

Supporting Information

For

**Bi-nuclear Ru(II) complexes of bis-chalcone and bis-flavonol: Synthesis,
characterization, photo cleavage of DNA and Topoisomerase I inhibition Activity**

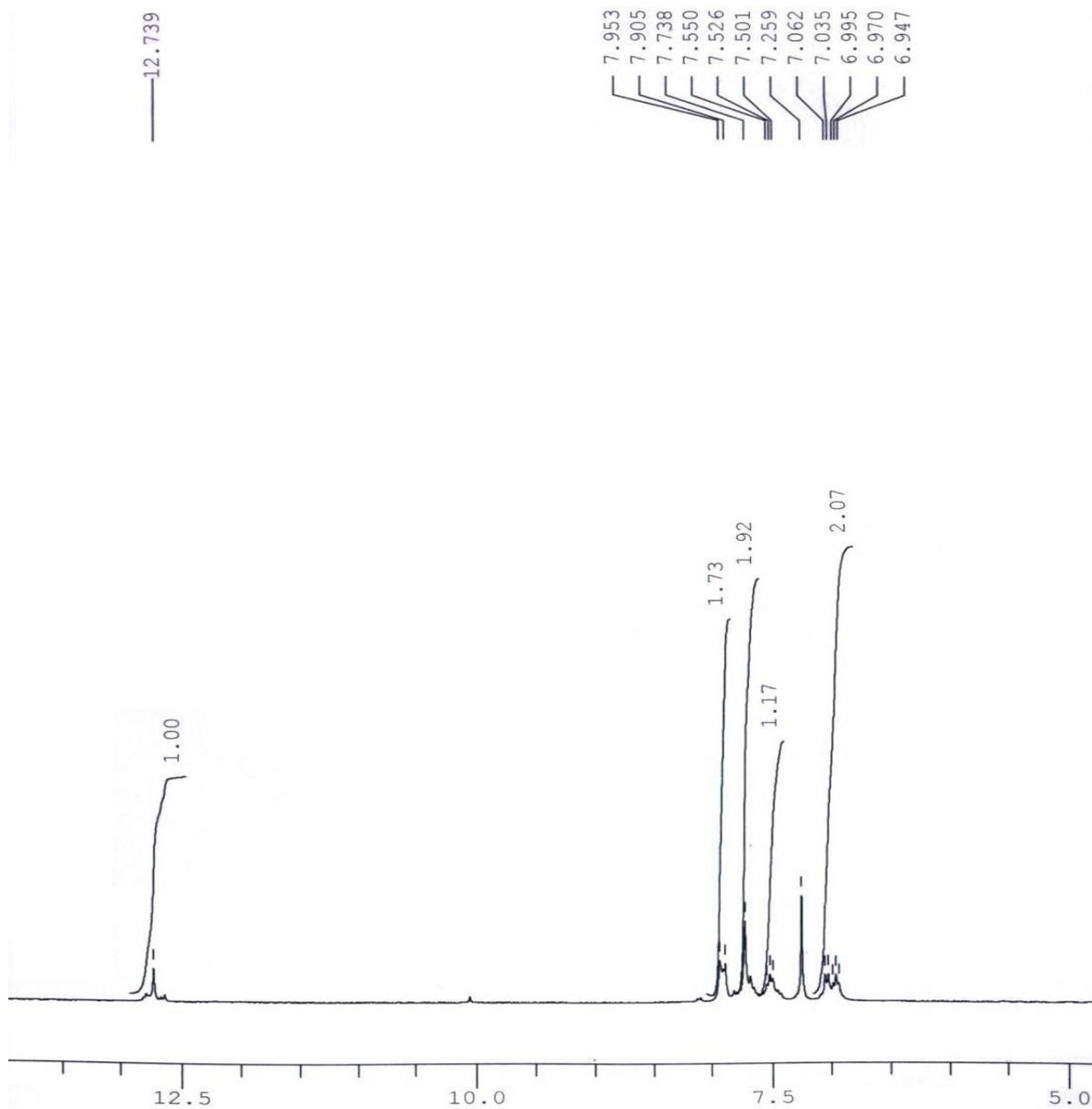
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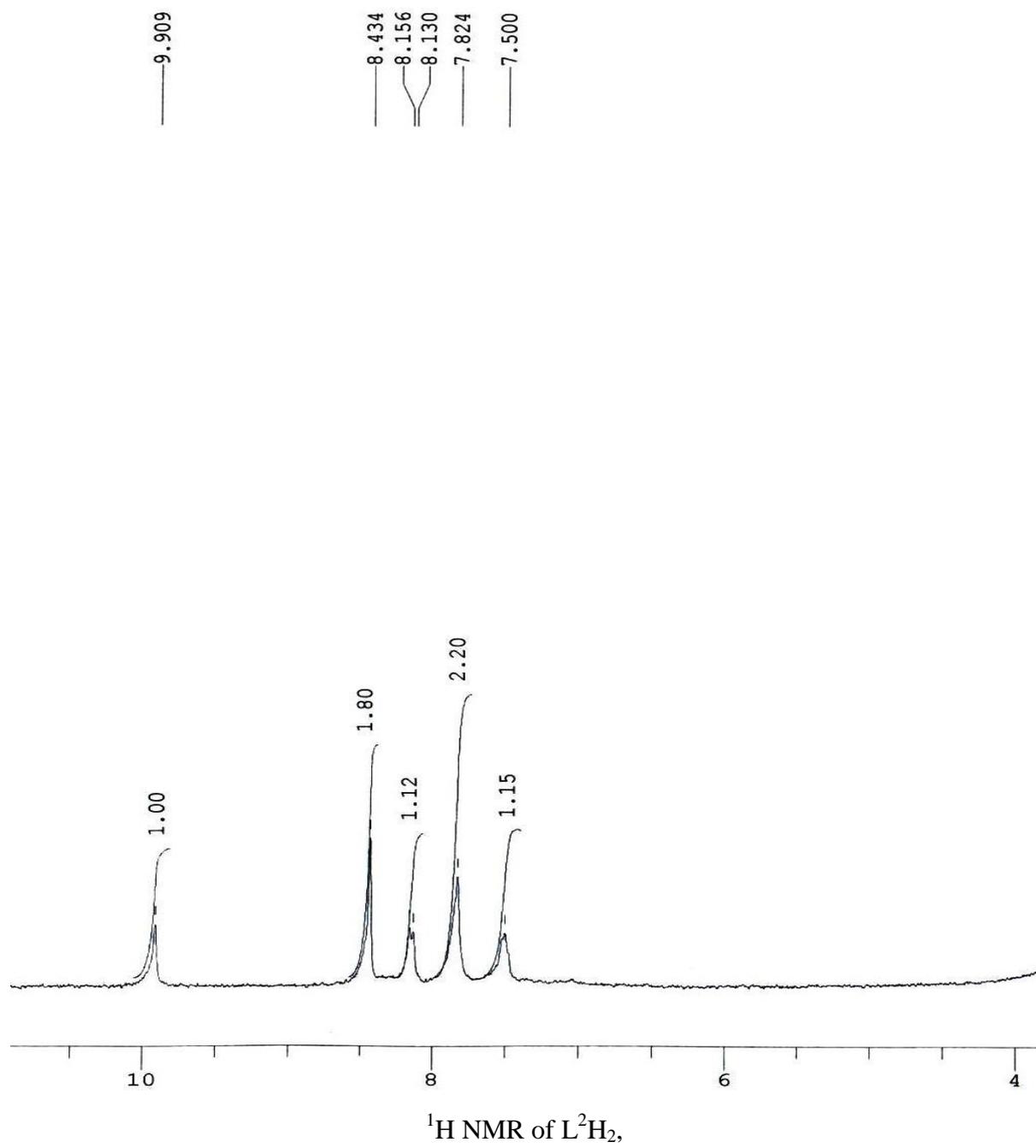
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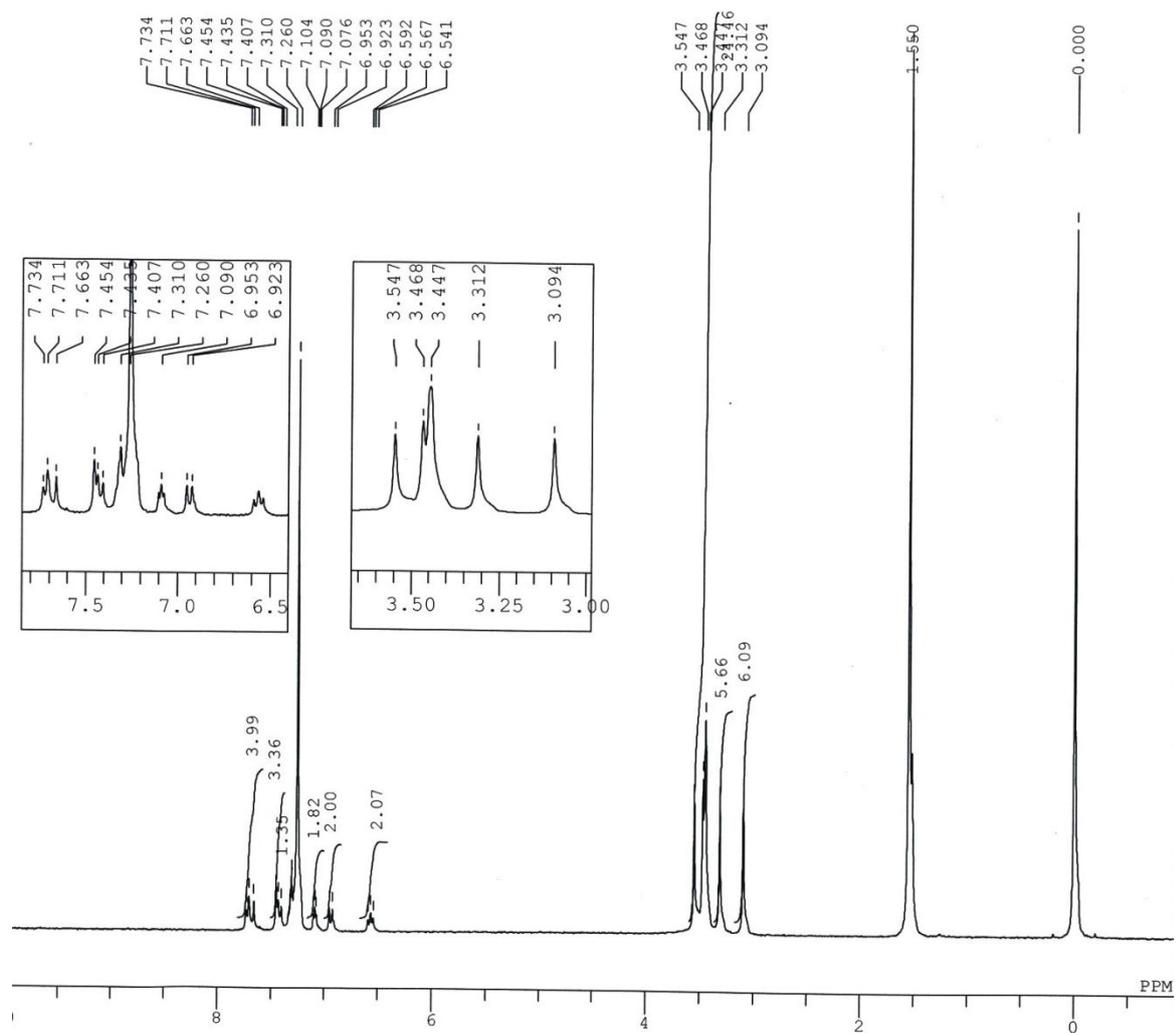
¹ H NMR spectra of L ¹ H ₂ , L ² H ₂ , complexes 1 and 2S1
ESI-MS of complexes 1 and 2S2
Molecular structure of L ¹ H ₂S3
Summary of crystallographic data for L ¹ H ₂S4
Selected bond length (Å) and bond angle (°) for L ¹ H ₂S5
Ladder like structural motif owing to C-H...π weak interactions along 'c' axis in L ¹ H ₂S6
Absorption pattern of ethidium bromide bound to DNA separately by complex 1 and 2 . [DNA] = 10 μM, [complexes 1 and 2] = 0 – 0.325 μMS7
Emission pattern of complexes bound to DNA with replacement EB. [DNA] = 10 μM, [complexes 1 and 2] = 0.325 μM, EB= 10 μMS8
Absorption spectra of the both complexes on increasing the concentration of saltS9
Ethidium bromide stained agarose gel (1%) of pBR322 plasmid DNA (300 ng μL ⁻¹) in presence of 100 μM L ¹ H ₂ , L ² H ₂ , 1 and 2S10
Effects of different concentrations of 1 and 2 on the activity of DNA topoisomerase I.	...S11

S1

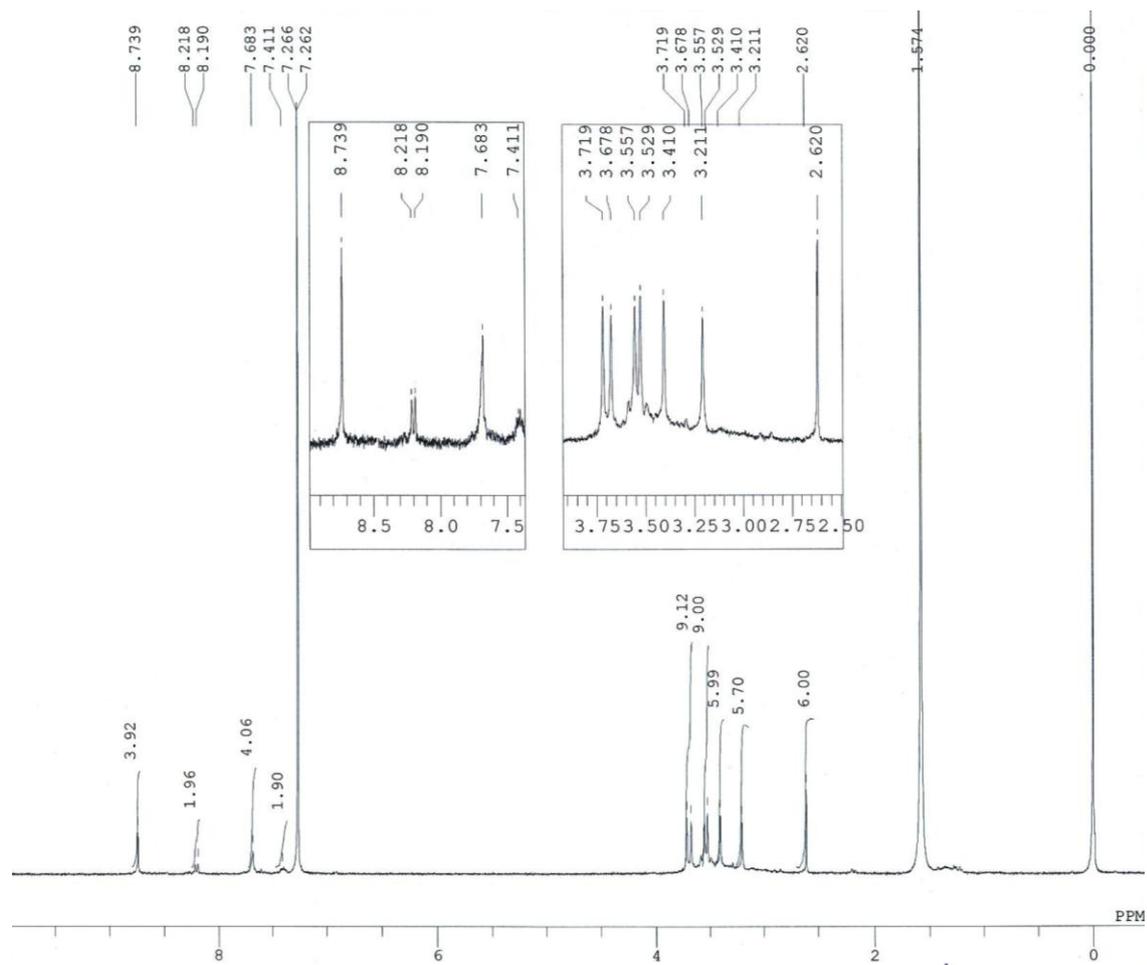


^1H NMR of L^1H_2 ,



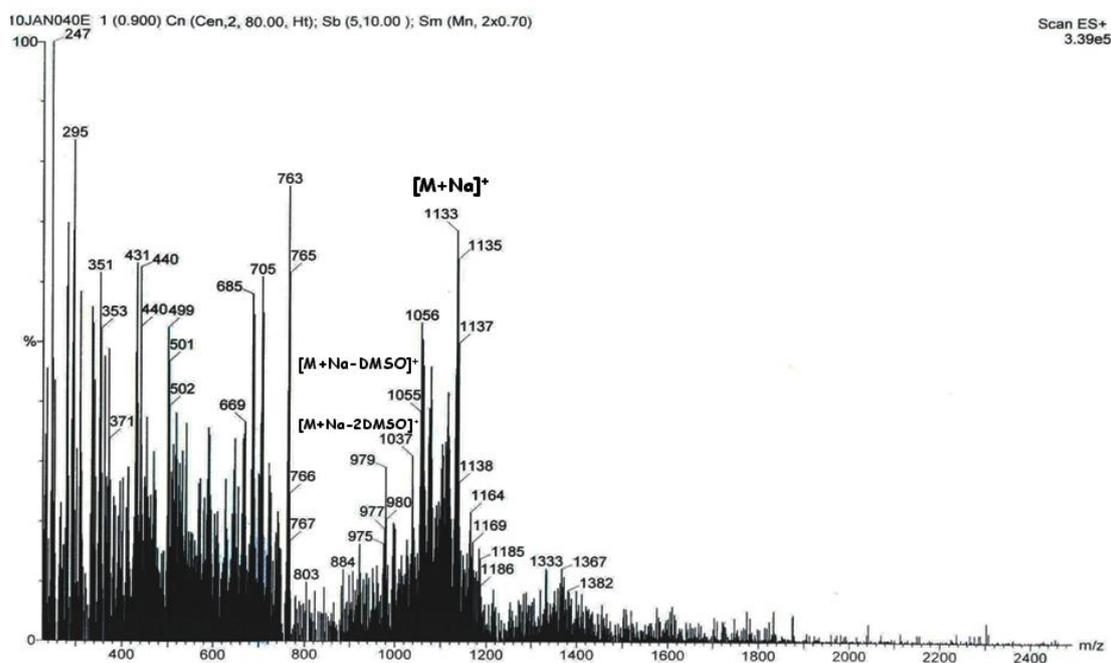


¹H NMR of complex 1

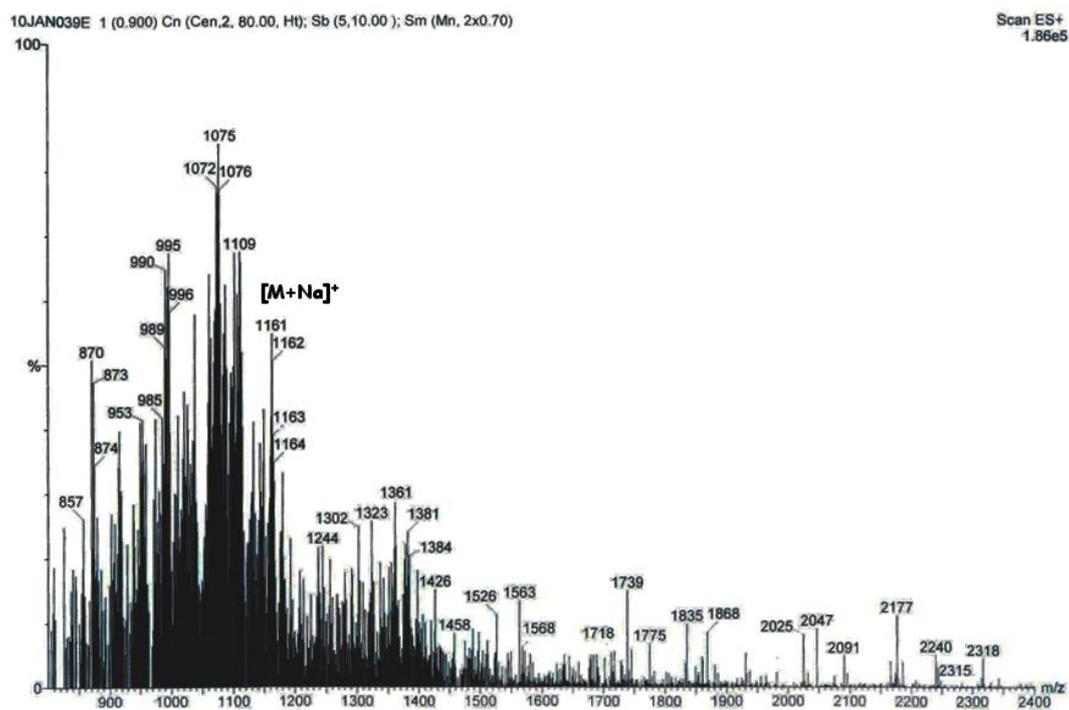


^1H NMR of complex 2

S2

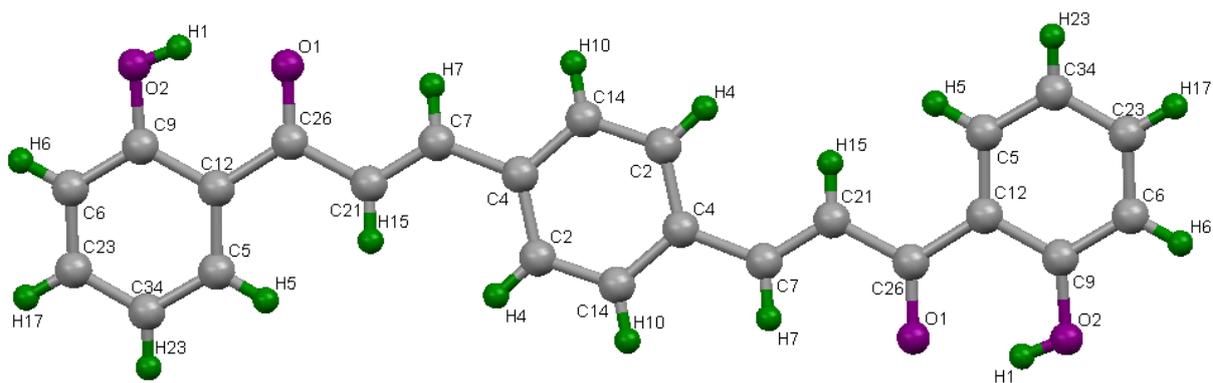


ESI-MS of complex 1



ESI-MS of complex 2

S3



Molecular structure of L^1H_2

S4

Summary of Crystallographic data for L¹H₂

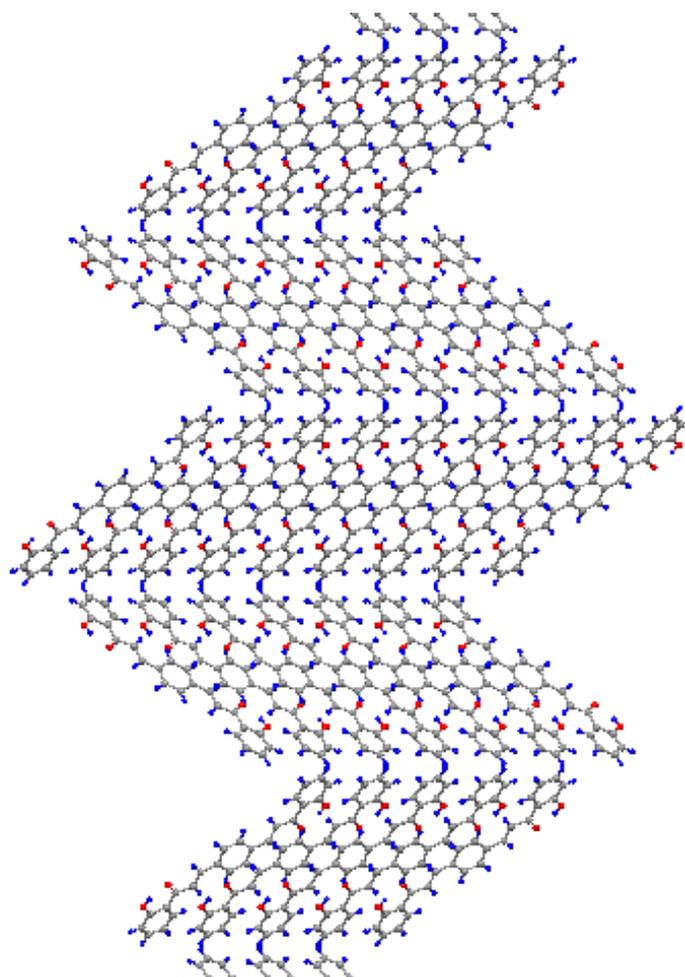
Parameters	L ¹ H ₂
Formula	C ₂₄ H ₁₈ O ₄
M	370.38
Crystal system	Monoclinic
Temperature	293(2) K
Space group	<i>P</i> 21/ <i>c</i>
<i>a</i> /Å	4.967(5)
<i>b</i> /Å	27.181(14)
<i>c</i> /Å	7.764(7)
α (°)	90
β (°)	117.55(6)
γ (°)	90
<i>V</i> /Å ³	929.3(13)
<i>Z</i>	2
<i>D_c</i> /Mg·m ⁻³	1.324
Reflns. collected	3448
Reflns. unique	2580
<i>R</i> (<i>int</i>)	0.0532
Refinement method	Full-matrix, least squares on <i>F</i> ²
<i>wR</i> ₂	0.0538
<i>R</i> ₁	0.0532
<i>GoF</i>	0.735

S5

Selected bond lengths (Å) and angles (°)

L ¹ H ₂			
O(3)-C(17)	1.245(2)	C(2)-C(1)-C(16)	123.01(16)
O(4)-C(35)	1.342(2)	O(2)-C(12)-C(26)	117.78(17)
C(8)-C(23)	1.405(2)	C(12)-O(2)-H(2)	109.5
O(2)-H(2)	0.8200	C(39)-C(18)-H(18)	119.4

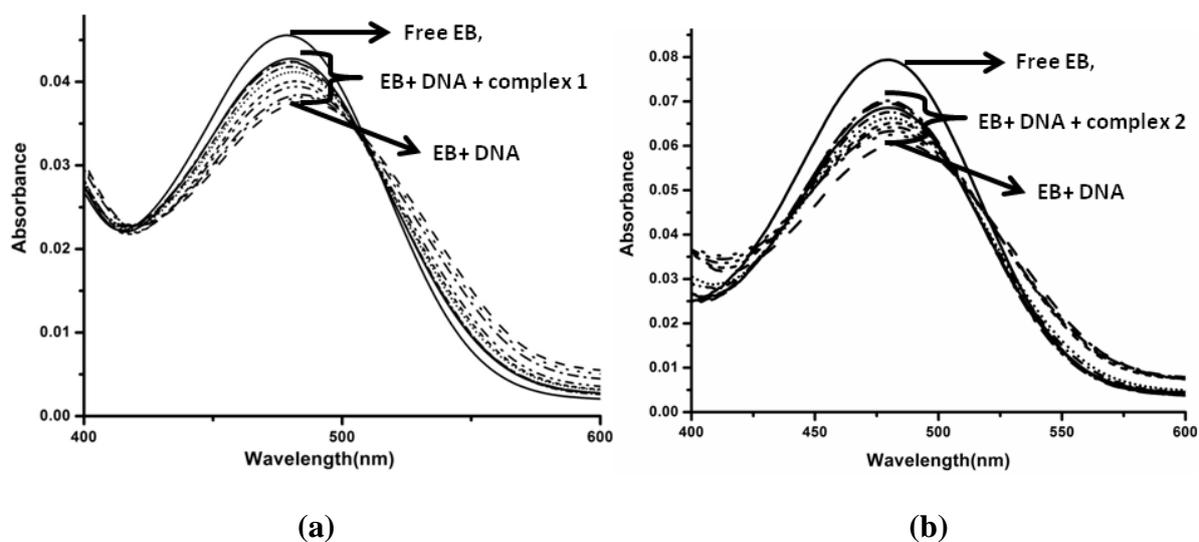
S6



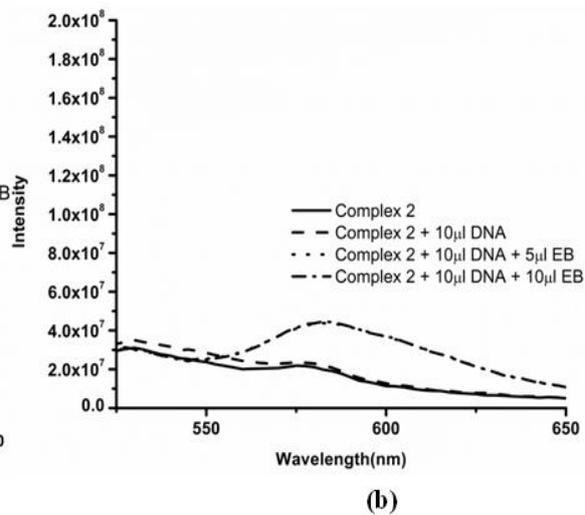
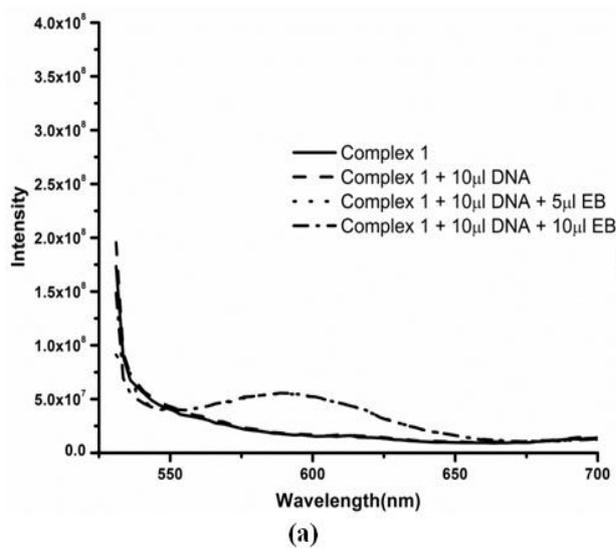
Ladder like supramolecular structure of L¹H₂

Competitive binding of complexes with EB bound DNA using spectroscopic titrations

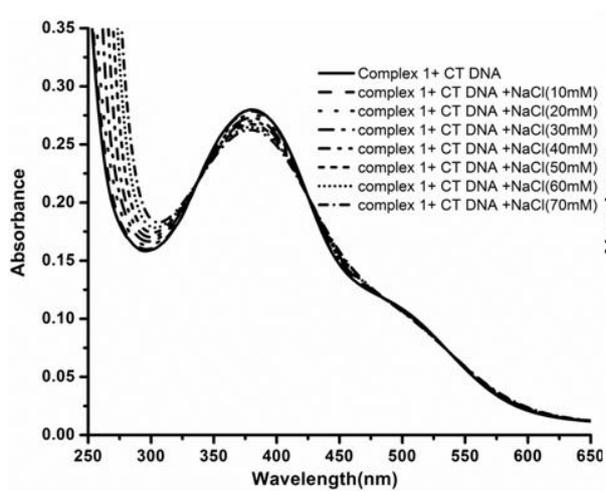
The competitive binding experiments were performed on Jasco UV-630 spectrophotometer. Absorption titrations were performed by keeping the concentration of the EB (10 μM), DNA (10 μM) constant and by varying [complexes **1** and **2**] = 0 – 0.325 μM . It is well known that free ethidium bromide shows absorbance at 490 nm. After addition of CT-DNA (10 μM), a decrease observed in absorbance supported intercalation of EB into DNA base stacks. However, on addition of complexes (**1** and **2**) separately to EB-DNA solution, absorbance again increased and finally gets saturated. Thus, some fraction of EB bound initially to DNA is displaced by both complexes indicating that there is competitive binding of complexes (**1** and **2**) with EB for DNA.



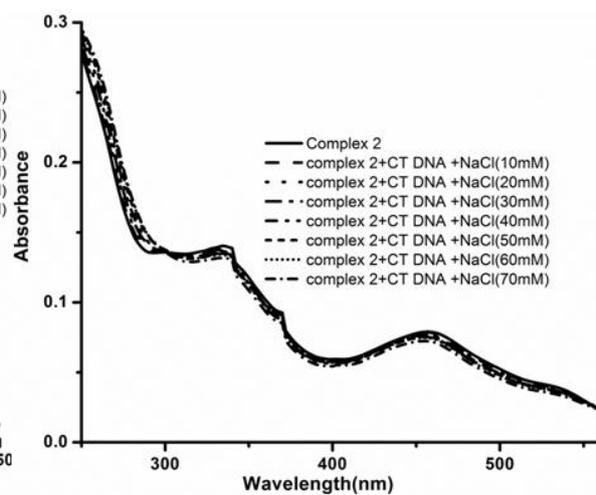
S8



S9

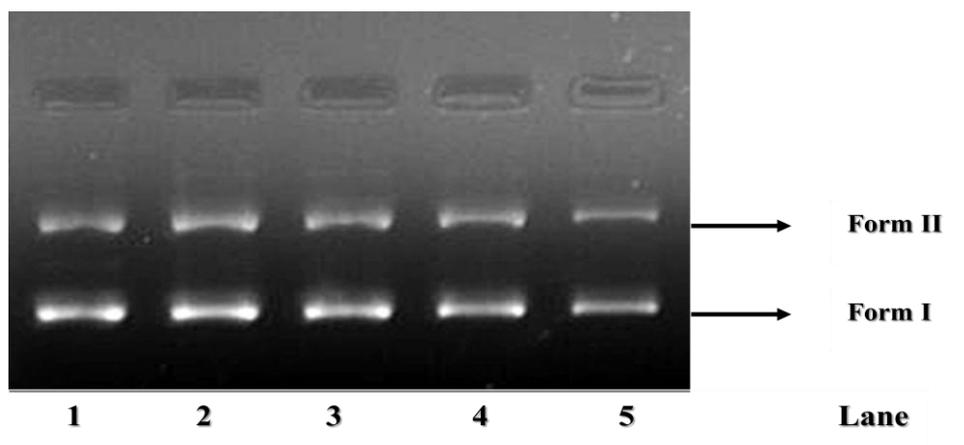


(a)



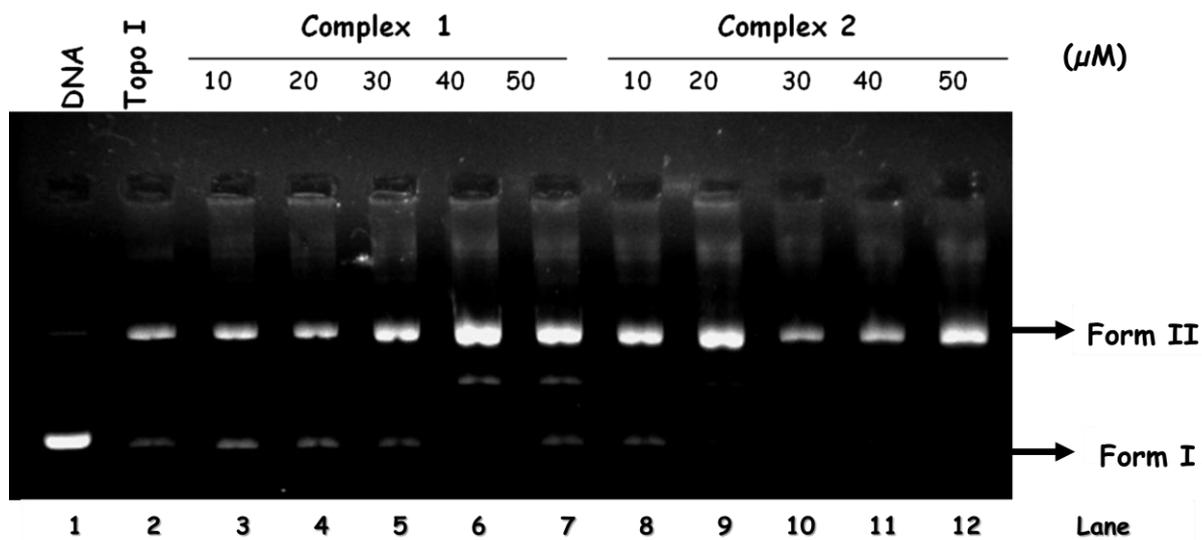
(b)

S10



Ethidium bromide stained agarose gel (1 %) of pBR322 plasmid DNA ($300 \text{ ng } \mu\text{L}^{-1}$) after 1 h of incubation in dark. Lane 1: DNA control; Lane 2: DNA + L¹H₂ (100 μM); Lane 3: DNA + L²H₂ (100 μM), Lane 4: DNA + complex **1** (100 μM); Lane 5: DNA + complex **2** (100 μM).

S11



Effects of different lower concentrations of complexes **1** and complex **2** on the activity of DNA topoisomerase I.