Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Exploration on the Drug Solubility Enhancement in Aqueous Medium with the Help of Endo-Functionalized Molecular Tubes: A Computational Approach

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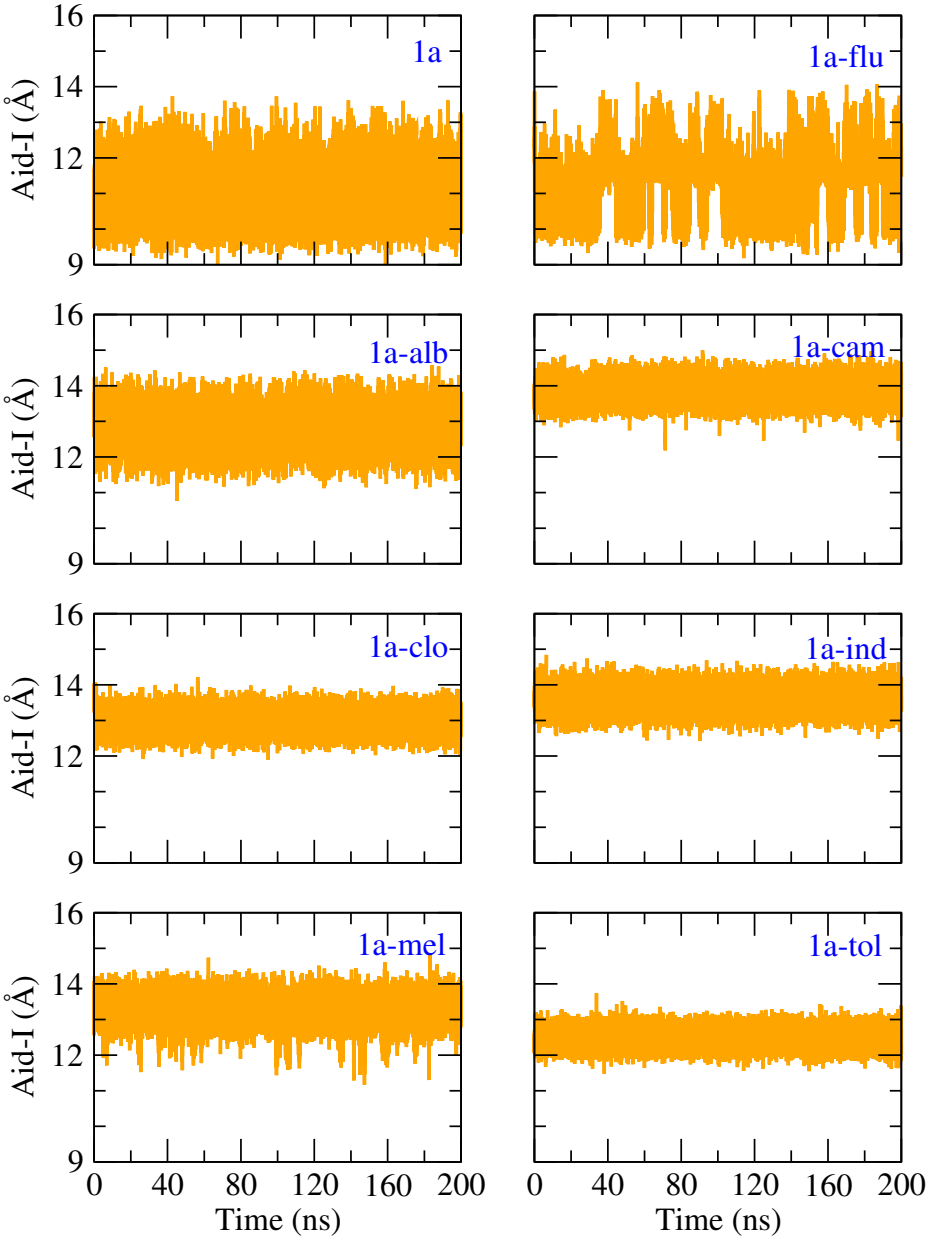

FIG. S1: Diameter-I (Aid-I) of host-1a as a function of simulation time of all the systems.

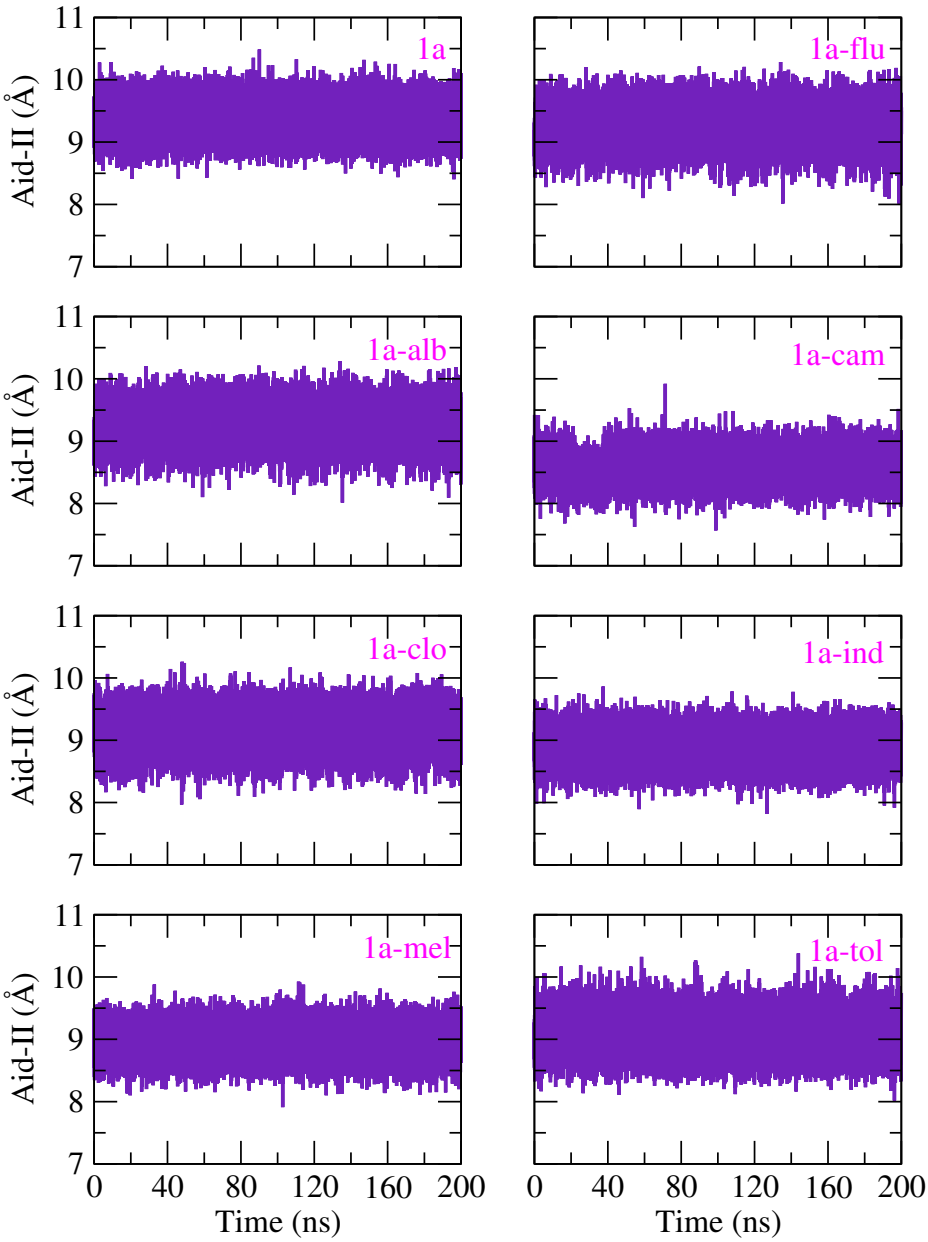

FIG. S2: Diameter-II (Aid-II) of host-1a as a function of simulation time of all the systems.

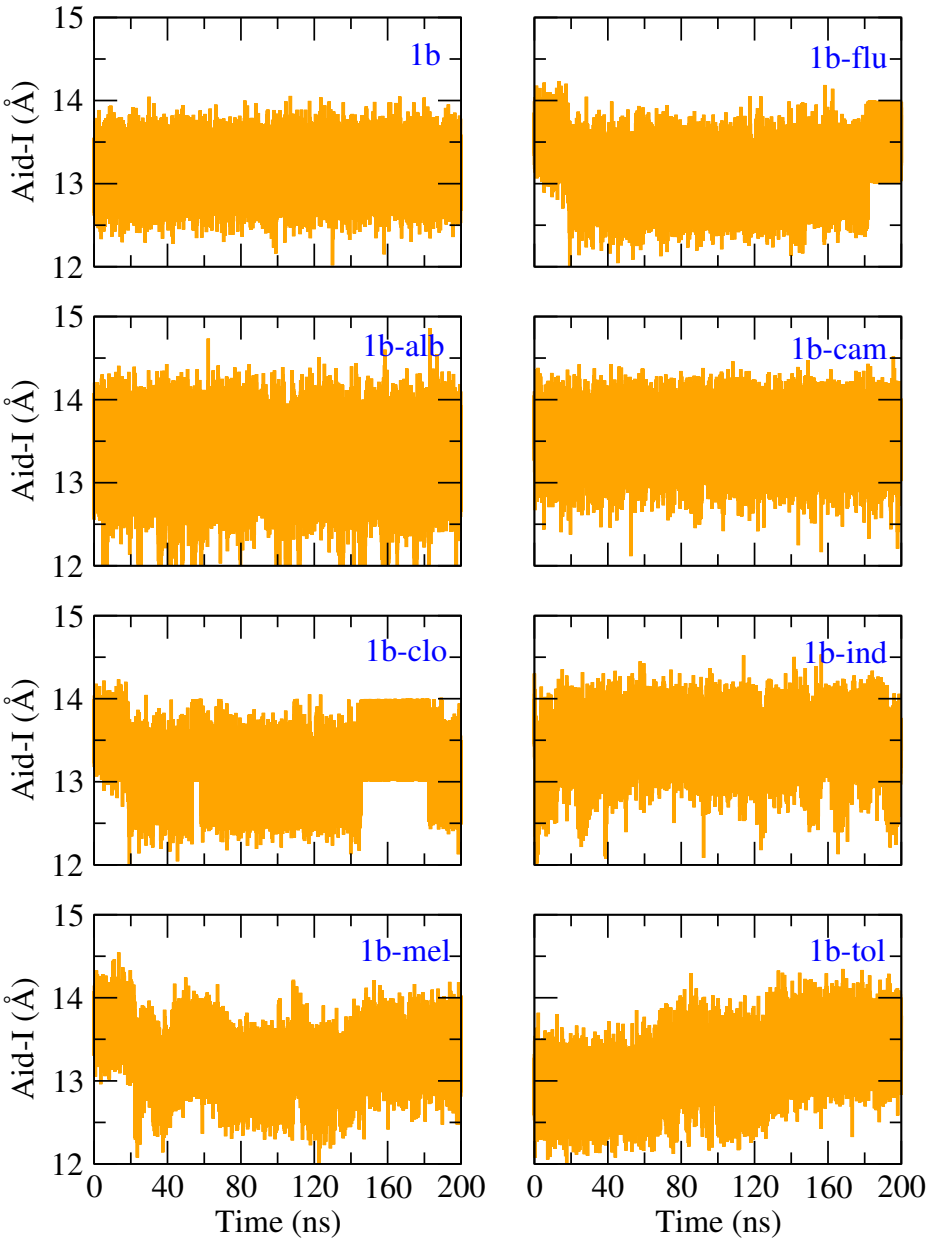

FIG. S3: Diameter-I (Aid-I) of host-1b as a function of simulation time of all the systems.

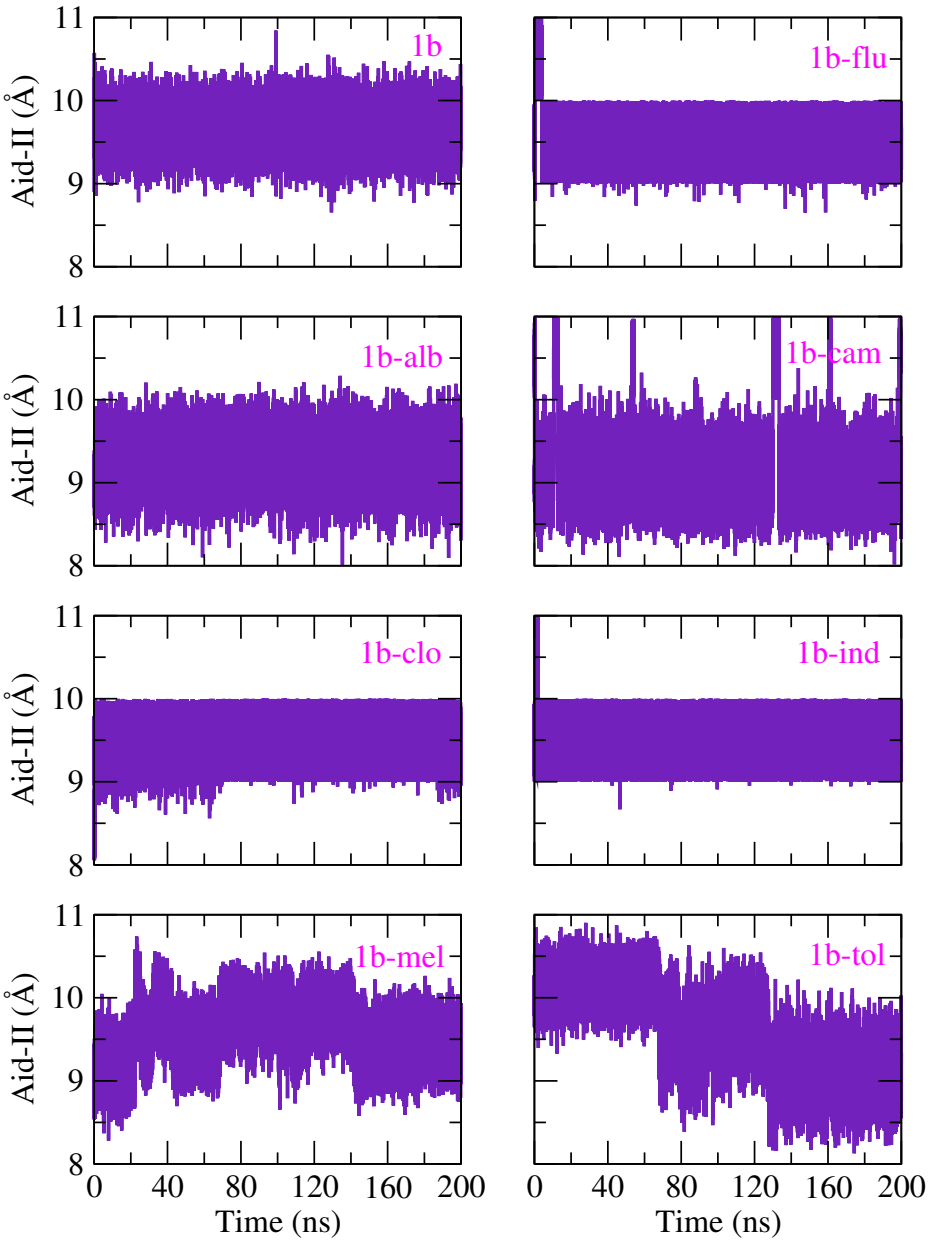

FIG. S4: Diameter-II (Aid-II) of host-1b as a function of simulation time of all the systems.

TABLE S1: Partial charges of all the atomic sites of the fluorouracil drug molecule. e is the elementary charge.

Fluorouracil			
Atom	Charge (e)	Atom	Charge (e)
C1	0.7874	C2	0.0703
N7	-0.6750	F9	-0.2015
C4	0.8568	C3	-0.0721
O11	-0.6462	H12	0.2305
H5	0.3937	N6	-0.5375
O8	-0.5912	H10	0.3848

TABLE S2: Partial charges of all the atomic sites of the albendazole drug molecule. e is the elementary charge.

Albendazole			
Atom	Charge (e)	Atom	Charge (e)
N4	-0.7675	S1	-0.3095
C12	1.0687	C20	-0.1676
N5	-0.8007	H21, H22	0.0716
N6	-1.0461	C23	0.3594
C14	1.2086	H24, H25	-0.0647
O2	-0.4316	C26	-0.1721
C30	-0.1089	H27, H28, H29	0.0353
H31, H32, H33	0.1155	H15	0.1782
O3	-0.7352	C8	0.4166
H19	0.4484	C11	-0.3531
H16	0.5054	H17	0.2244
C7	0.1115	C13	-0.2315
C10	-0.2334	H18	0.1727
C9	0.1970		

TABLE S3: Partial charges of all the atomic sites of the camptothecin drug molecule. e is the elementary charge.

Camptothecin			
Atom	Charge (e)	Atom	Charge (e)
C11	0.0154	H40, H41, H42	0.0748
N5	-0.1692	H27	0.2444
C9	0.0816	C14	0.5157
C12	-0.4140	N6	-0.7053
C8	0.1328	H25, H26	0.1131
C7	0.2674	C13	-0.1683
O2	-0.6703	C18	-0.2131
H30	0.4347	H29	0.2028
C17	0.7466	C19	-0.0118
O1	-0.4773	C21	-0.2147
C16	0.2255	C23	-0.1868
C10	-0.2387	H33	0.1663
C15	0.6393	H31	0.1652
O3	-0.6783	C20	0.6009
H28, H35	0.0716	C22	-0.3669
O4	-0.6013	H32	0.2017
C36	0.0975	C24	-0.0957
H37, H38	-0.0065	H34	0.1561
C39	-0.2629		

TABLE S4: Partial charges of all the atomic sites of the clopidogrel drug molecule. e is the elementary charge.

Clopidogrel			
Atom	Charge (e)	Atom	Charge (e)
N5	-0.0593	O3	-0.3669
C6	-0.4245	C21	-0.1299
C9	0.0941	H28, H36, H37	0.1118
C11	-0.1573	O4	-0.6146
S2	-0.0526	H35	0.1719
C15	-0.2011	C12	0.4159
C13	-0.4434	C17	-0.3234
C10	0.3733	C19	-0.0939
C7	-0.3412	H26	0.1524
H33, H34	0.1488	H24	0.1723
H22	0.2220	C16	-0.1636
H23	0.2347	Cl1	-0.1010
H29, H30	0.0631	C18	-0.0141
H31, H32	0.1768	H25	0.1329
C8	-0.4118	C20	-0.2603
C14	0.9012	H27	0.1757

TABLE S5: Partial charges of all the atomic sites of the indomethacin drug molecule. e is the elementary charge.

Indomethacin			
Atom	Charge (e)	Atom	Charge (e)
O3	-0.5671	C25	0.0418
C15	0.9159	H36, H37, H41	0.0549
N6	-0.4466	C17	-0.2333
C9	0.2449	C13	-0.3535
C8	0.1174	H29	0.2182
C7	-0.3357	H32	0.2020
C10	0.2542	H28	0.2214
C14	-0.2909	C18	-0.3199
H30, H31, H39	0.1064	C21	-0.0516
C11	0.0204	C23	-0.0654
C19	0.8856	H35	0.1322
O4	-0.7404	H33	0.1262
H38	0.4777	C20	-0.0516
O5	-0.6323	H40	0.1262
H26, H27	0.0478	C22	-0.0654
C12	-0.3541	H34	0.1322
C16	0.3285	C24	0.0013
O2	-0.4145	Cl1	-0.1029

TABLE S6: Partial charges of all the atomic sites of the melphalan drug molecule. e is the elementary charge.

Melphalan			
Atom	Charge (e)	Atom	Charge (e)
N5	-0.1862	C11	0.6896
C9	-0.2840	C18	0.6256
C16	-0.2445	O3	-0.7339
Cl1	-0.1873	H31	0.5043
H28, H29	0.1888	O4	-0.5886
H20, H21	0.1860	H34	-0.0027
C10	-0.2840	N35	-1.0242
C17	-0.2445	H36, H37	0.3750
Cl2	-0.1873	H19, H33	0.2200
H30, H32	0.1888	H27	0.1918
H22, H23	0.1860	H24, H25	0.2431
C6	0.3352	C12	-0.3403
C13	-0.3403	C7	-0.8721
C15	-0.3703	C14	-0.3703
C8	0.5470	H26	0.1918

TABLE S7: Partial charges of all the atomic sites of the tolfenamic acid drug molecule. e is the elementary charge.

Tolfenamic acid			
Atom	Charge (e)	Atom	Charge (e)
N4	-0.9493	O3	-0.6179
C6	0.7531	H17	0.4820
C7	-0.4953	C5	0.2579
C13	-0.0102	C30	0.2876
C15	-0.3774	C9	-0.1587
C14	0.0465	Cl1	-0.0986
C10	-0.4551	C26	-0.3754
H19	0.1850	H27, H28, H29	0.1167
H23	0.1428	C8	-0.1918
H24	0.1837	H18	0.1795
H22	0.1513	C11	-0.2676
C16	0.9141	H20	0.1863
O2	-0.6397	C12	-0.0479
H25	0.4166	H21	0.1483

TABLE S8: Descriptions of all the randomly packed systems used for this work. N_{host} is the numbers of the host, $N_{\text{NH}_4^+}$ is the numbers of the ammonium ion, N_{drug} is the numbers of the drug molecules, and N_{wat} is the number of water molecules. The molar concentration of the host molecule is represented by M_{host}. Host-1a and host-1b are represented by 1a and 1b, respectively. 1a-cam-ran, 1b-clo-ran, etc., is the systems of host-1a and host-1b with the drug cam, clo respectively, etc. These systems with the 'ran' terms created by randomly packed the drug molecule inside the simulation box.

System	N_{host}	$N_{\text{NH}_4^+}$	N_{drug}	N_{wat}	Box volume (nm^3)	M_{host} (M)
1a-flu-ran	1	4	1	5079	156.63	0.0106
1a-alb-ran	1	4	1	5617	175.03	0.0095
1a-cam-ran	1	4	1	5343	163.60	0.0107
1a-clo-ran	1	4	1	5411	169.23	0.0098
1a-ind-ran	1	4	1	5979	186.98	0.0089
1a-mel-ran	1	4	1	5616	174.98	0.0095
1a-tol-ran	1	4	1	5558	171.54	0.0098
1b-flu-ran	1	4	1	5596	172.26	0.0096
1b-alb-ran	1	4	1	5643	175.43	0.0095
1b-cam-ran	1	4	1	5338	163.61	0.0101
1b-clo-ran	1	4	1	5498	171.72	0.0097
1b-ind-ran	1	4	1	5431	170.72	0.0097
1b-mel-ran	1	4	1	5416	169.22	0.0098
1b-tol-ran	1	4	1	5264	164.53	0.0101

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