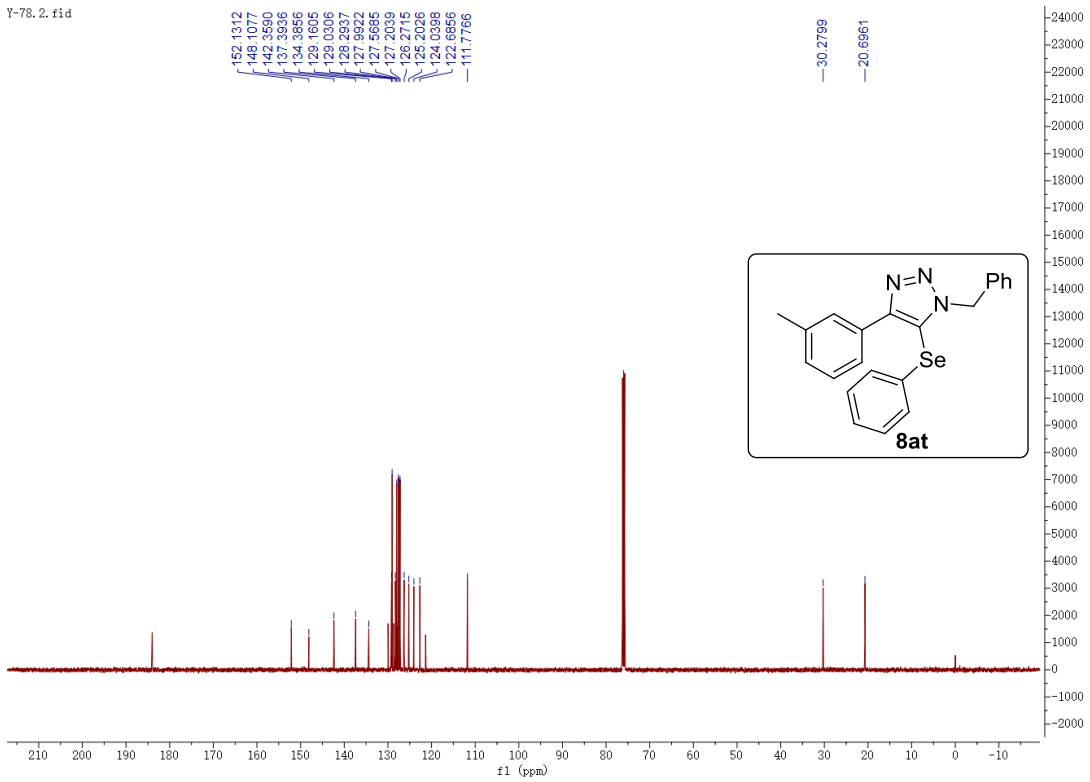
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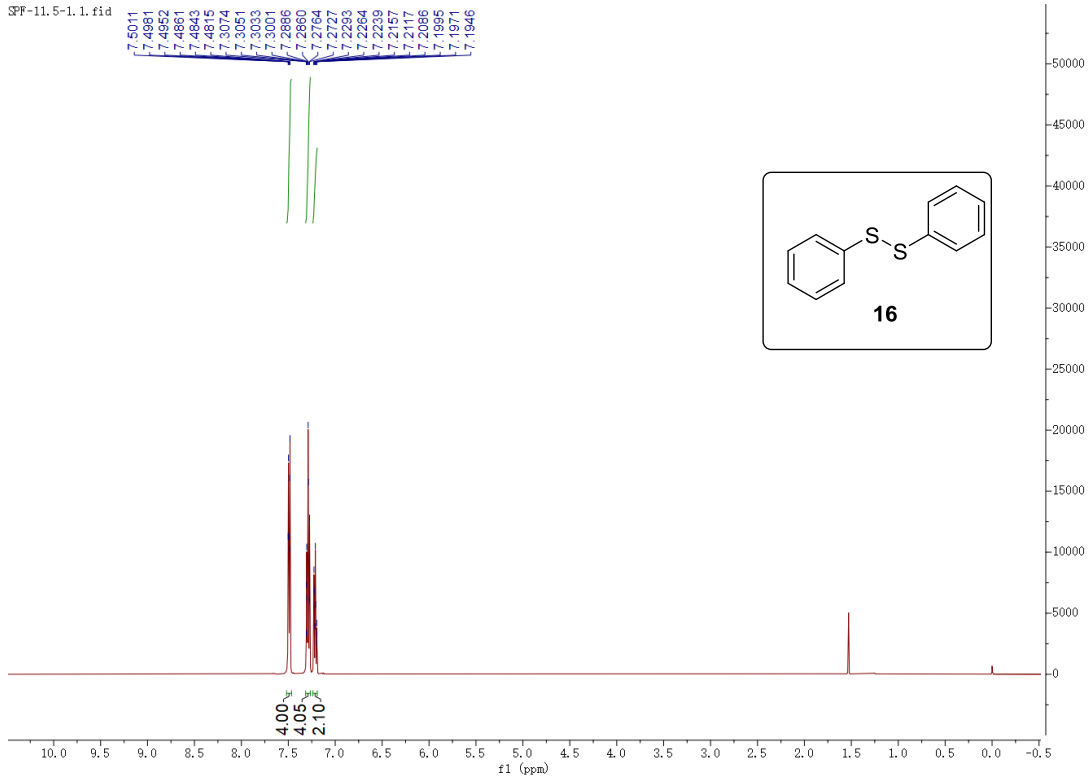
Ph
N
Se
8at
f1 (ppm)

Compound 16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S
S
16
4.00
4.05
2.10
f1 (ppm)