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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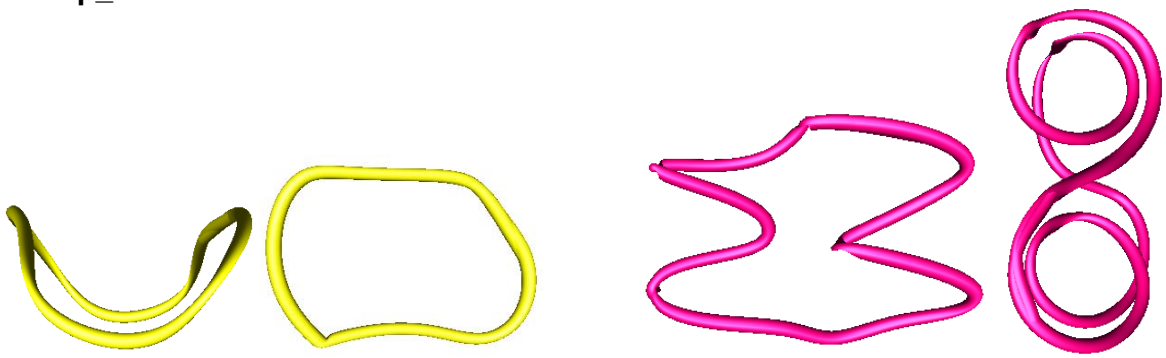
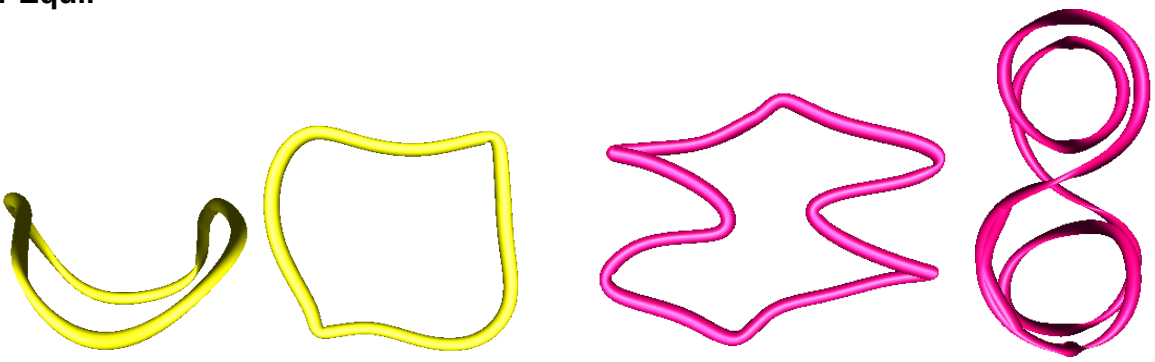
(file *_esi-001)

CD14 **CD26**

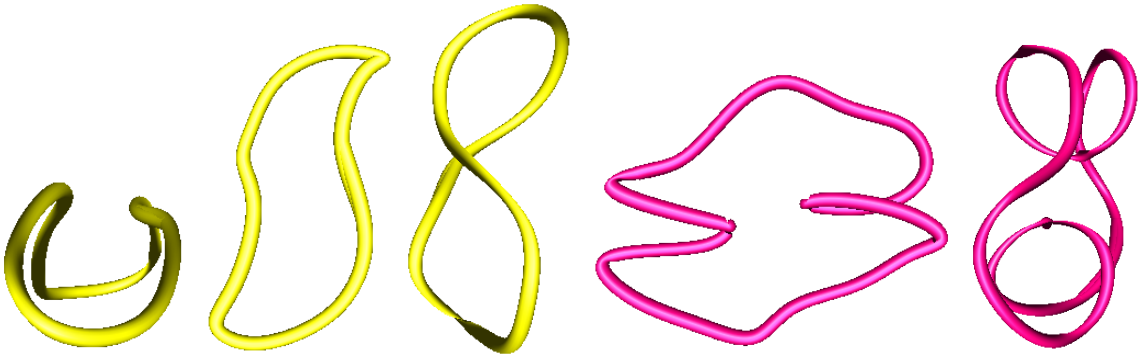
After tleap_3



After Equil



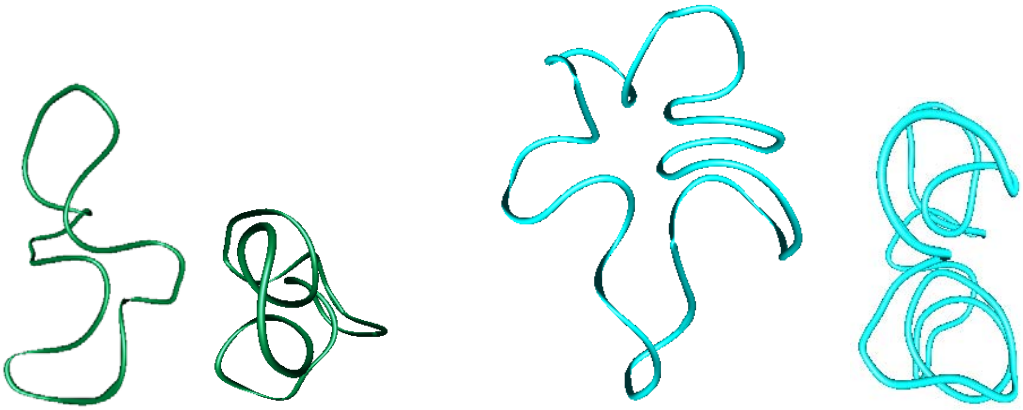
After 500 ps MD



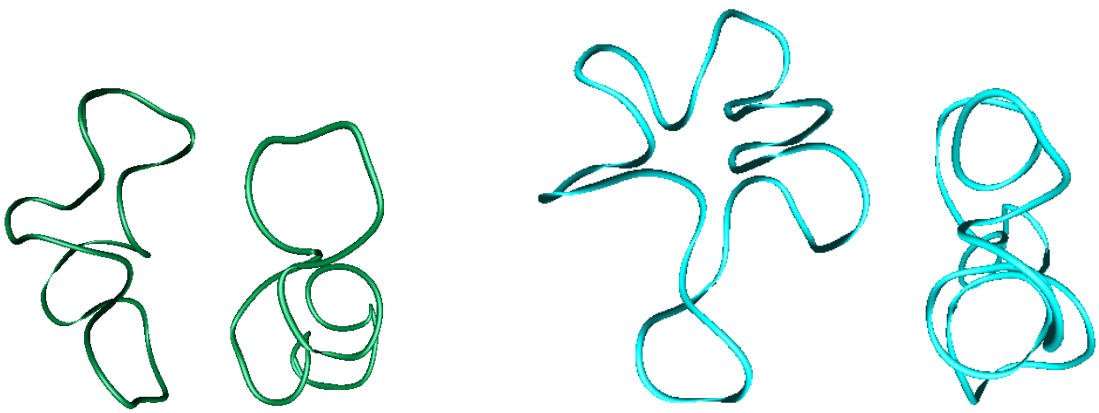
CD40 **CD70**

After tleap_3

After Equil



After 500 ps MD



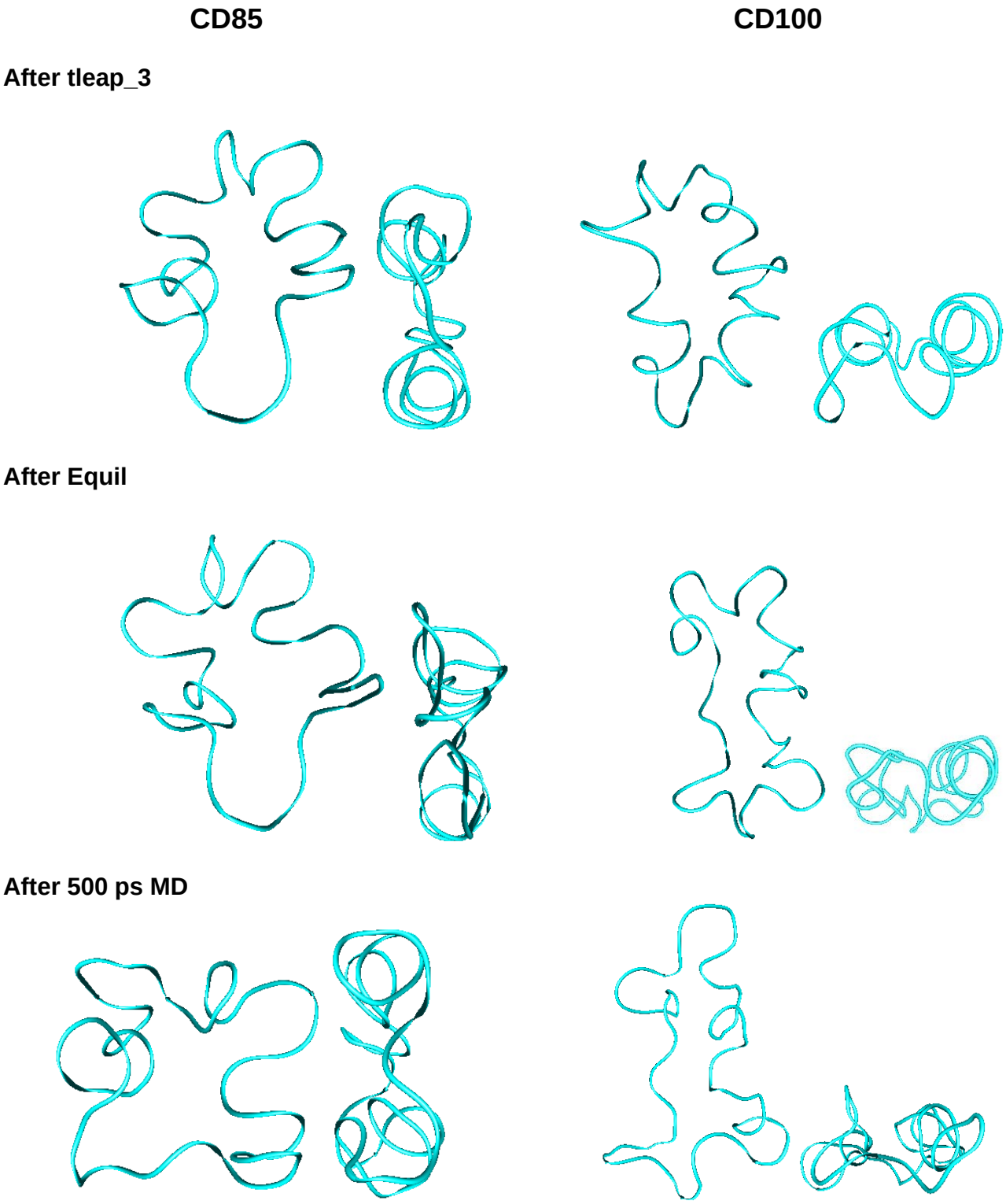


Fig. S1. Geometries (two different views) of the macrorings at different stages during the preparation of the systems for conformational search with molecular dynamics simulations: Starting geometries, before the productive simulation and after the preliminary 500.0 ps simulation.

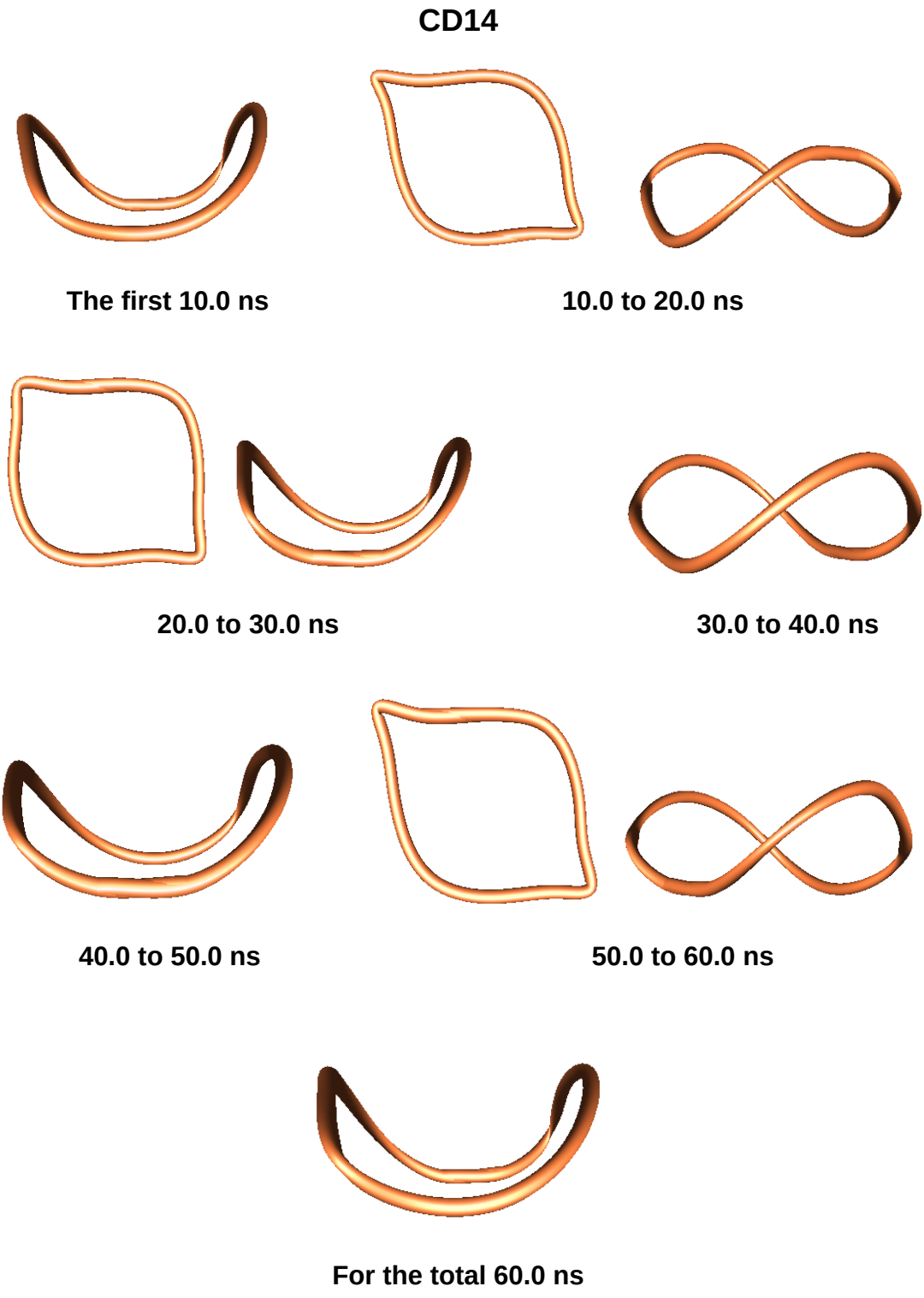


Fig. S2. Averaged structures obtained from analyses of the simulation trajectory of CD14 decomposed to 10.0 ns time intervals, and comparison with the geometry averaged over the whole simulation trajectory.

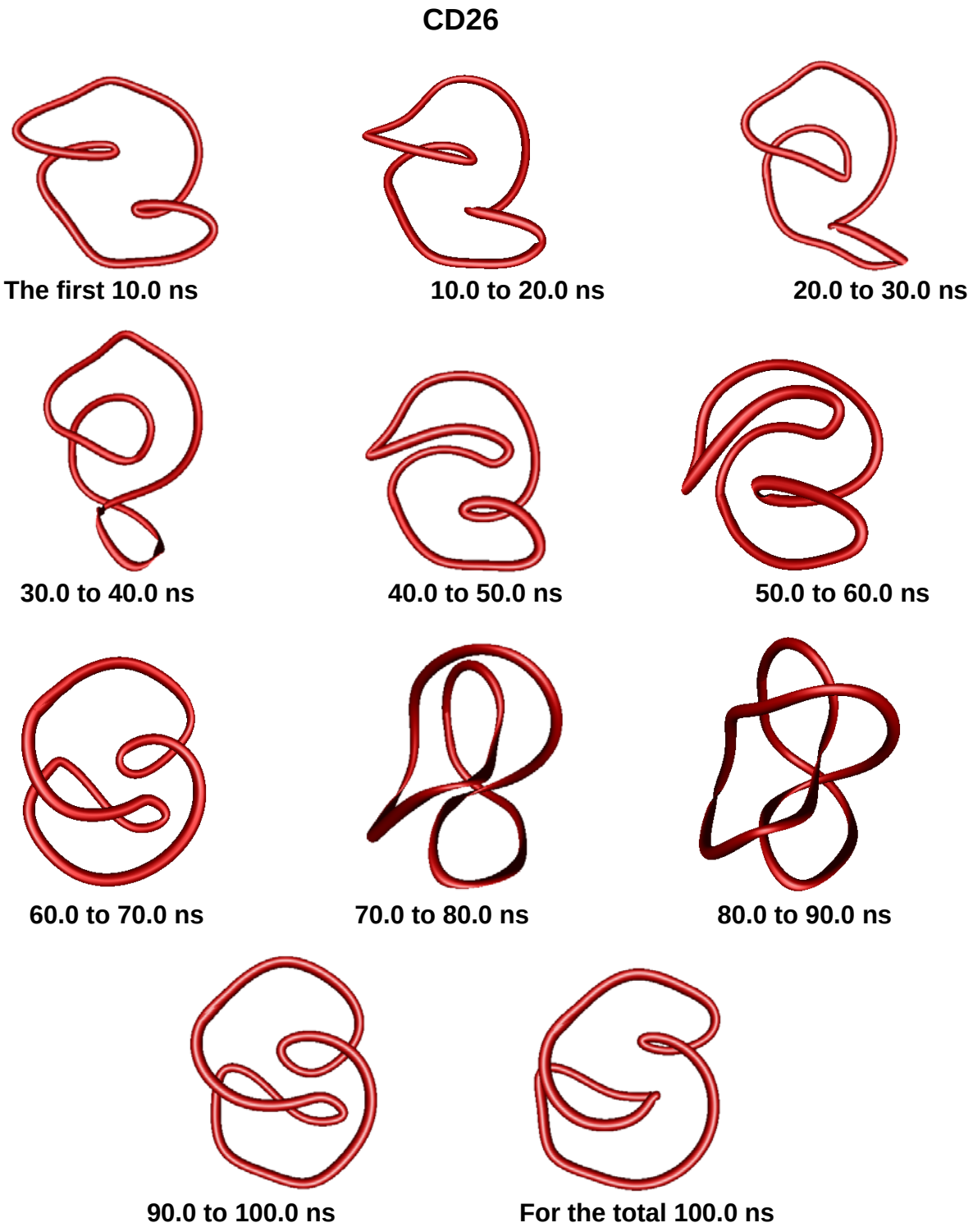


Fig. S3. Averaged structures obtained from analyses of the simulation trajectory of CD26 decomposed to 10.0 ns time intervals, and comparison with the geometry averaged over the whole simulation trajectory.

CD40

The first 10.0 ns

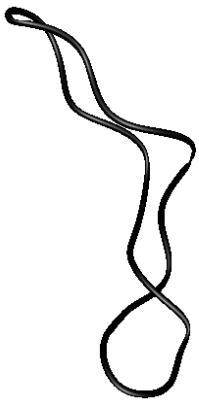
10.0 to 20.0 ns

20.0 to 30.0 ns

30.0 to 40.0 ns

40.0 to 50.0 ns

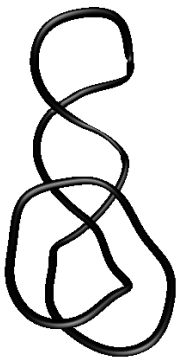
50.0 to 60.0 ns



60.0 to 70.0 ns

70.0 to 80.0 ns

80.0 to 90.0 ns

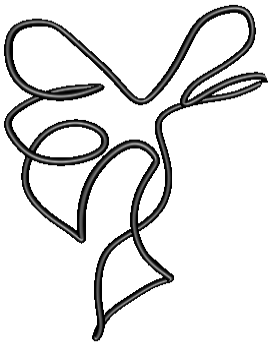


90.0 to 100.0 ns

For the first 70.0 ns

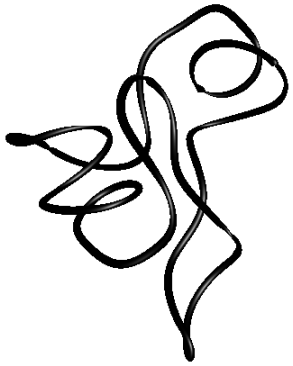
For 100.0 ns

CD70

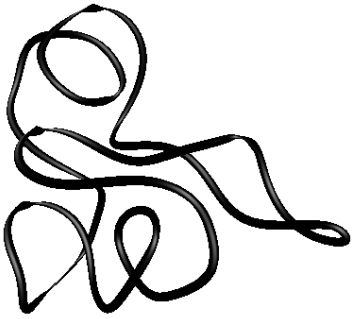


The first 10.0 ns

10.0 to 20.0 ns

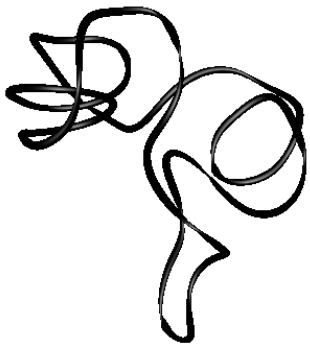


20.0 to 30.0 ns

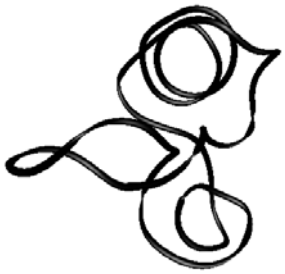


30.0 to 40.0 ns

40.0 to 50.0 ns



50.0 to 60.0 ns

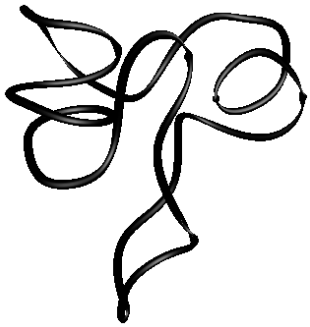


60.0 to 70.0 ns

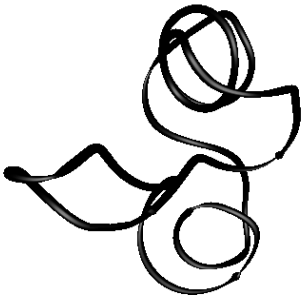
70.0 to 80.0 ns

80.0 to 90.0 ns

90.0 to 100.0 ns

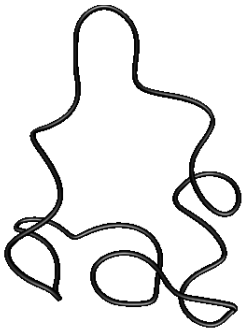


For the first 60.0 ns

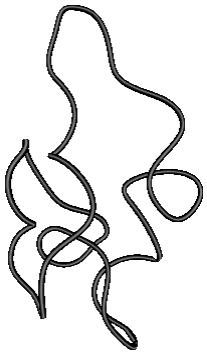


For 100.0 ns

CD85

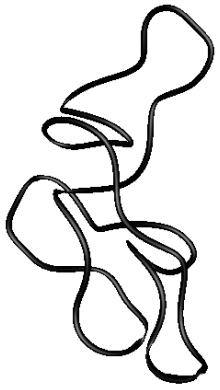


The first 10.0 ns

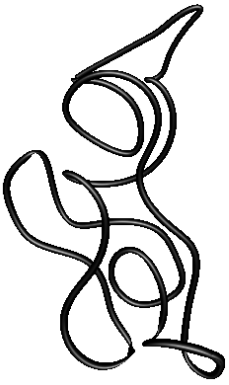


10.0 to 20.0 ns

20.0 to 30.0 ns



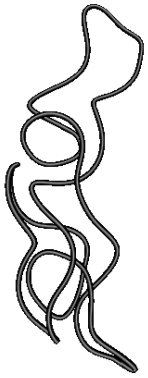
30.0 to 40.0 ns



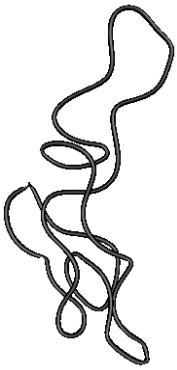
40.0 to 50.0 ns

50.0 to 60.0 ns

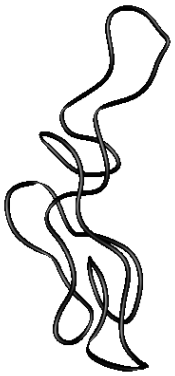
60.0 to 70.0 ns



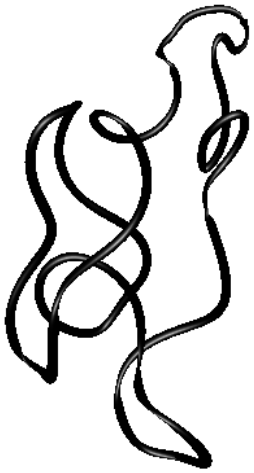
70.0 to 80.0 ns



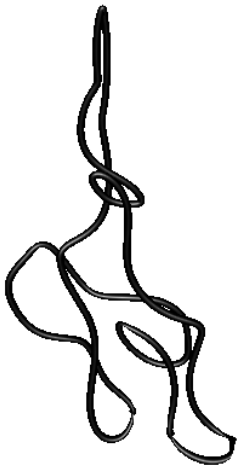
80.0 to 90.0 ns



90.0 to 100.0 ns

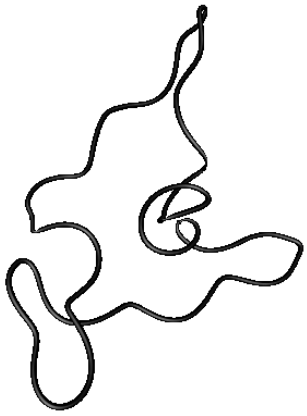


For the first 60.0 ns

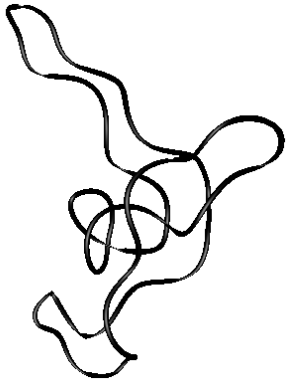


For 100.0 ns

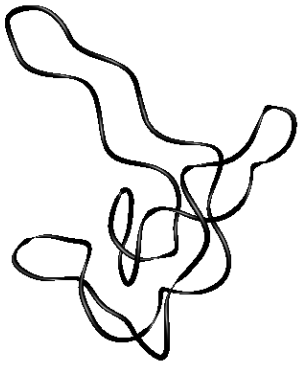
CD100



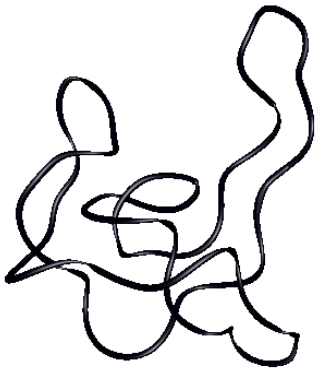
The first 10.0 ns



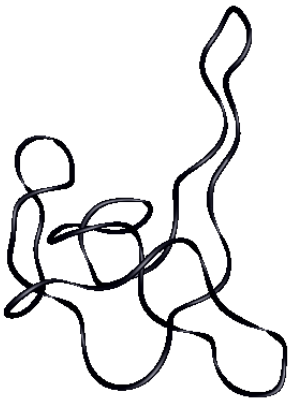
10.0 to 20.0 ns



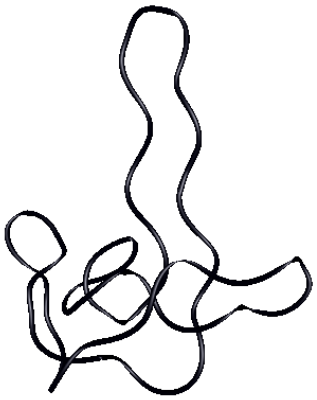
20.0 to 30.0 ns



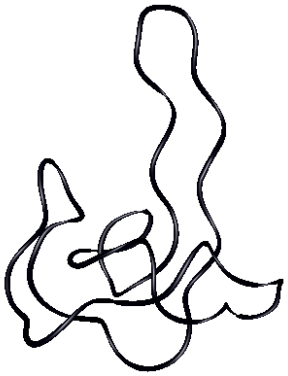
30.0 to 40.0 ns



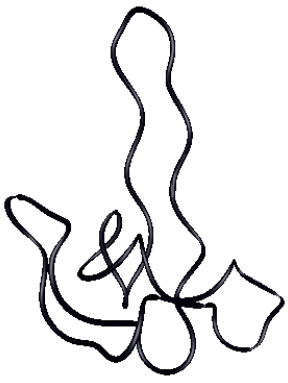
40.0 to 50.0 ns



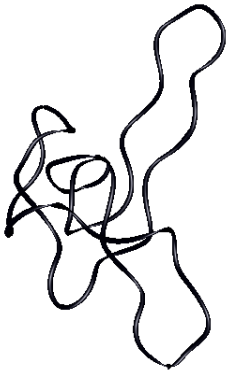
50.0 to 60.0 ns



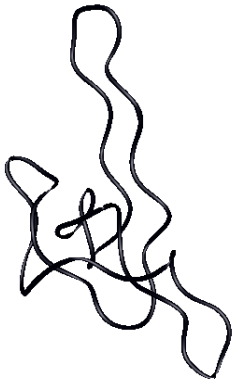
60.0 to 70.0 ns



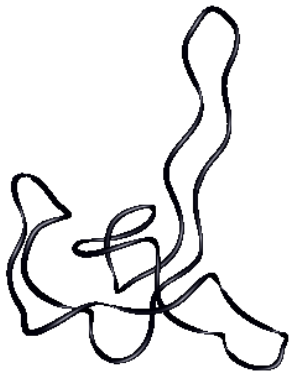
70.0 to 80.0 ns



80.0 to 90.0 ns



90.0 to 100.0 ns



For 100.0 ns

Fig. S4. Averaged structures obtained from analyses of the simulation trajectories of CDn (n=40,70,85,100) decomposed to 10.0 ns time intervals. Comparison with averages for longer simulation time intervals.

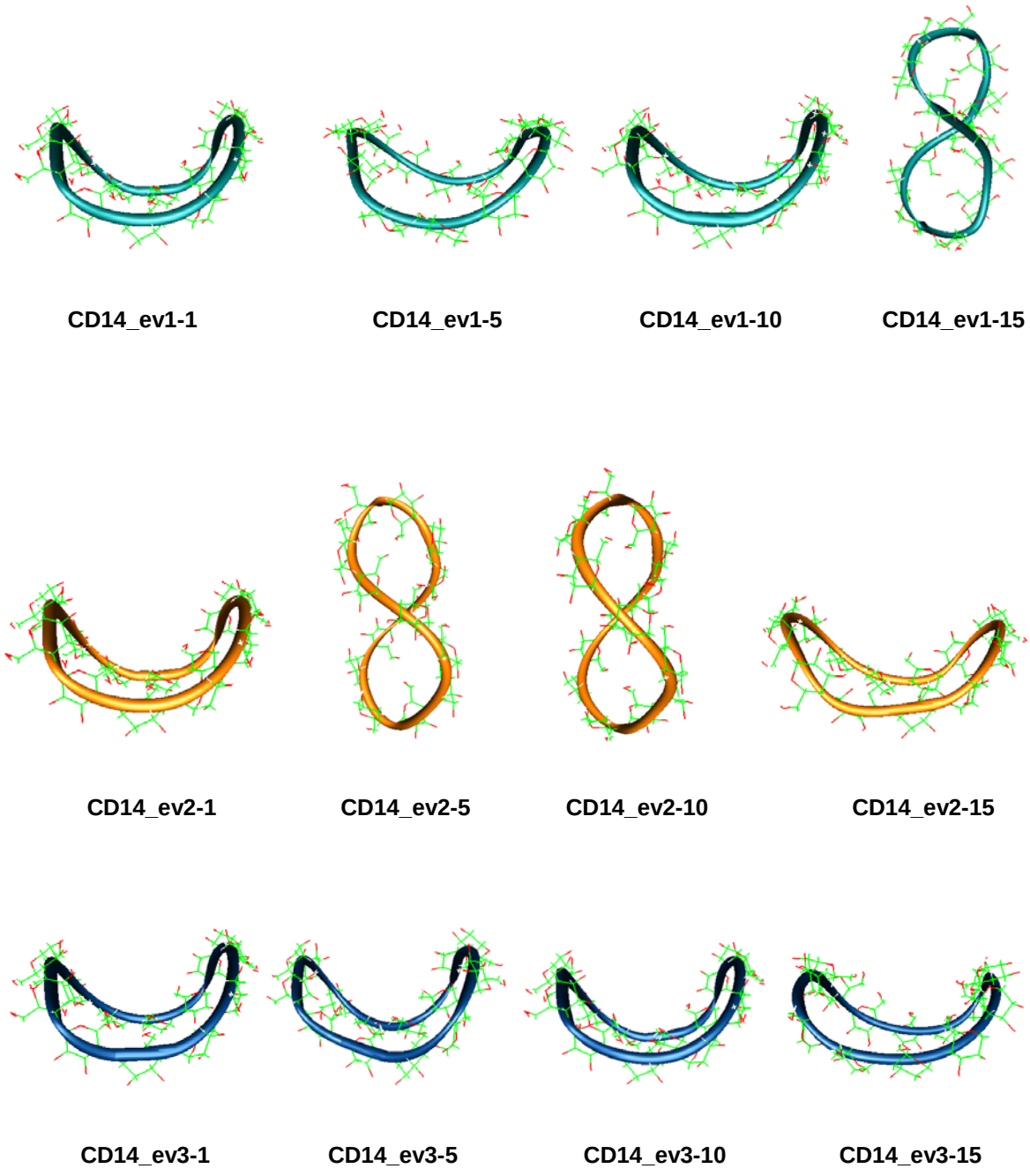
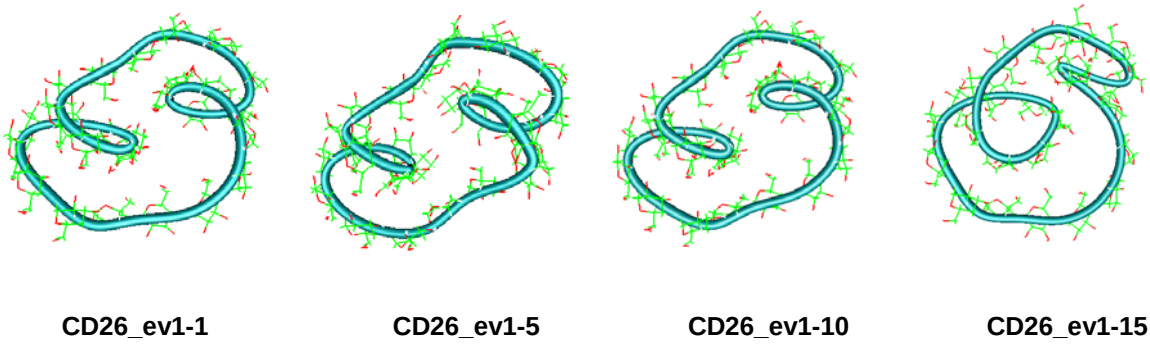
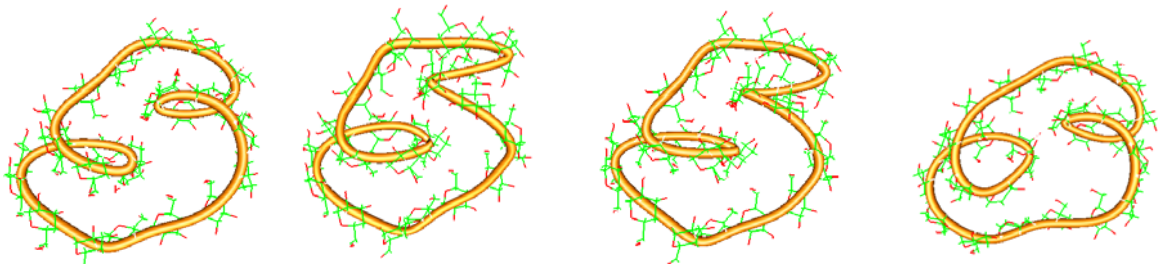


Fig. S5. Snapshots (with sequential numbers 1, 5, 10 and 15) of the first three animated eigenvectors (**ev1**, **ev2**, **ev3**) having the largest contribution to the total variance of the atomic fluctuations of CD14 (PCA analysis; 60.0 ns).

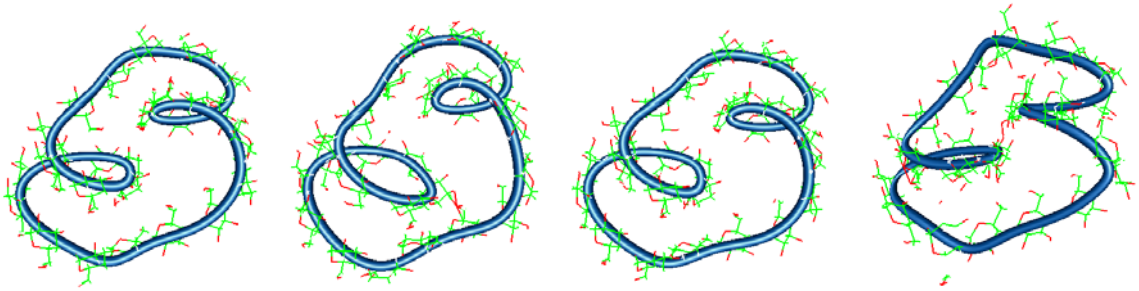
(a)



CD26_ev1-1 CD26_ev1-5 CD26_ev1-10 CD26_ev1-15



CD26_ev2-1 CD26_ev2-5 CD26_ev2-10 CD26_ev2-15



CD26_ev3-1 CD26_ev3-5 CD26_ev3-10 CD26_ev3-15

(b)

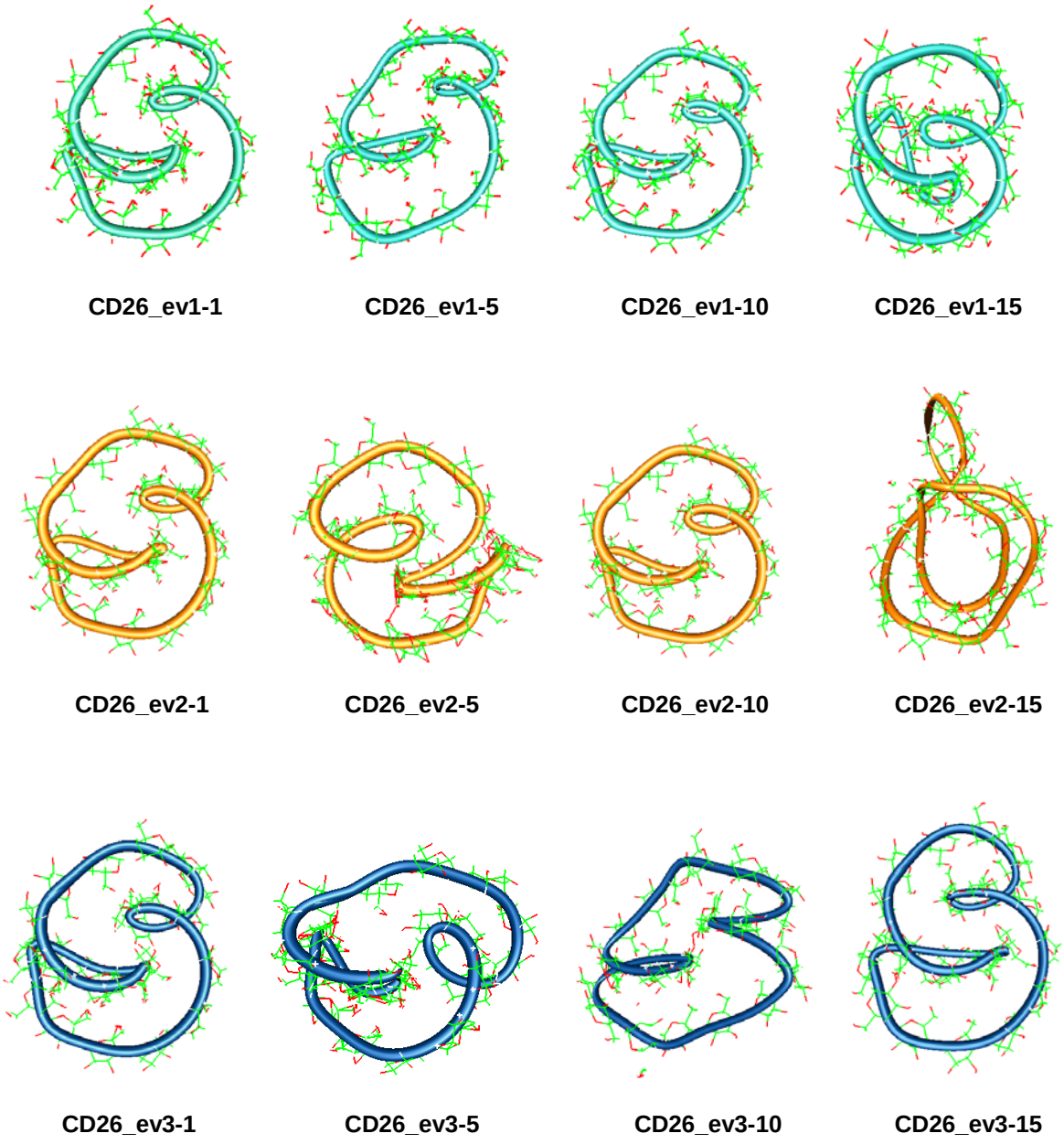


Fig. S6. Snapshots (with sequential numbers 1, 5, 10 and 15) of the first three animated eigenvectors (**ev1**, **ev2**, **ev3**) having the largest contribution to the total variance of the atomic fluctuations of CD26 (PCA analysis: (a) 10.0 ns; (b) 100.0 ns).

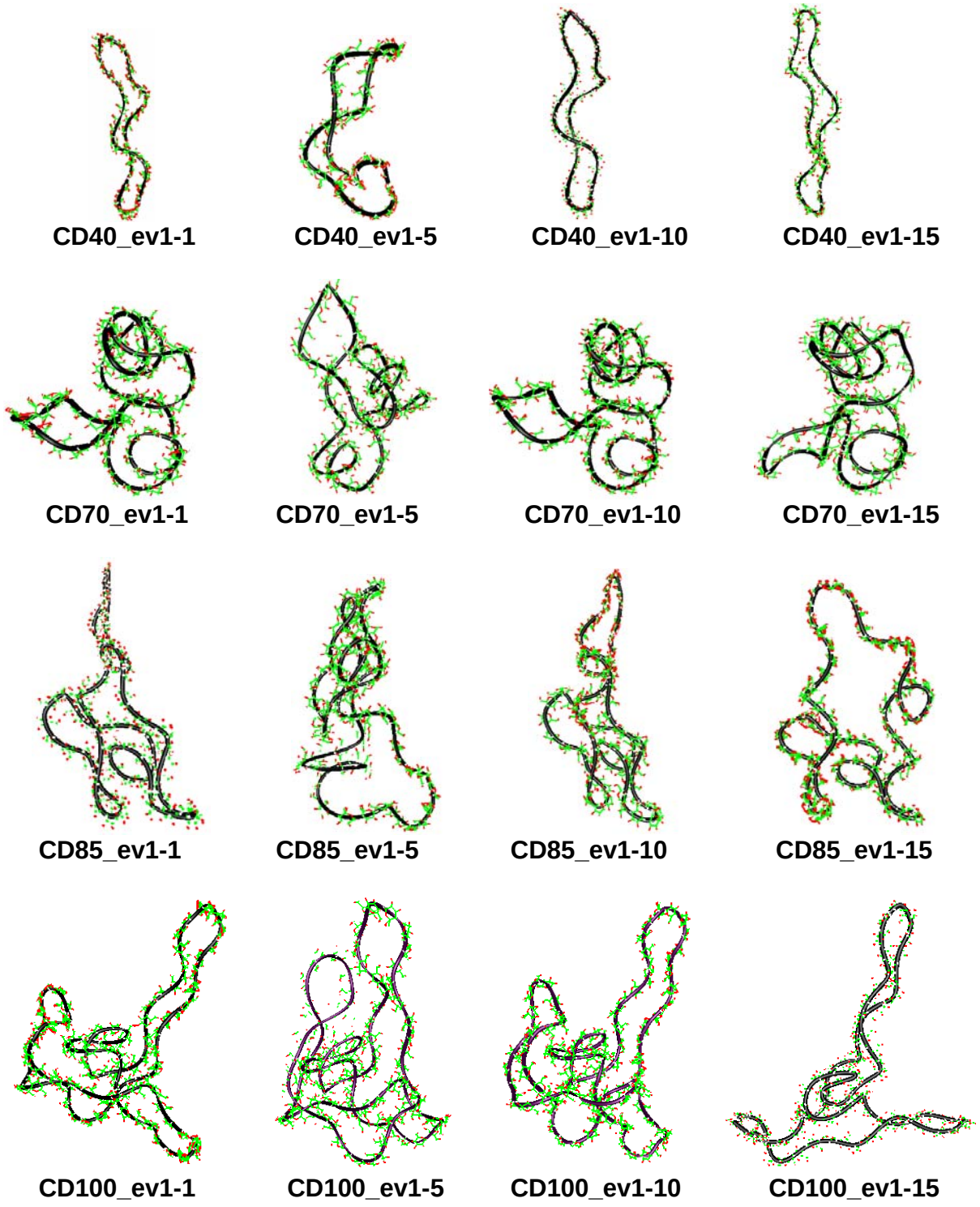


Fig. S7. Snapshots (with sequential numbers 1, 5, 10 and 15) of the first animated eigenvectors (**ev1**) having the largest contribution to the total variance of the atomic fluctuations of CDn (n = 40, 70, 85, 100).