Electronic Supplementary Information (ESI)

DNA cleavage activity of linear trinuclear copper(II) complexes

Arup Kumar Das [a *], Susnata Karmakar [a],

Figures and Tables

Fig. S1. IR spectrum of (*a*)$[Cu_3^{II}(L^2)_4(2\text{-picolinate})_2(OClO_3)_2][ClO_4]_2.2CH_3COCH_3.2CH_3OH$ (1), and (b) $[Cu_3^{II}(L^2)_4(2,6\text{-dipicolinate})_2][ClO_4]_2.6CH_3OH.2H_2O$ (2).

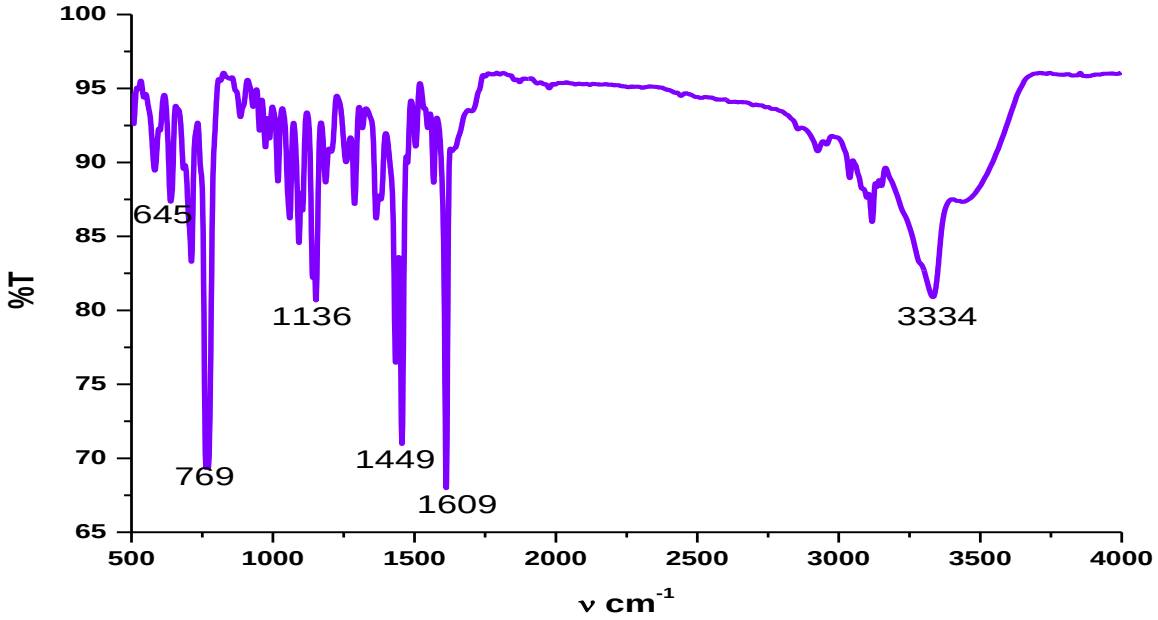
Fig. S2. UV-VIS spectra (in DMF) of (*a*) $[Cu_3^{II}(L^2)_4(2\text{-picolinate})_2(OClO_3)_2][ClO_4]_2.2CH_3COCH_3.2CH_3OH$ (1), and (b) $[Cu_3^{II}(L^2)_4(2,6\text{-dipicolinate})_2][ClO_4]_2.6CH_3OH.2H_2O$ (2).

Fig. S3. UV-VIS spectra (in DMF) of (*a*) $CuSO4.5H_2O$ (b) $[Cu_3^{II}(L^2)_4(2\text{-picolinate})_2(OClO_3)_2][ClO_4]_2.2CH_3COCH_3.2CH_3OH$ (1), and (c) $[Cu_3^{II}(L^2)_4(2,6\text{-dipicolinate})_2][ClO_4]_2.6CH_3OH.2H_2O$ (2) with P-DNA at different concentration.

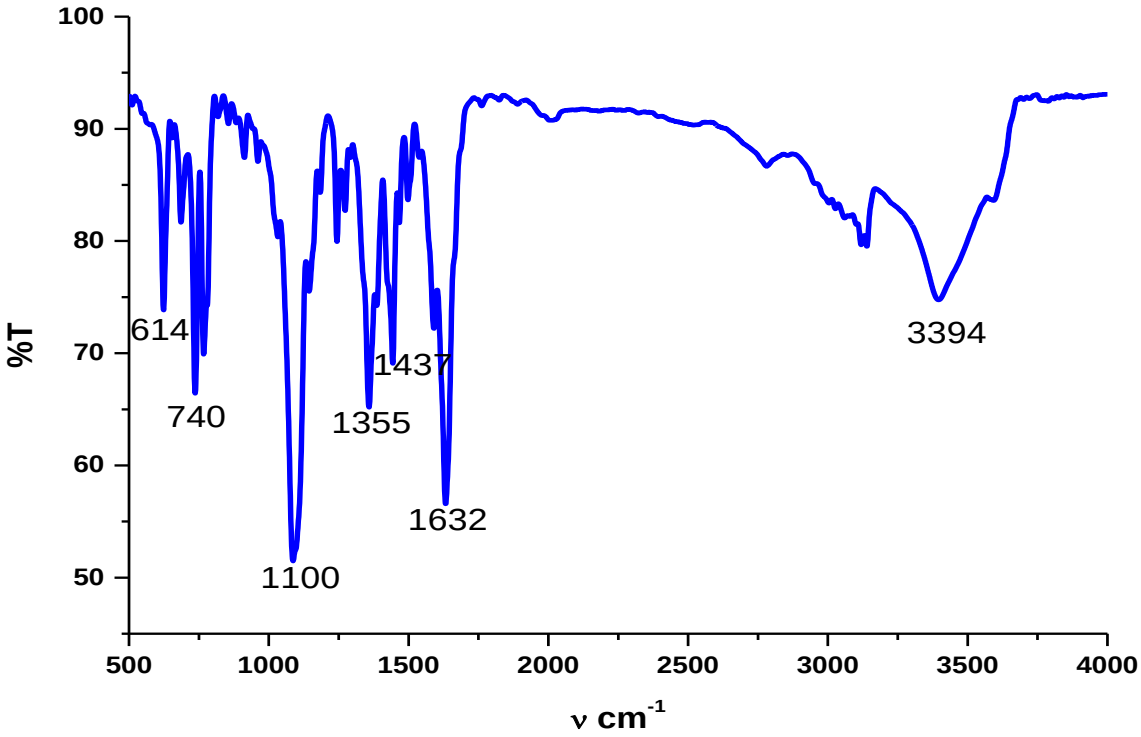
Table. S1. Data collection and structure refinement parameters for $[Cu^{II}_3(L^2)_4(2\text{-picolinate})_2\text{-}(OClO_3)_2](ClO_4)_2\bullet 2CH_3COCH_3\bullet 2CH_3OH$ (**1**), and $[Cu^{II}_3(L^2)_4(2,6\text{-dipicolinate})_2](ClO_4)_2\bullet 6CH_3OH\bullet 2H_2O$ (**2**).

Table. S2. Selected bond lengths (Å) and angles (°) of $[Cu_3(L^2)_4(2\text{-picolinate})_2(OClO_3)_2]\text{-}(ClO_4)_2\bullet 2CH_3COCH_3\bullet 2CH_3OH$ (**1**), and $[Cu_3(L^2)_4(2,6\text{-dipicolinate})_2](ClO_4)_2\bullet 6CH_3OH\bullet 2H_2O$ (**2**).

(a)



(b)



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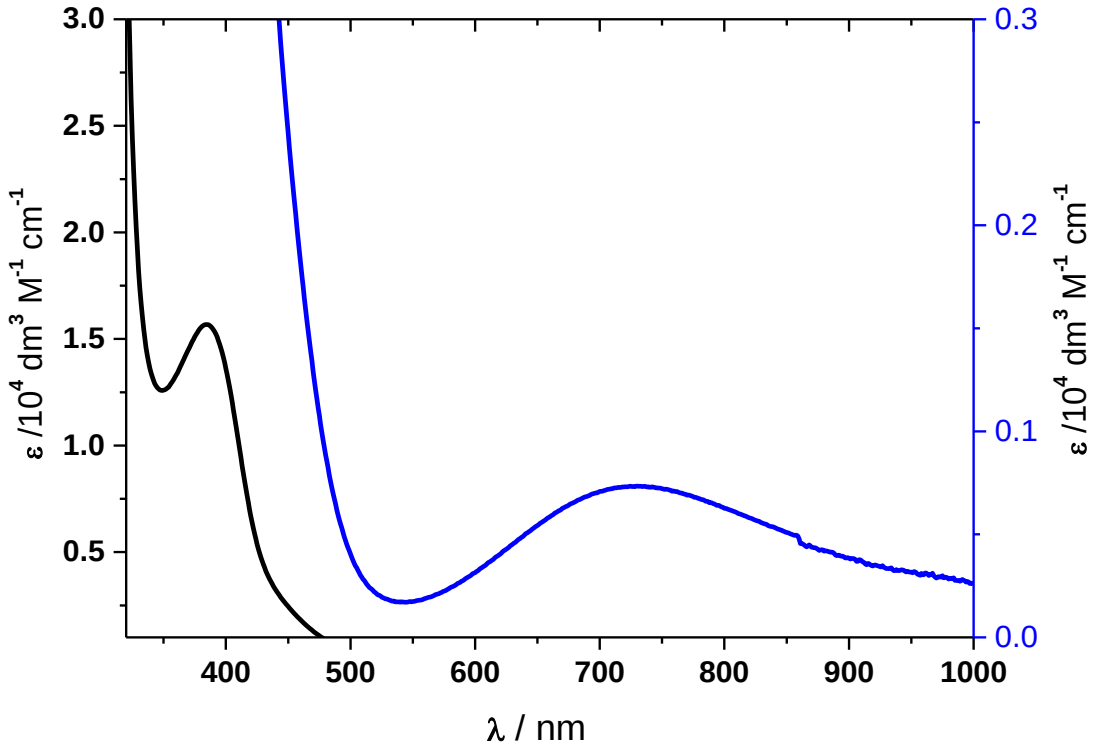
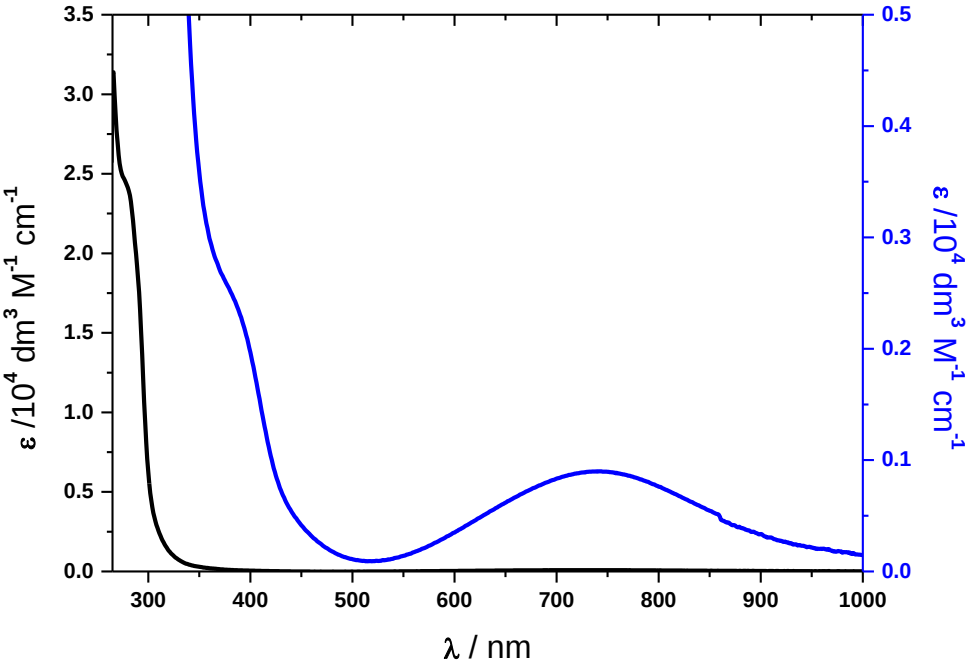


(b)



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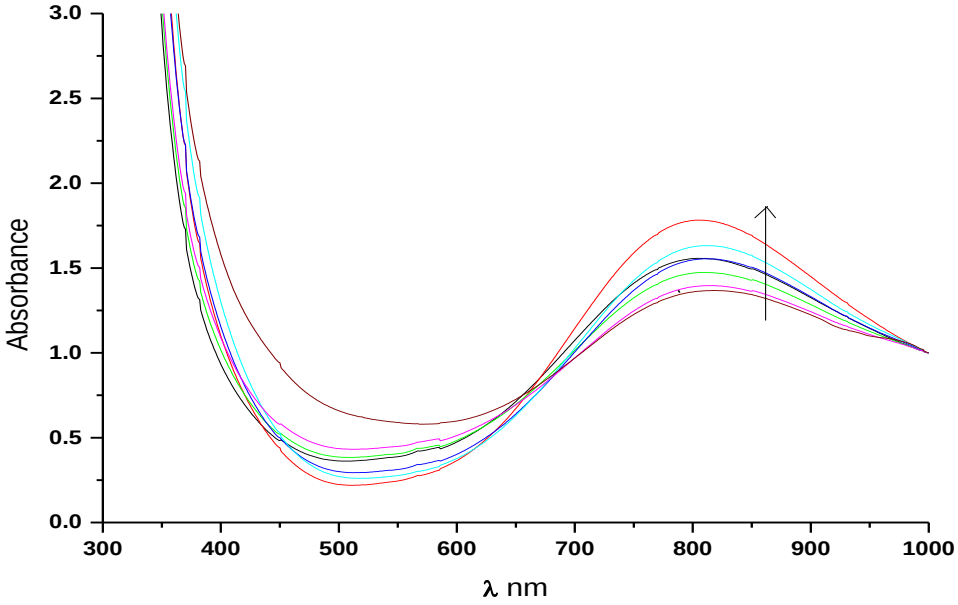
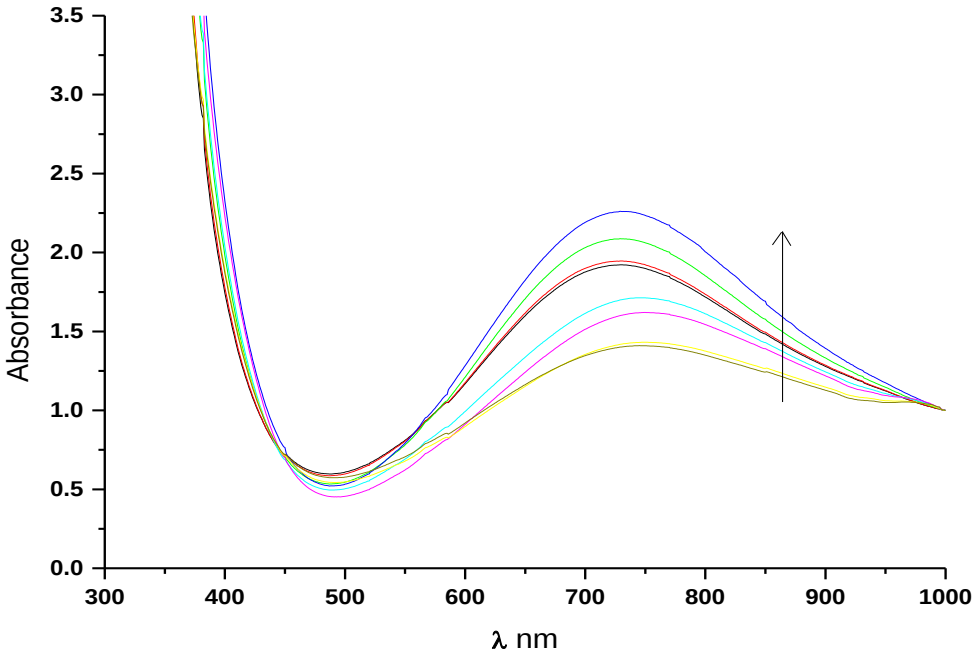
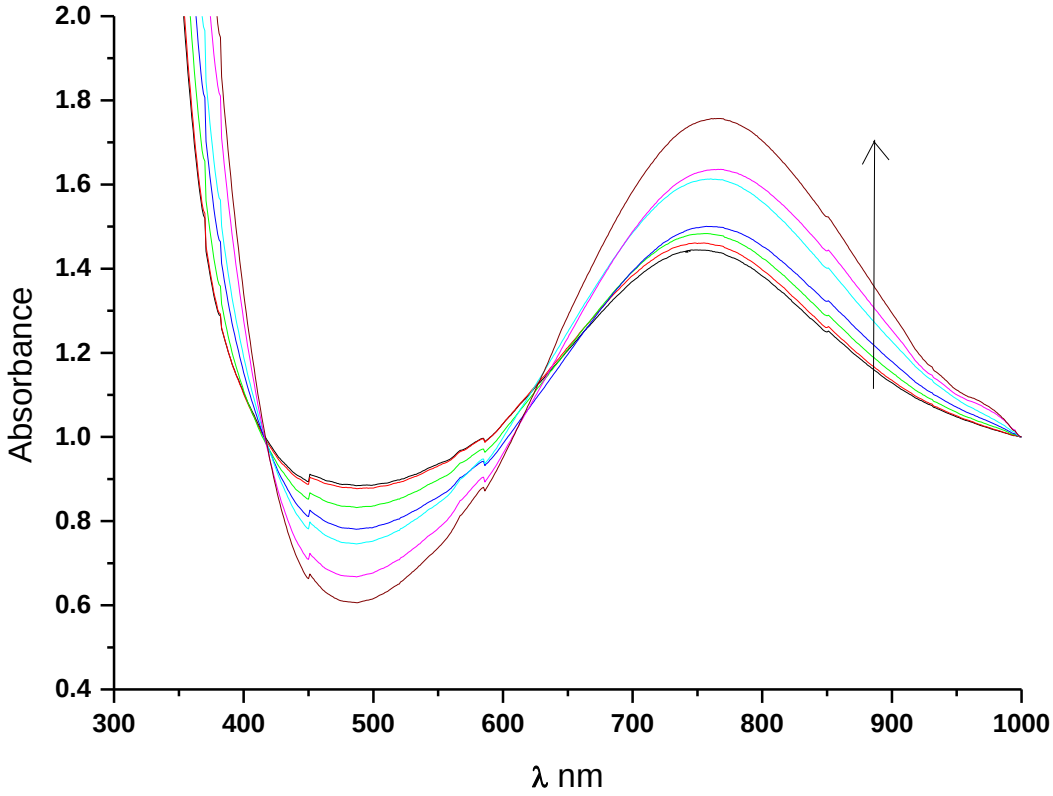

Absorbance
λ nm
3.0
2.5
2.0
1.5
1.0
0.5
0.0
300
400
500
600
700
800
900
1000

(b)


Absorbance
λ nm
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
300
400
500
600
700
800
900
1000

(c)



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	1	**2**
Formula	$C_{80}H_{80}Cl_4N_{14}Cu_3O_{24}$	$C_{80}H_{86}Cl_2N_{14}Cu_3O_{24}$
Formula weight	1954.06	1889.20
Crystal color, habit	blue, block	blue, block
T / K	100(10)	100(10)
Crystal system	Triclinic	Monoclinic
Space group	$P\bar{1}$	$C2/c$
a/Å	12.6131(6)	20.9979(4)
b/Å	12.7714(5)	14.3682(3)
c/Å	14.4145(7)	27.2294(6)
α/°	88.583(4)	90
β/°	78.027(4)	94.892(2)
γ/°	69.131(4)	90
V/Å^3	2119.39(18)	8185.2(3)
Z	2	8
D_c/g cm^{-3}	1.5309	1.531
μ/mm^{-1}	0.957	0.925
Reflections measured	15508	16215
Unique reflections/R_{int}	7389/0.0316	7162/0.0262
Reflections used $I > 2\sigma(I)$]	6136	6583
R_1 [a], wR_2 [b] [$I > 2\sigma(I)$]	$R_1 = 0.0603$ [a] $wR_2 = 0.1577$ [b]	$R_1 = 0.0535$ [a] $wR_2 = 0.1536$ [b]
R_1 [a], wR_2 [b] (all data)	$R_1 = 0.0733$ [a] $wR_2 = 0.1695$ [b]	$R_1 = 0.0573$ [a] $wR_2 = 0.1576$ [b]
GOF on F^2	1.0673	1.031

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1		**2**	
Cu1–N2	1.995(3)	Cu1–N3	1.981(3)
Cu1–N3	1.991(3)	Cu1–N4	1.987(3)
Cu1–N4	2.155(3)	Cu1–N5	2.230(3)
Cu1–N6	2.076(3)	Cu1–N6	2.053(3)
Cu1–O2	2.057(3)	Cu1–O1	2.022(3)
Cu2–N1	1.971(3)	Cu2–N1	1.903(4)
Cu2–O1	1.954(3)	Cu2–N2	1.985(4)
Cu1···Cu2*	4.654	Cu2–O1	2.352(2)
		Cu2–O3	2.039(2)
		Cu1···Cu2*	4.119
N2–Cu1–N3	175.67(13)	N3–Cu1–N4	177.18(12)
N2–Cu1–N4	79.49(13)	N3–Cu1–N6	102.15(11)
N2–Cu1–N6	100.45(14)	N3–Cu1–O1	149.85(10)
N2–Cu1–O2	89.82(12)	N4–Cu1–O1	92.39(10)
N3–Cu1–N4	104.15(13)	N5–Cu1–N3	79.87(12)
N3–Cu1–N6	80.39(14)	N5–Cu1–N4	97.99(12)
N3–Cu1–O2	87.11(12)	N5–Cu1–N6	110.44(11)
N4–Cu1–N6	113.13(12)	N5–Cu1–O1	99.49(10)
N4–Cu1–O2	102.28(11)	N6–Cu1–N4	80.29(11)
N6–Cu1–O2	144.31(12)	N6–Cu1–O1	149.85(10)
N1–Cu2–O1	90.66(12)	N1–Cu2–O1	104.66(6)
N1–Cu2–O1	83.34(12)	N1–Cu2–O3	79.87(7)
		N2–Cu2–O1	75.34(6)
		N2–Cu2–O3	100.13(7)
		O1–Cu2–O1	150.67(12)
		O3–Cu2–O1	99.69(9)
		O3–Cu2–O1	85.46(9)
		O3–Cu2–O3	159.73(15)
		Cu1–O1–Cu2	140.60(12)