Experimental and Theoretical Study of the Inclusion Complexes of Epinephrine with β-Cyclodextrin, 18-Crown-6 and Cucurbit[7]uril

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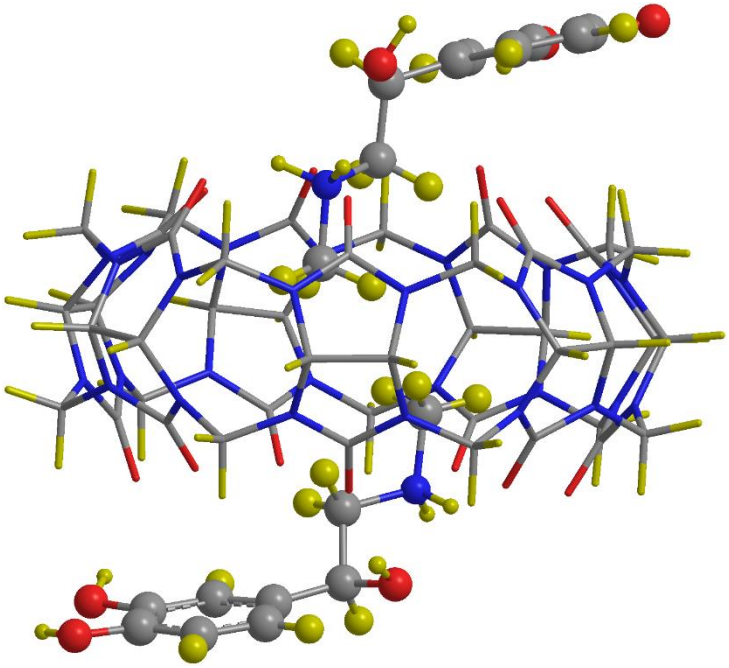
(a)



(b)

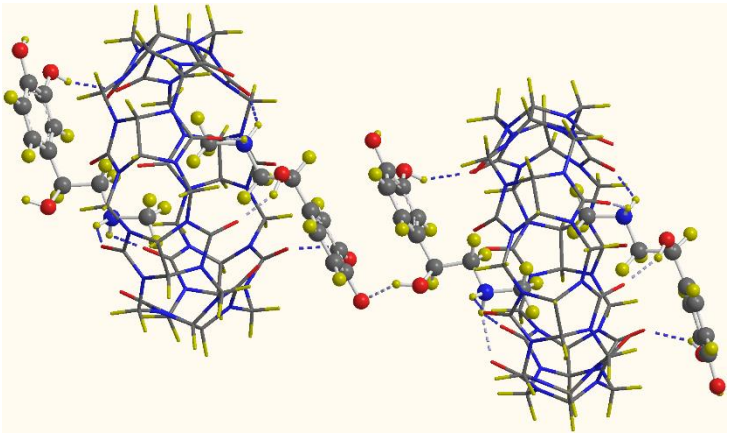
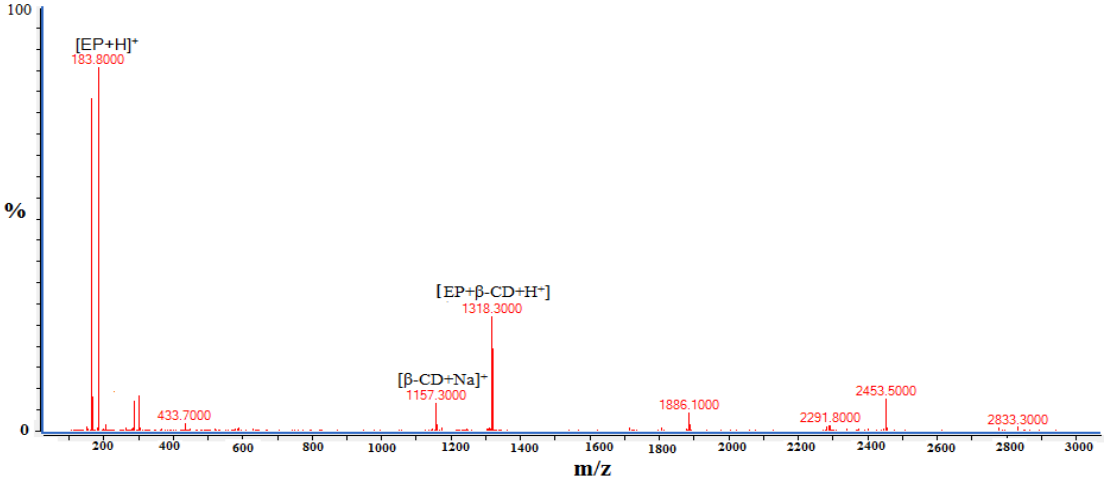
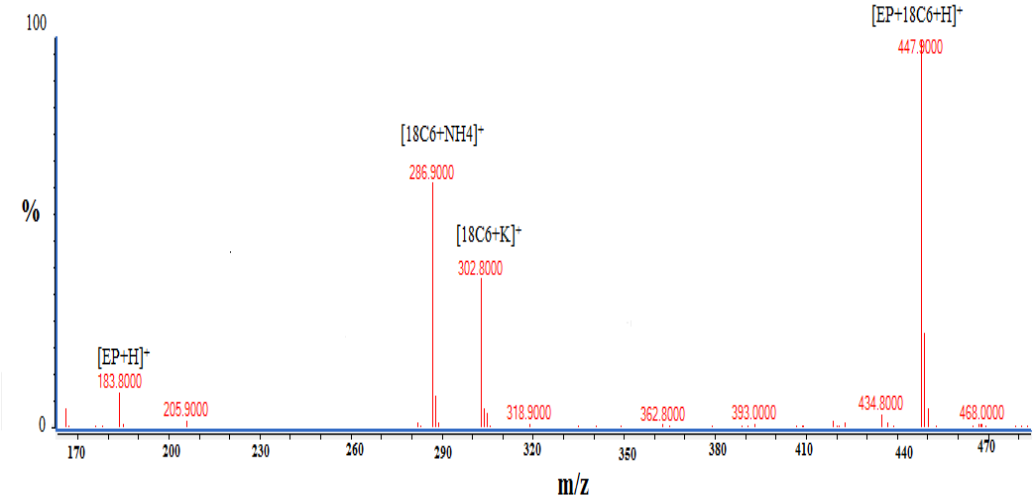


Figure S1 Plausible structures of (a) EP-CB7-EP complex (b) Face-to-face aggregation of EP-CB7-EP complex

(a)


100
%
0
[EP+H]+
183.8000
[EP+β-CD+H+]
1318.3000
[β-CD+Na]+
1157.3000
433.7000
1886.1000
2291.8000
2453.5000
2833.3000
200
400
600
800
1000
1200
1400
1600
1800
2000
2200
2400
2600
2800
3000
m/z

(b)


100
%
0
[EP+18C6+H]+
447.9000
[18C6+NH4]+
286.9000
[18C6+K]+
302.8000
[EP+H]+
183.8000
205.9000
318.9000
362.8000
393.0000
434.8000
468.0000
170
200
230
260
290
320
350
380
410
440
470
m/z

(c)

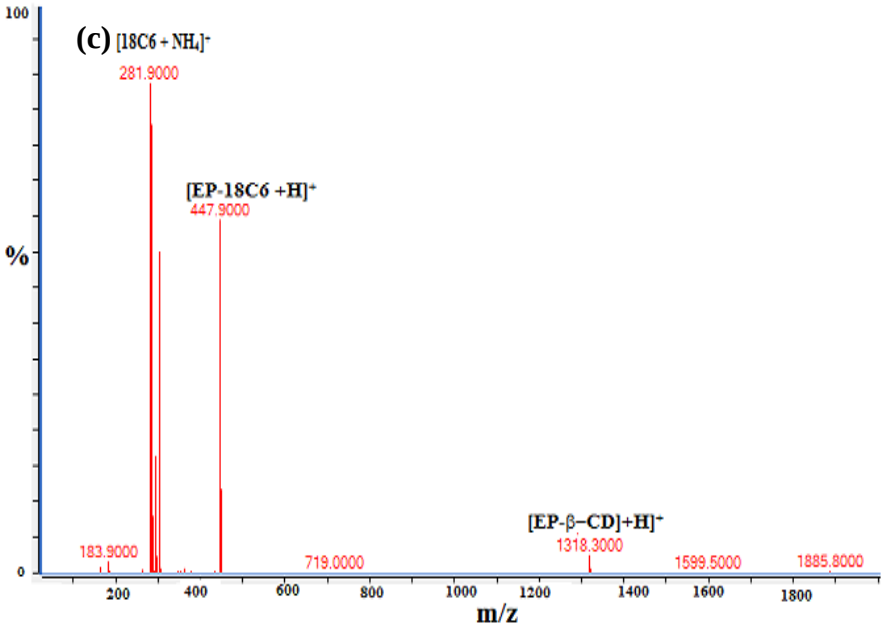

100
%
0
[18C6 + NH4]+
281.9000
[EP-18C6 +H]+
447.9000
183.9000
719.0000
[EP-β-CD]+H]+
1318.3000
1599.5000
1885.8000
200
400
600
800
1000
1200
1400
1600
1800
m/z

Figure S2a ESI-MS Spectra of (a) EP-βCD (b) EP -18C6 (c) EP-βCD-18C6.

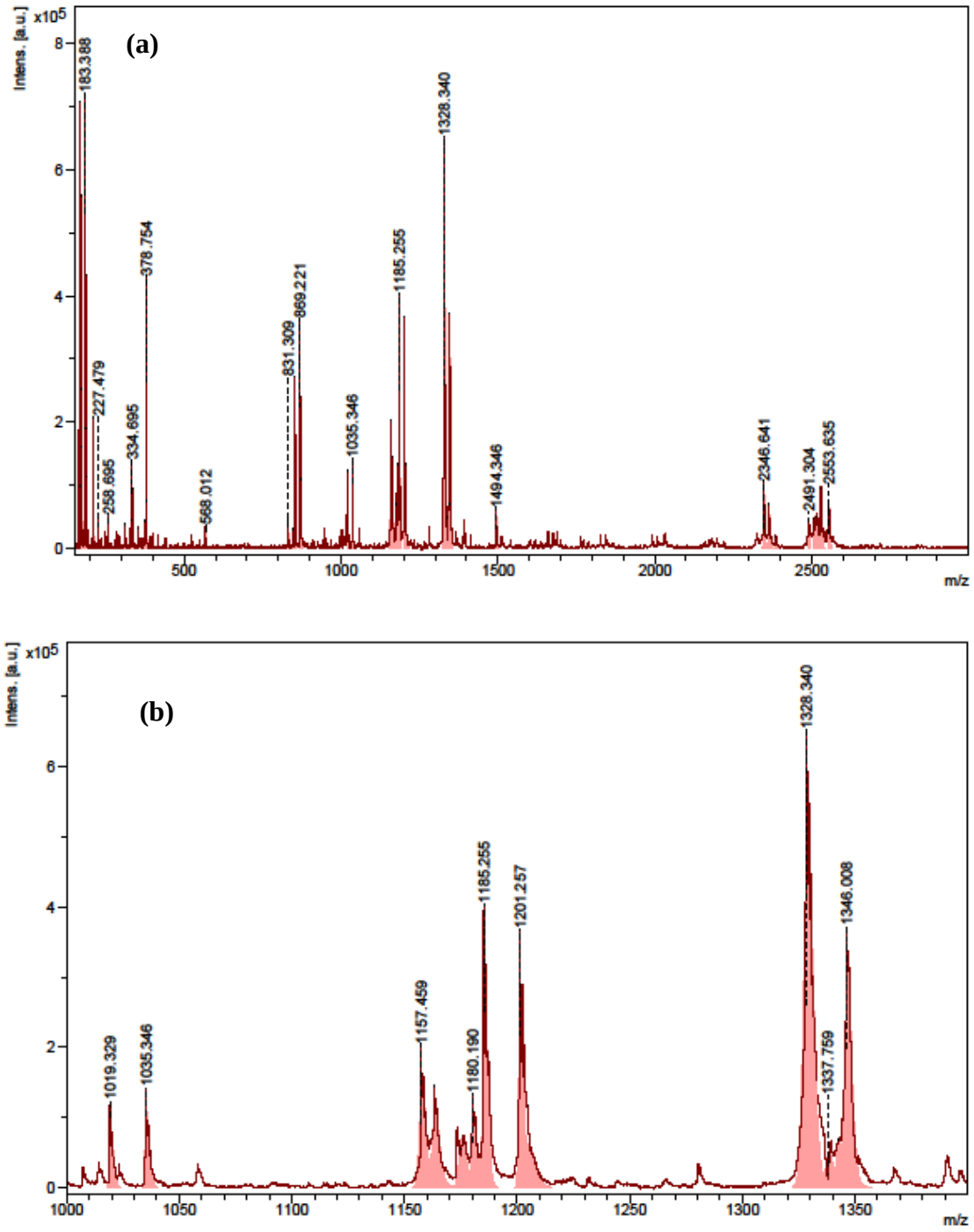


Figure S2 MALDI-TOF spectrum for EP-βCD-CB7 in ACC matrix (a) in m/z range 400-3000 (b) the m/z region from 1000-14000.

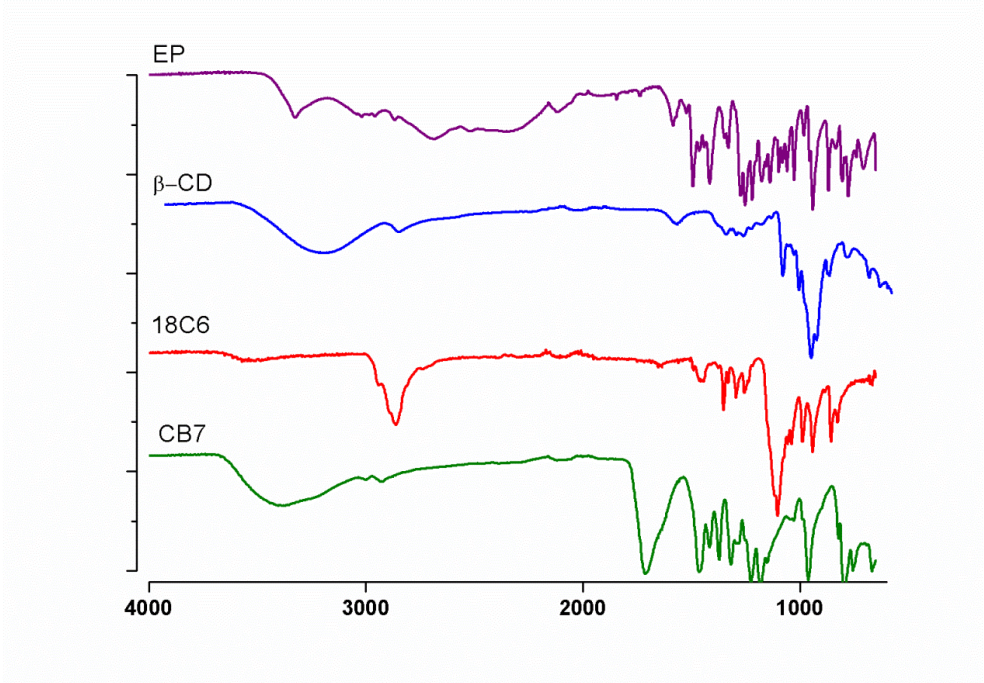
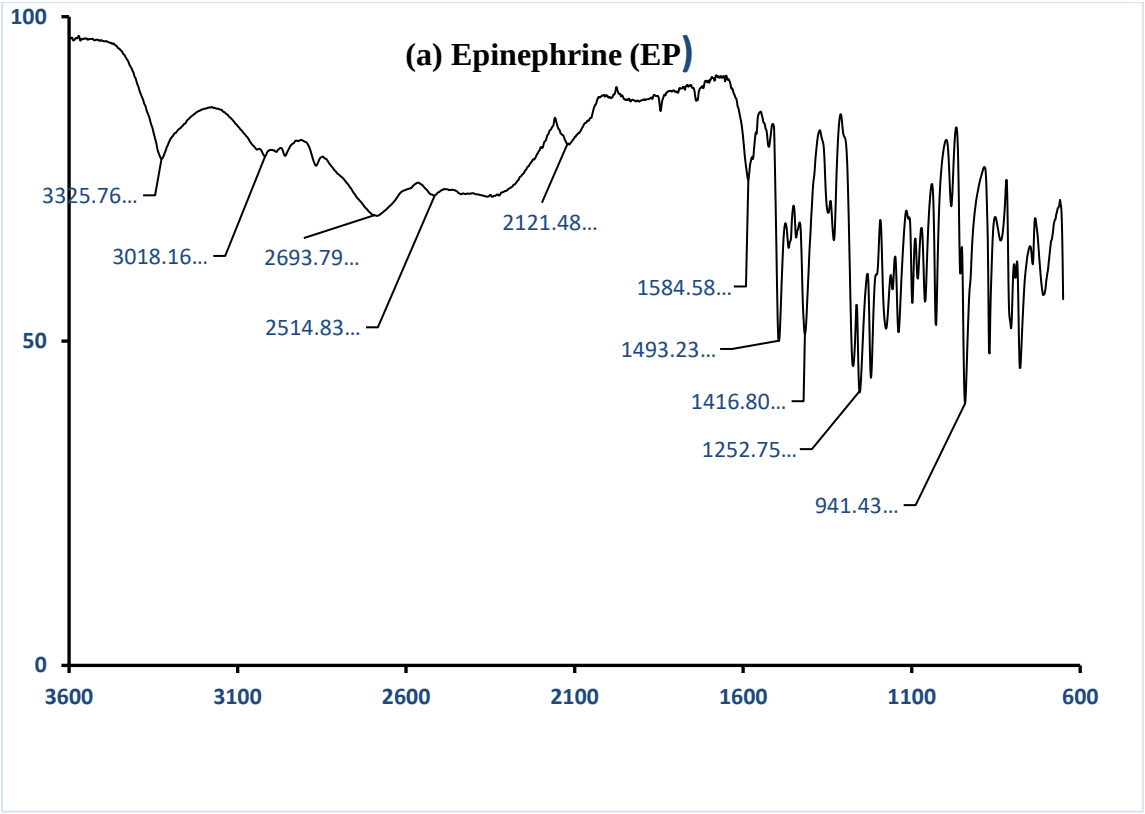
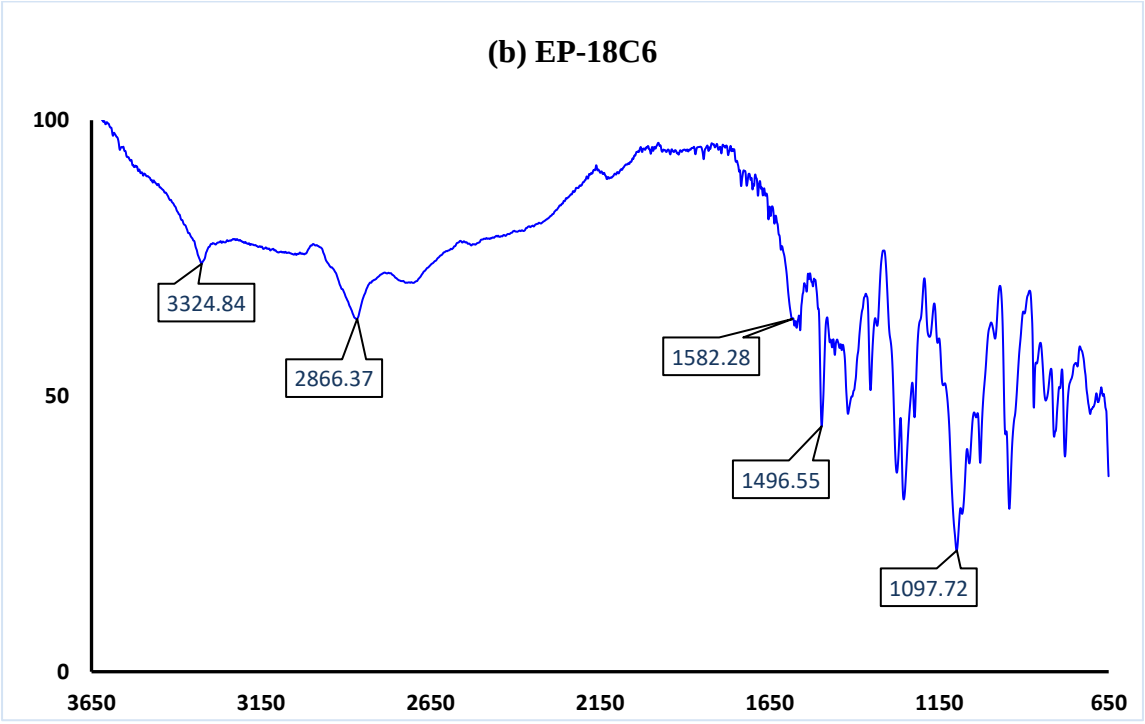
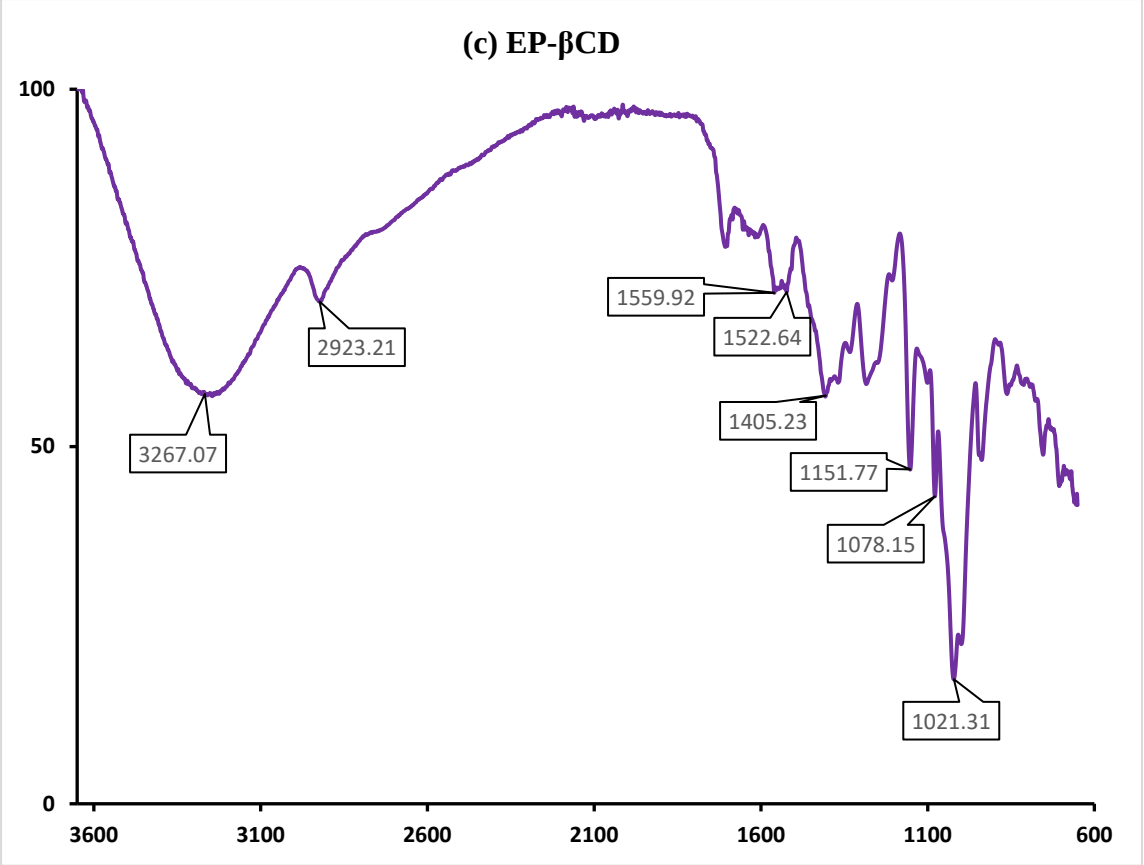
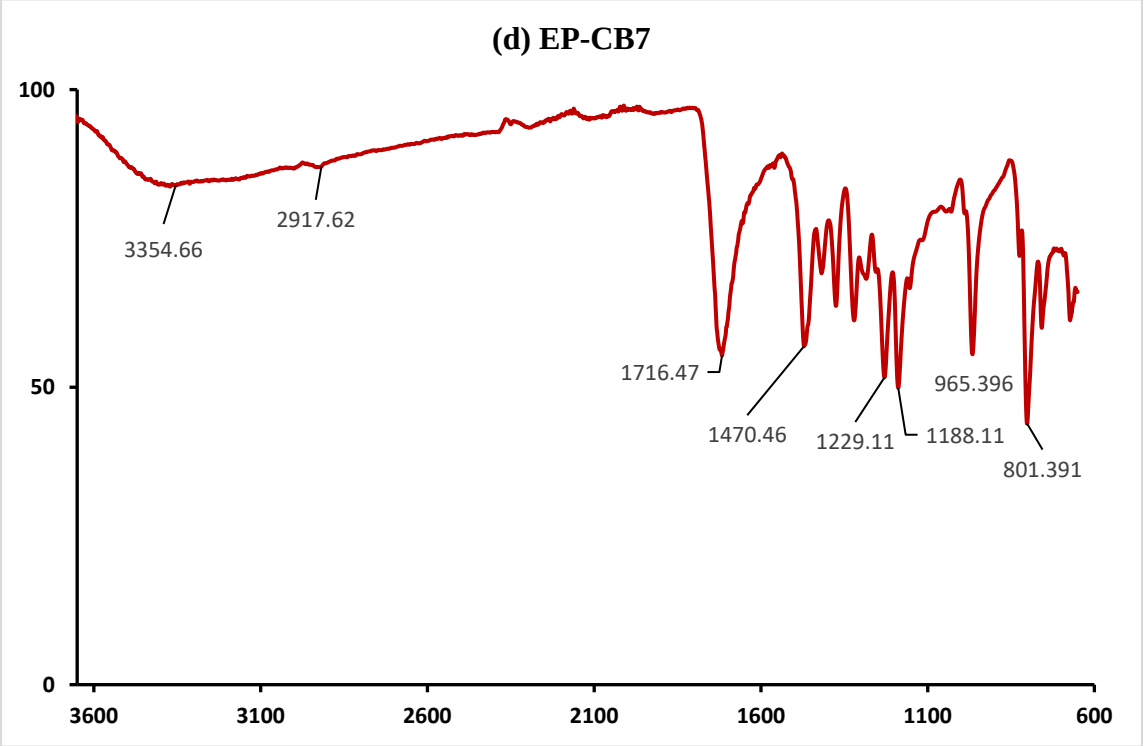


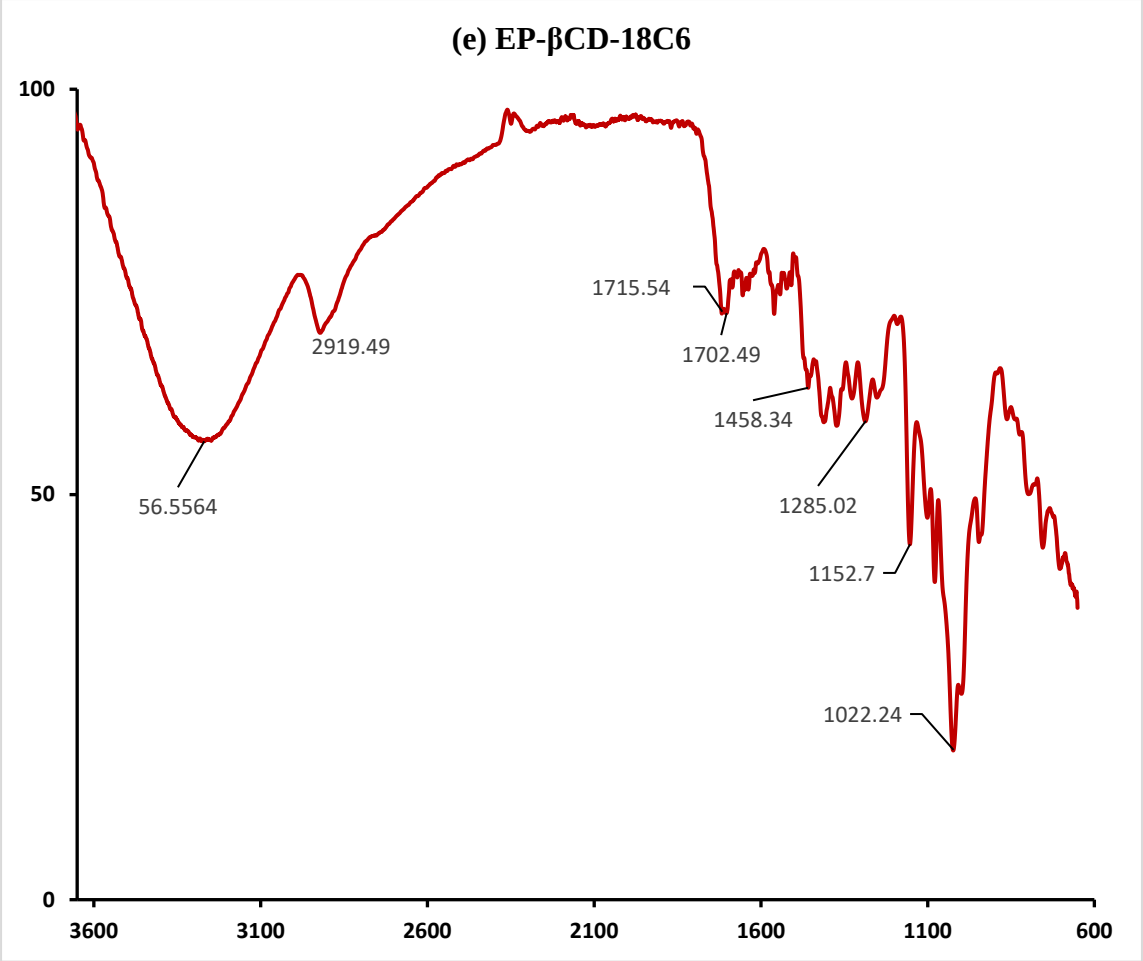
Figure S3a FT-IR spectra of pure compounds


(a) Epinephrine (EP)
100
50
0
3600
3100
2600
2100
1600
1100
600
3325.76...
3018.16...
2693.79...
2514.83...
2121.48...
1584.58...
1493.23...
1416.80...
1252.75...
941.43...


(b) EP-18C6
100
50
0
3650
3150
2650
2150
1650
1150
650
3324.84
2866.37
1582.28
1496.55
1097.72


(c) EP-βCD
100
50
0
3600
3100
2600
2100
1600
1100
600
3267.07
2923.21
1559.92
1522.64
1405.23
1151.77
1078.15
1021.31


(d) EP-CB7
100
50
0
3600
3100
2600
2100
1600
1100
600
3354.66
2917.62
1716.47
1470.46
1229.11
1188.11
965.396
801.391


(e) EP-βCD-18C6
100
50
0
3600
3100
2600
2100
1600
1100
600
56.5564
2919.49
1715.54
1702.49
1458.34
1285.02
1152.7
1022.24

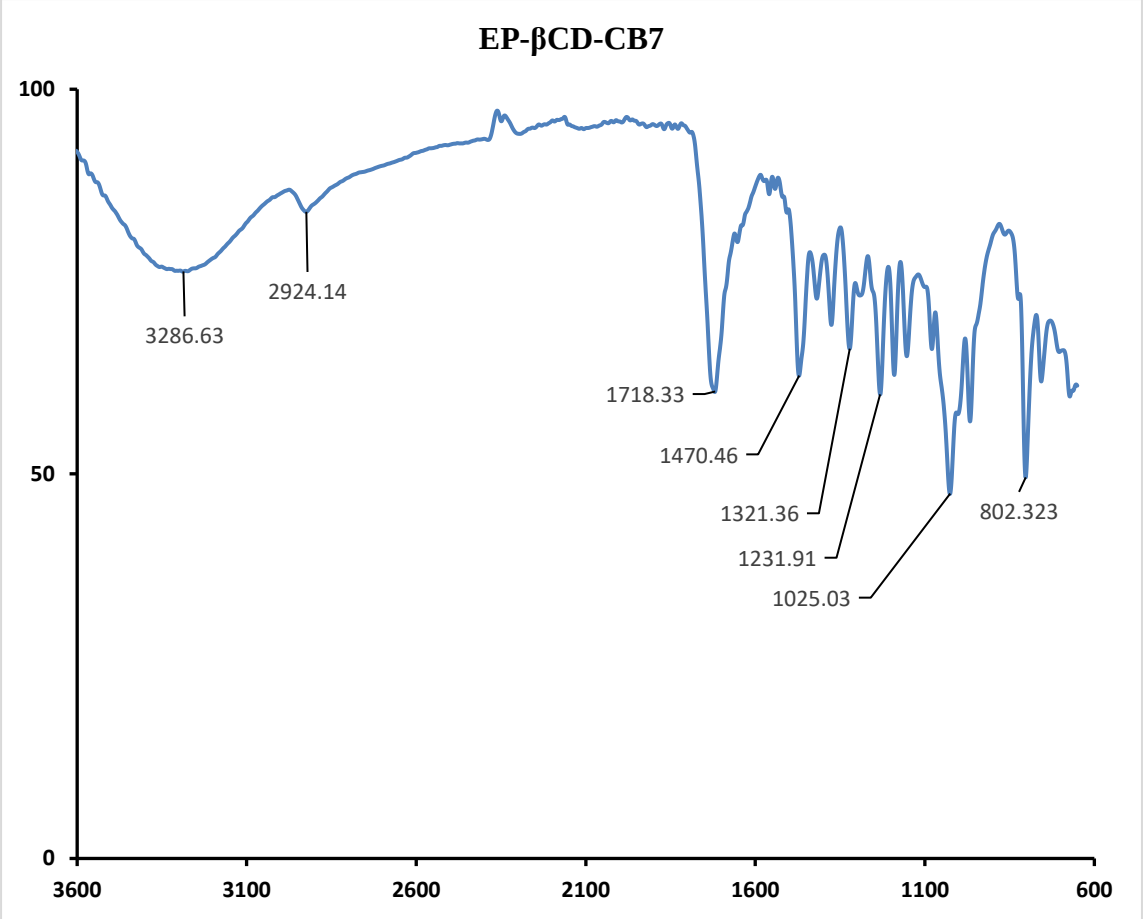


Figure S3b FT-IR spectra of EP and EP-hosts complexes prepared by lyopholization.

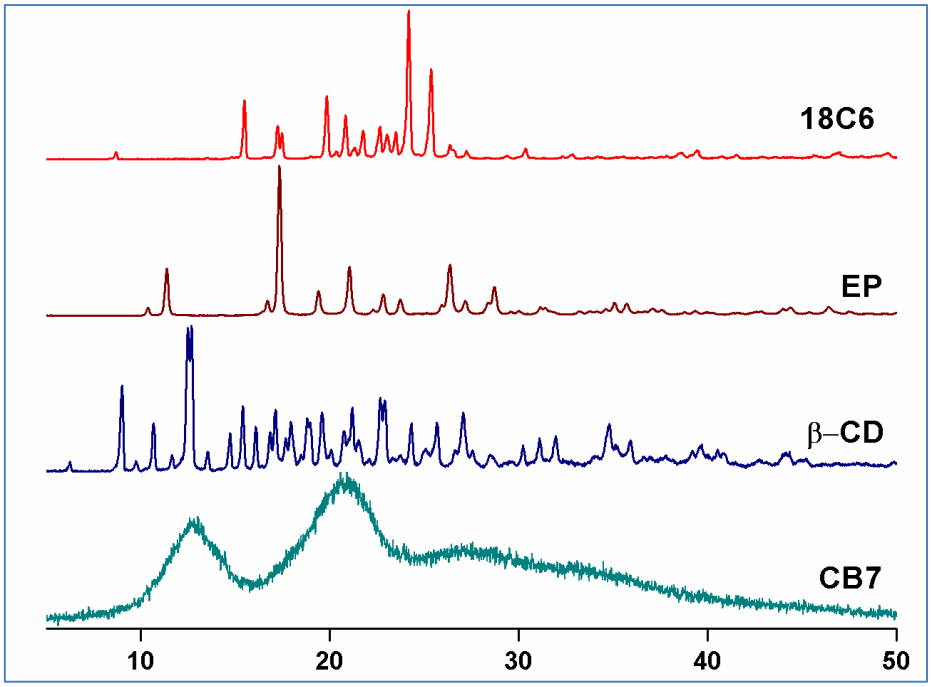


Figure S4a PXRD patterns of pure guest and hosts.

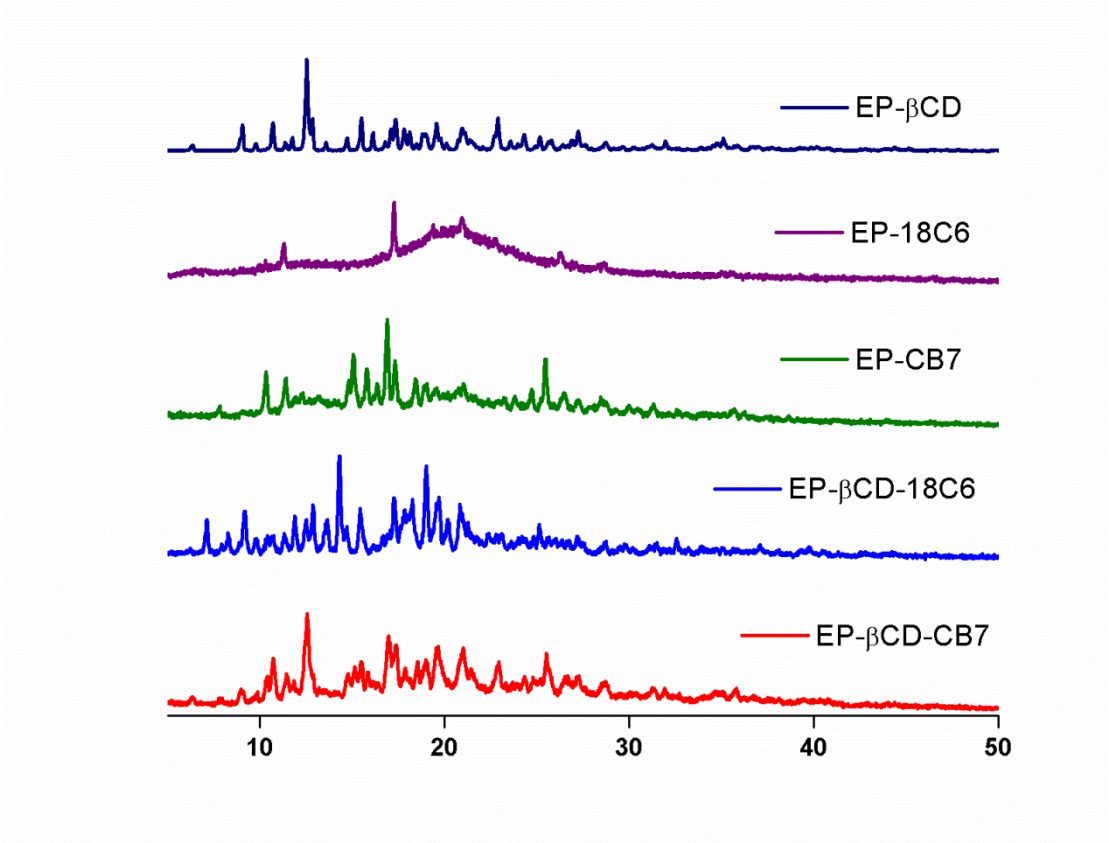


Figure S4b PXRD patterns of physical mixture

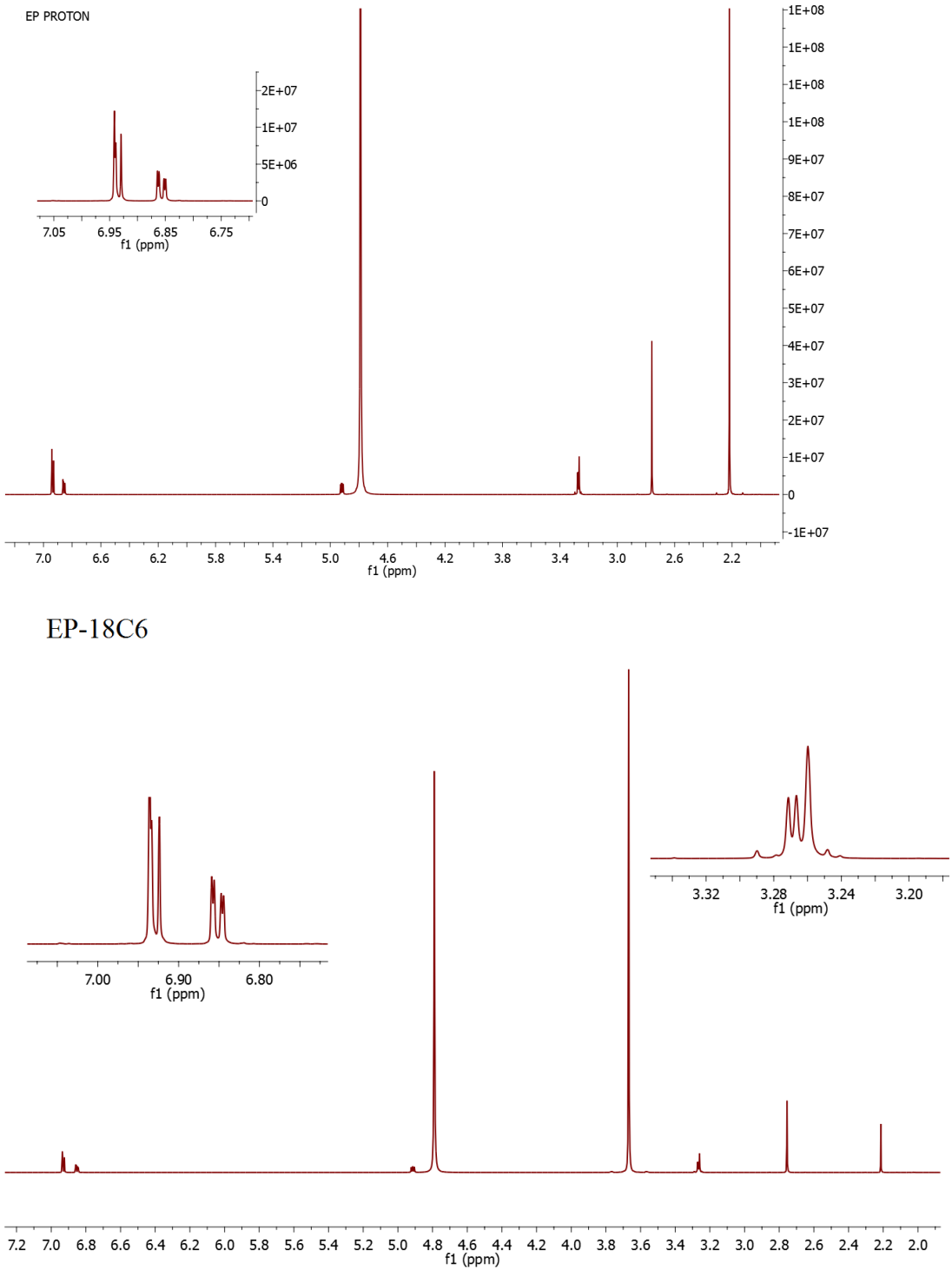


Figure S5a [1]HNMR spectra of the pure EP and EP-18C6 complex.

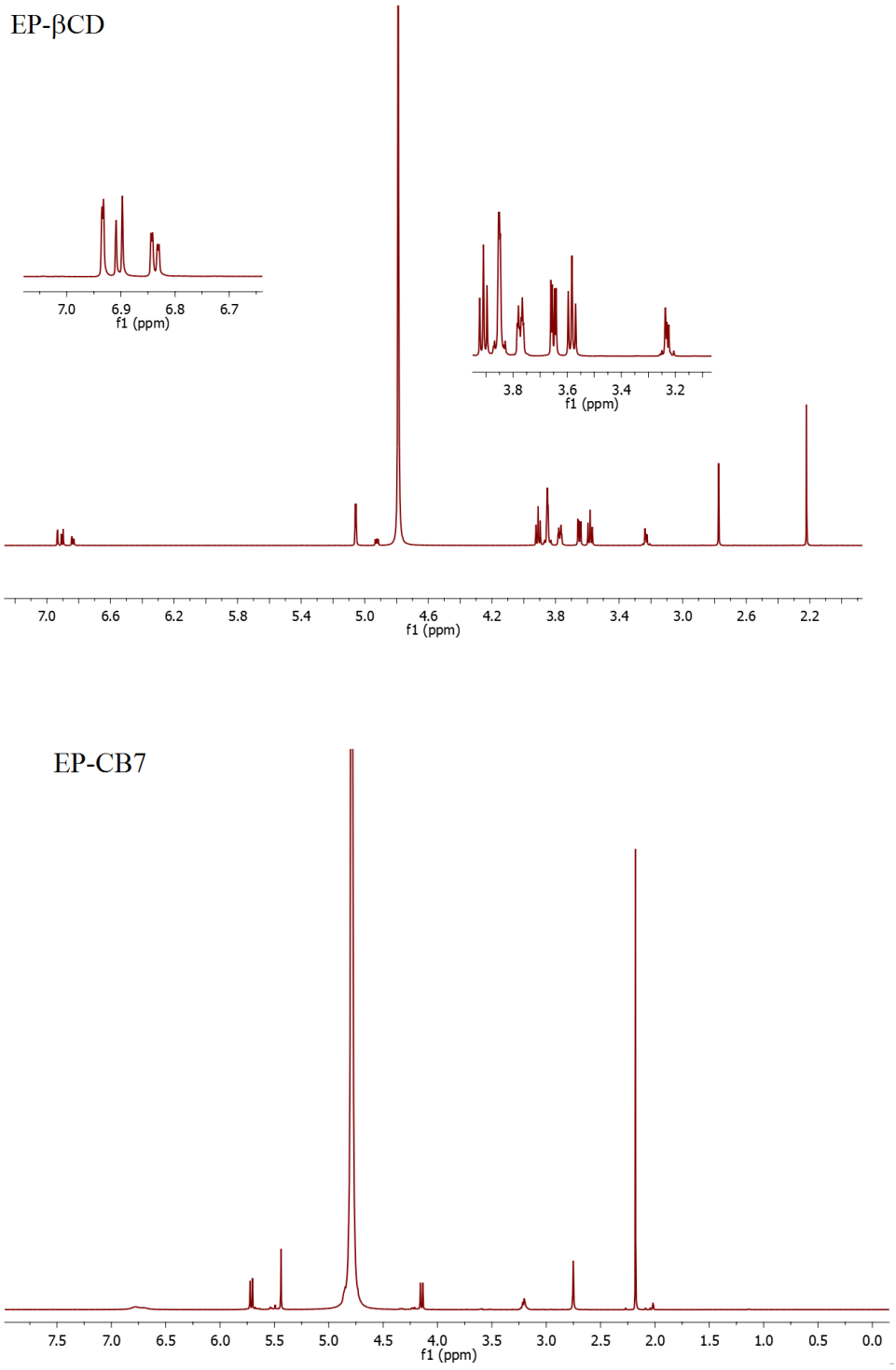


Figure S5b ^{1}HNMR spectra of the pure EP-βCD and EP-CB7 complexes.

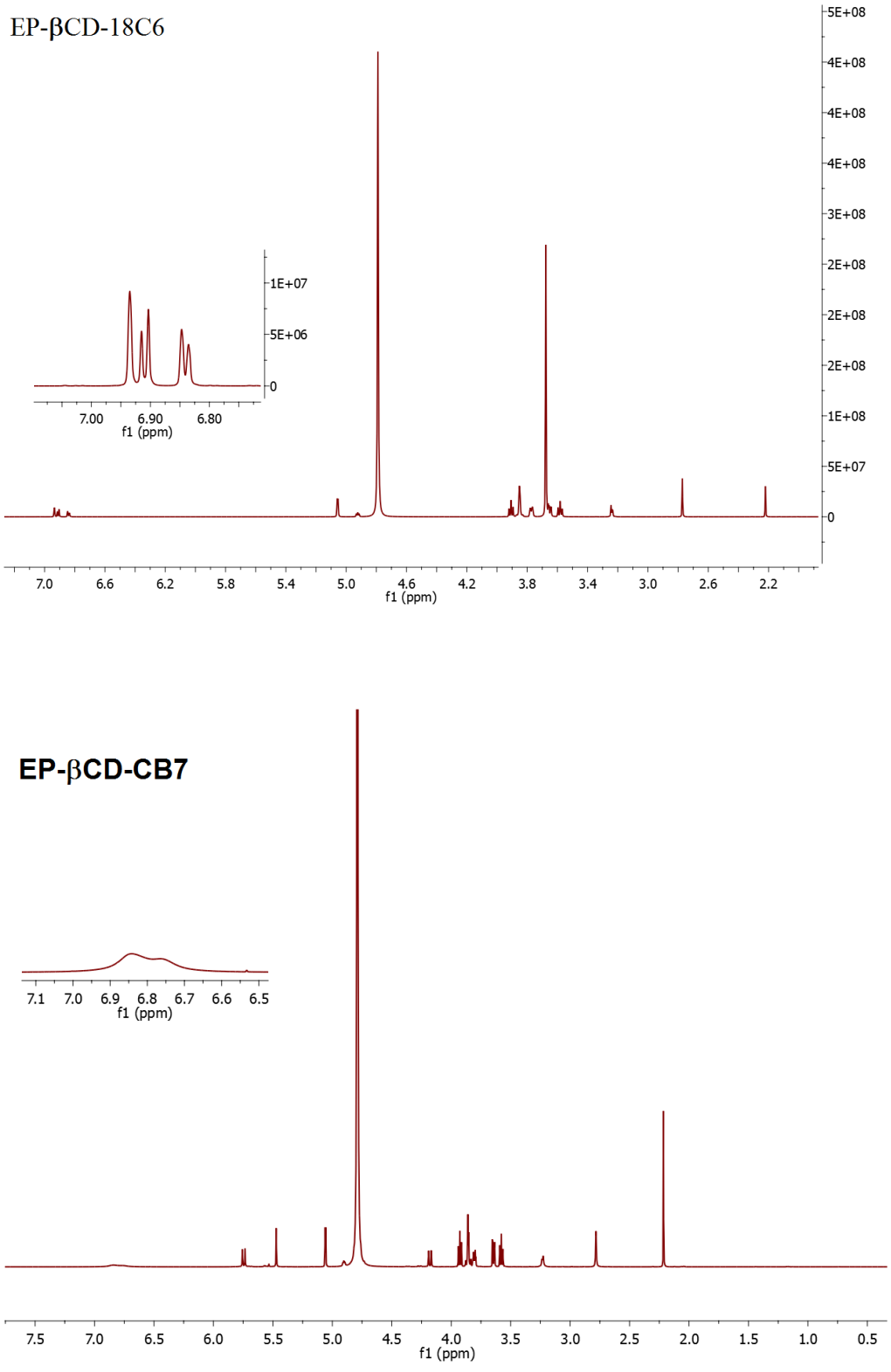


Figure S5c [1]HNMR spectra of the pure EP-βCD-18C6 and EP-βCD-CB7 complexes.

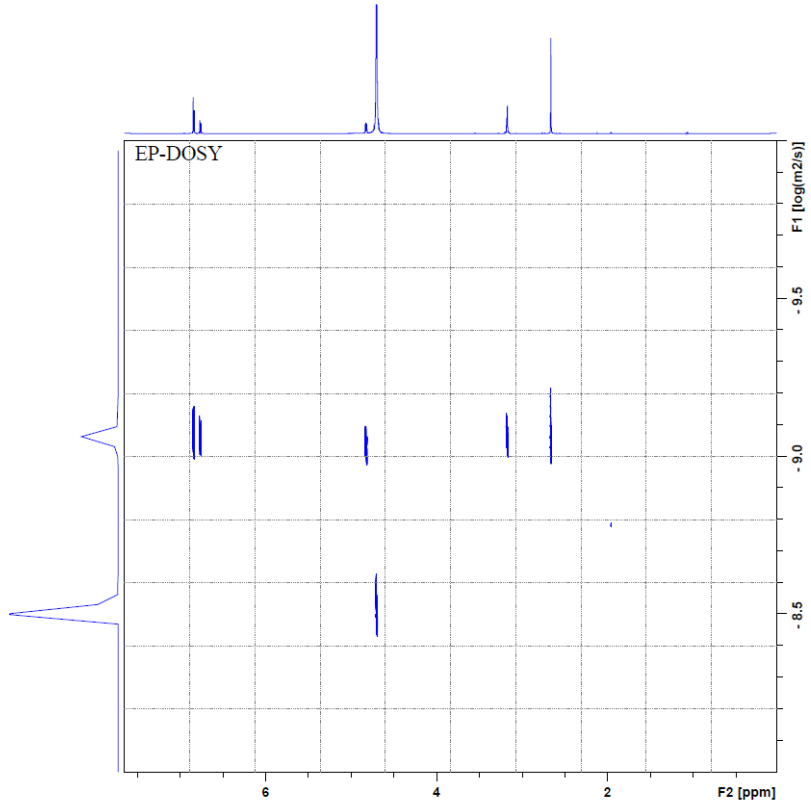


Figure S6a DOSY spectrum of EP.

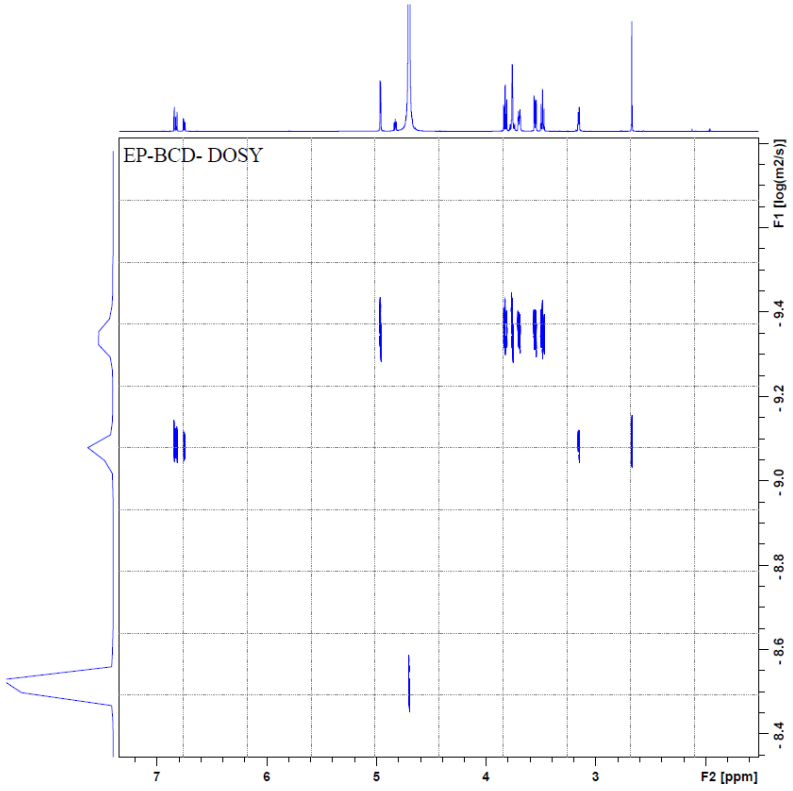


Figure S6b DOSY spectrum of EP-βCD.

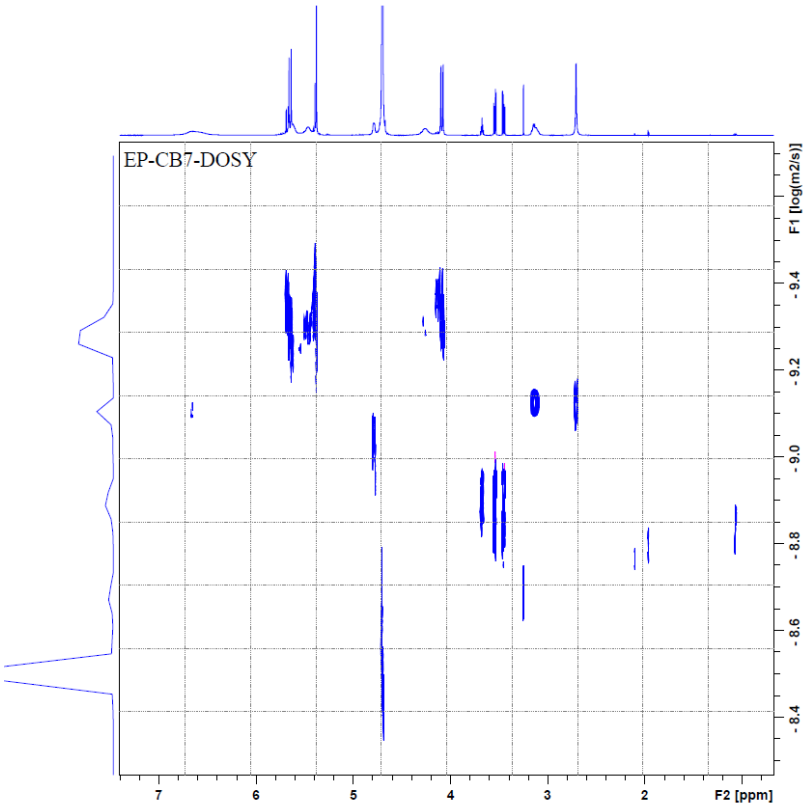


Figure S6c DOSY spectrum of EP-CB7.

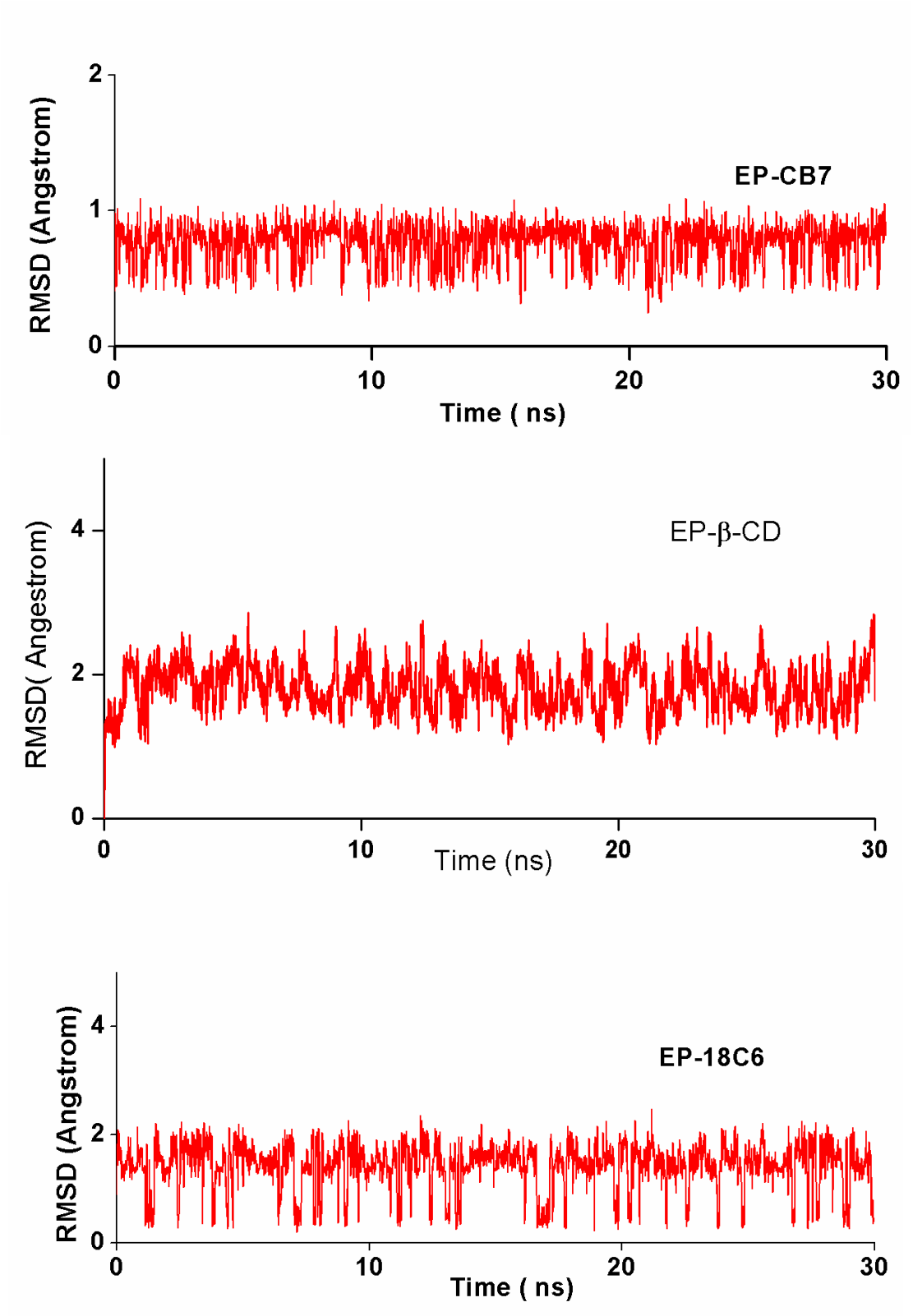


Figure S7 The time dependence of the root-mean-square deviations (RMSD) of atomic positions in the MD simulated binary complexes from those in the corresponding energy minimized structure.

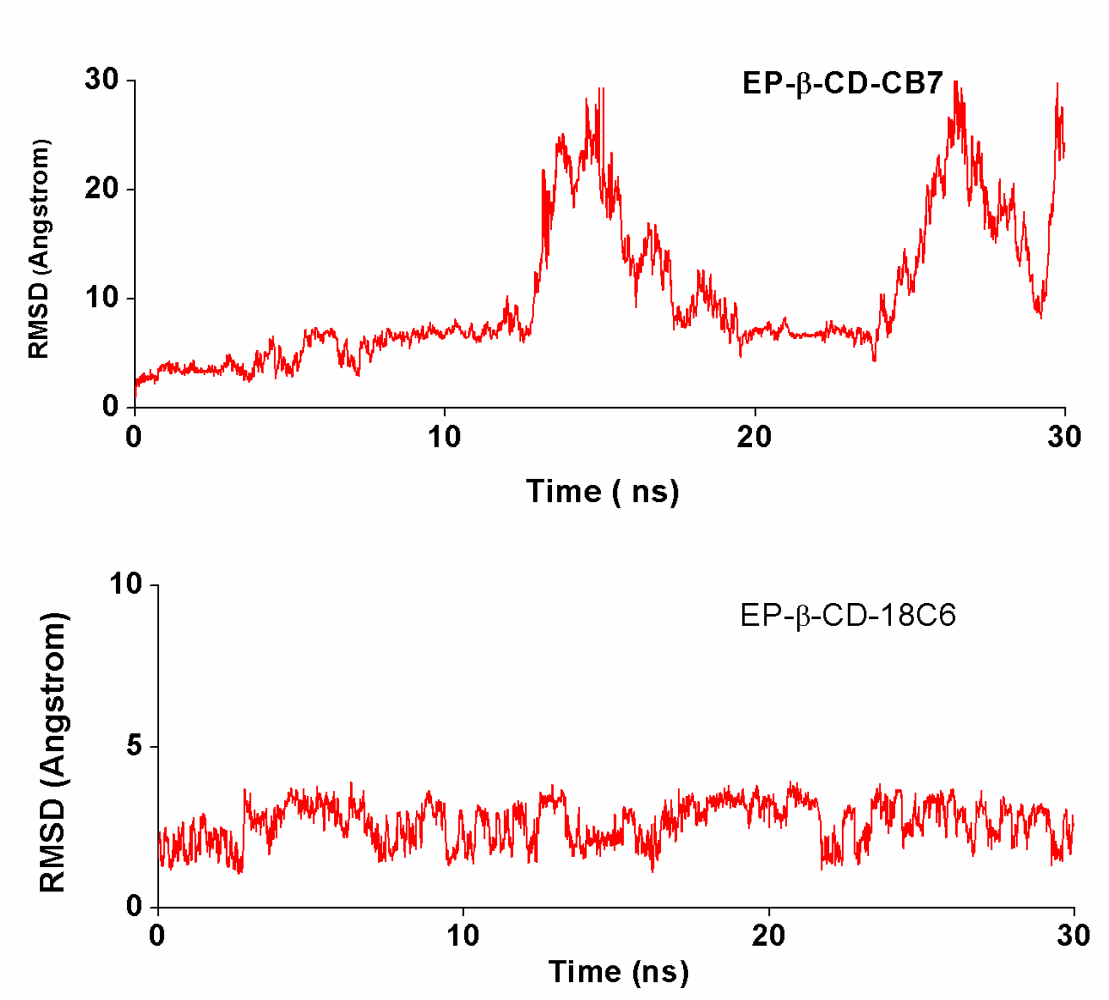


Figure S7b The time dependence of the root-mean-square deviations (RMSD) of atomic positions in the MD simulated ternary complex from those in the corresponding energy minimized structure.

(a)

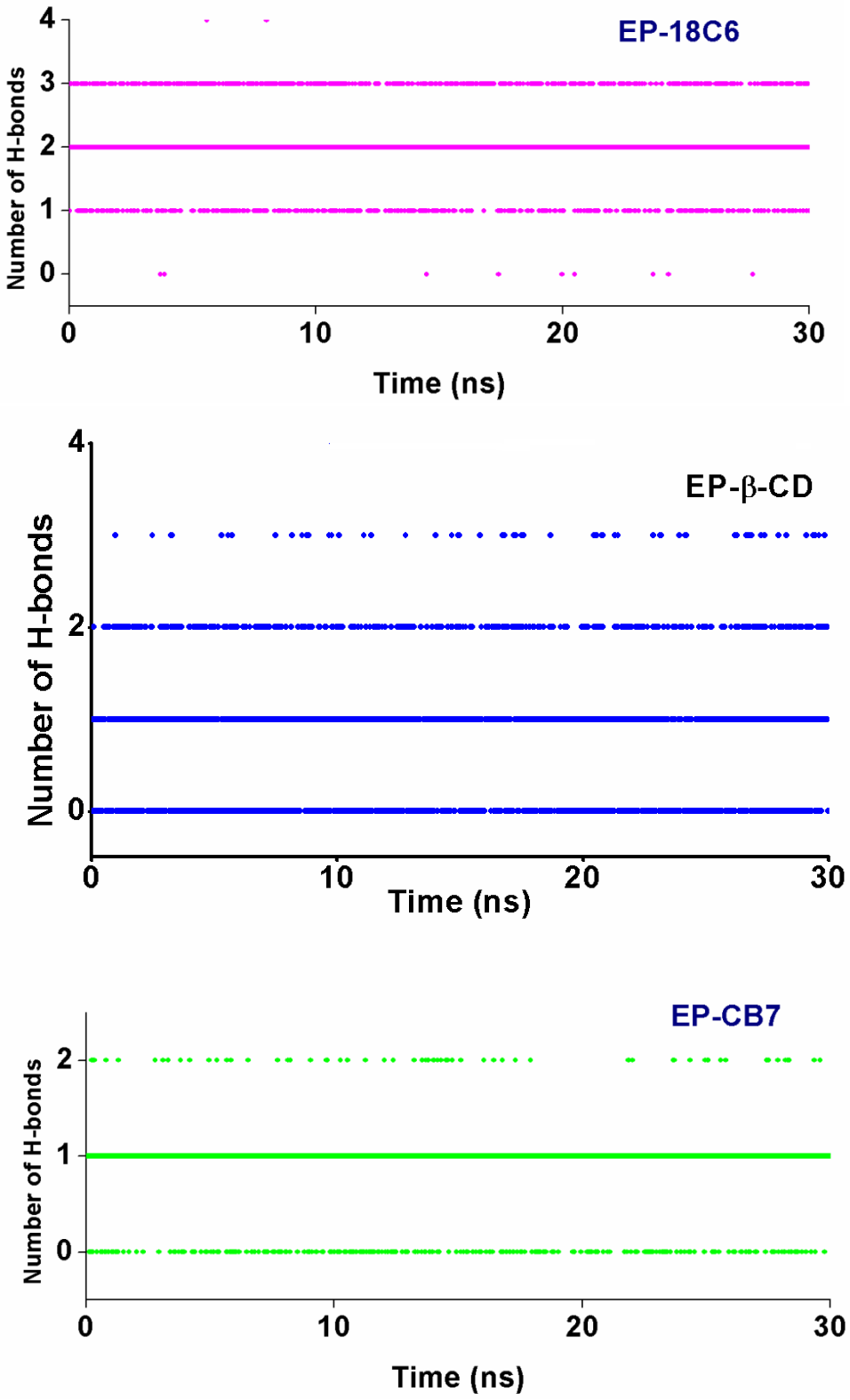
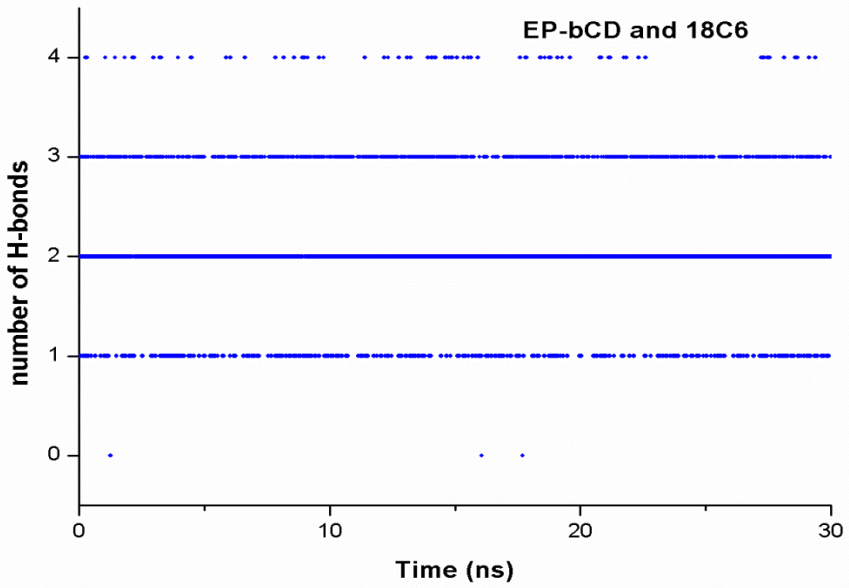
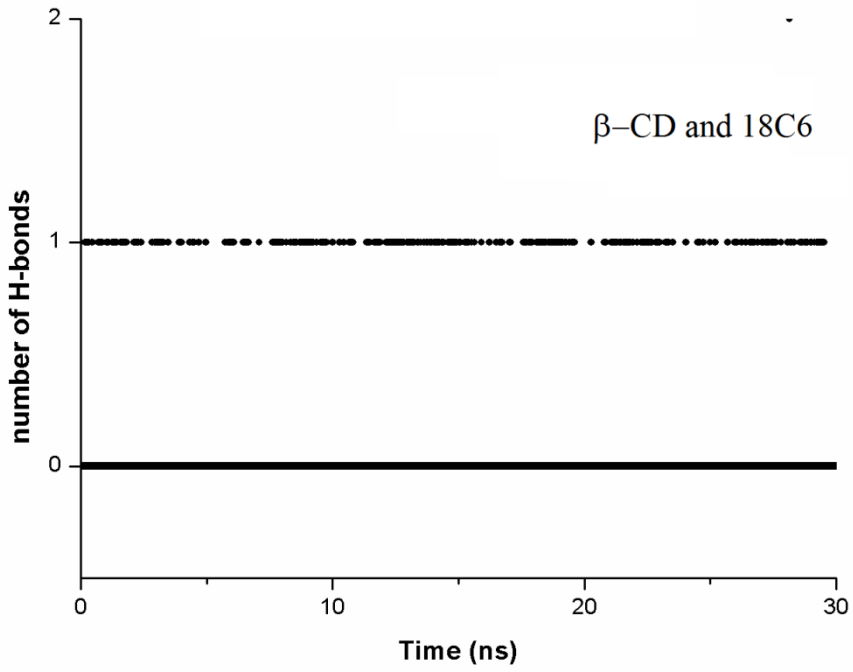


Figure S8a Hydrogen bonding interaction obtained from MD trajectories for binary complexes.


EP-bCD and 18C6
number of H-bonds
0
1
2
3
4
0
10
20
30
Time (ns)


β–CD and 18C6
number of H-bonds
0
1
2
0
10
20
30
Time (ns)

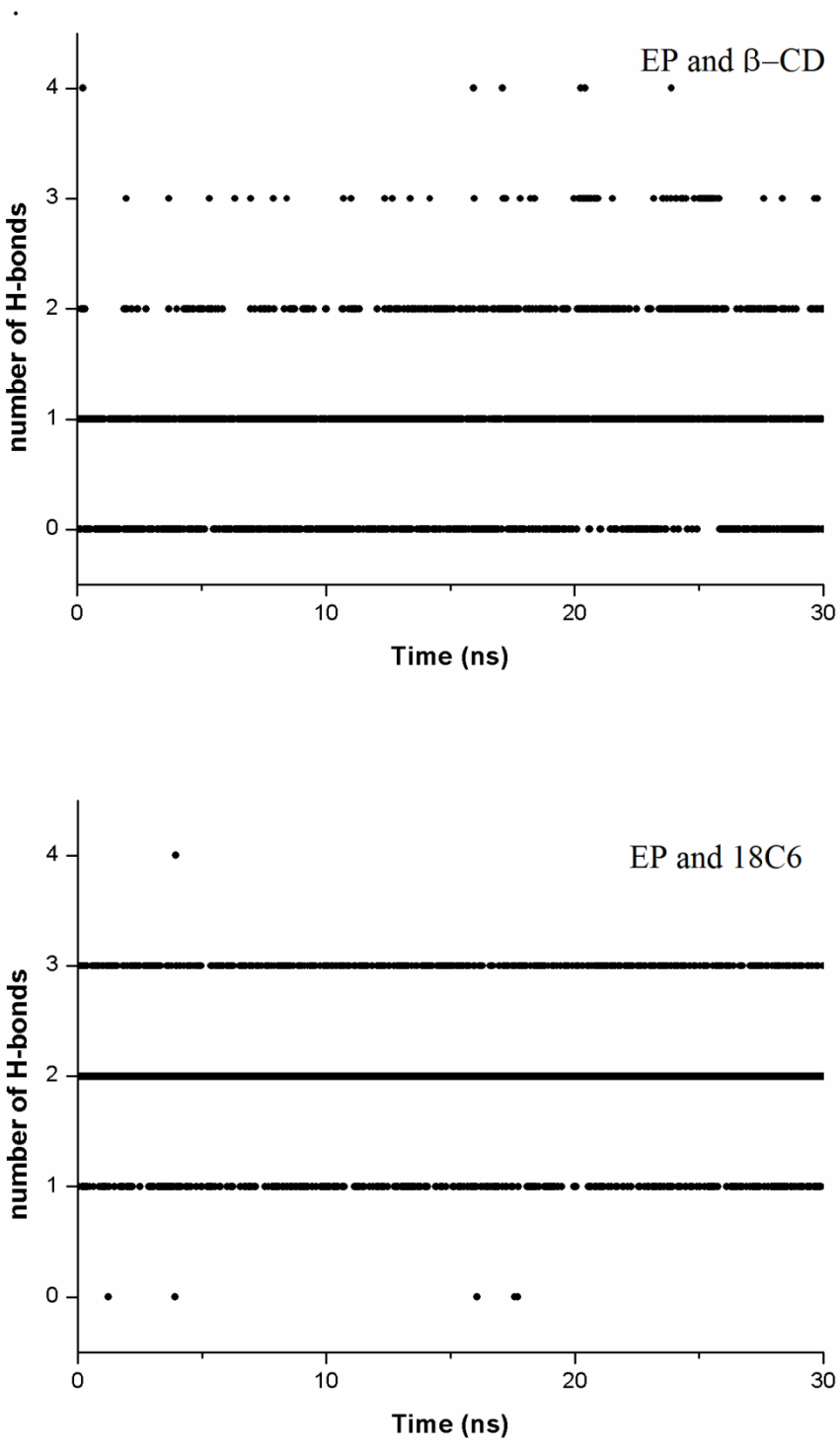


Figure S8b Hydrogen bonding interaction obtained from MD trajectories for EP-bCD-18C6 complex.

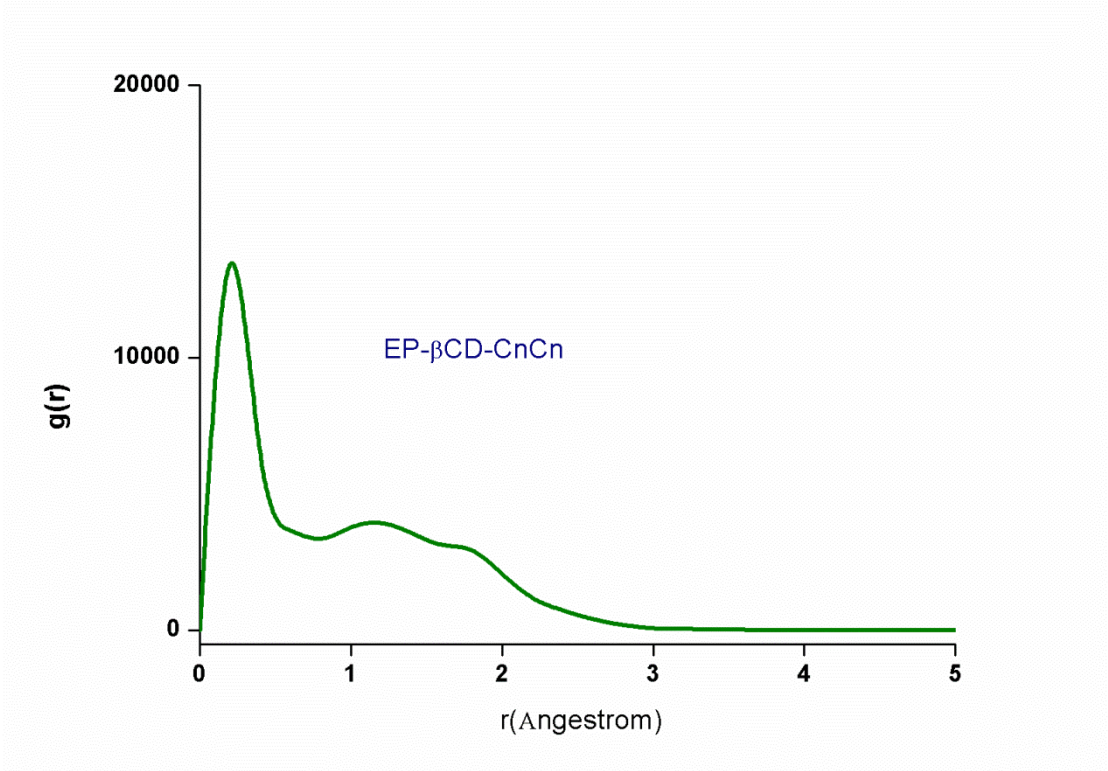


Figure S9 The RDF of center of mass of host and guest plotted as a function of separation distance *r* (Å) in EP-βCD complex.

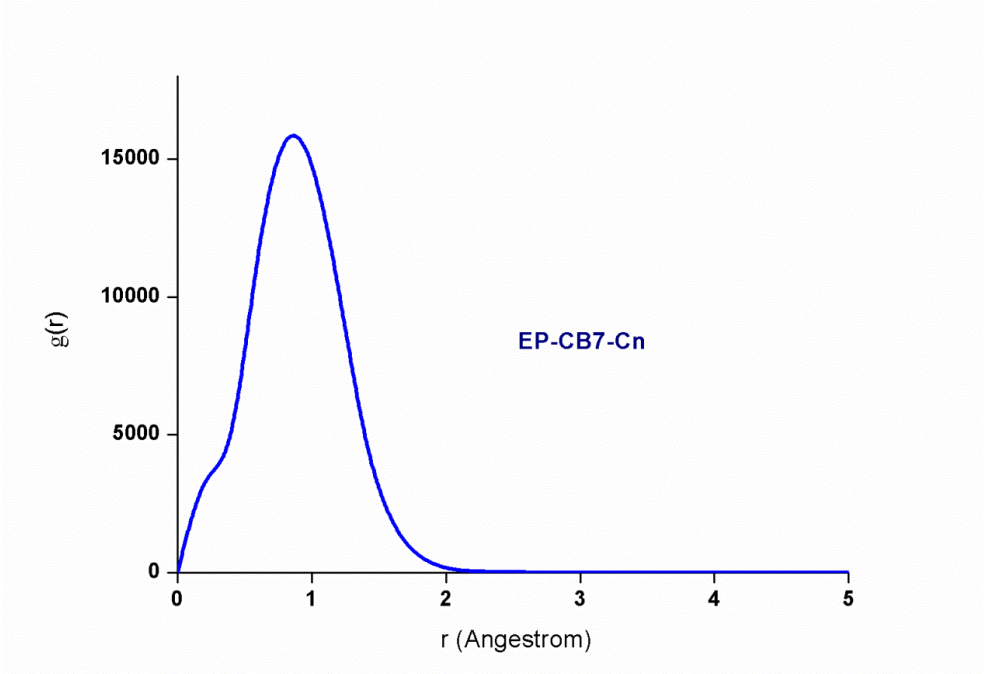


Figure S10 The RDF of center of mass of host and guest plotted as a function of separation distance *r* (Å) in EP-CB7 complex