

## **Supplementary information**

### **Nitrosyl/diphenylphosphine-ruthenium complexes as inhibitors of MDA-MB-231 breast cancer cells**

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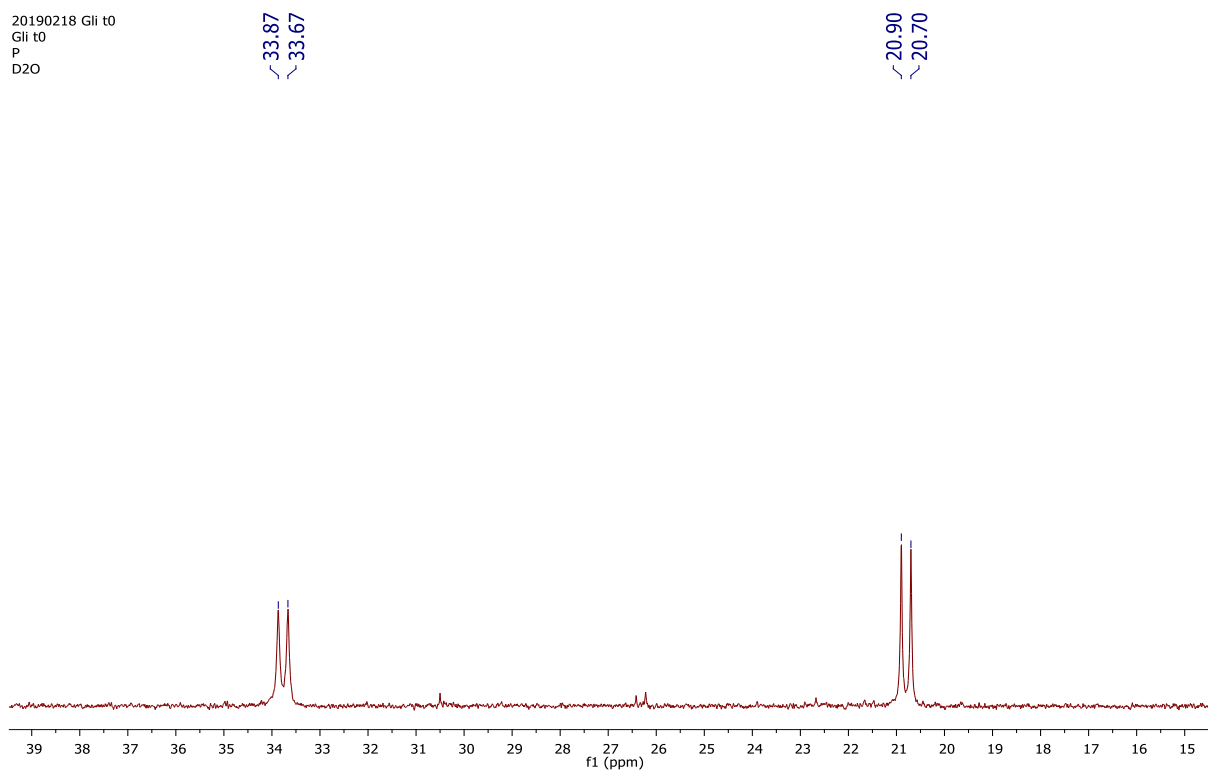
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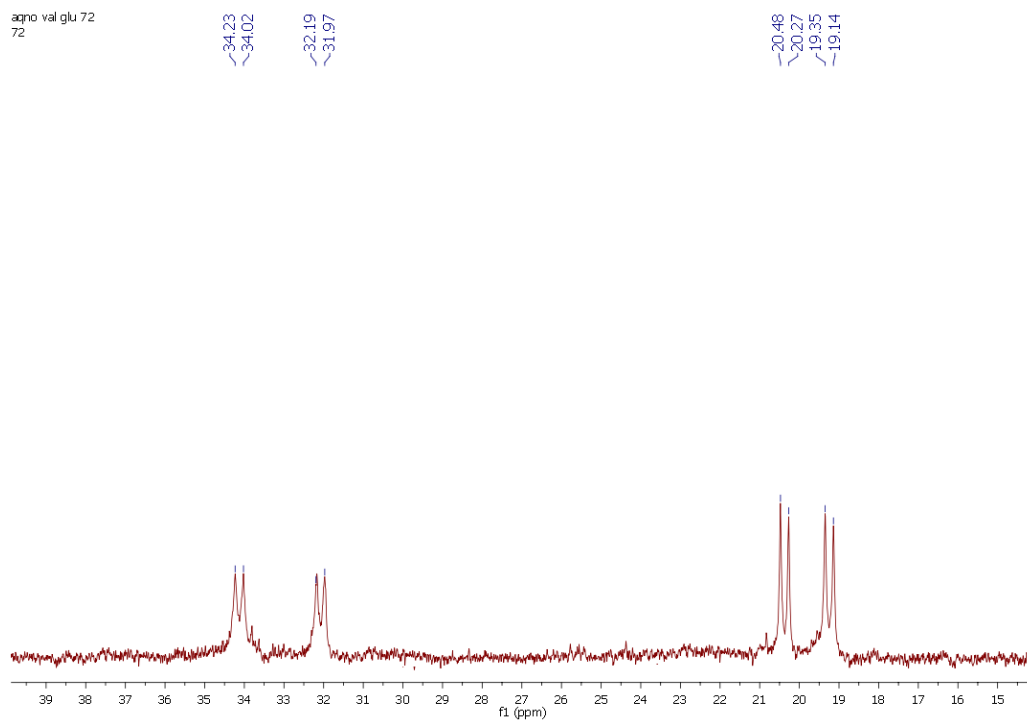
Alzir A. Batista (daab@ufscar.br) Tel.: +55 16 3351-8285.

20190218 Gli t0  
Gli t0  
P  
D2O

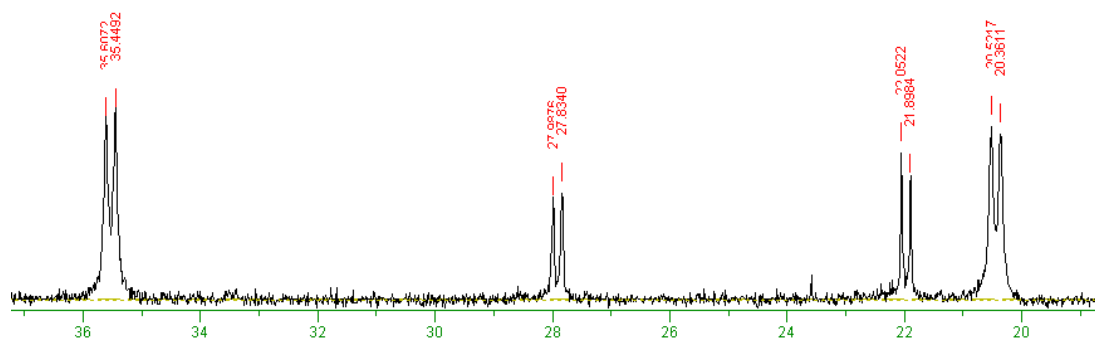


**Fig. S1** -  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum for **1**, in  $\text{CH}_2\text{Cl}_2/\text{D}_2\text{O}$  at 298K.

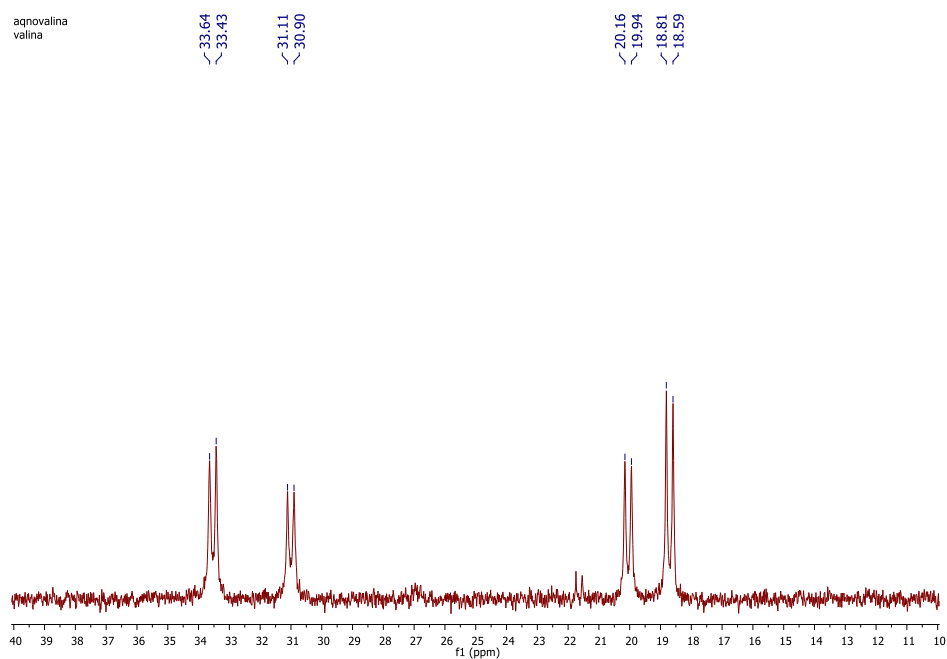
aqno val gli 72  
72



**Fig. S2** -  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum for **2**, in  $\text{CH}_2\text{Cl}_2/\text{D}_2\text{O}$  at 298K.

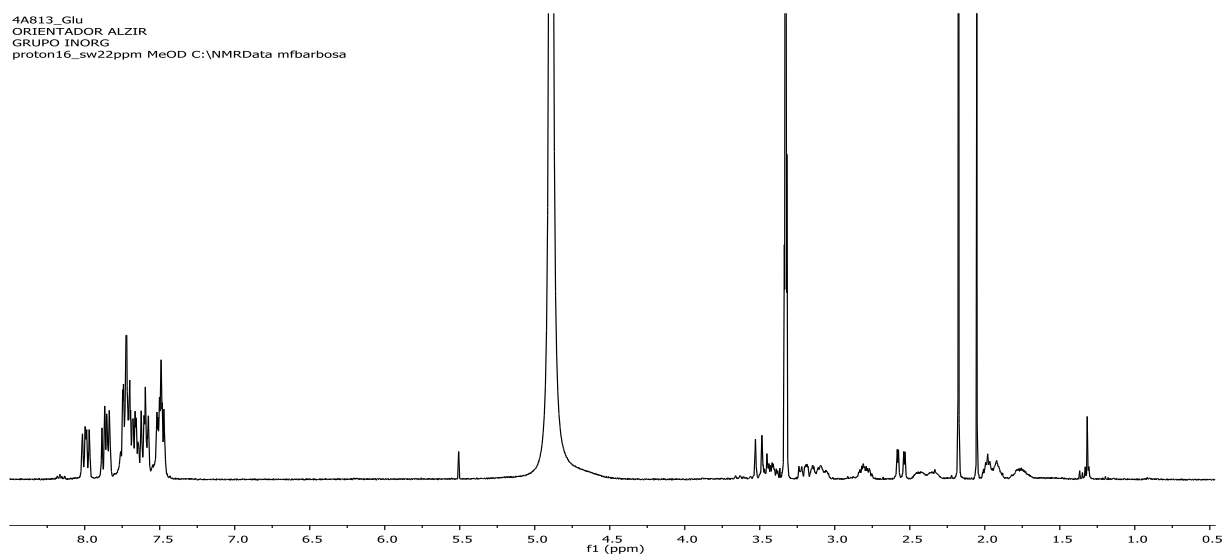


**Fig. S3** -  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum for **3**, in  $\text{CH}_2\text{Cl}_2/\text{D}_2\text{O}$  at 298K.



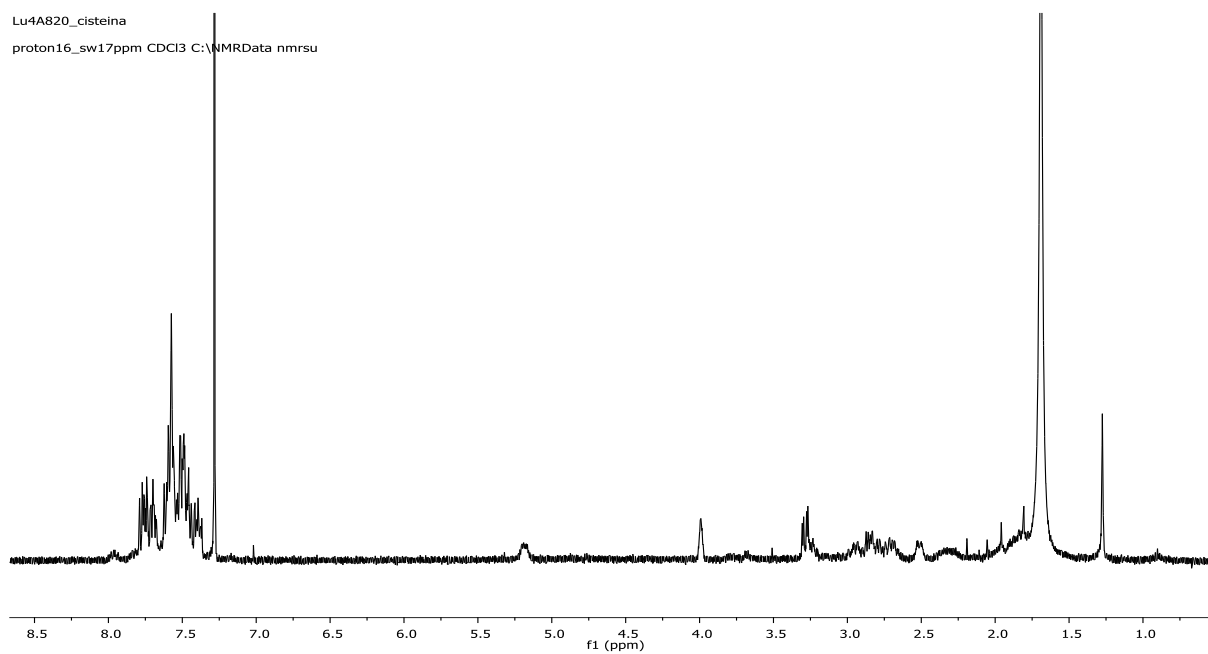
**Fig. S4** -  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum for **4**, in  $\text{CH}_2\text{Cl}_2/\text{D}_2\text{O}$  at 298K.

4A813\_Glu  
ORIENTADOR ALZIR  
GRUPO INORG  
proton16\_sw22ppm MeOD C:\NMRData mfbarbosa

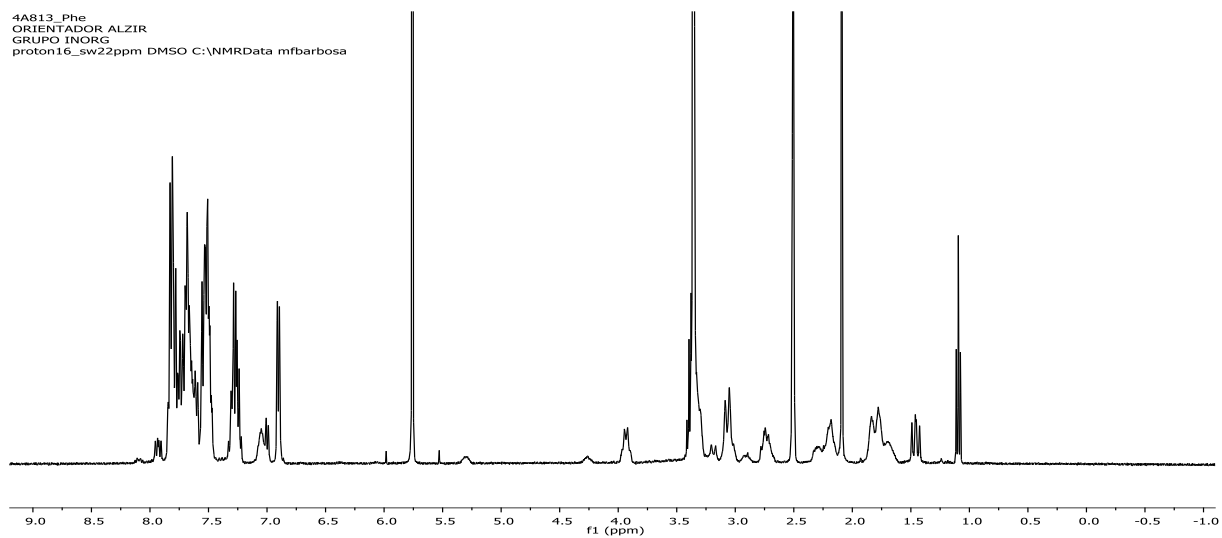


**Fig. S5** - <sup>1</sup>H NMR spectrum for **1**, in CDCl<sub>3</sub>.

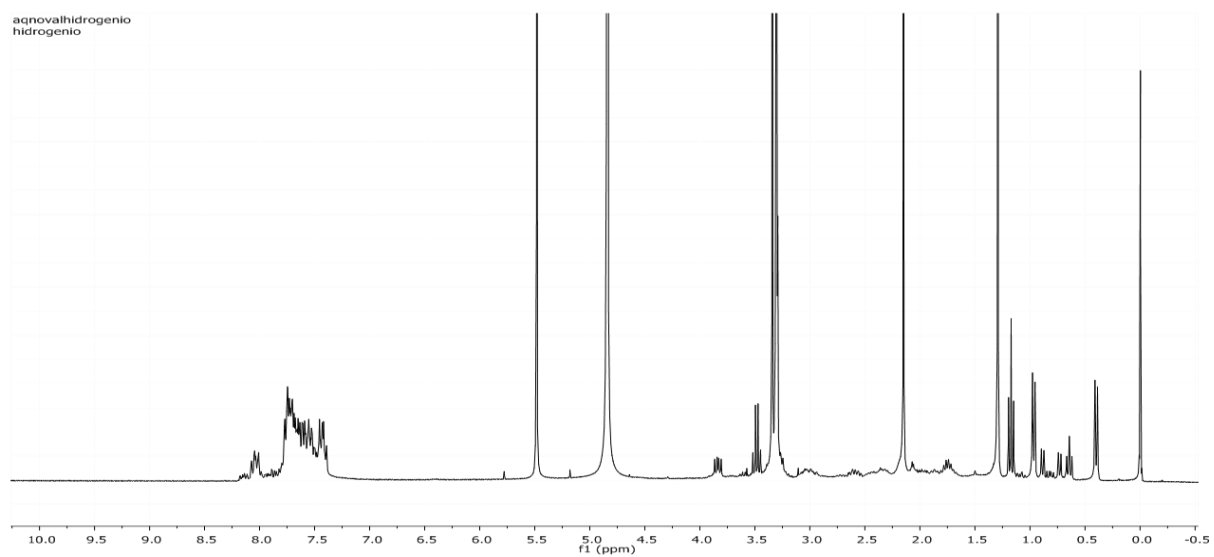
Lu4A820\_cisteina  
proton16\_sw17ppm CDCl3 C:\NMRData nmrsu



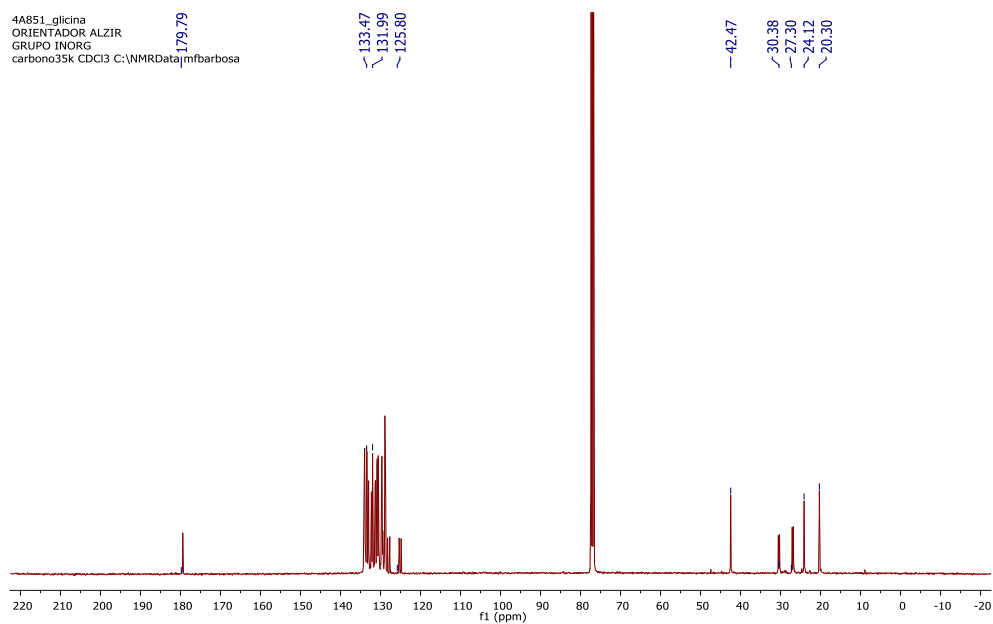
**Fig. S6** - <sup>1</sup>H NMR spectrum for **2**, in CDCl<sub>3</sub>.



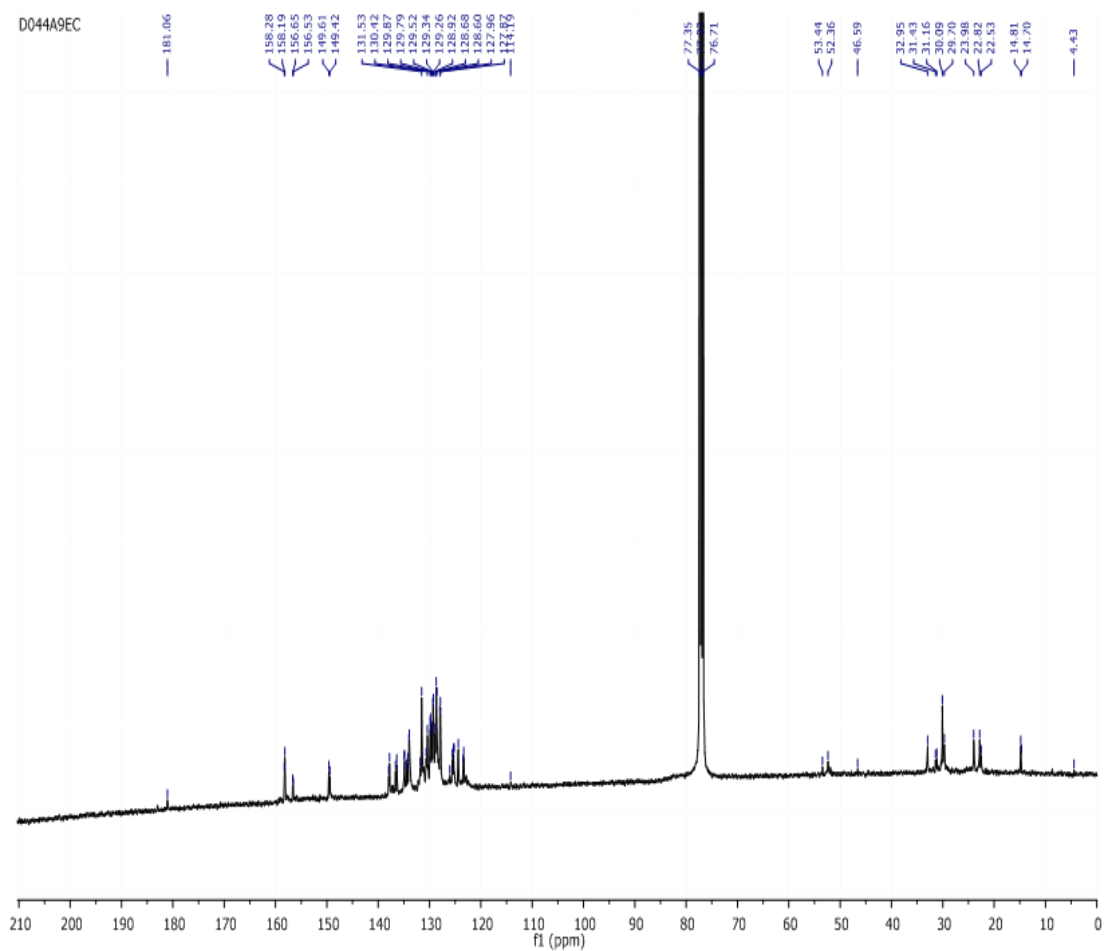
**Fig. S7** -  $^1\text{H}$  NMR spectrum for **3**, in  $\text{CDCl}_3$ .



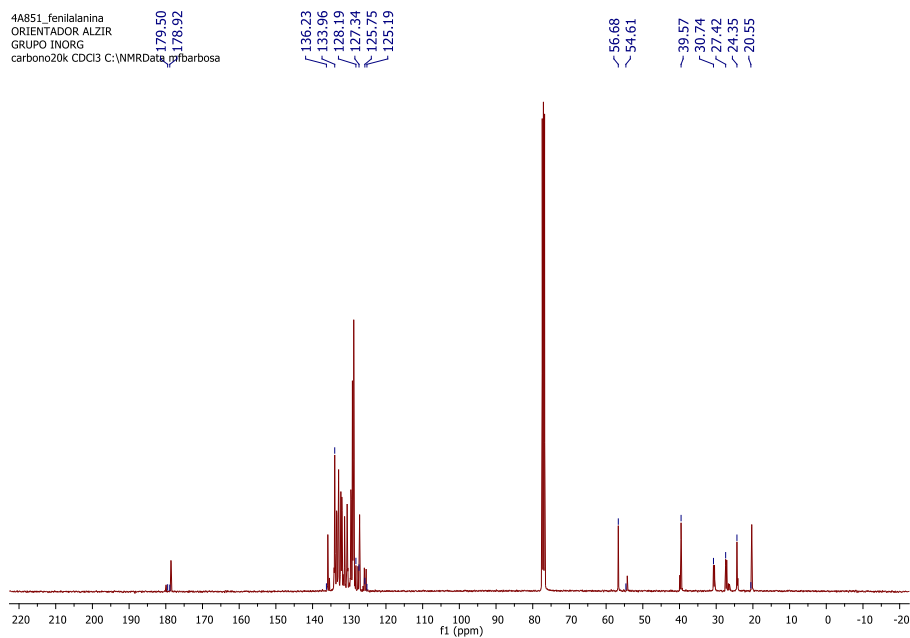
**Fig. S8** -  $^1\text{H}$  NMR spectrum for **4**, in  $\text{CDCl}_3$ .



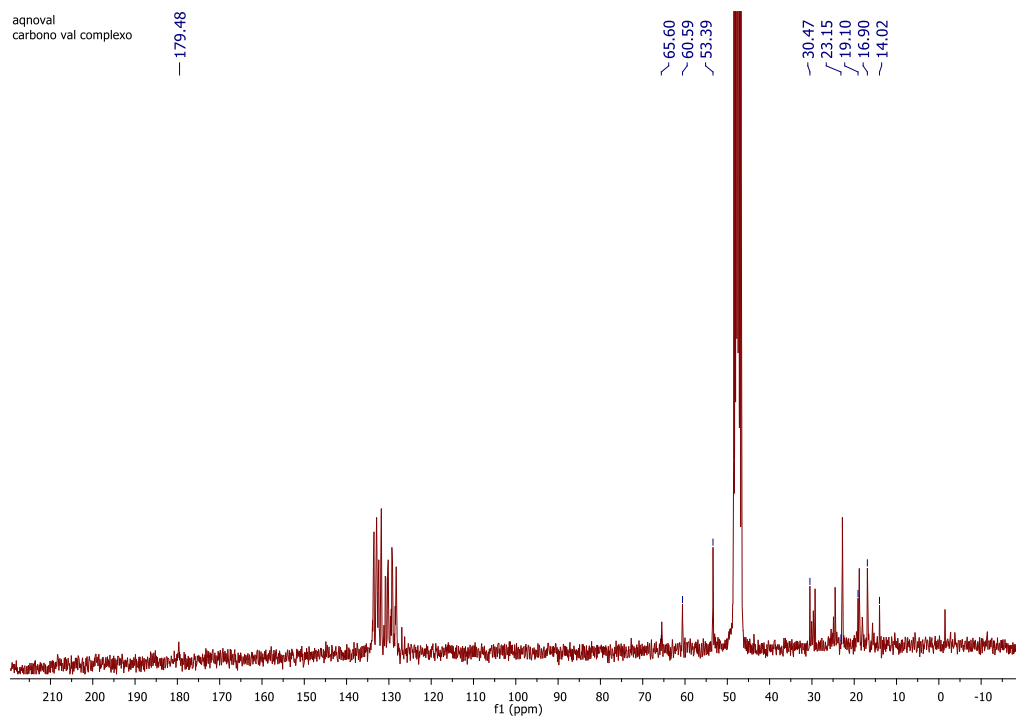
**Fig. S9** -  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum for **1**, in  $\text{CDCl}_3$ .



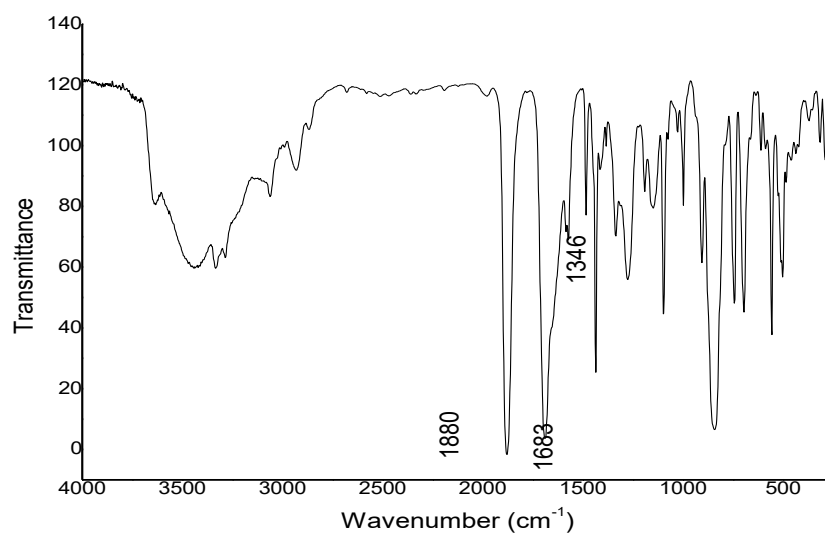
**Fig. S10** -  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum for **2**, in  $\text{CDCl}_3$ .



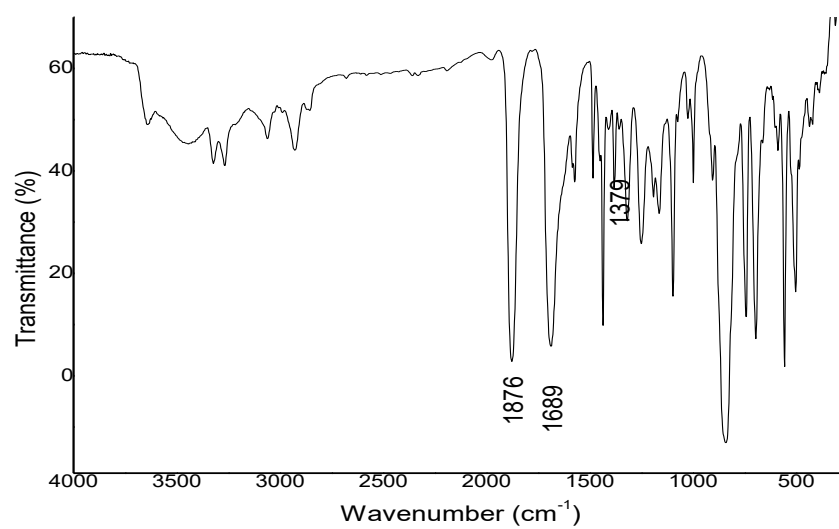
**Fig. S11**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum for **3**, in  $\text{CDCl}_3$ .



**Fig. S12**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum for **4**, in  $\text{CDCl}_3$ .

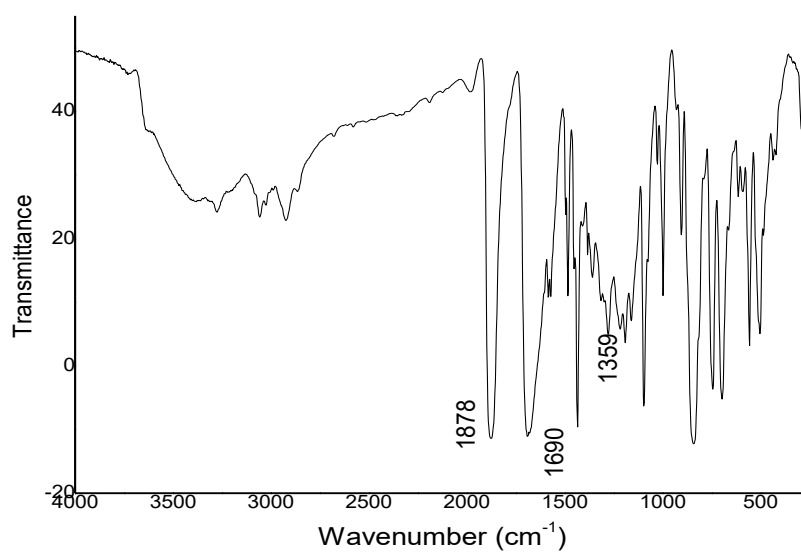


**Fig. S13** - Infrared spectrum for **1**, in KBr pallet.

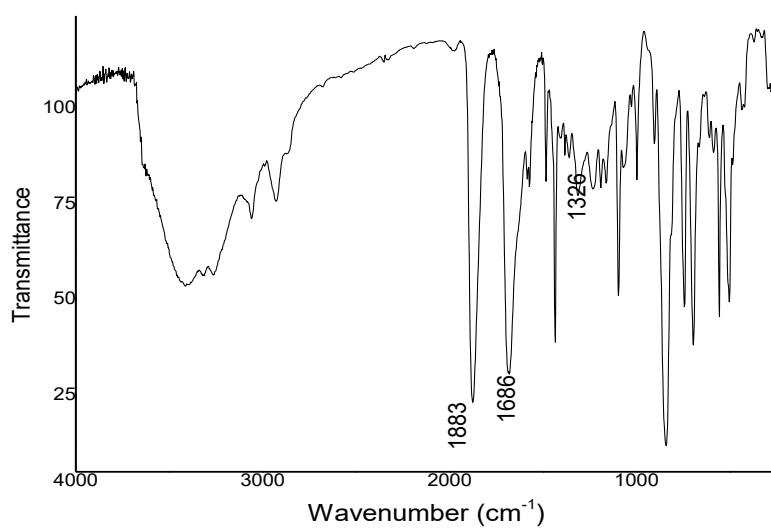


**Fig. S14** - Infrared spectrum for **2**, in KBr pallet.

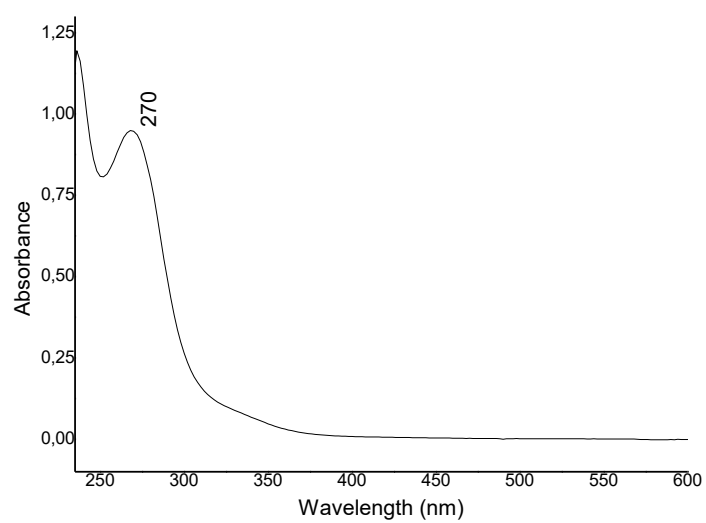




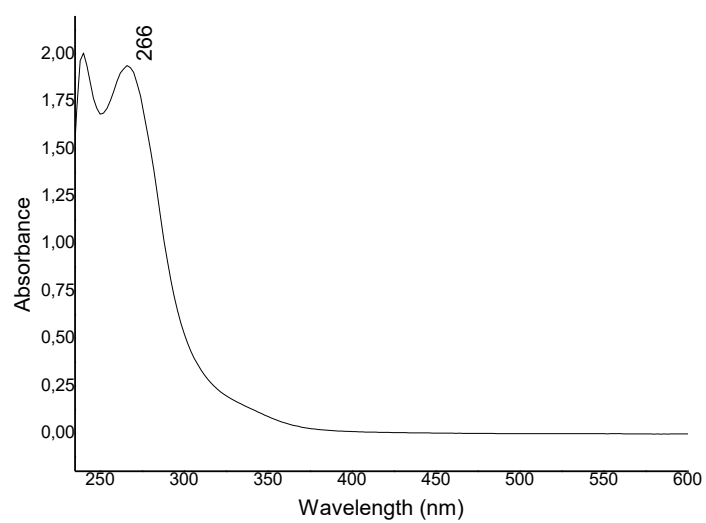
**Fig. S15** - Infrared spectrum for **3**, in KBr pallet.



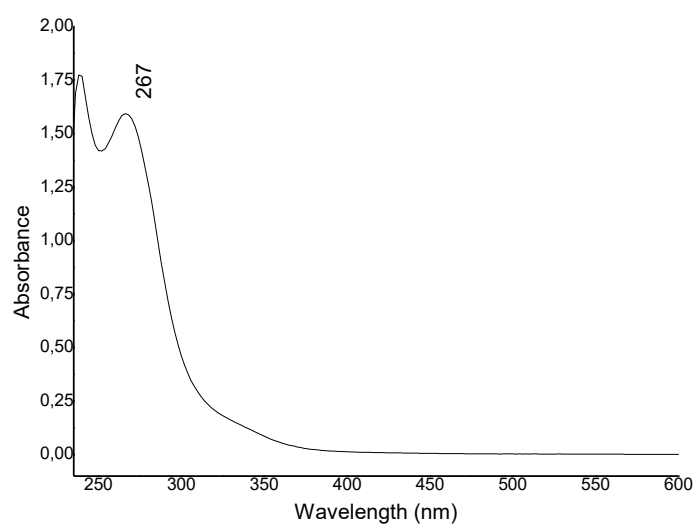
**Fig. S16** - Infrared spectrum for **4**, in KBr pallet.



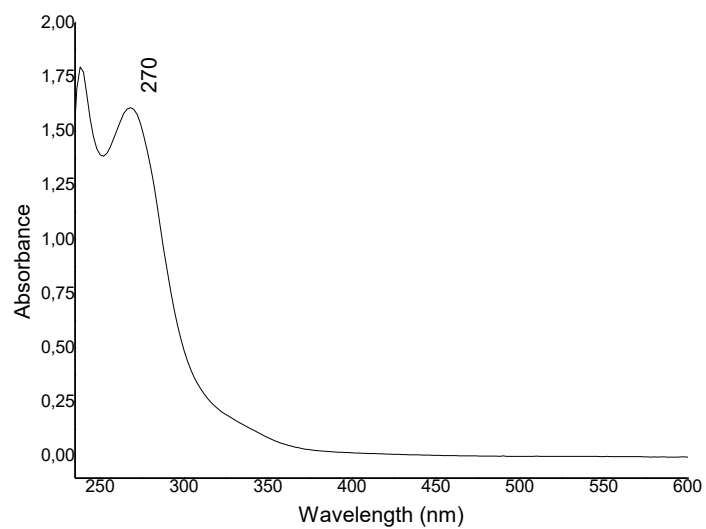
**Fig. S17** - UV-Vis spectrum for **1**, in CH<sub>2</sub>Cl<sub>2</sub>



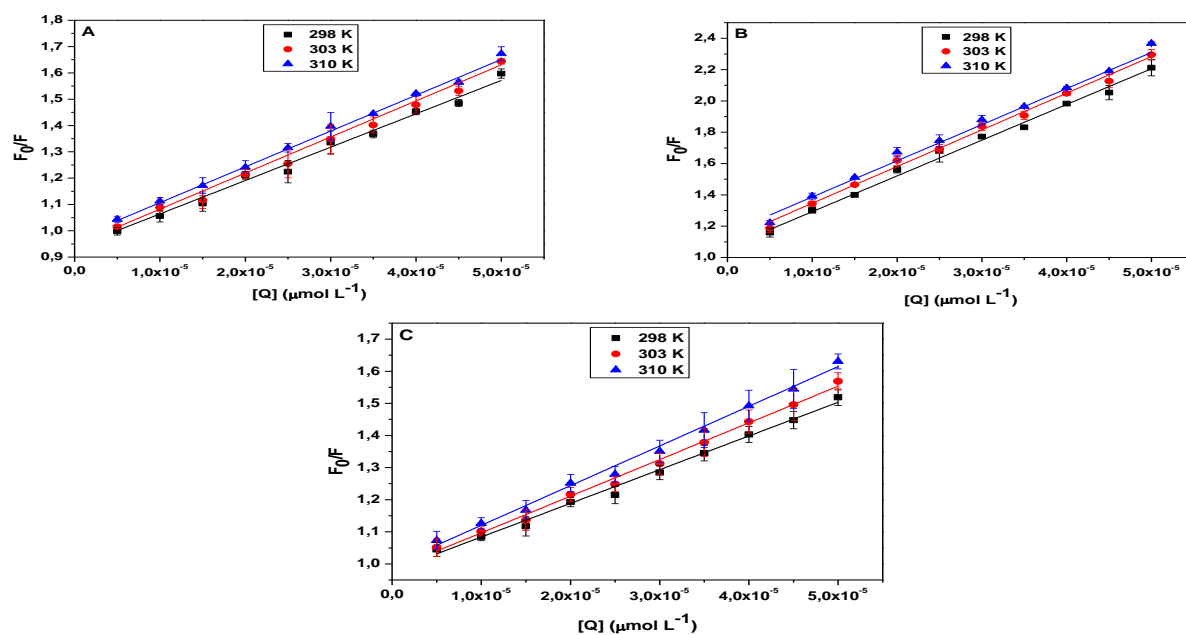
**Fig. S18** - UV-Vis spectrum for **2**, in CH<sub>2</sub>Cl<sub>2</sub>



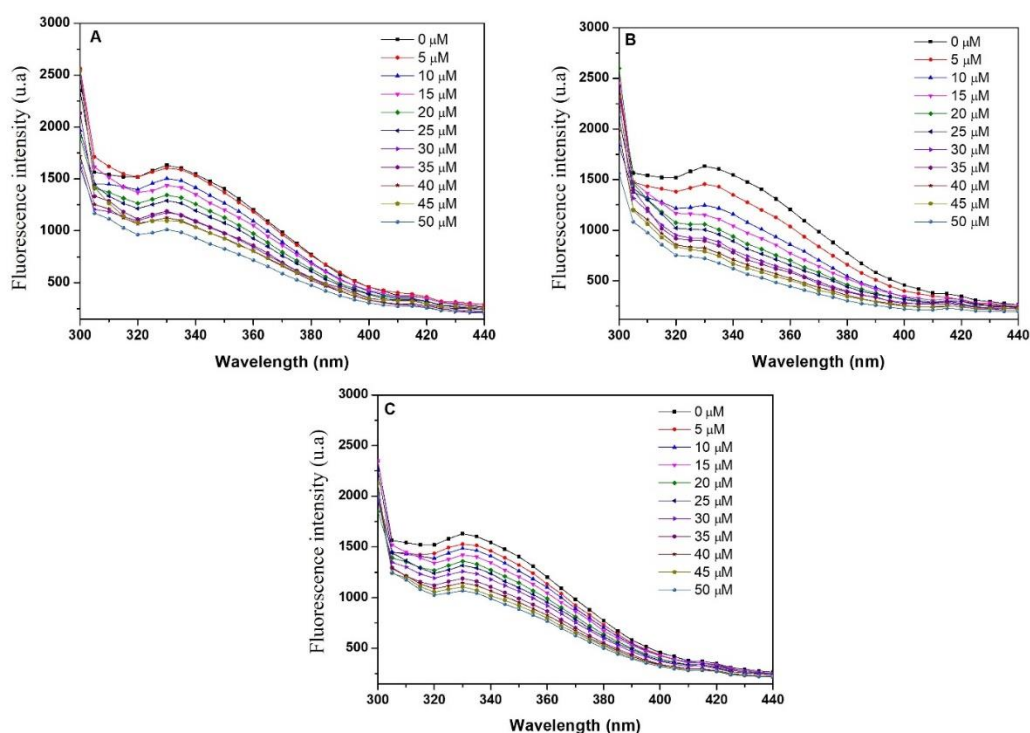
**Fig. S19** - UV-Vis spectrum for **3**, in  $\text{CH}_2\text{Cl}_2$



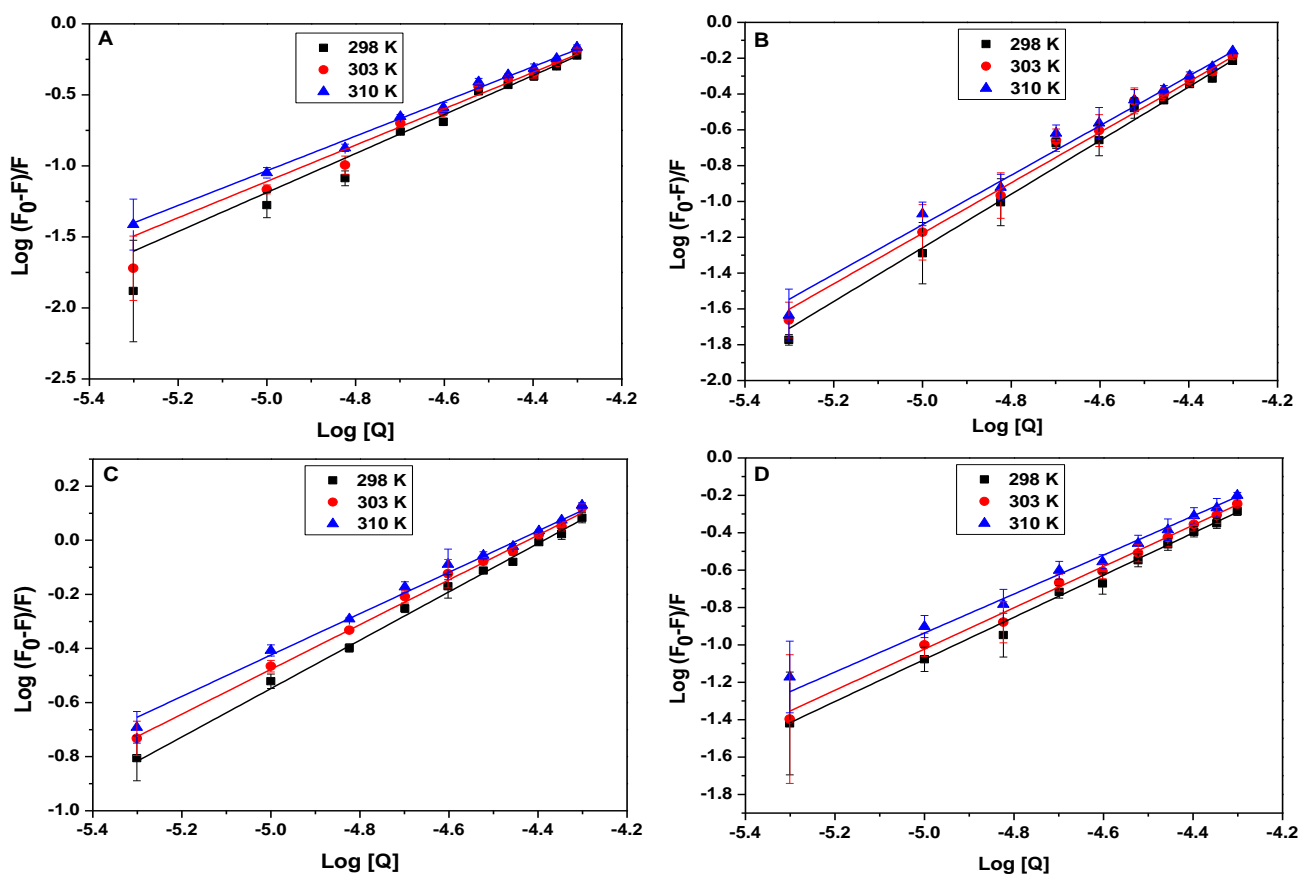
**Fig. S20** - UV-Vis spectrum for **4**, in  $\text{CH}_2\text{Cl}_2$



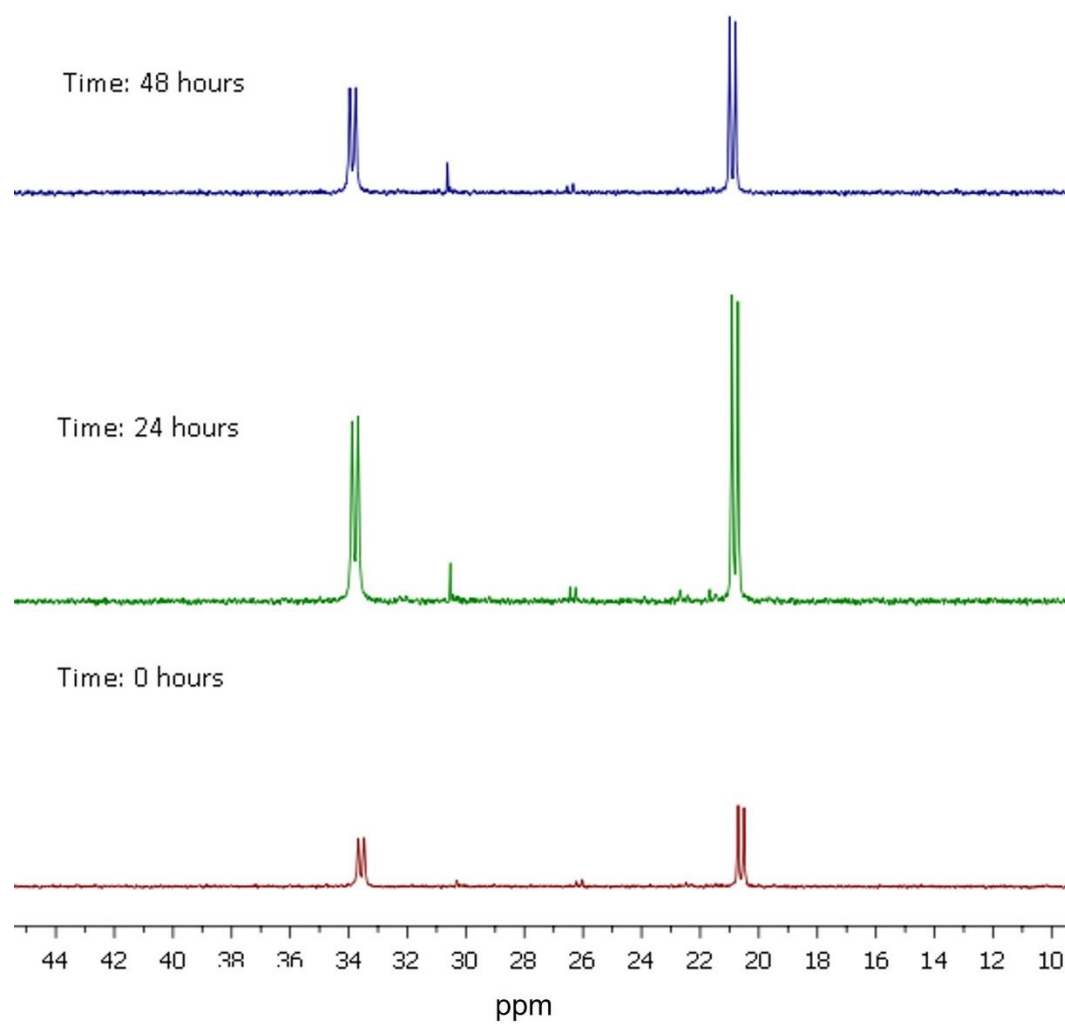
**Fig. S21** - Stern-Volmer plots for the quenching of HSA fluorescence by A)  $[\text{RuCl}(\text{NO})(\text{Ala})(\text{dppb})]\text{PF}_6$ , B)  $[\text{RuCl}(\text{NO})(\text{Phe})(\text{dppb})]\text{PF}_6$  and C)  $[\text{RuCl}(\text{NO})(\text{Val})(\text{dppb})]\text{PF}_6$ .



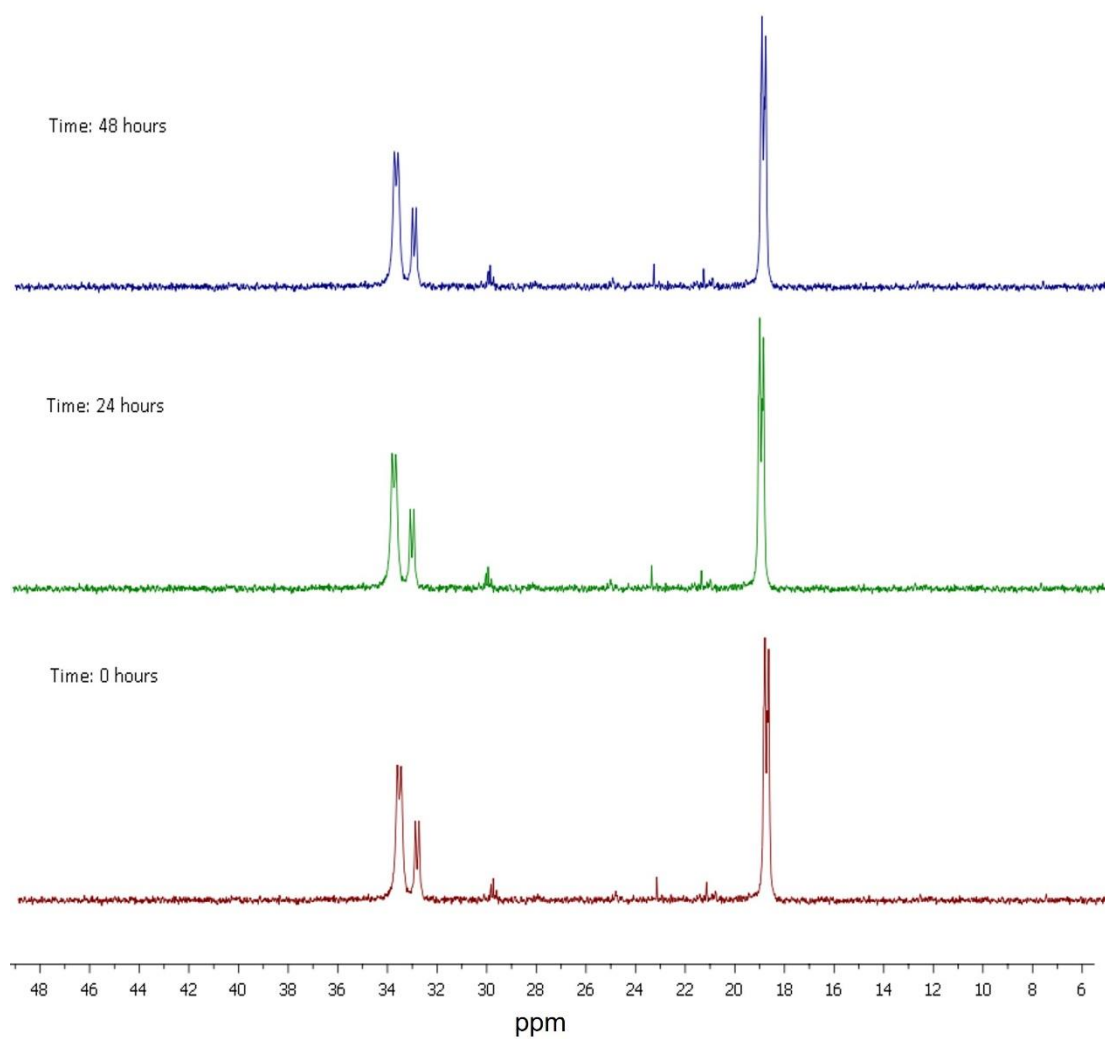
**Fig. S22** - Fluorescence spectrum of A) HSA +  $[\text{RuCl}(\text{NO})(\text{Ala})(\text{dppb})]\text{PF}_6$ , B) HSA +  $[\text{RuCl}(\text{NO})(\text{Phe})(\text{dppb})]\text{PF}_6$  and C) HSA +  $[\text{RuCl}(\text{NO})(\text{Val})(\text{dppb})]\text{PF}_6$ . Concentration da HSA =  $5.0 \mu\text{mol L}^{-1}$ ,  $\lambda_{\text{ex.}} = 280 \text{ nm}$ , pH = 7.4 e T = 298 K.



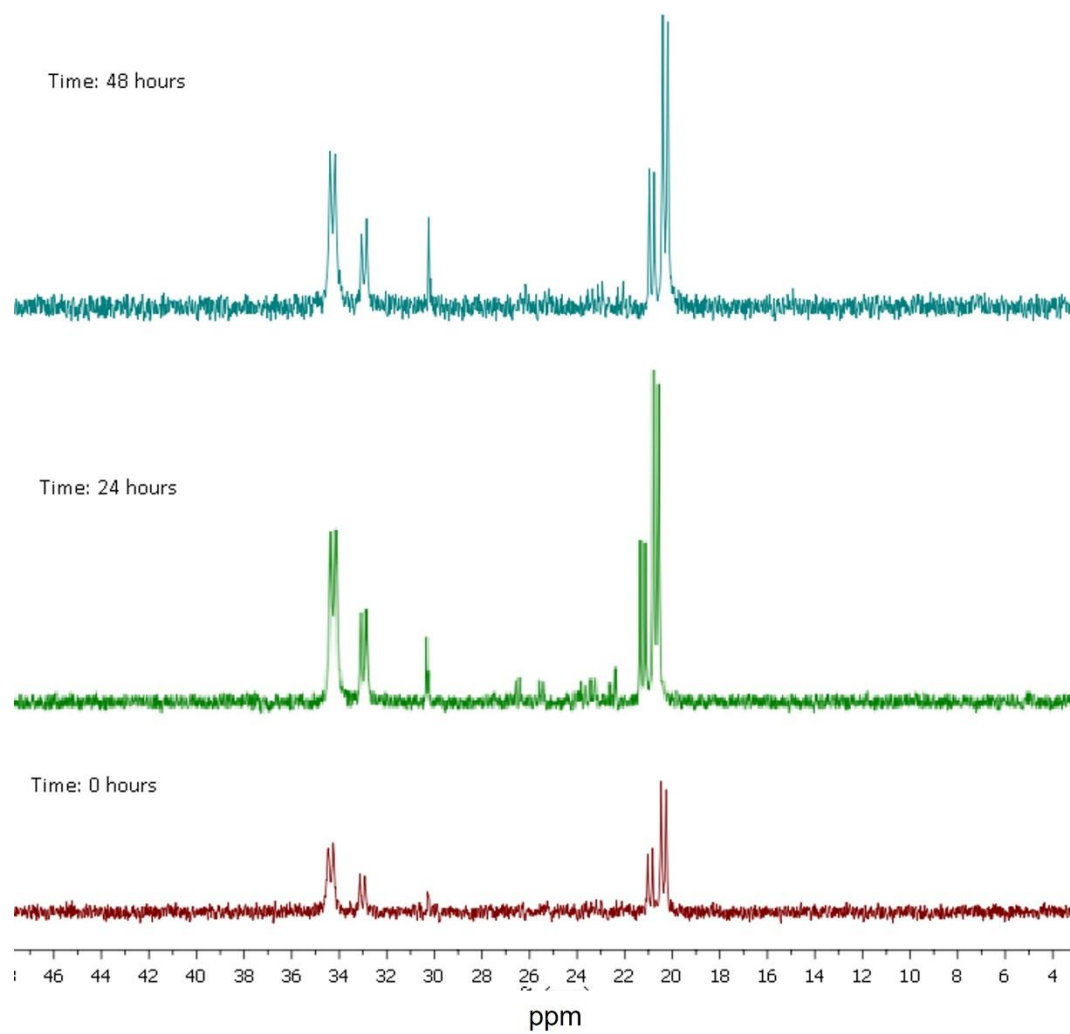
**Fig. S23** - Plot of  $\log[(F_0 - F) / F]$  vs.  $\log[Q]$ : **A)** [RuCl(NO)(Gly)(dppb)]PF<sub>6</sub>; **B)** [RuCl(NO)(Ala)(dppb)]PF<sub>6</sub>, **C)** [RuCl(NO)(Phe)(dppb)]PF<sub>6</sub> and **D)** [RuCl(NO)(Val)(dppb)]PF<sub>6</sub>.



**Fig. S24** -  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum for **1**, in  $\text{DMSO-d}_6$

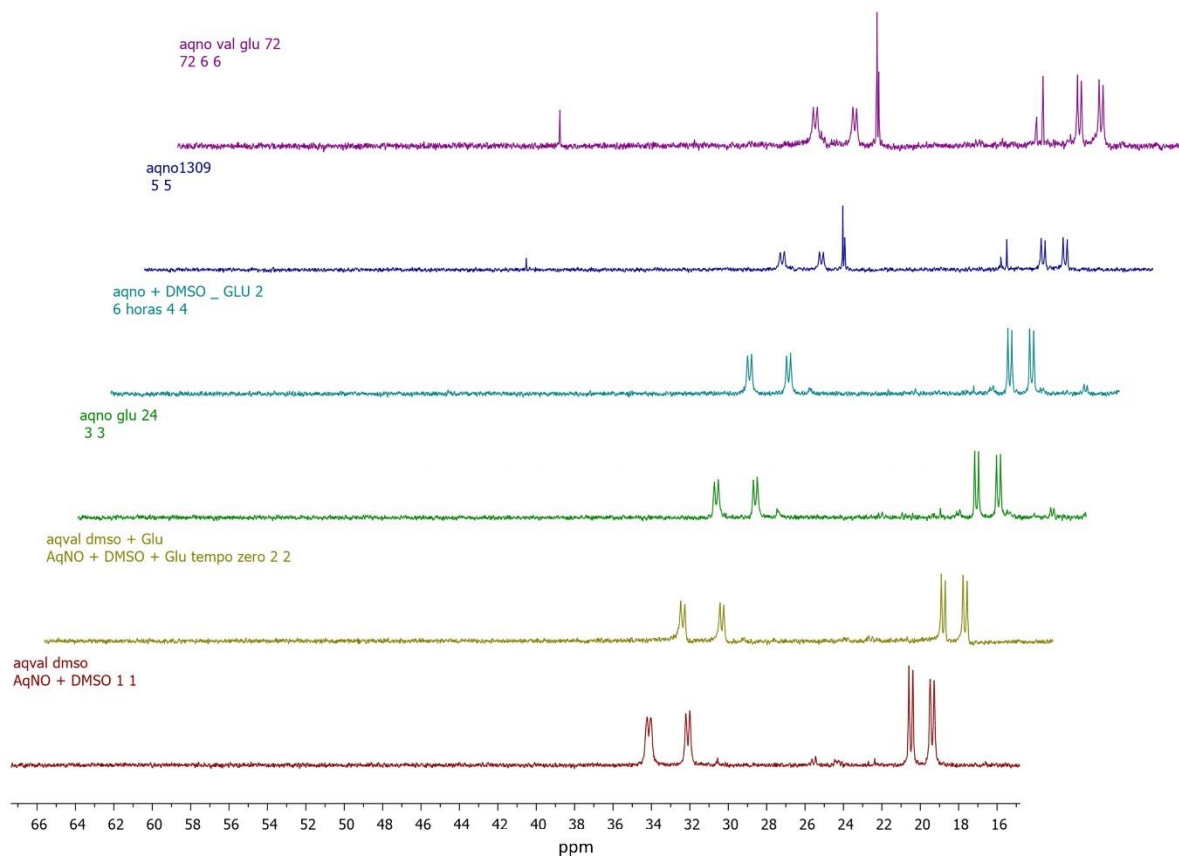


**Fig. S25** -  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum for **2**, in  $\text{DMSO-d}_6$

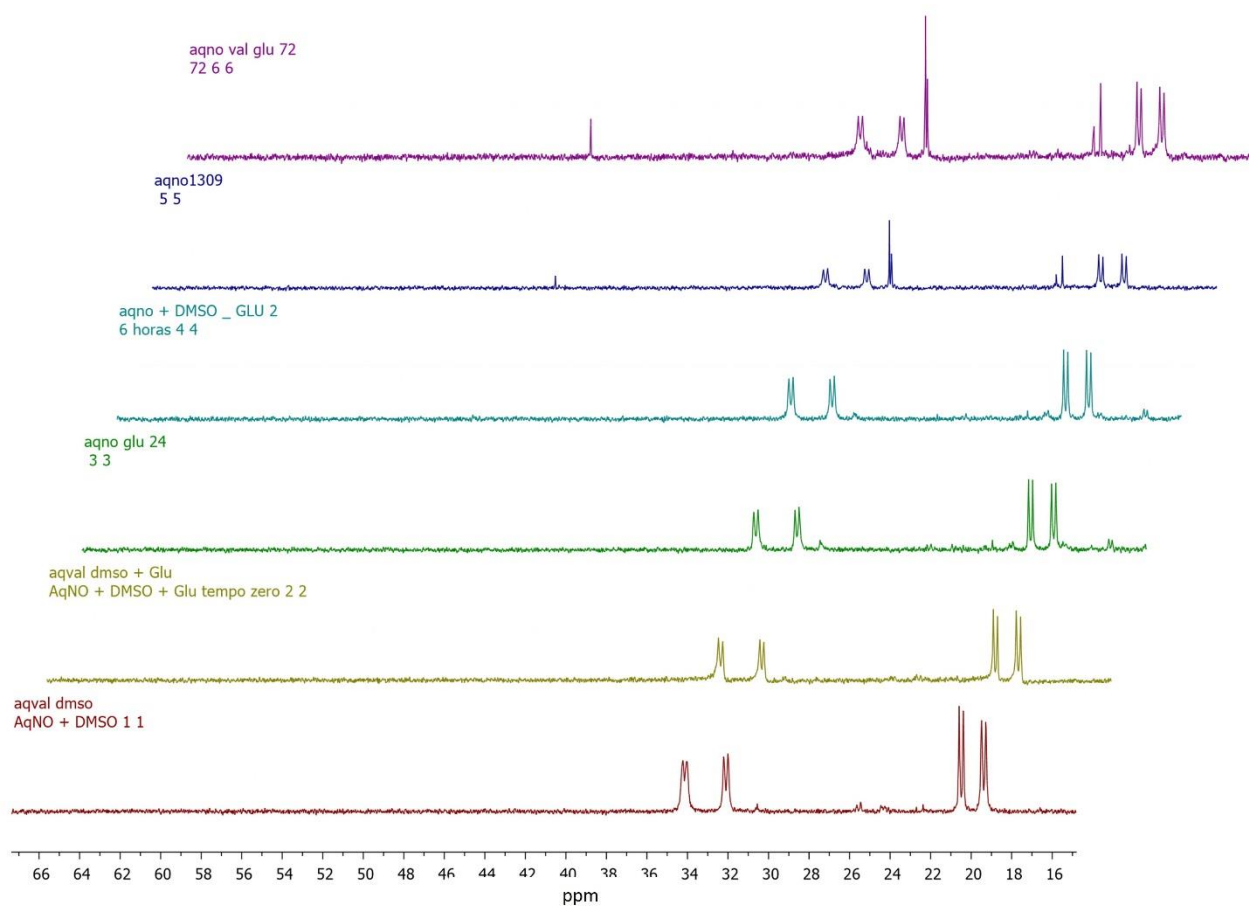


**Fig. S26** -  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum for **3**, in  $\text{DMSO-d}_6$





**Fig. S27** -  $^{31}\text{P}\{^1\text{H}\}$  NMR (using an external capillary with  $\text{D}_2\text{O}$ ), compound (**1**), DMSO/DMEM / GSH solution 1:1:5. (Time: 0, 6, 24, 48 and 72 hours).



**Fig. S28** -  $^{31}\text{P}\{^1\text{H}\}$  NMR (using an external capillary with  $\text{D}_2\text{O}$ ), compound (4), DMSO/DMEM /GSH solution 1:1:5. (Time: 0, 6, 24, 48 and 72 hours).