Supplementary Data

Remote loading of Curcumin-in-modified β-cyclodextrins into liposomes through transmembrane pH gradient

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Legends for Supplementary Fig.s

Fig. S1 The molecular structure of Curcumin.
Fig. S2 Conformation structure of β-cyclodextrin.
Fig. S3 Conformation structure of 6-OTs-βCD.
Fig. S4 Mass spectrum of 6-O-Monotosyl-6-deoxy-β-cyclodextrin (**6-**βCD OTs) on the negative mode.
Fig. S**5** ^{1}H-NMR spectrum of βCD in the d_6-DMSO solvent.
Fig. S**6** ^{1}H-NMR spectrum of 6-OTs-βCD in the d_6-DMSO solvent.
Fig. S7 The absorption spectra of CRM (0.18 mM), βCD (0.22 mM) and CRM: βCD complex at pH 7 .
Fig. S**8** Absorption spectra of [CRM] = 0.18 mM with increasing concentrations of a) βCD , b) E-βCD and c) D-βCD from 0.00-0.54 mM.
Fig. S9 TGA thermograms for a) CRM-βCD, b) CRM-E-βCD and c) CRM-D-βCD.
Fig. S10 ^{1}H-NMR specrums for βCD , CRM and CRM-βCD complex in d_6-DMSO.
Fig. S11 ^{1}H-NMR spectrum for E-βCD, CRM and CRM-EβCD complex in d_6-DMSO.
Fig. S12 ^{1}H-NMR spectrum for D-βCD, CRM and CRM-DβCD complex in d_6-DMSO.

Legends for Supplementary Tables

Table S1 A summary table for DSC exothermic peaks of CRM with different βCD complexes
Table S2 Chemical shifts (δ) of CRM-βCD complexe and their corresponding precursors. where δo, δc and Δδo represent the chemical shifts for free compound, the complex and the chemical shift difference, respectively.
Table S3 Chemical shifts (δ) of CRM-E-βCD complex and their corresponding precursors.
Table S4 Chemical shifts (δ) of CRM-D-βCD complexe and their corresponding precursors.

Fig. S1

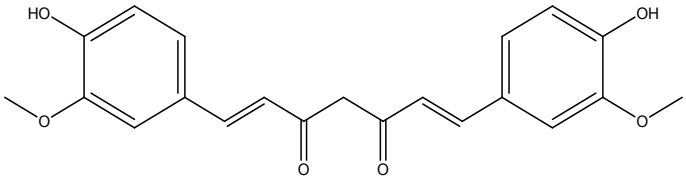


Fig. S2

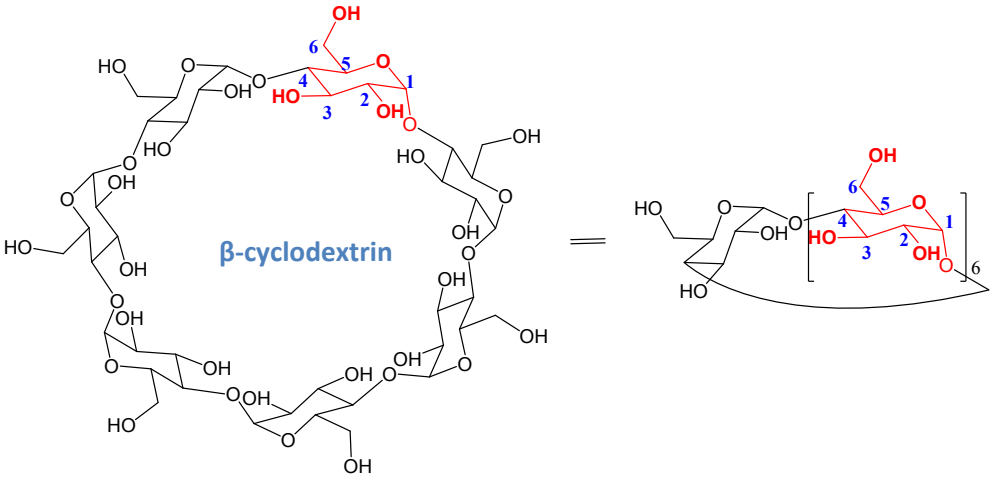
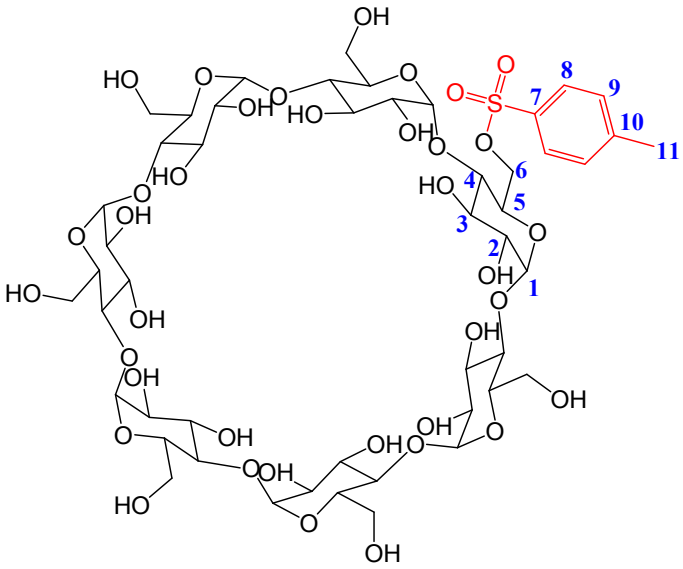


Fig. S3



$C_{49}H_{76}O_{37}S$
Exact Mass: 1288.3786

Fig. S4

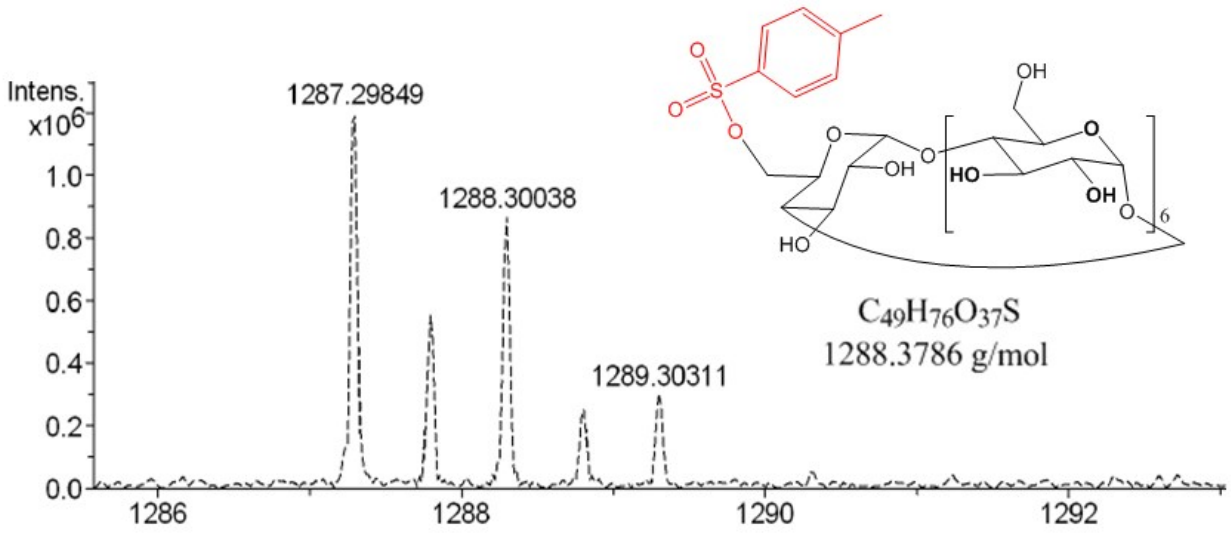

Intens.
x10^6
1.0
0.8
0.6
0.4
0.2
0.0
1287.29849
1288.30038
1289.30311
1286
1288
1290
1292
OH
HO
OH
HO
OH
O
6
C49H76O37S
1288.3786 g/mol

Fig. S5

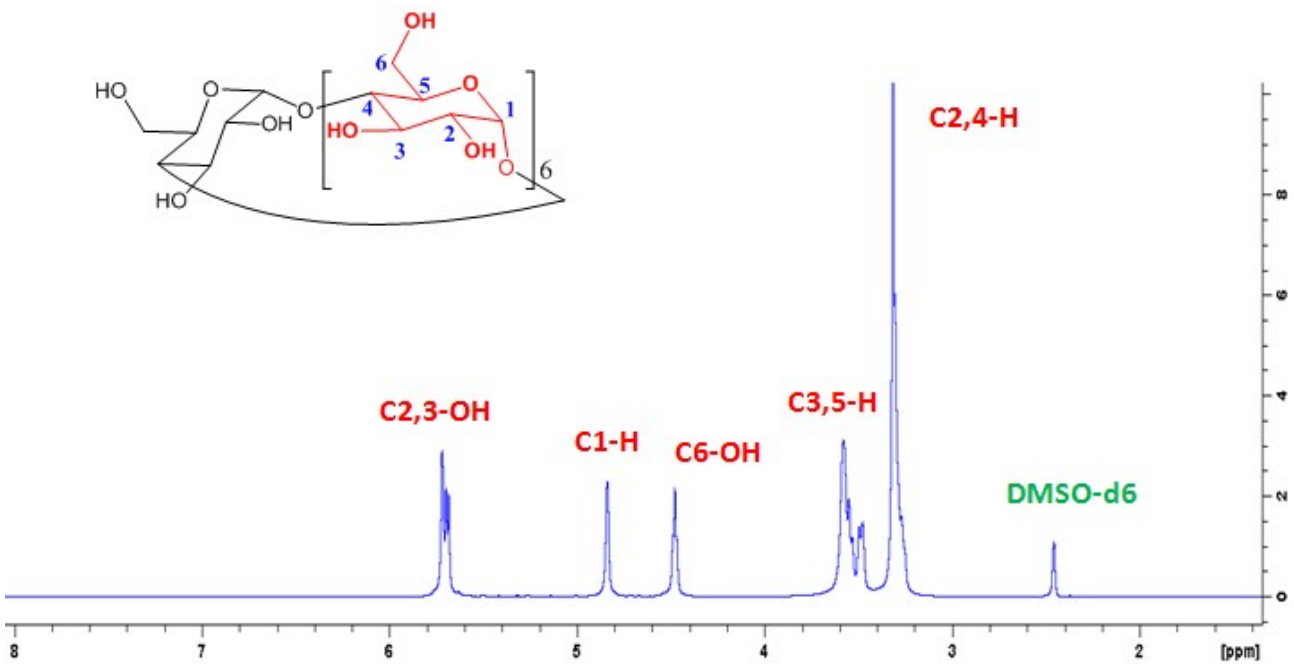


Fig. S6

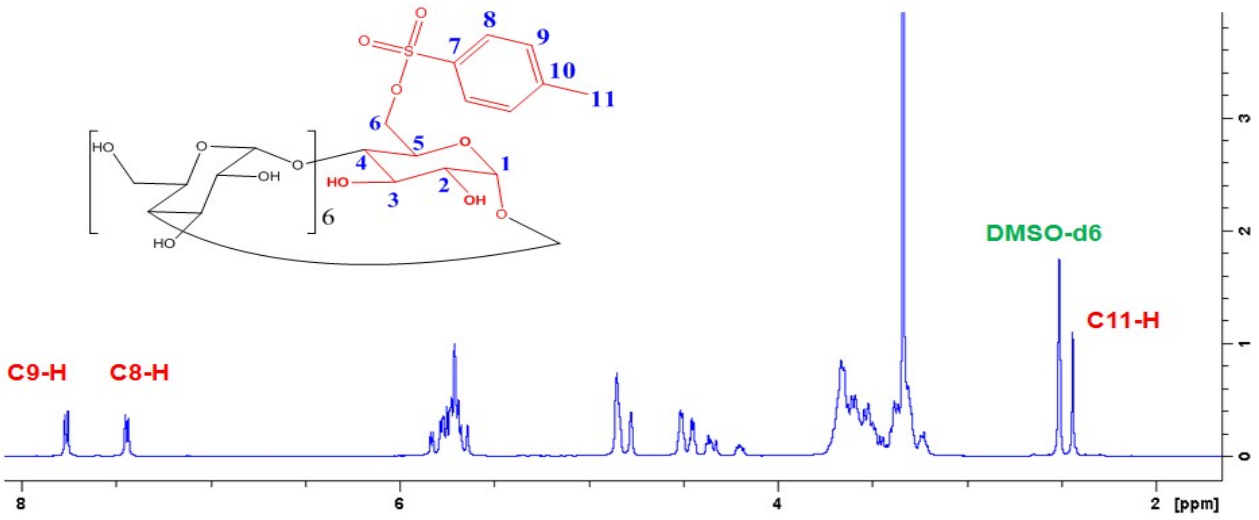


Fig. S7

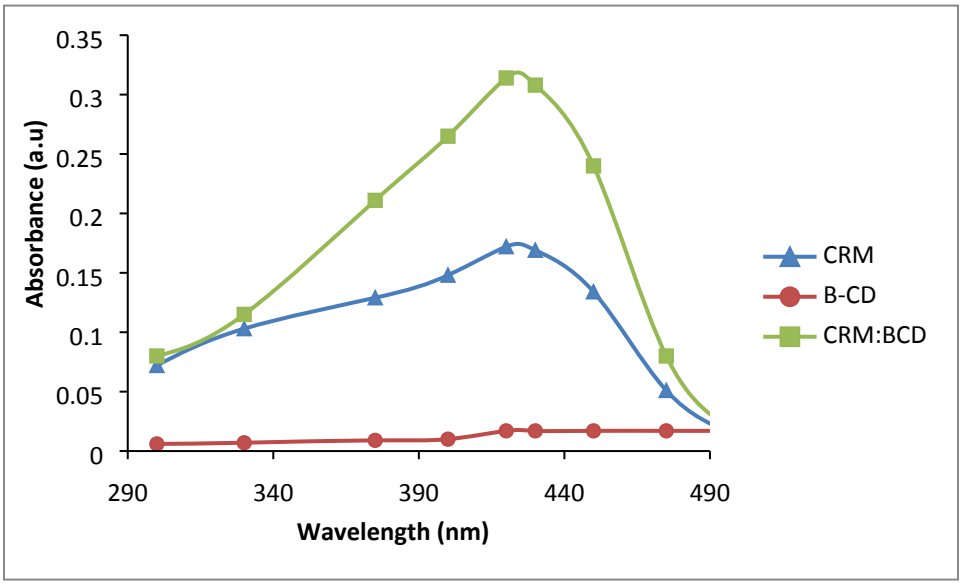

0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
Absorbance (a.u)
290
340
390
440
490
Wavelength (nm)
CRM
B-CD
CRM:BCD

Fig. S8

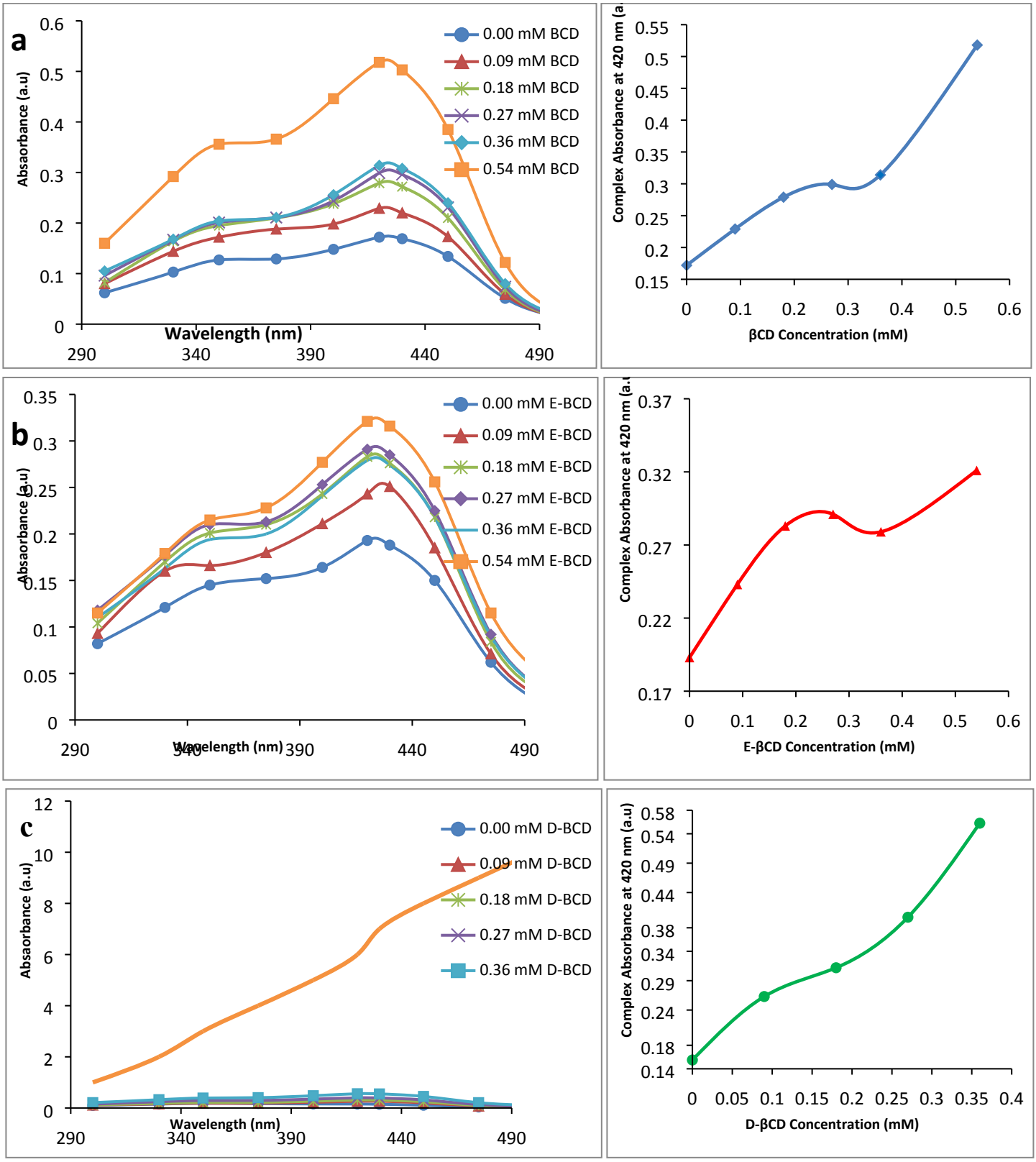
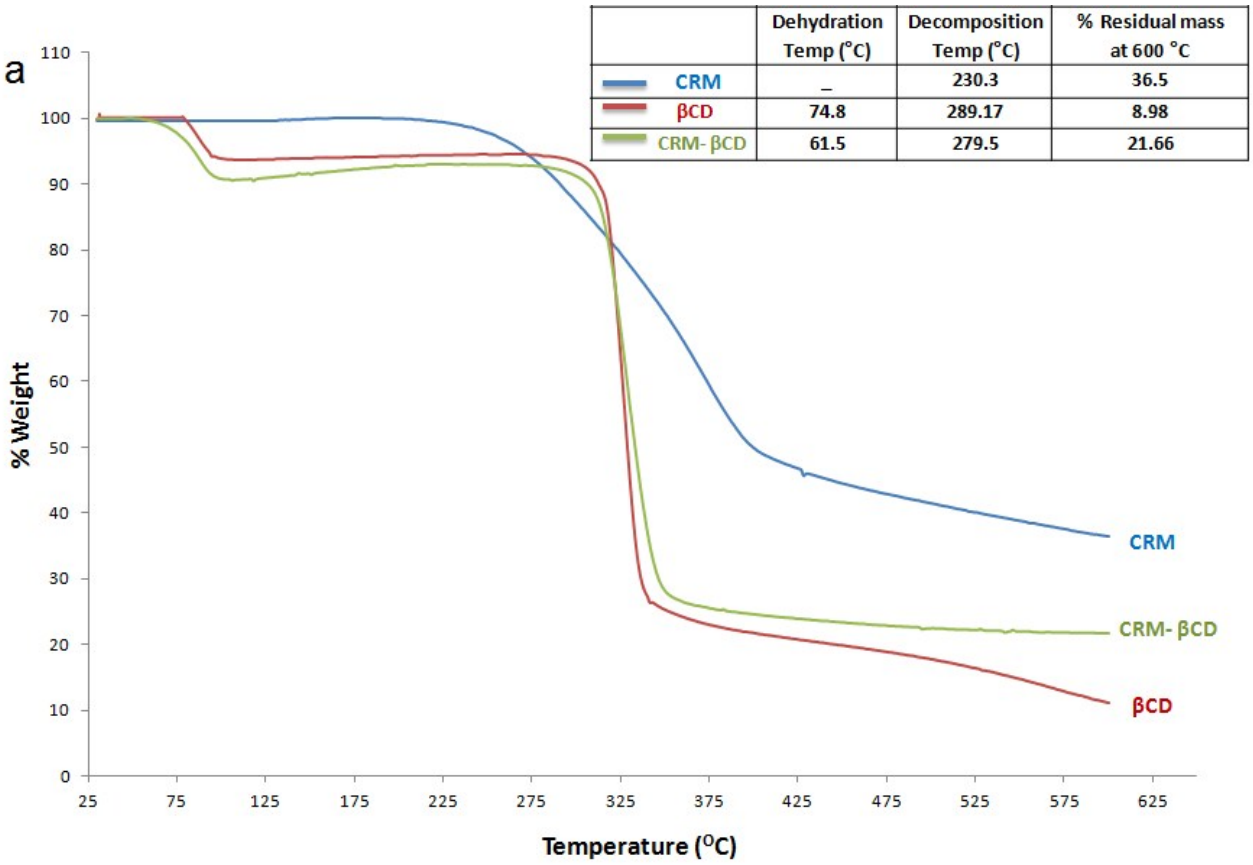

a
Absaorbance (a.u)
Wavelength (nm)
0.00 mM BCD
0.09 mM BCD
0.18 mM BCD
0.27 mM BCD
0.36 mM BCD
0.54 mM BCD
Complex Absorbance at 420 nm (a.
βCD Concentration (mM)
b
Absaorbance (a.u)
Wavelength (nm)
0.00 mM E-BCD
0.09 mM E-BCD
0.18 mM E-BCD
0.27 mM E-BCD
0.36 mM E-BCD
0.54 mM E-BCD
Complex Absorbance at 420 nm (a.
E-βCD Concentration (mM)
c
Absaorbance (a.u)
Wavelength (nm)
0.00 mM D-BCD
0.09 mM D-BCD
0.18 mM D-BCD
0.27 mM D-BCD
0.36 mM D-BCD
Complex Absorbance at 420 nm (a.u)
D-βCD Concentration (mM)

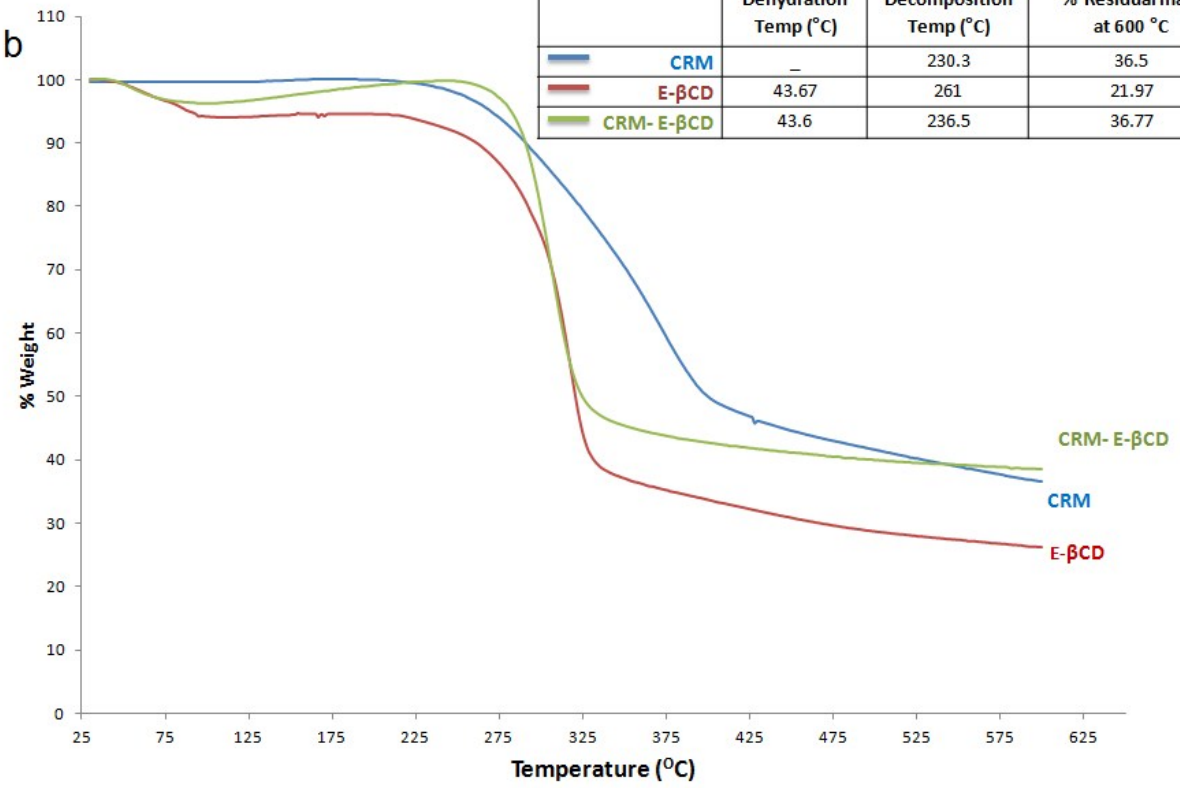
Fig. S9



	Dehydration Temp (°C)	Decomposition Temp (°C)	% Residual mass at 600 °C
CRM	_	230.3	36.5
βCD	74.8	289.17	8.98
CRM- βCD	61.5	279.5	21.66

b

	Dehydration Temp (°C)	Decomposition Temp (°C)	% Residual mass at 600 °C
CRM	_	230.3	36.5
E-βCD	43.67	261	21.97
CRM- E-βCD	43.6	236.5	36.77



c

	Dehydration Temp (°C)	Decomposition Temp (°C)	% Residual mass at 600 °C
CRM	_	230.3	36.5
D-βCD	47.3	224	26.19
CRM-D-βCD	42.3	252.83	38.59

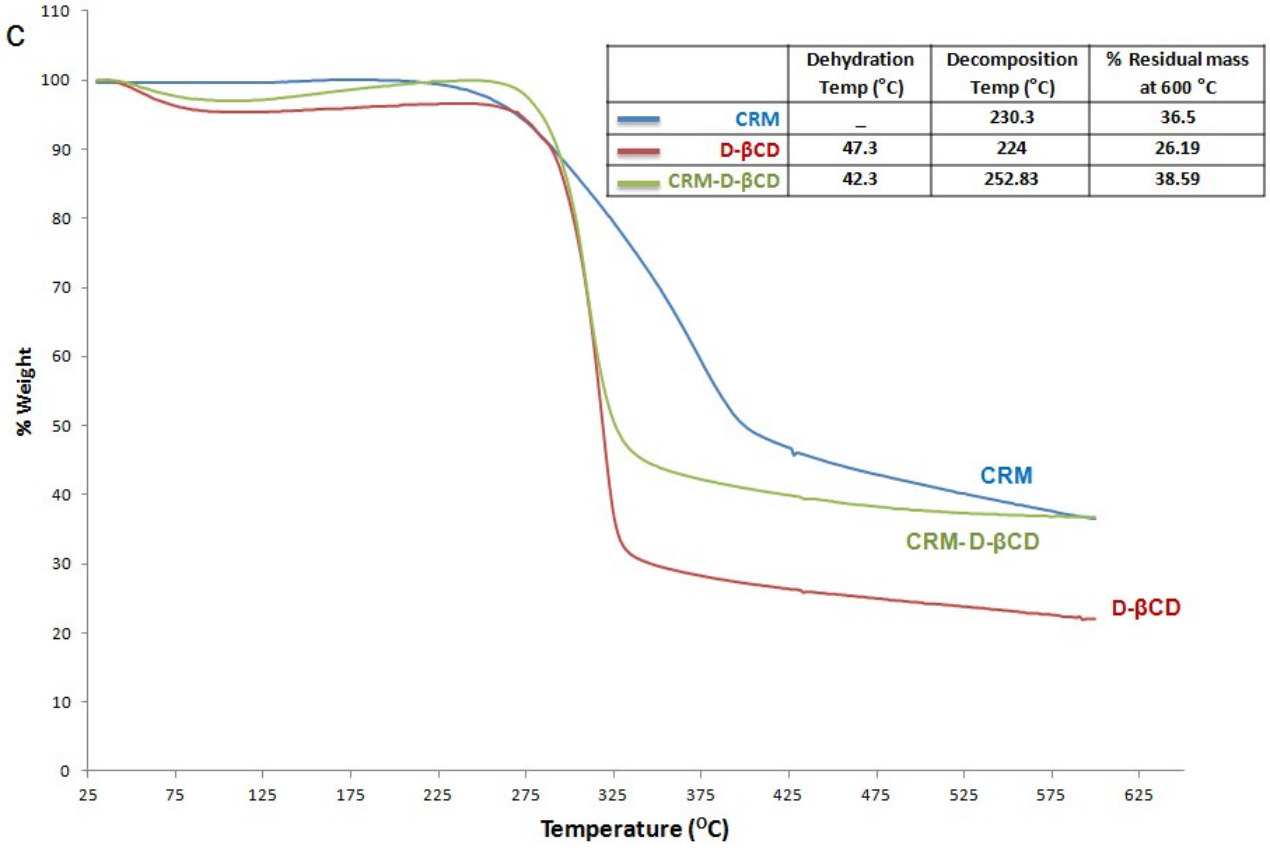


Fig. S10

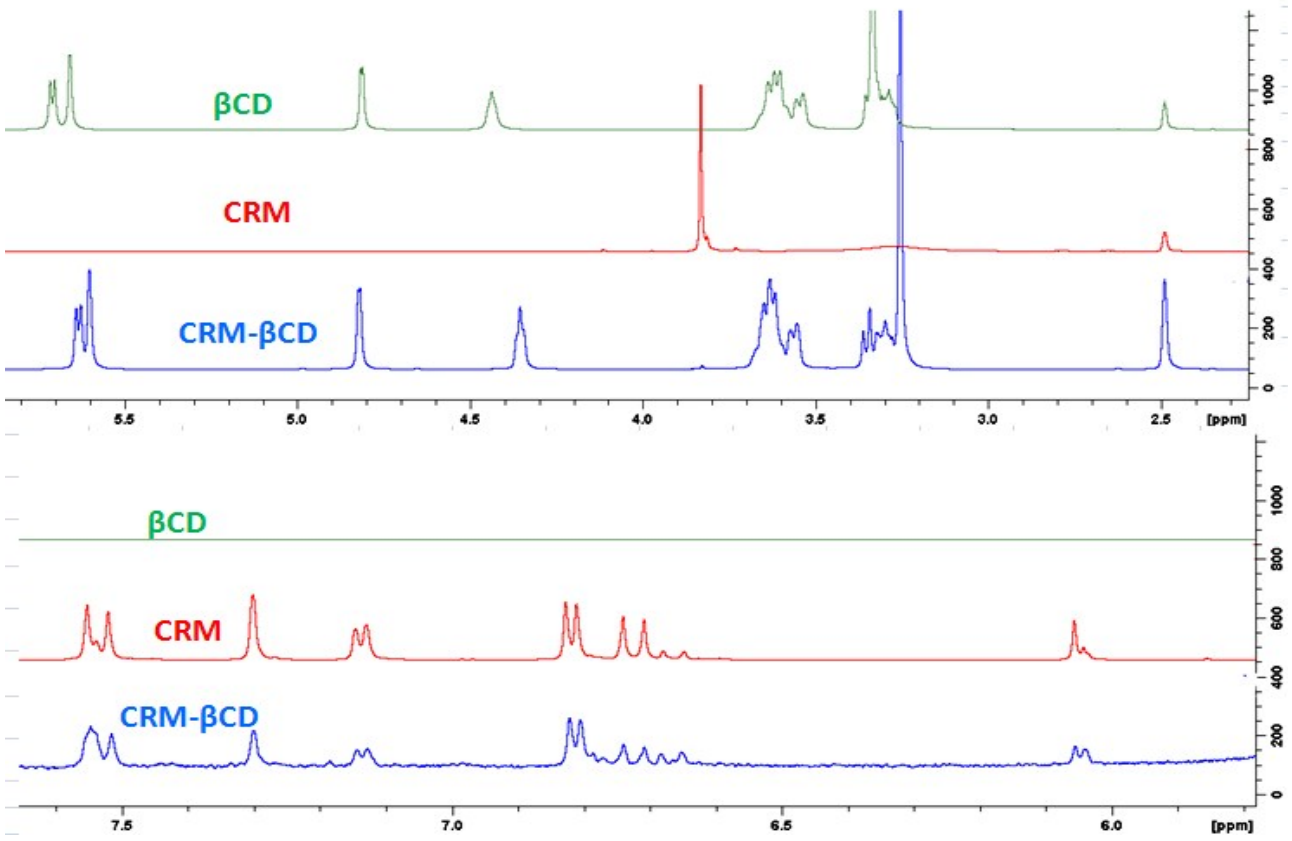

βCD
CRM
CRM-βCD
5.5
5.0
4.5
4.0
3.5
3.0
2.5
[ppm]
1000
800
600
400
200
0
βCD
CRM
CRM-βCD
7.5
7.0
6.5
6.0
[ppm]
1000
800
600
400
200
0

Fig. S11

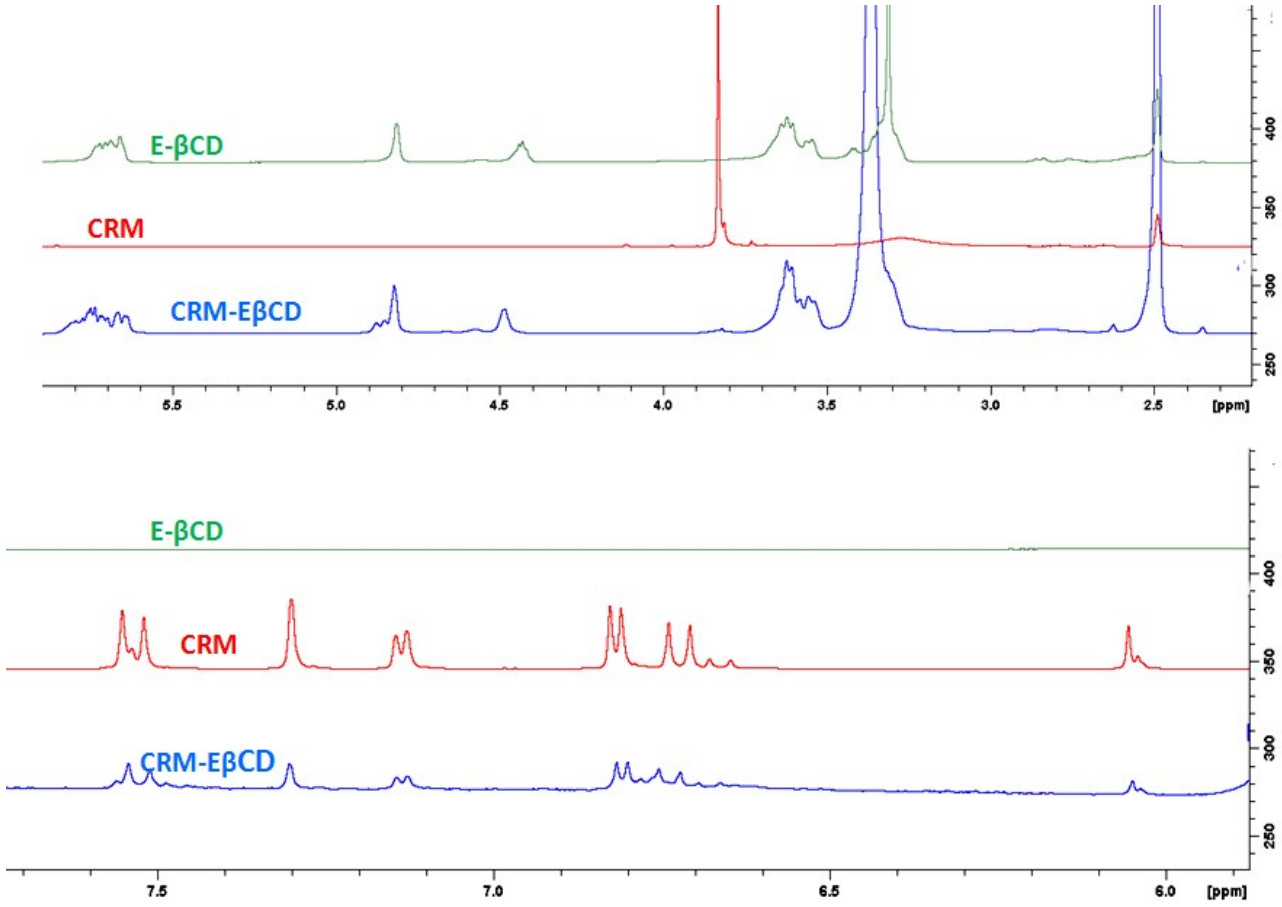

E-βCD
CRM
CRM-EβCD
5.5
5.0
4.5
4.0
3.5
3.0
2.5
[ppm]
400
350
300
250
E-βCD
CRM
CRM-EβCD
7.5
7.0
6.5
6.0
[ppm]
400
350
300
250

Fig. S12

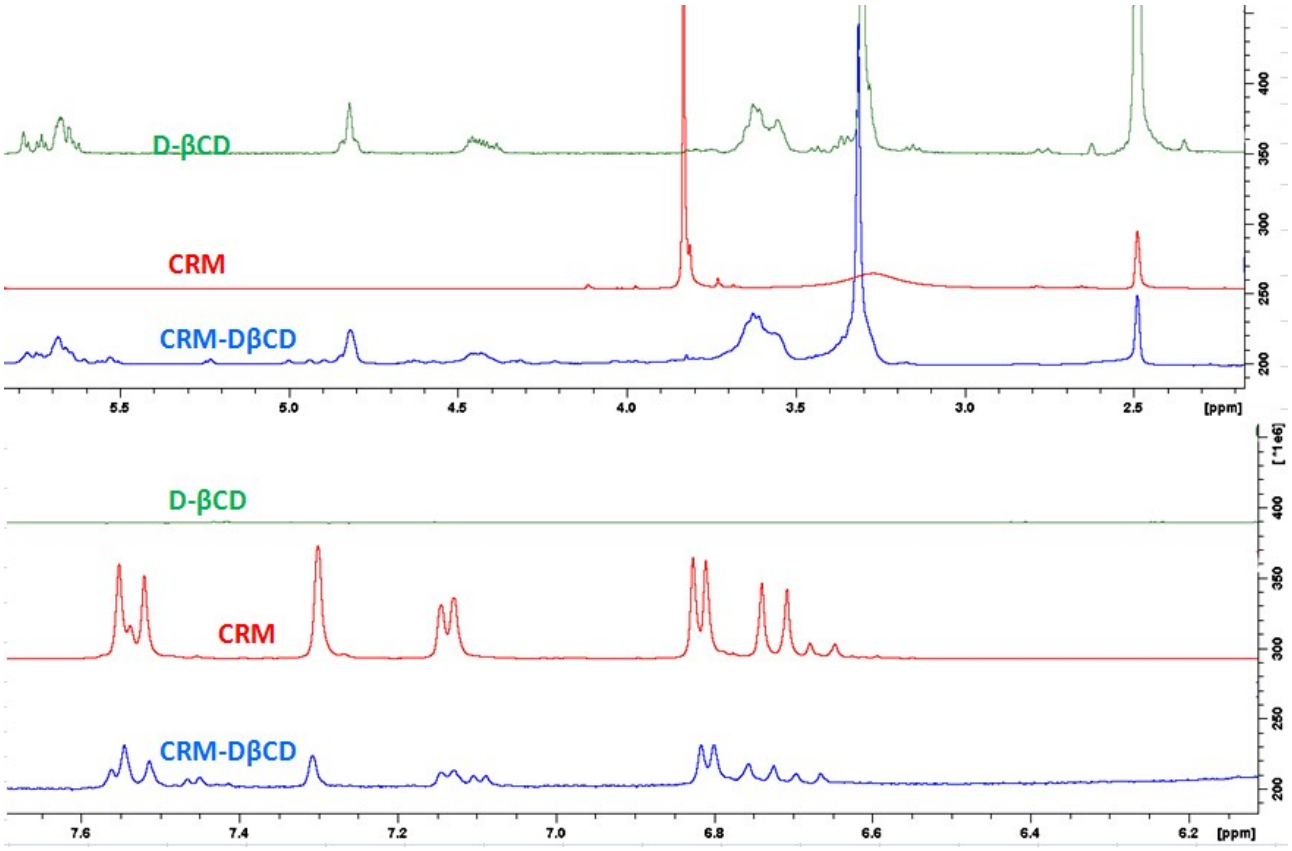

D-βCD
CRM
CRM-DβCD
5.5
5.0
4.5
4.0
3.5
3.0
2.5
[ppm]
400
350
300
250
200
[*1e6]
D-βCD
CRM
CRM-DβCD
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
[ppm]

Table S1

No	Sample	Exothermic peak (°C)
1	CRM	177.3
2	βCD	131.6
3	E-βCD	96.6
4	D-βCD	96.0
5	CRM-βCD	122.0
7	CRM-E-βCD	93.6
6	CRM-D-βCD	86.7

Table S2

	Proton	δo	δc	Δδo
βCD	H1	4.4384	4.3564	-0.0820
	H2	3.2887	3.2986	0.0099
	H3	3.6202	3.6331	0.0129
	H4	3.3363	3.3439	0.0076
	H5	3.5462	3.5642	0.0180
Curcumin	Ha	6.0559	6.0546	-0.0013
	Hb	6.8176	6.8119	-0.0057
	Hc	7.5311	7.5272	-0.0039
	Hd	6.6789	6.6825	0.0036
	He	7.1375	7.1350	-0.0025
	Hf	5.8550	Not visible	
	Hg	3.8329	3.8299	-0.0030
	Hh	7.3013	7.2999	-0.0014

Table S3

	Proton	δo	δc	Δδo
E-βCD	H1	4.8182	4.8234	0.0052
	H2	3.2893	3.3146	0.0253
	H3	3.6223	3.6245	0.0022
	H4	3.3129	3.3635	0.0506
	H5	3.5558	3.5448	-0.0110
Curcumin	Ha	6.0559	6.0496	-0.0063
	Hb	6.8180	6.8094	-0.0086
	Hc	7.5524	7.5432	-0.0092
	Hd	6.7398	6.7543	0.0145
	He	7.1375	7.1364	-0.0011
	Hf	5.8245	Not visible	
	Hg	3.8330	3.8215	-0.0115
	Hh	7.3010	7.3035	0.0025

Table S4

	Proton	δ_o	δ_c	$\Delta\delta_o$
D-βCD	H1	4.8215	4.8197	-0.0018
	H2	3.3046	3.3159	0.0113
	H3	3.6140	3.6181	0.0041
	H4	3.3471	3.3615	0.0144
	H5	3.5550	3.5643	0.0093
Curcumin	Ha	6.0560	6.0477	-0.0083
	Hb	6.8180	6.8083	-0.0097
	Hc	7.5205	7.5140	-0.0065
	Hd	6.7082	6.7249	0.0167
	He	7.1373	7.1373	0.0000
	Hf	5.8551	Not visible	
	Hg	3.8330	3.8245	-0.0085
	Hh	7.3011	7.3077	0.0066