Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Molecular Simulations of Zwitterlation-induced Conformation and Dynamics Variation of Glucagon-like Peptide-1 and Insulin

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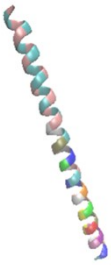
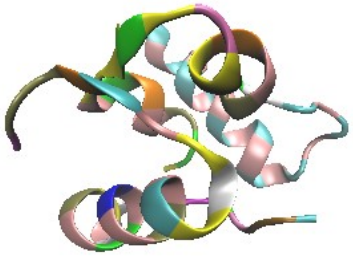
Table S1. The sequence of GLP-1.

	Sequence
GLP-1	HAEGTFTSDVSSYLEGQAAKEFIAWLVKGR

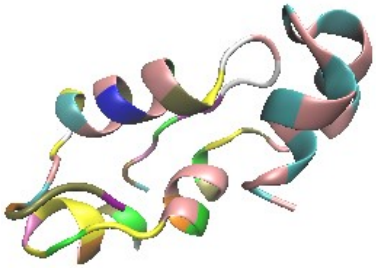
(a)



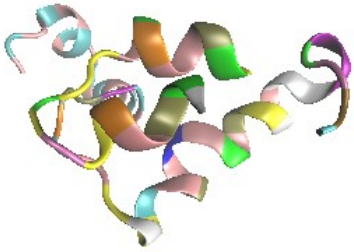
(b)



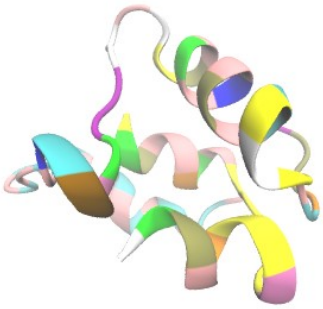
(c)



(d)

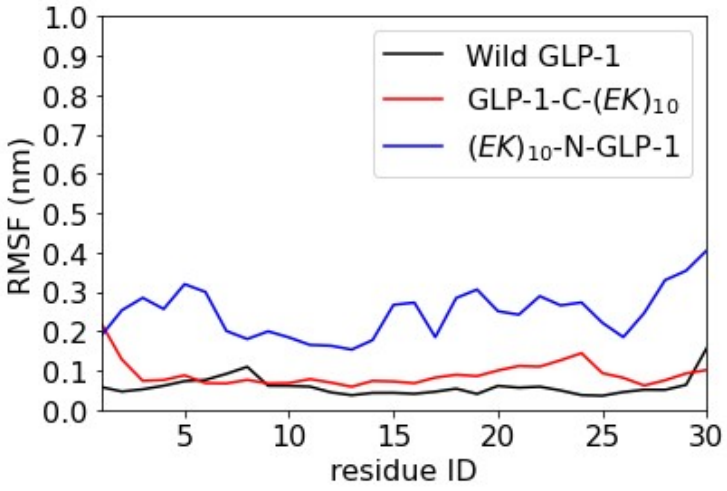


(e)



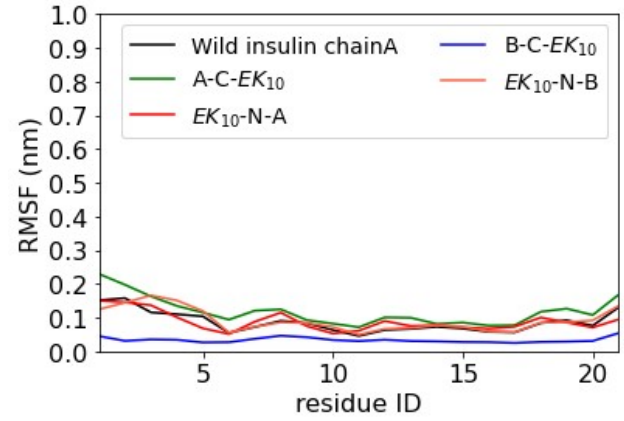
(f)

Figure S1. The Rosetta predicted structure of (a) $(EK)_{10}$-N-GLP-1, (b) GLP-1-C-$(EK)_{10}$, (c) $(EK)_{10}$-N-insulin-A, (d) insulin-A-C-$(EK)_{10}$, (e) $(EK)_{10}$-N-insulin-B, (f) insulin-B-C-$(EK)_{10}$. These structures predicted by Rosetta Server, colored by residue name. The protein: new-cartoon model, colored based on the residue name.

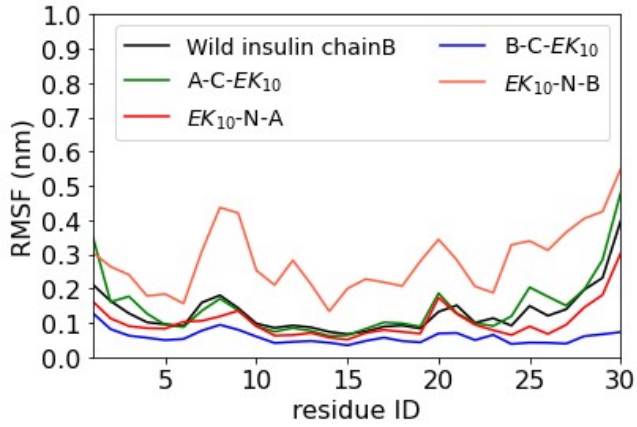


(a)

Figure S2. RMSF of C_α atoms on GLP-1



(a)



(b)

Figure S3. RMSF of C_α atoms on insulin (a) Chain A and (b) Chain B

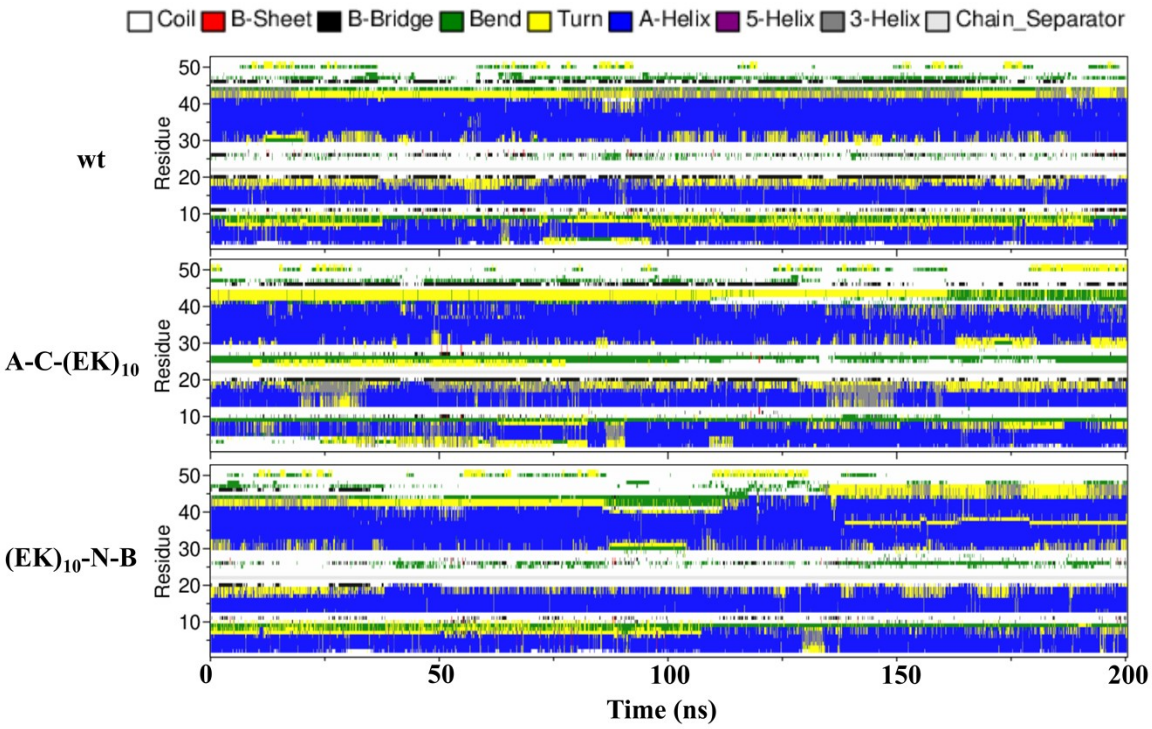


Figure S4. Secondary structure analysis of residues verse simulation time for insulin protein and the protein-peptide conjugates.