Solid-state Supramolecular Architectures of a Series of Hg(II) Halide Coordination Compounds Based on Hydroxyl-substituted Schiff Base Ligands

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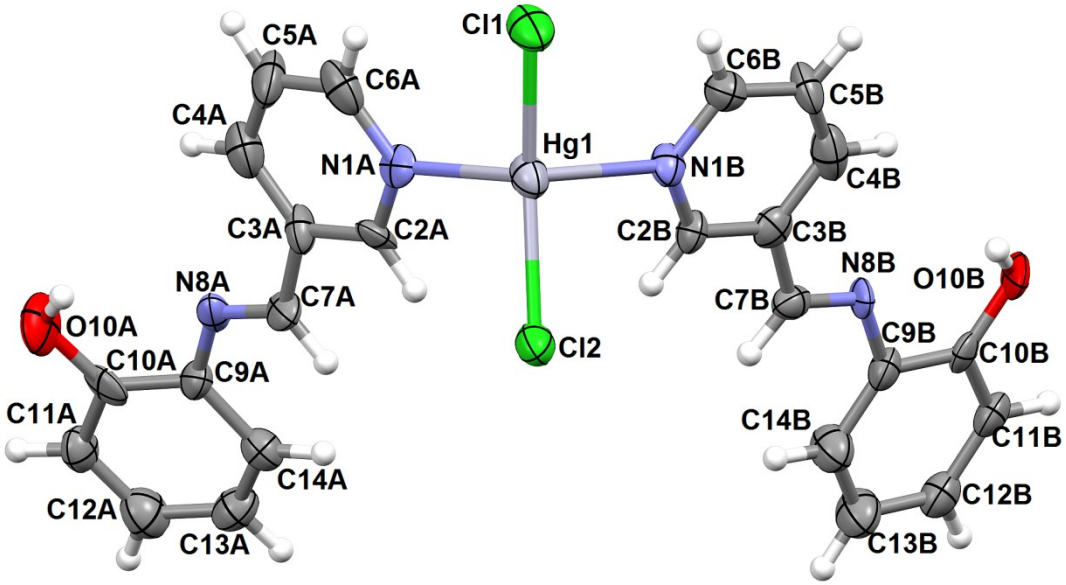
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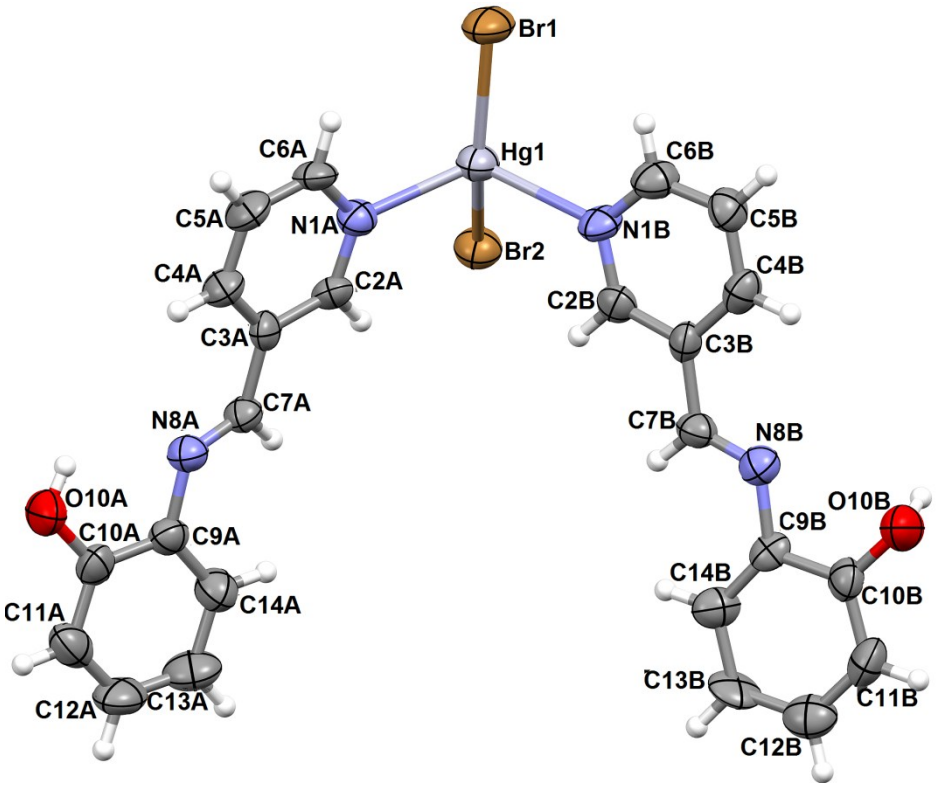
C6A
C4A
N1A
Hg1
N1B
C6B
C5B
C4B
C3A
C2A
C2B
C3B
N8A
C7A
O10A
C10A
C9A
Cl2
N8B
O10B
C7B
C9B
C10B
C11A
C14A
C12A
C13A
C14B
C11B
C12B
C13B

(a)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C6A
Hg1
C6B
C5A
N1A
N1B
C5B
Br2
C4A
C2A
C4B
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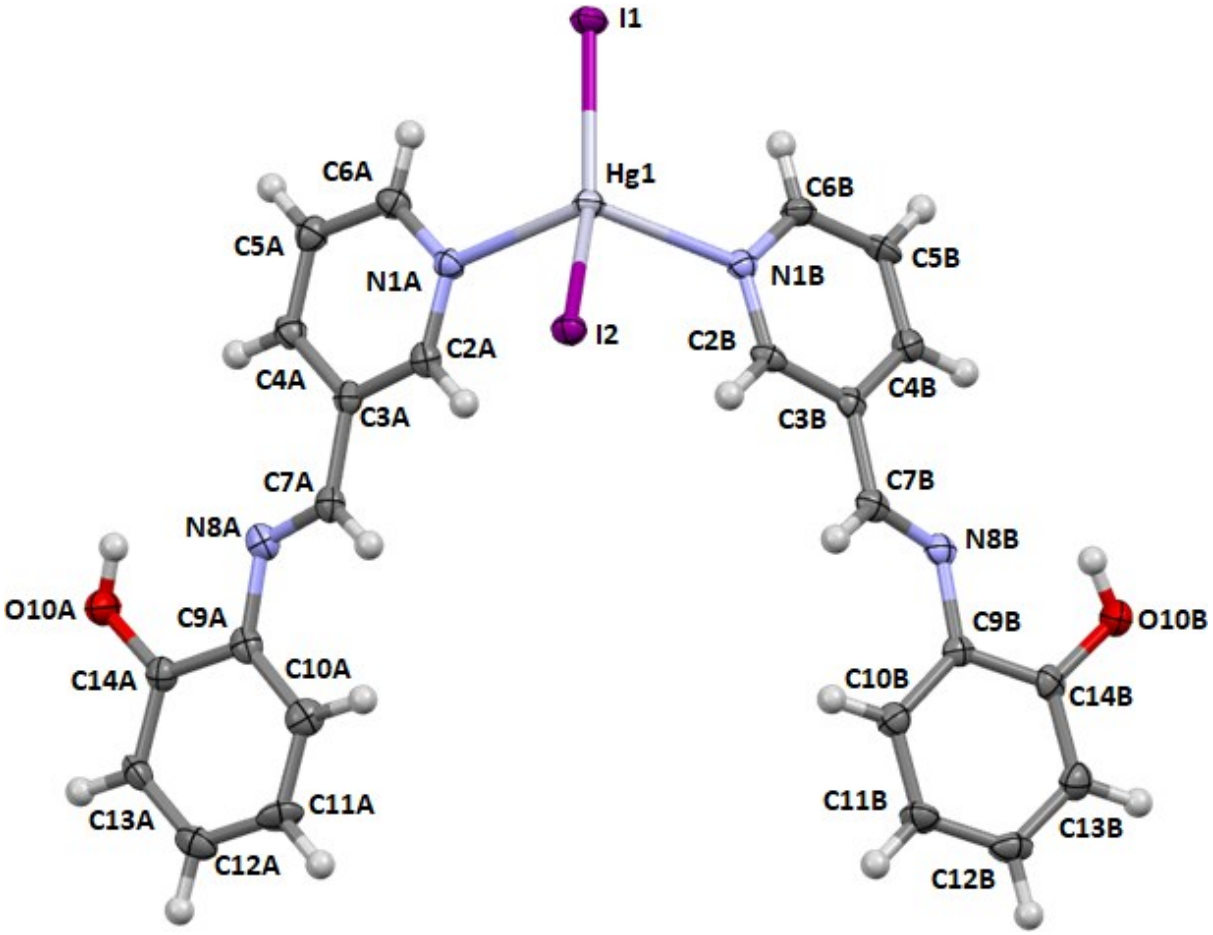
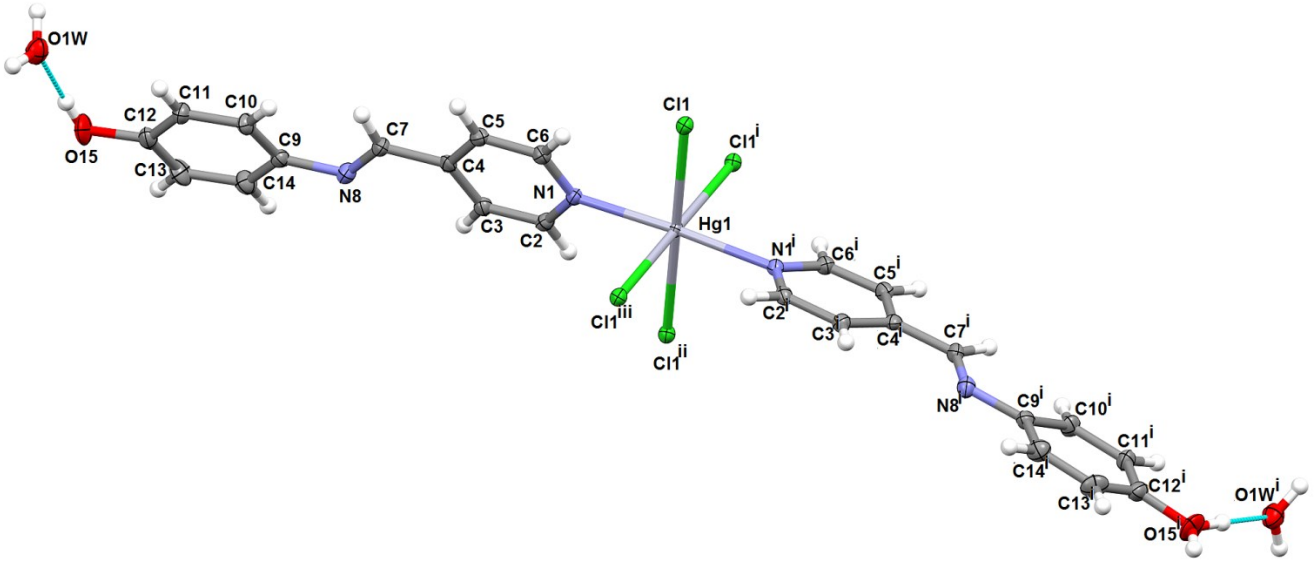
C3B
C7A
N8A
C7B
N8B
O10A
C10A
C9A
O10B
C9B
C14B
C11A
C14A
C10B
C13B
C12A
C13A
C11B
C12B

(b)


I1
Hg1
I2
C6A
C5A
N1A
C2A
C4A
C3A
C7A
N8A
O10A
C9A
C14A
C10A
C13A
C11A
C12A
C6B
C5B
N1B
C2B
C4B
C3B
C7B
N8B
C9B
O10B
C10B
C14B
C11B
C13B
C12B

(c)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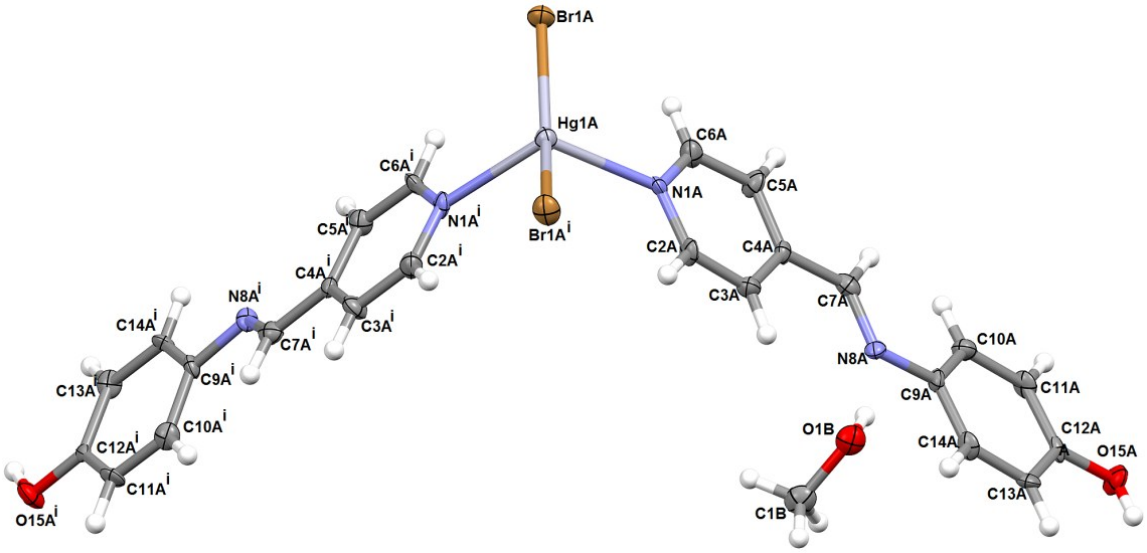
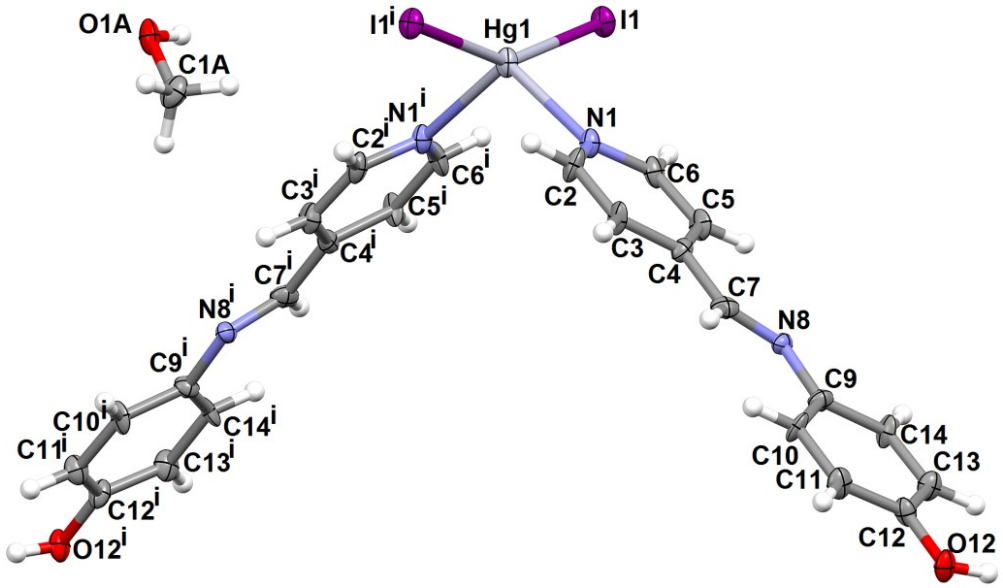
O15
C11
C10
C12
C9
C13
C14
N8
C7
C5
C6
C4
N1
C3
C2
Cl1
Cl1i
Hg1
Cl1iii
Cl1ii
N1i
C6i
C5i
C2i
C3i
C4i
C7i
N8i
C9i
C10i
C11i
C14i
C13i
C12i
O15i
O1Wi

(d)



(e)



(f)

Figure S1. Molecular structure of compound **1**(a), **2** (b), **3** (c), **4**(d), **5** (e) and **6** (f) with all non-hydrogen atoms labelled. Thermal displacement given as 50% probability in the crystal structure. For structure **4**, i: ½-x,y, 1-z; ii: ½-x,1+y, 1-z; x, 1+y, z. For structure **5**, i: -x,1-y, z. For structure **6**, i: 1-x,1-y, z.

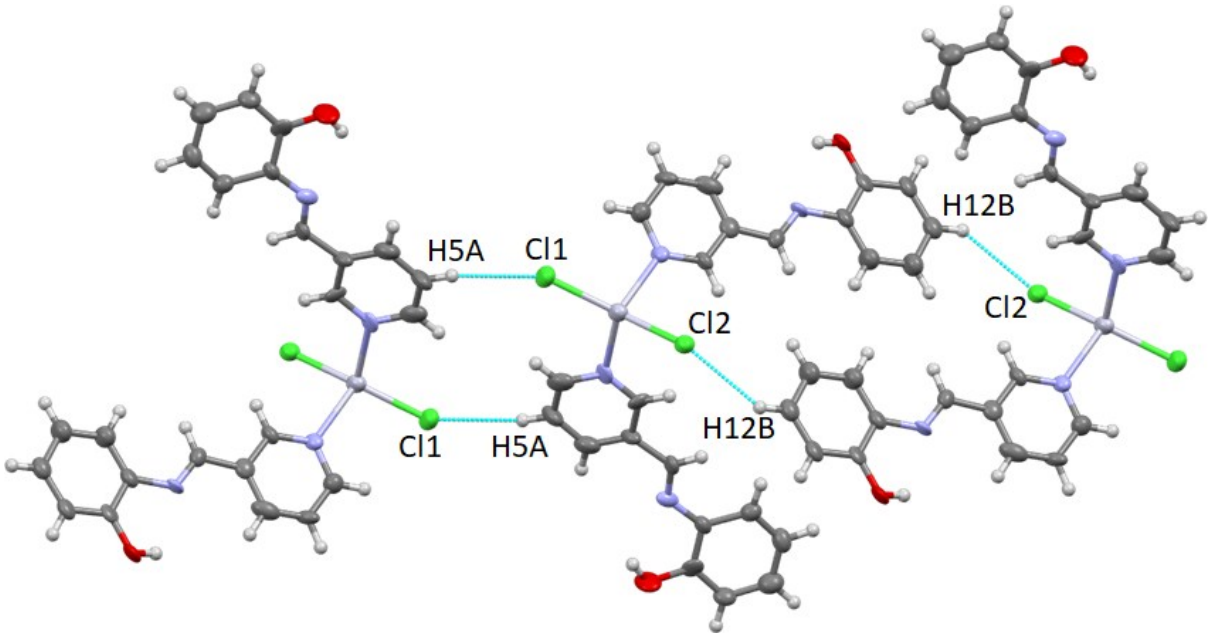


Figure S2: Expanded view of compound **1** showing the reciprocal interaction between C5A–H5A···Cl1 (2.792(6) Å, 145.4(17)°) and C12B–H12B···Cl2 (2.858(6) Å, 138.8(14)°).

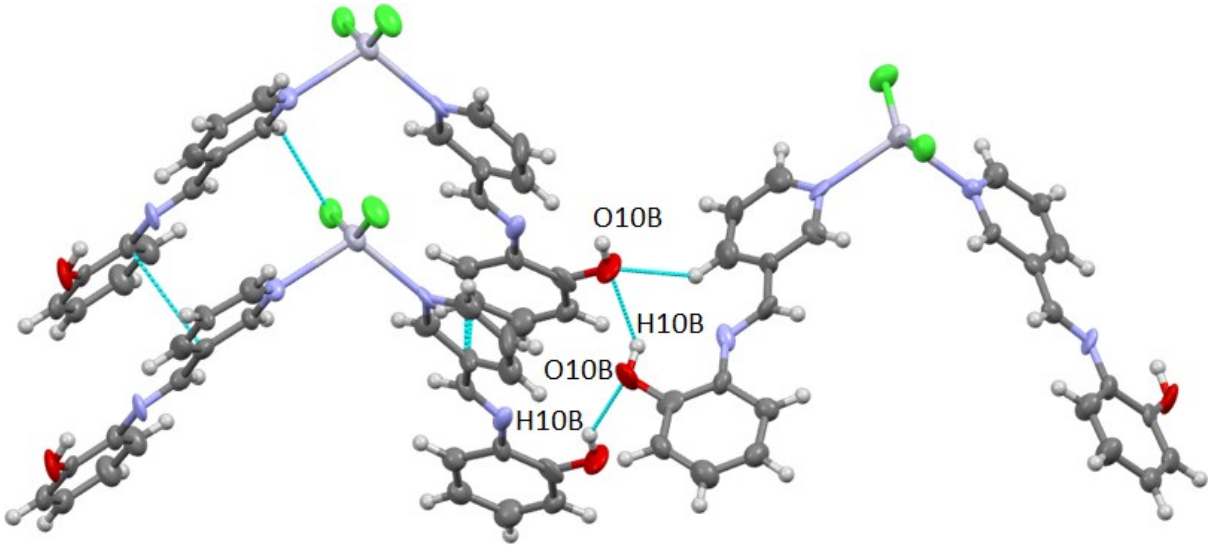


Figure S3: Expanded view of compound **1** hydrogen bonding between the phenol groups (O10B–H10B···O10B (2.251(18) Å, 140.2(7)°)).

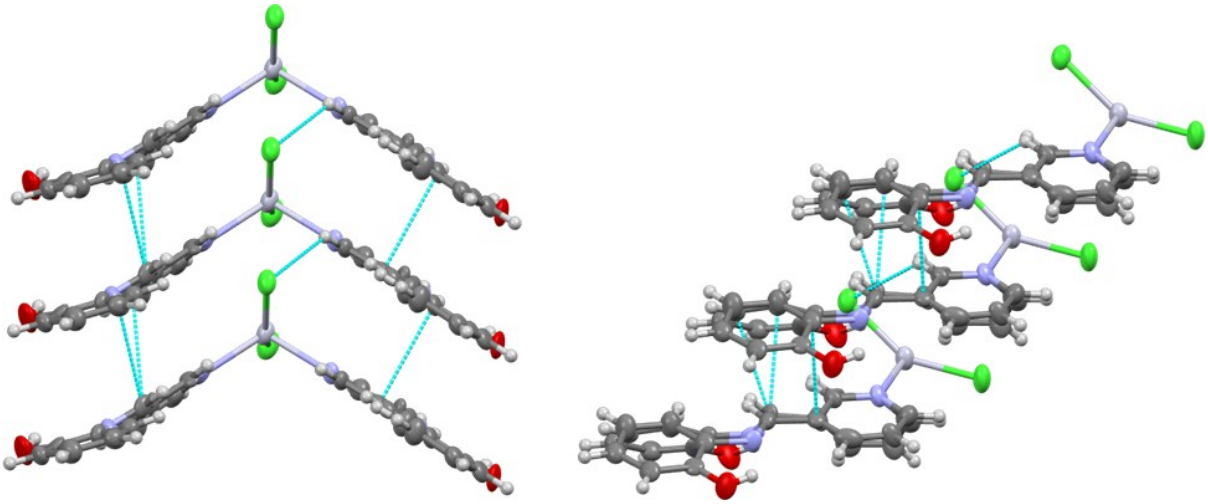


Figure S4: Expanded view of compound **1** showing front (left) and side (right) view of the stacking pattern. Hg···Hg separation is 4.796(4) Å.

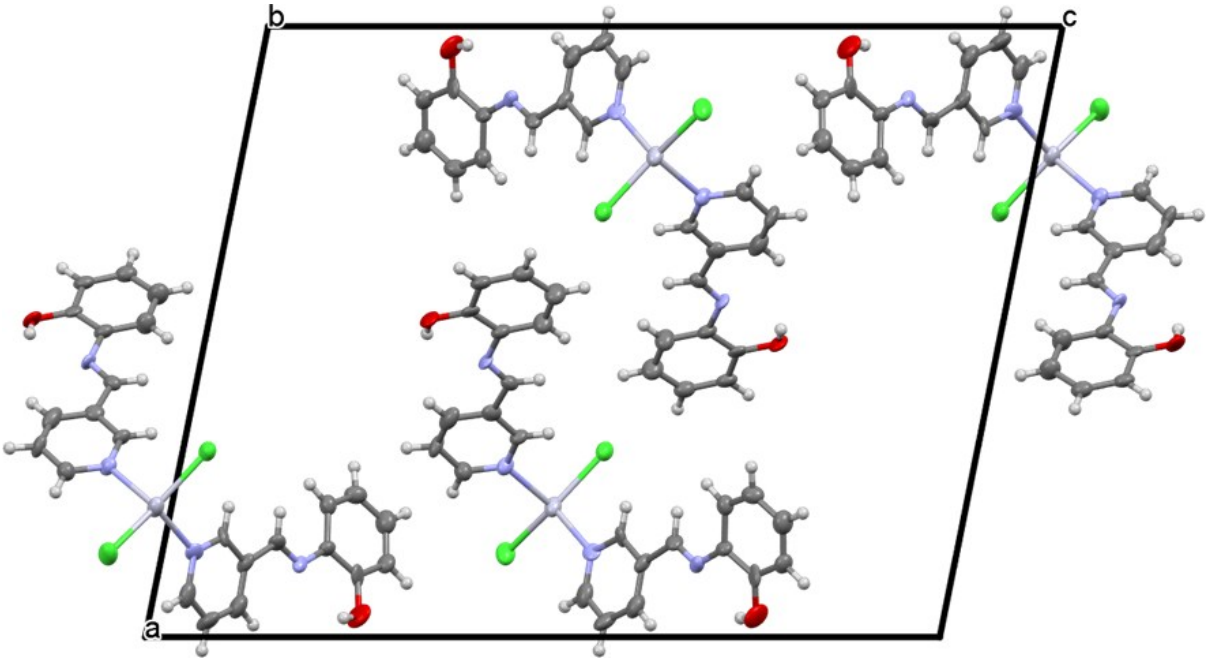


Figure S5: Crystal packing of compound **1** looking down the *b*-axis.

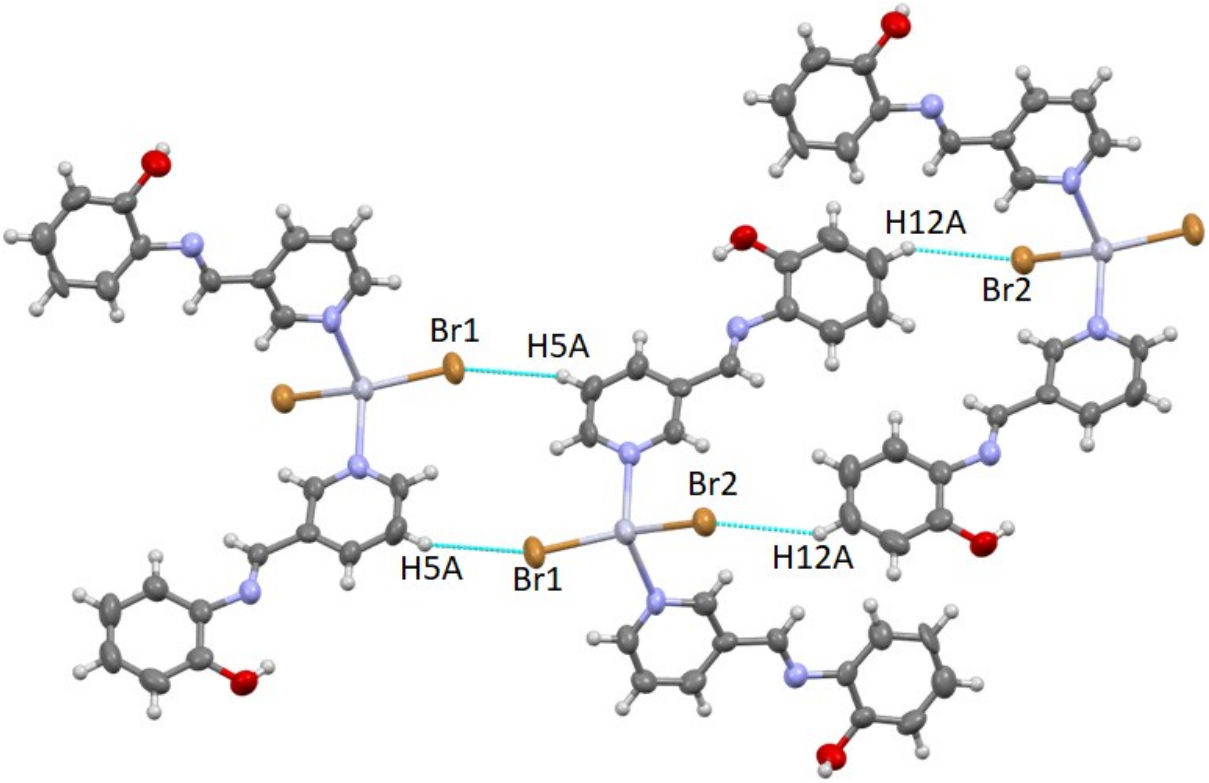


Figure S6: Expanded view of compound **2** showing the reciprocal interaction between C5A–H5A···Br1 (3.029(15) Å, 134.0(9)°) and C12A–H12A···Br2 (3.079(14) Å, 145.9(10)°).

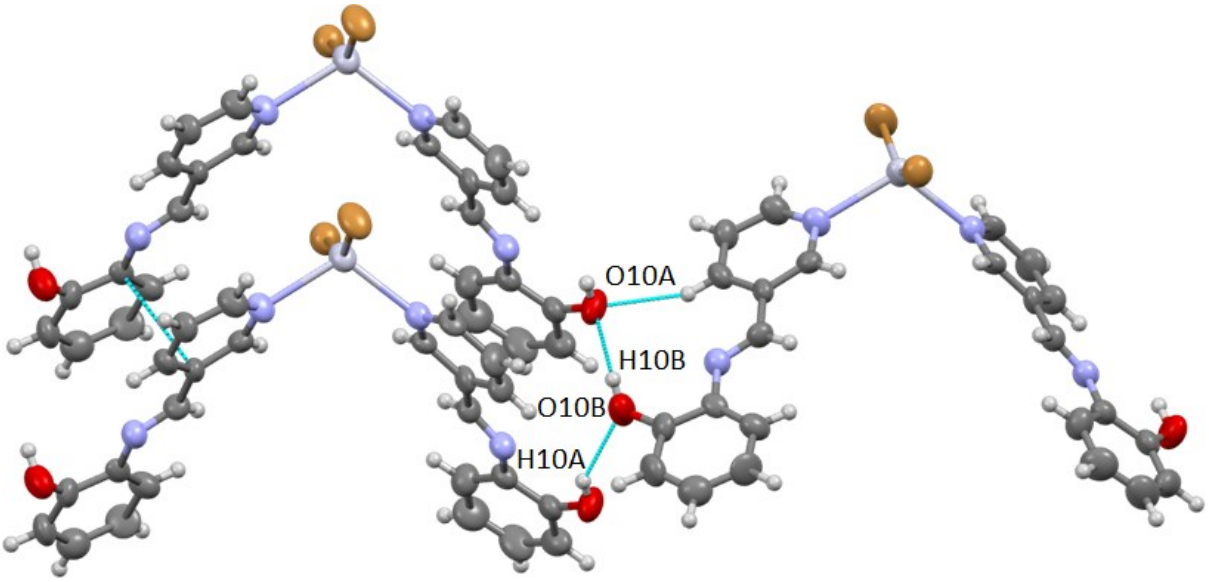


Figure S7: Expanded view of compound **2** hydrogen bonding between the phenol groups (O10B–H10B···O10A (2.397(10) Å, 123.5(8)°)) and (O10A–H10A···O10B (2.317(10) Å, 141.3(7)°)).

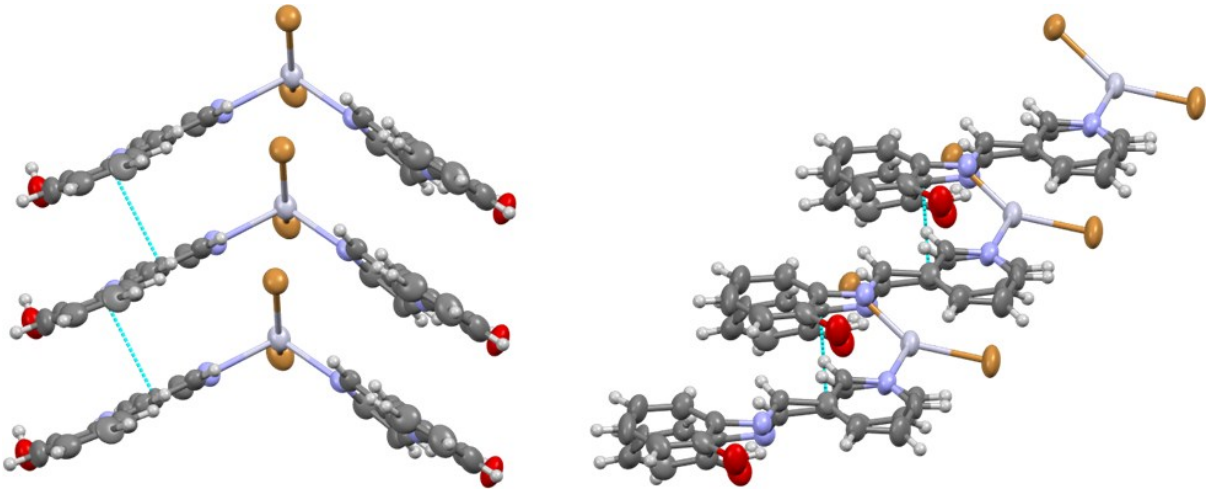


Figure S8: Expanded view of compound **2** showing front (left) and side (right) view of the stacking pattern. Hg···Hg separation is 4.931(14) Å.

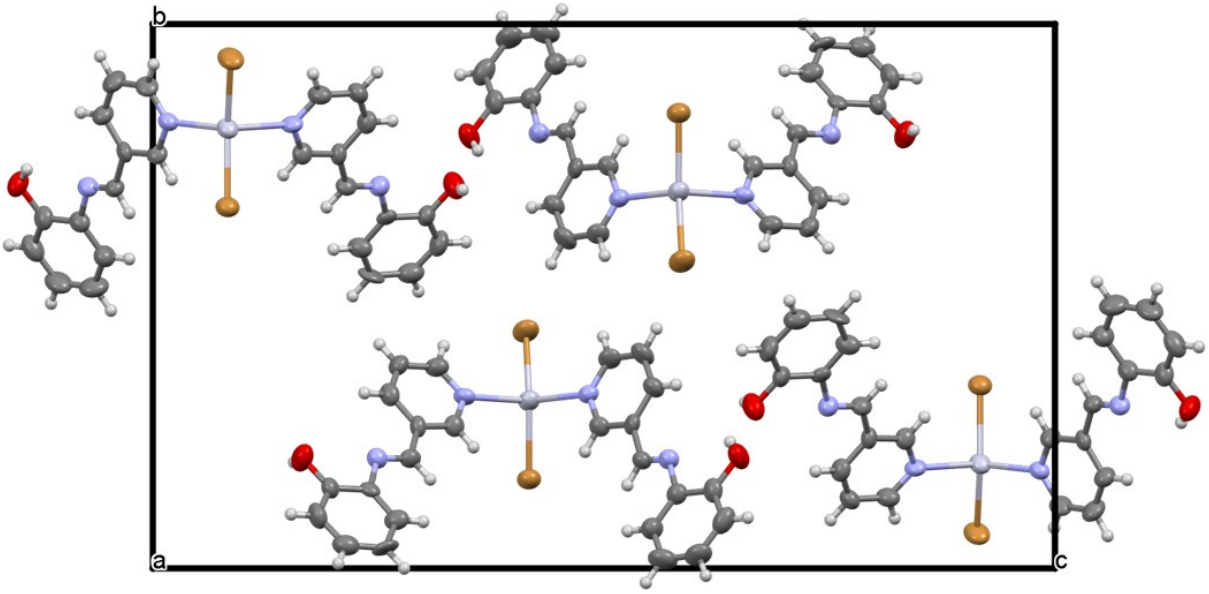


Figure S9: Crystal packing of compound **2** looking down the *a*-axis.

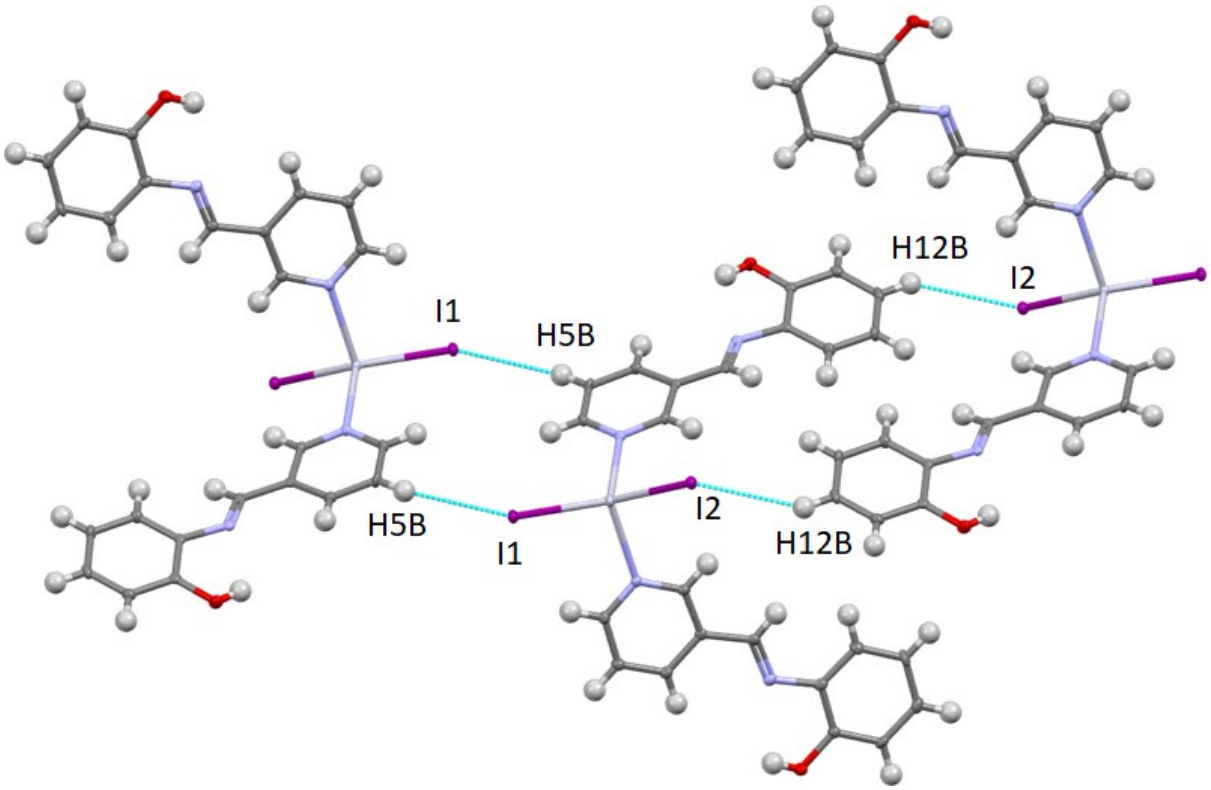


Figure S10: Expanded view of compound **3** showing the reciprocal interaction between C5B–H5B···I1 (3.087(1) Å, 135.0(3)°) and C12B–H12B···I2 (3.132(1) Å, 141.2(2)°).

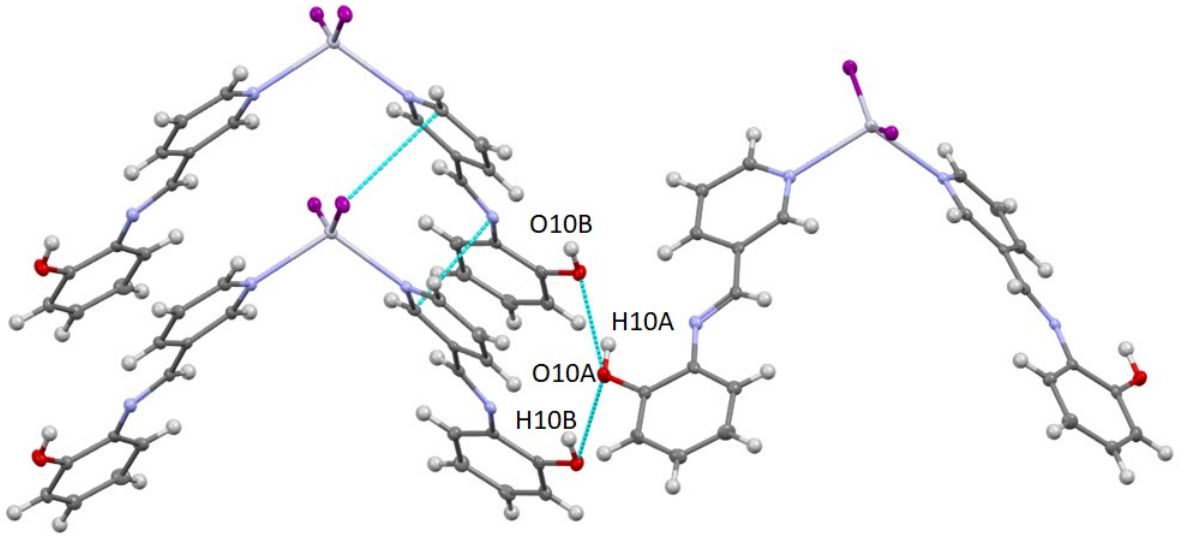


Figure S11: Expanded view of compound **3** hydrogen bonding between the phenol groups (O10B–H10B···O10A (2.230(4) Å, 142.0(5)°)) and (O10A–H10A···O10B (2.070(5) Å, 152.0(5)°)).

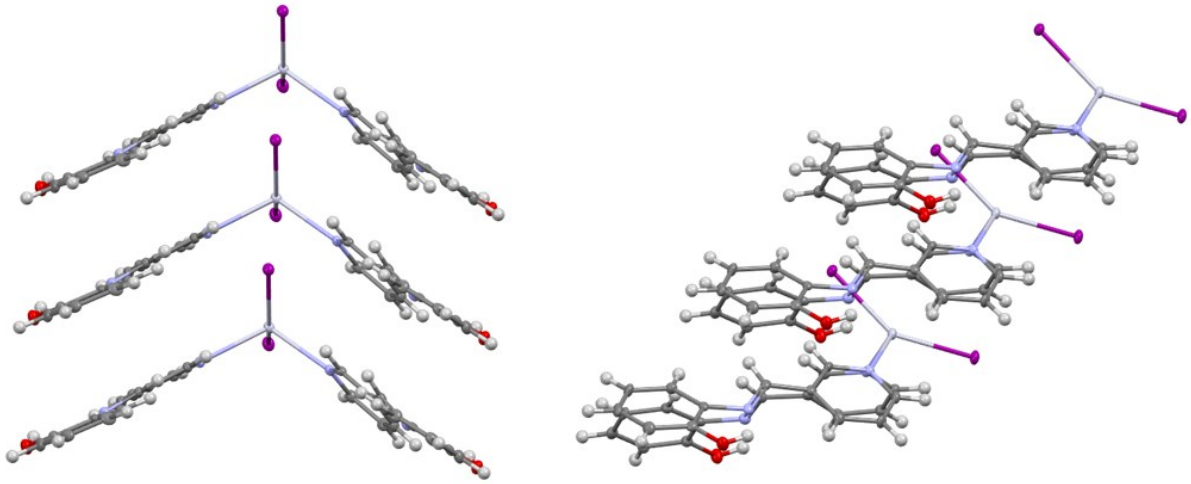


Figure S12: Expanded view of compound **3** showing front (left) and side (right) view of the stacking pattern. Hg···Hg separation is 4.913(3) Å.

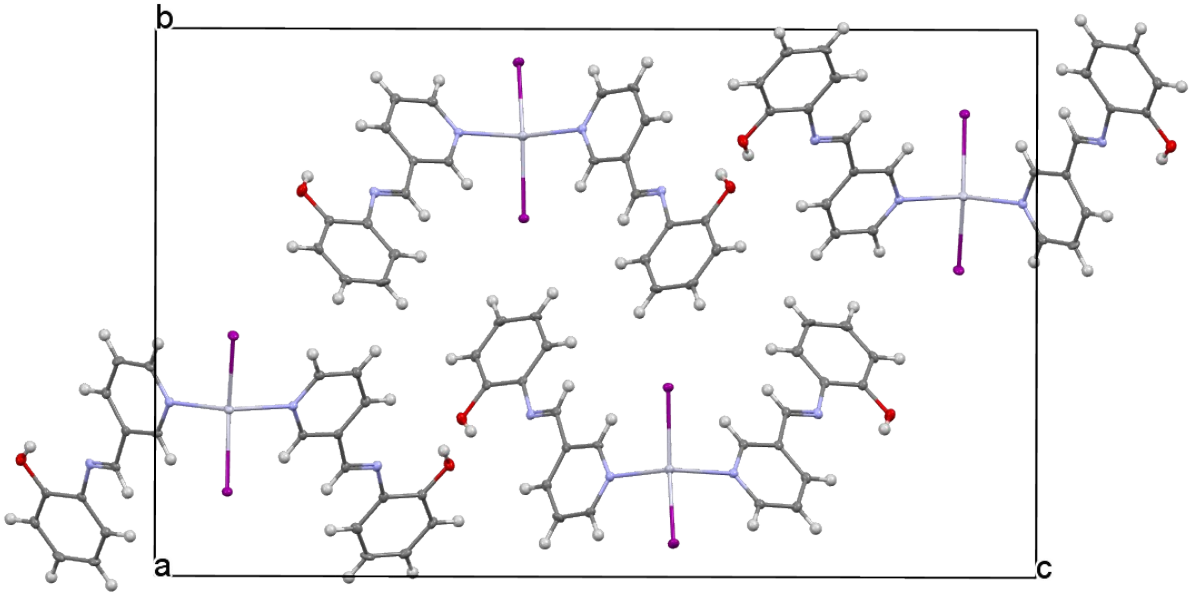


Figure S13: Crystal packing of compound **3** looking down the *a*-axis.

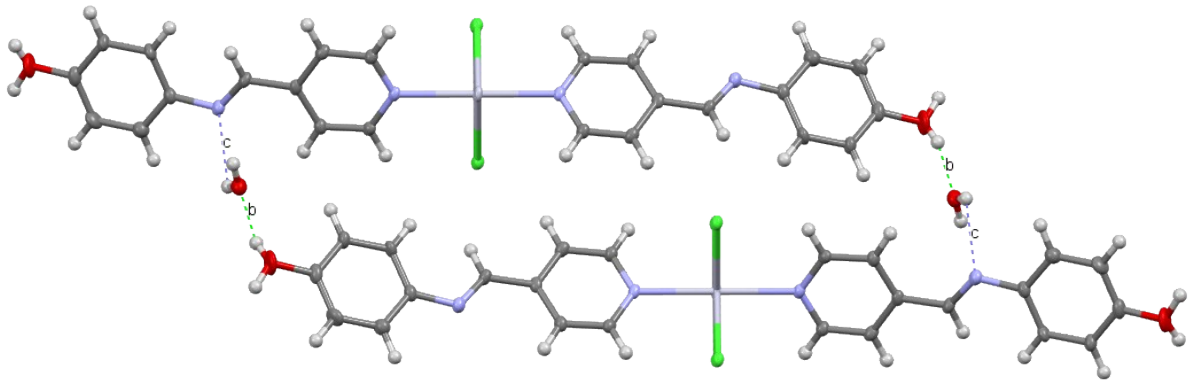


Figure S14: Expanded structure of compound **4** showing the solvent interactions between molecules.

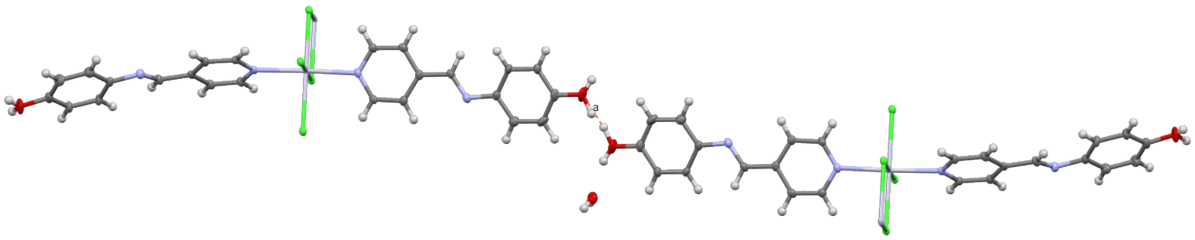


Figure S15: Expanded structure of compound **4** showing the hydrogen bonding between molecular units.

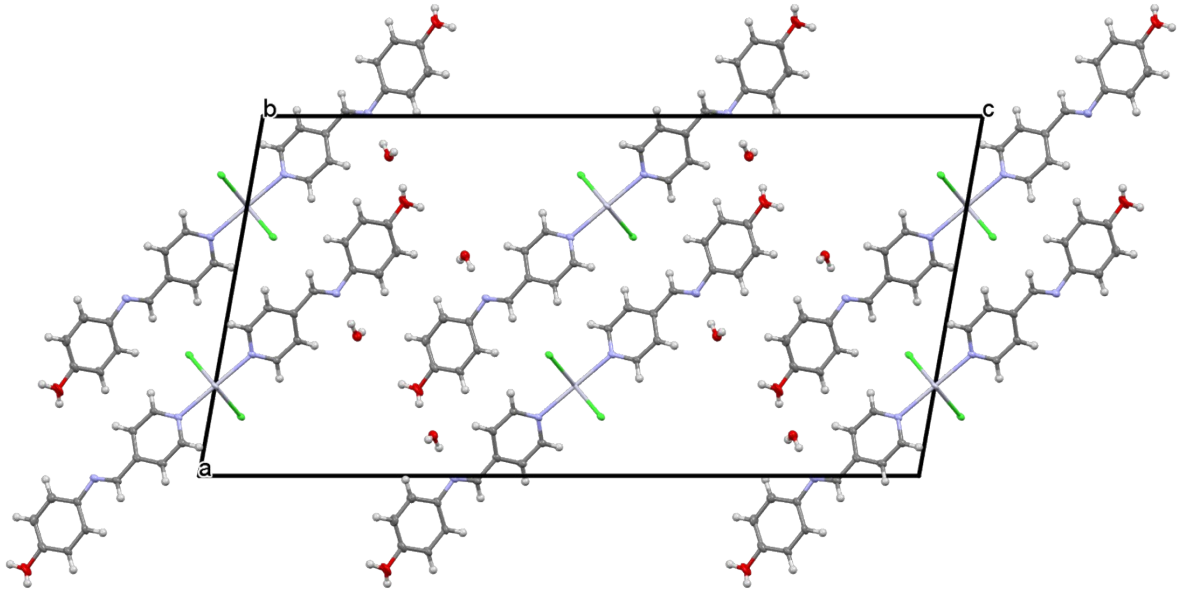


Figure S16: Crystal packing of compound **4** looking down the *b*-axis.

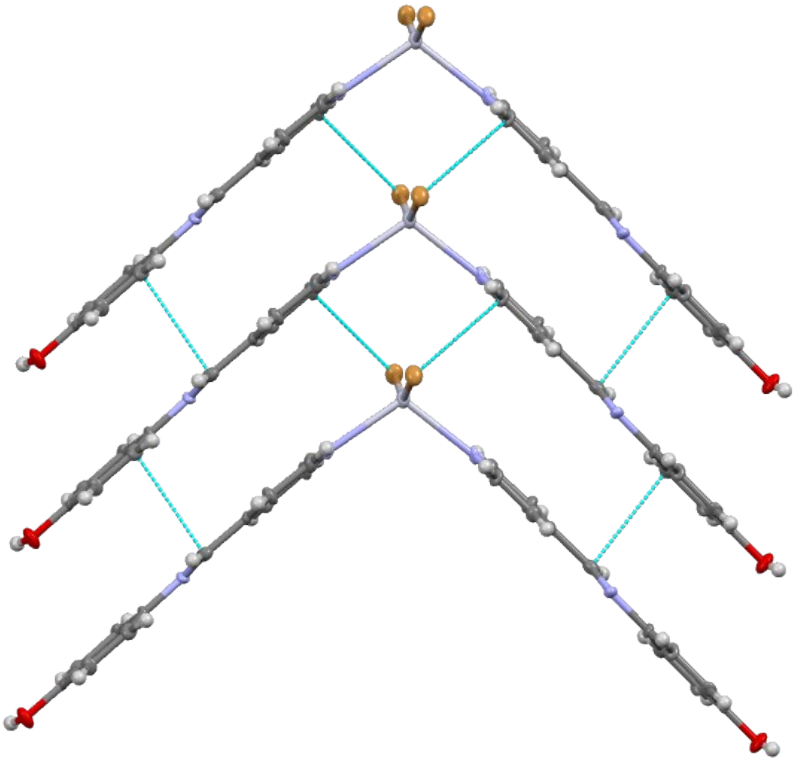


Figure S17: Expanded structure of compound **5** showing the stacking pattern.

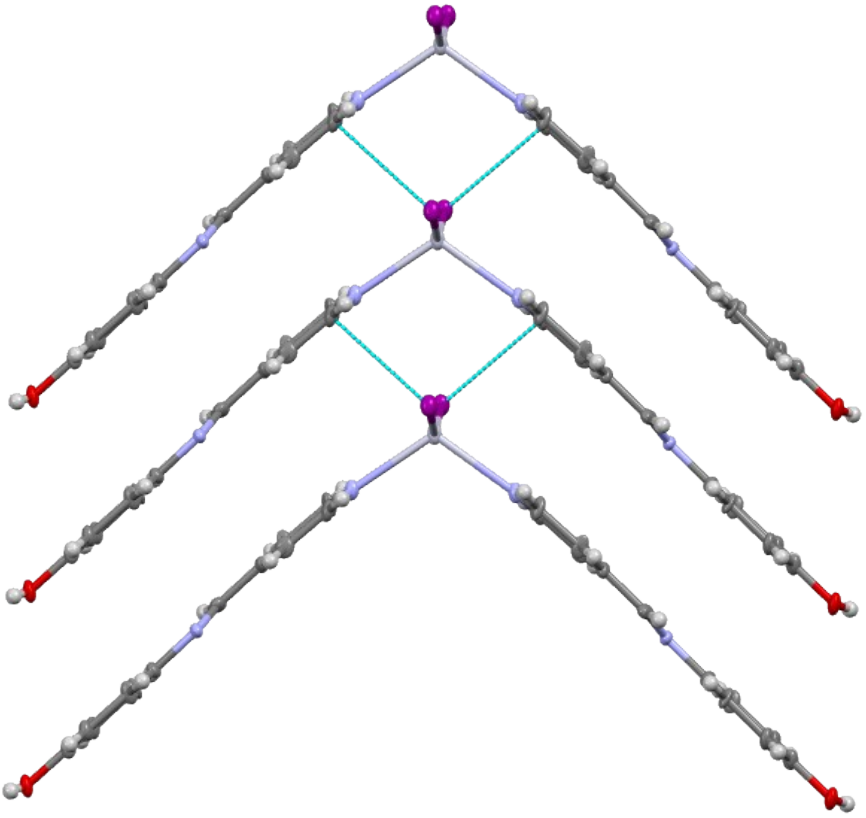


Figure S18: Expanded structure of compound **6** showing the stacking pattern

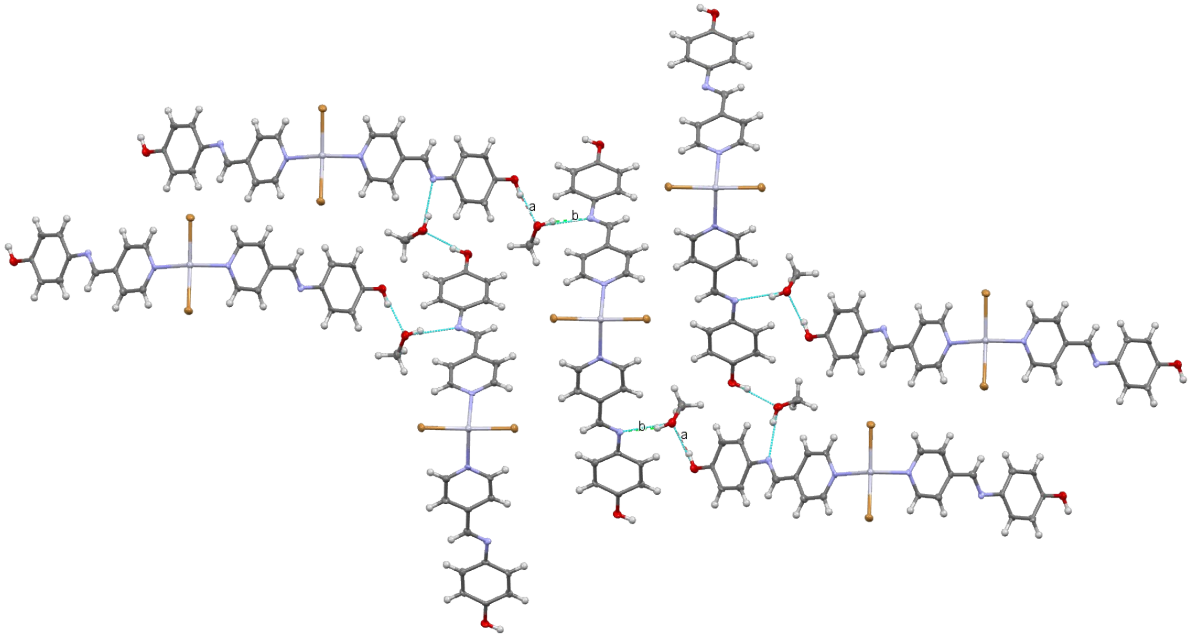


Figure S19: Expanded structure of compound **5** showing the hydrogen bonding between individual molecular units and solvent molecules.

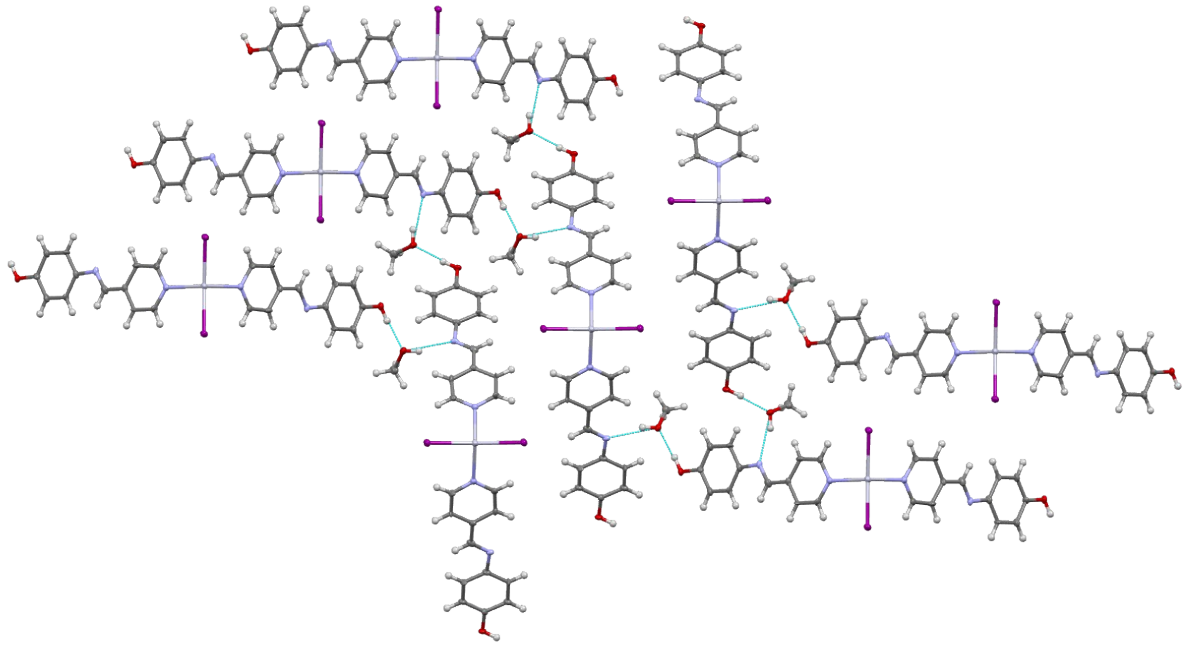


Figure S20: Expanded structure of compound **6** showing the hydrogen bonding between individual molecular units and solvent molecules.

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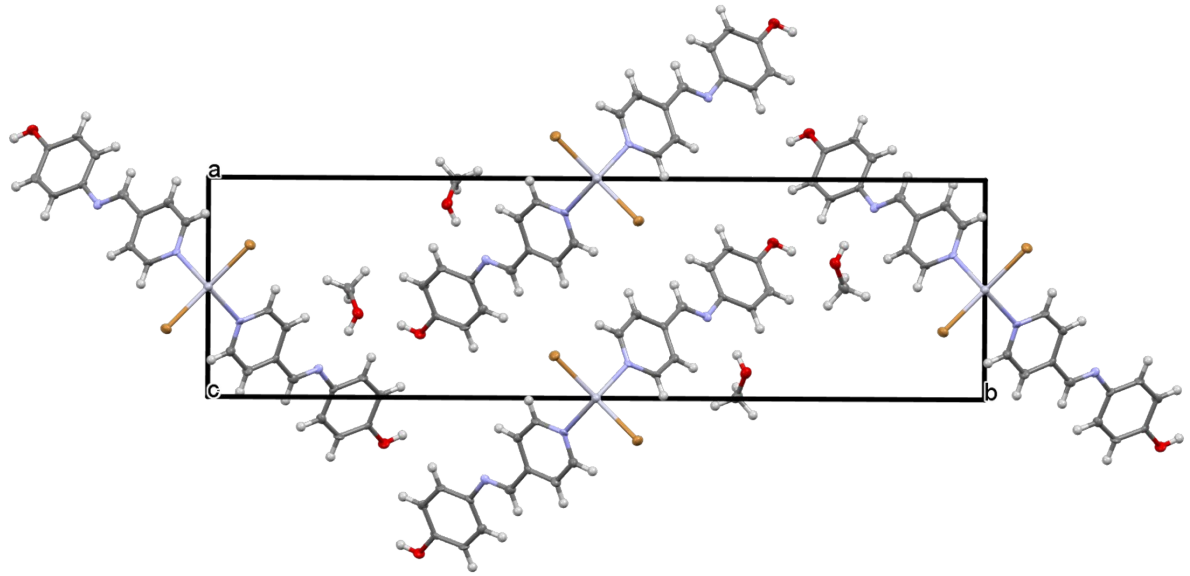


Figure S21: Crystal packing of compound **5** looking down the *c*-axis

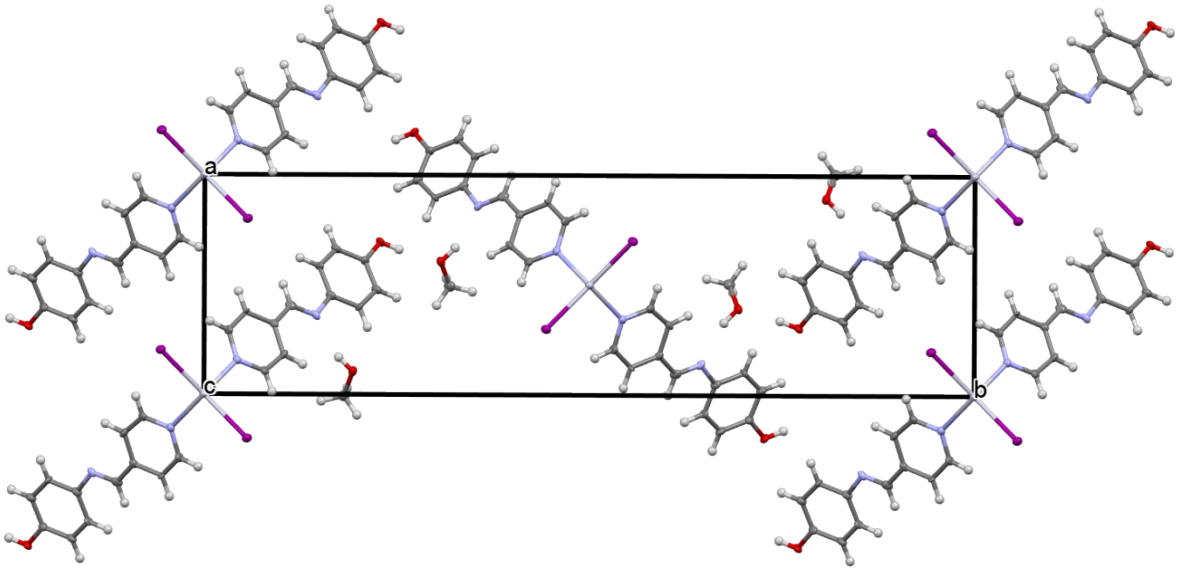
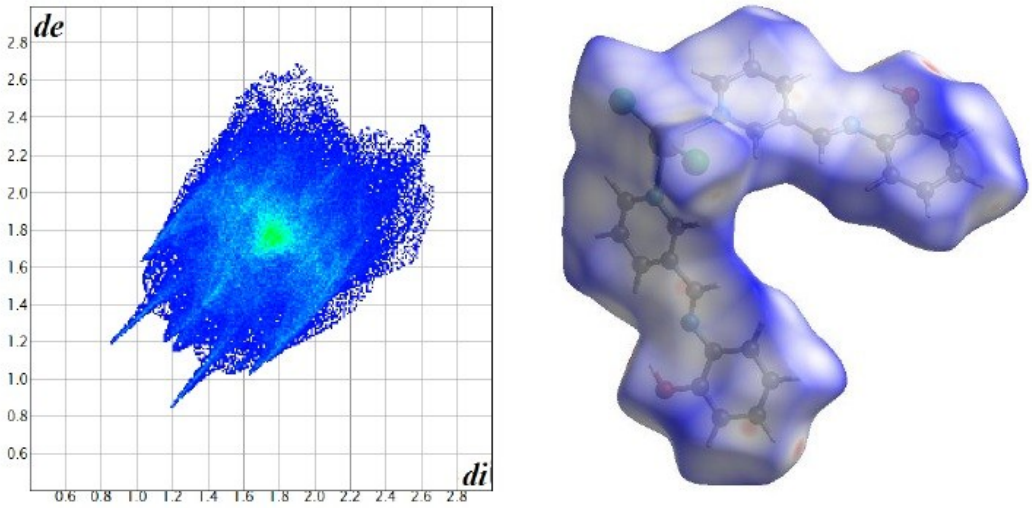


Figure S22: Crystal packing of compound **6** looking down the *c*-axis


de
di
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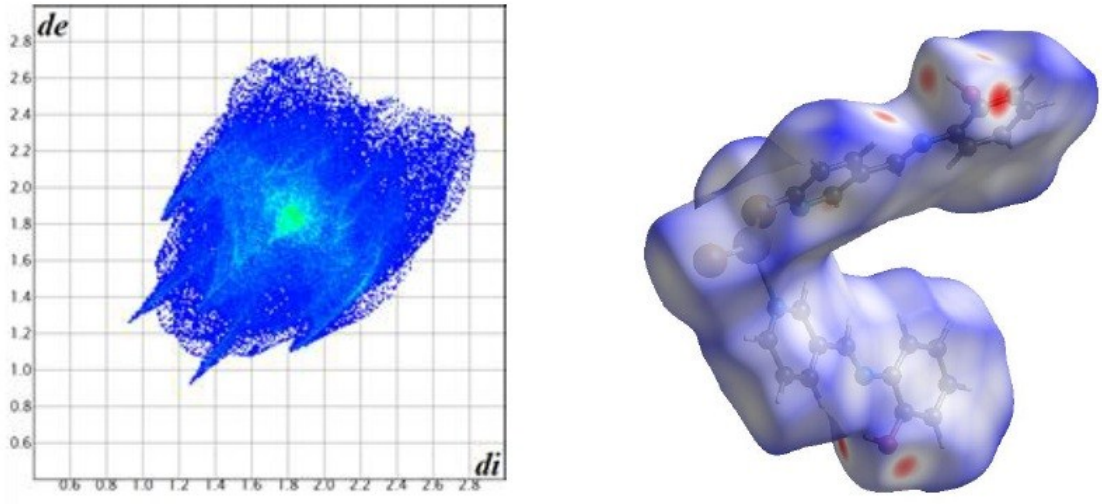
(a)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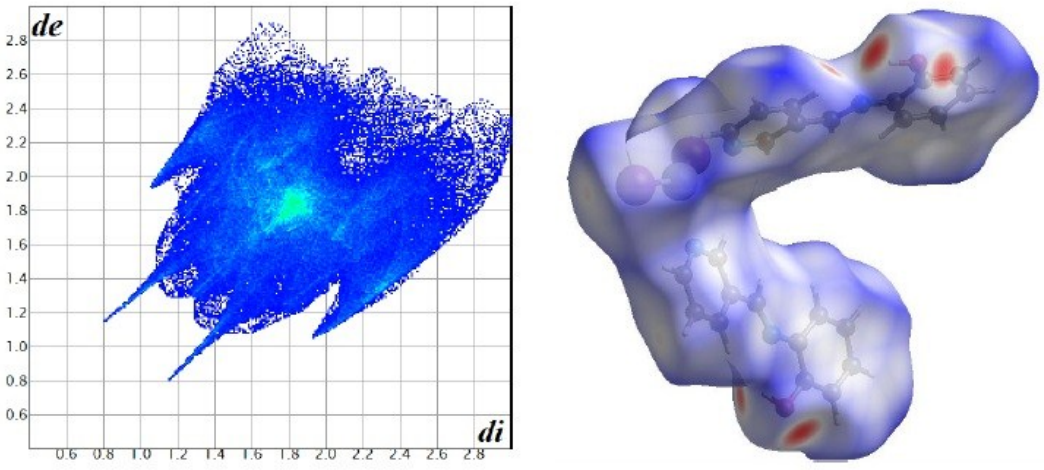
(b)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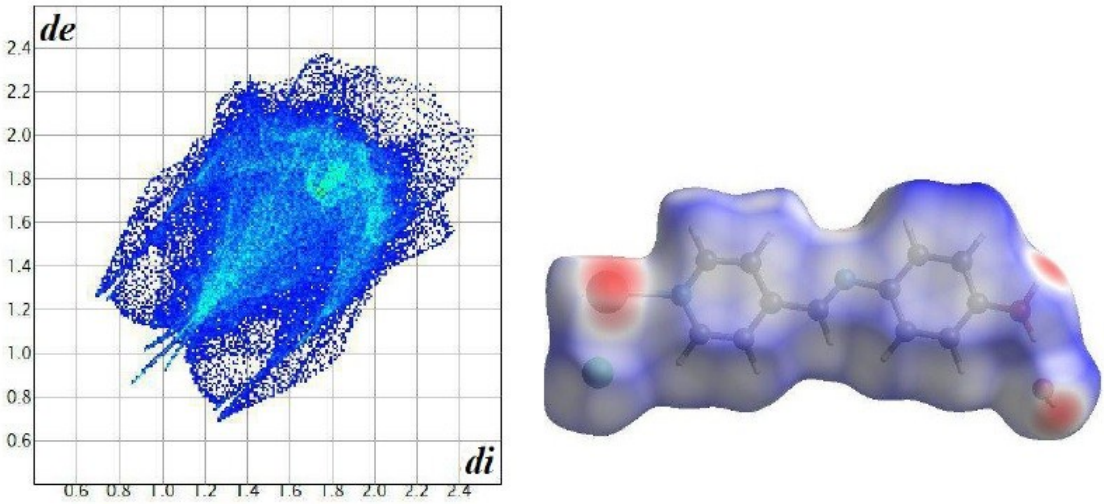
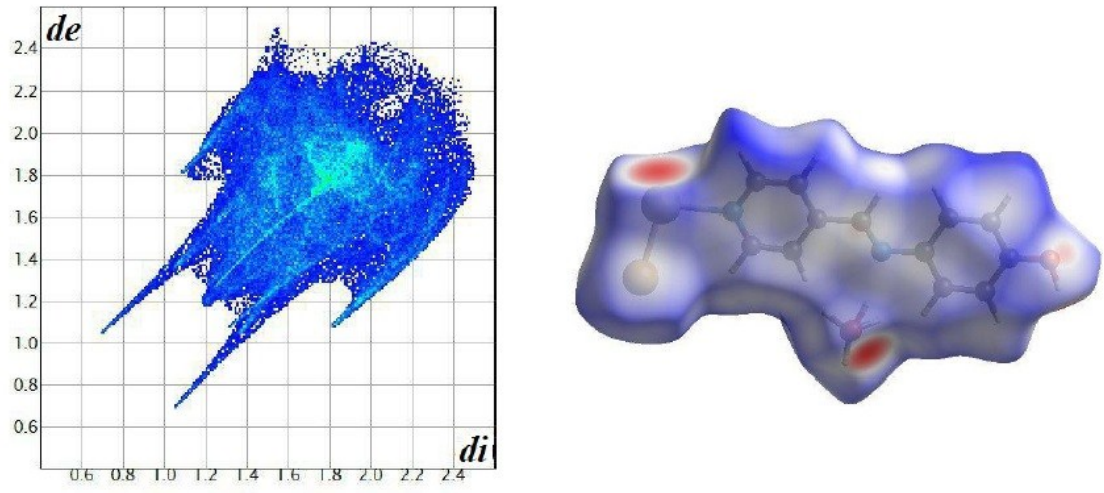
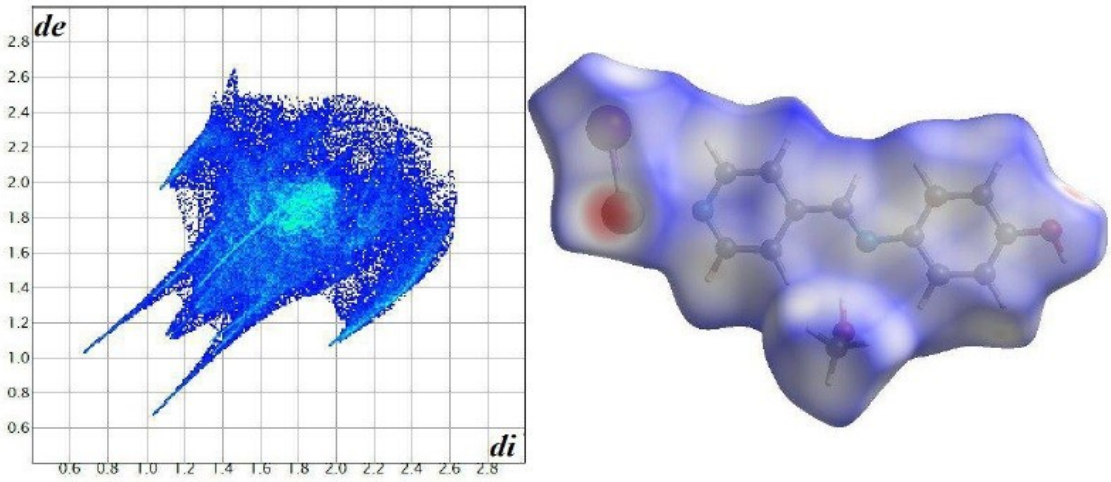
(c)



(d)



(e)



(f)

Figure S23: Fingerprint plots and d_{norm} mapped on Hirshfeld surfaces for compounds **1**(a), **2** (b), **3** (c), **4**(d), **5** (e) and **6** (f).