Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary information

Co(II) and Zn(II) Pyrazolyl-benzimidazole complexes with remarkable antibacterial activity

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Table S1. Selected bond lengths and bond angles of coordination complexes **C1-C3**.

Bond length (Å)		Bond angles (°)	
C1			
Co(1)–N(3)	2.005(2)	N(3)–Co(1)–N(2)	92.38(11)
Co(1)–N(2)	2.012(3)	N(3)–Co(1)–Cl(2)	113.62(8)
Co(1)–Cl(2)	2.2286(10)	N(2)–Co(1)–Cl(2)	116.49(8)
Co(1)–Cl(1)	2.2495(10)	N(3)–Co(1)–Cl(1)	112.51(8)
		N(2)–Co(1)–Cl(1)	109.18(9)
		Cl(2)–Co(1)–Cl(1)	111.38(4)
C2			
Co(1)–N(2)	1.989(7)	N(2)–Co(1)–N(3)	91.7(3)
Co(1)–N(3)	1.994(8)	N(2)–Co(1)–Cl(2)	113.3(3)
Co(1)–Cl(2)	2.218(3)	N(3)–Co(1)–Cl(2)	115.0(3)
Co(1)–Cl(1)	2.234(3)	N(2)–Co(1)–Cl(1)	108.0(3)
Co(2)–N(6)	1.993(8)	N(3)–Co(1)–Cl(1)	113.1(3)
Co(2)–N(7)	2.018(7)	C(l2)–Co(1)–Cl(1)	113.67(13)
Co(2)–Cl(3)	2.229(3)	N(6)–Co(2)–N(7)	91.5(3)
Co(2)–Cl(4)	2.259(3)	N(6)–Co(2)–Cl(3)	115.4(3)
		N(7)–Co(2)–Cl(3)	108.8(2)
		N(6)–Co(2)–Cl(4)	115.9(3)
		N(7)–Co(2)–Cl(4)	108.6(2)
		C(l3)–Co(2)–Cl(4)	113.87(12)
C3			
Zn(1)–N(3)	2.023(4)	N(3)–Zn(1)–N(1)	91.29(15)
Zn(1)–N(1)	2.030(4)	N(3)–Zn(1)–Cl(1)	108.48(11)
Zn(1)–Cl(1)	2.2099(14)	N(1)–Zn(1)–Cl(1)	122.48(11)
Zn(1)–Cl(2)	2.2551(13)	N(3)–Zn(1)–Cl(2)	110.91(11)
Zn(2)–N(7)	2.018(4)	N(1)–Zn(1)–Cl(2)	109.71(12)
Zn(2)–N(5)	2.041(4)	C(l1)–Zn(1)–Cl(2)	111.90(5)
Zn(2)–Cl(4)	2.2056(18)	N(7)–Zn(2)–N(5)	89.40(15)
Zn(2)–Cl(3)	2.2080(14)	N(7)–Zn(2)–Cl(4)	110.90(12)
		N(5)–Zn(2)–Cl(4)	106.51(13)
		N(7)–Zn(2)–Cl(3)	115.02(11)
		N(5)–Zn(2)–Cl(3)	108.51(12)
		C(l4)–Zn(2)–Cl(3)	121.28(7)

Table S2. Hydrogen bonding parameters of coordination complexes **C1**-**C3**.

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (˚)	Symmetry operation for A
C1					
N(1)–H(1)···Cl(1)	0.86	2.49	3.253(3)	149	1-x, 1/2+y, 3/2-z
C(5)–H(5A)···Cl(1)	0.97	2.75	3.653(3)	155	1-x, 1-y, 1-z
C2					
N(1)–H(1)···Cl(4)	0.86	2.52	3.374(8)	176	x, -1+y, z
O(1)–H(1E)···Cl(2)	0.85	2.50	3.179(17)	138	x, y, z
N(5)–H(5)···Cl(1)	0.86	2.38	3.203(10)	160	x, 1+y, z
C(15)–H(15B)···Cl(1)	0.97	2.79	3.71(3)	159	x, 1+y, z
C(17)–H(17C)···Cl(2)	0.96	2.77	3.624(15)	149	x, 1+y, z
C(21)–H(21A)···O1)	0.97	2.29	3.09(3)	139	x, y, z
C3					
N(2)–H(2)···Cl(3)	0.86	2.37	3.197(4)	160	x, y, z
N(6)–H(6)···Cl(2)	0.86	2.45	3.293(4)	168	x, y, z
C(21)–H(21A)···Cl(1)	0.97	2.83	3.773(6)	166	-1/2+x, -1/2+y, z

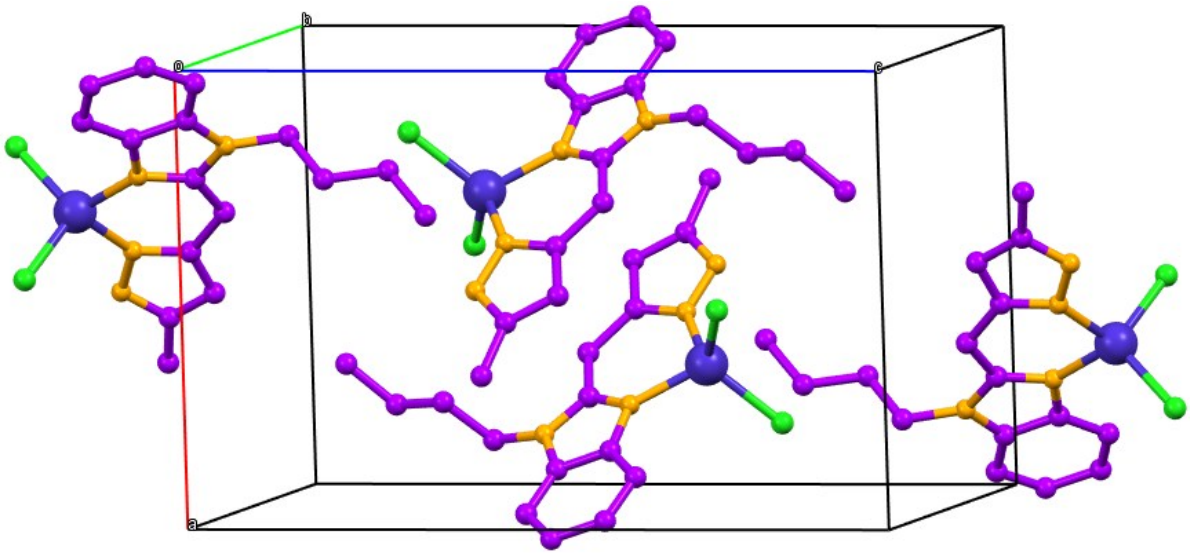

Figure S1. Unit cell content of **C1**.

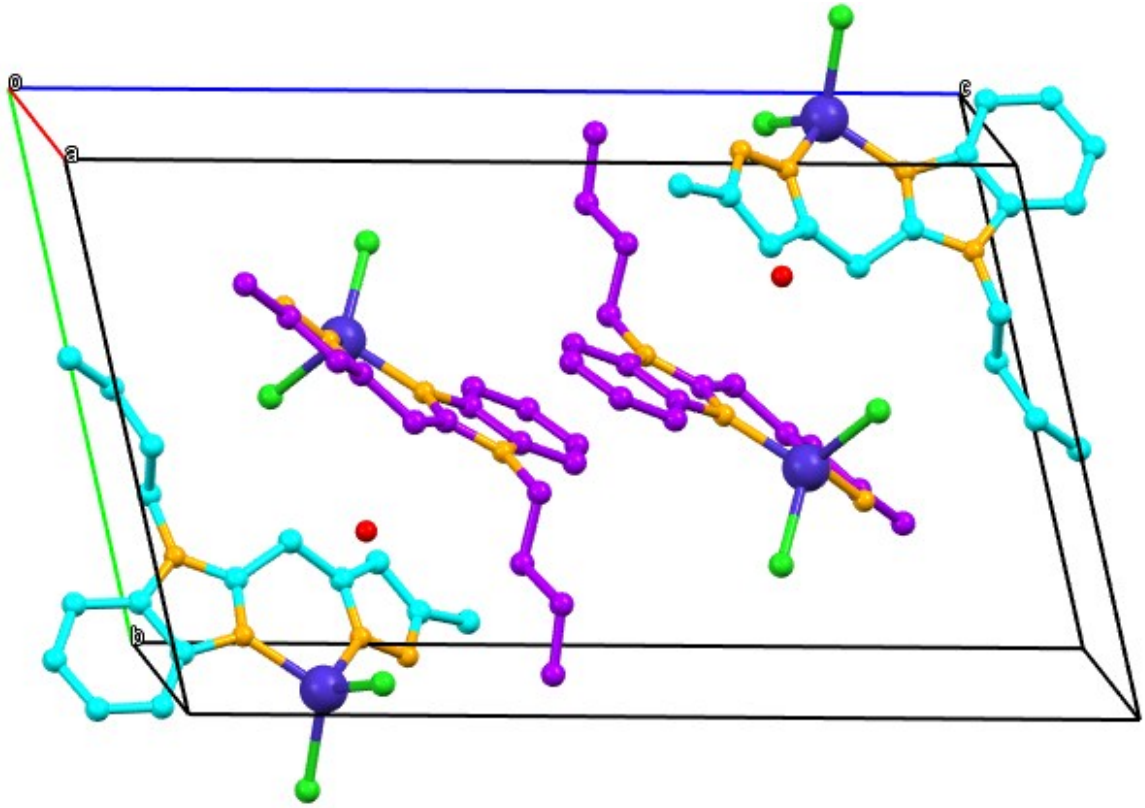

Figure S2. Unit cell content of **C2**.

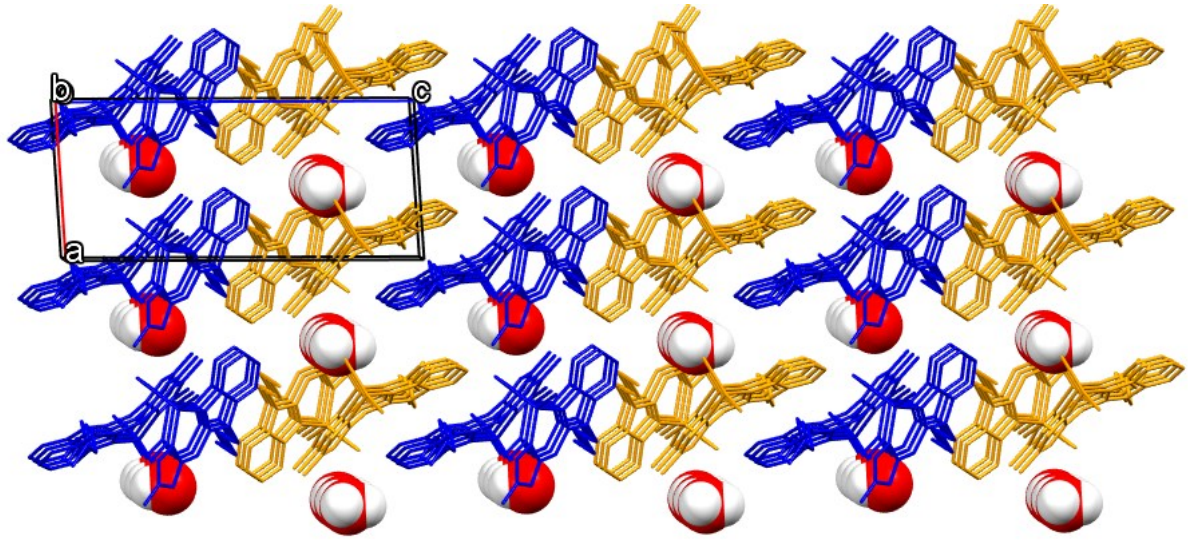

Figure S3. Overall crystal packing of **C2** displaying the inclusion of water molecules in its voids.

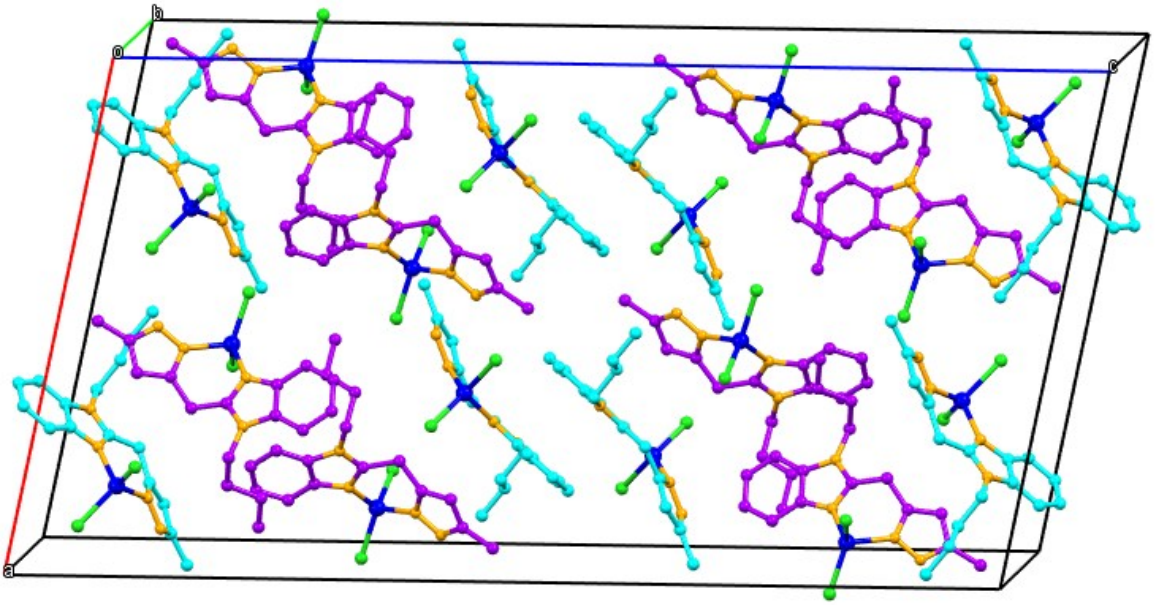

Figure S4. Unit cell content of **C3**.

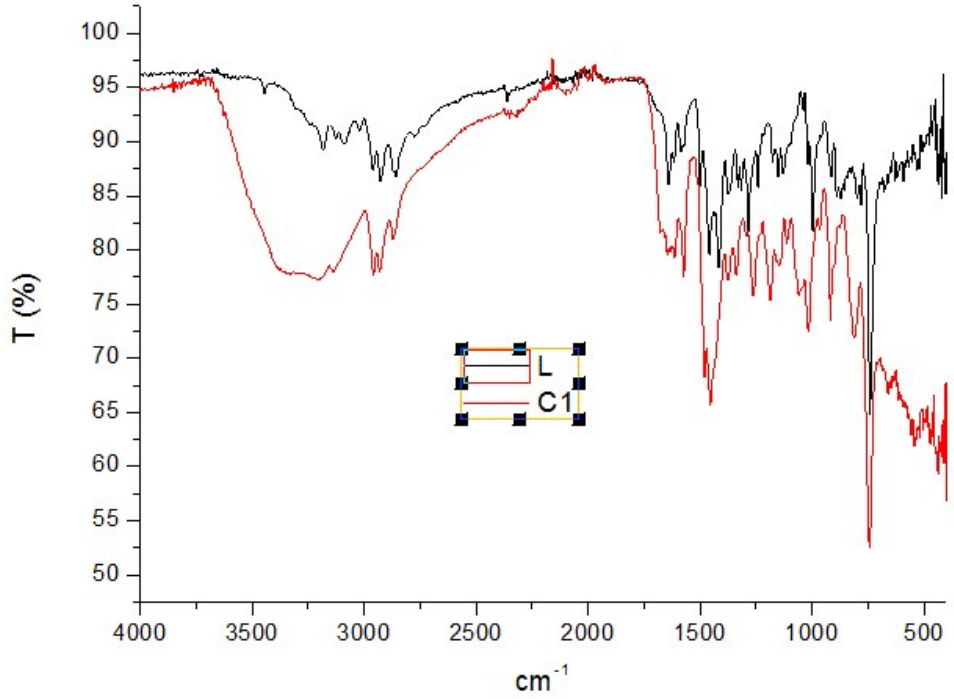

Figure S5. FT-IR comparison plot of **C1** and **L**.

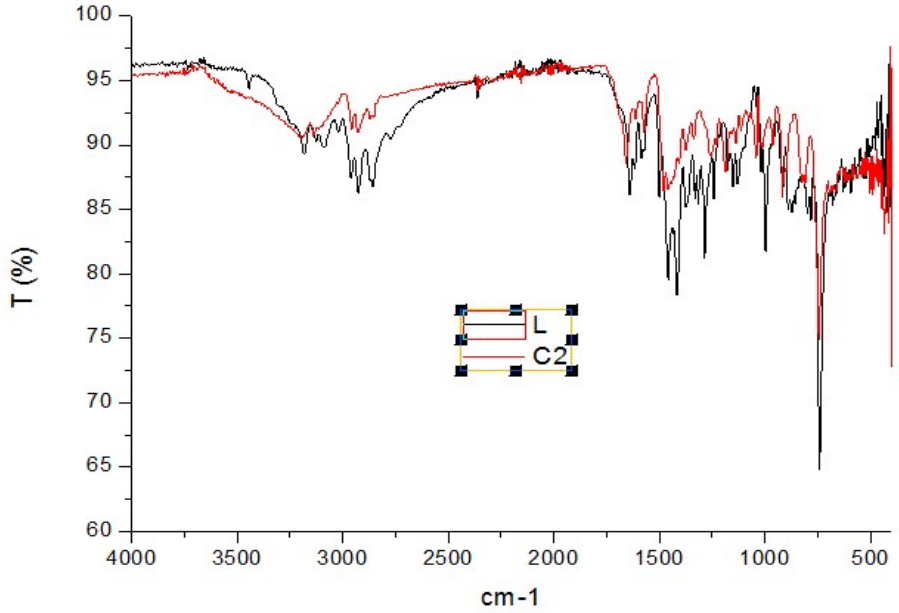

Figure S6. FT-IR comparison plot of **C2** and **L**.

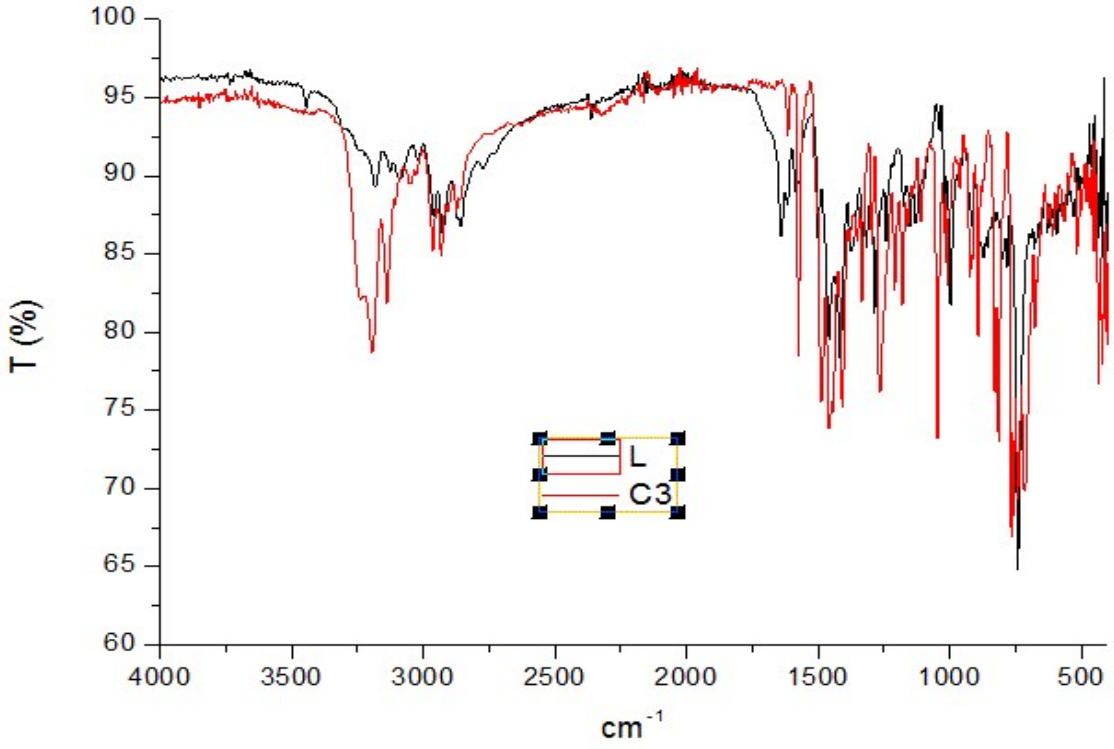

Figure S7. FT-IR comparison plot of **C3** and **L**.

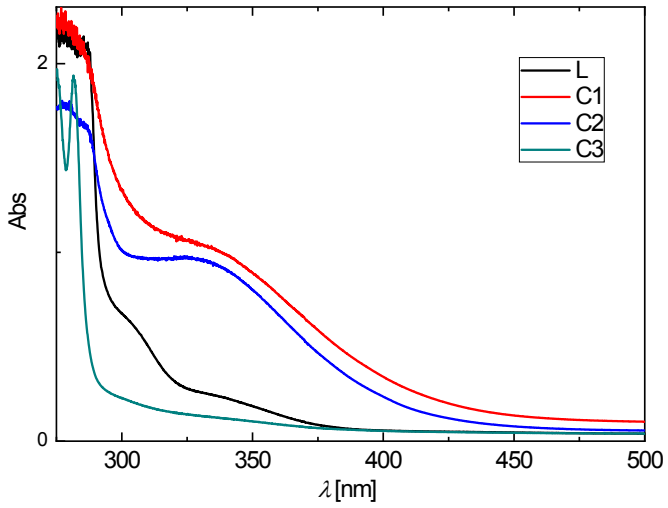

Figure S8. UV/Vis comparison plot of **C1-C3** and **L**.

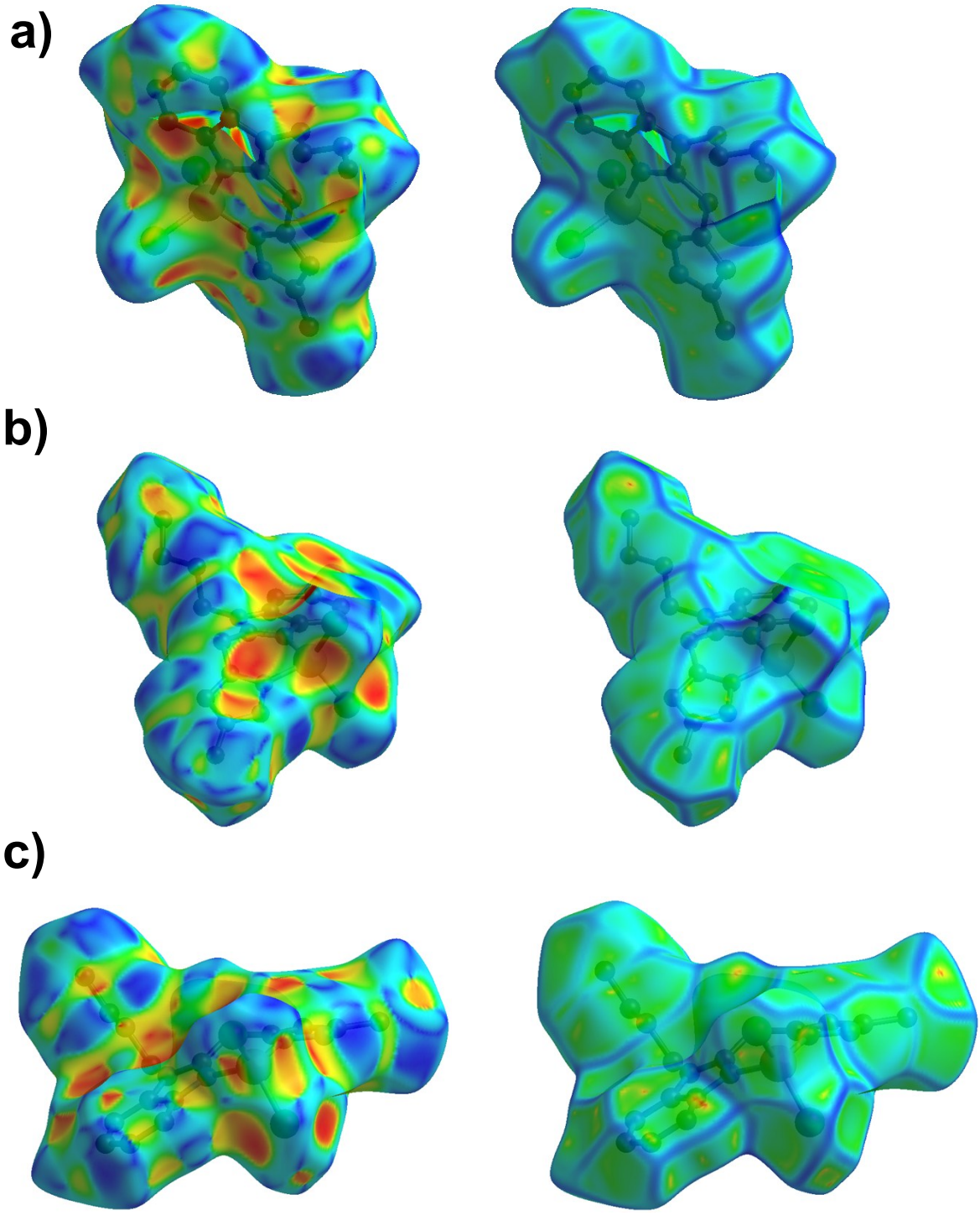

Figure S9. shape index (shown in *left* side) and curvedness (shown in *right* side) of **C1** (a), **C2** (b), and **C3** (c).

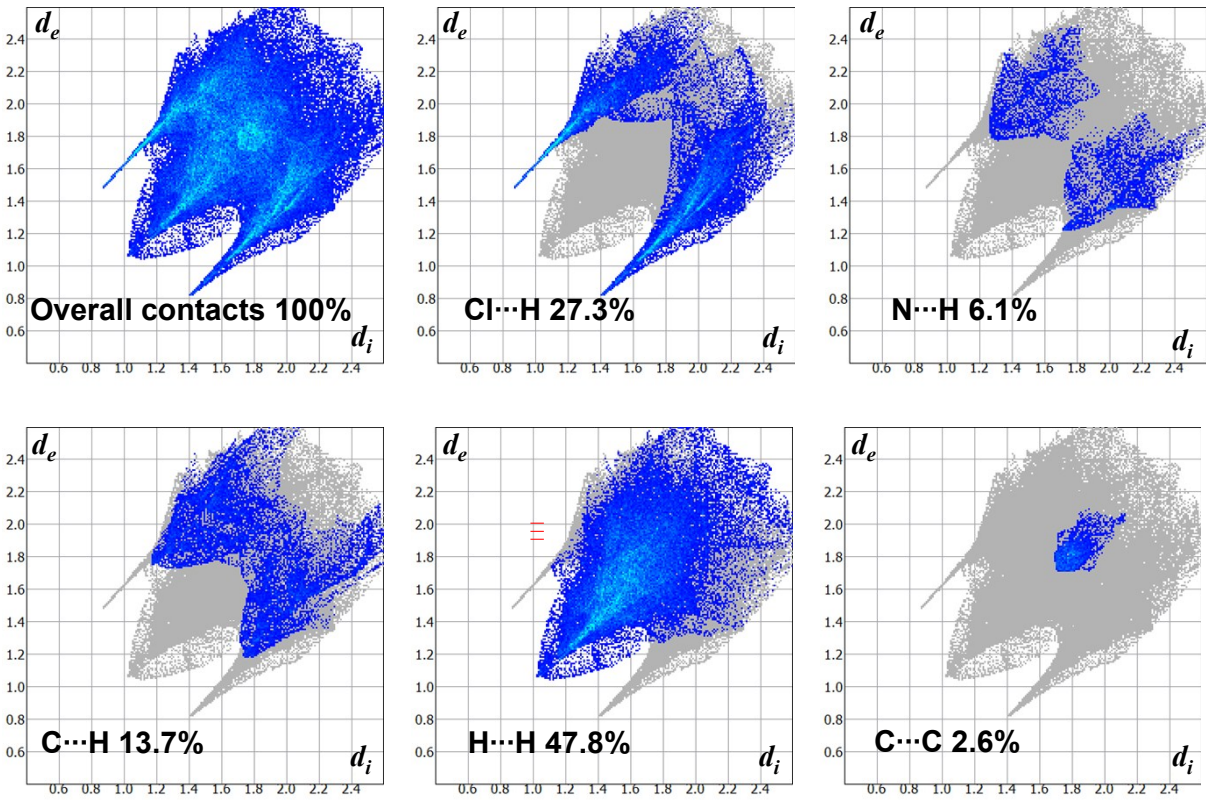

Figure S10. 2D Fingerprint plots derived from Hirshfeld surfaces, displaying various intermolecular interactions for **C2**.

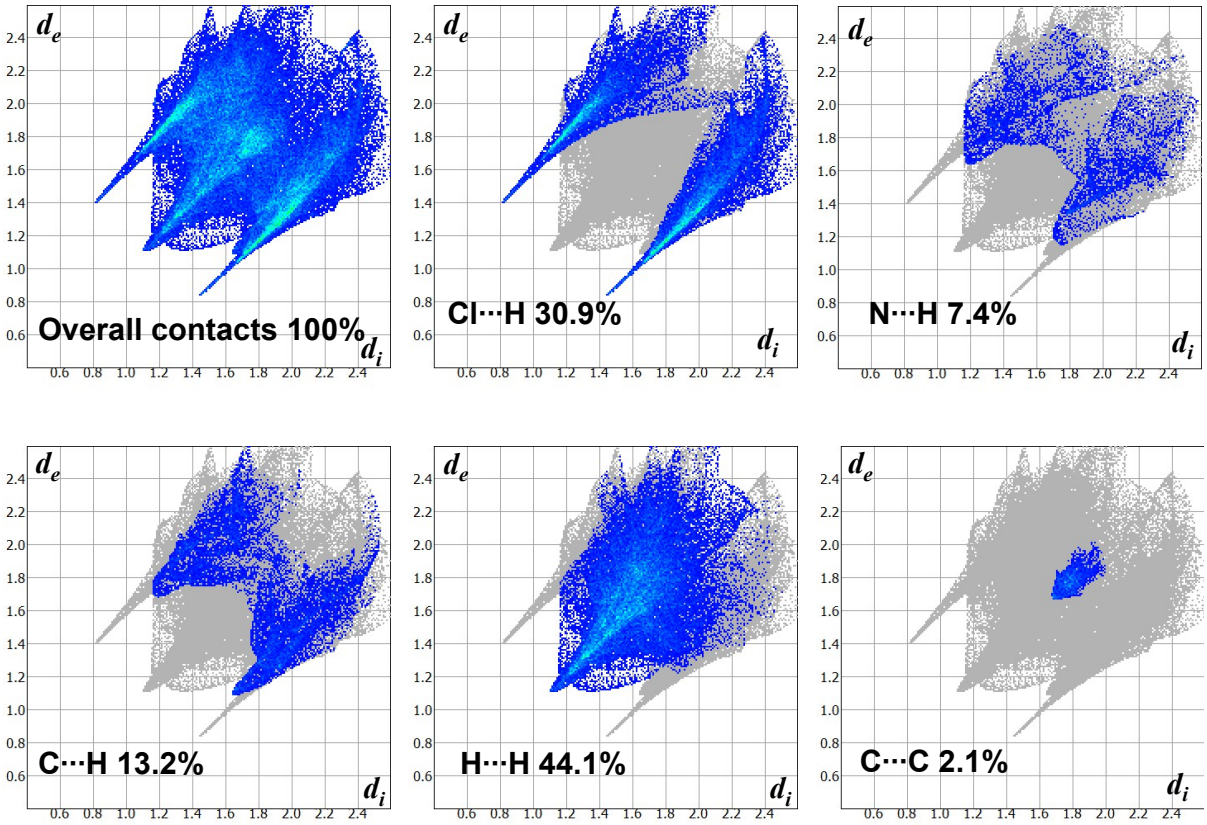

Figure S11. 2D Fingerprint plots derived from Hirshfeld surfaces, displaying various intermolecular interactions for **C3**.