ELECTRONIC SUPPLEMENTARY INFORMATION

Computational study on the intramolecular self-organization of the macrorings of some 'giant' cyclodextrins (CDn, n = 40, 70, 85, 100)

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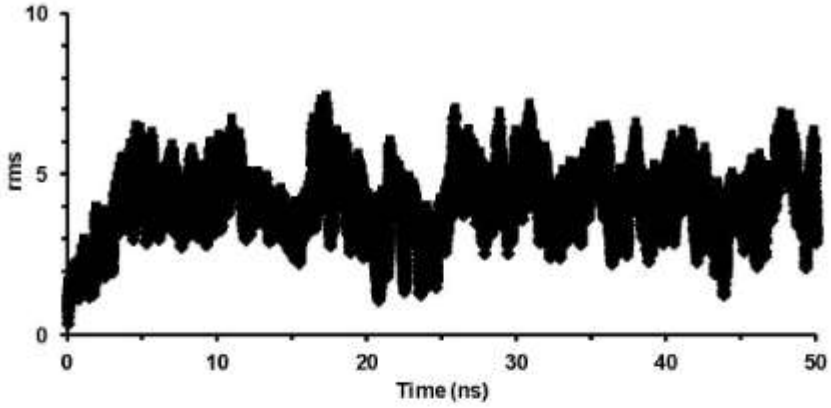
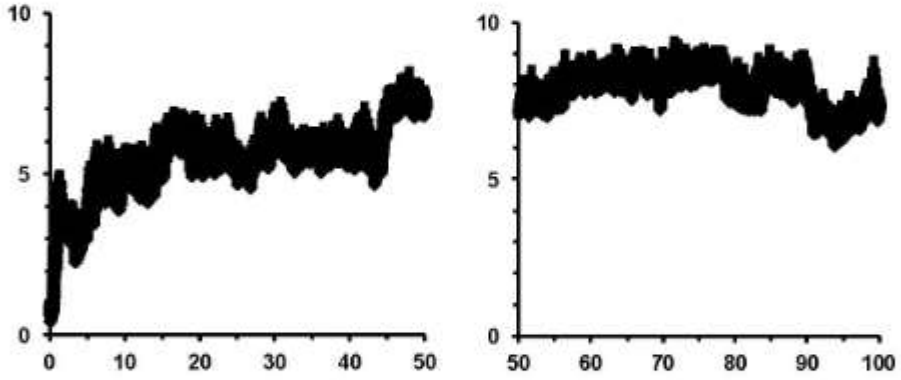
(continued file *_si-002)

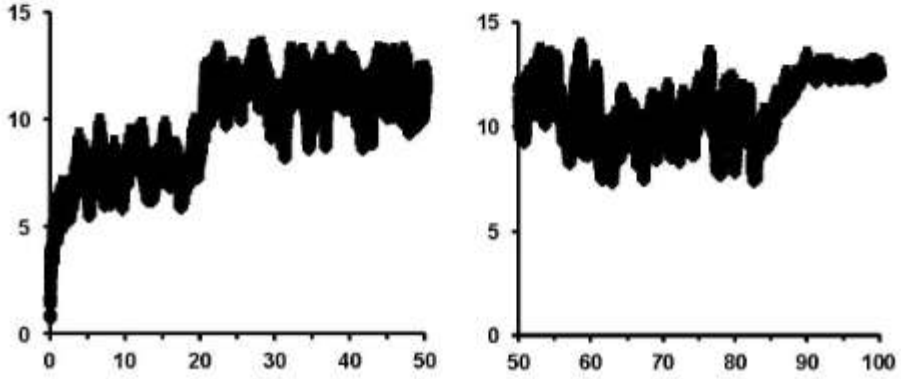
CD14



CD26



CD40



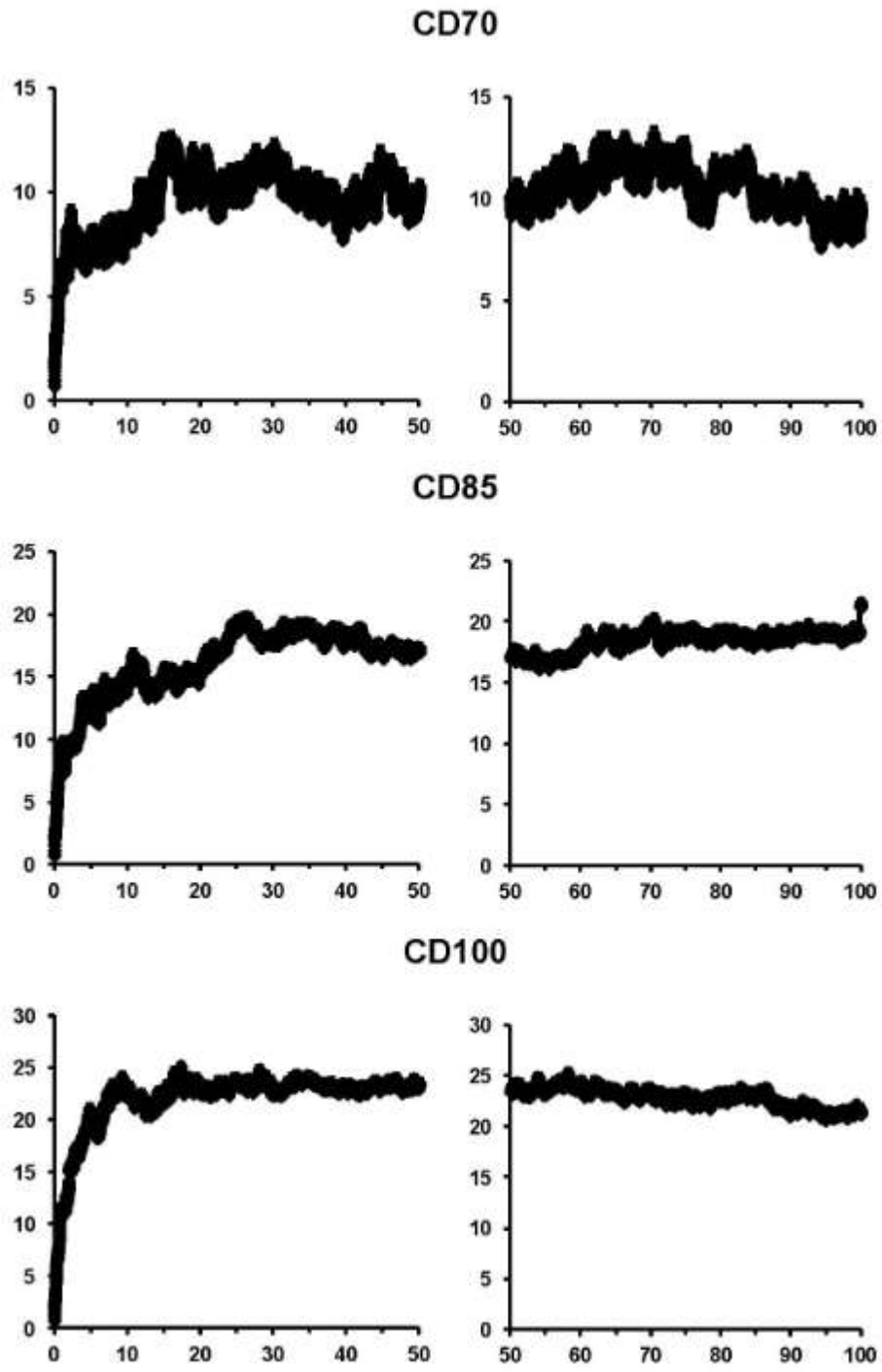


Fig. S8. Rms deviations of atomic coordinates (in Å) relative to the starting set of coordinates.

Table S1. - Computed Distances (Å), Bond Angles and Dihedral Angles (in degrees) of Neighboring Glucose Units Obtained from the MD Simulations in Water and Comparison with Experimental Determinations (experimental data from Table 1 of Ref. [1] and Ref. [23])[a]

		CD6	**CD7**	**CD8**	**CD9**	**CD10**	**CD14**	**CD26**[b]
I. Experimental Data								
Number of glucose units		6	7	8	9	10	14	26
Cavity diameter		4.7-5.3	6.0-6.5	7.5-8.3				
Height of the cone		7.9±1	7.9±1	7.9±1				
Volume of the cavity		174	262	472				
Φ	av.	109.2	109.8	108.9	112.1	99.4	103.4	103.6
	min.	102.0	102.3	103.6	88.4	94.1	96.6	91.1
	max.	114.9	118.6	123.2	141.2	102.1	110.2	115.3
Ψ	av.	128.8	127.6	127.1	124.7	106.1	112.6	115.3
	min.	115.1	114.2	111.9	97.6	96.3	103.6	97.4
	max.	148.7	140.0	138.5	144.5	122.0	135.2	131.4
O4(n)…O4(n-1) …O4(n-2)	av.	119.9	128.3	134.9	136.6	138.2	138.2	126.4
	min.	116.9	125.2	133.5	125.7	126.7	131.6	117.9
	max.	122.3	132.5	136.9	149.9	145.9	142.5	136.7
O4(n)…O4(n-1)	av.	4.24	4.38	4.50	4.49	4.49	4.54	4.39
	min.	4.16	4.27	4.43	4.26	4.36	4.45	4.11
	max.	4.30	4.50	4.59	4.73	4.63	4.61	4.56
O2(n)…O3(n-1)	av.	2.98	2.88	2.82	2.91	2.93	2.83	2.86
	min.	2.90	2.80	2.76	2.74	2.85	2.76	2.65
	max.	3.15	2.98	2.91	3.23	3.01	2.90	3.10

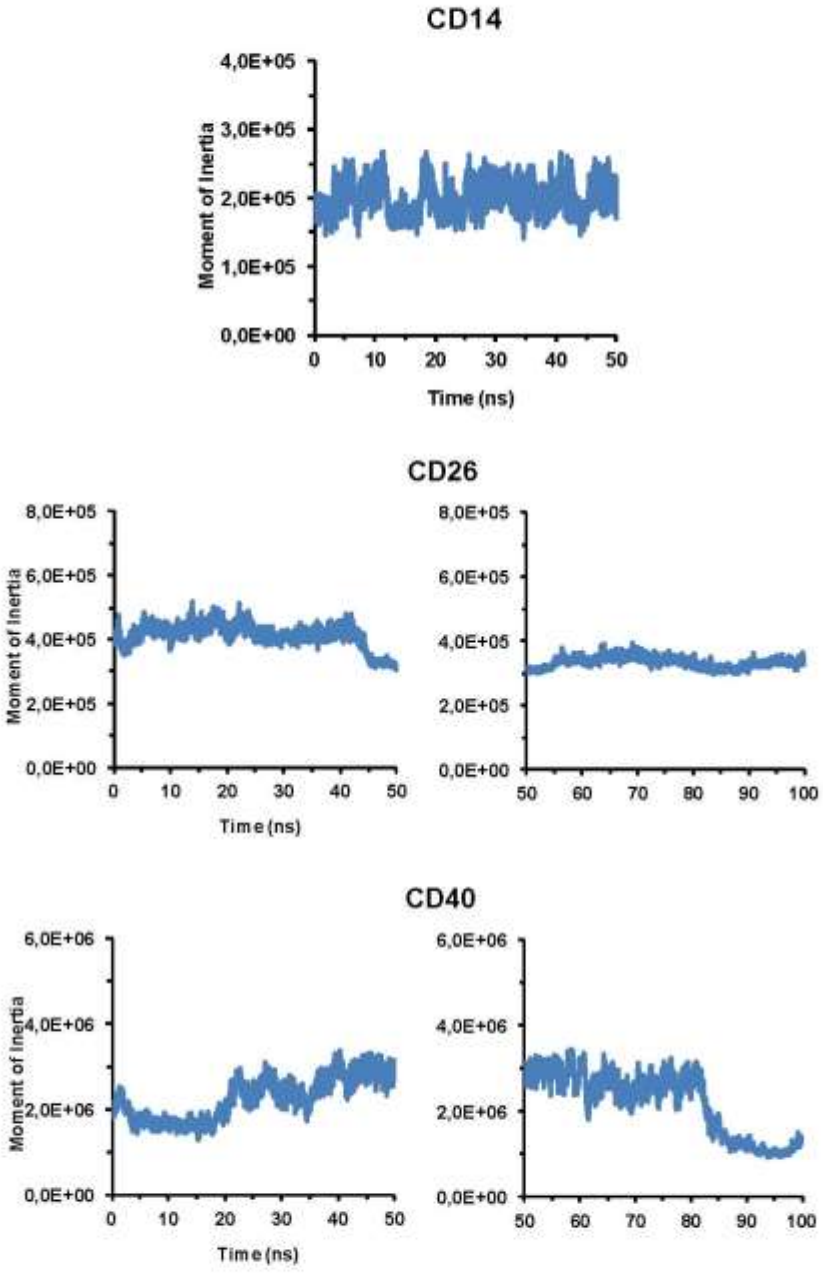
Table S1. – (continued)

II. Computed Data								
	O4(n)…O4(n-1)				**O2(n)…O3(n-1)**			
	av.	rms	max.	min.	av.	rms	max.	min.
CD14	4.7	0.2	5.9	3.6	3.8	0.5	6.3	2.4
CD26	4.7	0.2	6.0	3.0	3.8	0.5	6.6	2.4
CD40	4.7	0.2	5.9	2.7	3.7	0.6	6.3	2.4
CD70	4.7	0.2	5.9	2.8	3.6	0.5	6.5	2.4
CD85	4.7	0.2	5.9	2.6	3.7	0.5	6.3	2.5
CD100	4.7	0.2	6.1	2.9	3.8	0.5	6.6	2.4
	C1(n)—O4(n-1)—C4(n-1)				**O4(n)…O4(n-1)…O4(n-2)**			
	av.	rms	max.	min.	av.	rms	max.	min.
CD14	115.5	3.7	134.3	99.0	138.4	9.6	179.5	81.1
CD26	115.8	3.8	135.4	98.2	135.1	10.0	179.7	62.6
CD40	115.1	3.8	134.4	97.9	142.3	8.9	179.9	78.8
CD70	115.3	3.7	136.1	98.5	139.3	8.1	179.9	78.4
CD85	115.3	3.8	135.2	97.9	139.9	8.2	179.8	75.5
CD100	115.3	3.8	138.9	97.8	141.4	8.0	179.9	70.7
	O4(n)…O4(n-1)…O4(n-2)…O4(n-3)				**O3(n)…C4(n)…C1(n+1)…O2(n+1)**			
	av.		rms		av.		rms	
CD14	-5.2		27.6		-18.8		25.7	
CD26	-4.1		22.6		-16.7		24.6	
CD40	-28.7		35.6		-42.8		29.1	
CD70	-15.9		27.1		-27.7		25.1	
CD85	-25.3		28.8		-37.3		25.3	
CD100	-29.9		30.1		-42.2		25.9	

Table S1. – (continued)

	Φ **O5(n)—C1(n)—O4(n-1)—C4(n-1)**		**Ψ** **C1(n)—O4(n-1)—C4(n-1)—C3(n-1)**	
	av.	rms	av.	rms
CD14	88.2	15.9	81.4	16.1
CD26	89.1	14.2	81.5	18.9
CD40	86.4	16.3	93.5	19.6
CD70	90.9	15.7	91.8	17.4
CD85	86.6	15,4	91.6	16.1
CD100	84.4	14.9	88.7	17.2

[a] Units are: distances (Å), angles (°), volumes (Å^3). [b] The data refer to the helical part.


CD14
4,0E+05
3,0E+05
2,0E+05
1,0E+05
0,0E+00
Moment of Inertia
0
10
20
30
40
50
Time (ns)
CD26
8,0E+05
6,0E+05
4,0E+05
2,0E+05
0,0E+00
Moment of Inertia
0
10
20
30
40
50
Time (ns)
50
60
70
80
90
100
CD40
6,0E+06
4,0E+06
2,0E+06
0,0E+00
Moment of Inertia
0
10
20
30
40
50
Time (ns)
50
60
70
80
90
100

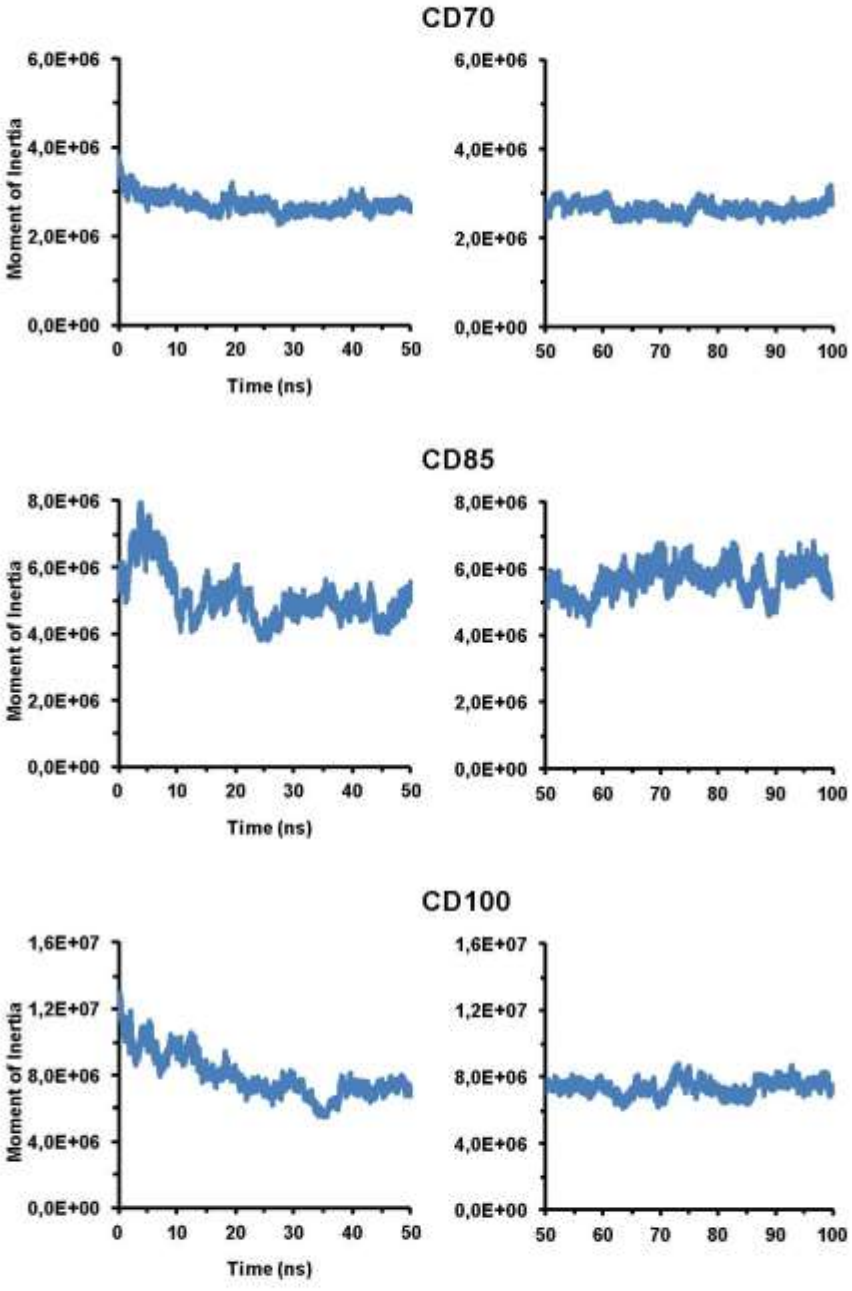
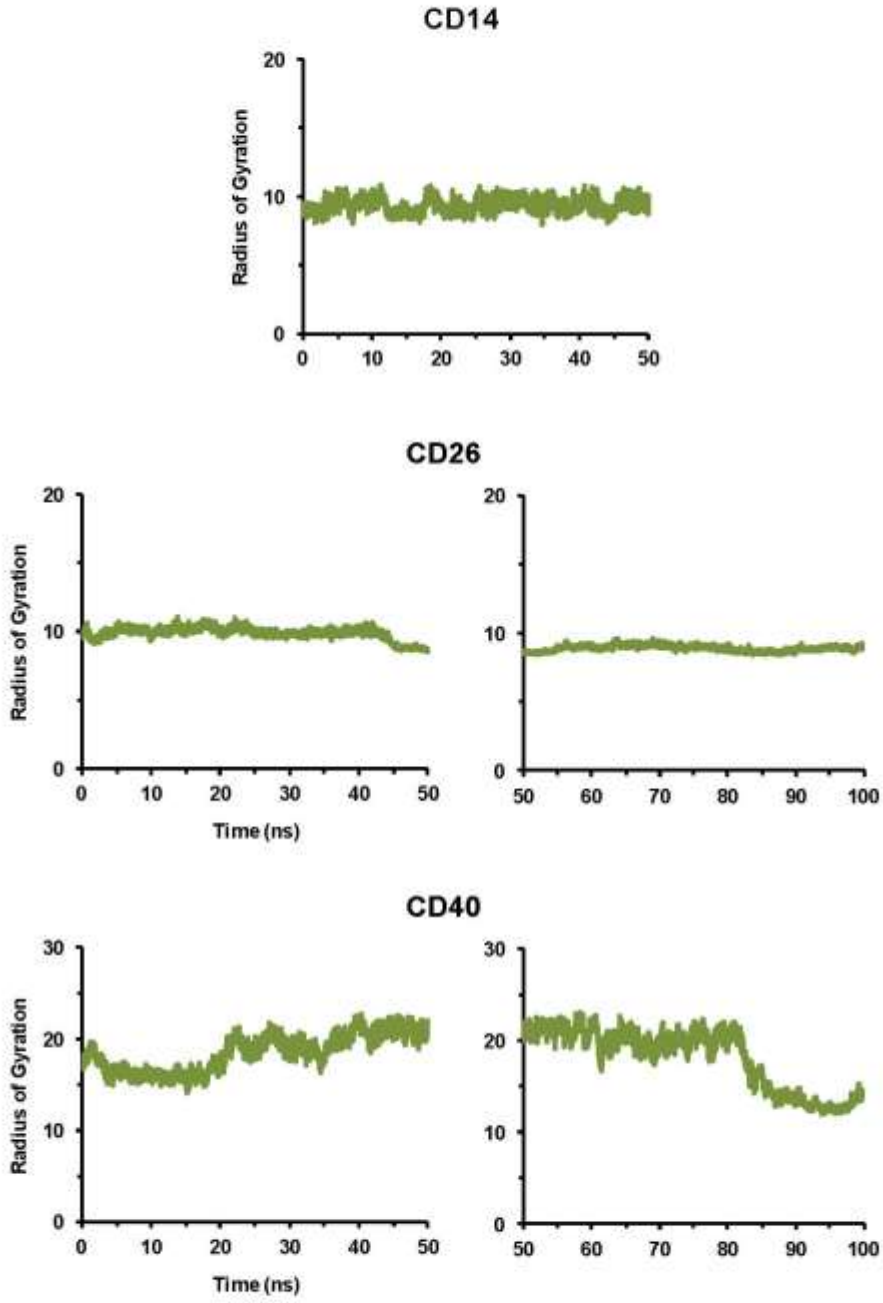


Fig. S9. Variation with the time of the moments of inertia.


CD14
Radius of Gyration
20
10
0
0
10
20
30
40
50
CD26
Radius of Gyration
20
10
0
0
10
20
30
40
50
20
10
0
50
60
70
80
90
100
Time (ns)
CD40
Radius of Gyration
30
20
10
0
0
10
20
30
40
50
30
20
10
0
50
60
70
80
90
100
Time (ns)

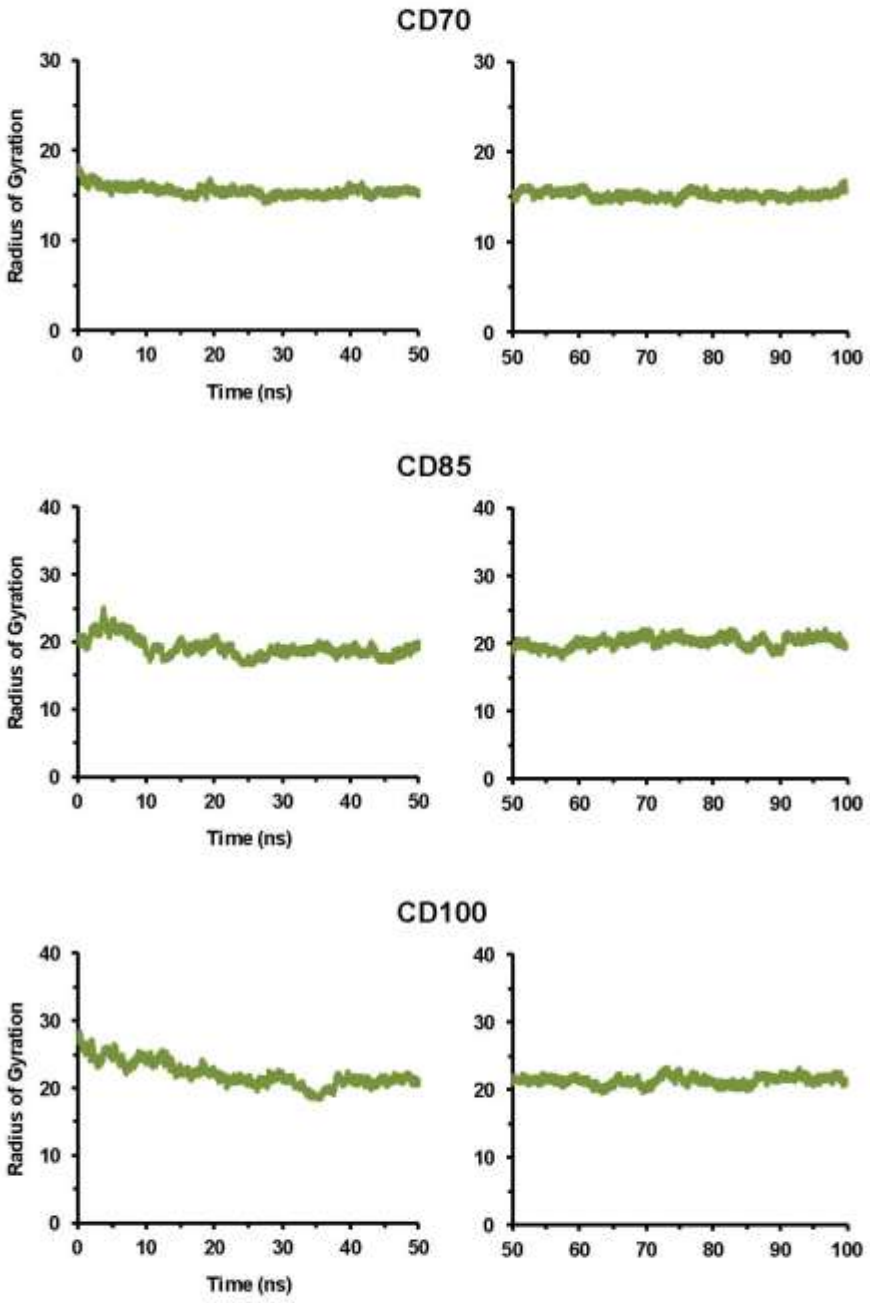
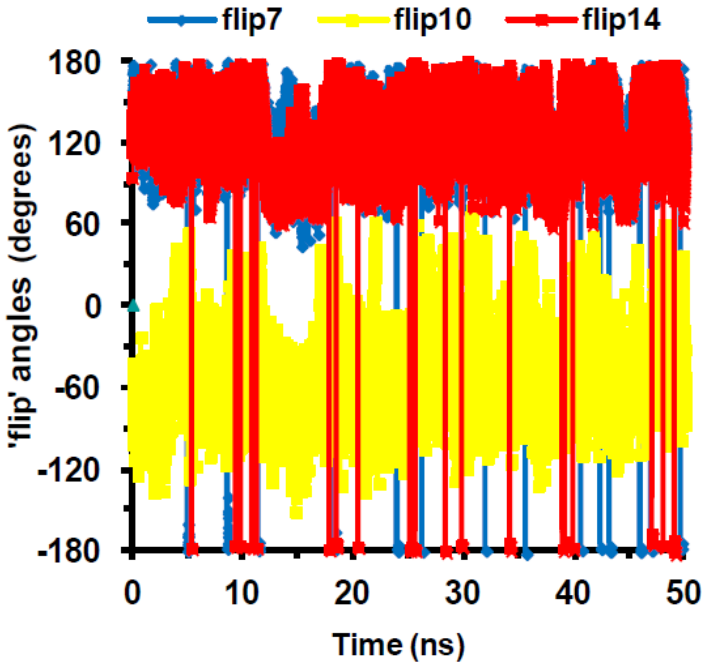
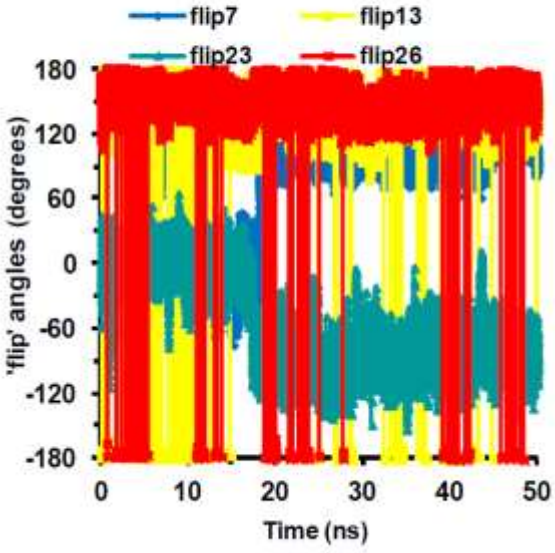


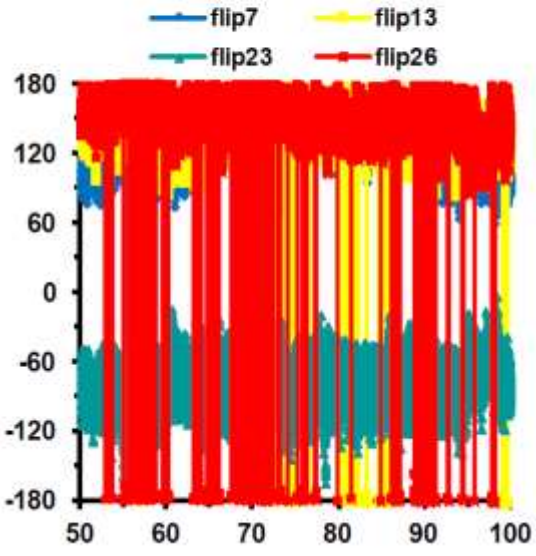
Fig. S10. Variation with the time of the radius of gyration.

CD14

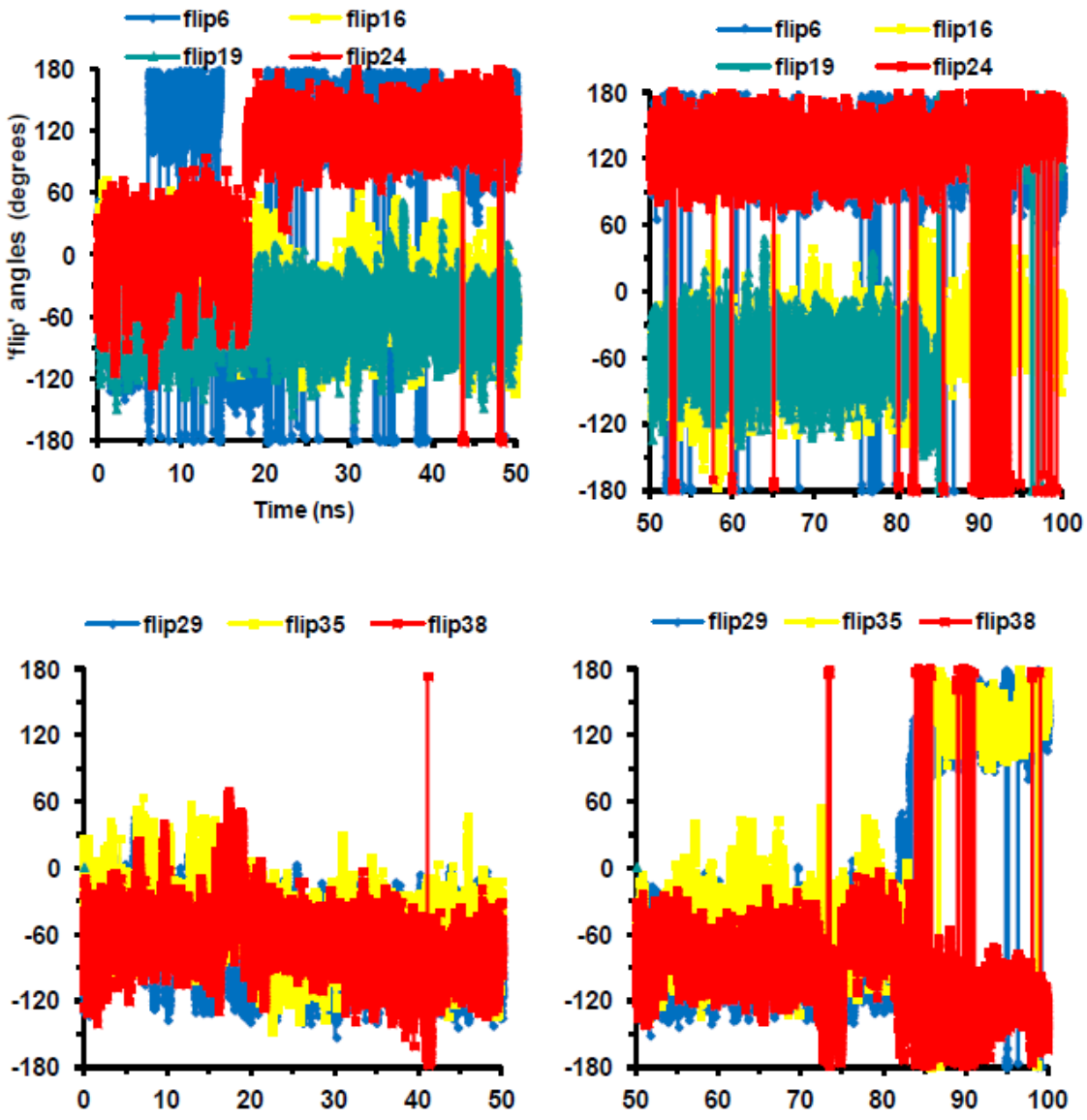

flip7
flip10
flip14
180
120
60
0
-60
-120
-180
'flip' angles (degrees)
0
10
20
30
40
50
Time (ns)

CD26

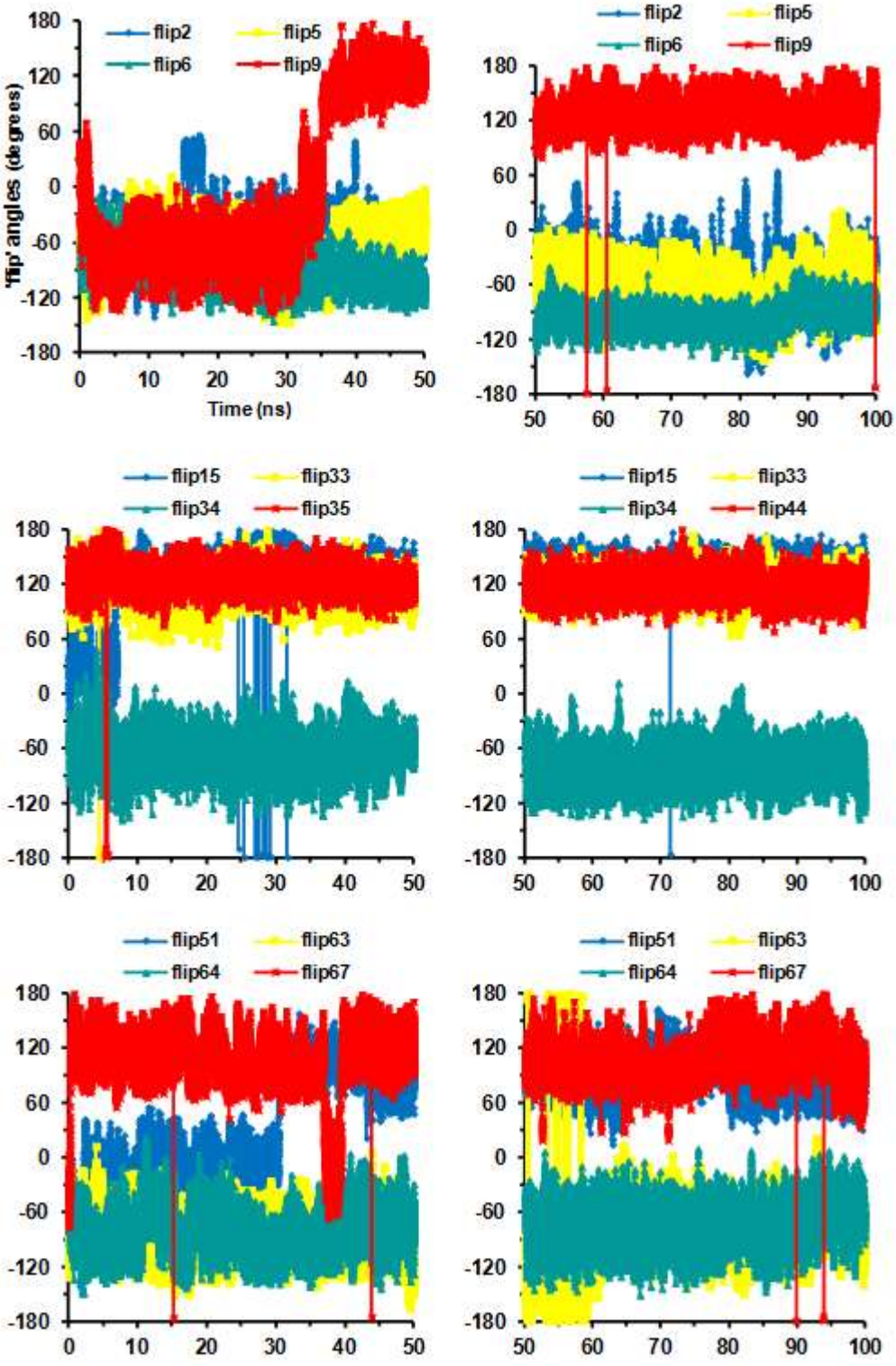

flip7
flip13
flip23
flip26
180
120
60
0
-60
-120
-180
'flip' angles (degrees)
0
10
20
30
40
50
Time (ns)


flip7
flip13
flip23
flip26
180
120
60
0
-60
-120
-180
50
60
70
80
90
100

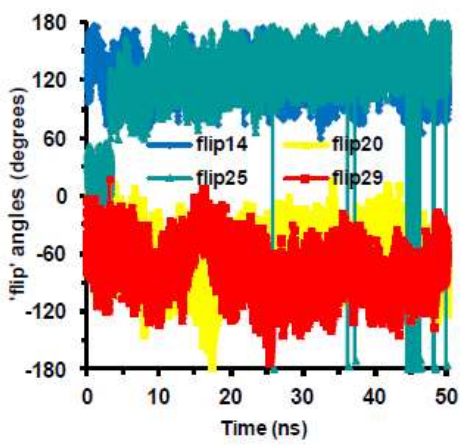
CD40

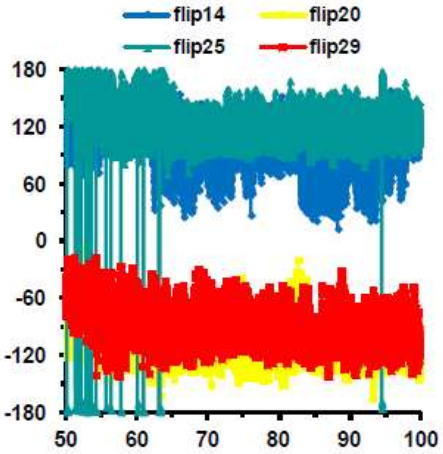

flip6
flip16
flip19
flip24
'flip' angles (degrees)
Time (ns)
flip29
flip35
flip38

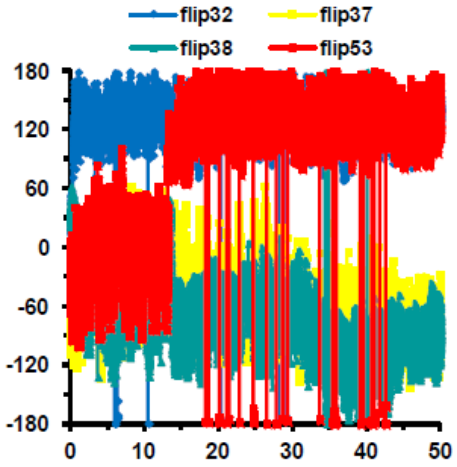
CD70


flip2
flip5
flip6
flip9
'flip' angles (degrees)
Time (ns)
flip15
flip33
flip34
flip35
flip44
flip51
flip63
flip64
flip67

CD85


'flip' angles (degrees)
Time (ns)
flip14
flip20
flip25
flip29


flip14
flip20
flip25
flip29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flip37
flip38
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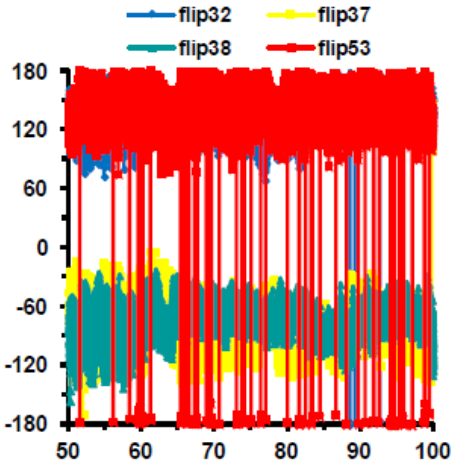
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flip38
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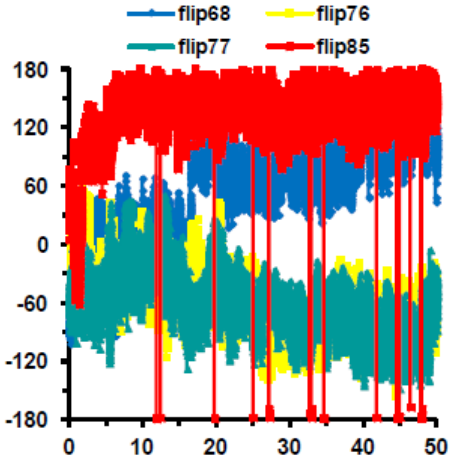
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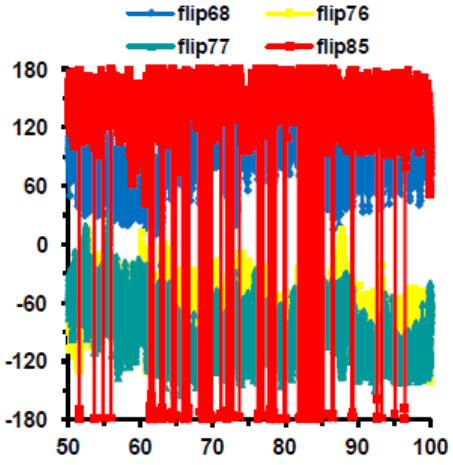
flip76
flip77
flip85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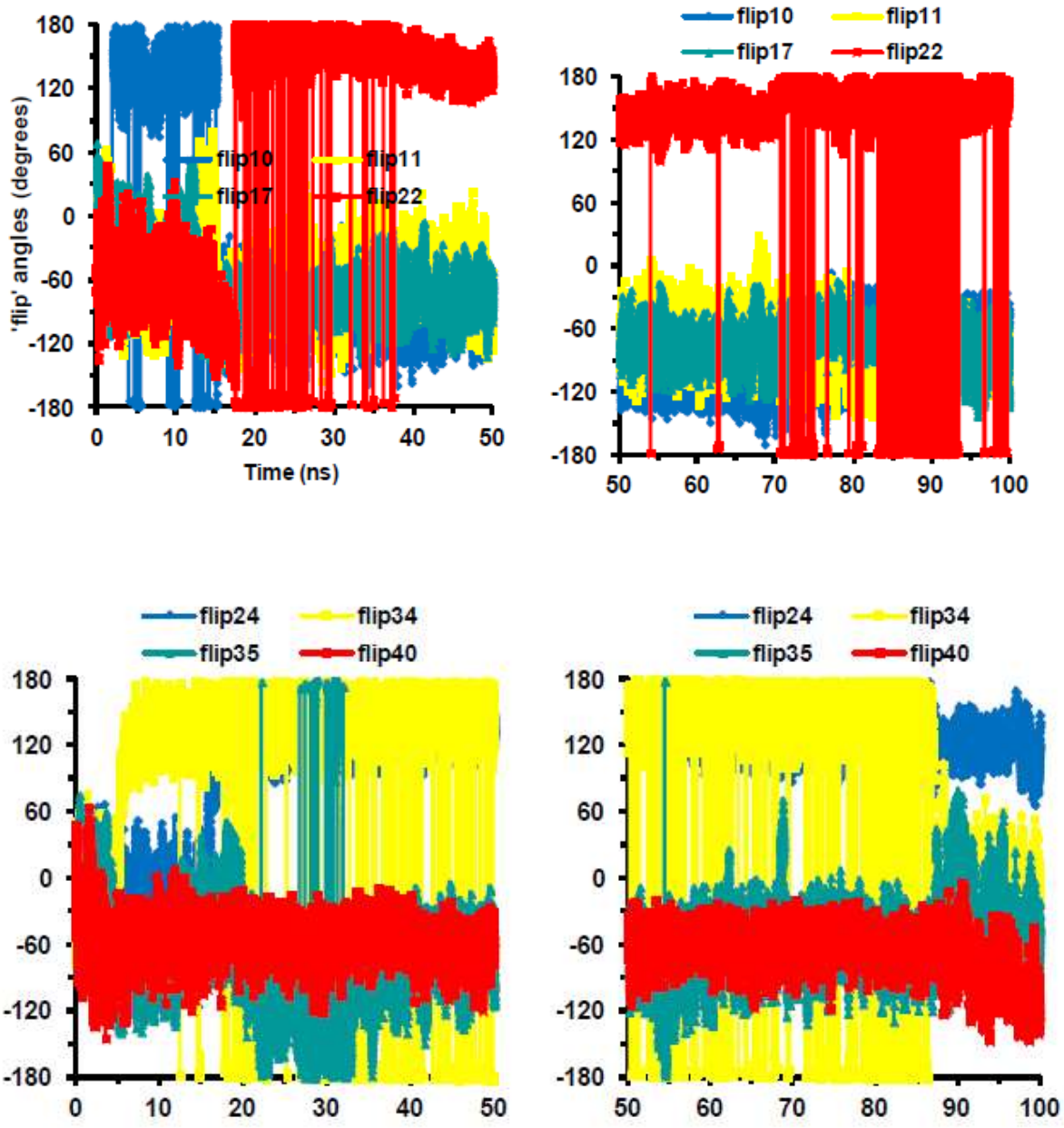
flip85

CD100


'flip' angles (degrees)
Time (ns)
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flip11
flip17
flip22
flip24
flip34
flip35
flip40

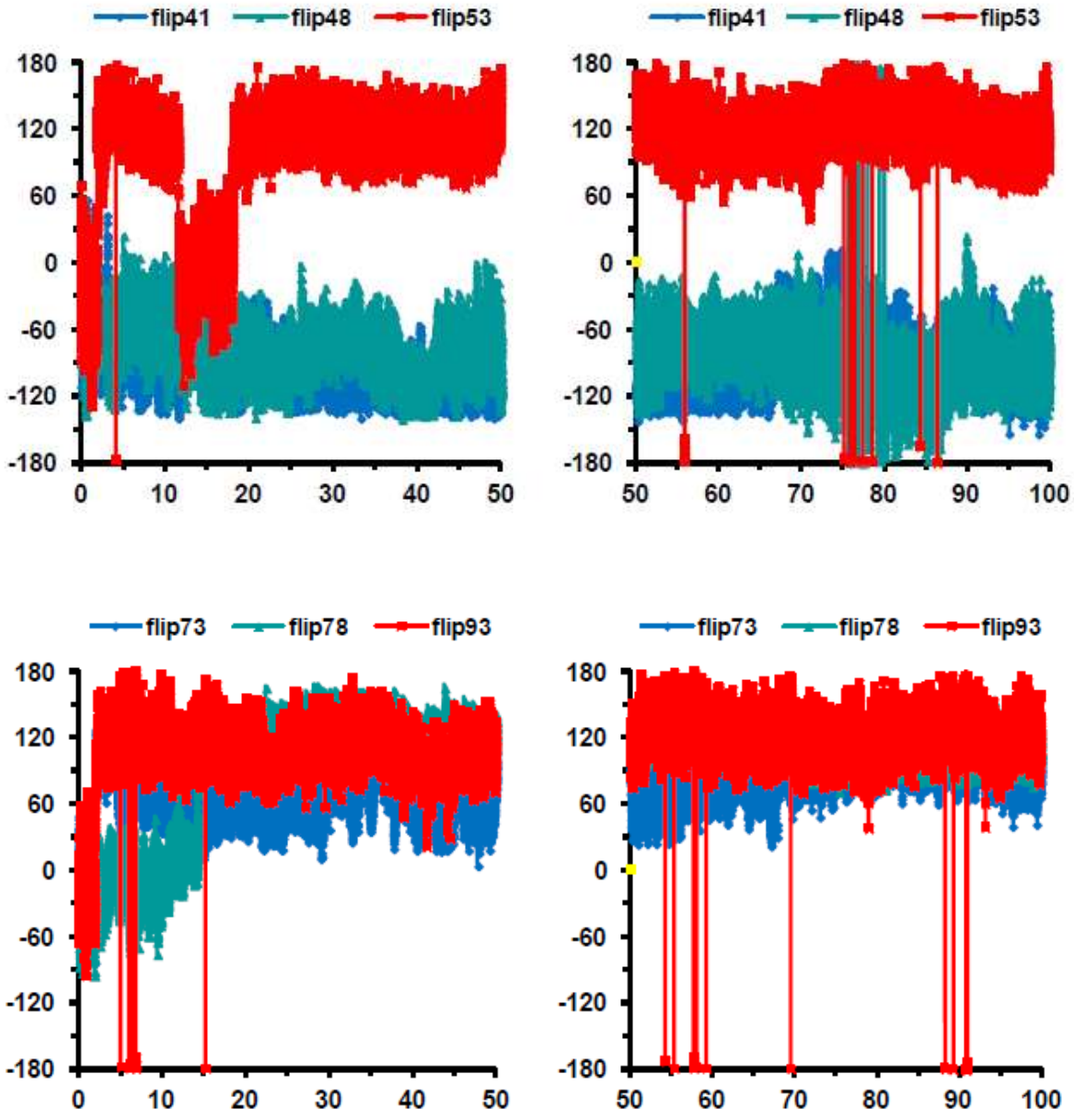
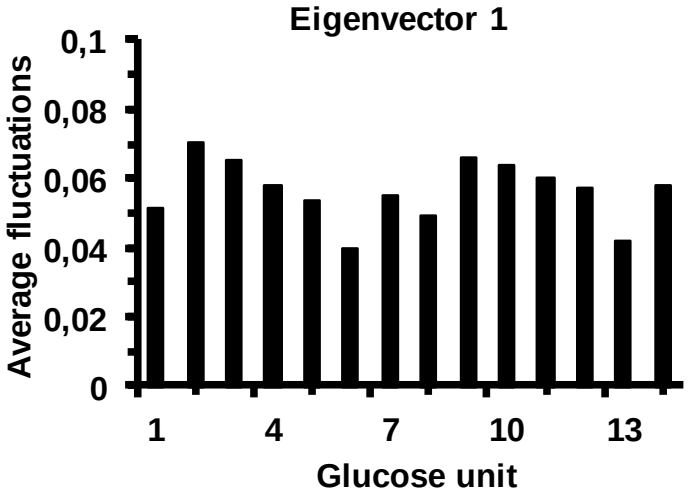


Fig. S11. Variation of *flip* angles.

CD14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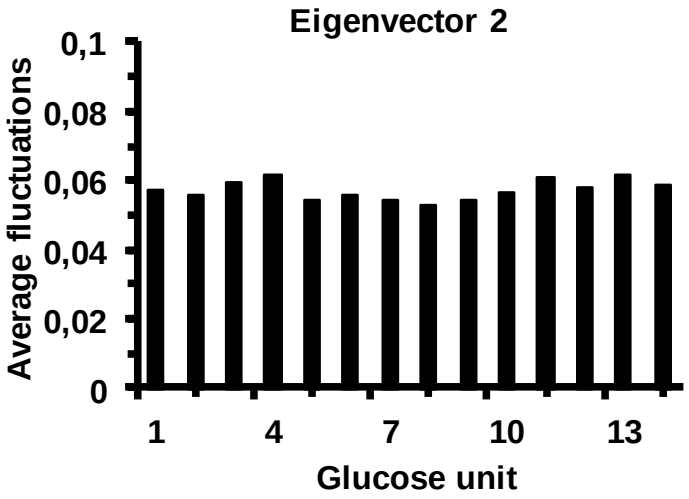
0,06
0,04
0,02
0
1
4
7
10
13
Glucose unit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0,08
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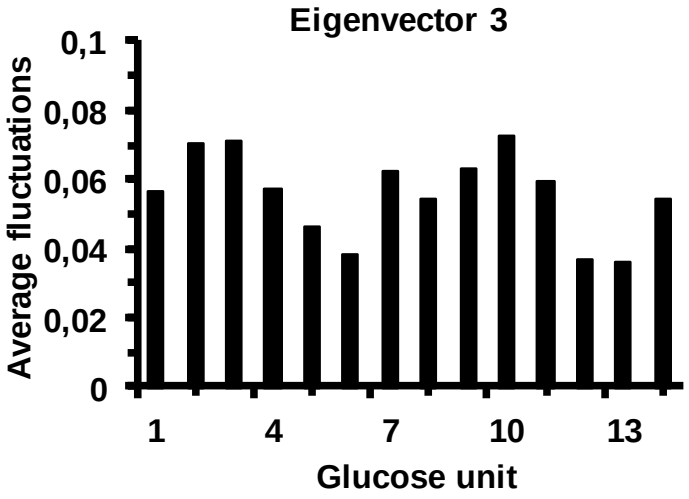
0,04
0,02
0
1
4
7
10
13
Glucose unit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Average fluctuations
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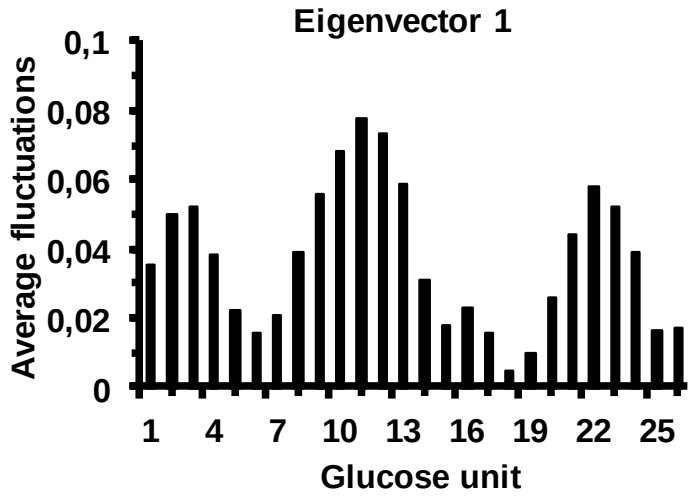
0,06
0,04
0,02
0
1
4
7
10
13
Glucose unit

CD26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0,02
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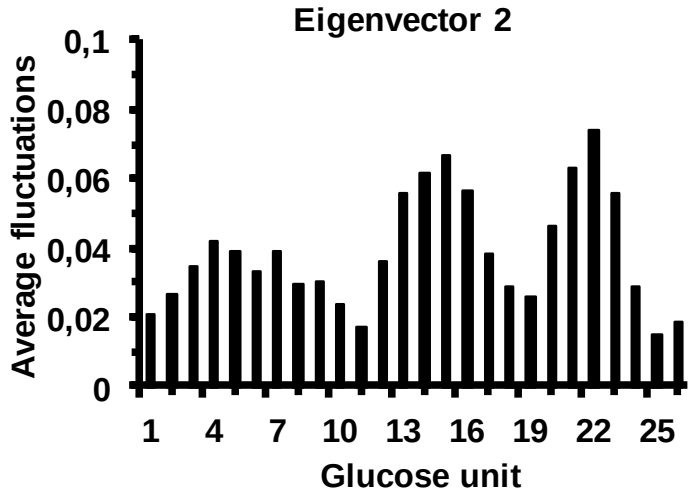
Glucose unit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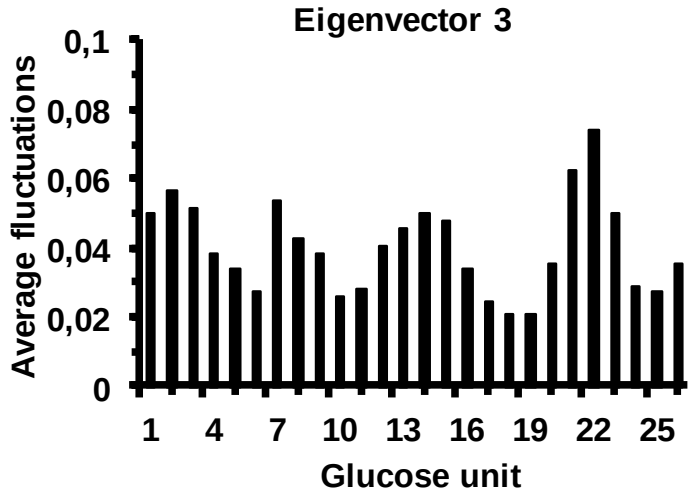
Glucose unit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0,06
0,04
0,02
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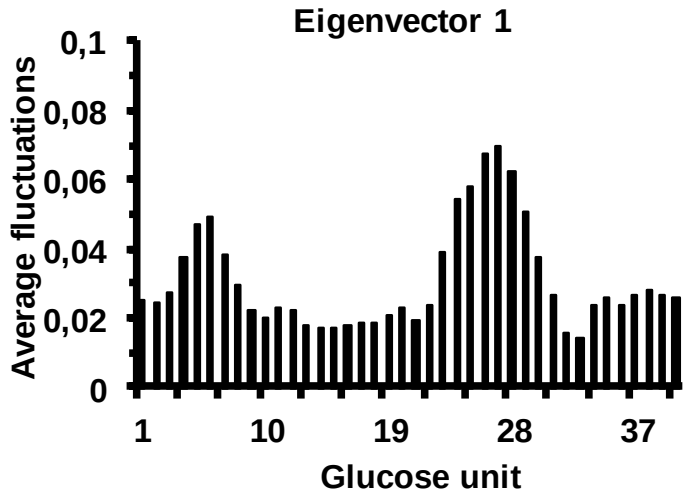
1 4 7 10 13 16 19 22 25
Glucose unit

CD40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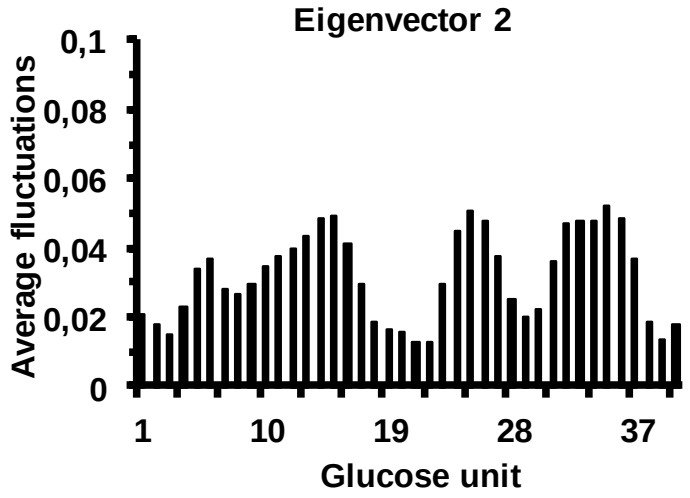
0,08
0,06
0,04
0,02
0
1
10
19
28
37
Glucose unit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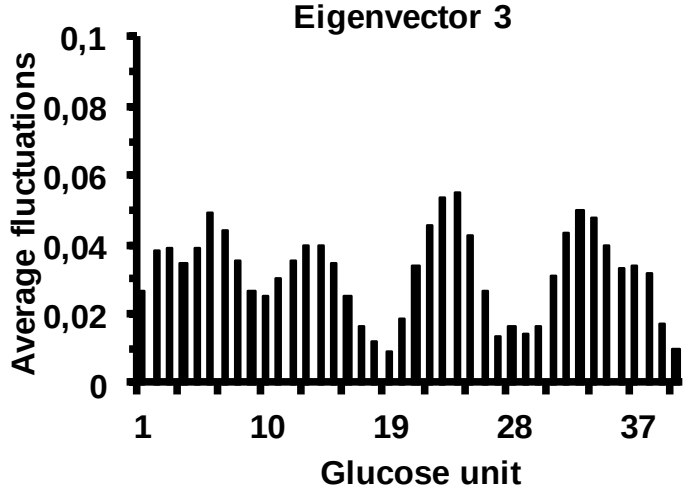
0,02
0
1
10
19
28
37
Glucose unit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0,02
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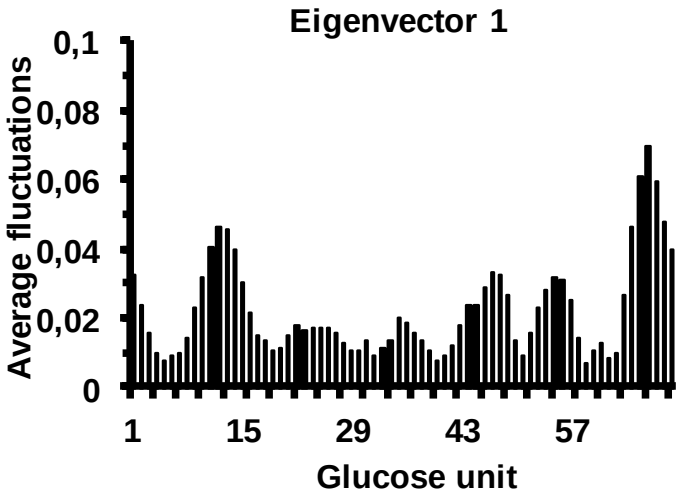
1
10
19
28
37
Glucose unit

CD70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Average fluctuations
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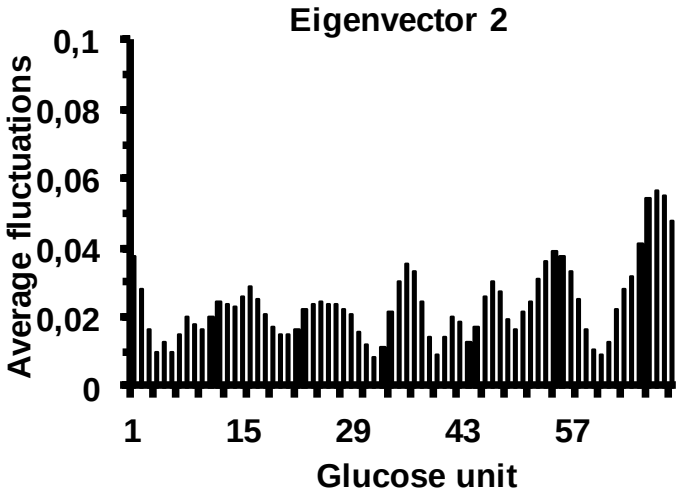
0,06
0,04
0,02
0
1
15
29
43
57
Glucose unit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Average fluctuations
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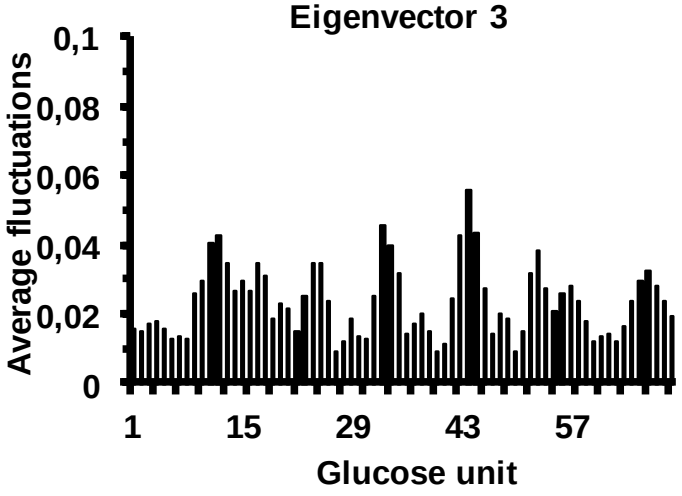
0,06
0,04
0,02
0
1
15
29
43
57
Glucose unit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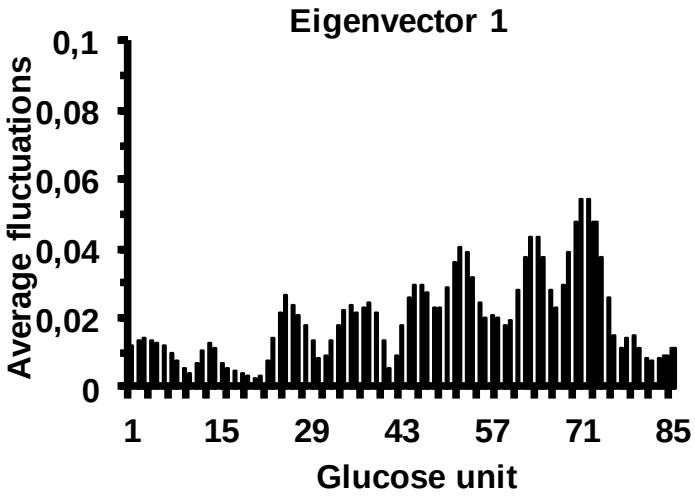
Average fluctuations
0,1
0,08
0,06
0,04
0,02
0
1
15
29
43
57
Glucose unit

CD85


Eigenvector 1
Average fluctuations
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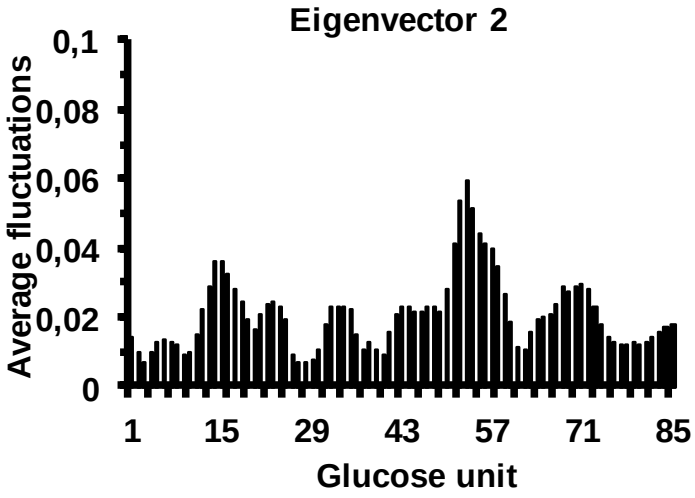
0,08
0,06
0,04
0,02
0
1
15
29
43
57
71
85
Glucose unit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Average fluctuations
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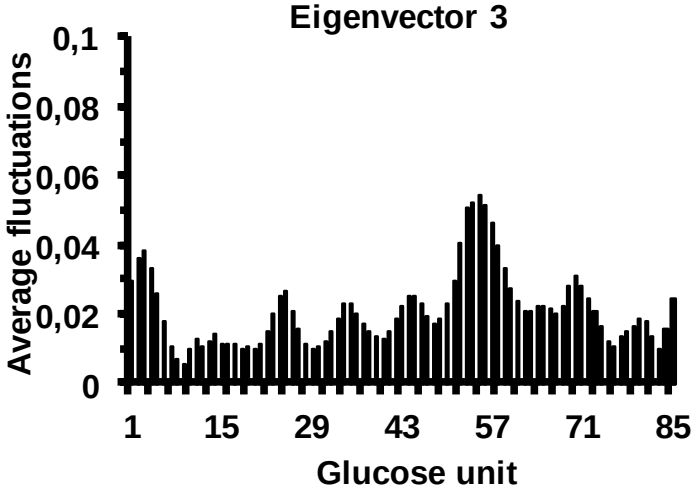
0,06
0,04
0,02
0
1
15
29
43
57
71
85
Glucose unit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Average fluctuations
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0,06
0,04
0,02
0
1
15
29
43
57
71
85
Glucose unit

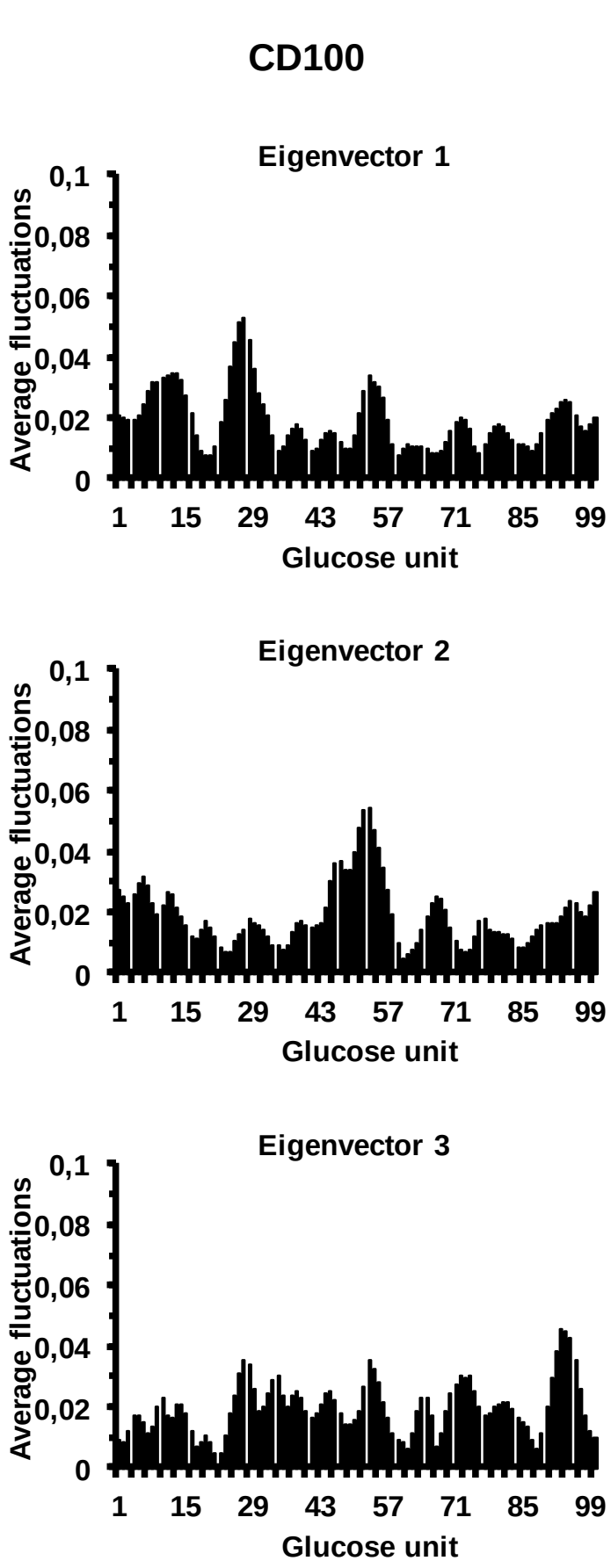

Fig. S12. Fluctuations of atomic coordinates (in Å) for each residue, averaged over the first three animated eigenvectors.

Table S2. - Principal component analysis of the conformational variations[a]

Simulation interval (from … ns to … ns)	0.0 to 10.0	10.0 to 20.0	20.0 to 30.0	30.0 to 40.0	40.0 to 50.0	50.0 to 60.0	60.0 to 70.0	70.0 to 80.0	80.0 to 90.0	90.0 to 100	0.0 to 100.0[b]
CD14 (N_{at} = 294; Q = 90.1 – 90.5)											
N_{ev}	12	9	13	16	13						13
total variance	1683.5	2253.2	1683.6	1390.4	1645.3						1892.1
explained variance	1516.2	2039.4	1520.9	1255.8	1483.9						1709.5
CD26 (N_{at} = 546; Q = 90.0 – 90.4)											
N_{ev}	12	24	44	56	8	41	58	58	55	41	9
total variance	3644.2	2393.6	1258.5	968.9	3899.8	1295.5	969.6	932.7	955.1	1281.0	6797.9
explained variance	3292.7	2156.4	1132.8	872.1	3515.7	1166.2	873.9	840.2	859.9	1153.6	6141.8
CD40 (N_{at} = 840; Q = 90.1 – 91.4)											
N_{ev}	14	11	13	13	14	12	13	12	6	14	11
total variance	19218.3	18319.4	13949.6	16552.6	12388.3	14800.9	12927.9	15464.4	37342.9	6681.8	44633.3
explained variance	17435.9	16611.7	12631.9	15009.1	11164.9	13412.2	11648.4	13979.2	34139.6	6019.1	40503.7
CD70 (N_{at} = 1470; Q = 90.1 – 90.6)											
N_{ev}	15	18	18	24	18	20	29	10	22	21	14
total variance	20169.9	14187.1	13807.1	9864.5	12321.8	8866.4	7344.0	16254.8	9006.4	8994.1	33504.8
explained variance	18252.7	12819.7	12479.1	8890.4	11142.2	7997.4	6613.1	14629.6	8122.8	8117.7	30356.1
CD85 (N_{at} = 1785; Q = 90.0 – 90.5)											
N_{ev}	10	12	7	13	12	18	12	18	16	17	11
total variance	89693.3	45322.4	50322.7	29070.6	25217.4	18831.6	27613.1	14297.9	16731.0	14072.6	108727.9
explained variance	80738.9	40896.6	45515.0	26198.7	22756.2	16951.6	24907.6	12894.7	15104.8	12717.6	98074.3
CD100 (N_{at} = 2100; Q = 90.1 – 90.5)											
N_{ev}	8	10	20	12	23	24	22	18	16	19	14
total variance	176660.6	79654.6	27849.8	36672.4	21895.7	22860.6	22920.8	32124.5	32417.5	26596.8	135510.1
explained variance	159402.1	72075.6	25109.7	33039.4	19758.3	20657.9	20703.0	28932.8	29191.7	24038.7	122336.7

Table S2 (continued)

Eigenvector	Eigenvalues										
CD14											
1	841.3	1299.3	743.0	541.8	761.5						797.8
2	232.9	361.8	283.9	310.4	271.6						407.5
3	151.9	116.0	210.7	100.6	161.0						163.6
4	89.1	72.9	73.4	68.8	84.6						80.4
5	57.6	64.9	51.4	66.3	50.9						70.2
6	40.3	46.9	44.1	38.2	35.0						49.6
7	26.4	35.6	26.5	23.3	28.9						35.2
8	20.0	23.9	21.5	20.7	23.7						23.8
9	16.8	18.1	19.8	17.4	18.2						21.8
10	15.9		15.3	16.0	15.5						20.0
CD26											
1	2061.6	659.9	326.8	264.5	2908.9	549.9	269.2	242.3	333.1	361.0	4414.2
2	433.8	393.3	267.3	108.5	289.2	167.1	124.1	115.4	89.7	212.1	664.4
3	298.6	254.4	102.8	100.7	107.5	71.8	68.1	95.2	57.3	134.4	346.6
4	121.0	186.1	78.4	61.6	62.6	53.5	47.2	50.0	52.2	78.7	238.1
5	95.3	149.8	49.1	38.6	52.6	43.4	38.7	37.8	35.5	53.7	146.0
6	89.6	91.1	40.3	34.2	39.4	31.2	35.2	31.2	31.0	39.4	119.1
7	51.2	67.0	25.7	24.3	29.3	22.6	30.5	28.3	25.2	33.3	87.4
8	44.3	54.4	22.8	18.0	26.3	19.1	24.6	19.7	23.7	26.6	67.8
9	31.0	50.0	21.7	17.3		17.1	20.5	15.7	22.2	21.8	58.1
10	24.9	42.2	17.3	14.6		16.1	18.0	13.7	15.3	17.4	
CD40											
1	5634.8	8177.1	4768.6	6002.5	3572.4	5560.9	4378.3	4778.7	23260.4	2988.5	20073.1
2	4147.6	3014.8	2323.4	2628.9	1785.4	3164.4	2997.8	4060.1	6453.5	1113.9	6052.1
3	2706.6	2254.7	1554.5	2340.4	1514.4	1431.1	1053.1	1982.2	2409.5	747.1	4675.7
4	1348.9	869.0	1031.2	964.2	986.5	888.1	711.2	794.3	716.4	239.0	2804.9
5	880.2	573.6	804.4	699.5	806.0	494.1	590.2	627.0	702.5	207.7	1573.7
6	639.3	507.9	536.1	643.9	595.1	458.3	409.3	381.4	597.2	147.6	1369.4
7	492.4	380.8	431.2	455.3	404.8	410.0	382.6	350.7		119.9	1303.4
8	406.3	260.9	305.1	342.6	329.7	287.8	313.7	302.7		107.4	819.4
9	296.0	236.2	245.8	244.6	299.2	278.9	237.9	247.1		85.7	672.9
10	240.7	176.3	185.7	225.8	247.2	170.8	205.1	191.1		71.7	627.6

Table S2 (continued)

CD70											
1	7156.1	5836.1	5460.9	3238.7	4399.1	3564.0	2314.4	9748.3	3991.3	3003.1	15107.3
2	4038.5	2059.1	2481.7	1885.3	2620.2	1948.8	1249.4	1525.9	1025.4	1656.3	5593.4
3	2099.7	943.1	1121.8	835.0	1021.7	747.6	720.5	952.1	731.3	994.3	3037.1
4	1226.9	846.6	880.8	518.1	771.1	393.1	436.8	693.8	541.3	670.2	1573.1
5	1134.4	742.8	576.2	377.9	505.9	223.8	348.2	426.9	384.5	498.7	1213.8
6	841.3	560.4	556.6	335.7	390.7	204.8	244.1	347.1	259.6	256.4	763.4
7	410.7	338.0	240.2	283.6	276.4	163.8	218.2	314.8	212.3	200.5	557.4
8	247.1	326.3	180.1	222.1	252.0	136.2	166.5	245.5	160.7	121.1	504.4
9	217.5	212.3	162.1	175.1	178.6	92.1	109.2	207.2	136.6	104.3	451.8
10	206.1	169.7	141.2	157.8	132.3	89.9	104.3	168.0	100.2	91.1	392.0
CD85											
1	40823.8	16007.2	21070.8	16585.0	12007.9	6672.7	11726.5	4432.6	7586.0	5140.9	43704.9
2	17840.0	10234.6	17097.4	2480.1	4729.8	3040.9	5378.3	3391.5	2069.1	2492.4	21650.6
3	6240.6	6616.4	3850.8	2096.2	1890.8	1934.5	2275.8	1651.9	1460.8	2035.5	10601.0
4	4538.1	1986.4	1444.8	1238.0	978.9	1118.2	1847.2	792.4	980.6	626.3	6922.6
5	3017.3	1155.4	814.6	794.5	846.5	975.8	855.1	489.5	671.3	575.1	4475.0
6	2183.0	988.9	677.7	628.6	580.5	657.7	812.3	339.7	554.5	445.0	2829.7
7	1902.8	932.2	558.9	549.7	494.8	415.9	546.1	312.3	376.3	279.3	2589.7
8	1710.6	760.5		488.7	346.1	404.5	396.8	286.9	278.6	210.8	1806.5
9	1298.4	697.3		387.5	283.9	328.5	338.0	233.2	246.2	189.3	1374.8
10	1184.4	615.1		294.7	233.9	269.0	263.9	209.5	199.2	144.1	1159.5
CD100											
1	92038.1	37147.9	8384.4	15510.8	6552.1	6355.5	6855.0	8211.5	11351.2	8389.3	57385.7
2	26561.1	13866.3	4913.5	7668.5	3930.4	3283.0	4466.6	6566.8	6312.1	3175.3	25051.1
3	20329.2	7998.3	2923.7	3540.6	2335.7	2354.1	2291.7	3416.1	3267.5	3020.4	8829.6
4	7230.3	3645.0	2313.0	1491.8	1422.3	1531.3	1323.8	2588.8	2117.8	2434.6	6477.9
5	4437.4	2886.2	1201.6	1208.7	850.3	1286.6	1264.8	1827.8	1304.8	1505.7	4841.6
6	4053.7	1695.4	864.9	970.1	803.8	1173.6	766.5	1560.1	1070.9	1343.7	4100.8
7	2719.4	1574.4	809.6	869.1	644.4	737.6	675.3	831.1	763.0	913.0	3299.5
8	2032.8	1268.3	673.6	522.6	478.8	606.9	459.2	694.3	615.8	549.8	2655.4
9		1120.1	438.7	421.1	415.6	478.1	378.0	608.3	418.2	481.8	2500.7
10		873.6	406.4	334.1	331.1	418.6	350.5	502.3	392.3	377.9	2081.5

Table S2 (continued)

Eigenvector	Weight (%)										
CD14											
1	56.4	63.7	49.9	45.0	52.5						47.8
2	15.6	17.7	19.1	25.8	18.7						24.4
3	10.2	5.7	14.1	8.4	11.1						9.8
4	6.0	3.6	4.9	5.7	5.8						4.8
5	3.9	3.2	3.5	5.5	3.5						4.2
6	2.7	2.3	3.0	3.2	2.4						3.0
7	1.8	1.7	1.8	1.9	2.0						2.1
8	1.3	1.2	1.4	1.7	1.6						1.4
9	1.1	0.9	1.3	1.4	1.3						1.3
10	1.1	0.0	1.0	1.3	1.1						1.2
CD26											
1	63.4	33.9	34.3	38.8	82.7	55.4	39.8	37.3	48.6	36.9	71.9
2	13.3	20.2	28.1	15.9	8.2	16.8	18.4	17.8	13.1	21.7	10.8
3	9.2	13.1	10.8	14.8	3.1	7.2	10.1	14.7	8.4	13.7	5.6
4	3.7	9.6	8.2	9.0	1.8	5.4	7.0	7.7	7.6	8.0	3.9
5	2.9	7.7	5.2	5.7	1.5	4.4	5.7	5.8	5.2	5.5	2.4
6	2.8	4.7	4.2	5.0	1.1	3.1	5.2	4.8	4.5	4.0	1.9
7	1.6	3.4	2.7	3.6	0.8	2.3	4.5	4.4	3.7	3.4	1.4
8	1.4	2.8	2.4	2.6	0.7	1.9	3.6	3.0	3.5	2.7	1.1
9	1.0	2.6	2.3	2.5		1.7	3.0	2.4	3.2	2.2	0.9
10	0.8	2.2	1.8	2.1		1.6	2.7	2.1	2.2	1.8	
CD40											
1	33.6	49.7	39.1	41.3	33.9	42.3	38.8	34.8	68.1	51.3	50.2
2	24.7	18.3	19.1	18.1	16.9	24.1	26.6	29.6	18.9	19.1	15.1
3	16.1	13.7	12.8	16.1	14.4	10.9	9.3	14.5	7.1	12.8	11.7
4	8.0	5.3	8.5	6.6	9.4	6.8	6.3	5.8	2.1	4.1	7.0
5	5.2	3.5	6.6	4.8	7.6	3.8	5.2	4.6	2.1	3.6	3.9
6	3.8	3.1	4.4	4.4	5.6	3.5	3.6	2.8	1.7	2.5	3.4
7	2.9	2.3	3.5	3.1	3.8	3.1	3.4	2.6	0.0	2.1	3.3
8	2.4	1.6	2.5	2.4	3.1	2.2	2.8	2.2	0.0	1.8	2.0
9	1.8	1.4	2.0	1.7	2.8	2.1	2.1	1.8	0.0	1.5	1.7
10	1.4	1.1	1.5	1.6	2.3	1.3	1.8	1.4	0.0	1.2	1.6

Table S2 (continued)

CD70											
1	40.7	48.5	46.3	40.3	41.7	47.1	39.1	66.6	52.9	39.5	51.7
2	23.0	17.1	21.0	23.5	24.8	25.8	21.1	10.4	13.6	21.8	19.2
3	11.9	7.8	9.5	10.4	9.7	9.9	12.2	6.5	9.7	13.1	10.4
4	7.0	7.0	7.5	6.5	7.3	5.2	7.4	4.7	7.2	8.8	5.4
5	6.5	6.2	4.9	4.7	4.8	3.0	5.9	2.9	5.1	6.6	4.2
6	4.8	4.7	4.7	4.2	3.7	2.7	4.1	2.4	3.4	3.4	2.6
7	2.3	2.8	2.0	3.5	2.6	2.2	3.7	2.2	2.8	2.6	1.9
8	1.4	2.7	1.5	2.8	2.4	1.8	2.8	1.7	2.1	1.6	1.7
9	1.2	1.8	1.4	2.2	1.7	1.2	1.8	1.4	1.8	1.4	1.5
10	1.2	1.4	1.2	2.0	1.3	1.2	1.8	1.1	1.3	1.2	1.3
CD85											
1	50.6	40.0	46.3	64.9	53.6	42.2	48.0	36.5	52.6	42.4	45.0
2	22.1	25.6	37.6	9.7	21.1	19.2	22.0	27.9	14.3	20.5	22.3
3	7.7	16.5	8.5	8.2	8.4	12.2	9.3	13.6	10.1	16.8	10.9
4	5.6	5.0	3.2	4.8	4.4	7.1	7.6	6.5	6.8	5.2	7.1
5	3.7	2.9	1.8	3.1	3.8	6.2	3.5	4.0	4.7	4.7	4.6
6	2.7	2.5	1.5	2.5	2.6	4.2	3.3	2.8	3.8	3.7	2.9
7	2.4	2.3	1.2	2.2	2.2	2.6	2.2	2.6	2.6	2.3	2.7
8	2.1	1.9	0.0	1.9	1.5	2.6	1.6	2.4	1.9	1.7	1.9
9	1.6	1.7	0.0	1.5	1.3	2.1	1.4	1.9	1.7	1.6	1.4
10	1.5	1.5	0.0	1.2	1.0	1.7	1.1	1.7	1.4	1.2	1.2
CD100											
1	57.7	51.5	36.6	47.7	36.9	34.9	36.4	30.6	41.1	37.8	49.0
2	16.7	19.2	21.4	23.6	22.1	18.0	23.7	24.5	22.9	14.3	21.4
3	12.8	11.1	12.8	10.9	13.1	12.9	12.2	12.7	11.8	13.6	7.5
4	4.5	5.1	10.1	4.6	8.0	8.4	7.0	9.7	7.7	11.0	5.5
5	2.8	4.0	5.2	3.7	4.8	7.1	6.7	6.8	4.7	6.8	4.1
6	2.5	2.4	3.8	3.0	4.5	6.4	4.1	5.8	3.9	6.1	3.5
7	1.7	2.2	3.5	2.7	3.6	4.0	3.6	3.1	2.8	4.1	2.8
8	1.3	1.8	2.9	1.6	2.7	3.3	2.4	2.6	2.2	2.5	2.3
9	0.0	1.6	1.9	1.3	2.3	2.6	2.0	2.3	1.5	2.2	2.1
10	0.0	1.2	1.8	1.0	1.9	2.3	1.9	1.9	1.4	1.7	1.8

[a] N_{at} – number of atoms; N_{ev} – number of eigenvectors; Q - quality of the compression (%). [b] 0.0 to 50.0 ns for CD14.