Supporting Information

Synthesis, bioevaluation and molecular docking study of new piperazine and amide linked dimeric 1,2,3-triazoles

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Experimental:

Synthesis of 1,4-di(prop-2-yn-1-yl)piperazine (1)

In a round bottom flask the mixture of piperazine (0.01 mol), NaH and propargyl bromide (0.02 mol) dissolved in DMF. The solution was stirred at room temperature for 2 h. The progress of the reaction was monitored by TLC using ethyl acetate: hexane (1:9) as a solvent system. After completion of the reaction, the reaction mixture was poured on crushed ice. Ethyl acetate was added to the mixture and the organic layer was separated. The aqueous layer was extracted with 3 x 10 mL of ethyl acetate and the combined organic layers were dried over $MgSO_4$. Solvent was removed under reduced pressure, and the off white solid of 1,4-di(prop-2-yn-1-yl)piperazine (**1**) was obtained which was sufficiently pure to use without further work up.[1]

Synthesis of azides (2a-r)

a) Synthesis of intermediates

In a round bottom flask, primary or secondary amines (0.1 mol) and triethyl amine were dissolved in DCM and stirred at 0 °C. 2-Chloroacetyl chloride (0.1 mol) was added to

reaction mixture drop wise with continuous stirring on magnetic stirrer. After the addition, the ice bath was removed and the reaction mixture was stirred at room temperature for 4 h. The progress of the reaction was monitored by TLC using ethyl acetate: hexane (1:9) as a solvent system. After completion of the reaction, the reaction mixture was poured on crushed ice and neutralised by adding acetic acid to it. The obtained solid intermediates of respective amines were filtered, dried and crystallised in ethanol.

b) Synthesis of azides (2a-r)

The freshly synthesized above intermediates were heated at 100 °C with sodium azide (0.1 mol) in DMF-H_2O for 6 h. The progress of the reaction was monitored by TLC using ethyl acetate: hexane (1:9) as a solvent system. The reaction mixture was poured on crushed ice. Ethyl acetate was added to the mixture and the organic layer was separated. The organic layers were dried over $MgSO_4$ and solvent was removed under reduced pressure. All the azides **(2a-r)** were synthesized from respective amines, were obtained as solid compounds except azide **(2e)** obtained from o-anisidine in liquid state. This azide **(2e)** was extracted in organic layer using ethyl acetate and solvent is removed under reduced pressure. After this it was used for further reaction without any purification. All the newly synthesized solid azides were crystallised in ethanol and then used for further reaction.[2]

Synthesis of 2,2'-(4,4'-(piperazine-1,4-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis (N,N-dimethylacetamide) (3a)

The compound (**3a**) was obtained by Cu (I)-catalyzed 1,3-dipolar cycloaddition reaction between 1,4-di(prop-2-yn-1-yl)piperazine (**1**) and azide (**2a**) as dark greenish solid; Yield: 68 %; Mp: 182-185 °C; ^{1}H NMR (400 MHz, DMSO-d_6, δ_H ppm) 2.75 (s, 4H, piperazinyl-H), 2.91 (s, 4H, piperazinyl-H), 4.16 (s, 12H, 4×CH_3), 4.73 (s, 4H, piperazinyl N-CH_2), 5.59 (s, 4H, triazolyl N-CH_2), 8.66 (s, 2H, triazolyl-H); ^{13}C NMR (100 MHz, DMSO-d_6, δ_C ppm) 39.3, 60.7, 70.3, 72.9, 129.7, 133.6, 159.0; HRMS (ESI) calcd. for $C_{18}H_{31}N_{10}O_2$ M+H^+: 419.2632; found 419.2638.

Synthesis of 2,2'-(4,4'-(piperazine-1,4-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis (N-phenylacetamide) (3b)

The compound (**3b**) was obtained by Cu (I)-catalyzed 1,3-dipolar cycloaddition reaction between 1,4-di(prop-2-yn-1-yl)piperazine (**1**) and azide (**2b**) as dark greenish solid; Yield: 94

%; Mp: >270 °C; ^{1}H NMR (400 MHz, DMSO-d_6, δ_H ppm) 2.95 (s, 4H, piperazinyl-H), 3.02 (s, 4H, piperazinyl-H), 4.78 (s, 4H, piperazinyl N-CH_2), 5.38 (s, 4H, triazolyl N-CH_2), 7.14-7.63 (m, 10H, Ar-H), 8.68 (s, 2H, triazolyl-H), 10.58 (s, 2H, amido N-H); ^{13}C NMR (100 MHz, DMSO-d_6, δ_C ppm) 24.5, 70.2, 72.8, 116.9, 119.3, 133.1, 133.5, 135.1, 138.5, 162.0; HRMS (ESI) calcd. for $C_{26}H_{31}N_{10}O_2$ M+H^+: 515.2632; found 515.2636.

Synthesis of 2,2'-(4,4'-(piperazine-1,4-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis (N-(o-tolyl)acetamide) (3c)

The compound (**3c**) was obtained by Cu (I)-catalyzed 1,3-dipolar cycloaddition reaction between 1,4-di(prop-2-yn-1-yl)piperazine (**1**) and azide (**2c**) as brownish solid; Yield: 90 %; Mp: 158-160 °C; ^{1}H NMR (400 MHz, DMSO-d_6, δ_H ppm) 2.30 (s, 6H, 2×CH_3), 2.80 (s, 4H, piperazinyl-H), 2.96 (s, 4H, piperazinyl-H), 4.79 (s, 4H, piperazinyl N-CH_2), 5.58 (s, 4H, triazolyl N-CH_2), 7.24-8.03 (m, 8H, Ar-H), 8.71 (s, 2H, triazolyl-H), 9.91 (s, 2H, amido N-H); ^{13}C NMR (100 MHz, DMSO-d_6, δ_C ppm) 18.3, 31.3, 36.3, 70.3, 125.3, 126.1, 126.2, 126.6, 131.0, 132.2, 132.2, 162.9, 171.2; HRMS (ESI) calcd. for $C_{28}H_{35}N_{10}O_2$ M+H^+: 543.2945; found 543.2947.

Synthesis of 2,2'-(4,4'-(piperazine-1,4-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis (N-(m-tolyl)acetamide) (3d)

The compound (**3d**) was obtained by Cu (I)-catalyzed 1,3-dipolar cycloaddition reaction between 1,4-di(prop-2-yn-1-yl)piperazine (**1**) and azide (**2d**) as light greenish solid; Yield: 87 %; Mp: 188-190 °C; ^{1}H NMR (400 MHz, DMSO-d_6, δ_H ppm) 2.34 (s, 6H, 2×CH_3), 2.85 (s, 4H, piperazinyl-H), 3.09 (s, 4H, piperazinyl-H), 4.79 (s, 4H, piperazinyl N-CH_2), 5.52 (s, 4H, triazolyl N-CH_2), 6.98-7.47 (m, 8H, Ar-H), 8.70 (s, 2H, triazolyl-H), 10.46 (s, 2H, amido N-H); ^{13}C NMR (100 MHz, DMSO-d_6, δ_C ppm) 21.7, 60.7, 70.3, 72.8, 116.9, 120.3, 125.1, 129.3, 131.2, 136.4, 138.7, 163.4, 175.0; HRMS (ESI) calcd. for $C_{28}H_{35}N_{10}O_2$ M+H^+: 543.2945; found 543.2946.

Synthesis of 2,2'-(4,4'-(piperazine-1,4-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis (N-(p-tolyl)acetamide) (3e)

The compound (**3e**) was obtained by Cu (I)-catalyzed 1,3-dipolar cycloaddition reaction between 1,4-di(prop-2-yn-1-yl)piperazine (**1**) and azide (**2e**) as dark greenish solid; Yield: 88 %; Mp: 210-211 °C; ^{1}H NMR (400 MHz, DMSO-d_6, δ_H ppm) 2.29 (s, 6H, 2×CH_3), 2.77 (s,

4H, piperazinyl-H), 2.93 (s, 4H, piperazinyl-H), 4.67 (s, 4H, piperazinyl N-CH_2), 5.39 (s, 4H, triazolyl N-CH_2), 7.17-7.49 (m, 8H, Ar-H), 8.02 (s, 2H, triazolyl-H), 10.41 (s, 2H, amido N-H); ^{13}C NMR (100 MHz, DMSO-d_6, δ_C ppm) 26.7, 62.2, 66.6, 70.8, 119.6, 122.2, 126.6, 129.6, 140.1, 144.1, 163.2; HRMS (ESI) calcd. for $C_{28}H_{35}N_{10}O_2$ M+H^+: 543.2945; found 543.2948.

Synthesis of 2,2'-(4,4'-(piperazine-1,4-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis (N-(3-methoxyphenyl)acetamide) (3f)

The compound (**3f**) was obtained by Cu (I)-catalyzed 1,3-dipolar cycloaddition reaction between 1,4-di(prop-2-yn-1-yl)piperazine (**1**) and azide (**2f**) as brownish solid; Yield: 84 %; Mp: 157-160 °C; ^{1}H NMR (400 MHz, DMSO-d_6, δ_H ppm) 2.96 (s, 4H, piperazinyl-H), 3.12 (s, 4H, piperazinyl-H), 3.94 (s, 6H, 2OCH_3), 5.01 (s, 4H, piperazinyl N-CH_2), 5.71 (s, 4H, triazolyl N-CH_2), 6.92-8.25 (m, 8H, Ar-H), 8.91 (s, 2H, triazolyl-H), 10.80 (s, 2H, amido N-H); ^{13}C NMR (100 MHz, DMSO-d_6, δ_C ppm) 31.5, 36.5, 53.4, 55.8, 105.8, 110.0, 112.2, 112.5, 124.8, 130.5, 140.2, 160.3, 164.8; HRMS (ESI) calcd. for $C_{28}H_{35}N_{10}O_4$ M+H^+: 575.2843; found 575.2890.

Synthesis of 2,2'-(4,4'-(piperazine-1,4-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis (N-(4-methoxyphenyl)acetamide) (3g)

The compound (**3g**) was obtained by Cu (I)-catalyzed 1,3-dipolar cycloaddition reaction between 1,4-di(prop-2-yn-1-yl)piperazine (**1**) and azide (**2g**) as light greenish solid; Yield: 88 %; Mp: 203-205 °C; ^{1}H NMR (400 MHz, DMSO-d_6, δ_H ppm) 2.75 (s, 4H, piperazinyl-H), 2.91 (s, 4H, piperazinyl-H), 3.73 (s, 6H, 2OCH_3), 4.12 (s, 4H, piperazinyl N-CH_2), 5.29 (s, 4H, triazolyl N-CH_2), 6.91 (d, 4H, Ar-H), 7.49 (d, 4H, Ar-H), 8.03 (s, 2H, triazolyl-H), 10.34 (s, 2H, amido N-H); ^{13}C NMR (100 MHz, DMSO-d_6, δ_C ppm) 31.3, 36.3, 55.7, 58.0, 114.5, 119.4, 121.3, 132.3, 132.8, 156.1, 162.9; HRMS (ESI) calcd. for $C_{28}H_{35}N_{10}O_4$ [M+H]$^+$: 575.2843; found 575.2852.

Synthesis of 2,2'-(4,4'-(piperazine-1,4-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis (N-(2-chlorophenyl)acetamide) (3h)

The compound (**3h**) was obtained by Cu (I)-catalyzed 1,3-dipolar cycloaddition reaction between 1,4-di(prop-2-yn-1-yl)piperazine (**1**) and azide (**2h**) as light greenish solid; Yield: 77 %; Mp: 193-195 °C; ^{1}H NMR (400 MHz, DMSO-d_6, δ_H ppm) 2.75 (s, 4H, piperazinyl-H),

2.91 (s, 4H, piperazinyl-H), 4.73 (s, 4H, piperazinyl N-CH_2), 5.59 (s, 4H, triazolyl N-CH_2), 7.25-7.75 (m, 8H, Ar-H), 8.66 (s, 2H, triazolyl-H), 10.16 (s, 2H, amido N-H); ^{13}C NMR (100 MHz, DMSO-d_6, δ_C ppm) 52.1, 55.6, 61.2, 126.0, 126.4, 126.5, 126.9, 127.0, 127.7, 129.8, 130.2, 165.0; HRMS (ESI) calcd. for $C_{26}H_{28}Cl_2N_{10}O_2Na$ M+Na: 605.4671; found 605.4712.

Synthesis of 2,2'-(4,4'-(piperazine-1,4-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis (N-(3-chlorophenyl)acetamide) (3i)

The compound (**3i**) was obtained by Cu (I)-catalyzed 1,3-dipolar cycloaddition reaction between 1,4-di(prop-2-yn-1-yl)piperazine (**1**) and azide (**2i**) as brownish green solid; Yield: 80 %; Mp: 179-180 °C; ^{1}H NMR (400 MHz, DMSO-d_6, δ_H ppm) 2.82 (s, 4H, piperazinyl-H), 2.98 (s, 4H, piperazinyl-H), 4.82 (s, 4H, piperazinyl N-CH_2), 5.58 (s, 4H, triazolyl N-CH_2), 7.25-7.87 (m, 8H, Ar-H), 8.73 (s, 2H, triazolyl-H), 10.82 (s, 2H, amido N-H); ^{13}C NMR (100 MHz, DMSO-d_6, δ_C ppm) 31.3, 36.3, 52.9, 118.2, 119.3, 131.1, 133.7, 134.8, 140.1, 162.9, 164.8; HRMS (ESI) calcd. for $C_{26}H_{29}Cl_2N_{10}O_2$ M+H^+: 583.1853; found 583.1850.

Synthesis of 2,2'-(4,4'-(piperazine-1,4-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis (N-(4-chlorophenyl)acetamide) (3j)

The compound (**3j**) was obtained by Cu (I)-catalyzed 1,3-dipolar cycloaddition reaction between 1,4-di(prop-2-yn-1-yl)piperazine (**1**) and azide (**2j**) as light greenish solid; Yield: 84 %; Mp: >270 °C; ^{1}H NMR (400 MHz, DMSO-d_6, δ_H ppm) 2.75 (s, 4H, piperazinyl-H), 2.91 (s, 4H, piperazinyl-H), 4.73 (s, 4H, piperazinyl N-CH_2), 5.46 (s, 4H, triazolyl N-CH_2), 7.55-7.75 (m, 8H, Ar-H), 8.66 (s, 2H, triazolyl-H), 10.09 (s, 2H, amido N-H); ^{13}C NMR (100 MHz, CD_3OD, δ_C ppm) 41.7, 53.6, 74.9, 100.3, 102.0, 115.0, 116.9, 120.0, 121.7, 163.2; HRMS (ESI) calcd. for $C_{26}H_{29}Cl_2N_{10}O_2$ M+H^+: 583.1853; found 583.1858.

Synthesis of 2,2'-(4,4'-(piperazine-1,4-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis (N-(2-nitrophenyl)acetamide) (3k)

The compound (**3k**) was obtained by Cu (I)-catalyzed 1,3-dipolar cycloaddition reaction between 1,4-di(prop-2-yn-1-yl)piperazine (**1**) and azide (**2k**) as yellowish brown solid; Yield: 81 %; Mp: 185-187 °C; ^{1}H NMR (400 MHz, DMSO-d_6, δ_H ppm) 2.90 (s, 4H, piperazinyl-H), 3.06 (s, 4H, piperazinyl-H), 4.89 (s, 4H, piperazinyl N-CH_2), 5.71 (s, 4H, triazolyl N-CH_2), 7.59-8.14 (m, 8H, Ar-H), 8.79 (s, 2H, triazolyl-H), 10.94 (s, 2H, amido N-H);^{13}C NMR (100

MHz, DMSO-d_6, δ_C ppm) 52.8, 62.2, 62.2, 70.2, 125.6, 125.6, 126.0, 126.5, 130.7, 134.7, 142.9, 165.2, 168.8; HRMS (ESI) calcd. for $C_{26}H_{29}N_{12}O_6$ M+H^+: 605.2334; found 605.2341.

Synthesis of 2,2'-(4,4'-(piperazine-1,4-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis (N-(3-nitrophenyl)acetamide) (3l)

The compound (**3l**) was obtained by Cu (I)-catalyzed 1,3-dipolar cycloaddition reaction between 1,4-di(prop-2-yn-1-yl)piperazine (**1**) and azide (**2l**) as dark brownish solid; Yield: 77 %; Mp: 133-135 °C; ^{1}H NMR (400 MHz, DMSO-d_6, δ_H ppm) 2.90 (s, 4H, piperazinyl-H), 3.06 (s, 4H, piperazinyl-H), 4.96 (s, 4H, piperazinyl N-CH_2), 5.72 (s, 4H, triazolyl N-CH_2), 7.81-8.15 (m, 8H, Ar-H), 8.78 (s, 2H, triazolyl-H), 11.24 (s, 2H, amido N-H);^{13}C NMR (100 MHz, DMSO-d_6, δ_C ppm) 31.3, 36.3, 70.2, 113.8, 118.9, 125.7, 130.9, 131.3, 139.8, 148.4, 162.9, 165.3; HRMS (ESI) calcd. for $C_{26}H_{29}N_{12}O_6$ M+H^+: 605.2334; found 605.2337.

Synthesis of 2,2'-(4,4'-(piperazine-1,4-diylbis(methylene))bis(1H-1,2,3-triazole-4,1-diyl))bis (N-(4-nitrophenyl)acetamide) (3m)

The compound (**3m**) was obtained by Cu (I)-catalyzed 1,3-dipolar cycloaddition reaction between 1,4-di(prop-2-yn-1-yl)piperazine (**1**) and azide (**2m**) as greenish solid; Yield: 83 %; Mp: 245-247 °C; ^{1}H NMR (400 MHz, DMSO-d_6, δ_H ppm) 2.94 (s, 4H, piperazinyl-H), 3.10 (s, 4H, piperazinyl-H), 4.80 (s, 4H, piperazinyl N-CH_2), 5.73 (s, 4H, triazolyl N-CH_2), 8.03-8.20 (m, 8H, Ar-H), 8.82 (s, 2H, triazolyl-H), 11.36 (s, 2H, amido N-H); ^{13}C NMR (100 MHz, DMSO-d_6, δ_C ppm) 31.3, 36.3, 60.7, 72.8, 112.9, 119.6, 125.6, 126.8, 143.2, 148.4, 163.0; HRMS (ESI) calcd. for $C_{26}H_{29}N_{12}O_6$ M+H^+: 605.2334; found 605.2339.

Experimental protocol for biological activity

***In vitro Mtb* MABA assay**

The antitubercular activity of newly synthesized Compounds (**3a-r**) have been screened for their *in vitro* effects against *Mtb H37Rv* (ATCC 27294) by using microplate Almar Blue assay (MABA)[3] for determination of MIC in triplicates. The MIC (in µg/mL) was recorded as the lowest concentration/highest dilution of the compounds/control drugs that completely inhibited the growth of *Mtb* cultures. The MIC values of compounds (**3a-r**) have been compared with standard drugs (Rifampicin, Isoniazid, Ethambutol and Ciprofoxacin). The experimental method for antitubercular activity is briefly described as follows-

Initially, the inoculum was prepared from fresh LJ medium re-suspended in 7H9-S medium (7H9 broth, 0.1% casitone, 0.5% glycerol, supplemented oleic acid, albumin, dextrose, and catalase OADC), adjusted to a McFarland tube No. 1, and diluted 1:20; 100 µl was used as inoculum. Each drug stock solution was thawed and diluted in 7H9-S at four-fold the final highest concentration tested. Serial two-fold dilutions of each drug were prepared directly in a sterile 96-well microtiter plate using 100µl 7H9-S. A growth control containing no antibiotic and a sterile control were also prepared on each plate. Sterile water was added to all perimeter wells to avoid evaporation during the incubation. The plate was covered, sealed in plastic bags and incubated at 37 ºC in normal atmosphere. After 7 days incubation, 30 µl of alamar blue solution was added to each well, and the plate was re-incubated overnight. A change in colour from blue (oxidised state) to pink (reduced) indicated the growth of bacteria, and the MIC was defined as the lowest concentration of drug that prevented this change in colour.

***In vitro* antifungal activity**

Antifungal activity was determined by standard agar dilution method as per CLSI (formerly, NCCLS) guidelines[4] These newly synthesized compounds were screened for their *in vitro* antifungal activity against five human pathogenic fungal strains such as *Candida albicans* (NCIM 3471), *Fusarium oxysporum* (NCIM 1332), *Aspargillus flavus* (NCIM 539), *Aspargillus niger* (NCIM 1196) and *Candida neoformans* (NCIM 576). The synthesized compounds and standard miconazole were dissolved in DMSO solvent. The medium yeast nitrogen base was dissolved in phosphate buffer pH 7 and it was autoclaved at 110 ℃ for 10 min. With each set, a growth control without the antifungal agent and solvent control DMSO were included. The fungal strains were freshly subcultured onto Sabouraud dextrose agar (SDA) and incubated at 25 ℃ for 72 h. The fungal cells were suspended in sterile distilled water and diluted to get 105 cells/mL. Ten microliters of standardized suspension was inoculated onto the control plates and the media incorporated with the antifungal agents. The inoculated plates were incubated at 25 ℃ for 48 h. The readings were taken at the end of 48 and 72 h. The MIC was the lowest concentration of drug preventing growth of macroscopically visible colonies on drug containing plates when there was visible growth on the drug free control plates.

General procedure for antioxidant activity

The antioxidant activity of all the synthesized compounds have been assessed *in vitro* by the 1,1-diphenyl-2-picrylhydrazyl (DPPH) radical scavenging assay[5] and the results were compared with standard synthetic antioxidant BHT (Butylated Hydroxy Toluene). The hydrogen atom or electron donation ability of the compounds were measured from the bleaching of the purple coloured methanol solution of 1,1-diphenyl-1-picrylhydrazyl (DPPH). The spectrophotometric assay uses the stable radical DPPH as a reagent. 1 mL of various concentrations of the test compounds (5, 10, 25, 50 and 100 mg/mL) in methanol was added to 4mL of 0.004% (w/v) methanol solution of DPPH. The reaction mixture was incubated at 37 °C. The scavenging activity on DPPH was determined by measuring the absorbance at 517 nm after 30 min. All tests were performed in triplicate and the mean values were entered. The percent of inhibition (I %) of free radical production from DPPH was calculated by the following equation

$$\% \text{ of scavenging} = (A_{control} - A_{sample})/(A_{sample} \times 100)$$

Where, $A_{control}$ is the absorbance of the control (DPPH radical without test sample) A_{sample} is the absorbance of the test sample (DPPH radical with test sample). The control contains all reagents except the test samples.

Molecular docking study

Molecular docking studies were performed using with *Glide* (Grid-Based Ligand Docking With Energetics) program[6] integrated in the Schrodinger molecular modeling package (Schrodinger, LLC, New York, NY, 2015). With this purpose, the crystal structure of mycobacterial enoyl-ACP reductase (InhA) complexed with its inhibitor was retrieved from the protein data bank (PDB) (pdb code: 4TZK) and refined using the *protein preparation wizard* .The 3D structures of the triazole derivatives to be docked were sketched using the *build* panel in Maestro and their geometries were optimized using *LigPrep* module. Both the enzyme as well as ligand structures were subjected to energy minimization, before submitting the docking simulations, until their average RMSD reached 0.01Å. The active site of InhA was defined using the *receptor grid generation panel*. This active site grid was defined by a box having a dimension of 10X10X10Å centered on the co-crystallized ligand in the crystal complex. The co-ordinates of native ligand served as the reference to define the active site of a ligand with respect to the target. Following this, the ligands were subjected to flexible docking against the InhA structure using with extra precision (i.e., with GlideXP) scoring

function to identify their mode of binding and the affinities. The output files obtained in the form of docking poses were visualized and quantitatively analysed for the thermodynamic elements of interactions with the residues lining the active site of the enzyme using the *Maestro's* Pose Viewer utility.

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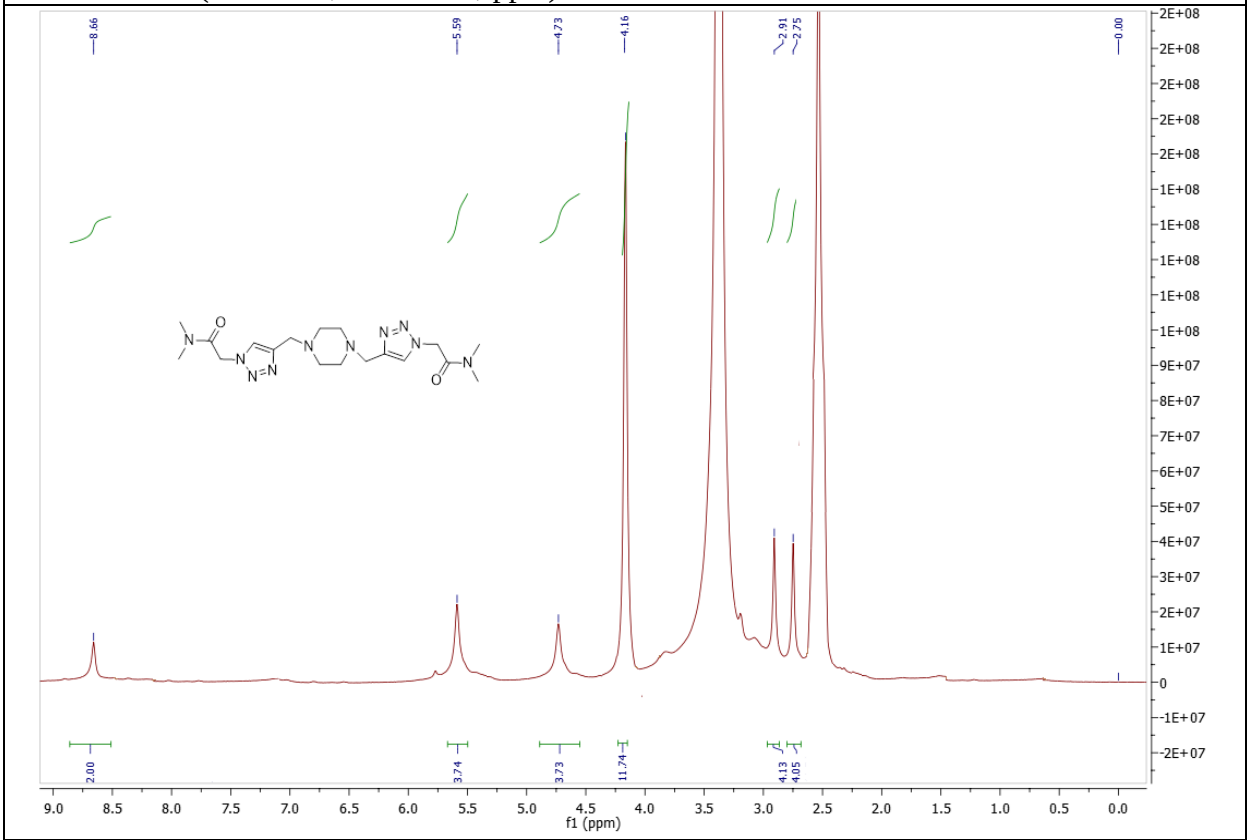
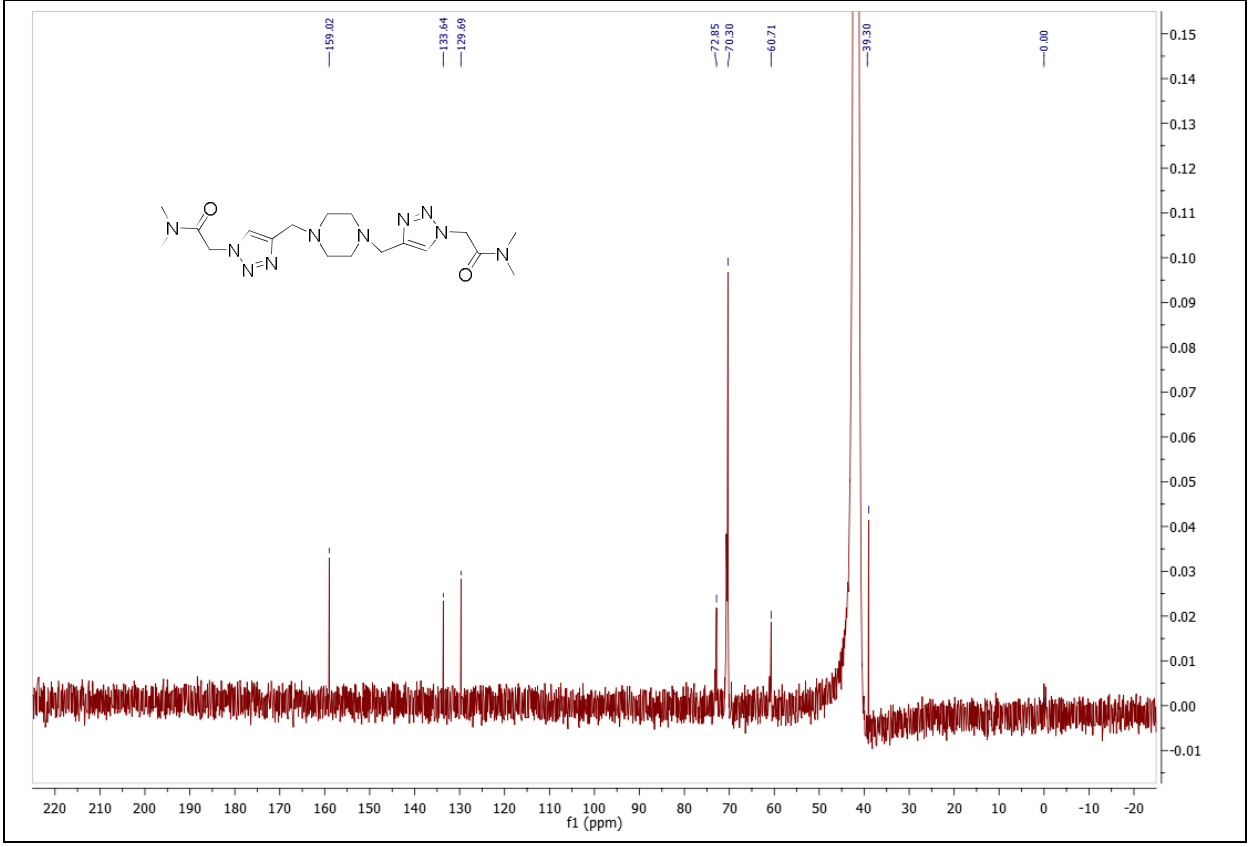
^{1}H NMR, ^{13}C NMR and HRMS:

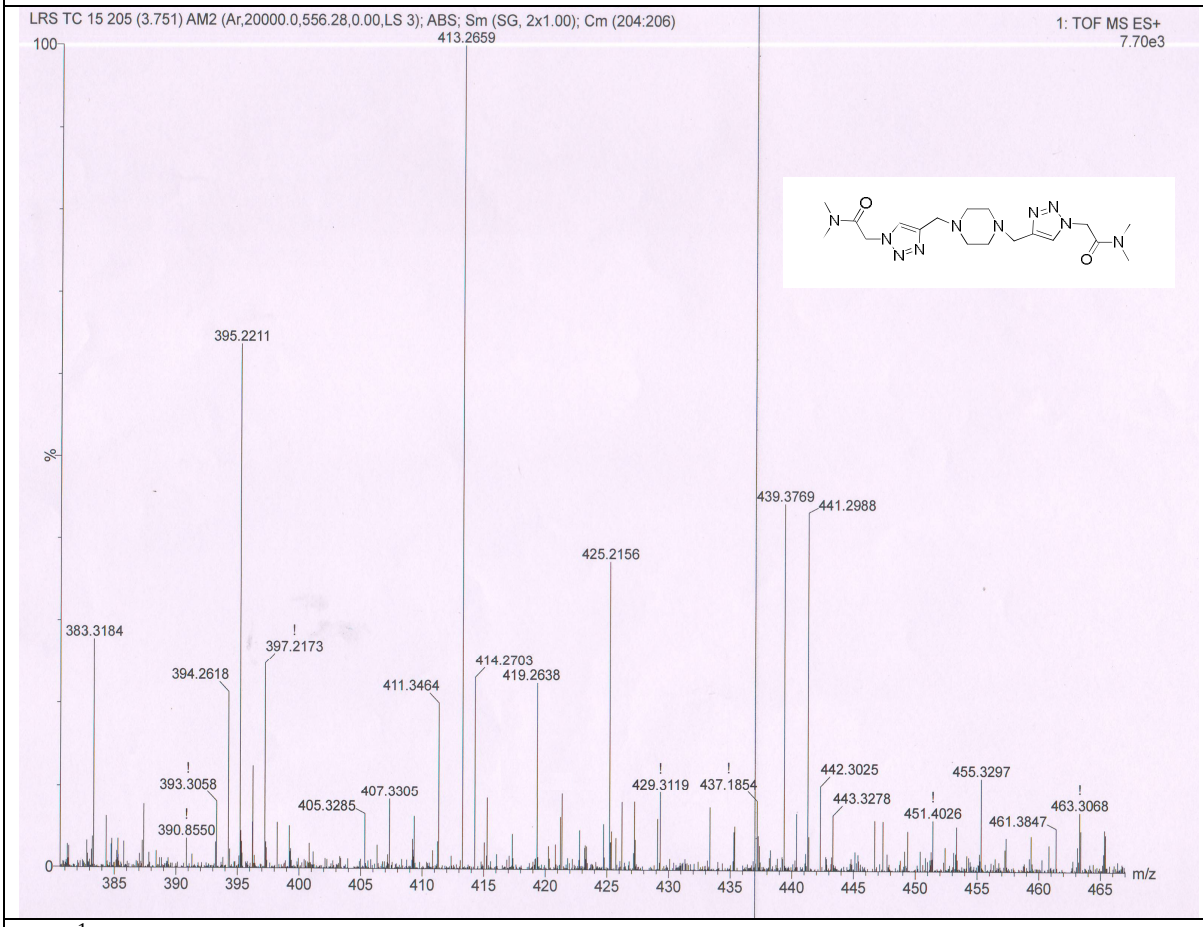
3a : ^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)



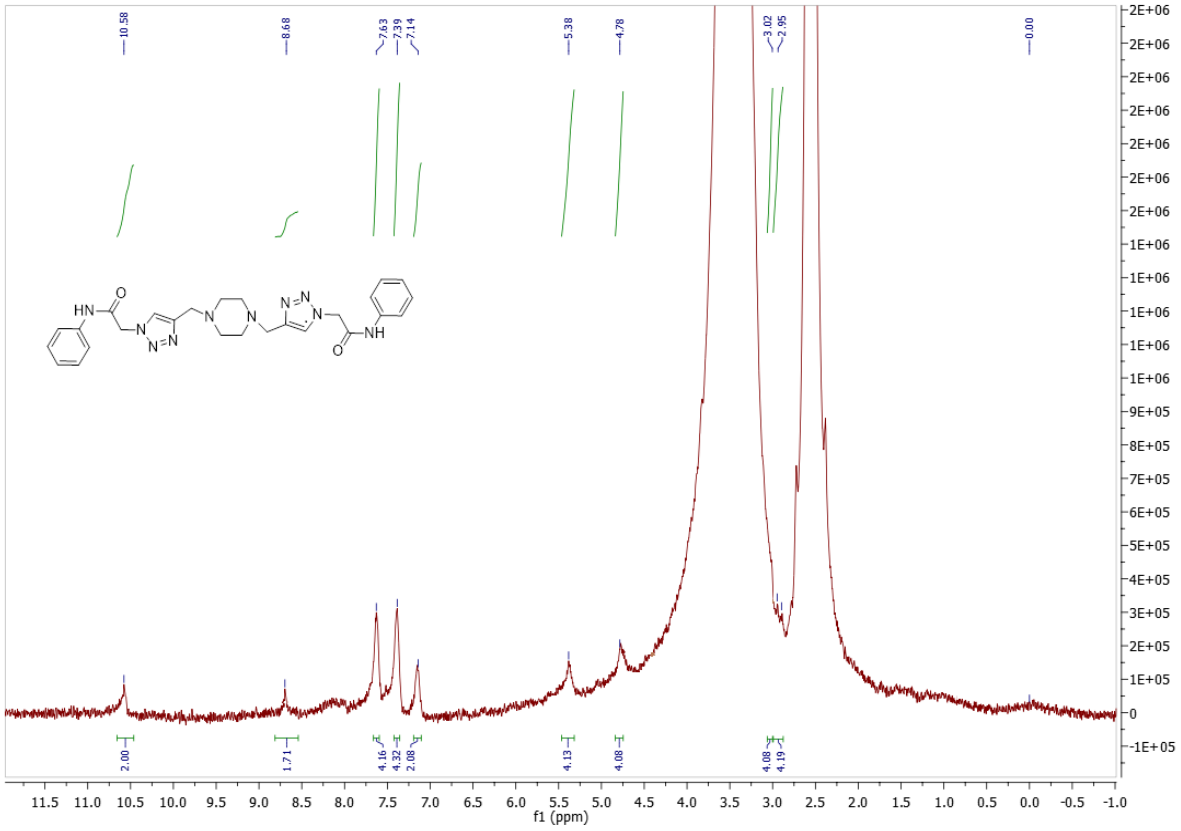
3a : ^{13}C NMR (100 MHz, DMSO-d$_6$, ppm)



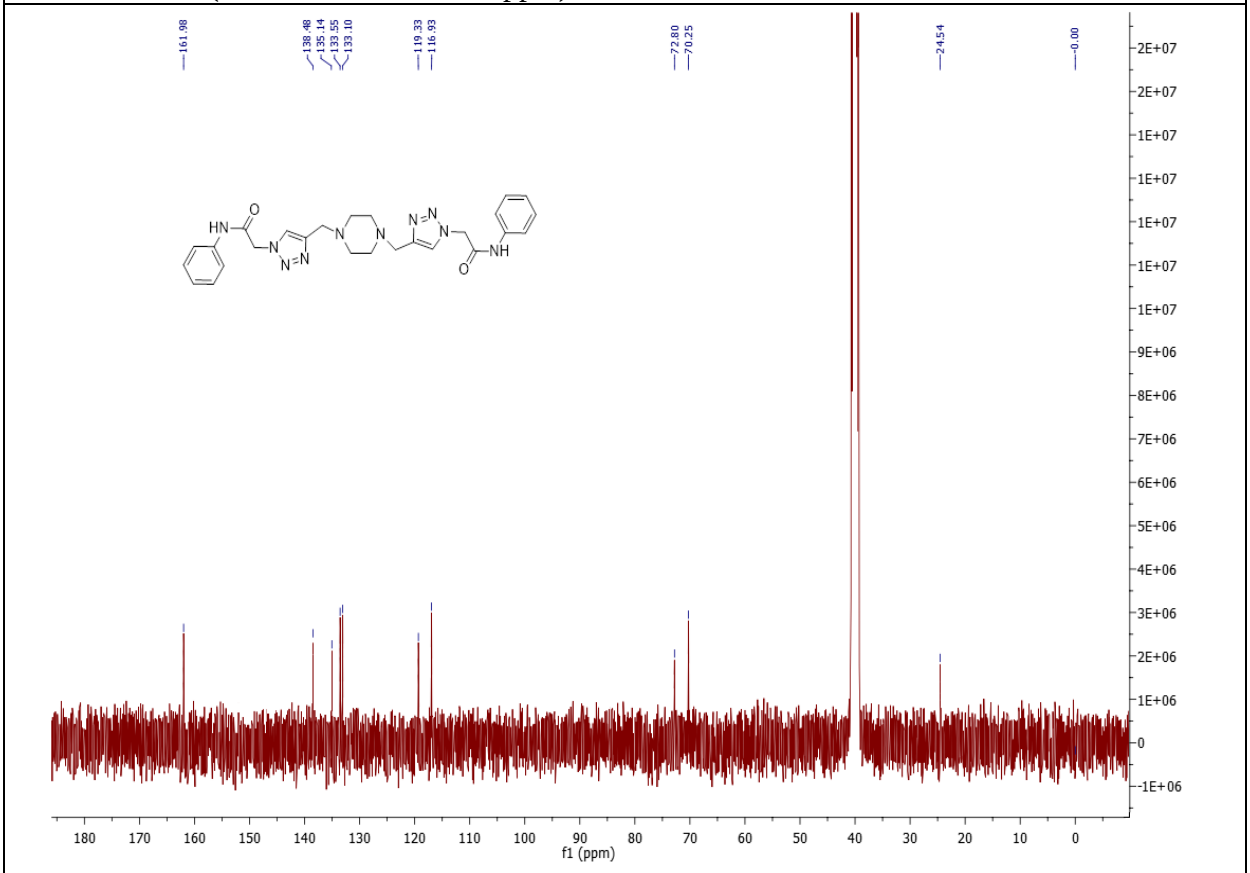
3a : HRMSz



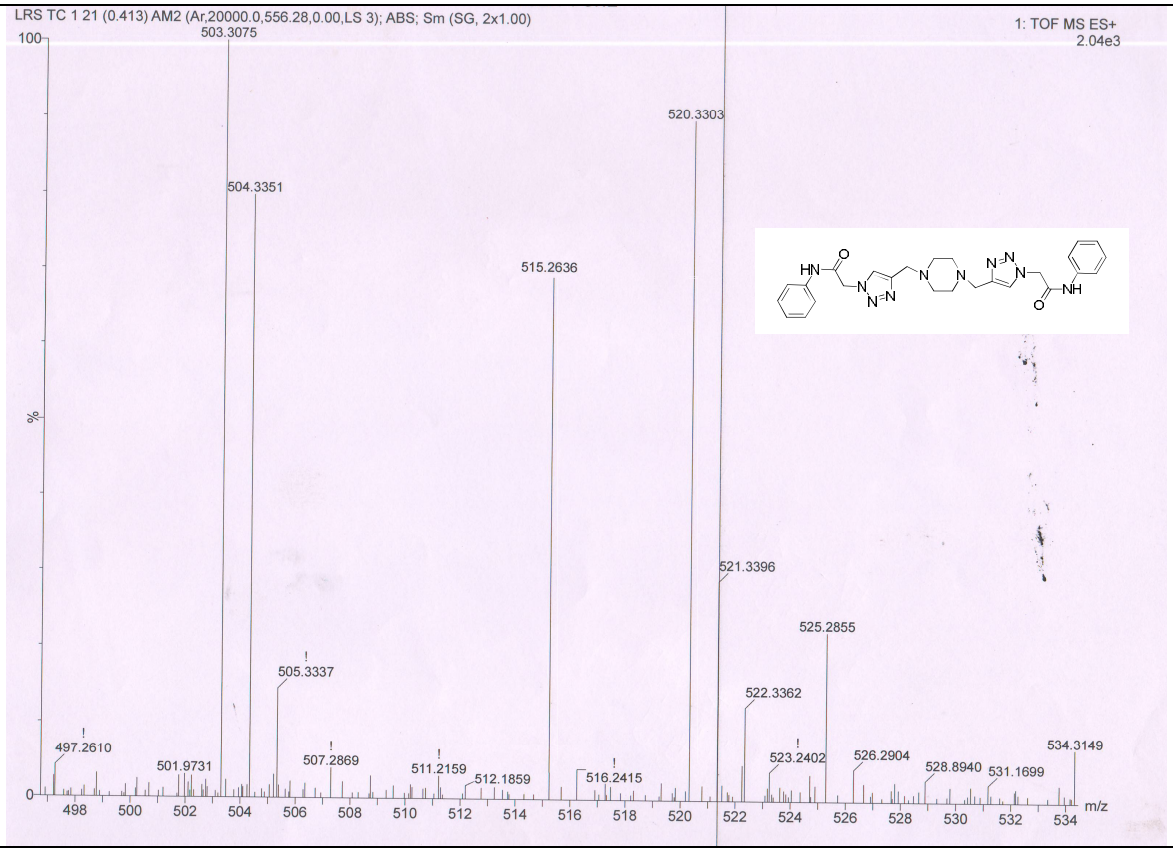
3b : ^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)



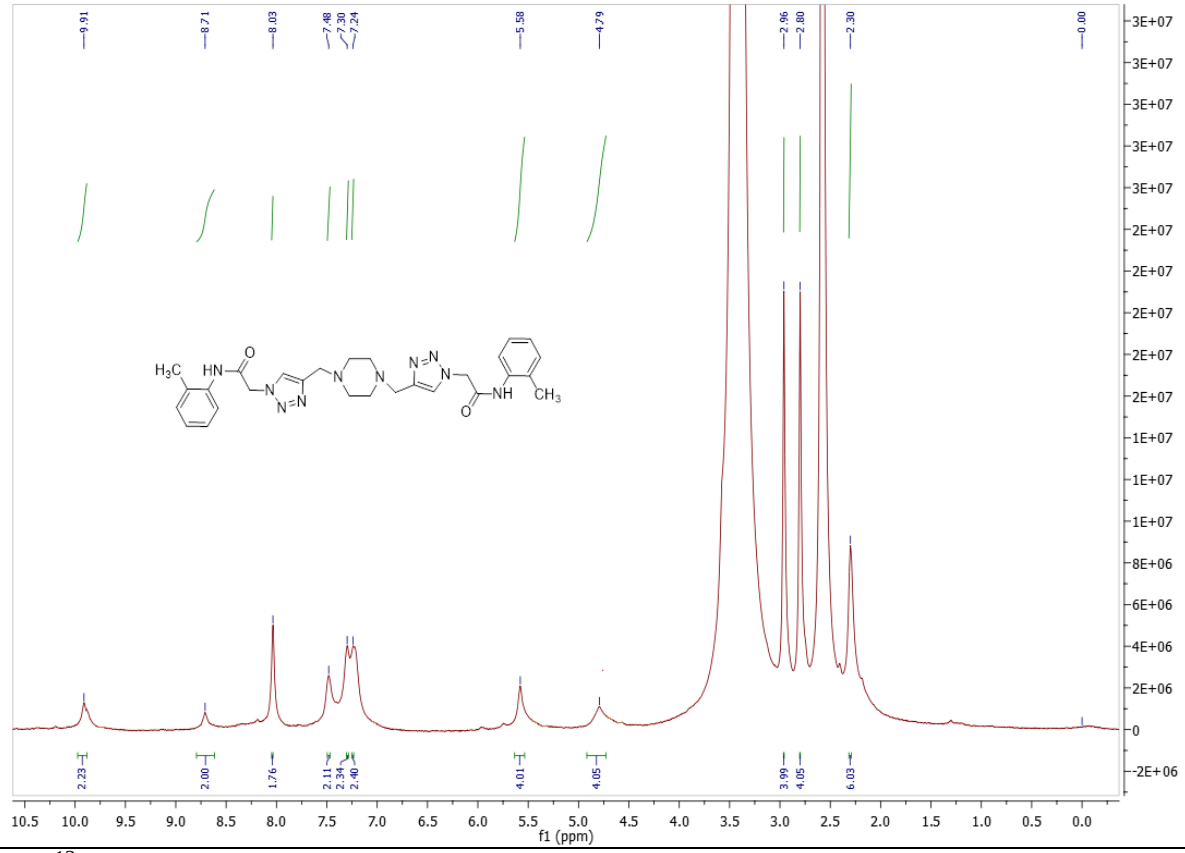
3b : ^{13}C NMR (100 MHz, DMSO-d_6, ppm)



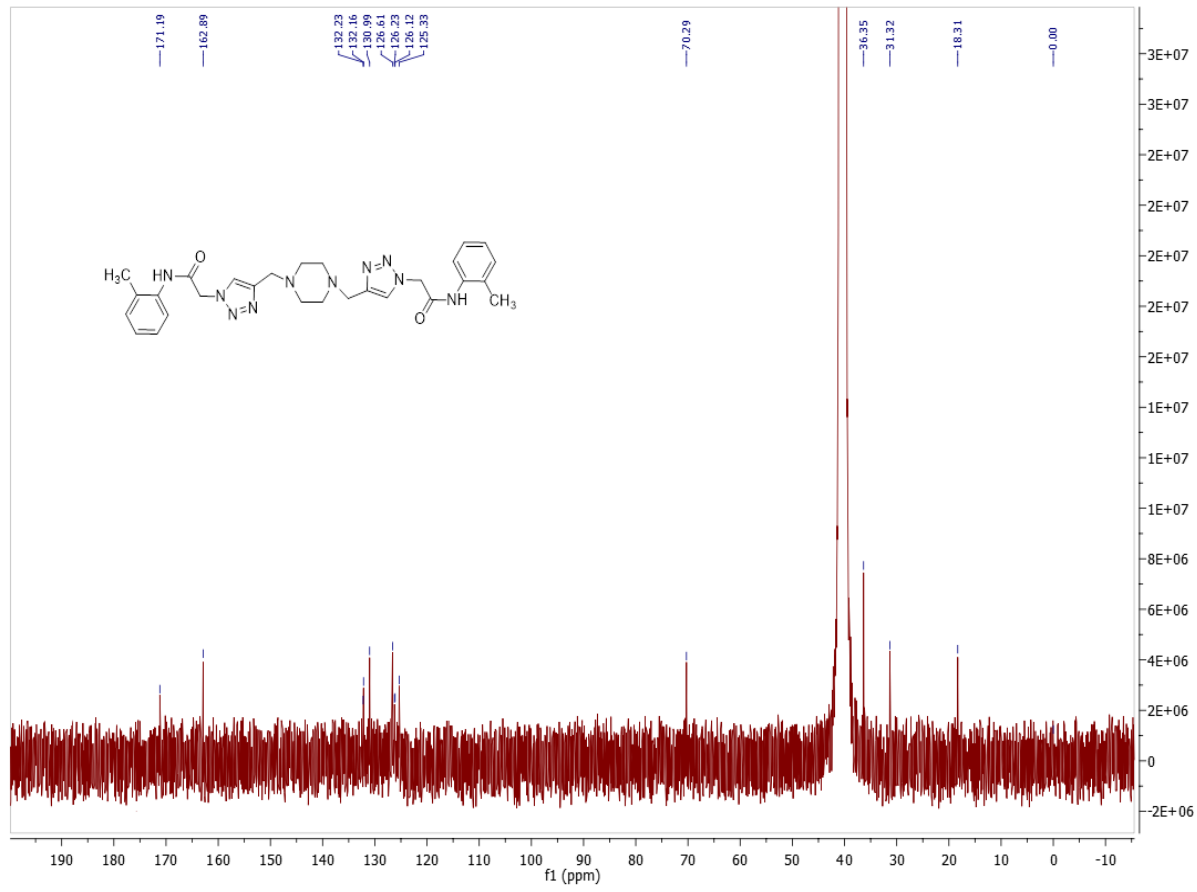
3b: HRMS



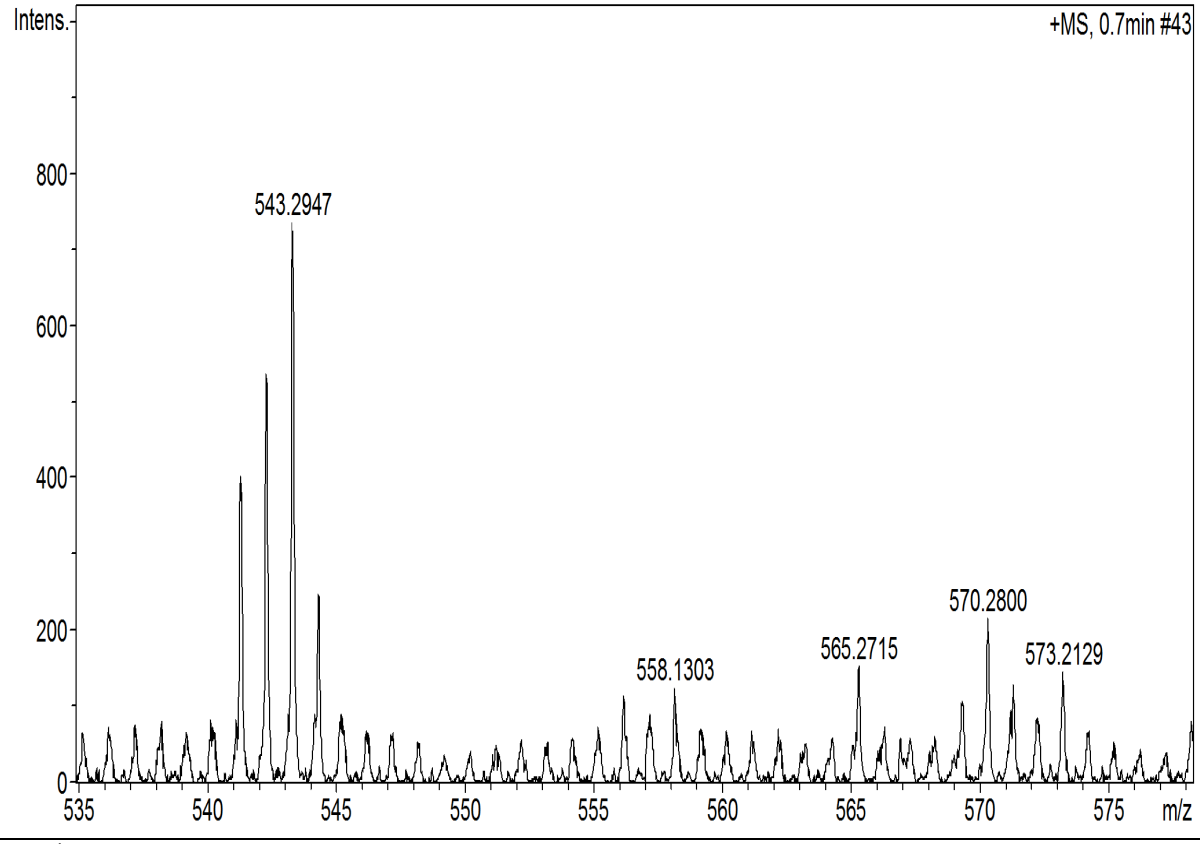
3c: ^{1}H NMR (400 MHz, DMSO-d_6, ppm)



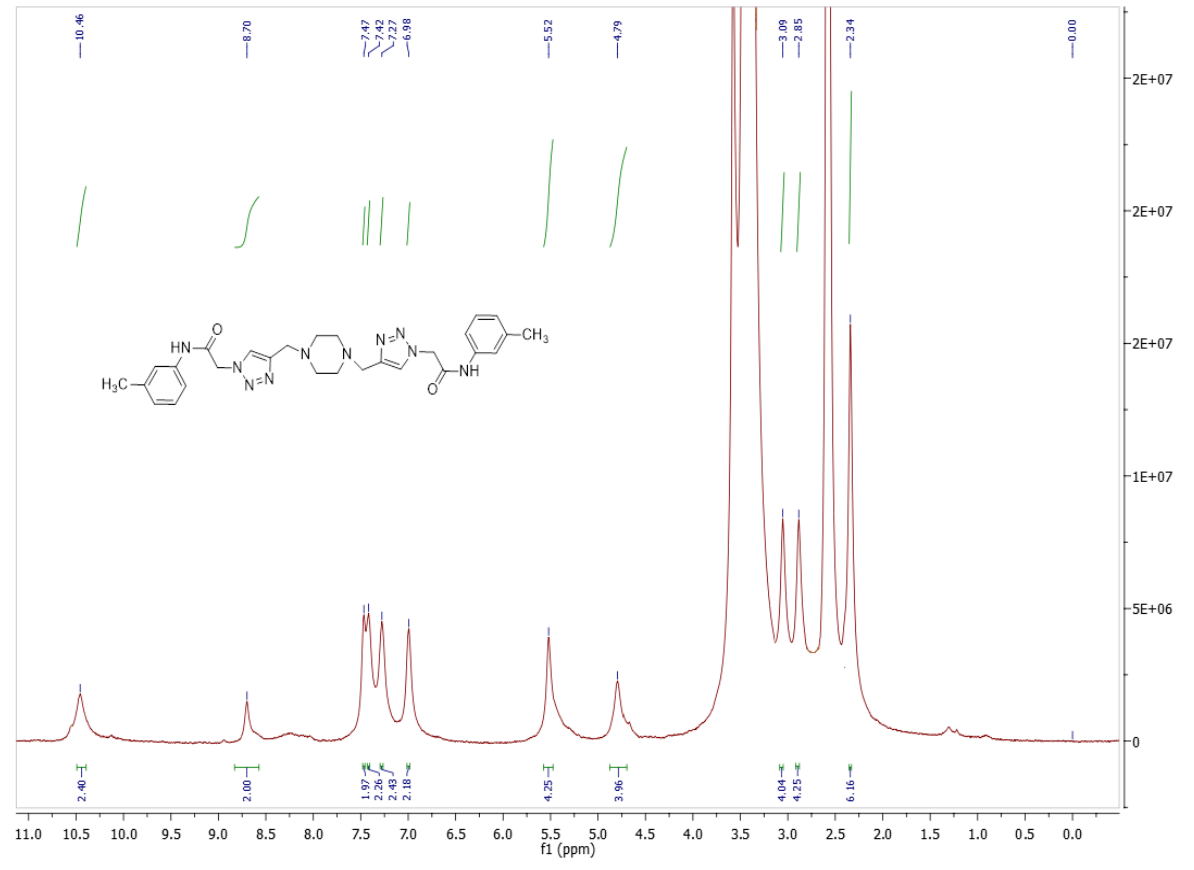
3c : ^{13}C NMR (100 MHz, DMSO-d_6, ppm)



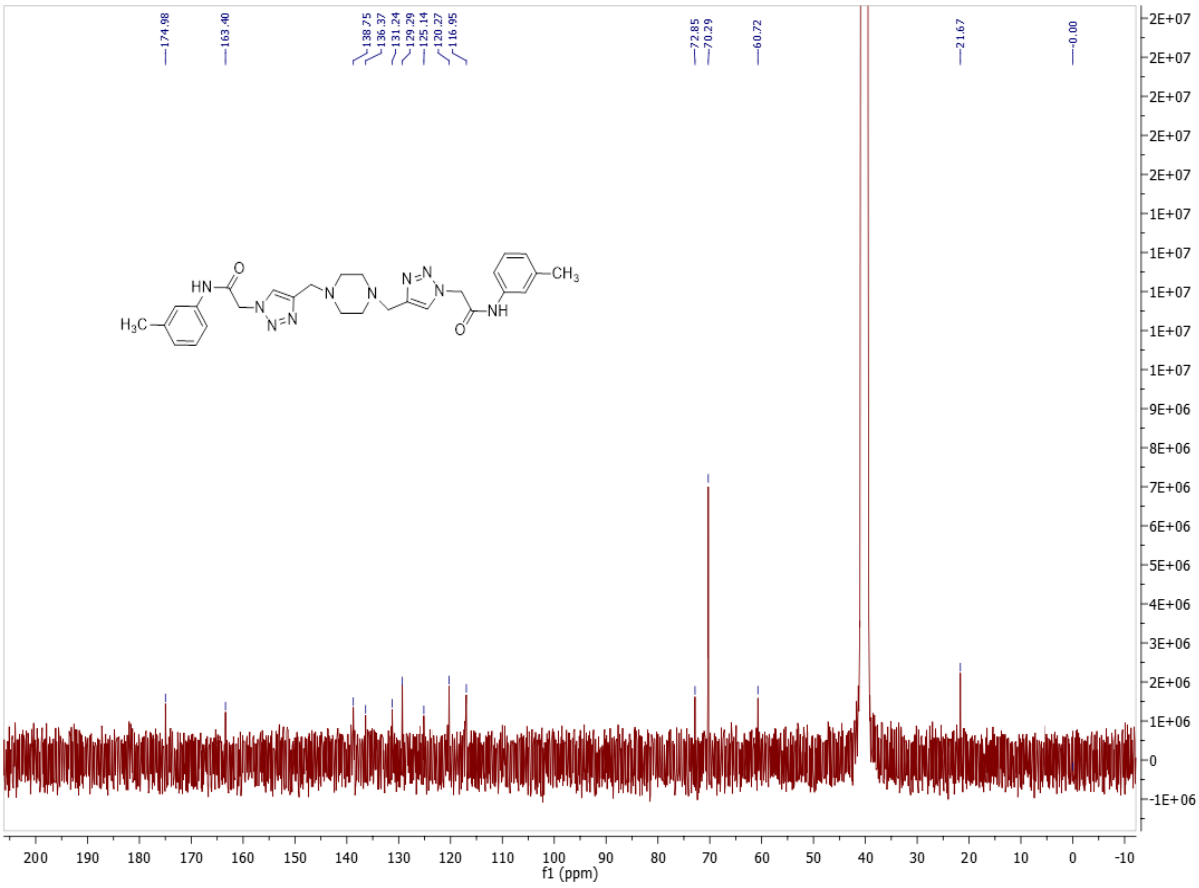
3c : HRMS



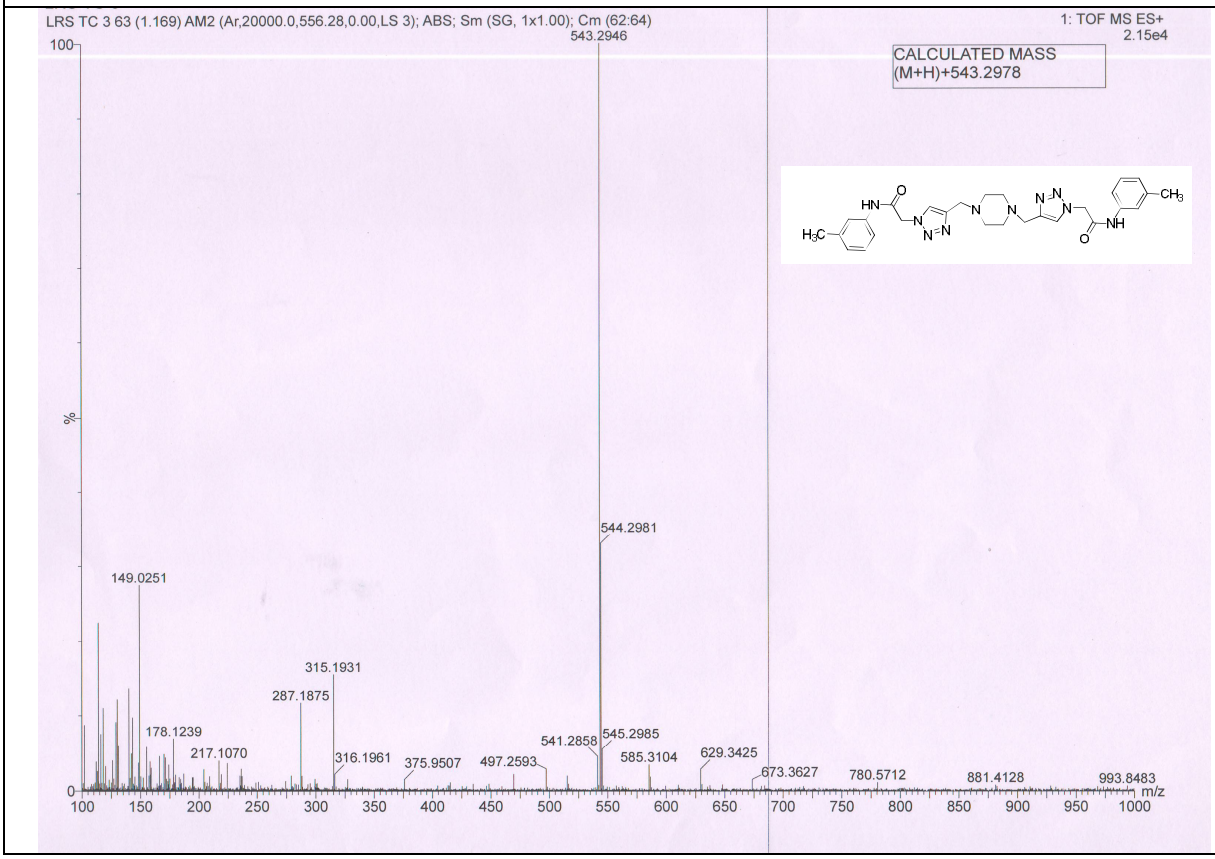
3d : ^{1}H NMR (400 MHz, DMSO-d_6, ppm)



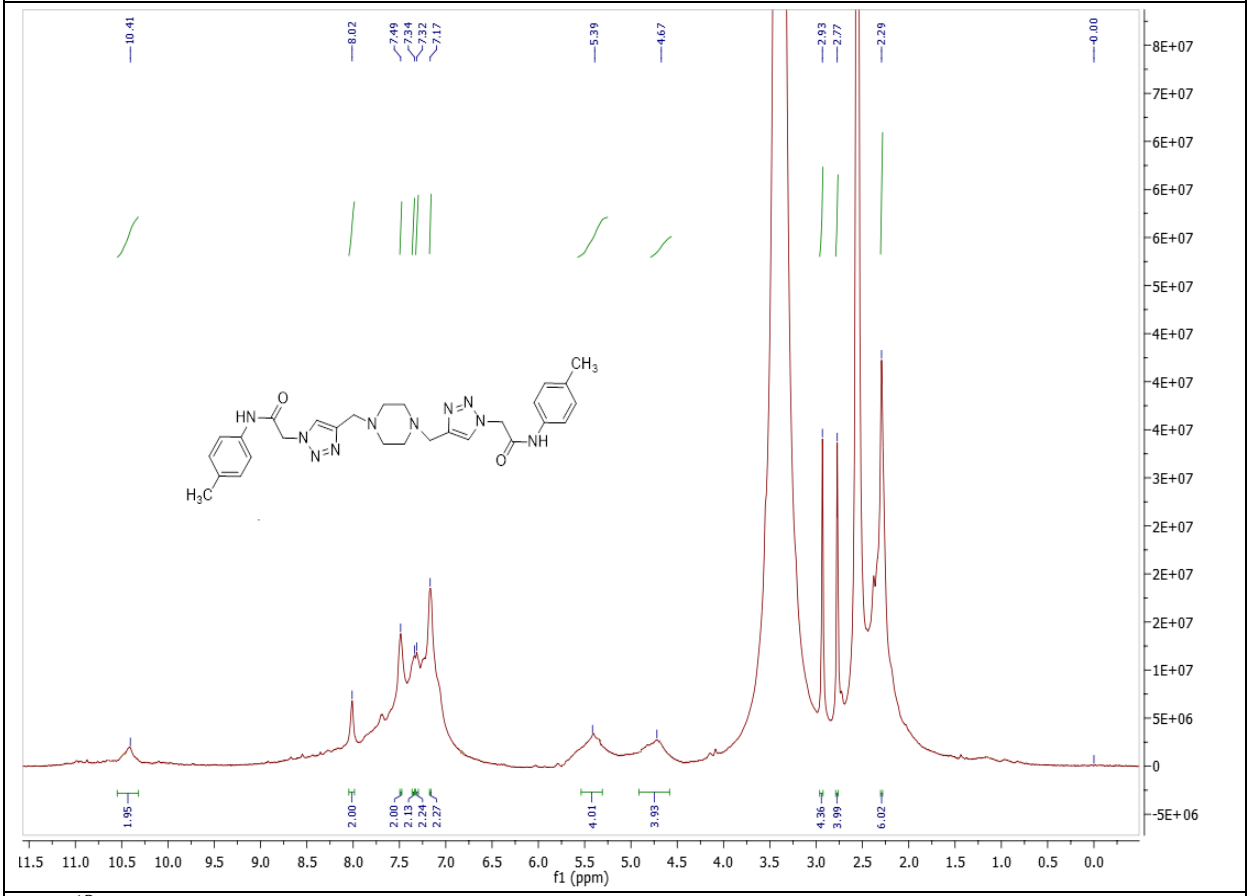
3d : ^{13}C NMR (100 MHz, DMSO-d_6, ppm)



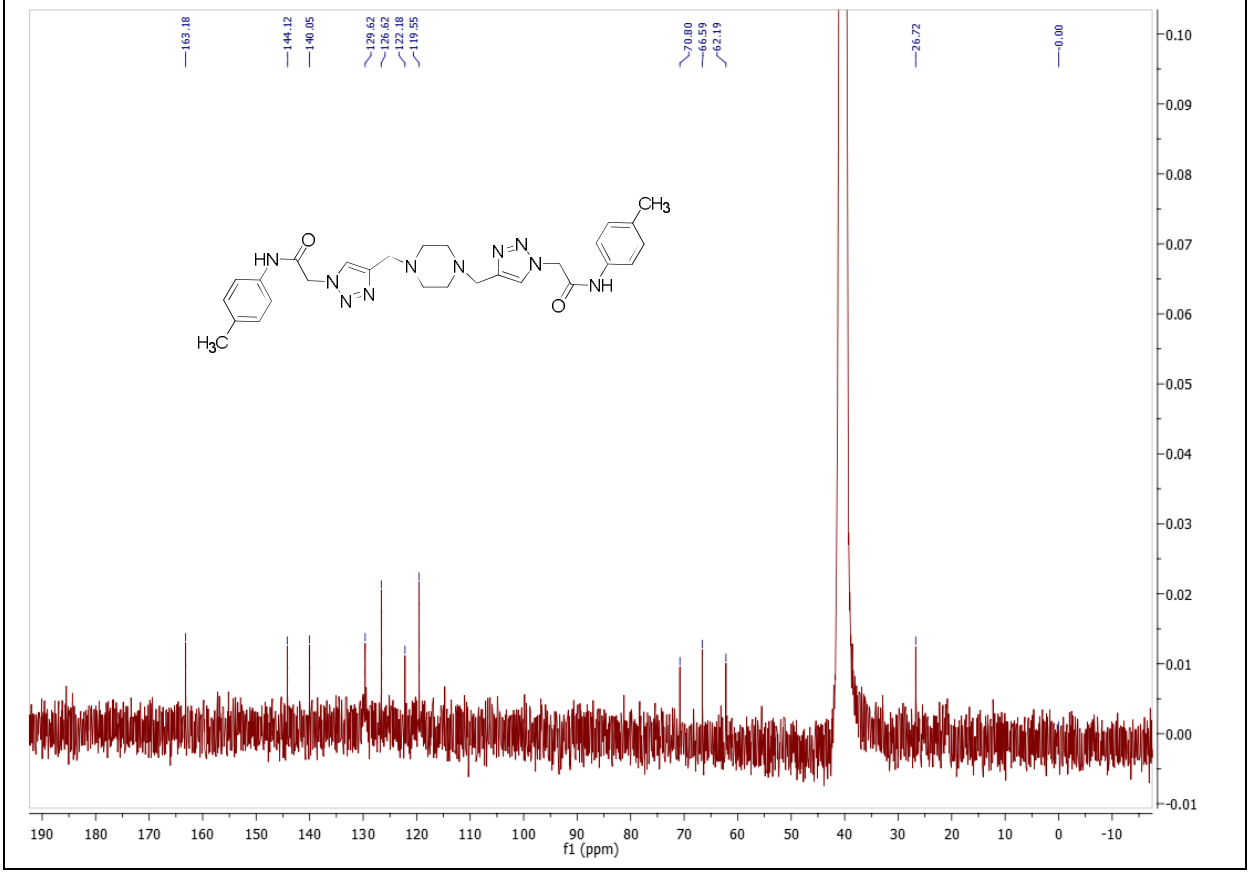
3d: HRMS



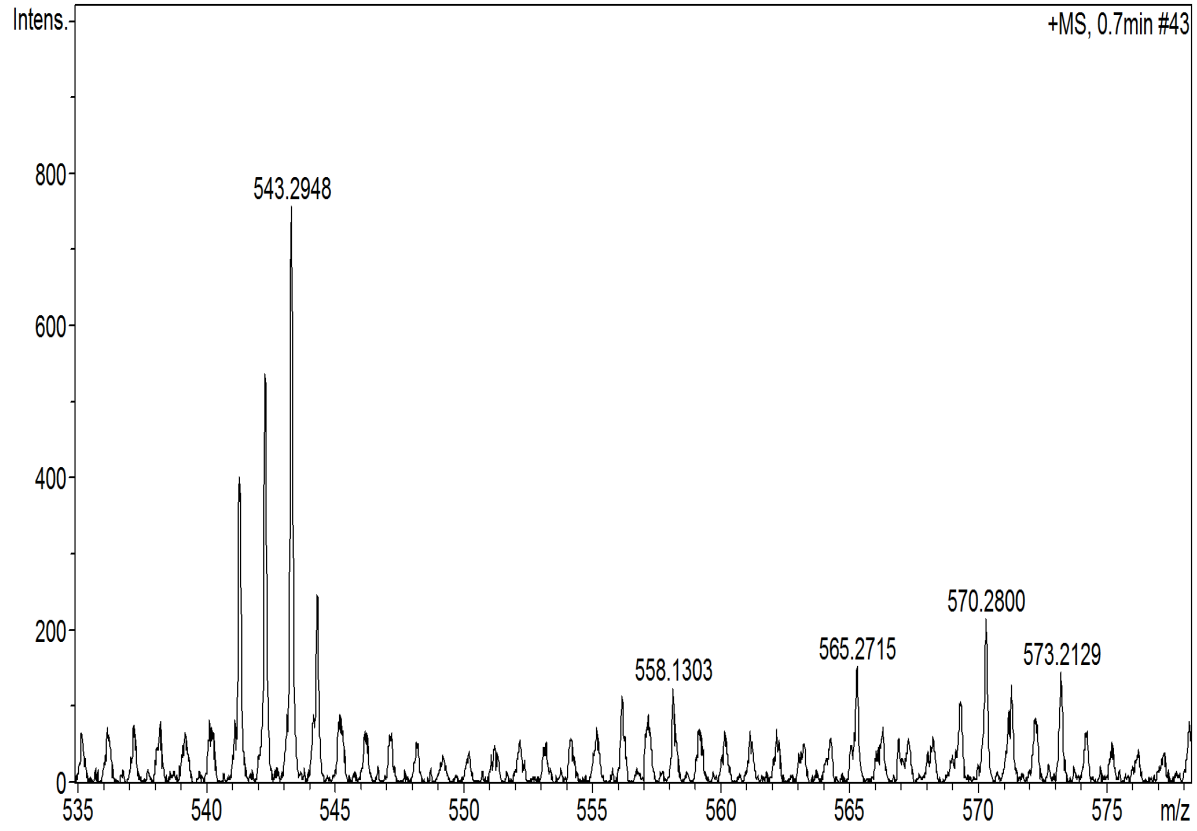
3e : ^{1}H NMR (400 MHz, DMSO-d_6, ppm)



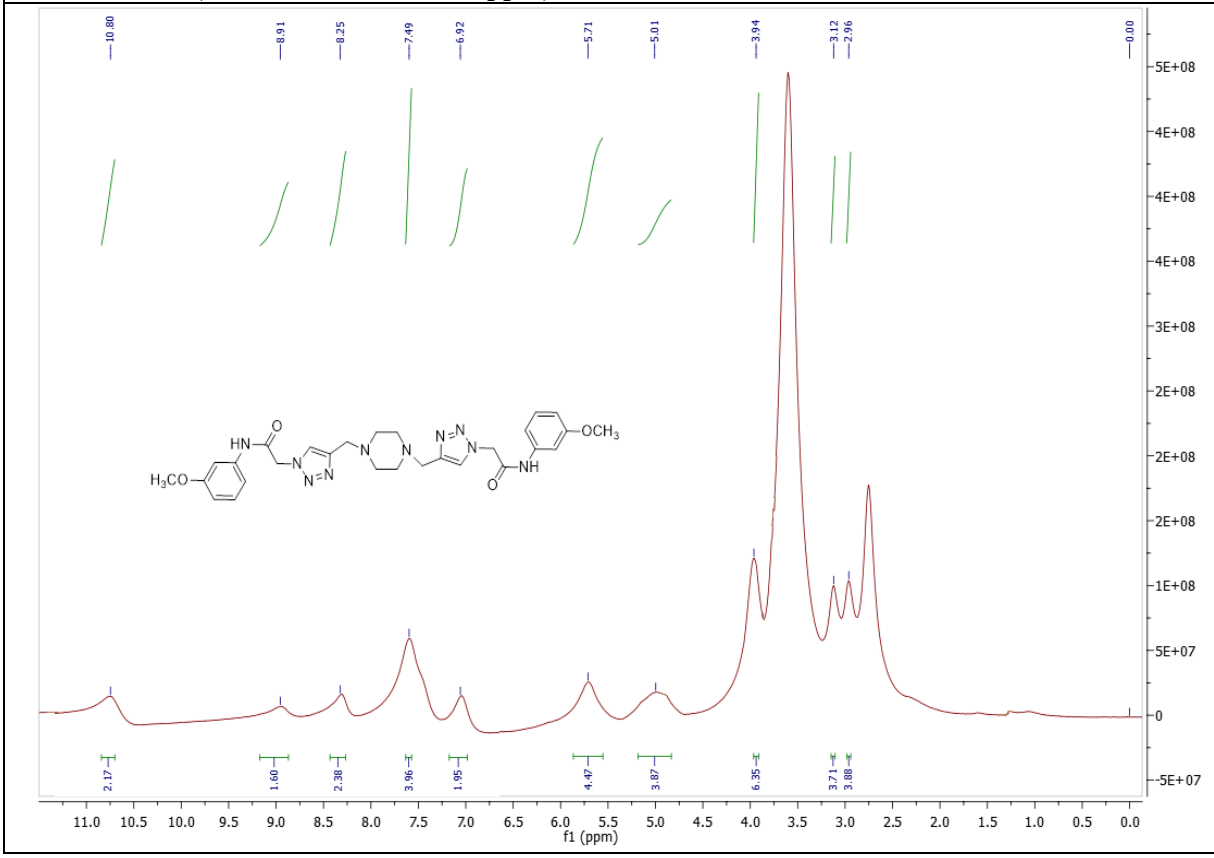
3e : ^{13}C NMR (100 MHz, DMSO-d_6, ppm)



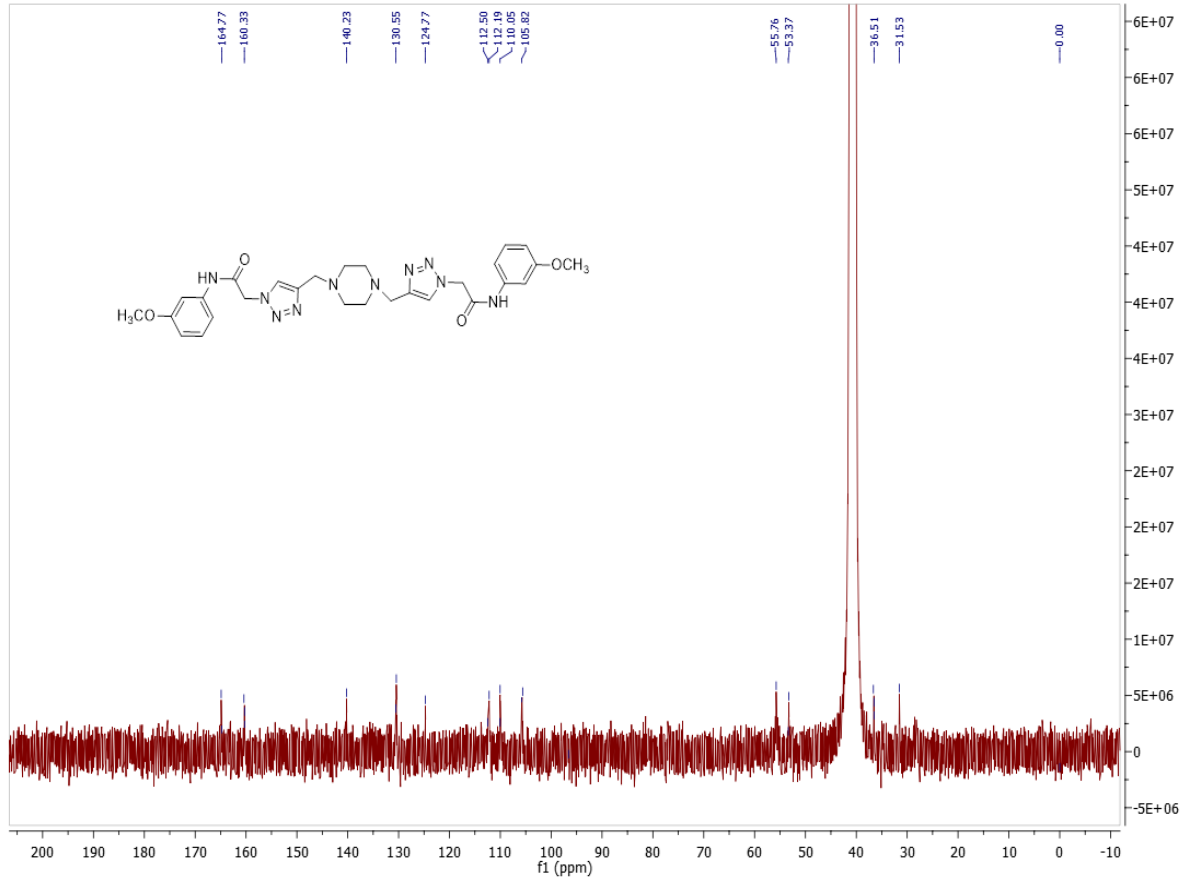
3e : HRMS



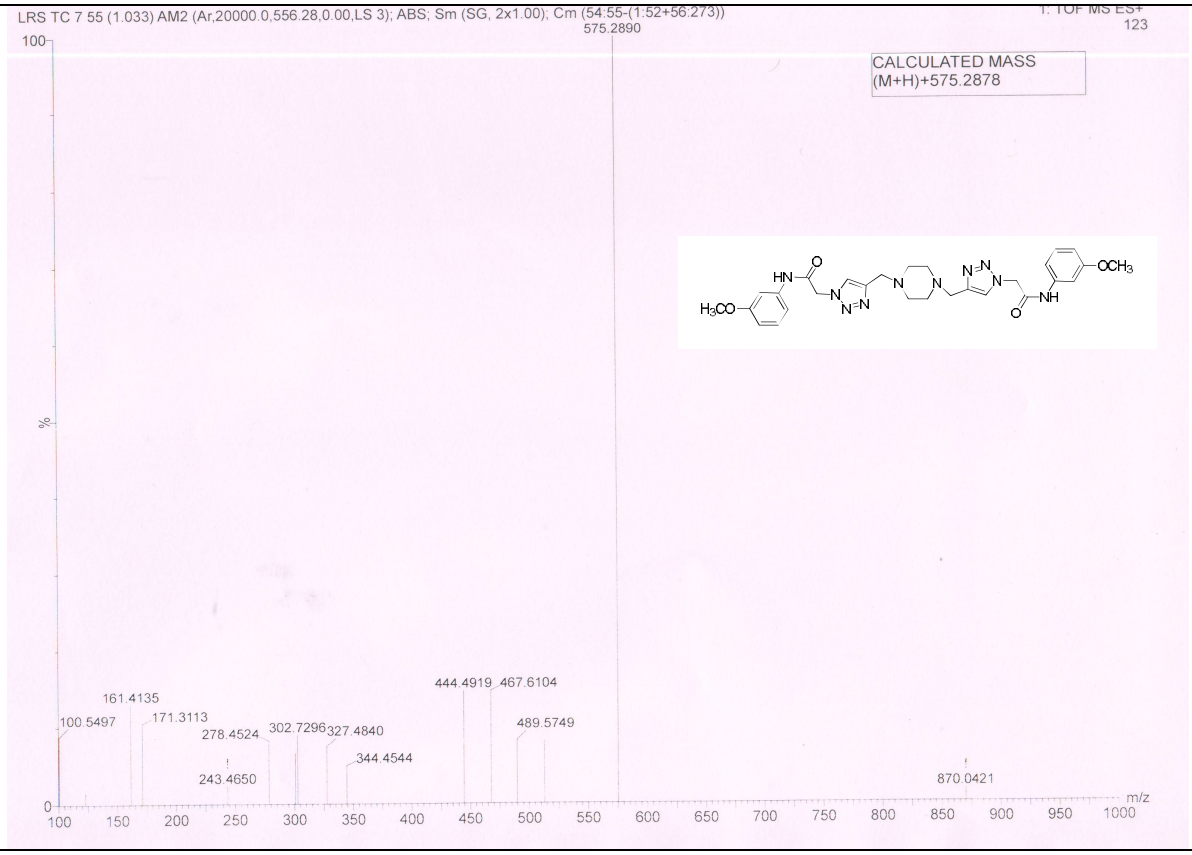
3f : ^{1}H NMR (400 MHz, DMSO-d_6, ppm)



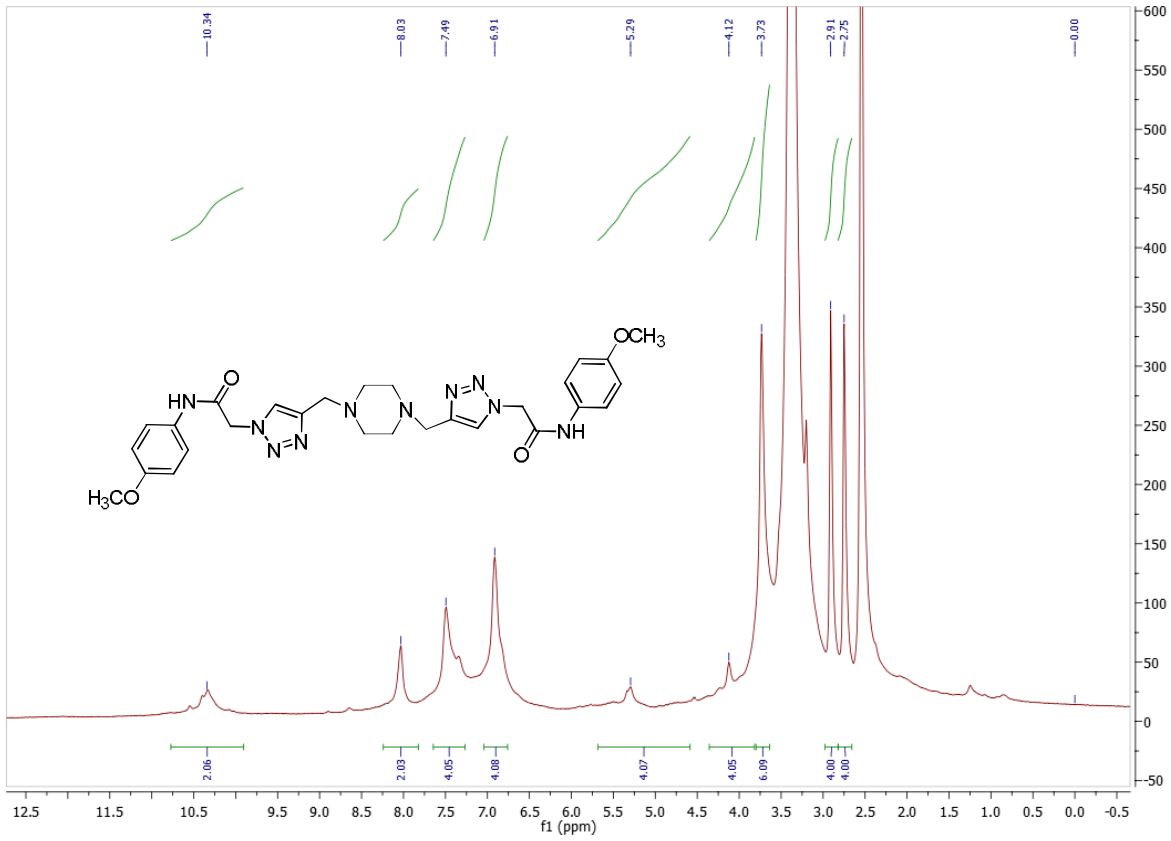
3f : ^{13}C NMR (100 MHz, DMSO-d_6, ppm)



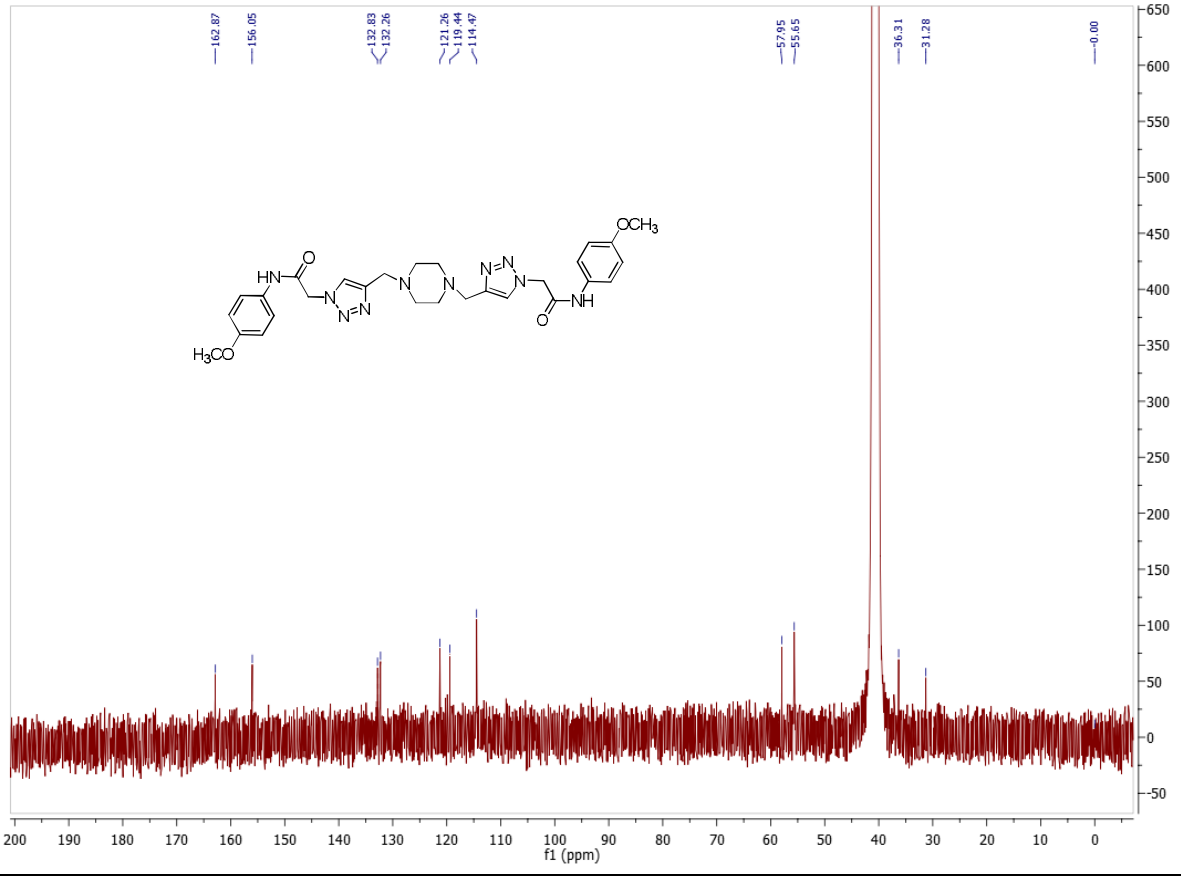
3f: HRMS



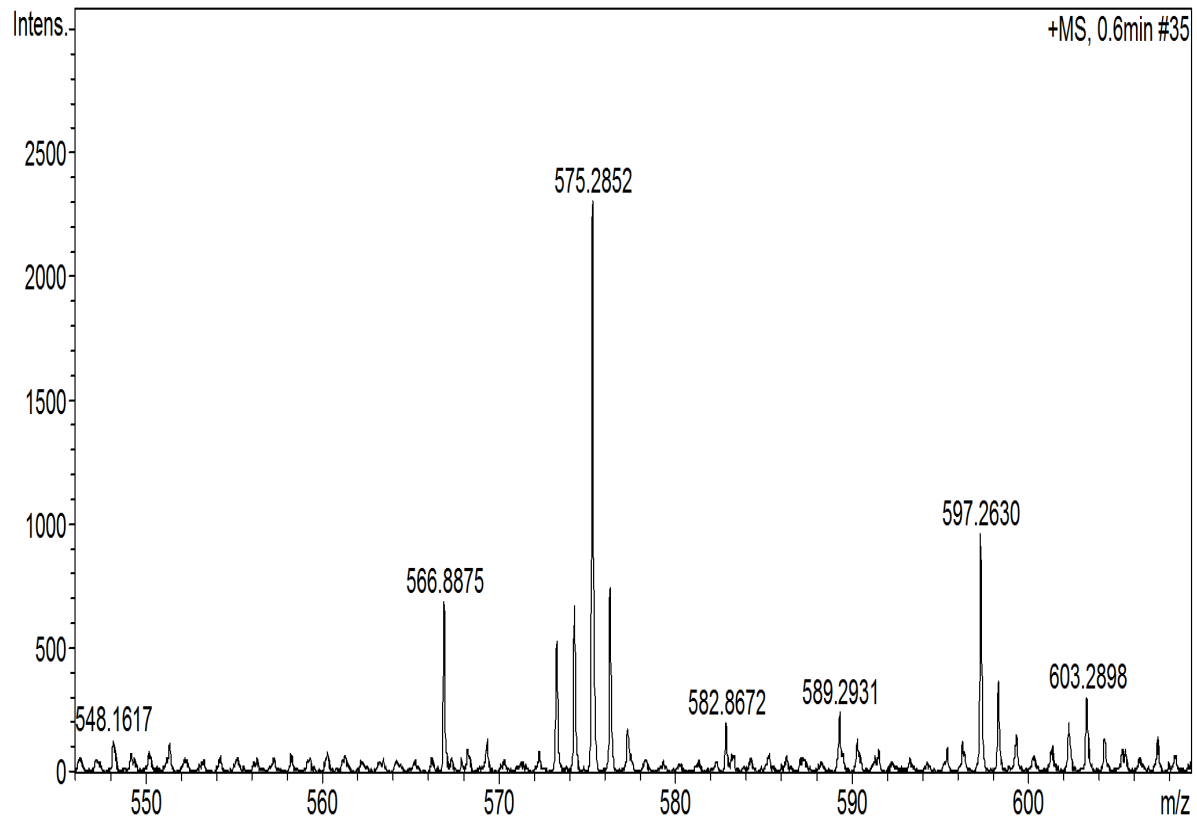
3g : ^{1}H NMR (400 MHz, DMSO-d_6, ppm)



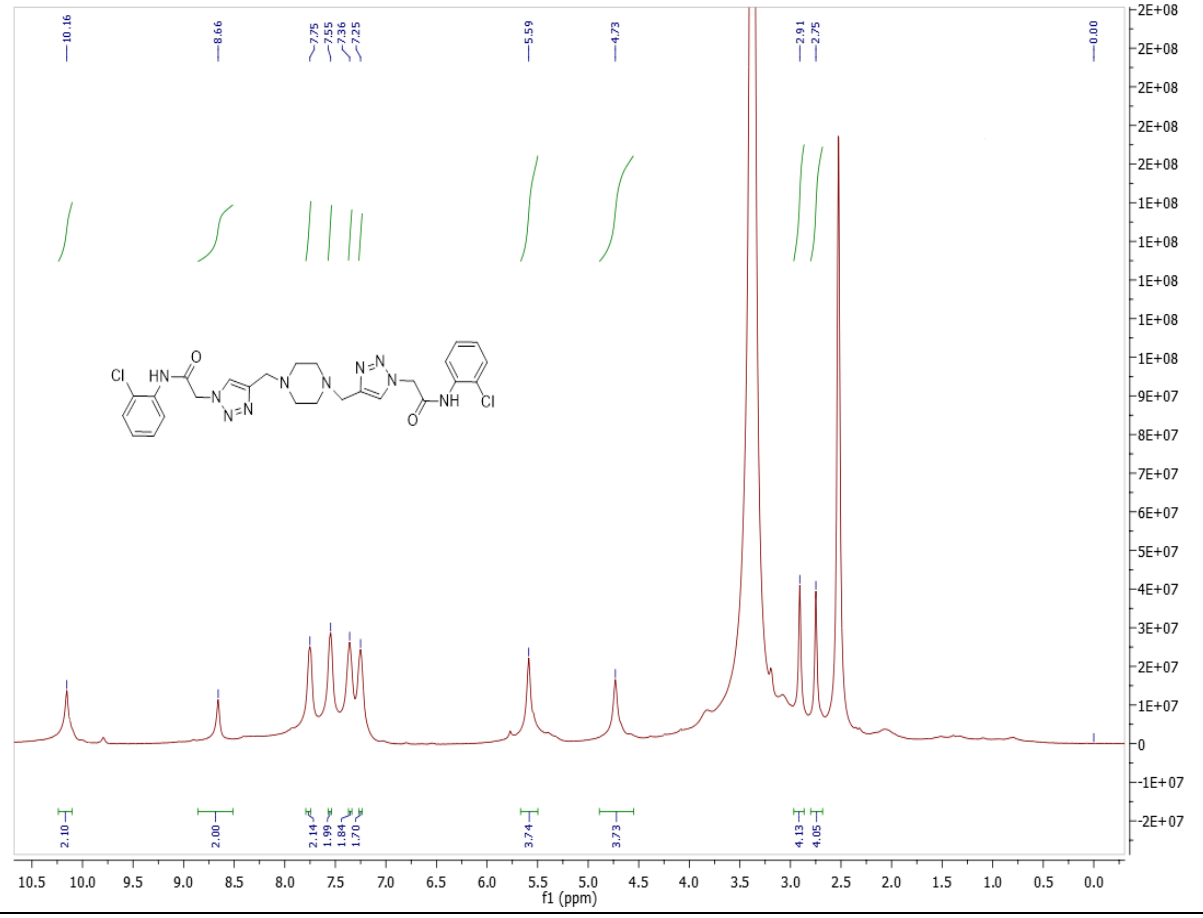
3g : ^{13}C NMR (100 MHz, DMSO-d_6, ppm)



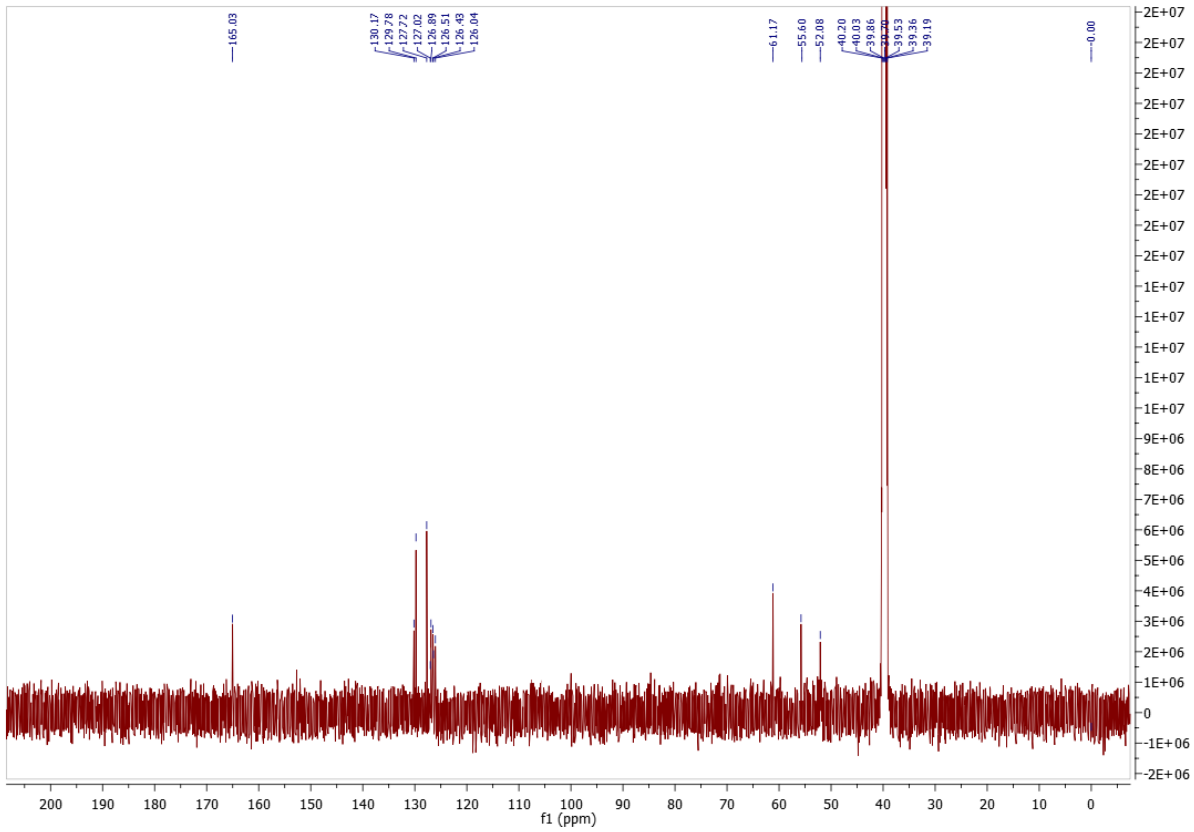
3g : HRMS



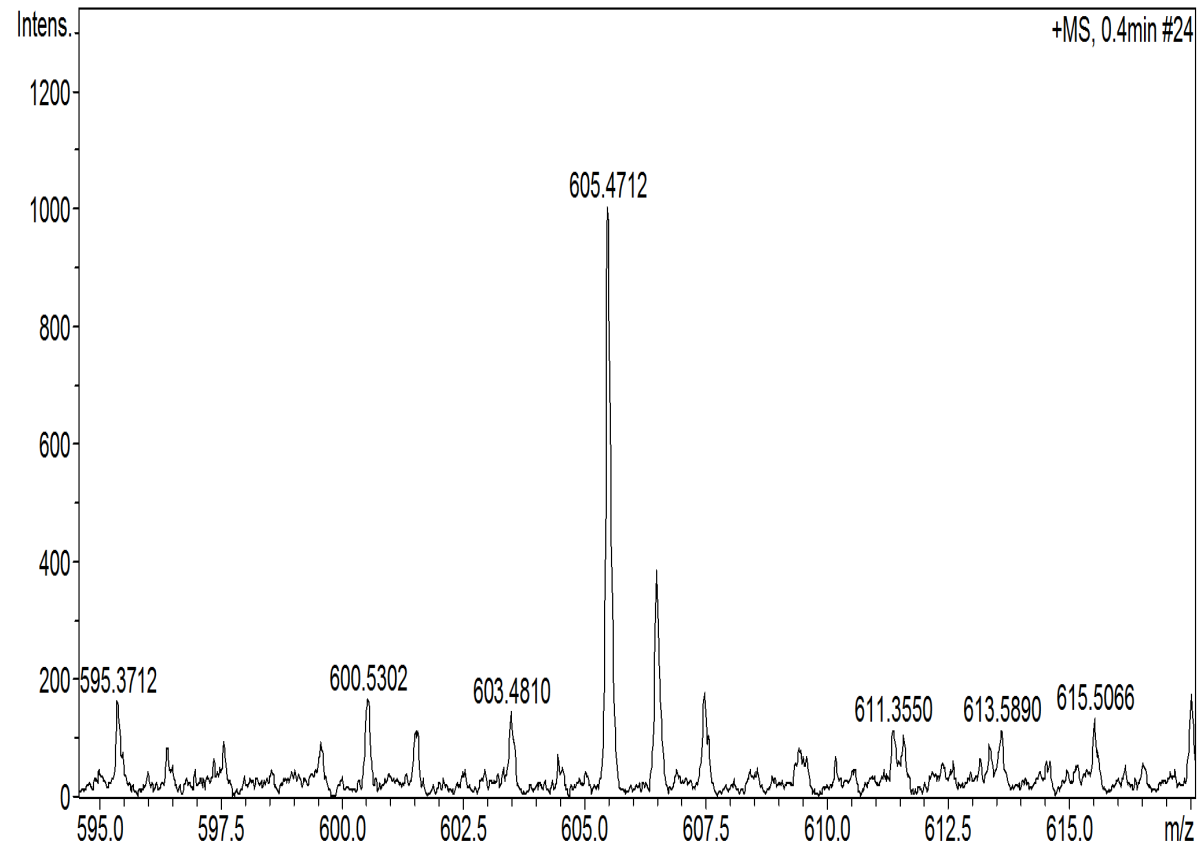
3h : ^{1}H NMR (400 MHz, DMSO-d$_6$, ppm)



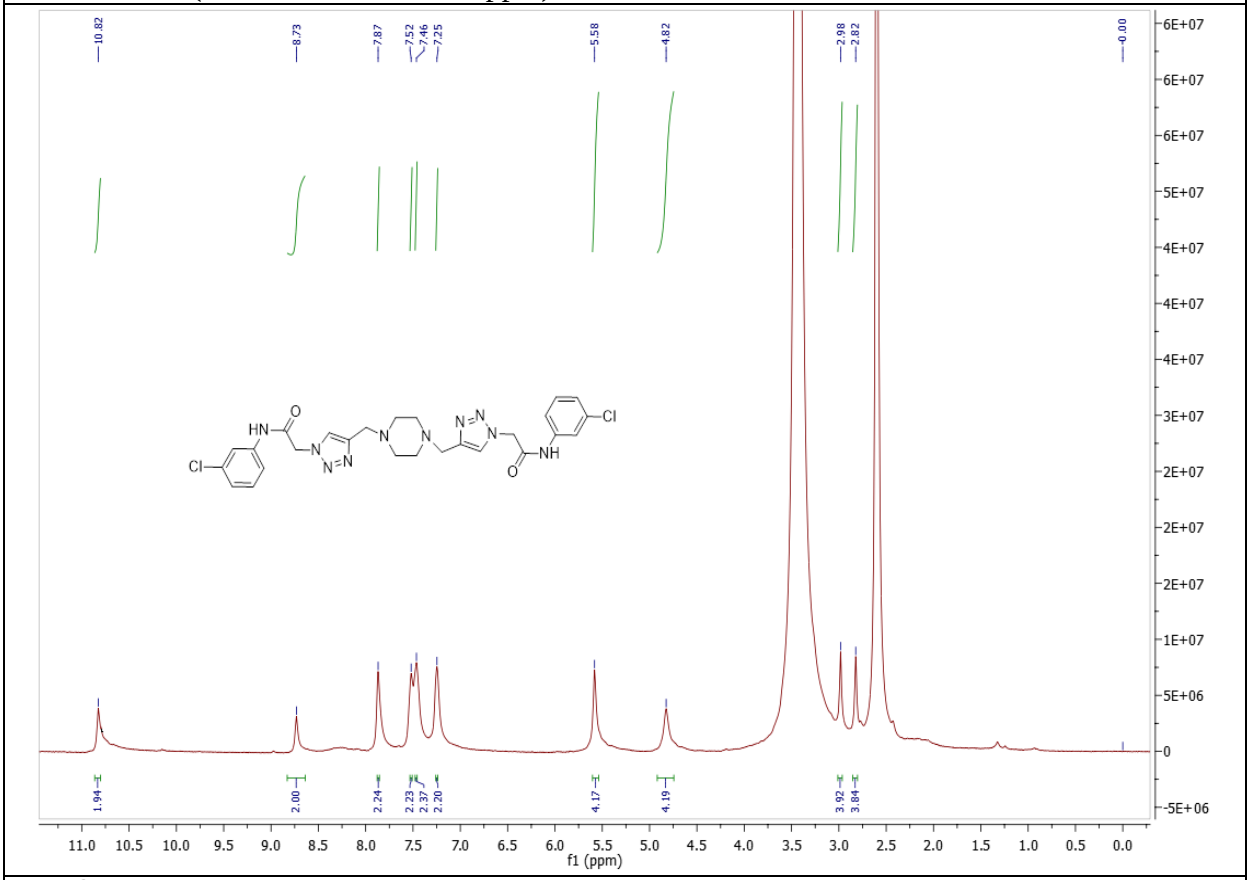
3h : ^{13}C NMR (100 MHz, DMSO-d_6, ppm)



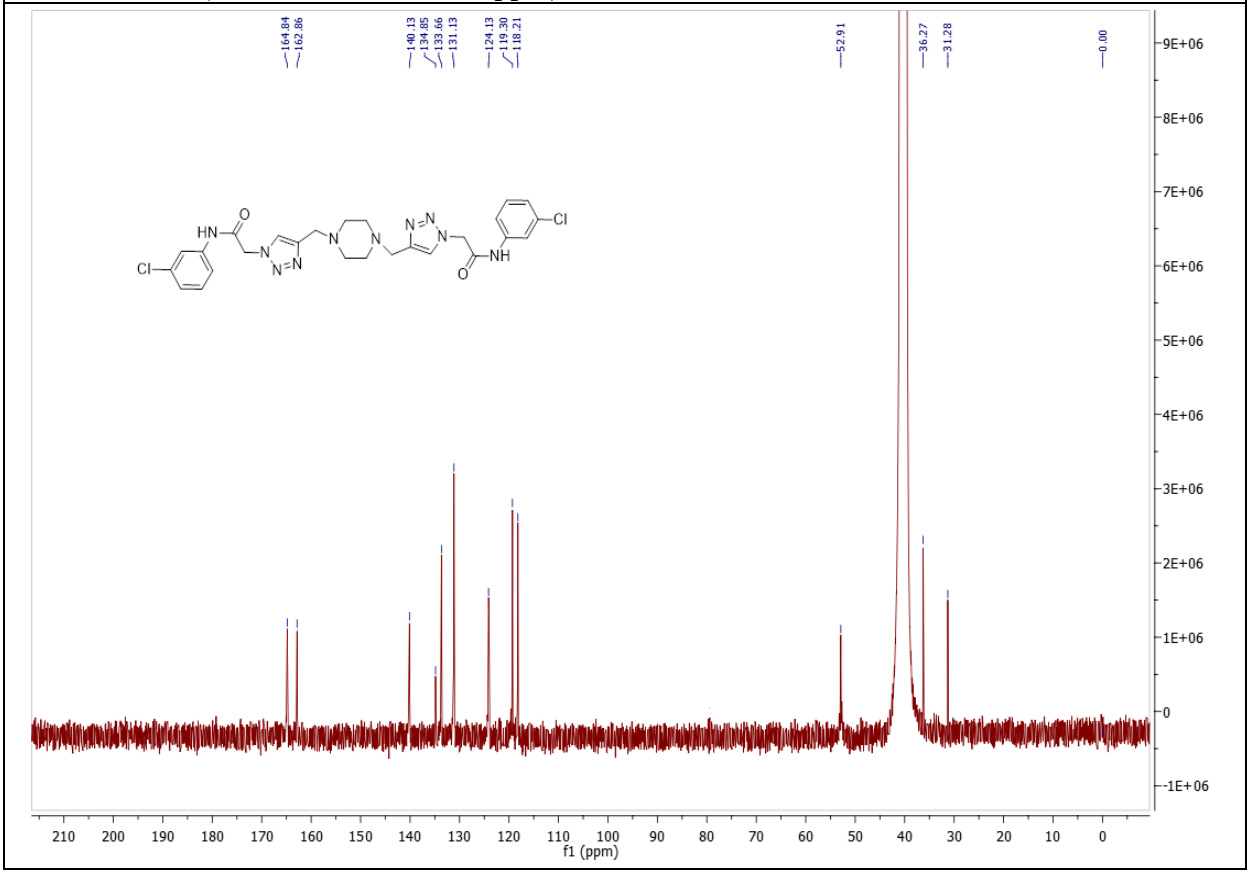
3h : HRMS



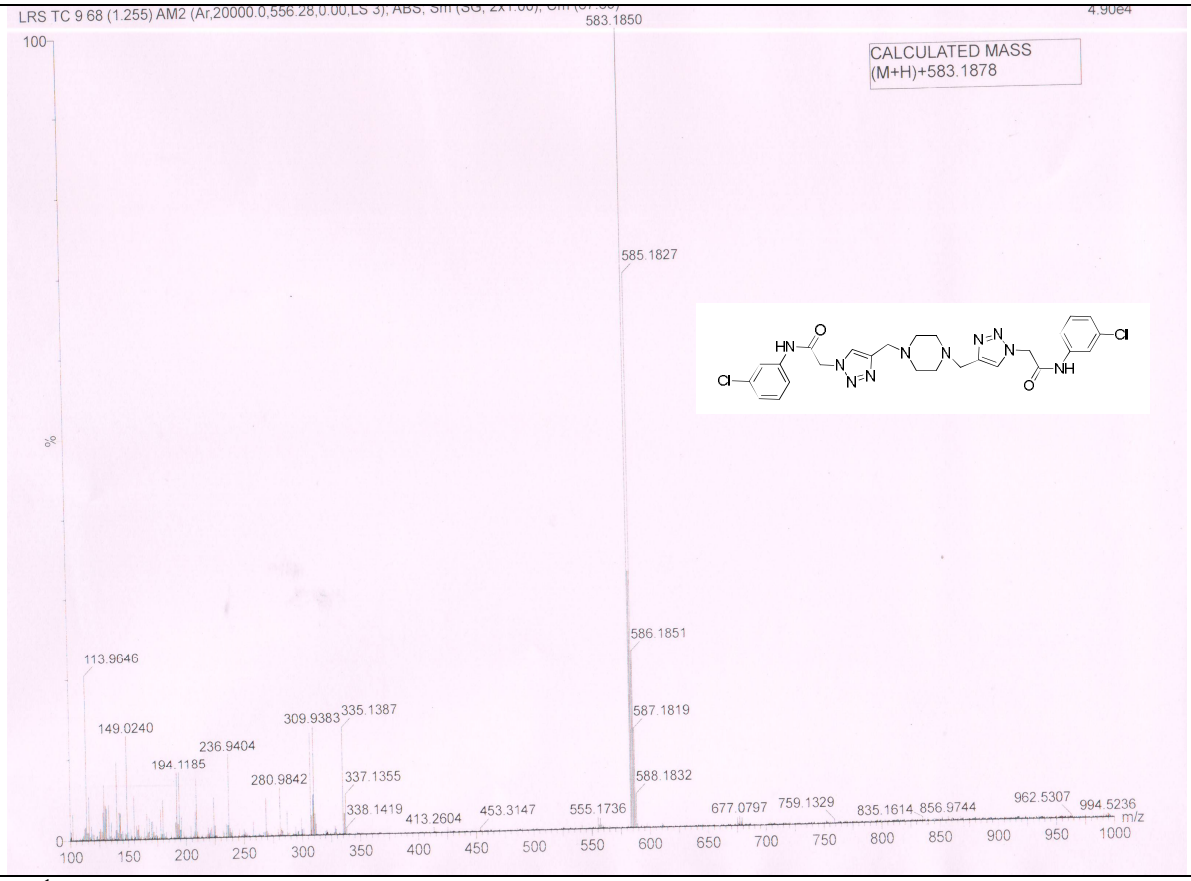
3i : ^{1}H NMR (400 MHz, DMSO-d_6, ppm)



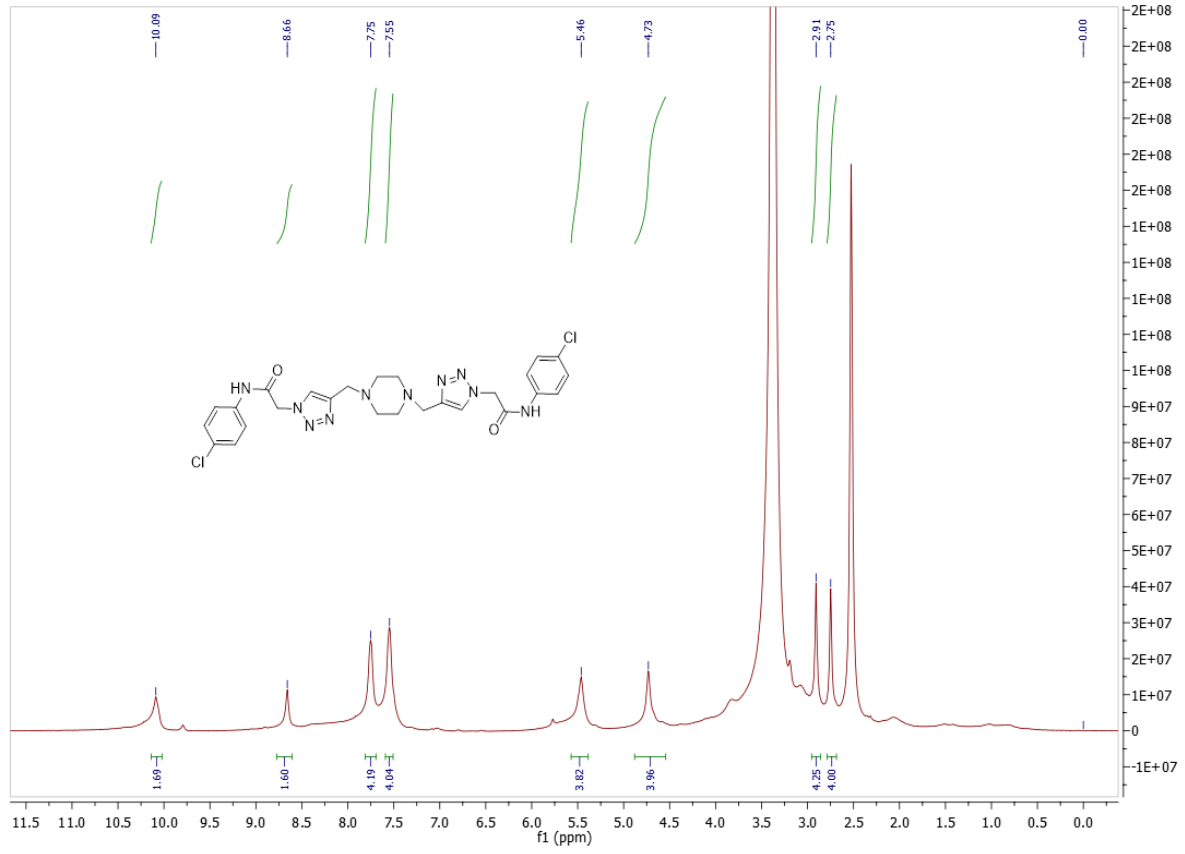
3i : ^{13}C NMR (100 MHz, DMSO-d_6, ppm)



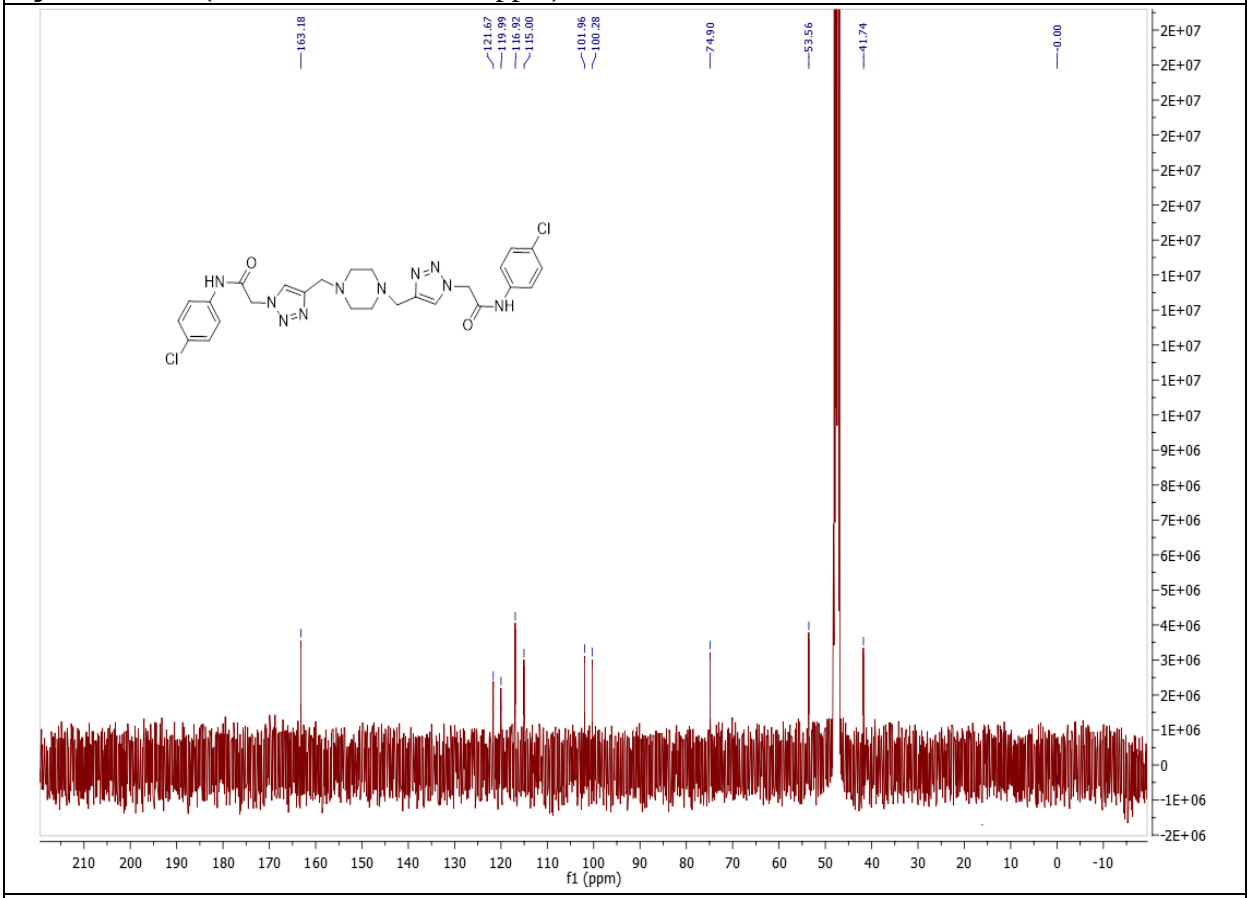
3i: HRMS



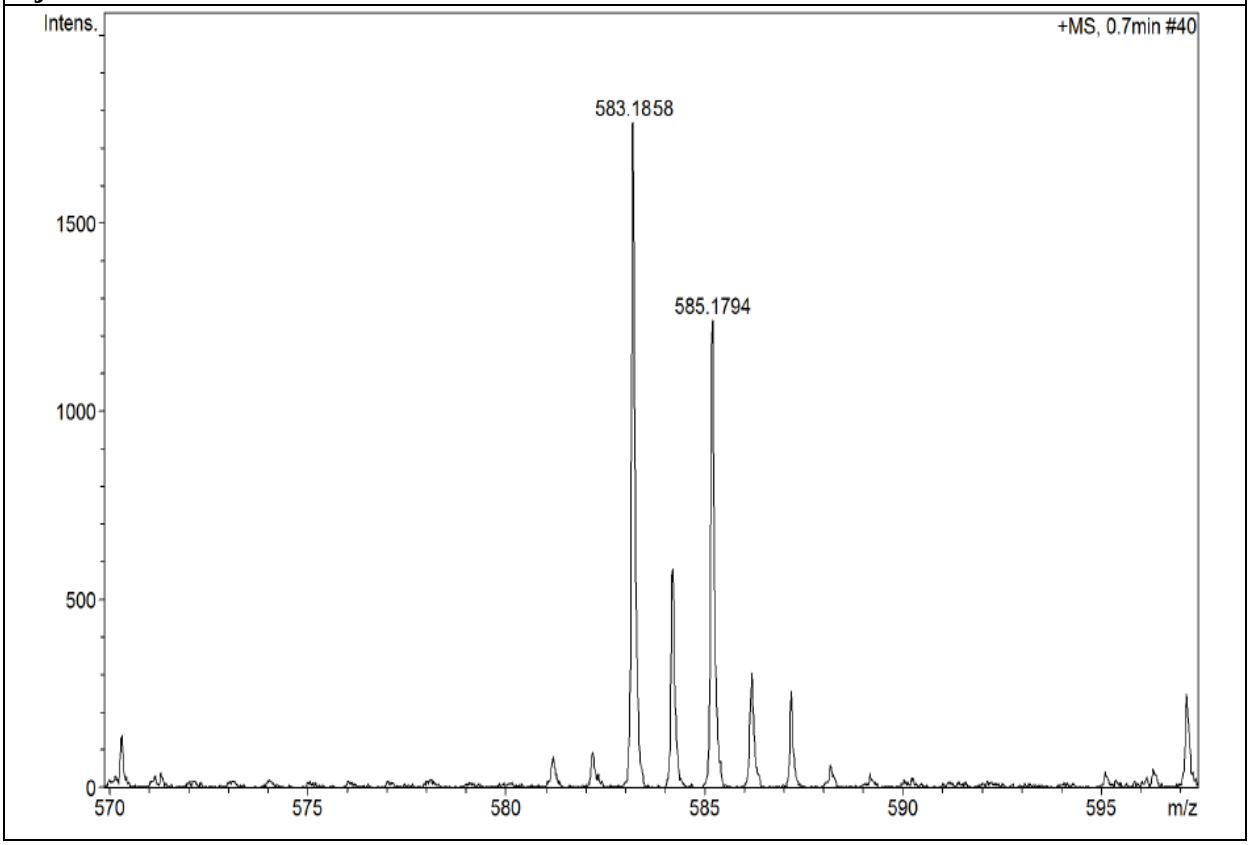
3j : ^{1}H NMR (400 MHz, DMSO-d_6, ppm)



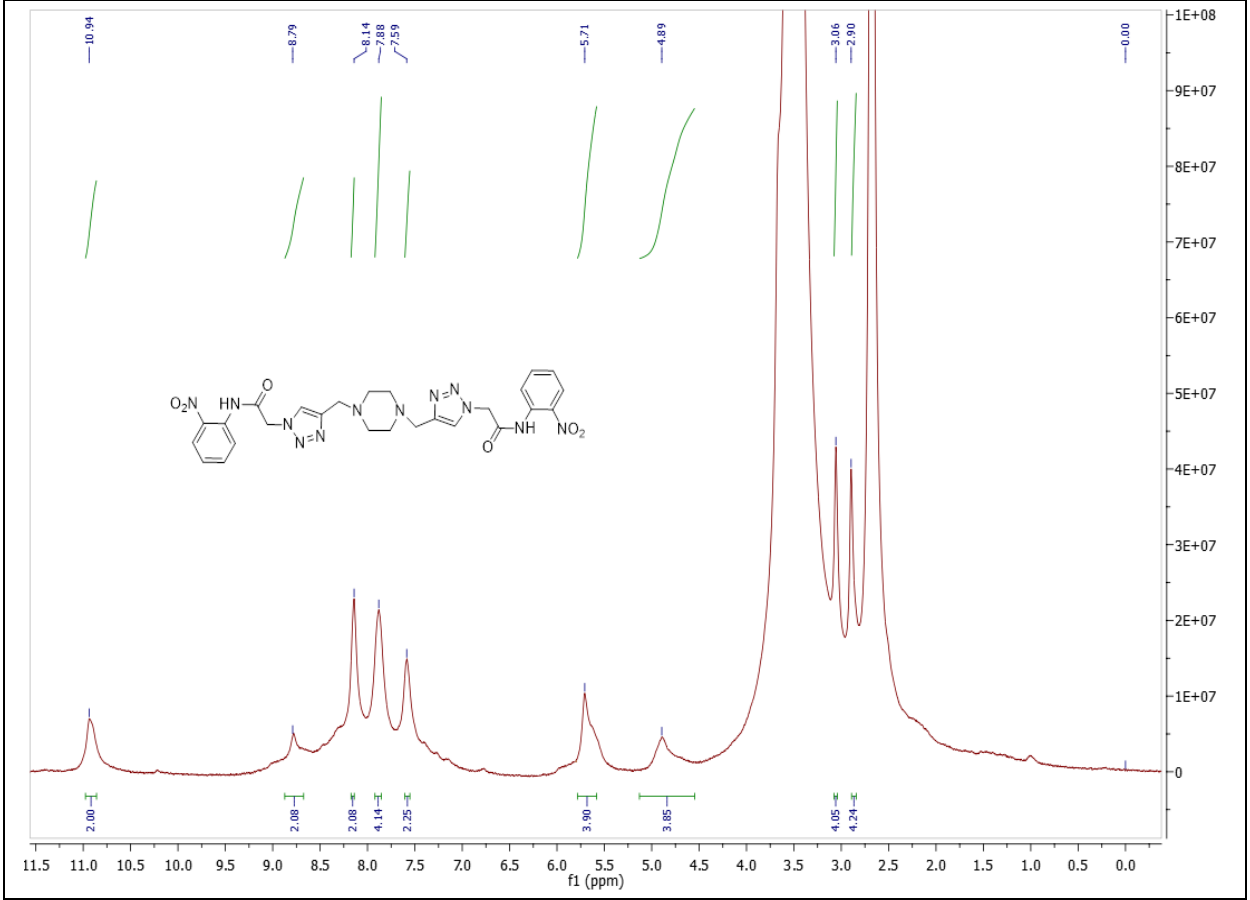
3j : ^{13}C NMR (100 MHz, DMSO-d_6, ppm)



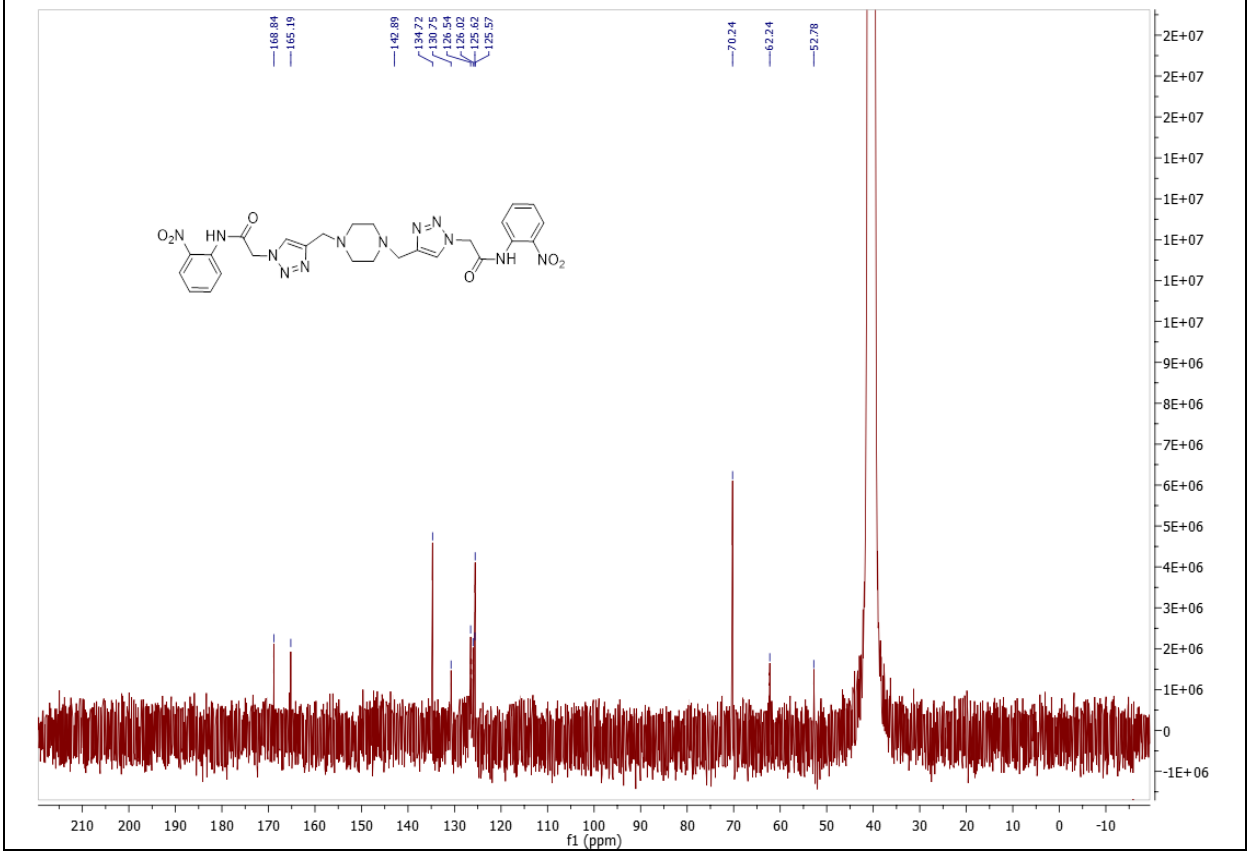
3j: HRMS



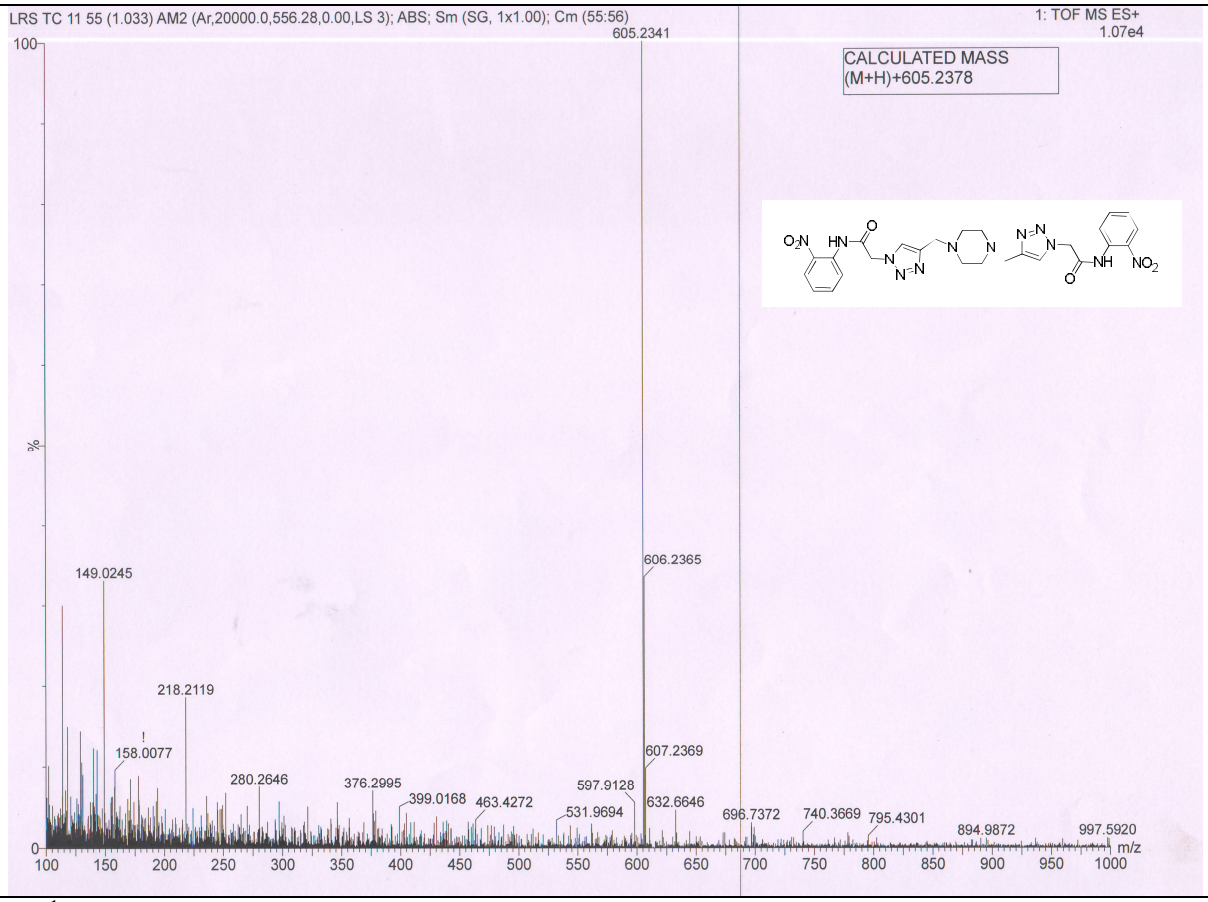
3k : ^{1}H NMR (400 MHz, DMSO-d_6, ppm)



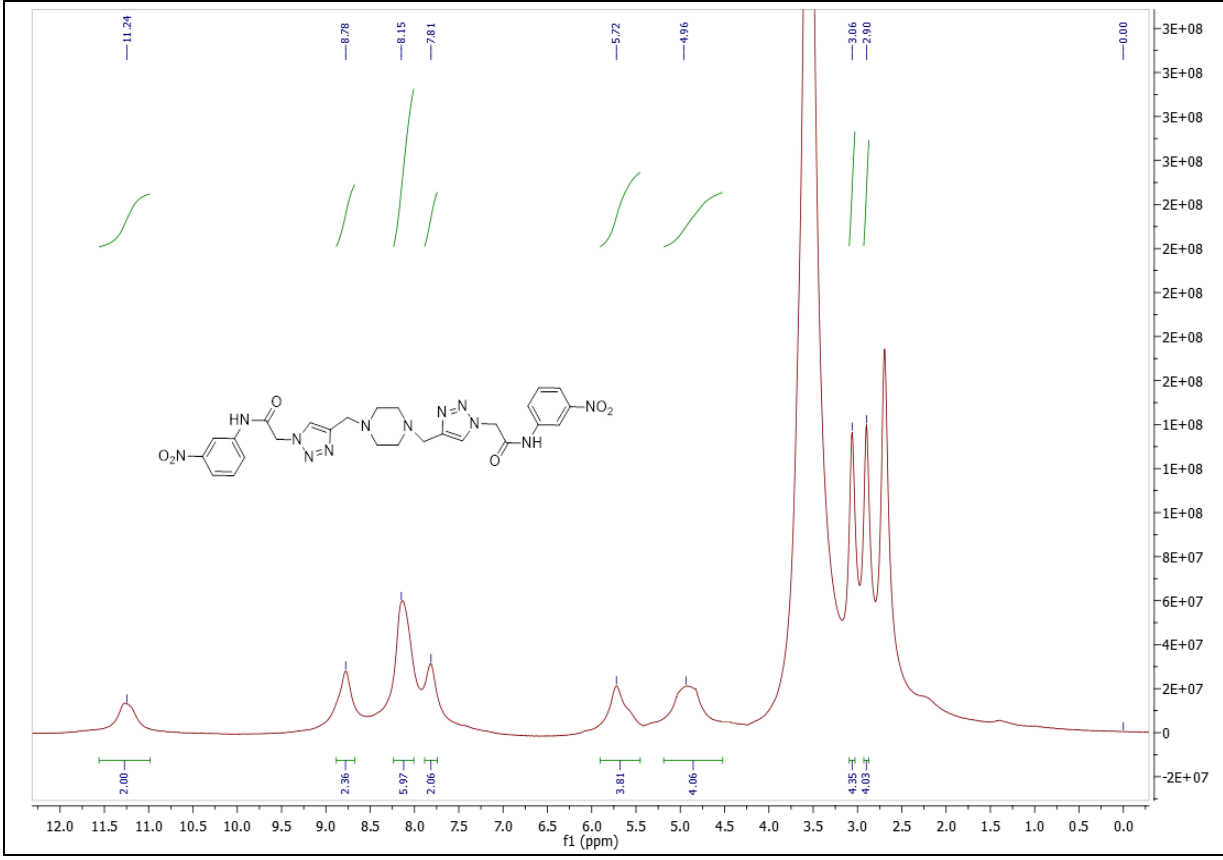
3k : ^{13}C NMR (100 MHz, DMSO-d_6, ppm)



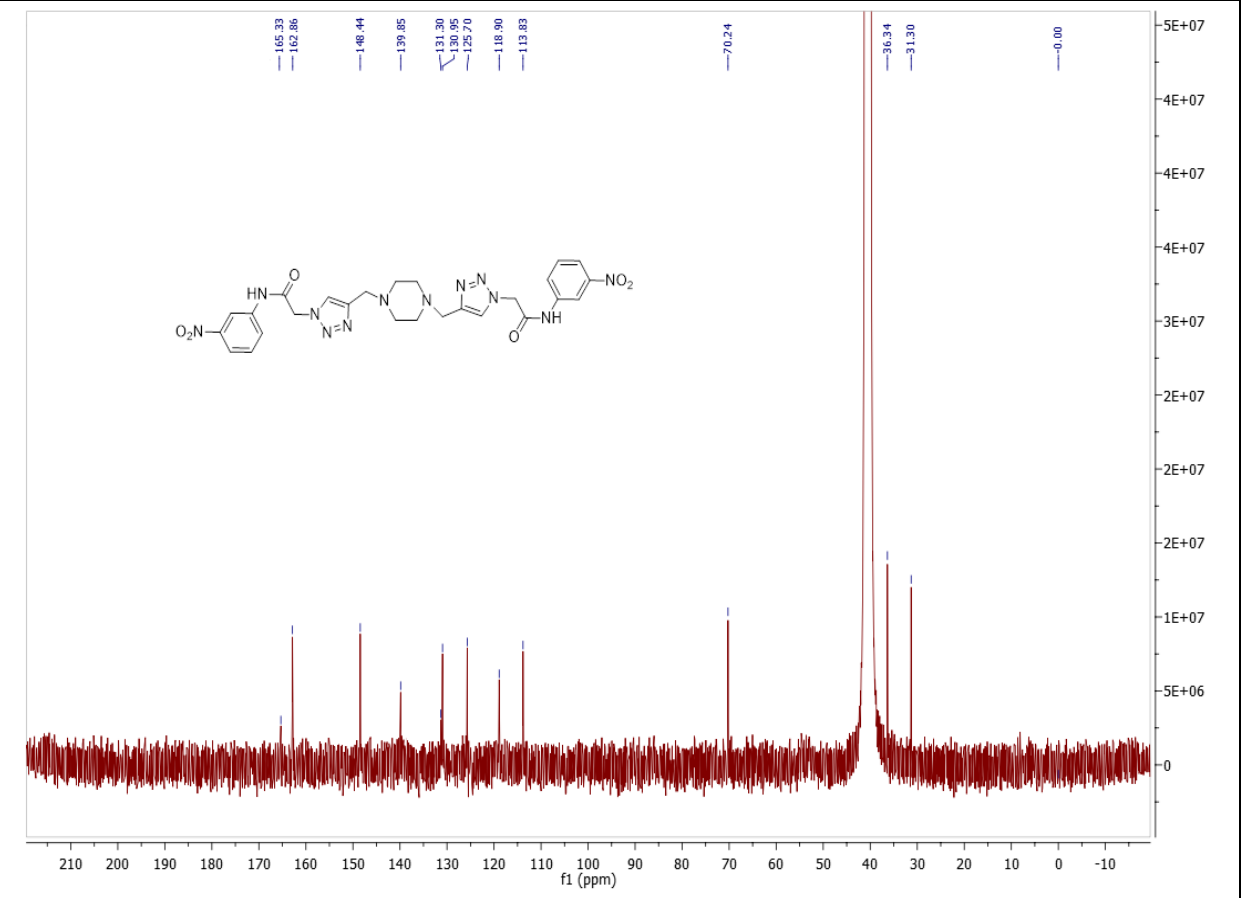
3k: HRMS



3l : ^{1}H NMR (400 MHz, DMSO-d_6, ppm)



3l : ^{13}C NMR (100 MHz, DMSO-d_6, ppm)



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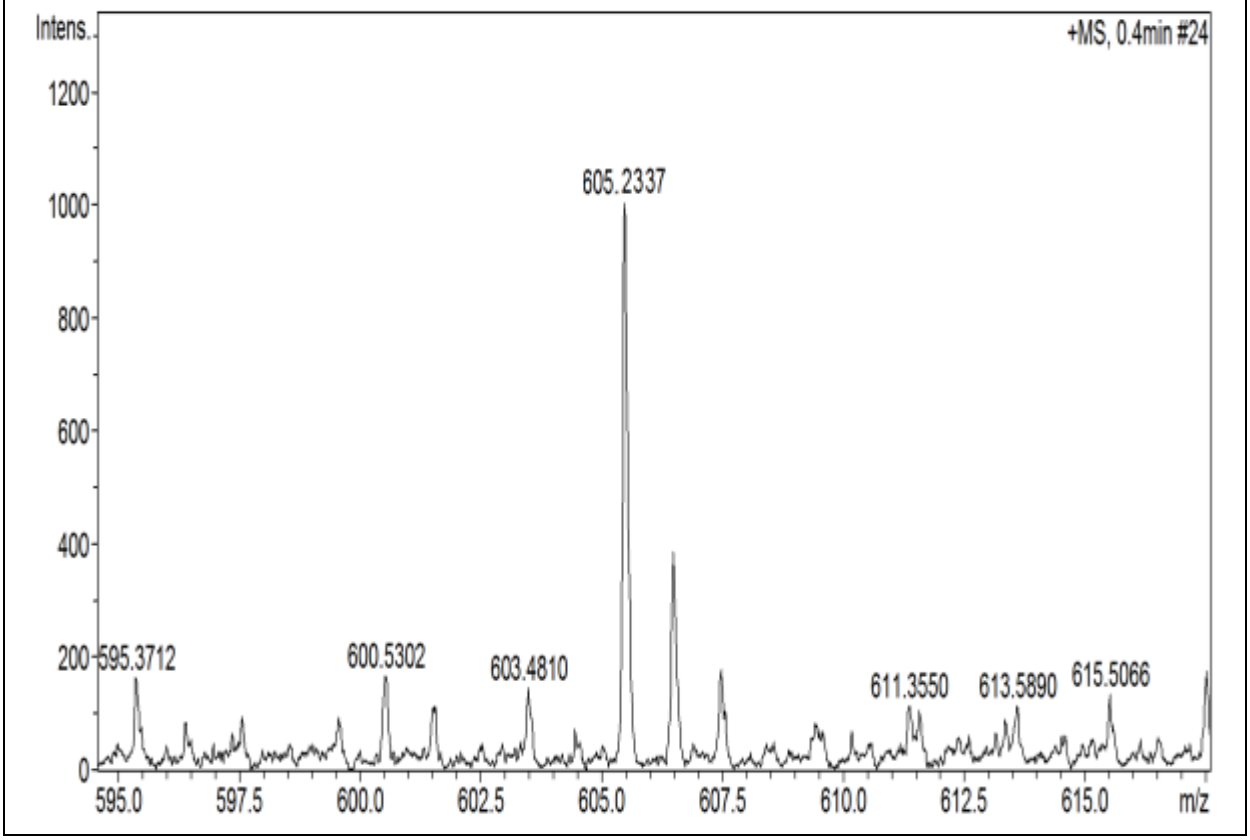
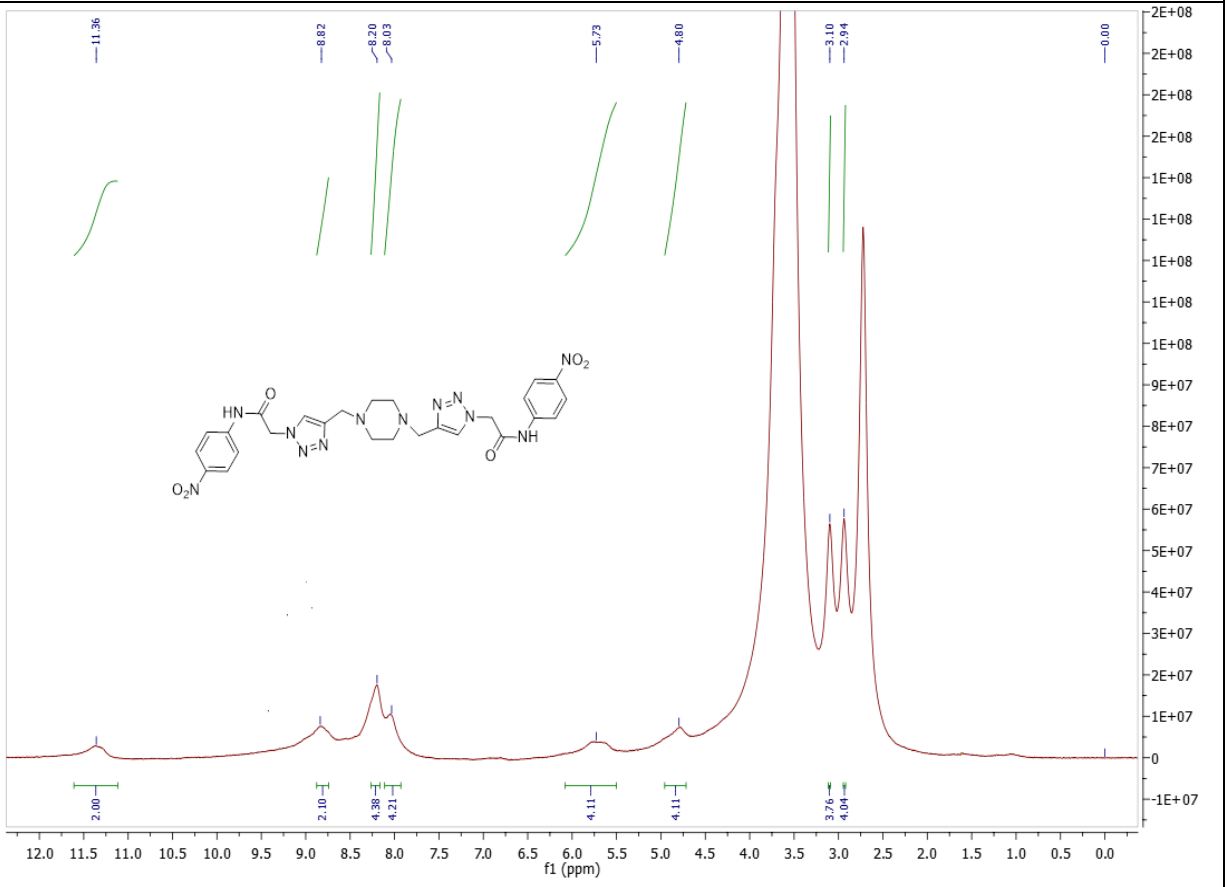
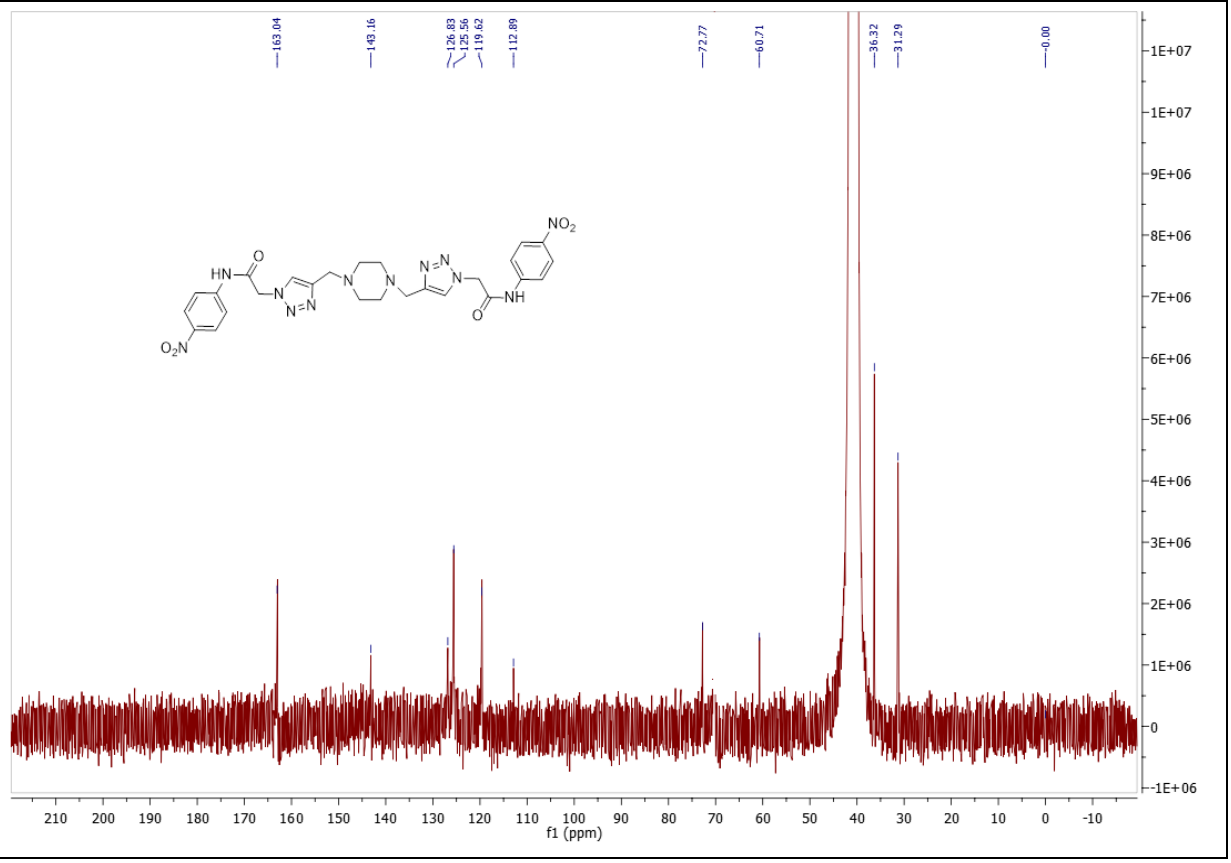


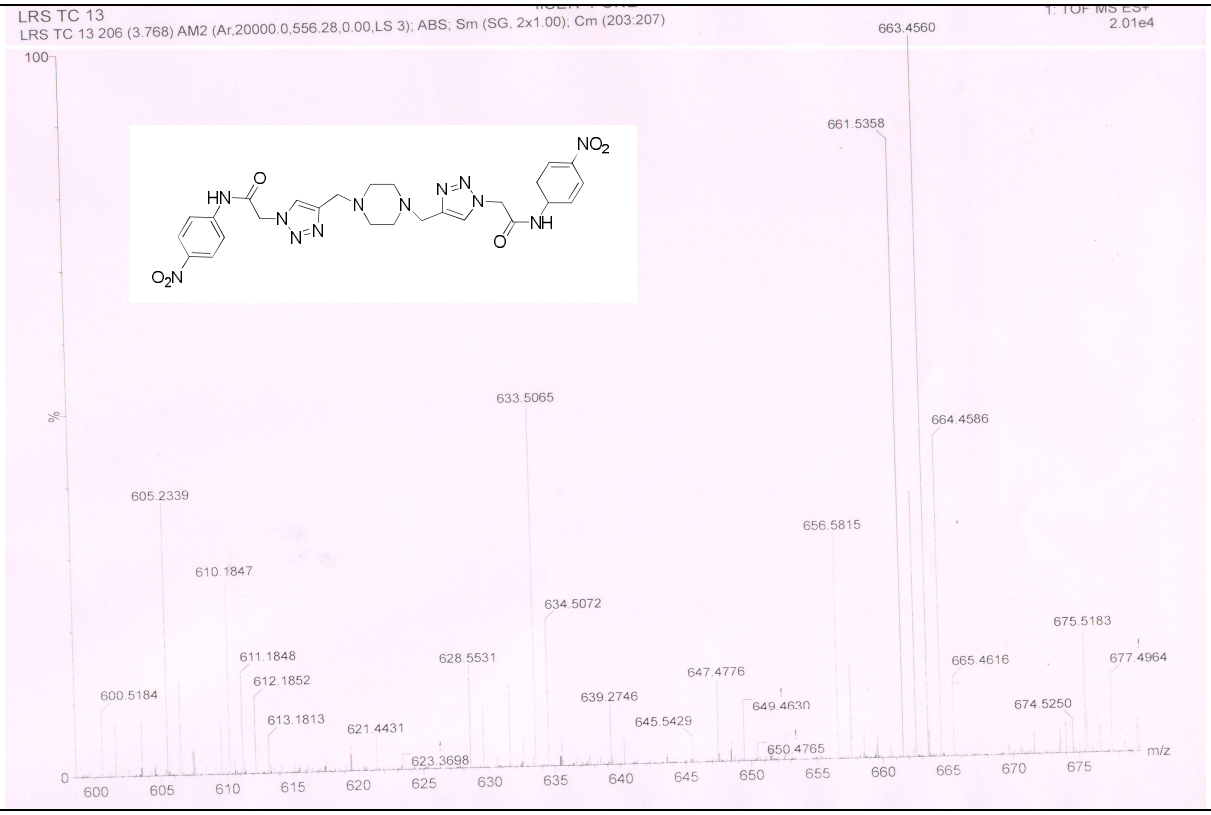
3m : ^{1}H NMR (400 MHz, DMSO-d_6, ppm)



3m : ^{13}C NMR (100 MHz, DMSO-d_6, ppm)



3m: HRMS


LRS TC 13
LRS TC 13 206 (3.768) AM2 (Ar,20000.0,556.28,0.00,LS 3); ABS; Sm (SG, 2x1.00); Cm (203:207)
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