

Preparation of Tryptanthrin Derivates Bearing a Thiosemicarbazone Moiety to Inhibit SARS-CoV-2 Replication

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Context>

Figure S1: Titration and titration curves of **PAA-TSC** receptor with Fe(III) ion

Figure S2: Titration and titration curves of **PAA-TSC** receptor with Fe(II) ion

Figure S3: Titration and titration curves of **T8H-TSC** receptor with Cu(II) ion

Figure S4: Titration and titration curves of **T8H-TSC** receptor with Fe(III) ion

Figure S5: Titration and titration curves of **T8H-TSC** receptor with Fe(II) ion

Figure S6: Colour change after addition of Cu(II) ion to receptors (**PAA-TSC** and **T8H-TSC**)

Figure S7: Infrared spectra of **PAA-TSC** receptor and its complex with Cu(II) ion

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Figure S9: Infrared spectra of **T8H-TSC** receptor and its complex with Cu(II) ion

Figure S10: Raman spectra of **T8H-TSC** receptor and its complex with Cu(II) ion.

Table S1: Determination of limit of detection and linear range for **PAA-TSC** and **T8H-TSC** complexes with Cu (II) and Fe(II/III)

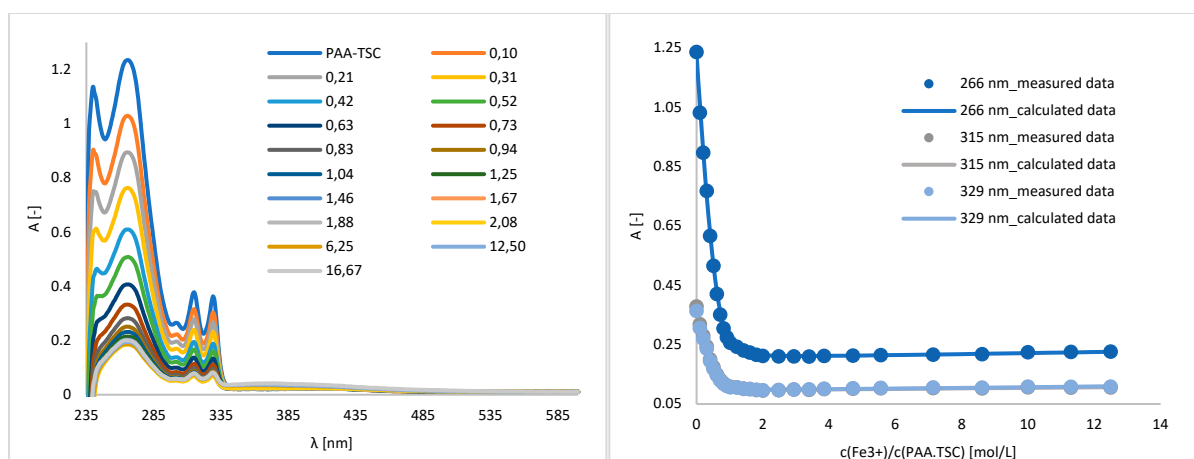


Figure S1: Titration and titration curves of **PAA-TSC** receptor with Fe(III) ion in water (water/DMSO, 99:1, v/v). Titration curves were measured at the absorption maxima (266 nm, 315 nm, 329 nm) of **PAA-TSC** receptor.

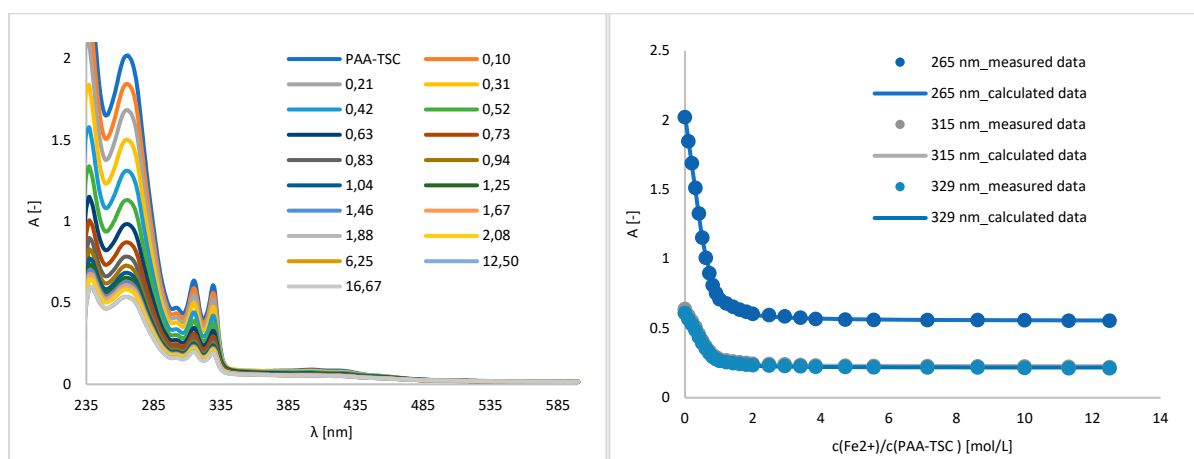


Figure S2: Titration and titration curves of **PAA-TSC** receptor with Fe(II) ion in water (water/DMSO, 99:1, v/v). Titration curves were measured at the absorption maxima (265 nm, 315 nm, 329 nm) of **PAA-TSC** receptor.

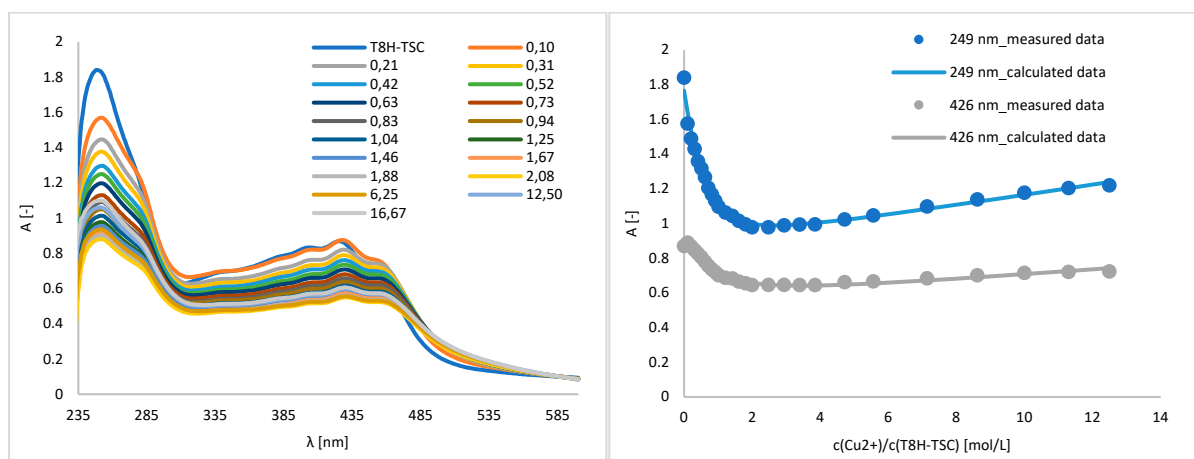


Figure S3: Titration and titration curves of **T8H-TSC** receptor with Cu(II) ion in water (water/DMSO, 99:1, v/v). Titration curves were measured at the absorption maxima (249 nm, 426 nm) of **T8H-TSC** receptor.

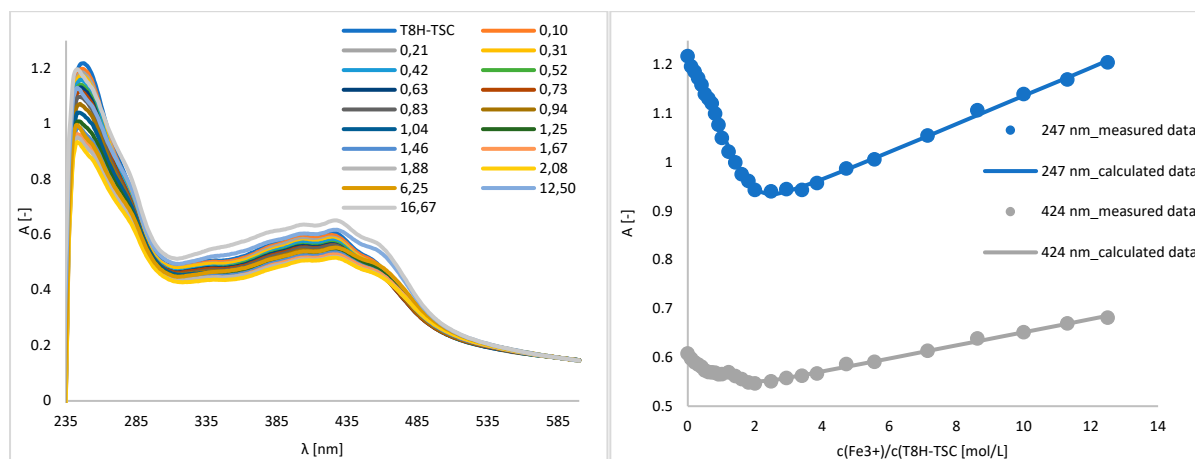


Figure S4: Titration and titration curves of **T8H-TSC** receptor with Fe(III) ion in water (water/DMSO, 99:1, v/v). Titration curves were measured at the absorption maxima (247 nm, 424 nm) of **T8H-TSC** receptor.

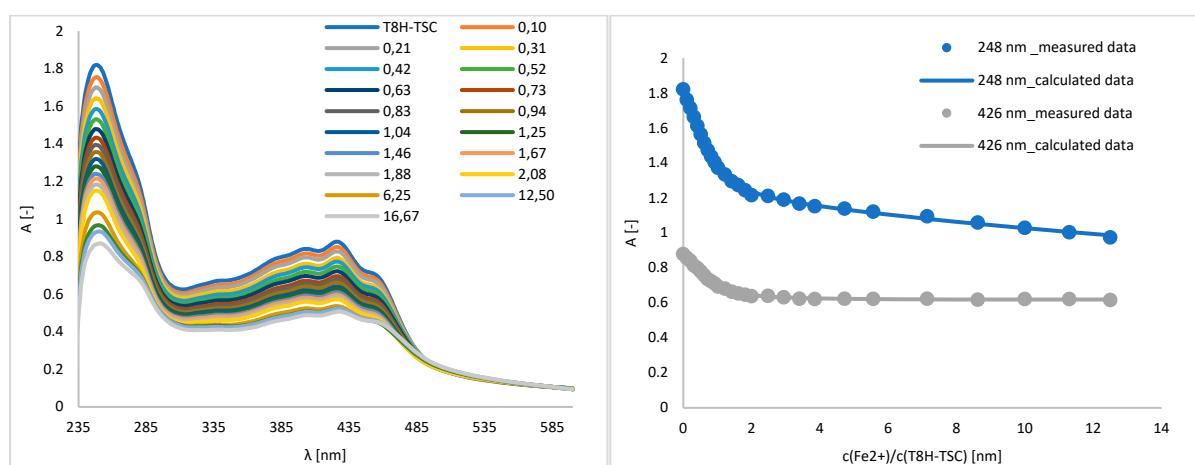


Figure S5: Titration and titration curves of **T8H-TSC** receptor with Fe(II) ion in water (water/DMSO, 99:1, v/v). Titration curves were measured at the absorption maxima (248 nm, 426 nm) of **T8H-TSC** receptor.



Figure S6: Colour change after addition of Cu(II) ion to receptors (**PAA-TSC** and **T8H-TSC**). **PAA-TSC** receptor (left) showed a green coloration of the solution and **T8H-TSC** receptor (right) showed a brown coloration of the solution. Receptors were dissolved in dichloromethane in 1:1 ratio.

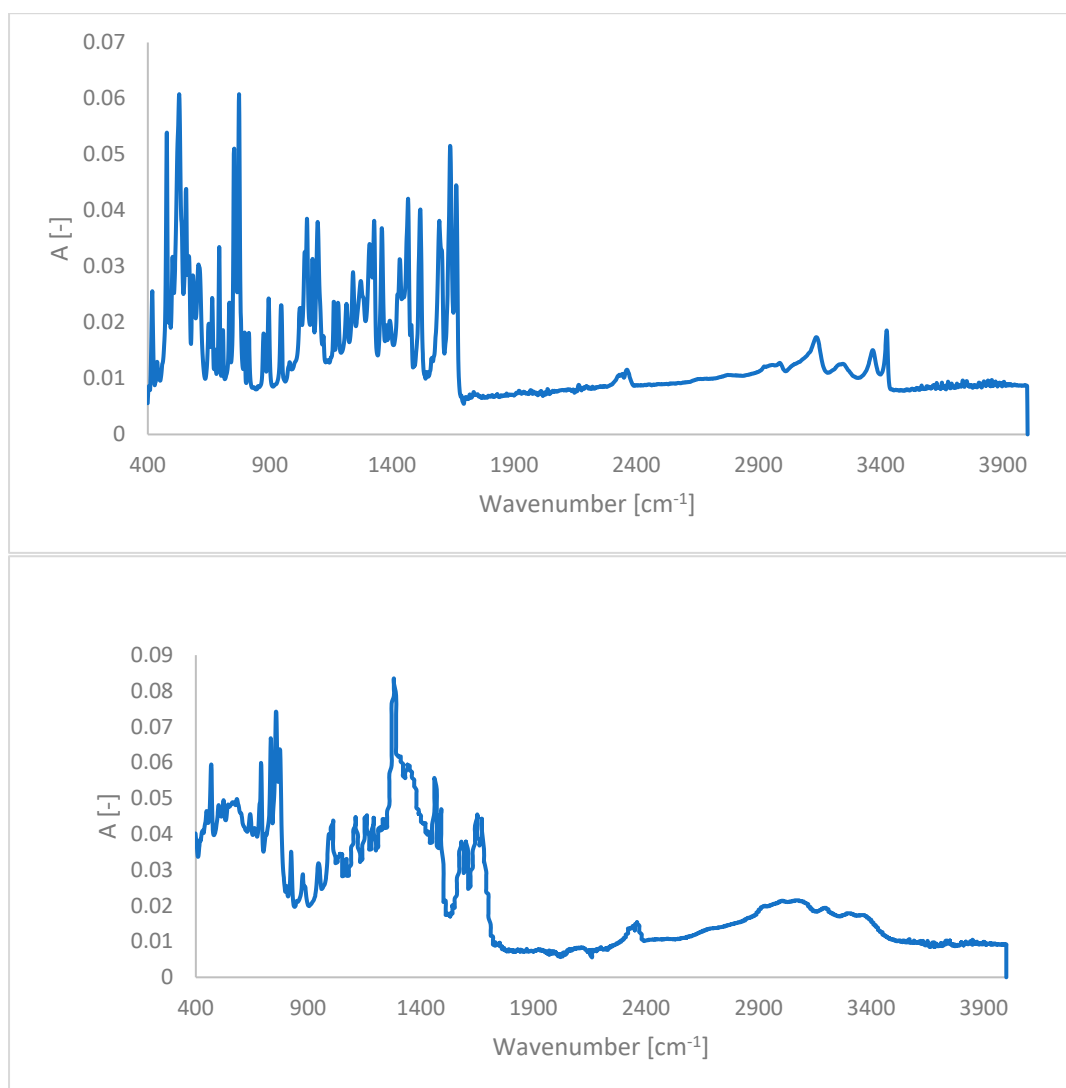


Figure S7: Infrared spectra of **PAA-TSC** receptor (up) and its complex with Cu(II) ion (down).

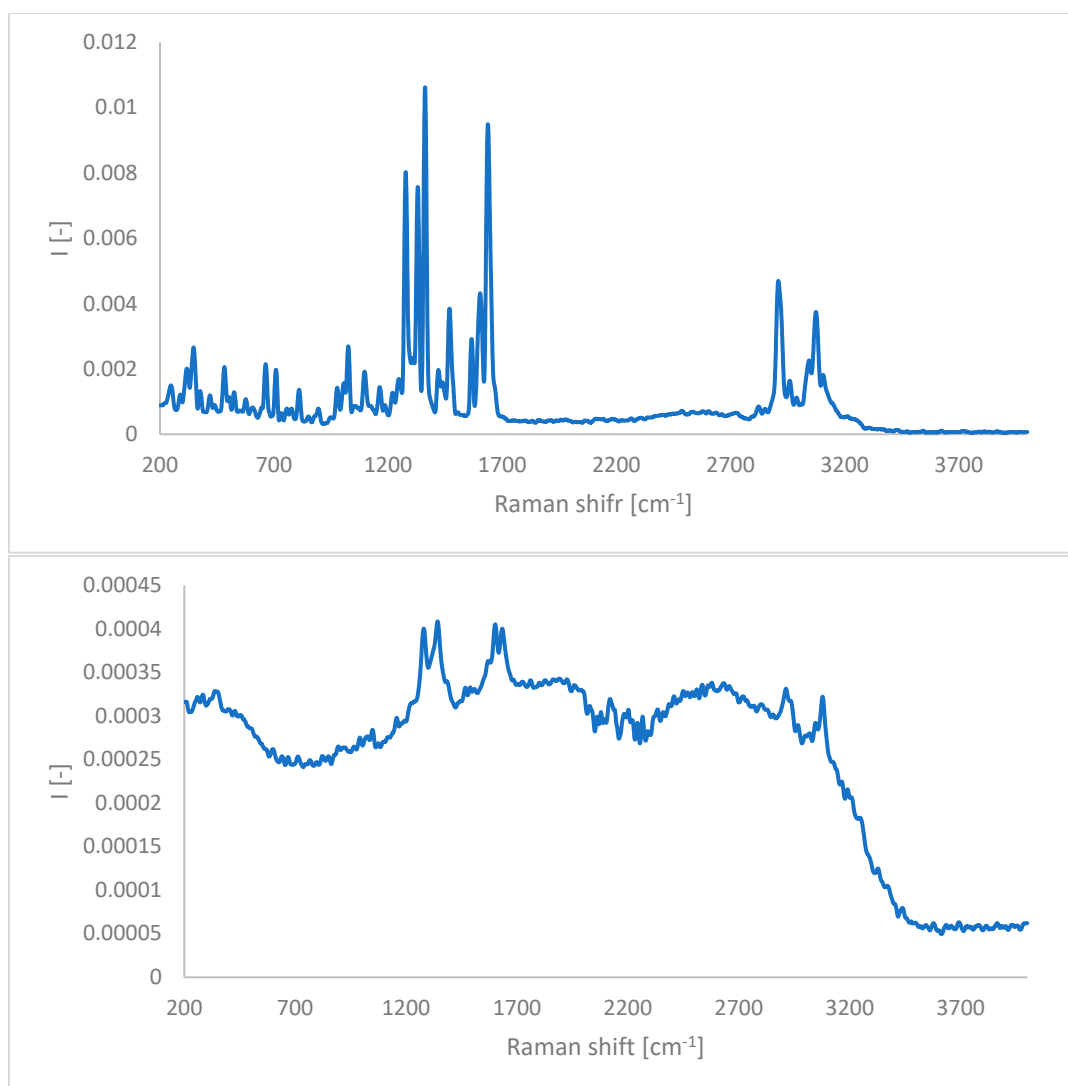


Figure S8: Raman spectra of **PAA-TSC** receptor (up) and its complex with Cu(II) ion (down).

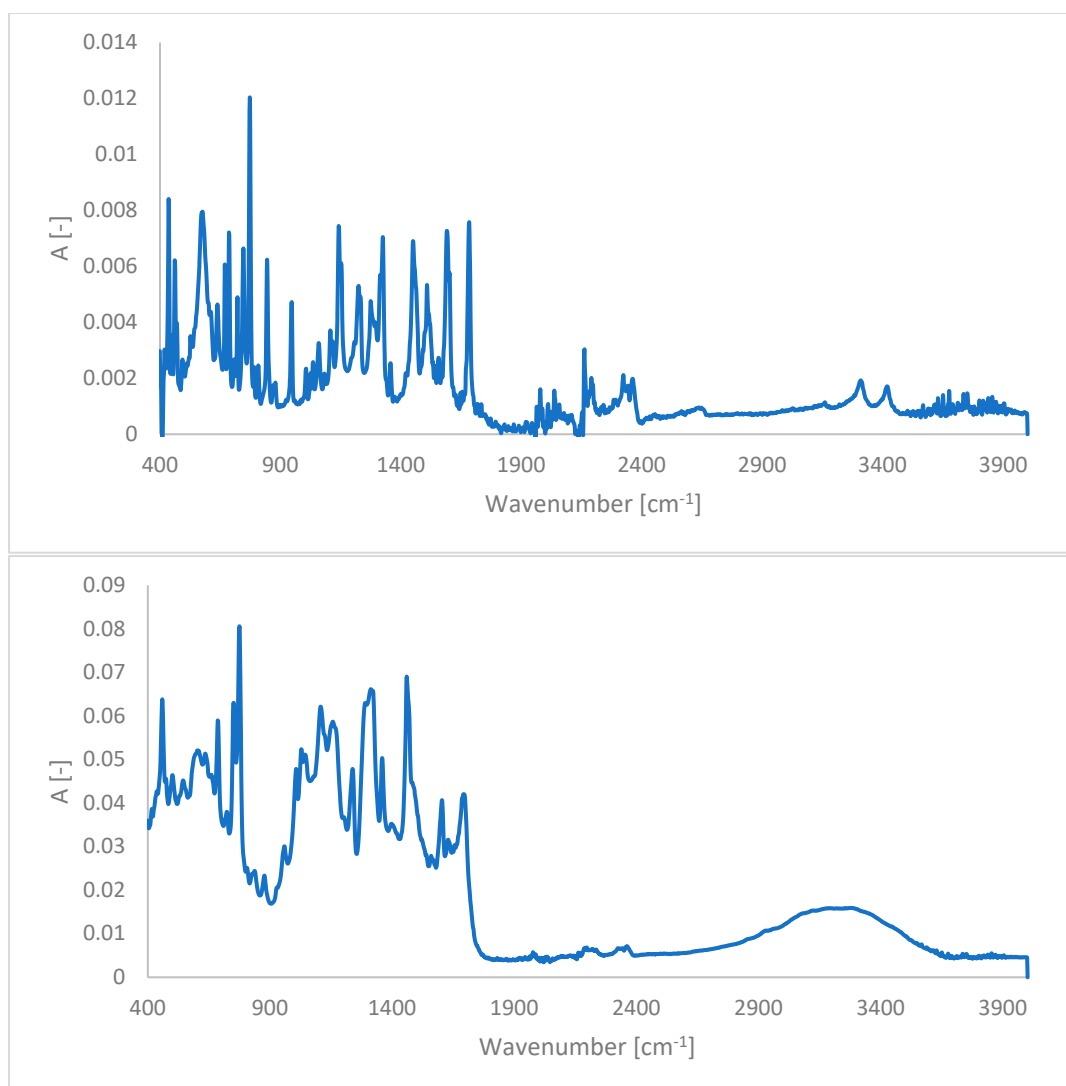


Figure S9: Infrared spectra of **T8H-TSC** receptor (up) and its complex with Cu(II) ion (down).

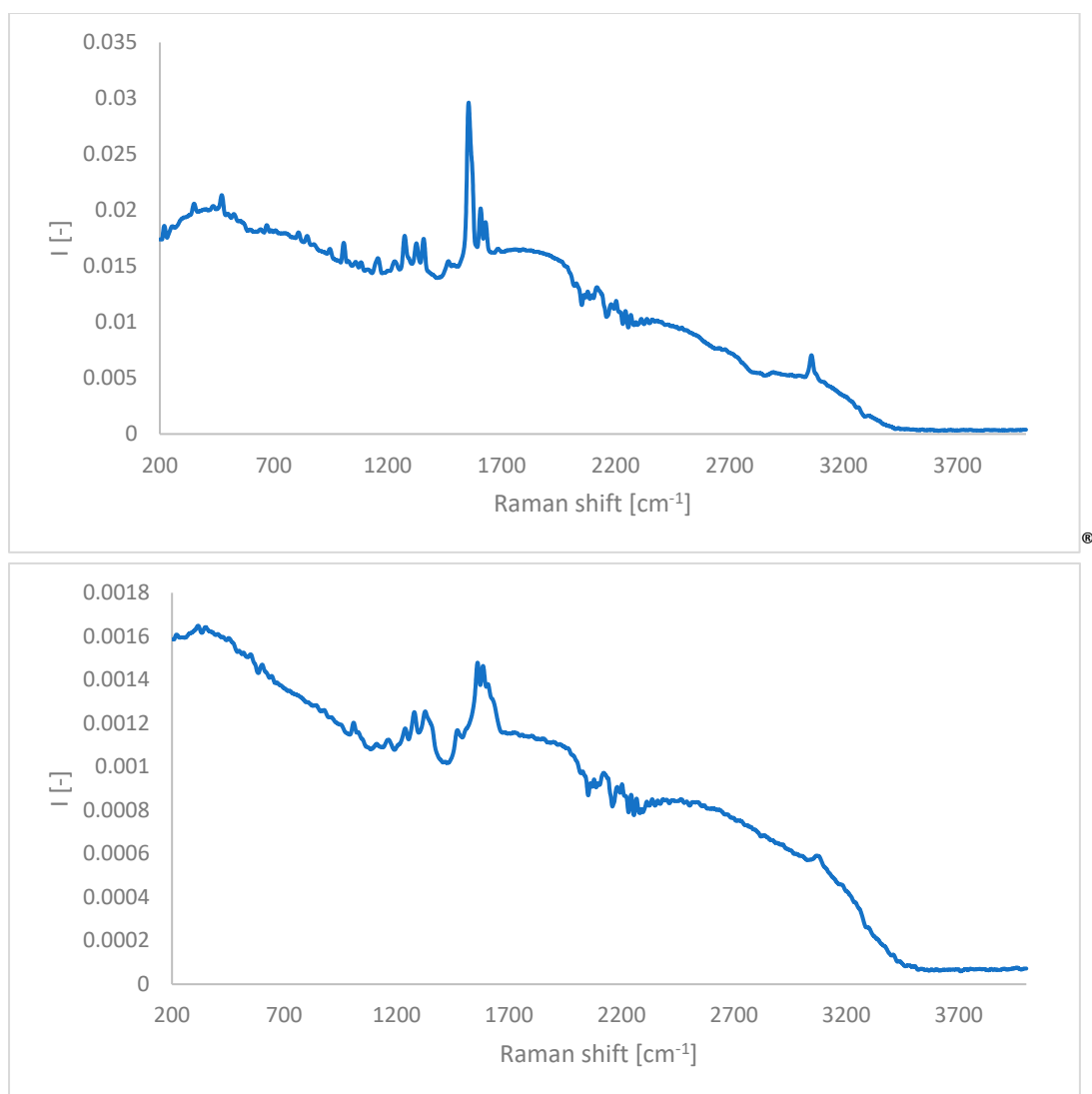


Figure S10: Raman spectra of **T8H-TSC** receptor (up) and its complex with Cu(II) ion (down).

Table S1: Determination of limit of detection and linear range for PAA-TSC and T8H-TSC complexes with Cu(II) and Fe(II/III) in their absorption maxima.

Compound	Wavelength	Limit of detection [M]	Linear range [M]
PAA-TSC -Cu(II)	265	$1.14 \cdot 10^{-5}$	$0\text{-}5 \cdot 10^{-5}$
	315	$1.33 \cdot 10^{-5}$	
	329	$1.74 \cdot 10^{-5}$	
PAA-TSC -Fe(III)	265	$8.29 \cdot 10^{-6}$	$0\text{-}6 \cdot 10^{-5}$
	315	$7.63 \cdot 10^{-6}$	
	329	$7.63 \cdot 10^{-6}$	
PAA-TSC -Fe(II)	265	$9.43 \cdot 10^{-6}$	$0\text{-}7 \cdot 10^{-5}$

	315	$9.62 \cdot 10^{-6}$	$0-8 \cdot 10^{-5}$
	329	$9.67 \cdot 10^{-6}$	
T8H-TSC-Cu(II)	249	$2.75 \cdot 10^{-6}$	$0-8 \cdot 10^{-5}$
	426	$1.01 \cdot 10^{-5}$	$0-1 \cdot 10^{-4}$
T8H-TSC-Fe(III)	247	$1.63 \cdot 10^{-5}$	$0-1.6 \cdot 10^{-4}$
	424	$6.81 \cdot 10^{-6}$	$0-6.17 \cdot 10^{-5}$
T8H-TSC-Fe(II)	248	$6.60 \cdot 10^{-6}$	$0-1 \cdot 10^{-4}$
	426	$8.06 \cdot 10^{-6}$	