Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information

Effect of Mixture of Ionic Liquids and Water on the Structure and Stability of Insulin Dimer: A Combined DFT and MD Simulations Study

N. Giri Lakshman[†,‡] S. M. Esther Rubavathy,[†,‡] S. Priyankha,[†,‡] K. Palanisamy,[†] and M. Prakash*[,†]

[†] *Department of Chemistry, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur - 603 203, Chengalpattu, Tamil Nadu, India.*

[‡]***These authors are contributed equally to this work***

*Corresponding Authors: Muthuramalingam Prakash: Phone: +914427417142 and +914427417832. Email: prakashspm@gmail.com and prakashm4@srmist.edu.in

Table S1: The average values of RMSD, RMSF, and Rg of the systems

Systems	RMSD (nm)	RMSF (nm)	Rg (nm)
Protein-water	0.162	0.095	1.125
Protein-[Cho] [Ger]	0.122	0.077	1.022
Protein-[Cho] [Tau]	0.132	0.086	1.099
Protein--[Cho] [Ger] [Tau]	0.192	0.114	1.043

Radial distribution function (RDF) was calculated to identify the interaction of choline, taurate, and geranate ions with water. **Fig. S1** displays the RDF plots of water containing choline, geranate, and taurate ions. When we compared [Cho] [Tau] ILs sharp peak was observed for the cation Choline with water at 1.5 nm than the taurate water. Also, higher peaks were observed for the geranate anions. It shows that the geranate ions have strongly interacted with the protein. We conclude that the [Cho] [Ger] ILs show sharp peaks in the RDF plots. This shows that the [Cho] [Ger] ILs stabilises the insulin protein

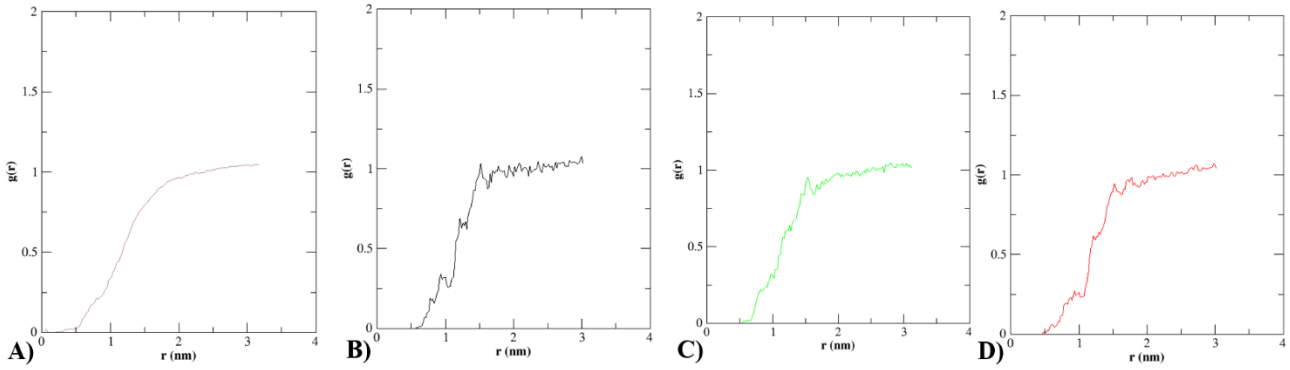

Fig. S1. RDF plots for the protein and ILs **A)** protein-water **B)** protein-[Cho] [Ger] **C)** protein-[Cho] [Tau] **D)** protein-[Cho] [Ger] [Tau] ILs.

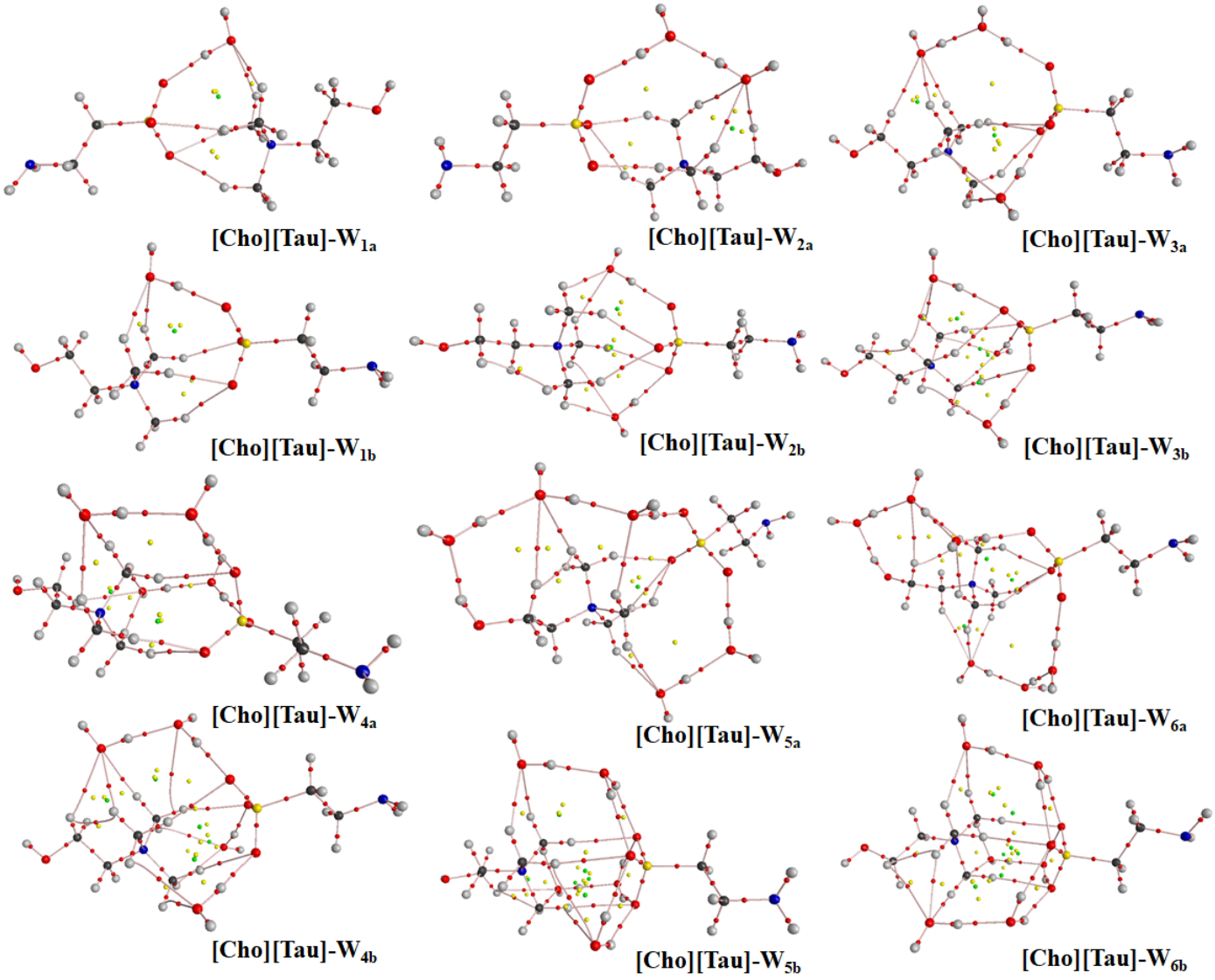

Fig. S2. Electron topography of most stable geometries of [Cho] [Tau] with W_n (n=1-6) models are displayed, where red colour represents the bond critical points.

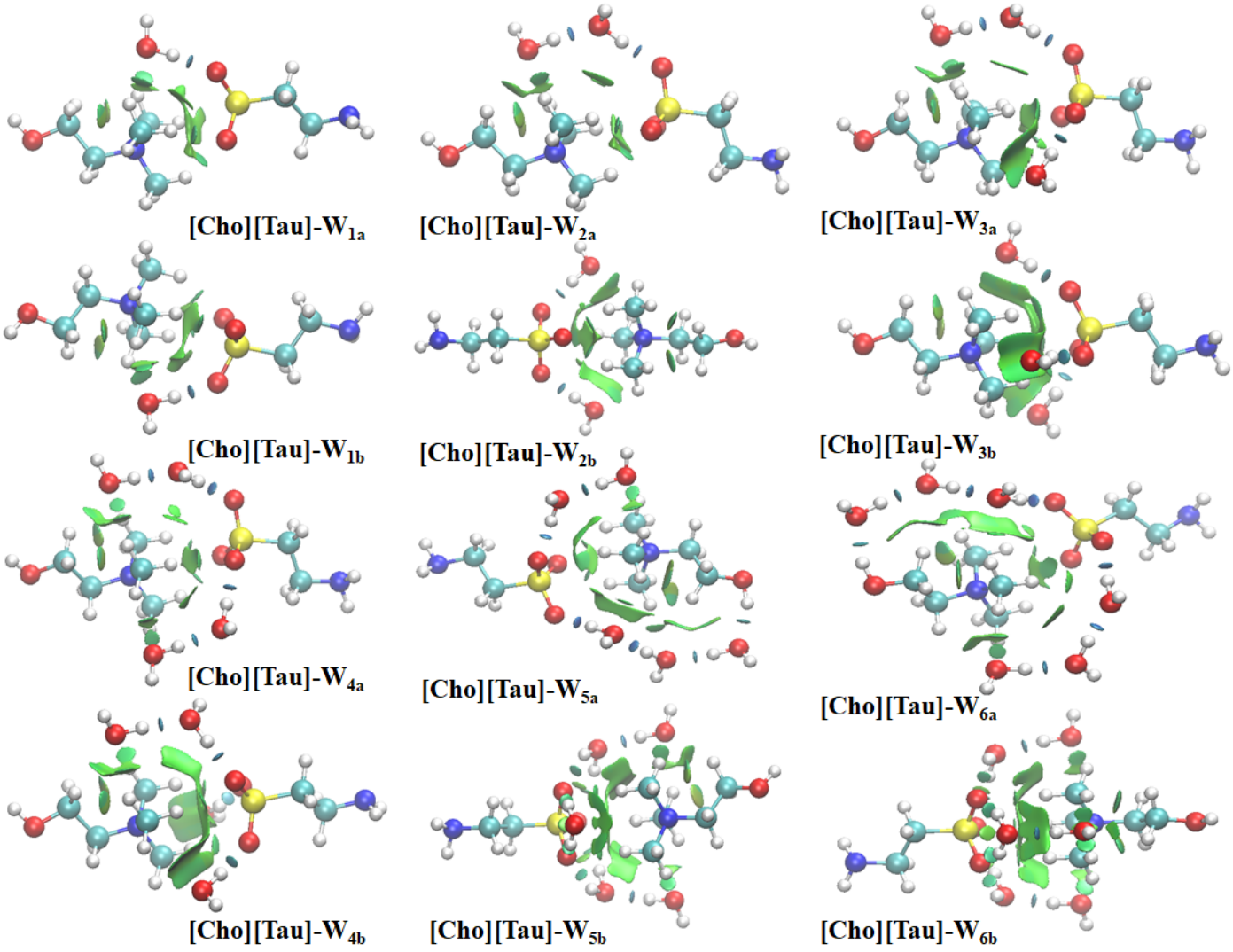

Fig. S3. NCI plots of [Cho] [Tau] W_n (n=1-6) models, interactions of weak (green), strong (blue) are shown.

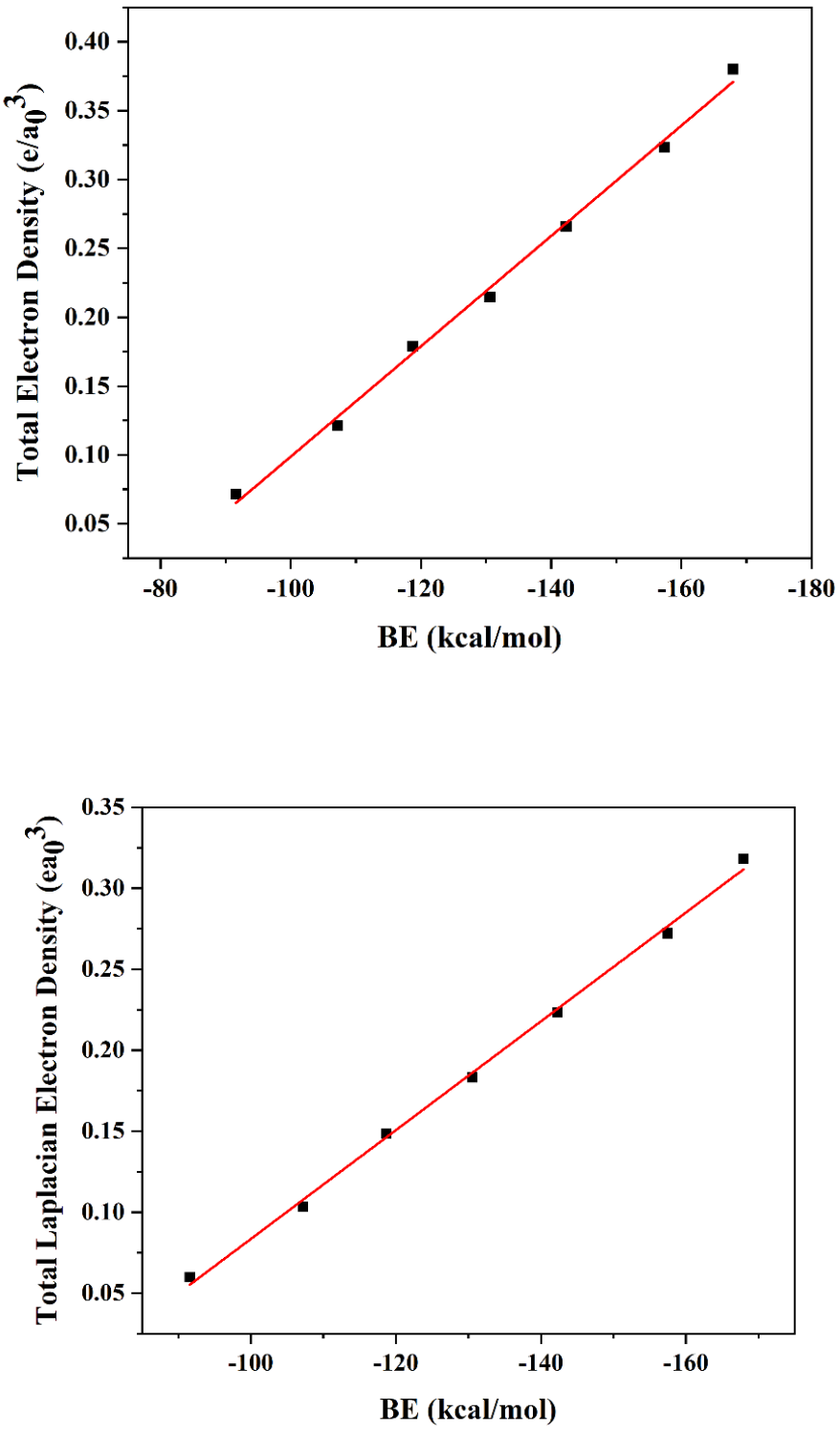

Fig. S4. Correlation between binding energy and total electron density (Σ ($\rho(r_c)$) and total laplacian electron density ($\nabla^2\rho(r_c)$) of [Cho] [Tau] W_n (n=0-6) clusters.