Supporting Information

Molecular Dynamics Investigations of An Indicator Displacement Assay

Mechanism in Liquid Crystal Sensor

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1. **Snapshot of β-CD/SDS inclusion complex calculated using QM/MM MD method.**

2. **The end-to-end distance distribution of SDS in bulk water and in β-CD.**

3. **Hydrogen bond occupancy analysis for β-CD/SDS complex with SHAKE. algorithm not applied to maintain all covalent bonds involving hydrogen atoms.**

4. **Distances of COMs between b-CD and molecules of MB, SDS and DA calculated at M06-2x/6-31G(d) level of theory.**
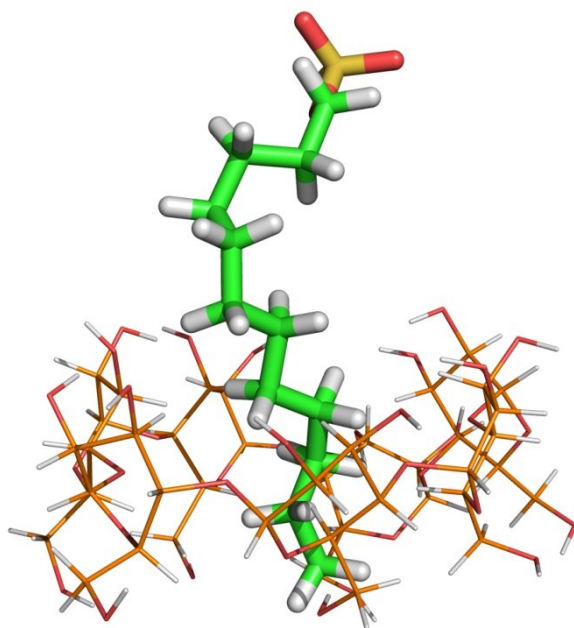
Figure S1. Snapshot of β-CD/SDS inclusion complex calculated using QM/MM MD method. For better view, all water molecules are not shown here.
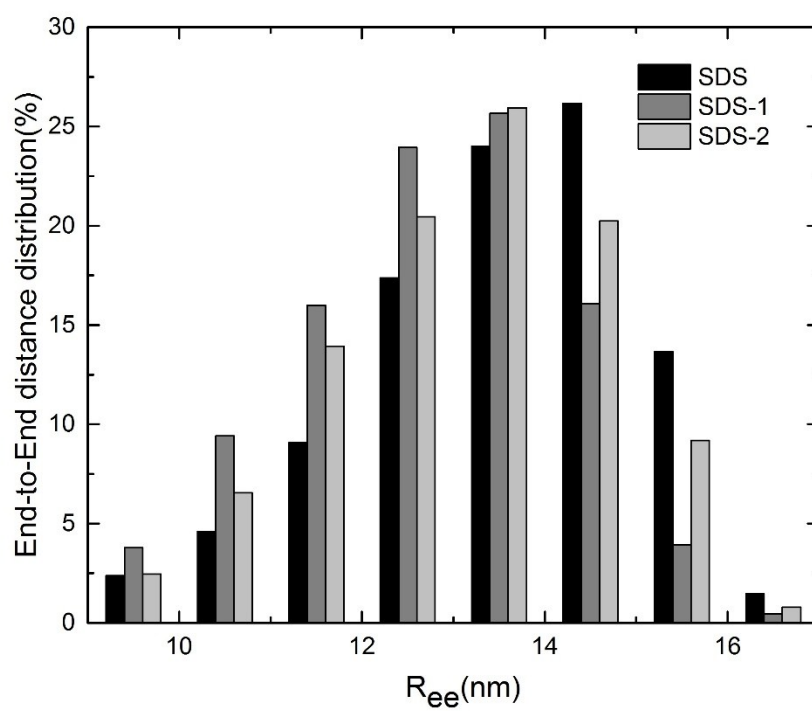
Figure S2. The end-to-end distance distribution of SDS in bulk water and in β-CD.

Table S1. Hydrogen bond occupancy analysis between β-CD and SDS-1*

H-Bond	Percentage (%)**
SDS@O2···β-CD-6@O2	11.80
SDS@O1···β-CD-6@O3	11.26
SDS@O2···β-CD-5@O3	11.20
SDS@O3···β-CD-7@O2	10.76
SDS@O2···β-CD-7@O2	9.76
SDS@O2···β-CD-6@O3	9.54
SDS@O1···β-CD-7@O2	8.66
SDS@O3···β-CD-6@O3	6.84

*SHAKE algorithm was not applied to maintain all covalent bonds involving hydrogen atoms for the SDS/β-CD inclusion complex.

**The occupancy percentage of the specific hydrogen bonds formation during the investigated time period (5 ns). The hydrogen bond is considered to be formed when the distance between acceptor and donor atoms is less than 3.0 Å and the acceptor···H-donor angle is greater than 135°.

Table S2. Distances of COMs of β-CD and MB, SDS, and DA calculated using M06-2X/6-31G(d) level of theory. For comparison, the average values extracted from MD simulation are also included.

	MB	SDS-1	SDS-2	DA-1	DA-2
MD	1.15±0.62	2.58±1.05	3.32±1.35	1.78±1.02	1.01±0.46
DFT	0.99	2.28	2.18	0.95	0.81