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

Supplementary Material

Controlling the Self-assembly of Human Calcitonin: A Theoretical Approach from Molecular Dynamics Simulation

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(Dated: May 6, 2021)

Systems	N_{hCT}	N_{inh}	N_W	Box length (Å)	M_P (mM)
T1 (hCT+sCT)	5	5	10000	70.29	23.9
T2 (hCT+phCT)	5	5	10000	70.24	23.9
T3 (hCT+DM hCT)	5	5	10000	70.19	24.0
T4 (hCT+N17H hCT)	5	5	10000	70.27	23.9
T5 (hCT+Y12L hCT)	5	5	10000	70.21	24.0

TABLE S1: N_{hCT} , N_{inh} , and N_W represent the number of hCT, inhibitor peptides and water molecules respectively. M_P represents the peptide concentration in millimolar.

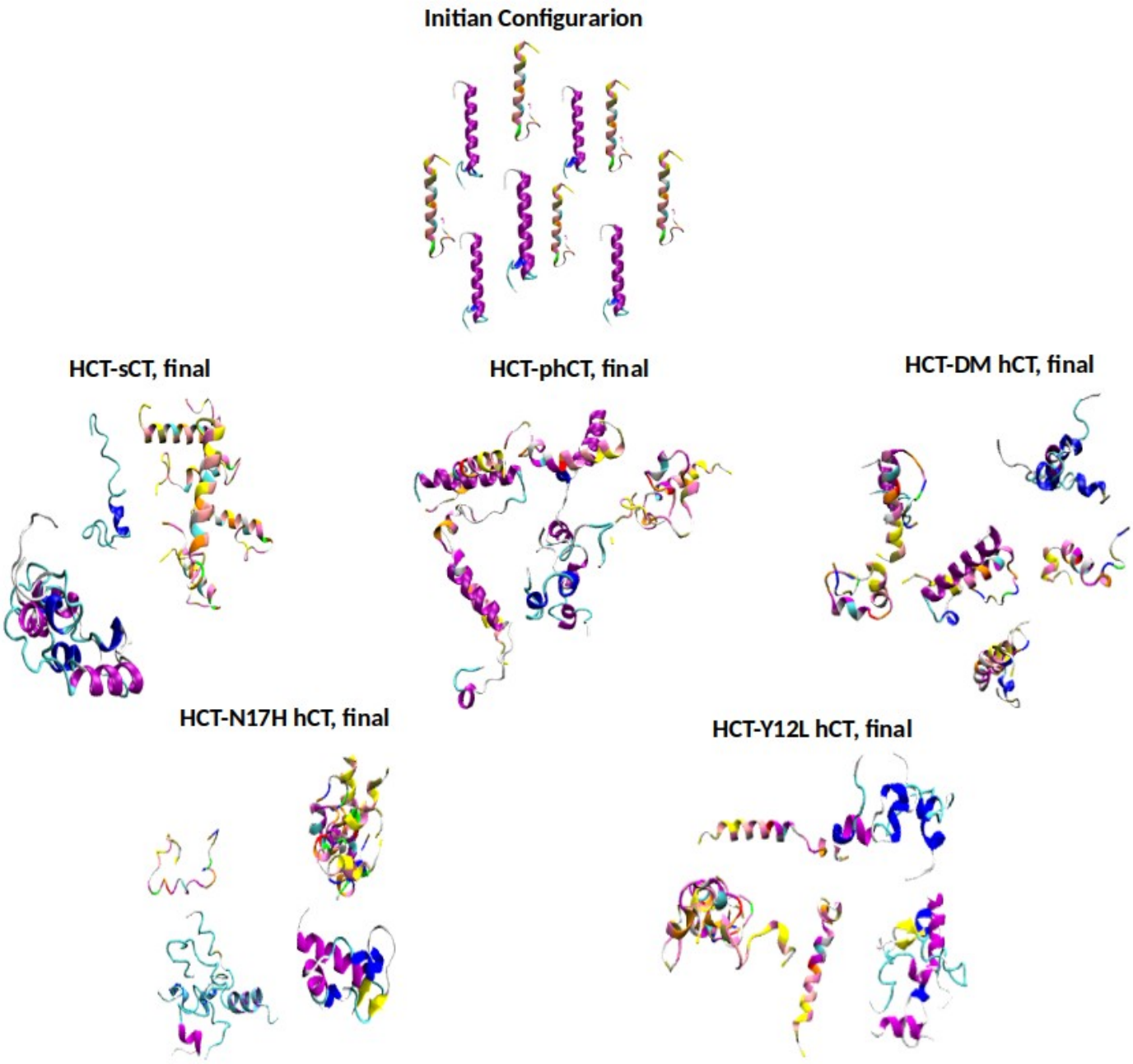

FIG. S1: Snapshot of hCT peptides (pink) and inhibitor peptides (colored according to resname) at starting and end of the simulation for different systems. As all the initial structures are visually similar, only one snapshot is provided. Water molecules are left off due to visual clarity.

Systems	Helix	β-sheet	Coil	Turn
S0 (hCT+no inhibitor)	36.88 (± 0.76)	2.66 (± 0.09)	43.66 (± 0.97)	16.80 (± 0.36)
T1 (hCT+sCT)	39.21 (± 0.56)	1.23 (± 0.03)	43.44 (± 1.11)	16.12 (± 0.21)
T2 (hCT+phCT)	49.56 (± 0.67)	0	38.02 (± 0.93)	12.42 (± 0.27)
T3 (hCT+DM hCT)	48.91 (± 0.61)	0	38.11 (± 0.81)	12.98 (± 0.29)
T4 (hCT+N17H hCT)	38.73 (± 0.68)	3.78 (± 0.09)	42.78 (± 0.78)	14.71 (± 0.24)
T5 (hCT+Y12L hCT)	39.19 (± 0.60)	3.43 (± 0.07)	41.02 (± 0.84)	16.36 (± 0.30)

TABLE S2: Percentage of Helix, β-Sheet, coil and turn conformations of hCT for the systems T1 to T5. Standard deviations are calculated using block average method and included in the parenthesis.