

## Electronic Supplementary Information

### “A colorimetric and fluorescent turn-on chemosensor operative in aqueous media for $Zn^{2+}$ based on a multifunctionalized spirobenzopyran derivative”

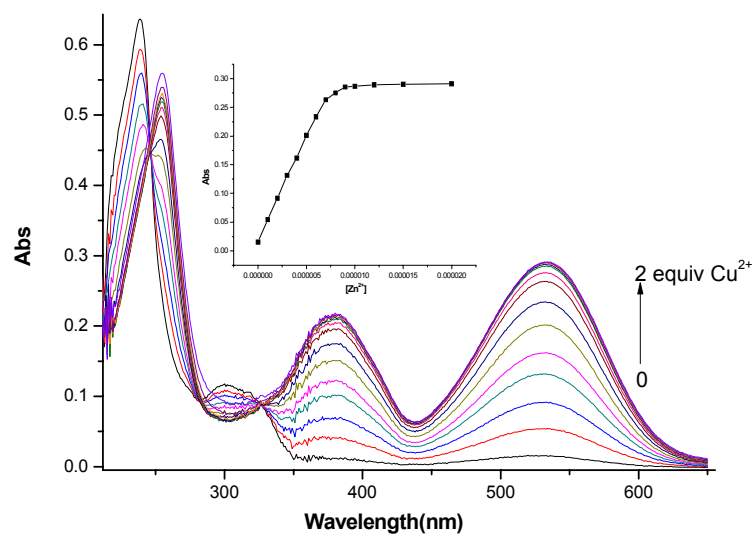
Jian-Fa Zhu, Han Yuan, Wing-Hong Chan\* and Albert W. M. Lee

Department of Chemistry, Hong Kong Baptist University, Kowloon Tong, Hong Kong SAR, China

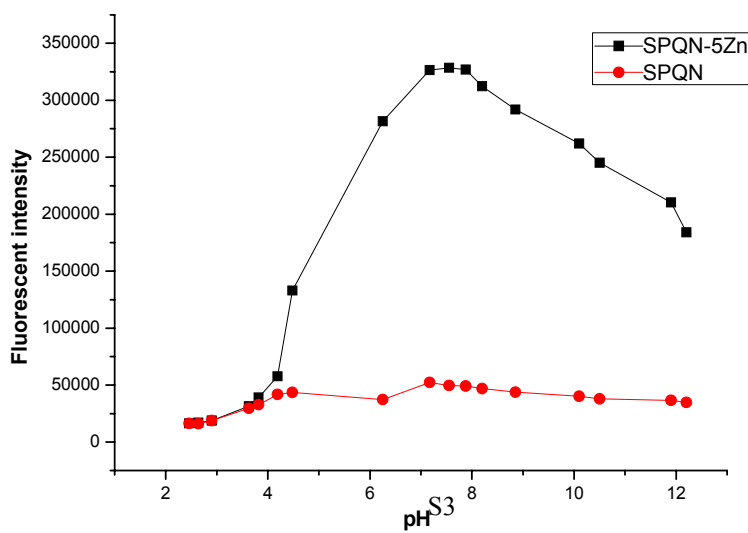
Fax: +852 3411 7348; Tel: +852 3411 7076; Email: [whchan@hkbu.edu.hk](mailto:whchan@hkbu.edu.hk)

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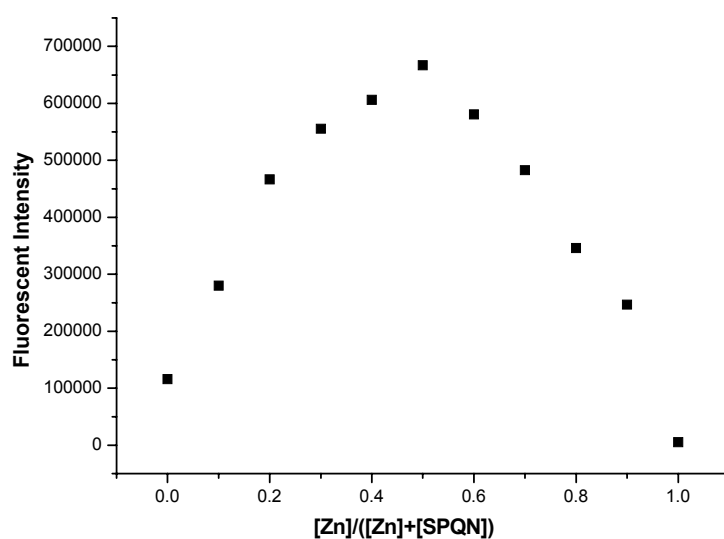
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| Figure S8     | Fluorescence spectra ( $\lambda_{\text{ex}} = 326 \text{ nm}$ ) of <b>SPQN</b> (10 $\mu\text{M}$ ) in buffer solution (50 mM, HEPES, 50% ethanol, pH = 7.4) in the presence of different concentration of $\text{Zn}^{2+}$ (exceeding 1 equiv) | S6  |
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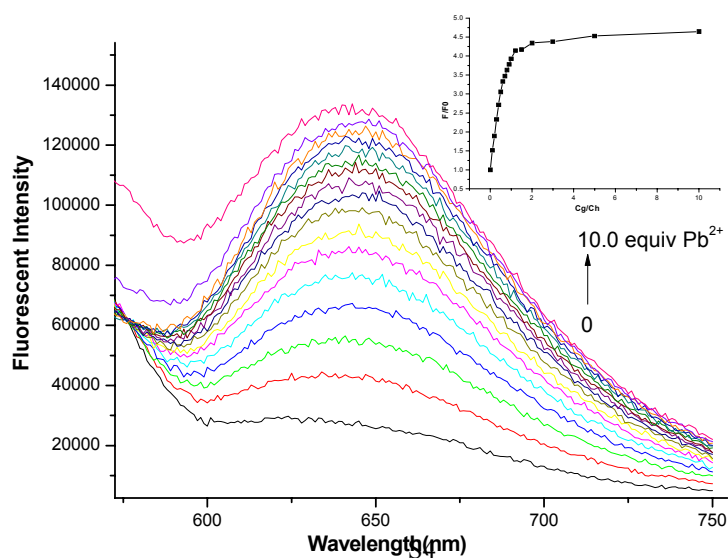
**Fig. S1** UV-vis spectra of SPQN (10 μM) upon the titration of Cu<sup>2+</sup> (0 – 2 equiv) in buffer solution (50 mM HEPES, 50% ethanol, pH = 7.4)



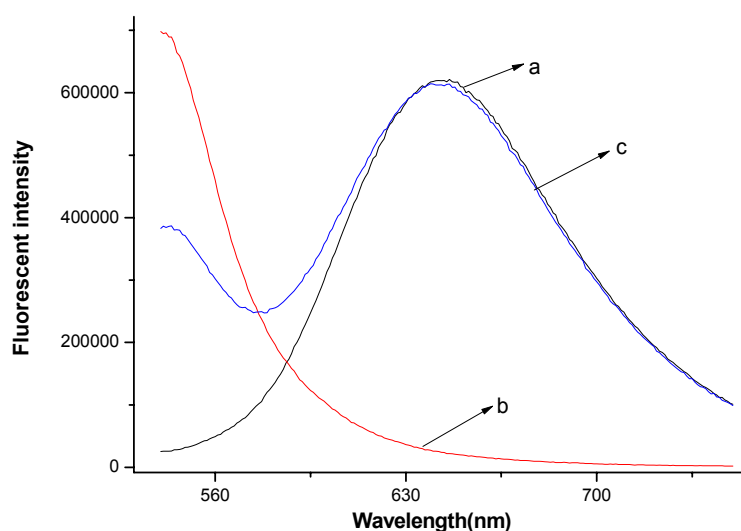
**Fig. S2** Fluorescence intensity of SPQN (10  $\mu\text{M}$ ) at various pH values in ethanol/water (2:8, v/v) solution in the absence and presence of  $\text{Zn}^{2+}$  (5 equiv).



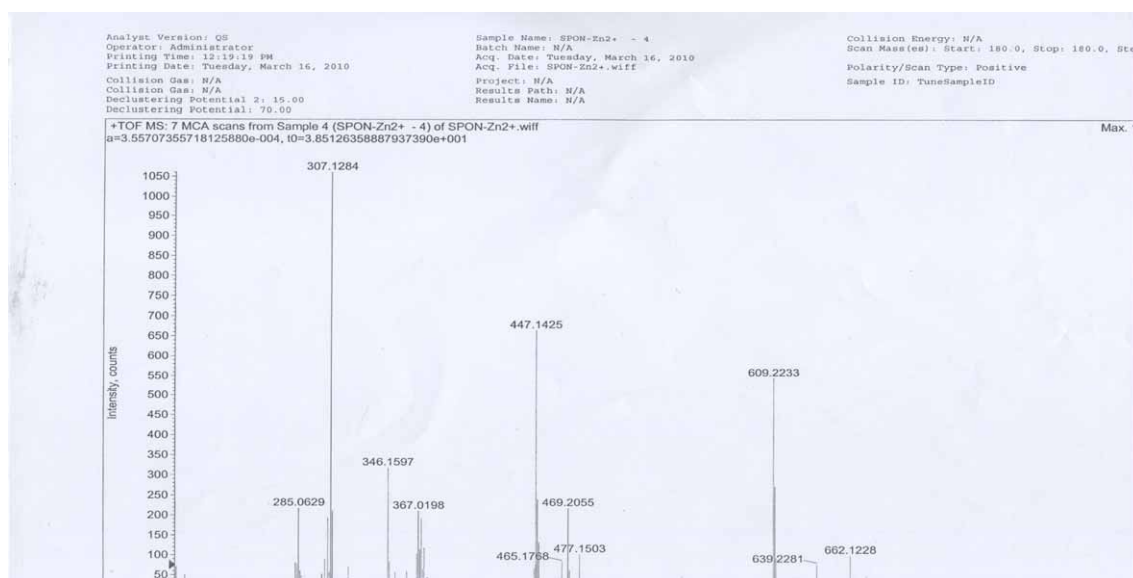
**Fig. S3** Job's plot by fluorescence method of the complex between SPQN and  $\text{Zn}^{2+}$ .



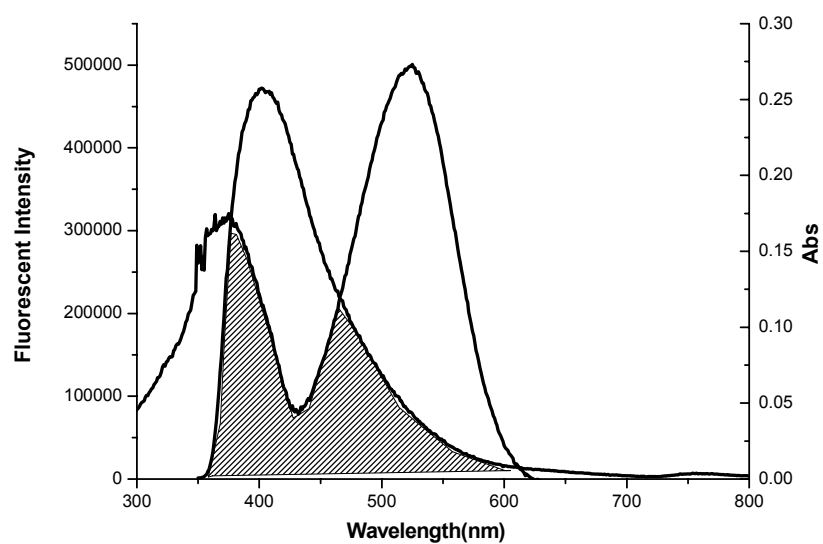
**Fig. S4** Fluorescence spectra ( $\lambda_{\text{ex}} = 515 \text{ nm}$ ) of  $10 \mu\text{M}$  SPQN upon the titration of  $\text{Pb}^{2+}$  (0 – 10.0 equiv) in buffer solution (50 mM, HEPES, 50% ethanol, pH = 7.4); inset: fluorescence intensity ratio as a function of  $\text{Pb}^{2+}$  concentration



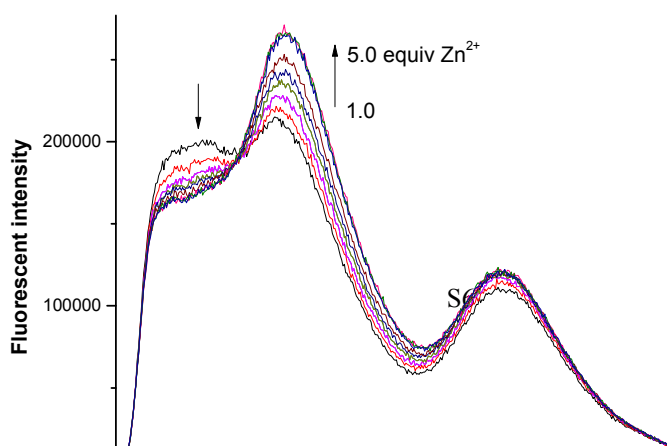
**Fig. S5** Plot of fluorescence intensity changes of SPQN ( $10 \mu\text{M}$ ) by adding (a) 1 equiv of  $\text{Zn}^{2+}$ ; (b) (a) + 1 equiv of EDTA; (c) (b) + 1 equiv of  $\text{Zn}^{2+}$



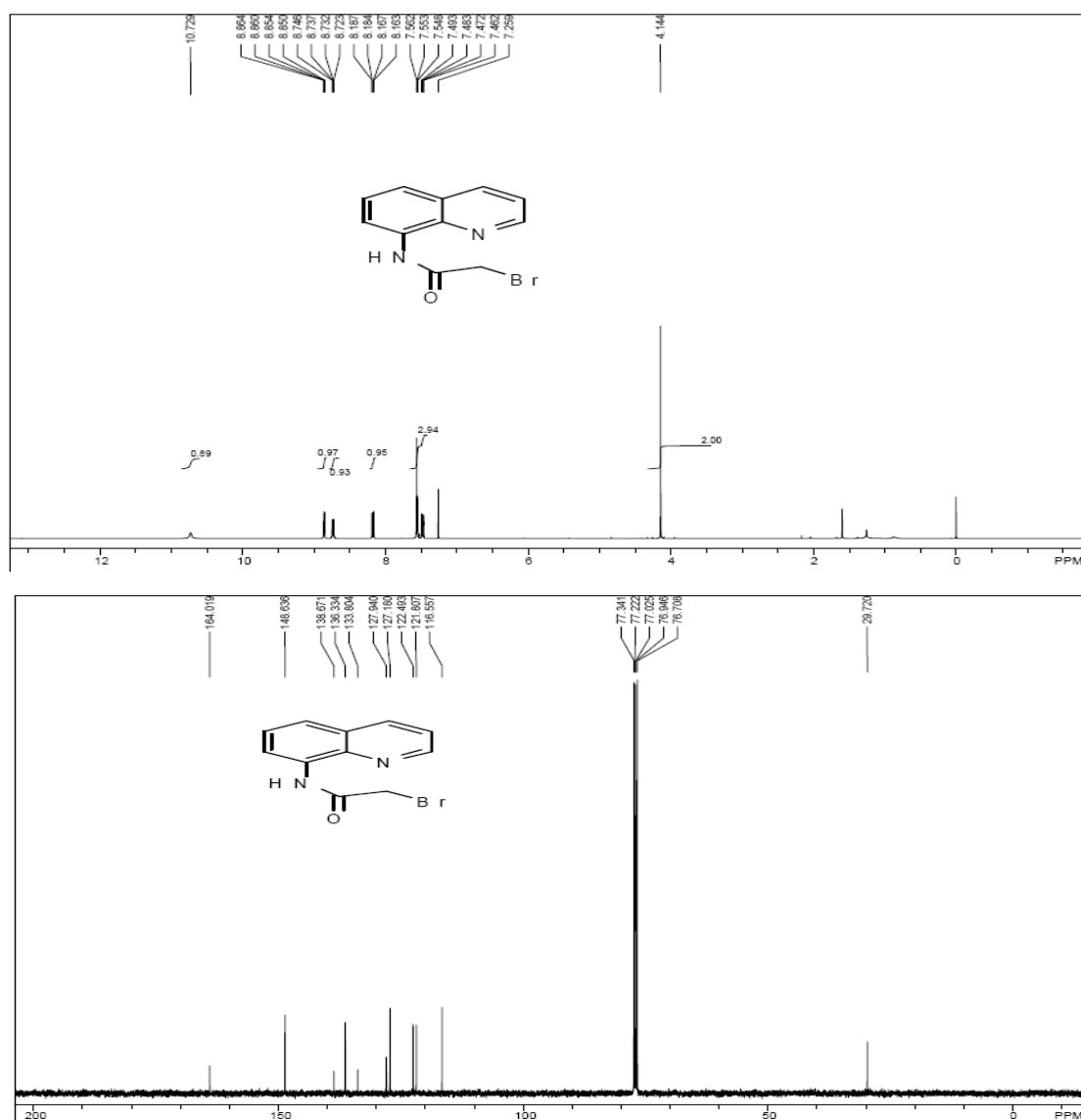
**Fig. S6** MADLI-TOF HRMS spectrum of SPQN-Zn<sup>2+</sup> showing [M + Zn - H]<sup>+</sup> peak at 609.2233



**Fig. S7** The overlapping of the emissive peak of the quinoline moiety of SPQN ( $\lambda_{\text{ex}} = 326 \text{ nm}$ ) and the absorption peak of SPQN-Zn<sup>2+</sup> complex



**Fig. S8** Fluorescence spectra ( $\lambda_{\text{ex}} = 326 \text{ nm}$ ) of SPQN (10  $\mu\text{M}$ ) in buffer solution (50 mM, HEPES, 50% ethanol, pH = 7.4) in the presence of different concentration of  $\text{Zn}^{2+}$  (exceeding 1 equiv)



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Operator: Administrator  
Printing Time: 09:57:53 AM  
Printing Date: Friday, February 26, 2010  
Collision Gas: N/A  
Decustering Potential: 2; 15.00  
Decustering Potential: 55.00

Sample Name: QN-Br-1  
Batch Name: N/A  
Acq. Date: Friday, February 26, 2010  
Acq. File: QN-Br-1.wiff  
Project: N/A  
Results Path: N/A  
Results Name: N/A

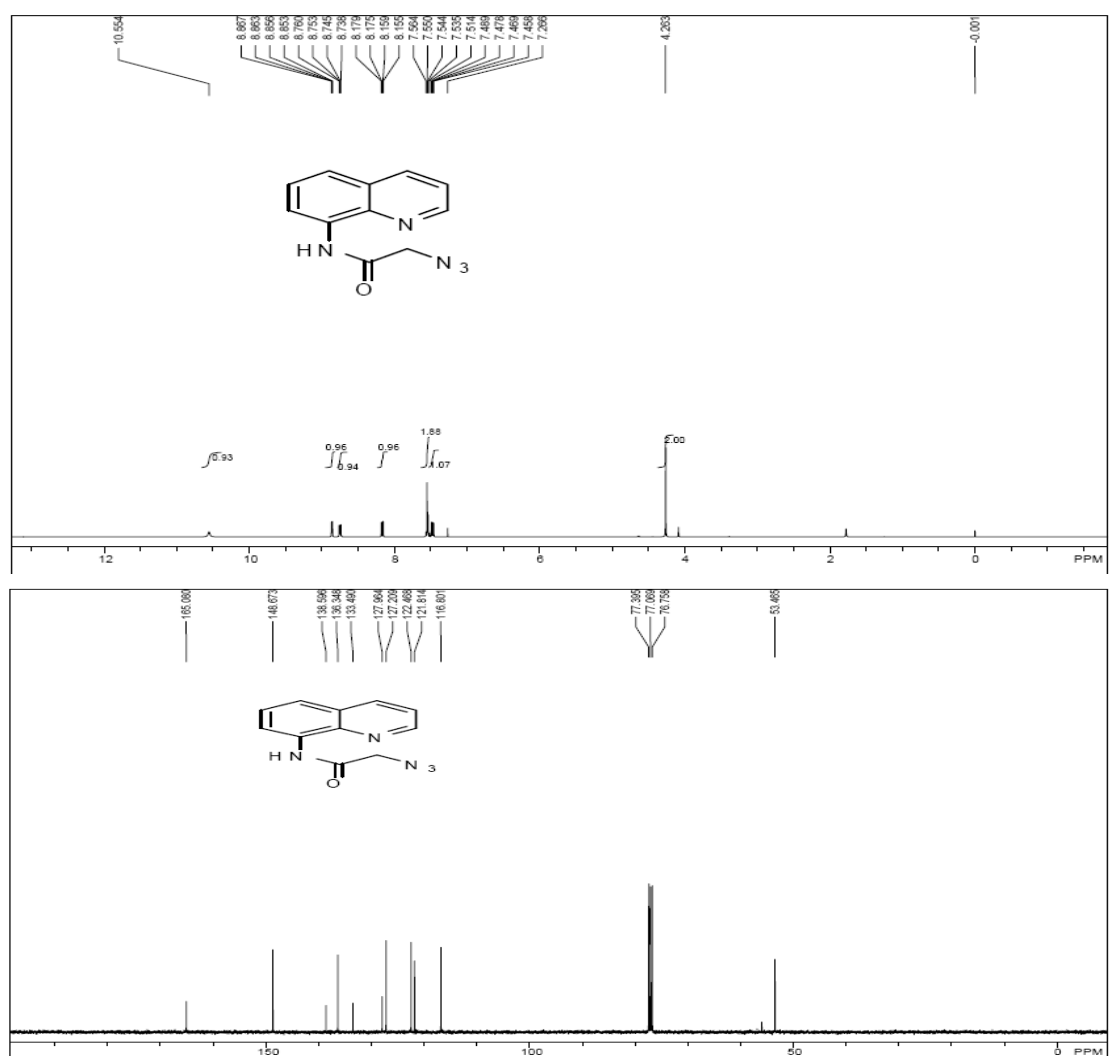
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Polarity/Scan Type: Positive  
Sample ID: TuncSampleID

+TOF MS: 18 MCA scans from QN-Br-1.wiff

Max. 426



**Fig. S9-11** Spectral data of compound **3** ( $^1\text{H}$  NMR;  $^{13}\text{C}$  NMR; HRMS)





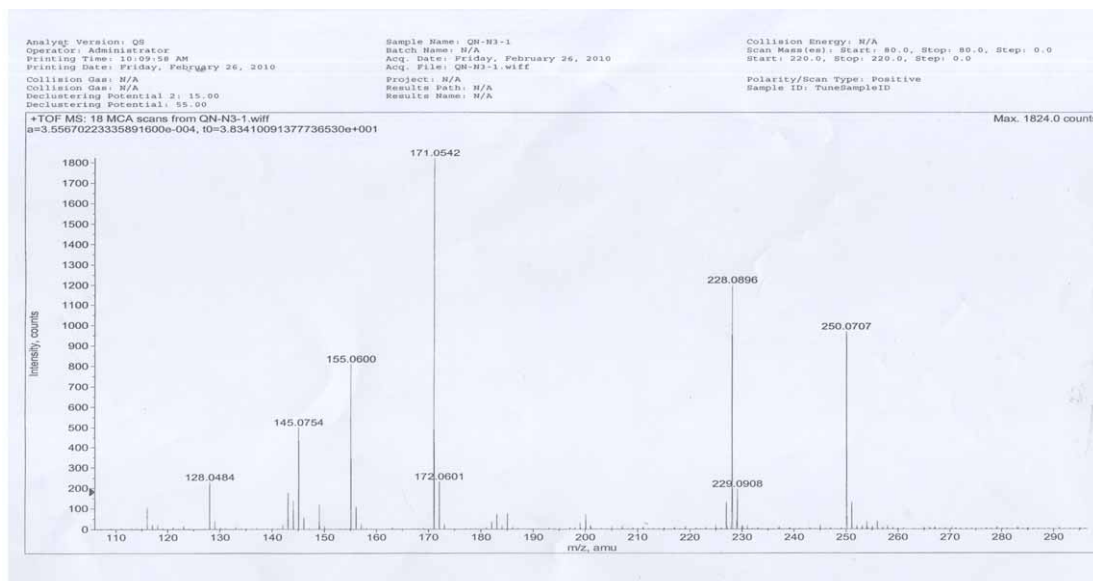
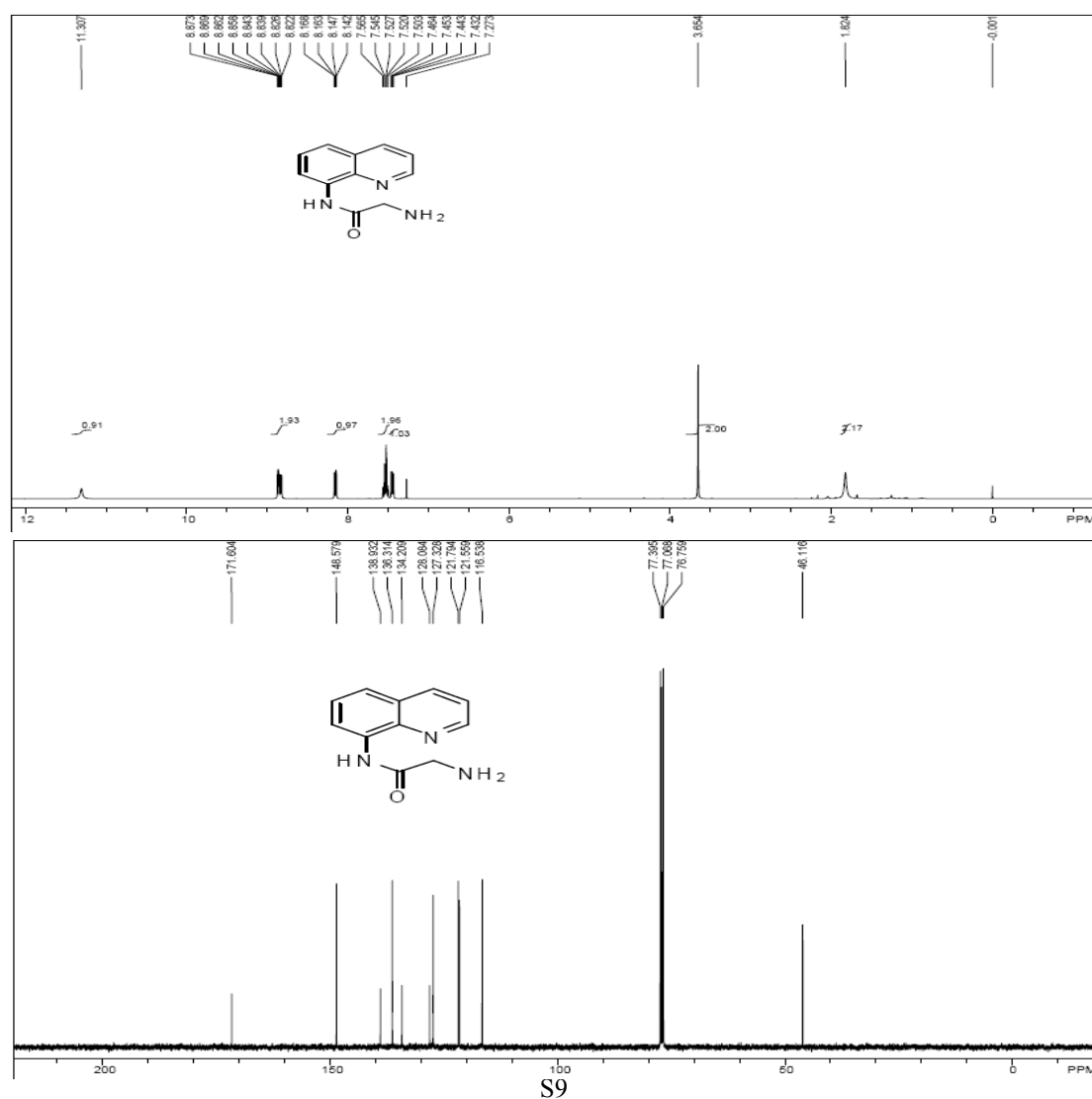
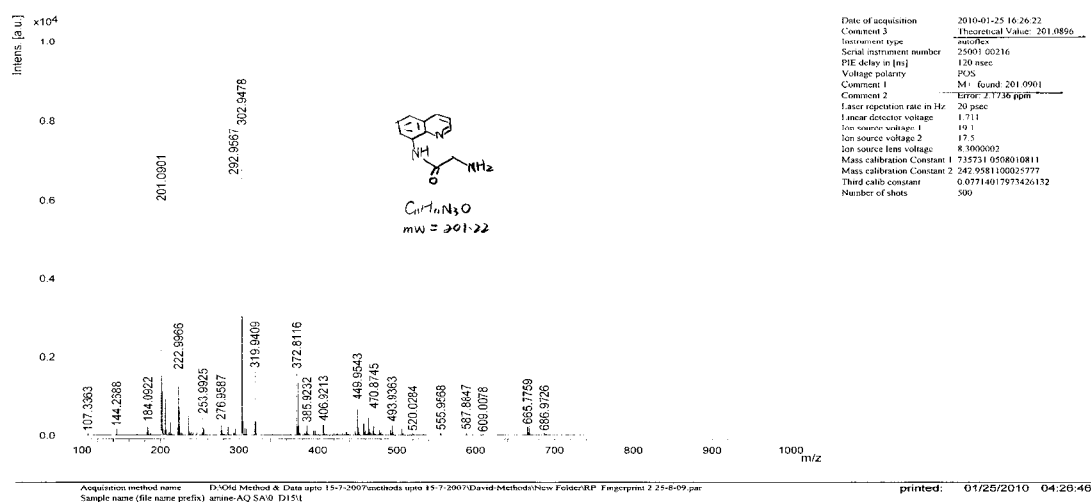


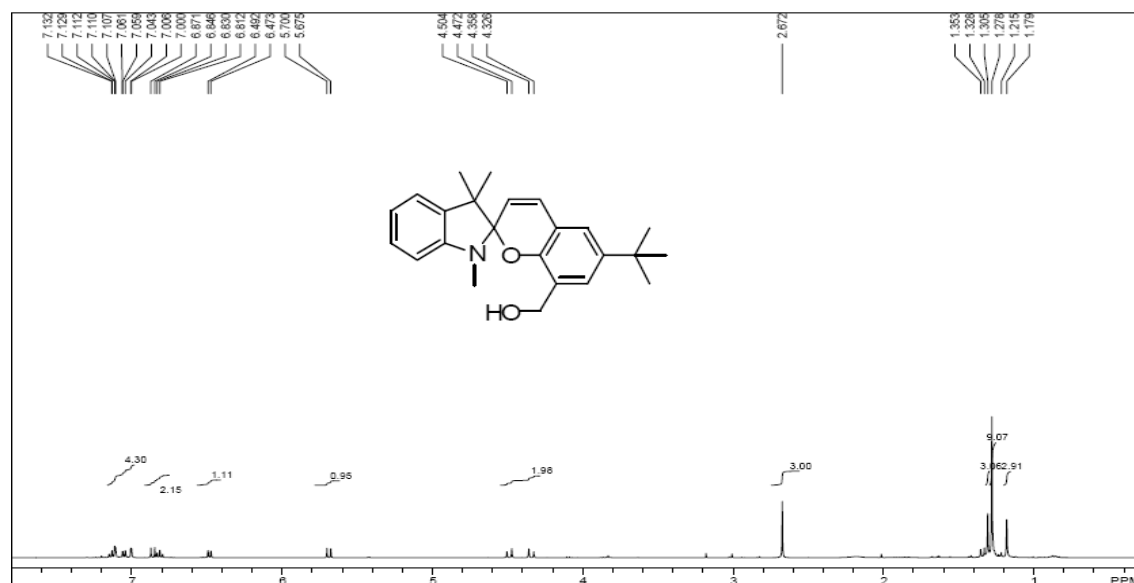
Fig. S12-14 Spectral data of compound **4** ( $^1\text{H}$  NMR;  $^{13}\text{C}$  NMR; HRMS)



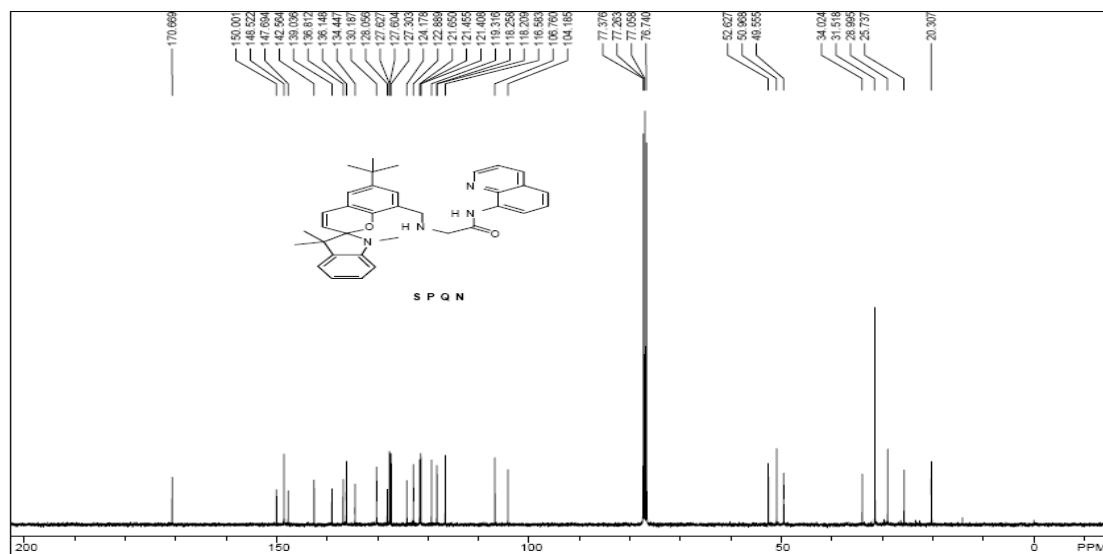
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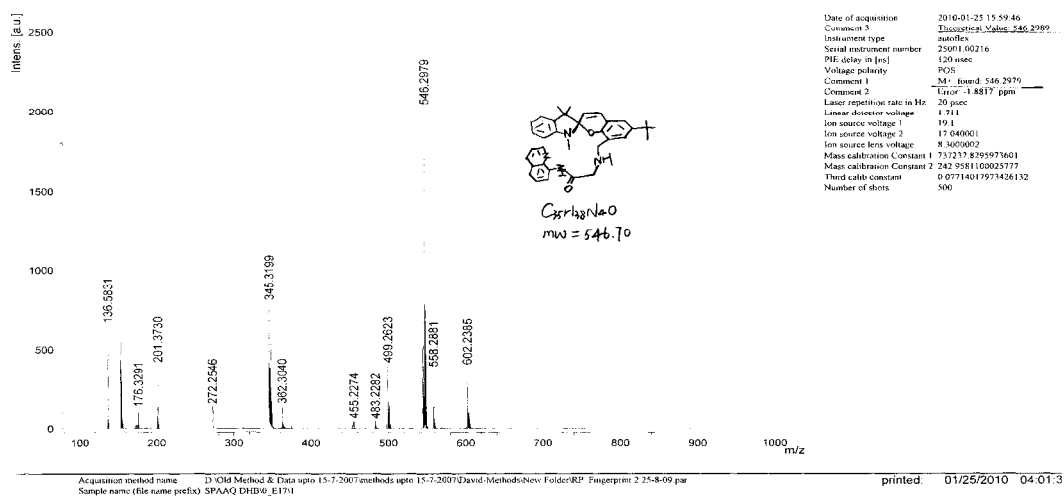
**Fig. S15-17** Spectral data of compound **5** ( $^1\text{H}$  NMR;  $^{13}\text{C}$  NMR; HRMS)







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**Fig. S21-23** Spectral data of compound **5** ( $^1\text{H}$  NMR;  $^{13}\text{C}$  NMR; HRMS)