SYNTHESIS, CRYSTAL STRUCTURE, HIRSHFELD SURFACE ANALYSIS OF ISOMERIC ((1-(4-NITROPHENYL)- 1H-1,2,3-TRIAZOL-4(5)-YL) METHOXY) BENZALDEHYDE COMPOUNDS

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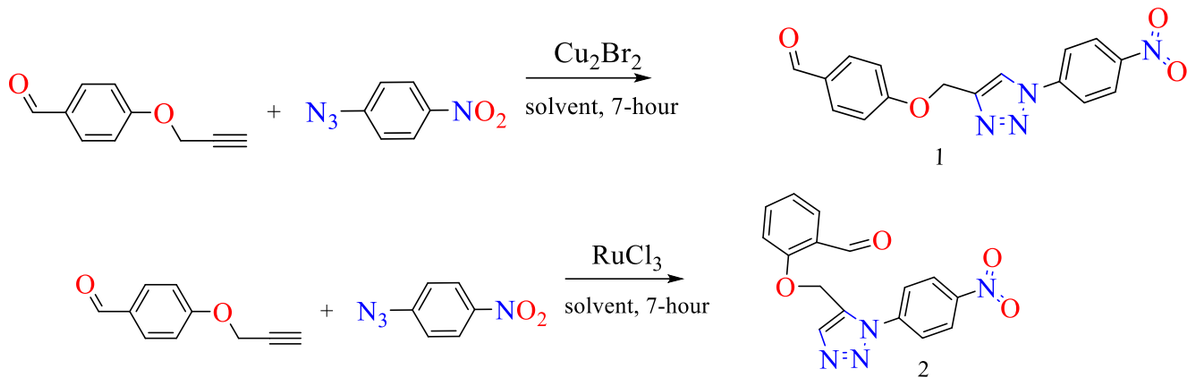
INTRODUCTION & AIM

Among nitrogen-containing heterocyclic compounds, triazoles have high pharmacological properties and are therefore of interest for structural and physico-chemical studies. Structurally, triazoles can be divided into two different subsets: 1,2,3-triazole and 1,2,4-triazole. Due to their structural characteristics, 1,2,3- and 1,2,4-triazoles can accommodate a wide range of substituents (electrophiles and nucleophiles) around their core structures, opening the way for the synthesis of various new bioactive substances [1]. Although it has been more than 120 years since the initial discovery of the method for the synthesis of 1,2,3-triazoles by cross-alkynes and azides, the interest in this chemical class of molecules has been increasing rapidly in the last 20 years. The reason for this is the introduction of catalytic methods for cyclization reaction which made the generation of 1,2,3-triazole derivatives widely accessible for pharmacological applications. With the advancement of click chemistry, scientific work on these 5-membered heterocyclic compounds is growing rapidly [2]. Here, we report the synthesis and structural characterization of 2-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methoxy) benzaldehyde (**1**) and 3-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methoxy) benzaldehyde (**2**) using X-ray crystallography.

Keywords: crystal structures, 1,2,3-triazoles, hydrogen bond networks, Hirshfeld surface analysis

METHOD

Compound **1** and **2**: para-bromophenylazide, prop-2-yn-1-yl-2-(4-nitrophenoxy) acetate, *copper (I) bromide and ruthenium (III) chloride* (respectively: **1** and **2**) and toluene were placed into a flask with a reflux condenser, which was heated on an oil bath at the boiling point of toluene (110 ^{0}C) for 7 h. The progress of the reaction was monitored by thin layer chromatography. Over time, a precipitate began to form in the reaction mixture.



As a result, product **1** and **2** were obtained. Melting point: compound **1** =144-146 ^{0}C and compound **2** =150-152 ^{0}C, Rf_1 =0.55 and Rf_2 =0.55 (system: benzene: methanol – 10:1). The colourless single crystals suitable for X-ray diffraction were grown from ethanol at room temperature within two weeks.

RESULTS & DISCUSSION

The structures of compounds 1 and 2 were established by single crystal X-ray diffraction and the identified conformations were described in the context of their stabilizing intra- and inter-molecular interactions, particularly highlighting the significant hydrogen bonds of the crystals. The following figures show the significant hydrogen bonds.

2-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl) methoxy) benzaldehyde (compound **1)**

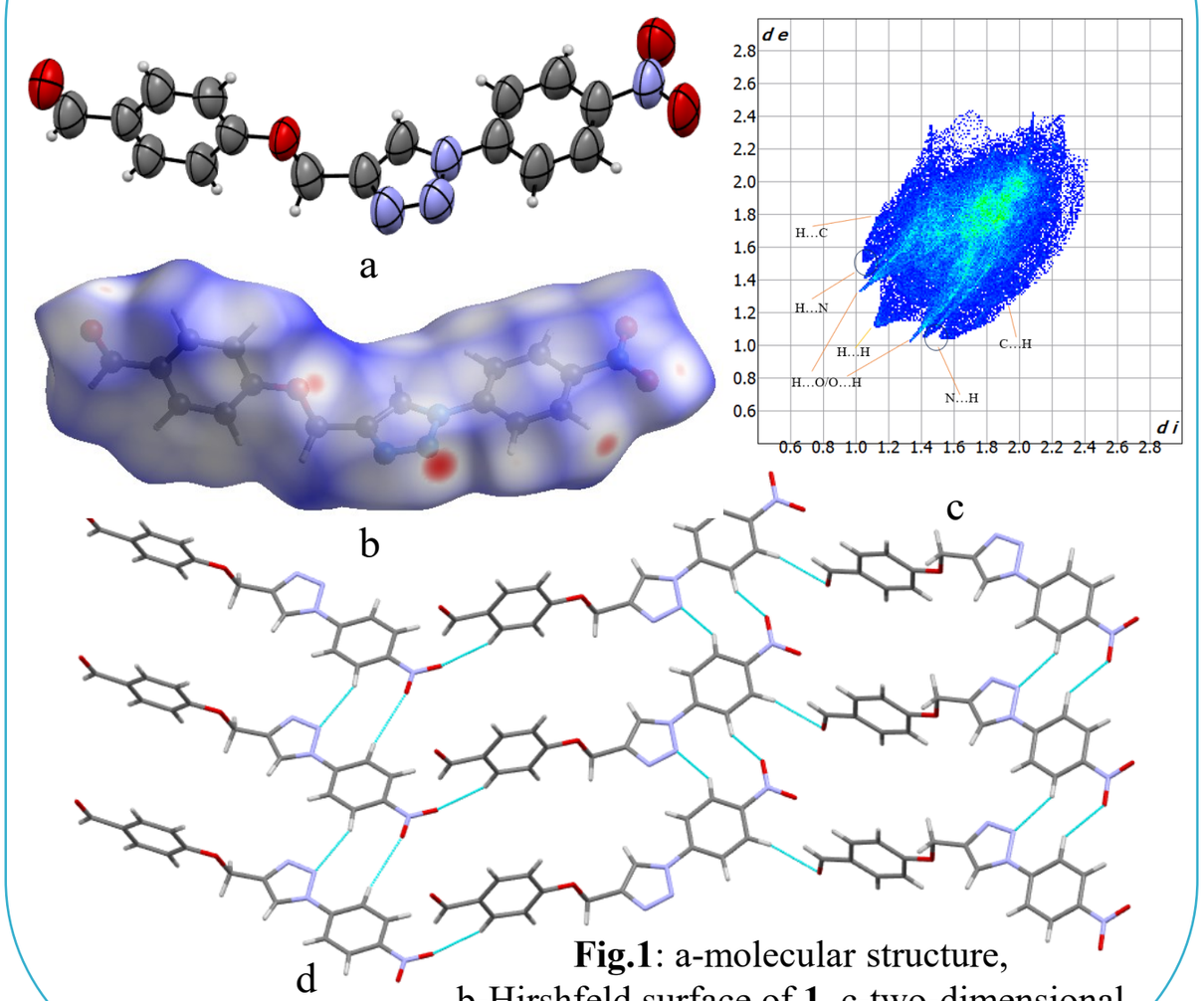


Fig.1: a-molecular structure, b-Hirshfeld surface of **1,** c-two-dimensional fingerprint plot, d-crystal packing of **1**

3-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl) methoxy) benzaldehyde (compound **2**)

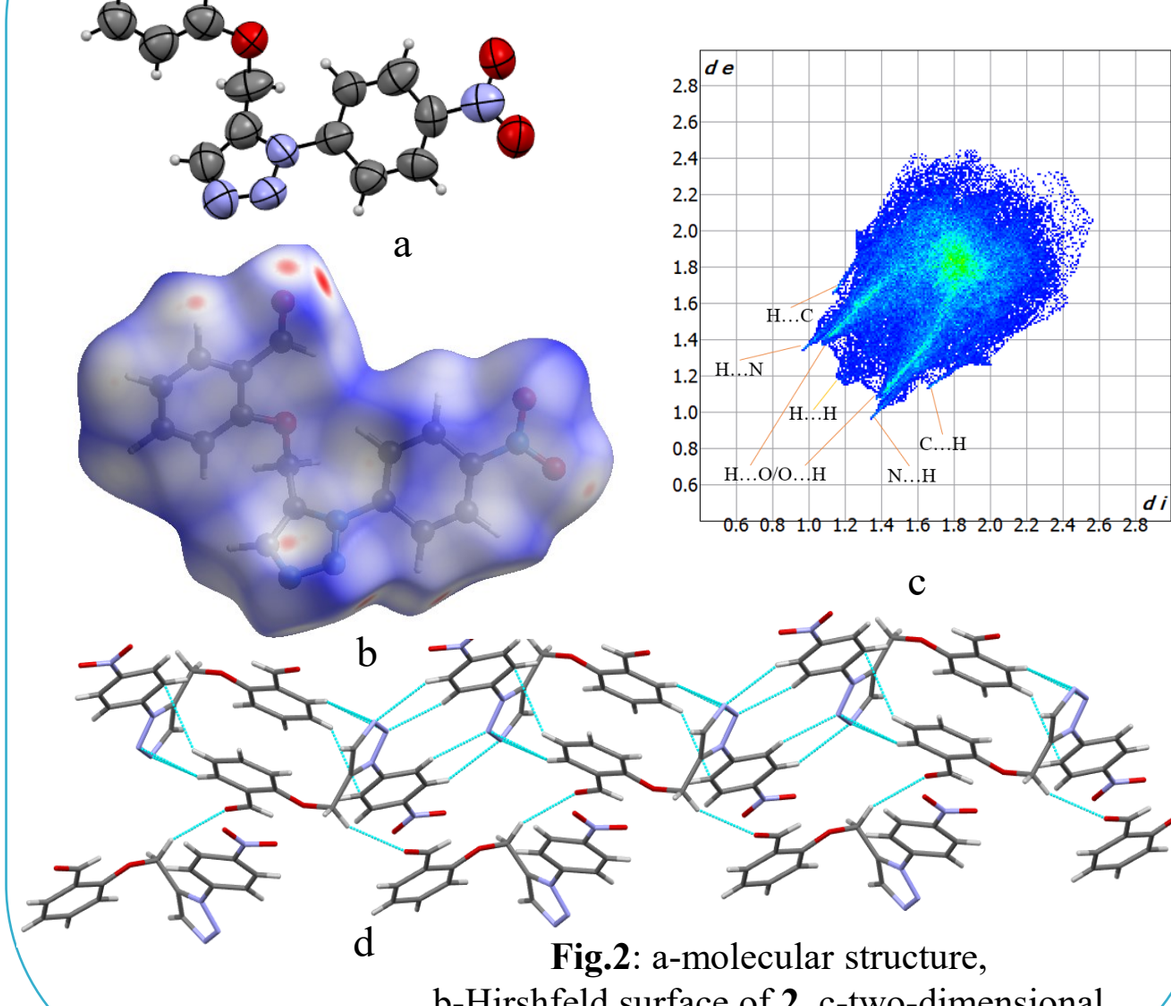


Fig.2: a-molecular structure, b-Hirshfeld surface of **2,** c-two-dimensional fingerprint plot, d-crystal packing of **2**

CONCLUSION

For molecular crystals, These analyses were performed to determine intermolecular interactions in **1** and **2**. According to our results, the molecules are associated by intra- and intermolecular hydrogen bonds, C—H···π and N—O···π stacking interactions. The three-dimensional Hirshfeld surface analysis and two-dimensional fingerprint plots revealed that the structures are dominated by H···H, H···C/C···H, H···N/N···H and H···O/O···H contacts. In future, we will synthesis their complexes with 3d elements, and will analysis synergism property of those compounds.

ACKNOWLEDGEMENTS/ REFERENCES

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