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Crystal structures of 5-bromo-1-arylpyrazoles and their halogen bonding features

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Contents

1. X-ray crystallography

Table 1S. Bond distances (Å) and angles (▪) for compounds **1**-**5**

Compound 1		Compound 2		Compound 3		Compound 4		Compound 5	
Br1-C7	1.843(4)	Br1-C8	1.846(9)	Br1-C9	1.856(3)	Br1-C10	1.855(4)	Br1-C4	1.906(4)
F1-C4	1.361(4)	Cl1-C5	1.728(12)	O1-C12	1.194(4)	O1-C13	1.193(4)	Br2-C10	1.855(4)
O1-C10	1.203(4)	O1-C11	1.188(12)	O2-C12	1.325(4)	O2-C13	1.326(4)	O1-C13	1.191(5)
O2-C10	1.324(5)	O2-C11	1.333(11)	O2-C13	1.443(4)	O2-C14	1.453(4)	O2-C13	1.327(5)
O2-C11	1.448(5)	O2-C12	1.429(12)	O3-C14	1.179(4)	O3-C15	1.194(4)	O2-C14	1.451(4)
O3-C12	1.200(4)	O3-C13	1.186(12)	O4-C14	1.322(4)	O4-C15	1.329(4)	O3-C15	1.199(5)
O4-C12	1.314(4)	O4-C13	1.325(13)	O4-C15	1.447(4)	O4-C16	1.443(4)	O4-C15	1.332(5)
O4-C13	1.449(4)	O4-C14	1.452(12)	N1-N2	1.356(3)	N1-N2	1.354(4)	O4-C16	1.450(4)
N1-N2	1.351(4)	N1-N2	1.362(10)	N1-C1	1.443(4)	N1-C1	1.445(4)	N1-N2	1.366(4)
N1-C1	1.437(4)	N1-C1	1.420(12)	N1-C9	1.344(3)	N1-C10	1.358(4)	N1-C1	1.434(5)
N1-C7	1.357(4)	N1-C8	1.377(11)	N2-C11	1.327(4)	N2-C12	1.332(4)	N1-C10	1.350(4)
N2-C9	1.327(4)	N2-C10	1.333(11)	C1-C2	1.385(5)	C1-C2	1.370(6)	N2-C12	1.324(5)
C1-C2	1.374(5)	C1-C2	1.381(14)	C1-C6	1.370(4)	C1-C6	1.387(5)	C1-C2	1.387(5)
C1-C6	1.373(5)	C1-C6	1.412(14)	C2-C3	1.389(4)	C2-C3	1.379(6)	C1-C6	1.388(5)
C2-C3	1.373(5)	C2-C3	1.380(15)	C3-C4	1.374(5)	C3-C4	1.377(6)	C2-C3	1.382(5)
C3-C4	1.362(6)	C2-C7	1.481(15)	C3-C7	1.504(5)	C4-C5	1.369(6)	C3-C4	1.372(5)
C4-C5	1.357(6)	C3-C4	1.399(16)	C4-C5	1.375(6)	C5-C6	1.391(6)	C4-C5	1.371(5)
C5-C6	1.377(6)	C4-C5	1.366(15)	C5-C6	1.393(5)	C6-C7	1.502(6)	C5-C6	1.393(5)
C7-C8	1.382(5)	C5-C6	1.399(14)	C6-C8	1.495(5)	C7-C8	1.515(6)	C6-C7	1.517(5)
C8-C9	1.408(5)	C8-C9	1.395(13)	C9-C10	1.366(4)	C7-C9	1.522(6)	C7-C8	1.517(5)
C8-C12	1.481(5)	C9-C10	1.418(12)	C10-C11	1.403(4)	C10-C11	1.371(5)	C7-C9	1.529(5)
C9-C10	1.488(5)	C9-C13	1.469(13)	C10-C14	1.481(4)	C11-C12	1.400(4)	C10-C11	1.375(5)
		C10-C11	1.491(14)	C11-C12	1.481(4)	C11-C15	1.475(5)	C11-C12	1.406(5)
						C12-C13	1.481(5)	C11-C15	1.481(5)
								C12-C13	1.494(6)

Compound 1		Compond 2		Compound 3		Compound 4		Compound 5	
		C11-O2-C12	116.1(8)	C12-O2-C13	115.8(3)	C13-O2-C14	115.5(3)	C13-O2-C14	115.2(4)
C10-O2-C11	115.5(3)								
		C13-O4-C14	117.3(9)	C14-O4-C15	116.4(3)	C15-O4-C16	116.0(3)	C15-O4-C16	114.5(3)
C12-O4-C13	116.1(3)								
N2-N1-C1	119.6(3)	N2-N1-C1	121.1(7)	N2-N1-C1	119.8(2)	N2-N1-C1	121.2(3)	N2-N1-C1	120.3(3)
N2-N1-C7	112.1(3)	N2-N1-C8	111.1(8)	C9-N1-N2	111.3(2)	N2-N1-C10	111.4(3)	C10-N1-N2	111.0(3)
C7-N1-C1	128.3(3)	C8-N1-C1	127.8(8)	C9-N1-C1	128.9(2)	C10-N1-C1	127.4(3)	C10-N1-C1	128.5(4)
		C10-N2-N1	104.7(7)						
C9-N2-N1	104.7(3)			C11-N2-N1	104.4(2)	C12-N2-N1	104.6(3)	C12-N2-N1	104.7(3)
C2-C1-N1	120.2(3)	C2-C1-N1	121.5(9)	C2-C1-N1	117.4(3)	C2-C1-N1	117.5(3)	C2-C1-N1	118.6(4)
C6-C1-N1	118.8(4)	C2-C1-C6	122.5(10)	C6-C1-N1	119.1(3)	C2-C1-C6	123.0(4)	C2-C1-C6	122.4(4)
C6-C1-C2	121.0(4)	C6-C1-N1	115.8(9)	C6-C1-C2	123.5(3)	C6-C1-N1	119.5(4)	C6-C1-N1	119.0(4)
C3-C2-C1	119.9(4)	C1-C2-C7	121.4(10)	C1-C2-C3	120.0(3)	C1-C2-C3	119.6(4)	C3-C2-C1	119.6(4)
C4-C3-C2	117.9(4)	C3-C2-C1	117.0(10)	C2-C3-C7	120.5(4)	C4-C3-C2	119.1(5)	C4-C3-C2	118.3(4)
F1-C4-C3	117.8(5)	C3-C2-C7	121.6(10)	C4-C3-C2	117.2(3)	C5-C4-C3	120.3(4)	C3-C4-Br1	118.8(4)
C5-C4-F1	118.8(4)	C2-C3-C4	122.5(11)	C4-C3-C7	122.3(4)	C4-C5-C6	122.3(4)	C5-C4-Br1	118.7(3)
C5-C4-C3	123.4(4)	C5-C4-C3	119.2(10)	C3-C4-C5	122.0(3)	C1-C6-C5	115.7(4)	C5-C4-C3	122.4(4)

C4-C5-C6	118.5(4)	C4-C5-Cl1	119.6(9)	C4-C5-C6	121.7(4)	C1-C6-C7	123.0(4)	C4-C5-C6	120.4(4)
C1-C6-C5	119.2(4)	C4-C5-C6	121.0(11)	C1-C6-C5	115.6(3)	C5-C6-C7	121.4(4)	C1-C6-C5	116.9(4)
N1-C7-Br1	121.2(3)	C6-C5-Cl1	119.4(9)	C1-C6-C8	122.9(3)	C6-C7-C8	110.4(4)	C1-C6-C7	122.6(4)
N1-C7-C8	107.1(3)	C5-C6-C1	117.7(9)	C5-C6-C8	121.5(3)	C6-C7-C9	111.7(4)	C5-C6-C7	120.4(4)
C8-C7-Br1	131.8(3)	N1-C8-Br1	120.9(7)	N1-C9-Br1	121.2(2)	C8-C7-C9	111.6(5)	C6-C7-C8	111.2(3)
C7-C8-C9	103.9(3)	N1-C8-C9	108.1(8)	N1-C9-C10	108.4(2)	N1-C10-Br1	121.8(3)	C6-C7-C9	111.3(4)
C7-C8-C12	123.3(3)	C9-C8-Br1	131.0(7)	C10-C9-Br1	130.4(2)	N1-C10-C11	107.6(3)	C8-C7-C9	111.3(4)
C9-C8-C12	132.3(3)	C8-C9-C10	102.6(7)	C9-C10-C11	103.6(2)	C11-C10-Br1	130.5(3)	N1-C10-Br2	121.1(3)
N2-C9-C8	112.2(3)	C8-C9-C13	126.3(9)	C9-C10-C14	127.0(3)	C10-C11-C12	104.2(3)	N1-C10-C11	108.2(4)
N2-C9-C10	117.6(3)	C10-C9-C13	131.0(9)	C11-C10-C14	129.4(3)	C10-C11-C15	128.1(3)	C11-C10-Br2	130.6(3)
C8-C9-C10	129.9(3)	N2-C10-C9	113.5(8)	N2-C11-C10	112.3(2)	C12-C11-C15	127.5(3)	C10-C11-C12	103.5(3)
O1-C10-O2	124.3(4)	N2-C10-C11	118.5(8)	N2-C11-C12	119.9(3)	N2-C12-C11	112.2(3)	C10-C11-C15	126.4(4)
O1-C10-C9	124.4(4)	C9-C10-C11	127.5(8)	C10-C11-C12	127.3(3)	N2-C12-C13	120.2(3)	C12-C11-C15	129.9(4)
O2-C10-C9	111.1(3)	O1-C11-O2	123.9(10)	O1-C12-O2	124.7(3)	C11-C12-C13	127.5(3)	N2-C12-C11	112.5(4)
O3-C12-O4	124.0(4)	O1-C11-C10	123.7(10)	O1-C12-C11	123.1(3)	O1-C13-O2	124.4(4)	N2-C12-C13	119.3(4)
O3-C12-C8	123.3(4)	O2-C11-C10	112.1(9)	O2-C12-C11	112.2(3)	O1-C13-C12	123.3(4)	C11-C12-C13	128.2(4)
O4-C12-C8	112.5(3)	O3-C13-O4	125.2(10)	O3-C14-O4	125.6(3)	O2-C13-C12	112.2(4)	O1-C13-O2	125.0(5)
		O3-C13-C9	124.7(11)	O3-C14-C10	124.2(3)	O3-C15-O4	124.3(3)	O1-C13-C12	123.4(4)
		O4-C13-C9	110.0(9)	O4-C14-C10	110.1(3)	O3-C15-C11	124.4(3)	O2-C13-C12	111.6(4)
						O4-C15-C11	111.3(3)	O3-C15-O4	125.6(4)
								O3-C15-C11	124.2(4)
								O4-C15-C11	110.3(4)

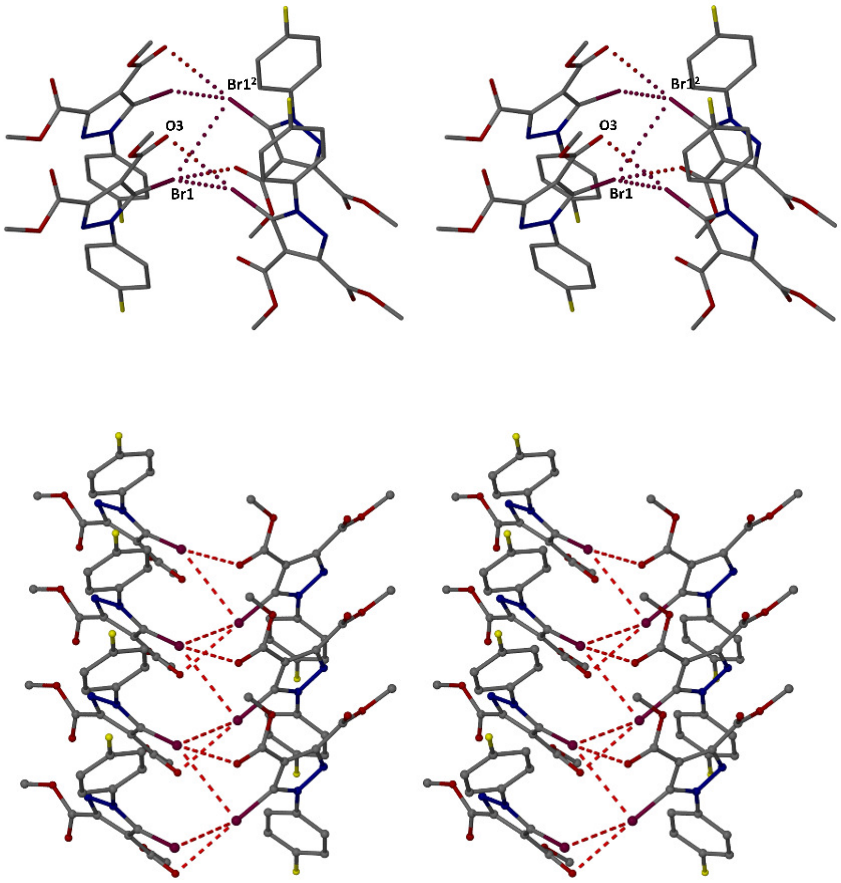


Figure.1S. Stereoscopic view of a short length of a continuous array of halogen bond interactions (top) and a longer representative chain of molecules (bottom) to illustrate the trifurcated halogen bonding. These interactions form a continuum running parallel to the crystal b-axis.

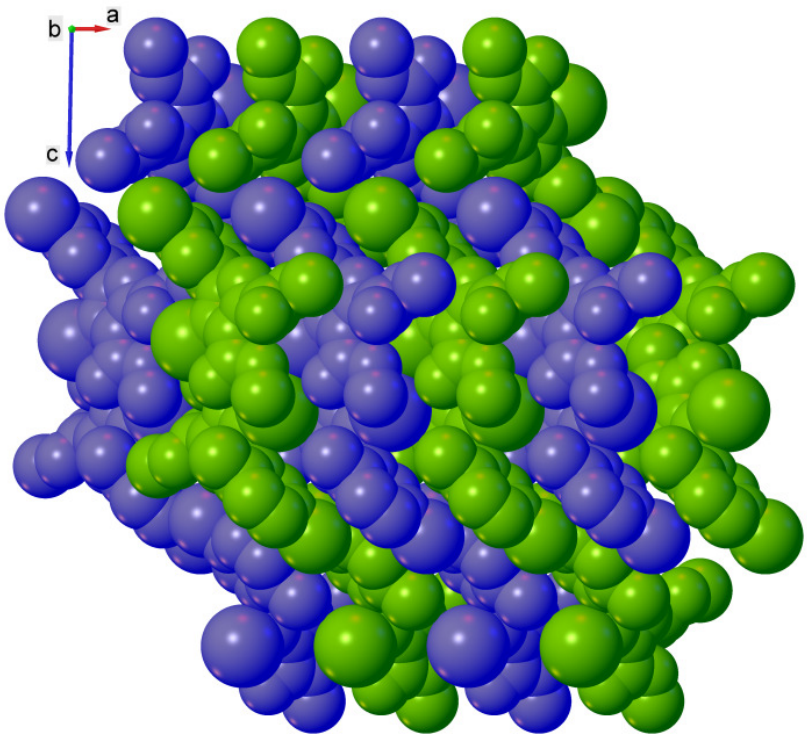


Figure 2S. View of crystal structure in crystal **2** viewed along the *b*-axis showing the parallel packing of 2D layers, space filling representation.

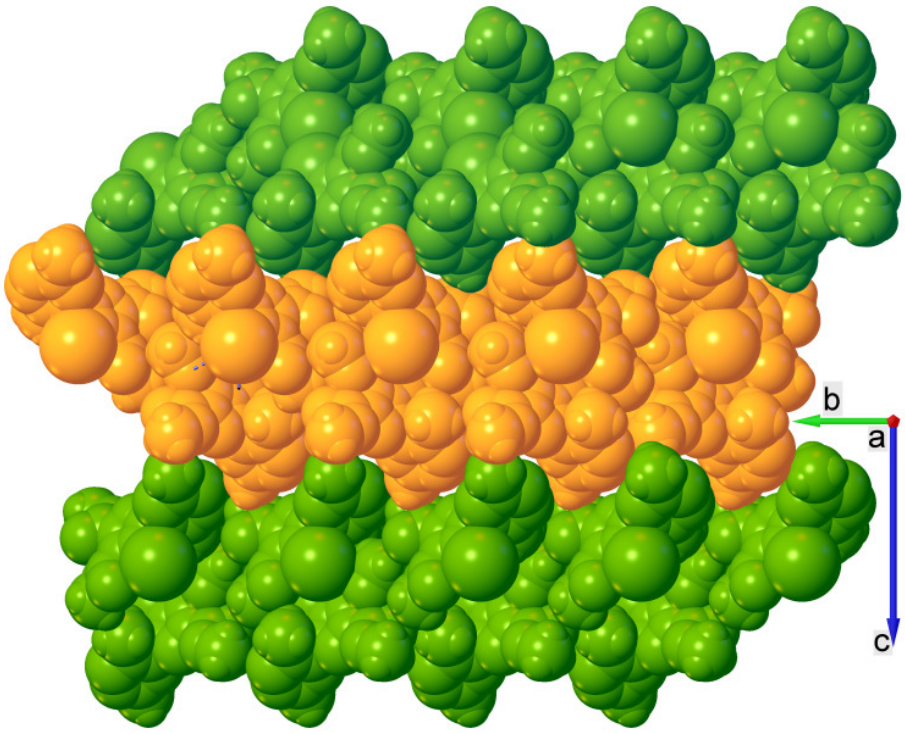


Figure 3S. View of the crystal packing showing the parallel arrangement of 2D layers in crystal **3**, space filling representation.

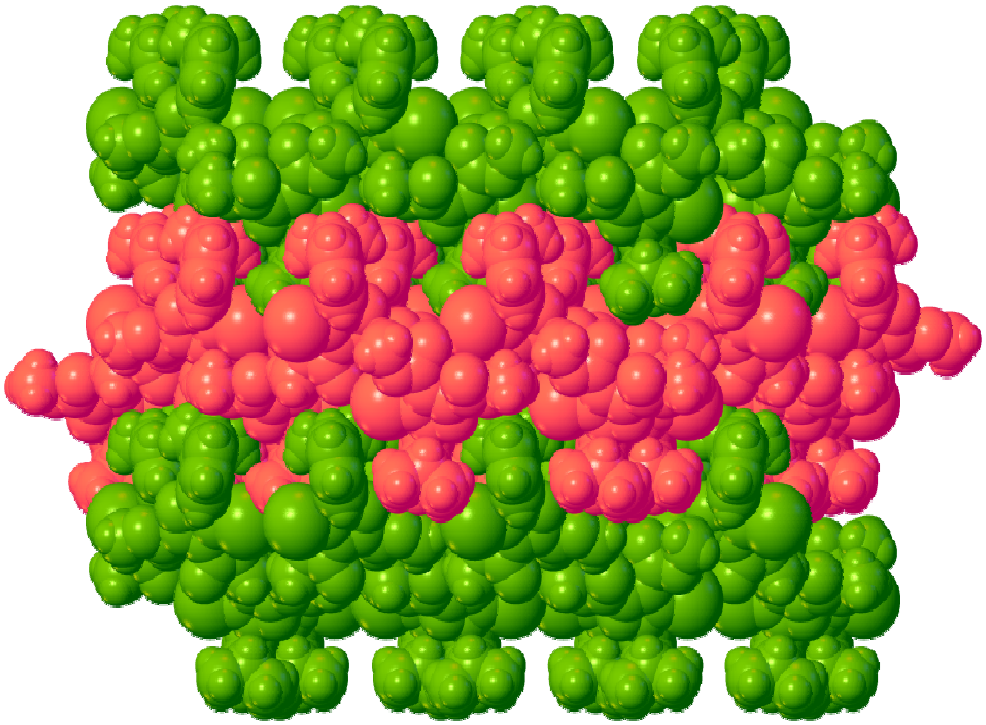
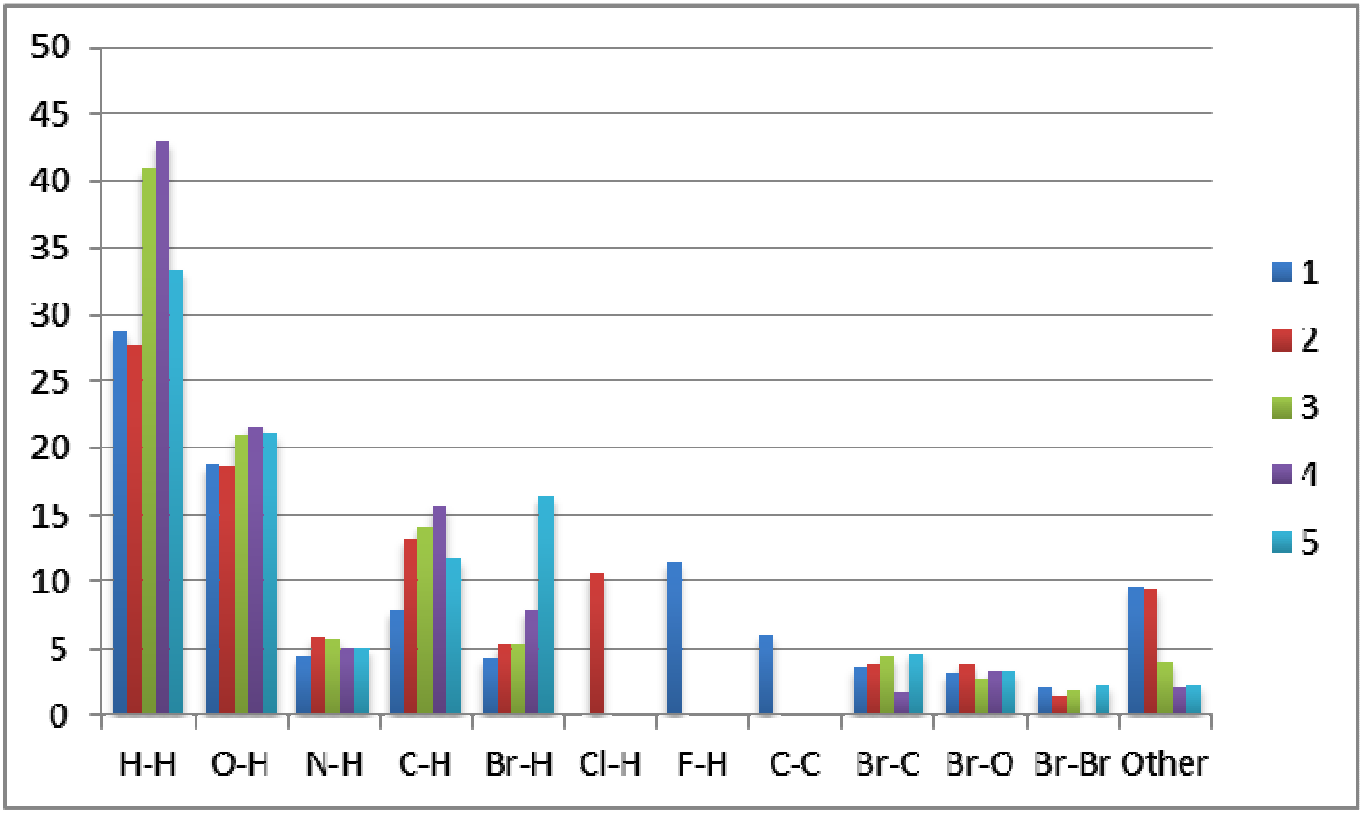


Figure 4S. View of the crystal packing showing the parallel arrangement of 2D layers in crystal **3**, space filling representation.

1. Hirshfield analysis



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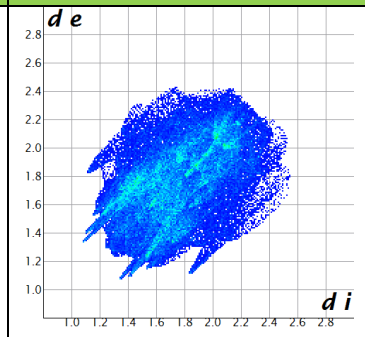
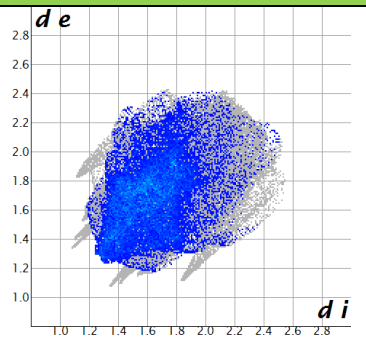
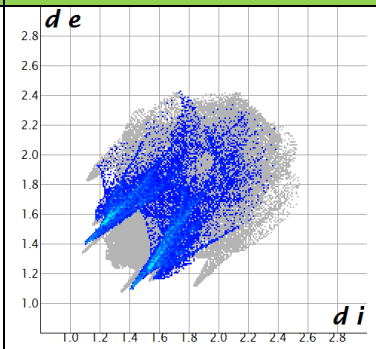
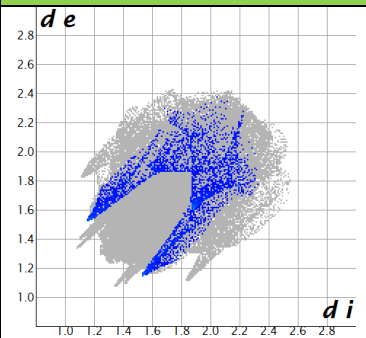
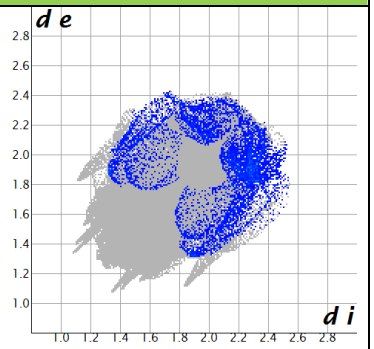
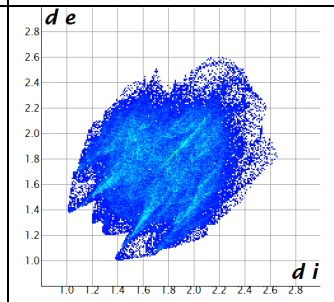
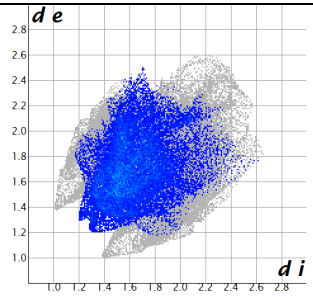
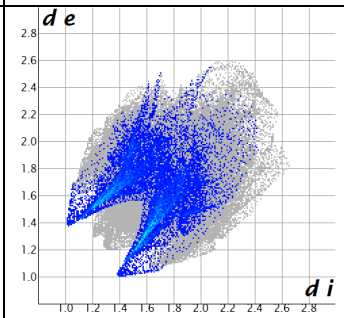
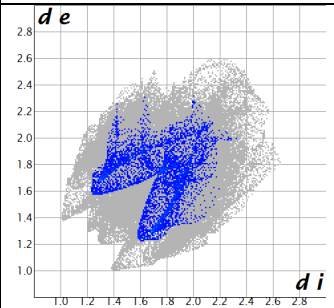
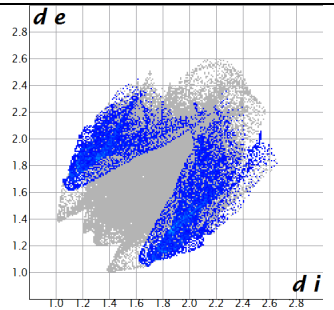
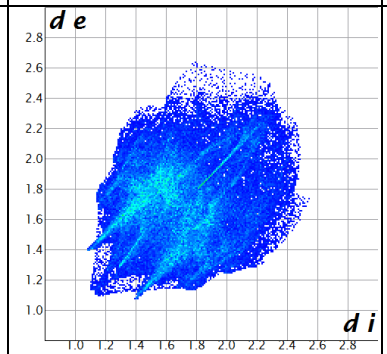
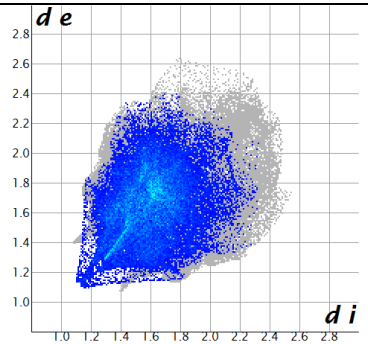
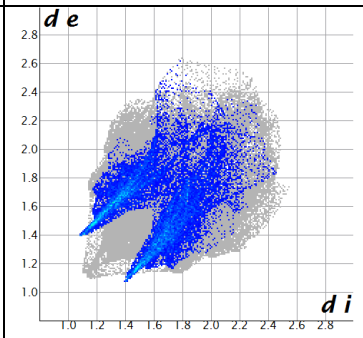
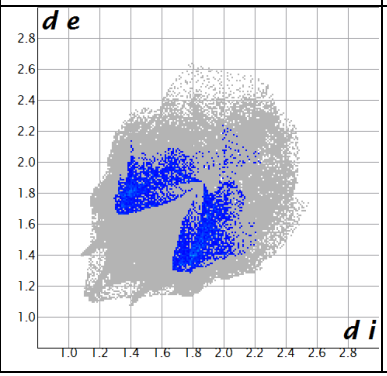
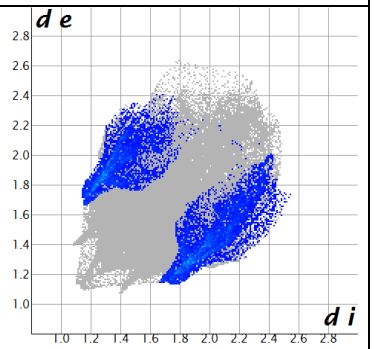
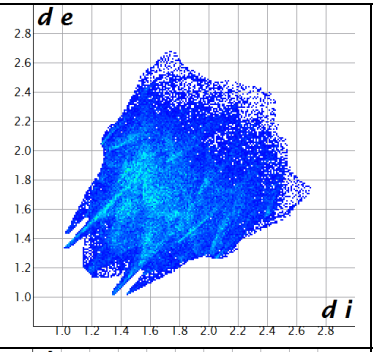
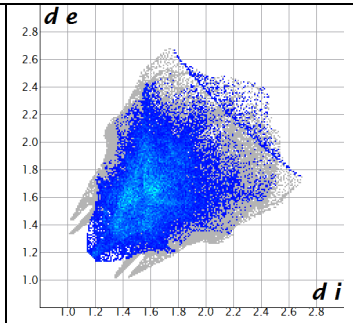
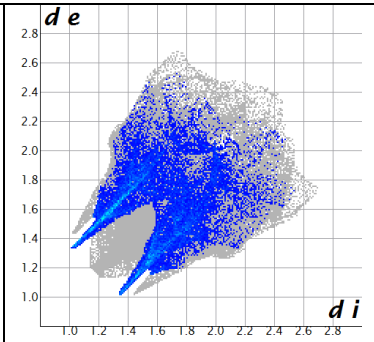
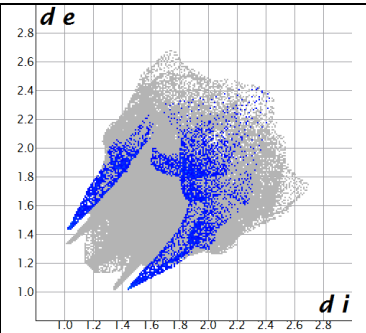
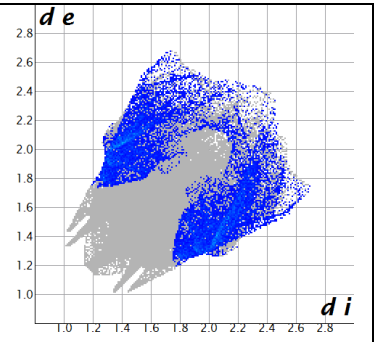
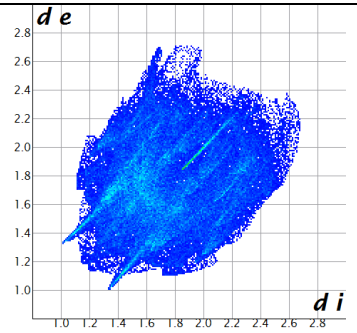
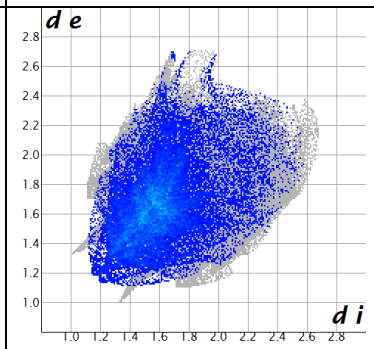
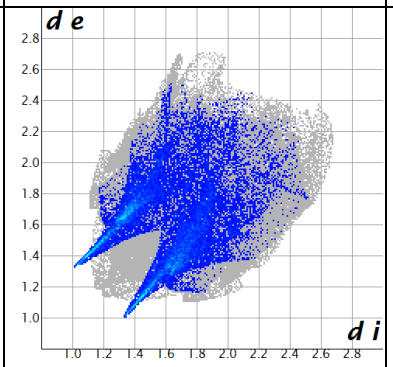
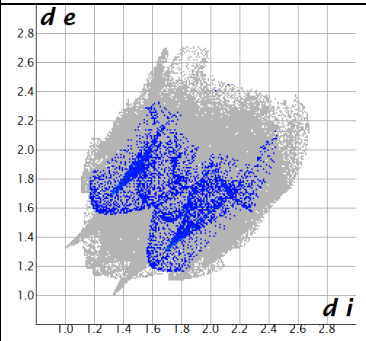
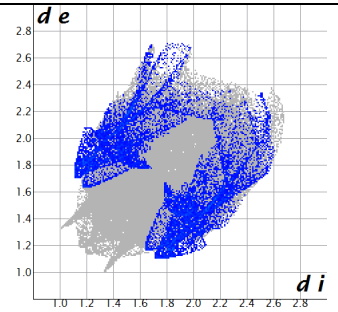
1					
2					
3					

4					
5					
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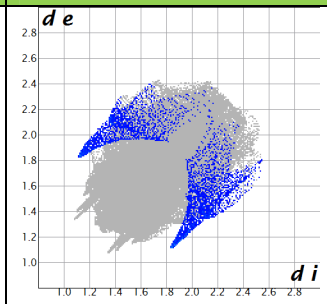
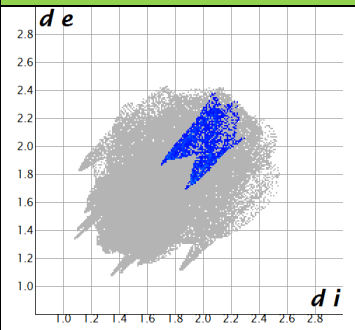
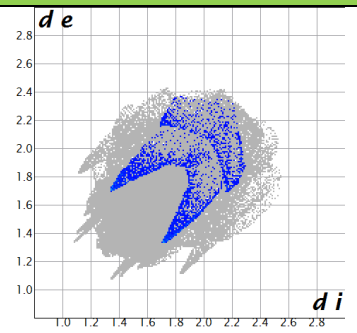
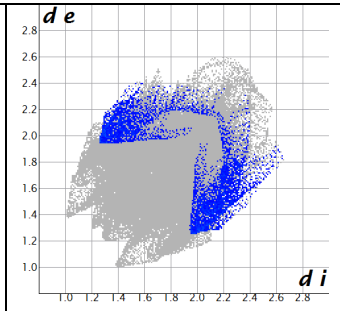
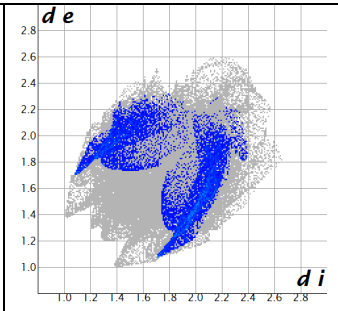
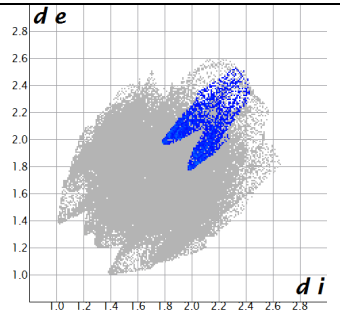
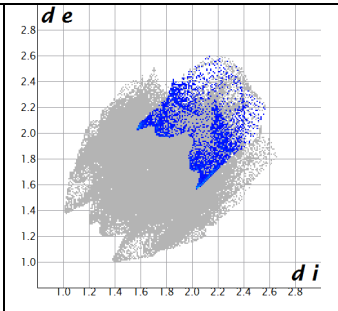
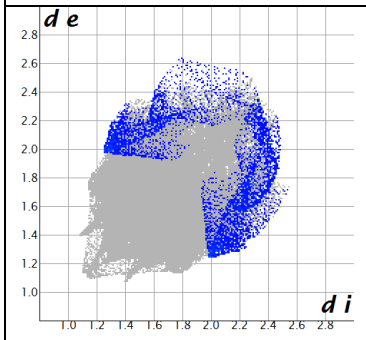
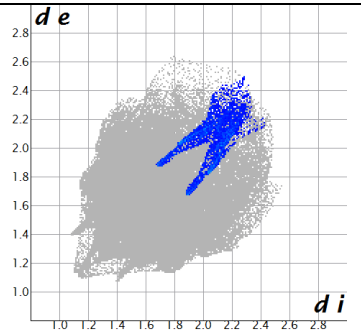
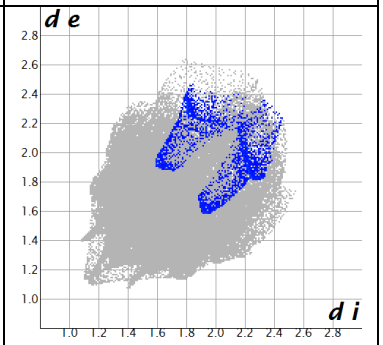
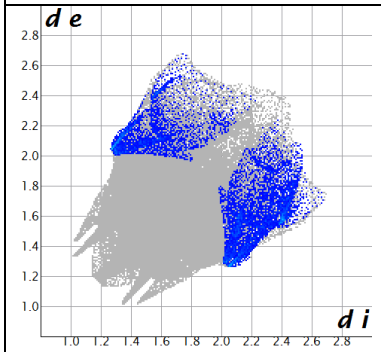
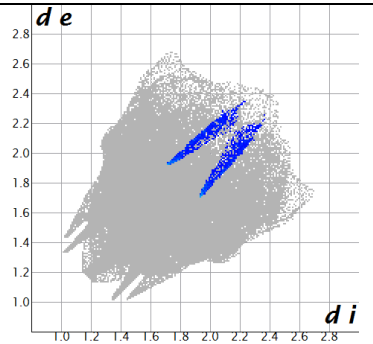
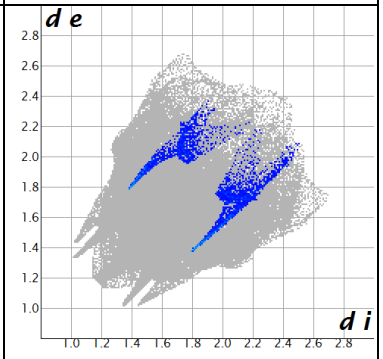
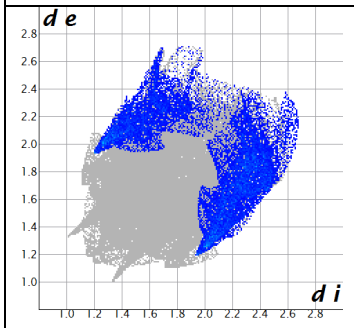
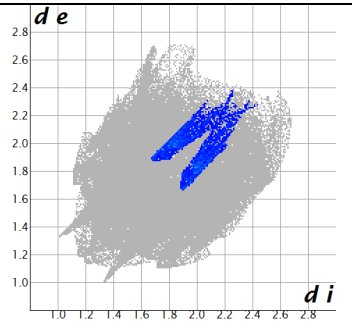
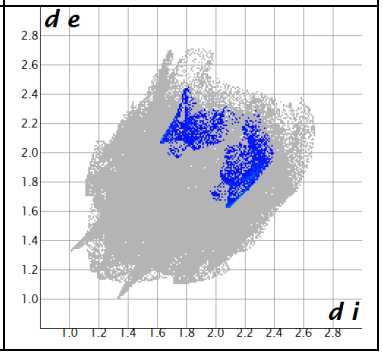
			NA		

					
			NA		
			NA		
4			NA		

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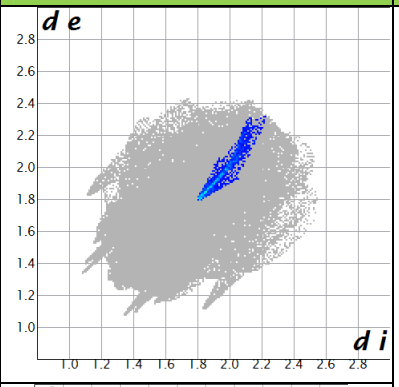
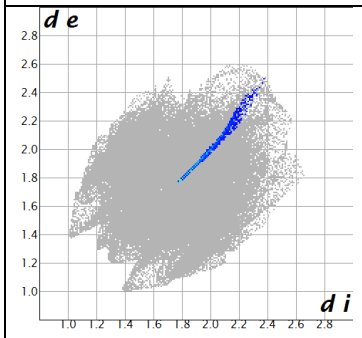
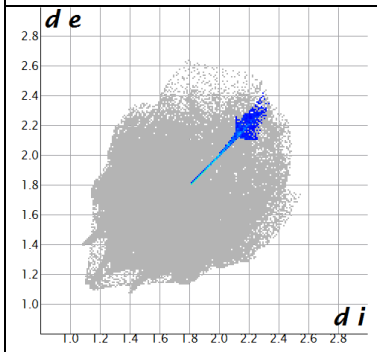
1			
2			
3			
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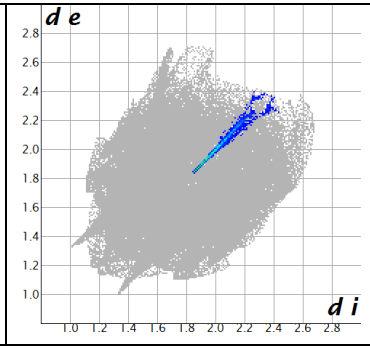
5		 d e 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 d i 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4 2.6 2.8	