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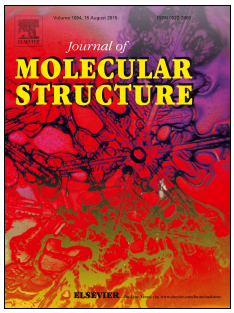


Synthesis, crystal structure and theoretical analysis of intermolecular interactions in two biologically active derivatives of 1,2,4-triazoles

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# Synthesis, Crystal Structure and Theoretical Analysis of intermolecular interactions in two biologically active derivatives of 1,2,4-triazoles.

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## Highlights

- Synthesis of two biologicallyactive derivatives of 1,2,4-triazoles has been reported.
- Role in different intermolecular interaction in crystal packing.
- Quantitative investigation of the nature and strength of intermolecular interactions.

## Abstract

In the present study, we have synthesized and structurally characterized two biologically active derivatives of 1,2,4 triazoles, namely 3-(4-fluoro-3-phenoxyphenyl)-1-(piperidin-1-ylmethyl)-1H-1,2,4-triazole-5(4H)-thione **(TR)** and 1-((3-(4-fluoro-3-phenoxyphenyl)-5-(methylthio)-1H-1,2,4-triazol-1-yl)methyl)piperidine**(TR1)** via single crystal X-ray diffraction. Both the structures show the presence of various intermolecular interactions in the crystalline solid such as C-H…F, C-H…S, C-H…N, C-H…O, C-H…π, and π…π intermolecular interactions. The role of these interactions in molecular packing was analyzed, and the nature of these interactions was evaluated through computational procedures using PIXEL. Hirshfeld analysis further reveals that the contribution of H…F interactions was more prominent towards packing as compared to H…N/O intermolecular interactions.

## Keywords

1,2,4-triazoles, crystal structure, intermolecular interactions, Hirshfeld analysis, PIXEL.