

Supporting Information

For

Thermodynamic Consequences of Incorporating 4-Substituted Proline Derivatives into a Small Helical Protein[†]

Tong-yuan Zheng, Yu-Ju Lin, Jia-Cherng Horng*

Department of Chemistry, National Tsing Hua University, Hsinchu,
Taiwan 30013, R.O.C.

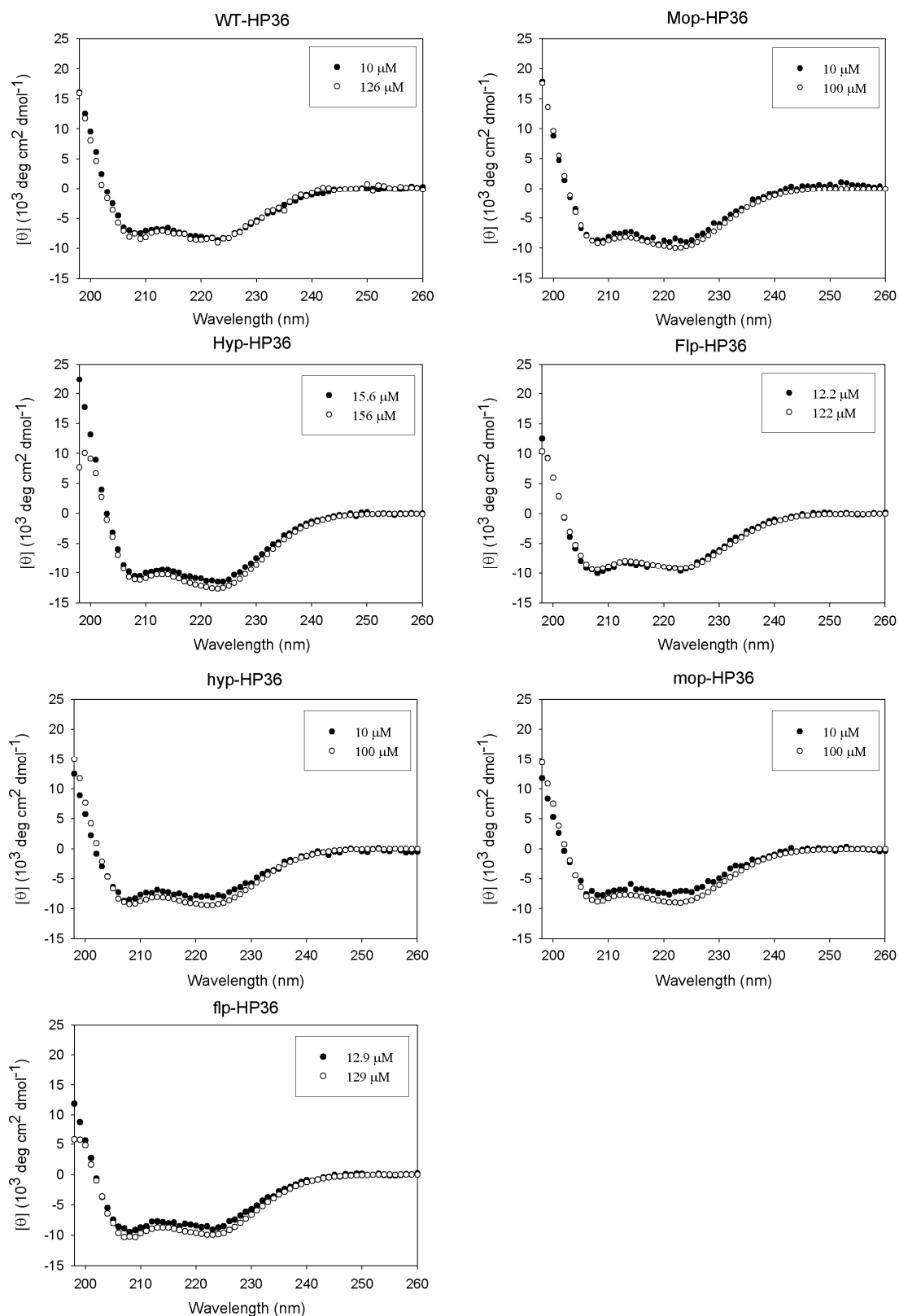
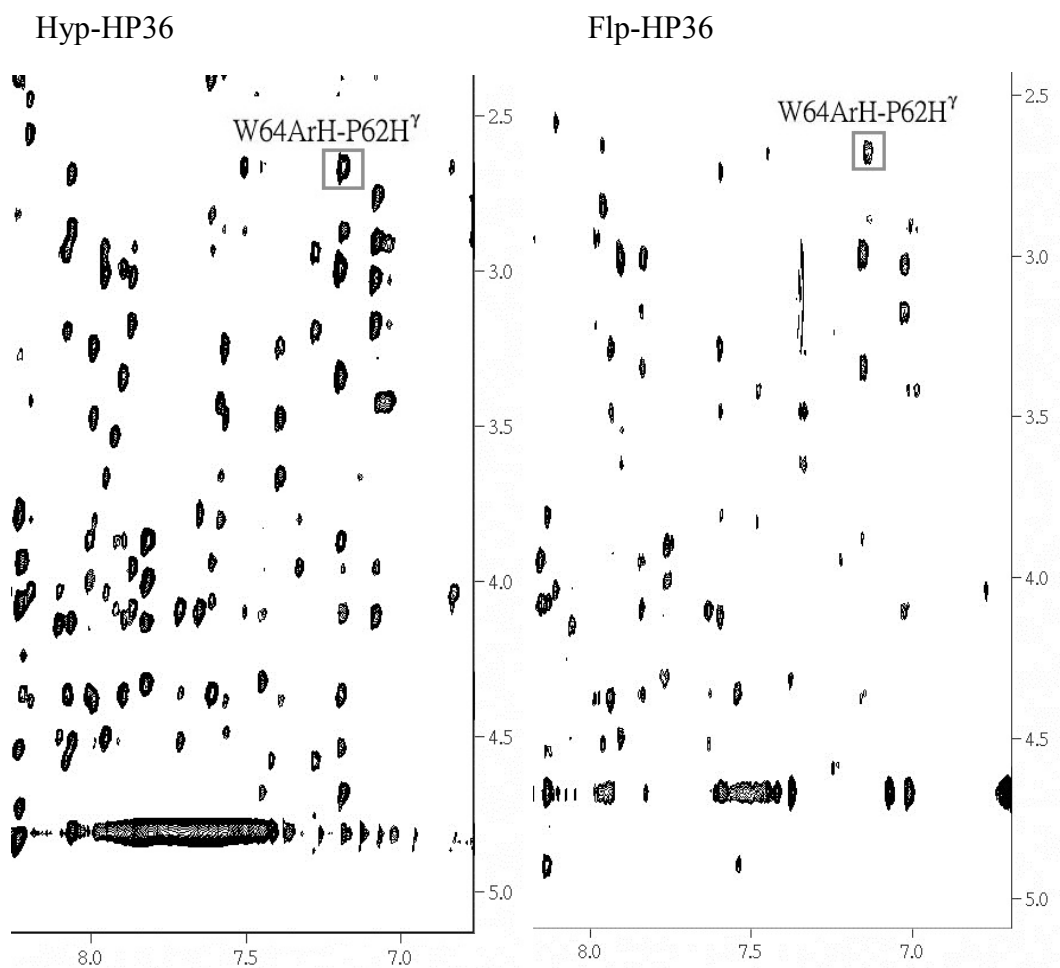
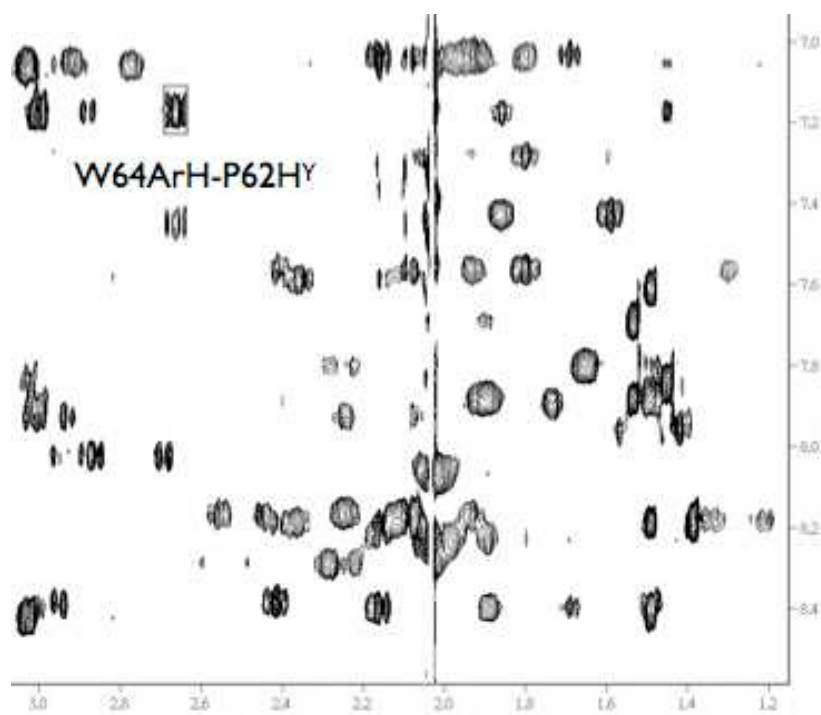


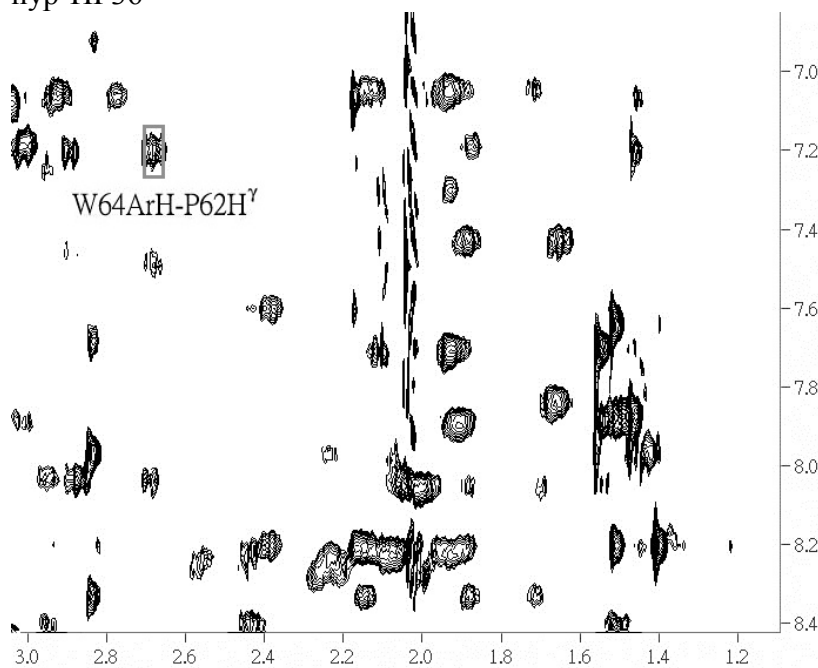
Figure S1. Far-UV CD spectra for HP36 and its mutants at different concentrations and 25 °C.



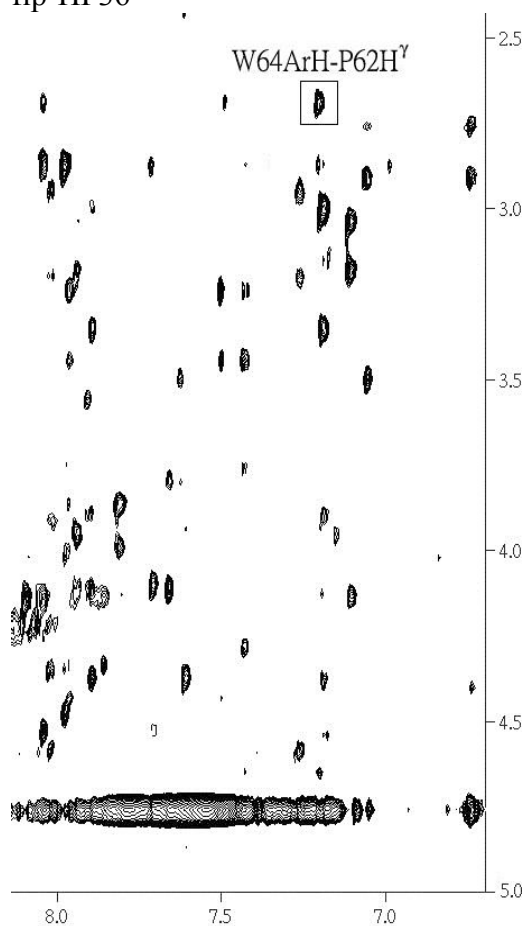
Mop-HP36



hyp-HP36



flp-HP36



mop-HP36

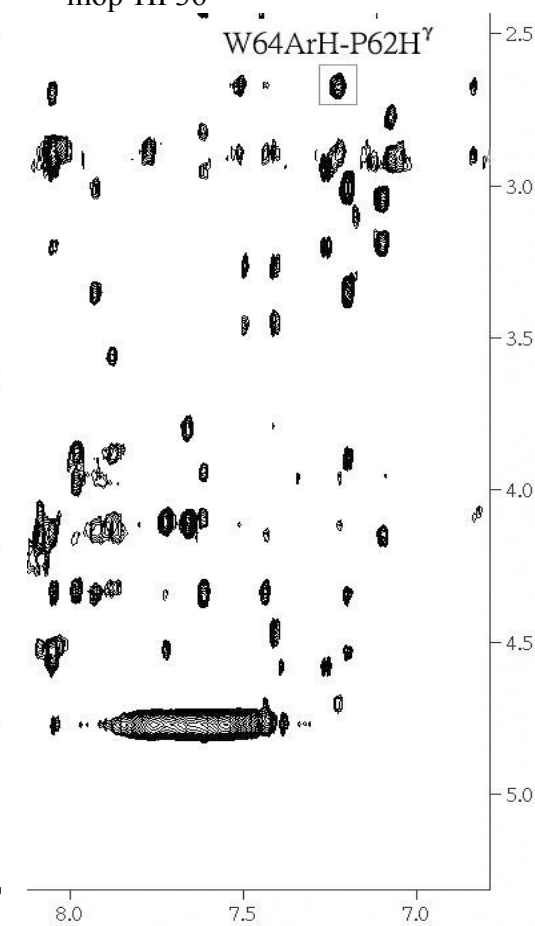
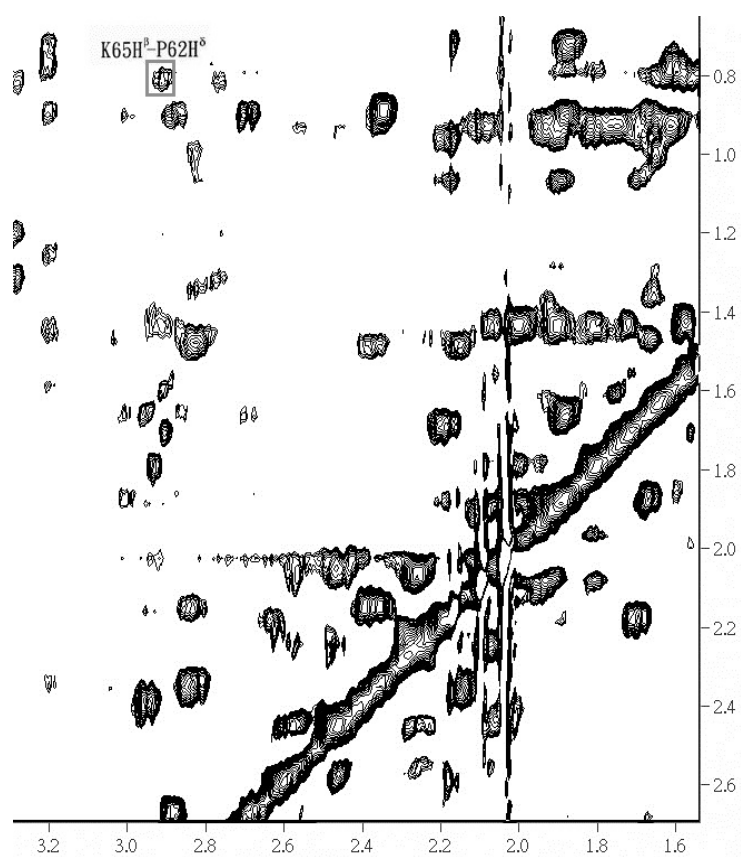
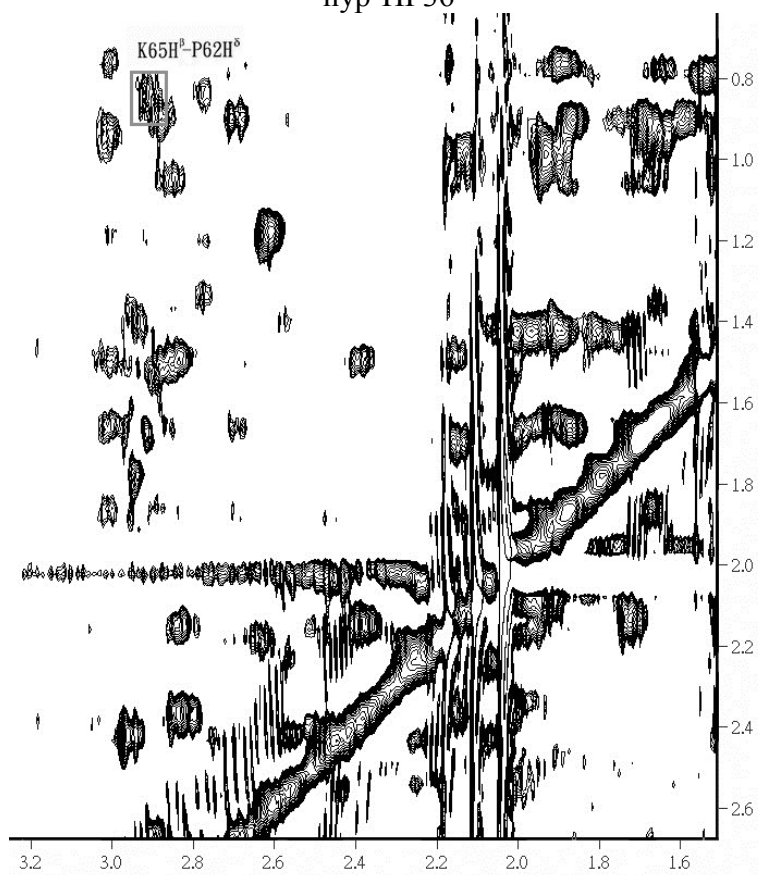


Figure S2. Excerpts of NOESY spectra for the HP36 mutants: the NOE cross-peaks between aromatic H of W64 and C^γH of proline derivatives (labeled as P62) are indicated.

Hyp-HP36



hyp-HP36



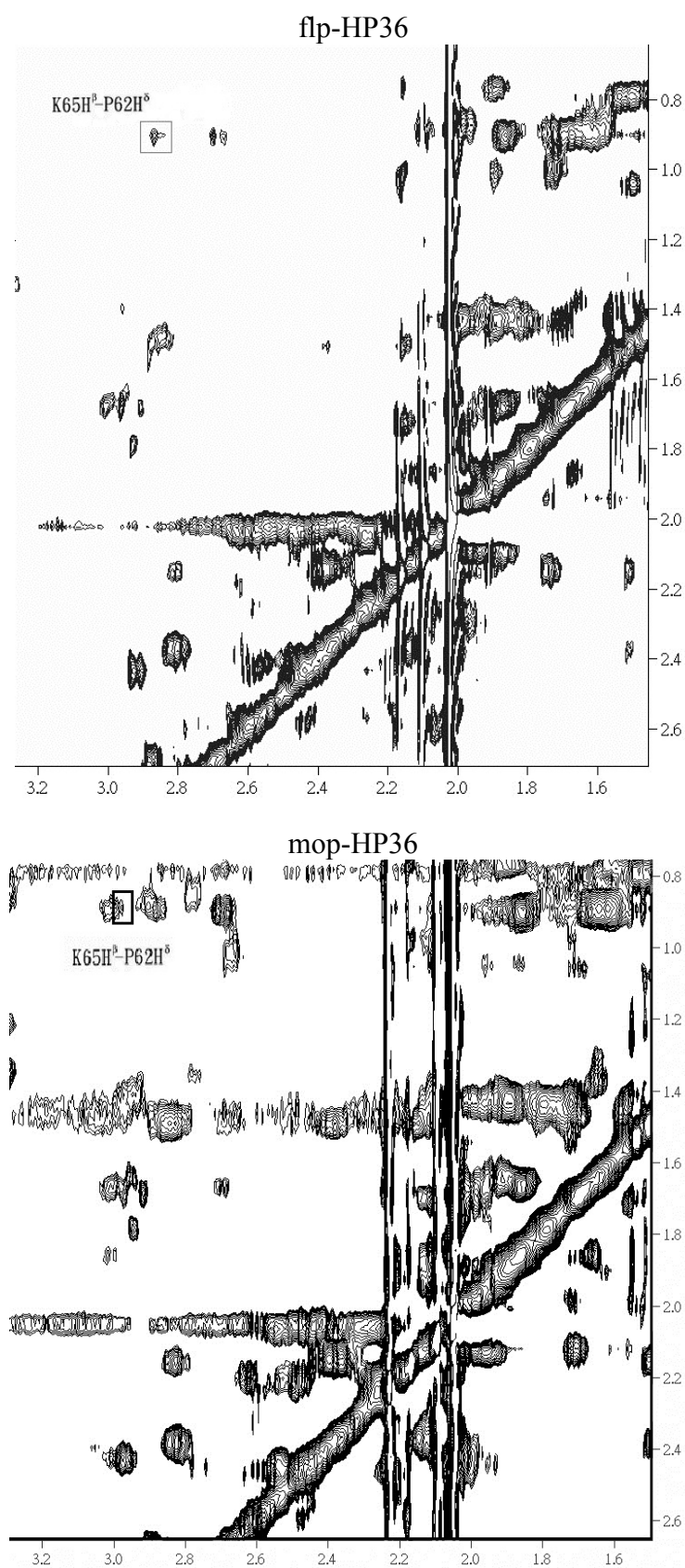


Figure S3. Excerpts of NOESY spectra for four of the HP36 mutants: the NOE cross-peaks between $C^{\beta}H$ of K65 and $C^{\delta}H$ of proline derivatives (labeled as P62) are indicated.

Table S1. Chemical shifts of the corresponding NOE cross-peaks for the HP36 mutants

Protein	δ (ppm)			
	W64 ArH	P62 C ^{γ} H	K65 C ^{β} H	P62 C ^{δ} H
Hyp-HP36	7.185	2.664	0.809	2.931
Flp-HP36	7.143	2.674	--	--
Mop-HP36	7.166	2.665	--	--
hyp-HP36	7.200	2.681	0.831	2.926
flp-HP36	7.195	2.687	0.902	2.873
mop-HP36	7.226	2.667	0.887	2.858

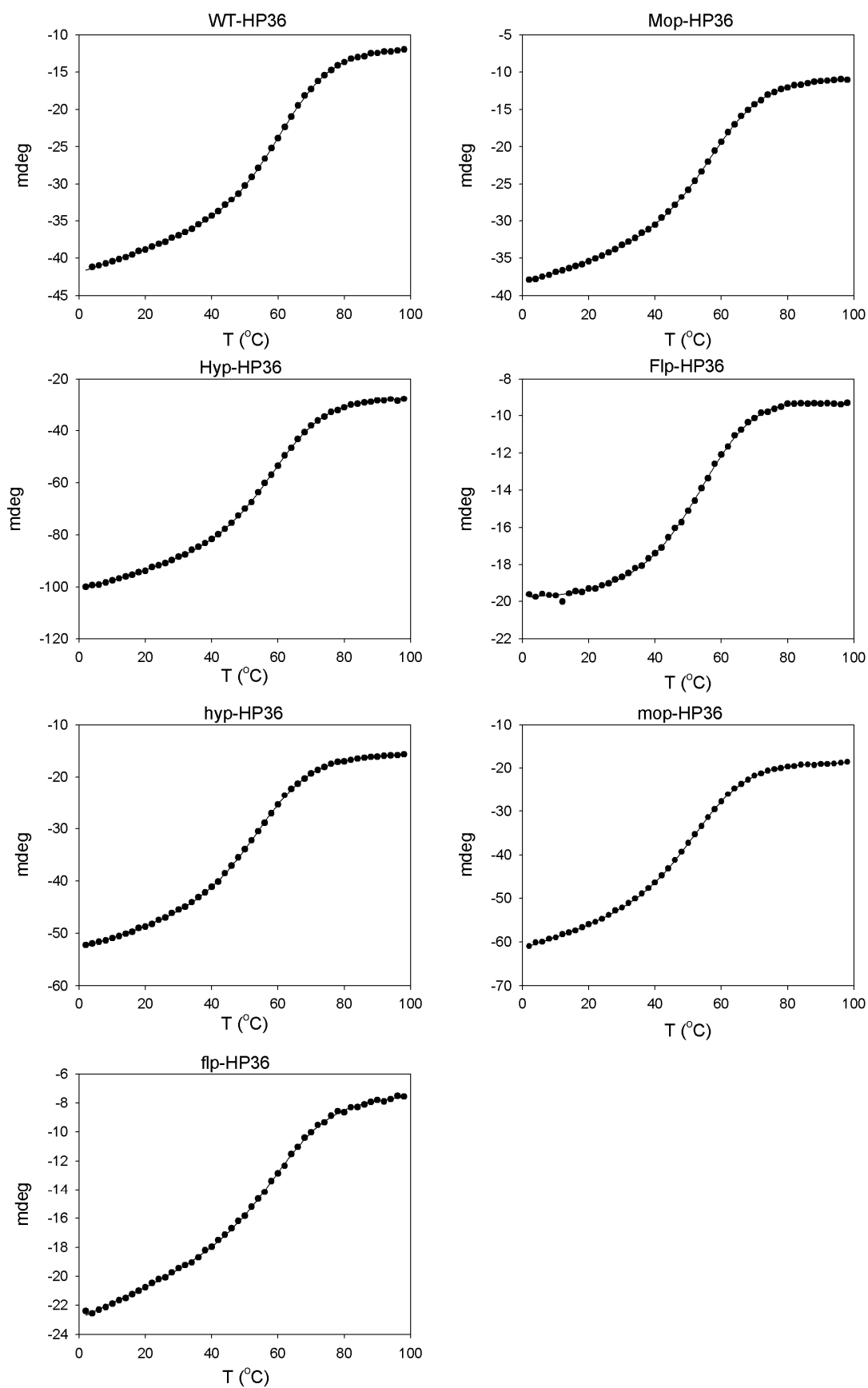


Figure S4. CD raw data of thermal unfolding curves for HP36 and its mutants.

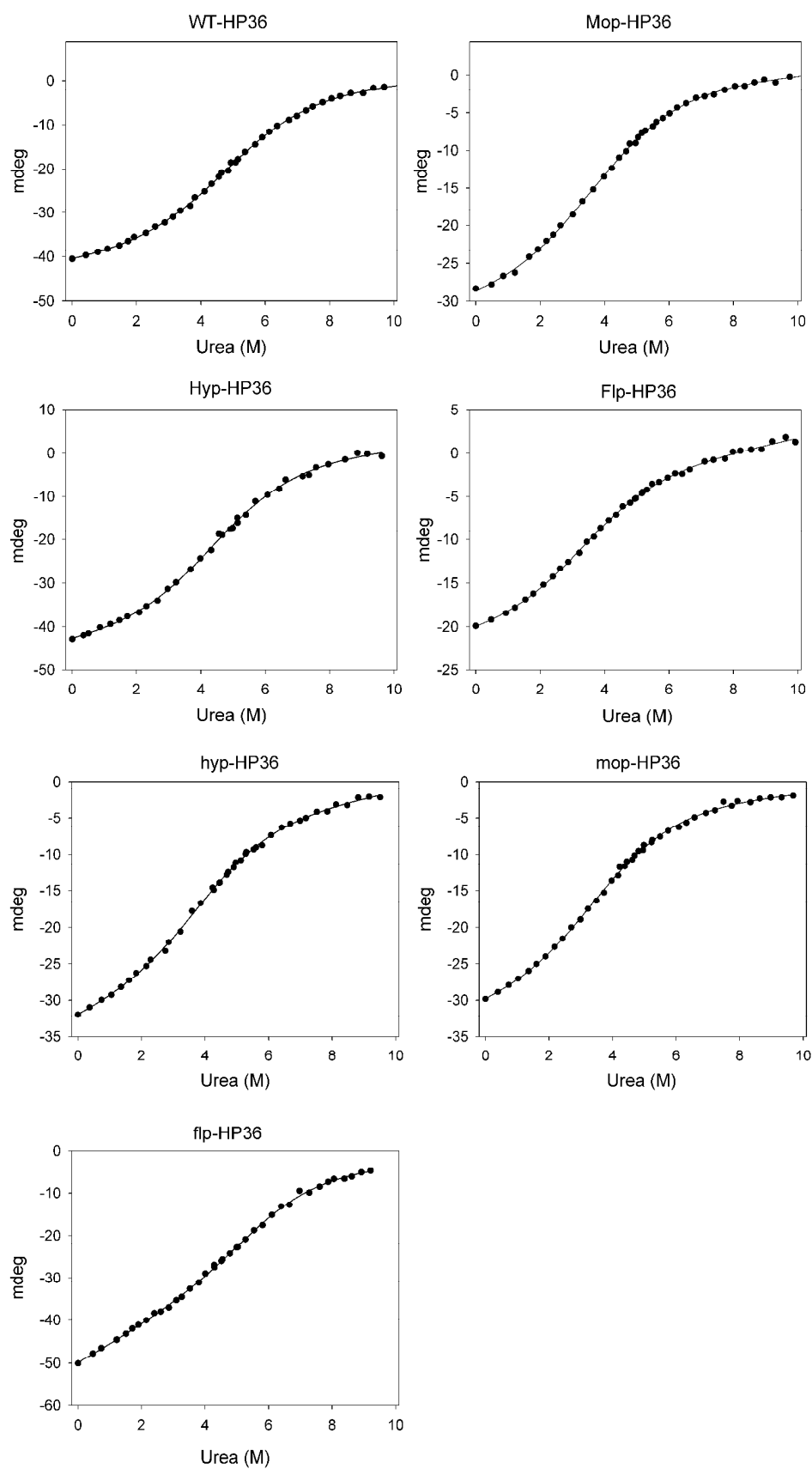


Figure S5. CD raw data of urea-induced unfolding curves for HP36 and its mutants.