SUPPORTING INFORMATION

Synthesis, characterisation, nuclease and cytotoxic activity of phosphate-free and phosphate-containing copper 4′-(N-methylpyridinium)-2,2′:6′,2″ terpyridine complexes

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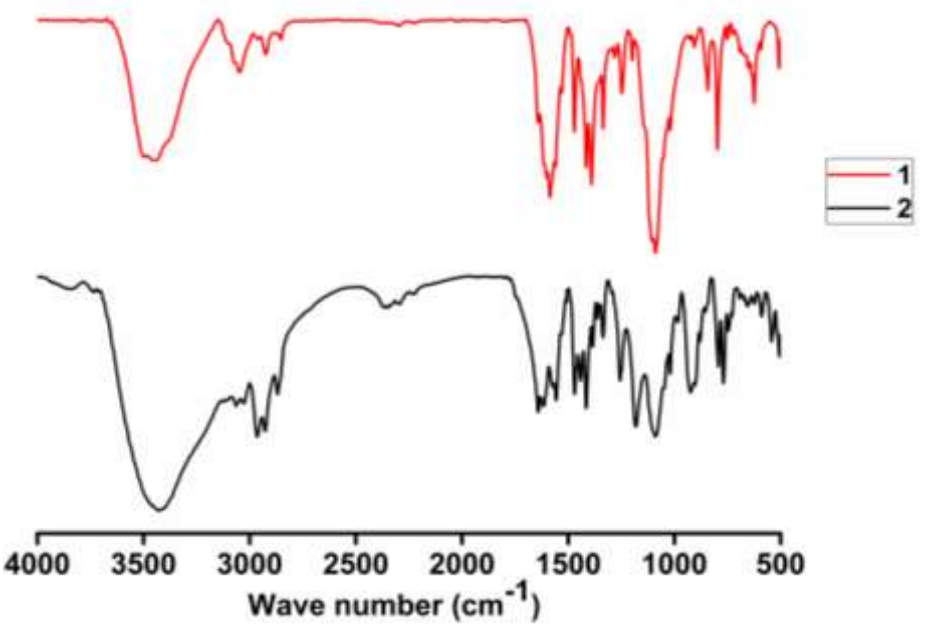

Figure S1. FT-IR spectra of **1** and **2** (as KBr disc)

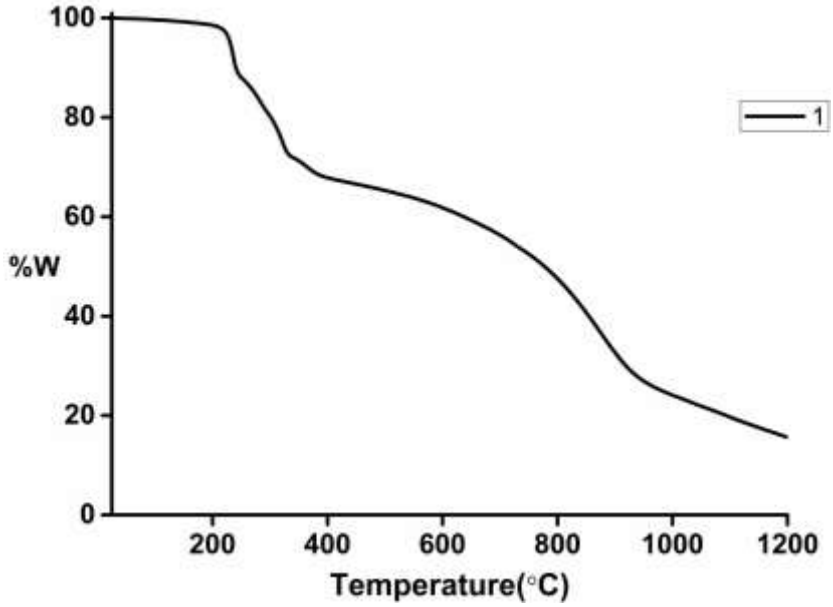

Figure S2. TGA trace of **1**.

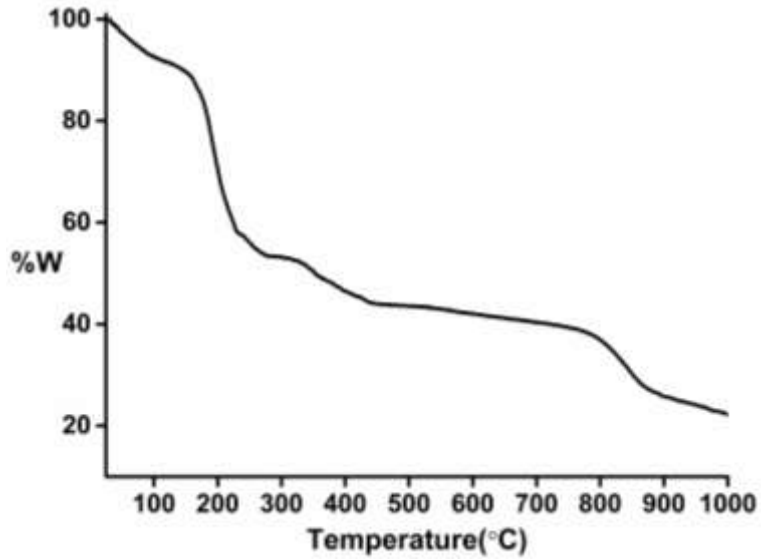

Figure S3. TGA trace of **2**.

Table S1. Selected bond lengths [Å] and angles [°] of complex **1**

Cu(1)-O(1)	1.909(5)	O(1)-Cu(1)-N(2)	173.4(2)
Cu(1)-N(2)	1.958(6)	O(1)-Cu(1)-N(1)	101.2(2)
Cu(1)-N(3)	2.037(6)	N(2)-Cu(1)-N(1)	79.2(2)
Cu(1)-N(1)	2.022(6)	O(1)-Cu(1)-N(3)	98.3(2)
Cu(1)- I(1)	2.121(2)	N(2)-Cu(1)-N(3)	80.2(2)
O(1)-C(22)	1.290(9)	O(1)-Cu(1)-I(1)	101.95(16)
O(2)-C(22)	1.235(9)	N(2)-Cu(1)-I(1)	84.66(16)

Table S2. Selected bond lengths [Å] and angles [°] of complex **2**

Cu(1)-O(5)	1.895(2)	O(5)-Cu(1)-N(2)	158.46(11)
Cu(1)-O(1)	2.147(2)	O(5)-Cu(1)-N(3)	96.61(10)
Cu(1)-N(2)	1.949(3)	N(2)-Cu(1)-N(3)	79.46(10)
Cu(1)-N(3)	2.048(3)	O(5)-Cu(1)-N(1)	99.82(10)
Cu(1)-N(1)	2.058(3)	N(2)-Cu(1)-N(1)	79.20(10)
P(1)-O(1)	1.507(2)	N(3)-Cu(1)-N(1)	156.73(11)
P(1)-O(2)	1.484(3)	O(5)-Cu(1)-O(1)	106.61(9)
P(1)-O(3)	1.569(2)	N(2)-Cu(1)-O(1)	94.93(10)
P(1)-O(4)	1.636(2)	N(3)-Cu(1)-O(1)	97.66(9)
P(2)-O(5)	1.528(2)	N(1)-Cu(1)-O(1)	93.32(9)
P(2)-O(6)	1.520(2)	O(7)-P(2)-O(6)	114.19(13)
P(2)-O(7)	1.505(2)	O(7)-P(2)-O(5)	114.48(13)
P(2)-O(8)	1.641(2)	O(6)-P(2)-O(5)	111.87(13)

Table S3. Hydrogen bonds for complex **2** [Å and °]

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(3)-H(3)...O(6)	0.84	1.73	2.557(3)	167.6
C(7)-H(7)...O(7)#2	0.95	2.42	3.357(4)	167.8
C(15)-H(15)...O(7)	0.95	2.41	3.341(4)	167.8
C(17)-H(17)...O(7)#2	0.95	2.38	3.329(4)	172.5
C(20)-H(20)...O(1)#1	0.95	2.30	3.218(4)	162.1
C(21)-H(21A)...O(9)#1	0.98	2.38	3.337(5)	165.0
C(21)-H(21B)...O(10)#3	0.98	2.46	3.430(7)	172.6
C(46)-H(46C)...O(3)	0.98	2.51	3.461(8)	162.1
O(9)-H(9B)...O(10)#4	0.85	2.07	2.913(5)	172.2

Table S4. Shape measures of the penta coordinate CuN_3O_2 copper centres.

Structure [ML5]	**1**	**2**
PP-5	34.433	31.425
vOC-5	4.333	1.785
TBPY-5	7.158	4.775
SPY-5	**2.402**	**1.006**
JTBPY-5	11.278	6.866

Label	Symmetry	Shape
PP-5	D5h	Pentagon
vOC-5	C4v	Vacant octahedron
TBPY-5	D3h	Trigonal bipyramid
SPY-5	C4v	Spherical square pyramid
JTBPY-5	C2v	Johnson trigonal bipyramid J12