Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information to Amyloid-β Fibril Disruption by C_{60} — Molecular Guidance for Rational Drug Design

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Table I: Partial contributions to the binding free energy, ΔG^{bind}, following MM/PBSA analysis of C_{60}/Aβ-pentamer complexes in type I - III coordination (Δ refers to Complex $-(A\beta)_{5,\text{isolated}}$ $-C_{60,\text{isolated}}$).

Coordination	ΔMM^{vdW} $\left[\frac{kcal}{mol}\right]$	ΔMM^{Eel} $\left[\frac{kcal}{mol}\right]$	ΔPB $\left[\frac{kcal}{mol}\right]$	$\Delta\gamma_{eff}SA^{(a)}$ $\left[\frac{kcal}{mol}\right]$	ΔG^{bind} $\left[\frac{kcal}{mol}\right]$
Type I Complex	-49.21	-0.16	16.55	-2.56	-35.38
Type II Complex	-43.72	-0.17	11.57	-2.64	-34.95
Type III Complex	-67.40	-0.14	13.21	-3.18	-57.51

$^{(a)}$ effective surface tension $\times$ surface area

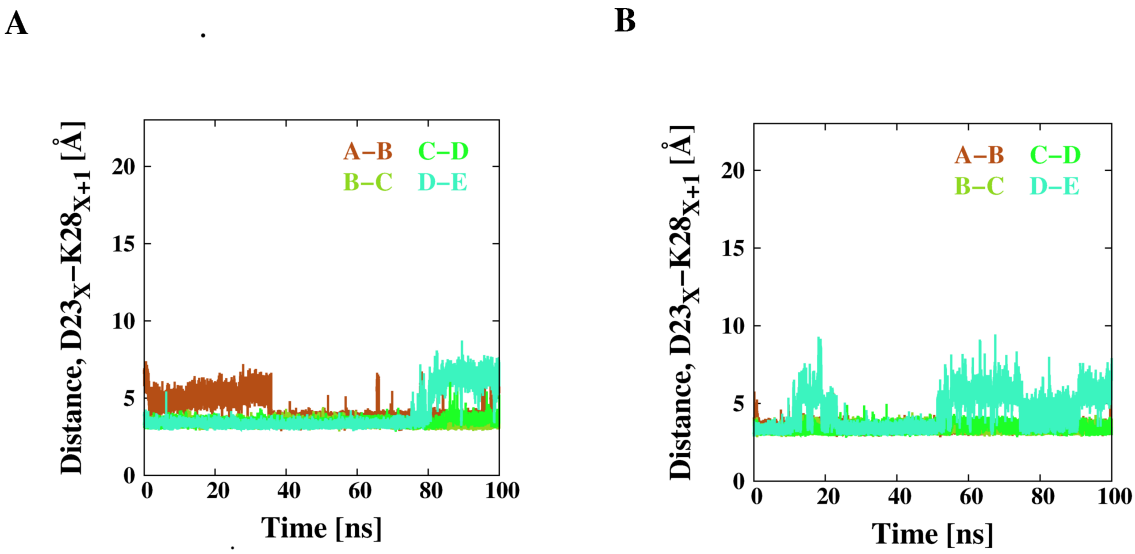

Figure I: **Inter-chain salt bridge between residues** $D23_X$ **and** $K28_{X+1}$ (A) Maintenance of the inter-chain salt bridge between residues $D23_X$ and $K28_{X+1}$ as observed during 100 ns of MD simulation of the wt Aβ pentamer (colors as in Fig 4A of the parent document). (B) Maintenance of the inter-chain salt bridge between residues $D23_X$ and $K28_{X+1}$ as observed during 100 ns of MD simulation of the complex C_{60}/Aβ pentamer (type III coordination, colors as in Fig 4A of the parent document). Little variation is seen thus indicating overall stability and maintenance of the inter-chain salt bridge in either system.