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

Supporting Information

A Computational Approach on the Stereoselective Binding of Peptides from Aqueous Medium with Endo-Functionalized Molecular Tubes

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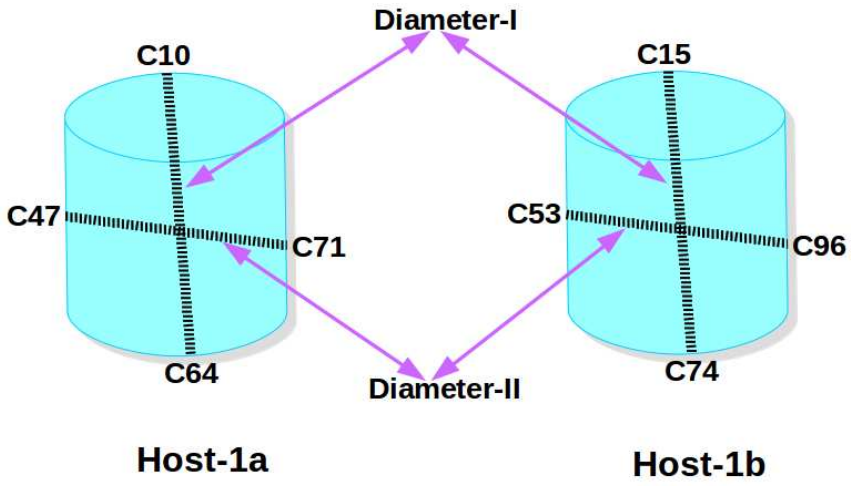

FIG. S1: Schematic representation of the two internal diameters of host-1a and host-1b are displayed as diameter-I and diameter-II.

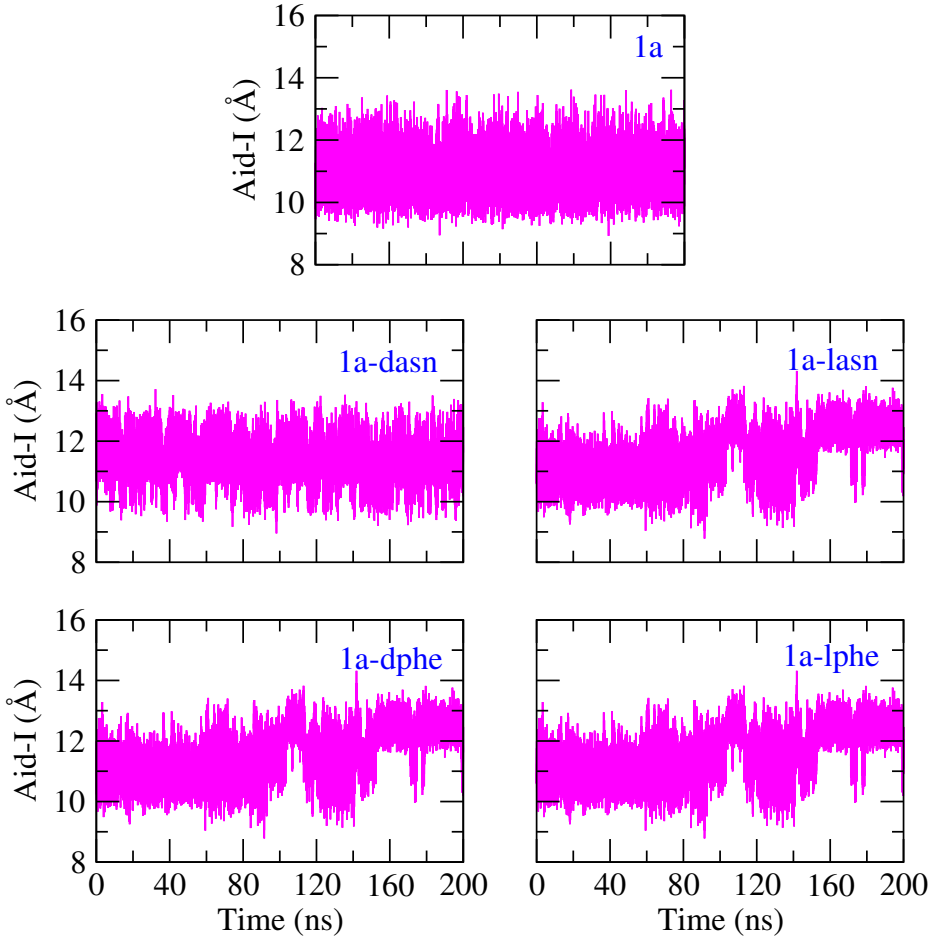

FIG. S2: Diameter-I (Aid-I) of host-1a as a function of simulation time of all the host-1a containing systems.

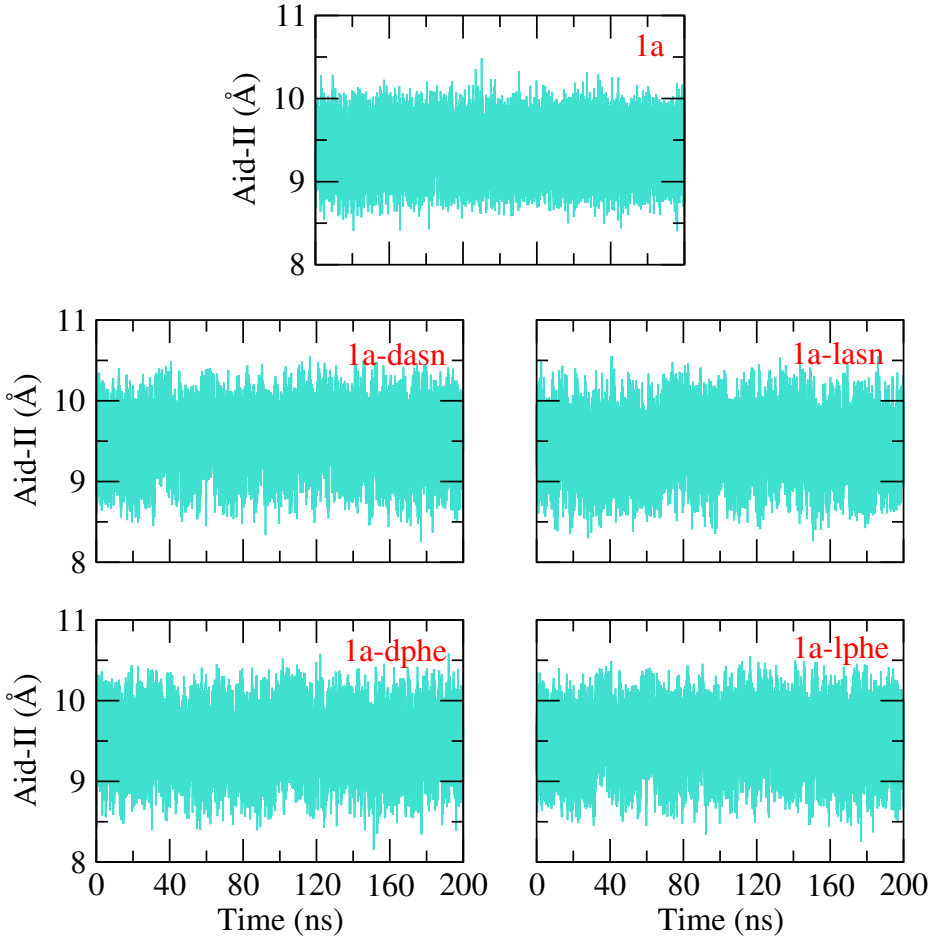

FIG. S3: Diameter-II (Aid-II) of host-1a as a function of simulation time of all the host-1a containing systems.

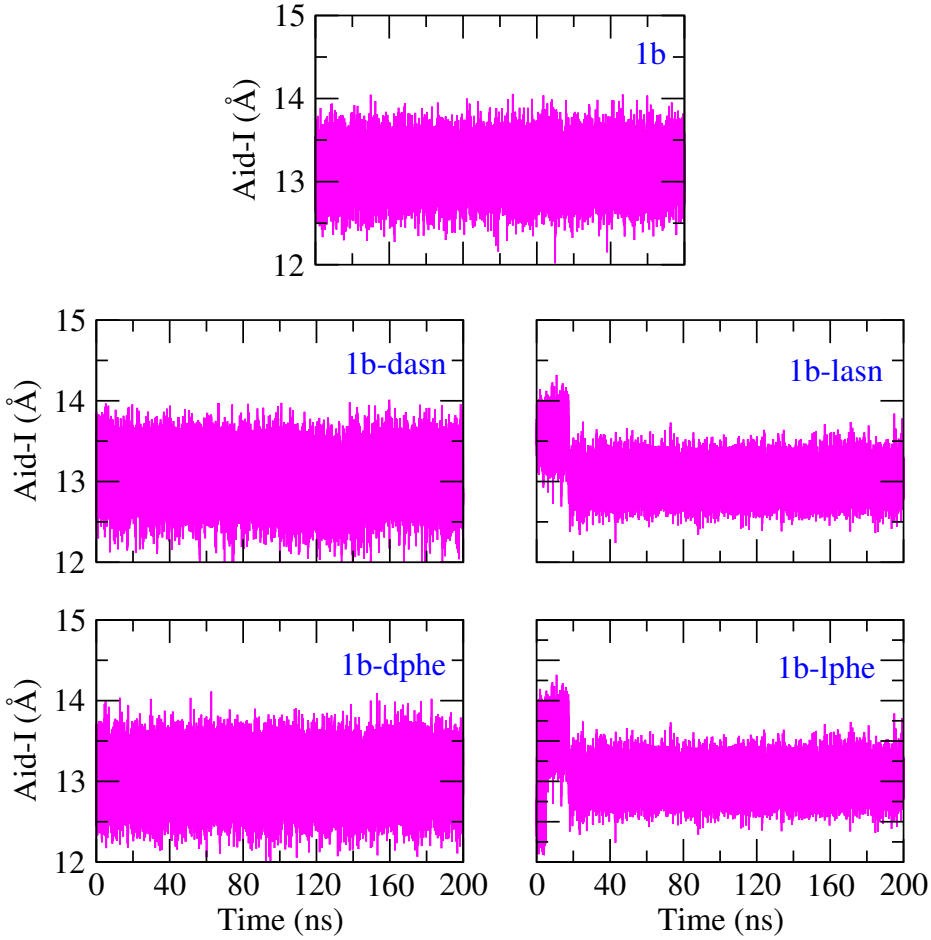

FIG. S4: Diameter-I (Aid-I) of host-1b as a function of simulation time of all the host-1b containing systems.

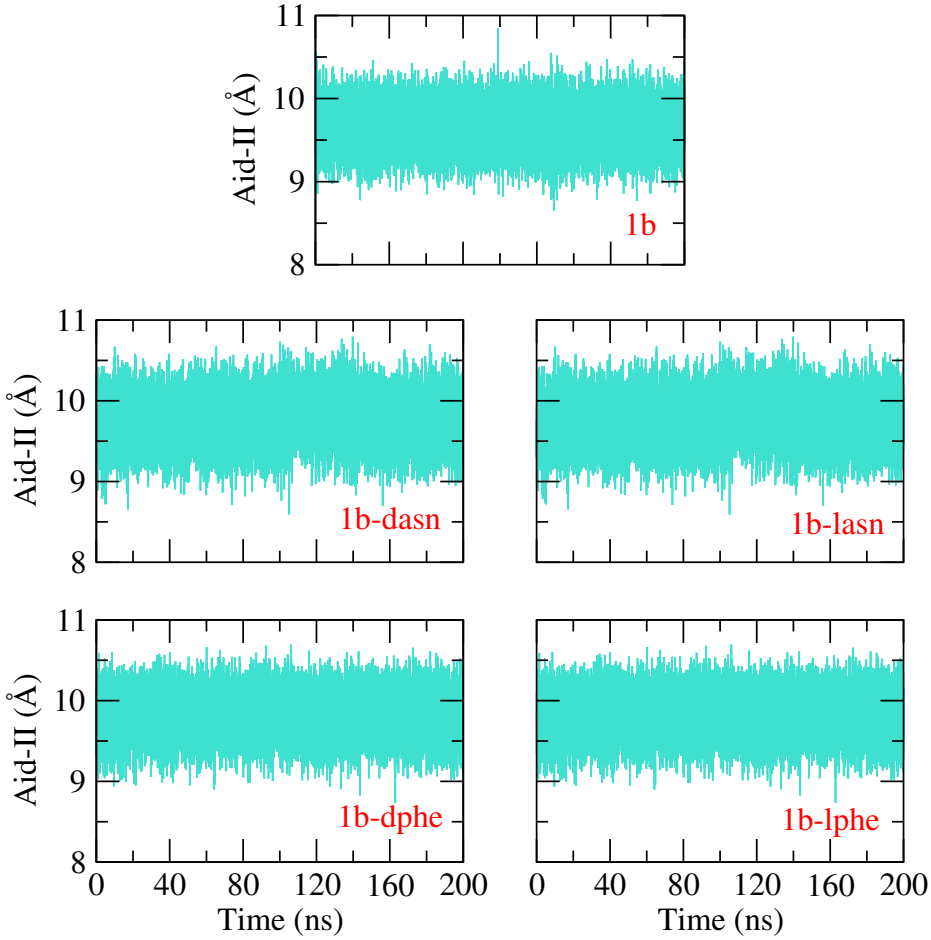

FIG. S5: Diameter-II (Aid-II) of host-1b as a function of simulation time of all the host-1b containing systems.

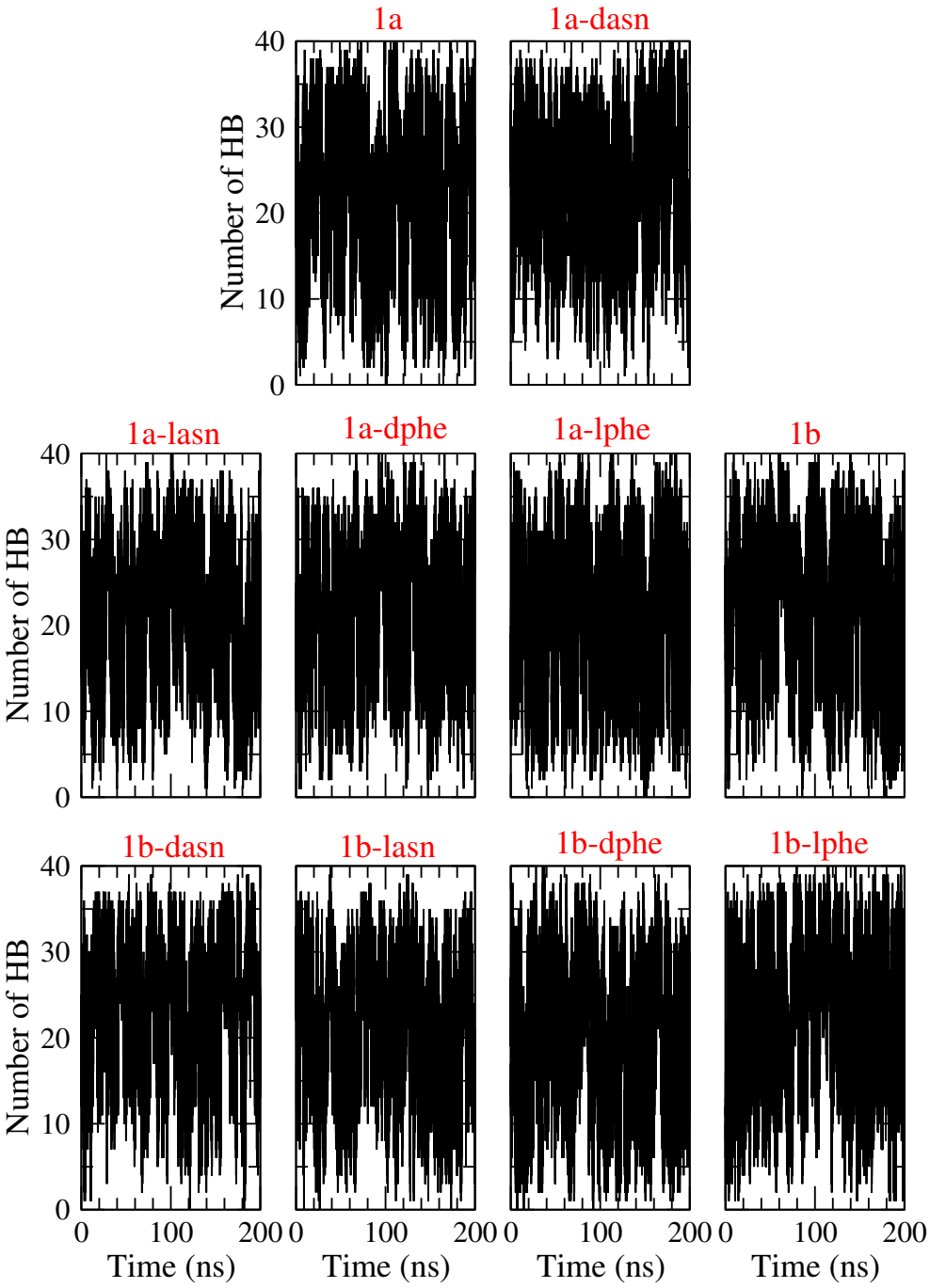

FIG. S6: Time series of the host-water hydrogen bonds of all the systems.

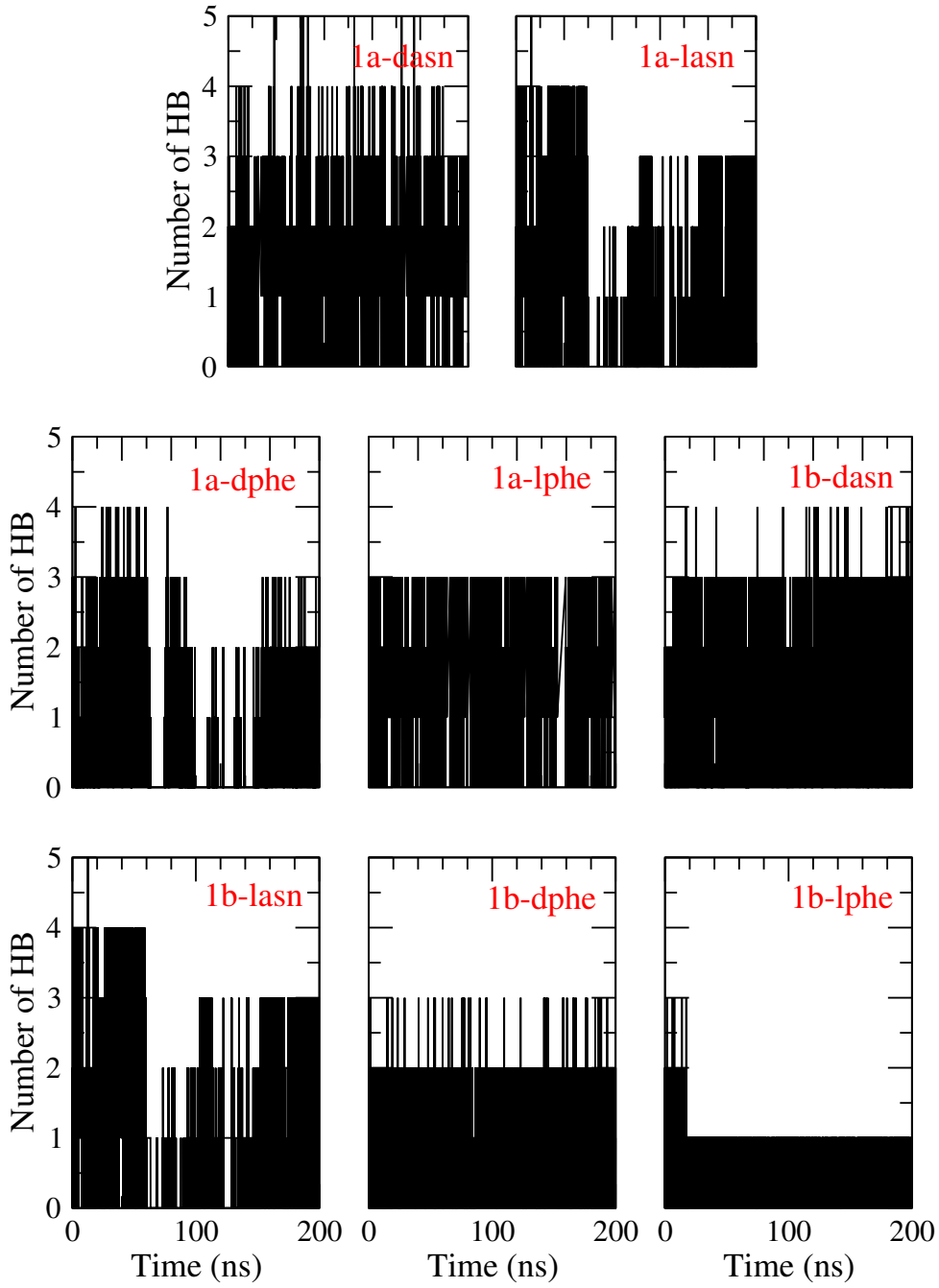

FIG. S7: Time series of the host-peptide hydrogen bonds of all the peptide containing systems.

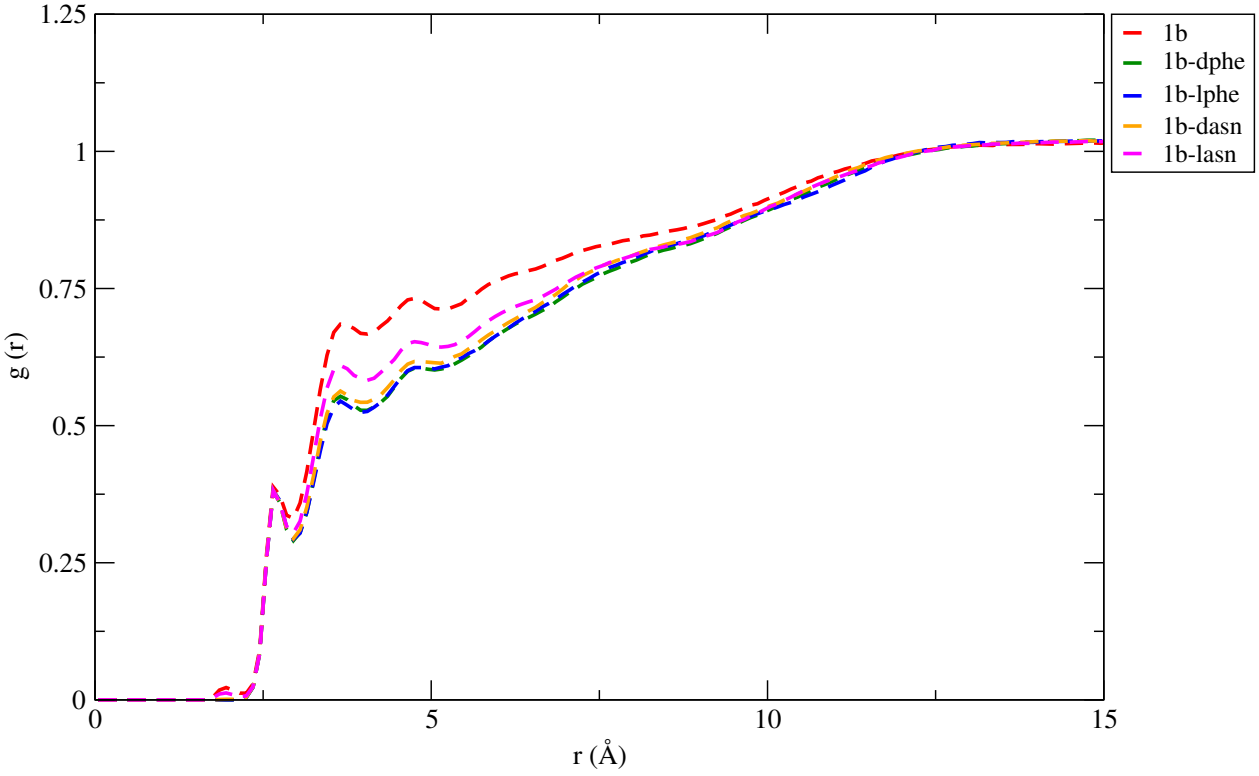

FIG. S8: Radial distribution function of water molecules with the surface of the host-1b for the systems 1b, 1b-dasn, 1b-lasn, 1b-dphe and 1b-lphe are represented here.

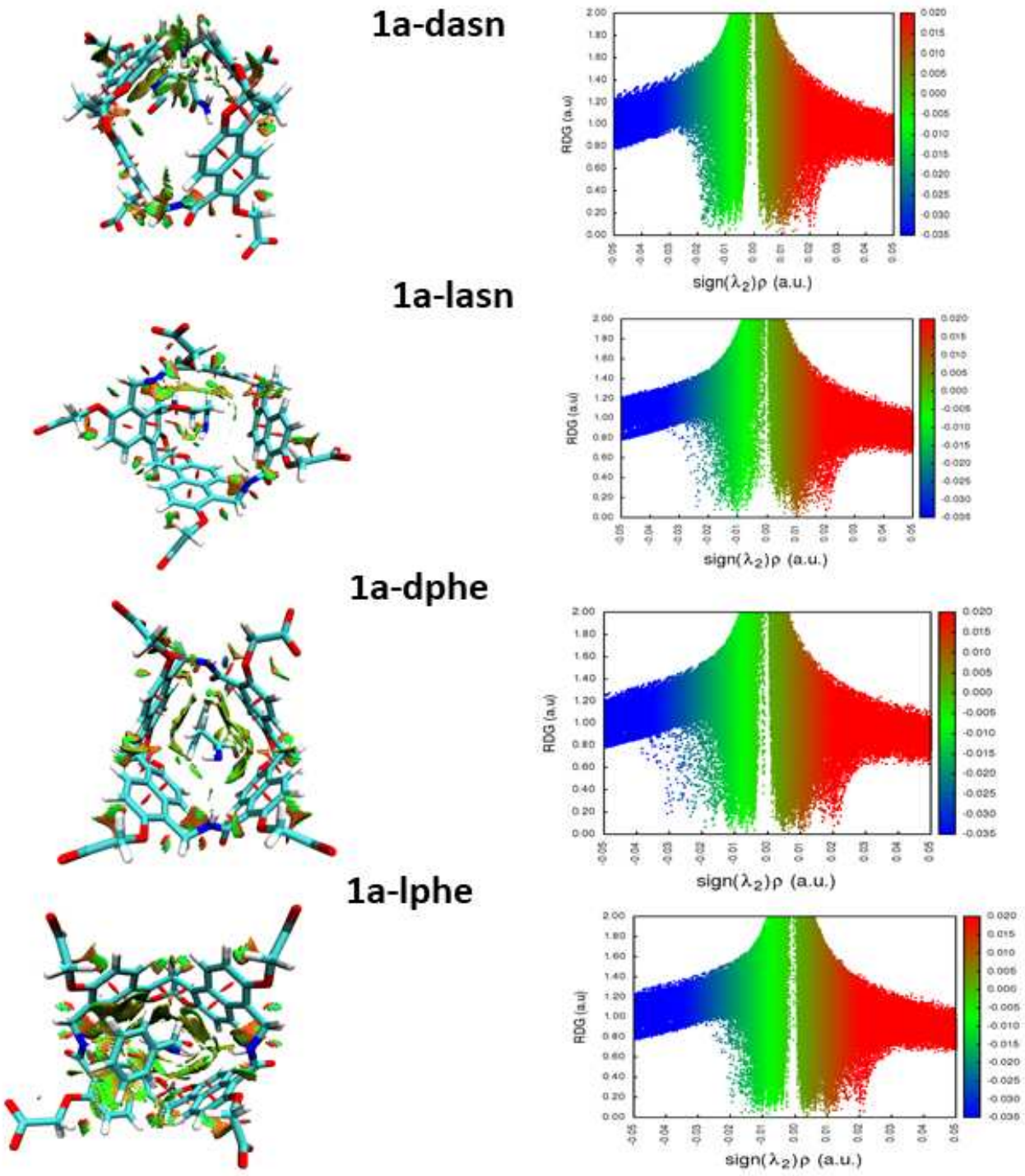

FIG. S9: Color-filled RDG isosurfaces delimitate non-covalent interaction (NCI) regions in 1a-dasn, 1a-lasn, 1a-dphe and 1a-lphe systems.

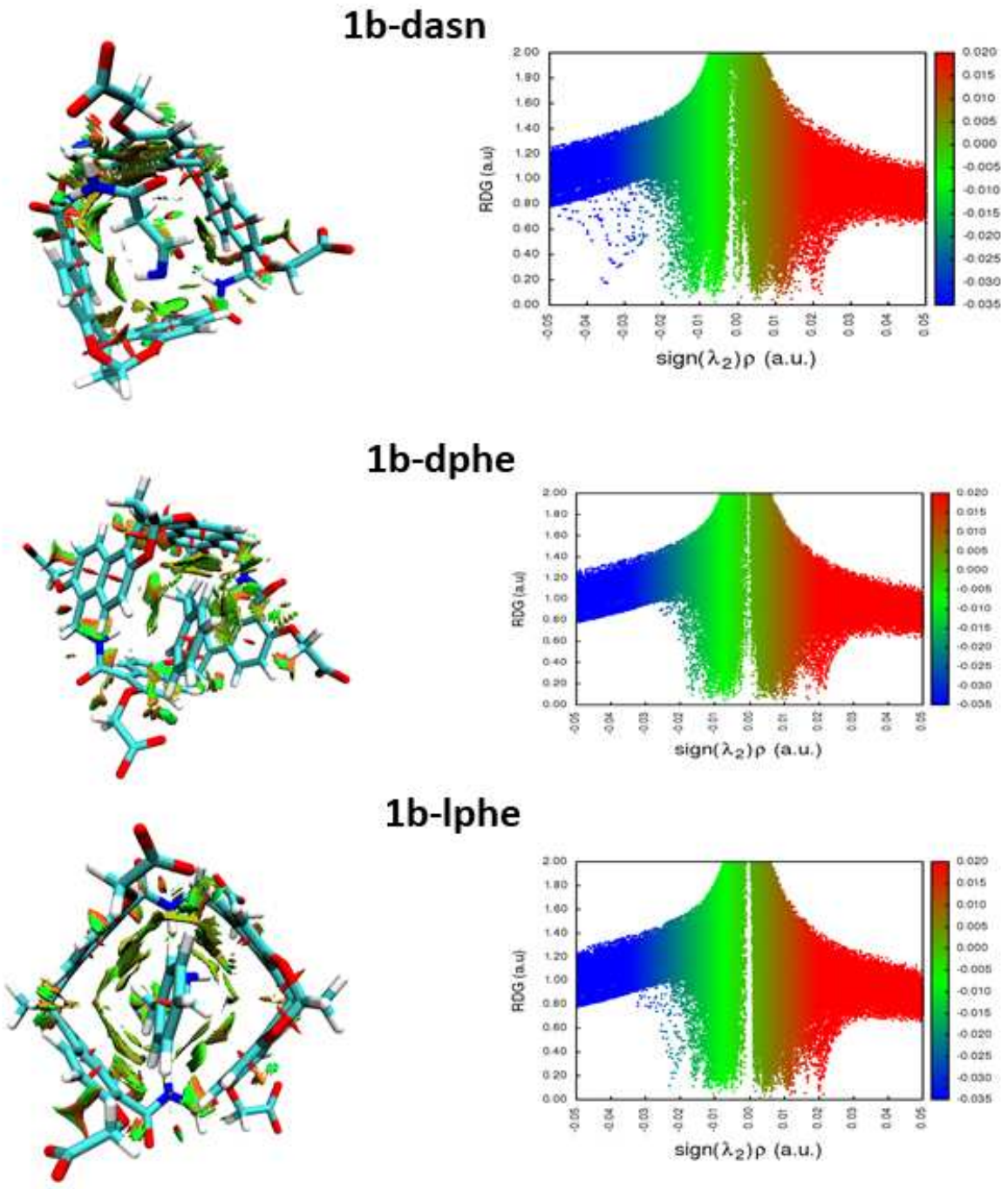

FIG. S10: Color-filled RDG isosurfaces delimitate non-covalent interaction (NCI) regions in 1b-dasn, 1b-dphe and 1b-lphe systems.

TABLE S1: Specifics of all the systems for normal MD simulation. N_{host}, $N_{\text{NH}_4^+}$, N_{pep}, and N_{wat} represent the numbers of the host molecules, ammonium ions, peptide, and water molecules, respectively. M_{host} designates the concentration of the host molecules expressed in molarity. 1a and 1b are the host-1a and host-1b, respectively. 1a-dasn, 1b-lphe, etc., are the systems having dasn, lphe, etc., as the model peptides and the receptors are host-1a and host-1b respectively. Systems 1a and 1b are pure host-water systems without any peptide molecule.

System	N_{host}	$N_{\text{NH}_4^+}$	N_{pep}	N_{wat}	Box volume (nm^3)	M_{host} (M)
1a	1	4	0	2280	70.58	0.0235
1a-dasn	1	4	1	2278	70.47	0.0236
1a-lasn	1	4	1	2279	70.48	0.0236
1a-dphe	1	4	1	2279	70.65	0.0235
1a-lphe	1	4	1	2279	70.77	0.0235
1b	1	4	0	2321	71.43	0.0232
1b-dasn	1	4	1	2320	71.69	0.0231
1b-lasn	1	4	1	2318	72.00	0.0230
1b-dphe	1	4	1	2319	71.72	0.0231
1b-lphe	1	4	1	2319	71.98	0.0230
1a-dasn-ran	1	4	1	5535	169.13	0.0098
1a-lphe-ran	1	4	1	5832	178.34	0.0093
1b-lasn-ran	1	4	1	5543	169.77	0.0098
1b-dphe-ran	1	4	1	5833	178.15	0.0093

TABLE S2: The water-water hydrogen bond distribution and the average number of hydrogen bonds per water molecule, $\langle n_{HB} \rangle$, within 5.0 Å from the surface for all the systems are presented here. The data for bulk is included for comparison.

System	f_0	f_1	f_2	f_3	f_4	f_5	f_6	$\langle n_{HB} \rangle$
bulk	0.002	0.033	0.175	0.394	0.353	0.042	0.001	3.19
1b	0.006	0.069	0.253	0.391	0.253	0.027	0.000	2.89
1b-dasn	0.006	0.067	0.247	0.395	0.256	0.028	0.000	2.91
1b-lasn	0.006	0.070	0.254	0.391	0.252	0.027	0.000	2.90
1b-dphe	0.005	0.065	0.246	0.396	0.260	0.028	0.000	2.93
1b-lphe	0.005	0.067	0.250	0.393	0.257	0.027	0.000	2.91

TABLE S3: The amplitudes a_i's and the time constants τ_i's for the tri-exponential fit of the water-water intermittent hydrogen bond time correlation functions are represented here.

System	a_1	τ_1 (ps)	a_2	τ_2 (ps)	a_3	τ_3 (ps)
bulk	0.09	15.36	0.55	2.40	0.36	0.28
1b	0.09	23.42	0.43	3.64	0.48	0.38
1b-dasn	0.10	16.54	0.42	3.75	0.48	0.39
1b-lasn	0.04	42.30	0.42	4.55	0.51	0.43
1b-dphe	0.13	13.83	0.43	3.26	0.44	0.32
1b-lphe	0.12	13.24	0.43	3.08	0.44	0.32

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