Supplementary Material

Synthesis of a Novel 1,2,3-Triazoles Scaffold Using a Heterogeneous Multifunctional Copper Photocatalyst for In Vitro Investigation via Click Reaction

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Experimental Procedures

1. Experimental Section

1.1General characterization

All chemicals purchased from Merck, Aldrich, Acros, or Fluka were used without further purification. NMR spectra were recorded by BRUKERDRX-400AVANCE Advance spectrometer. Gas chromatography was performed by Trace GC ultra Thermo Company equipped with FID detector and Rtx®-1 capillary column. Melting points of products were measured with Electrothermal 9100 apparatus and were uncorrected. Nicolet IR100 instrument recorded IR spectra (with spectroscopic grade KBr), and spectra were obtained over the region of 400–4000 cm^{-1}. Thermogravimetric analysis was performed by STA504 weight change from 0 °C to 1000 °C. Field Emission Scanning Electron Microscopy (FE-SEM) images were recorded by Tescan MIRA3 FE-SEM. Transmission Electron Microscope (TEM) images were recorded by Philips EM208S and Carl Zeiss. Inductively coupled plasma atomic emission spectroscopy (ICP) was investigated by vista-pro. Vibrating sample magnetometer (VSM) was measured by Kavir magnetic-alternative gradient force magnetometer. X-ray diffraction pattern (XRD) was determined by Philips X-Pert 1710 diffraction meter. Differential Reflectance Spectroscopy was analyzed by Shimadzu UV-2450/2550. Photoluminescence (PL) spectra were obtained by RF6000 Shimadzu fluorescence spectrophotometer. Surface environment was investigated by X-ray photoelectron spectroscopy XPS measured by UHV analysis system SPECS using 1486.6 eV Al Kα as exciting X-ray source. CHNS was determined by elemental analyzer.

1.2 Electrochemical characterization

The electrochemical experiments were carried out using a Potentiostat/ Galvanostat (IVIUM Vertex), with a conventional three-electrode setup for the current-voltage (I-V) characteristic measurements. The electrolyte, reference electrodes, and gas purging were all held in a four-neck glass cell. A platinum plate and a glassy carbon (GC) electrode with an area of 0.031415 cm2 were employed as the working electrode and counter electrode. Ag/AgCl electrode with a saturated KCl solution was used as the reference electrode. For photocatalyst ink preparation, 1 mg of powder (the as-prepared photocatalysts) was dispersed in 100 µL of H2O-EtOH, and 40 µL

of Nafion solution (5 Wt.%, Aldrich), stirred for 24h. 5 µL of the dispersed mixture was dripped on a Glassy carbon electrode surface (as a working electrode) and dried under an IR lamp. The CV response of the samples was measured in 0.02 M Fe^{3+} /Fe^{2+} and KCl 1M solution at a scan rate of 30mV/s. This route for electrochemical impedance spectroscopy (EIS) was carried out. The open circuit potential and ac voltage amplitude (3mV) with frequency varying from 10mHz to 100KHz were scanned. The Mott-Schottky measurement was probed in the potential range of -1 to +1.5 V (vs. Ag/AgCl) with a frequency of 500 Hz. For Mott-Schottky analysis, 3 mg of powder was dispersed in 100 µl H2O-EtOH using an ultrasonic bath for 10 min. 3 µl of the dispersed mixture was dripped on the electrode surface and left to dry under an IR lamp. Then 1 µl of Nafion solution (5 Wt.%, Aldrich)was added to the surface and allowed to dry by the same method. It should be noted thatThe Mott-Schottky measurement was measured in Na_2SO_4 (0.2 M).

1.3 Preparation of AlZn-Cu (using a specific 3:7.5:1.5 mol/mol ratio**)**

The coprecipitation approach involved dissolving 7.5 mmol of $Zn(Cl)_2$, 3 mmol of $Al(Cl)_3$, and 1.5 mmol of $Cu(Cl)_2$ in 50 ml of deionized water. An alkaline solution (0.2 M NaOH) was added dropwise to the LDH solution while continuously stirring until the pH reached 10. The suspension was stirred for 24 hours at 60 °C.

1.4 Preparation of Magnetic AlZn-Cu(using a specific 6.5:3:7.5:1.5 mol/mol ratio**)**

To synthesize the core-shell magnetic Fe_3O_4/AlZn-Ni-LDH nano-catalyst, Fe_3O_4 nanoparticles were first created [23]. Similar to previous methods, the coprecipitation route was used to create the layered double-hydroxide solution. 7.5 mmol of $Zn(Cl)_2$, 3 mmol of $Al(Cl)_3$, and 1.5 mmol of $Cu(Cl)_2$ were dissolved in 50 ml of deionized water. Dropwise addition of alkaline solutions (0.2 M NaOH) was made to the LDH solution while continuously stirring, maintaining pH at 10. To fabricate the LDH materials on the magnetic support, 100 ml of dispersed Fe3O4 (6.5mmol:1.5g) nanoparticles required dropwise addition of LDH solution. The suspension was stirred at 60 °C for 24 hours. After being separated by an external magnet, the nanoparticles were washed three times in water. The chloride and water absorbed between the interlayers of Fe_3O_4/AlZn-Cu LDH were removed by calcining at 380 °C.

1.5 General Procedure for 2-(Prop-2-yn-1-yloxy)naphthalene-1,4-dione

For the synthesis of 2-(prop-2-yn-1-yloxy)naphthalene-1,4-dione, 2-hydroxynaphthalene-1,4-dione (1 mmol) and K_2CO_3 (1.2 mmol) were ground in a mortar to remove moisture, then DMF was added to the mortar and transferred to clean round-bottom tubes. Propargyl bromide (1.2 eq) was added after grinding, and the mixture was stirred for 12 hours at room temperature. TLC was used to monitor the progress of the reaction. The solvent was removed by a vacuum pump, and the reaction mixture was then extracted with H_2O and EtOAc (4 × 10 mL). The organic layer was dried using anhydrous Na_2SO_4, the solvent was evaporated, and the product was crystallized with a small amount of EtOH and shocked with cooled water. Two drops of HCl (37%) were added to the beaker, and extraction was performed again with ethyl acetate.

1.6 General Procedure for 2-Chloro-N-phenylacetamide

To synthesize 2-chloro-N-phenylacetamide, aniline (0.5 mmol) and triethylamine (0.55 mmol) in dried dichloromethane (DCM) (3 mL) were stirred. Chloroacetyl chloride (1.1 mmol) was then slowly added. After addition, the mixture was stirred at room temperature for 24h, worked up with water, and the aqueous DCM layer was extracted with DCM (2 × 10 mL). The combined organic phases were washed with hydrochloric acid (2 drops) and extracted with ethyl acetate and water (2 × 10 mL). The yellow powder was obtained after drying.

1.7 General Procedure for Click Reaction

For the click reaction, 2-(prop-2-yn-1-yloxy)naphthalene-1,4-dione (1.2 mmol), 2-chloro-N-phenylacetamide (1 mmol), and K_2CO_3 (1.2 mmol) were combined with 20 mg of Fe_3O_4/AlZn-Cu catalyst and added to a mixture of EtOH-H2O-DMSO (1:1:2) at 25°C under domestic light (20w). TLC was used to monitor completion. After removing the catalyst with a large magnet, the solvent was evaporated by a vacuum pump. The reaction mixture was then extracted with H_2O and EtOAc (4 × 10 mL). The organic layer was dried using anhydrous Na2SO4. The purification of the compound was done using silica gel.The catalyst was washed with acetone and ethanol and reused.

2. Figures

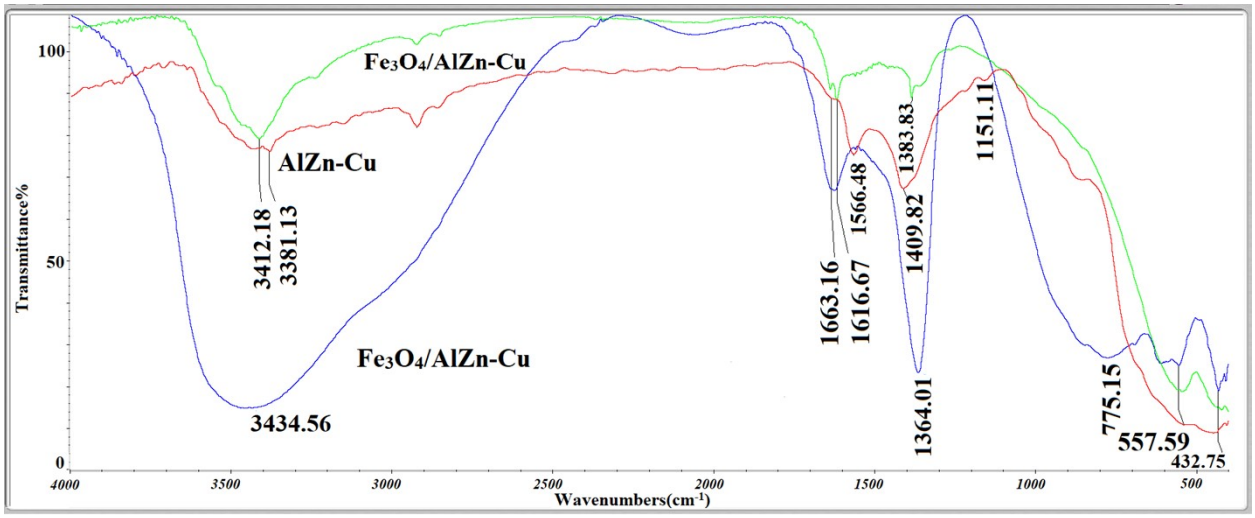
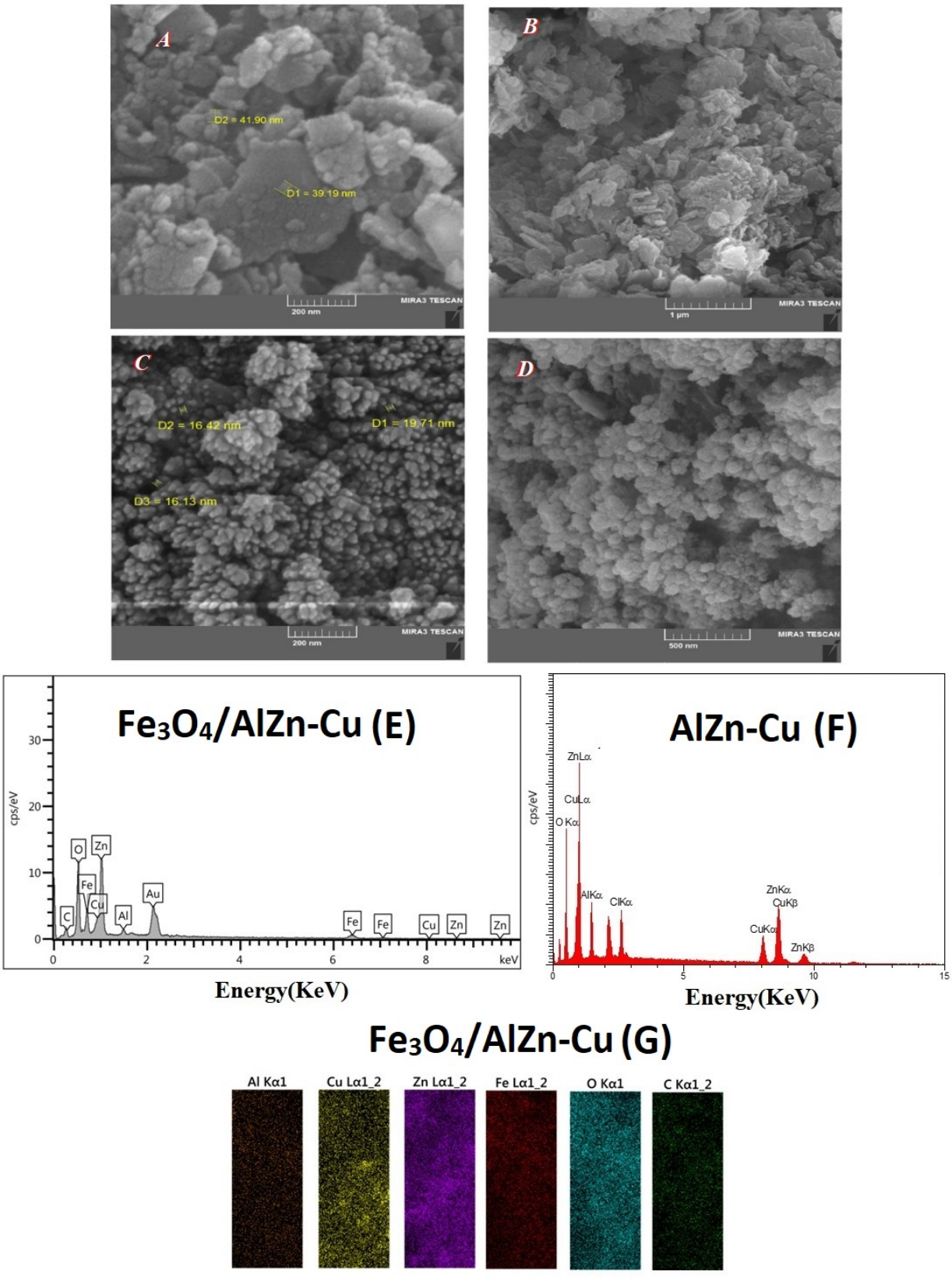


Fig.S$_1$. FT-IR spectrum of preparation of the catalyst



FigureS2. SEM images of AlZn-Cu (A, B), Fe_3O_4@AlZn-Cu before furnace (C), Fe_3O_4@AlZn-Cu after furnace (D) EDS images of FeO_4@AlZn-Cu (E) AlZn-Cu (F) Element Mapping (G)

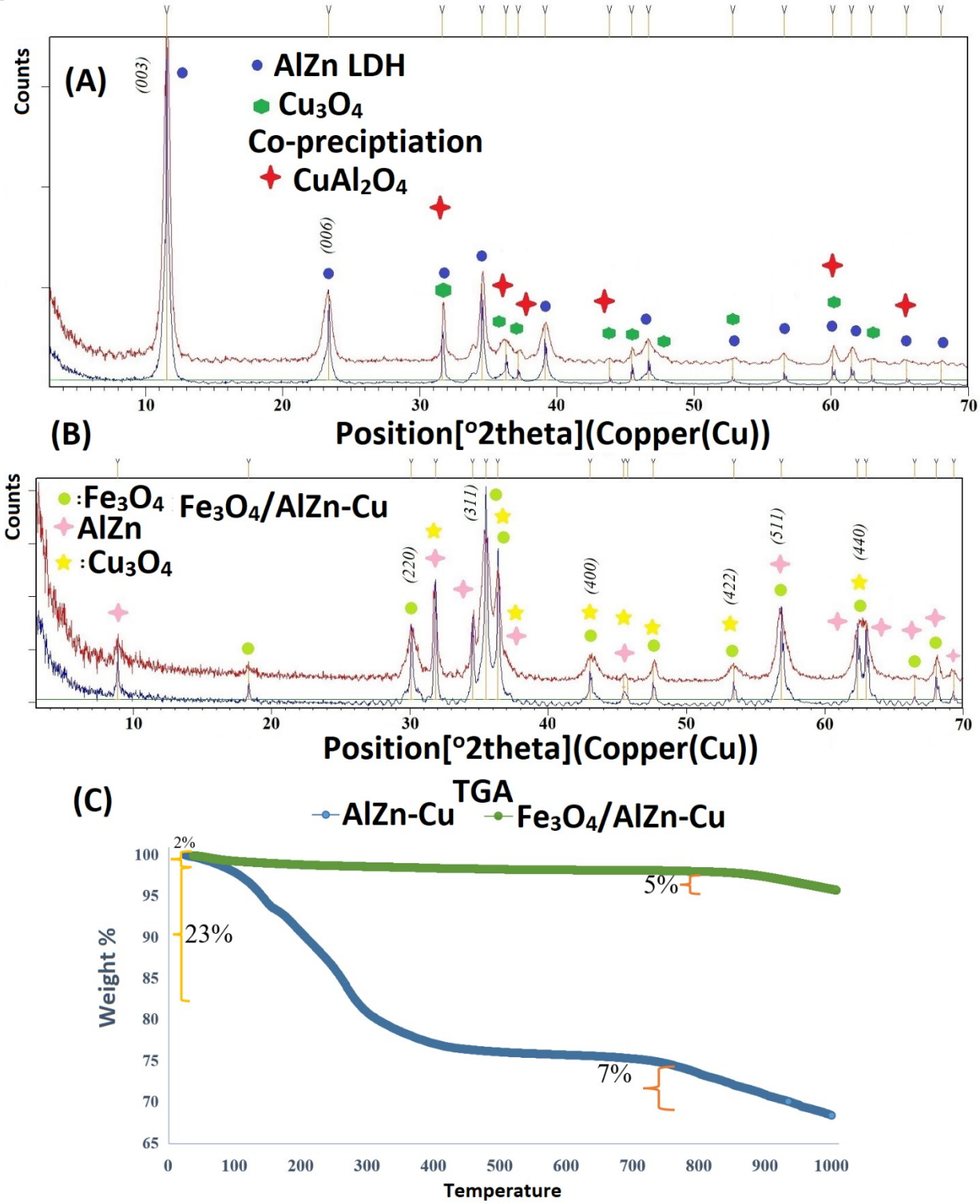


Figure S_3. XRD pattern of AlZn-Cu (A), Fe_3O_4/AlZn-Cu (B) TGA of AlZn-Cu(Green) ,and Fe_3O_4@AlZn-Cu(Blue) (C)

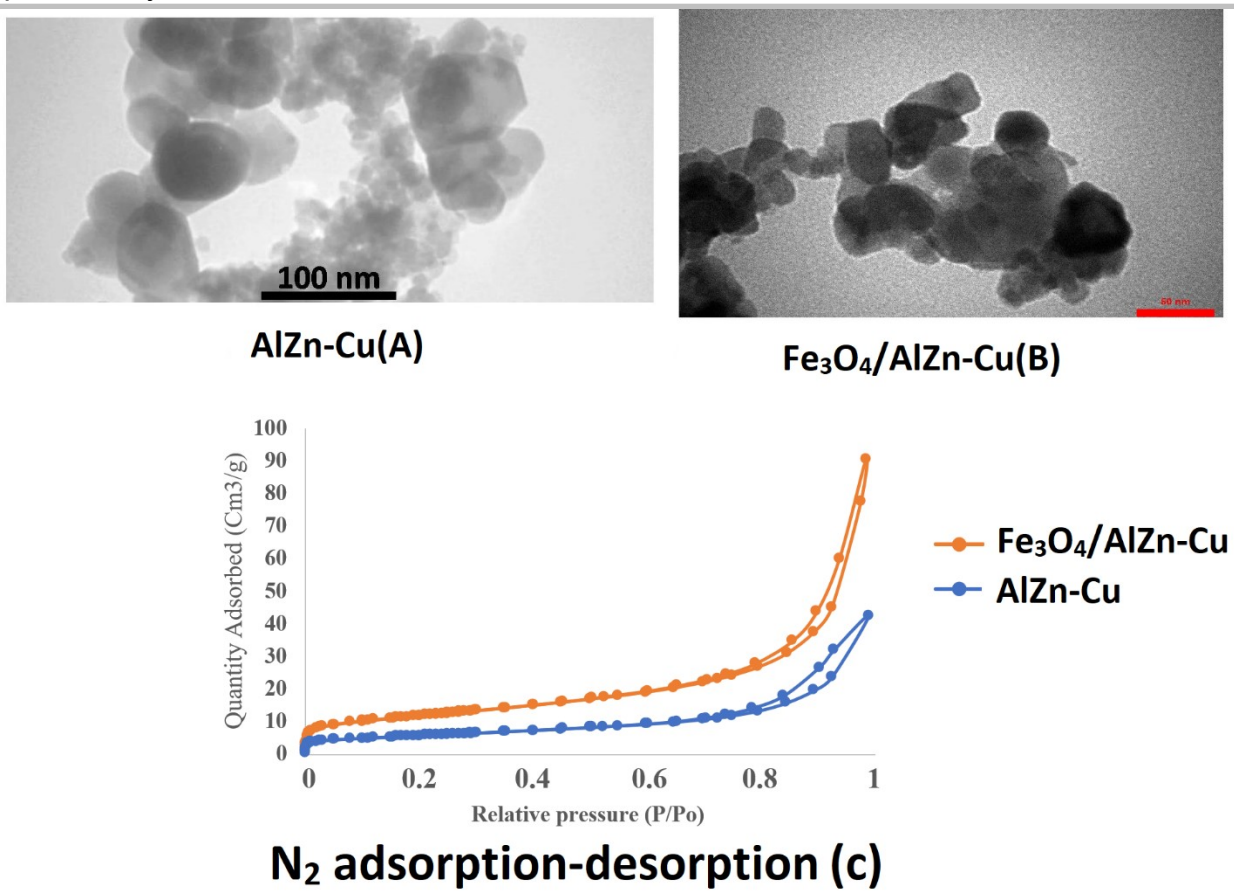


Fig.S4. TEM images of AlZn-Cu(A), Fe_3O_4/AlZn-Cu(B) N_2 adsorption-desorption isotherms of AlZn-Cu, and Fe_3O_4@AlZn-Cu(C)

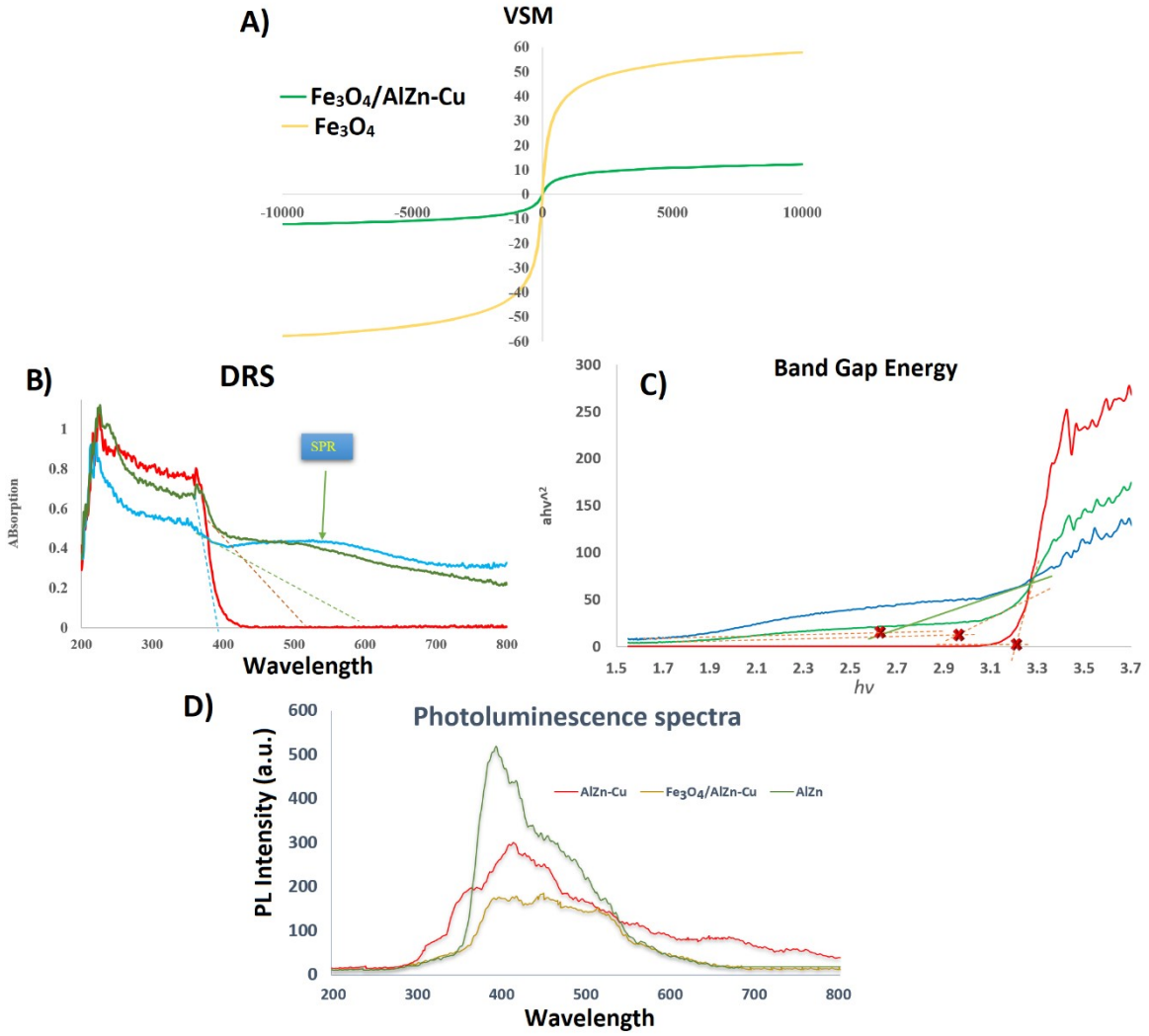


Fig.S5 VSM curve of Fe_3O_4@AlZn-Cu **(A)** UV–Vis diffuse reflectance of Al-Zn , AlZn-Cu , and Fe_3O_4/AlZn-Cu **(B)** The obtained band gaps from the curves of $(ahv)^2$ versus hν for Al-Zn (Red), AlZn-Cu (Green), and Fe_3O_4/AlZn-Cu (Blue) **(C)** Photo-luminescence spectra of Al-Zn(green), AlZn-Cu(Red), and Fe_3O_4/AlZn-Cu(Yellow) **(D)**

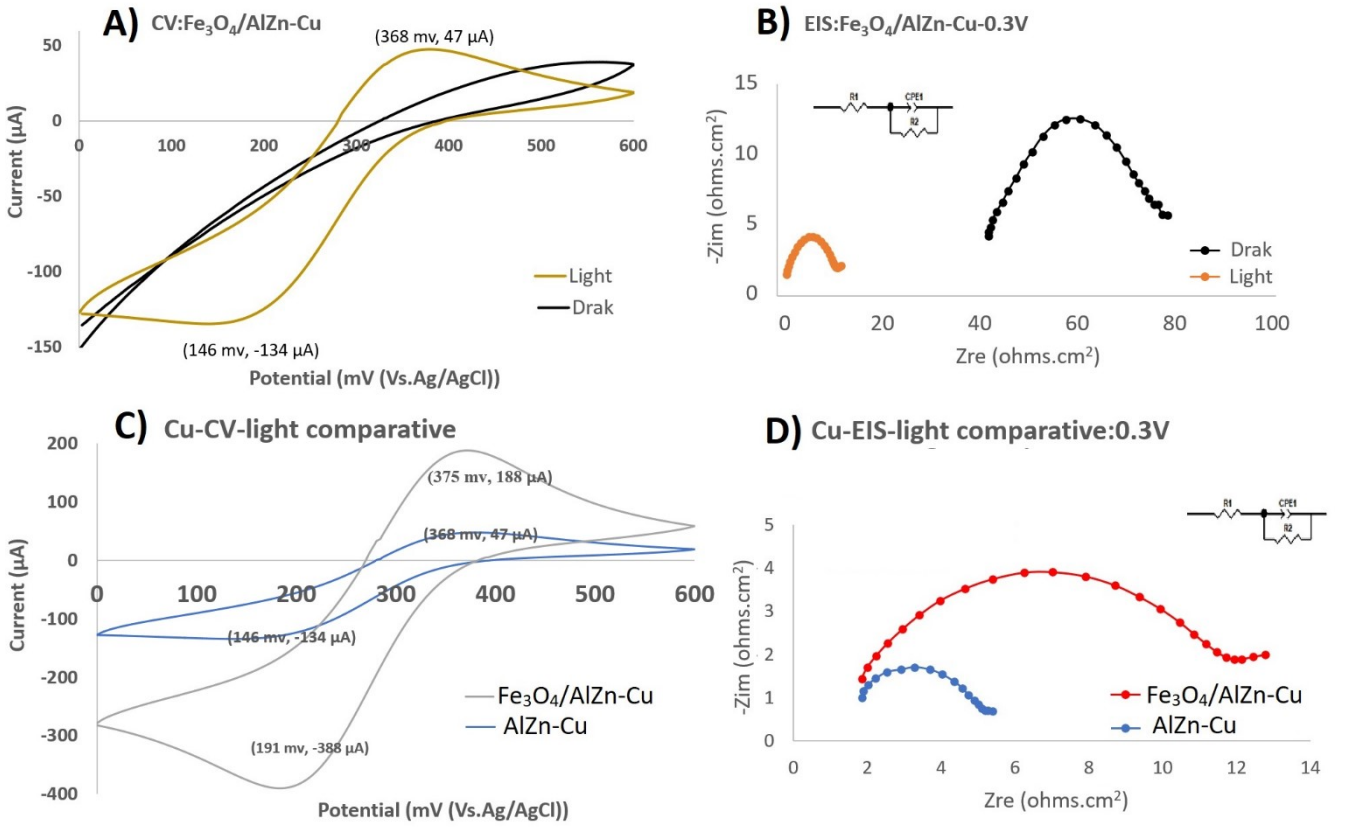


Fig.S$_6$ the cyclic voltammogram of $K_3Fe(CN)_6/K_4Fe(CN)_6$. in the dark and light Using Fe_3O_4/AlZn-Cu as photocatalyst **(A)** EIS Response of L_2S-M: Fe_3O_4/AlZn-Cu at 0.3 V light and dark **(B)** The comparative of the cyclic voltamgram of $K_3Fe(CN)_6/K_4Fe(CN)_6$ using Fe_3O_4/AlZn-Cu and AlZn-Cu as photocatalyst in light **(C)** Comparative Nyquist plots, of of AlZn-Cu and Fe_3O_4/AlZn-Cu at 0.3v in light **(D)**

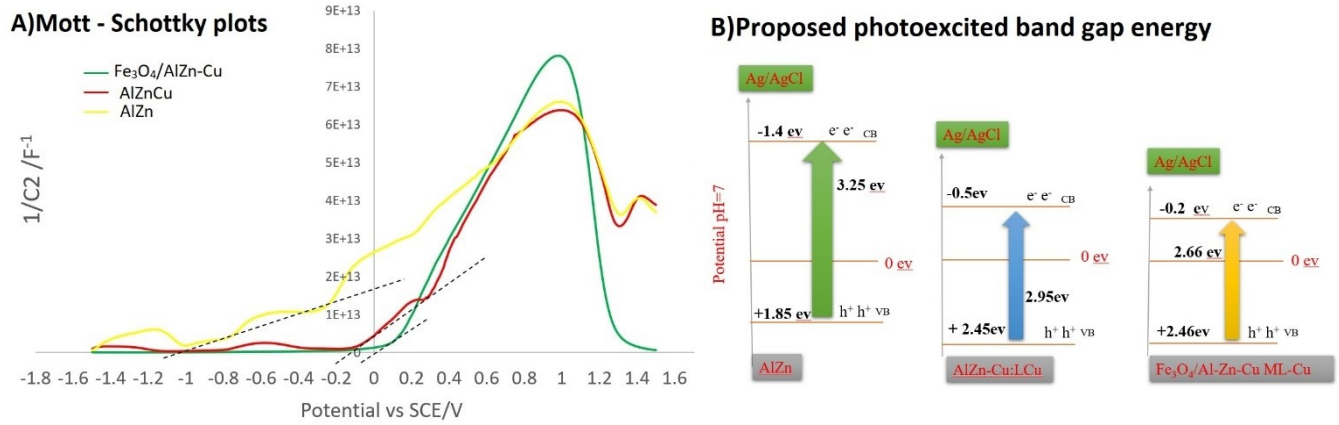


Fig.S$_7$ Mott - Schottky plots of AlZn , AlZnCu ,and Fe_3O_4/AlZn-Cu at 500 Hz **(A)** Proposed photoexcited band gap for the AlZn, AlZn-Cu, and Fe_3O_4/AlZn-Cu with Mott – Schottky test **(B)**

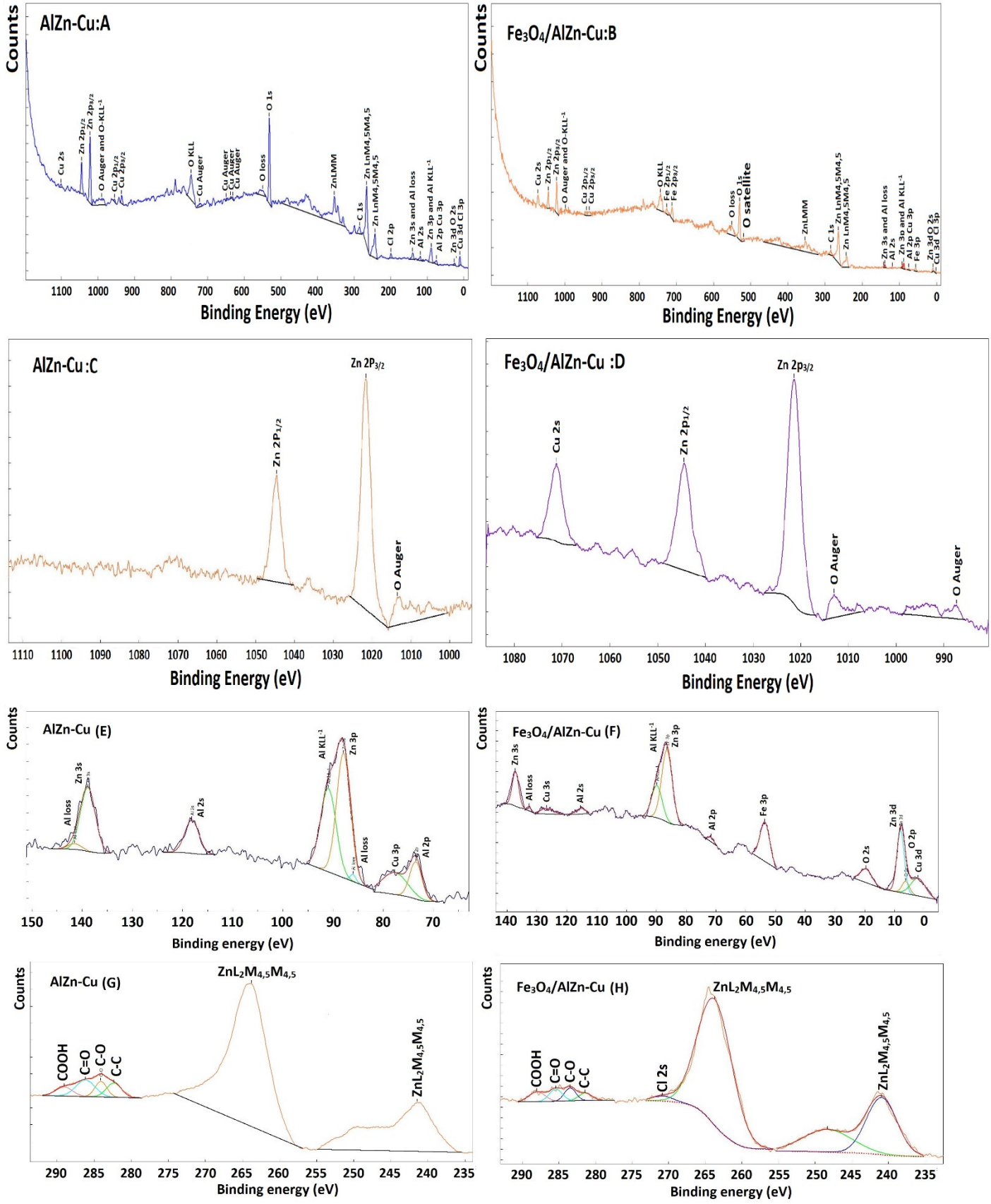


Fig. S$_8$ X-ray photoelectron spectroscopy (XPS) survey spectrum of AlZn-Cu, and Fe_3O_4/AlZn-Cu **(A and B),** X-ray photoelectron spectroscopy (XPS) expand of ZnO, **(C and D),** X-ray photoelectron spectroscopy (XPS) expand of Al_2O_3**(E and F),** X-ray photoelectron spectroscopy (XPS) expand of carbon**(I and J)**

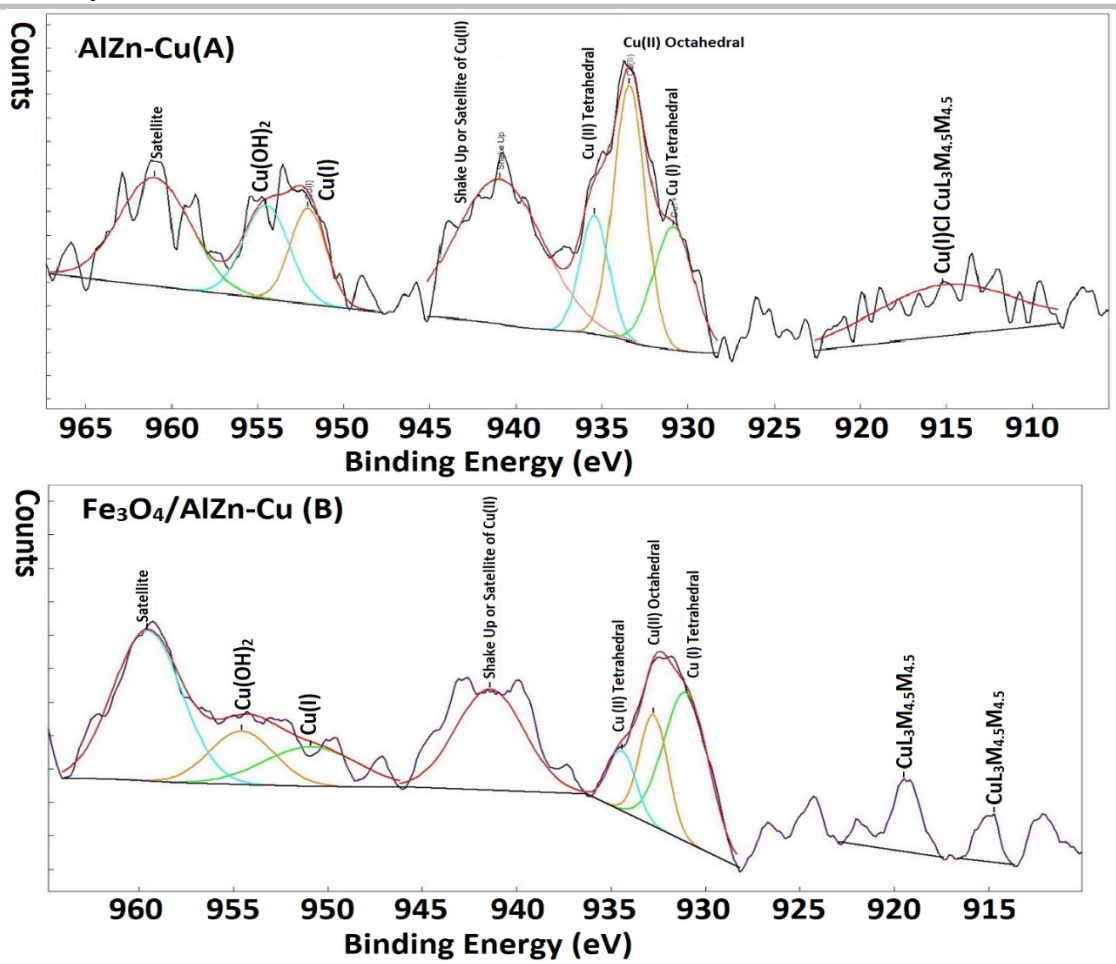


Fig. S$_9$ X-ray photoelectron spectroscopy (XPS) expand of copper for AlZn-Cu **(A) ,** X-ray photoelectron spectroscopy (XPS) expand of copper for AlZn-Cu **(B)**

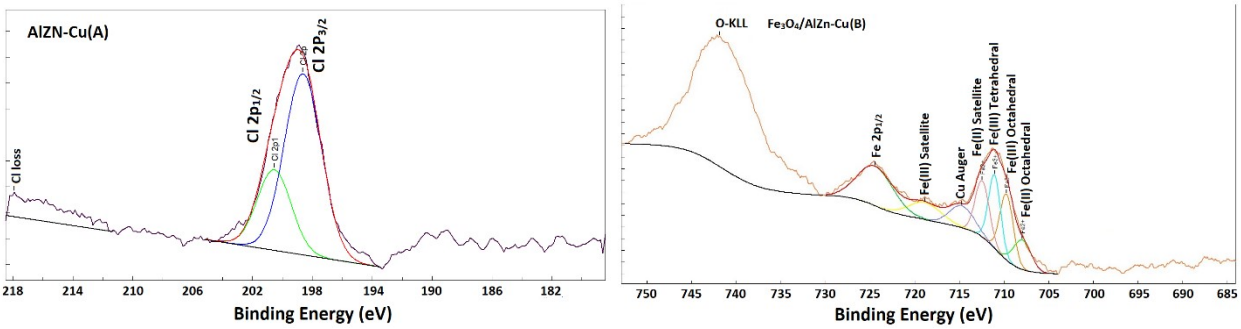


Fig. S$_{10}$ X-ray photoelectron spectroscopy (XPS) expand of Chlorine (A) and Fe_3O_4 (B)

Proposed Mechanism :

Previous studies have reported successfully reducing 3d transition metals [1-3] using photocatalytic substrates as co-catalysts [4-9]. In this study, a new photocatalyst (PC) in the form of $ZnAl_2O_4$ LDH was investigated and found to act as an effective co-catalyst. The study suggested that through doping and creating a composite structure, $ZnAl_2O_4$ LDH exhibited photo-induced electron transfer (PET) [10]. It is proposed that PC reduces copper, a process previously observed with ascorbic acid or natural compounds [11] and subsequently facilitates the click

reaction [12]. However, when TEMPO was introduced into the reaction, the catalyst activity was inhibited, indicating that TEMPO halted the LDH photocatalysis [13].

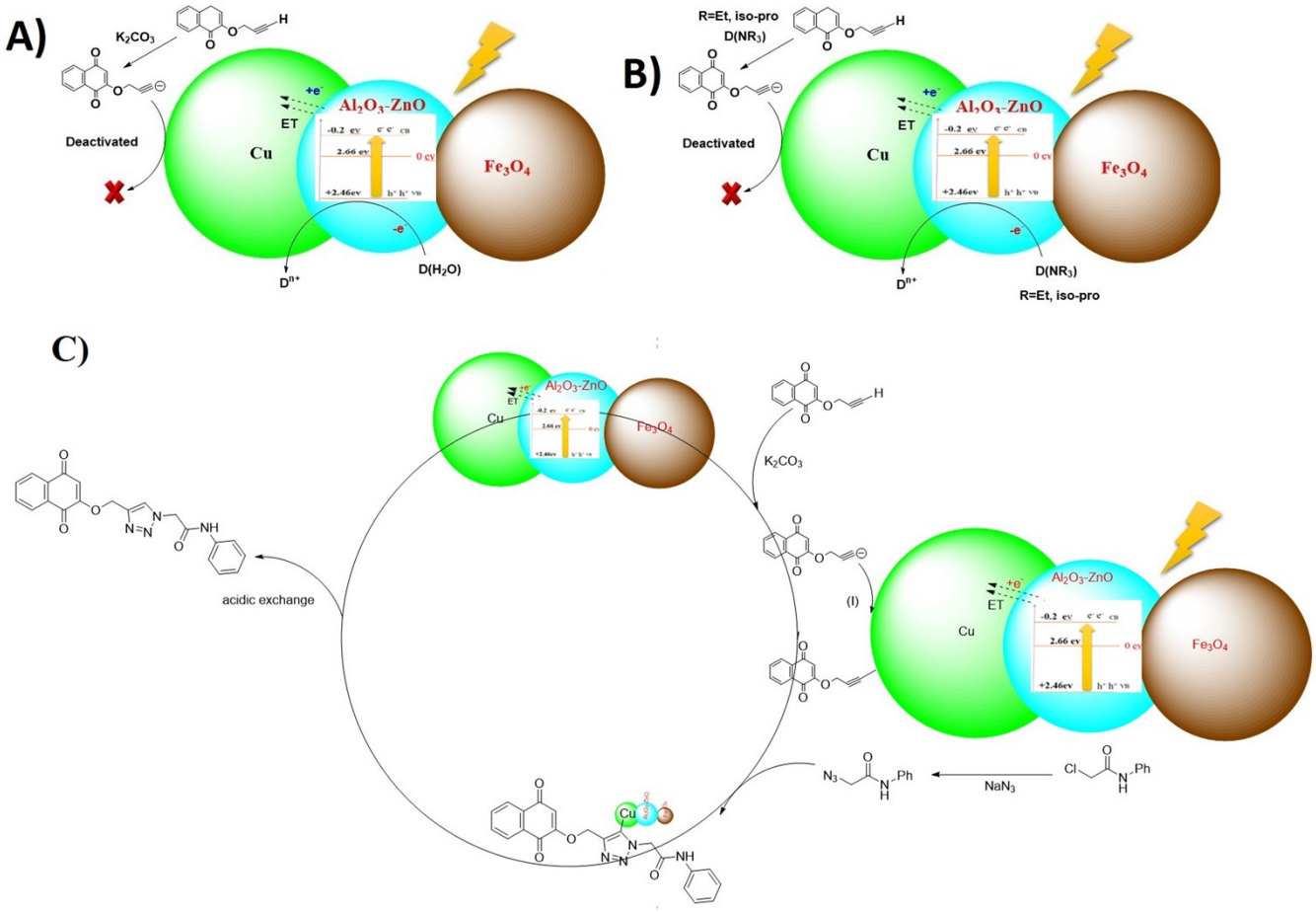


Fig. S_{11} Evaluation of proposed mechanisms for catalysis

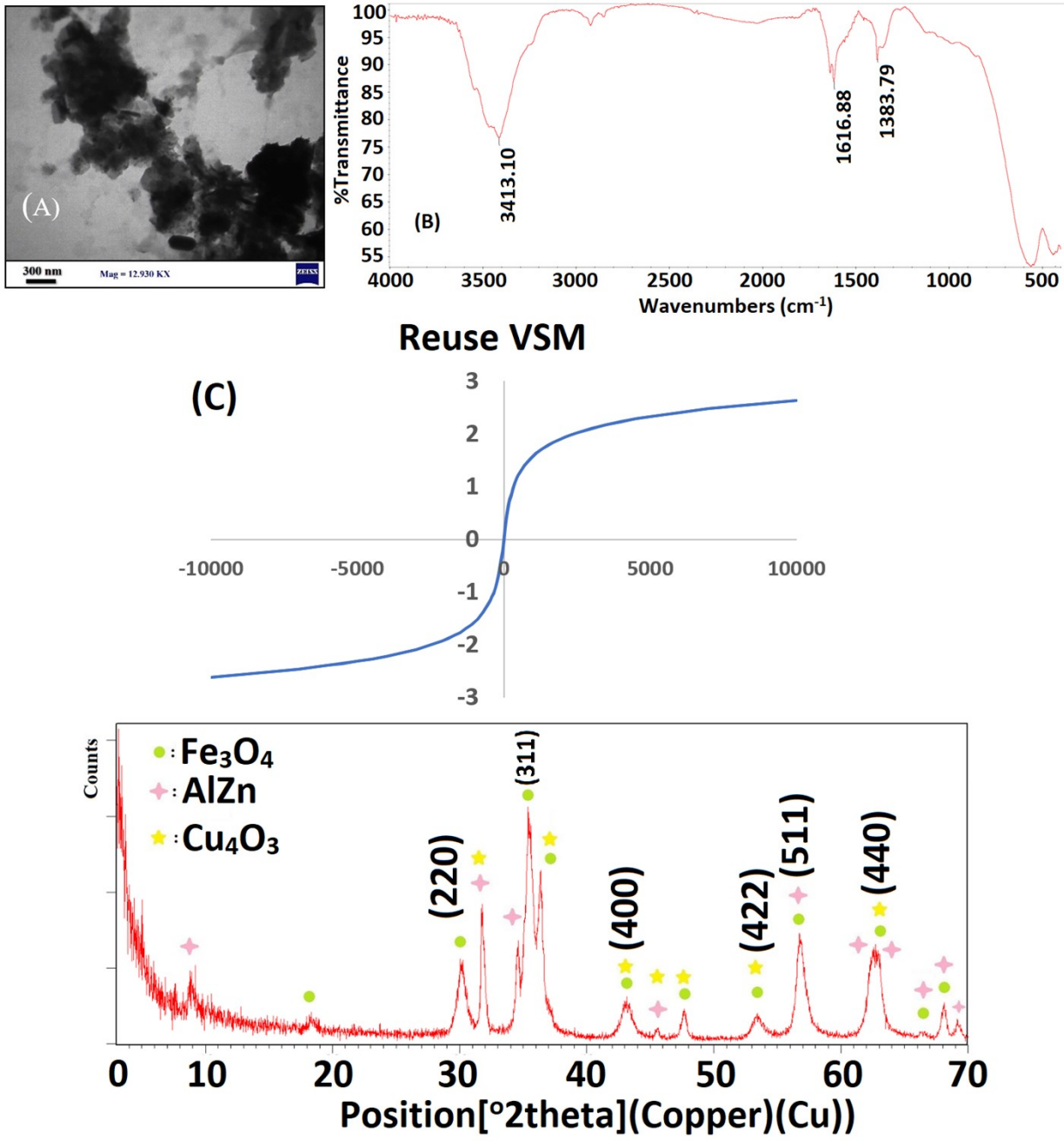


Fig. S_{12}Reused TEM image (A) and Reused FT-IR spectrum (B) reused VSM curve (C)Reused XRD Pattern

3.Characterization of Products

Also, All of Crude data are available at: https://zenodo.org/record/7680323 (DOI: 10.5281/zenodo.7680323)

2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)-N-phenylacetamide (3a):

Cream solid, M.P.: 200-202 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 5.29 (s, 2H, N-CH_2), 5.40 (s, 2H, O-CH_2), 6.67 (s, 1H, C-H, quinon), 7.09 (t, J = 8 Hz, 1H, ArH), 7.34 (t, J = 8 Hz, 2H, ArH), 7.59 (d, J = 8 Hz, 2H, ArH), 7.81 – 7.91 (m, 2H, ArH), 8.00 (td, J = 8.4, 0.8 Hz, 2H, ArH), 8.37 (s, 1H, C-H, Triazole), 10.51 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 52.71, 62.83, 111.38, 119.66, 124.26, 126.04, 126.60, 127.71, 129.41, 131.31,

131.95,134.16, 135.01, 138.87, 141.06, 159.64, 164.60, 179.99, 185.05.; IR (KBr) 3345, 1710, 1670, 1243, 1123 cm^{-1}. Mass (M/Z:20ev):387. **Anal. calcd for $C_{21}H_{16}N_4O_4$** (387): C, 64.94; H: 4.15; N, 14.43 Found: C, 64.98 H: 4.19; N, 14.40.

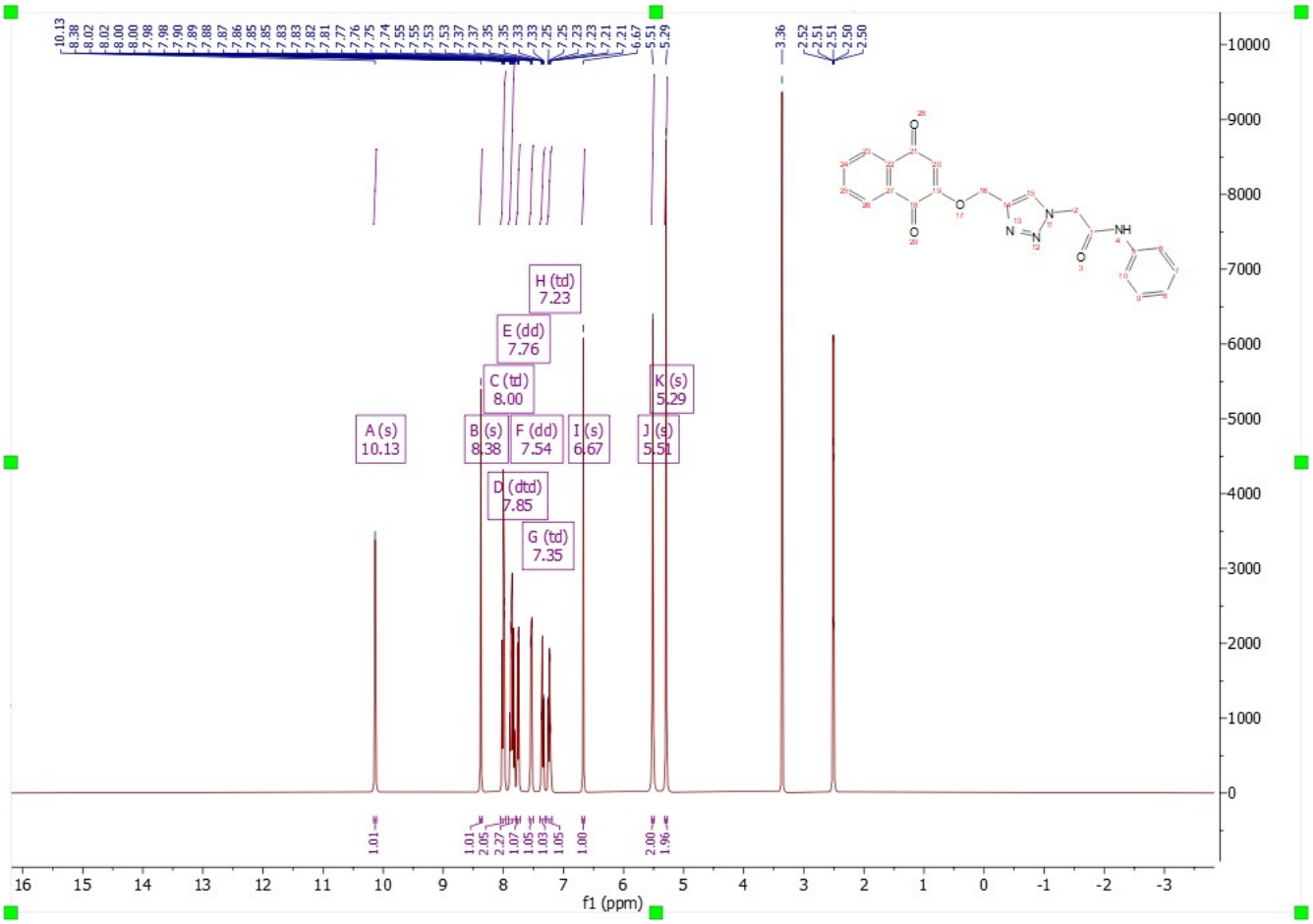


Fig. S_{13} ^{1}HNMR of 3a

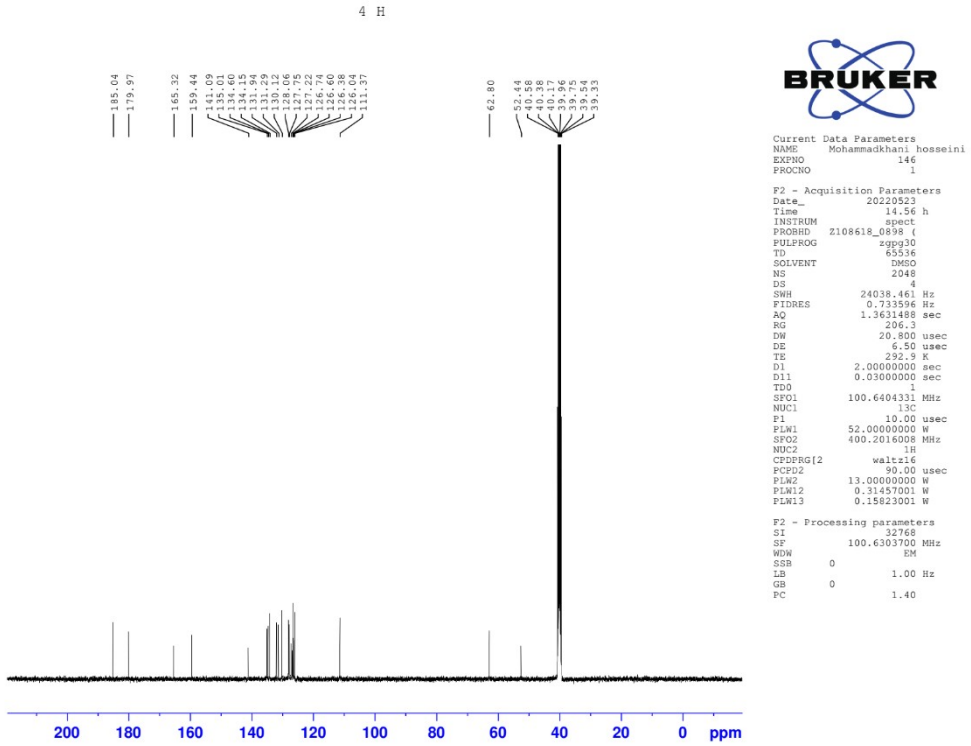


Fig. S_{14} ^{13}CNMR of 3a

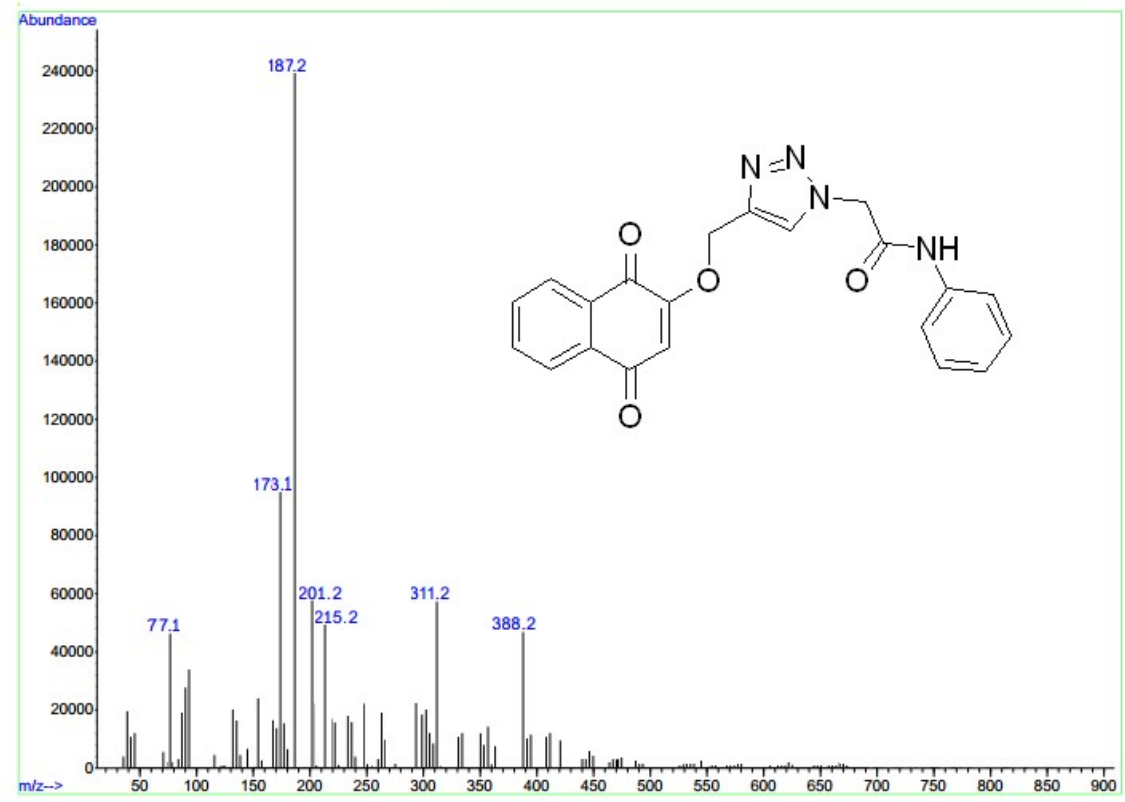


Fig. S_{15} Mass spectroscopy of 3a

N-(2-chlorophenyl)-2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)acetamide (3b): Cream solid; isolated yield: 63%, m.p.: 218-220 °C;; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 5.29 (s, 2H, N-CH_2), 5.29 (s, 2H, N-CH_2), 5.51 (s, 2H, O-CH_2), 6.66 (s, 1H, C-H, quinon), 7.231 (t, J = 7.2 Hz, 1H, ArH), 7.35 (t, J = 7.2 Hz, 2H, ArH), 7.54 (d, J = 7.2 Hz, 2H, ArH), 7.75 (d, J = 7.2 Hz, 2H, ArH), 7.91-7.82 (m, 2H, ArH), 8.01 (td, J = 8, 0.8 Hz, 2H, ArH), 8.37 (s, 1H, C-H, Triazole), 10.13 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 52.44, 62.80, 111.37, 126.04, 126.38, 126.60, 126.74, 127.22, 127.75, 128.06, 130.12, 131.29, 131.94, 134.15, 134.60, 135.01, 141.49, 159.44, 165.32, 179.97, 185.04; MS (EI, 20 eV): IR (KBr) 3798,3432,3248, 3051,2927,1991 ,1677,1606, 1502,1452, 1375, 1301, 1252, 1119, 1057, 872,756. cm^{-1}m/z: 424 **Anal. calcd for $C_{21}H_{15}ClN_4O_4$** (424): C, 59.65; H, 3.58; N, 13.25;Found: C, 59.63; H, 3.60; N, 13.26;

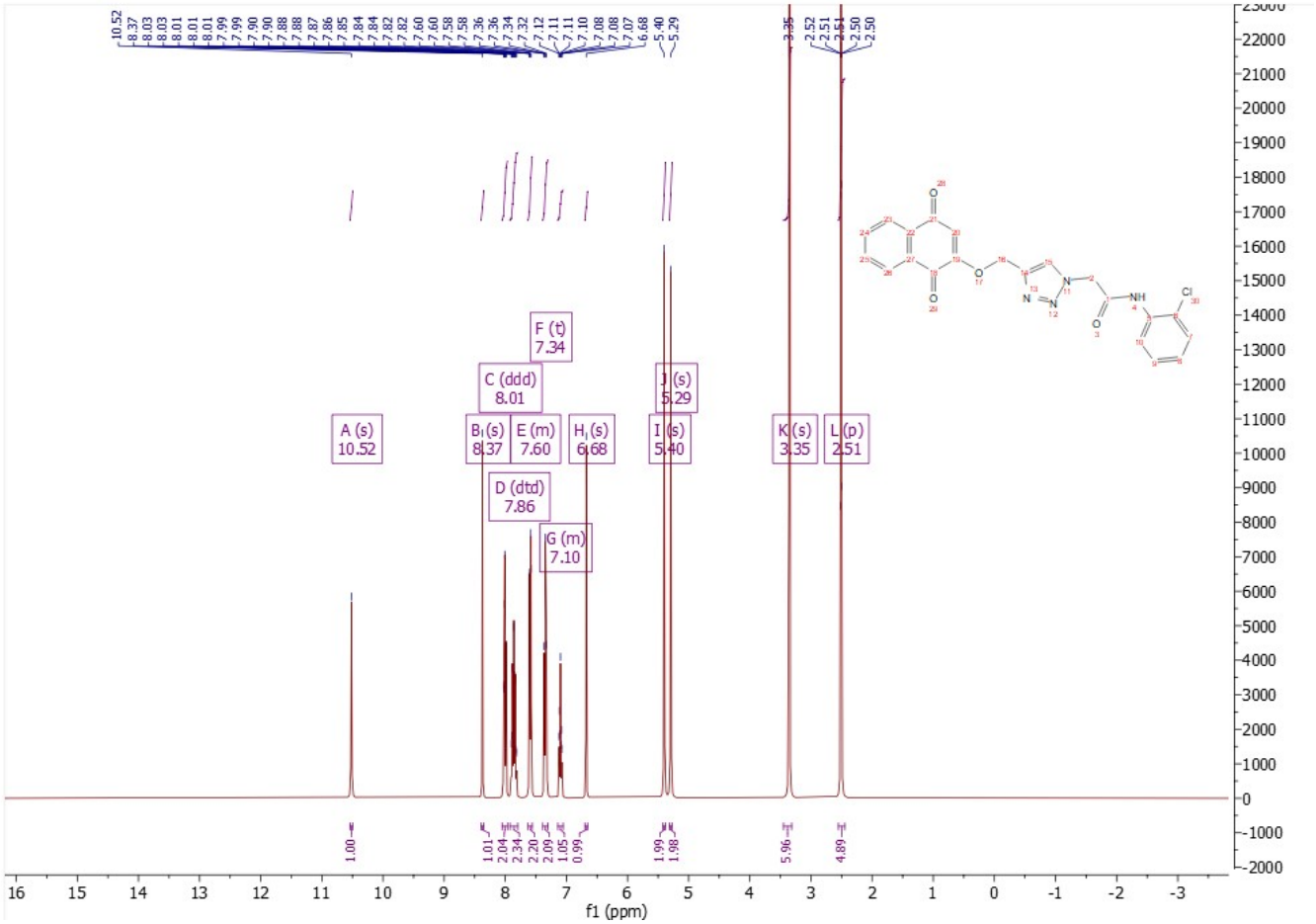


Fig. S_{16} ^{1}HNMR of 3b

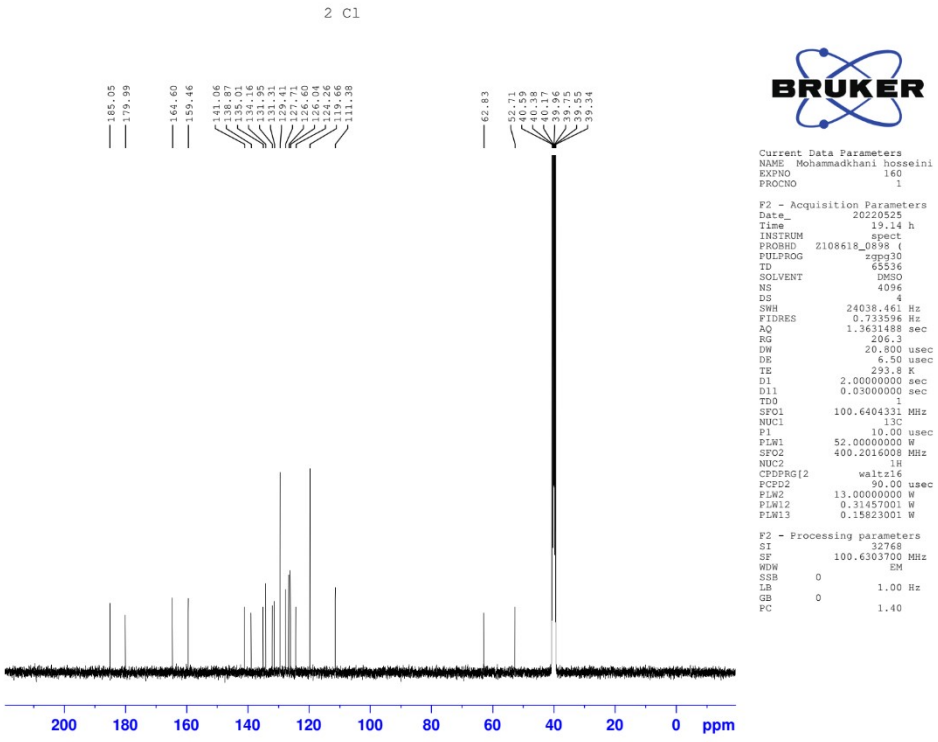


Fig. S_{17} ^{13}CNMR of 3b

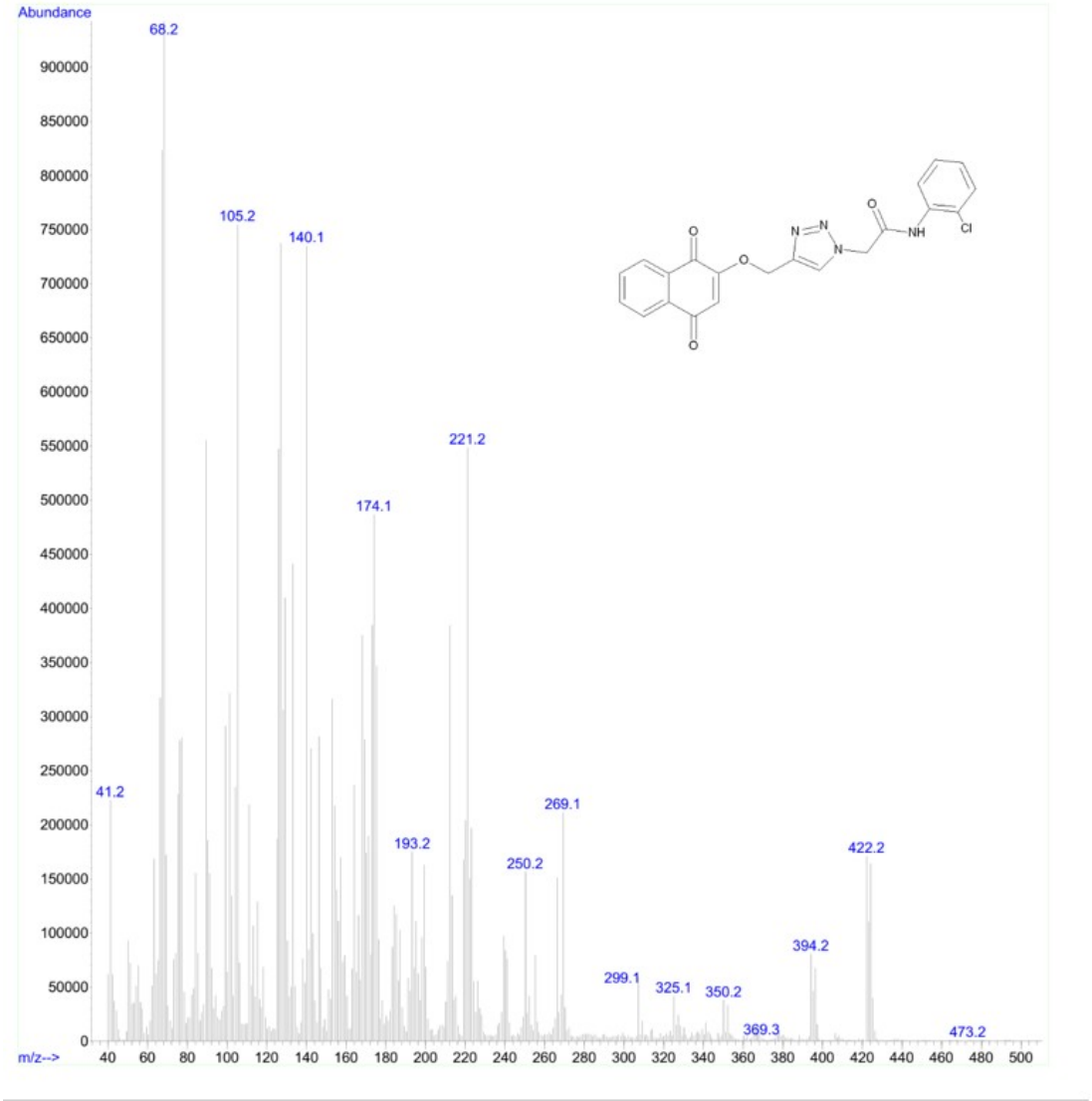


Fig. S_{18} Mass spectroscopy of 3b

N-(4-chlorophenyl)-2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)acetamide (3c): Cream solid; isolated yield: 79%, m.p.: 229-230 °C;; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 5.29 (s, 2H, N-CH_2), 5.40 (s, 2H, O-CH_2), 6.67 (s, 1H, C-H, quinon), 7.40 (d, J = 8.8 Hz, 2H, ArH), 7.62 (d, J = 8.8 Hz, 2H, ArH), 7.81-7.90 (m, 2H, ArH), 8.00 (td, J = 8.2, 0.8 Hz, 2H, ArH), 8.37 (s, 1H, C-H, Triazole), 10.65 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 52.71, 62.82, 111.38, 121.24, 126.04, 126.60, 127.7, 127.83, 129.34, 131.30, 134.15, 135.01, 137.82, 141.09, 159.45, 164.82, 179.98, 185.04; IR (KBr): 3896, 3584 ,3269, 2961,2882,1946 ,1677,1606, 1496,1413, 1319, 1260, 1252, 1189, 1021, 970,745 cm^{-1} Mass (M/Z:20ev): 422-424 **Anal. calcd for $C_{21}H_{15}ClN_4O_4$** (422-424): C, 59.65; H: 3.58; N, 13.25 Found: C, 59.63 H: 3.55; N, 13.22.

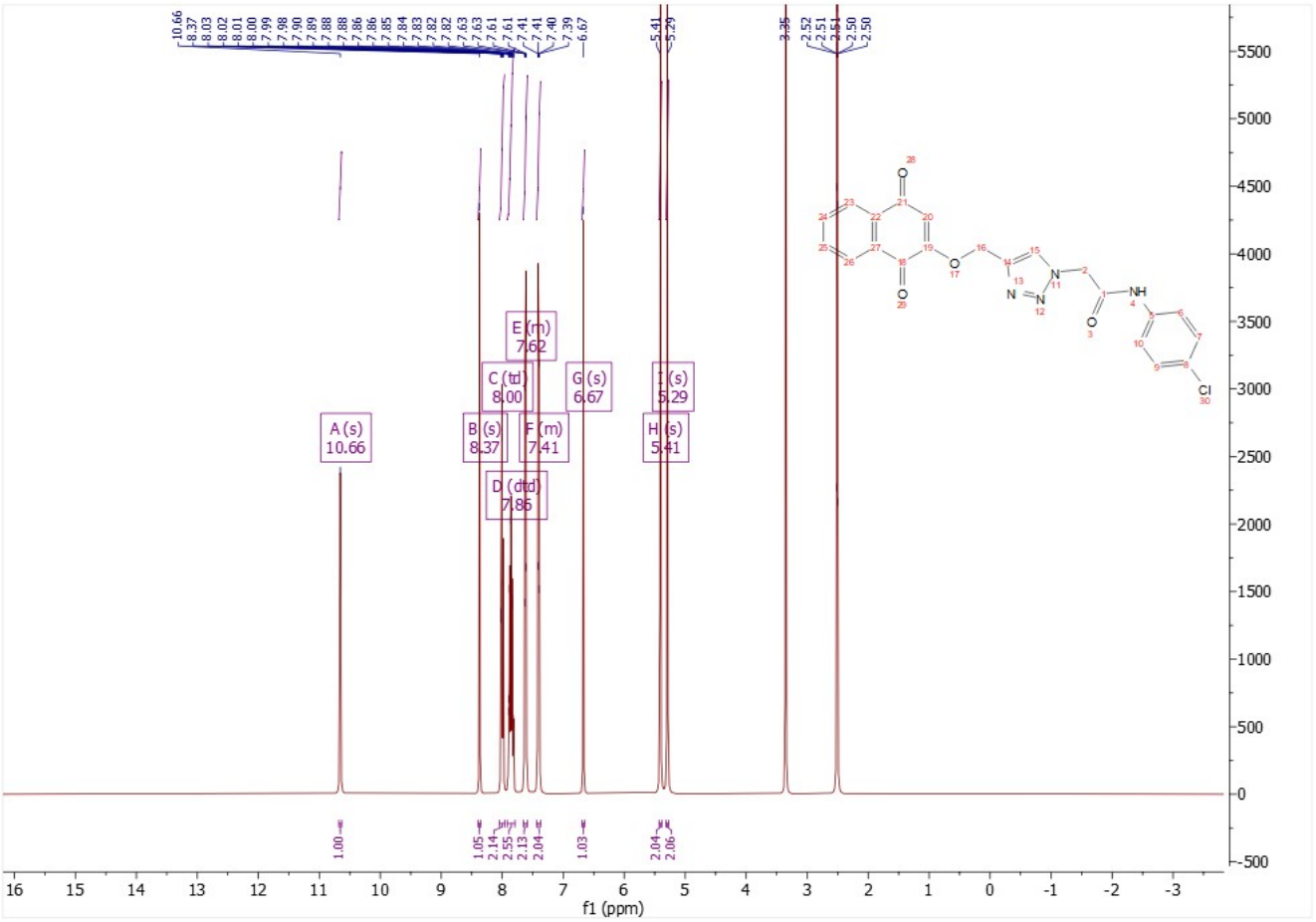


Fig. S_{19} ^{1}HNMR of 3c

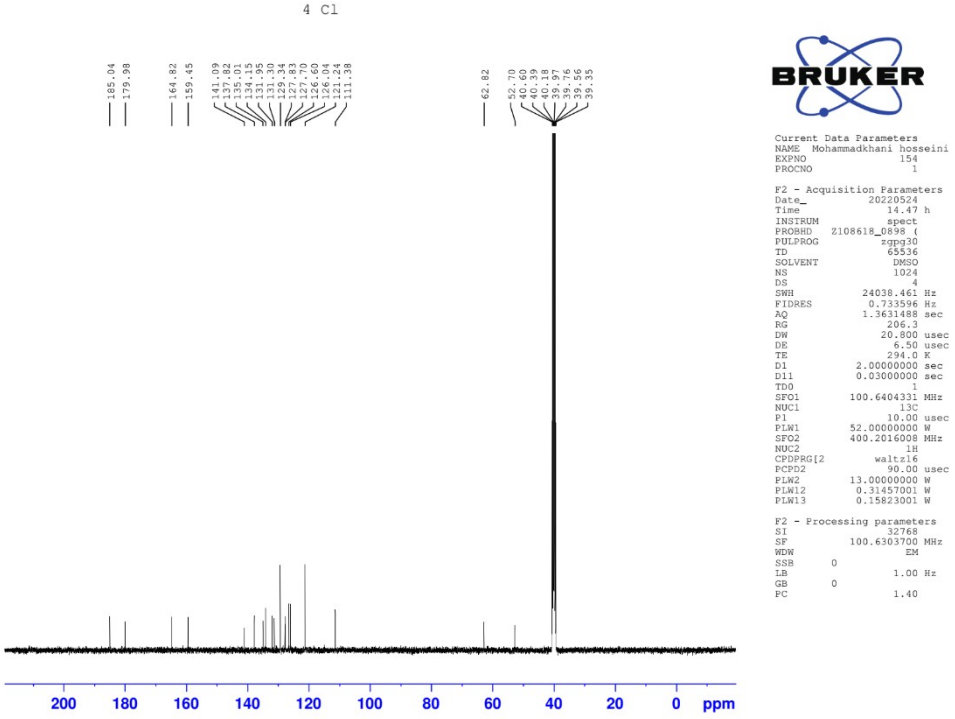



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Fig. S_{20} ^{13}CNMR of 3c

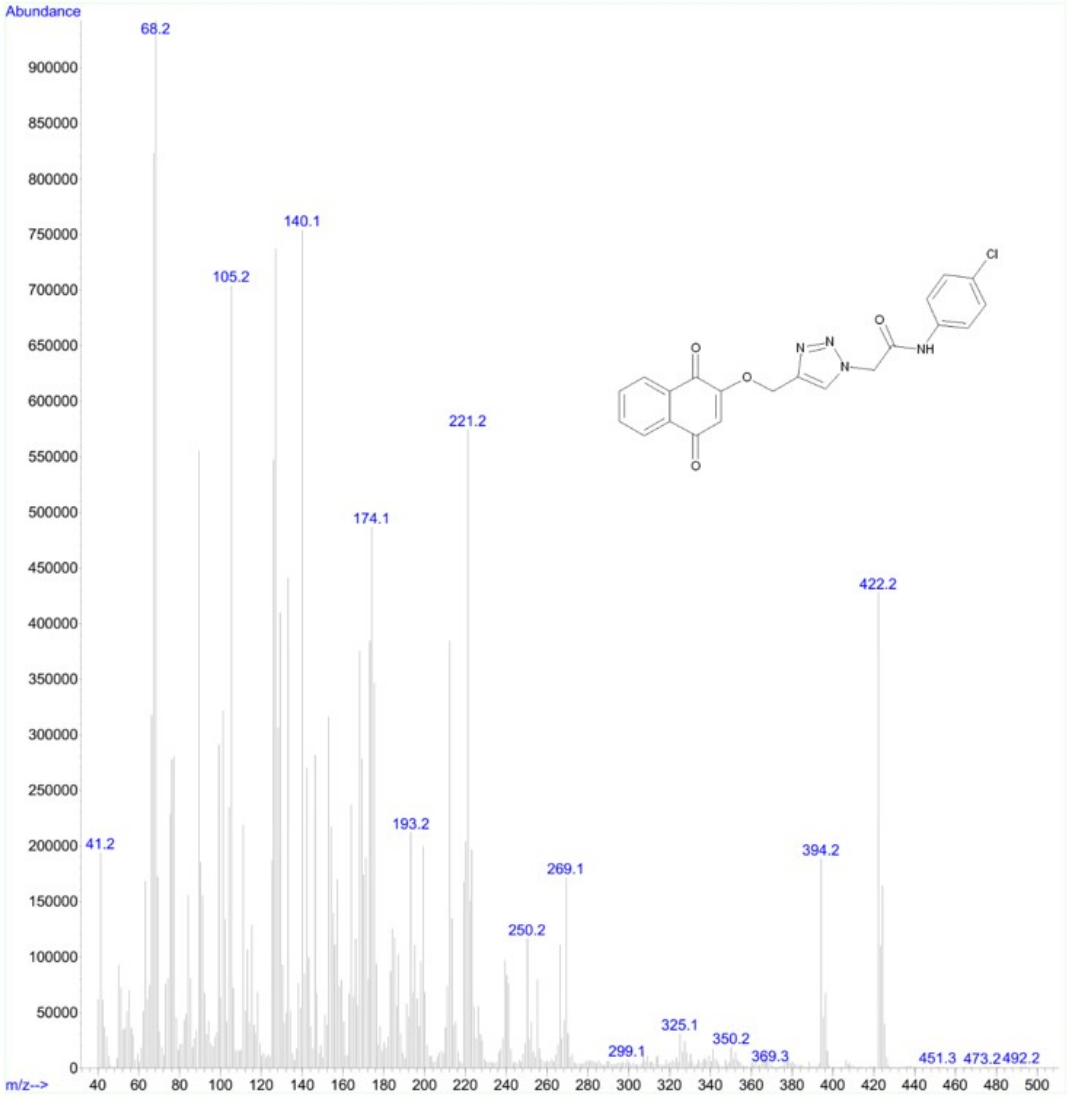


Fig. S_{21} Mass spectroscopy of 3c

N-(3-bromophenyl)-2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)acetamide (3d): Yellow solid; isolated yield: 84%, m.p.: 233-235 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 5.29 (s, 2H, N-CH_2), 5.41 (s, 2H, O-CH_2), 6.67 (s, 1H, C-H, quinon), 7.27 -7.40 (m, 2H, ArH), 7.49 (d, J = 7.2 , 1H, ArH), 7.81-7.91 (m, 2H, ArH), 7.92 (s, 1H, ArH), 8.01 (td, J = 8.4, 0.8 Hz, 2H, ArH), 8.37 (s, 1H, C-H, Triazole), 10.70 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 52.70, 62.81, 111.38, 118.47, 122.04, 122.13, 126.05, 126.61, 126.91, 127.72, 131.31, 131.46, 131.95, 134.16, 135.02, 140.41, 141.09, 159.45, 165.09, 179.98,185.06, IR (KBr) 3779,3580,3299,2957,2900,2838,2044, 1661, 1621, 1550 ,1454 ,1343 ,1298 ,1242 ,1166

,1028,832,699 cm^{-1}; Mass (M/Z:20ev): 468 . **Anal. calcd for $C_{21}H_{15}BrN_4O_4$** (468): C, 53.98; H, 3.24; N, 11.99; Found:

): C, 53.97; H, 3.25; N, 12.00.

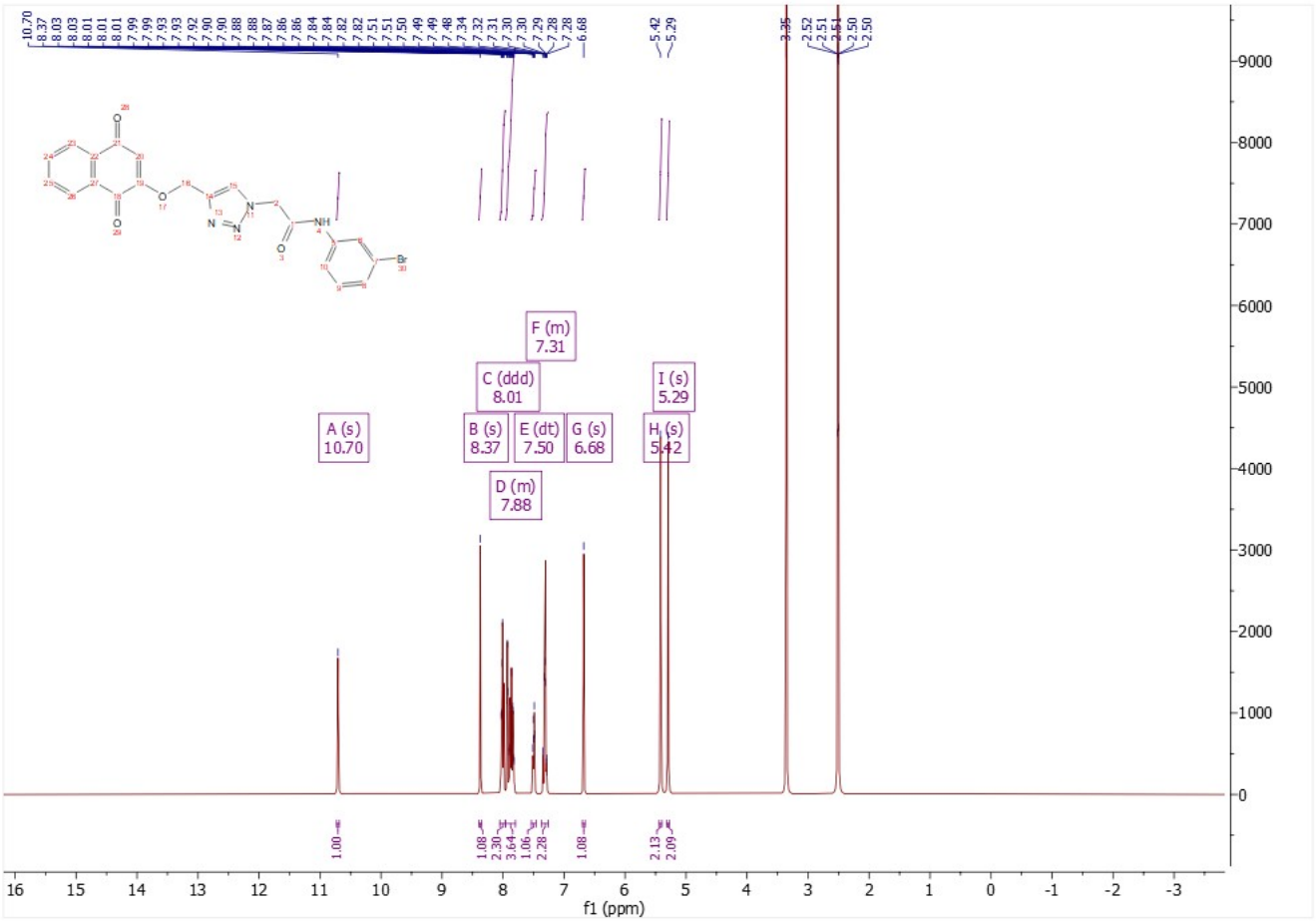


Fig. S_{22} ^{1}HNMR of 3d

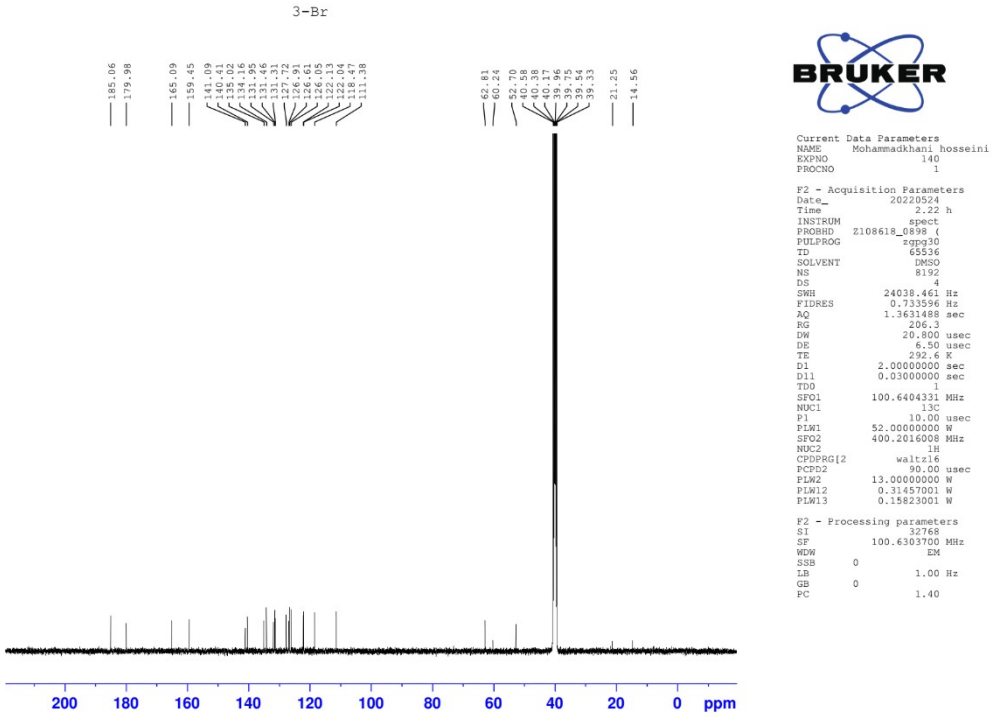


Fig. S_{23} ^{13}CNMR of 3d

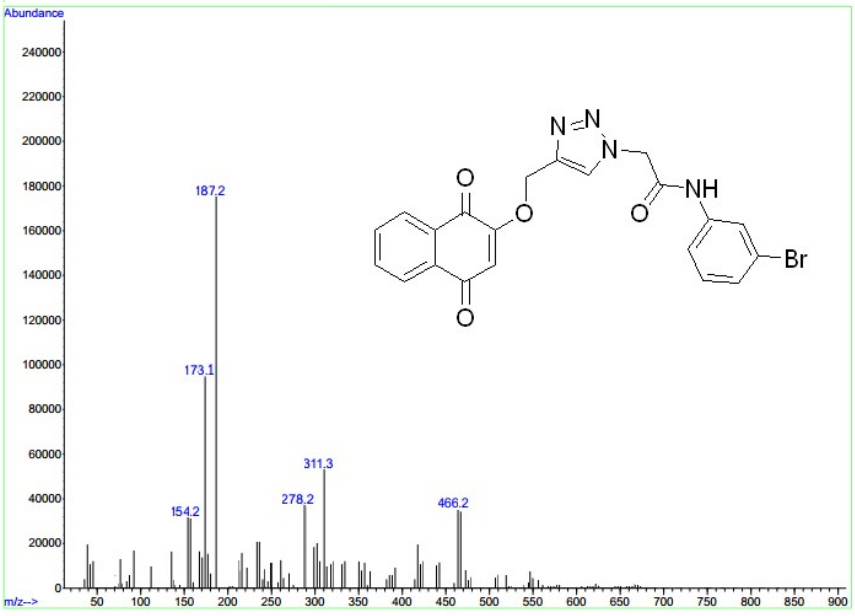


Fig. S_{24} Mass spectroscopy of 3d

N-(4-bromophenyl)-2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)acetamide (3e): Yellow solid; isolated yield: 79%, m.p.: 245-247 °C;; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 5.29 (s, 2H, N-CH_2), 5.40 (s, 2H, O-CH_2), 6.67 (s, 1H, C-H, quinon), 7.52 (d, J = 8.8, 2H, ArH), 7.56 (d, J = 8.8, 2H, ArH), 7.81-7.91 (m, 2H, ArH), 7.97 – 8.04 (td, J = 8.2, 0.8, 2H, ArH), 8.37 (s, 1H, C-H, Triazole), 10.65 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 52.72, 62.82, 111.38, 115.89, 121.61, 126.05, 126.61, 127.71,

131.31, 131.95, 132.25, 134.16, 135.02, 138.24, 141.08, 159.45, 164.85, 179.98, 185.05, IR (KBr) :3779, 3434,3280,2997,2944,2836,2004,1666, 1605, 1548, 1457, 1301, 1247, 1122,1044,961,831,780,722, cm^{-1}. Mass (M/Z:20ev): 466-468 **Anal. calcd for $C_{21}H_{15}BrN_4O_4$** (466): C, 53.98; H: 3.24; N, 11.99 Found: C, 53.96 H: 3.22; N, 12.01.

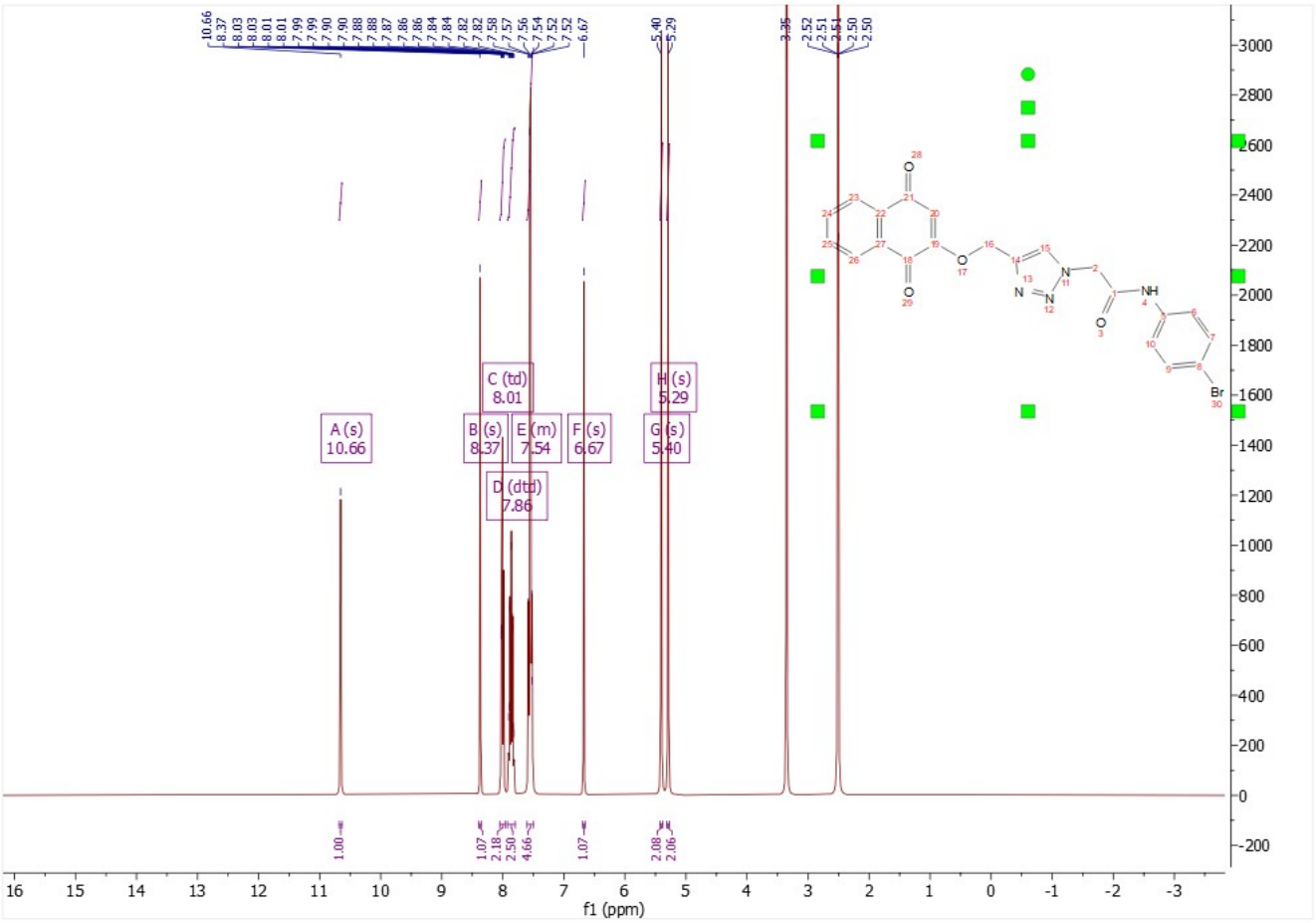


Fig. S_{25} ^{1}HNMR of 3e

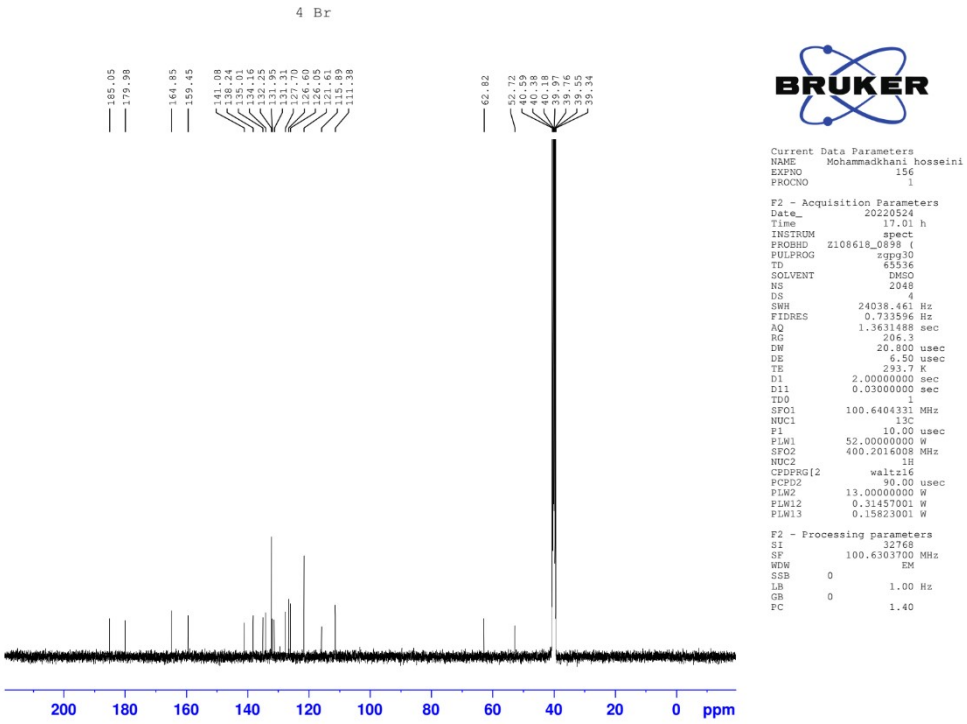


Fig. S_{26} ^{13}CNMR of 3e

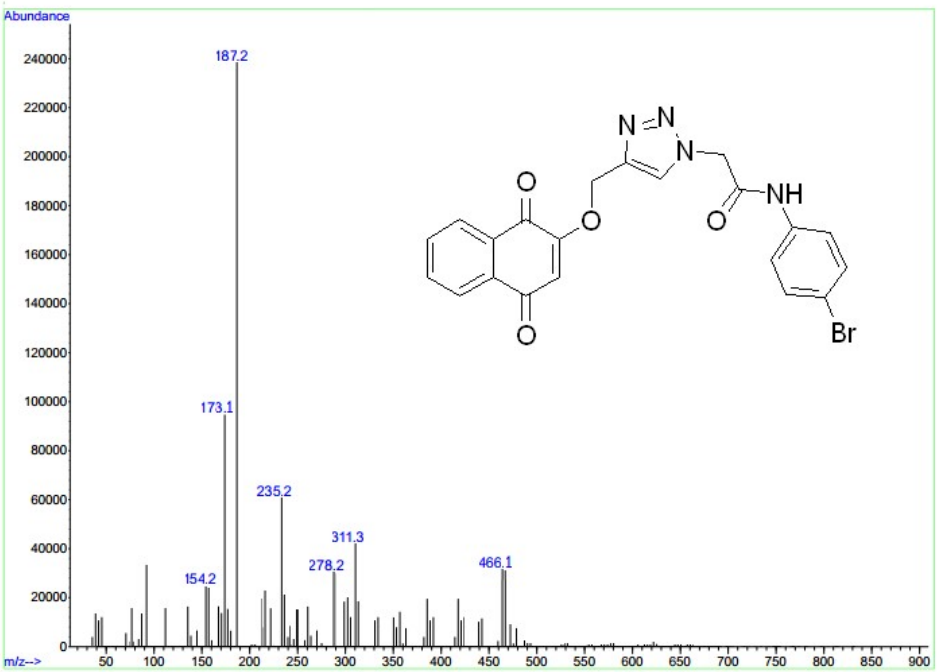


Fig. S_{27} Mass spectroscopy of 3e

2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)-N-(2-nitrophenyl)acetamide (3f): Yellow solid; isolated yield: 83%, m.p.: 259-261 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 5.28 (s, 2H, N-CH_2), 5.49 (s, 2H, O-CH_2), 6.66 (s, 1H, C-H, quinon), 7.42 (t, J = 7.6 Hz, 1H, ArH), 7.63–7.79 (m, 3H, ArH), 7.79 – 7.90 (m, 2H, ArH), 7.97 (d, J = 6.8 Hz, 1H, ArH), 8.08 (d, J = 6.8 Hz, 1H, ArH), 8.34

(s, 1H, C-H, Triazole), 1075 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 52.27, 62.77, 111.38, 125.42, 126.04, 126.65, 131.28, 131.95, 134.15, 134.66, 135.05, 137.79, 139.04, 141.09, 159.44, 165.38, 165.53, 179.97, 185.04, IR (KBr) 3742, 3266 ,2950 ,2884 ,2030 ,1882 ,1671, 1603, 1546, 1487, 1396, 1338, 1286, 1244, 1188, 1073, 1009, 918, 962, 860,cm^{-1}. Mass (M/Z:20ev): 433, **Anal. calcd for $C_{21}H_{15}N_5O_6$** (433): C, 58.20; H: 3.49; N, 16.16 Found: C, 58.18 H: 3.47; N, 16.13.

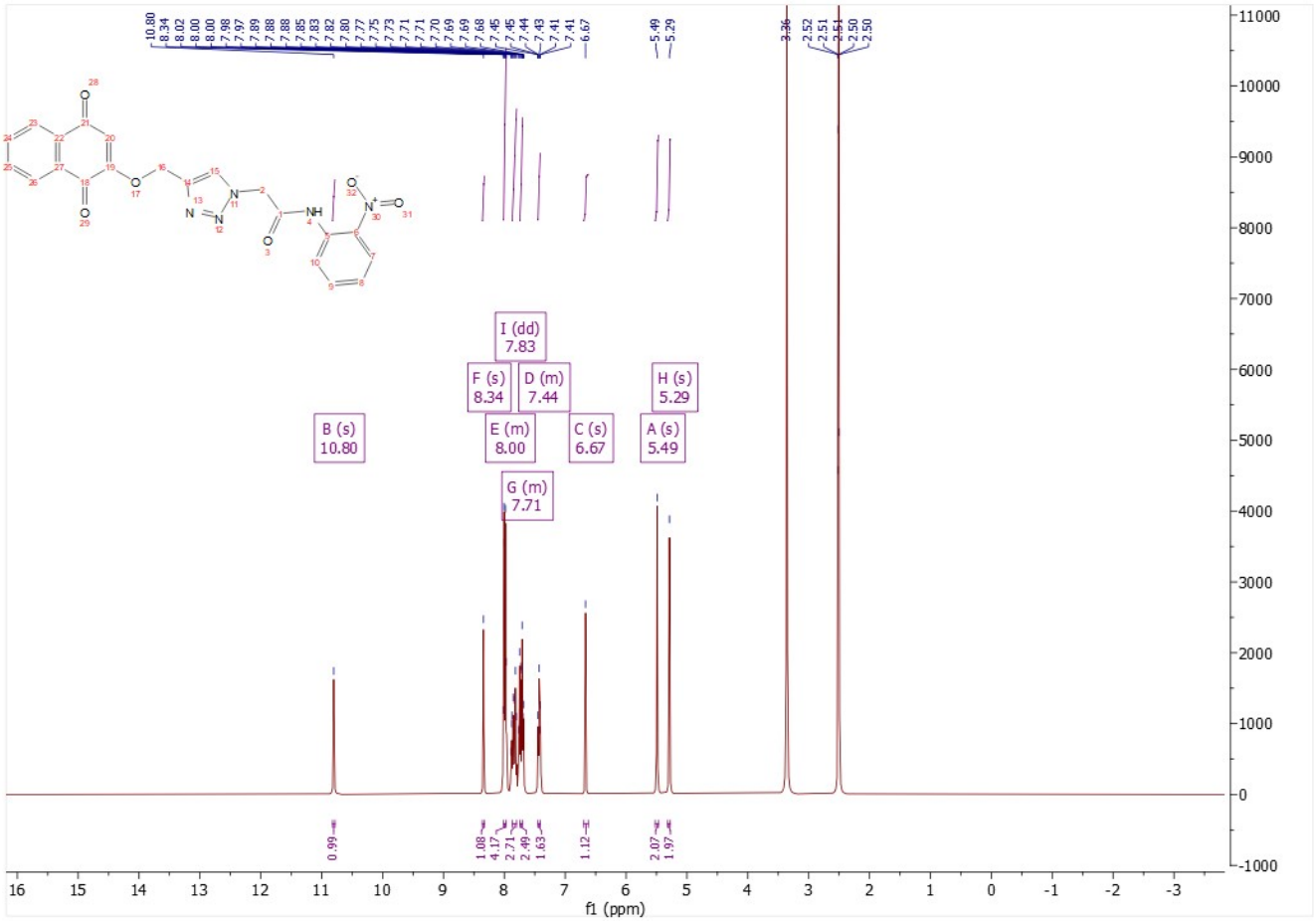


Fig. S_{28} ^{1}HNMR of 3f

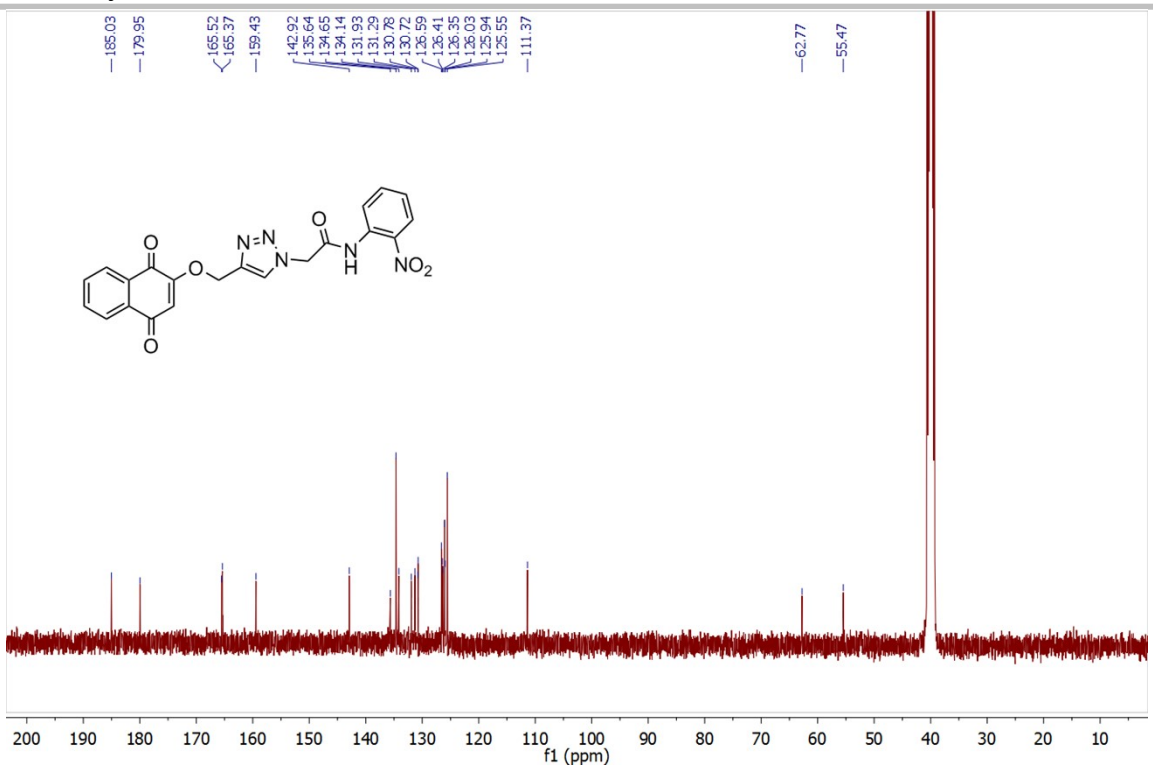


Fig. S_{29} ^{13}CNMR of 3f

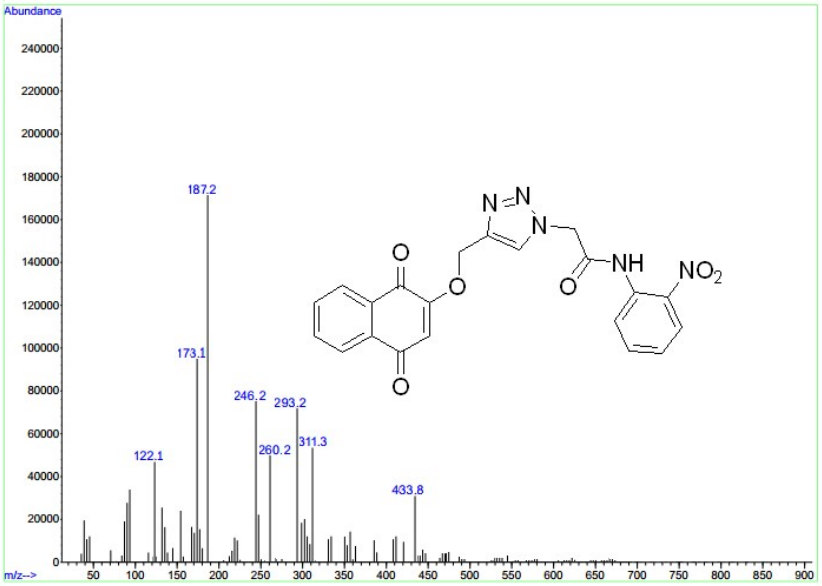


Fig. S_{30} Mass spectroscopy of 3f

2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-methoxyphenyl)acetamide (3g): Cream solid; isolated yield: 62%, m.p.: 235-237 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 3.72 (s, 3H, O-CH_3), 5.28 (s, 2H, N-CH_2), 5.36 (s, 2H, O-CH_2), 6.66 (s, 1H, C-H, quinon), 6.91 (d, J = 9.2 Hz, 2H, ArH), 7.50 (d, J = 9.2 Hz, 2H, ArH), 7.8-7.9 (m, 2H, ArH), 8.00 (td, J = 7.4, 0.8 Hz, 2H, ArH), 8.37 (s, 1H, C-H, Triazole), 10.38 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 52.64, 55.61, 62.82, 11.36, 114.47, 121.20, 126.04, 126.59, 127.70, 131.29, 131.93, 131.96, 134.14, 135.00, 141.05, 155.98, 159.44, 164.05, 179.97, 185.04;IR (KBr) : 3551, 3245, 3041, 2863, 1955, 1673, 1579,

1530,144,1350,1210,971,844,801,730 cm^{-1} Mass (M/Z:20ev):418 **Anal. calcd for $C_{22}H_{18}N_4O_5$** (418): C, 63.15; H: 4.34; N, 13.39 Found: C, 63.13 H: 4.32; N, 13.42.

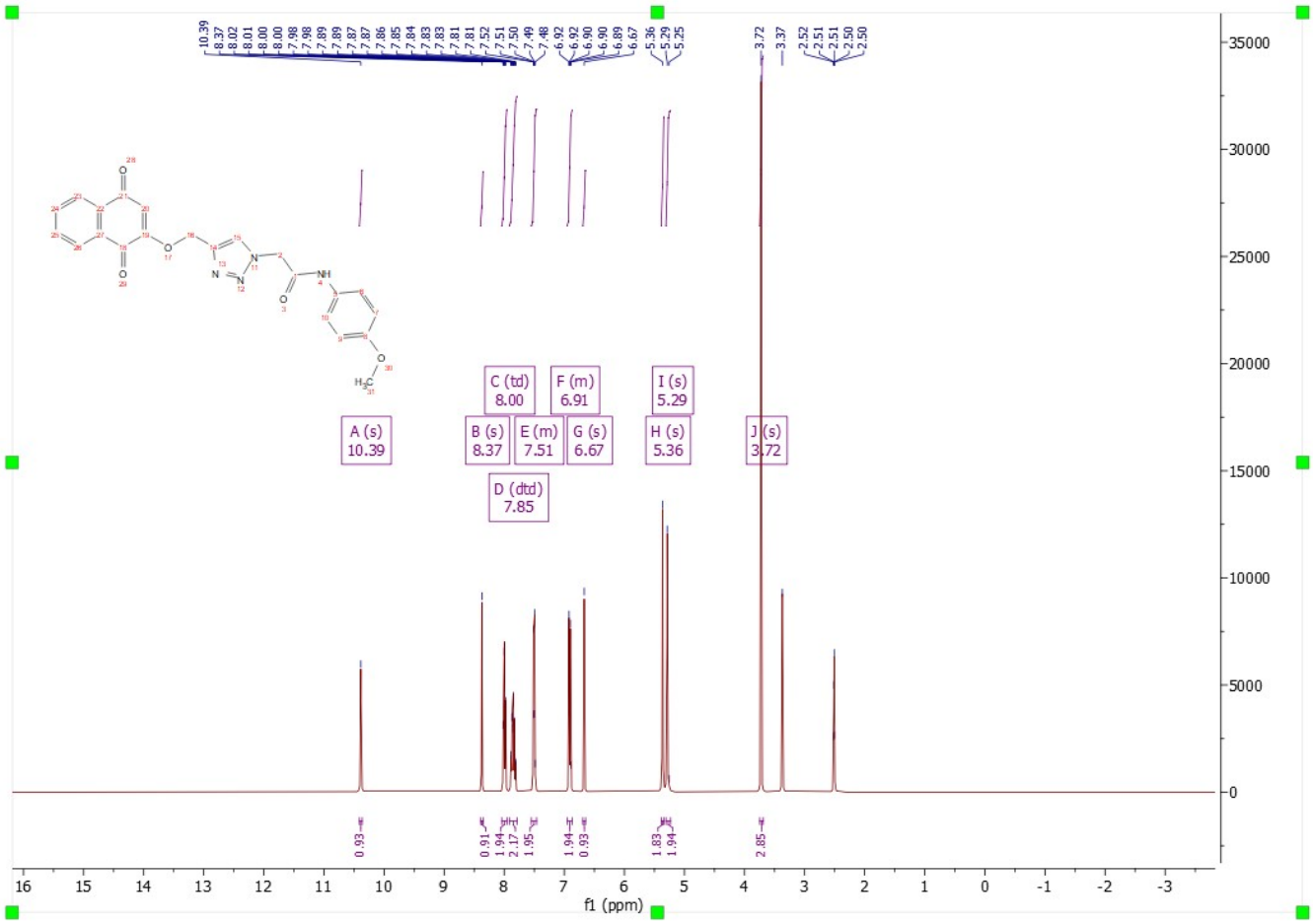
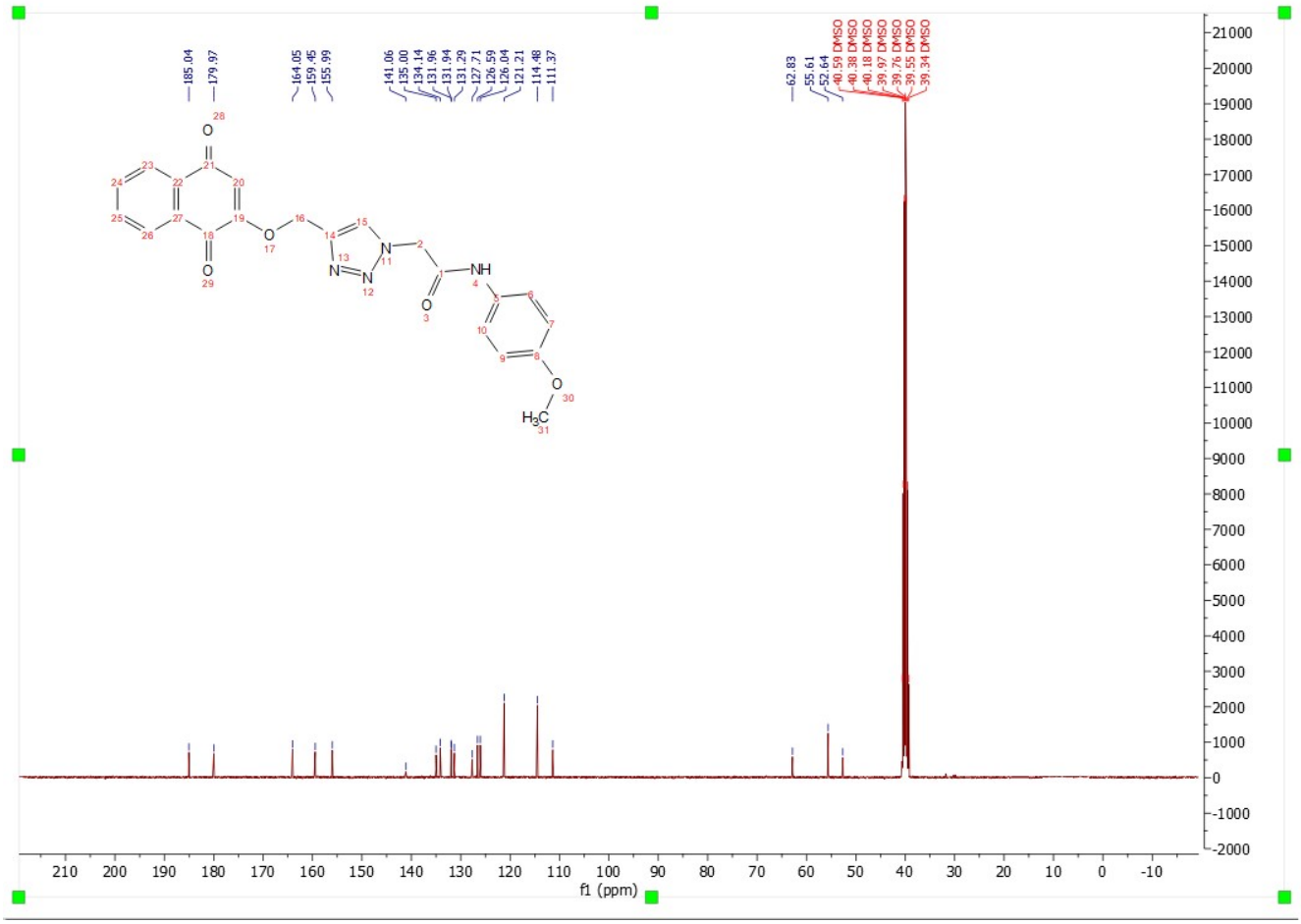


Fig. S_{31} ^{1}HNMR of 3g



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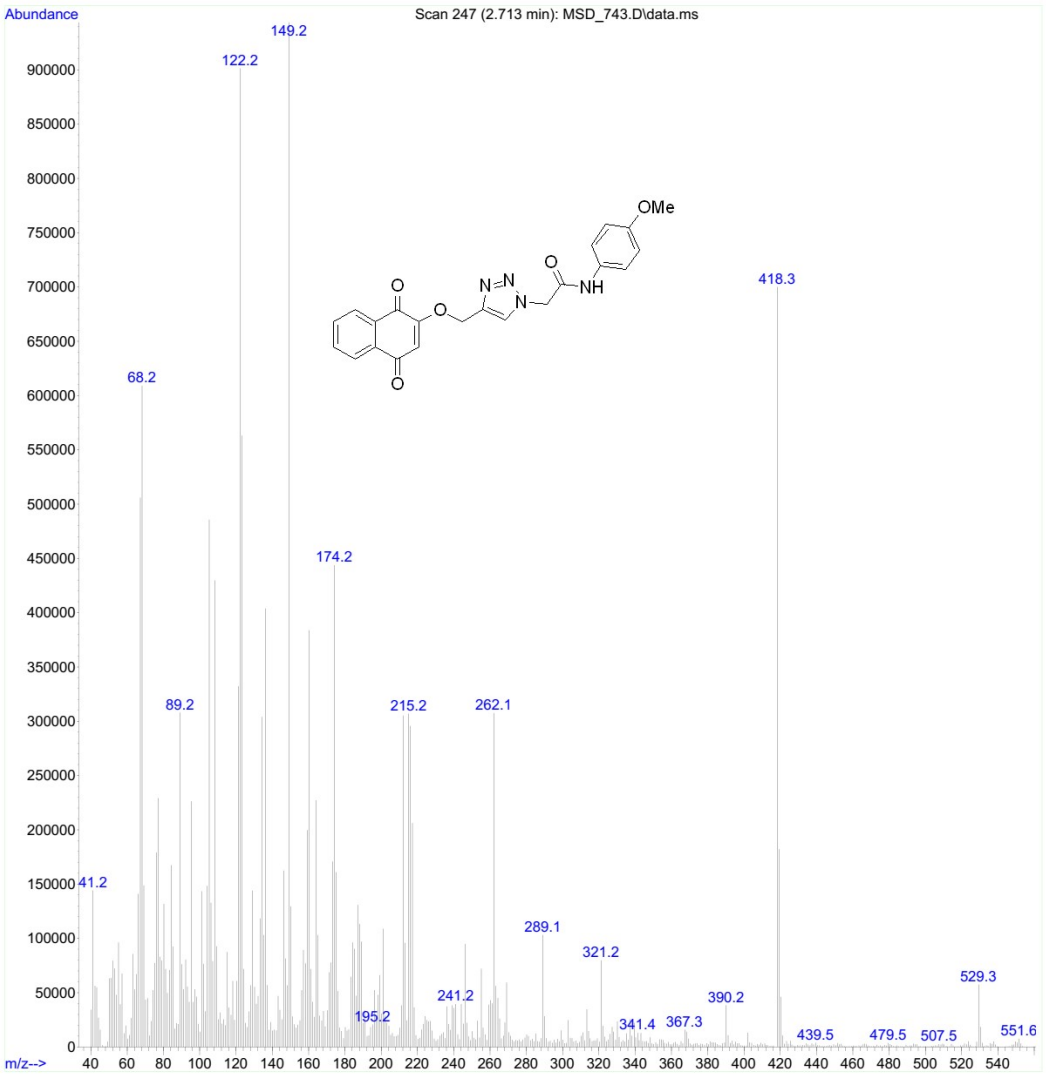


Fig. S_{33} Mass spectroscopy of 3g

2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)-N-(p-tolyl)acetamide (3h): Cream solid; isolated yield: 68%, m.p.: 244-246 °C;; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 2.25 (s, 3H, -CH_3), 5.28 (s, 2H, O-CH_2), 5.37 (s, 2H, O-CH_2), 6.67 (s, 1H, C-H, quinon), 7.14 (d, J = 8.4 Hz, 2H, ArH), 7.47 (d, J = 8.4 Hz, 2H, ArH), 7.81-7.91(m, 2H, ArH), 8.00 (td, J = 8.2, 0.8 Hz, 2H, ArH), 8.36 (s, 1H, C-H, Triazole), 10.43 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 20.92, 52.69, 62.82, 111.37, 119.65, 126.04, 126.60, 127.71, 129.78, 131.30, 131.95, 133.22,134.15, 135.01, 136.36, 141.04, 159.45, 164.33, 179.98, 185.05;IR (KBr) 3797,3592,3271,3037, 2941,1948, 1676,1583,1535,14303, 1278, 1175, 1049, 911,786 cm^{-1} Mass (M/Z:20ev):402 **Anal. calcd for $C_{22}H_{18}N_4O_4$** (402): C, 65.66; H: 4.51; N, 13.92 Found: C, 65.63 H: 4.49; N, 13.90.

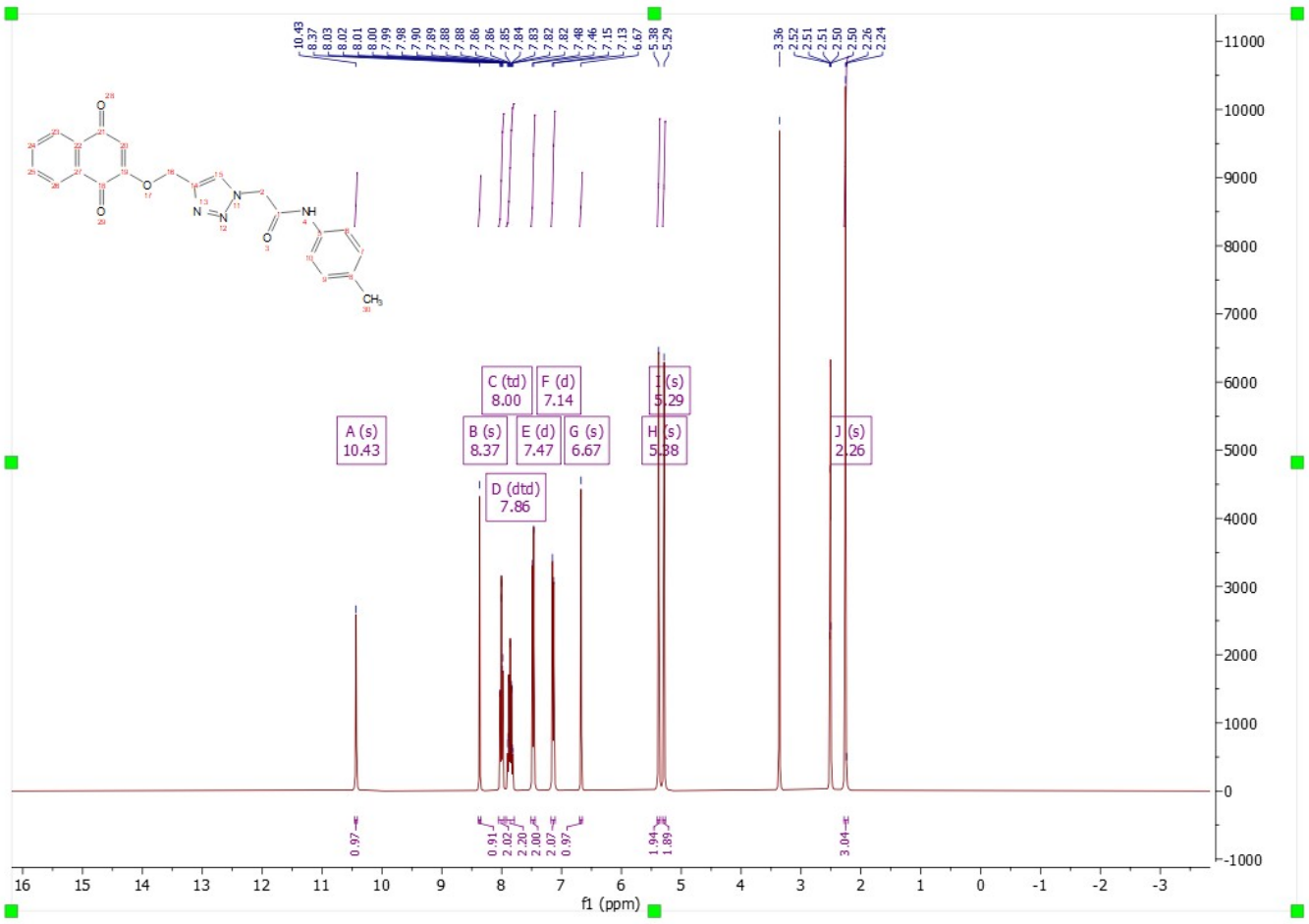
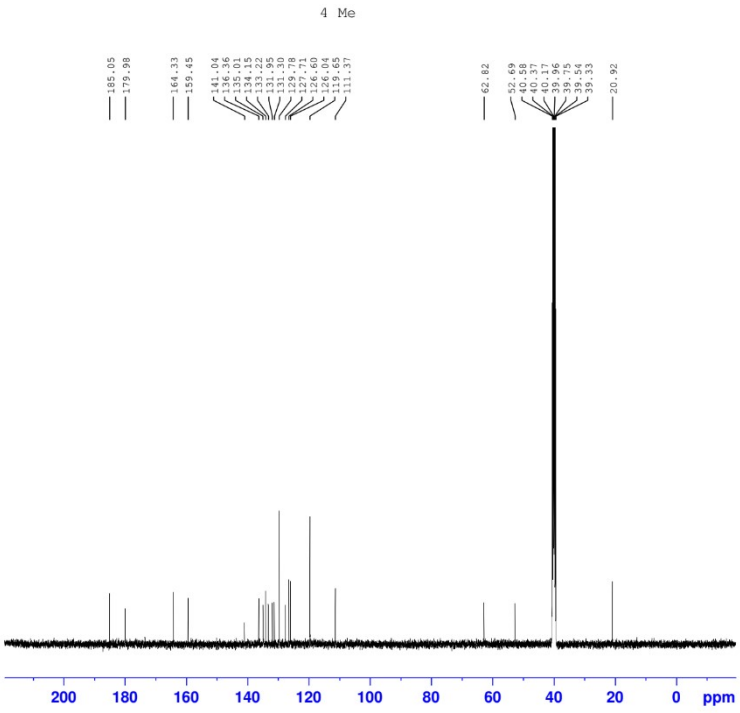


Fig. S_{34} ^{1}HNMR of 3h



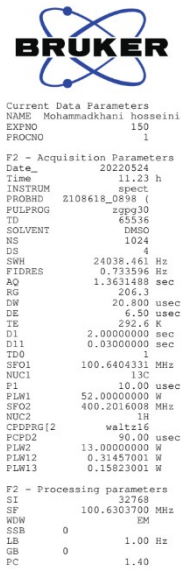


Fig. S_{35} ^{13}CNMR of 3h

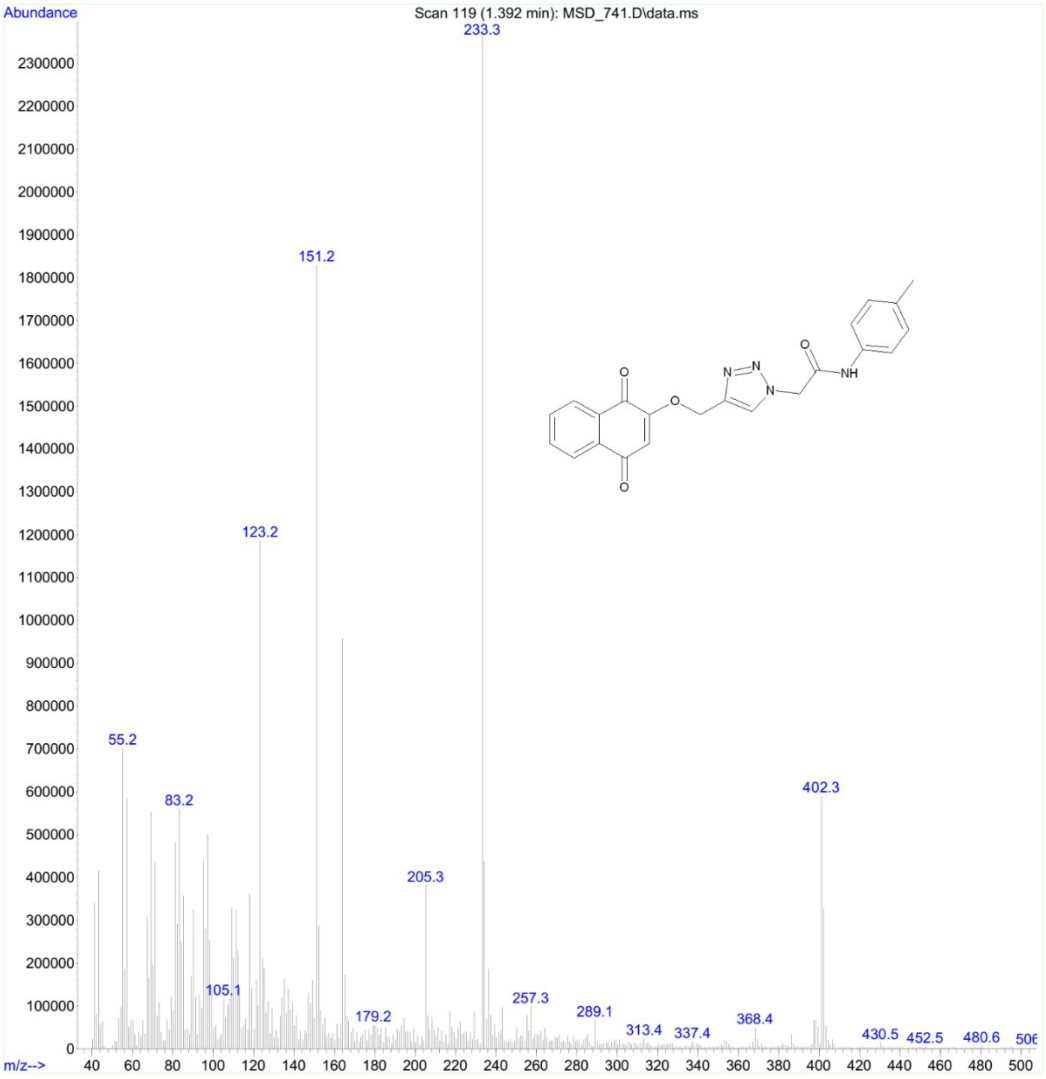


Fig. S_{36} Mass spectroscopy of 3h

2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)-N-(2-methyl-3-nitrophenyl)acetamide (3i): Cream solid; isolated yield: 71%, m.p.: 226-228 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 2.31 (s, 3H, -CH_3), 5.29 (s, 2H, N-CH_2), 5.50 (s, 2H, O-CH_2), 6.67 (s, 1H, C-H, quinon), 7.45 (t, J = 8.1 Hz, 1H, ArH), 7.71 (d, J = 8.0 Hz, 1H, ArH), 7.76 (d, J = 8.0 Hz, 1H, ArH), 7.81-7.91 (m, 2H, ArH), 8.00 (td, J = 8, 0.8 Hz, 2H, ArH), 8.38 (s, 1H, C-H, Triazole), 10.29 (s, 1H, NH). ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 14.27, 52.35, 62.82, 111.39, 121.69, 126.04, 126.60, 126.96, 127.31, 127.69, 130.30, 131.30, 131.95, 134.16, 135.02, 137.74, 141.10, 151.38, 159.45, 165.45, 179.98, 185.04; IR (KBr) 3340, 1708, 1673, 1550, 1354, 1260, 1108 cm^{-1} Mass (M/Z:20ev):447 **Anal. calcd for $C_{22}H_{17}N_5O_6$** (447): C, 59.06; H: 3.83; N, 15.65 Found: C, 59.04 H: 3.81; N, 15.63.

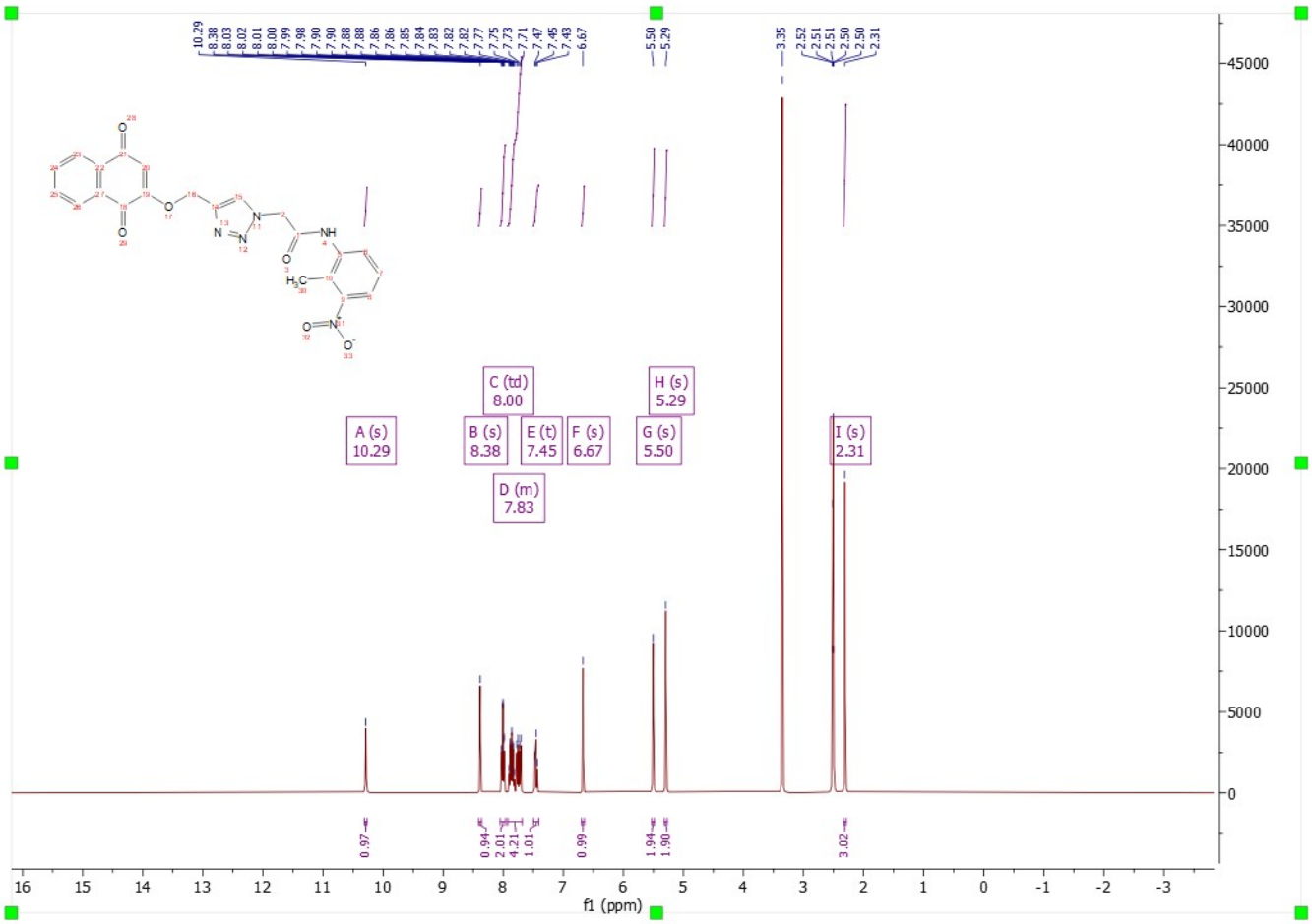


Fig. S_{37} ^{1}HNMR of 3i

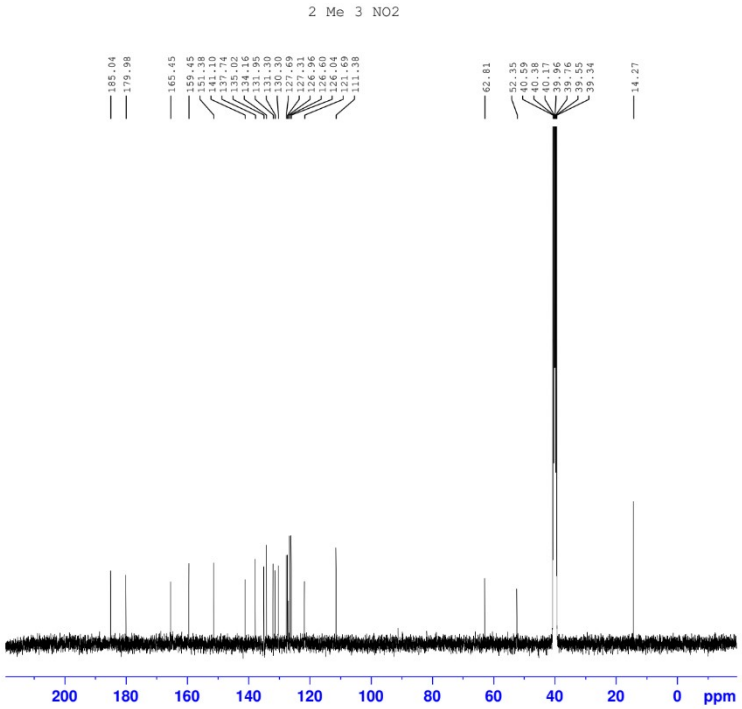


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Fig. S_{38} ^{13}CNMR of 3i

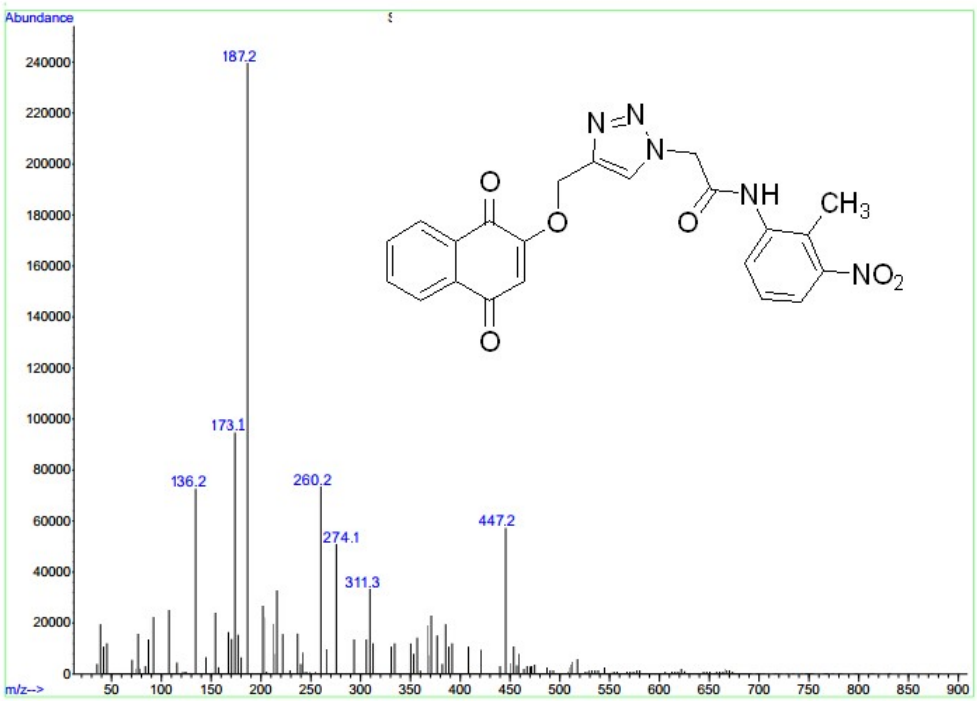

Fig. S_{39} Mass spectroscopy of 3i

N-(3-chloro-2-methylphenyl)-2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)acetamide (3j): Cream solid; isolated yield: 72%, m.p.: 251-253°C ;^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 2.27 (s, 3H, -CH_3), 5.28 (s, 2H, N-CH_2), 5.46 (s, 2H, O-CH_2), 6.66 (s, 1H, C-H, quinon), 7.22 (t, J = 8.0 Hz, 1H, ArH), 7.32 (d, J = 8 Hz, 1H, ArH), 7.38 (d, J = 8 Hz, 1H, ArH), 7.85 (m, 2H, ArH), 8.00 (td, J = 8, 0.8 Hz, 2H, ArH), 8.37 (s, 1H, C-H, Triazole), 10.11 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 15.58, 52.36, 62.81, 111.37, 124.79, 126.04, 126.60, 126.91, 127.46, 127.70, 130.84, 131.29, 131.94, 134.15, 134.34, 135.01, 137.46, 141.07, 159.44, 165.12, 179.98, 185.04,; IR (KBr) 3356, 1703, 1663, 1272, 1111 cm^{-1} Mass : (M/Z:20ev):436 **Anal. calcd for $C_{22}H_{17}ClN_4O_4$** (436): C, 60.49; H: 3.92; N, 12.83 Found: C, 60.52 H: 3.91; N, 12.83.

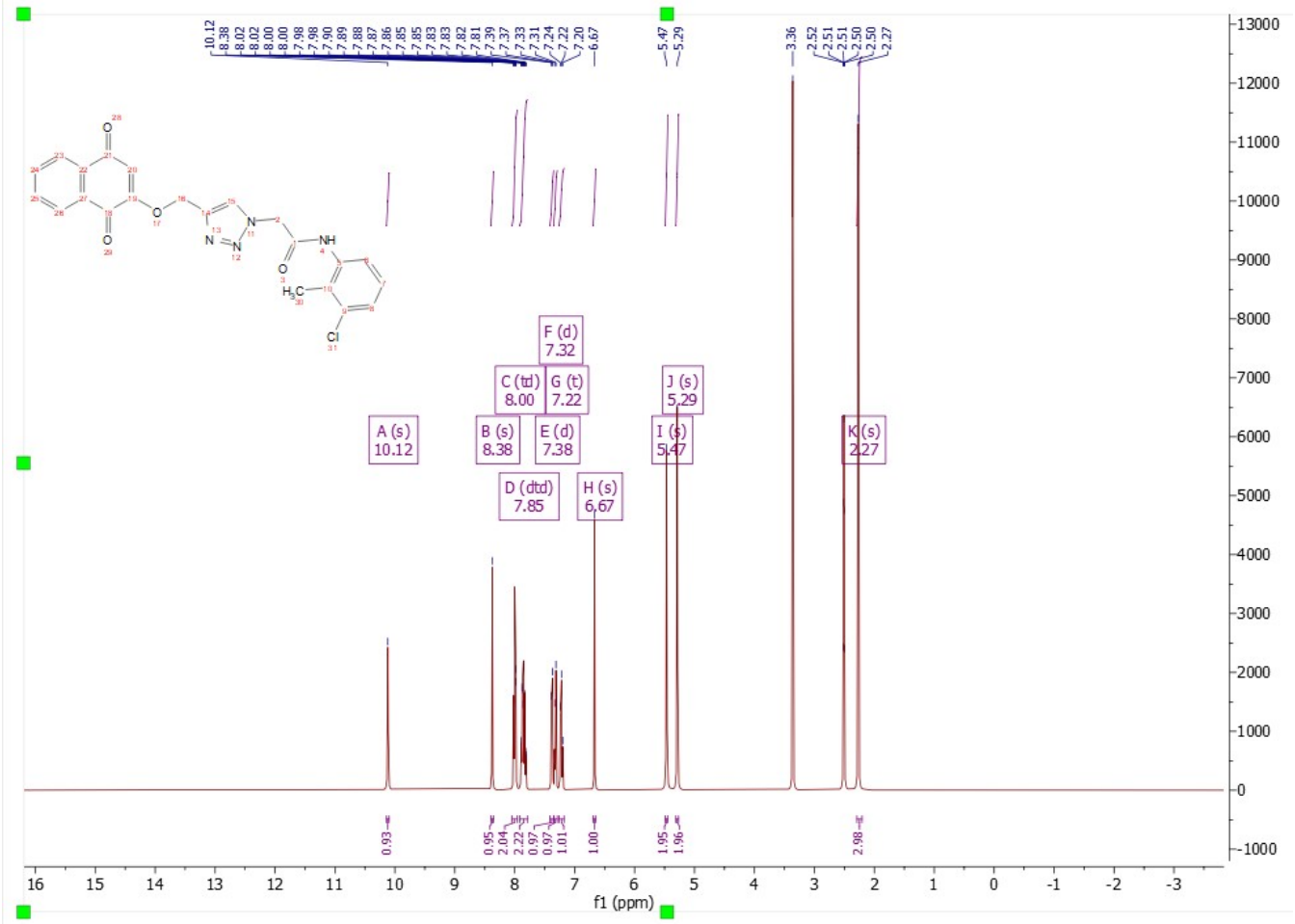

Fig. S_{40} ^{1}HNMR of 3j

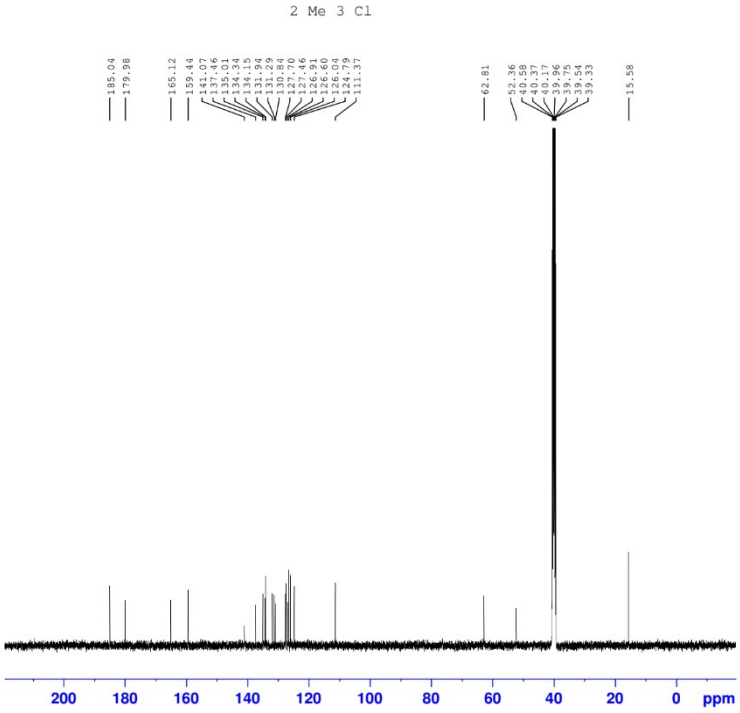


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Fig. S_{41} ^{13}CNMR of 3j

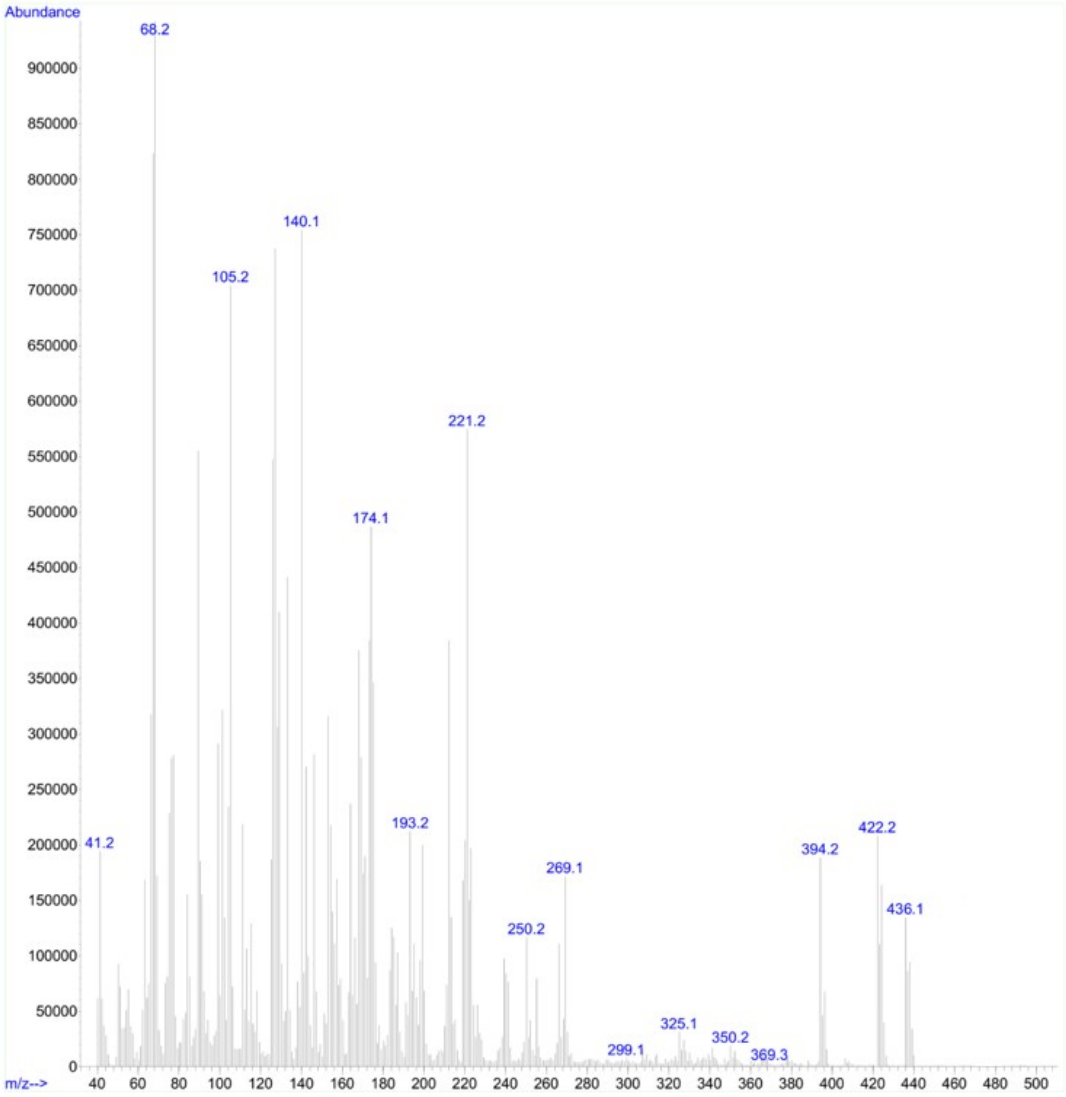

Fig. S_{42} Mass spectroscopy of 3j

N-(2,4-difluorophenyl)-2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)acetamide (3k): Cream solid; isolated yield: 78%, m.p.: 222-224°C; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 5.28 (s, 2H, N-CH_2), 5.48 (s, 2H, O-CH_2), 6.66 (s, 1H, C-H, quinon), 7.09 (td, J = 28.5, 0.7 Hz, 1H, ArH), 7.37 (td, J = 28.5, 0.7 Hz, 1H, ArH), 7.81 – 7.91 (m, 3H, ArH), 7.99 (td, J = 8, 0.8 Hz, 2H, ArH), 8.37 (s, 1H, C-H, Triazole), 10.38 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm), 52.39, 62.80, 104.79 (d, $J_{C\text{-}F}$= 27, Hz, ArCH), 111.36, 111.78 (d, $J_{C\text{-}F}$= 22, ArCH), 122.45 125.70 126.03, 126.58, 127.73, 131.28, 131.93, 134.14, 134.99, 141.10, 155.23 (d, $J_{C\text{-}F}$= 130Hz, ArCH), 159.12 (d, $J_{C\text{-}F}$= 130Hz, ArCH), 159.43, 165.29, 179.96, 185.03;IR (KBr) 3343, 1707, 1674, 1242, 1100 cm^{-1} Mass (M/Z:20ev):424 **Anal. calcd for $C_{21}H_{14}F_2N_4O_4$** (424): C, 59.44; H: 3.33; N, 13.20 Found: C: 59.42 H: 3.31; N, 13.19.

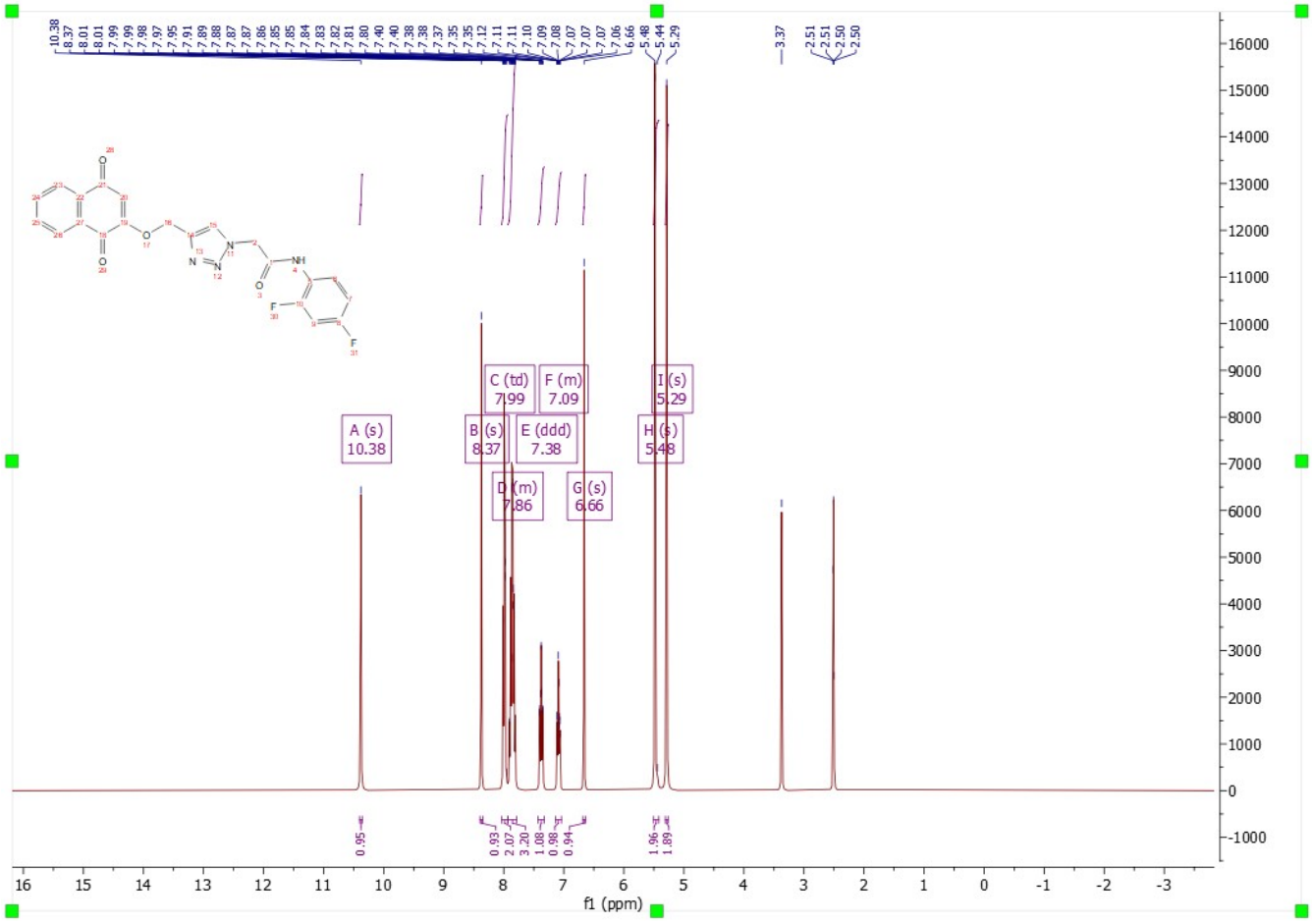

Fig. S_{43} ^{1}HNMR of 3k

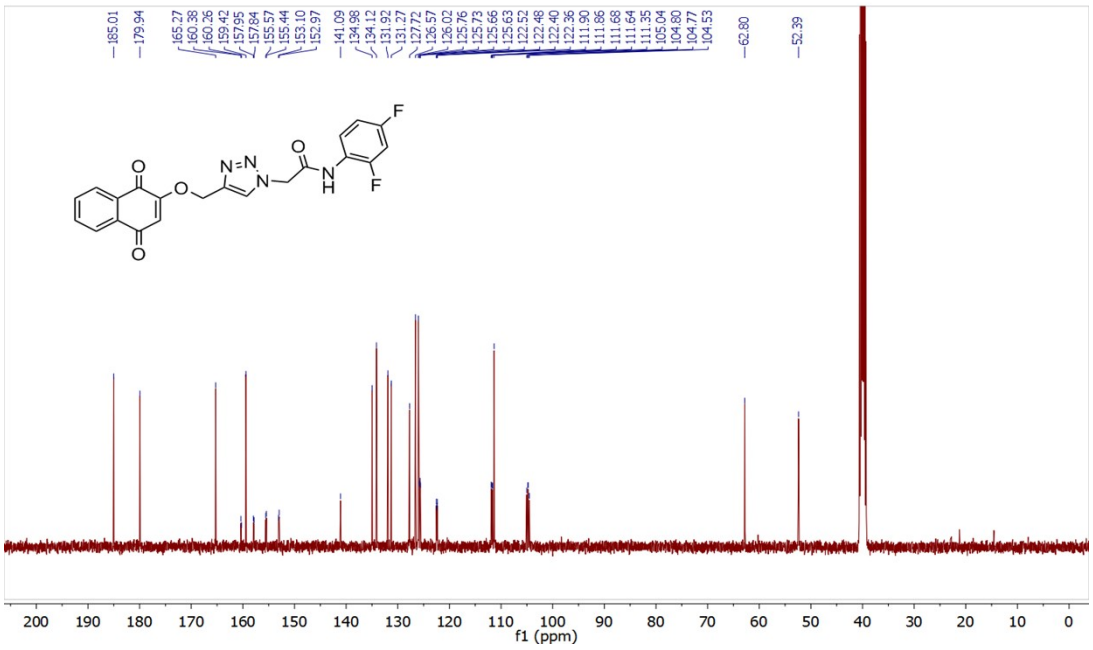

Fig. S_{44} ^{13}CNMR of 3k

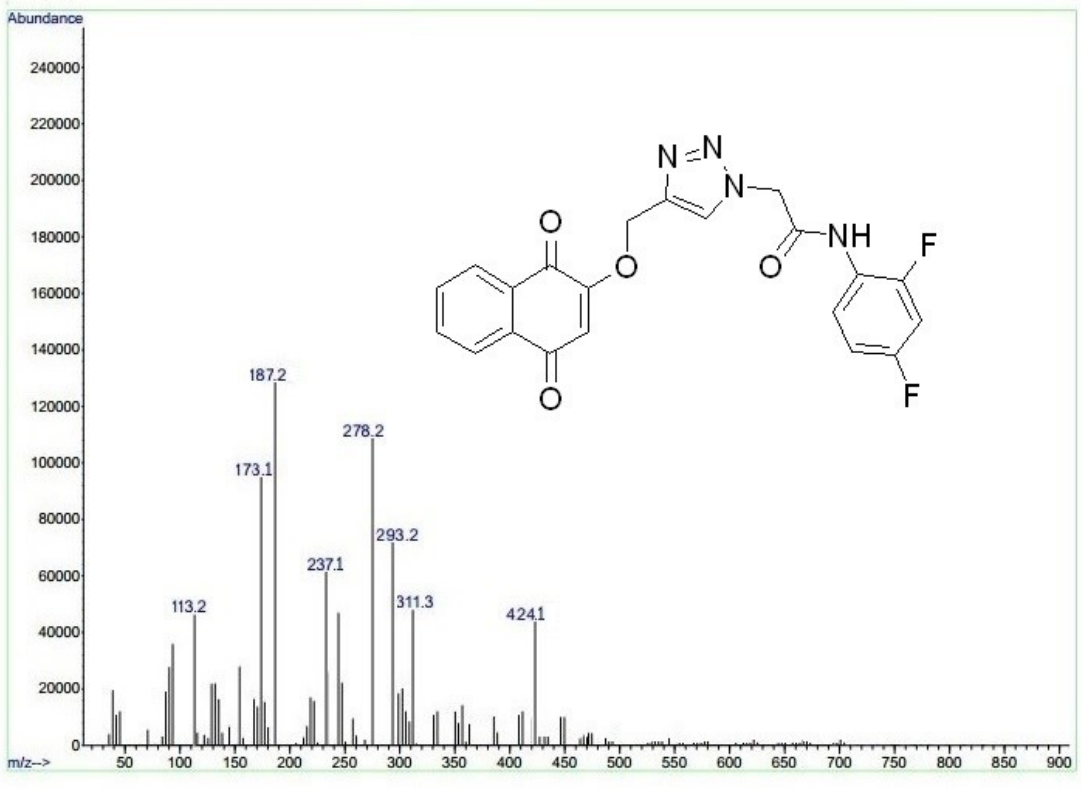

Fig. S_{45} Mass spectroscopy of 3k

N-(3-chloro-4-fluorophenyl)-2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)acetamide (3l): Cream solid; isolated yield: 76%, m.p.: 249-251°C; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm), 5.29 (s, 2H, N-CH_2) , 5.41 (s, 2H, O-CH_2), 6.66 (s, 1H, C-H, quinon), 7.38 – 7.50 (m, 2H, ArH), 7.80 – 8.1 (m, 3H, ArH), 8.00 (td, J = 8.2, 0.8 Hz, 2H, ArH), 8.37 (s, 1H, C-H, Triazole), 10.75 (s, 1H, NH);^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm), 52.64, 62.81, 111.38, 117.67 (d, $J_{C\text{-}F}$ = 22 Hz, ArCH), 119.78 (d, $J_{C\text{-}F}$= 18 Hz, ArC_q), 120.05 (d, $J_{C\text{-}F}$ = 7 Hz, ArCH), 121.16, 126.04, 126.59, 127.72, 131.28, 131.93, 134.14, 135.00, 136.09141.10, 153.81 (d, $J_{C\text{-}F}$= 241 Hz, C_q, C-F), 159.43, 165.02, 179.97, 185.03;IR (KBr) 3595, 3276, 3089, 1922, 1788, 1687, 1572, 1499, 1343,1251,1182,1111,967,853,737 cm$^{-1;}$ Mass (M/Z:20ev):442 **Anal. calcd for $C_{21}H_{14}ClFN_4O_4$** (442): C, 57.22; H: 3.20; N, 12.71 Found: C, 57.20 H: 3.17; N, 12.74.

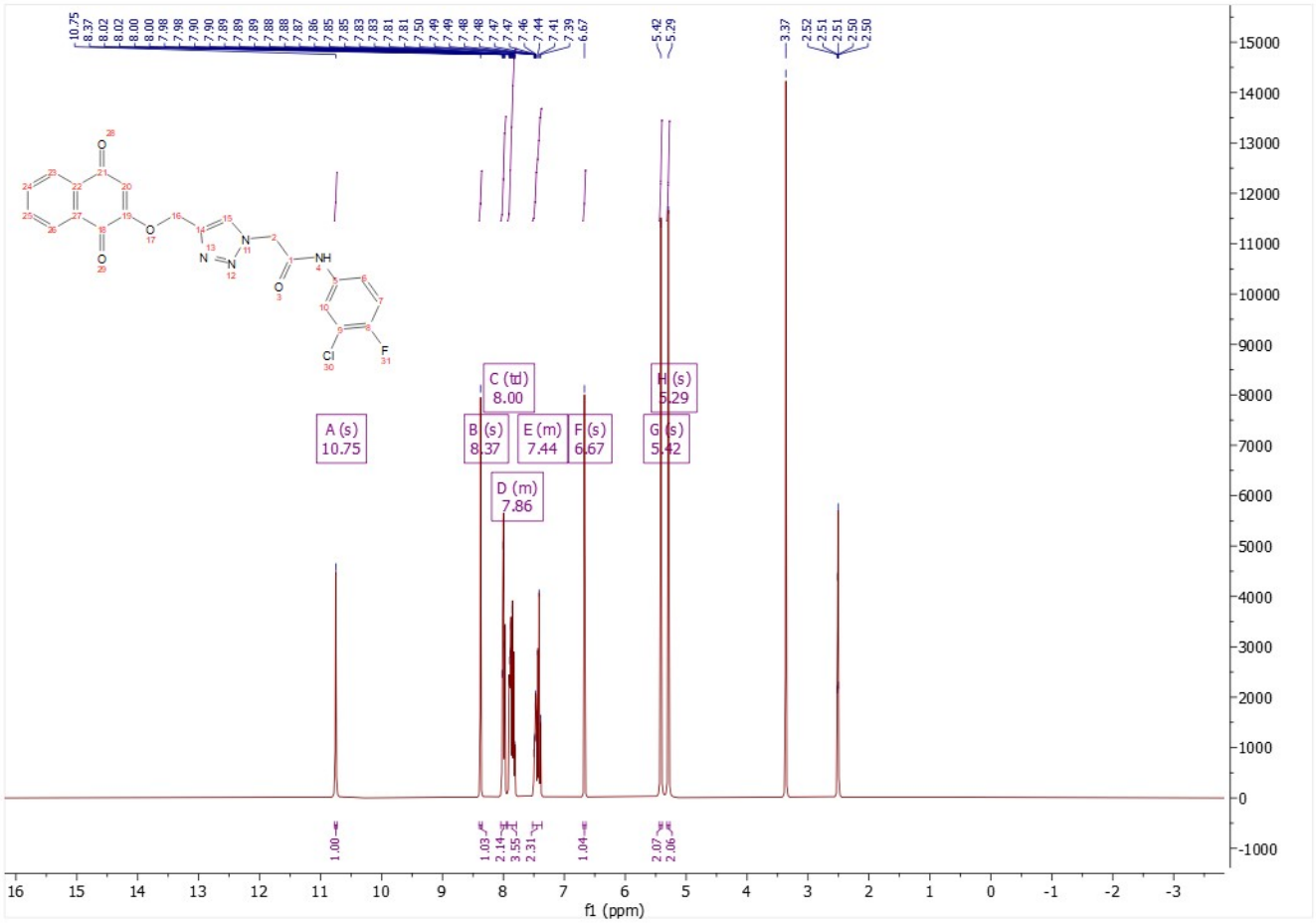

Fig. S_{46} ^{1}HNMR of 3l

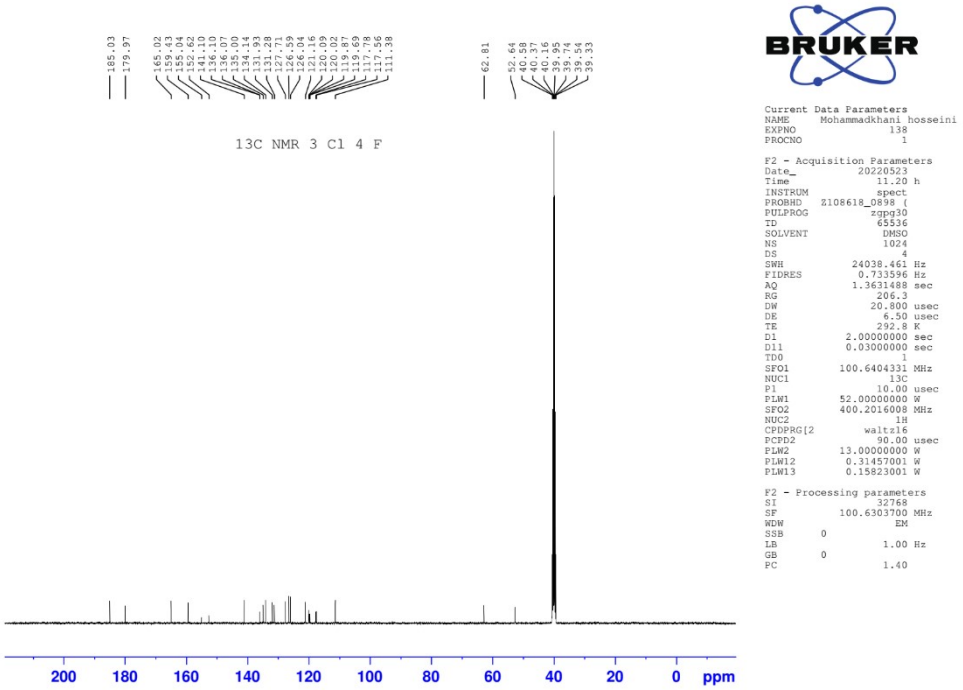

Fig. S_{47} ^{13}CNMR of 3l

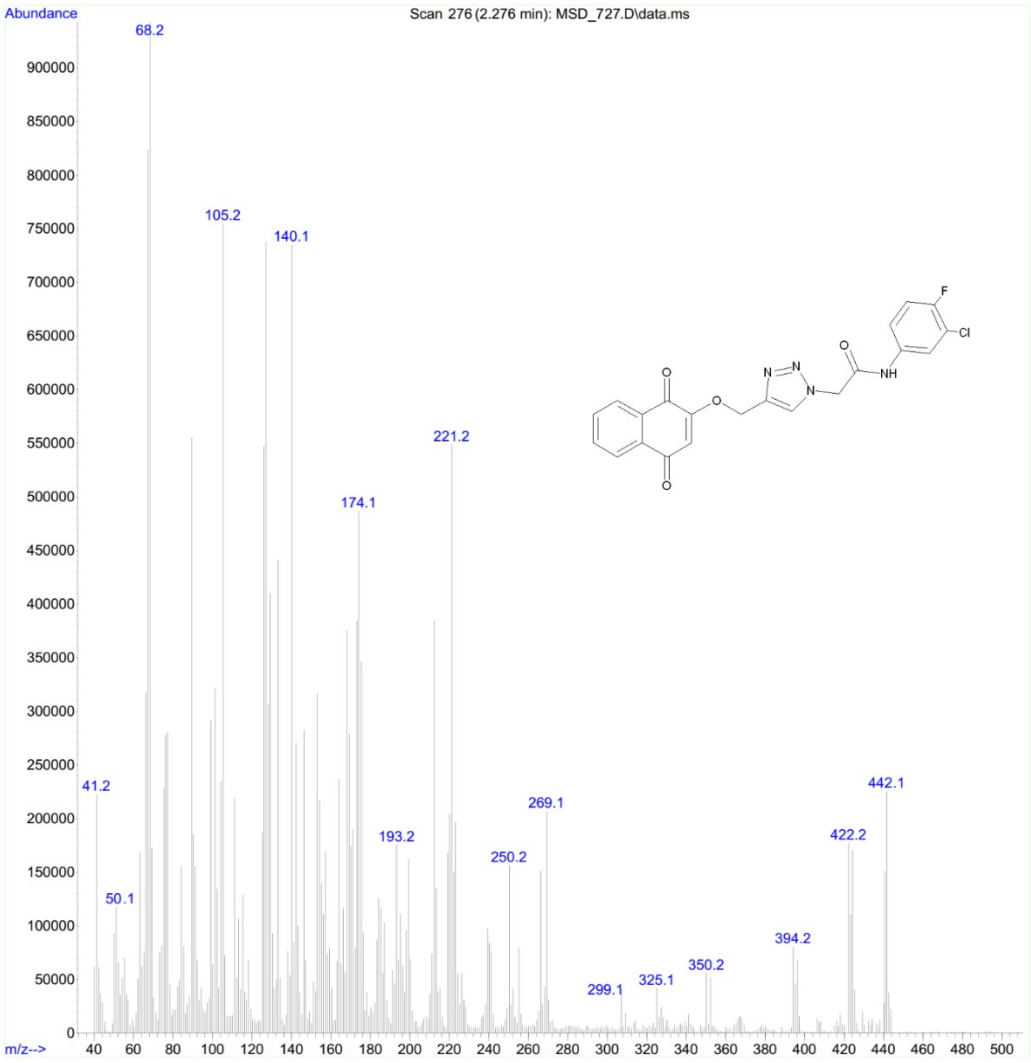

Fig. S_{48} Mass spectroscopy of 3l

N-benzyl-2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)acetamide (3m): Cream solid; isolated yield: 67%, m.p.: 218-220°C; ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm) 4.34 (d, J = 6 Hz, 2H, NH-CH_2), 5.23 (s, 2H, N-CH_2), 5.27 (s, 2H, O-CH_2), 6.67 (s, 1H, C-H, quinon), 7.23 – 7.38 (m, 5H, ArH), 7.81 – 7.91 (m, 2H, ArH), 8.00 (td, J = 8.2, 0.8 Hz, 2H, ArH), 8.31 (s, 1H, C-H, Triazole), 8.86 (t, J = 5.6 Hz, 1H, NH);^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm) 42.85, 52.10, 62.81, 111.37, 126.04, 126.60, 127.49, 127.59, 127.88, 128.85, 131.30, 131.95, 134.16, 135.01, 139.16, 140.97, 159.45, 165.83, 179.98, 185.05; IR (KBr) 3349, 1701, 1665, 1263, 1155 cm^{-1} Mass (M/Z:20ev):402 **Anal. calcd for $C_{22}H_{18}N_4O_4$** (402): C, 65.66; H, 4.51; N, 13.92 Found: C, 65.65; H, 4.50; N, 13.90

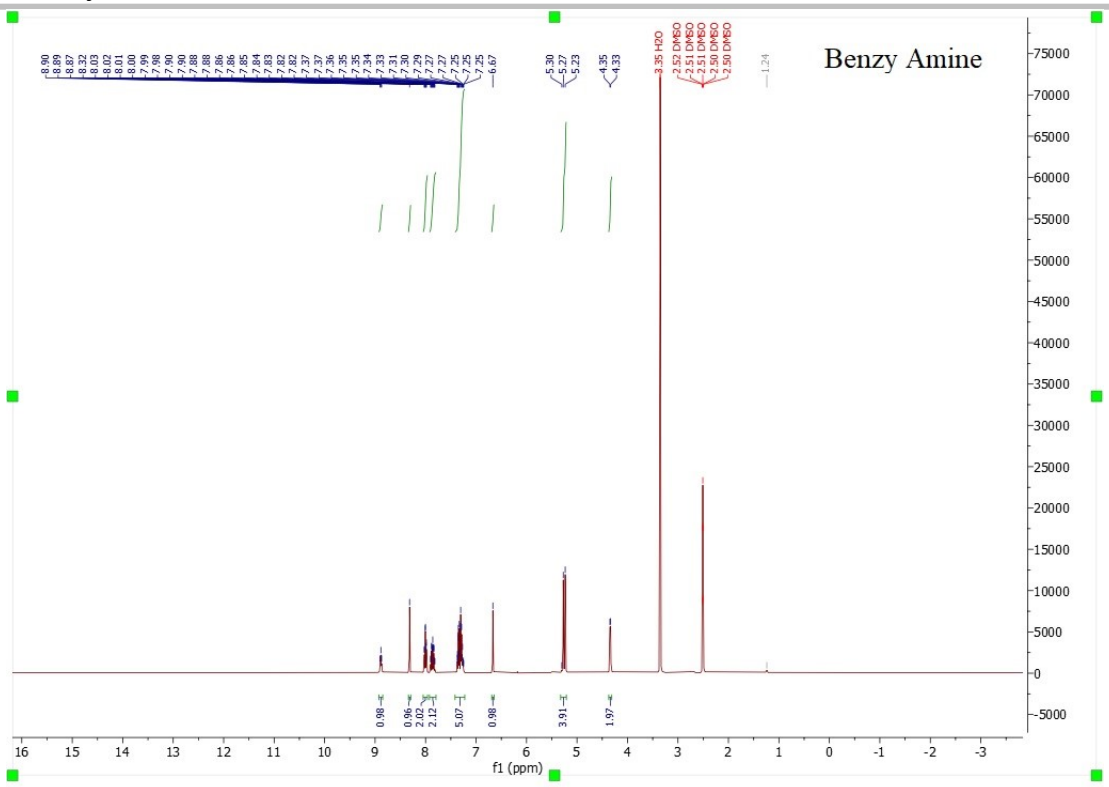

Fig. S_{49} ^{1}HNMR of 3m

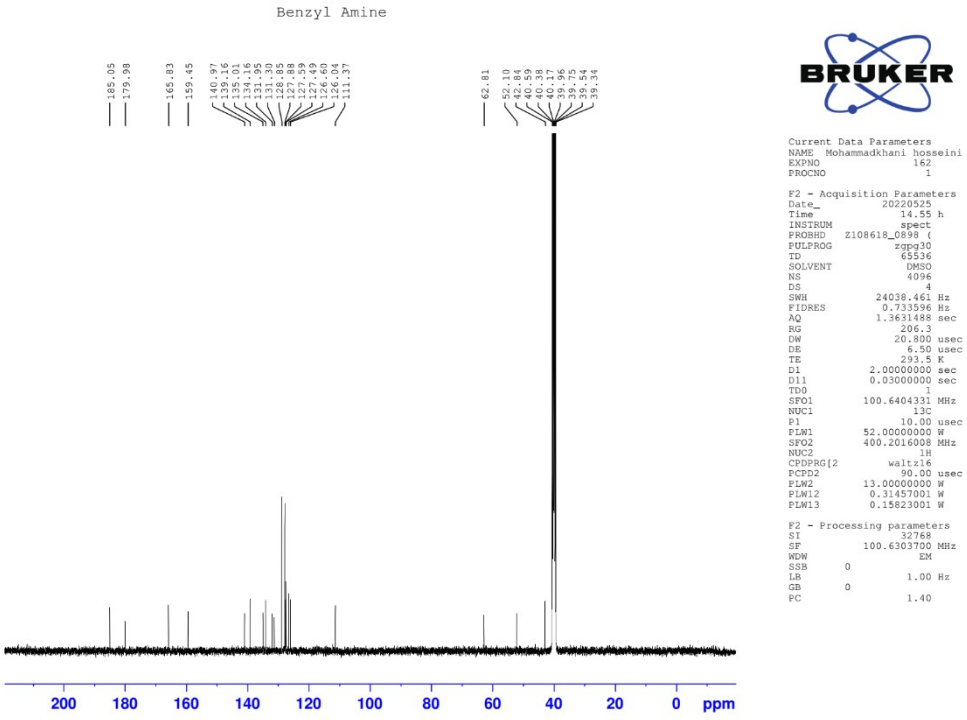

Fig. S_{50} ^{13}CNMR of 3m

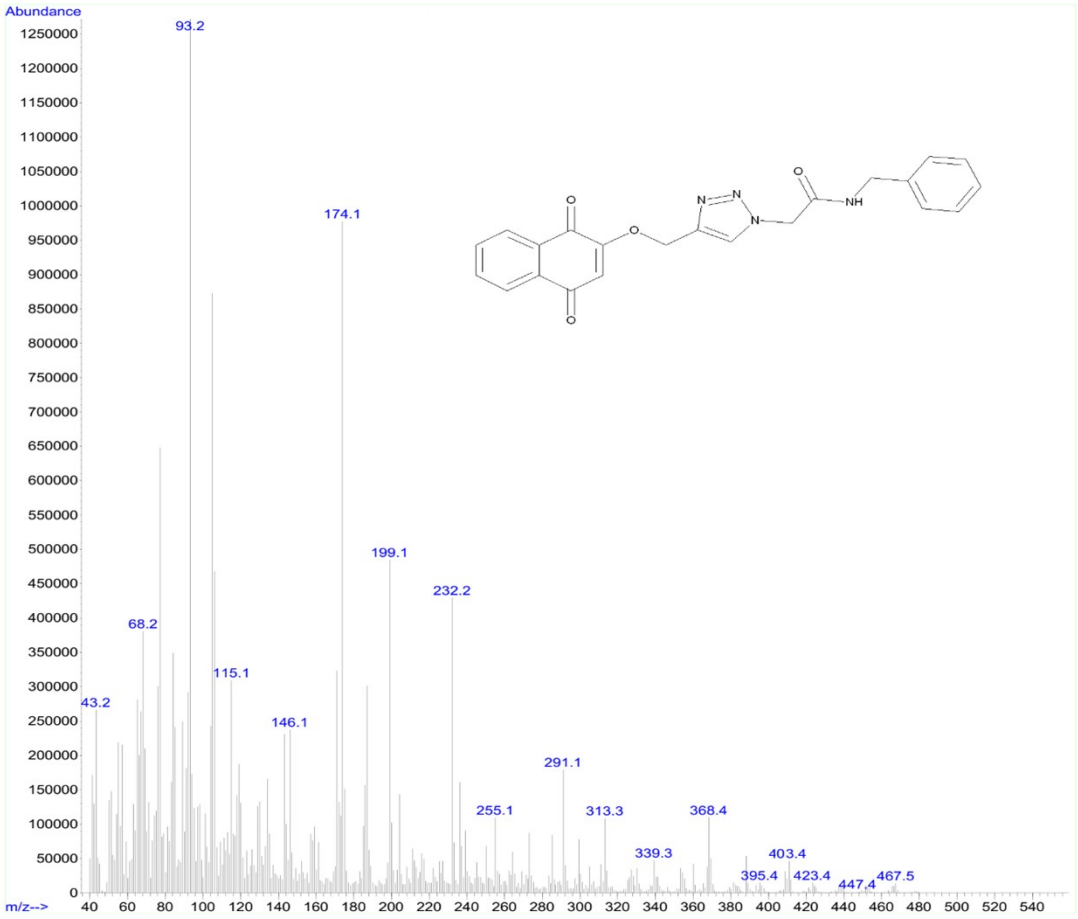

Fig. S_{51} Mass spectroscopy of 3m

N-(2,4-dimethylphenyl)-2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)acetamide (3n); 1H NMR (400 MHz, DMSO) δ 9.81 (s, 1H), 8.37 (s, 1H), 8.00 (td, J = 7.3, 1.6 Hz, 2H), 7.85 (dtd, J = 16.7, 7.4, 1.5 Hz, 2H), 7.17 – 7.03 (m, 4H), 6.67 (s, 1H), 5.44 (s, 2H), 5.29 (s, 2H), 2.17 (s, 6H). ^{13}C NMR (101 MHz, DMSO) δ 185.03, 179.98, 164.44, 159.45, 141.04, 135.55, 135.00, 134.66, 134.15, 131.95, 131.30, 129.38, 128.68, 128.43, 128.24, 127.64, 127.24, 126.59, 126.04, 111.38, 62.82, 52.13, 18.51, 7.91.FT-IR(KBr): 3747, 3480, 3414, 2935, 2109, 1654, 1606, 1532, 1480 ,1394 ,1303 ,1241 ,1203 ,1048 ,780 ,700 cm^{-1} Mass (M/Z:20ev):416 **Anal. calcd for $C_{23}H_{20}N_4O_4$** (416): C, 66.34; H, 4.84; N, 13.45; Found: 66.33; H, 4.85; N, 13.44

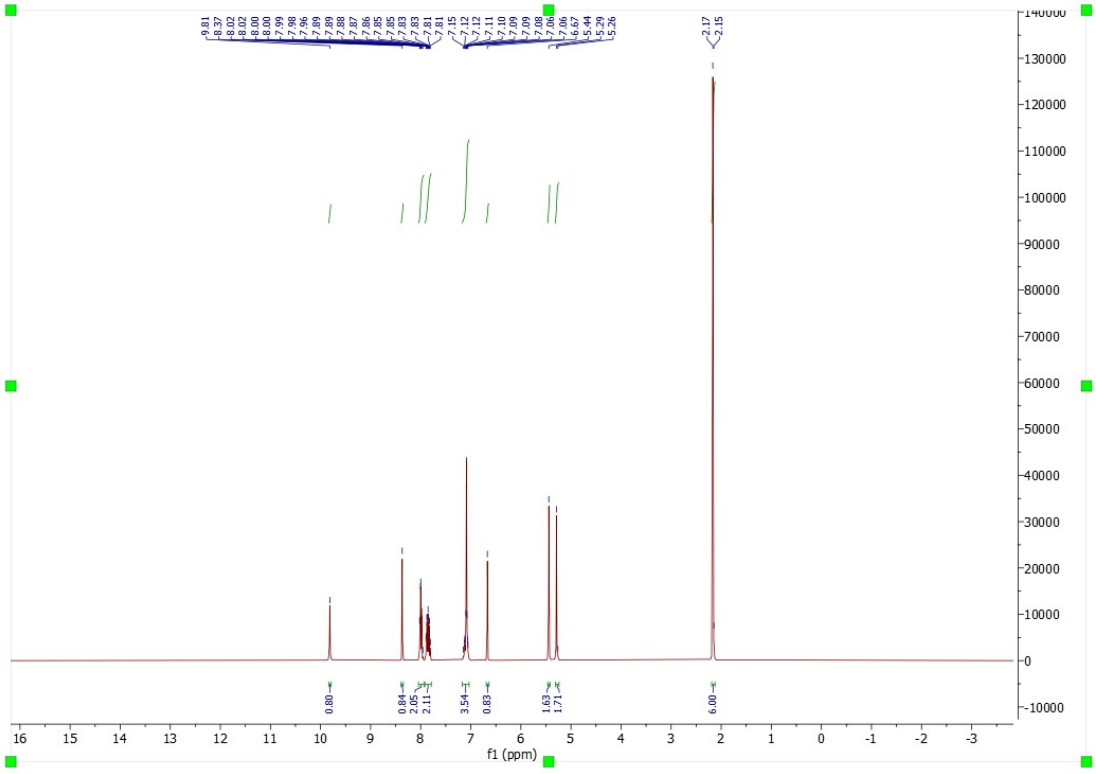

Fig. S_{52} ^{1}HNMR of 3n

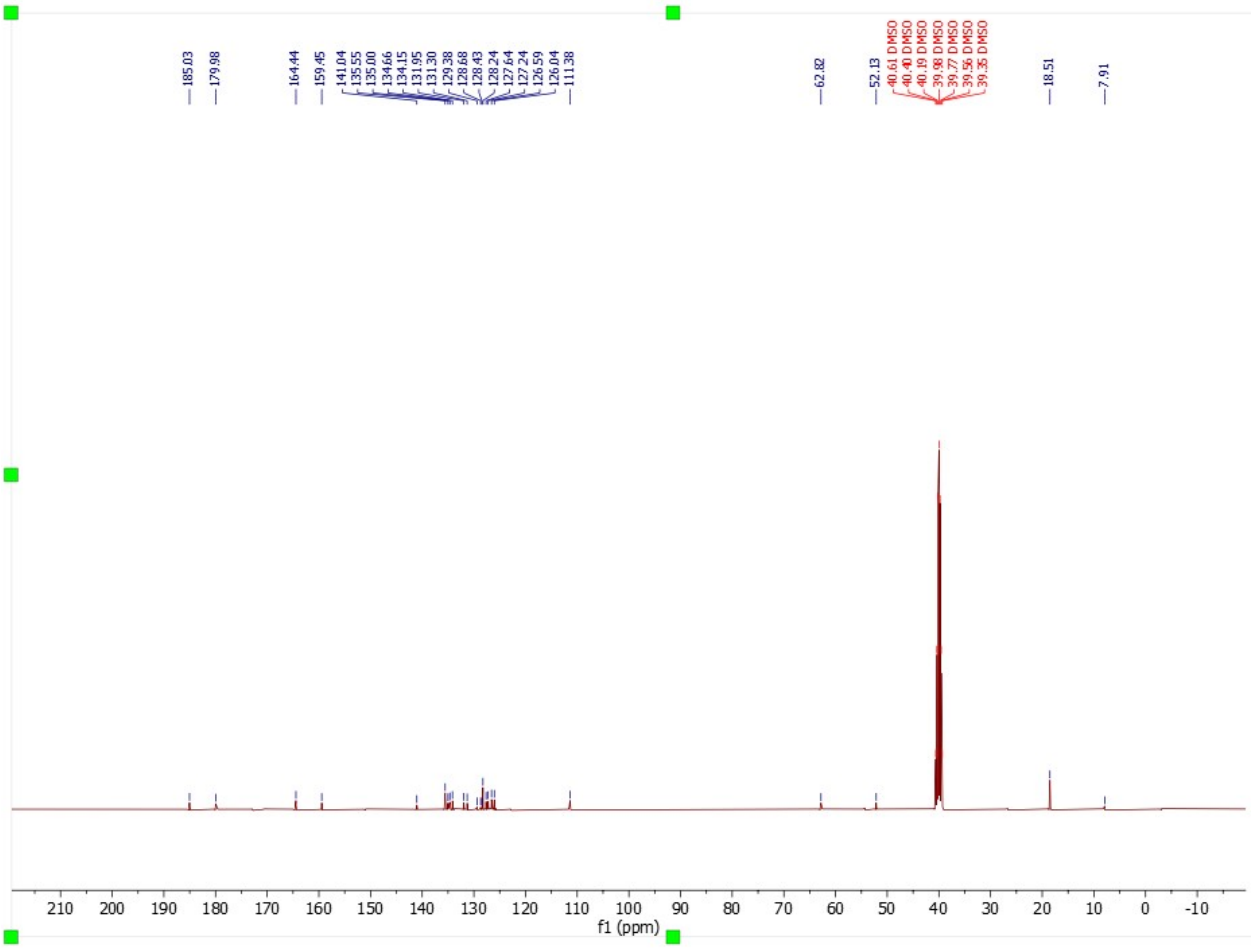

Fig. S_{53} ^{13}CNMR of 3n

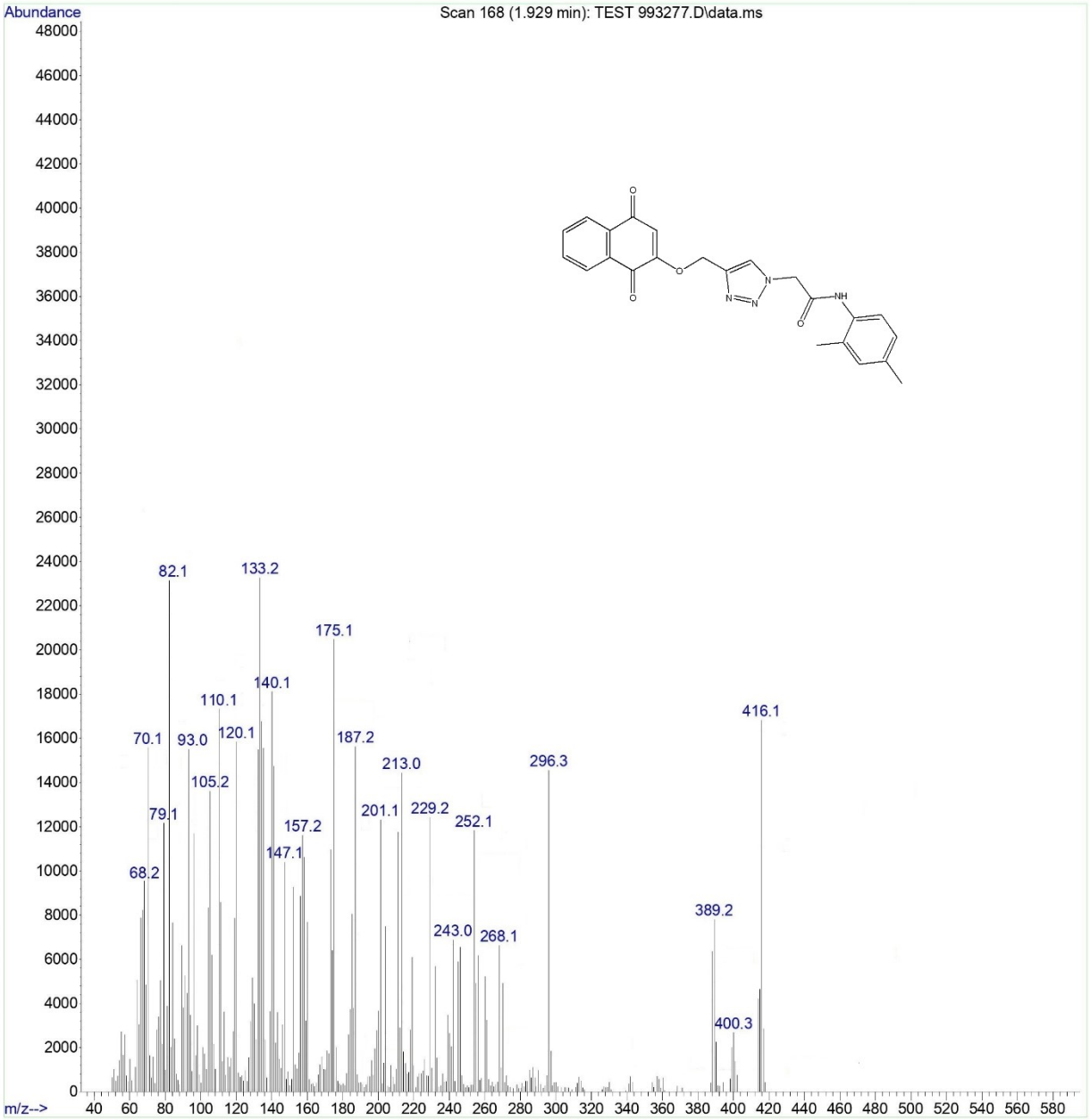

Fig. S_{54} Mass spectroscopy of 3n

2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)-N-(2-methyl-4-nitrophenyl)acetamide (3o): ^{1}H NMR (400 MHz, DMSO) δ 10.10 (s, 1H), 8.39 (s, 1H), 8.21 – 8.10 (m, 2H), 8.08 (dd, *J* = 9.0, 2.8 Hz, 2H), 8.03 – 7.93 (m, 4H), 7.86 (dtd, *J* = 16.6, 7.4, 1.6 Hz, 3H), 6.67 (s, 1H), 5.56 (s, 2H), 5.30 (s, 2H), 2.42 (s, 4H).^{13}C NMR (101 MHz, DMSO) δ 185.04, 179.99, 165.70, 159.45, 143.96, 142.58, 141.14, 135.01, 134.16, 131.95, 131.81, 131.30, 127.74, 126.60, 126.04, 123.73, 122.33, 111.39, 62.82, 52.68, 18.32.. FT-IR(KBr): 3763, 3420, 2930, 2117, 1658, 1608, 1537, 1486 ,1389 ,1299 ,1225 ,1206 ,1038 ,780 ,720 cm^{-1}, Mass (M/Z:20ev):447, **Anal. calcd for $C_{23}H_{20}N_4O_4$** (447): C, 59.06; H, 3.83; N, 15.65 Found: C, 59.05; H, 3.82; N, 15.68.

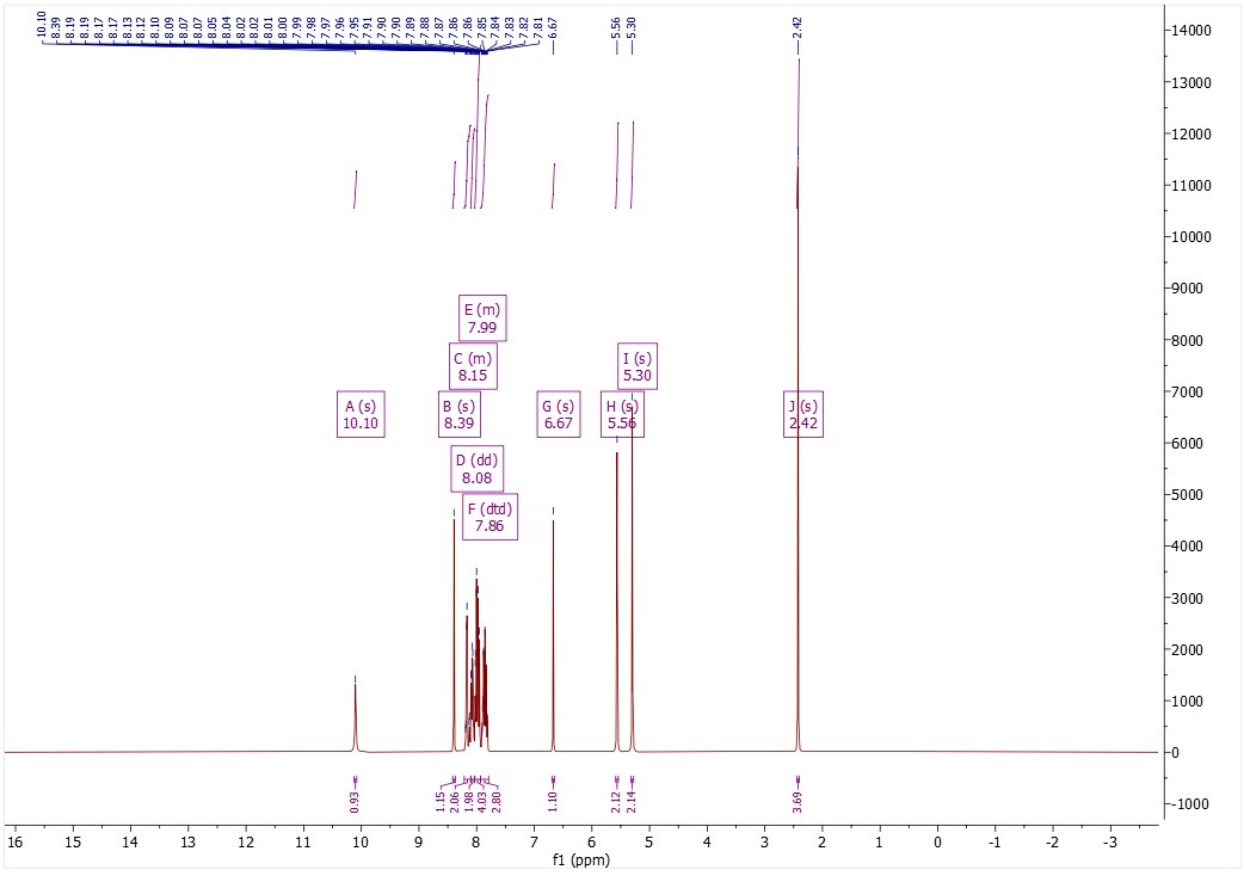

Fig. S_{55} ^{1}HNMR of 3o

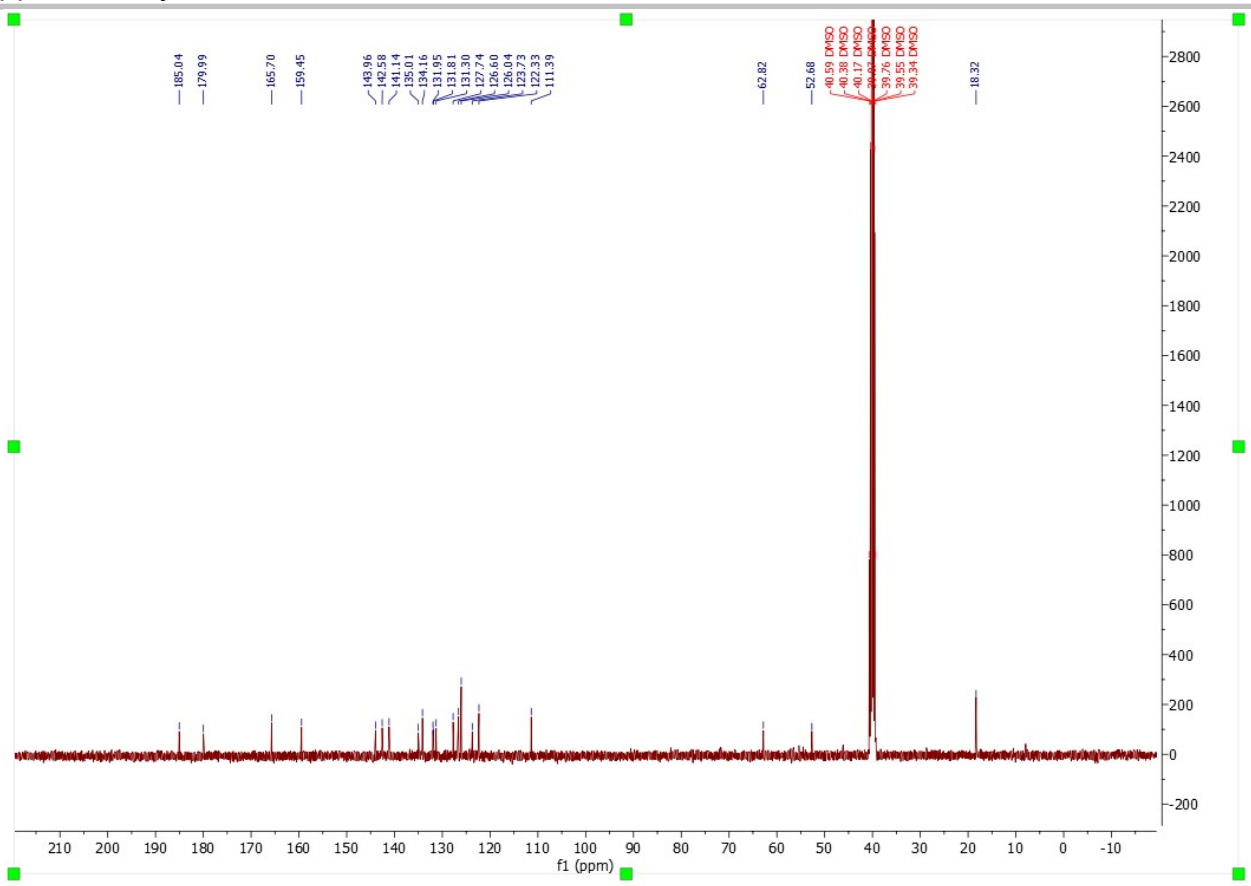

Fig. S_{56} ^{13}CNMR of 3o

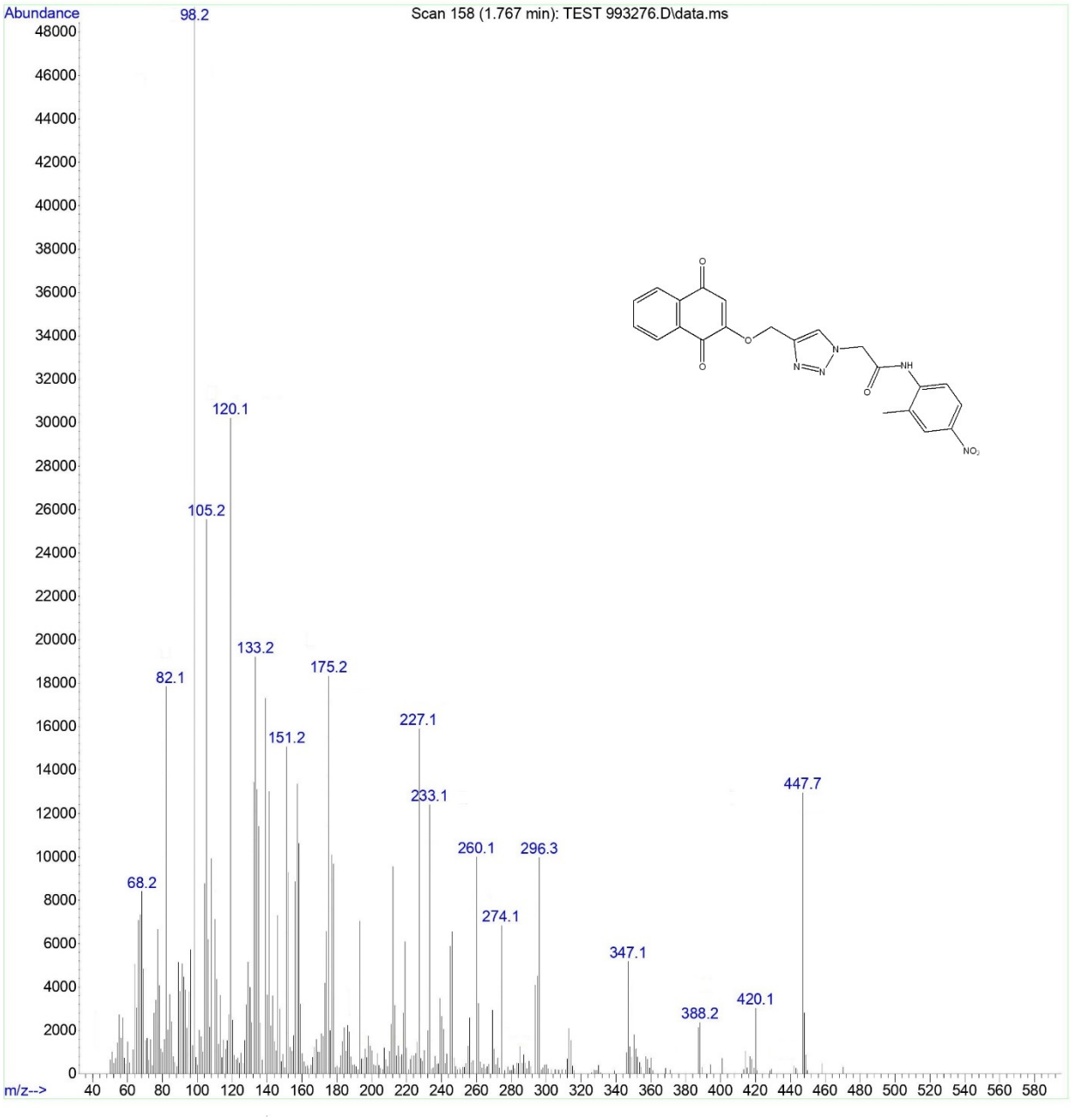

Fig. S_{57} Mass spectroscopy of 3o

N-(2,6-dimethylphenyl)-2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)acetamide (3p); ^{1}H NMR (400 MHz, DMSO) δ 9.81 (s, 1H), 8.36 (s, 1H), 8.00 (td, *J* = 7.3, 1.6 Hz, 2H), 7.85 (dtd, *J* = 16.6, 7.4, 1.5 Hz, 2H), 7.09 (d, *J* = 1.3 Hz, 3H), 6.67 (s, 1H), 5.44 (s, 1H), 5.29 (s, 2H), 2.17 (s, 6H), 1.24 (s, 1H), 0.86 (t, *J* = 6.6 Hz, 1H).^{13}C NMR (101 MHz, DMSO) δ 185.04, 179.98, 164.44, 159.45, 141.03, 135.55, 135.01, 134.65, 134.15, 131.95, 131.30, 128.24, 127.64, 127.25, 126.60, 126.04, 111.38, 62.81, 52.12, 31.77, 29.18, 22.58, 18.51, 14.44, FT-IR(KBr): 3761, 3474, 3416, 2932, 2113, 1657, 1609, 1536, 1483 ,1392 ,1300 ,1241 ,1207 ,1051 ,773 ,715 cm^{-1} Mass (M/Z:20ev):416, **Anal. calcd for $C_{23}H_{20}N_4O_4$** (416): 66.34; H, 4.84; N, 13.45 Found: 66.34; H, 4.82; N, 13.46

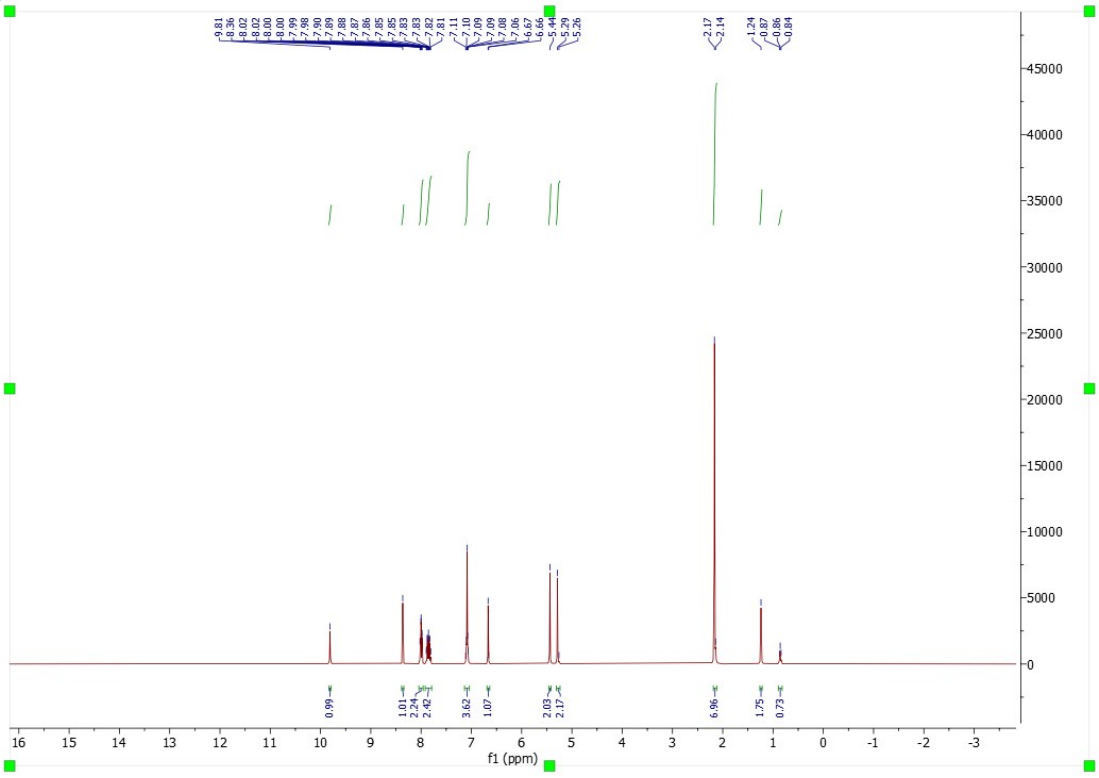

Fig. S_{58} ^{1}HNMR of 3p

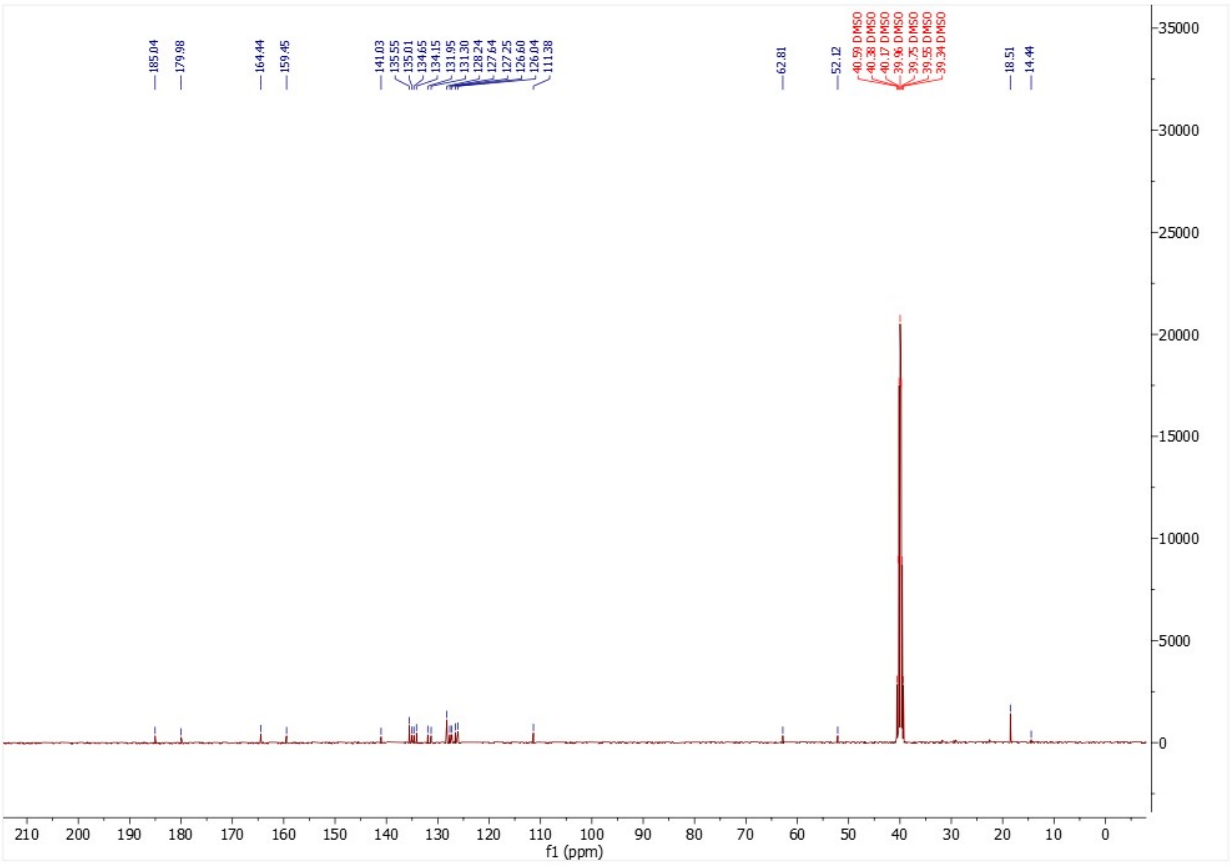

Fig. S_{59} ^{13}CNMR of 3p

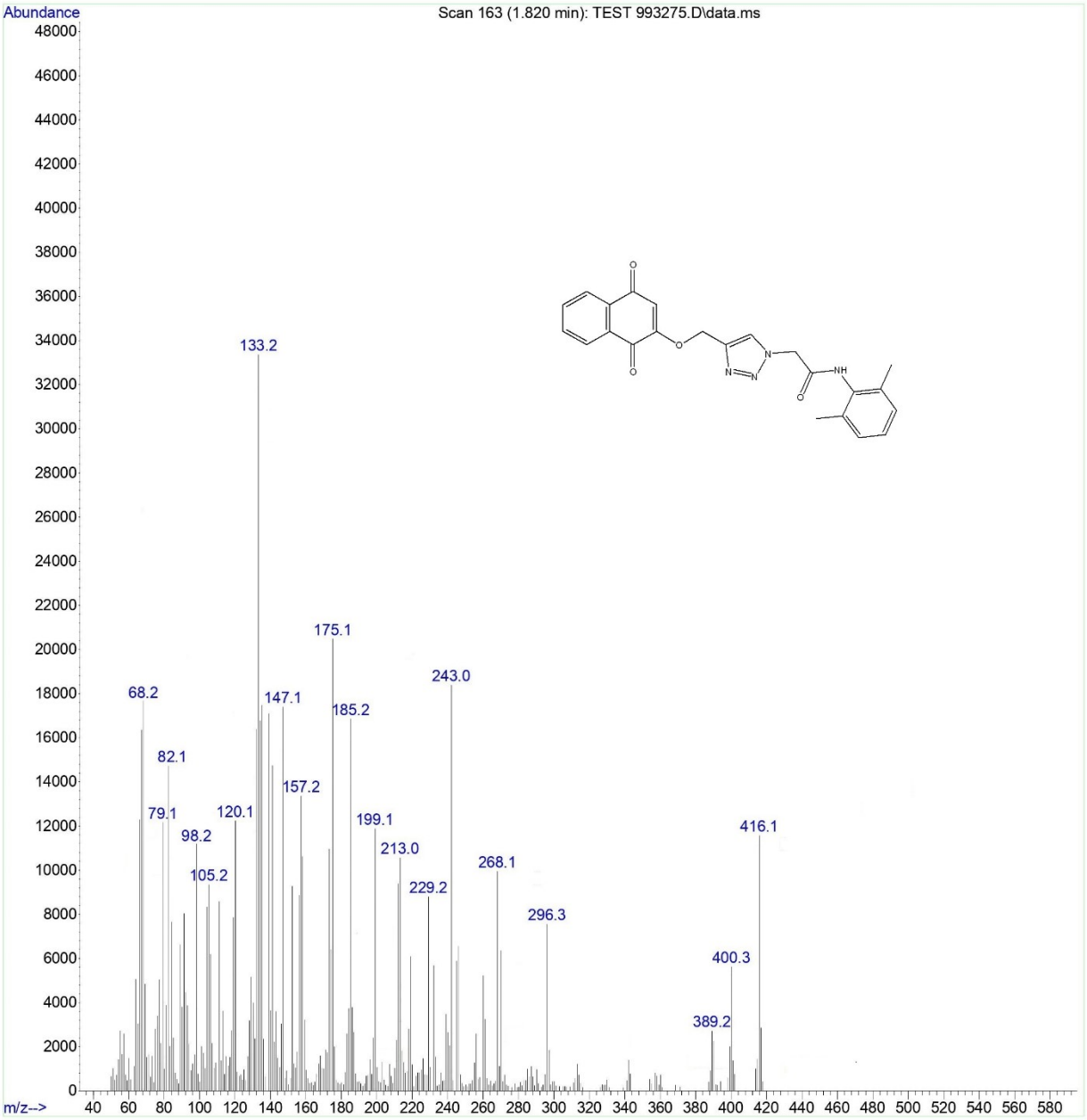

Fig. S_{60} Mass spectroscopy of 3p

2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)-N-(2-iodophenyl)acetamide (3q): orange solid; M.P.: 202-205 °C ^{1}H NMR (400 MHz, DMSO) δ 10.00 (s, 1H), 8.37 (s, 1H), 8.00 (td, *J* = 7.4, 1.6 Hz, 2H), 7.93 – 7.81 (m, 3H), 7.67 – 7.54 (m, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.02 (t, *J* = 7.7 Hz, 1H), 6.66 (s, 1H), 5.46 (s, 2H), 5.29 (s, 2H). ^{13}C NMR (101 MHz, DMSO) δ 185.03, 182.80, 165.05, 159.44, 141.11, 139.58, 139.13, 135.00, 134.15, 131.95, 131.30, 130.31, 129.28, 128.57, 127.71, 126.60, 126.04, 111.39, 96.49, 62.82, 52.49. FT-IR(KBr):3757,3476,3418,2958,2117, 1684,1653, 1611, 1583, 1529, 1477,1434 ,1333 ,1295, 1243, 1204, 1164, 1045,1012, 855,757,724,617,491 cm^{-1} Mass (M/Z:20ev): (514): **Anal. calcd for $C_{21}H_{15}IN4O_4$ (**514) C, 49.05; H: 2.94; N, 10.89 Found: C, 49.03 H: 2.95; N, 10.92.

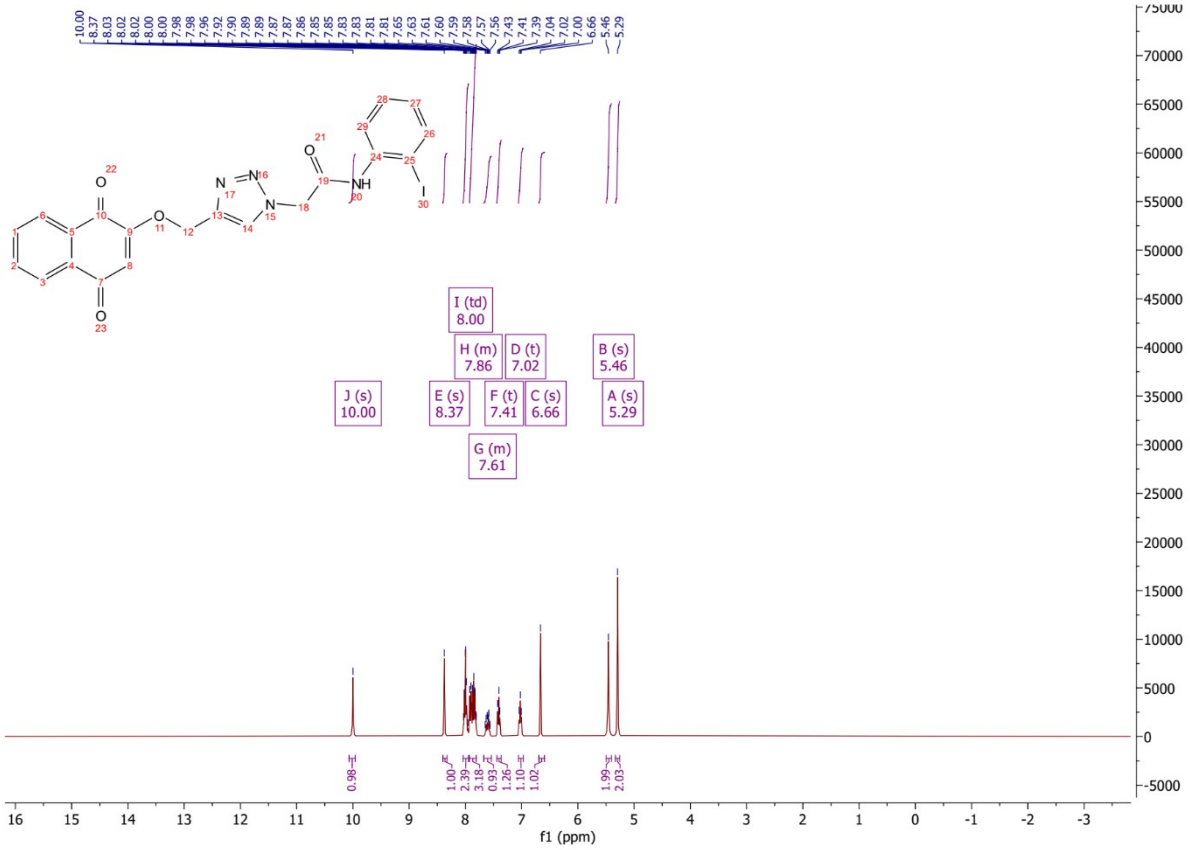

Fig. S_{61} ^{1}HNMR of 3q

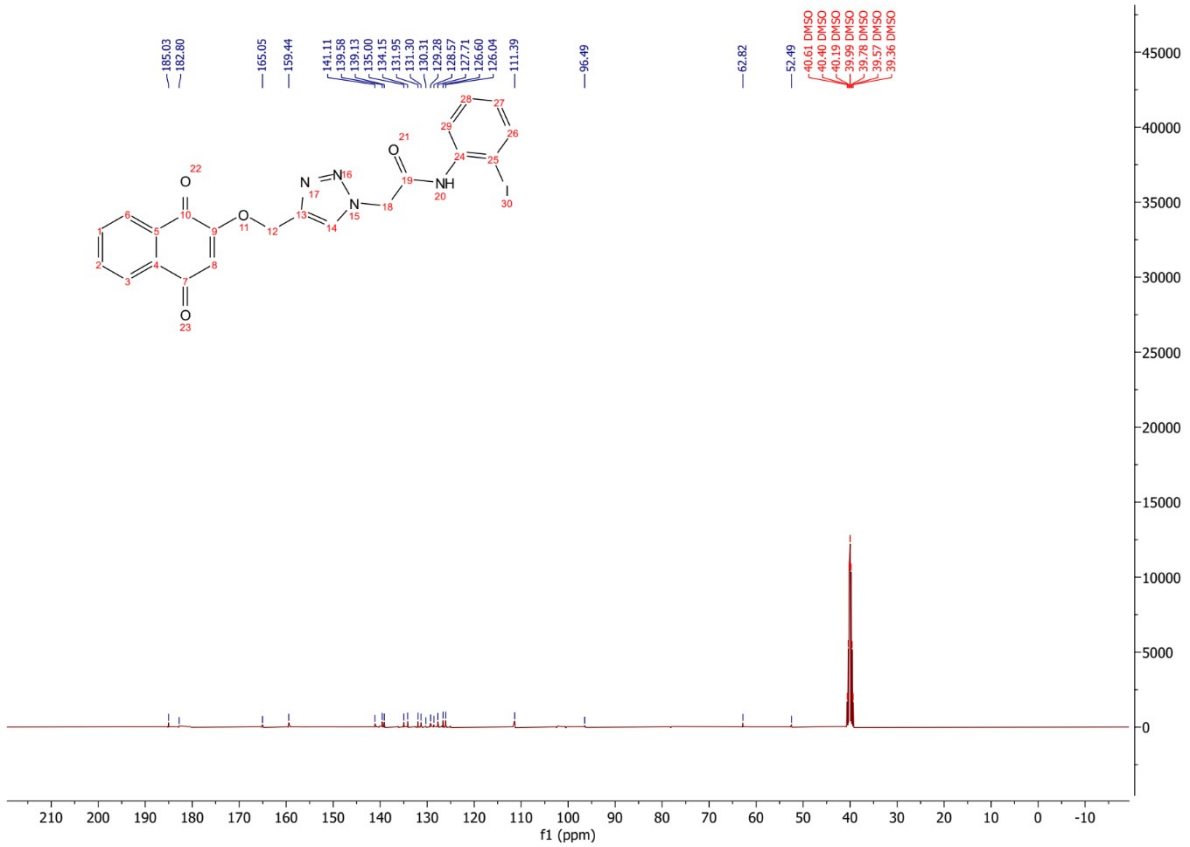

Fig. S_{62} ^{13}CNMR of 3q

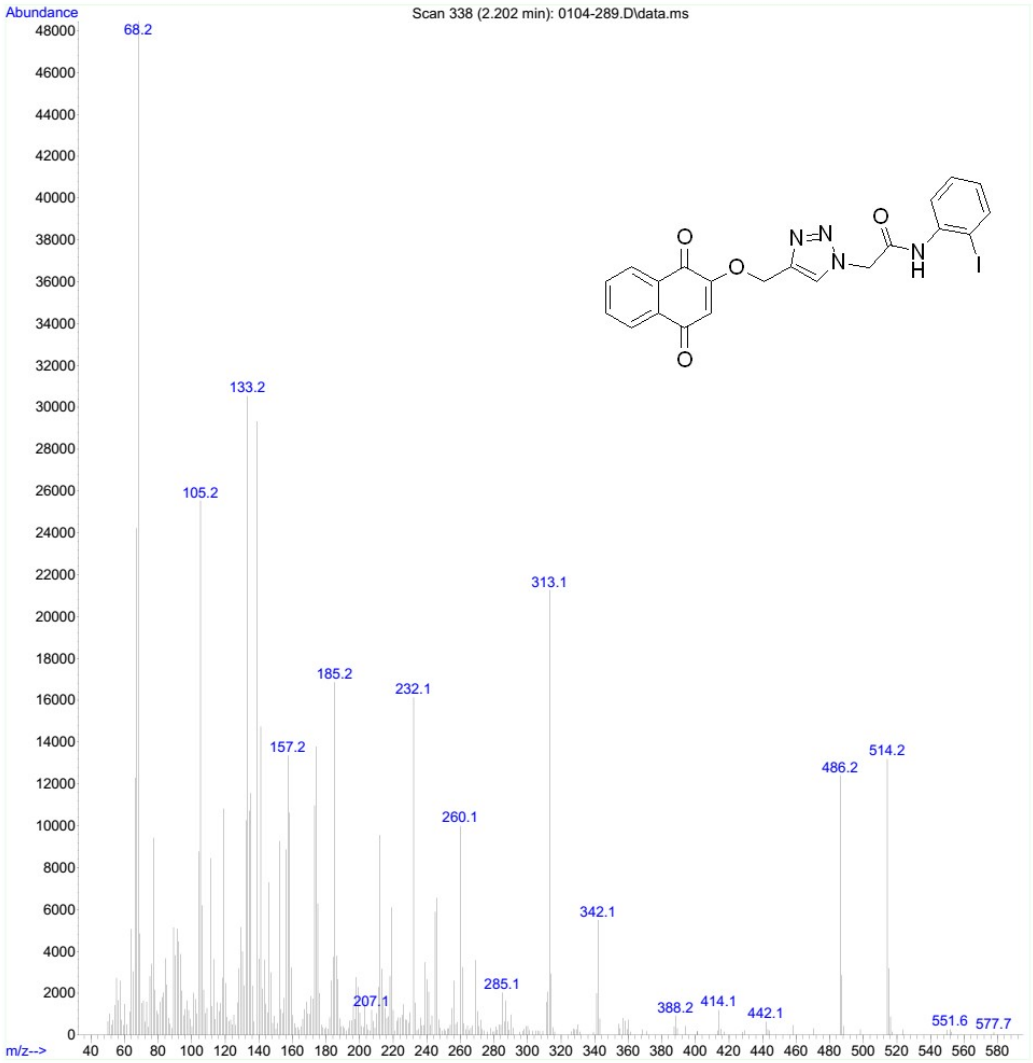

Fig. S_{63} Mass spectroscopy of 3q

2-(4-(((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-iodophenyl)acetamide (3r)m.p.:213-215: ^{1}H NMR (400 MHz, DMSO) δ 10.62 (s, 1H), 8.36 (s, 1H), 8.01 (dd, *J* = 9.0, 7.2 Hz, 2H), 7.86 (dtd, *J* = 16.6, 7.4, 1.6 Hz, 2H), 7.68 (d, *J* = 8.4 Hz, 3H), 7.43 (dd, *J* = 8.8, 2.0 Hz, 3H), 6.67 (s, 1H), 5.40 (s, 2H), 5.29 (s, 3H). ^{13}C NMR (101 MHz, DMSO) 185.03, 179.98, 165.05, 158.64, 141.11, 139.58, 139.13, 135, 134.15, 131.95, 131.5, 127.71, 126.60, 126.04, 125.05, 111.39, 96.82, 62.82, 55.5. FT-IR(KBr): 3759, 3476, 3419, 2935, 2115, 1654, 1611, 1538, 1486 ,1394 ,1301 ,1245 ,1203 ,1053 ,1009 ,823 ,776 ,719 ,613,494 cm^{-1} Mass (M/Z:20ev):514 **Anal. calcd for $C_{21}H_{15}IN4O_4$** (514): C, 49.05; H: 2.94; N, 10.89 Found: C, 49.07 H: 2.92; N, 10.91.

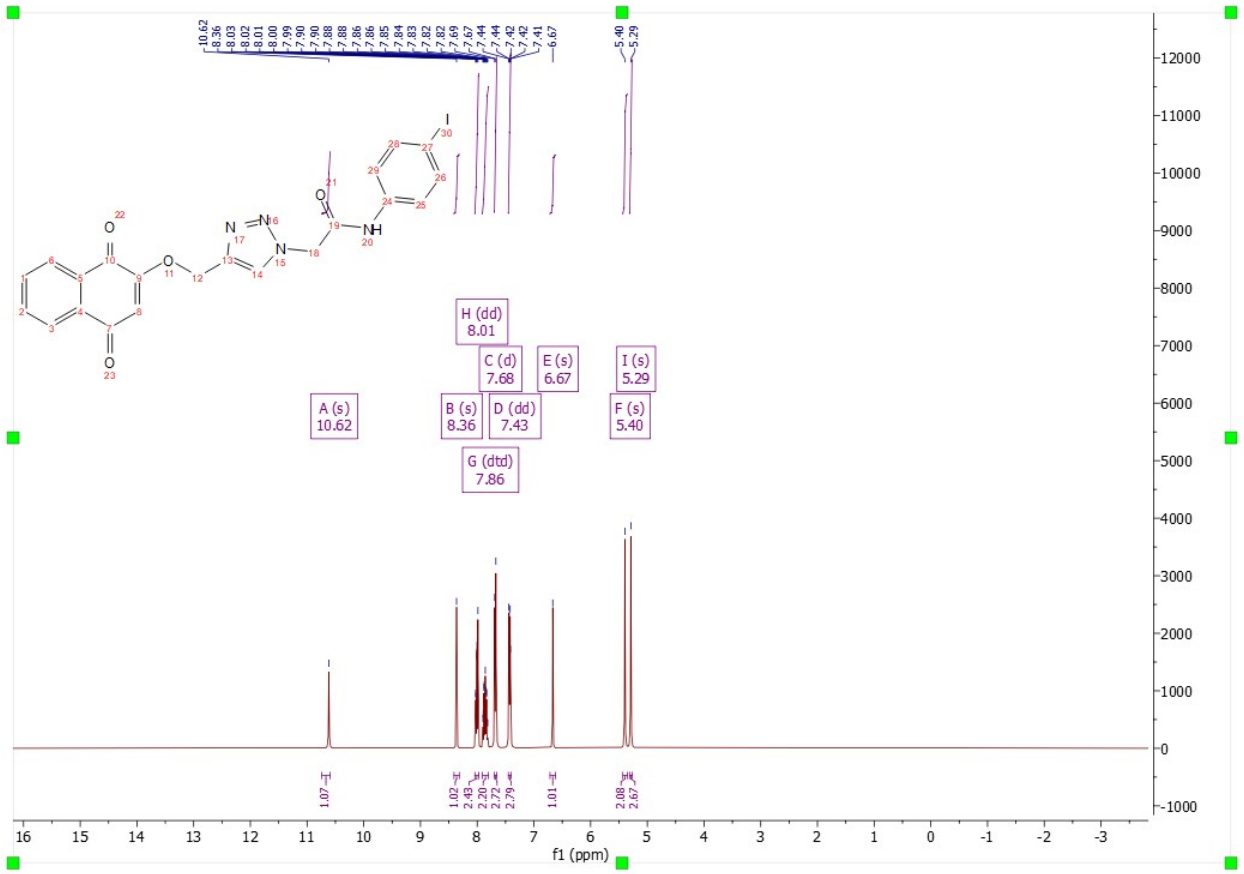

Fig. S_{64} ^{1}HNMR of 3r

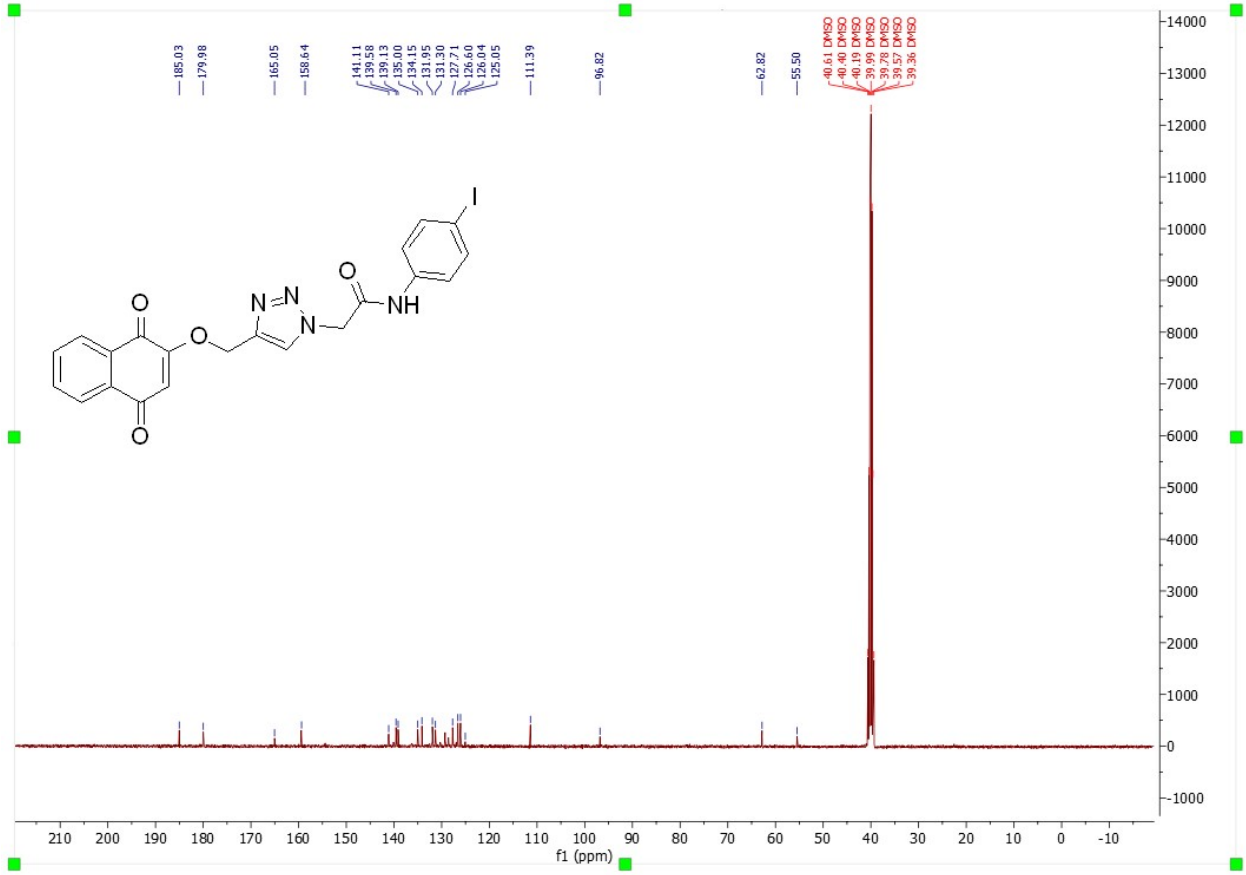

Fig. S_{65} ^{13}CNMR of 3r

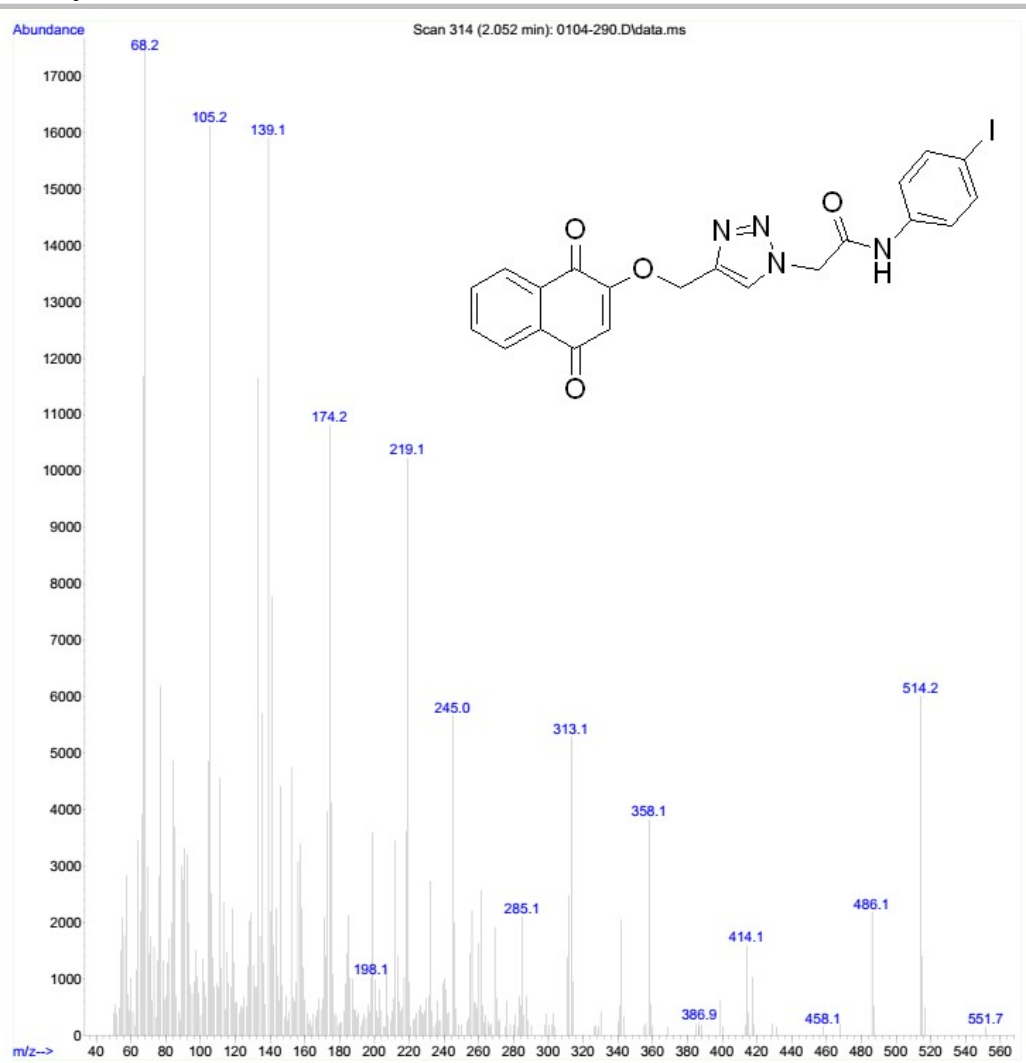

Fig. S_{66} Mass spectroscopy of 3r

4.Author Contributions:

A.M. and S.S. : cooperated on All parts, the conceptualization of the research project, the writing-original draft of the manuscript, writing- review & editing of the manuscript equally.

M.M.: Just cooperated on the investigation of the medicinal chemistry research project.

A.H. and S.A.P.: Supervision and corresponded on the project, Data curation, validation of resources, writing- reviewing as well as editing the manuscript.

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