S100A9 induces aggregation-prone conformation in Abeta peptides: A combined experimental and simulation study

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Aβ_{12-24} protonation state		
Residue ID	*pKa* Value	Charge States
HIS-13	5.5	-1^{ε}
HIS-14	7.6	$+1^{\varepsilon,\delta}$
LYS-16	9.7	+1
GLU-22	4.5	−1
ASP-23	4.4	−1

Table S1 The protonation state of Aβ_{12-24} titratable residues at $pH = 7$.

ε - H on C (epsilon-1).
ε, δ - H on C (epsilon-1) and C (delta-2).

The temperatures of the 108 replicas in our Aβ-S100A9 REMD simulations are as following:
315.00 K, 315.97 K, 316.94 K, 317.92 K, 318.91 K, 319.89 K, 320.88 K, 321.88 K, 322.88 K, 323.89 K, 324.90 K, 325.91 K, 326.93 K, 327.96 K, 328.99 K, 330.02 K, 331.06 K, 332.11 K, 333.15 K, 334.21 K, 335.27 K, 336.33 K, 337.40 K, 338.47 K, 339.55 K, 340.64 K, 341.73 K, 342.82 K, 343.92 K, 345.03 K, 346.14 K, 347.26 K, 348.38 K, 349.51 K, 350.64 K, 351.78 K, 352.92 K, 354.07 K, 355.23 K, 356.39 K, 357.56 K, 358.73 K, 359.91 K, 361.10 K, 362.29 K, 363.49 K, 364.69 K, 365.90 K, 367.12 K, 368.34 K, 369.57 K, 370.80 K, 372.04 K, 373.29 K, 374.54 K, 375.81 K, 377.07 K, 378.35 K, 379.63 K, 380.92 K, 382.21 K, 383.51 K, 384.82 K, 386.14 K, 387.46 K, 388.79 K, 390.13 K, 391.47 K, 392.82 K, 394.18 K, 395.55 K, 396.92 K, 398.31 K, 399.69 K, 401.09 K, 402.50 K, 403.91 K, 405.33 K, 406.76 K, 408.20 K, 409.64 K, 411.10 K, 412.56 K, 414.03 K, 415.51 K, 417.00 K, 418.49 K, 420.00 K, 421.51 K, 423.04 K, 424.57 K, 426.11 K, 427.66 K, 429.22 K, 430.79 K, 432.36 K, 433.95 K, 435.55 K, 437.16 K, 438.77 K, 440.40 K, 442.04 K, 443.68 K, 445.34 K, 447.01 K, 448.69 K, 450.38 K and 452.07 K.
The temperatures of the 64 replicas in our Aβ dimer REMD simulations are as following:
315.00 K, 316.88 K, 318.77 K, 320.67 K, 322.57 K, 324.49 K, 326.42 K, 328.35 K, 330.29 K, 332.26 K, 334.22 K, 336.19 K, 338.17 K, 340.16 K, 342.16 K, 344.17 K, 346.19 K, 348.22 K, 350.26 K, 352.31 K, 354.37 K, 356.44 K, 358.52 K, 360.61 K, 362.71 K, 364.83 K, 366.95 K, 369.07 K, 371.21 K, 373.37 K, 375.53 K, 377.70 K, 379.88 K, 382.07 K, 384.27 K, 386.48 K, 388.71 K, 390.94 K, 393.18 K, 395.44 K, 397.71 K, 399.99 K, 402.28 K, 404.58 K, 406.89 K, 409.21 K, 411.55 K, 413.89 K, 416.25 K, 418.62 K, 421.00 K, 423.39 K, 425.79 K, 428.21 K, 430.64 K, 433.11 K, 435.56 K, 438.02 K, 440.49 K, 442.98 K, 445.48 K, 447.99 K, 450.51 K and 453.04 K.

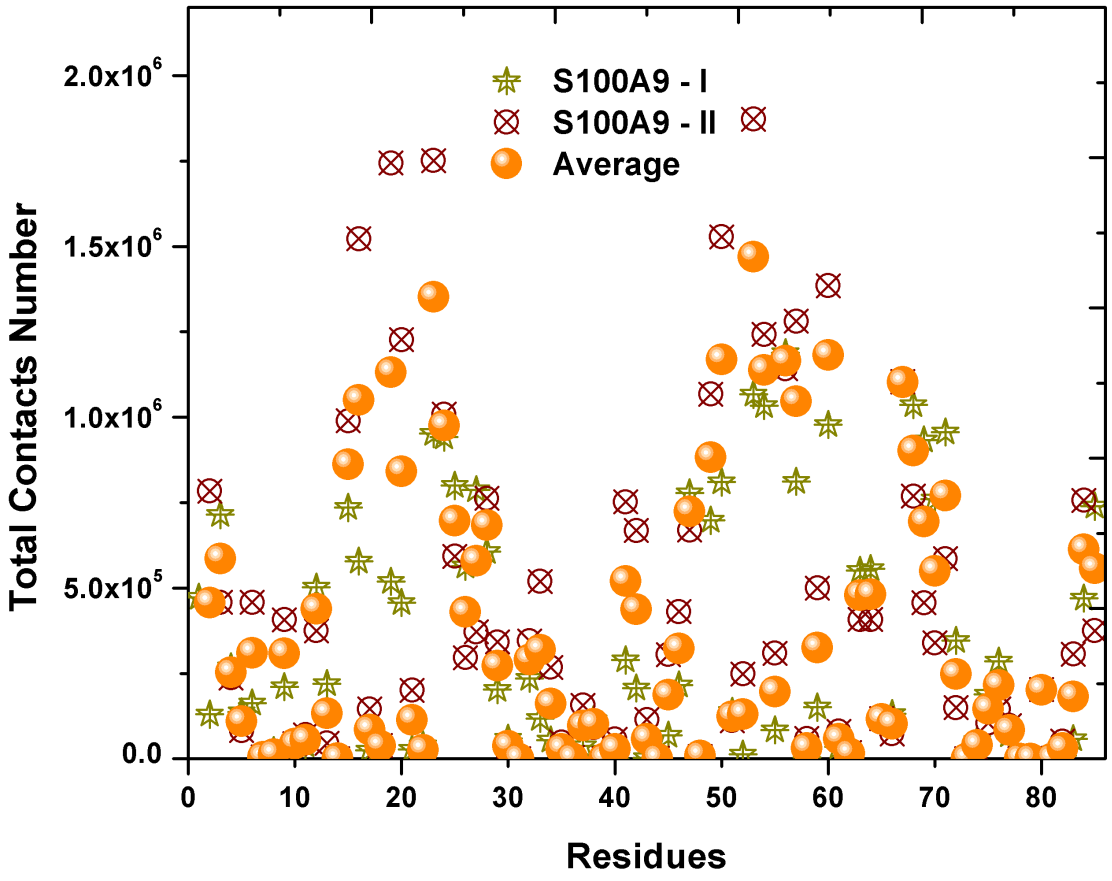

Fig. S1 A plot of the contact between S100A9 and Aβ_{12-24} peptides at the level of amino acids. The contacts were defined as atom pairs within a cut-off distance of 5 Å. The analysis was based on an ensemble of trajectories at 315 K. The average cumulative number of contacts of amino acids of S100A9 homodimer towards Aβ_{12-24} peptides. Note that S100A9-I indicates the first S100A9 consitutes the homodimer and S100A9-II indicates the second one.

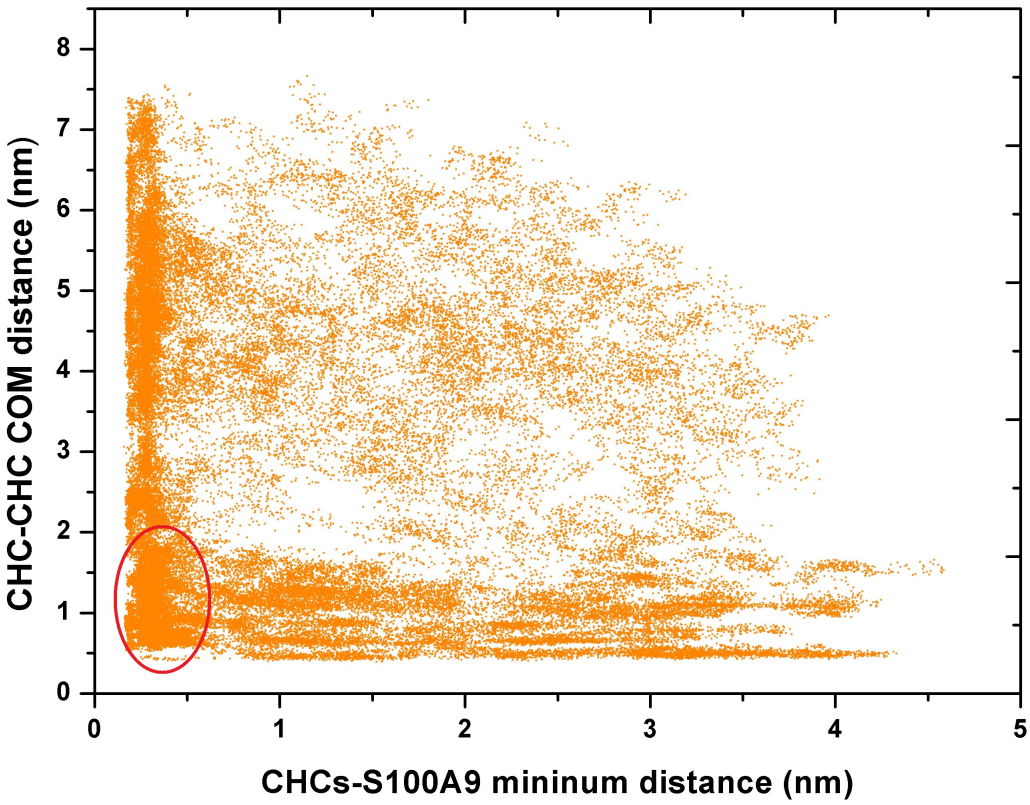

Fig. S2 A plot of the density distribution of the CHC-CHC COM distance with respect to the minimal distance towards S100A9 at 315 K. The x-axis indicates the minimum distance between CHCs and S100A9, while the y-axis gives the COM distance between the two CHCs. Note that the red circle indicates the densest distribution area.