The Crucial Role of Lattice Water in Directing Supramolecular Networks of Deferiprone Analogues: A Combined X-ray and DFT Study

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Table S1. Crystal data and structure refinement parameters for **3**, **4**, **5** and **6**

Empirical formula	$C_8H_{13}NO_6S$ (**3**·H_2O)	$C_{12}H_{17}N_3O_6$ (**4**·$2H_2O$)	$C_{11}H_{17}N_3O_{3.5}Cl$ (**5**·HCl·$1.5H_2O$)	$C_{22}H_{34}N_6O_8CuCl_2$ (**6**)
Formula Weight	251.25	299.28	282.72	644.99
Temperature (K)	100	100	100	100
Crystal system	Orthorhombic	Triclinic	Monoclinic	Triclinic
Space group	$P2_12_12_1$	P-1	P2/c	P-1
a, b, c (Å)	6.8391(3) 11.2218(5) 13.7253(6)	7.0597(9) 8.8765(11) 11.2263(14)	51.723(3) 7.3982(4) 13.4262(8)	8.1875(5) 8.7569(5) 9.8704(6)
α, β, γ (°)	90 90 90	89.195(4) 88.506(4) 68.574(4)	90 97.29(2) 90	94.856(2) 103.393(2) 103.024(2)
Volume (Å^3)	1053.38(8)	654.65(14)	5096.1(5)	663.69(7)
Z/Density(calc.) (Mg/m^3)	4/1.584	2/1.518	24/1.474	1/1.614
Absorption coeff (mm^{-1})	2.922	1.049	0.310	1.083
F(000)	528.0	316.0	2384.0	335.0
Crystal size (mm^3)	0.49 x 0.22 x 0.17	0.25 x 0.09 x 0.07	0.194 x 0.172x 0.062	0.173 x 0.164 x 0.123
2θ range for data collection (°)	10.182 to 136.57	10.706 to 136.906	4.764 to 56.628	4.286 to 56.63
Limiting indices	$-7 \le h \le 8$, $-13 \le k \le 13$, $-16 \le l \le 16$	$-8 \le h \le 8$, $-10 \le k \le 10$, $-13 \le l \le 13$	$-68 \le h \le 68$, $-9 \le k \le 9$, $-17 \le l \le 17$	$-10 \le h \le 10$, $-11 \le k \le 11$, $-13 \le l \le 113$
Reflections collected	24647	23230	53532	311377
Independent reflections	1890 [R_{int} = 0.0468]	2386 [R_{int} = 0.0565]	6331 [R_{int} = 0.0517]	3289 [R_{int} = 0.0388]
Data/restraints/parameters	1890/0/152	2386/0/199	6331/0/382	3289/0/202
Goodness-of-fit on F^2	1.123	1.137	1.131	1.087
Final R indices [I > 2σ(I)]	R1=0.0271, wR2=0.0677	R1=0.0525, wR2=0.1400	R1=0.0389, wR2=0.1005	R1=0.0222, wR2=0.583
R indices (all data)	R1=0.0271, wR2=0.0677	R1=0.0530, wR2=0.1405	R1=0.0418, wR2=0.1025	R1=0.0222, wR2=0.0584
Largest diff. peak and hole (e.Å^3)	0.32 and -0.32	0.54 and -0.56	0.52 and -0.35	0.34 and -0.54