Alteration of the Regiospecificity of Human Heme Oxygenase-1 by Unseating of the Heme but not Disruption of the Distal Hydrogen Bonding Network

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Supporting Information : One Table (chemical shift for assigned residues) and one figure (TOCSY spectra).

Table S1: Chemical Shift for Assigned Residues in K18E/E29K/R183E-hHO1-PH-CN and Wild-type hHO1-PH-CN[a]

		mutant	wild-type			mutant	wild-type
Lys22	$C_{\alpha}H$	6.37	6.18	Ser142	$C_{\alpha}H$	2.79	2.66
	$C_{\beta}H$	3.08	3.00		$C_{\beta 1}H$	-2.47	-3.35
	$C_{\gamma}H$	2.92	2.82		$C_{\beta 2}H$	-3.37	-5.25
His25	C H	9.07	9.24	Leu164	$C_{\alpha}H$	5.45	5.37
	$C_{\delta 2}H$	12.04	9.99				
	$C_{\alpha}H$	4.20	4.01	Ala165	NH	12.03	12.05
					$C_{\alpha}H$	4.03	3.98
Ala28	$C_{\alpha}Hs$	-2.15	-2.25		$C_{\beta}H_3$	1.54	1.49
	$C_{\alpha}H$	2.45	2.25				
				Phe166	NH	11.62	11.56
Phe47	$C_{\beta}Hs$	6.30	6.41		$C_{\beta}Hs$	5.90	5.89
	$C_{\beta}Hs$	7.06	7.59		$C_{\beta}Hs$	6.72	6.78
	$C_{\delta}H$	7.18	7.68		$C_{\delta}H$	8.12	8.18
Tyr58	NH	9.12	9.11	Phe167	$C_{\delta}H$	8.16	8.19
	$C_{\delta}H$	7.88	7.83		$C_{\zeta}H$	8.77	8.77
	$C_{\beta}Hs$	7.22	7.04		$C_{\varepsilon}H$	8.11	8.11
Phe95	$C_{\beta}Hs$	6.05	5.97	Phe207	$C_{\beta}Hs$	5.27	6.50
	$C_{\delta}H$	6.19	6.13		$C_{\beta}Hs$	6.13	5.85
	$C_{\zeta}H$	6.75	6.69		$C_{\zeta}H$	8.10	-
Tyr134	$C_{\beta}Hs$	6.77	6.71	Phe214	$C_{\beta}Hs$	6.41	6.62
	$C_{\beta}Hs$	6.60	6.45		$C_{\beta}Hs$	6.54	6.95
					$C_{\zeta}H$	7.06	7.78
Thr135	$C_{\alpha}H$	2.41	2.65				
	$C_{\beta}H$	3.25	3.10				
	$C_{\gamma}H_3$	-0.51	0.01				

a) Chemical shifts in ppm, referenced to DSS, in ^2H_2O solution, 60 mM in phosphate, pH 7.2 at 25•C.

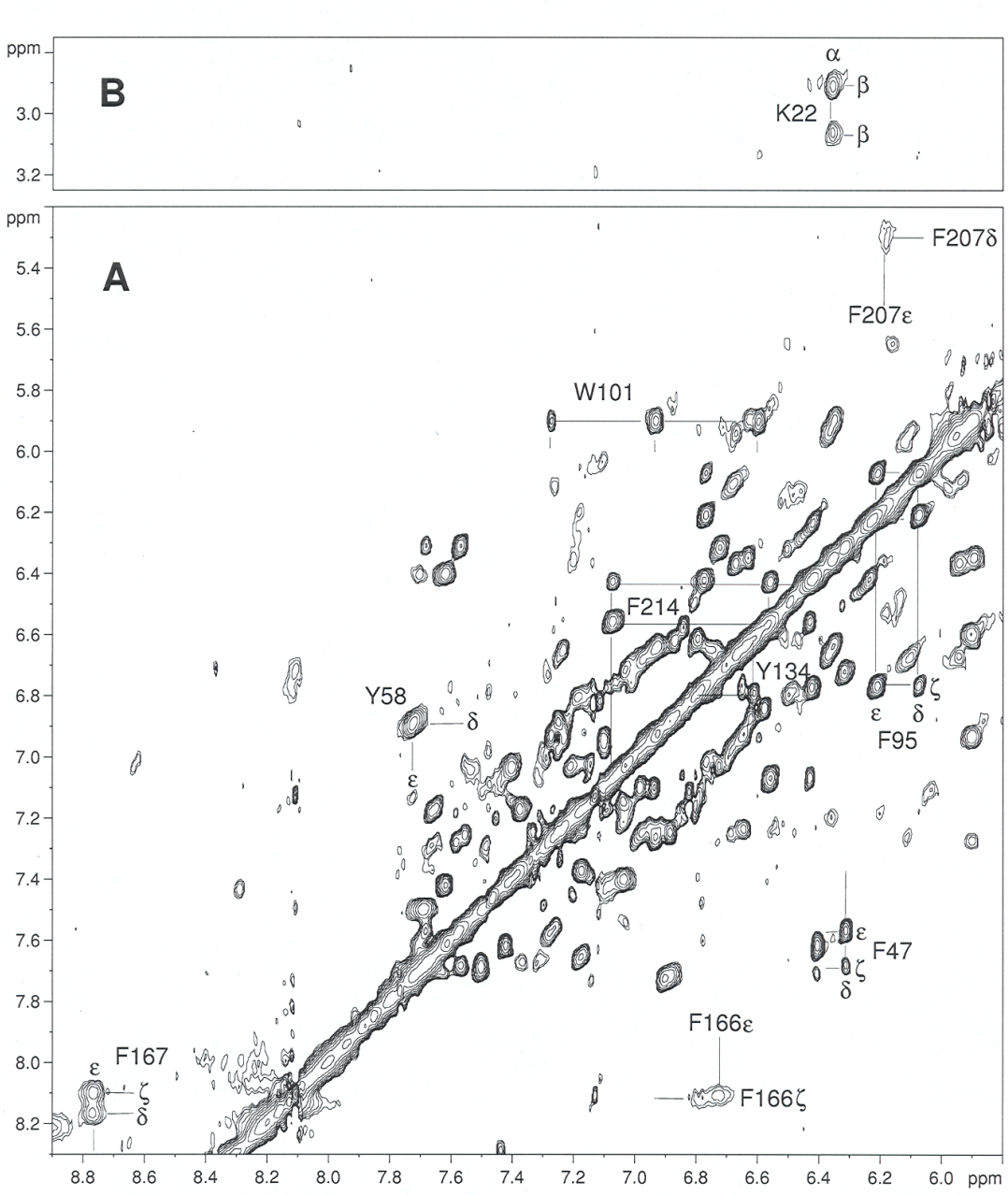

Figure S1: Portion of the 600 MHz ^{1}H NMR TOCSY spectrum (mixing time 25 ms, repetition rate 2 s^{-1}) of K18E/E29K/R183E-hHO1-PH-CN in $^{2}H_2O$ 60 mM in phosphate, pH 7.2 at 25°C illustrating the scalar connectivities for (**A**) aromatic residues Phe47, Tyr58, Phe95, Trp101, Tyr134, Phe166, Phe167, Phe207 and Phe214, and (**B**) the

strongly low-field dipolar-shifted Lys22. Cross peaks are labeled by one-letter code for residue, residue number and proton position.