

Supporting material (Text S1) for:

Structural similarities and differences between amyloidogenic and non-amyloidogenic Islet Amyloid Polypeptide (IAPP) sequences and implications for the dual physiological and pathological activities of these peptides

Author Affiliation:

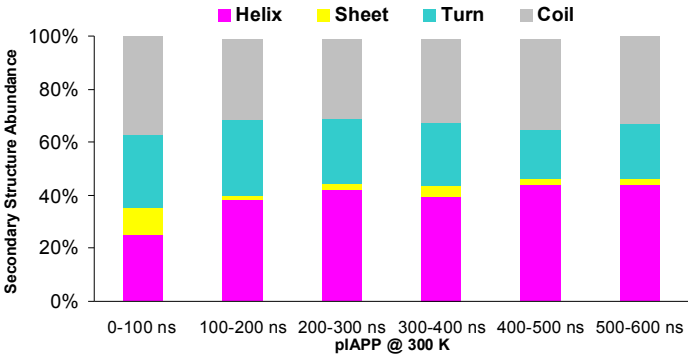
Chun Wu, Joan-Emma Shea^{*}

Department of Chemistry and Biochemistry, University of California Santa Barbara,
Santa Barbara, CA 93106

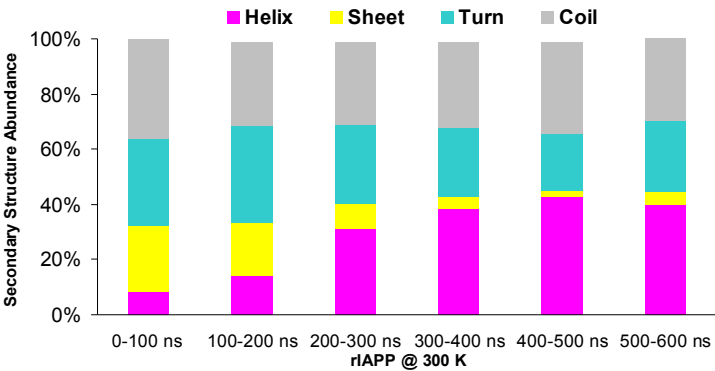
Table S1. The calcitonin family of peptides. Three structural features are conserved (conserved residues are in red): 1) a disulfide bond close to N-termini; 2) a region of putative amphipathic α -helix; 3) a C-terminal amidation. CGRP: calcitonin gene-related peptide

	S-S	
Human IAPP	KC	NTATCATQRLANFLVHS SNNFGA I LSS TNVGSNT Y-NH2
Calcitonin	CG	NLSTCMLGTYTQDFNKFHTF PQT A IGVGA P-NH2
Adrenomedullin	GC	RFGTCTVQKLAHQIYQFT DKDKDNVAPR NK I SP Q G Y-NH2
α CGRP	AC	DTATCVTHRLAGLLSRSGGVVKNNFVP TNVGSKA F-NH2
β CGRP	AC	NTATCVTHRLAGLLSRSGGMVKSNFVP TNVGSKA F-NH2

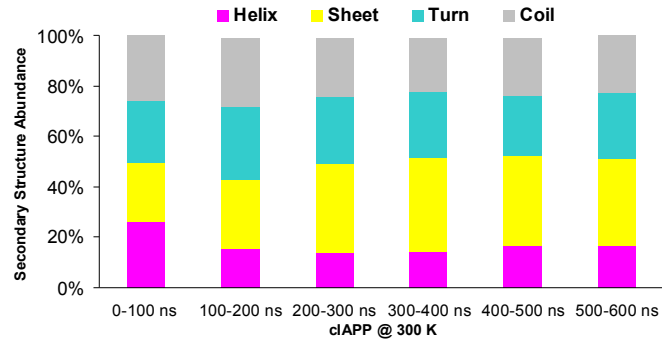
Table S2 the convergence within last 300 ns of the REMD simulations. A total 600 ns sampling at 300 K is equally divided into six blocks for secondary and tertiary structure Hanalysis. A, E: pig IAPP; B, F: rat IAPP; C, G: cat IAPP; D, H: human IAPP



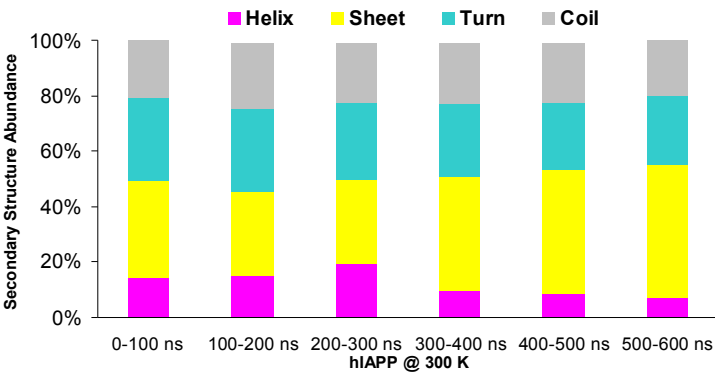
A



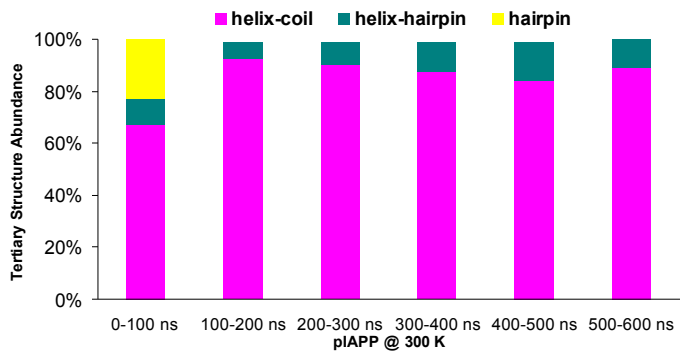
B



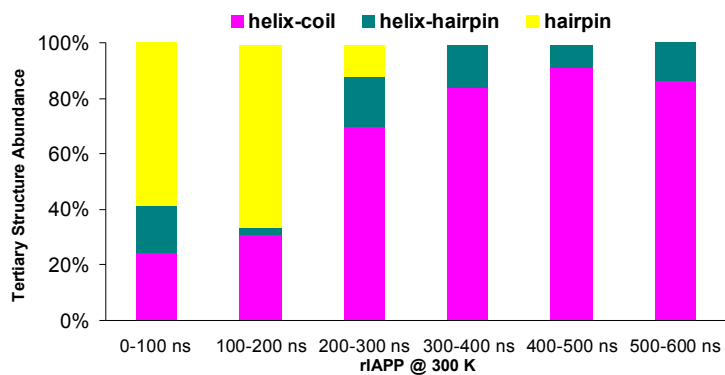
C



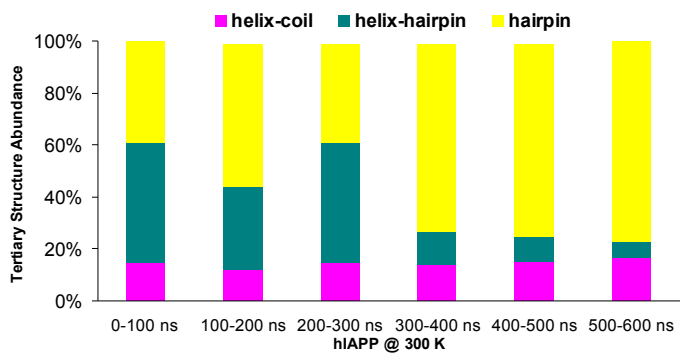
D



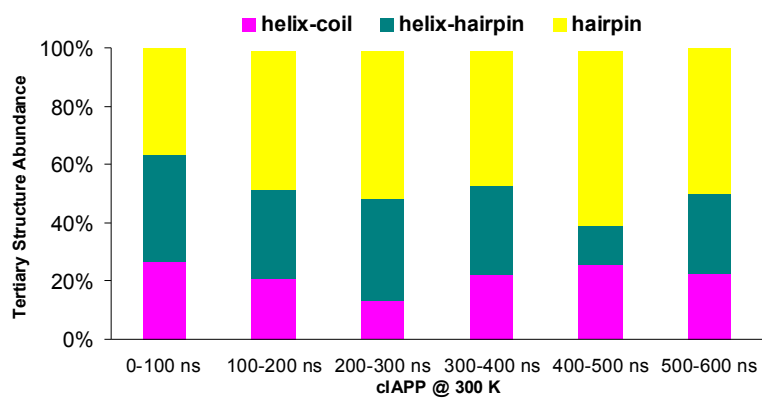
E



F

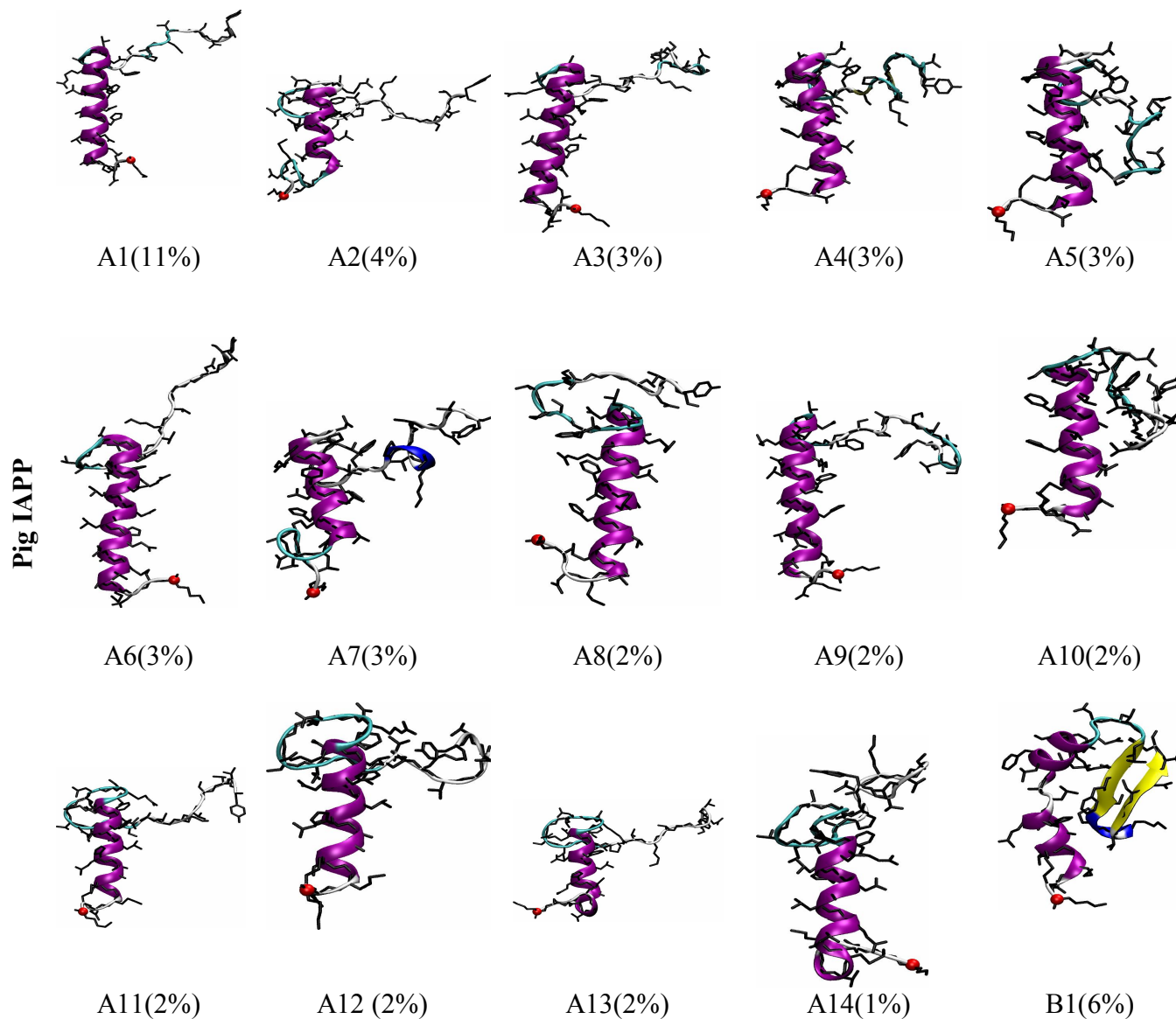


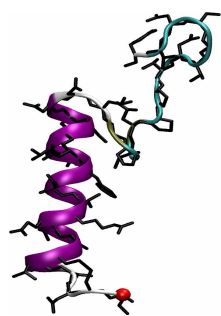
G



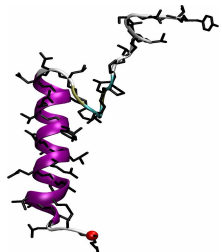
H

Table S3 Representative structures of the top 15 structural families for each IAPP peptide from the clustering analysis (500-600 ns) with a cutoff C α rmsd of 3.0 Å. A1-B1: pig IAPP, C1-D1: rat IAPP, E1-G6: cat IAPP, H1-J6 human IAPP. The abundance is shown in parenthesis. The backbone is in cartoon; α -helical, β -sheet, β -bridged, turn and coiled conformations are colored in purple, yellow, tan, cyan and white respectively. The N-terminus is shown by a red ball.

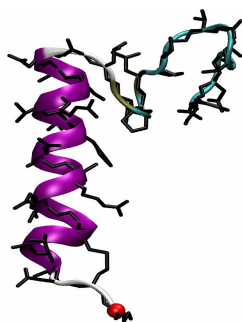




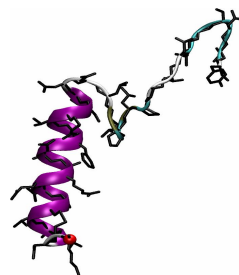
C1(9%)



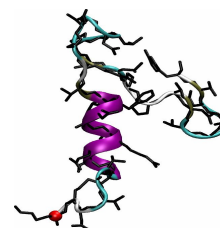
C2(9%)



C3(3%)

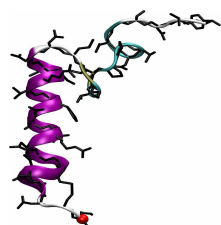


C4(3%)

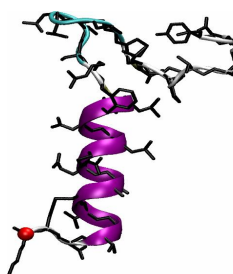


C5(3%)

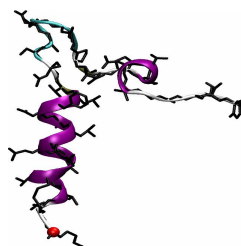
Rat IAPP



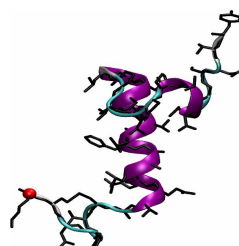
C6(2%)



C7(2%)



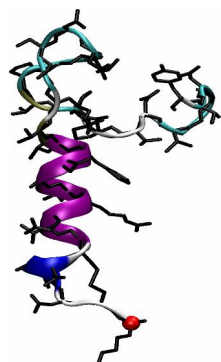
C8(2%)



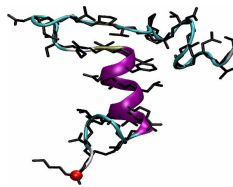
C9(2%)



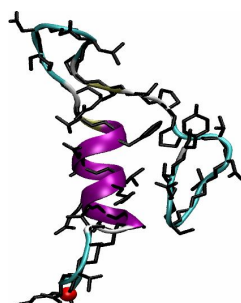
C10(1%)



C11(1%)



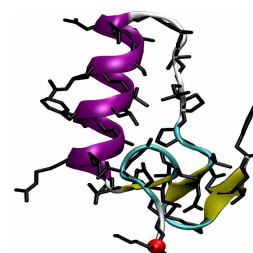
C12(1%)



C13(1%)

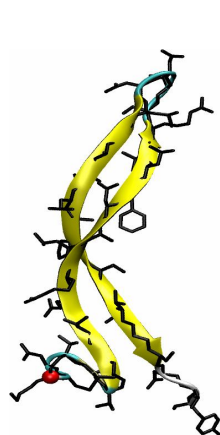


C14(1%)

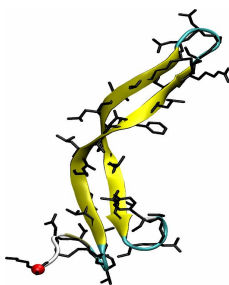


D1(4%)

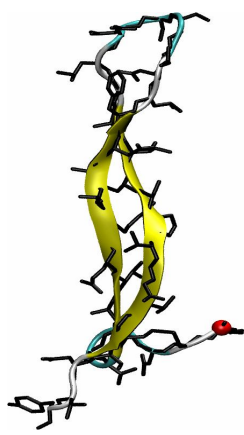
Cat IAPP



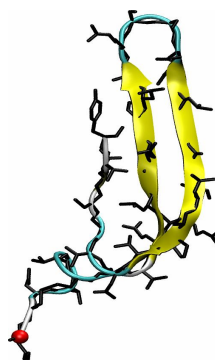
E1(13%)



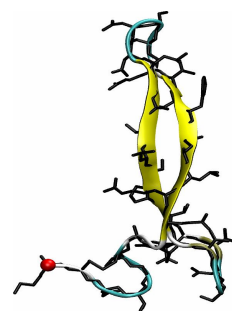
E2(5%)



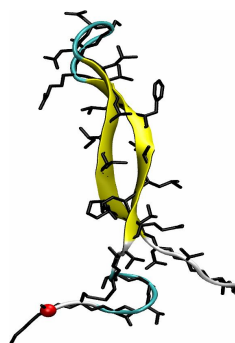
E3(5%)



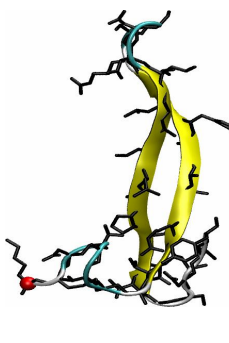
E4(4%)



E5(4%)



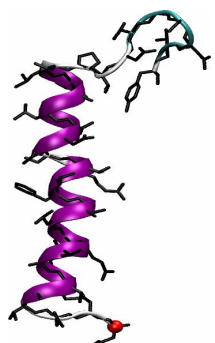
E6(3%)



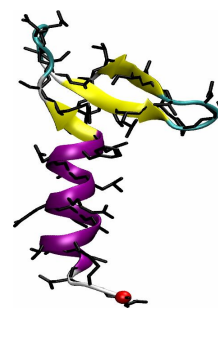
E7(1%)



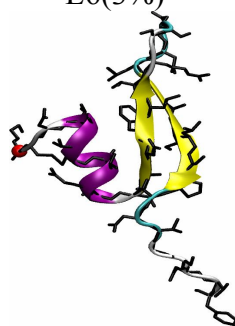
F1(1%)



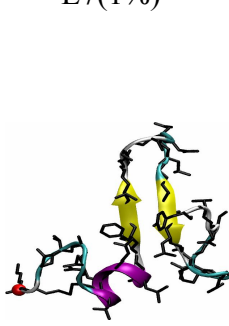
F2(1%)



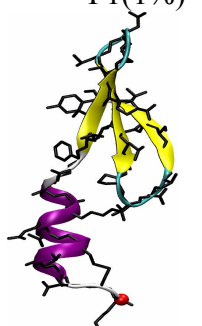
G1(6%)



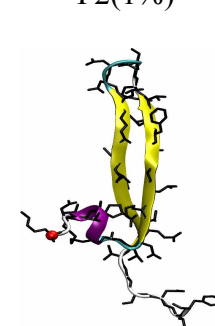
G2(4%)



G3(2%)



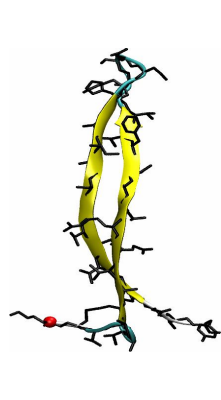
G4(2%)



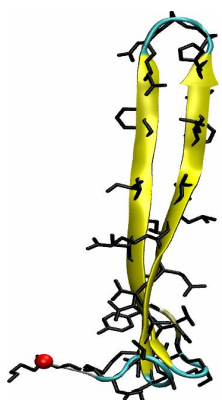
G5(1%)



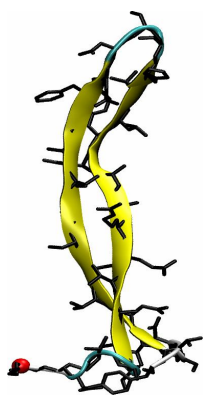
G6(1%)



H1(29%)



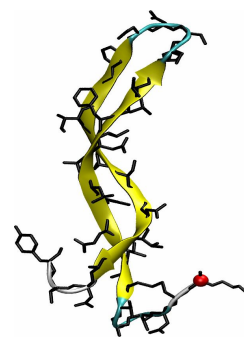
H2(26%)



H3(4%)

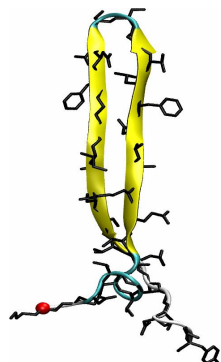


H4(3%)

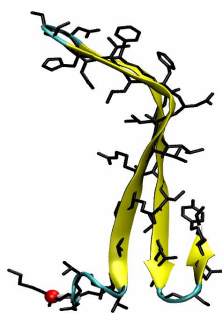


H5(2%)

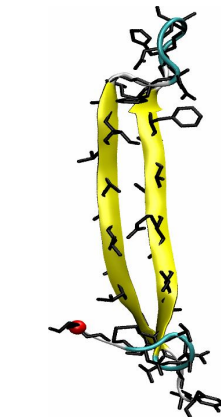
Human IAPP



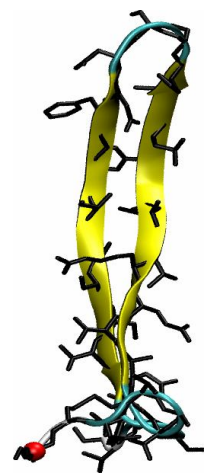
H6(2%)



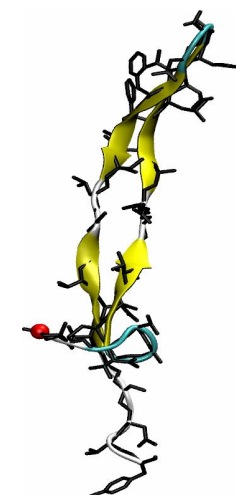
H7(2%)



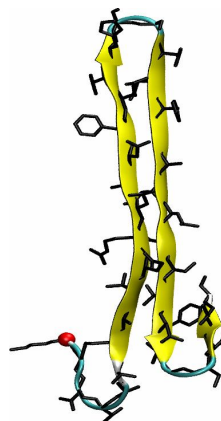
H8(1%)



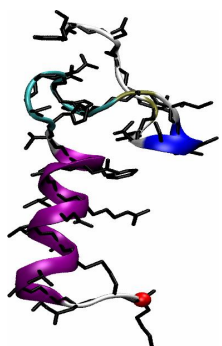
H9(1%)



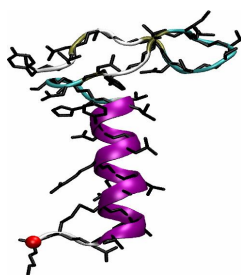
H10(1%)



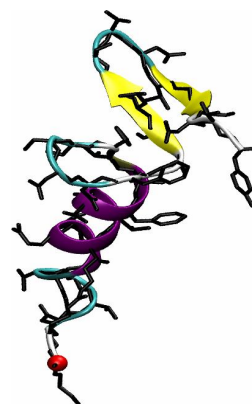
H11(1%)



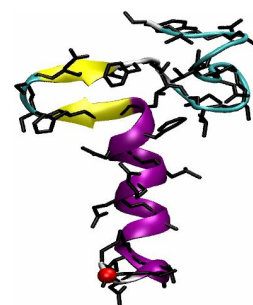
I1(2%)



I2(1%)



J1(2%)



J2(1%)