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Electronic Supplementary Information for

Selective Binding and Highly Sensitive Fluorescent Sensor of Palmatine and Dehydrocorydaline Alkaloids by Cucurbit[7]uril

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Fig. S1 Fluorescence spectra of P in the presence and absence of CB7 or β -CD host in aqueous phosphate buffer solution (pH 7.2) at 298.15 K. The concentration of P is $1.25 \times 10^{-5} \text{ mol dm}^{-3}$.



Fig. S2 Fluorescence spectra of DHC in the presence and absence of CB7 or β -CD host in aqueous phosphate buffer solution (pH 7.2) at 298.15 K. The concentration of DHC is 1.42×10^{-5} mol dm⁻³.



Fig. S3 Visible emission observed from samples of P and CB7, β -CD and glycoluril. Left to right: P, P + CB7, P + β -CD and P + glycoluril.



Fig. S4 Visible emission observed from samples of DHC and CB7, β -CD and glycoluril. Left to right: DHC, DHC + CB7, DHC + β -CD and P + glycoluril.



Fig. S5 Fluorescence spectra of P($1.86 \times 10^{-5} \text{ mol dm}^{-3}$), DHC(1.81 mol dm^{-3}) and the mixture of P and DHC($1.90 \times 10^{-5} \text{ mol dm}^{-3}$ for P and $1.85 \times 10^{-5} \text{ mol dm}^{-3}$ for DHC) in the absence and presence of about 1 mol equivalent of CB7 in aqueous phosphate buffer solution (pH 7.2) at 298.15 K($\lambda_{ex} = 348 \text{ nm}$).



Fig. S6 Fluorescence spectral changes of the mixture of P and DHC $(1.90 \times 10^{-5} \text{ mol} \text{ dm}^{-3} \text{ for P and } 1.85 \times 10^{-5} \text{ mol dm}^{-3} \text{ for DHC})$ with the addition of CB7 (0, 1eq, 2eq, 3eq, 4eq, 5eq, 6eq, 8eq, 11eq and 17eq) in aqueous phosphate buffer solution (pH 7.2) at 298.15 K($\lambda_{ex} = 348 \text{ nm}$).



Fig. S7 Job's plot for inclusion complexation of P with CB7 ([P]+[CB7]= 2.65×10^{-5} mol dm⁻³) in phosphate buffer solution (pH 7.2)



Fig. S8 Job's plot for inclusion complexation of DHC with CB7 ([DHC]+[CB7]= 2.92×10^{-5} mol dm⁻³) in phosphate buffer solution (pH 7.2)

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Fig. S9 ¹H NMR spectra (300 MHz, 0.2 M NaCl-D₂O, 298 K) of P + 1.1 equiv of CB7, P, DHC + 1.1 equiv of CB7 and DHC. The concentrations of P and DHC are 1.2 and 1.1×10^{-3} mol dm⁻³, respectively.

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Fig. S10 Possible structures of P-CB7 and DHC-CB7 constructed according to MD simulation.