Supplementary data

1. Method for the calculation of *K*s values

After validating the 1:1 host/guest stoichiometry, the inclusion complexation of the guest cinchona alkaloid (CA) with the host CyDs can be expressed by eqn. (1).

$$\mathrm{CyD} + \mathrm{CA} \underset{}{\overset{K_S}{\rightleftharpoons}} \mathrm{CyD \cdot CA} \qquad (1)$$

The relative fluorescence intensity change of guest cinchona alkaloid (ΔF) upon addition of host CyD, where $\Delta F = F$ (with host CyD) $- F$ (without host CyD), was assumed to be proportional to the concentration of inclusion complex formed by CyD with cinchona alkaloid, *i.e.*, $\Delta F = \alpha[\mathrm{CyD \cdot CA}]$. The proportionality coefficient α was taken as a sensitivity factor for the fluorescence change upon inclusion complexation.

$$K_S = \frac{[\mathrm{CyD \cdot CA}]}{[\mathrm{CyD}][\mathrm{CA}]} = \frac{[\mathrm{CyD \cdot CA}]}{([\mathrm{CyD}]_0 - [\mathrm{CyD \cdot CA}])([\mathrm{CA}]_0 - [\mathrm{CyD \cdot CA}])} = \frac{\Delta F / a}{([\mathrm{CyD}]_0 - \Delta F / a)([\mathrm{CA}]_0 - \Delta F / a)} \qquad (2)$$

Then, the effective stability constant (K_S) can be expressed by eqn. (2):
Where $[\mathrm{CyD}]_0$ and $[\mathrm{CA}]_0$ denoted the initial concentrations of host CyD and guest cinchona alkaloid, respectively. Subsequently, eqn. (2) can be solved for ΔF to give

$$\Delta F = \{\alpha([\mathrm{CyD}]_0 + [\mathrm{CA}]_0 + 1/K_S) - \sqrt{\alpha^2([\mathrm{CyD}]_0 + [\mathrm{CA}]_0 + 1/K_S)^2 - 4\alpha^2[\mathrm{CA}]_0[\mathrm{CyD}]_0}\}/2 \qquad (3)$$

eqn. (3). Using a nonlinear least squares curve-fitting method, we can obtain the complex stability constant (*K*s) for each host-guest combination from the analysis of the sequential changes of fluorescence intensity (ΔF) at various CyD concentrations.

2. Method for the inclusion complexation stoichiometry

The inclusion complexation stoichiometry was determined as follows: To examine the inclusion complexation stoichiometry between cyclodetxrin and alkaloid, a continuous variation experiment (Job's experiment) was performed (cyclodextrin/QUN as an example). For each experiment, solutions containing cyclodextrin and QUN at the

following 13 molar ratios (0:10, 1:9, 2:8, 3:7, 4:6, 4.5:5.5, 5:5, 5.5:4.5, 6:4, 7:3, 8:2, 9:1, 10:0) were prepared. The final combined concentration ([cyclodextrin + QUN]) of the solution was kept 5 μM, and the fluorescence intensity at 380 nm (the emission maximum of QUN) of the solution was measured to be $F_{(CyD+QUN)}$. In the control experiments, the fluorescence intensity of QUN with the same concentration as that in the cyclodextrin/QUN solution was also measured to be F_{QUN}. Then, the Job's plot was drawn as a function of $\Delta F = F_{(CyD+QUN)}-F_{QUN}$ against the molecular fraction of cyclodextrin in the cyclodextrin/QUN solution.