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

SUPPORTING INFORMATION

For

Kinetic and Thermodynamic Stability Comparison for Fibrillar Form of Small Amyloid-β(1-42) Oligomers Using Scaled Molecular Dynamics

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RMSD plots for 2NAO.pdb and 5KK3.pdb system from Equilibration:

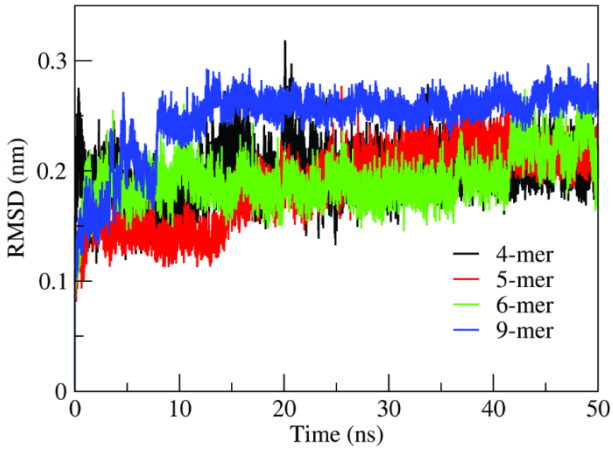

Figure S1 RMSD vs time plot for 4-mer (black), 5-mer (red), 6-mer (green) and 9-mer (blue) oligomers of 2NAO.pdb system after equilibration.

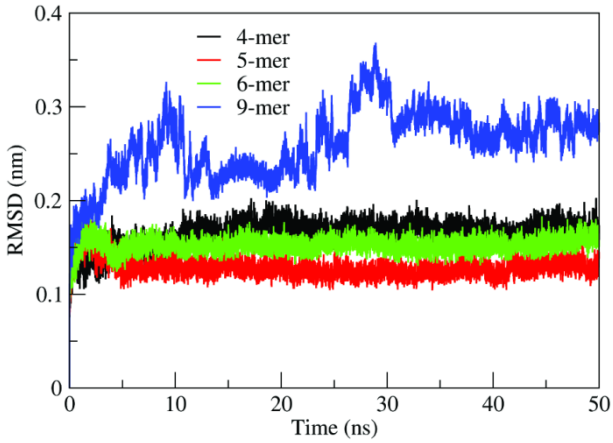

Figure S2 RMSD vs time plot for 4-mer (black), 5-mer (red), 6-mer (green) and 9-mer (blue) oligomers of 5KK3.pdb system after equilibration.

RMSD vs time and Q vs time plot for 5KK3.pdb system from sMD:

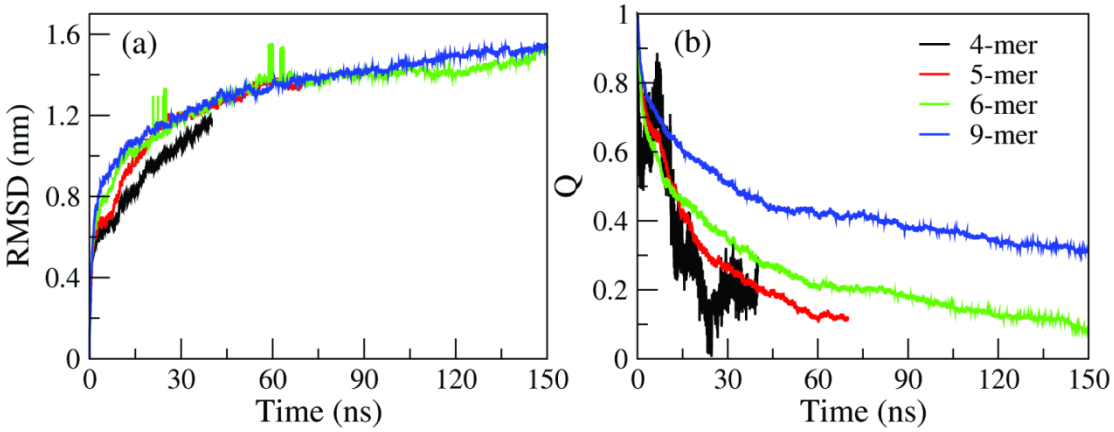

Figure S3 The RMSD plot (a) and the fraction of native contact, Q plot (b) for the oligomers of 5KK3.pdb system obtained from averaging of 10 independent sMD simulations.

Representative plot for fitting of Q vs time data:

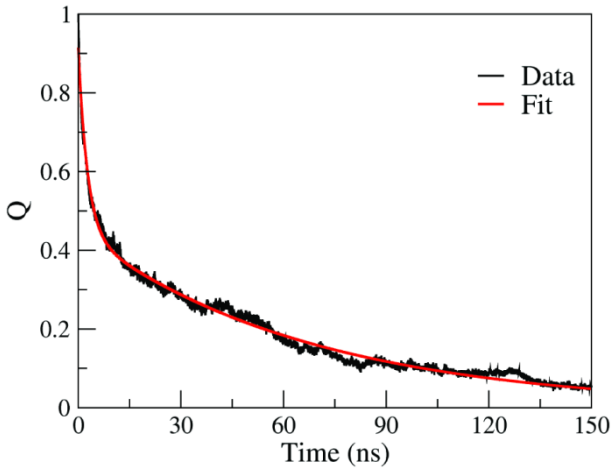

Figure S4 Bi-exponential fitting of Q vs time plot from one of the systems. The black line shows the original data and red line shows fitted data.

Q vs time plot and timescales obtained through fitting for 5KK3.pdb:

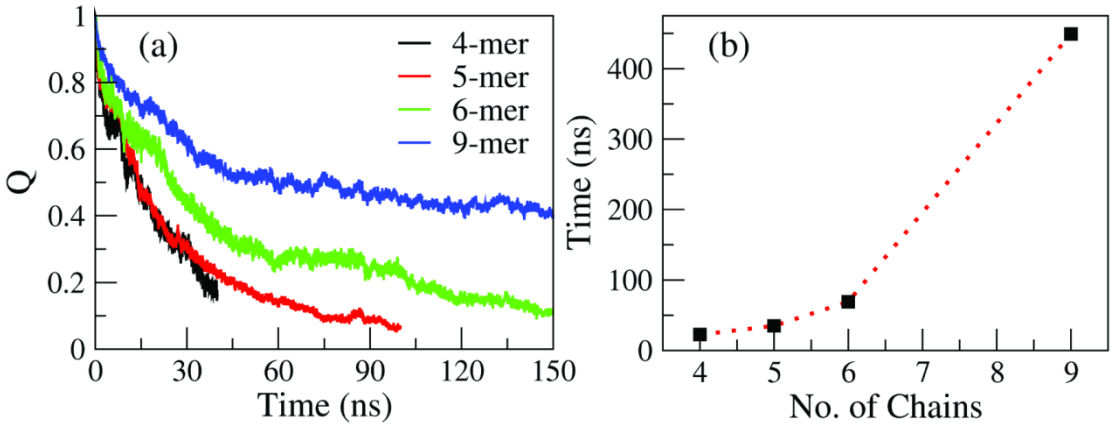

Figure S5 The Q values between middle chains vs time plot for different oligomers of 5KK3.pdb (a) and the timescales obtained by fitting the Q values (b). The red dashed line in (b) is shown only to guide the eyes.

Comparison of Q vs time plot for different segments of oligomers of 5KK3.pdb system:

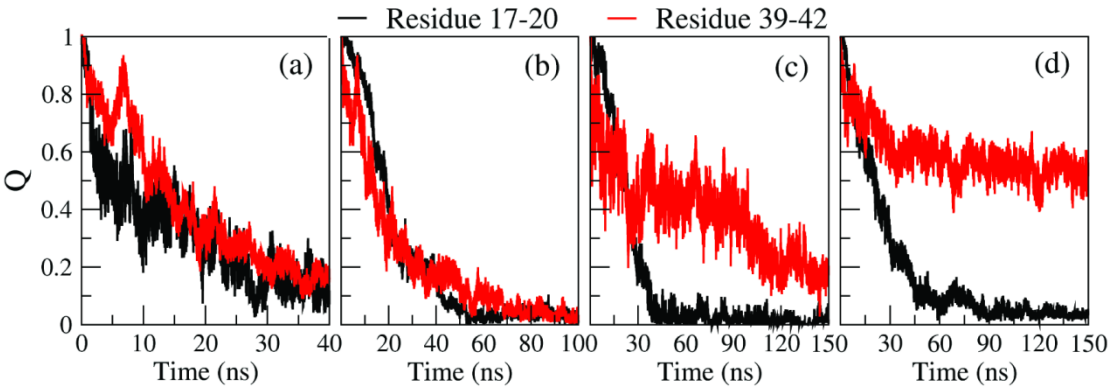

Figure S6 Q vs time plots for residues 17-20 from the CHC segment (black lines) and residues 39-42 from the C-terminus end (red lines) for 4-mer (a), 5-mer (b), 6-mer (c) and 9-mer (d) from the 5KK3.pdb system.

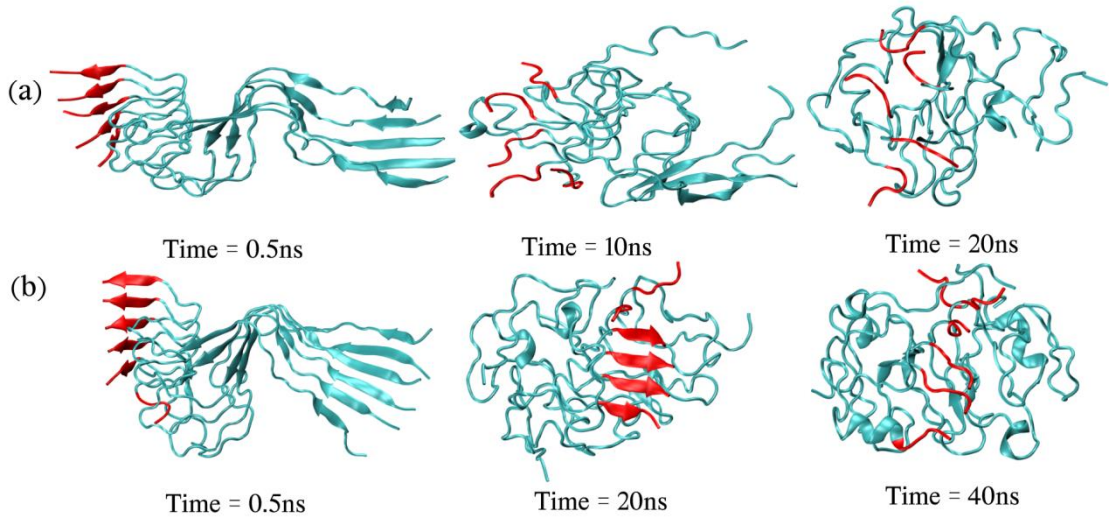

Figure S7 Structure evolutions of 5-mer (a) and 6-mer (b) oligomers of 2NAO.pdb system from simulations at $\lambda = 0.45$. The timesteps at which frames have been extracted are given below each figure. The red portions indicate four residues at the C-terminus end for each 42 residue chain.

Terminal chain Q vs time plot for 5KK3.pdb system:

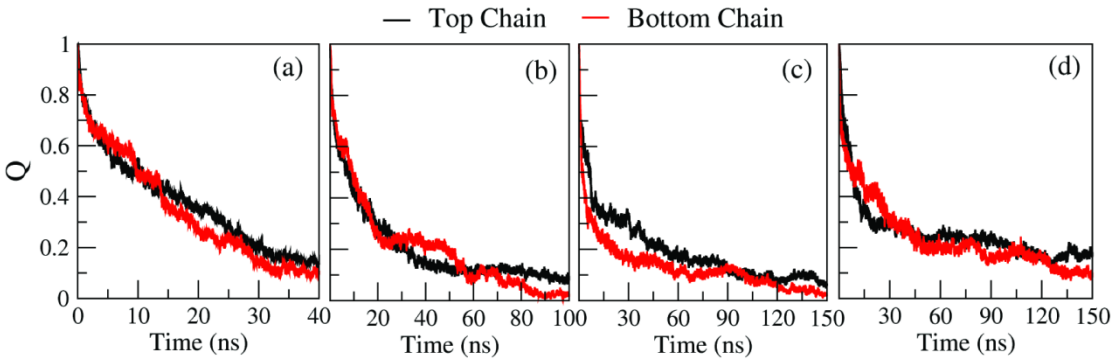

Figure S8 Q vs time plots for the terminal chains of 4-mer (a), 5-mer (b), 6-mer (c) and 9-mer (d) for 5KK3.pdb system. The black and red lines represent the top and bottom chain of the oligomers as indicated in Fig 1 in the main paper.

Timescale of terminal chains' dissociation:

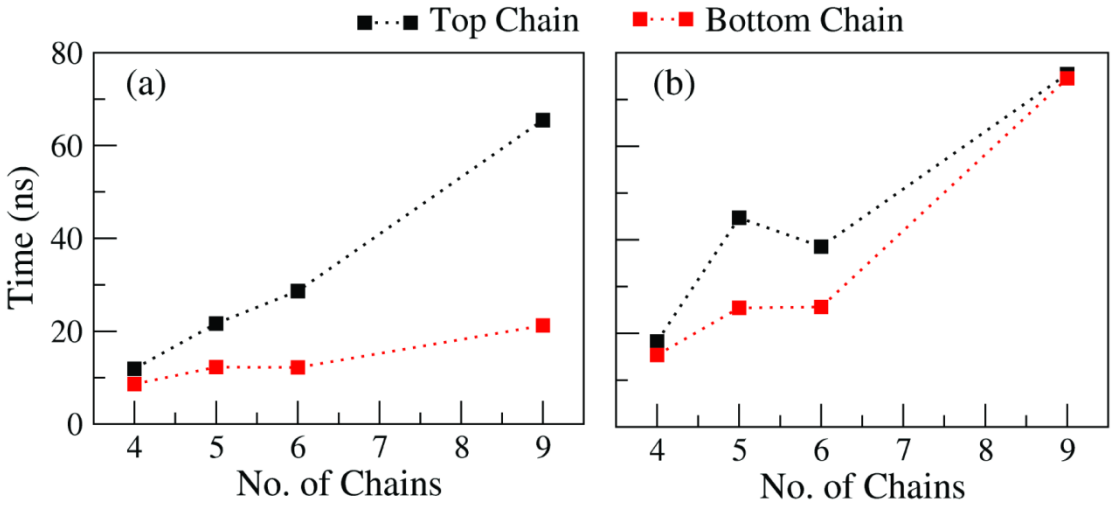

Figure S9 Time required for complete breaking of native contacts of terminal chains form different oligomers of 2NAO.pdb system (a) and 5KK3.pdb system (b). The black and red squares represent the timescales for top and bottom chain respectively. The dashed lines are used only to guide the eyes.

Total interaction energy distribution for different segments of 5KK3.pdb:

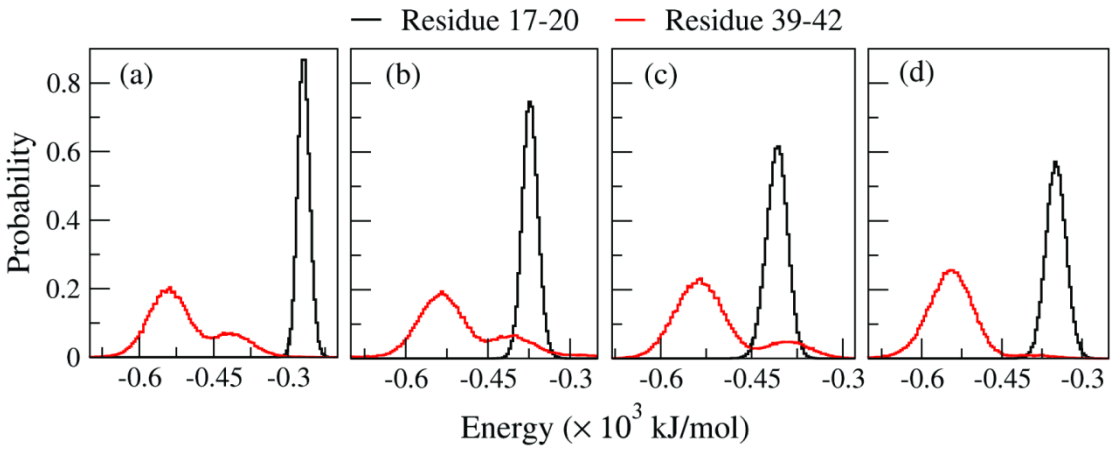

Figure S10 Total interaction energy distribution for residues 17-20 (black lines) and residues 39-42 (red lines) for 4mer (a), 5-mer (b), 6-mer (c) and 9-mer (d) oligomer of 5KK3.pdb system.

Protein-protein interaction energy distribution for 2NAO.pdb and 5KK3.pdb systems:

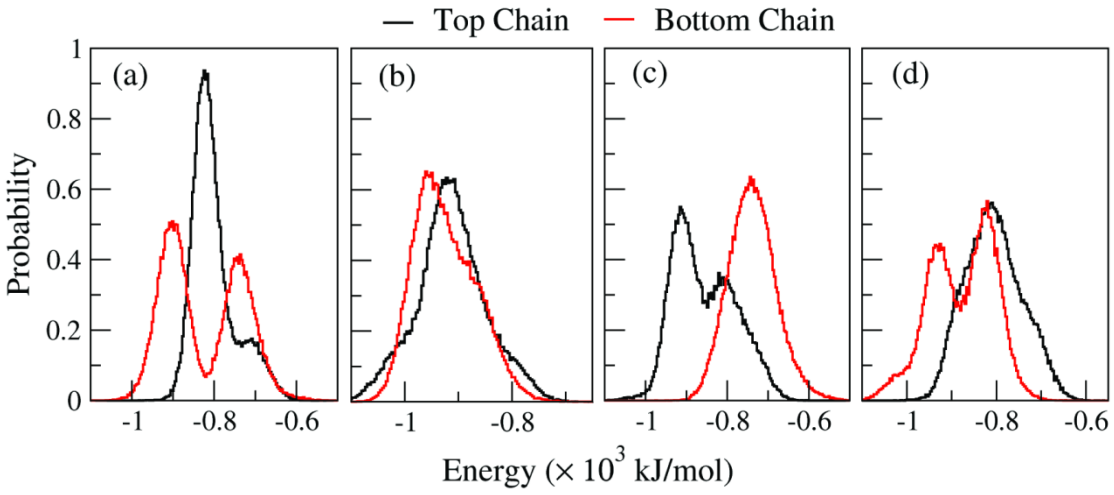

Figure S11 Interaction energy between top (black line) and bottom (red line) end chain with rest of the protein atoms for 4-mer (a), 5-mer (b), 6-mer (c) and 9-mer (d) oligomer of 2NAO.pdb system.

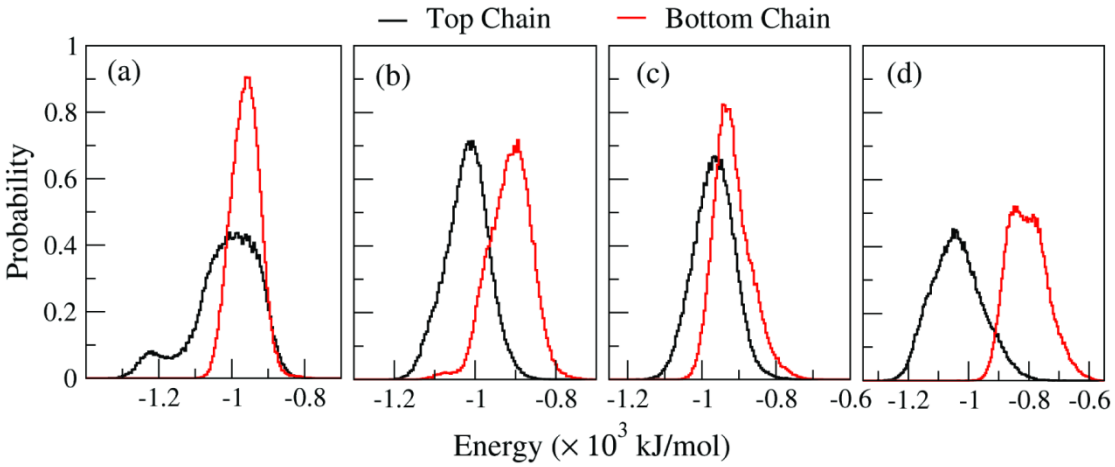

Figure S12 Interaction energy between top (black line) and bottom (red line) end chain with rest of the protein atoms for 4-mer (a), 5-mer (b), 6-mer (c) and 9-mer (d) oligomer of 5KK3.pdb system.

Protein-water interaction energy distribution for 2NAO.pdb and 5KK3.pdb systems:

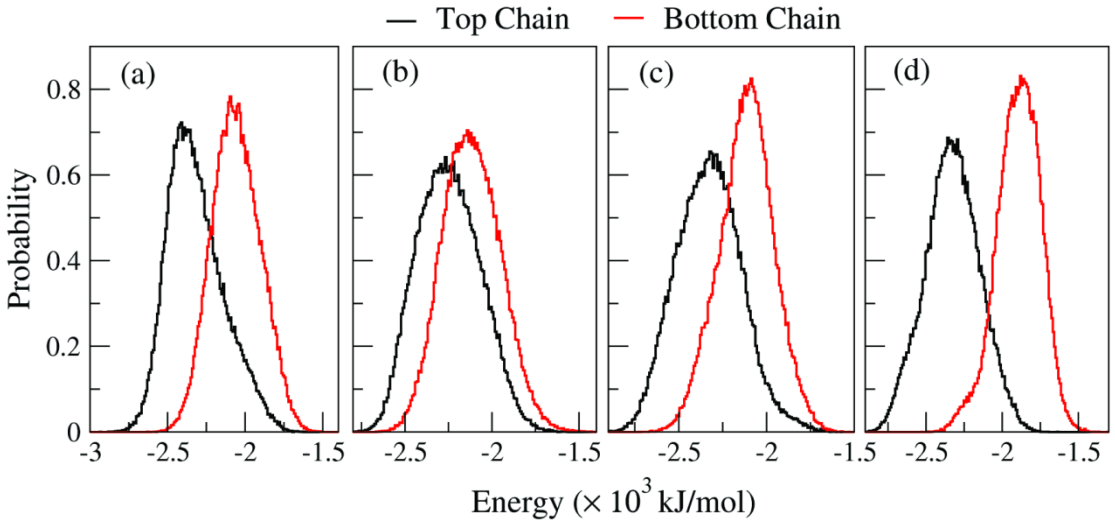

Figure S13 Interaction energy between top (black line) and bottom (red line) end chain with water molecules from the system for 4-mer (a), 5-mer (b), 6-mer (c) and 9-mer (d) oligomer of 2NAO.pdb system.

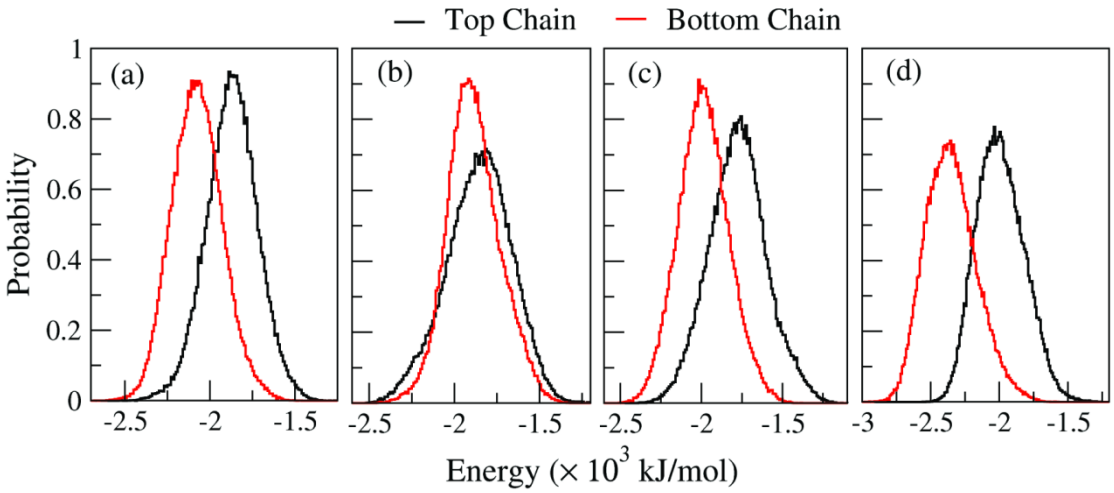

Figure S14 Interaction energy between top (black line) and bottom (red line) end chain with water molecules from the system for 4-mer (a), 5-mer (b), 6-mer (c) and 9-mer (d) oligomer of 5KK3.pdb system.

Total interaction energy distribution for terminal chains of 5KK3.pdb:

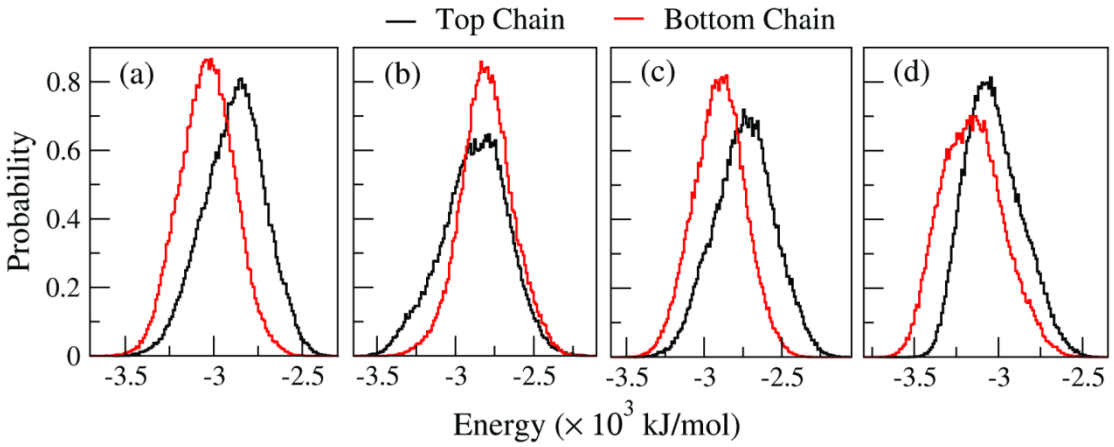

Figure S15 Distribution of total interaction energy for top (black line) and bottom (red line) chain for 4-mer (a), 5-mer (b), 6-mer (c) and 9-mer (d) oligomer of 5KK3.pdb system. The interaction energy shown in the plot represents sum of protein-protein and protein-water interaction energies.

MM-PBSA calculation results:

Table S1: Binding free energies between terminal chains and the rest of the protein from MM-PBSA calculations.

System								
	4-mer		**5-mer**		**6-mer**		**9-mer**	
Chain	**Top**	**Bottom**	**Top**	**Bottom**	**Top**	**Bottom**	**Top**	**Bottom**
van der Waal energy (kj/mol)	-463.33	-491.19	-468.68	-531.28	-474.07	-483.63	-421.51	-408.99
Electrostattic energy (kj/mol)	-40.19	376.76	105.79	250.69	161.01	399.07	85.68	432.2
Polar solvation energy (kj/mol)	454.86	252.36	370.86	517.32	313.95	314.84	451.46	506.56
SASA energy (kj/mol)	-48.84	-52.00	-50.07	-54.86	-47.28	-52.57	-47.47	-48.38
Binding energy (kj/mol)	-97.5	85.92	-42.11	181.87	-46.39	177.7	68.16	481.39