

A green approach to offset the perturbation action of 1-butyl-3-methylimidazolium iodide on α -chymotrypsin

P. Madhusudhana Reddy, R. Umapathi and P. Venkatesu*

Department of Chemistry, University of Delhi, Delhi-110 007, India.

E-mail: venkatesup@hotmail.com; pvenkatesu@chemistry.du.ac.in (P. Venkatesu)

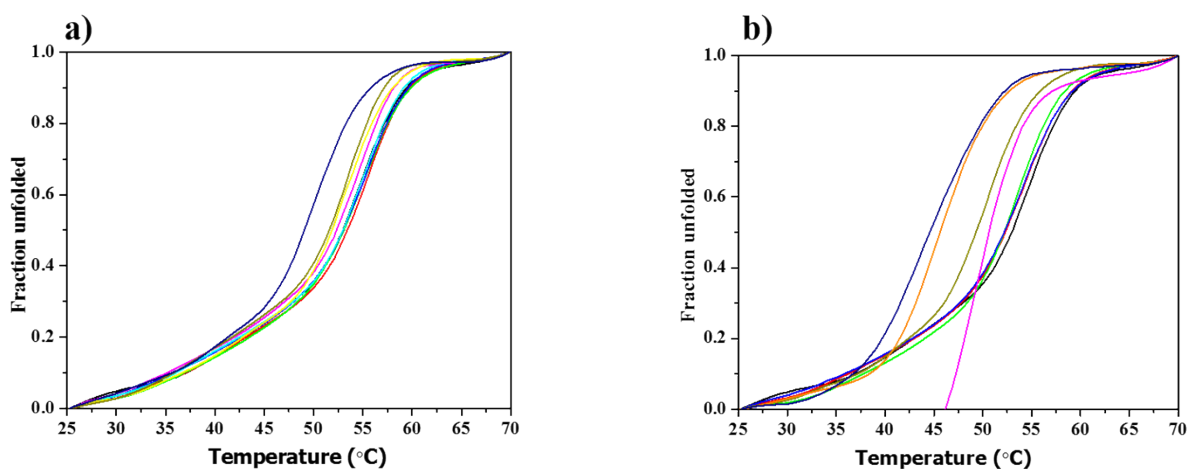


Fig. S1 Fraction of unfolded α -chymotrypsin (CT) in tris-HCl buffer in the presence of [Bmim][Br] (a); [Bmim][I] (b). The black, red, green, blue, cyan, magenta, yellow, dark yellow and navy color lines represent CT in buffer, 0.025, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3 and 0.6 M, respectively, of [Bmim][Br] in panel a; black, red, green, blue, magenta, dark yellow, orange and navy color lines represent CT in buffer, 0.025, 0.05, 0.1, 0.2, 0.3, 0.4 and 0.6 M, respectively, of [Bmim][I] in panel b.

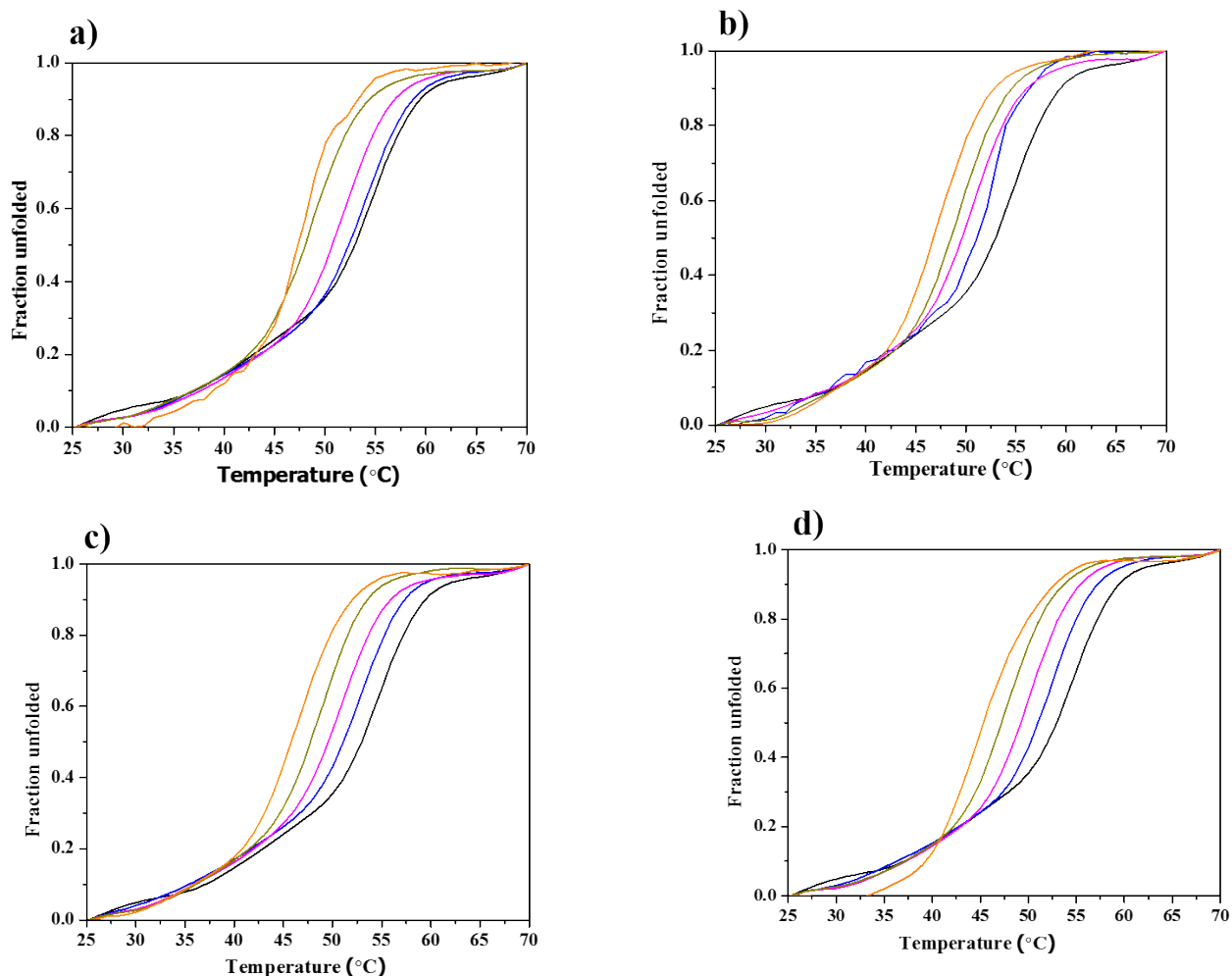


Fig. S2 Fraction of unfolded α -chymotrypsin (CT) in tris-HCl buffer in the presence of [Bmim][Br] + [Bmim][I] mixture. The blue, magenta, dark yellow and orange lines represent mole ratios of [Bmim][Br] + [Bmim][I] mixture as 0.025:0.1, 0.025:0.2, 0.025:0.3 and 0.025:0.4 M respectively, in panel a; 0.5:0.1, 0.5:0.2, 0.5:0.3 and 0.5:0.4 M respectively, in panel b; 0.1:0.1, 0.1:0.2, 0.1:0.3 and 0.1:0.4 M respectively, in panel c; 0.2:0.1, 0.2:0.2, 0.2:0.3 and 0.2:0.4 M respectively, in panel d. The black color line represents in all panels α -chymotrypsin (CT) in tris-HCl buffer.

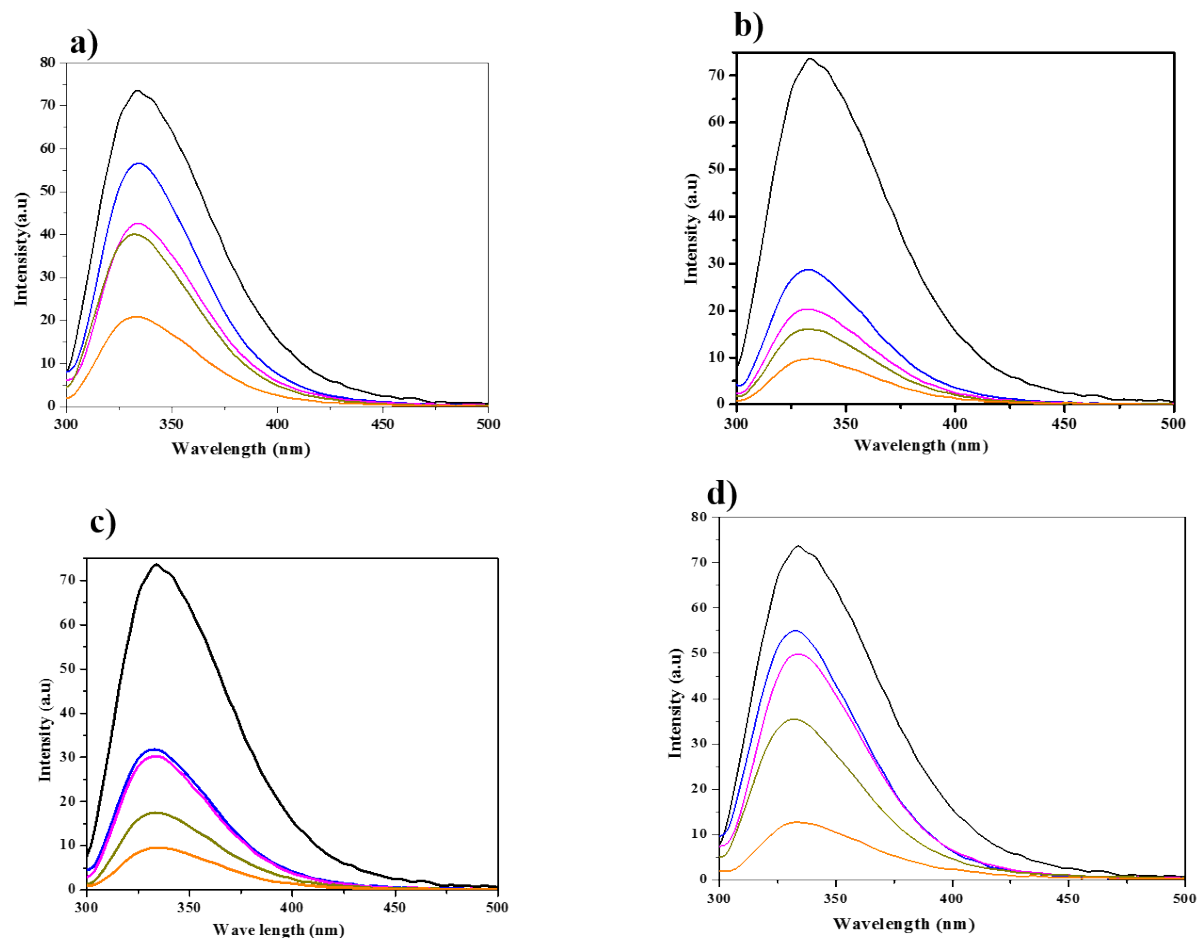


Fig. S3 Fluorescence intensity changes for α -chymotrypsin (CT) in tris-HCl buffer in the presence of [Bmim][Br] + [Bmim][I] mixture. The blue, magenta, dark yellow and orange lines represent mole ratios of [Bmim][Br] + [Bmim][I] mixture as 0.025:0.1, 0.025:0.2, 0.025:0.3 and 0.025:0.4 M respectively, in panel a; 0.5:0.1, 0.5:0.2, 0.5:0.3 and 0.5:0.4 M respectively, in panel b; 0.1:0.1, 0.1:0.2, 0.1:0.3 and 0.1:0.4 M respectively, in panel c; 0.2:0.1, 0.2:0.2, 0.2:0.3 and 0.2:0.4 M respectively, in panel d. The black color line represents in all panels α -chymotrypsin (CT) in tris-HCl buffer.

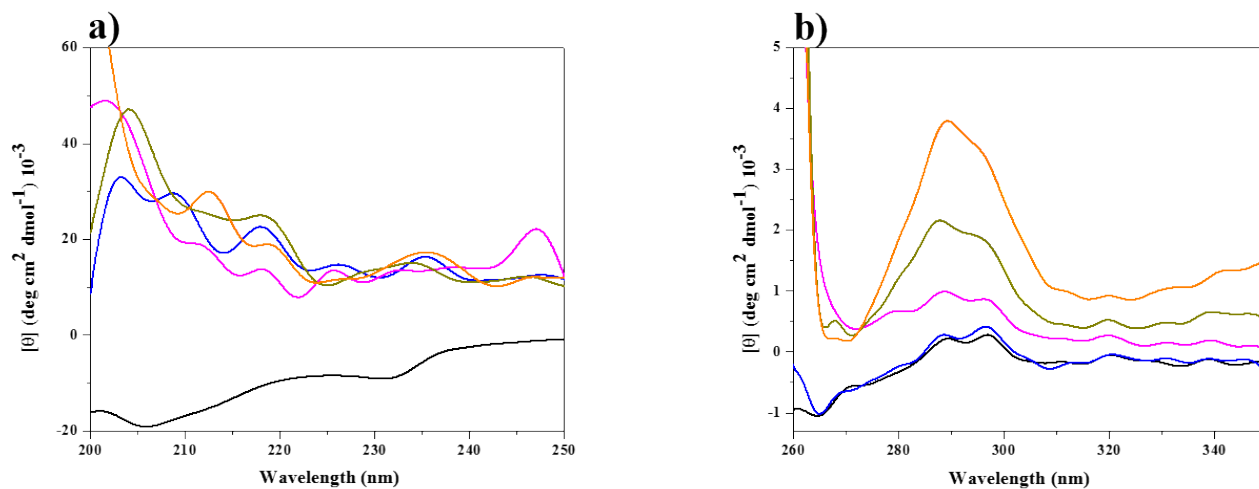


Fig. S4 Far (a) and near (b) UV-CD spectra for α -chymotrypsin (CT) in tris-HCl in the presence of presence of [Bmim][Br] + [Bmim][I] mixture. The blue, magenta, dark yellow and orange lines represent mole ratios of [Bmim][Br] + [Bmim][I] mixture as 0.025:0.1, 0.025:0.2, 0.025:0.3 and 0.025:0.4 M respectively, in panels a and b. The black color line represents in both the panels is α -chymotrypsin (CT) in tris-HCl buffer.

Table S1. Transition temperature (T_m), enthalpy change (ΔH) Gibbs free energy changes (ΔG_u) and heat capacity change (ΔC_p) at 25 °C for the α -chymotrypsin (CT) in tris HCl in the presence of various concentrations of ionic liquids (ILs) and ionic liquid mixtures determined by fluorescence spectroscopy.^a

Sample	T_m / °C	ΔH / k Cal mol ⁻¹	ΔG_u / k Cal mol ⁻¹	ΔC_p / k Cal mol ⁻¹ K ⁻¹
Buffer	53.1	55.76	4.01	1.04
0.025 M [Bmim][Br]	53.5	59.63	4.31	1.10
0.05 M [Bmim][Br]	53.3	52.93	3.81	0.98
0.1 M [Bmim][Br]	53.1	58.90	4.24	1.10
0.15 M [Bmim][Br]	52.9	55.42	3.98	1.03
0.2 M [Bmim][Br]	52.4	61.01	4.34	1.15
0.25 M [Bmim][Br]	51.8	60.31	4.25	1.15
0.3 M [Bmim][Br]	51.6	62.93	4.41	1.20
0.6 M [Bmim][Br]	49.1	64.67	4.34	1.31
0.025 M[Bmim][I]	52.3	57.82	4.10	1.09
0.05 M[Bmim][I]	52.2	66.39	4.71	1.26
0.1 M[Bmim][I]	52.1	57.18	4.05	1.09
0.2 M[Bmim][I]	50.6	97.70	5.74	1.92
0.3 M[Bmim][I]	49.3	66.08	4.45	1.33
0.4 M[Bmim][I]	45.6	67.44	4.23	1.48
0.6 M[Bmim][I]	44.5	54.48	3.35	1.23
0.025 M [Bmim][Br] + 0.1 M [Bmim][I]	52.3	61.97	4.36	1.18
0.025 M [Bmim][Br] + 0.2 M [Bmim][I]	50.6	64.71	4.46	1.27
0.025 M [Bmim][Br] + 0.3 M [Bmim][I]	48.2	65.50	4.48	1.31
0.025 M [Bmim][Br] + 0.6 M [Bmim][I]	47.4	88.32	5.75	1.86

0.4 M [Bmim][I]				
0.05 M [Bmim][Br] +	51.1	83.64	5.82	1.63
0.1 M [Bmim][I]				
0.05 M [Bmim][Br] +	49.5	64.98	4.39	1.31
0.2 M [Bmim][I]				
0.05 M [Bmim][Br] +	48.5	69.71	4.63	1.43
0.3 M [Bmim][I]				
0.05 M [Bmim][Br] +	46.6	70.84	4.54	1.52
0.4 M [Bmim][I]				
0.1 M [Bmim][Br] +	51.1	62.55		
0.1 M [Bmim][I]			4.35	1.21
0.1 M [Bmim][Br] +	49.6	62.46		
0.2 M [Bmim][I]			4.23	1.25
0.1 M [Bmim][Br] +	47.7	67.16		
0.3 M [Bmim][I]			4.39	1.40
0.1 M [Bmim][Br] +	45.8	67.44		
0.4 M [Bmim][I]			4.19	1.49
0.2 M [Bmim][Br] +	51.1	67.88		
0.1 M [Bmim][I]			4.72	1.32
0.2 M [Bmim][Br] +	49.2	69.53		
0.2 M [Bmim][I]			4.68	1.41
0.2 M [Bmim][Br] +	47.2	69.66		
0.3 M [Bmim][I]			4.51	1.47
0.2 M [Bmim][Br] +	45.3	64.89		
0.4 M [Bmim][I]			4.05	1.43

^aEach Value is the average over three measurements. The error in T_m doesnot exceeds 0.1°C. The estimated relative uncertainties in (ΔH), (ΔC_p) and (ΔG_u) are around 2% of the reported values.