Supporting information

PEG-Containing Ruthenium Phthalocyanines as Photosensitizers for Photodynamic Therapy: Synthesis, Characterization and *in vitro* Evaluation

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1. Characterization of Ruthenium(bisbenzonitrile)phthalocyanine ($Ru(PhCN)_2Pc$)

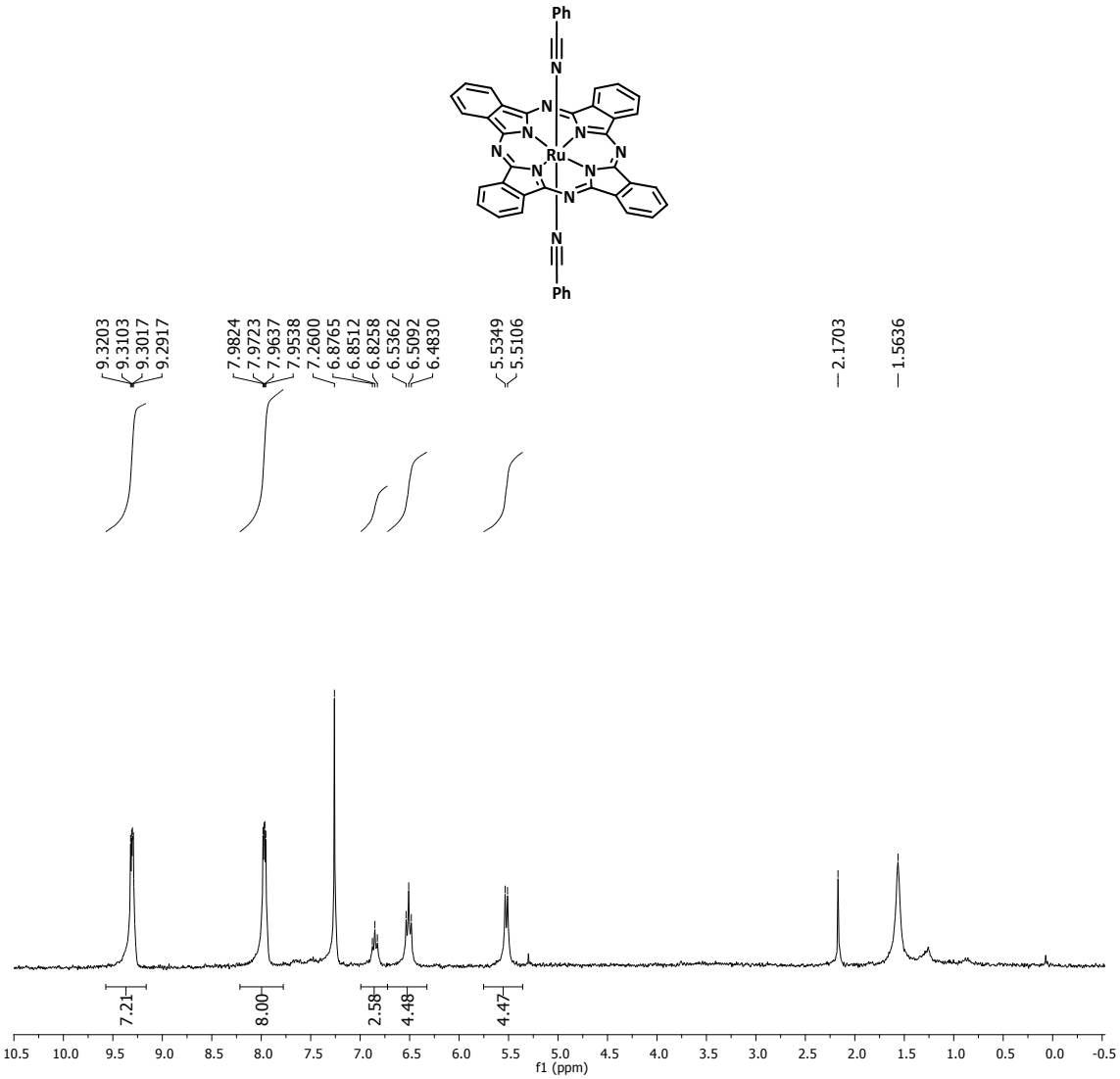


Figure S 1 – ^1H NMR spectrum of **$Ru(PhCN)_2Pc$** in $CDCl_3$.

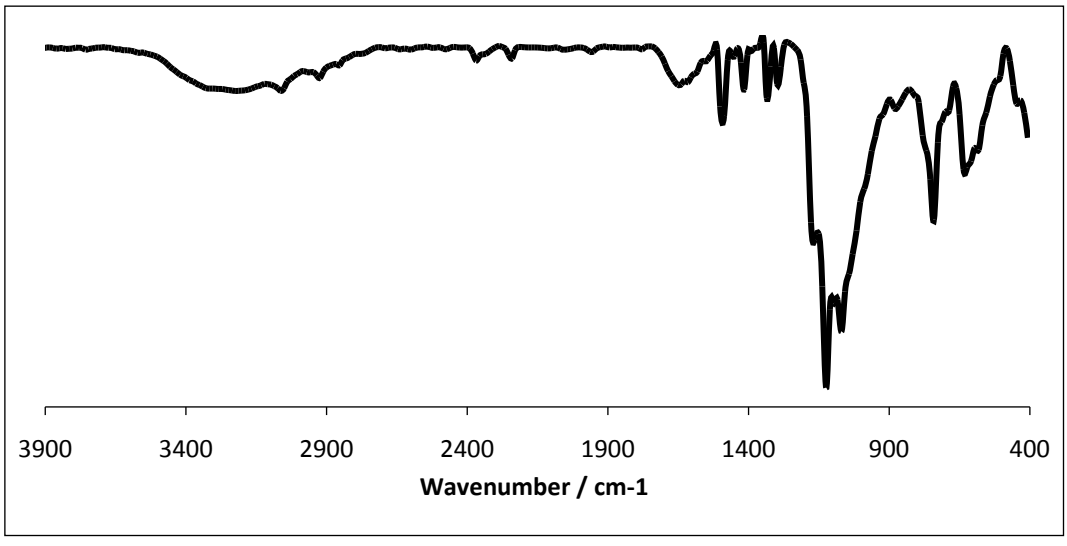


Figure S 2 – IR spectrum of **$Ru(PhCN)_2Pc$** in KBr**.**

2. Characterization of Pyridine-3,5-dicarboxylic acid bis-(2-[2-(hydroxy-ethoxy)-ethoxy]-ethyl) ester (L1).

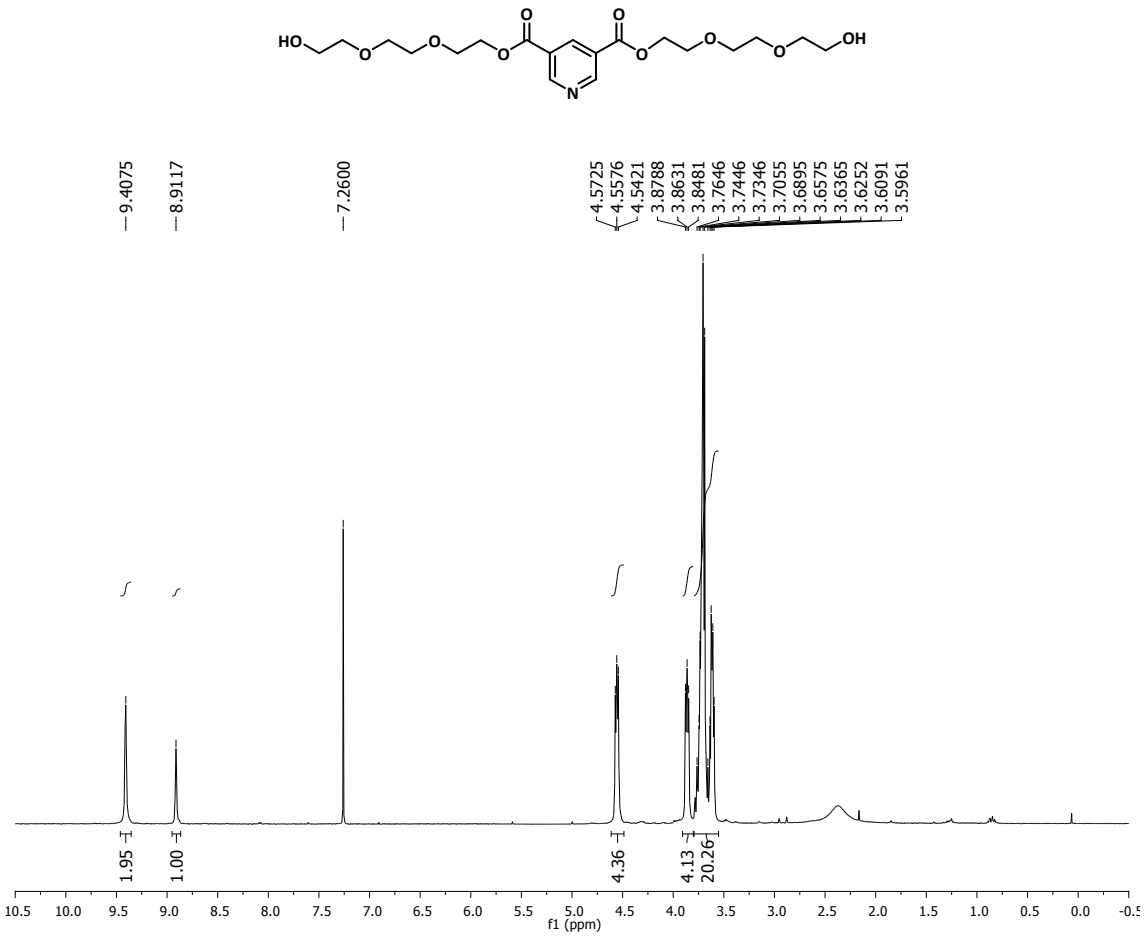


Figure S 3 - ^{1}H NMR spectrum of **L1** in $CDCl_3$.

3. Characterization of Pyridine-3,5-dicarboxylic acid bis-(2-[2-(dimethylamine)-ethoxy]-ethyl) ester (L2).

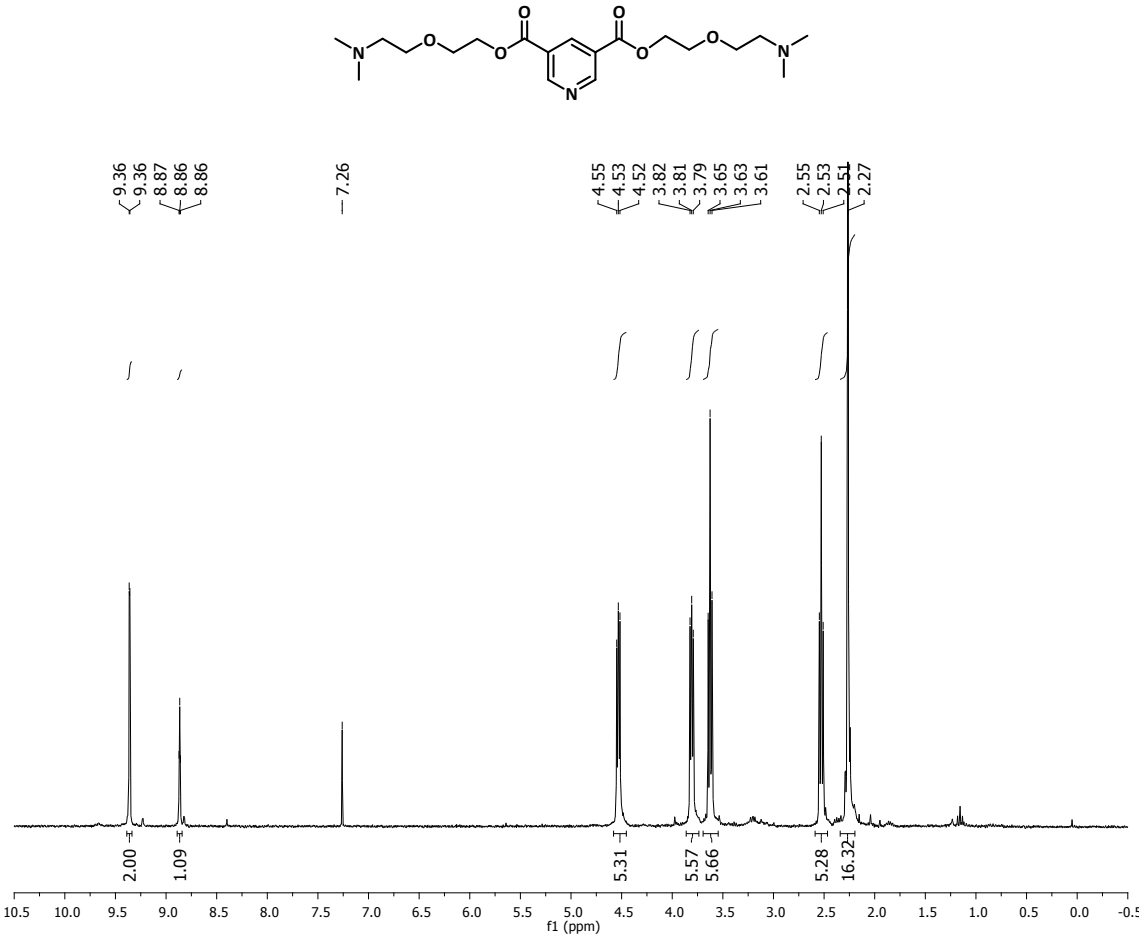


Figure S 4 – ^{1}H NMR spectrum of **L2** in $CDCl_3$.

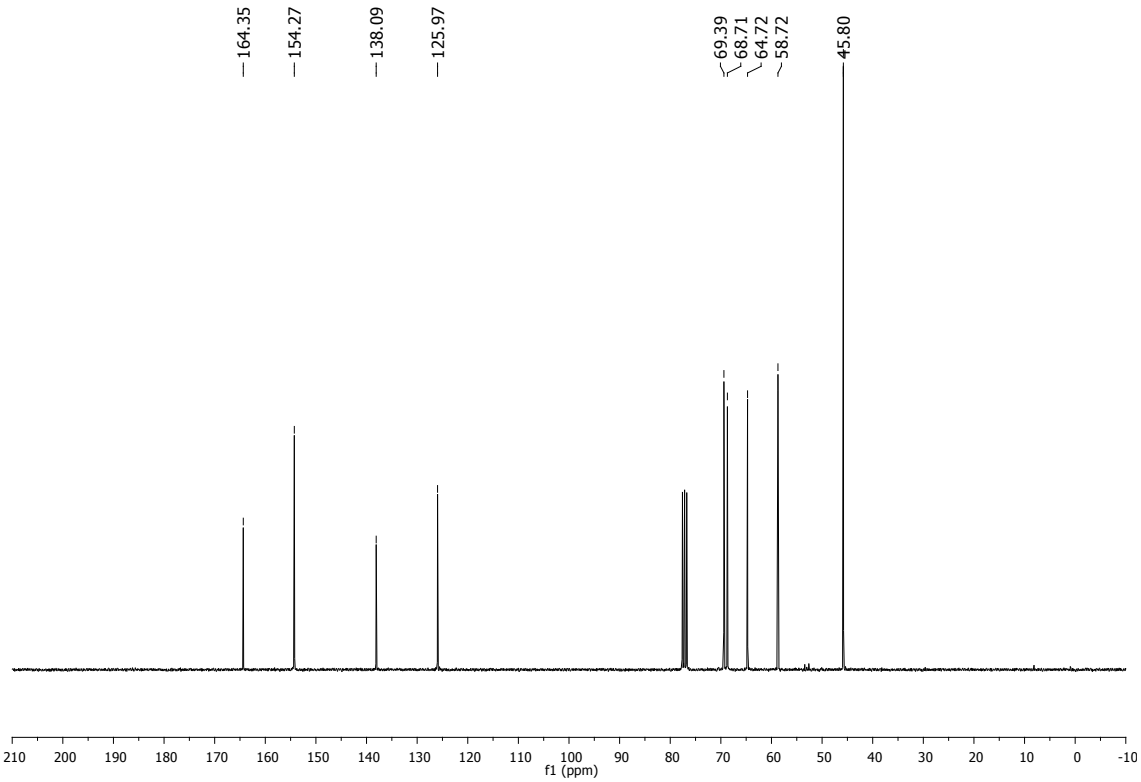


Figure S 5 – ^{13}C NMR spectrum of **L2** in $CDCl_3$.

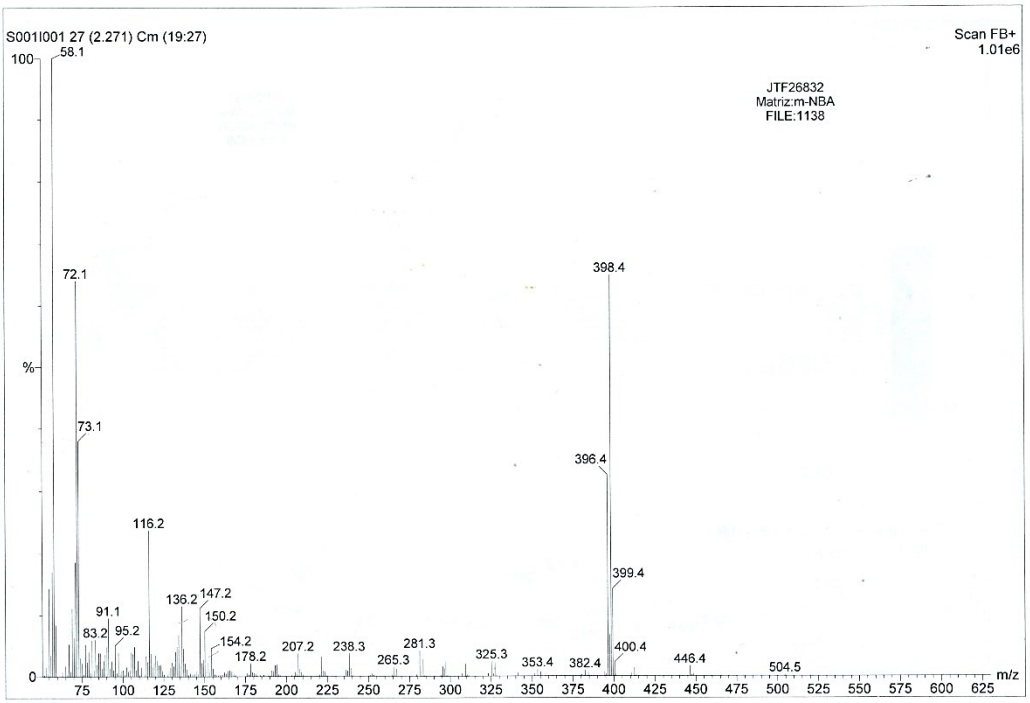


Figure S 6 - MS (FAB, *m*-NBA) spectrum of **L2.**

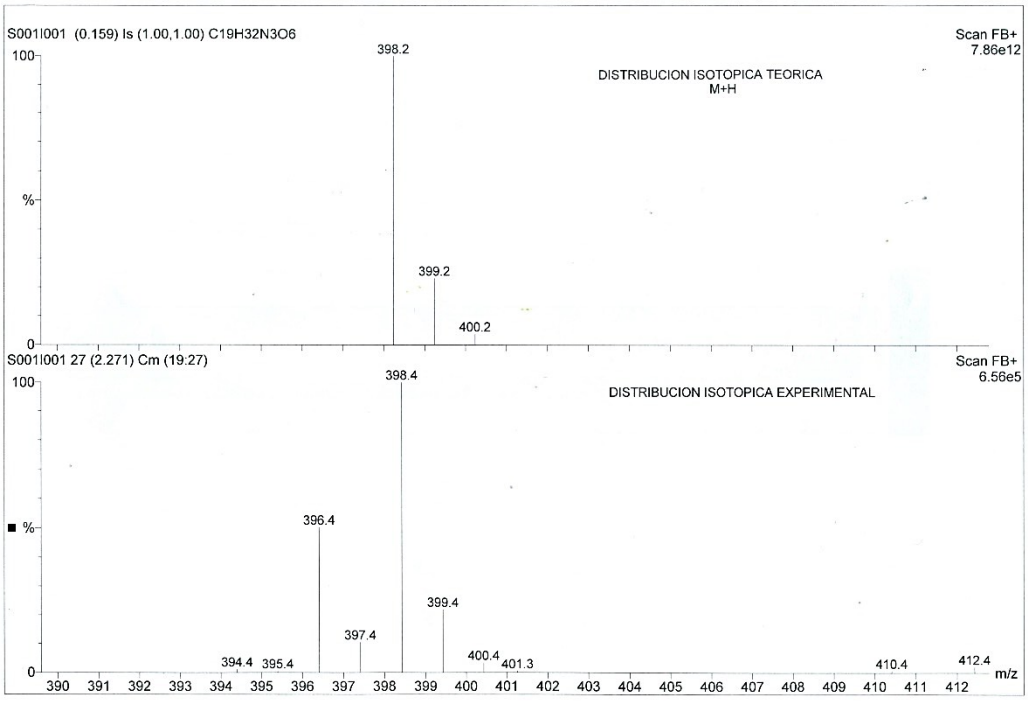


Figure S 7 – MS (FAB, *m*-NBA) spectrum of **L2**; predicted isotopic pattern (top) and experimental isotopic pattern (botton).

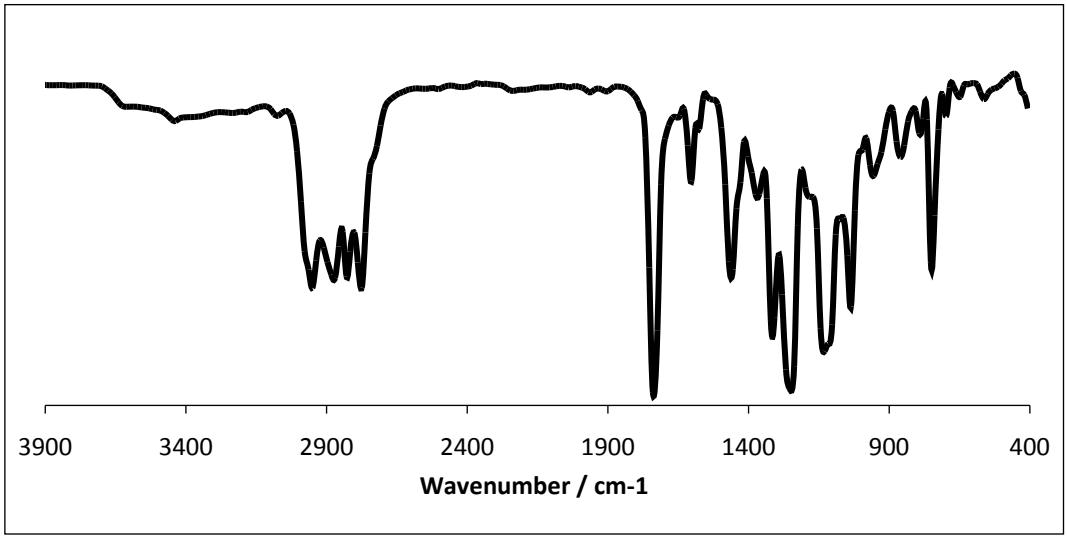


Figure S 8 – IR spectrum of **L2.**

4. Characterization of Bis(3,4,5-tris(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)benzyl) pyridine-3,5-dicarboxylate (L3).

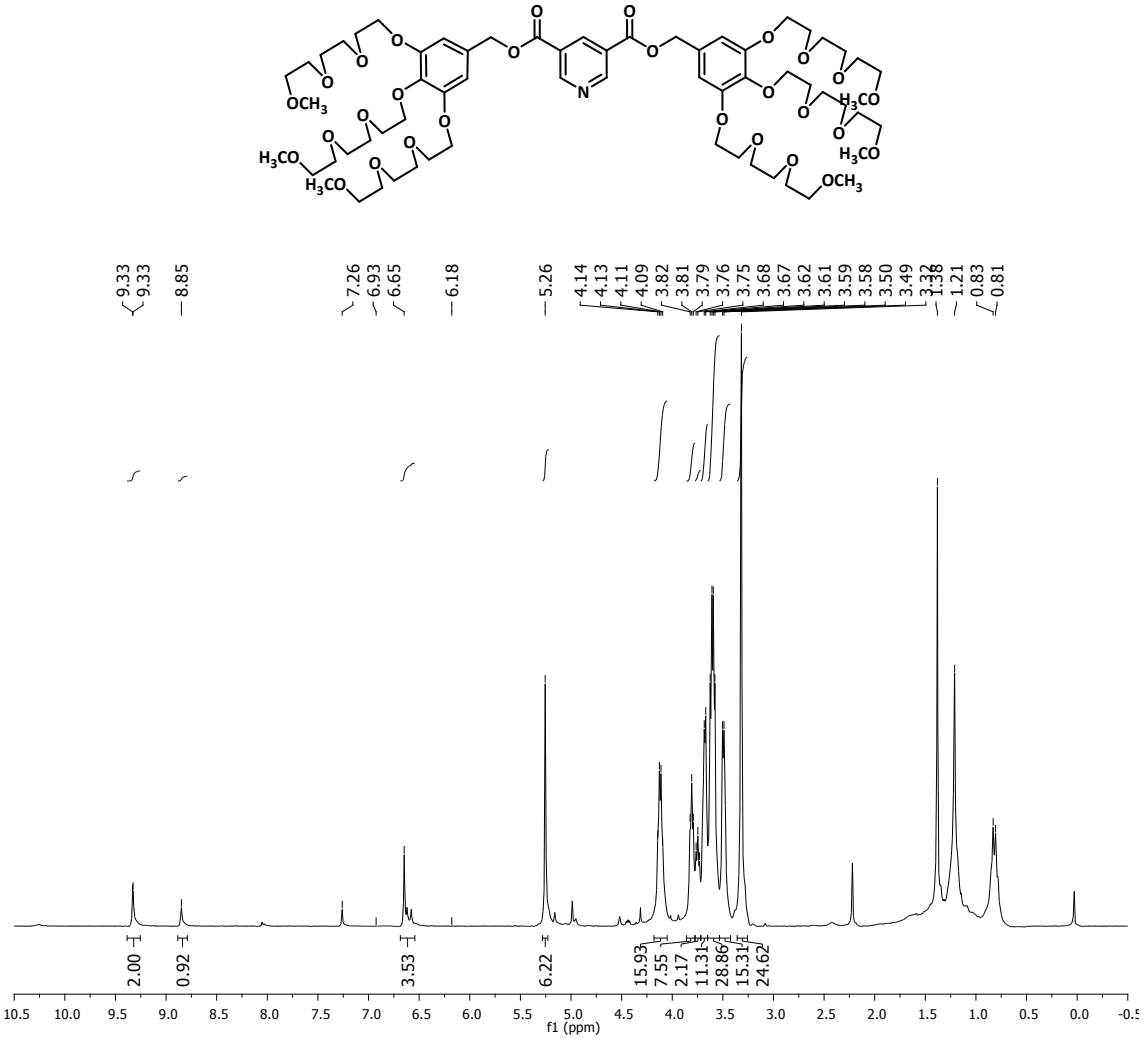


Figure S 9 – ^{1}H NMR spectrum of **L3** in $CDCl_3$.

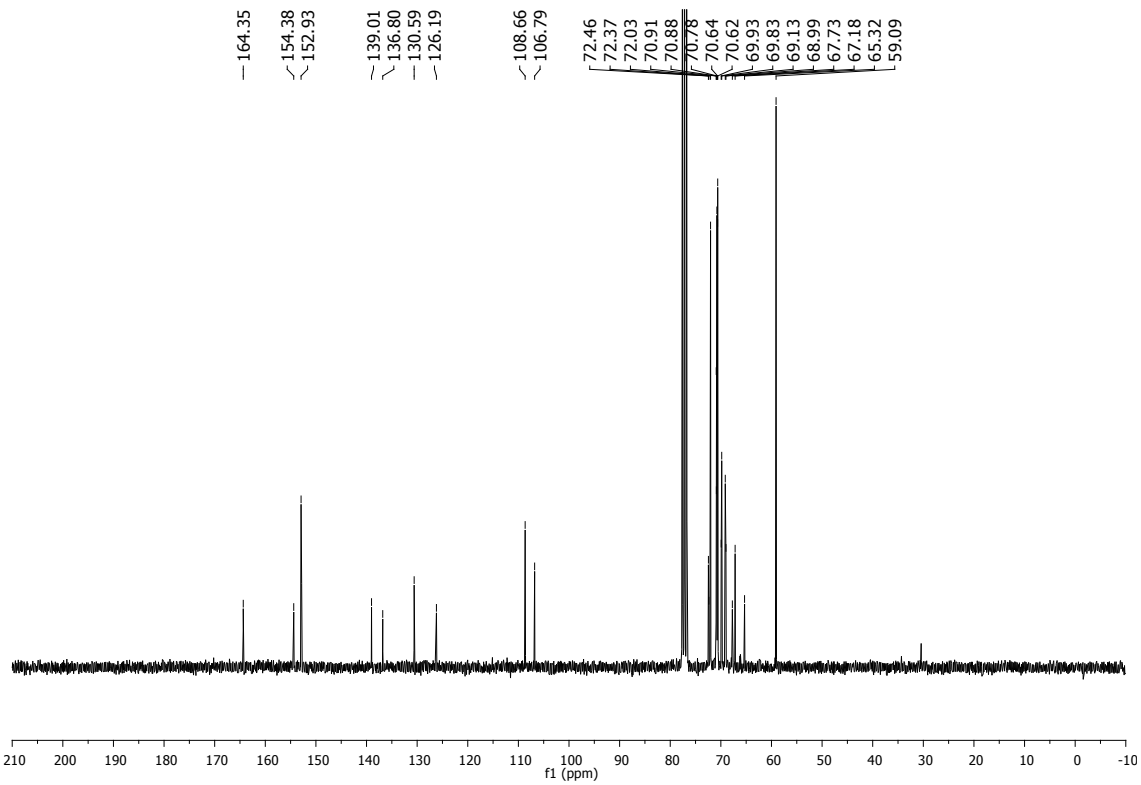


Figure S 10 – ^{13}C NMR spectrum of **L3** in $CDCl_3$.

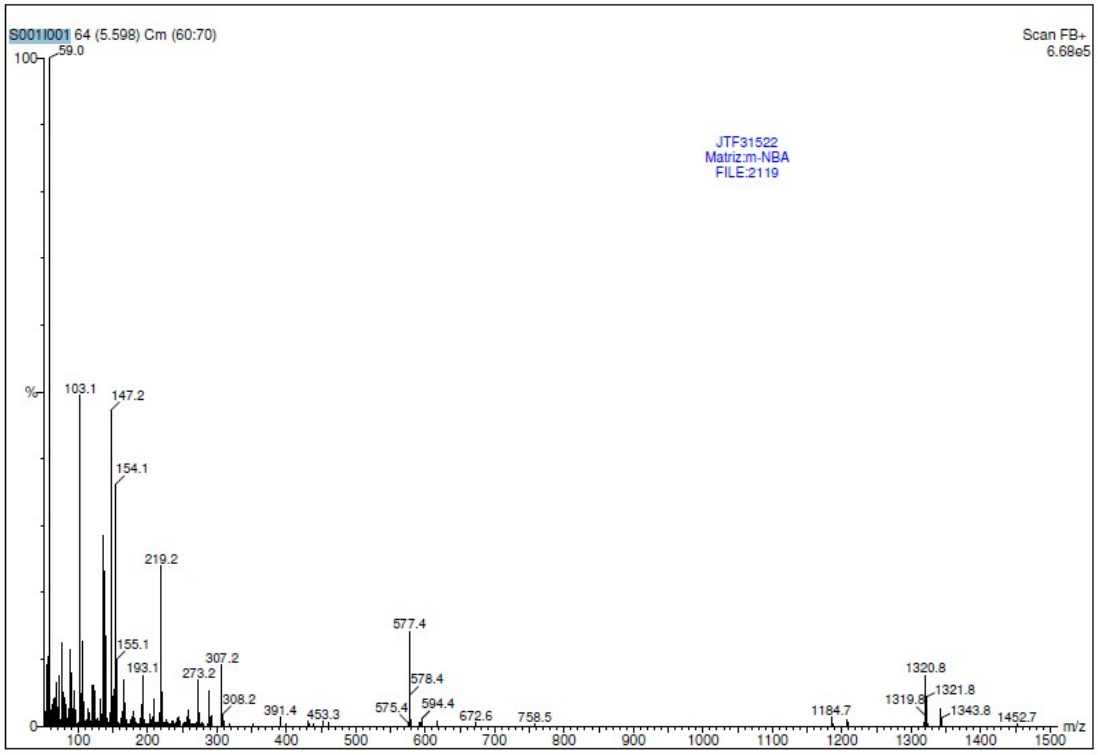


Figure S 11 – MS (FAB$^+$, *m*-NBA) spectrum of **L3.**

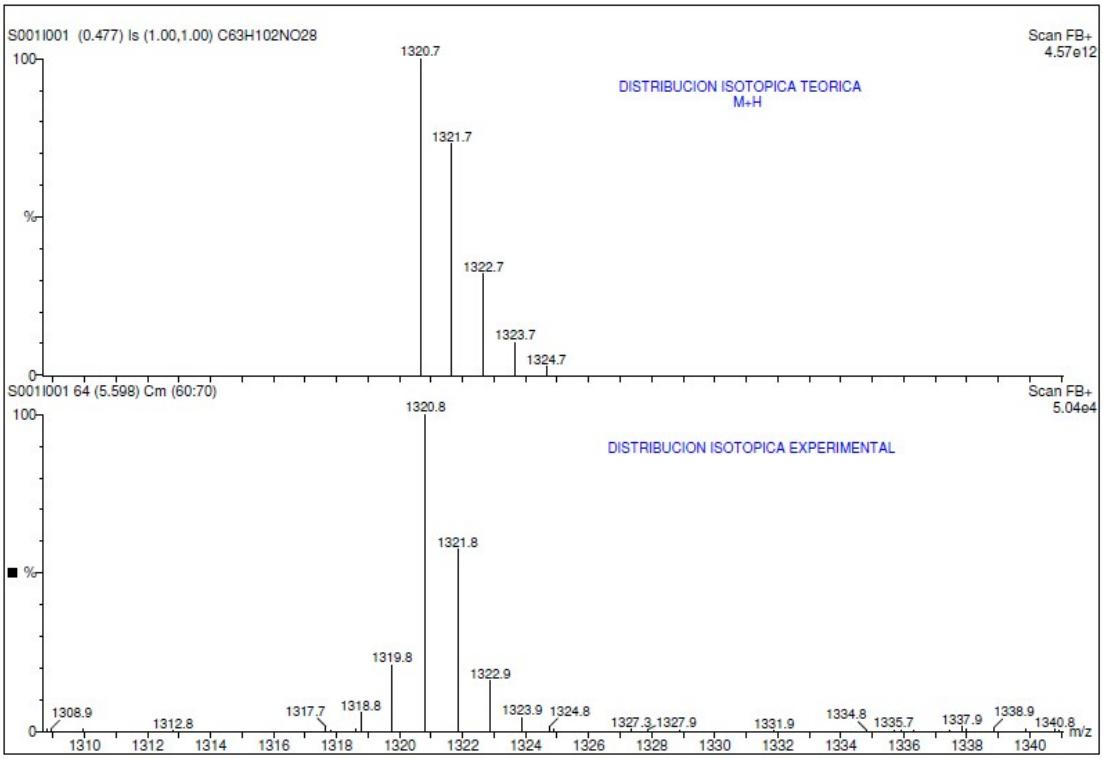


Figure S 12 - MS (FAB$^+$, *m*-NBA) spectrum of **L3**; predicted isotopic pattern (top) and experimental isotopic pattern (botton).

5. Characterization of $Ru(L1)_2Pc$

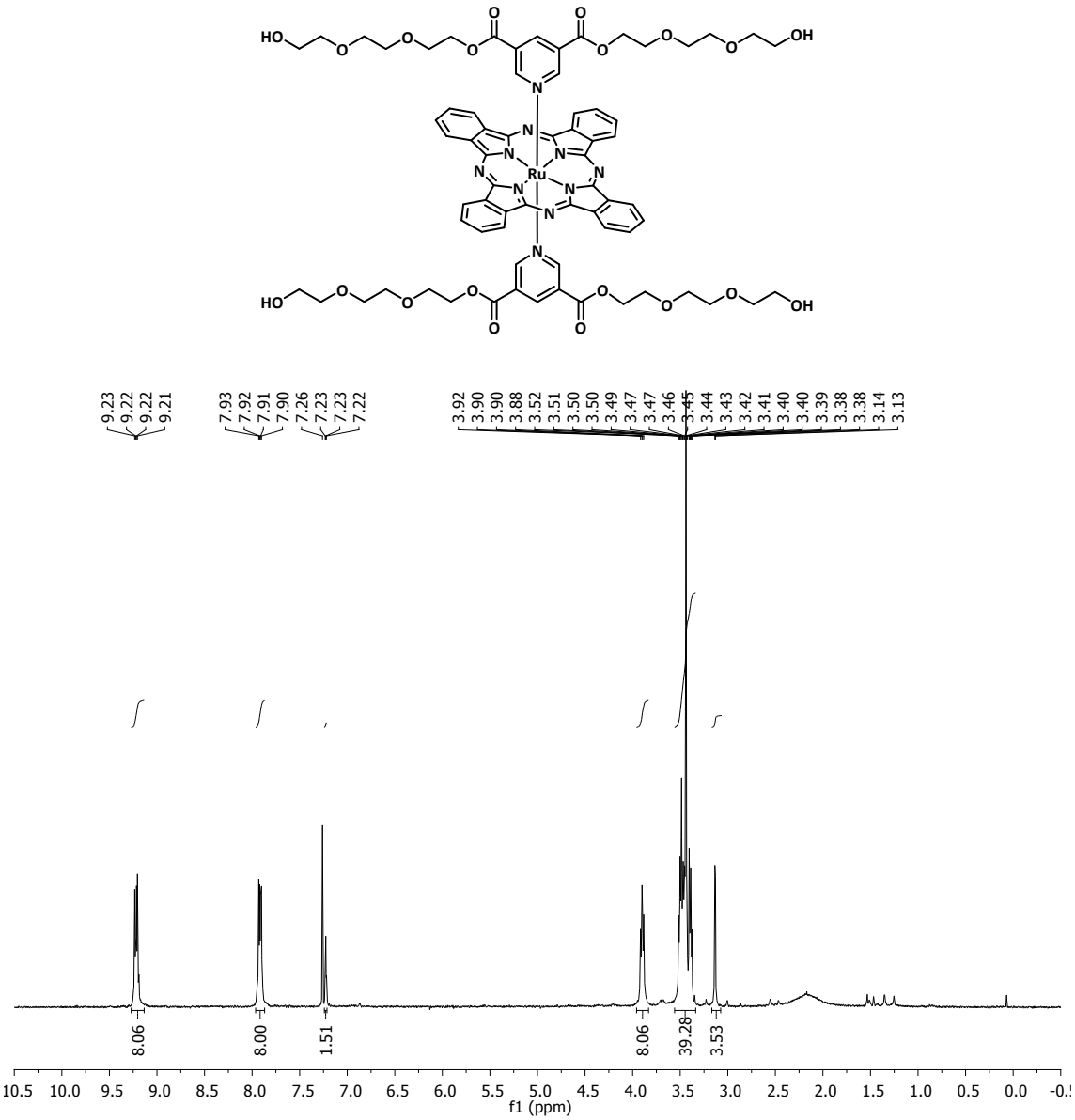


Figure S 13 - ^{1}H NMR spectrum of **$Ru(L1)_2Pc$** in $CDCl_3$.

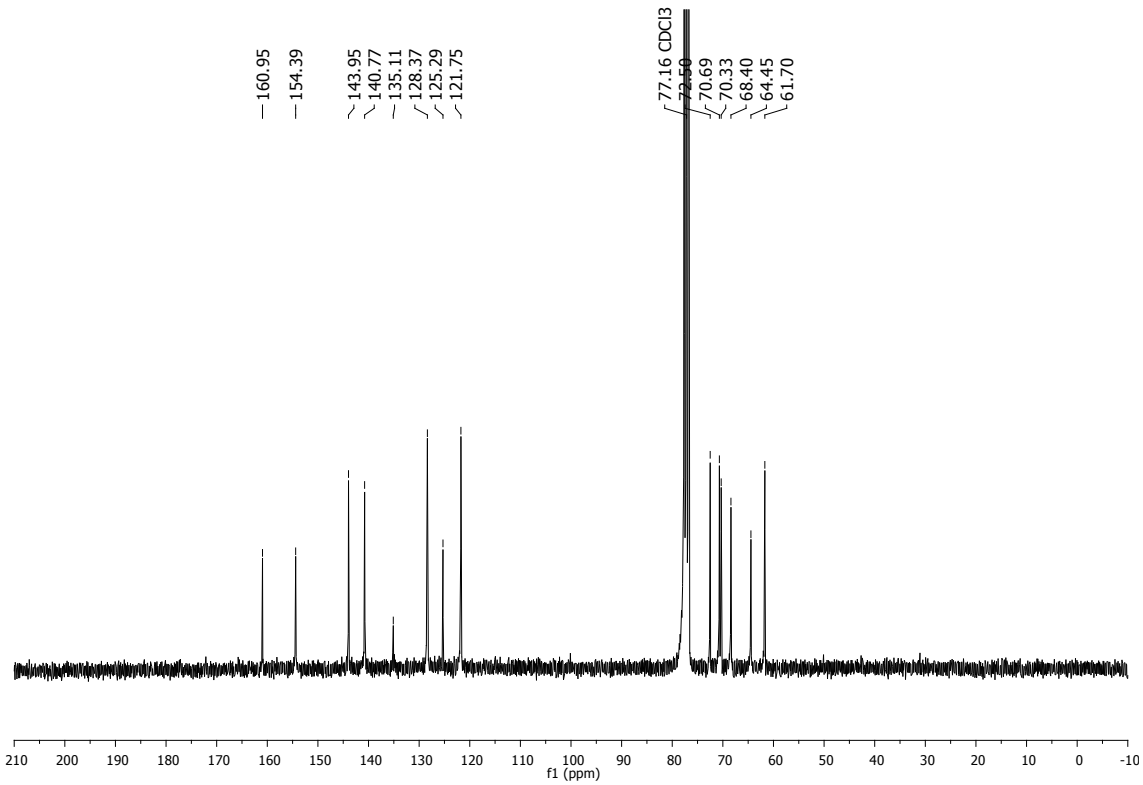


Figure S 14 – ^{13}C NMR spectrum of **Ru(L1)$_2$Pc** in $CDCl_3$.

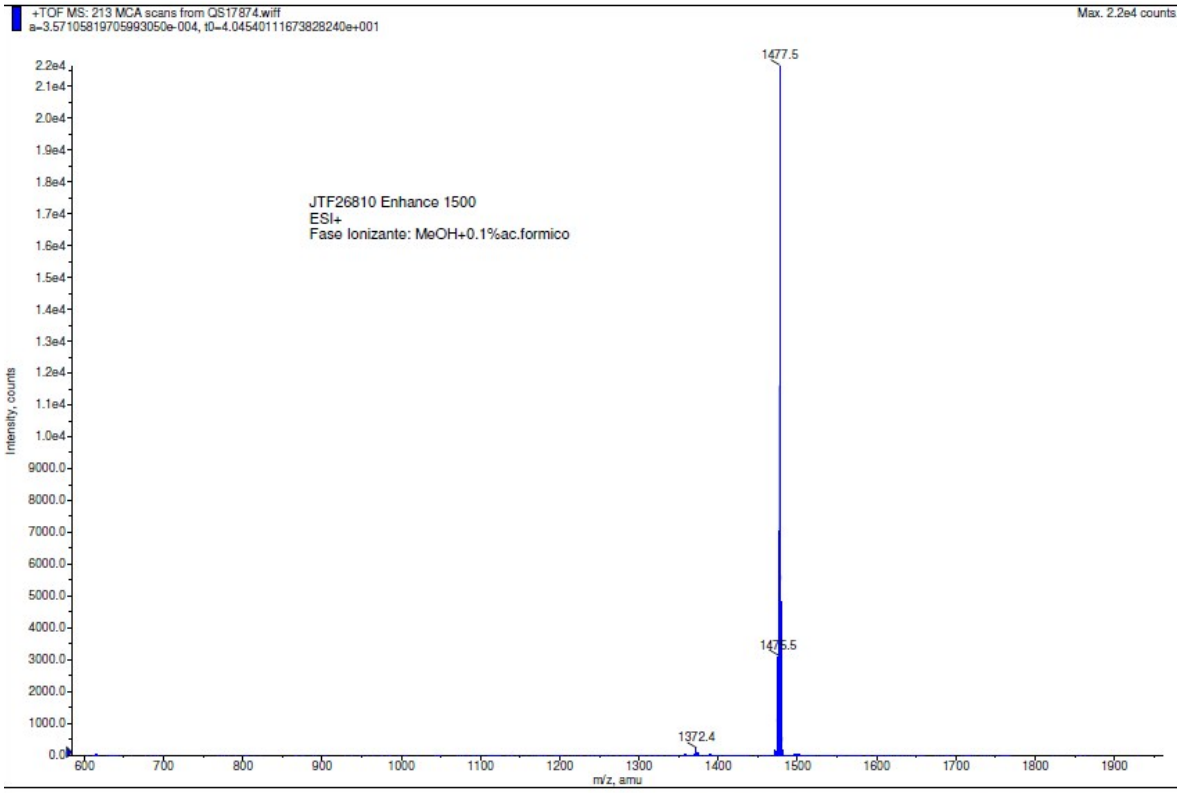


Figure S 15 – MS (ESI+) spectrum of **Ru(L1)$_2$Pc.**

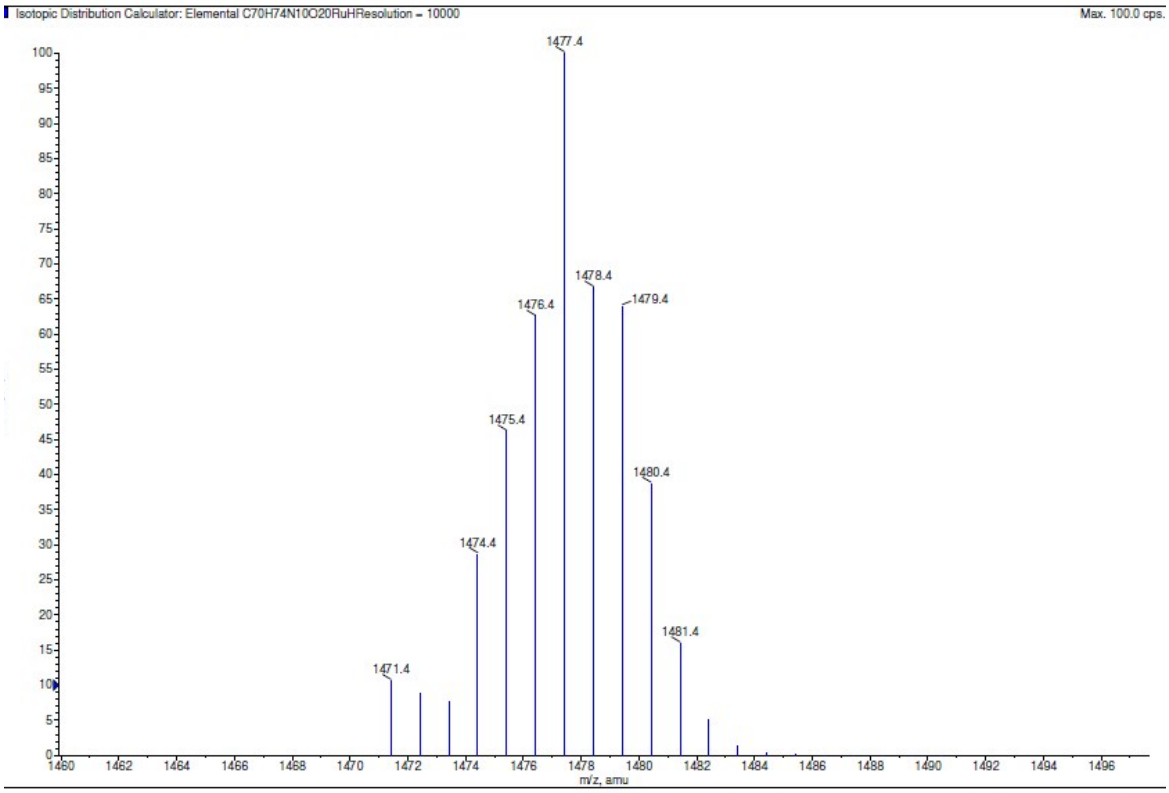


Figure S 16 – MS (ESI+) spectrum of **Ru(L1)$_2$Pc**; predicted isotopic pattern.

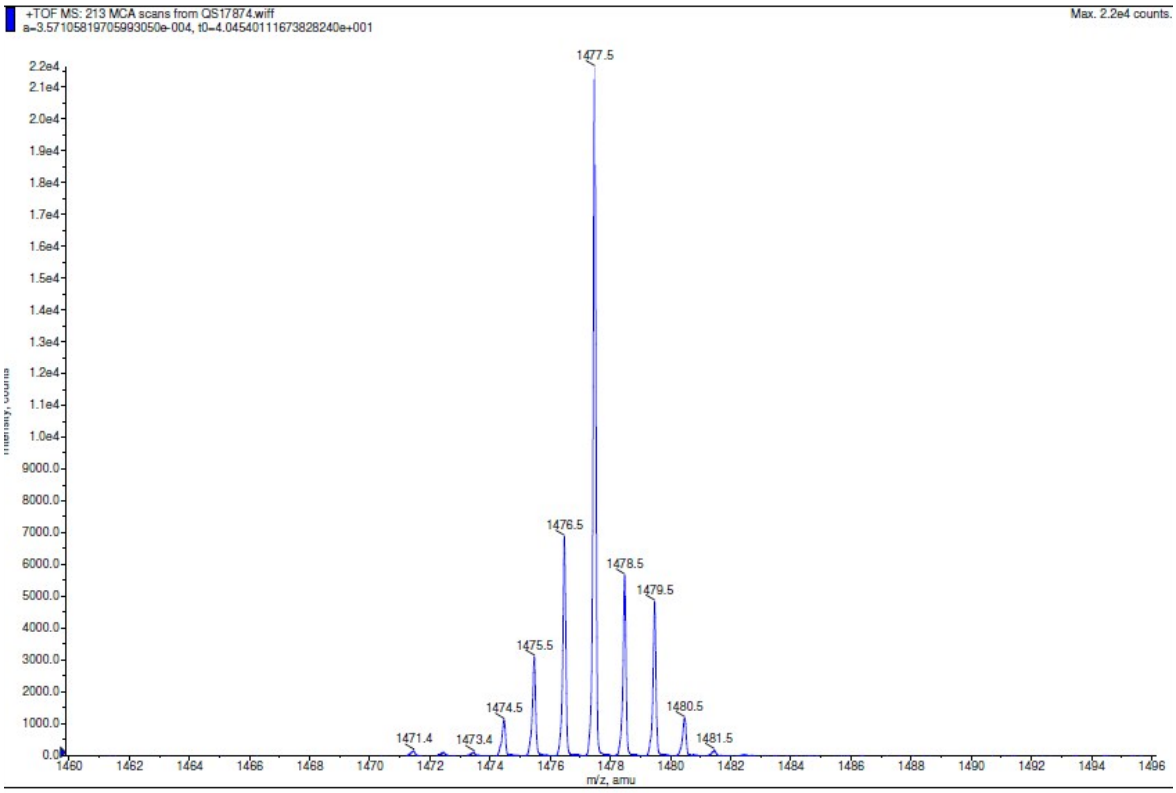


Figure S 17 – MS (ESI+) spectrum of **Ru(L1)$_2$Pc**; experimental isotopic pattern.

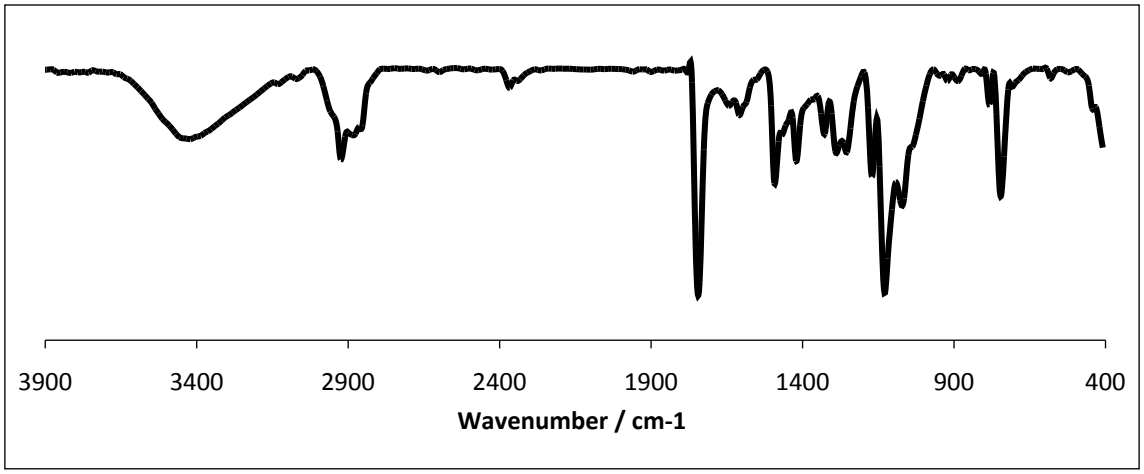


Figure S 18 – IR spectrum of **Ru(L1)$_2$Pc.**

6. Characterization of Ru(L2)$_2$Pc

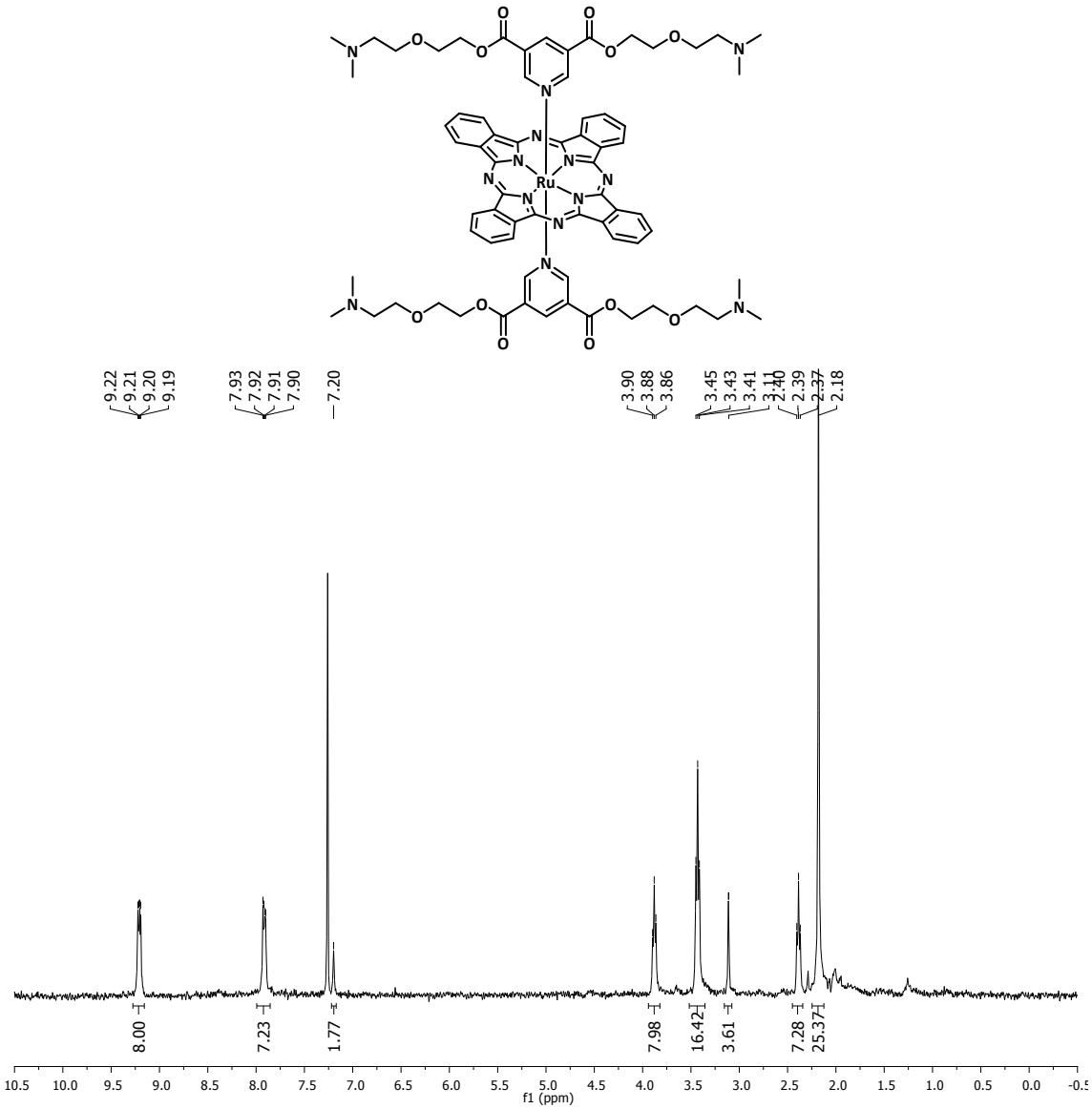


Figure S 19 – ^{1}H NMR spectrum of **Ru(L2)$_2$Pc** in $CDCl_3$.

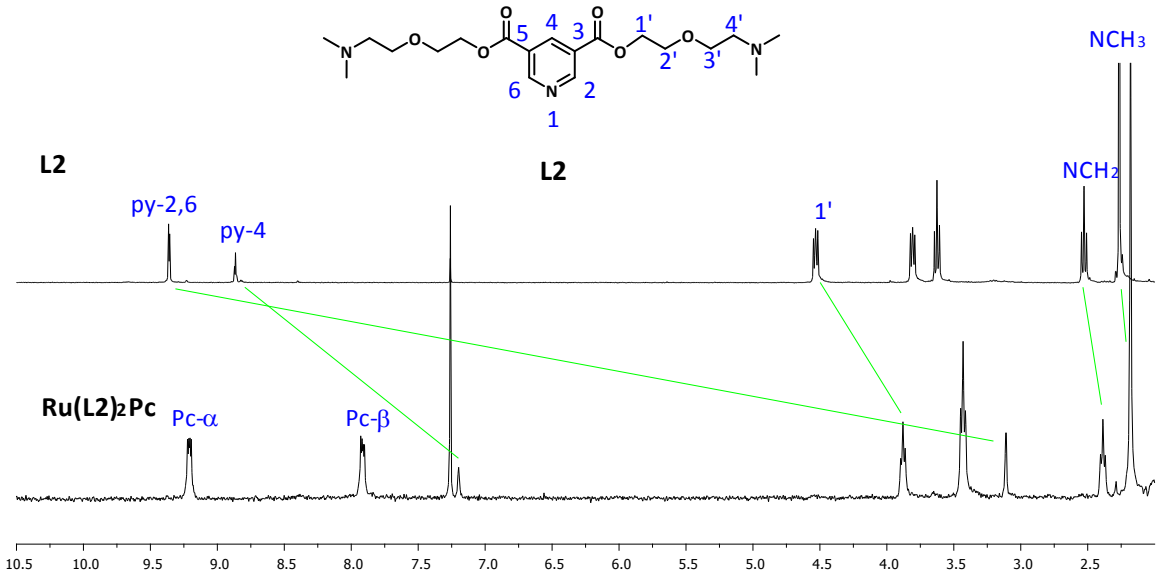


Figure S 20 – Comparative ^{1}H NMR spectra in $CDCl_3$ of non-coordinated **L2** and **Ru(L2)$_2$Pc.**

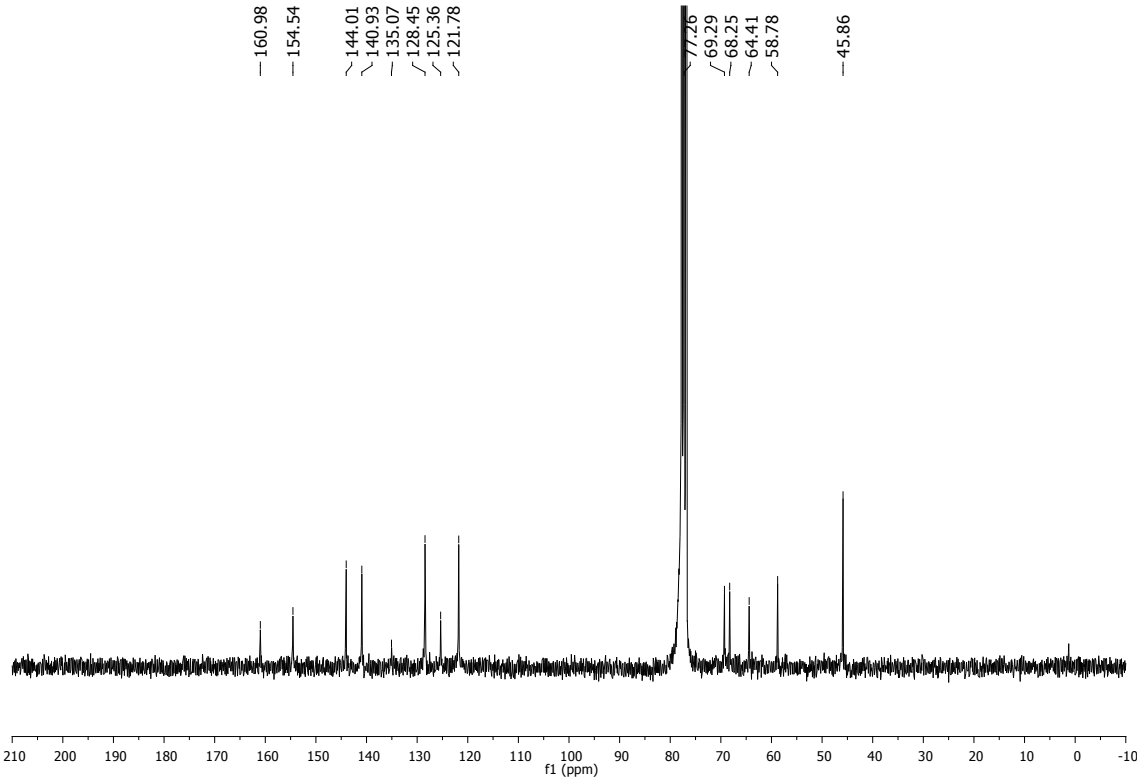


Figure S 21 – ^{13}C NMR spectrum of **Ru(L2)$_2$Pc** in $CDCl_3$.

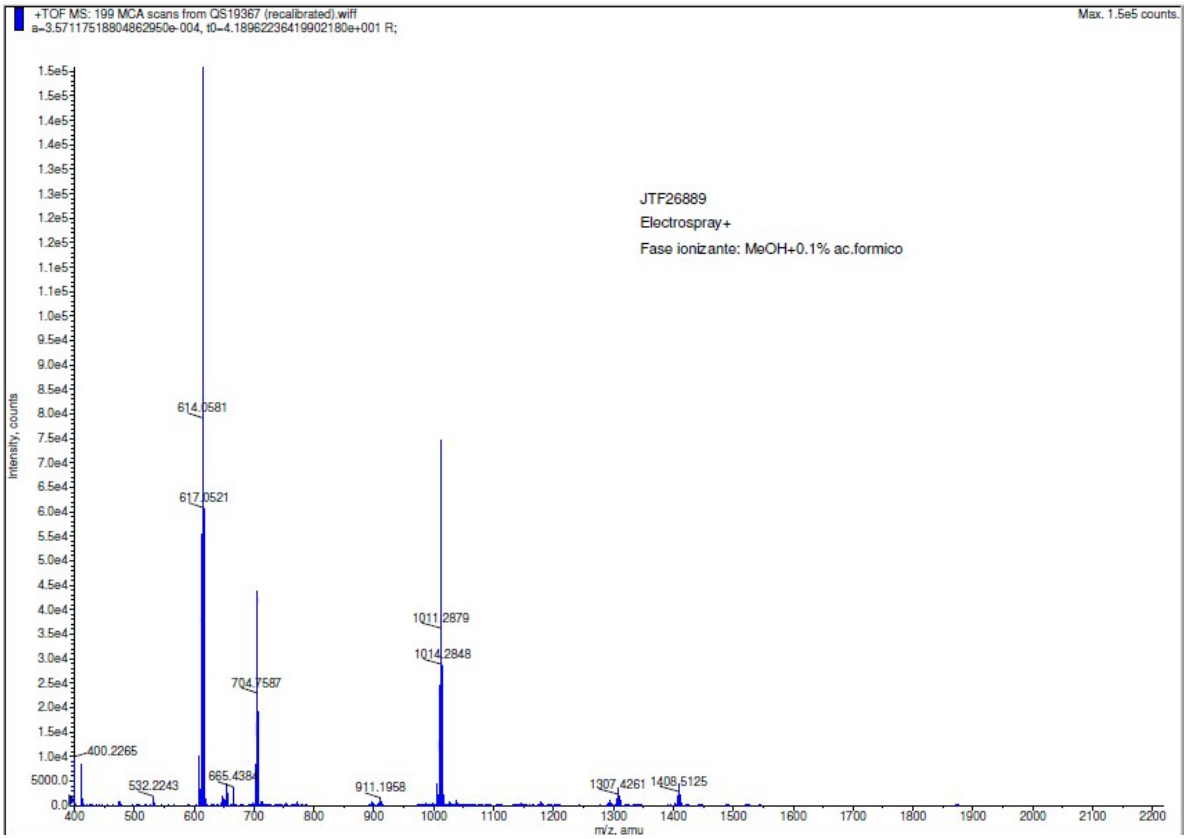


Figure S 22 – MS (ESI+) spectrum of **Ru(L2)$_2$Pc.**

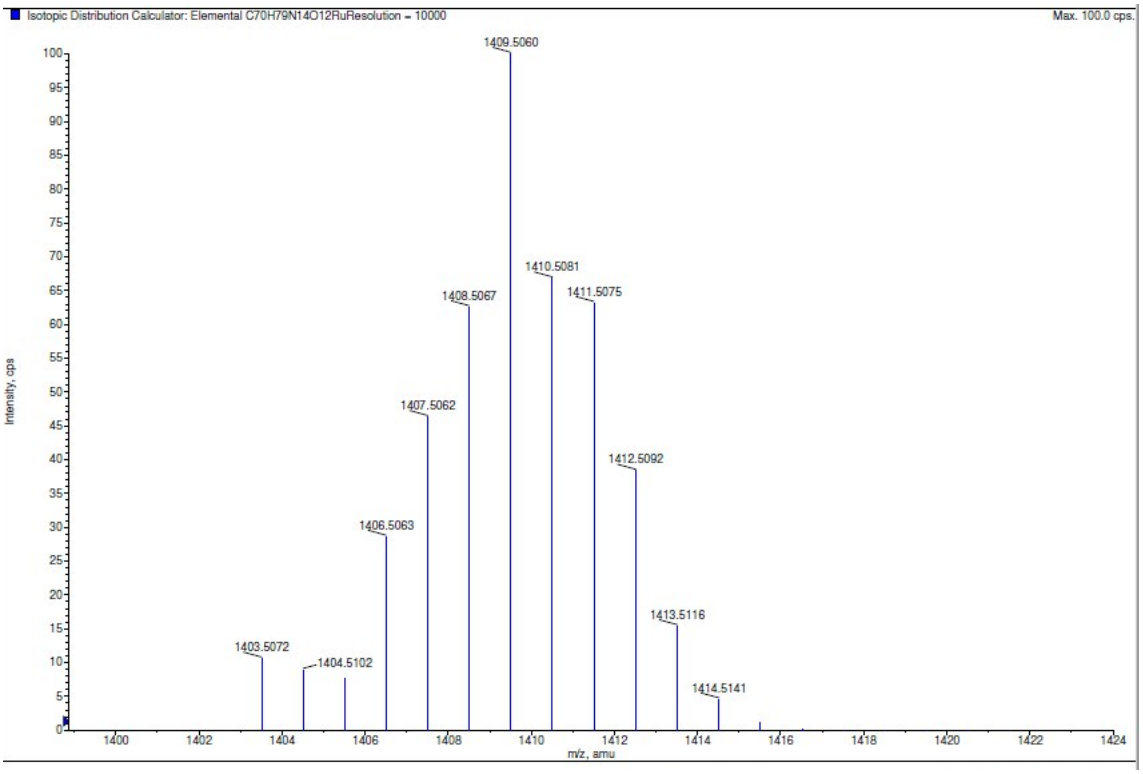


Figure S 23 – MS (ESI+) spectrum of **Ru(L2)$_2$Pc;** predicted isotopic pattern.

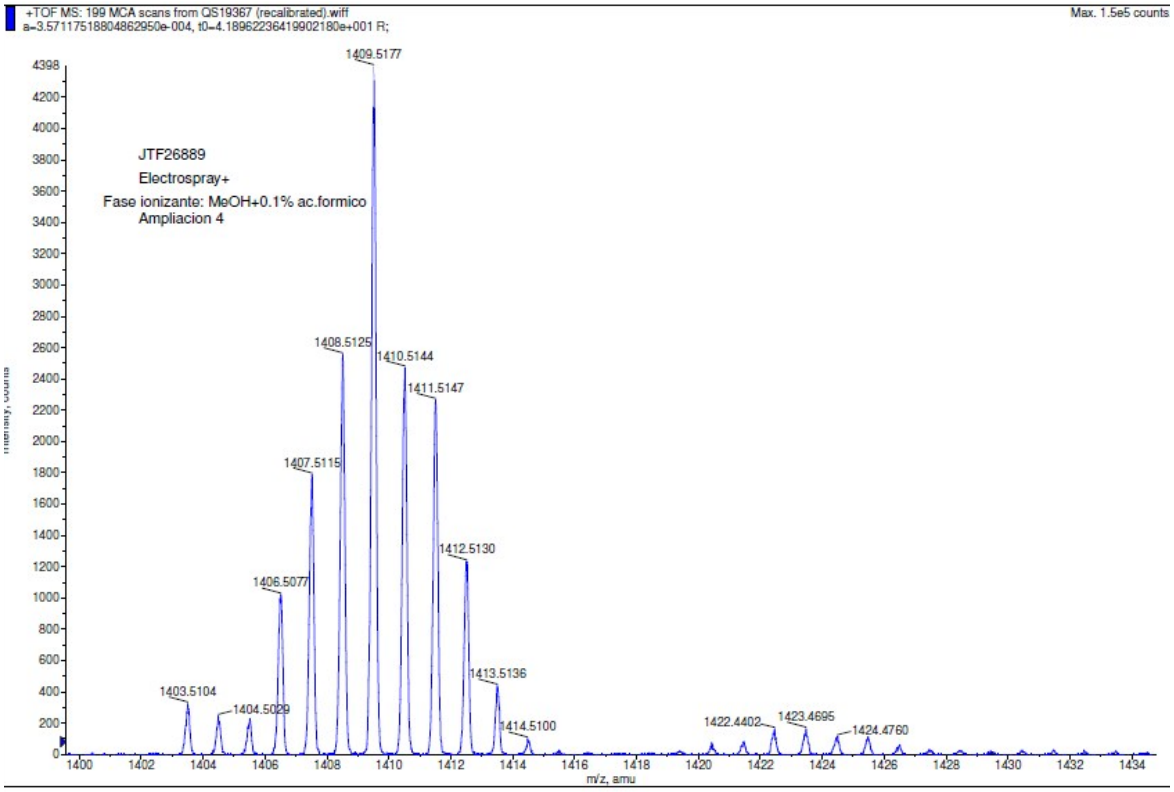


Figure S 24 – MS (ESI+) spectrum of **Ru(L2)$_2$Pc;** experimental isotopic pattern.

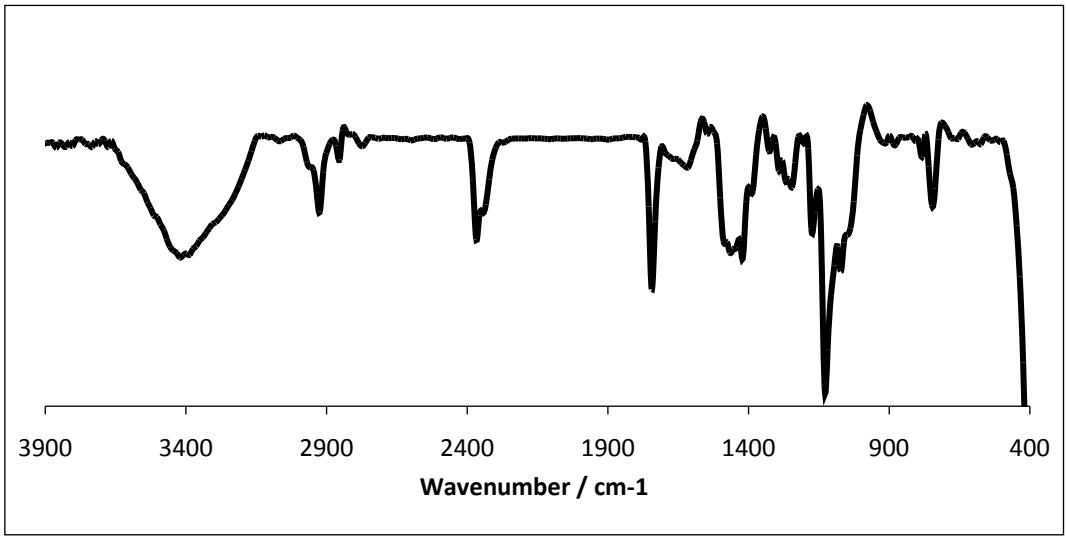
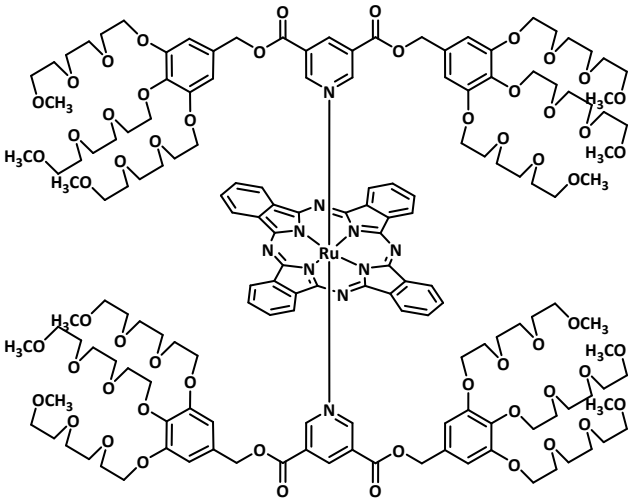


Figure S 25 – IR spectrum of **Ru(L2)$_2$Pc.**

7. Characterization of $Ru(L3)_2Pc$



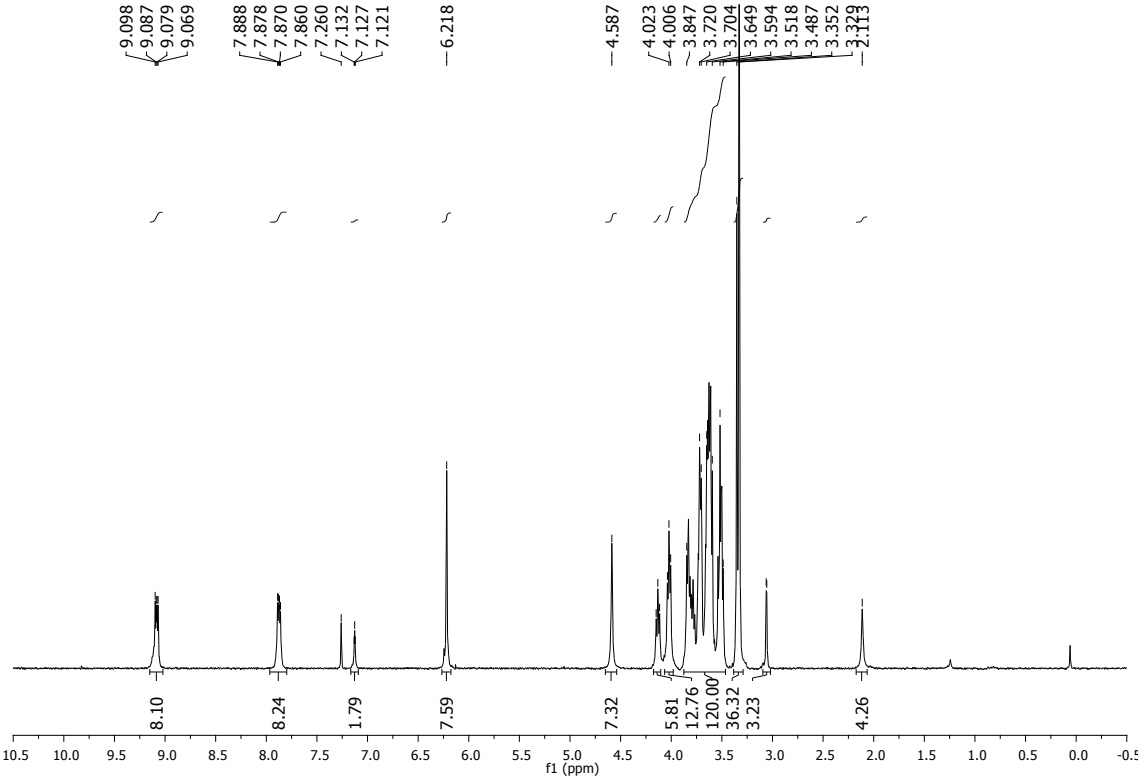


Figure S 26 – ^{1}H NMR spectrum of **$Ru(L3)_2Pc$** in $CDCl_3$.

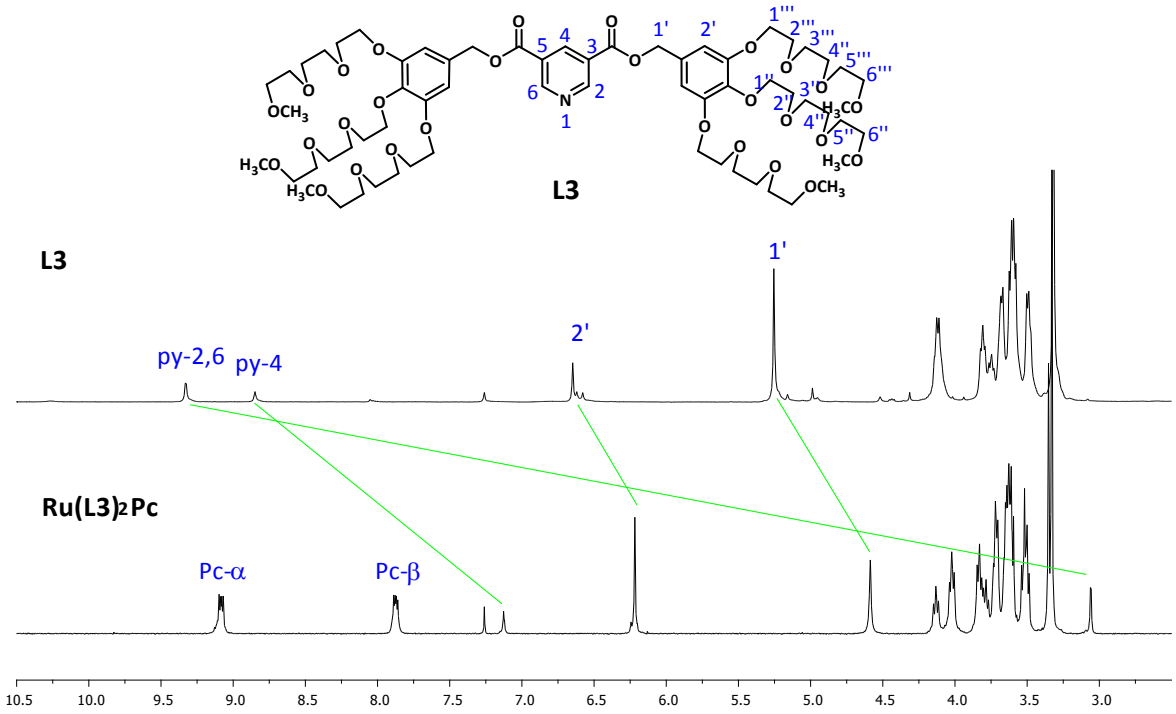


Figure S 27 – Comparative ^{1}H NMR spectra in $CDCl_3$ of non-coordinated **L3** and **$Ru(L3)_2Pc$.**

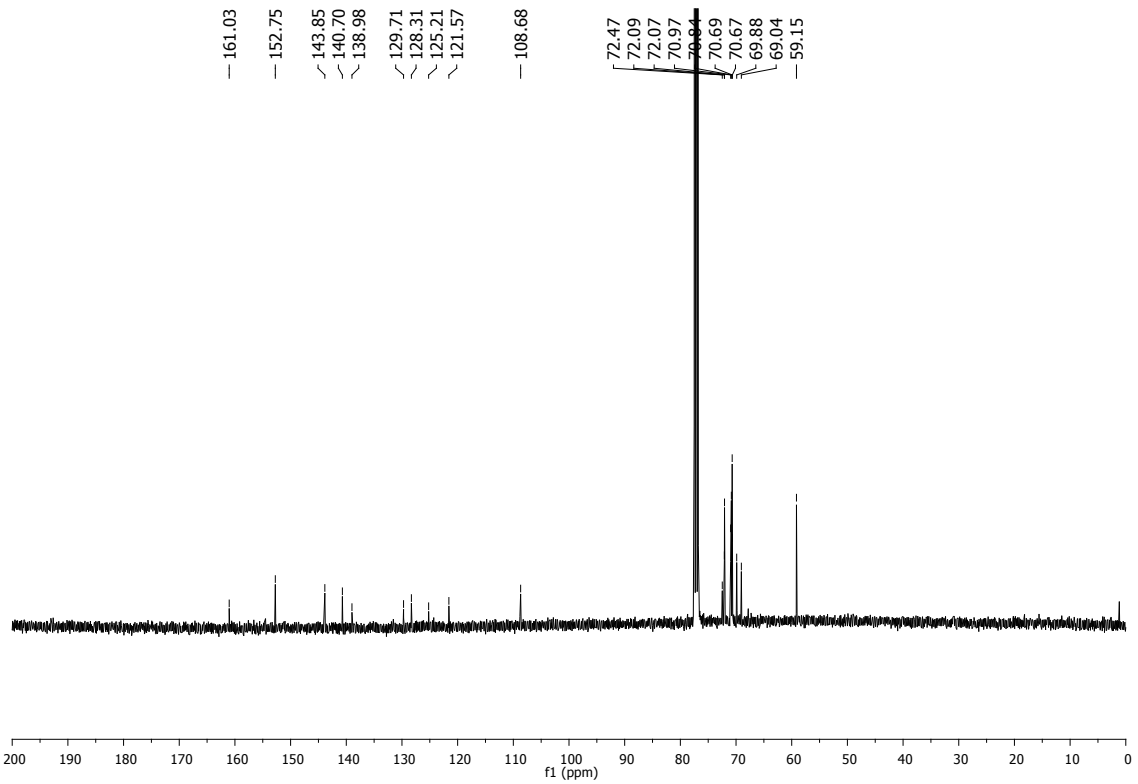


Figure S 28 – ^{13}C NMR spectrum of **$Ru(L3)_2Pc$** in $CDCl_3$.

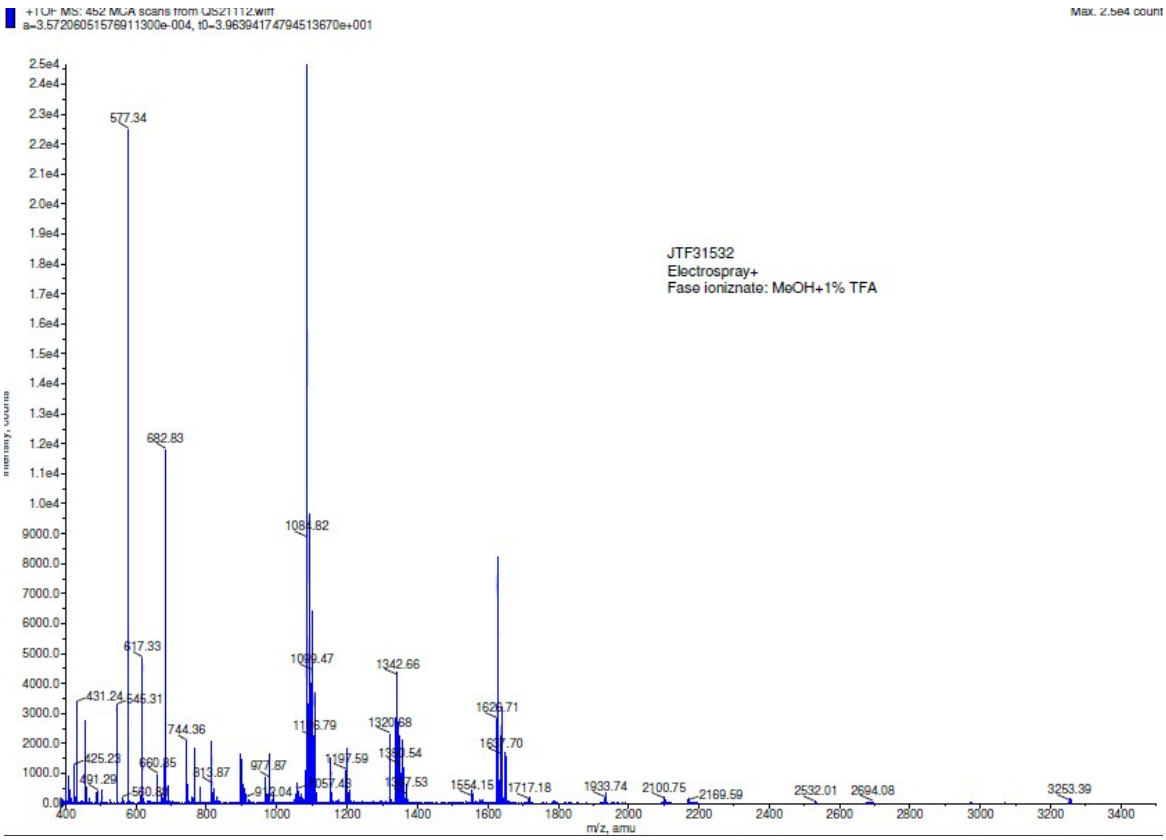


Figure S 29 – MS (ESI$^+$, MeOH + 1%TFA) of **Ru(L3)$_2$Pc.**

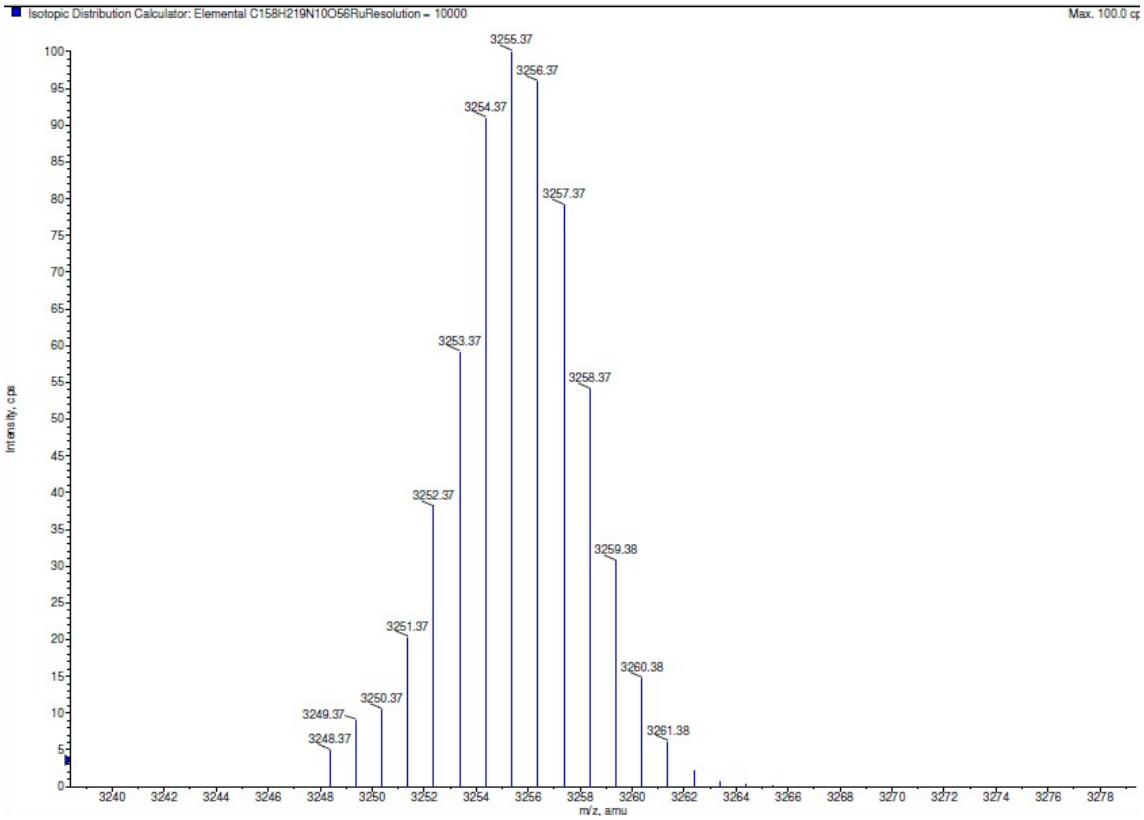


Figure S 30 – MS (ESI$^+$, MeOH + 1%TFA) of **Ru(L3)$_2$Pc**; predicted isotopic pattern.

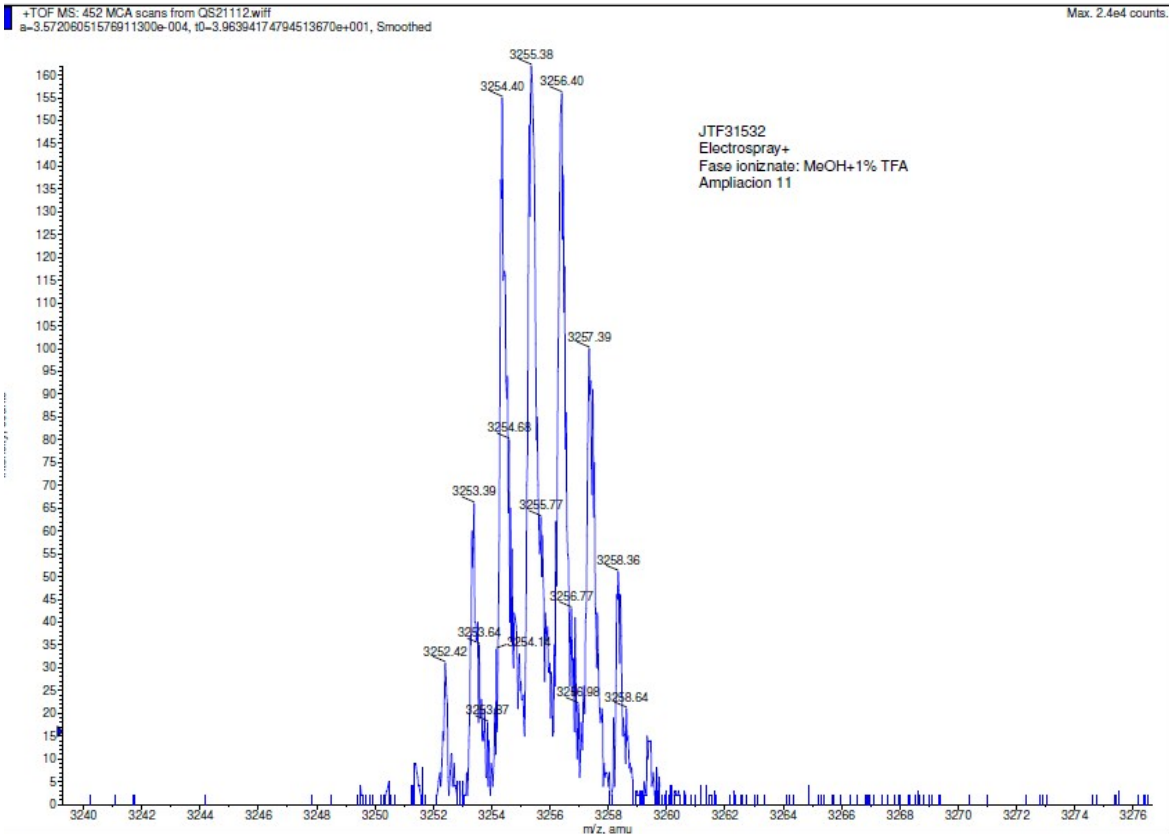


Figure S 31 – MS (ESI$^+$, MeOH + 1%TFA) of **Ru(L3)$_2$Pc**; experimental isotopic pattern.

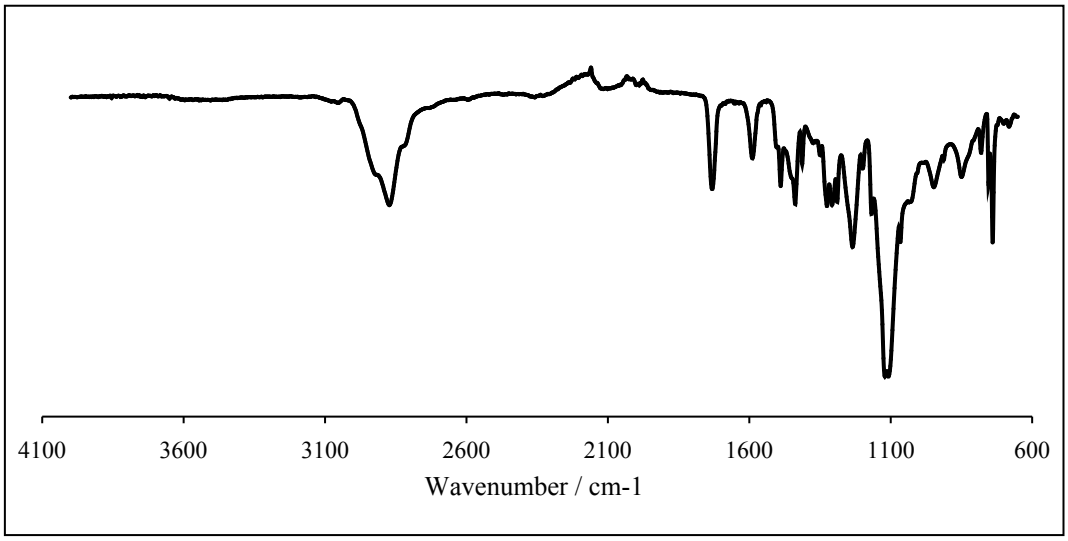


Figure S 32 – IR spectrum of **Ru(L3)$_2$Pc.**

8. Dark toxicities of $Ru(L)_2Pcs$

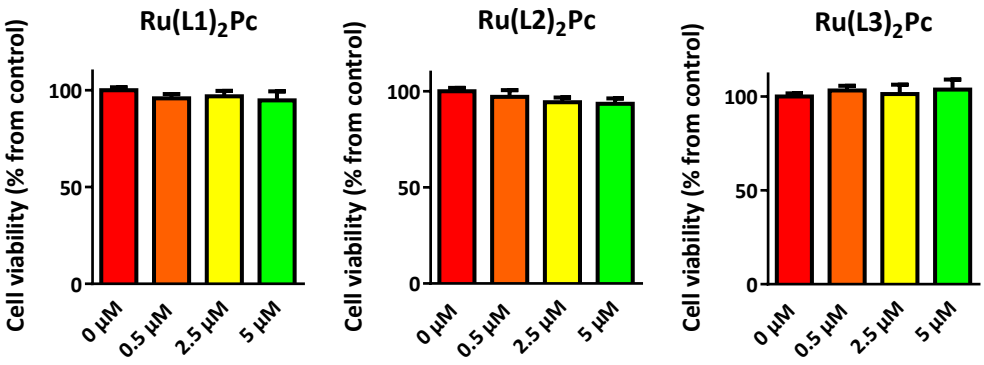


Figure S 33 – Dark toxicity evaluated 24h after incubation with **RuL_2Pcs** for 2h; data are the mean value ± S.E.M. of at least three independent experiments performed in triplicates. *(p≤0.05), **(p≤0.01), ***(p≤0.001), **** (p≤0.0001) significantly different from control cells.