Electronic Supplementary Material (ESI) for CrystEngComm

Supporting information

belonging to the manuscript

Construction of Homo- and Heterometallic-Pyridine-2,3-Dicarboxylate Metallosupramolecular Networks with Structural Diversity: 1D T5(2) Water Tape and Unexpected Coordination Mode of Pyridine-2,3-dicarboxylate

Fatih Semerci[a, b], Okan Zafer Yeşilel[*,a], Cihan Darcan[c], Murat Taş[d], Seda Keskin[e], Hakan Dal[f]

[a]Department of Chemistry, Faculty of Arts and Sciences, Eskişehir Osmangazi University, 26480 Eskişehir, Turkey

[b]Department of Chemistry, Faculty of Arts and Sciences, Kırklareli University, 39100 Kırklareli, Turkey

[c]Department of Molecular Biology and Genetic, Faculty of Arts and Sciences, Bilecik Şeyh Edebali University, 11000 Bilecik Gülümbe, Turkey

[d]Department of Chemistry, Faculty of Arts and Sciences, Giresun University, Giresun, Turkey

[e]Department of Chemical and Biological Engineering, Koç University, İstanbul, Turkey

[f]Department of Chemistry, Faculty of Sciences, Anadolu University, Eskişehir, Turkey

Contents:

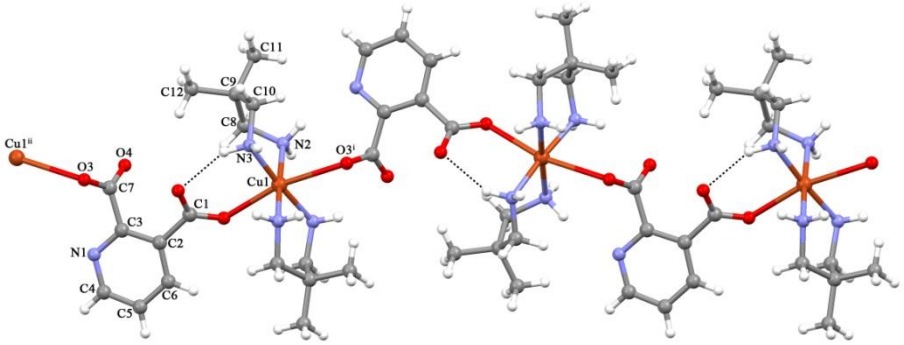


Fig S1. View of the coordination environment of Cu(II) metal centers, the steric effect of methyl groups within the 1,3-diamino-2,2-dimethylpropane ligand and the unexpected coordination mode of the pydc in **1**

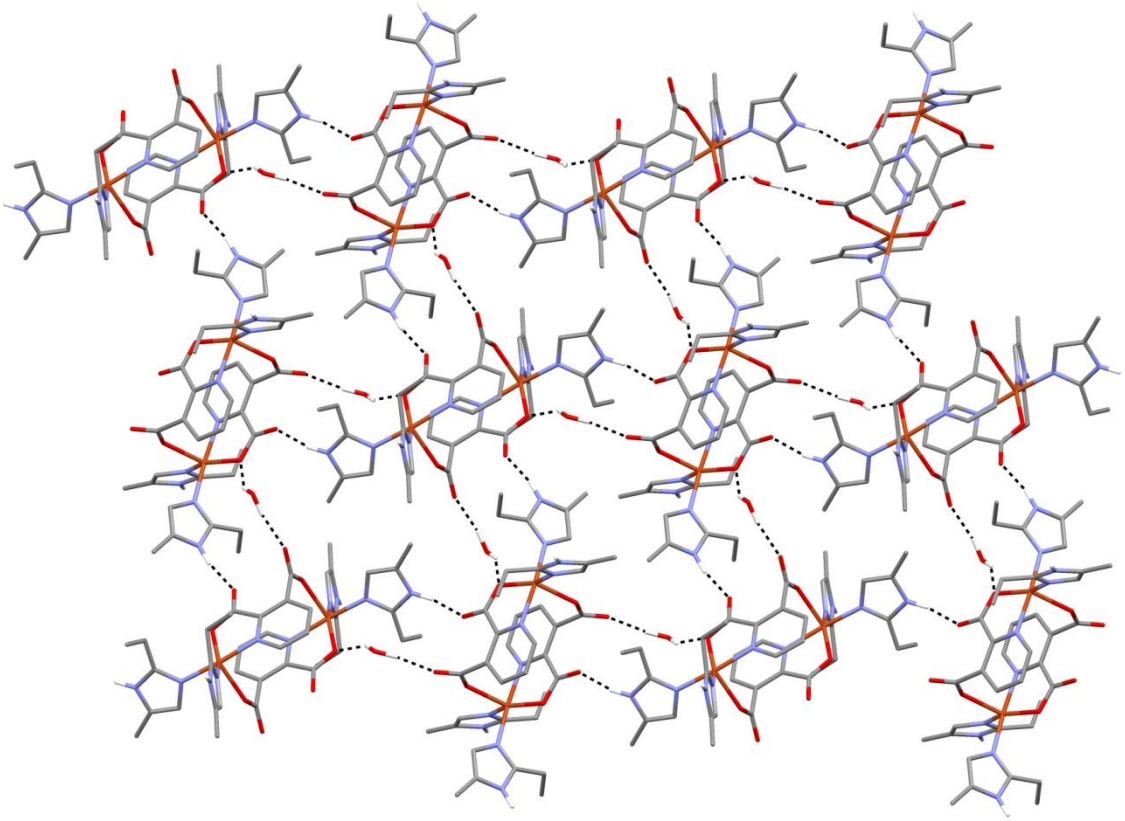
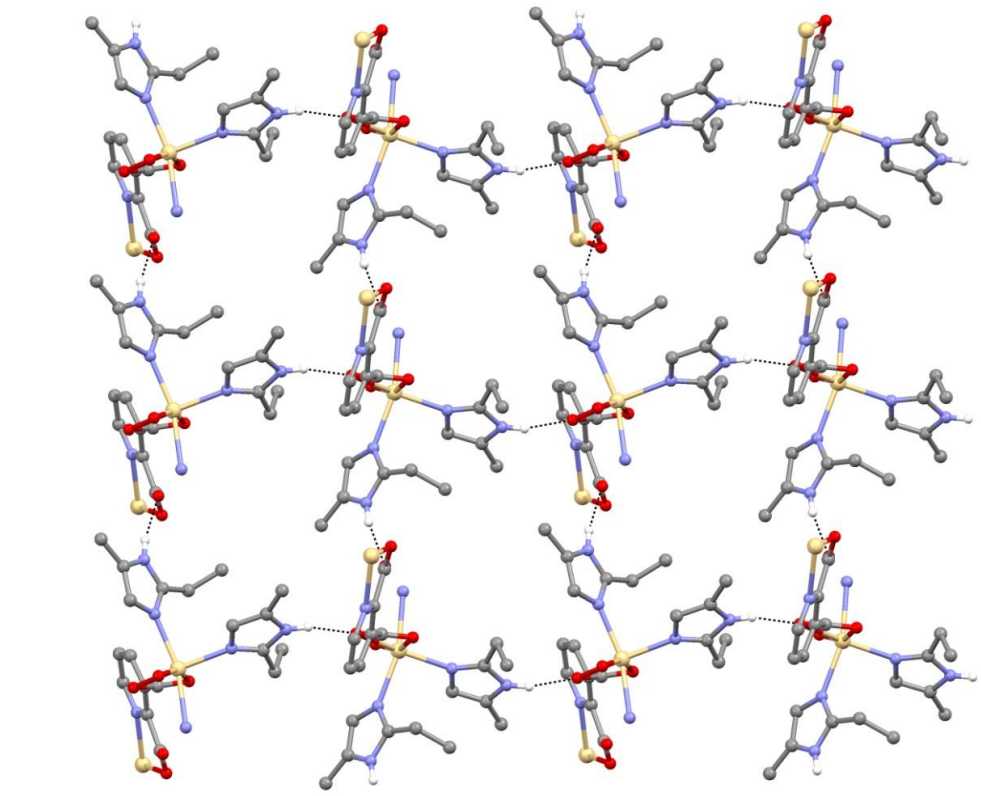
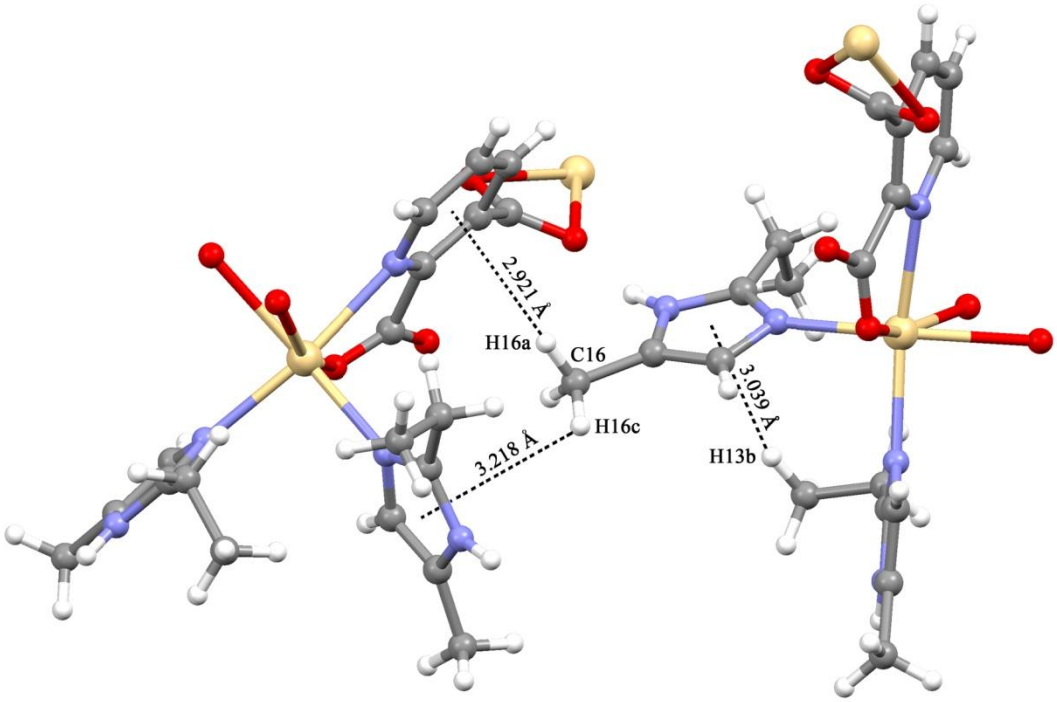


Fig S2. View of hydrogen bonding interactions of **2**

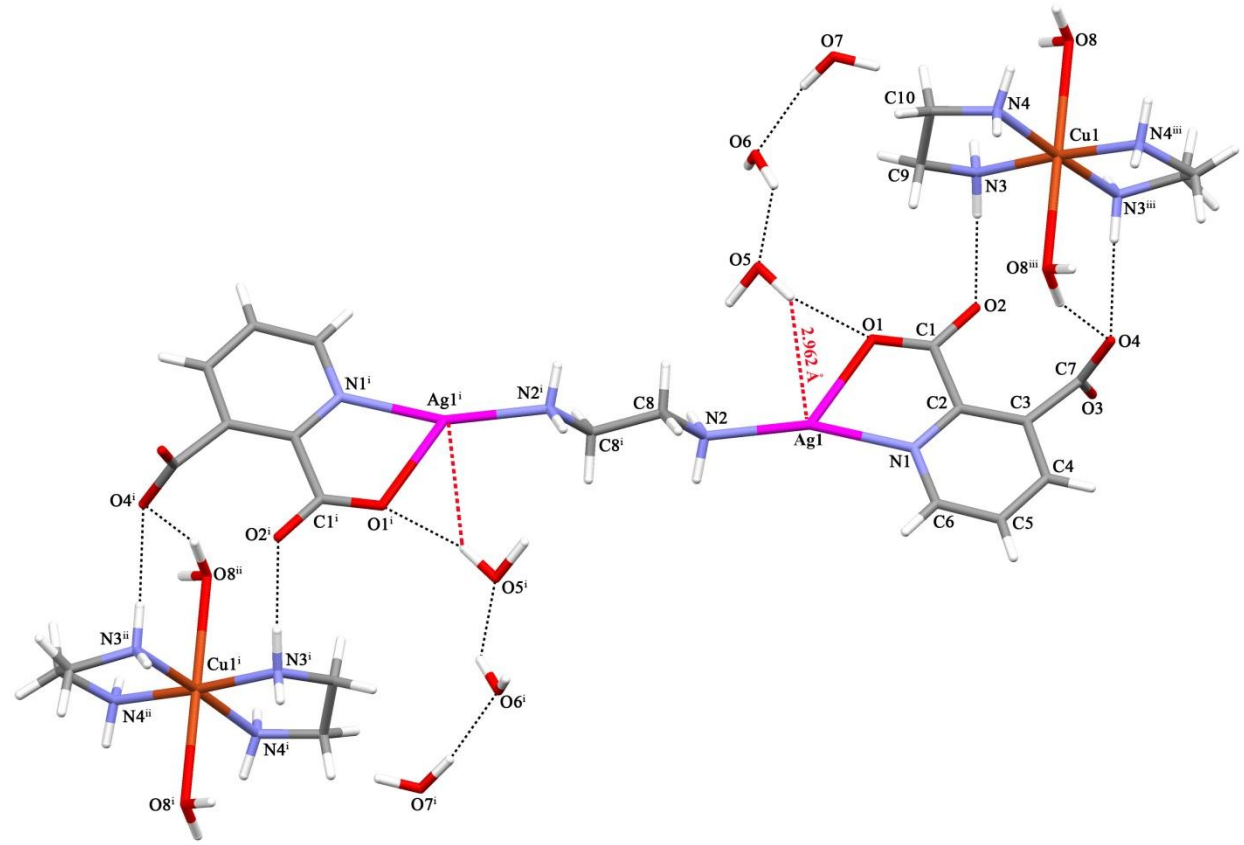


(a)

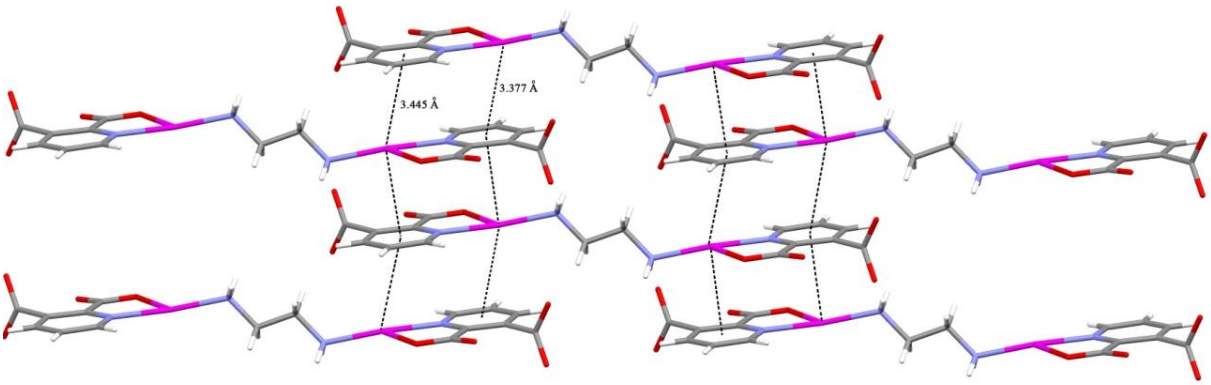


(b)

Fig. S3. (a) View of the N–H···O hydrogen interactions and **(b)** intermolecular C-H···π interactions in **3**



(a)



(b)

Fig. S4. (a) A view of the different coordination modes of the ethylenediamine ligands with atom-labeling scheme in **4** and (**b**) View of the intermolecular Ag···π interactions and stacking of [Ag_2pydc_2(μ-en)] units in **4**

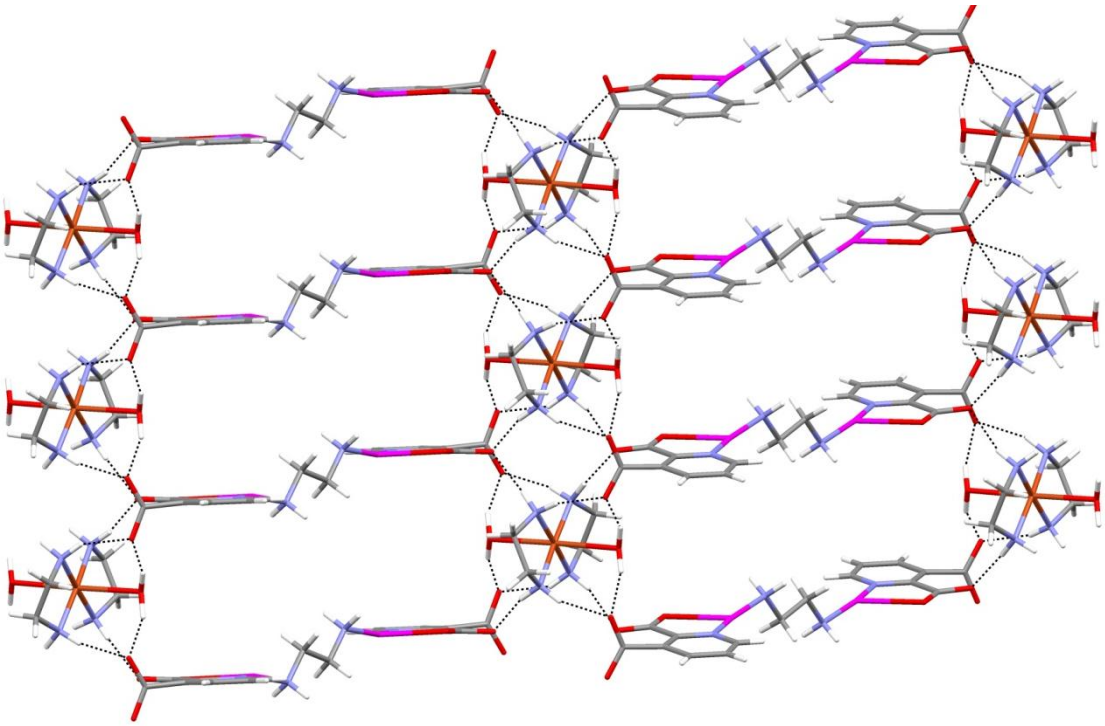
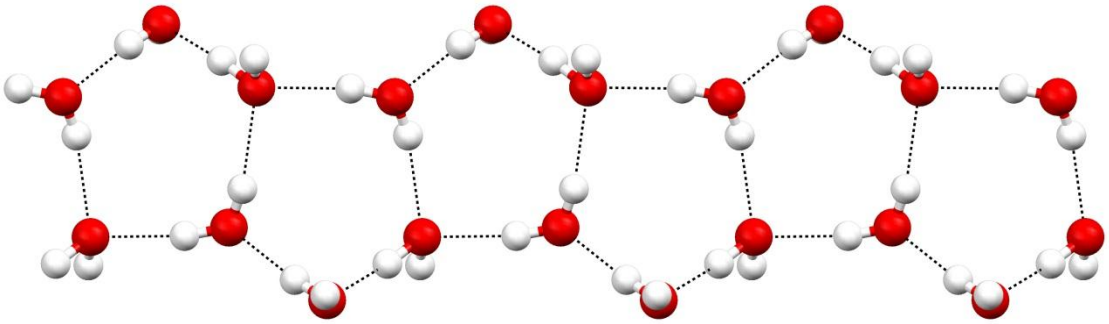
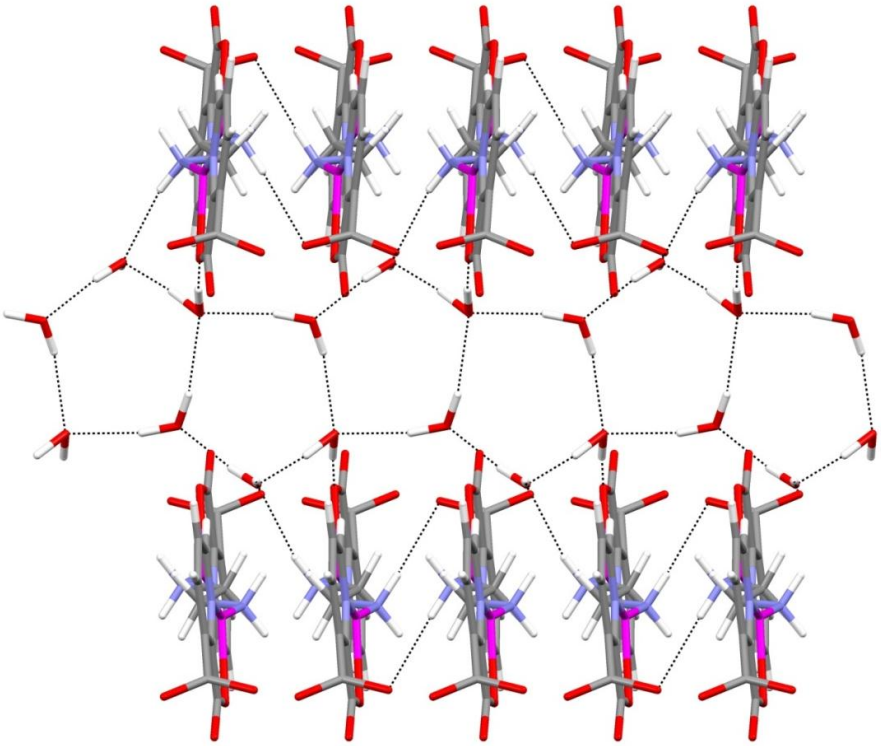


Fig S5. View of $[Cu(H_2O)_2(en)_2]^{2+}$ complex ions settled between the layers by using their aqua ligands and NH_2 parts of en ligands



(a)



(b)

Fig. S6. (a) View of the 1D T5(2) water tape in **4** and (b) The water tape interact with the complex unit

Table S1. Selected bond lengths (Å) and angles (º) for **1**

Bond lenghts			
Chain 1		***Chain 2***	
Cu1-N2	2.022 (3)	Cu2-N6	2.018 (3)
Cu1-N3	2.032 (3)	Cu2-N7	2.029 (3)
Cu1-N4	2.030 (3)	Cu2-N8	2.027 (3)
Cu1-N5	2.007 (3)	Cu2-N9	2.028 (4)
Cu1-O1	2.388 (3)	Cu2-O5	2.348 (3)
Cu1-O3^{i}	2.638(4)	Cu2-O8^{ii}	2.597(3)
Bond angles			
Chain 1		***Chain 2***	
N5-Cu1-N2	173.74 (15)	N6-Cu2-N8	87.93 (13)
N5-Cu1-N4	92.61 (14)	N6-Cu2-N9	173.08 (15)
N2-Cu1-N4	90.90 (14)	N8-Cu2-N9	88.14 (14)
N5-Cu1-N3	88.23 (14)	N6-Cu2-N7	92.83 (14)
N2-Cu1-N3	87.90 (14)	N8-Cu2-N7	175.95 (14)
N4-Cu1-N3	175.81 (14)	N9-Cu2-N7	90.70 (14)
N5-Cu1-O1	88.35 (12)	N6-Cu2-O5	88.91 (12)
N2-Cu1-O1	96.98 (14)	N8-Cu2-O5	96.43 (12)
N4-Cu1-O1	87.44 (12)	N9-Cu2-O5	97.20 (14)
N3-Cu1-O1	96.69 (12)	N7-Cu2-O5	87.56 (12)
O1-Cu1-O3^{i}	167.62(10)	O5-Cu2-O8^{ii}	167.41(11)
N2 -Cu1- O3^{i}	91.91(13)	N6-Cu2- O8^{ii}	82.35(10)
N3-Cu1- O3^{i}	92.21(12)	N7-Cu2- O8^{ii}	83.86(12)
N4-Cu1- O3^{i}	83.81(12)	N8-Cu2- O8^{ii}	92.32(12)
N5-Cu1- O3^{i}	83.32(12)	N9-Cu2- O8^{ii}	92.13(13)

Symmetry codes: (i) ½+x, ½−y, ½+z; (ii) −½+x, ½−y, −½+z

Table S2. Selected bond lengths (Å) and angles (º) for **2**

Bond lenght			
$Cu1^{i}$ -O3	2.191 (2)	Cu1-N4	1.979 (2)
Cu1-N1	2.017 (2)	Cu1-N2	1.987 (2)
Cu1-O1	1.986 (2)		
Bond angle			
$N1\text{-}Cu1\text{-}O3^{i}$	88.93 (8)	N4-Cu1-O1	89.46 (9)
$O1\text{-}Cu1\text{-}O3^{i}$	116.22 (7)	$N2\text{-}Cu1\text{-}O3^{i}$	94.71 (8)
O1-Cu1-N1	80.69 (8)	N2-Cu1-N1	94.63 (9)
$N4\text{-}Cu1\text{-}O3^{i}$	90.95 (9)	N2-Cu1-O1	148.46 (9)
N4-Cu1-N1	168.94 (9)	N2-Cu1-N4	96.40 (10)

Symmetry codes: (i) −x+1, −y+1, −z+2.

Table S3. Selected bond lengths (Å) and angles (º) for **3**

Bond lenghts			
Cd1-O3	2.295 (4)	Cd1-N1	2.337 (5)
Cd1-N2	2.261 (6)	Cd1-N4	2.275 (6)
Cd1-O1^{i}	2.377 (5)	Cd1-O2^{i}	2.462 (5)
Bond angles			
N2-Cd1-O3	91.45 (2)	O1^{i}-Cd1-O3	159.45 (2)
N1-Cd1-O3	72.03 (2)	O1^{i}-Cd1-N2	101.93 (2)
N1-Cd1-N2	160.60 (2)	O1^{i}-Cd1-N1	91.58 (2)
N4-Cd1-O3	93.41 (2)	O1^{i}-Cd1-N4	101.40 (2)
N4-Cd1-N2	92.70(2)	O2^{i}-Cd1-O3	111.56 (2)
N4-Cd1-N1	98.30 (2)	O2^{i}-Cd1-N2	88.50 (2)
O2^{i}-Cd1-N4	154.97 (2)	O2^{i}-Cd1-N1	88.23 (2)
O2^{i}-Cd1-O1i	54.09 (2)		

Hydrogen Bond Geometry				
D–H···A	**D–H**	**H···A**	**D···A**	**D– H···A**
N3-H3···O4^{ii}	0.860(8)	1.886(8)	2.729(8)	166,34(7)
N5-H5···O2^{iii}	0.860(1)	1.911(8)	2.751(8)	165,19(8)

Symmetry codes: (i) x−1/2, −y+3/2, −z+1; (ii) x−1/2, −y+1/2, −z+1; (iii) −x+2, y−1/2, −z+3/2; (iv) x-1/2, −y-1/2, 1-z;

Table S4. Selected bond lengths (Å) and angles (º) for **4.**

Bond lengths			
Cu1-O8	2.614 (5)	Ag1-N2	2.157 (4)
Cu1-N3	2.005 (5)	Ag1-O1	2.452(5)
Cu1-N4	2.012 (5)	Ag1-N1	2.178 (5)
Bond angles			
N3i-Cu1-N3	94.40 (3)	N2-Ag1-O1	124.88 (2)
N3i-Cu1-N4^{i}	84.40 (3)	N2-Ag1-N1	161.21 (2)
N3-Cu1-N4^{i}	176.27 (2)	N1-Ag1-O1	71.18 (2)
O8-Cu1-N3	90.55 (2)	N4-Cu1-N4^{i}	96.90 (4)
O8-Cu1-N4	85.91 (2)		

Symmetry codes: (i) −x, y, −z+3/2; (ii) −x+1/2, −y+1/2, −z+1.

Table S5. Selected bond lengths (Å) and angles (º) for **5**

Bond lengths			
Cu1–N1	2.134 (7)	Cd1–O4	1.947 (4)
Cu1–O1	1.700 (4)	Cd1–O6	2.291 (6)
Cu1–O3	2.737 (4)	Cd1–O7	2.798 (7)
Bond angles			
N1–Cu1–O3^{i}	98.58 (2)	O4^{ii}–Cd1–O7	99.23 (2)
N1–Cu1–N1^{i}	180.00(3)	O6–Cd1–O7	78.10 (3)
N1–Cu1–O3	81.42(2)	O6^{ii}–Cd1–O7	101.91 (3)
O1–Cu1–N1^{i}	99.63 (2)	O4–Cd1–O4^{ii}	180.00 (2)
O1–Cu1–O3^{iii}	83.85 (2)	O4–Cd1–O6	95.44 (2)
O1–Cu1–O3^{iv}	96.15 (2)	O6–Cd1–O6^{ii}	180.00 (2)
O1–Cu1–O1^{i}	180.00(3)	O4–Cd1–O6^{ii}	84.60 (2)
O3–Cu1–O3	180.00(3)	O4–Cd1–O7	80.77 (2)
O1–Cu1–N1	80.37 (2)		

Symmetry codes: (i) −x+1, −y+2, −z+1; (ii) −x+1/2, −y+1/2, −z+1/2; (iii) 1-x, 1-y, 1-z; (iv) x, y+1, z

Table S6. Selected hydrogen bonding geometry (Å, °) for **1**

D–H···A	**H···A**	**D···A**	**D–H···A**
N8-H8B···O6	2.15	2.961 (5)	150
N3-H3A···O2	2.17	2.980 (5)	150
N6-H6A···O2^{i}	2.17	3.062 (5)	170
N6-H6B···O3^{i}	2.35	3.022 (4)	131
N4-H4B···O4^{i}	2.21	3.021 (4)	150
N8-H8A···O2^{i}	2.48	2.979 (4)	115
N2-H2B···O7^{ii}	2.06	2.932 (5)	163
N7-H7A···O7^{iii}	2.14	2.965 (4)	152
N3-H3B···O6^{iii}	2.49	2.965 (5)	113
N5-H5A···O8^{iii}	2.37	3.048 (5)	132
N5-H5B···O6^{iii}	2.21	3.094 (5)	168
N9-H9A···O4^{iv}	2.10	2.973 (5)	162
N7-H7B···O4^{iv}	2.25	3.061 (4)	150

Symmetry codes: (i) x+½, −y+½, z+½; (ii) x−1, y, z; (iii) x−½, −y+½, z−½; (iv) x+1, y, z.

Table S7. Selected hydrogen bonding geometry (Å, °) for **2** and **3**

Complex 2				
X-H···Cu	**H···Cu**	**X···Cu**		**X-H···Cu**
C9-H9A···Cu	2.920(2)	3.462(5)		116.37(1)
C15-H15A···Cu	2.969(1)	3.459(3)		112.52(1)
D-H···A	**D-H**	**H···A**	**D···A**	**D-H···A**
O5-H5a···O1^{i}	0.85(5)	2.117(5)	2.918(3)	157,06(5)
N3-H3···O4^{ii}	0.79(3)	1.939(3)	2.725(3)	172,46(4)
O5-H5B···O4	0.85(4)	2.060(4)	2.870(4)	160,15(4)
N5-H5···O2^{iii}	0.86(4)	1.908(4)	2.718(4)	158,82(4)
Complex 3				
N3-H3···O4^{ii}	0.860(8)	1.886(8)	2.729(8)	166,34(7)
N5-H5···O2^{iii}	0.860(1)	1.911(8)	2.751(8)	165,19(8)

Symmetry codes for **2**: (i) −*x*+½, *y*−½, −*z*+3/2. (ii) 3/2-x, ½+y, 3/2-z, (iii) ½-x, ½+y, 3/2-z; for **3**: (ii) x−½, −y+½, −z+1; (iii) −x+2, y−½, −z+3/2.

Table S8. Selected hydrogen bonding geometry (Å, °) for **4**

D–H···A	**D–H**	**H···A**	**D···A**	**D–H···A**
O5–H1O5···O1	0.89 (1)	1.90 (1)	2.771 (7)	164 (1)
N3–H3A···O2	0.90	2.02	2.922 (7)	177
O7–H2O7···O6	0.902 (5)	1.842 (5)	2.735 (7)	170.5 (3)
O6–H2O6···O5	0.90 (1)	2.07 (1)	2.854 (7)	146 (1)
O6–H1O6···O5^{iv}	0.91 (1)	1.96 (1)	2.834 (8)	162 (1)
O5–H2O5···O7^{iv}	0.988 (6)	1.921 (5)	2.883 (8)	163.5 (3)
N2–H2B···O7^{iv}	0.90	2.14	3.025 (7)	169
N2–H2A···O3^{v}	0.90	2.16	3.046 (6)	167
O7–H1O7···O4^{i}	0.89 (1)	1.98 (1)	2.836 (6)	162 (1)
N3–H3B···O4^{i}	0.90	2.16	3.036 (6)	166
O8–H1O8···O4^{i}	0.988 (5)	1.849 (4)	2.786 (6)	157.3 (3)
N4–H4A···O2^{vi}	0.90	2.07	2.939 (7)	161
O8–H2O8···O3^{vii}	0.906 (5)	1.983 (4)	2.861 (7)	163.1 (3)
N4–H4B···O3^{vii}	0.90	2.31	3.117 (6)	149

Symmetry codes: (i) −x, y, −z+3/2; (iii) x, −y+1, z−1/2; (iv) −x+1/2, y−1/2, −z+3/2; (v) −x, −y, −z+1; (vi) x, y+1, z; (vii) −x, y+1, −z+3/2; (viii) x−1/2, −y+1/2, z−1/2; (ix) −x, −y+1, −z+1.

Table S9. Selected hydrogen bonding geometry (Å, °) for **5**

D-H···A	**H···A**	**D···A**	**D-H···A**
O6–H6B···O3	1.85	2.532 (8)	135
O7–H7A···O3	2.65	2.957 (8)	103
O7–H7B···O2	1.80	2.605 (8)	156
C-O···π	**C-O**	**O···π**	**C-O···π**
C7-O2···Cg^{i}	1.129(8)	3.711(8)	94.93(6)

Symmetry codes: (i) -x,2-y,-z Cg refer to center of the pyridine ring

Table S10. The MIC value (µg/mL) of synthesized complexes on studied microorganisms

	Wild type					**Clinical isolates**				
Complexes	a	b	c	d	e	f	g	h	i	j
1	2250	>4500	>4500	>4500	4500	NT	NT	NT	NT	NT
2	1300	1300	1300	1300	1300	NT	NT	NT	NT	NT
3	Did not disolved in DMSO, water, ethanol and methanol									
4	47	47	47	47	47	47	47	47	47	47
5	47	23	93.5	187	187	47	93.5	187	187	93.5

NT: not tested, a- E. coli, b- S. aureus, c- B. cereus, d- P. aeruginosa, e- C. albicans, f- MRSA, g- E. coli, h- A. baumannii, i- M. morganii, j- E. aerogenes