Supplementary Information for:

Providing evidence on the requirements to achieve supramolecular materials based on metal-nucleobase entities

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S1. Tables of most relevant coordination bonds.

Table S1. Most relevant coordination bonds (Å) for compound **1**.[a]

Compound **1**	
Bonds	
Cu1–N3	2.025(4)
Cu1–N9^{i}	2.020(4)
Cu1–Cl1	2.402(2)
Cu1···Cu1^{i}	3.035(2)

[a]Symmetry codes: (i) –x, –y, z.

Table S2. Most relevant coordination bonds (Å) for compound **2**.

Compound **2**			
Bonds			
Co1–N3	2.115(2)	Co2–N9	2.105(2)
Co1–O1w	2.122(2)	Co2–Cl2	2.511(1)
Co1–O2w	2.154 (2)	Co2–Cl3	2.474(1)
Co1–Cl1	2.436(1)	Co1···Co2	3.476(2)
Co1–Cl2	2.411(1)		
Co1–Cl3	2.482(1)		

Table S3. Most relevant coordination bonds (Å) for compound **3**.[a]

Compound **3**			
Bonds			
Cu1–N29	1.987(4)	Cu1–Cl2A	2.242(3)
Cu1–N19	1.991(5)	Cu1–Cl1A	2.350(3)
Cu1–O1w	2.134(5)	Cu1–Cl2B^{i}	2.260(4)
		Cu1···Cu1^{i}	3.658(4)

[a]Symmetry codes: (i) –x+1, –y, –z+1.

Table S4. Most relevant coordination bonds (Å) for compound **4**.

Compound **4**	
Bonds	
Co1–O1w	2.091(1)
Co1–N7	2.149(2)

Table S5. Most relevant coordination bonds (Å) for compound **5**.[a]

Compound **5**			
Bonds			
Cu1–O2^{i}	1.952(4)	Cu2–O6^{ii}	1.962(4)
Cu1–O1	1.955(4)	Cu2–O7	1.982(4)
Cu1–O3	1.967(4)	Cu2–N11	2.211(5)
Cu1–O4^{i}	1.977(4)	Cu1···Cu1^{i}	2.643(1)
Cu1–N17	2.211(5)	Cu1···Cu2	7.643(1)
Cu2–O5	1.957(4)	Cu2···Cu2^{ii}	2.662(1)
Cu2–O8^{ii}	1.959(4)		

[a] Symmetry codes: (i) –x+1, –y, –z; (ii) –x+1, –y+1, –z+1.

Table S6. Most relevant coordination bonds (Å) for compound **6**.[a]

Compound **6**			
Bonds			
Co1–O2w	2.086(1)	Co1–O2w^{i}	2.086(1)
Co1–O1w	2.122(1)	Co1–O1w^{i}	2.122(1)
Co1–N9	2.128(1)	Co1–N9^{i}	2.128(1)

[a] Symmetry code: (i) –x+2, –y+1, –z+1.

S2. Tables of non-covalent interactions.

Table S7. Structural parameters (Å, º) for non-covalent interactions in compound **2**.[a]

D–H···A[b]	H···A	D···A	D–H···A
N7–H7···O3w	1.92	2.731(3)	157.1
N6–H6A···Cl3^{i}	2.70	3.435(2)	144.6
N6–H6B···O3w	2.23	3.054(3)	161.6
O1w–H11···N1^{ii}	1.93	2.785(3)	176.4
O2w–H21···Cl1^{iii}	2.20	3.055(2)	168.8
O1w–H12···O2w^{iv}	2.08	2.859(2)	153.6
O3w–H31···O1w^{v}	2.30	3.071(2)	141.4
O3w–H32···Cl1^{vi}	2.24	3.1437(19)	163.5

[a] Symmetry code: (i) x, y–1,z; (ii)–x+2, –y–1,–z+3; (iii) –x+1, –y, –z+3 (iv); –x+2, –y, –z+3; (v) –x+3, –y–1, –z+2; (vi) –x+2, –y–1, –z+2. [b] **D**: donor; **A**: acceptor.

Table S8. Structural parameters (Å, º) for non-covalent interactions in compound **3**.[a]

D–H···A[b]	H···A	D···A	D–H···A
O1w–H2w ··Cl1B^{i}	1.92	2.786(10)	153.9
N13–H13 ··O1w	1.86	2.576(6)	139.4
N23–H23·· O1w	1.93	2.604(6)	133.9
N13–H13·· Cl1B^{i}	2.66	3.389(6)	143.8
N23–H23 ··Cl1B^{i}	2.68	3.393(6)	141.8
N11–H11 ··O26^{ii}	1.90	2.723(6)	161.1
N12–H12A ··Cl1A^{i}	2.60	3.421(6)	161.1
N12–H12A ··Cl1B^{i}	2.37	3.182(6)	158.4
N12–H12B ··O26^{ii}	2.42	3.105(6)	137.5
N17–H17 ··Cl4^{iii}	2.27	3.118(5)	170.0
N21–H21···Cl3^{iv}	2.31	3.123(5)	156.8
N22–H22A···Cl1A^{i}	2.62	3.429(7)	156.4
N22–H22A···Cl1B^{i}	2.36	3.172(7)	156.7
N22–H22B···Cl3^{iv}	2.52	3.274(6)	147.5
N27–H27···O16^{v}	1.90	2.754(6)	174.7

[a] Symmerty code: (i) –x+1, –y+1, –z+1; (ii) x, y, z+1; (iii) x+1, y, z+1; (iv) x, y+1, z; (v) x, y, z–1. [b] **D**: donor; **A**: acceptor.

Table S9. Structural parameters (Å, º) for non-covalent interactions in compound **4**.[a]

Hydrogen bonding interactions.[a]

D–H···A[b]	H···A	D···A	D–H···A
N6–H6A···N1^{i}	2.12	2.974(3)	175.6
N6–H6B···O1w	2.31	2.980(2)	135.3
N6–H6B···O1w^{II}	2.31	2.980(2)	135.3
O1w–H1A···Cl1^{III}	2.13	3.073(1)	167.2
O1w–H1B···O2w	1.93	2.771(2)	171.2
O2w–H2A···N3^{iv}	2.06	2.920(2)	156.6
O2w–H2B···Cl1	2.35	3.209(2)	171.4

π-π interactions[c]

Ring···Ring[d]	Angle	DC	α	DZ	DXY
Ring(1)···Ring(1)^{v}	0	3.9521(8)	31.62	3.3654(1)	2.072

[a] Symmetry: (i) –x+1,–y+1,–z+1; (ii) x,–y+1,z; (iii)–x+2,–y+1,–z+1; (iv) –x+3/2,–y+3/2,–z+3/2; (v) –x+3/2, y–1/2, –z+3/2. [b] **D**: donor; **A**: acceptor. [c] Angle: Dihedral Angle between Planes I and J (º), DC: Distance between ring centroids (Å), α: Angle Cg(I)—>Cg(J) vector and normal to plane I (°), DZ: Perpendicular distance of Cg(I) on ring J (Å), DXY: Slippage. [d] Ring 1: N1, C2, N3, C4, N9, C6.

Table S10. Structural parameters (Å, º) for non-covalent interactions in compound **5**.[a]

Hydrogen bonding interactions.[a]			
D–H···A[b]	H···A	D···A	D–H···A
N16–H16A···O7	1.96	2.793(6)	162.3
N16–H16B···O3	1.94	2.801(6)	178.1
O9–H9···O5^{i}	2.04	2.835(6)	161.8

[a] Symmetry code: (i) –x+1, –y+1, –z+1. [b] **D**: donor; **A**: acceptor.

Table S11. Structural parameters (Å, º) for non-covalent interactions in compound **6**.[a]

Hydrogen bonding interactions.[a]

D–H···A[b]	H···A	D···A	D–H···A
O1w–H11···N7^{i}	2.24	3.020(2)	149.8
O1w–H12···N7^{ii}	2.11	2.902(2)	151.1
O2w–H21···N3^{iii}	1.94	2.737(2)	153.4
O2w–H22···O4w^{iv}	1.81	2.709(2)	169.4
O3w–H31···O1w	2.19	2.979(2)	153.7
O4w–H41···N1	1.90	2.827(2)	164.0
O4w–H42···O3w^{v}	1.82	2.673(2)	175.5

π–π stacking interactions.[c]

Ring···Ring[d]	Angle	DC	α	DZ	DXY
Ring1–Ring1^{vi}	2	3.6908(9)	19.22	3.4987(6)	1.1752
Ring1–Ring1^{vii}	2	3.6908(9)	18.56	3.4851(6)	1.2149
Ring1–Ring2^{vi}	1.79(8)	3.6505(8)	18.26	3.4958(6)	1.1434
Ring2–Ring1^{vii}	1.79(8)	3.6506(8)	16.74	3.4668(6)	1.1438
Ring2–Ring2^{vi}	1	3.7471(8)	22.24	3.4857(6)	1.3750
Ring2–Ring2^{vii}	1	3.7472(8)	21.53	3.4684(6)	1.4183

[a] Symmetry: (i) –x+2, y–1/2, –z+3/2; (ii) x, –y+3/2, z+1/2; (iii) –x+2, –y+1, –z+1; (iv) x+1, –y+3/2, z+1/2; (v) –x+1, y+1/2, –z+3/2; (vi) x, 3/2–y,–1/2+z; (vii) x, 3/2–y, 1/2+z; [b] **D**: donor; **A**: acceptor. [c] Angle: Dihedral Angle between Planes I and J (º), DC: Distance between ring centroids (Å), α: Angle Cg(I)—>Cg(J) vector and normal to plane I (°), DZ: Perpendicular distance of Cg(I) on ring J (Å), DXY: Slippage. [d] Ring1: N7, C5, C4, N9, C8; Ring 2: N1, C2, N3, C4, C5, C6.

S3. X-ray diffraction patterns

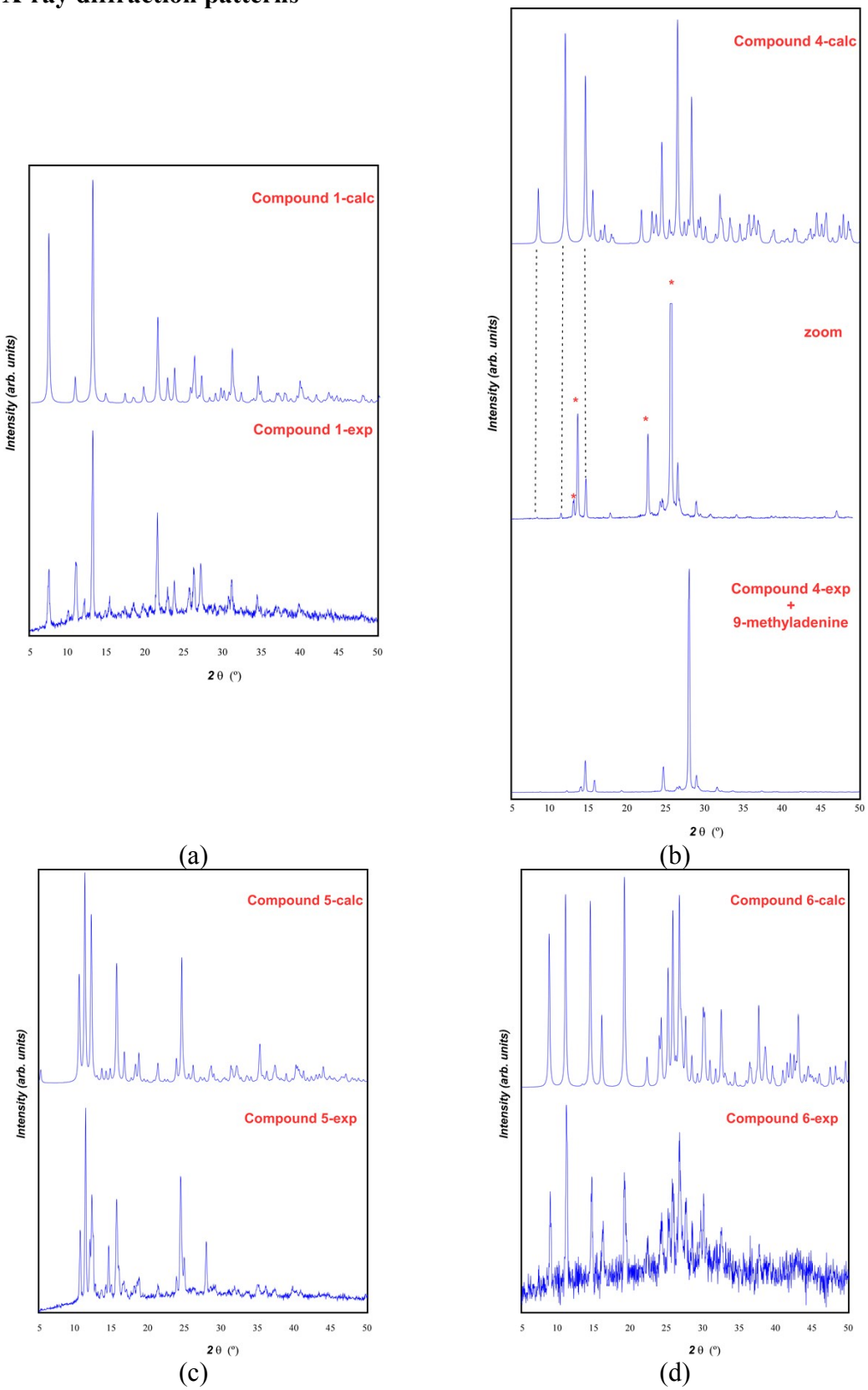

Figure S1. Experimental and calculated X-ray diffraction patterns of: (a) compound **1**, (b) compound **4**, (c) compound **5** and (d) compound **6**. Note that compound **4** appears cocrystallized with 9-methyladenine, so a zoom has been included in order to show more clearly the peaks corresponding to compound **4**. * corresponds to the peaks assigned to 9-methyladenine, and some discontinuous lines have been included which correspond to compound **4**.

S4. Thermogravimetric data

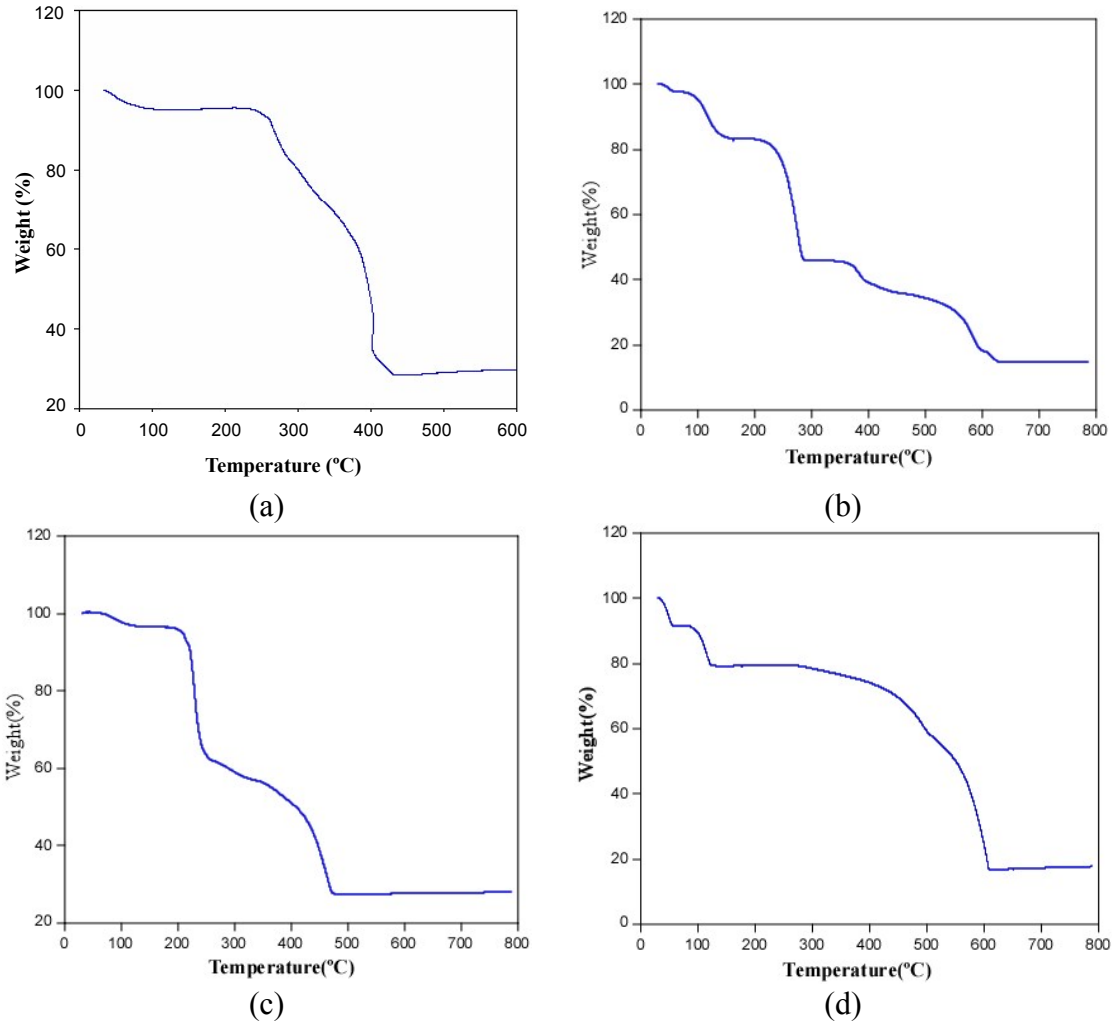

Figure S2. Thermogravimetric data of: (a) compound **1**, (b) compound **4**, (c) compound **5** and (d) compound **6**.