Supporting Information

A Combination of a Fluorescent Dye and a Zn-S cluster and its Biological Application as a Stain for Bacteria

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Materials and General Procedures

All starting materials and solvents were purchased from commercial sources and used without further purification. The IR spectra in the range 4000-400 cm^{-1} were recorded on a PerkinElmer Spectrum One FT-IR Spectrometer. Elemental analyses were carried out in Chemical & MicroAnalytical Services Pty. Ltd., Belmont, VIC, Australia. UV-vis spectra were recorded on UV-1650 PC spectrophotometer (double cell mode, baseline correction was performed a wavelength scan from 800 nm to 200 nm). ^1H NMR spectra were recorded on an INOVA 400 spectrometer (400 MHz, $(CD_3)_2SO$, 25^oC). Fluorescence measurements were performed on Varian Cary Eclipse fluorescence spectrophotometer.

Crystallography

Crystal data, details of the data collection and refinement are summarized in Table 1. Crystal structure was solved using direct methods (SHELXTL V5.1[1]) from single-

crystal data collected at 130 K on a Bruker SMART/CCD area detector diffractometer fitted with Mo K_α radiation (λ = 0.71073 Å) and a graphite monochromator. Structure refinements were performed using the SHELX97 program,[2] which uses a full-matrix least-squares refinement based on F^2. Absorption corrections were performed using the SADABS program.[3]

Note: Some unsatisfactory aspects in relation to the refinement have arisen as a consequence of a low reflection to parameter ratio for this structure. The reason for the low ratio is the relatively weak nature of the diffraction. The surface $–SC_6H_5$ ligands have severe disorder and this is responsible for the elevated agreement values (*R* values) found for this structure. Despite these difficulties, the atomic positions are well resolved in the crystal structure analysis.

References:

(1) Sheldrick, G. M. *SHELXTL V5.1 Software Reference Manual*, Bruker AXS, Inc., Madison, USA, **1997**.

(2) Sheldrick, G. M. SHELX97, *Programs for Crystal Structure Analysis*; Institüt für Anorganische Chemie der Universität: Göttingen, Germany, **1998**.

(3) Sheldrick, G. M. *SADABS, V2.01, Empirical Absorption Correction Program*, Institüt für Anorganische Chemie der Universität: Göttingen, Germany, **1996**.

Table1. Summary of crystal and structure refinement data for compound **1**

Compound	**1**
Empirical formula	$C_{105}H_{93}N_3OS_{16}Zn_8$
Formula weight	2449.13
Crystal system	Monoclinic
Space group	*C2/c*
a / Å	27.752(9)
b / Å	25.752(8)
c / Å	33.771(11)
α / °	90
β / °	103.656(5)
γ / °	90
V / Å^3	23453(13)
Z	8
Dc / Mg m^{-3}	1.334
Abs coeff. / mm^{-1}	1.934
Max. and min. transmission	0.671 and 0.609
F(000)	9240
Crystal size / mm	0.47 × 0.22 × 0.21
θ / deg	1.17 to 27.59
Limiting indices	-35 ≤ h ≤ 31
	-25 ≤ k ≤ 33
	-43 ≤ l ≤ 42
Reflns collected / unique	67119 / 26441
	[R(int) = 0.2729]
Data / restraints / params	26441 / 0 / 534
Goodness-of-fit on F^2	1.012
Final R indices [I>2σ(I)]	R_1 = 0.1640
	wR_2 = 0.3800
R indices (all data)	R_1 = 0.3798
	wR_2 = 0.4952

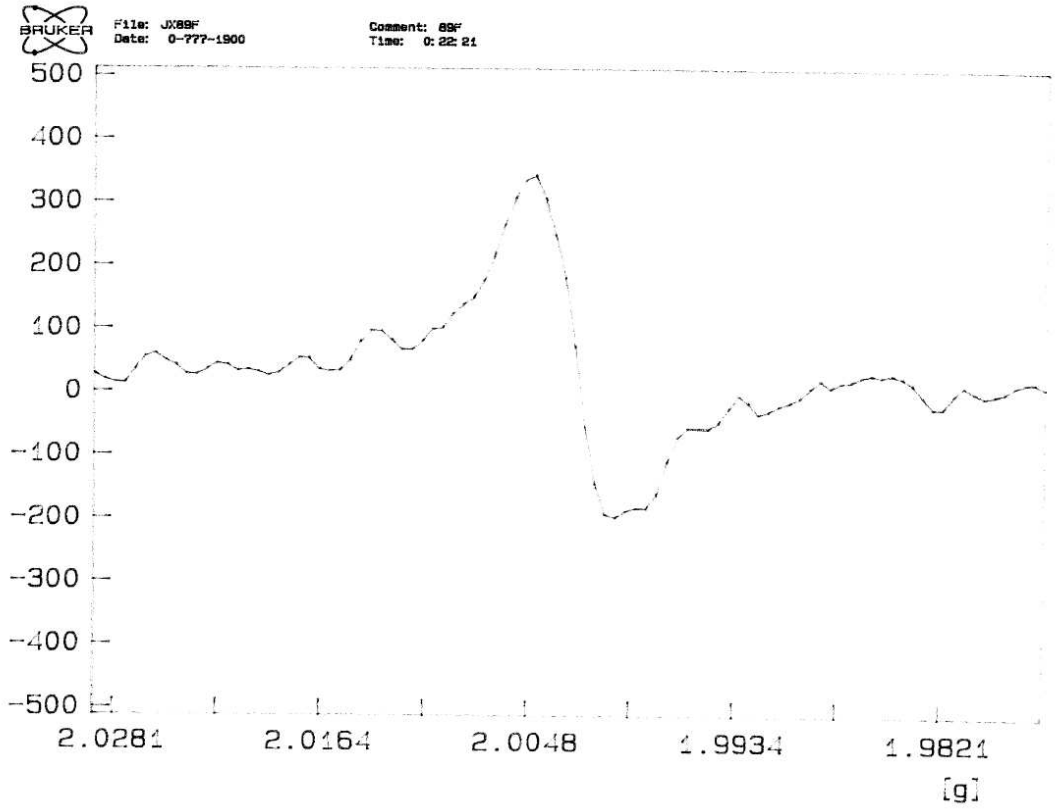
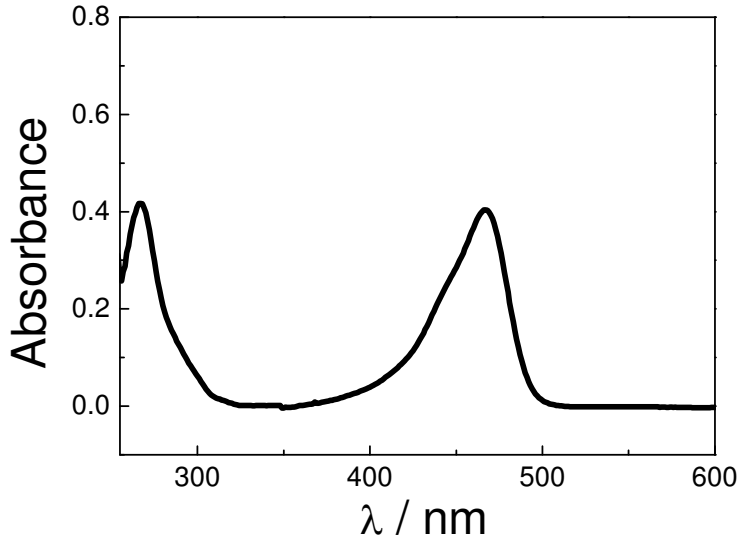
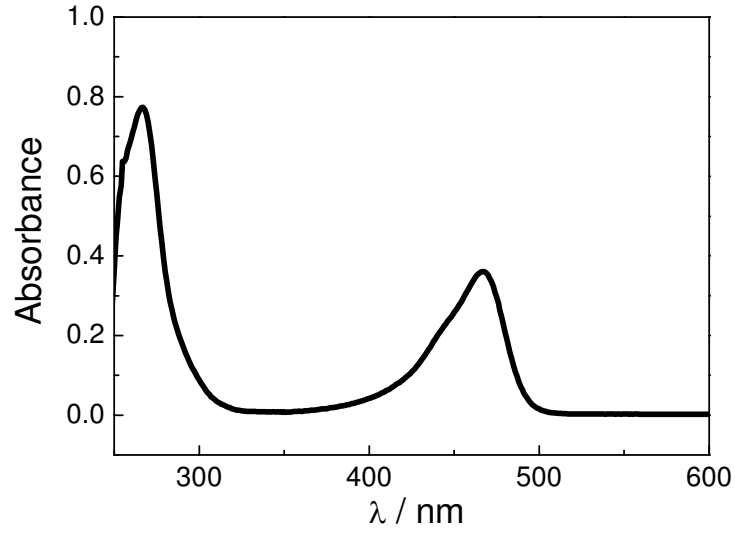


Figure S1. ESR spectrum of **1** at room temperature.



(a)



(b)

Figure S2. (a) UV-vis spectrum of Acridine Yellow G ($c = 1.0 \times 10^{-5}$ M in DMSO). (b) UV-vis spectrum of **1** ($c = 1.0 \times 10^{-5}$ M in DMSO).

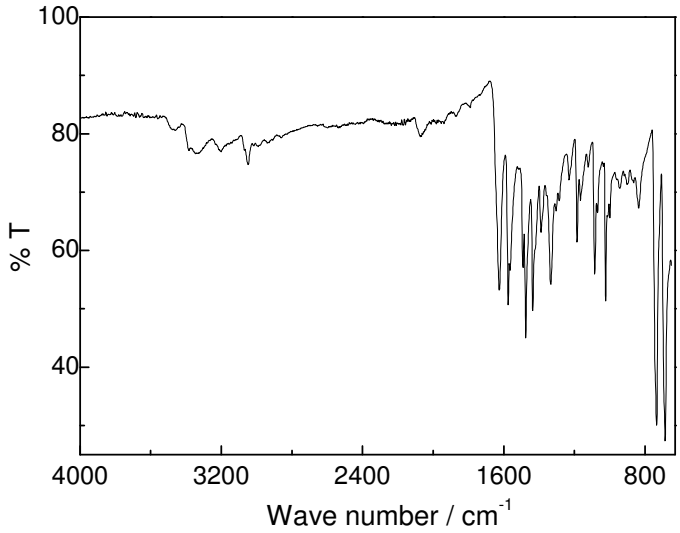


Figure S3. FT-IR spectrum of compound **1**.

(a) (b)

Figure S4. Photos of compound **1** in DMSO solution (c = 1.0 × 10^{-6} M): (a) under daylight and (b) under UV irradiation (λ = 365 nm).