Supplementary Information

Computational Study of Multicharged Cyclodextrin Derivatives with Deep Cavities for High-Affinity Host-Guest Recognition

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Table S1 Summary of Vina docking scores for the twelve host–guest complexes.

Complexes	Vina docking scores (kJ/mol)
ROC@SUG	-24.26
ROC@ADA	-31.11
PAR@host 1	-17.73
PAR@host 2	-23.31
ROC@host 3	-30.84
ROC@host 4	-31.87
ROC@host 5	-32.00
ROC@host 6	-32.63
SIM@host 7	-19.18
LID@host 2	-18.87
NEO@host 2	-22.04
EDR@host 2	-19.46

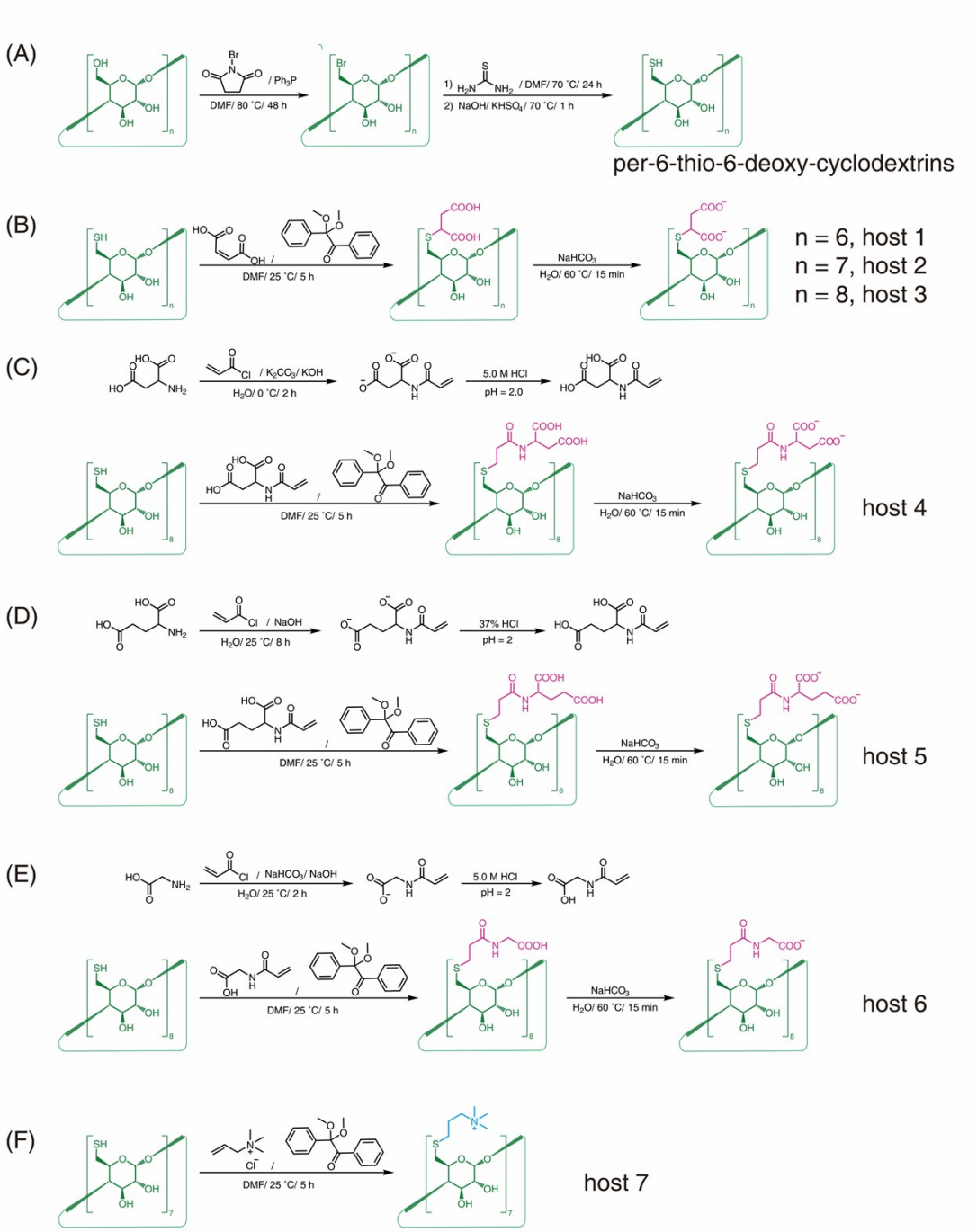

Fig. S1 Schematic diagrams of all possible synthetic routes for the hosts. Among them, (A) represents the synthesis of the intermediate product of per-6-thio-6-deoxy-cyclodextrins, where n can be 6, 7, or 8, and (B-F) represent the synthetic routes of host 1-7.

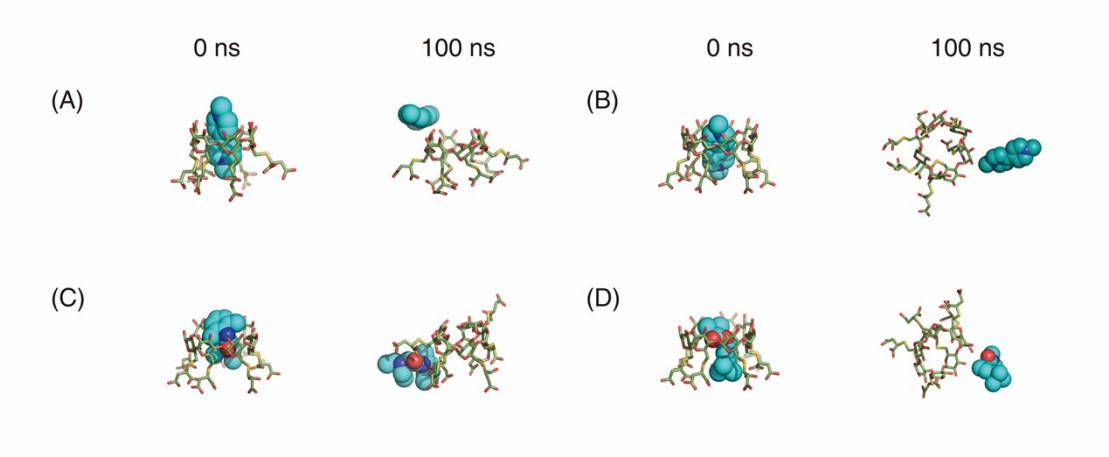

Fig. S2 Initial (0 ns) and post-simulation (100 ns) binding conformations of the four unstable complexes, where (A-D) correspond to PAR@host 1, PAR@host 2, LID@host 2, and NEO@host 2 complexes, respectively.

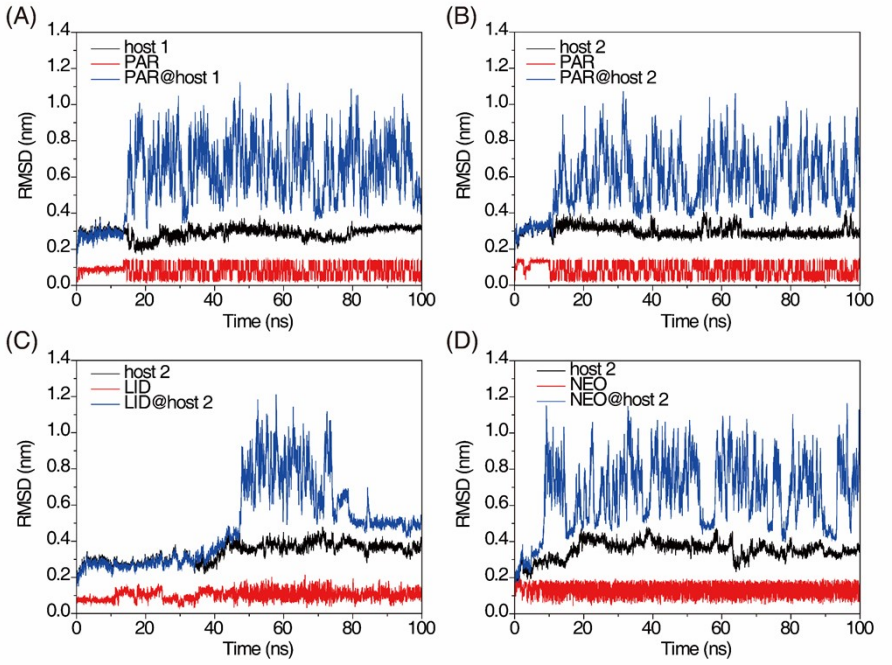

Fig. S3 Changes in the root mean square deviation (RMSD) of all unstable host-guest complexes over time.

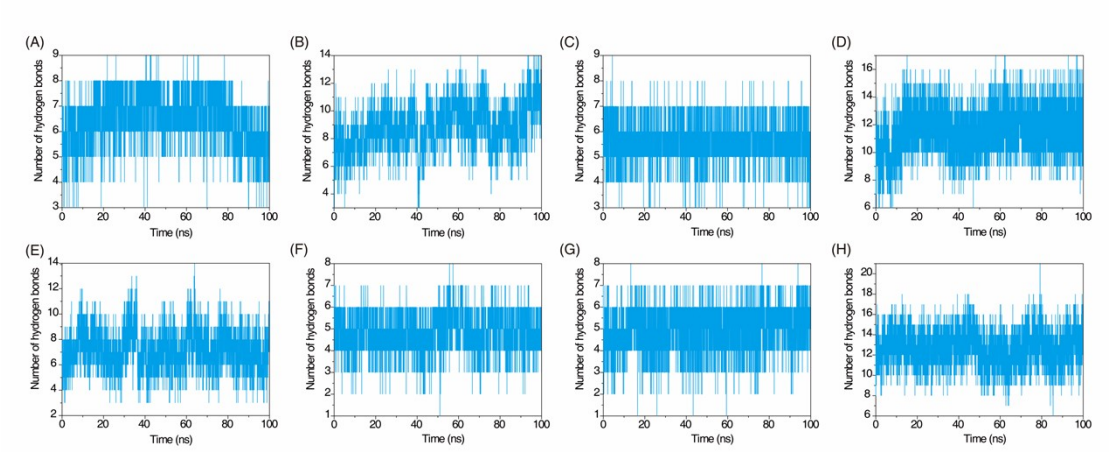

Fig. S4 The variation of the number of intramolecular hydrogen bonds in the hosts of the eight complexes over time. (A-H) correspond to ROC, ADA, host 3, host 4, host 6, host 7, host 2, and host 5, respectively.

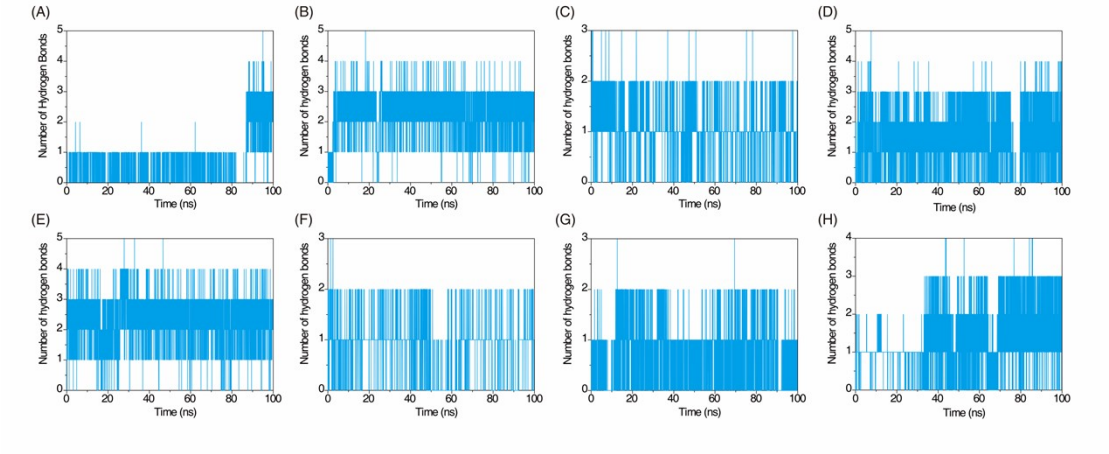

Fig. S5 The variation of the number of hydrogen bonds between the host and guest molecules in eight complexes over time. (A-H) represent ROC@SUG, ROC@ADA, ROC@host 3, ROC@host 4, ROC@host 6, SIM@host 7, EDR@host 2, and ROC@host 5, respectively.

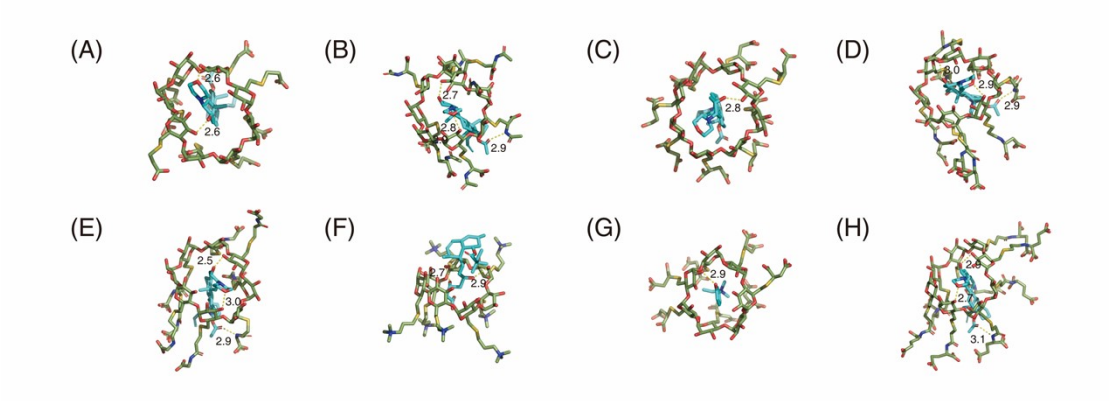

Fig. S6 Three-dimensional structures of all host–guest complexes with hydrogen bonds (yellow dashed lines) and distances (Å) indicated. (A-H) represent ROC@SUG, ROC@ADA, ROC@host 3, ROC@host 4, ROC@host 6, SIM@host 7, EDR@host 2, and ROC@host 5, respectively.