SUPPORTING INFORMATION

Molecular Dynamics of Large-Ring Cyclodextrins: Principal Component Analysis of the Conformational Interconversions

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The names of the structures used for some of the figures in the Supporting Information were composed by *i)* the cyclodextrin abbreviation and *ii)* a number indicating the simulation time (in nanoseconds) and referring approximately to the moment of the simulation at which this structure has been picked up from the MD simulation trajectory file (a snapshot). In this way, CD14-2.0 represents a snapshot of the structure for CD14 after 2.0 ns MD simulation.

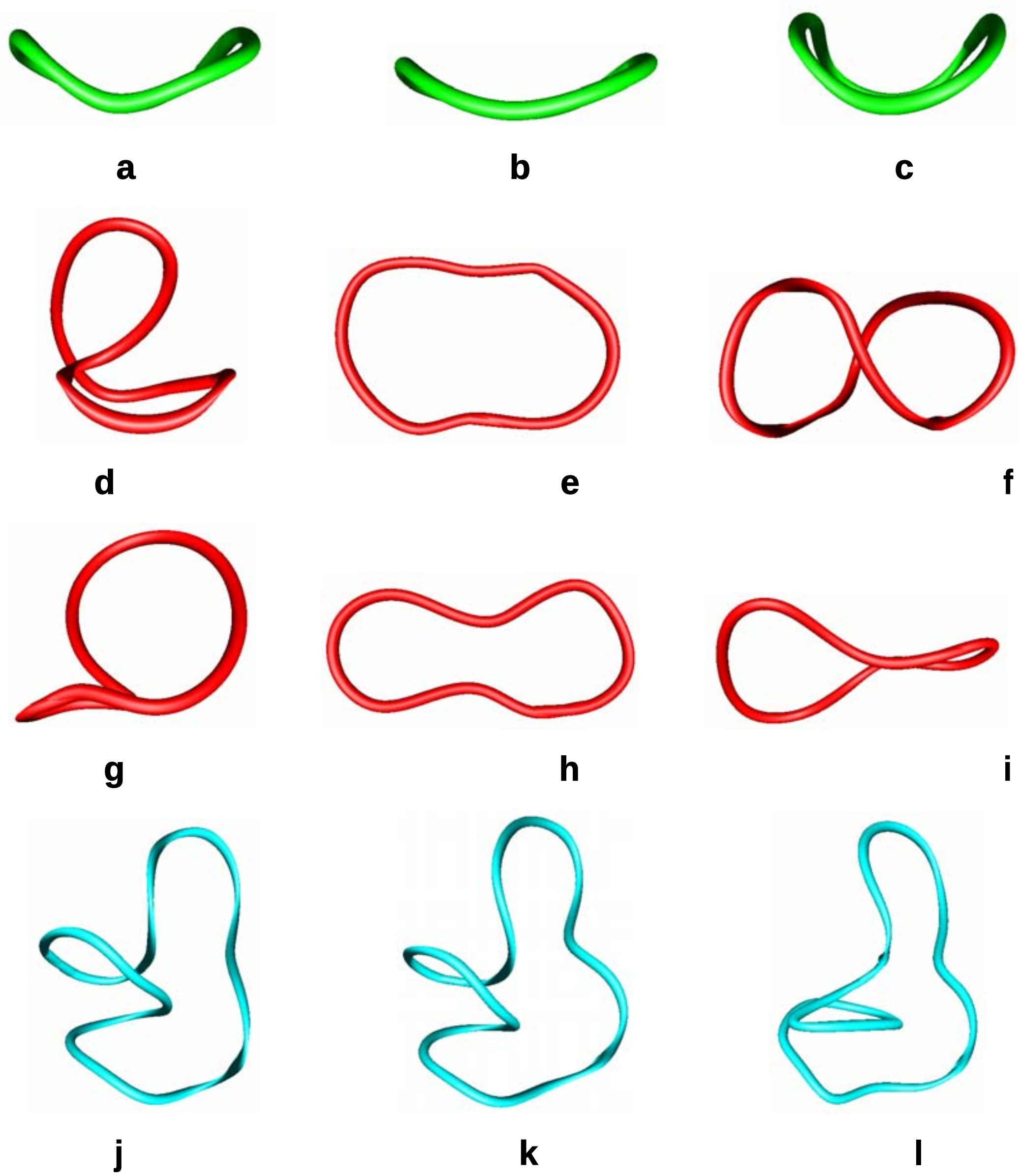


Figure 1S. Typical appearances of some of the structural motifs:[1] a) CD10-2.5, the most common form; b) CD10-5.5, the most opened form; c) CD10-19.0, the most closed form; d) CD14-1.5, two loops in perpendicular planes; e) CD14-5.0, the most open conformation; f) CD14-7.0, shaped as number eight; g) CD14-11.0, a big circular loop with a small helical turn; h) CD14-17.0, symmetrically squeezed open form ("a dumbbell"); i) CD14-20.0, two loops in perpendicular planes; j) CD26-3.5, a two turn helix with an extended helical portion; k) CD26-12.5, two turn helix with an arc and a loop of six glucose units; l) CD26-20.0, one turn helix with elongated loop and an arc.

CD10

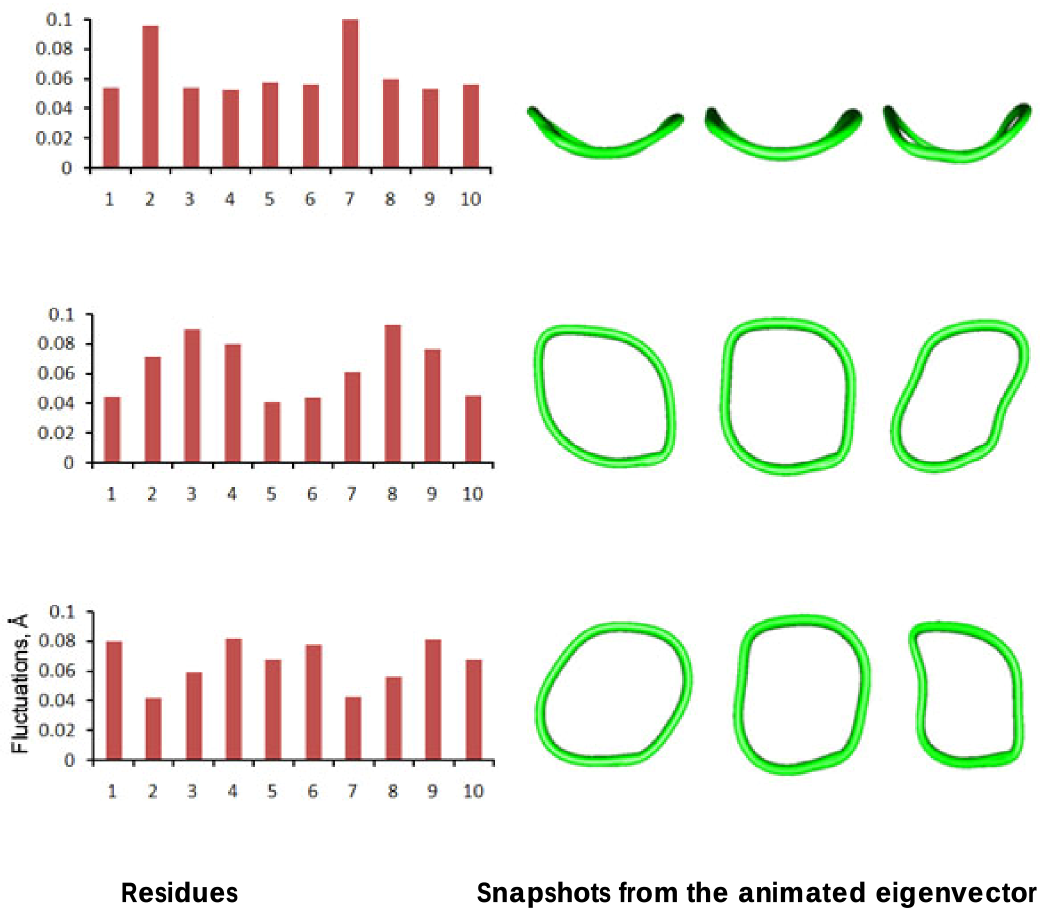


Figure 2S. The first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectory of CD10.[1] Fluctuations of atomic coordinates (in Å), averaged per residue (on the left), and snapshots of the corresponding animated eigenvectors (on the right).

CD14

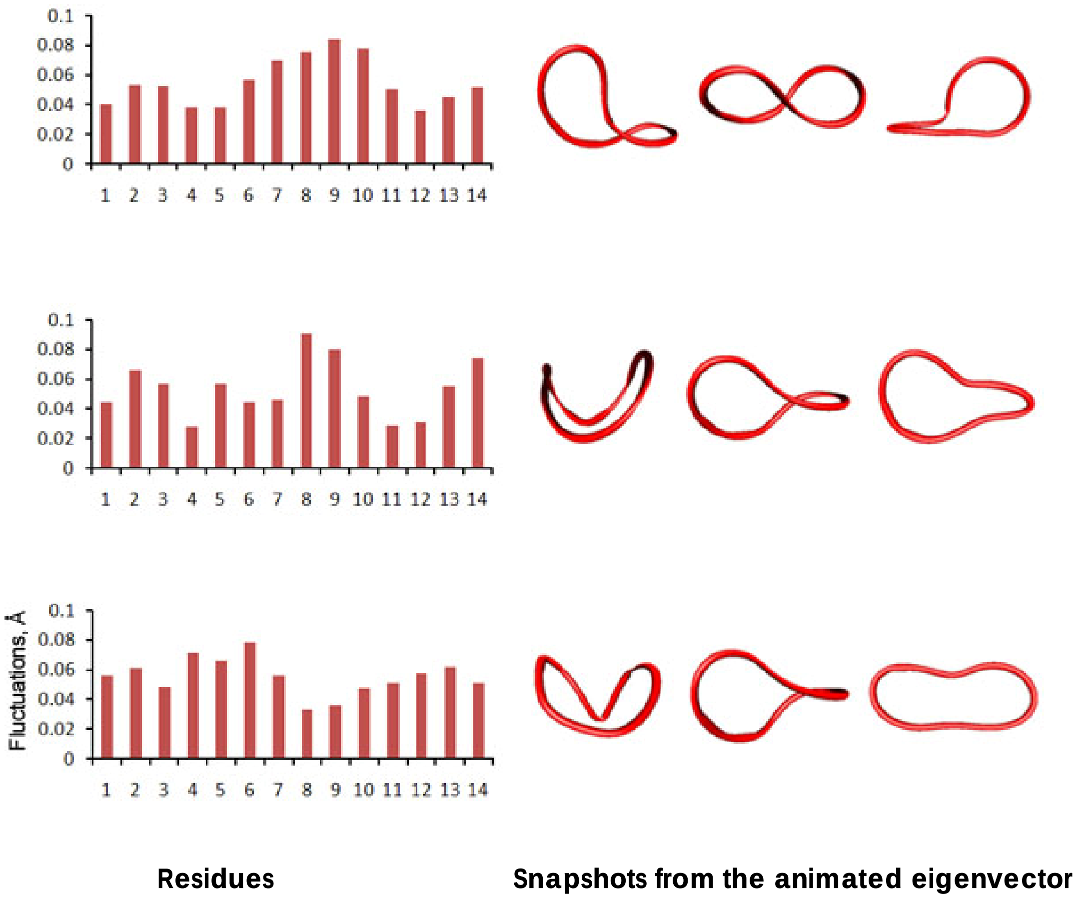


Figure 3S. The first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectory of CD14.[1] Fluctuations of atomic coordinates (in Å), averaged per residue (on the left), and snapshots of the corresponding animated eigenvectors (on the right).

CD26

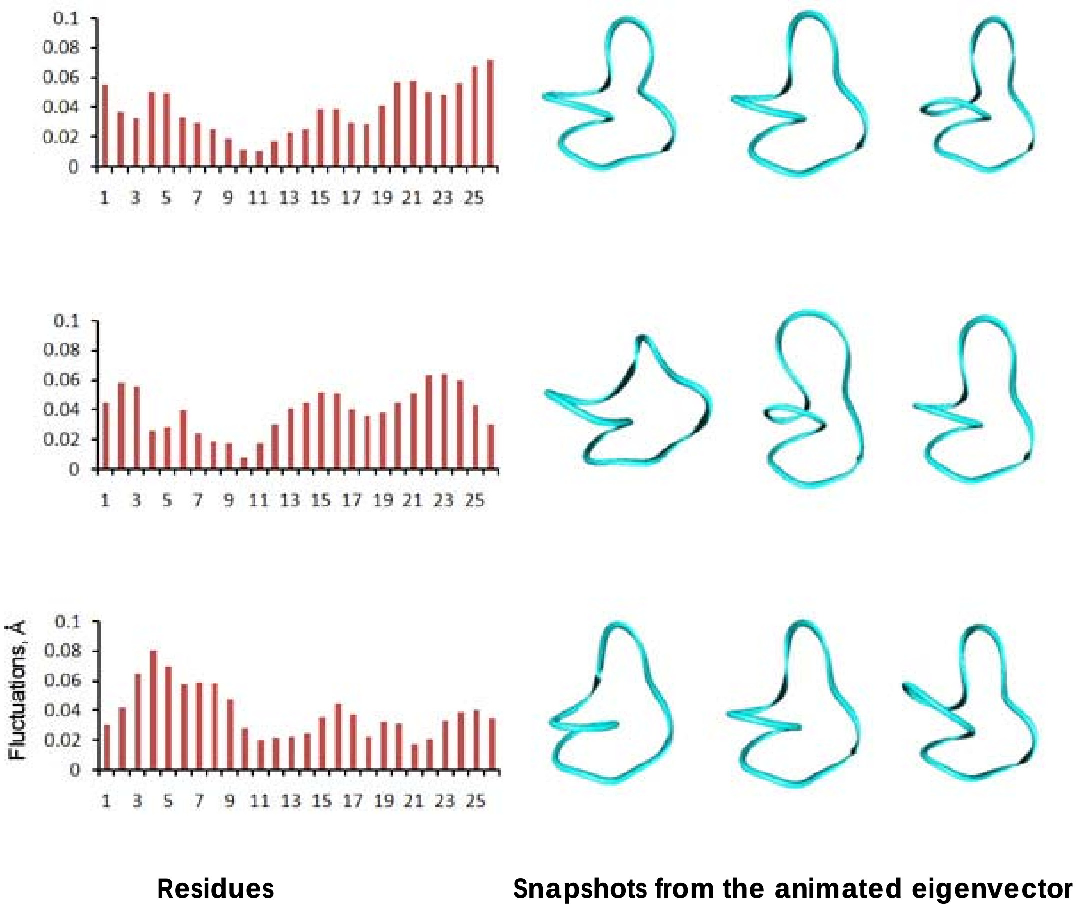


Figure 4S. The first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectory of CD26.[1] Fluctuations of atomic coordinates (in Å), averaged per residue (on the left), and snapshots of the corresponding animated eigenvectors (on the right).

CD26*

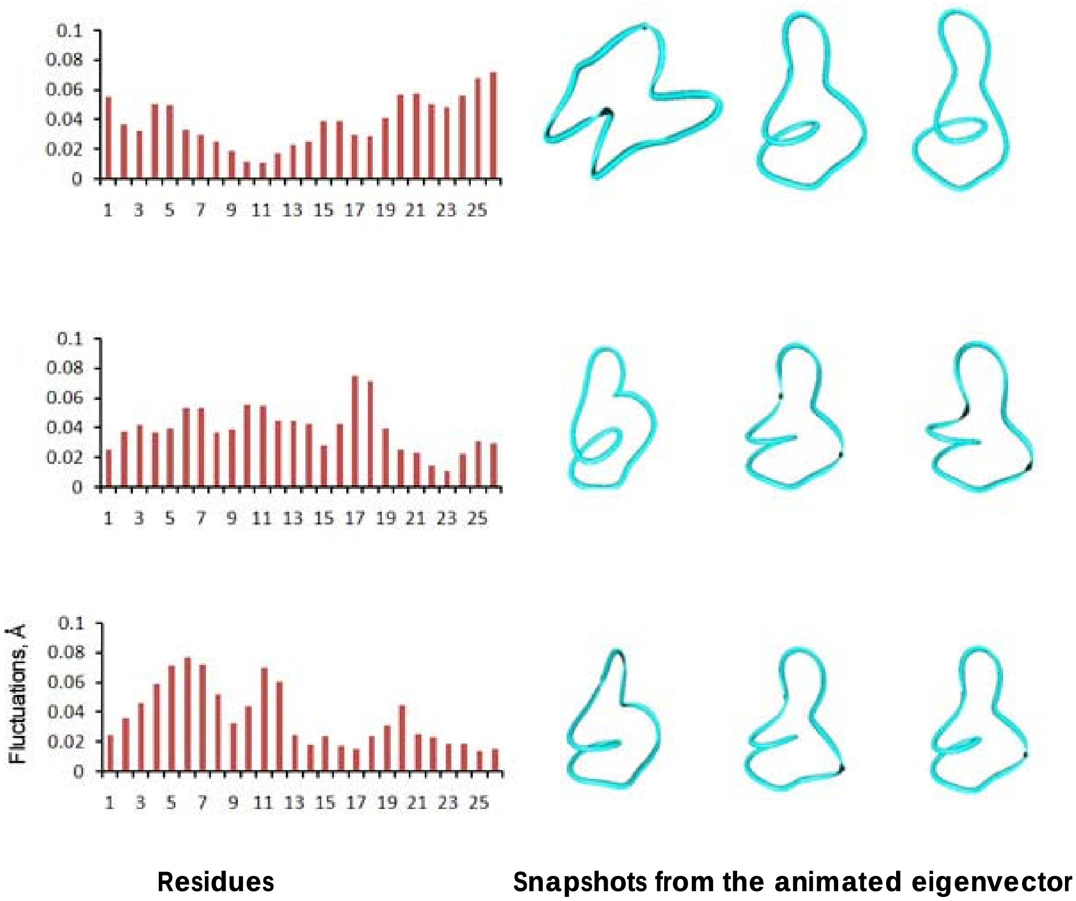
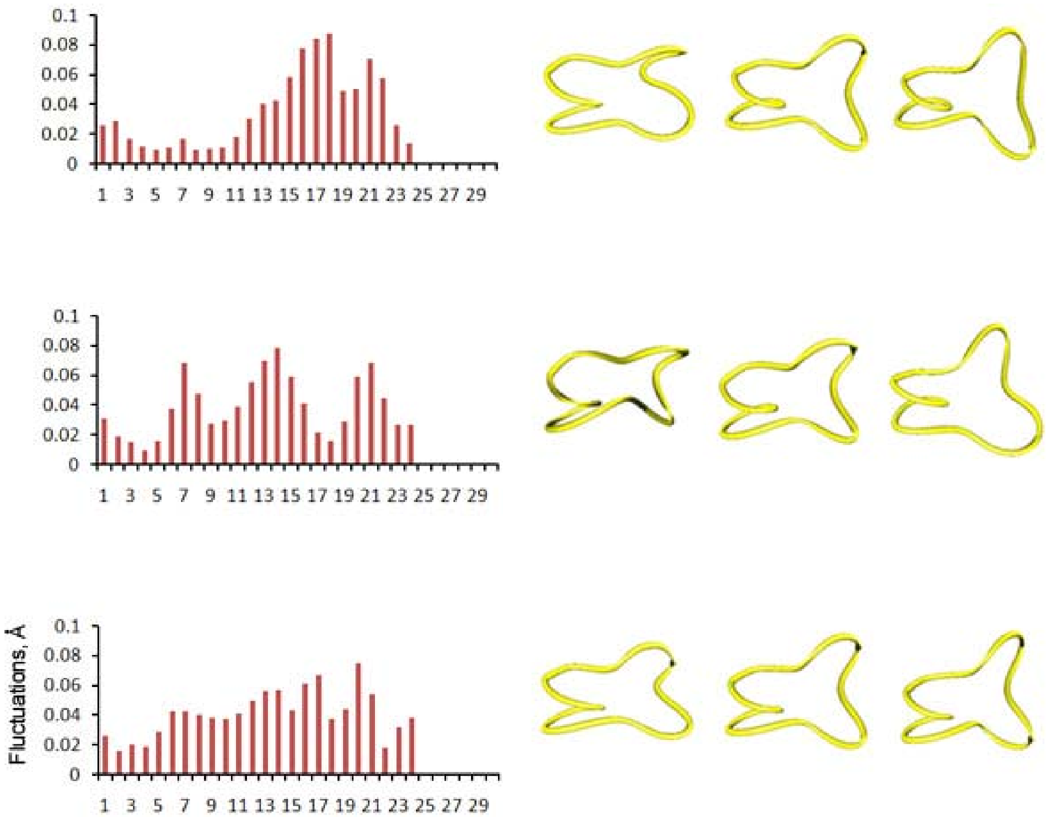


Figure 5S. The first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectory of CD26***.**[1] Fluctuations of atomic coordinates (in Å), averaged per residue (on the left), and snapshots of the corresponding animated eigenvectors (on the right).

CD24



Residues **Snapshots from the animated eigenvector**

Figure 6S. The first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectory of CD24**.**[2] Fluctuations of atomic coordinates (in Å), averaged per residue (on the left), and snapshots of the corresponding animated eigenvectors (on the right).

CD25

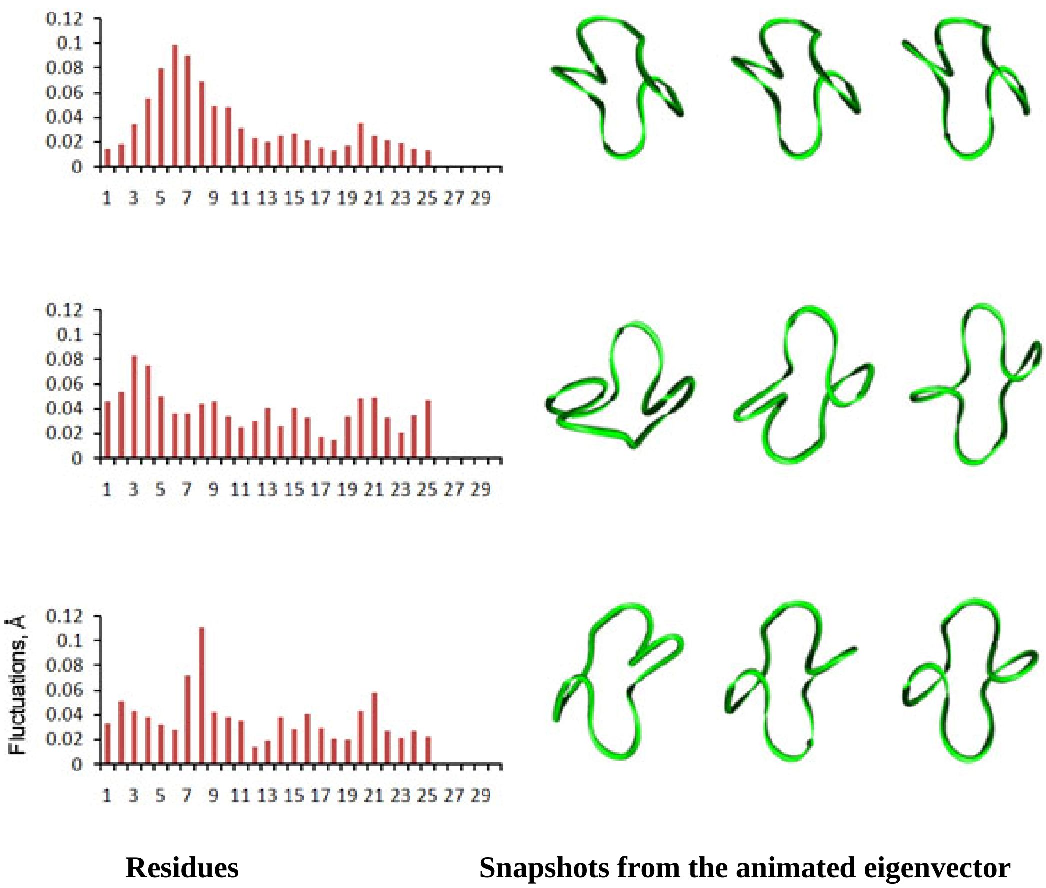
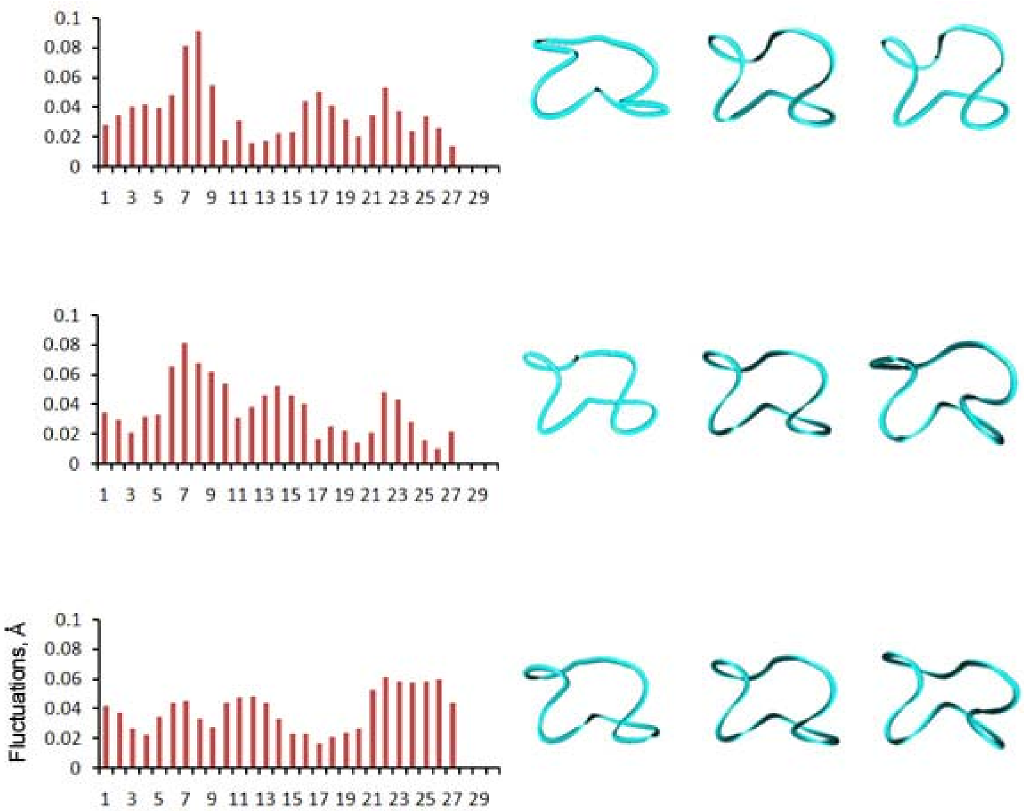


Figure 7S. The first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectory of CD25**.**[2] Fluctuations of atomic coordinates (in Å), averaged per residue (on the left), and snapshots of the corresponding animated eigenvectors (on the right).

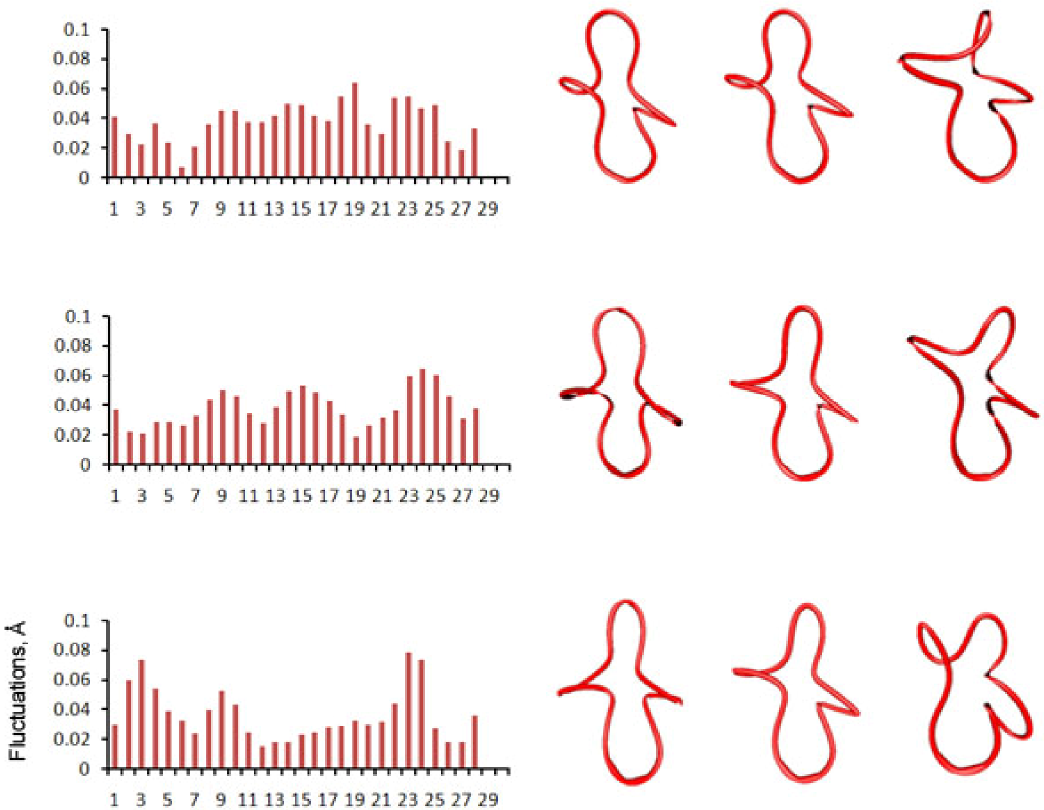
CD27



Residues **Snapshots from the animated eigenvector**

Figure 8S. The first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectory of CD27**.**[2] Fluctuations of atomic coordinates (in Å), averaged per residue (on the left), and snapshots of the corresponding animated eigenvectors (on the right).

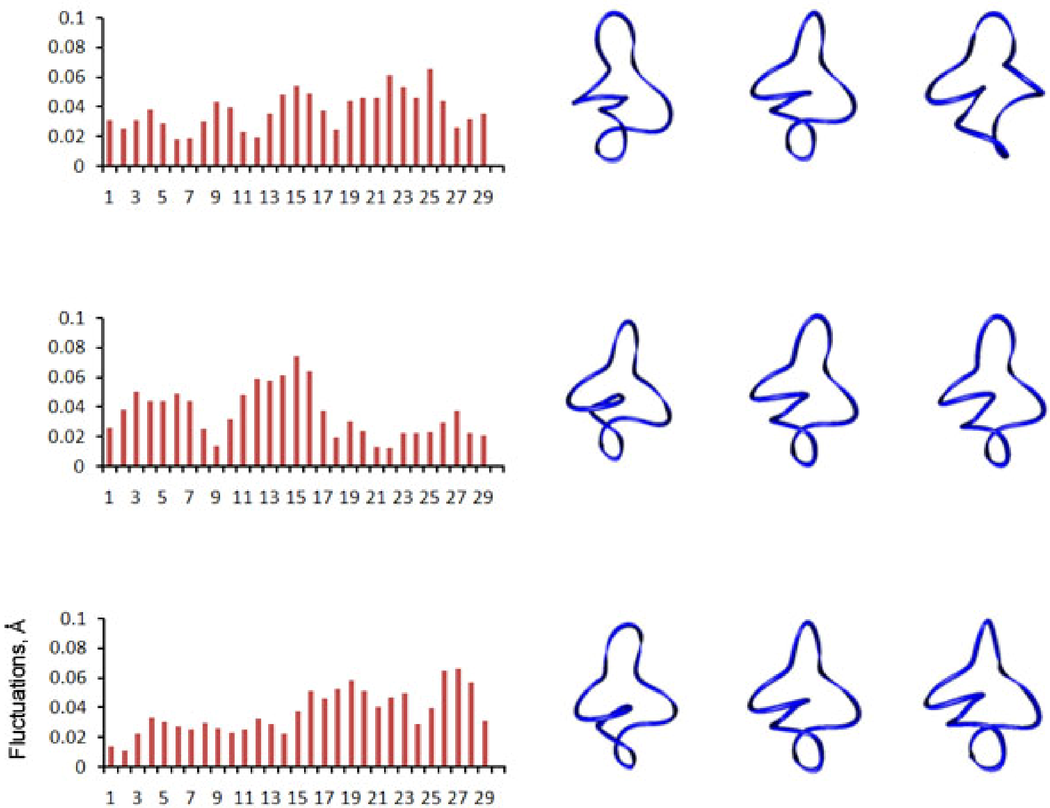
CD28



Residues **Snapshots from the animated eigenvector**

Figure 9S. The first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectory of CD28**.**[2] Fluctuations of atomic coordinates (in Å), averaged per residue (on the left), and snapshots of the corresponding animated eigenvectors (on the right).

CD29



Residues **Snapshots from the animated eigenvector**

Figure 10S. The first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectory of CD29.[2] Fluctuations of atomic coordinates (in Å), averaged per residue (on the left), and snapshots of the corresponding animated eigenvectors (on the right).

CD30

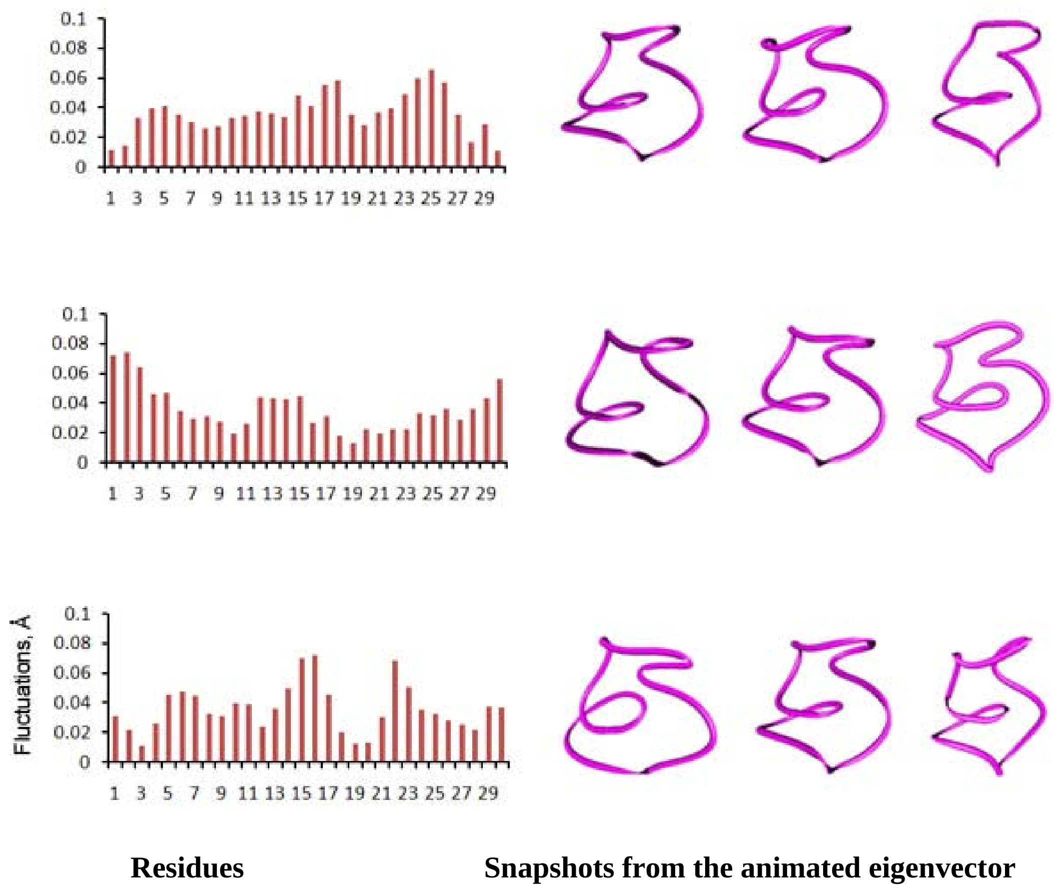


Figure 11S. The first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectory of CD30**.**[2] Fluctuations of atomic coordinates (in Å), averaged per residue (on the left), and snapshots of the corresponding animated eigenvectors (on the right).

TABLE S-1: Principal Component Analysis of the Simulation Trajectories of CD10, CD14 and CD26

Part 1: For the first 10.0 ns

	CD10		CD14		CD26		CD26*	
Number of atoms	210		294		546		546	
Number of eigenvectors	67		23		19		17	
Total variance	273		2134		6031		6775	
Explained variance	259		2028		5730		6452	
Quality of the compression	95.1%		95.0%		95.0%		95.2%	
Eigenvectors	**Eigenvalues/Weight (%)**							
1	62	24.0	893	44.0	3617	63.1	3891	60.3
2	35	13.4	317	15.6	767	13.4	1101	17.1
3	25	9.6	253	12.5	360	6.3	403	6.3
4	21	7.9	190	9.4	263	4.6	272	4.2
5	15	5.9	82	4.0	147	2.6	162	2.5
6	10	4.0	68	3.4	125	2.2	124	1.9
7	9	3.4	39	1.9	85	1.5	87	1.3
8	9	3.3	32	1.6	69	1.2	81	1.2
9	7	2.6	24	1.2	55	1.0	70	1.1
10	6	2.2	20	1.0	45	0.8	60	0.9

TABLE S-1 (continued)

Part 2: From 10.0 ns to 20.0 ns

	CD10		CD14		CD26		CD26*	
Number of atoms	210		294		546		546	
Number of eigenvectors	68		17		36		62	
Total variance	269		2822		3267		1869	
Explained variance	255		2688		3107		1776	
Quality of the compression	95.1%		95.3%		95.1%		95.0%	
Eigenvectors	**Eigenvalues/Weight (%)**							
1	58	22.8	1564	58.2	1226	39.5	685	39.9
2	33	13.0	398	14.8	487	15.7	230	13.4
3	29	11.5	331	12.3	310	10.0	190	11.1
4	21	8.2	89	3.3	190	6.1	108	6.3
5	15	5.7	78	2.9	145	4.7	83	4.8
6	10	3.8	50	1.9	135	4.4	66	3.8
7	10	3.7	36	1.3	95	3.1	43	2.5
8	7	2.7	26	1.0	77	2.5	38	2.2
9	6	2.4	21	0.8	62	2.0	31	1.8
10	6	2.4	18	0.7	50	1.6	25	1.5

TABLE S-2: Principal Component Analysis of the Simulation Trajectories of Cyclodextrins Obtained by Using CD26-Derived Starting Geometries

Part 1: For the first 5.0 ns

	CD24	**CD25**	**CD27**	**CD28**	**CD29**	**CD30**
Number of atoms	504	525	567	588	609	630
Number of eigenvectors	35	66	32	53	36	47
Total variance	2235	1203	3129	2205	3174	2330
Explained variance	2124	1143	2973	2095	3017	2214
Quality of the compression (%)	95.1	95.0	95.0	95.0	95.1	95.0

Eigenvectors	**Eigenvalues/Weight (%)**											
1	1073	50.5	450	39.4	1225	41.2	629	30.0	1297	43.0	1082	48.8
2	303	14.3	167	14.6	676	22.7	389	18.5	690	22.9	317	14.3
3	164	7.7	96	8.4	275	9.3	200	9.5	256	8.5	175	7.9
4	134	6.3	69	6.0	153	5.1	165	7.9	132	4.4	119	5.4
5	71	3.4	48	4.2	107	3.6	99	4.7	89	3.0	79	3.6
6	50	2.3	40	3.5	95	3.2	87	4.2	73	2.4	63	2.8
7	41	1.9	37	3.2	72	2.4	69	3.3	62	2.1	54	2.4
8	38	1.8	24	2.1	48	1.6	62	2.9	49	1.6	39	1.7
9	34	1.6	22	1.9	42	1.4	47	2.2	48	1.6	29	1.3
10	26	1.2	18	1.5	32	1.1	33	1.6	35	1.2	23	1.0

TABLE S-2 (continued)

Part 2: From 5.0 ns to 10.0 ns

	CD24		CD25		CD27		CD28		CD29		CD30	
Number of atoms	504		525		567		588		609		630	
Number of eigenvectors	32		80		31		33		61		35	
Total variance	2454		1071		3675		3433		1683		3410	
Explained variance	2334		1018		3491		3265		1599		3242	
Quality of the compression (%)	95.1		95.0		95.0		95.1		95.0		95.1	
Eigenvectors	**Eigenvalues/Weight (%)**											
1	961	41.2	330	32.4	1631	46.7	1495	45.8	725	45.3	1538	47.4
2	670	28.7	144	14.1	560	16.0	661	20.2	181	11.3	526	16.2
3	136	5.8	96	9.4	274	7.9	321	9.8	123	7.7	239	7.4
4	120	5.1	81	7.9	225	6.4	141	4.3	94	5.9	175	5.4
5	101	4.3	45	4.4	147	4.2	115	3.5	65	4.0	132	4.1
6	61	2.6	34	3.4	94	2.7	85	2.6	52	5.9	106	3.3
7	41	1.7	29	2.9	83	2.4	54	1.6	35	2.2	81	2.5
8	33	1.4	27	2.6	60	1.7	49	1.5	33	2.1	62	1.9
9	27	1.2	20	2.0	54	1.5	36	1.1	26	1.6	59	1.8
10	21	0.9	18	1.7	52	1.5	35	1.1	23	1.5	45	1.4

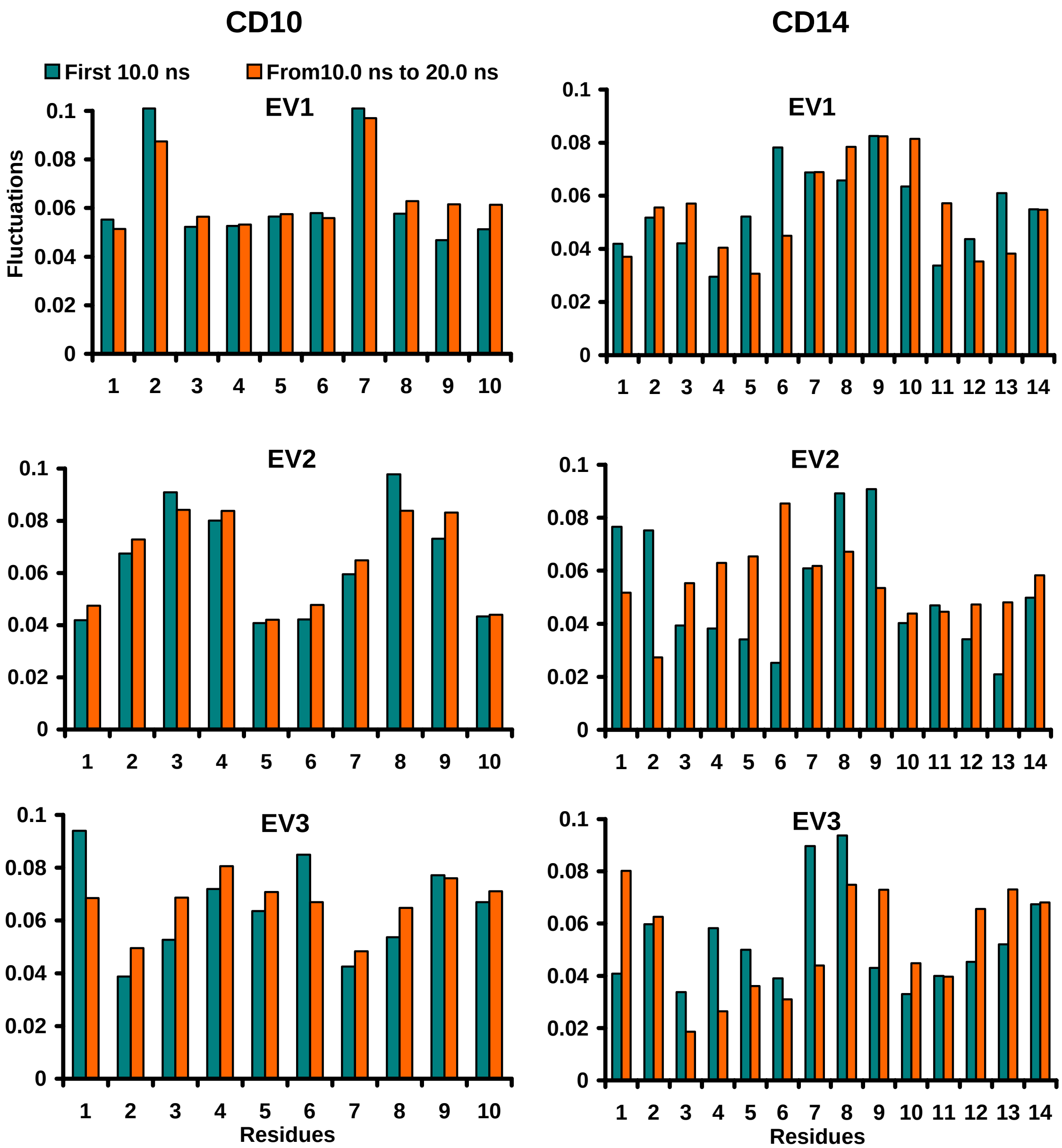


Figure 12S. Decomposition for periods of 10.0 ns of the fluctuations of atomic coordinates (in Å), averaged per residue, for the first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectories of CD10 and CD14.[1]

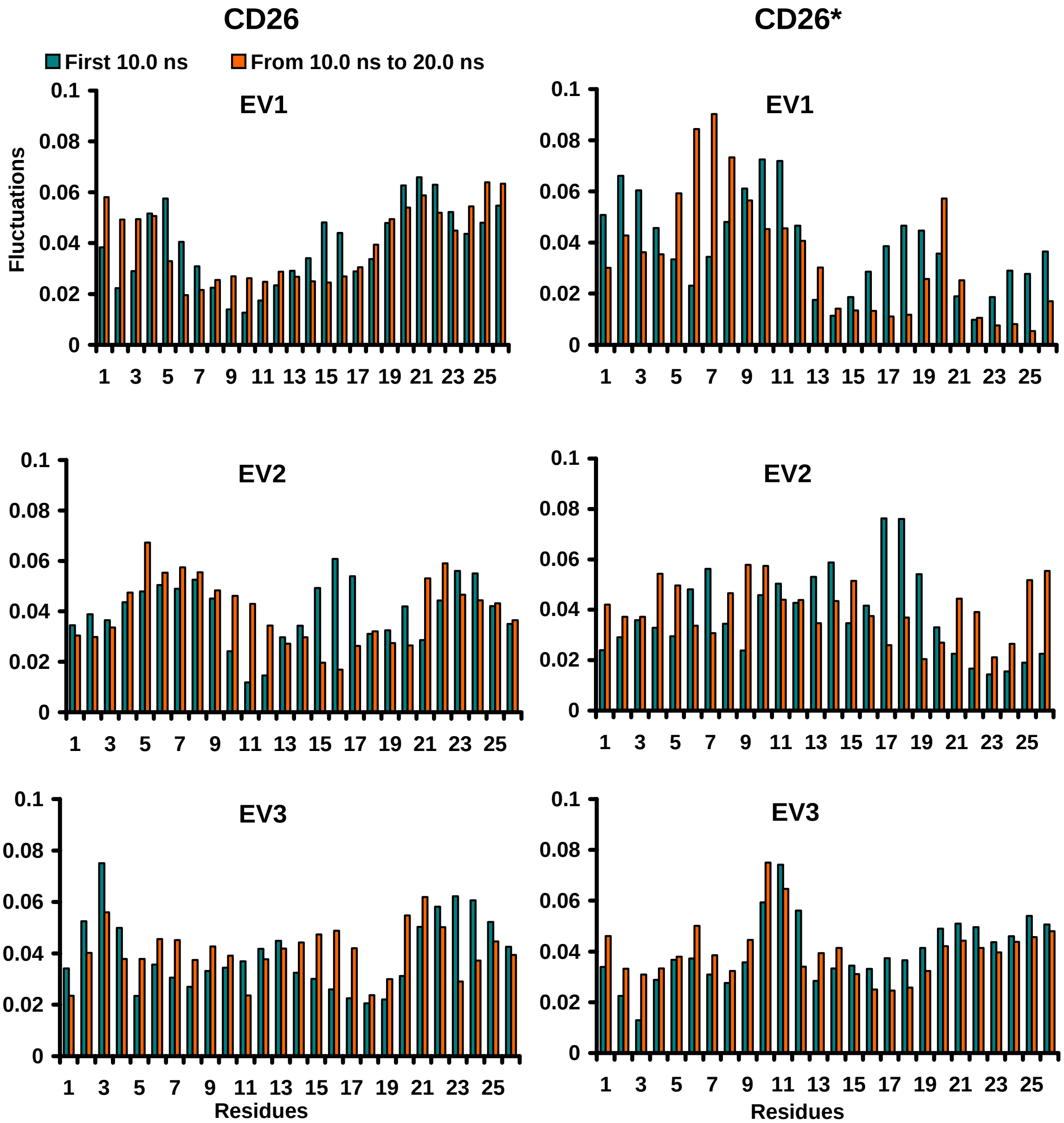


Figure 13S. Decomposition for periods of 10.0 ns of the fluctuations of atomic coordinates (in Å), averaged per residue, for the first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectories of CD26 and CD26*.[1]

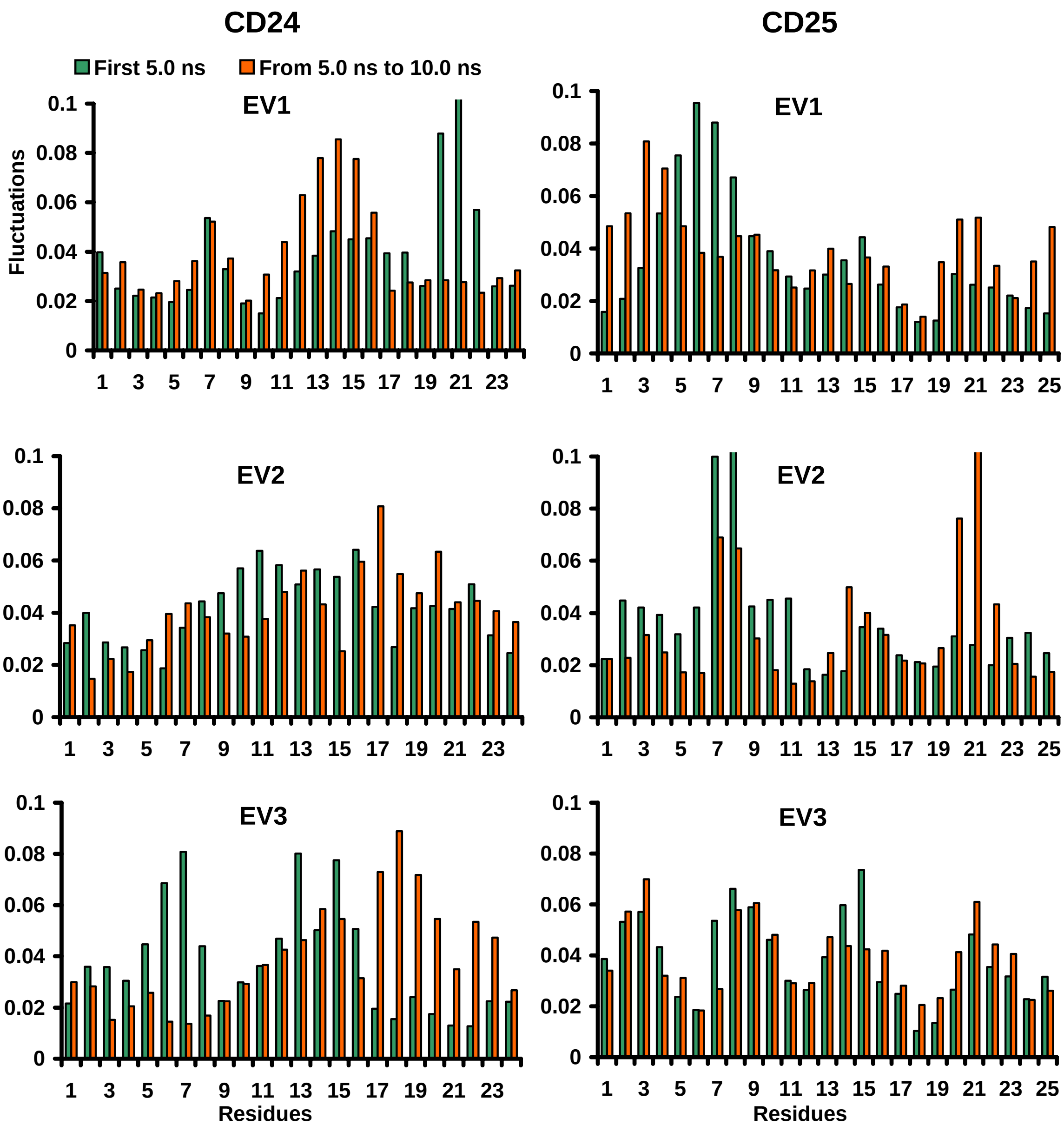


Figure 14S. Decomposition for periods of 5.0 ns of the fluctuations of atomic coordinates (in Å), averaged per residue, for the first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectories of CD24 and CD25.[2]

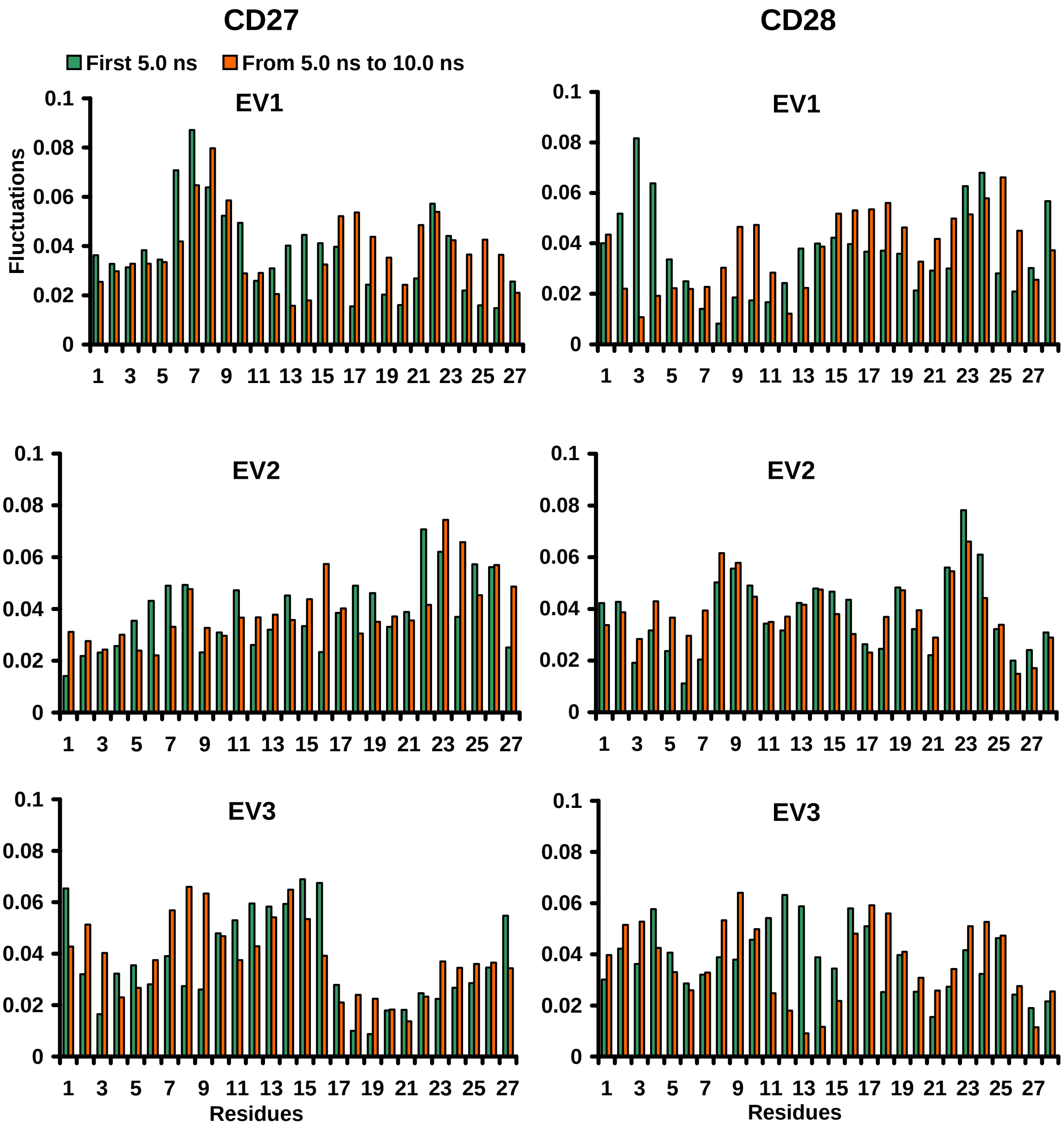


Figure 15S. Decomposition for periods of 5.0 ns of the fluctuations of atomic coordinates (in Å), averaged per residue, for the first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectories of CD27 and CD28.[2]

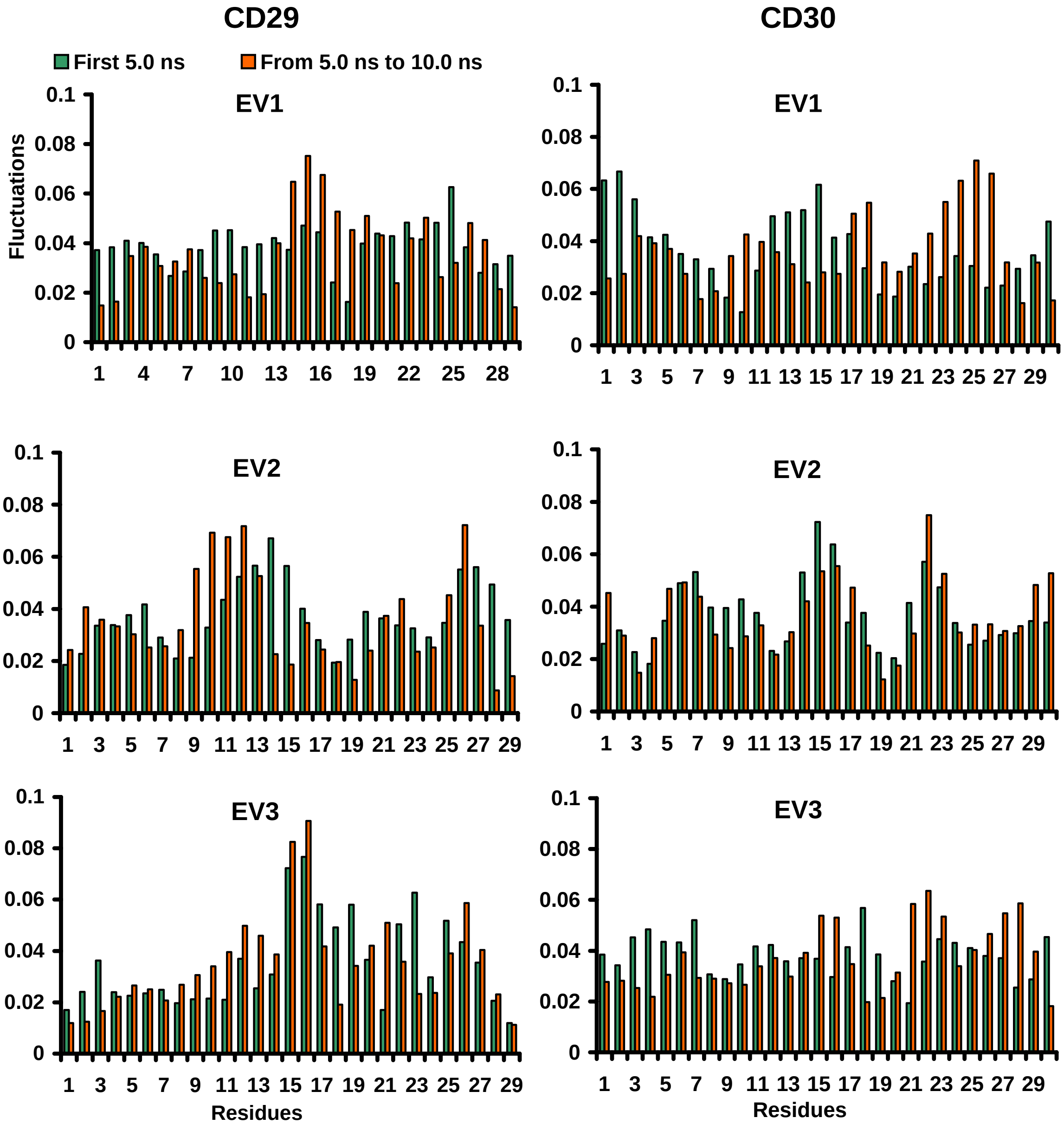


Figure 16S. Decomposition for periods of 5.0 ns of the fluctuations of atomic coordinates (in Å), averaged per residue, for the first three eigenvectors having the largest contribution to the total variance estimated by the PCA analysis of the simulation trajectories of CD27 and CD28.[2]

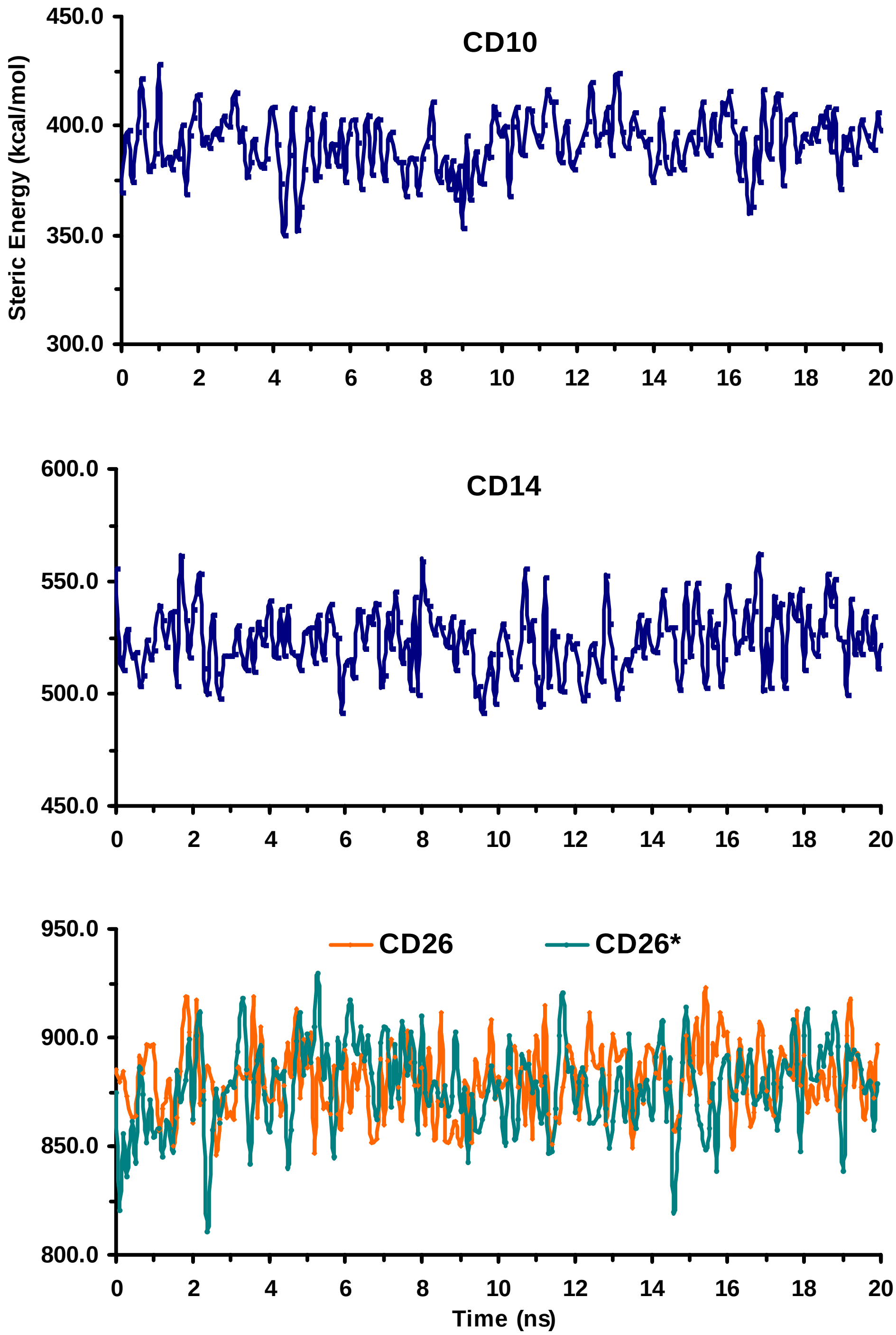


Figure 17S. Minimized total steric energies of snapshots from the simulation trajectories of CD10, CD14, CD26 and CD26* obtained with the NMODE module of AMBER.[1] The sampled structures were extracted with a step 100.0 ps.

References

[1] Gotsev, M. G.; Ivanov, P. M. *ARKIVOC* **2007** *(xiii)* 167-189.

[2] Gotsev, M. G.; Ivanov, P. M. *Int. J. Quantum Chem.* **2007**, *10*, 1657-1672.

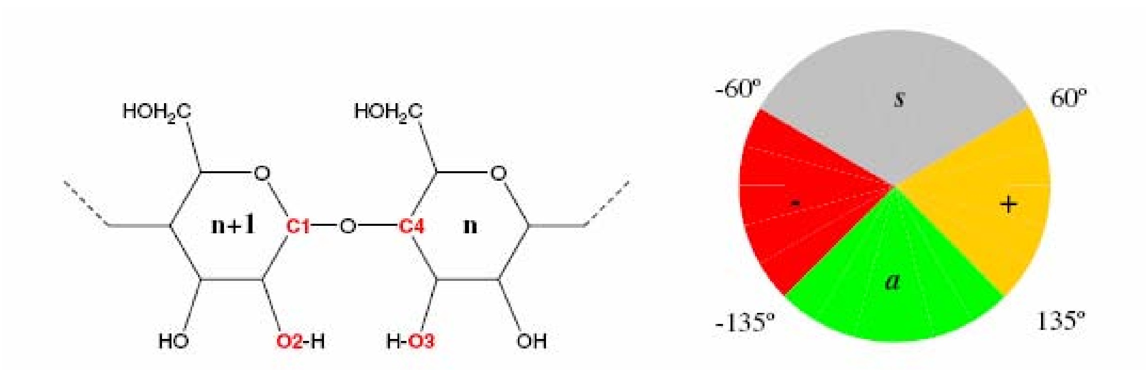


Figure 18S. Definition of the relative orientation for a pair of glucose units as derived from the *flip* dihedral angle (O3(n)···C4(n)···C1(n+1)···O2(n+1)).

TABLE S-3: Values of the *flip* dihedral angles designated by a letter-code (Fig. 17S) and extracted in steps of 500.0 ps from the simulation trajectories of CD10, CD14, CD26 and CD26*.

CD10	flip1	flip2	flip3	flip4	flip5	flip6	flip7	flip8	flip9	flip10
2	s	+	-	s	-	s	+	-	s	s
500	s	a	-	-	s	-	a	-	s	s
1000	-	+	s	s	s	s	a	-	s	s
1500	s	a	-	s	s	s	a	-	-	s
2000	s	+	-	s	s	s	a	s	-	s
2500	s	a	s	-	s	-	+	s	-	s
3000	s	a	s	-	s	s	a	-	s	s
3500	s	+	-	s	s	s	+	s	s	s
4000	s	+	s	-	s	s	a	-	-	s
4500	s	a	s	s	s	s	+	-	s	s
5000	s	+	s	s	s	s	a	-	s	-
5500	s	a	s	-	s	s	a	-	-	s
6000	s	a	-	s	s	s	a	s	s	s
6500	s	+	-	s	s	s	a	-	s	s
7000	s	+	s	s	s	s	+	-	s	s
7500	s	a	-	s	s	s	+	s	s	s
8000	-	a	-	s	s	-	+	s	-	s
8500	s	a	-	s	s	s	a	-	s	-
9000	-	+	s	s	s	-	+	s	s	s
9500	s	a	-	s	s	-	+	s	s	s
10000	s	a	s	-	s	s	+	s	s	s
10500	s	+	s	s	s	s	+	-	s	-
11000	s	a	-	s	s	s	a	-	s	s
11500	-	+	s	s	s	s	+	s	-	s
12000	s	a	-	s	s	s	a	s	-	s
12500	s	+	s	s	-	-	+	s	-	s
13000	s	+	s	-	s	s	a	-	s	s
13500	s	+	-	-	s	-	+	s	-	s
14000	s	a	s	s	s	-	+	-	s	s
14500	s	+	s	s	s	-	a	-	s	s
15000	s	+	-	s	-	s	+	-	s	-
15500	s	a	-	s	s	s	a	-	-	s
16000	s	+	s	-	s	-	a	-	s	s
16500	-	+	s	s	-	s	+	s	s	s
17000	s	+	s	s	s	s	+	s	s	s
17500	-	a	-	s	s	s	+	-	s	s
18000	s	+	-	s	s	-	a	-	s	s
18500	s	a	-	s	s	s	a	-	s	s
19000	s	a	s	s	s	-	+	s	s	-
19500	-	+	s	s	s	s	a	-	s	s
20000	s	+	-	s	s	s	+	-	-	s

CD14	flip1	flip2	flip3	flip4	flip5	flip6	flip7	flip8	flip9	flip10	flip11	flip12	flip13	flip14
2	s	s	s	s	s	-	+	s	s	s	-	s	s	a
500	s	-	s	s	s	s	+	-	s	s	s	s	s	+
1000	s	s	s	s	s	s	a	-	s	s	-	s	s	a
1500	s	s	s	-	s	s	-	-	s	-	s	s	-	+
2000	s	s	s	s	s	s	s	-	s	s	s	s	s	a
2500	s	s	s	-	s	s	s	-	-	s	-	s	s	a
3000	s	-	-	s	s	s	-	-	-	-	s	s	s	+
3500	-	-	s	s	s	s	-	-	-	s	s	s	s	a
4000	s	s	-	s	s	s	-	-	-	s	s	-	s	a
4500	s	s	s	s	s	s	-	-	s	s	s	s	s	a
5000	s	s	-	s	s	s	a	-	-	s	-	s	s	a
5500	s	s	s	-	s	s	a	-	s	s	s	s	s	a
6000	s	s	s	s	s	s	a	-	-	s	s	s	s	+
6500	s	s	s	s	s	-	-	s	s	s	s	s	s	a
7000	s	-	s	-	s	s	-	-	-	s	s	-	s	+
7500	s	-	s	s	s	-	a	s	-	s	s	s	s	a
8000	s	s	-	s	s	s	a	s	-	s	s	s	s	a
8500	s	-	s	s	s	s	a	-	s	s	s	s	s	a
9000	s	s	s	s	s	s	-	s	-	s	s	s	s	a
9500	s	s	s	s	s	s	a	-	s	s	-	s	s	a
10000	s	s	s	-	s	-	-	-	s	s	s	s	-	a
10500	s	s	s	s	s	-	-	s	s	s	s	s	-	a
11000	s	s	s	s	s	-	-	s	s	s	s	s	s	a
11500	-	s	s	s	s	-	-	s	s	s	s	s	-	a
12000	s	-	s	s	s	s	-	-	-	s	s	s	-	a
12500	-	s	s	s	s	s	s	s	-	s	s	s	s	a
13000	s	-	s	s	s	s	s	-	-	s	s	-	s	a
13500	-	s	s	s	s	s	s	s	s	s	-	s	s	a
14000	s	s	s	s	s	s	s	-	-	s	s	s	s	+
14500	-	s	-	s	s	s	s	-	-	s	s	s	s	a
15000	s	s	s	s	s	s	-	-	-	-	s	s	s	a
15500	-	-	s	s	s	s	-	-	-	s	s	s	s	-
16000	-	-	s	s	s	s	s	-	-	s	s	s	s	-
16500	-	-	s	s	s	-	-	-	-	s	s	s	s	-
17000	-	-	s	s	s	-	-	-	-	s	s	s	-	-
17500	-	s	s	s	s	-	-	-	s	s	s	s	-	-
18000	-	s	s	s	s	-	-	-	s	s	s	s	-	-
18500	s	s	s	s	s	-	-	-	s	s	s	-	-	-
19000	-	s	s	s	s	-	-	-	s	s	s	s	-	-
19500	-	s	s	s	s	-	-	-	s	s	s	-	-	-
20000	-	s	s	s	s	-	-	-	s	s	s	s	-	s

CD26	flip1	flip2	flip3	flip4	flip5	flip6	flip7	flip8	flip9	flip10	flip11	flip12	flip13	flip14	flip15	flip16	flip17	flip18	flip19	flip20	flip21	flip22	flip23	flip24	flip25	flip26
2	-	s	s	s	s	-	s	s	s	s	s	s	a	s	s	s	s	s	s	s	-	s	s	s	s	-
500	s	s	s	s	s	-	s	s	s	s	s	s	a	s	s	s	s	s	s	s	-	s	s	s	s	-
1000	s	-	s	s	s	-	s	s	s	s	s	s	a	s	-	s	s	s	s	s	s	s	s	s	s	-
1500	-	s	s	s	s	s	s	s	-	s	s	s	a	s	-	s	s	s	-	s	s	s	s	s	s	-
2000	s	s	s	s	s	s	s	s	s	s	s	s	a	s	-	s	s	s	-	s	s	s	s	-	s	-
2500	s	s	s	s	s	s	s	s	s	s	s	s	a	s	s	s	s	-	-	-	s	s	s	s	-	s
3000	s	s	s	s	s	s	s	s	s	s	s	s	a	-	s	s	-	-	-	s	s	s	s	-	s	s
3500	s	s	s	s	s	-	s	s	s	s	s	s	a	s	s	s	-	-	-	s	s	s	-	s	-	s
4000	s	s	s	s	s	s	s	s	s	s	s	s	a	s	-	s	s	-	-	s	s	s	s	-	-	s
4500	-	s	s	s	s	s	s	s	s	s	s	s	a	-	s	s	-	-	-	s	s	s	s	-	s	s
5000	s	s	s	s	s	s	s	s	s	s	s	s	a	s	-	s	-	-	-	s	s	s	-	s	-	s
5500	s	s	s	s	s	s	s	s	s	s	s	s	a	-	s	-	-	-	s	s	s	s	s	s	s	s
6000	s	s	s	s	s	s	s	s	s	s	s	s	a	-	s	s	-	-	-	s	s	s	s	-	-	s
6500	s	s	s	s	s	s	s	s	s	s	s	s	a	s	s	s	-	-	-	s	s	s	s	-	s	s
7000	s	s	s	s	s	s	s	s	s	s	s	-	a	-	s	s	s	-	-	s	s	s	s	-	-	s
7500	s	s	-	s	s	s	s	s	s	s	s	-	a	s	s	s	s	-	-	s	s	s	s	-	-	s
8000	s	s	s	s	s	s	s	s	s	s	s	s	+	s	s	s	-	-	-	-	s	s	s	-	s	s
8500	s	s	s	s	s	s	s	s	s	s	s	s	+	s	s	-	-	-	s	-	s	s	s	s	-	s
9000	s	s	s	s	s	s	s	s	s	s	s	s	+	s	s	s	s	-	-	s	s	s	s	s	-	s
9500	s	s	s	s	s	s	s	s	s	s	s	s	a	-	s	s	-	-	s	-	s	s	s	-	s	-
10000	s	s	-	s	s	s	s	s	s	s	-	s	a	-	-	s	s	-	-	s	s	s	s	s	s	s
10500	s	s	s	s	s	s	s	s	s	s	s	s	a	s	s	-	-	s	-	s	s	s	s	s	-	s
11000	s	s	s	s	s	s	s	s	s	-	s	s	a	s	-	s	s	-	s	s	s	s	s	s	-	s
11500	s	s	s	s	s	s	s	s	s	s	s	s	a	s	-	s	s	-	-	s	s	s	s	-	-	s
12000	s	s	s	s	s	s	s	s	s	s	s	s	a	s	s	s	s	-	-	s	-	s	s	s	s	-
12500	s	s	s	-	s	s	s	s	s	s	s	s	a	-	s	s	s	-	-	-	s	s	s	s	s	s
13000	s	s	s	s	s	s	s	s	s	s	s	s	a	-	s	s	s	-	-	s	s	s	s	s	s	s
13500	s	s	s	s	s	s	s	s	s	s	s	s	a	-	s	s	s	-	-	s	s	s	s	s	s	s
14000	s	s	s	s	s	s	s	s	s	s	s	s	a	-	s	-	s	-	-	s	s	s	s	s	s	-
14500	s	s	s	s	s	s	s	s	s	s	s	s	a	s	s	s	-	-	-	-	s	s	s	s	s	-
15000	s	s	s	s	s	s	s	s	s	s	s	s	+	s	s	-	s	s	-	-	s	s	s	s	s	-
15500	s	s	s	s	s	s	s	s	s	s	s	s	a	-	s	s	-	s	-	-	s	s	s	s	s	-
16000	s	s	s	s	s	s	s	s	s	s	s	s	a	-	s	s	s	-	-	s	s	s	s	s	-	-
16500	s	s	s	s	s	s	s	s	s	s	s	s	a	s	-	s	s	s	-	-	s	s	s	s	s	-
17000	s	s	s	s	s	s	s	s	s	s	-	s	a	s	-	s	s	-	-	s	s	s	s	s	s	s
17500	s	s	s	s	s	s	s	s	s	s	s	-	a	s	s	s	s	-	-	-	s	s	s	s	-	-
18000	s	s	s	s	s	s	s	s	s	s	s	s	a	s	-	s	-	-	-	s	s	s	s	s	s	-
18500	s	s	s	s	s	s	s	s	s	s	s	s	a	-	s	-	s	s	-	-	s	s	s	s	s	-
19000	s	s	s	s	s	s	s	s	s	s	s	s	a	-	-	s	s	s	-	-	s	s	s	s	s	-
19500	s	s	s	s	s	s	s	s	s	s	s	-	a	s	s	s	-	s	-	-	s	s	s	s	s	-
20000	s	s	s	s	s	s	s	s	s	s	s	-	a	s	s	s	s	s	-	-	s	s	s	s	-	s

CD26*	flip1	flip2	flip3	flip4	flip5	flip6	flip7	flip8	flip9	flip10	flip11	flip12	flip13	flip14	flip15	flip16	flip17	flip18	flip19	flip20	flip21	flip22	flip23	flip24	flip25	flip26
2	s	s	-	s	s	s	s	s	s	s	s	s	a	s	s	s	s	s	s	s	s	s	s	s	s	a
500	s	s	-	s	s	-	s	s	-	s	s	s	a	s	-	s	s	-	s	s	s	s	s	s	s	a
1000	s	s	s	s	s	-	s	s	s	s	s	s	a	-	s	s	s	s	s	s	s	s	s	s	s	a
1500	s	s	s	s	s	s	s	s	s	s	s	s	a	s	s	s	s	s	s	s	s	s	s	s	s	a
2000	s	s	s	s	s	-	s	s	-	s	s	s	a	s	s	s	s	s	s	s	s	s	s	s	s	a
2500	s	s	s	s	s	-	s	s	s	s	s	s	a	s	-	s	s	s	s	s	s	s	s	s	s	a
3000	s	-	s	s	s	s	s	s	s	s	s	s	a	s	s	s	s	s	s	s	s	s	s	s	s	a
3500	s	s	s	s	s	-	s	-	s	s	s	s	-	s	s	s	s	s	s	s	s	s	s	s	s	a
4000	s	-	s	s	s	s	-	-	s	s	s	s	-	s	-	s	s	s	s	s	s	s	s	s	s	a
4500	-	s	s	-	-	-	s	s	s	s	s	s	-	s	s	s	s	s	s	s	s	s	s	s	-	a
5000	s	-	s	s	-	-	s	s	-	s	s	-	s	s	s	s	s	s	-	s	s	s	s	s	s	a
5500	s	-	s	s	-	-	-	s	s	s	s	s	s	s	s	s	s	s	s	s	s	s	s	s	s	a
6000	s	s	s	s	-	-	-	s	s	s	s	s	-	s	s	s	s	s	s	s	s	s	s	s	s	a
6500	s	s	s	-	s	-	-	-	s	s	s	-	s	s	s	-	s	s	s	s	s	s	s	s	s	a
7000	s	-	s	s	s	-	-	s	s	s	s	s	-	-	s	s	s	s	s	s	s	s	s	s	s	a
7500	s	s	s	s	s	-	-	-	s	s	s	s	s	-	s	s	s	s	s	s	s	s	s	s	-	+
8000	s	s	s	-	-	s	-	s	s	s	s	-	-	-	s	s	s	-	s	s	s	s	s	s	s	+
8500	s	s	s	-	s	-	-	s	s	s	s	s	-	-	s	-	s	s	s	s	s	s	s	s	s	a
9000	-	s	s	-	s	-	-	-	s	s	s	s	-	s	s	-	s	s	s	s	s	s	s	s	s	a
9500	-	s	s	s	s	s	-	-	s	s	s	-	-	-	s	s	s	s	s	s	s	s	s	s	s	a
10000	s	s	s	s	-	s	-	-	s	s	s	s	-	-	s	s	s	s	s	s	s	s	s	s	s	a
10500	s	s	s	-	s	-	-	-	s	s	s	s	-	-	-	s	s	s	s	s	s	s	s	s	s	a
11000	s	-	s	s	s	-	-	-	s	s	s	s	-	-	s	s	s	s	s	s	s	s	s	s	s	a
11500	s	s	s	s	s	s	-	-	s	s	s	s	-	s	-	s	s	s	s	s	s	s	s	s	s	a
12000	s	s	s	s	s	-	-	s	s	s	-	s	-	-	s	s	s	s	s	s	s	s	s	s	s	+
12500	s	s	s	s	s	s	s	-	s	s	s	s	-	s	-	s	s	s	s	s	s	s	-	s	s	a
13000	s	s	s	s	s	s	-	-	s	s	s	s	-	s	-	s	s	s	s	s	s	s	s	s	s	a
13500	s	s	s	s	s	s	-	-	s	s	s	s	-	-	-	s	s	s	s	s	s	s	s	s	s	a
14000	s	s	-	-	s	-	-	-	s	s	s	s	-	s	-	s	s	s	s	s	s	s	s	s	s	+
14500	s	s	s	s	s	s	-	s	s	s	s	s	-	-	s	s	s	s	s	s	s	s	s	s	s	a
15000	-	s	-	s	s	-	-	-	s	s	s	-	-	s	-	s	s	s	s	s	s	s	s	s	s	a
15500	s	s	-	s	s	-	-	s	s	s	s	s	-	-	s	s	s	s	-	s	s	s	s	s	s	a
16000	-	s	-	s	s	-	-	s	s	s	s	s	-	-	s	s	s	s	s	s	s	s	s	s	s	a
16500	-	s	-	-	s	-	s	s	s	s	s	-	s	-	s	s	s	s	s	s	s	s	s	s	s	a
17000	s	-	-	s	-	s	-	s	s	s	s	s	-	s	-	s	s	s	s	-	s	s	s	s	s	+
17500	-	s	s	s	s	-	s	s	s	s	s	-	-	-	s	s	s	s	s	s	s	s	s	s	s	a
18000	s	s	s	s	s	s	-	s	s	s	s	s	-	-	s	s	s	s	s	s	s	s	s	s	s	a
18500	-	s	s	-	-	s	-	s	s	s	s	-	-	s	s	s	s	s	s	s	s	s	s	s	s	a
19000	s	s	s	s	-	-	s	s	s	s	s	s	-	-	s	s	s	s	s	s	s	s	s	s	s	a
19500	s	s	s	s	-	-	-	-	s	s	s	s	-	s	-	s	s	s	s	s	s	s	s	s	s	a
20000	-	s	s	s	s	s	-	s	s	s	s	s	-	-	-	s	s	s	s	s	s	s	s	s	s	a