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Synthesis, Characterization, Crystal Structure and Hirshfeld Surface Studies of Schiff Base Derivatives

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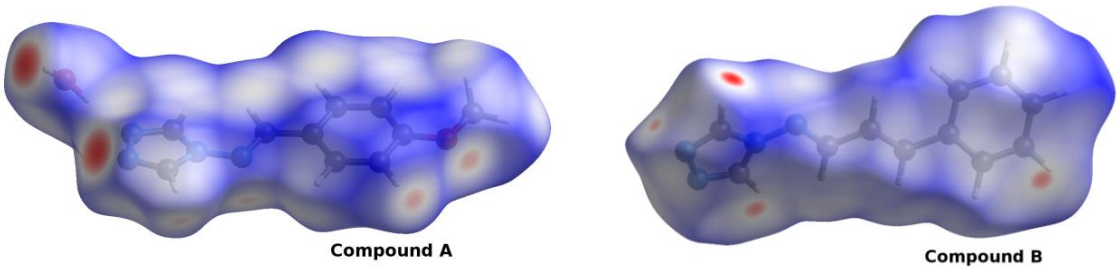
Abstract: Schiff bases are the important constituent of many natural sources and have variety of biological activities. The synthesised Compound A contains triazole group, triazoleposses antimicrobial, anti-inflammatory characteristic properties. Synthesised compound was characterized using various techniques and finally confirmed it structure, using X-ray diffraction (XRD) method, and found that the structure of crystal is triclinic with space group P-1, and ORTEP diagrams with 50% probability level displacement ellipsoids drawn, and Hirshfeld surface analysis with intermolecular interaction in crystal structures and employing fingerprint plots and molecular surface contours.

Keywords: Hirshfeld Surface, Schiff Base, X-ray Diffraction, Crystals Structure.

Graphical Abstract



Specification Details

Subject	:	Oraganic and analytical chemistry, Crystallography
Compounds	:	(Z)-1-(4-methoxyphenyl)-N-(4H-1,2,4-triazol-4-yl)methanimine and (Z1,2E)-3-phenyl-N-(4H-1,2,4-triazol-4-yl) prop-2-en-1-imine
Category	:	Crystallography, computational simulations Data format X-ray diffraction method of single crystal
Type	:	Process and analysed
Method	:	Compounds were synthesized, characterized by spectral analysis, x-ray diffraction method
Accessibility	:	CCDC-1818661 and CCDC-1883899

INTRODUCTION

Schiff base are the compounds having azomethine group (-CH=N-). Schiff base compounds was discovered in 1864 by Hugo Schiff. These type of compounds usually prepared by the condensation method by amines with carbonyl compound. Aromatic aldehydes of schiff base have conjugated *system* are more stable than aliphatic aldehydes and easily polymerizable. Each year number of papers are

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published on schiff base. However, the enormous potential of Schiff bases provides lot of opportunity for creativity in chemicals. Another important class of heterocyclic compounds is triazoles having benzo-fused structure [1]. Heterocyclic systems containing 1,2,4-triazole aroused great interest because of their application in important areas as diverse as pharmacology, agriculture, industry [2]. Triazoles have lot of application in the medical field [3]. Triazole have pronounced anti-inflammatory, anti-microbial, anti convulsant, antihypoxic, hypoglycemic, anti-tumor and other properties [4]. 1,2,4-triazole are used in medicine which are available in markets nucleusis like Ribavirin, letrozoles etc[5]. Schiff bases compouns are used in many reactions like addition, ring closure etc. [6]. The schiff base structure find major role in the field of chemistry and biology [7]. Schiff bases structures is to improve protein, vitamins etc, in some reactions it is use as ligands [8]. Schiff base derivatives possess antifungus, anticancer, antimicrobial, antitumor etc [9]. Schiff bases have lot of application medicines, reactions, biology. Metal complex of schiff base has effective scavengers of reactive oxygen species ROS acting as anti-oxidants thereby reducing the incidence of certain cancers [10].

PROCEDURE

Synthesis of (*Z*)-1-(4-Methoxyphenyl)-*N*-(4*H*-1,2,4-Triazol-4-yl) Methanimine (Compound-A)

4-amino-4H-1,2,4-triazole 00.8408g (00.01mole) and anisaldehyde 1.3615g (0.01 mol) and 10 ml of absolute alcohol are taken in a RB flask, 2-3 drops of sulfuric acid was added and was refluxed for about 3 hours at 98^0. Using TLC reaction was monitered for completion, (mobile phase: hexane and ethyl acetate in 1:2 ratio), and was filtered, and solid is separated and recrystallized uing ethyl aceto acetate. Using slow evaporation technique the crystals were grown. **MP:273 K.** The reaction is shown in the Fig. 1a

Synthesis of (1*Z*,2*E*)-3-Phenyl-*N*-(4*H*-1,2,4-triazol-4-yl) Prop-2-en-1-Imine (Compound-B)

4-amino-4H-1,2,4-triazole 00.8408g (00.01mole) and cinnamaldehyde 1.3216g (0.01 mol) and 15ml of absolute alcohol are taken in a RB flask, 2-3 drops of sulfuric acid was added and refluxed about 3 hours at 98^0C. Using TLC reaction was monitered for completion, (mobile phase: hexane and ethyl acetate in 1:2 ratio), and was filtered and solid is separated and recrystallized using ethyl ace to acetate. Using slow evaporation technique the crystals were grown. **MP:457 K.** The reaction is shown in Fig.2

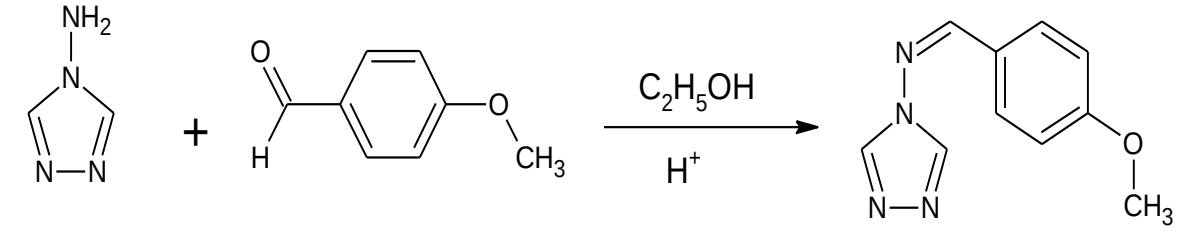


Figure 1: Synthetic scheme -compound-A

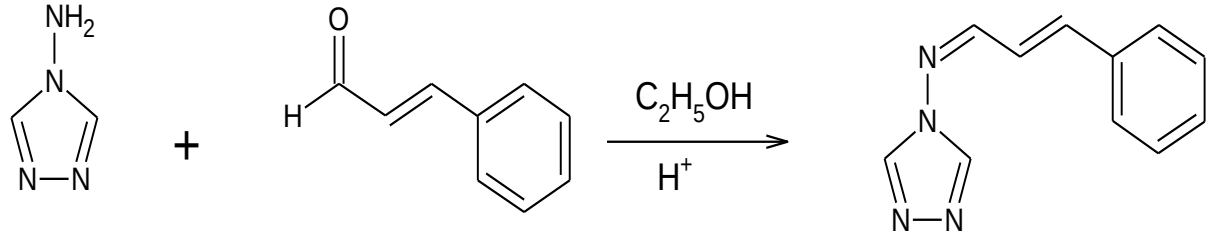


Figure 2: Synthetic scheme - compound-B

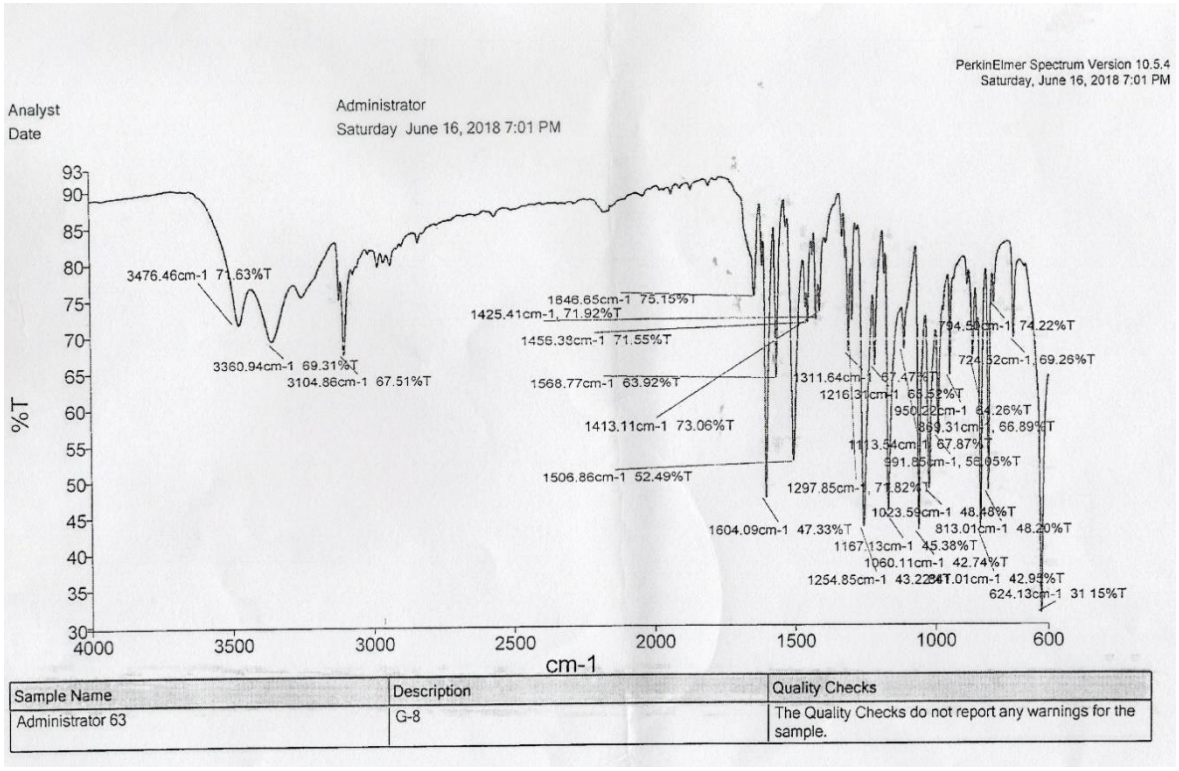
Spectral Data

IR-Spectra: The characteristic absorption band of the synthesized compound-A and compound-B are as follows.

Compound-A: **IR -** The peak at 1604cm^{-1} are due to C=N, at 1060 cm^{-1} and 991 cm^{-1} by C-Oand N-N, aromatic C-H at 3104 cm^{-1}.

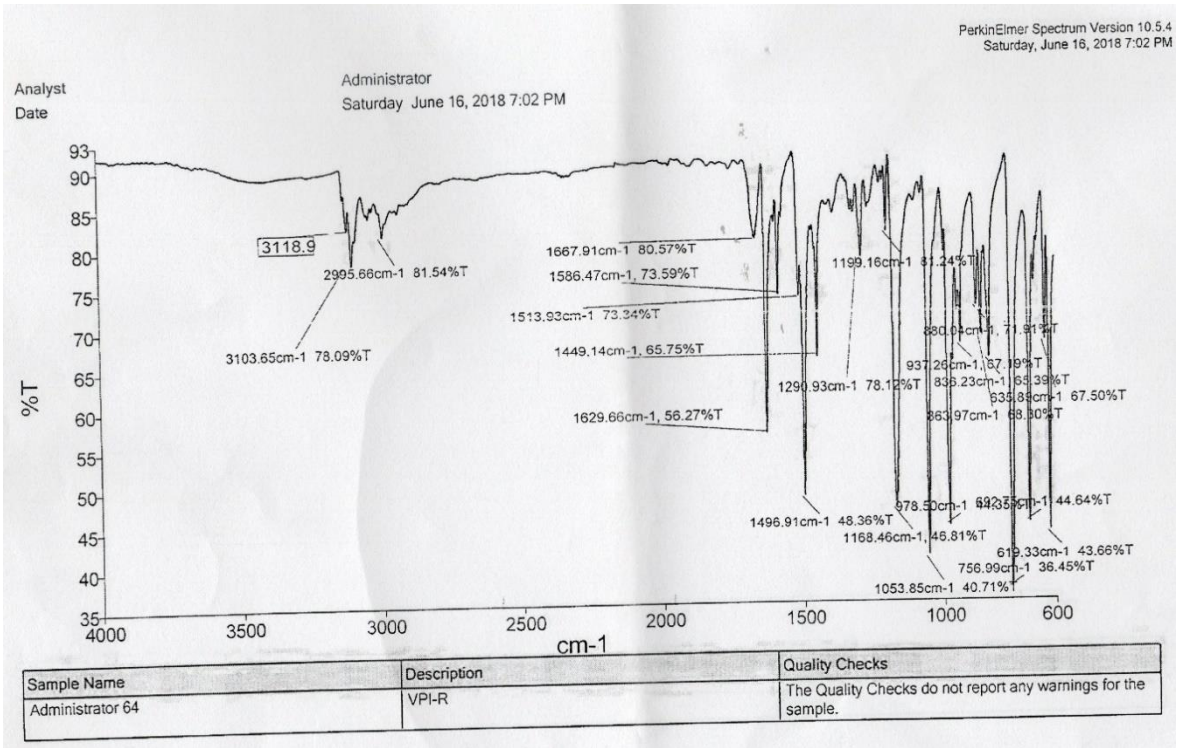
Compound-B: **IR** - The peak obtained at 1629 cm^{-1} are due to C=N, at 991 $cm^{-1}$is N-N, at 3103 $cm^{-1}$by CH in aromatic group, C=C at 1496 cm^{-1}.

Compound-A



Sample Name	Description	Quality Checks
Administrator 63	G-8	The Quality Checks do not report any warnings for the sample.

Compound-B



Sample Name	Description	Quality Checks
Administrator 64	VPI-R	The Quality Checks do not report any warnings for the sample.

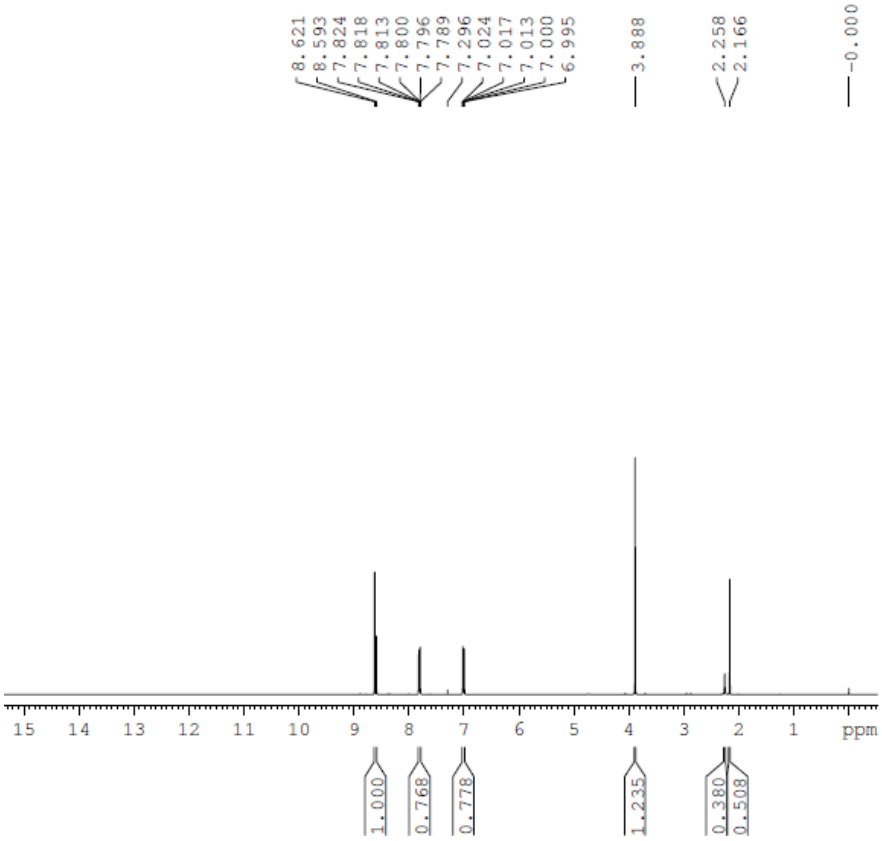
^{1}H NMR Spectra

The ^{1}H NMR peak values in δ -ppm of compound –A and compound –B are as follows.

Compound-A : NMR – ^{1}H δ03.89 (3H, S, OCH_3), δ06.99-7.81 (4H, m, Aromatic), δ08.59 (1H, S, N=CH (triazole)), δ 8.62 (1H, S, CH).

Compound-B : NMR – ^{1}H, δ06.99(1H, S, CH), δ07.02 (1H, S, CH), δ07.24-07.56 (5H, m, Aromatic), δ08.40 (1H,S, CH), δ08.55 (1H, S, N=CH (triazole)).

Compound-A

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PROCNO                       1

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PULPROG                   zg
TD                     32050
SOLVENT                CDC13
NS                        32
DS                         0
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FIDRES              0.200008 Hz
AQ                  2.4999001 sec
RG                       101
DW                    78.000 usec
DE                     6.50 usec
TE                     298.0 K
D1                2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
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P1                     13.50 usec
PL1                    -3.00 dB
PL1W            13.42244530 W
SFO1            400.2330017 MHz

F2 - Processing parameters
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LB                     0.30 Hz
GB           0
PC                     1.00
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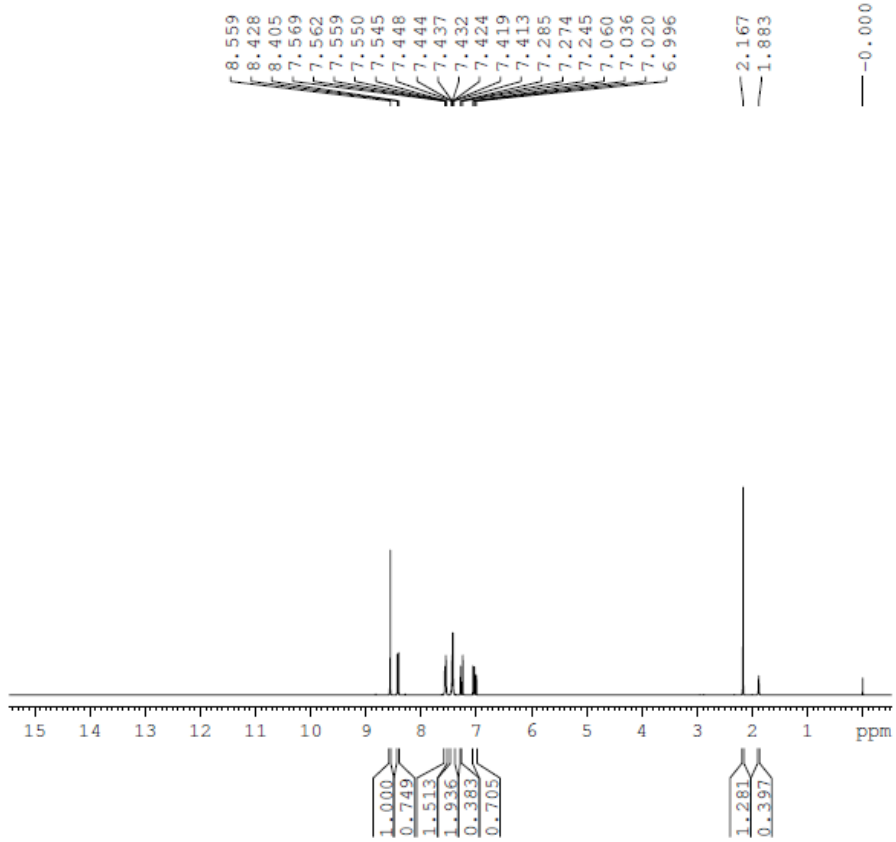
Compound-B

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NS                        32
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SWH                 6410.256 Hz
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AQ                  2.4999001 sec
RG                       101
DW                    78.000 usec
DE                     6.50 usec
TE                     298.0 K
D1                2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                       1H
P1                     13.50 usec
PL1                    -3.00 dB
PL1W            13.42244530 W
SFO1            400.2330017 MHz

F2 - Processing parameters
SI                      131072
SF                400.2300146 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

Crystallographic Data Collection and Structure Refinement

Schiff base crystals obtained by Slow evaporation technique are choose for XRD study, data of intensity of x ray was taken at 293K on RigakuXtaLAB Mini diffractometer at 50 kV and 12 mA, X-ray generator is operated using MoK$_\alpha$ radiation of 0.71173 Å wavelength, by fixing χ value at 55° and changing φ from 0°-360°,data were collected 00.5° of width in scan and exploring it for 4s,50 mm the sample to detector distance.Using Crystal cleardata of intensity was done[11]. By direct methodstructure of crystal was done andby usingleast square technique onF2byUsing program SHELXS and SHELXL, crystals were refined[12-13]. Anisotropically nonhydrogen atom was refined, geometrically positioned the H atom, CH= -00.96A^o, by ridings modelsU_{iso}[H]=01.2 U_{eq}[C], U$_{iso}$[H]=01.5U_{eq}[Cmethyll] it was refined. Repeating many times of refinement,no peak of chemicals significance was found in Fourier's mapand the residual is saturated to desired value and calculation of geometrical was done by PLATON program[14]. The packing diagramswas obtained using the MERCURY Software [15].

Hirshfelds Surface Analysis

The intermolecular interactions was quantified and to visualize the moleculars surfaces, the Hirshfelds surface analysIs (HSA) by crystal Explorer [16] software is the unique tool. In HSA the d_{norm} surface and the fingerprint plots defined by d_i and d_e, in the crystalline environment qualitative and quantitative information of the intermolecular interactions is involved. The distance from the nearest nucleus inside to Hirshfeld surface is d_i and $d_e$outside the surface. The molecular surface is normalized (equation 1) using d_i, d_e and van der Waal's distance.

RESULT AND DISCUSION

By X ray diffractions analysis the three dimensional structures of the compounds (A) and (B) was confirmed, compound A's crystal structure was found to be Triclinic and space group P1, whereas thecompound B's crystal structure Orthorhombic with $P2_12_12_1$. ORTEP diagrams of molecules A and B, at 5.0% Probability levelsdisplacement ellipsoids drawn are mentioned in **Fig.3**. the structure refinement and crystal data details are mentioned below in **Table1.**

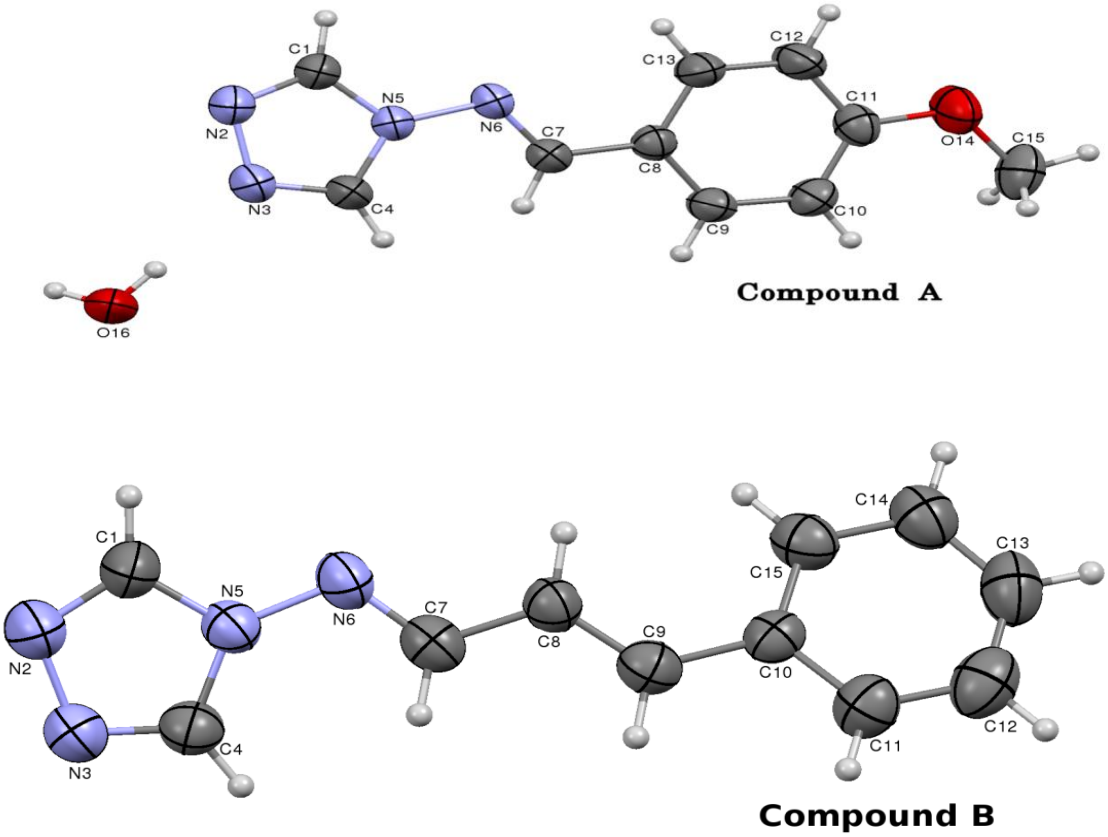


Figure 3: ORTEP diagram

Table 1: Summary of structure refinement and Crystals information

Parameter	Compound A	Compound B
CCDC deposit No.	CCDC 1818661	CCDC 1883899
Molecular formula	$C_{10}H_{12}N_4O_2$	$C_{11}H_{10}N_4$
Formula weight	220.24	198.23
Temperatures	293K	293K
Wavelengths	00.71074A^o	00.71074A^o
Crystals type	Triclinic	Orthorhombics
Space. groups	P1	$P2_12_12_1$
Unit-cells dimention	a. =07.310 [3]A^o b.= 08.011[3]A^o c.= 10.105 [4]A^o α.=102.548[8]^0 β= 98.566[7]^0 γ.= 100.730[8]^0	a = 05.643[7]A^o b = 09.277[12]A^o c = 19.770[3]A^o α = 9o^0 β = 9o^0 γ = 9o^0
Volume	556.3[4]A^{o3}	1035.0[19]A^{o3}
Z	2	4
Density[calc]	01.315Mgm^{-3}	01.272 Mgm^{-3}
AbsorptiOn coeff	00.096 m m^{-1}	00.082 m m^{-1}
F_{000}	232	416
Crystals size	0.31 × 0.27× 0.24 m m	0.33 × 0.26× 0.21 m m
Data collection θ range	03.23^o to 27.47^o	3.01^o to 27.50^o
Index ranges	-9≤h ≤9 -10 ≤ k ≤6 -12 ≤ l ≤13	-4 ≤ h≤7 -9 ≤ k≤11 -23≤ l≤ 25
Reflection Collected.	3252	4218
Independent reflection	2492 [R_{in}= 0.0157]	2338 [R_{in}= 0.1006]
Absorption correction	Multiscan	Multiscan
Refinement methods	FUll Matrix least square on F^2	Full Matrix least square on F^2
Data/ parameter/restrain	2492/ 149/ 0	2338/ 136/0
Goodness of fit on F^2	01.047	01.069
R indices [I>2σ(I)	R1 = 00.52, wR2 = 00.1295	R1 = 00.0759, wR2 = 00.1789
R *indice* [full data]	R1 = 00.078,wR2 = 00.1414	R1=00.125, wR2= 00.2149
Large dif Peak and Hole	00.184 & -00.210 eA^{-3}	00.181 and -00.184 eA^{-3}

Structure of Crystals

By XRD technique Compounds (A and B) structures was determined. The obtained schiff basecompounds bond angles and bond lengths when compared with standard values are found in good agreement, this data is listed in the **Table 2** and **Table 3**. The dihedral angle and torsion angles describes the molecular spatial orientation, the torsion angles is given **Table 4.**

Table 2: Compound A&B, bond lengths (A^o)

Compound A	bond lengths	Compound B	Bond lengths
N_2-C_1	01.299 (02)	N_2-C_1	01.304(05)
N_2 - N_3	01.385(02)	N_2 - N_3	01.402(05)
N_3 - C_4	01.301(02)	N_3 - C_4	01.300 (05)
N_5 - C_1	01.343(02)	N_5 - C_1	01.356 (05)
N_5 - C_4	01.356 (02)	N_5 - C_4	01.359 (05)
N_5 - N_6	01.408 (02)	N_5 - N_6	01.396(05)
N_6 - C_7	01.271(02)	N_6 - C_7	01.273 (05)
C_7 - C_8	01.458(02)	C_7 - C_8	01.425 (05)
C_8 - C_9	01.380(02)	C_8 - C_9	01.342 (05)
C_9 - C_{10}	01.388 (02)	C_9 - C_{10}	01.461 (05)
C_{10} - C_{11}	01.375 (02)	C_{10} - C_{11}	01.399 (05)
C_{11} - C_{12}	01.390 (02)	C_{12} - C_{13}	01.372 (07)
C_{12} - C_{13}	01.367(02)	C_{13} - C_{14}	01.371 (06)
O_{14} - C_{15}	01.421 (03)	C_{14} - C_{15}	01.389 (06)
O_{14} - C_{11}	01.359 (02)	C_{10} - C_{15}	01.395 (05)
C_8 - C_{13}	01.397 (02)	C_{11} - C_{12}	01.380 (06)

Table 3: Bond angles (⁰)

Compound A	Bond angles	Compound B	Bond angles
N_3-N_2-C_1	106.28(14)	N_3-N_2-C_1	106.1(03)
N_2-N_3-C_4	107.58(13)	N_2-N_3-C_4	107.0(03)
N_6-N_5-C_4	132.76(14)	N_6-N_5-C_4	133.1(03)
C_1-N_5-C_4	105.05(13)	N_6-N_5-C_1	122.6(03)
N_6-N_5-C_1	122.19(12)	C_1-N_5-C_4	104.3(03)
N_5-N_6-C_7	115.16(12)	N_5-N_6-C_7	115.9(03)
N_2-C_1-N_5	111.20(14)	N_2-C_1-N_5	111.5(03)
N_3-C_4-N_5	109.89(14)	N_3-C_4-N_5	111.0(03)
N_6-C_7-C_8	121.95(14)	N_6-C_7 - C_8	119.1 (03)
C_7- C_8- C_{13}	122.12(15)	C_7 - C_8 - C_9	122.3(03)
C_9-C_8-C_{13}	118.13(14)	C_8 - C_9 - C_{10}	127.0(03)
C_7 - C_8 - C_9	118.76(14)	C_9 - C_{10} - C_{11}	119.7(03)
C_8 - C_9 - C_{10}	121.97(14)	C_9-C_{10}-C_{15}	121.7 (03)
C_9 - C_{10} - $C11$	119.01(15)	C_{11}-C_{10}-C_{15}	118.5(03)
O_{14}-C_{11}-C_{12}	115.44(15)	C_{10}-C_{11}-C_{12}	120.9 (04)
C_{10} - $C11$ - $C12$	119.96(15)	C_{11} - C_{12} - C_{13}	119.3 (04)
O_{14}-$C11$-C_{10}	124.58(15)	C_{12}-C_{13}-C_{14}	121.6(04)
C_{11}-C_{12}-C_{13}	120.60(16)	C_{13} - C_{14} - C_{15}	119.4 (04)
C_8 - C_{13}-C_{12}	120.44(15)	C_{10}-C_{15}-C_{14}	120.4(04)
C_{11}-O_{14}-C_{15}	118.93(14)		

Table 4: Torsion angles (°)

Compound A	Torsion angles	Compound B	Torsion angles
C_1 - N_2 - N_3-C_4	00.08(18)	C_1- N_2- N_3-C_4	- 00.6(04)
N_3-N_2-C_1-N_5	00.52(18)	N_3-N_2-C_1-N_5	00.3(04)
N_2-N_3-C_4-N_5	−00.65(18)	N_2-N_3-C_4-N_5	00.7(04)
C_1-N_5-N_6-C_7	−168.43(14)	C_1-N_5-N_6-C_7	162.4(03)
C_4-N_5-N_6-C_7	10.6(02)	C_4-N_5-N_6-C_7	−18.0(03)
N_6-N_5-C_1-N_2	178.35(13)	N_6-N_5-C_1-N_2	179.9(03)
C_4-N_5-C_1-N_2	−00.91(18)	C_4-N_5-C_1-N_2	00.1(03)
N_6-N_5-C_4-N_3	−178.19(15)	N_6-N_5-C_4-N_3	179.8(03)
C_1-N_5-C_4-N_3	00.94(17)	C_1-N_5-C_4-N_3	−00.6(03)
N_5-N_6-C_7-C_8	179.83(13)	N_5-N_6-C_7-C_8	176.8(03)
N_6-C_7-C_8-C_9	179.19(15)	N_6-C_7-C_8-C_9	−178.9(03)
N_6-C_7-C_8-C_{13}	−00.21(02)	C_7-C_8-C_9-C_{10}	174.2 (03)
C_7-C_8-C_9-C_{10}	−178.53(14)	C_8-C_9-C_{10}-C_{11}	170.3 (04)
C_{13}-C_8-C_9-C_{10}	00.90(02)	C_8-C_9-C_{10}-C_{15}	−13.2(06)
C_7-C_8-C_{13}-C_{12}	178.93(16)	C_9-C_{10}-C_{11}-C_{12}	175.5(04)
C_9-C_8-C_{13}-C_{12}	−00.51(02)	C_{15}-C_{10}-C_{11}-C_{12}	−01.3(05)
C_8-C_9-C_{10}-C_{11}	−00.52(02)	C_9-C_{10}-C_{15}-C_{14}	−176.9(03)
C_9-C_{10}-C_{11}-O_{14}	178.19(15)	C_{11}-C_{10}-C_{15}-C_{14}	−00.3(05)
C_9-C_{10}-C_{11}-C_{12}	−00.41(02)	C_{10}-C_{11}-C_{12}-C_{13}	01.1(06)
O_{14}-C_{11}-C_{12}-C_{13}	−177.90(17)	C_{11}-C_{12}-C_{13}-C_{14}	00.5(07)
C_{10}-C_{11}-C_{12}-C_{13}	00.81(03)	C_{12}-C_{13}-C_{14}-C_{15}	−01.9(06)
C_{11}-C_{12}-C_{13}-C_8	−00.4(03)	C_{13}-C_{14} - C_{15} - C_{10}	01.8(05)
C_{15}-O_{14}-C_{11}-C_{10}	00.3(02)		
C_{15}-O_{14}-C_{11}-C_{12}	178.92(17)		

In the structure of compound A, consists of six membered methoxyphenyl and a five membered triazole ring connected through the azomethine group. The compounds crystal structure revealed that it is crystallized with a water molecule, its non-planar, and Dihedral angle is 10.36(9)ºbetween its rings. The distance in bond of N6-C7 found 1.271(2) Å, which is similar to the reported schiff base structure which was reported earlier and compareable [17]. In the phenyl ring the methoxy group attached is in the same plane with the torsions angle of 0.3(2)º about C10-C11-O14-C15. the molecules structure shows two types of hydrogen bonding ie intra & inter, of the type O-H...N and C-H...O. By$\pi\cdots\pi$ interactions the structure is stablized[18-20]. Cg(1)--- Cg(2),is the center of the ring (C1/N2/N3/C4/N5) is Cg1 and the rings center (C8/C9/C10/C11/C12/C13) is Cg2, and*Cg1-Cg2* distances is 04.412(2)Aº, α = 10.36(9)°, β =

40.2°, γ = 37.6°, the perpendicular distances is*Cg*1on Cg2 found to be -3.4941(7) Å, the perpendicular distances of *Cg2* on *Cg*1 found to be 3.3691[7] A, the symetry code and a symmetry codes -x,1-y,-z. Packing diagram was taken along c axis represented in Fig 4. The bridging of molecules through C-H-O hydrogen bond interactions forms $R_2^2(8)$ ring motif [21-22] and the supra-molecular architecture exhibited by the O—H...N interactions of water molecule involved in the crystals structure is shown in **Fig. 5**.

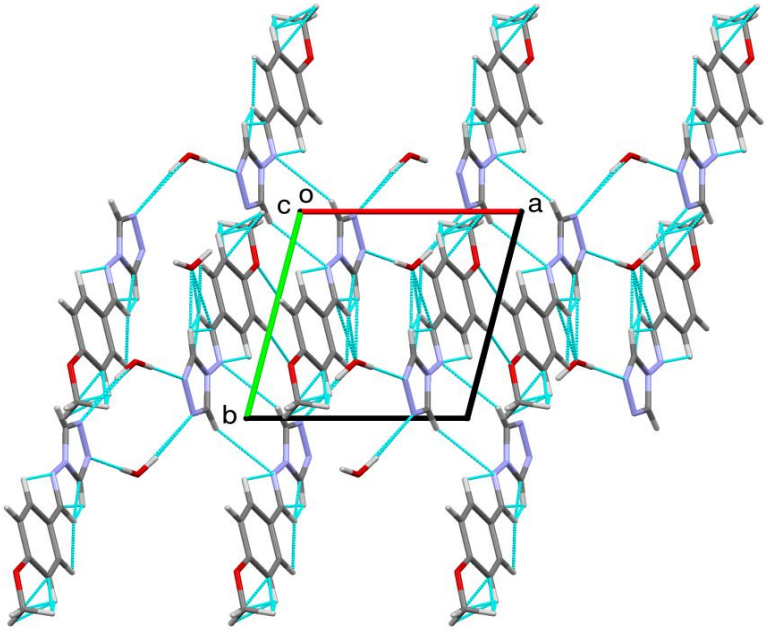


Figure 4: Packing diagramalong c axis of compound A

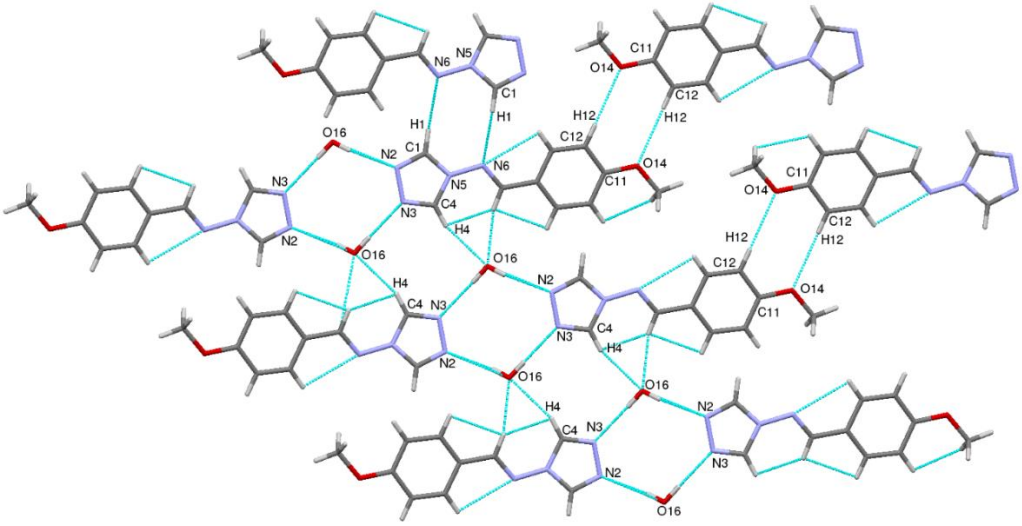


Figure 5: The R_2^2 [8] ringsformed by intermolecular C-H--O and hydrogen bond interactions and the supra-molecular architecture exhibited by the O—H···N interactions

In structure of compound B, it has a 5member membered triazole group and a phenyl group which is six memberedwhich is connected by the carbon chain-azomethine group. The compound B crystal structure found to be orthorhombic with space group $P2_12_12_1$. The molecule is found to be non-planar,and its dihedral angle is 33.9(2)^0 between two rings. The bond distance of azomethine N6-C7 bond is 1.273(5) Å. The compound B has intermolecular hydrogen bonds due to which the structure is stabilised and its in the form C-H--N, it also shows interaction of the typeπ--πandC—H···π ; C14—H14···*Cg*(2), centriod of the (C10/C11/C12/C13/C14/C15) ring is Cg(2) with a distance 03.510(6)A^o of C-Cg, 2.82 Å of H--Cg distance, angle of C-H--Cgangle of 132^o with *-1/2 +x, -1/2-y, -1-z*symmetry code. The packing diagram is represented in **Fig.6**. The molecules which form bridgeing forms supra molecular self

assemblies through hydrogen bond C-H--N[23] is represented in the**Fig7**. Compound A and B 's hydrogen bond are given in **Table 5**.

Table 5: Hydrogen bond interaction prameters [A^{o},^{o}]

D-H--A	D-H	H-A	D-A	D-H-A
O(16)–H(16B)...N(3)*	0.85	02.05	02.893(2)	176
O(16)–H(16A)...N(2)^{i}	0.85	02.19	03.016(2)	166
C(4)-H(4)..O(16)^{ii}	0.93	02.38	03.279(2)	162
C(7)–H(7)..O(16)^{ii}	0.93	02.34	03.220(2)	157
C(12)–H(12)...O(14)^{iii}	0.93	02.59	03.507(3)	171

*Intra; I: 1-x, -y, 1-z; II: 1-x, 1-y, 1-z; III: -x, 1-y, -1-z.

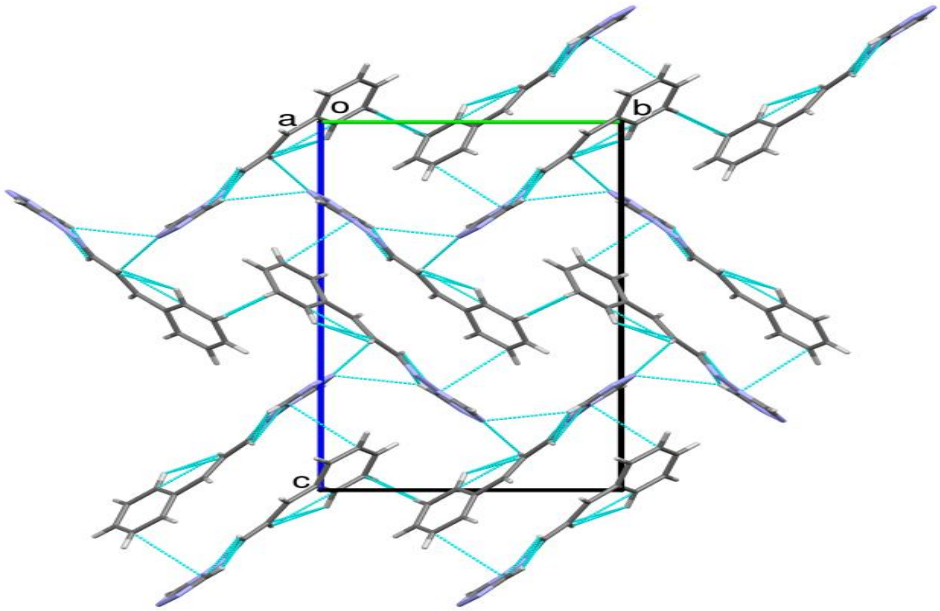


Figure 6: Packing diagram along a-axis

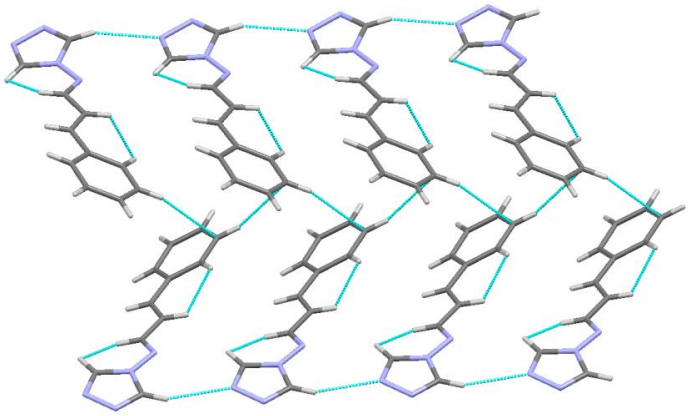


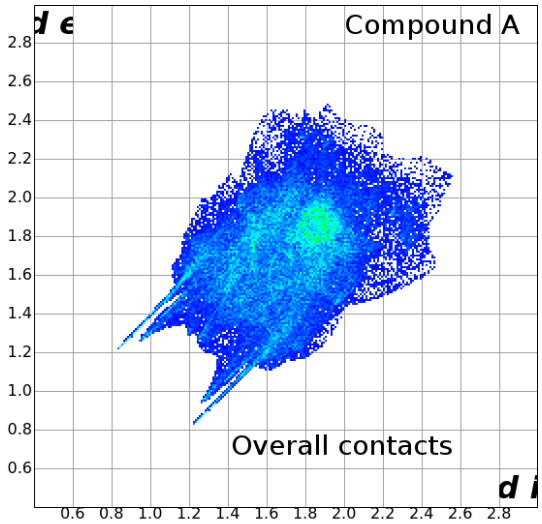
Figure 7: Supra-molecular self assemblies exhibited by the C—H···N interactions

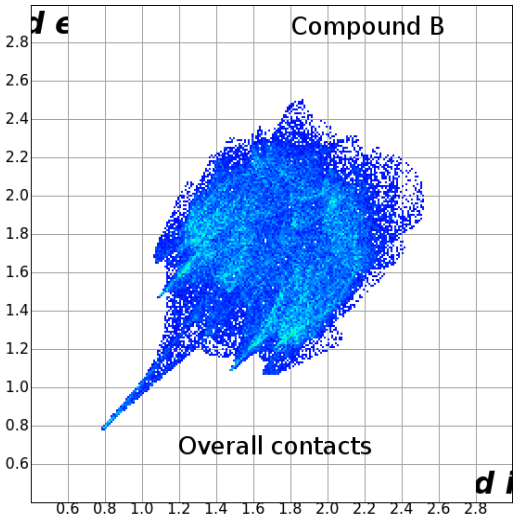
Hirshfeld Surfaces Study

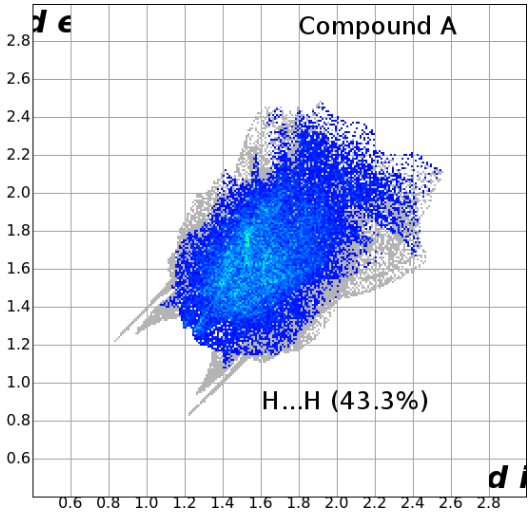
Calculation and analysis of crystallographic information and Hirshfelds surfaces study was was done by crystal explorer software [16]. The d_{norm} plots for compound Amapping with colours scale-00.446au(Blue) ---01.153au(Red) and for compound B -0.560au(blue) to1.320au(red), respectively. In the range of 0.6-2.8A^{0}, 2D fingerprint plots [24-26] were displayed, *di* and *deare the* distance scales.

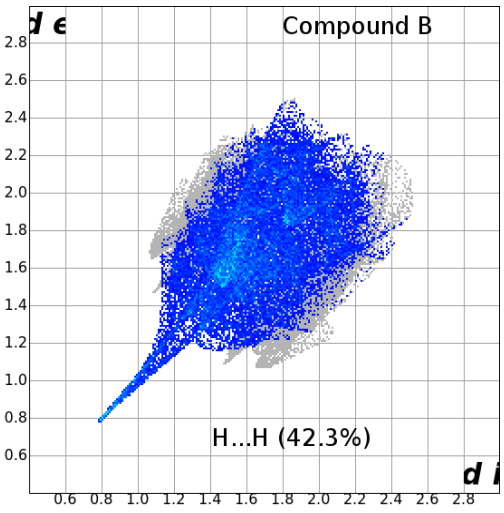
The fingerprint plots analysis helps to find the % contribution of intermoleculars individual contactsTo molecular total surfaces. In fingerprints regions plots, colour codes indicated the intercontacts frequency of occurrence, zero occurance represented by white color, minute or little apperance by blue colour, red & green represents more occurances of any data for (di, de)pairs[17]. In Compound-A, the H--H (43.3%), N···H (19.4%), O--H (13.6%) and C--H (13.2%) contacts has contributes to the total molecular surface. Whereas, in compound B, H···H (42.3%), C···H (30.2%) and N-H(24.8%) contributes forsurfaces

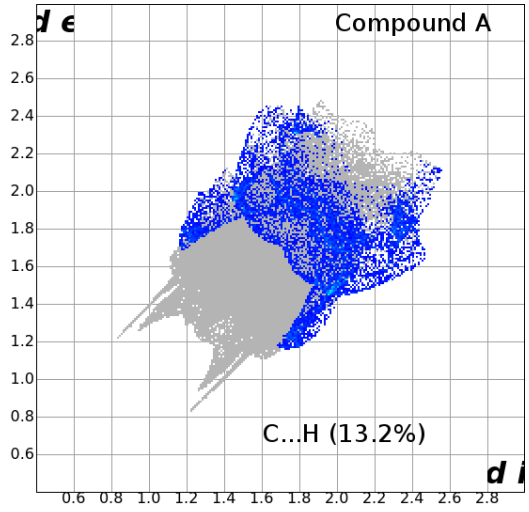
total areas represented in **Fig 8**. By using shape index and conventional mapping of d_{nor}, the molecular surfaces close contact are highlighted repreented in the **Fig. 9**. On theMolecular Hirshfeld surface the inter-molecular contacts were determined by their colour codes at different regions, the short contact is indicated by red colour, longer contact by blue colour and contacts around the vdW radi by white colour. The concave region of red colour represents π-stackings interaction, The convex region of blue colour represents the molecules ring atoms shape index in hirshfelds [28-29].

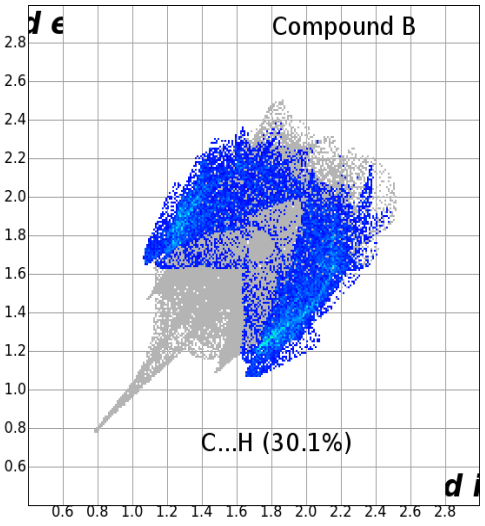












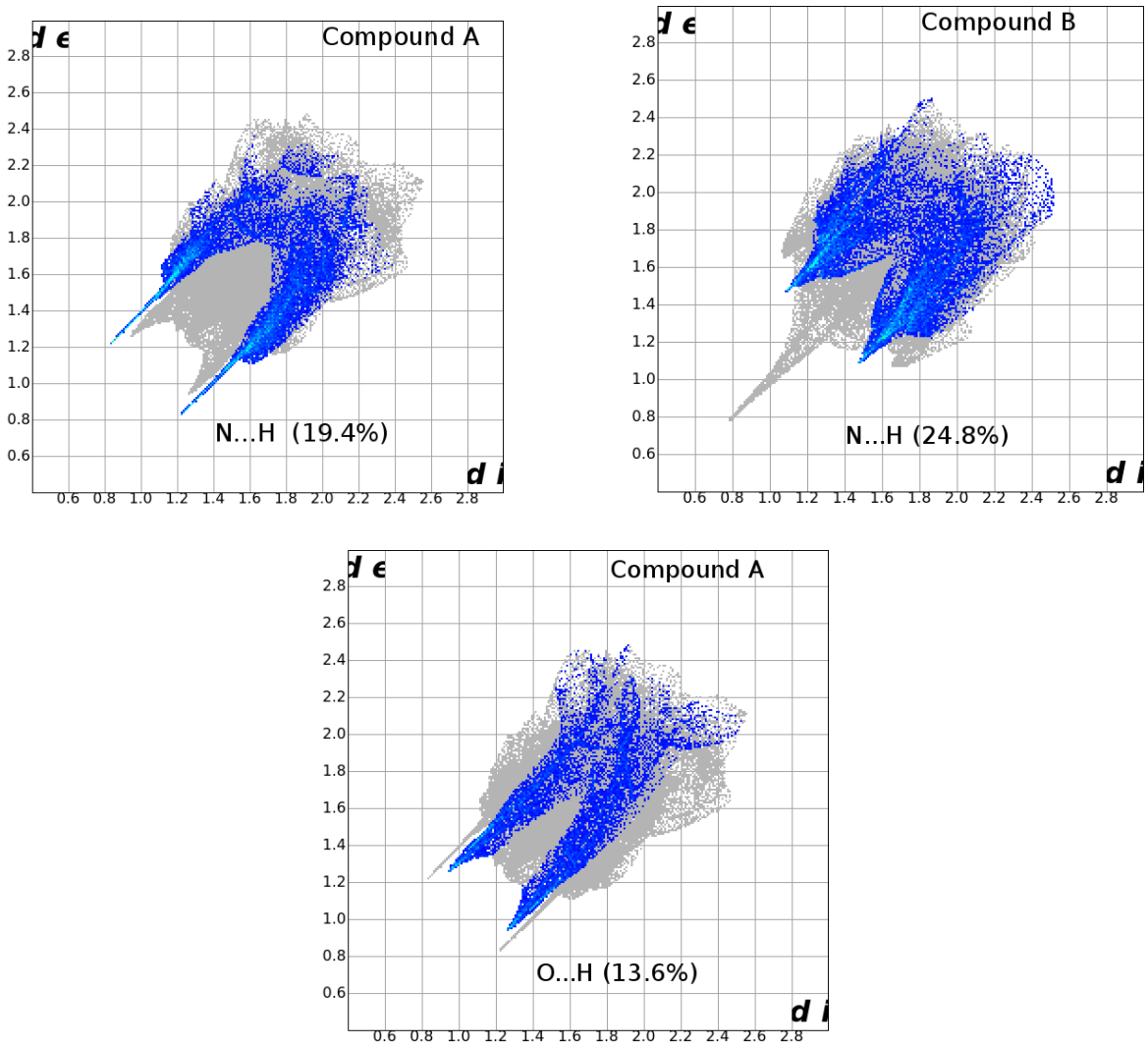
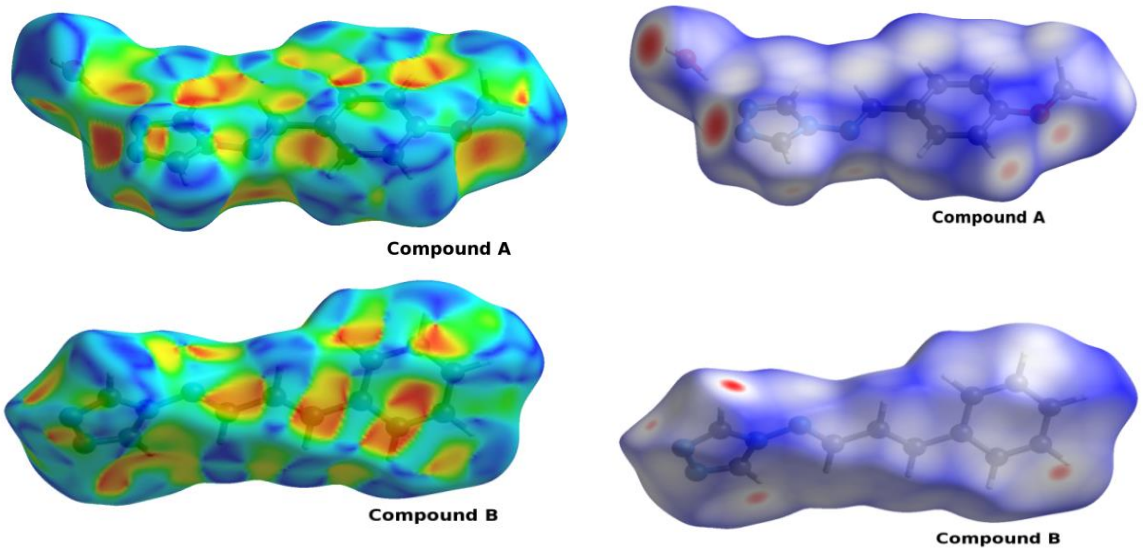


Figure 8: Compund A and B's Finger print plots representing each interactions showing the individual contribution



[A] **[B]**

Figure 9: d_{norm}[A] & shape index [B] of compound A &B moleculars contact on Hirshfeld surface mapped

CONCLUSIONS

A novel schiff base derivaties of compound A was synthesised and characterized and compared with compound B. The structure was confirmed by XRD technique which revealed that the compound A crystal is Triclinic in structure and space group P1, whereas compound B is orthorhombic with space group $P2_12_12_1$. Compound A is non-planar,dihedrals angle between 2 rings is $10.36(9)^0$, whereas compound B is non-planar, dihedrals angle $33.9(2)^0$. The bond distance of azomethine N6-C7 of compound A is 1.271(2) Å, whereas in compound B is 1.273(5)Å,which confirms the compound of the type Schiff base. Compound A structure exhibits hydrogen bondinginter & intra, C-H--O & O-H--N, by$\pi\cdots\pi$ interactions the structure is stabilised, in compound B intermolecular hydrogen bonds stabilises the structure C-H--N, it also shows π--π and C-H--πinteractions.

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