ELECTRONIC SUPPLEMENTARY INFORMATION

Organic co-crystals of 1,3-bis(4-pyridyl)azulene with a series of hydrogen-bond donors

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Table S1. Summary of sorption parameters for **5**.

Parameters	Values
A_{BET} (m2/g)	13
Total pore volume (cm3/g)	0.26
Modal pore width (nm)	26
Consistency parameters derived from the BET analyses	
P/P$_o$ range	0.13–0.27
C	39.2
V_m (cm^3/g)	2.92
P/Po(V_m)	0.137
θ(P/P$_o$)	0.138
R	0.999

Table S2. Contributions (%) of various types of close contacts to the Hirshfeld surface area as obtained from 2D fingerprints, summed for one or two non-equivalent azbipy molecules and the unit structure.

Atom	**1**	**2**		**3**		**4**		**5**		**6**	
	azbipy	azbipy	total	azbipy	total	azbipy	total	azbipy	total	azbipy	total
C···H	29.0	29.0	30.9	20.5	24.0	30.8	29.1	13.5	14.8	12.8	13.6
C···C	10.3	9.8	6.7	6.6	4.6	9.6	8.7	7.2	9.7	13.0	9.7
C···N	0.0	0.3	0.4	1.0	0.7	3.3	2.7	1.8	1.4	4.1	2.3
N···N	0.0	0.0	0.0	0.1	0.1	0.2	0.1	0.1	0.1	0.4	0.2
H···H	44.7	45.9	44.0	45.4	41.9	40.1	39.5	50.0	41.7	44.5	39.4
N···H	16.0	10.9	9.3	8.5	4.7	9.0	6.8	5.1	3.4	2.4	2.3
O···H	-	2.4	6.6	16.9	21.1	6.4	12.2	17.5	22.9	21.1	29.6
O···C	-	1.1	1.3	0.5	2.0	0.6	0.8	4.1	2.3	1.8	1.9
O···N	-	0.6	0.7	0.5	0.3	0.1	0.0	0.6	0.8	0.0	0.0
O···O	-	0.0	0.0	0.0	0.6	0.0	0.0	0.0	0.0	0.0	0.9

Figure S1. FTIR spectra of the systems investigated in this paper.

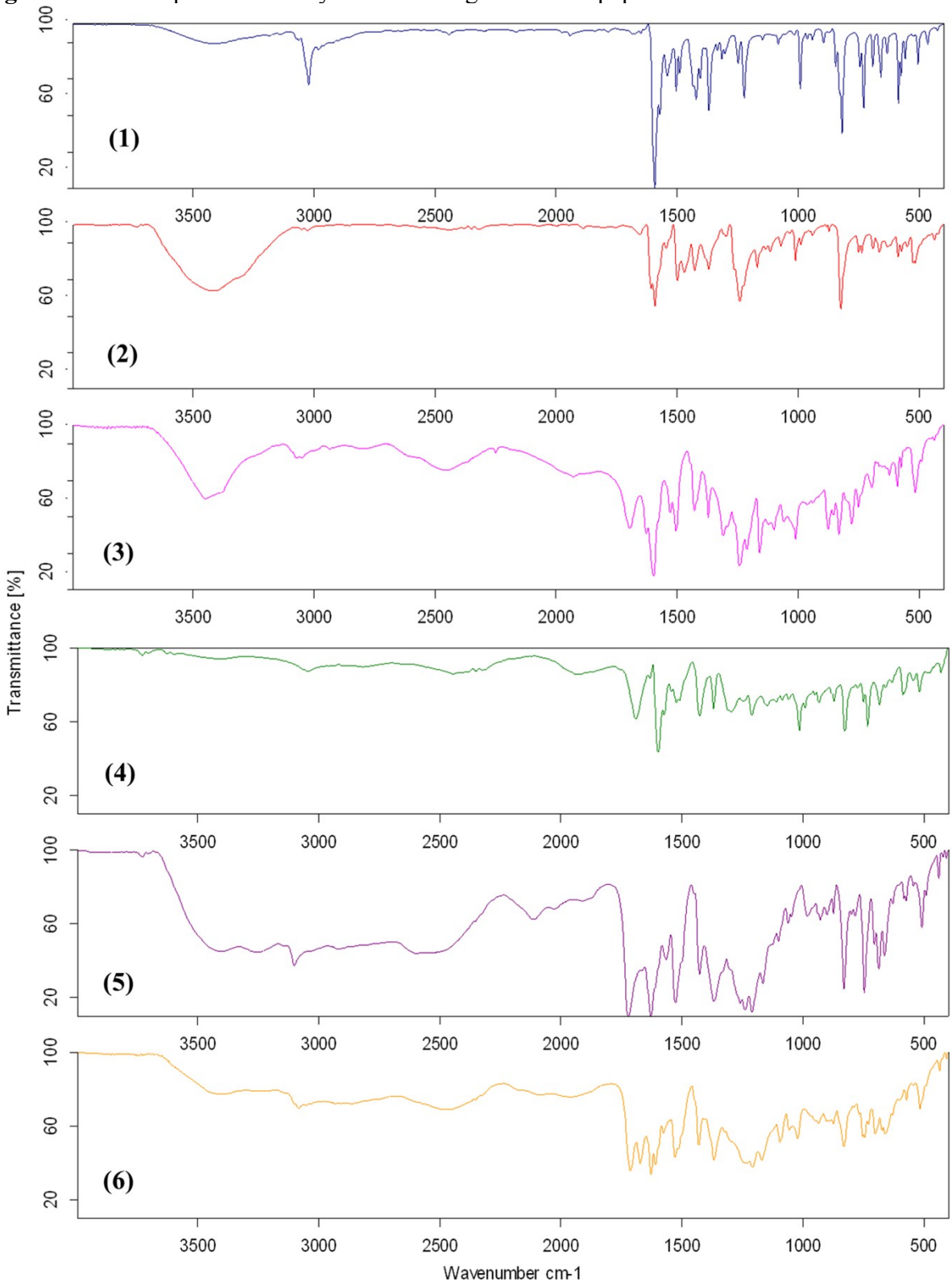
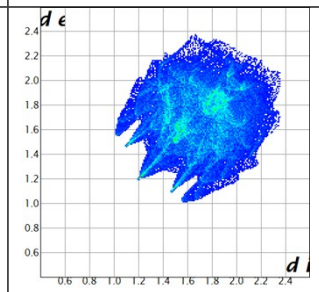
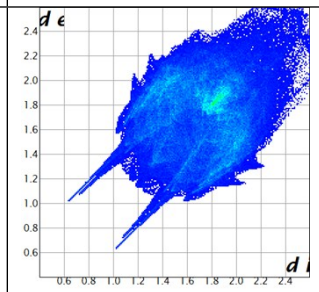
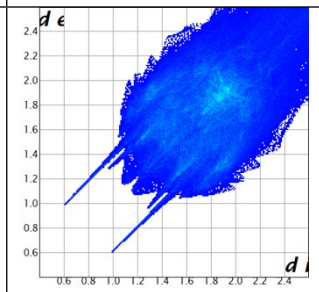
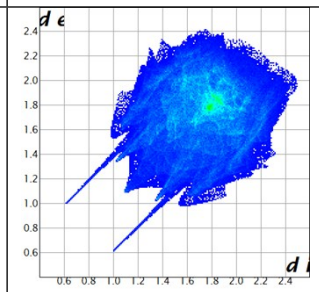
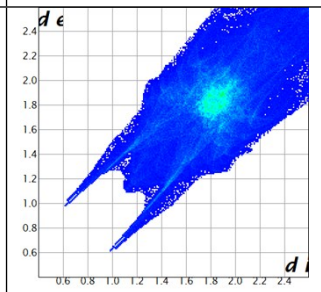
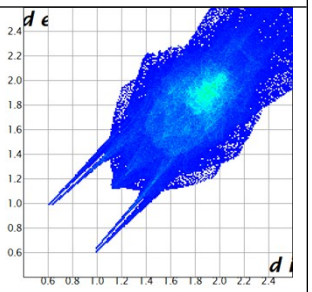
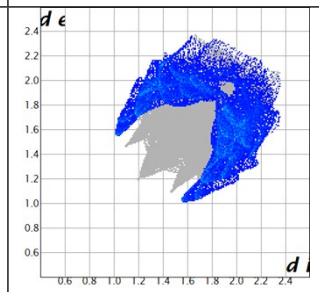
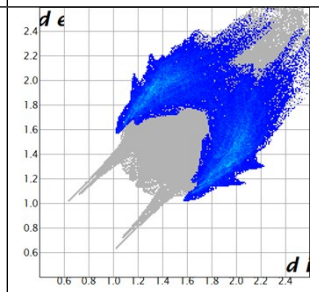
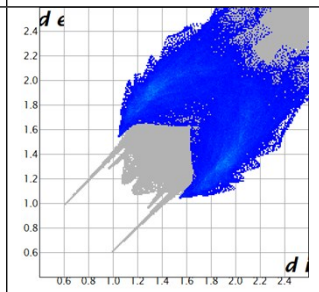
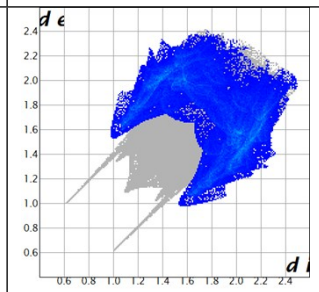
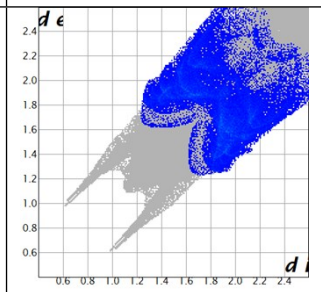
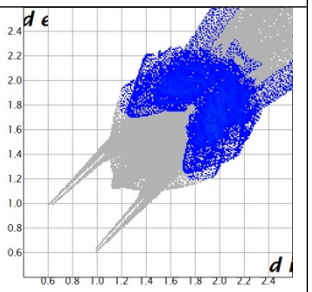
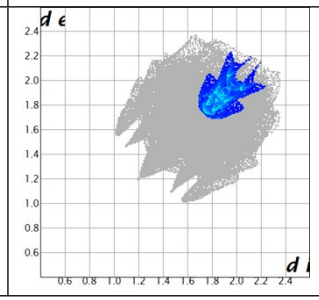
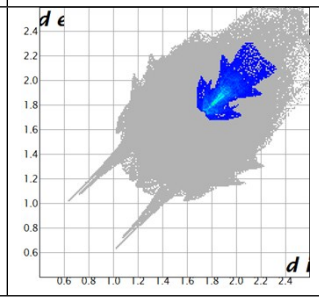
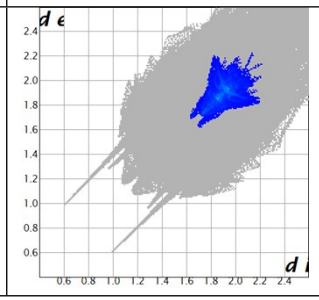
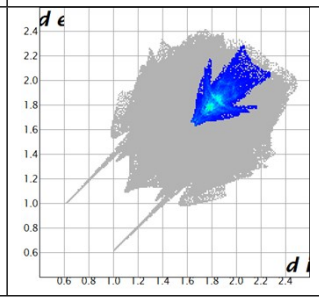
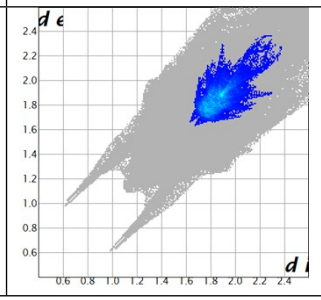
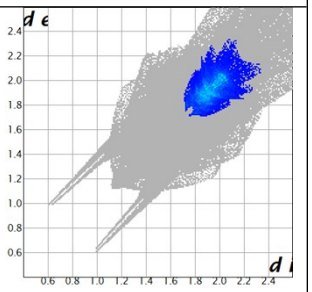
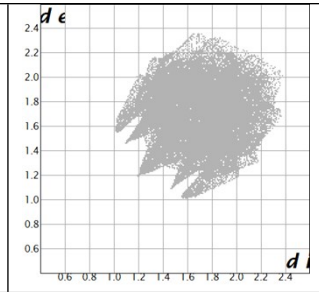
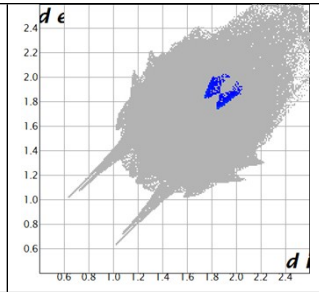
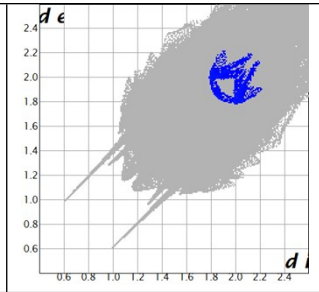
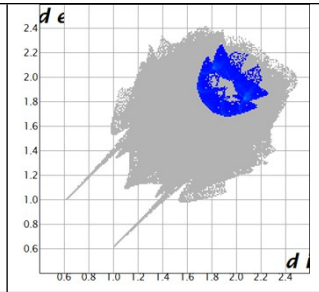
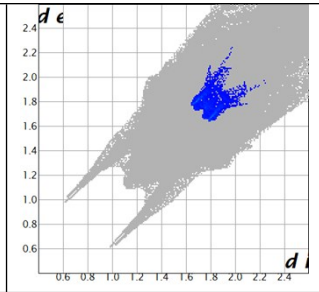
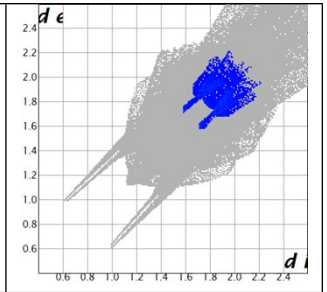
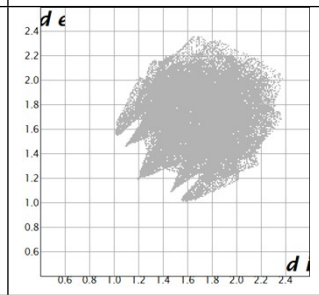
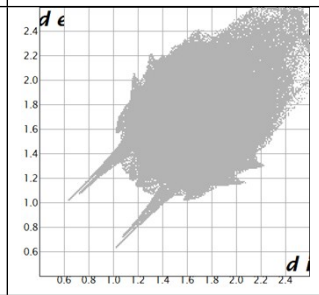
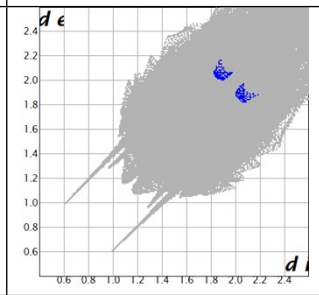
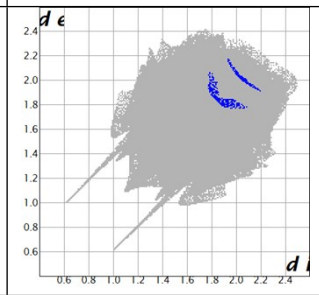
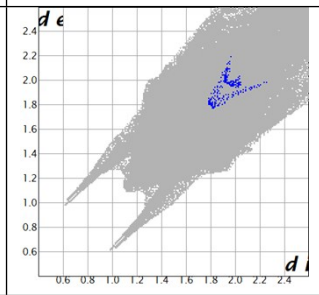
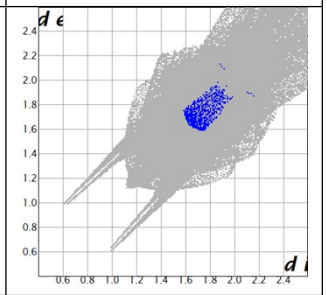
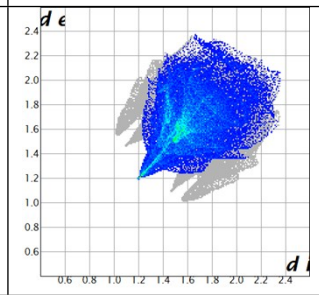
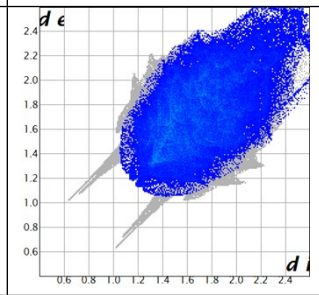
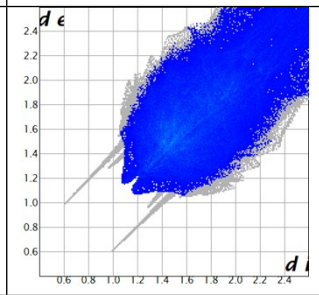
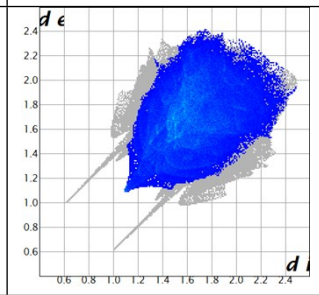
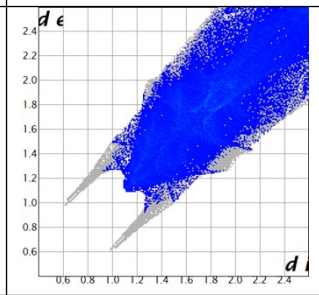
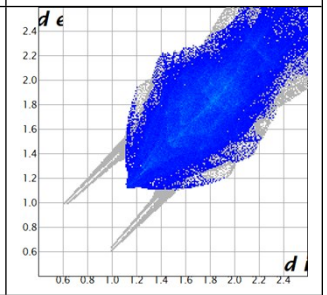
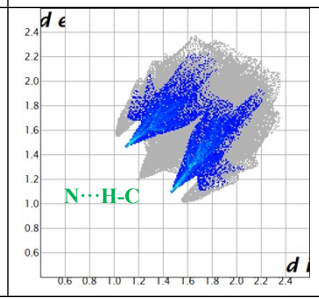
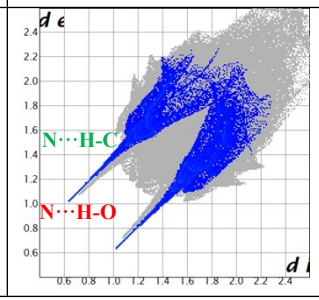
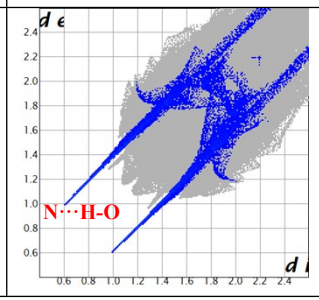
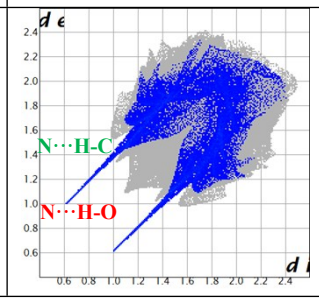
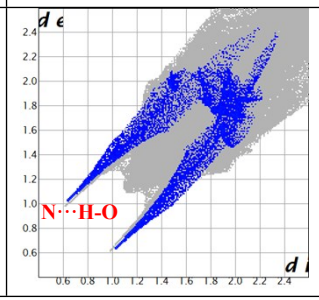
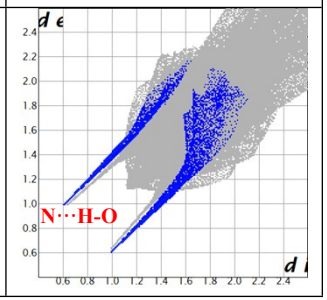


Figure S2. 2D fingerprint plots decomposed on types of close contacts for non-equivalent molecules in the studied crystals.

Atoms	**1**	**2**	**3**	**4**	**5**	**6**
All						
C···H						
C···C						

C···N						
N···N						
H···H						
N···H						

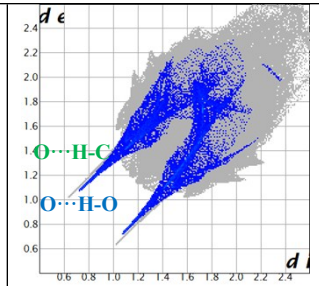
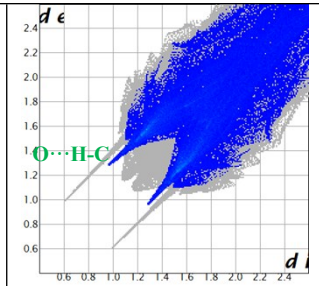
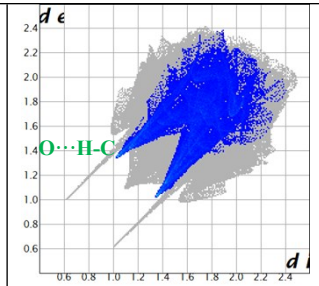
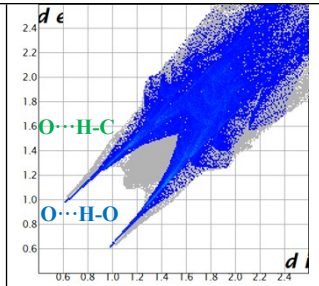
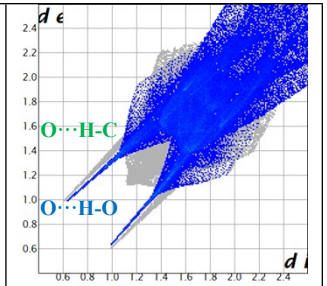
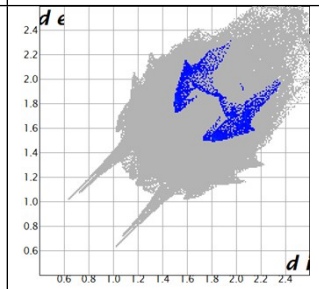
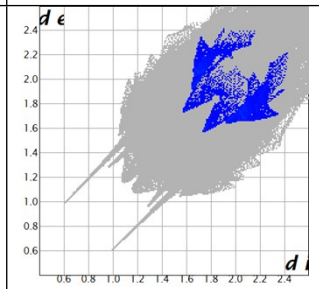
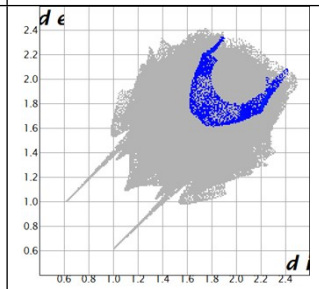
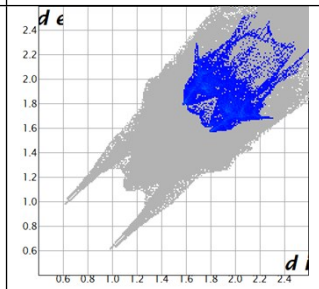
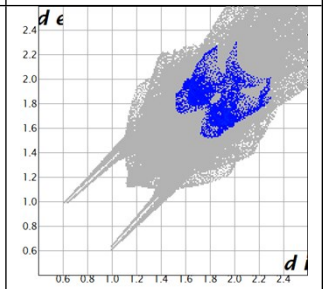
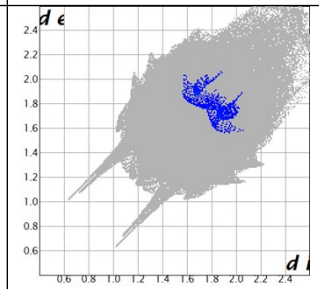
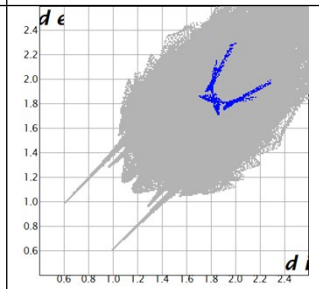
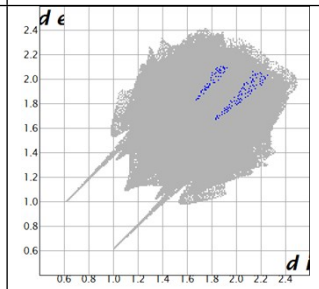
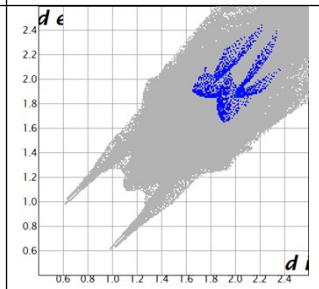
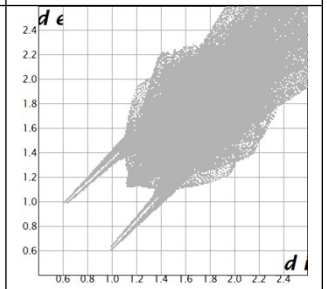
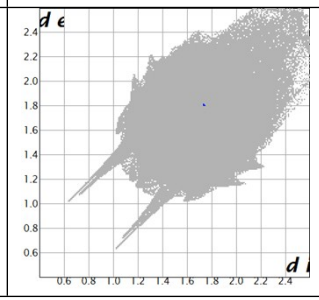
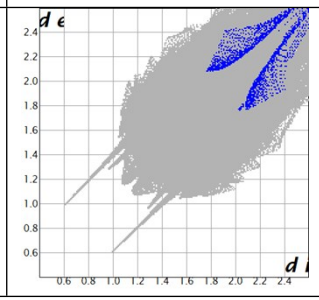
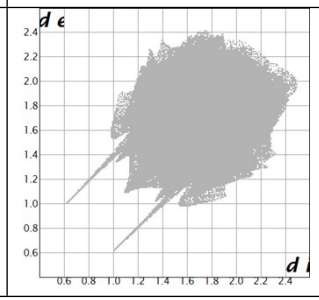
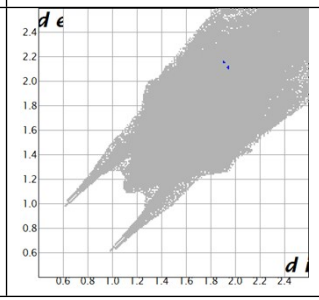
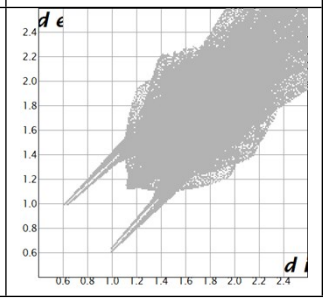
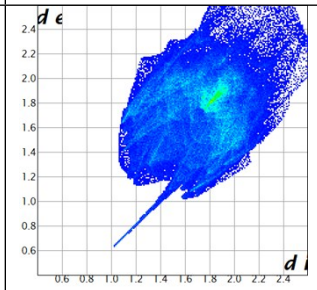
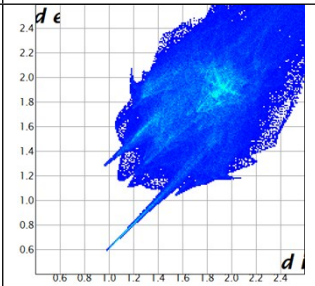
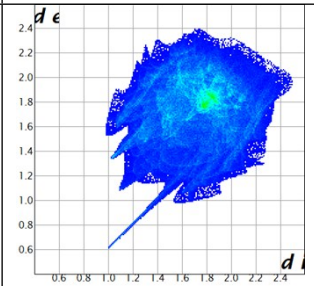
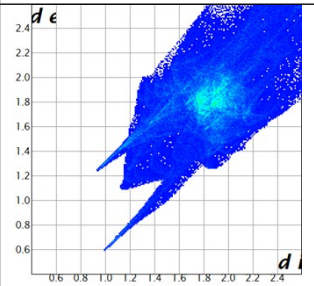
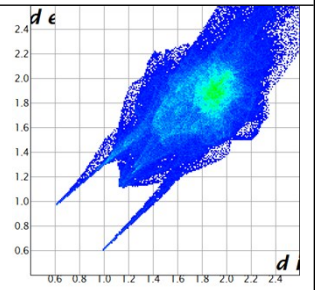
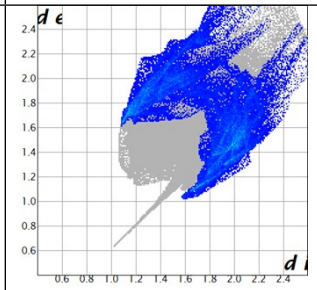
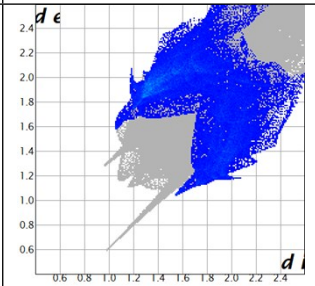
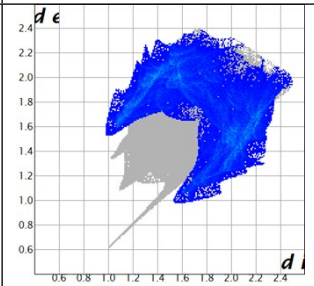
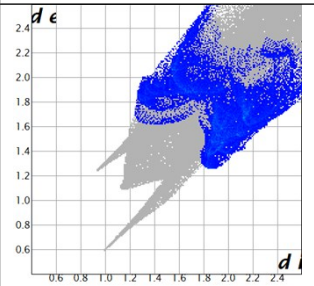
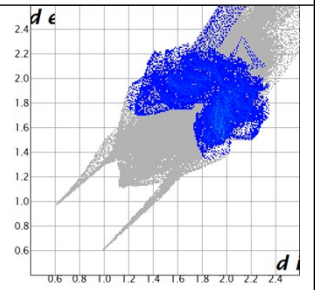
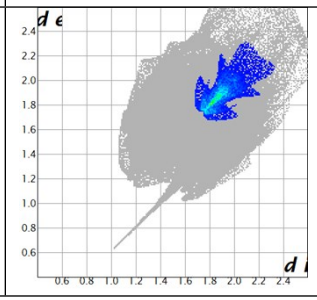
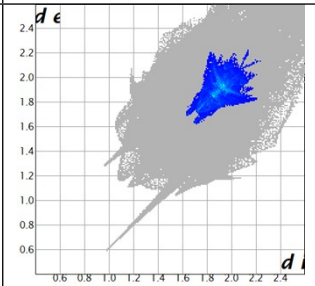
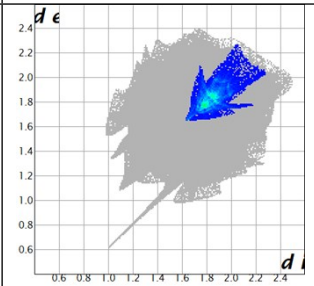
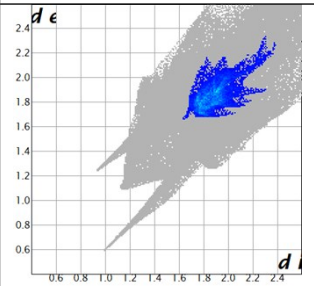
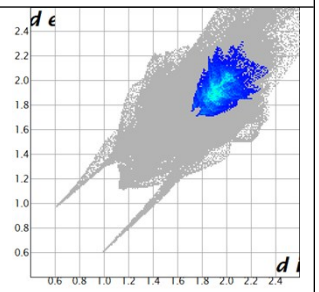
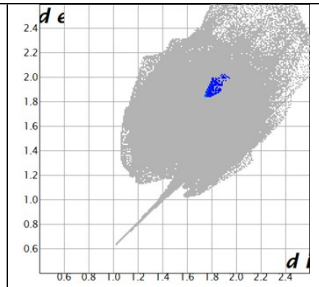
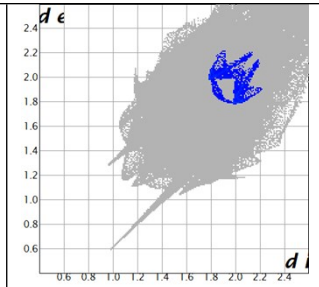
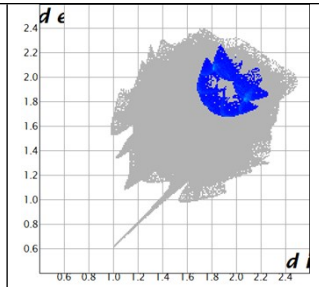
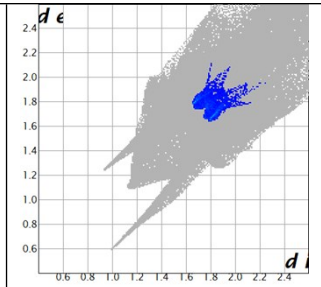
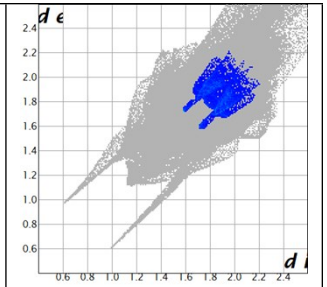
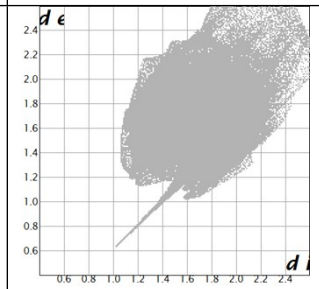
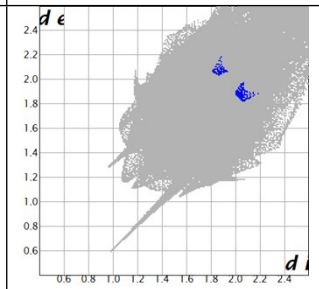
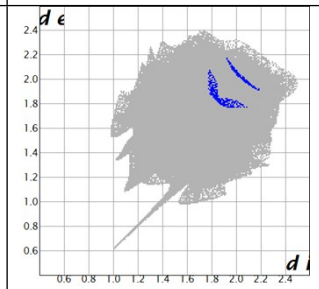
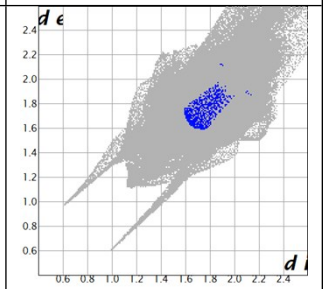
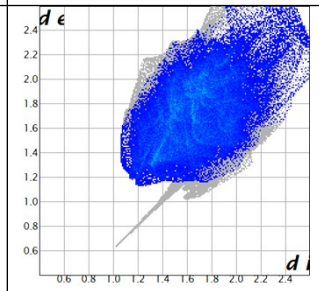
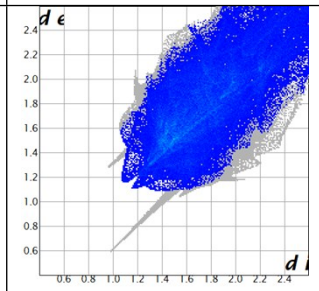
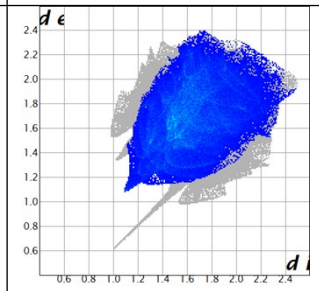
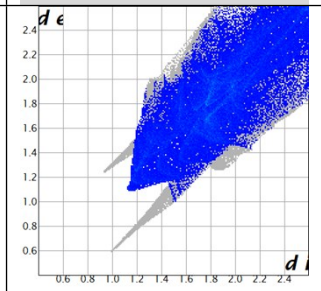
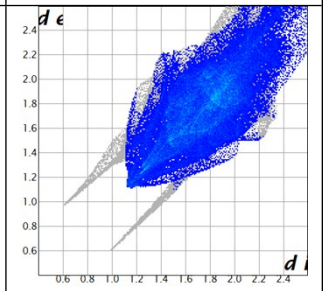
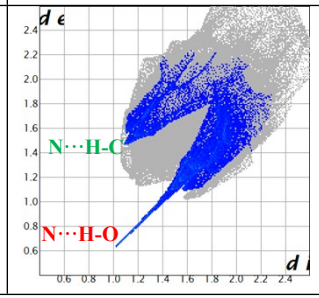
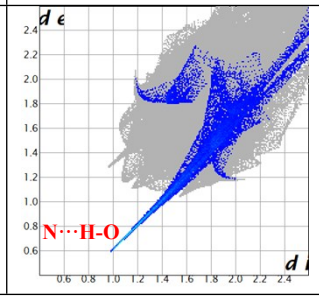
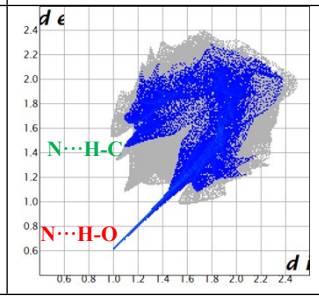
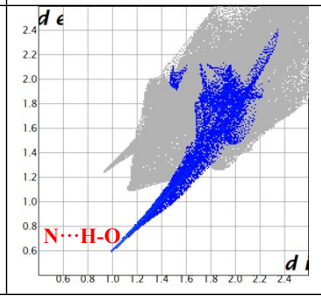
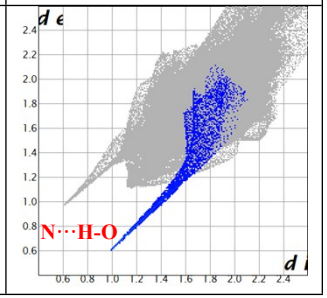
O···H	-					
O···C	-					
O···N	-					
O···O	-					

Figure S3. 2D fingerprint plots decomposed on types of close contacts for one or two non-equivalent azbbpy molecules in the studied crystals.

Atoms	1	2	3	4	5	6
All						
C···H						
C···C						

C···N						
N···N						
H···H						
N···H	N···H-C					

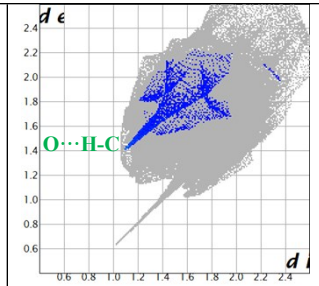
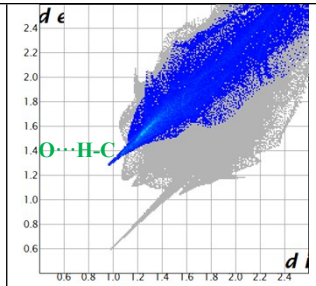
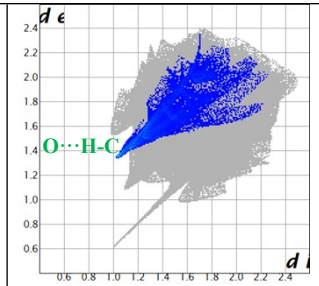
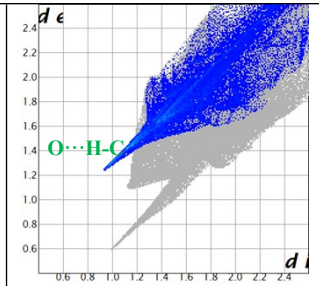
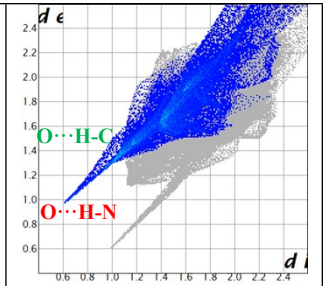
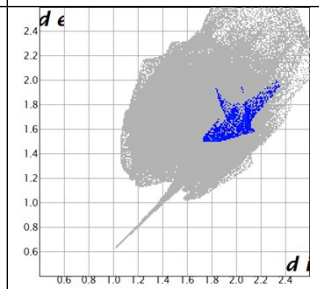
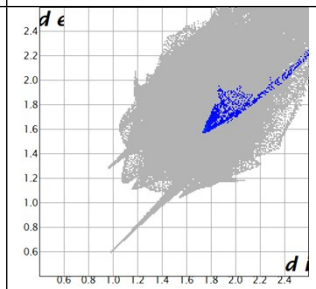
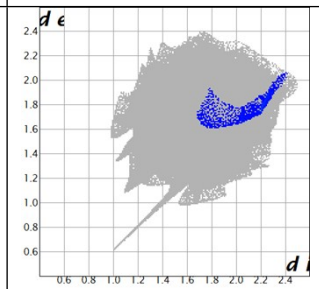
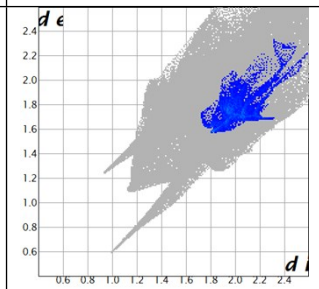
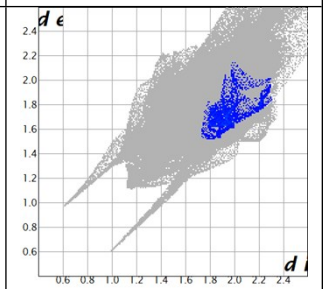
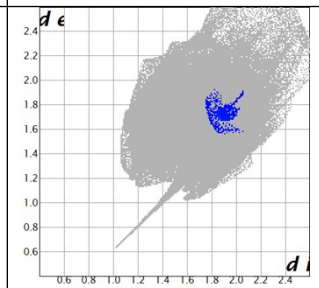
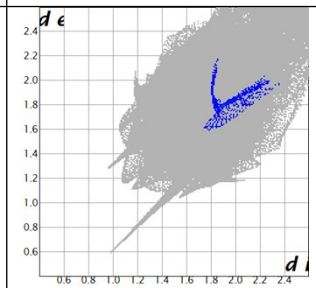
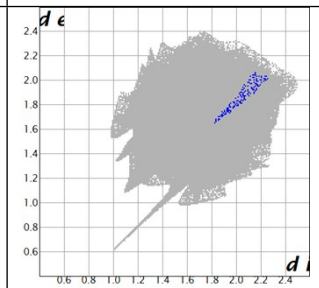
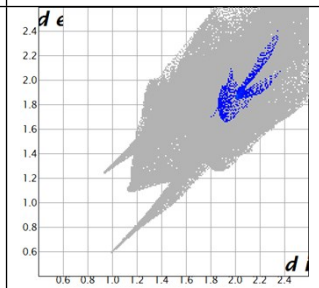
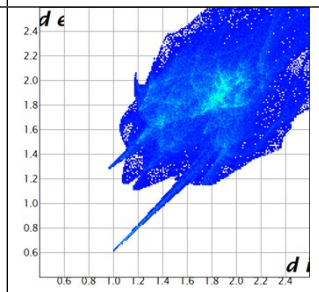
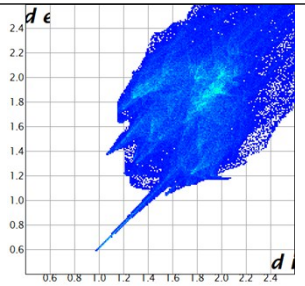
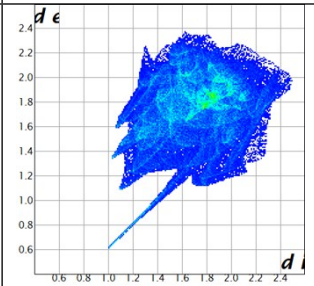
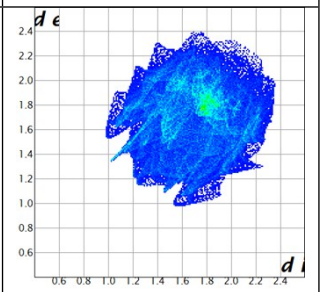
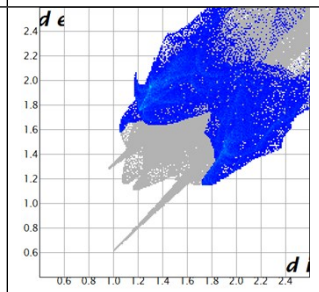
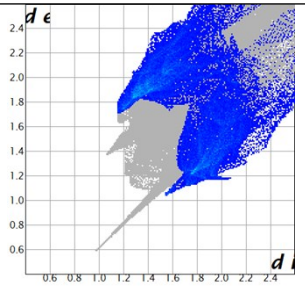
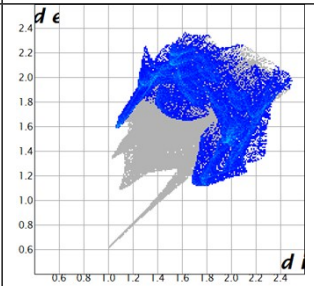
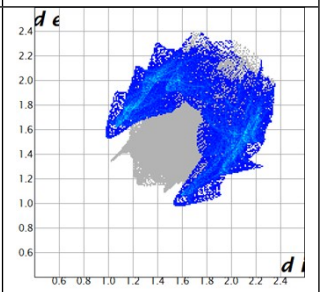
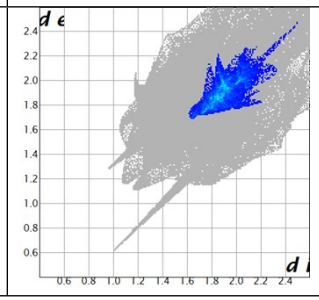
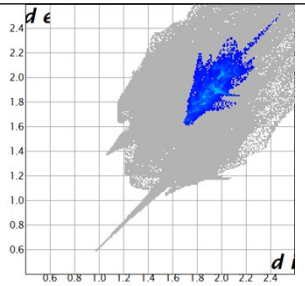
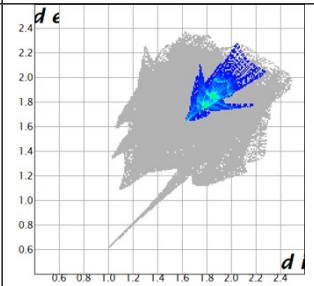
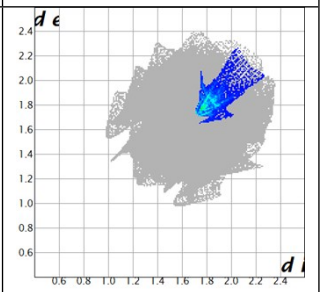
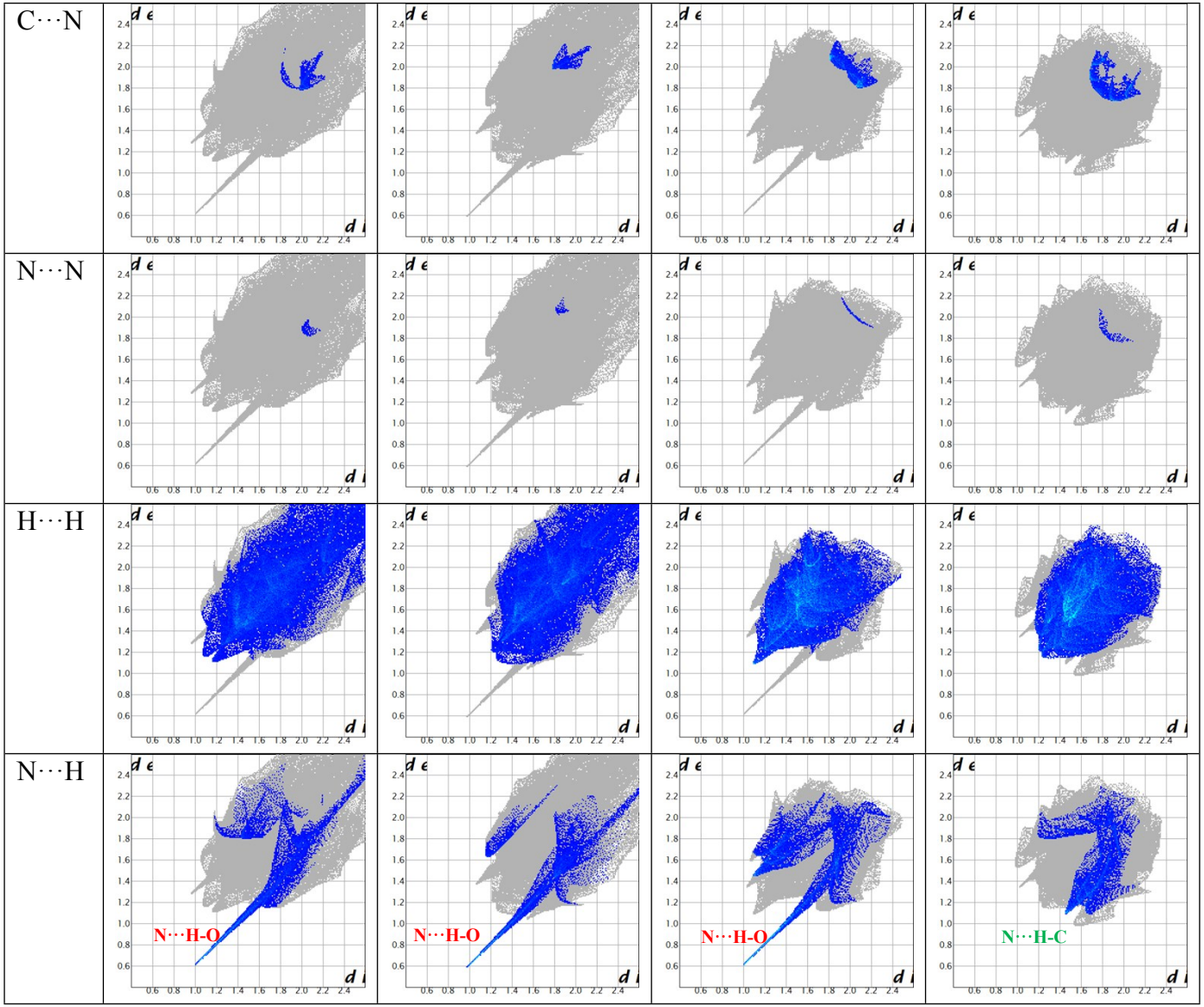
O···H	-					
O···C	-					
O···N	-					
O···O	-	-	-	-	-	-

Figure S4. 2D fingerprint plots decomposed on types of close contacts for each non-equivalent azbbpy molecule in crystals **3** and **4**.

Atoms	**3A**	**3B**	**4A**	**4B**
All				
C···H				
C···C				


C···N
N···N
H···H
N···H
N···H-O
N···H-O
N···H-O
N···H-C

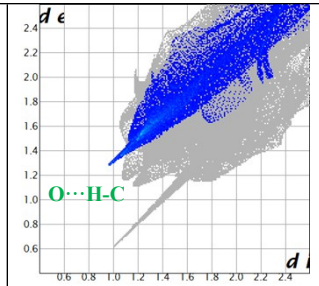
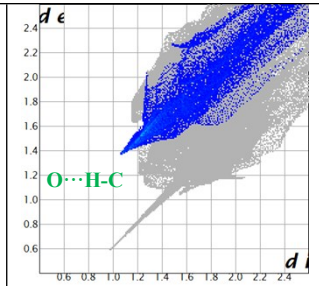
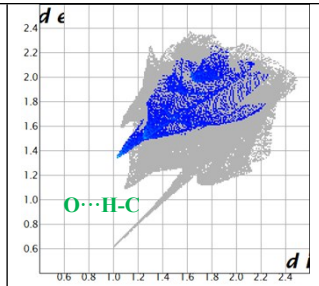
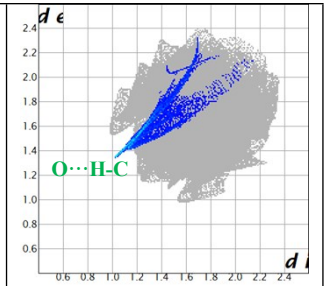
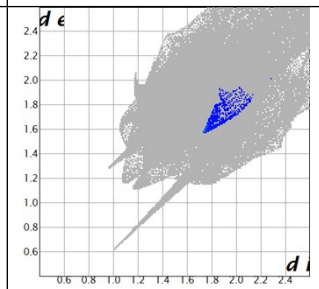
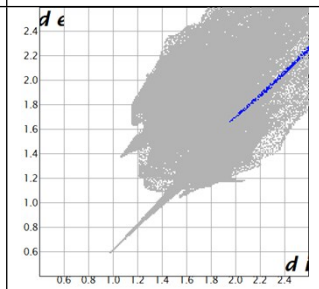
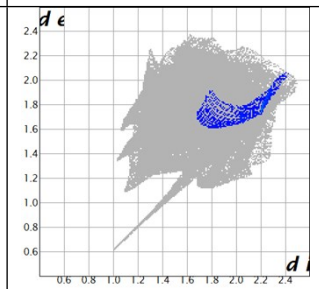
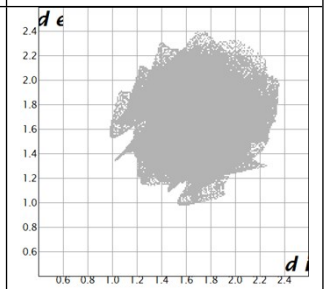
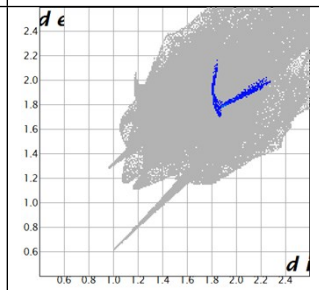
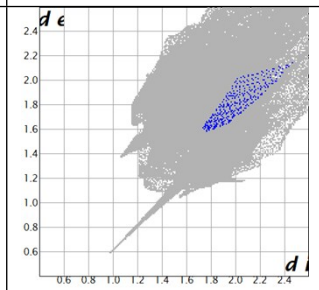
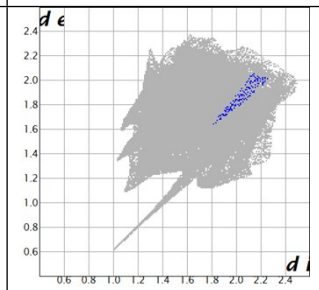
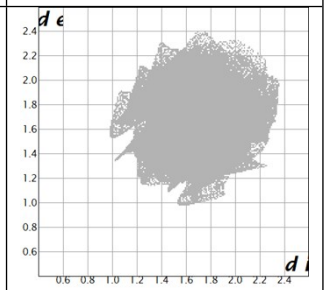
O…H				
O…C				
O…N				
O…O	-	-	-	-

Figure S5. TG curves for compounds 2 – 5.

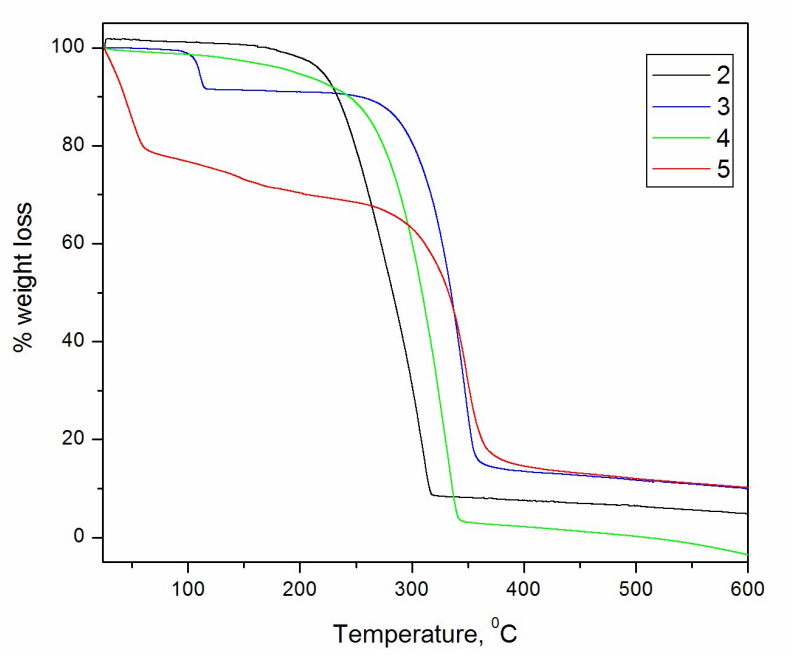


Figure S6. Pore distribution curve for **5** fitted using N_2 at 77 K on carbon (slit/cylindrical pores, QSDFT adsorption branch model).

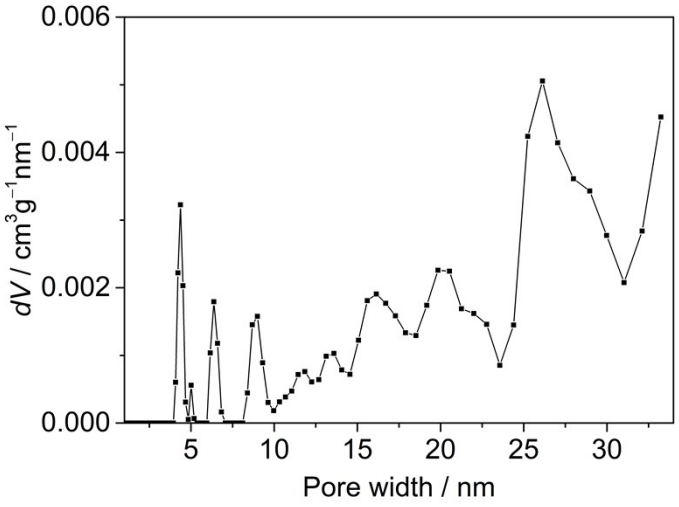


Figure S7. Fluorescence emission spectra: a) azbbpy in CH_2Cl_2 solution (λ_{ex} = 425 nm); b) solids (λ_{ex} = 400 nm)