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环糊精对阿斯巴甜的甜感增强作用及二者相互作用热力学

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Sweetness Enhancement of Aspartame in the Presence of Cyclodextrins and the Thermodynamics in Binding

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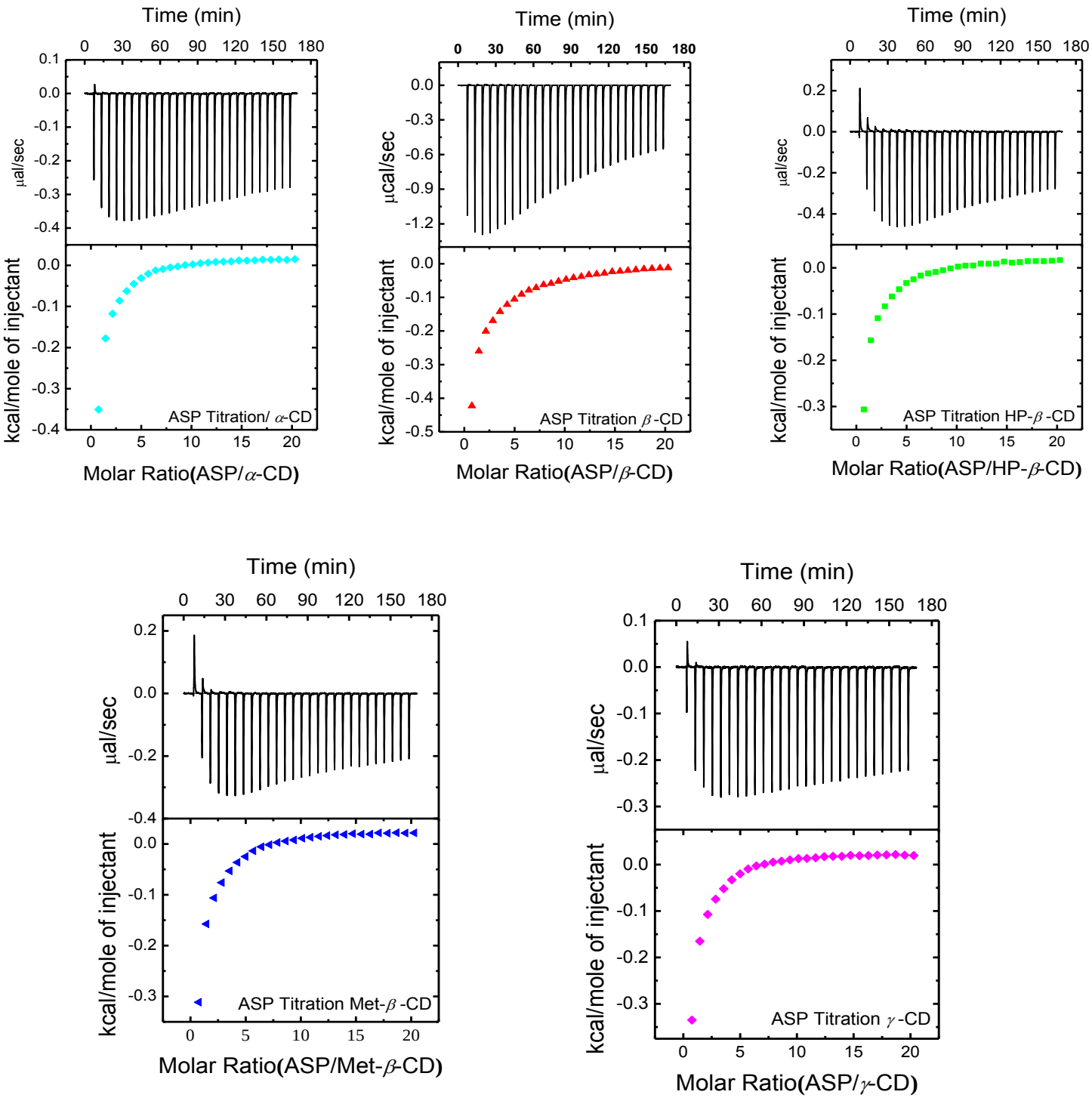

Fig.S1 Isothermal Titration Calorimetry for the interaction of 30 mmol Ł$^{-1}$ aspartame with 0.1 mmol Ł$^{-1}$ different CDs

Raw data were obtained as a plot of heating rate (μcal·s^{-1}) against time (min) (upper panel). Each peak area representing the amount of heat enthalpy change per mole of injected CDs (ΔH, kcal mol^{-1}, 1 kcal mol^{-1} = 4.187 kJ mol^{-1}) against molar ratio (aspartame/CDs) (lower panel).

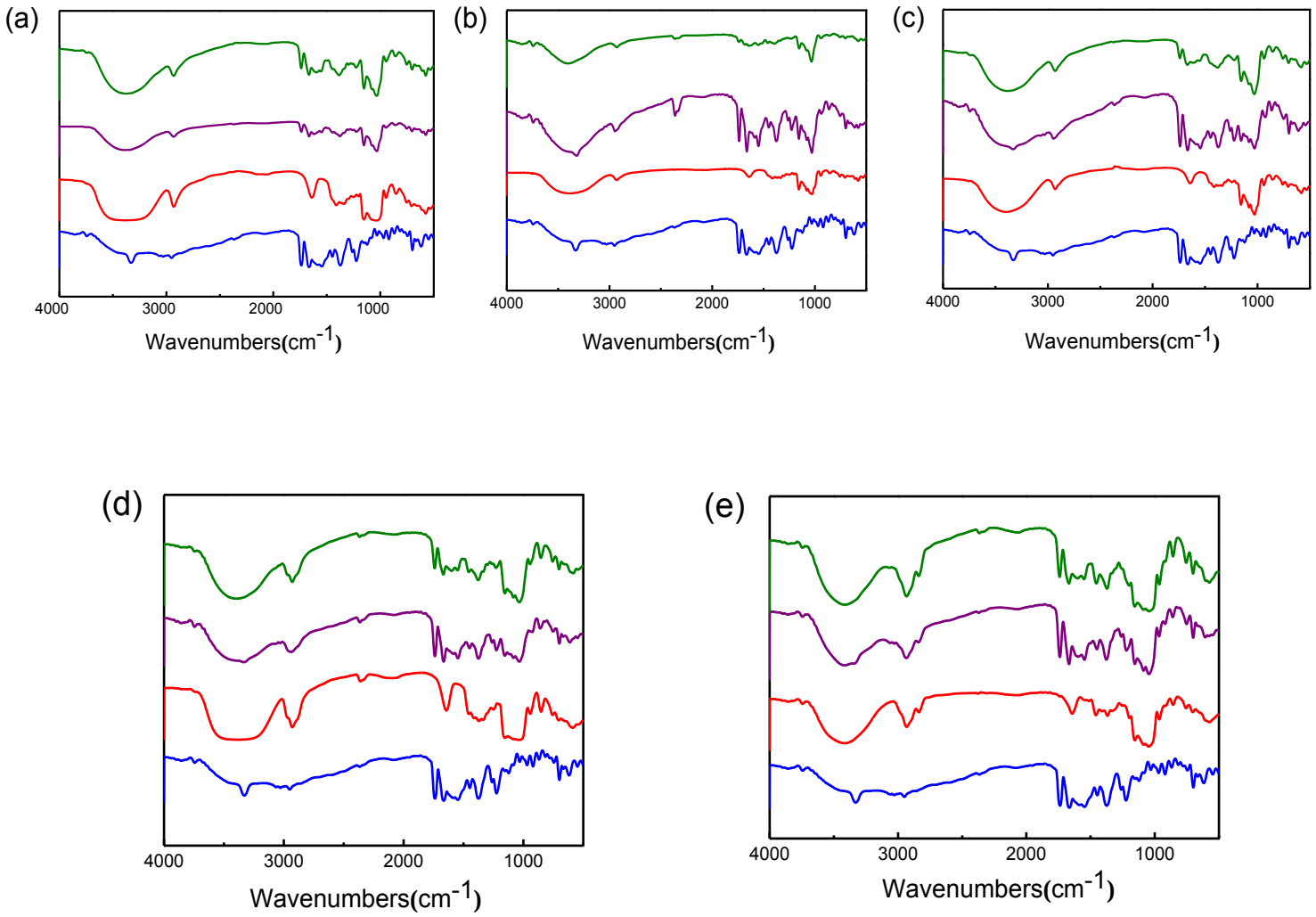

Fig.S2 FT-IR spectra of aspartame (blue), different kinds of CD (red), physical mixture (purple) and inclusion complex (olive)

(a) *α*-CD; (b) *β*-CD; (c) *γ*-CD; (d) HP-*β*-CD; (e) Met-*β*-CD

The FT-IR spectrum of the physical mixture did not differ significantly from those of the single components. However, there are changes in the frequencies of the complex when compared with those of the pure substrate. The bands located at 1375.76–1228.91 cm^{-1} shifted and diminished. The broad peak in the spectrum of aspartame/*β*-CD complex was increased in intensity owing to the increase in the number of hydroxyl groups. These results suggested a partial or complete shielding of

chromophores in the CD cavity and are therefore rationalized as being indicative of complex formation.

Table S1 Chemical shift (δ) values of the protons of aspartame and β-CD in D_2O

Proton	Free	Complexed	$\Delta\delta$
		β-CD	
H1	4.989	4.963	0.026
H2	3.578	3.561	0.017
H3	3.883	3.806	0.077
H4	3.502	3.479	0.023
H5	3.773	3.640	0.133
H6	3.794	3.754	0.040
		Aspartame	
Ha	7.248	7.234	0.014
Hb	7.307	7.282	0.025
Hb’	7.274	7.253	0.021
Hc	7.187	7.179	0.008
Hc’	7.173	7.165	0.008
Hd	3.143	3.141	0.002
He	4.626	4.625	0.001
Hf	3.637	3.825	0.188
Hj	2.684	2.689	0.005
Hh	4.067	4.069	0.003

From Table S1, we can see that the complexation-induced chemical shift of H3, H5 protons ($\Delta\delta$ = 0.077, 0.133) of β-CD are those expected as a result of interaction with those protons of the aspartame Ha, Hb, Hb′, Hc, Hc′, Hf ($\Delta\delta$ = 0.014, 0.025, 0.021, 0.008, 0.008, 0.188) which are oriented towards the β-CD cavity, confirming the interaction of aspartame and β-CD.