

ESI

# Structural and biological properties of copper fenamates with diethylnicotinamide: Preparation, structure, spectral properties and Hirshfeld surface analysis

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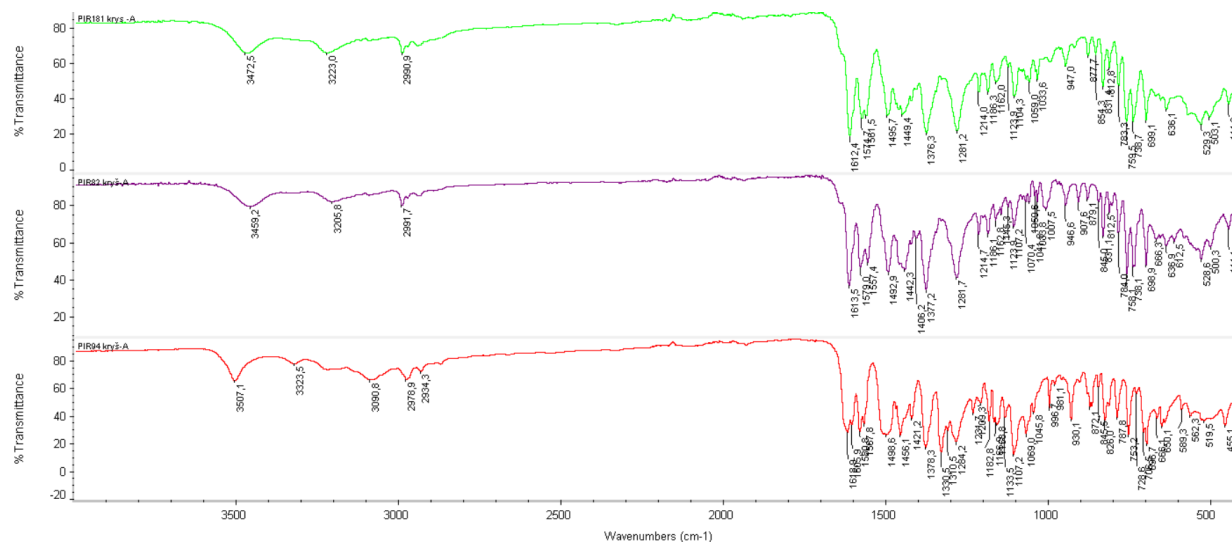
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**Table S1.** Selected hydrogen-bond parameters for 1–5.

<i>D</i> —H... <i>A</i>	<i>D</i> —H (Å)	H... <i>A</i> (Å)	<i>D</i> ... <i>A</i> (Å)	<i>D</i> —H... <i>A</i> (°)
<b>1</b>				
O1—H1WA...O2 <sup>i</sup>	0.90(2)	1.85(2)	2.7289(15)	166(2)
O1—H1WB...O3 <sup>ii</sup>	0.92(3)	1.95(3)	2.8533(16)	168(2)
N3—H3...O2	0.98(2)	1.79(2)	2.6310(16)	142(2)
C14—H14...F2 <sup>iii</sup>	1.05(2)	2.42(2)	3.1950(17)	131(1)
<b>3</b>				
O1—H1WA...O2 <sup>iv</sup>	0.93(1)	1.84(1)	2.7386(8)	161(1)
O1—H1WB...O3 <sup>v</sup>	0.93(1)	1.88(1)	2.7993(8)	167(1)
N3—H3A...O2	1.03(1)	1.80(2)	2.6429(10)	137(1)
N3A—H3AA...O2A	1.02(2)	1.83(5)	2.537(6)	123(4)
<b>5</b>				
O1—H1WA...O2 <sup>iv</sup>	0.95(2)	1.81(2)	2.7282(11)	163(1)
O1—H1WB...O3 <sup>v</sup>	0.96(2)	1.89(2)	2.8279(12)	168(1)
N3—H3A...O2	1.02(2)	1.80(2)	2.6577(19)	139(2)
N3A—H3AA...O2A	1.01(2)	1.78(5)	2.528(6)	133(5)
<b>2</b>				
N3—H3...O2	1.00(1)	1.82(1)	2.6692(11)	141(1)
C3—H3A...O3 <sup>i</sup>	1.07(1)	2.45(1)	3.2141(12)	128(1)
C4—H4...O3 <sup>vi</sup>	1.06(1)	2.66(1)	3.4789(12)	134(1)
C21—H21...O3 <sup>vii</sup>	1.06(1)	2.39(1)	3.4356(17)	170(1)
C23—H23...N4	1.09(1)	2.24(1)	2.9129(14)	118(1)
<b>4</b>				
N3—H3...O2	1.01(2)	1.81(2)	2.6725(15)	142(2)
C3—H3A...O3 <sup>viii</sup>	1.08(2)	2.44(2)	3.1999(18)	126(1)
C4—H4...O3 <sup>ix</sup>	1.09(2)	2.42(2)	3.2810(17)	135(1)
C21—H21...O3 <sup>x</sup>	1.06(2)	2.43(2)	3.4356(18)	158(2)
C23—H23...N4	1.04(2)	2.21(2)	2.8988(19)	122(1)

Symmetry codes: (i) 1-*x*, 1-*y*, 2-*z*; (ii) 1+*x*, +*y*, 1+*z*; (iii) 1+*x*, 1/2-*y*, 1/2+*z*; (iv) 1-*x*, 1-*y*, 1-*z*; (v) +*x*, 1+*y*, +*z*; (vi) 1+*x*, +*y*, +*z*; (vii) 1-*x*, 2-*y*, 1-*z*; (viii) 1-*x*, 1-*y*, -*z*; (ix) -1+*x*, +*y*, +*z*; (x) 1-*x*, -*y*, 1-*z*.

a)



b)

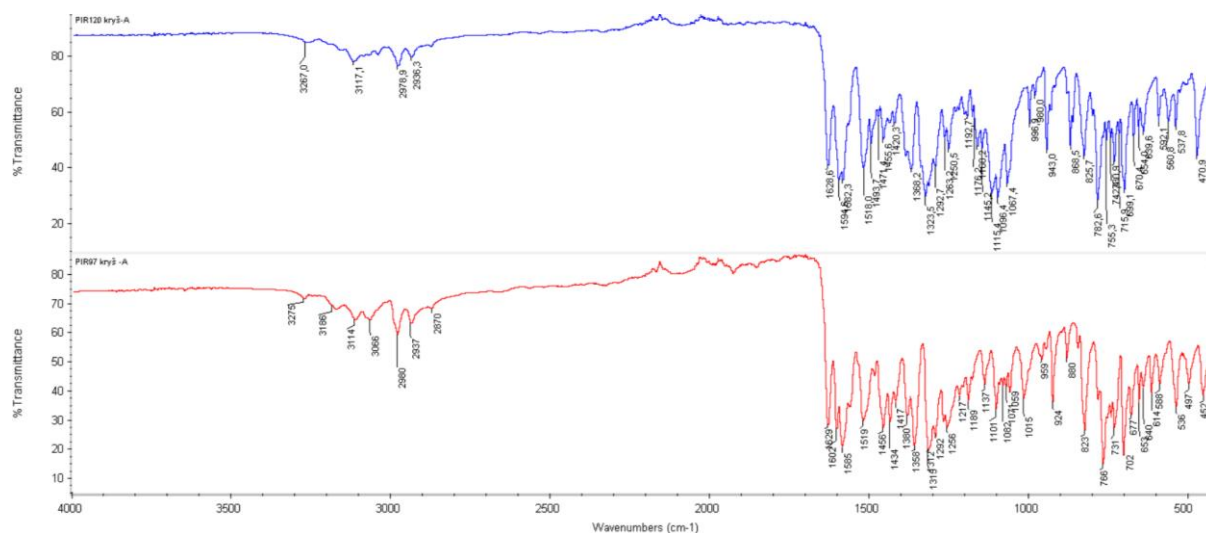


Figure S1. ATR IR spectra of solid samples of a) complexes 1, 3, 5; b) complexes 2 and 4.

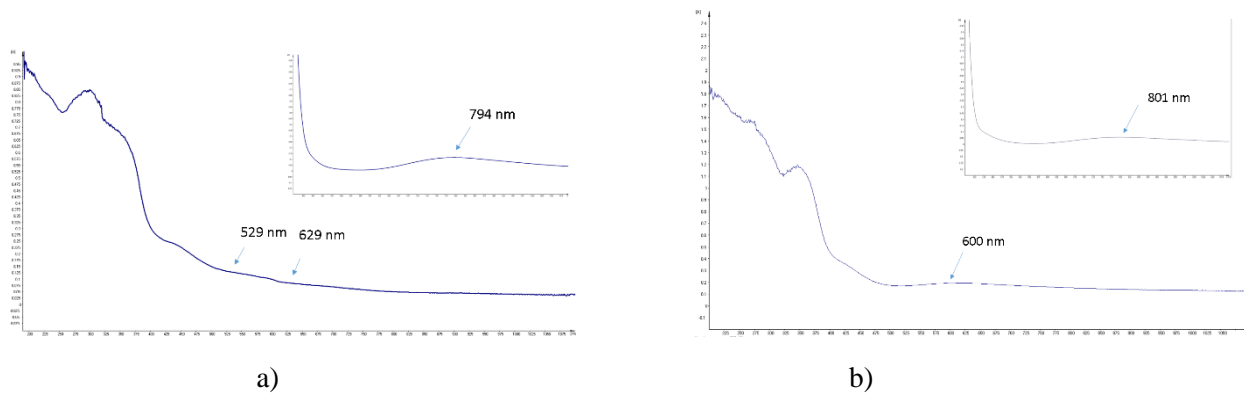


Figure S2. UV-Vis spectrum of nujol mulls of a) 4 and b) 5. Inset: d-d transition of DMSO solutions.

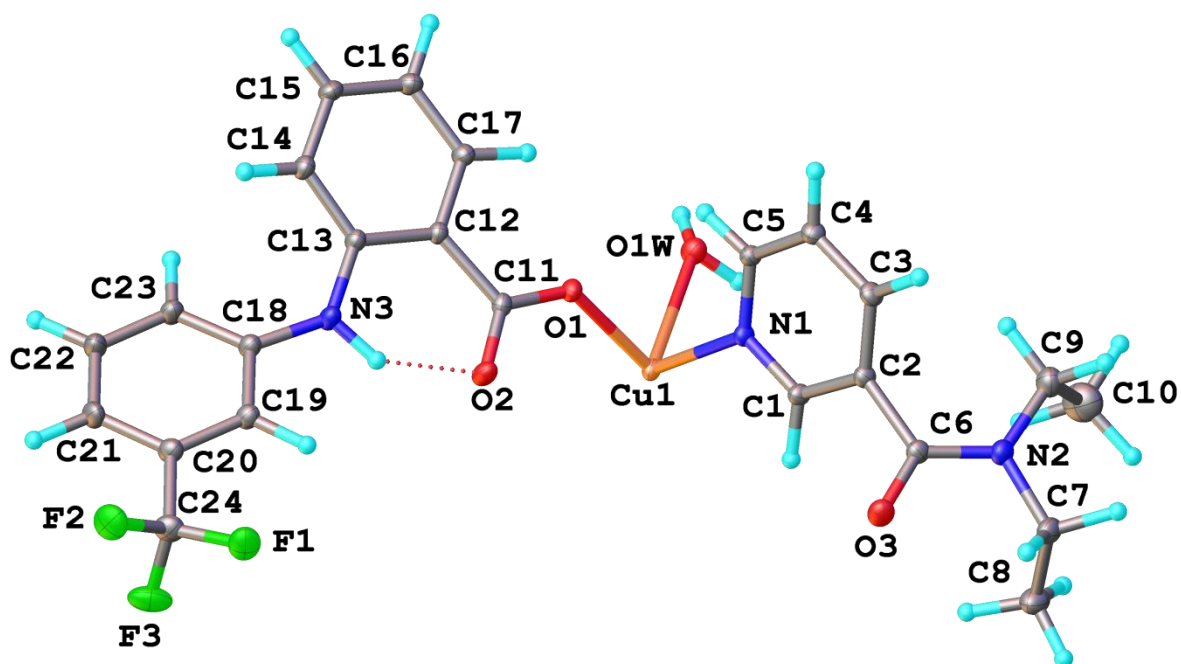


Figure S3. ORTEP-like representation of the asymmetric part of the crystal structure of complex 1.

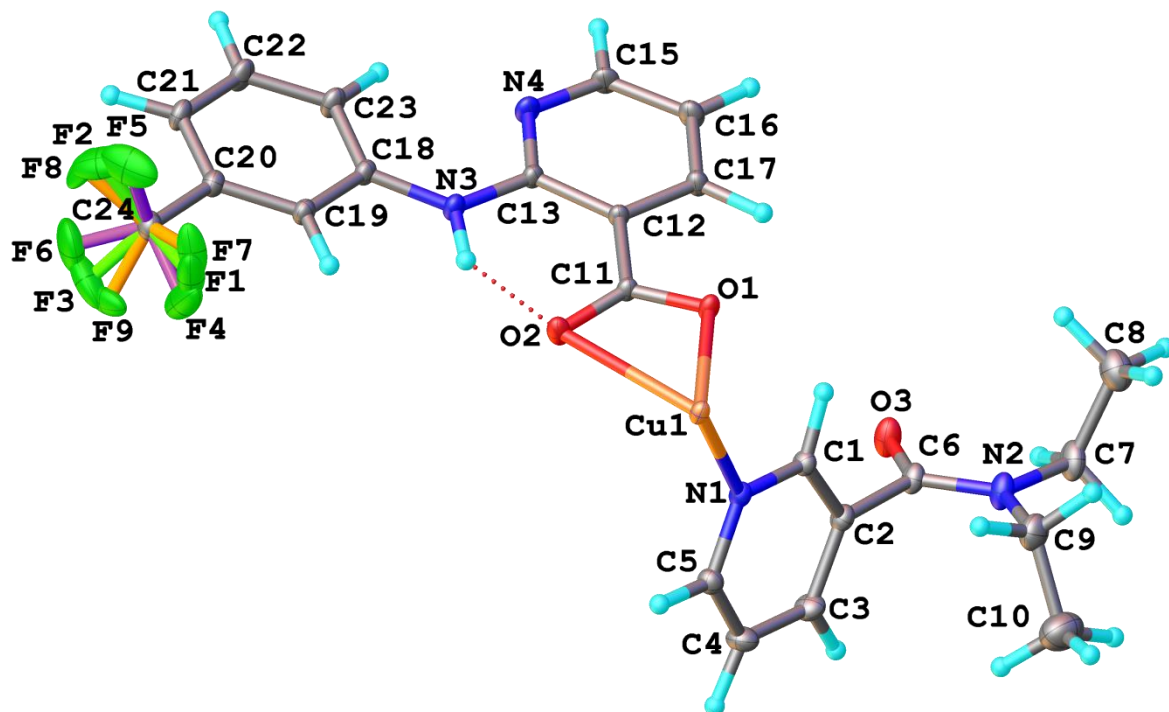
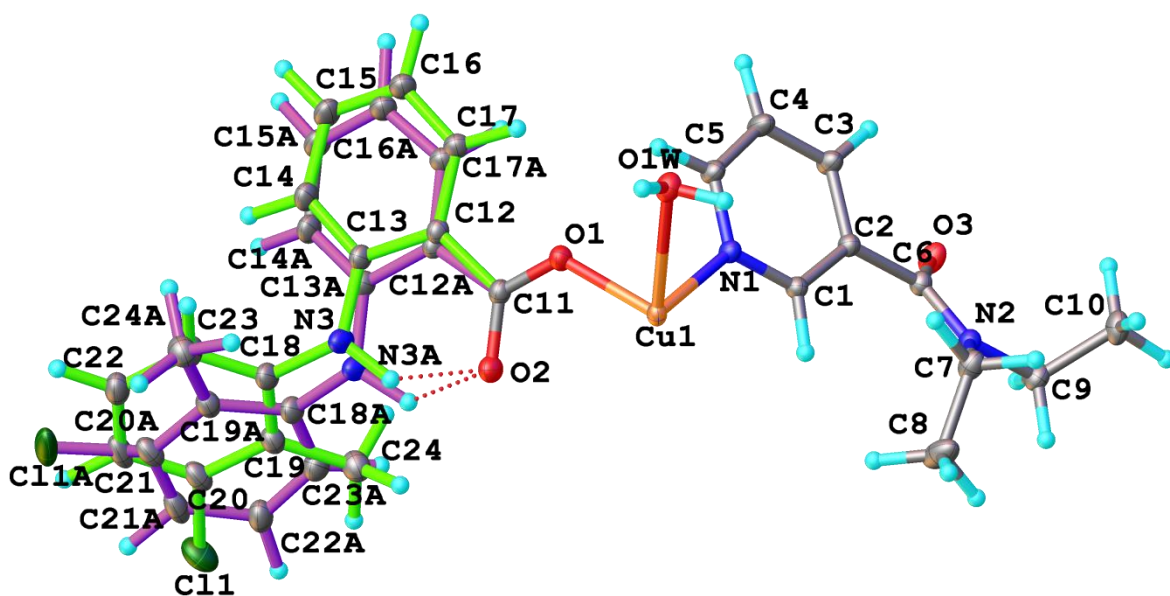


Figure S4. ORTEP-like representation of the asymmetric part of the crystal structure of 2.



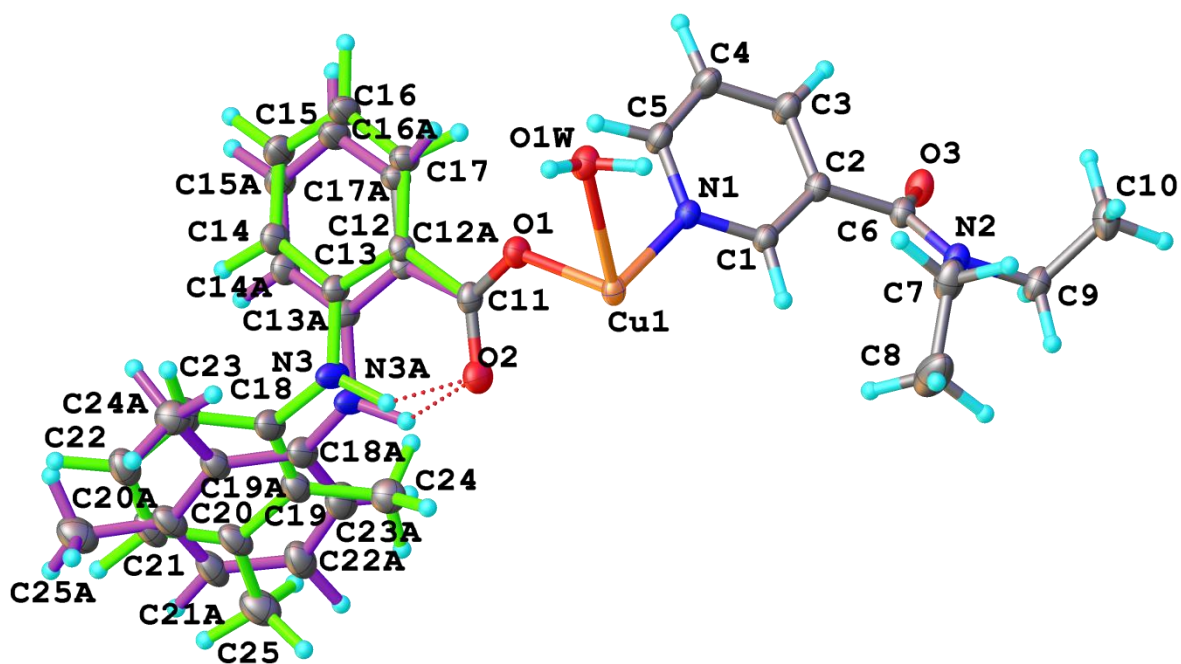
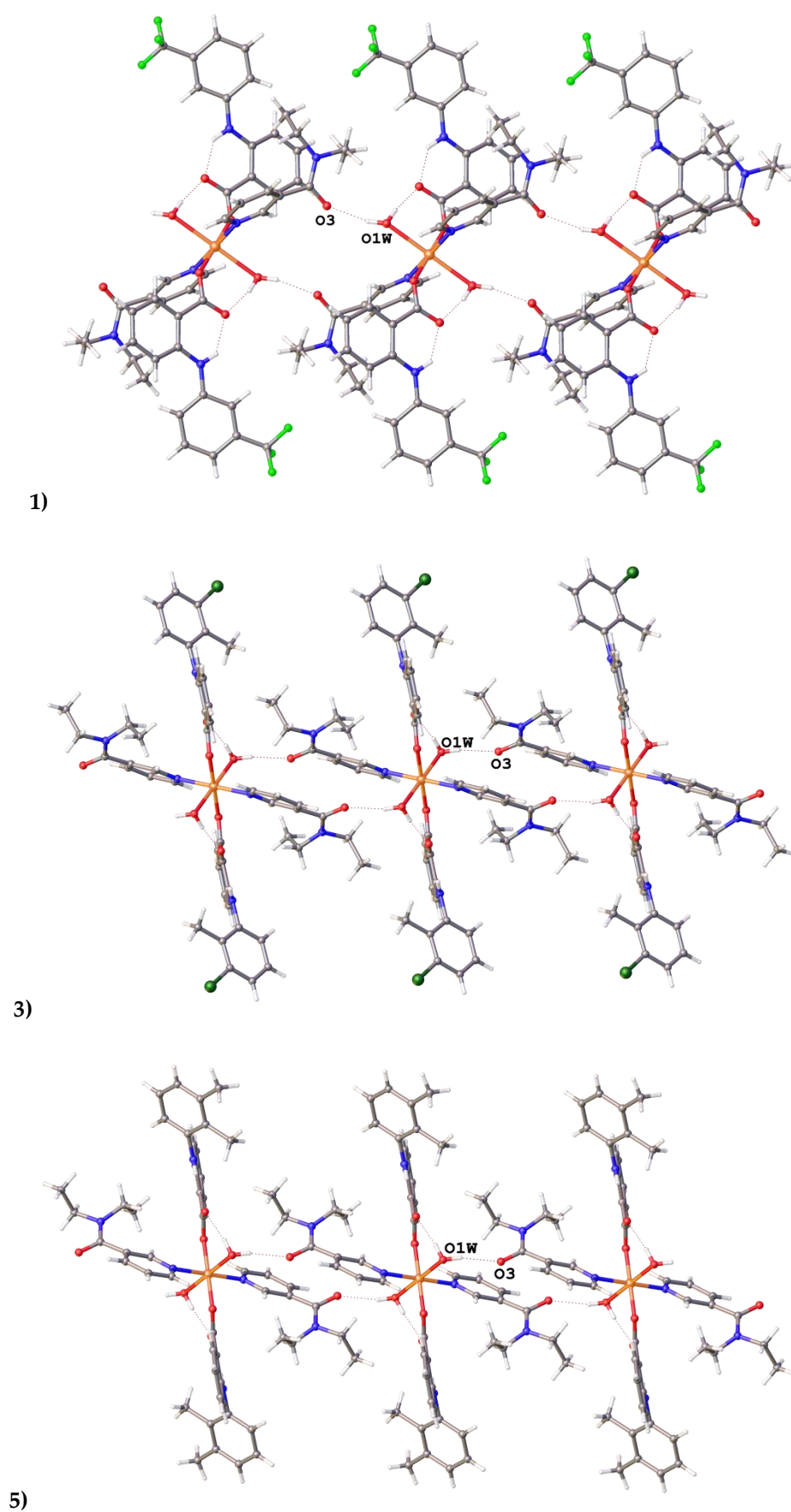
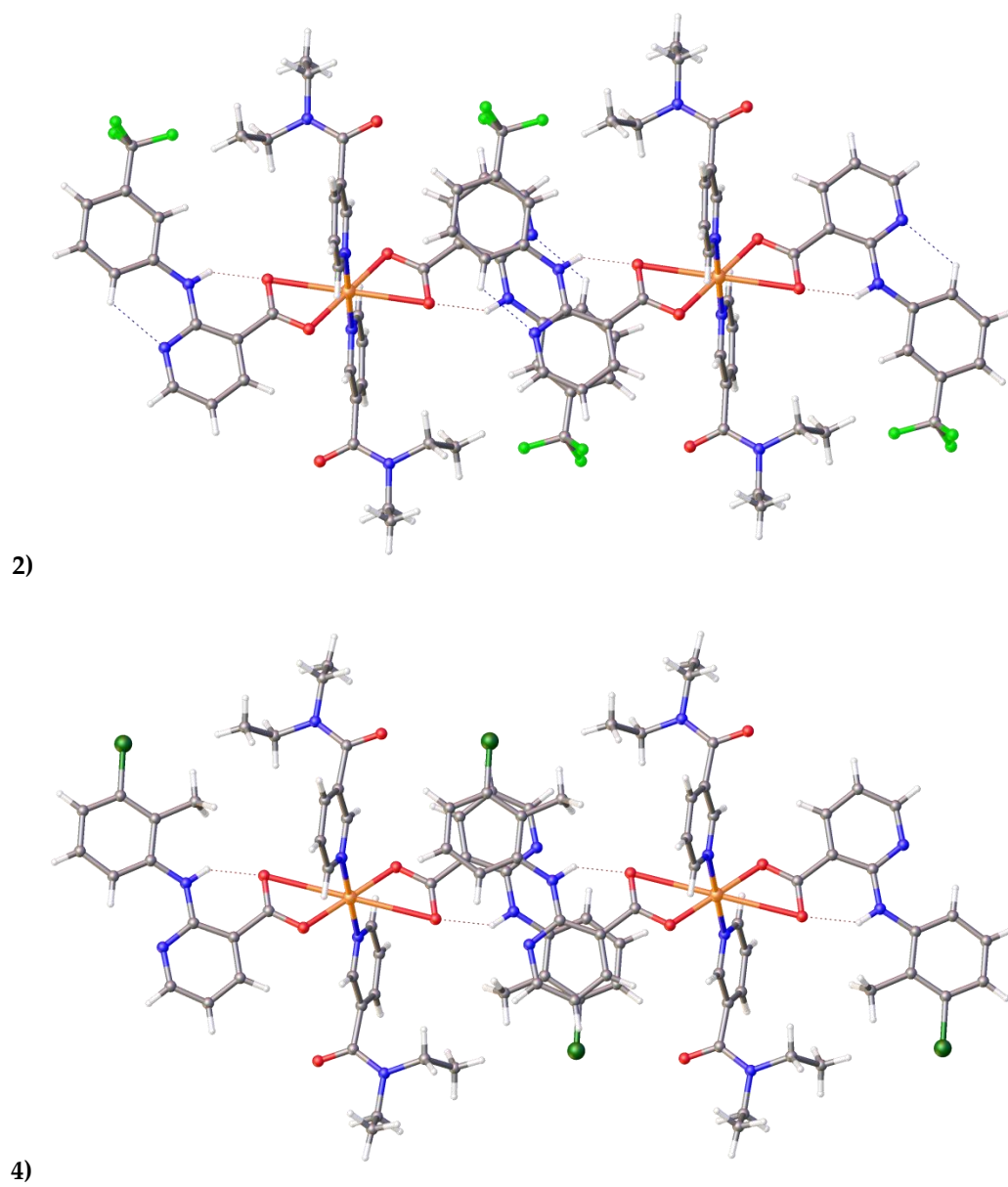


Figure S7. ORTEP-like representation of the asymmetric part of the crystal structure of 5.

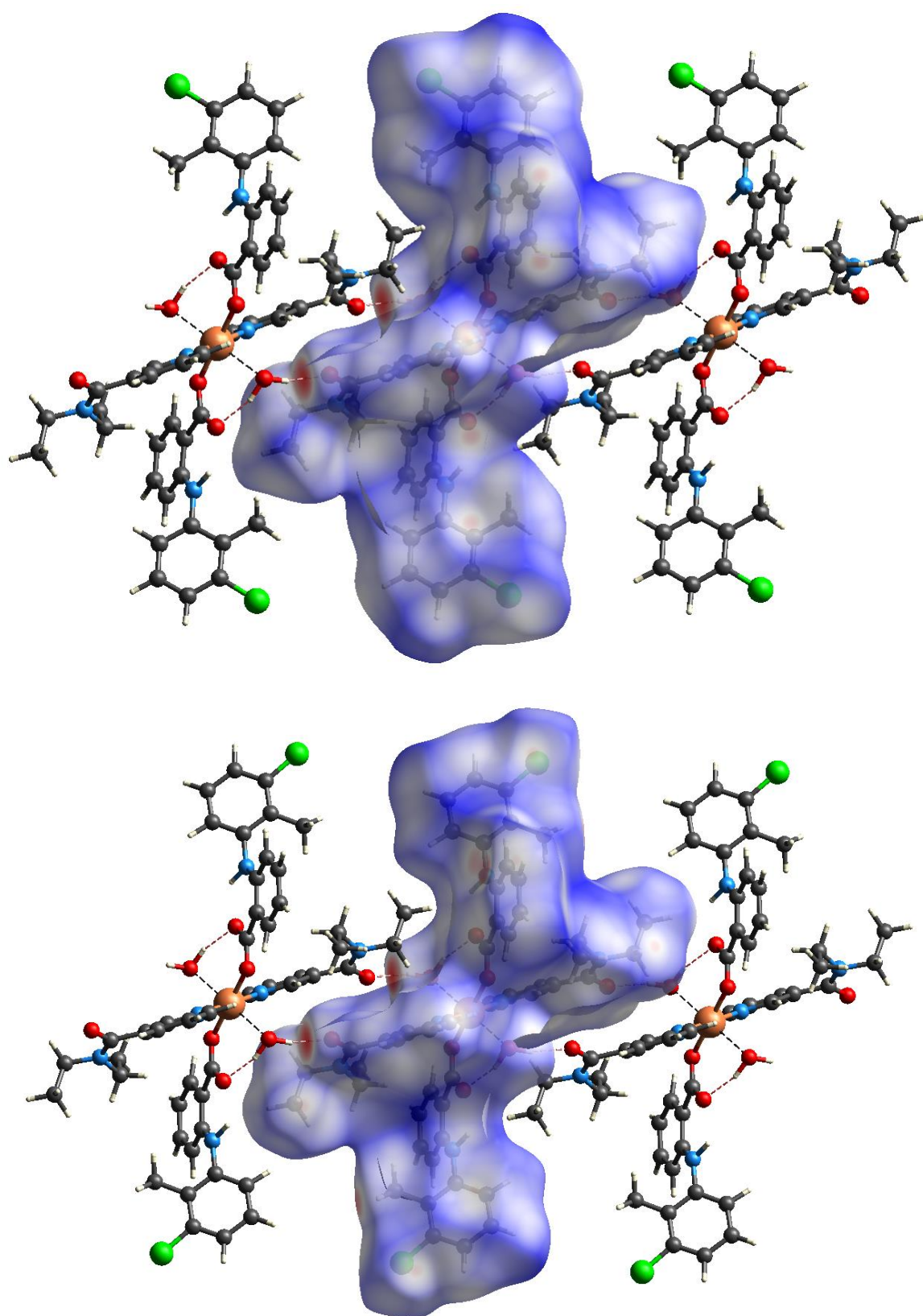


**Figure S8.** Comparison of 1D supramolecular chains formed by O–H...O hydrogen bonds in the crystal structure of 1, 3 and 5.

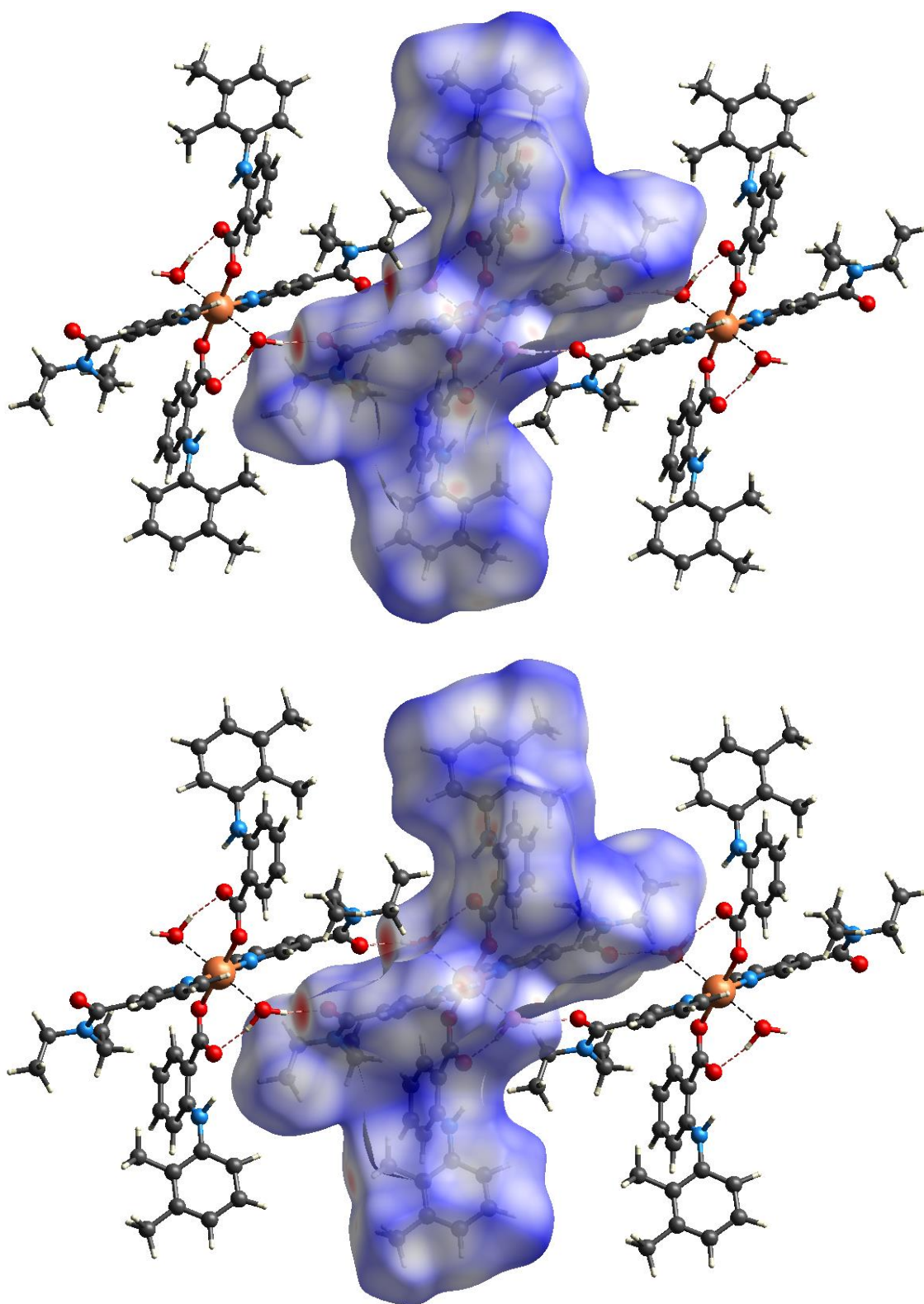


**Figure S9.** Comparison of  $\pi$ - $\pi$  stacking interactions in the crystal structure of **2** and **4**.

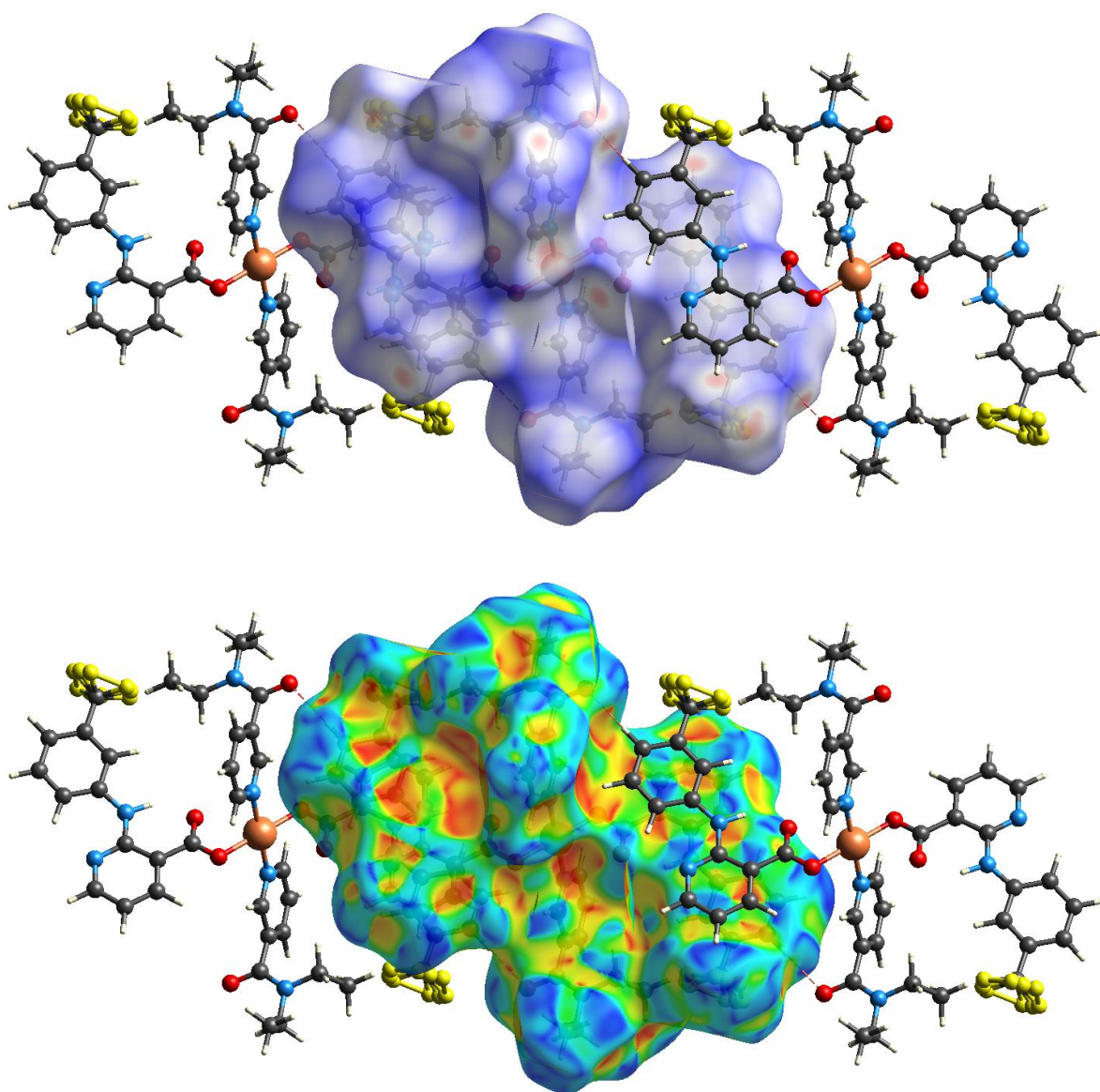




**Figure S10.** View of the three-dimensional Hirshfeld surface of **3** plotted over  $d_{\text{norm}}$  in the range - 0.6001 to 1.3768 a.u. The Hirshfeld surfaces are shown separately for the main (top) and minor (bottom) part of the disorder.

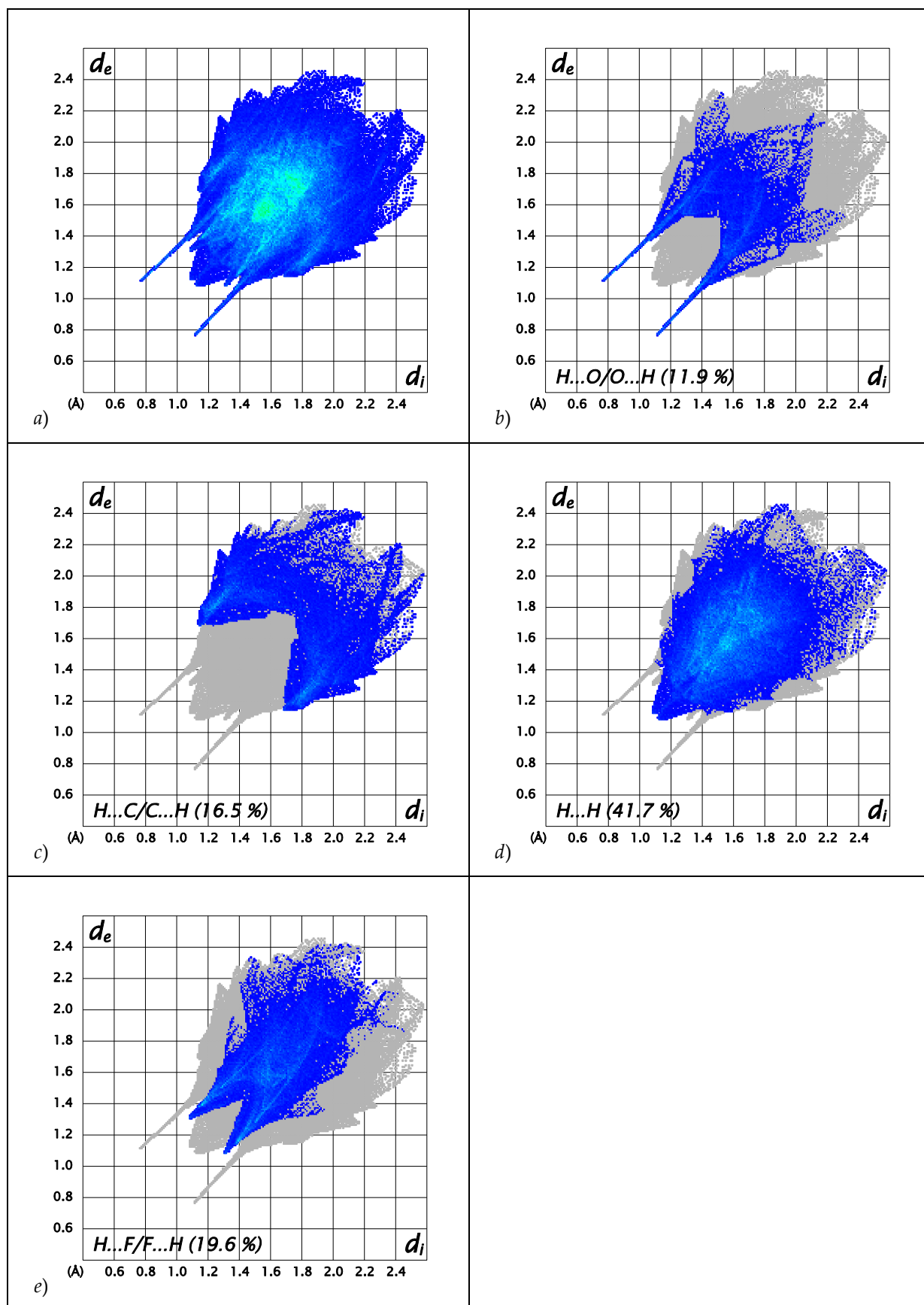


**Figure S11.** View of the three-dimensional Hirshfeld surface of **5** plotted over  $d_{\text{norm}}$  in the range -0.5814 to 1.4120 a.u. The Hirshfeld surfaces are shown separately for the main (top) and minor (bottom) part of the disorder.

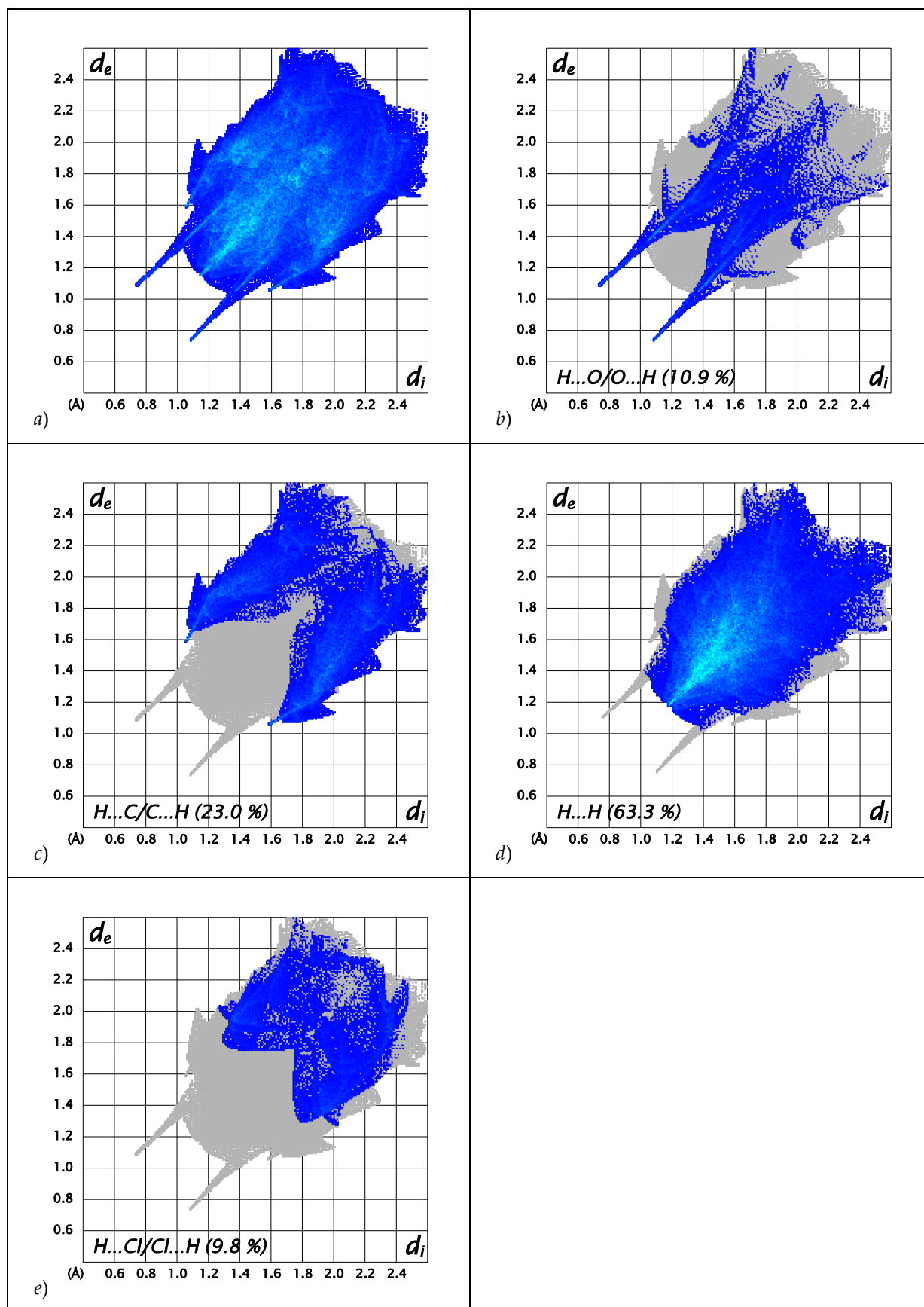


**Figure S12.** View of the three-dimensional Hirshfeld surface of **2** plotted over  $d_{\text{norm}}$  in the range - 0.5000 to 1.4110 a.u. (top) and shape-index (bottom).

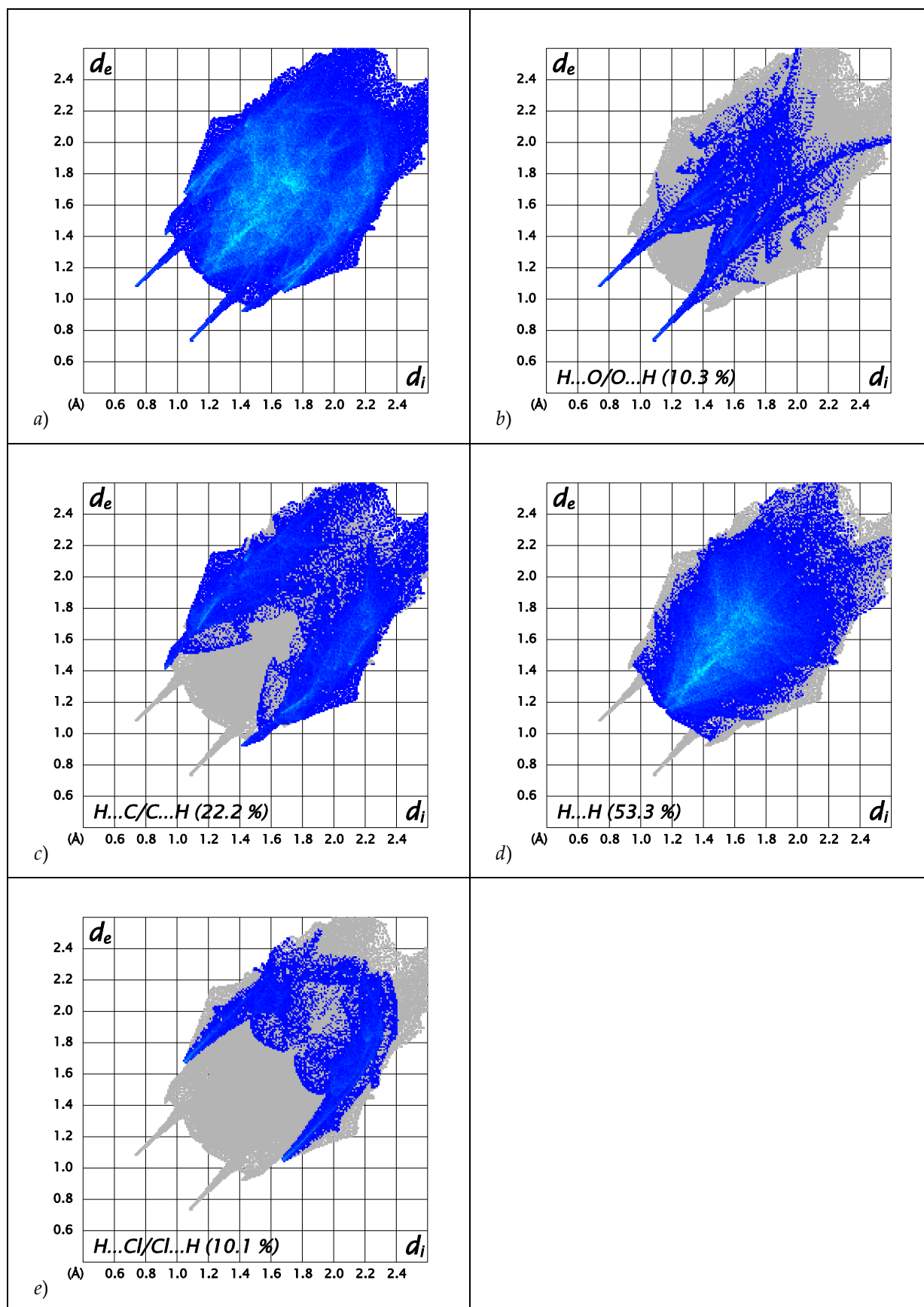




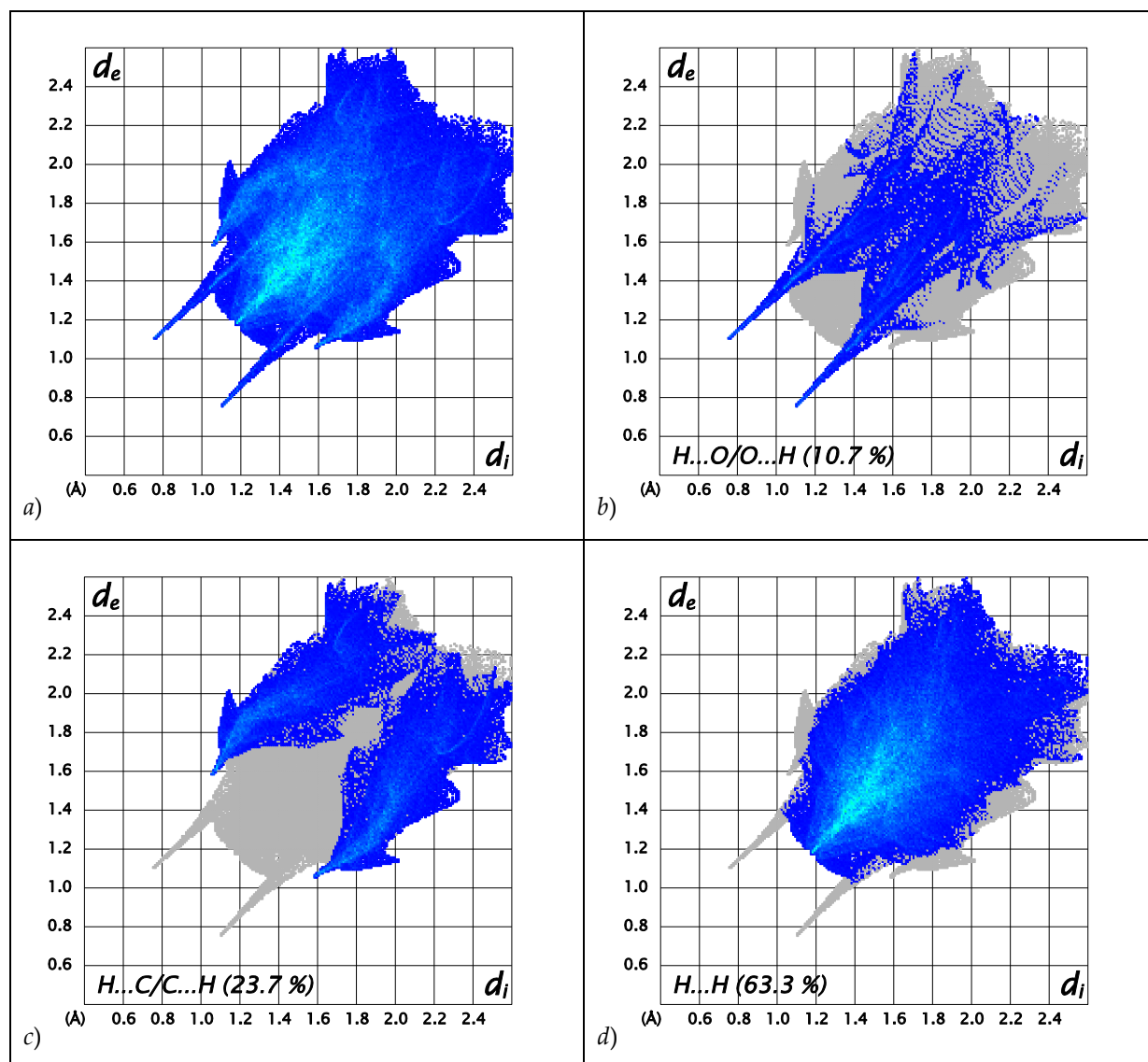
**Figure S13.** The full two-dimensional fingerprint plots of **1**, showing (a) all interactions, (b)  $H\cdots O/O\cdots H$ , (c)  $H\cdots C/C\cdots H$ , (d)  $H\cdots H$  and (e)  $H\cdots F/F\cdots H$  interactions.



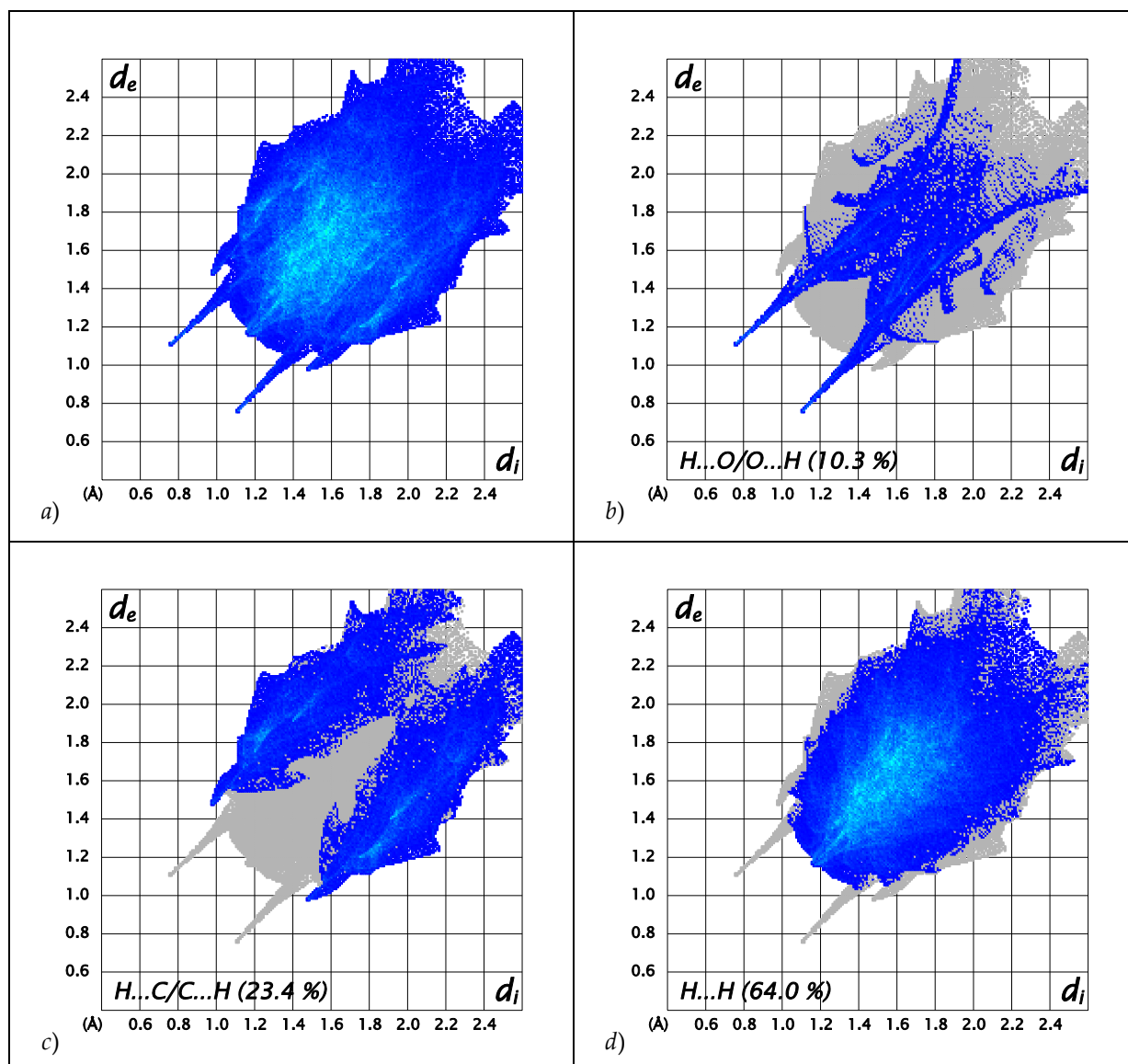
**Figure S14.** The full two-dimensional fingerprint plots of **3** (main part), showing (a) all interactions, (b)  $H\cdots O/O\cdots H$ , (c)  $H\cdots C/C\cdots H$ , (d)  $H\cdots H$  and (e)  $H\cdots Cl/Cl\cdots H$  interactions.



**Figure S15.** The full two-dimensional fingerprint plots of **3** (minor part), showing (a) all interactions, (b)  $H\cdots O/O\cdots H$ , (c)  $H\cdots C/C\cdots H$ , (d)  $H\cdots H$  and (e)  $H\cdots Cl/Cl\cdots H$  interactions.



**Figure S16.** The full two-dimensional fingerprint plots of 5 (main part), showing (a) all interactions, (b)  $H\cdots O/O\cdots H$ , (c)  $H\cdots C/C\cdots H$  and (d)  $H\cdots H$  interactions.



**Figure S17.** The full two-dimensional fingerprint plots of **5** (minor part), showing (a) all interactions, (b)  $H\cdots O/O\cdots H$ , (c)  $H\cdots C/C\cdots H$  and (d)  $H\cdots H$  interactions.



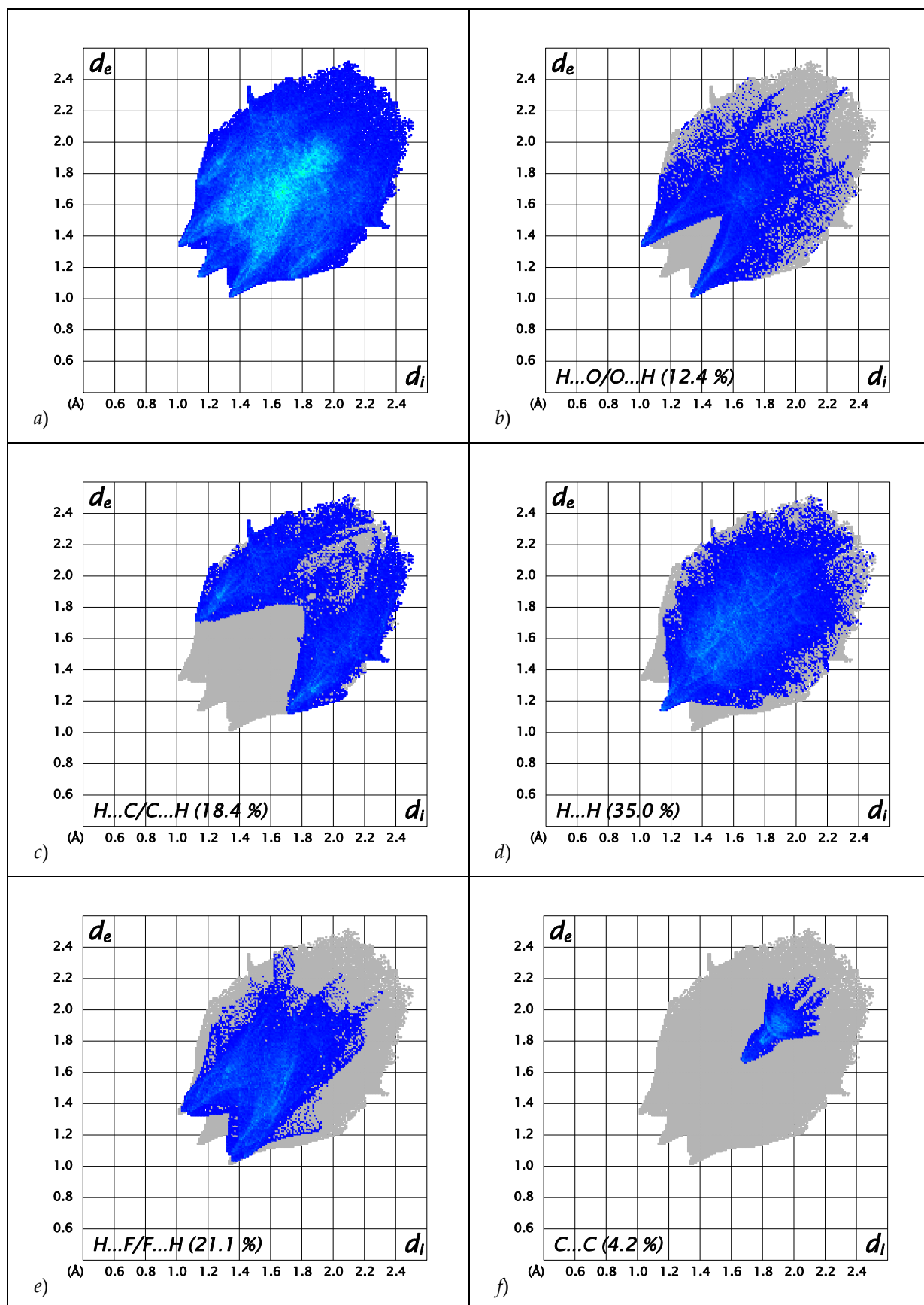


Figure S18. The full two-dimensional fingerprint plots of 2, showing (a) all interactions, (b)  $H...O/O...H$ , (c)  $H...C/C...H$ , (d)  $H...H$ , (e)  $H...F/F...H$  and (f)  $C...C$  interactions.

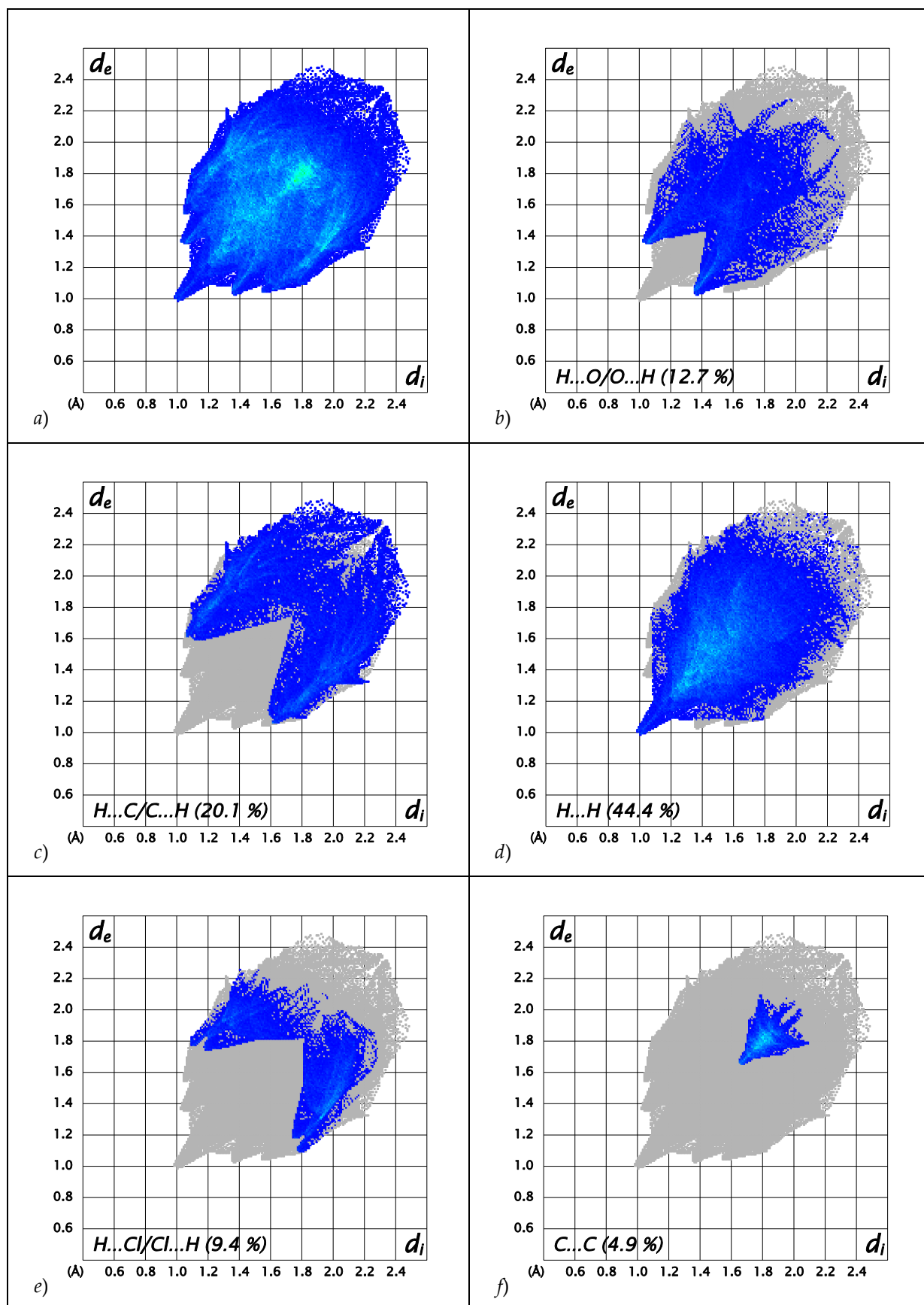


Figure S19. The full two-dimensional fingerprint plots of 4, showing (a) all interactions, (b)  $H...O/O...H$ , (c)  $H...C/C...H$ , (d)  $H...H$ , (e)  $H...Cl/Cl...H$  and (f)  $C...C$  interactions.

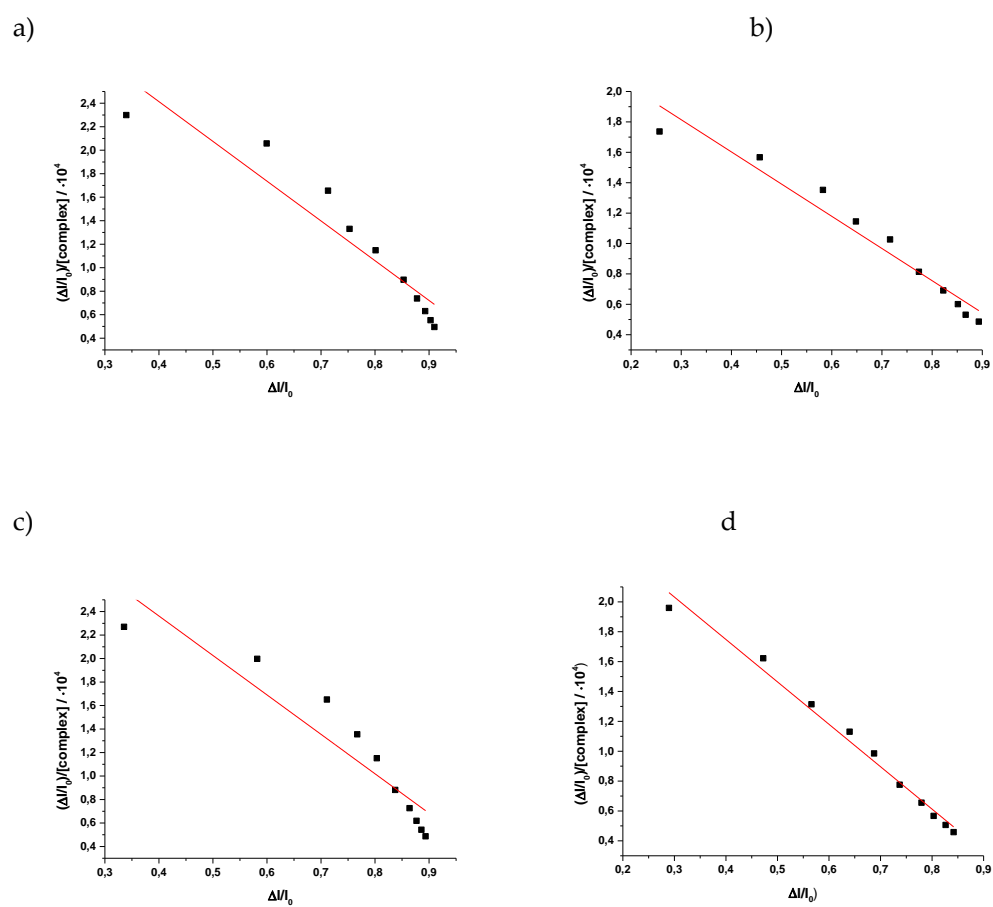


Figure S20. Scatchard plot of BSA for complex a) 1, b) 2, c) 3, d) 4.