Preferential Regulation of Transient Protein-Protein Interaction by the Macromolecular Crowders

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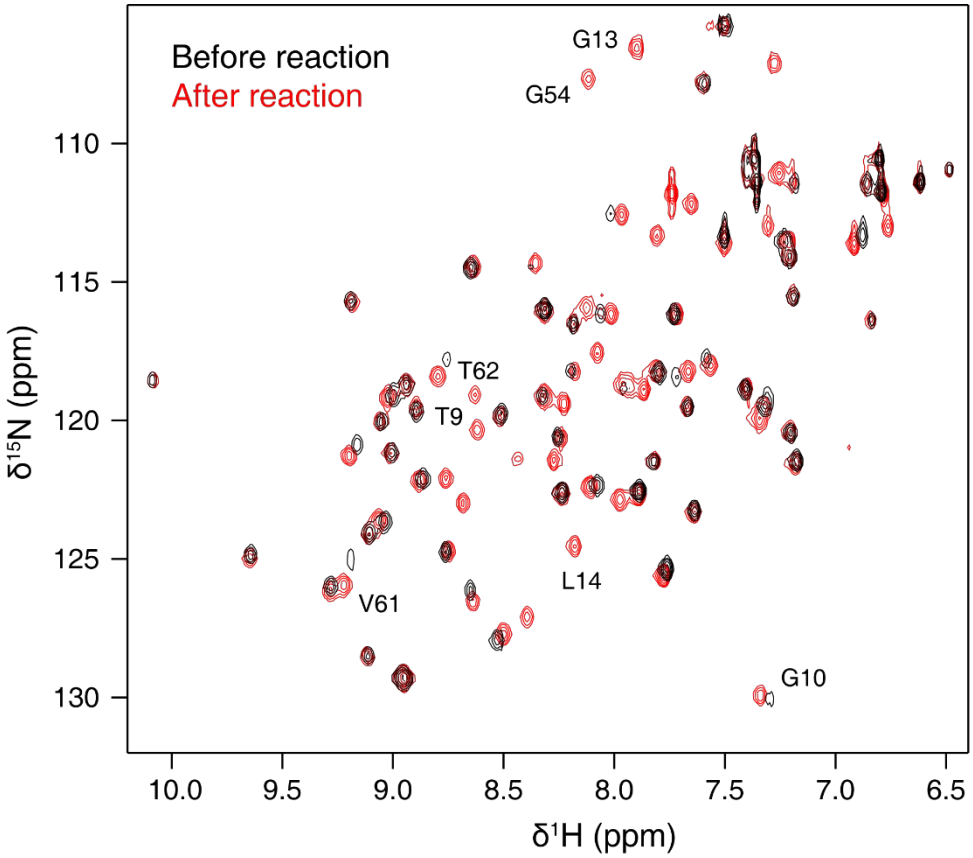

Figure S1. The overlaid ^{1}H-^{15}N HSQC spectra of ^{15}N isotopically labeled HPr before (black) and after (red) phosphoryl transfer from EIN in dilute buffer. The amide signals labeled with HPr residues were used to determine the phosphoryl transfer rate between EIN and HPr.

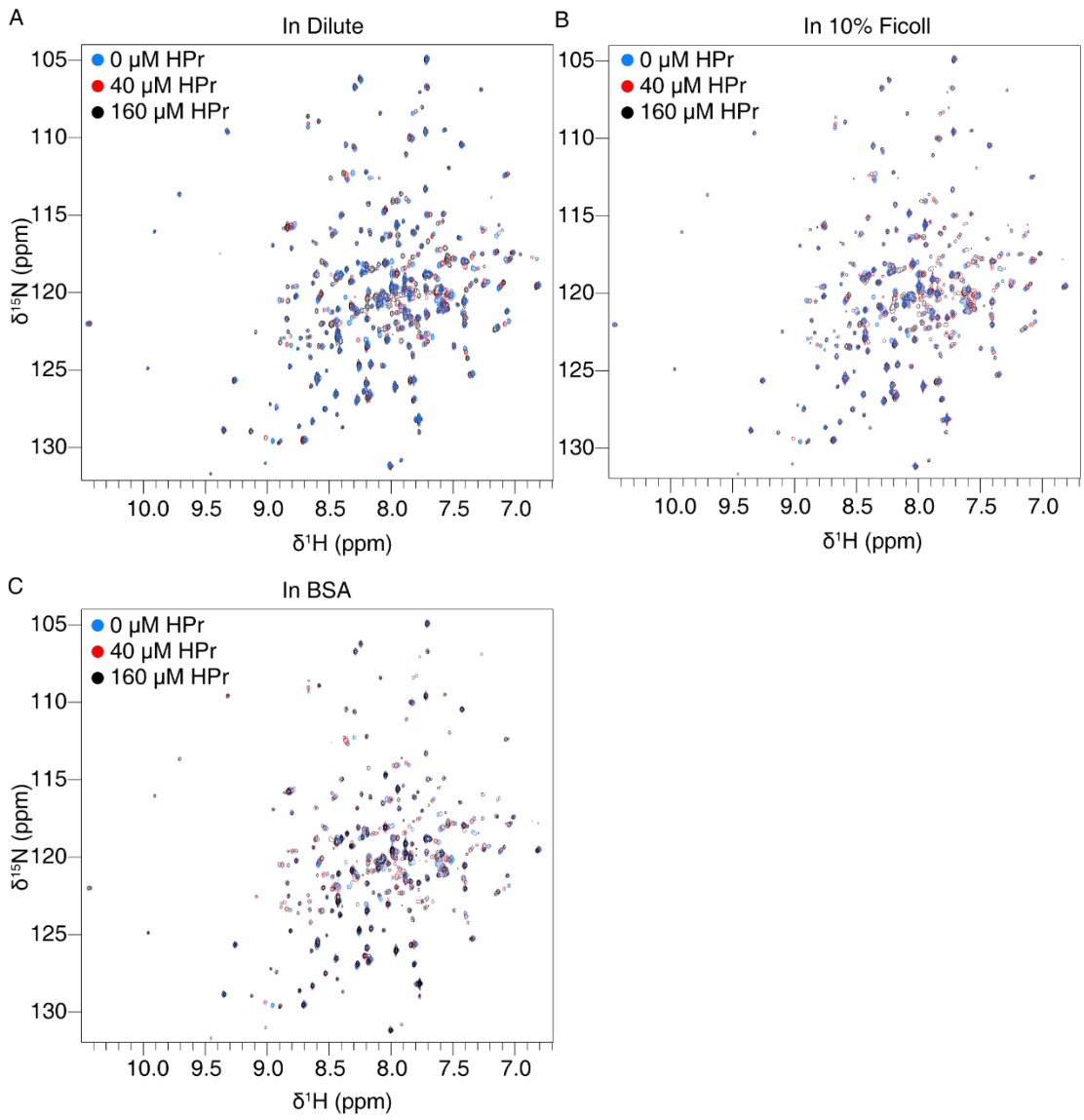

Figure S2. (A) The superimposed ^{1}H-^{15}N HSQC spectra of $^{2}H/^{15}N$ EIN (200 μM in 20 mM Tris•HCl 150 mM NaCl and pH 7.4) titrated with unlabeled HPr at increasing concentration. (B) and (C) show the ^{1}H-^{15}N HSQC spectra monitoring the same titration experiments but conducted in 10% (w/v) Ficoll-70 and in 10% (w/v) BSA, respectively.

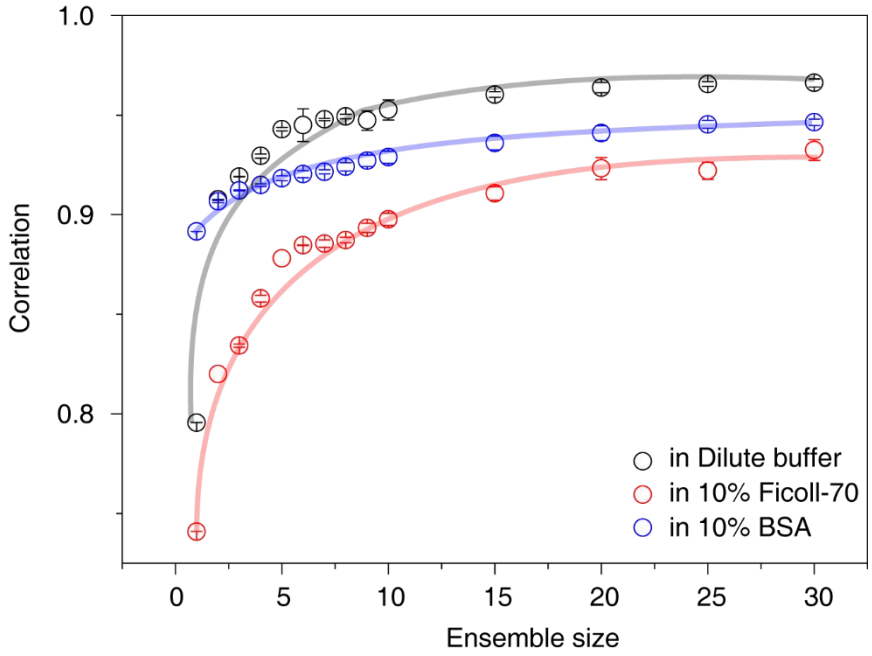

Figure S3. The plot of ensemble size against the correlation between the experimental PRE input and the theoretical PRE of the calculated ensemble. The error bars show the standard deviations of the correlation of 10 sets of the calculated ensemble. The black, red and blue cycles show calculation for the ensembles in dilute buffer, in Ficoll-70 and in BSA, respectively.

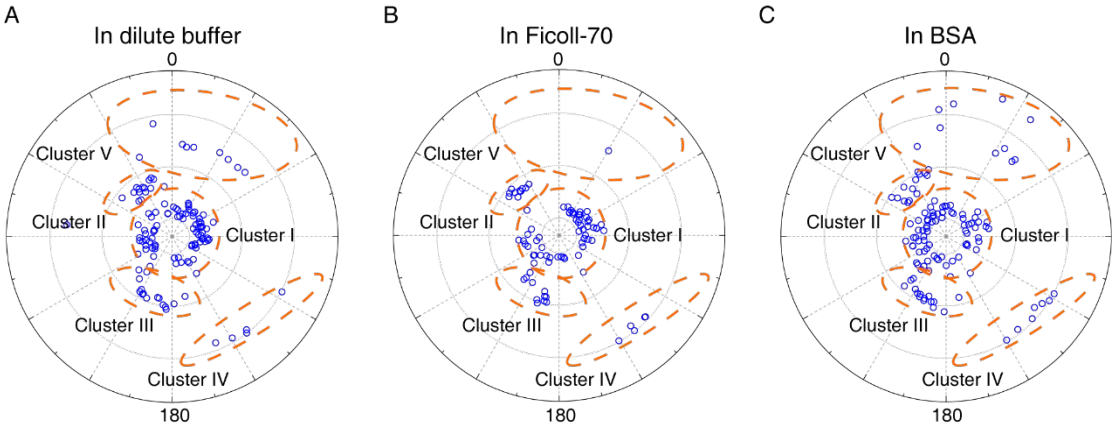

Figure S4. Two dimensional projection of the ensemble EIN-HPr structures in dilute buffer (A), in Ficoll-70 environment (B) and in BSA (C) environment. The orgin of polar coordinates is the mass center of EIN, and the blue cycles represent the mass center of HPr molecules on EIN surface. The clustering of HPr molecules are marked using dashed cycles.

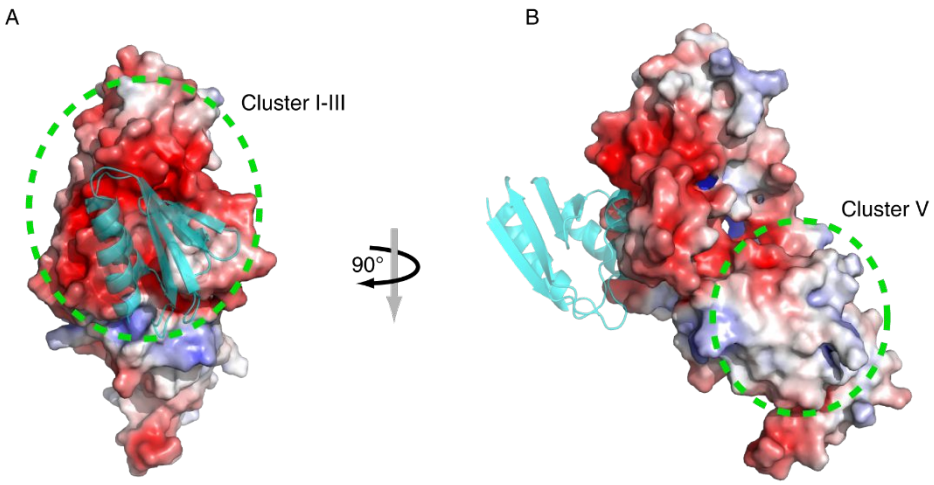

Figure S5. The specific structure of EIN and HPr (PDB code: 3EZA). Panel B shows the 90° rotated view of Panel A. The surface charge of EIN is shown as surface, and HPr is shown as cartoon in cyan. The Cluster I-III and Cluster V regions are higlighted using green cycles.

REFERENCES