Supplementary Material

Host–Guest Inclusion System of Luteolin with Polyamine-β-cyclodextrin: Preparation, Characterisation, Anti-oxidant and Anti-cancer Activity

Manshuo Liu,^A Rongqiang Liao,^A Yulin Zhao,^B and Bo Yang^{A,C}

^AFaculty of Life Science and Technology, Kunming University of Science and Technology, Kunming 650500, China.

^BFaculty of Chemical Engineering, Kunming University of Science and Technology, Kunming 650500, China.

^CCorresponding author. Email: yangb_2015@163.com

Contents

The stoichiometry for the inclusion complex of LU with TETA-βCD (Fig.S1).

The stoichiometry for the inclusion complex of LU with NH_2 - β CD (Fig.S2).

The stoichiometry for the inclusion complex of LU with DETA- β CD (Fig.S3).

The absorption spectral of inclusion complex of LU with NH₂-βCD (Fig.S4).

The absorption spectral of inclusion complex of LU with EN- β CD (Fig.S5).

The absorption spectral of inclusion complex of LU with TETA- β CD (Fig.S6).

The speciation plot for the inclusion complex of LU with NH_2 - βCD (Fig.S7).

The speciation plot for the inclusion complex of LU with EN- β CD (Fig.S8).

The speciation plot for the inclusion complex of LU with TETA-βCD(Fig.S9).

The ¹H NMR spectra of LU in the absence and presence of EN- β CD and TETA- β CD

in D2O at 25 °C, respectively (Fig.S7).

The ROESY spectrum of LU/NH₂ - β CD complex (Fig.S8).

The ROESY spectrum of LU/DETA-βCD complex (Fig.S9).

The ROESY spectrum of LU/TETA-βCD complex (Fig.S10).

The scanning electron microphotographs of inclusion complex of LU with NH₂- β CD, EN- β CD and TETA- β CD, respectively (Fig.S11).



Fig.S1. Job plot for the Lu/TETA - β CD system at λ em: 430 nm ([Lu]+[TETA- β CD]=4.0×10⁻⁵ M) in pH 7.4 buffer.



Fig.S2. Job plot for the Lu/NH₂ - β CD system at λ em: 430 nm ([Lu]+[NH₂- β CD]=4.0×10⁻⁵M) in pH 7.4 buffer.



Fig.S3. Job plot for the Lu/DETA- β CD system at λ em: 430 nm ([Lu]+[DETA- β CD]=4.0×10⁻⁵ M) in pH 7.4 buffer.



Fig.S4. Fluorescence emission spectra of LU (4.0×10^{-5} mol/L) containing various concentrations of NH₂- β CD (from a to g: 0.0×10^{-4} , 0.1×10^{-4} , 0.3×10^{-4} , 0.4×10^{-4} , 0.6×10^{-4} , 0.6×10^{-4} , and 0.8×10^{-4} mol/L of NH₂- β CD); emission at 509 nm. (B) Nonlinear least-squares curve-fitting analyses for the inclusion complexation.



Fig.S5. (A) Fluorescence emission spectra of LU (4.0×10⁻⁵ mol/L) containing various concentrations of EN-βCD (from a to j: 0.0×10⁻⁴, 0.1×10⁻⁴, 0.2×10–4, 0.3×10⁻⁴, 0.4×10⁻⁴, 0.5×10⁻⁴, 0.6×10⁻⁴, 0.7×10⁻⁴, 0.8×10⁻⁴ and 1.0×10⁻⁴ mol/L of EN-βCD); emission at 509 nm. (B) Nonlinear least-squares curve-fitting analyses for the inclusion complexation.



Fig.S6. (A) Fluorescence emission spectra of LU (4.0×10⁻⁵ mol/L) containing various concentrations of TETA-βCD (from a to j: 0.0×10⁻⁴, 0.1×10⁻⁴, 0.2×10–4, 0.3×10⁻⁴, 0.4×10⁻⁴, 0.5×10⁻⁴, 0.6×10⁻⁴ and 0.7×10⁻⁴ mol/L of TETA-βCD); emission at 509 nm.
(B) Nonlinear least-squares curve-fitting analyses for the inclusion complexation.



Fig.S7.Speciation plot for NH₂- β CD (red curve) and LU/DETA- β CD complex (black curve) at λ_{UV} : 353 nm in pH 7.4 buffer.



Fig.S8.Speciation plot for EN- β CD (red curve) and LU/DETA- β CD complex (black curve) at λ_{UV} : 353 nm in pH 7.4 buffer.



Fig.S9. Speciation plot for TETA- β CD (red curve) and LU/DETA- β CD complex (black curve) at λ_{UV} : 353 nm in pH 7.4 buffer.



Fig.S10. ¹H NMR spectra of LU in the absence and presence of EN-βCD and TETA-βCD in D₂O at 25 °C, respectively. a: LU/NH₂-βCD complex, b:EN-βCD, c:
LU/TETA-βCD complex, d: TETA-βCD (it shows the enlarged NMR spectrum from approximately (6.0-7.7 ppm in the left box.).



Fig.S11. ROESY spectrum of LU/NH₂- β CD complex in D₂O.



Fig.S12. ROESY spectrum of LU/DETA- β CD complex in D₂O.



Fig.S13. ROESY spectrum of LU/TETA- β CD complex in D₂O.



(c)



(b)



Fig.S14. Scanning electron microphotographs: (a) LU/NH₂ - β CD inclusion complex; (b) LU/EN - β CD inclusion complex; (c) LU/DETA - β CD inclusion complex;