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

1.1 General 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 K\(_{\alpha}\) 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 cm\(^2\) 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
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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 that the Mott-Schottky measurement was measured in Na$_2$SO$_4$ (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$_3$O$_4$/AlZn-Ni-LDH nano-catalyst, Fe$_3$O$_4$ 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$_3$O$_4$/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
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For the synthesis of 2-(prop-2-yn-1-yloxy)naphthalene-1,4-dione, 2-hydroxynaphthalene-1,4-dione (1 mmol) and K$_2$CO$_3$ (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$_2$O and EtOAc (4 × 10 mL). The organic layer was dried using anhydrous Na$_2$SO$_4$, 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$_2$CO$_3$ (1.2 mmol) were combined with 20 mg of Fe$_3$O$_4$/AlZn-Cu catalyst and added to a mixture of EtOH-H$_2$O-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$_2$O and EtOAc (4 × 10 mL). The organic layer was dried using anhydrous Na$_2$SO$_4$. The purification of the compound was done using silica gel. The catalyst was washed with acetone and ethanol and reused.
2. Figures

Fig. S1. FT-IR spectrum of preparation of the catalyst
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Figure S2. SEM images of AlZn-Cu (A, B), Fe₃O₄@AlZn-Cu before furnace (C), Fe₃O₄@AlZn-Cu after furnace (D) EDS images of FeO₄@AlZn-Cu (E) AlZn-Cu (F) Element Mapping (G)

2. SEM images of AlZn-Cu (A, B), Fe₃O₄@AlZn-Cu before furnace (C), Fe₃O₄@AlZn-Cu after furnace (D) EDS images of FeO₄@AlZn-Cu (E) AlZn-Cu (F) Element Mapping (G)
Figure S3. XRD pattern of AlZn-Cu (A), Fe$_3$O$_4$/AlZn-Cu (B) TGA of AlZn-Cu(Green), and Fe$_3$O$_4$/AlZn-Cu(Blue) (C)
Fig. S4. TEM images of AlZn-Cu(A), Fe₃O₄/AlZn-Cu(B) N₂ adsorption-desorption isotherms of AlZn-Cu, and Fe₃O₄@AlZn-Cu(C)
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Fig. S5 VSM curve of Fe$_3$O$_4$/AlZn-Cu (A) UV–Vis diffuse reflectance of Al-Zn, AlZn-Cu, and Fe$_3$O$_4$/AlZn-Cu (B) The obtained band gaps from the curves of $(ahv)^2$ versus $hv$ for Al-Zn (Red), AlZn-Cu (Green), and Fe$_3$O$_4$/AlZn-Cu (Blue) (C) Photo-luminescence spectra of Al-Zn(green), AlZn-Cu(Red), and Fe$_3$O$_4$/AlZn-Cu(Yellow) (D)
Fig. S6 the cyclic voltammogram of K$_3$Fe(CN)$_6$/K$_4$Fe(CN)$_6$ in the dark and light using Fe$_3$O$_4$/AlZn-Cu as photocatalyst (A)

EIS Response of L$_2$S-M: Fe$_3$O$_4$/AlZn-Cu at 0.3 V light and dark (B) The comparative of the cyclic voltamgram of K$_3$Fe(CN)$_6$/K$_4$Fe(CN)$_6$ using Fe$_3$O$_4$/AlZn-Cu and AlZn-Cu as photocatalyst in light (C) Comparative Nyquist plots of AlZn-Cu and Fe$_3$O$_4$/AlZn-Cu at 0.3V in light (D)

Fig. S7 Mott - Schottky plots of AlZn, AlZnCu, and Fe$_3$O$_4$/AlZn-Cu at 500 Hz (A) Proposed photoexcited band gap energy for the AlZn, AlZn-Cu, and Fe$_3$O$_4$/AlZn-Cu with Mott – Schottky test (B)
Fig. S8. X-ray photoelectron spectroscopy (XPS) survey spectrum of AlZn-Cu, and Fe$_3$O$_4$/AlZn-Cu (A and B), X-ray photoelectron spectroscopy (XPS) expand of ZnO, (C and D), X-ray photoelectron spectroscopy (XPS) expand of Al$_2$O$_3$(E and F), X-ray photoelectron spectroscopy (XPS) expand of carbon(I and J).
Proposed Mechanism:

Previous studies have reported successfully reducing 3d transition metals\textsuperscript{1-3} using photocatalytic substrates as co-catalysts\textsuperscript{4-9}. In this study, a new photocatalyst (PC) in the form of ZnAl\textsubscript{2}O\textsubscript{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\textsubscript{2}O\textsubscript{4} LDH exhibited photo-induced electron transfer (PET)\textsuperscript{10}. It is proposed that PC reduces copper, a process previously observed with ascorbic acid or natural compounds\textsuperscript{11} and subsequently facilitates the click
reaction\textsuperscript{12}. However, when TEMPO was introduced into the reaction, the catalyst activity was inhibited, indicating that TEMPO halted the LDH photocatalysis\textsuperscript{13}.

Fig. S\textsubscript{11} Evaluation of proposed mechanisms for catalysis
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,
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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 C₂₁H₁₆N₄O₄ (387): C, 64.94; H: 4.15; N, 14.43 Found: C, 64.98 H: 4.19; N, 14.40.

Fig. S₁₃: HNMR of 3a
Fig. S14 $^{13}$C-NMR of 3a

Fig. S15 Mass spectroscopy of 3a
Supplementary Material

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-\(d_6\)) \(\delta\) (ppm) 5.29 (s, 2H, N-\(\text{CH}_2\)), 5.29 (s, 2H, N-\(\text{CH}_2\)), 5.51 (s, 2H, O-\(\text{CH}_2\)), 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); \(^1\)C NMR (100 MHz, DMSO-\(d_6\)) \(\delta\) (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 cm\(^{-1}\); m/z: 424.


Fig. S\(_{16}\) \(^1\)HNMR of 3b
Fig. S17 $^{13}$C NMR 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-$d_6$) $\delta$ (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-$d_6$) $\delta$ (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

Fig. S_{19} \textsuperscript{1}HNMR of 3c

4 Cl

Fig. S_{20} \textsuperscript{13}CNMR of 3c
N-(3-bromophenyl)-2-(4-((1,4-dioxo-1,4-dihydropyrene-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-$d_6$) $\delta$ (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-$d_6$) $\delta$ (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
Supplementary Material


Fig. S22/HNMR of 3d
N-(4-bromophenyl)-2-(4-((1,4-dioxo-1,4-dihydronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-ylacetamide (3e): Yellow solid; isolated yield: 79%, m.p.: 245-247 °C; ¹H NMR (400 MHz, DMSO-d₆) δ (ppm) 5.29 (s, 2H, N-CH₂), 5.40 (s, 2H, O-CH₂), 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); ¹³C NMR (100 MHz, DMSO-d₆) δ (ppm) 52.72, 62.82, 111.38, 115.89, 121.61, 126.05, 126.61, 127.71,
Supplementary Material


Fig. S₂₅ ¹HNMR 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
Supplementary Material

(s, 1H, C-H, Triazole), 1075 (s, 1H, NH); $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ (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, 1717, 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$_5$O$_6$: C, 58.20; H: 3.49; N, 16.16 Found: C, 58.18 H: 3.47; N, 16.13.

Fig. S31: $^1$H NMR 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-$d_6$) $\delta$ (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-$d_6$) $\delta$ (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,
Supplementary Material


Fig. S₃ ¹H NMR of 3g
Fig. S32: $^{13}$CNMR of 3g
Supplementary Material

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-$d_6$) $\delta$ (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-$d_6$) $\delta$ (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, 1430, 1278, 1175, 1049, 911, 786 cm$^{-1}$ Mass (M/Z:20ev):402

Fig. S4 $^1$HNMR of 3h

Fig. S5 $^{13}$CNMR 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-$d_6$) $\delta$ (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, $J = 8.0, 0.8$ Hz, 2H, ArH), 8.38 (s, 1H, C-H, Triazole), 10.29 (s, 1H, NH). $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ (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$_5$O$_6$ (447): C, 59.06; H: 3.83; N, 15.65 Found: C, 59.04 H: 3.81; N, 15.63.
Fig. S2: $^1$H NMR of 3i

Fig. S3: $^{13}$C NMR 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-$d_6$) $\delta$ (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-$d_6$) $\delta$ (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$_4$O$_4$ (436): C, 60.49; H: 3.92; N, 12.83 Found: C, 60.52 H: 3.91; N, 12.83.
Fig. S40 1H NMR of 3j

Fig. S41 13C NMR of 3j
**N-(2,4-difluorophenyl)-2-(4--((1,4-dioxo-1,4-dihydrophtalaln-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-$d_6$) $\delta$ (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-$d_6$) $\delta$ (ppm), 52.39, 62.80, 104.79 (d, $J_{C-F} = 27$ Hz, ArCH), 111.36, 111.78 (d, $J_{C-F} = 22$, ArCH), 122.45 125.70 126.03, 126.58, 127.73, 131.28, 131.93, 134.14, 134.99, 141.10, 155.23 (d, $J_{C-F} = 130$Hz, ArCH), 159.12 (d, $J_{C-F} = 130$Hz, 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$_2$N$_4$O$_4$ (424): C, 59.44; H: 3.33; N, 13.20 Found: C: 59.42 H: 3.31; N, 13.19.
Fig. S41 $^1$HNMR of 3k

Fig. S42 $^{13}$CNMR of 3k
N-(3-chloro-4-fluorophenyl)-2-(4-((1,4-dioxo-1,4-dihyronaphthalen-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) $\delta$ (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) $\delta$ (ppm), 52.64, 62.81, 111.38, 117.67 (d, $J_{C-F} = 22$ Hz, ArCH), 119.78 (d, $J_{C-F} = 18$ Hz, ArC$_q$), 120.05 (d, $J_{C-F} = 7$ Hz, ArCH), 121.16, 126.04, 126.59, 127.72, 131.28, 131.93, 134.14, 135.00, 136.09, 141.10, 158.41, 159.43, 165.02, 179.97, 185.03; IR (KBr) 3595, 3276, 3089, 1922, 1788, 1687, 1572, 1499, 1343, 1141, 1082, 1011, 967, 853, 737 cm$^{-1}$; Mass (M/Z:20ev):442 Anal. calcd for C$_{21}$H$_{14}$ClF$_{13}$N$_4$O$_4$: C, 57.22; H: 3.20; N, 12.71 Found: C, 57.20 H: 3.17; N, 12.74.
Fig. S46 HNMR of 31

Fig. S47 13CNMR of 31
N-benzyl-2-((1,4-dioxo-1,4-dihyronaphthalen-2-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)acetamide (3m):
Cream solid; isolated yield: 67%, m.p.: 218-220°C; 1H NMR (400 MHz, DMSO-\textit{d}_6) \delta (ppm) 4.34 (d, \textit{J} = 6 Hz, 2H, NH-\textit{CH}_2), 5.23 (s, 2H, N-\textit{CH}_2), 5.27 (s, 2H, O-\textit{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, \textit{J} = 8.2, 0.8 Hz, 2H, ArH), 8.31 (s, 1H, C-H, Triazole), 8.86 (t, \textit{J} = 5.6 Hz, 1H, NH); 13C NMR (100 MHz, DMSO-\textit{d}_6) \delta (ppm) 42.85, 52.10, 62.81, 111.37, 126.04, 126.60, 127.49, 127.59, 127.88, 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\textsuperscript{-1}; Mass (M/Z:20ev): 402 Anal. calcd for C\textsubscript{22}H\textsubscript{18}N\textsubscript{4}O\textsubscript{4} (402): C, 65.66; H, 4.51; N, 13.92 Found: C, 65.65; H, 4.50; N, 13.90
Supplementary Material

Fig. S_{49} \textsuperscript{1}H NMR of 3m

Benzy1 Amine

Fig. S_{50} \textsuperscript{13}C NMR 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). 13C 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_{4}O_{4}: C, 66.34; H, 4.84; N, 13.45; Found: 66.33; H, 4.85; N, 13.44
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) $\delta$ 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) $\delta$ 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$_4$O$_4$: C, 59.06; H, 3.83; N, 15.65 Found: C, 59.05; H, 3.82; N, 15.68.
Fig. S5 \( ^1 \text{HNMR} \) of 3o
Fig. S_{56}^{13}CNMR 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) \(\delta\) 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). \(^1\)C NMR (101 MHz, DMSO) \(\delta\) 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. S58 ¹H NMR of 3p

Fig. S59 ¹³C NMR of 3p
Fig. S6. 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 ¹H NMR (400 MHz, DMSO) δ 10.00 (s, 1H), 8.37 (s, 1H), 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). ¹³C 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 C₂₁H₁₅IN₄O₄ (514) C, 49.05; H: 2.94; N, 10.89 Found: C, 49.03 H: 2.95; N, 10.92.
Fig. S61: 1H NMR of 3q
Fig. S6: 13CNMR 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

1H NMR (400 MHz, DMSO) \( \delta \) 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)

13C 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\(_{15}\)IN\(_4\)O\(_4\): C, 49.05; H, 2.94; N, 10.89

Found: C, 49.07 H, 2.92; N, 10.91
Supplementary Material

Fig. S64 1HNMR of 3r

Fig. S65 13CNMR of 3r
Supplementary Material

Fig. S6. 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.

5. References

Supplementary Material