

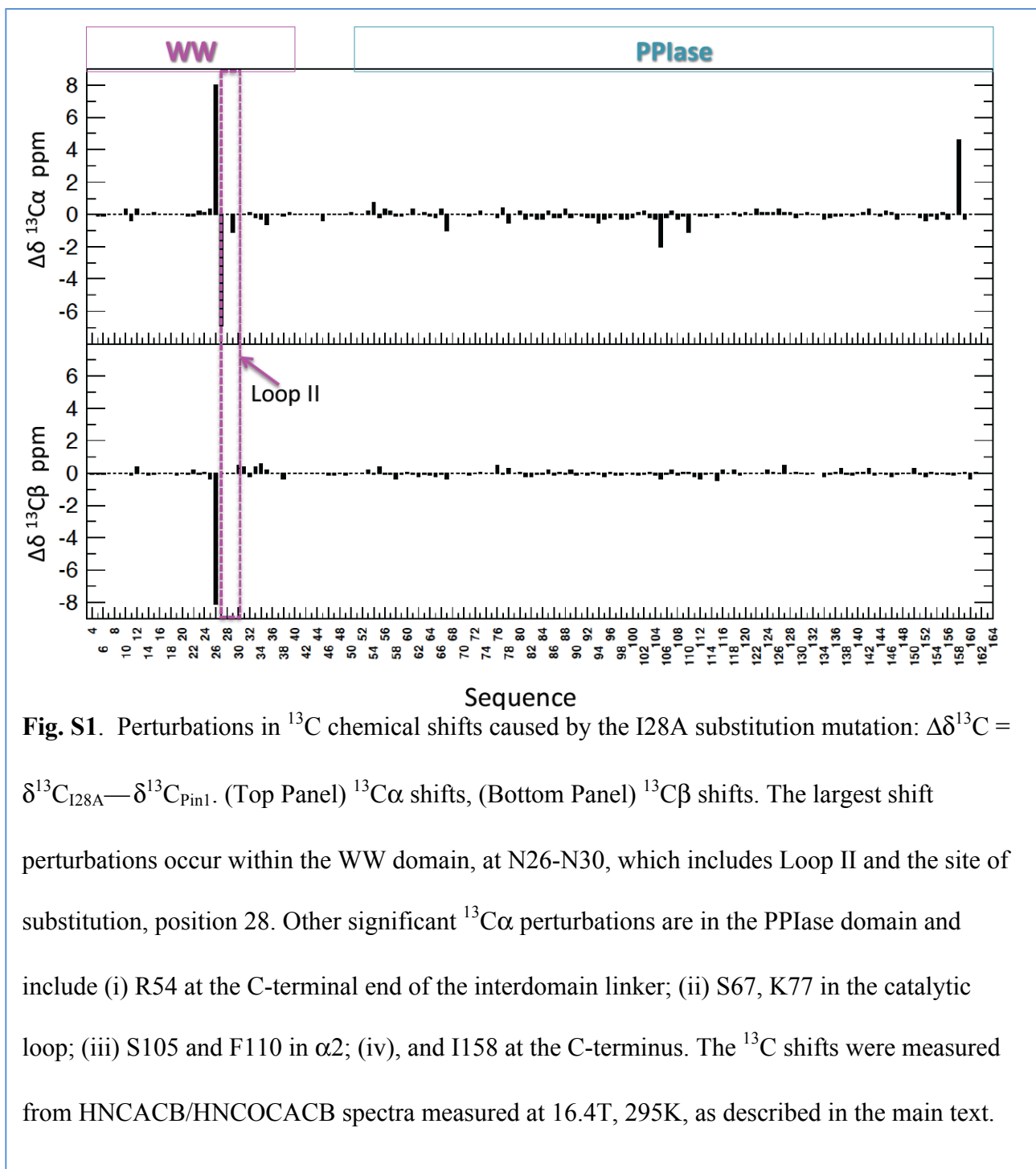
## Supplementary Material

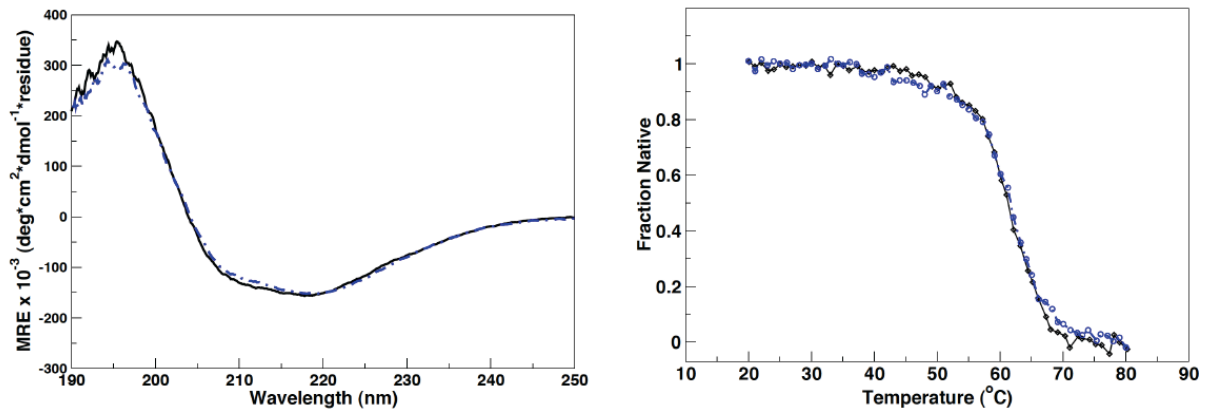
### **Interdomain Interactions Support Interdomain Communication in Human Pin1**

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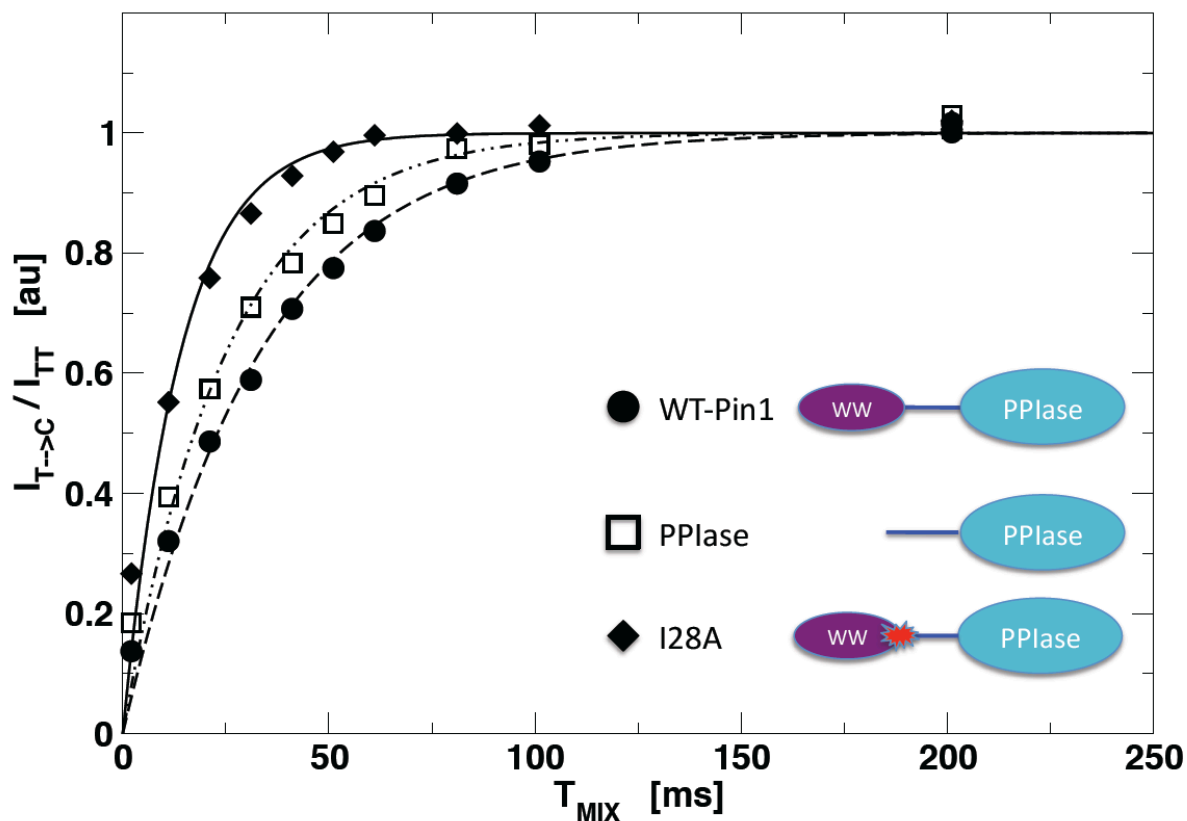
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Four (4) Supplementary Figures, S1, S2, S3, and S4, on four separate pages below.

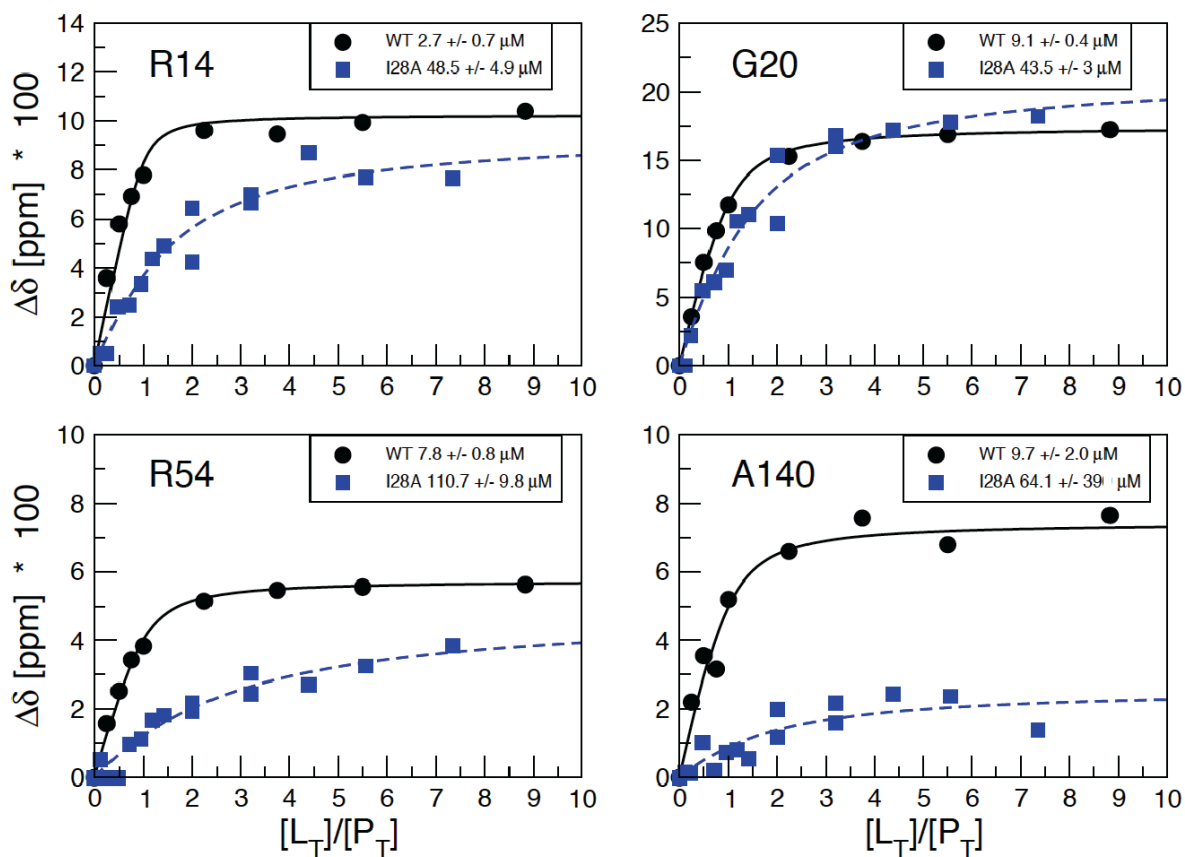




**Fig. S2.** (Left panel) Far-UV CD wave scans at 20 °C of WT Pin1 (black solid trace) and I28A (blue dashed-dotted trace). (Right panel) Thermal denaturation (monitored at 200 nm, WT Pin1 (black,  $T_{m, WT} = 62.5 \pm 0.2$  °C) and I28A (blue,  $T_{m, I28A} = 62.1 \pm 0.2$  °C). In both panels, the WT and I28A traces are nearly the same.



**Fig. S3.**  $^1\text{H}$ - $^1\text{H}$  EXSY build-up curves of pThr5 methyl protons of 2mM Cdc25C phosphopeptide in the presence of 50 $\mu\text{M}$  I28A, WT Pin1, or WT PPIase at 295K, 18.8 T, in buffer consisting of 30 mM  $\text{D}_4$ -imidazole (pH 6.6), 5 mM  $\text{D}_{10}$ -DTT, 30 mM NaCl, 0.03%  $\text{NaN}_3$ , and 90%  $\text{H}_2\text{O}$ /10%  $\text{D}_2\text{O}$ . The raw data and curve fits have been normalized with respect to the limiting plateau value at long  $T_{\text{mix}}$ . The vertical axis is the ratio of intensity of trans $\rightarrow$  cis exchange cross-peak ( $I_{\text{T}\rightarrow\text{C}}$ ), over that of the trans diagonal peak ( $I_{\text{TT}}$ ). Filled diamonds and black solid line are I28A ( $k_{\text{EXSY}} = 73 \pm 2 \text{ s}^{-1}$ ), open squares and dashed-dotted line are the isolated PPIase domain ( $k_{\text{EXSY}} = 41.4 \pm 1.0 \text{ s}^{-1}$ ), and filled circles and dashed line are WT full-length ( $k_{\text{EXSY}} = 31.3 \pm 0.5 \text{ s}^{-1}$ ).



**Fig. S4.** Binding isotherms for residues in the WW domain (R14 and G20) and PPIase domain (R54 and A140) from  $^{15}\text{N}$ - $^1\text{H}$  chemical shifts perturbations at 295 K, 16.4T in buffer consisting of 30 mM  $\text{D}_4$ -imidazole (pH 6.6), 5 mM  $\text{D}_{10}$ -DTT, 30 mM NaCl, 0.03%  $\text{NaN}_3$ , and 90%  $\text{H}_2\text{O}/10\%$   $\text{D}_2\text{O}$ . The horizontal axis is the ratio of total Cdc25C phosphopeptide over total protein. WT isotherms are the black dots and solid lines, I28A isotherms are blue squares and dashes. Fitted  $K_d$  values are: R14  $K_d^{\text{WT}} = 2.7 \pm 0.7 \mu\text{M}$ ,  $K_d^{\text{I28A}} = 48.5 \pm 4.9 \mu\text{M}$ ; G20  $K_d^{\text{WT}} = 9.1 \pm 0.4 \mu\text{M}$ ,  $K_d^{\text{I28A}} = 43.5 \pm 3.0 \mu\text{M}$ ; R54  $K_d^{\text{WT}} = 7.8 \pm 0.8 \mu\text{M}$ ,  $K_d^{\text{I28A}} = 110.7 \pm 9.8 \mu\text{M}$ ; A140  $K_d^{\text{WT}} = 9.7 \pm 2.0 \mu\text{M}$ ,  $K_d^{\text{I28A}} = 64.1 \pm 39.0 \mu\text{M}$ .