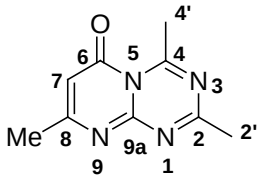
Table III Crystallographic data and refinement parameter for **6a**, **4i** and **14**



	6a[15a]	**4i**	**14**
Empirical formula	C8 H9 N5 O	C_{10} H_{13} N_5 O.3H_2O	C_{14} H_{20} N_6 O
Formula weight	191.20	273.30	288.36
Temperature, K	100(2)	223(2)	100(2)
λ, Å	0.71073	0.71073	0.71073
Crystal system	Orthorhombic	Monoclinic	Orthorhombic
Space group	Pna2(1)	P2(1)/c	Pna2(1)
Unit cell dimensions	a = 11.1369(19) Å; α = 90° b = 18.913(3) Å; β = 90°;c = 4.0311(7) Å; γ = 90°	a = 9.1448(13) Å; α = 90° b = 6.7638(10) Å; β = 94.610(3)°; c = 22.369(3) Å; γ = 90°	a = 7.4179(9) Å; α= 90° b = 11.2238(15) Å; β= 90° c = 17.288(2) Å; γ = 90°
Volume, $Å^3$	849.1(3)	1379.2(3)	1439.4(3)
Z	4	4	4
$Density_{calculated}$, mg/m^3	1.496	1.316	1.331
μ, mm^{-1}	0.107	0.103	0.090
Crystal size, mm^3	0.60 x 0.08 x 0.06	0.58 x 0.36 x 0.16	0.34 x 0.30 x 0.12
Theta range for data collection	2.15 to 27.49°	2.23 to 27.50°	2.16 to 27.48°
Index ranges	-13<=h<=14, -24<=k<=22, -5<=l<=4	-11<=h<=8, -8<=k<=8, -29<=l<=28	-7<=h<=9, -14<=k<=14, -22<=l<=18
Independent reflections	5774	9324	2799 [R(int) = 0.0389]
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	1825 / 1 / 137	3155 / 0 / 200	2799 / 1 / 196
Goodness-of-fit on F^2	1.134	1.079	1.061

Final R indices [$I>2\sigma(I)$]	R1 = 0.0565, wR2 = 0.1148	R1 = 0.0530, wR2 = 0.1473	R1 = 0.0478, wR2 = 0.118
R indices (all data)	R1 = 0.0657, wR2 = 0.1185	R1 = 0.0611, wR2 = 0.1559	R1 = 0.0519, wR2 = 0.1193
Bond distance, Å			
N1-C2	1.324	1.329	1.340(3)
C2-N2’	1.492	1.331	1.344(3)
C2-N3	1.344	1.377	1.354(3)
N3-C4	**1.321**	**1.289**	**1.315(3)**
C4-4’	1.311	1.492	1.410(3)
C4-N5	**1.419**	**1.409**	**1.438(2)**
N5-C6	**1.448**	**1.458**	**1.449(3)**
C6-C7	1.418	1.412	1.426(3)
C7-C8	1.362	1.361	1.359(3)
C8-N9	1.357	1.362	1.363(3)
N9-C9a	1.314	1.317	1.323(3)
N5-C9a	1.410	1.415	1.414(3)
Involvement of amino group (directly attached to the ring) in π-electron delocalization with the pyrimido[1,2-*a*][1,3,5]triazine nucleus	evident as N3C4N5N4’ bond lengths are equal	evident as N1C2N3N2’ bond lengths are equal	evident as N1C2N3N2’ bond lengths are equal
Key features	refer reference 15a	1) Water forms a complex intermolecular hydrogen bonding network with the carbonyl oxygen of one molecule and pyrimidine ring nitrogen of another molecule. 2) Strong inverse aromatic π-π stacking between triazine rings with interplanar distance of 3.357 Å.	1) NMe2 group of position 4 side chain of the molecules are stacked along the a axis making π- π interactions [N⊙⊙⊙N distance 3.732 (2)Å] 2) The methyl groups of the two dimethylamino fragments are involved in the formation of weak intermolecular C-H⊙⊙⊙O hydrogen bonds with the lone pairs of carbonyl group of the heterocyclic system

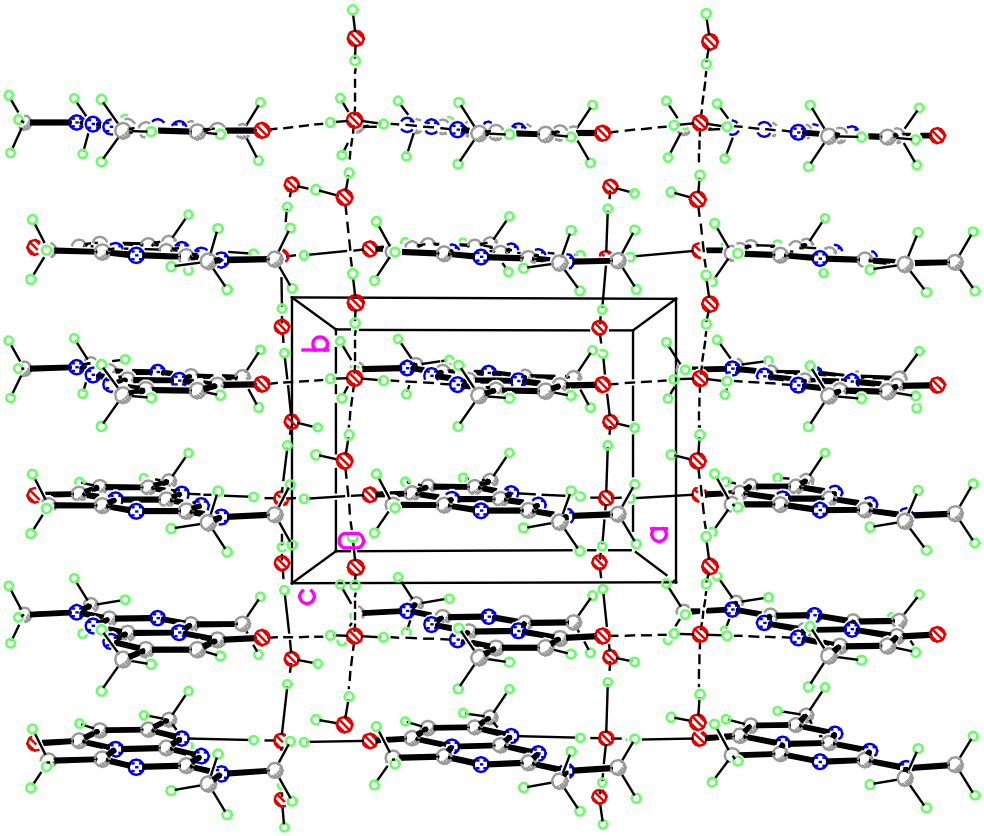


Fig 5 Molecular packing along c axis showing water channel in **4i**.

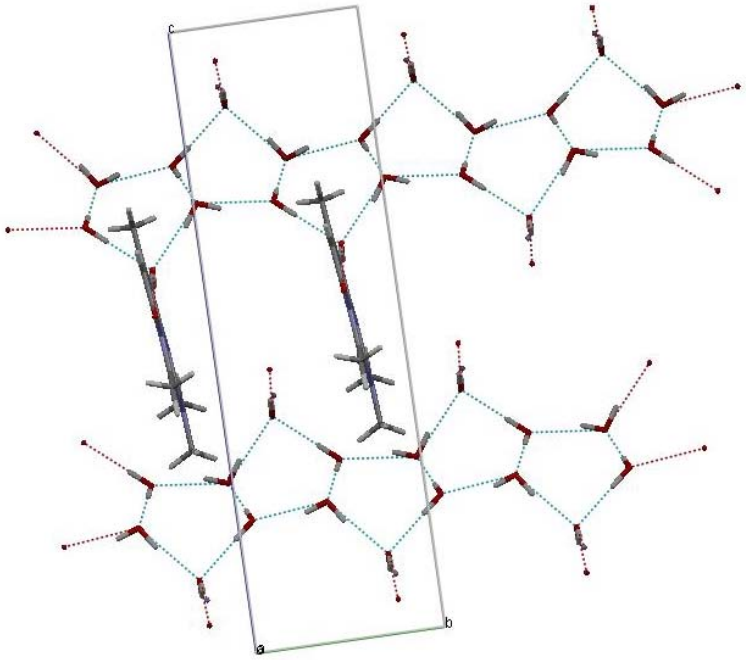


Fig 6 Closer look of water channel in **4i** shows cyclic pentamer connected to form tape like water cluster which propagates infinitely along b axis.