Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Synthesis, structure elucidation and DFT studies of a new coumarin derived Zn(II) complex: *In vitro* DNA/HSA binding profile and pBR322 cleavage pathway

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Table S1. Selected Geometrical Parameters Bond Length (Å) and Bond Angles (°) in **1.**

Geometrical Parameters	**Experimental from X-ray data**	**Theoretical calculations**
Zn1–O1	2.064(4)	2.0641
Zn1–O9	2.101(4)	2.1011
Zn1–O2W	2.075(5)	2.0752
Zn1–O2W	2.121(4)	2.1202
Zn1–O3W	2.087(5)	2.0874
Zn1–O4W	2.098(4)	2.0981

Table S2. Selected Bond Distances (Å) and Bond Angles (°) in **1.**

1

Zn1 O1 2.064(4)	Zn1 O9 2.101(4)	Zn1 O1W 2.075(5)
Zn1 O2W 2.121(4)	Zn1 O3W 2.087(5)	Zn1 O4W 2.098(4)
O1 Zn1 O1W 97.73(17)	O1 Zn1 O3W 85.88(17)	O1W Zn1 O3W 176.36(19)
O1 Zn1 O4W 89.05(16)	O1W Zn1 O4W 85.99(18)	O3W Zn1 O4W 93.58(18)
O1 Zn1 O9 174.35(17)	O1W Zn1 O9 87.92(17)	O3W Zn1 O9 88.47(16)
O4W Zn1 O9 91.16(16)	O1 Zn1 O2W 94.68(17)	O1W Zn1 O2W 83.48(17)
O3W Zn1 O2W 96.78(18)	O4W Zn1 O2W 169.21(19)	O9 Zn1 O2W 86.12(16)

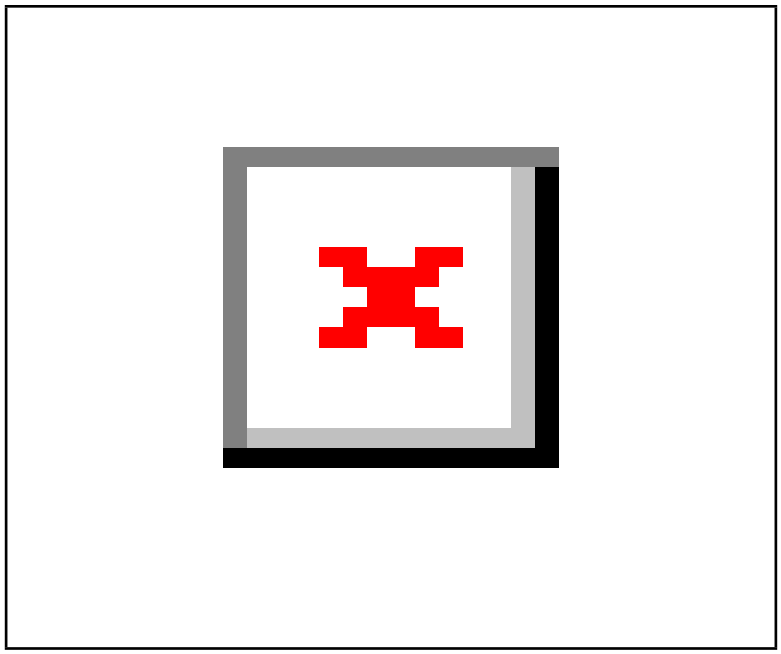

Fig. S1. Thermogravimetric analysis of Complex **1**.

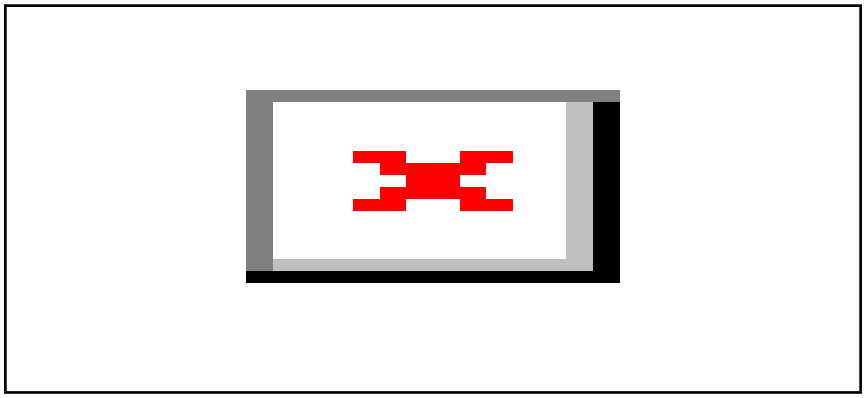

Fig. S2. PXRD of Complex **1**.

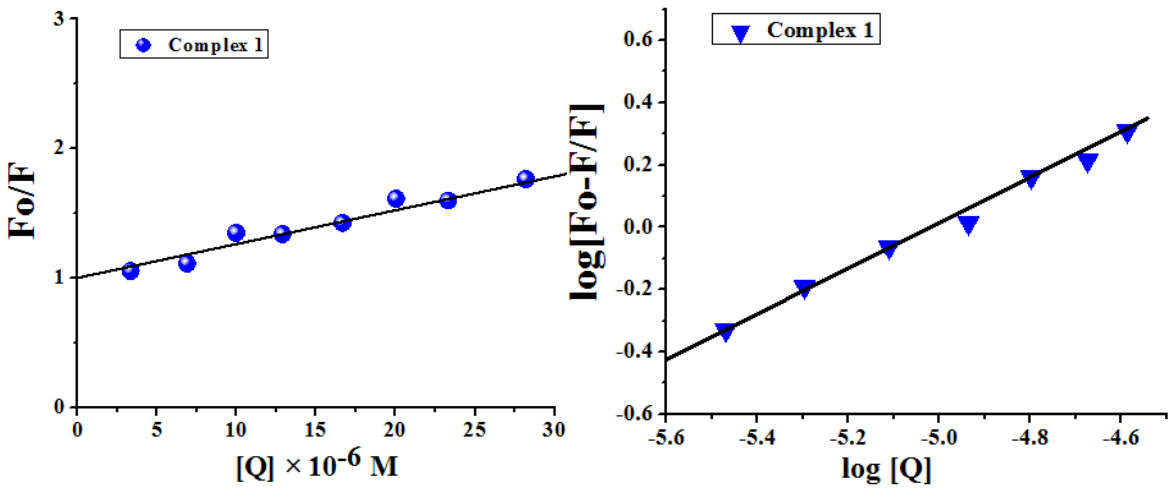

Fig. S3. (a) Stern–Volmer plots showing HSA tryptophan quenching caused by complex **1** at room temperature (pH 7.40, λ_{ex} = 295 nm, λ_{em} = 327 nm); (b) Logarithmic plot of the fluorescence quenching of HSA for the calculation of binding constant (K) and number of binding sites (n) for complex **1** HSA at room temperature.

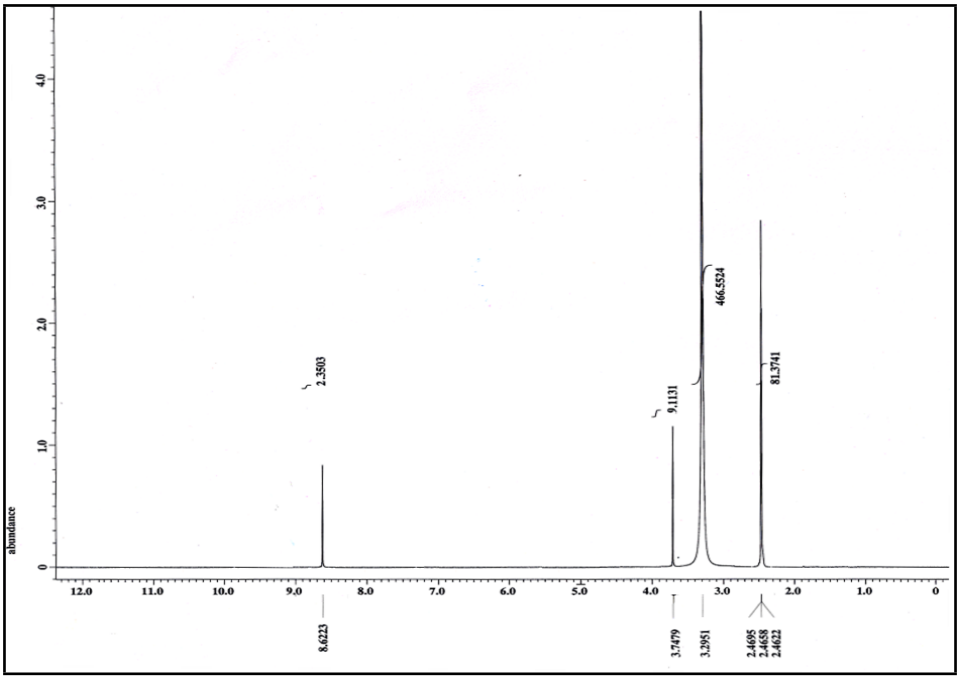

Fig. S4. [1]HNMR spectrum of Triester.

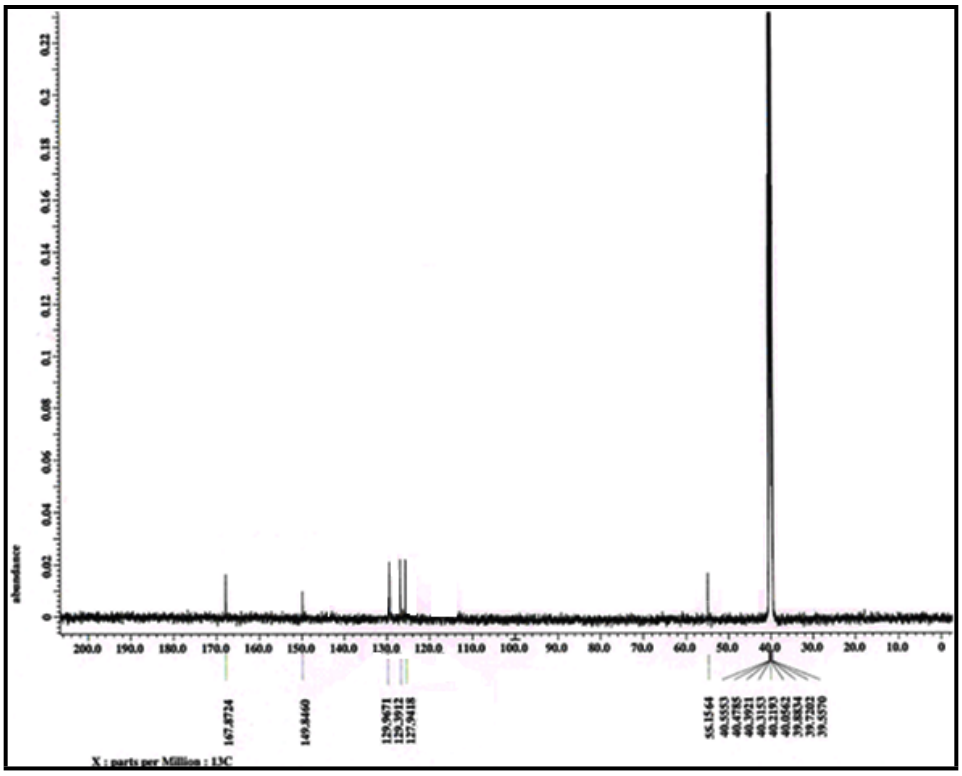

Fig. S5. ^{13}C NMR spectrum of Triester.

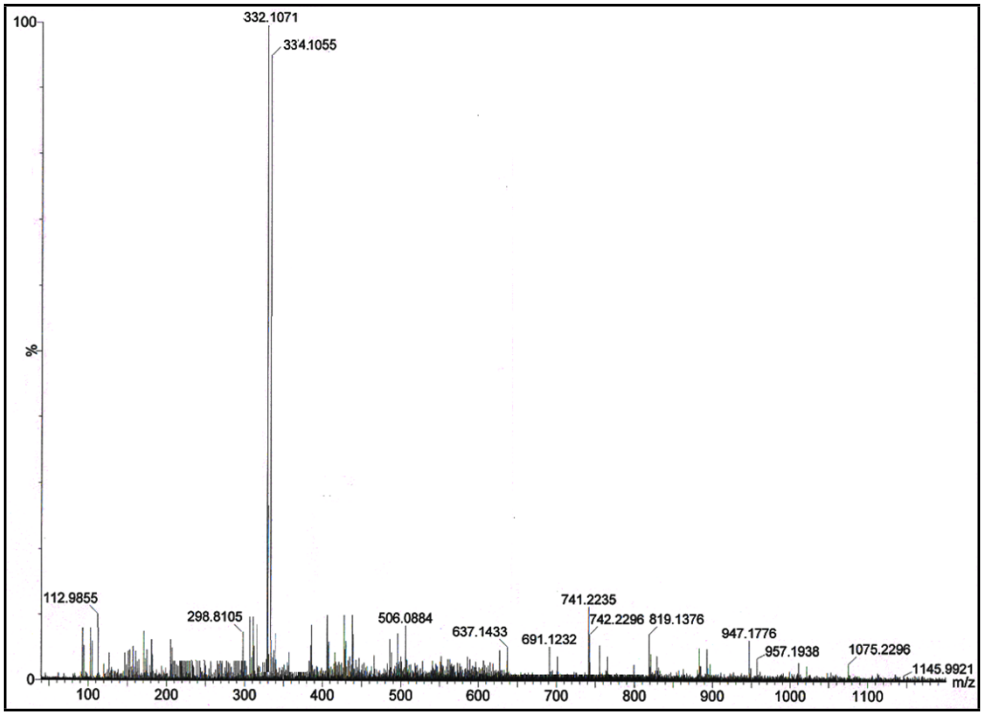

Fig. S6. ESI-MS spectrum of Triester.

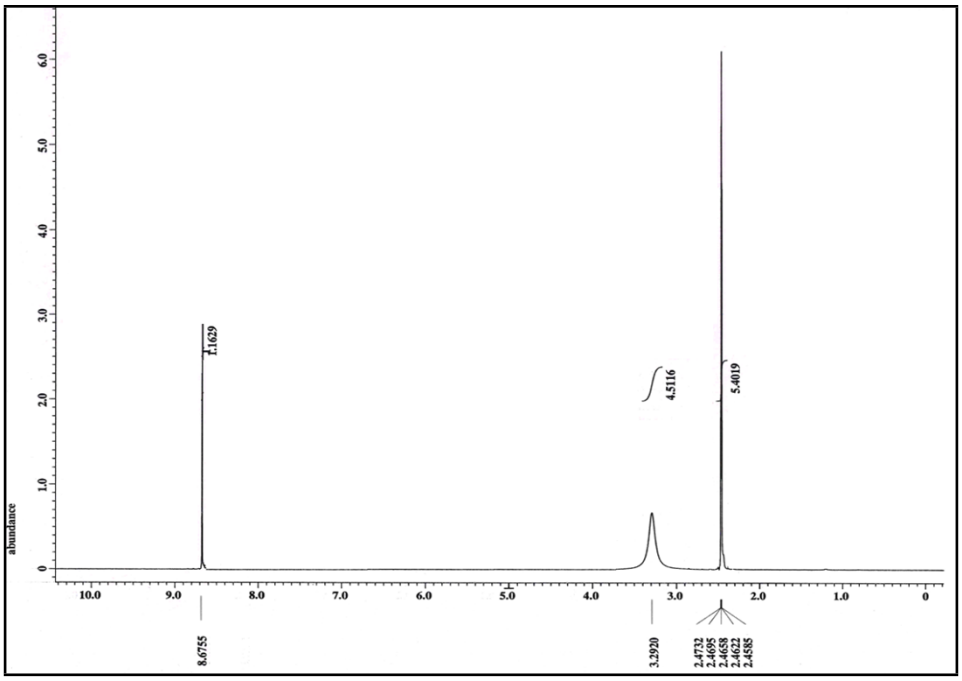

Fig. S7. ^{1}HNMR spectrum of H_6L.

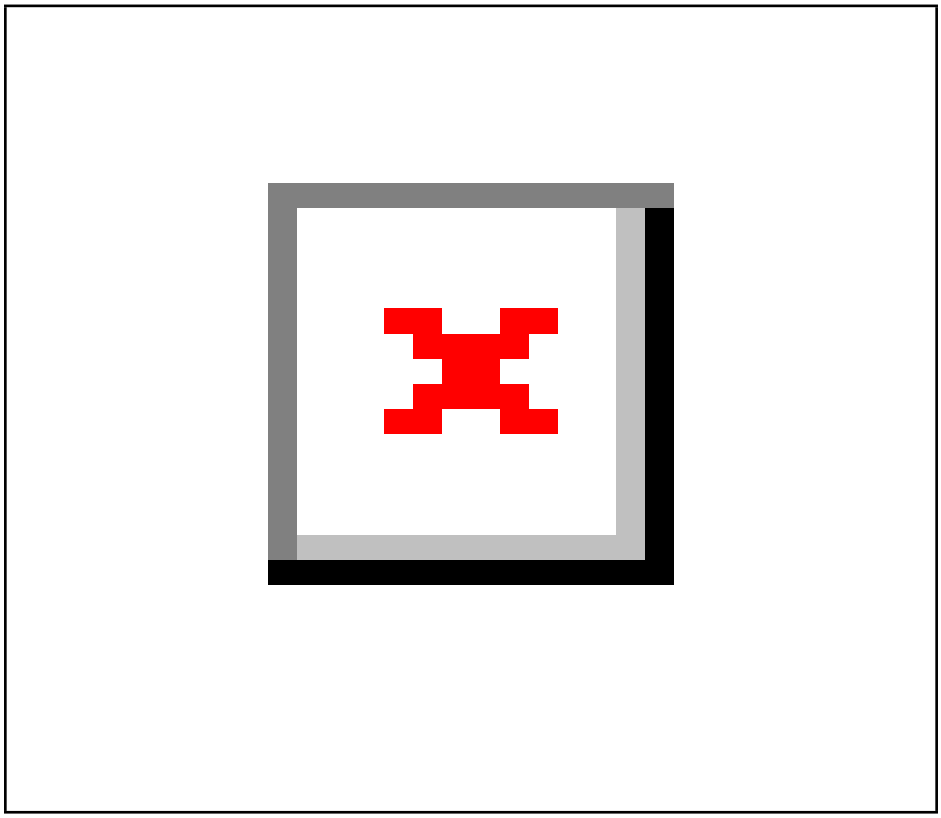

Fig. S8. ^{13}C NMR spectrum of H_6L.

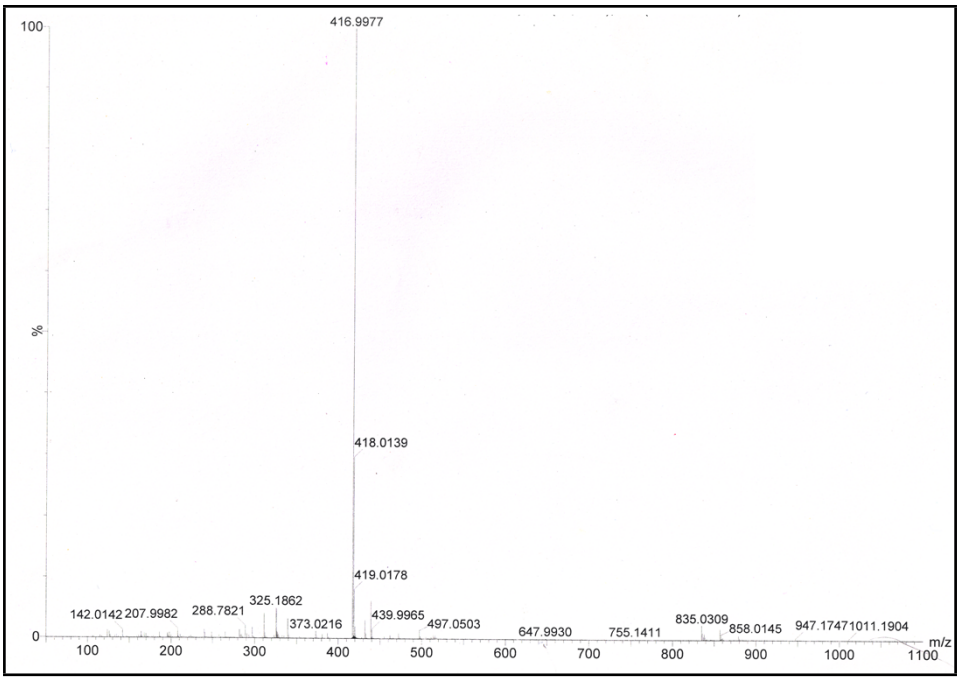

Fig. S9. ESI-MS spectrum of H_6L.

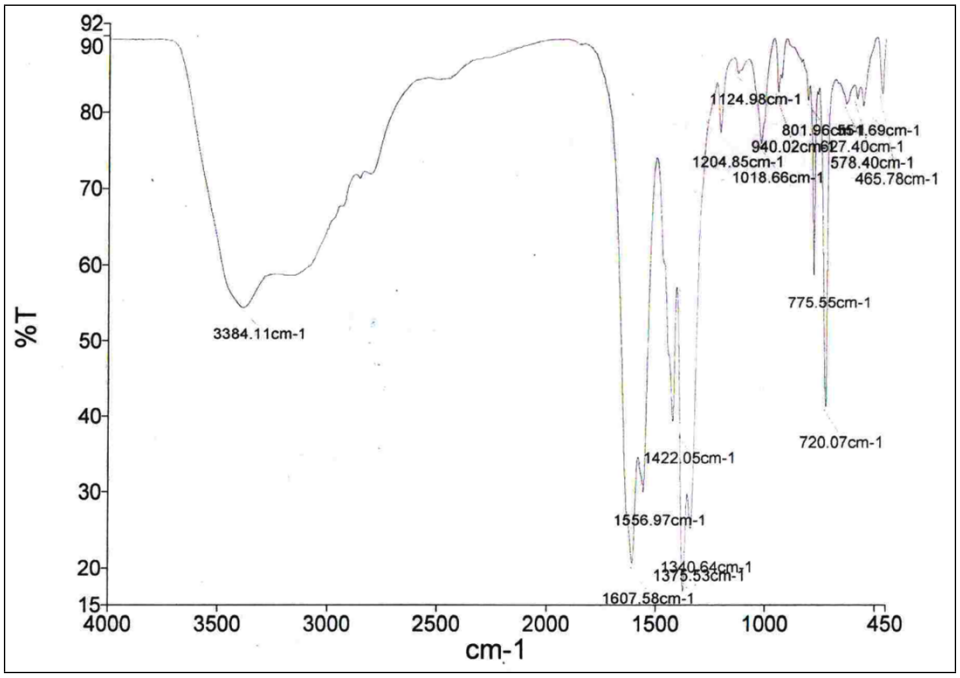

Fig. S10. IR spectrum of Complex **1**.

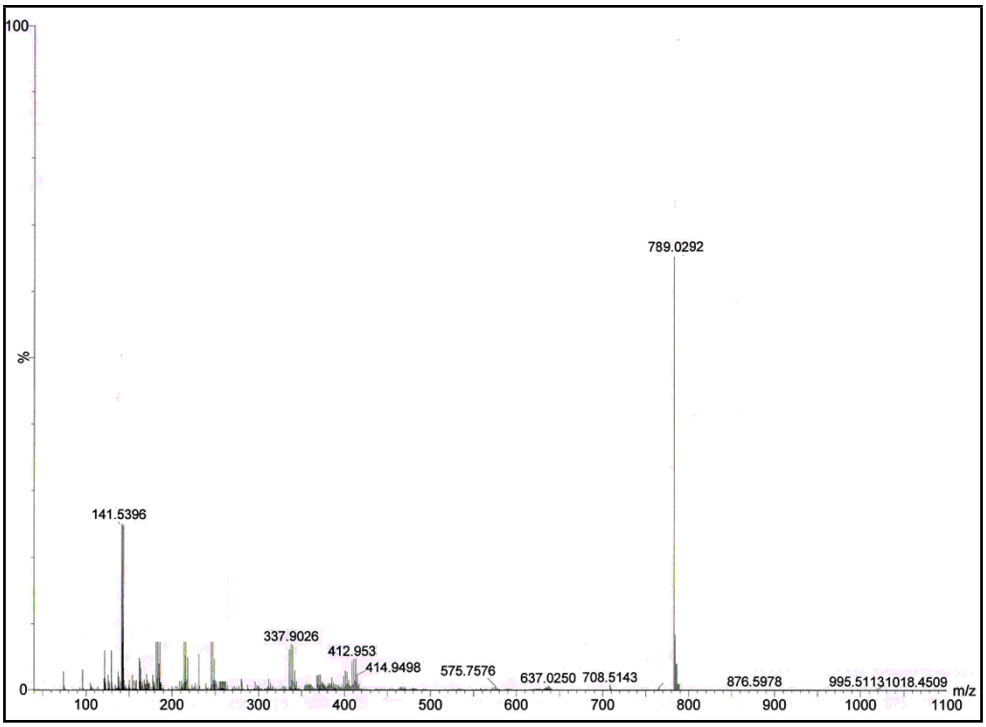

Fig. S11. ESI-MS of Complex **1**.