Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Combining PeT and ICT Mechanism into One Chemosensor for the Highly Sensitive and Selective Detection of Zinc

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Photophysical properties of ZS1

Table S1 Photophysical properties of the probe.

entry	λ_{ab} (nm)	λ_{em} (nm)	Φ^a	ε / M^{-1} cm^{-1}
ZS1	360	465	0.033	11598
ZS1+Zn^{2+}	366	522	0.175[b]	12145

(a) The quantum yield (Φ) of **ZS1** and **ZS1**-Zn^{2+} system were determined according to the literature.[1] (b) Φ was determined in the present of 10.0 equiv. of Zn^{2+}.

$$\Phi_{Sample} = \frac{\Phi_{QS} \cdot A_{QS} \cdot F_{Sample} \cdot \lambda_{exQS} \cdot \eta^2_{Sample}}{A_{Sample} \cdot F_{QS} \cdot \lambda_{exSample} \cdot \eta^2_{QS}}$$

Where Φ is quantum yield; A is absorbance at the excitation wavelength; F is integrated area under the corrected emission spectra; λ_{ex} is the excitation wavelength; η is the refractive index of the solution; the Sample and QS refer to the sample and the standard, respectively. We chose quinine sulfate in 0.1N H_2SO_4 as standard, which has the quantum yield of 0.546.[2]

Additional spectroscopic data

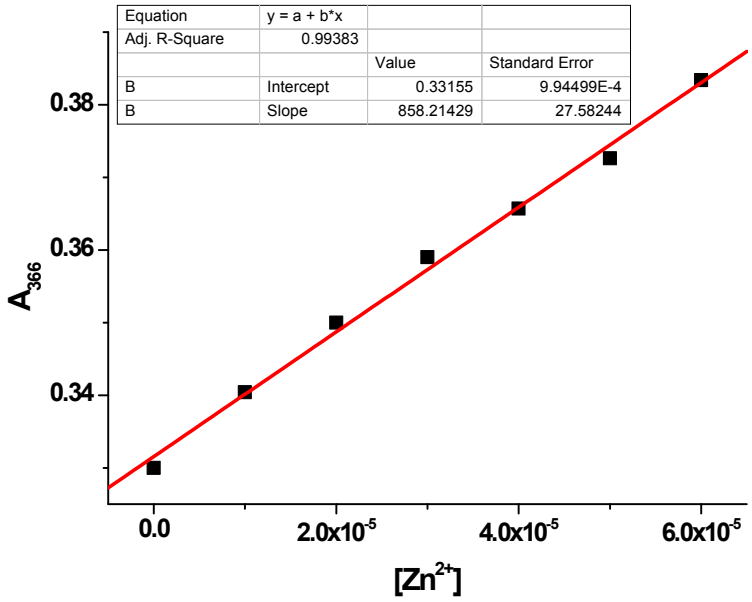


Fig. S1 UV-vis absorption of **ZS1** (20.0 μM) at 366 nm as a function of Zn^{2+} concentration (0-6.0 equiv.) in Tirs-HCl buffer solution (10 mM, pH 7.2, containing 1% CH_3CN).

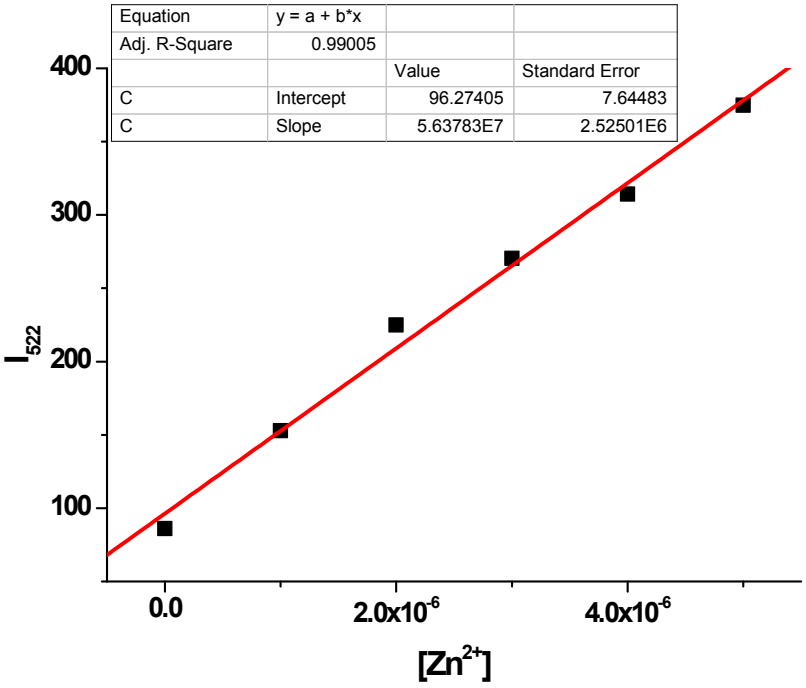


Fig. S2 Calibration curve of **ZS1** (1.0 μM) with Zn^{2+} (10 mM Tirs-HCl buffer, pH 7.2, containing 1% CH_3CN, λ_{ex} = 360 nm), slit = 5/5. The detection limit (DL) of Zn^{2+} ions using **ZS1** was determined from the following equation: [3]

$$DL = 3*\sigma/K$$

Where σ is the standard deviation of the blank solution; K is the slope of the calibration curve.

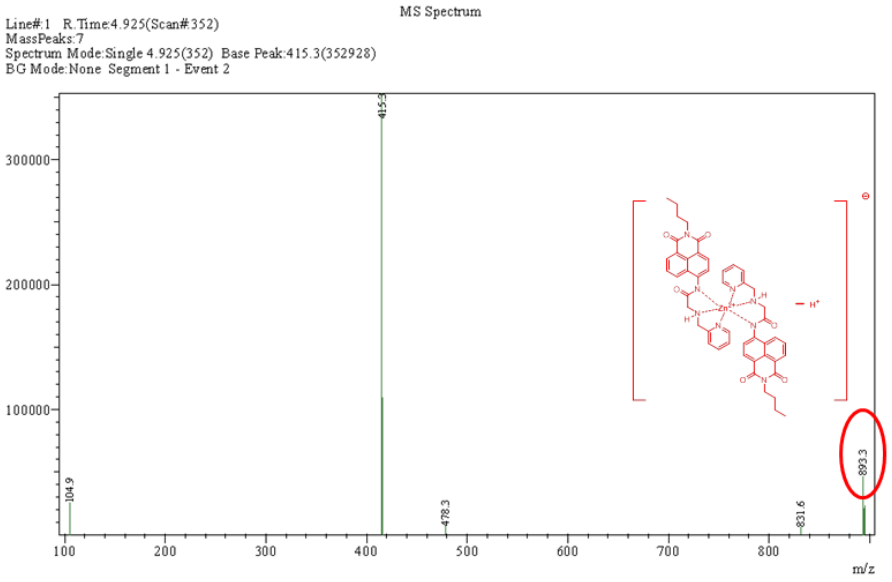


Fig. S3 HPLC-MS (ESI) spectrum of **ZS1**-Zn^{2+} system (in Tris-HCl solution) shows the peak of **ZS1**-Zn^{2+} complex. [**ZS1**-Zn complex -H]$^{-}$ = 893.3 (*calcd*. for 893.3, $C_{48}H_{45}N_8O_6Zn$).

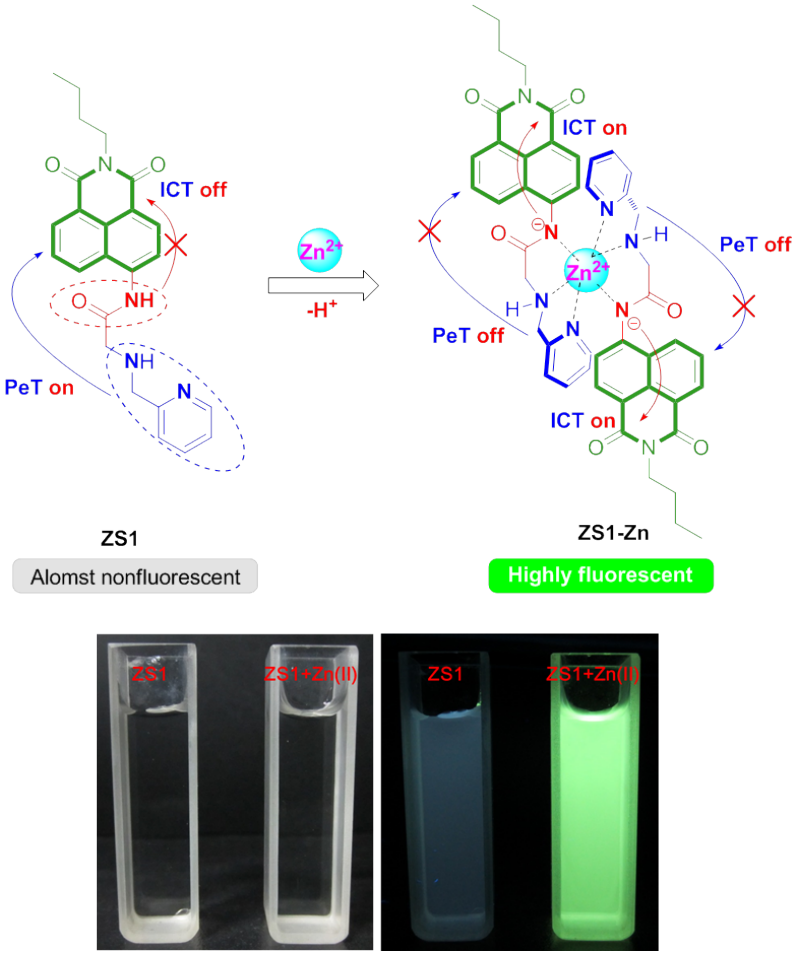


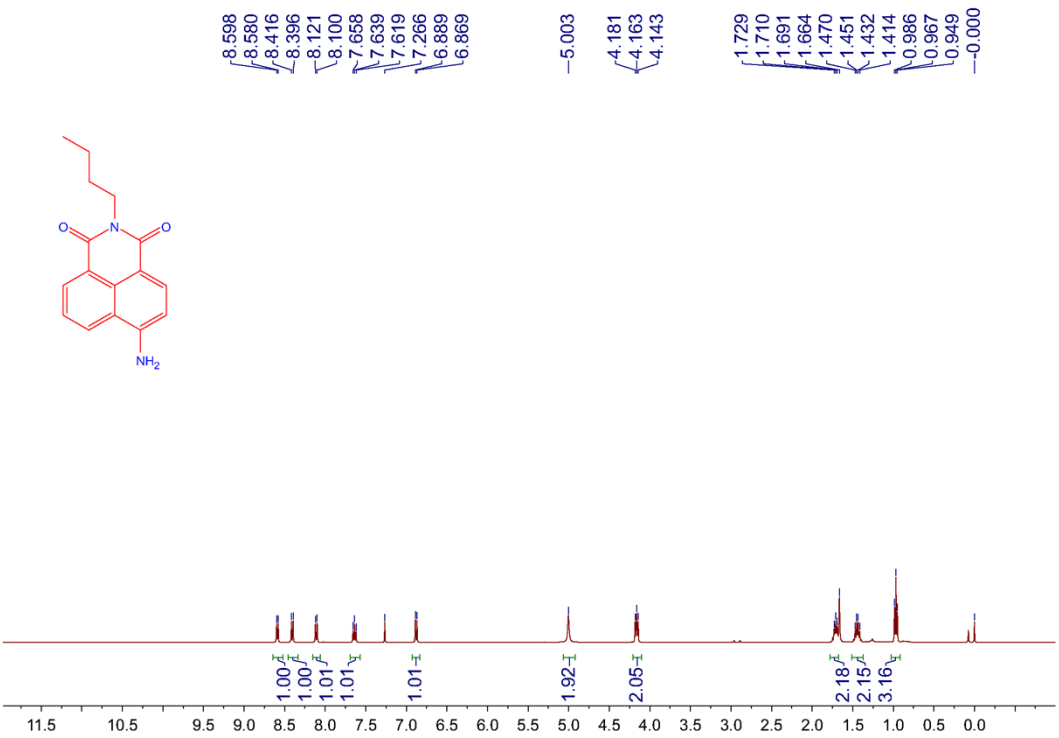
Fig. S4 The color changes of **ZS1** in the absence and presence of Zn^{2+}.

Cell lines and imaging experiments

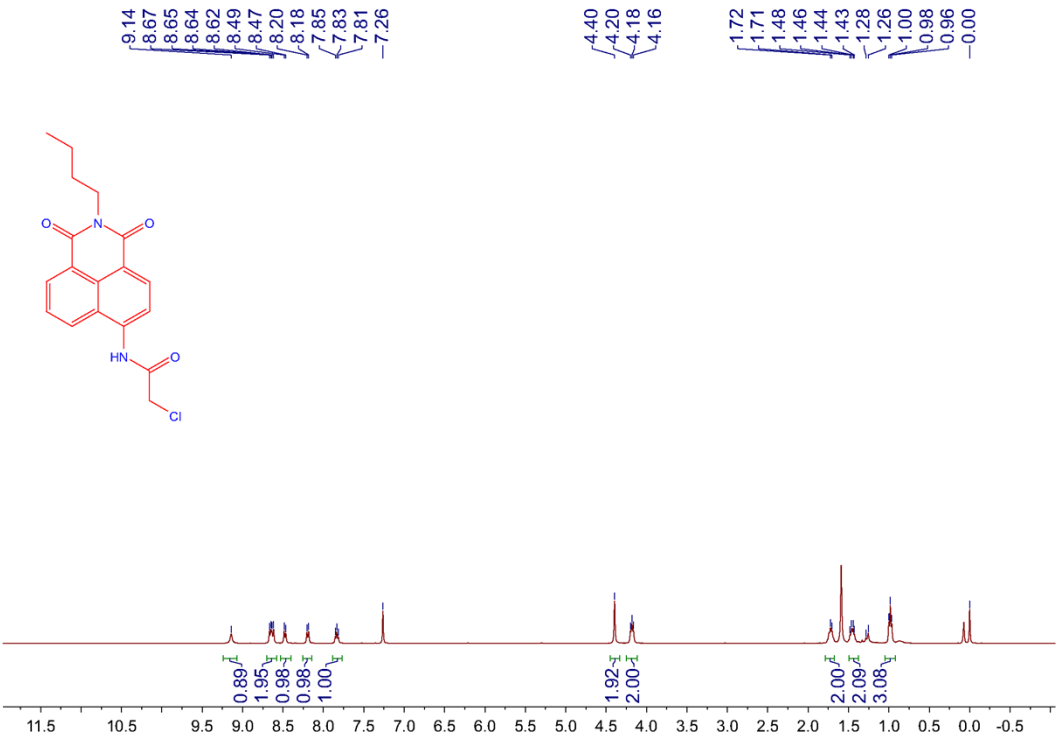
HeLa cells were cultured in DMEM (Invitrogen, Carlsbad, CA), supplemented with 10% fetal bovine serum in a humidified atmosphere of 5% CO_2 at 37 ^oC. For imaging experiments, **e**xponentially growing cells (at a density of 20000-40000 cells per well, respectively) were seeded in 24-well plate. Cells were cultured at 37 ^oC in a 5% CO_2 atmosphere for 24 h before they were exposed to reagents. After the staining steps as described in figure captions, the images were collected upon excitation using the corresponding filters for DAPI (blue). Furthermore, MTT assay was employed to evaluate the cytotoxicity of ZS1 and it turned out that this probe is virtually nontoxic to HeLa cells even at 20 μM after 24 h incubation.

The characterization data of compounds

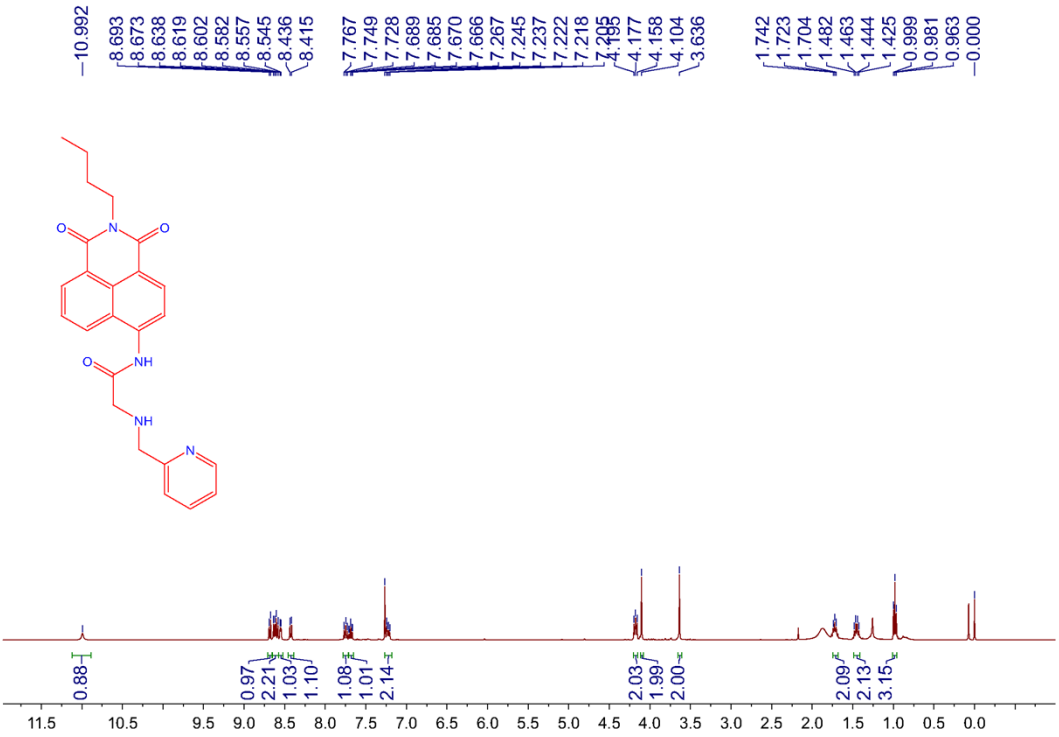
^{1}H NMR of compound **1**



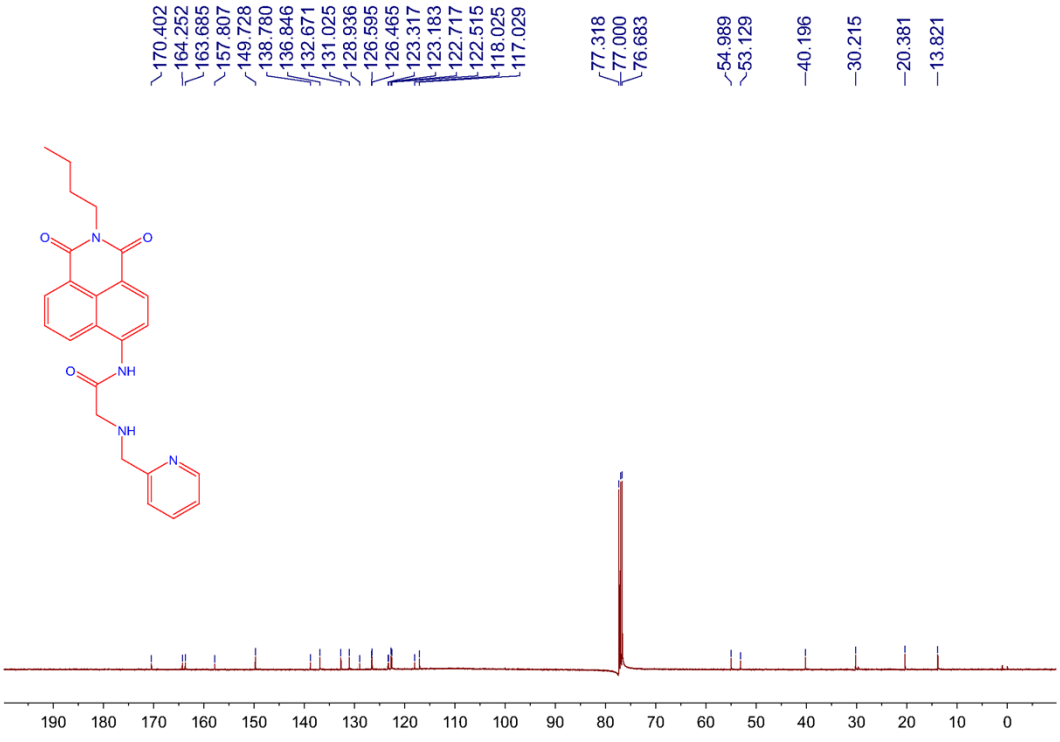
^{1}H NMR of compound **2**



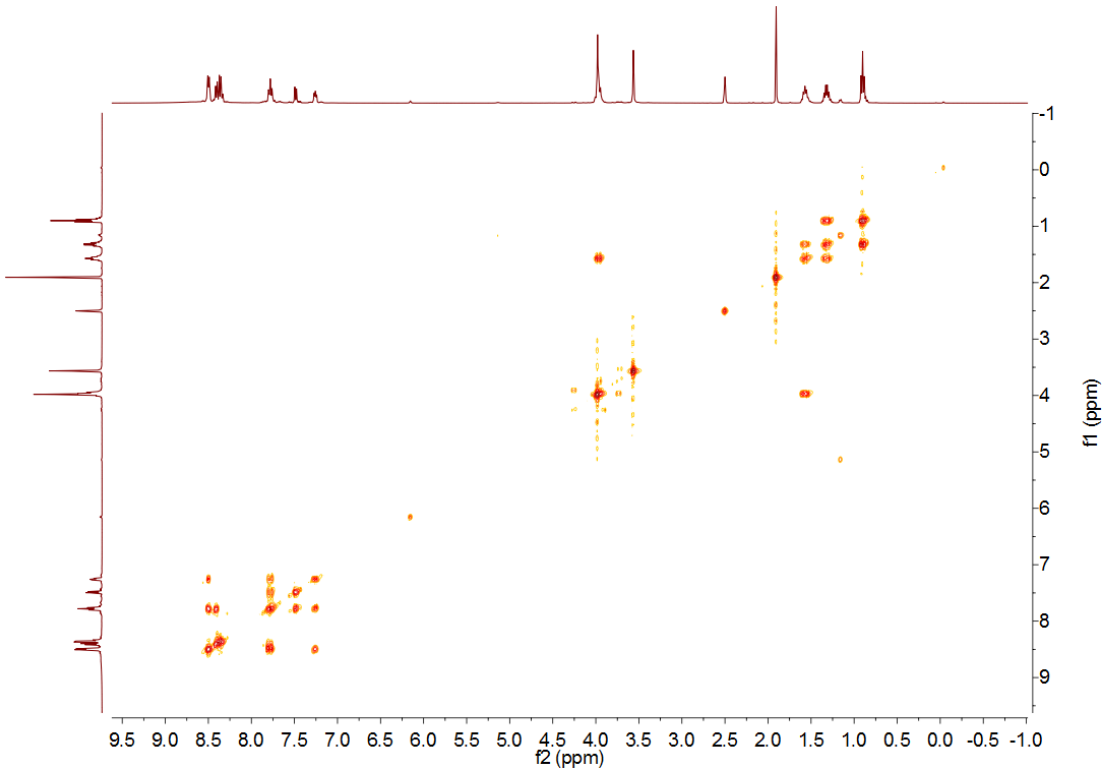
^{1}H NMR of compound **3** (**ZS1**)



^{13}C NMR of compound **3** (**ZS1**)

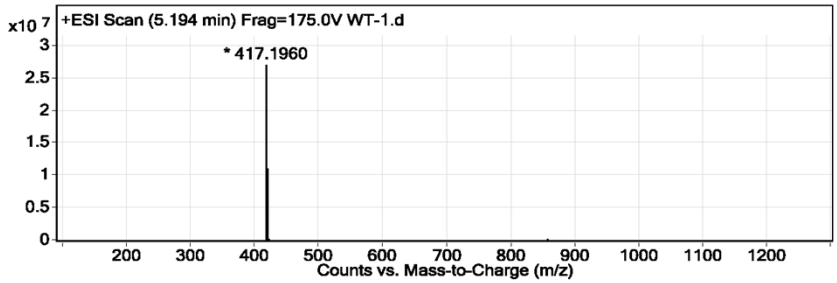


2D NMR of compound **3** (**ZS1**)



HRMS (ESI-TOF) of compound **3** (**ZS1**)

Qualitative Analysis Report



Peak List

m/z	z	Abund
417.196	1	27108390
417.3741		1931938.4
418.1967	1	11177915
419.1991	1	1907391.8

References

1 R. A. Velapoldi, H. H. Tønnesen, *J. Fluoresc*., 2004, **14**, 465-472.

2 D. F. Eaton, *Pure Appl. Chem*., 1988, **60**, 1107-1114.

3 (*a*) J. T. Yeh, P. Venkatesan and S. P. Wu, *New J. Chem*., 2014, **38**, 6198-6204. (*b*) A. Roy, D. Kand, T. Saha and P. Talukdar, *Chem. Commun*., 2014, **50**, 5510-5513.