

**AIE-active Ir(III) complexes with tunable emissions,  
mechanoluminescence and the application for data security  
protection**

Zhongming Song,<sup>a</sup> Rui Liu,<sup>\*a</sup> Yuhao Li,<sup>b</sup> Hong Shi,<sup>c</sup> Jinyang Hu,<sup>a</sup> Xiao Cai<sup>a</sup> and  
Hongjun Zhu<sup>\*a</sup>

<sup>a</sup> *Department of Applied Chemistry, College of Chemistry and Molecular Engineering,  
Nanjing Tech University, Nanjing 211816, P. R. China.*

<sup>b</sup> *College of Science, University of Shanghai for Science and Technology, Shanghai  
200093, P. R. China.*

<sup>c</sup> *Jiangsu Vocational College of Information Technology, Wuxi 214153, P. R. China.*

\*Corresponding author. Phone: +86-25-58139539. Fax: +86-25-58139539. E-mail:

rui.liu@njtech.edu.cn (R. Liu)

\*Corresponding author. Phone: +86-25-83172358. Fax: +86-25-83587428. E-mail:

zhuhj@njtech.edu.cn (H. Zhu)

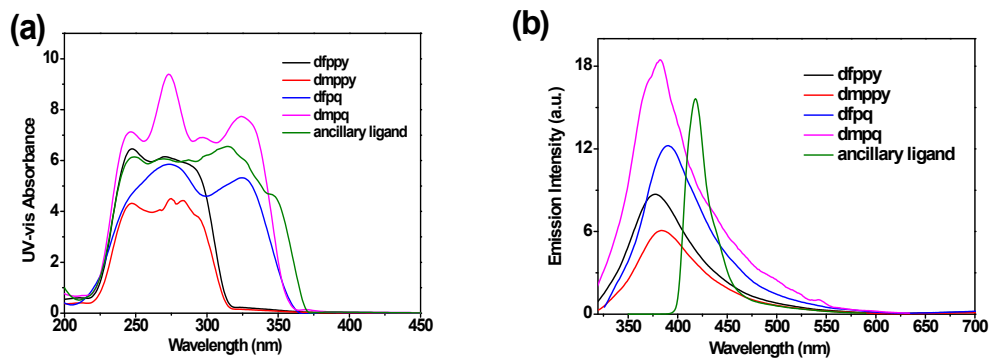
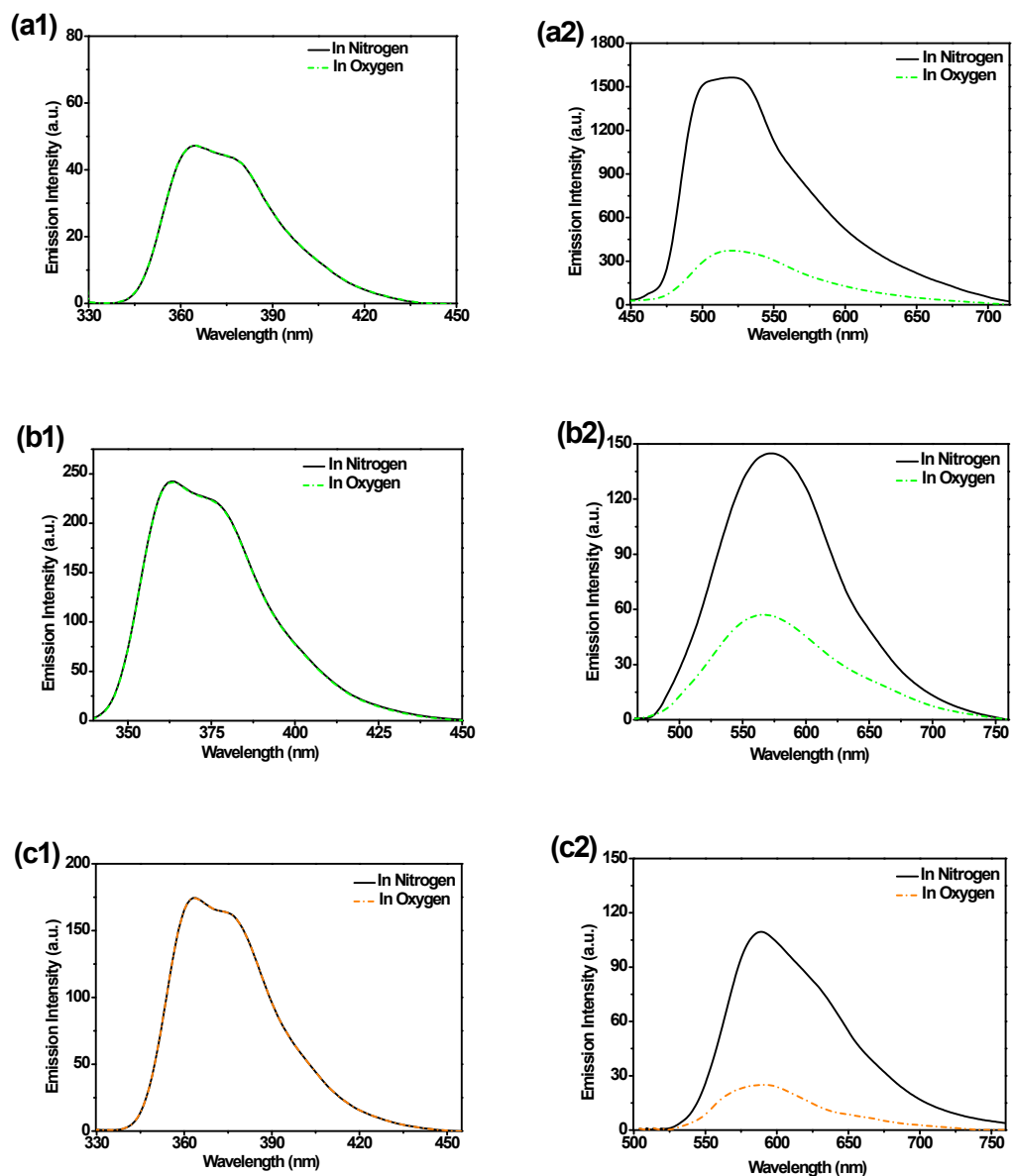
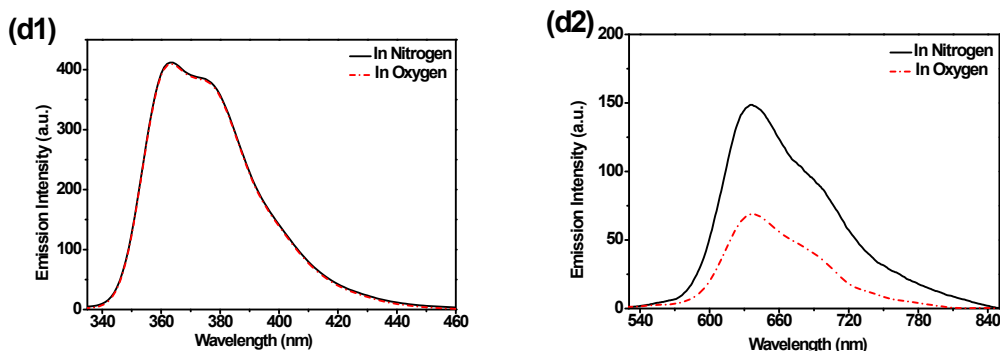
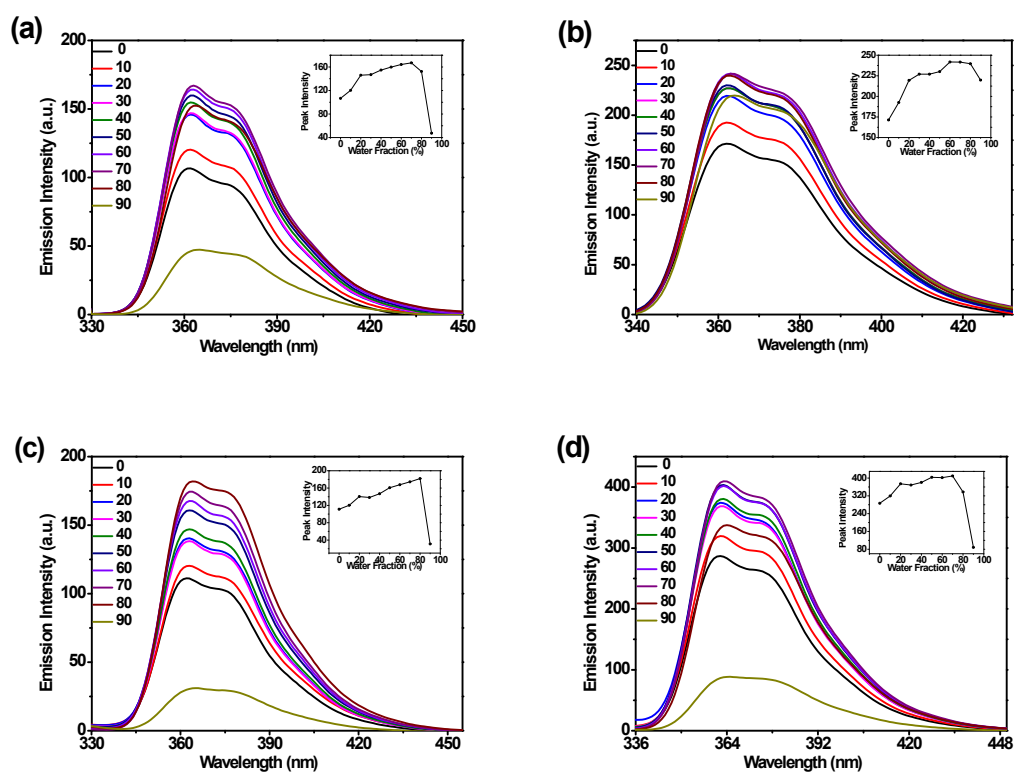


Fig. S1 Absorption and emission spectra of ligands in  $\text{CH}_2\text{Cl}_2$  solution at room temperature.

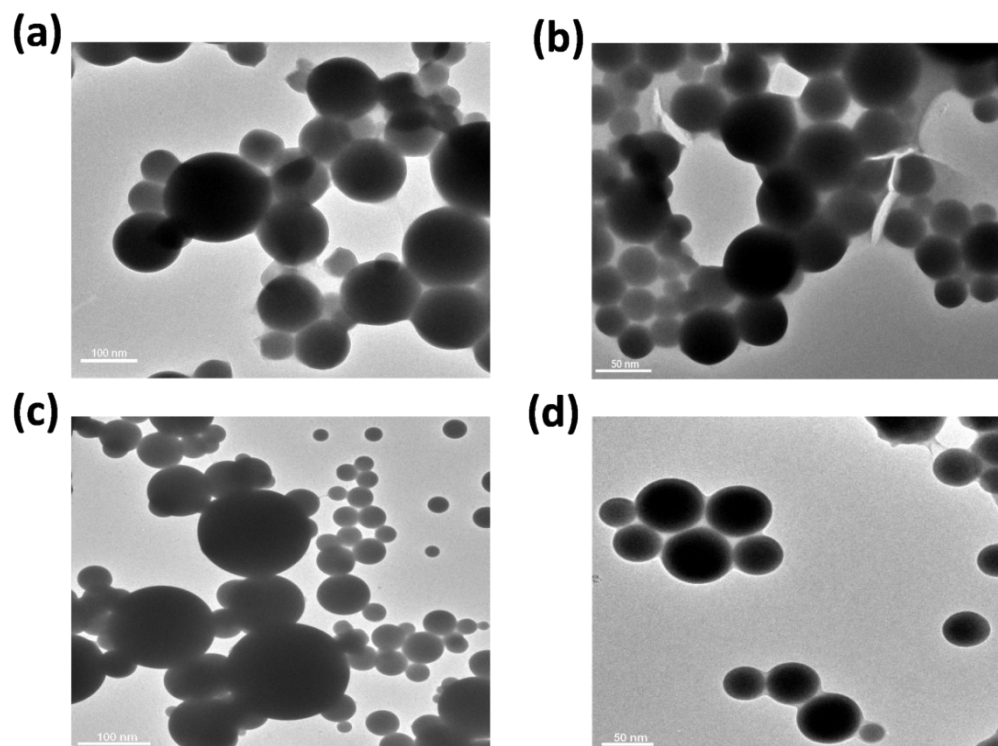




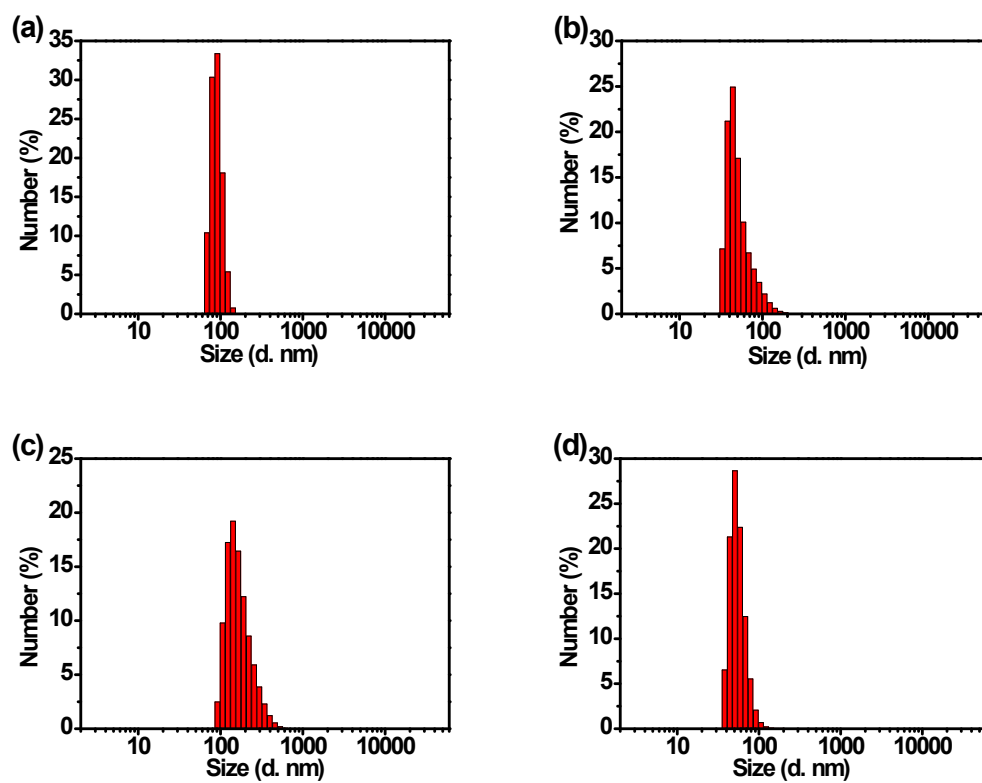
**Fig. S2** Emission spectra of complexes **1** (a1, a2), **2** (b1, b2), **3** (c1,c2) and **4** (d1,d2) in solution (MeCN/H<sub>2</sub>O=1:9, v/v) under nitrogen and oxygen atmosphere, respectively.



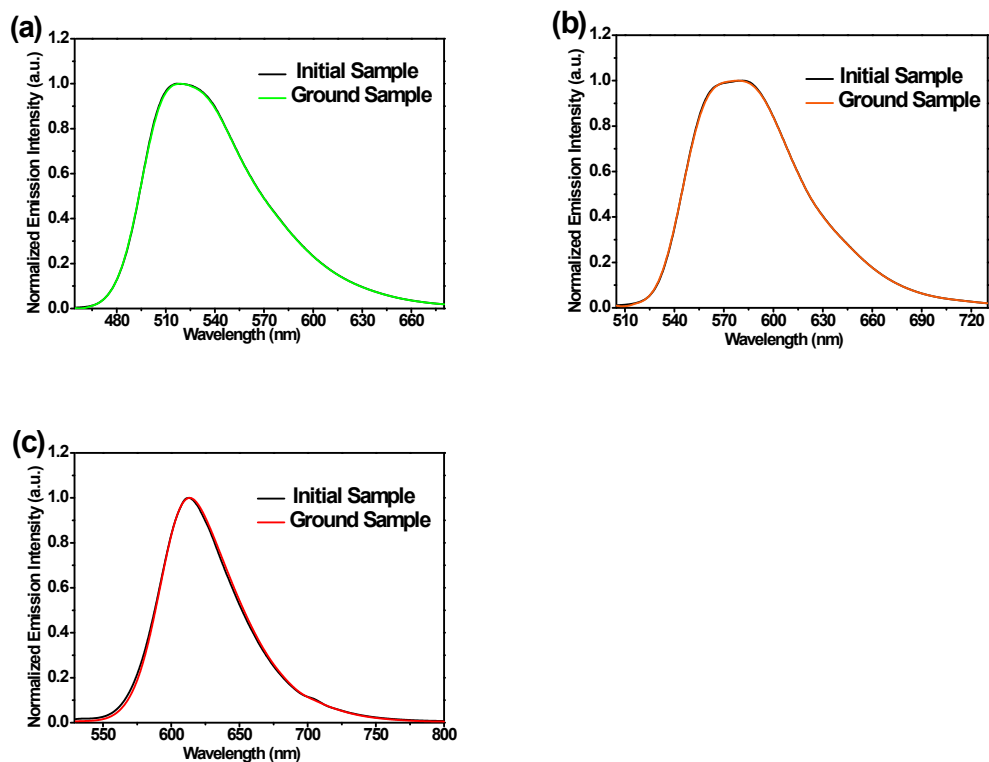
**Fig. S3** Emission spectra of complexes **1**(a), **2** (b), **3**(c) and **4**(d) ( $c = 1.0 \times 10^{-5}$  M) in MeCN/water mixtures with different water fraction (0-90%) ( $\lambda_{exc} = 271$  nm for **1**;  $\lambda_{exc} = 298$  nm for **2**;  $\lambda_{exc} = 298$  nm for **3**;  $\lambda_{exc} = 298$  nm for **4**). The insets and the photographs show the complexes in different water fraction mixtures under 365 nm UV illumination.



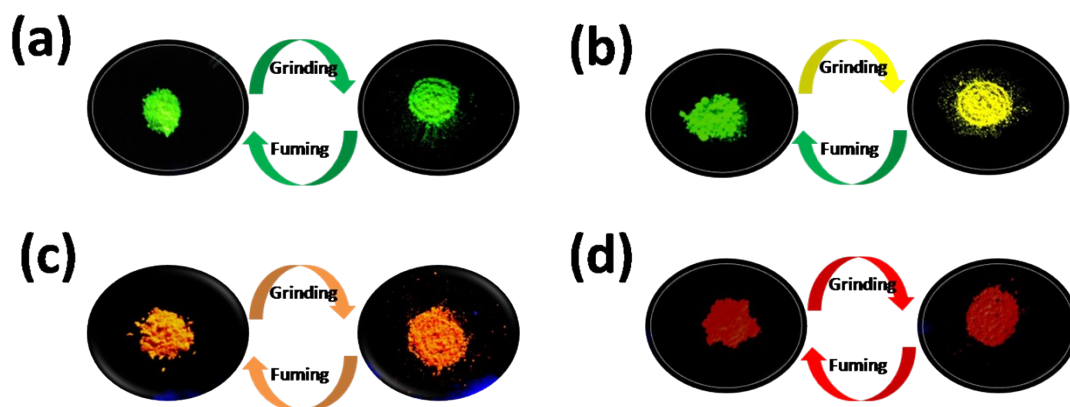
**Fig. S4** Transmission electron microscopy (TEM) images of complexes 1 (a), 2 (b), 3 (c) and 4 (d) in MeCN/water mixture (3: 7, v/v).



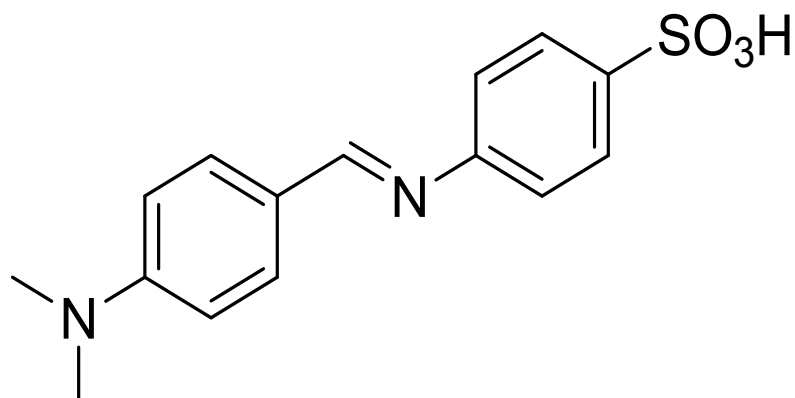
**Fig. S5** Particle size distributions of complexes 1 (a), 2 (b), 3 (c) and 4 (d) in MeCN/water mixture (3: 7, v/v).



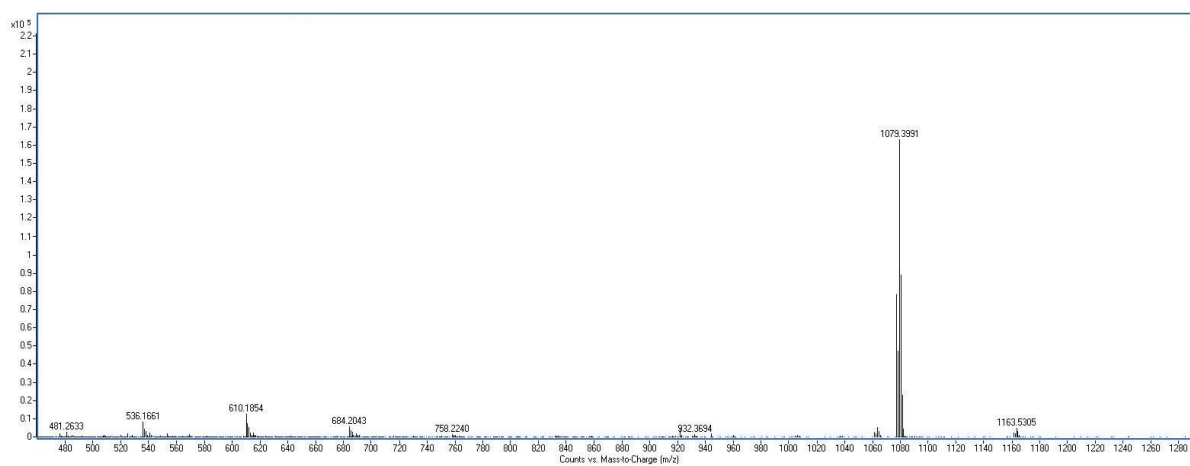
**Fig. S6** Emission spectra of complexes **1**(a), **3**(b) and **4**(c) for initial and grinded samples in solid states ( $\lambda_{\text{exc}} = 396$  nm for **1**;  $\lambda_{\text{exc}} = 429$  nm for **3**;  $\lambda_{\text{exc}} = 360$  nm for **4**).



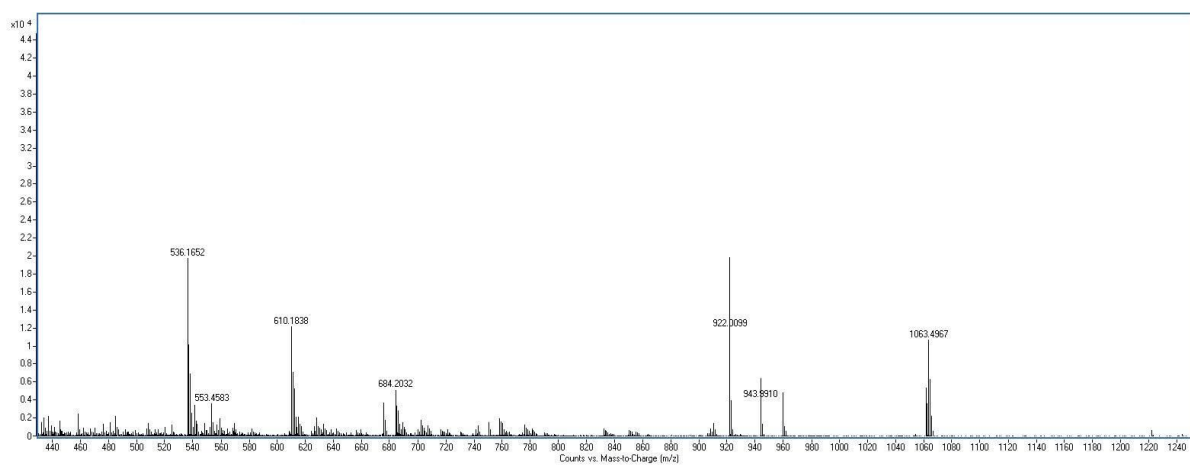
**Fig. S7** Photographs of complexes **1** (a), **2** (b), **3** (c) and **4** (d) by reversible grinding-fuming under 365 nm UV illumination at room temperature.



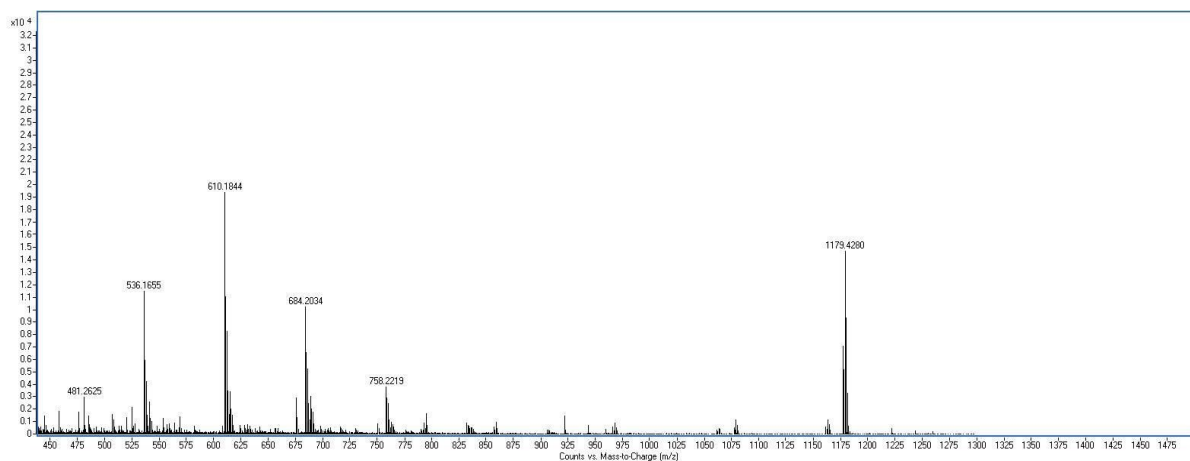
**Fig. S8** Chemical structure of the dye (*E*)-4-sulphonic-4'-dimethylaminoazastilbene (SDMAB) used in this study.



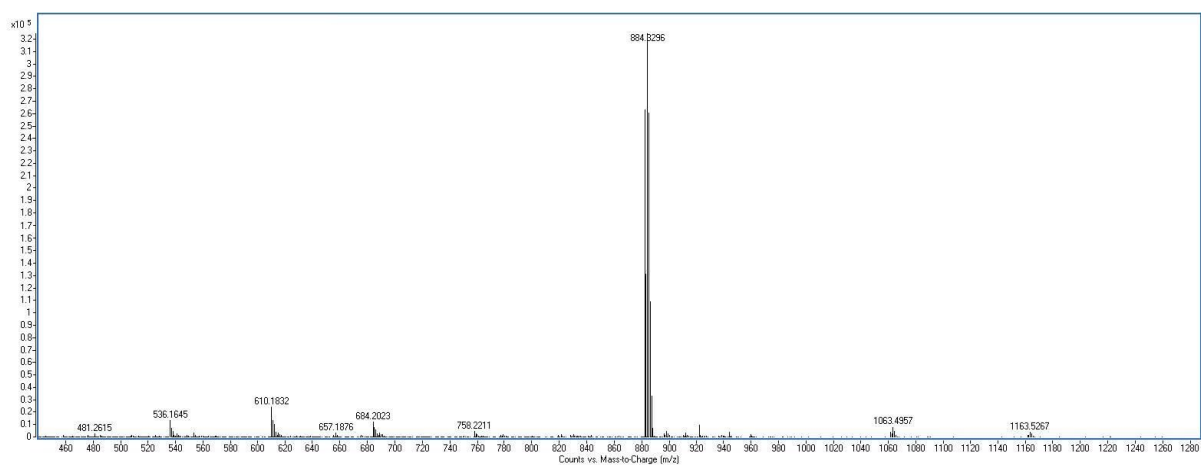
**Fig. S9** HRMS (ESI-TOF) spectrum of complex 1.



**Fig. S10** HRMS (ESI-TOF) spectrum of complex 2.



**Fig. S11** HRMS (ESI-TOF) spectrum of complex 3.



**Fig. S12** HRMS (ESI-TOF) spectrum of complex 4.