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## **Supporting Information (SI)**

## Host-guest complexation of APP+ with cucurbit[7]uril. Theoretical and experimental studies on the supramolecular inhibition of its cytotoxicity on SERT.

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## Content

**Figure S2(A).** Fluorescence decay of **AAP**<sup>+</sup> (1.6  $\mu$ M) in aqueous solution (blue line). Excitation wavelength at 458 nm and emission wavelength at 512 nm. The instrument response function is also shown in the figure (red line)......2

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**Figure S4.** Fluorescence decay of **AAP**<sup>+</sup> (1.6  $\mu$ M) in dichloromethane. Excitation wavelength at 458 nm and emission wavelength at 512 nm. The instrument response function is also shown in the figure (red line)......4

**Figure S5.** ITC enthalpogram for the binding of **APP**<sup>+</sup> with CB[7] at 25°C in 0.01 M Phosphate-buffered saline (PBS).



**Figure S1.** UV-Vis spectrophotometric host-guest titration of **AAP**<sup>+</sup> (2  $\mu$ M) with CB[7] in aqueous solution.



**Figure S2(A).** Fluorescence decay of **AAP**<sup>+</sup> (1.6  $\mu$ M) in aqueous solution (blue line). Excitation wavelength at 458 nm and emission wavelength at 512 nm. The instrument response function is also shown in the figure (red line).



**Figure S2(B).** Fluorescence decay of **AAP**<sup>+</sup> (1.6  $\mu$ M) in the presence of CB[7] (16.3  $\mu$ M) (blue line). Excitation wavelength at 458 nm and emission wavelength at 512 nm. The instrument response function is also shown in the figure (red line).



**Figure S3.** Fluorescence decay of **AAP**<sup>+</sup> (1.6  $\mu$ M) in acetonitrile. Excitation wavelength at 458 nm and emission wavelength at 512 nm. The instrument response function is also shown in the figure (red line).



**Figure S4.** Fluorescence decay of **AAP**<sup>+</sup> (1.6  $\mu$ M) in dichloromethane. Excitation wavelength at 458 nm and emission wavelength at 512 nm. The instrument response function is also shown in the figure (red line).



**Figure S5.** ITC enthalpogram for the binding of **APP**<sup>+</sup> with CB[7] at 25°C in 0.01 M Phosphate-buffered saline (PBS).