

## Electronic Supplementary Information (ESI)

### Acid–base regulated inclusion complexes of $\beta$ -cyclodextrin with 1-[2-(4-fluorophenyl)-2-oxoethyl]-4,4'-bipyridinium dichloride displaying multistimuli-responsive chromic behaviors and photomodulable fluorescence

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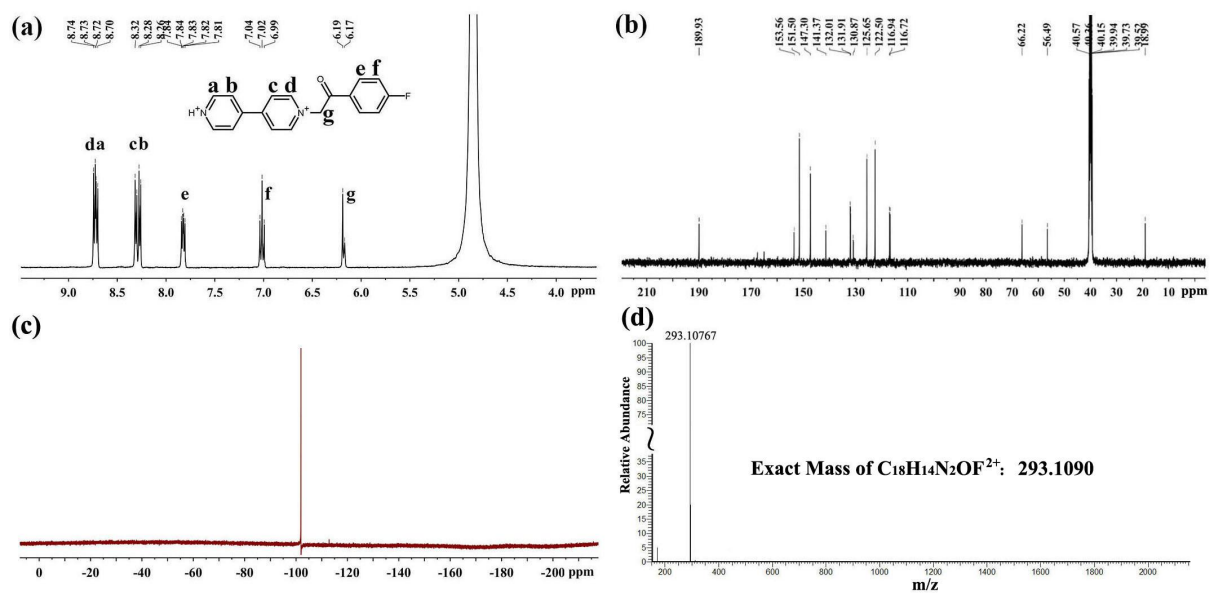


Figure S1. (a)  $^1\text{H}$  NMR (400 MHz,  $\text{D}_2\text{O}$ ), (b)  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-d}_6$ ), (c)  $^{19}\text{F}$  NMR (400 MHz,  $\text{D}_2\text{O}$ ) and (d) HRMS spectra of FOV· $\text{Cl}_2$ .

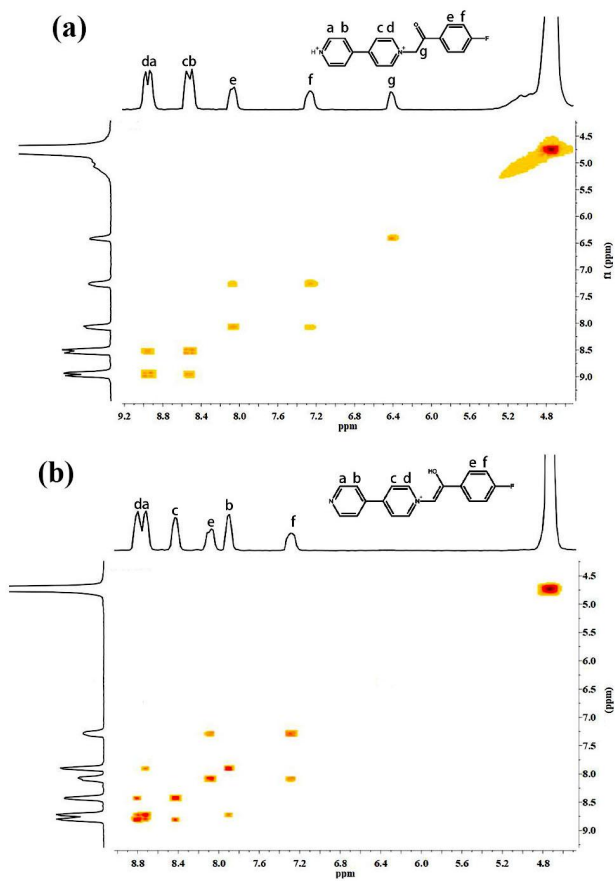


Figure S2. 2D Cosy NMR of FOV·Cl<sub>2</sub> and FHV·Cl.

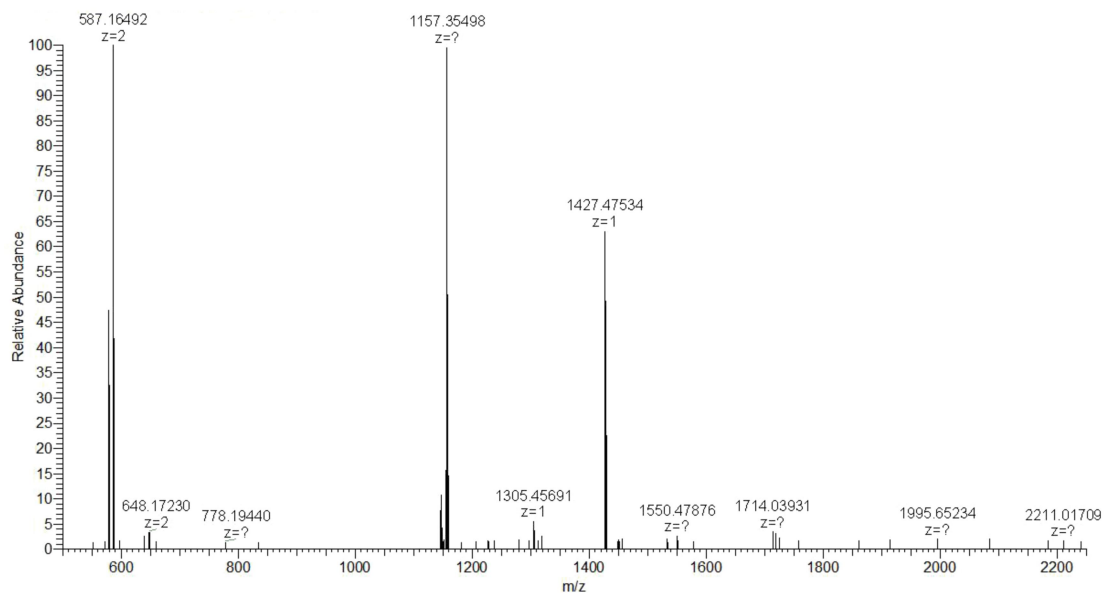


Figure S3. ESI-MS of inclusion complex FOV<sup>2+</sup>@β-CD. The peak found at m/z 1427.47534 corresponds to {FOV·Cl<sub>2</sub>+β-CD-Cl<sub>2</sub>} (calculated for {C<sub>18</sub>H<sub>14</sub>N<sub>2</sub>OF<sup>+</sup> +C<sub>42</sub>H<sub>70</sub>O<sub>35</sub>}, 1427.4788).

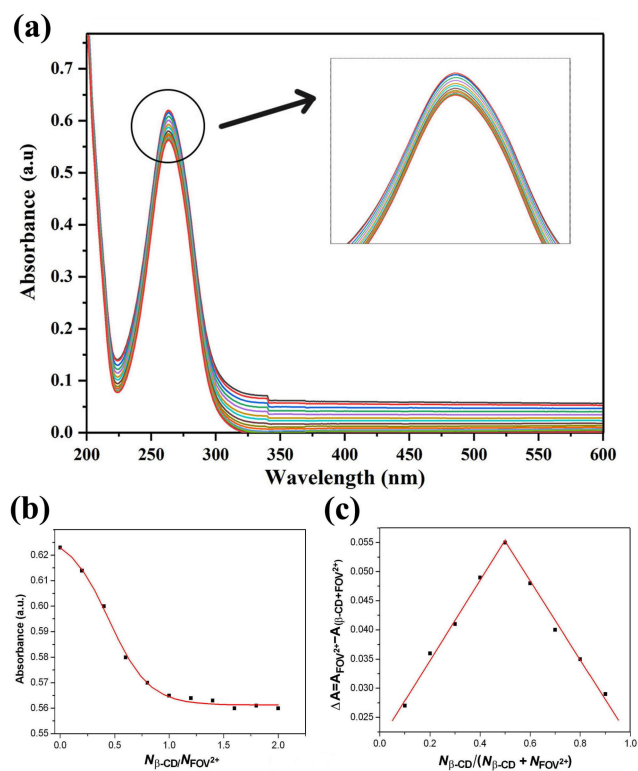


Figure S4. (a) Change in absorption spectra of  $\text{FOV}\cdot\text{Cl}_2$  ( $2.0 \times 10^{-5} \text{ mol}\cdot\text{L}^{-1}$ ) with increasing concentration of  $\beta$ -CD. (b) The curve of absorbance intensity vs.  $N_{\beta\text{-CD}}/N_{\text{FOV}\cdot\text{Cl}_2}$ . (c) Continuous variation Job's plot for the  $\beta$ -CD and  $\text{FOV}\cdot\text{Cl}_2$  on the basis of UV spectra.

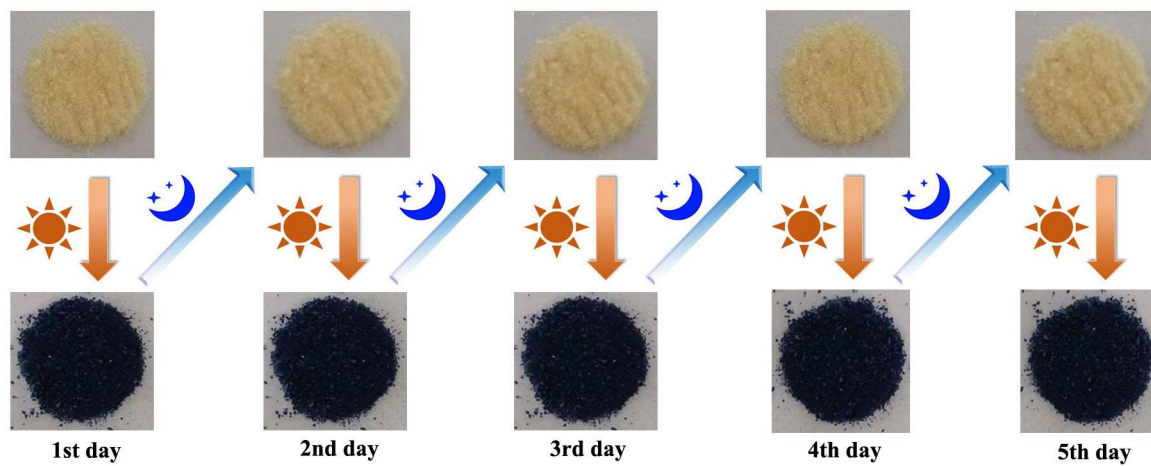


Figure S5. Photographs showing the reversible colour change can occur multiple times.

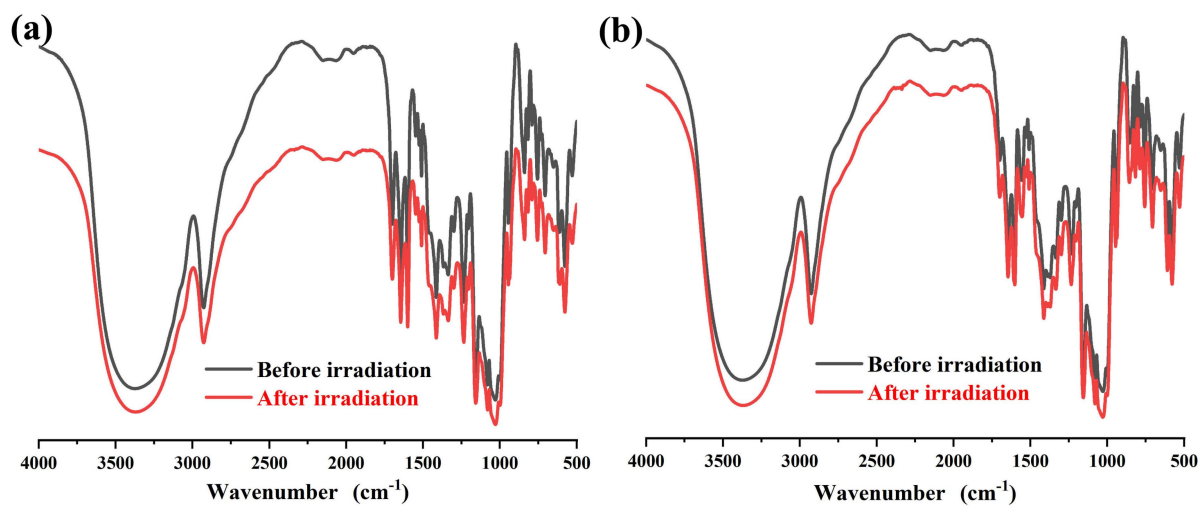


Figure S6. IR spectra of inclusion complexes (a) FOV<sup>2+</sup>@ $\beta$ -CD and (b) FHV<sup>+</sup>@ $\beta$ -CD before and after irradiation.

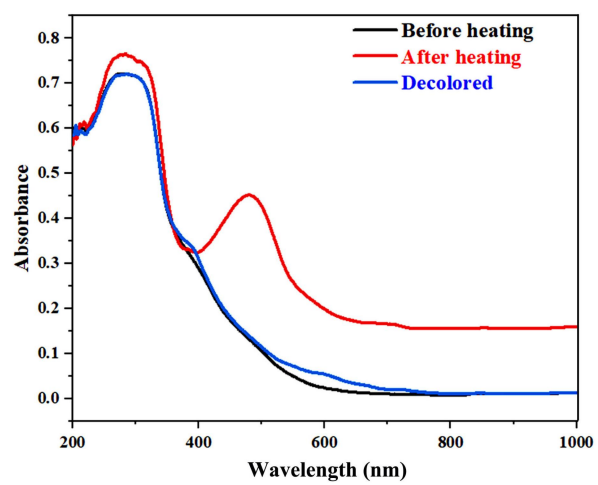


Figure S7. Solid-state UV-vis absorption spectra of FOV<sup>2+</sup>@β-CD before and after heating .



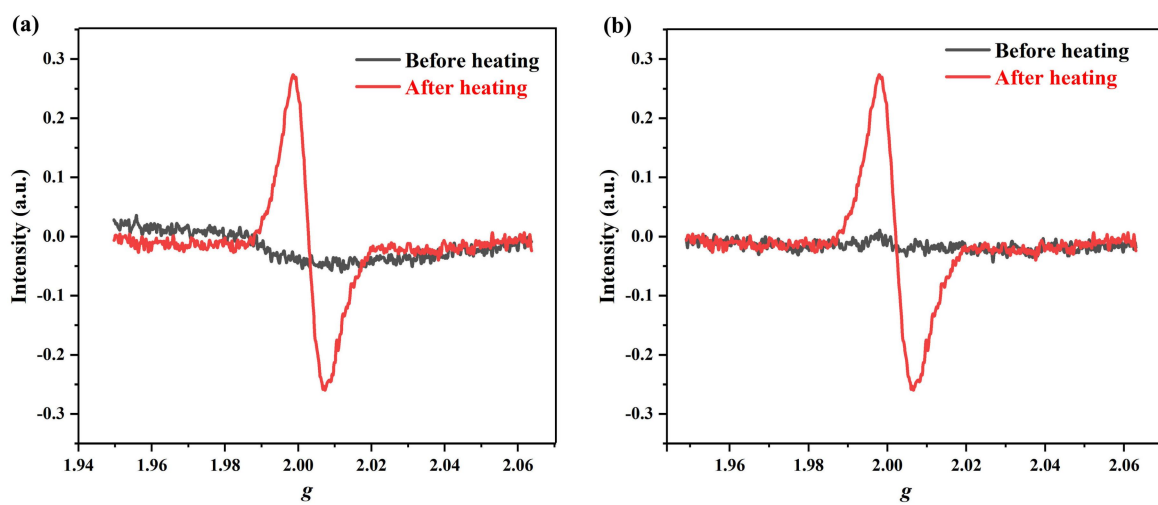


Figure S8. ESR spectra of the  $\text{FOV}^{2+}@ \beta\text{-CD}$  (a) and  $\text{FHV}^{+}@ \beta\text{-CD}$  (b) before and after heating.

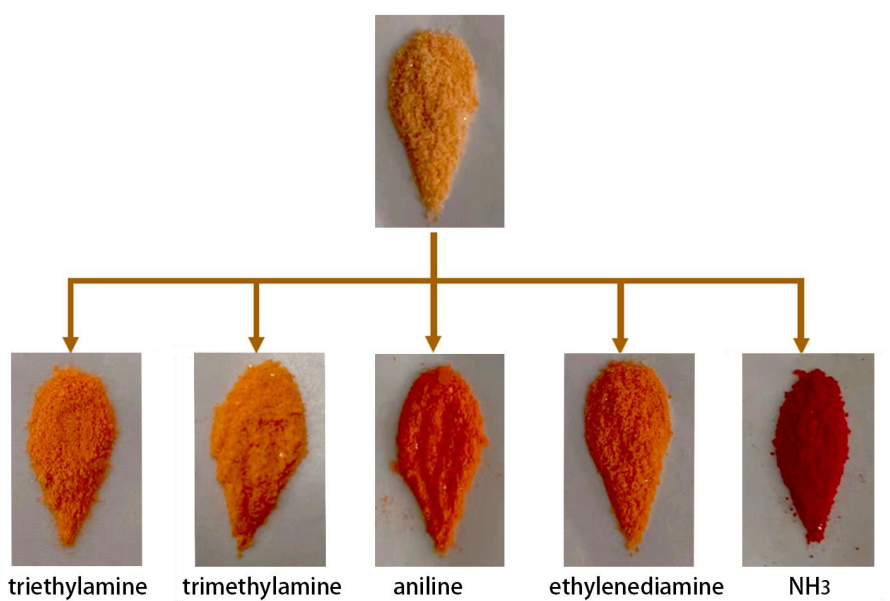


Figure S9. Photographs of the FHV<sup>2+</sup>@β-CD treated with vapors of ammonia and organic amines.

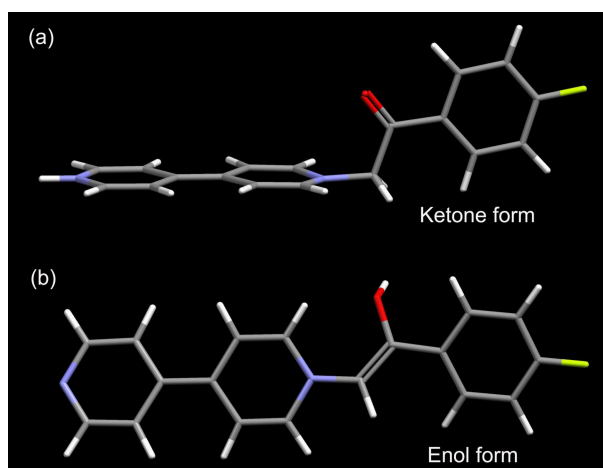


Figure S10. Energy minimized structures of  $\text{FOV}^{2+}$  (a) and  $\text{FHV}^+$  (b) in the gas phase.