Utility of 5-Cyanotryptophan Fluorescence as a Sensitive Probe of Protein Hydration

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Supporting Information

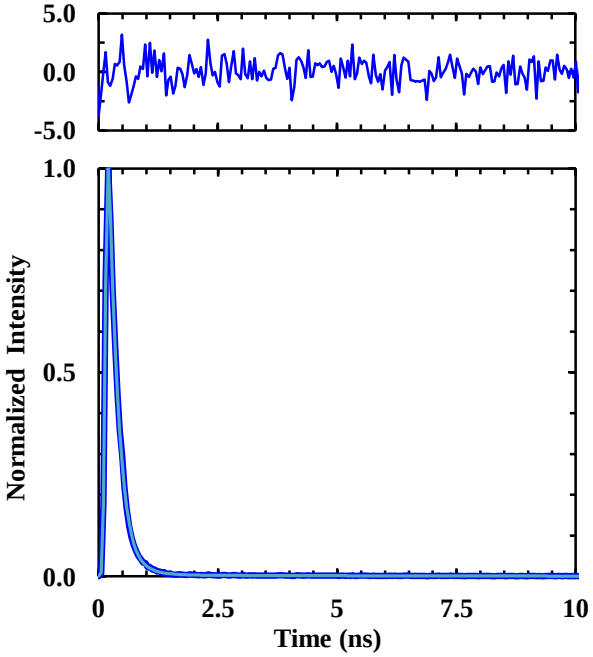

Figure S1. Fluorescence decay kinetics of 5CI in D_2O. The smooth line is a fit to a double-exponential function. The residuals of the fits are shown in the top panel and the resulting fitting parameters are listed in Table 1.

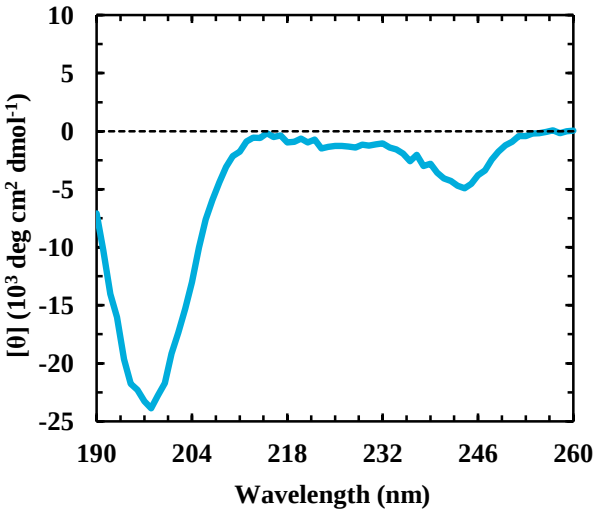

Figure S2. CD spectrum of $2W_{CN}P$ in H_2O at 1.0 °C.

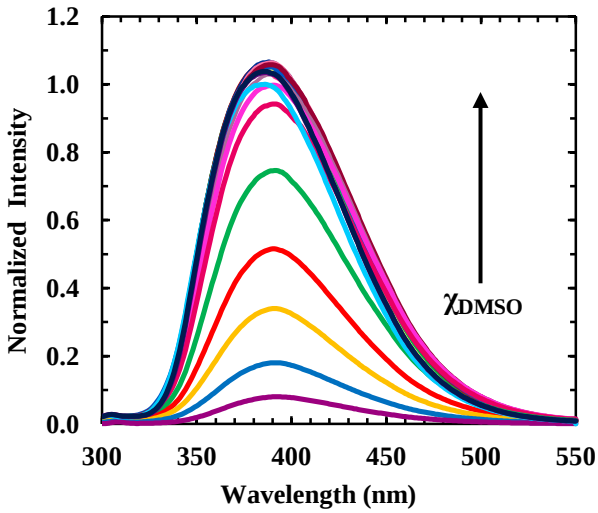

Figure S3. Fluorescence spectra of $2W_{CN}P$ in DMSO-H_2O mixtures with different molar fractions of DMSO (χ_{DMSO}).

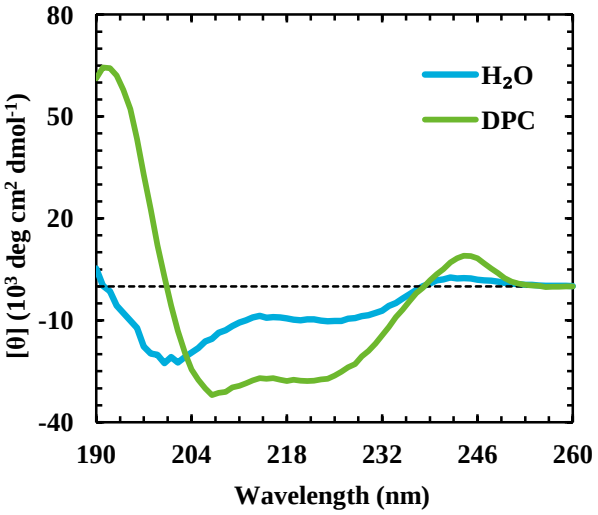

Figure S4. CD spectra of MPXW$_{CN}$ in H_2O and in DPC micelles at 25.0 °C, as indicated.

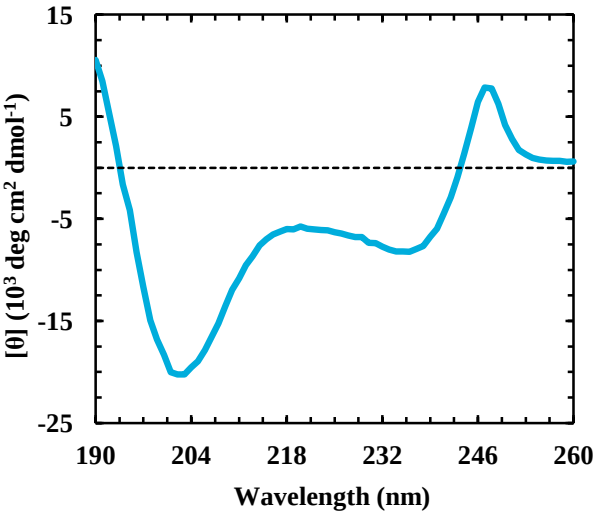

Figure S5. Far UV CD spectrum of TC2W$_{CN}$ in H_2O at 1.0 °C. The strong CD couplet at 247 and 236 nm, arising from the exciton coupling between the two Trp$_{CN}$ sidechains, indicates that the peptide is folded. It is worth noting that the Trp$_{CN}$–Trp$_{CN}$ exciton CD band is different from that of Trp–Trp and hence, can be used as a stand-alone structure reporter. We are currently exploring this potential application and will report the findings in a future publication.