

## Supporting Information

for

### **Ultrasound-assisted One-Pot Synthesis of tetrazolo[1,5-*a*]pyrimidines and their pharmacological evaluations**

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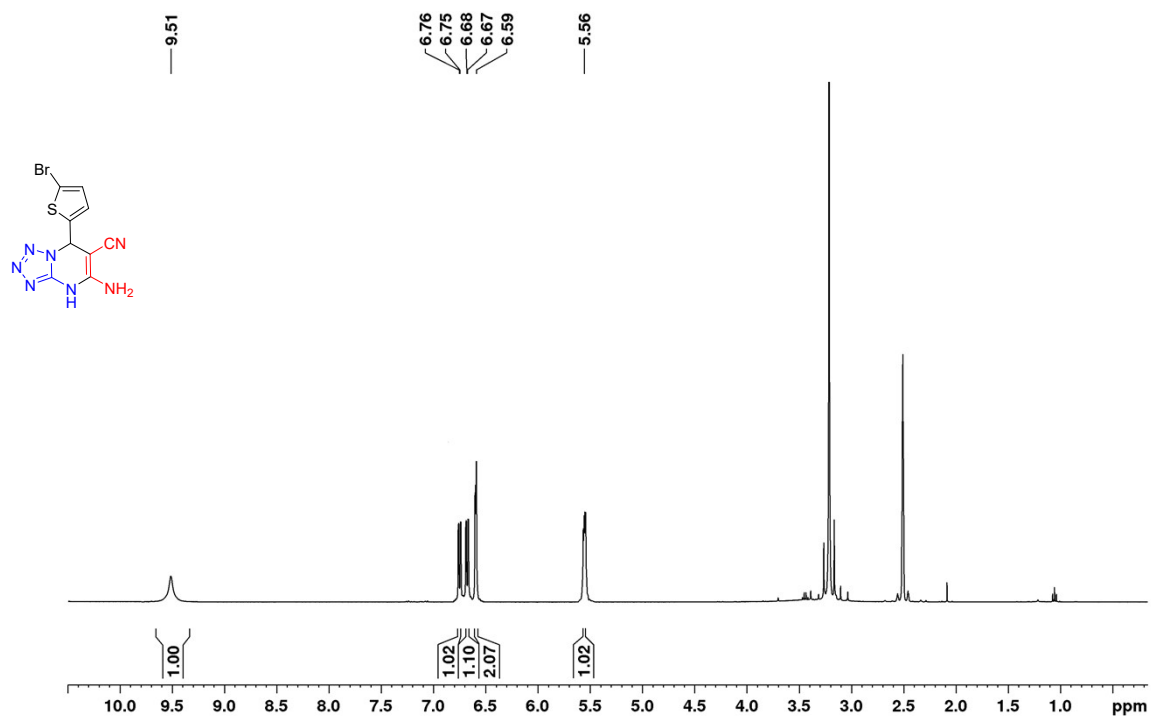
## 1. General method

The chemicals necessary for the reactions were sourced from Sigma-Aldrich, TCI, and Sisco Research Laboratories Pvt. Ltd. in India. Since these chemicals were used as received, no additional purification was required. Reaction progress was monitored using thin-layer chromatography (TLC) on aluminum plates coated with F254 silica gel 60. Melting points of the synthesized compounds were determined using the open capillary tube method, with the data recorded as observed. Nuclear magnetic resonance (NMR) spectra were collected using a 500 MHz JOEL JNM-ECX500II (delta) spectrometer equipped with proton noise decoupling mode and a standard 5mm probe. Samples were dissolved in deuterated DMSO, using d6 as a standard reference. The following abbreviations were used to describe the <sup>1</sup>H NMR signals: "s" for singlet, "d" for doublet, "t" for triplet, "q" for quartet, "dd" for double doublet, and "m" for multiplet. Chemical shifts are reported in parts per million (ppm), and coupling constants (J) are given in Hertz (Hz).

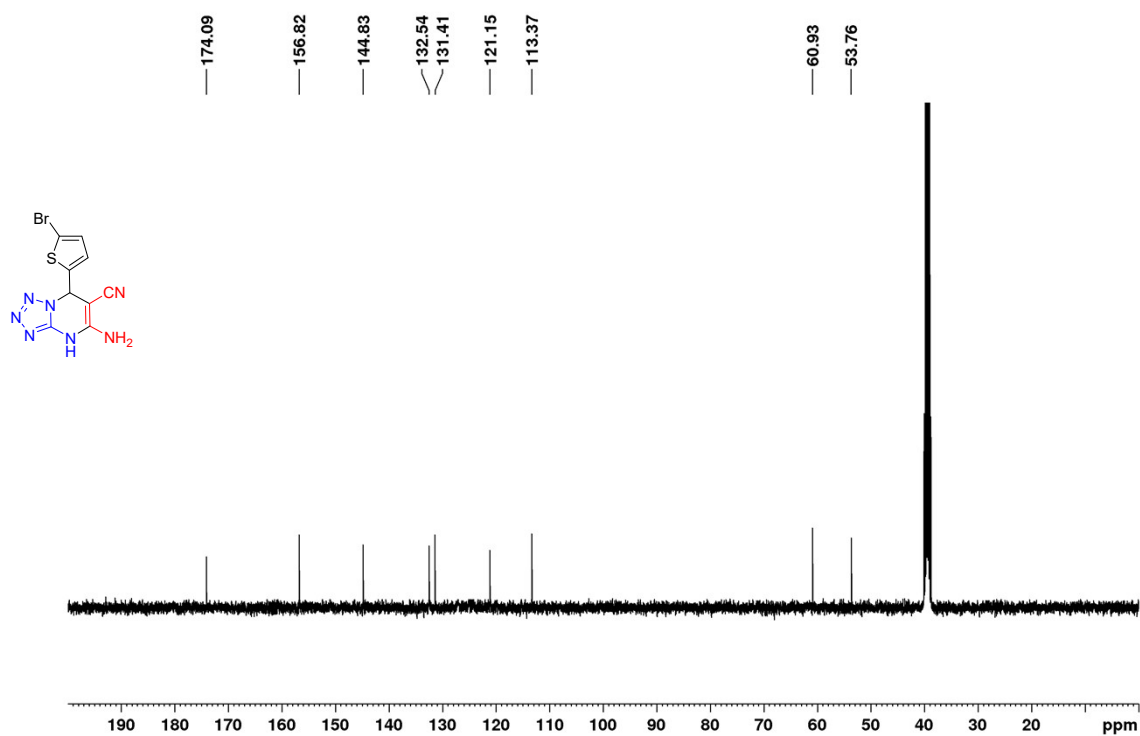
## 2. General procedure for the synthesis of tetrazolo[1,5-a]pyrimidine 4(a-l)

Compounds **4(a-l)** were synthesized via an ultrasound-assisted protocol by reacting 5-aminotetrazole (**1**, **1 mmol**) with either malononitrile (**2a**, **1 mmol**) or acetylacetone (**2b**, **1 mmol**) and a range of heterocyclic aromatic aldehydes (**3(a-f)**, **1 mmol**) in the presence of acetic acid. The reactions were carried out under ultrasonic irradiation (130 W, 28 kHz) for 12–15 minutes. Reaction progress was periodically checked using thin-layer chromatography (TLC). Upon completion, the reaction mixture was allowed to cool to ambient temperature, and water was added to induce precipitation. The resulting solid product was isolated by filtration, washed with a small quantity of ethanol followed by hot water, and dried to obtain the purified compounds.

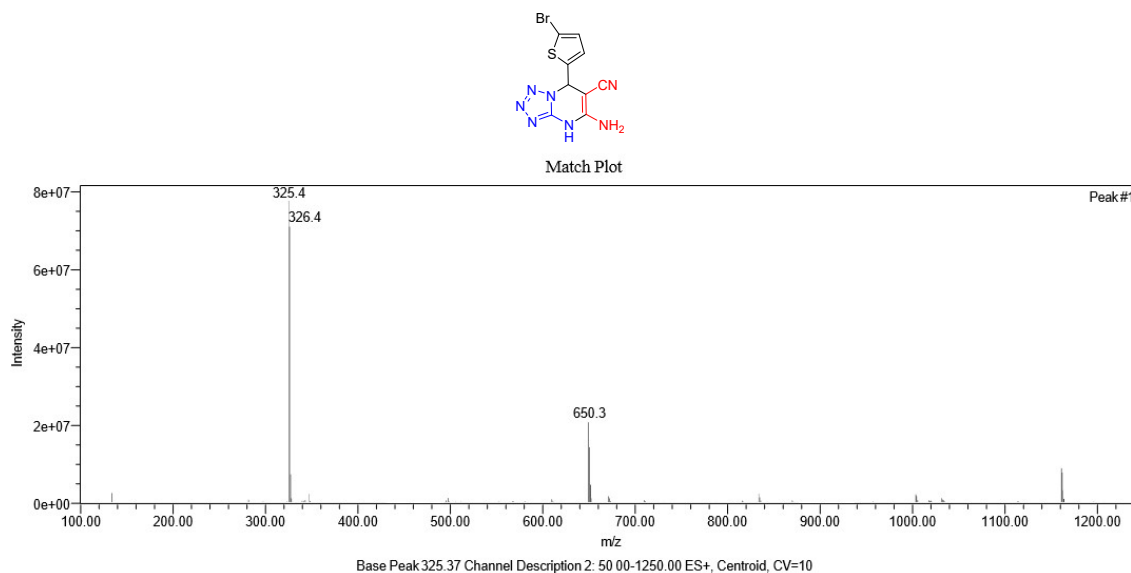
### 3. Scanned copies of $^1\text{H}$ NMR, $^{13}\text{C}$ NMR and MS spectra for all compounds (4a-l)



**Fig S1:**  $^1\text{H}$ -NMR of 5-amino-7-(5-bromothiophen-2-yl)-4,7-dihydro-1H-tetrazolo[1,5-a]pyrimidin-6-carbonitrile (**4a**)



**Fig S2:** <sup>13</sup>C-NMR of 5-amino-7-(5-bromothiophen-2-yl)-4,7-dihydro-1H-tetrazolo[1,5-a]pyrimidin-6-carbonitrile (**4a**)



**Fig S3:** MS of 5-amino-7-(5-bromothiophen-2-yl)-4,7-dihydro-1H-tetrazolo[1,5-a]pyrimidin-6-carbonitrile (**4a**)

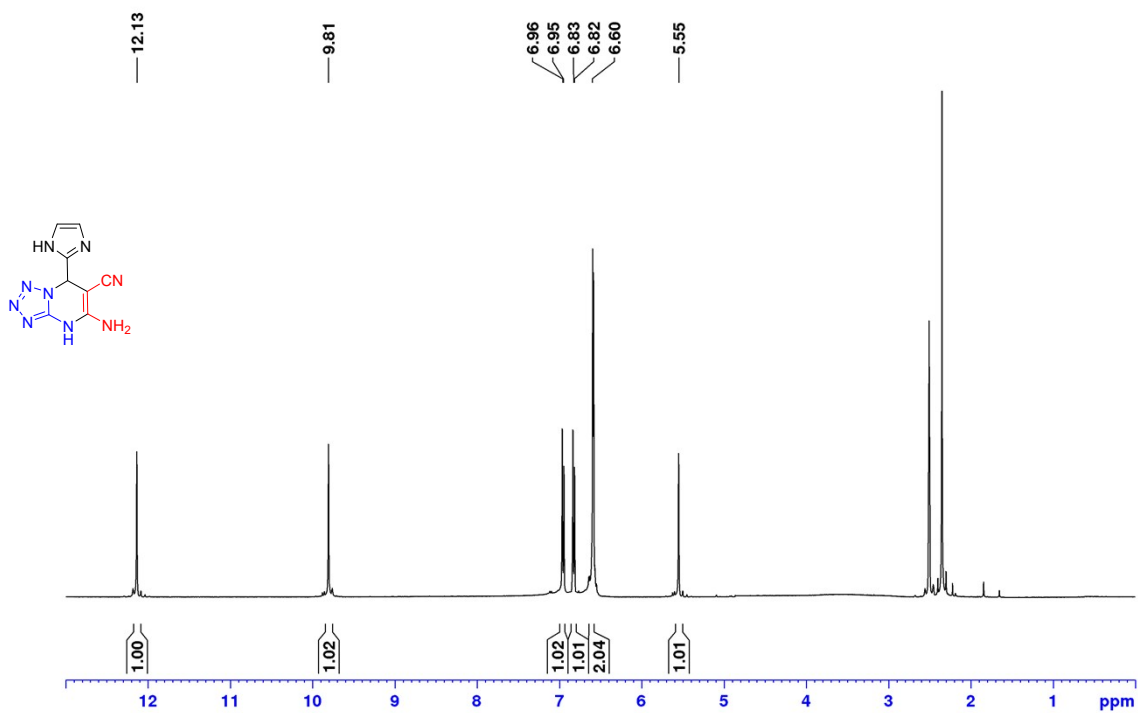
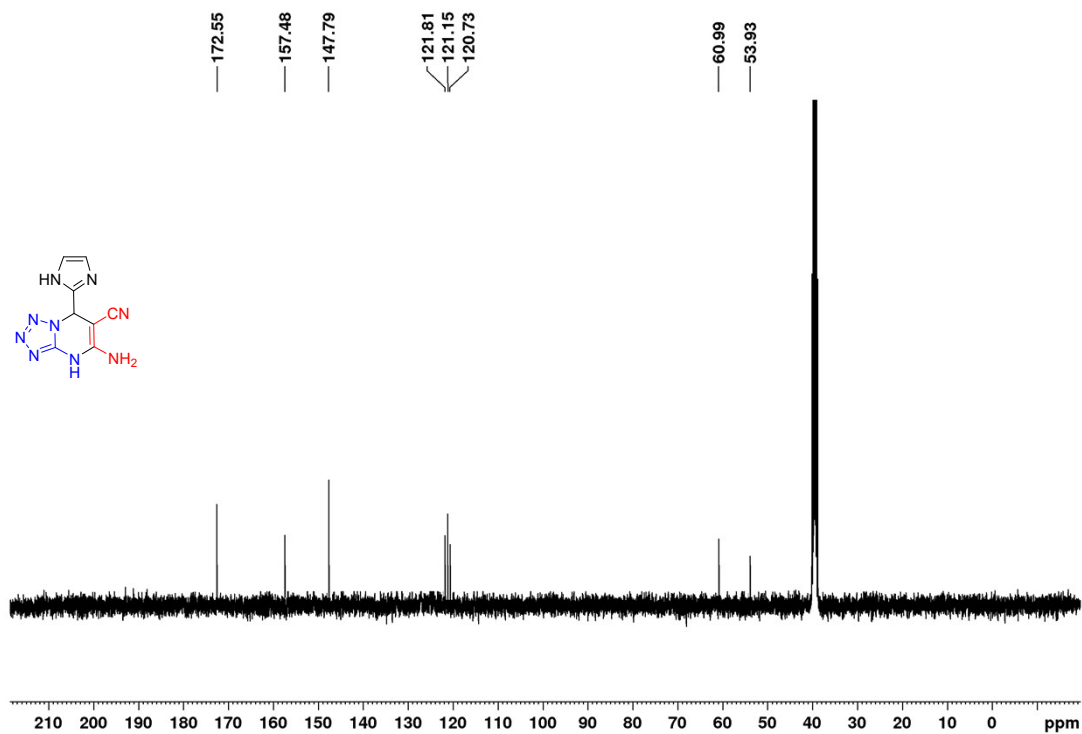
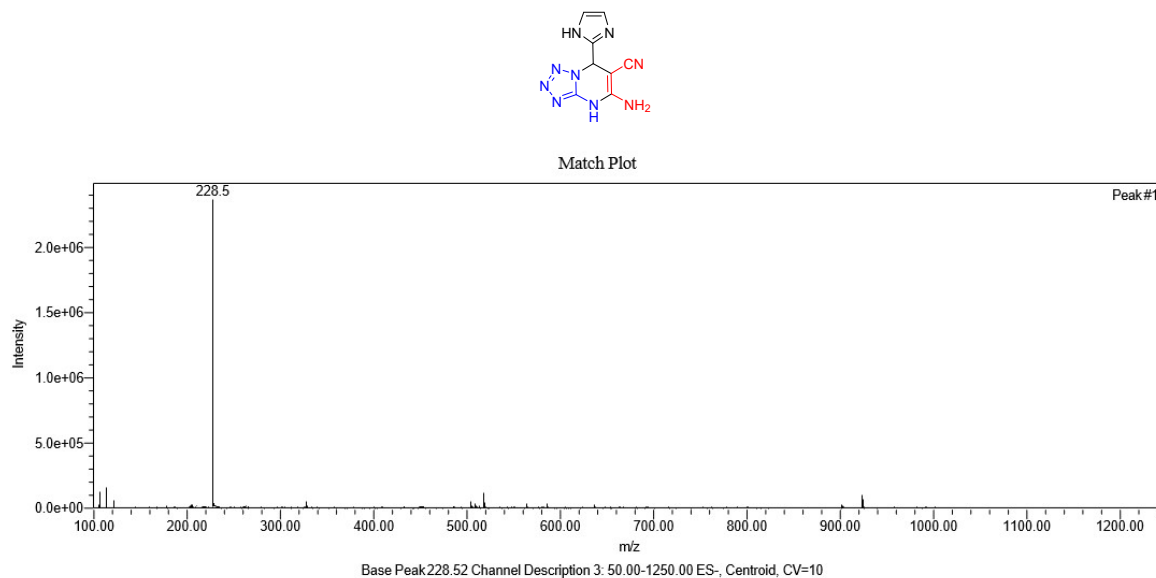


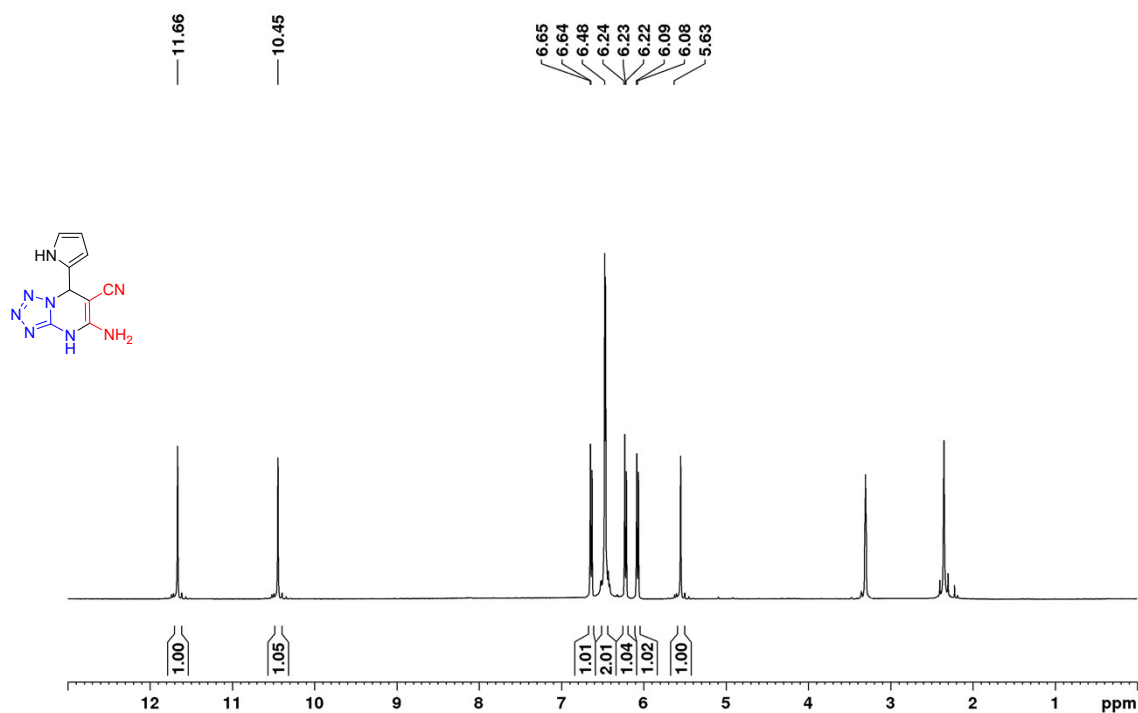
Fig S4: <sup>1</sup>H-NMR of 5-amino-7-(1H-imidazol-2-yl)-4,7-dihydro-1,5-benzotetrazolo[1,5-a]pyrimidin-6-carbonitrile (4b)



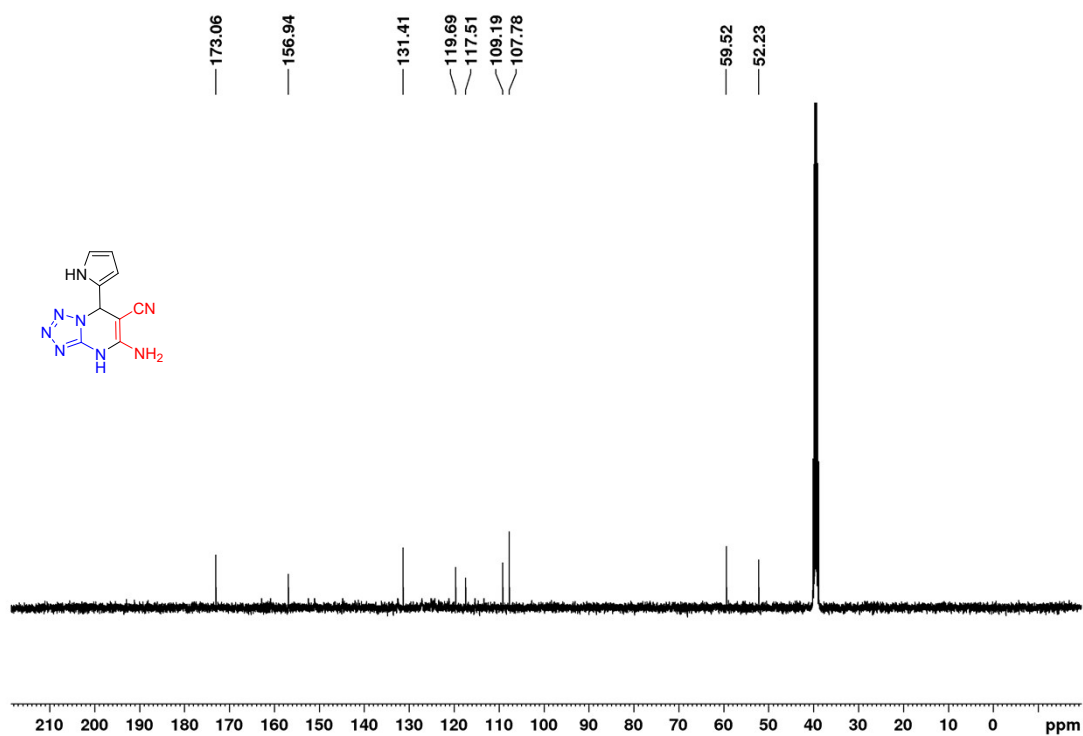
**Fig S5:**  $^{13}\text{C}$ -NMR of 5-amino-7-(1H-imidazol-2-yl)-4,7-dihydro-tetrazolo[1,5-a]pyrimidine-6-carbonitrile (**4b**)



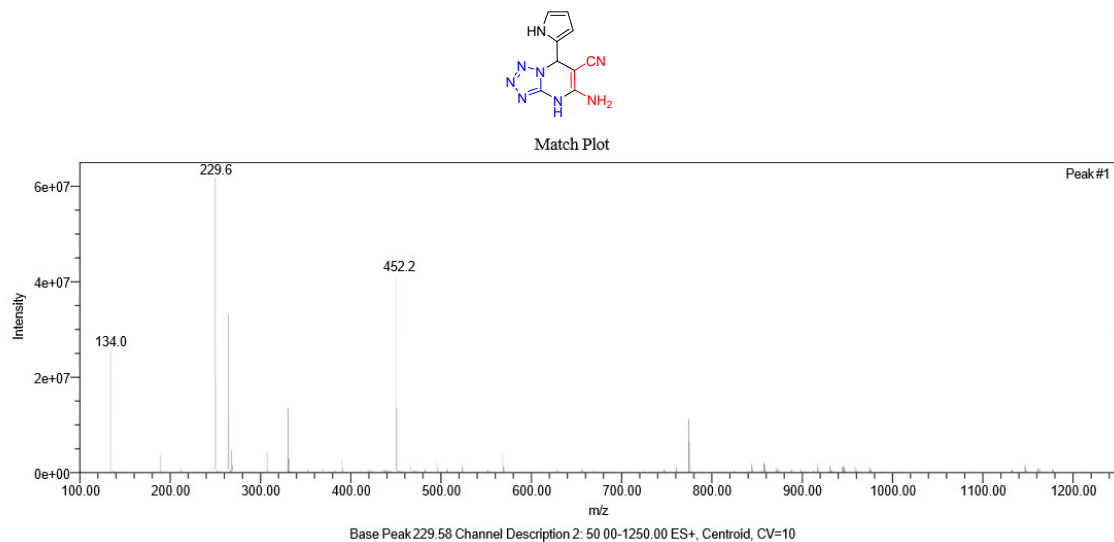
**Fig S6:** MS of 5-amino-7-(1H-imidazol-2-yl)-4,7-dihydro-tetrazolo[1,5-a]pyrimidine-6-carbonitrile (**4b**)



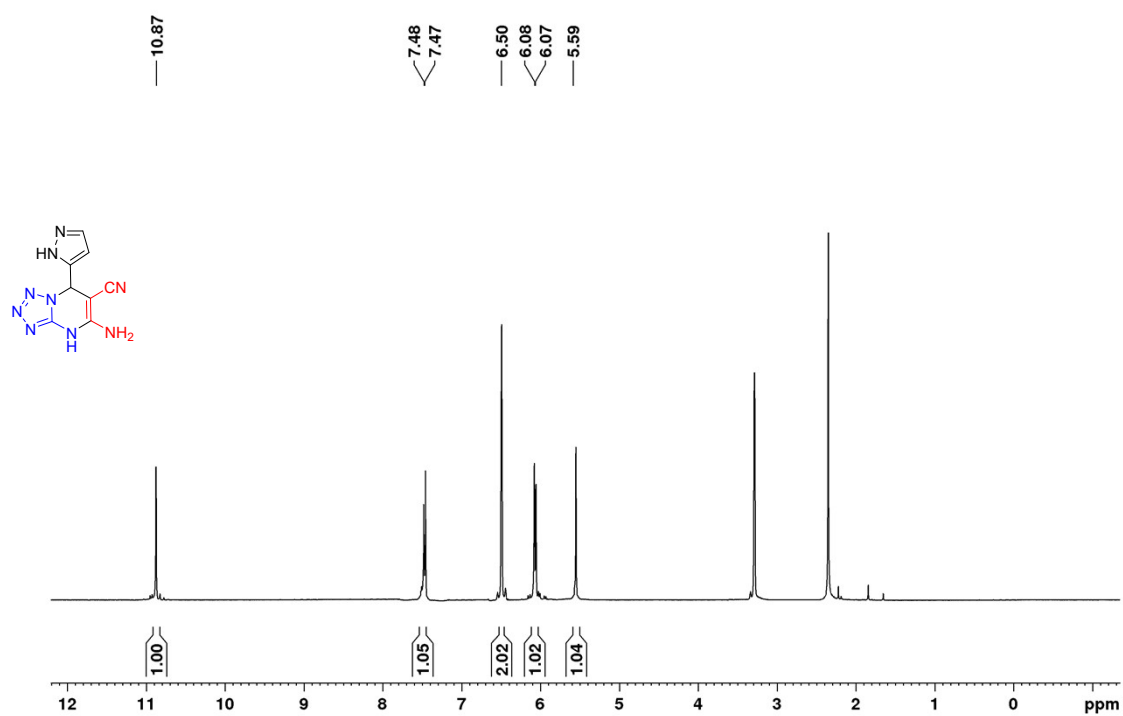
**Fig S7:**  $^1\text{H}$ -NMR of 5-amino-7-(1H-pyrrol-2-yl)-4,7-dihydro-tetrazolo[1,5-a]pyrimidine-6-carbonitrile (**4c**)



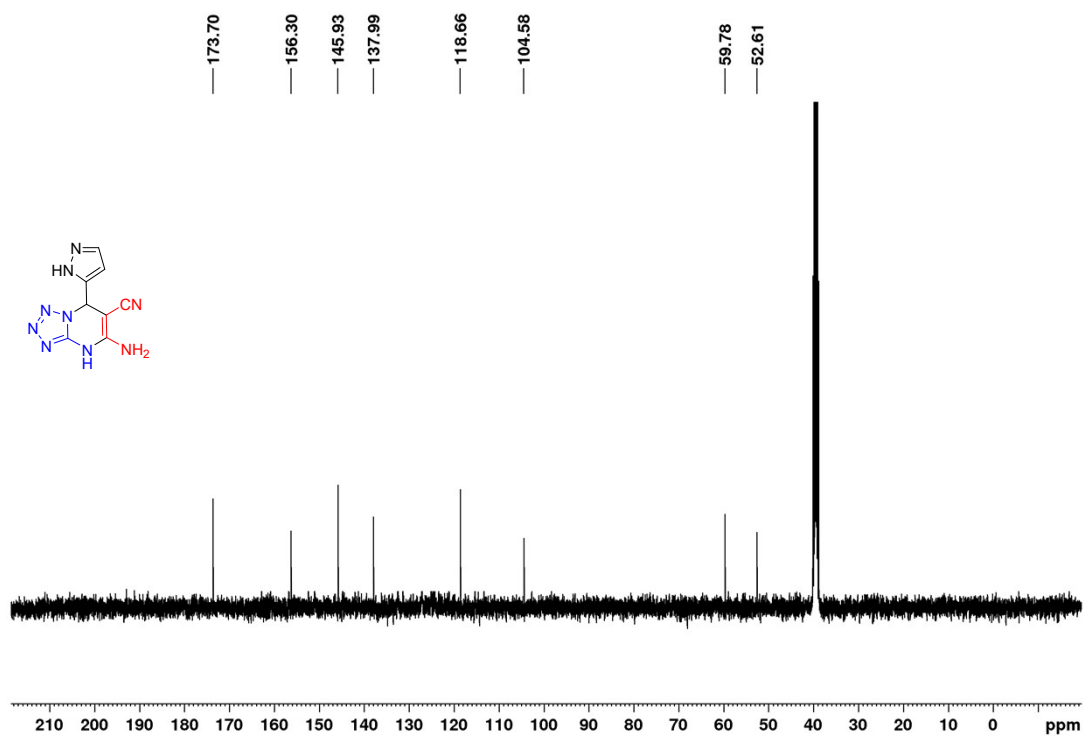
**Fig S8:** <sup>13</sup>C-NMR of 5-amino-7-(1H-pyrrol-2-yl)-4,7-dihydro-1,2,4-triazolo[1,5-a]pyrimidine-6-carbonitrile (**4c**)



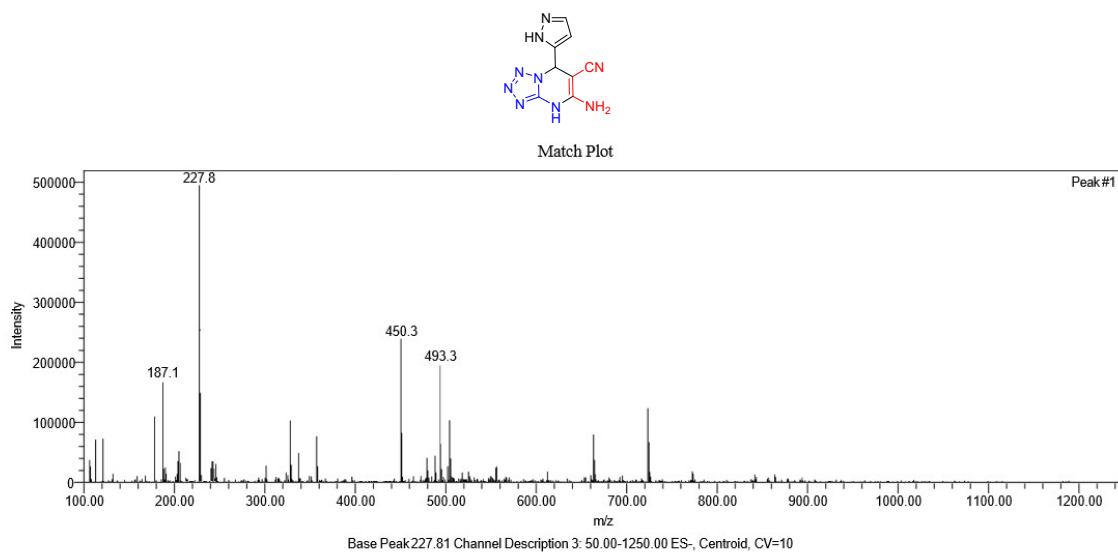
**Fig S9:** MS of 5-amino-7-(1H-pyrrol-2-yl)-4,7-dihydro-1,2,4-triazolo[1,5-a]pyrimidine-6-carbonitrile (**4c**)



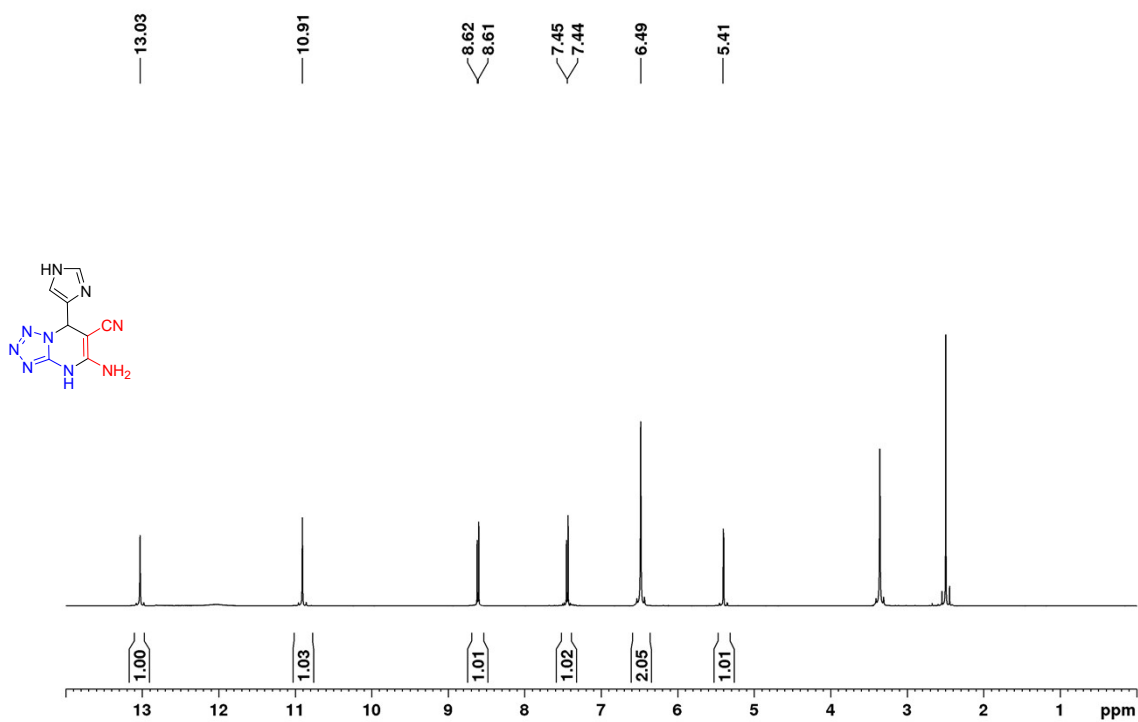
**Fig S10:** <sup>1</sup>H-NMR of 5-amino-7-(1H-pyrazol-5-yl)-4,7-dihydro-1,2,4-triazolo[1,5-a]pyrimidin-6-carbonitrile (4d)



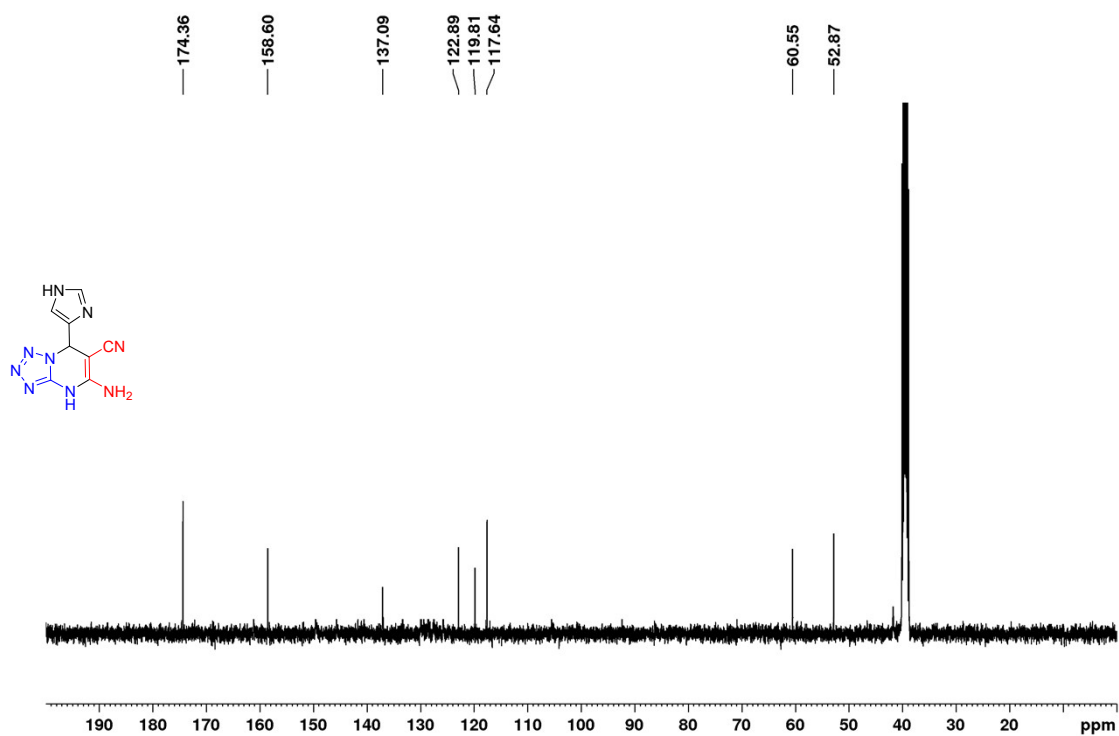
**Fig S11:**  $^{13}\text{C}$ -NMR of 5-amino-7-(1H-pyrazol-5-yl)-4,7-dihydro-tetrazolo[1,5-a]pyrimidine-6-carbonitrile (**4d**)



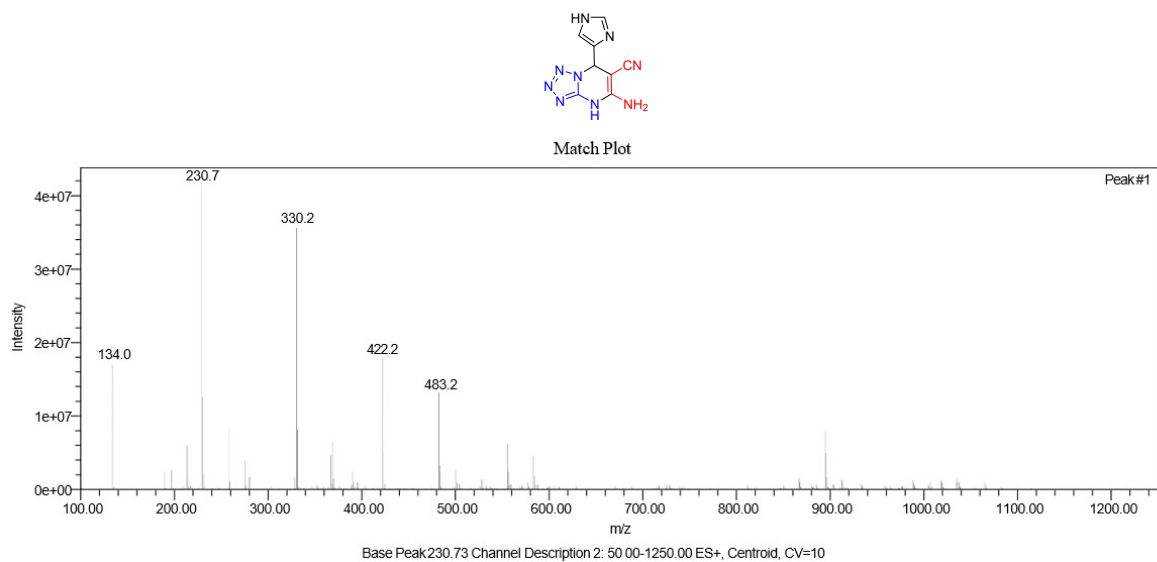
**Fig S12:** MS of 5-amino-7-(1H-pyrazol-5-yl)-4,7-dihydro-tetrazolo[1,5-a]pyrimidine-6-carbonitrile (**4d**)



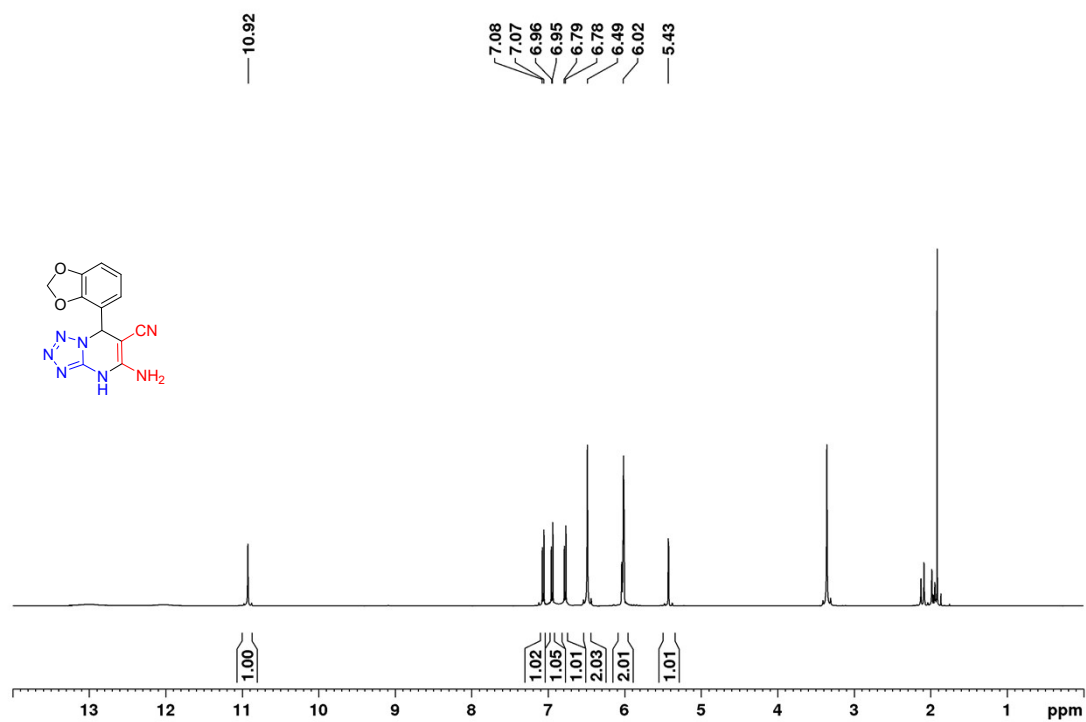
**Fig S13:**  $^1\text{H}$ -NMR of 5-amino-7-(1H-imidazol-4-yl)-4,7-dihydro-tetrazolo[1,5-a]pyrimidine-6-carbonitrile (**4e**)



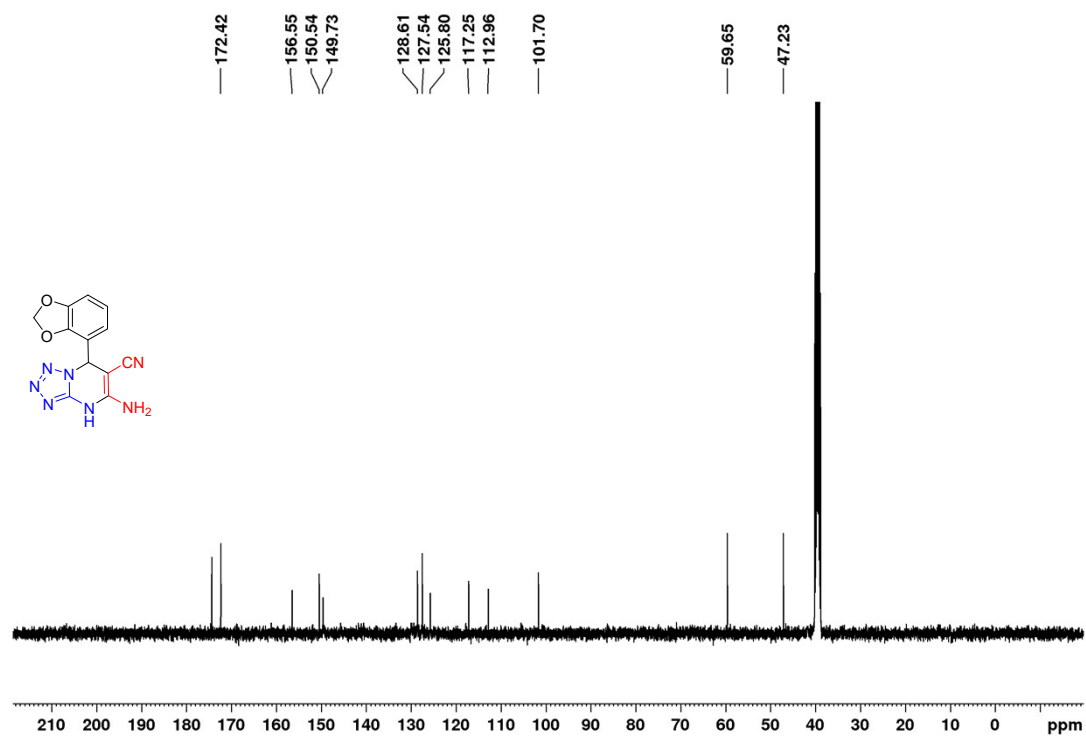
**Fig S14:** <sup>13</sup>C-NMR of 5-amino-7-(1H-imidazol-4-yl)-4,7-dihydro-1,2,4-triazolo[1,5-a]pyrimidin-6-carbonitrile (**4e**)



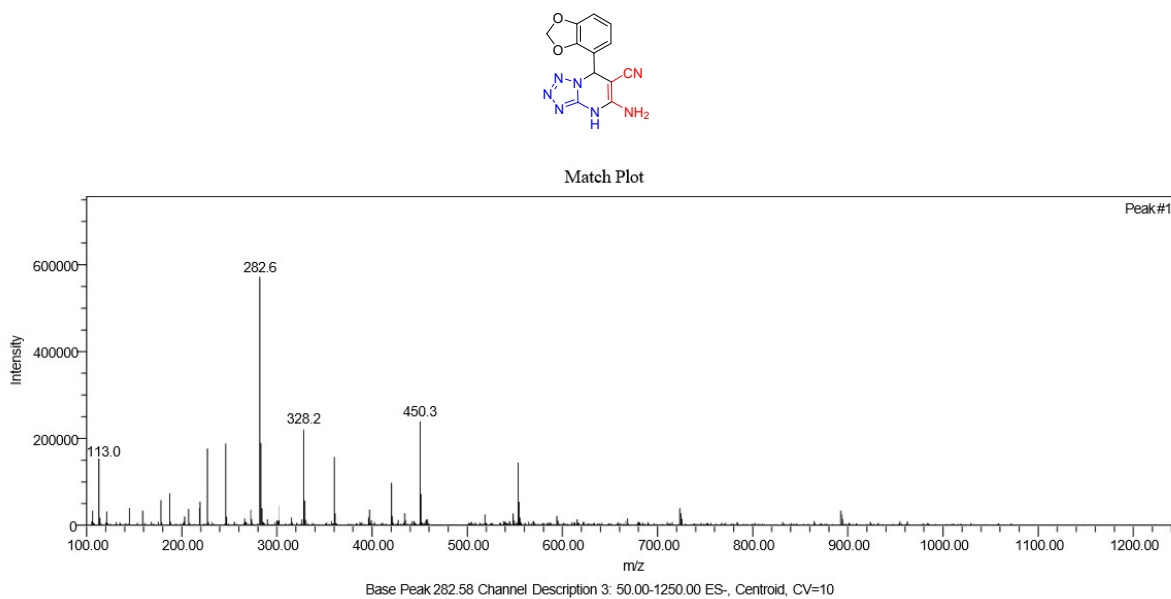
**Fig S15:** MS of 5-amino-7-(1H-imidazol-4-yl)-4,7-dihydro-1,2,4-triazolo[1,5-a]pyrimidin-6-carbonitrile (**4e**)



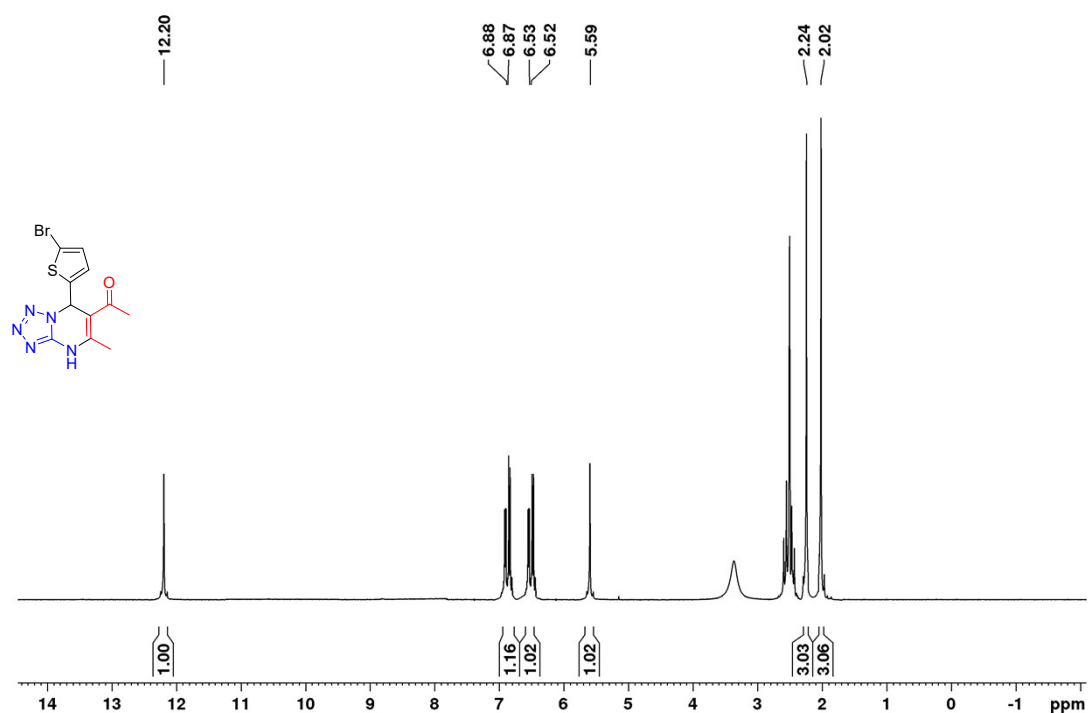
**Fig S16:** <sup>1</sup>H-NMR of 5-amino-7-(benzo[d][1,3]dioxol-4-yl)-4,7-dihydro-1H-tetrazolo[1,5-a]pyrimidin-6-carbonitrile (**4f**)



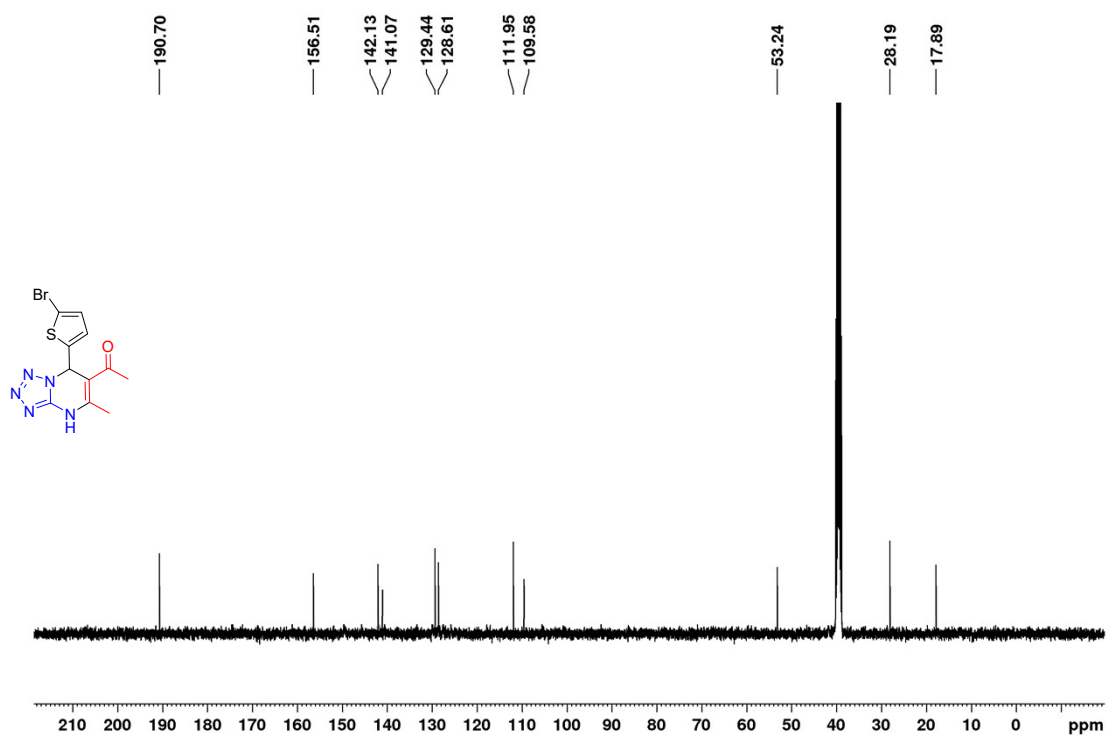
**Fig S17:**  $^{13}\text{C}$ -NMR of 5-amino-7-(benzo[d][1,3]dioxol-4-yl)-4,7-dihydro-tetrazolo[1,5-a]pyrimidine-6-carbonitrile (**4f**)



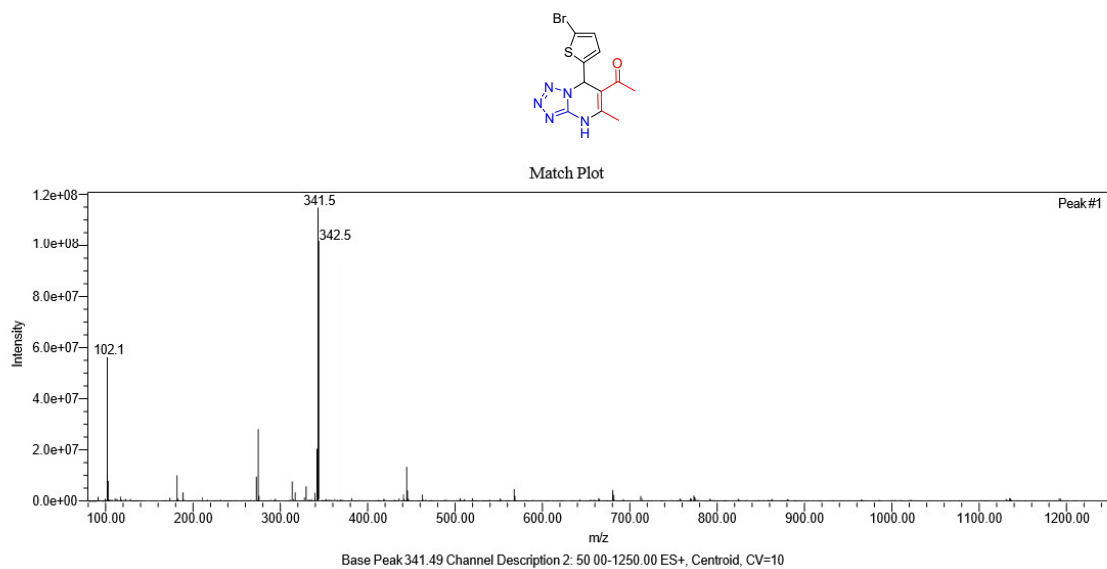
**Fig S18:** MS of 5-amino-7-(benzo[d][1,3]dioxol-4-yl)-4,7-dihydro-tetrazolo[1,5-a]pyrimidine-6-carbonitrile (**4f**)



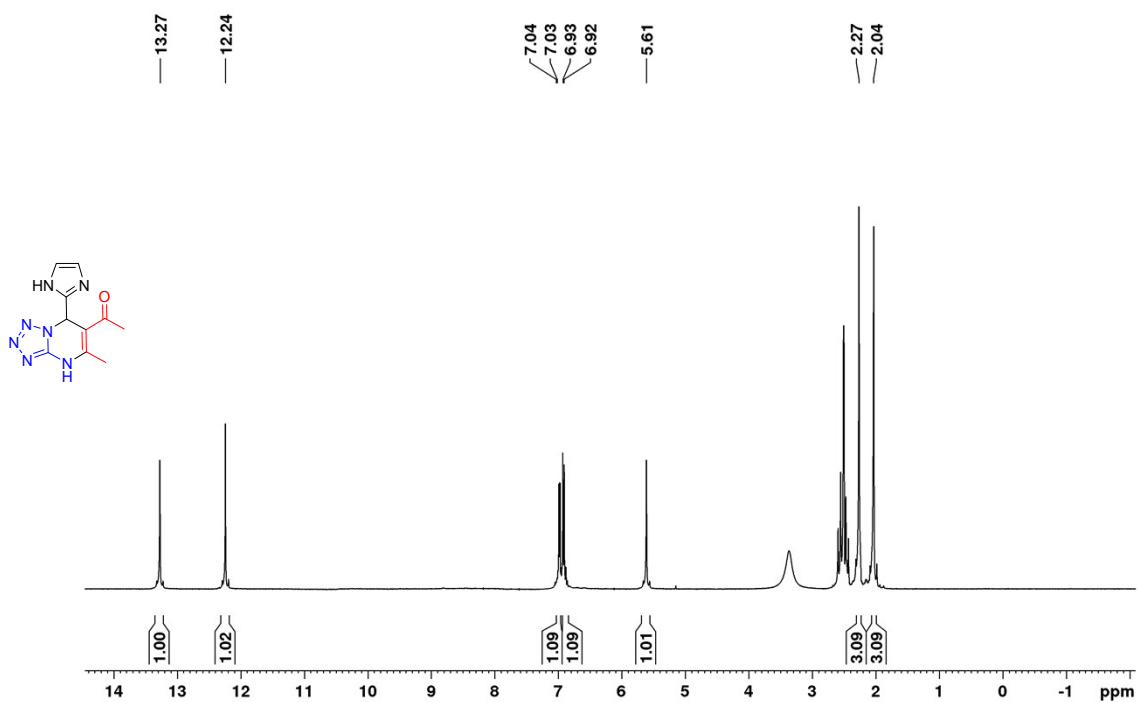
**Fig S19:**  $^1\text{H}$ -NMR of 1-(7-(5-bromothiophen-2-yl)-5-methyl-4,7-dihydro-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4g**)



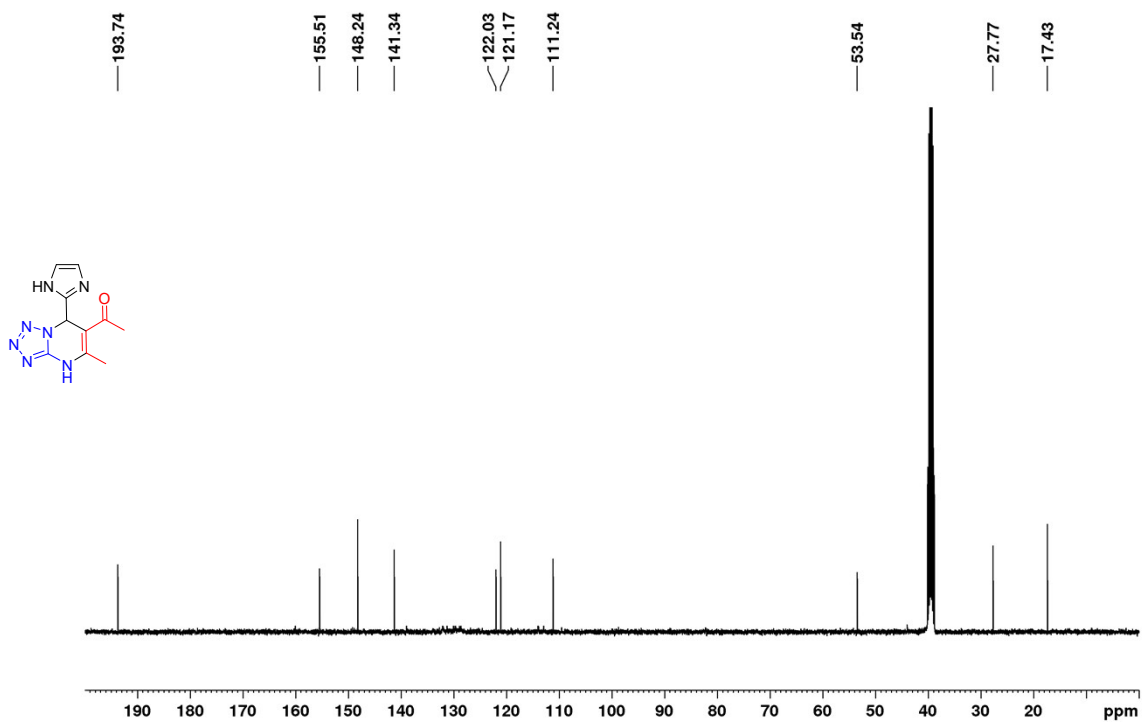
**Fig S20:** <sup>13</sup>C-NMR of 1-(7-(5-bromothiophen-2-yl)-5-methyl-4,7-dihydro-1H-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4g**)



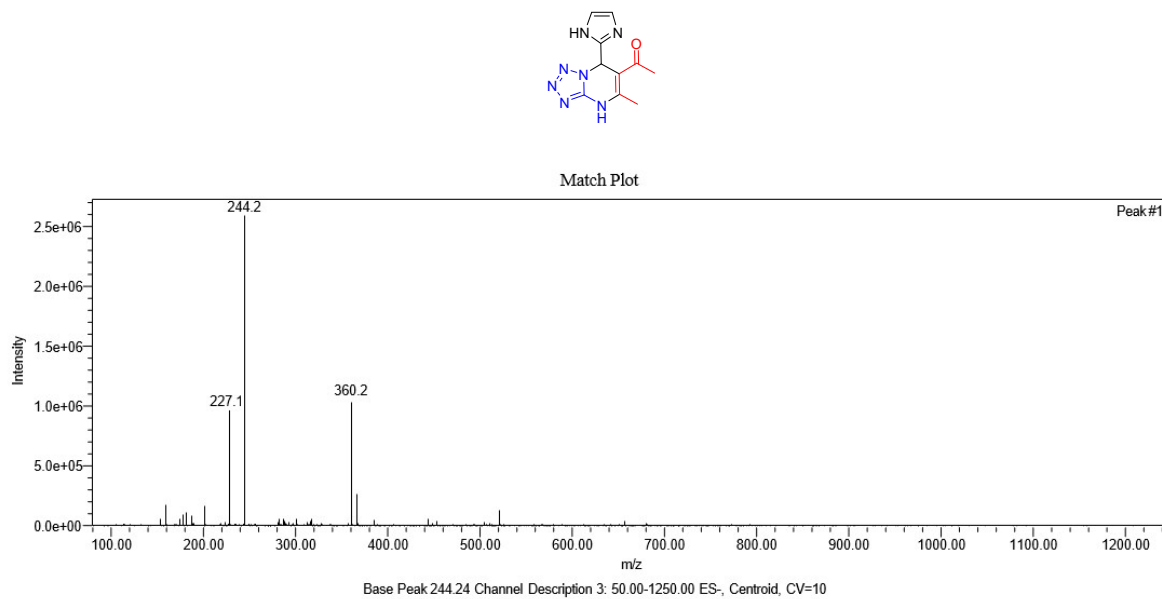
**Fig S21:** MS of 1-(7-(5-bromothiophen-2-yl)-5-methyl-4,7-dihydro-1H-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4g**)



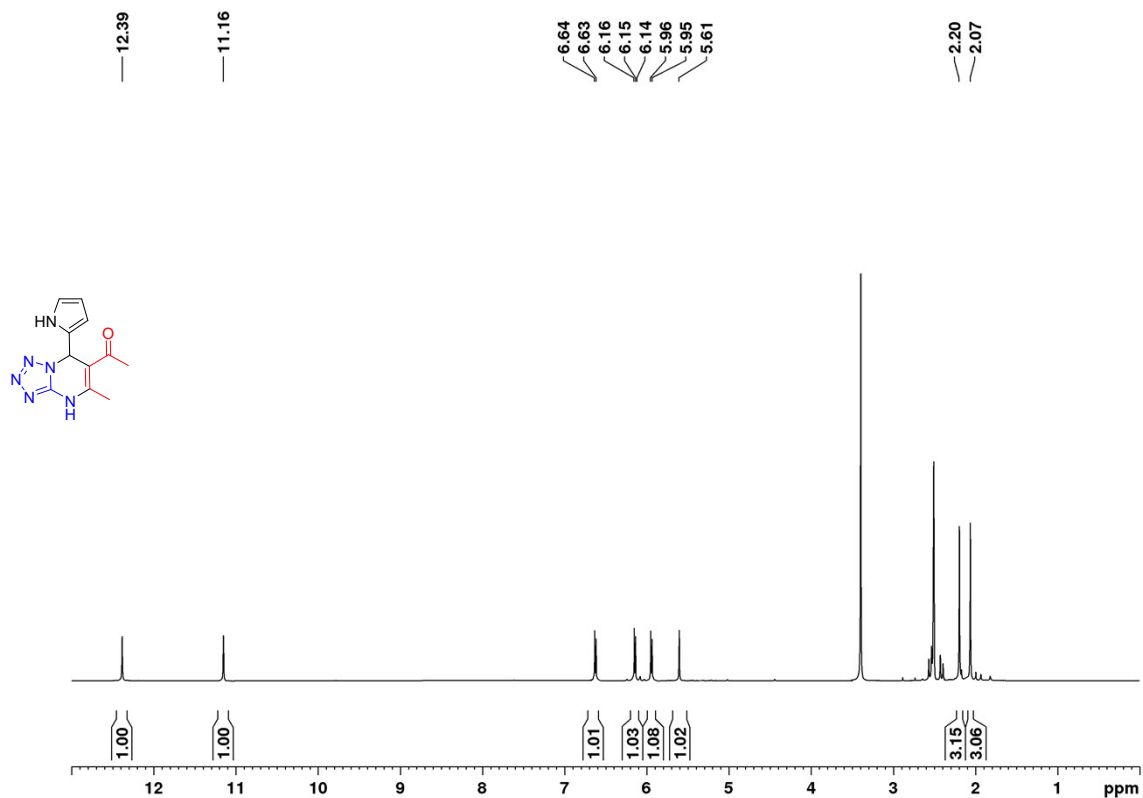
**Fig S22:** <sup>1</sup>H-NMR of 1-(7-(1H-imidazol-2-yl)-5-methyl-4,7-dihydro-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4h**)



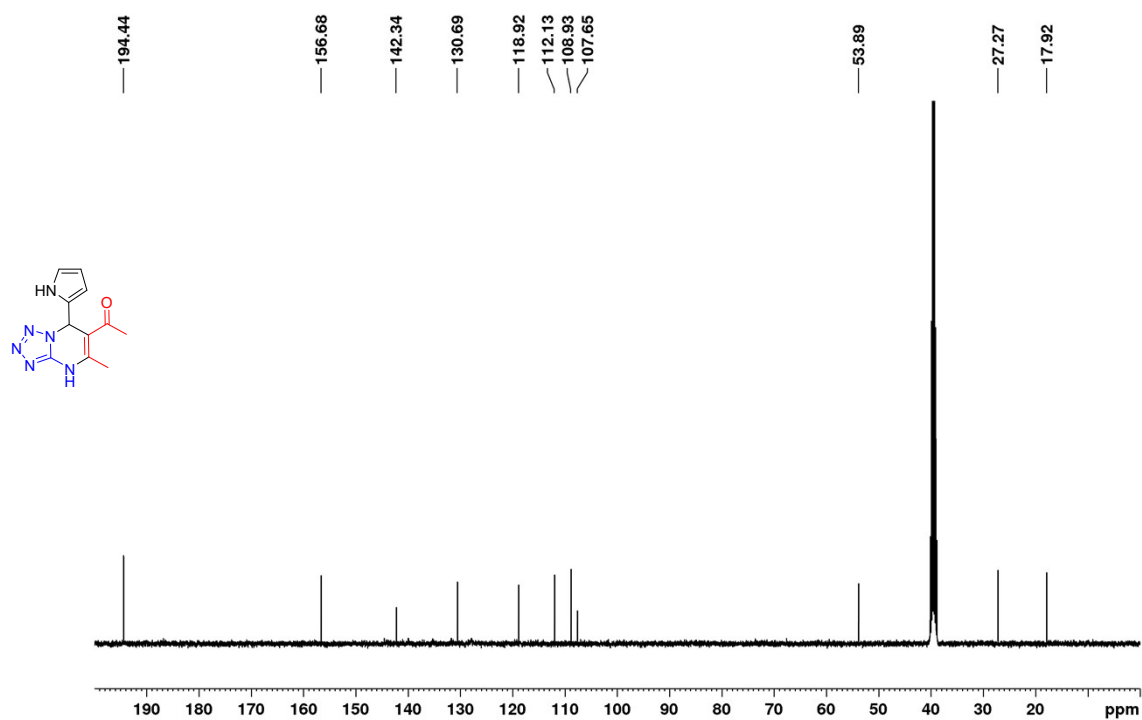
**Fig S23:**  $^{13}\text{C}$ -NMR of 1-(7-(1H-imidazol-2-yl)-5-methyl-4,7-dihydro-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4h**)



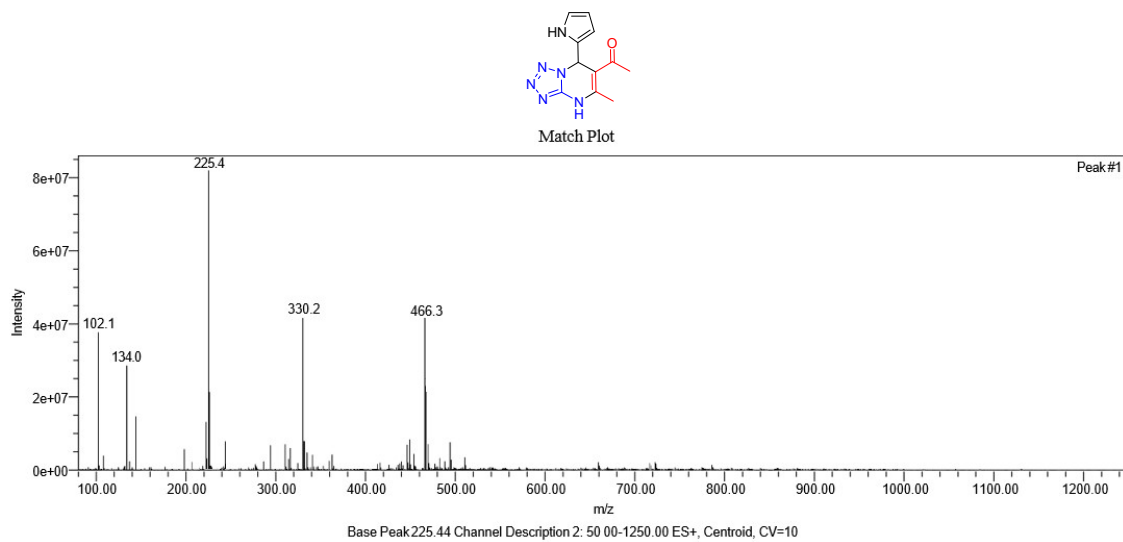
**Fig S24:** MS of 1-(7-(1H-imidazol-2-yl)-5-methyl-4,7-dihydro-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4h**)



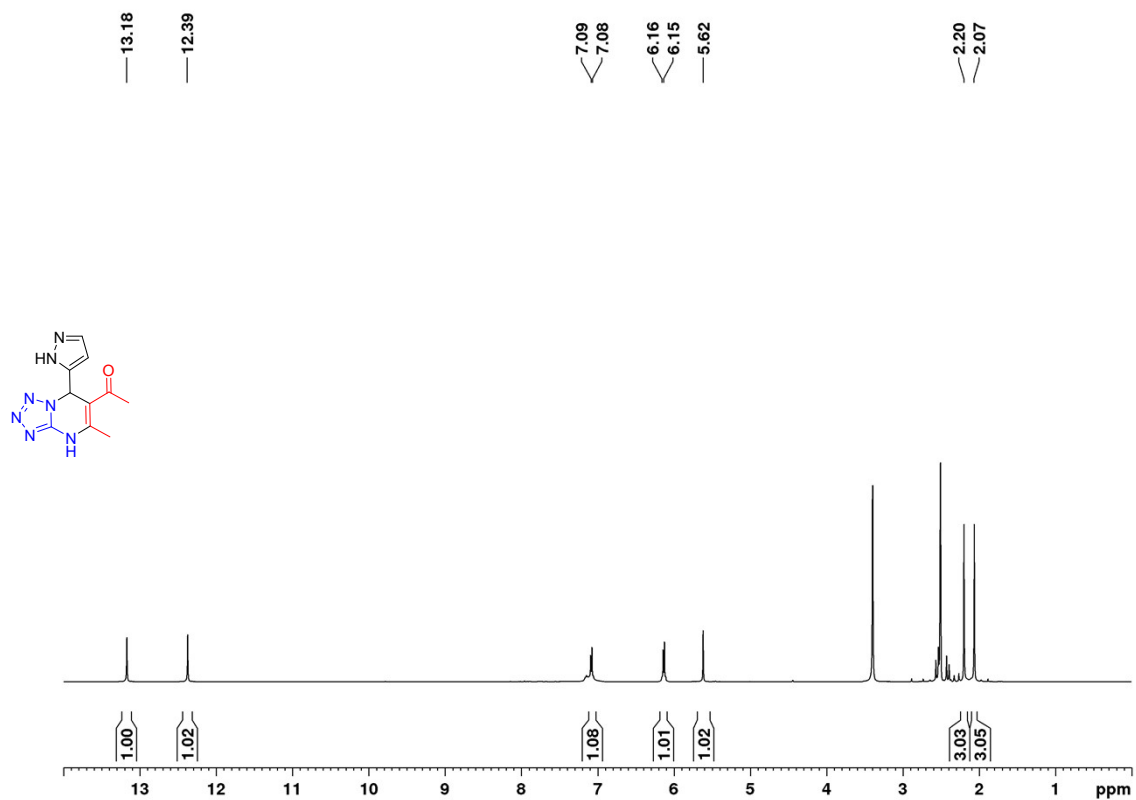
**Fig S25:**  $^1\text{H}$ -NMR of 1-(5-methyl-7-(1H-pyrrol-2-yl)-4,7-dihydro-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4i**)



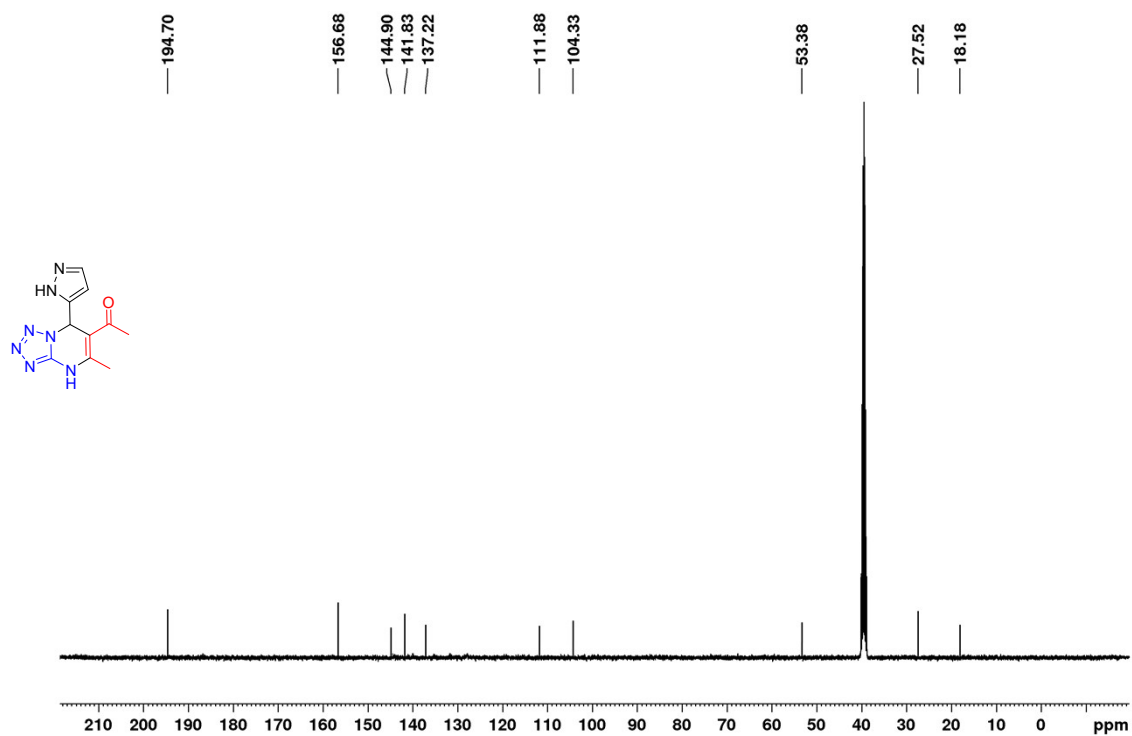
**Fig S26:** <sup>13</sup>C-NMR of 1-(5-methyl-7-(1H-pyrrol-2-yl)-4,7-dihydro-1H-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4i**)



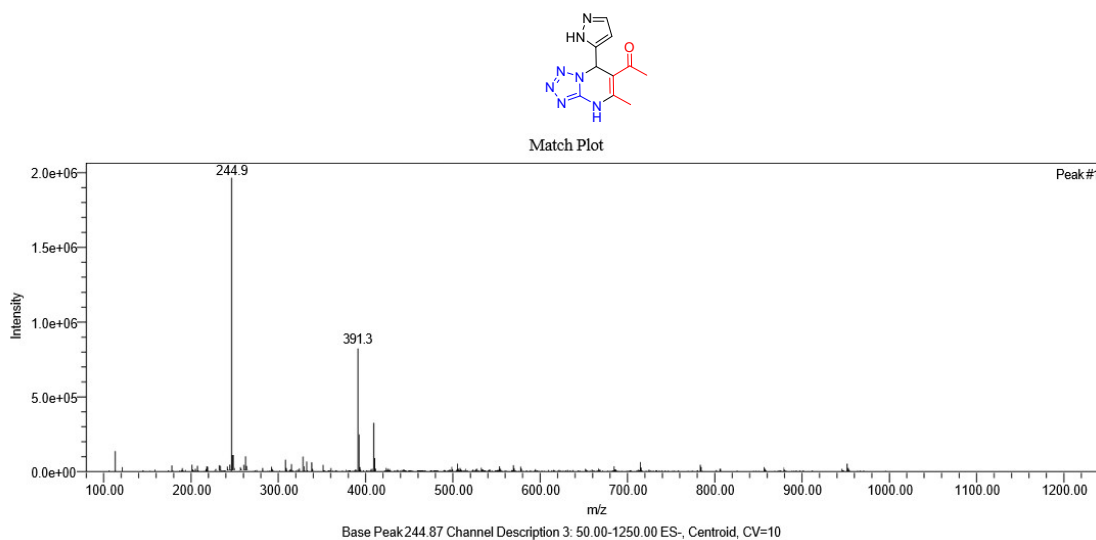
**Fig S27:** MS of 1-(5-methyl-7-(1H-pyrrol-2-yl)-4,7-dihydro-1H-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4i**)



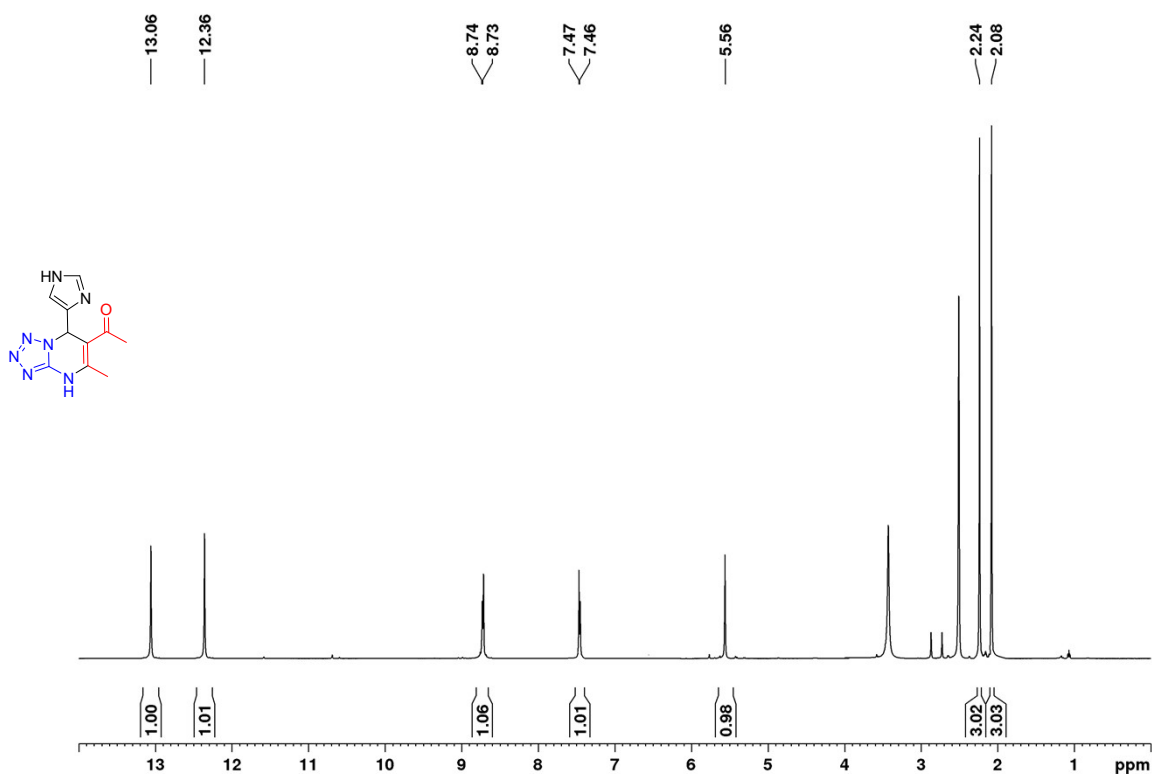
**Fig S28:** <sup>1</sup>H-NMR of 1-(5-methyl-7-(1H-pyrazol-5-yl)-4,7-dihydro-1,2,4-triazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4j**)



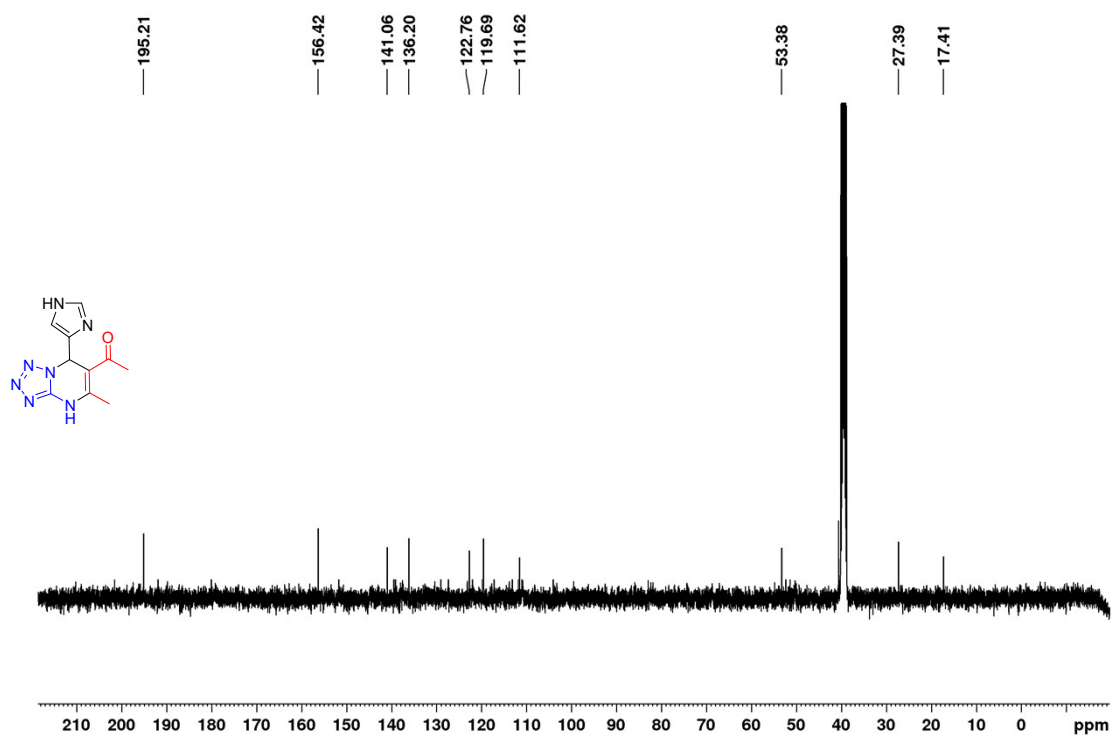
**Fig S29:**  $^{13}\text{C}$ -NMR of 1-(5-methyl-7-(1H-pyrazol-5-yl)-4,7-dihydro-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4j**)



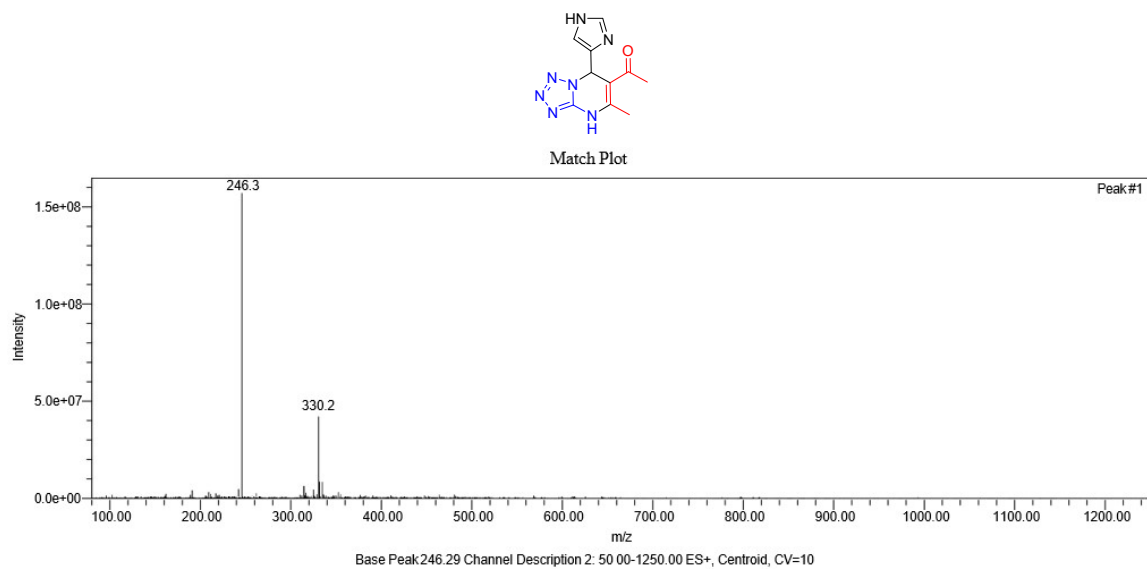
**Fig S30:** MS of 1-(5-methyl-7-(1H-pyrazol-5-yl)-4,7-dihydro-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4j**)



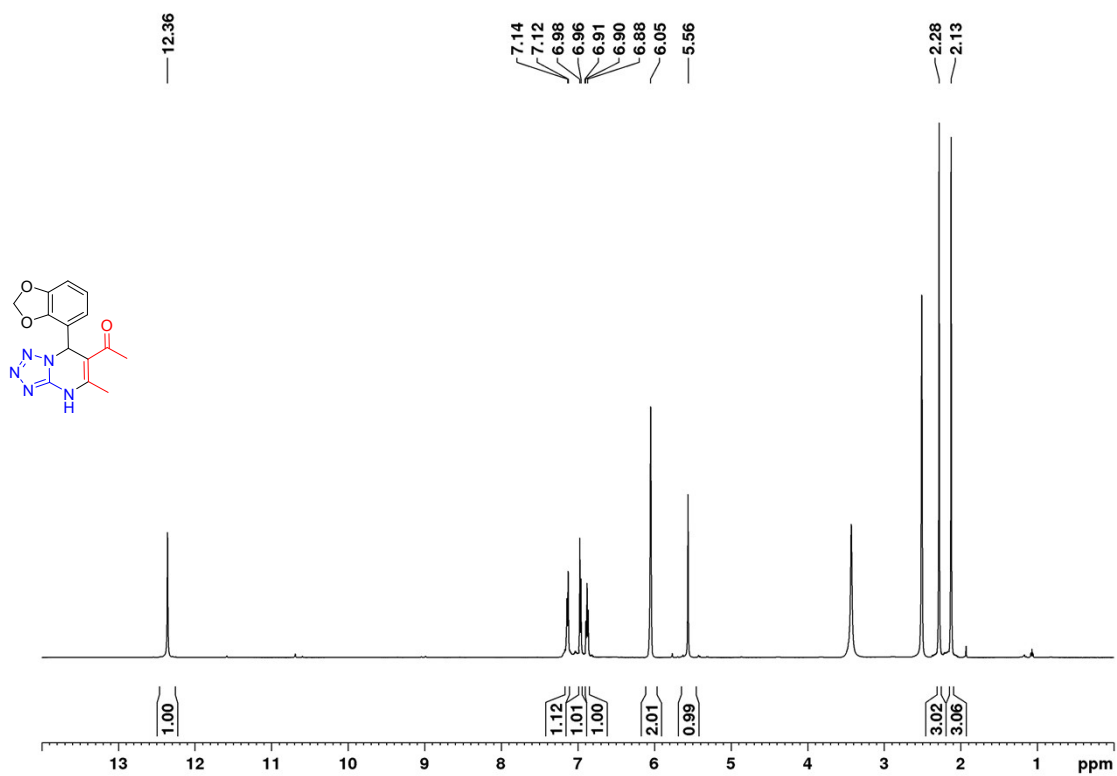
**Fig S31:**  $^1\text{H}$ -NMR of 1-(7-(1H-imidazol-4-yl)-5-methyl-4,7-dihydro-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4k**)



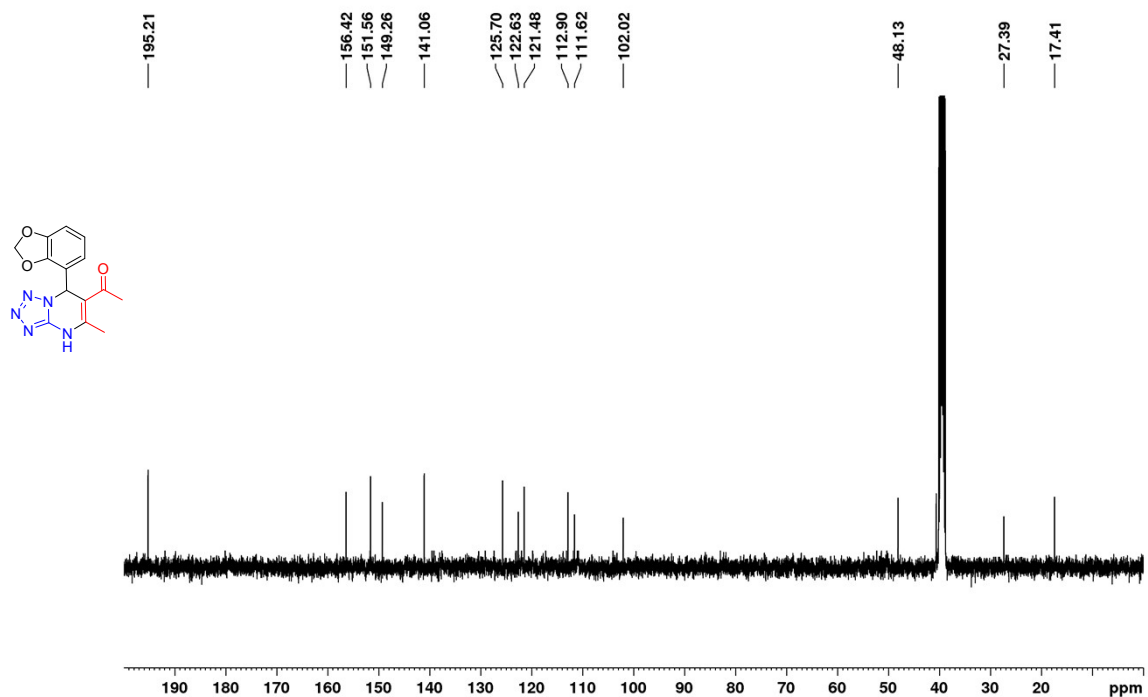
**Fig S32:** <sup>13</sup>C-NMR of 1-(7-(1H-imidazol-4-yl)-5-methyl-4,7-dihydro-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4k**)



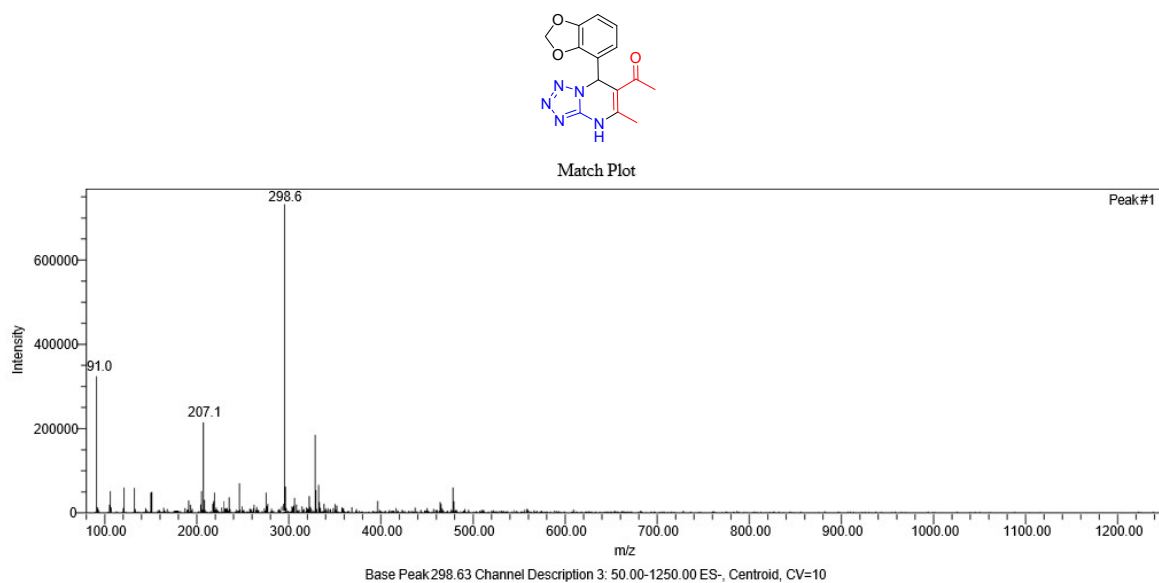
**Fig S33:** MS of 1-(7-(1H-imidazol-4-yl)-5-methyl-4,7-dihydro-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4k**)



**Fig S34:** <sup>1</sup>H-NMR of 1-(7-(benzo[d][1,3]dioxol-4-yl)-5-methyl-4,7-dihydro-1H-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4I**)



**Fig S35:**  $^{13}\text{C}$ -NMR of 1-(7-(benzo[d][1,3]dioxol-4-yl)-5-methyl-4,7-dihydro-1H-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4I**)



**Fig S36:** MS of 1-(7-(benzo[d][1,3]dioxol-4-yl)-5-methyl-4,7-dihydro-1H-tetrazolo[1,5-a]pyrimidin-6-yl)ethan-1-one (**4I**)