Supporting Information for:

Complexation of drug amifampridine with Cu(II), Zn(II) and Cd(II) ions, and its dimerization with the magic of Mn(II) salts. Potential anti-COVID-19 and anticancer activities

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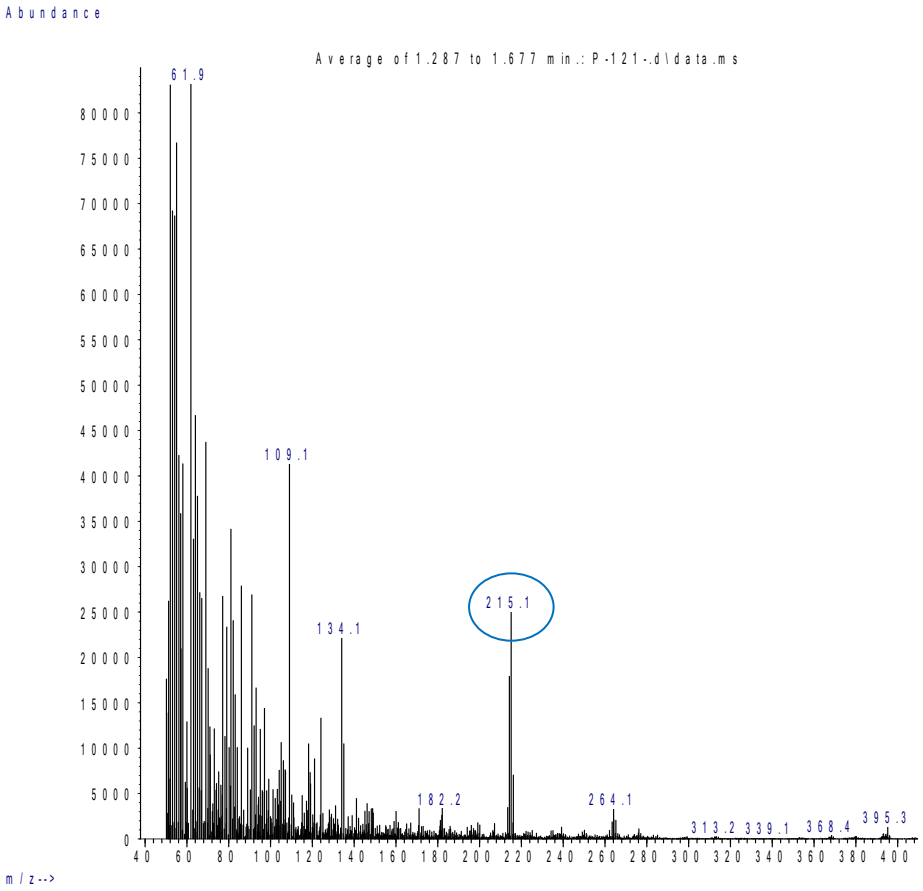


Figure S1. Mass spectrum of [AmpDimer]Cl (**3**).

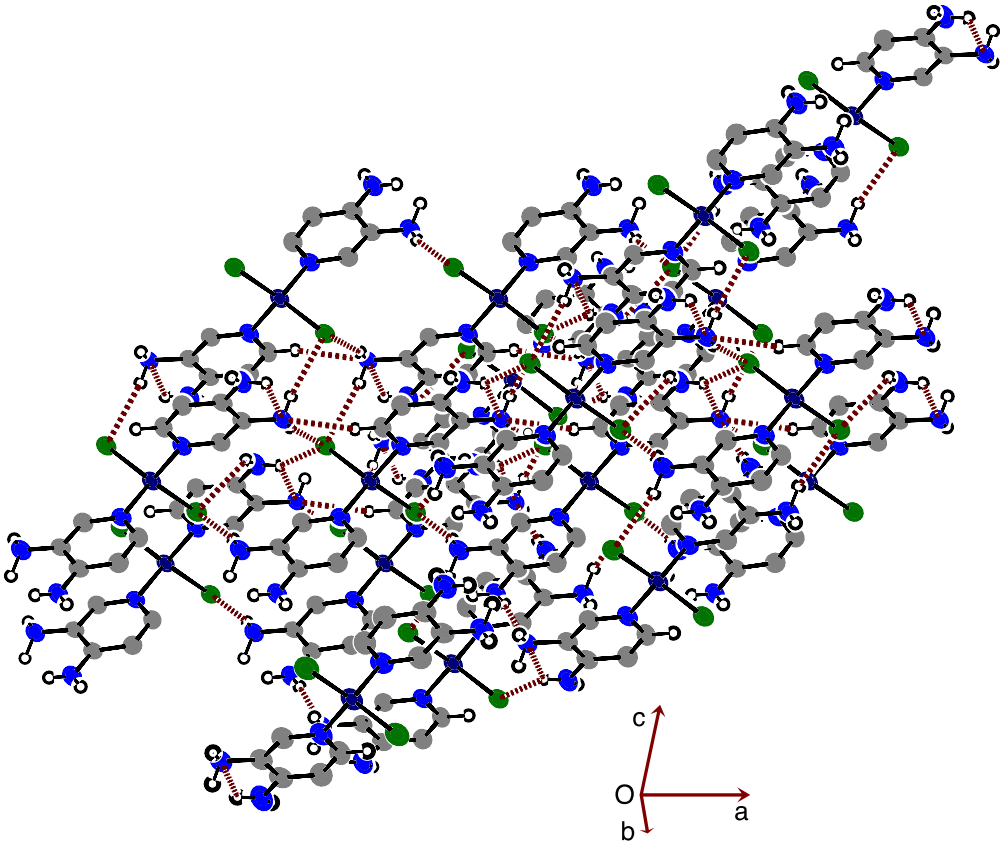


Figure S2. ORTEP diagram of $[Zn(AMP)_2Cl_2]$ (**1**) showing the hydrogen bonds (Zn: dark blue; Cl: green; N: blue; C: grey). Ellipsoids are drawn at the 50% level. Only H-atoms (open circles) on donor atoms are shown.

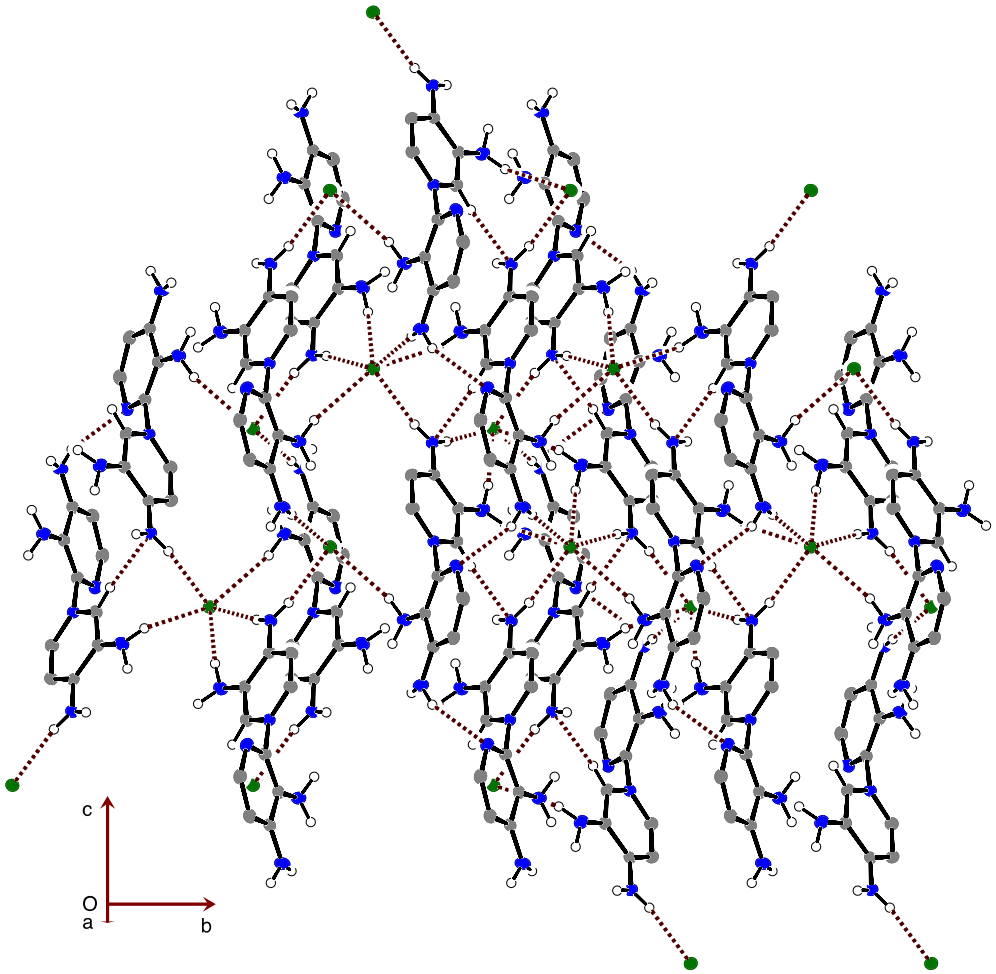


Figure S3. ORTEP diagram of [AmpDimer]Cl (**3**) showing the hydrogen bonds (Cl: green; N: blue; C: grey). Ellipsoids are drawn at the 50% level. Only H-atoms (open circles) on donor atoms are shown**.**

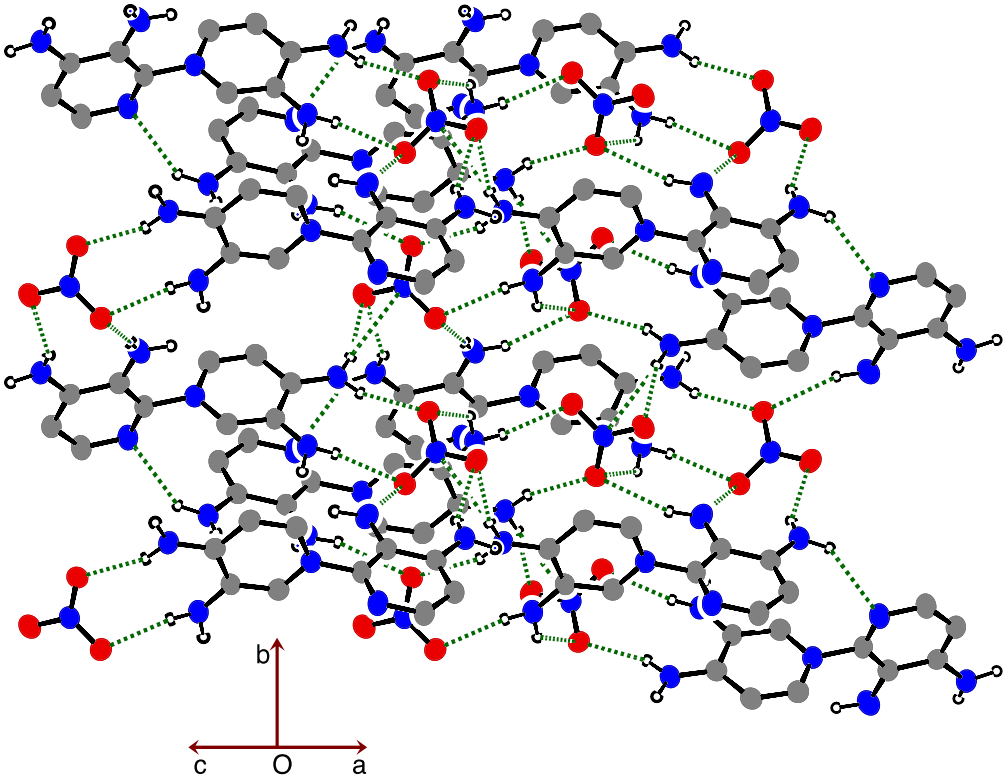


Figure S4. ORTEP diagram of [AmpDimer]NO_3 (**4**) showing the hydrogen bonds (O: Red; N: blue; C: grey). Ellipsoids are drawn at the 25% level. Only H-atoms (open circles) on donor atoms are shown.

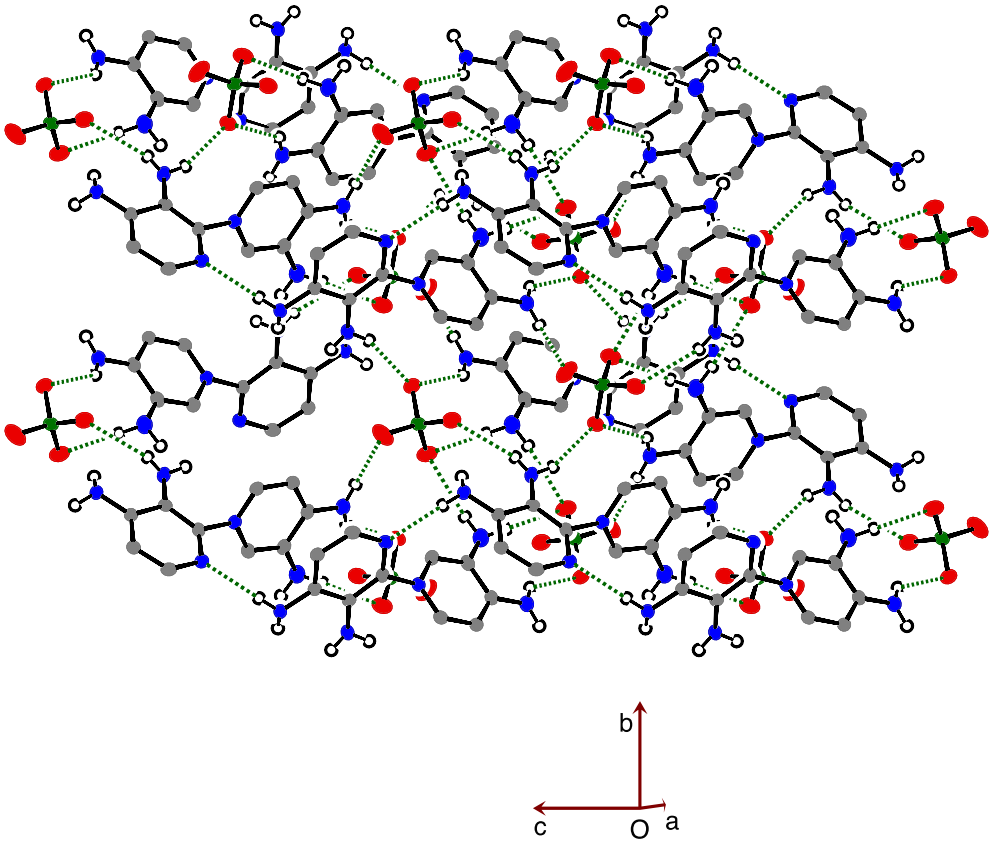


Figure S5. ORTEP diagram of [AmpDimer]ClO_4 (**5**) showing the hydrogen bonds (Cl: green; O: Red; N: blue; C: grey). Ellipsoids are drawn at the 50% level. Only H-atoms (open circles) on donor atoms are shown.

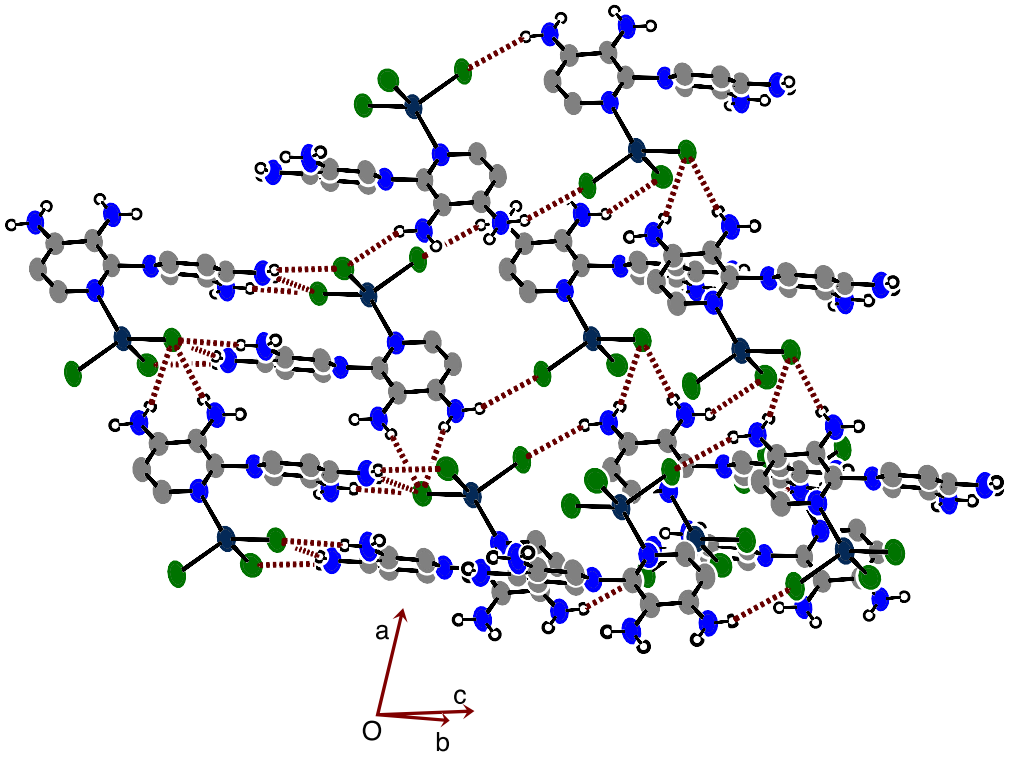


Figure S6. ORTEP diagram of [Cd(AmpDimer)Cl_3] (**7**) showing the hydrogen bonds (Cd: Dark blue; Cl: green; N: blue; C: grey). Ellipsoids are drawn at the 50% level. Only H-atoms (open circles) on donor atoms are shown.

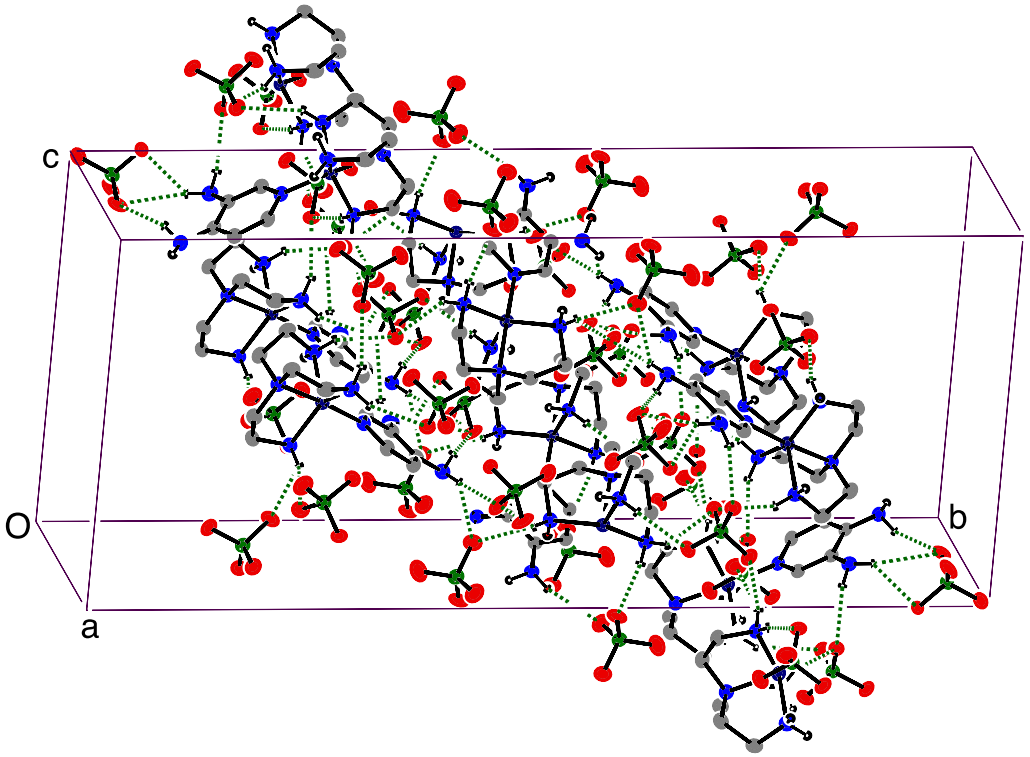


Figure S7. ORTEP diagram of [Cu(tren)(AMP)]$(ClO_4)_2$ (**8**) showing the hydrogen bonds (Cu: Dark blue; Cl: green; O: red; N: blue; C: grey). Ellipsoids are drawn at the 10% level. Only H-atoms (open circles) on donor atoms are shown. [Cd(tren)(AMP)]$(ClO_4)_2$ **(10)** is isomorphous.

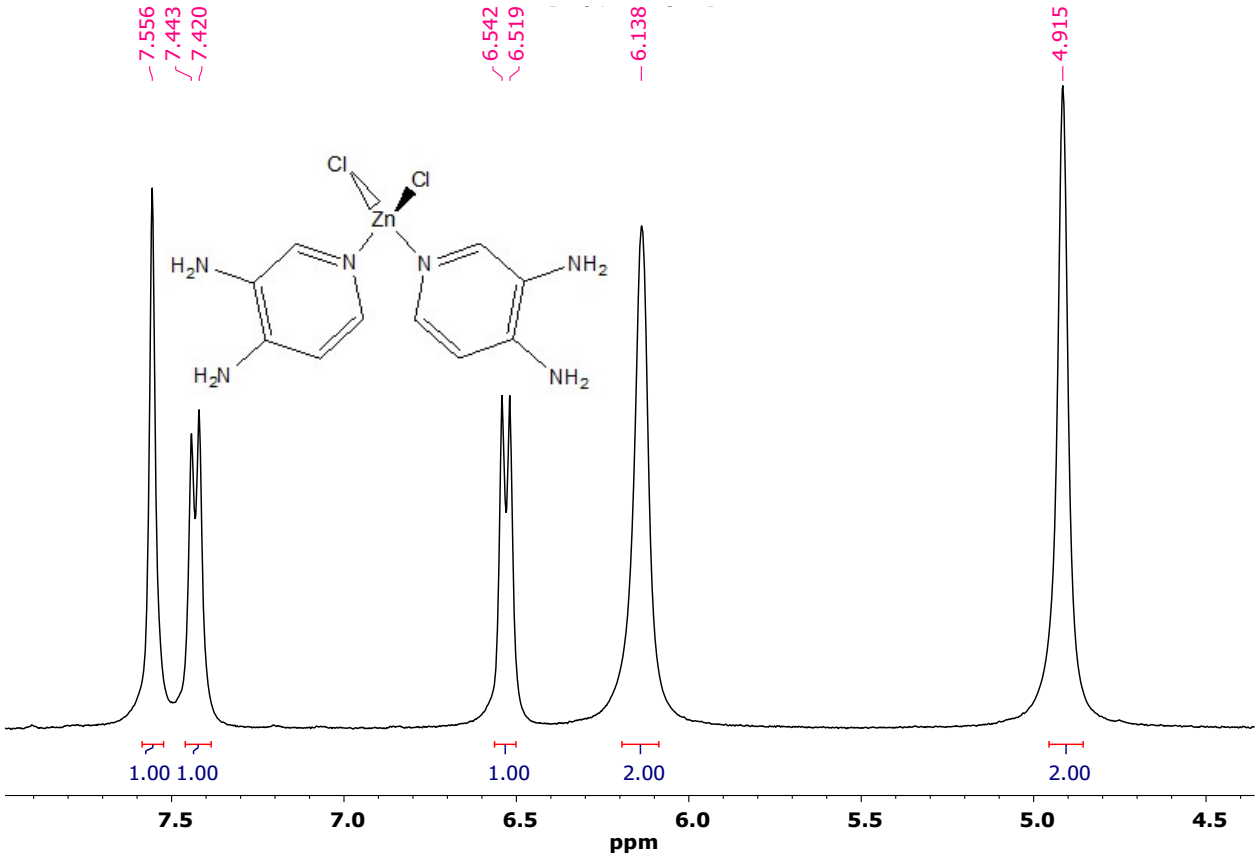


Figure S8. ^{1}H NMR spectrum of $[Zn(AMP)_2Cl_2]$ (**1**) in DMSO-d_6.

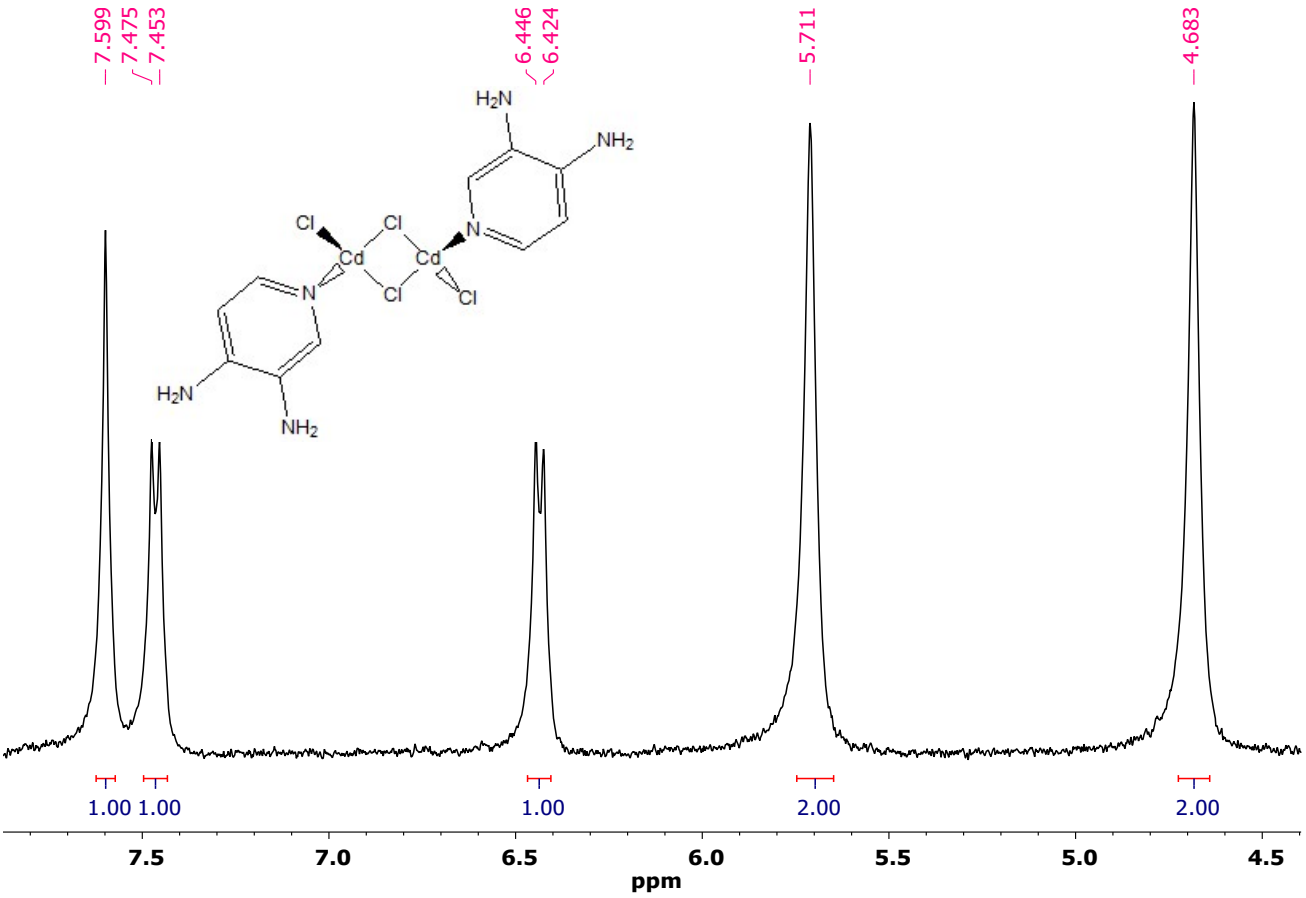


Figure S9. ^{1}H NMR spectrum of $[Cd_2(AMP)_2(\mu\text{-}Cl)_2Cl_2]$ (**2**) in DMSO-d_6.

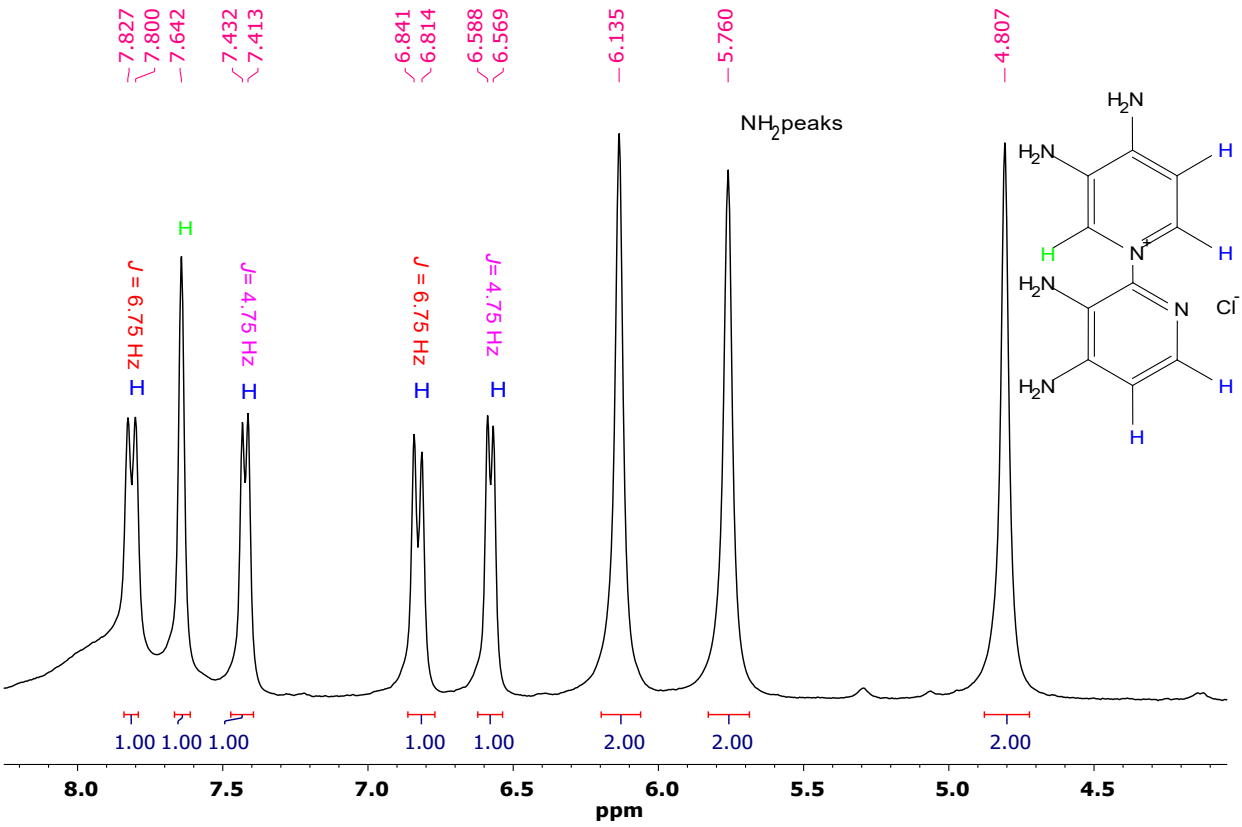


Figure S10. ^{1}H NMR spectrum of [AmpDimer]Cl (**3**) in DMSO-d_6.

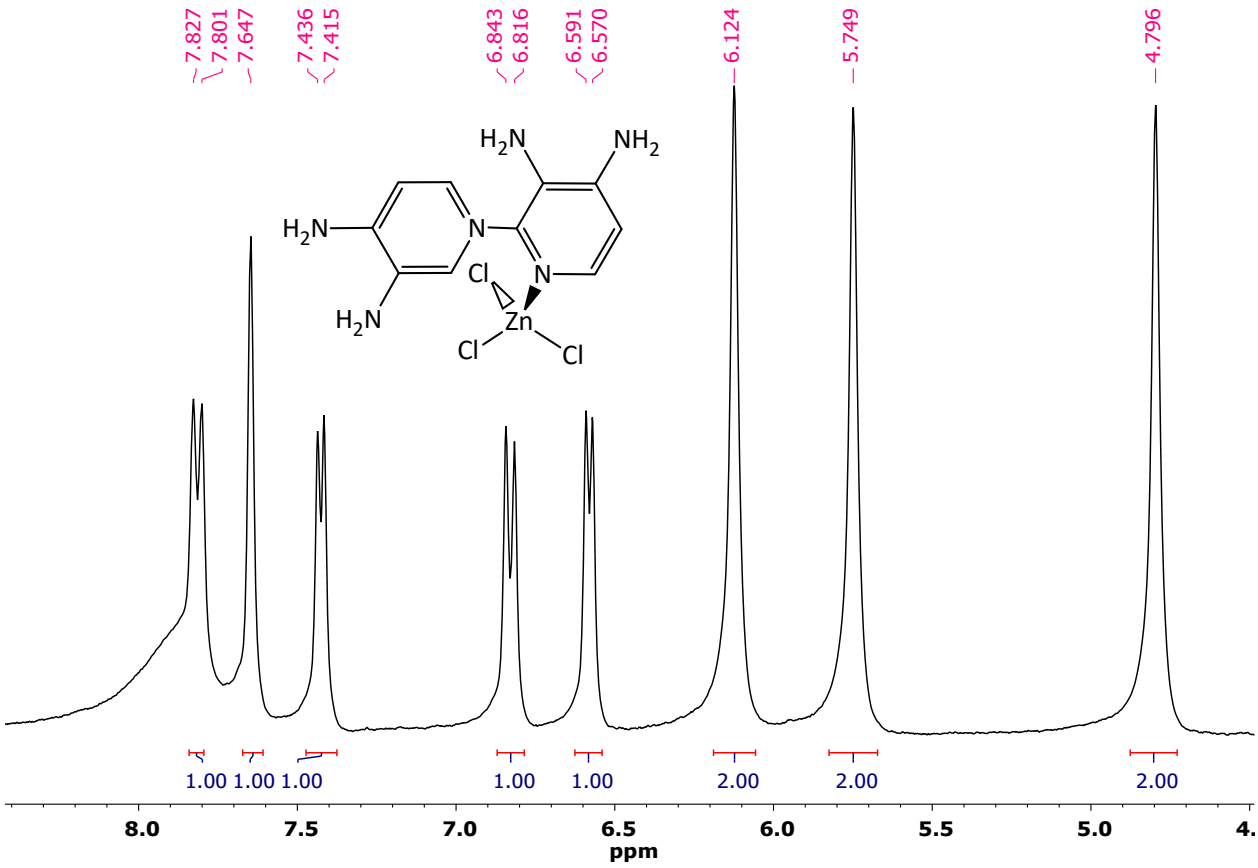


Figure S11. ^{1}H NMR spectrum of [Zn(AmpDimer)Cl_3] (**6**) in DMSO-d_6.

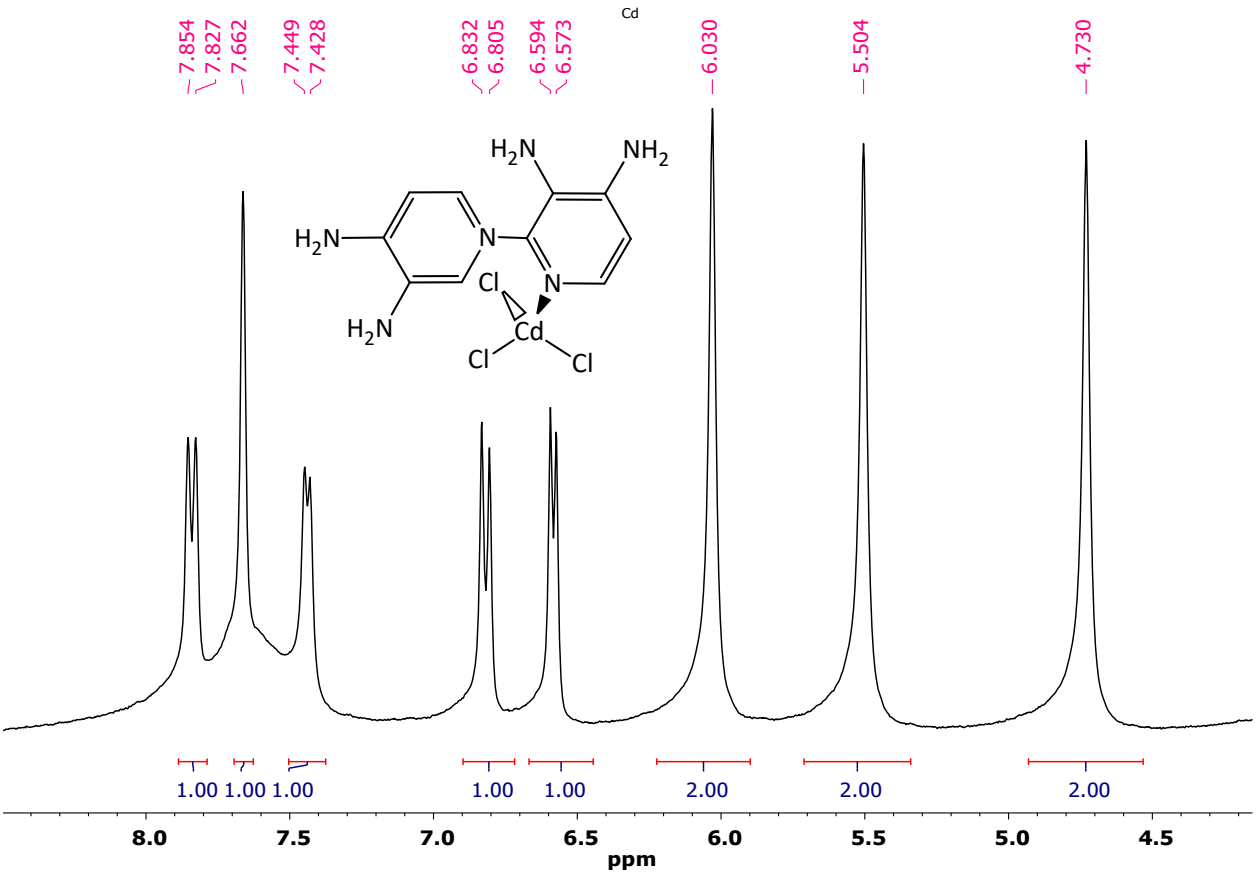
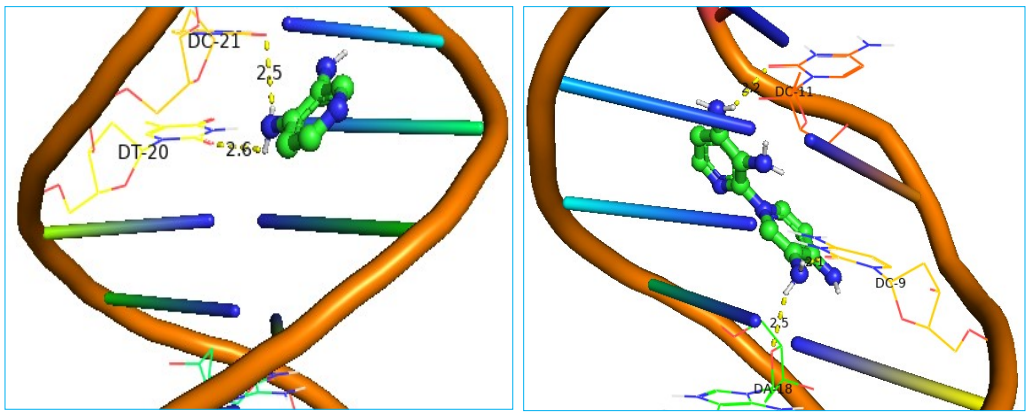


Figure S12. ^{1}H NMR spectrum of [Cd(AmpDimer)Cl_3] (**7**) in DMSO-d_6.



(a) (b)

(c) (d)

Figure S13. Molecular docking 3D visualization of AMP (a), $[AmpDimer]^+$ cation (b), $[Zn(AMP)_2Cl_2]$ (c) and 5-FU (d) in the interaction with DNA (PDB ID: 1BNA), which shows the bond lengths between atoms of above compounds and 1BNA nucleotides.

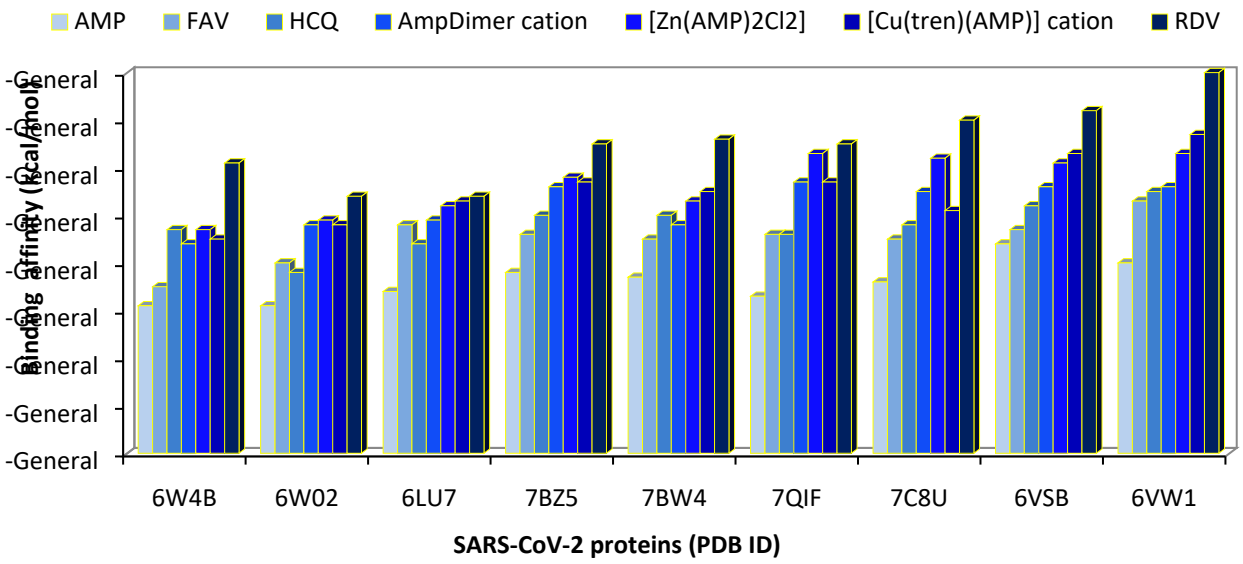


Figure S14. Comparison of binding affinity (kcal/mol) of AMP, $[AmpDimer]^{+}$ cation, $[Zn(AMP)_2Cl_2]$, $[Cu(tren)(AMP)]^{2+}$ cation, FAV, HCQ and RDV in the interaction with essential proteins of SARS-CoV-2.

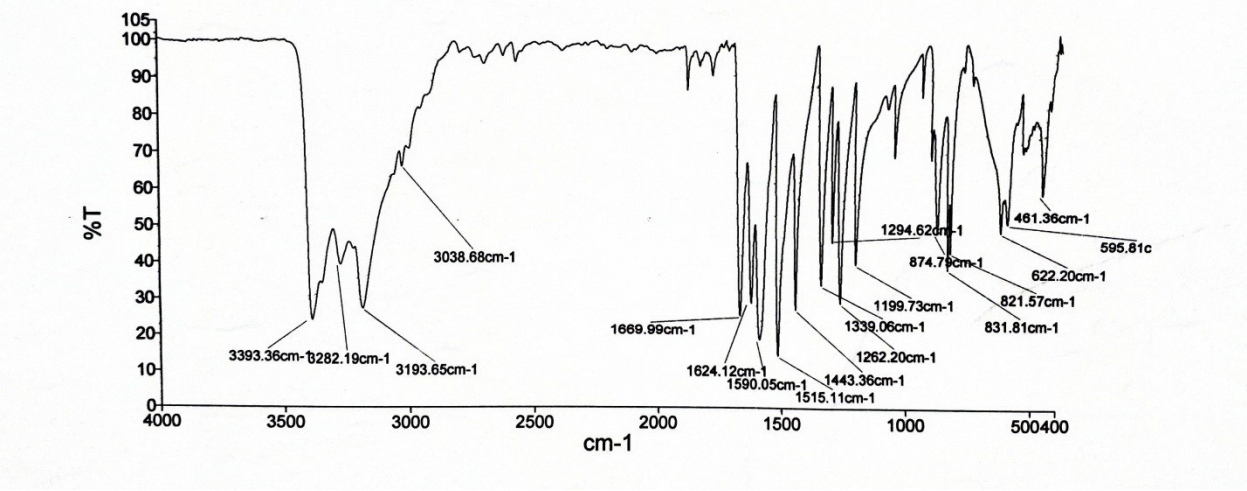


Figure S15. FT-IR (KBr disc) spectrum of AMP.

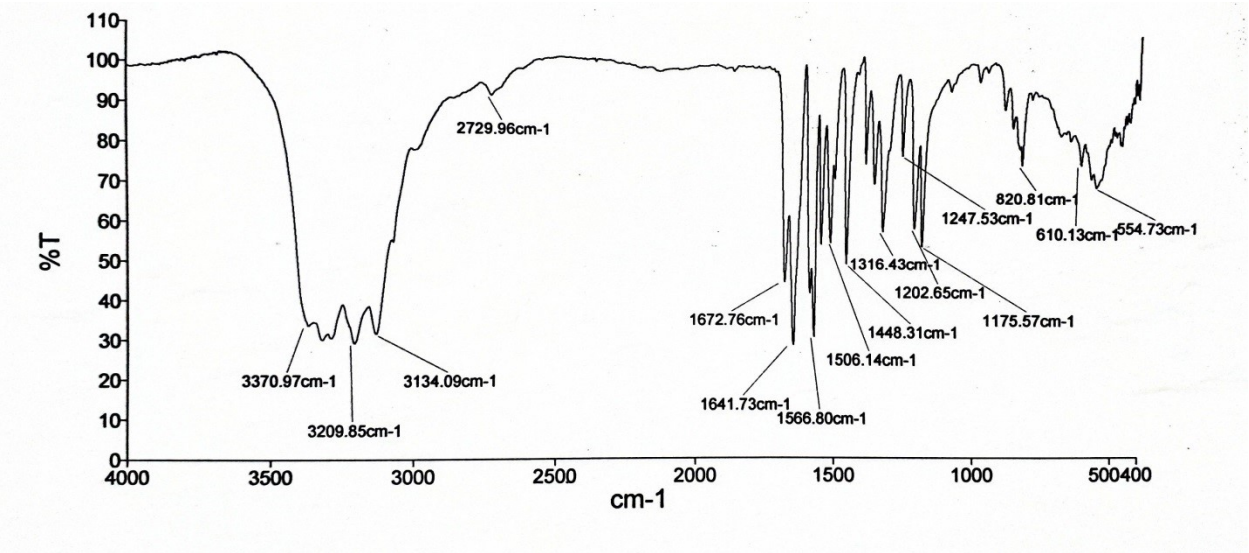


Figure S16. FT-IR (KBr disc) spectrum of [AmpDimer]Cl (**3**).

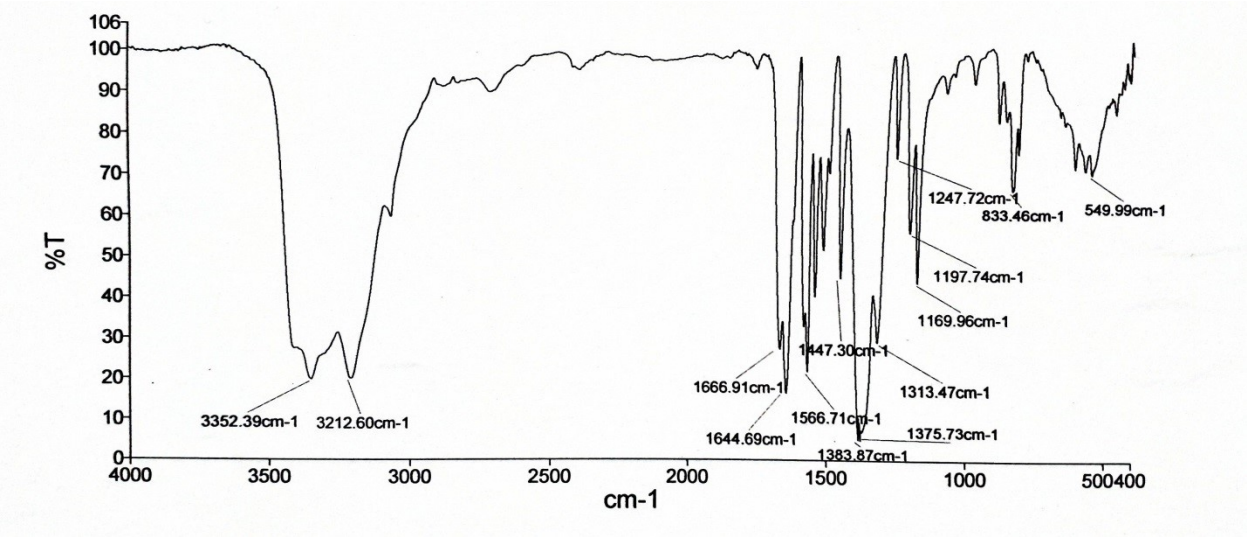


Figure S17. FT-IR (KBr disc) spectrum of [AmpDimer]NO_3 (**4**).

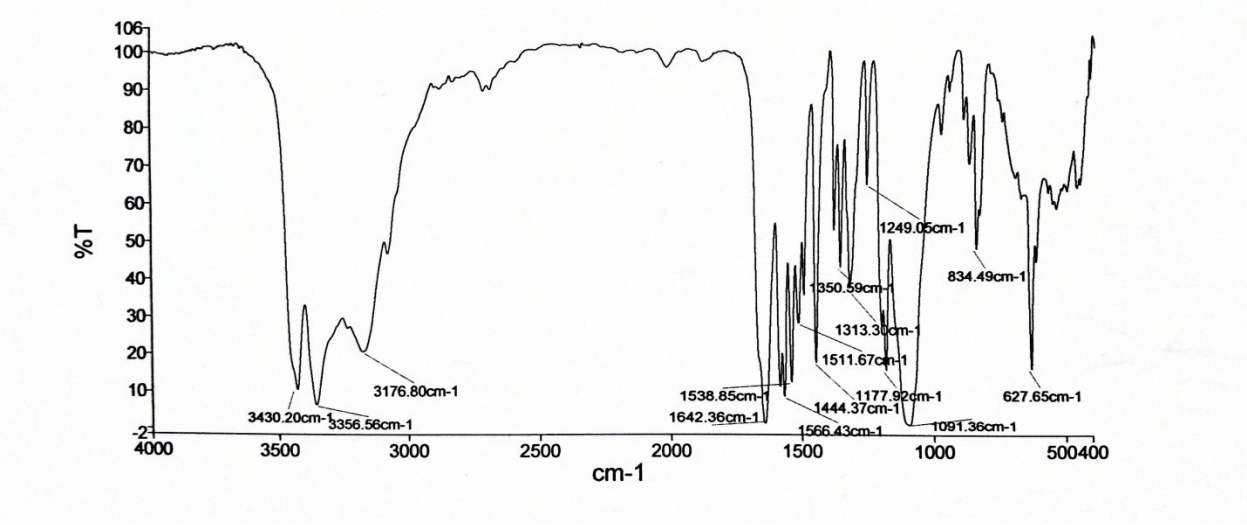


Figure S18. FT-IR (KBr disc) spectrum of [AmpDimer]ClO_4 (**5**).

Table S1. Hydrogen Bonds for $[Zn(AMP)_2Cl_2]$ (**1**)

D-H…A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N2-H2A…Cl2^{i}	0.96(3)	2.43(3)	3.368(2)	166(2)
N2-H2B…Cl2^{ii}	0.87(3)	2.55(3)	3.403(3)	166(3)
N3-H3A…N5^{iii}	0.87(3)	2.31(3)	3.170(3)	169(3)
N5-H5A…Cl1^{iv}	0.85(3)	2.54(3)	3.388(2)	171(3)
N5-H5B…Cl1^{v}	0.82(3)	2.71(3)	3.527(2)	171(3)
N6-H6A…Cl1^{vi}	0.84(4)	2.91(3)	3.459(2)	125(3)
N6-H6B…Cl2^{vii}	0.78(3)	2.95(3)	3.484(3)	128(3)
C1-H1…Cl1	0.95	2.84	3.463(3)	123.9
C6-H6…Cl2	0.95	2.89	3.482(3)	121.5
C10-H10…N5^{ii}	0.95	2.55	3.481(3)	165.6

Symm. Code: i: -x,2-y,1-z; ii: -1+x,+y,+z; iii: 1-x,1-y,1-z; iv: 1-x,1-y,2-z; v: 1+x,+y,+z; vi: 1+x,-1+y,+z; vii: +x,-1+y,+z.

Table S2. Hydrogen Bonds for [AmpDimer]Cl (**3**)

D-H…A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N2-H2A…Cl1^{i}	0.88(2)	2.44(2)	3.3074(12)	168.4(16)
N2-H2B…Cl1	0.86(2)	2.42(2)	3.2615(12)	168.7(17)
N3-H3A…Cl1^{ii}	0.90(2)	2.72(2)	3.5103(13)	146.7(16)
N3-H3B…Cl1^{i}	0.93(2)	2.44(2)	3.3475(12)	164.8(16)
N5-H5A…Cl1^{iii}	0.88(2)	2.49(2)	3.3462(13)	165.2(17)
N5-H5B…N4^{ii}	0.88(2)	2.30(2)	3.1007(16)	151.2(19)
N6-H6A…Cl1^{iv}	0.92(2)	2.64(2)	3.5331(12)	166.0(16)
C5-H5...N2^{ii}	0.947(18)	2.514(18)	3.4259(17)	161.6(14)

Symm Code: i: -x,1/2+y,3/2-z; ii: +x,3/2-y,-1/2+z; iii: +x,+y,-1+z; iv: +x,1/2-y,-1/2+z

Table S3. Hydrogen Bonds for [AmpDimer]NO_3 (**4**)

D-H…A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N2-H2A…O3^{i}	0.90(5)	2.17(6)	3.034(12)	162(4)
N2-H2A…N7^{i}	0.90(5)	2.59(5)	3.424(10)	154(4)
N2-H2A…O3A^{i}	0.90(5)	2.07(8)	2.95(6)	165(5)
N2-H2B…O2	0.90(5)	2.06(5)	2.920(11)	158(4)
N2-H2B…O1A	0.90(5)	2.40(5)	3.22(2)	152(4)
N2-H2B…O2A	0.90(5)	2.01(7)	2.82(5)	149(4)
N2-H2B…N7A	0.90(5)	2.55(6)	3.45(4)	175(5)
N5-H5A..N4^{ii}	0.90(5)	2.41(5)	3.184(6)	144(4)
N5-H5B…O3^{iii}	0.80(5)	2.30(5)	3.017(11)	149(5)
N5-H5B…O3A^{iii}	0.80(5)	2.36(8)	3.12(5)	158(5)
N6-H6A…O1^{iii}	0.74(6)	2.36(6)	3.102(6)	177(6)
N6-H6A…O1A^{iii}	0.74(6)	2.33(6)	3.04(2)	161(6)
N6-H6B…O2^{iv}	0.92(6)	2.29(6)	3.179(10)	162(4)
N6-H6B…O2A^{iv}	0.92(6)	2.19(7)	3.07(5)	161(5)
N3-H3A…O1	0.90(7)	2.13(7)	2.954(7)	152(5)
N3-H3B…O2^{ii}	0.89(7)	2.36(6)	3.011(13)	130(5)
N3A-H3AA…O3A^{i}	0.8907(11)	2.40(4)	3.19(4)	148(2)

Symm Code: i: 1-x,1/2+y,3/2-z; ii: +x,1/2-y,-1/2+z; iii: 1-x,1/2+y,1/2-z; iv: 1-x,1-y,1-z

Table S4. Hydrogen Bonds for for [AmpDimer]ClO_4 (**5**)

D-H…A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N2-H2A…O1^{i}	0.869(5)	2.183(13)	3.011(4)	159(3)
N2-H2B…O4	0.869(5)	2.27(3)	2.947(3)	135(3)
N3-H3A…O2	0.91(4)	2.42(4)	3.178(4)	142(3)
N3-H3B…O2^{ii}	0.91(4)	2.46(4)	3.316(4)	158(3)
N5-H5A…N4^{iii}	0.85(3)	2.26(4)	3.103(3)	169(3)
N6-H6A…O4^{iv}	0.83(4)	2.39(4)	3.171(3)	157(3)
N6-H6B…O3^{v}	0.80(4)	2.45(4)	3.219(3)	161(3)
C1-H1…N5^{vi}	0.95	2.61	3.380(4)	138.6

Symm Code: i: 1-x,1/2+y,3/2-z; ii: 1-x,-y,1-z; iii: +x,1/2-y,-1/2+z; iv: 1-x,1-y,1-z; v: 1-x,1/2+y, 1/2-z; vi: -x,1-y,-z

Table S5. Hydrogen Bonds for [Cd(AmpDimer)Cl_3] (**7**)

D-H…A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N2-H2A…Cl2[i]	0.88	2.63	3.458(4)	156.9
N2-H2B…Cl3[ii]	0.88	2.64	3.444(5)	152.8
N3-H3A…Cl1[iii]	0.88	2.75	3.481(5)	141.0
N3-H3B…Cl3[ii]	0.88	2.58	3.416(5)	159.8
N6-H6A…Cl1[iv]	0.88	2.57	3.197(6)	129.2
N6-H6B…Cl3[iv]	0.88	2.47	3.336(7)	169.2
N5-H5A…Cl1[v]	0.88	2.54	3.204(8)	133.0
N5-H5B…Cl3[iv]	0.88	2.54	3.400(7)	167.0
N5A-H5AA…N2[vi]	0.88	2.29	3.047(13)	144.4
N5A-H5AA…N3[vi]	0.88	2.62	3.094(12)	114.6
N5A-H5AB…N6	0.88	1.99	2.462(14)	111.8

Symm Code: i: 1-x,1-y,-z; ii: 1+x,-1+y,+z; iii: 1+x,+y,+z; iv: 1-x,2-y,1-z; v: 1-x,1-y,1-z; vi: +x,1+y,+z

Table S6. Selected Torsion Angles (°) for [Cu(tren)(AMP)]$(ClO_4)_2$ (**8**) and [Cd(tren)(AMP)]$(ClO_4)_2$ (**10**)

(8, cation 1)		(8, cation 2)		(10, cation 1)	
Torsion Angles					
N1-C1-C2-N2	-53.7(4)	N8-C12-C13-N9	-50.8(4)	N1-C1-C2-N2	-57.5(4)
N1-C3-C4-N3	-51.9(3)	N8-C14-C15-N10	-51.4(4)	N1-C3-C4-N3	-56.1(3)
N1-C5-C6-N4	-50.0(3)	N8-C16-C17-N11	-49.5(4)	N1-C5-C6-N4	-57.2(3)
N2-Cu1-N5-C7	21.2(3)	N9-Cu2-N12-C18	85.4(3)	N2-Cd1-N5-C7	22.9(3)
N2-Cu1-N5-C11	-167.7(2)	N9-Cu2-N12-C22	-87.6(2)	N2-Cd1-N5-C11	-164.5(2)
N3-Cu1-N5-C7	142.7(3)	N10-Cu2-N12-C18	-157.2(3)	N3-Cd1-N5-C7	146.0(2)
N3-Cu1-N5-C11	-46.2(3)	N10-Cu2-N12-C22	29.9(3)	N3-Cd1-N5-C11	-41.4(2)
N4-Cu1-N5-C7	-94.5(3)	N11-Cu2-N12-C18	-48.5(3)	N4-Cd1-N5-C7	-99.5(3)
N4-Cu1-N5-C11	76.6(2)	N11-Cu2-N12-C22	138.5(2)	N4-Cd1-N5-C11	73.1(2)

Table S7. Hydrogen Bonds for [Cu(tren)(AMP)]$(ClO_4)_2$ (**8**)

D-H…A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N2-H2A…O8^{i}	0.91	2.47	3.241(4)	142.1
N2-H2A…O3A^{ii}	0.91	2.55	3.074(9)	116.8
N2-H2B…O11^{iii}	0.91	2.21	3.105(9)	166.7
N2-H2B…O9A^{iii}	0.91	2.49	3.279(4)	145.9
N2-H2B…O11A^{iii}	0.91	2.53	3.395(4)	158.3
N3-H3A…N6^{ii}	0.91	2.32	3.222(4)	171.9
N3-H3B…O10^{iv}	0.91	2.39	2.966(11)	121.3
N3-H3B..O10A^{iv}	0.91	2.42	3.061(3)	127.6
N3-H3B…O13	0.91	2.48	3.267(6)	145.2
N3-H3B..O13A	0.91	2.40	2.989(6)	122.7
N4-H4A...O16	0.91	2.12	2.929(5)	147.6
N4-H4A…O16A	0.91	2.25	3.147(6)	170.0
N4-H4B…O6^{i}	0.91	2.31	3.119(4)	147.3
N6-H6A…O11A^{v}	0.88	2.39	3.122(4)	141.2
N6-H6B...O9^{vi}	0.88	2.54	3.389(15)	162.7
N6-H6B...O10A^{vi}	0.88	2.21	3.079(4)	168.7
N7-H7A…O15A	0.89	2.40	3.062(6)	131.8
N7-H7B…O11A^{v}	0.88	2.33	3.091(4)	144.0
C3-H3D...O14A^{iv}	0.99	2.52	3.408(6)	149.1
C4-H4C…O13A	0.99	2.44	3.120(5)	125.4
C6-H6D…O15^{v}	0.99	2.58	3.543(6)	163.9
C6-H6D…O16A^{v}	0.99	2.59	3.486(7)	149.9
C8-H8…O9^{vi}	0.95	2.53	3.360(13)	146.7
C8-H8…O9A^{vi}	0.95	2.45	3.326(4)	153.7
C11-H11…O13	0.95	2.60	3.543(6)	173.3
N9-H9A…O1^{vii}	0.91	2.34	3.176(5)	152.5
N9-H9A..O3A^{vii}	0.91	2.46	3.156(10)	133.9
N9-H9B...O4^{viii}	0.91	2.31	3.209(5)	171.7
N9-H9B...O4A^{viii}	0.91	2.49	3.389(13)	168.0
N10-H10A…O2A^{viii}	0.91	2.05	2.837(11)	144.3
N10-H10B…O8^{i}	0.91	2.43	3.238(4)	148.6
N11-H11A…O4^{ii}	0.91	2.28	3.098(5)	150.0
N11-H11A…O4A^{ii}	0.91	2.20	3.070(8)	160.2
N11-H11B…O7^{ix}	0.91	2.33	3.191(4)	156.8
N13-H13A…O15^{v}	0.89	2.46	3.237(6)	147.4
N13-H13B…O13^{iv}	0.88	2.31	3.186(6)	169.0
N14-H14A…O7^{i}	0.89	2.32	3.144(4)	153.9
N14-H14B…O14^{v}	0.88	2.44	3.055(6)	127.0
N14-H14B…O15^{v}	0.88	2.54	3.407(7)	166.6
N14-H1…O15A^{v}	0.88	2.20	2.951(6)	142.3
C12-H12A…O3A^{vii}	0.99	2.52	3.269(13)	132.4
C13-H13C…O9A^{i}	0.99	2.49	3.414(4)	154.9
C14-H14C…O12^{i}	0.99	2.41	3.179(16)	134.4
C15-H15A…O1A^{ii}	0.99	2.59	3.494(16)	151.7
C17-H17A…O2A^{vii}	0.99	2.49	3.462(12)	167.0
C18-H18…O2^{vii}	0.95	2.48	3.353(6)	152.0
C18-H18…O1A^{vii}	0.95	2.33	3.133(9)	141.3
C22-H22...O2^{viii}	0.95	2.54	3.348(6)	142.5

Symm Code: i: 1/2+x,3/2-y,-1/2+z; ii: -1+x,+y,+z; iii: +x,+y,-1+z; iv: -x,1-y,1-z; v: 1-x,1-y,1-z; vi: 1+x,+y,-1+z; vii: -3/2+x,3/2-y,1/2+z; viii: -1/2+x,3/2-y,1/2+z; ix: -1/2+x,3/2-y,-1/2+z

Table S8. Selected Bond Lengths (Å), Angles and Torsion Angles (°) for [Cd(tren)(AMP)]$(ClO_4)_2$ (**10**)

		Component:	**1**	**2(A)**	**3(B)**
		Occupancy:	0.368(2)	0.345(2)	0.2871(11)
Bond Lengths					
Cd1-N1	2.384(2)	Cd2-N8	2.409(5)	2.395(6)	2.427(6)
Cd1-N2	2.278(3)	Cd2-N9	2.244(7)	2.286(7)	2.328(7)
Cd1-N3	2.312(3)	Cd2-N10	2.295(7)	2.261(7)	2.231(8)
Cd1-N4	2.279(3)	Cd2-N11	2.312(6)	2.297(6)	2.305(7)
Cd1-N5	2.246(2)	Cd2-N12	2.238(5)	2.248(5)	2.242(6)
Angles					
N2-Cd1-N1	77.31(9)	N9-Cd2-N8	76.9(3)	76.1(3)	73.4(3)
N2-Cd1-N3	117.20(10)	N9-Cd2-N10	108.4(4)	106.8(4)	104.7(4)
N2-Cd1-N4	116.22(10)	N9-Cd2-N11	119.1(5)	118.8(5)	117.1(5)
N3-Cd1-N1	76.76(9)	N10-Cd2-N8	76.0(3)	78.2(3)	77.8(3)
N4-Cd1-N1	77.89(9)	N11-Cd2-N8	75.8(3)	76.5(3)	75.2(3)
N4-Cd1-N3	112.52(10)	N10-Cd2-N11	116.0(5)	119.4(5)	119.8(5)
N5-Cd1-N1	172.19(9)	N12-Cd2-N8	166.8(4)	169.6(4)	158.4(4)
N5-Cd1-N2	110.44(10)	N12-Cd2-N9	115.0(3)	107.3(3)	97.3(3)
N5-Cd1-N3	98.20(9)	N12-Cd2-N10	104.1(4)	109.4(3)	123.7(4)
N5-Cd1-N4	98.90(9)	N12-Cd2-N11	92.6(4)	93.4(4)	92.8(4)
Torsion Angles					
N1-C1-C2-N2	-57.5(4)	N8-C12-C13-N9	52.9(14)	49.2(16	-57.1(12)
N1-C3-C4-N3	-56.1(3)	N8-C14-C15-N10	55.8(15)	40(2)	-61(2)
N1-C5-C6-N4	-57.2(3)	N8-C16-C17-N11	53(2)	48(2)	-52(3
N2-Cd1-N5-C7	22.9(3)	N9-Cd2-N12-C18	155(2)	160(3)	134(2)

N2-Cd1-N5-C11	-164.5(2)	N9-Cd2-N12-C22	-24.8(17)	-33.6	-39.9(16)
N3-Cd1-N5-C7	146.0(2)	N10-Cd2-N12-C18	37(3)	44(3)	21(2)
N3-Cd1-N5-C11	-41.4(2)	N10-Cd2-N12-C22	-143.3(15)	-149.1(15)	-153.0(15)
N4-Cd1-N5-C7	-99.5(3)	N11-Cd2-N12-C18	-81(3)	-78(3)	-108(2)
N4-Cd1-N5-C11	73.1(2)	N11-Cd2-N12-C22	99.1(16)	88.1(16)	77.9(17)

Table S9. Hydrogen Bonds for [Cd(tren)(AMP)]$(ClO_4)_2$ (**10**)

D-H…A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N2-H2A…O9A[i]	0.91	2.56	3.085(8)	117.4
N2-H2A…O15[ii]	0.91	2.38	3.174(4)	146.1
N2-H2A…O15A[ii]	0.91	2.19	3.089(19)	172.2
N2-H2B…O7[i]	0.91	2.29	3.130(4)	153.1
N3-H3A…N6[iii]	0.91	2.33	3.232(4)	172.2
N3-H3B…O1	0.91	2.26	2.890(4)	126.4
N3-H3B…O3A	0.91	2.59	3.423(9)	153.0
N4-H4A..O4	0.91	2.37	3.207(5)	153.5
N4-H4A…O1A	0.91	2.03	2.856(10)	150.5
N4-H4A..O1B	0.91	2.16	2.933(12)	142.6
N4-H4B…O2B[iv]	0.91	2.56	3.099(16)	118.6
N4-H4B…O16[ii]	0.91	2.56	3.201(4)	127.9
N4-H4B…O16A[ii]	0.91	2.37	3.04(2)	130.2
N6-H6A…O5[v]	0.878(5)	2.229(8)	3.105(5)	176(4)
N6-H6B…O6[vi]	0.878(5)	2.235(11)	3.085(5)	163(3)
N7-H7A…O3	0.878(5)	2.33(2)	3.009(5)	135(3)
N7-H7B…O5[v]	0.878(5)	2.289(14)	3.128(4)	160(3)
C2-H2D…O14A[iv]	0.99	2.49	3.20(2)	128.4
C4-H4C…O1	0.99	2.54	3.152(4)	120.2
C4-H4C…O1B	0.99	2.58	3.315(11)	131.1
C4-H4D…O4A[iii]	0.99	2.59	3.368(8)	135.3
C4-H4D…O4B[iii]	0.99	2.48	3.192(10)	128.9
C6-H6D…O4A[iv]	0.99	2.46	3.340(11)	147.8
C6-H6D…O4B[iv]	0.99	2.49	3.338(16)	143.7
C8-H8…O7[vi]	0.95	2.38	3.260(4)	153.8
C11-H11…O3A	0.95	2.50	3.433(9)	166.4
C11-H11…O3B	0.95	2.49	3.365(12)	153.3
N9-H9A…O15[iii]	0.91	2.53	3.263(12)	138.0
N9-H9B…O10	0.91	2.57	3.303(14)	138.5
N10-H10A…O13	0.91	2.59	3.459(9)	159.7
N10-H10A…O14	0.91	2.54	3.012(7)	112.6
N10-H10B…O11[vii]	0.91	2.31	3.150(11)	152.7
N11-H11A…O11	0.91	2.38	3.201(18)	150.1
N11-H11B…O9[viii]	0.91	2.22	3.096(19)	161.0
N13-H13B…O8[v]	0.879(5)	2.38(7)	2.886(10)	116(5)
N14-H14A…O3	0.879(5)	1.98(4)	2.474(9)	114(4)
N9A-H9AA…O15A[iii]	0.91	2.51	3.33(2)	149.9
N9A-H9AB…O10A	0.91	2.30	3.000(15)	133.2
N10A-H10D…O11A[vii]	0.91	2.54	3.356(15)	149.7
N10A-H10D…O14A	0.91	2.27	2.83(2)	119.4
N11A-H11C…O11A	0.91	2.44	3.31(2)	158.7
N11A-H11D…O9A[viii]	0.91	2.45	3.26(2)	149.2
N11A-H11D…O15A[ix]	0.91	2.51	3.22(2)	135.7
C13A-H13H…O12A[vii]	0.99	2.47	3.293(17)	140.6
C14A-H14G…O8[viii]	0.99	2.51	3.331(11)	140.4
C17A-H17C…O7	0.99	2.57	3.38(2)	139.3
C18A-H18A…O12A[viii]	0.95	2.44	3.30(2)	151.0
C22A-H22A…O13A[iii]	0.95	2.39	2.90(2)	112.9
N14A-H14E…O12A	0.880(5)	2.60(4)	3.39(2)	150(6)
N14A-H14F…O2A	0.880(5)	2.31(2)	3.16(2)	160(4)
N9B-H9BA…O11B[vii]	0.91	1.81	2.716(14)	170.7
N10B-H10E…Cl3B[viii]	0.91	2.65	3.463(13)	148.9
N10B-H10E…O10B[viii]	0.91	2.13	3.005(15)	162.4
N11B-H11E…O10B	0.91	2.49	3.27(2)	144.0
C13B-H13K…O10B	0.99	2.33	3.256(14)	155.3
C13B-H13L…O12B[vii]	0.99	2.59	3.285(16)	126.8
C14B-H14K…O8[viii]	0.99	2.49	3.026(10)	114.0
C16B-H16F…O7	0.99	2.59	3.189(9)	118.7
C17B-H17F…O9B[viii]	0.99	2.57	3.40(4)	141.1
C19B-H19B…O3B[viii]	0.95	2.49	3.37(2)	154.0

Symm Code: i: 1/2-x,1/2+y,1/2-z; ii: 2-x,1-y,1-z; iii: -1+x,+y,+z; iv: 1-x,1-y,1-z; v: 1/2+x,1/2-y,-1/2+z; vi: 3/2-x,1/2+y,1/2-z; vii: 1/2+x,1/2-y,1/2+z; viii: 1+x,+y,+z; ix: -1/2+x,1/2-y,-1/2+z