Zn(II) Detection and Biological Activity of a Macrocycle Containing a Bis(oxadiazole)pyridine Derivative as Fluorophore

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Table of Contents

	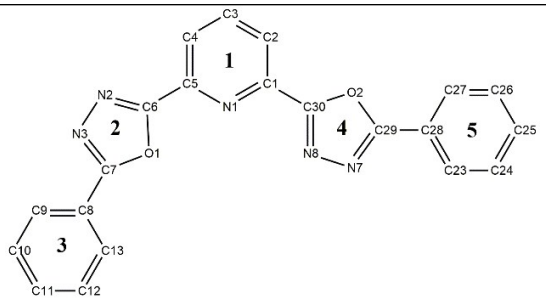				
		2	3	4	5
A	1	4.4(1)	12.3(1)	22.6(2)	68.6(2)
	2		8.7(2)	25.4(2)	72.7(2)
	3			26.6(2)	76.2(2)
	4				50.0(2)
B	1	7.9(2)	12.7(2)	17.0(2)	64.3(4)/61.7(4)
	2		5.5(2)	20.5(2)	71.3(4)/54.9(4)
	3			21.3(2)	73.7(4)/52.9(3)
	4				53.2(4)/74.1(3)

Table S1. Angle between the mean planes 1,2,3,4 and 5. For the B molecules, due to disorder, two value (For Ba and Bb respectively) are reported for the angles involving the plane number 5.

Table S2. Protonation constants (log *K*) of ligand **L** spectrofluorimetrically determined in 0.15 mol dm^{-3} $NaClO_4$ water/acetonitrile 70/30 v/v solvent mixture at 298.1 K.

Reaction	Log *K*
$\mathbf{L} + H^+ = H\mathbf{L}^+$	6.9(1)[a]
$H\mathbf{L}^+ + H^+ = H_2\mathbf{L}^{2+}$	4.8(2)
$H_2\mathbf{L}^{2+} + H^+ = H_3\mathbf{L}^{3+}$	2.2(1)

[a]Values in parentheses are the standard deviations on the last significant figure.

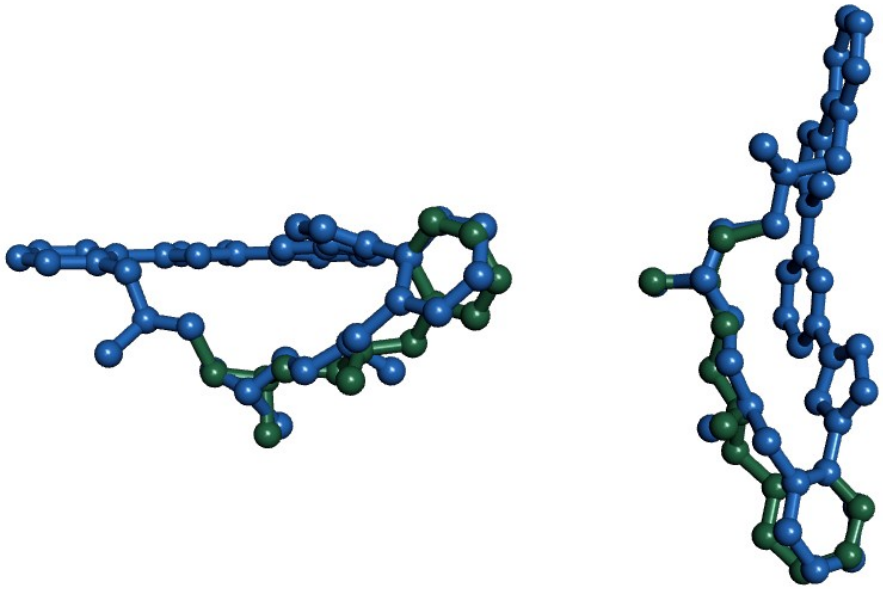

Figure S1. Superimposition of the a (green) and b (pale blue) model of the B independent molecules of **L**.

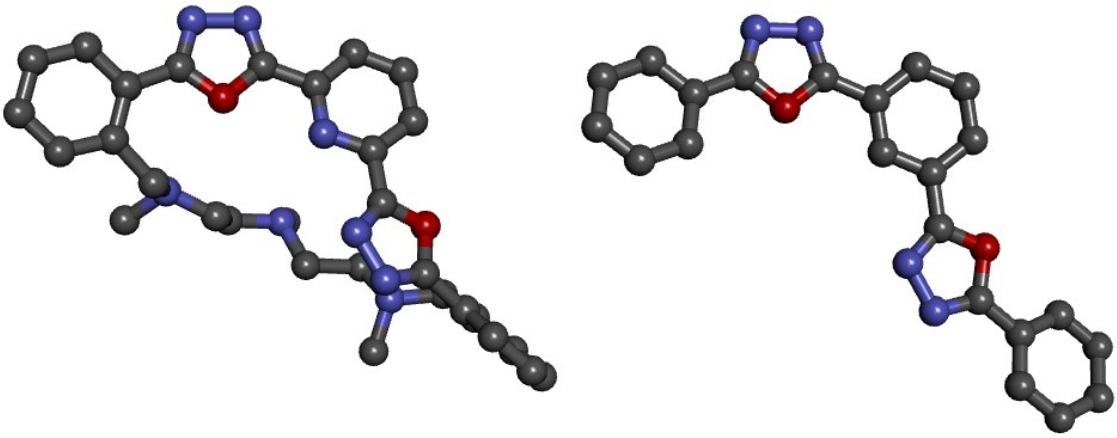

Figure S2. Left = ball and stick representation of the A molecule in **L**. Right = ball and stick representation of SEQRIR.

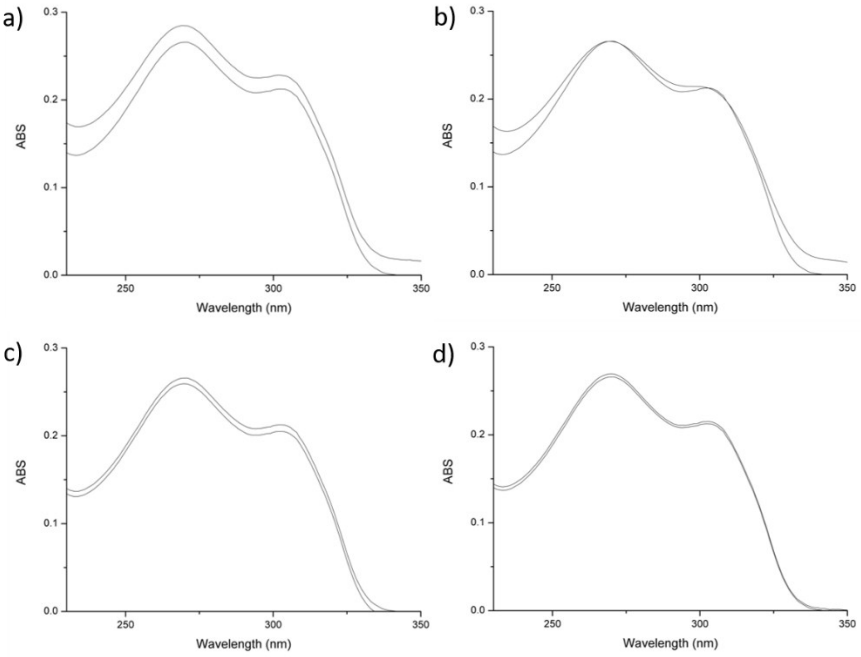

Figure S3. Absorption spectra of **L** recorded in water/acetonitrile 70/30 v/v in the presence of a HEPES buffer (10^{-3} mol dm^{-3}) at pH = 7.0 and after addition of 2 equivalents of a) $Ni(ClO_4)_2$, b) $Cu(ClO_4)_2$, c) $Zn(ClO_4)_2$ and d) $Cd(ClO_4)_2$. ([**L**] = $2 \cdot 10^{-5}$ mol dm^{-3}).

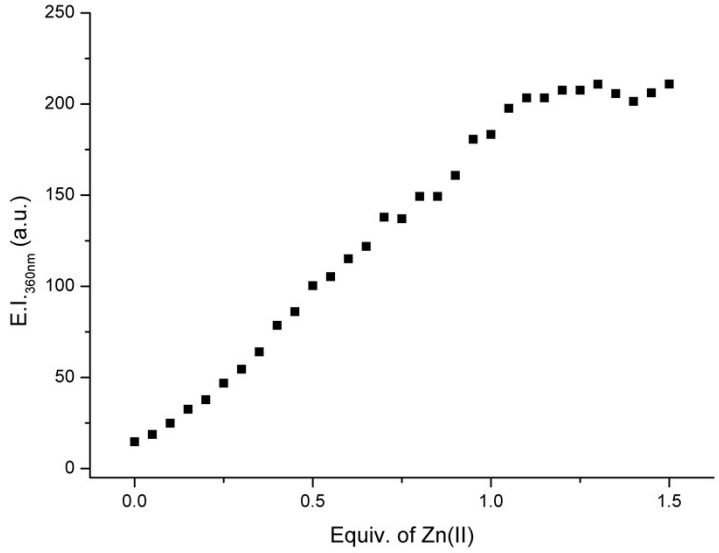

Figure S4. Variation of the emission intensity at 360 nm as a function of the added Zn(II) registered in water/acetonitrile 70/30 v/v in the presence of a HEPES buffer (10^{-3} mol dm^{-3}) at pH = 7.0 (λ_{ex} = 300 nm, [**L**] = $2 \cdot 10^{-5}$ mol dm^{-3}).

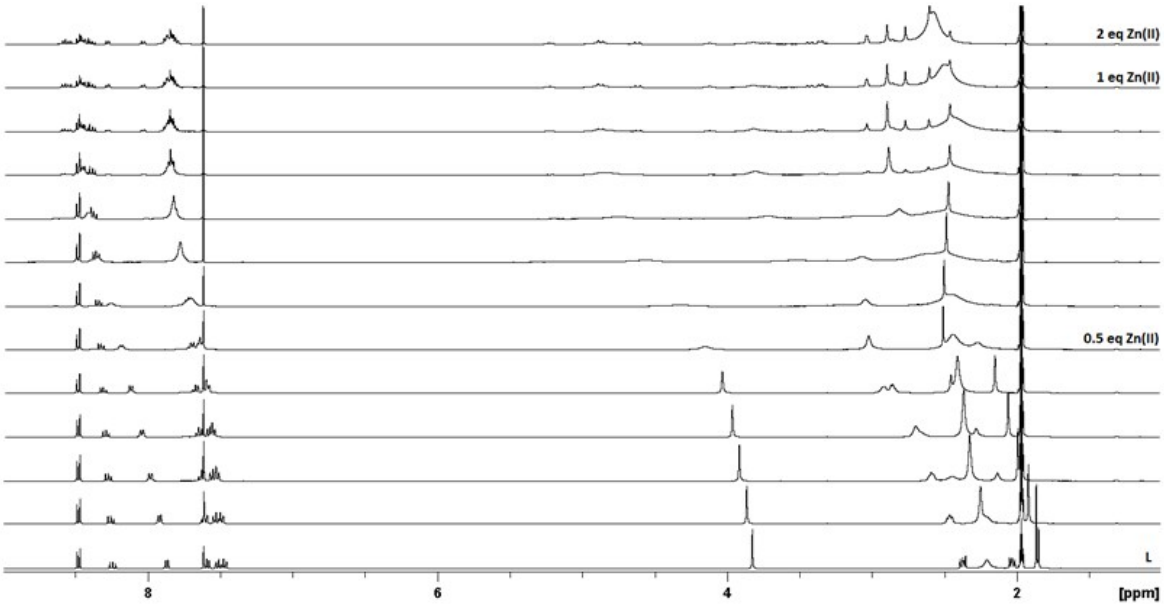

Figure S5. ^{1}H-NMR spectra of **L** recorded in acetonitrile-*d3* with step-to-step addition of Zn(II) ion as perchlorate salt. ([**L**] = $1 \cdot 10^{-2}$ mol dm^{-3}, [Zn(II)] = $5 \cdot 10^{-2}$ mol dm^{-3}, 298 K)