Supplementary Materials

Metadynamics supports molecular dynamics simulation-based binding affinities of eucalyptol and beta-cyclodextrins inclusion complexes

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Figure Caption

Fig. S1 RMSD plots of all atoms in the inclusion complex for the five eucalyptol/βCDs: (a-b) eucalyptol/βCD, (c-d) eucalyptol/2,6-DMβCD, (e-f) eucalyptol/2-HPβCD, (g-h) eucalyptol/6-HPβCD and (i-j) eucalyptol/2,6-DHPβCD obtained from the other two independent simulations**.**

Fig. S2 Distances between the centers of mass of eucalyptol and the CD molecules in (a-b) eucalyptol/βCD, (c-d) eucalyptol/2,6-DMβCD, (e-f) eucalyptol/2-HPβCD, (g-h) eucalyptol/6-HPβCD and (i-j) eucalyptol/2,6-DHPβCD inclusion complexes obtained from the other two independent simulations**.**

Fig. S3 The distributions of (a) the intramolecular hydrogen bond distances, $O3_{(n)}$−$O2_{(n+1)}$, and (b) the distances between the adjacent glycosidic oxygens, $O4_{(n)}$−$O4_{(n+1)}$, of βCDs in ligand bound form.

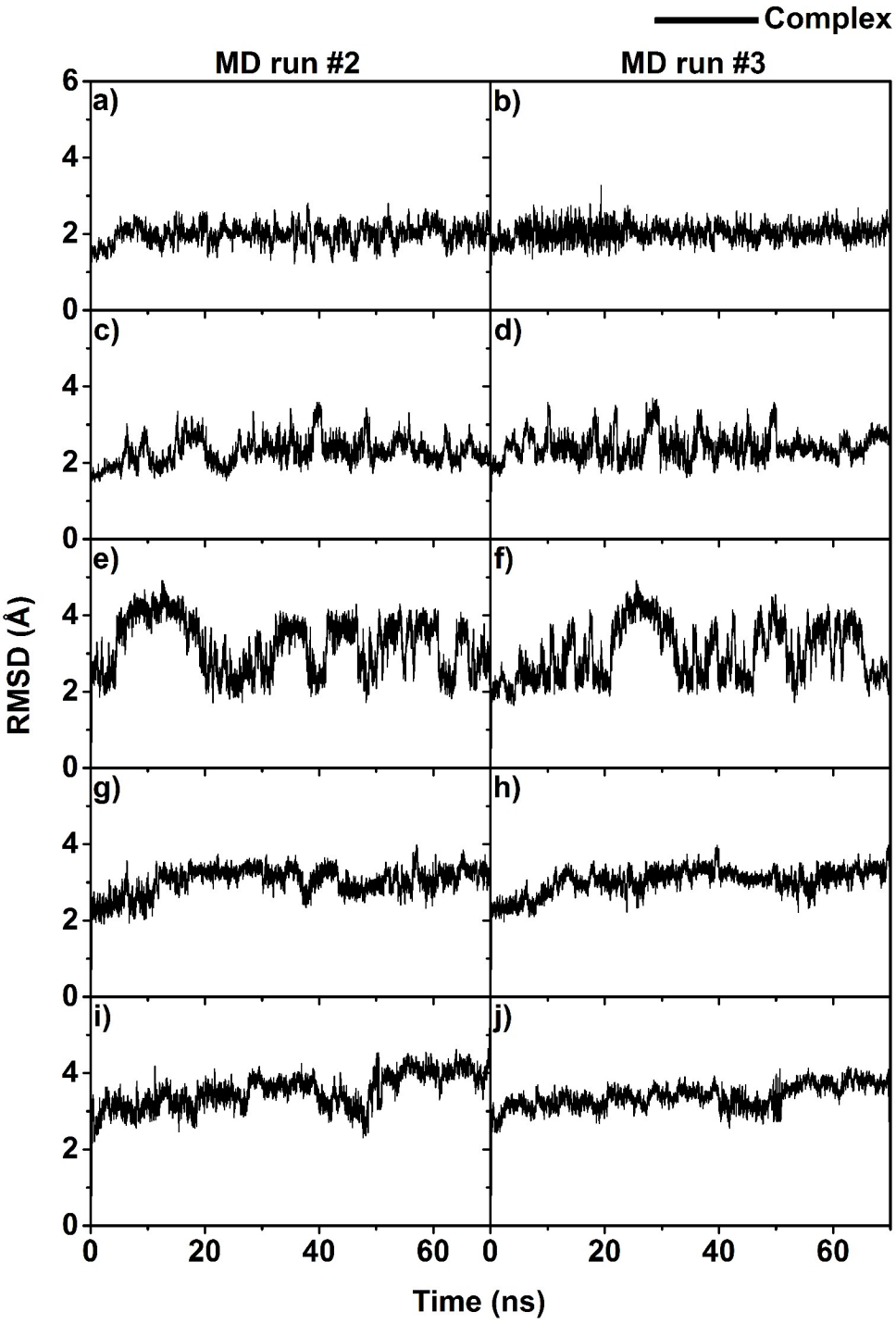
Complex
MD run #2
MD run #3
a)
b)
c)
d)
e)
f)
g)
h)
i)
j)
RMSD (Å)
Time (ns)
0
2
4
6
0
20
40
60

Figure S1

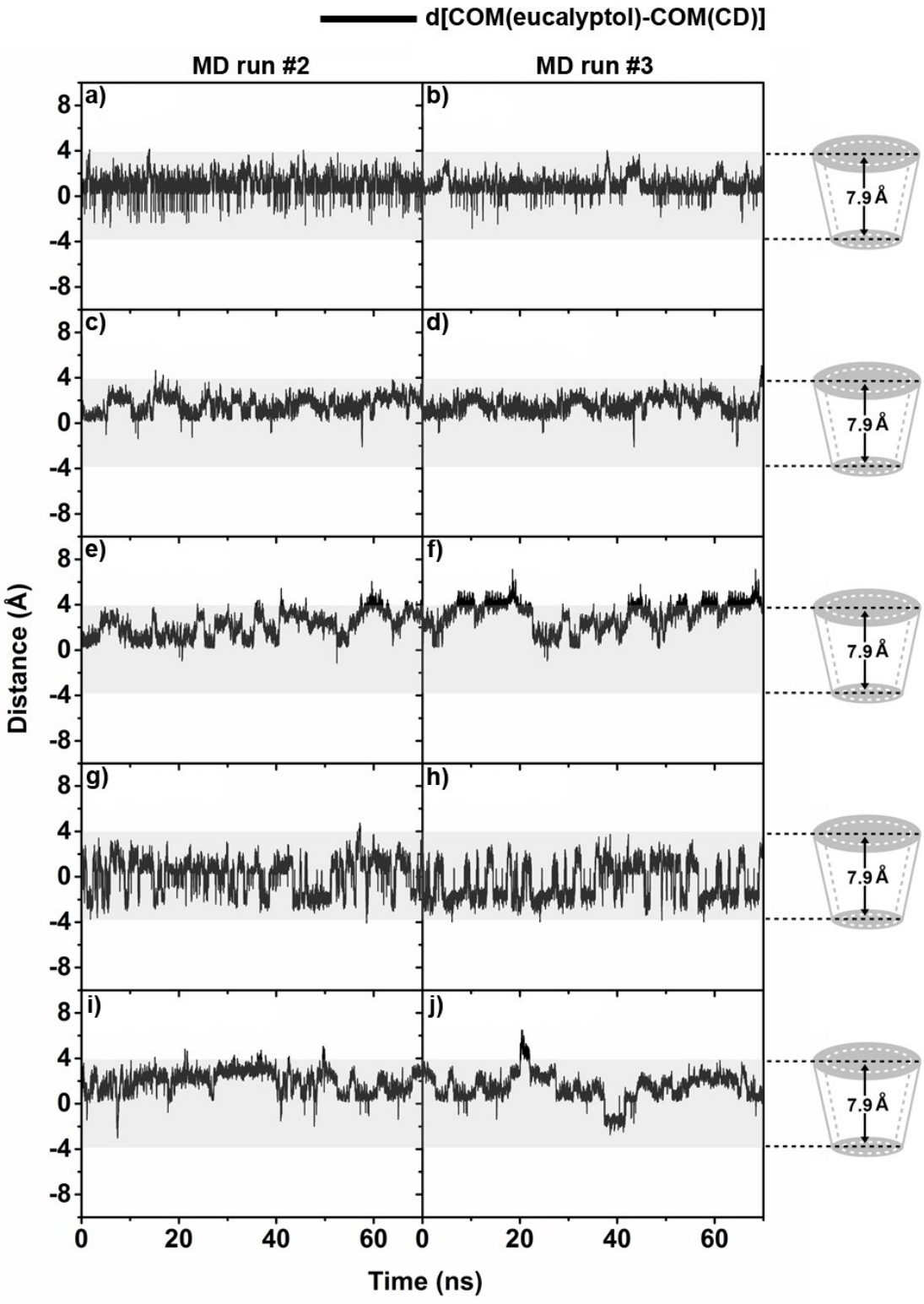
d[COM(eucalyptol)-COM(CD)]
MD run #2
MD run #3
a)
b)
c)
d)
e)
f)
g)
h)
i)
j)
8
4
0
-4
-8
7.9 Å
Distance (Å)
0
20
40
60
Time (ns)

Figure S2

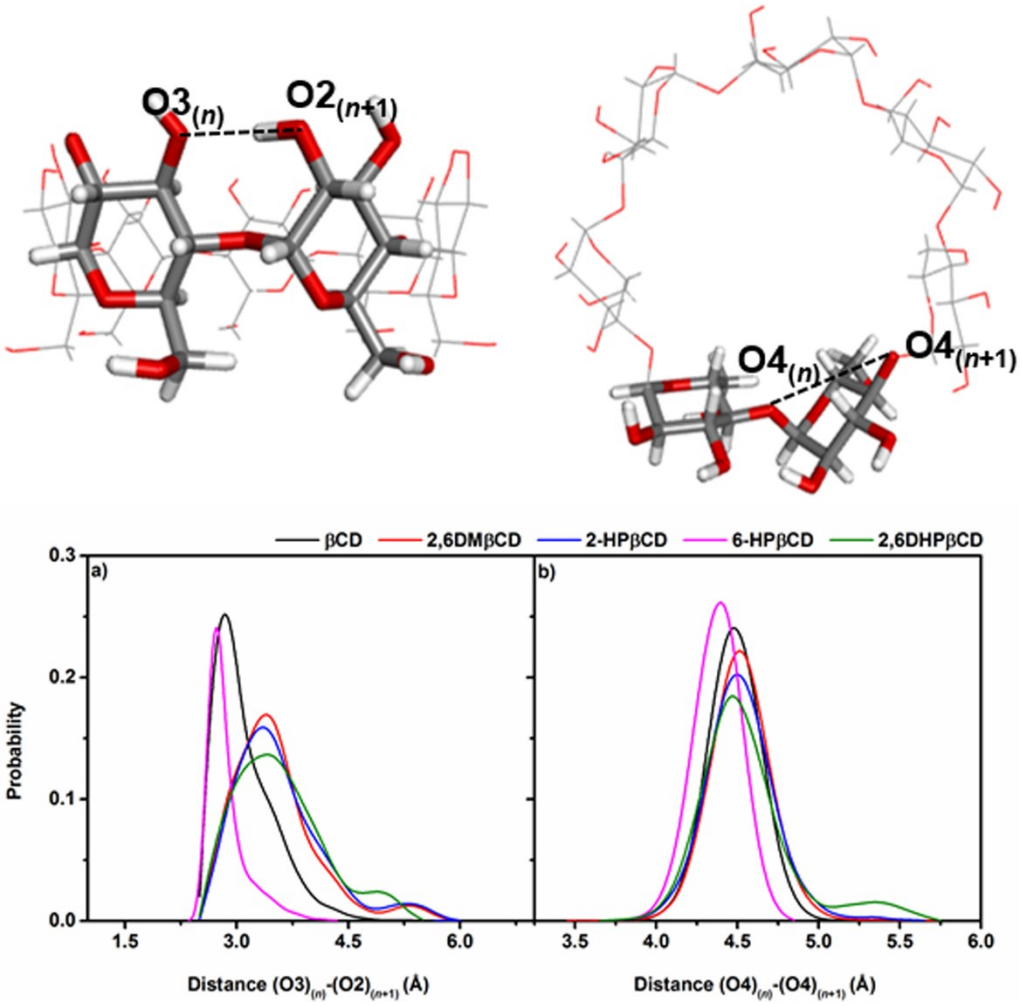
O3(n)
O2(n+1)
O4(n)
O4(n+1)
βCD
2,6DMβCD
2-HPβCD
6-HPβCD
2,6DHPβCD
a)
b)
Probability
0.0
0.1
0.2
0.3
1.5
3.0
4.5
6.0
3.5
4.0
4.5
5.0
5.5
6.0
Distance (O3)(n)-(O2)(n+1) (Å)
Distance (O4)(n)-(O4)(n+1) (Å)

Figure S3