Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information

Propeller-shaped molecules with thiazole hub: structural landscape and hydrazone cap mediated tunable host behavior in 4-hydrazino-1,3-thiazoles

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Table S. Geometrical parameters of H-bonds and angles (D=donor atom; A= acceptor atom)[a]

Compound	D–H···A	D–H/ Å	H···A)/Å	D···A/ Å	D–H···A/ deg
IPHAT 1	N(3)-H(3)...O(1)	1.002(10)	1.85(2)	2.625(4)	131(2)
	N(2)-H(2)...O(1')	1.003(10)	1.895(15)	2.869(4)	163(3)
	O(1')-H(1')...N(4)#1	0.950(10)	2.01(2)	2.892(4)	154(4)
	O(1')-H(1'')...O(1')#1	0.954(10)	1.922(16)	2.864(4)	169(6)
IPHAT 2	N(1)-H(1)...O(2) #2	0.82(3)	2.06(3)	2.867(3)	166(3)
	N(3)-H(3)...O(1)	0.85(3)	1.91(3)	2.606(3)	139(2)
	O(2)-H(2A)...O(2)	0.89(3)	1.963(3)	2.847(3)	171(3)
	O(2)-H(2B)...N(4)	0.79(4)	2.10(4)	2.882(3)	171(4)
BzHAT.MeOH	N(2)-H(2A)...O(1')#3	0.86	1.95	2.811(2)	174
	N(3)-H(3A)...O(1)	0.86	2.09	2.7060(18)	128
	O(1')-H(1')...O(1)	0.82	1.90	2.719(2)	176
BzHAT.EtOH	O(2)-H(2)...O(1)#4	0.82	1.99	2.739(2)	150
	N(1)-H(1)...O(2)#5	0.86	1.91	2.767(2)	178
	N(3)-H(3)...O(1)	0.86	2.08	2.713(2)	129
CyHAT	N(12)-H(12)...N(23))#6	0.86	2.17	3.001	160
	N(22)-H(22)...N(13)#7	0.86	2.10	2.945	164
	N(14)-H(14)...O(16)	0.86	2.07	2.678	127

[a] Symmetry codes : (#1) -x+1, y-1/2, -z+1/2; (#2) -x+1, y+1/2, -z+3/2; (#3) -x+3/2, y+1/2, -z+1/2; (#4) -x, -y, -z+1; (#5) x+1/2, -y+1/2, z-1/2; (#6) x, y-1, z;(#7) x, 1+y, z.

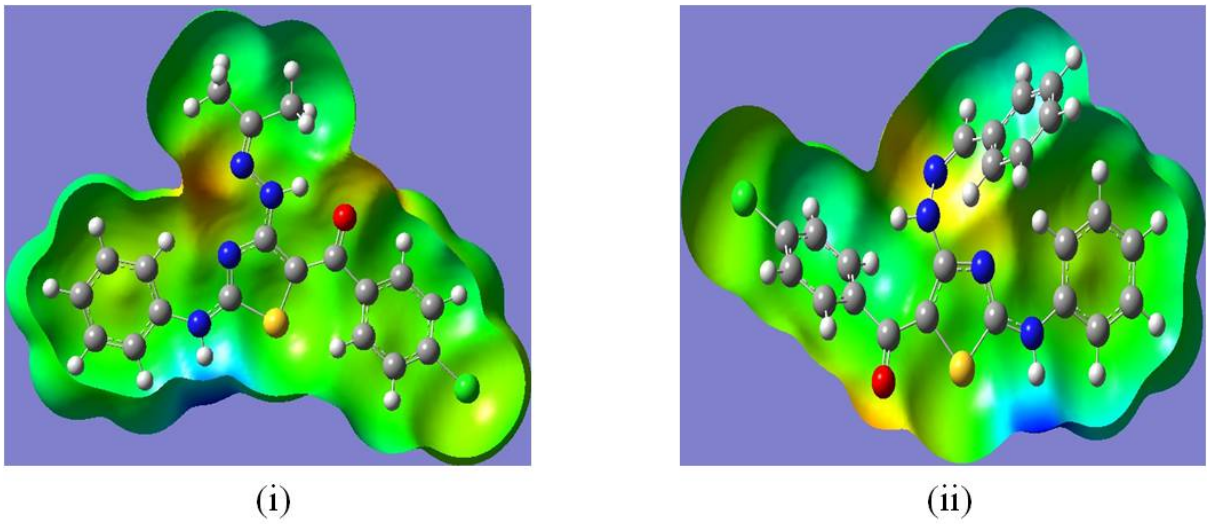

Fig.S1 Optimized geometries of (i) IPHAT 2 and (ii) BzHAT. Electron density map is given. Calculations were done with 6-31G basis set, Gaussian 09 program.

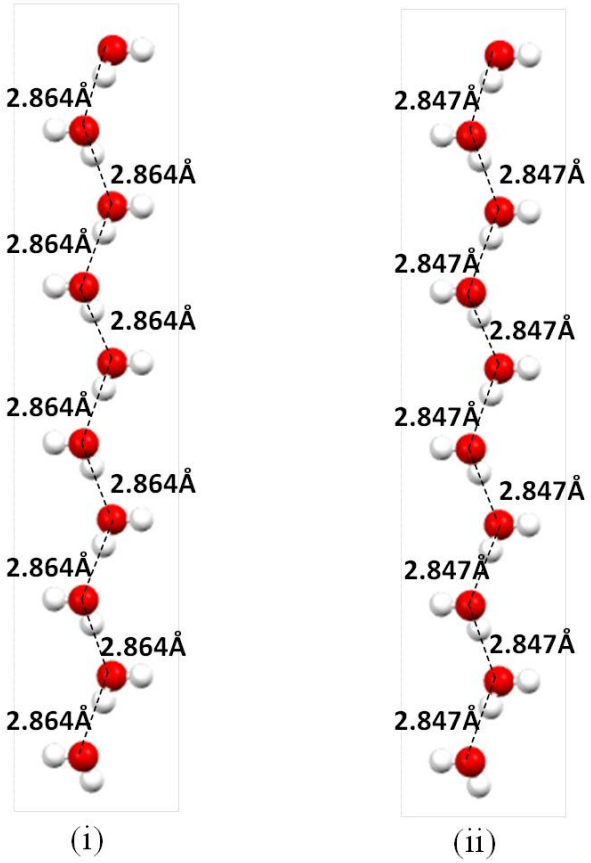

Fig. S2 Distance between adjacent water molecules comparable to aquaporin in the 1D water chain of (i) IPHAT 1 and (ii) IPHAT 2. Molecules are viewed along *a* axis.

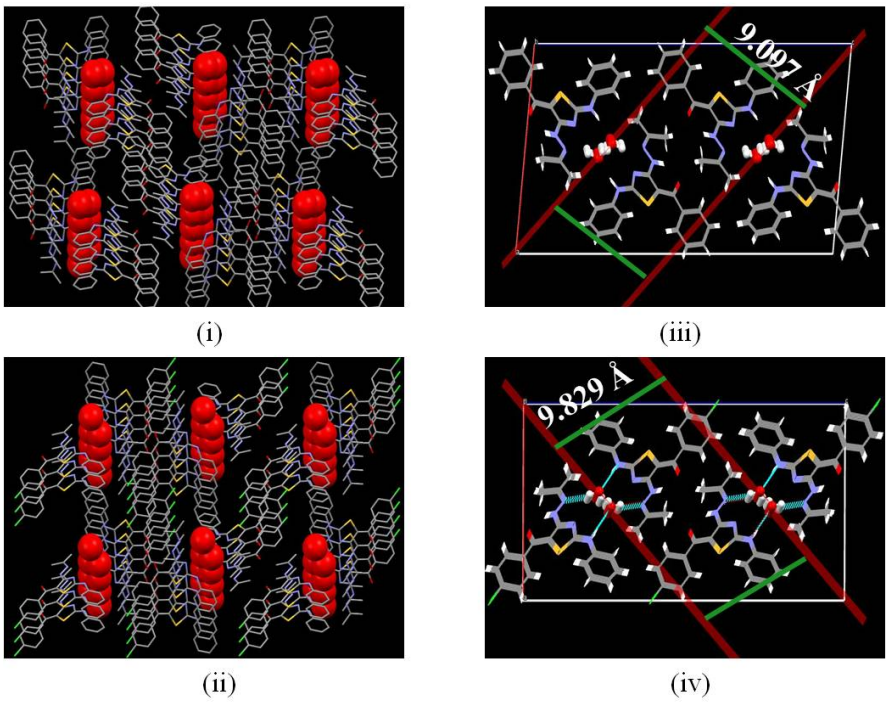

Fig. S3 View of superstructures formed by (i) IPHAT 1 and (ii) IPHAT 2 in the *ac* plane. Water molecules are in CPK representation. View of the two parallel water planes in the unit cell of (iii) IPHAT 1 and (iv) IPHAT 2 perpendicular to *ac* plane. Distances between the water planes are marked. Water molecules are shown in ball and stick representation.

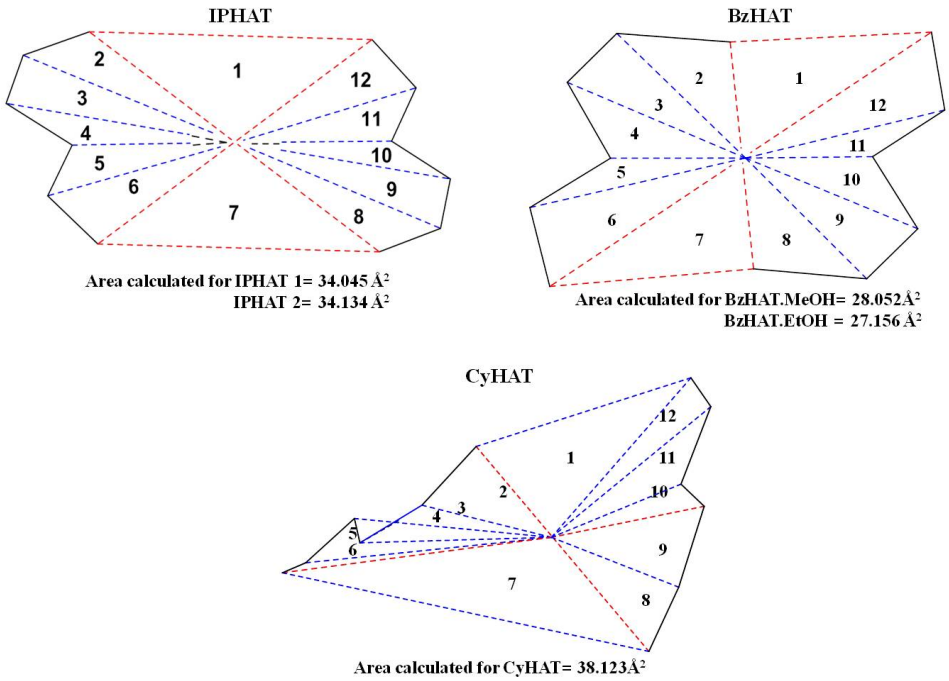

Fig. S4 N-rich cannel area enclosing water molecules. Area of triangles was calculated using Heron's formula[1] ($\Delta = \sqrt{s(s-a)(s-b)(s-c)}$ where $s = \frac{a+b+c}{2}$)

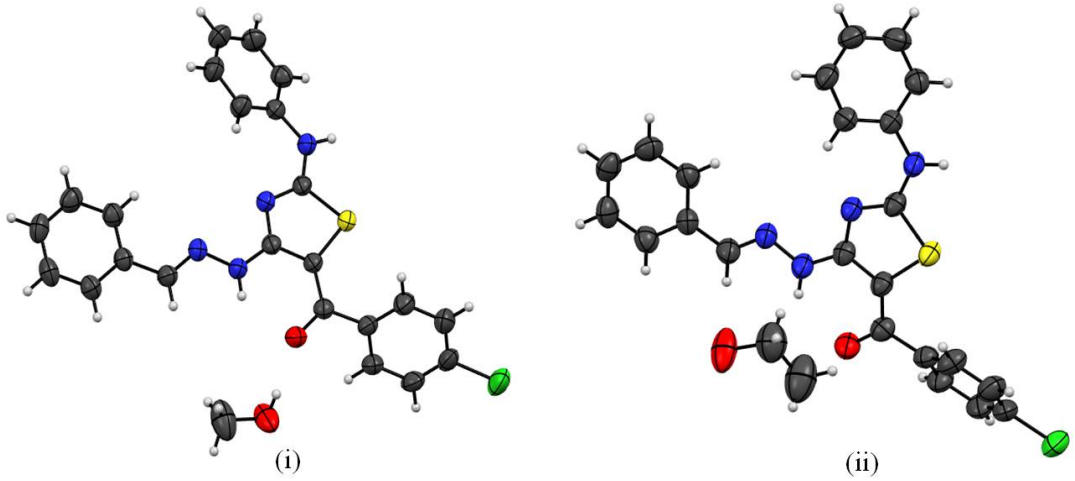

Fig. S5 ORTEP views of molecular structures of (i) BzHAT-1.MeOH and (ii) BzHT-1.EtOH with 50% probability level.

References

1 Dunham, W., *Journey through genius*. ed.; Wiley: 1990.