10.1071/CH14495\_AC

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Australian Journal of Chemistry 2015, 68 (6), 946-955

## **Supplementary Material**

## Host–Guest Inclusion System of Scutellarin with Polyamine-β-Cyclodextrin: Preparation, Characterisation, and Anti-Cancer Activity

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Fig.S1. Job plot for the SCU/NH<sub>2</sub>- $\beta$ CD system at  $\lambda$ em: 474nm ([SCU]+[NH<sub>2</sub>- $\beta$ CD]=3.0×10<sup>-5</sup>M) in pH 10.5 buffer.



Fig.S3. Job plot for the SCU/TETA- $\beta$ CD system at  $\lambda$ em: 474nm ([SCU]+[ TETA- $\beta$ CD]=3.0×10<sup>-5</sup>M) in pH 10.5 buffer.



Fig.S4. (A) Fluorescence emission spectra of SCU (3.0×10<sup>-5</sup> mol/L) containing various concentrations of NH<sub>2</sub>-βCD (from a to j: 0.0×10<sup>-3</sup>, 0.5×10<sup>-3</sup>, 1.0×10<sup>-3</sup>, 1.2×10<sup>-3</sup>, 1.4×10<sup>-3</sup>, 1.6×10<sup>-3</sup>, 1.8×10<sup>-3</sup>, 2.0×10<sup>-3</sup>, 2.50×10<sup>-3</sup> and 3.0×10<sup>-3</sup> mol/L of NH<sub>2</sub>-βCD); emission at 474 nm. (B) Nonlinear least-squares curve-fitting analyses for the inclusion complexation.



Fig.S5. (A) Fluorescence emission spectra of SCU  $(3.0 \times 10^{-5} \text{ mol/L})$  containing various concentrations of  $\beta$ CD (from a to i:  $0.0 \times 10^{-4}$ ,  $1.0 \times 10^{-3}$ ,  $1.2 \times 10^{-3}$ ,  $1.4 \times 10^{-3}$ ,  $1.6 \times 10^{-3}$ ,  $1.8 \times 10^{-3}$ ,  $2.0 \times 10^{-3}$ ,  $2.5 \times 10^{-3}$ ,  $3.0 \times 10^{-3}$  mol/L of  $\beta$ CD); emission at 474 nm. (B) Nonlinear least-squares curve-fitting analyses for the inclusion complexation



Fig.S6. (A) Fluorescence emission spectra of SCU  $(3.0 \times 10^{-5} \text{ mol/L})$  containing various concentrations of EN- $\beta$ CD (from a to h:  $0.0 \times 10^{-4}$ ,  $0.25 \times 10^{-3}$ ,  $0.5 \times 10^{-3}$ ,  $0.6 \times 10^{-3}$ ,  $0.8 \times 10^{-3}$ ,  $1.0 \times 10^{-3}$ ,  $2.0 \times 10^{-3}$ ,  $1.25 \times 10^{-3}$ ,  $1.5 \times 10^{-3}$  mol/L of EN- $\beta$ CD); emission at 474 nm. (B) Nonlinear least-squares curve-fitting analyses for the inclusion complexation.



Fig.S7. <sup>1</sup>H NMR spectra of SCU in the absence and presence of NH<sub>2</sub>-βCD and DETA-βCD in D2O at25 °C, respectively. a: NH<sub>2</sub>-βCD, b: SCU/NH<sub>2</sub>-βCD complex, c: DETA-βCD, d: SCU/DETA-βCD complex(it shows the enlarged NMR spectrum from approximately 5.5–8 ppm in the left box.).