Supporting Information

Protein Charge Transfer Absorption Spectra: An Intrinsic Probe to Monitor Structural and Oligomeric Transitions in Proteins

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Figure S1  Disorder prediction plots

Figure S1: Intrinsic disorder prediction plots of the proteins for [A] PEST Wt; [B] PEST M1 and [C] DHN1 as obtained by various predictors. Disorder prediction was determined using Genesilico MetaDisorder server. (L. P. Kozlowski and J. M. Bujnicki, BMC Bioinformatics, 2012, 13, 111.)
**Figure S2** Purification of PEST Wt and PEST M1

**Figure S2**: 15 % Reducing SDS-PAGE showing a single band of purified proteins for [A] PEST Wt and [B] PEST M1. Apparent molecular weight of PEST proteins on SDS-PAGE is approximately 15 kDa because of its anomalous mobility.
Figure S3  Mass Spectra of PEST Wt and PEST M1

Figure S3: Mass spectra of [A] PEST Wt and [B] PEST M1. The mass calculated from sequence were 8341.61 and 8527.82 Da.
Figure S4  Purification of DHN1

Figure S4: 15% Reducing SDS-PAGE shows the single band of purified DHN1 at 19 kDa. Higher molecular weight of DHN1 on SDS-PAGE is observed due to its anomalous mobility.
Figure S5  Mass Spectrum of DHN1

Figure S5: Mass spectrum of Dehydrin (DHN1). The mass calculated from sequence was 16955.33 Da.
Figure S6  Comparison of absorption spectra with simulated scatter

**Figure S6**: Comparison of absorbance spectra with simulated Rayleigh scatter (using $1/\lambda^4$ dependence) for [A] PEST Wt; [B] PEST M1; [C] DHN1 and [D] HEWL aggregate formed in Glycine buffer (pH 2.0).
Figure S7  PEST Wt, PEST M1 and DHN1 exist as a monomer in solution

Figure S7: Variation of ProCharTS absorbance with protein concentration for [A] PEST Wt; [B] PEST M1 and [C] DHN1 at chosen wavelengths.
Figure S8  Absorption spectrum of DHN1 in 0.1 N NaOH

Figure S8: Absorption spectrum of DHN1 in 0.1 N NaOH. Inset shows DHN1 spectrum after subtracting contribution of Phe and Tyr (260 to 326 nm).
Figure S9  Percent change in absorbance at different pH with respect to pH 7

Figure S9: Percent change in absorption intensity measured every 25 nm at specified pH among the proteins [A] PEST Wt; [B] PEST M1; [C] DHN1 and [D] α3C with respect to pH 7. The change in absorbance at selected wavelengths were calculated as [(Absorbance at chosen pH – Absorbance at pH 7)/Absorbance at pH 7]×100.
Figure S10: Change in secondary structure content in [A] PEST Wt and [B] PEST M1 at various pH and in deionized water.
Figure S11: Fitted CD spectra of [A] PEST Wt and [B] PEST M1 by using DichroWeb server at pH 3 and 9.
Figure S12: CD spectra of DHN1 and $\alpha_3$C at various pH.

Figure S12: CD spectra of [A] 12.5 $\mu$M DHN1 and [B] 30 $\mu$M $\alpha_3$C at various pH.
Figure S13: Percent change in absorption intensity measured every 25 nm at specified temperature among the proteins [A] PEST Wt; [B] PEST M1 and [C] DHN1 with respect to room temperature (25 °C). The change in absorbance at selected wavelengths were calculated as [(Absorbance at chosen temperature – Absorbance at 25°C)/Absorbance at 25 °C]×100.
Figure S14: Secondary structure content of PEST Wt and M1 at various temperatures

Figure S14: Change in secondary structure content in [A] PEST Wt and [B] PEST M1 at different temperatures.
Figure S15: Fitted CD spectra of [A] PEST Wt and [B] PEST M1 by using DichroWeb server at 25 and 85 °C.
Figure S16: Percent change in absorption intensity measured at 25 nm intervals among the proteins [A] PEST Wt; [B] PEST M1; [C] DHN1 and [D] α3C in 250 mM NaCl and 250 mM KCl with respect to absorption of proteins in deionised water. The change in absorbance were calculated at selected wavelengths as [(Absorbance in salt – Absorbance in water)/Absorbance in water]×100.
**Figure S17** Concentration dependence of ProCharTS on concentration of HEWL aggregates

![Graph showing concentration dependence of ProCharTS on HEWL aggregates](image)

**Figure S17: ProCharTS of HEWL aggregates formed at pH 12.2:** Difference absorption spectra of 10 day old HEWL aggregates for different monomer concentrations is shown. All absorbance measurements were done immediately after transfer in 0.1 M sodium bicarbonate buffer (pH 9.3). Difference spectra are generated by subtracting the spectra of fresh HEWL monomer of same concentration in the same buffer as the transferred aggregates.