

Electronic Supporting Information

Structural conformations of calixarene-based receptors and their implications for molecular recognition.

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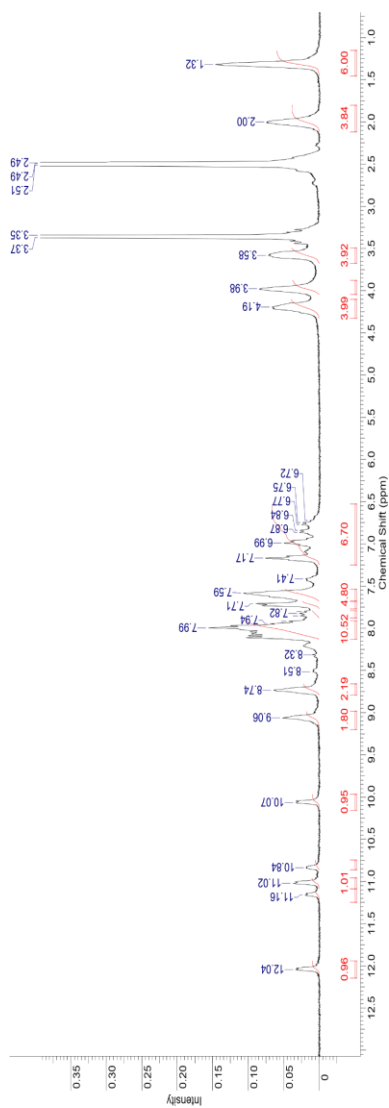
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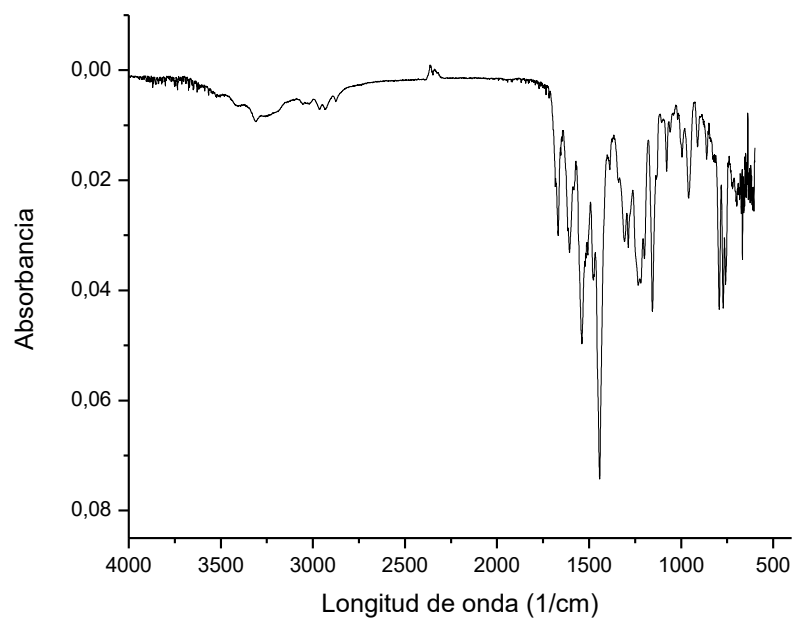
1.- Characterization of I; 5,17- N-(pyridin-2-yl)-2-naphthamide-thiosemicarbazone-25,27-dipropoxy- 26,28-dihydroxycalix[4]arene, pinched cone

Figure S1: Spectra for I: (a) ¹H NMR and (b) FT-IR.

(a) ¹H NMR

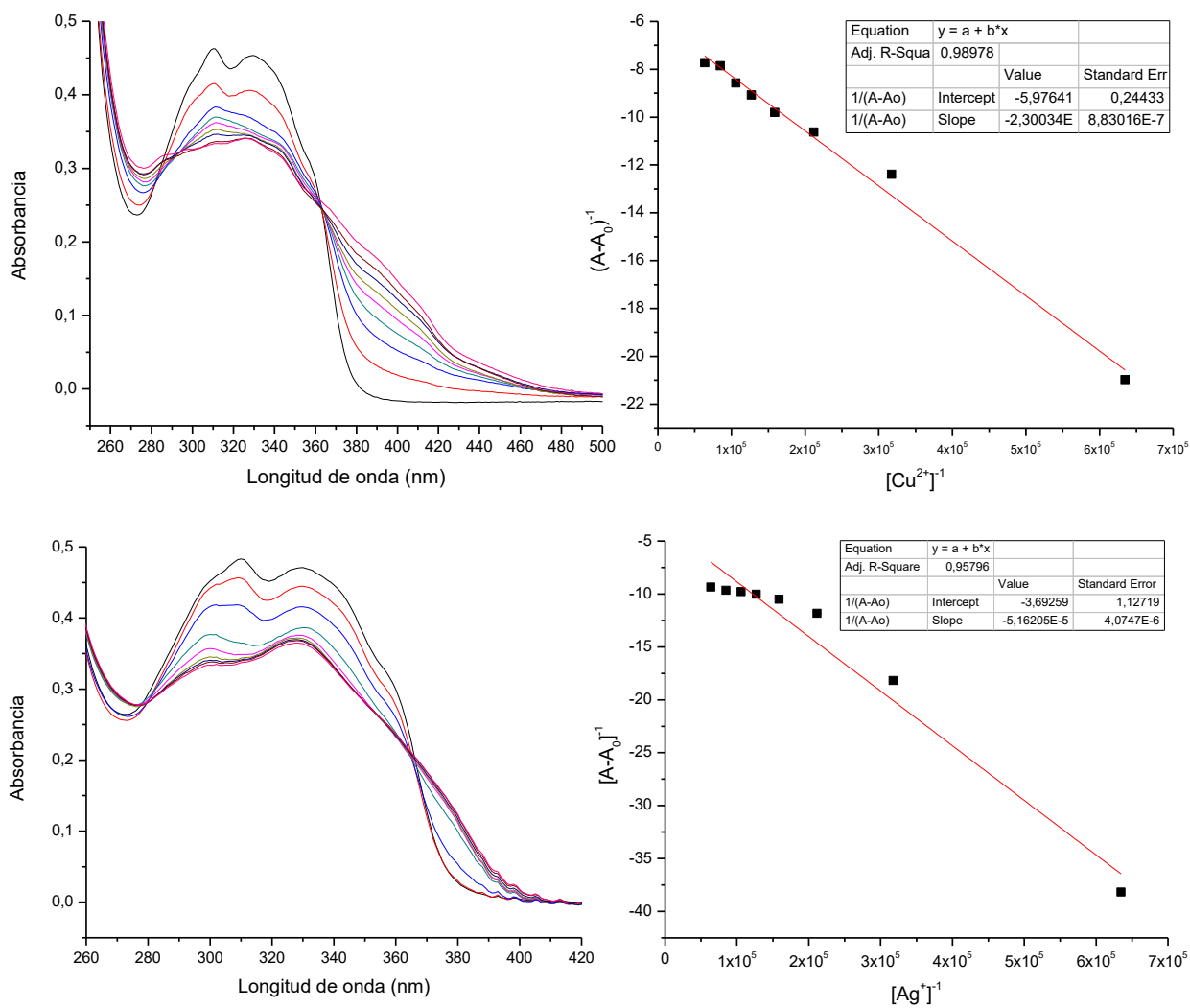


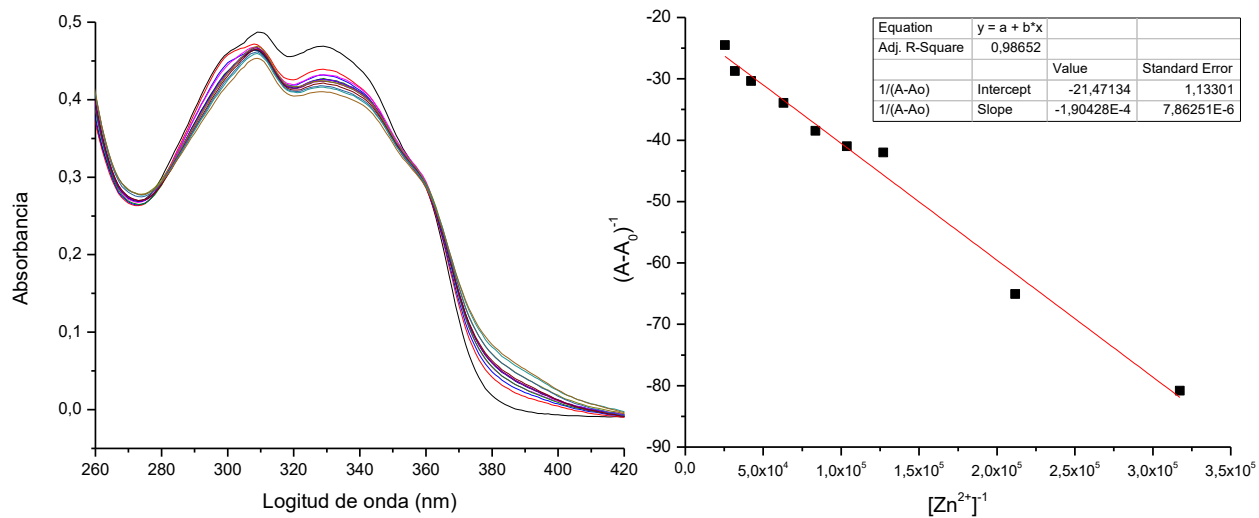
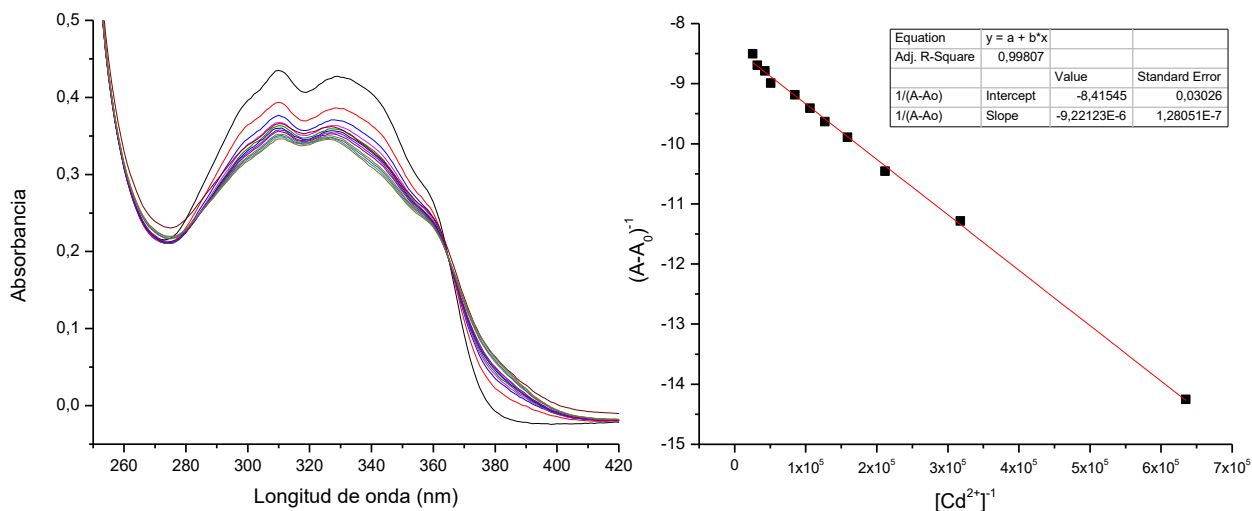
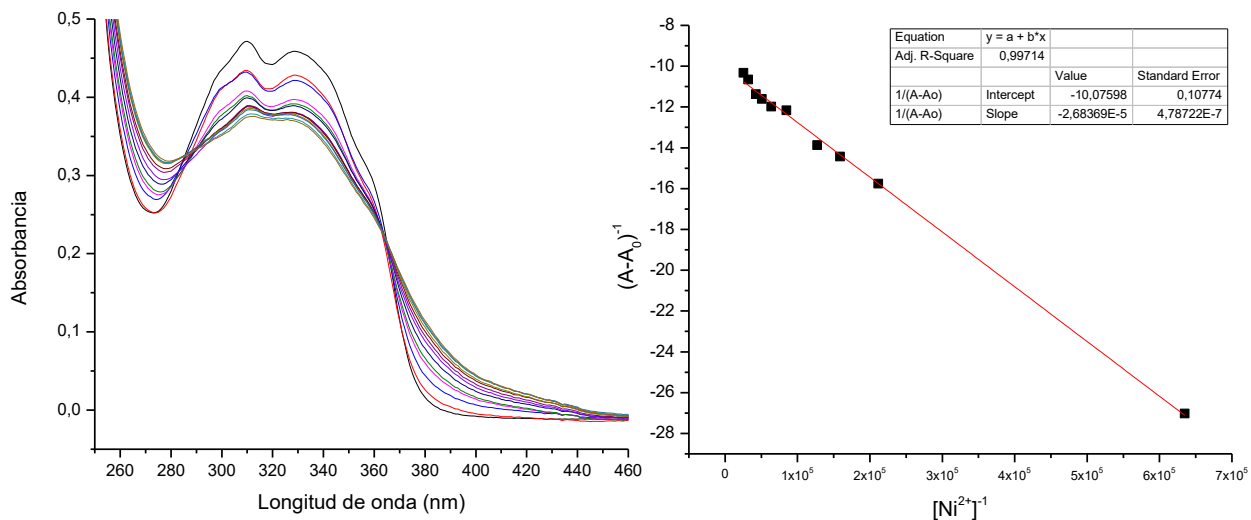
(b) FT-IR

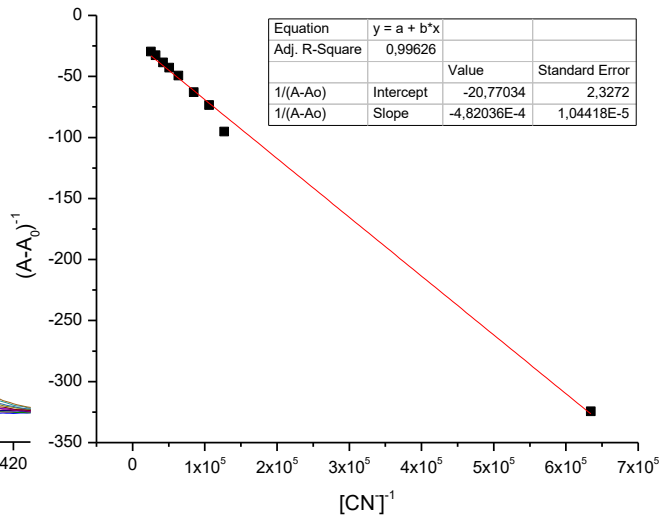
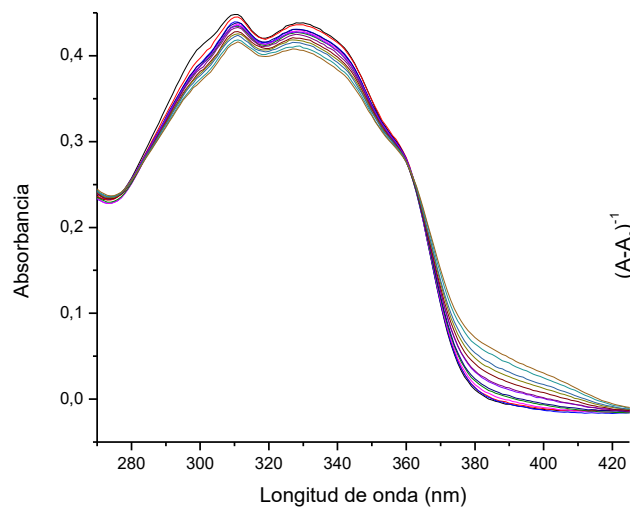
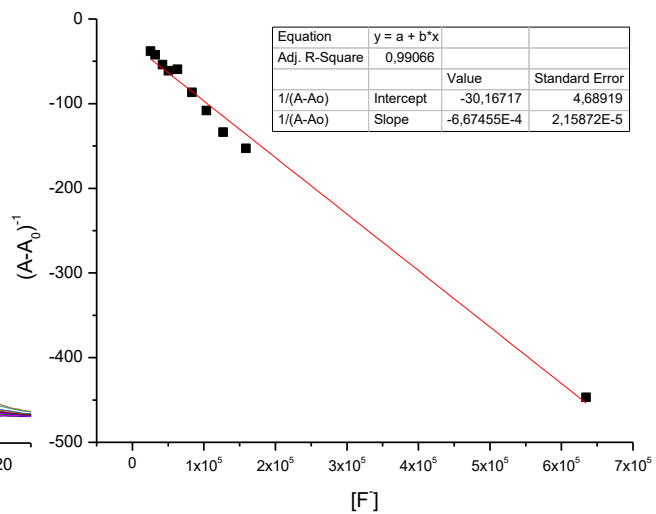
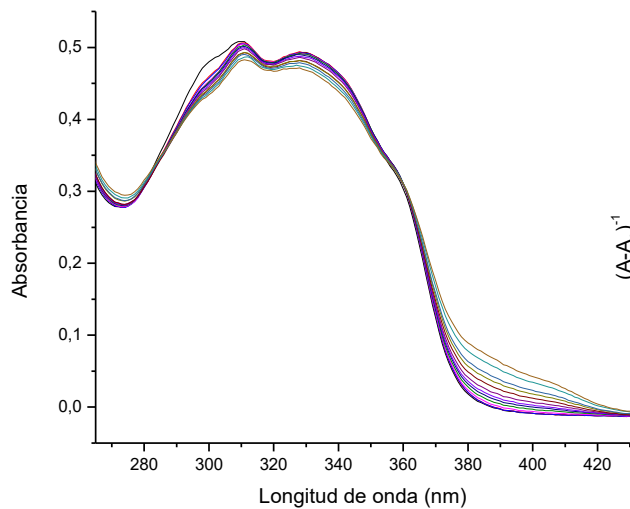


2.- Determination of the association constant by absorption titration.

Figure S2. The binding constant of I has been derived based on the Benesi–Hildebrand equation using absorption titration a) Cu^{2+} , b) Ag^+ , c) Ni^{2+} , d) Cd^{2+} , e) Zn^{2+} , f) F^- and g) CN^- .

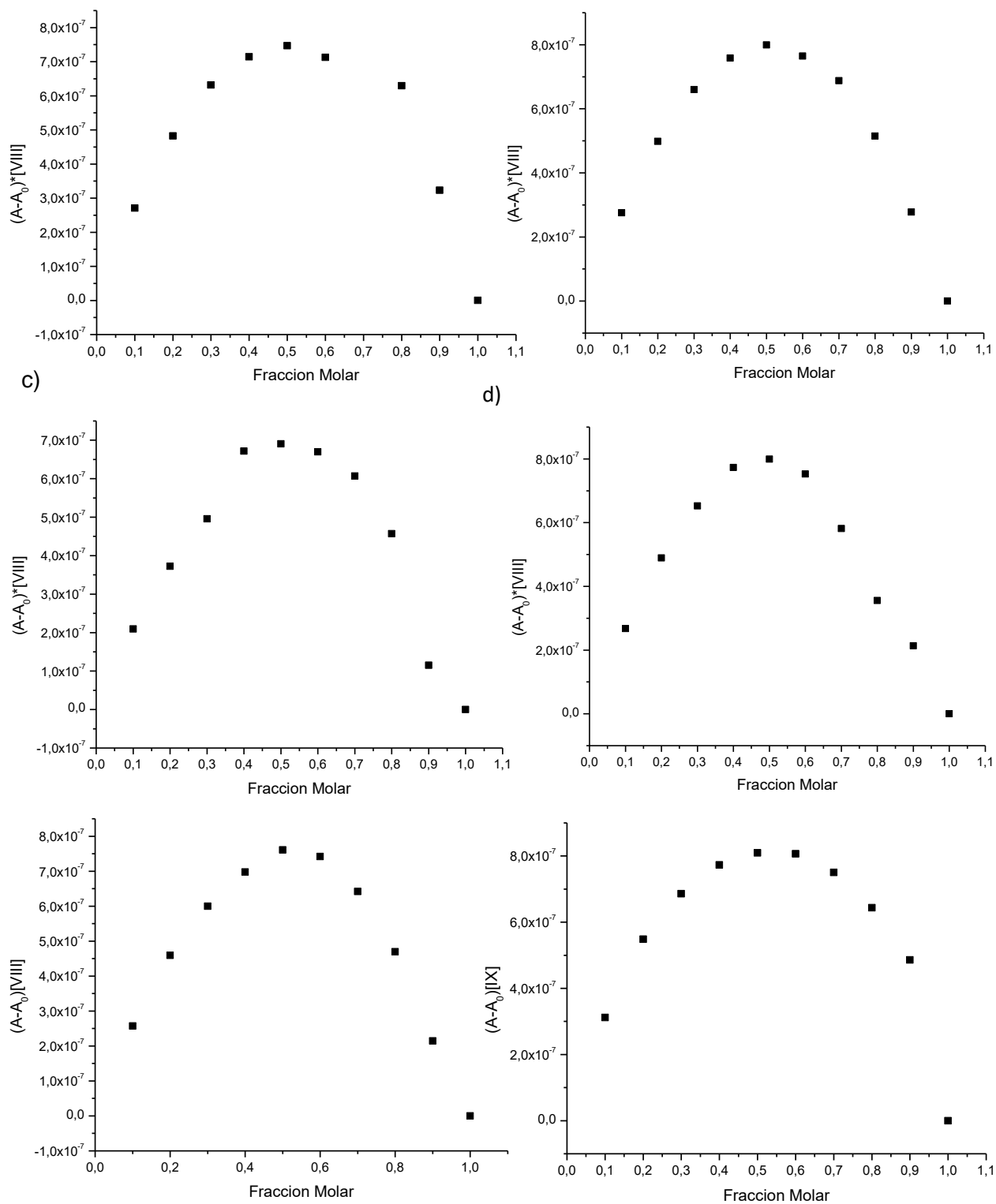


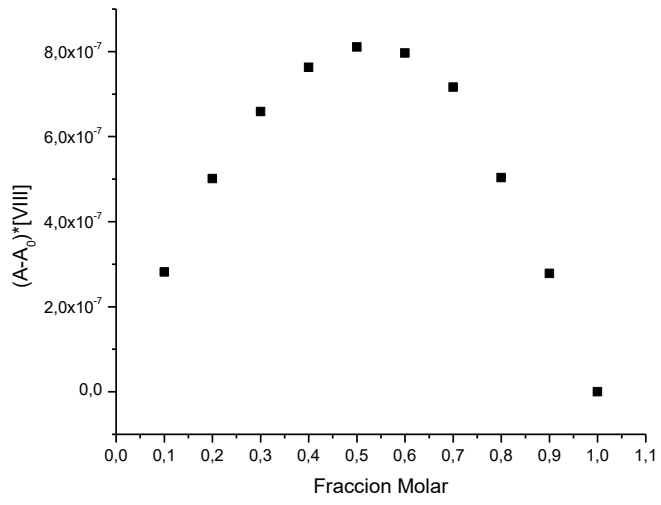




3.- Determination of the stoichiometry.

Figure S3. Continuous variation plot for receptor I from absorbance measurements in CH₃CN: a) Cu²⁺, b) Ag⁺, c) Ni²⁺, d) Cd²⁺, e) Zn²⁺, f) F⁻ and g) CN⁻.

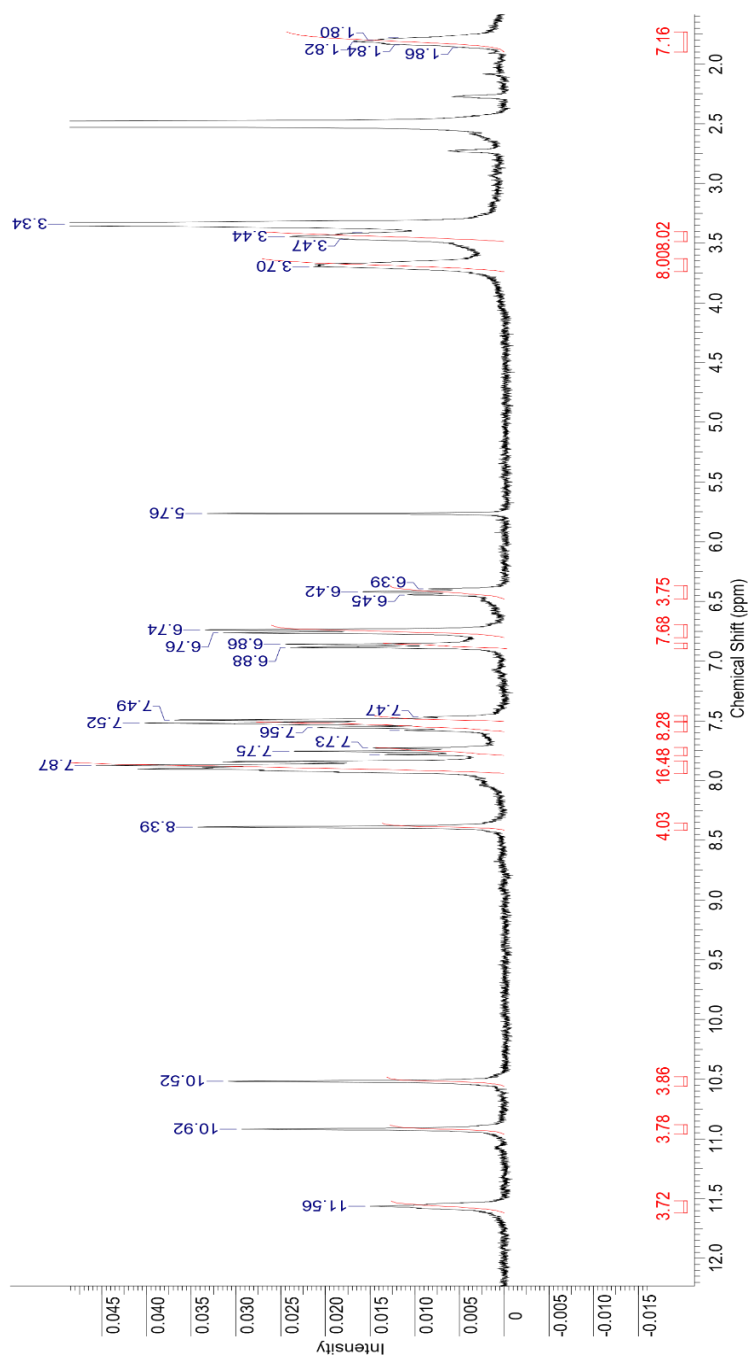




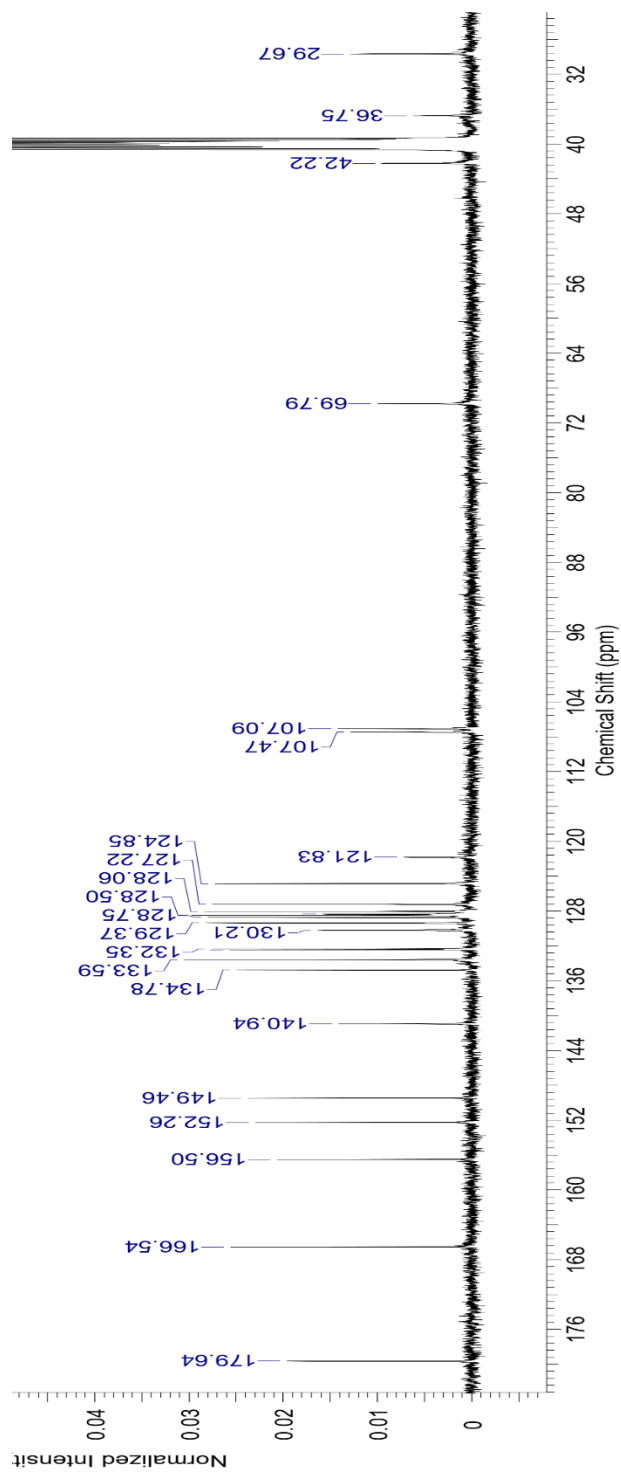
4.- Characterization of II; 25,26,27,28-tetra[3-(3-(6-(2-naphthamido)pyridin-2-yl)thioureido) propyloxy]calix[4]arene, 1,3-alternate.

Figure S1: Spectra for II: (a) ^1H NMR; (b) ^{13}C NMR; (c) FT-IR; and (d) ESI-TOF.

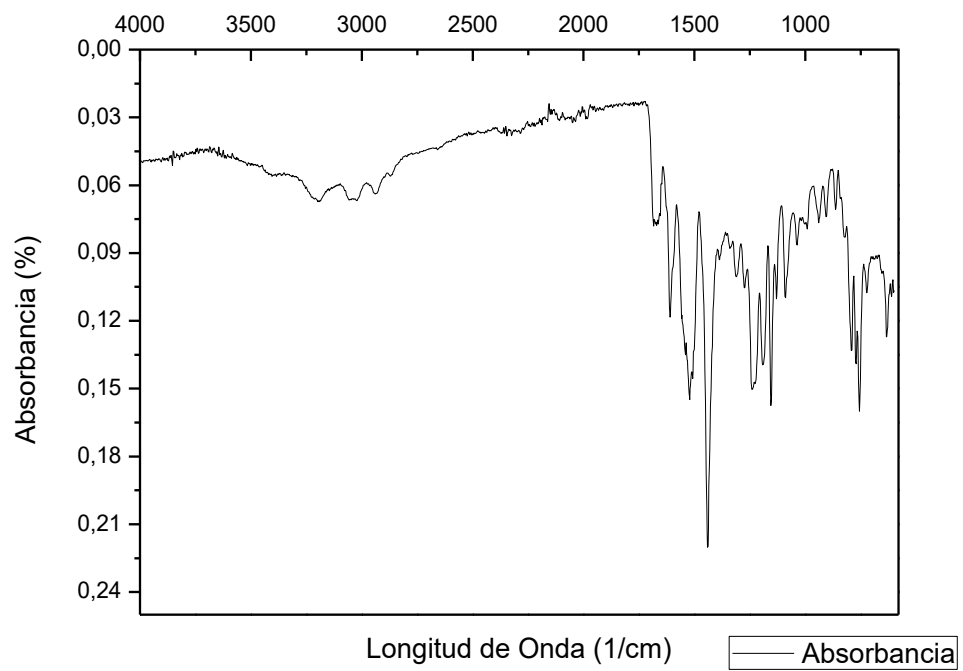
(a) ^1H NMR



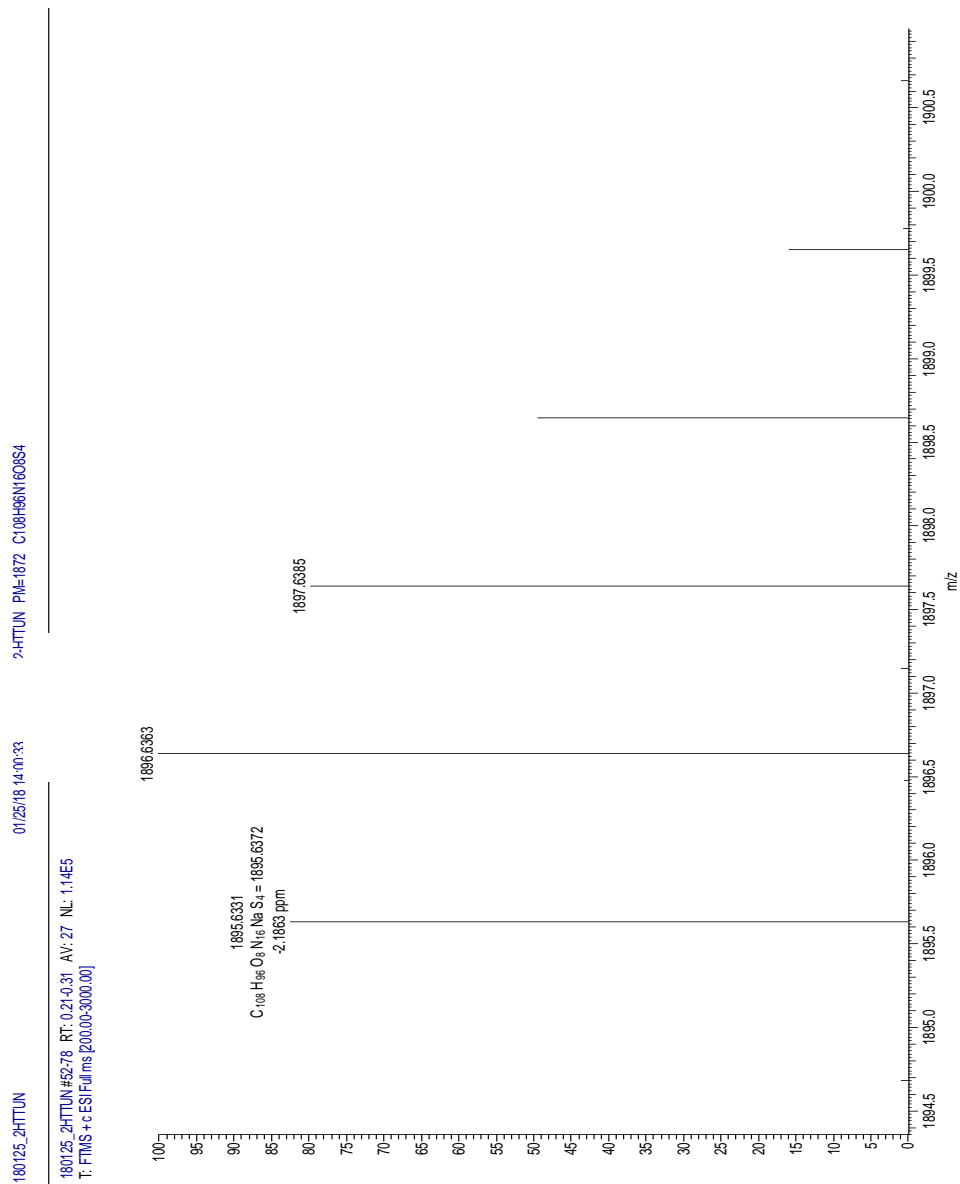
(b) ^{13}C NMR



(c) FT-IR

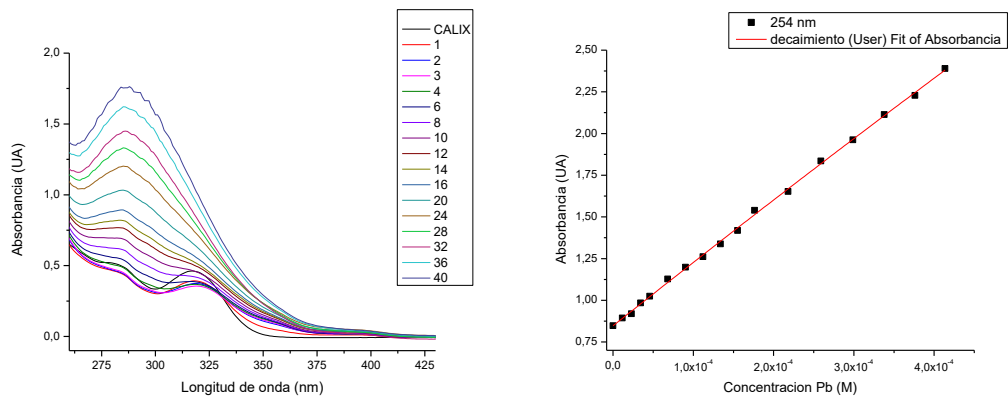


(d) ESI-TOF



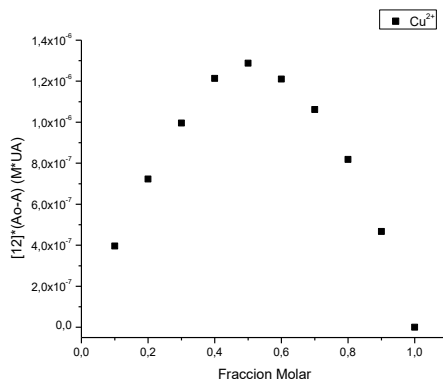
5.- Determination of the association constant by absorption titration.

Figure S2. The binding constant of II has been derived based on the Benesi–Hildebrand equation using absorption titration with (a) Cu^{2+} .



6.- Determination of the stoichiometry.

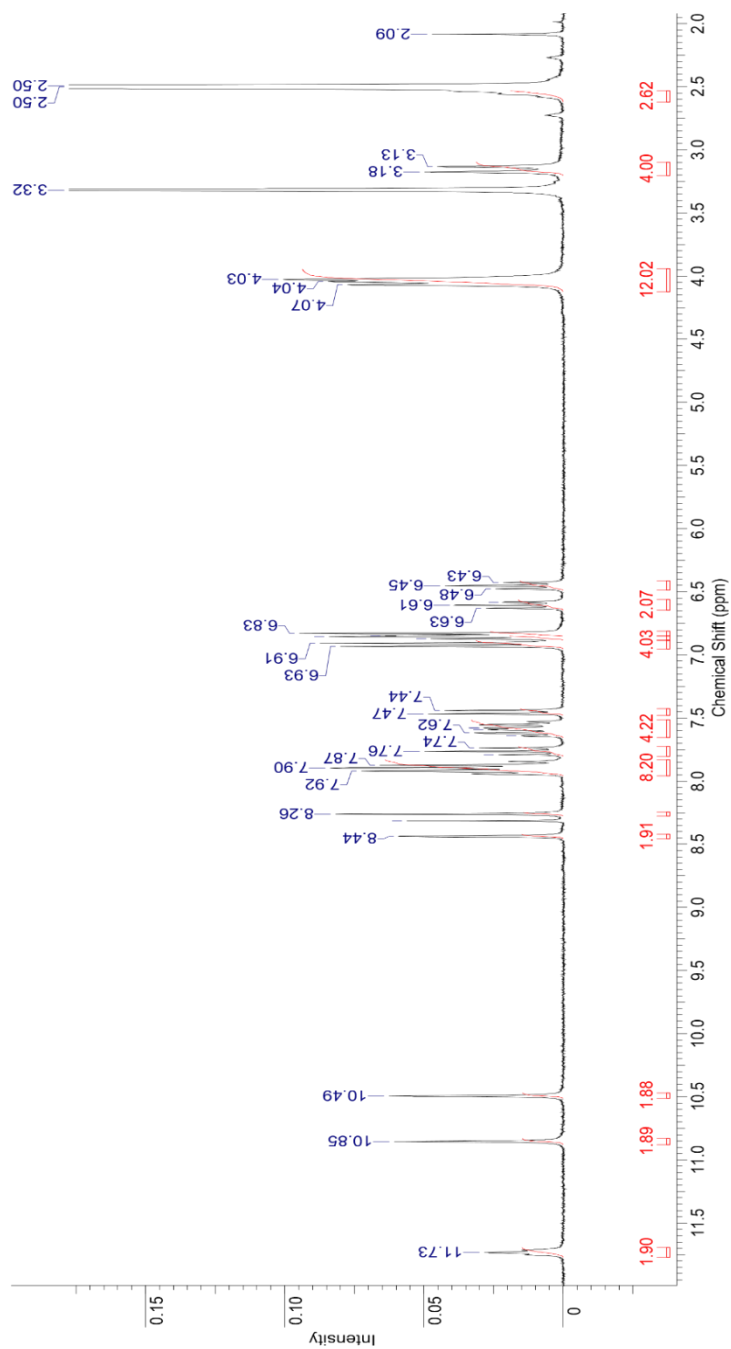
Figure S3. Continuous variation plot for receptor II from absorbance measurements in CH_3CN .



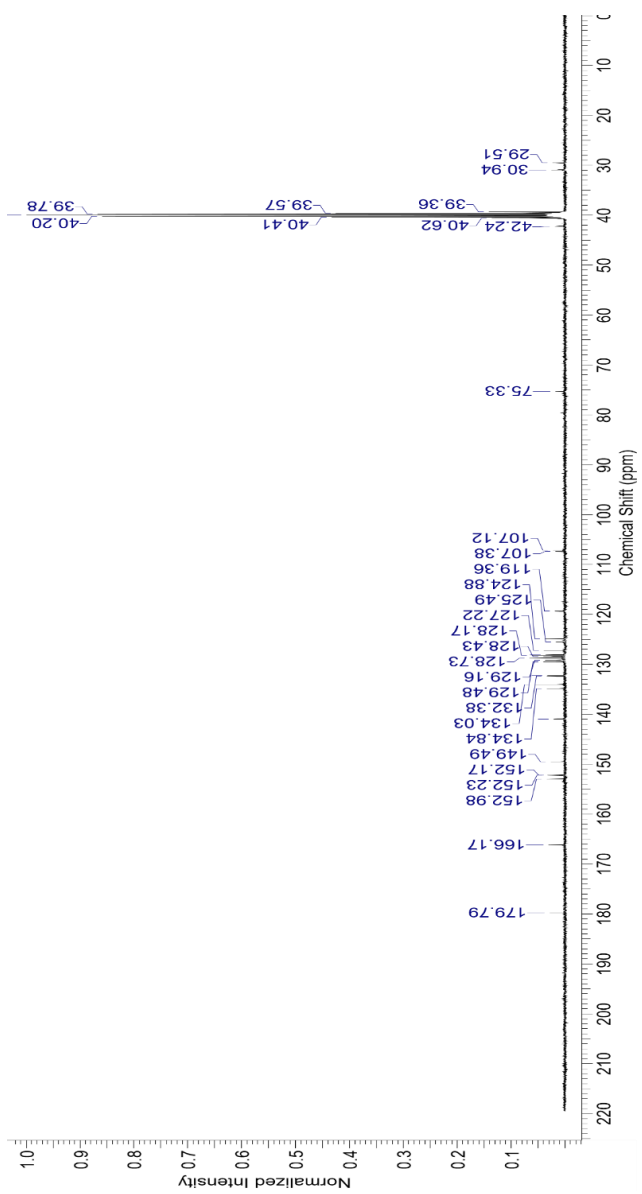
7.- Characterization of III; 25,27-bis[3-(6-(2-naphthamido)pyridin-2-thioureido)propyloxy]-26,28-dihydroxychalix[4]arene, cone.

Figure S1: Spectra for III: (a) ^1H NMR; (b) ^{13}C NMR; (c) FT-IR and (d) ESI-TOF.

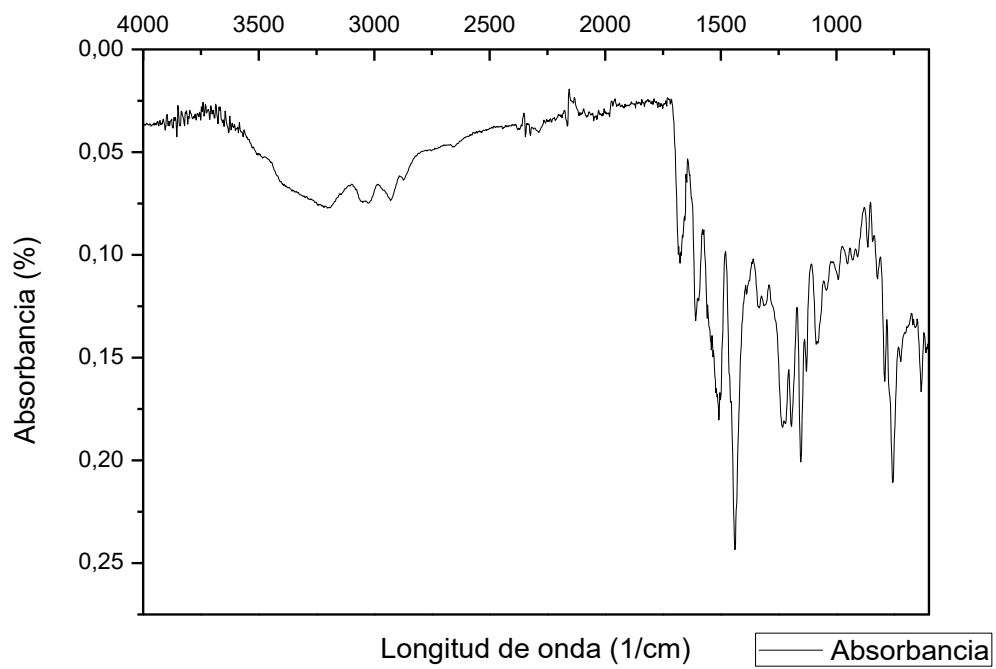
(a) ^1H NMR



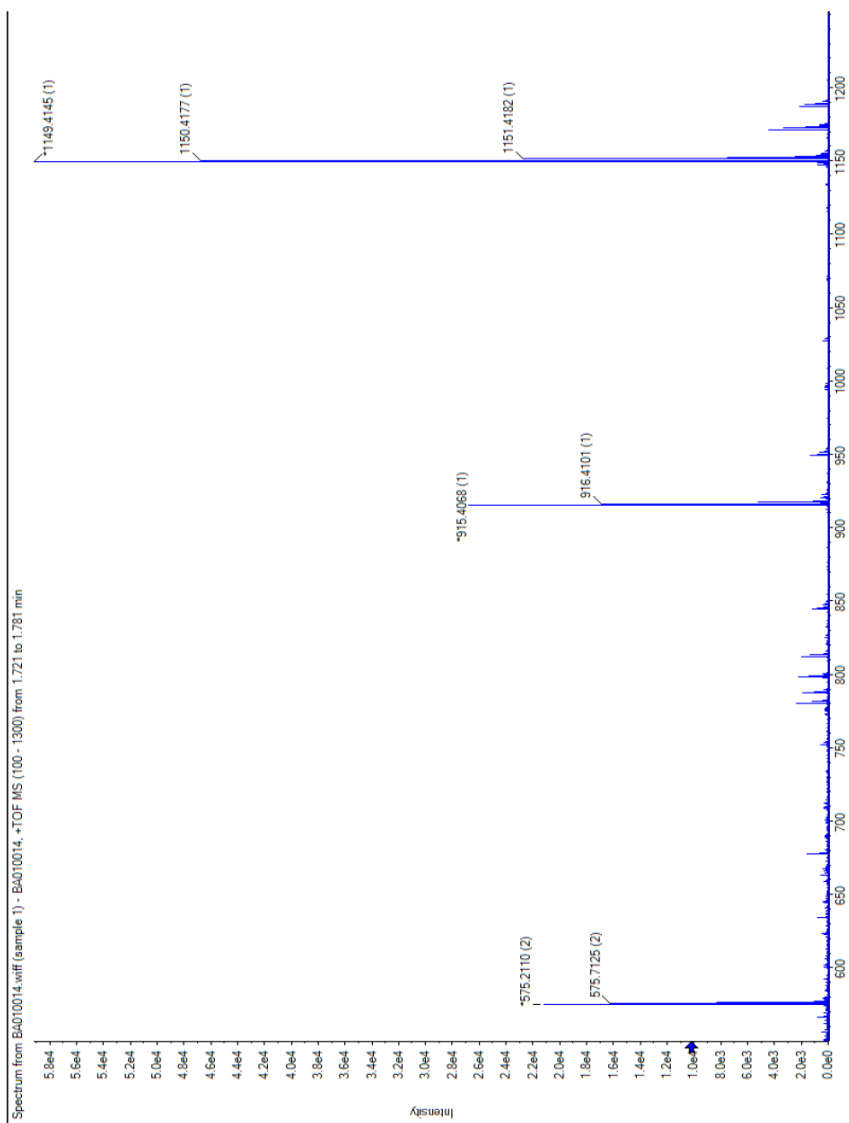
(b) ^{13}C NMR



(c) FT-IR

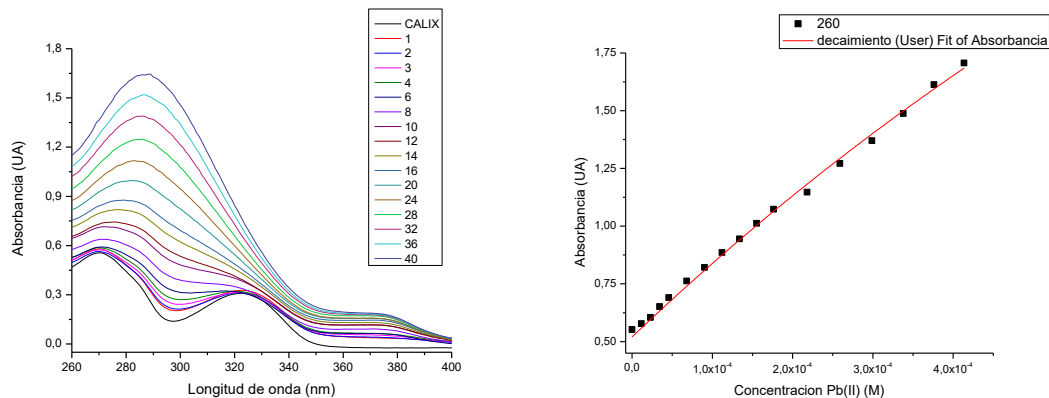


(d) ESI-TOF



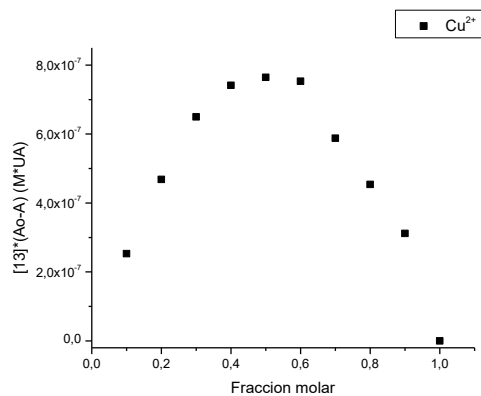
8.- Determination of the association constant by absorption titration.

Figure S2. The binding constant of III has been derived based on the Benesi–Hildebrand equation using absorption titration with Cu^{2+} .



9.- Determination of the stoichiometry.

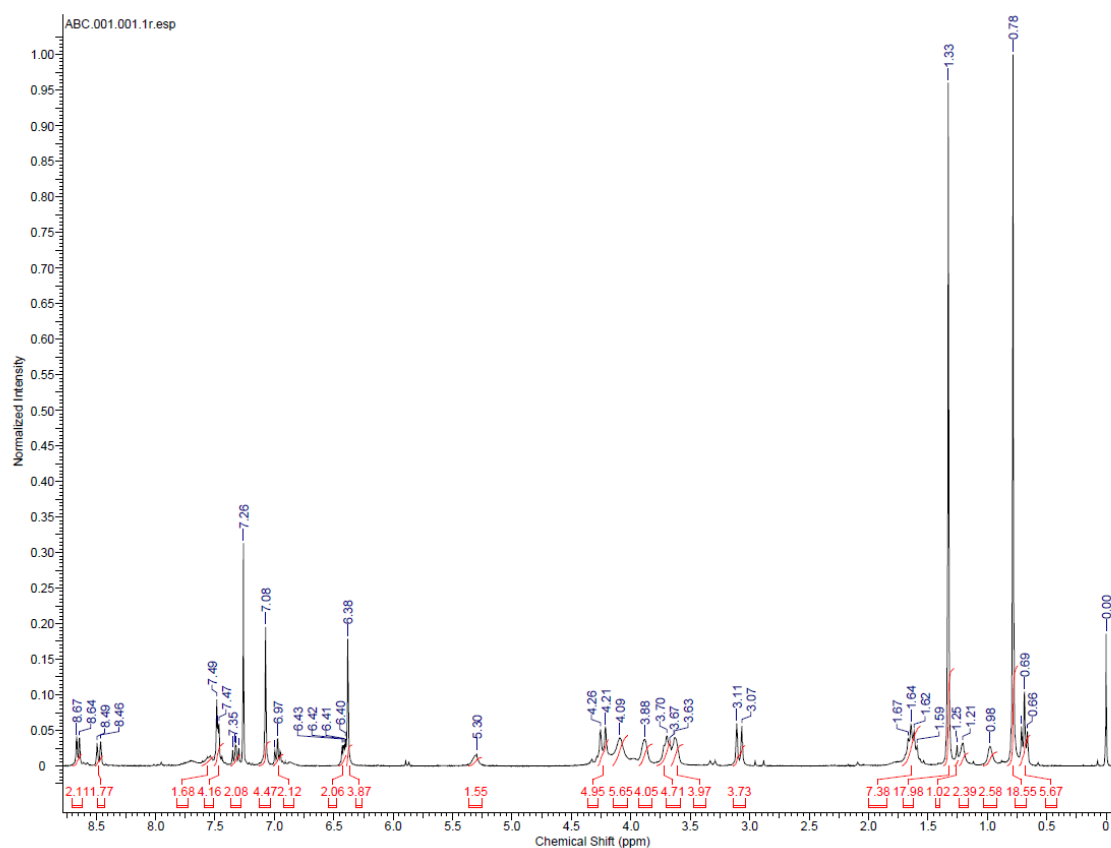
Figure S3. Continuous variation plot for receptor III from absorbance measurements in CH_3CN .



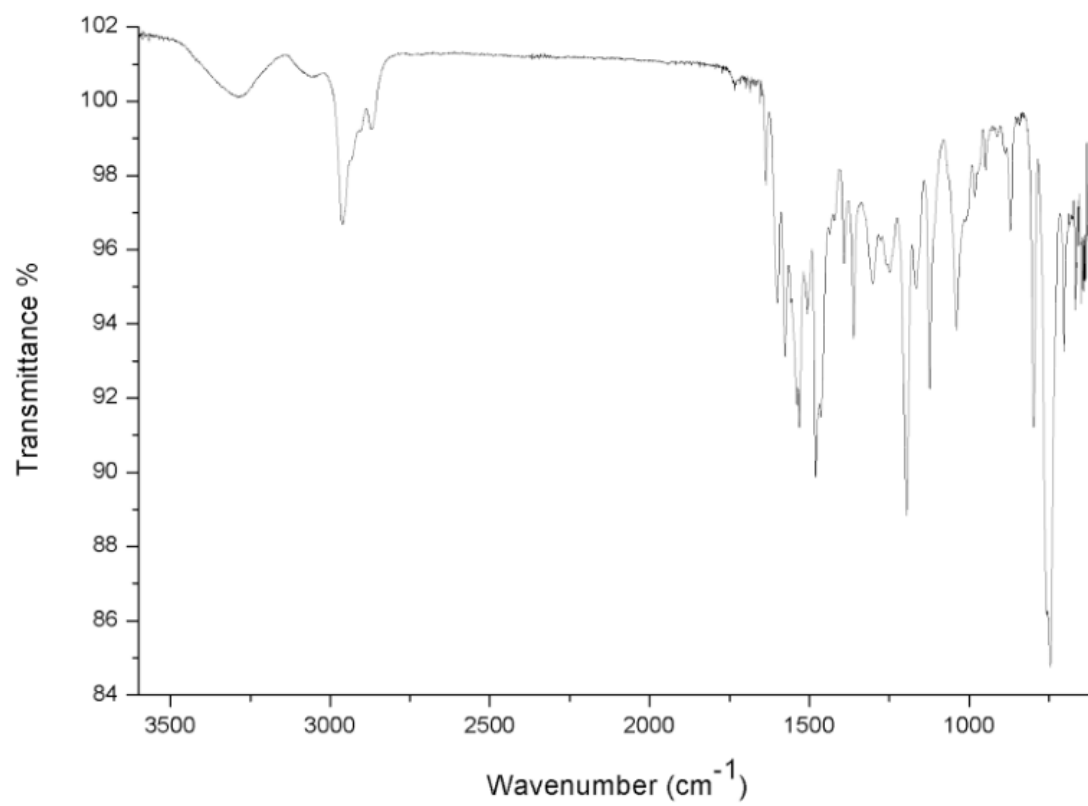
10.- Characterization of IV; 5,11,17,23-tetra-tert-butyl-25,27-bis[3-(6-(N-diethylamino)-2-pyridinyl)-1,2,3-triazolo[1,5-a]pyridine)ethoxy]-26,28-dipropoxycalix[4]arene, cone.

Figure S1: Spectra for IV: (a) ¹H NMR; (b) FT-IR and (c) ESI-TOF.

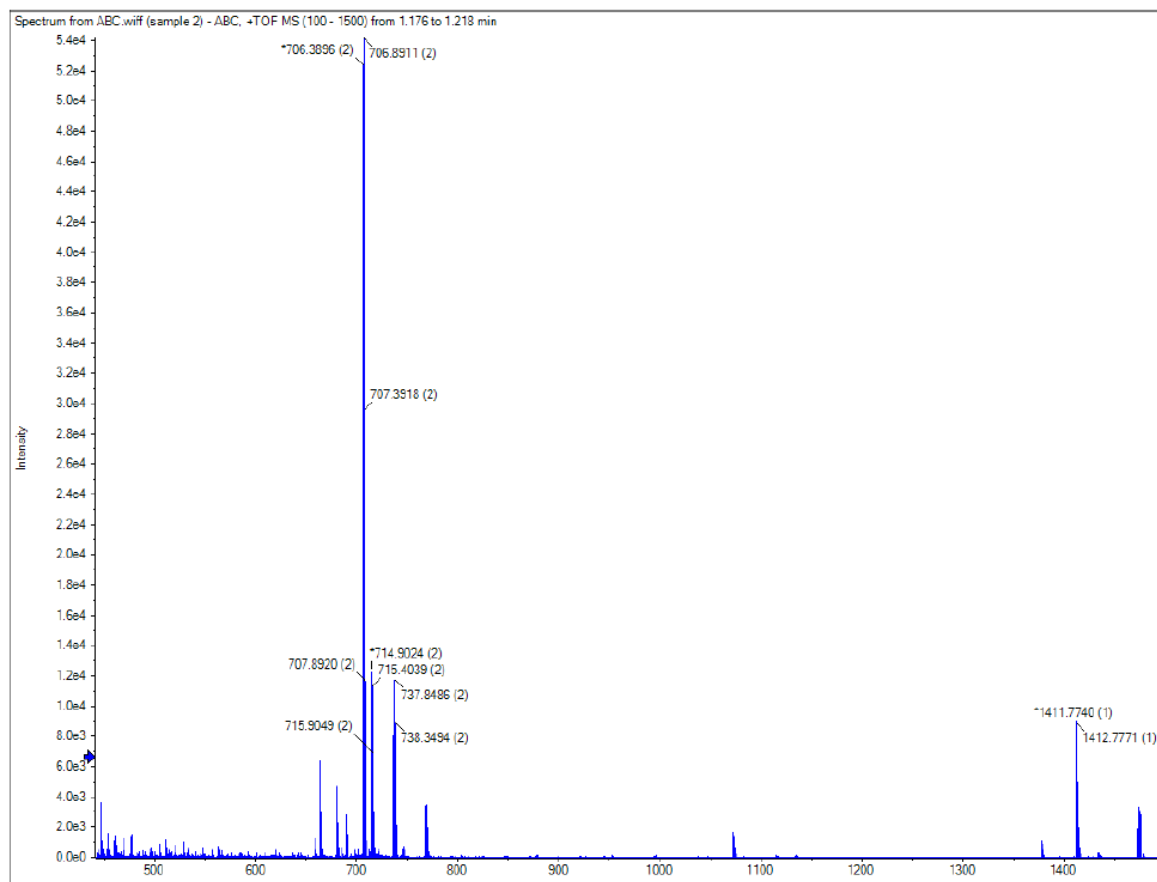
(a) ¹H NMR



(b) FT-IR

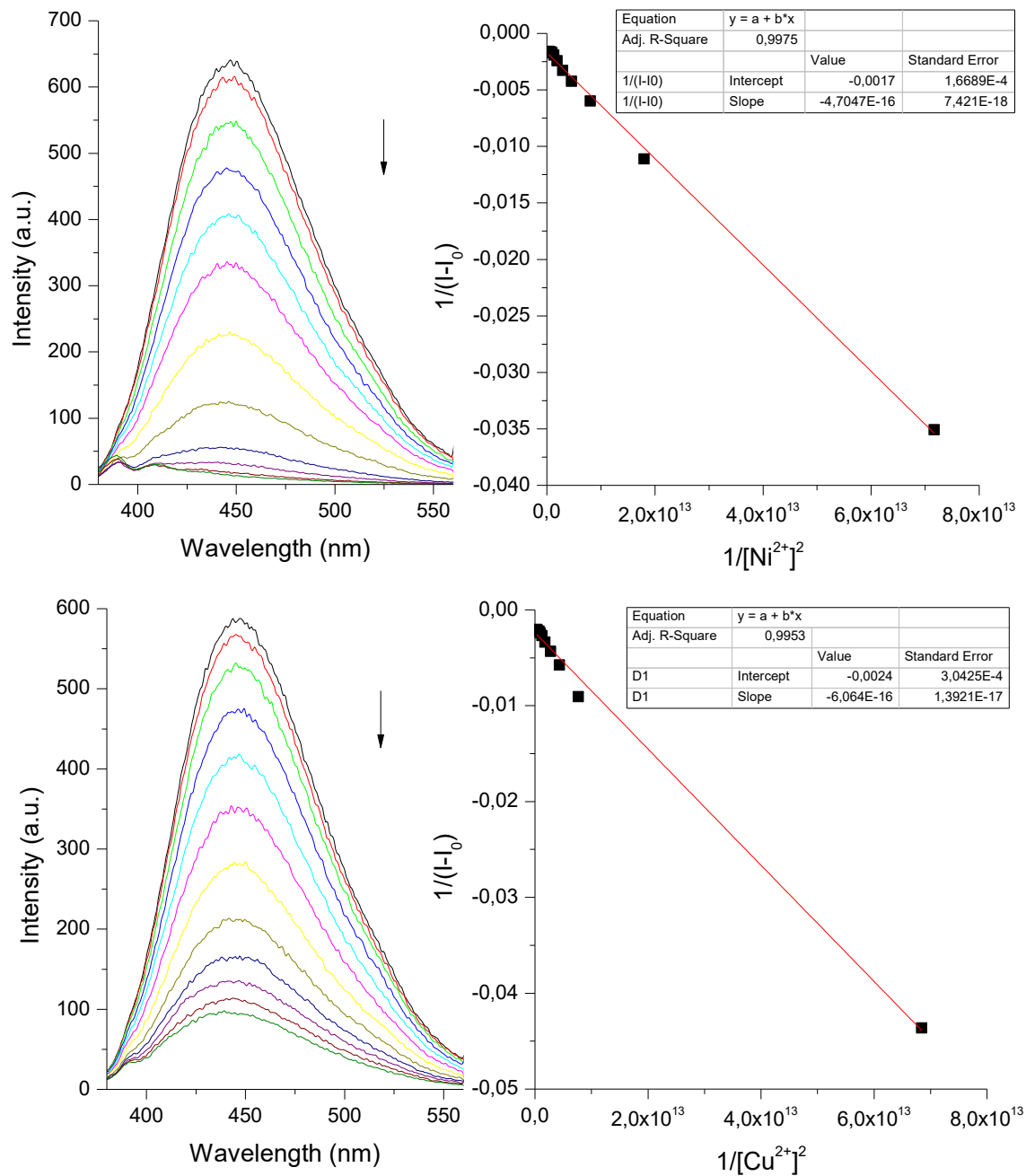


(c) ESI-TOF



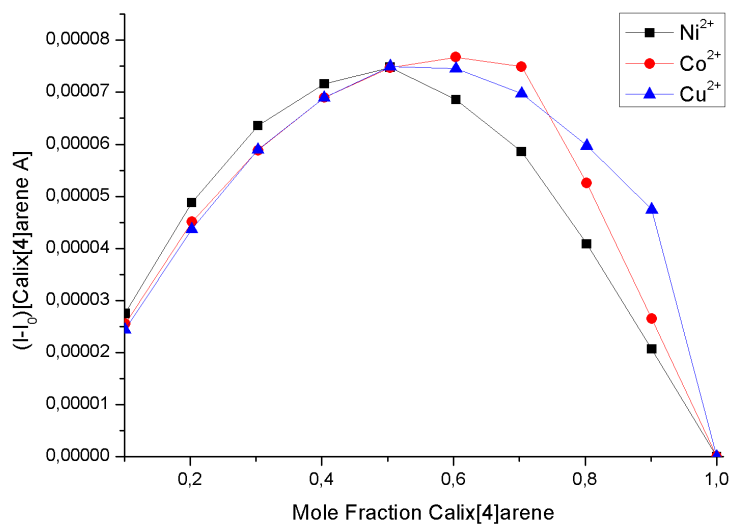
11.- Determination of the association constant by fluorescent titration.

Figure S2. The binding constant of IV has been derived based on the Benesi–Hildebrand equation using fluorescent titration with (a) Ni^{2+} and (b) Cu^{2+} .



12.- Determination of the stoichiometry.

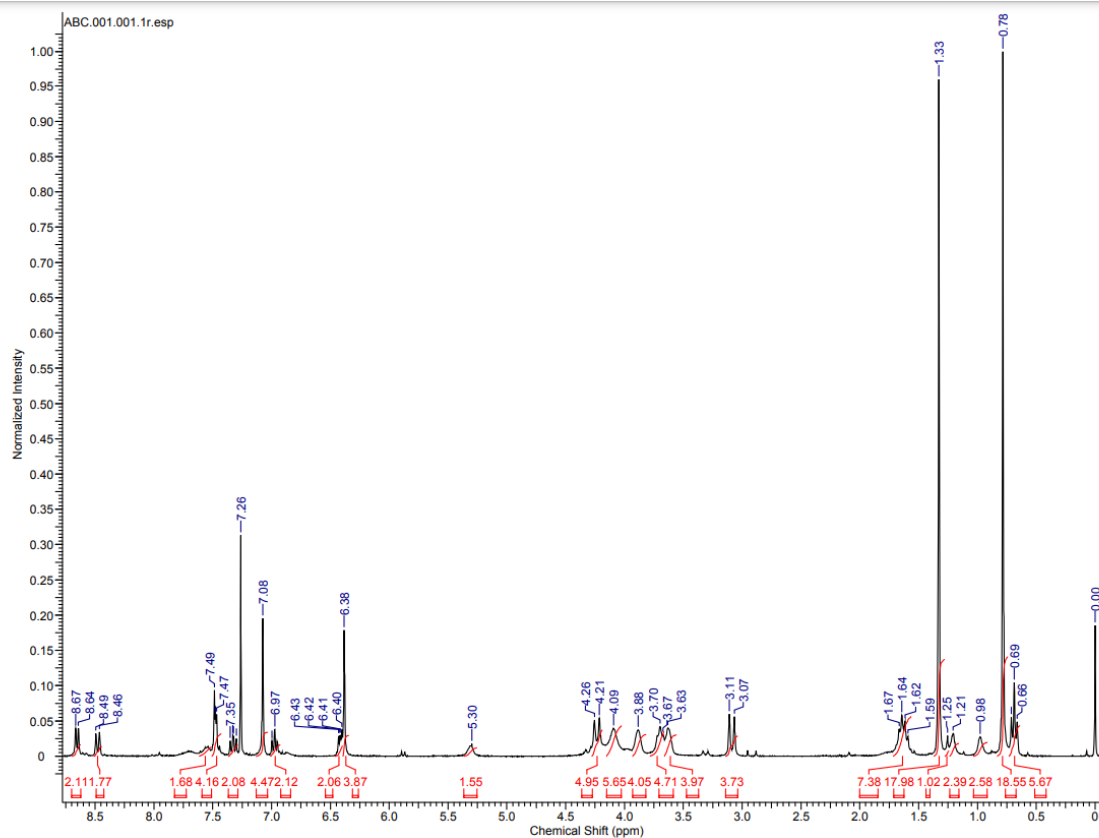
Figure S3. Continuous variation plot for receptor IV from fluorescence measurements at 450 nm in CH₃CN. (a) Ni²⁺; (b) Co²⁺ and (c) Cu²⁺.



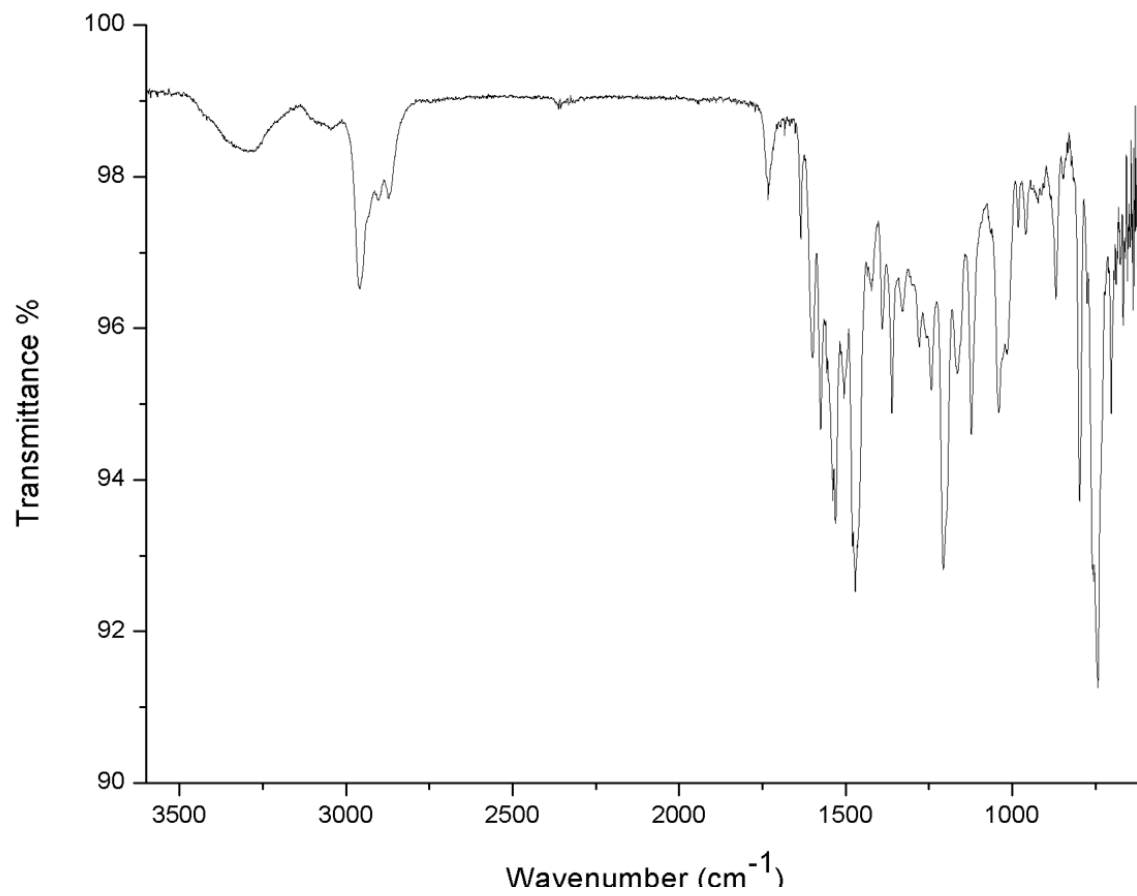
13.- Characterization of V; 5,11,17,23-tetra-tert-butyl-25,27-bis[3-(6-(N-diethylamino)-2-pyridinyl)-1,2,3-triazolo[1,5-a]pyridine)ethoxy]-26,28-dipropoxycalix[4]arene, 1,3-alternate.

Figure S1: Spectra for V: (a) ^1H NMR; (b) FT-IR and (c) ESI-TOF.

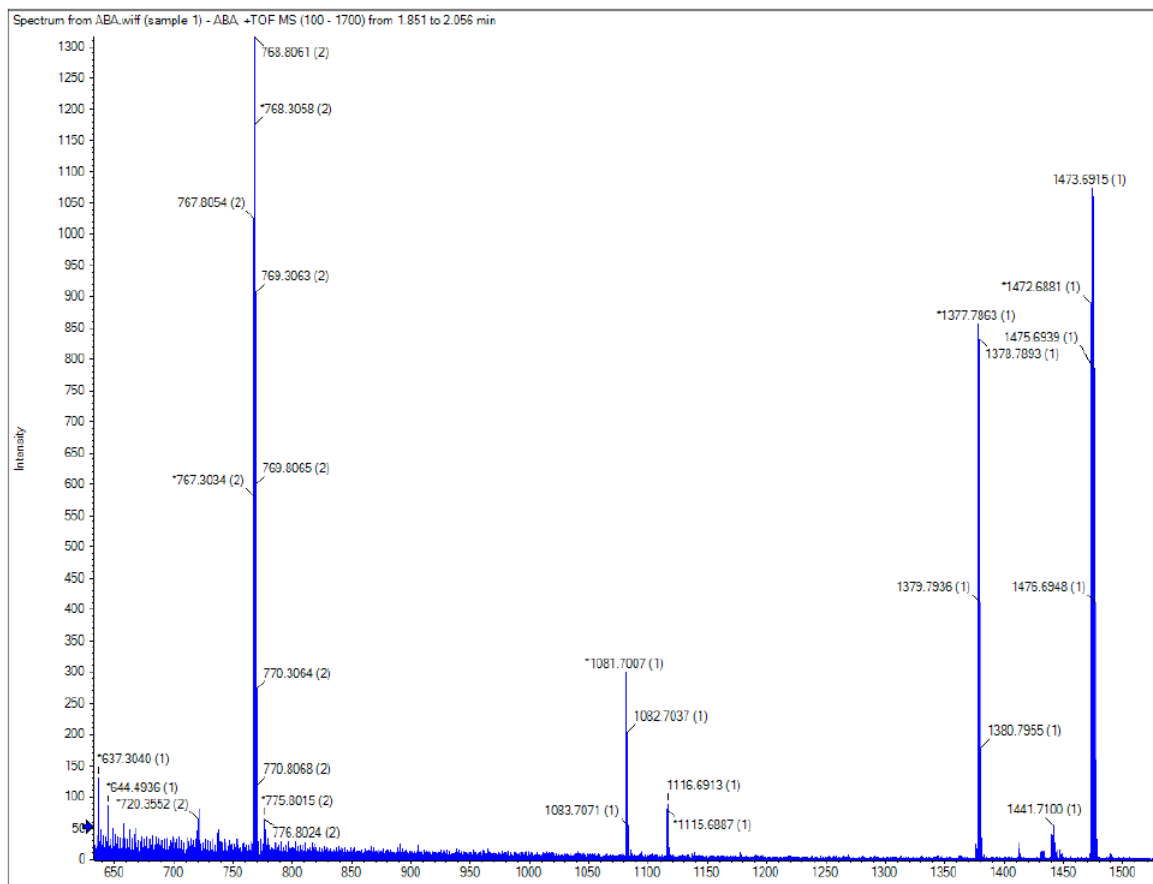
(a) ^1H NMR



(b) FT-IR

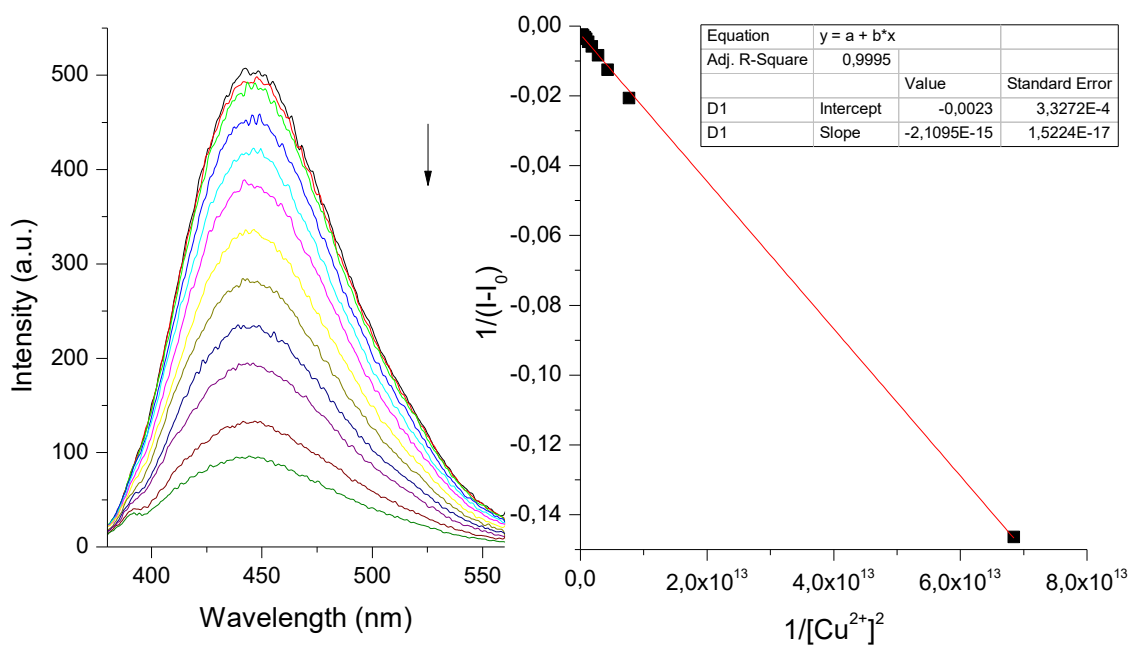
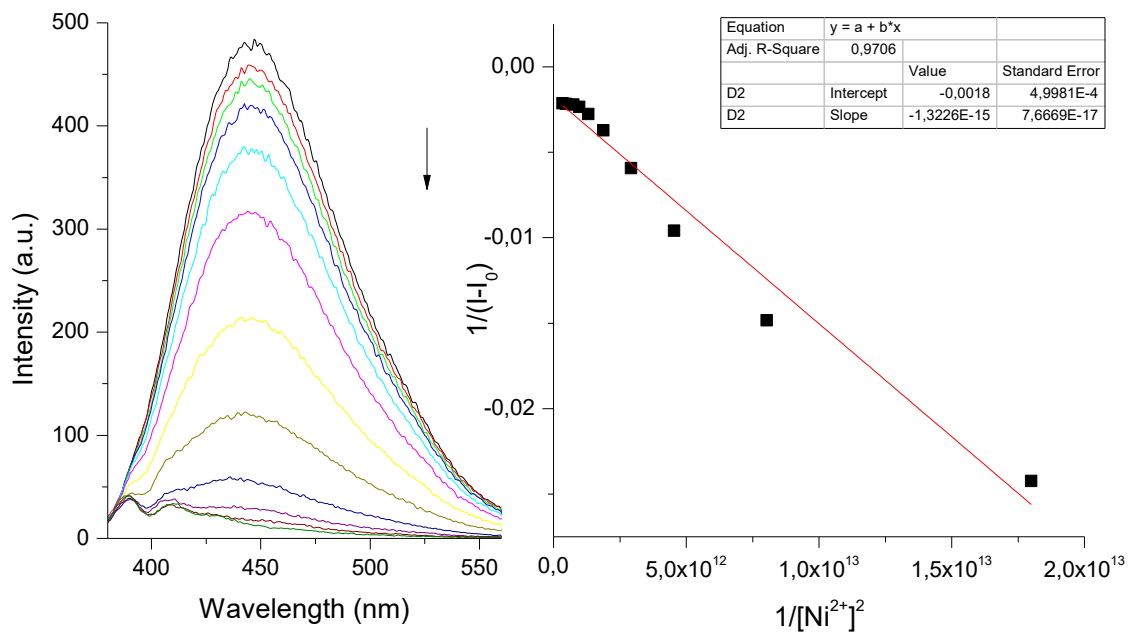


(c) ESI-TOF



14.- Determination of the association constant by fluorescent titration.

Figure S2. The binding constant of V has been derived based on the Benesi–Hildebrand equation using fluorescent titration with (a) Ni^{2+} and (b) Cu^{2+} .



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15.- Determination of the stoichiometry.

Figure S3. Continuous variation plot for receptor V from fluorescence measurements at 450 nm in CH₃CN. (a) Ni²⁺; (b) Co²⁺ and (c) Cu²⁺.

