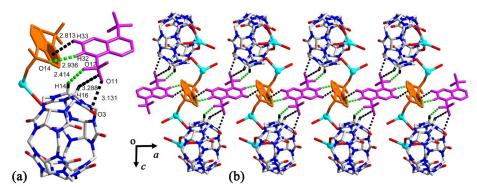
## Sulfonate Ligands-Induced Formation of Alkali Metal - Cucurbit[5]uril-based Assemblies

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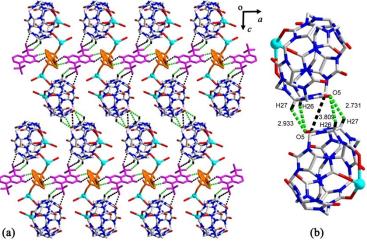
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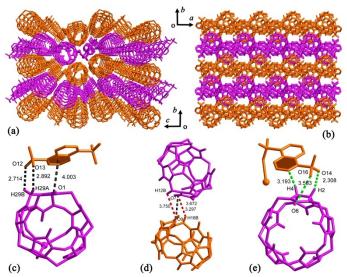
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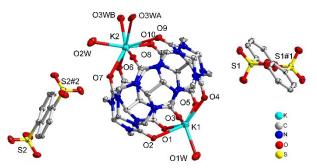
**Fig. S1** (a) The interaction among the sulfonate ligands 1,5-NAS<sup>2-</sup> and the outer surface of Q[5] molecules; (b) The ternary Q[5]-Na<sup>+</sup>-1,5-NAS<sup>2-</sup> supramolecular chain.



**Fig. S2.** (a) The 2D supramolecular layer (a) constructed from the  $Q[5]-Na^+-1,5-NAS^{2-}$  chains through the hydrogen bonding interactions between adjacent Q[5] (b).



**Fig.S3.** The 3D supramolecular structure of assembly **3** along (a) *a*-axis; (b) and *c*-axis; (c) through the noncovalent interactions between Q[5]s (d) and those between Q[5] and  $NDS^{2-}$  (c, e).



**Fig. S4**. The coordination environment of Na<sup>+</sup> in assembly **3** with displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms was omitted for clarity.

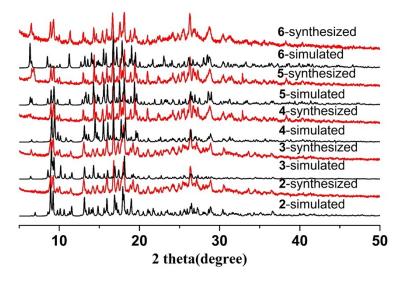


Fig. S5 PXRD patterns of 2-6.

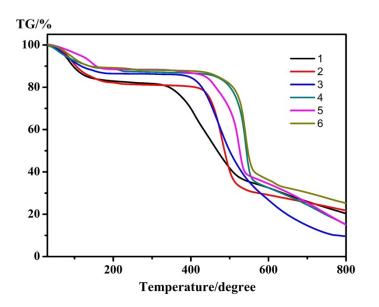


Fig. S6 TG curve of 2-6.

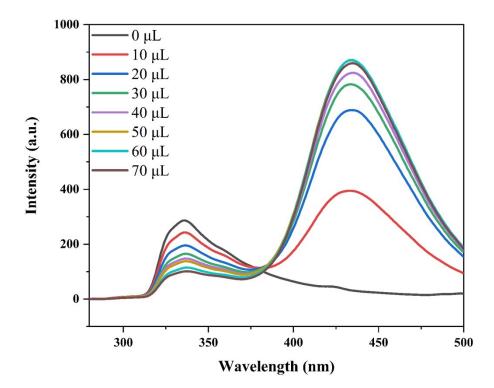
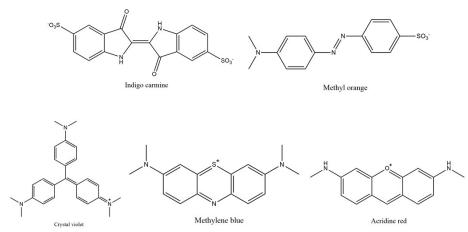


Fig. S7 Change in emission intensities of 2 with the gradual addition of NFX.



**Fig.S8** The structure of the dyes used in this work.

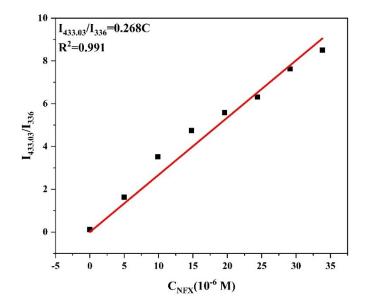
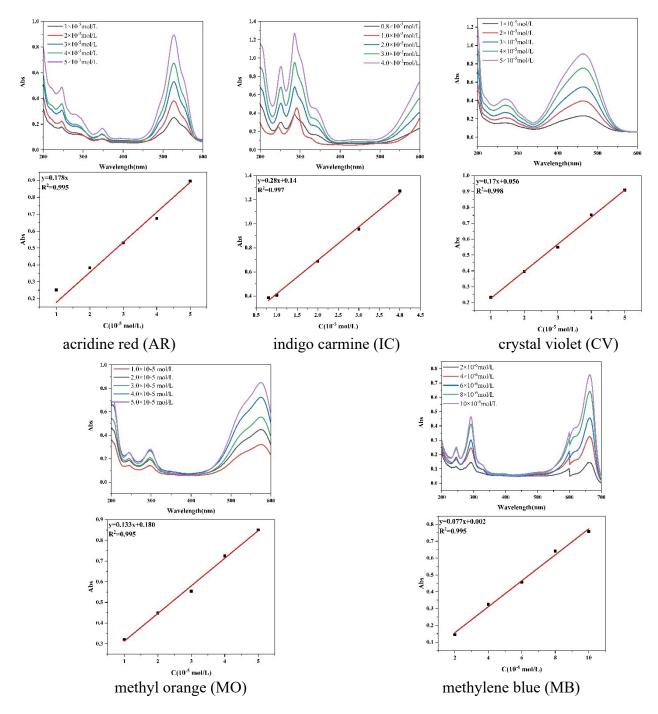


Fig. S9 Linear relationship between different concentrations of NFX and value of  $I_{433}/I_{336}$ ...



**Fig S10**. The standard curve of the five dyes including acridine red (AR), indigo carmine (IC), crystal violet (CV), methyl orange (MO) and methylene blue (MB).

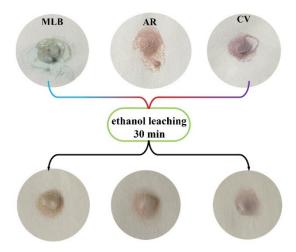


Fig S11. Compound 2 adsorbing cationic dye has been recycled and regenerate through ethanol leaching.