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Supporting information for article:

A comparison of three crystalline forms of miconazole: solvent-free, ethanol monosolvate and hemihydrate

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Table S1 Geometric parameters [Å, °] of aromatic π-π interactions.

Structure	Interaction	*Cg*(I)···*Cg*(J)	α	*Cg*(I)$_{perp}$	*Cg*(J)$_{perp}$	Slippage
MIC	*Cg*(1)···*Cg*(1)^{iii}	3.663(2)	0.0(3)	3.311(2)	3.311(2)	1.566
	Cg(2)···*Cg*(3)^{iv}	3.826(2)	6.2(2)	3.580(1)	3.491(1)	1.565
	Cg(2)···*Cg*(3)^{v}	3.934(2)	6.2(2)	3.601(1)	3.686(1)	1.373
MIC-EtOH	*Cg*(2)···*Cg*(2)^{ii}	4.098(1)	0.0(1)	3.606(1)	3.606(1)	1.947
	Cg(3)···*Cg*(3)^{iii}	3.847(1)	0.0(1)	3.474(1)	3.474(1)	1.653
	Cg(3)···*Cg*(3)^{iv}	4.460(1)	0.0(1)	3.638(1)	3.638(1)	2.581
MIC-0.5H$_2$O	*Cg*(3)···*Cg*(6)^{iv}	3.946(2)	6.0(1)	3.704(1)	3.739(1)	1.262
	Cg(3)···*Cg*(6)^{v}	4.136(2)	6.0(1)	3.655(1)	3.706(1)	1.835

Symmetry codes: MIC (iii) –*x*+2, -*y*, −*z*+1; (iv) *x*, −*y*+1/2, *z*+1/2; (v) *x*+1, −*y*+1/2, *z*+1/2; MIC-EtOH (i) *x*+1, *y*, *z*; (ii) −*x*+1, −*y*, −*z*; (iii) −*x*+2, −*y*+1, −*z*+1; (iv) –*x*+1, −*y*+1, −*z*+1; MIC-0.5H$_2$O (iv) *x*−1, *y*, *z*; (v) *x*−2, *y*, *z*.

Cg(I)···*Cg*(J) – distance between ring centroids; α - dihedral angle between planes I and J; *Cg*(I)$_{perp}$ and *Cg*(J)$_{perp}$ - (interplanar spacing) perpendicular distance of *Cg*(I) on ring J and *Cg*(J) on ring I, respectively; slippage - distance between *Cg*(I) and perpendicular projection of *Cg*(J) on ring I.

Cg(1) and *Cg*(4) (in molecule B) – a centre-of-gravity of imidazole ring; *Cg*(2) and *Cg*(5) (in molecule B) – a centre-of-gravity of the phenyl ring (C6-C11); Cg(3) and *Cg*(6) (in molecule B) - a centre-of-gravity of the phenyl ring (C13-C18).

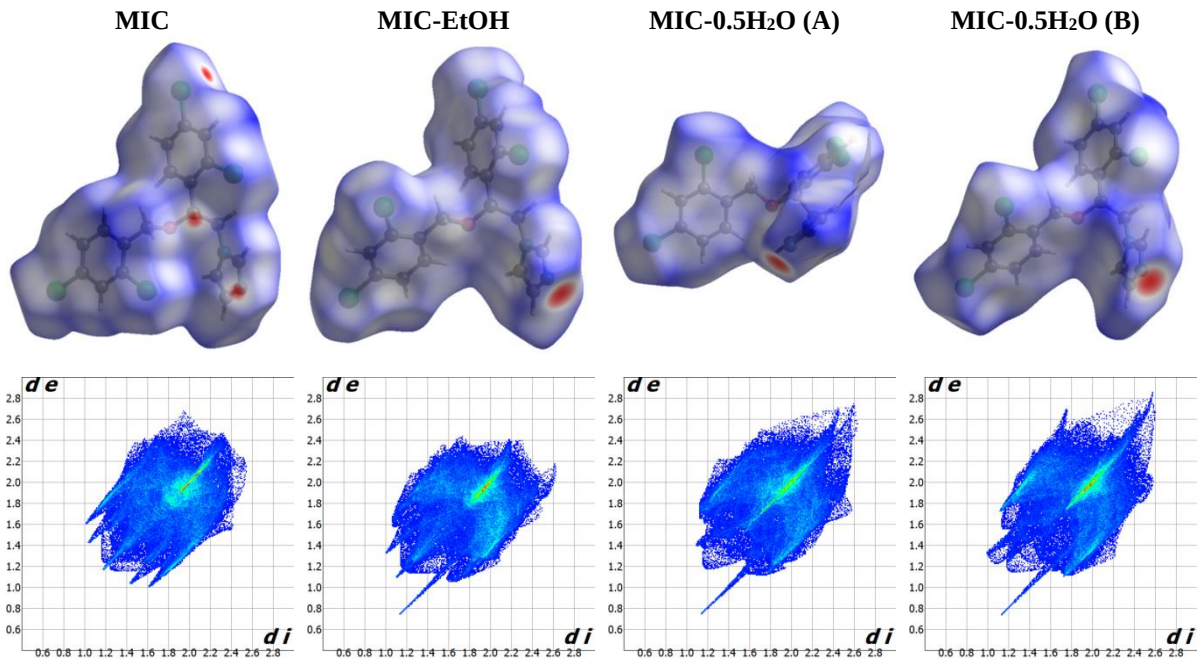
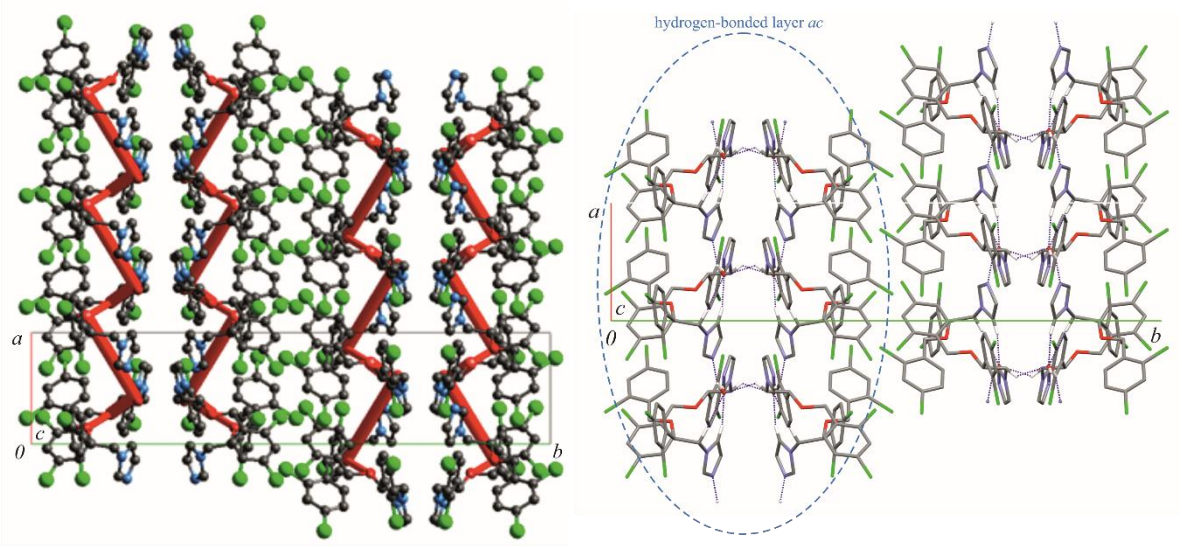
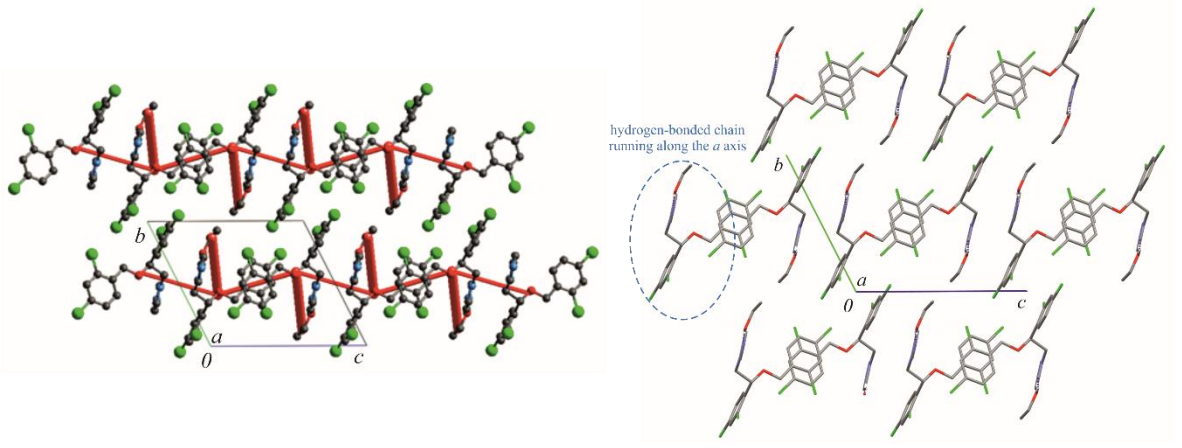


Figure S1 Hirshfeld surface with d_{norm} mapped on it and the corresponding fingerprint plot for three forms of miconazole (MIC, MIC-EtOH, MIC-0.5H_2O).



a *b*

Figure S2 Diagram of the electrostatic energy (red) (*a*) and hydrogen-bonded layer-motifs (*b*) for MIC-0.5H_2O (viewed along the *c* axis). Energy tube scale factor of 80 and an energy threshold of 20 kJ mol^{-1} were used.



a *b*

Figure S3 Diagram of the electrostatic energy (red) (*a*) and hydrogen-bonded chain-motifs (*b*) for MIC-EtOH (viewed along the *a* axis). Energy tube scale factor of 80 and an energy threshold of 20 kJ mol^{-1} were used.

Table S2 Final Cartesian coordinates (X, Y, Z in Å) for the gas-phase structure of miconazole (MIC-opt) optimized at the B3LYP/6-311++G(3df,3pd) level of theory.

Atom	X	Y	Z
Cl	-3.725417	1.231915	1.629867
Cl	-5.349191	-3.471123	-0.408011
Cl	3.206458	1.542905	1.225724
Cl	6.128841	-2.626932	-0.489599
O	0.186382	0.318258	-0.232519
N	-0.576085	3.100067	-1.003718
N	-0.102740	5.216047	-0.522484
C	-1.113541	0.849853	-0.038701
C	-1.355069	1.887196	-1.147482
C	-1.039436	4.301504	-0.546007
C	1.027994	4.587636	-0.985281
C	0.760094	3.281901	-1.288463
C	-2.183702	-0.230973	-0.095852
C	-3.387349	-0.145210	0.605103
C	-4.363093	-1.130692	0.519726
C	-4.134942	-2.229070	-0.294573
C	-2.955302	-2.348455	-1.016572
C	-1.998718	-1.350549	-0.907922
C	0.728876	-0.322541	0.926030
C	2.086505	-0.870249	0.592347
C	3.257094	-0.112844	0.684372
C	4.498936	-0.642539	0.355745
C	4.575393	-1.957816	-0.076399
C	3.437426	-2.745608	-0.178296
C	2.212709	-2.190077	0.158713
H	-1.161770	1.360692	0.926971
H	-1.136342	1.423527	-2.110509
H	-2.407128	2.167716	-1.145510
H	-2.068924	4.440488	-0.256666
H	1.966192	5.108635	-1.074154
H	1.375047	2.479034	-1.650054
H	-5.281514	-1.038905	1.078927
H	-2.790587	-3.206759	-1.651136
H	-1.071588	-1.436271	-1.457881
H	0.074734	-1.141885	1.238884
H	0.787017	0.398833	1.745285
H	5.388382	-0.037219	0.438440
H	3.510873	-3.770422	-0.510445
H	1.321325	-2.800136	0.086794