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Supporting information

A Spectroscopic and Molecular dynamic simulation approach towards the stabilizing effect of ammonium based Ionic Liquids on Bovine serum albumin

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1.Circular dichroism spectra

1.1 Far UV CD spectra figures

Figure S1. Thermal unfolding and refolding of BSA in N2 IL with concentrations, (a) 0, Buffer solution; (b) $2*10^{-6}$ M; (c) $2*10^{-5}$ M; (d) $2*10^{-4}$ M; (e) $2*10^{-3}$ M, each sample was subjected to a heating cycle of 25-90-25 ^{0}C. [Intial 25 ^{0}C (Black), 90 ^{0}C (Red) and Final 25 ^{0}C (Blue)]

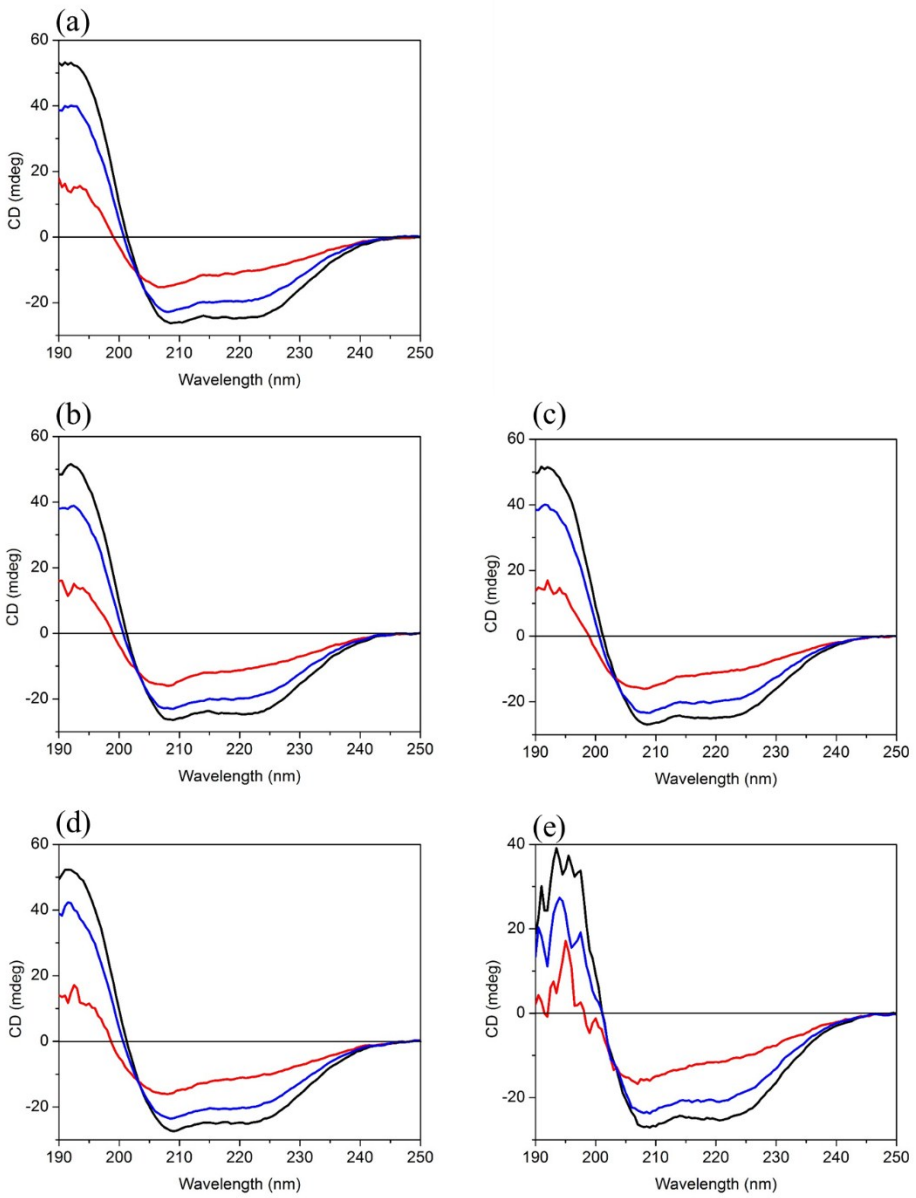


Figure S2. Thermal unfolding and refolding of BSA in N4 IL with concentrations, (a) $2*10^{-6}$ M; (b) $2*10^{-5}$ M; (c) $2*10^{-4}$ M; (d) $2*10^{-3}$ M, each sample was subjected to a heating cycle of 25-90-25 ^{0}C. [Intial 25 ^{0}C (Black), 90 ^{0}C (Red) and Final 25 ^{0}C (Blue)]

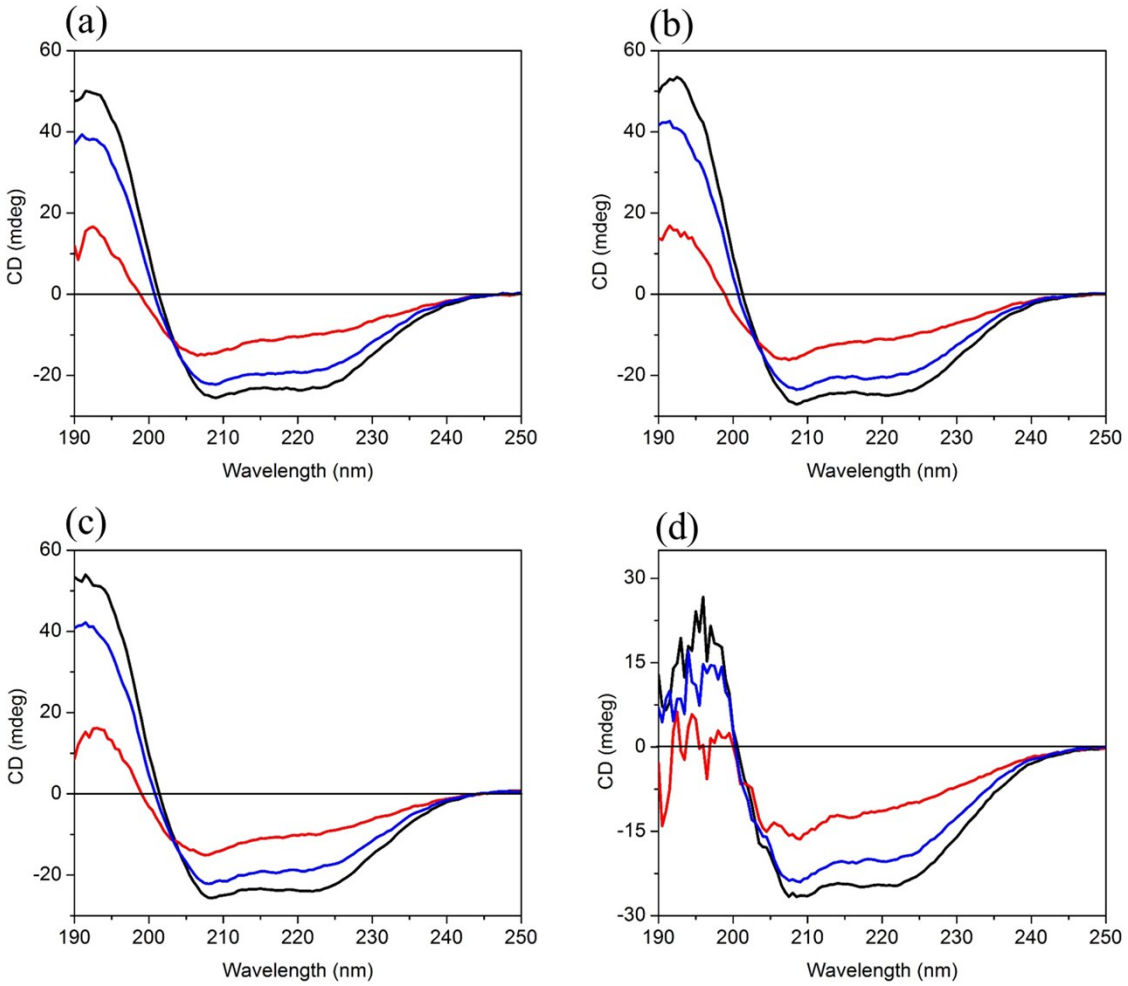
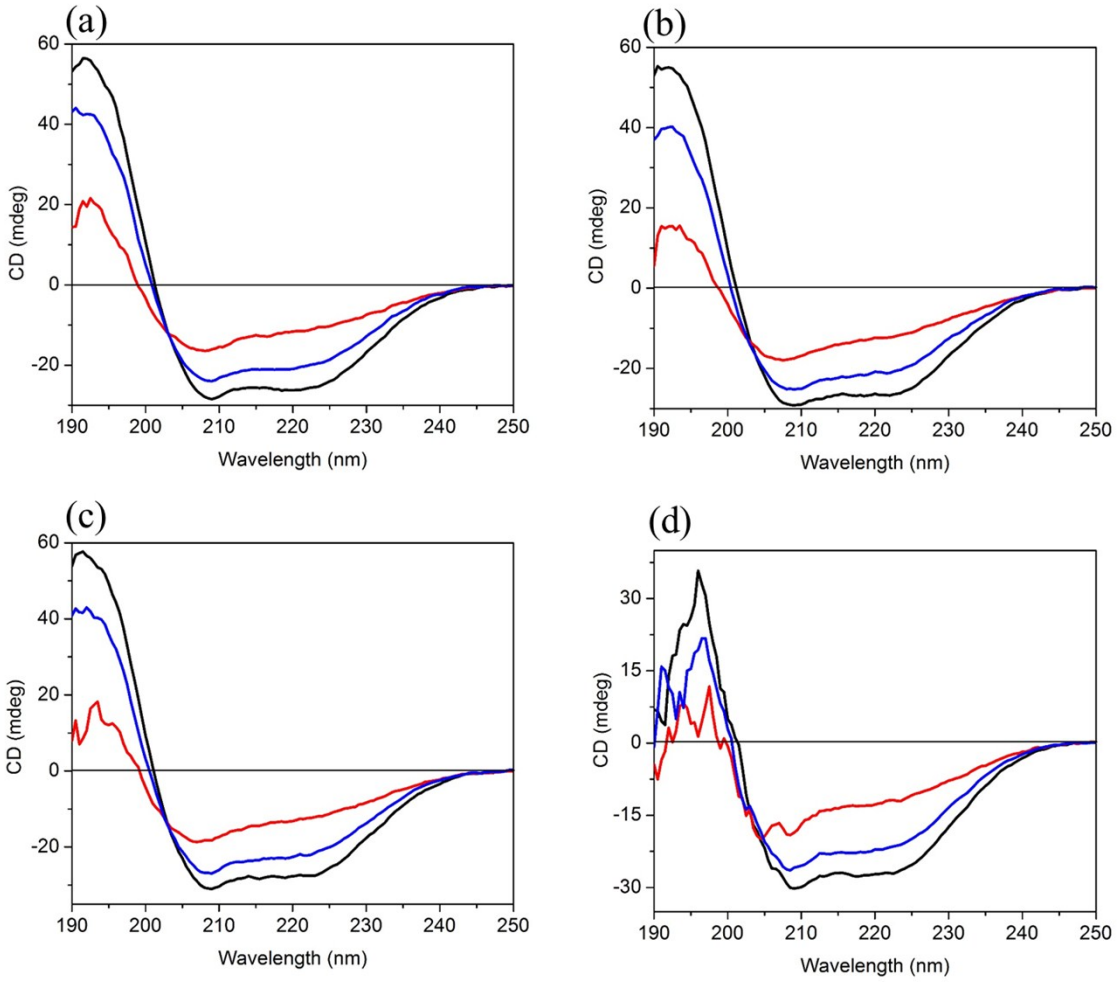


Figure S3. Thermal unfolding and refolding of BSA in N6 IL with concentrations, (a) $2*10^{-6}$ M; (b) $2*10^{-5}$ M; (c) $2*10^{-4}$ M; (d) $2*10^{-3}$ M, each sample was subjected to a heating cycle of 25-90-25 ^{0}C. [Intial 25 ^{0}C (Black), 90 ^{0}C (Red) and Final 25 ^{0}C (Blue)]



1.2 Near UV CD spectra figures

Figure S4. Thermal unfolding and refolding of BSA in N2 IL with concentrations, (a) $2*10^{-6}$ M; (b) $2*10^{-5}$ M; (c) $2*10^{-4}$ M; (d) $2*10^{-3}$ M; (e) $2*10^{-2}$ M; (f) $2*10^{-1}$ M; each sample was subjected to a heating cycle of 25-90-25 ^{0}C. [Intial 25 ^{0}C (Black), 90 ^{0}C (Red) and Final 25 ^{0}C (Blue)]

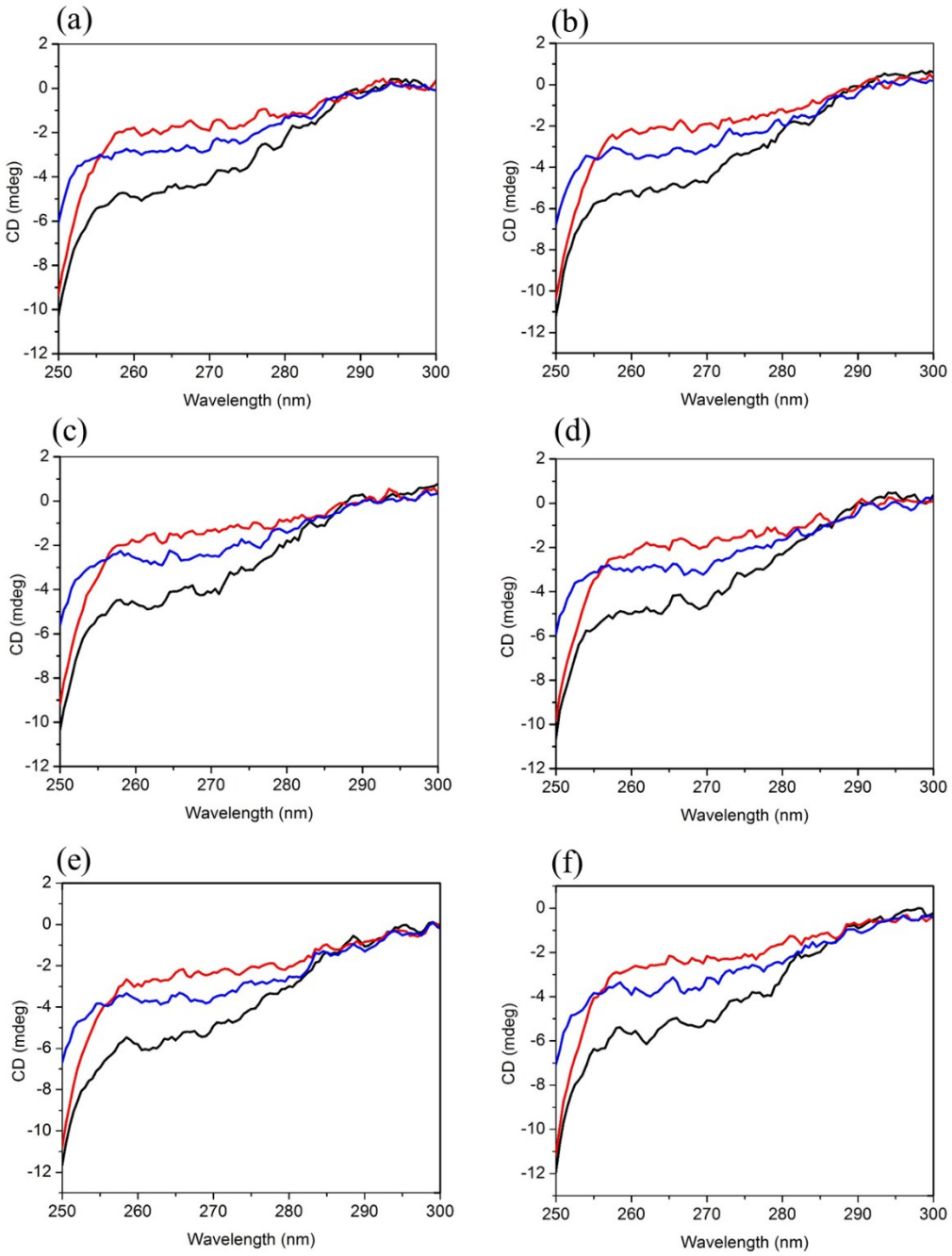


Figure S5. Thermal unfolding and refolding of BSA in N4 IL with concentrations, (a) $2*10^{-6}$ M; (b) $2*10^{-5}$ M; (c) $2*10^{-4}$ M; (d) $2*10^{-3}$ M; (e) $2*10^{-2}$ M; (f) $2*10^{-1}$ M; each sample was subjected to a heating cycle of 25-90-25 ^{0}C. [Intial 25 ^{0}C (Black), 90 ^{0}C (Red) and Final 25 ^{0}C (Blue)]

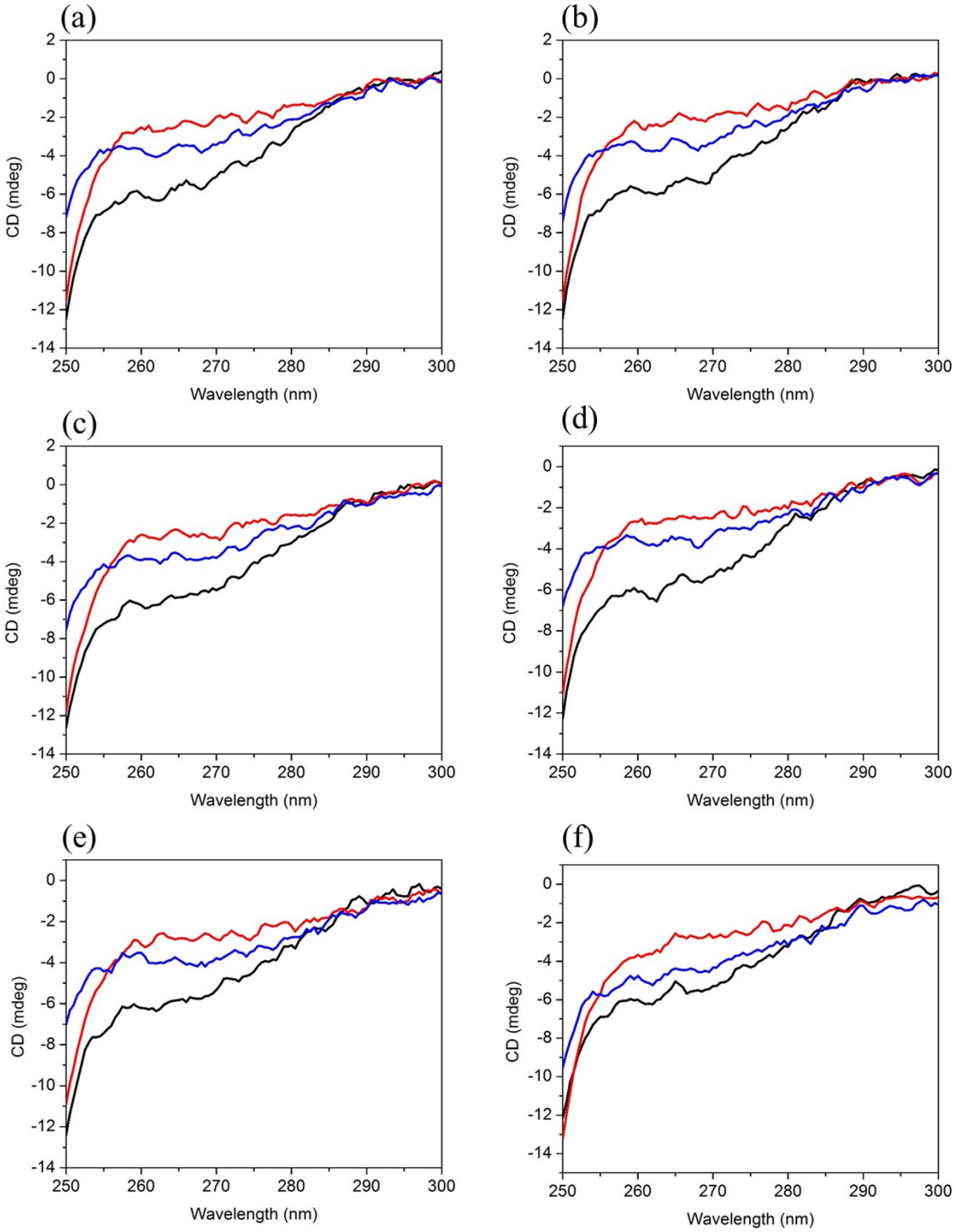
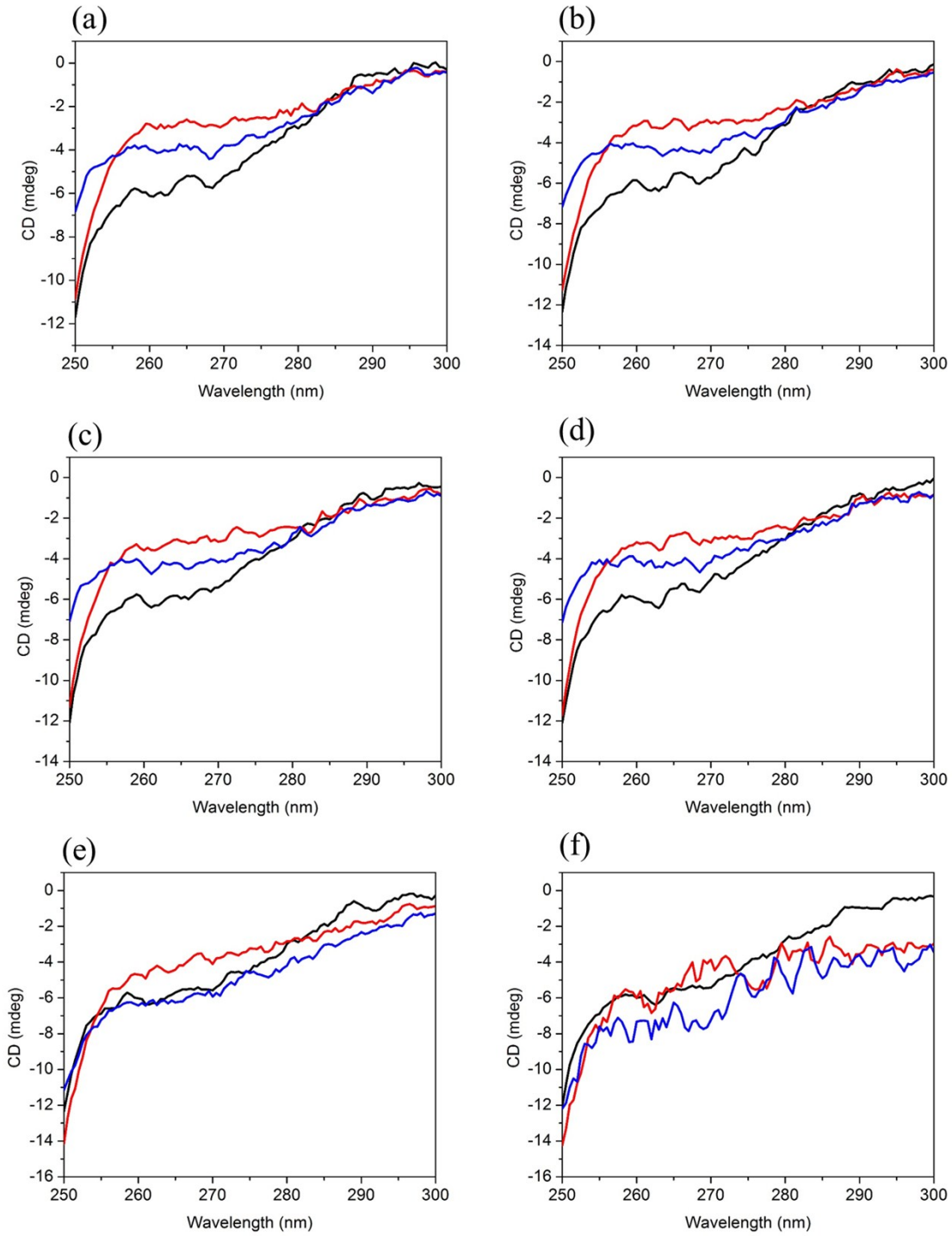


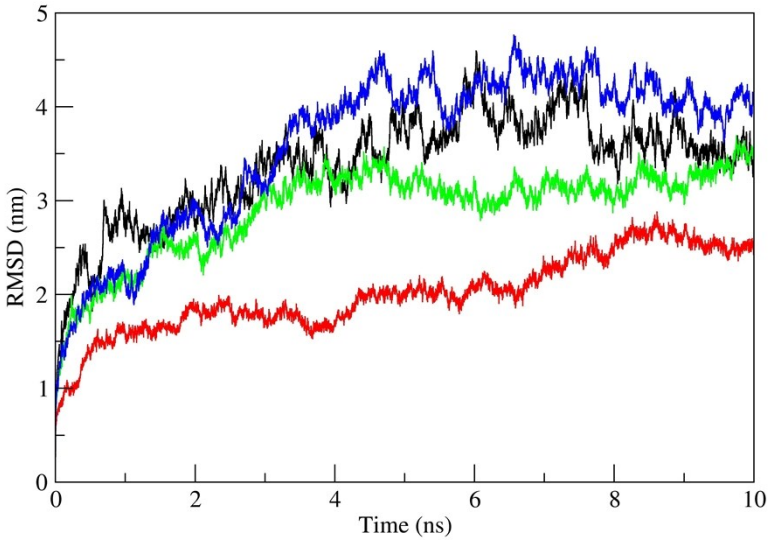
Figure S6. Thermal unfolding and refolding of BSA in N6 IL with concentrations, (a) $2*10^{-6}$ M; (b) $2*10^{-5}$ M; (c) $2*10^{-4}$ M; (d) $2*10^{-3}$ M; (e) $2*10^{-2}$ M; (f) $2*10^{-1}$ M; each sample was subjected to a heating cycle of 25-90-25 ^{0}C. [Intial 25 ^{0}C (Black), 90 ^{0}C (Red) and Final 25 ^{0}C (Blue)]



2. Molecular dynamic simulation

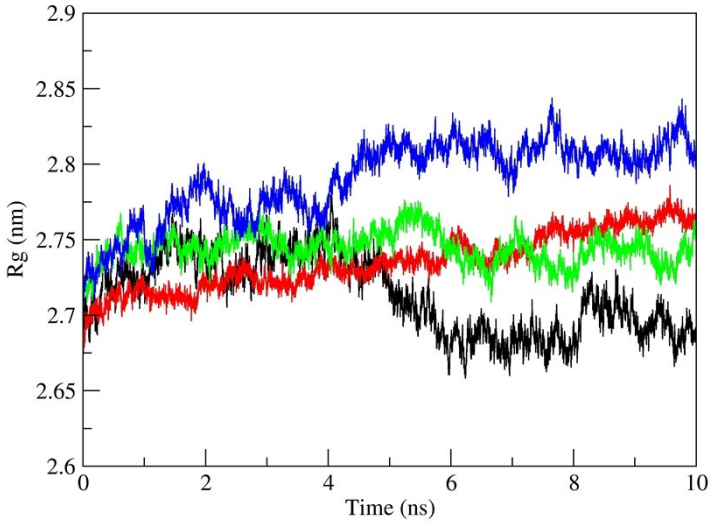
2.1. RMSD plot

Figure S7. Time dependence of root mean square deviations (RMSDs). C_α RMSD values for BSA in aqueous (Black), N2 (Blue), N4 (Green) and N6 (Red) medium during 10 ns molecular dynamics simulation



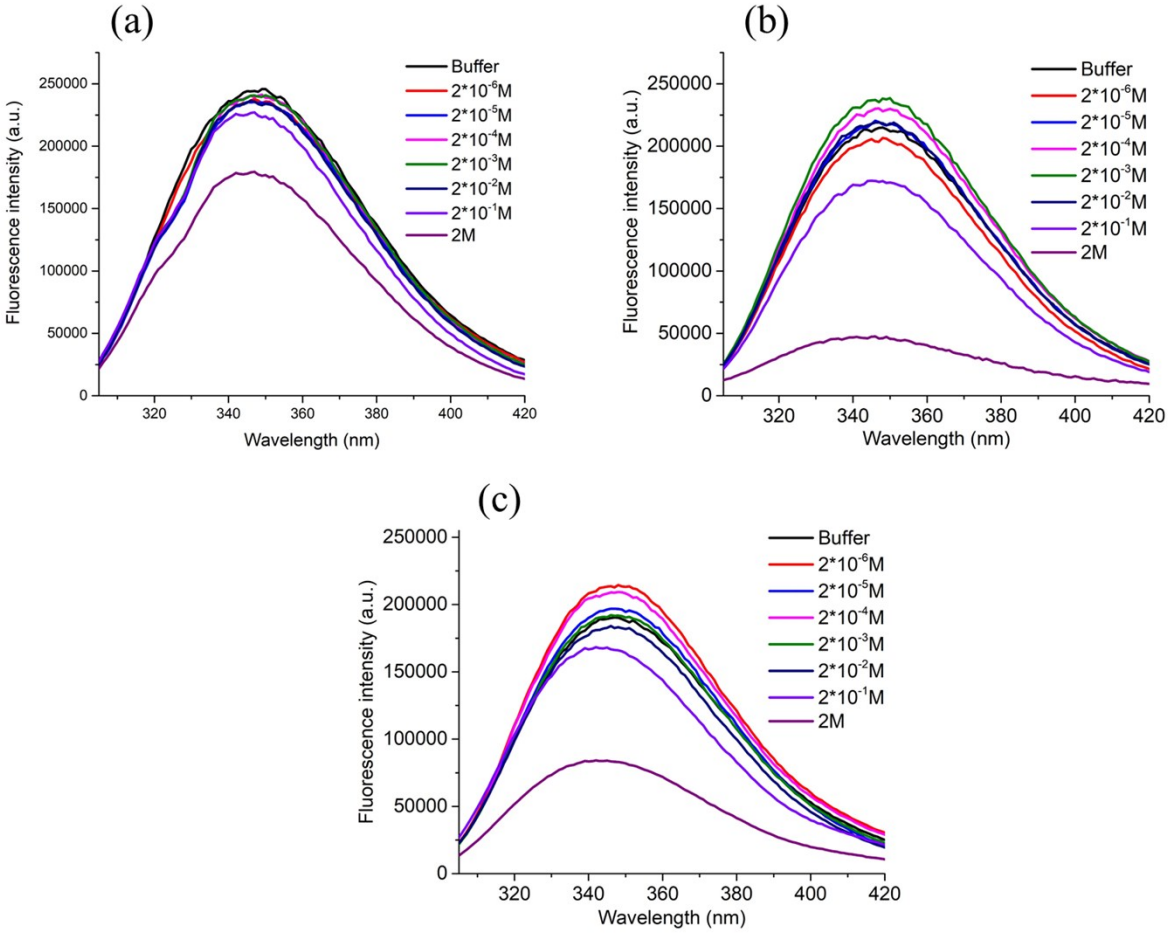
2.1. R_g plot

Figure S8. Time evolution of the radius of gyration (Rg) of BSA in aqueous (Black), N2 (Blue), N4 (Green) and N6 (Red) medium during 10 ns molecular dynamics simulation



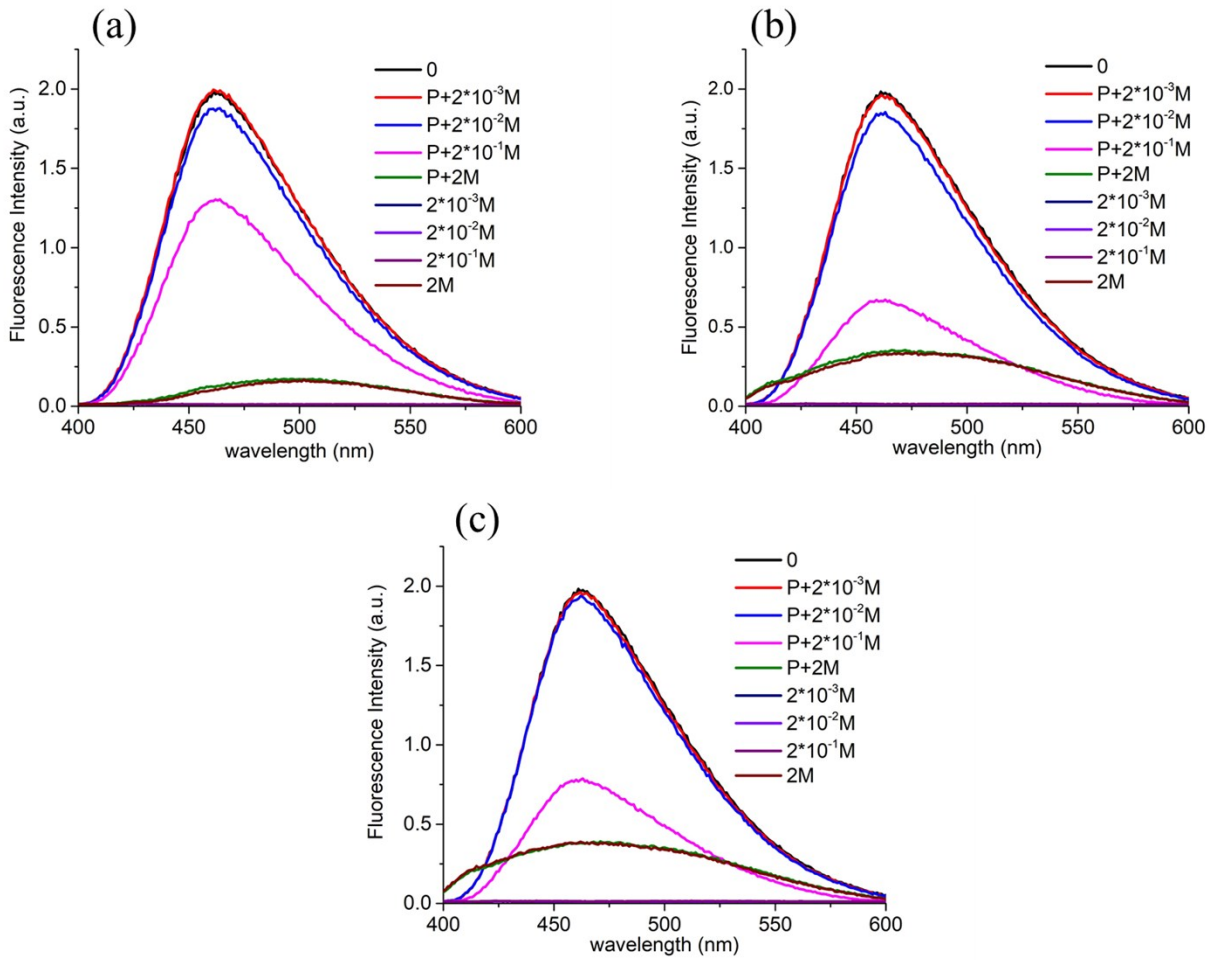
3. Fluorescence spectra

Figure S9. Fluorescence spectra of intrinsic tryptophan with excitation at 295 nm in presence of IL (0, $2*10^{-6}$, $2*10^{-5}$, $2*10^{-4}$, $2*10^{-3}$, $2*10^{-2}$ M, $2*10^{-1}$**,** 2M) ; (a) N2, (b) N4, and (c) N6



4. ANS Fluorescence spectra

Figure S10. Raw data of ANS fluorescence in the presence of BSA+ IL (0, $2*10^{-3}$, $2*10^{-2}$, $2*10^{-1}$, 2 M) system as well as free IL ($2*10^{-3}$, $2*10^{-2}$, $2*10^{-1}$, 2 M); (a) N2, (b) N4, and (c) N6 [“P” represents protein, BSA]



5. Fluorescence lifetime decay

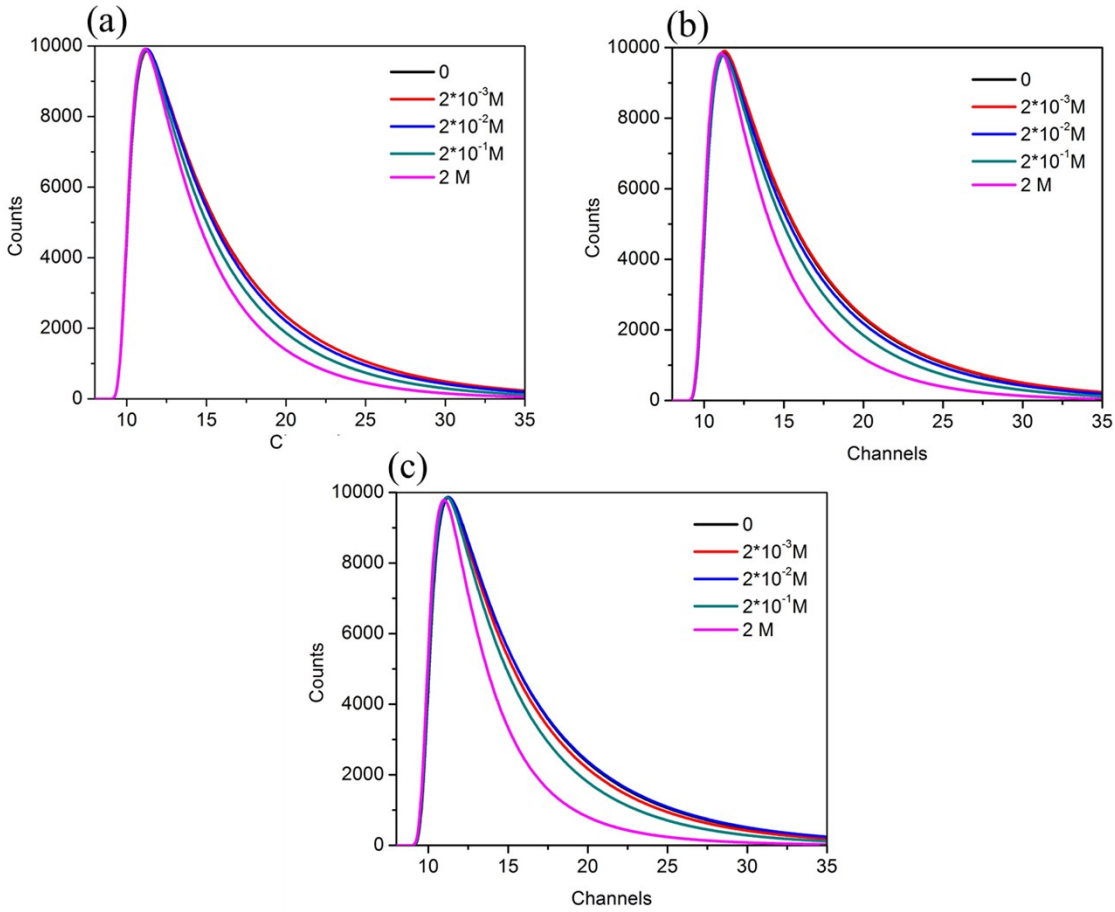



Figure S11. Time resolved fluorescence decay of BSA in ILs with different concentrations (0, $2*10^{-3}$, $2*10^{-2}$, $2*10^{-1}$, 2 M); (a) N2, (b) N4 and (c) N6