New bis-tetraamine ligand with a chromophoric 4-(9-anthracenyl)-2,6-dimethylpyridinyl linker for glyphosate and ATP sensing

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Supporting Information

(4 pages; with this one)

Table S1. Crystallographic data of compound **5**.

Table S2. Logarithm of the complexation constants, log K_{alh}, and log β for the ligands with **PMG** (I = 0.1 M (NaCl); T = 298 K). Charges are omitted for the sake of clarity.

Table S3. Logarithm of the complexation constants, log K_{alh}, and log β for the ligands with **ATP** (I = 0.1 M (NaCl); T = 298 K). Charges are omitted for the sake of clarity.

Figure S1: Variation of the absorption spectra of a 1.69×10^{-5} M aqueous solution of **L1** as a function of pH (I = 0.1 M (NaCl), T = 298.0 ± 0.2 K). (1) pH = 2.63; (2) pH = 10.96 (uncorrected for dilution).

Figure S2: Variation of the absorption spectra of a 2.55×10^{-4} M aqueous solution of **L2** as a function of pH (I = 0.1 M (NaCl), T = 298.0 ± 0.2 K). (1) pH = 2.64; (2) pH = 11.18 (uncorrected for dilution).

Figure S3: "Naked eyes" fluorimetric experiment. Picture presenting the variation of the fluorescence under a UV lamp (λ_{exc} = 312 nm) of samples containing **L1**, **L1** + **ATP** and **L1** + **PMG** in a stoichiometric amount (4×10^{-3} M, pH 7, in H_2O)

Table S1. Crystallographic data of compound **5**.

Empirical formula	$C_{25}\ H_{21}\ N\ O_4$
Formula weight ($g.mol^{-1}$)	399.43
Sample dimensions (mm)	0.14 × 0.12 × 0.08
Crystal system / space group	Monoclinic, C2/c
Z	4
a (Å)	14.0913(17)
b (Å)	10.8393(9)
c (Å)	13.9585(15)
α = γ (°)	90
β (°)	110.917
v ($Å^3$)	1991.5(4)
T (K)	170(2)
λ (Å)	0.71073
μ (mm^{-1})	0.090
D_x ($Mg.m^{-3}$)	1.332
Measured reflections	2465
Unique reflections	3517; 1580 with I > 2σ(I)
F(000)	840
θ	23,5 ° < θ < 28;28°
$R_{int.}$	0.0693
h	-18→18
k	-14→ 12
l	-18 → 18
R_1 [I > 2σ (I) and all data]	0.003 and 0.1458
wR_2 [I > 2σ (I) and all data]	0,076 and 0.0989
S	0,911
w [I > 2σ (I)]	$1/[\sigma^2+ (0.0306P)^2+0.000P]$ [b]
$\Delta\rho_{max}$ (e $Å^{-3}$)	0.211
$\Delta\rho_{min}$ (e $Å^{-3}$)	-0.157

[a] Refinement on all F^2, 139 parameters, 0 restraint
[b] $P = (F_o^2 + 2\ F_c^2)\ /3$

Table S2. Logarithm of the complexation constants, log K_{alh}, and log β for the ligands with **PMG** (I = 0.1 M (NaCl); T = 298 K). Charges are omitted for the sake of clarity.

	L1		**L2**	
A+L=AL	4.65			
A+L=AL		4.65(2)		
A+L+H=ALH	14.95 *(10.30)*		14.55	
A+LH=ALH		4.53(2)		4.10(3)
A+L+2H=ALH_2	24.91 *(9.96)*		24.41*(9.86)*	
AH+LH= ALH_2		4.37(2)		3.84(3)
A+L+3H=ALH_3	34.48 *(9.57)*		34.44*(10.03)*	
AH+LH_2=ALH_3		4.32(2)		4.09(4)
A+L+4H=ALH_4	43.38 *(8.90)*		43.39*(8.95)*	
AH+LH_3=ALH_4		4.23(2)		4.02(4)
A+L+5H=ALH_5	51.78 *(8.40)*		52.02*(8.63)*	
AH+LH_4=ALH_5		4.21(3)		4.08(3)
A+L+6H=ALH_6	58.72 *(6.94)*		59.04*(7.02)*	
AH+LH_5=ALH_6		4.35(3)		4.16(2)
A+L+7H=ALH_7	64.68 *(5.96)*		64.98*(5.94)*	
AH+LH_6=ALH_7		4.47(3)		4.21(2)
A+L+8H=ALH_8	70.50 *(5.82)*		70.87*(5.90)*	
AH_2+LH_6=ALH_8		4.89(3)		4.70(4)
A+L+9H=ALH_9	75.56 *(5.06)*		75.97*(5.10)*	
AH_2+LH_7=ALH_9		4.59(4)		4.41(5)
A+L+10H=ALH_{10}	80.27 *(4.71)*		80.97*(5.00)*	
AH_2+LH_8=ALH_{10}		4.68(4)		4.64(5)
A+L+11H=ALH_{11}	83.06 *(2.79)*		83.21*(2.23)*	
AH_3+LH_8=ALH_{11}		5.34(6)		4.65(4)
I = 0.1 M (NaCl); T = 298 K				

Table S3. Logarithm of the complexation constants, log K_{alh}, and log β for the ligands with **ATP** (I = 0.1 M (NaCl); T = 298 K). Charges are omitted for the sake of clarity.

	L1		**L2**	
A+L=AL	3.22			
A+L=AL		3.22(1)		
A+L+H=ALH	13.34 *(10.12)*		14.26	
A+LH=ALH		2.92(1)		3.81(1)
A+L+2H=ALH_2	22.50 *(9.16)*		24.01 *(9.75)*	
A+LH_2=ALH_2		2.46(1)		3.78(1)
A+L+3H=ALH_3	32.16 *(9.66)*		33.40 *(9.39)*	
A+LH_3=ALH_3		3.13(1)		4.15(1)
A+L+4H=ALH_4	40.80 *(8.64)*		42.02 *(8.62)*	
A+LH_4=ALH_4		3.35(1)		4.20(2)
A+L+5H=ALH_5	48.99 *(8.19)*		50.07 *(8.05)*	
A+LH_5=ALH_5		4.74(2)		5.48(2)
A+L+6H=ALH_6	56.37 *(7.38*		57.31 *(7.24)*	
AH+LH_5=ALH_6		5.36(2)		5.78(2)
A+L+7H=ALH_7	63.00 *(6.63)*		64.03 *(6.72)*	
AH+LH_6=ALH_7		6.15(2)		6.61(2)
A+L+8H=ALH_8	68.80 *(5.80)*		69.95 *(5.92)*	
AH+LH_7=ALH_8		6.58(2)		7.14(1)
A+L+9H=ALH_9	72.88 *(4.08)*		73.67 *(3.72)*	
AH+LH_8=ALH_9		6.05(2)		6.09(1)
A+L+10H=ALH_{10}	75.80 *(2.92)*		76.46 *(2.79)*	
AH+LH_8=ALH_{10}		4.66(2)		4.55(1)
A+L+11H=ALH_{11}	78.15 *(2.35)*			
AH_3+LH_8=ALH_{11}		5.21(4)		
I = 0.1 M (NaCl); T = 298 K				

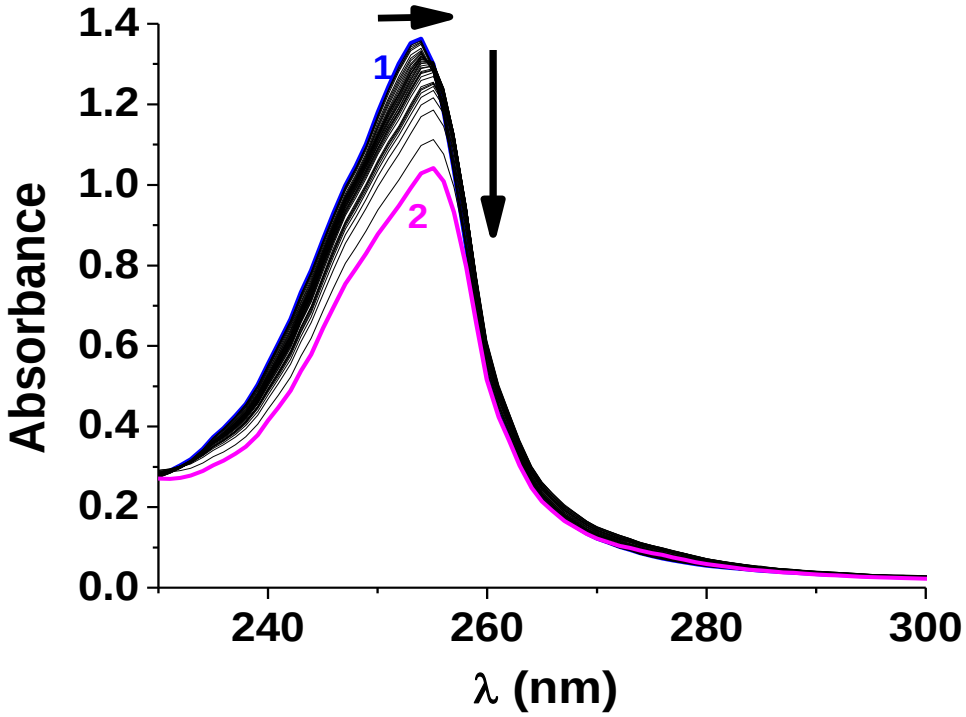


Figure S1: Variation of the absorption spectra of a 1.69 × 10^{-5} M aqueous solution of **L1** as a function of pH (*I* = 0.1 M (NaCl), *T* = 298.0 ± 0.2 K). (1) pH = 2.63; (2) pH = 10.96 (uncorrected for dilution).

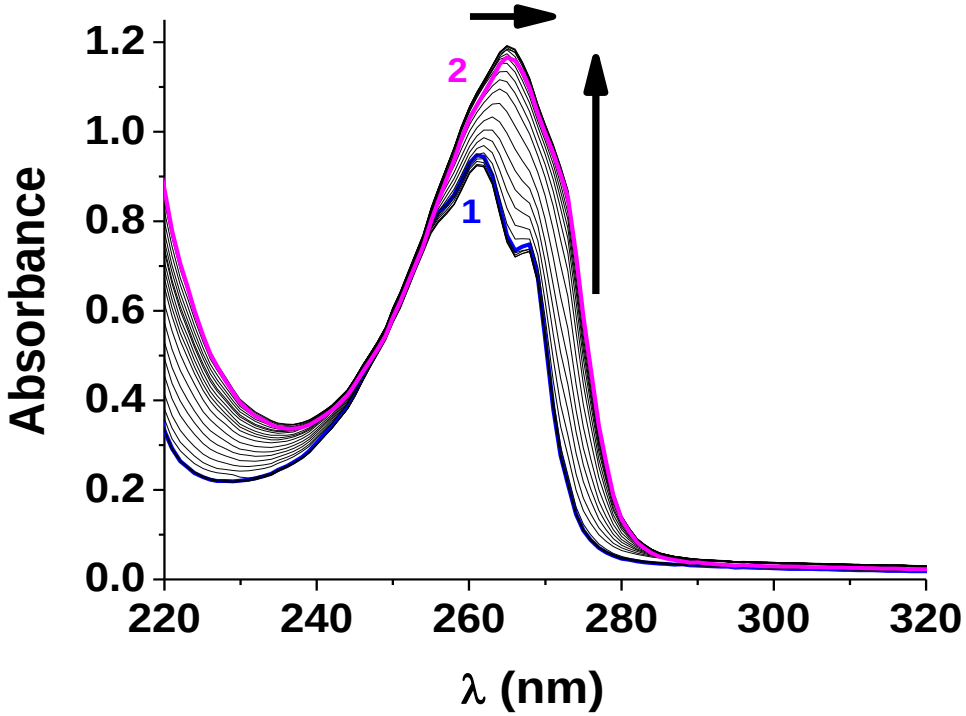
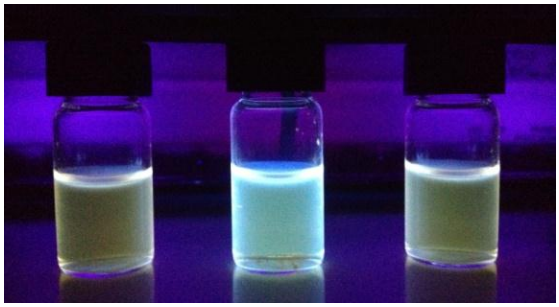


Figure S2: Variation of the absorption spectra of a 2.55 × 10^{-4} M aqueous solution of **L2** as a function of pH (*I* = 0.1 M (NaCl), *T* = 298.0 ± 0.2 K). (1) pH = 2.64; (2) pH = 11.18 (uncorrected for dilution).



L1 **L1+ATP** **L1+PMG**

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