4. Materials and methods

The Solvents, reagents and chemicals used in the present work were purchased from Aldrich, E. Merck, Spectrochem P. Ltd., and S. D. Fine Chem. P. Ltd., BD Biosciences P. Ltd., Himedia P. Ltd. and used without further purification. The reactions were monitored by thin layer chromatography (TLC) carried out on 0.25mm E. Merck silica gel plates (silica gel 60 F254). Purification of synthesized compounds was performed by column chromatographic technique using silica gel 100-200 mesh (E. Merck). Few compounds were purified by Flash Chromatography technique using ISCO Combiflash Companion.

The purity of the synthesised compounds was checked by TLC on silica gel 60 F254 (E. Merck) aluminum plates. Melting points were determined using laboratory melting point apparatus (Toshniwal P. Ltd.) and are uncorrected. Chemical tests were performed to confirm the presence of functional groups and required elements.

UV absorption was detected in UV-2450 spectrophotometer (Shimadzu) to find the λ max of the compounds. IR spectra of the synthesized compounds were recorded on FT-IR Affinity-1 (Shimadzu) IR Spectrometer. Mass spectra were recorded on GC-MS-QP5050A (Shimadzu). NMR spectra were recorded on Bruker 400 MHz spectrometer using DMSO-d6 as the solvent.

The log P and pKa of the compounds was determined by HPLC method. Chromatographic runs were performed on Shimadzu UFLC system. Inertsil® ODS-4, (GL Sciences Inc.) and Gemini 5μ C18 110A (150 x 4.6 mm, particle size 4.7-5.3 μm, Phenomenex) columns were used for the determination of logP and pKa respectively. Metabolic stability assay was performed using Microsorb-MV 100 C18, (Varian) column.
4.1. Molecular modeling studies

The protein structure of CYP 121 (PDB code: 4G2G) and CYP 125 (PDB code: 3IW2) were obtained from online data base (www.pdb.org). Molecular docking studies were carried out using Schrodinger 2010.

**Ligand preparation**

Chemical structures were drawn using ChemDraw Ultra 2008. 1,2,4-triazoles derivatives were designed to built a chemical library and were optimized using Lig Prep module in Schrodinger 2010. The desalt process and generation of Epik state was performed prior to minimization of ligands. 32 conformers were generated for each ligand with retention of specific chiralities. The ligands were minimized using OPLS_2005 force field. The most stable isomer per ligand was selected for further studies.

**Protein preparation**

The protein structures were obtained from PDB (CYP 121 (4G2G) and CYP 125 (3IW2). The protein was optimized for docking studies using protein preparation wizard in Schrodinger 2010. The missing links and missing loops in the protein were rectified by capping and looping the missing residues respectively using Prime wizard. The active site was selected at the position of reference ligand. The water molecules were deleted beyond 5 Å from the active site. The final refinement of the protein was performed using exhaustive sampling. The convergence to RMSD was taken as 0.30 Å. Energy minimization of the protein was carried out using OPLS_2005 force field.

**Grid generation**

The grid was generated in the protein by selecting the position of reference ligand as the centroid of active site. The default Vander Waal (VdW) scaling factor and partial cutoff were taken as 1.0 and 0.25 respectively for the grid generation. The grid was generated without considering per-atom scaling factors.

**Docking studies**

The docking studies were performed by Glide, applying Standard precession. The non-planar conformations were penalized for amide bonds in the ligands. Using VdW radius scaling factor 0.8 and partial cutoff 0.15, the docking was performed. The limits for the ligands to be
docked were kept at <300 atoms and <50 rotatable bonds. After the docking was finished, the post docking minimization was performed for 5 poses per ligand and the per residue interactions of docked ligands in active site was determined up to 12 Å from the grid centre. The ligands RMSD, docking score and residue interactions were compared with the reference ligand.
4.2. Synthetic Schemes:

Scheme 1a

5a. R = H, R¹ = CH₃, 5b. R = H, R¹ = C₂H₅, 5c. R = H, R¹ = C₃H₇, 5d. R = H, R¹ = C₄H₉, 5e. R = H, R¹ = C₅H₁₁, 5f. R = H, R¹ = C₆H₁₃, 5g. R = H, R¹ = 2-CH₃Ph, 5h. R = H, R¹ = 3-ºCH₂Ph, 5i. R = H, R¹ = 4-ºCH₂Ph, 5j. R = H, R¹ = 4-FPh, 5k. R = H, R¹ = 4-C₂H₅Ph, 5l. R = H, R¹ = 4-ºC₂H₅Ph, 5m. R = H, R¹ = 3,4-ºCH₂Ph

6a. R = CH₃, R¹ = CH₃, 6b. R = CH₃, R¹ = C₂H₅, 6c. R = CH₃, R¹ = C₃H₇, 6d. R = CH₃, R¹ = C₄H₉, 6e. R = CH₃, R¹ = C₅H₁₁, 6f. R = CH₃, R¹ = C₆H₁₃, 6g. R = CH₃, R¹ = Ph, 6h. R = CH₃, R¹ = 2-CH₃Ph, 6i. R = CH₃, R¹ = 4-ºCH₂Ph, 6j. R = CH₃, R¹ = 3-ºCH₂Ph, 6k. R = CH₃, R¹ = 4-ºCH₂Ph, 6l. R = CH₃, R¹ = 2-ClPh, 6m. R = CH₃, R¹ = 4-ClPh, 6n. R = CH₃, R¹ = 4-FPh, 6o. R = CH₃, R¹ = -ºCH₂Ph, 6p. R = CH₃, R¹ = 4-ºC₂H₅Ph, 6q. R = CH₃, R¹ = 4-ºC₂H₅Ph, 6r. R = CH₃, R¹ = 3,4-ºCH₂Ph

*Reagents and Conditions:
(i) MeOH, Conc. H₂SO₄ (Cat.) reflux, 4h. (ii) N₂H₄·2H₂O (99%), MeOH, reflux, 9h. (iii) CS₂, Et₃N, MeOH, reflux, 10h. (iv) N₂H₄·2H₂O (99 %), EtOH, reflux, 12h. (v) Dry Dioxane, R¹COCl, reflux, 10h.
**Scheme 2**

R-COOH + H₂N - S - H₂N NH₂ → R N - N - SH → R N - N - SH

7a. R = CH₃, 7b. R = C₂H₅, 7c. R = C₃H₇,
8a. R = CH₃, R¹ = H, 8b. R = C₂H₅, R¹ = H, 8c. R = C₃H₇, R¹ = H.
9a. R = CH₃, R¹ = CH₃, 9b. R = C₂H₅, R¹ = CH₃, 9c. R = C₃H₇, R¹ = CH₃.

**Reagents and Conditions:**
(i) 180-200 °C, 1 h. (ii) 10 % NaOH (aq), reflux, 1 h. (iii) R¹COCl, Dry Dioxane, reflux, 8 h.

**Scheme 3**

R¹ = H, 8d-o
R¹ = CH₃, 9d-o

13d. R = H, 13e. R = 2-CH₃, 13f. R = 4-CH₃, 13g. R = 3-OCH₃, 13h. R = 4-OCH₃, 13i. R = 2-Cl, 13j. R = 4-Cl,
13k. R = 4-F, 13m. R = -CH₂OCH₃, 13n. R = 4-C₂H₅, 13a. R = 4-OC₂H₅, 13o. R = 3,4-OC₂H₅.
8d. R = 2-CH₃, R¹ = H, 8e. R = 4-CH₃, R¹ = H, 8f. R = 3-OCH₃, R¹ = H, 8g. R = 4-OCH₃, R¹ = H, 8h. R = 4-Cl,
R¹ = H, 8i. R = 4-F, R¹ = H, 8j. R = 4-C₂H₅, R¹ = H, 8k. R = 4-OC₂H₅, R¹ = H, 8l. R = 3,4-OC₂H₅,
R¹ = H.
9d. R = H, R¹ = CH₃, 9e. R = 2-CH₃, R¹ = CH₃, 9f. R = 4-CH₃, R¹ = CH₃, 9g. R = 2-Cl, R¹ = CH₃, 9h. R = 4-Cl,
R¹ = CH₃, 9i. R = 3-OCH₃, R¹ = CH₃, 9j. R = 4-OCH₃, R¹ = CH₃, 9k. R = 4-F, R¹ = CH₃, 9l. R = 4-C₂H₅,
R¹ = CH₃, 9m. R = 4-OC₂H₅, R¹ = CH₃, 9n. R = 3,4-OCH₃, R¹ = CH₃, 9o. R = -CH₂OCH₃, R¹ = CH₃.

**Reagents and Conditions:**
(i) MeOH, Conc. H₂SO₄ (Cat.), reflux, 4 h. (ii) N₂H₄·2H₂O (99%), MeOH, reflux, 9 h. (iii) CS₂, Et₃N, MeOH,
reflux, 10 h. (iv) N₂H₄·2H₂O (99 %), EtOH, reflux, 12 h. (v) Dry Dioxane, R¹COCl, reflux, 10 h.
Reagents and Conditions:
(i) NH₄SCN, EtOH, reflux, 4h. (ii) 4% NaOH(aq), reflux, 1h. (iii) R¹X, Et₃N, EtOH, reflux, 4h.

Reagents and Conditions: (i) MeOH, Conc. H₂SO₄ (Cat.), reflux, 4h. (ii) N₂H₄·2H₂O (99 %), MeOH, reflux, 9h.
(iii) NH₄SCN, EtOH, reflux, 4h. (iv) 4% NaOH(aq), reflux, 1h. (v) R¹X, Et₃N, EtOH, reflux, 4h.
Design, synthesis and evaluation of Antimycobacterial activity of triazoles

Scheme 6a

2a-b
2a. R=H
2b. R=CH₃

21a, 22a
21a. R=H, R₁=H
22a. R=CH₃, R₁=2,4-Cl

23a, 24a
23a. R= H, R₁=H
24a. R=CH₃, R₁=2,4-Cl

23 b. R= H, R₁=H, R₂= CH₃, 23 c. R= H, R₁=H, R₂= C₆H₅, 23 d. R= H, R₁=H, R₂= -CH₂Ph, 24 b. R= CH₃, R₁=2,4-Cl, R₂= CH₃, 24 c. R= CH₃, R₁=2,4-Cl, R₂= C₆H₅, 24 d. R= CH₃, R₁=2,4-Cl, R₂= -CH₂Ph

Scheme 7a

17a-b
17a. R= 3-OPh
17b. R= 4-OPh

25a, 26a, 27a
25a. R= 4-OPh, R₁=H
26a. R= 4-OPh, R₁=2,4-Cl
27a. R= 3-OPh, R₁=2,4-Cl

28a, 29a, 30a
28a. R= 4-OPh, R₁=H
29a. R= 4-OPh, R₁=2,4-Cl
30a. R= 3-OPh, R₁=2,4-Cl

28 b. R= 4-OPh, R₁=H, R₂= CH₃, 28 c. R= 4-OPh, R₁=H, R₂= C₆H₅, 28 d. R= 4-OPh, R₁=H, R₂= -CH₂Ph, 29 b. R= 4-OPh, R₁=2,4-Cl, R₂= CH₃, 29 c. R= 4-OPh, R₁=2,4-Cl, R₂= C₆H₅, 29 d. R= 4-OPh, R₁=2,4-Cl, R₂= -CH₂Ph, 30 b. R= 3-OPh, R₁=2,4-Cl, R₂= CH₃, 30 c. R= 3-OPh, R₁=2,4-Cl, R₂= C₆H₅, 30 d. R= 3-OPh, R₁=2,4-Cl, R₂= -CH₂Ph,

*Reagents and Conditions:
(i) ArNCS, EtOH, reflux, 4h. (ii) 4% NaOH (aq), reflux, 1h. (iii) R₁X, Et₃N, EtOH, reflux, 4h.
Design, synthesis and evaluation of Antimycobacterial activity of triazoles

**Scheme 8**

\[ \text{R} \quad \begin{array}{c} \text{O} \\ \text{N} \\ \text{NH}_2 \\ \text{R} \end{array} \quad \text{2a-b} \]

- **2a.** R = H
- **2b.** R = CH₃

\[ \begin{array}{c} \text{N} \\ \text{NH} \\ \text{R} \end{array} \quad \text{31a-b} \]

- **31a.** R = H
- **31b.** R = CH₃

\[ \begin{array}{c} \text{N} \\ \text{NH} \\ \text{R} \\ \text{R} \end{array} \quad \text{32a-h} \]

- **32a.** R = H
- **32b.** R = H, R¹ = 2-CH₃
- **32c.** R = H, R¹ = 4-CH₃
- **32d.** R = H, R¹ = 4-Cl
- **32e.** R = H, R¹ = 4-F

\[ \begin{array}{c} \text{N} \\ \text{NH} \\ \text{R} \\ \text{R} \end{array} \quad \text{33a-d} \]

- **33a.** R = CH₃
- **33b.** R = H, R¹ = 2-CH₃
- **33c.** R = CH₃, R¹ = 3-OCH₃
- **33d.** R = CH₃, R¹ = 4-F

*aReagents and Conditions:* (i) Triphosgene, DIPEA, N₂, DCM, rt, 0.5h. (ii) ArNHNH₂, Dry toluene, reflux, 3h.

**Scheme 9**

\[ \begin{array}{c} \text{O} \\ \text{NH} \\ \text{NH}_2 \end{array} \quad \text{17b} \]

\[ \begin{array}{c} \text{O} \\ \text{N} \\ \text{SH} \end{array} \quad \text{34a} \]

\[ \begin{array}{c} \text{O} \\ \text{N} \\ \text{SH} \end{array} \quad \text{35a} \]

- **35a.** R = C₃H₇
- **35b.** R = C₄H₉
- **35c.** R = C₅H₁₁
- **35d.** R = Ph
- **35e.** R = Cyclohexyl
- **35f.** R = Cyclobutyl

*bReagents and Conditions:*

(i) CS₂, Et₃N, MeOH, reflux, 10 h. (ii) N₂H₄·2H₂O (99 %), EtOH, reflux, 12 h. (iii) Dry Dioxane, ROC₁, reflux, 10 h.
4.3. Experimental section

**General procedure for the preparation of carboxylic acid methyl esters (3a-b, 10d-o and 16a-b):**\(^{45}\) To the solution of carboxylic acid (0.01 mole) in methanol (10 mL), catalytic amount of sulphuric acid was added and refluxed for 4 h. The reaction completion was monitored by TLC using hexane: ethyl acetate (9:1) as mobile phase. The solvent was removed under reduced pressure. The product obtained was purified by column chromatography using hexane: ethyl acetate (9:1) as mobile phase.

**General procedure for the preparation of carboxylic acid hydrazide (1a-b, 11d-o and 17a-b):**\(^{45}\) To the solution of ester (0.01 mole) in methanol (10 mL), hydrazine hydrate (0.05 mole) (99%) was added and refluxed for 9 h. The reaction was monitored by using TLC using hexane: ethyl acetate (9:1) as mobile phase. The solvent was removed under reduced pressure and the product obtained was treated with 4-5 mL of ice cold water. The solid obtained was filtered under vacuum and dried. The product obtained was purified by column chromatography using hexane: ethyl acetate (9:1) as mobile phase.

**General procedure for the preparation of 5-Aryl-[1,3,4]oxadiazole-2-thiol (1a-b, 12d-o and 34a):**\(^{55-68}\) To the solution of acid hydrazide (0.01 mole) in methanol (10 mL), (0.02 mole) triethylamine and (0.02 mole) carbon disulphide were added and refluxed for 10 h. The progress of the reaction was monitored by TLC using hexane: ethyl acetate (8:2) as mobile phase. The solvent was removed under reduced pressure and the product obtained was dissolved in 100 mL of cold water and acidified with concentrated HCl to pH 6-7. The precipitate obtained was filtered, washed with cold water and dried. The product was purified by column chromatography using hexane: ethyl acetate (8:2) as mobile phase.

**General procedure for the preparation of 4-Amino-5-Alkyl-4H-[1,2,4]triazole-3-thiol (7a-c):**\(^{44,69}\) A mixture of aliphatic carboxylic acid (0.01 mole) and thiosemicarbazide (0.02 mole) was heated on an oil bath at 95-100°C for 1 h. The progress of the reaction was monitored by TLC using hexane: ethyl acetate (1:1) using mobile phase. The solid obtained was dissolved in 10% NaOH (aq) (6-8 mL), refluxed for 1 h and cooled. The reaction mixture was acidified using concentrated HCl to pH 6. The precipitate obtained was filtered, washed with water and dried. The crude product was purified by column chromatography using hexane: ethyl acetate (1:1) as mobile phase.
General procedure for the preparation of 4-Amino-5-Aryl-4H-[1,2,4]triazole-3-thiol (4a-b, 13d-o and 35a): To the solution of the oxadiazole (0.01 mole) in absolute ethanol, hydrazine hydrate 99% (0.01 mole) was added and refluxed for 12 h. The progress of the reaction was monitored by TLC using hexane: ethyl acetate (7:3) as mobile phase. At the end, the solvent was removed under reduced pressure. The concentrated product was added to 100 mL of cold water and acidified with concentrated HCl to pH 5. The product obtained was filtered, washed with water and dried. Purification was done by column chromatography using hexane: ethyl acetate (7:3) as mobile phase.

General procedure for the preparation of N-(3-Mercapto-5-Aryl-[1,2,4]triazol-4-yl)-amide (5a-m, 6a-r, 8d-l, 9d-o and 36a-f): To a solution of amino triazole (0.001 mole) in dry dioxane, (0.0012 moles) acid chloride was added drop wise with stirring. After the addition, the reaction mixture was refluxed for 10 h and monitored by TLC using chloroform: methanol (9:1) as mobile phase. The solvent was removed under reduced pressure and the product was purified by column chromatography using chloroform: methanol (9:1) as mobile phase.

General procedure for the preparation of 5-Aryl-4H-[1,2,4]triazole-3-thiol (15a, 19a and 20a): To the solution of acid hydrazide (0.01 mole) in 20% aqueous Ethanol (10 mL), HCl (0.001 mole) and ammonium thiocyanate (0.03 mole) were added and refluxed for 2 h. The reaction was monitored by TLC chloroform: methanol (9:1) as mobile phase. The solvent was removed under reduced pressure and the solid obtained was washed with alcohol and dried. The solid obtained was dissolved in 10% NaOH (aq.) (6 mL) and refluxed for 1 h and cooled. The reaction mixture was neutralized with concentrated HCl to pH 7. The solid obtained was filtered, washed with water and dried. The product was purified by column chromatography using chloroform: methanol (9:1) as mobile phase.

General procedure for the preparation of 3-Acylsulfanyl-5-aryl-4H-[1,2,4]triazole (15b-d, 19b-d and 20b-d): To the solution of triazole-3-thiol (0.01 mole) in absolute alcohol (10 mL), triethylamine (0.02 mole) was added and stirred. To this solution, alkyl/aryl halides (0.02 mole) was added drop wise and refluxed for 3 h. The reaction was monitored by TLC using chloroform: methanol (9:1) as mobile phase. The solvent was removed under reduced pressure and the crude product obtained was washed with water and purified by column chromatography. The product was purified by column chromatography using chloroform: methanol (9:1) as mobile phase.
General procedure for the preparation of 4,5-Diaryl-4H-[1,2,4]triazole-3-thiol (23a, 24a, 28a, 29a and 30a): To the solution of acid hydrazide (0.001 mole) in absolute alcohol (10mL), phenyl isothiocyanate (0.001 mole) was added and refluxed for 2h. The reaction was monitored by TLC using chloroform: methanol (9:1) as mobile phase. The solvent was removed under reduced pressure and the solid obtained was washed with alcohol and dried. (21a, 22a, 25a, 26a and 27a) The solid was dissolved in 10 % NaOH (aq.) (6mL), refluxed for 1h and cooled. The reaction mixture was neutralized with concentrated HCl to pH 7. The solid obtained was filtered, washed with water and dried. The product was purified by column chromatography using chloroform: methanol (9:1) as mobile phase.

General procedure for the preparation of 3-Acylsulfanyl-4,5-diphenyl-4H-[1,2,4]triazole (23b-d, 24b-d, 28b-d, 29b-d and 30b-d): To the solution of triazole-3-thiol (23a, 24a, 28a, 29a and 30a) (0.01 mole) in absolute alcohol (10mL), triethylamine (0.02 mole) was added and stirred. To this solution, alkyl/aryl halides (0.02 mole) was added drop wise and refluxed for 3h. The reaction was monitored by TLC using chloroform: methanol (9:1) as mobile phase. The solvent was removed under reduced pressure. The crude product was washed with water, dried and purified by column chromatography. The product was purified by column chromatography using chloroform: methanol (9:1) as mobile phase.

General procedure for the preparation of 5-Aryl-3H-[1,3,4]oxadiazol-2-one (31a-b): To a solution of acid hydrazide (0.002 mole) in dichloromethane (50mL), DIPEA (0.004 mole) was added and stirred under an inert atmosphere of Nitrogen gas. To this reaction mixture, triphosgene (0.0008 mole) dissolved in dichloromethane (10mL) was added drop wise with the help of a syringe. The reaction mixture was stirred at room temperature for 30 minutes. The reaction was monitored by TLC using hexane: ethyl acetate (1:1) as mobile phase. The solvent was removed under reduced pressure and the crude product was purified by column chromatography. The product was purified by column chromatography using hexane: ethyl acetate (1:1) as mobile phase.

General procedure for the preparation of N-(5-Oxo-3-aryl-1,5-dihydro-[1,2,4]triazol-4-yl)-arylamide (32a-h and 33a-d): To the solution of aryl oxadiazole-2-one (0.001 mole) in dry toluene, acid hydrazide (0.002 mole) was added and refluxed for 3h. The reaction was monitored by TLC using chloroform: methanol (9:1) as mobile phase. The solvent was removed under reduced pressure and crude product was purified by column chromatography. The product was purified by column chromatography using chloroform: methanol (9:1) as mobile phase.
Table 1: Physical properties of synthesized compounds (5a-m)

<table>
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<tr>
<th>S.No.</th>
<th>Code</th>
<th>R</th>
<th>Mol. Wt.</th>
<th>Rf a</th>
<th>M.P. (°C)</th>
<th>Yield (%)</th>
<th>λmax. b (nm)</th>
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<td>5a</td>
<td>-CH₃</td>
<td>236</td>
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<td>150-152</td>
<td>70</td>
<td>256</td>
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<td>0.31</td>
<td>160</td>
<td>68</td>
<td>255.8</td>
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<td>172-174</td>
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<td>255</td>
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<tr>
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<td>5e</td>
<td>-C₅H₁₁</td>
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<td>0.5</td>
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</table>

*Mobile phase= Chloroform: Methanol (9:1), *Solvent= Methanol.
Table 2: Physical properties of synthesized compounds (6a-r)

![Chemical structure of 6a-r](image)

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Code</th>
<th>R</th>
<th>M.W.</th>
<th>R_f</th>
<th>M.P. (°C)</th>
<th>Yield (%)</th>
<th>λ_max. (nm)</th>
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<tr>
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*aMobile phase= Chloroform: Methanol (9:1). bSolvent= Methanol.
**Table 3: Physical properties of synthesized compounds (8a-l)**

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<th>Yield (%)</th>
<th>( \lambda_{\text{max.}} )^b (nm)</th>
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^aMobile phase= Chloroform: Methanol (9:1), ^bSolvent= Methanol.
Table 4: Physical properties of synthesized compounds (9a-o)

![Chemical structure](image)

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<th>Yield (%)</th>
<th>λmax.&lt;sup&gt;b&lt;/sup&gt; (nm)</th>
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<sup>a</sup>Mobile phase= Chloroform: Methanol (9:1), <sup>b</sup>Solvent= Methanol.
Table 5: Physical properties of synthesized compounds (15a-30d)

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*Mobile phase= Chloroform: Methanol (9:1), Solvent= Methanol.*
### Table 6: Physical properties of synthesized compounds (32a-33d)

![Chemical structure](https://example.com/structure.png)

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Code</th>
<th>R</th>
<th>R¹</th>
<th>M.Wt.</th>
<th>Rf a</th>
<th>M.P. (°C)</th>
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</thead>
<tbody>
<tr>
<td>90</td>
<td>32a</td>
<td>-H</td>
<td><img src="https://example.com/benzene.png" alt="苯环" /></td>
<td>282</td>
<td>0.5</td>
<td>212-214</td>
<td>44</td>
<td>268.8</td>
</tr>
<tr>
<td>91</td>
<td>32b</td>
<td>-H</td>
<td><img src="https://example.com/benzene.png" alt="苯环" /> <img src="https://example.com/methyl.png" alt="甲基" /></td>
<td>296</td>
<td>0.52</td>
<td>186-188</td>
<td>54</td>
<td>269.2</td>
</tr>
<tr>
<td>92</td>
<td>32c</td>
<td>-H</td>
<td><img src="https://example.com/benzene.png" alt="苯环" /> <img src="https://example.com/methyl.png" alt="甲基" /></td>
<td>296</td>
<td>0.51</td>
<td>206-208</td>
<td>74</td>
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</tr>
<tr>
<td>93</td>
<td>32d</td>
<td>-H</td>
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<td>264.6</td>
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<tr>
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<td>32e</td>
<td>-H</td>
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<tr>
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<td>312</td>
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<td>25</td>
<td>269.2</td>
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<tr>
<td>96</td>
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<td>-H</td>
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<tr>
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<td>-H</td>
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<td>268.6</td>
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<tr>
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<td><img src="https://example.com/benzene.png" alt="苯环" /> <img src="https://example.com/methyl.png" alt="甲基" /></td>
<td>296</td>
<td>0.5</td>
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<tr>
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<td>-CH₃</td>
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<td>206-208</td>
<td>52</td>
<td>273.6</td>
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<td>-CH₃</td>
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<tr>
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<td>-CH₃</td>
<td><img src="https://example.com/benzene.png" alt="苯环" /> <img src="https://example.com/methyl.png" alt="甲基" /> <img src="https://example.com/formic_acid.png" alt="甲酸" /> <img src="https://example.com/methyl.png" alt="甲基" /> <img src="https://example.com/chlorine.png" alt="氯原子" /> <img src="https://example.com/hydrogen.png" alt="氢原子" /></td>
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*Mobile phase= Chloroform: Methanol (9:1), Solvent= Methanol.
Table 7: Physical properties of synthesized compounds (36a-f)

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<th>S.No.</th>
<th>Code</th>
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<th>M.P. (°C)</th>
<th>Yield (%)</th>
<th>λ_max. (nm)</th>
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<td>-C_3H_7</td>
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<td>0.35</td>
<td>184-186</td>
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<td>103</td>
<td>36b</td>
<td>-C_4H_9</td>
<td>368</td>
<td>0.4</td>
<td>174-176</td>
<td>48</td>
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<tr>
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<td></td>
<td>366</td>
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<td>212-214</td>
<td>50</td>
<td>258.2</td>
</tr>
</tbody>
</table>

4.4. Spectral data and characterization

4-Amino-5-pyrazin-2-yl-4H-[1,2,4]triazole-3-thiol (4a): FTIR (KBr, cm⁻¹): 3458 (N-H, str.), 3197 (C-H, str.), 2988 (S-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 5.96 (s, 2H), 8.29 (dd, J=2.4 Hz and 1.6 Hz, 1H), 8.81 (d, J=2.4 Hz, 1H), 9.26 (d, J=1.6 Hz, 1H), 14.19 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 141.48, 144.96, 145.05, 146.34, 146.91, 166.81. GCMS (EI, m/z) 194 (M)+.

4-Amino-5-(5-methyl-pyrazin-2-yl)-4H-[1,2,4]triazole-3-thiol (4b): FTIR (KBr, cm⁻¹): 3458 (N-H, str.), 3115 (C-H, str.), 2372 (S-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.48 (s, 3H), 5.96 (s, 2H), 8.70 (d, J=1.2 Hz, 1H), 9.12 (d, J=1.6 Hz, 1H), 14.13 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 21.78, 138.56, 143.84, 144.49, 147.03, 155.68, 166.57. GCMS (EI, m/z) 208 (M)+.

4-Amino-5-methyl-4H-[1,2,4]triazole-3-thiol (7a): FTIR (KBr, cm⁻¹): 3510 (N-H, str.), 2965 (Ar-H, str.), 2346 (S-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.23 (s, 3H), 5.50 (s, 2H), 13.37 (s, 1H); GCMS (EI, m/z) 130 (M)+.

4-Amino-5-ethyl-4H-[1,2,4]triazole-3-thiol (7b): FTIR (KBr, cm⁻¹): 3443 (N-H, str.), 3105 (C-H, str.), 2965 (Ar-H, str.), 2300 (S-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.23 (s, 3H), 4.06 (s, 2H), 5.52 (s, 2H), 7.10 (s, 3H), 12.67 (s, 1H); GCMS (EI, m/z) 144 (M)+.

4-Amino-5-propyl-4H-[1,2,4]triazole-3-thiol (7c): FTIR (KBr, cm⁻¹): 3435 (N-H, str.), 3086 (C-H, str.), 2997 (Ar-H, str.), 2367 (S-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 0.93 (t, J=7.6 Hz, 2H), 1.61 - 1.67 (m, 2H), 2.60 (t, J=7.2 Hz, 3H), 4.06 (s, 2H), 5.25 (s, 2H), 13.40 (s, 1H); GCMS (EI, m/z) 158 (M)+.

4-Amino-5-phenyl-4H-[1,2,4]triazole-3-thiol (13a): FTIR (KBr, cm⁻¹): 3466 (N-H, str.), 3151(C-H, str.), 3070 (Ar-H, str.), 2316 (S-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 5.77 (s, 2H), 7.50-7.53 (m, 3H), 7.99-8.02 (m, 2H), 13.89 (s, 1H); GCMS (EI, m/z) 192 (M)+.

4-Amino-5-o-tolyl-4H-[1,2,4]triazole-3-thiol (13e): FTIR (KBr, cm⁻¹): 3442 (N-H, str.), 3234 (C-H, str.), 3095 (Ar-H, str.), 2368 (S-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.25 (s, 3H), 5.53 (s, 2H), 7.28- 7.36 (m, 2H), 7.41-7.48 (m, 2H), 13.84 (s, 1H); GCMS (EI, m/z) 206 (M)+.

4-Amino-5-p-tolyl-4H-[1,2,4]triazole-3-thiol (13f): FTIR (KBr, cm⁻¹): 3433 (N-H, str.), 3244 (C-H, str.), 2926 (Ar-H, str.), 2368 (S-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.38 (s, 3H), 5.76 (s, 2H), 7.34 (d, J= 8.4 Hz, 2H), 7.92 (d, J=8 Hz, 2H), 13.84 (s, 1H); GCMS (EI, m/z) 206 (M)+.

4-Amino-5-(3-methoxy-phenyl)-4H-[1,2,4]triazole-3-thiol (13g): FTIR (KBr, cm⁻¹): 3425 (N-H, str.), 3186 (C-H, str.), 3045 (Ar-H, str.), 2364 (S-H, str.), 1280 (Assym. Ar-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 3.82 (s, 3H), 5.78 (s, 2H), 7.09- 7.12 (m, 1H), 7.45 (t, J= 8 Hz, 1H), 7.56- 7.59 (m, 2H), 13.91 (s, 1H); GCMS (EI, m/z) 222 (M)+.

4-Amino-5-(4-methoxy-phenyl)-4H-[1,2,4]triazole-3-thiol (13h): FTIR (KBr, cm⁻¹): 3433 (N-H, str.), 3005 (Ar-H, str.), 2362 (S-H, str.), 1280 (Assym. Ar-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 3.83 (s, 3H), 5.76 (s, 2H), 7.10 (dd, J= 7.2 Hz and 2.4 Hz, 2H), 8.00 (t, J= 6.8 Hz and 2 Hz, 2H), 13.80 (s, 1H); GCMS (EI, m/z) 222 (M)+.
4-Amino-5-(2-chloro-phenyl)-4H-[1,2,4]triazole-3-thiol (13i): FTIR (KBr, cm⁻¹): 3400 (N-H, str.), 3076 (Ar-H, str.), 2366 (S-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 5.49 (s, 2H), 7.47-7.51 (m, 1H), 7.59-7.61 (m, 3H), 13.96 (s, 1H); GCMS (EI, m/z) 226 (M⁺).

4-Amino-5-(4-chloro-phenyl)-4H-[1,2,4]triazole-3-thiol (13j): FTIR (KBr, cm⁻¹): 3425 (N-H, str.), 2933 (Ar-H, str.), 2362 (S-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 5.77 (s, 2H, -NH₂), 8.06 (dd, J = 6.4 Hz and 1.6 Hz, 2H), 7.61 (dd, J = 6.8 Hz and 2 Hz, 2H), 13.95 (s, 1H); GCMS (EI, m/z) 226 (M⁺).

4-Amino-5-(4-fluoro-phenyl)-4H-[1,2,4]triazole-3-thiol (13k): FTIR (KBr, cm⁻¹): 3365 (N-H, str.), 3041 (Ar-H, str.), 2368 (S-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 5.76 (s, 2H), 8.09 (dd, J = 6.8 Hz and 2 Hz, 2H), 7.39 (dd, J = 6.8 Hz and 2 Hz, 2H), 13.90 (s, 1H); GCMS (EI, m/z) 210 (M⁺).

4-Amino-5-phenoxy methyl-4H-[1,2,4]triazole-3-thiol (13l): FTIR (KBr, cm⁻¹): 3444 (N-H, str.), 3011 (C-H, str.), 2906 (Ar-H, str.), 2352 (S-H, str.), 1179 (Sym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 5.21 (s, 2H), 5.64 (s, 2H), 7.29-7.33 (m, 5H), 13.77 (s, 1H); GCMS (EI, m/z) 222 (M⁺).

4-Amino-5-(4-ethyl-phenyl)-4H-[1,2,4]triazole-3-thiol (13m): FTIR (KBr, cm⁻¹): 3456 (N-H, str.), 3112 (C-H, str.), 3055 (Ar-H, str.), 2368 (S-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 1.21 (t, J = 15.2 Hz and 7.6 Hz, 3H) 2.69 (dd, J = 15.2 Hz and 7.6 Hz, 2H), 5.75 (s, 2H), 7.93 (dd, J = 6.8 Hz and 2 Hz, 2H), 7.36 (d, J = 8.4 Hz, 2H), 13.84 (s, 1H, -SH); GCMS (EI, m/z) 220 (M⁺).

4-Amino-5-(4-ethoxy-phenyl)-4H-[1,2,4]triazole-3-thiol (13n): FTIR (KBr, cm⁻¹): 3535 (N-H, str.), 2991 (Ar-H, str.), 2345 (S-H, str.) 1256 (Assym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 1.35 (t, J = 14 Hz and 7.2 Hz, 3H), 4.11 (dd, J = 14 Hz and 6.8 Hz, 2H), 5.74 (s, 2H), 7.05 (dd, J = 6.8 Hz and 2 Hz, 2H), 7.96 (dd, J = 6.8 Hz and 2 Hz, 2H), 13.77 (s, 1H); GCMS (EI, m/z) 236 (M⁺).

4-Amino-5-(3,4-dimethoxy-phenyl)-4H-[1,2,4]triazole-3-thiol (13o): FTIR (KBr, cm⁻¹): 3446 (N-H, str.), 3022 (Ar-H, str.), 2367 (S-H, str.), 1180 (Sym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 3.82 (t, J = 14.4 Hz and 4.8 Hz, 6H), 5.77 (s, 2H), 7.09 (d, J = 8.8 Hz, 1H), 7.57 (d, J = 2 Hz, 1H), 7.66 (dd, J = 8.4 Hz and 2 Hz, 1H), 13.80 (s, 1H); GCMS (EI, m/z) 252 (M⁺).

5-Pyrazin-2-yl-3H-[1,3,4]oxadiazol-2-one (31a): FTIR (KBr, cm⁻¹): 3427 (N-H, str.), 3070 (Ar-H, str.), 2364 (S-H, str.), 1616 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 8.81 (s, 2H), 9.13 (s, 1H), 12.98 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 139.71, 142.85, 145.25, 146.87, 152.13, 154.71. GCMS (EI, m/z) 164 (M⁺).

5-(5-Methyl-pyrazin-2-yl)-3H-[1,3,4]oxadiazol-2-one (31b): FTIR (KBr, cm⁻¹): 3483 (N-H, str.), 3043 (Ar-H, str.), 2368 (S-H, str.), 1663 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.59 (s, 3H), 8.69 (s, 1H), 8.98 (s, 1H), 12.89 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 21.82, 136.89, 141.72, 144.87, 152.35, 154.74, 156.37. GCMS (EI, m/z) 178 (M⁺).

N-(3-Mercapto-5-pyrazin-2-yl-[1,2,4]triazol-4-yl)-acetamide (5a): FTIR (KBr, cm⁻¹): 3345 (N-H, str.), 3041 (Ar-H, str.), 1691 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 1.99 (s,
3H), 8.77 (d, J= 2.4 Hz and 1.6 Hz, 1H), 8.80 (d, J= 2.4 Hz, 1H), 9.10 (d, J= 1.6 Hz, 1H), 11.46 (s, 1H), 14.39 (s, 1H); GCMS (EI, m/z) 236 (M)+.

**N-(3-Mercapto-5-pyrazin-2-yl-[1,2,4]triazol-4-yl)-propionamide (5b):** FTIR (KBr, cm⁻¹): 3407 (N-H, str.), 3047(Ar-H, str.), 2771 (S-H, str.), 1741 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): 6 1.00 (t, J= 7.2 Hz, 3H), 2.67- 2.72 (m, 2H), 8.80 (dd, J= 2.4 Hz and 1.6 Hz, 1H), 8.68 (d, J= 2.4 Hz, 1H), 9.26 (d, J= 1.6 Hz, 1H), 11.46 (s, 1H), 14.81 (s, 1H); GCMS (EI, m/z) 250 (M)+.

**N-(3-Mercapto-5-pyrazin-2-yl-[1,2,4]triazol-4-yl)-butyramide (5c):** FTIR (KBr, cm⁻¹): 3319 (N-H, str.), 3095 (Ar-H, str.), 2368 (S-H, str.), 1741 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 0.82 (t, J= 7.2 Hz, 3H), 1.47- 1.56 (m, 2H), 2.71 (dd, 2H), 8.80 (d, J= 2.4 Hz, 1H), 8.67 (d, J= 1.6 Hz, 1H), 9.26 (s, 1H), 11.44 (s, 1H), 14.79 (s, 1H); GCMS (EI, m/z) 264 (M)+.

**Pentanoic acid (3-mercapto-5-pyrazin-2-yl-[1,2,4]triazol-4-yl)-amide (5d):** FTIR (KBr, cm⁻¹): 3341 (N-H, str.), 3167 (C-H, str.), 1712 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 0.857(t, J= 7.2Hz, 3H), 1.19- 1.28 (m, 2H), 1.45- 1.52 (m, 2H), 2.77 (t, J= 7.2 Hz, 2H), 8.74 (dd, J= 2.4 Hz and 1.6 Hz, 1H), 8.79 (d, J= 2.4 Hz, 1H), 9.09 (d, J= 1.6 Hz, 1H), 11.44 (s, 1H), 14.37 (s, 1H); LCMS (ESI, m/z) 279.03 (M+H)+.

**Hexanoic acid (3-mercapto-5-pyrazin-2-yl-[1,2,4]triazol-4-yl)-amide (5e):** FTIR (KBr, cm⁻¹): 3300 (N-H, str.), 3163 (C-H, str.), 2956 (Ar-H, str.), 2605 (S-H, str.), 1714 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 0.84 (t, J= 7.2 Hz, 3H), 1.18- 1.27 (m, 4H), 1.46- 1.54 (m, 2H), 2.26 (t, J= 7.2 Hz, 2H), 8.74 (dd, J= 2.4 Hz and 1.6 Hz, 1H), 8.80 (d, J= 1.6 Hz, 1H), 9.09 (d, J= 1.6 Hz, 1H), 11.44 (s, 1H), 14.38 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 14.29, 22.23, 24.74, 31.00, 33.41, 140.97, 143.99, 144.80, 146.69, 147.69, 169.37, 171.63. LCMS (ESI, m/z) 294.88 (M+H)+.

**Heptanoic acid (3-mercapto-5-pyrazin-2-yl-[1,2,4]triazol-4-yl)-amide (5f):** FTIR (KBr, cm⁻¹): 3348 (N-H, str.), 3153 (C-H, str.), 2956 (Ar-H, str.), 2370 (S-H, str.), 1680 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 0.85 (t, J= 6.8 Hz, 3H), 1.51(t, J= 6.8 Hz, 2H), 1.21- 1.24 (m, 6H), 2.26 (t, J= 7.2 Hz, 2H), 8.74 (dd, J= 2.4 Hz and 1.6 Hz, 1H), 8.80 (d, J= 1.6 Hz, 1H), 9.09 (d, J= 1.6 Hz, 1H), 11.46 (s, 1H), 14.37 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 14.37, 22.42, 25.03, 29.50, 31.37, 33.47, 140.97, 143.99, 144.79, 146.69, 147.31, 169.38, 171.63. GCMS (EI, m/z) 306 (M)+.

**N-(3-Mercapto-5-pyrazin-2-yl-[1,2,4]triazol-4-yl)-2-methyl-benzamide (5g):** FTIR (KBr, cm⁻¹): 3390 (N-H, str.), 3032 (Ar-H, str.), 1707 (C=O, str.); ¹³CNMR (100 MHz, DMSO-d₆): δ 19.56, 126.17, 128.21, 131.19, 133.45, 136.94, 141.00, 144.00, 144.81, 146.81, 147.13, 167.79, 169.62. GCMS (EI, m/z) 312 (M)+.

**N-(3-Mercapto-5-pyrazin-2-yl-[1,2,4]triazol-4-yl)-3-methoxy-benzamide (5h):** FTIR (KBr, cm⁻¹): 3385 (N-H, str.), 3099 (Ar-H, str.), 3034 (C-H, str.), 1685 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 3.81 (s, 3H), 7.19- 7.22 (m, 1H), 7.42- 7.44 (m, 1H), 7.46- 7.50 (m, 2H), 8.66- 8.67 (dd, J= 2.4 Hz and 1.6 Hz, 1H), 8.76 (d, J= 2.4 Hz, 1H), 9.17 (d, J= 1.6 Hz, 1H), 12.03 (s, 1H), 14.49 (s, 1H); GCMS (EI, m/z) 328 (M)+.

**N-(3-Mercapto-5-pyrazin-2-yl-[1,2,4]triazol-4-yl)-4-methoxy-benzamide (5i):** FTIR (KBr, cm⁻¹): 3338 (N-H, str.), 2960 (Ar-H, str.), 2681 (S-H, str.), 1693 (C=O, str.), 1290 (Assym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 3.81 (s, 3H), 7.04 (d, J= 8.8 Hz, 2H); 7.72
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(d, J=8.8 Hz, 2H), 8.87- 8.88 (dd, J= 2.4 Hz and 1.6 Hz, 1H), 9.00 (d, J= 2.4 Hz, 1H), 9.20 (d, J= 1.6 Hz, 1H), 12.29 (s, 1H), 14.09 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-d$_6$): $\delta$ 55.87, 113.29, 119.05, 120.46, 130.46, 133.00, 140.92, 143.89, 144.90, 146.77, 147.25, 159.78, 165.52, 169.69. GCMS (EI, m/z) 328 (M)$^+$. 

4-Fluoro-N-(3-mercapto-5-pyrazin-2-yl-[1,2,4]triazol-4-yl)-benzamide (5j): FTIR (KBr, cm$^{-1}$): 3340 (N-H, str.), 3039 (Ar-H, str.), 2964 (C-H, str.), 2360 (S-H, str.), 1697 (C=O, str.); $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ 7.30- 7.42 (m, 2H), 7.96- 8.00 (m, 2H), 8.64- 8.65 (dd, J= 2.4 Hz and 1.6 Hz, 1H), 8.76 (d, J= 2.4 Hz, 1H), 9.177 (d, J= 1.6 Hz, 1H), 12.11 (s, 1H), 14.51 (s, 1H); GCMS (EI, m/z) 316 (M)$^+$. 

4-Ethyl-N-(3-mercapto-5-pyrazin-2-yl-[1,2,4]triazol-4-yl)-benzamide (5k): FTIR (KBr, cm$^{-1}$): 3068 (Ar-H, str.), 2960 (C-H, str.), 2682 (S-H, str.), 1691 (C=O, str.); $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ 1.22 (t, J= 7.6 Hz, 3H), 2.65- 2.71 (dd, J= 15.2 Hz and 7.6 Hz, 2H), 7.39 (d, J= 8 Hz, 2H), 7.84 (d, J= 8 Hz, 2H), 8.65- 8.66 (dd, J= 2.4 Hz and 1.6 Hz, 1H), 8.76 (d, J= 2.4 Hz, 1H), 9.16 (d, J= 1.6 Hz, 1H), 11.96 (s, 1H), 14.47 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-d$_6$): $\delta$ 15.74, 28.62, 128.57, 129.15, 140.96, 143.89, 144.90, 145.15, 146.10, 146.73, 147.38, 149.50, 164.65, 165.64, 169.70. GCMS (EI, m/z) 326 (M)$^+$. 

4-Ethoxy-N-(3-mercapto-5-pyrazin-2-yl-[1,2,4]triazol-4-yl)-benzamide (5l): FTIR (KBr, cm$^{-1}$): 3347 (N-H, str.), 2989 (Ar-H, str.), 2466 (S-H, str.), 1691 (C=O, str.), 1269 (Assym. C=O-C, str.), 873; $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ 1.36 (t, J= 7.2 Hz and 14 Hz, 3H), 4.08- 4.14 (dd, J= 7.2 Hz and 14 Hz, 2H), 7.06 (dd, J= 8.8 Hz, 2H), 7.85- 7.88 (m, 2H), 8.64- 8.65 (dd, J= 2.4 Hz and 1.6 Hz, 1H), 8.75 (d, J= 2.4 Hz, 1H), 9.14 (d, J= 1.6 Hz, 1H), 11.86 (s, 1H), 14.45 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-d$_6$): $\delta$ 14.95, 63.82, 15.33, 117.09, 129.43, 143.09, 144.46, 144.53, 149.50, 150.93, 161.01, 162.56, 168.32. GCMS (EI, m/z) 342 (M)$^+$. 

N-(3-Mercapto-pyrazin-2-yl-[1,2,4]triazol-4-yl)-3,4-dimethoxy-benzamide (5m): FTIR (KBr, cm$^{-1}$): 3080 (Ar-H, str.), 3034 (C-H, str.), 2364 (S-H, str.), 1680 (C=O, str.), 1253 (Assym. C-O-C, str.), 1134 (Sym. C-O-C, str.); $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ 3.78-3.83 (m, 6H), 7.11 (d, J= 8.4 Hz, 1H), 7.45 (d, J= 2 Hz, 1H), 7.59 (dd, J= 8.4 Hz and 2 Hz, 1H), 8.65- 8.66 (dd, J= 2.4 Hz and 1.6 Hz, 1H), 8.76 (d, J= 2.4 Hz, 1H), 9.15 (d, J= 1.6 Hz, 1H), 11.88 (s, 1H), 14.46 (s, 1H); LCMS (ESI, m/z) 359.07 (M+H)$^+$. 

N-[3-Mercapto-(5-methyl-pyrazin-2-yl]-[1,2,4]triazol-4-yl]-acetamide (6a): FTIR (KBr, cm$^{-1}$): 3223 (N-H, str.), 2956 (Ar-H, str.), 2368 (S-H, str.), 1722 (C=O, str.); $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ 1.98 (s, 3H), 2.07 (s, 3H), 8.60 (d, J= 0.8 Hz, 1H), 8.94 (d, J= 1.2 Hz, 1H), 9.11 (d, J= 1.2 Hz, 1H), 11.42 (s, 1H), 14.73 (s, 1H); LCMS (ESI, m/z) 251.06 (M+H)$^+$. 

N-[3-Mercapto-(5-methyl-pyrazin-2-yl]-[1,2,4]triazol-4-yl]-propionamide (6b): FTIR (KBr, cm$^{-1}$): 2956 (Ar-H, str.), 2368 (S-H, str.), 1672 (C=O, str.), 1577 (C-C, str.); $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ 1.04 (t, J= 7.6 Hz, 2H), 2.24- 2.28 (q, J=7.6 Hz, 3H), 2.56 (s, 3H), 8.64 (d, J= 0.8 Hz, 1H), 8.95 (d, J= 1.2 Hz, 1H), 11.37 (s, 1H), 14.30 (s, 1H); LCMS (ESI, m/z) 265.08(M+H)$^+$. 

N-[3-Mercapto-(5-methyl-pyrazin-2-yl]-[1,2,4]triazol-4-yl]-butyramide (6c): FTIR (KBr, cm$^{-1}$): 2956 (Ar-H, str.), 2368 (S-H, str.), 1635 (C-O, str.), 1558 (C-C, str.); $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ 0.87 (t, J= 7.4Hz, 3H), 1.49- 1.56 (m, 2H), 2.24 (t, J= 7.2 Hz, 2H), 2.56 (s, 3H), 8.63 (d, J= 1.2 Hz, 1H), 8.94 (d, J= 1.6 Hz, 1H), 11.40 (s, 1H), 14.30 (s, 1H);
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13C NMR (100 MHz, DMSO-d6): δ 13.90, 18.59, 21.76, 35.41, 138.11, 142.82, 144.37, 147.51, 156.13, 169.23, 171.48. LCMS (ESI, m/z) 280.09 (M+H)+.

Pentanoic acid [3-mercapto-5-(5-methyl-pyrazin-2-yl)-[1,2,4]triazol-4-yl]-amide (6d): FTIR (KBr, cm−1): 3340 (N-H, str.), 2972 (Ar-H, str.), 2823 (C-H, str.), 1710 (C=O, str.), 1521 (C-C, str.); 1H NMR (400 MHz, DMSO-d6): δ 0.85 (t, J = 7.4 Hz, 3H), 1.22-1.26 (m, 2H), 1.45-1.52 (m, 2H), 2.26 (t, J = 7.2 Hz, 2H), 2.57 (s, 3H), 8.63 (d, J = 0.8 Hz, 1H), 8.93 (d, J = 1.2 Hz, 1H), 11.41 (s, 1H), 14.30 (s, 1H); LCMS (ESI, m/z) 294.82 (M+H)+.

Hexanoic acid [3-mercapto-5-(5-methyl-pyrazin-2-yl)-[1,2,4]triazol-4-yl]-amide (6e): FTIR (KBr, cm−1): 3340 (N-H, str.), 3018 (Ar-H, str.), 2951 (Ar-H, str.), 2825 (C-H, str.), 2357 (S-H, str.), 1701 (C=O, str.), 1521 (C-C, str.); 1H NMR (400 MHz, DMSO-d6): δ 0.84 (t, J = 7 Hz, 3H), 1.25-1.27 (m, 2H), 1.46-1.53 (m, 4H), 2.25 (t, J = 7.4 Hz, 2H), 2.57 (s, 3H), 8.63 (d, J = 0.8 Hz, 1H), 8.93 (d, J = 1.6 Hz, 1H), 11.41 (s, 1H), 14.30 (s, 1H); LCMS (ESI, m/z) 307.13 (M+H)+.

Heptanoic acid [3-mercapto-5-(5-methyl-pyrazin-2-yl)-[1,2,4]triazol-4-yl]-amide (6f): FTIR (KBr, cm−1): 3330 (N-H, str.), 3018 (Ar-H, str.), 2937 (C-H, str.), 2357 (S-H, str.), 1708 (C=O, str.), 1494 (C-C, str.); 1H NMR (400 MHz, DMSO-d6): δ 0.85 (t, J = 6.4 Hz, 3H), 1.20-1.23 (m, 6H), 1.50 (t, J = 6.8 Hz, 2H), 2.25 (t, J = 7.4 Hz, 2H), 2.56 (s, 3H), 8.63 (d, J = 0.8 Hz, 1H), 8.93 (d, J = 1.2 Hz, 1H), 11.41 (s, 1H), 14.29 (s, 1H); 13C NMR (100 MHz, DMSO-d6): δ 14.35, 21.75, 22.44, 25.03, 28.48, 31.38, 33.47, 138.10, 142.87, 144.37, 147.61, 156.11, 169.23, 171.58. LCMS (m/z) 321.14 (M+H)+.

N-[3-Mercapto-5-(5-methyl-pyrazin-2-yl)-[1,2,4]triazol-4-yl]-benzamide (6g): FTIR (KBr, cm−1): 3323 (N-H, str.), 3018 (Ar-H, str.), 2357 (S-H, str.), 1701 (C=O, str.), 1521 (C-C, str.); 1H NMR (400 MHz, DMSO-d6): δ 2.52 (s, 3H), 7.57 (t, J = 7.6 Hz, 2H), 7.64 (t, J = 7.2 Hz, 1H), 7.89-7.91 (dd, J = 7.2 Hz and 5.2 Hz, 2H), 8.55 (d, J = 0.8 Hz, 1H), 9.02 (d, J = 1.2 Hz, 1H), 12.04 (s, 1H), 14.42 (s, 1H); 13C NMR (100 MHz, DMSO-d6): δ 21.73, 128.26, 129.21, 131.74, 133.15, 138.09, 142.75, 144.49, 147.53, 156.25, 165.72, 169.51. LCMS (+ESI, m/z) 313.08 (M+H)+.

N-[3-Mercapto-5-(5-methyl-pyrazin-2-yl)-[1,2,4]triazol-4-yl]-2-methyl-benzamide (6h): FTIR (KBr, cm−1): 3340 (N-H, str.), 2972 (Ar-H, str.), 2357 (S-H, str.), 1701 (C=O, str.), 1492 (C-C, str.); 1H NMR (400 MHz, DMSO-d6): δ 2.38 (s, 3H), 2.51 (s, 3H), 7.33-7.34 (dd, J = 8.4 Hz and 2.4 Hz, 2H), 7.51-7.53 (m, 1H), 7.82 (d, J = 8.4 Hz, 2H), 8.54 (d, J = 0.8 Hz, 1H), 9.00 (d, J = 1.6 Hz, 1H), 11.42 (s, 1H), 14.39 (s, 1H); LCMS (+ESI, m/z) 327.09 (M+H)+.

N-[3-Mercapto-5-(5-methyl-pyrazin-2-yl)-[1,2,4]triazol-4-yl]-4-methyl-benzamide (6i): FTIR (KBr, cm−1): 3398 (N-H, str.), 2980 (Ar-H, str.), 2357 (S-H, str.), 1664 (C=O, str.), 1494 (C-C, str.); 1H NMR (400 MHz, DMSO-d6): δ 2.38 (s, 3H), 2.51 (s, 3H), 7.36 (d, J = 8 Hz, 2H), 7.82 (d, J = 8.4 Hz, 2H), 8.54 (d, J = 0.8 Hz, 1H), 9.00 (d, J = 1.6 Hz, 1H), 11.42 (s, 1H), 14.39 (s, 1H); 13C NMR (100 MHz, DMSO-d6): δ 21.58, 21.72, 128.30, 128.90, 129.71, 138.09, 142.74, 143.38, 144.48, 147.61, 156.23, 165.58, 169.54. LCMS (+ESI, m/z) 327.09 (M+H)+.

N-[3-Mercapto-5-(5-methyl-pyrazin-2-yl)-[1,2,4]triazol-4-yl]-3-methoxy-benzamide (6j): FTIR (KBr, cm−1): 3234, 3018 (Ar-H, str.), 2850 (C-H, str.), 2366 (S-H, str.), 1662 (C=O, str.), 1467 (C-C, str.), 1261 (Assym. C-O-C, str.); 1H NMR (400 MHz, DMSO-d6): δ 2.52 (s, 3H), 3.68 (s, 3H), 3.85 (s, 3H), 6.77-6.79 (m, 2H), 7.25-7.27 (m, 2H), 7.78-7.80 (m, 3H), 8.11 (d, J = 8.4 Hz, 2H), 8.63 (d, J = 0.8 Hz, 1H), 9.00 (d, J = 1.6 Hz, 1H), 11.42 (s, 1H), 14.39 (s, 1H); 13C NMR (100 MHz, DMSO-d6): δ 21.58, 21.72, 128.30, 128.90, 129.71, 138.09, 142.74, 143.38, 144.48, 147.61, 156.23, 165.58, 169.54. LCMS (+ESI, m/z) 327.09 (M+H)+.
3H), 3.81 (s, 3H), 7.19- 7.22 (m, 1H), 7.43- 7.50 (m, 3H), 8.56 (d, J= 0.8 Hz, 1H), 9.01 (d, J= 1.6 Hz, 1H), 12.01 (s, 1H), 14.50 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-$d_6$): δ 21.73, 55.72, 113.29, 120.46, 130.44, 133.01, 138.05, 142.74, 144.50, 147.50, 156.28, 159.77, 165.45, 169.50. LCMS (+ESI, m/z) 343.09 (M+H)$^+$.  

N-[3-Mercapto-5-(5-methyl-pyrazin-2-yl)-1,2,4]triazol-4-yl]-4-methoxy-benzamide (6k): FTIR (KBr, cm$^{-1}$): 3340 (N-H, str.), 3018 (Ar-H, str.), 2980 (C-H, str.), 2357 (S-H, str.), 1662 (C=O, str.), 1467 (C=C, str.), 1261(Sym. C-O-C, str.); $^1$H NMR (400 MHz, DMSO-$d_6$): δ 2.55 (s, 3H), 3.83 (s, 3H), 7.06- 7.08 (dd, J= 12.4 Hz and 6.8 Hz, 3H), 7.87- 7.90 (dd, J= 6.8 Hz and 2 Hz, 1H), 8.56 (d, J= 0.8 Hz, 1H), 9.01 (d, J= 1.6 Hz, 1H), 12.01 (s, 1H), 14.42 (s, 1H); LCMS (+ESI, m/z) 343.09 (M+H)$^+$.  

2-Chloro-N-[3-mercaptopo-5-(5-methyl-pyrazin-2-yl)-1,2,4]triazol-4-yl]-benzamide (6l): FTIR (KBr, cm$^{-1}$): 3016 (Ar-H, str.), 2355 (S-H, str.), 1705 (C=O, str.); $^1$H NMR (400 MHz, DMSO-$d_6$): δ 2.52 (s, 3H), 7.65 (dd, J= 6.8 Hz and 2 Hz, 1H), 7.94- 7.90 (m, 3H), 8.54 (d, J= 1.2 Hz, 1H), 9.02 (d, J= 1.2 Hz, 1H), 12.41 (s, 1H), 14.44 (s, 1H); LCMS (+ESI, m/z) 347.03 (M+H)$^+$.  

4-Chloro-N-[3-mercaptopo-5-(5-methyl-pyrazin-2-yl)-1,2,4]triazol-4-yl]-benzamide (6m): FTIR (KBr, cm$^{-1}$): 3022 (Ar-H, str.), 2897 (C-H, str.), 2384 (S-H, str.), 1678 (C=O, str.), 1467 (C-C, str.); $^1$H NMR (400 MHz, DMSO-$d_6$): δ 2.60 (s, 3H), 7.33- 7.36 (m, 2H), 7.80- 7.83 (m, 2H), 8.74 (d, J= 1.2 Hz, 1H), 9.03 (d, J= 1.2 Hz, 1H), 12.20 (s, 1H), 14.20 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-$d_6$): δ 21.74, 129.22, 130.18, 131.62, 138.02, 130.48, 138.27, 142.74, 144.45, 147.33, 156.28, 164.86, 166.93, 169.45. LCMS (+ESI, m/z) 347.04 (M+H)$^+$.  

4-Fluoro-N-[3-mercaptopo-5-(5-methyl-pyrazin-2-yl)-1,2,4]triazol-4-yl]-benzamide (6n): FTIR (KBr, cm$^{-1}$): 3022 (Ar-H, str.), 2899 (C-H, str.), 2368 (S-H, str.), 1678 (C=O, str.); $^1$H NMR (400 MHz, DMSO-$d_6$): δ 2.63 (s, 3H), 7.36 (t, J = 8.8 Hz, 2H), 7.79- 7.83 (m, 2H), 8.74 (s, 1H), 9.03 (s, 1H), 12.20 (s, 1H), 14.20 (s, 1H); LCMS (+ESI, m/z) 331.21 (M+H)$^+$.  

N-[3-Mercapto-5-(5-methyl-pyrazin-2-yl)-1,2,4]triazol-4-yl]-2-phenoxy-acetamide (6o): FTIR (KBr, cm$^{-1}$): 3022 (Ar-H, str.), 2887 (C-H, str.), 2360 (S-H, str.), 1712 (C=O, str.), 1284 (Assym. C-O-C, str.); $^1$H NMR (400 MHz, DMSO-$d_6$): δ 2.62 (s, 3H), 5.05 (s, 2H), 6.89- 6.94 (m, 3H), 7.20- 7.24 (m, 2H), 8.70 (d, J = 1.2 Hz, 1H), 9.08 (d, J = 1.6 Hz, 1H), 12.07 (s, 1H), 14.05 (s, 1H); LCMS (+ESI, m/z) 343.09 (M+H)$^+$.  

4-Ethyl-N-[3-mercaptopo-5-(5-methyl-pyrazin-2-yl)-1,2,4]triazol-4-yl]-benzamide (6p): FTIR (KBr, cm$^{-1}$): 3024 (Ar-H, str.), 2935 (C-H, str.), 2362 (S-H, str.), 1691 (C=O, str.); $^1$H NMR (400 MHz, DMSO-$d_6$): δ 1.22 (t, J = 7.6 Hz, 3H), 2.52 (s, 3H), 2.65- 2.71 (dd, J = 15.2 Hz and 7.6 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H), 7.84 (d, J = 8.4 Hz, 2H), 8.55 (d, J = 1.2 Hz, 1H), 9.00 (d, J = 1.6 Hz, 1H), 11.93 (s, 1H), 14.40 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-$d_6$): δ 15.76, 21.72, 28.62, 127.58, 128.01, 128.40, 128.56, 129.16, 130.09, 142.74, 144.50, 147.63, 149.48, 156.23, 165.58, 169.54. LCMS (+ESI, m/z) 341.11 (M+H)$^+$.  

4-Ethoxy-N-[3-mercaptopo-5-(5-methyl-pyrazin-2-yl)-1,2,4]triazol-4-yl]-benzamide (6q): FTIR (KBr, cm$^{-1}$): 3305 (N-H, str.), 2989 (Ar-H, str.), 2937 (C-H, str.), 2366 (S-H, str.), 1683 (C=O, str.), 1500 (C-C, str.), 1261 (Assym. C-O-C, str.); $^1$H NMR (400 MHz, DMSO-$d_6$): δ 1.36 (t, J = 6.8 Hz, 3H), 2.51 (s, 3H), 4.07- 4.14 (m, 2H), 7.06 (d, J = 8.8 Hz, 2H), 7.85- 7.88 (m, 2H), 2H), 8.54 (d, J = 1.2 Hz, 1H), 8.99 (d, J = 1.6 Hz, 1H), 11.84 (s, 1H), 14.38 (s, 1H); LCMS (+ESI, m/z) 357.10 (M+H)$^+$.  

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N-[3-Mercapto-5-(5-methyl-pyrazin-2-yl)-1,2,4]triazol-4-yl]-3,4-dimethoxy-benzamide (6r): FTIR (KBr, cm⁻¹): 3419 (N-H, str.), 3022 (Ar-H, str.), 2887 (C-H, str.), 2353 (S-H, str.), 1695 (C=O, str.), 1469 (C-C, str.), 1192 (Sym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.52 (s, 3H), 3.82 (s, 3H), 3.83 (s, 3H), 7.46-7.05 (m, 2H), 7.50-7.59 (m, 2H), 8.55 (d, J = 1.2 Hz, 1H), 9.00 (d, J = 1.6 Hz, 1H), 11.86 (s, 1H), 14.39 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 21.72, 56.10, 56.21, 121.36, 121.95, 123.66, 124.24, 142.75, 144.54, 147.75, 148.94, 152.15, 152.89, 156.22, 165.90, 169.57. LCMS (+ESI, m/z) 373.10 (M+H)⁺.

Pyrazine-2-carboxylic acid (3-mercapto-5-methyl-[1,2,4]triazol-4-yl)-amide (8a): FTIR (KBr, cm⁻¹): 3010 (Ar-H, str.), 2360 (S-H, str.), 1710 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.18 (s, 3H), 8.86 (d, J = 2.4 Hz and 1.6 Hz, 1H), 8.99 (d, J = 2.4 Hz, 1H), 9.25 (d, J = 1.6Hz, 1H), 12.14 (s, 1H), 13.64 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 10.49, 143.39, 144.35, 144.60, 149.28, 150.25, 162.57, 167.38. GCMS (EI, m/z) 236 (M)⁺.

Pyrazine-2-carboxylic acid (3-ethyl-5-mercapto-[1,2,4]triazol-4-yl)-amide (8b): FTIR (KBr, cm⁻¹): 3082 (Ar-H, str.), 2904 (C-H, str.), 2360 (S-H, str.), 1681 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 1.16 (t, J = 7.6 Hz, 3H), 2.54 (dd, J = 15.2 Hz and 7.6 Hz, 2H), 8.85-8.86 (dd, J = 2.4 Hz and 1.6 Hz, 1H), 9.00 (d, J = 2.4 Hz, 1H), 9.251 (d, J = 1.6 Hz, 1H), 12.04 (s, 1H), 13.71 (s, 1H); GCMS (EI, m/z) 250 (M)⁺.

Pyrazine-2-carboxylic acid (3-mercaptopropl-[1,2,4]triazol-4-yl)-amide (8c): FTIR (KBr, cm⁻¹): 3082 (Ar-H, str.), 2956 (C-H, str.), 2360 (S-H, str.), 1707 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 0.90 (t, J = 7.2 Hz, 3H), 1.58-1.64 (dd, J = 14.8 Hz and 7.6 Hz, 2H), 2.46 (m, 2H), 8.85-8.86 (dd, J = 2.4 Hz and 1.6 Hz, 1H), 9.00 (d, J = 2.4 Hz, 1H), 9.25 (d, J = 1.6 Hz, 1H), 12.04 (s, 1H), 13.71 (s, 1H); GCMS (EI, m/z) 264 (M)⁺.

Pyrazine-2-carboxylic acid (3-mercapto-5-o-tolyl-[1,2,4]triazol-4-yl)-amide (8d): FTIR (KBr, cm⁻¹): 3340 (N-H, str.), 3145 (Ar-H, str.), 2895 (C-H, str.), 2360 (S-H, str.), 1741 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.30 (s, 3H), 3.79-7.2 (m, 1H), 7.43-7.46 (m, 1H), 7.66 (d, J = 8 Hz, 2H), 8.86 (dd, J = 2.4 Hz and 1.6 Hz, 1H), 8.99 (d, J = 2.4 Hz, 1H), 9.183 (d, J = 1.2Hz, 1H), 12.36 (s, 1H), 14.14 (s, 1H); GCMS (EI, m/z) 312 (M)⁺.

Pyrazine-2-carboxylic acid (3-mercapto-5-p-tolyl-[1,2,4]triazol-4-yl)-amide (8e): FTIR (KBr, cm⁻¹): 2995 (C-H, str.), 2360 (S-H, str.), 1716 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.30 (s, 3H), 7.29 (d, J = 8 Hz, 2H), 7.66 (d, J = 8 Hz, 2H), 8.86 (dd, J = 2.4 Hz and 1.6 Hz, 1H), 8.99 (d, J = 2.4 Hz, 1H), 9.183 (d, J = 1.2Hz, 1H), 12.30 (s, 1H), 14.14 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 21.41, 122.25, 127.72, 130.04, 141.53, 143.07, 144.47, 144.53, 149.51, 151.10, 162.54, 168.48. LCMS (+ESI, m/z) 313.08 (M+H)⁺.

Pyrazine-2-carboxylic acid [3-mercaptopropl-(3-methoxy-phenyl)-[1,2,4]triazol-4-yl]-amide (8f): FTIR (KBr, cm⁻¹): 3340 (N-H, str.), 3116, 3066 (Ar-H, str.), 2374 (S-H, str.), 1710 (C=O, str.), 1220 (Assym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 3.81 (s, 3H), 7.19-7.22 (m, 1H), 7.42-7.50 (m, 3H), 8.66-8.67 (dd, J = 2.4 Hz and 1.6 Hz, 1H), 8.76 (d, J = 2.4 Hz, 1H), 9.17 (d, J = 1.6 Hz, 1H), 12.03 (s, 1H), 14.49 (s, 1H); GCMS (EI, m/z) 328 (M)⁺.

Pyrazine-2-carboxylic acid [3-mercaptopropl-(4-methoxy-phenyl)-[1,2,4]triazol-4-yl]-amide (8g): FTIR (KBr, cm⁻¹): 3240 (N-H, str.), 3066 (Ar-H, str.), 2841 (C-H, str.), 2374 (S-H, str.), 1710 (C=O, str.), 1220 (Assym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 3.17 (s, 3H), 7.04 (d, J = 8.8 Hz, 2H), 7.29 (d, J = 8.8 Hz, 2H), 8.87 (s, 1H), 9.00 (d, J = 2.4 Hz, 1H), 9.20 (s, 1H), 12.29 (s, 1H), 14.09 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 55.83, 114.97,
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117.24, 129.43, 143.08, 144.47, 144.54, 149.51, 150.91, 161.72, 162.55, 168.33. GCMS (EI, m/z) 328 (M+) 

Pyrazine-2-carboxylic acid [3-(4-chloro-phenyl)-5-mercapto-[1,2,4]triazol-4-yl]-amide (8h): FTIR (KBr, cm⁻¹): 3068 (Ar-H, str.), 2374 (S-H, str.), 1714 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 7.56-7.59 (dd, J = 6.8 Hz and 2 Hz, 2H), 7.77-7.79 (dd, J = 6.8 Hz and 2 Hz, 2H), 8.85-8.86 (dd, J = 2.4 Hz and 1.6 Hz, 1H), 9.00 (d, J = 2.4 Hz, 1H), 9.19 (d, J = 1.6 Hz, 1H), 12.31 (s, 1H), 14.27 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 129.43, 130.18, 130.46, 138.07, 140.89, 143.88, 144.86, 146.76, 147.09, 164.90, 169.61. GCMS (EI, m/z) 332 (M+) 

Pyrazine-2-carboxylic acid [3-(4-fluoro-phenyl)-5-mercapto-[1,2,4]triazol-4-yl]-amide (8i): FTIR (KBr, cm⁻¹): 3068 (Ar-H, str.), 2370 (S-H, str.), 1749 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 7.31-7.37 (m, 2H), 7.79-7.84 (m, 2H), 8.40-8.44 (dd, J = 2.4 Hz and 1.6 Hz, 2H), 8.99 (d, J = 2.4 Hz, 1H), 9.19 (d, J = 1.6 Hz, 1H), 12.30 (s, 1H), 14.30 (s, 1H); GCMS (EI, m/z) 316 (M+) 

Pyrazine-2-carboxylic acid [3-(4-ethyl-phenyl)-5-mercapto-[1,2,4]triazol-4-yl]-amide (8j): FTIR (KBr, cm⁻¹): 3398 (N-H, str.), 3174 (Ar-H, str.), 2370 (S-H, str.), 1737 (C=O, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 1.16 (t, J = 7.6 Hz, 3H), 2.57-2.63 (dd, J = 7.6 Hz, 2H), 7.33 (d, J = 8 Hz, 2H), 7.68 (d, J = 8 Hz, 2H), 8.86 (t, J = 1.6 Hz, 1H), 8.99 (d, J = 2.4 Hz, 1H), 9.19 (d, J = 1.6 Hz, 1H), 12.30 (s, 1H), 14.14 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 15.58, 28.45, 122.49, 127.80, 128.89, 143.07, 144.47, 144.54, 147.61, 149.52, 151.07, 162.59, 168.48. GCMS (EI, m/z) 326 (M+) 

Pyrazine-2-carboxylic acid [3-(4-ethoxy-phenyl)-5-mercapto-[1,2,4]triazol-4-yl]-amide (8k): FTIR (KBr, cm⁻¹): 3174 (C-C, str.), 3109, 2956 (Ar-H, str.), 2370 (S-H, str.), 1672 (C=O, str.), 1201 (Assym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 1.30 (t, J = 7.2Hz, 3H), 4.00-4.05 (dd, J = 6.8 Hz, 2H), 7.01 (d, J = 8.8 Hz, 2H), 7.67-7.70 (dd, J = 2 Hz, 2H), 8.87 (t, J = 1.6 Hz, 1H), 8.99 (d, J = 2.4 Hz, 1H), 9.19 (d, J = 1.6 Hz, 1H), 12.28 (s, 1H), 14.07 (s, 1H); GCMS (EI, m/z) 342 (M+) 

Pyrazine-2-carboxylic acid [3-(3,4-dimethoxy-phenyl)-5-mercapto-[1,2,4]triazol-4-yl]-amide (8l): FTIR (KBr, cm⁻¹): 3487 (N-H, str.), 2895 (C-H, str.), 2368 (S-H, str.), 1635 (C=O, str.), 1195 (Sym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 3.83 (s, 3H), 3.80 (s, 3H), 7.11 (d, J = 8.4 Hz, 1H), 7.46 (d, J = 2 Hz, 1H), 7.59 (dd, J = 8.4 Hz and 2 Hz, 1H), 8.66 (t, J = 1.6 Hz, 1H), 8.75 (d, J = 2.4 Hz, 1H), 9.15 (d, J = 1.6 Hz, 1H), 12.28 (s, 1H), 14.07 (s, 1H); LCMS (ESI, m/z) 359.07 (M+H)⁺ 

5-Methyl-pyrazine-2-carboxylic acid (3-mercapto-5-methyl-[1,2,4]triazol-4-yl)-amide (9a): FTIR (KBr, cm⁻¹): 3332 (N-H, str.), 2916 (Ar-H, str.), 2378 (S-H, str.), 1692 (C=O, str.), 1458 (Ar C-C, str.); 

5-Methyl-pyrazine-2-carboxylic acid (3-ethyl-5-mercapto-[1,2,4]triazol-4-yl)-amide (9b): FTIR (KBr, cm⁻¹): 3034 (Ar-H, str.), 2898 (C-H, str.), 2362 (S-H, str.), 1700 (C=O, str.), 1400 (Ar C-C, str.); ¹³C NMR (100 MHz, DMSO-d₆): δ 9.70, 21.77, 26.95, 138.12, 142.74, 144.38, 147.40, 156.13, 169.21, 172.45.
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5-Methyl-pyrazine-2-carboxylic acid (3-mercapto-5-propyl-[1,2,4]triazol-4-yl)-amide (9c): FTIR (KBr, cm\(^{-1}\)): 3415 (N-H, str.), 2967 (Ar-H, str.), 2372 (S-H, str.), 1712 (C=O, str.); LCMS (+ESI, m/z) 279.09 (M+H\(^+\)).

5-Methyl-pyrazine-2-carboxylic acid (3-mercapto-5-phenyl-[1,2,4]triazol-4-yl)-amide (9d): FTIR (KBr, cm\(^{-1}\)): 3024 (Ar-H, str.), 2887 (C-H, str.), 2362 (S-H, str.), 1714 (C=O, str.); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 2.62 (s, 3H), 7.47-7.51 (m, 3H), 7.74-7.77 (m, 2H), 8.74 (s, 1H), 9.03 (s, 1H), 12.23 (s, 1H), 14.19 (s, 1H); LCMS (+ESI, m/z) 313.08 (M+H\(^+\)).

5-Methyl-pyrazine-2-carboxylic acid (3-mercapto-5-o-tolyl-[1,2,4]triazol-4-yl)-amide (9e): FTIR (KBr, cm\(^{-1}\)): 3462 (N-H, str.), 3136 (Ar-H, str.), 2821 (C-H, str.), 2370 (S-H, str.), 1710 (C=O, str.); LCMS (+ESI, m/z) 327.09 (M+H\(^+\)).

5-Methyl-pyrazine-2-carboxylic acid (3-mercapto-5-p-tolyl-[1,2,4]triazol-4-yl)-amide (9f): FTIR (KBr, cm\(^{-1}\)): 3462 (N-H, str.), 3136 (Ar-H, str.), 2821 (C-H, str.), 2370 (S-H, str.), 1714 (C=O, str.), 1400 (Ar-C-C, str.); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 2.38 (s, 3H), 2.51 (s, 3H), 7.36 (d, \(J=8\) Hz, 2H), 7.82 (d, \(J=8\) Hz, 2H), 8.54 (d, \(J=1.2\) Hz, 1H), 9.00 (d, \(J=1.6\) Hz, 1H), 11.92 (s, 1H), 14.39 (s, 1H); LCMS (+ESI, m/z) 327.09 (M+H\(^+\)).

5-Methyl-pyrazine-2-carboxylic acid [3-mercapto-5-(3-methoxy-phenyl)-[1,2,4]triazol-4-yl]-amide (9g): FTIR (KBr, cm\(^{-1}\)): 3473 (N-H, str.), 3136 (Ar-H, str.), 2823 (C-H, str.), 2370 (S-H, str.), 1714 (C=O, str.), 1494 (Ar-C-C, str.), 1147 (Sym. C-O-C, str.); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 2.52 (s, 3H), 3.82 (s, 3H), 7.19-7.22 (m, 1H), 7.43-7.50 (m, 2H), 8.56 (d, \(J=1.2\) Hz, 1H), 9.01 (d, \(J=1.2\) Hz, 1H), 12.01 (s, 1H), 14.42 (s, 1H); LCMS (+ESI, m/z) 343.21 (M+H\(^+\)).

5-Methyl-pyrazine-2-carboxylic acid [3-mercapto-5-(4-methoxy-phenyl)-[1,2,4]triazol-4-yl]-amide (9h): FTIR (KBr, cm\(^{-1}\)): 3473 (N-H, str.), 2821 (C-H, str.), 2370 (S-H, str.), 1698 (C=O, str.), 1456 (Ar-C-C, str.); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 2.51 (s, 3H), 3.83 (s, 3H), 7.06-7.08 (dd, \(J=6.8\) Hz and 2Hz, 2H), 7.87-7.90 (dd, \(J=6.8\) Hz and 2Hz, 2H), 8.54 (d, \(J=1.2\) Hz, 1H), 8.99 (d, \(J=1.2\) Hz, 1H), 11.85 (s, 1H), 14.38 (s, 1H); LCMS (+ESI, m/z) 343.09 (M+H\(^+\)).

5-Methyl-pyrazine-2-carboxylic acid [3-(2-chloro-phenyl)-5-mercapto-[1,2,4]triazol-4-yl]-amide (9i): FTIR (KBr, cm\(^{-1}\)): 3091 (Ar-H, str.), 2939 (C-H, str.), 2370 (S-H, str.), 1712 (C=O, str.), 1541 (Ar-C-C, str.); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 2.52 (s, 3H), 7.54-7.56 (dd, \(J=6.8\) Hz and 2Hz, 1H), 7.63-7.66 (m, 1H), 7.90-7.94 (m, 2H), 8.54 (d, \(J=1.2\) Hz, 1H), 9.02 (d, \(J=1.2\) Hz, 1H), 12.14 (s, 1H), 14.44 (s, 1H); \(^1\)C NMR (100 MHz, DMSO-\(d_6\)): \(\delta\) 22.07, 124.02, 127.78, 130.70, 132.17, 133.25, 133.61, 140.22, 143.46, 144.03, 149.25, 159.19, 162.77, 167.97. LCMS (+ESI, m/z) 347.04 (M+H\(^+\)).

5-Methyl-pyrazine-2-carboxylic acid [3-(4-chloro-phenyl)-5-mercapto-[1,2,4]triazol-4-yl]-amide (9j): FTIR (KBr, cm\(^{-1}\)): 3178, 2945 (Ar-H, str.), 2821 (C-H, str.), 2368 (S-H, str.), 1722 (C=O, str.); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 2.63 (s, 3H), 7.36-7.32 (m, 2H), 7.83-7.79 (m, 2H), 8.74 (d, \(J=1.2\) Hz, 1H), 9.03 (d, \(J=1.2\) Hz, 1H), 12.20 (s, 1H), 14.20 (s, 1H); LCMS (+ESI, m/z) 347.04 (M+H\(^+\)).

5-Methyl-pyrazine-2-carboxylic acid [3-(4-fluoro-phenyl)-5-mercapto-[1,2,4]triazol-4-yl]-amide (9k): FTIR (KBr, cm\(^{-1}\)): 3124 (Ar-H, str.), 2821 (C-H, str.), 2368 (S-H, str.), 1714 (C=O, str.); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 2.62 (s, 3H), 7.32-7.36 (m, 2H), 7.79-7.83
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(m, 2H), 8.74 (d, J = 1.2 Hz, 1H), 9.03 (d, J = 1.6 Hz, 1H), 12.21 (s, 1H), 14.21 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-d$_6$): δ 22.11, 116.67, 116.89, 130.37, 130.46, 140.29, 143.53, 144.10, 150.30, 159.31, 162.78, 168.60. LCMS (+ESI, m/z) 331.07 (M+H)$^+$.  

5-Methyl-pyrazine-2-carboxylic acid [3-(4-ethyl-phenyl)-5-mercapto-[1,2,4]triazol-4-yl]-amide (9I): FTIR (KBr, cm$^{-1}$): 3276 (N-H, str.), 2948 (Ar-H, str.), 2387 (S-H, str.), 1692 (C=O, str.); $^{1}$H NMR (400 MHz, DMSO-d$_6$): δ 1.22 (t, J = 7.6 Hz, 3H), 2.52 (s, 3H), 2.71-2.65 (dd, J = 7.6 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H), 7.84 (d, J = 8.4 Hz, 2H), 8.55 (d, J = 0.8 Hz, 1H), 9.00 (d, J = 1.2 Hz, 1H), 11.93 (s, 1H), 14.40 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-d$_6$): δ 15.00, 22.10, 63.81, 115.30, 117.14, 129.42, 140.42, 143.51, 144.08, 150.97, 159.21, 160.99, 162.71, 168.36. LCMS (+ESI, m/z) 357.09 (M+H)$^+$.  

5-Methyl-pyrazine-2-carboxylic acid [3-(4-ethoxy-phenyl)-5-mercapto-[1,2,4]triazol-4-yl]-amide (9m): FTIR (KBr, cm$^{-1}$): 3334 (N-H, str.), 3001 (Ar-H, str.), 2842 (C-H, str.), 2360 (S-H, str.), 1706 (C=O, str.), 1277 (Assym. C-O-C, str.); $^{1}$H NMR (400 MHz, DMSO-d$_6$): δ 1.30 (t, J = 7 Hz, 3H), 2.63 (s, 3H), 4.00-4.05 (dd, J = 14 Hz and 7.2 Hz, 2H), 6.99-7.01 (m, 2H), 7.66-7.69 (m, 2H), 8.74 (d, J = 1.2 Hz, 1H), 9.04 (d, J = 1.6 Hz, 1H), 12.19 (s, 1H), 14.06 (s, 1H); LCMS (+ESI, m/z) 337.09 (M+H)$^+$.  

5-Methyl-pyrazine-2-carboxylic acid [3-(3,4-dimethoxy-phenyl) -5-mercapto-[1,2,4]triazol-4-yl] -amide (9n): FTIR (KBr, cm$^{-1}$): 3300 (N-H, str.), 2887 (C-H, str.), 2866 (C-H, str.), 2378 (S-H, str.), 1709 (C=O, str.), 1256 (Assym. C-O-C, str.); $^{1}$H NMR (400 MHz, DMSO-d$_6$): δ 2.51 (s, 3H), 3.85 (s, 3H), 3.88 (s, 3H), 7.05-7.11 (dd, J = 8.4 Hz, 1H), 7.46-7.59 (m, 2H), 8.55 (s, 1H), 9.00 (d, J = 1.2 Hz, 1H), 11.86 (s, 1H), 14.39 (s, 1H); LCMS (+ESI, m/z) 343.09 (M+H)$^+$.  

5-Methyl-pyrazine-2-carboxylic acid (3-mercapto-5-phenoxymethyl-[1,2,4]triazol-4-yl)-amide (9o): FTIR (KBr, cm$^{-1}$): 3321 (N-H, str.), 2956 (Ar-H, str.), 2830 (C-H, str.), 2372 (S-H, str.), 1712 (C=O, str.), 1250 (Assym. C-O-C, str.); $^{1}$H NMR (400 MHz, DMSO-d$_6$): δ 2.62 (s, 3H), 5.05 (s, 2H), 6.89-6.94 (m, 3H), 7.20-7.24 (m, 2H), 8.70 (d, J = 1.6 Hz, 1H), 9.08 (d, J = 1.6 Hz, 1H), 12.08 (s, 1H), 14.06 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-d$_6$): δ 22.08, 59.70, 115.45, 122.02, 129.90, 140.59, 143.54, 143.90, 148.98, 157.85, 158.97, 162.56, 168.51. LCMS (+ESI, m/z) 343.09 (M+H)$^+$.  

5-Pyrizin-2-yl-4H-[1,2,4]triazole-3-thiol (15a): FTIR (KBr, cm$^{-1}$): 3286, 3080 (Ar-H, str.), 2380 (S-H, str.); $^{1}$H NMR (400 MHz, DMSO-d$_6$): δ 8.76 (d, J = 2.4 Hz, 1H), 8.75 (d, J = 1.2 Hz, 1H), 9.18 (d, J = 1.2 Hz, 1H), 13.91 (s, 1H), 14.13 (s, 1H); LCMS (+ESI, m/z) 180.14(M+H)$^+$.  

2-(5-Methylsulfanyl-4H-[1,2,4]triazol-3-yl)-pyrazine (15b): FTIR (KBr, cm$^{-1}$): 3479 (N-H, str.), 3026 (Ar-H, str.), 2343 (S-H, str.); LCMS (+ESI, m/z) 194.04 (M+H)$^+$.  

2-(5-Sec-Butylsulfanyl-4H-[1,2,4]triazol-3-yl)-pyrazine (15c): FTIR (KBr, cm$^{-1}$): 3479 (N-H, str.), 3086 (Ar-H, str.); $^{1}$H NMR (400 MHz, DMSO-d$_6$): δ 0.99 (t, J = 7.4Hz, 3H), 1.36 (d, J = 6.8 Hz, 3H), 1.64-1.74 (m, 3H), 8.75 (s, 2H), 9.21 (s, 1H), 15.01 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-d$_6$): δ 11.63, 21.33, 29.66, 44.22, 142.98, 144.93, 146.04. LCMS (+ESI, m/z) 236.20 (M+H)$^+$.  

2-(5-Benzylsulfanyl-4H-[1,2,4]triazol-3-yl)-pyrazine (15d): FTIR (KBr, cm$^{-1}$): 3479 (N-H, str.), 3032 (Ar-H, str.); $^{1}$H NMR (400 MHz, DMSO-d$_6$): δ 4.43 (s, 2H), 7.43-7.21 (m, 5H).
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8.75 (s, 2H), 9.24 (d, \(J = 0.8\) Hz, 1H), 15.02 (s, 1H); \(^{13}\)C NMR (100 MHz, DMSO-\(d_6\)): \(\delta\) 36.00, 127.75, 128.91, 129.36, 138.13, 142.99, 144.96, 146.12. LCMS (+ESI, \(m/z\)) 270.08 (M+H)+.

5-(3-Phenoxy-phenyl)-4H-[1,2,4]triazole-3-thiol (19a): FTIR (KBr, \(cm^{-1}\)) 3593 (N-H, str.), 3093 (Ar-H, str.), 2989 (C-H, str.), 2368 (S-H, str.), 1485 (Ar C-C, str.);

3-Methylsulfanyl-5-(3-phenoxy-phenyl)-4H-[1,2,4]triazole (19b): FTIR (KBr, \(cm^{-1}\)) 3593 (N-H, str.), 3093 (Ar-H, str.), 2895 (C-H, str.), 1485 (Ar C-C, str.), 1230 (Assym. C-O-C, str.); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 2.64 (s, 3H), 7.09 (m, 3H), 7.19 (s, 1H), 7.43- 7.54 (m, 4H), 7.73 (s, 1H), 14.06 (s, 1H); LCMS (+ESI, \(m/z\)) 284.09 (M+H)+.

3-sec-Butylsulfanyl-5-(3-phenoxy-phenyl)-4H-[1,2,4]triazole (19c): FTIR (KBr, \(cm^{-1}\)) 3593 (N-H, str.), 3043 (Ar-H, str.), 2823 (C-H, str.), 1467 (Ar C-C, str.), 1230 (Assym. C-O-C, str.); \(^{13}\)C NMR (100 MHz, DMSO-\(d_6\)): \(\delta\) 11.62, 21.28, 29.70, 115.89, 119.46, 121.29, 124.33, 130.65, 131.22, 156.73, 157.72. LCMS (+ESI, \(m/z\)) 326.34 (M+H)+.

3-Benzylsulfanyl-5-(3-phenoxy-phenyl)-4H-[1,2,4]triazole (19d): FTIR (KBr, \(cm^{-1}\)) 3593 (N-H str.), 3128 (Ar-H, str.), 2927 (Ar-H, str.), 1494 (Ar C-C, str.), 1246 (Assym. C-O-C, str.); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 4.44 (s, 2H), 7.10- 7.29 (m, 8H), 7.29- 7.44 (m, 4H), 7.58- 7.77 (m, 3H), 14.52 (s, 1H); \(^{13}\)C NMR (100 MHz, DMSO-\(d_6\)): \(\delta\) 35.63, 115.51, 116.12, 119.54, 121.39, 124.33, 127.59, 128.81, 129.36, 130.69, 131.48, 133.22, 137.76, 152.09, 154.98, 156.57, 156.76, 157.75, 157.86, 159.98. LCMS (+ESI, \(m/z\)) 360.34 (M+H)+.

5-(4-Phenoxy-phenyl)-4H-[1,2,4]triazole-3-thiol (20a): FTIR (KBr, \(cm^{-1}\)) 3477 (S-H, str.), 3161 (Ar-H, str.), 2366 (S-H, str.), 1485 (Ar C-C, str.), 1213 (Assym. C-O-C, str.); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 2.51 (s, 3H), 7.21 (m, 5H), 7.44 (s, 2H), 7.96 (s, 1H); LCMS (+ESI, \(m/z\)) 270.06 (M+H)+.

3-Methylsulfanyl-5-(4-phenoxy-phenyl)-4H-[1,2,4]triazole (20b): FTIR (KBr, \(cm^{-1}\)) 3479 (N-H, str.), 2997 (Ar-H, str.), 1494 (Ar C-C, str.), 1182 (Sym. C-O-C, str.); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 2.51 (s, 3H), 7.21 (m, 5H), 7.44 (s, 2H), 7.96 (s, 1H); LCMS (+ESI, \(m/z\)) 284.08(M+H)+.

3-sec-Butylsulfanyl-5-(4-phenoxy-phenyl)-4H-[1,2,4]triazole (20c): FTIR (KBr, \(cm^{-1}\)) 3473 (N-H, str.), 3126 (Ar-H, str.), 2850 (C-H, str.), 1419 (Ar C-C, str.); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 0.98 (t, \(J = 7.4\) Hz, 3H), 1.34 (d, \(J = 6.8\) Hz, 3H), 1.58-1.73 (m, 3H), 7.06- 7.10 (m, 3H), 7.20 (t, \(J = 7.6\) Hz, 2H), 7.40- 7.44 (dd, \(J = 8.4\) Hz and 7.6 Hz, 2H), 7.97 (d, \(J = 8.8\) Hz, 2H); \(^{13}\)C NMR (100 MHz, DMSO-\(d_6\)): \(\delta\) 11.65, 21.35, 29.71, 118.95, 119.71, 124.53, 128.33, 130.68. LCMS (+ESI, \(m/z\)) 326.28 (M+H)+.

3-Benzylsulfanyl-5-(4-phenoxy-phenyl)-4H-[1,2,4]triazole (20d): FTIR (KBr, \(cm^{-1}\)) 3566 (N-H, str.), 3126 (Ar-H, str.), 2848 (C-H, str.), 1417 (Ar C-C, str.), 1182 (Sym. C-O-C, str.); \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 4.45 (s, 2H), 7.08- 7.10 (m, 5H), 7.20- 7.23 (m, 2H), 7.27-7.31 (m, 2H), 7.39- 7.45 (dd, \(J = 8\) Hz and 7.6 Hz, 2H), 7.96 (d, \(J = 7.2\) Hz, 3H), 14.36 (s, 1H); \(^{13}\)C NMR (100 MHz, DMSO-\(d_6\)): \(\delta\) 35.64, 118.91, 119.94, 124.76, 127.59, 128.59, 128.83, 128.98, 130.73, 138.59, 155.22, 156.11, 159.14, 159.80. LCMS (+ESI, \(m/z\)) 360.11 (M+H)+.
4-Phenyl-5-pyrazin-2-yl-4H-[1,2,4]triazole-3-thiol (23a): FTIR (KBr, cm⁻¹): 3028 (Ar-H, str.), 2368 (S-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 7.35-7.46 (m, 5H), 8.44 (s, 1H), 8.66 (s, 1H), 9.03 (s, 1H), 14.46 (s, 1H); GCMS (EI, m/z) 255 (M)⁺.

2-(5-Methylsulfanyl-4-phenyl-4H-[1,2,4]triazol-3-yl)-pyrazine (23b): FTIR (KBr, cm⁻¹): 3300 (N-H, str.), 2926 (Ar-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.5 (s, 3H), 7.41-7.52 (m, 5H), 8.41 (s, 1H), 8.63 (s, 1H), 9.20 (s, 1H); LCMS (+ESI, m/z) 271.07 (M+H)⁺.

2-(5-sec-Butylsulfanyl-4-phenyl-4H-[1,2,4]triazol-3-yl)-pyrazine (23c): FTIR (KBr, cm⁻¹): 3479 (N-H, str.), 2964 (Ar-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 0.91 (d, J = 6.4 Hz, 3H), 1.35 (s, 3H), 1.66 (d, J = 6.4 Hz, 2H), 3.66 (d, J = 5.6 Hz, 1H), 7.39 (m, 2H), 7.51 (m, 3H), 8.41 (s, 1H), 8.63 (s, 1H), 9.19 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 11.54, 21.17, 29.48, 45.35, 127.97, 129.81, 130.03, 134.75, 142.82, 144.15, 144.72, 145.43, 151.77, 153.64. LCMS (+ESI, m/z) 312.12 (M+H)⁺.

2-(5-Benzylsulfanyl-4-phenyl-4H-[1,2,4]triazol-3-yl)-pyrazine (23d): FTIR (KBr, cm⁻¹): 3034 (Ar-H, str.), 2926 (Ar-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 4.45 (s, 2H), 7.23-7.51 (m, 10H), 8.37-8.38 (dd, J = 2.4 Hz and 1.2 Hz, 1H), 8.61 (d, J = 2.4 Hz, 1H), 9.18 (d, J = 1.2 Hz, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 36.44, 127.76, 128.01, 128.96, 129.51, 129.86, 130.11, 134.52, 137.35, 142.73, 144.15, 144.67, 145.48, 151.93, 153.90. LCMS (+ESI, m/z) 346.10 (M+H)⁺.

4-(2,4-Dichloro-phenyl)-5-(5-methyl-pyrazin-2-yl)-4H-[1,2,4]triazole-3-thiol (24a): FTIR (KBr, cm⁻¹): 3390 (N-H, str.), 3037 (Ar-H, str.), 2912 (C-H, str.), 2378 (S-H, str.), 1496 (Ar-C-C, str.); ¹⁵N NMR (400 MHz, DMSO-d₆): δ 2.00 (s, 3H), 7.61 (s, 2H), 7.88 (s, 1H), 8.33 (s, 1H), 9.07 (s, 1H), 9.85 (s, 1H), 14.54 (s, 1H); LCMS (+ESI, m/z) 339.98 (M+H)⁺.

2-[4-(2,4-Dichloro-phenyl)-5-methylsulfanyl-4H-[1,2,4]triazol-3-yl]-5-methyl-pyrazine (24b): FTIR (KBr, cm⁻¹): 3510 (N-H, str.), 3037 (Ar-H, str.), 2929 (Ar-H, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.51 (s, 3H), 2.63 (s, 3H), 7.62-7.73 (m, 2H), 7.96 (d, J = 18.4 Hz, 1H), 8.31 (d, J = 19.2 Hz, 1H), 9.20 (d, J = 18.4 Hz, 1H); LCMS (+ESI, m/z) 355.99 (M+H)⁺.

2-[5-sec-Butylsulfanyl-4-(2,4-dichloro-phenyl)-4H-[1,2,4]triazol-3-yl]-5-methyl-pyrazine (24c): FTIR (KBr, cm⁻¹): 3510 (N-H, str.), 3037 (Ar-H, str.), 2966 (Ar-H, str.), 1496 (Ar-C-C, str.); ¹³C NMR (100 MHz, DMSO-d₆): δ 11.60, 21.11, 21.55, 29.52, 45.86, 129.03, 130.10, 131.79, 131.84, 132.07, 132.91, 135.81, 139.46, 142.79, 143.79, 151.52, 155.10. LCMS (+ESI, m/z) 394.06 (M+H)⁺.

2-[5-Benzylsulfanyl-4-(2,4-dichloro-phenyl)-4H-[1,2,4]triazol-3-yl]-5-methyl-pyrazine (24d): FTIR (KBr, cm⁻¹): 3510 (N-H, str.), 3024 (Ar-H, str.), 1467 (Ar-C-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.48 (s, 3H), 4.48 (s, 2H), 7.31 (d, J = 9.6 Hz, 3H), 7.37 (m, 2H), 7.58 (d, J = 7.2 Hz, 2H), 7.91 (m, 1H), 8.30 (s, 1H), 9.20 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 21.56, 36.65, 128.05, 128.96, 129.04, 130.16, 131.58, 131.76, 132.89, 135.91, 137.24, 139.37, 142.75, 143.79, 155.15. LCMS (+ESI, m/z) 429.03 (M+H)⁺.

3-Methylsulfanyl-5-(4-phenoxy-phenyl)-4H-[1,2,4]triazole (28b): FTIR (KBr, cm⁻¹): 3287 (N-H, str.), 3051 (Ar-H, str.), 1436 (Ar-C-C, str.), 1247 (Assym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.61 (s, 3H), 6.92 (d, J = 2.8 Hz, 2H), 6.93-7.05 (m, 2H),...
7.05-7.20 (m, 1H), 7.36 (d, J= 2.4 Hz, 2H), 7.36- 7.42 (m, 4H), 7.56 (m, 3H); LCMS (+ESI, m/z) 360.92 (M+H)⁺.

3-sec-Butylsulfanyl-5-(4-phenoxy-phenyl)-4-phenyl-4H-[1,2,4]triazole (28c): FTIR (KBr, cm⁻¹): 3277 (N-H, str.), 3059 (Ar-H, str.), 2968 (Ar-H, str.), 2879 (C-H, str.), 1485 (Ar C-C, str.), 1240 (Assym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 0.88 (s, 3H), 1.24 (m, 2H), 1.63 (d, J= 4.8 Hz, 1H), 1.68 (s, 3H), 6.91 (d, J= 6 Hz, 2H), 6.93 (d, J= 6 Hz, 2H), 7.05 (m, 2H), 7.41 (m, 4H), 7.55 (m, 3H); LCMS (+ESI, m/z) 402.82 (M+H)⁺.

3-Benzylsulfanyl-5-(4-phenoxy-phenyl)-4-phenyl-4H-[1,2,4]triazole (28d): FTIR (KBr, cm⁻¹): 3051 (Ar-H, str.), 1487 (Ar C-C, str.), 1246 (Assym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 4.37 (s, 2H), 6.91 (d, J= 8.8 Hz, 3H), 7.03 (d, J= 7.6 Hz, 2H), 7.19 (t, J= 7.6 Hz, 2H), 7.31- 7.34 (m, 5H), 7.41 (t, J=7.6 Hz, 2H), 7.49- 7.51 (m, 5H); ¹³C NMR (100 MHz, DMSO-d₆): δ 36.79, 118.17, 120.06, 124.82, 127.96, 128.15, 128.93, 129.47, 130.23, 120.39, 130.70, 134.49, 151.71, 154.38, 155.83, 158.71. LCMS (+ESI, m/z) 436.40 (M+H)⁺.

4-(2,4-Dichloro-phenyl)-5-(4-phenoxy-phenyl)-4H-[1,2,4]triazole-3-thiol (29a): FTIR (KBr, cm⁻¹): 3103 (Ar-H, str.), 2374 (S-H, str.), 1489 (Ar C-C, str.), 1242 (Assym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 6.97-7.07 (m, 3H), 7.21 (m, 3H), 7.23 (d, J= 5.6 Hz, 1H), 7.35- 7.43 (m, 3H), 7.68- 7.76 (m, 2H), 7.92- 7.76 (m, 1H), 14.22 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 118.19, 120.37, 125.10, 129.35, 129.96, 130.52, 130.77, 133.60, 133.65, 136.09. LCMS (+ESI, m/z) 415.00 (M+H)⁺.

4-(2,4-Dichloro-phenyl)-3-methylsulfanyl-5-(4-phenoxy-phenyl)-4H-[1,2,4]triazole (29b): FTIR (KBr, cm⁻¹): 3026 (Ar-H, str.), 1510 (Ar C-C, str.), 1215 (Assym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.62 (s, 3H), 6.98 (d, J= 6.8 Hz, 2H), 7.07 (d, J= 6 Hz, 2H), 7.21 (s, 1H), 7.42 (t, J=8.4 Hz, 4H), 7.71 (d, J= 8 Hz, 1H), 7.86 (d, J= 7.6 Hz, 1H), 7.98 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 15.17, 118.33, 120.22, 121.34, 124.93, 129.66, 129.80, 130.73, 130.93, 132.45, 133.10, 136.72, 152.99, 154.25, 155.69, 159.07. LCMS (+ESI, m/z) 430.03 (M+H)⁺.

3-Sec-Butylsulfanyl-4-(2,4-dichloro-phenyl)-5-(4-phenoxy-phenyl)-4H-[1,2,4]triazole (29c): FTIR (KBr, cm⁻¹): 2996 (Ar-H, str.), 1487 (Ar-C-C, str.), 1238 (Assym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 0.89 (s, 3H), 1.32 (s, 3H), 1.63 (m, 2H), 3.54 (s, 1H), 6.97-7.07 (m, 4H), 7.21- 7.41 (m, 5H), 7.70 (m, 1H), 7.83 (m, 1H), 7.96 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 11.46, 21.16, 29.53, 45.88, 118.29, 120.25, 124.95, 129.63, 129.73, 130.73, 136.54, 154.12, 155.67, 159.10. LCMS (+ESI, m/z) 471.34 (M+H)⁺.

3-Benzylsulfanyl-4-(2,4-dichloro-phenyl)-5-(4-phenoxy-phenyl)-4H-[1,2,4]triazole (29d): FTIR (KBr, cm⁻¹): 3032 (Ar-H, str.), 1483 (Ar C-C, str.), 1211 (Assym. C-O-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 4.47 (s, 2H), 6.97 (d, J= 6.4 Hz, 2H), 7.07 (d, J= 6 Hz, 2H), 7.22 (d, J= 5.2 Hz, 1H), 7.36- 7.42 (m, 10H), 7.64 (br, s, 2H), 7.96 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 37.01, 118.33, 120.25, 121.25, 124.95, 128.02, 128.95, 129.43, 129.68, 130.73, 130.84, 130.90, 132.30, 133.04, 136.65, 137.35, 151.64, 154.27, 155.66, 159.14. LCMS (+ESI, m/z) 505.05 (M+H)⁺.

4-(2,4-Dichloro-phenyl)-5-(3-phenoxy-phenyl)-4H-[1,2,4]triazole-3-thiol (30a): FTIR (KBr, cm⁻¹): 3084 (Ar-H, str.), 2376 (S-H, str.), 1487 (Ar C-C, str.), 1238 (Assym. C-O-C, str.); ¹³C NMR (100 MHz, DMSO-d₆): δ 116.48, 119.61, 121.24, 122.82, 124.76, 127.30,
129.34, 130.54, 130.67, 130.73, 131.42, 131.55, 133.33, 136.14, 149.90, 155.77, 157.56, 169.25.

4-(2,4-Dichloro-phenyl)-3-methylsulfanyl-5-(3-phenoxy-phenyl)-4H-[1,2,4]triazole (30b): FTIR (KBr, cm⁻¹): 3180 (Ar-H, str.), 1510 (Ar C-C, str.), 1267 (Assym. C-O-C, str.); LCMS (+ESI, m/z) 429.20 (M+H)⁺.

3-sec-Butylsulfanyl-4-(2,4-dichloro-phenyl)-5-(3-phenoxy-phenyl)-4H-[1,2,4]triazole (30c): FTIR (KBr, cm⁻¹): 3084 (Ar-H, str.), 3028 (C-H, str.), 1487 (Ar C-C, str.), 1234 (Assym. C-O-C, str.); ¹³C NMR (100 MHz, DMSO-d₆): δ 11.57, 21.33, 29.51, 45.95, 116.10, 119.68, 120.56, 122.61, 124.71, 128.28, 129.61, 130.65, 130.78, 130.98, 131.33, 132.27, 132.33, 132.75, 136.58, 153.78, 155.84, 157.63. LCMS (+ESI, m/z) 471.07 (M+H)⁺.

3-Benzylsulfanyl-4-(2,4-dichloro-phenyl)-5-(3-phenoxy-phenyl)-4H-[1,2,4]triazole (30d): FTIR (KBr, cm⁻¹): 3234, 3080 (Ar-H, str.), 3004, (C-H, str.), 1487 (Ar C-C, str.), 1242 (Assym. C-O-C, str.); LCMS (+ESI, m/z) 505.32 (M+H)⁺.

N-(5-Oxo-3-pyrazin-2-yl-1,5-dihydro-[1,2,4]triazol-4-yl)-benzamide (32a): FTIR (KBr, cm⁻¹): 3452 (N-H, str.), 3024 (Ar-H, str.), 1676 (C=O, str.), 1521 (Ar C-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 7.49- 7.56 (m, 3H), 7.91 (m, 2H), 8.76 (s, 1H), 8.89 (s, 1H), 9.17 (s, 1H), 10.24 (s, 1H), 10.52 (s, 1H); LCMS (+ESI, m/z) 283.09 (M+H)⁺.

2-Methyl-N-(5-oxo-3-pyrazin-2-yl-1,5-dihydro-[1,2,4]triazol-4-yl)-benzamide (32b): FTIR (KBr, cm⁻¹): 3313 (N-H, str.), 3066 (Ar-H, str.), 1678 (C=O, str.), 1577 (Ar C-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.37 (s, 3H), 7.26- 7.42 (m, 4H), 8.59 (s, 1H), 8.90 (s, 1H), 9.18 (s, 1H), 9.88 (s, 1H), 10.56 (s, 1H); LCMS (+ESI, m/z) 297.11 (M+H)⁺.

4-Methyl-N-(5-oxo-3-pyrazin-2-yl-1,5-dihydro-[1,2,4]triazol-4-yl)-benzamide (32c): FTIR (KBr, cm⁻¹): 3452 (N-H, str.), 3201 (Ar-H, str.), 1676 (C=O, str.), 1521 (Ar C-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 2.34 (s, 3H), 7.28 (d, J= 8 Hz, 2H), 7.80 (d, J= 8 Hz, 2H), 8.75 (dd, J= 2.4 Hz and 1.6 Hz, 1H), 8.87 (d, J= 2.4 Hz, 1H), 9.16 (d, J= 1.2 Hz, 1H), 10.24 (s, 1H), 10.40 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 21.47, 128.05, 129.30, 130.41, 142.05, 144.00, 144.14, 145.16, 148.16, 158.00, 163.24, 166.57. LCMS (+ESI, m/z) 297.11 (M+H)⁺.

4-Chloro-N-(5-oxo-3-pyrazin-2-yl-1,5-dihydro-[1,2,4]triazol-4-yl)-benzamide (32d): FTIR (KBr, cm⁻¹): 3452 (N-H, str.), 3018 (Ar-H, str.), 1676 (C=O, str.), 1519 (Ar C-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 7.57 (m, 2H), 7.92 (m, 2H), 8.77 (d, J= 8 Hz, 1H), 8.90 (d, J= 7.6 Hz, 1H), 9.18 (d, J= 8 Hz, 1H), 10.34 (s, 1H), 10.55 (s, 1H); ¹³C NMR (100 MHz, DMSO-d₆): δ 128.91, 129.98, 131.98, 136.96, 144.00, 144.14, 145.10, 148.20, 157.90, 163.31, 165.71. LCMS (+ESI, m/z) 326.13 (M+H)⁺.

4-Fluoro-N-(5-oxo-3-pyrazin-2-yl-1,5-dihydro-[1,2,4]triazol-4-yl)-benzamide (32e): FTIR (KBr, cm⁻¹): 3330 (N-H, str.), 3026 (Ar-H, str.), 1676 (C=O, str.), 1519 (Ar C-C, str.); ¹H NMR (400 MHz, DMSO-d₆): δ 7.28- 7.52 (dd, J= 8.8 Hz and 6.8 Hz, 2H), 7.94- 7.98 (dd, J= 8.8 Hz and 5.6 Hz, 2H), 8.74- 8.75 (dd, J= 2.4 Hz and 1.6 Hz, 1H), 8.88 (d, J= 2.4 Hz, 1H), 9.16 (d, J= 1.2 Hz, 1H), 10.24 (s, 1H), 10.48 (s, 1H); LCMS (+ESI, m/z) 301.19 (M+H)⁺.

3-Methoxy-N-(5-oxo-3-pyrazin-2-yl-1,5-dihydro-[1,2,4]triazol-4-yl)-benzamide (32f): FTIR (KBr, cm⁻¹): 3353 (N-H, str.), 3035 (Ar-H, str.), 1678 (C=O, str.), 1519 (Ar C-C, str.).
1210 (Assym. C-O-C, str.): $^1$H NMR (400 MHz, DMSO-$d_6$): δ 3.79 (s, 3H), 7.12 (t, $J= 1.4$ Hz, 1H), 7.39 (t, $J= 7.6$ Hz, 1H), 7.44- 7.48 (dd, $J= 7.6$ Hz and 1.4 Hz, 2H), 8.74- 8.75 (dd, $J= 2.4$ Hz and 1.6 Hz, 1H), 8.88 (d, $J= 2.4$ Hz, 1H), 9.16 (d, $J= 1.2$ Hz, 1H), 10.19 (s, 1H), 10.48 (s, 1H); LCMS (+ESI, m/z) 313.10 (M+H)$^+$.  

4-Methoxy-N-(5-oxo-3-pyrazin-2-yl-1,5-dihydro-[1,2,4]triazol-4-yl)-benzamide (32g): FTIR (KBr, cm$^{-1}$): 3255 (N-H, str.), 3018 (Ar-H, str.), 1676 (C=O, str.), 1519 (Ar C-C, str.), 1286 (Assym. C-O-C, str.); $^1$H NMR (400 MHz, DMSO-$d_6$): δ 3.81 (s, 3H), 7.01 (br, s, 2H), 7.88 (br, s, 2H), 8.75 (s, 1H), 8.88 (s, 1H), 9.16 (s, 1H), 10.10 (s, 1H), 10.53 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-$d_6$): δ 55.83, 114.00, 125.36, 129.92, 144.00, 144.13, 145,11, 148.18, 158.08, 162.34, 163.26, 166.17. LCMS (+ESI, m/z) 313.10 (M+H)$^+$.  

N-(5-Oxo-3-pyrazin-2-yl-1,5-dihydro-[1,2,4]triazol-4-yl)-2-phenoxy-acetamide (32h): FTIR (KBr, cm$^{-1}$): 3103 (Ar-H, str.), 1712 (C=O, str.), 1267 (Assym. C-O-C, str.); $^1$H NMR (400 MHz, DMSO-$d_6$): δ 4.62 (s, 2H), 7.03 (m, 3H), 7.36 (d, $J= 6$ Hz, 2H), 8.82 (s, 1H), 8.95 (s, 1H), 9.23 (s, 1H), 10.00 (s, 1H), 10.57 (s, 1H); LCMS (+ESI, m/z) 331.10 (M+H)$^+$.  

N-[3-(5-Methyl-pyrazin-2-yl)-5-oxo-1,5-dihydro-[1,2,4]triazol-4-yl]-benzamide (33a): FTIR (KBr, cm$^{-1}$): 3244, 3024 (Ar-H, str.), 1676 (C=O, str.), 1531 (Ar C-C, str.); $^1$H NMR (400 MHz, DMSO-$d_6$): δ 2.61 (s, 3H), 7.49 (d, $J= 2$ Hz, 2H), 7.56 (m, 1H), 7.91 (m, 2H), 8.65 (s, 1H), 9.04 (s, 1H), 10.24 (s, 1H), 10.45 (s, 1H); LCMS (+ESI, m/z) 297.09 (M+H)$^+$.  

2-Methyl-N-[3-(5-Methyl-pyrazin-2-yl)-5-oxo-1,5-dihydro-[1,2,4]triazol-4-yl]-benzamide (33b): FTIR (KBr, cm$^{-1}$): 3307 (N-H, str.), 3010 (Ar-H, str.), 1689 (C=O, str.), 1570 (Ar C-C, str.); $^1$H NMR (400 MHz, DMSO-$d_6$): δ 2.37 (s, 3H), 2.61 (s, 3H), 7.26- 7.42 (m, 4H), 8.57 (d, $J= 8$ Hz, 1H), 9.04 (s, 1H), 9.88 (s, 1H), 10.47 (s, 1H); LCMS (+ESI, m/z) 311.11 (M+H)$^+$.  

3-Methoxy-N-[3-(5-Methyl-pyrazin-2-yl)-5-oxo-1,5-dihydro-[1,2,4]triazol-4-yl]-benzamide (33c): FTIR (KBr, cm$^{-1}$): 3373 (N-H, str.), 3093 (Ar-H, str.), 2999 (Ar-H, str.), 1685 (C=O, str.), 1573 (Ar C-C, str.), 1261 (Assym.C-O-C, str.), $^1$H NMR (400 MHz, DMSO-$d_6$): δ 2.60 (s, 3H), 3.81 (s, 3H), 7.12 (s, 1H), 7.40 (d, $J= 6$ Hz, 1H), 7.47 (m, 2H), 8.65 (s, 1H), 9.03 (s, 1H), 10.23 (s, 1H), 10.45 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-$d_6$): δ 21.88, 55.75, 113.05, 118.07, 120.30, 129.94, 134.57, 142.36, 143.09, 143.51, 157.63, 158.01, 159.55, 163.43, 166.40. LCMS (+ESI, m/z) 327.23 (M+H)$^+$.  

4-Fluoro-N-[3-(5-Methyl-pyrazin-2-yl)-5-oxo-1,5-dihydro-[1,2,4]triazol-4-yl]-benzamide (33d): FTIR (KBr, cm$^{-1}$): 3731 (N-H, str.), 3026 (Ar-H, str.), 1670 (C=O, str.), 1533 (Ar C-C, str.); $^1$H NMR (400 MHz, DMSO-$d_6$): δ 2.60 (s, 3H), 7.33 (m, 2H), 7.88- 7.97 (m, 2H), 8.56 (s, 1H), 9.03 (s, 1H), 10.27 (s, 1H), 10.44 (s, 1H); LCMS (+ESI, m/z) 315.09 (M+H)$^+$.  

4-Amino-5-(4-phenoxy-phenyl)-2,4-dihydro-[1,2,4]triazole-3-thione (35a): FTIR (KBr, cm$^{-1}$): 3552 (N-H, str.), 2362 (S-H, str.), 1496 (Ar C-C, str.), 1246 (Assym. C-O-C, str.); $^1$H NMR (100 MHz, DMSO-$d_6$): δ 117.83, 118.33, 119.91, 120.00, 121.05, 124.75, 129.57, 130.50, 130.73, 149.48, 156.10, 159.15, 167.27. LCMS (+ESI, m/z) 285.19 (M+H)$^+$.  

N-[3-(4-Phenoxy-phenyl)-5-thioxo-1,5-dihydro-[1,2,4]triazol-4-yl]-butyramide (36a): FTIR (KBr, cm$^{-1}$): 3277 (N-H, str.), 3126, 2958 (Ar-H, str.), 2802 (C-H, str.), 2362 (S-H, str.), 1710 (C=O, str.), 1487 (Ar C-C, str.), 1240 (Assym. C-O-C, str.); $^1$H NMR (400 MHz, DMSO-$d_6$): δ 0.85 (d, $J= 4$ Hz, 3H), 1.56 (m, 2H), 2.26 (m, 2H), 7.11- 7.24 (m, 5H), 7.46 (d,
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$J= 2 \text{ Hz, 2H}$, 7.70 (d, $J= 2 \text{ Hz, 2H}$), 11.39 (s, 1H), 14.09 (s, 1H); LCMS (+ESI, m/z) 355.11 (M+H)$^+$. 

**Pentanoic acid [3-(4-phenoxy-phenyl)-5-thioxo-1,5-dihydro-[1,2,4]triazol-4-yl]-amide (36b):** FTIR (KBr, cm$^{-1}$): 3277 (N-H, str.), 2958 (Ar-H, str.), 2362 (S-H, str.), 1708 (C=O, str.), 1487 (Ar-C-H, str.), 1240 (Assym. C-O-C, str.); $^1$H NMR (400 MHz, DMSO-d$_6$): δ 0.84 (d, $J= 4.4\text{ Hz, 3H}$), 1.23 (m, 2H), 1.52 (d, $J= 4.4 \text{ Hz, 2H}$), 2.29 (d, $J= 4 \text{ Hz, 2H}$), 7.11-7.24 (m, 5H), 7.46-7.69 (m, 4H), 11.39 (s, 1H), 14.09 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-d$_6$): δ 14.05, 21.93, 27.22, 33.30, 118.47, 119.74, 120.14, 124.99, 129.87, 150.77, 159.72, 168.41, 172.05. LCMS (+ESI, m/z) 369.13 (M+H)$^+$. 

**Hexanoic acid [3-(4-phenoxy-phenyl)-5-thioxo-1,5-dihydro-[1,2,4]triazol-4-yl]-amide (36e):** FTIR (KBr, cm$^{-1}$): 3284 (N-H, str.), 2931 (Ar-H, str.), 2362 (S-H, str.), 1707 (C=O, str.), 1487 (Ar-C, str.), 1242 (Assym. C-O-C, str.); $^1$H NMR (400 MHz, DMSO-d$_6$): δ 0.83 (m, 3H), 1.22 (m, 5H), 1.52 (m, 2H), 2.28 (m, 2H), 7.10 (m, 4H), 7.24 (m, 1H), 7.46 (m, 2H), 7.68 (m, 2H), 11.39 (s, 1H), 14.09 (s, 1H); LCMS (+ESI, m/z) 383.15 (M+H)$^+$. 

**N-[3-(4-Phenoxy-phenyl)-5-thioxo-1,5-dihydro-[1,2,4]triazol-4-yl]-benzamide (36d):** FTIR (KBr, cm$^{-1}$): 2951 (Ar-H, str.), 2808 (C-H, str.), 2362 (S-H, str.), 1695 (C=O, str.), 1487 (Ar-C, str.), 1251 (Assym. C-O-C, str.); $^1$H NMR (400 MHz, DMSO-d$_6$): δ 7.22-7.11 (m, 5H), 7.43-7.43 (m, 2H), 7.59 (d, $J= 5.6 \text{ Hz, 2H}$), 7.59-7.67 (m, 1H), 7.78 (d, $J= 5.6 \text{ Hz, 2H}$), 7.78-7.95 (m, 2H), 12.00 (s, 1H), 14.21 (s, 1H); LCMS (+ESI, m/z) 389.10 (M+H)$^+$. 

**Cyclohexane carboxylic acid [3-(4-phenoxy-phenyl)-5-thioxo-1,5-dihydro-[1,2,4]triazol-4-yl]-amide (36e):** FTIR (KBr, cm$^{-1}$): 3277 (N-H, str.), 2931 (Ar-H, str.), 2854 (C-H, str.), 2362 (S-H, str.), 1705 (C=O, str.), 1500 (Ar C-C, str.), 1246 (Assym. C-O-C, str.); $^1$H NMR (400 MHz, DMSO-d$_6$): δ 1.18-1.26 (m, 4H), 1.63-1.69 (m, 4H), 1.88-1.69 (m, 1H), 2.34 (m, 1H), 7.11-7.22 (m, 4H), 7.45 (d, $J= 4.8 \text{ Hz, 2H}$), 7.69 (d, $J= 4.8 \text{ Hz, 2H}$), 11.26 (s, 1H), 14.00 (s, 1H); $^{13}$C NMR (100 MHz, DMSO-d$_6$): δ 25.35, 25.70, 29.05, 29.19, 40.62, 42.36, 118.52, 119.79, 119.91, 120.10, 124.95, 129.82, 130.76, 150.50, 155.83, 159.67, 168.39, 174.79. LCMS (+ESI, m/z) 395.15 (M+H)$^+$. 

**Cyclobutane carboxylic acid [3-(4-phenoxy-phenyl)-5-thioxo-1,5-dihydro-[1,2,4]triazol-4-yl]-amide (36f):** FTIR (KBr, cm$^{-1}$): 3342 (N-H, str.), 2958 (Ar-H, str.), 2387 (S-H, str.), 1710 (C=O, str.), 1500 (Ar c-C, str.), 1249 (Assym. C-O-C, str.); $^1$H NMR (400 MHz, DMSO-d$_6$): δ 1.80 (m, 2H), 2.08 (m, 4H), 7.11 (m, 4H), 7.24 (d, $J= 4.4 \text{ Hz, 1H}$), 7.45-7.68 (m, 4H), 11.22 (s, 1H), 14.09 (s, 1H); LCMS (+ESI, m/z) 367.11 (M+H)$^+$. 

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### Spectral data

**Fig. 18a.** Compound 4a. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 141.48, 144.96, 145.05, 146.34, 146.91, 166.81.

**Fig. 20a.** Compound 4a. GCMS (EI, m/z) 194 (M$^+$).
Fig. 18b. Compound 4b. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 21.78, 138.56, 143.84, 144.49, 147.03, 155.68, 166.57.

Fig. 20b. Compound 4b. GCMS (EI, m/z) 208 (M$^+$).
Fig. 19a. Compound 5d. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 0.857 (t, $J$ = 7.2 Hz, 3H), 1.19-1.28 (m, 2H), 1.45-1.52 (m, 2H), 2.77 (t, $J$ = 7.2 Hz, 2H), 8.74 (dd, $J$ = 2.4 Hz and 1.6 Hz, 1H), 8.79 (d, $J$ = 2.4 Hz, 1H), 9.09 (d, $J$ = 1.6 Hz, 1H), 11.44 (s, 1H), 14.37 (s, 1H);

Fig. 20c. Compound 5d. LCMS (+ESI, $m/z$) 279.10 (M+H)$^+$ of
Fig. 19b. Compound 5e. $^1$H NMR (400 MHz, DMSO-$d_6$) δ ppm 0.84 (t, $J$=7.2Hz, 3H), 1.27 (m, 4H), 1.54 (m, 2H), 2.26 (t, $J$=7.2Hz, 2H), 8.74 (d, 1.6Hz, 1H), 8.80 (d, $J$=2.4Hz, 1H), 9.09 (s, 1H), 11.44 (s, 1H), 14.38 (s, 1H);

Fig. 18c. Compound 5e. $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ ppm 14.29, 22.23, 24.74, 31.00, 33.41, 140.97, 143.99, 144.80, 146.69, 147.69, 169.37, 171.63.
Fig. 20d. Compound 5e. LCMS (+ESI, m/z) 293.11 (M+H)^+  

Fig. 19c. Compound 5i. $^1$H NMR (400 MHz, DMSO-$d_6$): δ 3.81 (s, 3H), 7.04 (d, $J$= 8.8 Hz, 2H); 7.72 (d, $J$=8.8 Hz, 2H), 8.87- 8.88 (dd, $J$= 2.4 Hz and 1.6 Hz, 1H), 9.00 (d, $J$= 2.4 Hz, 1H), 9.20 (d, $J$= 1.6 Hz, 1H), 12.29 (s, 1H), 14.09 (s, 1H);
Fig. 18d. Compound 5i. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 55.87, 113.29, 119.05, 120.46, 130.46, 133.00, 140.92, 143.89, 144.90, 146.77, 147.25, 159.78, 165.52, 169.69.

Fig. 20e. Compound 5i. GCMS (EI, $m/z$) 328 (M)$^+$. 
Fig. 19d. Compound 5l. $^1$H NMR (400 MHz, DMSO-$d_6$): δ 1.36 (t, $J$= 7.2 Hz and 14 Hz, 3H), 4.08- 4.14 (dd, $J$= 7.2 Hz and 14 Hz, 2H), 7.06 (d, $J$= 8.8 Hz, 2H), 7.85- 7.88 (m, 2H), 8.64- 8.65 (dd, $J$= 2.4 Hz and 1.6 Hz, 1H), 8.75 (d, $J$= 2.4 Hz, 1H), 9.14 (d, $J$= 1.6 Hz, 1H), 11.86 (s, 1H), 14.45 (s, 1H);

Fig. 18d. Compound 5l. $^{13}$C NMR (100 MHz, DMSO-$d_6$): δ 14.95, 63.82, 15.33, 117.09, 129.43, 143.09, 144.46, 144.53, 149.50, 150.93, 161.01, 162.56, 168.32.
**Fig. 20f.** Compound 5l. GCMS (EI, m/z) 342 (M)+.

**Fig. 19e.** Compound 6c. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 0.87 (t, $J$ = 7.4 Hz, 3H), 1.49-1.56 (m, 2H), 2.24 (t, $J$ = 7.2 Hz, 2H), 2.56 (s, 3H), 8.63 (d, $J$ = 1.2 Hz, 1H), 8.94 (d, $J$ = 1.6 Hz, 1H), 11.40 (s, 1H), 14.30 (s, 1H);
**Fig. 18e.** Compound 6c. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 13.90, 18.59, 21.76, 35.41, 138.11, 142.82, 144.37, 147.51, 156.13, 169.23, 171.48.

**Fig. 20g.** Compound 6c. LCMS (ESI, $m/z$) 280.09 (M+H)$^+$. 
Fig. 19f. Compound 6f. $^1$H NMR (400 MHz, DMSO-$d_6$): δ 0.85 (t, $J= 6.4$ Hz, 3H), 1.20-1.23 (m, 6H), 1.50 (t, $J= 6.8$ Hz, 2H), 2.25 (t, $J= 7.4$ Hz, 2H), 2.56 (s, 3H), 8.63 (d, $J= 0.8$ Hz, 1H), 8.93 (d, $J= 1.2$ Hz, 1H), 11.41 (s, 1H), 14.29 (s, 1H);

Fig. 18f. Compound 6f. $^{13}$C NMR (100 MHz, DMSO-$d_6$): δ 14.35, 21.75, 22.44, 25.03, 28.48, 31.38, 33.47, 138.10, 142.87, 144.37, 147.61, 156.11, 169.23, 171.58.
**Fig. 20h.** Compound 6f. LCMS (m/z) 321.14 (M+H)^+.

**Fig. 19g.** Compound 6i. $^1$H NMR (400 MHz, DMSO-$d_6$) δ ppm 2.38 (s, 3H, -CH$_3$), 2.51 (s, 3H, -CH$_3$), 7.36 (d, J=8Hz, 2H), 7.82 (d, J=8.4Hz, 2H), 8.54 (d, J=0.8Hz, 1H), 9.00 (d, J=1.6Hz, 1H), 11.42 (s, 1H, -NH), 14.39 (s, 1H, -SH);
Fig. 18g. Compound 6i. $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ ppm 21.58, 21.72, 128.30, 128.90, 129.71, 138.09, 142.74, 143.38, 144.48, 147.61, 156.23, 165.58, 169.54.

Fig. 20i. Compound 6i. LCMS (+ESI, $m/z$) 327.09 (M+H)$^+$. 
Fig. 19h. Compound 6m. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 2.60 (s, 3H), 7.33-7.36 (m, 2H), 7.80-7.83 (m, 2H), 8.74 (d, $J = 1.2$ Hz, 1H), 9.03 (d, $J = 1.2$ Hz, 1H), 12.20 (s, 1H), 14.20 (s, 1H);

Fig. 18h. Compound 6m. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 21.74, 129.22, 130.18, 131.62, 138.02, 130.48, 138.27, 142.74, 144.45, 147.33, 156.28, 164.86, 166.93, 169.45.
Fig. 20j. Compound 6m. LCMS (+ESI, m/z) 347.04 (M+H)+.

Fig. 19i. Compound 8a. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 2.18 (s, 3H), 8.86 (d, $J$= 2.4 Hz and 1.6 Hz, 1H), 8.99 (d, $J$= 2.4 Hz, 1H), 9.25 (d, $J$= 1.6Hz, 1H), 12.14 (s, 1H), 13.64 (s, 1H);
Fig. 18i. Compound 8a. $^{13}$C NMR (100 MHz, DMSO-$d_6$): δ 10.49, 143.39, 144.35, 144.60, 149.28, 150.25, 162.57, 167.38.

Fig. 20k. Compound 8a. GCMS (EI, $m/z$) 236 (M)$^+$. 
**Fig. 19j.** Compound 8e. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 2.30 (s, 3H), 7.29 (d, $J$ = 8 Hz, 2H) 7.66 (d, $J$ = 8 Hz, 2H), 8.86 (dd, $J$ = 2.4 Hz and 1.6 Hz, 1H), 8.99 (d, $J$ = 2.4 Hz, 1H), 9.183 (d, $J$ = 1.2Hz, 1H), 12.30 (s, 1H), 14.14 (s, 1H);

**Fig. 18j.** Compound 8e. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 21.41, 122.25, 127.72, 130.04, 141.53, 143.07, 144.47, 144.53, 149.51, 151.10, 162.54, 168.48.
Fig. 20. Compound 8e. LCMS (+ESI, m/z) 313.08 (M+H)+.

Fig. 19k. Compound 8j. $^1$H NMR (400 MHz, DMSO-$d_6$) δ ppm 1.16 (t, $J=7.6$Hz, 3H), 2.63 (dd, $J=7.6$Hz, 2H), 7.33 (d, $J=8$Hz, 2H), 7.68 (d, $J=8$Hz), 8.86 (t, $J=2.4$Hz and $1.6$Hz, 1H), 8.99 (d, $J=2.4$Hz, 1H), 9.19 (d, $J=1.6$Hz, 1H), 12.30 (s, 1H), 14.14 (s, 1H);
**Fig. 18k.** Compound 8j. $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ ppm 15.58, 28.45, 122.49, 127.80, 128.89, 143.07, 144.47, 144.54, 147.61, 149.52, 151.07, 162.59, 168.48.

**Fig. 20m.** Compound 8j. GCMS (EI, m/z) 326 (M)$^+$. 
**Fig. 19.** Compound 9k. $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ 2.62 (s, 3H), 7.32-7.36 (m, 2H), 7.79-7.83 (m, 2H), 8.74 (d, $J$= 1.2 Hz, 1H), 9.03 (d, $J$= 1.6 Hz, 1H), 12.21 (s, 1H), 14.21 (s, 1H);

**Fig. 18.** Compound 9k. $^{13}$C NMR (100 MHz, DMSO-d$_6$): $\delta$ 22.11, 116.67, 116.89, 130.37, 130.46, 140.29, 143.53, 144.10, 150.30, 159.31, 162.78, 168.60.
Fig. 20n. Compound 9k. LCMS (+ESI, m/z) 331.07 (M+H)^+. 

Fig. 19m. Compound 9m. \(^1\)H NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 1.22 (t, \(J=7.6\) Hz, 3H), 2.52 (s, 3H), 2.71- 2.65 (dd, \(J=7.6\) Hz, 2H), 7.39 (d, \(J=8.4\) Hz, 2H), 7.84 (d, \(J=8.4\) Hz, 2H), 8.55 (d, \(J=0.8\) Hz, 1H), 9.00 (d, \(J=1.2\) Hz, 1H), 11.93 (s, 1H), 14.40 (s, 1H);
**Fig. 18m.** Compound 9m. $^{13}$C NMR (100 MHz, DMSO-$d_6$): δ 15.00, 22.10, 63.81, 115.30, 117.14, 129.42, 140.42, 143.51, 144.08, 150.97, 159.21, 160.99, 162.71, 168.36.

**Fig. 20o.** Compound 9m. LCMS (+ESI, $m/z$) 357.09 (M+H)$^+$. 
Fig. 19n. Compound 9o. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 2.62 (s, 3H), 5.05 (s, 2H), 6.89-6.94 (m, 3H), 7.20-7.24 (m, 2H), 8.70 (d, $J=1.6$ Hz, 1H), 9.08 (d, $J=1.6$ Hz, 1H), 12.08 (s, 1H), 14.06 (s, 1H);

Fig. 18n. Compound 9o. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 22.08, 59.70, 115.45, 122.02, 129.90, 140.59, 143.54, 143.90, 148.98, 157.85, 158.97, 162.56, 168.51.
Fig. 20p. Compound 9o. LCMS (+ESI, m/z) 343.09 (M+H)^+.

Fig. 18o. Compound 15c. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 11.63, 21.33, 29.66, 44.22, 142.98, 144.93, 146.04.
Fig. 20q. Compound 15c. LCMS (+ESI, m/z) 236.20 (M+H)+.

Fig. 19o. Compound 15d. $^1$H NMR (400 MHz, DMSO-d$_6$): δ 4.43 (s, 2H), 7.43-7.21 (m, 5H), 8.75 (s, 2H), 9.24 (d, $J$= 0.8 Hz, 1H), 15.02 (s, 1H);
**Fig. 18p.** Compound 15d. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 36.00, 127.75, 128.91, 129.36, 138.13, 142.99, 144.96, 146.12.

**Fig. 19p.** Compound 19d. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 4.44 (s, 2H), 7.10 - 7.29 (m, 8H), 7.29 - 7.44 (m, 4H), 7.58 - 7.77 (m, 3H), 14.52 (s, 1H);
**Fig. 18q.** Compound 19d. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 35.63, 115.51, 116.12, 119.54, 121.39, 124.33, 127.59, 128.81, 129.36, 130.69, 131.48, 133.22, 137.76, 152.09, 154.98, 156.57, 156.76, 157.75, 157.86, 159.98.

**Fig. 20r.** Compound 19d. LCMS (+ESI, $m/z$) 360 (M+H)$^+$
**Fig. 19q.** Compound **23c.** $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 0.91 (d, $J = 6.4$ Hz, 3H), 1.35 (s, 3H), 1.66 (d, $J = 6.4$ Hz, 2H), 3.66 (d, $J = 5.6$ Hz, 1H), 7.39 (m, 2H), 7.51 (m, 3H), 8.41 (s, 1H), 8.63 (s, 1H), 9.19 (s, 1H);

**Fig. 18r.** Compound **23c.** $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 11.54, 21.17, 29.48, 45.35, 127.97, 129.81, 130.03, 134.75, 142.82, 144.15, 144.72, 145.43, 151.77, 153.64.
Fig. 20s. Compound 23c. LCMS (+ESI, m/z) 312.12 (M+H)+.

Fig. 19r. Compound 24d. δ 2.48 (s, 3H), 4.48 (s, 2H), 7.31 (d, \( J = 9.6 \text{ Hz} \), 3H), 7.37 (m, 2H), 7.58 (d, \( J = 7.2 \text{ Hz} \), 2H), 7.91 (m, 1H), 8.30 (s, 1H), 9.20 (s, 1H);
Fig. 18c. Compound 24d. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 21.56, 36.65, 128.05, 128.96, 129.04, 130.16, 131.58, 131.76, 132.89, 135.91, 137.24, 139.37, 142.75, 143.79, 155.15.

Fig. 20t. Compound 24d. LCMS (+ESI, m/z) 429.03 (M+H)$^+$. 
Fig. 19s. Compound 28d. $^1$H NMR (400 MHz, DMSO-$d_6$): δ 4.37 (s, 2H), 6.91 (d, $J$ = 8.8 Hz, 3H), 7.03 (d, $J$ = 7.6 Hz, 2H), 7.19 (t, $J$ = 7.6 Hz, 2H), 7.31-7.34 (m, 5H), 7.41 (t, $J$=7.6 Hz, 2H), 7.49-7.51 (m, 5H);

Fig. 18t. Compound 28d. $^{13}$C NMR (100 MHz, DMSO-$d_6$): δ 36.79, 118.17, 120.06, 124.82, 127.96, 128.15, 128.93, 129.47, 130.23, 120.39, 130.70, 134.49, 151.71, 154.38, 155.83, 158.71.
Design, synthesis and evaluation of Antimycobacterial activity of triazoles

![Graph and Compound Images]

**Fig. 20u.** Compound 28d. LCMS (+ESI, m/z) 436.40 (M+H)⁺.

**Fig. 19t.** Compound 29b. $^1$H NMR (400 MHz, DMSO-$_d_6$): $\delta$ 2.62 (s, 3H), 6.98 (d, $J$= 6.8 Hz, 2H), 7.07 (d, $J$= 6 Hz, 2H), 7.21 (s, 1H), 7.42 (t, $J$=8.4 Hz, 4H), 7.71 (d, $J$= 8 Hz, 1H), 7.86 (d, $J$= 7.6 Hz, 1H), 7.98 (s, 1H);
Fig. 18u. Compound 29b. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 15.17, 118.33, 120.22, 121.34, 124.93, 129.66, 129.80, 130.73, 130.93, 132.45, 133.10, 136.72, 152.99, 154.25, 155.69, 159.07.

Fig. 20v. Compound 29b. LCMS (+ESI, $m/z$) 430.03 (M+H)$^+$. 
Fig. 19u. Compound 32c. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 2.34 (s, 3H), 7.28 (d, $J$ = 8 Hz, 2H), 7.80 (d, $J$ = 8 Hz, 2H), 8.75 (dd, $J$ = 2.4 Hz and 1.6 Hz, 1H), 8.87 (d, $J$ = 2.4 Hz, 1H), 9.16 (d, $J$ = 1.2 Hz, 1H), 10.24 (s, 1H), 10.40 (s, 1H);

Fig. 18v. Compound 32c. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 21.47, 128.05, 129.30, 130.41, 142.05, 144.00, 144.14, 145.16, 148.16, 158.00, 163.24, 166.57.
Fig. 19v. Compound 32d. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 7.57 (m, 2H), 7.92 (m, 2H), 8.77 (d, $J = 8$ Hz, 1H), 8.90 (d, $J = 7.6$ Hz, 1H), 9.18 (d, $J = 8$ Hz, 1H), 10.34 (s, 1H), 10.55 (s, 1H);

Fig. 18w. Compound 32d. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 128.91, 129.98, 131.98, 136.96, 144.00, 144.14, 145.10, 148.20, 157.90, 163.31, 165.71.
Fig. 20w. Compound 32d. LCMS (+ESI, m/z) 326.13 (M+H)+.

Fig. 19w. Compound 33c. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 2.60 (s, 3H), 3.81 (s, 3H), 7.12 (s, 1H), 7.40 (d, $J=6$ Hz, 1H), 7.47 (m, 2H), 8.65 (s, 1H), 9.03 (s, 1H), 10.23 (s, 1H), 10.45 (s, 1H);
Fig. 18. Compound 33c. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 21.88, 55.75, 113.05, 118.07, 120.30, 129.94, 134.57, 142.36, 143.09, 143.51, 157.63, 158.01, 159.55, 163.43, 166.40.

Fig. 19. Compound 36b. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 0.84 (d, $J= 4.4$Hz, 3H), 1.23 (m, 2H), 1.52 (d, $J= 4.4$ Hz, 2H), 2.29 (d, $J= 4$ Hz, 2H), 7.11- 7.24 (m, 5H), 7.46- 7.69 (m, 4H), 11.39 (s, 1H), 14.09 (s, 1H);
Fig. 18y. Compound 36b. $^{13}$C NMR (100 MHz, DMSO-$d_6$): $\delta$ 14.05, 21.93, 27.22, 33.30, 118.47, 119.74, 120.14, 124.99, 129.87, 130.77, 150.53, 155.77, 159.72, 168.41, 172.05.

Fig. 20x. Compound 36b. LCMS (+ESI, m/z) 369.13 (M+H)$^+$. 
4.5. Antitubercular activity screening

The Anti Tubercular activity of synthesized compounds was determined by Microplate Alamar Blue Assay (MABA).  

**Bacterial strain:** *Mycobacterium tuberculosis* (H\(_{37}\)Rv)

**Requirements**

Middlebrook 7H9 broth (Difco), Bacto casitone (pancreatic digest of casein; Becton Dickinson), BBL Middlebrook OADC enrichment [(oleic acid, albumin, dextrose, catalase] Becton Dickinson], glycerol (Difco), polysorbate 80 (Difco), Alamar blue (Invitrogen), sterile water and deionised water (MilliQ, Millipore).

**Preparation of media**

**Media (A):** The media was prepared by mixing Glycerol (0.2 %), Casitone (0.1 %), Tween 80 (0.05 %) and 7H9 broth (0.47g/100 mL) in MilliQ water and made up to the desired volume and sterilized. To this media, OADC 10 % was added aseptically, mixed and stored at 4\(^\circ\)C. This media was used for the preparation of bacterial culture (*Mycobacterium tuberculosis* H\(_{37}\)Rv).

**Media (B):** The media was prepared by mixing Glycerol (0.2 %), Casitone (0.1 %) and 7H9 broth (0.47g/100 mL) in MilliQ water and made up to desired volume and sterilized. OADC 10 % was added aseptically and stored at 4\(^\circ\)C. This media is used for the dilution of compounds.

**Drug dilutions**

The stock solutions of the test compounds (20,000 μg/mL) were prepared in DMSO, filtered through 0.22 μ syringe filters and stored at -5 to 0\(^\circ\)C. The working solutions were prepared by diluting the stock solution to 400 μg/mL (4x) using media B. The working solutions were serially diluted in 96 well plates to achieve final concentrations 100, 50, 25, 12.5, 6.25 and 3.125 μg/mL.

**Bacterial culture**

*Mycobacterium tuberculosis* H\(_{37}\)Rv strain was grown on slants. 2.5mL of 7H9 broth was transferred to a sterile glass vial containing glass beads. A loop full of bacteria was suspended in the broth and vortexed for 1-2 minutes to break the lumps and obtain turbid suspension. The supernatant was transferred to another sterile vial and was left to sediment for 15 minutes. The turbidity of the suspension was compared with McFarland standard 1.0.
Inoculum preparation

0.333 mL of McFarland 1.0 bacterial suspension was diluted to 1 mL with 7H9 broth (without casitone) to give $2.0 \times 10^7$ cfu/ml, from which 0.5 mL was taken and diluted to 5 mL with media to give $2.0 \times 10^6$ cfu/ml. 1 mL of the bacterial suspension ($2.0 \times 10^6$ cfu/mL) was taken and diluted to 10 mL with media to give $2.0 \times 10^5$ cfu/ml. The suspension prepared was used within 20 minutes for the study.

Procedure

Antitubercular susceptibility testing was performed using clear flat bottomed 96-well microplates. Outer perimeter wells were filled with sterile water to avoid dehydration. 100 μL of media B was added to each well. Serial dilution of the test compounds were made in the microplate. Then 100 μL of inoculum was added to each well. The final concentration of the test samples were 100, 50, 25, 12.5, 6.25 and 3.125 μg/mL. DMSO was used as blank and additional control wells (positive and negative control) were also kept to minimize the experimental error. Plates were covered with sterile breath seals and kept for incubation at 37°C for 7 days. On 7th day, 20 μL of Alamar blue and 12.5 μL of tween 80 (20 %) were added to each well and kept for incubation at 37°C for 24 h. After incubation for 24 hours, the microplates were visualized to detect the change in colour of the wells. No change in colour (blue) in the wells indicated the sensitivity of Mycobacterium tuberculosis to the test compounds and pink colour indicated resistance of organism to them. MIC was determined by estimating the minimum concentration of the test compound required to stop mycobacterial growth.
4.5.1. Evaluation of Antitubercular activity against MDR strain

The compounds with MIC ≤ 20μg/mL (SI ≥ 10) against H$_{37}$Rv were evaluated for their activity against multidrug resistant strain of Mtb. BACTEC Mycobacteria Growth Indicator Tube (MGIT 960) automated system was used for the study. BACTEC MGIT 960 is a rapid qualitative procedure for the susceptibility testing of Mtb.\textsuperscript{110-113}

**Requirements**

Modified Middlebrook 7H9 Broth, BACTEC MGIT 960 tubes, BACTEC MGIT 960 instrument (BD Biosciences Pvt. Ltd.).

**Bacterial strain**

Clinical isolate of multi drug resistant *Mycobacterium tuberculosis* strain (resistant to isoniazid, rifampicin, pyrazinamide and streptomycin) was used.

**Principle**

BACTEC MGIT 960 is a non-radiometric method, which uses medium tubes containing fluorescent compound embedded in silicone on the bottom.\textsuperscript{113} The fluorescent compound is sensitive to the presence of oxygen dissolved in broth. The initial concentration of oxygen present in the tubes quenches the fluorescent emission. The actively growing bacteria consume the oxygen, which allows the compound to fluoresce. The test is based on the growth of Mtb isolate in sample tube compared to control tube, which is monitored continuously by instrument. The results were interpreted automatically and reports as susceptible or resistant.

**Preparation of Inoculum**

A loop full of bacteria was transferred into sterile tube with cap containing glass beads and 4 mL of 7H9 broth and vortexed for 1-2 minutes to break the lumps and the suspension was compared with McFarland 1.0 standard. 1mL of the supernatant suspension was transferred to new sterile BACTEC MGIT tube and kept in the BACTEC MGIT 960 instrument and observed for growth. The tube with day 1 or 2 positive growth was compared with McFarland 0.5 standard and is used for the inoculation. This is called as antimicrobial susceptibility testing (AST) inoculum.\textsuperscript{113}

**Growth control inoculum**

0.5 mL of AST inoculum was aseptically added to 4.5 mL of sterile saline to get the 1:10 growth control suspension. To the growth control tubes, 0.5 mL of 1:10 inoculum was added.
Test inoculum
0.5 mL of AST inoculum prepared was used without any further dilutions in the test compound MGIT tubes.

Test solutions
The stock solutions (20,000 μg/mL) were prepared in DMSO. The working solution was prepared by diluting the stock solution with sterile water to get different concentrations (80x).

Procedure
To each sterile 7mL MGIT tube, 0.8 mL of modified Middlebrook 7H9 broth and 0.1 mL of drug stock solution were added aseptically, and finally 0.5 mL of the test inoculum was added. The tubes were mixed gently. The control tube contained 0.8 mL of 7H9 broth and 0.5 mL of growth inoculum. Screening was carried out at four different concentrations for each compound (two higher and one lesser than MIC). All the MGIT inoculated tubes (4 drug containing and 1 growth control) were kept inside the BACTEC MGIT 960 instrument immediately and incubated for 12 days. The relative growth between drug tubes and control tube was determined and the results were interpreted automatically by the instrument. If the relative growth of tubes containing test compounds is higher than control, it indicates test compound is inactive against MDR strain. If the relative growth of tubes containing test compounds is lower than control, it indicates test compound is active against MDR strain.
4.6. Determination of Physico chemical properties

4.6.1. Lipophilicity (Log P)

The Log P of the synthesized compounds was determined by Reverse phase HPLC method.\textsuperscript{114-117}

Requirements

Octanol (HPLC grade, Spectrochem Pvt. Ltd.), deionised water (Millipore), MOPS (3-Morpholinopropane sulphonic acid) buffer (Spectrochem Pvt. Ltd.) and methanol (HPLC grade, Merck).

Procedure

A 0.25\% (v/v) amount of octanol was added to methanol, and octanol-saturated water was used to prepare the buffer. The mobile phase used, in all the cases, was 20 mM MOPS buffer (pH 7.4) and methanol (0.25\% v/v octanol) in varying proportions from 25 to 15\% v/v. All the chromatographic runs were performed on HPLC (LC-20AT, SPD-20A, Shimadzu) at ambient temperature, using Inertsil ODS-4 (5 \(\mu\)m, 4.6 x 150 mm, GL sciences Inc. Japan) column. A UV-Vis detector was used to monitor signals at 254, 260, 274, and 288 nm. Samples were dissolved in methanol and the solutions were diluted to get 10 \(\mu\)g/mL concentration. 10 \(\mu\)L of the sample solution was injected. The flow rate was 1-2 mL/min, depending on the lipophilicity range.

Triplicate runs were performed for each compound to get reproducible retention times. Pure methanol was injected to determine \(t_0\), i.e., the dead time, while \(t_R\) is the retention time for the analyte.

The capacity factor was calculated from the retention time by using the formula:

\[
\text{Capacity factor (K')} = \frac{(t_R-t_0)}{t_0}
\]

The capacity factors data (\(K'\)), obtained at various percentages of methanol (x-axis), were extrapolated to 0\% methanol (y-axis) and reported as \(K'_w\), using a linear procedure. In all cases, the square of the correlation coefficient was \(\geq 0.99\). The extrapolation of logarithmic capacity factor to 0\% methanol gave the Log P of the compound.
Table 8: RP-HPLC conditions used

<table>
<thead>
<tr>
<th>Compound</th>
<th>Flow rate (mL/min)</th>
<th>% Methanol</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 a-s</td>
<td>1</td>
<td>15, 20, 25</td>
</tr>
<tr>
<td>6 a-r</td>
<td>1</td>
<td>15, 20, 25</td>
</tr>
<tr>
<td>8 a-o</td>
<td>1</td>
<td>15, 20, 25</td>
</tr>
<tr>
<td>9 a-o</td>
<td>1</td>
<td>15, 20, 25</td>
</tr>
<tr>
<td>15c-d, 24a, 33c</td>
<td>2</td>
<td>40, 45, 50</td>
</tr>
<tr>
<td>19d, 23c, 30a-b, 35a</td>
<td>2</td>
<td>60, 65, 70</td>
</tr>
</tbody>
</table>
4.6.2. Dissociation constant (pKa)

pKa of selected compounds were determined using RP-HPLC.\textsuperscript{117-128}

**Requirements**

Acetonitrile (HPLC grade, Merck Pvt. Ltd.), deionised water (Millipore), Universal buffer (phosphoric acid, boric acid and acetic acid) and NaOH.

**Mobile phase**

Organic phase: Acetonitrile (5-10 %)

Aqueous phase: Universal buffer containing 3 components, each at a concentration of 0.004 M: Phosphoric acid, Boric acid and Acetic acid, and adjusted to pH 2, 4, 6, 7.4 and 10, using 0.02 M NaOH. The pH of the buffers used was measured at room temperature using Digital pH meter.

**Column used**

Gemini 5µ C18 110A (150 x 4.6 mm, particle size 4.7-5.3 µm, Phenomenex)

**Procedure**

All the chromatographic runs were performed on HPLC (LC-20AT, SPD-20A, SHIMADZU) at ambient temperature, using Gemini 5µ C18 110A (150 x 4.6 mm, particle size 4.7-5.3 µm, Phenomenex) column. A UV-Vis detector was used to monitor signals at 254, 260, 274, and 288 nm. Samples were dissolved in acetonitrile and diluted to get 10 μg/mL concentration. 10 μL of the sample solution was injected.

**Flow rate:** 1mL/min.

Column was allowed to equilibrate for 2h with each change in mobile phase composition. Triplicate runs were performed for each compound to get reproducible retention times. Pure Acetonitrile injected to determine $t_0$, i.e., the dead time, while $t_R$ is the retention time for the analyte. 4-nitrophenol and ciprofloxacin were used as standard compounds for the pKa determination. The pKa of the test analytes were determined using the following equation:

$$pKa = pH - \log \frac{k_{HA} - k}{k - k_A}$$

Where $k$ is the capacity factor of the sample at a given pH, $k_{HA}$ and $k_A$ are the capacity factors of unionized and fully ionized forms and pH is the pH of mobile phase used.

The calculated pKa values were compared with the graphical pKa values. P- Nitro phenol was used as standard reference in this study for validation of the method.
4.7. Microsomal Stability Assay

The synthesized compounds which have shown MIC $\leq$ 25 μg/mL, against Mtb H$_{37}$Rv strain with selectivity index $\geq$ 10 were taken for the determination of their metabolic stability using human liver microsomes.$^{129-135}$

Requirements

Human Liver Microsomes (BD Ultra Pool), NADPH A and B (BD Biosciences)

Phosphate buffer pH 7.4 (BD Biosciences), Testosterone (TCL Pvt. Ltd.)

Acetonitrile (Merck), DMSO (Merck)

Column used

Microsorb-MV 100 C18 column (250 x 4.6 mm) having particle size 5μm.

Test solution

Stock solution was prepared in DMSO: Acetonitrile (1:4 ratio) at a concentration of 5mM and stored at -20 °C until use.

Procedure

Human Liver Microsomes (20 mg protein/mL, BD Ultra Pool HLM 150) and NADPH regenerating system solutions A and B (1.3 mM NADP, 3.3 mM glucose 6-phosphate 0.4 U/mL glucose 6-phosphate dehydrogenase and 3.3 mM MgCl$_2$, BD Biosciences) were thawed in 37 °C water bath and kept on wet ice before use. To a 1.5mL micro centrifuge tube, 713 μL purified water, 200 μL 0.5 M potassium phosphate pH 7.4 buffer (BD Biosciences), 50 μL NADPH regenerating system solution A, 10 μL NADPH regenerating system solution B and 2 μL of 5mM test compound (10 μM final concentration) were added and mixed thoroughly by closing the tube. The components in the micro centrifuge were warmed to 37°C for 5 minutes in an incubator. After incubation, the metabolic reaction was initiated by the addition of 25 μL (0.5mg) Human Liver Microsomes. The contents were mixed by inverting the capped tube twice and kept in the incubator at 37 °C. After 0, 30 and 60 minutes, reaction was stopped by withdrawing 200 μL from the incubated tubes and added to micro centrifuge tubes (1.5mL) containing 200 μL of cold acetonitrile containing 0.2 μM propranolol as internal standard. The contents were mixed and centrifuged at 12000 rpm for 5 minutes. The supernatant was removed for analysis and pellet was stored at -20°C. The samples at 0, 30 and 60 minutes interval were analyzed by HPLC using RP-HPLC Microsorb-MV 100 C18 column (250 x 4.6 mm) having particle size 5μm. Acetonitrile: water (0.1% HCOOH) in gradient flow is used as mobile phase. Testosterone (TCL Pvt. Ltd.), was
used as standard for the assay. HPLC peak areas were integrated and expressed and a mean peak area value for each time point was calculated from the duplicates:

\[
\text{Peak area ratio (PAR)} = \frac{\text{Test compound peak area}}{\text{Internal standard peak area}}
\]

The % remaining of the test compounds were calculated as:

\[
% \text{ Remaining} = 100 \left( \frac{\text{Mean PAR}_{T60}}{\text{Mean PAR}_{T0}} \right)
\]
4.8. Cytotoxicity Screening

The cytotoxicity of the synthesized compounds were assessed by Microculture Tetrazolium Assay.\textsuperscript{136-139}

Reagents

Minimum Essential Medium Eagle (MEM, AT047-10x1L, HIMEDIA)

Fetal Bovine Serum (FBS, RM9970-500mL, HIMEDIA)

Trypsin Phosphate Versene Glucose (TPVG solution 1x, TCL022-100mL, HIMEDIA)

Phosphate Buffered Saline, pH 7.2 (PBS, TS1099-10x1L, HIMEDIA)

Antibiotic Antimycotic solution 100x Liquid (A002-20mL, HIMEDIA)

Thiazolyl Blue Tetrazolium Bromide reagent (MTT, AR, RM1131-500mG, HIMEDIA)

DMSO (AR, Spectrochem) and sterile deionised water (MilliQ, Millipore)

Cell cultures

1. Vero cells (African Green monkey kidney epithelial cells)
2. HepG2 cells (Human Hepato carcinoma cells)

Preparation of media

9.6 g of MEM was transferred to a 1L reagent bottle and dissolved in 900 mL of MilliQ water. To this solution, 3.6 g of sodium bicarbonate was added and mixed thoroughly. Then the volume was made up to 1L with sterile deionised water. The pH of the media was adjusted to 7.4 using pH meter. The media was filtered aseptically through 0.22 μm membrane filter. 10mL antibiotic solution (a mixture of penicillin, streptomycin and amphotericin) was added and the media was stored at 2-8 °C till use.

Preparation of Phosphate buffered saline (PBS)

9.9g of PBS dissolved in 900 mL MilliQ water and mixed. The final volume was adjusted to 1L and the pH was adjusted to 7.4 using 1N HCl or 1N NaOH. The solution was filtered aseptically through 0.22 μm membrane filter using vacuum. The solution was stored in dark at 2-8 °C till use.

Preparation of MTT reagent (2mg/mL)

200 mg of Thiazolyl Blue Tetrazolium Bromide (MTT) was added to sterile PBS 100 mL and mixed thoroughly to get a solution. It was stored in amber colored bottle at 0-5°C till use.

Propagation of cell culture

Cryo vials containing Vero cells and HepG2 cells (NCCLS, Pune) were thawed gently in 37 °C water bath. The cell suspension was transferred to a 15 mL sterile centrifuge tube containing 5 mL of MEM medium supplemented with 10 % fetal bovine serum and
centrifuged at 2000 rpm for 15 min at 25-27 °C to form cell pellet. The supernatant was discarded and again 5 mL of MEM supplemented with 10% FBS was added to the pellet and suspended in the centrifuge tube. The cell suspension was transferred aseptically to a tissue culture flask (25 cm²) with vented cap and kept for incubation at 37 °C with 5% CO₂. The growth and taxonomy of the cells were monitored daily under inverted microscope. The growth media was changed every 24 and 48 hours interval for HepG2 and Vero cells respectively. Cells were passaged into new tissue culture flask when it is observed > 90% confluent monolayer of cells.

**Plating of cells**

The growth medium from tissue culture flask (25 cm²) was decanted aseptically followed by gentle rinsing with 5 mL of MEM media. The cell monolayer was washed with 10 mL of PBS. To detach the cells from the cell flask, 0.5 mL of Trypsin solution was added and incubated at 37 °C for 2-3 minutes followed by gentle tapping and observed under microscope. To this flask, 5mL of MEM supplemented with 10% FBS was added to quench the Trypsin activity. The cells in the media were mixed uniformly with the help of a pipette, to break the cell lumps. The cells were counted using Hemocytometer. Then the cell suspension was diluted by calculated amount of MEM (10% FBS) to achieve a final concentration of 1x10⁵ cells/ mL for Vero cells and 0.5x10⁵ cells/mL for HepG2 cells. 100 μL of the cell suspension was added to each well in a 96 well Microplate, except the outer perimeter cells. The outer perimeter wells were filled with 100 μL of sterile water. The plates were kept for incubation at 37 °C with 5% CO₂ for 24 hours.

**Preparation of test samples** (stock solution 20,000 μg/mL in DMSO)

10 mg of test compound was weighed, transferred to a sterile micro centrifuge tube (1.5 mL), and dissolved in 0.5 mL sterile DMSO. The solution was filtered using 0.22 μm syringe filter, transferred into sterile vials (1.5mL), sealed with para film, labeled and stored at 2-8 °C till use.

**Assay Procedure**

The stock solutions of the test compounds were diluted in a 96 deep well plate aseptically with MEM (without FBS) to achieve concentrations 300, 250, 200, 150, 100 and 50 μg/mL. The 96 well plates containing the cells were taken and kept inverted on filter paper to remove the supernatant media and washed gently with PBS and decanted. 100μL of sterile water were added to outer perimeter wells. Then 100μL of each test compound dilutions were added to the wells. DMSO was used as control and the plates were incubated in incubator (5% CO₂) at 37 °C for 24 and 72 hours for HepG2 and Vero cells respectively.
After the incubation, plates were inverted on filter paper to remove the supernatant media followed by PBS washing. To this, 50 μL of MTT solution (2mg/mL) was added to each well in dark place and incubated for 3 hours. After the incubation, the MTT solution was removed from the well by inverting gently on filter paper and 50 μL of DMSO was added to each well and kept in dark place for 1-2 hours. Then the optical density readings of the plates were taken using Elisa reader at 540 nm.

**Determination of CC\textsubscript{50}**

\[
\text{% Cell Viability} = \frac{\text{Optical Density of Test}}{\text{Optical Density of Control}} \times 100
\]

\[
\text{% Cell Inhibition} = 100 - \text{% Cell Viability}
\]

CC\textsubscript{50} was calculated by extrapolating a graph with % cell inhibition on Y-axis against concentration of test compound on X-axis.