Supporting Information for

Tuning the Trapping of Epoxides by Endo-Functionalized Molecular Tubes in an Aqueous Medium: A Computational Study

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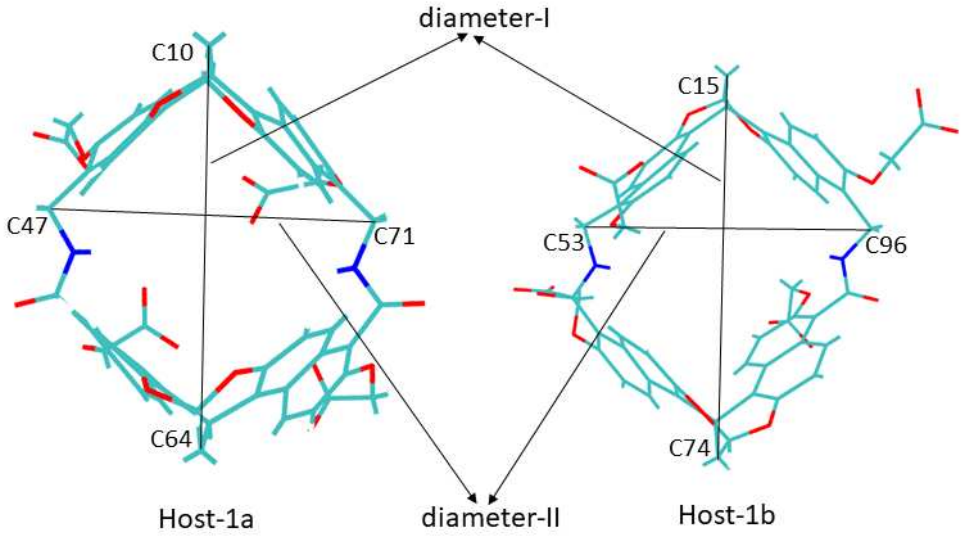

FIG. S1: Schematic representation of the two internal diameters of host-1a and host-1b are portrayed as diameter-I and diameter-II.

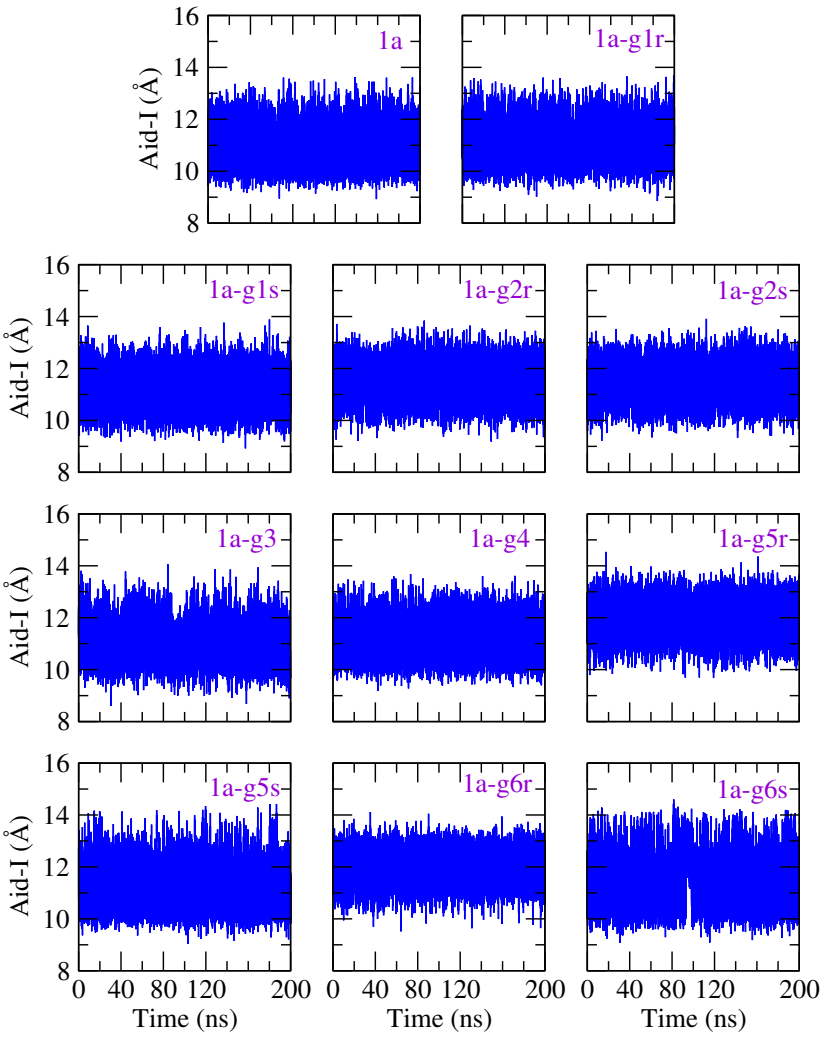

FIG. S2: Diameter-I (Aid-I) of host-1a as a function of simulation time for all systems.

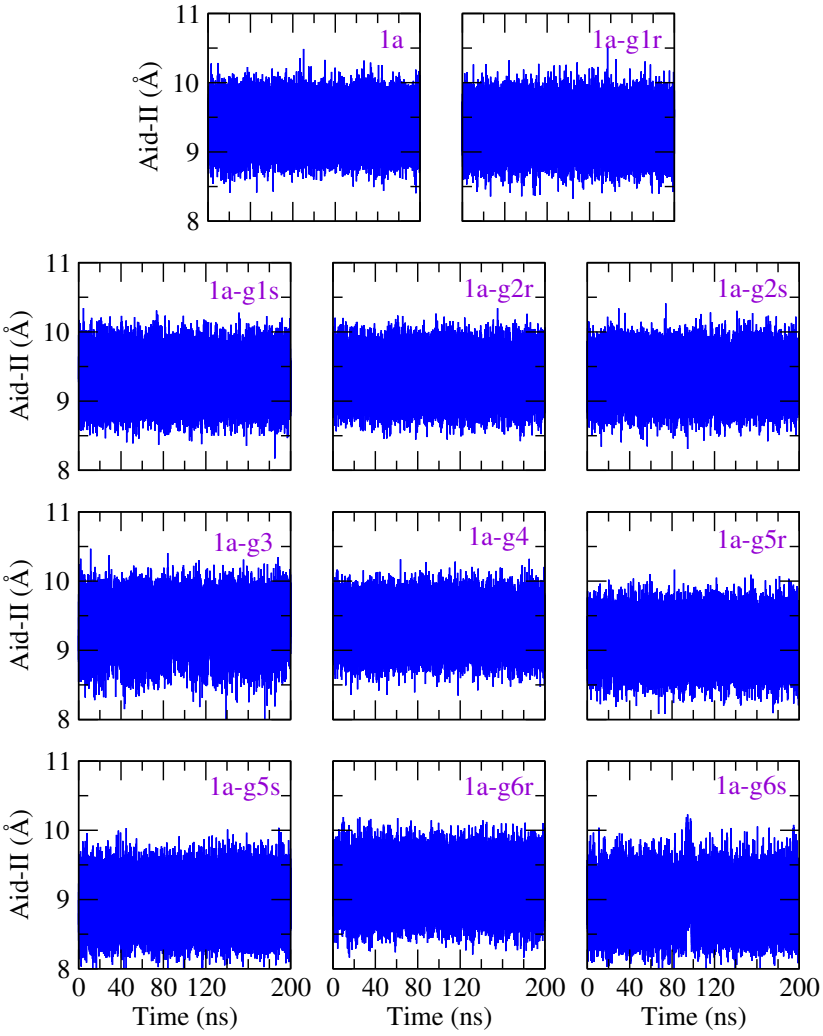

FIG. S3: Diameter-II (Aid-II) of host-1a as a function of simulation time for all systems.

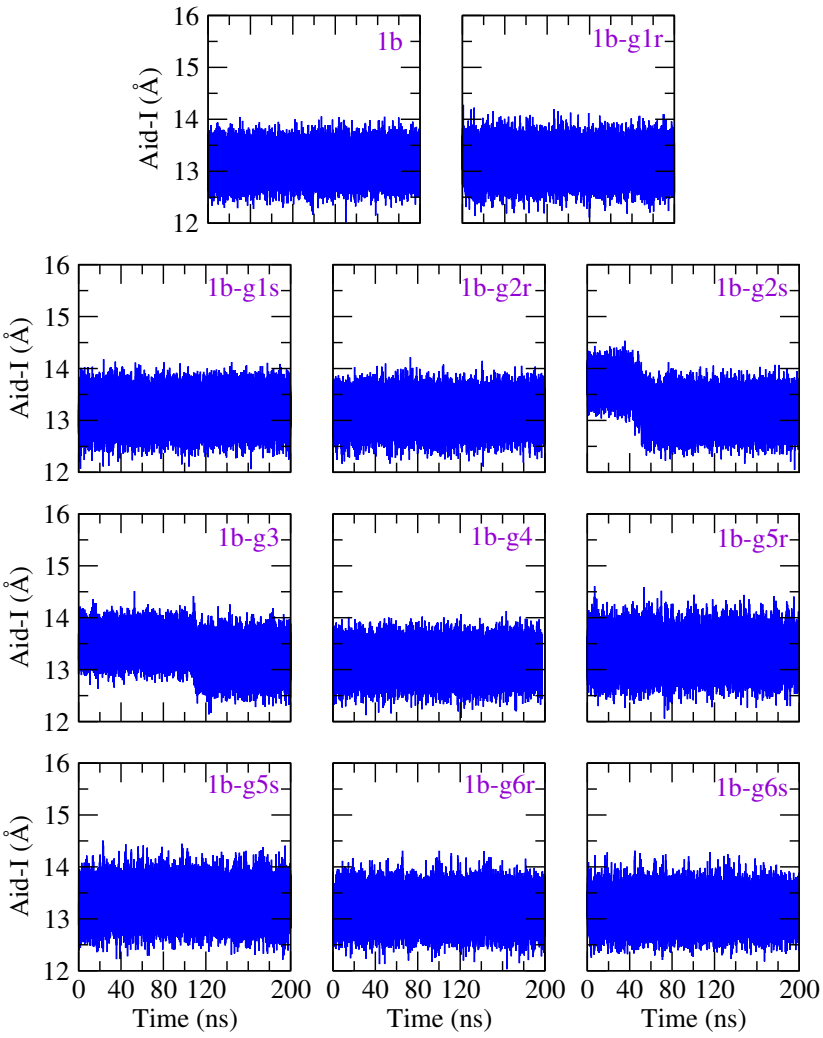

FIG. S4: Diameter-I (Aid-I) of host-1b as a function of simulation time for all systems.

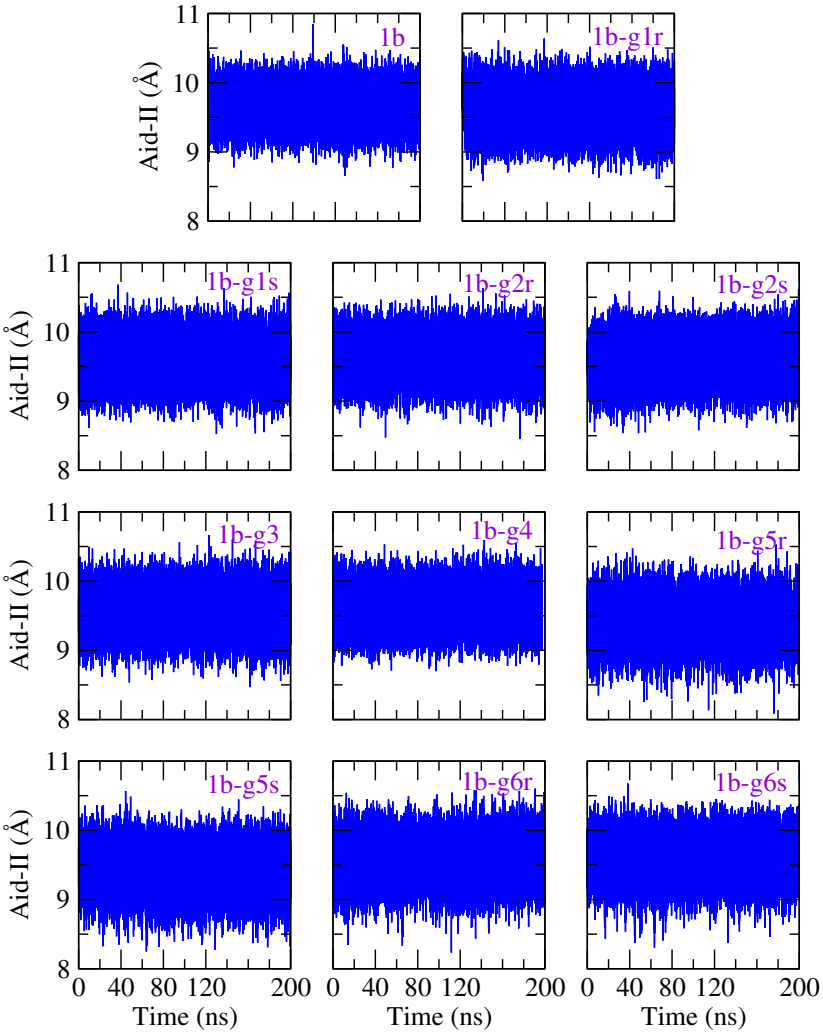

FIG. S5: Diameter-II (Aid-II) of host-1b as a function of simulation time for all systems.

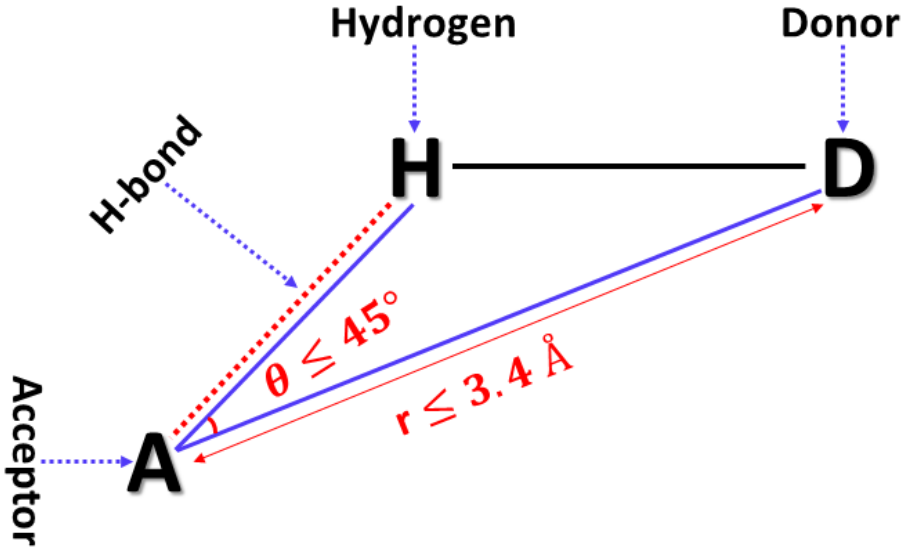

FIG. S6: The schematic representation of the imposed restrictions for hydrogen bond analysis.

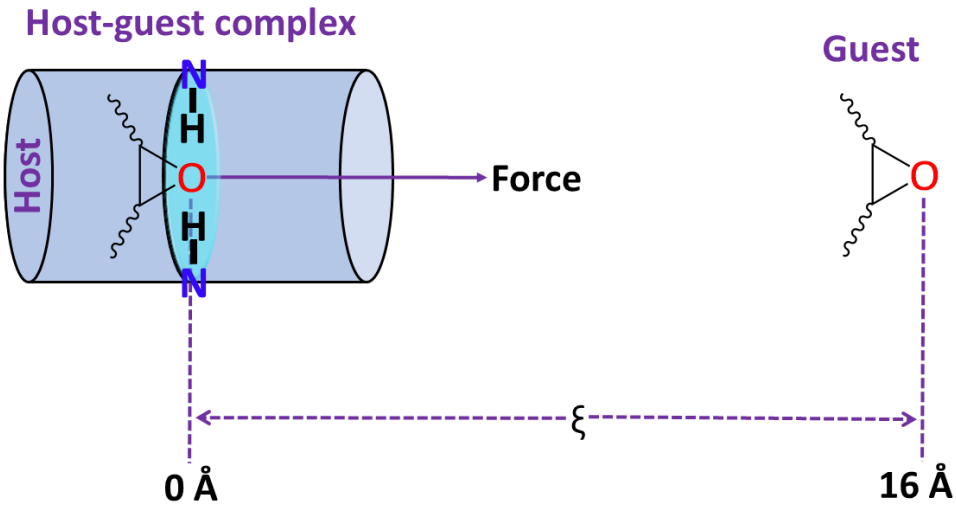

FIG. S7: Schematic representation of the umbrella sampling simulation by taking the host-guest center of mass (COM) - center of mass (COM) distance as the reaction coordinate.

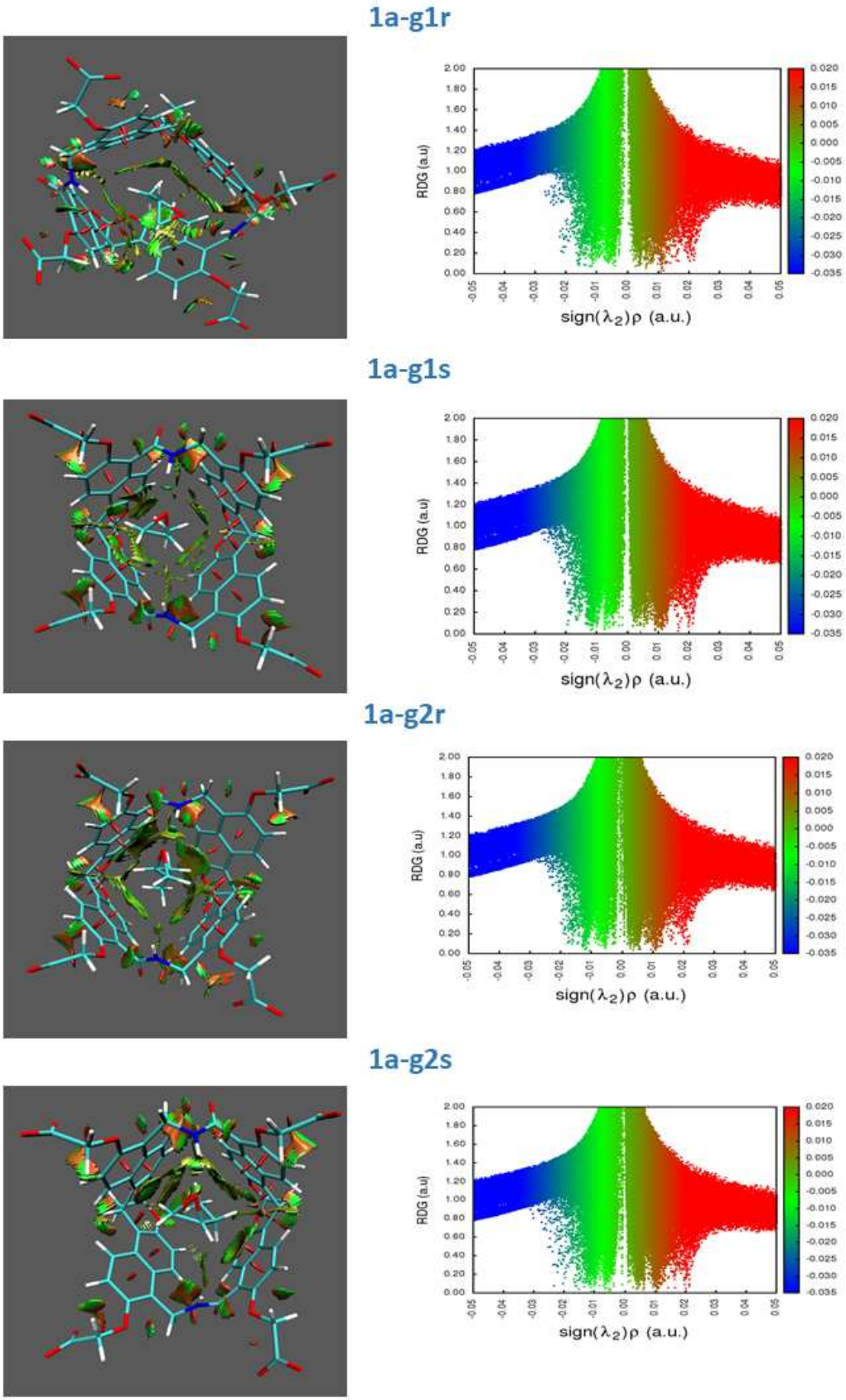

FIG. S8: Color-filled RDG isosurfaces delimitate non-covalent interaction (NCI) regions in 1a-g1r, 1a-g1s, 1a-g2r, and 1a-g2s systems.

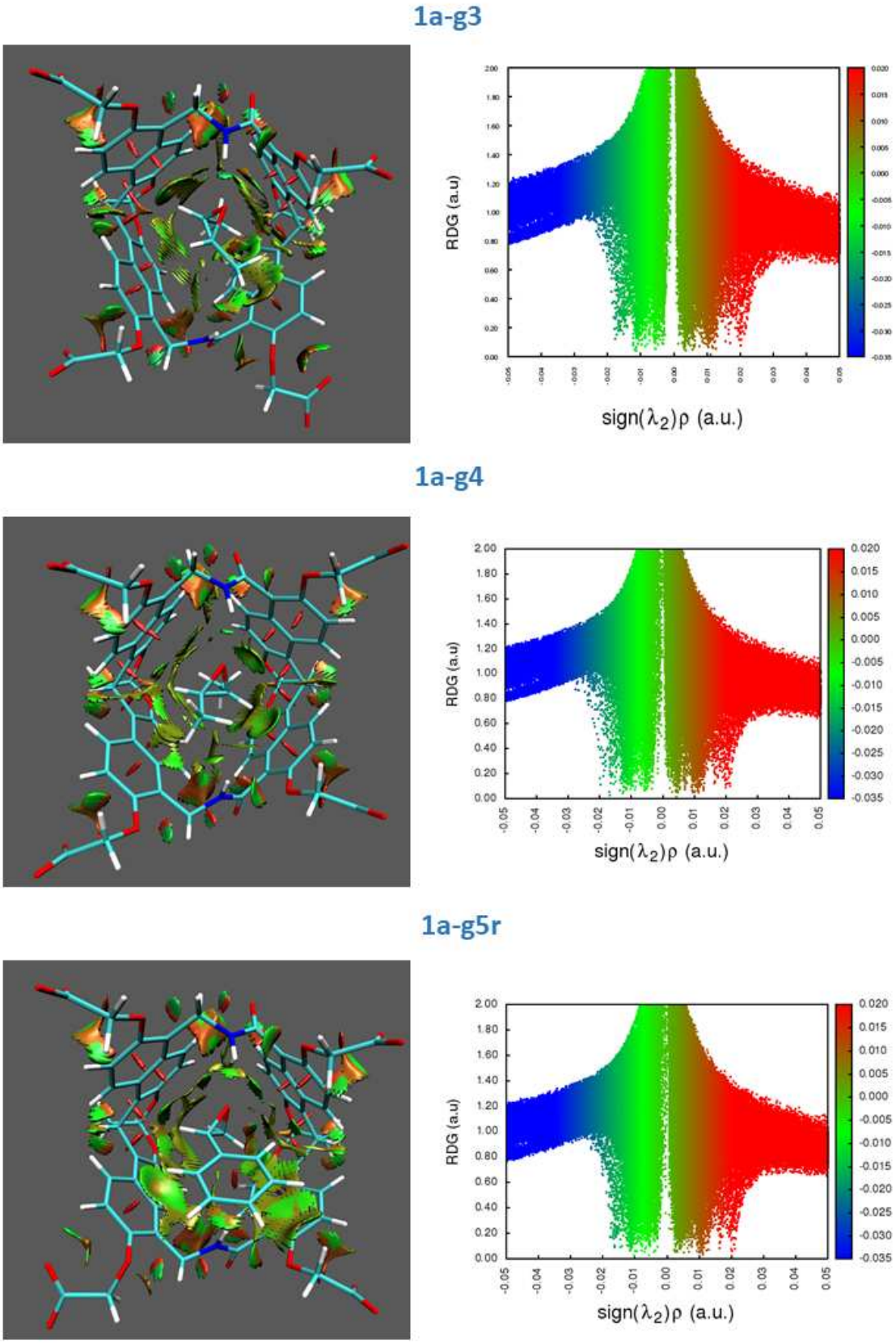

FIG. S9: Color-filled RDG isosurfaces delimitate non-covalent interaction (NCI) regions in 1a-g3, 1a-g4, and 1a-g5r systems.

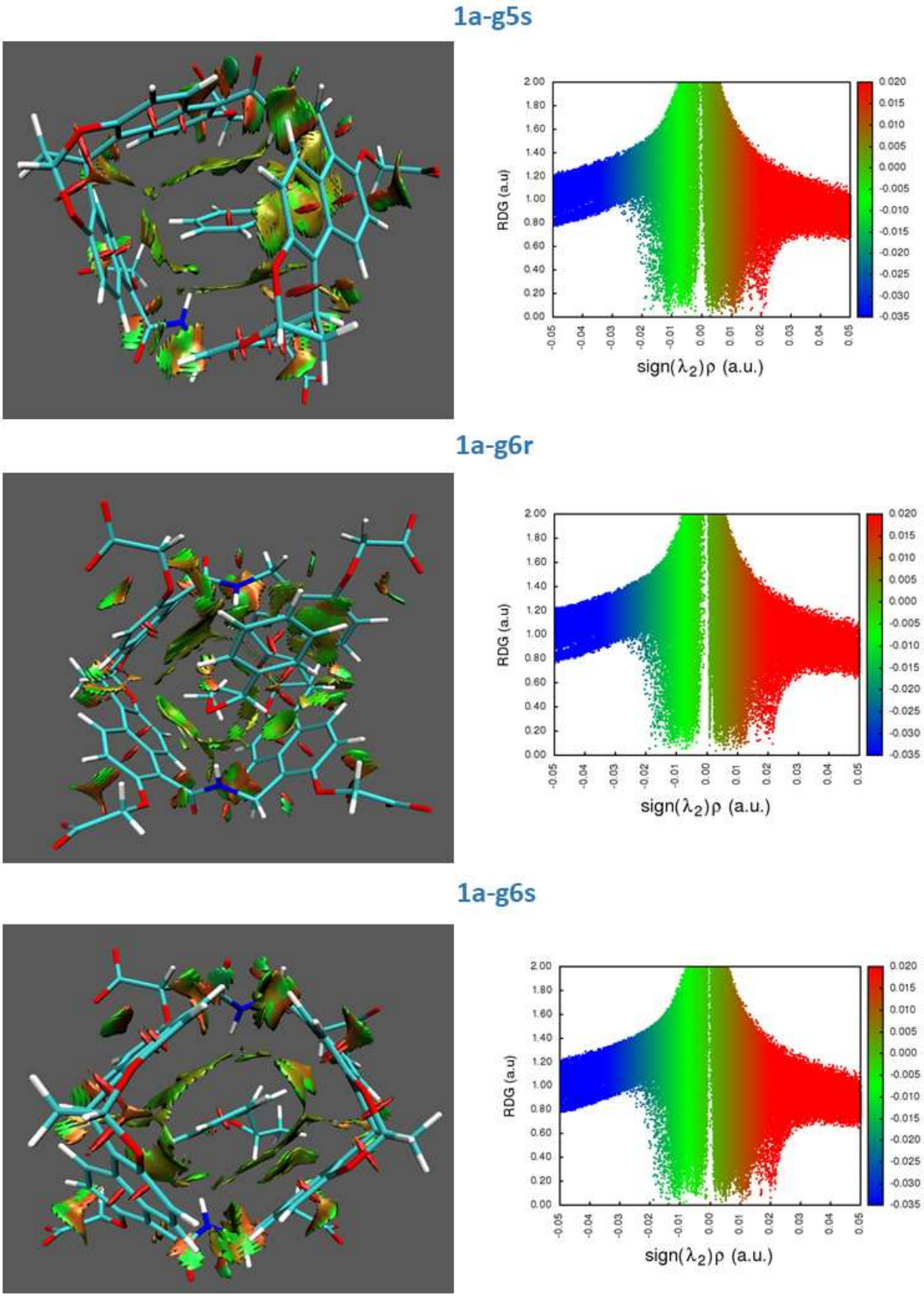

FIG. S10: Color-filled RDG isosurfaces delimitate non-covalent interaction (NCI) regions in 1a-g5s, 1a-g6r, and 1a-g6s systems.

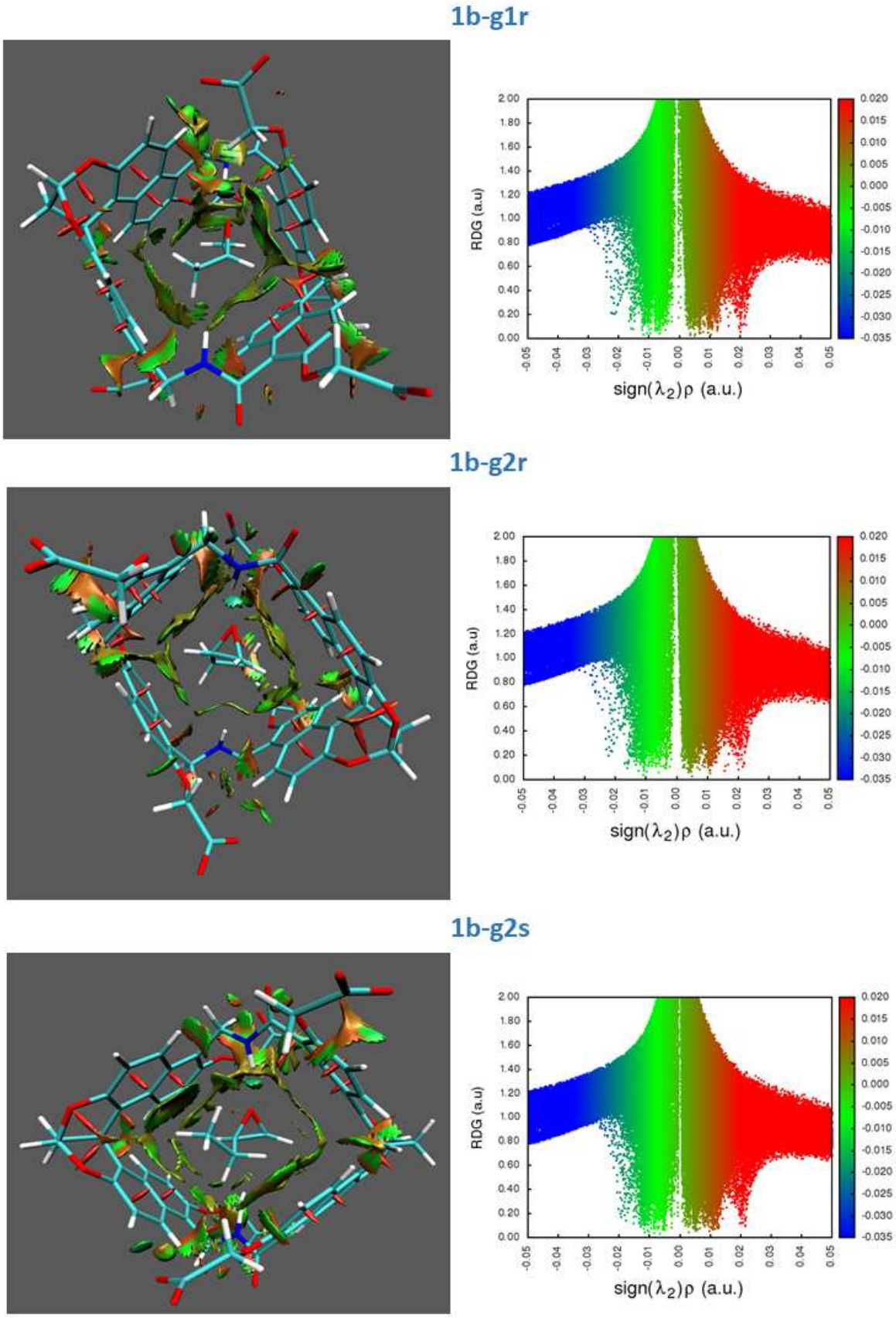

FIG. S11: Color-filled RDG isosurfaces delimitate non-covalent interaction (NCI) regions in 1b-g1r, 1b-g2r, and 1b-g2s systems.

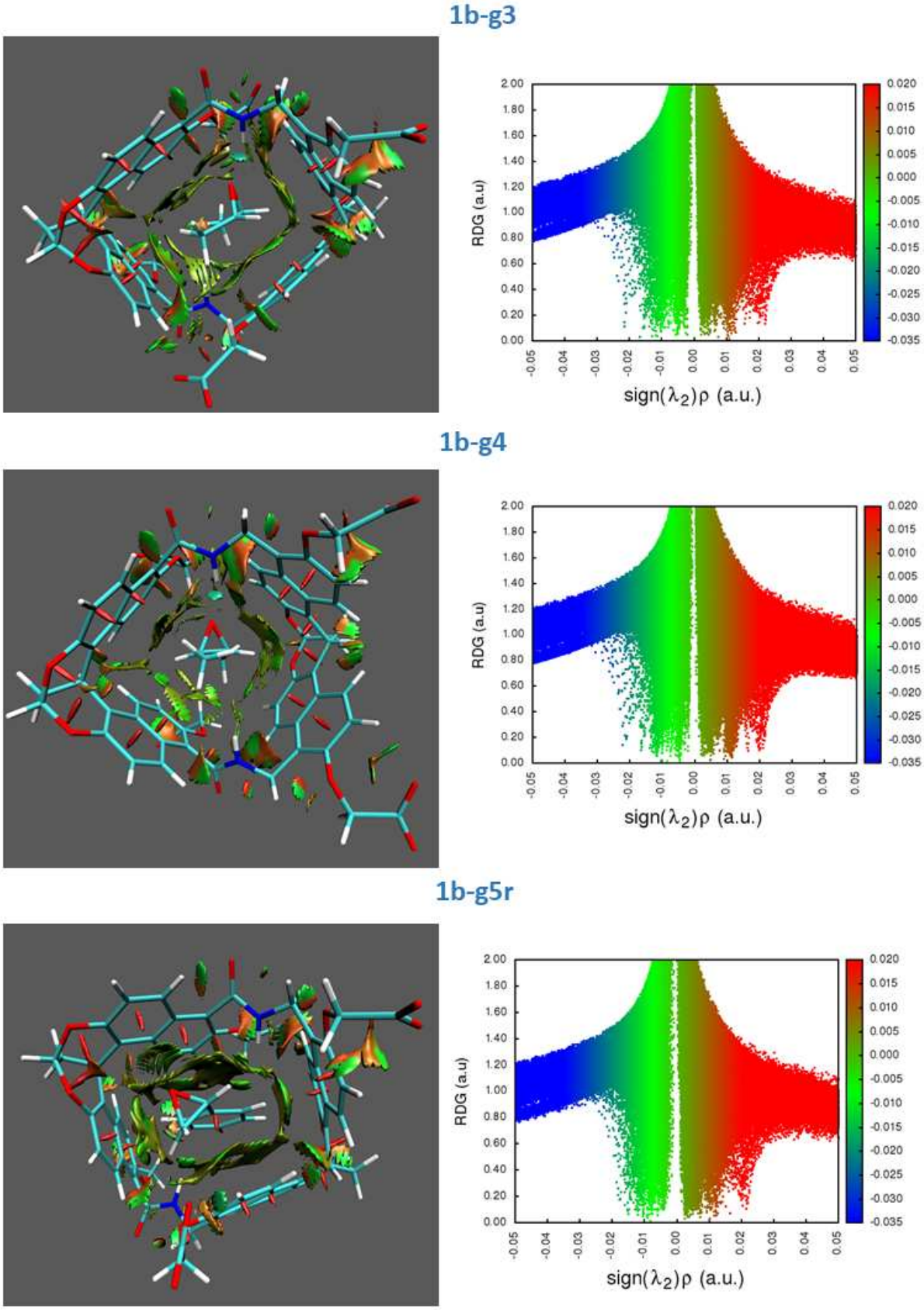

FIG. S12: Color-filled RDG isosurfaces delimitate non-covalent interaction (NCI) regions in 1b-g3, 1b-g4, and 1b-g5r systems.

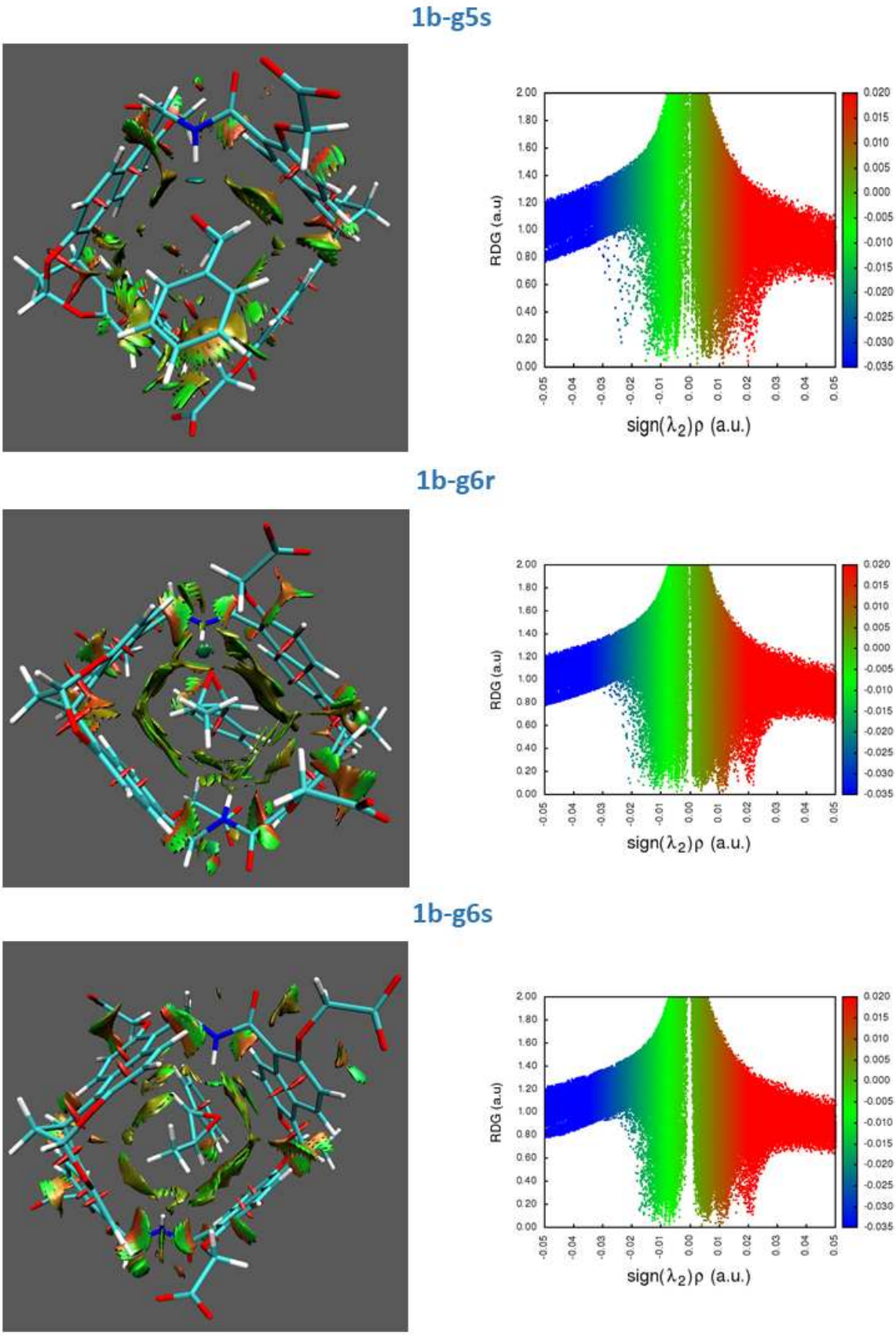

FIG. S13: Color-filled RDG isosurfaces delimitate non-covalent interaction (NCI) regions in 1b-g5s, 1b-g6r, and 1b-g6s systems.

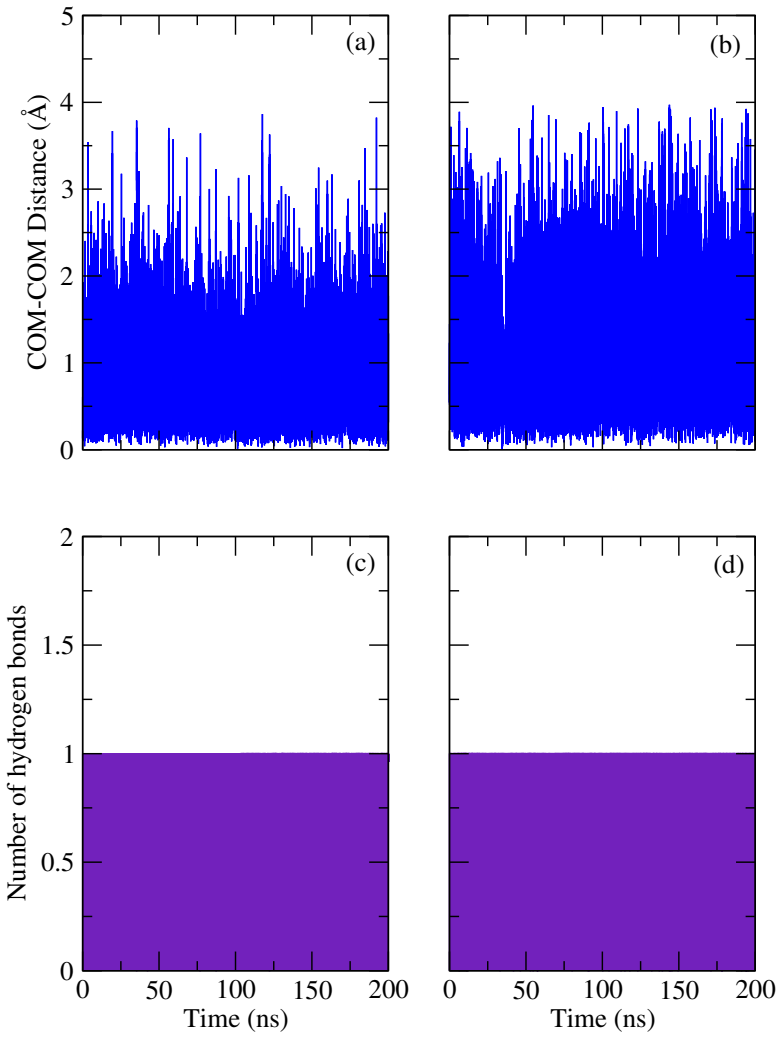

FIG. S14: Host-guest center of mass (COM) - center of mass (COM) distance and host-guest hydrogen bonds as a function of simulation time. (a) and (b) are for COM-COM distance for system 1a-g1r and 1b-g1r, respectively. (c) and (d) are the host-guest hydrogen bond values for system 1a-g1r and 1b-g1r, respectively.

TABLE S1: Partial charges of all the atomic sites of host-1a. e is the elementary charge.

host-1a					
Atom	Charge (e)	Atom	Charge (e)	Atom	Charge (e)
O1, O62	-0.5823	C41	0.6477	H37, H79	0.1771
C61	0.8341	C97	0.0211	H87, H88	0.0203
C10	-0.7799	H98, H99	0.0191	O90, O89	-0.7196
H11, H12	0.1558	C100, C108	1.0341	H73, H78	0.1737
C13	0.7208	O109, O110	-0.9125	H77	-0.0661
H14	-0.0346	O2, O5	-0.4183	H81, H82	0.1462
C56, C26	-0.4491	C42, C29	-0.2864	H83	-0.0432
C55, C25	0.1818	H43, H72	0.2007	H48, H74	0.0203
C53, C23	-0.3292	C44, C30	-0.2970	C57, C18	0.0776
C51, C21	0.2322	C45, C31	0.1471	C59, C17	-0.2162
C50, C20	0.4397	C63, C38	0.1321	C60, C16	-0.3960
C101, C91	-0.0935	C67, C36	-0.1179	C58, C15	0.5560
O3, O4	-0.3124	C66, C34	-0.4062	H85, H75	0.1879
H102, H105	0.0441	C65, C33	0.5554	H86, H76	0.2138
H92, H93	0.0441	O69, O68	-0.5962	H52, H22	0.1870
C94, C106	1.0770	C70	0.8723	H54, H24	0.1734
O113, O114	-0.9252	C64	-0.7891	H84	-0.0358
O111, O112	-0.9252	C39	0.8470	C40, C27	-0.5248
N6, N8	-0.6500	C32, C103	-0.5007	H35, H80	0.1750
C49, C19	-0.3002	O115, O116	-0.9125	C46, C104	0.9067
C47, C71	0.3091	C28	0.6477	H96, H107	0.0191
H7, H9	0.2978	C95	0.0211		

TABLE S2: Partial charges of all the atomic sites of host-1b. e is the elementary charge.

host-1b							
Atom	Charge (e)	Atom	Charge (e)	Atom	Charge (e)	Atom	Charge (e)
O5, O6	-0.6651	C85	-0.6899	C68	0.5877	H97, H98	0.0123
C20	0.5716	C84	0.5877	C66	-0.6117	H81	0.1708
C13	1.0925	C82	-0.6117	C65	-0.2608	O101, O102	-0.5940
C99, C100	-0.6651	C80	-0.2608	H103	0.1708	H14	-0.0695
C36	0.5716	C79	0.4658	H67	0.3942	C15	-1.0468
C37	-0.3272	O9, O10	-0.5802	H59	0.1657	H16, H17	0.1888
H38	0.1814	C72	0.8542	H61, H90	0.1740	H54, H55	0.0123
C39	-0.2464	C29	-0.2464	C77	0.9714	C18	1.0382
H40	0.1632	C64	0.4658	C74	-0.7070	H19	-0.1261
C41	0.2421	C63	-0.4062	H75, H76	0.0996	C21, C49	-0.5908
C42	-0.6232	C62	-0.0491	H32	0.1814	C22	0.1891
C43	0.4809	C60	-0.2565	H78	-0.1762	C23	-0.2887
O7, O8	-0.1990	C58	-0.2864	C92	-0.4062	H24	0.1635
C50	-0.2490	C57	0.5118	C91	-0.0491	C25	-0.2642
H51, H52	0.0636	O11, O12	-0.3156	C89	-0.2565	H104	0.1653
C96	0.5277	C69	0.0133	C87	-0.2864	C26	0.4809
C111	1.1483	H70, H71	-0.0031	C86	0.5118	H2	0.5133
O114, O116	-0.9397	H83	0.3942	H88	0.1657	C33	-0.2490
N1, N3	-1.1261	C112	1.0887	C93	0.0133	H34, H35	0.0636
C44	-0.2642	O113, O115	-0.9441	H94, H95	-0.0031	H4	0.5133
H45	0.1653	H73	-0.0469	C31	-0.3272	C105	1.1483
C46	-0.2887	C56	-0.6899	C106	1.0887	O107	-0.9397
H47	0.1635	C53	0.5277	O108, O110	-0.9441	O109	-0.9397
C48	0.1891	H30	0.1632	C28	0.2421	C27	-0.6232

TABLE S3: Partial charges of all the atomic sites of g1r. e is the elementary charge.

g1r			
Atom	Charge (e)	Atom	Charge (e)
C1	-0.1587	H8, H9, H10	0.1439
H4, H5	0.1406	C7	-0.4568
C2	0.1511	O3	-0.3514
H6	0.1029		

TABLE S4: Partial charges of all the atomic sites of g1s. e is the elementary charge.

g1s			
Atom	Charge (e)	Atom	Charge (e)
C1	-0.1567	H8, H9, H10	0.1443
H4, H5	0.1398	C7	-0.4586
C2	0.1522	O3	-0.3519
H6	0.1025		

TABLE S5: Partial charges of all the atomic sites of g2r. e is the elementary charge.

g2r			
Atom	Charge (e)	Atom	Charge (e)
C1	-0.0820	H8, H9	0.0409
O3	-0.3203	C7	-0.0042
H4, H5	0.1269	C10	-0.0408
C2	-0.1207	H11, H12, H13	0.0224
H6	0.1651		

TABLE S6: Partial charges of all the atomic sites of g2s. e is the elementary charge.

g2s			
Atom	Charge (e)	Atom	Charge (e)
C1	-0.0805	H8, H9	0.0405
O3	-0.3201	C7	-0.0018
H4, H5	0.1265	C10	-0.0437
C2	-0.1227	H11, H12, H13	0.0231
H6	0.1655		

TABLE S7: Partial charges of all the atomic sites of g3. e is the elementary charge.

g3			
Atom	Charge (e)	Atom	Charge (e)
C1	0.1306	C2	0.1306
H4, H5	0.0667	H7, H8, H9	0.0866
C6, C10	-0.2504	O3	-0.4133
H11, H12, H13	0.0866		

TABLE S8: Partial charges of all the atomic sites of g4. e is the elementary charge.

g4			
Atom	Charge (e)	Atom	Charge (e)
C1	0.1758	C2	0.1758
H4, H5	0.0997	H7, H8, H9	0.1346
C6, C10	-0.4692	O3	-0.4204
H11, H12, H13	0.1346		

TABLE S9: Partial charges of all the atomic sites of g5r. e is the elementary charge.

g5r			
Atom	Charge (e)	Atom	Charge (e)
C1	-0.1802	C8, C9	-0.2110
O3	-0.2629	C10, C12	-0.1454
H4, H5	0.1625	H15, H16	0.1527
C2	-0.1380	H11, H13	0.1420
H6	0.1591	C14	-0.1818
C7	0.2489	H17	0.1534

TABLE S10: Partial charges of all the atomic sites of g5s. e is the elementary charge.

g5s			
Atom	Charge (e)	Atom	Charge (e)
C1	-0.1821	C8, C9	-0.2134
O3	-0.2626	C10, C12	-0.1440
H4, H5	0.1632	H15, H16	0.1525
C2	-0.1393	H11, H13	0.1426
H6	0.1593	C14	-0.1832
C7	0.2525	H17	0.1536

TABLE S11: Partial charges of all the atomic sites of g6r. e is the elementary charge.

g6r			
Atom	Charge (e)	Atom	Charge (e)
C1	0.1517	C6	0.2133
O3	-0.3172	C7, C8	-0.2176
H4	0.1101	C9, C11	-0.1279
C17	-0.4362	H14, H15	0.1493
H18, H19, H20	0.1335	H10, H12	0.1389
C2	-0.1242	C13	-0.1979
H5	0.1593	H16	0.1553

TABLE S12: Partial charges of all the atomic sites of g6s. e is the elementary charge.

g6s			
Atom	Charge (e)	Atom	Charge (e)
C1	0.1519	C6	0.2153
O3	-0.3173	C7, C8	-0.2194
H4	0.1100	C9, C11	-0.1264
C17	-0.4379	H14, H15	0.1491
H18, H19, H20	0.1339	H10, H12	0.1392
C2	-0.1244	C13	-0.1993
H5	0.1593	H16	0.1556

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