Diversity-oriented synthesis of 1*H*-1,2,3-triazole tethered pyrazolo[5,1-b]quinazoline hybrids as antimicrobial agents and DFT study

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Supporting Information

Table of Contents

1. General Information.

All commercially available starting materials were purchased from Sigma-Aldrich and used without further purification. ^{1}H and ^{13}C NMR spectra were collected at 500 MHz and 125 MHz, on a Bruker Avance NEO spectrometer using DMSO-d_6 as solvent. Chemical shifts (δ) and coupling values (J) were given in parts per million (ppm) and in Hz respectively. Mass spectra were recorded on Shimadzu LCMS2020 mass spectrometer and the spectra were interpreted. Elemental analysis was carried out using EURO EA3000 elemental analyser instrument. Melting points were recorded on an ANALAB melting point apparatus and is uncorrected. Thin-layer chromatography (TLC) was performed using silica gel 60 F_{254} of 0.2 mm thickness (Merck) plates.

2. General procedure for the synthesis of pyrazolo[5,1-b]quinazolines 5(a-j)

Ethyl 5-amino-1*H*-pyrazole-4-carboxylate **[1; 1.0 mmol]**, dimedone or 1,3-cyclohexanedione **[2(a-b); 1.0 mmol]**, aromatic aldehyde **[3(a-f); 1.0 mmol]**, and TBAB **(10 mol %)**, in ethanol **(4 mL)** was poured into a 50-mL round bottom flask and heated in an oil bath at 60 ^{o}C temperature for the stipulated period and followed by addition of propargyl bromide **[4; 1.2 mmol]** and K_2CO_3 **(2.5 mmol)** in order to synthesize our target compound. The consumption of the starting material was monitoring by TLC (EtOAc : hexane, 5:5 v/v). Using a simple workup, the resulting reaction mixture was diluted with 5 mL water and solid mass was precipitated out. Then the precipitated solid was washed with water followed by EtOH (95 %) and dried under vacuum to obtain the pure products **5(a-j)** in excellent yields without any further purification, each of the synthesized compounds was distinguish by ^{1}H NMR, ^{13}C NMR, mass spectra and elemental analysis.

3. General procedure for the synthesis of 1H-1,2,3-triazole tethered pyrazolo[5,1-b]quinazoline hybrids 7(a-t)

An equimolar mixture of pyrazolo[5,1-b]quinazoline **[5(a-j); 1.0 mmol]**, substituted phenyl azides **[6(a-e); 1.0 mmol]** in 5 mL of H_2O was taken in a 50-mL round-bottomed flask. An aqueous solution of $CuSO_4.5H_2O$ **(10 mol %)** and sodium ascorbate **(20 mol %)** were added to it at room temperature and the mixture was starred for 30-40 min. The progress of the reaction was monitored by TLC (EtOAc : hexane, 7:3 v/v). After completing of the reaction, ice cold water (50 mL) was added to the reaction mixture. The precipitate thus formed was collected by filtration and washed with methanol to give targeted **7(a-t)** compounds. The products were characterized by ^{1}H NMR, ^{13}C NMR, mass spectra, and elemental analysis.

1. Scanned copies of ^{1}H NMR, ^{13}C NMR, and MS spectra for all compounds

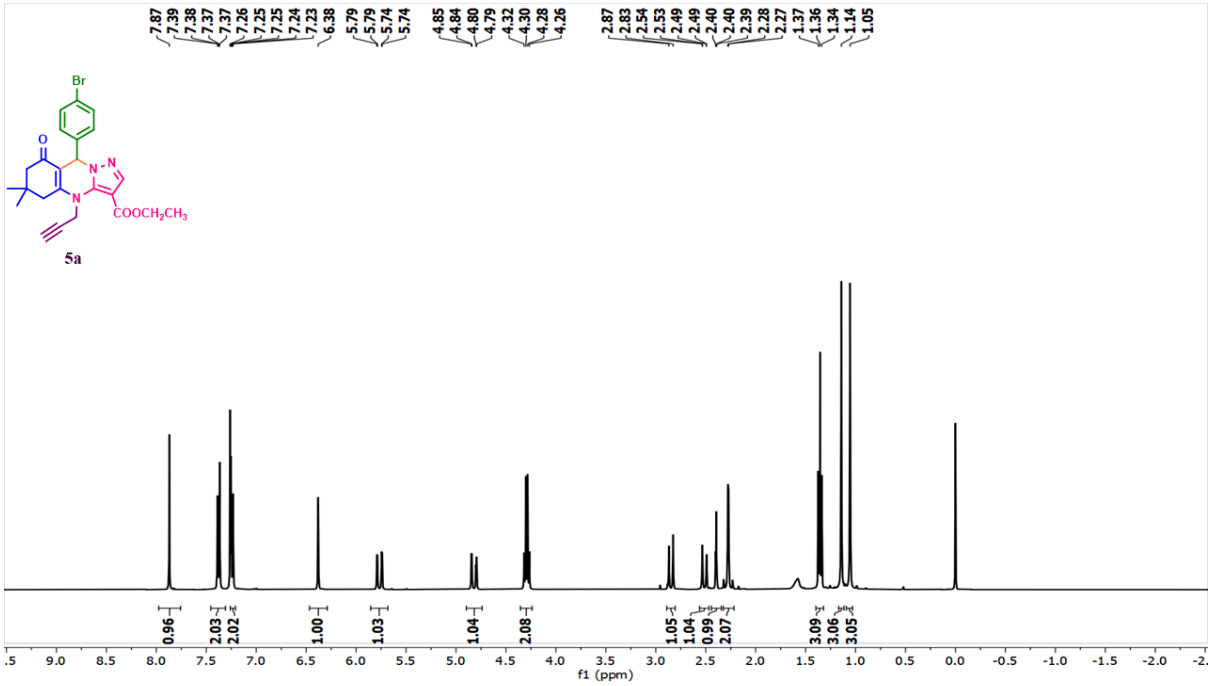

Figure S01. ^{1}H NMR spectrum of ethyl 9-(4-bromophenyl)-6,6-dimethyl-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5a).**

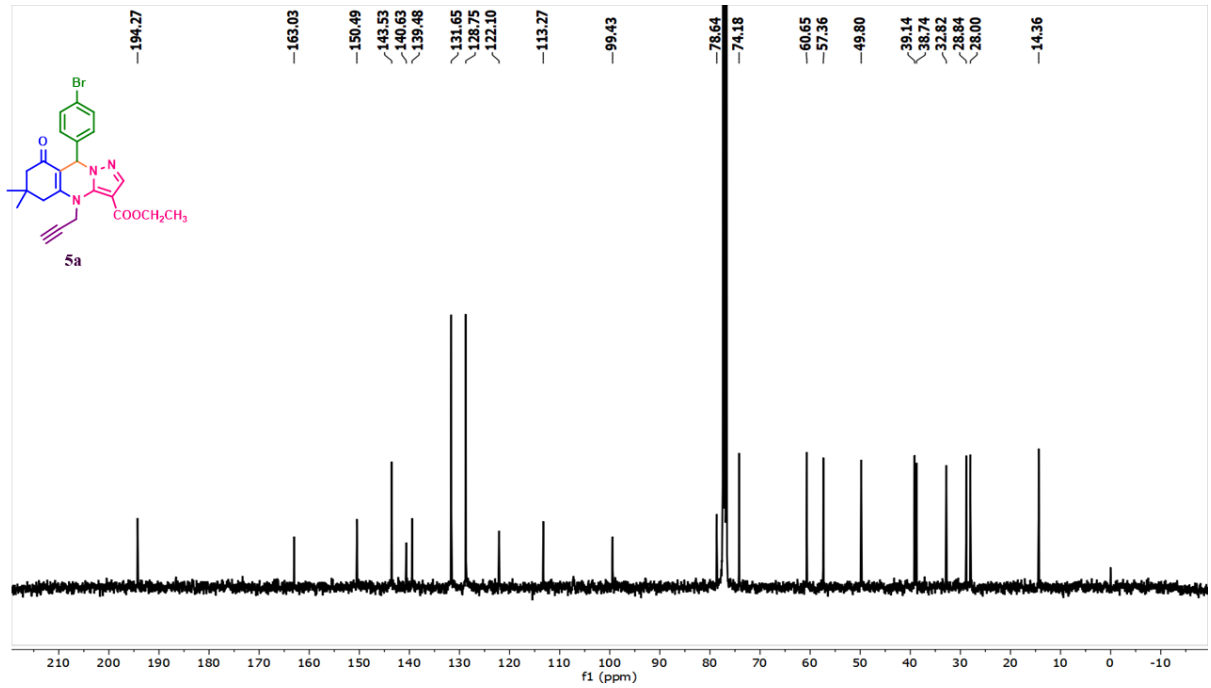

Figure S02. ^{13}C NMR spectrum of ethyl 9-(4-bromophenyl)-6,6-dimethyl-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5a).**

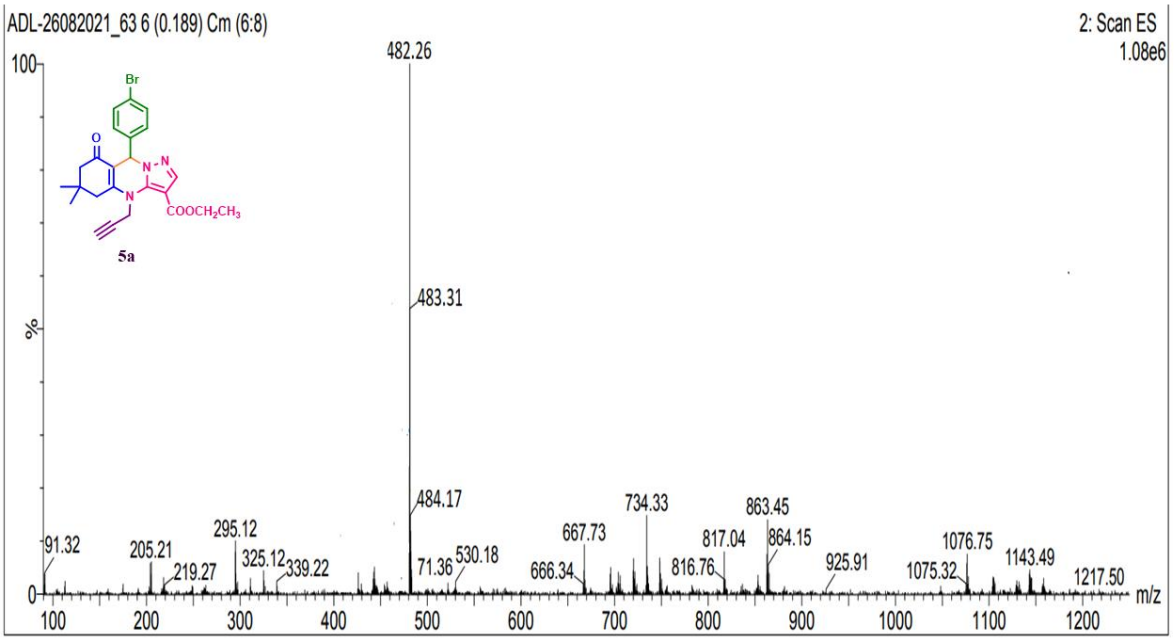

Figure S03. Mass spectrum of ethyl 9-(4-bromophenyl)-6,6-dimethyl-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5a).**

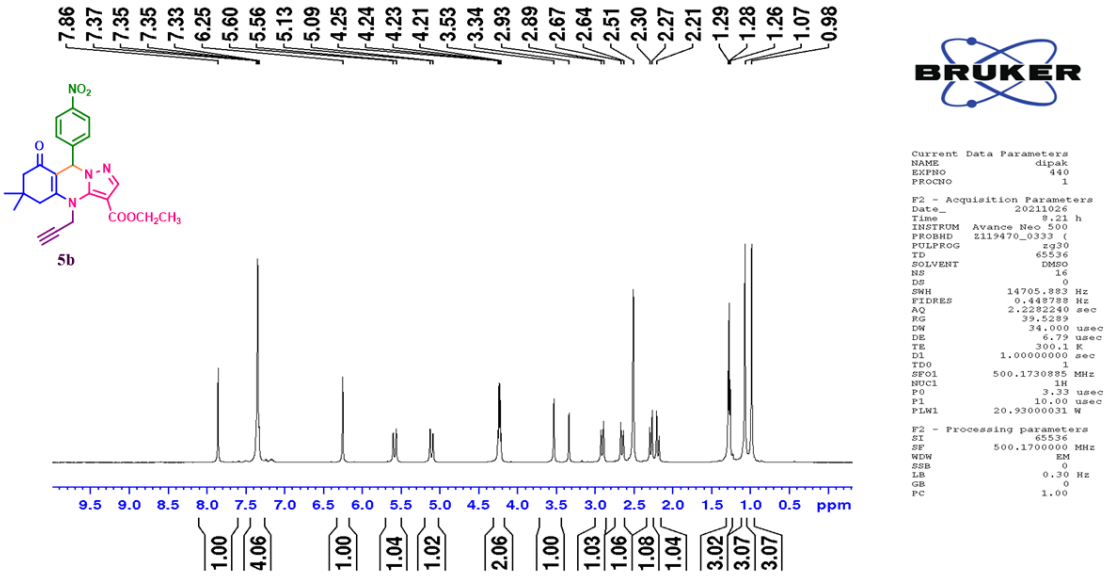

Figure S04. [1]H NMR spectrum of ethyl 6,6-dimethyl-9-(4-nitrophenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate ***(5b)*.**

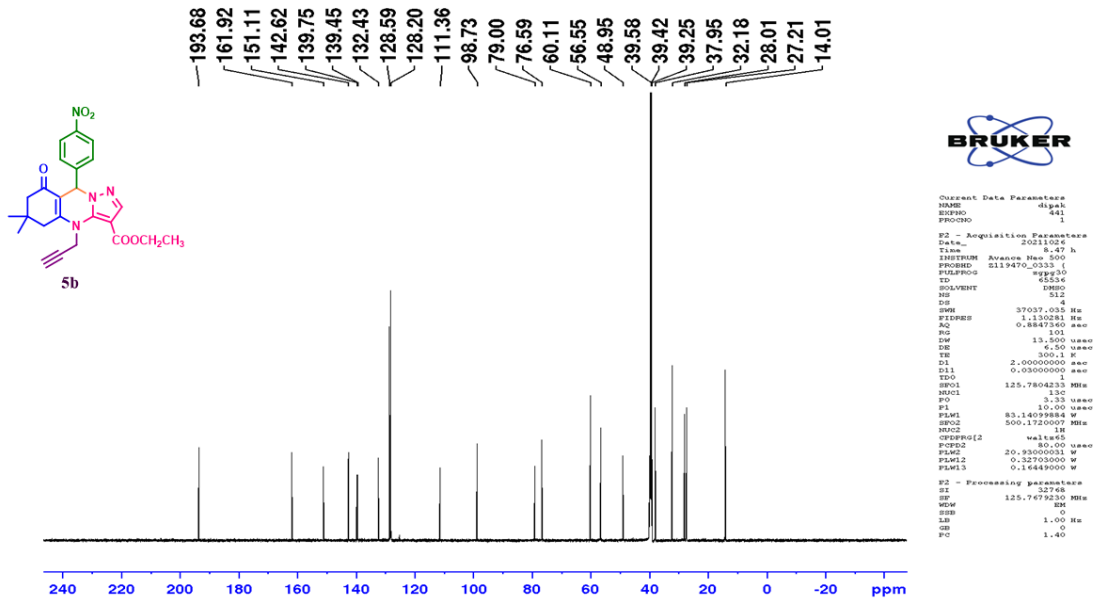

Figure S05. ^{13}C NMR spectrum of ethyl 6,6-dimethyl-9-(4-nitrophenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate ***(5b)*.**

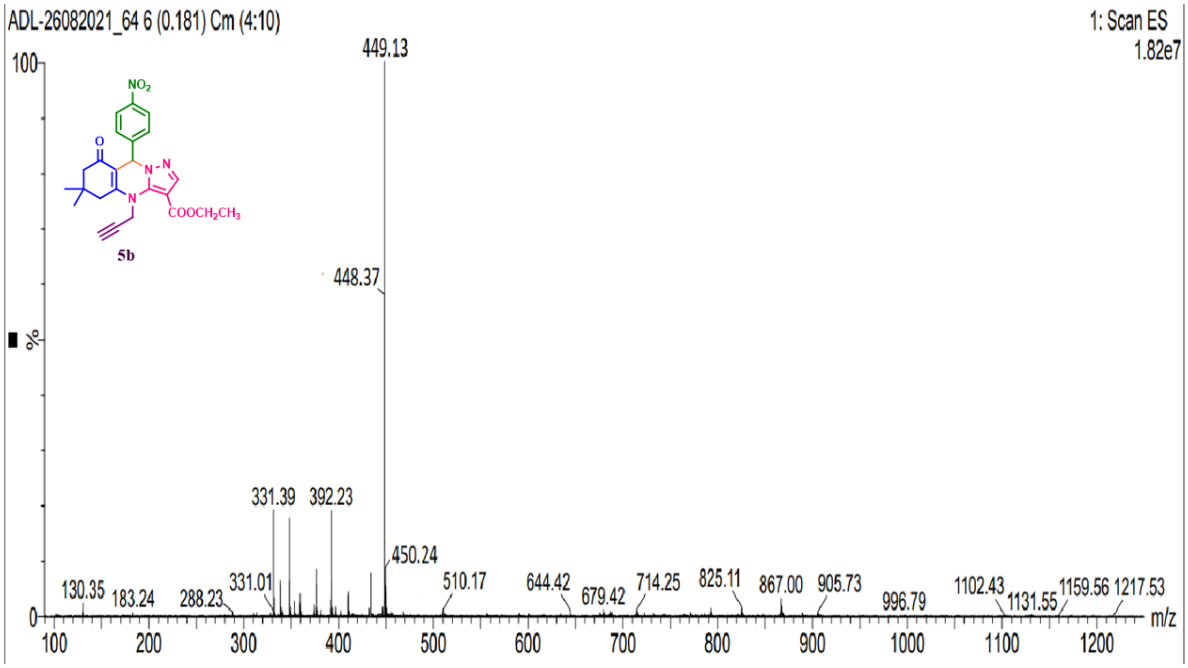

Figure S06. Mass spectrum of ethyl 6,6-dimethyl-9-(4-nitrophenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate ***(5b)*.**

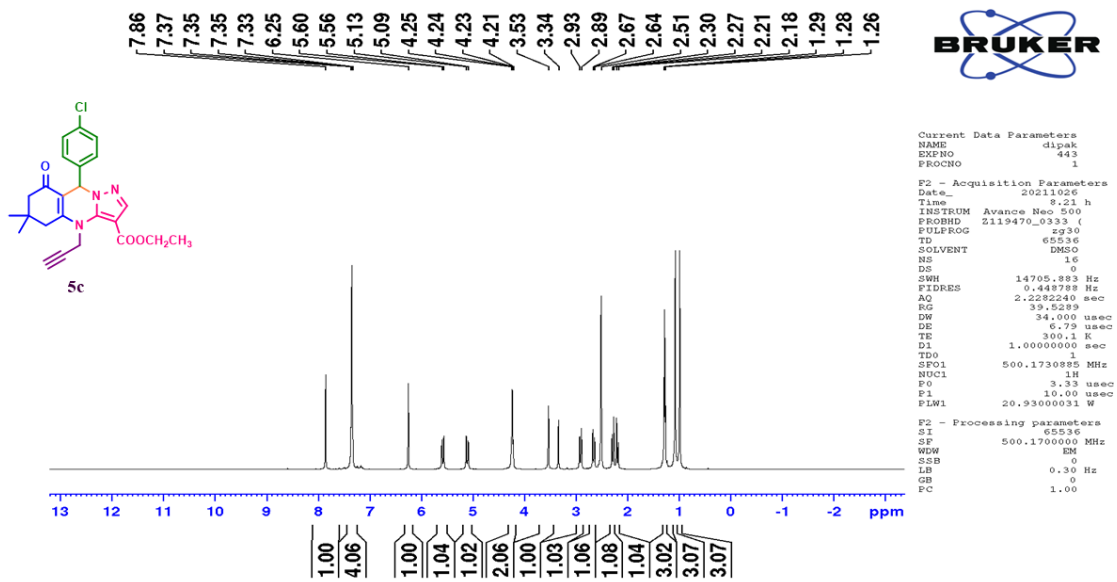

Figure S07. [1]H NMR spectrum of ethyl 9-(4-chlorophenyl)-6,6-dimethyl-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate ***(5c)*.**

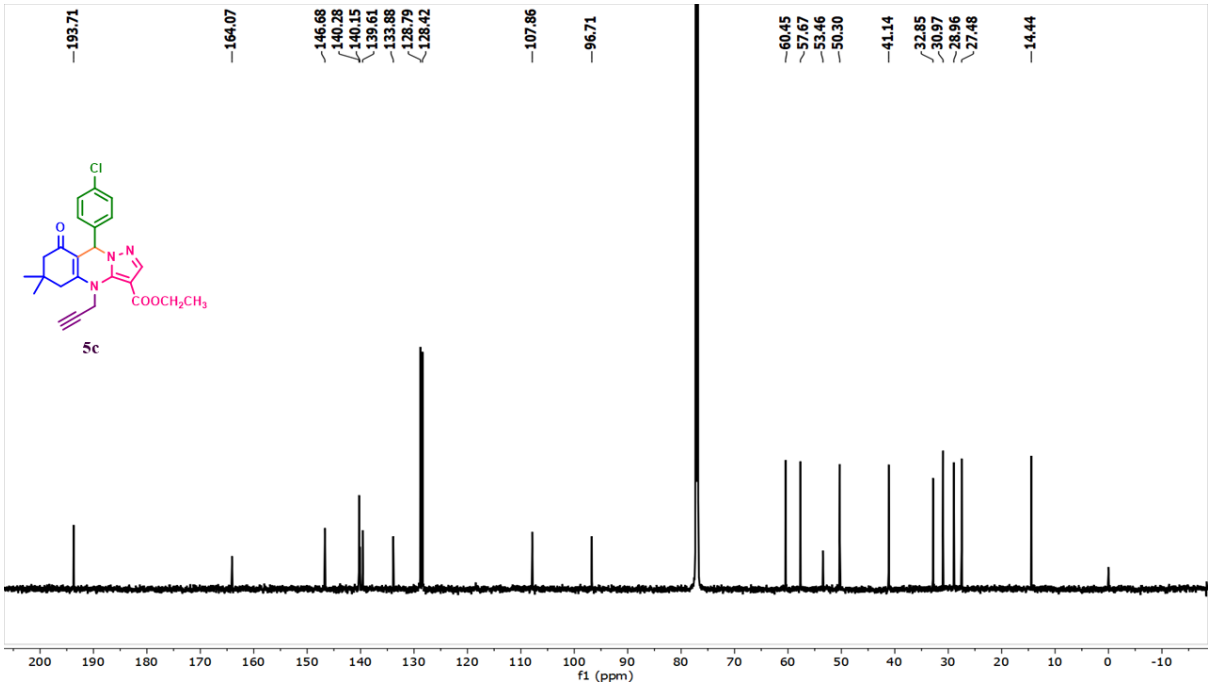

Figure S08. [13]C NMR spectrum of ethyl 9-(4-chlorophenyl)-6,6-dimethyl-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate ***(5c)*.**

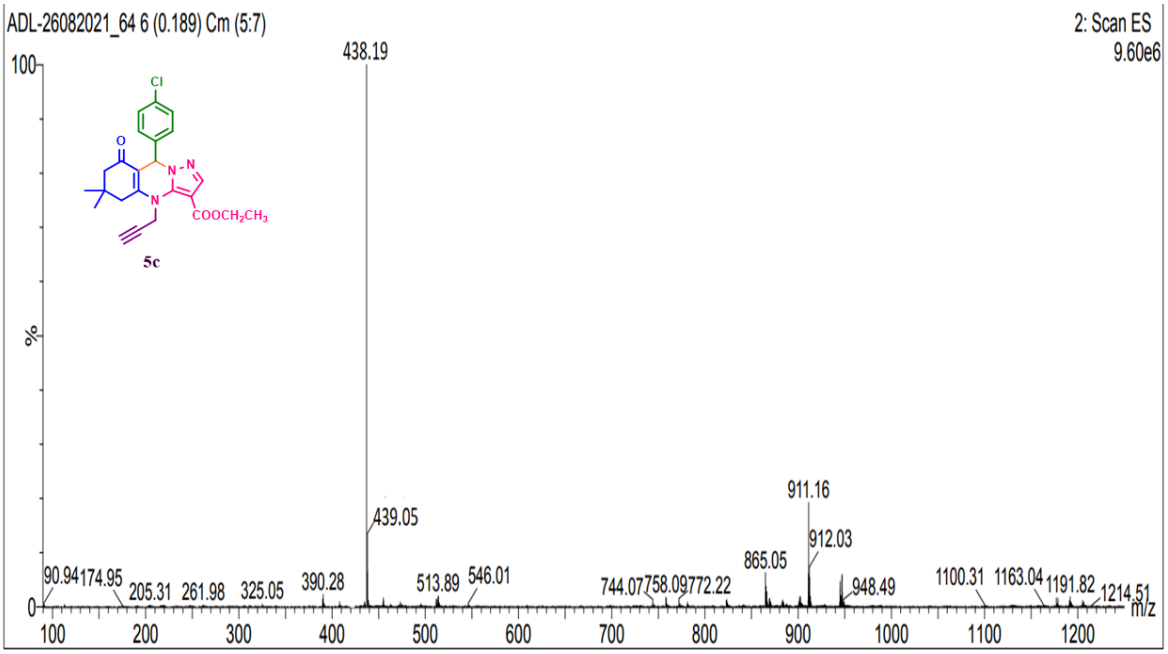

Figure S09. Mass spectrum of ethyl 9-(4-chlorophenyl)-6,6-dimethyl-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate ***(5c)*.**

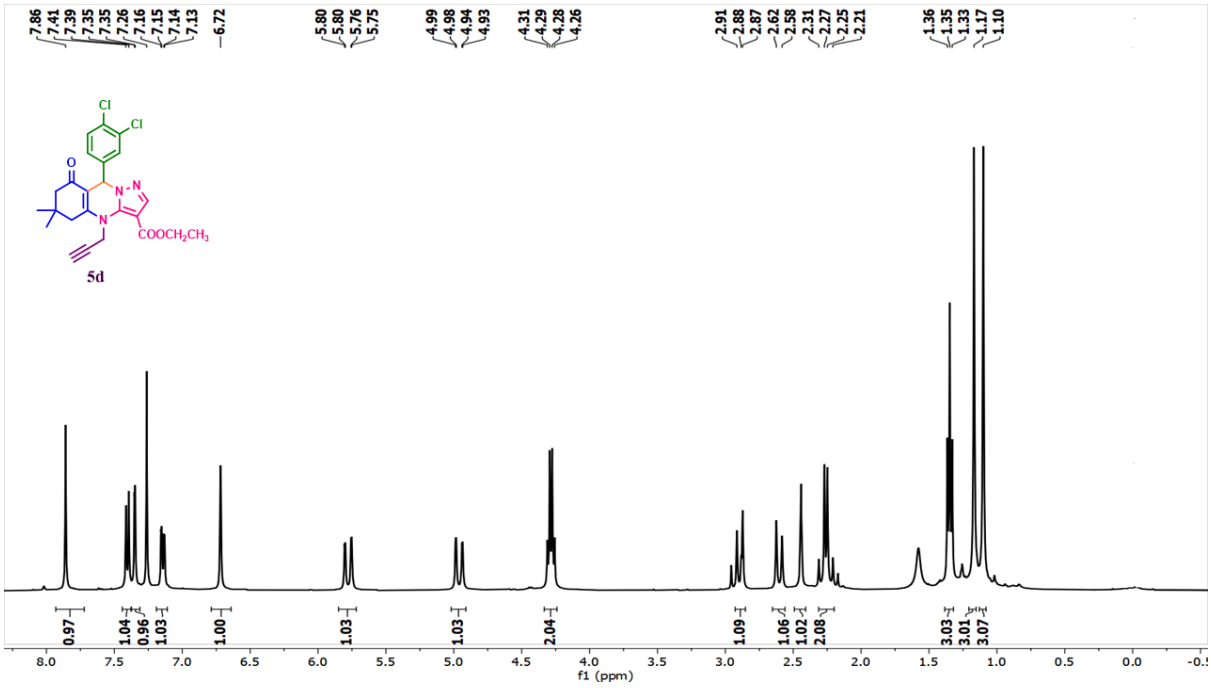

Figure S10. ^{1}H NMR spectrum of ethyl 9-(3,4-dichlorophenyl)-6,6-dimethyl-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5d).**

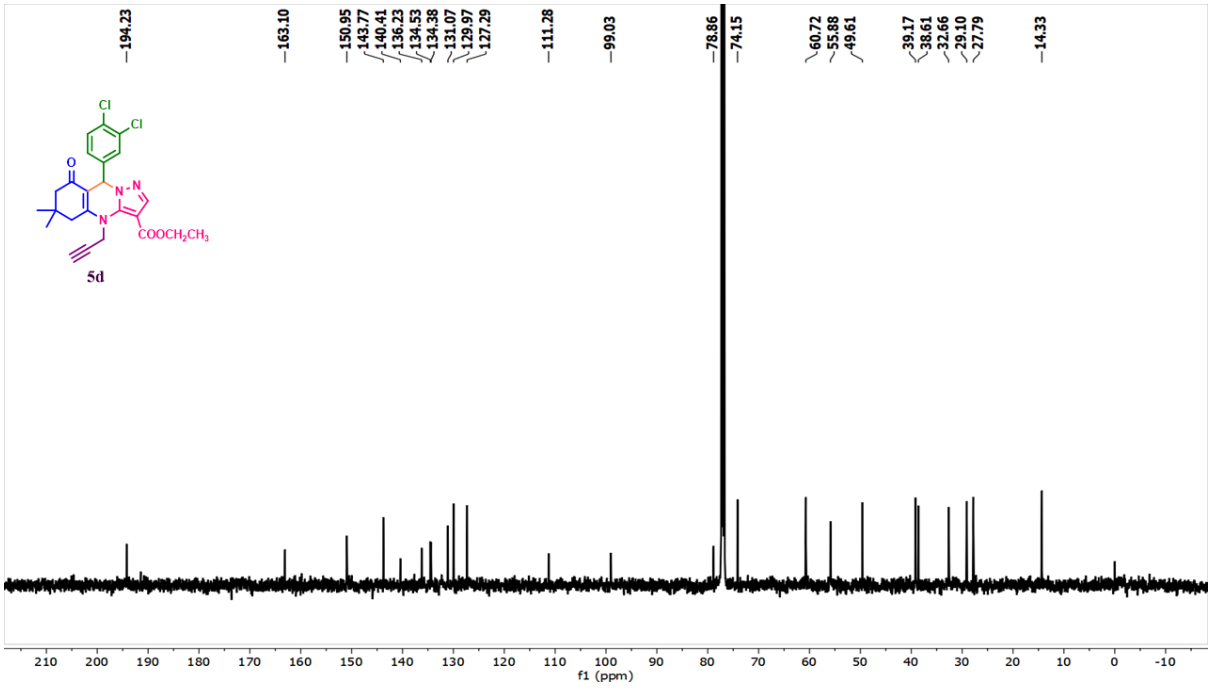

Figure S11. ^{13}C NMR spectrum of ethyl 9-(3,4-dichlorophenyl)-6,6-dimethyl-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5d).**

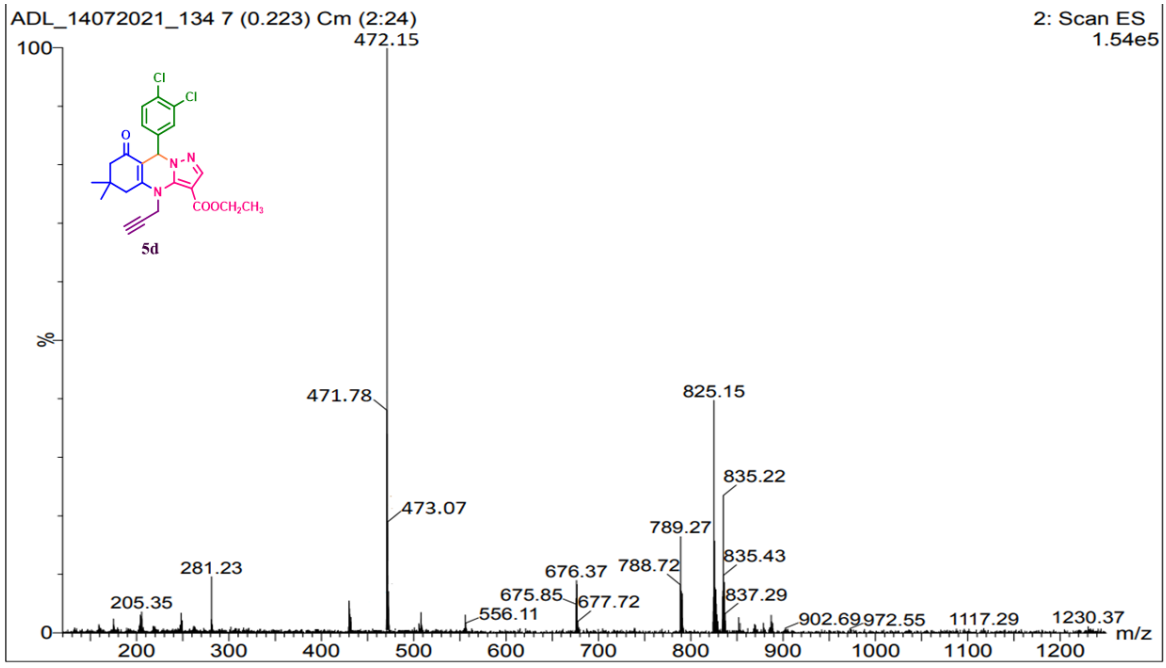

Figure S12. Mass spectrum of ethyl 9-(3,4-dichlorophenyl)-6,6-dimethyl-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5d).**

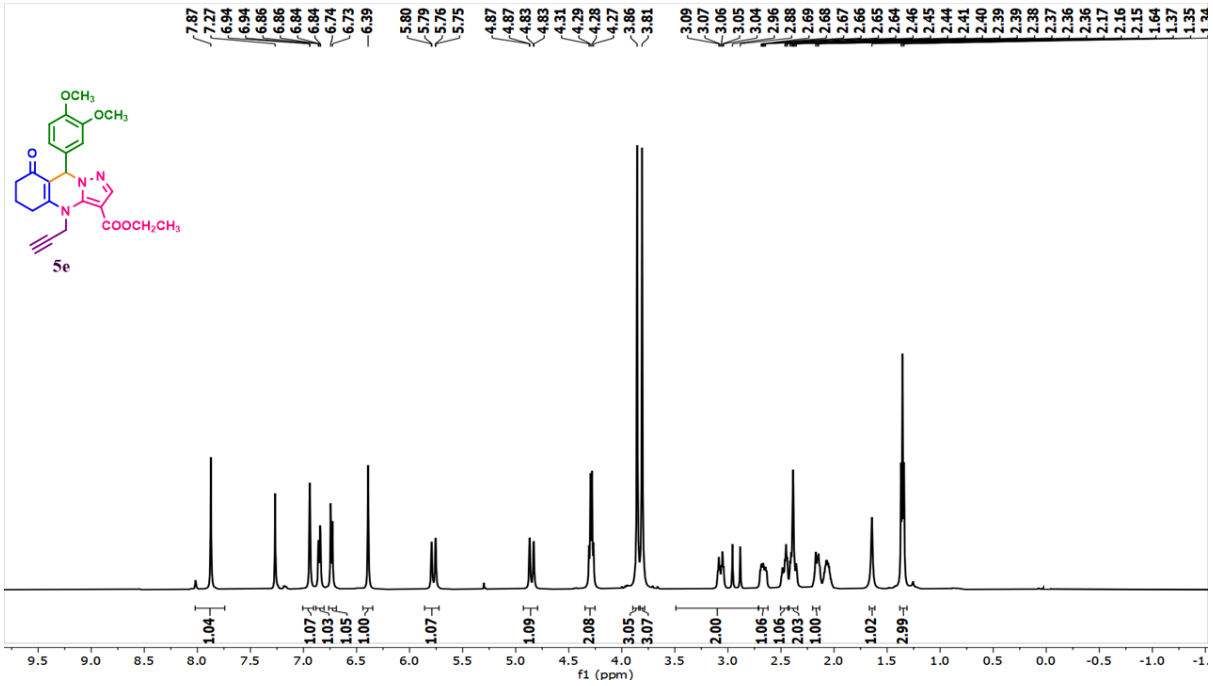

Figure S13. [1]H NMR spectrum of ethyl 9-(3,4-dimethoxyphenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5e).**

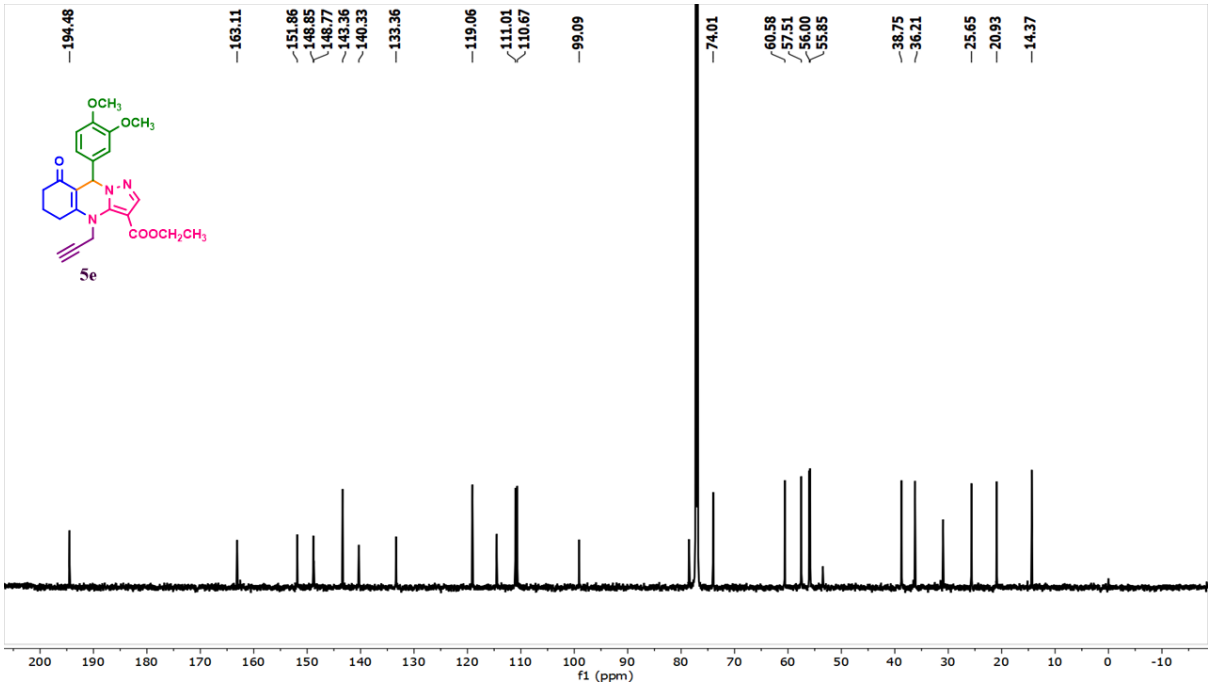

Figure S14. [13]C NMR spectrum of ethyl 9-(3,4-dimethoxyphenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5e).**

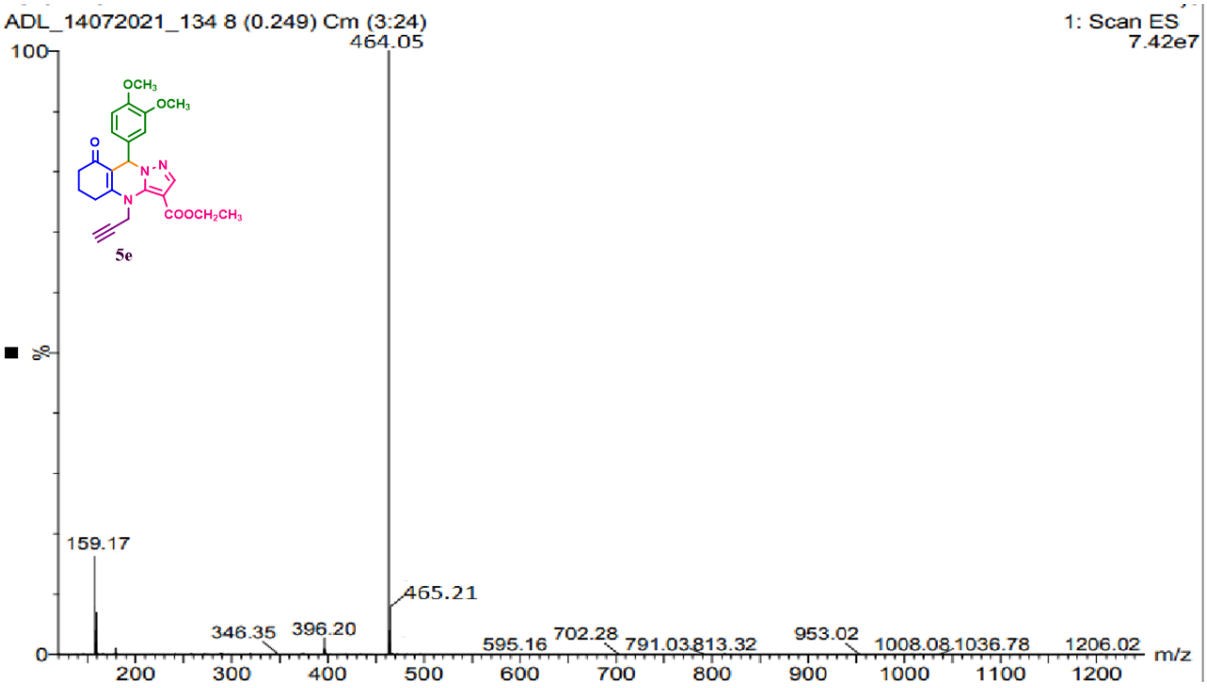

Figure S15. Mass spectrum of ethyl 9-(3,4-dimethoxyphenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5e).**

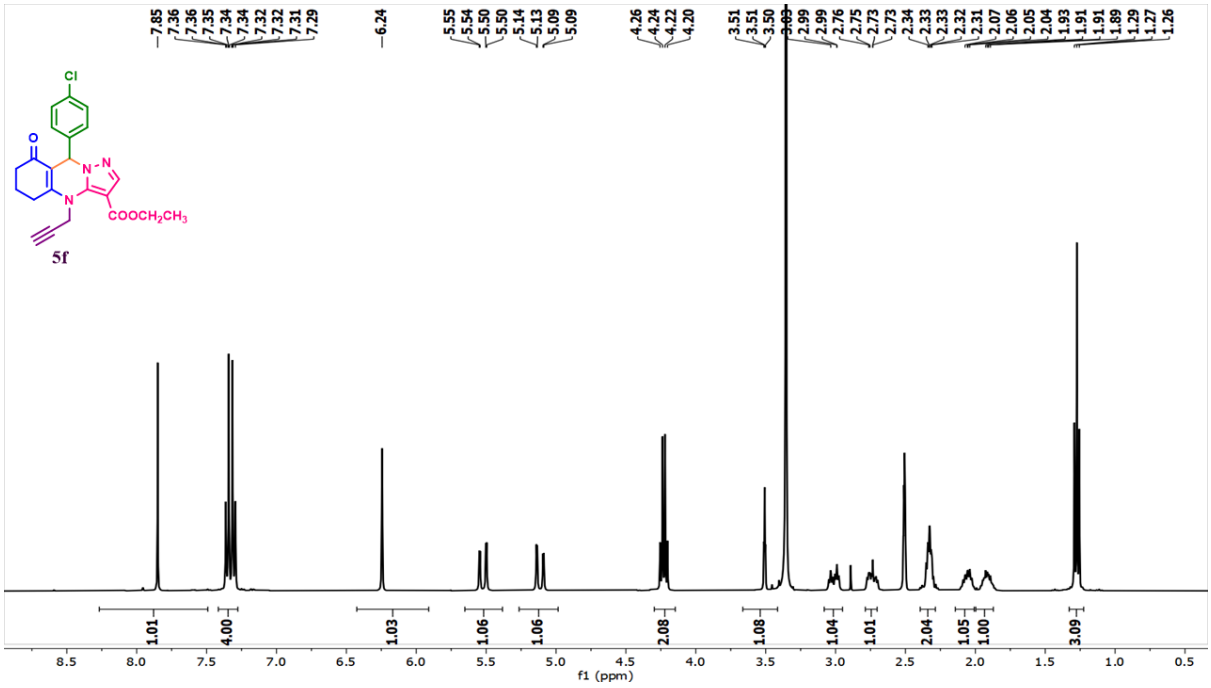

Figure S16. ^{1}H NMR spectrum of ethyl 9-(4-chlorophenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5f).**

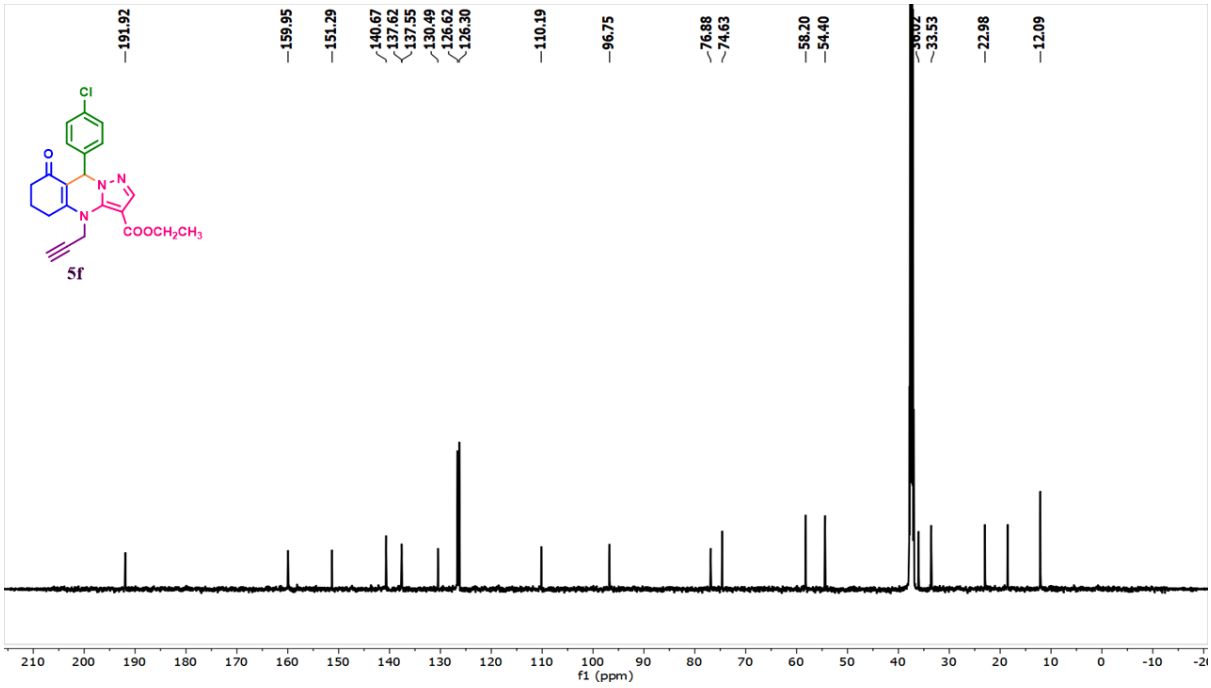

Figure S17. ^{13}C NMR spectrum of ethyl 9-(4-chlorophenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5f).**

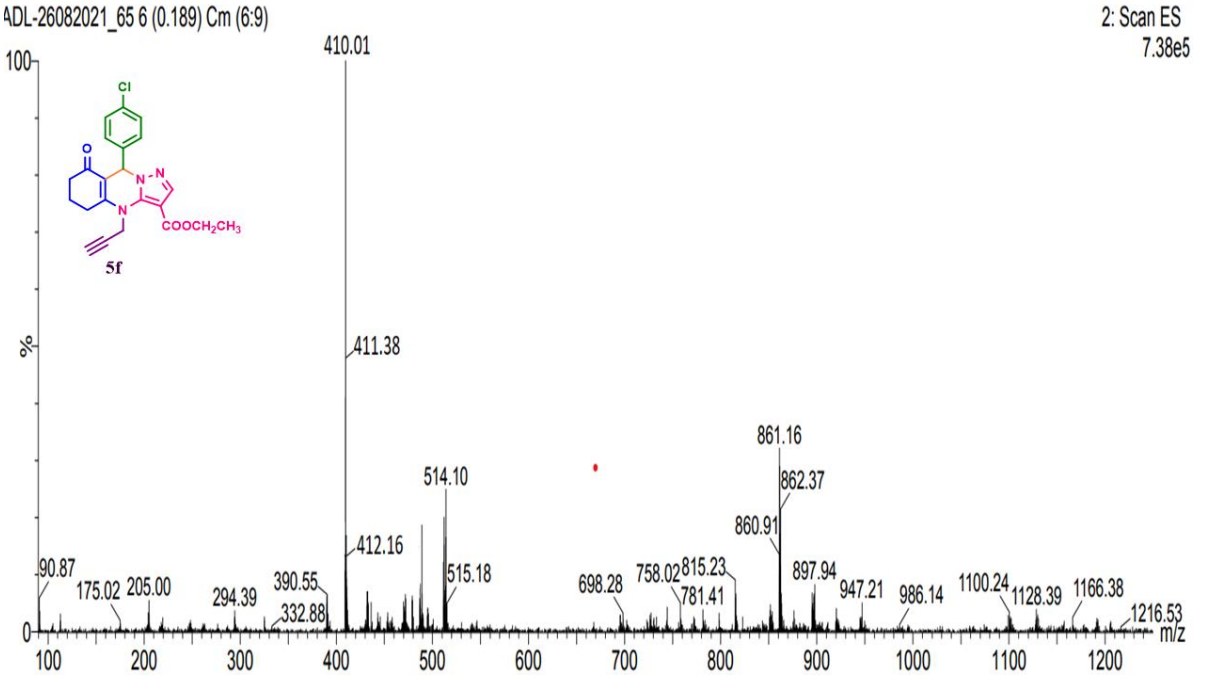

Figure S18. Mass spectrum of ethyl 9-(4-chlorophenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5f).**

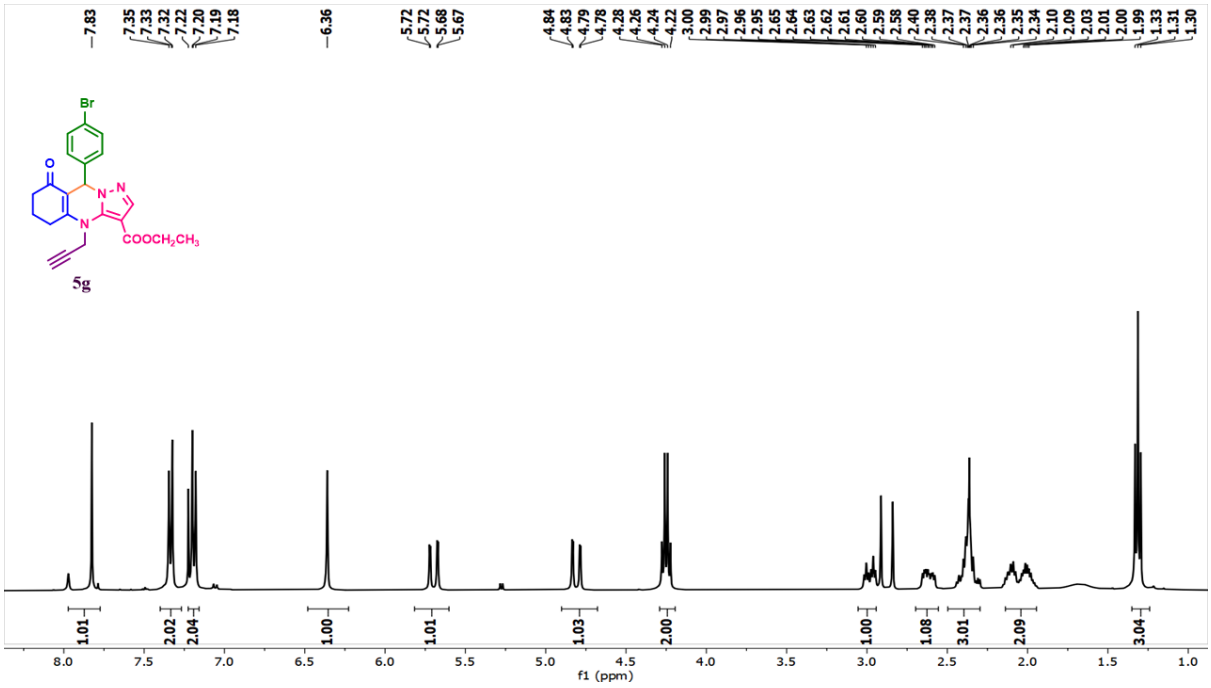

Figure S19. ^{1}H NMR spectrum of ethyl 9-(4-bromophenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5g).**

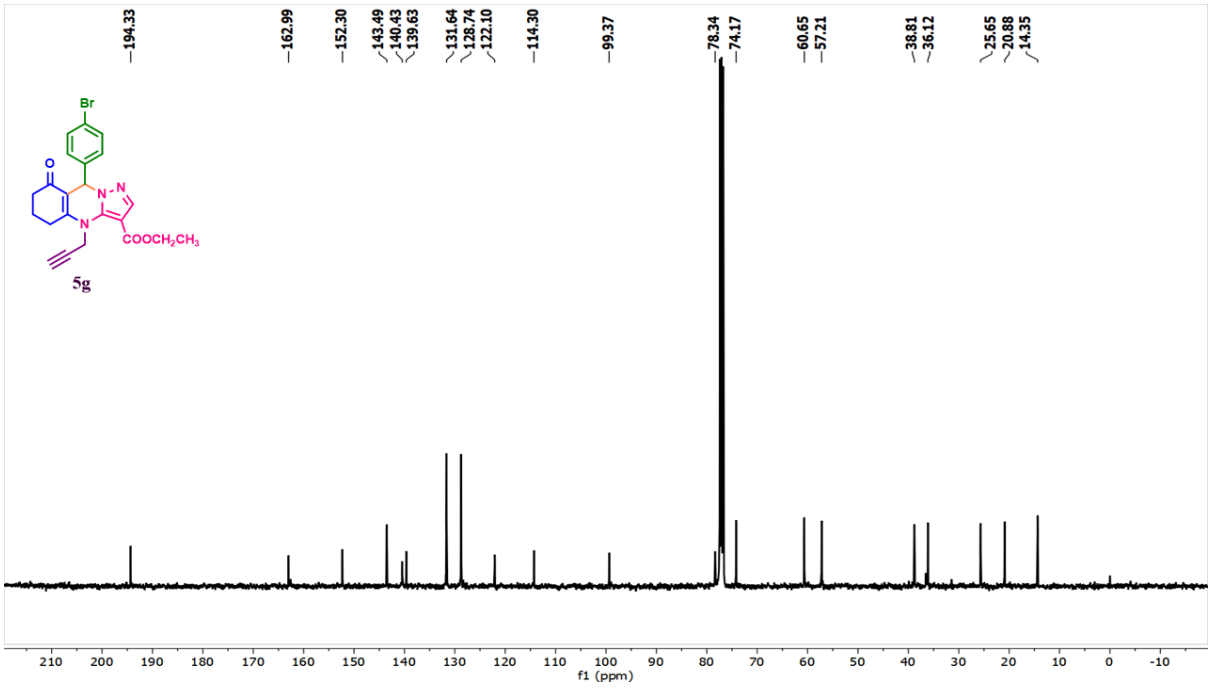

Figure S20. ^{13}C NMR spectrum of ethyl 9-(4-bromophenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5g).**

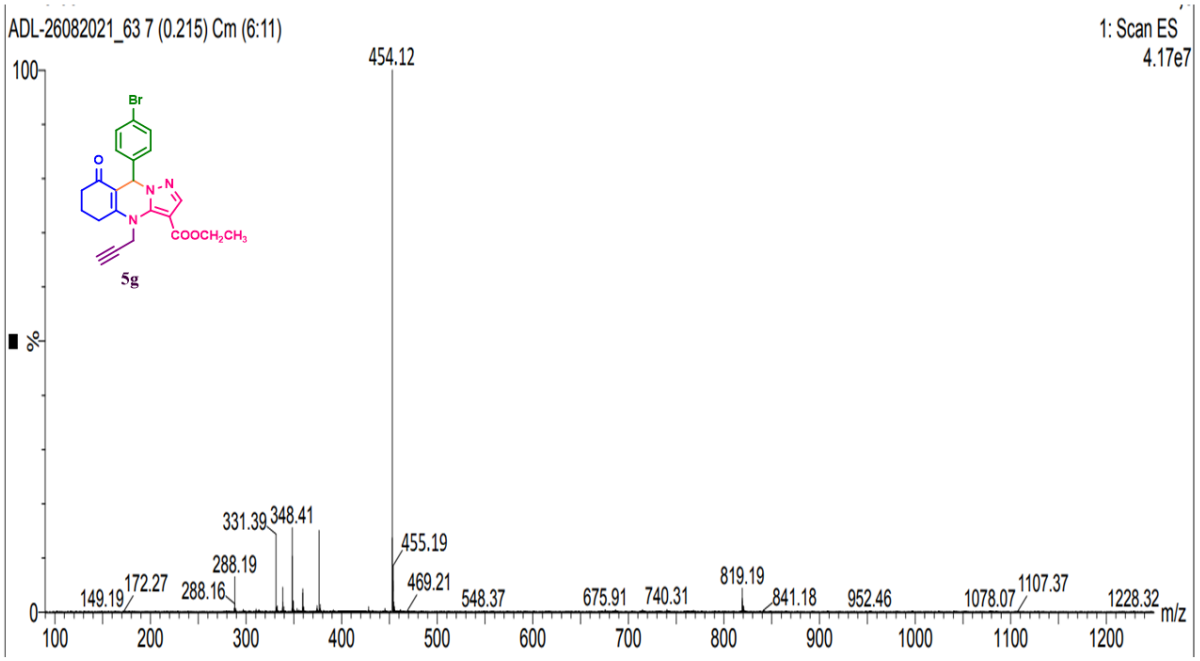

Figure S21. Mass spectrum of ethyl 9-(4-bromophenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5g).**

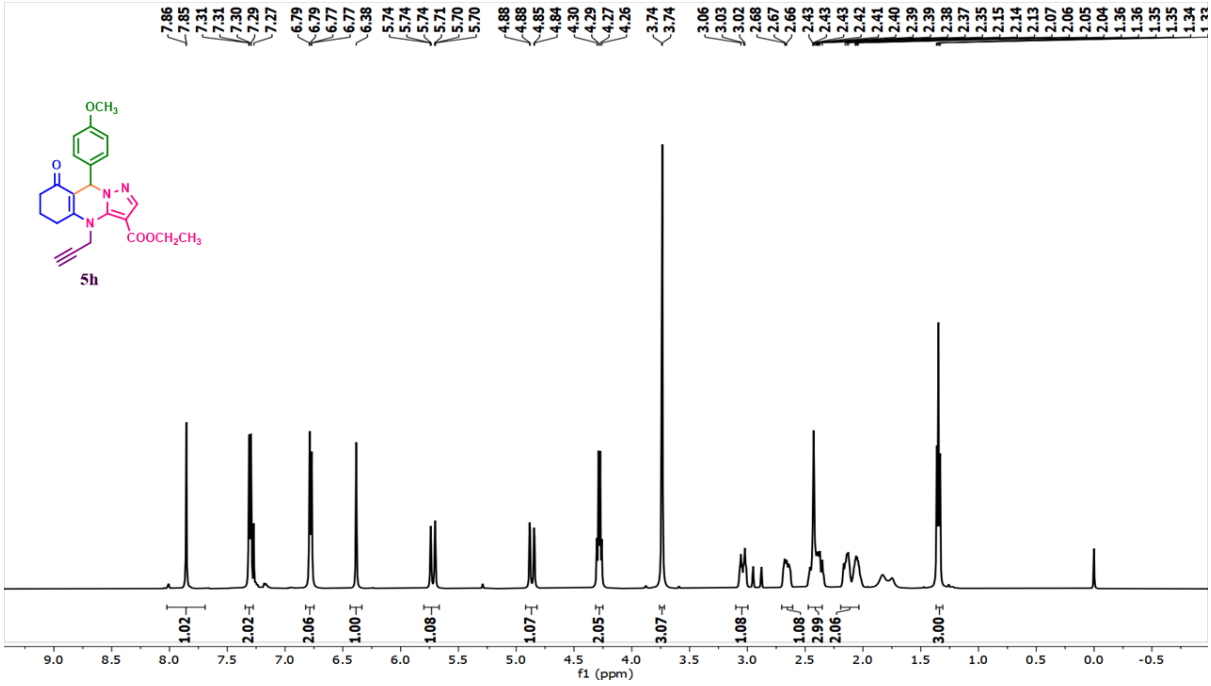

Figure S22. ^{1}H NMR spectrum of ethyl 9-(4-methoxyphenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5h).**

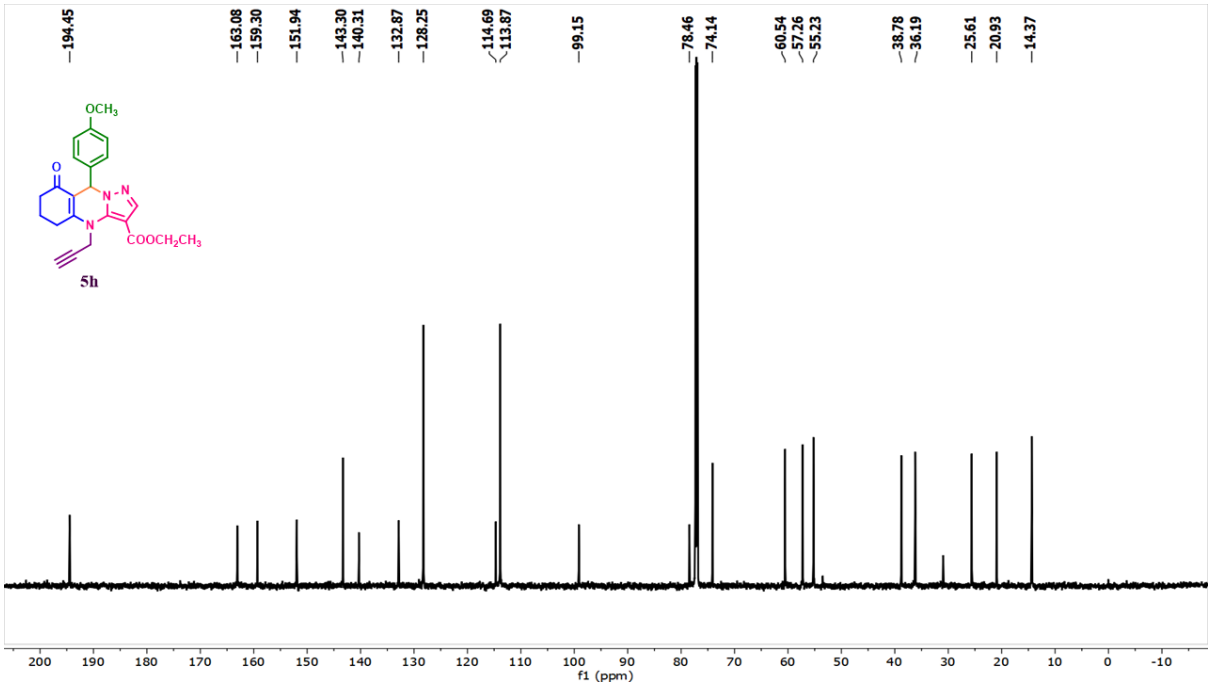

Figure S23. ^{13}C NMR spectrum of ethyl 9-(4-methoxyphenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5h).**

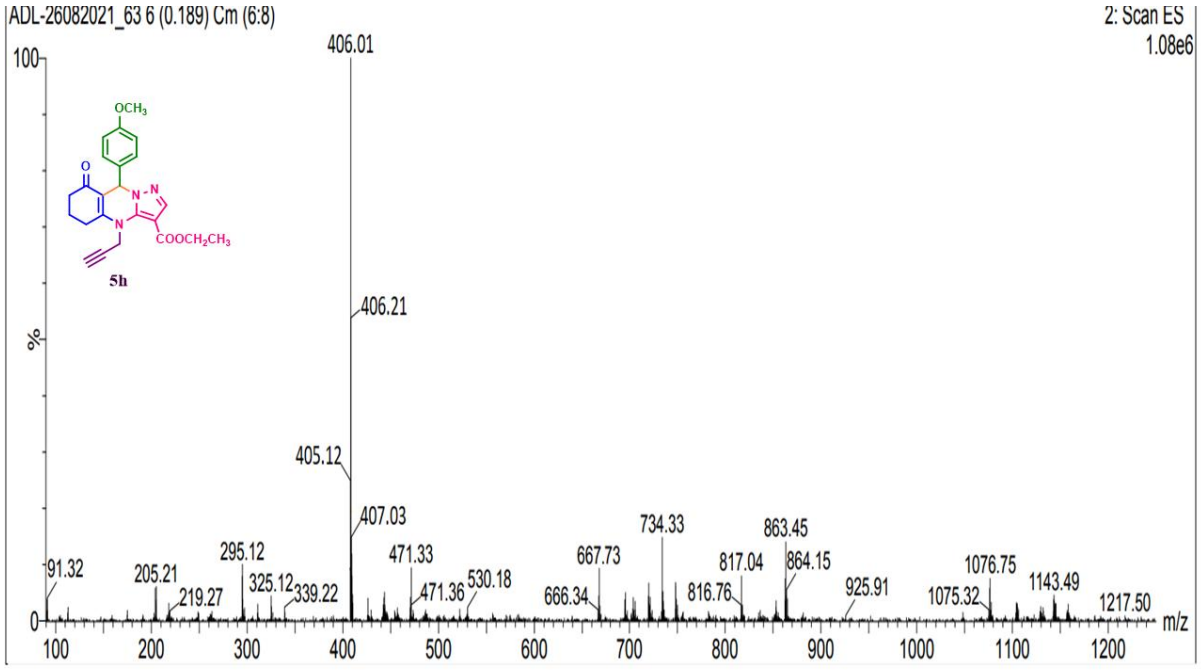

Figure S24. Mass spectrum of ethyl 9-(4-methoxyphenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5h).**

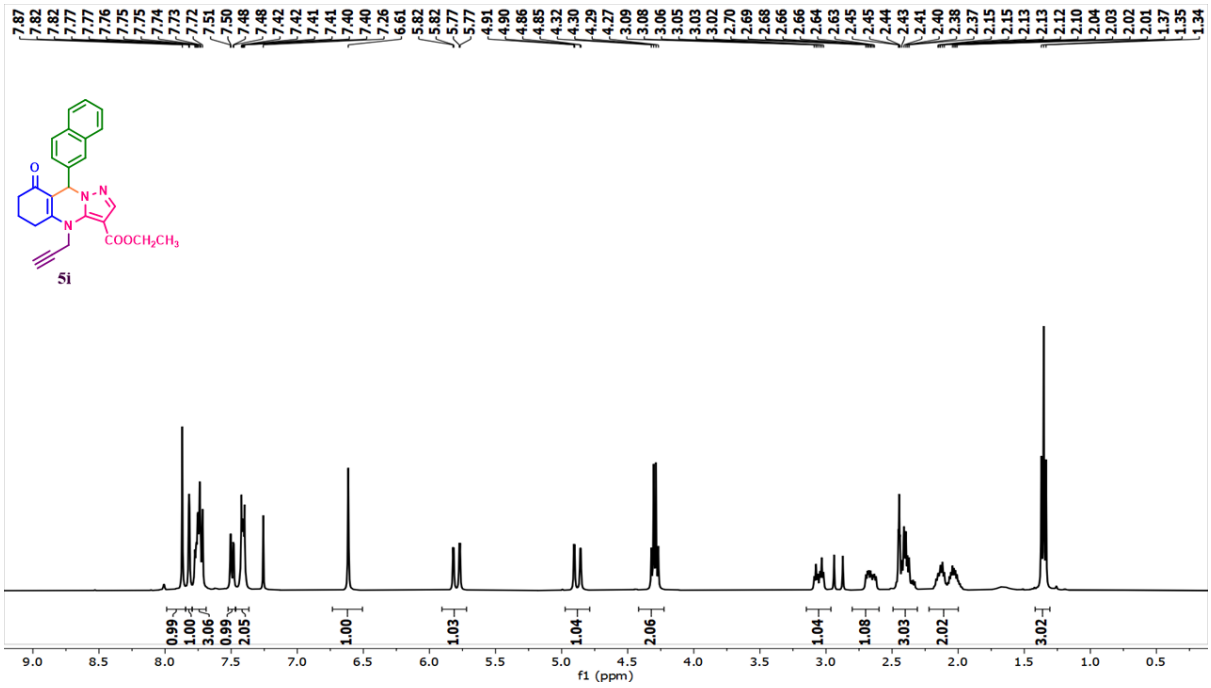

Figure S25. ^{1}H NMR spectrum of ethyl 9-(naphthalen-2-yl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5i).**

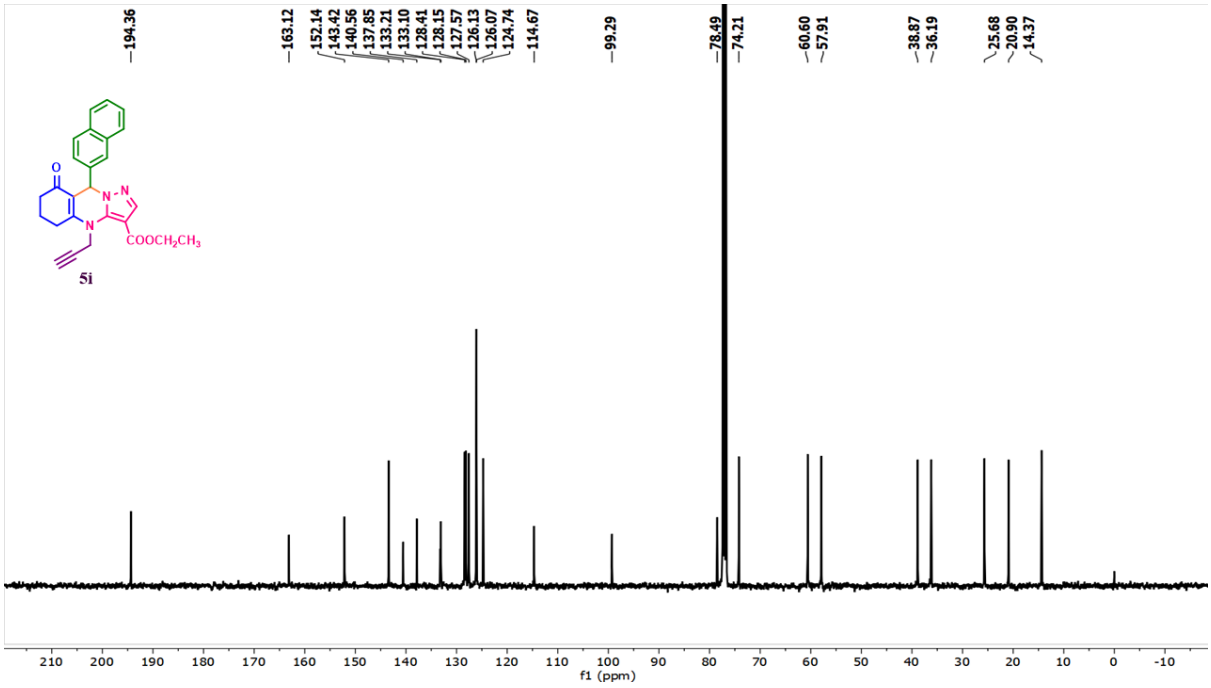

Figure S26. ^{13}C NMR spectrum of ethyl 9-(naphthalen-2-yl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5i).**

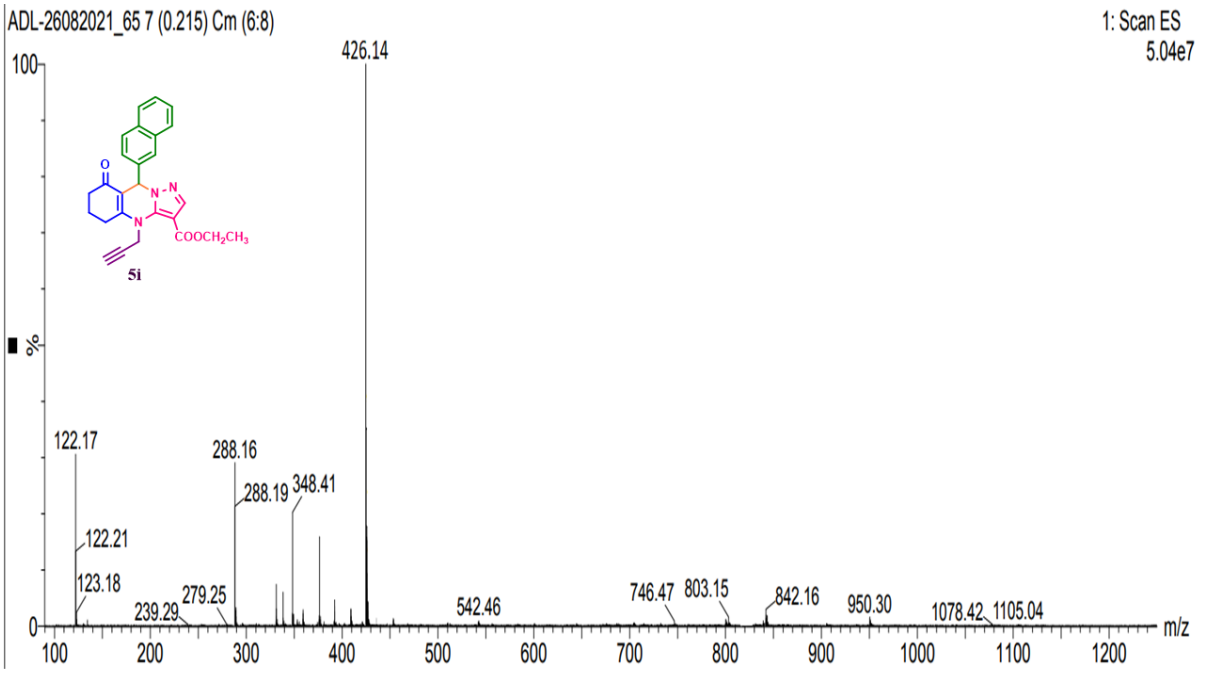

Figure S27. Mass spectrum of ethyl 9-(naphthalen-2-yl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5i).**

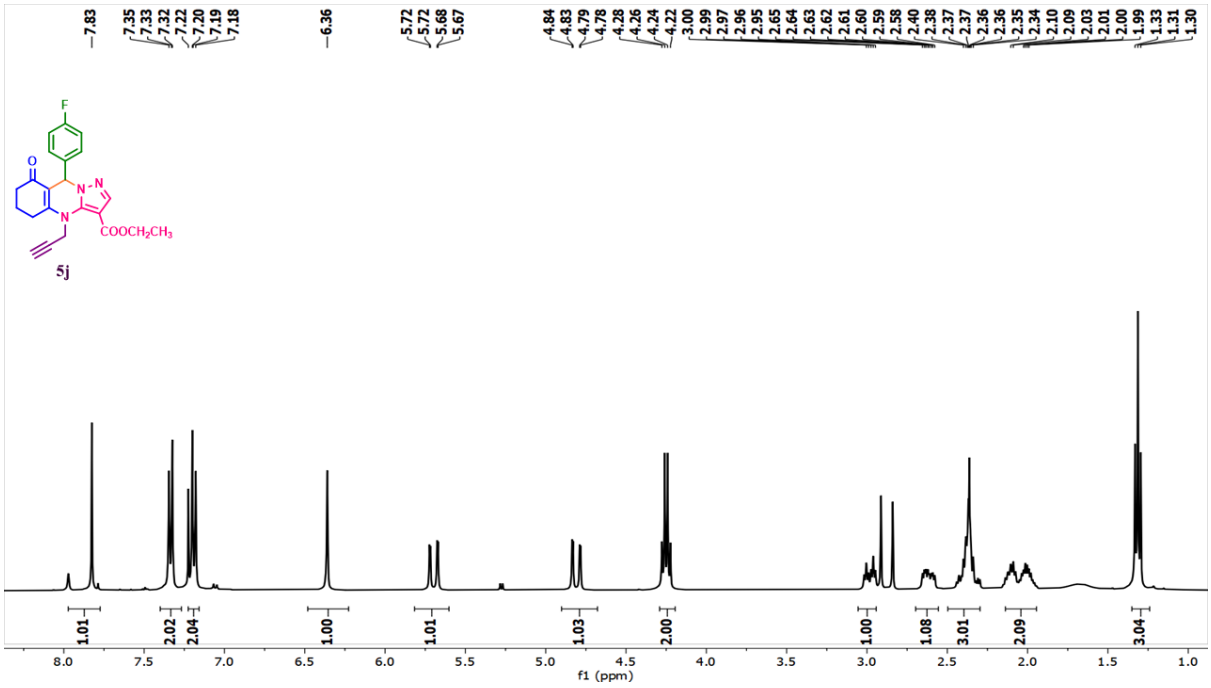

Figure S28. ^{1}H NMR spectrum of ethyl 9-(4-fluorophenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5j).**

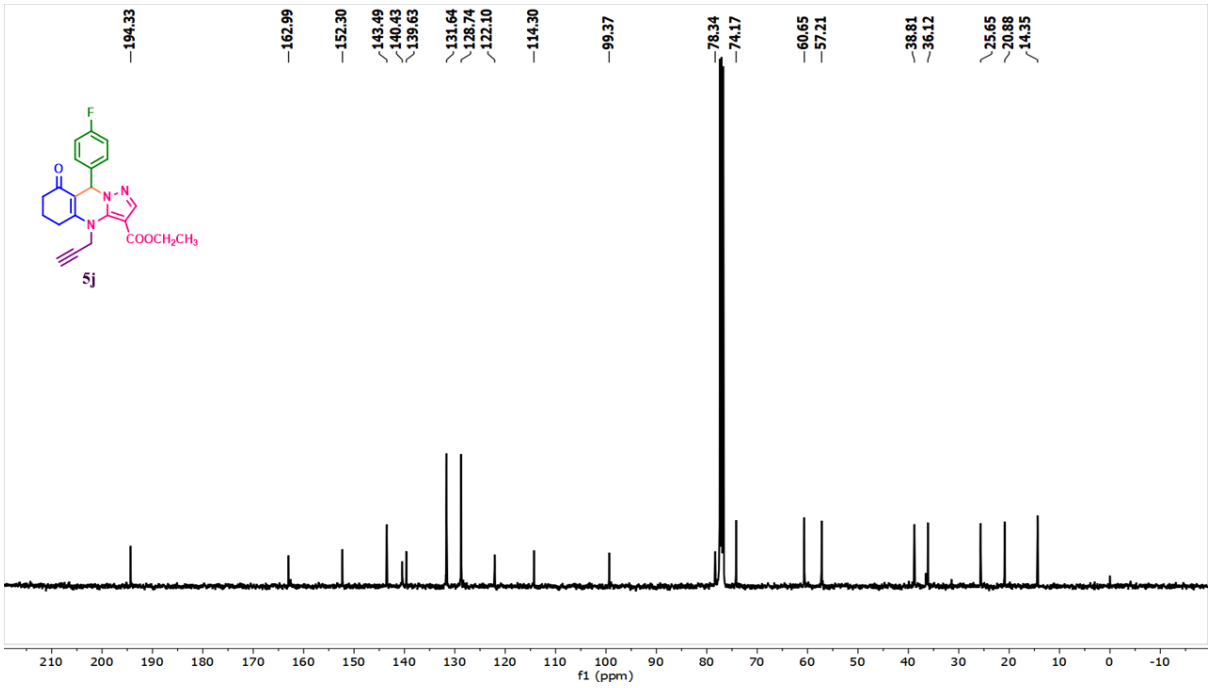

Figure S29. ^{13}C NMR spectrum of ethyl 9-(4-fluorophenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5j).**

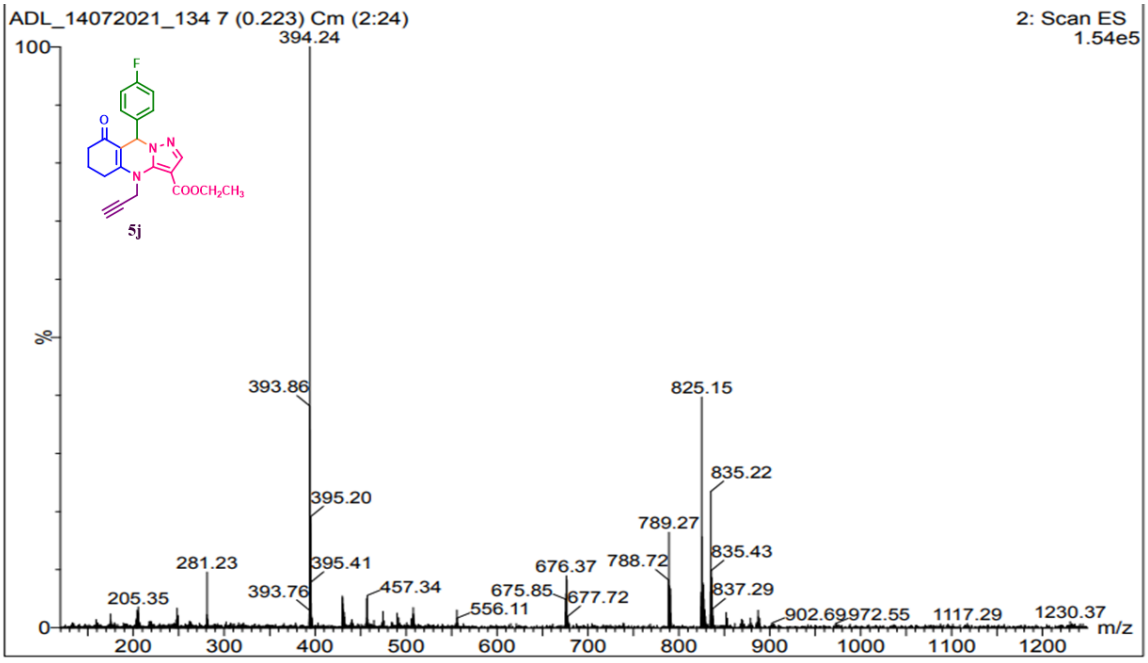

Figure S30. Mass spectrum of ethyl 9-(4-fluorophenyl)-8-oxo-4-(prop-2-yn-1-yl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(5j).**

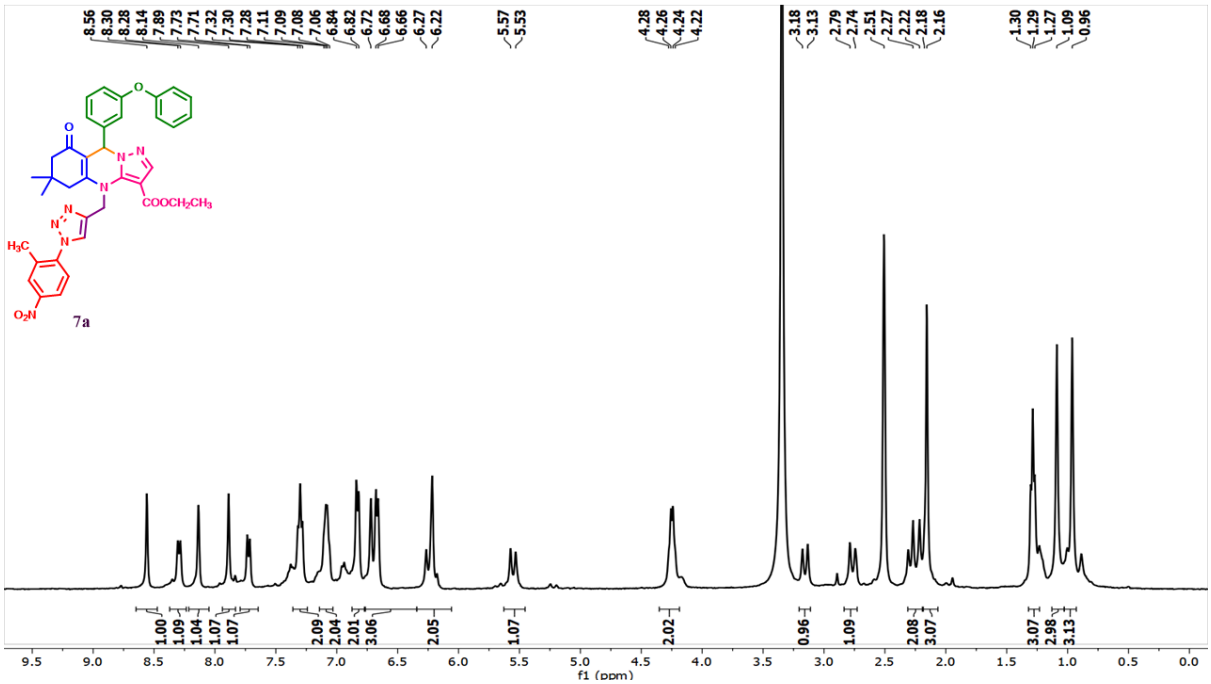

Figure S31. ^{1}H NMR spectrum of ethyl 6,6-dimethyl-4-((1-(2-methyl-4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methyl)-8-oxo-9-(3-phenoxyphenyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7a).**

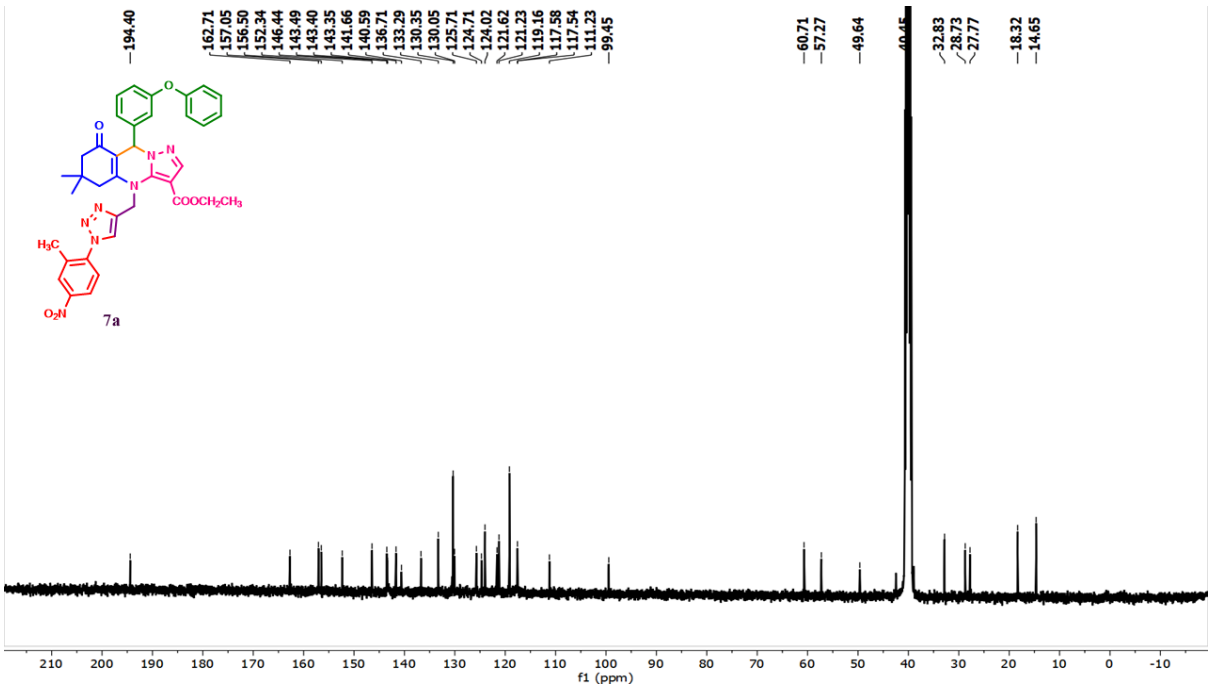

Figure S32. ^{13}C NMR spectrum of ethyl 6,6-dimethyl-4-((1-(2-methyl-4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methyl)-8-oxo-9-(3-phenoxyphenyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7a).**

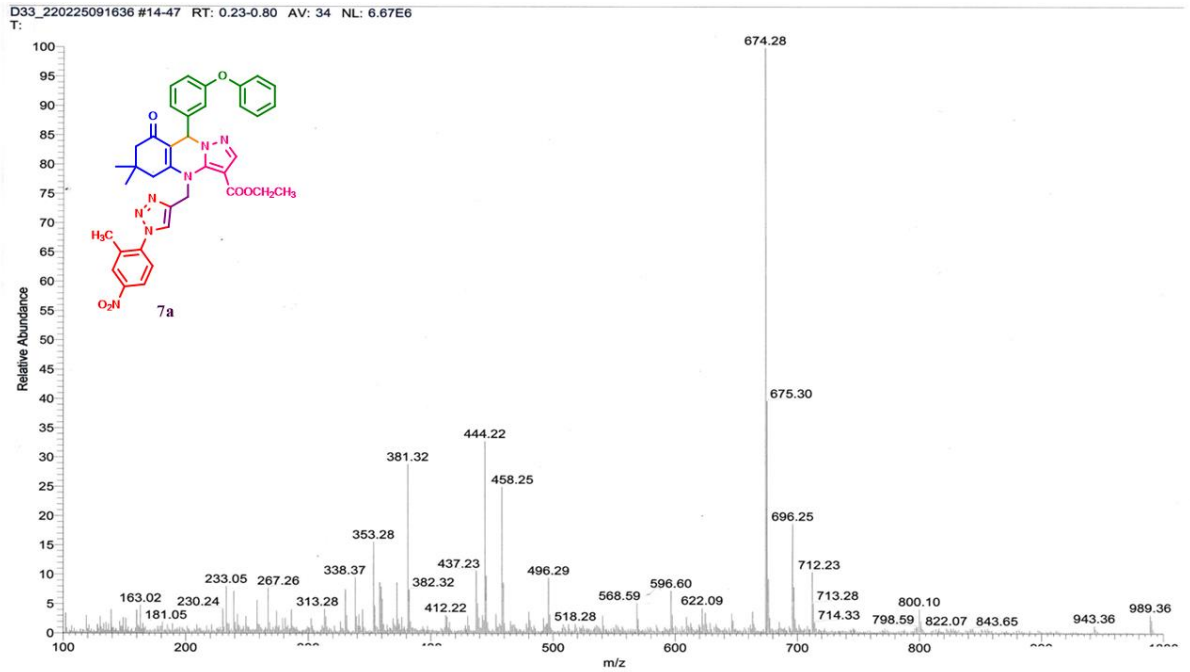

Figure S33. Mass s spectrum of ethyl 6,6-dimethyl-4-((1-(2-methyl-4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methyl)-8-oxo-9-(3-phenoxyphenyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7a).**

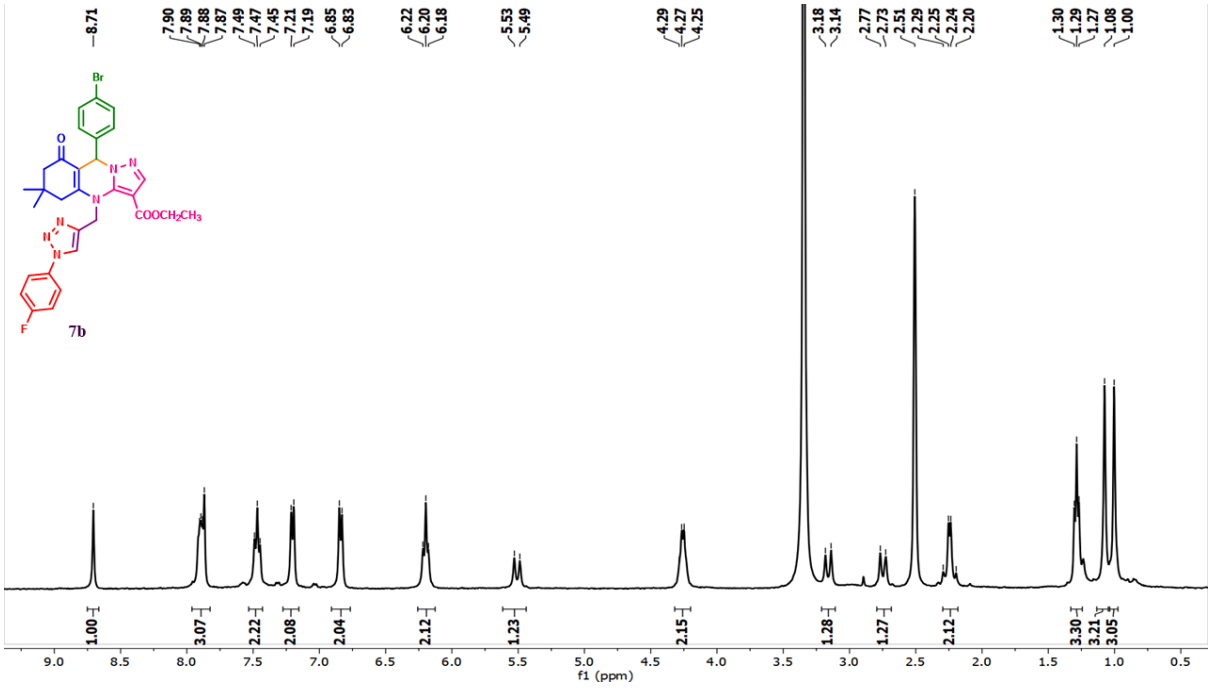

Figure S34. ^{1}H NMR spectrum of ethyl 9-(4-bromophenyl)-4-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-6,6-dimethyl-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7b).**

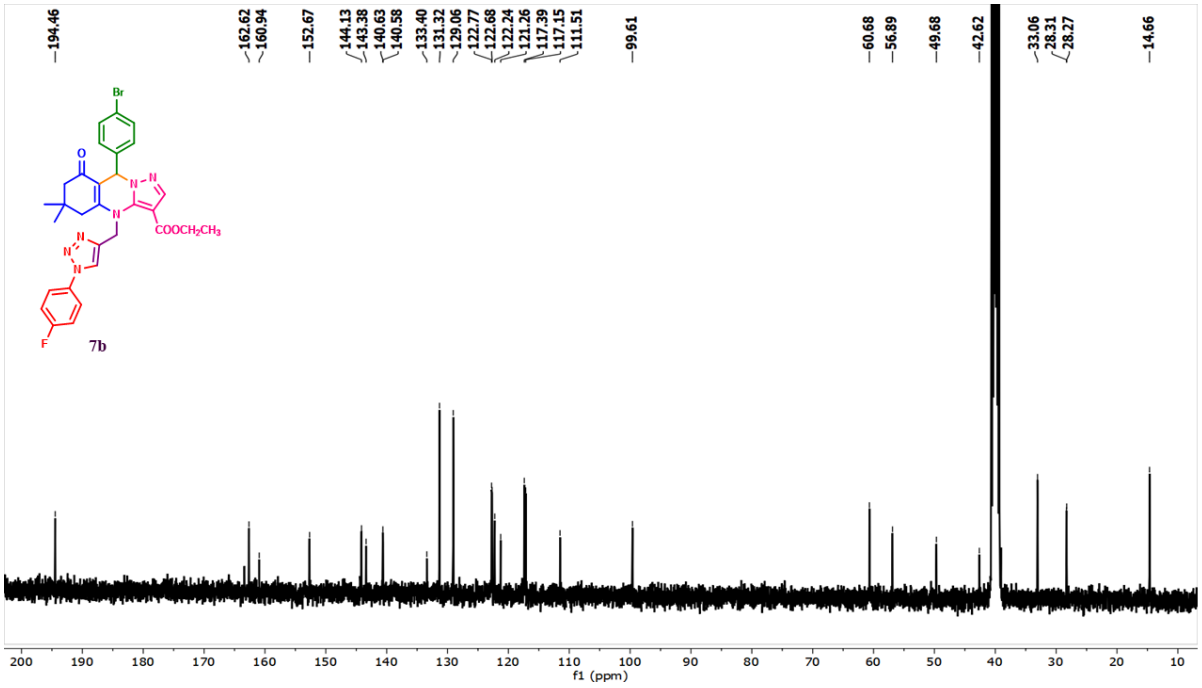

Figure S35. ^{13}C NMR spectrum of ethyl 9-(4-bromophenyl)-4-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-6,6-dimethyl-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7b).**

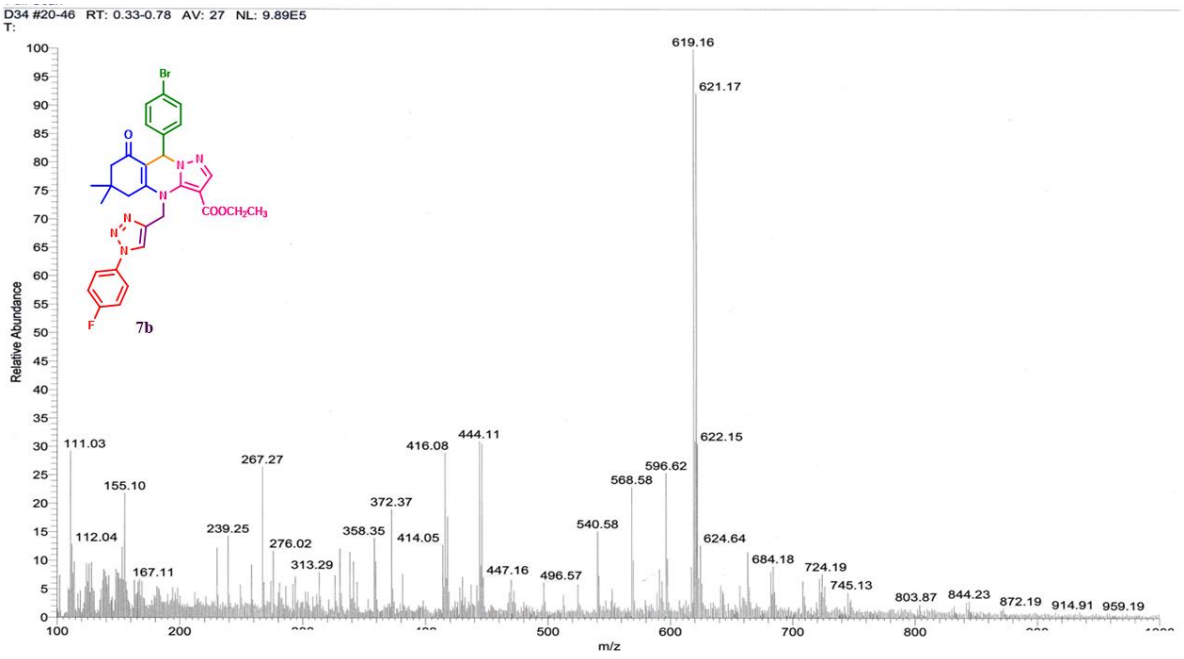

Figure S36. Mass spectrum of of ethyl 9-(4-bromophenyl)-4-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-6,6-dimethyl-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7b).**

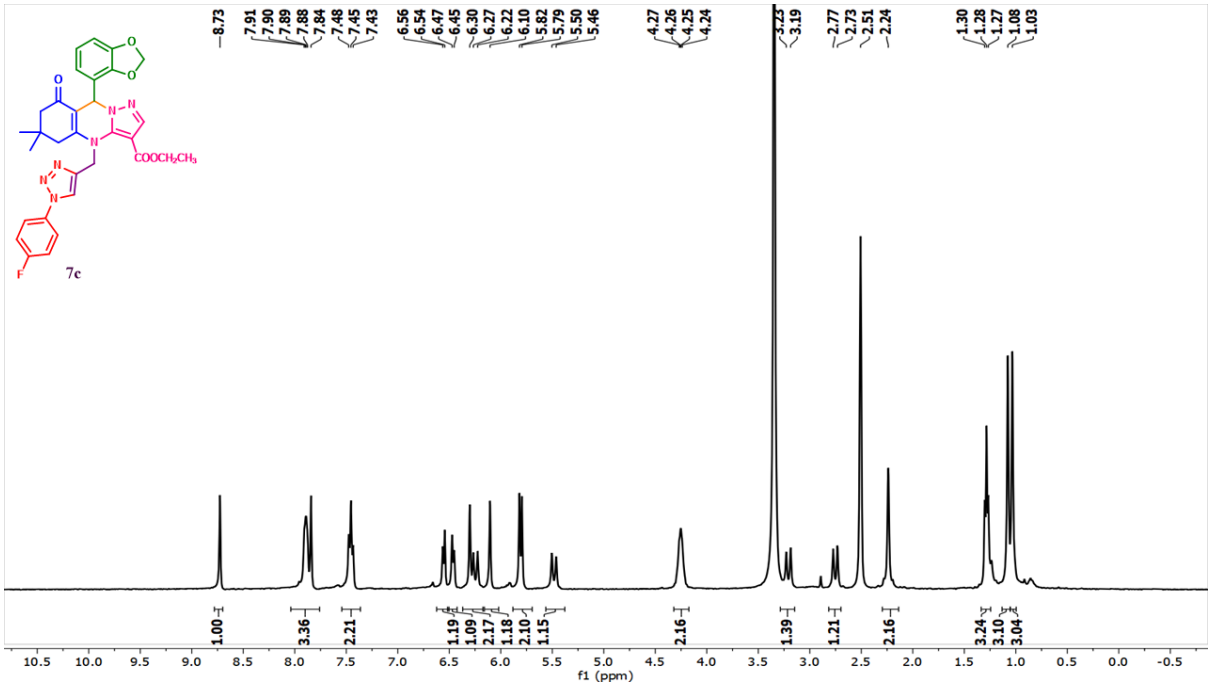

Figure S37. [1]H NMR spectrum of ethyl 9-(benzo[d][1,3]dioxol-4-yl)-4-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl) methyl)-6,6-dimethyl-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7c).**

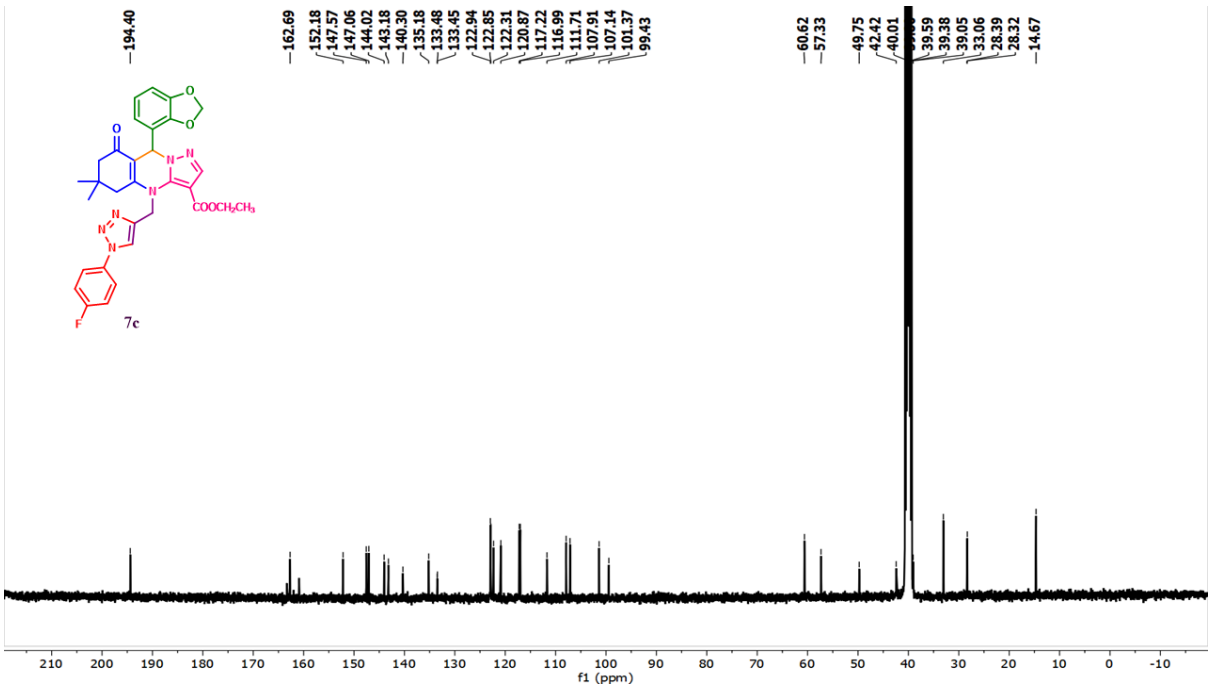

Figure S38. [13]C NMR s spectrum of ethyl 9-(benzo[d][1,3]dioxol-4-yl)-4-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl) methyl)-6,6-dimethyl-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7c).**

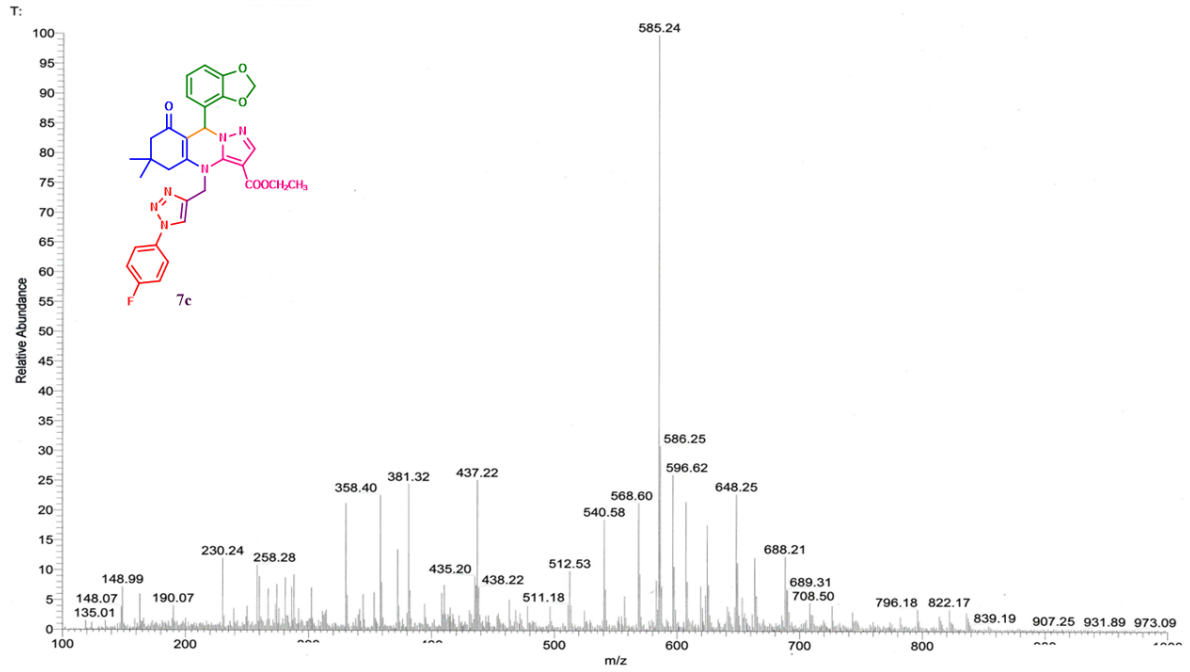

Figure S39. Mass spectrum of ethyl 9-(benzo[d][1,3]dioxol-4-yl)-4-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl) methyl)-6,6-dimethyl-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7c).**

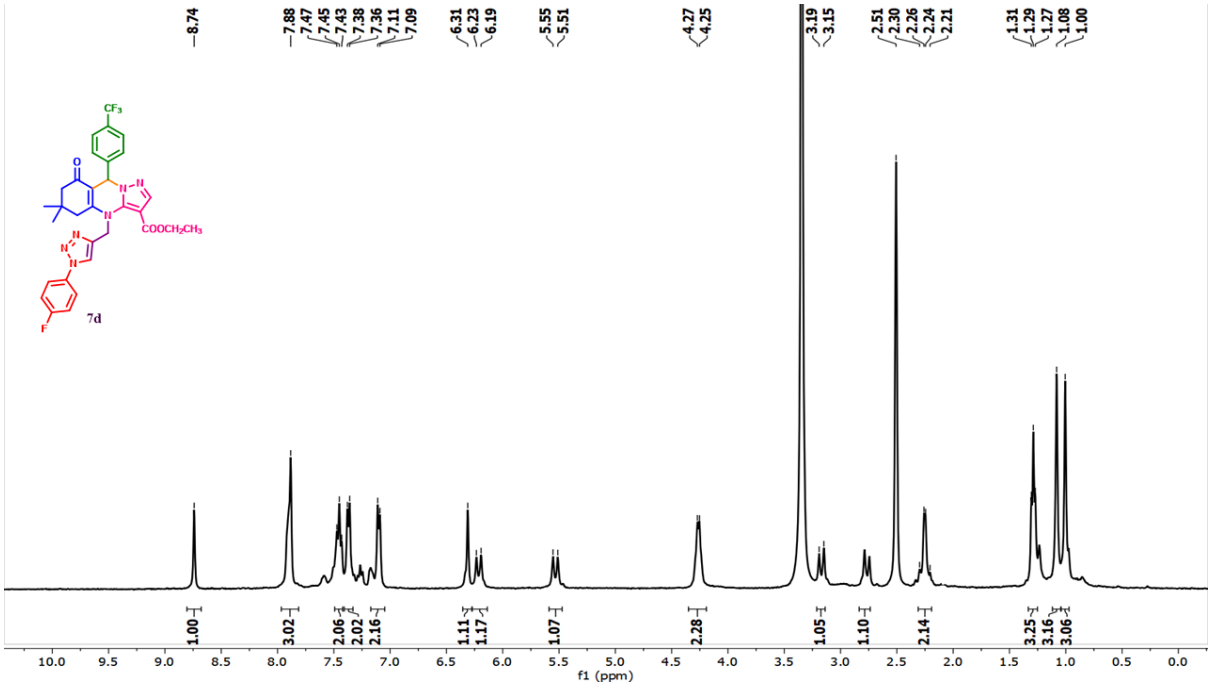

Figure S40. [1]H NMR spectrum of ethyl 4-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl) methyl)-6,6-dimethyl-8-oxo-9-(4-(trifluoromethyl)phenyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7d).**

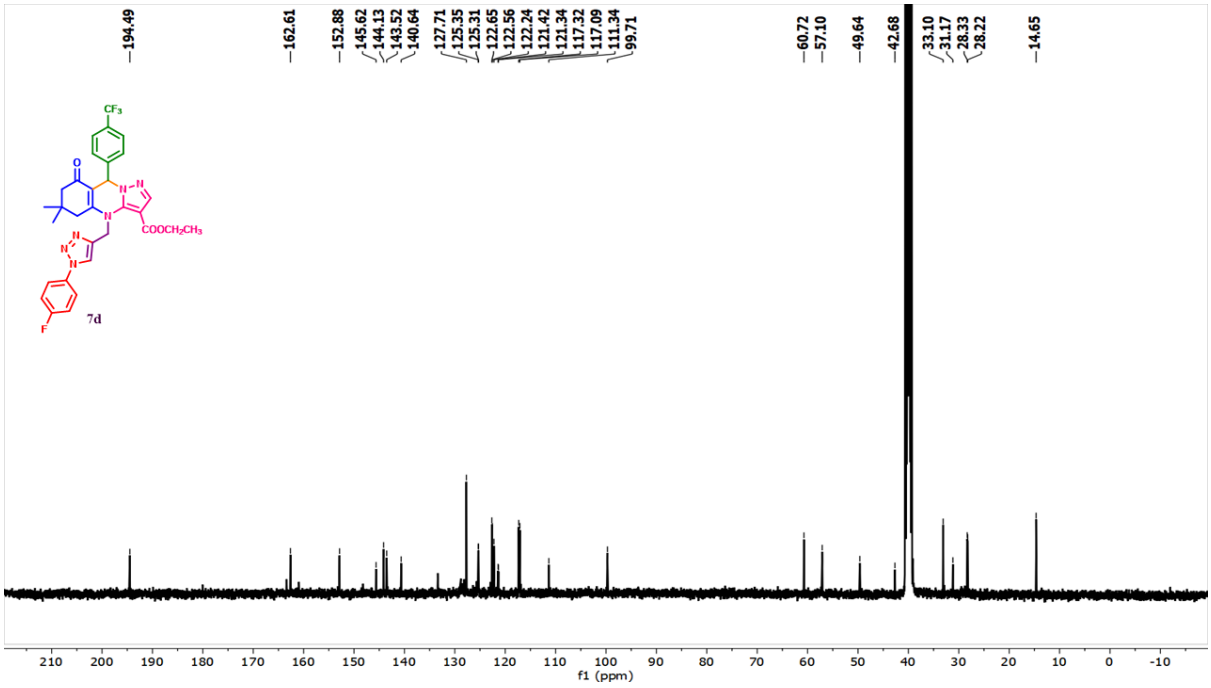

Figure S41. ^{13}C NMR spectrum of ethyl 4-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl) methyl)-6,6-dimethyl-8-oxo-9-(4-(trifluoromethyl)phenyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7d).**

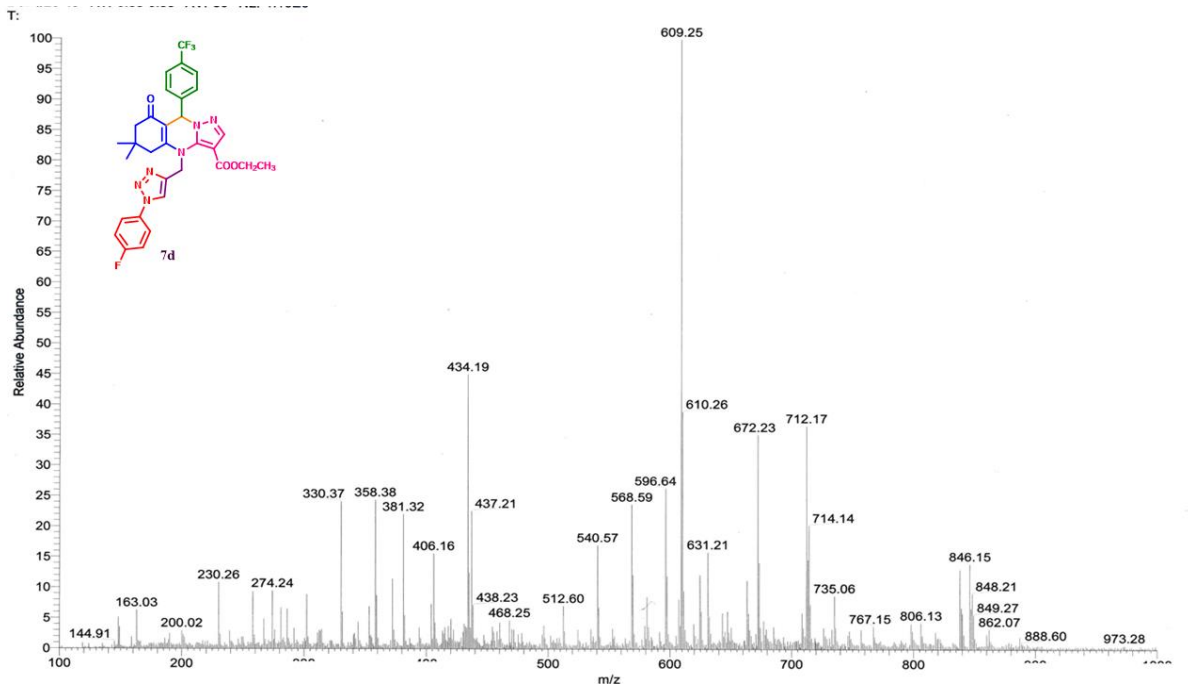

Figure S42. Mass spectrum of ethyl 4-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl) methyl)-6,6-dimethyl-8-oxo-9-(4-(trifluoromethyl)phenyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7d).**

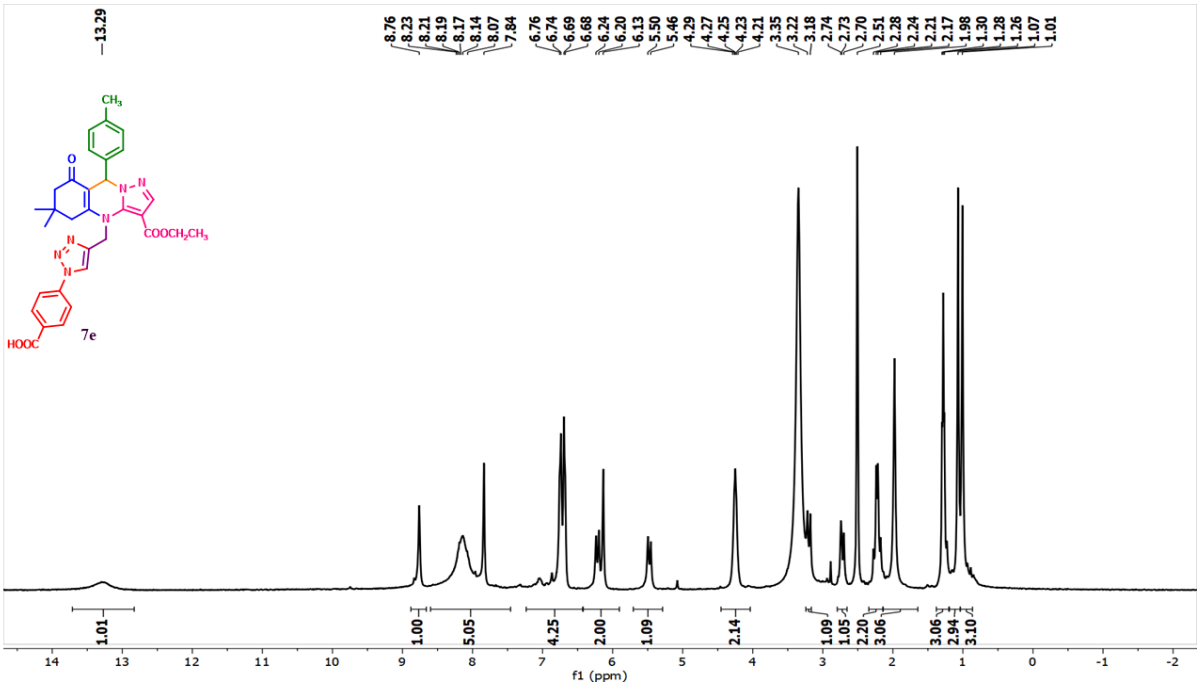

Figure S43. [1]H NMR spectrum of ethyl 4-(4-((3-(ethoxycarbonyl)-6,6-dimethyl-8-oxo-9-(p-tolyl)-5,7,8,9-tetrahydropyrazolo[5,1-b]quinazolin-4(6H)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)benzoic acid **(7e).**

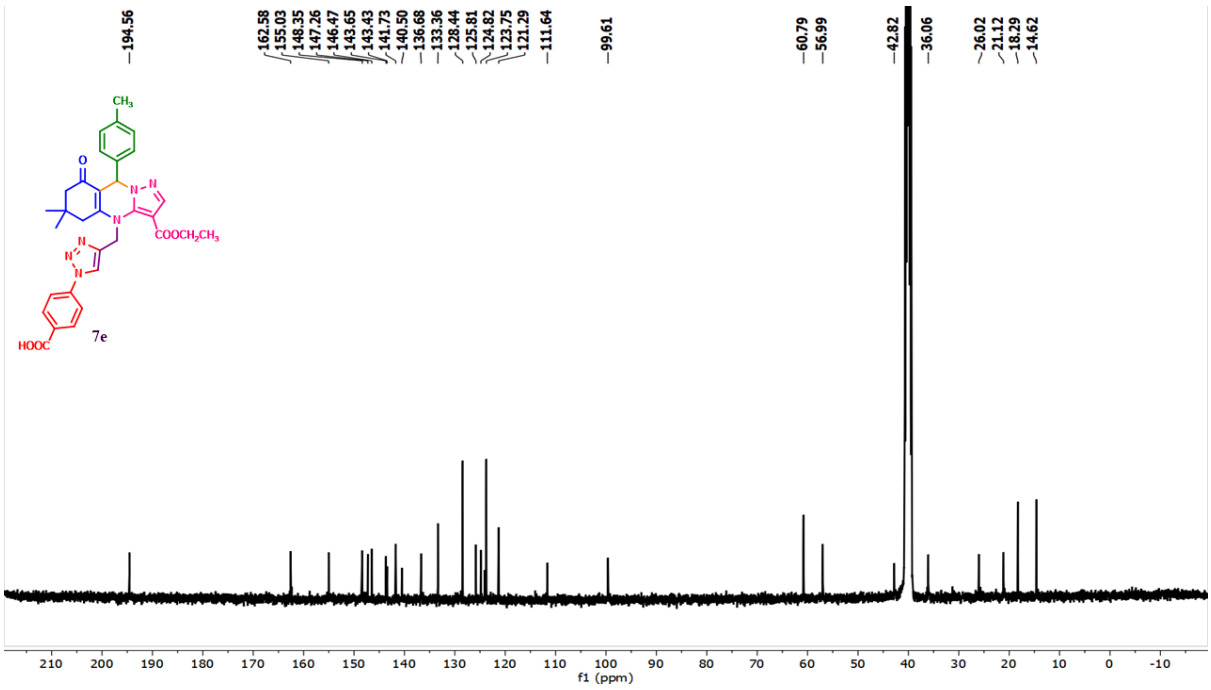

Figure S44. [13]C NMR spectrum of ethyl 4-(4-((3-(ethoxycarbonyl)-6,6-dimethyl-8-oxo-9-(p-tolyl)-5,7,8,9-tetrahydropyrazolo[5,1-b]quinazolin-4(6H)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)benzoic acid **(7e).**

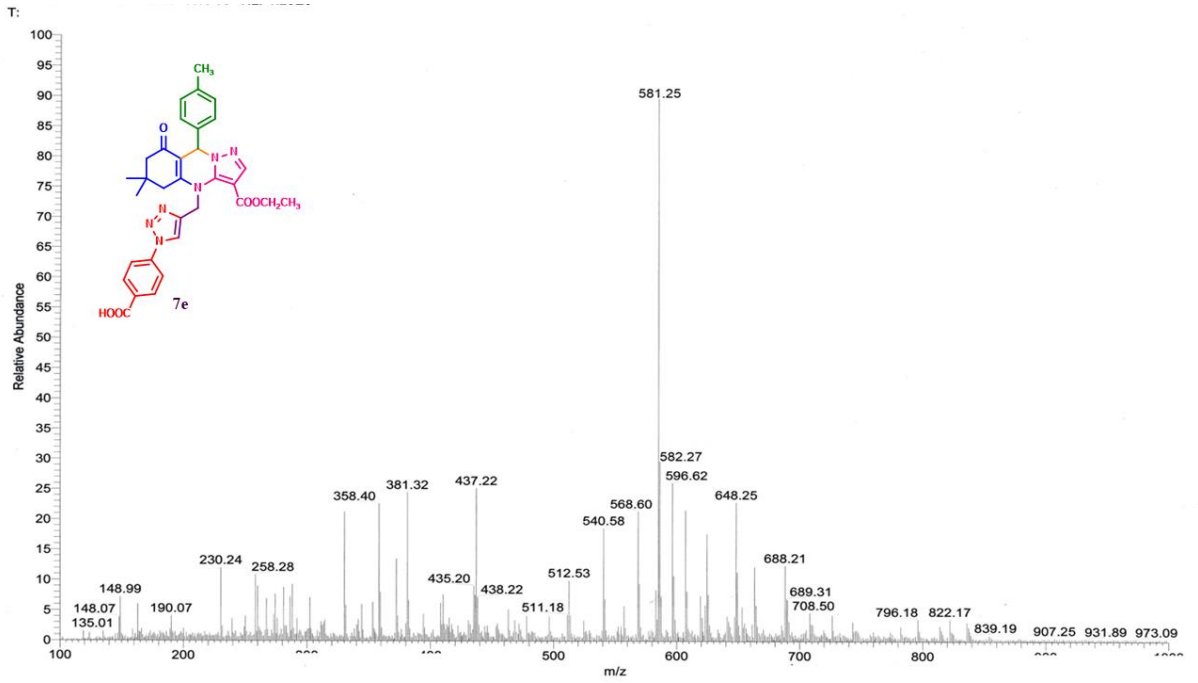

Figure S45. Mass spectrum of ethyl 4-(4-((3-(ethoxycarbonyl)-6,6-dimethyl-8-oxo-9-(p-tolyl)-5,7,8,9-tetrahydropyrazolo[5,1-b]quinazolin-4(6H)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)benzoic acid **(7e).**

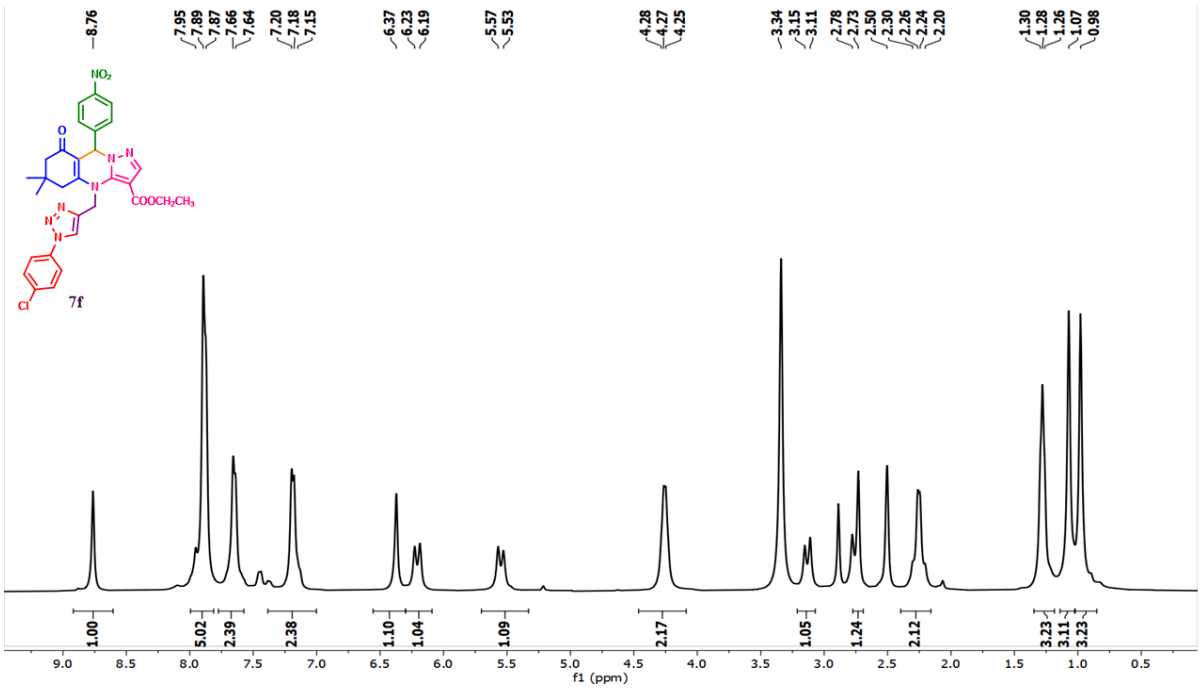

Figure S46. ^{1}H NMR spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-6,6-dimethyl-9-(4-nitrophenyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7f).**

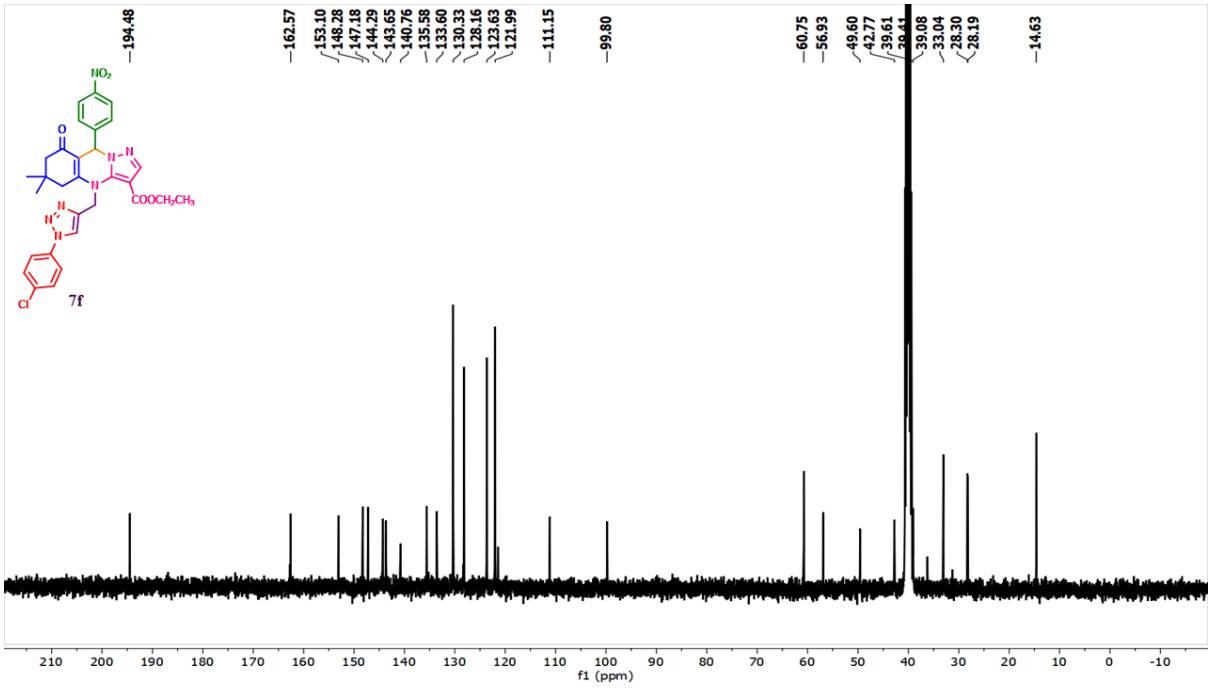

Figure S47. ^{13}C NMR spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-6,6-dimethyl-9-(4-nitrophenyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7f).**

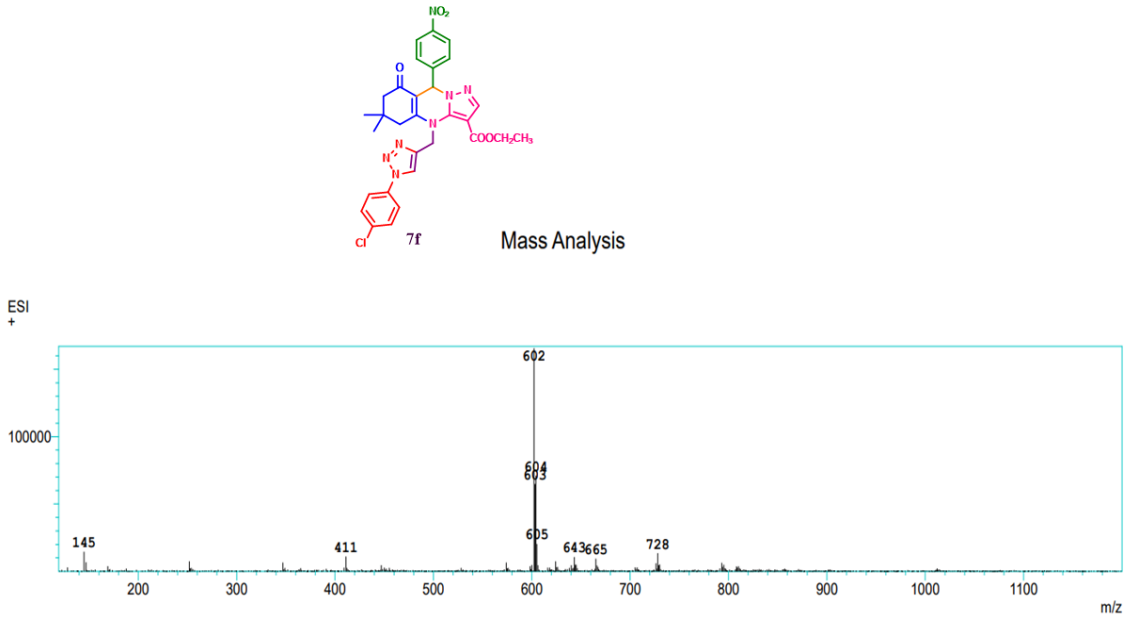

Figure S48. Mass spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-6,6-dimethyl-9-(4-nitrophenyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7f).**

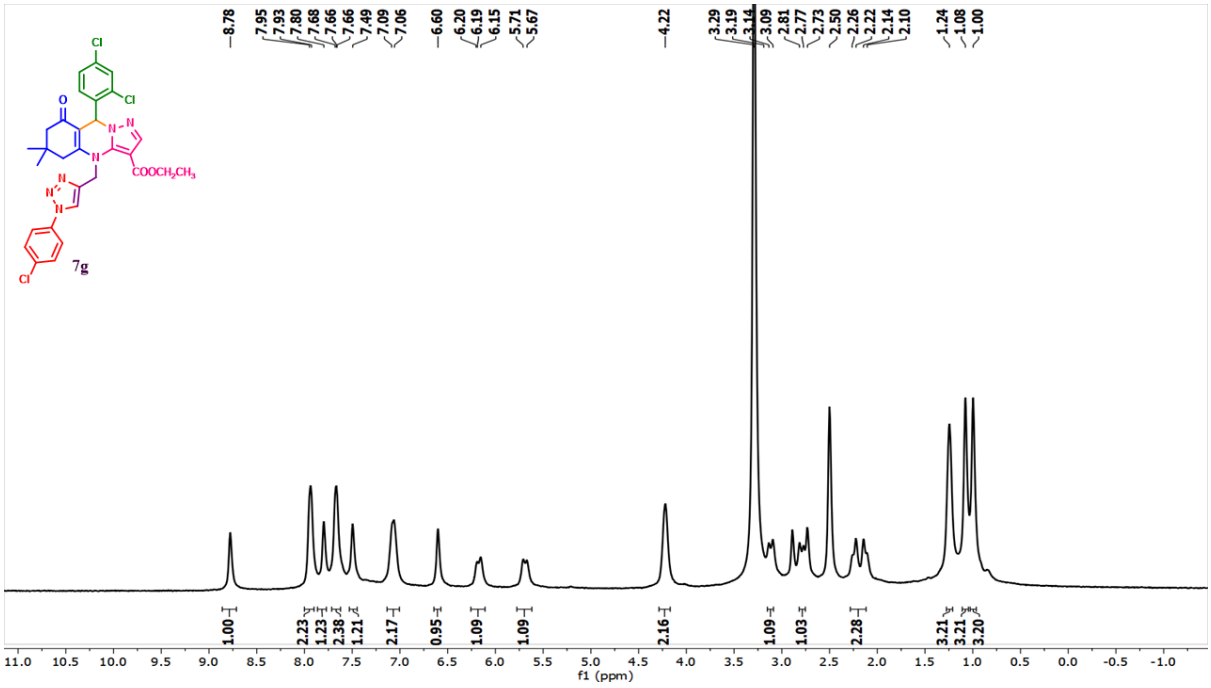

Figure S49. [1]H NMR spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(2,4-dichlorophenyl)-6,6-dimethyl-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7g).**

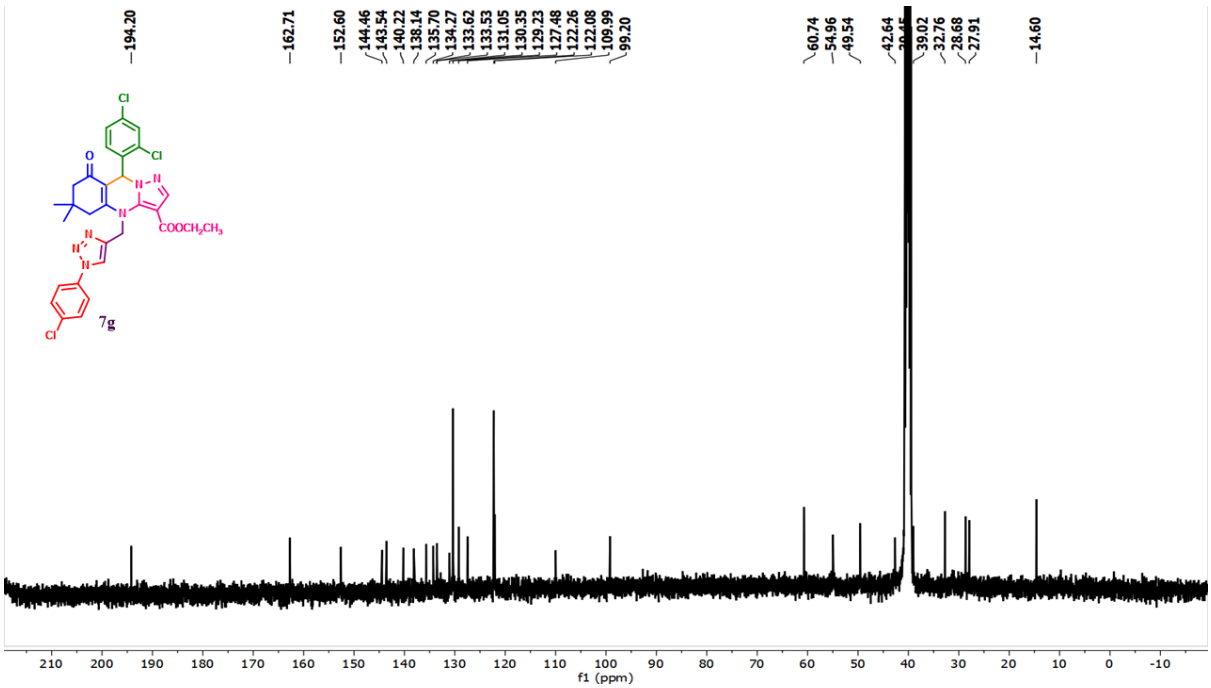

Figure S50. [13]C NMR spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(2,4-dichlorophenyl)-6,6-dimethyl-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7g).**

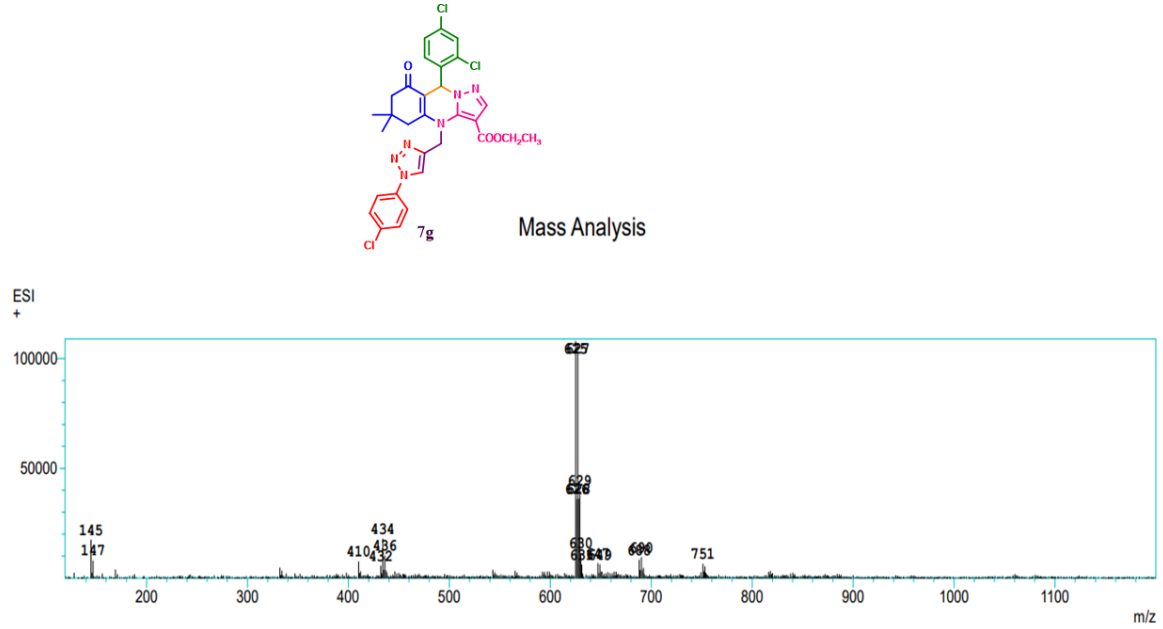

Figure S51. Mass spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(2,4-dichlorophenyl)-6,6-dimethyl-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7g).**

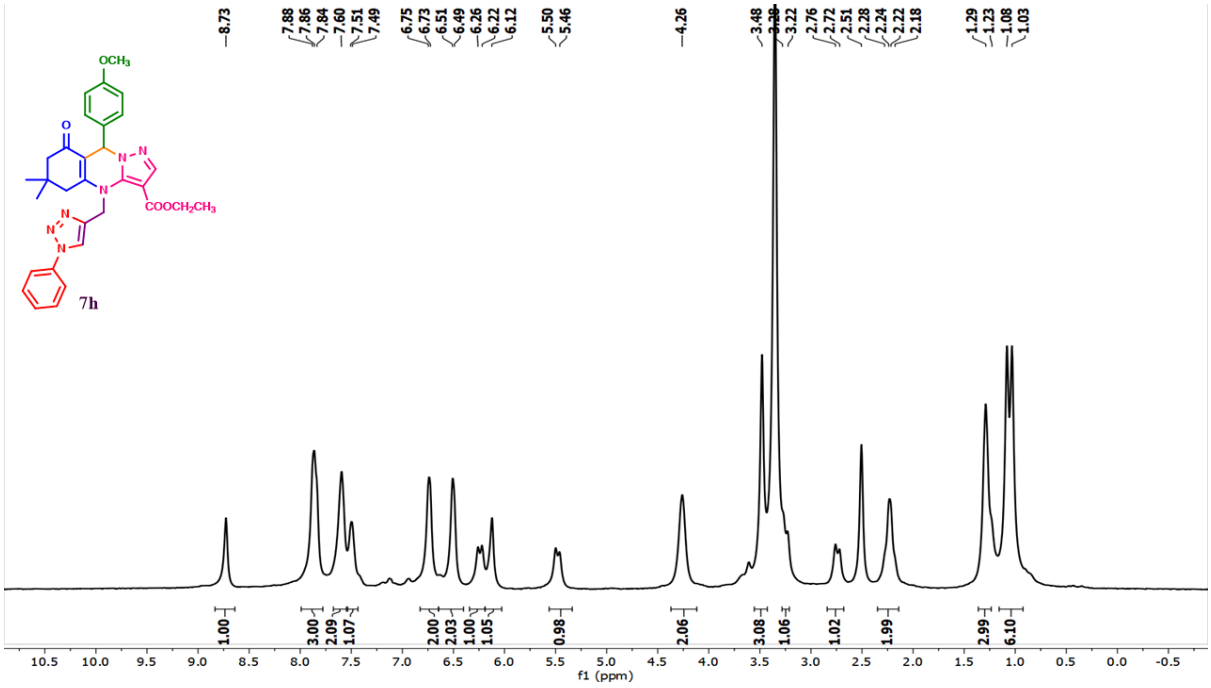

Figure S52. ^{1}H NMR spectrum of ethyl 9-(4-methoxyphenyl)-6,6-dimethyl-8-oxo-4-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7h).**

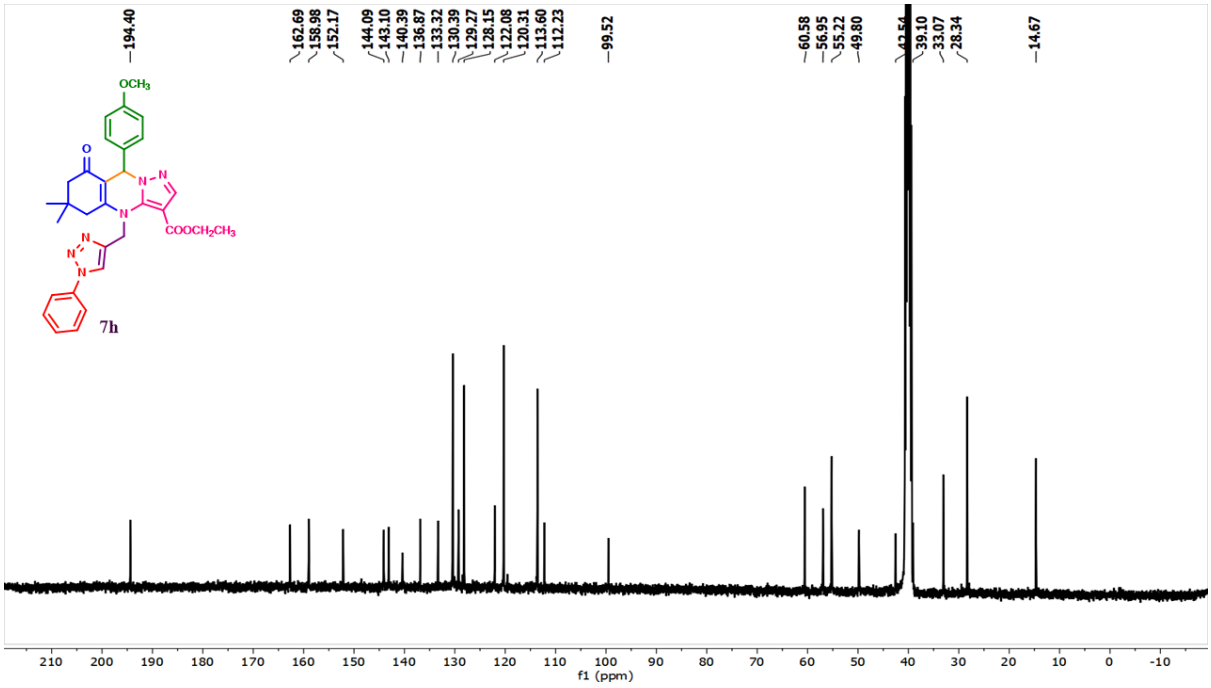

Figure S53. ^{13}C NMR spectrum of ethyl 9-(4-methoxyphenyl)-6,6-dimethyl-8-oxo-4-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7h).**

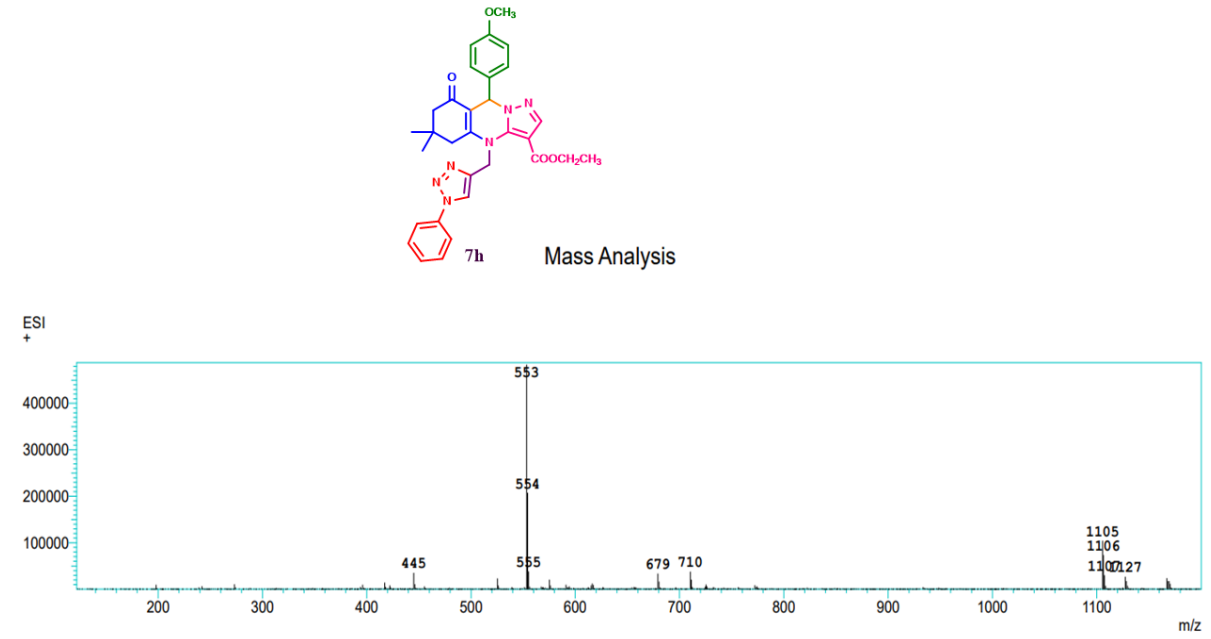

Figure S54. Mass spectrum of ethyl 9-(4-methoxyphenyl)-6,6-dimethyl-8-oxo-4-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7h).**

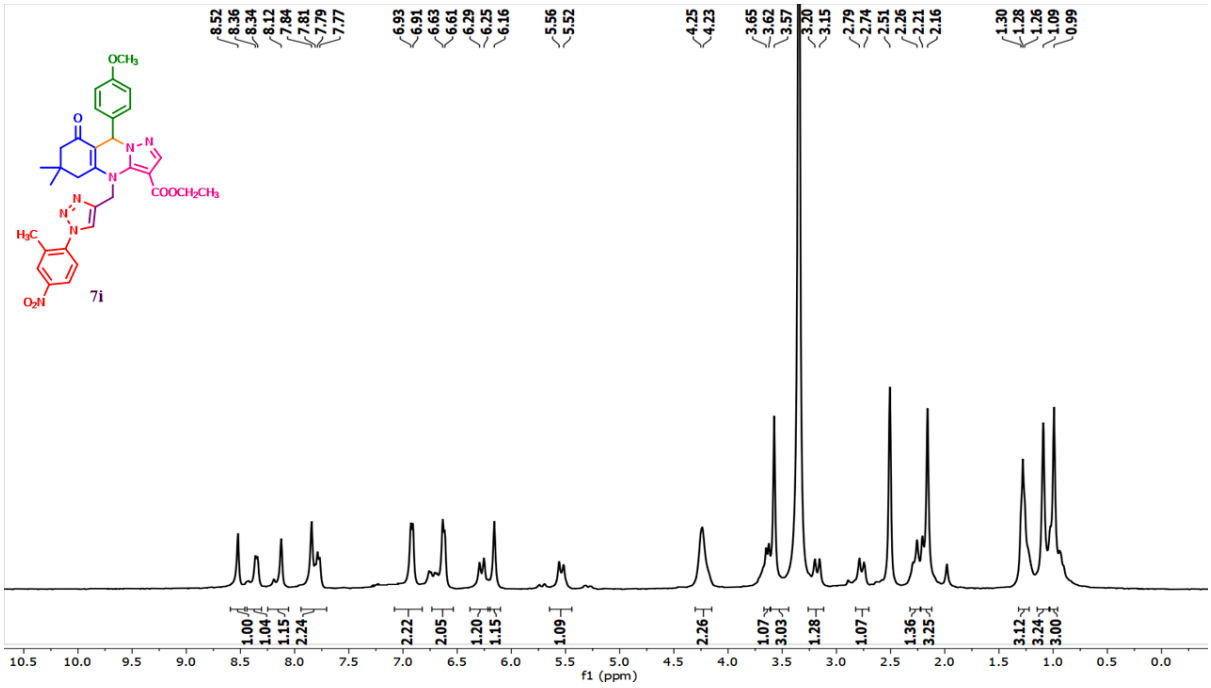

Figure S55. [1]H NMR spectrum of ethyl 9-(4-methoxyphenyl)-6,6-dimethyl-4-((1-(2-methyl-4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7i).**

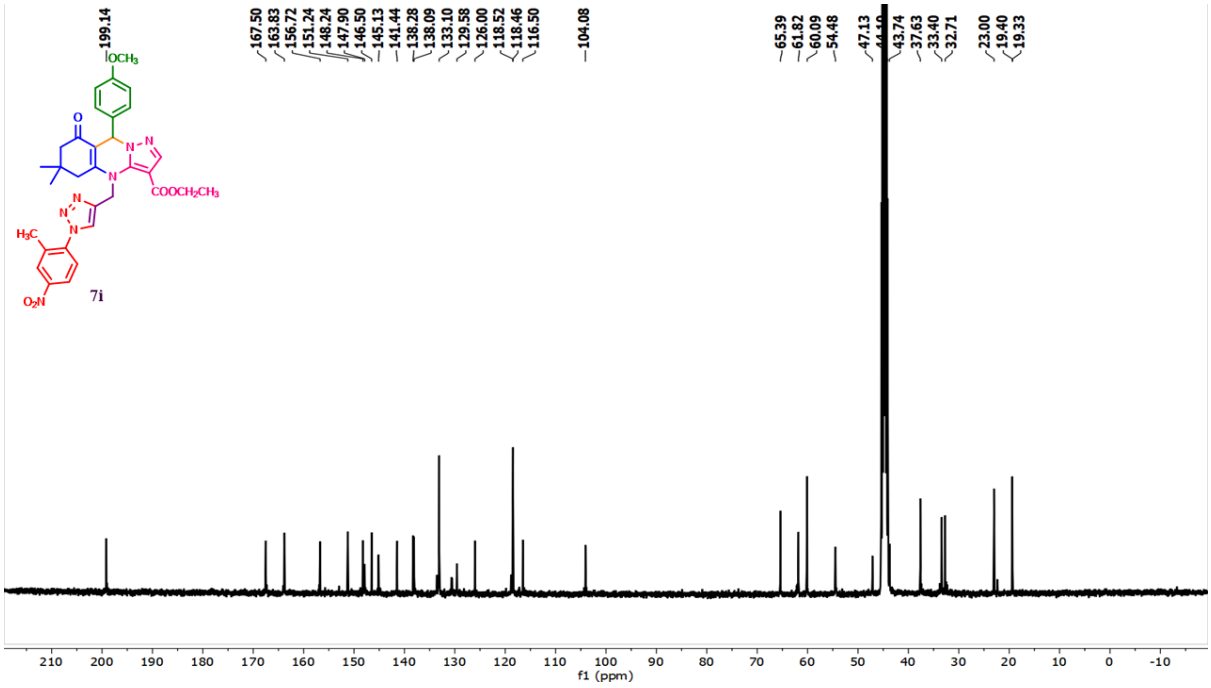

Figure S56. [13]C NMR spectrum of ethyl 9-(4-methoxyphenyl)-6,6-dimethyl-4-((1-(2-methyl-4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7i).**

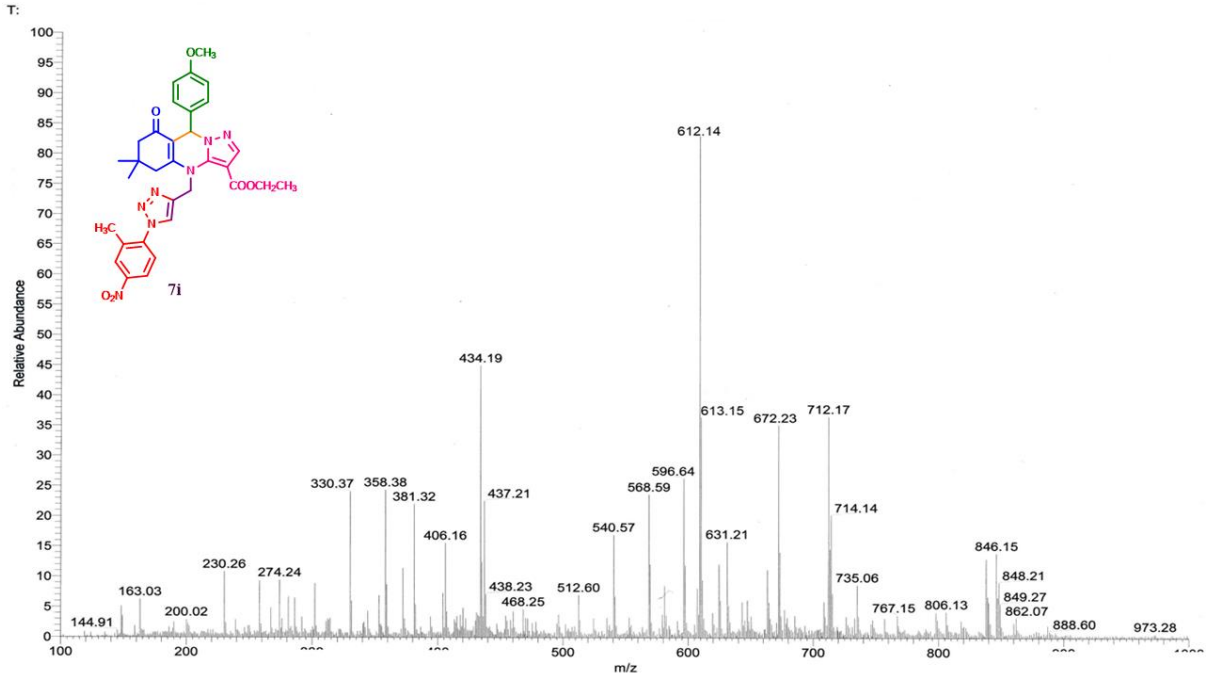

Figure S57. Mass spectrum of ethyl 9-(4-methoxyphenyl)-6,6-dimethyl-4-((1-(2-methyl-4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7i).**

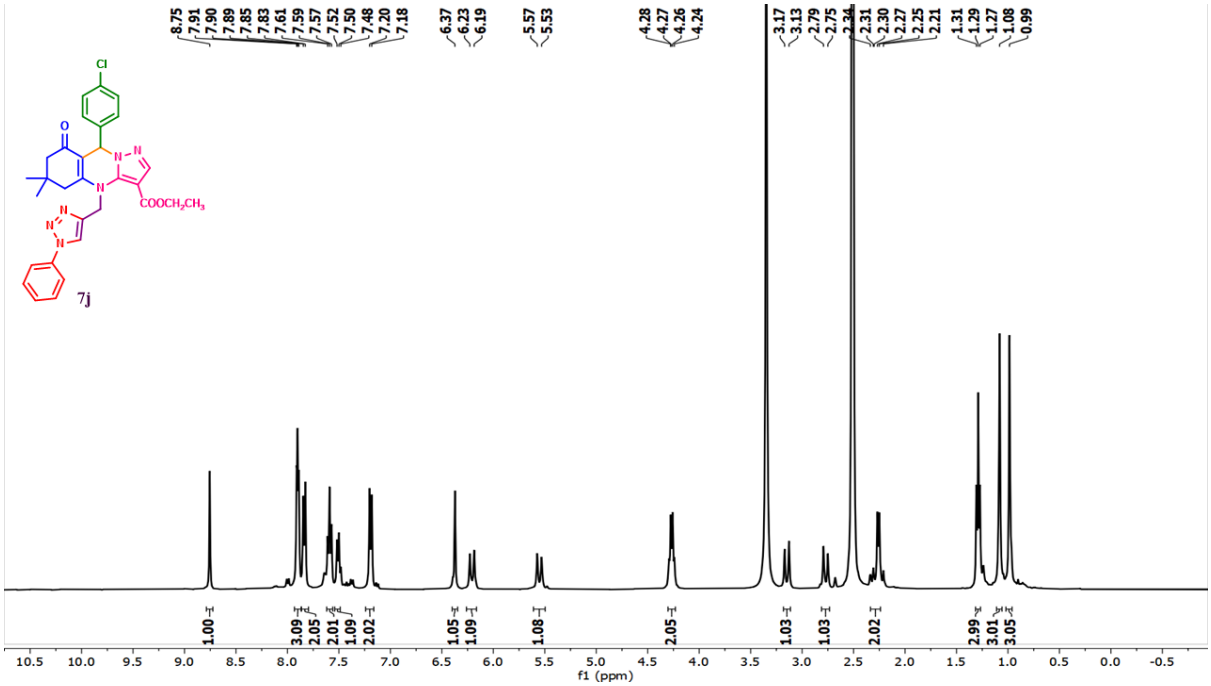

Figure S58. ^{1}H NMR spectrum of ethyl 9-(4-chlorophenyl)-6,6-dimethyl-8-oxo-4-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7j).**

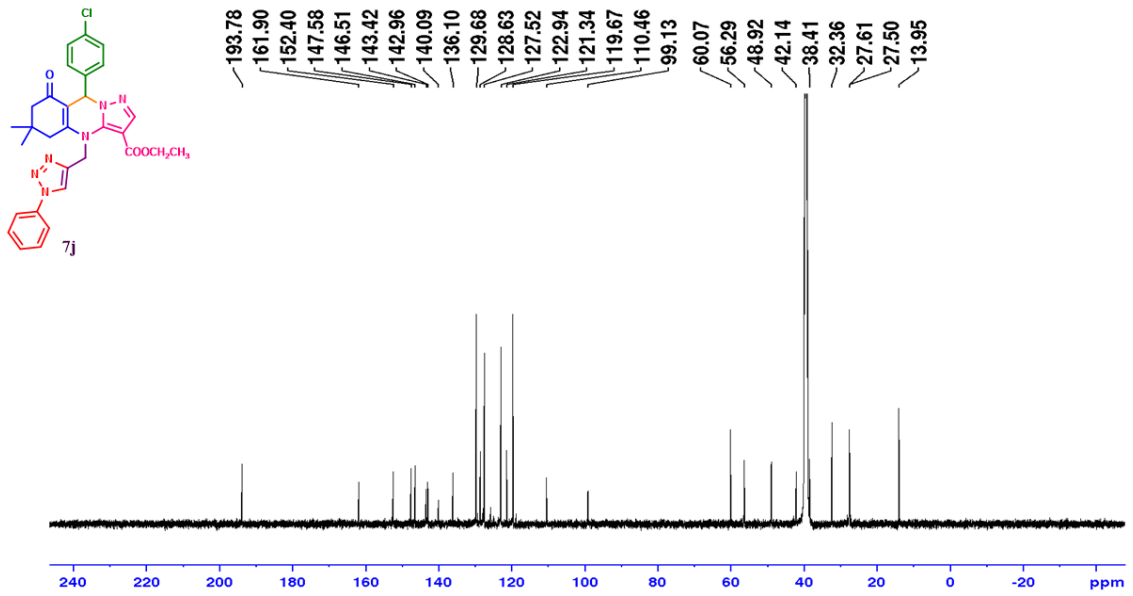

Figure S59. ^{13}C NMR spectrum of ethyl 9-(4-chlorophenyl)-6,6-dimethyl-8-oxo-4-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7j).**

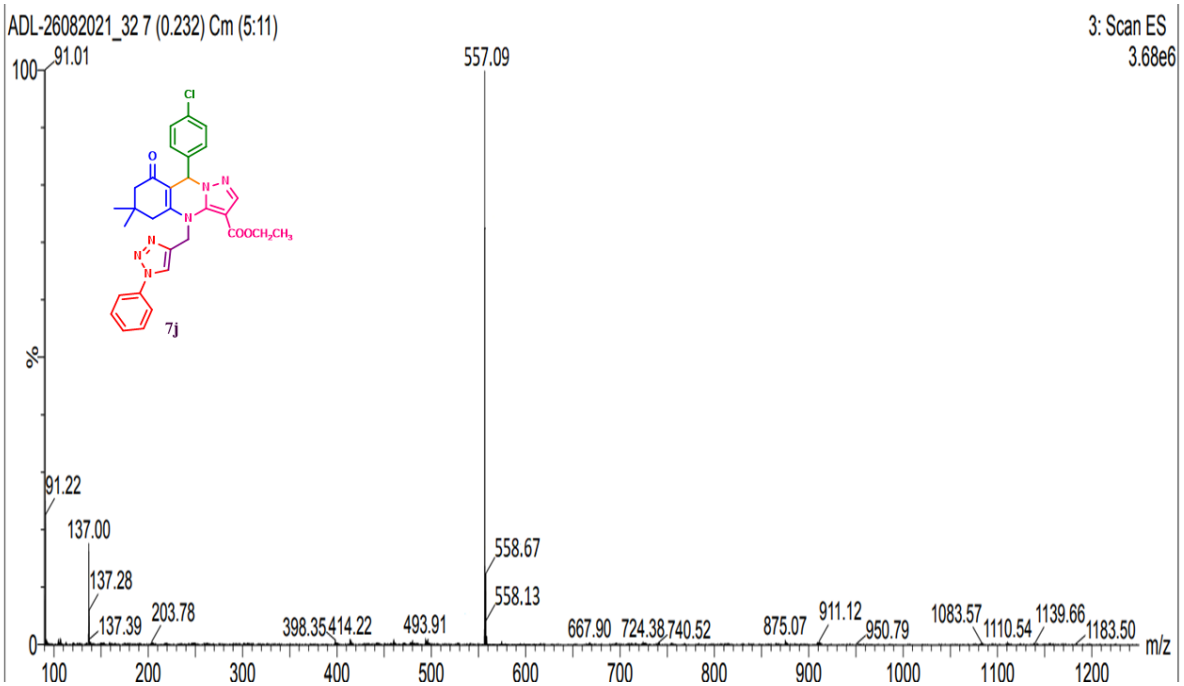

Figure S60. Mass spectrum of ethyl 9-(4-chlorophenyl)-6,6-dimethyl-8-oxo-4-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7j).**

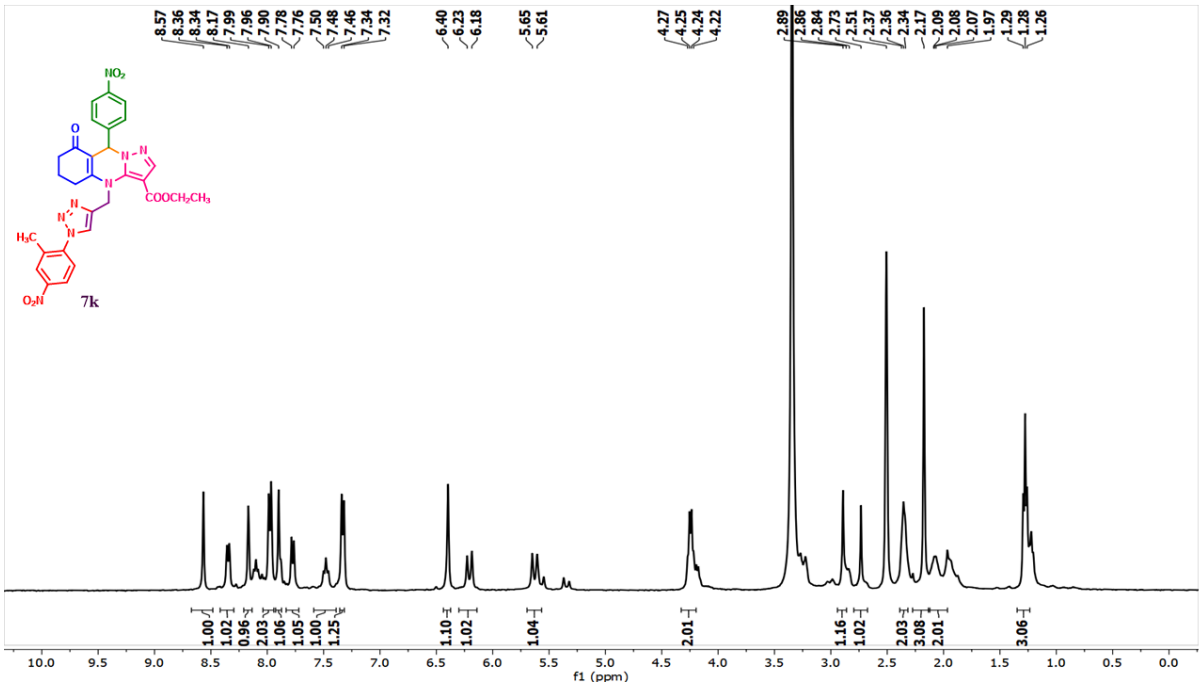

Figure S61. ^{1}H NMR spectrum of ethyl 4-((1-(2-methyl-4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(4-nitrophenyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7k).**

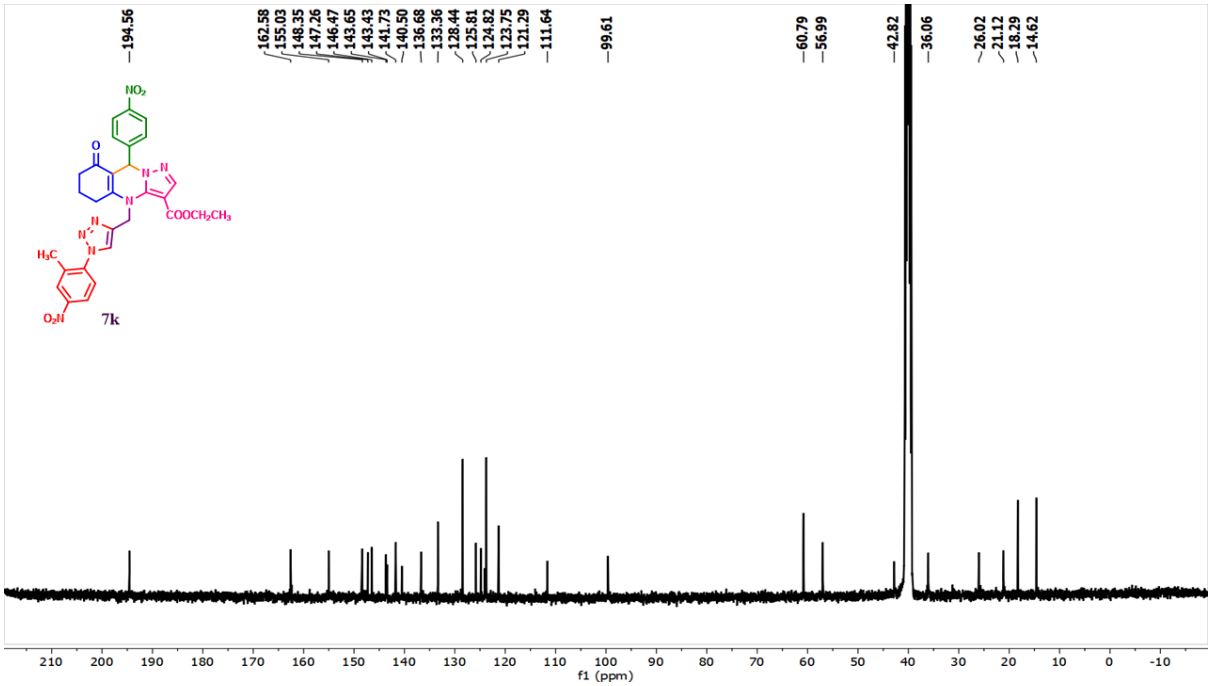

Figure S62. ^{13}C NMR spectrum of ethyl 4-((1-(2-methyl-4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(4-nitrophenyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7k).**

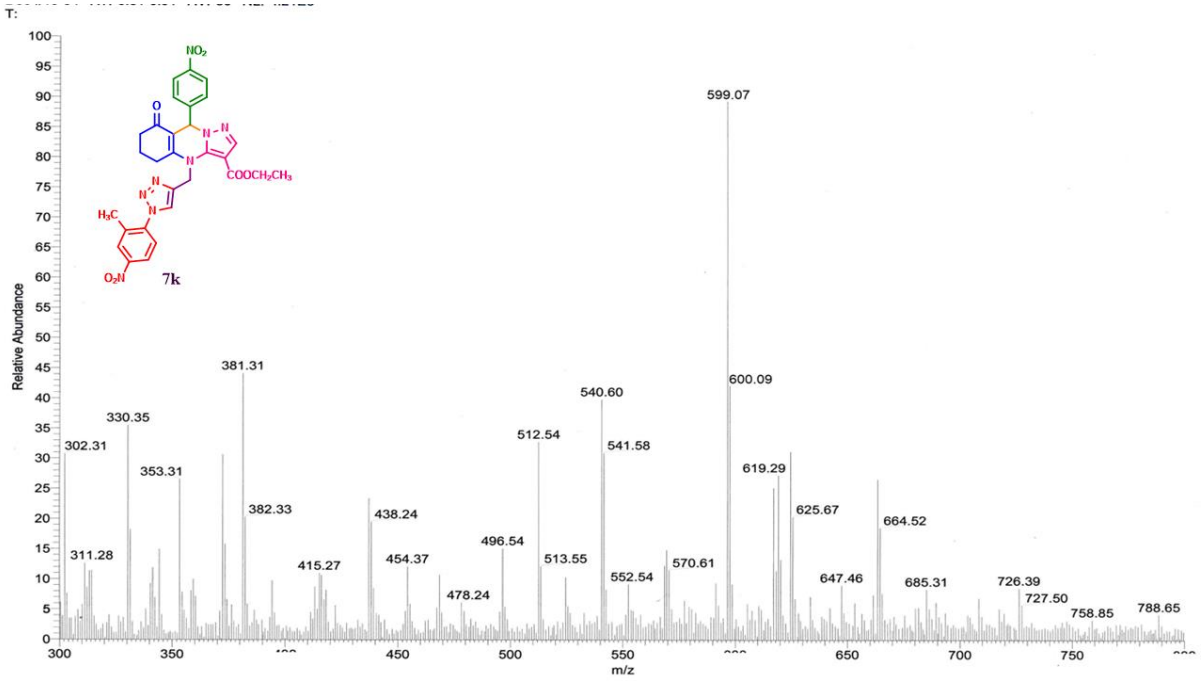

Figure S63. Maas spectrum of ethyl 4-((1-(2-methyl-4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(4-nitrophenyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7k).**

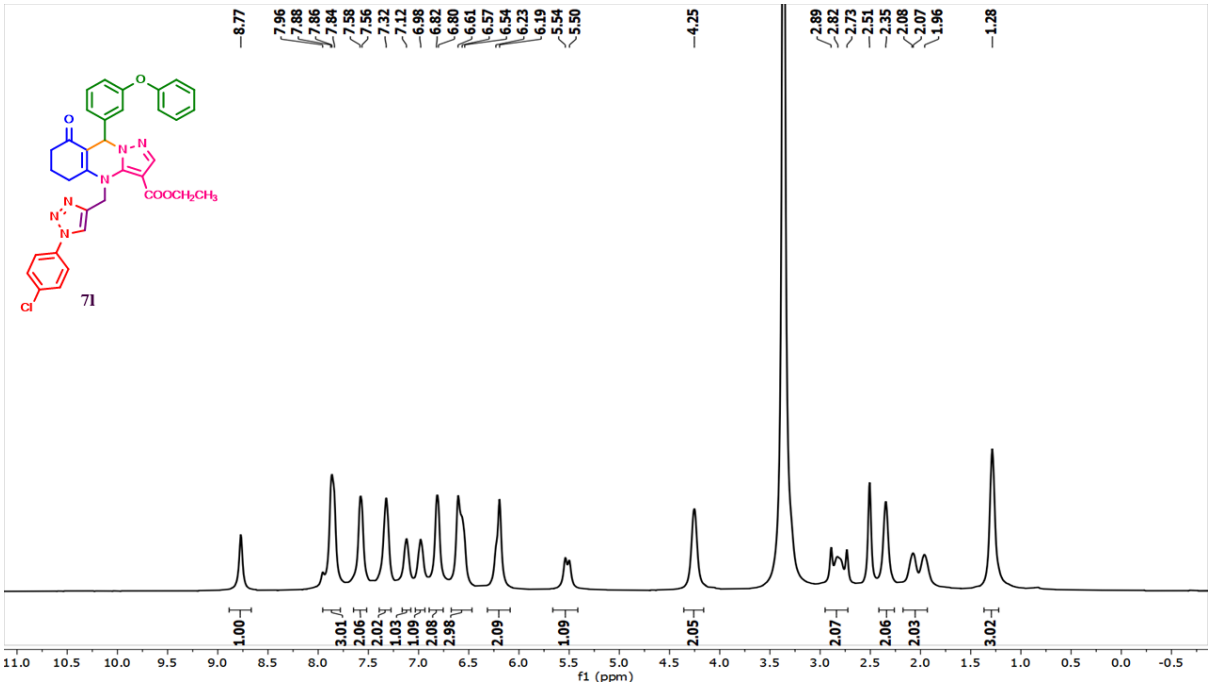

Figure S64. ^{1}H NMR spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-9-(3-phenoxyphenyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7l).**

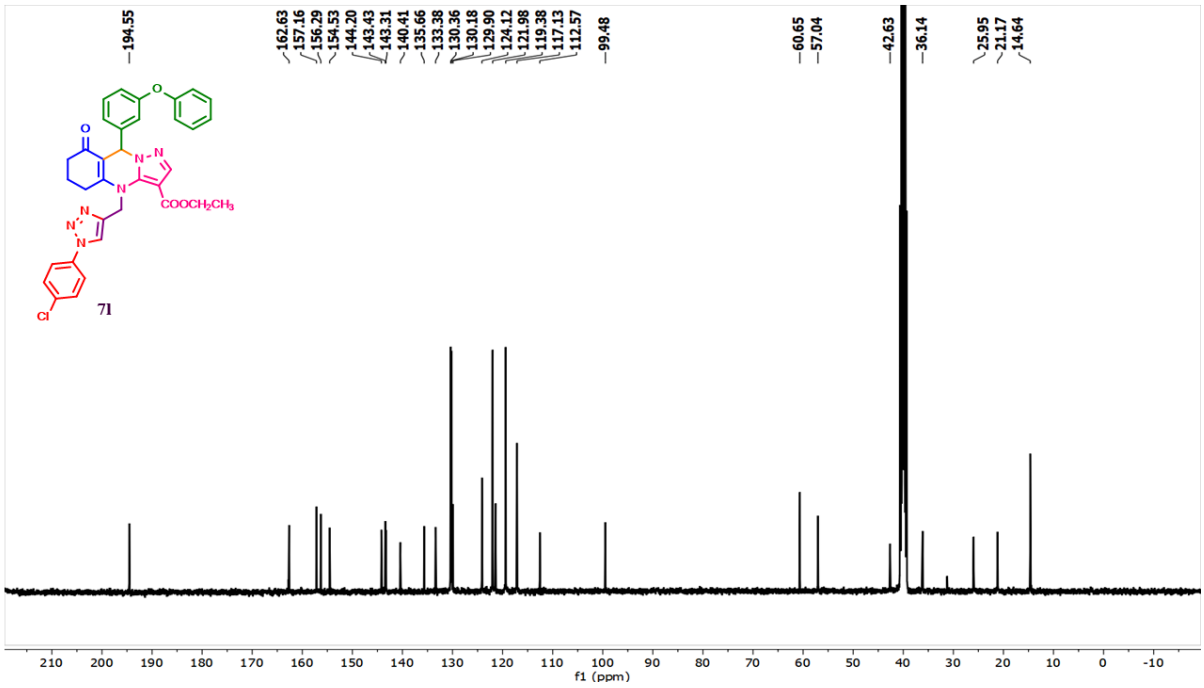

Figure S65. ^{13}C NMR spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-9-(3-phenoxyphenyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7l).**

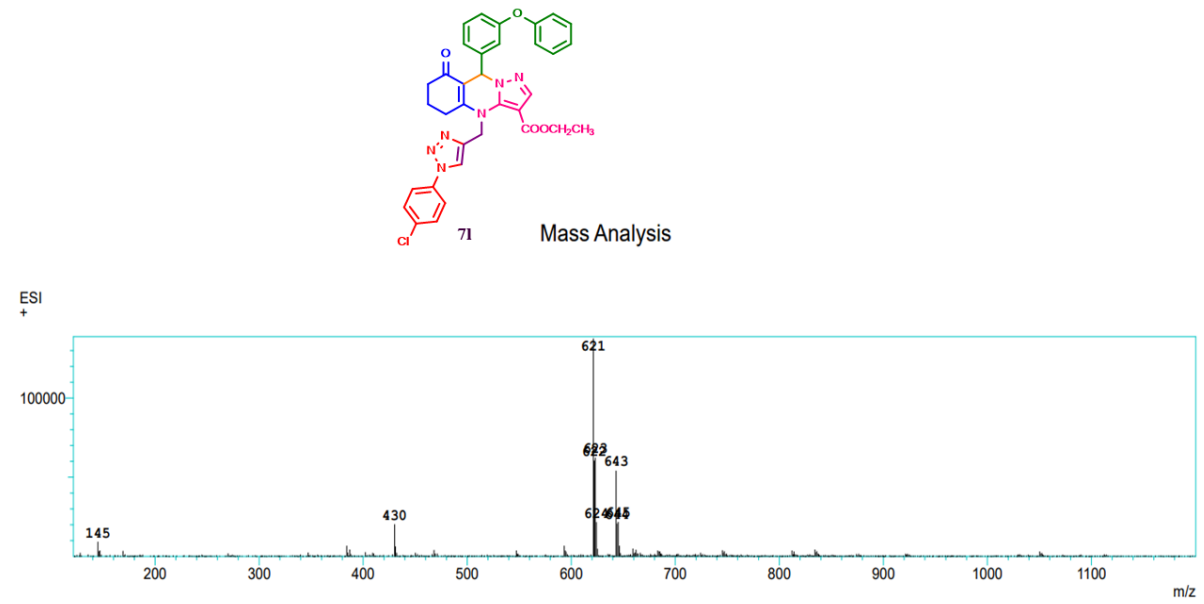

Figure S66. Maas spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-9-(3-phenoxyphenyl)-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7l).**

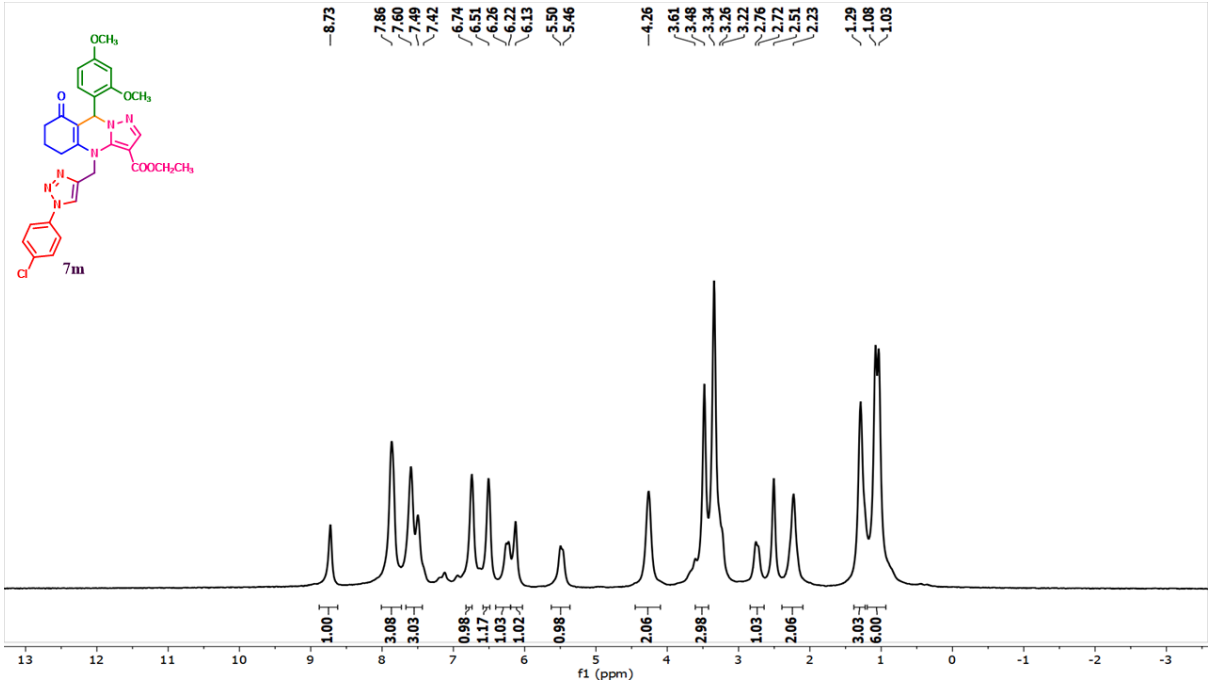

Figure S67. [1]H NMR spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(2,4-dimethoxyphenyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7m).**

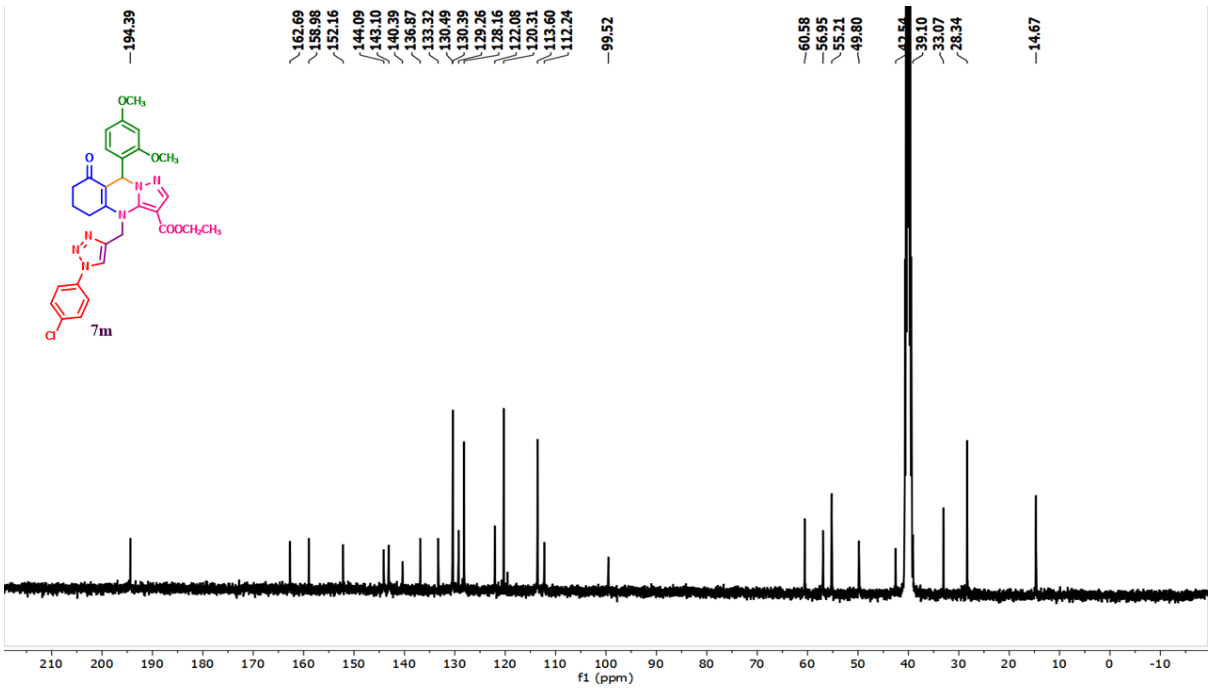

Figure S68. [13]C NMR spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(2,4-dimethoxyphenyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7m).**

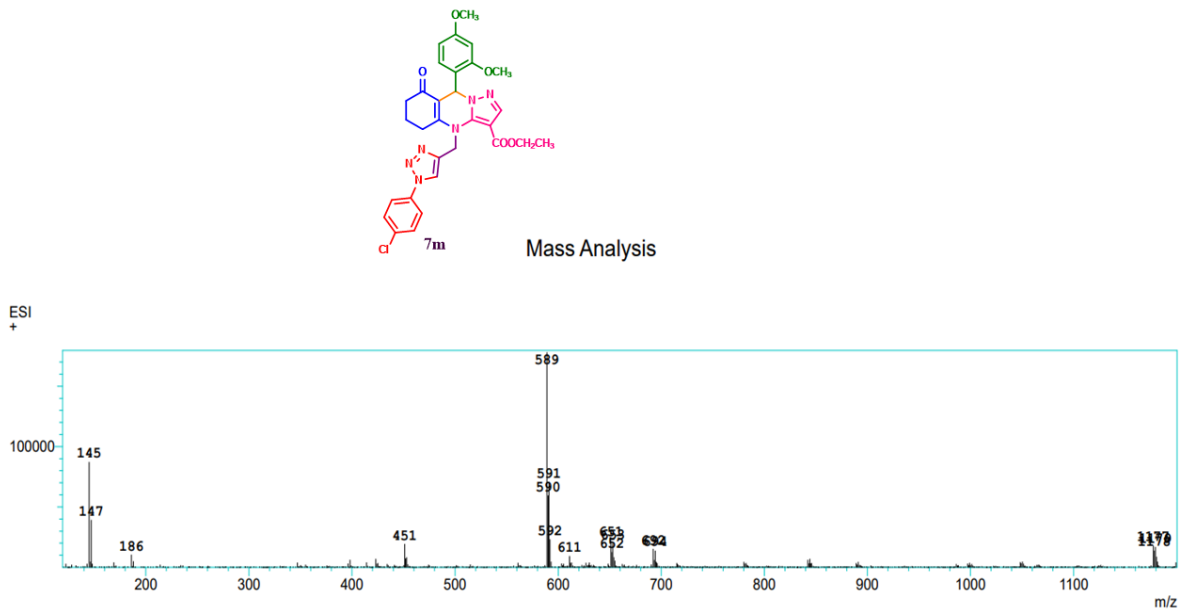

Figure S69. Maas spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(2,4-dimethoxyphenyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7m).**

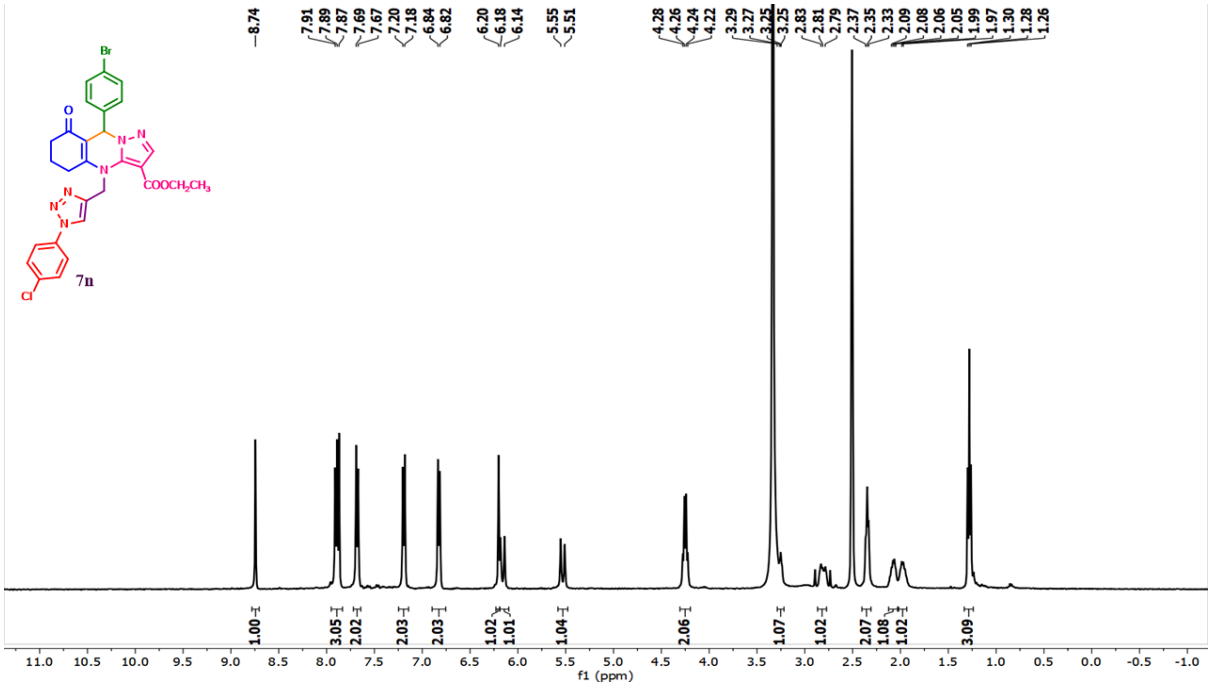

Figure S70. [1]H NMR spectrum of ethyl 9-(4-bromophenyl)-4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7n).**

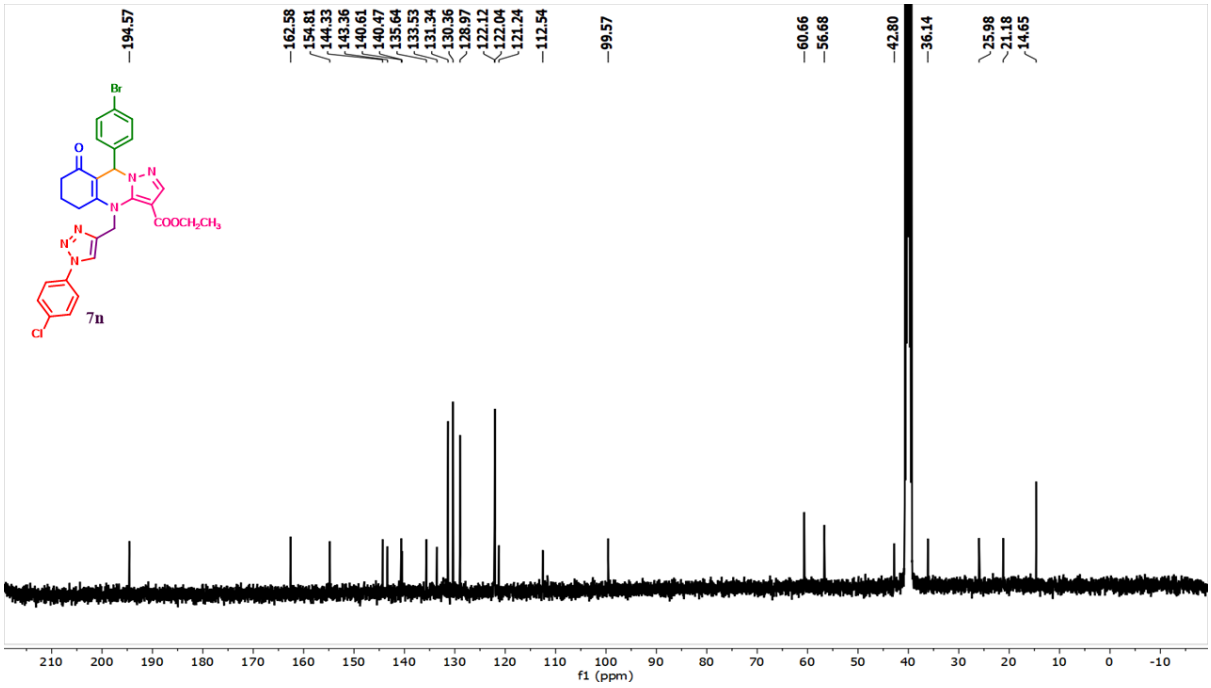

Figure S71. ^{13}C NMR spectrum ethyl 9-(4-bromophenyl)-4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7n).**

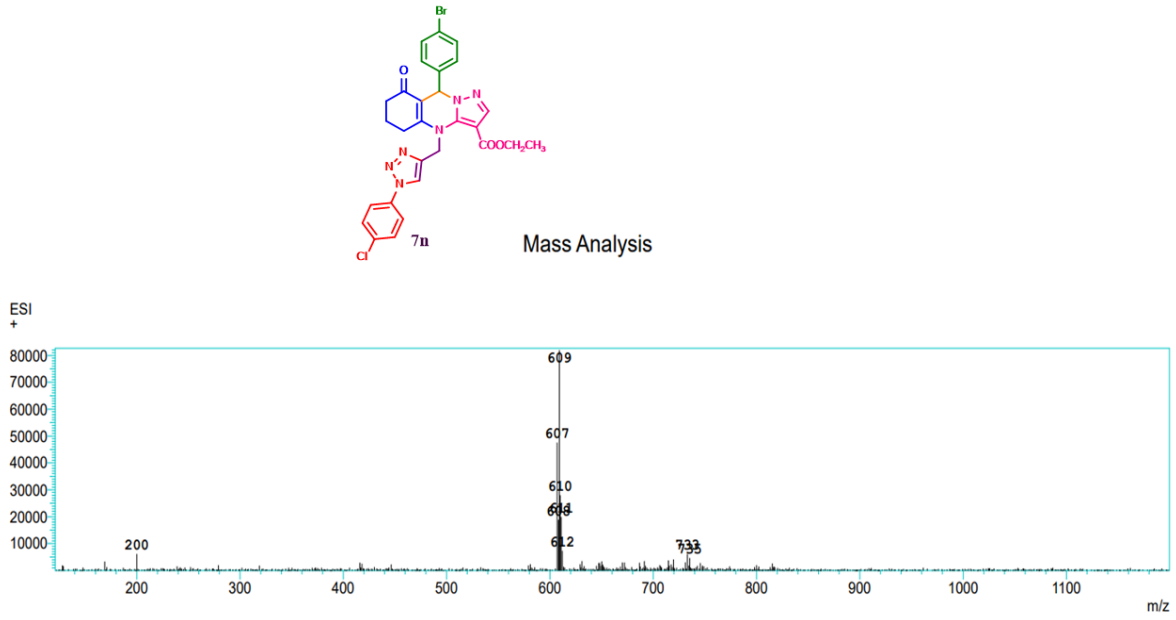

Figure S72. Maas spectrum of ethyl 9-(4-bromophenyl)-4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7n).**

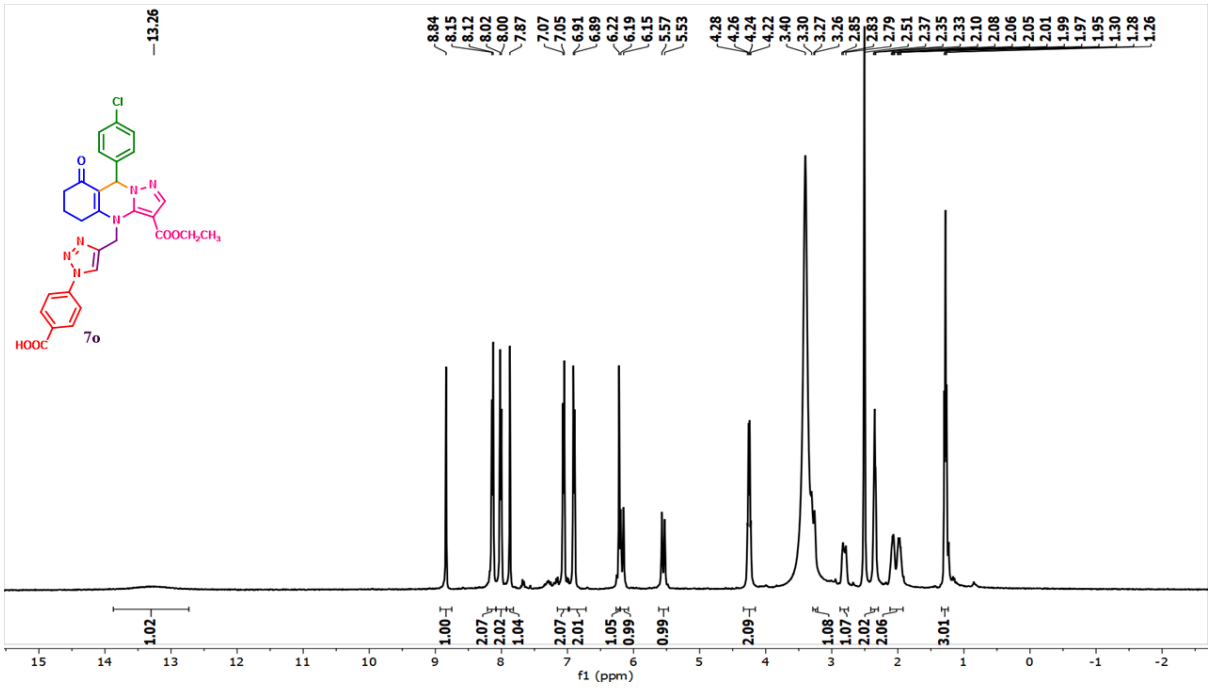

Figure S73. [1]H NMR spectrum ethyl 4-(4-((9-(4-chlorophenyl)-3-(ethoxycarbonyl)-8-oxo-5,7,8,9-tetrahydropyrazolo[5,1-b]quinazolin-4(6H)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)benzoic acid **(7o).**

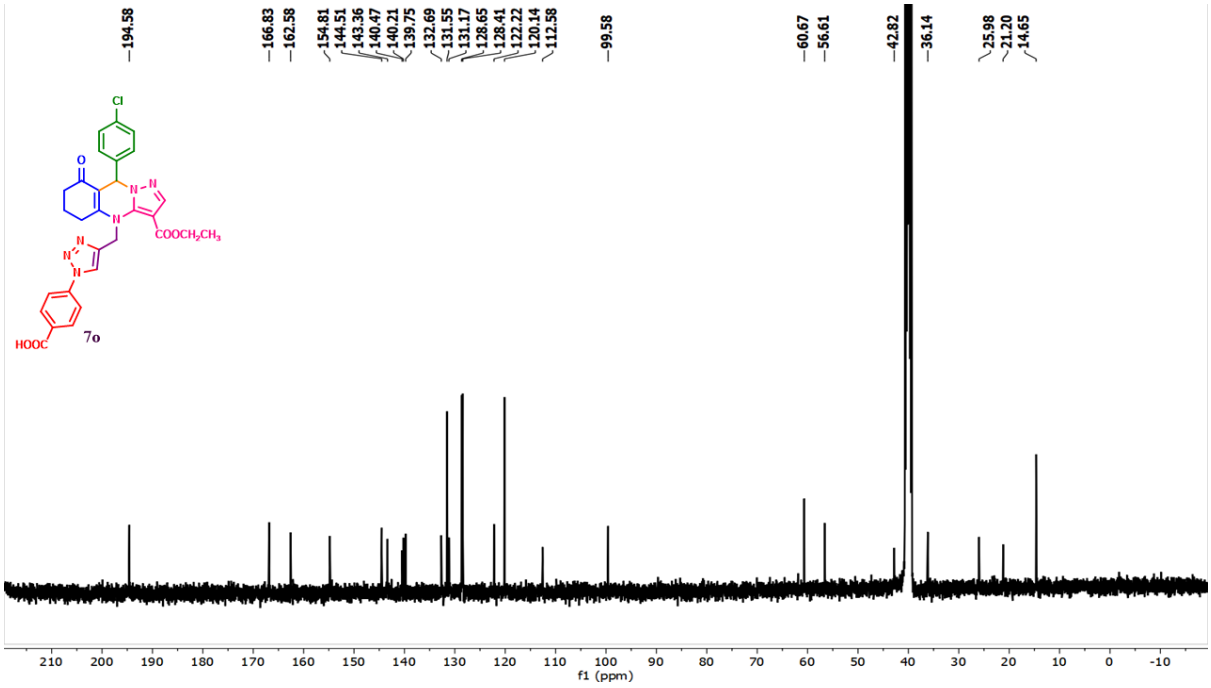

Figure S74. [13]C NMR spectrum of ethyl 4-(4-((9-(4-chlorophenyl)-3-(ethoxycarbonyl)-8-oxo-5,7,8,9-tetrahydropyrazolo[5,1-b]quinazolin-4(6H)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)benzoic acid **(7o).**

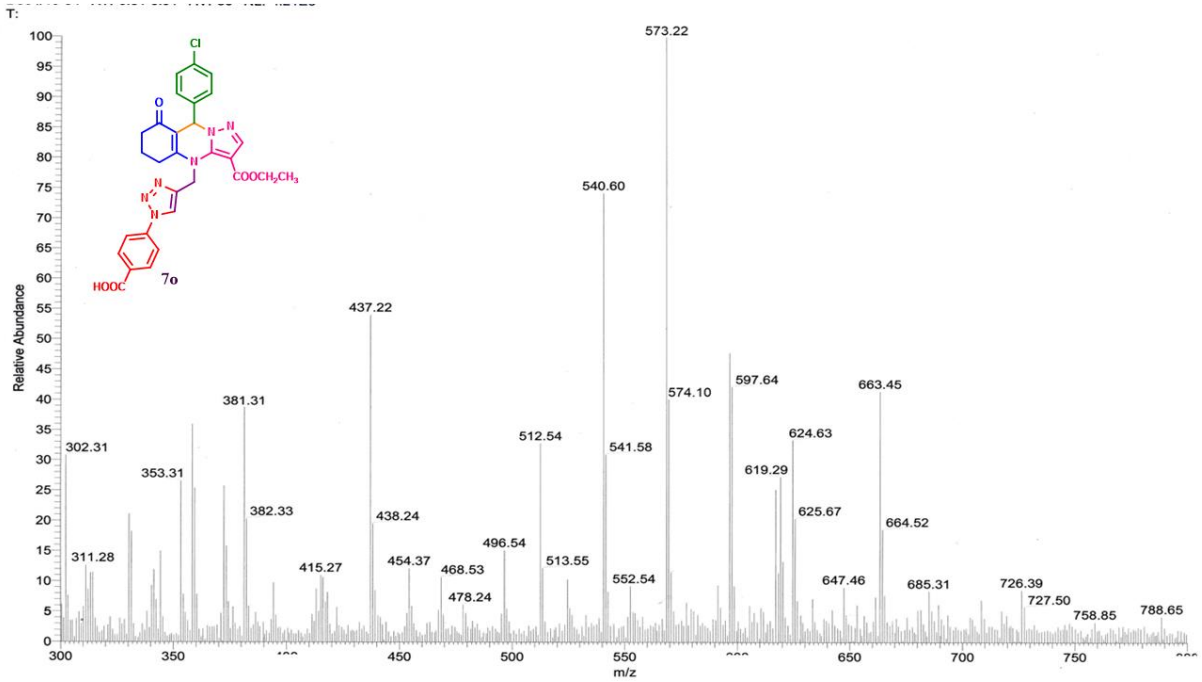

Figure S75. Maas spectrum of ethyl 4-(4-((9-(4-chlorophenyl)-3-(ethoxycarbonyl)-8-oxo-5,7,8,9-tetrahydropyrazolo[5,1-b]quinazolin-4(6H)-yl)methyl)-1*H*-1,2,3-triazol-1-yl)benzoic acid **(7o).**

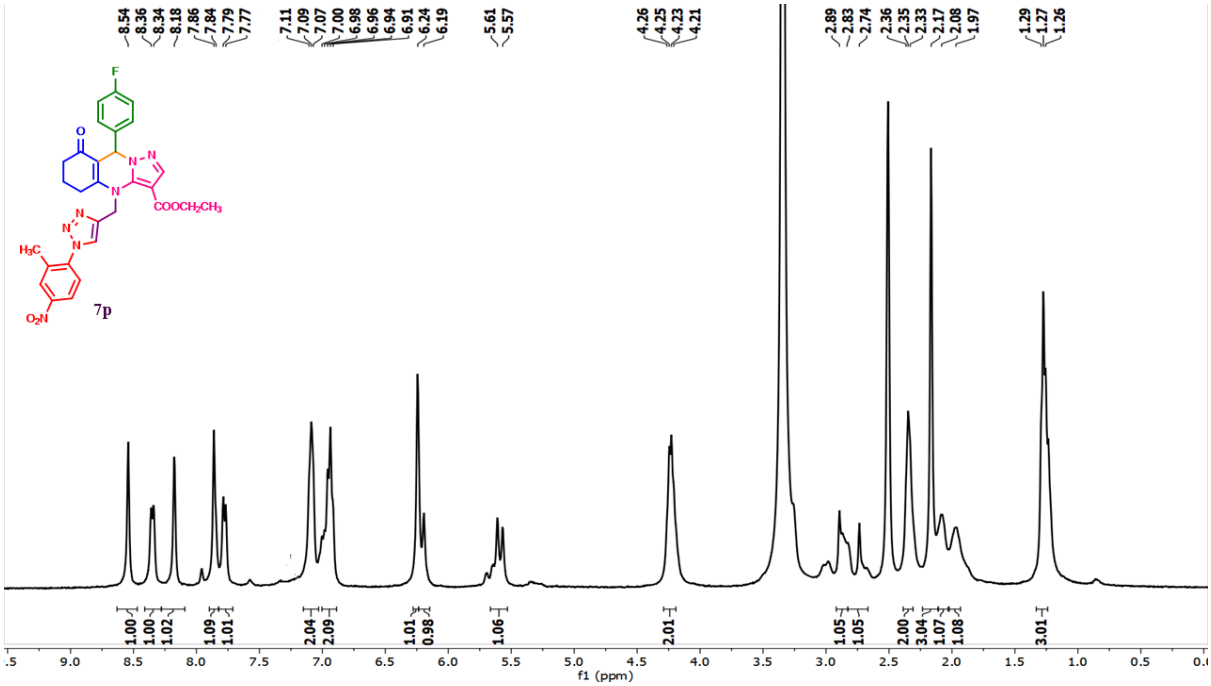

Figure S76. ^{1}H NMR spectrum of ethyl 9-(4-fluorophenyl)-4-((1-(2-methyl-4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7p).**

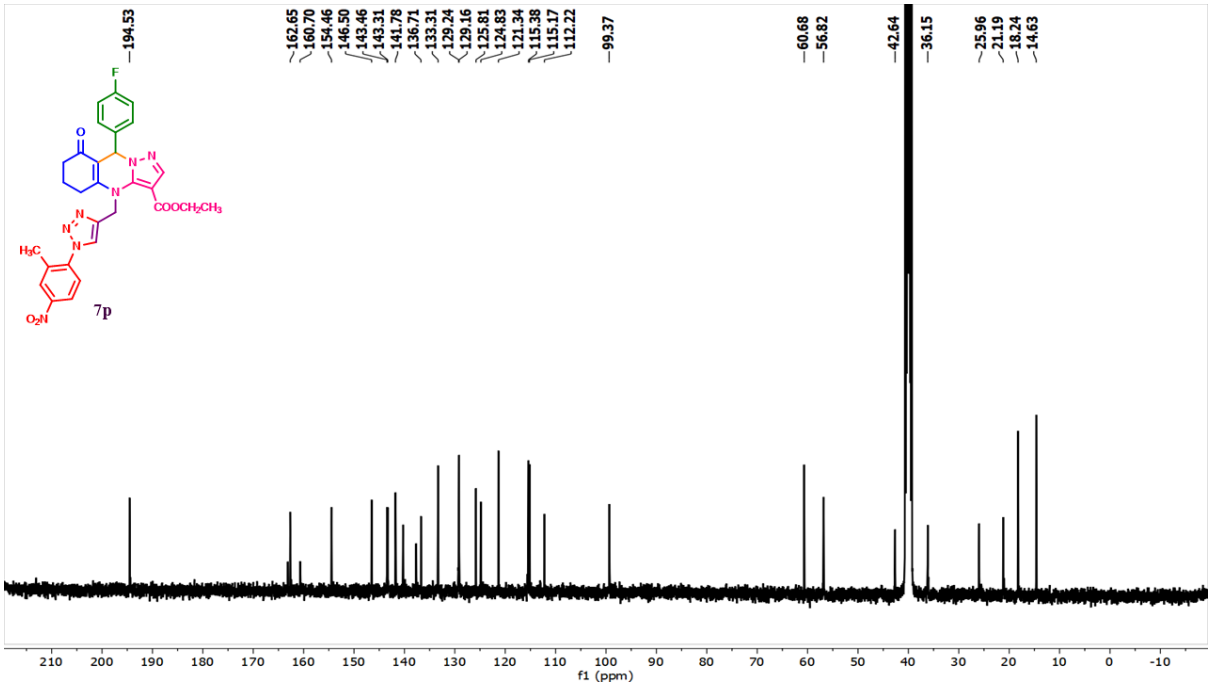

Figure S77. ^{13}C NMR spectrum of ethyl 9-(4-fluorophenyl)-4-((1-(2-methyl-4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7p).**

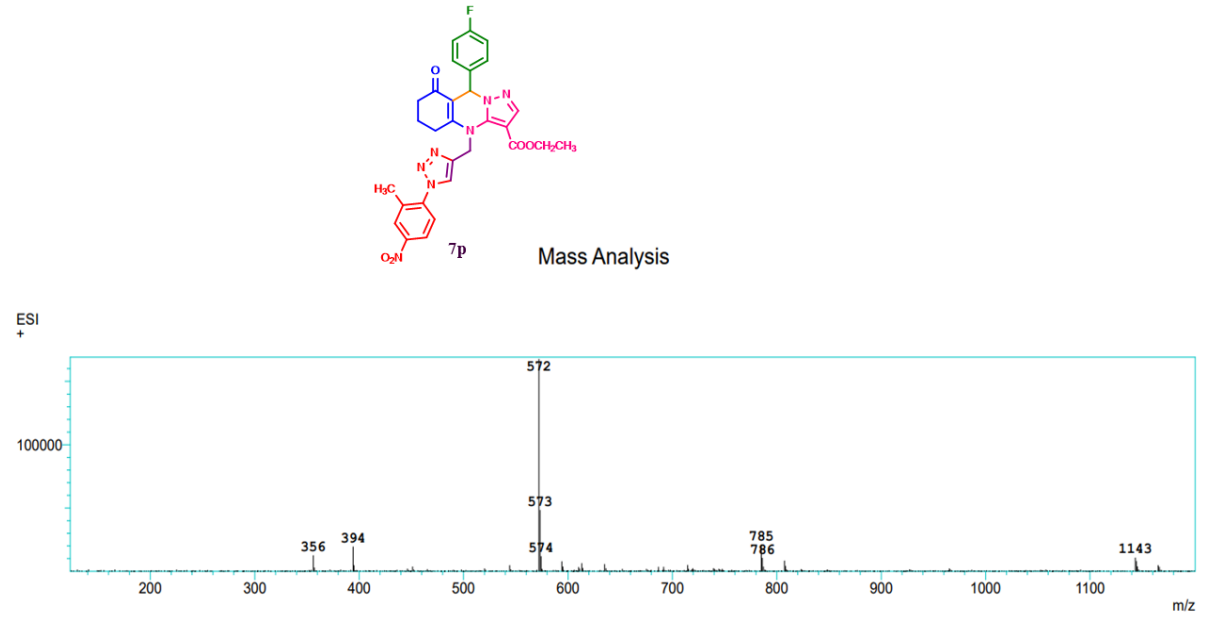

Figure S78. Maas spectrum of ethyl 9-(4-fluorophenyl)-4-((1-(2-methyl-4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7p).**

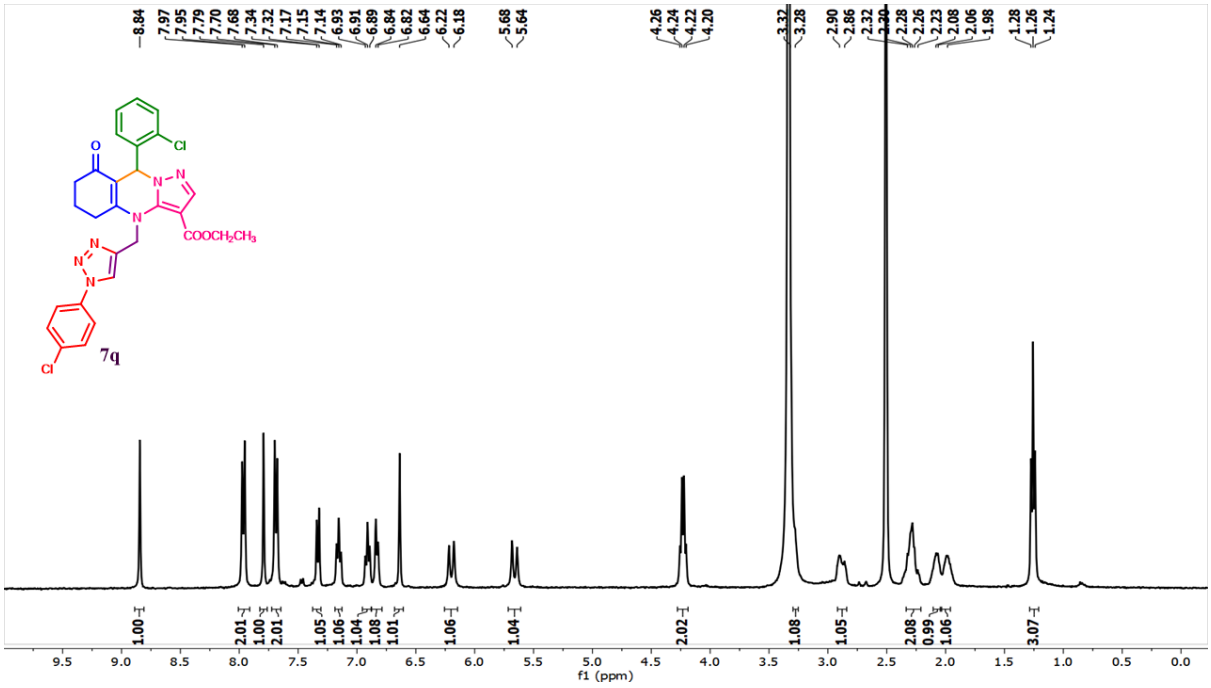

Figure S79. [1]H NMR spectrum of ethyl 9-(2-chlorophenyl)-4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7q).**

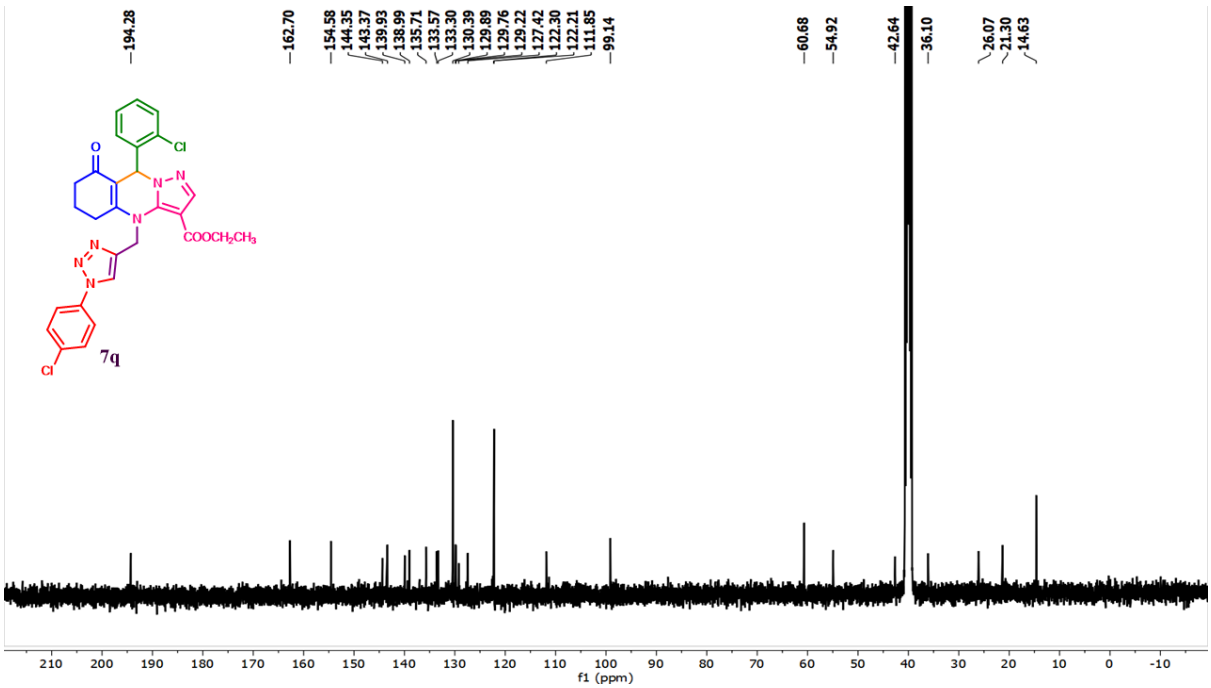

Figure S80. [13]C NMR spectrum of ethyl 9-(2-chlorophenyl)-4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7q).**

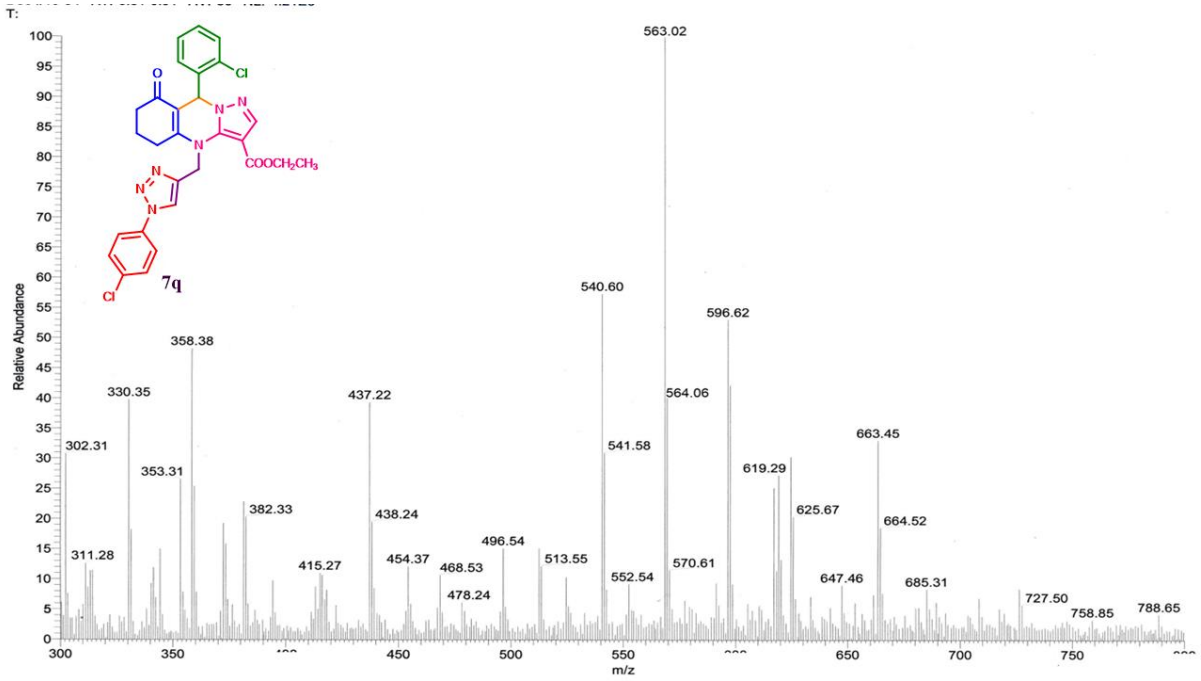

Figure S81. Maas spectrum of ethyl 9-(2-chlorophenyl)-4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7q).**

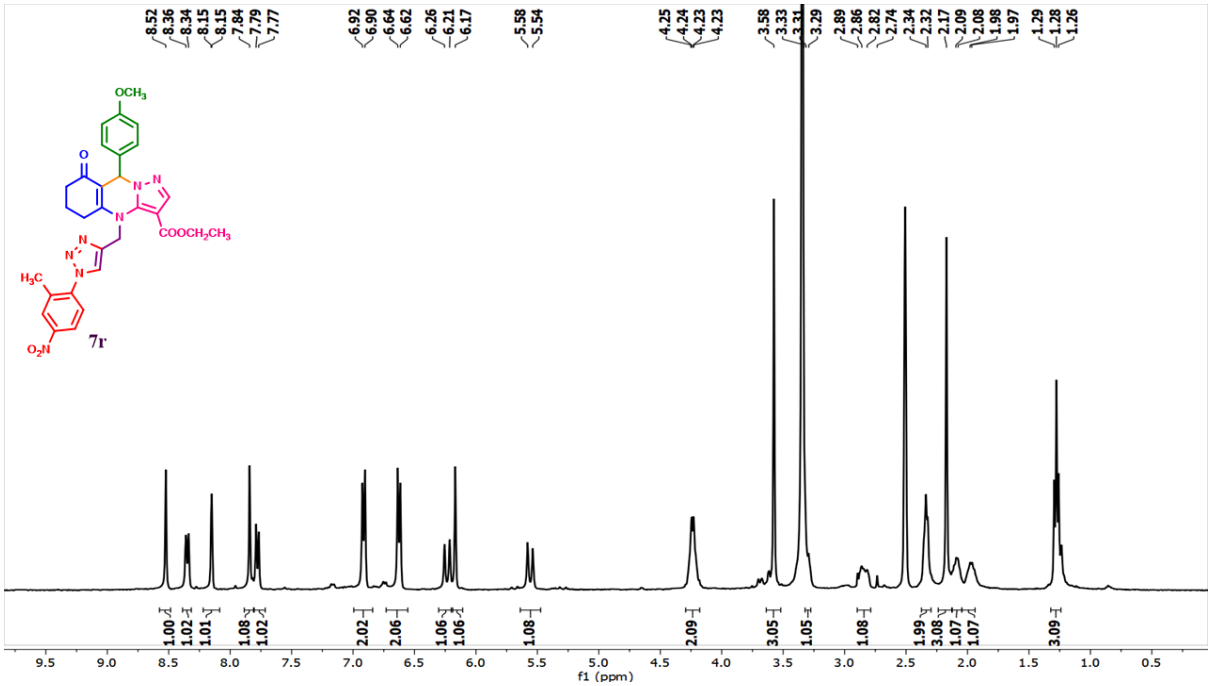

Figure S82. ^{1}H NMR spectrum of ethyl 9-(4-methoxyphenyl)-4-((1-(2-methyl-4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7r).**

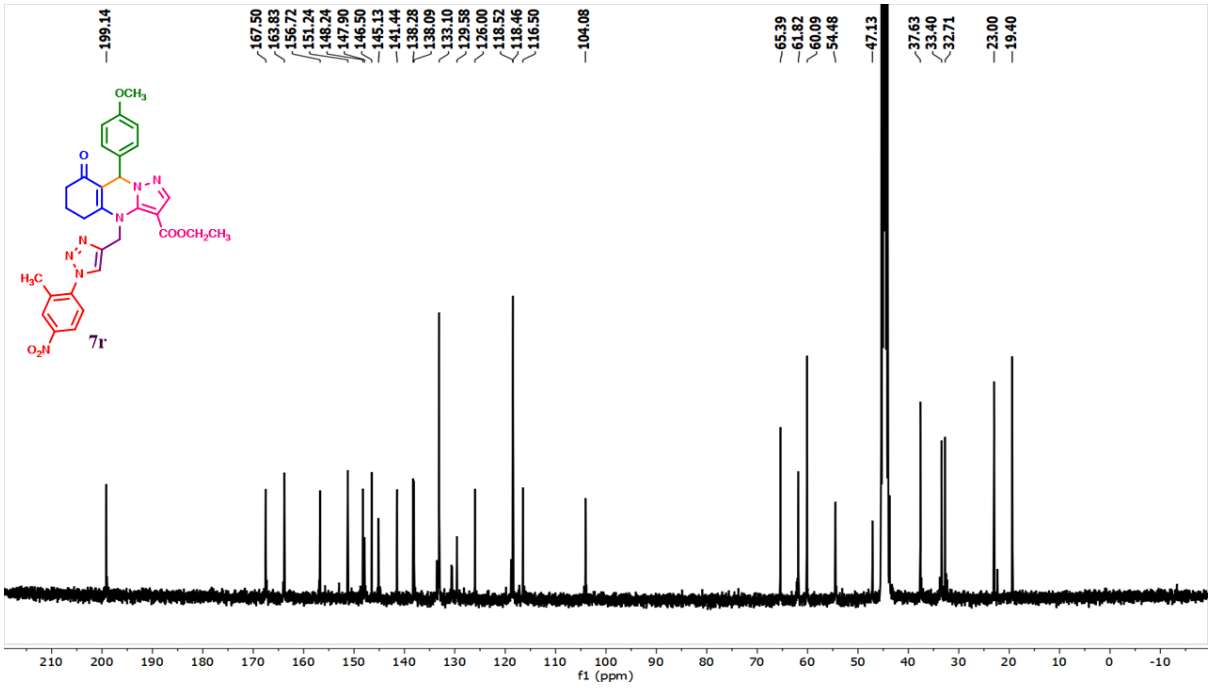

Figure S83. ^{13}C NMR spectrum of ethyl 9-(4-methoxyphenyl)-4-((1-(2-methyl-4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7r).**

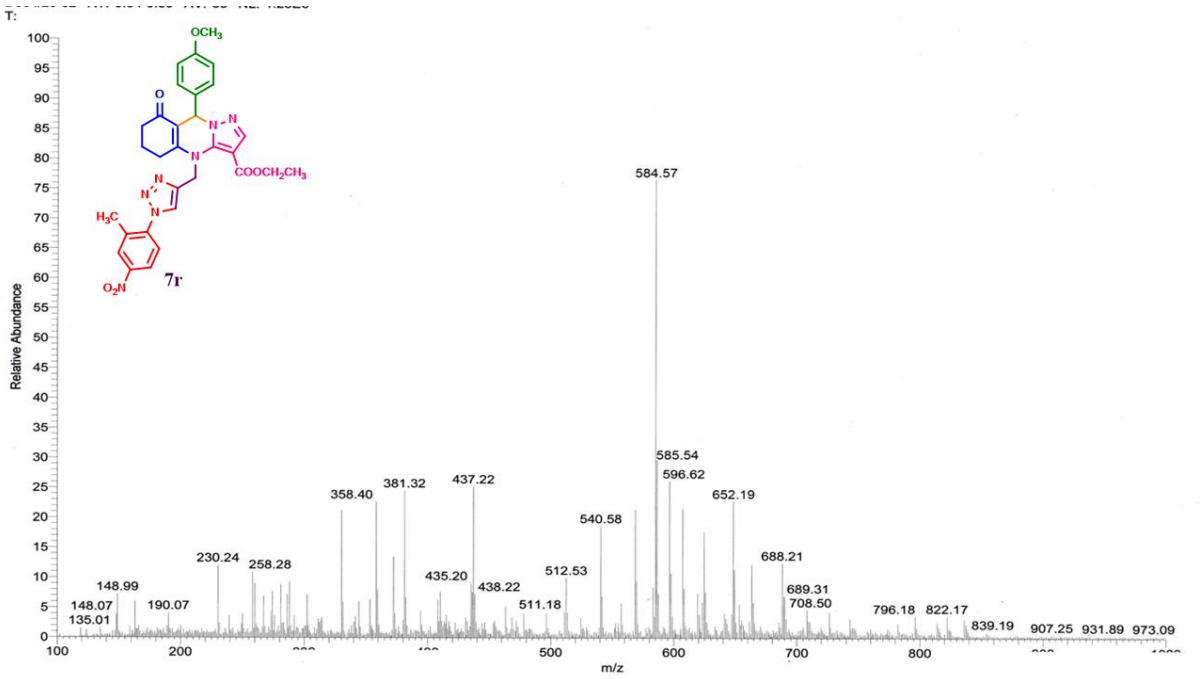

Figure S84. Maas spectrum of ethyl 9-(4-methoxyphenyl)-4-((1-(2-methyl-4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7r).**

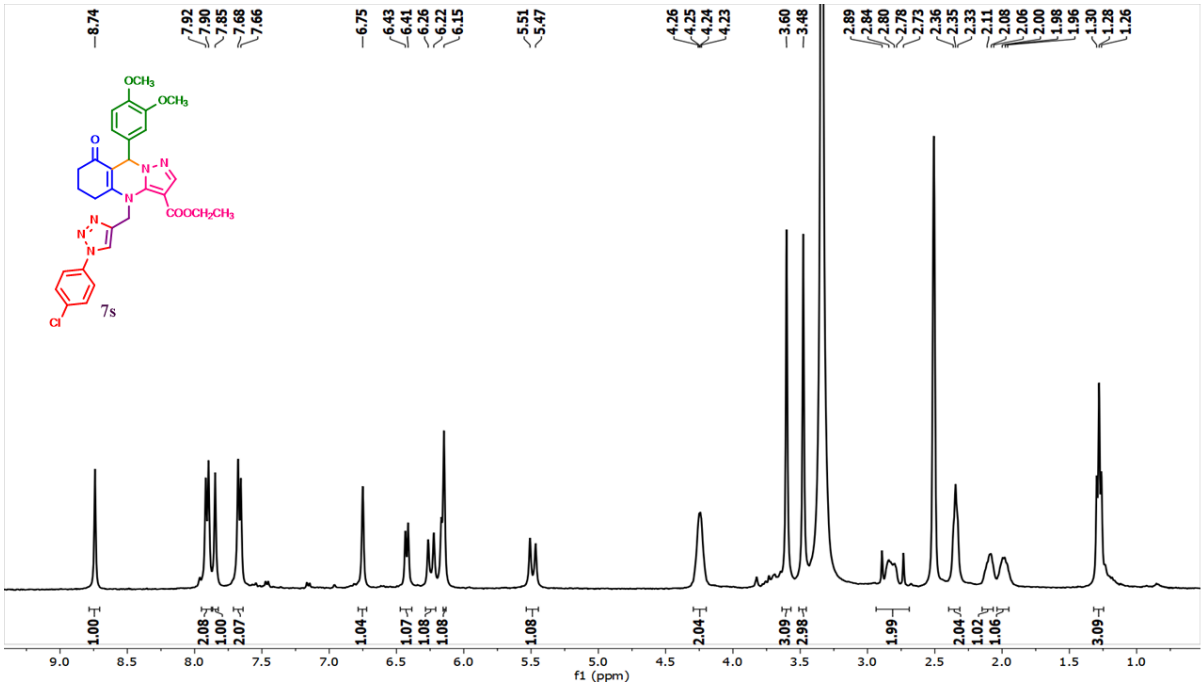

Figure S85. [1]H NMR spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(3,4-dimethoxyphenyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7s).**

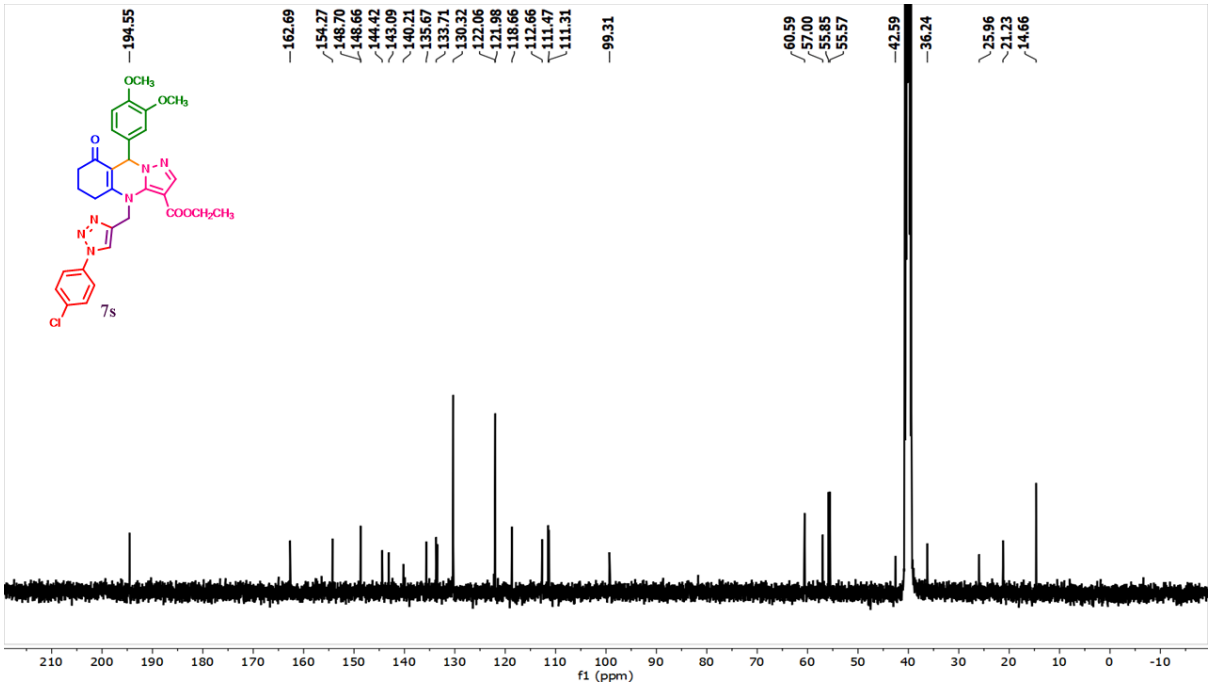

Figure S86. [13]C NMR spectrum ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(3,4-dimethoxyphenyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7s).**

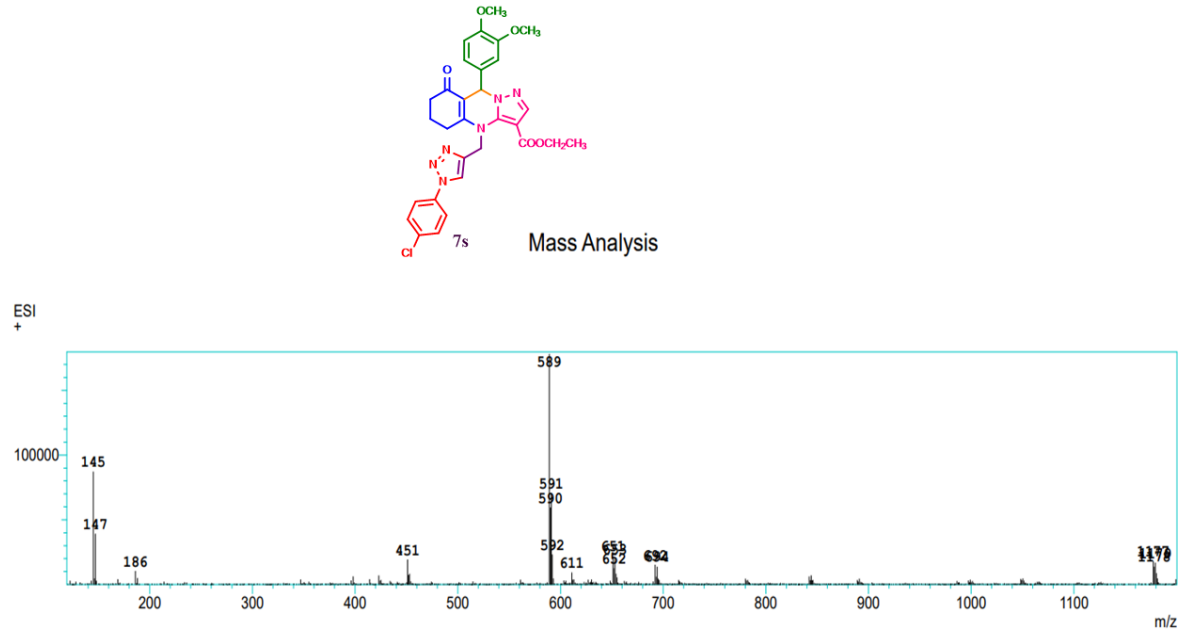

Figure S87. Maas spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(3,4-dimethoxyphenyl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7s).**

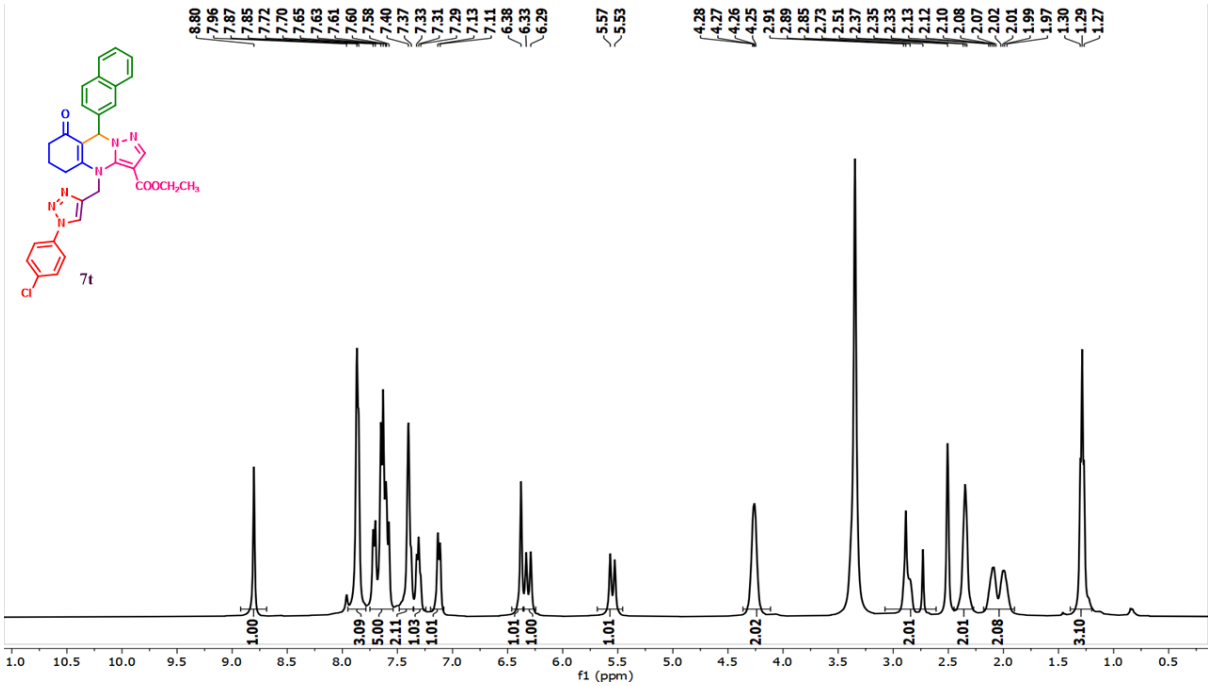

Figure S88. ^{1}H NMR spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(naphthalen-2-yl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7t).**

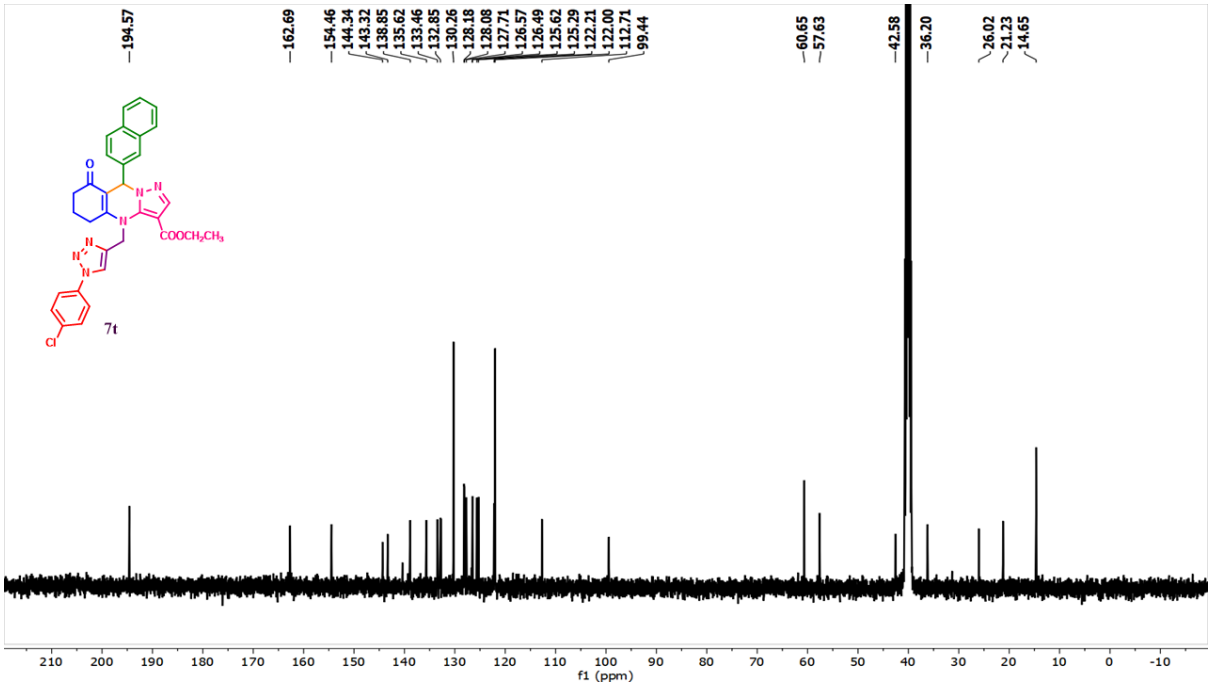

Figure S89. ^{13}C NMR spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(naphthalen-2-yl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7t).**

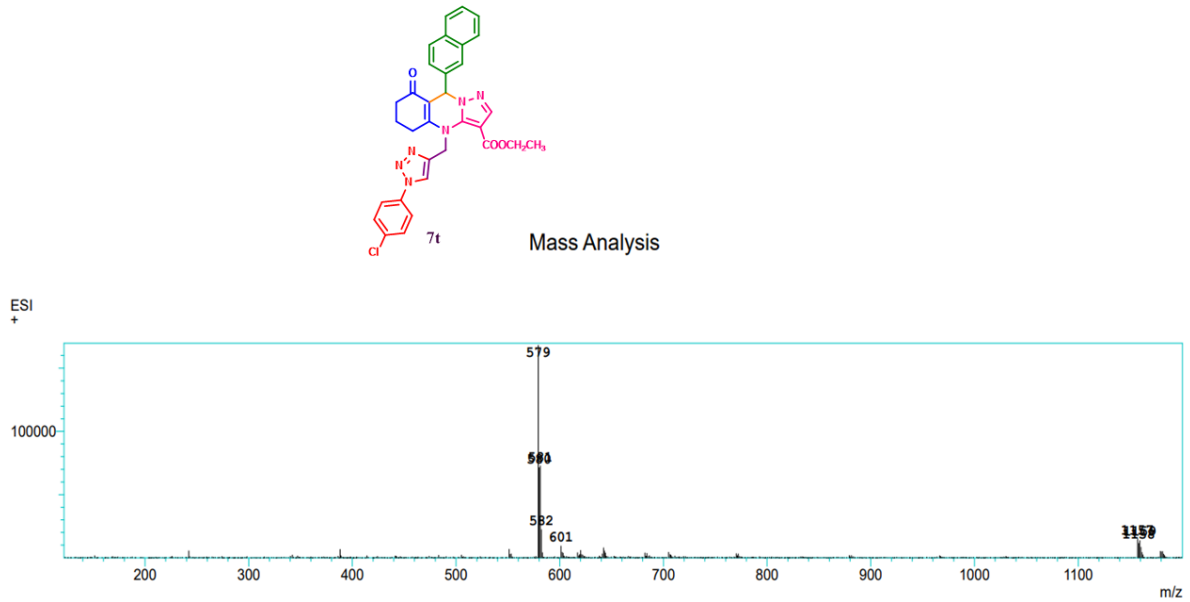

Figure S90. Maas spectrum of ethyl 4-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-9-(naphthalen-2-yl)-8-oxo-4,5,6,7,8,9-hexahydropyrazolo[5,1-b]quinazoline-3-carboxylate **(7t).**