Supporting Information

Visible-Light-Promoted Three-Component Cycloaddition Reaction: Synthesis of 4-Functionalized 1,5-Disubstituted 1,2,3-Triazoles

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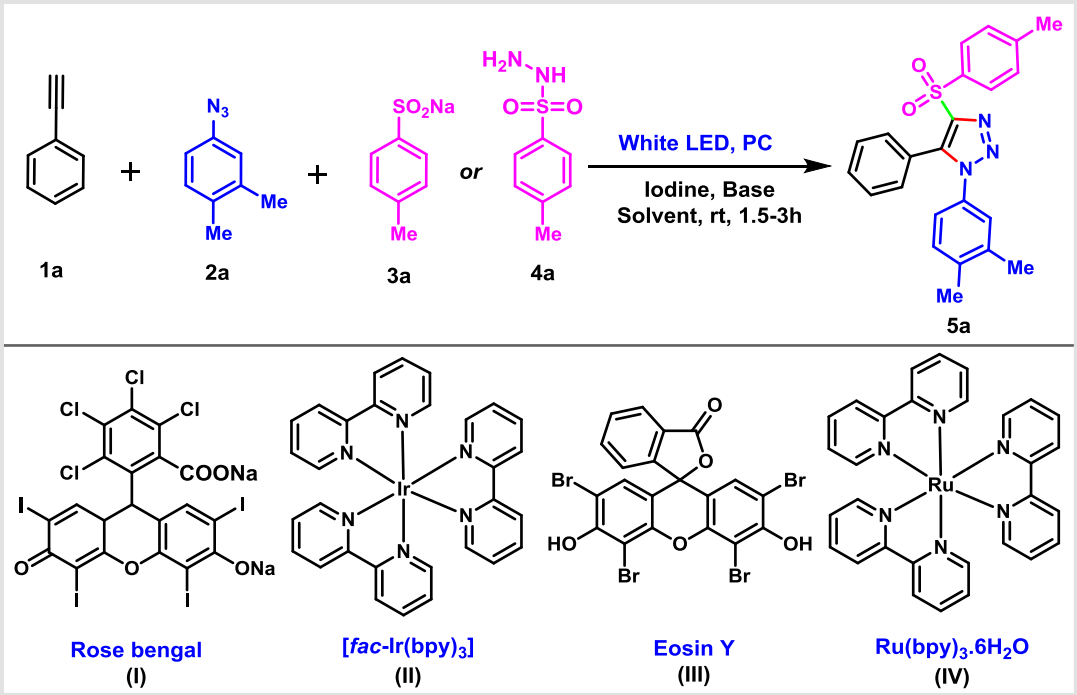
(1) General Information:

All the reactions were carried out under air unless otherwise noted. All the chemicals and reagents were purchased from commercial sources (Sigma-Aldrich or Merck chemical Co. and Alfa Aesar) and were used without further purification. Progresses of reactions were monitored by Thin Layer Chromatography (TLC). TLC was performed on Merck-percoated silica gel and 100-200 mesh silica gel was used for column chromatography. The chromatographic solvents are mentioned as v/v ratios. All the synthesized compounds were fully characterized by ^{1}H, ^{13}C-NMR, IR, and further confirmed through ESI-MS and HRMS analyses. IR spectra were recorded on a Perkin-Elmer FT-IR RXI spectrophotometer and values reported in cm^{-1}. NMR spectra were recorded with 400 MHz spectrometers for ^{1}H NMR, 100 MHz for ^{13}C-NMR respectively. The chemical shifts are reported in δ (ppm) relative to TMS (^{1}H), $CDCl_3$ as internal standards. Integrals are in accordance with assignments; coupling constants are given in Hz. ESI-MS spectra were obtained on a LCQ Advantage Ion trap mass spectrometer (Finnigan thermo Fischer scientific). High resolution mass spectra (HRMS) were measured with a Waters Micromass GCT instrument and accurate masses were reported for the molecular ion ($[M]^{+}$). All chemical shifts (δ) are reported in ppm and coupling constants (*J*) in Hz. All chemical shifts are reported relative to tetramethylsilane, and $CDCl_3$ (7.26 ppm for ^{1}H), and $CDCl_3$ (77.16 ppm for ^{13}C), and DMSO-d_6 (2.50 ppm for ^{1}H) and DMSO-d_6 (39.52 ppm for ^{13}C) respectively. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet.

A good quality Yellow color single crystal of size 0.32 x 0.28 x 0.08 mm, was selected under a polarizing microscope and was mounted on a glass fiber for data collection. Single crystal X-ray data for compound (**5n**) were collected on the Rigaku Kappa 3 circle diffractometer equipped with the AFC12 goniometer and enhanced sensitivity (HG) Saturn724+ CCD detector in the 4x4 bin mode using the monochromated Mo-Kα radiation generated from the microfocus sealed tube MicroMax-003 X-ray generator equipped with specially designed confocal multilayer optics. Data collection was performed using ω-scans of 0.5^{o} steps at 273 K. Cell determinations, data collection and data reduction was performed using the Rigaku CrystalClear-SM Expert 2.1 b24[1] software. Structure solution and refinement were performed by using SHELXTL-NT[2]. Refinement of coordinates and anisotropic thermal parameters of non-hydrogen atoms were carried out by the full-matrix least-squares method. The hydrogen

atoms attached to carbon atoms were generated with idealized geometries and isotropically refined using a riding model. Crystal data are summarized in Table S2.

(2) Optimization of Experiment Conditions:



Entry	Photocatalyst (2 mol %)	Base (1.0 equiv)	Solvent (v/v)	Yield (%)[b]
1	I	K_2CO_3	Ethanol/H_2O (1:1)	82/79
2	II	K_2CO_3	Ethanol/H_2O (1:1)	76/72
3	III	K_2CO_3	Ethanol/H_2O (1:1)	78/75
4	IV	K_2CO_3	Ethanol/H_2O (1:1)	72/69
5	**None**	**K_2CO_3**	**Ethanol/H_2O (1:1)**	**84/80**
6	None	Na_2CO_3	Ethanol/H_2O (1:1)	56/51
7	None	Cs_2CO_3	Ethanol/H_2O (1:1)	49/45
8	None	NaOH	Ethanol/H_2O (1:1)	43/50
9	None	KOH	Ethanol/H_2O (1:1)	48/52
10	None	DBU	Ethanol/H_2O (1:1)	34/30
11	None	DABCO	Ethanol/H_2O (1:1)	24/20
12	None	Et_3N	Ethanol/H_2O (1:1)	35/40
13	None	*t*-BuOK	Ethanol/H_2O (1:1)	15/19

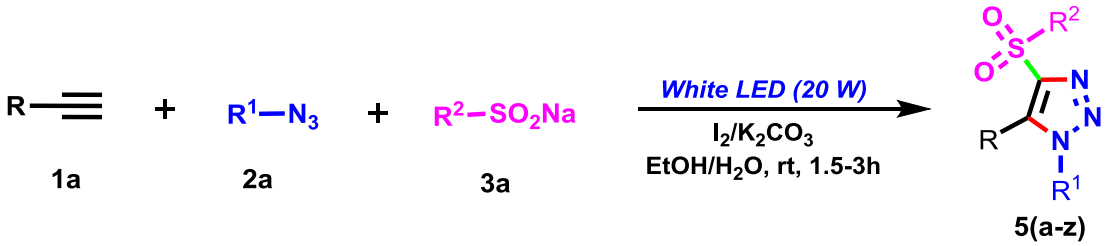
14	None	K_2CO_3	Ethanol	49/40
15	None	K_2CO_3	ACN	25/30
16	None	K_2CO_3	THF	12/16
17	None	K_2CO_3	DMF	trace/trace
18	None	K_2CO_3	DMSO	trace/trace
19	None	K_2CO_3	1,4-Dioxane	24/27
20	None	K_2CO_3	Toluene	15/11
21[c]	None	K_2CO_3	Ethanol/H_2O (1:1)	-/-
22[d]	None	K_2CO_3	Ethanol/H_2O (1:1)	84/80
23[e]	None	K_2CO_3	Ethanol/H_2O (1:1)	82/79
24[f]	None	K_2CO_3	Ethanol/H_2O (1:1)	21/15
25[g]	None	K_2CO_3	Ethanol/H_2O (1:1)	29/25
26[h]	None	K_2CO_3	Ethanol/H_2O (1:1)	22/18
27[i]	None	K_2CO_3	Ethanol/H_2O (1:1)	76/72
28[j]	None	K_2CO_3	Ethanol/H_2O (1:1)	35/30
29[k]	None	K_2CO_3	Ethanol/H_2O (1:1)	14/12

[a]**Reaction conditions:** Phenylacetylene **1a** (1.0 mmol), 4-Azido-1,2-dimethylbenzene **2a** (1.0 mmol), *p*-Toluenesulfinic acid sodium salt **3a** (1.2 mmol), or *p*-Toluenesulfonyl hydrazide **4a** (1.5 mmol), Iodine (1.0 equiv) and bases (1.0 equiv) under open-air atmosphere in solvents (2.0 mL) with 20 W white LED at room temperature for 1.5-3 h. [b]Yields of isolated products are given. [c]No light. [d]Under N_2 atmosphere. [e]Using CFL (30 W). [f]At 60 ºC, for 10h. [g]20 W white LED at 60 ºC for 10h. [h]20 W white LED at 80 ºC for 10h. [i]Using blue LED (455 nm) for 8h. [j]Using green LED (530 nm) for 8h. [k]Using red LED (660 nm) for 8h.

Table S1. Screening of reaction conditions for the regioselective 4-functionalized 1,5-disubstituted 1,2,3-triazoles

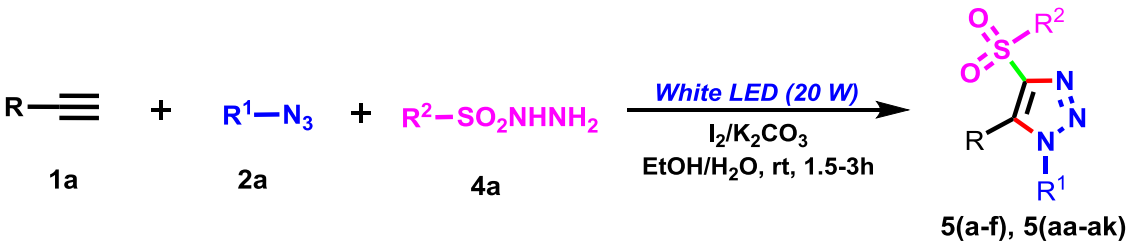
(3) Representative Experimental Procedure for the Synthesis of 4-Functionalized 1,5-Disubstituted 1,2,3-Triazoles 5(a-ak):

Method [A]: Using Arylacetylene and Arylazides with Arylsulfinic acid sodium salts;



In a 25 mL round-bottom flask equipped with a magnetic stirring bar charged with arylacetylene **1a** (1.0 mmol), arylazides **2a** (1.0 mmol), arylsulfinic acid sodium salt **3a** (1.2 mmol), iodine (1.0 equiv) and K_2CO_3 (1.0 equiv) in ethanol/water (2 mL) were stirred with the irradiation of a white LED (20 W) at room temperature under open air atmosphere for consumption of starting materials (confirmed by TLC). The reaction mixture was quenched by the addition of *satd. aq* sodium thiosulfate (2 mL) and extracted three times by ethyl acetate and water. The organic layer was further dried over anhydrous sodium sulfate, and the solvent was evaporated under vacuum. The resulting crude product was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (9:1) as the eluent to give the pure products **5(a-z)**.

Method [B]: Using Arylacetylene and Arylazides with Arylsulfonyl Hydrazides;



In a 25 mL round-bottom flask equipped with a magnetic stirring bar charged with arylacetylene **1a** (1.0 mmol), arylazides **2a** (1.0 mmol), arylsulfonyl hydrazides **4a** (1.5 mmol), iodine (1.0 equiv) and K_2CO_3 (1.0 equiv) in ethanol/water (2 mL) were stirred with the irradiation of a white LED (20 W) at room temperature under open air atmosphere for consumption of starting materials (confirmed by TLC). The reaction mixture was quenched by the addition of *satd. aq* sodium thiosulfate (2 mL) and extracted three times by ethyl acetate and water. The organic layer was further dried over anhydrous sodium sulfate, and the solvent was evaporated under vacuum. The resulting crude product was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (9:1) as the eluent to give the pure products **5(a-f)**, **5(aa-ak)**.

(4) UV-Vis Absorption Spectra

The UV-visible experiments were performed using a LABINDIA UV 3092 Spectrophotometer with a quartz cuvette of 1.0 cm path length. UV-Vis spectra of phenylacetylene **1a**, 4-Azido-1,2-dimethylbenzene **2a**, *p*-Toluenesulfinic acid sodium salt **3a**, *p*-Toluenesulfonyl hydrazide **4a**, Iodine and K_2CO_3 in EtOH ($5x10^{-5}$ M) are individual each and various combinations shown in Figure S1 to S8.

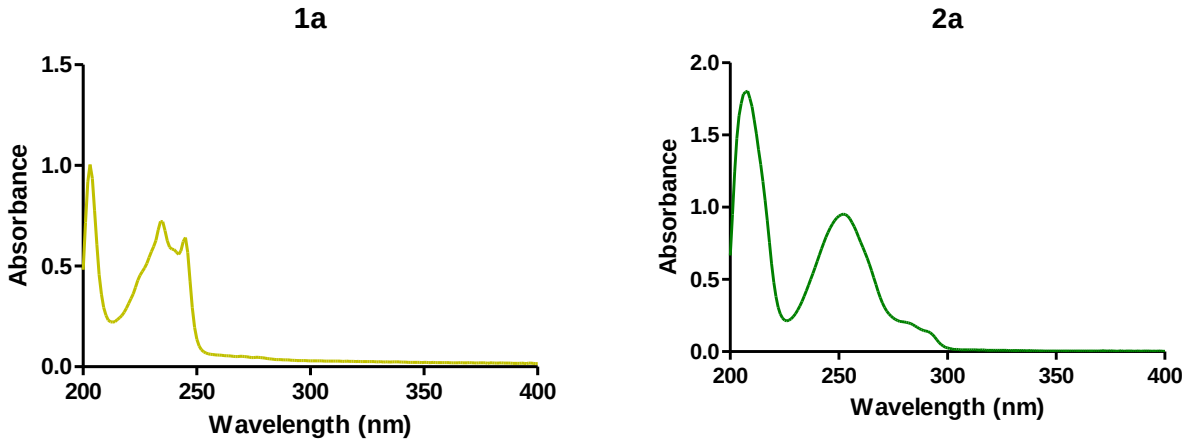


Figure S1. UV-Vis Absorption spectra of **1a** and **2a**

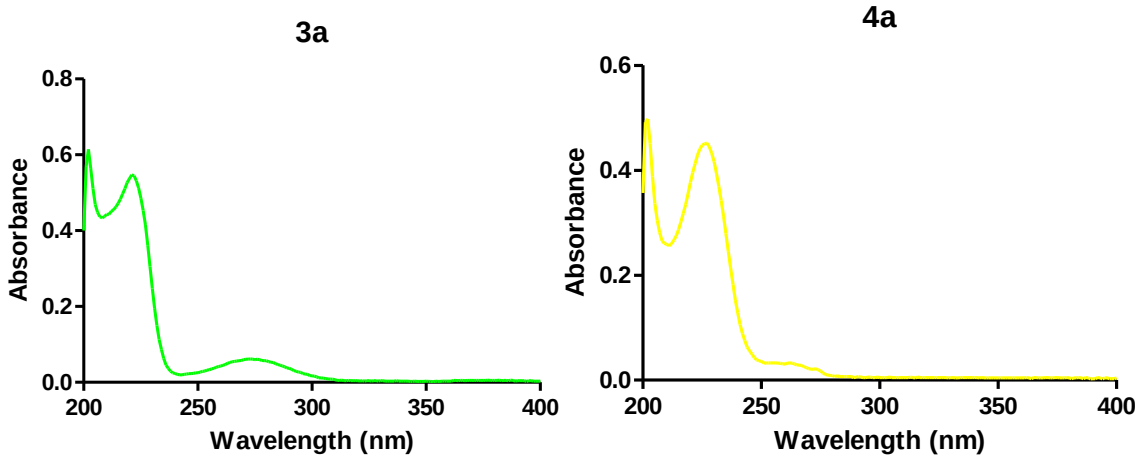


Figure S2. UV-Vis Absorption spectra of **3a** and **4a**

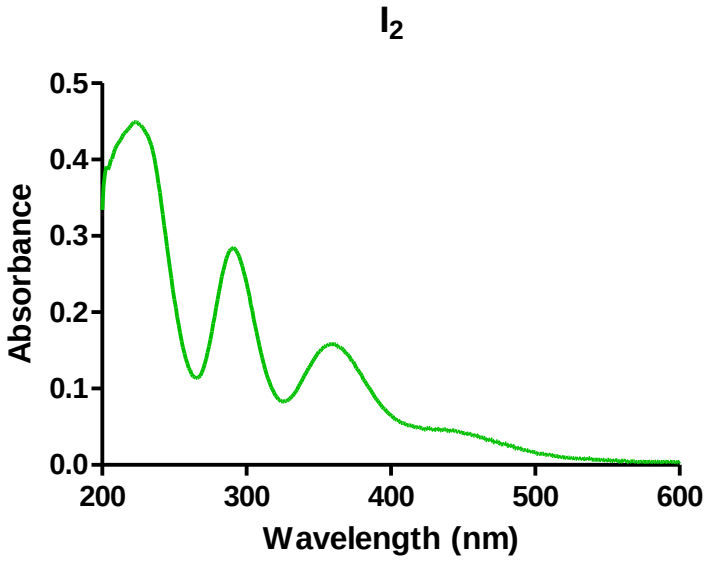


Figure S3. UV-Vis Absorption spectra of I_2

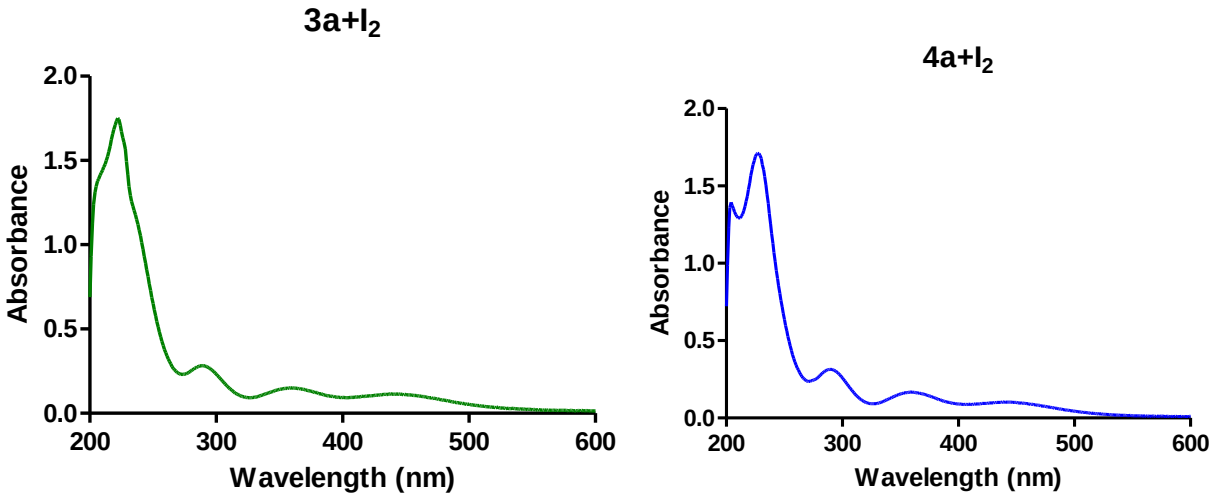


Figure S4. UV-Vis Absorption spectra mixture of **3a**, and **4a** with I_2

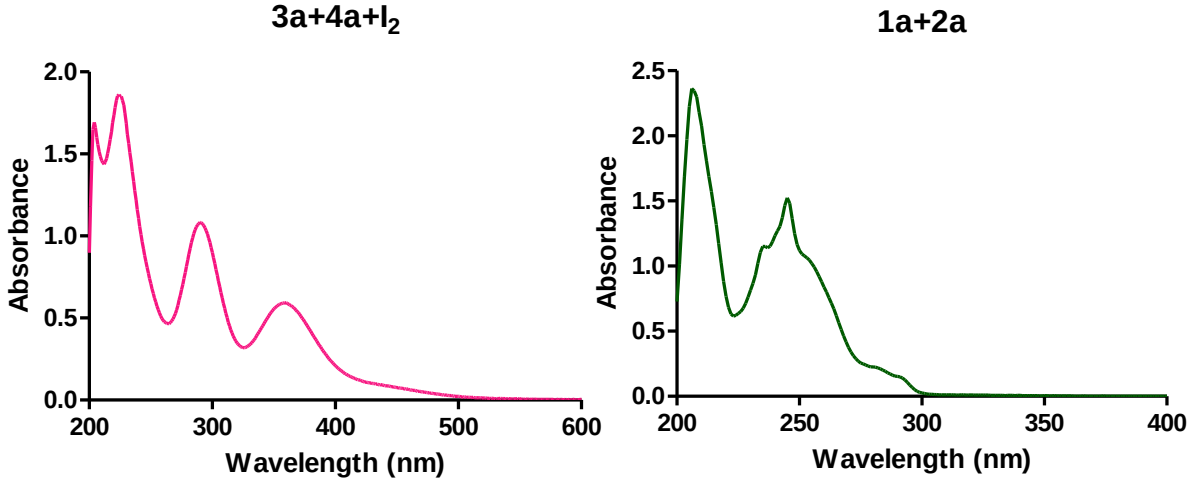


Figure S5. UV-Vis Absorption spectra mixture of both sulfone precursors **(3a, 4a)** with I_2 and mixture of **1a** and **2a**

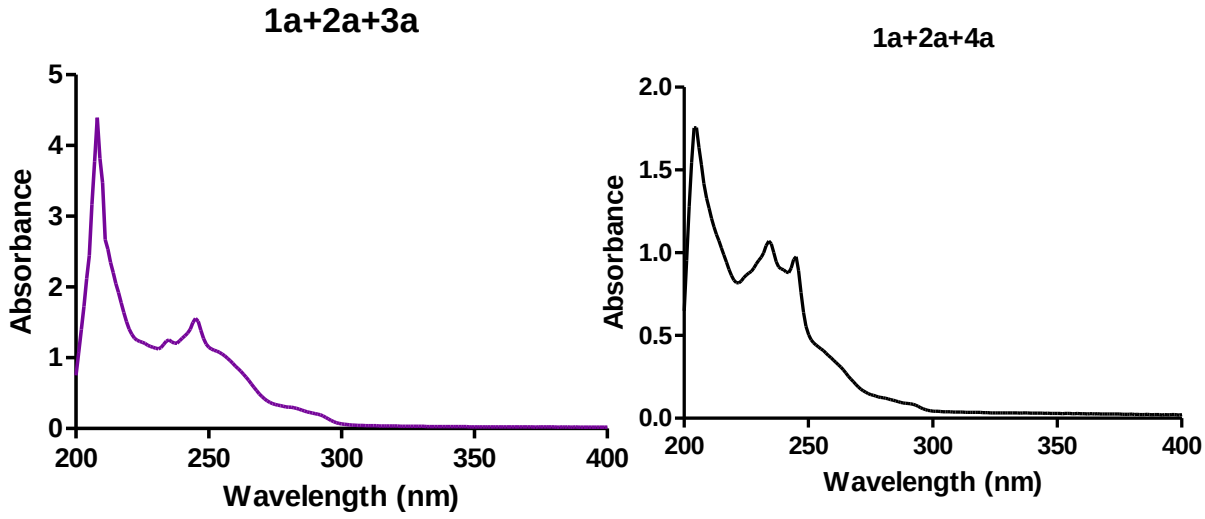


Figure S6. UV-Vis Absorption spectra mixture of **1a, 2a,** and **3a** and mixture of **1a, 2a** and **4a**

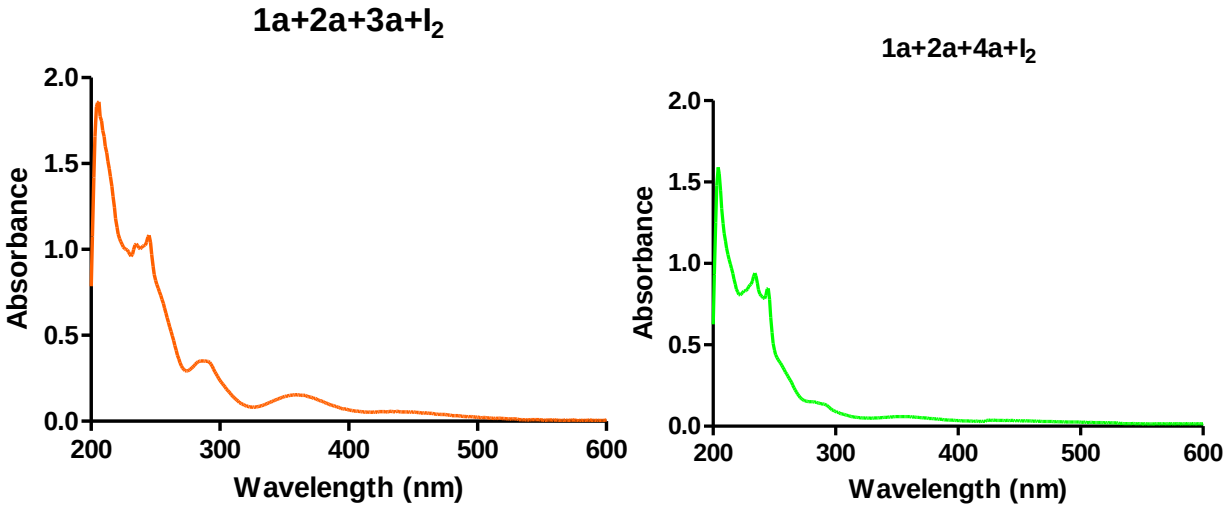


Figure S7. UV-Vis Absorption spectra mixture of **1a, 2a, 3a** and mixture of **1a, 2a, 4a** with I_2

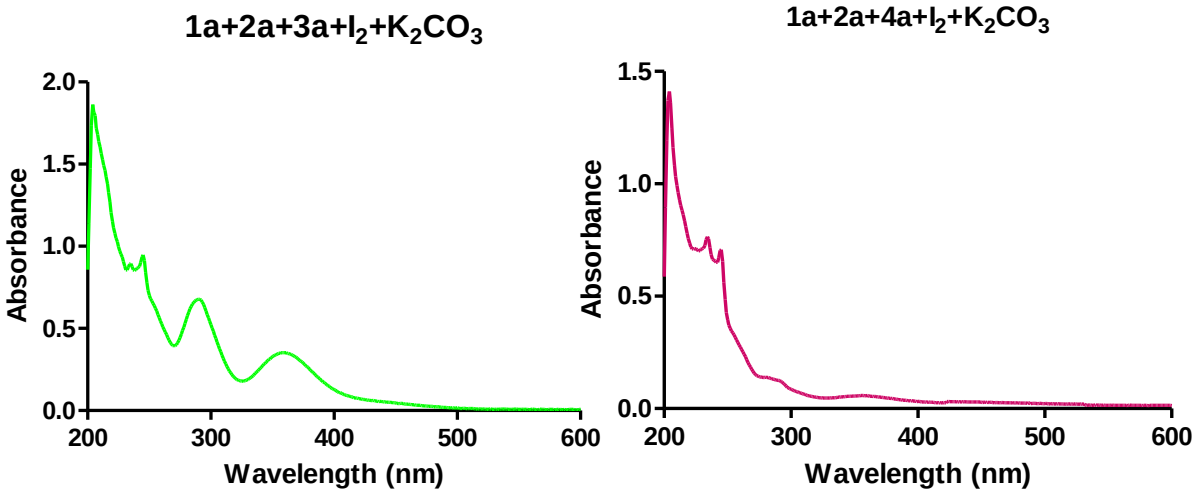


Figure S8. UV-Vis Absorption spectra mixture of **1a, 2a, 3a** and mixture of **1a, 2a, 4a** with I_2 and K_2CO_3

(5) Effect of Visible-light Irradiation: Light On/Off" Experiments

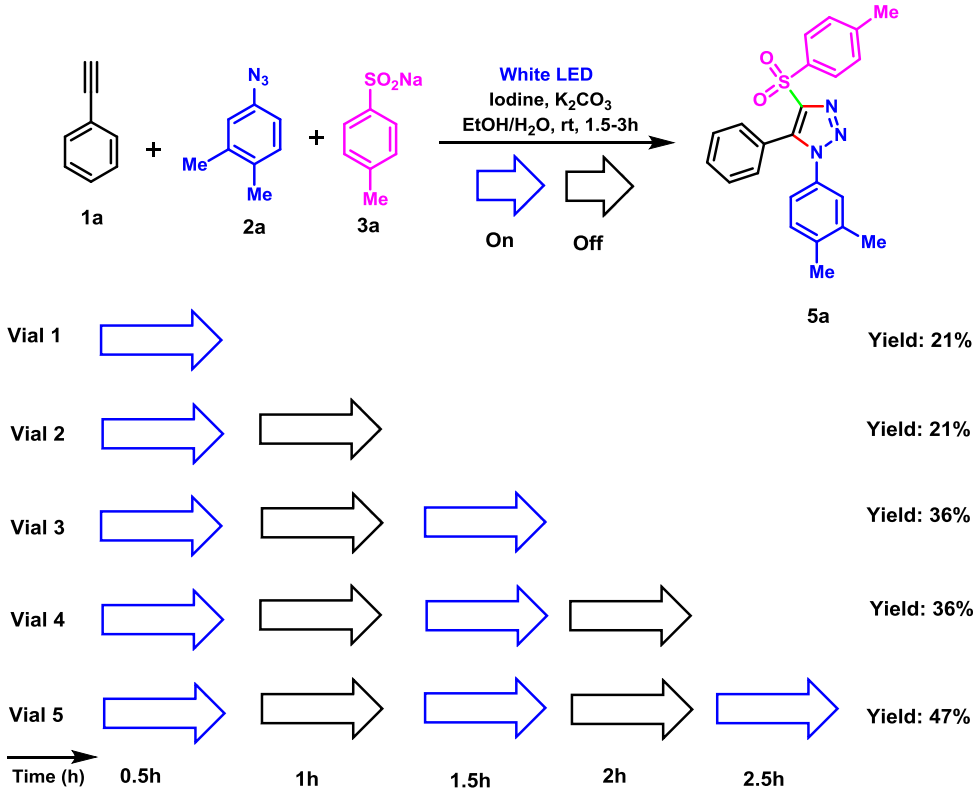


Figure S9. Visible-light Irradiation ON/OFF Experiments

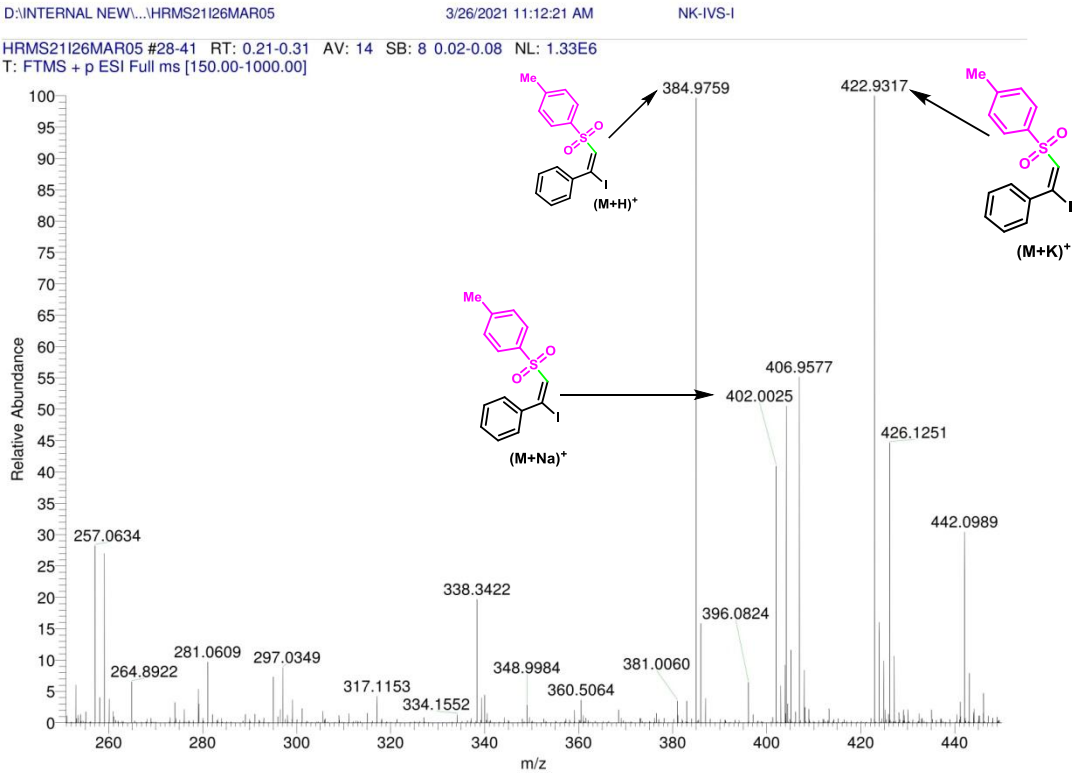


Figure S10. High Resolution Mass Spectrum of Reaction Mixture after 10min

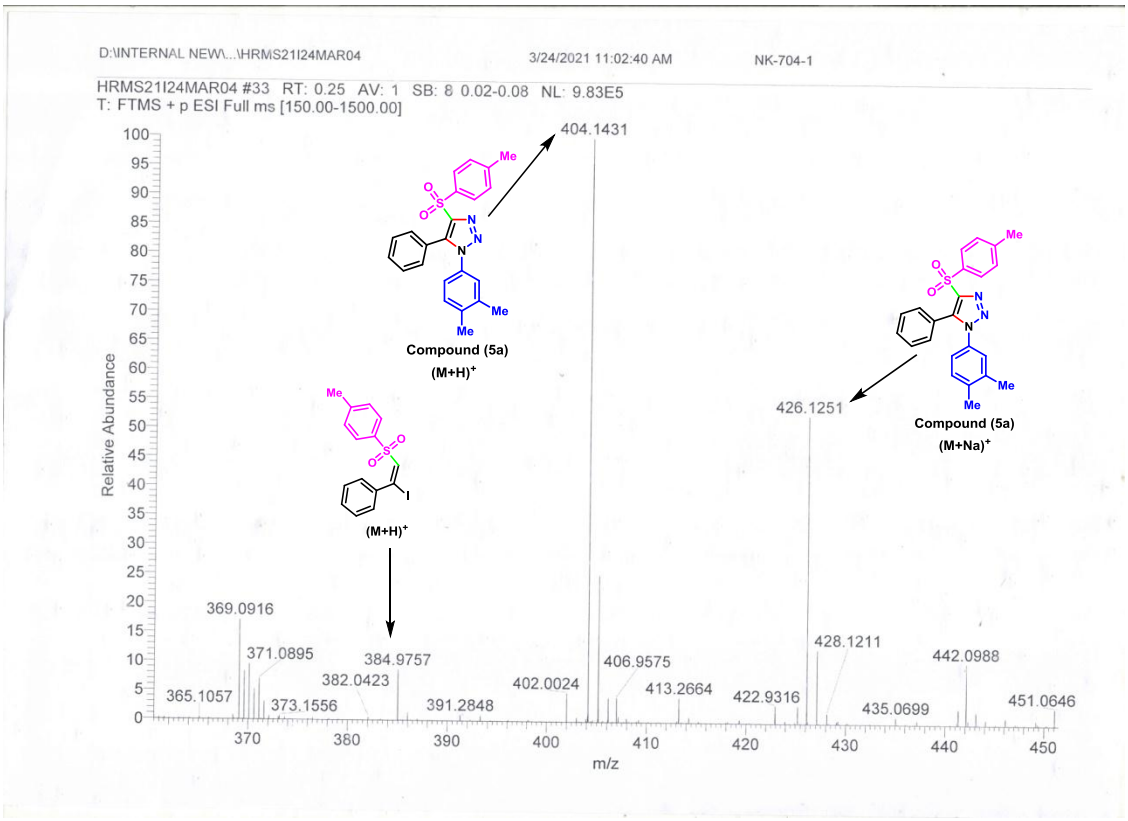


Figure S11. High Resolution Mass Spectrum of Reaction Mixture after 1h

(6) Determination of Light Flux and Quantum Yield

Determination of the light intensity at 455 nm (Blue LED)

The quantum yield was measured by standard ferrioxalate actinometry.[S1] The solutions were prepared and stored in dark room (to avoid the effect of light). A 0.15 M solution of ferrioxalate was prepared by dissolving potassium ferrioxalate hydrate (0.737 g) in H_2SO_4 (10 mL of 0.05 M solution) and buffer solution of phenanthroline was prepared by dissolving 1,10-phenanthroline (5.0 mg) and sodium acetate (1.13 g) in H_2SO_4 (5.0 mL of 0.5 M solution) were prepared.

To determine the light flux of the LED, the ferrioxalate solution (2.0 mL) was placed in a cuvette and irradiated for 10 seconds with blue LED (455 nm wavelength). After irradiation, the phenanthroline solution (0.5 mL) was added to the cuvette (1.0 cm path length) and the mixture was allowed to stir in the dark for 1 h to allow the ferrous ions to completely coordinate to the phenanthroline. The absorbance at 510 nm was measured by LABINDIA UV 3092 Spectrophotometer. A non-irradiated sample and other samples with different irradiation time (20 s) were also prepared in similar manner and the absorbance at 510 nm was recorded. Conversion was calculated using eq 1.

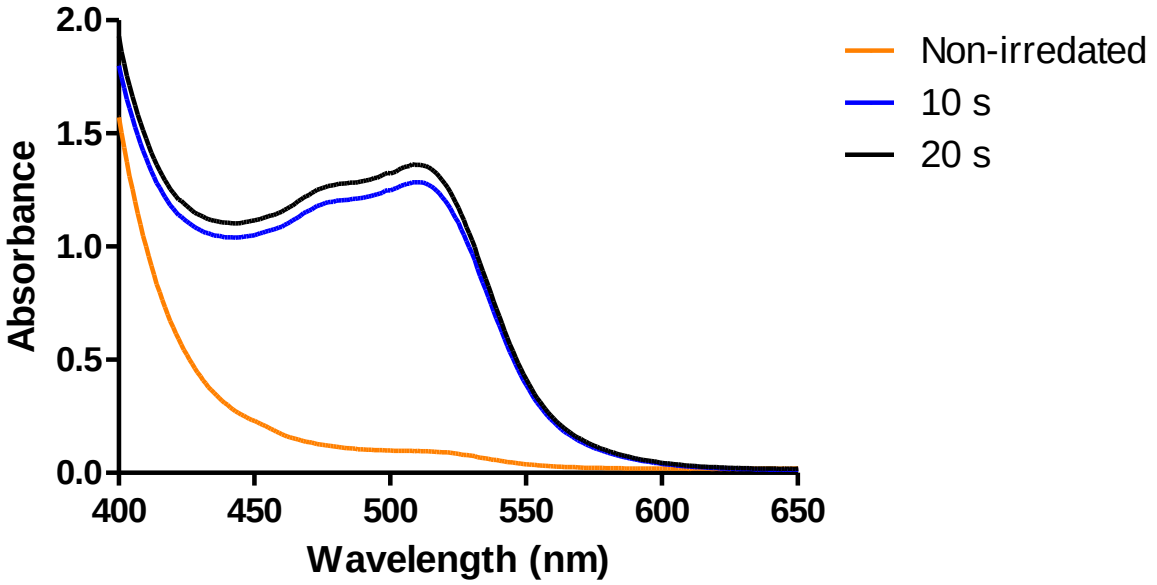


Figure S12. Absorption spectra of three irradiation experiments and non-irradiation experiment

$$mol\ of\ Fe^{2+} = \frac{V.\Delta A(510\ nm)}{l.\varepsilon} = \frac{(0.00250\ L).(1.187)}{(1.00\ cm).(11{,}100\frac{L}{mol\ cm})} = 2.6734\text{x}10^{-7}\ \text{mol} \qquad (1)$$

Where V is the total volume (0.00250 L) of the solution after addition of phenanthroline, ΔA is the difference in absorbance at 510 nm between the irradiated and non-irradiated solutions, l is the optical path length of the irradiation cell (1.0 cm), and ε is the molar absorptivity at 510 nm (11,100 L mol^{-1} cm^{-1}). The photon flux can be calculated using eq 2.

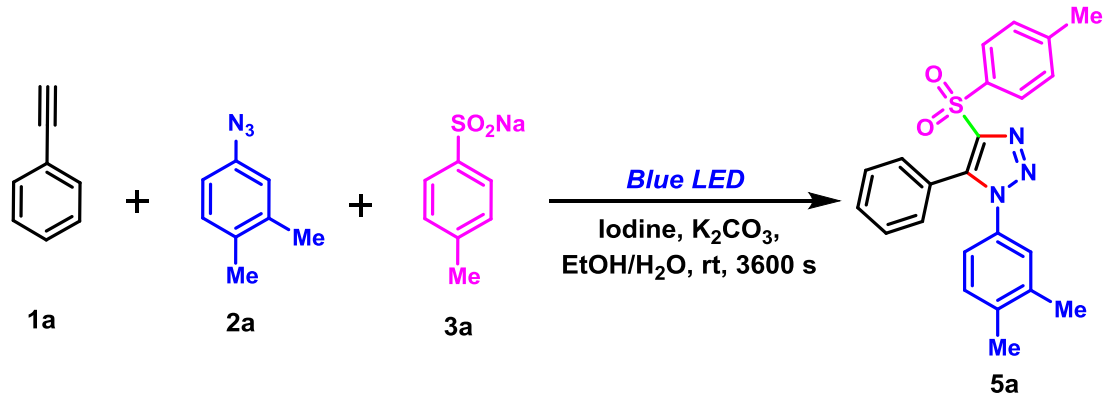
$$Photon\ flux = \frac{mol\ of\ Fe^{2+}}{\Phi.t.f} = \frac{2.6734X10^{-7}\ mol}{(1.01).(10s).(0.914)} = 2.8959\text{x}10^{-8}\ \text{einstein.s}^{-1} \qquad (2)$$

Where Φ is the quantum yield of the ferrioxalate actinometer (approximated as 1.01, which was reported for a 0.15 M solution at λ = 436 nm),[S1] t is the irradiation time, and f is the fraction of light absorbed at 455 nm (0.914). The fraction of light absorbed was determined by using eq 3.

$$f = 1\text{-}10^{-A} \qquad (3)$$

Where A is the absorbance (1.069) of the 0.15 M solution of potassium ferrioxalate at 455 nm

Determination of Quantum Yield



1a 2a 3a 5a

In a 25 mL round-bottom flask equipped with a magnetic stirring bar charged with phenylacetylene **1a** (1.0 mmol), 4-azido-1,2-dimethylbenzene **2a** (1.0 mmol), *p*-toluenesulfinic acid sodium salt **3a** (1.2 mmol), iodine (1.0 equiv) and K_2CO_3 (1.0 equiv) in ethanol/water (2 mL) were stirred with the irradiation of a blue LED (455 nm) at room temperature under open air atmosphere for consumption of starting materials (confirmed by TLC). The reaction mixture was quenched by the addition of *satd. aq* sodium thiosulfate (2 mL) and extracted three times by ethyl acetate and water. The organic layer was further dried over anhydrous sodium sulfate, and the solvent was evaporated under vacuum. The yield of product **5a** was measured to be 35 % (35×10^{-6} mol) by ^{1}H NMR analysis using CH_2Br_2 as internal standard. The reaction quantum yield (Φ) was determined using eq 4, where the light flux is 2.8959×10^{-8} einsteins.s^{-1} (determined by actinometry as described above), t is the reaction time (3600 s) and f (0.914) is the fraction of incident light determined using eq 3.

The quantum yield (Φ) was calculated by using:

$$\Phi = \frac{moles\ of\ product}{light\ flux.t.f} \qquad (4)$$

$$= \frac{35X10^{-6}mol}{(2.8959X10^{-8}einstein.s^{-1}).(3600\ s).(\ 0.914)} = 0.3673$$

The reaction quantum yield (Φ) was calculated to be 0.3673.

S1 (a) X. Li, C. Golz and M. Alcarazo, *Angew. Chem. Int. Ed*., 2021, **60**, 6943-6948. (b) C. B. Tripathi, T. Ohtani, M. T. Corbett and T. Ooi, *Chem. Sci*., 2017, **8**, 5622-5627. (c) D. Wang, F. Loose, P. J. Chirik and R. R. Knowles, *J. Am. Chem. Soc*., 2019, **141**, 4795-4799. (d) C. G. Hatchard, C. A. Parker and E. J. Bowen, *Proc. Roy. Soc. A*., 1956, **235**, 518-536. (e) M. A. Cismesia and T. P. Yoon, *Chem. Sci*., 2015, *6*, 5426-5434. (f) M. Kim, E. You, S. Park, and S. Hong, *Chem. Sci*., 2021, **12**, 6629-6637. (g) Y. Kim, K. Lee, G. R. Mathi, I. Kim, S. Hong, *Green Chem*., 2019, **21**, 2082-2087. (h) I. Kim, M. Min, D. Kang, K. Kim, and S. Hong, *Org. Lett*., 2017, **19**, 1394.

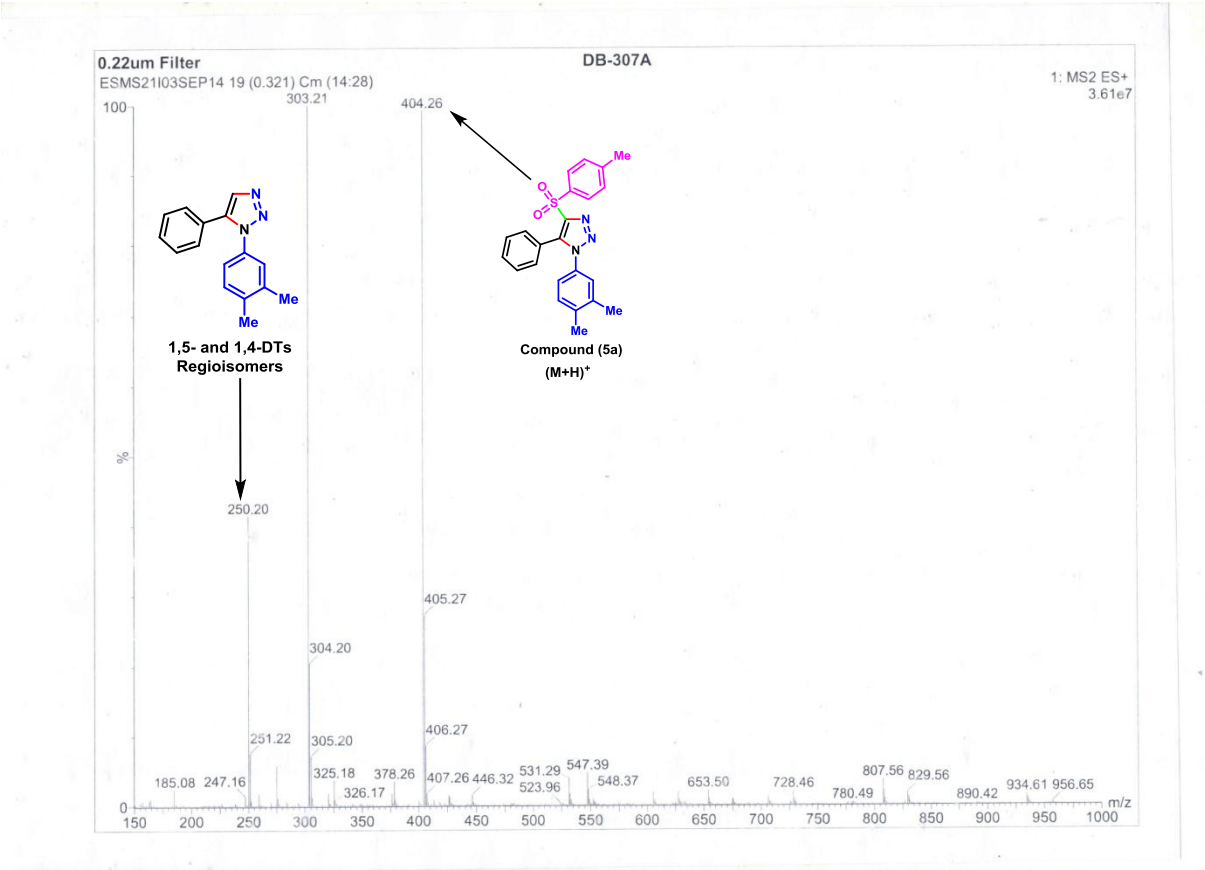


Figure S13. Mass Spectrum of Reaction Mixture under Thermal and Photo Condition

(7) Electron Spin-Resonance (ESR) spectroscopy experiments

Electron spin-resonance (ESR) spectra were recorded on a JEOL JES FA200 (X-band). The reactions were performed in glass vial (30 mL) under different conditions, then smaller fractions of the samples were transferred to the capillaries, and ESR spectra were recorded.

A mixture of iodine (0.2 mM), and DMPO (0.3 mM) in aqueous DMSO solution was irradiated without light for 5 minutes, then ESR spectrum was recorded and there was not observed signal (Fig. S14A). When the mixture of iodine (0.2 mM), and DMPO (0.3 mM) in aqueous DMSO solution was irradiated with 20W white LED for 5 minutes, and ESR spectrum was showed a new broad signal (Fig. S14B). Next, the mixture of DMPO (0.3 mM), iodine (0.2 mM), 4-methylbenzenesulfinate sodium salt (0.3 mM) (Fig. S14C), phenylacetylene (0.2 mM), and 4-azido-1,2-dimethylbenzene (0.2 mM) in aqueous DMSO solution was irradiated with 20W white LED for 5 minutes, and ESR spectrum was observed (Fig. S14D).

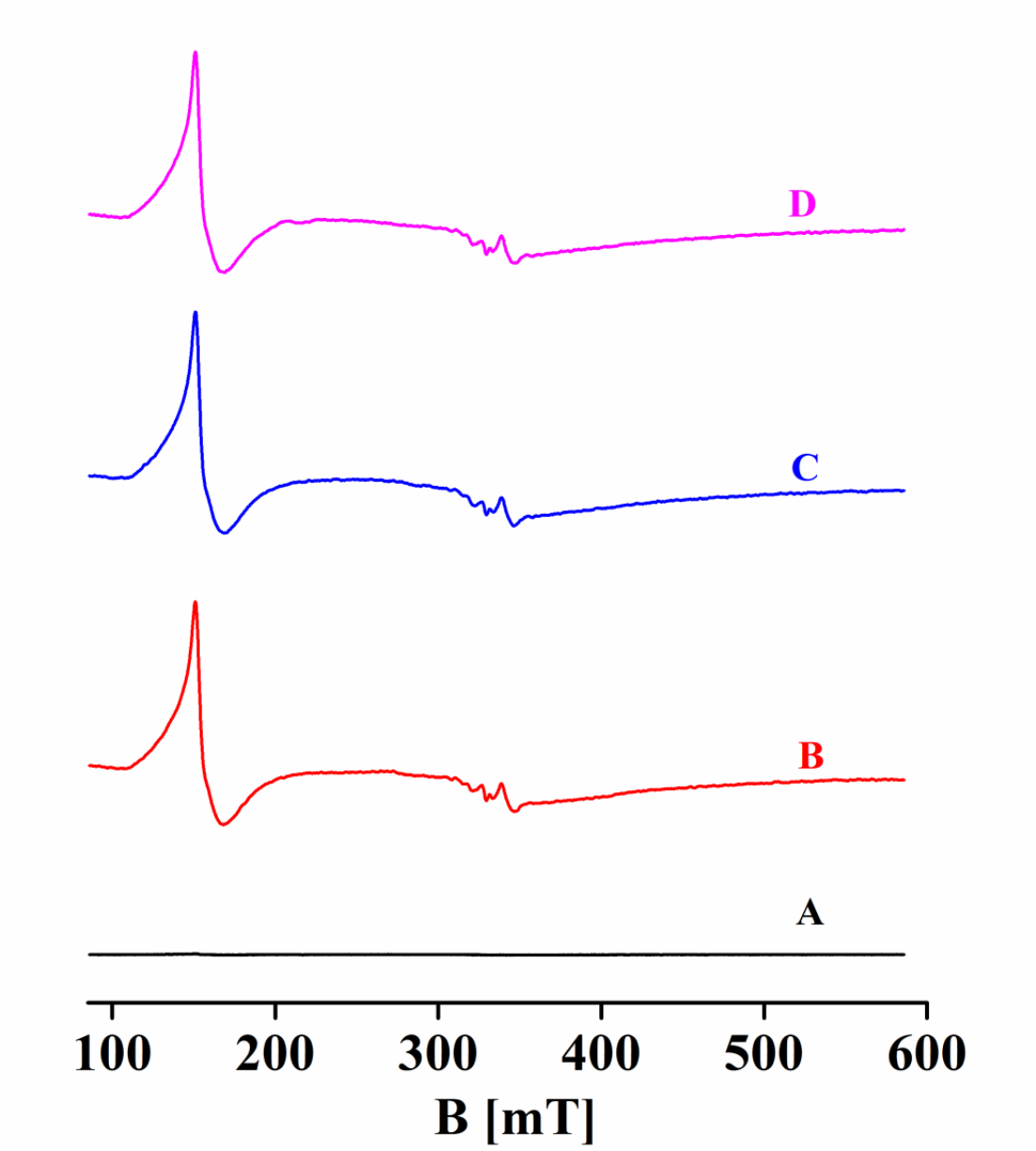
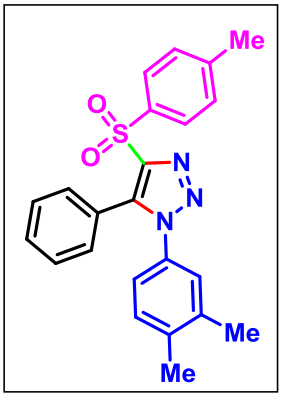


Figure S14. (A) ESR spectrum of mixture of iodine, and DMPO in aqueous DMSO solution under dark condition for 5 min. (B) ESR spectrum of mixture of iodine, and DMPO in aqueous DMSO solution under irradiation of 20 W white LED for 5 min. (C) ESR spectrum of mixture of iodine, 4-methylbenzenesulfinate sodium salt, and DMPO in aqueous DMSO solution under irradiation of 20 W white LED 5 min. (D) ESR spectrum of mixture of iodine, 4-methylbenzenesulfinate sodium salt, phenylacetylene, 4-azido-1,2-dimethylbenzene, and DMPO in aqueous DMSO solution under irradiation of 20 W white LED 5 min. ESR conditions: Frequency = 9159.993 MHz, Power = 0.995 mW, Modulation width = 2.0 mT, Centre field = 336.000 mT, Amplitude = 2.000 x 1 (modulation frequency 100 kHz), Sweep width = 2.5 x 100 mT, Sweep time = 30 sec, Time constant = 0.03 s, Temperature = -70 ^{o}C.

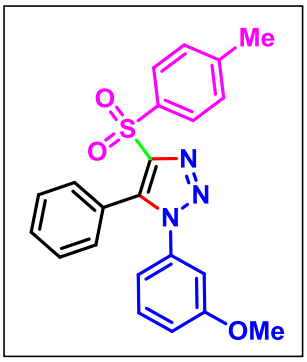
(8) Characterization Data for all the Synthesized Compounds:

1-(3,4-dimethylphenyl)-5-phenyl-4-tosyl-1*H*-1,2,3-triazole (5a):



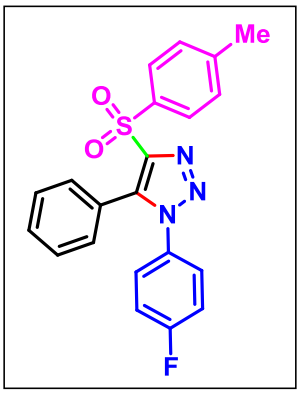
Off-white solid; yield 84% (method A) and 80% (method B); **mp:** 186-188 °C; **^{1}H NMR (400 MHz;CDCl$_3$):** δ 7.78 (d, *J* = 8.3 Hz, 2H), 7.50-7.46 (m, 1H), 7.42-7.38 (m, 2H), 7.29 (d, *J* = 2.1 Hz, 2H), 7.27 (d, *J* = 2.2 Hz, 2H), 7.09-7.05 (m, 2H), 6.86-6.83 (m, 1H), 2.42 (s, 3H), 2.25 (s, 3H), 2.20 (s, 3H); **^{13}C NMR (100 MHz; CDCl$_3$)** δ 145.9, 144.7, 138.7, 138.5, 138.1, 137.8, 133.1, 130.4, 130.3,130.2, 129.7, 128.4, 128.1, 126.0, 124.5, 122.2, 21.6, 19.6, 19.5; **IR (KBr) max** 3028, 2922, 1596, 1502, 1451, 1333, 1224, 1186, 1079, 921, 815, 700, 595; **ESI-MS (m/z)** = 404 [M+H]; **ESI-HRMS** for cald. **C$_{23}$H$_{21}$N$_3$O$_2$S;** (M+H), 404.1442; found: m/z 404.1428.

1-(3-methoxyphenyl)-5-phenyl-4-tosyl-1*H*-1,2,3-triazole (5b):



White solid; yield 82% (method A) and 79% (method B); **mp:** 171-173 °C. **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.79 (d, *J* = 8.3 Hz, 2H), 7.49 (tt, J_1 = 7.4 Hz and J_2 = 2.3 Hz, 1H), 7.44-7.40 (m, 2H), 7.31-7.29 (m, 3H), 7.27-7.26 (m, 1H), 7.24-7.22 (m, 1H), 6.95-6.92 (m, 1H), 6.79-6.76 (m, 2H), 3.68 (s, 3H), 2.42 (s, 3H); **^{13}C NMR (100 MHz, CDCl$_3$)** δ 160.0, 146.1, 144.8, 138.5, 137.6, 136.3, 130.4, 130.3, 130.0, 129.7, 128.5, 128.1, 124.4, 117.1, 115.9, 110.5, 55.4, 21.6; **IR (KBr) max** 3580, 2923, 1604, 1491, 1329, 1240, 1154, 1084, 1008, 859, 692, 602; **ESI-MS (m/z)** = 406 (M+H); **ESI-HRMS** for cald. **C$_{22}$H$_{19}$N$_3$O$_3$S;** (M+H), 406.1225; found: m/z 406.1228.

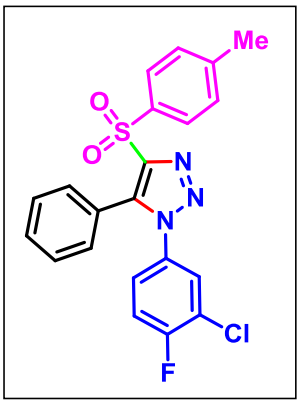
1-(4-fluorophenyl)-5-phenyl-4-tosyl-1*H*-1,2,3-triazole (5c):



Light yellow solid; yield 80% (method A) and 78% (method B); **mp:** 156-158 °C; **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.82 (dt, J_1 = 8.4 Hz and J_2 = 2.0 Hz, 2H), 7.49-7.43 (m, 2H), 7.42-7.35 (m, 3H), 7.31-7.28 (m, 4H), 7.26-7.22 (m, 1H), 7.13-7.08 (m, 1H), 2.43 (s, 3H); **^{13}C NMR (100 MHz, CDCl$_3$)** δ 163.8, 161.8, 146.2, 144.9, 138.6, 137.5, 131.5, 131.4, 130.6, 130.3, 129.8, 128.7, 128.1, 127.1, 124.1, 116.6, 116.4, 21.6; **IR (KBr) max** 3021, 2924, 1597, 1507, 1464, 1334, 1218, 1156, 999, 759, 664,541; **ESI-MS (m/z)** = 394

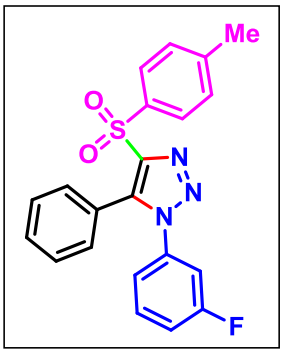
(M+H); **ESI-HRMS** for cald. **$C_{21}H_{16}FN_3O_2S$;** (M+H), 394.1025; found: m/z 394.1013.

1-(3-chloro-4-fluorophenyl)-5-phenyl-4-tosyl-1*H*-1,2,3-triazole (5d):



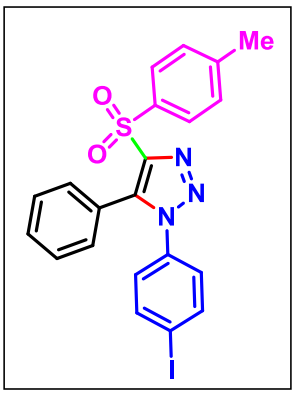
White solid; yield 78% (method A) and 75% (method B); **mp:** 152-154 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.78 (d, *J* = 8.2 Hz, 2H), 7.56-7.52 (m, 1H), 7.48-7.41 (m, 3H), 7.30-7.28 (m, 4H), 7.12 (t, *J* = 8.7 Hz, 1H), 7.07-7.04 (m, 1H), 2.42 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 159.7, 157.2, 146.3, 145.0, 138.7, 137.4, 131.8, 130.8, 130.3, 129.8, 128.8, 128.1, 127.6, 125.0, 124.9, 123.7, 122.3, 122.1, 117.4, 117.2, 21.6; **IR (KBr) max** 3021, 2922, 1597, 1500, 1333, 1266, 1155, 1080, 816, 763, 666, 595; ESI-MS (m/z) = 428 (M+H); **ESI-HRMS** for cald. **$C_{21}H_{15}FClN_3O_2S$;** (M+H), 428.0636; found: m/z 428.0632.

1-(3-fluorophenyl)-5-phenyl-4-tosyl-1*H*-1,2,3-triazole (5e):



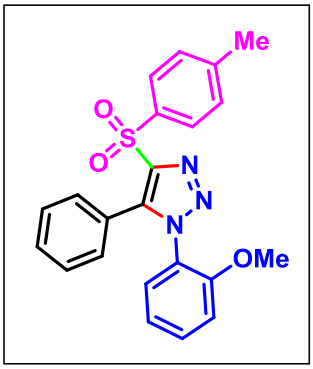
Light yellow solid; yield 80% (method A) and 77% (method B); **mp:** 154-156 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.79 (d, *J* = 8.3 Hz, 2H), 7.52 (tt, J_1 = 7.5 Hz and J_2 = 3.8 Hz, 1H), 7.46-7.42 (m, 2H), 7.37-7.33 (m, 1H), 7.31-7.28 (m, 4H), 7.16-7.11 (m, 1H), 7.05-7.00 (m, 2H), 2.42 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 163.6, 161.1, 146.3, 145.0, 138.6, 137.5, 136.5, 136.4, 130.8, 130.7, 130.3, 129.8, 128.7, 128.1, 123.9, 20.7, 117.1, 116.8, 112.9, 112.7, 21.6; **IR (KBr) max** 3021, 2923, 1605, 1491, 1335, 1216, 1155, 876, 760, 666, 599; **ESI-MS (m/z)** = 394 (M+H); **ESI-HRMS** for cald. **$C_{21}H_{16}FN_3O_2S$;** (M+H), 394.1025; found: m/z 394.1011.

1-(4-iodophenyl)-5-phenyl-4-tosyl-1*H*-1,2,3-triazole (5f):



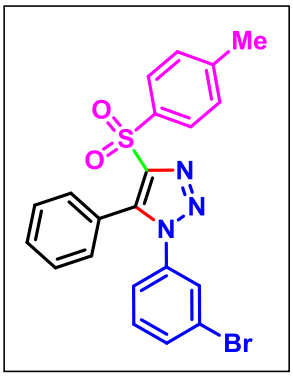
Light yellow solid; yield 78% (method A) and 76% (method B); **mp:** 184-186 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.78 (d, *J* = 8.3 Hz, 2H), 7.71-7.69 (m, 2H), 7.54-7.50 (m, 1H), 7.46-7.42 (m, 2H), 7.29-7.27 (m, 4H), 6.98 (dt, J_1 = 8.7 Hz and J_2 = 2.5 Hz, 2H), 2.42 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 146.4, 144.9, 138.6, 138.6, 138.4, 137.5, 135.1, 130.7, 130.3, 129.7, 128.7, 128.2, 126.5, 124.0, 95.6, 21.6; **IR (KBr) max** 2923, 1596, 1542, 1487, 1402, 1334, 1217, 1157, 1056, 992, 821, 700, 666, 585; **ESI-MS (m/z)** = 502 (M+H); **ESI-HRMS** for cald. **$C_{21}H_{16}IN_3O_2S$;** (M+H), 502.0086; found: m/z 502.0080.

1-(2-methoxyphenyl)-5-phenyl-4-tosyl-1*H*-1,2,3-triazole (5g):



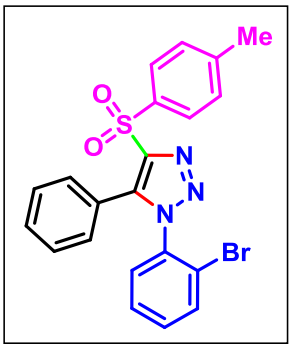
Light yellow solid; yield 75%; **mp:** 175-177 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.0 Hz, 2H), 7.43-7.27 (m, 9H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.84 (d, *J* = 8.3 Hz, 1H), 3.49 (s, 3H), 2.42 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 153.4, 145.1, 144.7, 140.4, 137.8, 132.0, 130.0, 129.8, 129.7, 128.4, 128.2, 127.9, 124.8, 124.2, 120.7, 112.1, 55.3, 21.6; **IR (KBr) max** 3583, 2923, 1602, 1504, 1465, 1331, 1155, 760, 663; **ESI-MS (m/z)** = 406 (M+H); **ESI-HRMS** for cald. **$C_{22}H_{19}N_3O_3S$;** (M+H), 406.1225; found: m/z 406.1213.

1-(3-bromophenyl)-5-phenyl-4-tosyl-1*H*-1,2,3-triazole (5h):



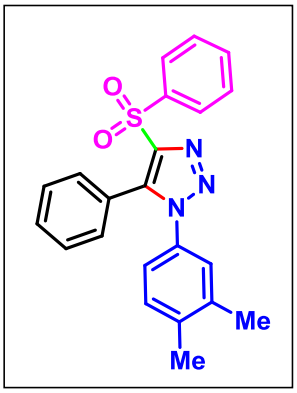
Light yellow solid; yield 70%; **mp:** 140-142 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.77 (d, *J* = 8.2 Hz, 2H), 7.55-7.51 (m, 3H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.30-7.28 (m, 4H), 7.21 (t, *J* = 8.0 Hz, 1H), 7.10-7.08 (m, 1H), 2.42 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 146.3, 145.0, 138.6, 137.5, 136.3, 132.9, 130.7, 130.6, 130.3, 129.8, 128.7, 128.1, 123.8, 123.5, 122.8, 21.6; IR (KBr) max 3020, 2923, 1588, 1478, 1333, 1218, 1156, 1083, 778, 666, 590; ESI-MS (m/z) = 454 (M+H); **ESI-HRMS** for cald. **$C_{21}H_{16}BrN_3O_2S$;** (M+H), 454.0225; found: m/z 454.0181.

1-(2-bromophenyl)-5-phenyl-4-tosyl-1*H*-1,2,3-triazole (5i):



Light yellow solid; yield 68%; **mp:** 149-151 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.83 (d, *J* = 8.3 Hz, 2H), 7.64-7.62 (m, 1H), 7.45-7.29 (m, 10H), 2.43 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 145.5, 144.9, 140.3, 137.6, 134.6, 133.7, 132.2, 130.5, 130.2, 129.8, 129.6, 128.3, 128.1, 123.6, 121.5, 21.6; **IR (KBr) max** 3020, 2923, 1597, 1482, 1447, 1333, 1217, 1156, 1082, 994, 759, 696, 666, 586; **ESI-MS (m/z)** = 454 (M+H); **ESI-HRMS** for cald. **$C_{21}H_{16}BrN_3O_2S$;** (M+H), 454.0225; found: m/z 454.0215.

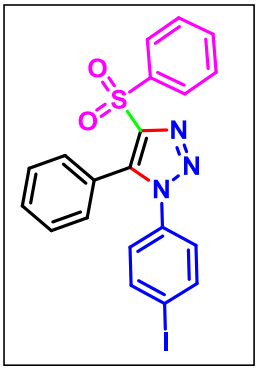
1-(3,4-dimethylphenyl)-5-phenyl-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5j):



White solid; yield 82%; **mp:** 153-155 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.91-7.88 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.50-7.46 (m, 3H), 7.42-7.39 (m, 2H), 7.29-7.26 (m, 2H), 7.10-7.06 (m, 2H), 6.86-6.83 (m, 1H), 2.25 (s, 3H), 2.20 (s, 3H); **^{13}C NMR (100 MHz,**

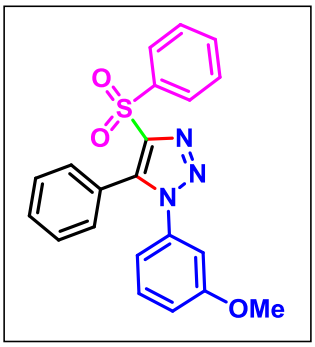
$CDCl_3$) δ 145.6, 140.7, 138.7, 138.1, 133.6, 133.0, 130.4, 130.3, 130.2, 129.0, 128.5, 128.0, 126.0, 124.4, 122.2, 19.7, 19.5; **IR (KBr) max** 3020, 2924, 1609, 1503, 1478, 1333, 1217, 1157, 1078, 995, 882, 757, 666, 562; **ESI-MS (m/z)** = 390 (M+H); **ESI-HRMS** for cald. **$C_{22}H_{19}N_3O_2S$;** (M+H), 390.1276; found: m/z 390.1276

1-(4-iodophenyl)-5-phenyl-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5k):



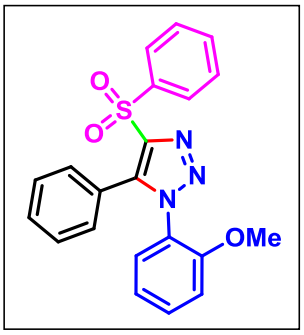
Yellow solid; yield 75%; **mp:** 154-156 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.85-7.83 (m, 2H), 7.65 (dt, J_1 = 8.7 Hz and J_2 = 2.5 Hz, 2H), 7.57-7.53 (m, 1H), 7.49-7.36 (m, 5H), 7.23-7.21 (m, 2H), 6.93 (dt, J_1 = 8.7 Hz and J_2 = 2.6 Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 146.0, 140.4, 138.7, 138.6, 135.0, 133.8, 130.7, 130.3, 129.1, 128.8, 128.1, 126.5, 123.9, 95.6; **IR (KBr) max** 3064, 2923, 1607, 1485, 1402, 1331, 1222, 1158, 1056, 992, 825, 753, 687, 664; **ESI-MS (m/z)** = 487 (M+H); **ESI-HRMS** for cald. **$C_{20}H_{14}IN_3O_2S$;** (M+H), 487.9929; found: m/z 487.9933.

1-(3-methoxyphenyl)-5-phenyl-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5l):



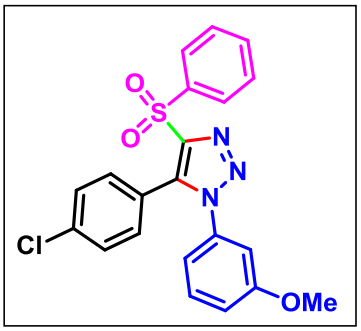
White solid; yield 79%; **mp:** 131-133 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.92-7.89 (m, 2H), 7.61 (tt, J_1 = 7.4 Hz and J_2 = 1.5 Hz, 1H), 7.52-7.47 (m, 3H), 7.44-7.40 (m, 2H), 7.31-7.28 (m, 2H), 7.27-7.22 (m, 1H), 6.95-692 (m, 1H), 6.79-6.77 (m, 2H), 3.8 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.0, 145.8, 140.5, 138.7, 136.2, 133.7, 130.5, 130.3, 130.1, 129.1, 128.6, 128.1, 124.3, 117.1, 115.9, 110.5, 55.4; **IR (KBr) max** 2924, 1606, 1491, 1329, 1240, 1156, 1084, 1007, 859, 768, 613; **ESI-MS (m/z)** = 392 (M+H); **ESI-HRMS** for cald. **$C_{21}H_{17}N_3O_3S$;** (M+H), 392.1069; found: m/z 392.1064.

1-(2-methoxyphenyl)-5-phenyl-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5m):



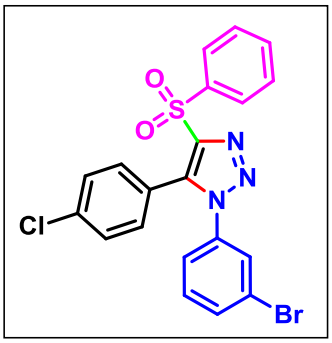
Light yellow solid; yield 70%; **mp:** 147-149 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.95-7.93 (m, 2H), 7.63-7.59 (m, 1H), 7.50 (t, J = 8.0 Hz, 2H), 7.44-7.37 (m, 3H), 7.36-7.28 (m, 4H), 7.04-7.00 (m, 1H), 6.85 (d, J = 8.3 Hz, 1H), 3.50 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 153.3, 144.7, 140.7, 133.6, 132.1, 130.1, 129.7, 129.0, 128.4, 128.1, 127.9, 124.6, 124.2, 120.8, 112.1, 55.3; **IR (KBr) max** 3016, 2927, 1602, 1504, 1469, 1330, 1285, 1253, 1158, 1087,996, 757, 688, 592; **ESI-MS (m/z)** = 392 (M+H); **ESI-HRMS** for cald. **$C_{21}H_{17}N_3O_3S$;** (M+H), 392.1069; found: m/z 392.1064.

5-(4-chlorophenyl)-1-(3-methoxyphenyl)-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5n):



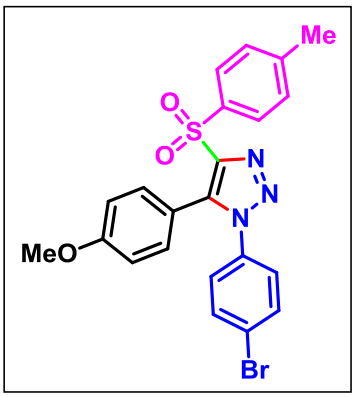
White solid; yield 73%; **mp:** 197-199 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.95-7.93 (m, 2H), 7.63 (tt, J_1 = 7.4 Hz and J_2 = 4.3 Hz, 1H), 7.54-7.50 (m, 2H), 7.41 (dt, J_1 = 8.6 Hz and J_2 = 2.3 Hz, 2H), 7.27-7.24 (m, 3H), 6.98-6.95 (m, 1H), 6.81 (t, J = 2.2 Hz, 1H), 6.75-6.72 (m, 1H), 3.74 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.2, 145.9, 140.3, 137.6, 137.0, 136.0, 133.9, 131.7, 130.2, 129.2, 129.0, 128.1, 122.7, 117.2, 116.0, 110.8, 55.5; **IR (KBr) max** 3582, 2922, 1606, 1473, 1329, 1240, 1157, 1090, 858, 759, 666; **ESI-MS (m/z)** = 426 (M+H); **ESI-HRMS** for cald. **$C_{21}H_{16}ClN_3O_3S$;** (M+H), 426.0679; found: m/z 426.0675.

1-(3-bromophenyl)-5-(4-chlorophenyl)-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5o):



Off-white solid; yield 74%; **mp:** 188-190 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.94-7.92 (m, 2H), 7.64 (tt, J_1 = 7.4 Hz and J_2 = 3.0 Hz, 1H), 7.60-7.58 (m, 1H), 7.55-7.51 (m, 3H), 7.44 (dt, J_1 = 8.6 Hz and J_2 = 2.4 Hz, 2H), 7.27-7.23 (m, 3H), 7.08-7.05 (m, 1H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 146.2, 140.2, 137.7, 137.3, 136.1, 134.0, 133.2, 131.7, 130.7, 129.2, 128.3, 128.1, 123.6, 123.1, 122.2; **IR (KBr) max** 3070, 2921, 2104, 1585, 1477, 1332, 1224, 1159, 1091, 999, 874, 758, 684, 595; **ESI-MS (m/z)** = 473 (M+H); **ESI-HRMS** for cald. **$C_{20}H_{13}ClBrN_3O_2S$;** (M+H), 473.9678; found: m/z 473.9662.

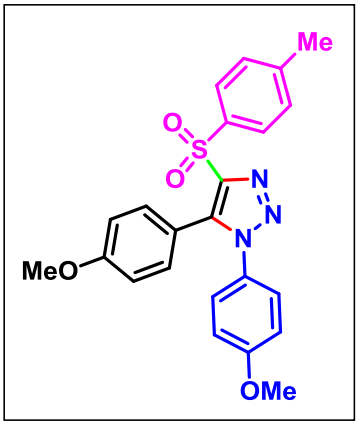
1-(4-bromophenyl)-5-(4-methoxyphenyl)-4-tosyl-1*H*-1,2,3-triazole (5p):



White solid; yield 72%; **mp:** 167-169 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.80 (d, J = 8.2 Hz, 2H), 7.52 (dt, J_1 = 8.8 Hz and J_2 = 4.8 Hz, 2H), 7.47 (dt, J_1 = 8.8 Hz and J_2 = 3.0 Hz, 1H), 7.29 (d, J = 8.0 Hz, 1H), 7.22 (dt, J_1 = 8.8 Hz and J_2 = 2.8 Hz, 2H), 7.13 (dt, J_1 = 6.8 Hz and J_2 = 4.8 Hz, 2H), 6.96-6.93 (m, 2H), 3.88 (s, 3H), 2.42 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.3, 146.0, 144.9, 138.5, 137.6, 134.5, 132.6, 131.8, 129.7, 128.1, 126.5, 123.8, 115.6, 114.3, 55.3, 21.6; **IR (KBr) max**

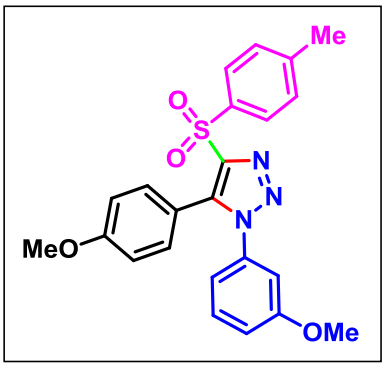
2922, 1610, 1490, 1401, 1331, 1296, 1255, 1156, 1064, 992, 833, 752, 668; **ESI-MS (m/z)** = 484 (M+H); **ESI-HRMS** for cald. **$C_{22}H_{18}BrN_3O_3S$;** (M+H), 484.0340; found: m/z 484.0318.

1,5-bis(4-methoxyphenyl)-4-tosyl-1*H*-1,2,3-triazole (5q):



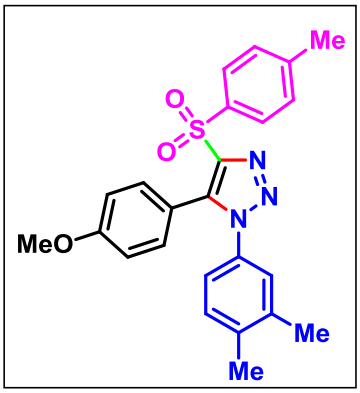
Light yellow solid; yield 78%; **mp:** 130-132 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.79 (d, *J* = 8.1 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 8.6 Hz, 2H), 7.15 (d, *J* = 8.9 Hz, 2H), 6.91 (d, *J* = 8.7 Hz, 2H), 6.86 (d, *J* = 8.9 Hz, 2H), 3.85 (s, 3H), 3.80 (s, 3H), 2.41 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.0, 160.3, 145.5, 144.7, 138.5, 137.8, 131.9, 129.7, 128.4, 128.1, 126.5, 116.1, 114.4, 114.0, 55.5, 55.3, 21.6; **IR (KBr) max** 3020, 2933, 2843, 1610, 1513, 1492, 1331, 1255, 1156, 1032, 835, 757, 669, 584; **ESI-MS (m/z)** = 436 (M+H); **ESI-HRMS** for cald. **$C_{23}H_{21}N_3O_4S$;** (M+H), 436.1331; found: m/z 436.1312.

1-(3-methoxyphenyl)-5-(4-methoxyphenyl)-4-tosyl-1*H*-1,2,3-triazole (5r):



White solid; yield 74%; **mp:** 151-153 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.80 (d, *J* = 8.2 Hz, 2H), 7.30-7.23 (m, 5H), 6.96-6.92 (m, 3H), 6.83-6.82 (m, 1H), 6.76 (d, *J* = 7.8 Hz, 1H), 3.87 (m, 3H), 3.72 (m, 3H), 2.42 (m, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.1, 160.1, 145.7, 144.7, 138.5, 137.7, 136.4, 131.8, 130.0, 129.7, 128.1, 117.2, 116.0, 115.8, 114.1, 110.7, 55.4, 55.3, 21.6; **IR (KBr) max** 2923, 1608, 1490, 1329, 1295, 1252, 1154, 1085, 1034, 839, 751, 666, 603; **ESI-MS (m/z)** = 436 (M+H); **ESI-HRMS** for cald. **$C_{23}H_{21}N_3O_4S$;** (M+H), 436.1331; found: m/z 436.1324.

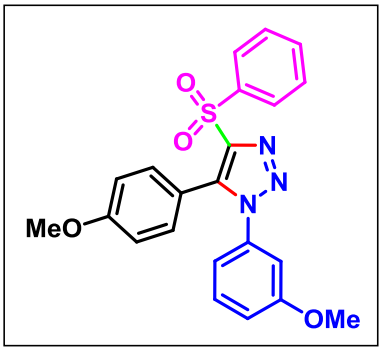
1-(3,4-dimethylphenyl)-5-(4-methoxyphenyl)-4-tosyl-1*H*-1,2,3-triazole (5s):



White solid; yield 83%; **mp:**189-191 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.79 (d, *J* = 8.2 Hz, 2H), 7.29 (d, *J* = 6.3 Hz, 2H), 7.23 (d, *J* = 8.7 Hz, 2H), 7.11-7.07 (m, 2H), 6.91 (d, *J* = 8.7 Hz, 2H), 6.86-6.83 (m, 1H), 3.86 (s, 3H), 2.42 (s, 3H), 2.26 (s, 3H), 2.22 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.0, 145.5, 144.6, 138.6, 138.4, 138.1, 137.9, 133.2, 131.9, 130.2, 129.7, 128.1, 126.1, 122.3, 116.2, 114.0, 55.3, 21.6, 19.7, 19.5; **IR (KBr) max** 3782, 3019, 2924, 2111, 1612, 1493, 1456,

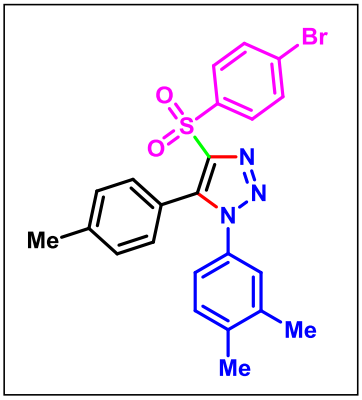
1332, 1296, 1218, 1181, 1154, 1078, 882, 757, 669, 595, 540; **ESI-MS (m/z)** = 434 (M+H); **ESI-HRMS** for cald. **$C_{24}H_{23}N_3O_3S$;** (M+H), 434.1538; found: m/z 434.1530.

1-(3-methoxyphenyl)-5-(4-methoxyphenyl)-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5t):



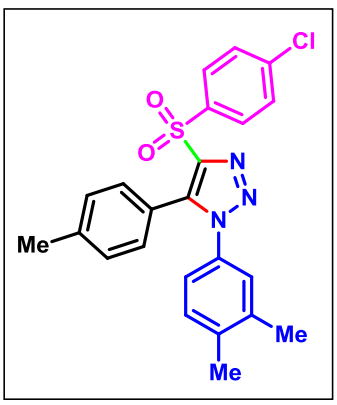
Light yellow solid; yield 80%; **mp:** 144-146 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.91 (d, *J* = 7.4 Hz, 2H), 7.59 (t, *J* = 6.8 Hz, 1H), 7.48 (t, *J* = 7.4 Hz, 2H), 7.25-7.21 (m, 3H), 6.93-6.91 (m, 3H), 6.82-6.75 (m, 2H), 3.85 (s, 3H), 3.71 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.2, 160.1, 145.4, 140.6, 138.8, 136.3, 133.7, 131.8, 130.1, 129.1, 128.0, 117.2, 115.9, 115.8, 114.1, 110.7, 55.5, 55.3; **IR (KBr) max** 2926, 1609, 1490, 1328, 1252, 1156, 1084, 856, 752, 687, 612; **ESI-MS (m/z)** = 422 (M+H); **ESI-HRMS** for cald. **$C_{22}H_{19}N_3O_4S$;** (M+H), 422.1174; found: m/z 422.1165.

4-((4-bromophenyl)sulfonyl)-1-(3,4-dimethylphenyl)-5-(*p*-tolyl)-1*H*-1,2,3-triazole (5u):



White solid; yield 81 %; **mp**: 188-190 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.73 (d, *J* = 8.5 Hz, 2H), 7.59 (d, *J* = 8.5 Hz, 2H), 7.19 (d, *J* = 7.9 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.09 (s, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 6.82 (d, *J* = 7.9 Hz, 1H), 2.39 (s, 3H), 2.23 (s, 3H), 2.20 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 145.0, 140.8, 139.7, 139.0, 138.7, 138.1, 133.0, 132.3, 130.2, 129.6, 129.3, 129.0, 126.1, 122.2, 121.1, 21.5, 19.7, 19.5; **IR (KBr) max** 3395, 2921, 1640, 1384, 1090, 1024, 834, 745, 662; **ESI-MS (m/z)** = 484 [M+H]; Analysis cald. for **$C_{23}H_{20}BrN_3O_2S$**: C, 57.27; H, 4.18; N, 8.71; Found: C, 57.20; H, 4.21; N, 8.70; **ESI-HRMS** for cald. **$C_{23}H_{20}BrN_3O_2S$**; **(M+H),** 484.0517; found: m/z 484.0516.

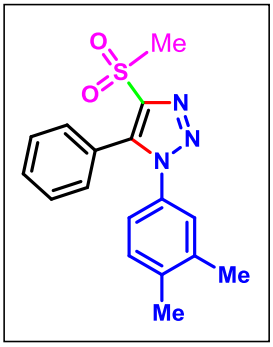
4-((4-chlorophenyl)sulfonyl)-1-(3,4-dimethylphenyl)-5-(*p*-tolyl)-1*H*-1,2,3-triazole (5v):



Off-white solid; yield 80 %; **mp**: 202-204 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 8.6 Hz, 2H), 7.42 (d, *J* = 8.6 Hz, 2H), 7.19 (d, *J* = 7.9 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.09 (s, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 6.82 (d, *J* = 7.9 Hz, 1H), 2.38 (s,

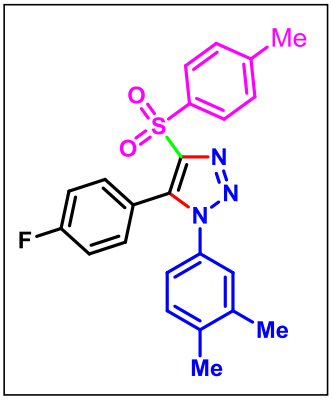
3H), 2.23 (s, 3H), 2.19 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 145.1, 140.8, 140.4, 139.2, 139.0, 138.7, 138.1, 133.0, 130.2, 129.6, 129.3, 126.1, 122.2, 121.1, 21.5, 19.7, 19.5; **IR (KBr) max** 3389, 2921, 1638, 1384, 1090, 758; **ESI-MS (m/z)** = 438 [M+H]; Analysis cald. for **$C_{23}H_{20}ClN_3O_2S$**: C, 63.08; H, 4.60; N, 9.60; Found: C, 63.10; H, 4.55; N, 9.63; **ESI-HRMS** for cald. **$C_{23}H_{20}ClN_3O_2S$**; **(M+H),** 438.1042; found: m/z 438.1039.

1-(3,4-dimethylphenyl)-4-(methylsulfonyl)-5-phenyl-1*H*-1,2,3-triazole (5w):



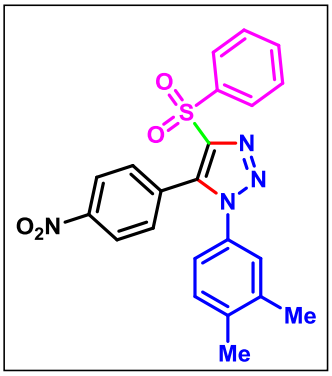
Light yellow oil; yield 75 %; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.44-7.39 (m, 1H), 7.39-7.34 (m, 4H), 7.12 (s, 1H), 7.09 (d, *J* = 8.0 Hz, 1H), 6.90-6.87 (m, 1H), 3.27 (s, 3H), 2.25 (s, 3H), 2.21 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 144.9, 138.9, 138.3, 138.2, 133.0, 130.5, 130.3, 128.6, 126.2, 124.0, 122.4, 43.5, 19.7, 19.5; **IR (KBr) max** 3398, 2925, 1638, 1384, 1145, 770, 697, 543; **ESI-MS (m/z)** = 328 [M+H]; Analysis cald. for **$C_{17}H_{17}N_3O_2S$**: C, 62.37; H, 5.23; N, 12.83; Found: C, 62.40; H, 5.30; N, 12.80; **ESI-HRMS** for cald. **$C_{17}H_{17}N_3O_2S$**; **(M+H),** 328.1119; found: m/z 328.1109.

1-(3,4-dimethylphenyl)-5-(4-fluorophenyl)-4-tosyl-1*H*-1,2,3-triazole (5x):



White solid; yield 78 %; **mp**: 143-145 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.77 (d, *J* = 8.2 Hz, 2H), 7.29-7.26 (m, 4H), 7.11-7.05 (m, 4H), 6.83-6.80 (m, 1H), 2.40 (s, 3H), 2.24 (s, 3H), 2.19 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 165.0, 162.4, 146.0, 144.9, 138.9, 138.3, 137.6, 137.5, 132.9, 132.6, 132.5, 130.3, 129.8, 128.1, 126.1, 122.3, 120.5, 120.4, 116.0, 115.7, 21.6, 19.7, 19.5; **IR (KBr) max** 3398, 2923, 1608, 1491, 1385, 1332, 1232, 1154, 1086, 827, 760, 674, 595; **ESI-MS (m/z)** = 422 [M+H]; Analysis cald. for **$C_{23}H_{20}FN_3O_2S$**: C, 65.54; H, 4.78; N, 9.97; Found: C, 65.60; H, 4.71; N, 9.91; **ESI-HRMS** for cald. **$C_{23}H_{20}FN_3O_2S$**; **(M+H),** 422.1334; found: m/z 422.1331.

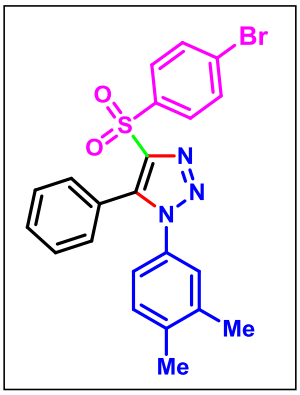
1-(3,4-dimethylphenyl)-5-(4-nitrophenyl)-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5y):



Off-white solid; yield 63 %; **mp**: 252-254 °C; **^{1}H NMR (400 MHz, DMSO-d_6)** δ 8.27 (d, *J* = 8.8 Hz, 2H), 7.87 (d, *J* = 8.6 Hz, 2H), 7.76 (t, *J* = 7.4 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 2H), 7.65 (t, *J* = 7.9 Hz, 2H), 7.33 (s, 1H), 7.16 (d, *J* = 8.1 Hz, 1H), 7.11-7.09 (m,

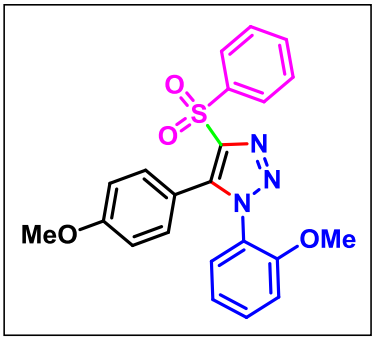
1H), 2.19 (s, 3H), 2.16 (s, 3H); **^{13}C NMR (100 MHz, DMSO-*d*$_6$)** δ 148.4, 144.8, 139.9, 139.0, 137.8, 137.6, 134.3, 132.3, 132.2, 131.1, 130.0, 129.6, 127.5, 126.8, 123.2, 123.1, 19.1, 18.9; **IR (KBr) max** 3397, 2921, 1640, 1523, 1341, 1090, 757, 606; **ESI-MS (m/z)** = 435 [M+H]; Analysis cald. for **$C_{22}H_{18}N_4O_4S$**: C, 60.82; H, 4.18; N, 12.90; Found: C, 60.80; H, 4.25; N, 12.88; **ESI-HRMS** for cald. **$C_{22}H_{18}N_4O_4S$**; **(M+H),** 435.1127; found: m/z 435.1123.

4-((4-bromophenyl)sulfonyl)-1-(3,4-dimethylphenyl)-5-phenyl-1*H*-1,2,3-triazole (5z):



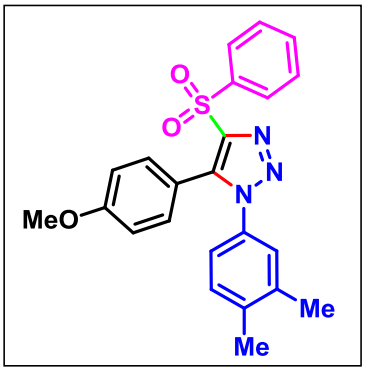
White solid; yield 84 %; **mp**: 177-179 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.73-7.70 (m, 2H), 7.60-7.57 (m, 2H), 7.49-7.45 (m, 1H), 7.41-7.37 (m, 2H), 7.27-7.24 (m, 2H), 7.07 (s, 1H), 7.05 (d, *J* = 8.1 Hz, 1H), 6.84-6.82 (m, 1H), 2.23 (s, 3H), 2.18 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 145.2, 139.6, 138.8, 138.2, 132.9, 132.4, 130.5, 130.3, 130.2, 129.6, 129.1, 128.5, 126.0, 124.2, 122.1, 19.7, 19.5; **IR (KBr) max** 3378, 1573, 1386, 1336, 1156, 1070, 822, 759, 698, 616; **ESI-MS (m/z)** = 470 [M+H]; Analysis cald. for **$C_{22}H_{18}BrN_3O_2S$**: C, 56.42; H, 3.87; N, 8.97; Found: C, 56.50; H, 3.80; N, 8.91; **ESI-HRMS** for cald. **$C_{22}H_{18}BrN_3O_2S$**; **(M+H),** 470.0361; found: m/z 470.0352.

1-(2-methoxyphenyl)-5-(4-methoxyphenyl)-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5aa):



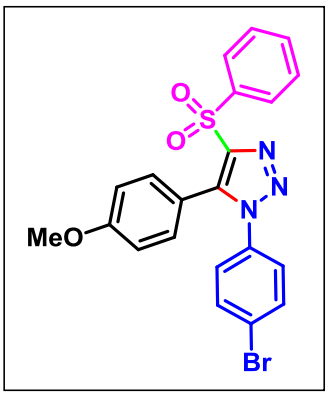
Light yellow solid; yield 72%; **mp:** 166-168 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.94-7.92 (m, 2H), 7.60 (t, *J* = 7.3 Hz, 1H), 7.49 (t, *J* = 7.9 Hz, 2H), 7.44-7.39 (m, 1H), 7.34-7.32 (m, 1H), 7.21-7.19 (m, 2H), 7.03-6.99 (m, 1H), 6.88-6.83 (m, 3H), 3.81 (s, 3H), 3.52 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.8, 153.5, 144.4, 140.8, 140.7, 133.6, 132.0, 131.2, 129.1, 129.0, 128.5, 128.0, 124.3, 120.8, 116.4, 113.5, 112.2, 55.5, 55.2; **IR (KBr) max** 3017, 2939, 2842, 1609, 1495, 1329, 1291, 1254, 1158, 1087, 836, 761, 666, 631, 560; **ESI-MS (m/z)** = 422 (M+H); **ESI-HRMS** for cald. **$C_{22}H_{19}N_3O_4S$;** (M+H), 422.1174; found: m/z 422.1162.

1-(3,4-dimethylphenyl)-5-(4-methoxyphenyl)-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5ab):



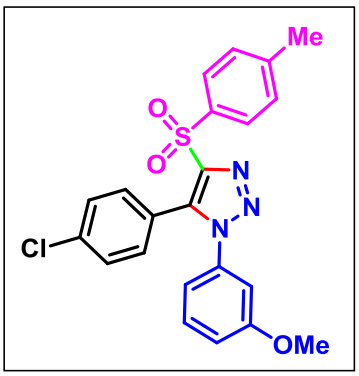
Light yellow solid; yield 79%; **mp:**148-150 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.91 (d, *J* = 7.6 Hz, 2H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.22 (d, *J* = 8.7 Hz, 2H), 7.09 (t, *J* = 9.1 Hz, 2H), 6.91 (d, *J* = 8.7 Hz, 2H), 6.85 (d, *J* = 7.8 Hz, 1H), 3.86 (s, 3H), 2.26 (s, 3H), 2.22 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.0, 145.2, 140.7, 138.7, 138.6, 138.1, 133.6, 133.1, 131.8, 130.2, 129.0, 127.9, 126.1, 122.3, 116.0, 114.0, 55.3, 19.7, 19.5; **IR (KBr) max** 3020, 2923, 1612, 1492, 1331, 1254, 1157, 1077, 882, 761, 666, 602; **ESI-MS (m/z)** = 420 (M+H); **ESI-HRMS** for cald. **$C_{23}H_{21}N_3O_3S$;** (M+H), 420.1382; found: m/z 420.1365.

1-(4-bromophenyl)-5-(4-methoxyphenyl)-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5ac):



White solid; yield 70%; **mp:** 154-156 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.93-7.90 (m, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.54-7.48 (m, 4H), 7.23-7.20 (m, 2H), 7.14-7.12 (m, 2H), 6.96-6.94 (m, 2H), 3.88 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.3, 145.6, 140.5, 138.7, 134.4, 133.8, 132.6, 131.8, 129.1, 128.0, 126.5, 123.9, 115.4, 114.3, 55.3; **IR (KBr) max** 3782, 2922, 1611, 1489, 1331, 1255, 1158, 1065, 993, 833, 722, 687, 589; **ESI-MS (m/z)** = 470 (M+H); **ESI-HRMS** for cald. **$C_{21}H_{16}BrN_3O_3S$;** (M+H), 470.0174; found: m/z 470.0166.

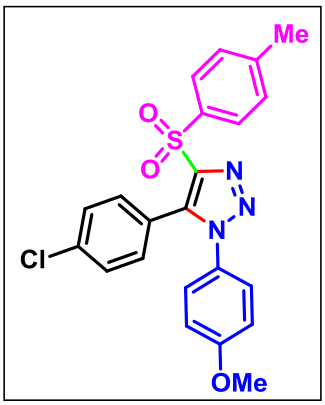
5-(4-chlorophenyl)-1-(3-methoxyphenyl)-4-tosyl-1*H*-1,2,3-triazole (5ad):



Off-white solid; yield 71%; **mp:** 160-162 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 7.1 Hz, 2H), 7.41 (d, *J* = 7.5 Hz, 2H), 7.33-7.25 (m, 5H), 6.97 (d, *J* = 7.9 Hz, 1H), 6.81 (s, 1H), 6.73 (d, *J* = 7.7 Hz, 1H), 3.73 (s, 3H), 2.43 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.2, 146.2, 145.1, 137.4, 136.9, 136.0, 131.7, 130.2, 129.8, 128.9, 128.1, 122.8, 117.2, 115.9, 110.9, 55.5, 21.6; **IR (KBr) max** 3582, 2922, 1605, 1470, 1330, 1241,

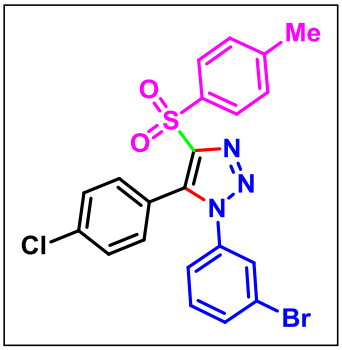
1155, 1090, 1042, 859, 750, 664, 590; **ESI-MS (m/z)** = 440 (M+H); **ESI-HRMS** for cald. **$C_{22}H_{18}ClN_3O_3S$;** (M+H), 440.0835; found: m/z 440.0831.

5-(4-chlorophenyl)-1-(4-methoxyphenyl)-4-tosyl-1*H*-1,2,3-triazole (5ae):



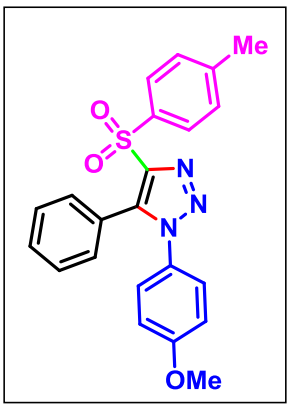
Light yellow solid; yield 72%; **mp:** 162-164 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 7.6 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 7.5 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 7.6 Hz, 2H), 6.88 (d, *J* = 7.6 Hz, 2H), 3.81 (s, 3H), 2.43 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.5, 146.0, 145.0, 137.5, 137.4, 136.8, 131.8, 131.7, 129.8, 128.9, 128.1, 127.9, 126.6, 122.9, 114.6, 55.5, 21.6; **IR (KBr) max** 3020, 2923, 1602, 1513, 1474, 1332, 1255, 1157, 1093, 834, 759, 668, 580; **ESI-MS (m/z)** = 440 (M+H); **ESI-HRMS** for cald. **$C_{22}H_{18}ClN_3O_3S$;** (M+H), 440.0835; found: m/z 440.0828.

1-(3-bromophenyl)-5-(4-chlorophenyl)-4-tosyl-1*H*-1,2,3-triazole (5af):



White solid; yield 69%; **mp:** 184-186 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 8.3 Hz, 2H), 7.60-7.57 (m, 1H), 7.54-7.53 (m, 1H), 7.45-7.42 (m, 2H), 7.32 (d, *J* = 7.9 Hz, 2H), 7.27-7.26 (m, 1H), 7.25-7.23 (m, 2H), 7.07-7.04 (m, 1H), 2.44 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 146.4, 145.2, 137.5, 137.2, 136.1, 133.2, 131.7, 130.7, 129.9, 129.1, 128.3, 128.1, 123.6, 123.0, 122.3, 21.7; **IR (KBr) max** 2923, 1590, 1477, 1439, 1334, 1218, 1156, 1017, 874, 759, 668, 590; **ESI-MS (m/z)** = 487 (M+H); **ESI-HRMS** for cald. **$C_{21}H_{15}ClBrN_3O_2S$;** (M+H), 387.9835; found: m/z 387.9816.

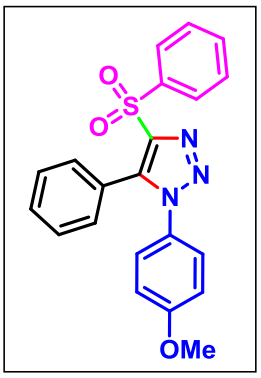
1-(4-methoxyphenyl)-5-phenyl-4-tosyl-1*H*-1,2,3-triazole (5ag):



Light Yellow solid; yield 79%; **mp:** 183-185 °C. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.78 (d, *J* = 8.3 Hz, 2H), 7.46 (tt, J_1 = 7.4 Hz and J_2 = 1.2 Hz, 1H), 7.42-7.38 (m, 2H), 7.29-7.27 (m, 4H), 7.14 (dt, J_1 = 9.0 Hz and J_2 = 3.3 Hz, 2H), 6.85 (dt, J_1 = 9.0 Hz and J_2 = 3.2 Hz, 2H), 3.80 (s, 3H), 2.42 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.3, 145.9, 144.8, 138.5, 137.7, 130.4, 130.3, 129.7, 128.5, 128.3, 128.1, 126.5, 124.4, 114.4, 55.5, 21.6; **IR (KBr) max** 3584, 2922, 2359, 1513, 1156, 1079, 921, 810, 705, 596; **ESI-MS (m/z)** = 406

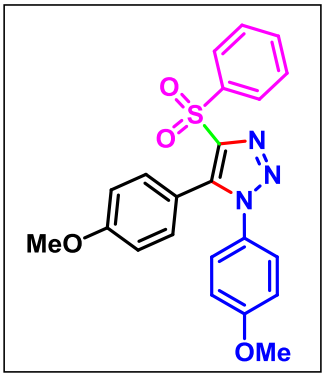
[M+H]; Analysis cald. for **$C_{22}H_{19}N_3O_3S$:** C, 65.17; H, 4.72; N, 10.36; Found: C, 65.20; H, 4.75; N, 10.38; **ESI-HRMS** for cald. **$C_{22}H_{19}N_3O_3S$**; **(M+H)**, 406.1225; found: m/z 406.1210.

1-(4-methoxyphenyl)-5-phenyl-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5ah):



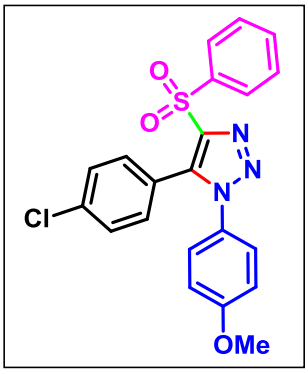
White solid; yield 79%; **mp:** 151-153 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.91-7.89 (m, 2H), 7.60 (tt, J_1 = 7.5 Hz and J_2 = 1.1 Hz, 1H), 7.50-746 (m, 3H), 7.43-7.39 (m, 2H), 7.30-7.28 (m, 1H), 7.27-7.26 (m, 1H), 7.15 (dt, J_1 = 9.0 Hz and J_2 = 2.1 Hz, 2H), 6.85 (dt, J_1 = 9.0 Hz and J_2 = 2.2 Hz, 2H), 3.80 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.4, 145.5, 140.6, 138.8, 133.7, 130.4, 130.3, 129.1, 128.5, 128.1, 128.0, 126.5, 124.3, 114.5, 55.5; **IR (KBr) max** 2924, 1607, 1513, 1448, 1329, 1255, 1159, 1072, 836, 765, 684, 664,583; **ESI-MS (m/z)** = 392 M+H]; Analysis cald. for **$C_{21}H_{17}N_3O_3S$**: C, 64.44; H, 4.38; N, 10.73; Found: C, 64.50; H, 4.35; N, 10.75; **ESI-HRMS** for cald. **$C_{21}H_{17}N_3O_3S$**; **(M+H)**, 392.1069; found: m/z 392.1058.

1,5-bis(4-methoxyphenyl)-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5ai):



Light yellow solid; yield 78%; **mp:**156-158 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.93-7.91 (m, 2H), 7.60 (t, J = 7.4 Hz, 1H), 7.49 (t, J = 7.9 Hz, 2H), 7.22 (d, J = 8.8 Hz, 2H), 7.16 (d, J = 9.0 Hz, 2H), 6.92 (d, J = 8.8 Hz, 2H), 6.87 (d, J = 9.0 Hz, 2H), 3.86 (s, 3H), 3.82 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 161.0, 160.3, 145.2, 140.7, 138.7, 133.6, 131.9, 129.0, 128.4, 128.0, 126.5, 116.0, 114.5, 114.1, 55.5, 55.3; **IR (KBr) max** 3782, 3020, 1610, 1513, 1330, 1255, 1161, 1073, 835, 758, 666; **ESI-MS (m/z)** = 422 [M+H]; Analysis cald. for **$C_{22}H_{19}N_3O_4S$**: C, 62.70; H, 4.54; N, 9.97; Found: C, 62.74; H, 4.50; N, 9.92; **ESI-HRMS** for cald. **$C_{22}H_{19}N_3O_4S$**; **(M+H),** 422.1174; found: m/z 422.1166.

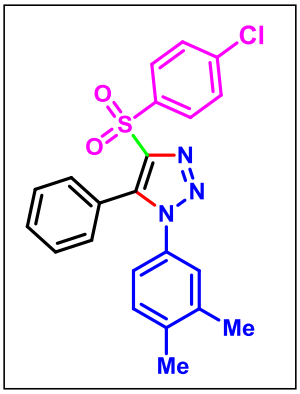
5-(4-chlorophenyl)-1-(4-methoxyphenyl)-4-(phenylsulfonyl)-1*H*-1,2,3-triazole (5aj):



Off-white solid; yield 73%; **mp**: 195-197 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.95-7.93 (m, 2H), 7.65-7.61 (m, 1H), 7.54-7.50 (m, 2H), 7.42-7.38 (m, 2H), 7.26-7.22 (m, 2H), 7.15-7.12 (m, 2H), 6.90.6.87 (m, 2H), 3.82 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 160.6, 145.7, 140.4, 137.6, 136.9, 133.8, 131.7, 129.2, 129.0, 128.1, 127.9, 126.5, 122.8, 114.6, 55.5; **IR (KBr) max** 3582, 1605, 1512,

1474, 1329, 1255, 1159, 1091, 1024, 834, 745, 662; **ESI-MS (m/z)** = 426 [M+H]; Analysis cald. for **$C_{21}H_{16}ClN_3O_3S$**: C, 59.22; H, 3.79; N, 9.87; Found: C, 59.20; H, 3.75; N, 9.90; **ESI-HRMS** for cald. **$C_{21}H_{16}ClN_3O_3S$**; **(M+H),** 426.0679; found: m/z 426.0656.

4-((4-chlorophenyl)sulfonyl)-1-(3,4-dimethylphenyl)-5-phenyl-1*H*-1,2,3-triazole (5ak):



White solid; yield 80 %; **mp**: 178-180 °C; **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81-7.77 (m, 2H), 7.49-7.44 (m, 1H), 7.43-7.37 (m, 4H), 7.27-7.25 (m, 2H), 7.07 (s, 1H), 7.05 (d, *J* = 8.1 Hz, 1H), 6.84-6.82 (m, 1H), 2.22 (s, 3H), 2.18 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 145.2, 140.4, 139.1, 138.8, 138.2, 132.9, 130.5, 130.3, 130.2, 129.5, 129.4, 128.5, 126.0, 124.2, 122.2, 19.7, 19.5; **IR (KBr) max** 3378, 1386, 1336, 1157, 1085, 766, 699, 626; **ESI-MS (m/z)** = 424 [M+H]; Analysis cald. for **$C_{22}H_{18}ClN_3O_2S$**: C, 62.33; H, 4.28; N, 9.91; Found: C, 62.30; H, 4.24; N, 9.98; **ESI-HRMS** for cald. **$C_{22}H_{18}ClN_3O_2S$**; **(M+H),** 424.0886; found: m/z 424.0879.

(9) NMR-Spectra of Compounds

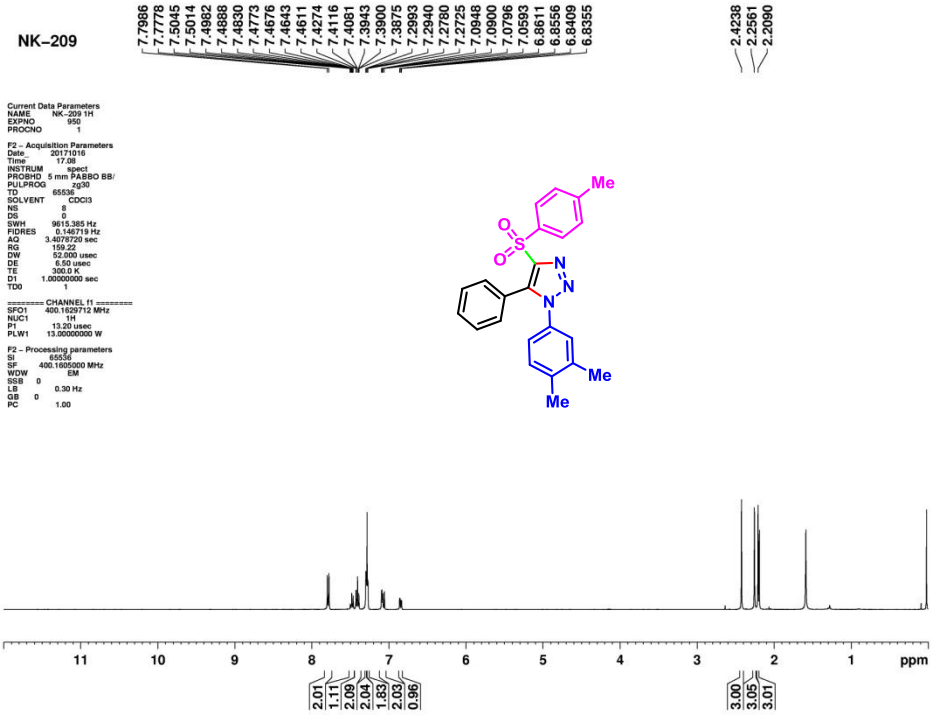


Figure S12: ^{1}H NMR of compound (5a)

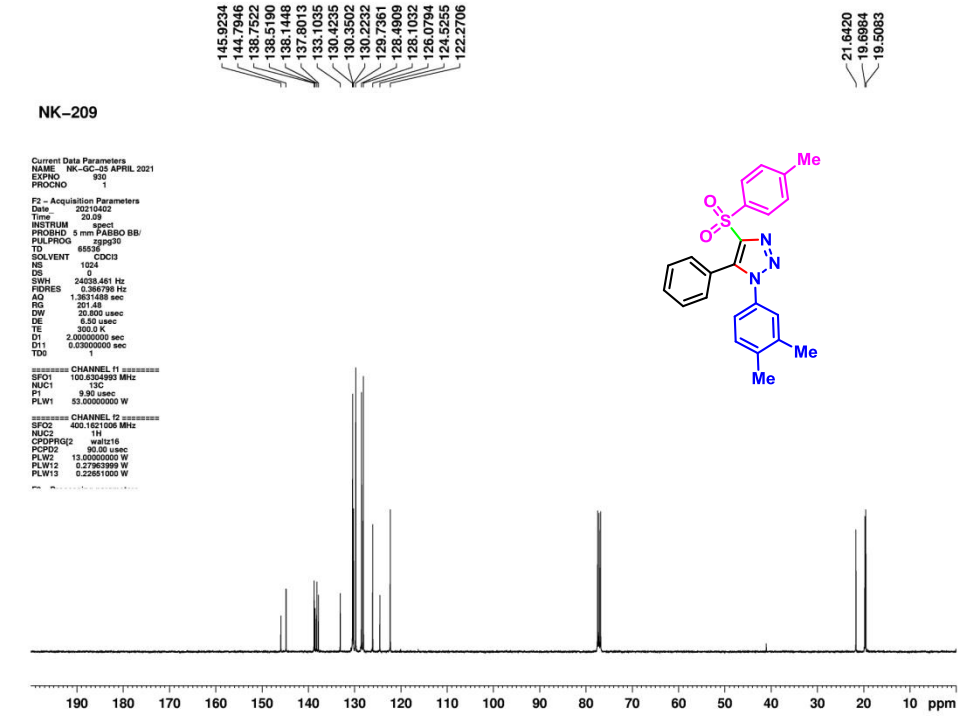


Figure S13: ^{13}C NMR of compound (5a)

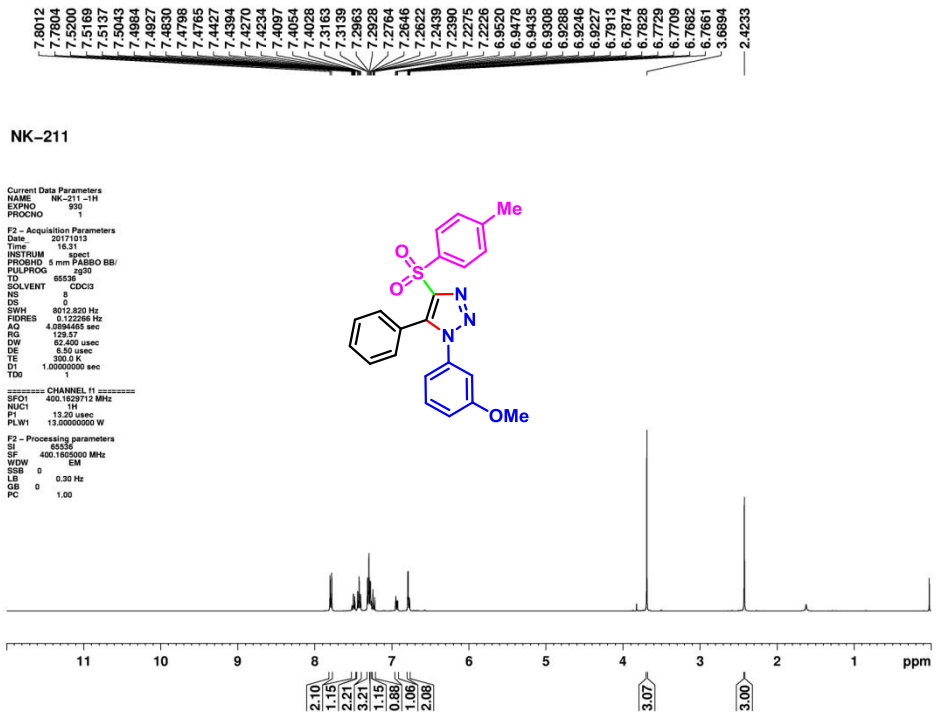


Figure S14: ^{1}H NMR of compound (5b)

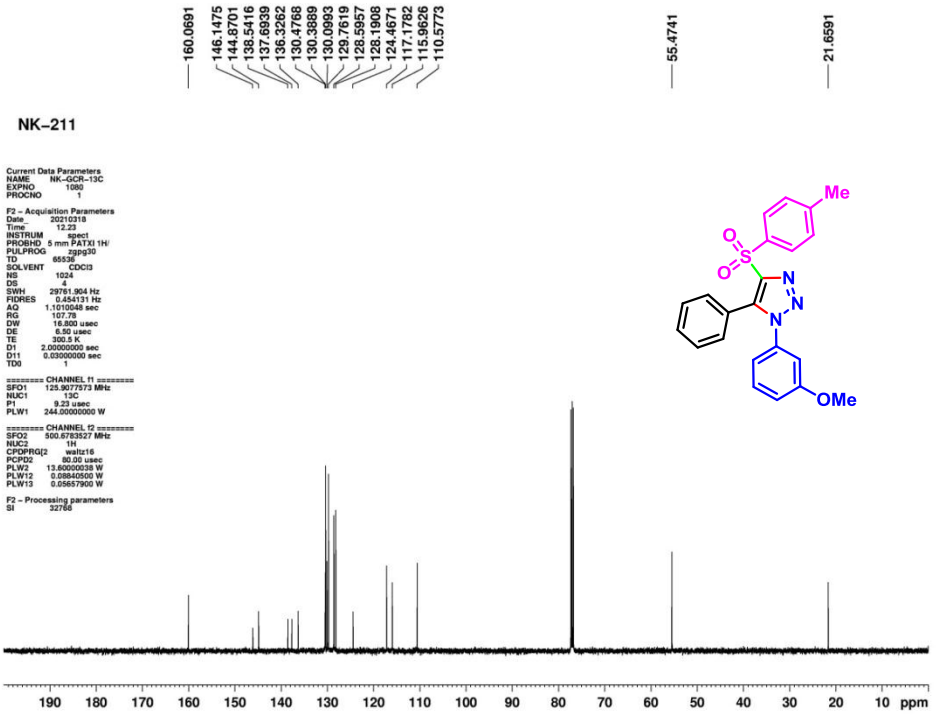


Figure S15: ^{13}C NMR of compound (5b)

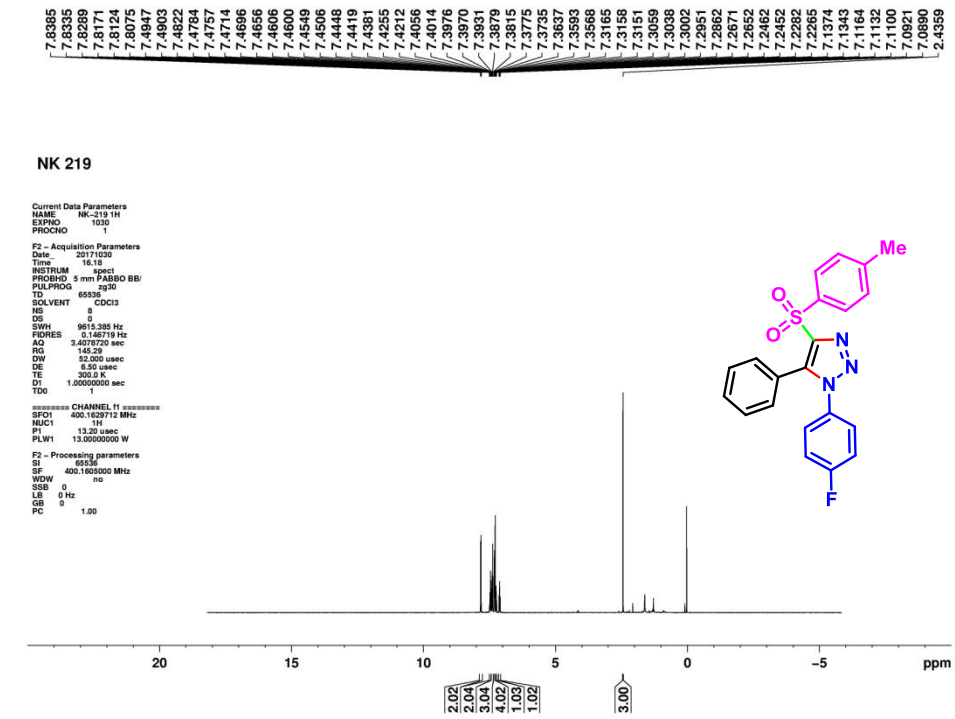


Figure S16: ^{1}H NMR of compound (5c)

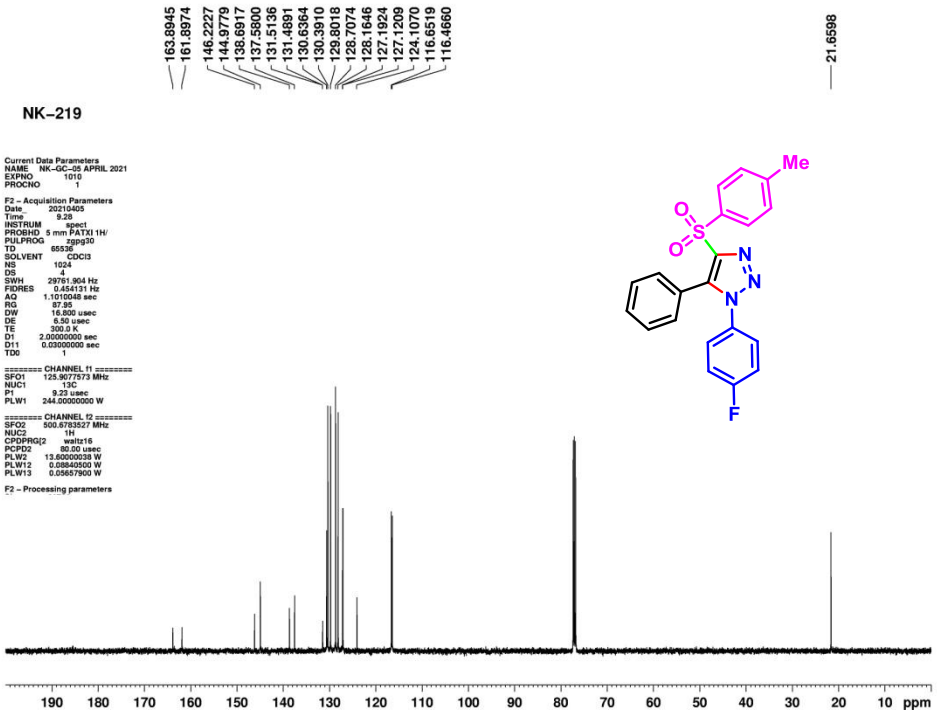


Figure S17: ^{13}C NMR of compound (5c)

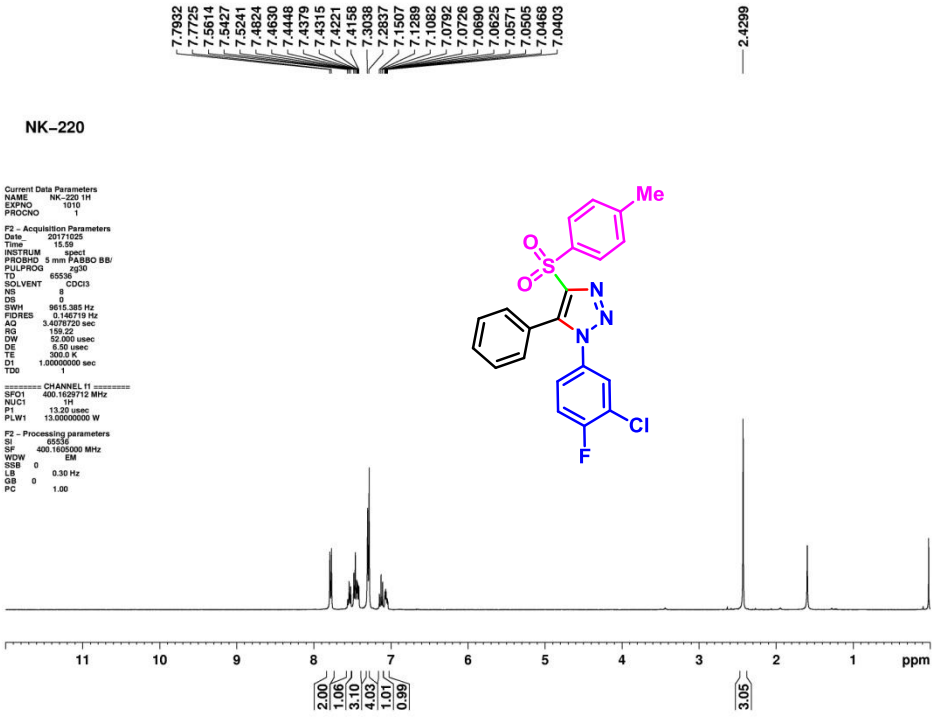


Figure S18: ^{1}H NMR of compound (5d)

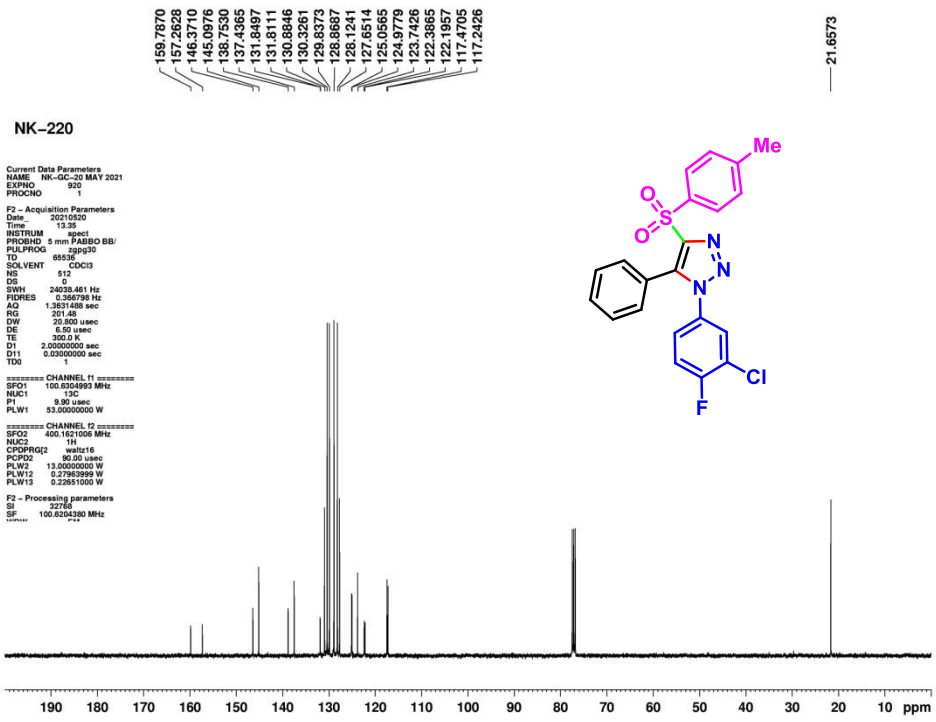


Figure S19:^{13}C NMR of compound (5d)

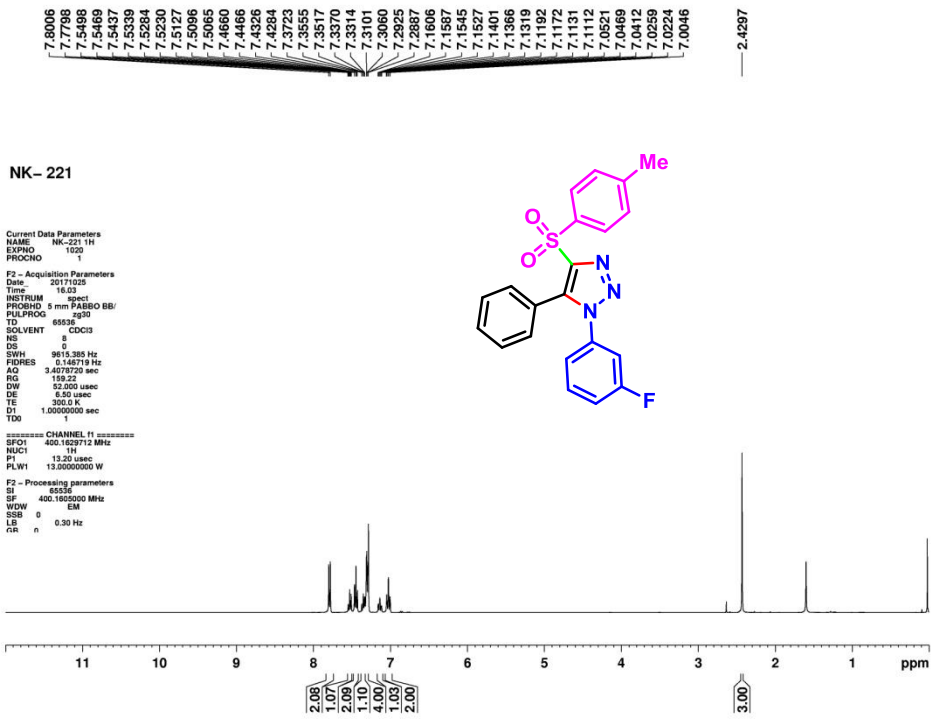


Figure S20: ^{1}H NMR of compound (5e)

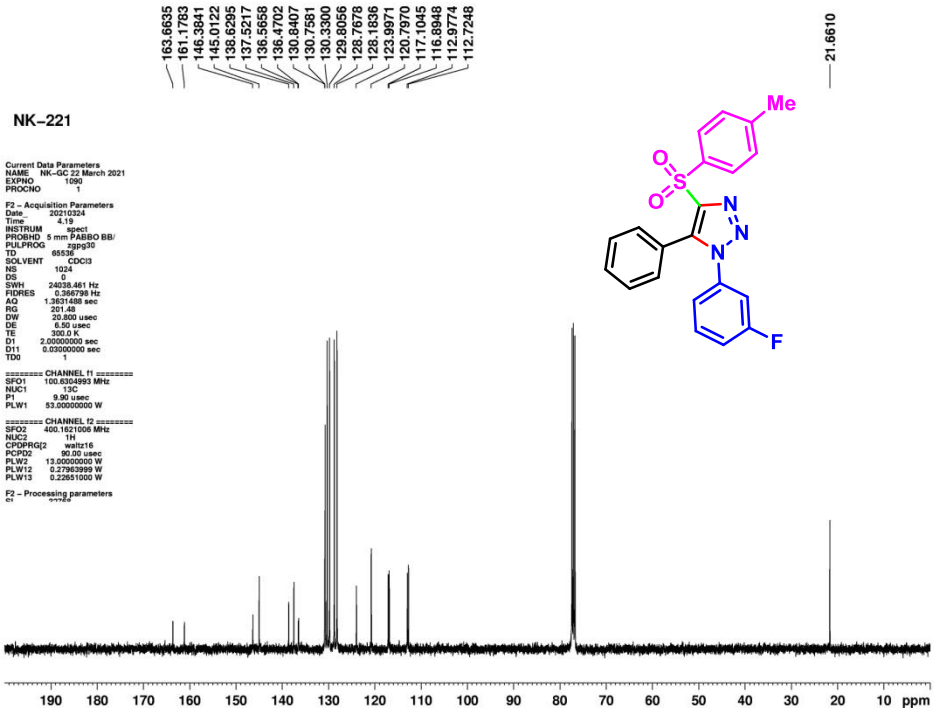


Figure S21: ^{13}C NMR of compound (5e)

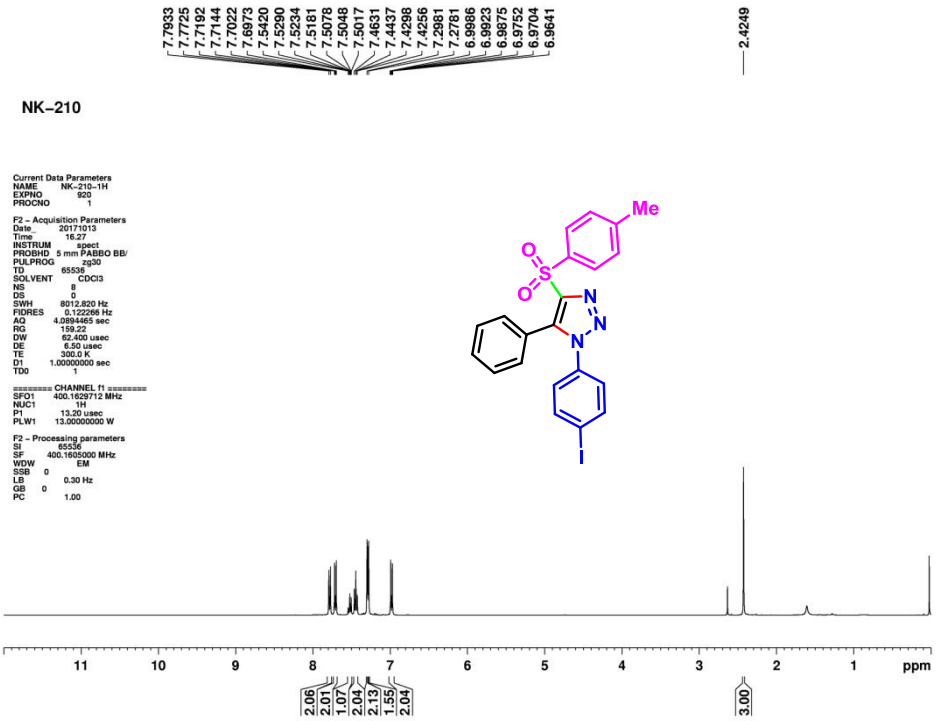


Figure S22: ^{1}H NMR of compound (5f)

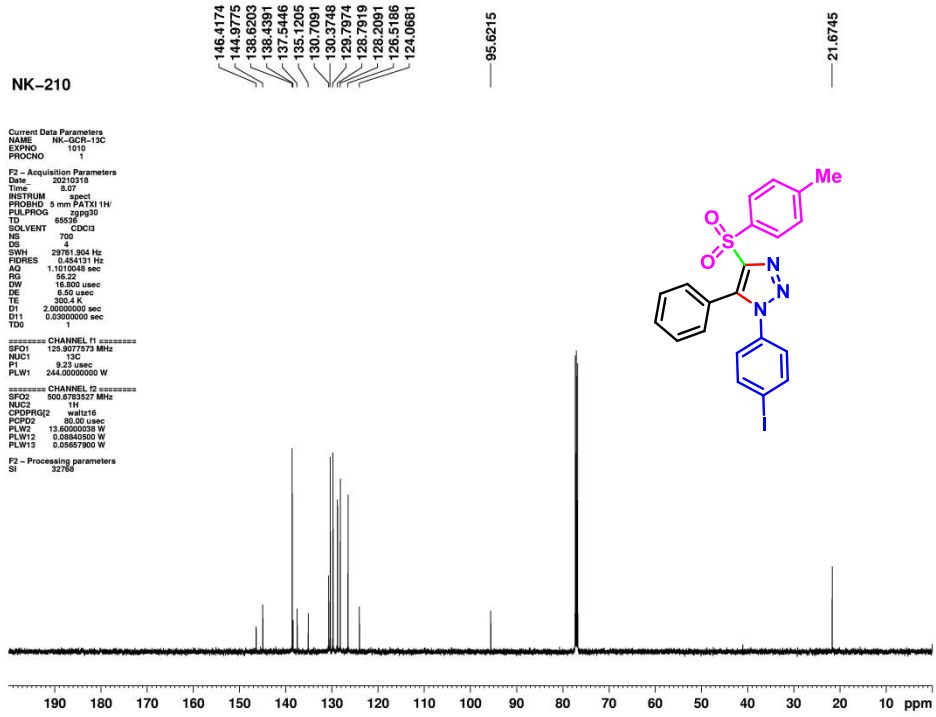


Figure S23: ^{13}C NMR of compound (5f)

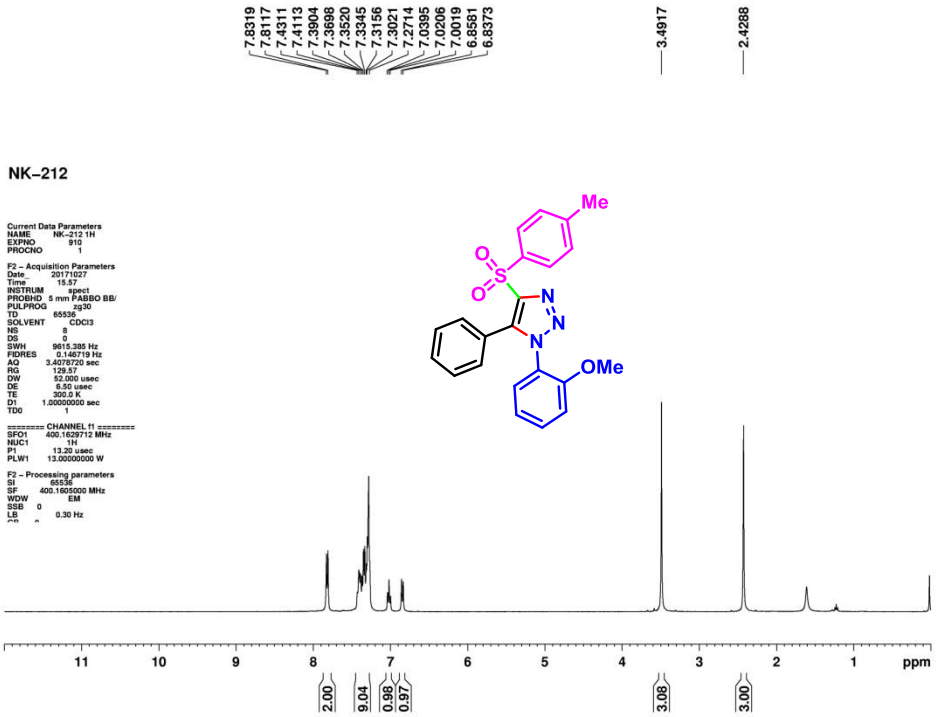


Figure S24: ^{1}H NMR of compound (5g)

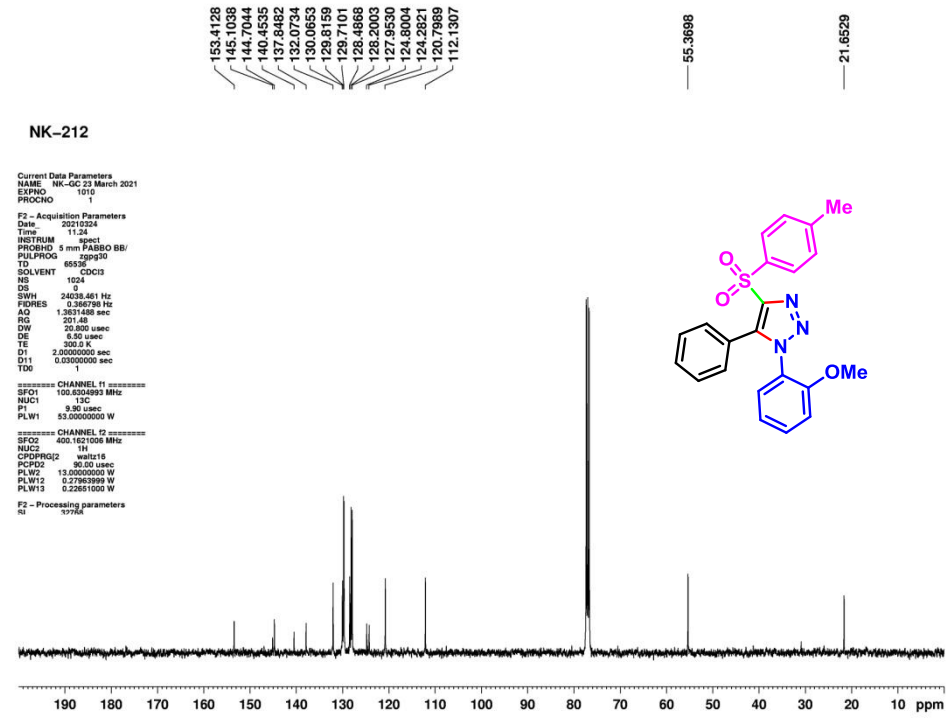


Figure S25: ^{13}C NMR of compound (5g)

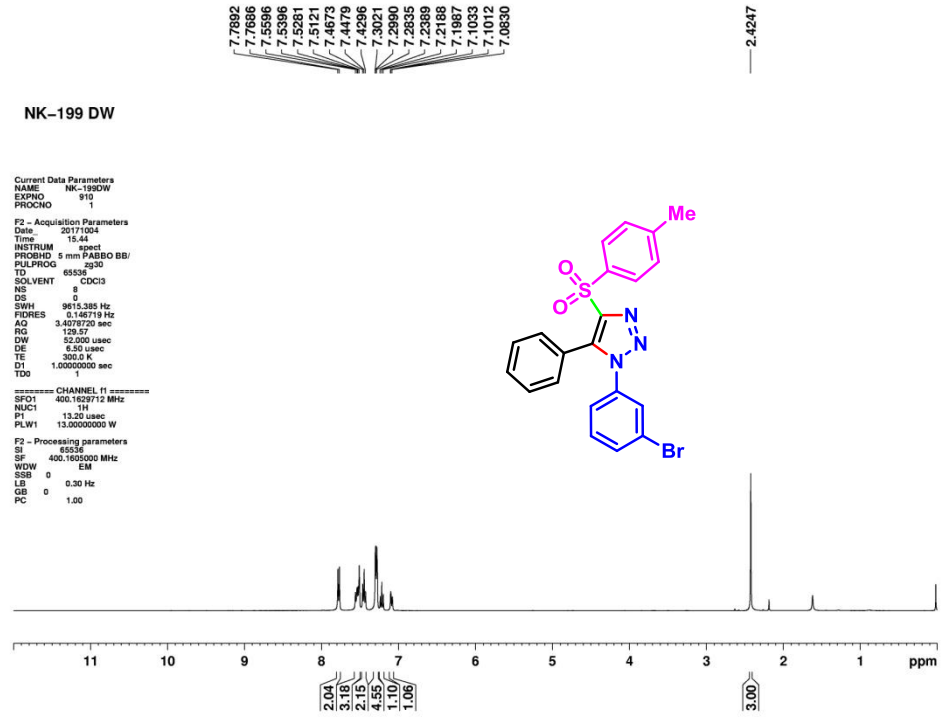


Figure S26: ^{1}H NMR of compound (5h)

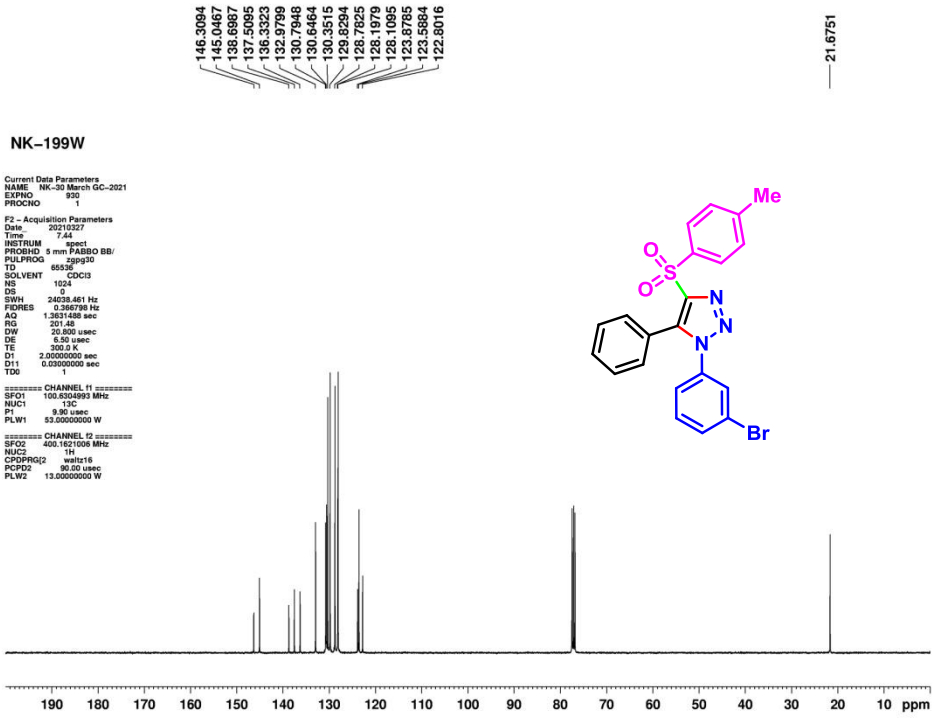


Figure S27: ^{13}C NMR of compound (5h)

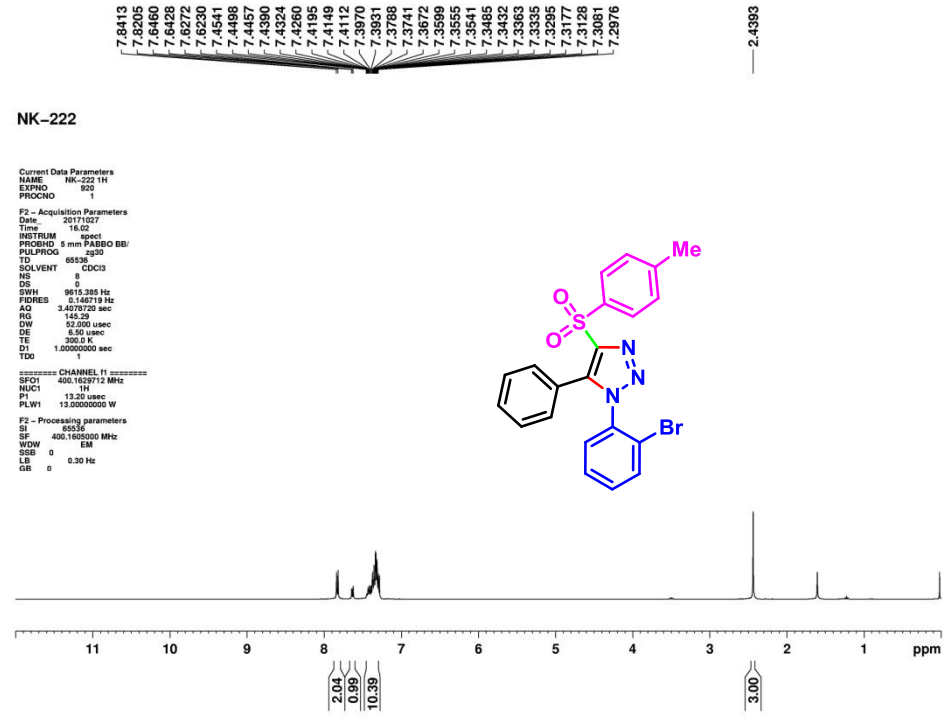


Figure S28: ^{1}H NMR of compound (5i)

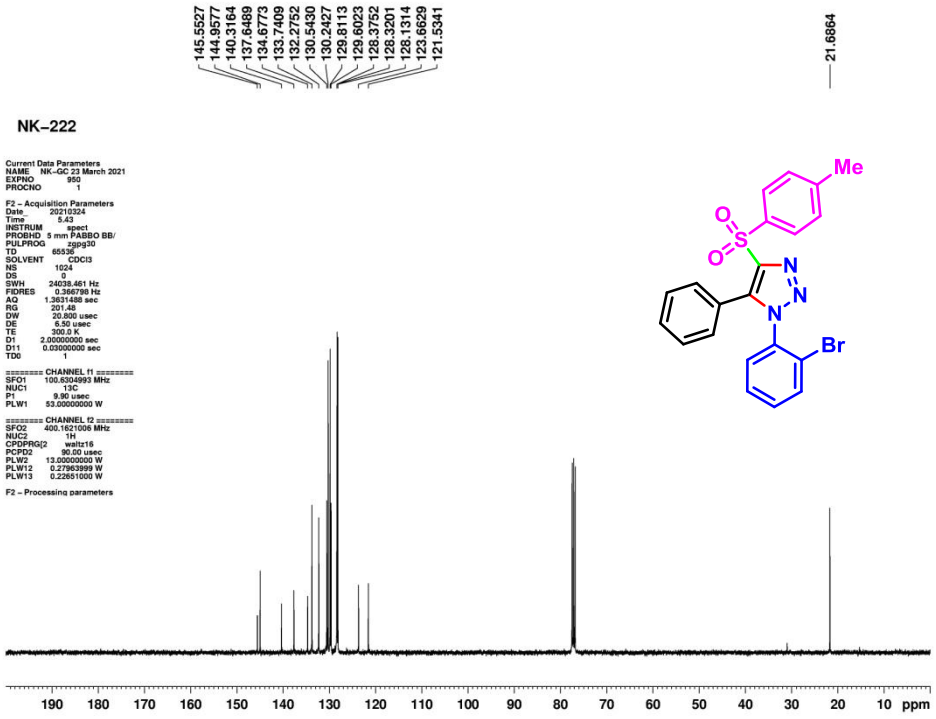


Figure S29: ^{13}C NMR of compound (5i)

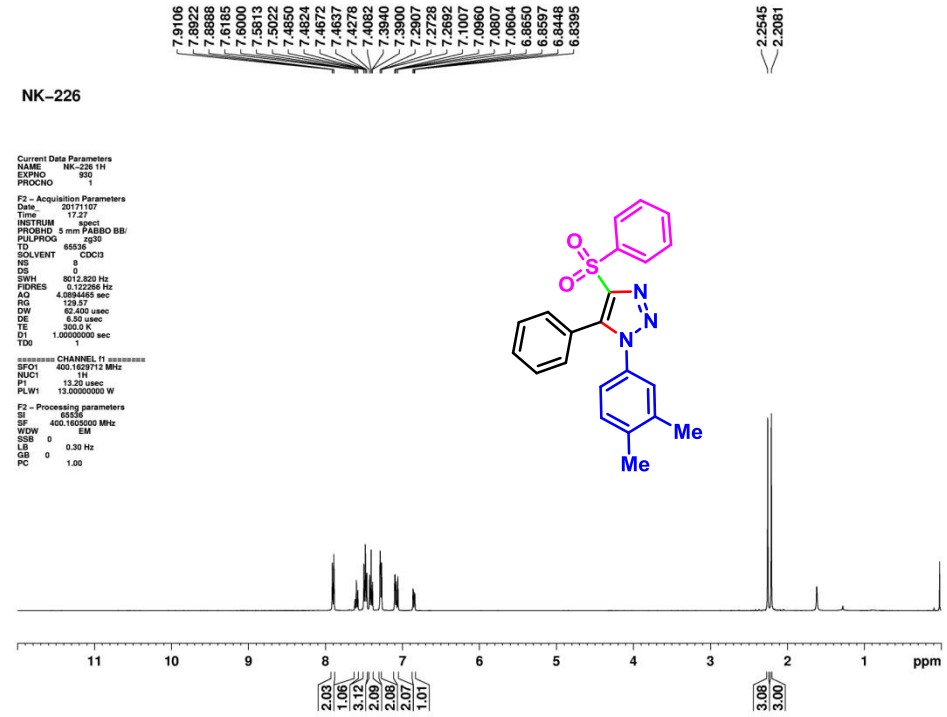


Figure S30: ^{1}H NMR of compound (5j)

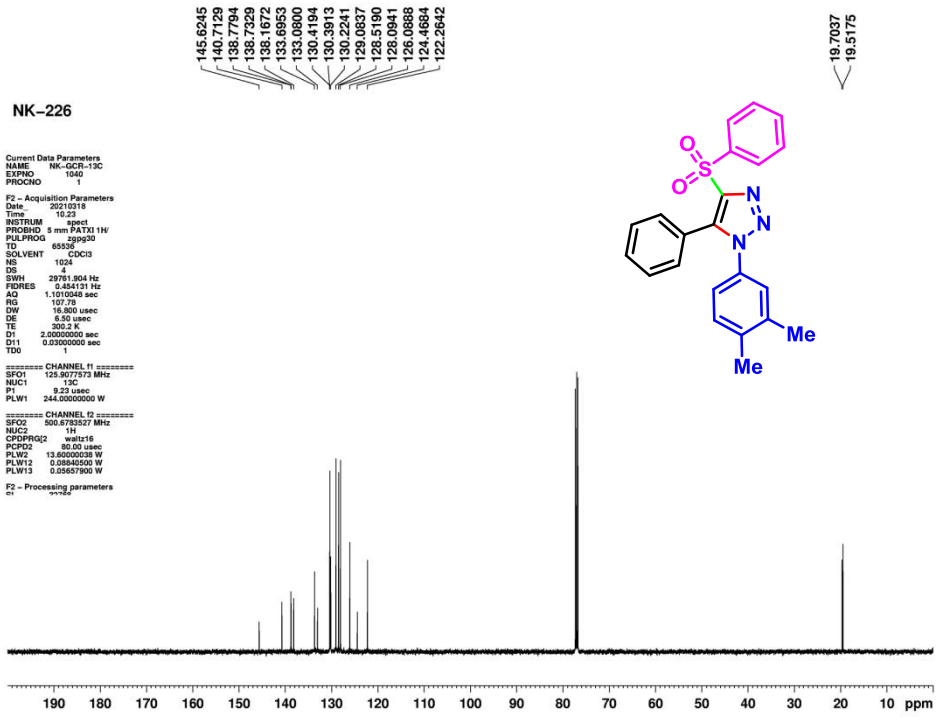


Figure S31: ^{13}C NMR of compound (5j)

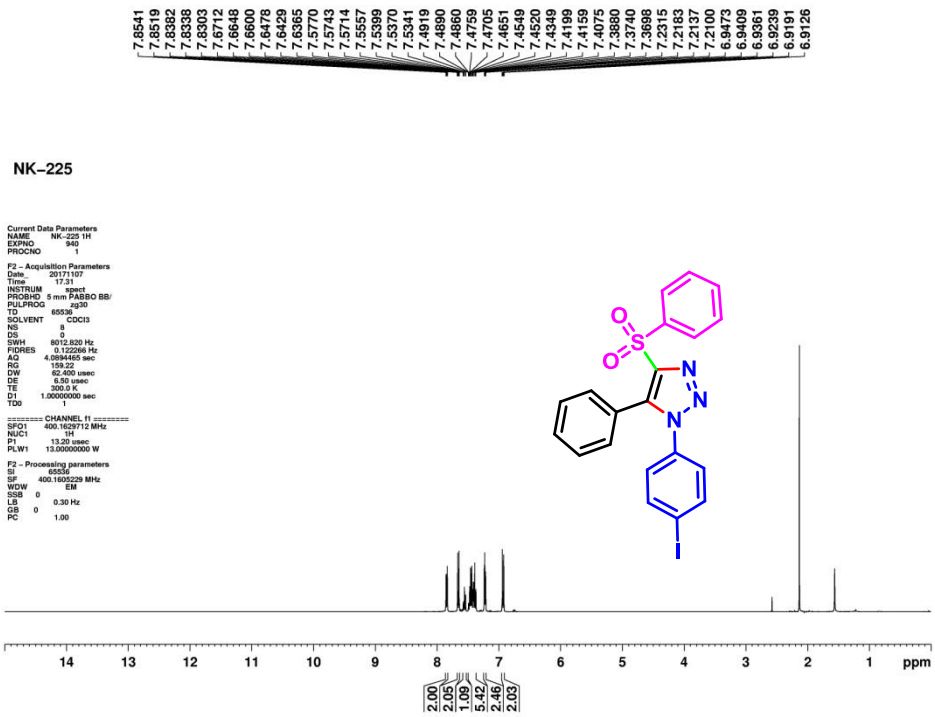


Figure S32: ^{1}H NMR of compound (5k)

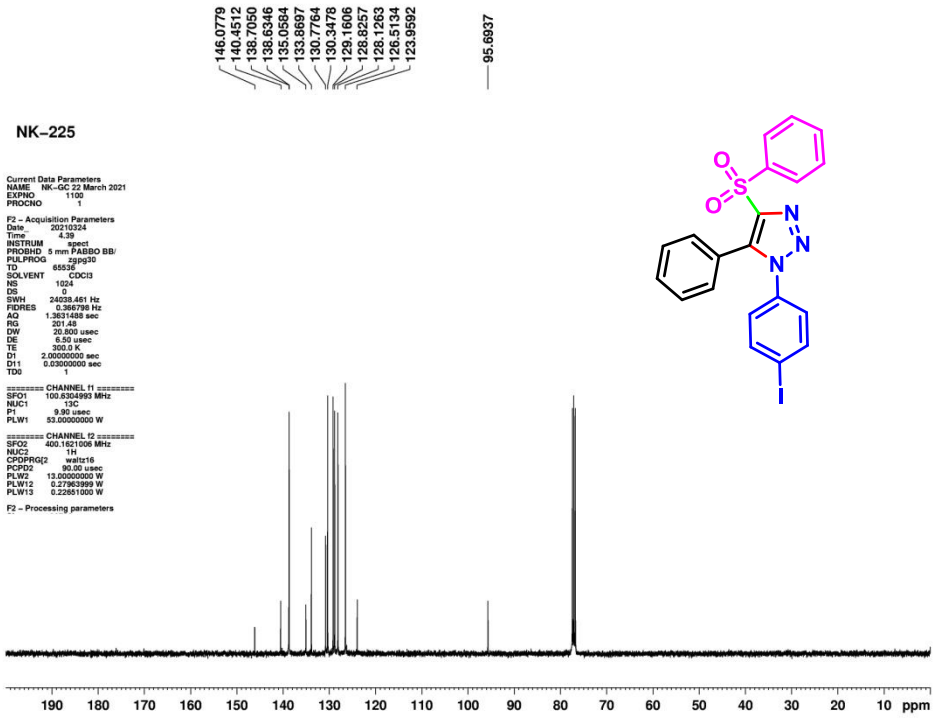


Figure S33: ^{13}C NMR of compound (5k)

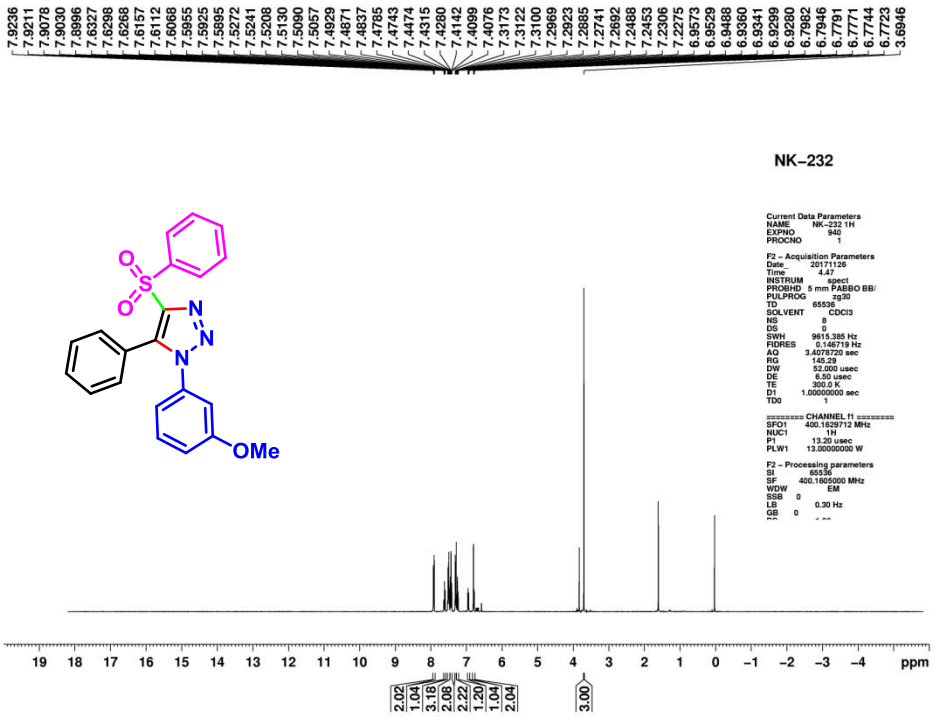


Figure S34: ^{1}H NMR of compound (5l)

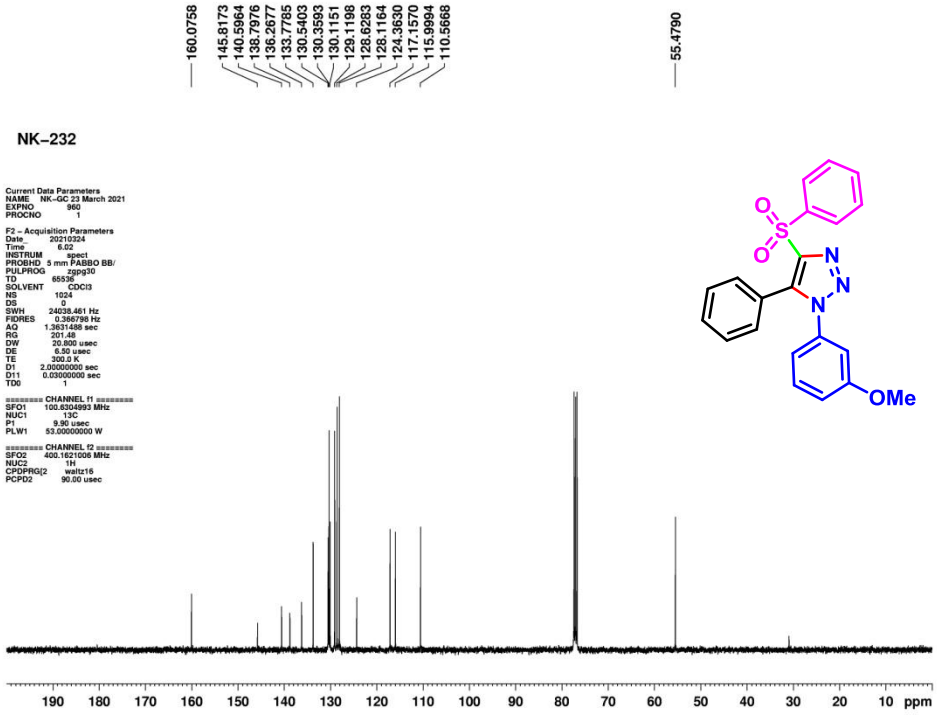


Figure S35: ^{13}C NMR of compound (5l)

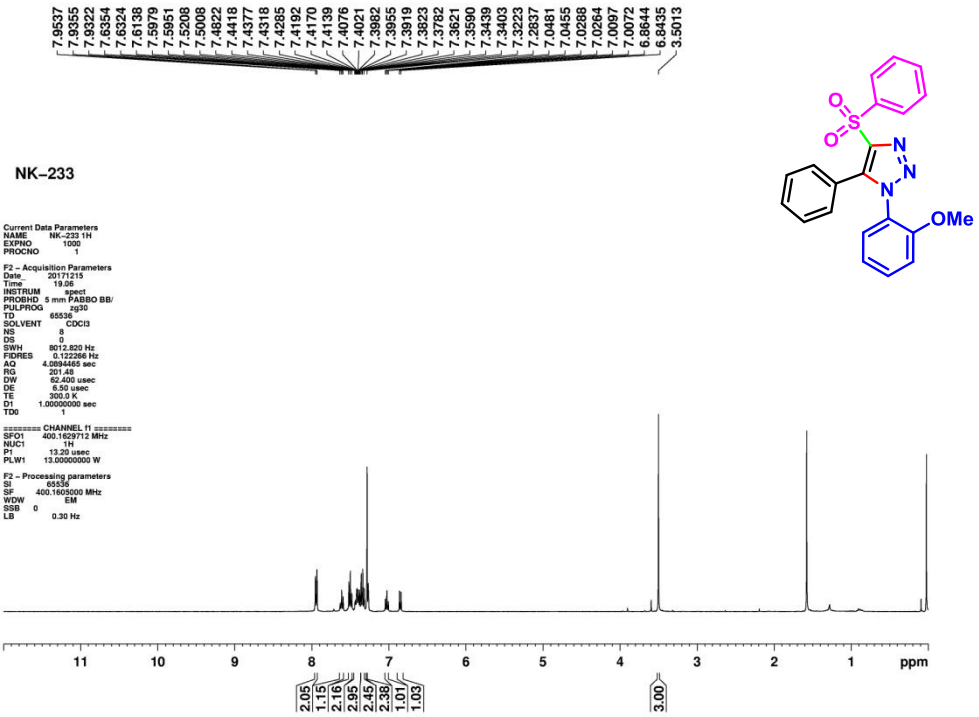


Figure S36: ^{1}H NMR of compound (5m)

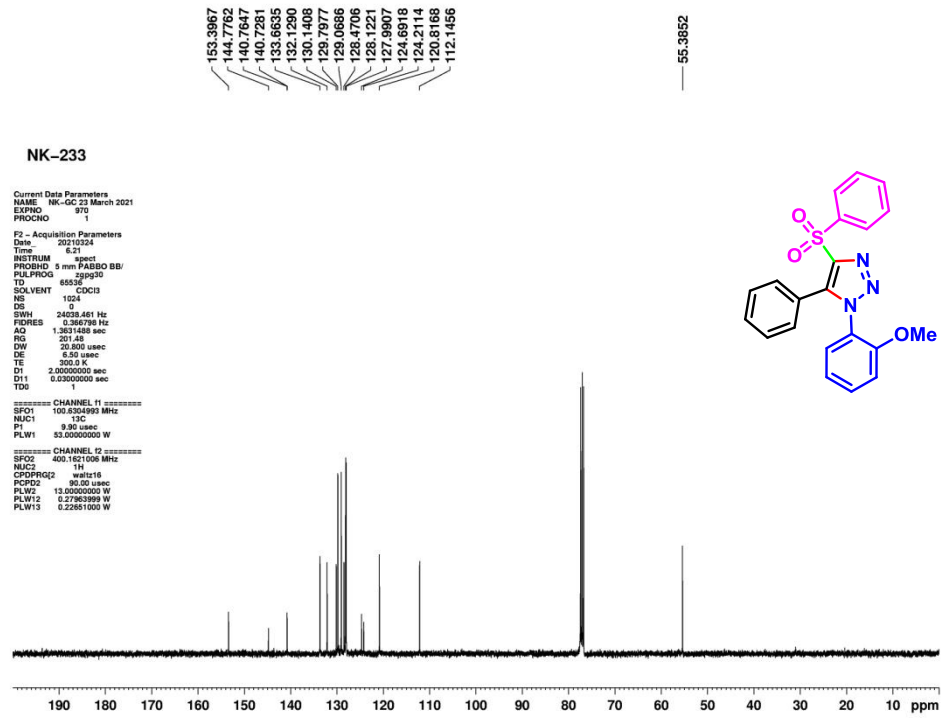


Figure S37: ^{13}C NMR of compound (5m)

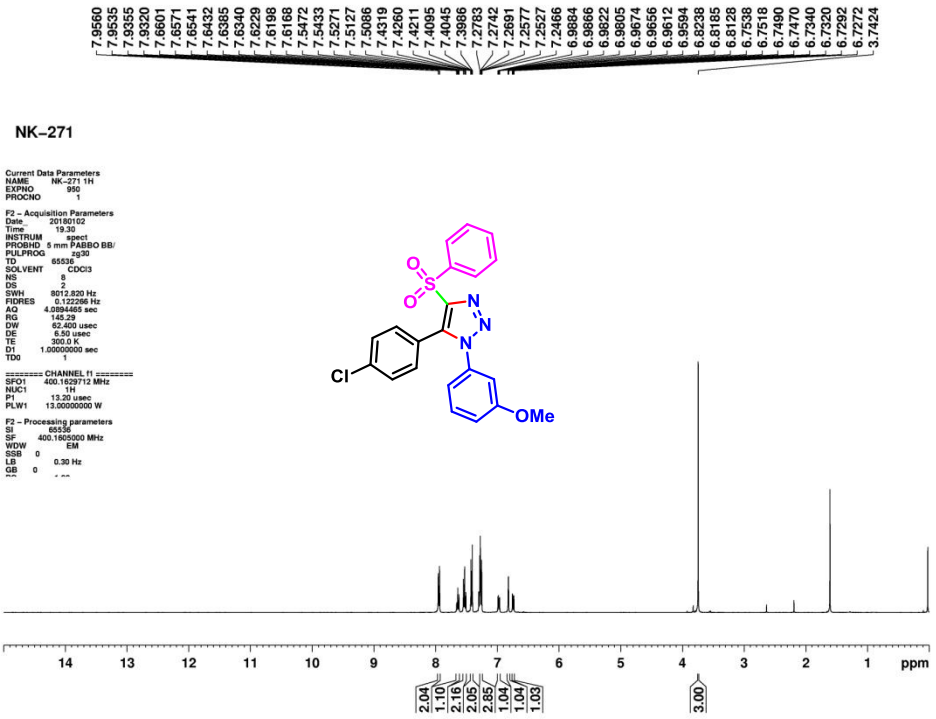


Figure S38: ^{1}H NMR of compound (5n)

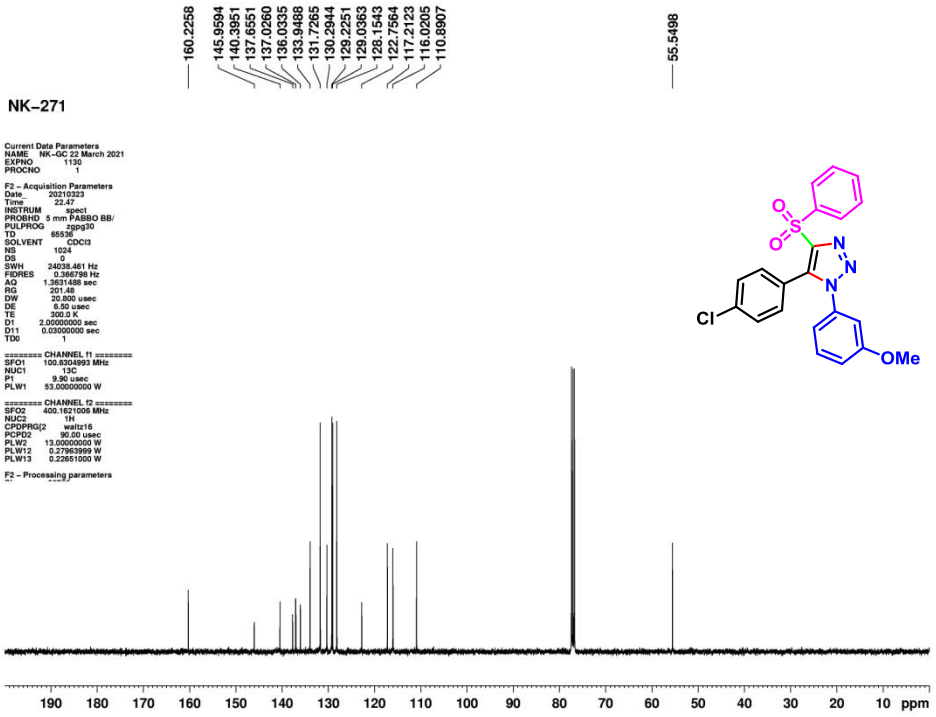


Figure S39: ^{13}C NMR of compound (5n)

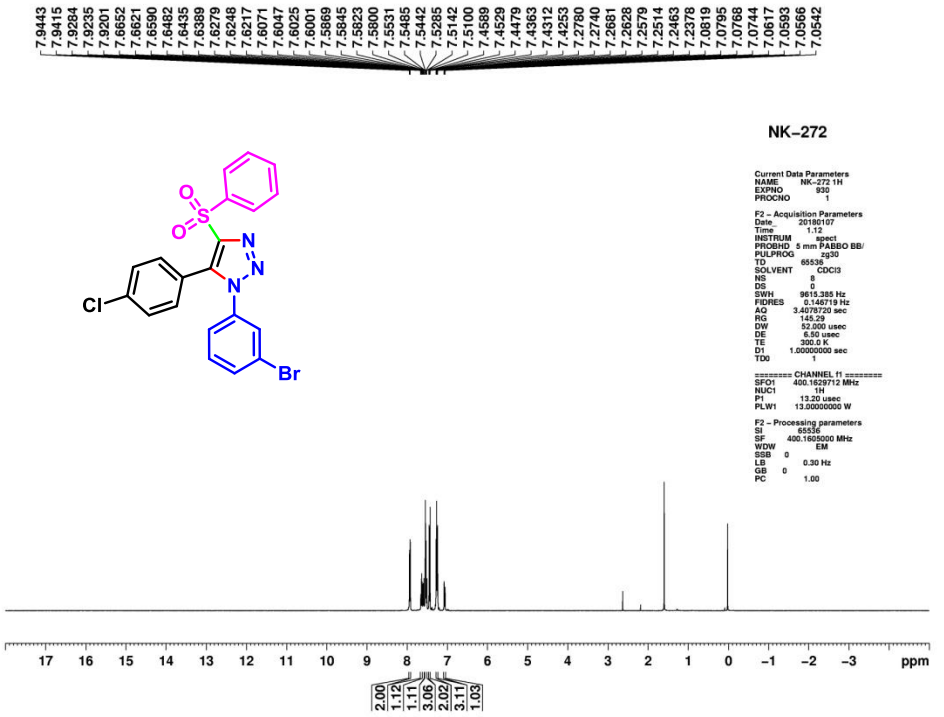


Figure S40: ^{1}H NMR of compound (5o)

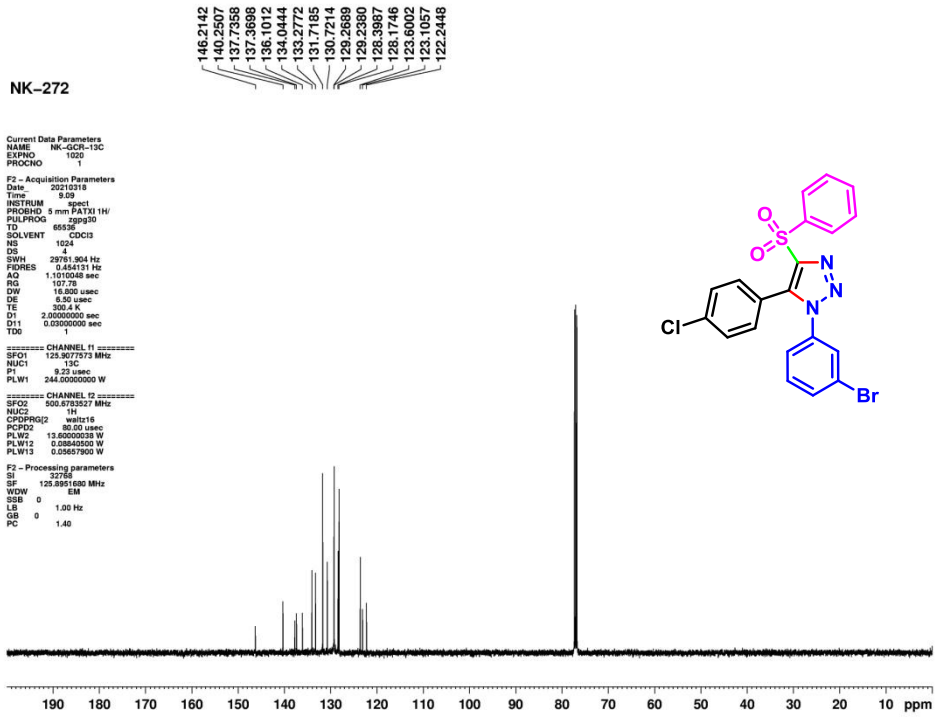


Figure S41: ^{13}C NMR of compound (5o)

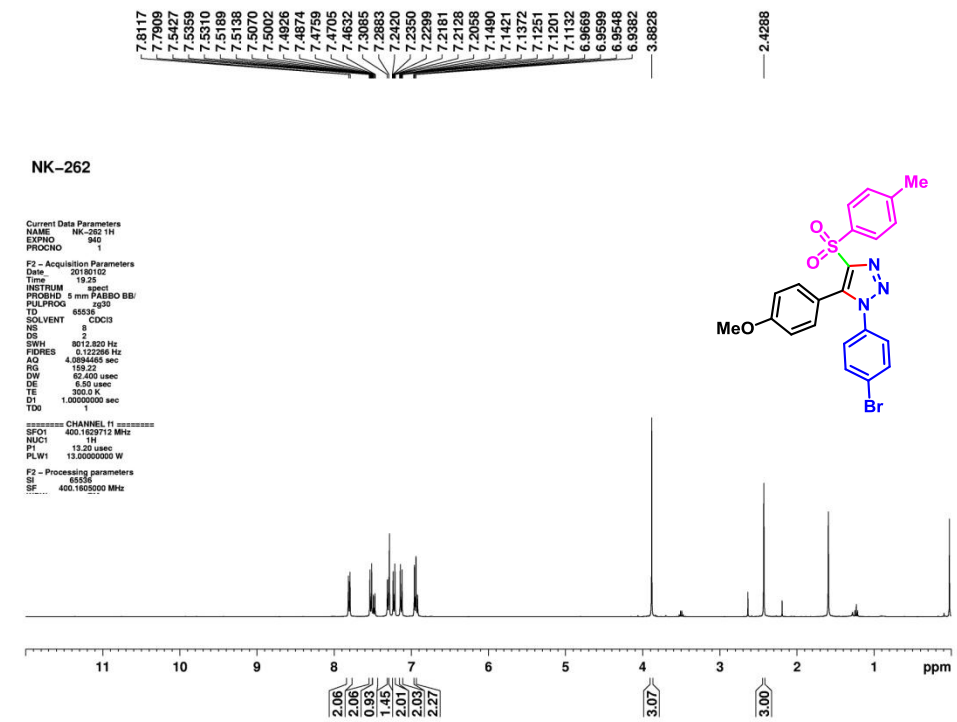


Figure S42: ^{1}H NMR of compound (5p)

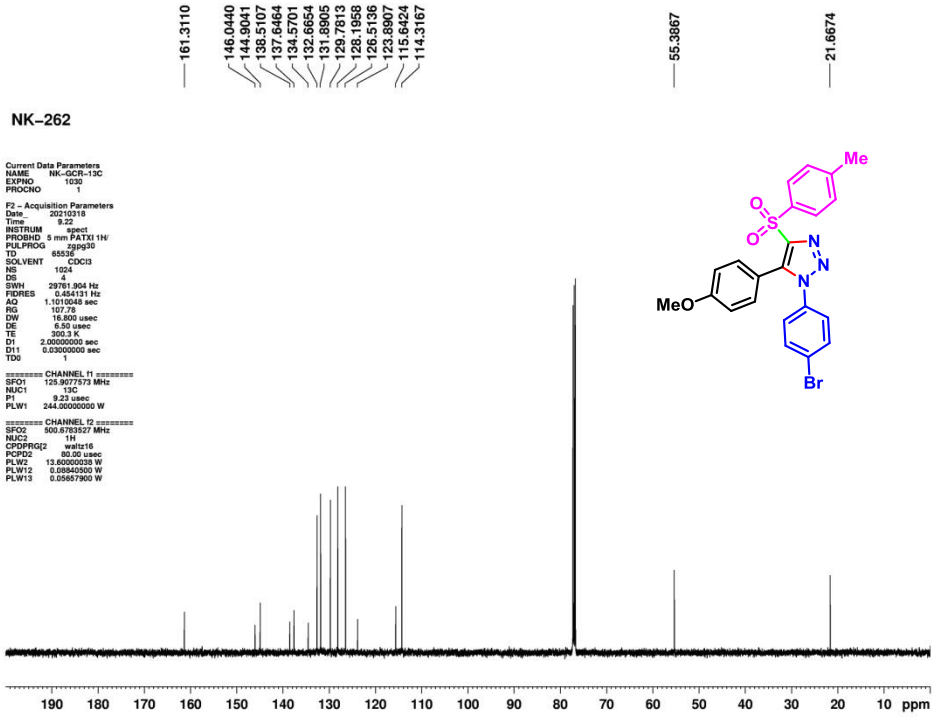


Figure S43: ^{13}C NMR of compound (5p)

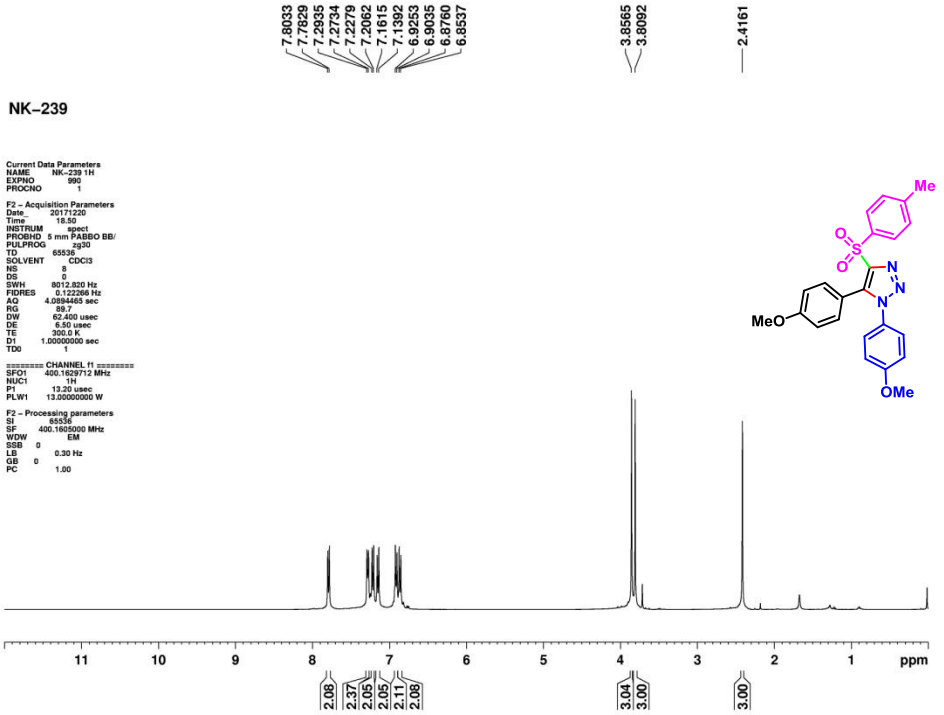


Figure S44: ^{1}H NMR of compound (5q)

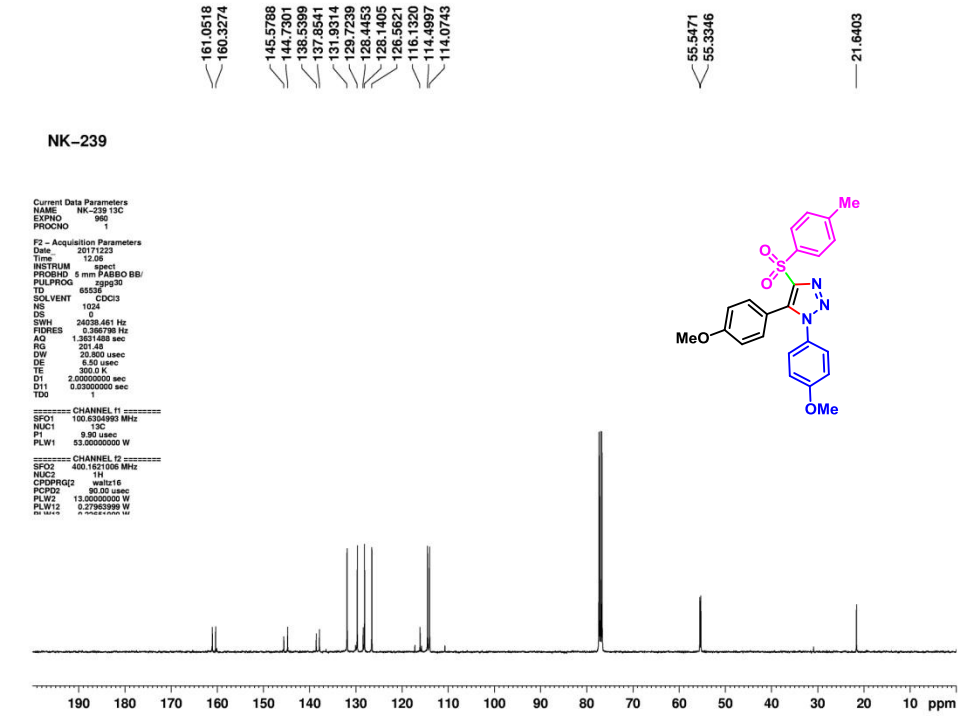


Figure S45: ^{13}C NMR of compound (5q)

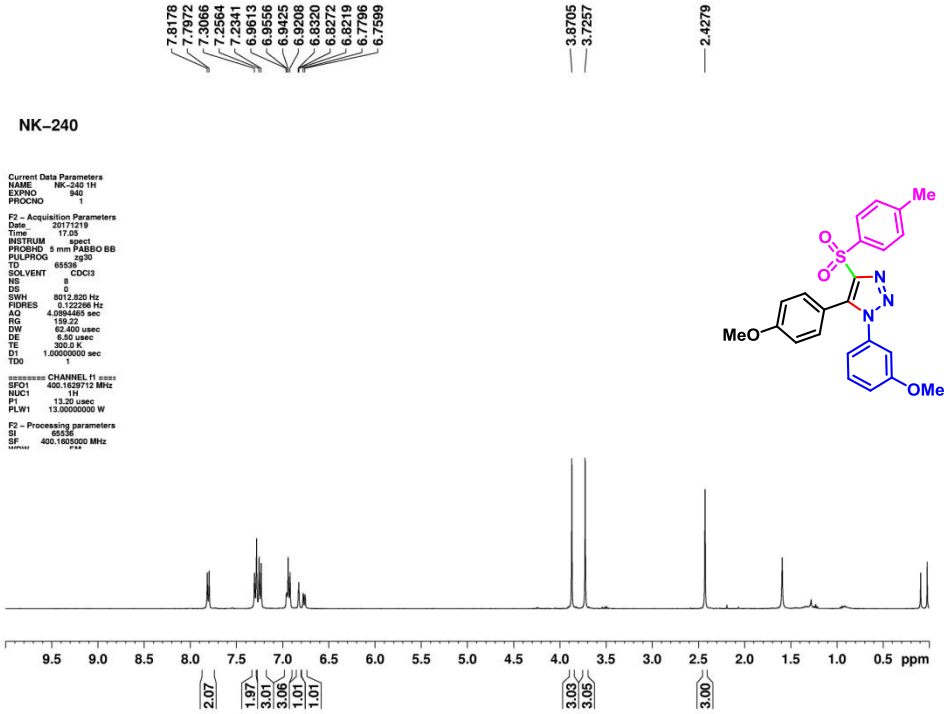


Figure S46: ^{1}H NMR of compound (5r)

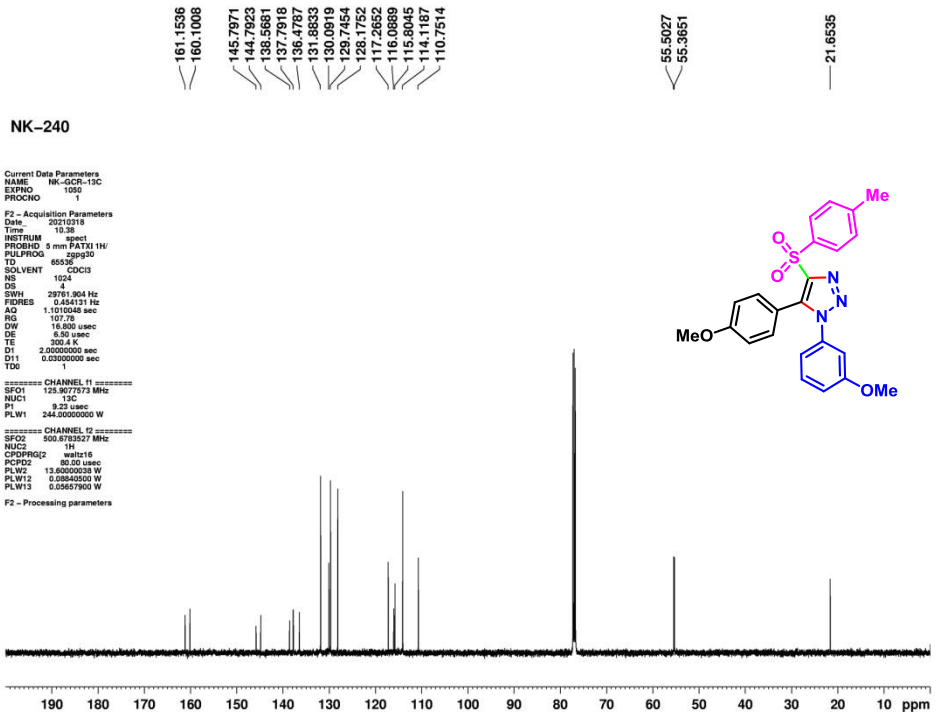


Figure S47: ^{13}C NMR of compound (5r)

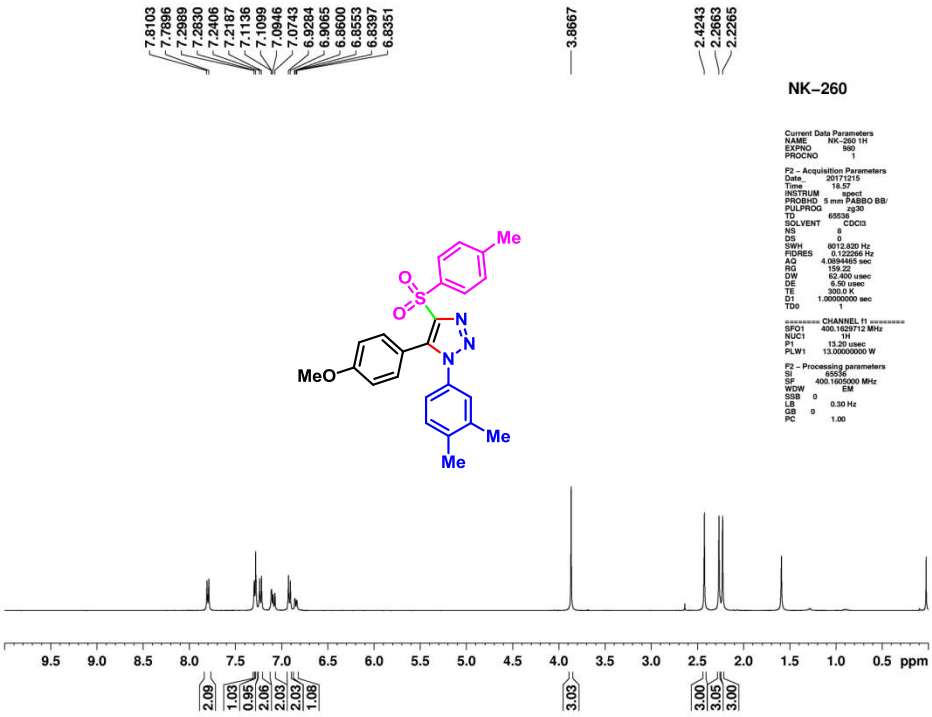


Figure S48: ^{1}H NMR of compound (5s)

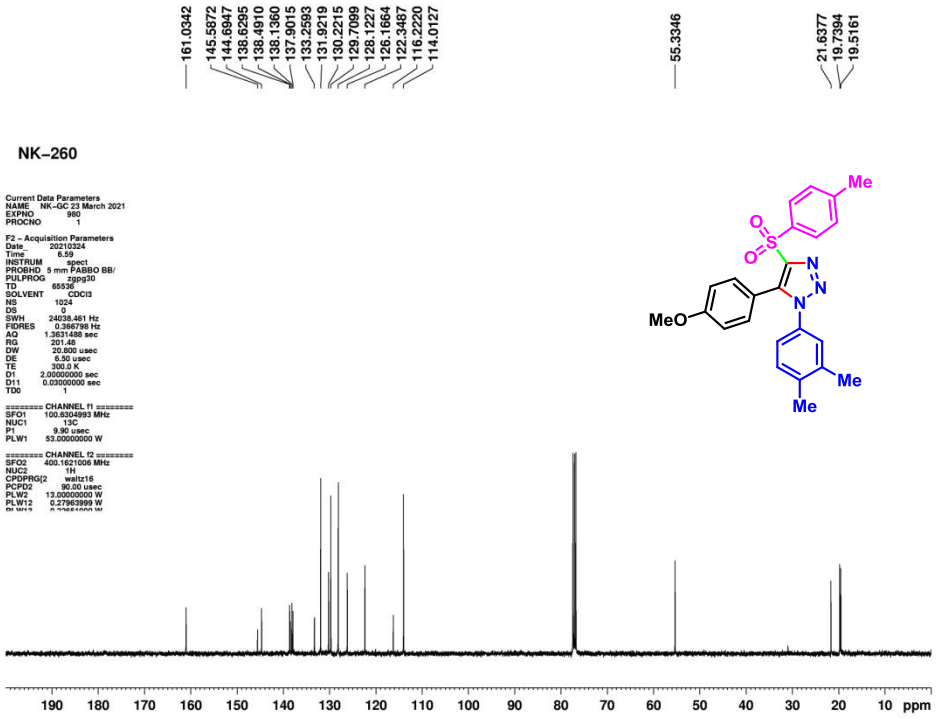


Figure S49: ^{13}C NMR of compound (5s)

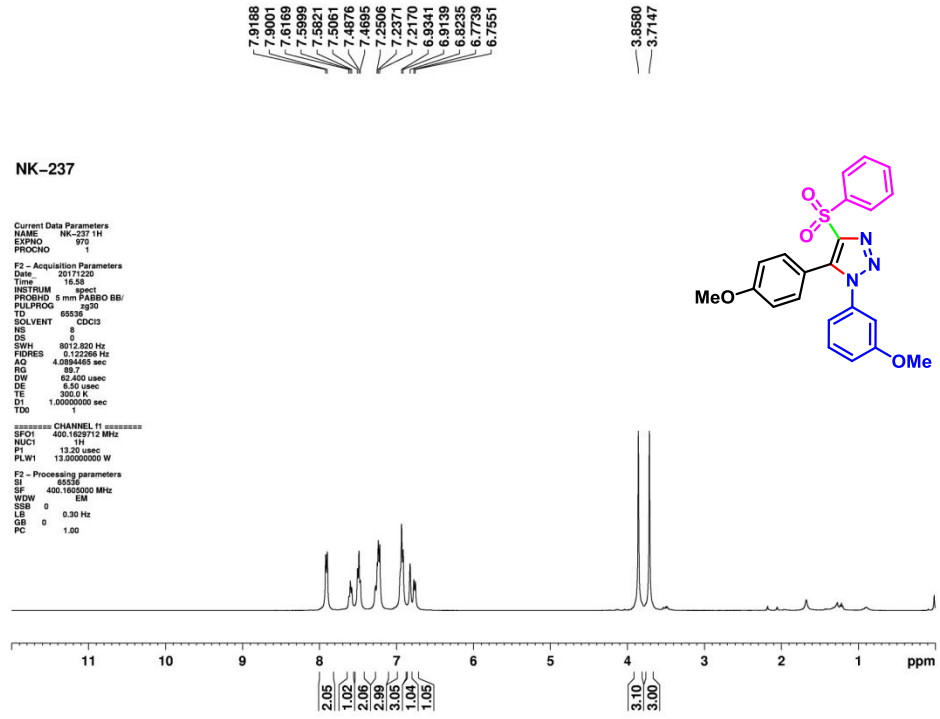


Figure S50: ^{1}H NMR of compound (5t)

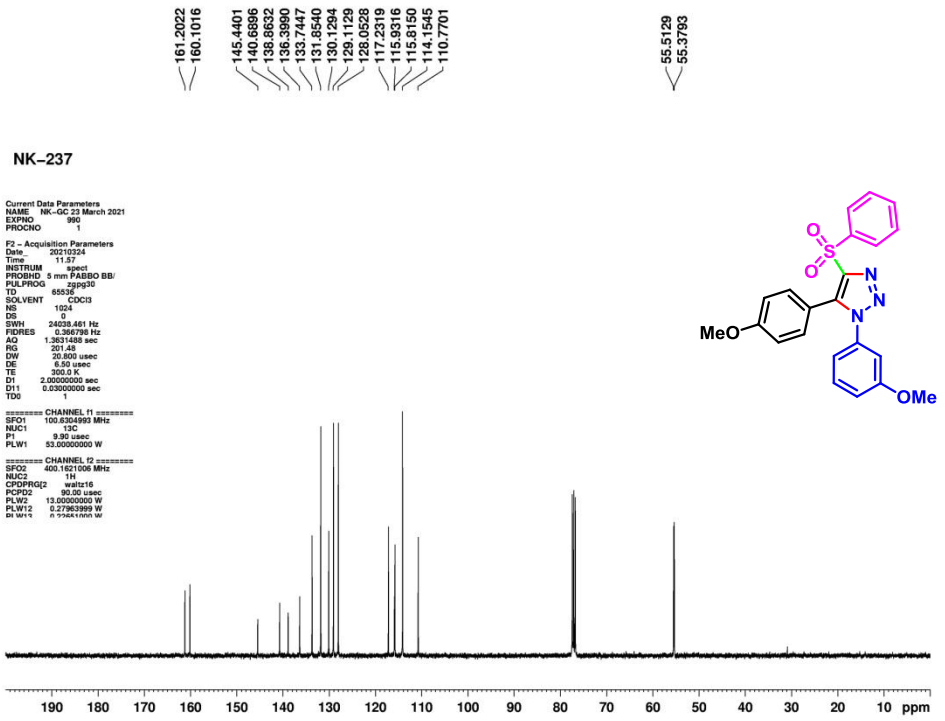


Figure S51: ^{13}C NMR of compound (5t)

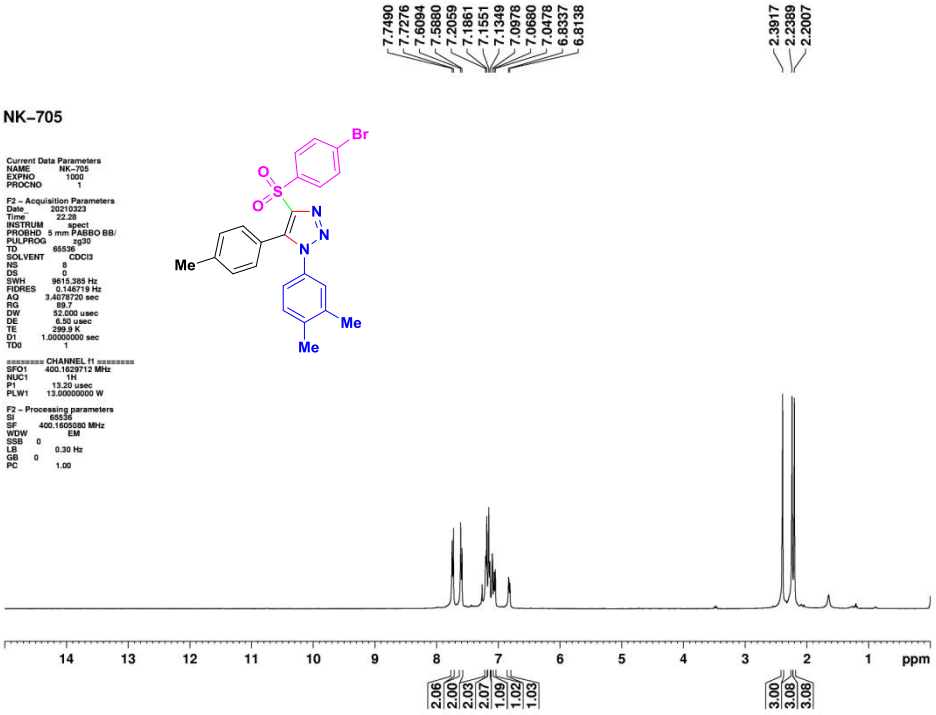


Figure S52: ^{1}H NMR of compound (5u)

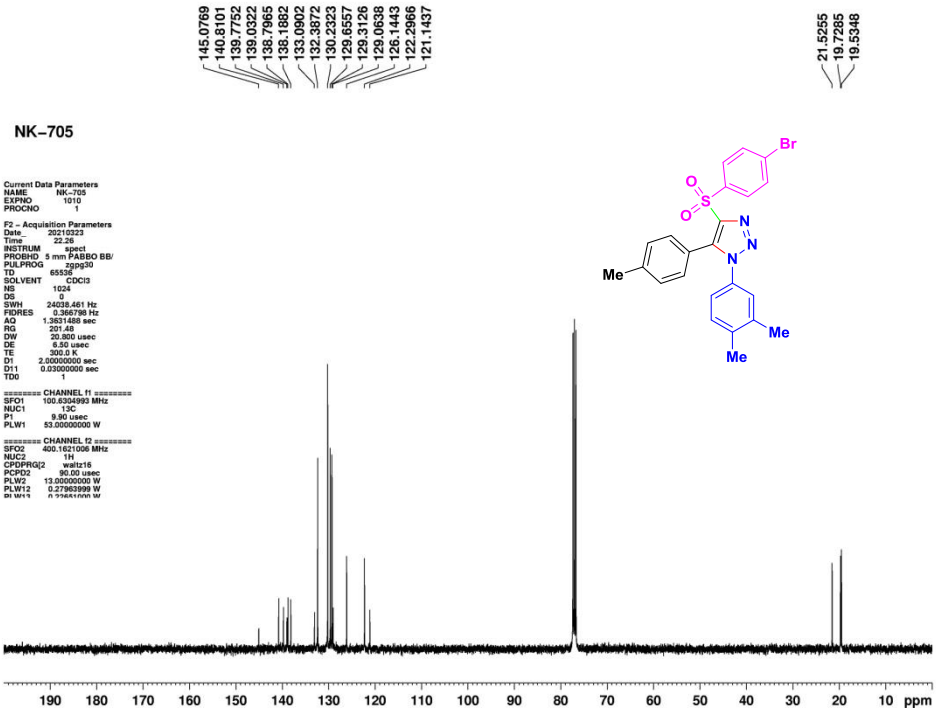


Figure S53: ^{13}C NMR of compound (5u)

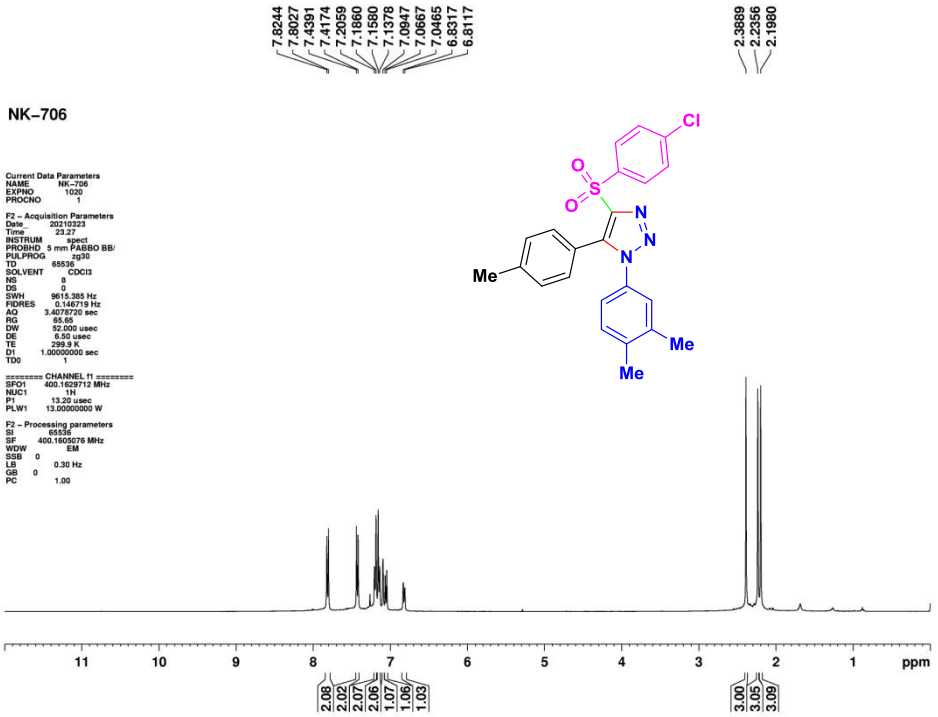


Figure S54: ^{1}H NMR of compound (5v)

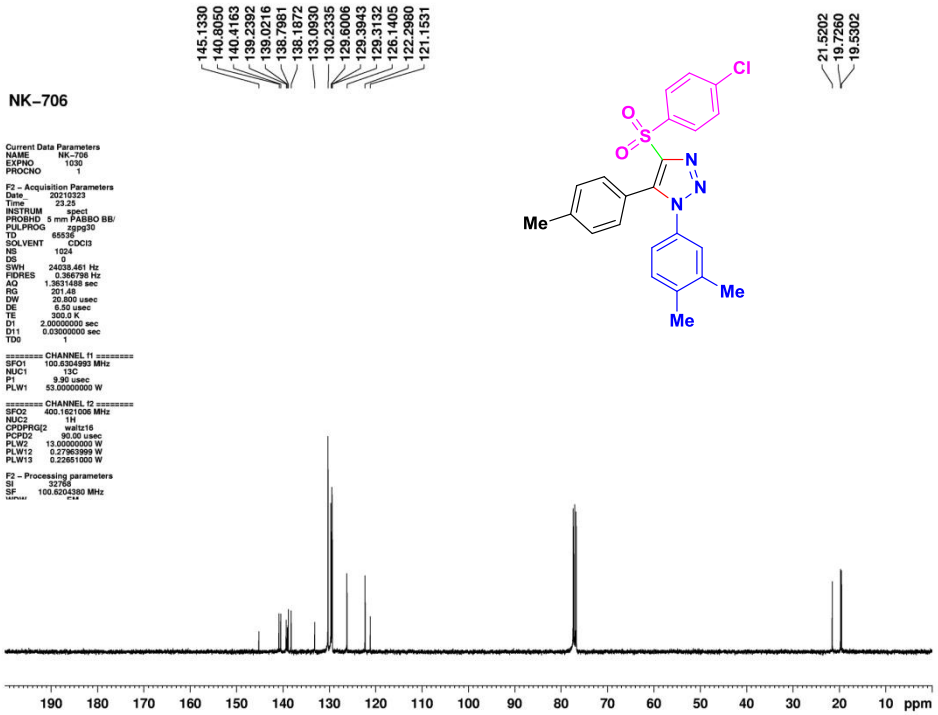


Figure S55: ^{13}C NMR of compound (5v)

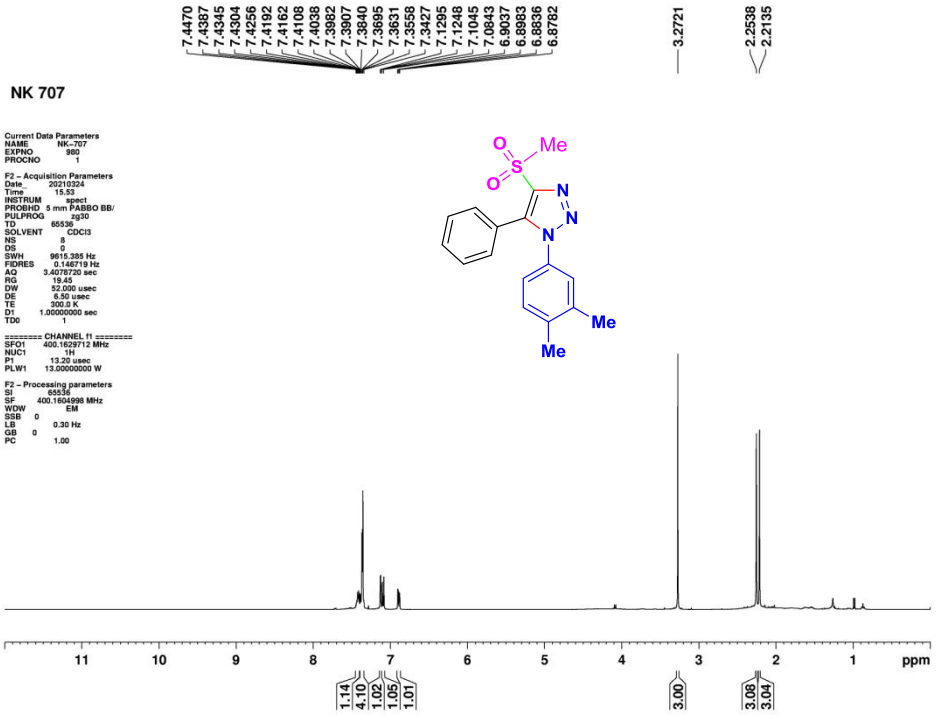


Figure S56: ^{1}H NMR of compound (5w)

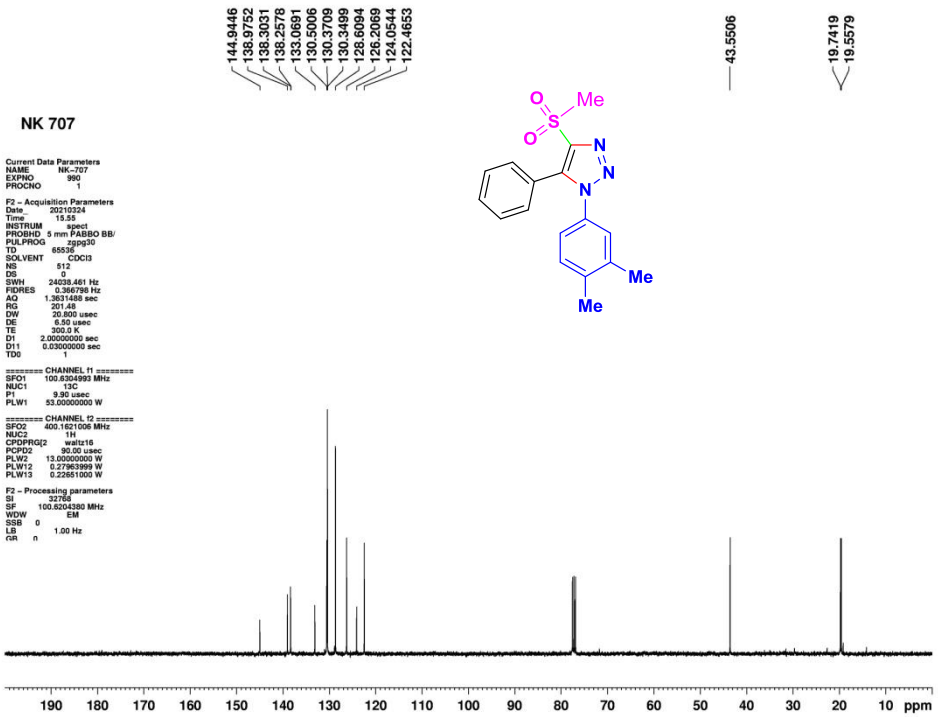


Figure S57: ^{13}C NMR of compound (5w)

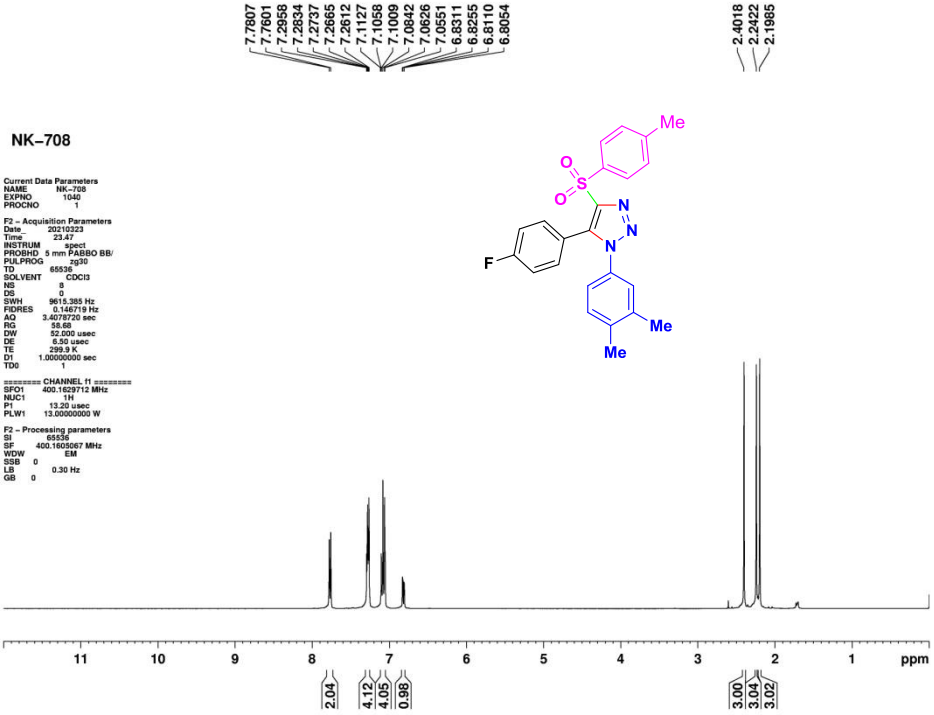


Figure S58: ^{1}H NMR of compound (5x)

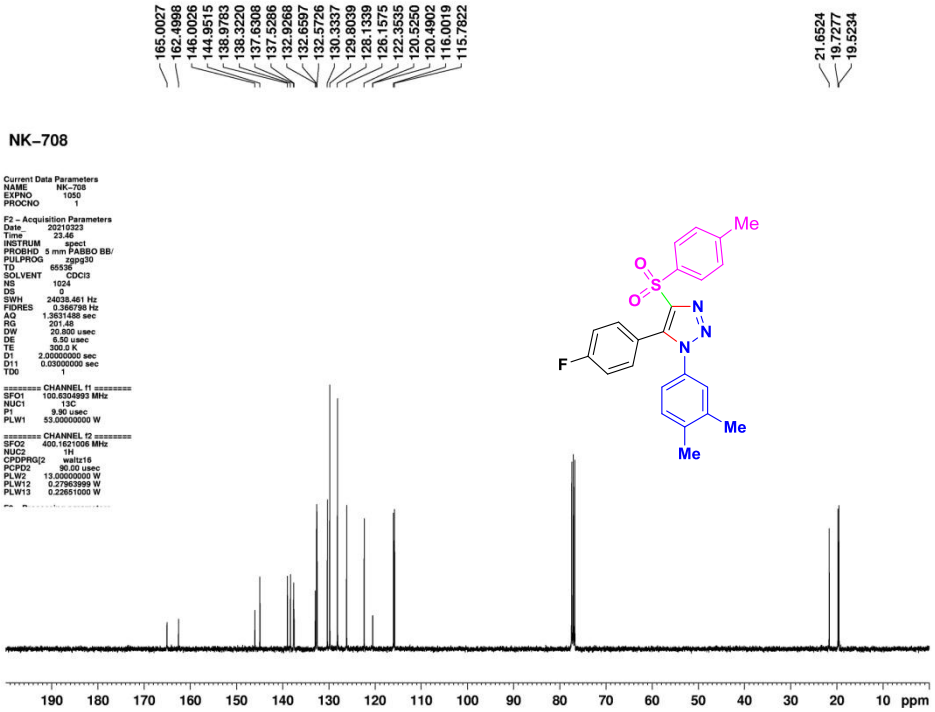


Figure S59: ^{13}C NMR of compound (5x)

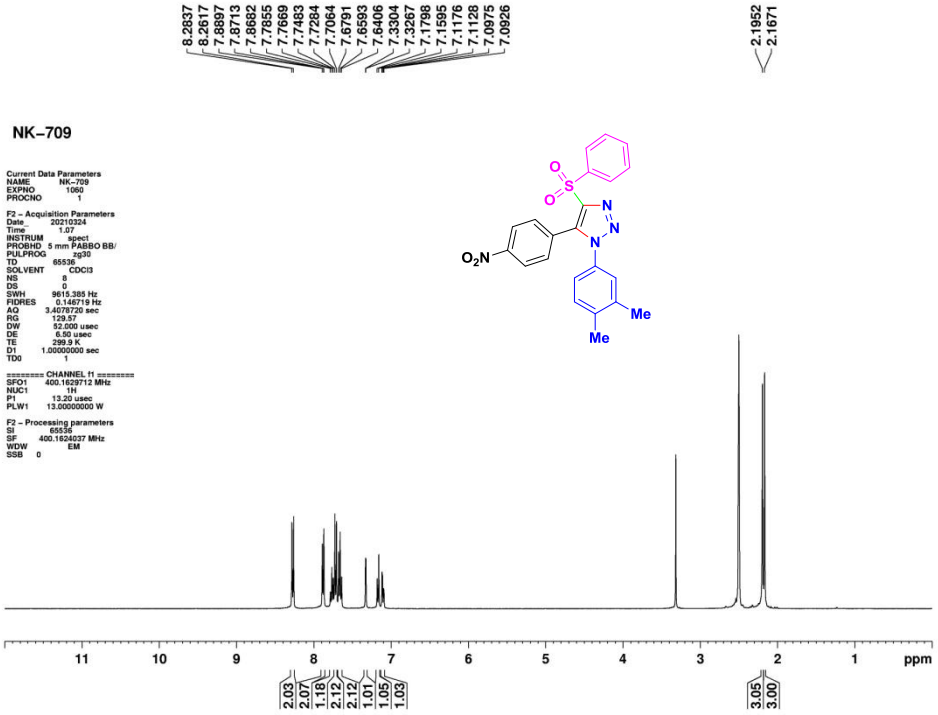


Figure S60: ^{1}H NMR of compound (5y)

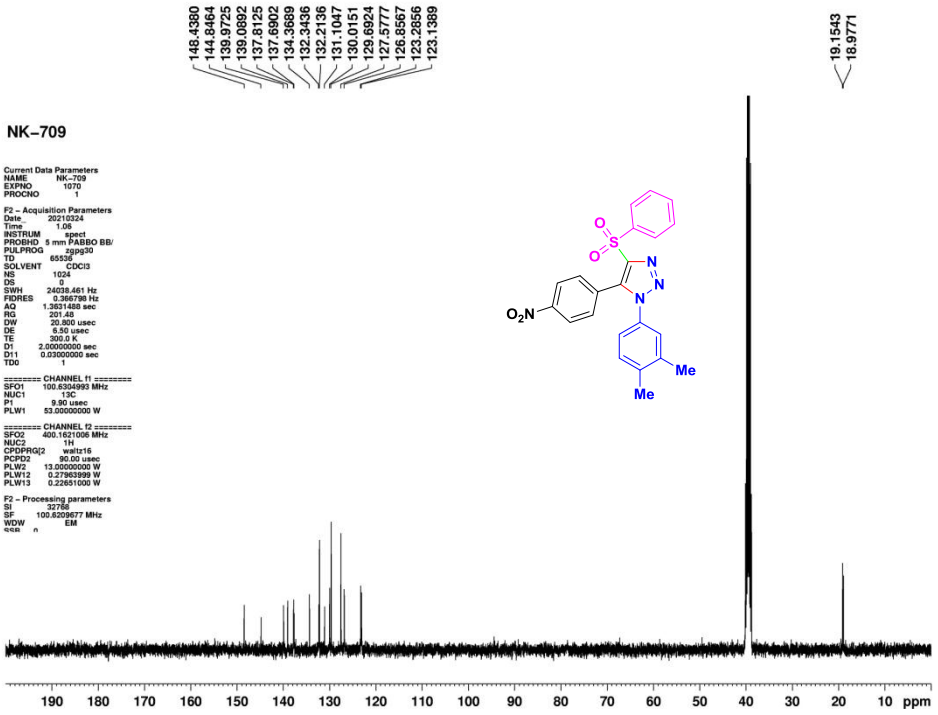


Figure S61: ^{13}C NMR of compound (5y)

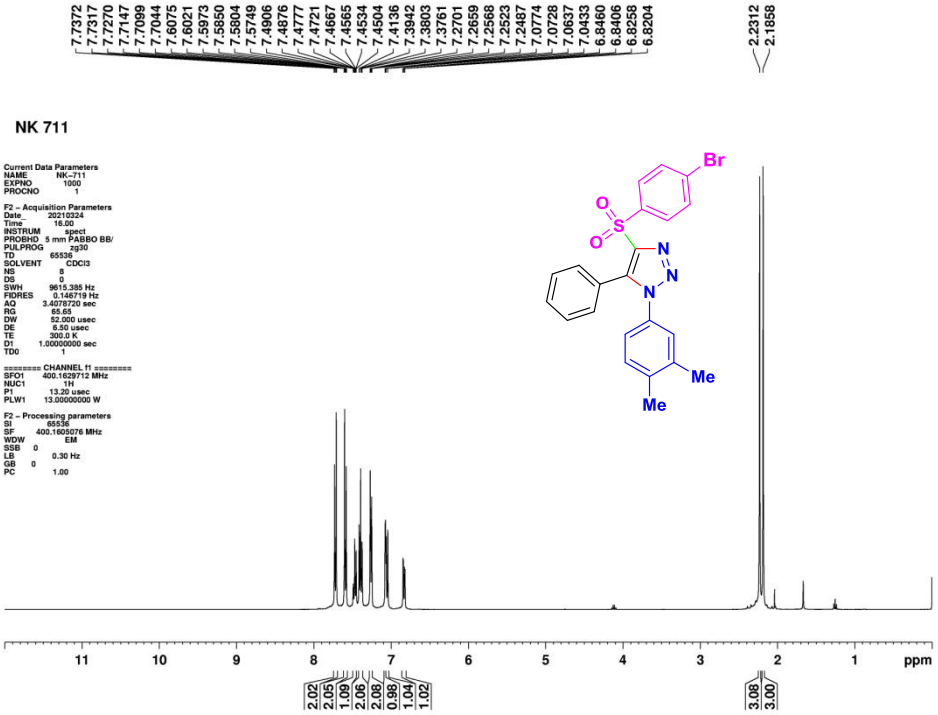


Figure S62: ^{1}H NMR of compound (5z)

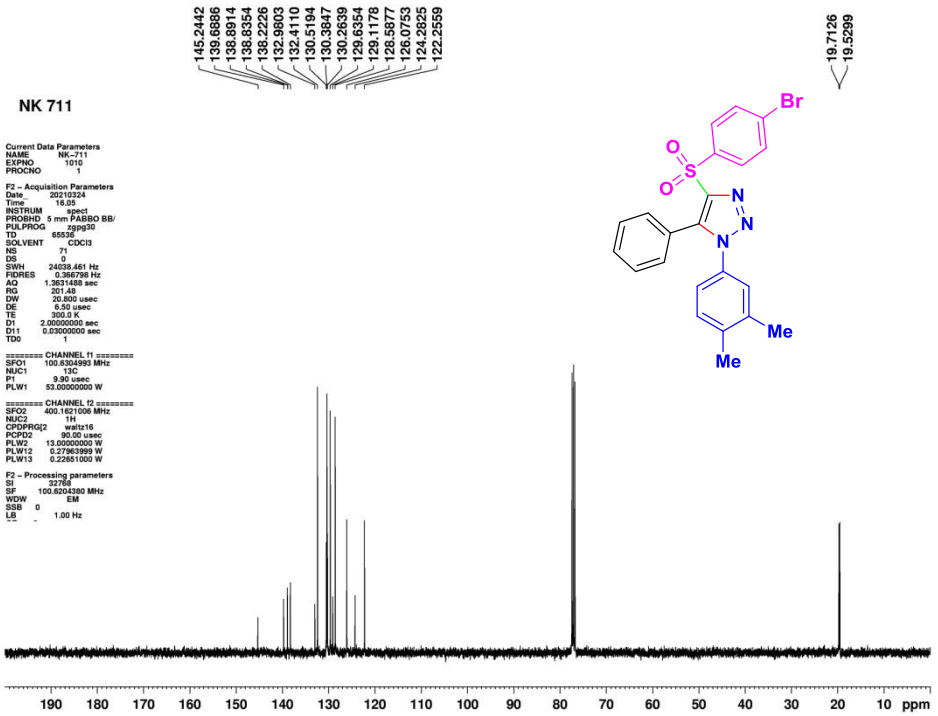


Figure S63: ^{13}C NMR of compound (5z)

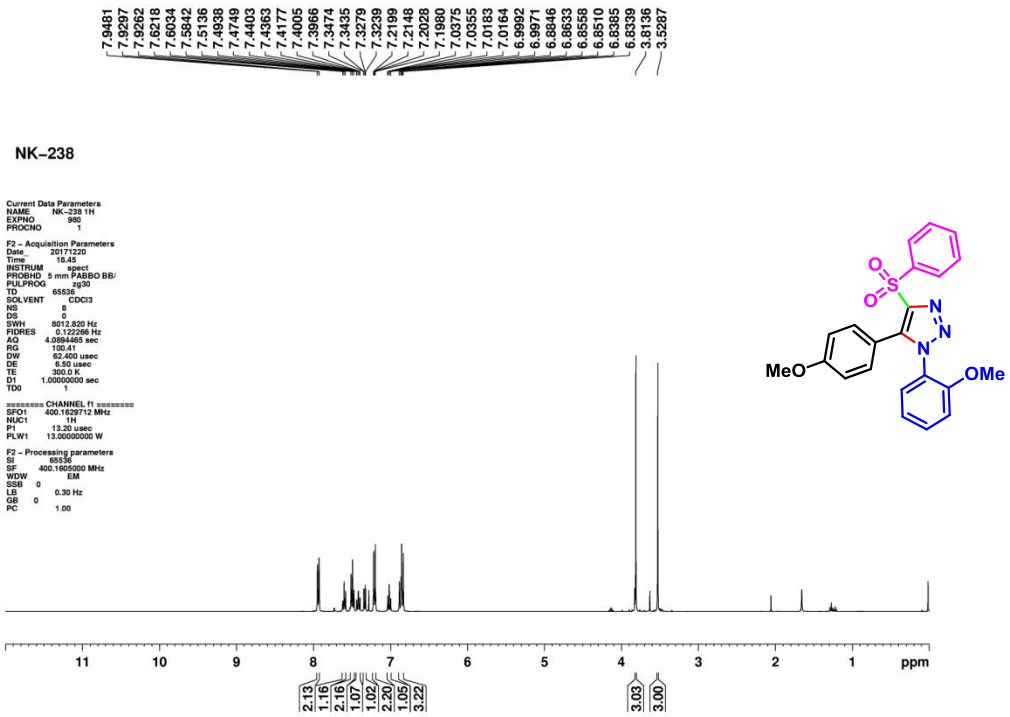


Figure S64: ^{1}H NMR of compound (5aa)

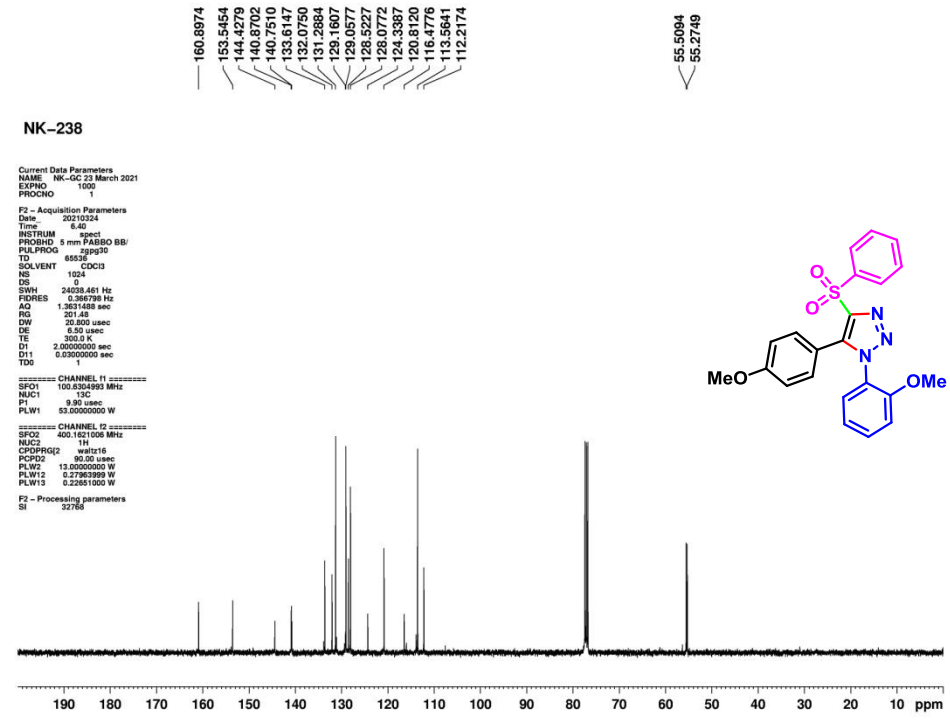


Figure S65: ^{13}C NMR of compound (5aa)

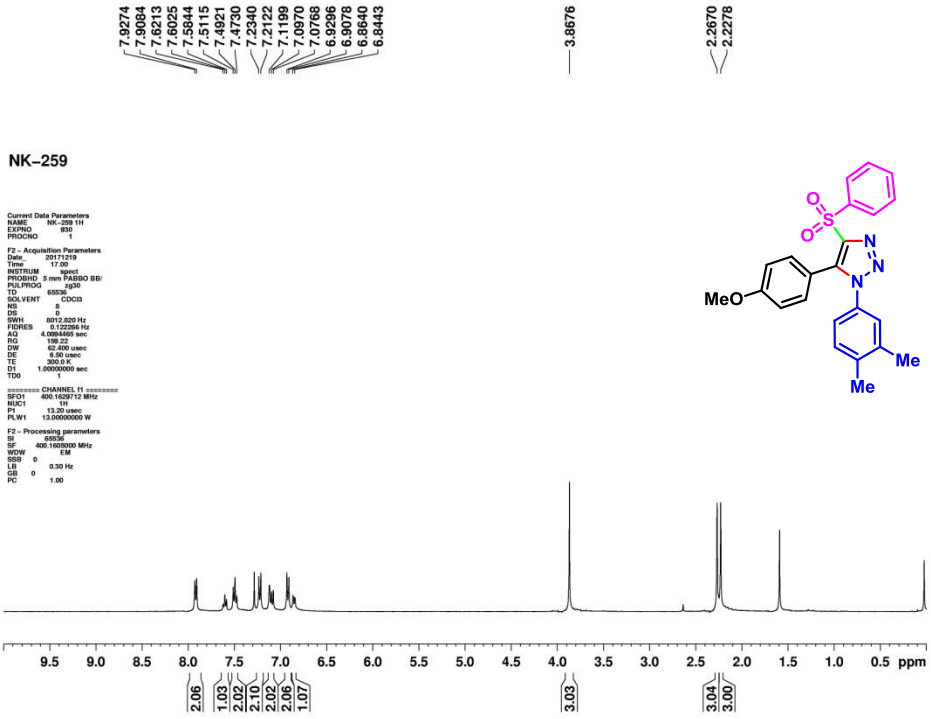


Figure S66: ^{1}H NMR of compound (5ab)

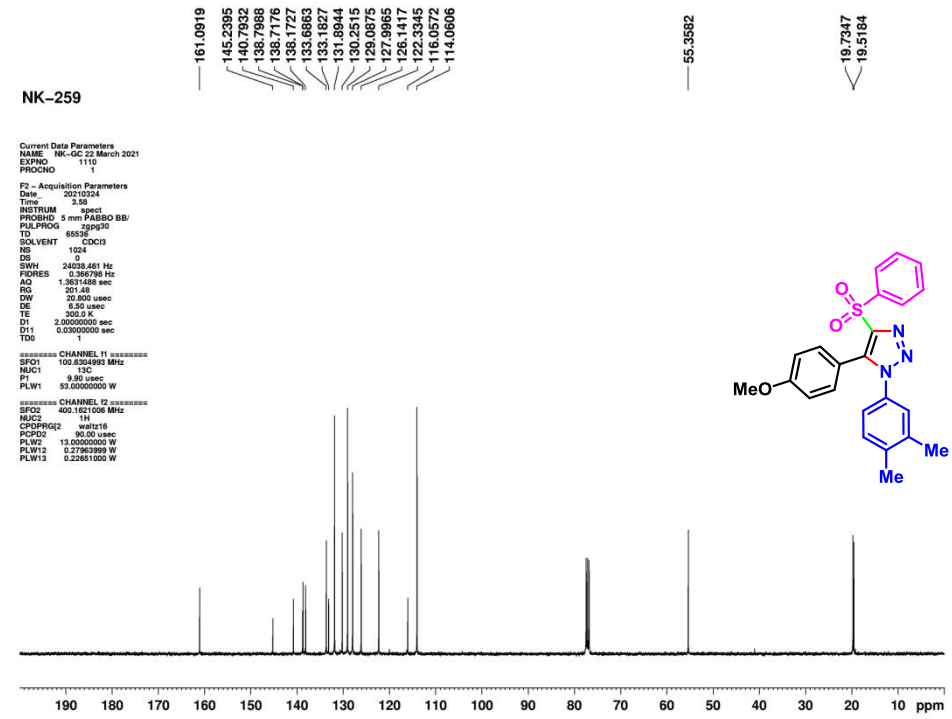


Figure S67: ^{13}C NMR of compound (5ab)

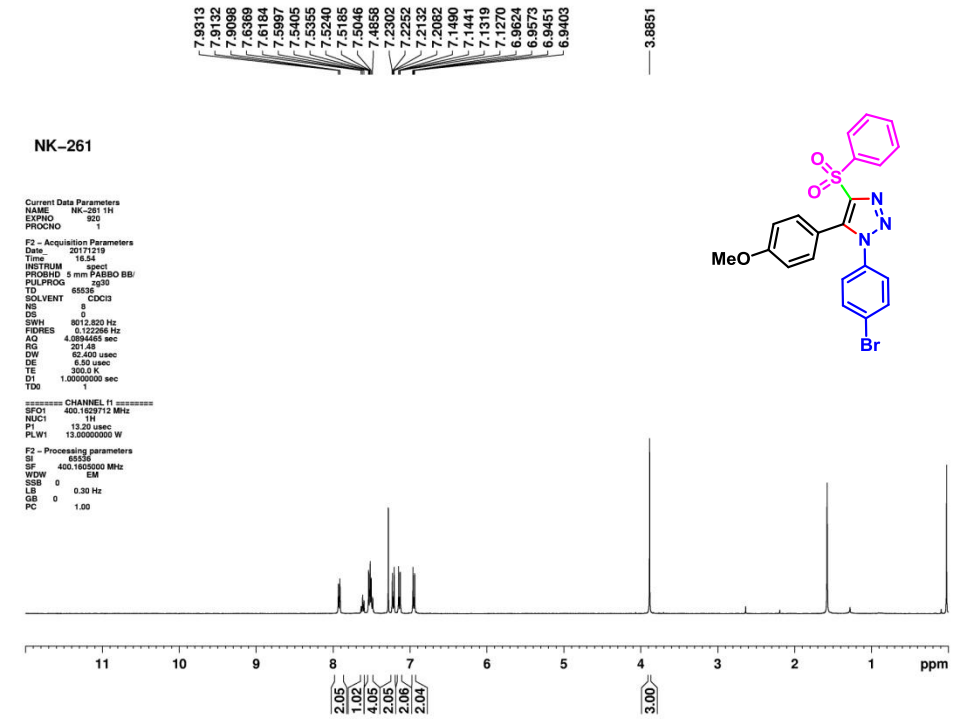


Figure S68: ^{1}H NMR of compound (5ac)

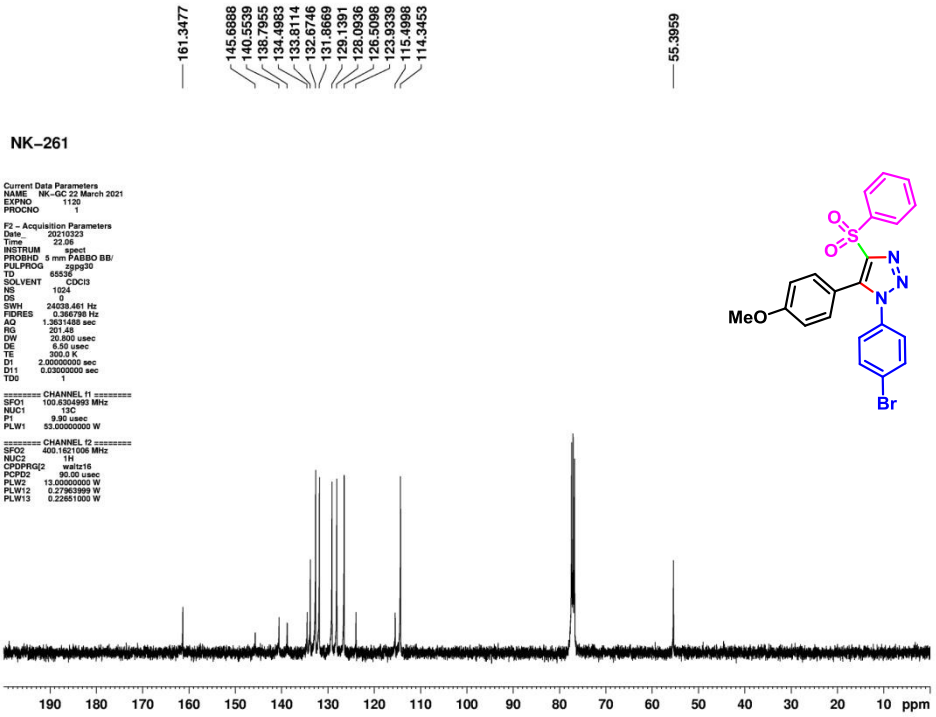


Figure S69: ^{13}C NMR of compound (5ac)

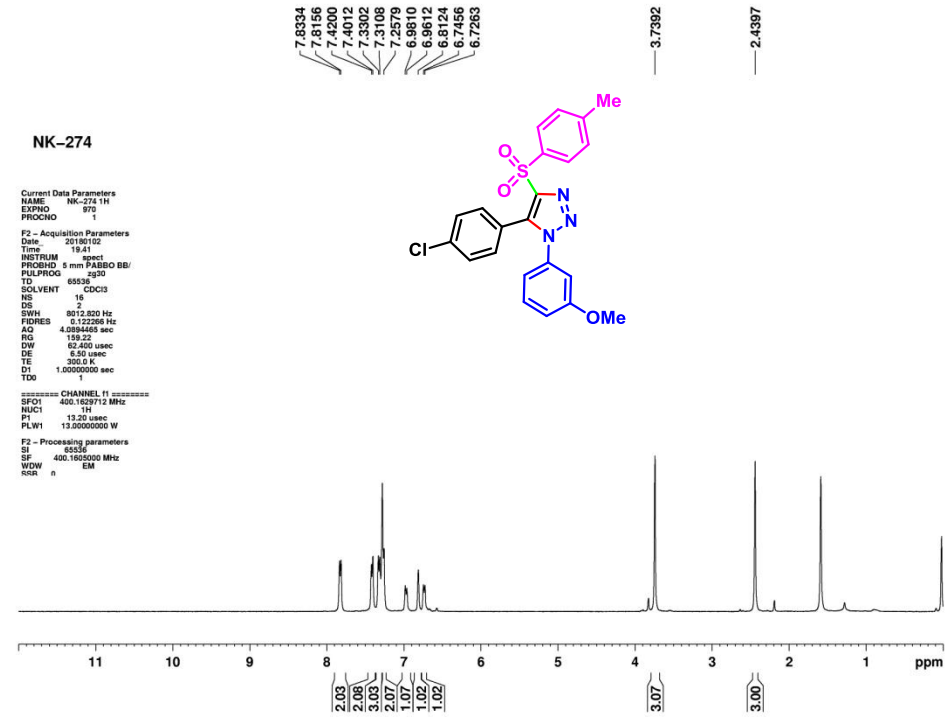


Figure S70: ^{1}H NMR of compound (5ad)

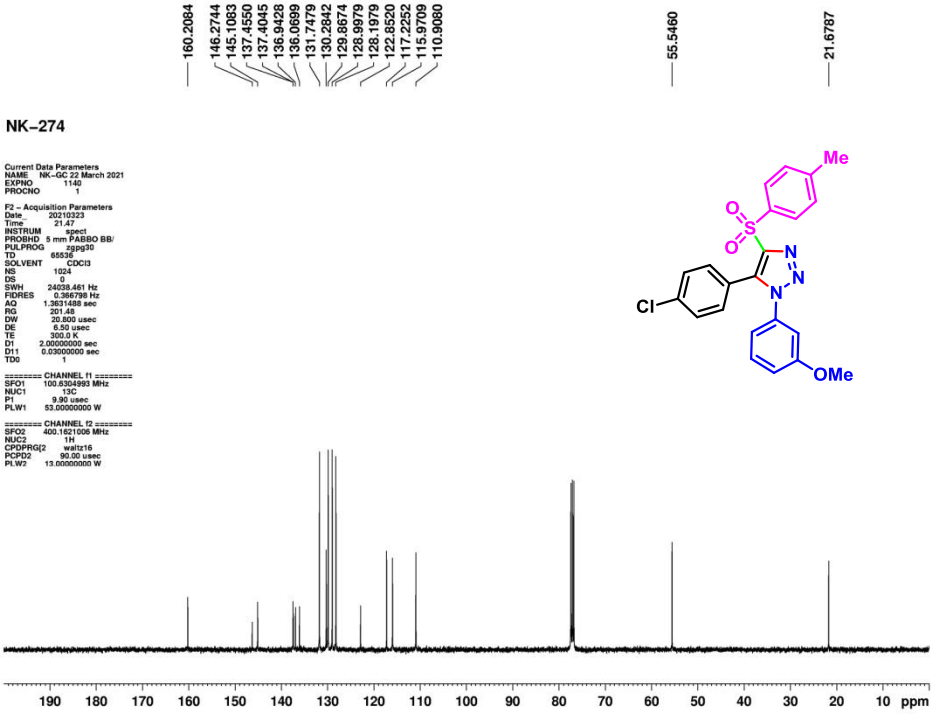


Figure S71: ^{13}C NMR of compound (5ad)

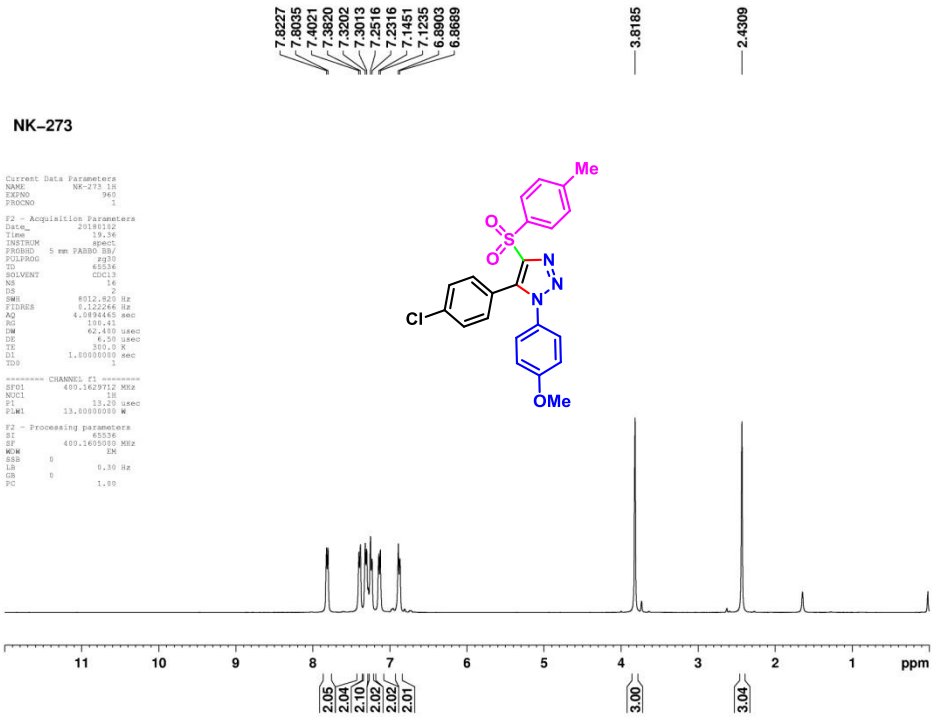


Figure S72: ^{1}H NMR of compound (5ae)

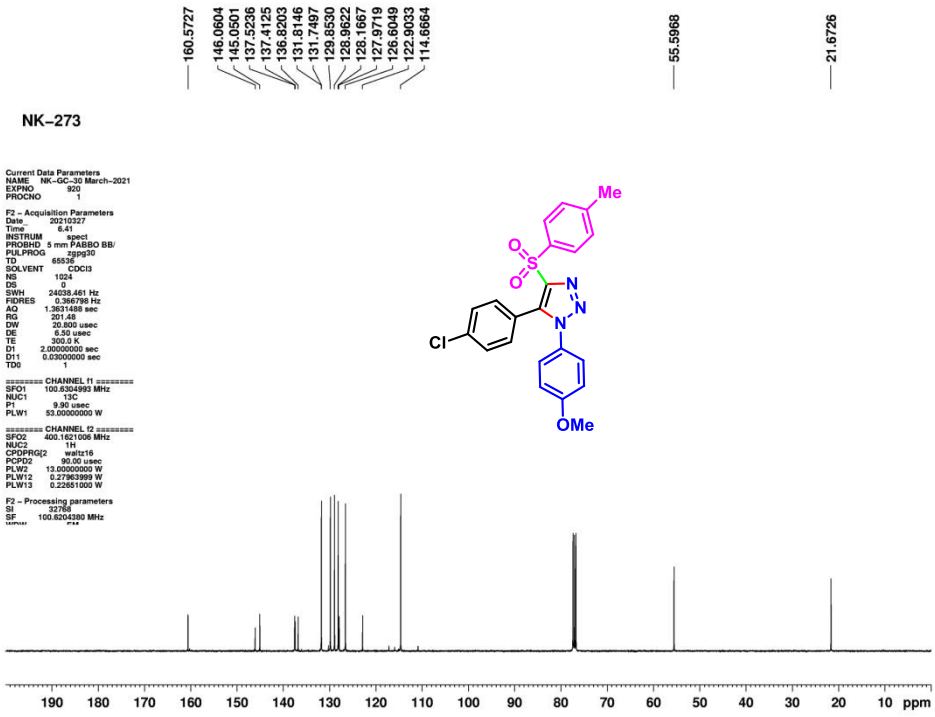


Figure S73: ^{13}C NMR of compound (5ae)

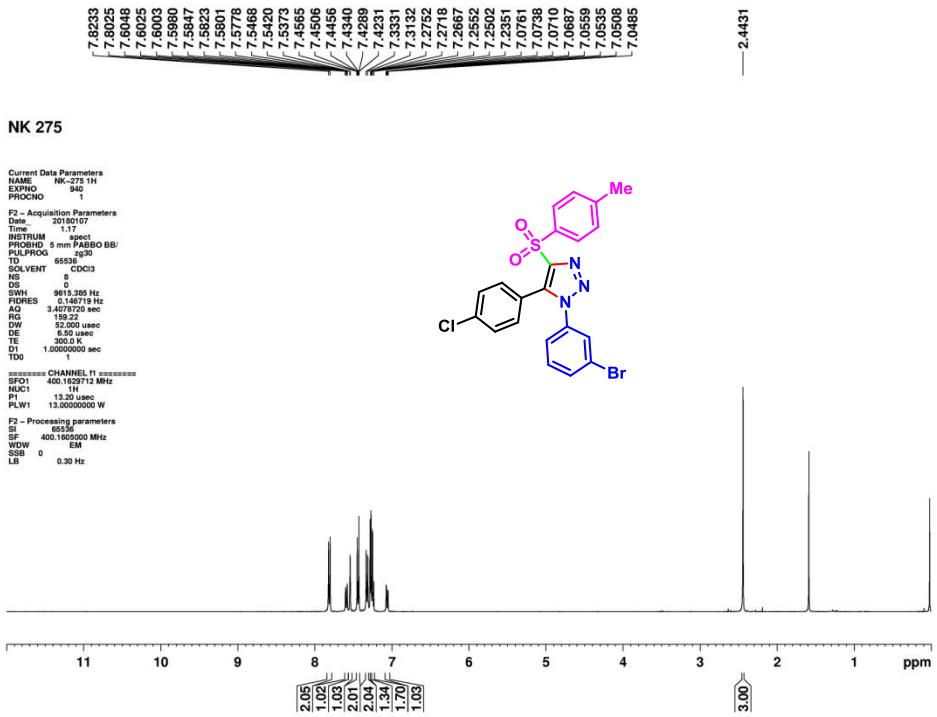


Figure S74: ^{1}H NMR of compound (5af)

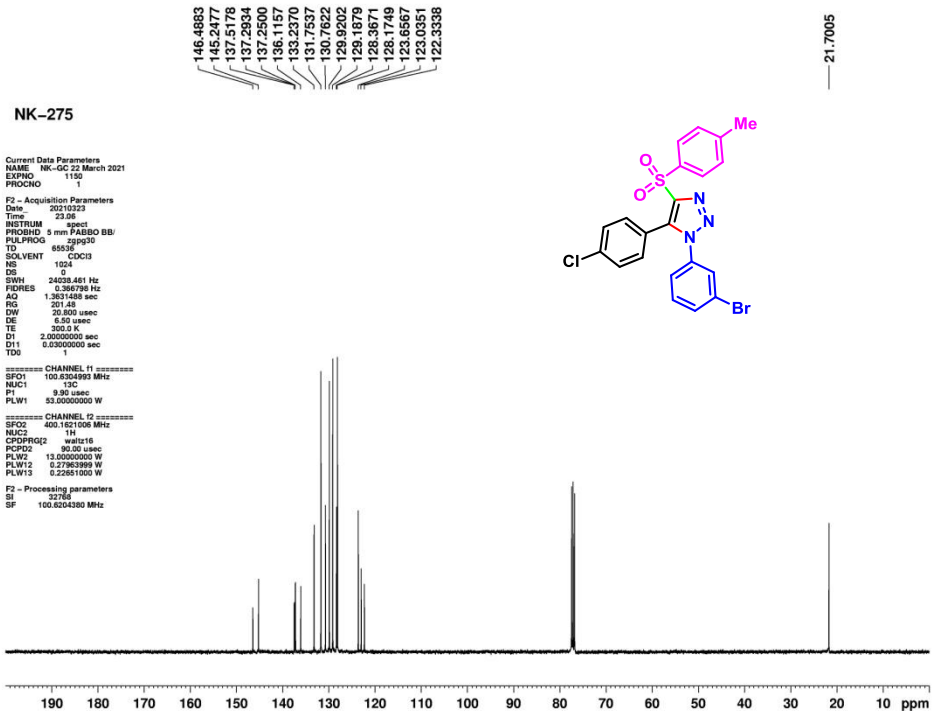


Figure S75: ^{13}C NMR of compound (5af)

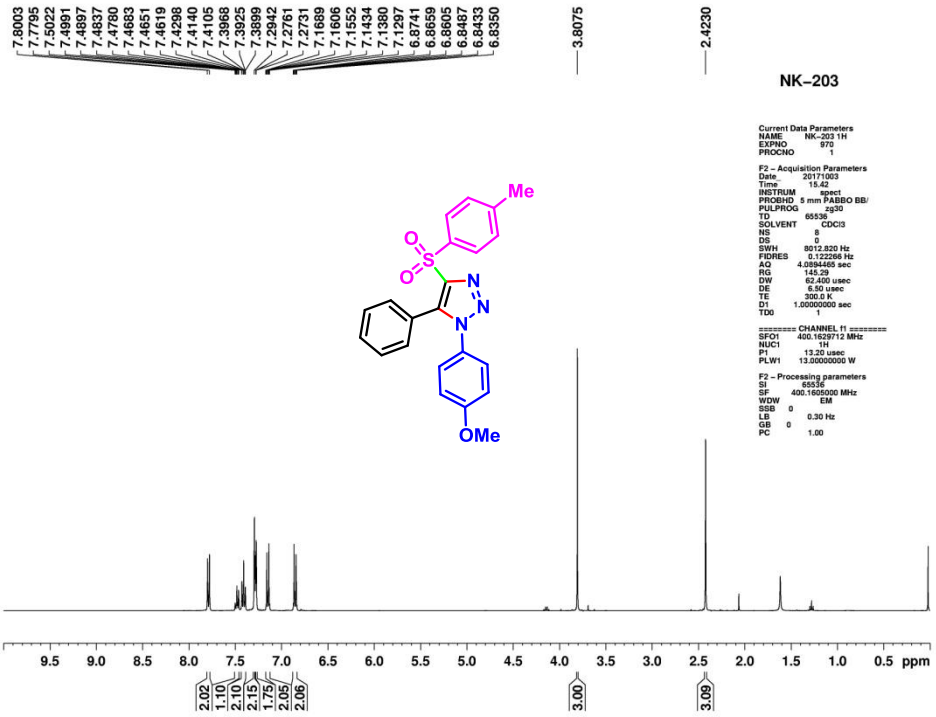


Figure S76: ^{1}H NMR of compound (5ag)

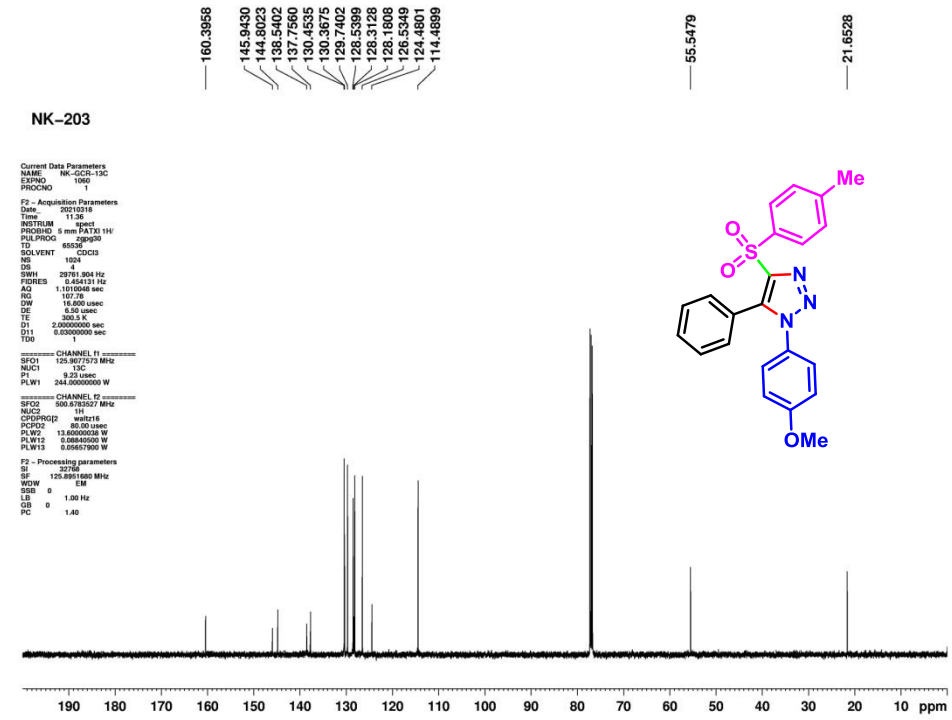


Figure S77: ^{13}C NMR of compound (5ag)

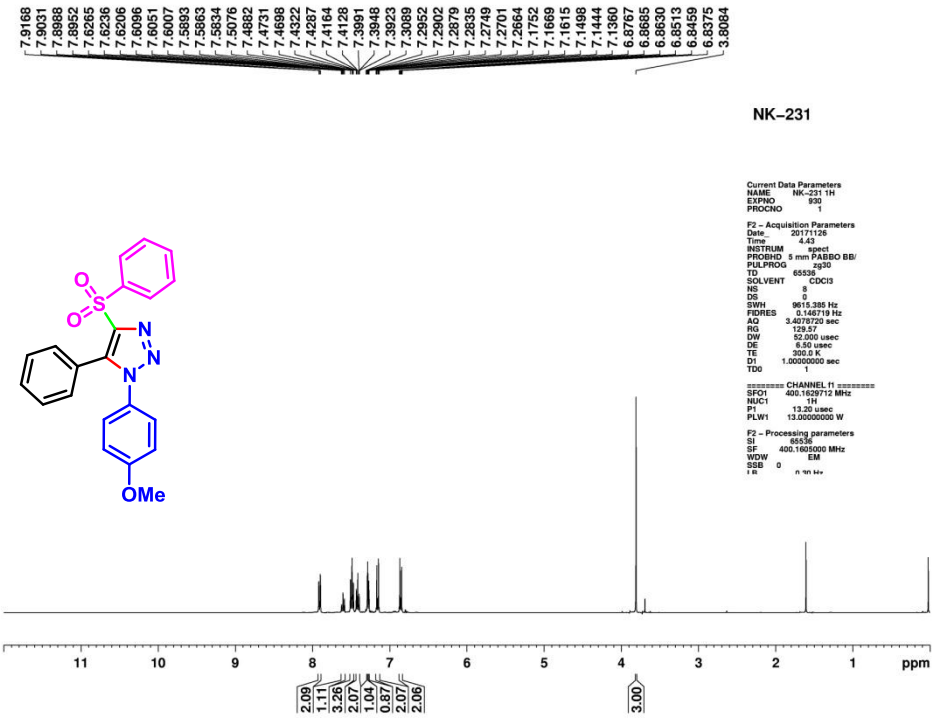


Figure S78: ^{1}H NMR of compound (5ah)

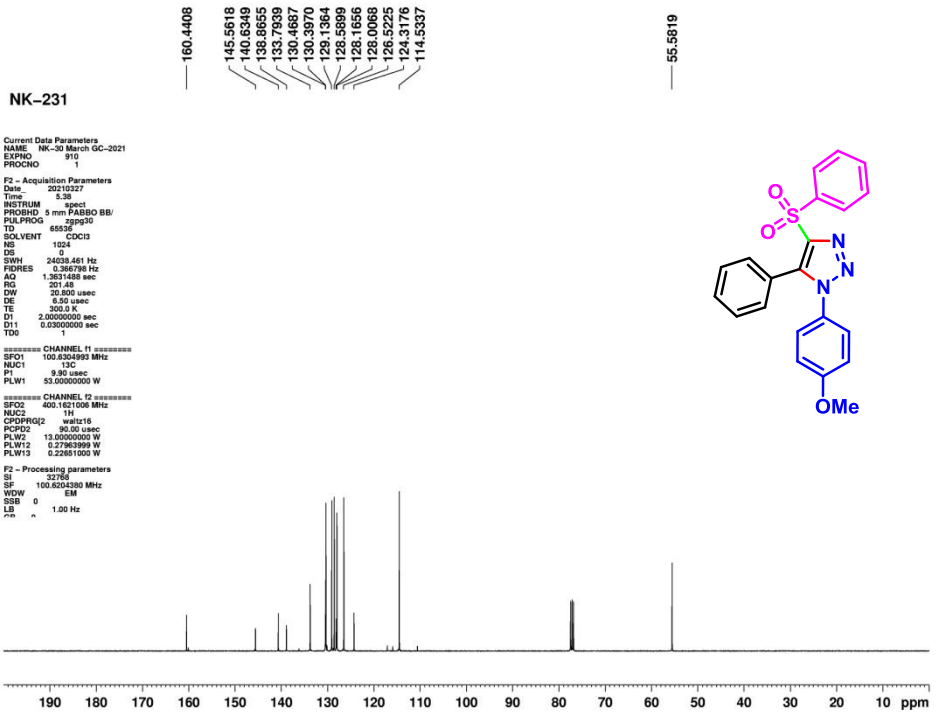


Figure S79: ^{13}C NMR of compound (5ah)

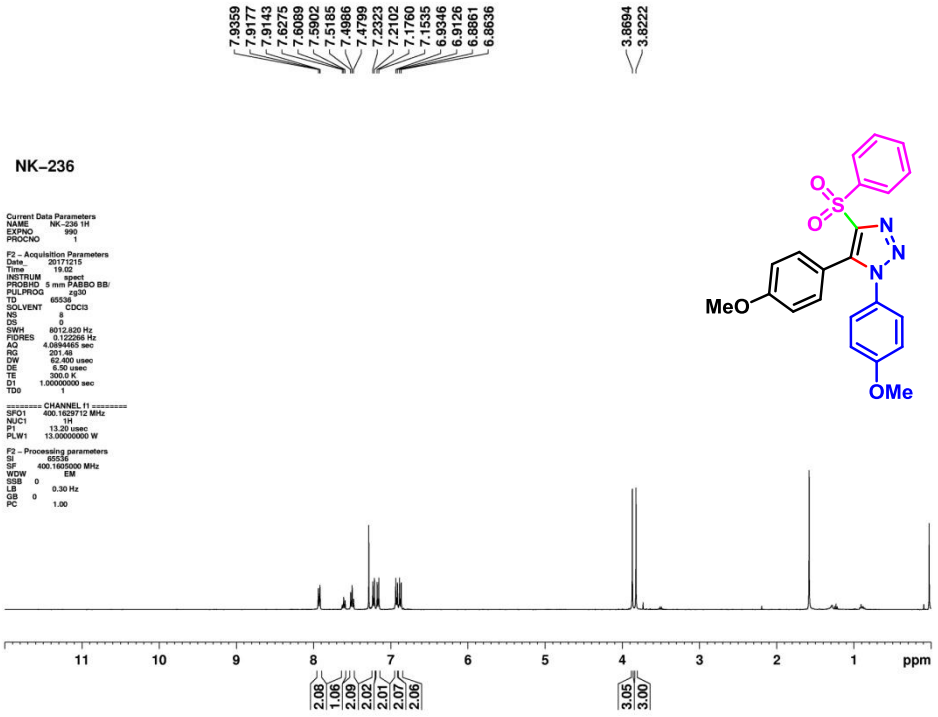


Figure S80: ^{1}H NMR of compound (5ai)

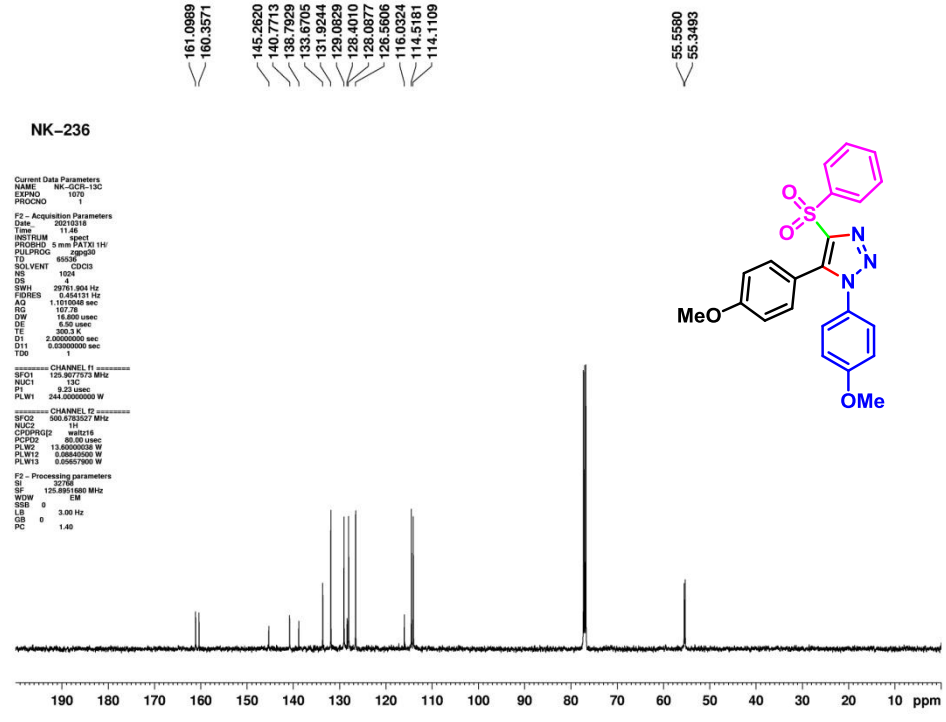


Figure S81: ^{13}C NMR of compound (5ai)

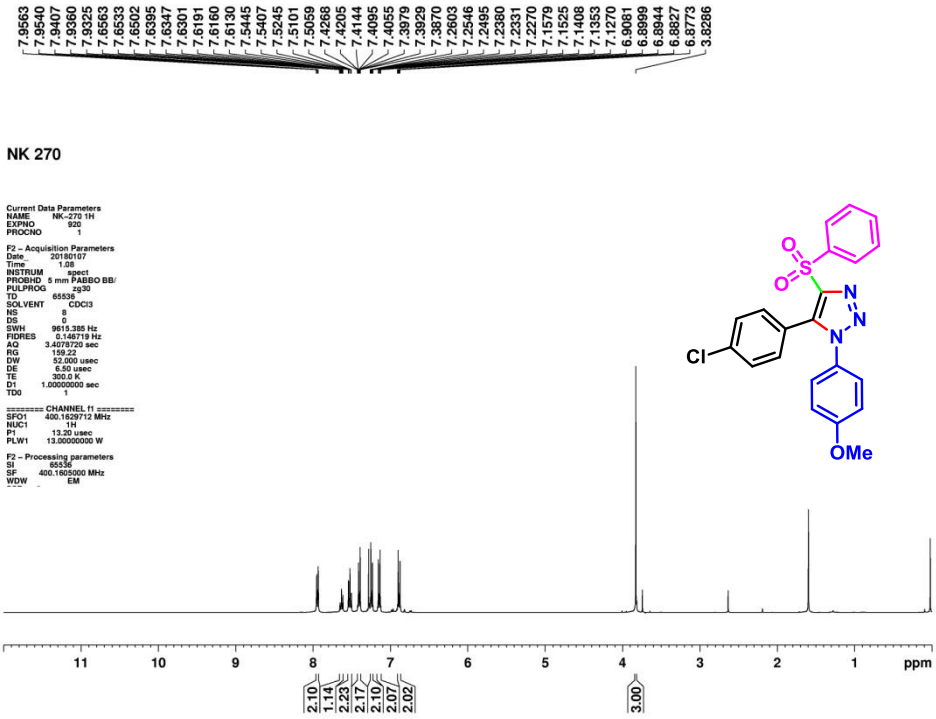


Figure S82: ^{1}H NMR of compound (5aj)

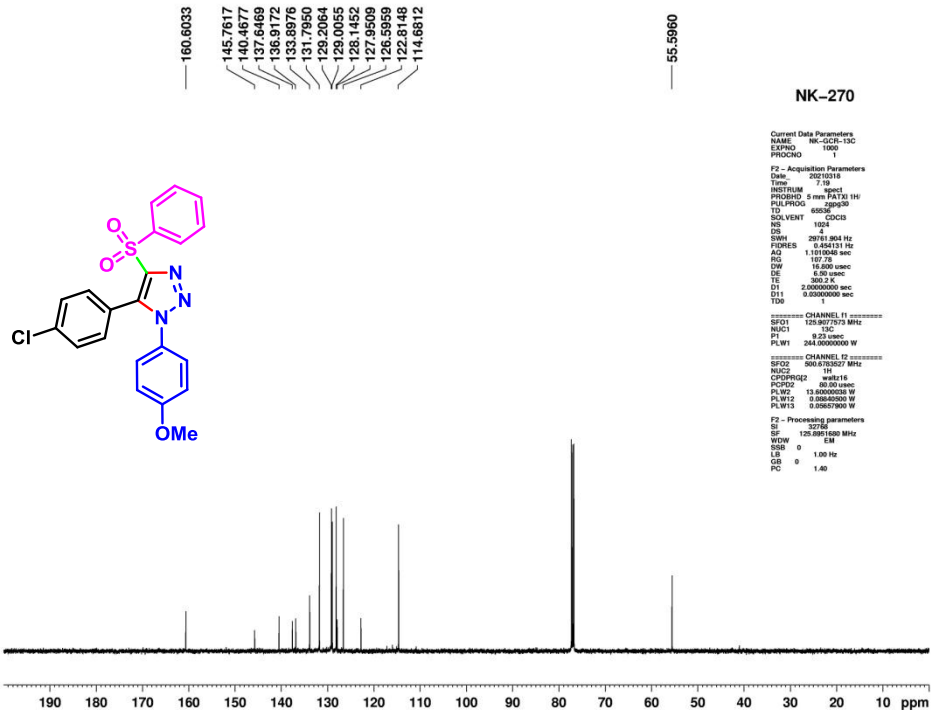


Figure S83: ^{13}C NMR of compound (5aj)

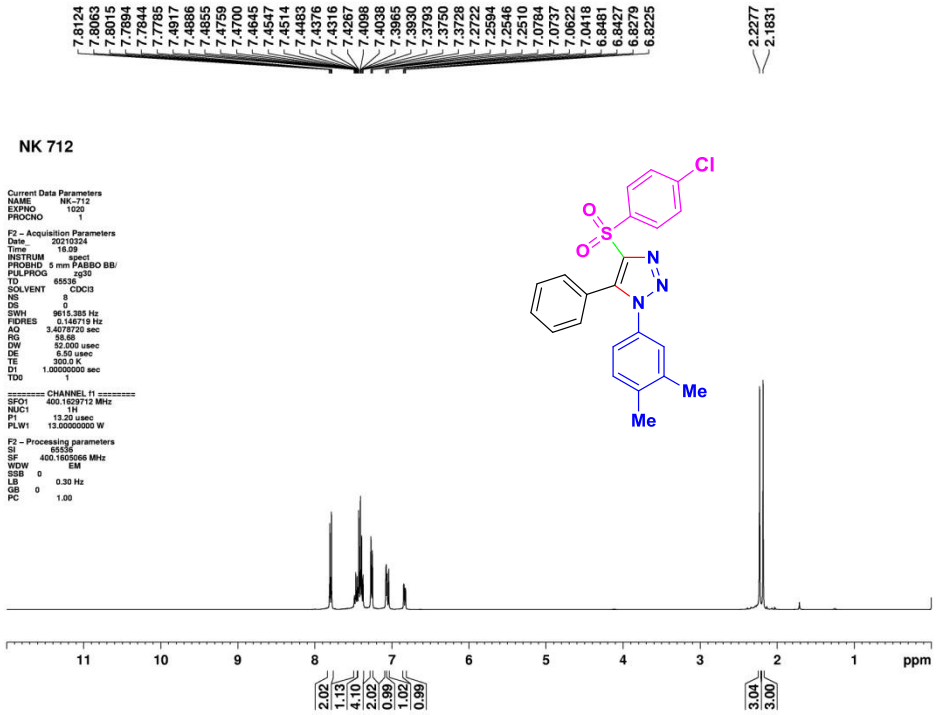


Figure S84: ^{1}H NMR of compound (5ak)

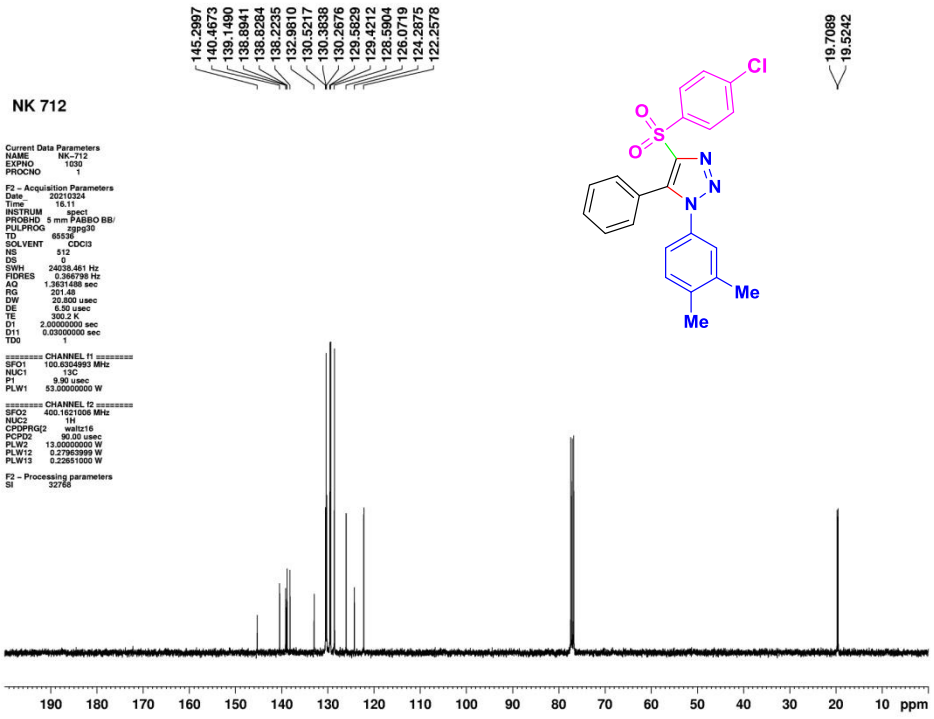


Figure S85: ^{13}C NMR of compound (5ak)

(10) X-Ray Data for Compound (5n)

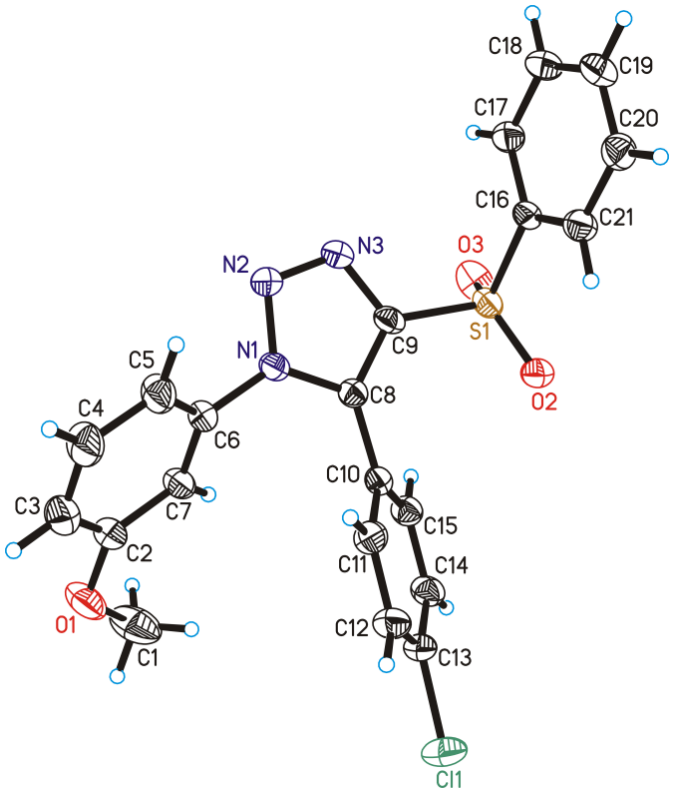


Figure S86 ORTEP diagram drawn with 30% ellipsoid probability for non-H atoms of the crystal structure of compound (**5n**).

X-Ray Data Collection and Structure Refinement Details:

A good quality Yellow color single crystal of size 0.32 x 0.28 x 0.08 mm, was selected under a polarizing microscope and was mounted on a glass fiber for data collection. Single crystal X-ray data for compound **5n** were collected on the Rigaku Kappa 3 circle diffractometer equipped with the AFC12 goniometer and enhanced sensitivity (HG) Saturn724+ CCD detector in the 4x4 bin mode using the monochromated Mo-Kα radiation generated from the microfocus sealed tube MicroMax-003 X-ray generator equipped with specially designed confocal multilayer optics. Data collection was performed using ω-scans of 0.5^{o} steps at 273K. Cell determinations, data collection and data reduction was performed using the Rigaku CrystalClear-SM Expert 2.1 b24[1] software. Structure solution and refinement were performed by using SHELXTL-NT[2]. Refinement of coordinates and anisotropic thermal parameters of non-hydrogen atoms were carried out by the full-matrix least-squares method. The hydrogen atoms attached to carbon atoms were generated with idealized geometries and isotropically refined using a riding model.

1. CrystalClear 2.1, Rigaku Corporation, Tokyo, Japan
2. Sheldrick, G. M. Acta Crystallogr., Sect. A 2008, 64, 112-122.

Supplementary:

Table S2 Crystal data and structure refinement details for (**5n**).

Compound	**5n**
Empirical formula	$C_{21}H_{16}ClN_3O_3S$
Formula weight	425.88
Temperature/K	273.15
Crystal system	triclinic
Space group	*P*-1
a/Å	8.3414(8)
b/Å	10.8615(11)
c/Å	11.6407(12)
α/°	69.332(3)
β/°	87.543(3)
γ/°	76.539(3)
Volume/Å^3	958.77(17)
Z	2
ρ_{calc}g/cm^3	1.475
μ/mm^{-1}	0.337
F(000)	440.0
Crystal size/mm^3	0.032 × 0.025 × 0.021
Radiation	synchrotron (λ = 0.71073)
2Θ range for data collection/°	5.026 to 56.718
Index ranges	$-11 \leq h \leq 11$, $-14 \leq k \leq 14$, $-15 \leq l \leq 15$
Reflections collected	20402
Independent reflections	4789 [R_{int} = 0.0375, R_{sigma} = 0.0309]
Data/restraints/parameters	4789/0/263
Goodness-of-fit on F^2	1.085
Final R indexes [I>=2σ (I)]	R_1 = 0.0346, wR_2 = 0.0836
Final R indexes [all data]	R_1 = 0.0411, wR_2 = 0.0887
Largest diff. peak/hole / e Å^{-3}	0.39/-0.46
CCDC No.	2092855