Synthesis and molecular structure of arene ruthenium(II) benzhydrazone complexes: Impact of substitution at chelating ligand and arene moiety on antiproliferative activity

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Table S1. Selected crystal data and structure refinement summary of **3** and **6.**

Complex	**3.**H_2O	**6**
Chemical formula	C_{23} H_{22} Cl N_3 O_3 Ru	C_{27} H_{28} Cl N_3 O_2 Ru
Formula weight	521.93	563.04
Crystal system	Monoclinic	Monoclinic
Space group	P2(1)/n	P2(1)/n
a (Å)	7.7924(4)	11.963(2)
b (Å)	10.7114(4)	12.838(3)
c (Å)	26.6417(12)	18.236(4)
α (°)	90	90
β (°)	91.178(2)	108.64(3).
γ (°)	90	90
Volume (Å3)	2223.25(17)	2654.0(9)
Z	4	4
ρ (g cm^{-3})	1.559	1.409
μ (mm^{-1})	0.855	0.719
Reflections collected	18192	20234
R1, wR2 [I≥ 2σ(I)]	0.0508, 0.1318	0.0460, 0.1212
Goodness–of–fit on F2	0.999	1.089

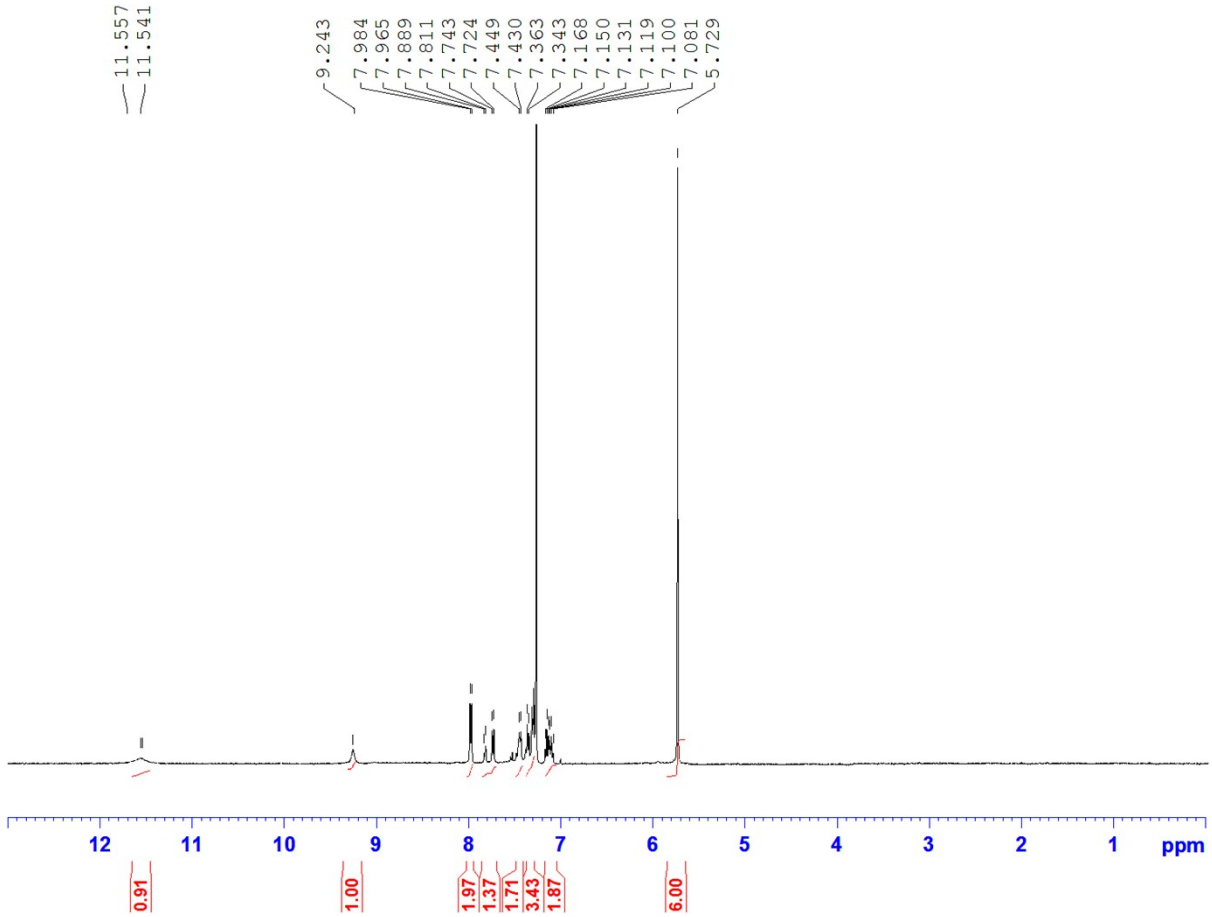


Figure S1. ^{1}H NMR spectrum of [Ru(η^6-C_6H_6)(Cl)(L1)] (**1**)

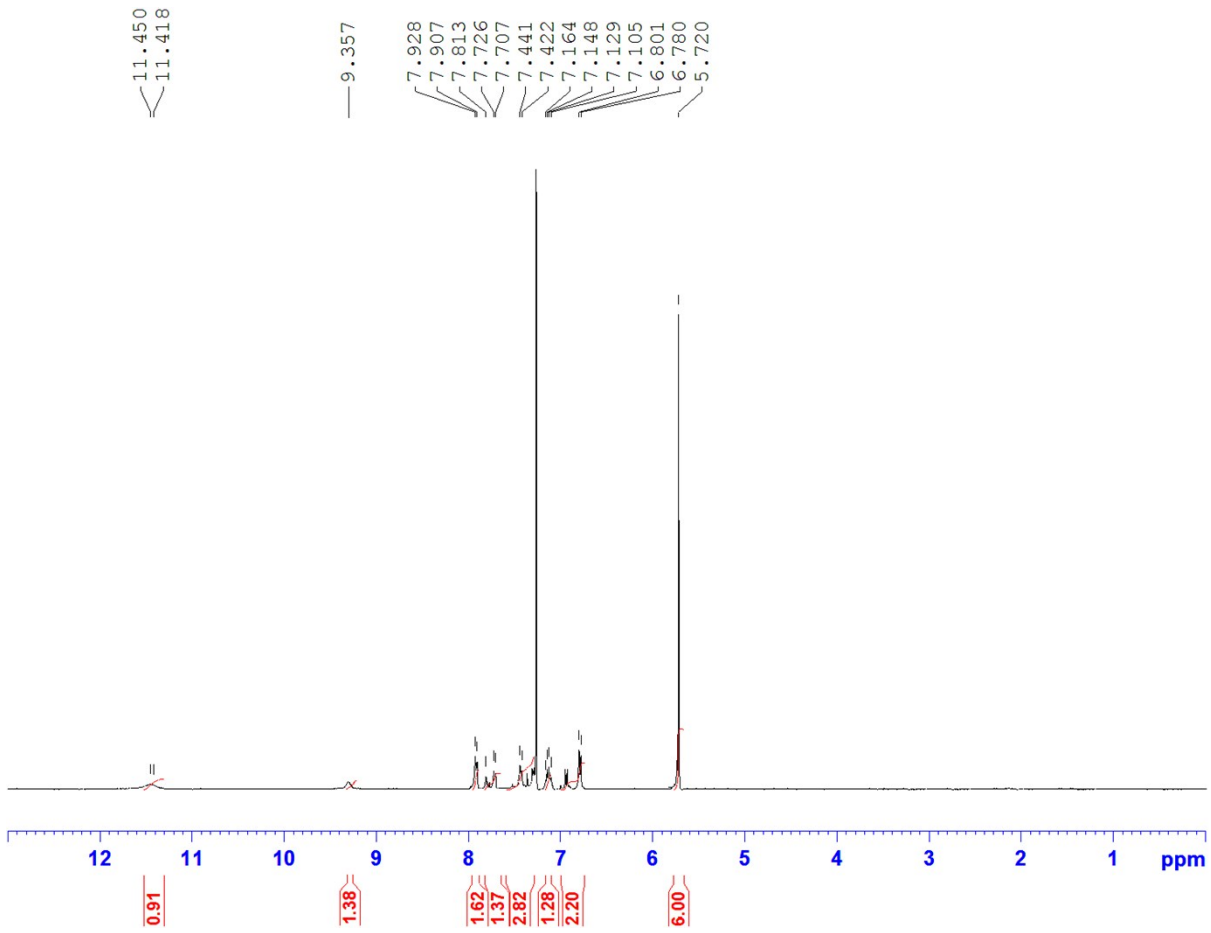
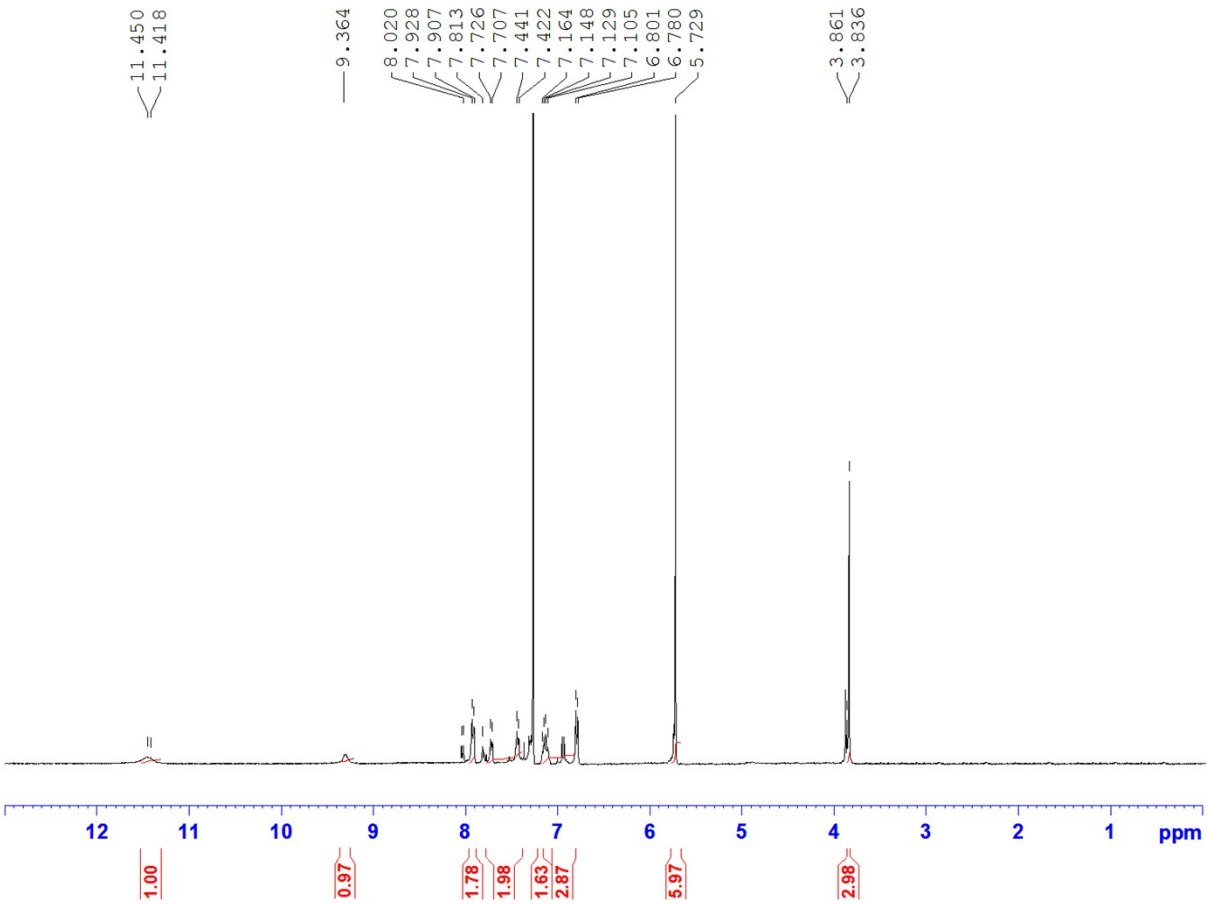


Figure S1. ^{1}H NMR spectrum of [Ru(η^6-C_6H_6)(Cl)(L2)] (**2**)



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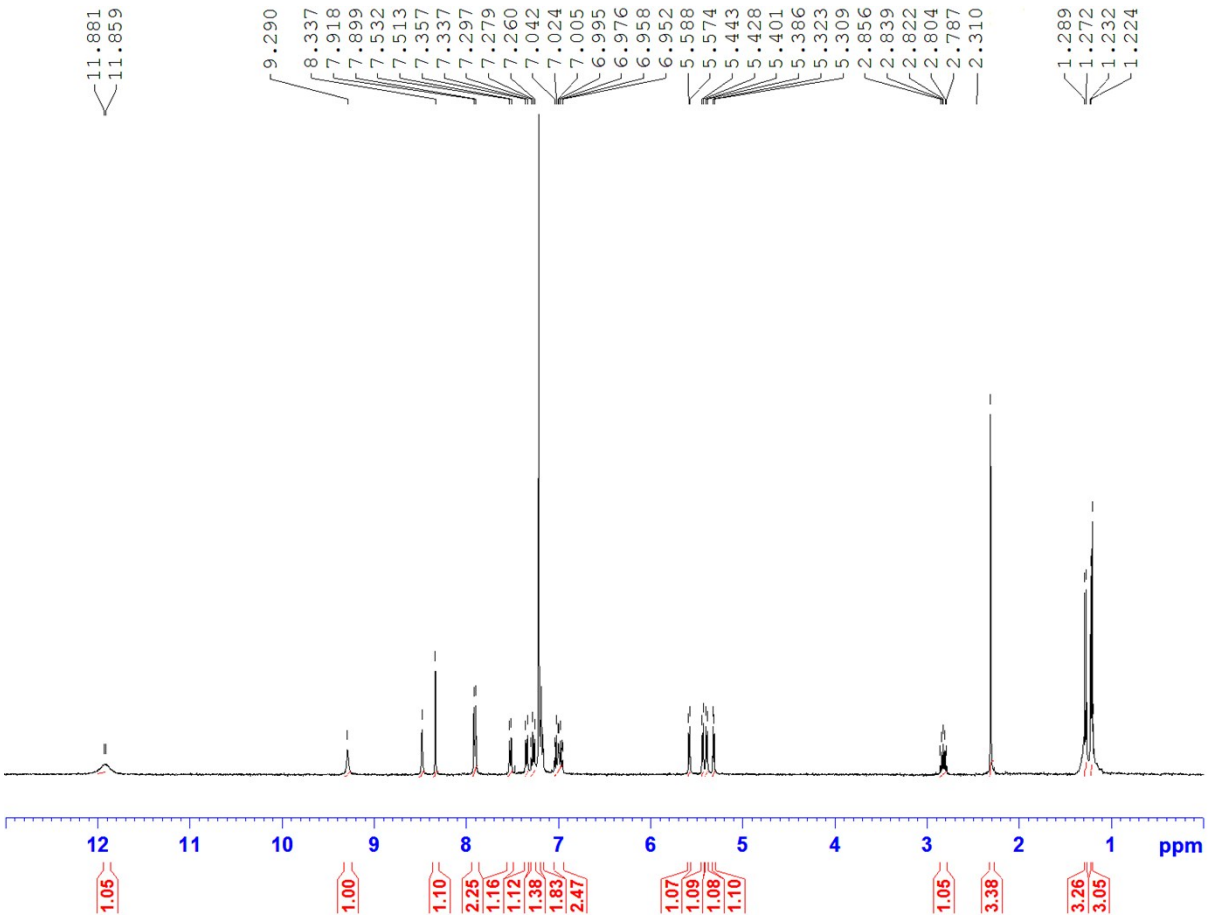


Figure S1. ^{1}H NMR spectrum of [Ru(η^{6}-p-cymene)(Cl)(L1)] (**4**)

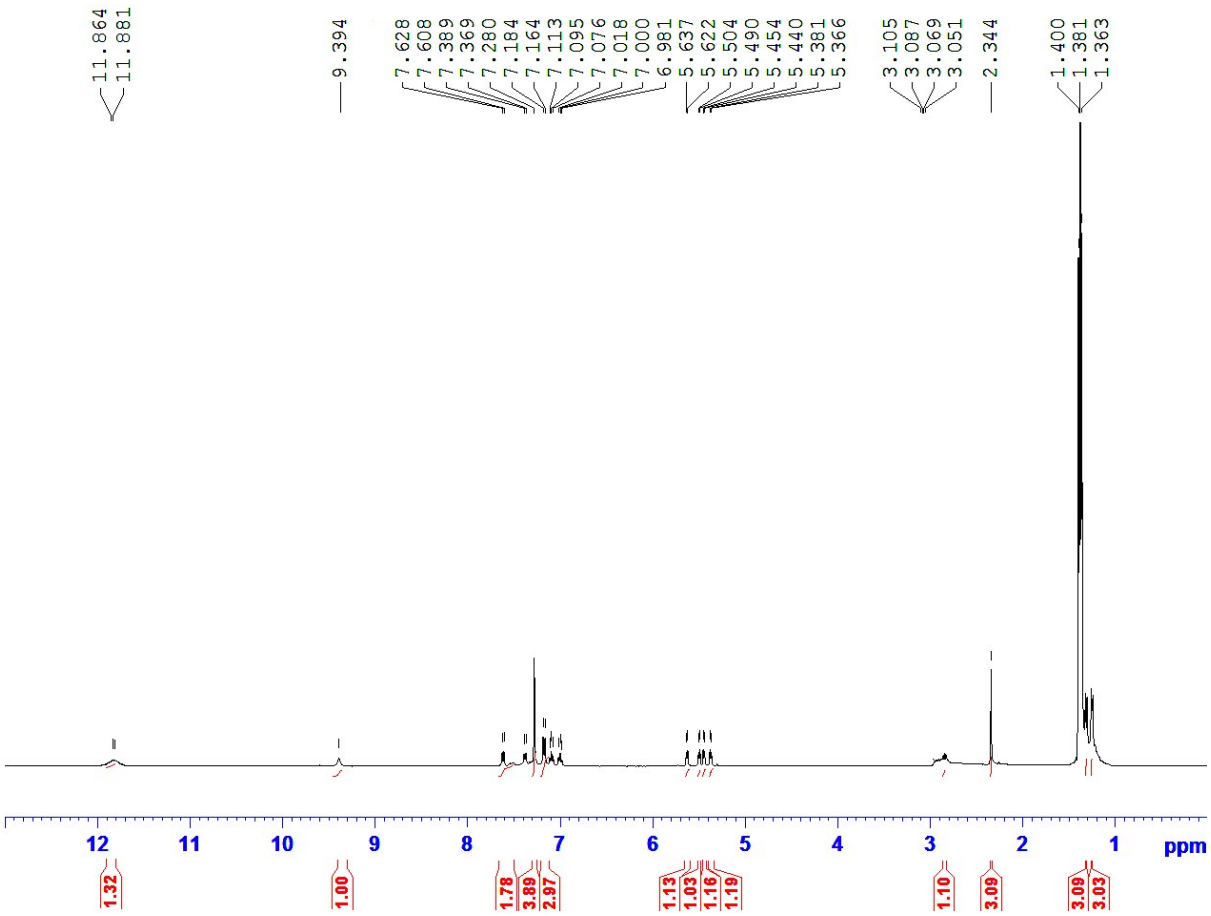
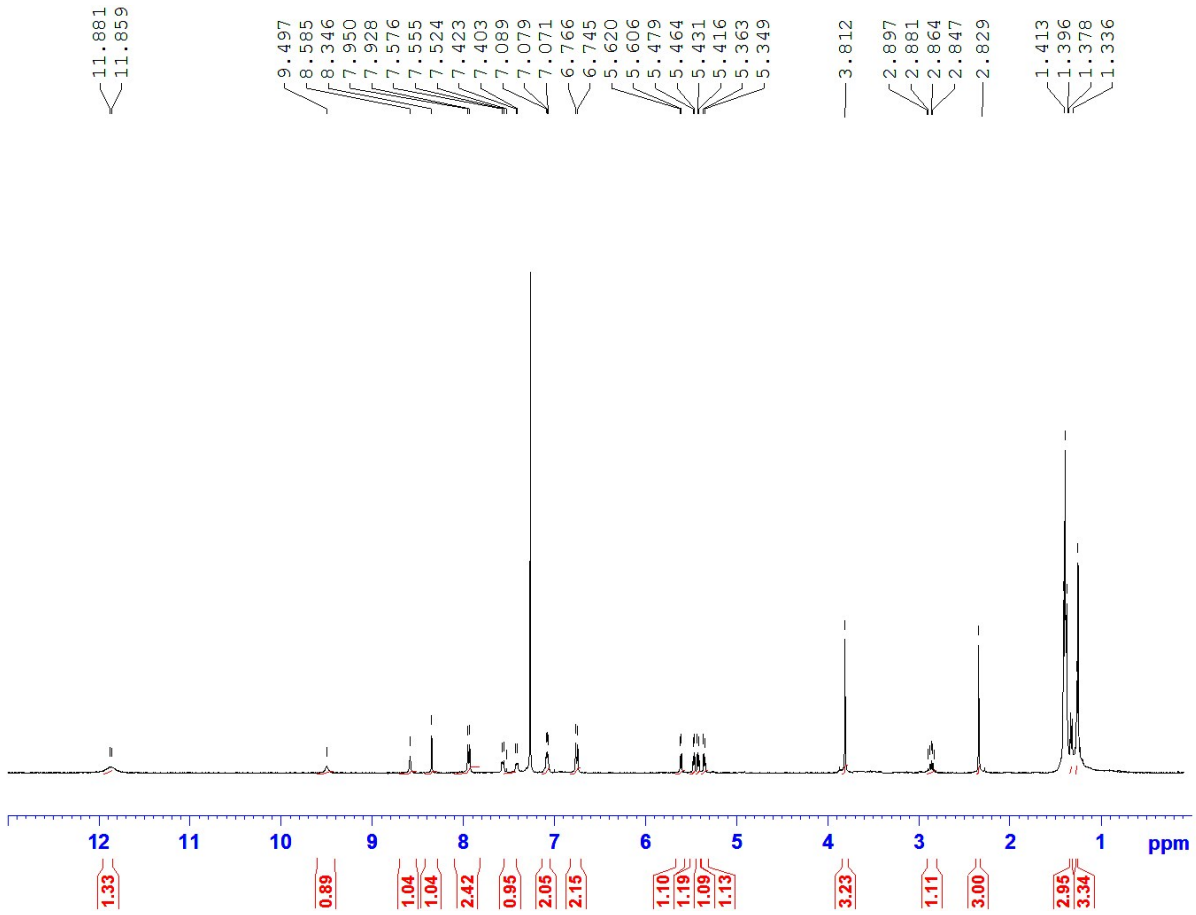


Figure S1. ^{1}H NMR spectrum of [Ru(η^6-p-cymene)(Cl)(L2)] (**5**)



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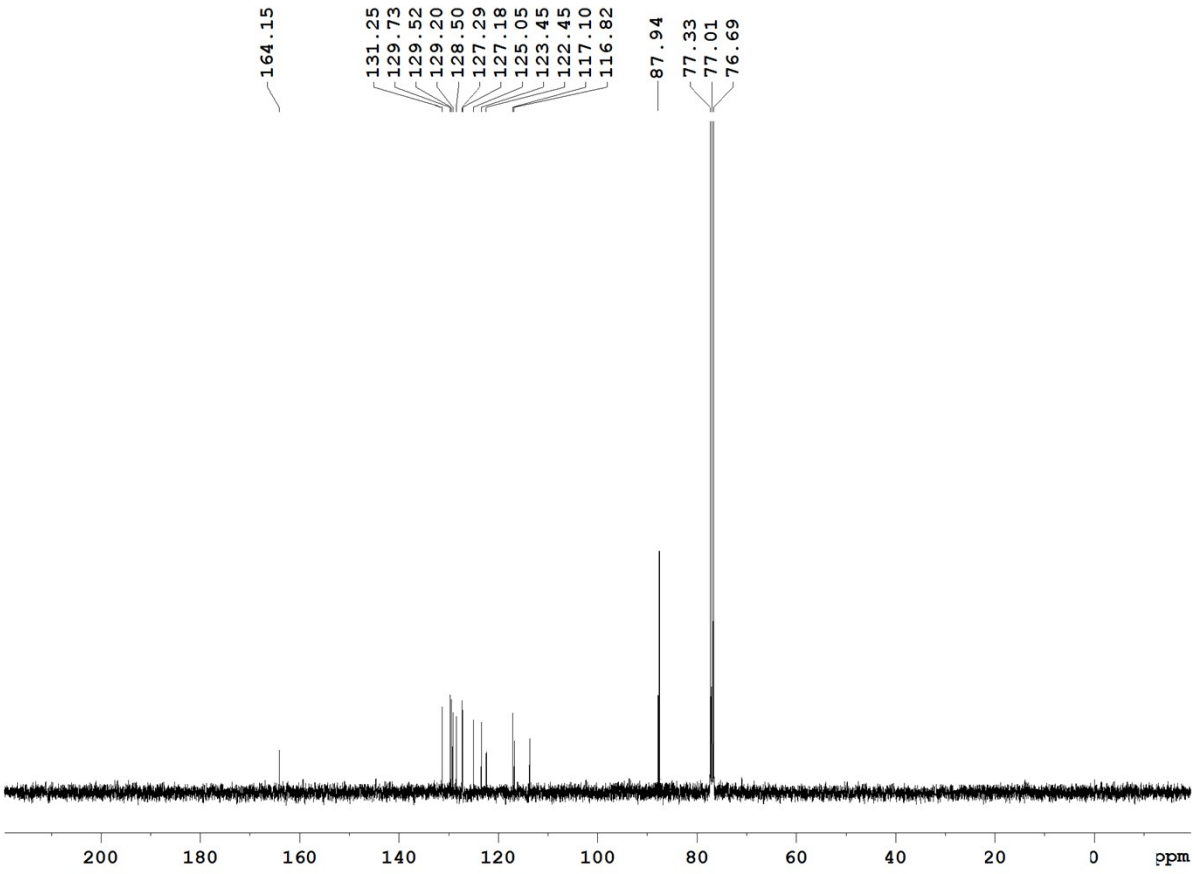


Figure S2. ^{13}C NMR spectrum of [Ru(η^6-C_6H_6)(Cl)(L1)] (**1**)

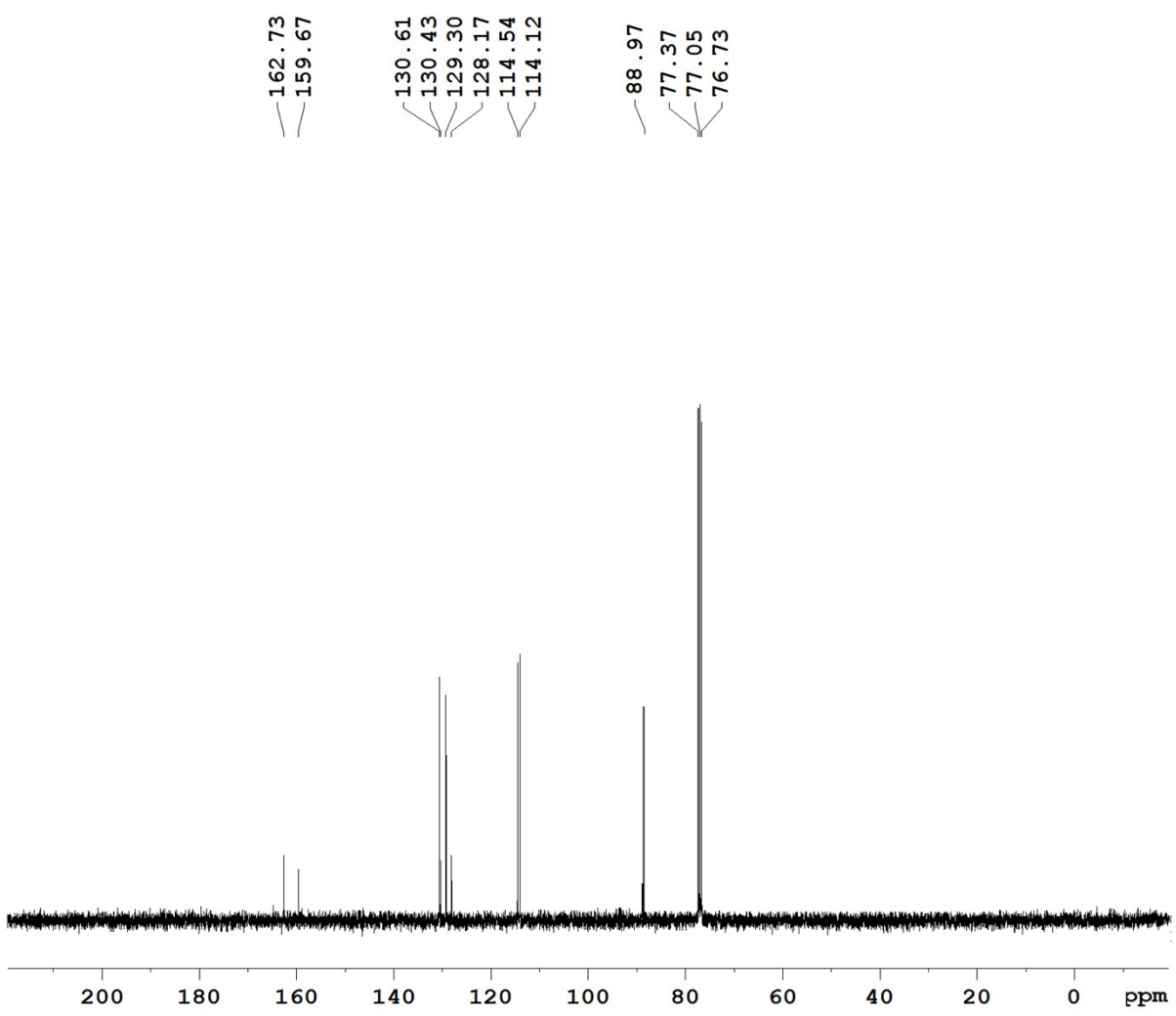
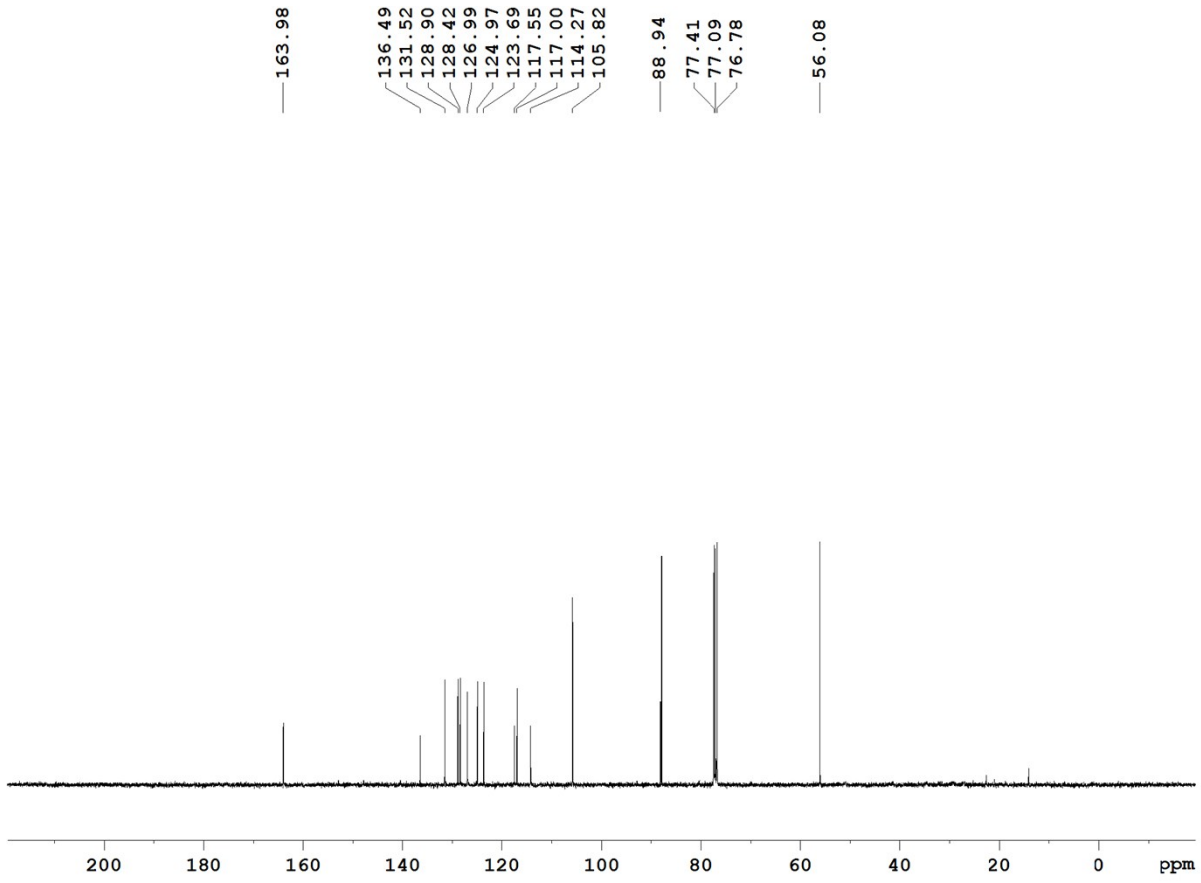


Figure S2. ^{13}C NMR spectrum of [Ru(η^6-C_6H_6)(Cl)(L2)] (**2**)



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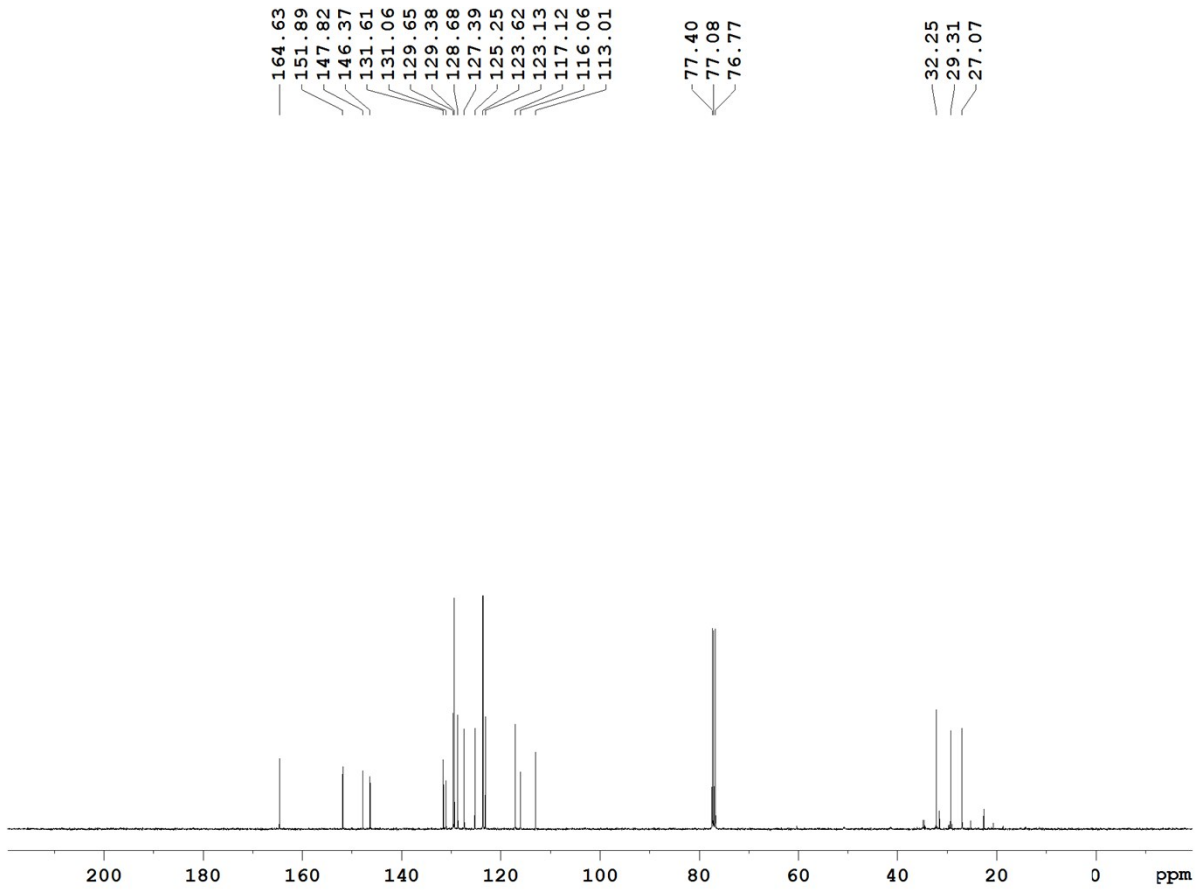

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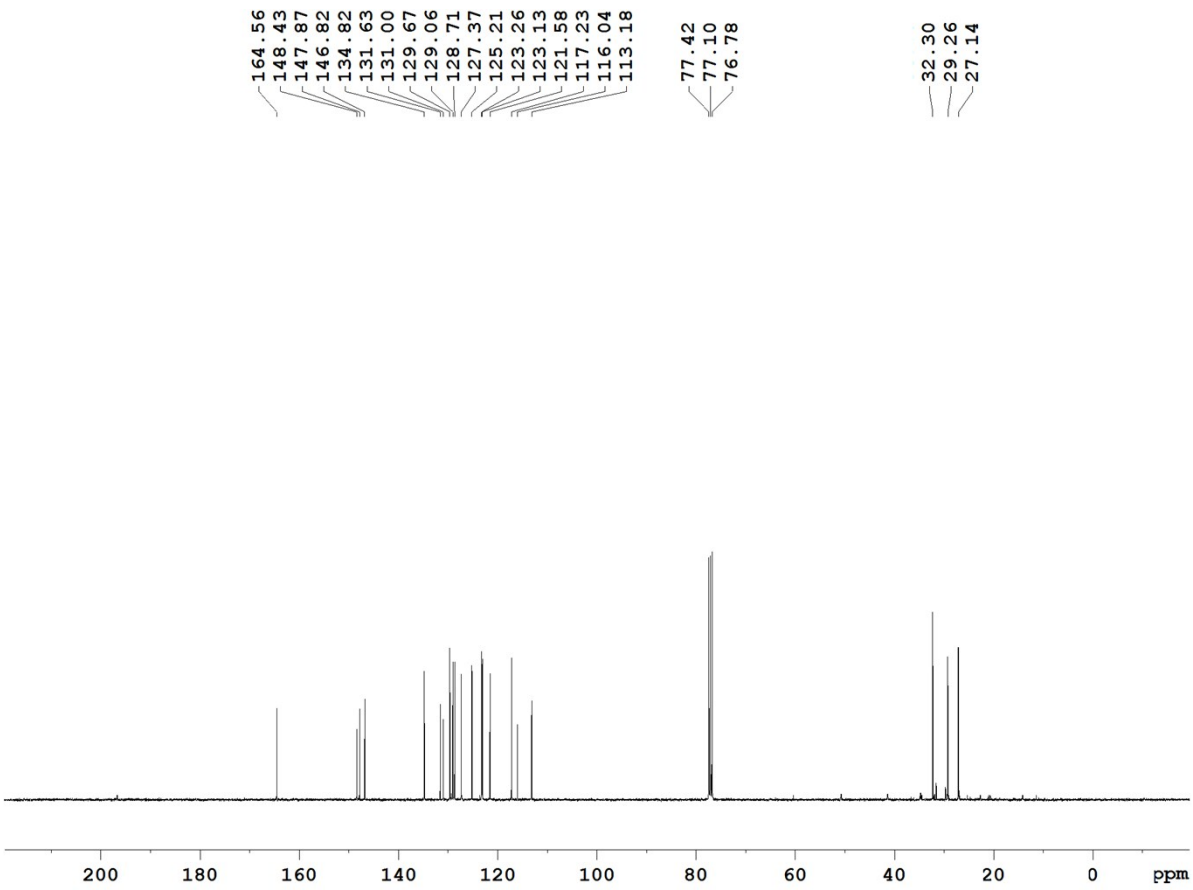

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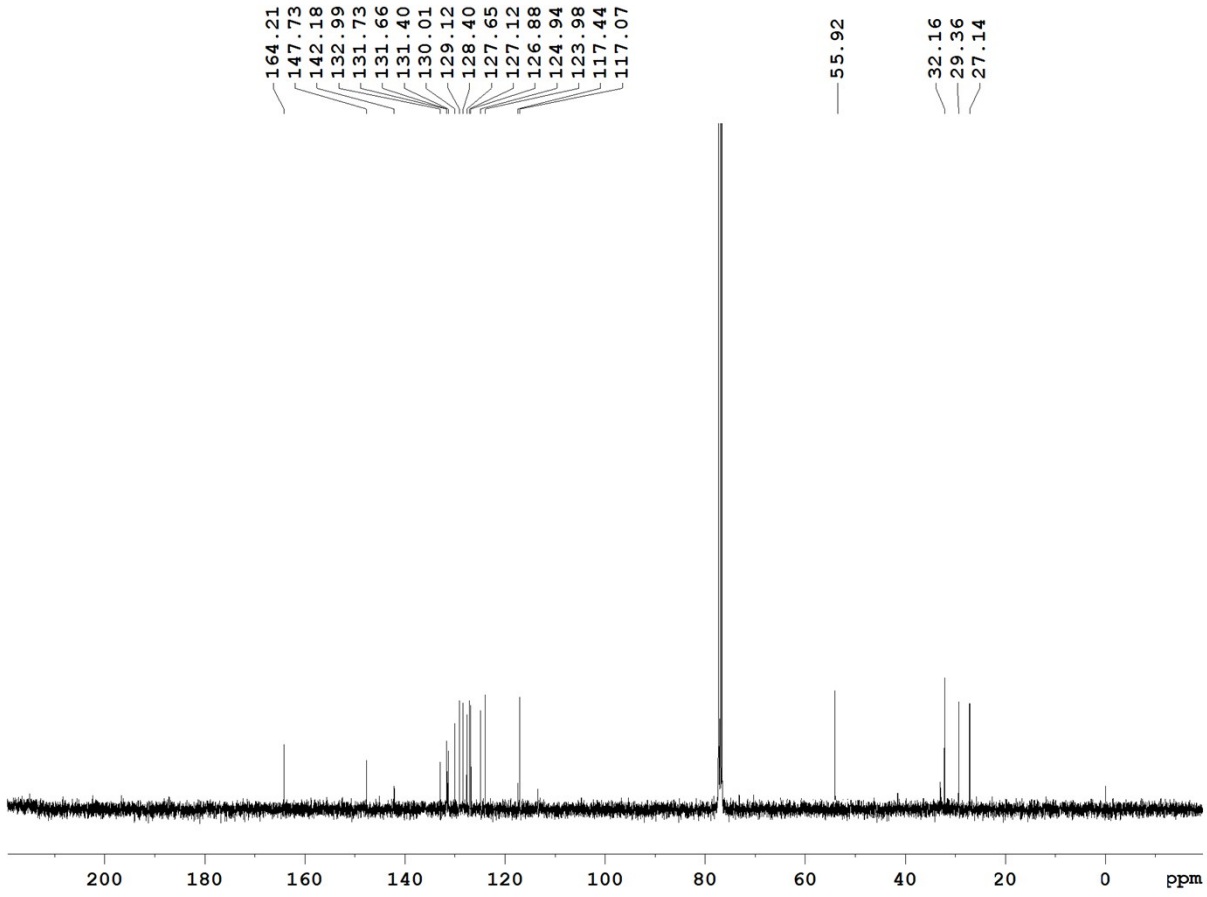

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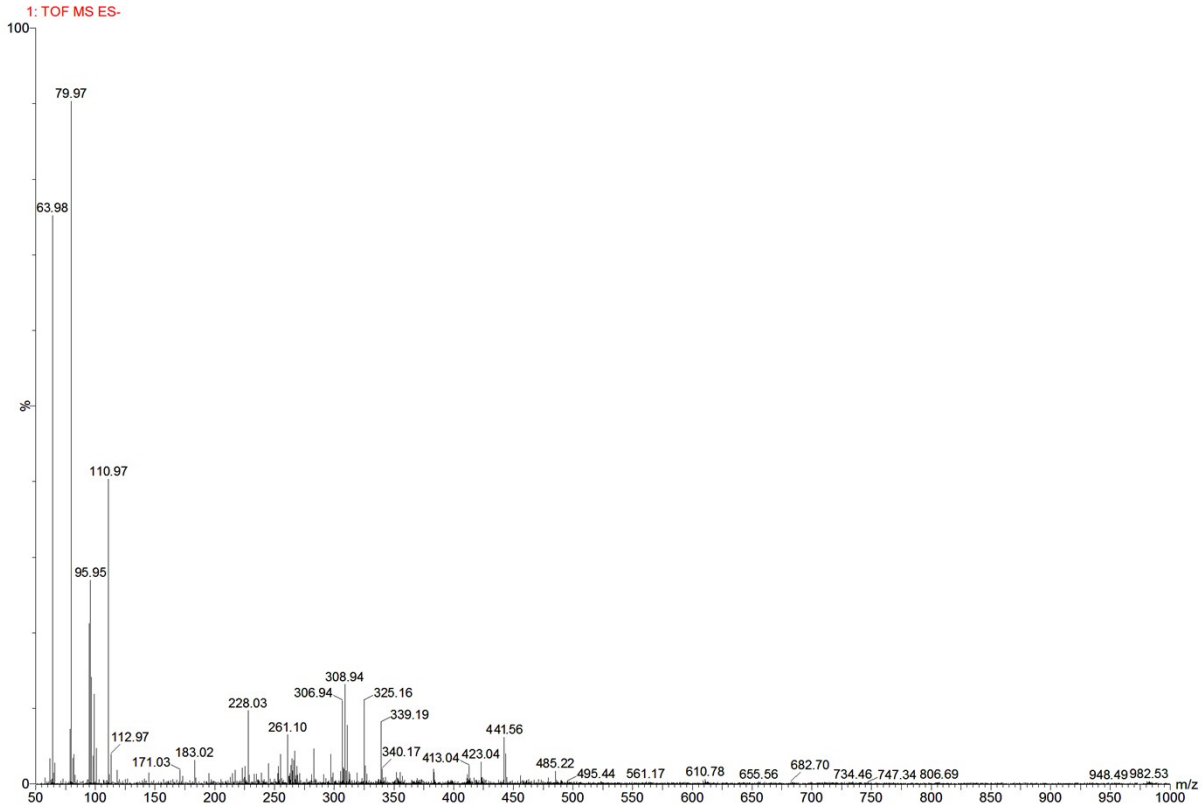
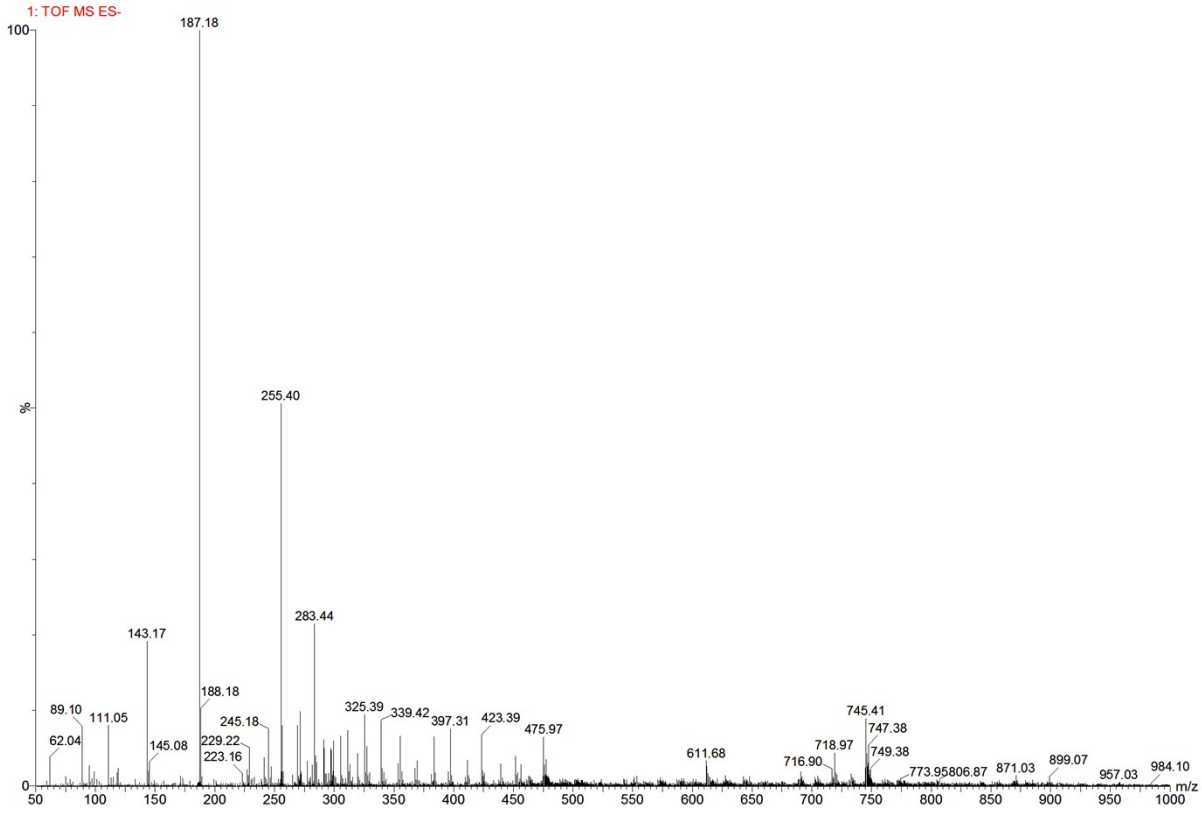


Figure S3: ESI-Mass spectrum of $[Ru(\eta^6\text{-}C_6H_6)(Cl)(L1)]$ (**1**)



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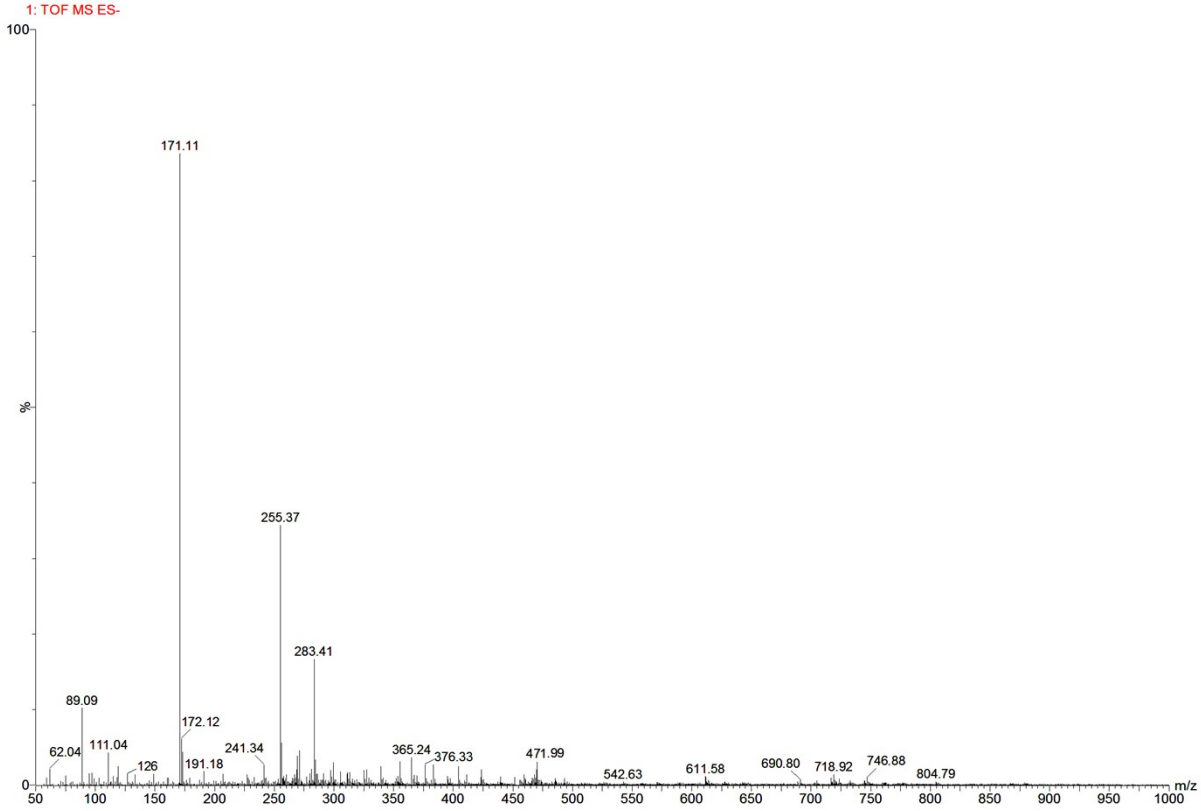

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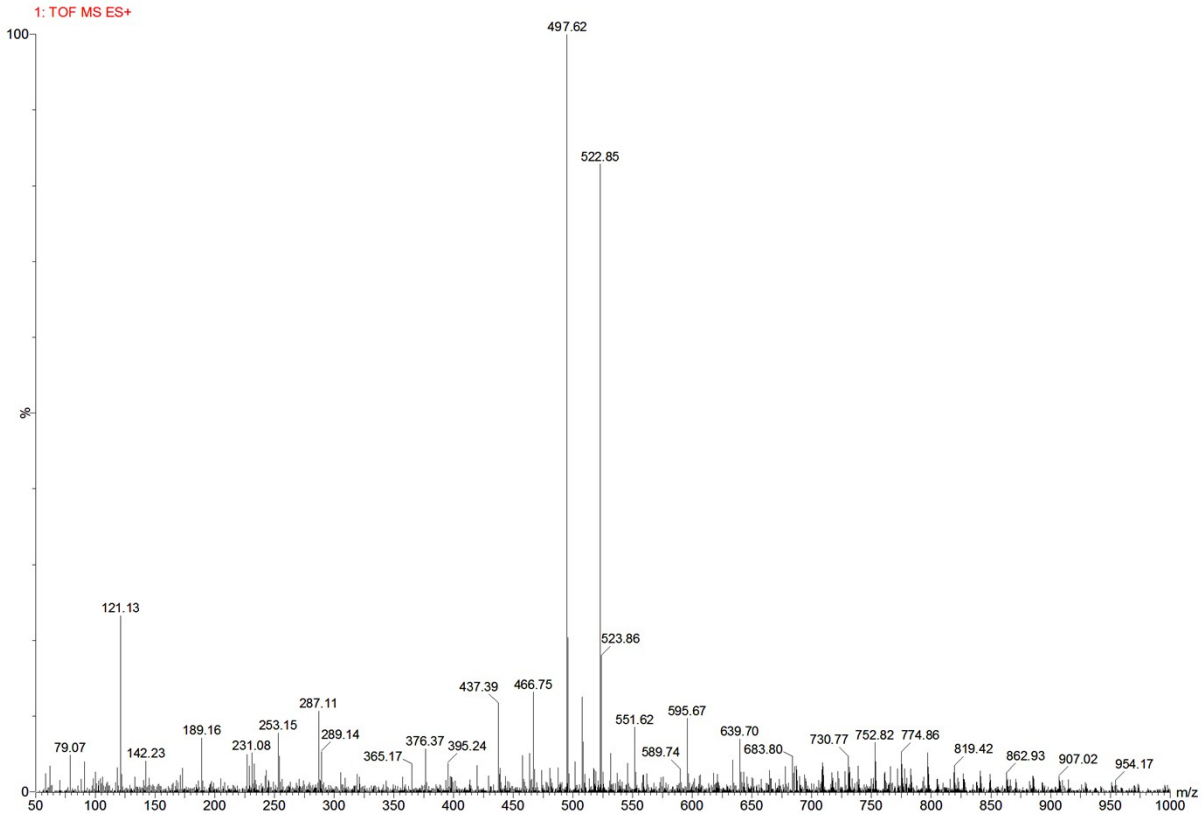

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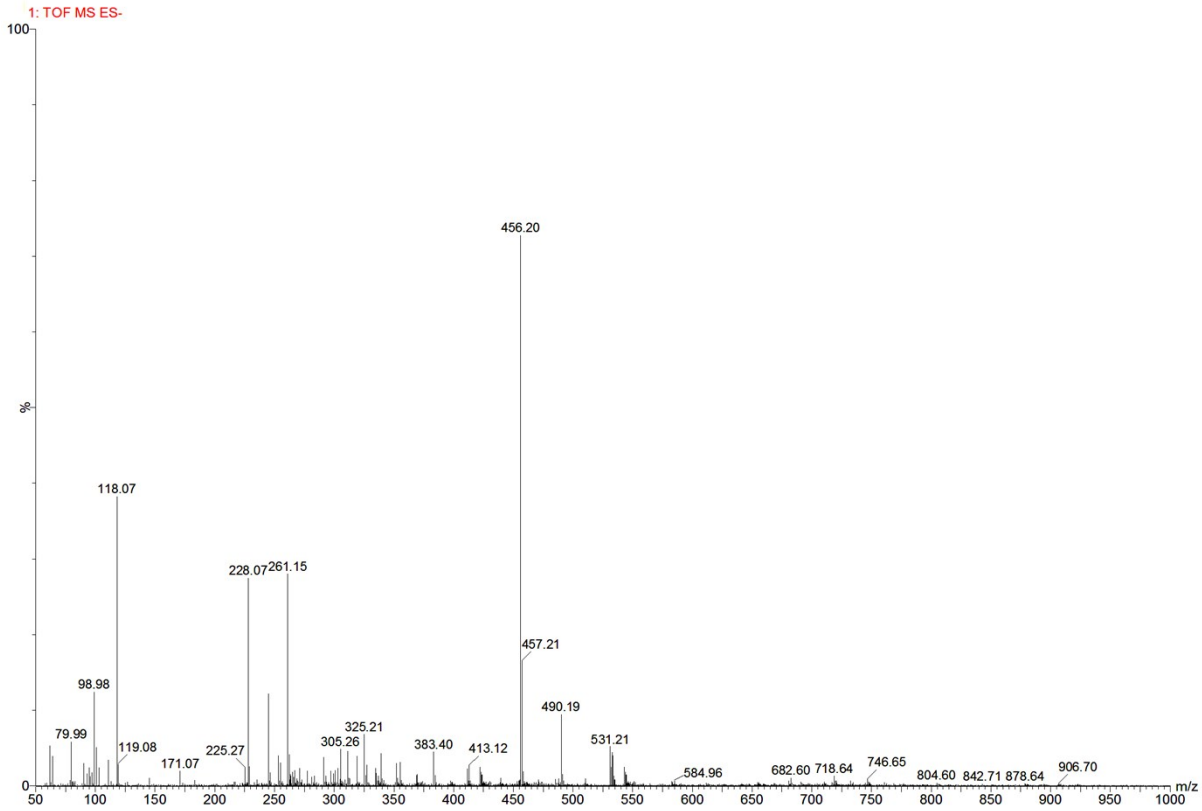

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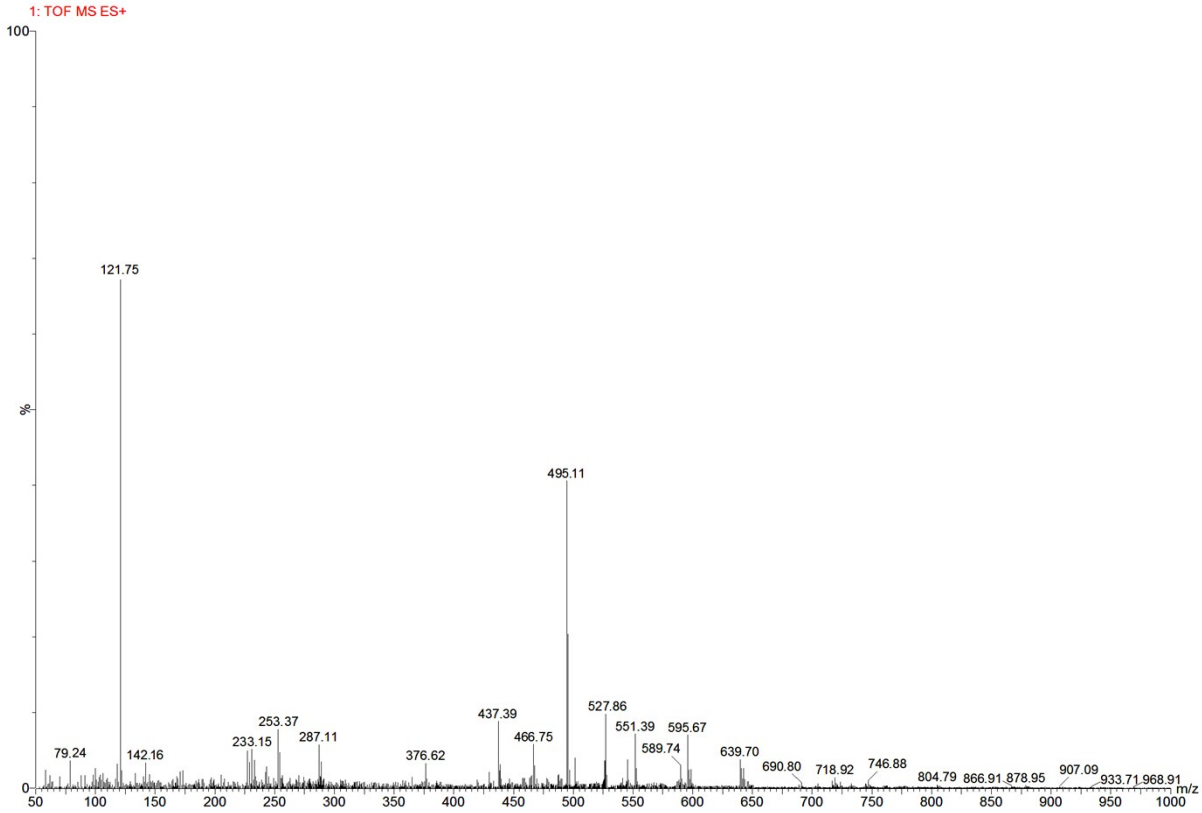

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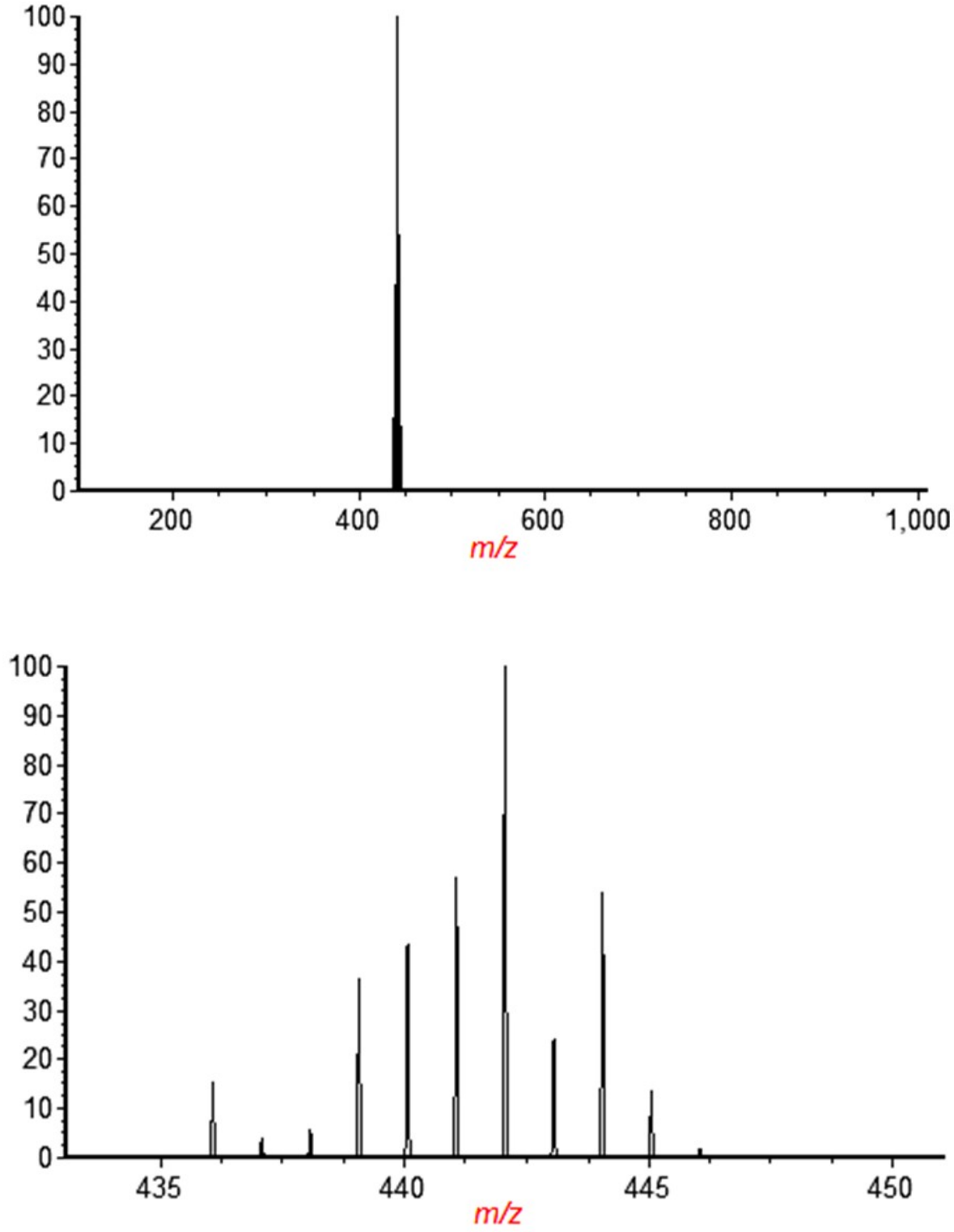

Figure S4: Theoretical Mass spectrum of [Ru(η^6-C_6H_6)(Cl)(L1)] (**1**)

Top: full spectrum, bottom: the theoretical isotopic patterns.

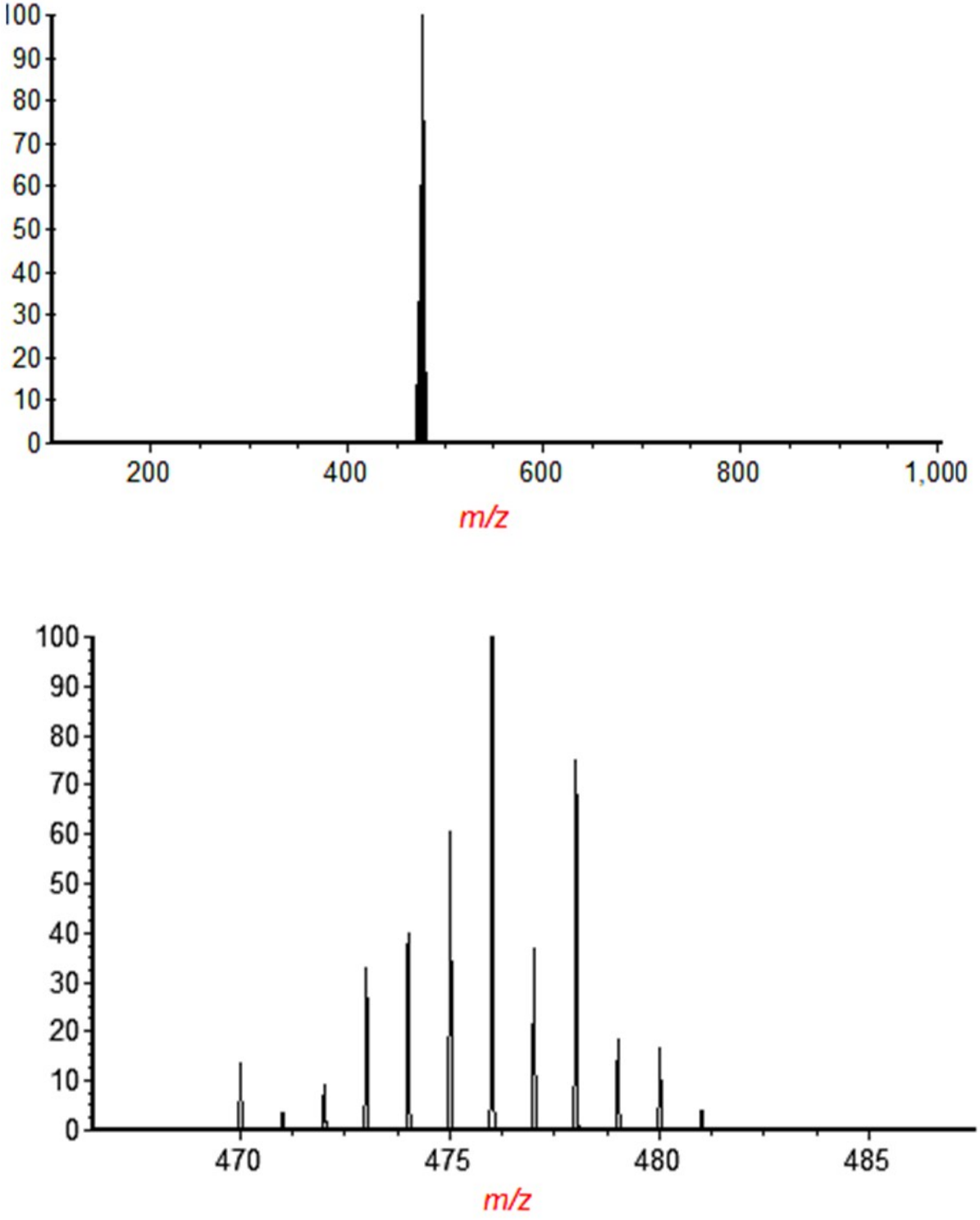

Figure S4: Theoretical Mass spectrum of [Ru(η^6-C_6H_6)(Cl)(L2)] (**2**)

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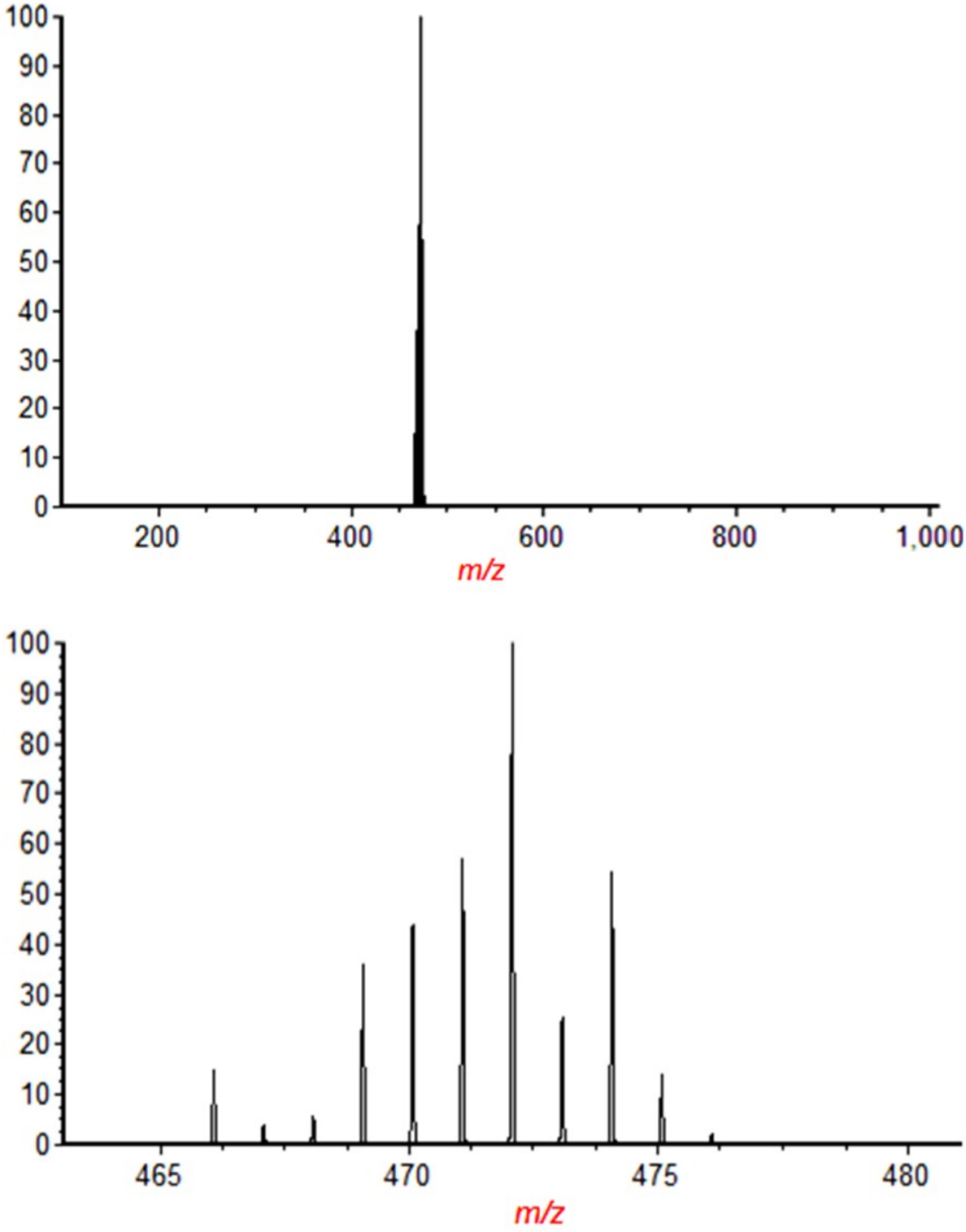

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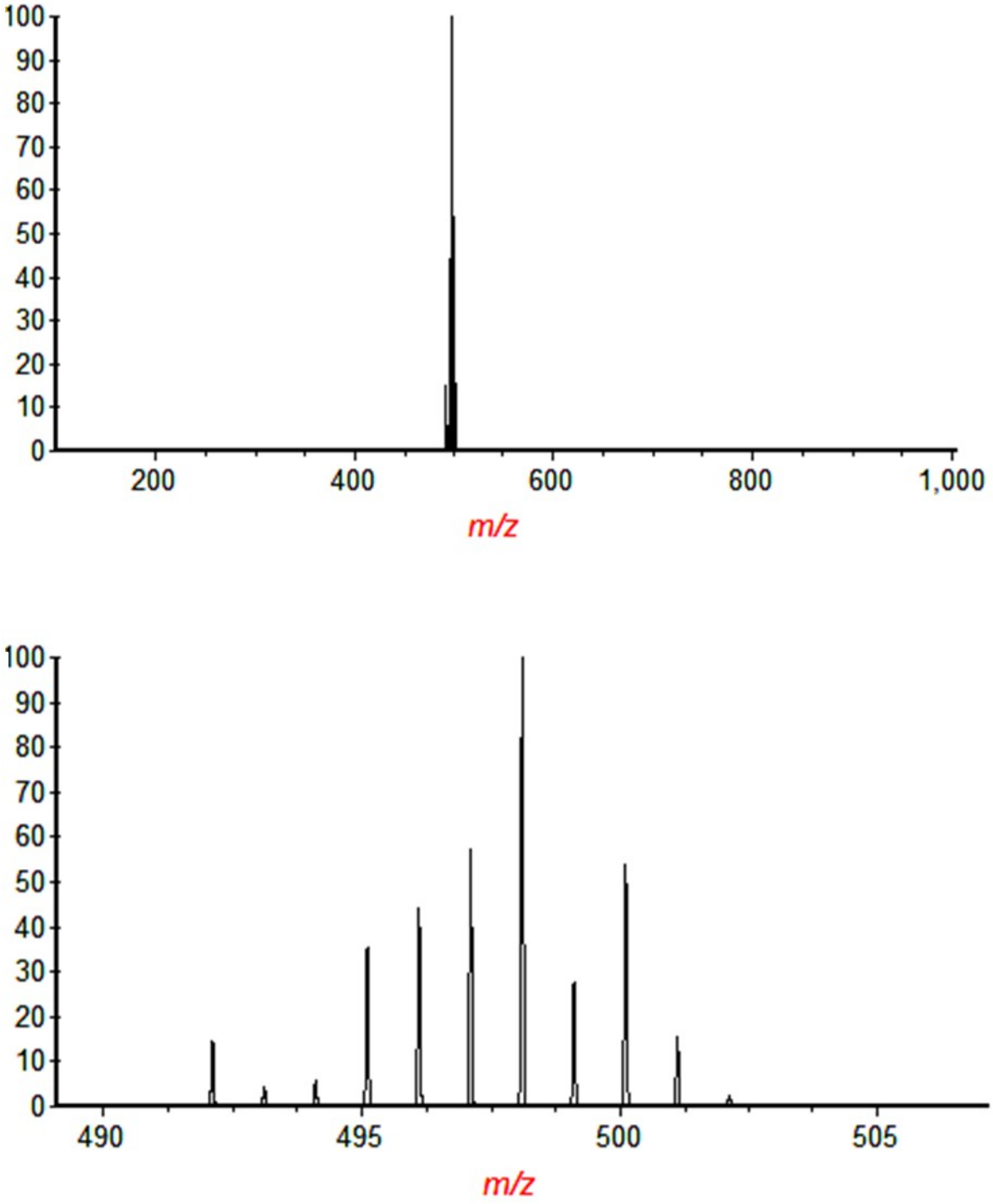

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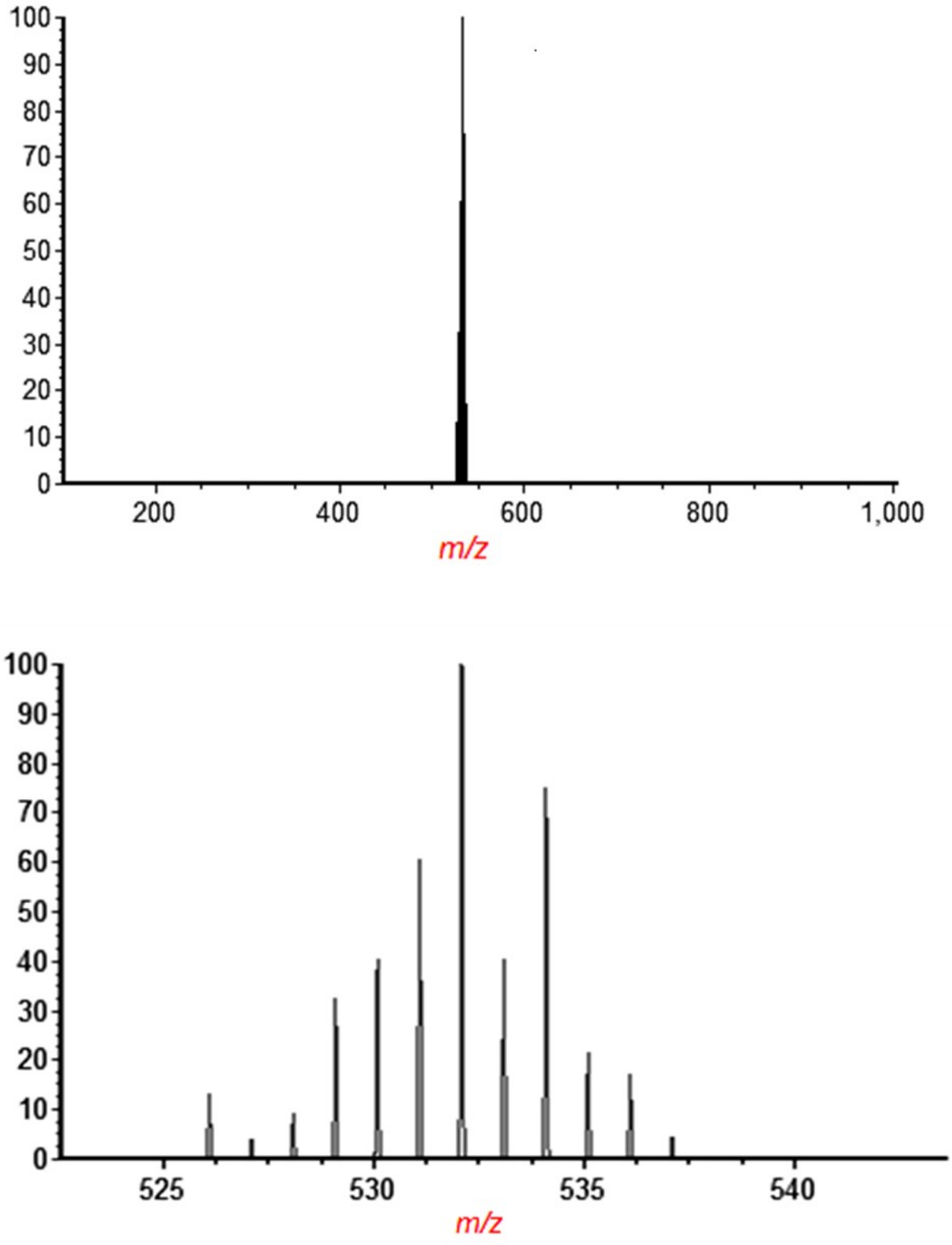

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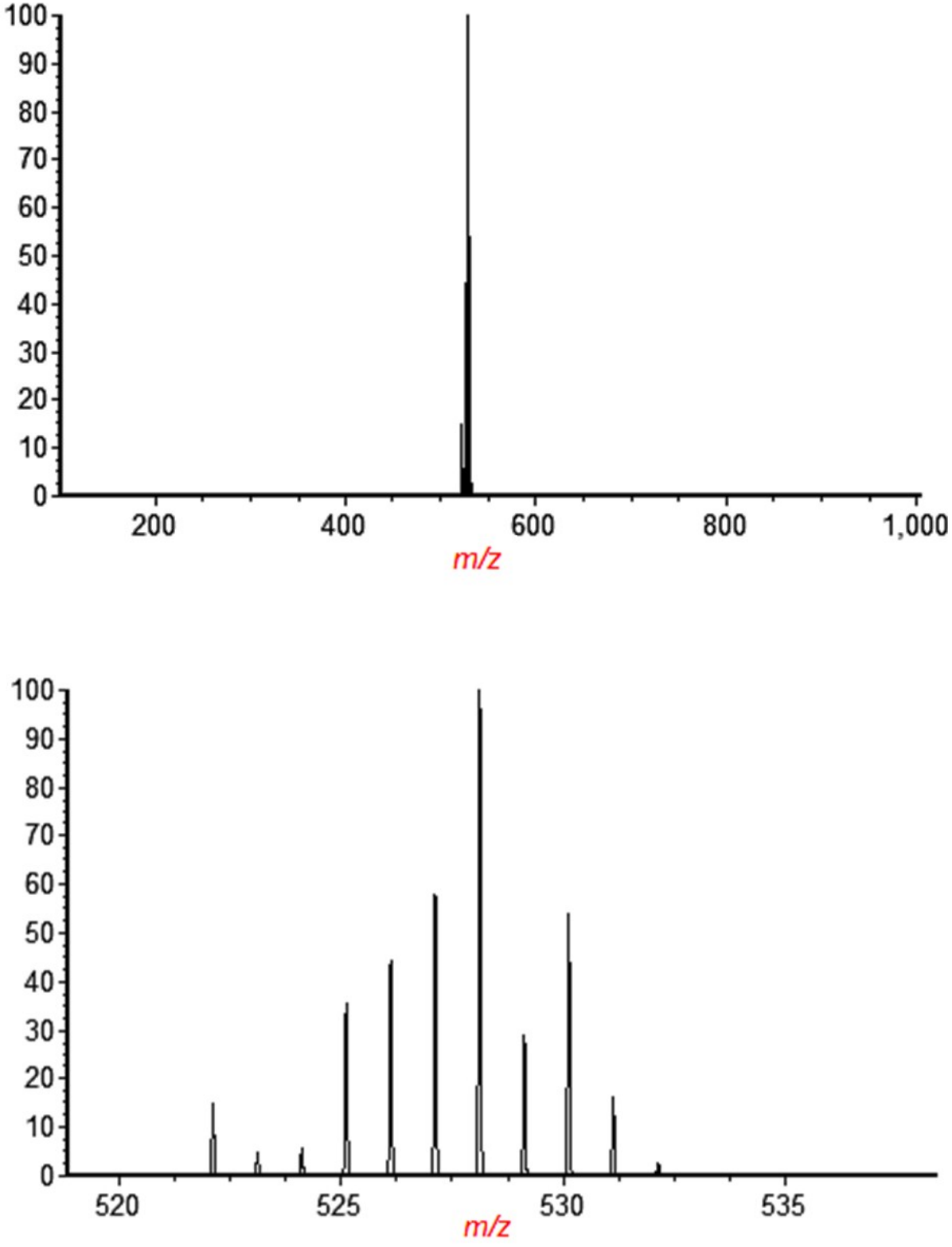

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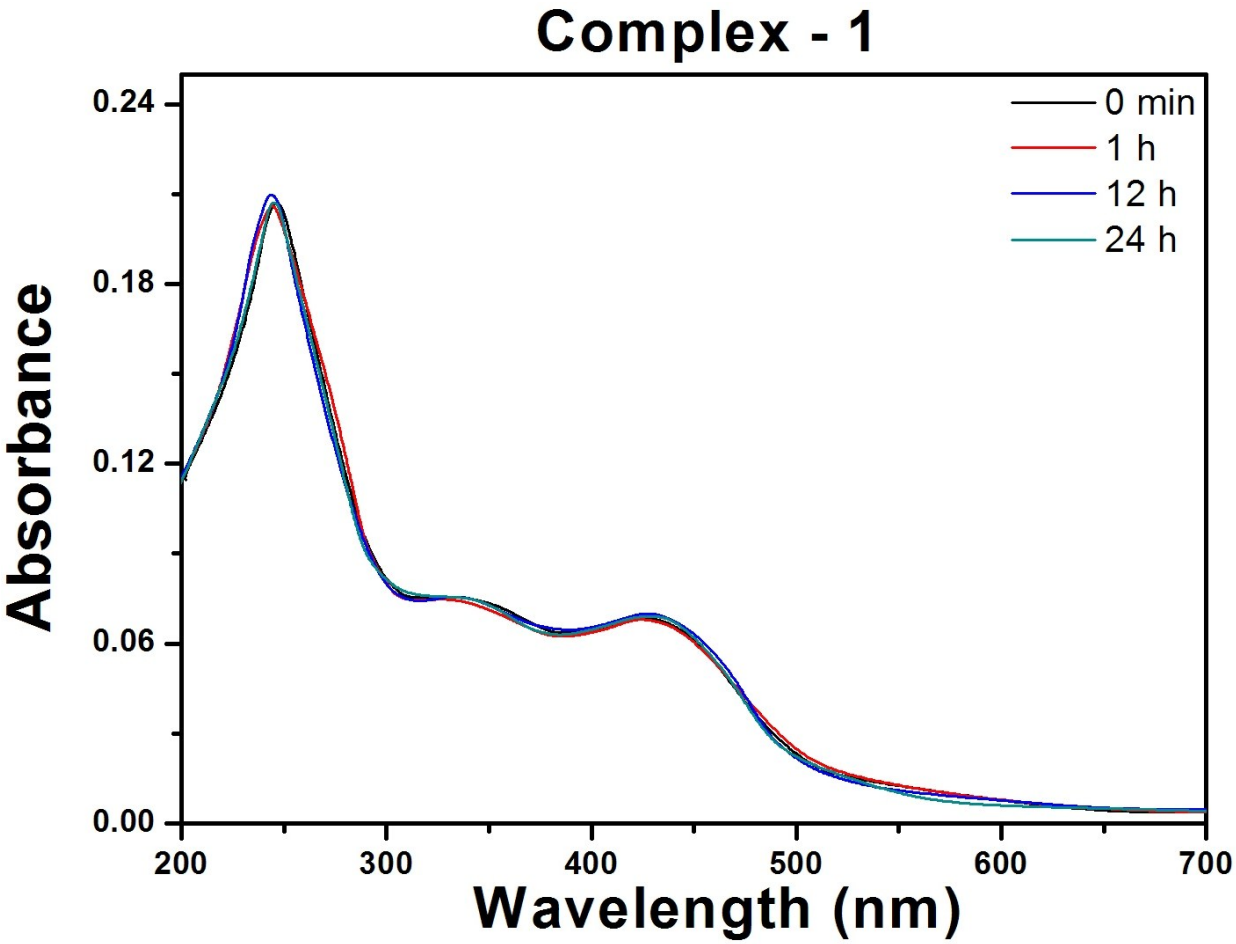
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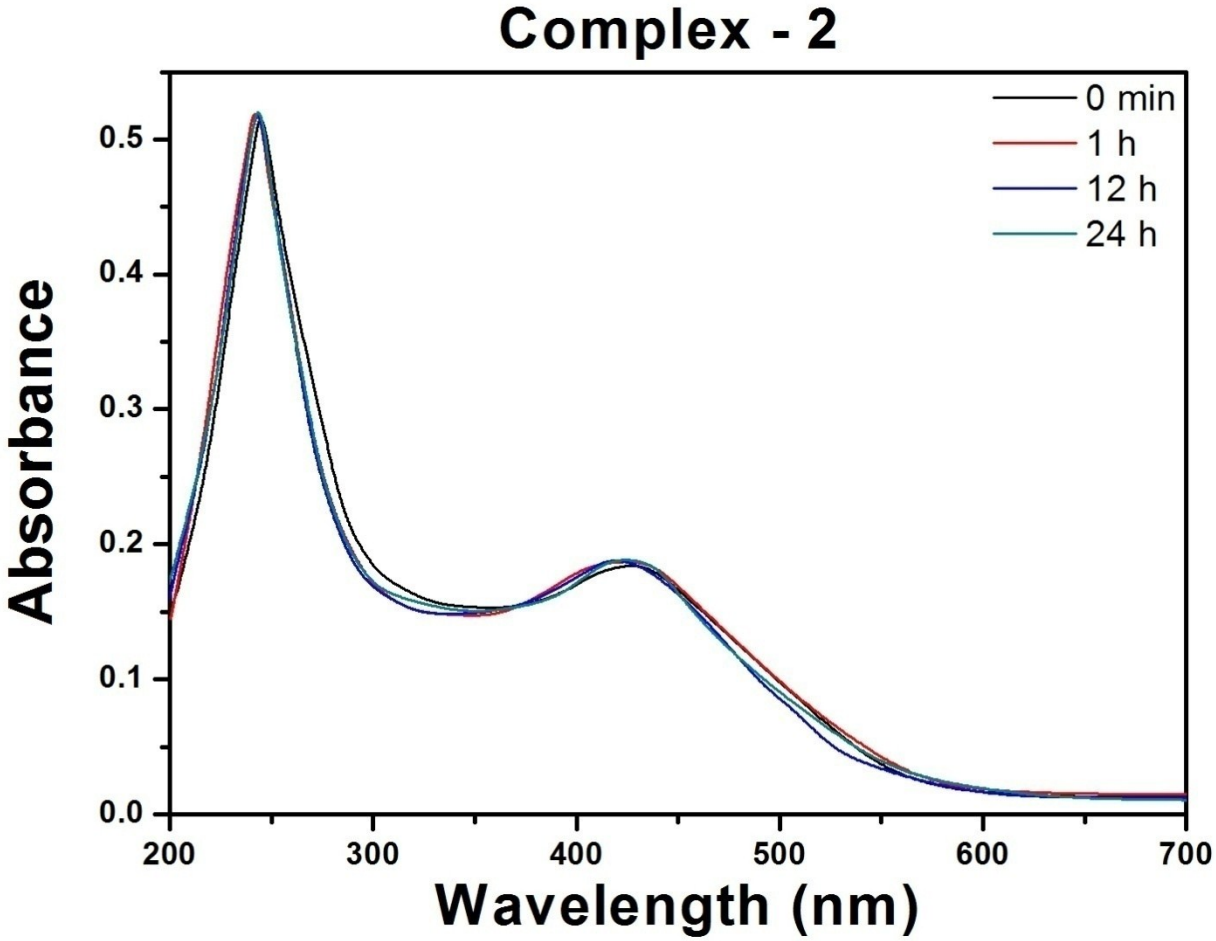
Wavelength (nm)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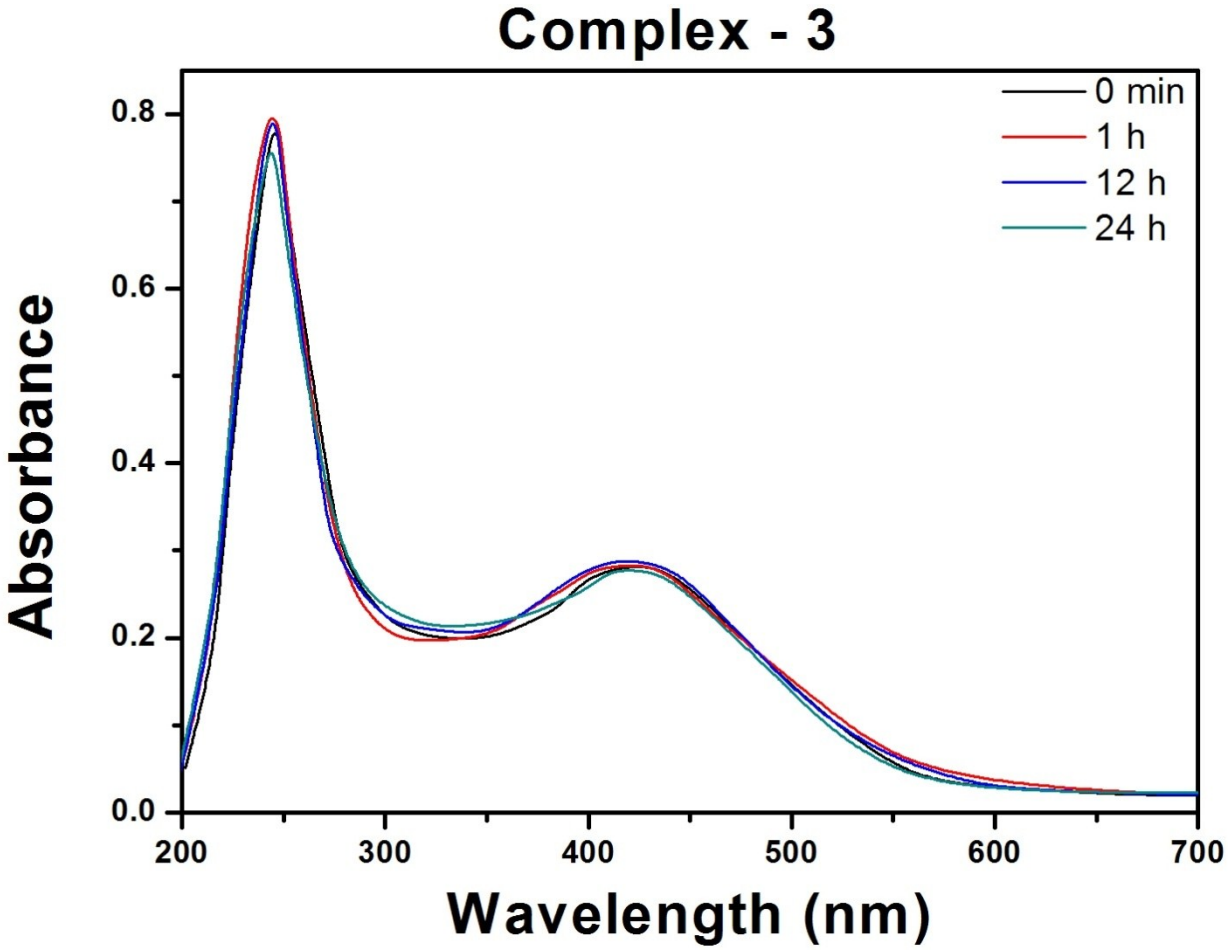
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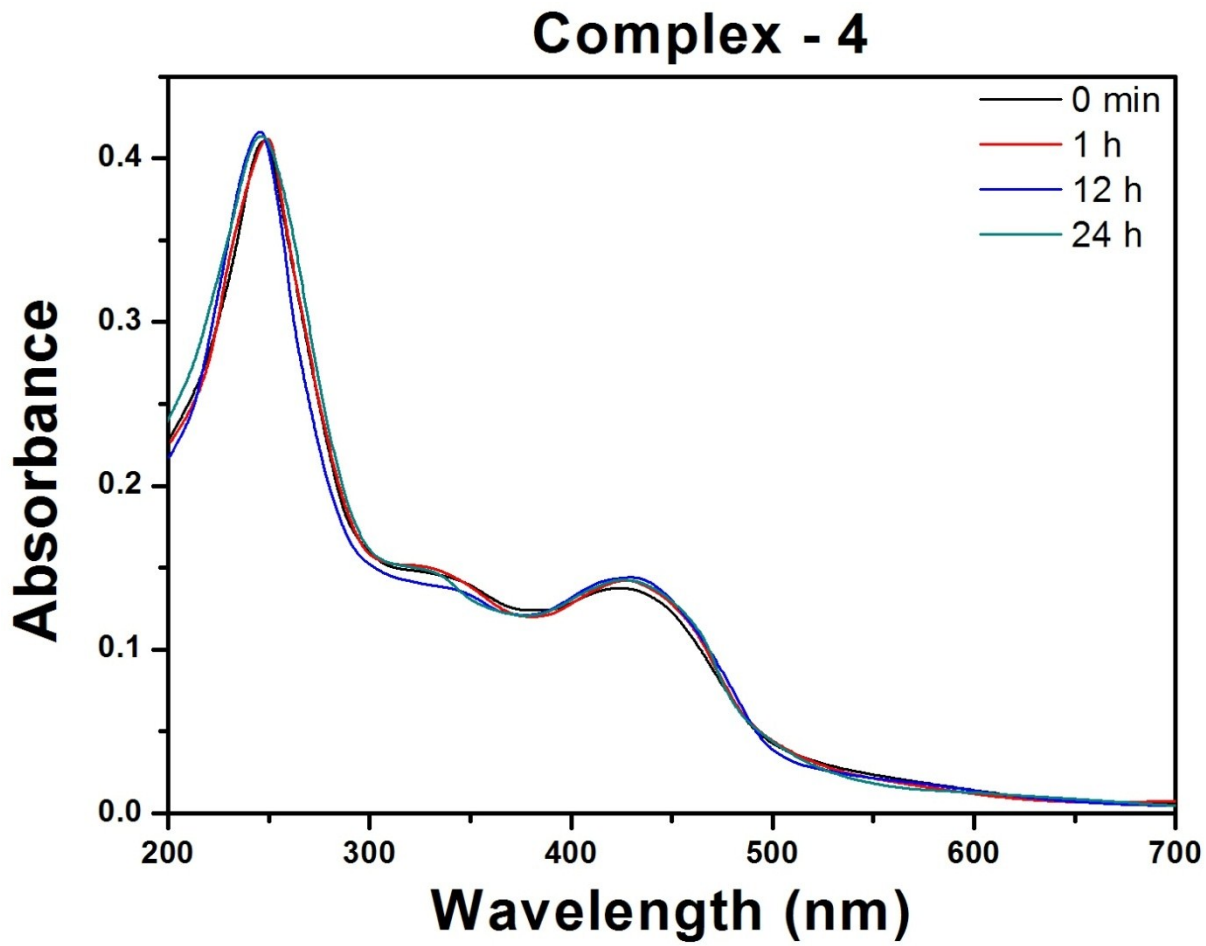
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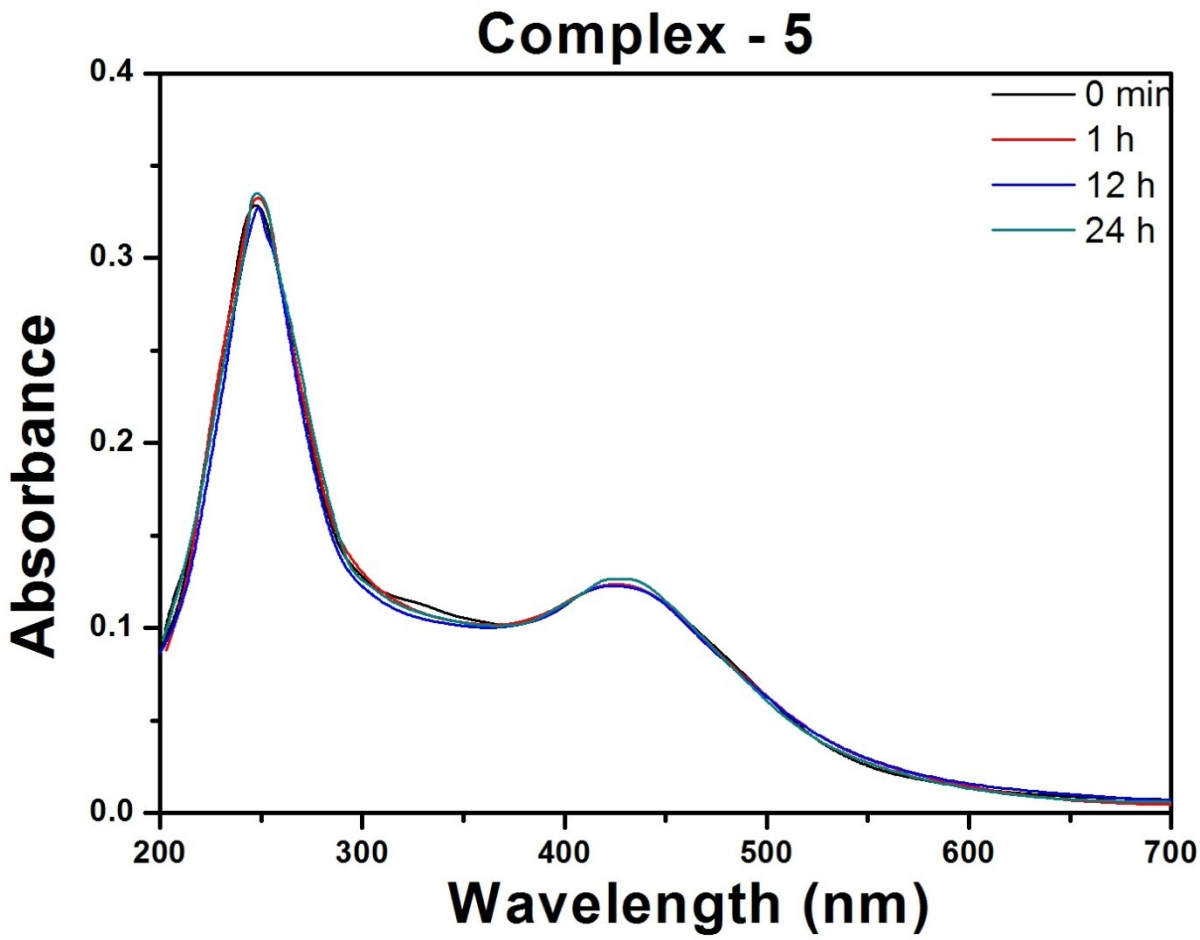
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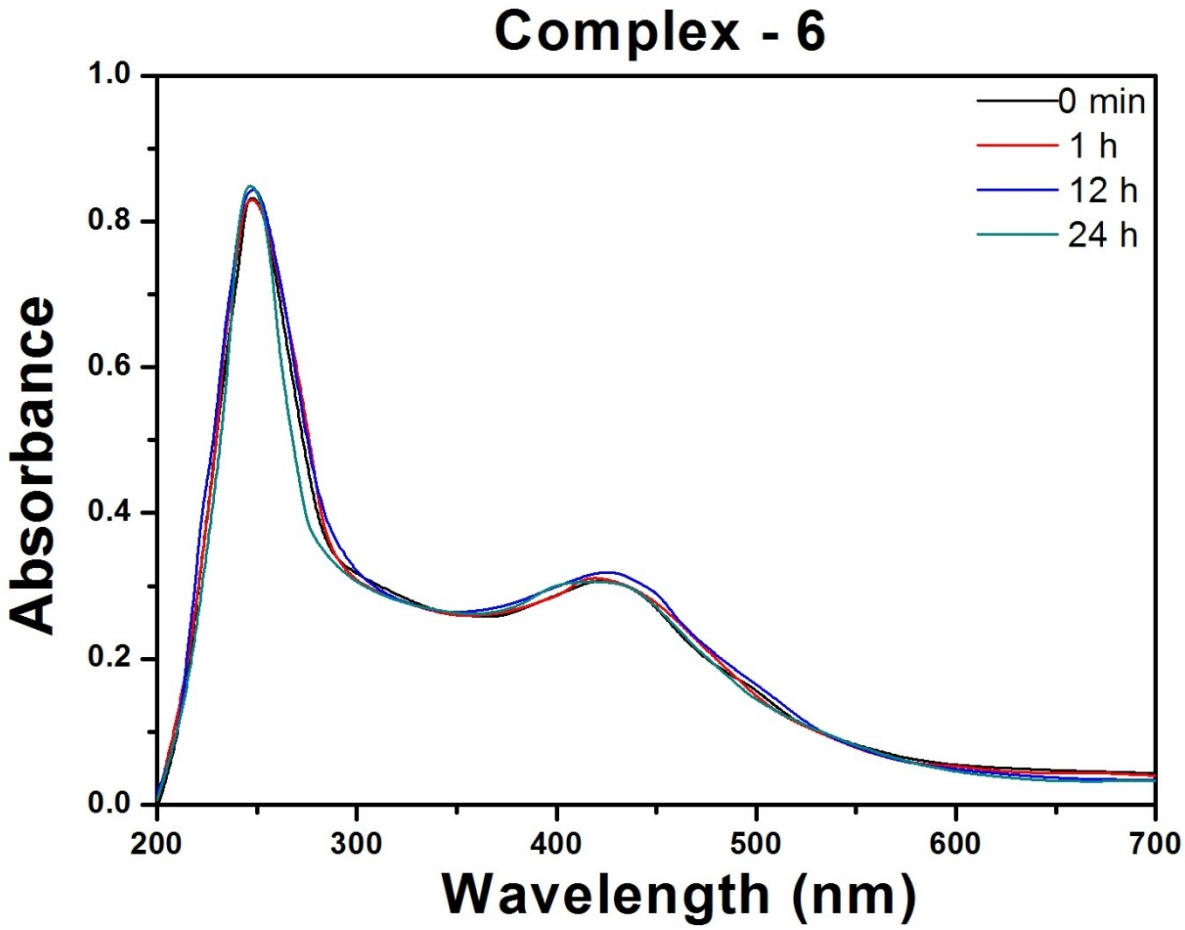

Figure S5. Stability studies UV spectrum of the complexes **1-6**

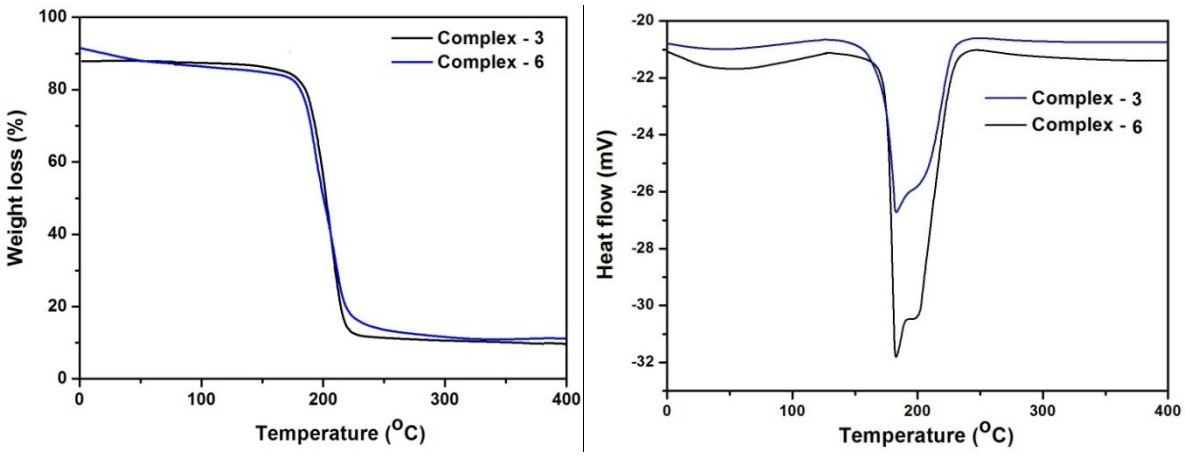

Figure S6: TGA and DTA curves of complexes **3** and **6**.

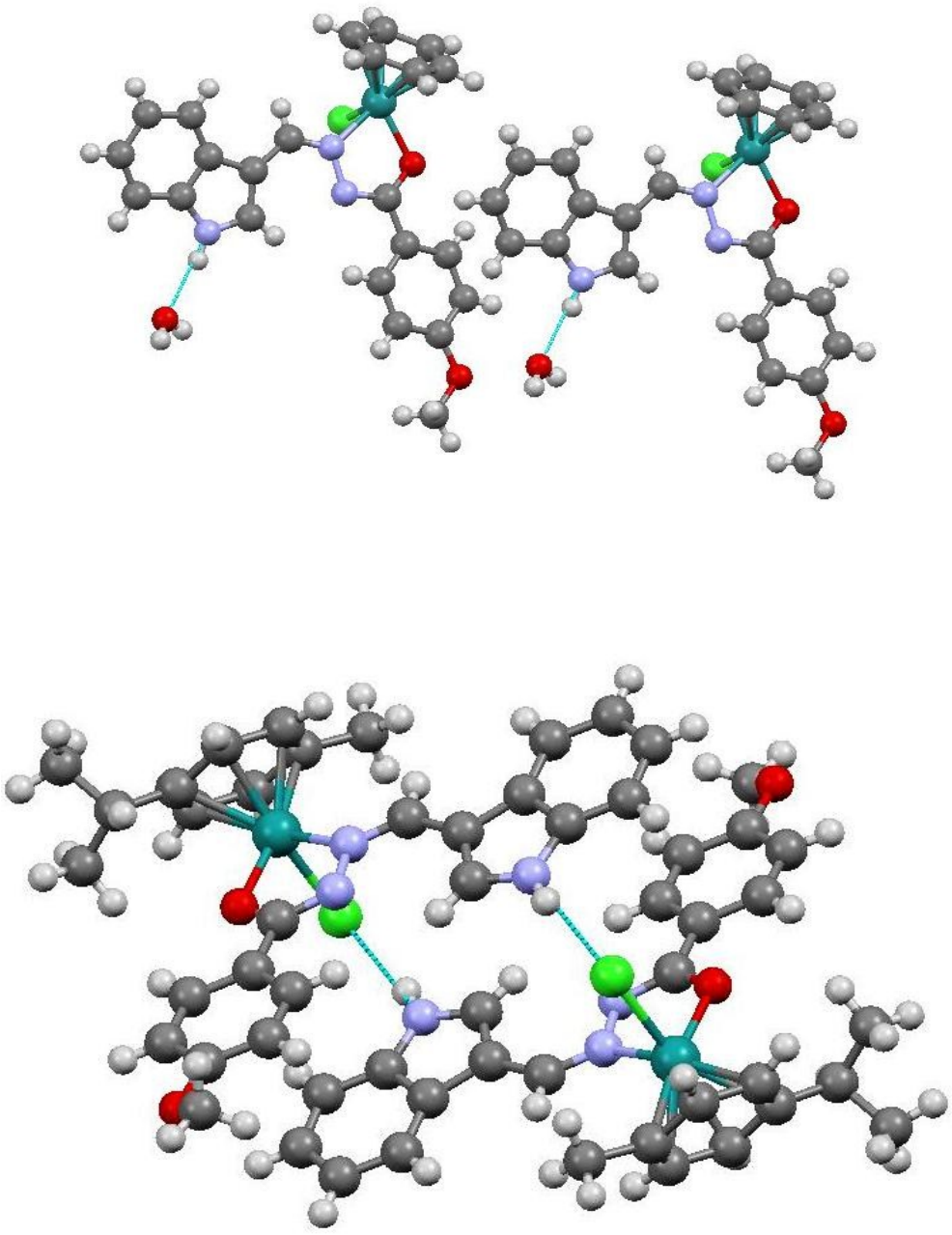

Figure S7. Intermolecular interaction of the complexes **3** and **6.**