

primary hydrogen bond backbone; **Fpm<sub>N</sub>** with N-H...N and **Fpm<sub>O</sub>** with N-H...O=C as primary interaction. The **Fom** isomer was unexpectedly found highly disordered with  $Z' = 6$ .

The most significant structural characteristic of the **Fxo** triad was formation of twisted dimmers through double N...H-N hydrogen bonding creating centrosymmetric  $R^2_2(8)$  rings. Formation of dimmers when pyridine nitrogen is in *ortho* position is already seen in analogue **Mxo** [2] isomers.

Computational modelling and conformational analyses of the **Fxx** isomers and their comparison with solid state structures showed that modelled structures generally comply with solid state conformations except in the **Fxm** isomers. Modelling of the **Fox** isomer triad suggested existence of intramolecular F...H-N bonding. Spectroscopic and crystallographic data supported this prediction.

This work represents the final step in the investigation of the four benzamide/carboxamide isomer grids with methyl/fluorine substituents (**Mxx** [1], **NxxF** [2], **NxxM** [3] and **Fxx**), by both solid state methods and computational modelling, with innovative approach in bridging two powerful structural methods together. The comparison of the four isomer grids revealed high degree of similarity regarding solid state aggregation and physicochemical properties, while correlated melting point values indicated significance of the substituent position on thermal behaviour, rather than the nature of substituent.

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**Keywords:** benzamides, solid-state, modelling

## MS73.P19

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### Analysis of Ethyl (2E)-3-(4-hydroxy-3,5-dimethoxyphenyl) prop-2-enoate

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In recent decades it has been discovered a wide range of biological activities for the derivatives of cinnamic acid. There are reports that the derivatives trans-cinnamic acid possess hepatoprotective activity, antimalarial, antimicrobial antioxidant and  $\alpha$ -glucosidase. Furthermore, *in vitro* tests showed regression of malignant cells in human tumors. The single crystal of Ethyl (2E)-3-(4-hydroxy-3,5-dimethoxyphenyl) prop-2-enoate (C<sub>13</sub>H<sub>16</sub>O<sub>5</sub>) was obtained by slow evaporation technique using as solvent ethyl ether. The structure was solved by Direct Methods and refined by full matrix Least Square methods on F<sup>2</sup> using WINGX package [1]. Non H atoms were refined anisotropically and all H atoms were placed geometrically except the hydrogen of the water molecule and of the hydrogen of the hydroxyl that were placed by D.W. Smith method [2], where the hydrogen are placed by estimating atomic charges by electronegativity equilibration. The compound crystallizes in the C2/c monoclinic space group and the cell dimensions are:  $a = 21.273(5)$  Å,  $b = 7.391(3)$  Å,  $c = 17.898(7)$  Å,  $\alpha = \gamma = 90^\circ$  and  $\beta = 92.64(3)^\circ$ ,  $Z = 8$  and  $V = 2811(2)$  Å<sup>3</sup>. 23018 measured reflections with 4279 unique and 2587 observed [ $I > 2\sigma(I)$ ]. The final residual factor  $R_1$  is 0.0607 for 181 refined parameters using 25 restraints. In the asymmetric unit there is a disordered water molecule that causes a partial disorder at the ester molecule, the disorder may be caused by a repulsive interaction between the hydrogen of the water molecule and of the hydroxyl of the ester molecule.

[1] S. L. Farrugia, *J. Journal Appl. Cryst.*, **1999**, *32*, 837. [2] M. Nardelli, *J. Appl. Cryst.*, **1999**, *32*, 563-571.

**Keywords:** cinnamic acid, X-ray diffraction, hydrogen bonds

## MS73.P20

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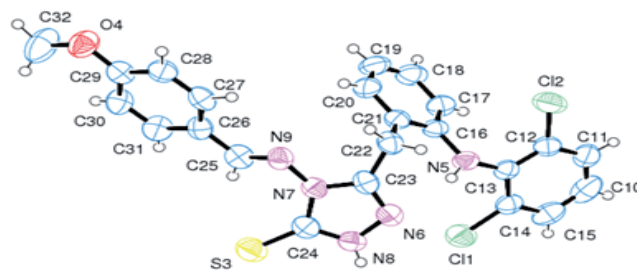
### X-ray structure of 4-methoxybenzylideneamino-5-substituted triazole derivative

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The crystal structure of the title derivative, 5-[2-[(2',6'-dichlorophenyl) amino] benzyl]-4-(4-methoxybenzylideneamino)-2H-1,2,4-triazole-3(4H)-thione (C<sub>23</sub>H<sub>19</sub>N<sub>3</sub>OSCl<sub>2</sub>) is determined by X-ray diffraction method and crystallizes in the Triclinic space group *P-1* with cell parameters  $a = 7.9438(4)$  Å,  $b = 10.9163(7)$  Å,  $c = 14.0384(8)$  Å,  $V = 1140.98(11)$  Å<sup>3</sup>,  $Z = 2$ ,  $D_{calc} = 1.410$  mg/m<sup>3</sup>,  $\mu = 0.402$  mm<sup>-1</sup>,  $F_{000} = 500$ ,  $\lambda(\text{MoK}\alpha) = 0.71073$  Å and the structure was refined to  $R = 0.0561$ .

Schiff bases are condensation products of primary amines with carbonyl compounds. The presence of lone pair of electrons in the SP<sup>2</sup> hybridised orbital of nitrogen atom of the azomethine group is of considerable chemical and biological importance. Schiff bases are some of the most widely used organic compounds. They are used as pigments and dyes, catalysts, intermediates in organic synthesis and polymer stabilisers. They have also been shown to exhibit broad range of biological activities including antimalarial, antibacterial, antifungal, antiviral and antitubercular/Imine or azomethine groups are present in various natural, natural-derived and non-natural compounds. The imine group present in such compounds has been shown to be critical to their biological activities.

The structure of 5-[2-[(2',6'-dichlorophenyl) amino] benzyl]-4-(4-methoxybenzylidene amino) -2H-1,2,4-triazole-3 (4H)-thione contains just one molecule in the asymmetric unit. The triazole ring makes dihedral angles of 24.81 (18)°, 69.94(19)° and 35.68(18)° with the three aromatic rings, respectively. The structure of the molecules is stabilized by intermolecular N-H...S and intramolecular C-H...S & N-H...N hydrogen bonds. In the crystal, molecules are stacked along *a* axis.



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**Keywords:** Crystal, Asymmetry, Diffractometer