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

Supporting information for:

Binding of fullerenes to amyloid beta fibrils: size matters

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Table S1: Summary of MD simulation details for all systems. τ_{total} is a total simulation time, while τ_{eq} stands for the equilibration time. Times are measured in ns. N_{water} refers to the number of water molecules in the box of size d_{box}.

System	τ_{total}	τ_{eq}	N_{water}	d_{box}(Å)
$5A\beta_{17-42}$	25	9	5448	65.08
$5A\beta_{17-42}$ +C20	40	17	6896	69.51
$5A\beta_{17-42}$ +C36	60	29	6901	69.60
$5A\beta_{17-42}$ +C60	100	71	5384	64.94
$5A\beta_{17-42}$ +C70	25	13	5610	65.69
$5A\beta_{17-42}$ +C84	25	13	5547	65.39
$12A\beta_{9-40}$	20	2.5	20260	99.20
$12A\beta_{9-40}$ +C20	20	7	20269	99.21
$12A\beta_{9-40}$ +C36	20	8	19883	98.66
$12A\beta_{9-40}$ +C60	20	8	20338	99.31
$12A\beta_{9-40}$ +C70	35	17	18752	96.96
$12A\beta_{9-40}$ +C84	39	25	18749	96.91

Table S2: Shown are amino acids which have the equilibrium contact population with fullerene exceeding 50%. Non-polar, basic polar, polar and acidic polar residues are colored gray, green, blue and orange, respectively.

Systems	N_{SC}	Important amino acids
$5A\beta_{17-42}$ +C20	12	A21-A, D23-A, F19-B, A21-B, D23-B, K28-B, I32-B, L34-B, A21-C, D23-C, I32-C, L34-C
$5A\beta_{17-42}$ +C36	13	L17-B, L17-C, F19-C, F19-D, A21-D, G38-D, A21-E, E22-E, V24-E, G37-E, G38-E, V39-E, I41-E
$5A\beta_{17-42}$ +C60	16	F20-A, A21-A, E22-A, D23-A, S26-A, K28-A, G29-A, A30-A, I31-A, I32-A, G33-A, L34-A, I31-B, I32-B, G33-B, L34-B
$5A\beta_{17-42}$ +C70	13	M35-A, V39-A, I41-A, A42-A, G33-B, M35-B, V39-B, I31-C, G33-C, M35-C, G33-D, M35-D, G33-E
$5A\beta_{17-42}$ +C84	11	G33-A, M35-A, I31-B, G33-B, M35-B, I31-C, I32-C, G33-C, M35-C, I31-D, G33-D
$12A\beta_{9-40}$ +C20	9	L17-B, Q15-C, L17-C, Q15-D, L17-D, V36-D, V36-E, G37-E, V36-F
$12A\beta_{9-40}$ +C36	13	F19-A, F20-A, D23-A, V24-A, G25-A, S26-A, I32-A, L34-A, A30-B, I32-B, L34-B, I32-C, L34-C
$12A\beta_{9-40}$ +C60	12	F19-D, L17-E, F19-E, L17-F, F19-F, G33-F, L34-F, V36-F, V40-F, M35-L, G38-L, V39-L
$12A\beta_{9-40}$ +C70	16	F19-E, A21-E, D23-E, L17-F, F19-F, A21-F, N27-F, K28-F, G29-F, A30-F, I31-F, I32-F, G33-F, Y10-L, V12-L, H14-L
$12A\beta_{9-40}$ +C84	20	F19-D, F19-E, A21-E, E22-E, D23-E, L17-F, F19-F, A21-F, D23-F, G25-F, S26-F, N27-F, K28-F, G29-F, A30-F, I31-F, I32-F, G9-L, Y10-L, V12-L

Table S3: Population of salt bridge ASP23-LYS28 for $5A\beta_{17-42}$ systems. Results were obtained in equilibrium

Chain	$5A\beta_{17-42}$	$5A\beta_{17-42}$ +C20	$5A\beta_{17-42}$ +C36	$5A\beta_{17-42}$ +C60	$5A\beta_{17-42}$ +C70	$5A\beta_{17-42}$ +C84
A	45.35	0	0	0	0.16	0
B	99.88	98.78	100	90.38	100	99.92
C	100	100	99.97	99.86	100	100
D	100	99.96	99.97	99.81	100	100
E	100	99.57	4.13	20.70	100	100

Table S4: Population of salt bridge ASP23-LYS28 for $12A\beta_{9-40}$ systems. Results were obtained in equilibrium

Chain	$12A\beta_{9-40}$	$12A\beta_{9-40}$ +C20	$12A\beta_{9-40}$ +C36	$12A\beta_{9-40}$ +C60	$12A\beta_{9-40}$ +C70	$12A\beta_{9-40}$ +C84
A	9.14	0	0	0	0	0
B	0.23	0	0	0	0	84.78
C	0.11	0	0	0	0	0
D	0	0	0	0	0	0
E	0	0	0	0	0	0
F	0	0	0	0	0	0
G	98.17	0	0	0	0	0
H	0	0	0	0	0	0
I	0	0	0	0	0	0
J	0	0	12.05	0	0	0
K	0	0	0.97	0	0	0
L	0	0	21.13	73.61	0	0

Table S5: Mean values of the number of fibril contacts for $5A\beta_{17-42}$ and $12A\beta_{9-40}$ with and without fullerenes. Results were obtained in equilibrium. The PDB structures of $5A\beta_{17-42}$ and $12A\beta_{9-40}$ have 161 and 503 FCs, respectively.

System	FC	System	FC
$5A\beta_{17-42}$	100.3	$12A\beta_{9-40}$	325.1
$5A\beta_{17-42}$ +C20	97.2	$12A\beta_{9-40}$ +C20	288.5
$5A\beta_{17-42}$ +C36	95.3	$12A\beta_{9-40}$ +C36	302.3
$5A\beta_{17-42}$ +C60	72.8	$12A\beta_{9-40}$ +C60	290.6
$5A\beta_{17-42}$ +C70	100.0	$12A\beta_{9-40}$ +C70	297.6
$5A\beta_{17-42}$ +C84	110.1	$12A\beta_{9-40}$ +C84	285.4

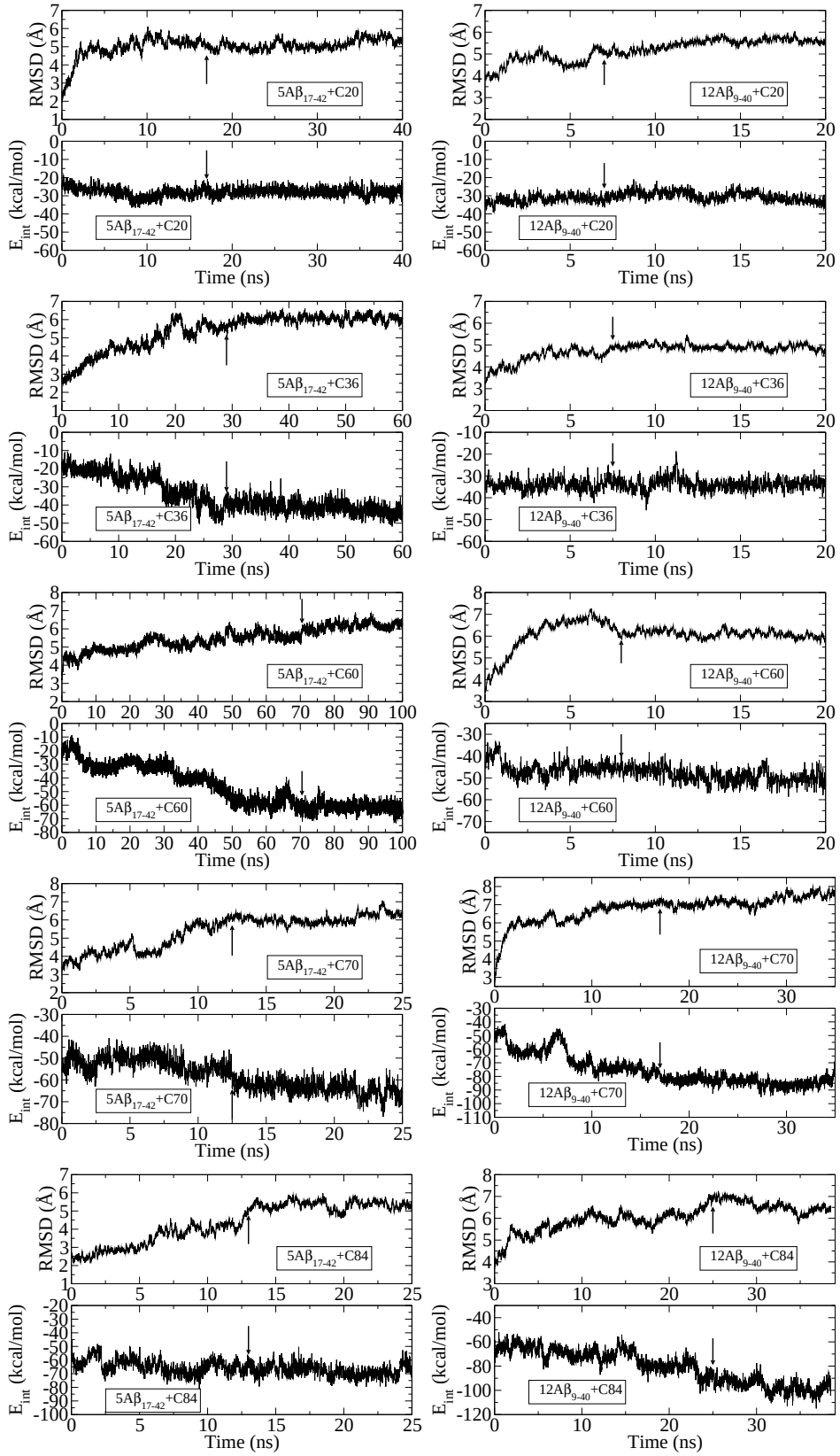

Figure S1: Time dependence of of root mean square deviation (RMSD) and interaction energy (E_{int}) for $5A\beta_{17-42}$ (left) and for $12A\beta_{9-40}$ (right). Arrow refers to τ_{eq} where the system reach equilibrium and snapshots collected after this moment were used for estimation of ΔG_{bind} by MM-PBSA method.

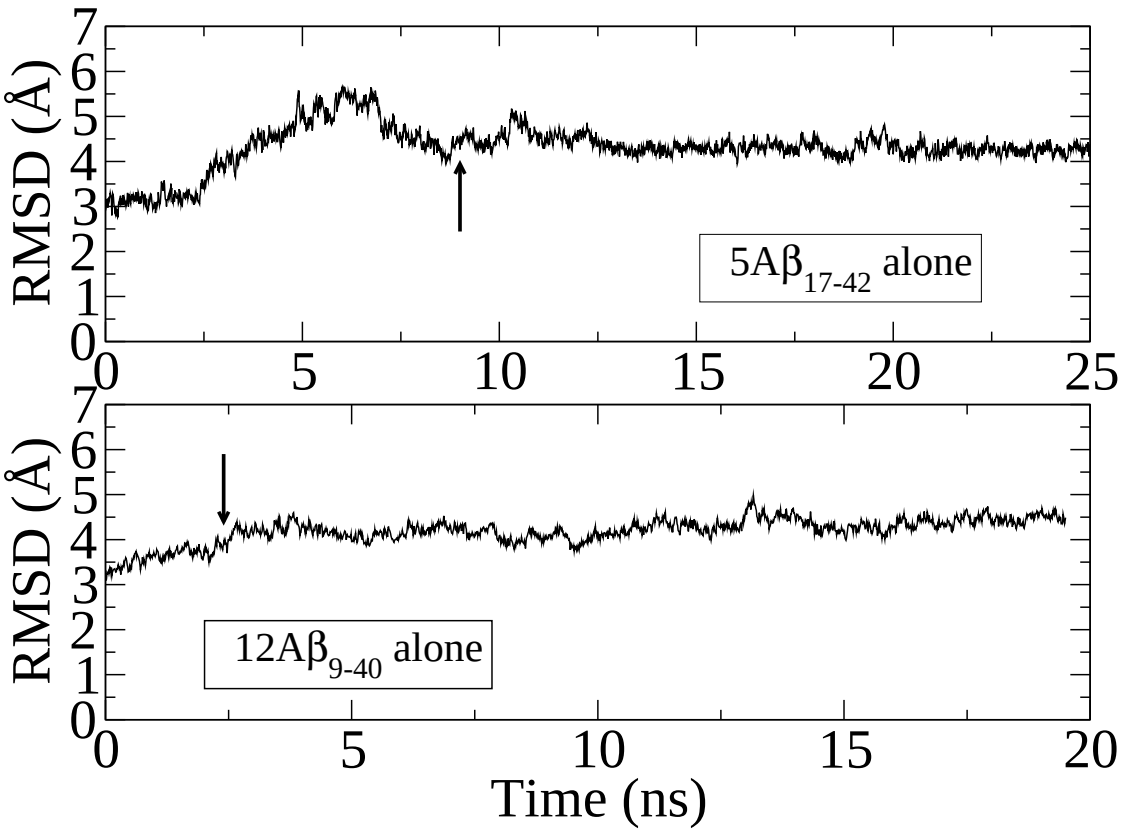

Figure S2: Evolution of RMSD of $5A\beta_{17-42}$ and $12A\beta_{9-40}$ without fullerenes. Arrow refers to the equilibration time τ_{eq}. Clearly these systems get equilibrated faster than those with fullerene.

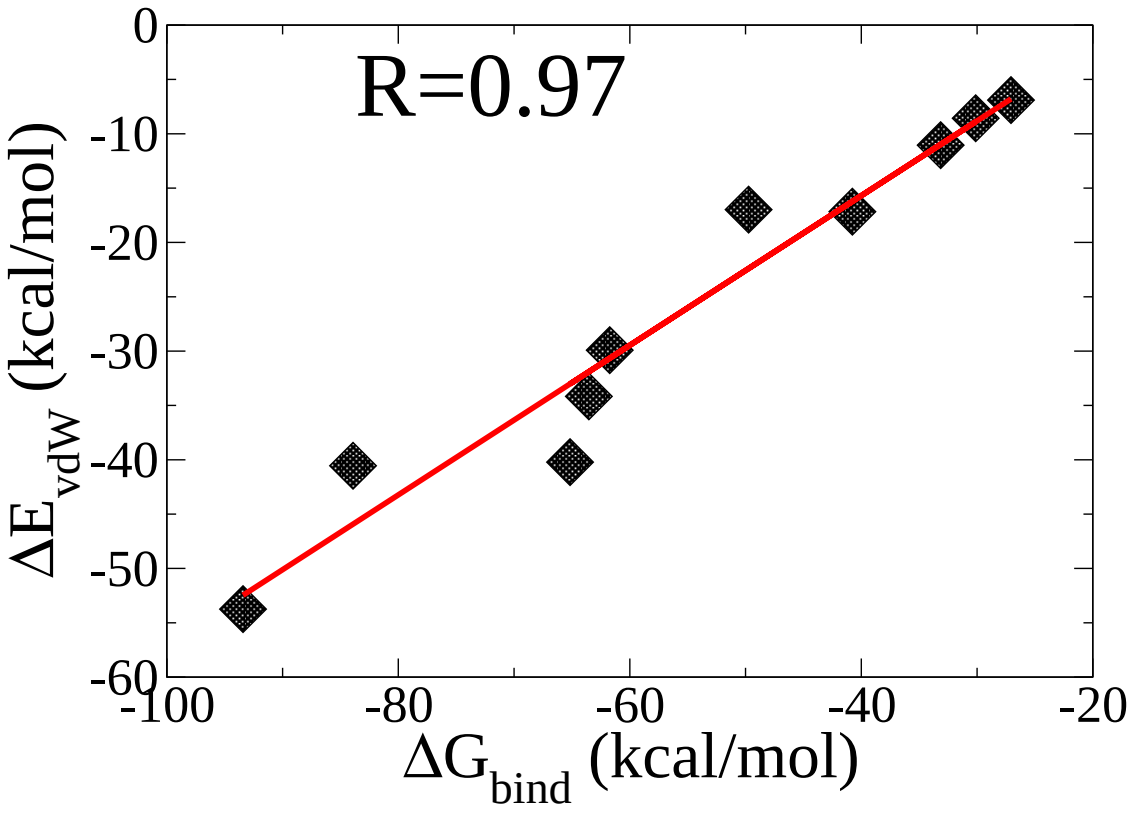

Figure S3: The correlation between ΔG_{bind} and vdW interaction energy. The correlation level R=0.97.

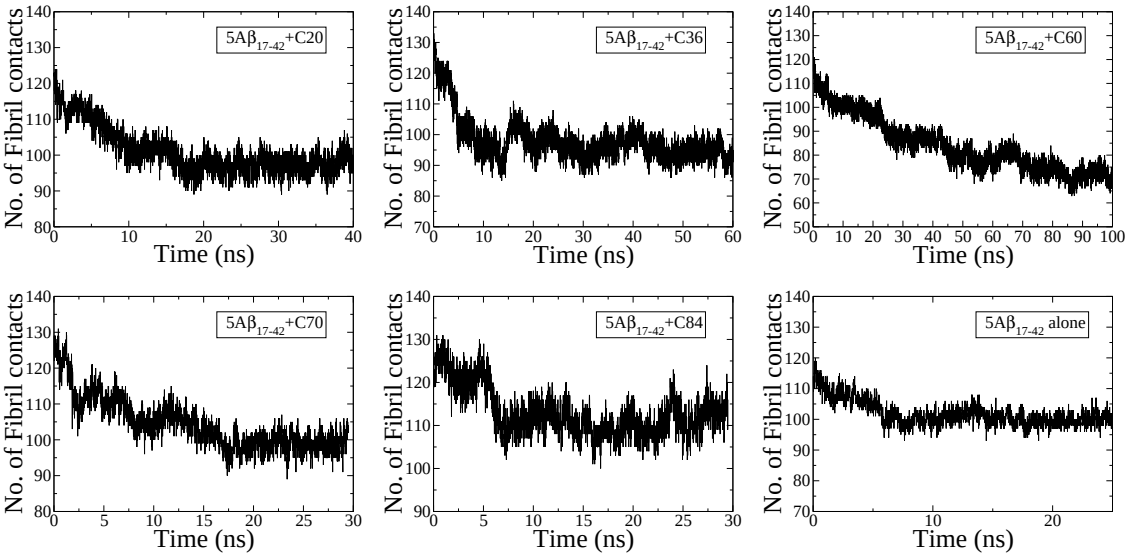

Figure S4: Evolution of fibril contacts for $5A\beta_{17-42}$ and complexes of $5A\beta_{17-42}$ +fullerenes. The PDB structure of $5A\beta_{17-42}$ has 161 FCs.

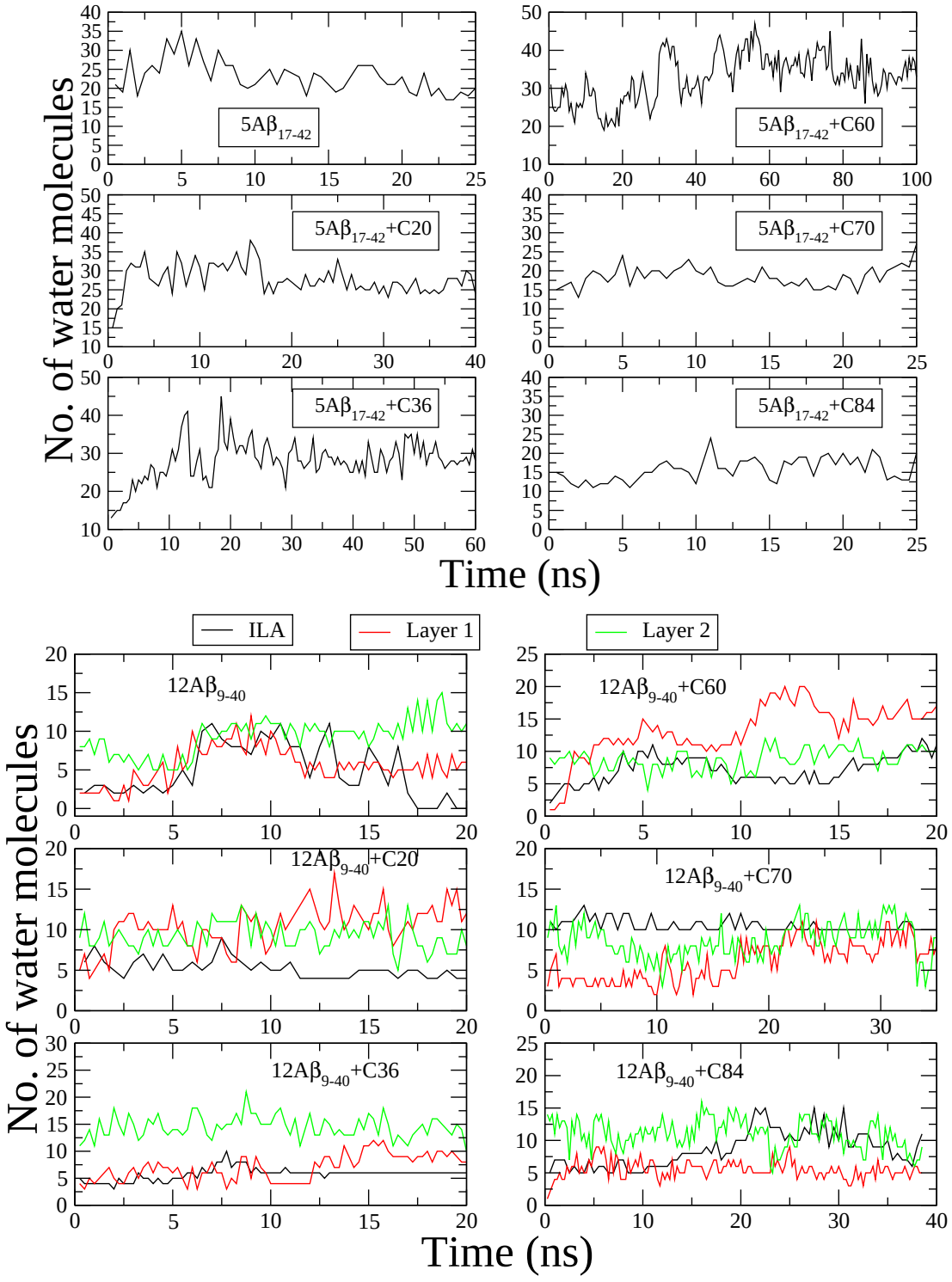

Figure S5: Time dependence of water molecules in the interior of $5A\beta_{17-42}$ (upper panel), and of two layers of $12A\beta_{9-40}$ and ILA (lower panel) in the presence and absence of fullerenes.

Movie 1. Movement of C20 in the complex with 5Aβ_{17-42} during MD simulations.

Movie 2. Movement of C84 in the complex with 5Aβ_{17-42} during MD simulations.

Movie 3. Movement of C60 in the complex with 5Aβ_{17-42} during MD simulations.

Movie 4. Movement of C60 in the complex with 12Aβ_{9-40} during MD simulations.

Movie 5. Movement of C36 in the complex with 5Aβ_{17-42} during MD simulations.

Movie 6. Movement of C36 in the complex with 12Aβ_{9-40} during MD simulations.

Movie 7. Movement of C70 in the complex with 12Aβ_{9-40} during MD simulations.

Movie 8. Movement of C84 in the complex with 12Aβ_{9-40} during MD simulations.

Coordinates of structures obtained in the best docking mode

In this section the coordinates of the structures, obtained in the best docking mode for all buckyballs with two targets 5Aβ_{17-42} and 12Aβ_{9-40}, are supplied in the PDB format. For instance, the coordinates of the 2BEG-C60 complex are stored in file "2begC60.pdb". In order to help a reader to quickly reproduce our plots in Pymol we also provide script files with extension pml. For example, to see the location of C60 near 2BEG as in Fig. 2 in the main text one has to type the command "pymol 2begC60.pml".