Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Naphthothiazole-Based Highly Selective and Sensitive Fluorescent and Colorimetric Chemosensor for Detection of Pollutant Metal Ions

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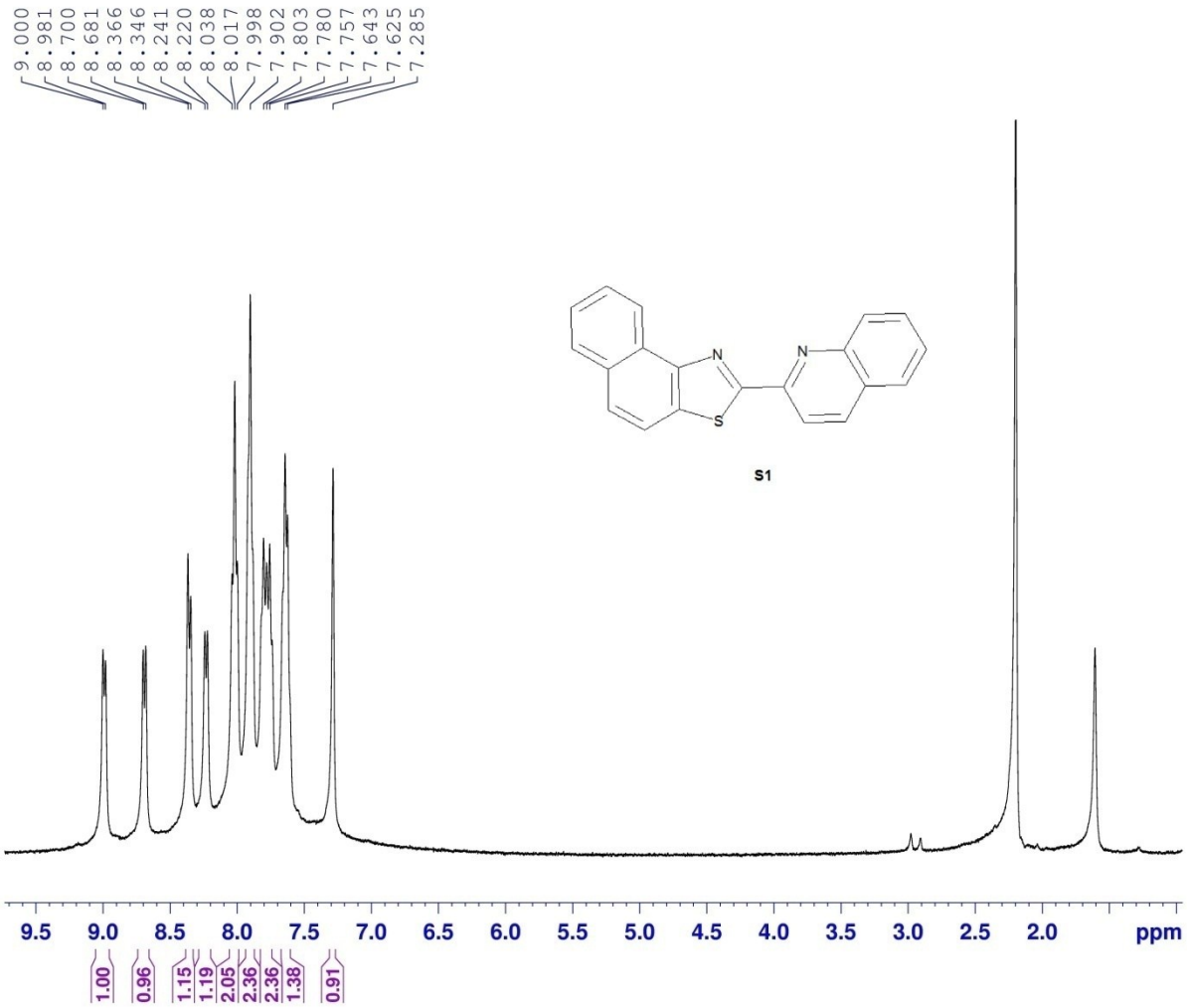
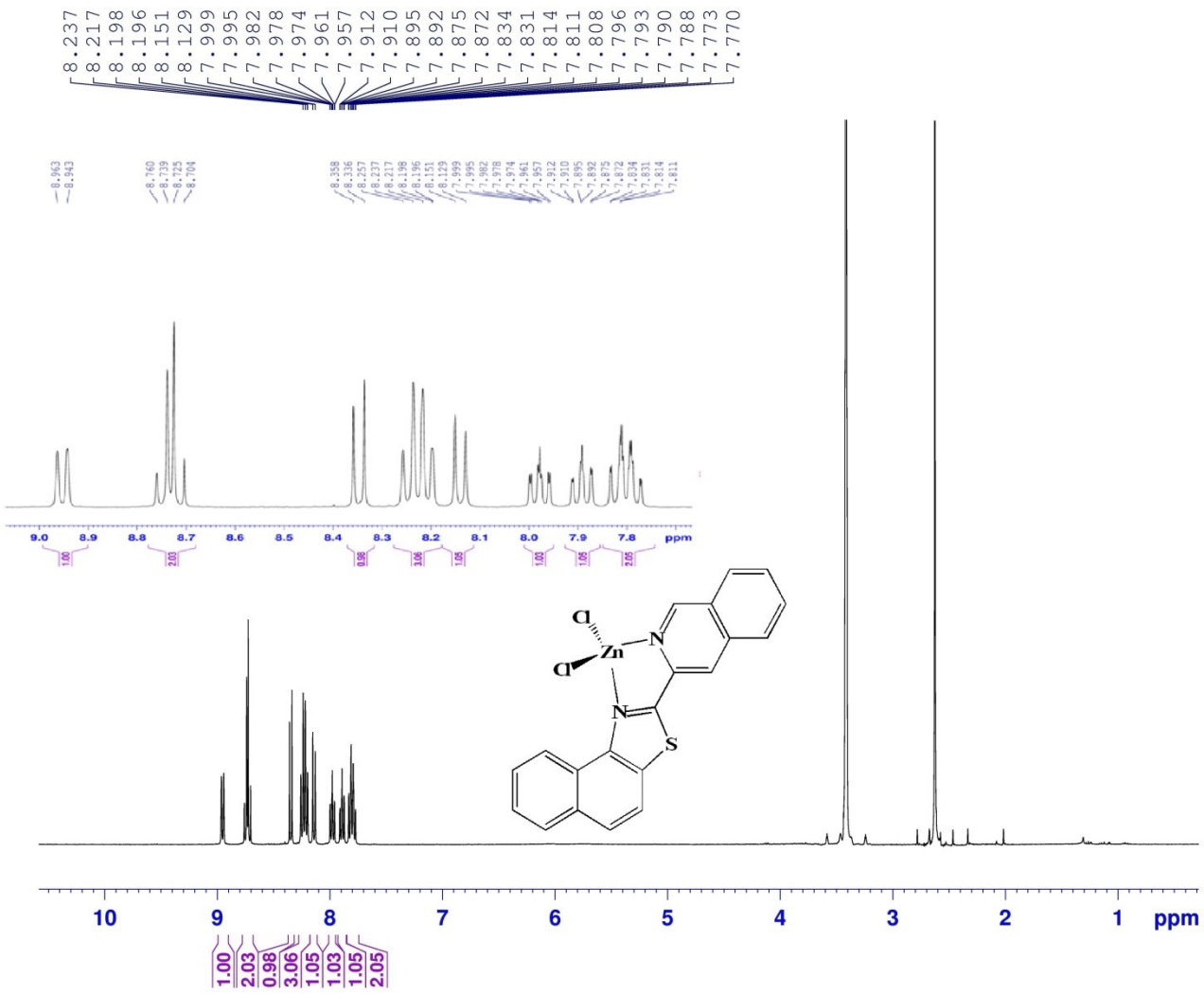
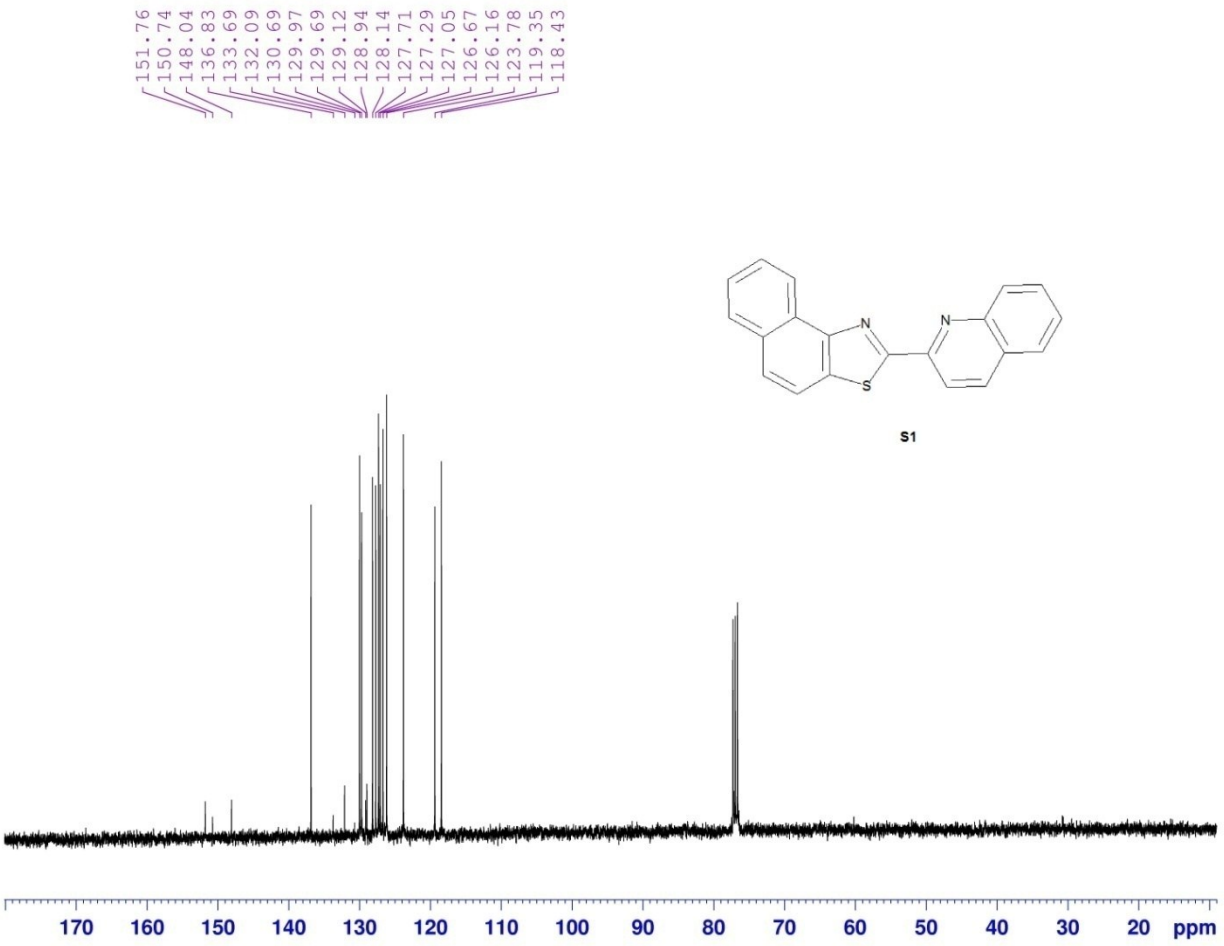


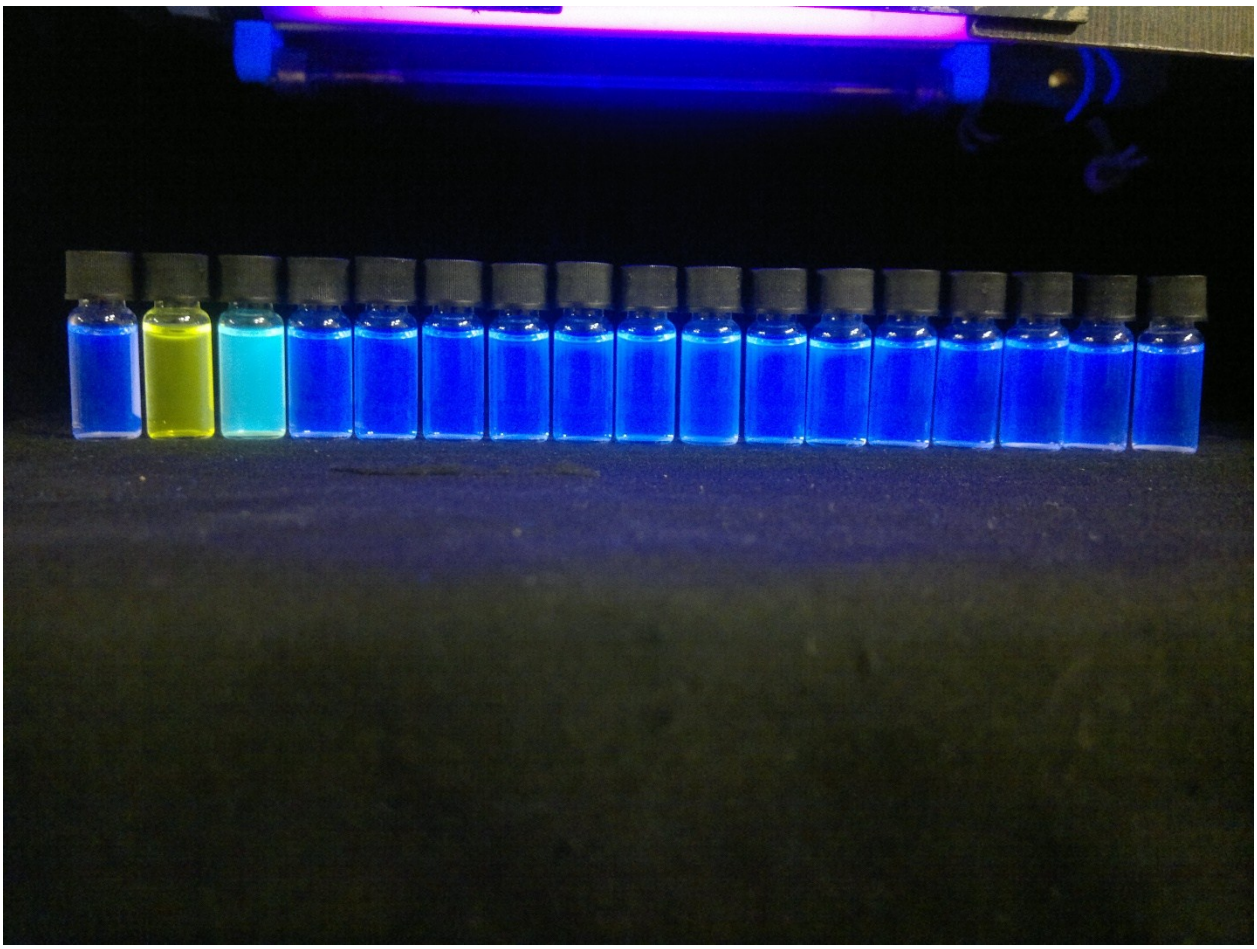
^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.28 (s, 1H), 7.63 (d, *J*= 7.2 Hz, 1H), 7.78 (t, *J*=9.2 Hz, 2H), 7.90 (s, 2H), 8.01 (t, *J*= 8.0 Hz, 2H), 8.23 (d, *J*= 8.4 Hz, 1H), 8.35 (d, *J*= 8.0 Hz, 1H), 8.69 (d, *J*= 7.6 Hz, 1H), 8.99 (d, *J*= 7.6 Hz, 1H).



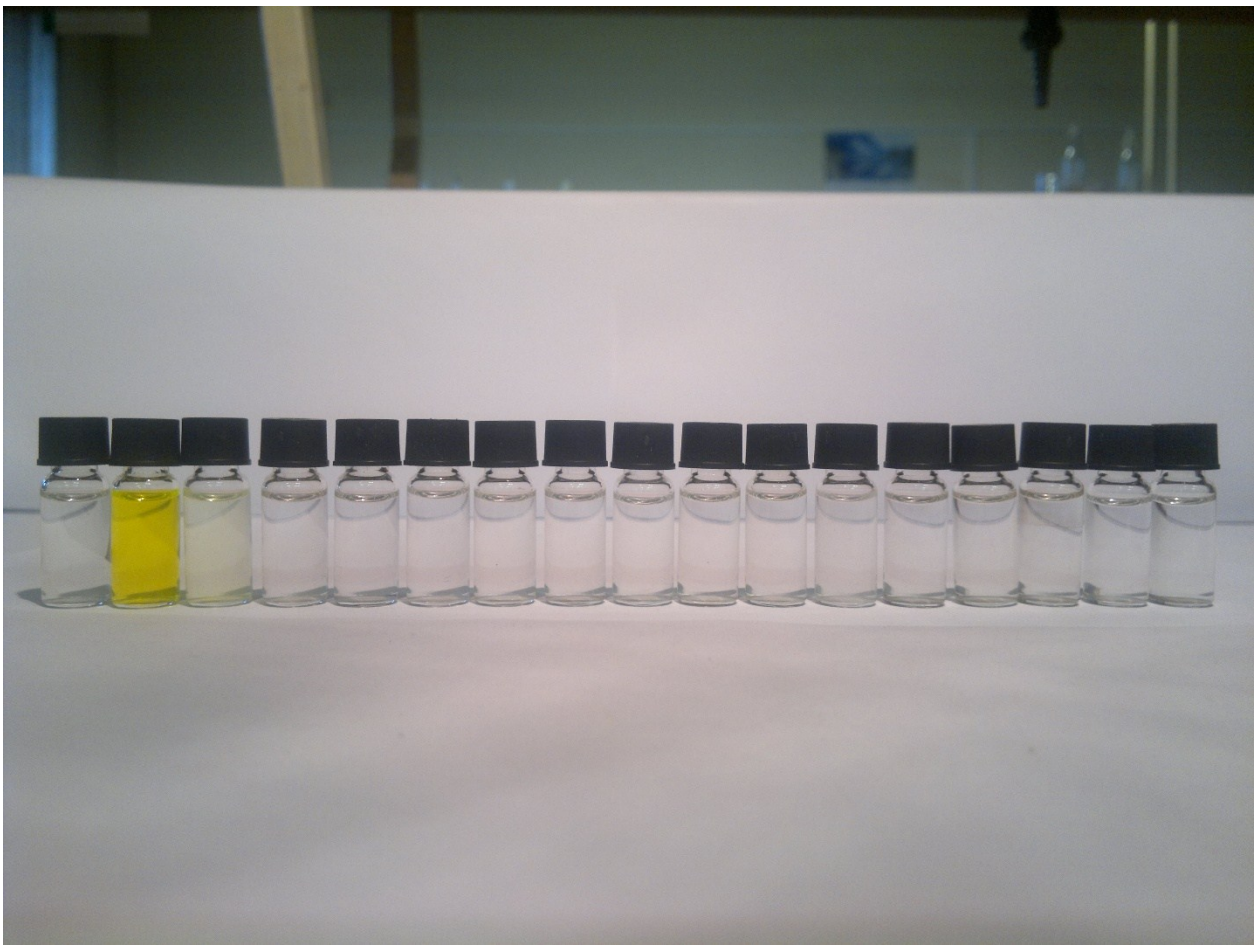
^{1}H NMR (400 MHz, DMSO-d_6) δ:7.78 (d, *J*= 8.0 Hz, 1H), 7.82 (d, *J*= 8.0 Hz, 1H), 7.89 (t, *J*= 8.3 Hz, 1H), 7.98 (t, *J*= 7.6 Hz, 1H), 8.14 (d, *J*= 8.4 Hz, 1H), 8.19-8.25 (m, 3H), 8.34 (d, *J*= 8 Hz, 1H), 8.71(d, *J*= 8.4 Hz, 1H), 8.75 (d, *J*= 8.4 Hz, 1H), 8.95 (d, *J*= 8 Hz, 1H).



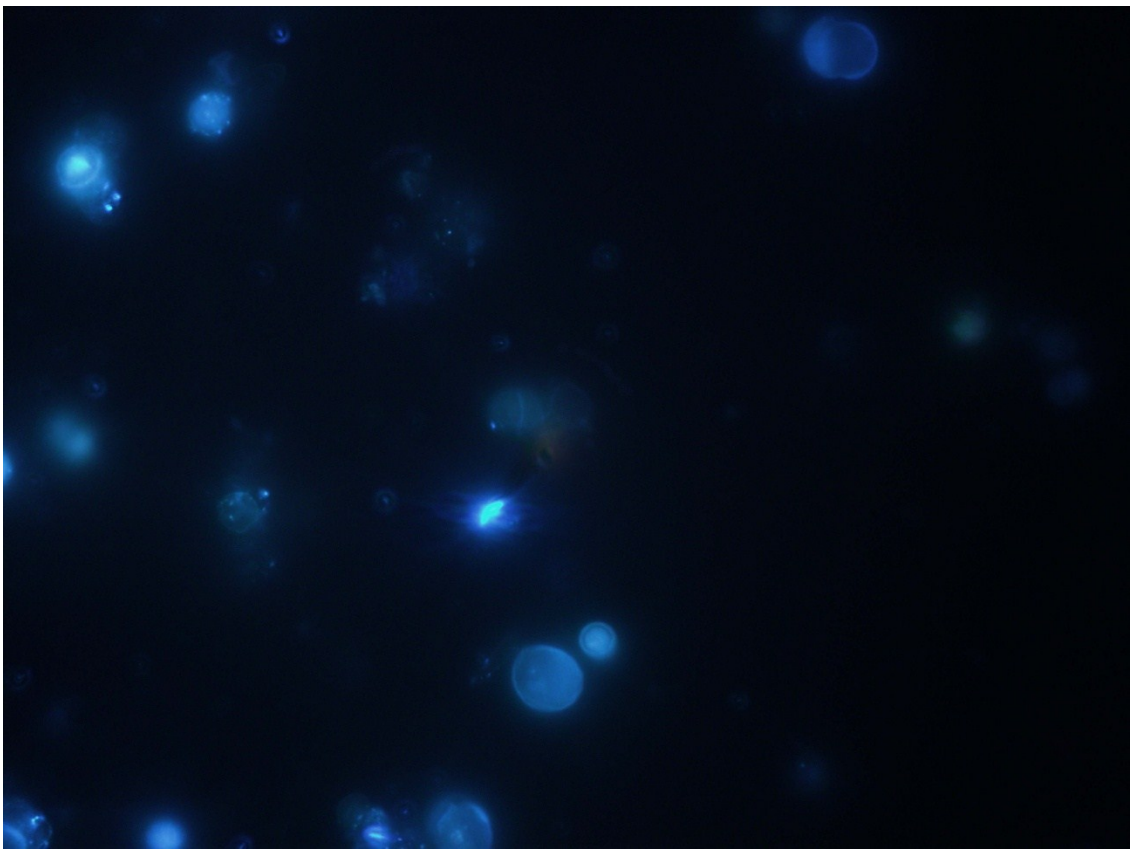
^{13}C NMR(100 MHz, DMSO-d_6) δ:118.4, 119.3, 123.8, 126.1, 126.7, 127.0, 127.3, 127.7, 128.1, 128.9, 129.1, 129.7, 129.6, 130.7, 132.1, 133.7, 136.8, 148.0, 150.7, 151.7.



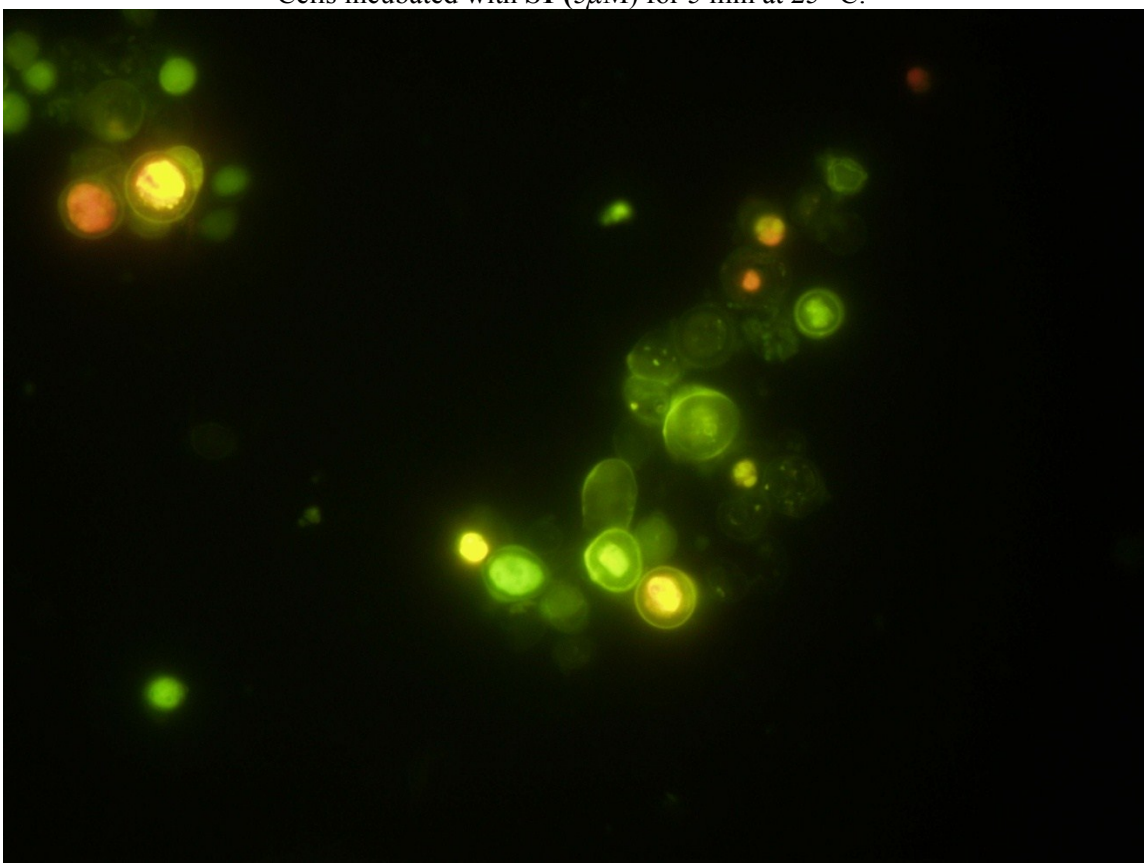
Fluorescence change upon addition of various metal cations to **S1** in CH_3CN-water under UV light.



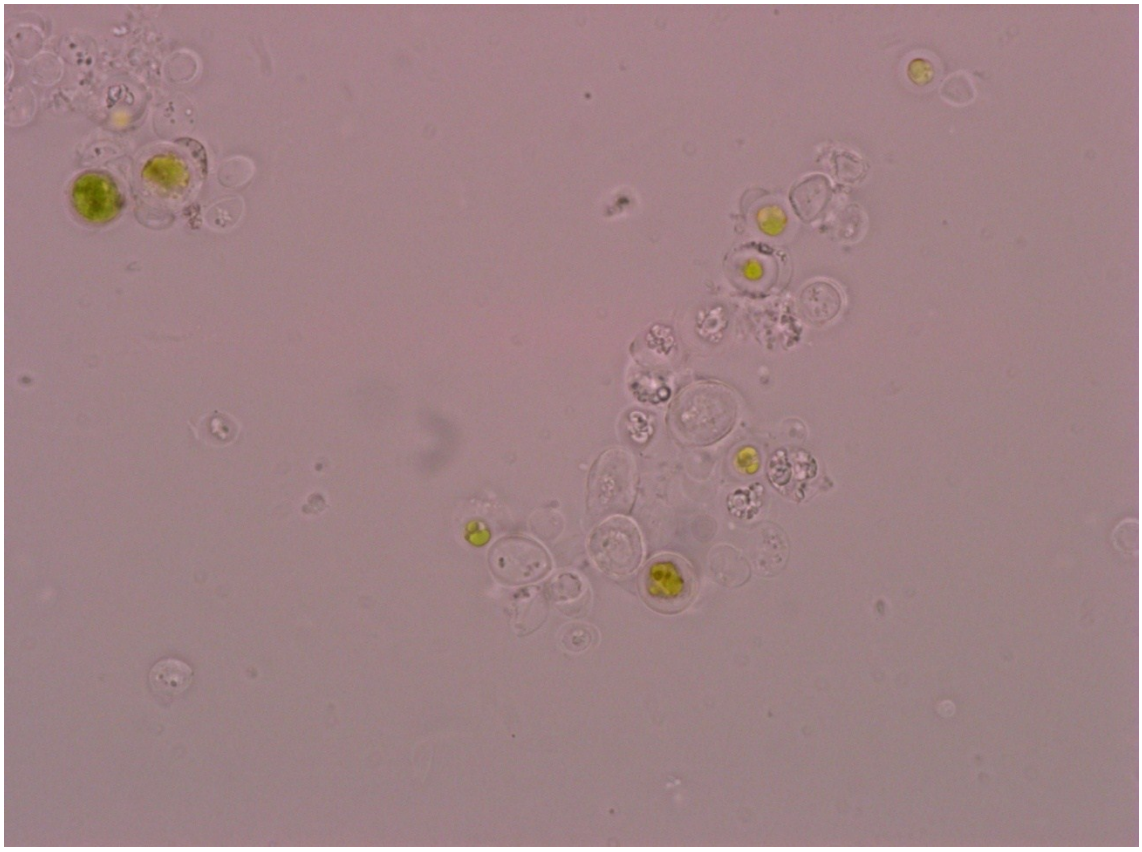
Color change upon addition of various metal cations to **S1** in CH_3CN-water under visible light.



Cells incubated with **S1 (**5μM) for 5 min at 25 °C.



Cells supplemented with $SnCl_2$(10 μM)for 1 h at 25 °C and stained with **S1**(5μM) at 25 °C for 5 min.



Brightfield image of the*scenedesmusobliquus* cells supplemented with $SnCl_2$(10 μM)for 1 h at 25 °C and stained with **S1**(5μM)at 25 °C for 5 min.

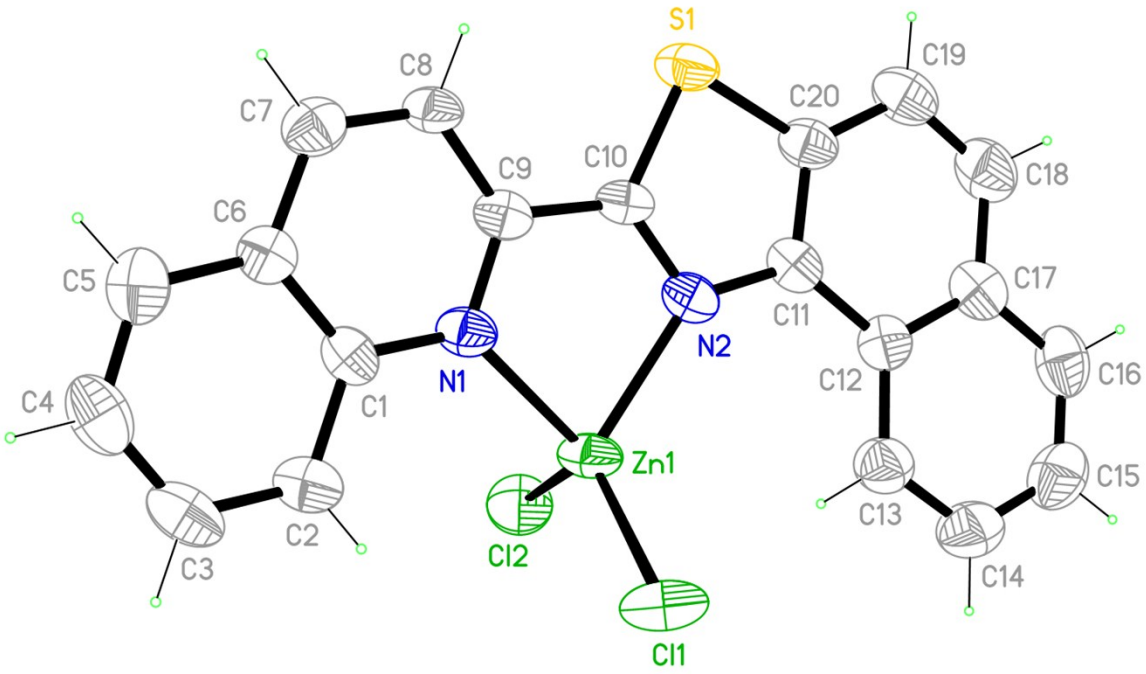


Fig. 1. ORTEP representation of single crystal formed between **S1** and**$ZnCl_2$**. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

Table 1. Crystal data and structure refinement for the complex compoundformed between **S1** and **$ZnCl_2$**.

Empirical formula	C20 H12 Cl2 N2 S Zn
Formula weight	448.65
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 7.6260(15) A alpha = 90 deg. b = 14.043(3) A beta = 98.269(3) deg. c = 16.787(3) A gamma = 90 deg.
Volume	1779.1(6) A^3
Z, Calculated density	4, 1.675 Mg/m^3
Absorption coefficient	1.804 mm^-1
F(000)	904

Theta range for data collection	2.90 to 27.10 deg.
Limiting indices	-9<=h<=9, -14<=k<=17, -21<=l<=21
Reflections collected / unique	12769 / 3889 [R(int) = 0.0362]
Completeness to theta = 27.10	98.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3889 / 0 / 235
Goodness-of-fit on F^2	1.112
Final R indices [I>2sigma(I)]	R1 = 0.0480, wR2 = 0.1218
R indices (all data)	R1 = 0.0803, wR2 = 0.1446
Largest diff. peak and hole	1.082 and -0.619 e.A^-3

Table 2. Bond lengths [A] and angles [deg] for the complex compound formed between **S1** and **$ZnCl_2$**.

Zn(1)-N(2)	2.073(3)
Zn(1)-N(1)	2.083(3)
Zn(1)-Cl(2)	2.1943(13)
Zn(1)-Cl(1)	2.2001(13)
S(1)-C(10)	1.703(4)
S(1)-C(20)	1.732(5)
N(2)-C(10)	1.311(5)
N(2)-C(11)	1.368(5)
N(1)-C(9)	1.314(5)
N(1)-C(1)	1.364(5)
C(5)-C(4)	1.342(7)
C(5)-C(6)	1.409(6)
C(5)-H(5)	0.9300
C(1)-C(2)	1.406(6)
C(1)-C(6)	1.408(6)
C(6)-C(7)	1.411(6)
C(12)-C(13)	1.396(6)
C(12)-C(17)	1.410(6)
C(12)-C(11)	1.436(6)
C(8)-C(7)	1.360(6)
C(8)-C(9)	1.392(6)
C(8)-H(8)	0.9300
C(11)-C(20)	1.388(6)

C(19)-C(18)	1.353(7)
C(19)-C(20)	1.404(6)
C(19)-H(19)	0.9300
C(2)-C(3)	1.359(7)
C(2)-H(2)	0.9300
C(13)-C(14)	1.353(7)
C(13)-H(13)	0.9300
C(10)-C(9)	1.479(6)
C(3)-C(4)	1.386(7)
C(3)-H(3)	0.9300
C(14)-C(15)	1.380(8)
C(14)-H(14)	0.9300
C(4)-H(4)	0.9300
C(17)-C(18)	1.406(6)
C(17)-C(16)	1.415(7)
C(18)-H(18)	0.9300
C(7)-H(7)	0.9300
C(16)-C(15)	1.343(7)
C(16)-H(16)	0.9300
C(15)-H(15)	0.9300

N(2)-Zn(1)-N(1)	80.91(14)
N(2)-Zn(1)-Cl(2)	110.52(10)
N(1)-Zn(1)-Cl(2)	109.13(10)
N(2)-Zn(1)-Cl(1)	117.14(11)
N(1)-Zn(1)-Cl(1)	113.53(10)
Cl(2)-Zn(1)-Cl(1)	119.20(5)
C(10)-S(1)-C(20)	89.5(2)
C(10)-N(2)-C(11)	111.9(3)
C(10)-N(2)-Zn(1)	109.6(3)
C(11)-N(2)-Zn(1)	137.8(3)
C(9)-N(1)-C(1)	118.1(4)
C(9)-N(1)-Zn(1)	113.3(3)
C(1)-N(1)-Zn(1)	128.6(3)
C(4)-C(5)-C(6)	119.7(5)
C(4)-C(5)-H(5)	120.1
C(6)-C(5)-H(5)	120.1
N(1)-C(1)-C(2)	118.3(4)
N(1)-C(1)-C(6)	121.9(4)
C(2)-C(1)-C(6)	119.8(4)
C(1)-C(6)-C(7)	117.7(4)
C(1)-C(6)-C(5)	118.8(4)
C(7)-C(6)-C(5)	123.4(4)
C(13)-C(12)-C(17)	118.5(4)
C(13)-C(12)-C(11)	124.7(4)
C(17)-C(12)-C(11)	116.8(4)
C(7)-C(8)-C(9)	119.1(4)
C(7)-C(8)-H(8)	120.5
C(9)-C(8)-H(8)	120.5

N(2)-C(11)-C(20)	113.9(4)
N(2)-C(11)-C(12)	126.6(4)
C(20)-C(11)-C(12)	119.5(4)
C(18)-C(19)-C(20)	117.7(4)
C(18)-C(19)-H(19)	121.1
C(20)-C(19)-H(19)	121.1
C(3)-C(2)-C(1)	119.1(4)
C(3)-C(2)-H(2)	120.4
C(1)-C(2)-H(2)	120.4
C(14)-C(13)-C(12)	121.3(5)
C(14)-C(13)-H(13)	119.3
C(12)-C(13)-H(13)	119.3
N(2)-C(10)-C(9)	121.2(4)
N(2)-C(10)-S(1)	115.1(3)
C(9)-C(10)-S(1)	123.7(3)
C(11)-C(20)-C(19)	122.7(4)
C(11)-C(20)-S(1)	109.6(3)
C(19)-C(20)-S(1)	127.7(4)
N(1)-C(9)-C(8)	123.9(4)
N(1)-C(9)-C(10)	114.1(4)
C(8)-C(9)-C(10)	122.1(4)
C(2)-C(3)-C(4)	120.8(4)
C(2)-C(3)-H(3)	119.6
C(4)-C(3)-H(3)	119.6
C(13)-C(14)-C(15)	120.3(5)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
C(5)-C(4)-C(3)	121.6(5)
C(5)-C(4)-H(4)	119.2
C(3)-C(4)-H(4)	119.2
C(18)-C(17)-C(12)	121.0(4)
C(18)-C(17)-C(16)	120.7(4)
C(12)-C(17)-C(16)	118.3(4)
C(19)-C(18)-C(17)	122.3(5)
C(19)-C(18)-H(18)	118.9
C(17)-C(18)-H(18)	118.9
C(8)-C(7)-C(6)	119.3(4)
C(8)-C(7)-H(7)	120.3
C(6)-C(7)-H(7)	120.3
C(15)-C(16)-C(17)	120.9(5)
C(15)-C(16)-H(16)	119.5
C(17)-C(16)-H(16)	119.5
C(16)-C(15)-C(14)	120.6(5)
C(16)-C(15)-H(15)	119.7
C(14)-C(15)-H(15)	119.7

Symmetry transformations used to generate equivalent atoms: