Electronic Supplementary Information

for

Synthesis of Fully-substituted 1,2,3-Triazoles via Copper(I)-Catalyzed Three-Component Coupling of Sulfoximines, Alkynes and Azides

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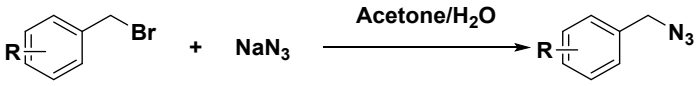
General Considerations

All experiments were conducted with a sealed pressure vessel. Flash column chromatography was performed over silica gel (300-400 mesh). ^{1}H NMR spectra were recorded on a Bruker AVIII-500M spectrometers, Chemical shifts (in ppm) were referenced to $CDCl_3$ (δ =7.26 ppm) as an internal standard. ^{13}C NMR spectra were obtained by using the same NMR spectrometers and were calibrated with $CDCl_3$ (δ = 77.0 ppm). Unless otherwise noted, materials obtained from commercial suppliers were used without further purification. Azide[1] and sulfoximines[2] were prepared following the known procedures.

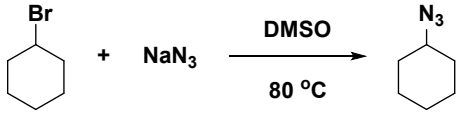
Experimental Procedures

Typical procedure for the synthesis of benzyl azides



In a 100 mL round-bottom flask, benzyl bromide (0.297 mL, 2.5 mmol) was dissolved in water (10 mL) and acetone (40 mL). Sodium azide (0.244 g, 3.75 mmol) was added in one portion, and the solution stirred overnight. Dichloromethane (50 mL) was added, and the organic layer separated. The aqueous layer was washed with dichloromethane (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and filtered. Solvent was removed under reduced pressure to give **1u** (0.335 g, quantitative) as a yellow oil. Spectroscopic data was consistent with previously reported results.

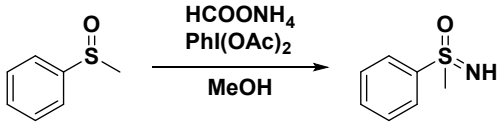
Typical procedure for the synthesis of other azide



In a 125 mL round-bottom flask, NaN_3 (0.715 g, 11 mmol) was dissolved in DMSO (20 mL) and stirred until homogeneous. Bromocyclopentane (1.072 mL, 10 mmol) was added, and the solution was stirred at 80°C overnight. Water (80 mL) was added, and the aqueous layer was extracted with ether (5 × 20 mL). The organic layers were combined, dried over anhydrous Na_2SO_4, and filtered. Solvent was removed under reduced pressure to give azidocyclohexane (1.15 g, quantitative yield) as a yellow oil.

Note: Azides are explosive substances that must be carefully handled and stored.

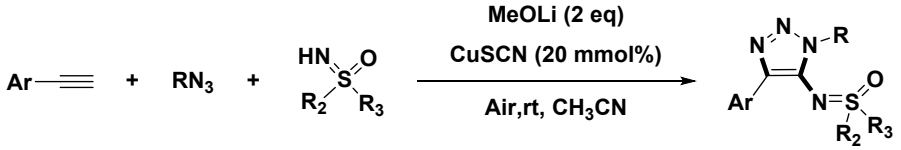
Typical procedure for the synthesis of NH Sulfoximines



The sulfoxide (1.50 mmol, 1.0 equiv.), $PhI(OAc)_2$ (1.45 g, 4.50 mmol, 3.0 equiv.) and ammonium carbamate (470 mg, 6. 0 mmol, 4.0 equiv.) were added to a 10 mL round bottom

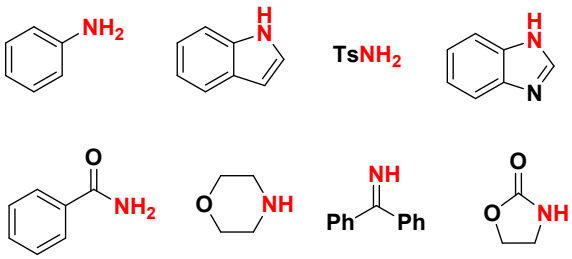
flask containing a stirrer bar. MeOH (3.0 mL, [0.5 M]) was added and the reaction was stirred for 30 min at 25 ºC in an open flask. The solvent was removed in vacuo and the crude residue was purified by flash column chromatography (SiO_2, dry loaded).

General procedure for the copper(I)-catalyzed three-component coupling of sulfoximines, alkynes and azides



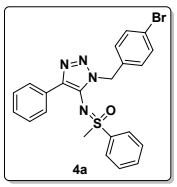
General reaction: azides (0.3 mmol), terminal alkynes (0.2 mmol), sulfoximines (0.3 mmol), CuSCN (0.04 mmol), and MeOLi (0.4 mmol) were added in dry MeCN (2.5 mL) and stirred for 12 h at room temperature in air. The reaction was monitored by TLC analysis. After the reaction was completed, the resulting mixture was evaporated to dryness and the crude product was purified with flash chromatography (silica gel, ethyl acetate: petroleum ether: =1:3).

Unsuccessful NH-containing compounds under standard conditions



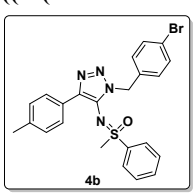
Characterization of Products

((1-(4-bromobenzyl)-4-phenyl-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4a).



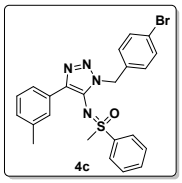
shallow yellow oil, 75.5 mg, 81% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 – 7.84 (m, 2 H), 7.69 – 7.67 (m, 2H), 7.59 – 7.56 (m, 1H), 7.44 – 7.39 (m, 6H), 7.32 – 7.28 (m, 1H), 7.22 – 7.20 (m, 2H), 5.60 – 5.53 (m, 2 H), 3.05 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.4, 137.3, 134.9, 134.8, 133.9, 131.6, 129.7, 129.4, 128.4, 127.7, 127.4, 126.8, 121.8, 50.2, 44.6. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{20}BrN_4OS^+$, 467.0536; Found: 467.0533.

((1-(4-bromobenzyl)-4-(p-tolyl)-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4b).



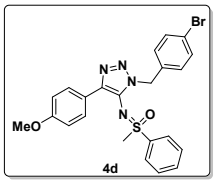
shallow yellow oil, 74.8 mg, 78% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ.7.75 – 7.70 (m, 4 H), 7.60 – 7.57 (m, 1 H), 7.43 – 7.40 (m, 4 H), 7.22 – 7.19 (m, 4 H), 5.58 – 5.52 (m, 2 H), 3.02 (s, 3 H), 2.38 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.5, 137.3, 137.0, 134.9, 134.5, 133.9, 131.6, 129.7, 129.4, 129.1, 128.7, 127.7, 126.6, 121.8, 50.1, 44.5, 21.3. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{22}BrN_4OS^+$, 481.0692; Found: 481.0692.

((1-(4-bromobenzyl)-4-(m-tolyl)-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4c).



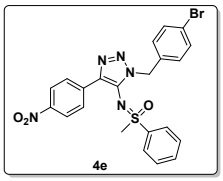
shallow yellow oil, 67.2 mg, 70% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ.7.72 – 7.64 (m, 4 H), 7.61 – 7.51 (m, 1 H), 7.44 – 7.40 (m, 4 H), 7.31 – 7.28 (m, 1 H), 7.22 – 7.19 (m, 2 H), 7.13-7.11 (m, 1 H), 5.56 (s, 2 H), 3.02 (s, 3 H), 2.38 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.9, 137.5, 137.3, 134.9, 134.7, 133.9, 131.6, 131.5, 129.7, 129.4, 128.3, 128.1, 127.7, 127.5, 123.8, 121.8, 50.1, 44.5, 21.4. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{22}BrN_4OS^+$, 481.0692; Found: 481.0695.

((1-(4-bromobenzyl)-4-(4-methoxyphenyl)-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4d).



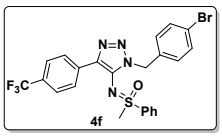
shallow yellow oil, 69.4 mg, 70% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ.7.76 – 7.74 (m, 2 H), 7.68 – 7.67 (m, 2 H), 7.60 – 7.56 (m, 1 H), 7.43 – 7.39 (m, 4 H), 7.21 – 7.19 (m, 2 H), 6.95 – 6.93 (m, 2 H), 5.58 – 5.58 (m, 2 H), 3.83 (s, 3 H), 3.03 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.9, 137.5, 137.1, 135.0, 134.2, 133.9, 131.6, 129.7, 129.4, 128.2, 127.7, 124.2, 121.8, 113.8, 55.3, 50.1, 44.6. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{22}BrN_4O_2S^+$, 497.0641; Found: 497.0647.

((1-(4-bromobenzyl)-4-(4-nitrophenyl)-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4e).



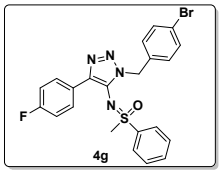
yellow solid, mp 121 – 123 °C, 46 mg, 45% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 – 8.24 (m, 2 H), 8.20 – 8.09 (m, 2 H), 7.64 – 7.61 (m, 3H), 7.45 – 7.40 (m, 4H), 7.23 – 7.19 (m, 2H), 5.62 – 5.54 (m, 2H), 3.10 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 146.5, 138.3, 137.1, 136.3, 135.1, 134.5, 134.2, 131.7, 129.6, 129.5, 127.4, 126.7, 123.8, 122.0, 50.4, 45.0. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{19}BrN_5O_3S^+$, 512.0386; Found: 512.0384.

((1-(4-bromobenzyl)-4-(4-(trifluoromethyl)phenyl)-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4f).



shallow yellow oil, 53.4 mg, 50% yield. ^{1}H NMR (500 MHz, CDCl3) δ. 7.86 – 7.79 (m, 2 H), 7.57 – 7.65 (m, 5 H), 7.46 – 7.39 (m, 4 H), 7.22 – 7.20 (m, 2 H), 5.55 (s, 2 H), 3.17 (s, 3 H). ^{13}C NMR (125 MHz, CDCl3) δ 137.2, 135.8, 135.5, 135.2, 134.7, 134.1, 131.7, 129.7, 129.5, 129.1 (q, *J* = 3.5 Hz), 127.6, 126.8, 125.7 (q, *J* = 270.2 Hz), 125.3 (q, *J* = 3.4 Hz), 122.0, 50.3, 44.8. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{19}BrF_3N_4OS^+$, 535.0410; Found: 535.0413. ^{19}F NMR (471 MHz, $CDCl_3$): -62.40.

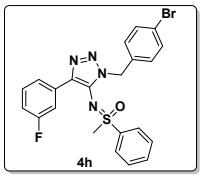
((1-(4-bromobenzyl)-4-(4-fluorophenyl)-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4g).



shallow yellow oil, 69.6 mg, 72% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ.7.78 – 7.75 (m, 2 H), 7.61 – 7.58 (m, 3 H), 7.45 – 7.38 (m, 4 H), 7.22 – 7.19 (m, 2 H), 7.10 – 7.06 (m, 2 H), 5.59 – 5.52 (m, 2 H), 3.08 (s, 3 H).

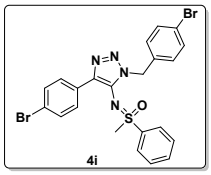
^{13}C NMR (125 MHz, $CDCl_3$) δ 163.1, 161.1, 137.4, 136.3, 134.8, 134.7, 134.0, 131.7, 129.7, 129.4, 128.8, 128.7, 127.6, 121.9, 115.4, 115.2, 50.2, 44.8. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{19}BrFN_4OS^+$, 485.0441; Found: 485.0440. ^{19}F NMR (471 MHz, $CDCl_3$): -114.39.

((1-(4-bromobenzyl)-4-(3-fluorophenyl)-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4h).



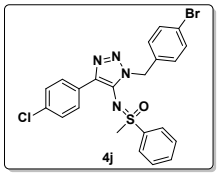
shallow yellow oil, 66.8 mg, 69% yield. ^{1}H NMR (500 MHz, CDCl3) δ. 7.68 – 7.66 (m, 3 H), 7.60 – 7.56 (m, 2 H), 7.44 – 7.34 (m, 5 H), 7.21 – 7.16 (m, 2 H), 7.01 – 6.97 (m, 1 H), 5.60 – 5.53 (m, 2 H), 3.12 (s, 3 H). ^{13}C NMR (125 MHz, CDCl3) δ 163.8, 161.9, 137.3, 136.1, 136.0, 135.1, 134.7, 134.0, 133.9, 133.8, 131.6, 130.0, 129.9, 129.7, 129.5, 127.5, 122.3, 122.2, 121.9, 114.1, 114.0, 113.5, 113.3, 50.2, 44.7. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{19}BrFN_4OS^+$, 485.0441; Found: 485.0431. ^{19}F NMR (471 MHz, $CDCl_3$): -112.81.

((1-(4-bromobenzyl)-4-(4-bromophenyl)-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4i).



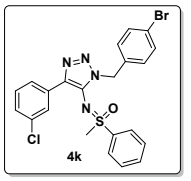
shallow yellow oil, 85.9 mg, 79% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ.7.72 – 7.69 (m, 2 H), 7.63 – 7.57 (m, 3 H), 7.51 – 7.50 (m, 2 H), 7.42 – 7.38 (m, 4 H), 7.20 – 7.16 (m, 2 H), 5.59 – 5.51 (m, 2 H) 3.09 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.3, 136.1, 135.0, 134.8, 134.0, 131.7, 131.5, 130.6, 129.7, 129.5, 128.3, 127.5, 121.9, 121.2, 50.2, 44.8. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{19}Br_2N_4OS^+$, 544.9641; Found: 544.9642.

((1-(4-bromobenzyl)-4-(4-chlorophenyl)-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4j).



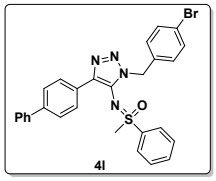
shallow yellow oil, 76.0 mg, 76% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ.7.77 – 7.76 (m, 2 H), 7.63 – 7.57 (m, 3 H), 7.44 – 7.35 (m, 6 H), 7.20 – 7.18 (m, 2 H), 5.59 – 5.52 (m, 2 H), 3.09 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.3, 136.1, 135.0, 134.8, 134.0, 133.0, 131.7, 130.2, 129.7, 129.5, 128.6, 128.1, 127.5, 121.9, 50.2, 44.8. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{19}BrClN_4OS^+$, 501.0146; Found: 501.0148.

((1-(4-bromobenzyl)-4-(3-chlorophenyl)-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4k).



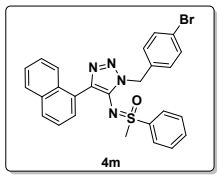
shallow yellow oil, 73 mg, 73% yield. ^{1}H NMR (500 MHz, CDCl3) δ. 7.86 – 7.85 (m, 1 H), 7.76 – 7.74 (m, 1 H), 7.68 – 7.66 (m, 2 H), 7.60 – 7.58 (m, 1 H), 7.45 – 7.41 (m, 4 H), 7.34 – 7.31 (m, 1 H), 7.28 – 7.25 (m, 1 H), 7.20 – 7.18 (m, 2 H), 5.60 – 5.54 (m, 2 H),3.11 (s, 3 H). ^{13}C NMR (125 MHz, CDCl3) δ 137.3, 135.8, 135.2, 134.7, 134.2, 134.0, 133.4, 131.7, 129.8, 129.7, 129.5, 127.5, 127.2, 126.6, 124.7, 121.9, 50.3, 44.6. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{19}BrClN_4OS^+$, 501.0146; Found: 501.0149.

((4-([1,1'-biphenyl]-4-yl)-1-(4-bromobenzyl)-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4l).



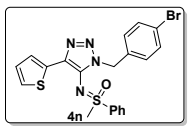
shallow yellow oil, 65.0 mg, 60% yield. ^{1}H NMR (500 MHz, $CDCl_3$) ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 – 7.89 (m, 2H), 7.76 – 7.70 (m, 2H), 7.70 – 7.63 (m, 4H), 7.62 – 7.55 (m, 1H), 7.52 – 7.35 (m, 7H), 7.26 – 7.17 (m, 2H), 5.68 – 5.44 (m, 2H), 3.12 (s, 3H).^{13}C NMR (125 MHz, $CDCl_3$) δ 140.6, 139.9, 137.5, 136.9, 134.9, 134.8, 134.0, 131.7, 130.7, 129.7, 129.4, 128.8, 127.7, 127.4, 127.1, 127.0, 126.9, 121.9, 50.2, 44.7. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{28}H_{24}BrN_4OS^+$, 543.0849; Found: 543.0847.

((1-(4-bromobenzyl)-4-(naphthalen-2-yl)-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4m).



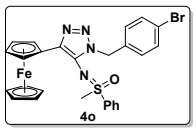
shallow yellow oil, 72.2 mg, 70% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.35 (s, 1 H), 8.05 – 8.03 (m, 1 H), 7.90 – 7.85 (m, 3H), 7.72 – 7.70 (m, 2H), 7.54 – 7.45 (m, 5H), 7.36 – 7.33 (m, 2 H), 7.25 – 7.24 (m, 2 H), 5.62 – 5.61 (m, 2H), 3.05 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.5, 137.2, 135.1, 134.9, 133.9, 133.4, 132.6, 131.7, 129.7, 129.4, 129.1, 128.1, 128.0, 127.7, 127.6, 126.2, 125.9, 125.4, 124.9, 121.9, 50.2, 44.5. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{26}H_{22}BrN_4OS^+$, 517.0692; Found: 517.0692.

((1-(4-bromobenzyl)-4-(thiophen-2-yl)-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4n).



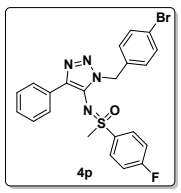
brown oil, 45.3 mg, 48% yield. ^{1}H NMR (500 MHz, CDCl3) δ. 7.86 – 7.79 (m, 2 H), 7.63 (t, J = 7.5 Hz, 1 H), 7.57 – 7.45 (m, 3 H), 7.42 – 7.39 (m, 2 H), 7.33 – 7.26 (m, 1 H), 7.20 – 7.05 (m, 3 H), 5.55 (s, 2 H), 3.17 (s, 3 H). ^{13}C NMR (125 MHz, CDCl3) δ 137.4, 134.7, 134.2, 134.0, 133.5, 133.0, 131.6, 129.6, 129.5, 127.8, 127.3, 124.5, 124.2, 121.8, 50.3, 44.9. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{18}BrN_4OS_2^+$, 473.0125; Found: 473.0125.

((1-(4-bromobenzyl)-4-(irondicyclopentadienyl-yl)-1H-1**,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4o).**



brown solid, mp 101 – 102 °C, 57.4 mg, 50% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ. 7.77 – 7.75 (m, 2 H), 7.64 – 7.58 (m, 1 H), 7.48 – 7.42 (m, 4 H), 7.17 – 7.14 (m, 2 H), 5.50 (s, 2 H), 4.78 – 4.72 (m, 2 H), 4.28 – 4.21 (m, 2 H), 4.17 (s, 5 H), 3.05 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.6, 135.9, 135.1, 134.0, 133.9, 131.6, 129.6, 129.5, 127.8, 121.7, 69.5, 68.1, 67.4, 67.1, 50.0, 44.7. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{26}H_{24}BrFeN_4OS^+$, 575.0198; Found: 575.0193.

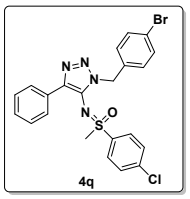
((1-(4-bromobenzyl)-4-phenyl-1H-1,2,3-triazol-5-yl)imino)(4-fluorophenyl)(methyl)-l6-sulfanone (4p).



shallow yellow oil, 70.6 mg, 73% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ.7.80 – 7.78 (m, 2 H), 7.65 – 7.62 (m, 2 H), 7.45 – 7.38 (m, 4 H), 7.33 – 7.28 (m, 1 H), 7.21 – 7.19 (m, 2 H), 7.05 – 7.01 (m, 2 H), 5.60 – 5.52 (m, 2 H), 3.07 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.1, 161.1, 137.4, 136.3, 134.8, 134.7, 134.0, 131.7, 129.7, 129.4, 128.8, 128.7, 127.9, 127.8, 127.6, 121.9,

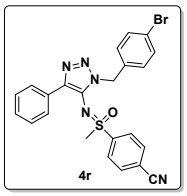
115.4, 115.2, 50.2, 44.8. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{19}BrFN_4OS^+$, 485.0441; Found: 485.0436. ^{19}F NMR (471 MHz, CDCl3): -102.52.

((1-(4-bromobenzyl)-4-phenyl-1H-1,2,3-triazol-5-yl)imino)(4-chlorophenyl)(methyl)-l6-sulfanone (4q).



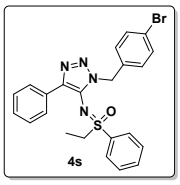
shallow yellow oil, 69.0 mg, 69% yield. ^1H NMR (500 MHz, $CDCl_3$) δ.7.79 – 7.71 (m, 2 H), 7.55 – 7.53 (m, 2 H), 7.46 – 7.39 (m, 4 H), 7.33 – 7.28 (m, 3 H), 7.21 – 7.19 (m, 2 H), 5.60 – 5.52 (m, 2 H), 3.08 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.8, 137.3, 135.8, 134.8, 134.5, 131.7, 131.5, 129.6, 129.1, 128.5, 127.5, 126.9, 121.9, 50.2, 44.7. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{19}BrClN_4OS^+$, 501.0146; Found: 501.0150.

4-(N-(1-(4-bromobenzyl)-4-phenyl-1H-1,2,3-triazol-5-yl)-S-methylsulfonimidoyl)benzonitrile (4r).



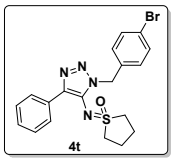
shallow yellow oil, 67.7 mg, 69% yield. ^1H NMR (500 MHz, $CDCl_3$) δ 7.69 – 7.66 (m, 4 H), 7.59 – 7.57 (m, 2H), 7.47 – 7.45 (m, 2H), 7.40 – 7.33 (m, 3H), 7.21 – 7.19 (m, 2 H), 5.60 – 5.51 (m, 2 H), 3.15 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.8, 137.3, 134.7, 133.9, 132.8, 131.7, 131.3, 129.6, 128.5, 128.3, 127.7, 127.1, 122.0, 117.5, 116.7, 50.3, 44.4. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{19}BrN_5OS^+$, 492.0488; Found: 492.0488.

((1-(4-bromobenzyl)-4-phenyl-1H-1,2,3-triazol-5-yl)imino)(ethyl)(phenyl)-l6-sulfanone (4s).



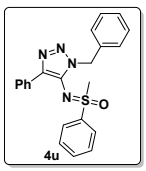
shallow yellow oil, 69.1 mg, 72% yield. ^1H NMR (500 MHz, $CDCl_3$) δ 7.82 – 7.81 (m, 2 H), 7.54 – 7.47 (m, 3H), 7.44 – 7.39 (m, 4H), 7.33 – 7.28 (m, 3H), 7.18 – 7.17 (m, 2 H), 5.65 – 5.54 (m, 2 H), 3.39 – 3.32 (m, 1 H), 3.20 – 3.13 (m, 1 H),.3.05 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.3, 135.2, 135.1, 135.0, 133.8, 131.8, 131.6, 129.6, 129.2, 128.5, 128.3, 127.3, 127.1, 121.7, 51.6, 50.3, 44.5. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{22}BrN_4OS^+$, 481.0692; Found: 481.0693.

1-((1-(4-bromobenzyl)-4-phenyl-1H-1,2,3-triazol-5-yl)imino)tetrahydro-1H-1l6-thiophene 1-oxide (4t).



shallow yellow oil, 43.0 mg, 50% yield. ^1H NMR (500 MHz, $CDCl_3$) δ. 7.95 – 7.93 (m, 2 H), 7.55 – 7.47 (m, 2 H), 7.43 – 7.37 (m, 2 H), 7.32 – 7.24 (m, 3 H), 5.55 (s, 2 H), 3.21 – 3.15 (m, 2 H), 3.00 – 2.94 (m, 2 H), 2.24 – 2.05 (m, 4 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.4, 135.6, 134.8, 131.7, 131.5, 129.7, 128.5, 127.5, 126.3, 121.9, 52.9, 50.0, 23.7. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{19}H_{20}BrN_4OS^+$, 431.0536; Found: 431.0536.

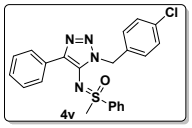
((1-benzyl-4-phenyl-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4u).



white solid, mp 128 – 130 °C, 55.8 mg, 72% yield. ^1H NMR (500 MHz, $CDCl_3$) δ 7.83 – 7.81 (m, 2 H), 7.65 – 7.63 (m, 2 H), 7.58 – 7.55 (m, 1H), 7.40 – 7.28 (m, 10 H), 5.62 (s, 2 H), 3.02 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.5, 137.0, 136.0, 134.9, 133.8, 131.7, 129.3, 128.5, 128.3, 127.9, 127.8,

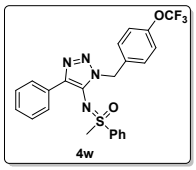
127.7, 127.3, 127.0, 50.8, 44.5. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{21}N_4OS^+$, 389.1431; Found: 389.1431.

((1-(4-chlorobenzyl)-4-phenyl-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4v).



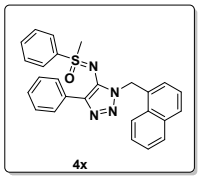
shallow yellow oil, 62.4 mg, 74% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ7.85 – 7.83 (m, 2 H), 7.72 – 7.64 (m, 2H), 7.61 – 7.53 (m, 1H), 7.45 – 7.35 (m, 4H), 7.34 – 7.22 (m, 5H), 5.68 – 5.47 (m, 2H), 3.05 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.4, 137.2, 134.8, 134.4, 133.9, 133.6, 131.6, 129.5, 129.4, 128.7, 128.4, 127.7, 127.3, 126.8, 50.1, 44.64. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{20}ClN_4OS^+$, 423.1041; Found: 423.1040.

Methyl(phenyl)((4-phenyl-1-(4-(trifluoromethoxy)benzyl)-1H-1,2,3-triazol-5-yl)imino)-l6-sulfanone (4w).



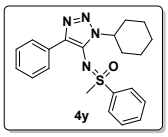
shallow yellow solid, mp 115 – 116 °C, 67.9 mg, 72% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 – 7.82 (m, 2H), 7.72 – 7.66 (m, 2H), 7.61 – 7.53 (m, 1H), 7.45 – 7.34 (m, 6H), 7.34 – 7.27 (m, 1H), 7.20 – 7.12 (m, 2H), 5.73 – 5.46 (m, 2H), 3.06 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$)) δ 148.7, 137.4, 137.2, 134.8, 134.6, 133.9, 131.7, 129.5, 129.4, 128.4, 127.7, 127.3, 126.8, 121.0, 120.5 (q, J = 271.2 Hz), 50.0, 44.6. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{2o}F_3N_4O_2S^+$, 473.1254; Found: 473.1257. ^{19}F NMR (471 MHz, $CDCl_3$): -57.81.

Methyl((1-(naphthalen-1-ylmethyl)-4-phenyl-1H-1,2,3-triazol-5-yl)imino)(phenyl)-l6-sulfanone (4x).



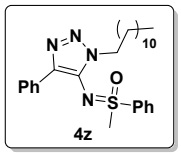
white solid, mp 125 – 127 °C, 65.7 mg, 75% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ. 8.27 – 8.25 (m, 1 H), 7.90 – 7.80 (m, 4 H), 7.57 – 7.49 (m, 5 H), 7.40 – 7.35 (m, 3 H), 7.32 – 7.25 (m, 3 H), 7.20 – 7.19 (m, 1 H), 6.12 – 5.05 (m, 2 H), 2.97 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.5, 137.0, 135.4, 133.7, 133.6, 131.8, 131.7, 131.0, 129.2, 128.7, 128.5, 128.3, 127.6, 127.3, 127.1, 126.6, 126.1, 125.9, 125.3, 123.3, 48.8, 44.6. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{26}H_{23}N_4OS^+$, 439.1587; Found: 439.1588.

((1-cyclohexyl-4-phenyl-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4y).



shallow yellow oil, 42.5 mg, 56% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 – 7.87 (m, 4 H), 7.65 – 7.62 (m, 1H), 7.50 – 7.41 (m, 4H), 7.32 – 7.28 (m, 1H), 4.56 – 4.50 (m, 1H), 3.02 (s, 3H), 2.15 – 1.90 (m, 6 H), 1.50 – 1.25 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.8, 136.6, 133.9, 133.4, 132.2, 129.4, 128.4, 127.8, 127.1, 126.7, 56.3, 44.0, 33.1, 25.6, 25.2. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{21}H_{25}N_4OS^+$, 381.1744; Found: 381.1744.

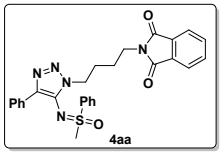
((1-dodecyl-4-phenyl-1H-1,2,3-triazol-5-yl)imino)(methyl)(phenyl)-l6-sulfanone (4z).



shallow yellow oil, 48.4 mg, 52% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ. 7.90 – 7.85 (m, 4 H), 7.63 – 7.60 (m, 1 H), 7.48 – 7.40 (m, 4 H), 7.32 – 7.28 (m, 1 H), 4.37 – 4.34 (m, 2 H), 3.04 (s, 3 H), 1.97 – 1.92 (m, 2 H), 1.41 – 1.26 (m, 18 H), 0.91 – 0.88 (m, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.8,

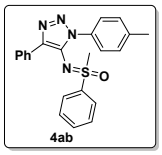
137.0, 134.3, 133.9, 132.0, 129.4, 128.4, 127.8, 127.1, 126.7, 47.4, 44.3, 31.9, 29.7, 29.6, 29.5, 29.3, 26.6, 22.7, 14.1. MS-ESI: *m/z* 247.1, $[M + H]^+$. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{27}H_{39}N_4OS^+$, 467.2839; Found: 467.2839.

2-(4-(5-((methyl(oxo)(phenyl)-l6-sulfanylidene)amino)-4-phenyl-1H-1,2,3-triazol-1-yl)butyl)isoindoline-1,3-dione (4aa).



shallow yellow oil, 53.8 mg, 54% yield. 1H NMR (500 MHz, CDCl3) δ 7.92 – 7.77 (m, 6H), 7.77 – 7.68 (m, 2H), 7.63 – 7.58 (m, 1H), 7.50 – 7.38 (m, 4H), 7.35 – 7.28 (m, 1H), 4.55 – 4.23 (m, 2H), 3.77 (t, *J* = 7.0 Hz, 2H), 3.05 (s, 3H), 2.09 – 1.97 (m, 2H), 1.90 – 1.72 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.3, 137.7, 137.0, 134.4, 133.9, 133.8, 132.1, 131.9, 129.4, 128.4, 127.7, 127.2, 126.7, 123.2, 46.6, 44.3, 37.4, 29.7, 27.0, 25.7 MS-ESI: *m/z* 247.1, $[M + H]^+$. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{27}H_{26}N_5O_3S^+$, 500.1751; Found: 500.1758.

Methyl(phenyl)((4-phenyl-1-(p-tolyl)-1H-1,2,3-triazol-5-yl)imino)-l6-sulfanone (4ab).



white solid, mp 135 – 137 °C, 43.4 mg, 56% yield. ^1H NMR (500 MHz, $CDCl_3$) δ. 8.00 – 7.98 (m, 2 H), 7.64 – 7.55 (m, 5 H), 7.45 – 7.28 (m, 7 H), 2.97 (s, 3 H), 2.46 (s, 3 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.7, 138.3, 137.7, 134.7, 134.1, 133.6, 131.5, 129.5, 129.2, 128.3, 127.5, 127.4, 127.0, 124.8, 44.6, 21.3. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{21}N_4OS^+$, 389.1431; Found: 389.1435.

References

[1] M. T. Berry, D. Castrejon, and J. E. Hein, *Org. Lett.,* 2014, **16**, 3676.

[2] M. Zenzola, R. Doran, L. Degennaro, R. Luisi and J. A. Bull, *Angew. Chem., Int. Ed.* 2016, **55**, 7203.

X-Ray Structure of 4u

Crystal data
Crystallographic data for compound **4u** (CCDC-
1511230) has been deposited with the Cambridge Crystallographic Data Center, Copi es of the data can be obtained, free of charge, on application to CCDC (Email:deposit @ccdc.cam.ac.uk).

Datablock: exp_4u

Bond precision: C-C = 0.0056 A Wavelength=0.71073
Cell: a=11.6535(8) b=9.6660(5) c=17.3752(12)
alpha=90 beta=98.934(6) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1933.5(2)	1933.4(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C22 H20 N4 O S	C22 H20 N4 O S
Sum formula	C22 H20 N4 O S	C22 H20 N4 O S
Mr	388.48	388.48
Dx,g cm-3	1.335	1.335
Z	4	4
Mu (mm-1)	0.188	0.188
F000	816.0	816.0
F000'	816.77	
h,k,lmax	15,13,23	15,12,23
Nref	5201	4456
Tmin,Tmax	0.914,0.945	0.766,1.000
Tmin'	0.910	

Correction method= # Reported T Limits: Tmin=0.766 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 0.857 Theta(max)= 29.118
R(reflections)= 0.0755(3271) wR2(reflections)= 0.2456(4456)
S = 1.022 Npar= 254

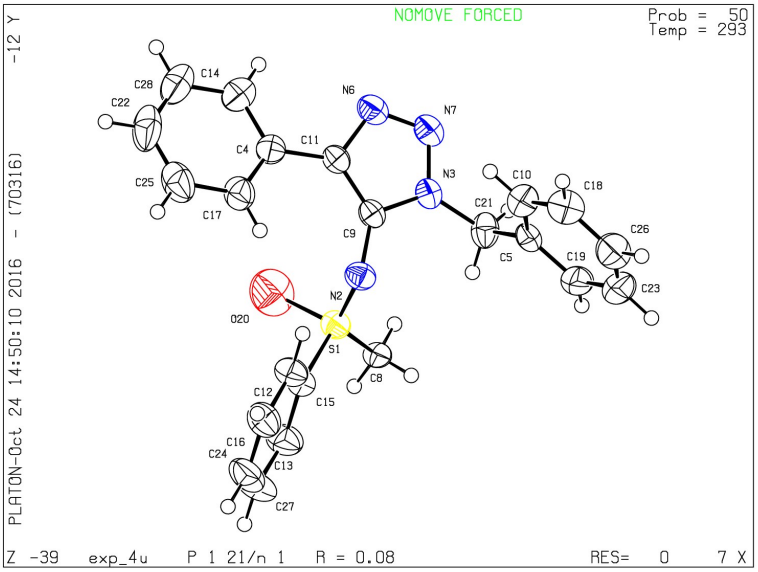
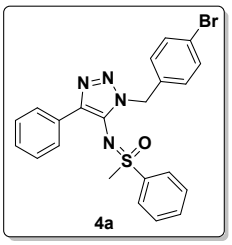
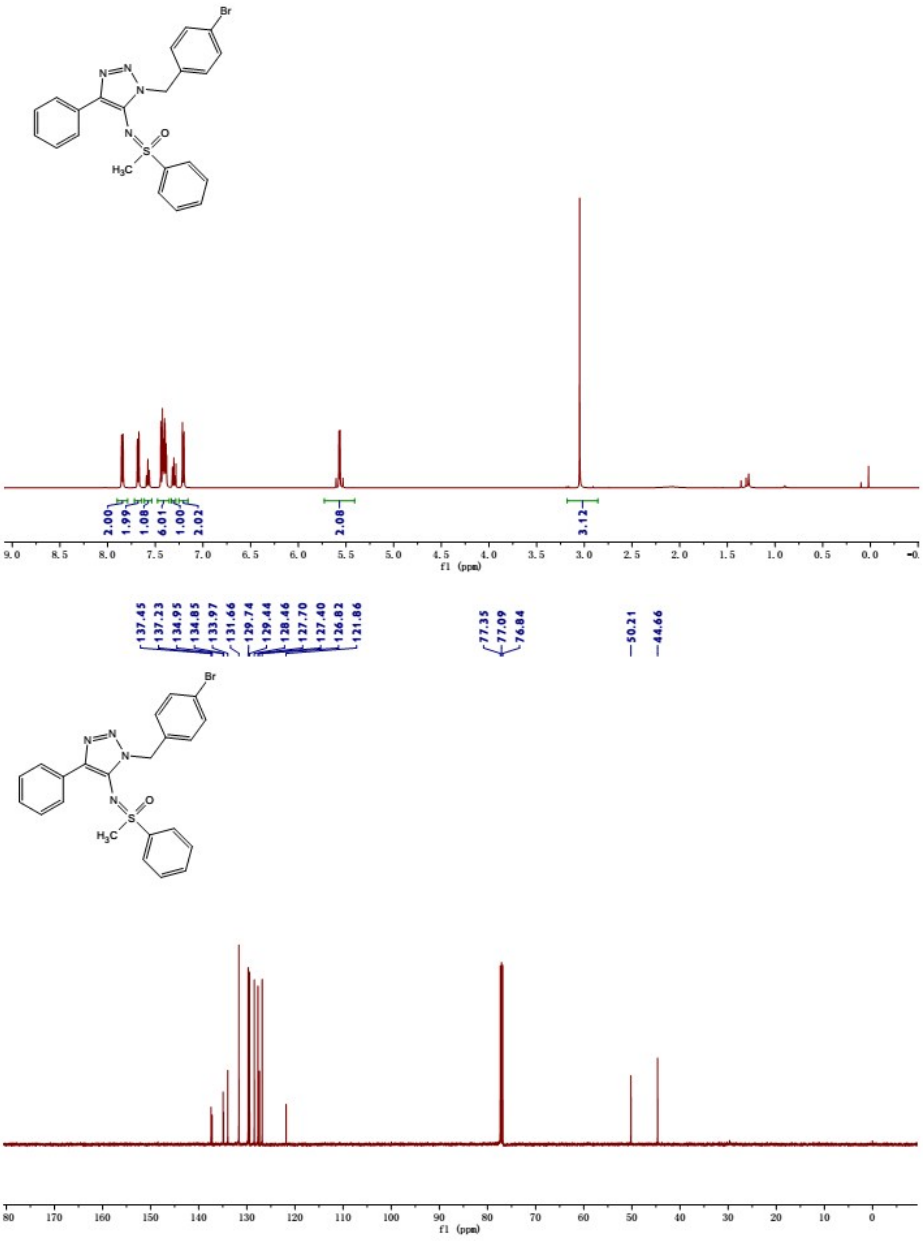
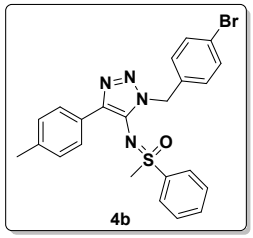


Figure 1: ORTEP view of the complex **4u** (Color scheme: C, gray; N, blue; O, red; S, yellow)

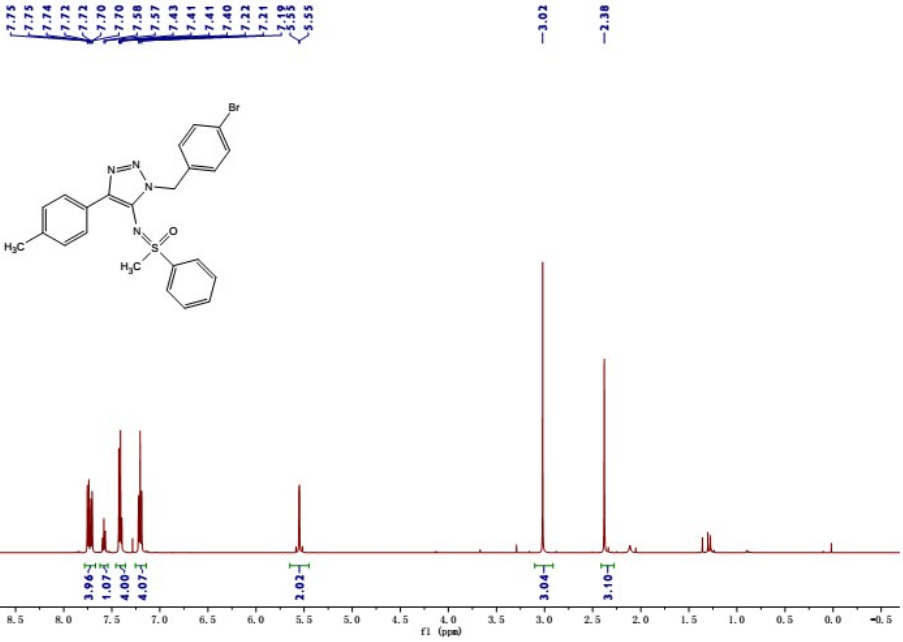
NMR Spectra of Products

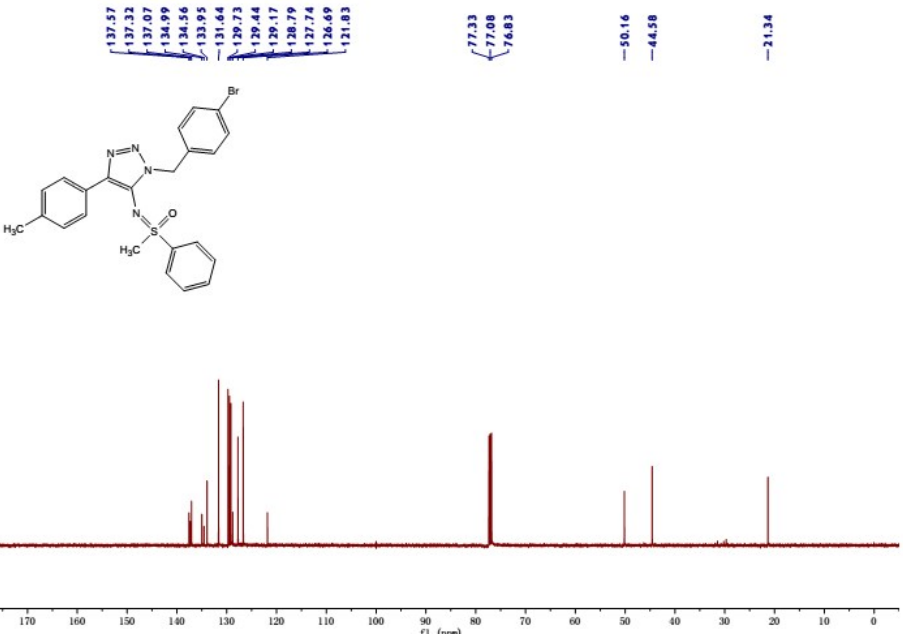





Br
N
N
N
N
O
S

4b


7.75
7.75
7.74
7.72
7.72
7.70
7.70
7.58
7.57
7.43
7.41
7.41
7.40
7.22
7.21
5.55
3.02
2.38
Br
H3C
H3C
3.96
1.07
4.00
4.07
2.02
3.04
3.10
f1 (ppm)


137.57
137.32
137.07
134.99
134.56
133.95
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129.73
129.44
129.17
128.79
127.74
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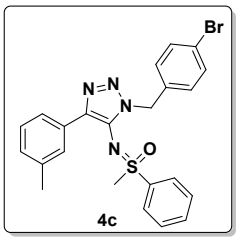
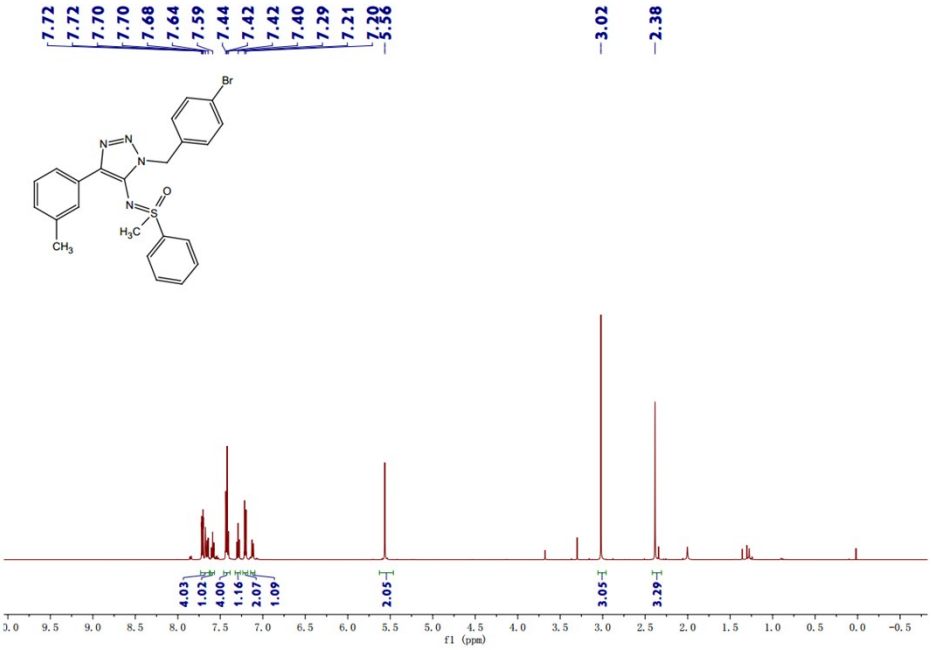
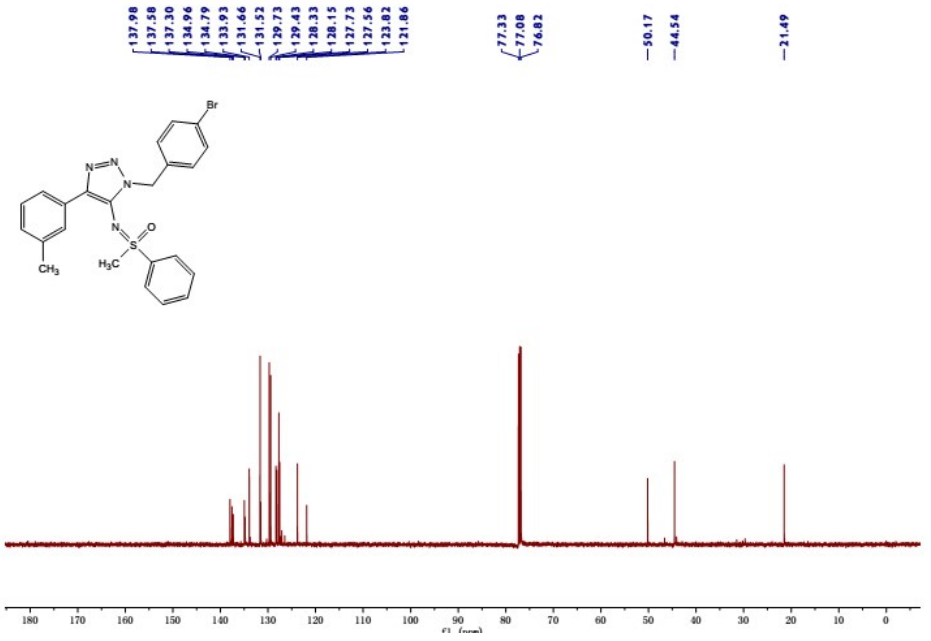
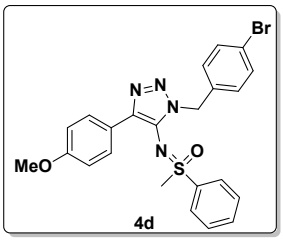
121.83
77.33
77.08
76.83
50.16
44.58
21.34
Br
H3C
H3C

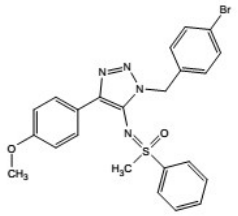

Br
N
N
N
N
O
S
4c

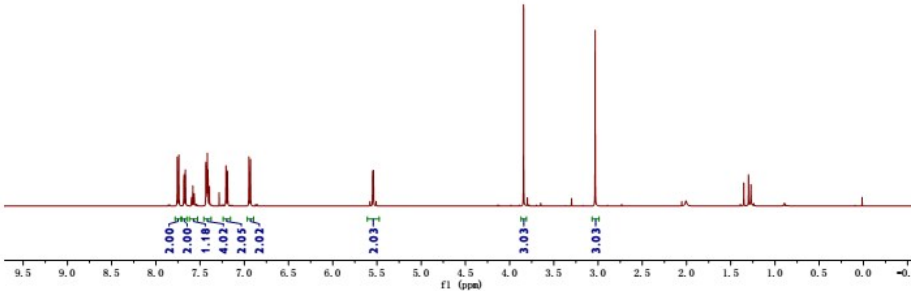

7.72
7.72
7.70
7.70
7.68
7.64
7.59
7.44
7.42
7.42
7.40
7.29
7.21
7.20
5.38
3.02
2.38
Br
CH3
H3C
4.03
1.02
4.00
1.16
2.07
1.09
2.05
3.05
3.29
f1 (ppm)


137.98
137.58
137.30
134.96
134.79
133.93
131.66
131.52
129.73
129.43
128.33
128.15
127.73
127.56
123.82
121.86
77.33
77.08
76.82
50.17
44.54
21.49
Br
CH3
H3C

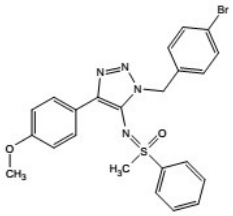

Br
N
N
N
MeO
N
S
O

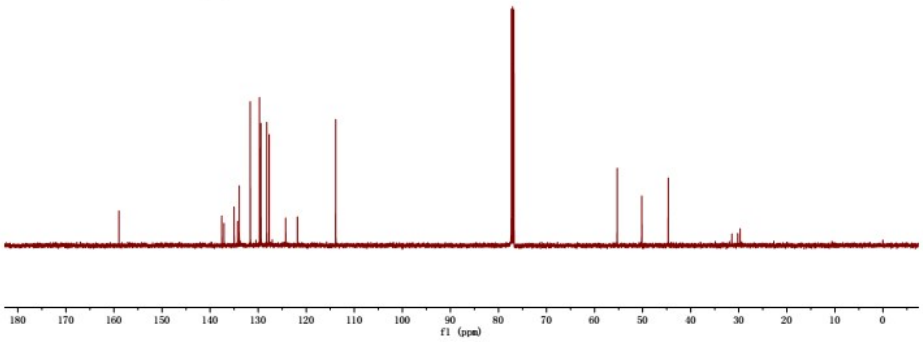
4d

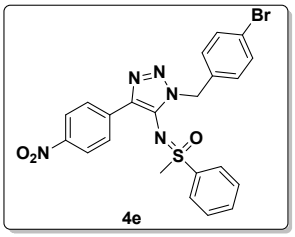

Br
O
CH3
H3C

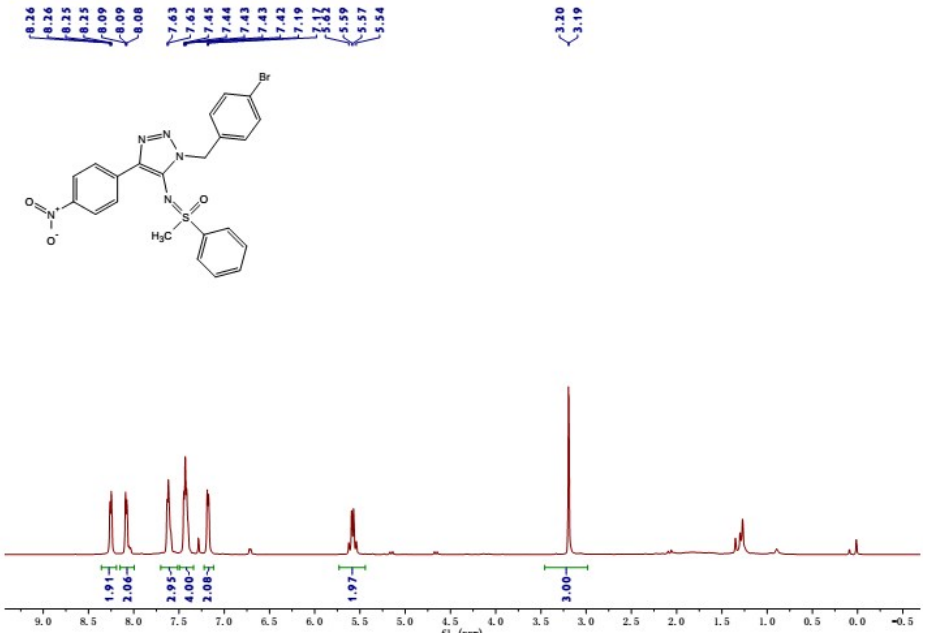

2.00
2.00
1.18
4.02
2.05
2.02
2.03
3.03
3.03
f1 (ppm)

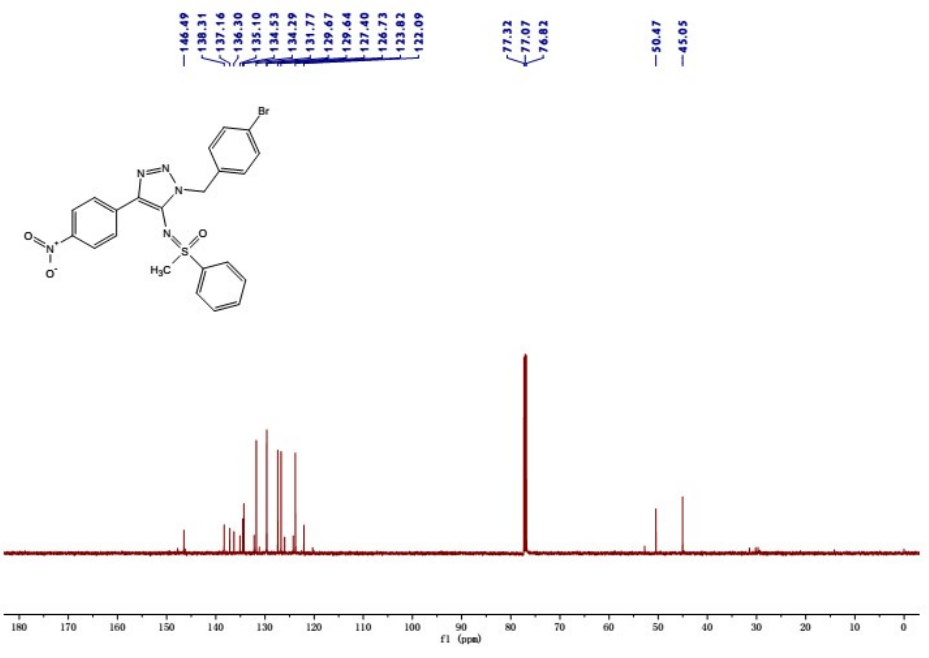

158.97
137.58
135.00
134.29
133.93
131.65
129.72
129.42
128.21
127.73
124.28
77.31
77.06
76.80
55.30
50.18
44.68

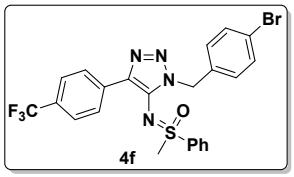

Br
O
CH3
H3C

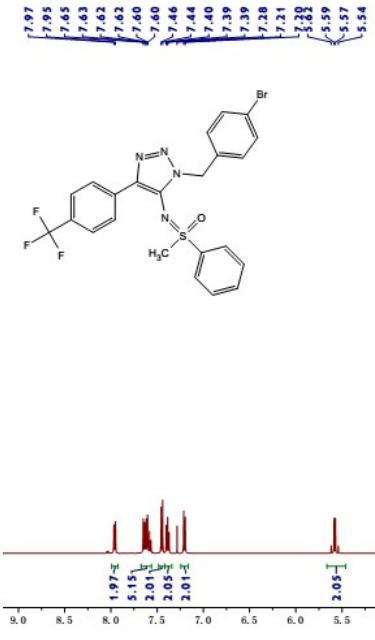

f1 (ppm)

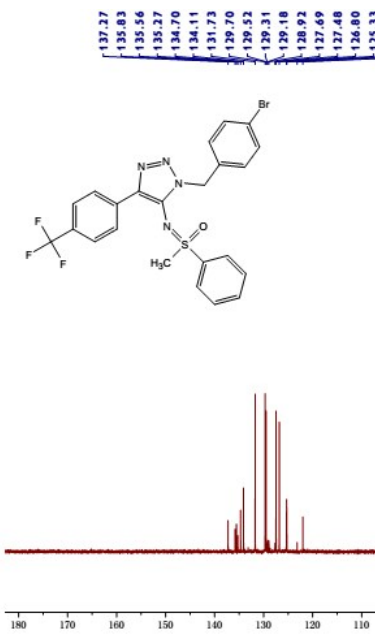

Br
N
N
N
N
O2N
O
S
4e


8.26
8.26
8.25
8.25
8.09
8.09
8.08
7.63
7.62
7.45
7.44
7.43
7.43
7.42
7.19
5.57
5.54
3.20
3.19
Br
1.91
2.04
2.95
4.00
2.08
1.97
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


146.49
138.31
137.16
136.30
135.10
134.53
134.29
131.77
129.67
129.64
127.40
126.73
123.82
122.09
77.32
77.07
76.82
50.47
45.05
Br
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Br
N=N
N
F3C
N
S
O
Ph
4f


7.97
7.95
7.65
7.63
7.62
7.62
7.60
7.60
7.46
7.44
7.40
7.39
7.39
7.28
7.21
5.59
5.57
5.54
3.14
Br
F
F
F
N=N
N
N
O
S
H3C
1.97
5.15
2.01
2.05
2.01
2.05
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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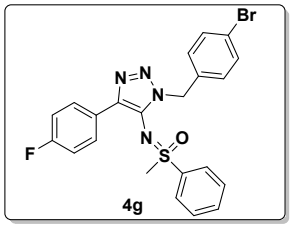
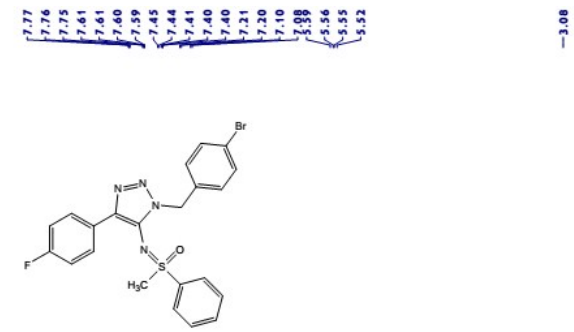
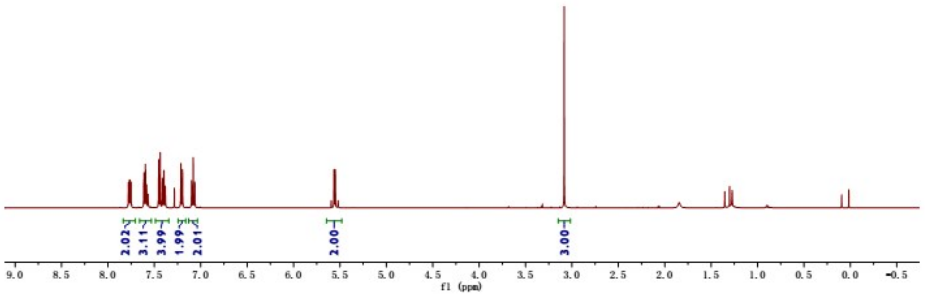
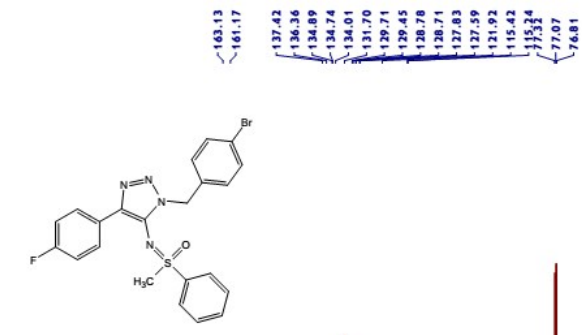
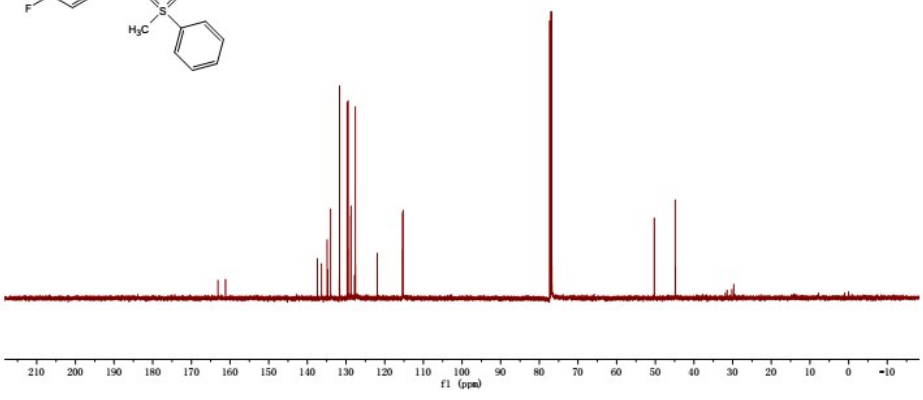
135.83
135.56
135.27
134.70
134.11
131.73
129.70
129.52
129.31
129.18
128.92
127.69
127.48
126.80
125.33
125.30
123.14
122.00
77.32
77.06
76.81
50.35
44.88
Br
F
F
F
N=N
N
N
O
S
H3C
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

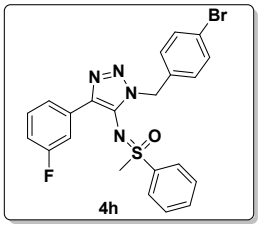

Br
F
4g


7.77
7.76
7.75
7.61
7.61
7.60
7.59
7.45
7.44
7.41
7.40
7.40
7.21
7.20
7.10
7.08
5.56
5.55
5.52
3.08
Br
F
H3C

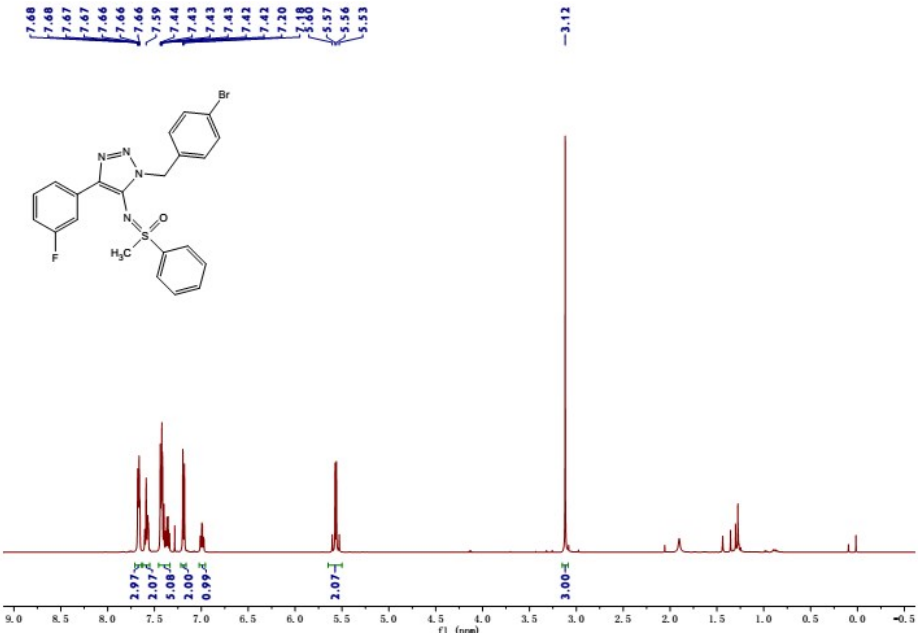

2.02
3.11
3.99
1.99
2.01
2.00
3.00
f1 (ppm)


163.13
161.17
137.42
136.36
134.89
134.74
134.01
131.70
129.71
129.45
128.78
128.71
127.83
127.59
121.92
115.42
115.24
77.32
77.07
76.81
50.26
44.85
Br
F
H3C


f1 (ppm)


Br
N
N
N
N
O
S
F

4h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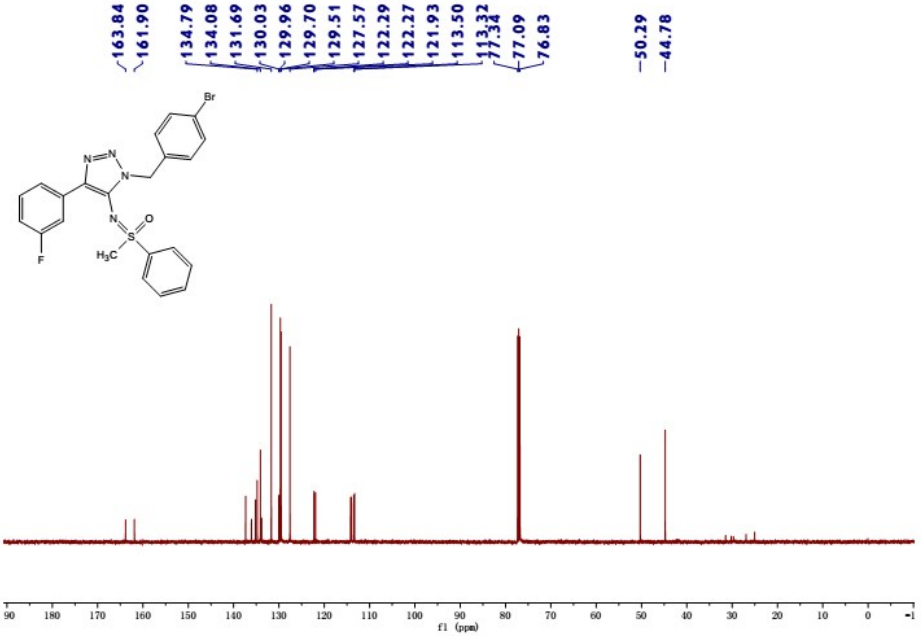
7.68
7.67
7.67
7.66
7.66
7.66
7.59
7.44
7.43
7.43
7.43
7.42
7.42
7.20
5.58
5.57
5.56
5.53
3.12
Br
N
N
N
N
O
S
F
H3C
2.97
2.07
5.08
2.00
0.99
2.07
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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134.08
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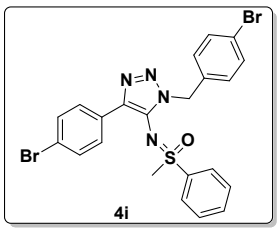
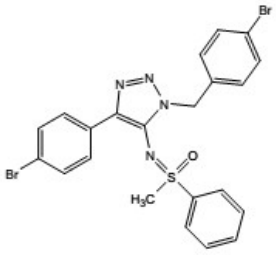
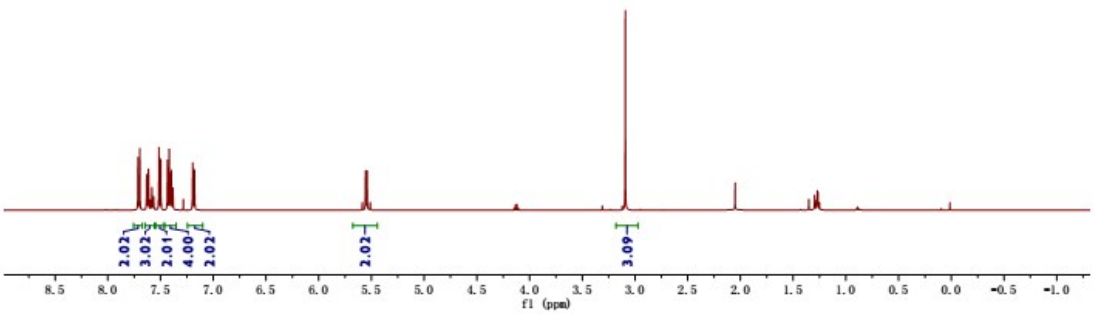
130.03
129.96
129.70
129.51
127.57
122.29
122.27
121.93
113.50
113.32
77.34
77.09
76.83
50.29
44.78
Br
N
N
N
N
O
S
F
H3C
90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


Br
N
N
N
N
O
S
Br

4i


7.71
7.70
7.63
7.62
7.61
7.51
7.50
7.43
7.42
7.41
7.40
7.40
7.19
7.18
5.55
5.54
5.51
3.09


Br
N
N
N
O
S
H3C
Br


2.02
3.02
2.01
4.00
2.02
2.02
3.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


137.34
136.14
135.03
134.81
134.06
131.70
131.54
130.67
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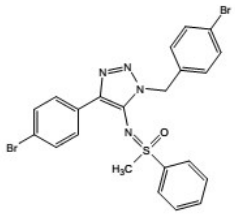
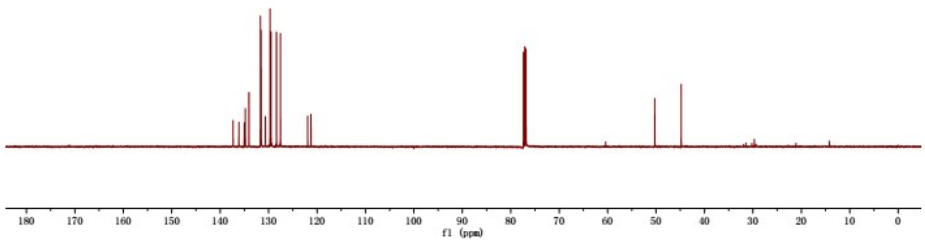
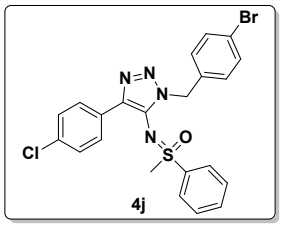
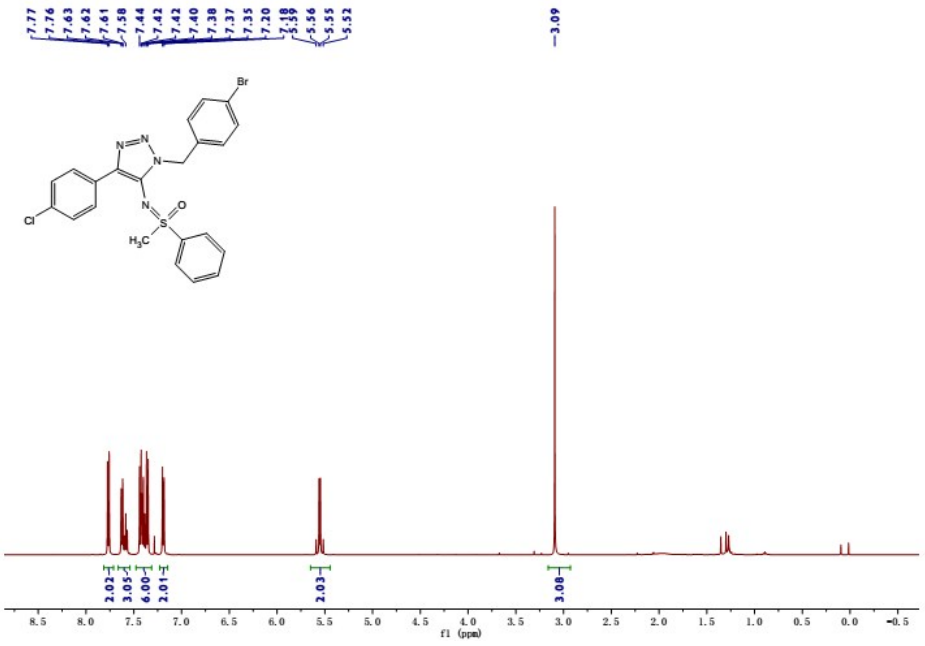
129.52
128.38
127.55
121.94
121.26
77.38
77.12
76.87
50.27
44.82

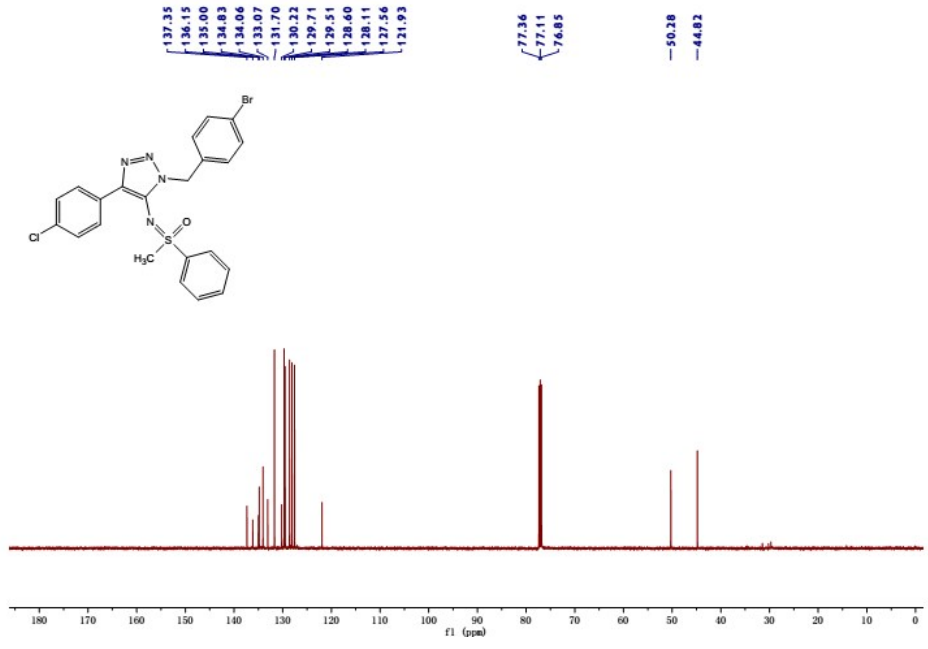

Br
N
N
N
O
S
H3C
Br

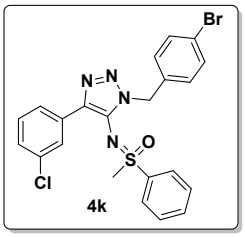

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

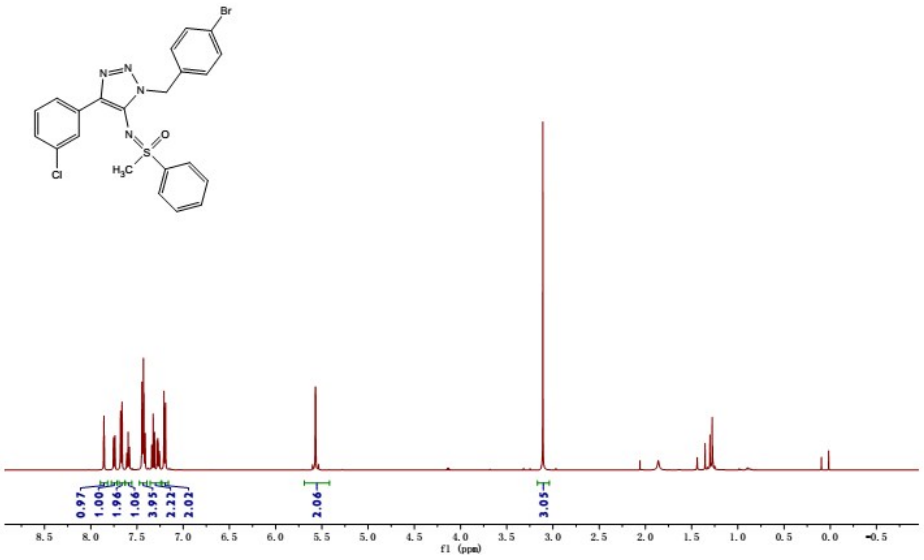

Br
Cl
N
N
N
N
O
S

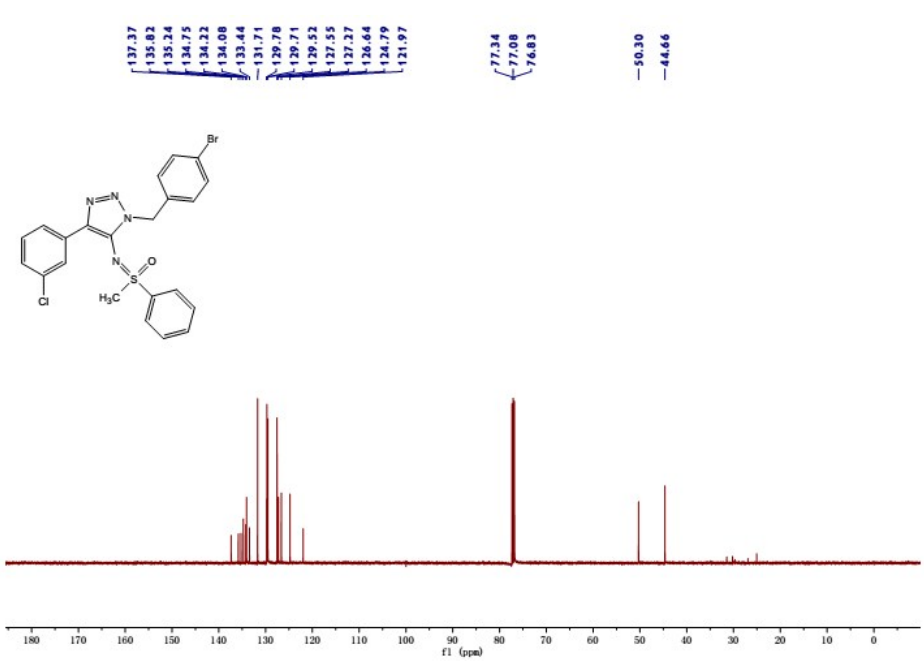
4j


7.77
7.76
7.63
7.62
7.61
7.58
7.44
7.42
7.42
7.40
7.38
7.37
7.35
7.20
5.59
5.56
5.55
5.52
3.09
Br
Cl
2.02
3.05
6.00
2.01
2.03
3.08
f1 (ppm)


137.35
136.15
135.00
134.83
134.06
133.07
131.70
130.22
129.71
129.51
128.60
128.11
127.56
121.93
77.36
77.11
76.85
50.28
44.82
Br
Cl
f1 (ppm)


Br
Cl
4k


Br
Cl
0.97
1.00
1.96
1.06
3.95
2.22
2.02
2.06
3.05
f1 (ppm)


137.37
135.82
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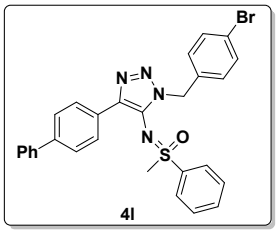
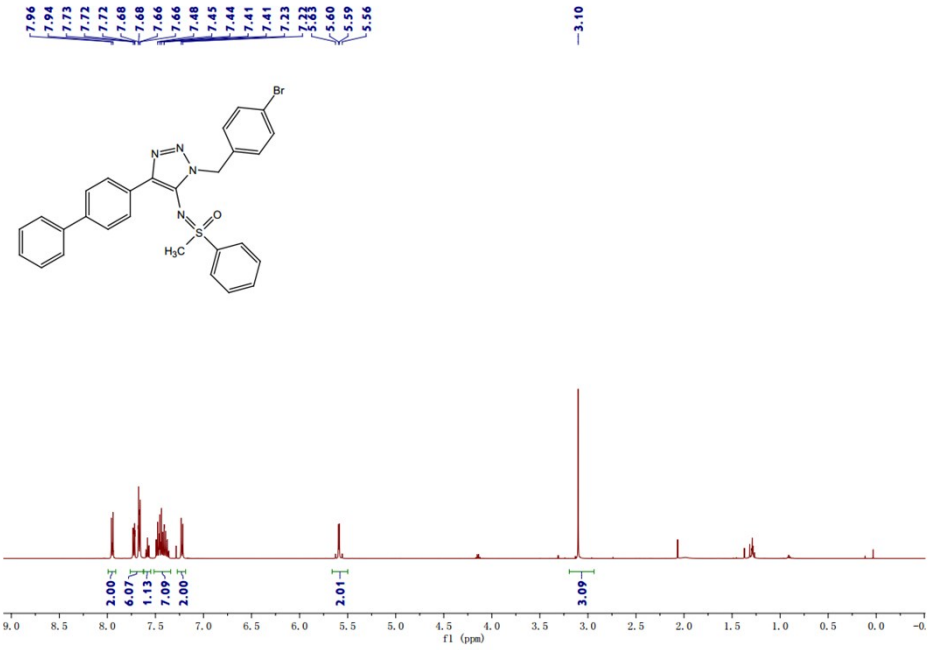
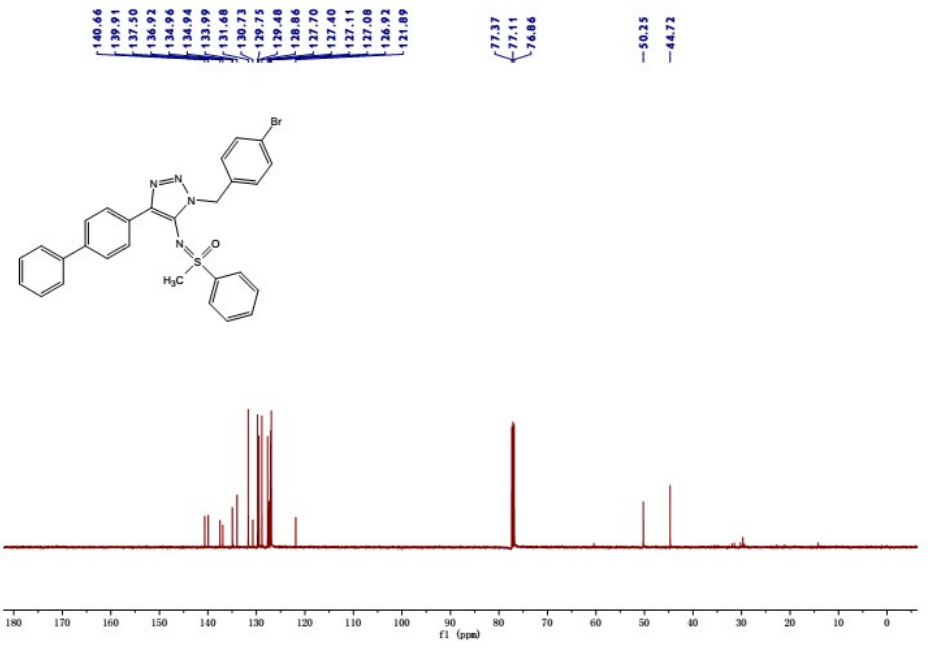
134.75
134.22
134.08
133.44
131.71
129.78
129.71
129.52
127.55
127.27
126.64
124.79
121.97
77.34
77.08
76.83
50.30
44.66
Br
Cl
f1 (ppm)


Br
Ph
4l


7.96
7.94
7.73
7.72
7.72
7.68
7.68
7.66
7.66
7.48
7.45
7.44
7.41
7.41
7.23
5.60
5.59
5.56
3.10
Br
2.00
6.07
1.13
7.09
2.00
2.01
3.09
f1 (ppm)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139.91
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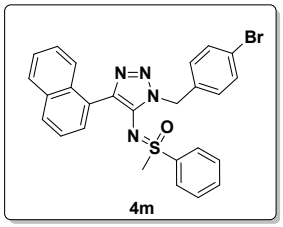
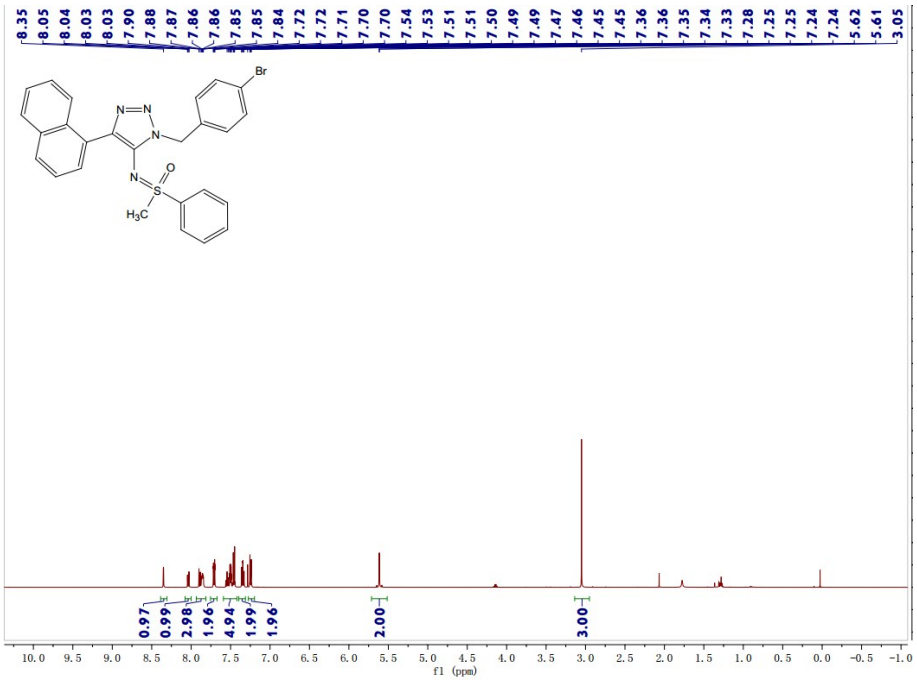
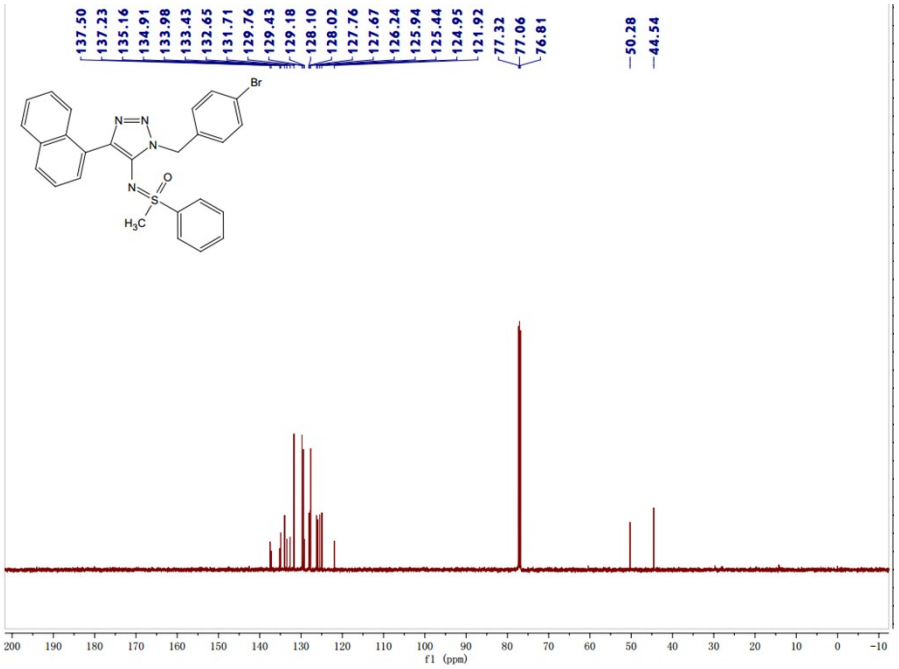
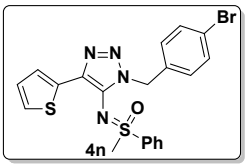
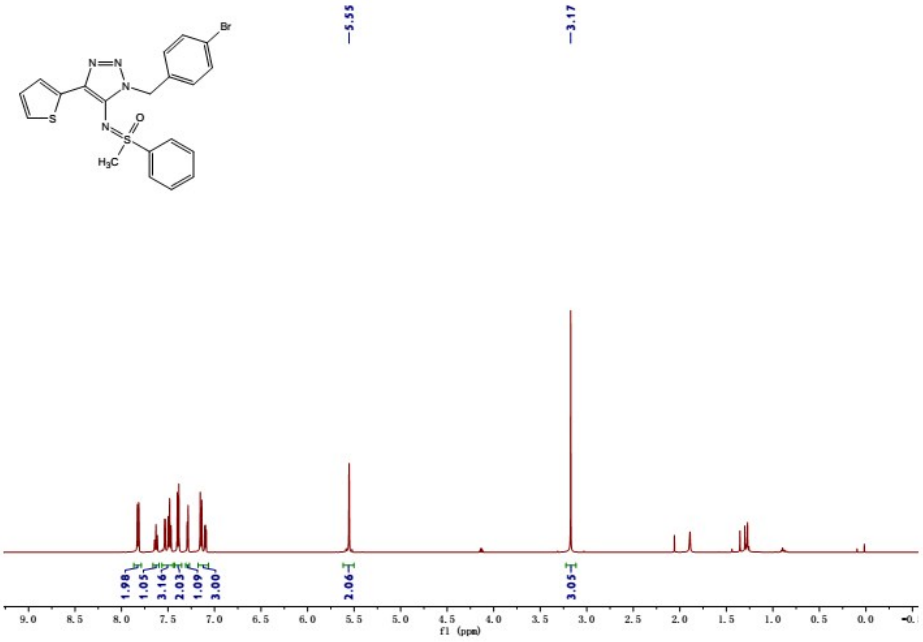
136.92
134.96
134.94
133.99
131.68
130.73
129.75
129.48
128.86
127.70
127.40
127.11
127.08
126.92
121.89
77.37
77.11
76.86
50.25
44.72
Br
f1 (ppm)

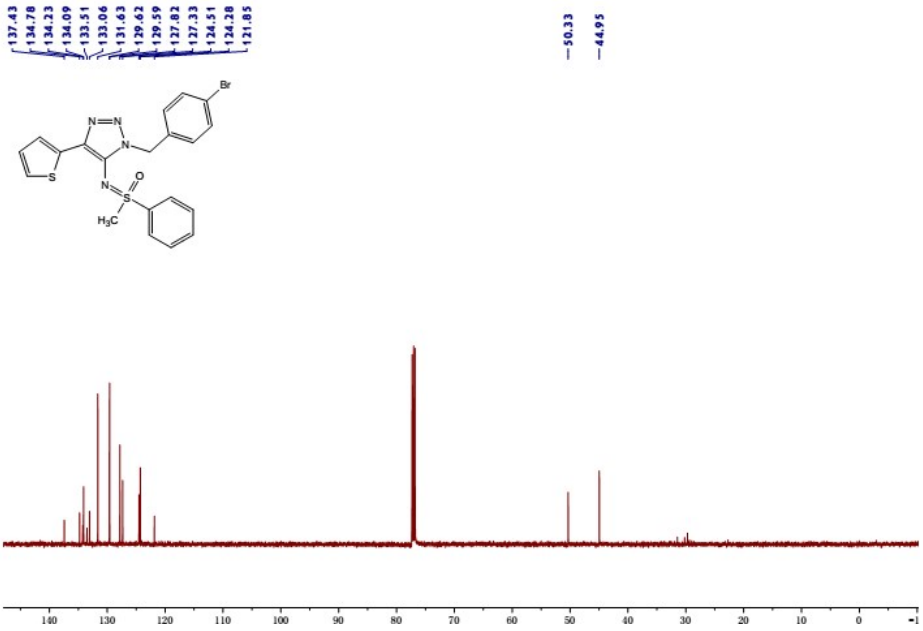

Br
N=N
N
N
O
S
4m

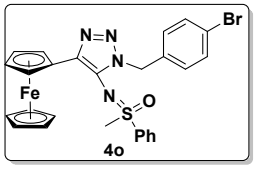

8.35 8.05 8.04 8.03 8.03 7.90 7.88 7.87 7.86 7.86 7.85 7.85 7.84 7.72 7.72 7.71 7.70 7.70 7.54 7.53 7.51 7.51 7.50 7.49 7.49 7.47 7.46 7.46 7.45 7.45 7.36 7.36 7.35 7.34 7.33 7.28 7.25 7.25 7.24 7.24 5.62 5.61 3.05
Br
N=N
N
N
O
S
H3C
0.97 0.99 2.98 1.96 4.94 1.99 1.96 2.00 3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


137.50 137.23 135.16 134.91 133.98 133.43 132.65 131.71 129.76 129.43 129.18 128.10 128.02 127.76 127.67 126.24 125.94 125.44 124.95 121.92 77.32 77.06 76.81 50.28 44.54
Br
N=N
N
N
O
S
H3C
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

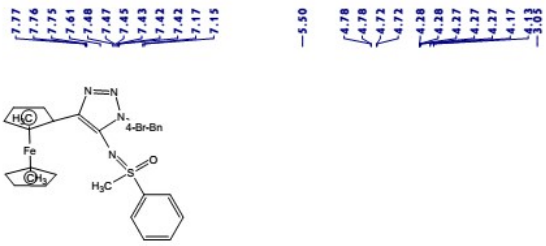

Br
N=N
N
S
N
S
O
Ph
4n


5.55
3.17
Br
N=N
N
S
N
S
O
H3C
1.98
1.05
3.16
2.03
1.09
3.00
2.06
3.05
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


137.43
134.78
134.23
134.09
133.51
133.06
131.63
129.62
129.59
127.82
127.33
124.51
124.28
121.85
50.33
44.95
Br
N=N
N
S
N
S
O
H3C
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


Br
N=N
N
Fe
N
S
O
Ph

4o


7.77
7.76
7.75
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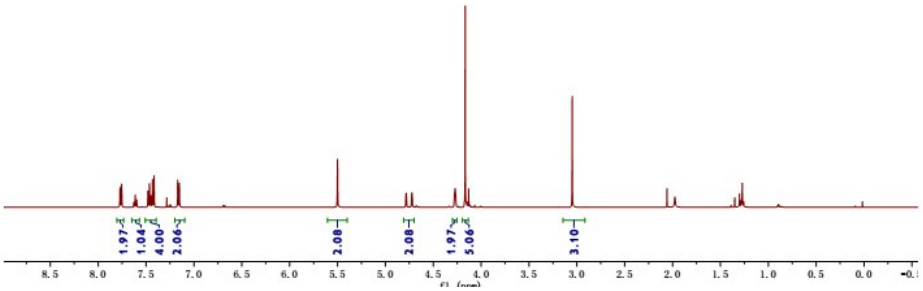
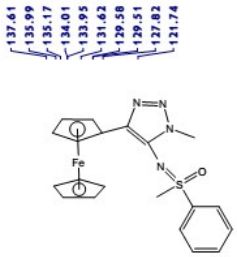
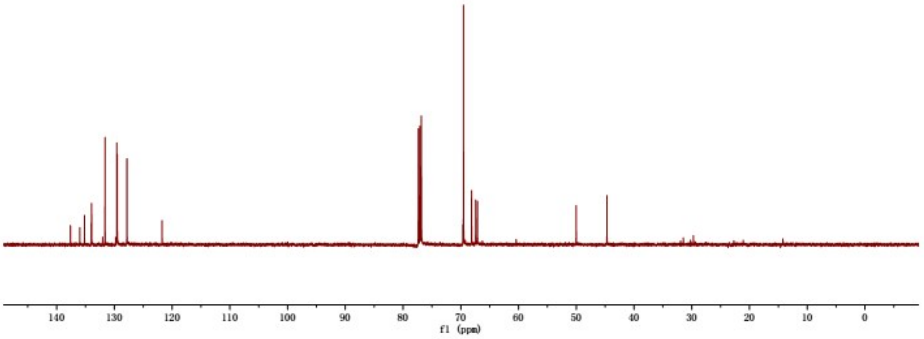
7.48
7.47
7.45
7.43
7.42
7.42
7.17
7.15
5.50
4.78
4.78
4.72
4.72
4.28
4.28
4.27
4.27
4.27
4.27
4.17
3.03
3.03

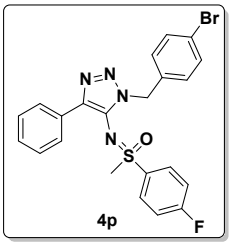
N=N
N
4-Br-Bn
HC
Fe
CH3
N
S
O
H3C


1.97
1.04
4.00
2.06
2.08
2.08
1.97
5.04
3.10
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

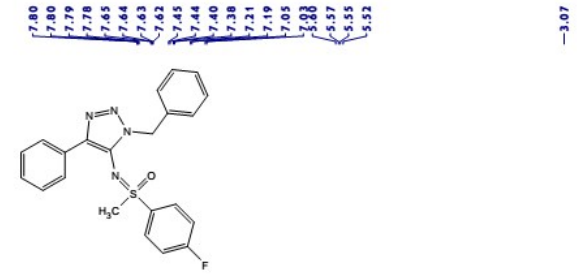

137.61
135.99
135.17
134.01
133.95
131.62
129.58
129.51
127.82
121.74
69.65
69.53
68.13
67.43
67.13
50.02
44.69

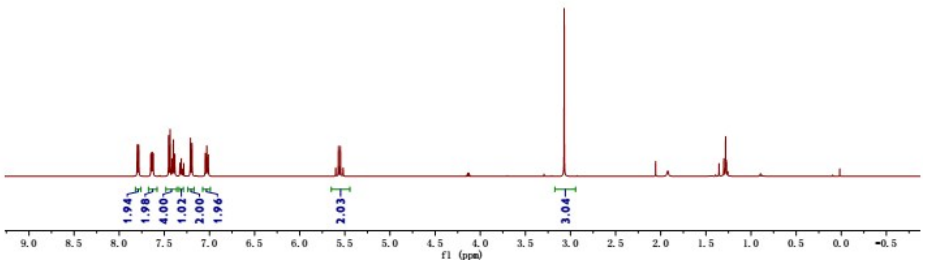
N=N
N
Fe
N
S
O

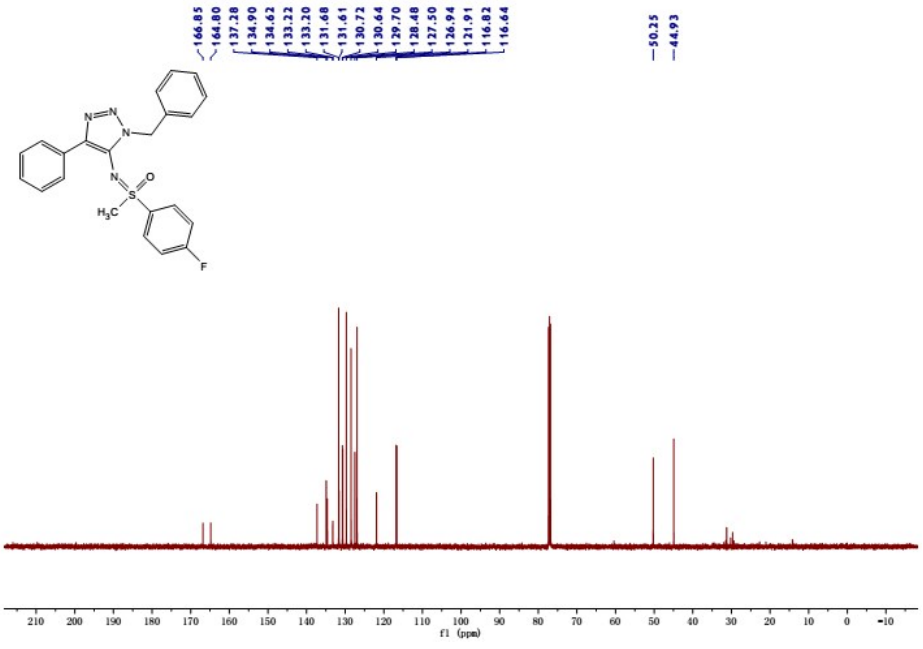

140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

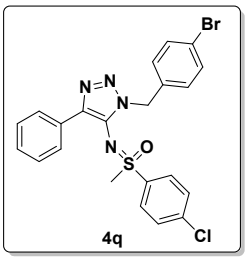

Br
N
N
N
N
O
S
F

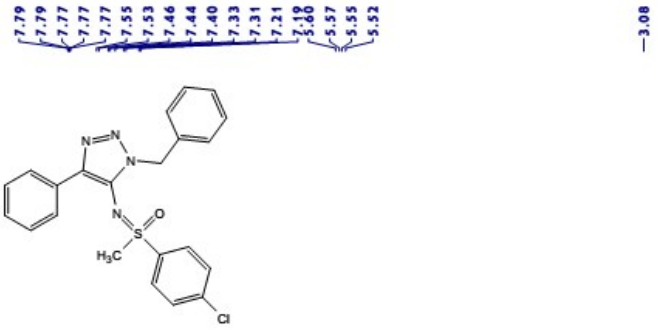
4p

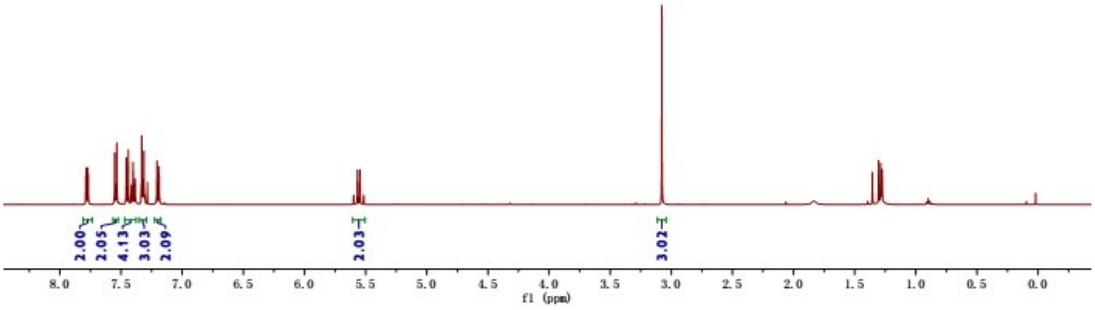

7.80
7.80
7.79
7.78
7.65
7.64
7.63
7.62
7.45
7.44
7.40
7.38
7.21
7.19
7.05
5.57
5.55
5.52
3.07

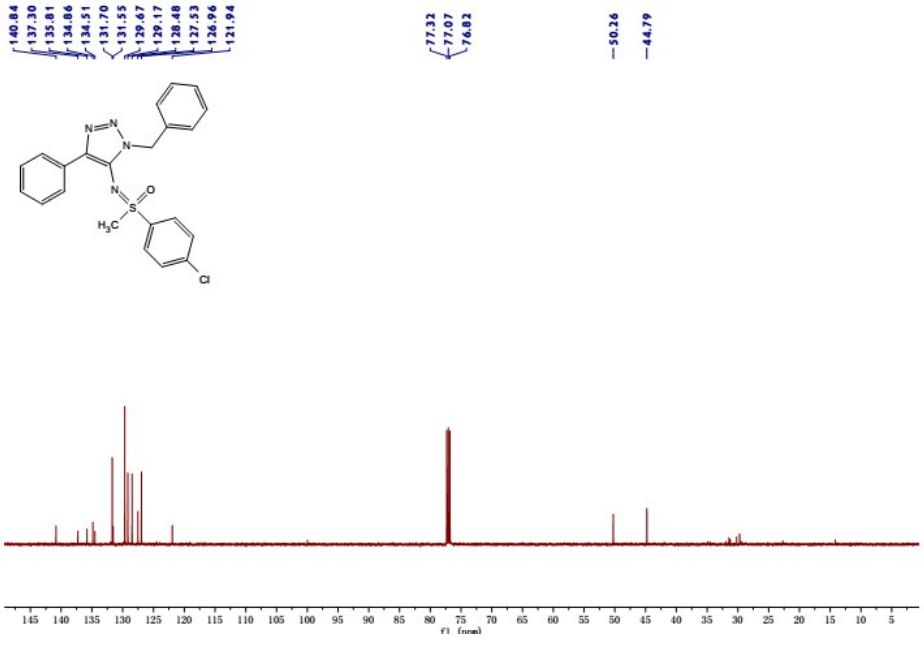

1.94
1.98
4.00
1.02
2.00
1.96
2.03
3.04
f1 (ppm)

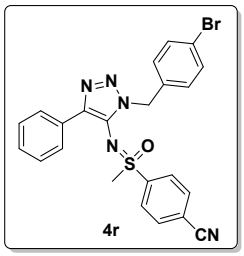

166.85
164.80
137.28
134.90
134.62
133.22
133.20
131.68
131.61
130.72
130.64
129.70
128.48
127.50
126.94
121.91
116.82
116.64
50.25
44.93
f1 (ppm)

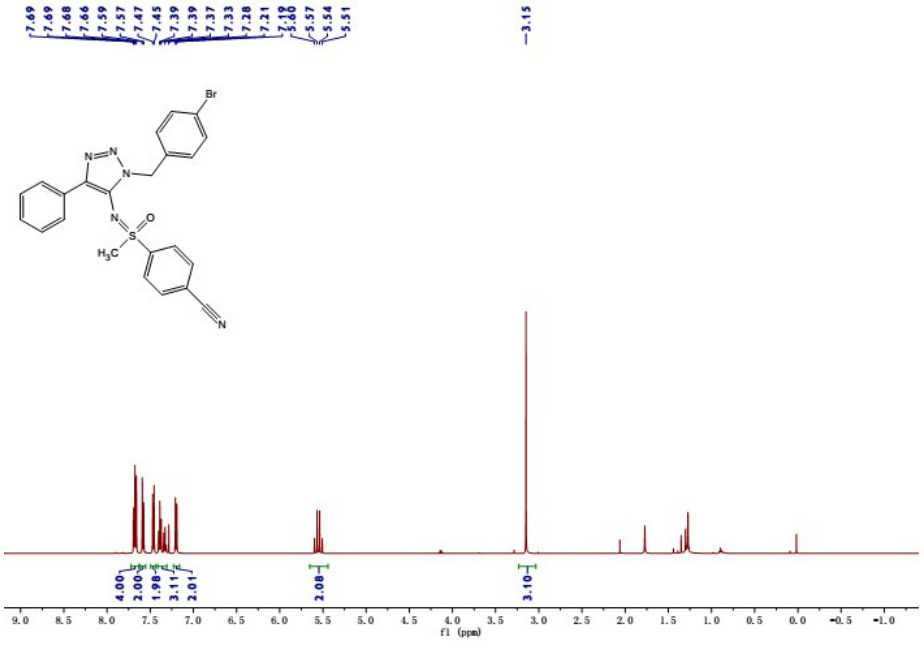

Br
N
N
N
N
O
S
Cl
4q

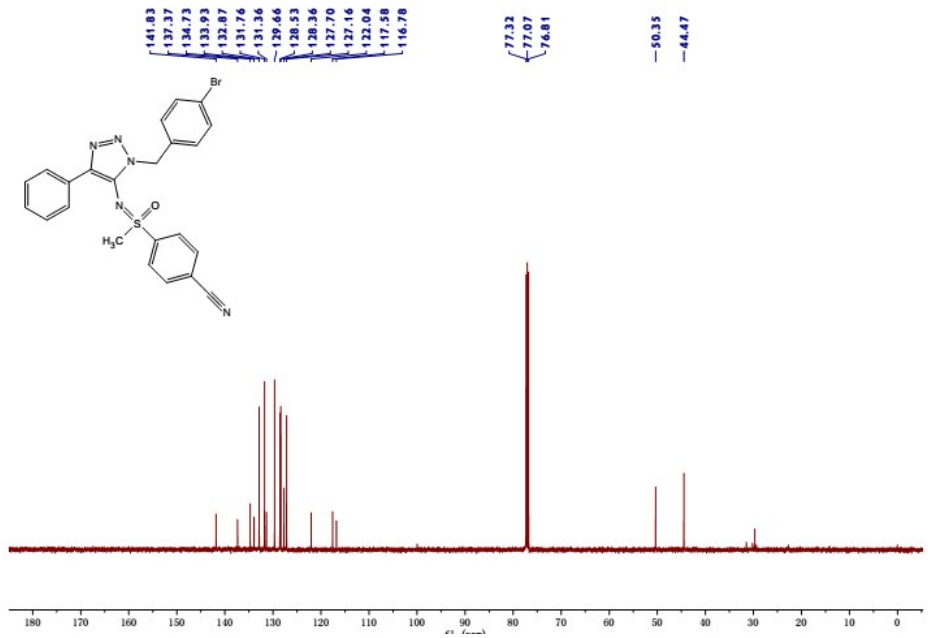

7.79
7.79
7.77
7.77
7.77
7.77
7.55
7.53
7.46
7.44
7.40
7.33
7.31
7.21
5.60
5.57
5.55
5.52
3.08
N
N
N
O
S
H3C
Cl


2.00
2.05
4.13
3.03
2.09
2.03
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


140.84
137.30
135.81
134.86
134.51
131.70
131.55
129.67
129.17
128.48
127.53
126.96
121.94
77.32
77.07
76.82
50.26
44.79
N
N
N
O
S
H3C
Cl
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
f1 (ppm)


Br
N
N
N
O
S
CN
4r


7.69
7.69
7.68
7.66
7.59
7.57
7.47
7.45
7.39
7.39
7.37
7.33
7.28
7.21
5.57
5.54
5.51
3.15
Br
N
O
H3C
N
4.00
2.00
1.98
3.11
2.01
2.08
3.10
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


141.83
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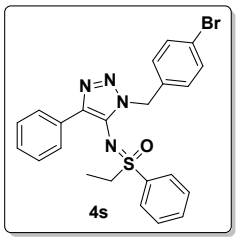
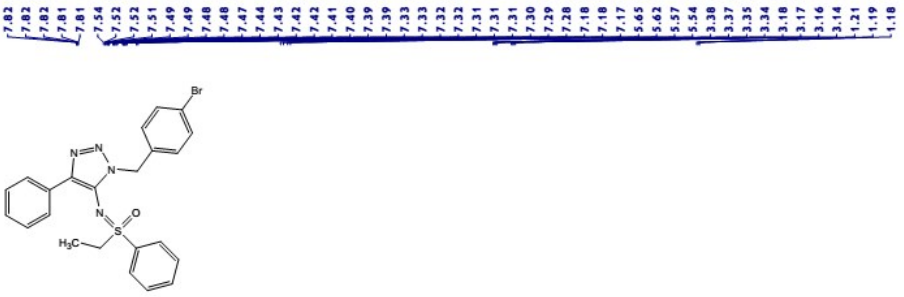
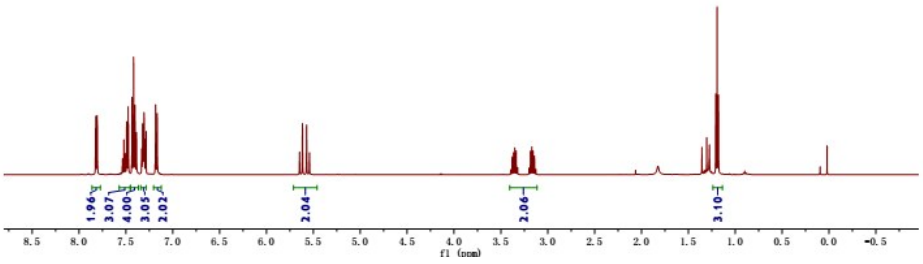
133.93
132.87
131.76
131.36
129.66
128.53
128.36
127.70
127.16
122.04
117.58
116.78
77.32
77.07
76.81
50.35
44.47
Br
N
O
H3C
N
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


Br
N
N
N
N
O
S
4s



Br
N
N
N
N
O
S
H3C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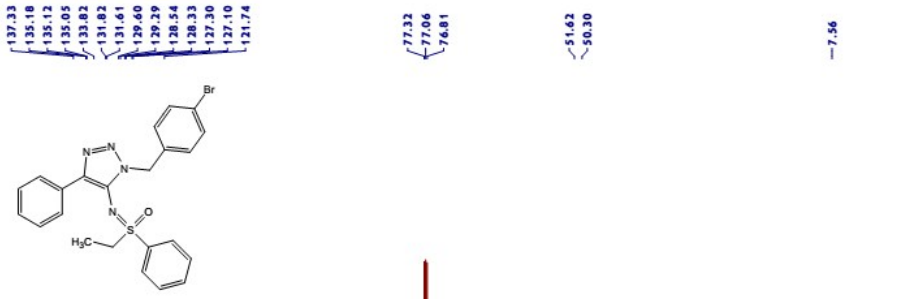
3.07
4.00
3.05
2.02
2.04
2.06
3.10
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


137.33
135.18
135.12
135.05
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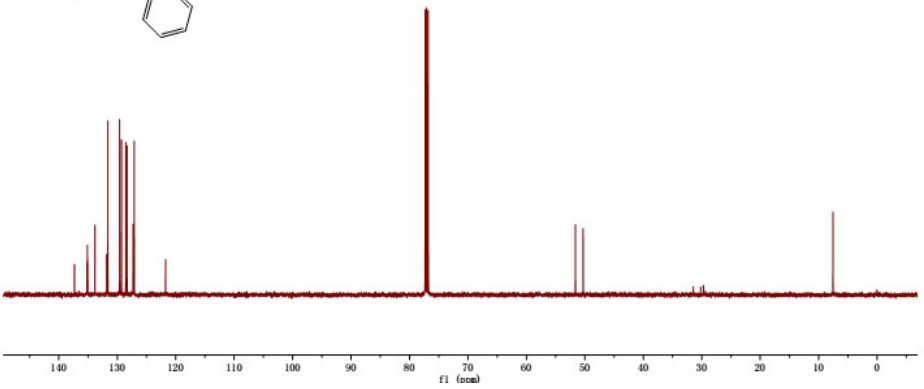
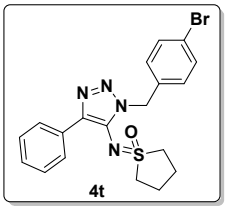
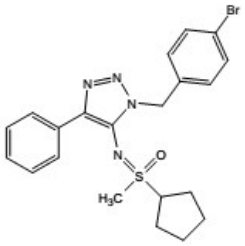
131.82
131.61
129.60
129.29
128.54
128.33
127.30
127.10
121.74
77.32
77.06
76.81
51.62
50.30
7.56

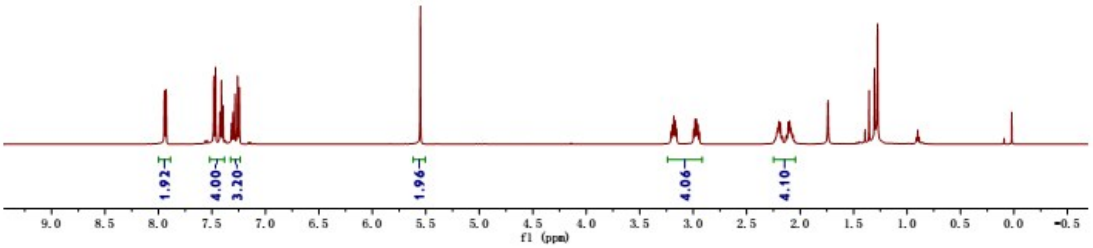
Br
N
N
N
N
O
S
H3C

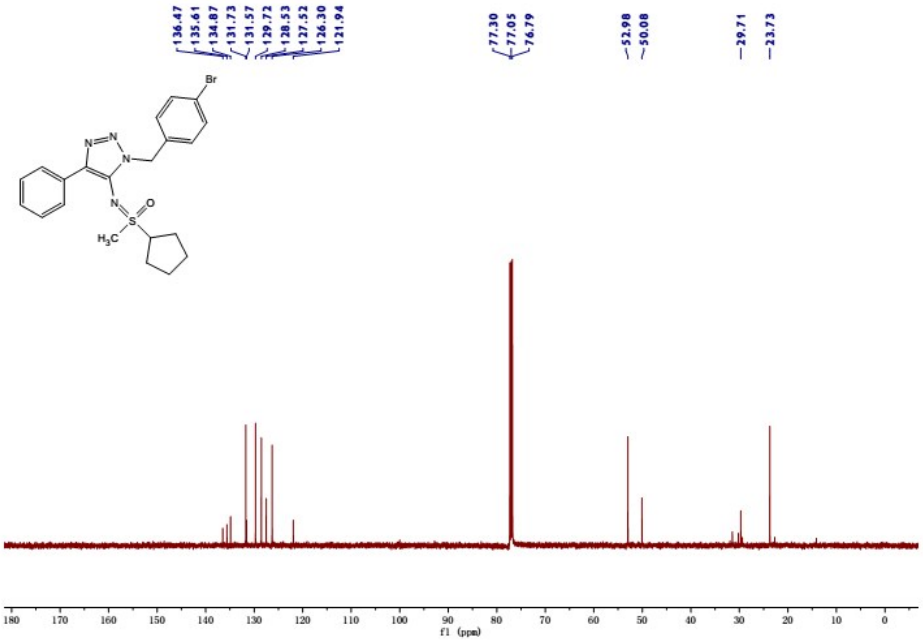

140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Br
N
N
N
O
N
S
4t


7.95
7.94
7.93
7.48
7.47
7.43
7.41
7.40
7.32
7.30
7.28
7.26
7.24
5.55
3.21
3.19
3.18
3.17
3.15
3.00
2.98
2.97
2.96
2.94
2.22
2.21
2.20
2.18
2.17
2.17
2.16
2.13
2.11
2.10
2.09
2.08
2.06


Br
N
N
N
N
O
S
H3C


1.92
4.00
3.20
1.96
4.06
4.10
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


136.47
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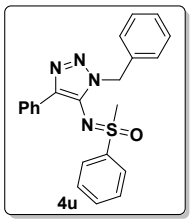
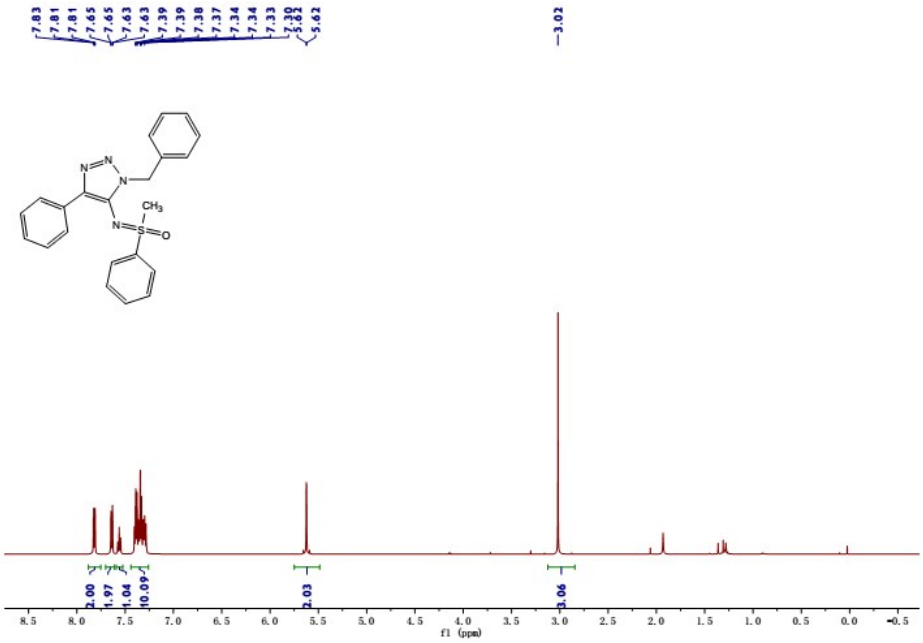
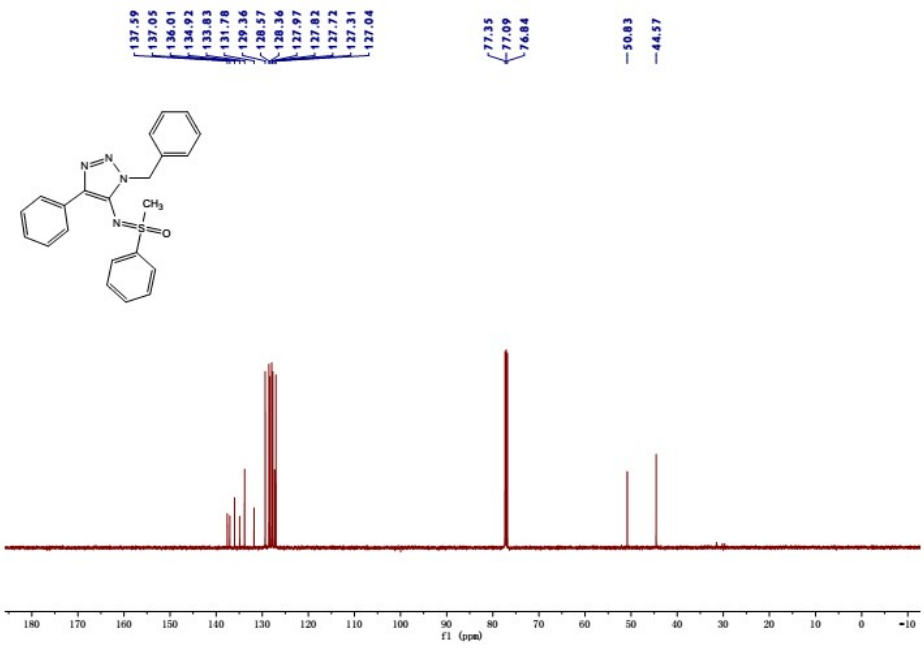
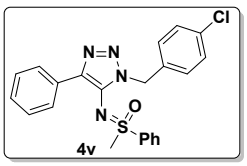
134.87
131.73
131.57
129.72
128.53
127.52
126.30
121.94
77.30
77.05
76.79
52.98
50.08
29.71
23.73
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

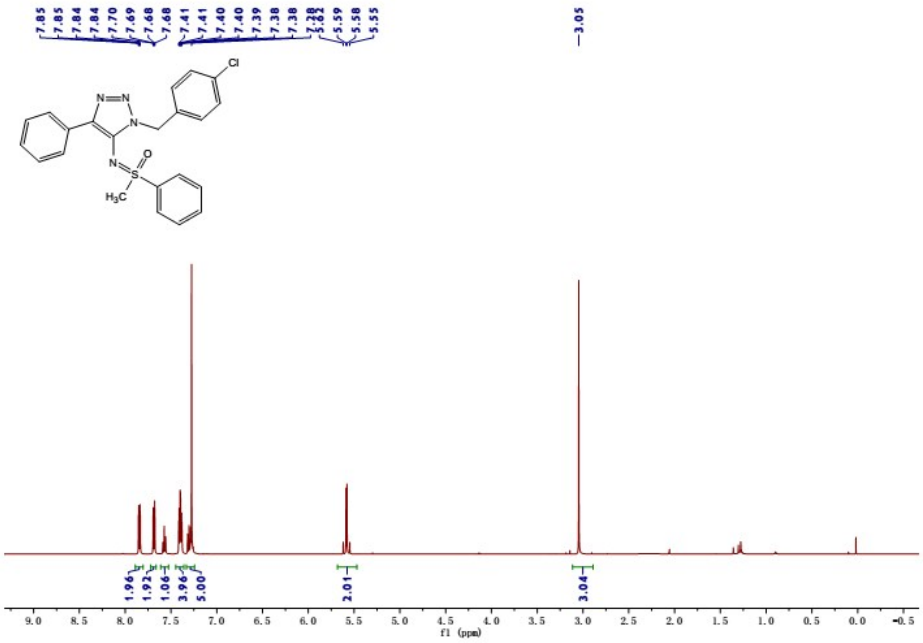
Br
N
N
N
N
O
S
H3C

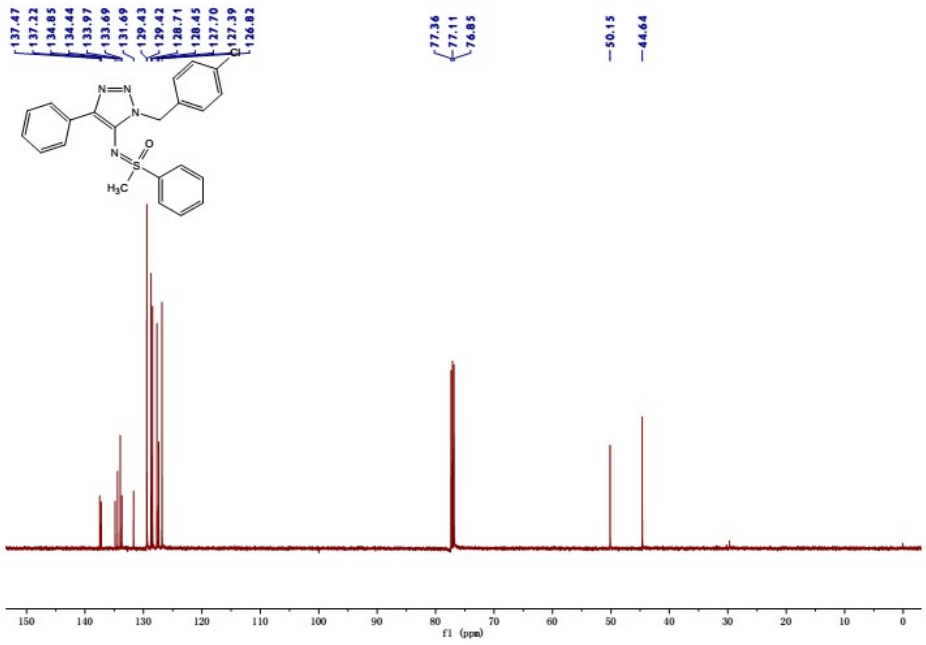

Ph
4u

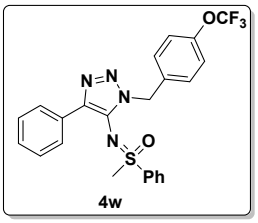

7.83
7.81
7.81
7.65
7.65
7.63
7.63
7.39
7.39
7.38
7.37
7.34
7.34
7.33
5.62
3.02
CH3
2.00
1.97
1.04
10.09
2.03
3.06
f1 (ppm)


137.59
137.05
136.01
134.92
133.83
131.78
129.36
128.57
128.36
127.97
127.82
127.72
127.31
127.04
77.35
77.09
76.84
50.83
44.57
CH3
f1 (ppm)

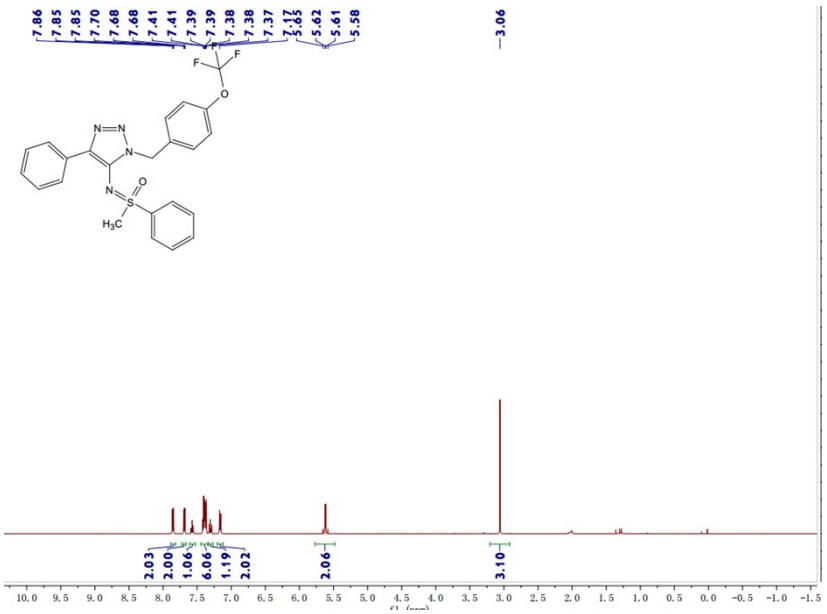

Cl
N=N
N
N
O
S
Ph
4v

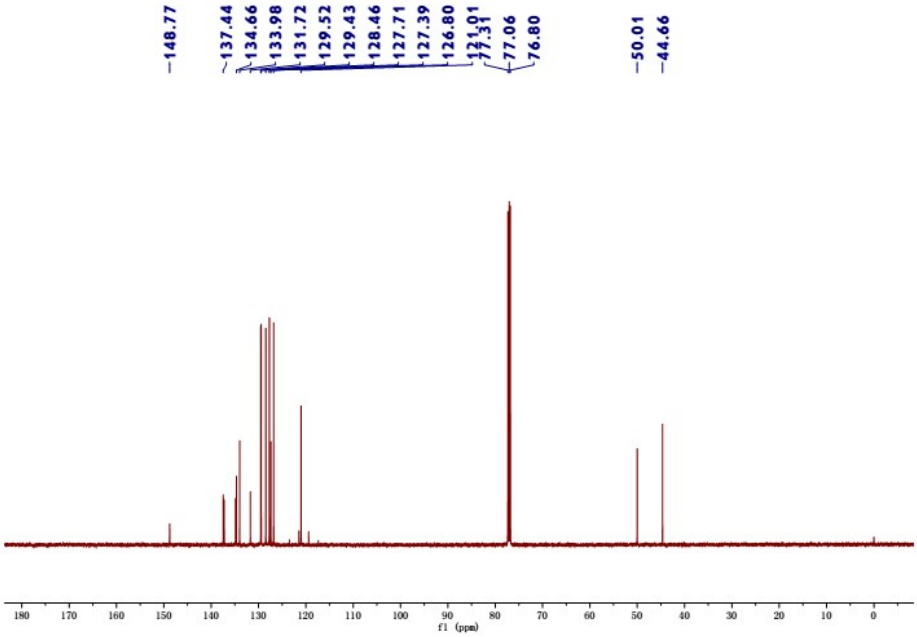

7.85
7.85
7.84
7.84
7.70
7.69
7.68
7.68
7.41
7.41
7.40
7.40
7.39
7.38
7.38
5.59
5.58
5.55
3.05
Cl
N=N
N
N
O
S
H3C
1.94
1.92
1.06
3.96
5.00
2.01
3.04
f1 (ppm)

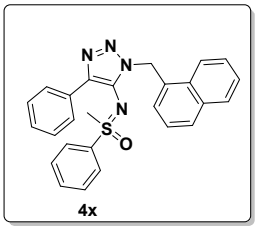

137.47
137.22
134.85
134.44
133.97
133.69
131.69
129.43
129.42
128.71
128.45
127.70
127.39
126.82
77.36
77.11
76.85
50.15
44.64
Cl
N=N
N
N
O
S
H3C
f1 (ppm)

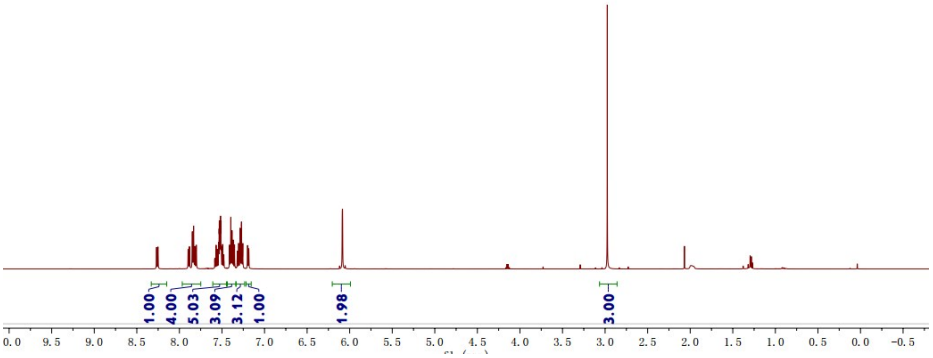

OCF3
N
N
N
O
S
Ph

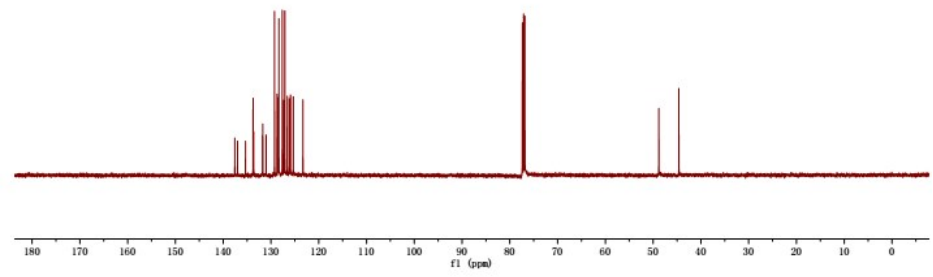
4w

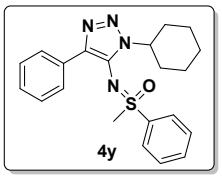

7.86
7.85
7.85
7.70
7.68
7.68
7.41
7.41
7.39
7.39
7.38
7.38
7.37
7.17
5.65
5.62
5.61
5.58
3.06
F
F
F
O
N
N
N
O
S
H3C
2.03
2.00
1.06
6.06
1.19
2.02
2.06
3.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5

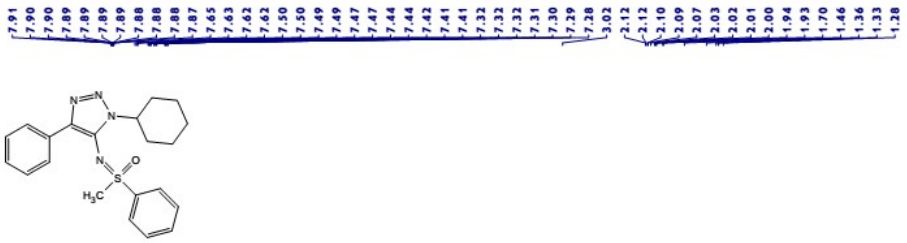

148.77
137.44
134.66
133.98
131.72
129.52
129.43
128.46
127.71
127.39
126.80
121.01
77.31
77.06
76.80
50.01
44.66
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

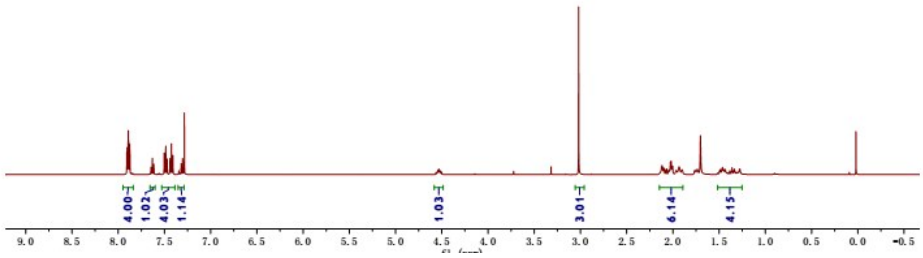

4x

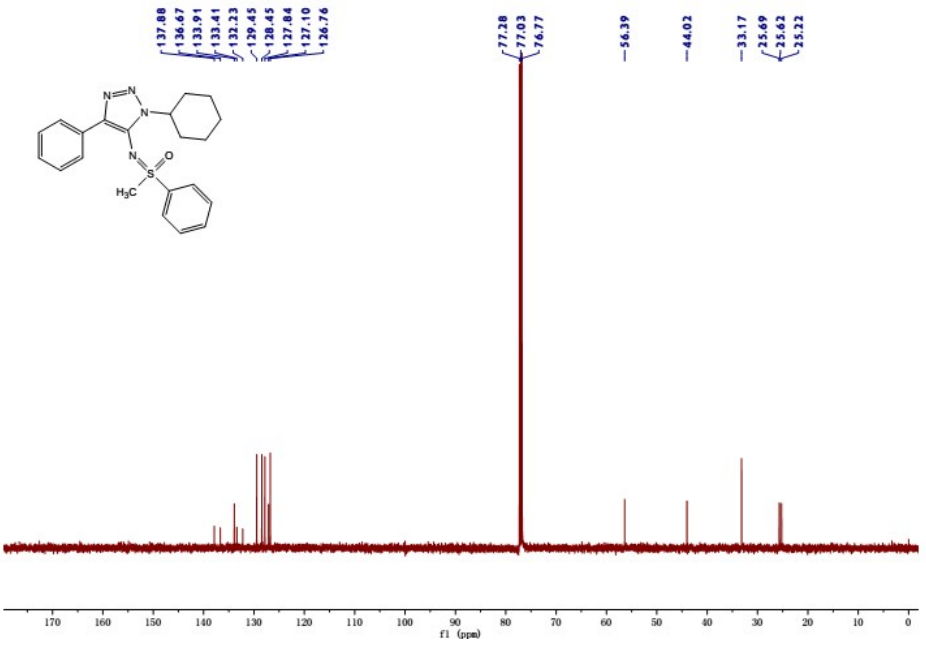


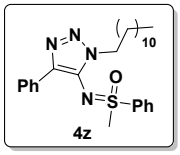


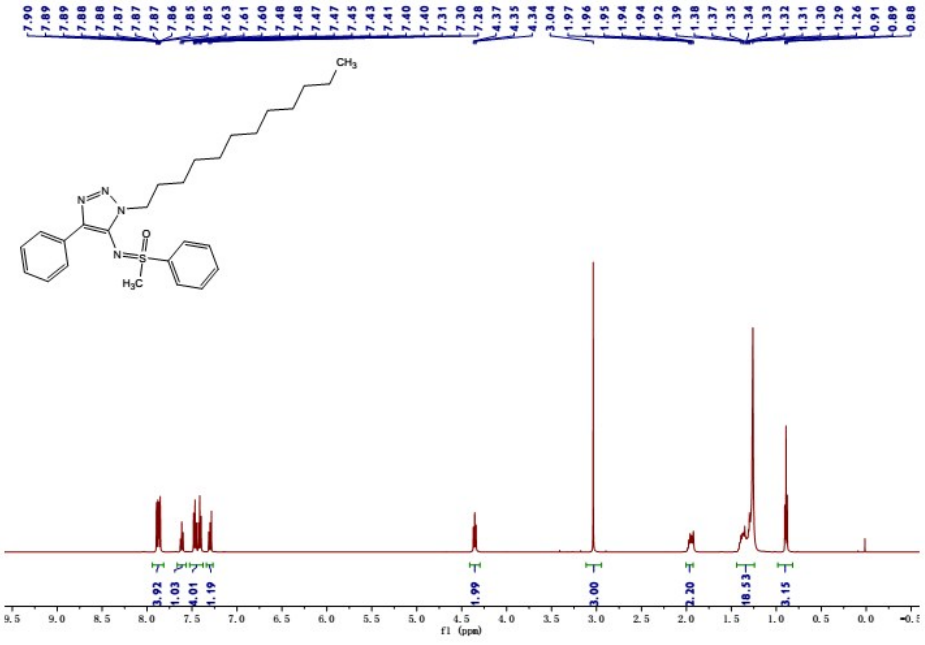

4y

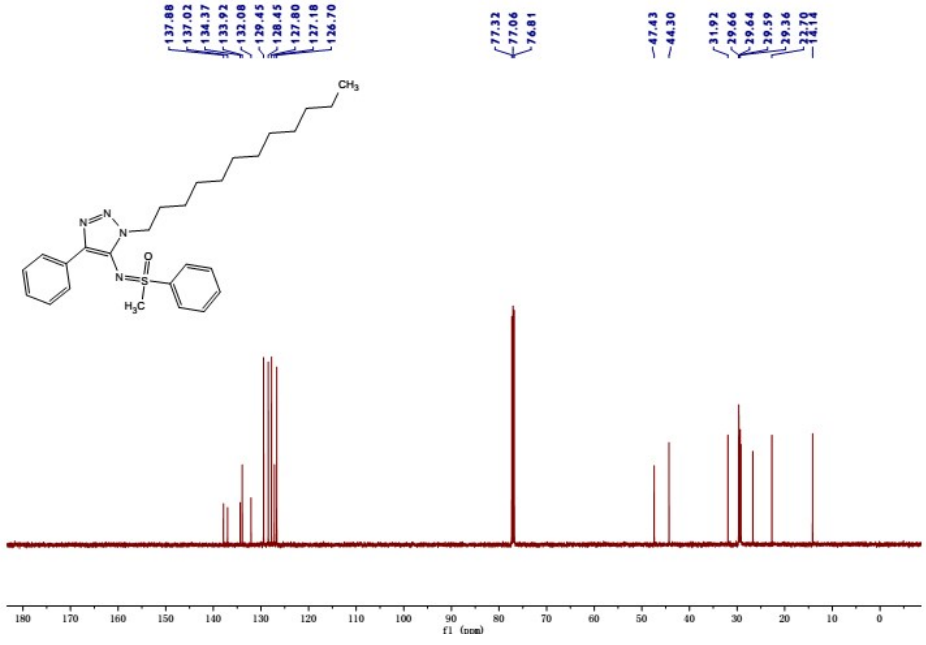


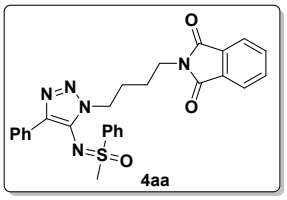


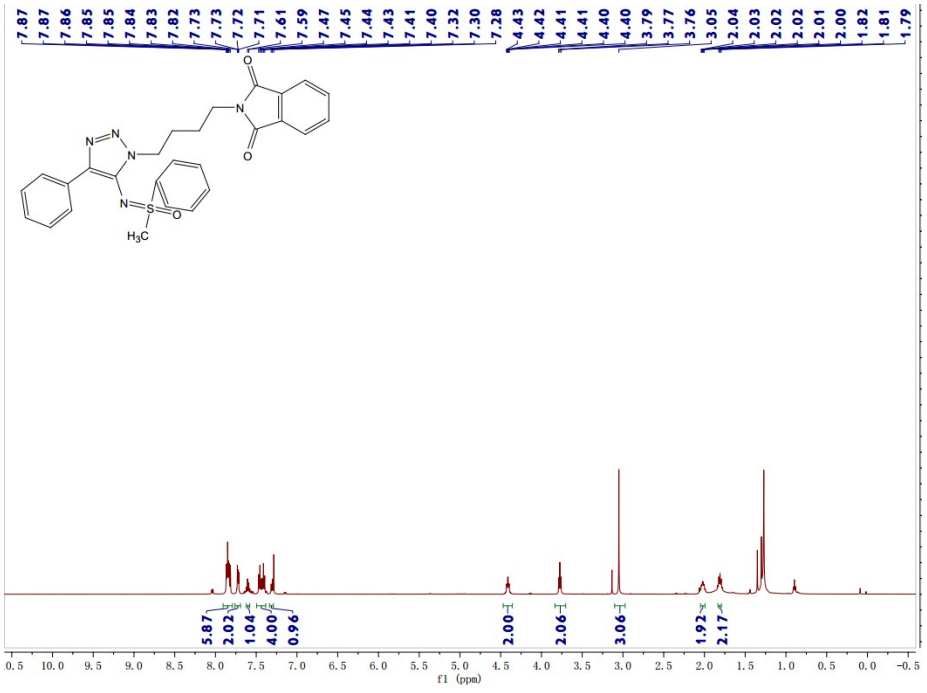


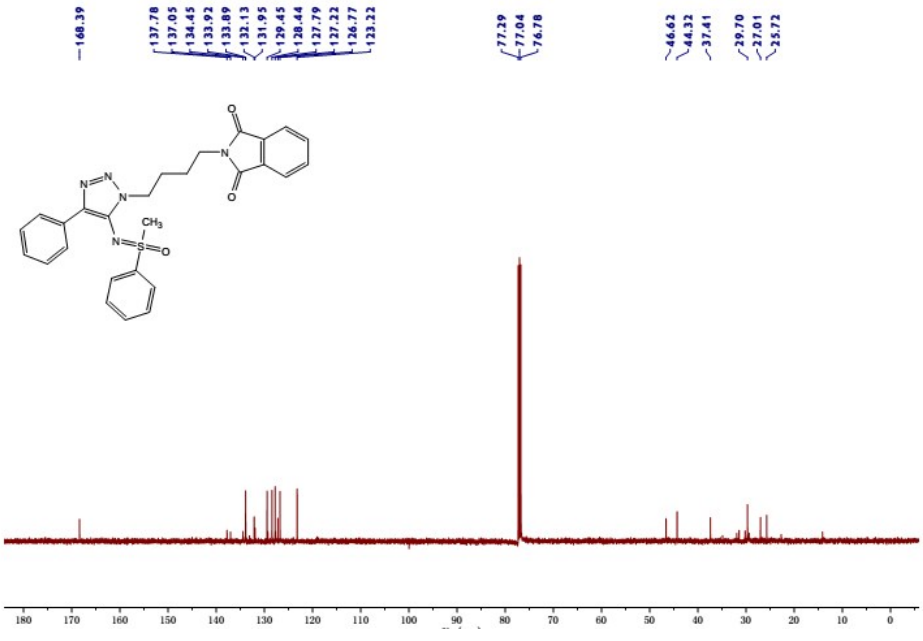

Ph
Ph
10
4z

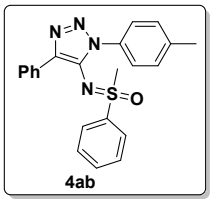

CH3
H3C
f1 (ppm)

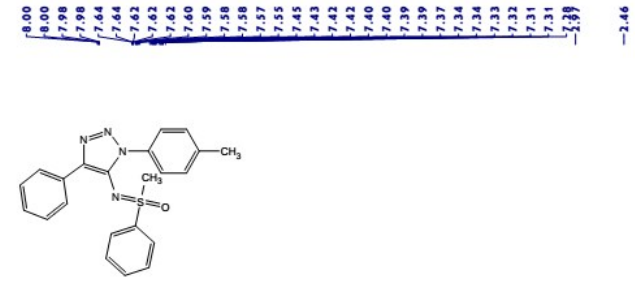

CH3
H3C
f1 (ppm)

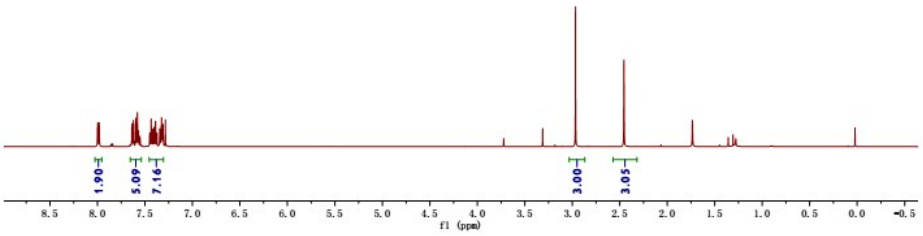

Ph
Ph
4aa

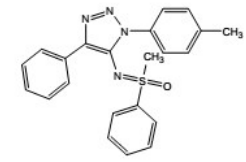

7.87 7.87 7.86 7.85 7.85 7.84 7.83 7.82 7.73 7.73 7.72 7.71 7.61 7.59 7.47 7.45 7.44 7.43 7.41 7.40 7.32 7.30 7.28
4.43 4.42 4.41 4.41 4.40 4.40 3.79 3.77 3.76 3.05 2.04 2.03 2.02 2.02 2.01 2.00 1.82 1.81 1.79
5.87 2.02 1.04 4.00 0.96 2.00 2.06 3.06 1.92 2.17
f1 (ppm)


168.39
137.78 137.05 134.45 133.92 133.89 132.13 131.95 129.45 128.44 127.79 127.32 126.77 123.22
77.29 77.04 76.78
46.62 44.32 37.41 29.70 27.01 25.72


Ph
N
S
O
4ab




1.90
5.09
7.16
3.00
3.05
f1 (ppm)



f1 (ppm)