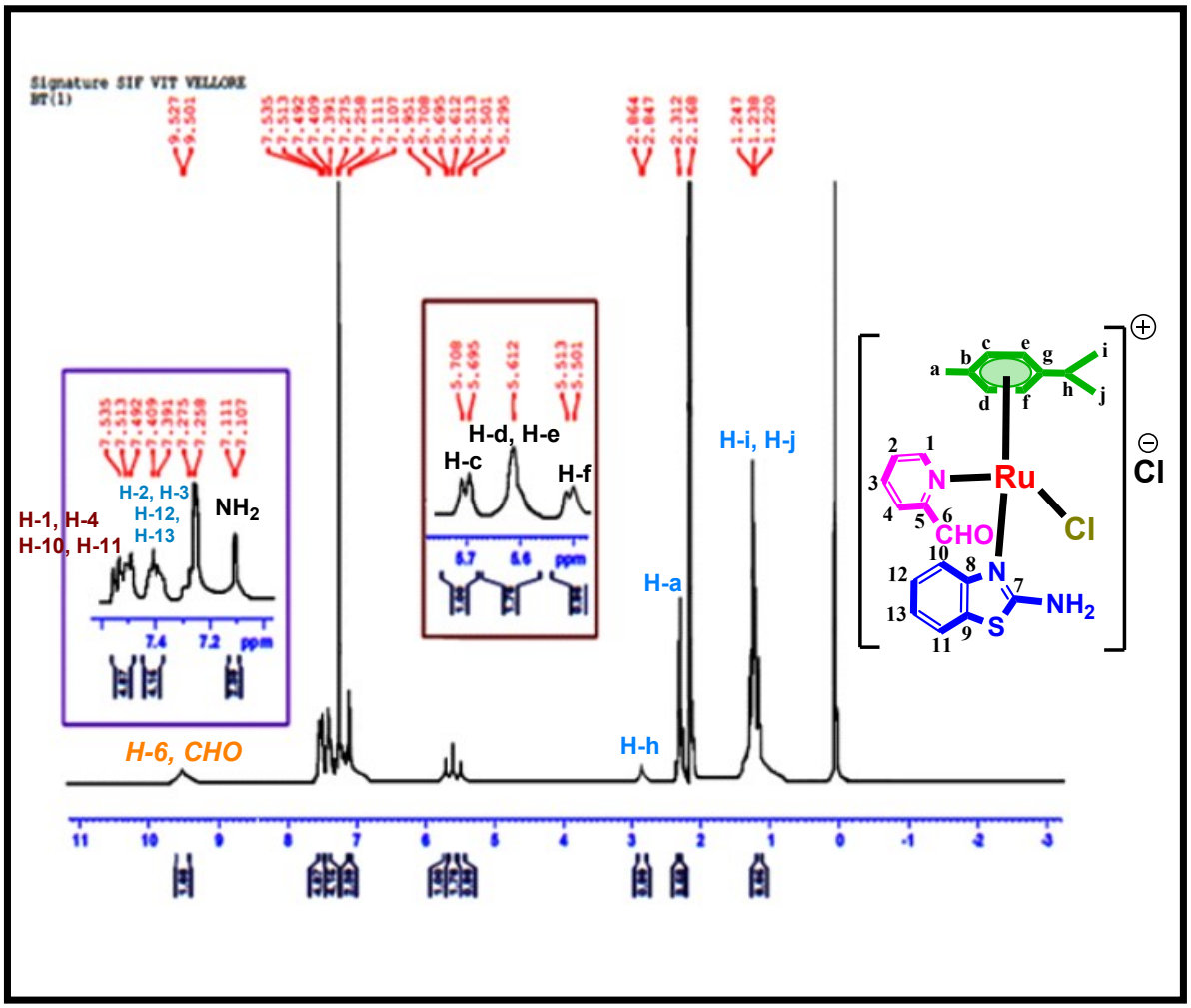
Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

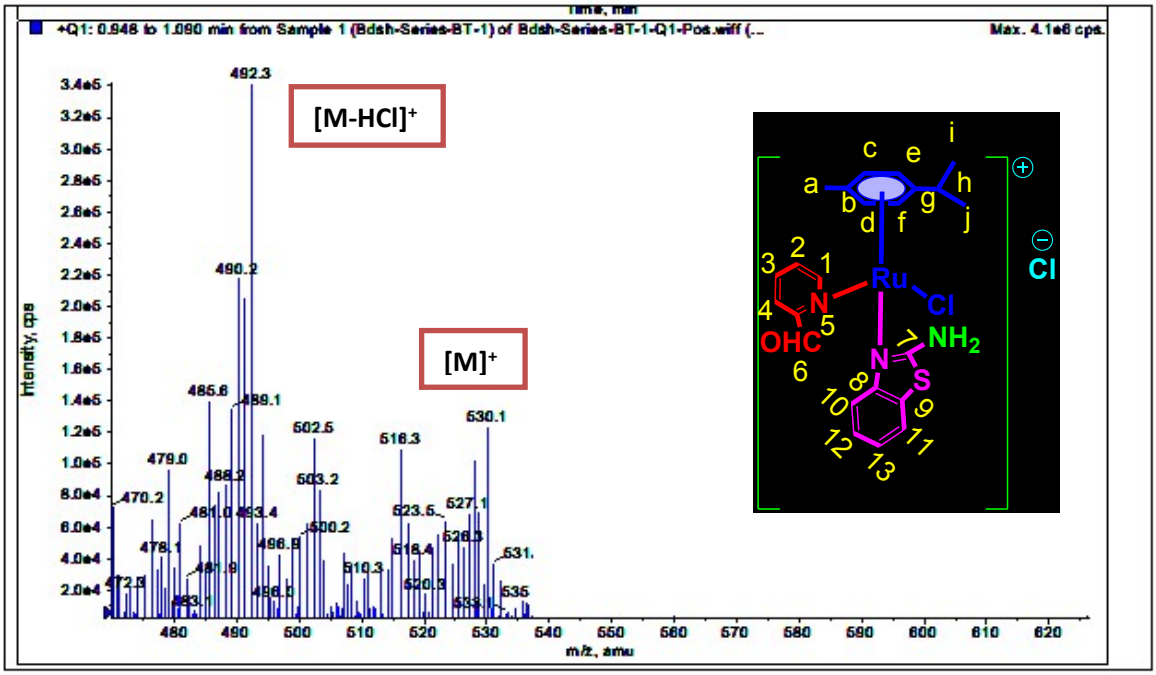
Ruthenium(II) *p*-cymene complex of pyridine-2-carboxaldehyde and 2-amino benzothiazole based ligand: A cytoselective and *in vitro* live cell imaging agent†

Anuja PK, Priyankar Paira*

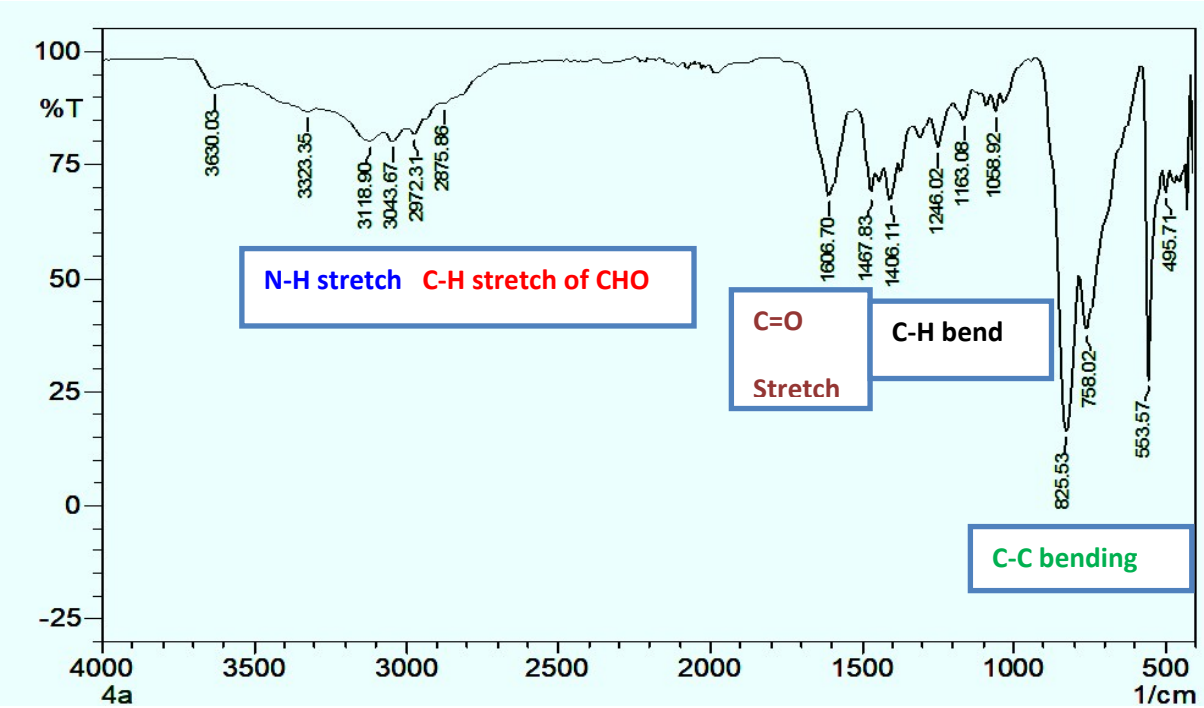
^{1}H NMR spectra of complex RuL1



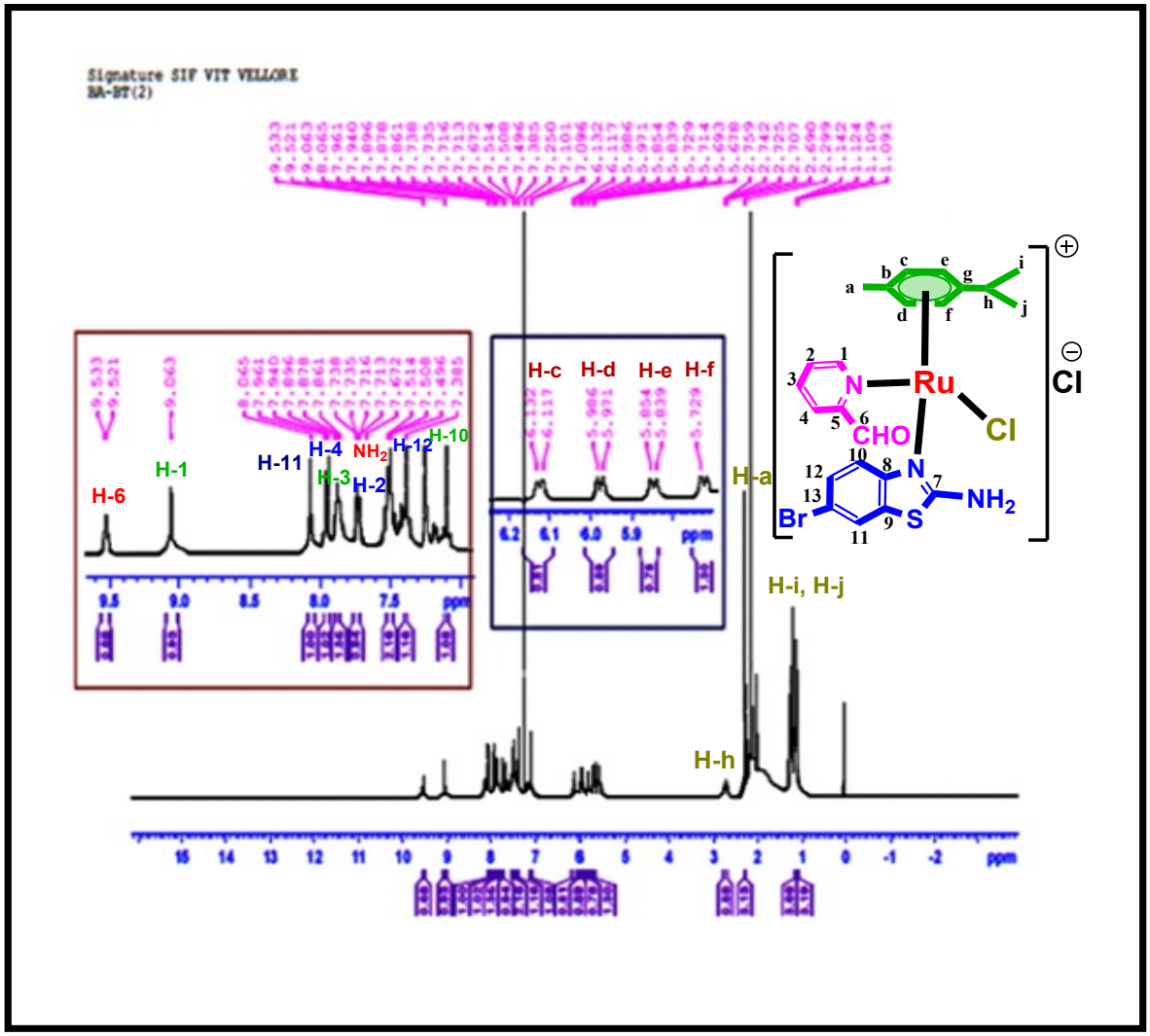
ESI-MS of complex RuL1



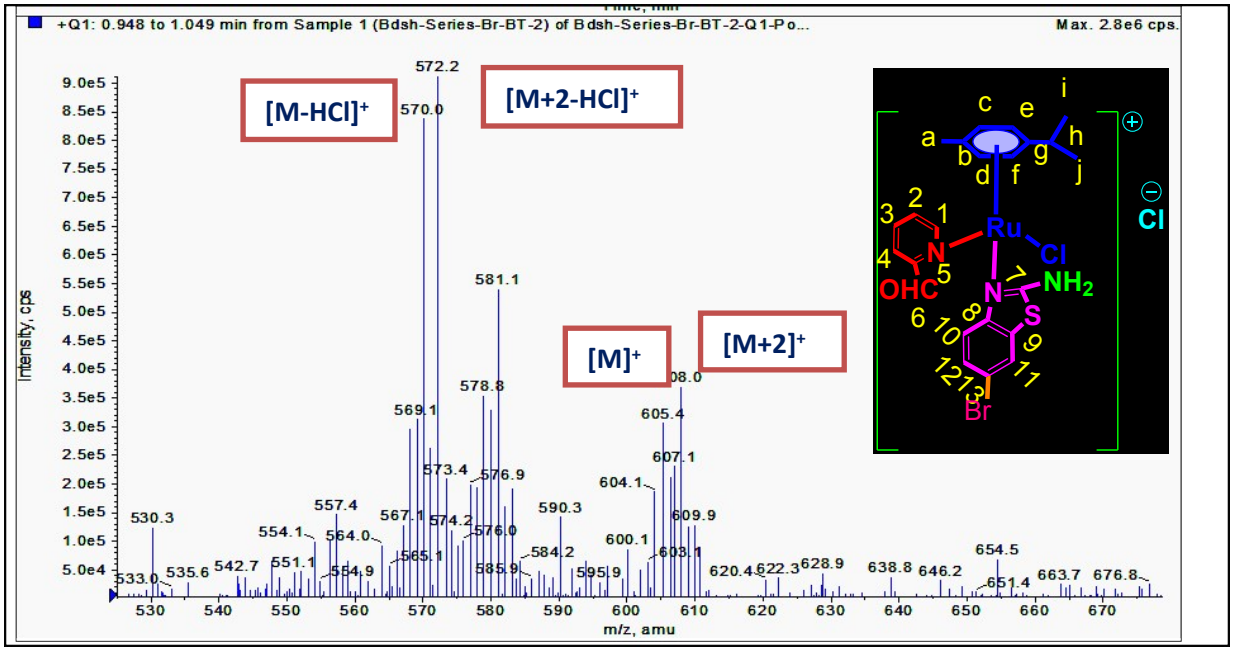
IR spectra of RuL1



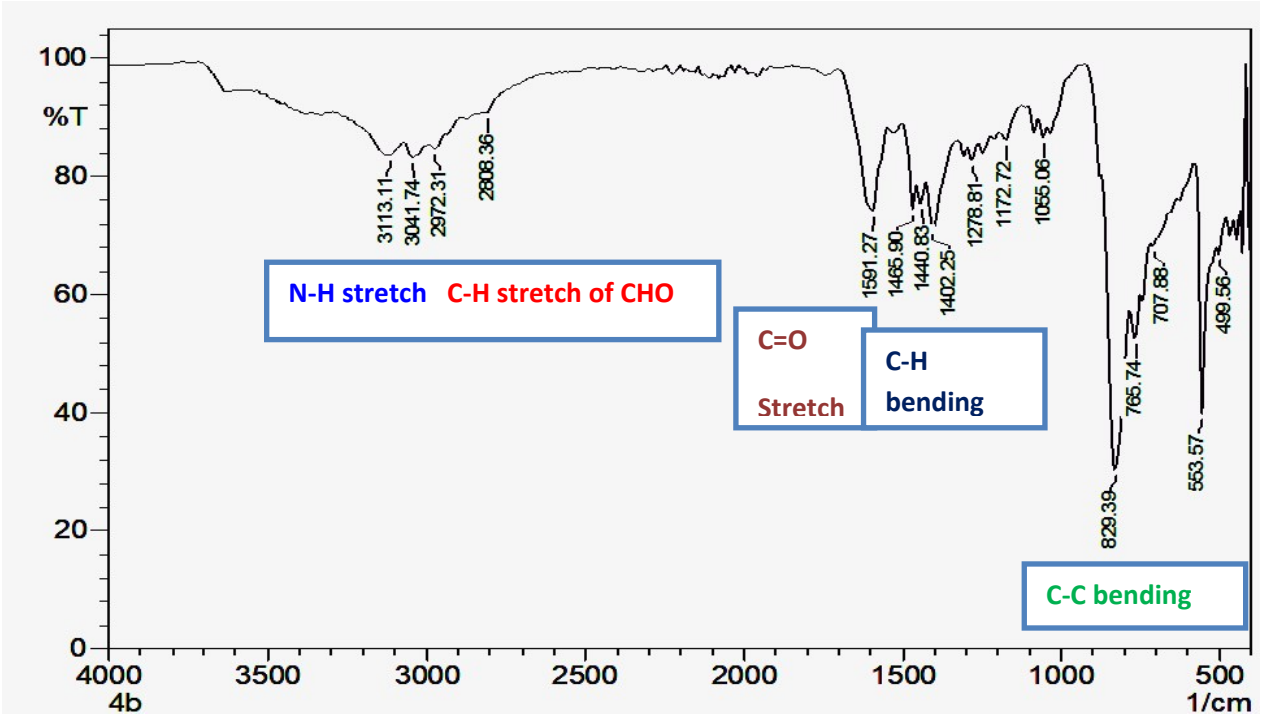
^{1}H NMR of complexRuL2



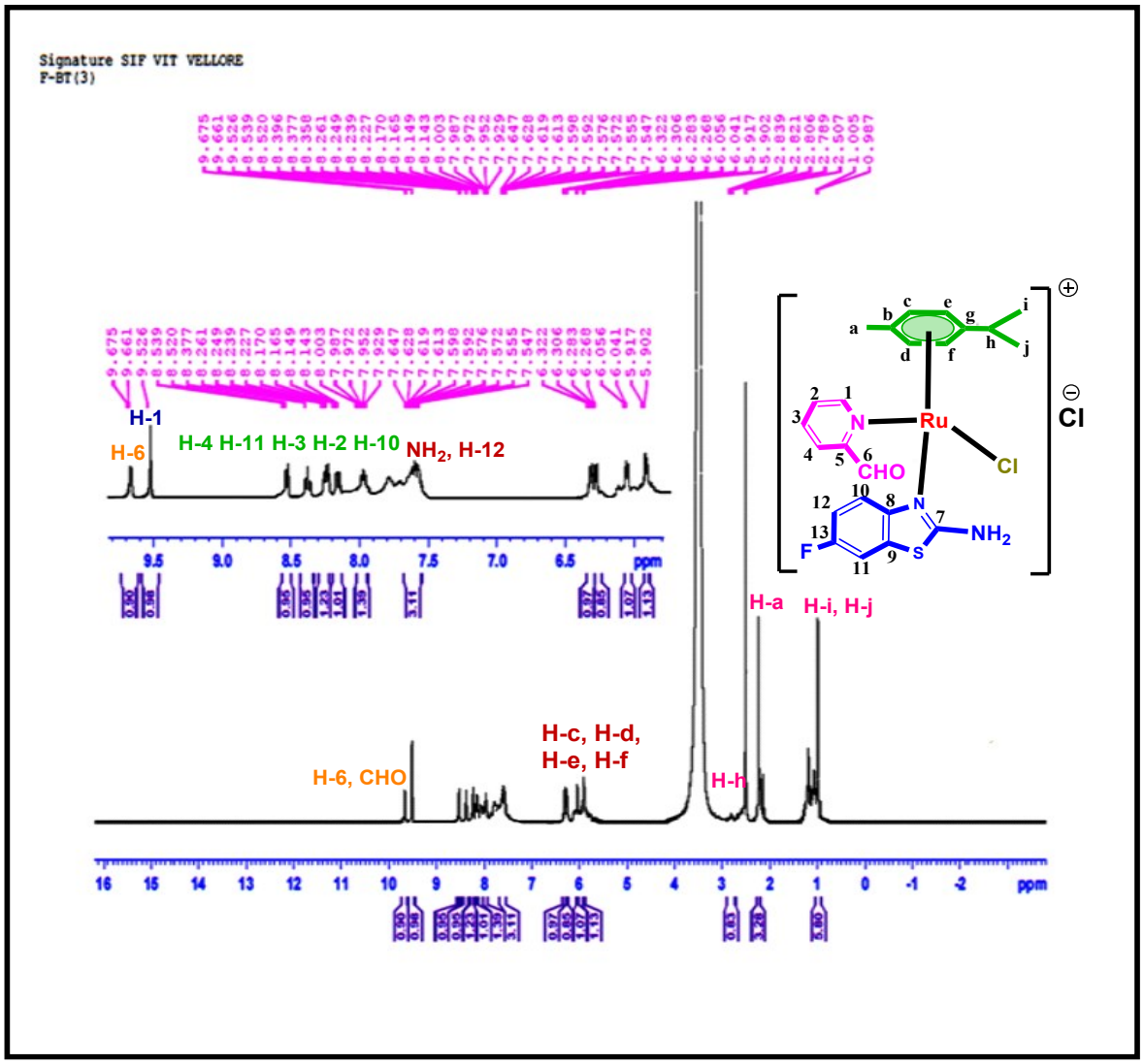
ESI-MS of complex RuL2



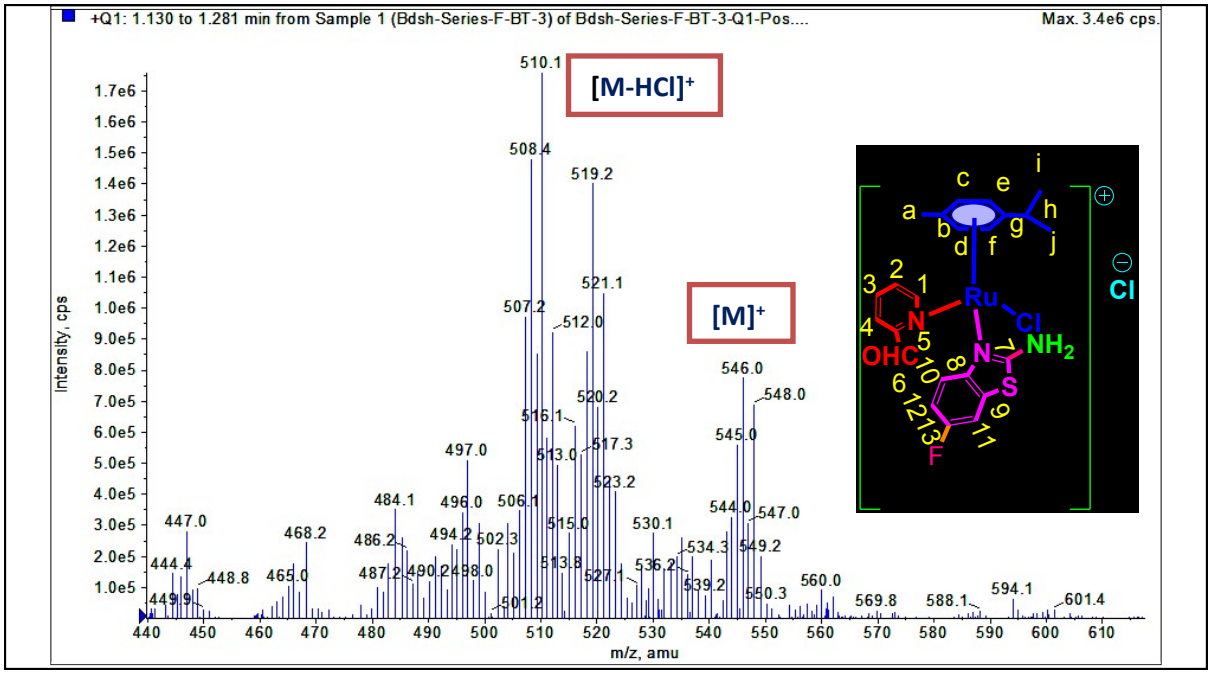
IR spectra of RuL2



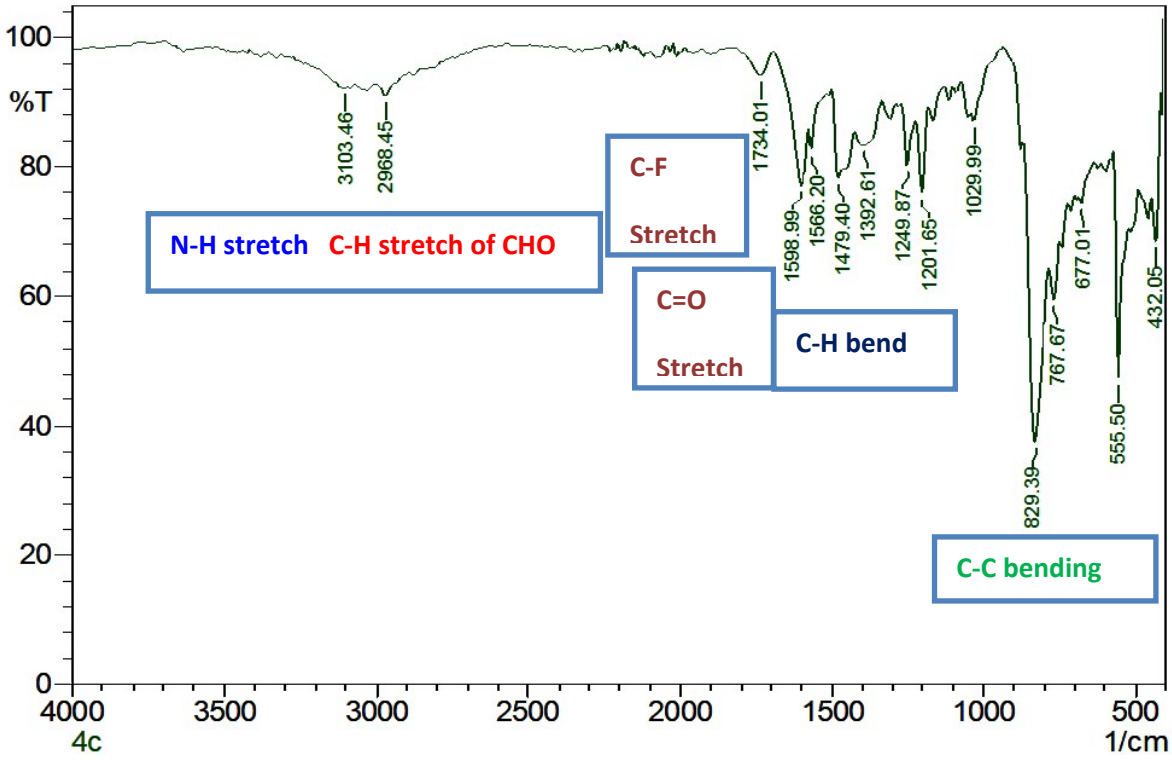
^{1}H NMR of RuL3



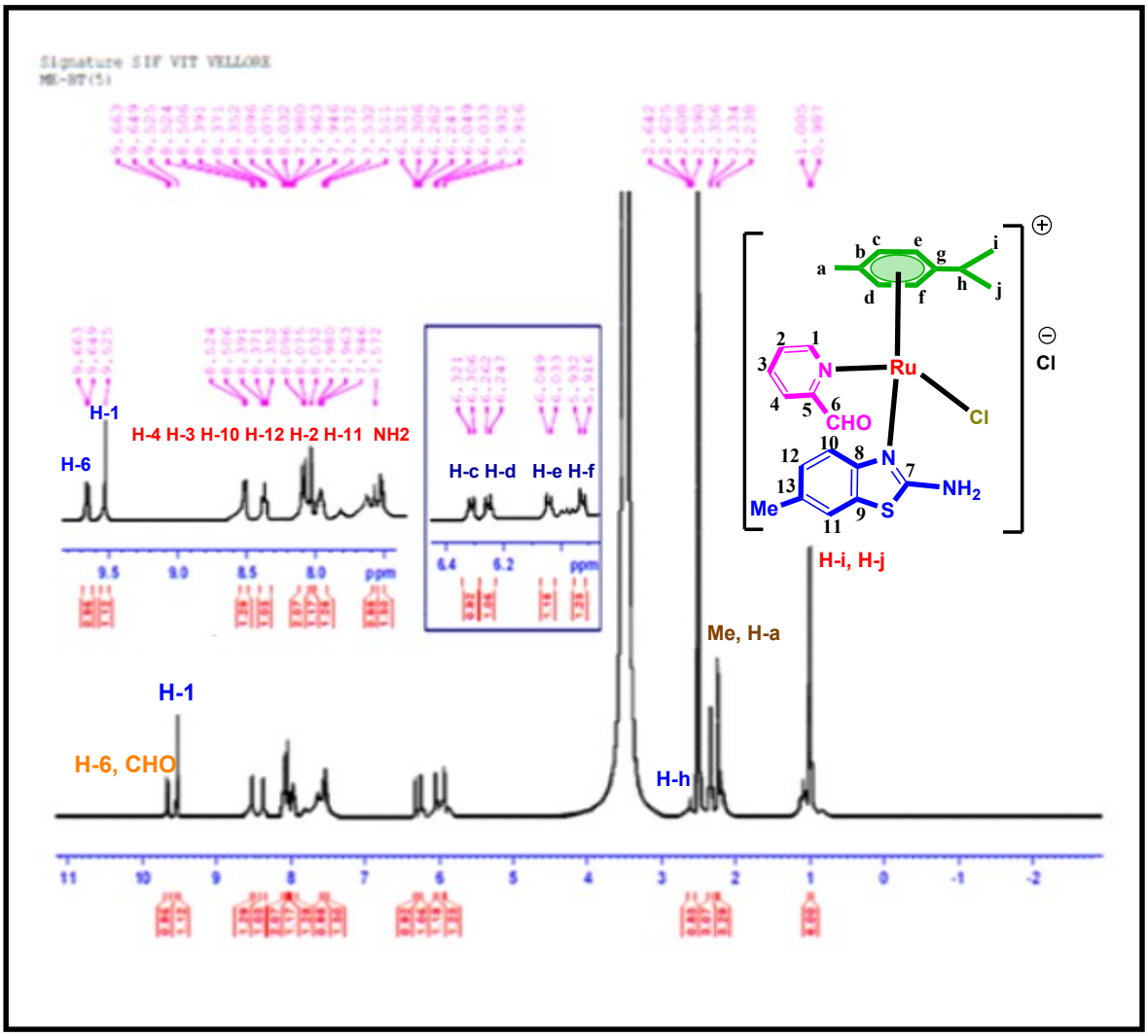
ESI-MS of complex RuL3



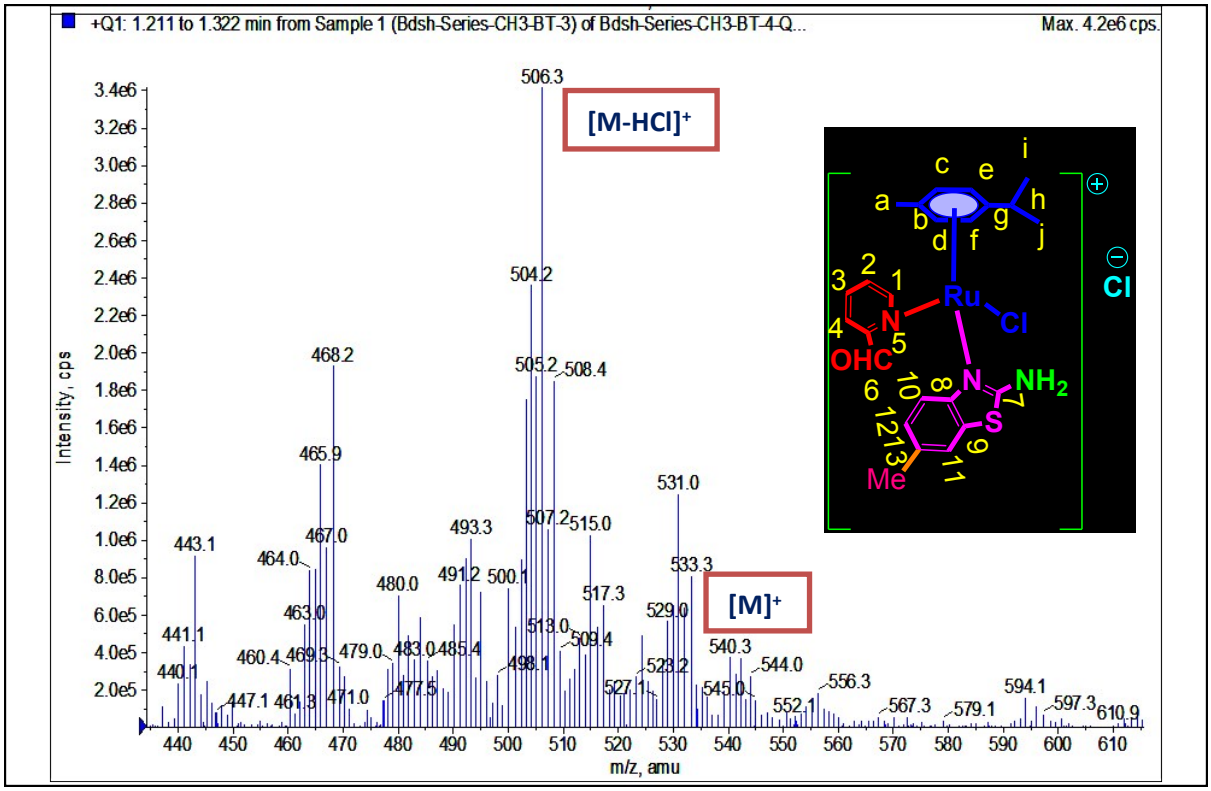
IR spectra of complex RuL3



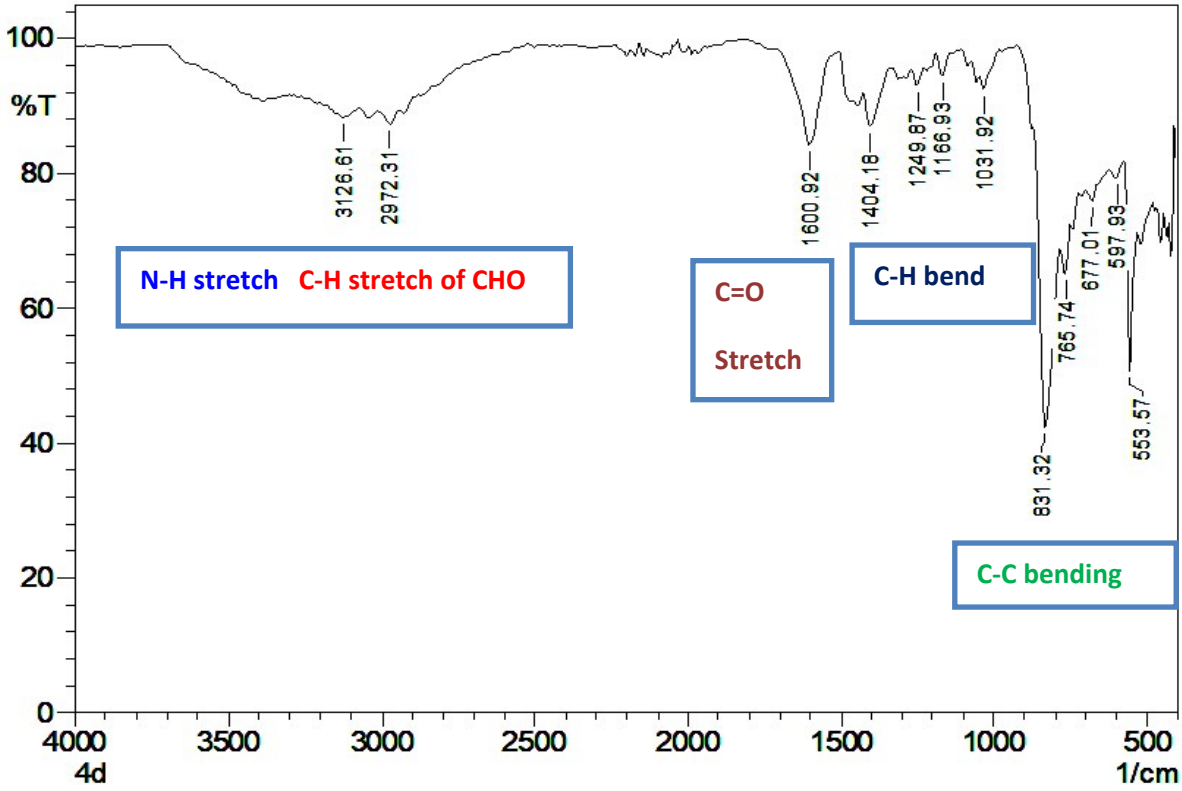
^{1}H NMR of RuL4



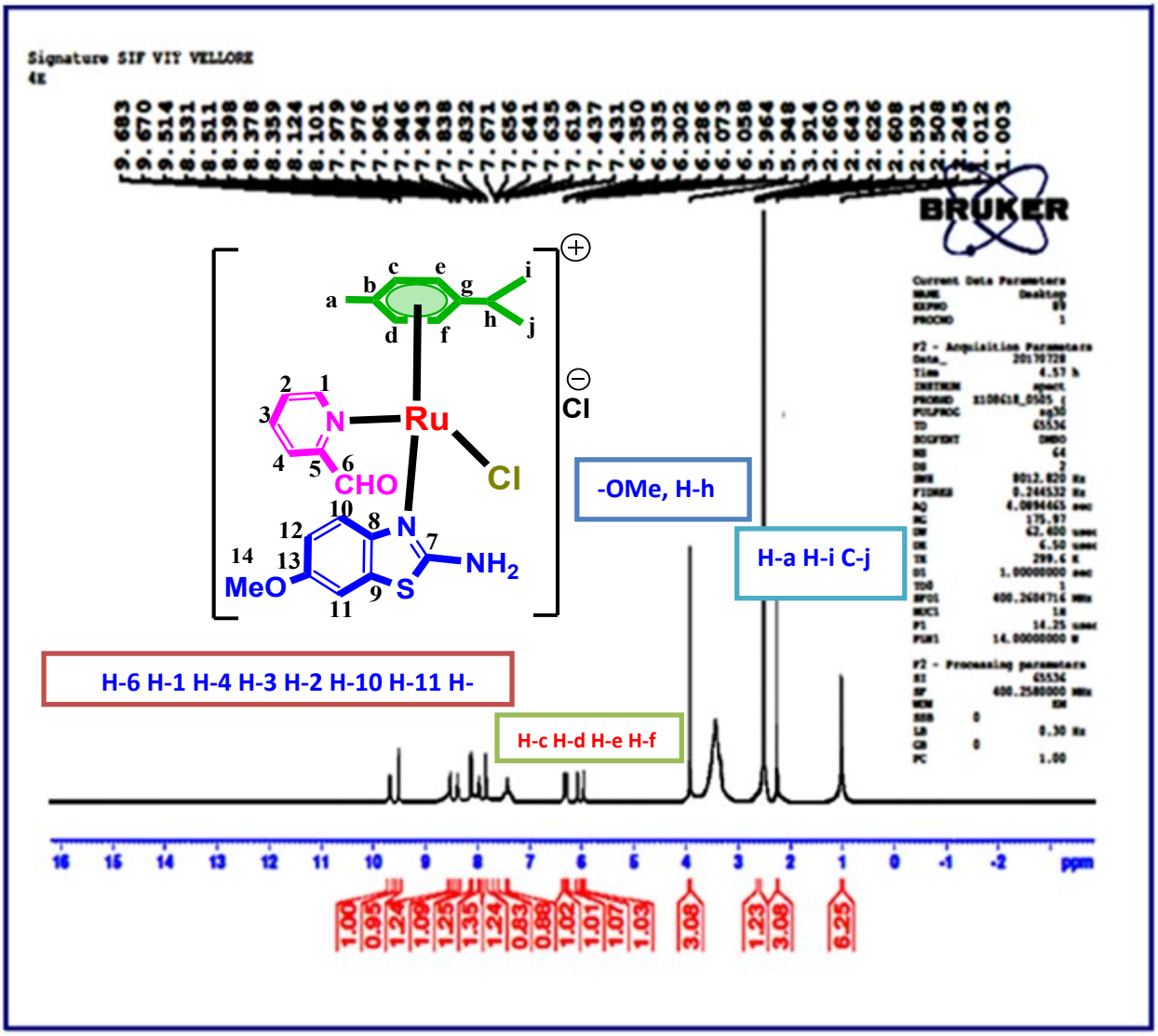
ESI-MS of complex RuL4



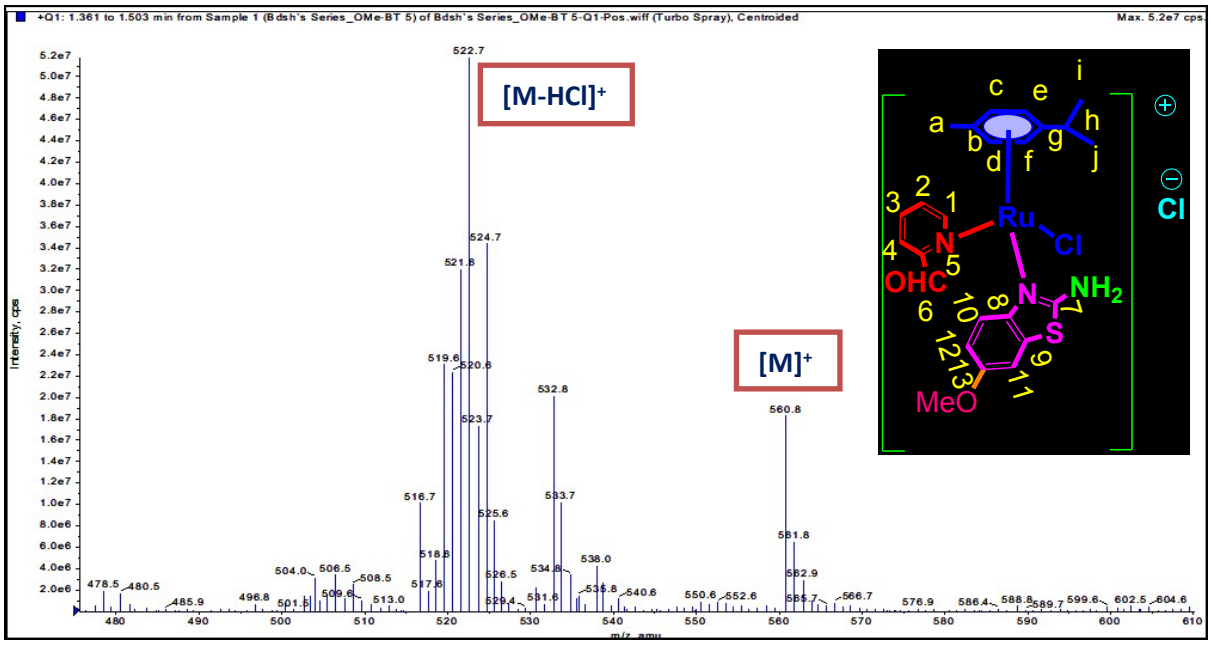
IR spectra of complex RuL4



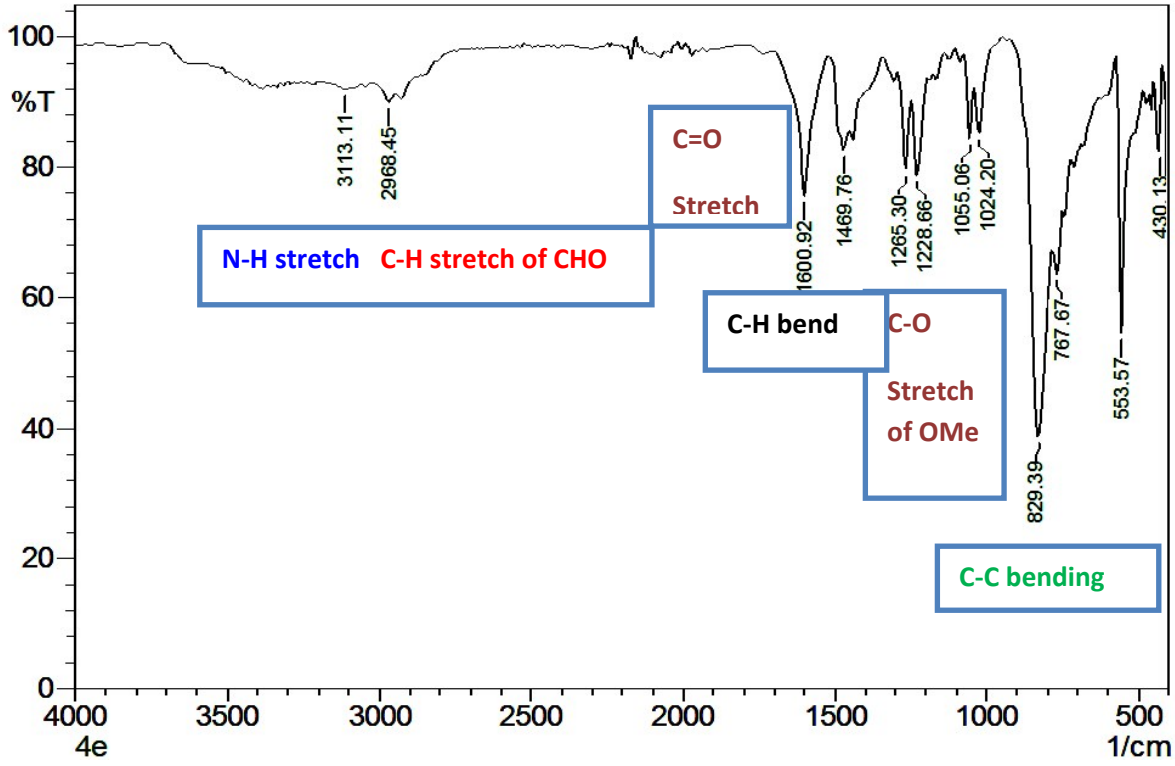
^{1}H NMR of RuL5



ESI-MS of complex RuL5



IR spectra of RuL5



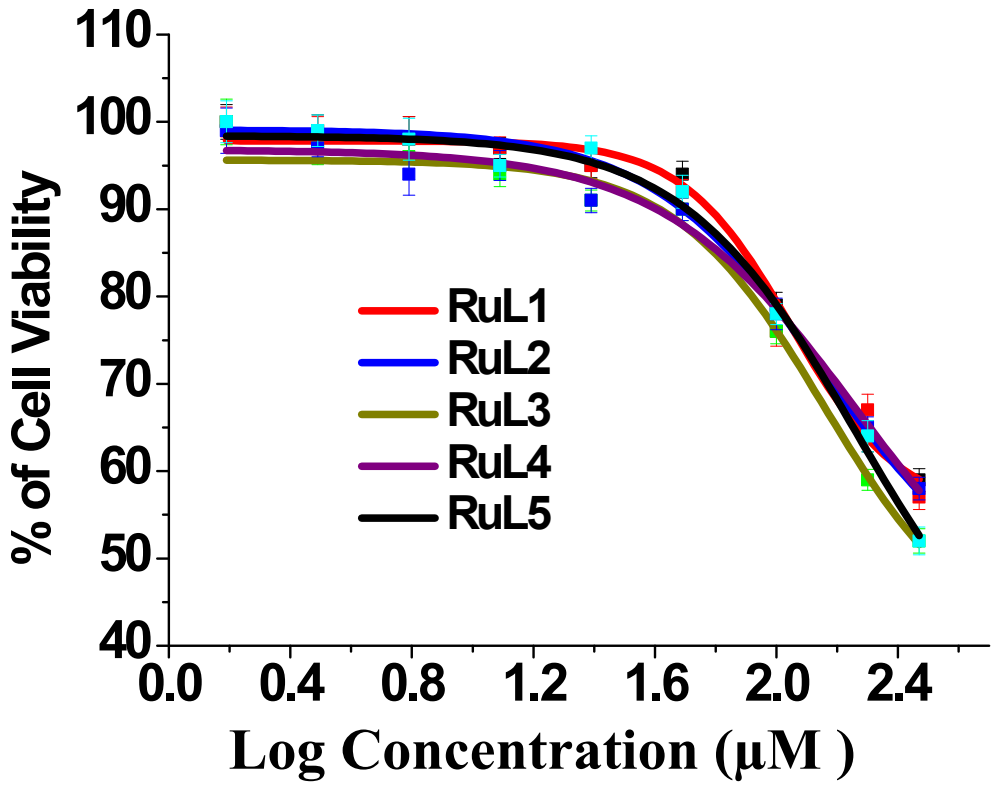


Fig. S1 *In vitro* dose–response curves for complexes (**RuL1-RuL5**) against HEK-293 cells treated under 48 h CO_2 incubation.

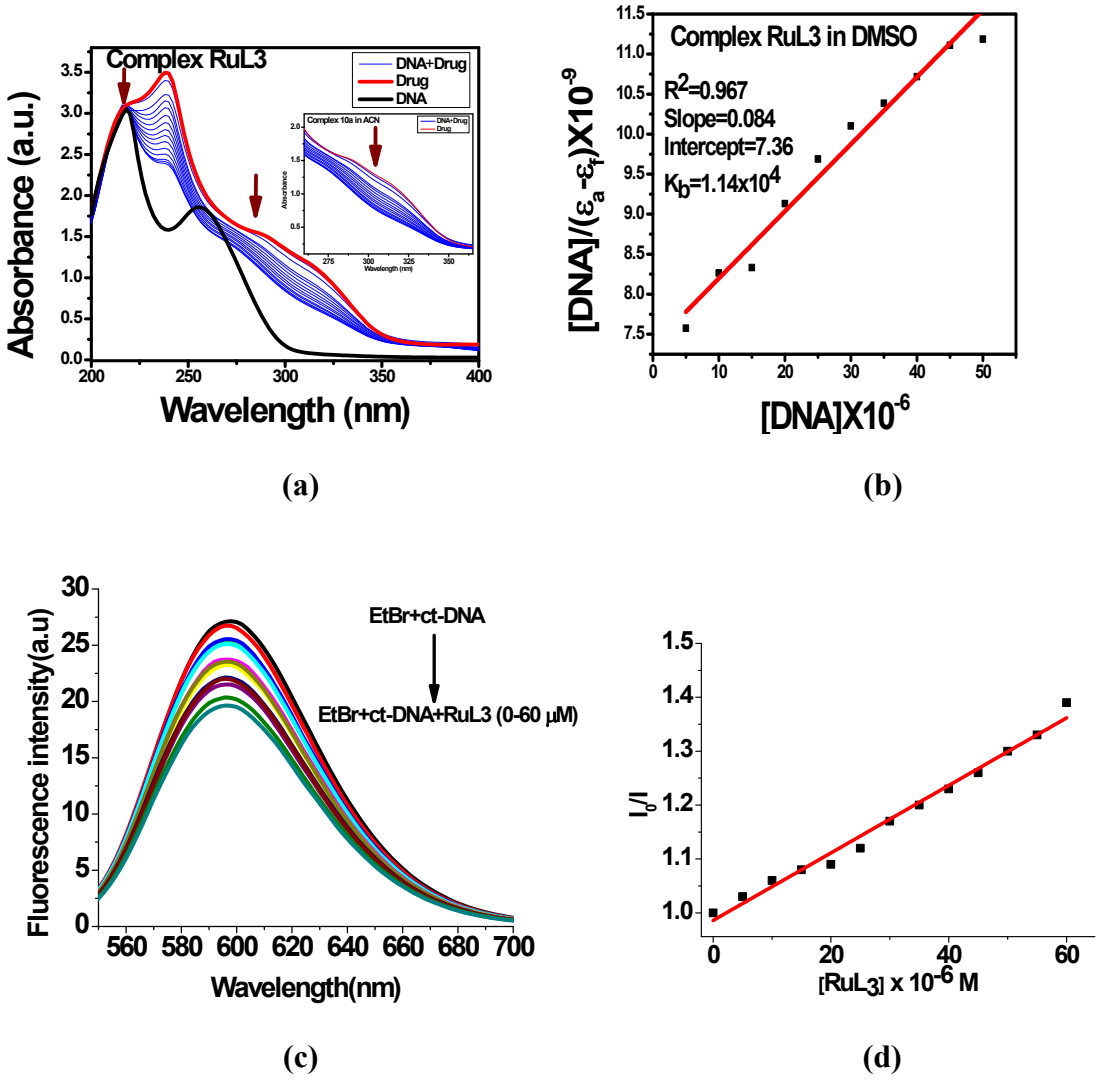
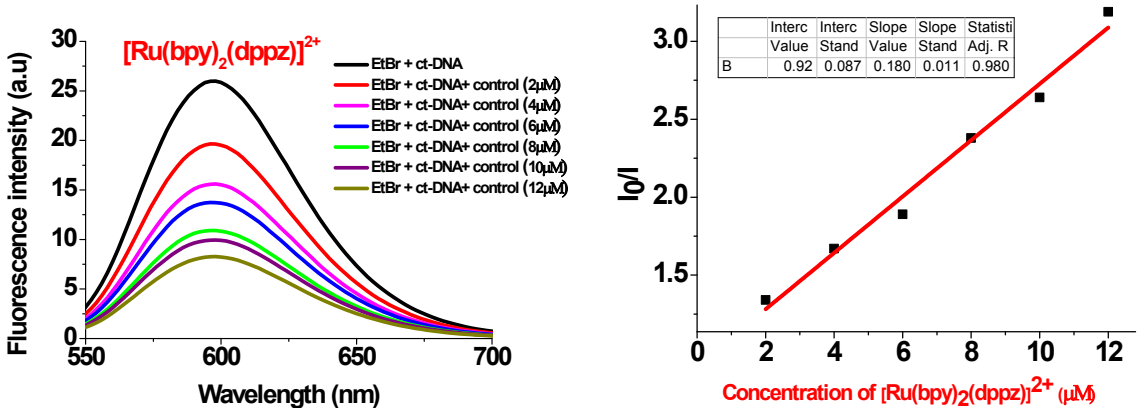


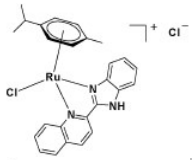
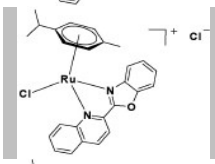
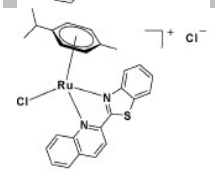
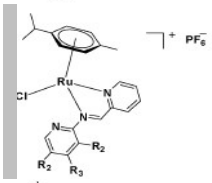
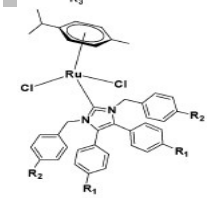
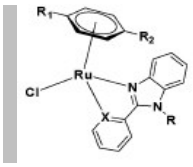
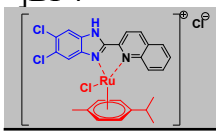
Fig. S2. (a) UV-Vis absorption spectrum of complex **RuL3** in absence and in presence of 10-100 μM of ct-DNA in TrisHCl buffer (pH 7.8, T = 25 °C). (b) plot of [DNA]/(ε_a- ε_f) vs [DNA]. (c) Ethidium bromide fluorescence quenching study with complex **RuL3**. (d) Stern Volmer plot of I_0/I *vs.* [**RuL3**]



(a) (b)

Fig. S3. (a) Ethidium bromide fluorescence quenching study with control DNA intercalator $[Ru(bpy)_2(dppz)]^{2+}$ (b) Stern Volmer plot of I_0/I *vs.* [control]

Table S1 Comparison of the IC_{50} values of previously reported Ru-*p*-cymene complexes against cancer cell lines

Complex	**IC_{50} (μM)**		
	Cell lines		
	HeLa	MCF-7	references
	-	2.64	1
	-	18.21	1
	-	7.36	1
	-	7.76-25.42	2
	-	10.2±1.2	3
	-	26-300	4
[(p-cym)RuCl(HL1]BF4	-	68±3	4
	3.52±1.7	-	5

References:

1. T. A. Khan, K. Bhar, R. Thirumoorthi, T. Roy, A. K. Sharma, *New J. Chem.,* 2020, 44, 239—257.
2. (a) G. R. Jadhav, S. Sinha, M. Chhabra and P. Paira, Bioorg. Med. Chem. Lett., 2016, 26, 2695–2700. (b) U. Ndagi, N. Mhlongo and M. E. Soliman, Drug Des., Dev. Ther., 2017, 11, 599.
3. F. Hackenberg, H. Mu¨ller-Bunz, R. Smith, W. Streciwilk, X. Zhu and M. Tacke, Organometallics, 2013, 32, 5551–5560.
4. M. Martı´nez-Alonso, N. Busto, F. A. Jalo´n, B. R. Manzano, J. M. Leal, A. M. Rodrı´guez, B. Garcı´a and G. Espino, Inorg. Chem., 2014, 53, 11274–11288.
5. A Mondal, U Sen, N Roy, V Muthukumar, SK Sahoo, B Bose, P Paira*, Dalton Transactions 2021, 50 (3), 979-997