Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Docking and in vitro molecular biology studies of p-anisidine appended 1-hydroxy-2-acetonapthanone Schiff base Lanthanum(III) complexes

Content

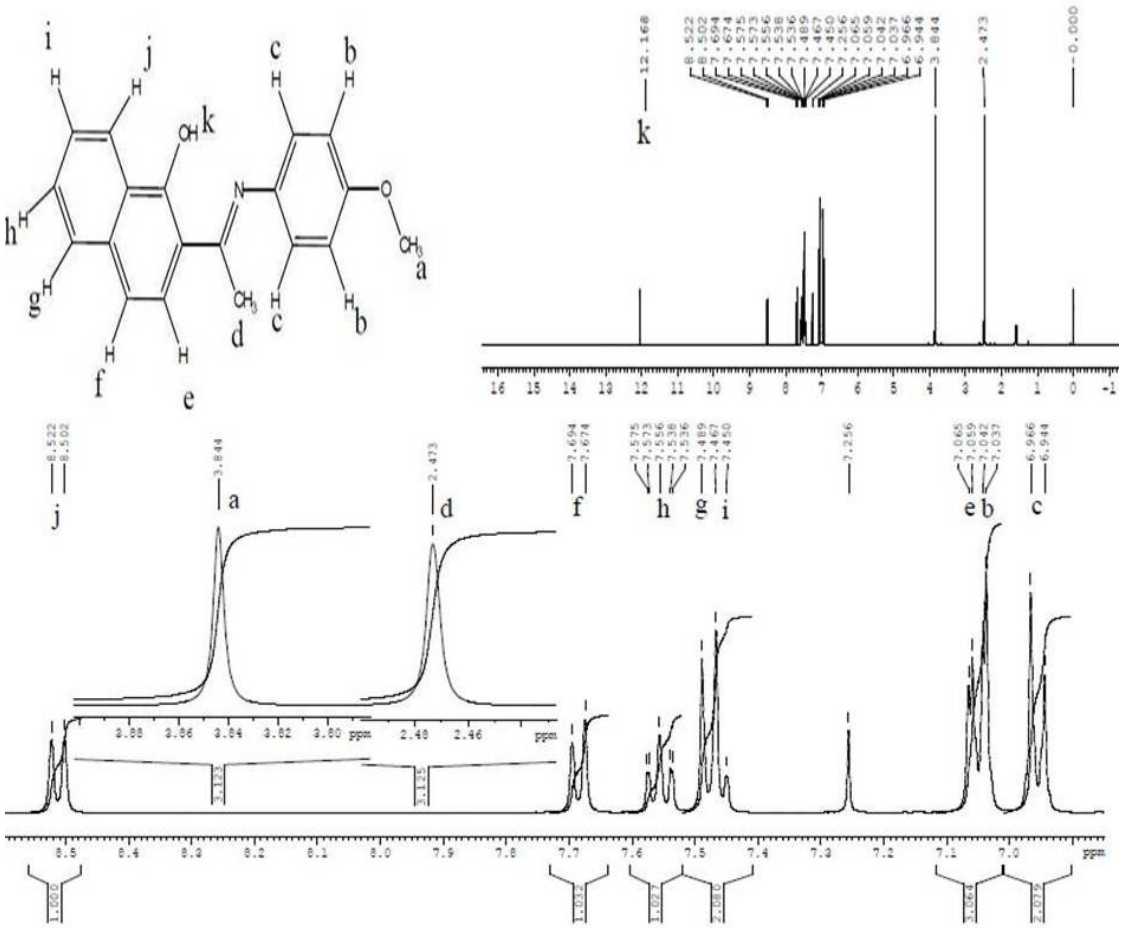
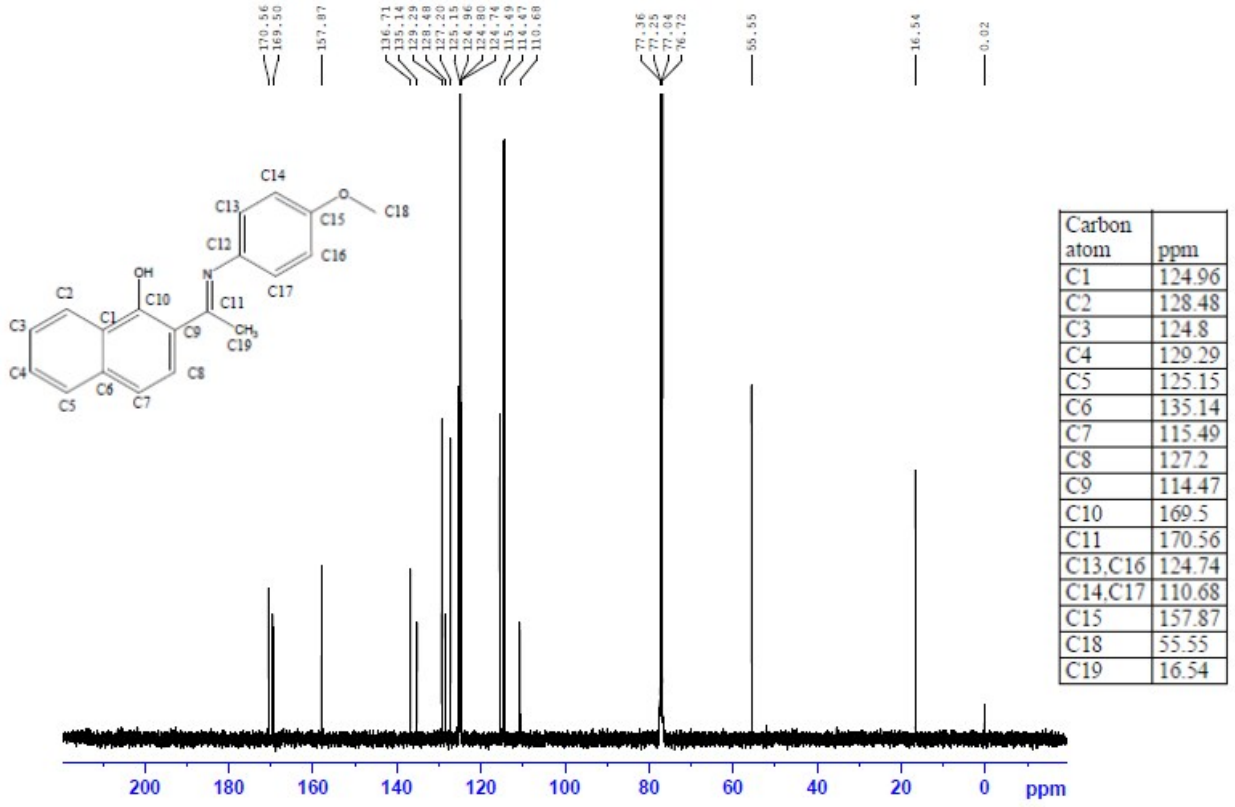


Figure S1. ^{1}H NMR spectrum of ligand 3 in $CDCl_3$ at 25°C.



Carbon atom	ppm
C1	124.96
C2	128.48
C3	124.8
C4	129.29
C5	125.15
C6	135.14
C7	115.49
C8	127.2
C9	114.47
C10	169.5
C11	170.56
C13,C16	124.74
C14,C17	110.68
C15	157.87
C18	55.55
C19	16.54

Figure S2. ^{13}C-NMR spectrum of ligand 3 in $CDCl_3$ at 25°C.

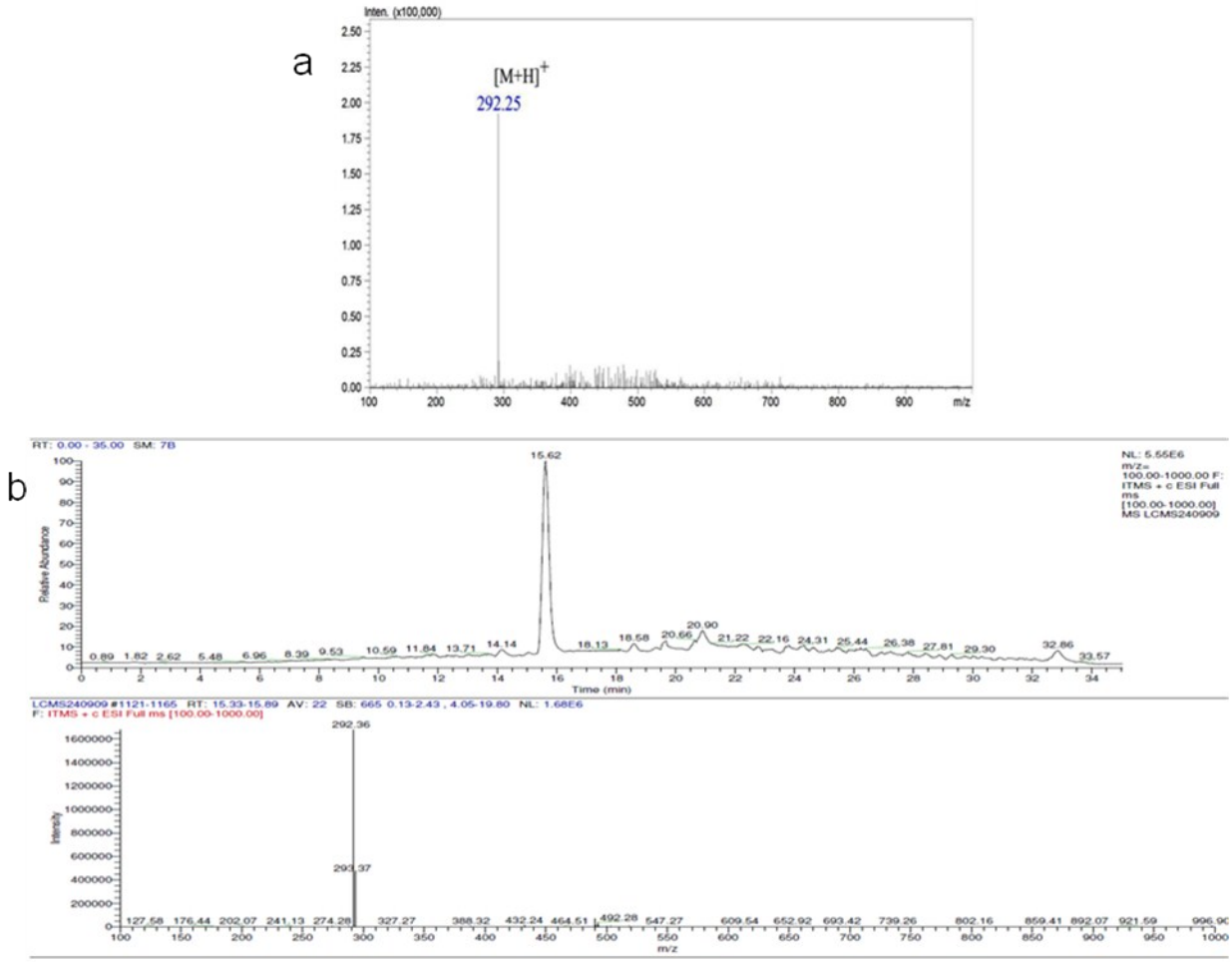


Figure S3. (a) ESI direct mass spectrum, (b) LC-MS chromatogram, and (c) total ion MS spectrum of LCMS for ligand 3.

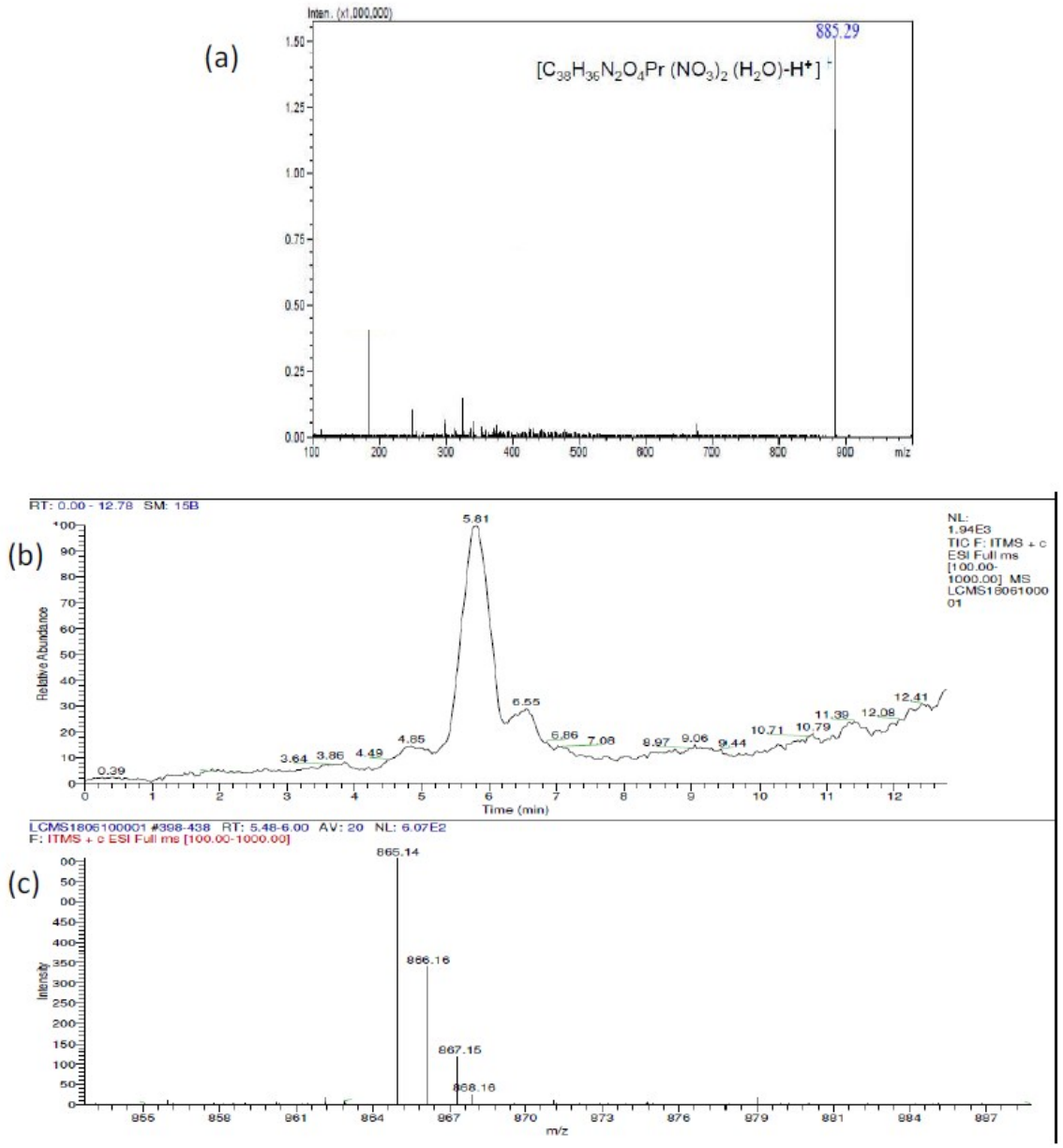


Figure S4. (a) ESI direct mass spectrum, (b) LC-MS chromatogram, and (c) total ion MS spectrum of LCMS for complex 4.

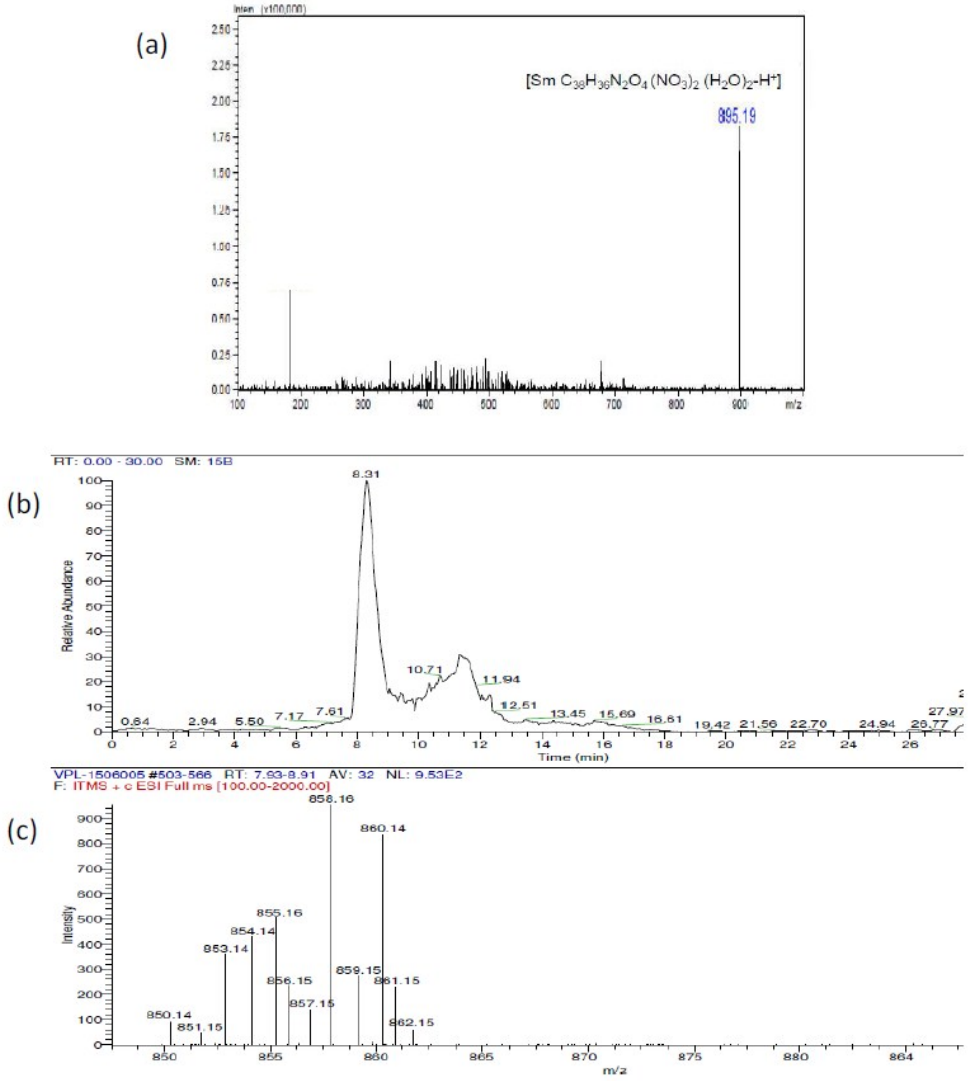


Figure S5. ESI direct mass spectrum, (b) LC-MS chromatogram, and (c) total ion MS spectrum of LCMS for complex 5.

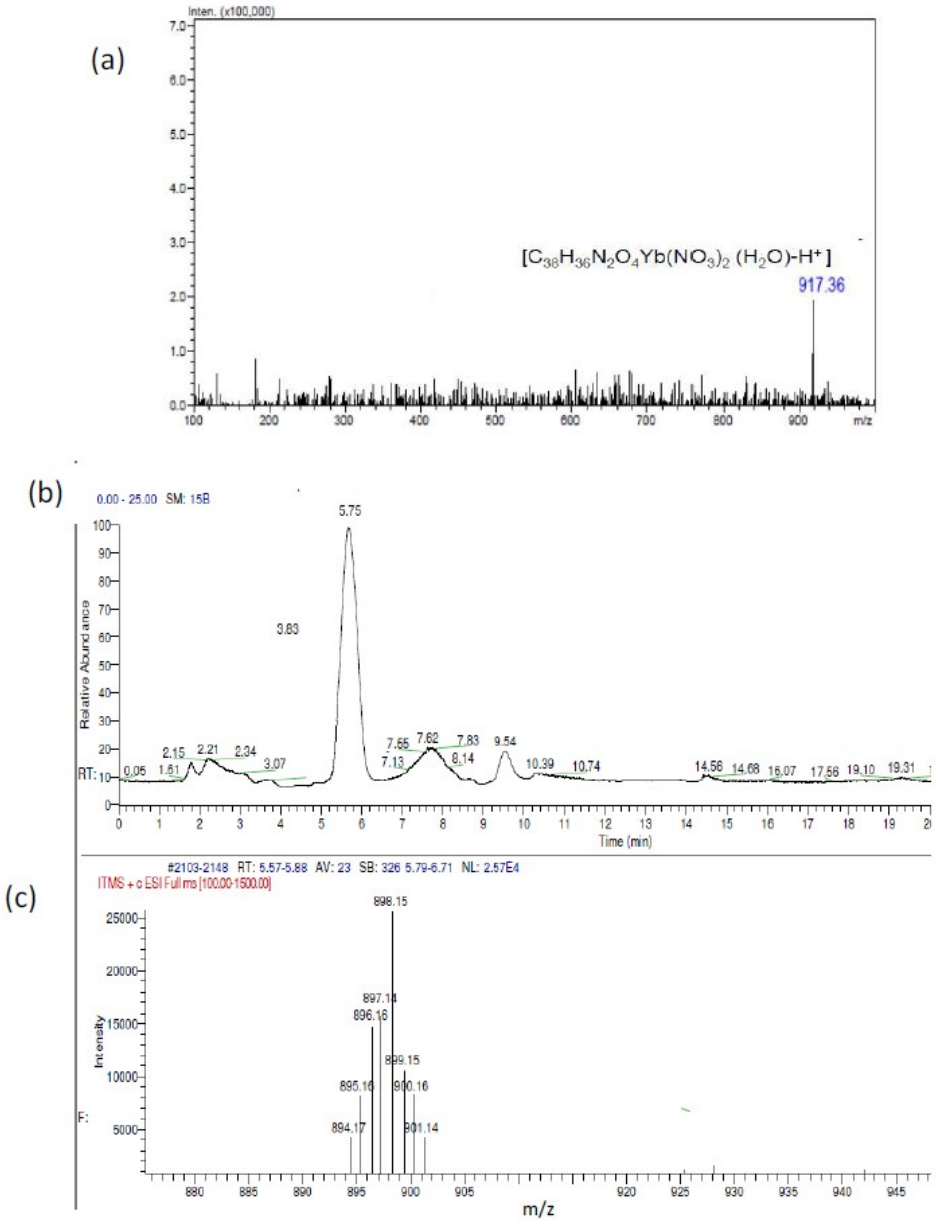


Figure S6 ESI direct mass spectrum, (b) LC-MS chromatogram, and (c) total ion MS spectrum of LCMS for complex 6.

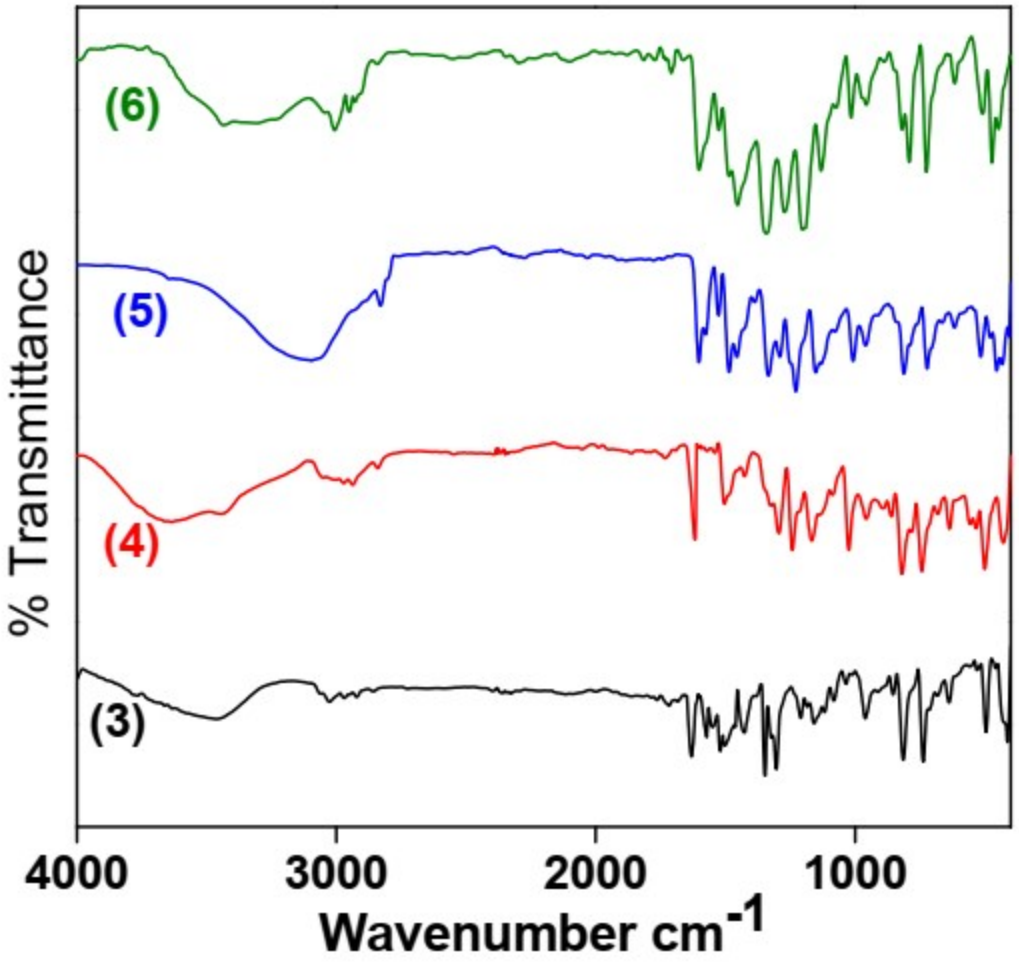


Figure S7 FTIR spectral comparison of 3, 4, 5, and 6.

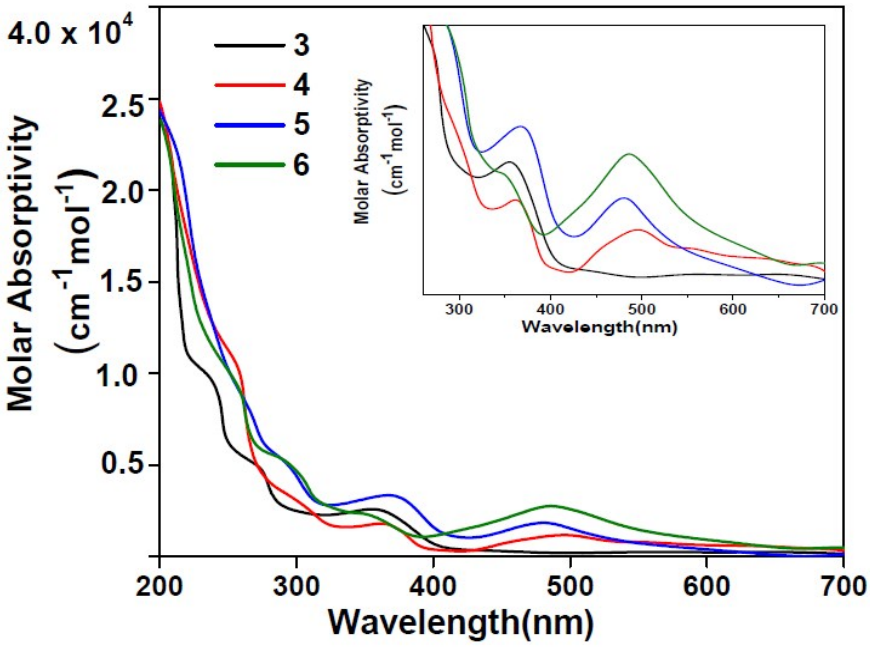


Figure S8 Electronic absorption spectra of 3, 4, 5, and 6 in methanol.

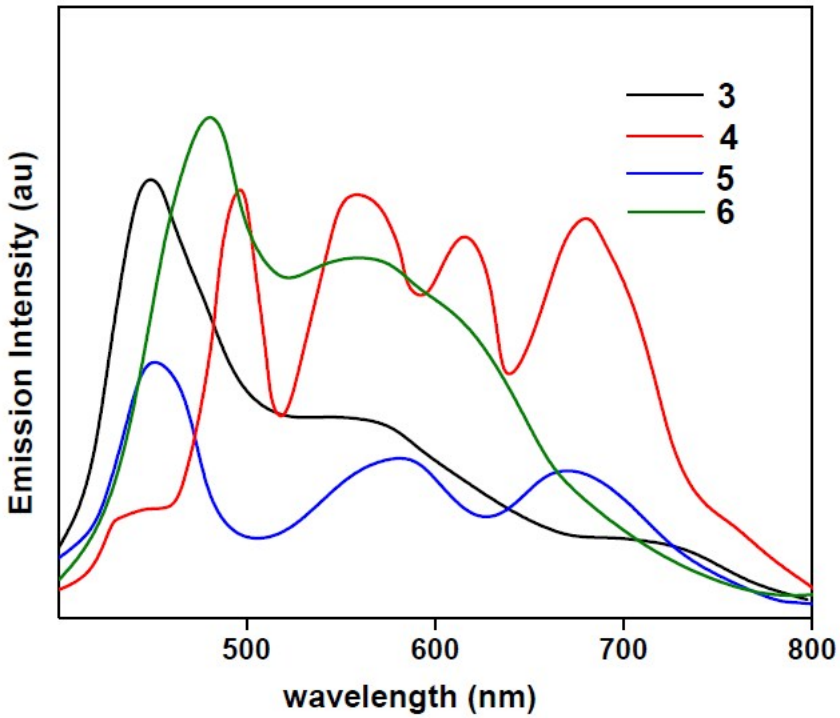


Figure S9. Emission spectra of 3, 4, 5, and 6 in ethanol excited at λ_{ex} 300 nm.

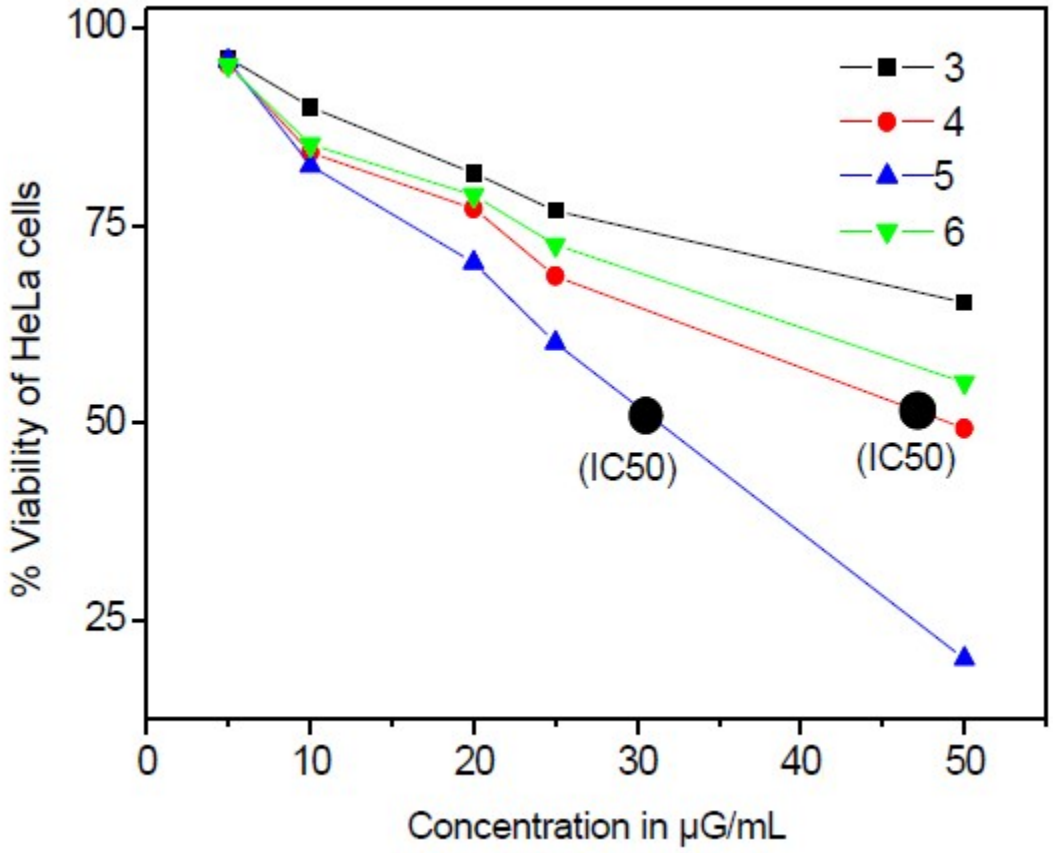


Figure S10. Concentration versus viability plot of incubated HeLa cells with varying. concentrations of the ligand and complexes.

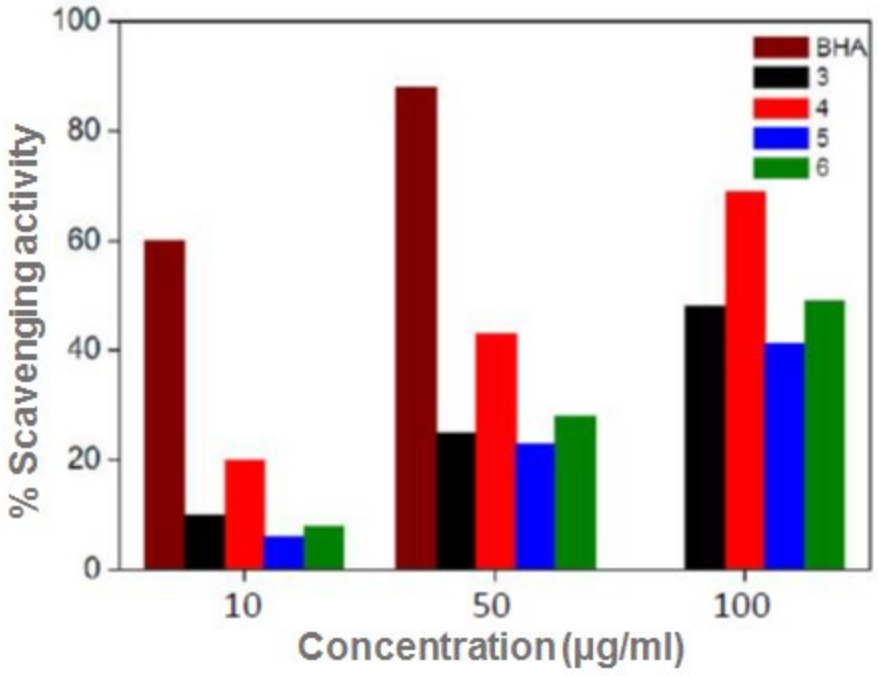


Figure S11. DPPH free radical scavenging activity of 3, 4, 5, and 6.

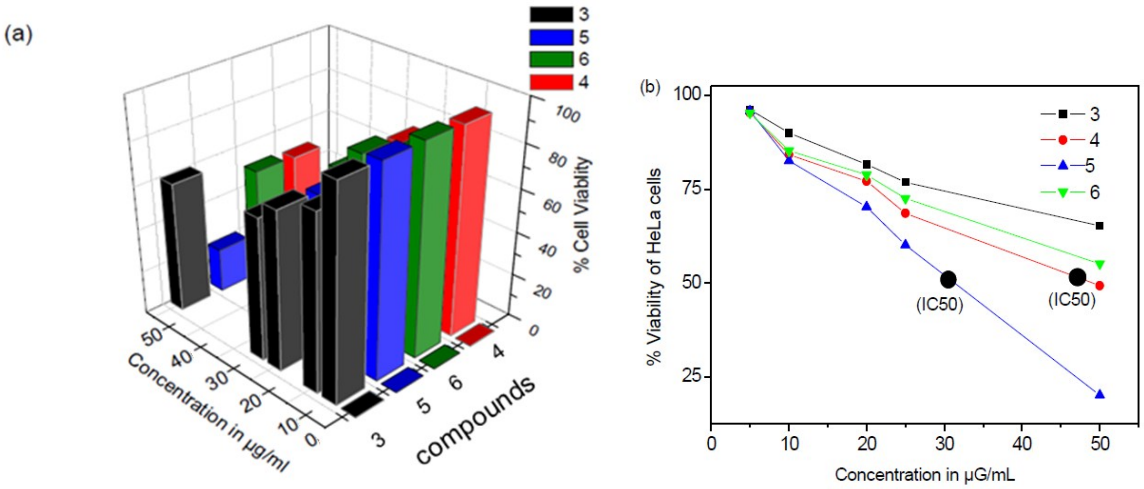


Figure S12. Concentration versus viability plot of incubated HeLa cells with varying concentrations of the ligand and complexes. (a) 3D bar diagram of cell viability of ligand and complexes. (b) Regression plot for the estimation of IC_{50} values from the test concentrations.

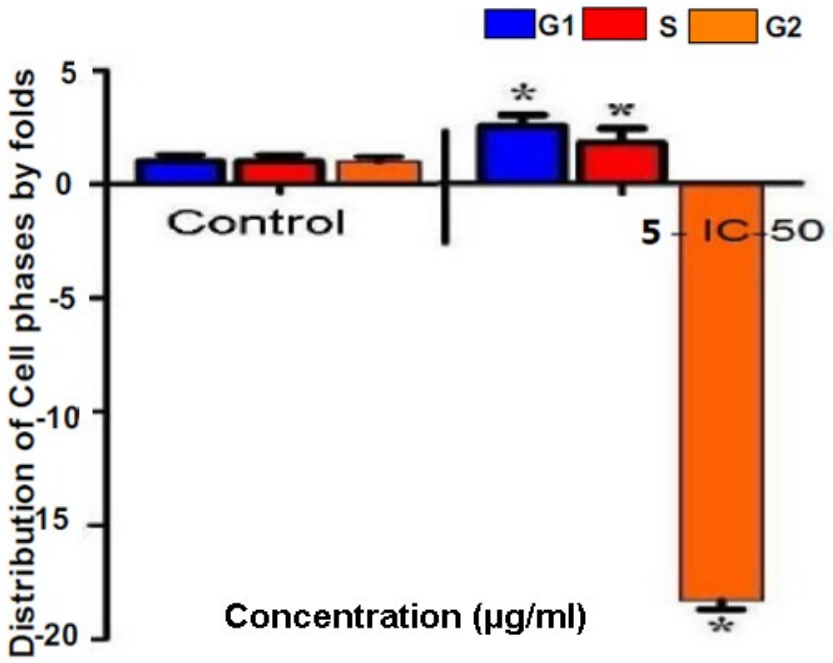


Figure S13. Histogram showing the percent distribution of cells in G2, S, and G1.

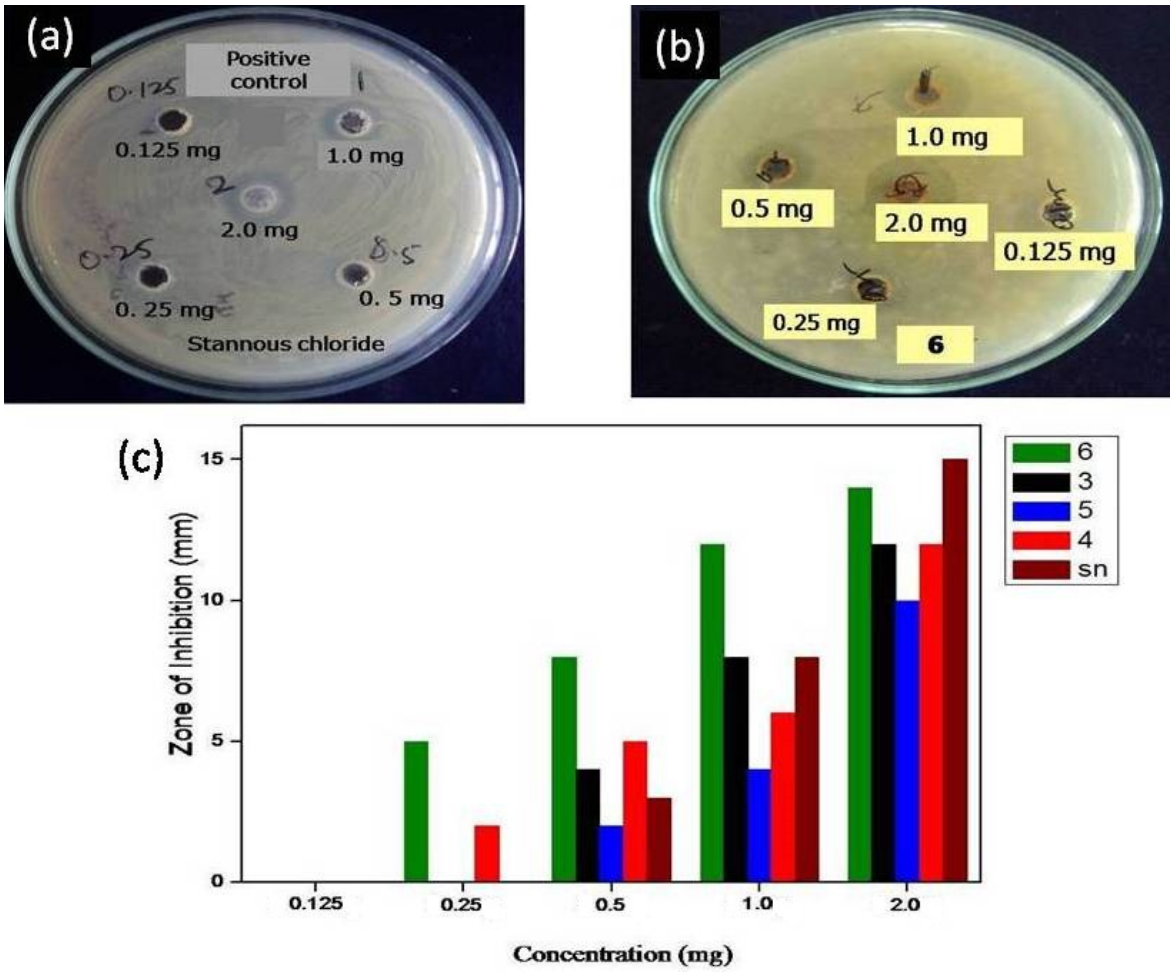


Figure S14. Carcinogenicity/cytotoxicity/mutagenicity screening (a) positive control-stannous chloride at various levels (2, 1, 0.5, 0.25, 0.125 mg) tested, (b) representative sample 6 at various levels (2, 1, 0.5, 0.25, 0.125 mg) tested, and (c) graphical representation of the concentration vs zone of inhibition.

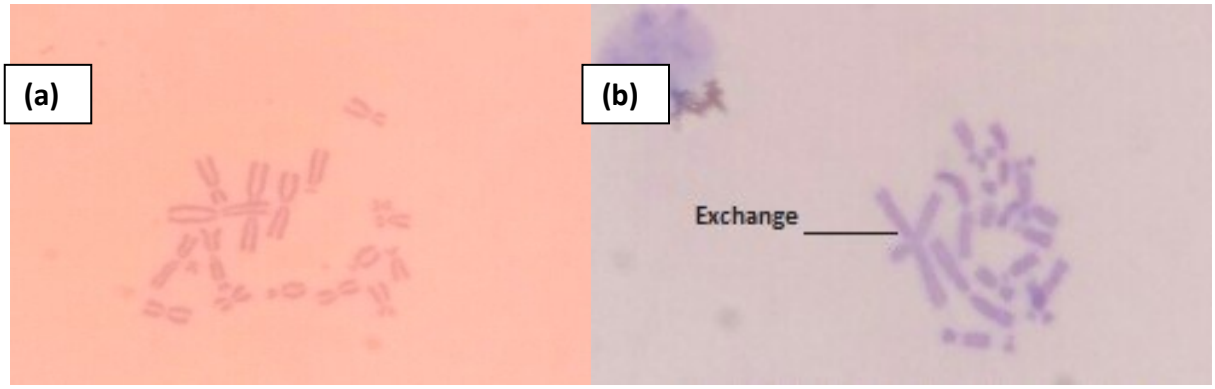


Figure S15. Representative image for chromosomal aberration of (a) complex 5 treated with cell line with normal metaphase, (b) Mitomycin treated cells with metaphase aberration exchange.

Table: S1 LCMS-MS-Mass spectrometry optimized selected parameters for the compounds.

Compound	Retention time (t_R)	Precursor ion (m/z)	CE (V)	Product ion (m/z)	CE (V)	Tube Lens
4	5.81 min	885.29	11	865.14, 866.16, 867.15 and 868.16	22	72
5	8.31 min	895.19	15	850.14, 851.15, 853.14, 855.16, 856.16, 857.15, 858.15, 859.15, 860.14, 861.15 and 862.15.	19	74
6	5.75 min	917.36	18	894.17, 895.16, 896.16, 897.14, 898.15, 899.15, 900.16 and 901.14	18	76

Table S2. Intercalation of L1HSm with DNA (PDB ID: 1BNA; Q-site finder) and preferential binding site from the docked structure.

B-DNA DODECAMER			LIHSm	Geometric Shape Complementarity Score	DISTANCE Å	H-BOND
DA 18	B	O4’	C	5136	—	—
DC 9	A	O2	C			

The -DNA DODECAMER,

1. **Atom of DA position 18 O4’ is bond to ligand of atom C.**

734	ATOM	343	N3	DA B	17	15.700	22.472	2.783	1.00	38.96	N
735	ATOM	344	C4	DA B	17	16.791	21.706	3.002	1.00	28.24	C
736	ATOM	345	P	DA B	18	19.803	27.141	2.526	1.00	46.11	P
737	ATOM	346	OP1	DA B	18	19.796	28.478	1.888	1.00	49.20	O
738	ATOM	347	OP2	DA B	18	20.953	26.858	3.426	1.00	43.48	O
739	ATOM	348	O5'	DA B	18	18.396	26.939	3.241	1.00	40.83	O
740	ATOM	349	C5'	DA B	18	17.203	27.028	2.452	1.00	40.72	C
741	ATOM	350	C4'	DA B	18	16.035	26.958	3.388	1.00	66.52	C
742	ATOM	351	O4'	DA B	18	15.856	25.612	3.850	1.00	44.25	O
743	ATOM	352	C3'	DA B	18	16.101	27.861	4.615	1.00	63.34	C
744	ATOM	353	O3'	DA B	18	14.890	28.608	4.757	1.00	55.65	O
745	ATOM	354	C2'	DA B	18	16.368	26.844	5.724	1.00	34.49	C
746	ATOM	355	C1'	DA B	18	15.561	25.655	5.243	1.00	29.45	C
747	ATOM	356	N9	DA B	18	16.104	24.373	5.755	1.00	20.03	N
748	ATOM	357	C8	DA B	18	17.411	23.967	5.830	1.00	16.51	C
749	ATOM	358	N7	DA B	18	17.539	22.706	6.276	1.00	20.58	N
750	ATOM	359	C5	DA B	18	16.266	22.309	6.480	1.00	21.66	C

2. **Atom of DC position 9 O2 is bond to ligand of atom C.**

```
552 ATOM    161  C6   DT A   8       9.545  18.548   4.904  1.00 20.28           C
553 ATOM    162  P    DC A   9       5.531  23.071   3.209  1.00 48.97           P
554 ATOM    163  OP1  DC A   9       4.648  24.244   3.269  1.00 62.33           O
555 ATOM    164  OP2  DC A   9       5.010  21.905   2.470  1.00 51.53           O
556 ATOM    165  O5'  DC A   9       6.926  23.547   2.611  1.00 43.99           O
557 ATOM    166  C5'  DC A   9       7.636  24.627   3.249  1.00 50.86           C
558 ATOM    167  C4'  DC A   9       8.897  24.853   2.457  1.00 46.66           C
559 ATOM    168  O4'  DC A   9       9.638  23.627   2.448  1.00 42.69           O
560 ATOM    169  C3'  DC A   9       8.717  25.240   0.998  1.00 56.96           C
561 ATOM    170  O3'  DC A   9       9.470  26.414   0.667  1.00 63.54           O
562 ATOM    171  C2'  DC A   9       9.126  23.965   0.253  1.00 50.41           C
563 ATOM    172  C1'  DC A   9      10.241  23.483   1.157  1.00 41.08           C
564 ATOM    173  N1   DC A   9      10.524  22.022   1.015  1.00 37.23           N
565 ATOM    174  C2   DC A   9      11.814  21.603   0.840  1.00 40.54           C
566 ATOM    175  O2   DC A   9      12.691  22.447   0.670  1.00 43.89           O
567 ATOM    176  N3   DC A   9      12.106  20.297   0.873  1.00 32.57           N
568 ATOM    177  C4   DC A   9      11.141  19.395   1.046  1.00 24.65           C
569 ATOM    178  N4   DC A   9      11.461  18.075   1.089  1.00 27.84           N
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Table S3. Molecular docking data of HSA (PDB ID: 1h9z; Q-site finder) and preferential binding site of L1HSm(5) from the docked structure.

Serum Albumin		Ligand	Geometrical shape complementary score	Distance Å	H-Bond
TRY 150	OH	O	5492	3.07	4
TRY 150	OH	O		3.23	
TRY 150	OH	O		2.68	
TRY 150	OH	N		2.94	

The protein Serum Albumin,

1. Amino acid Tyrosine of position 150 of atom OH is bond to ligand of atom O.
2. Amino acid Tyrosine of position 150 of atom OH is bond to ligand of atom O.
3. Amino acid Tyrosine of position 150 of atom OH is bond to ligand of atom O.
4. Amino acid Tyrosine of position 150 of atom OH is bond to ligand of atom N.

Table: S4 Chromosome aberration test in cultured CHO-K1 cells with different concentrations of L1HSm (5).

Concentration (mg/mL)	Treatment duration (h)	No. of Aberrant cells	No. of non Aberrant cells	*P* value	
				4 h	21 h
Negative control (0.0)	4	2	298	0.546	0.881
	21	3	297		
1.25	4	2	298		
	21	1	299		
2.5	4	1	299		
	21	3	297		
5.0	4	4	296		
	21	2	298		
Positve control (0.3 µg Mitomycin C)	4	16	284	0.001*	0.001*
	21	18	282		

* Significant