

Proximal influences in two-on-two globins: Effect of the Ala69Ser replacement on *Synechocystis* sp. PCC 6803 hemoglobin

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Supplementary Information

Figures S1-S4 contain portions of the NOESY spectrum used to assign resonances for S6803 rHb-R in the ferric, *bis*-histidine state.

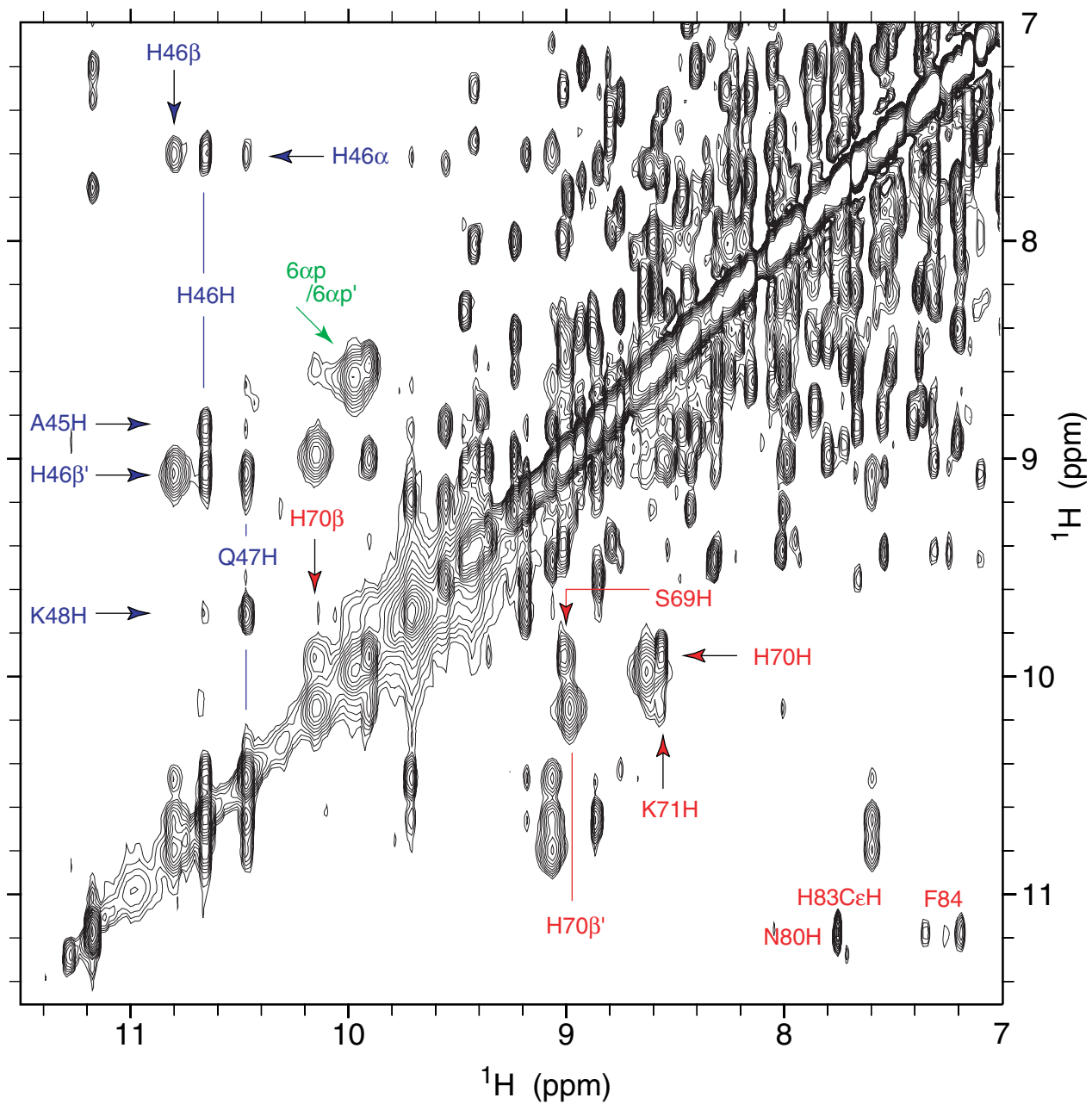


FIGURE S1: Portion of the NOESY spectrum of S6803 rHb-R collected in $^1\text{H}_2\text{O}:$ $^2\text{H}_2\text{O}$ 95:1 at 25°C and pH 7.3. Axial histidine assignments are as indicated, in blue for the distal side, red for the proximal side and green for the heme. Chemical shifts are listed in Table 1.

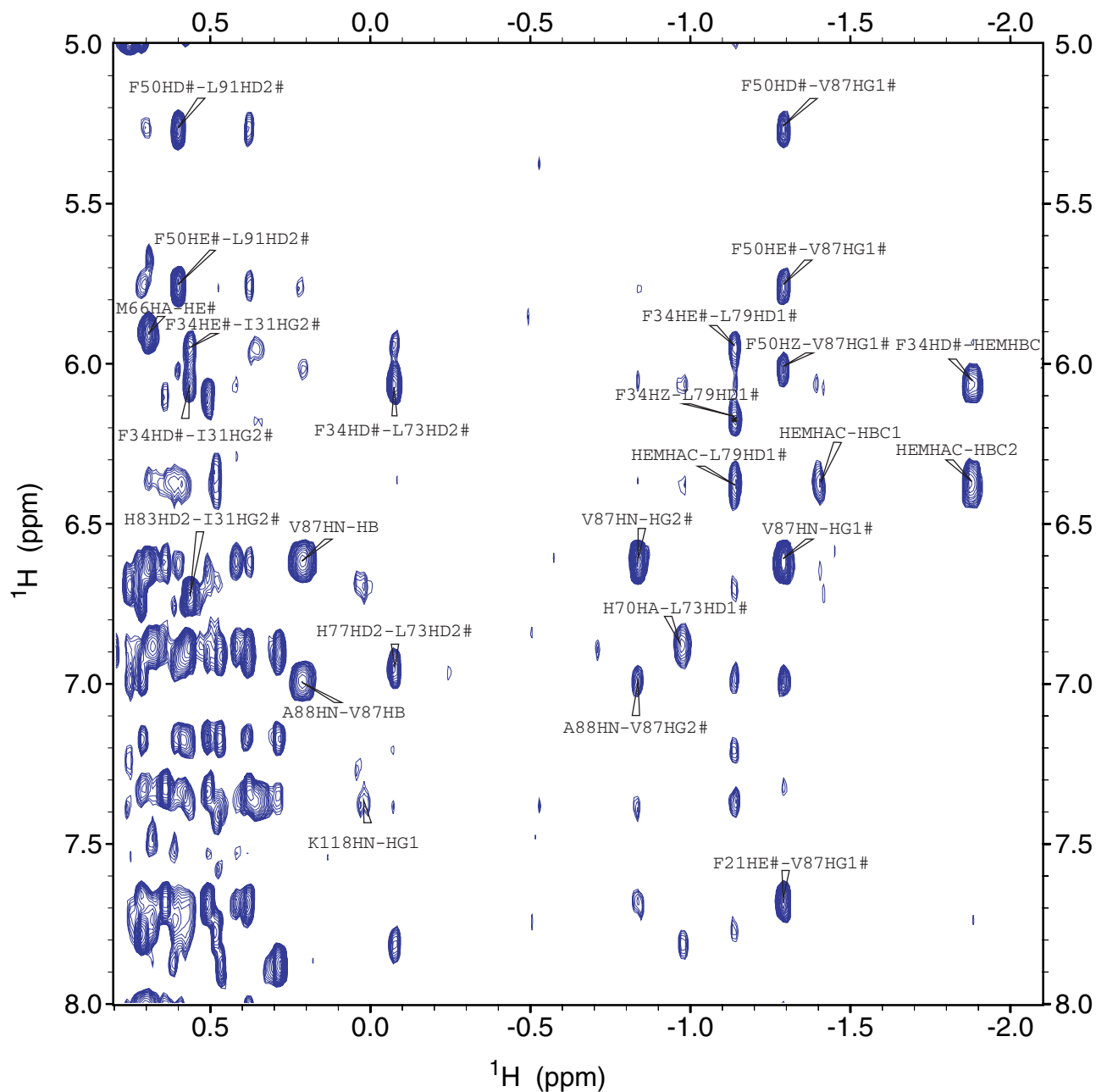


FIGURE S2: Portion of the same NOESY spectrum as in Figure S1. The nomenclature used is that of X-PLOR and the pdb for the heme group. Each peak is marked with two labels; the first label applies in the indirect dimension. The region contains a number of aromatic/CH₃ NOEs observed in the wild-type protein.

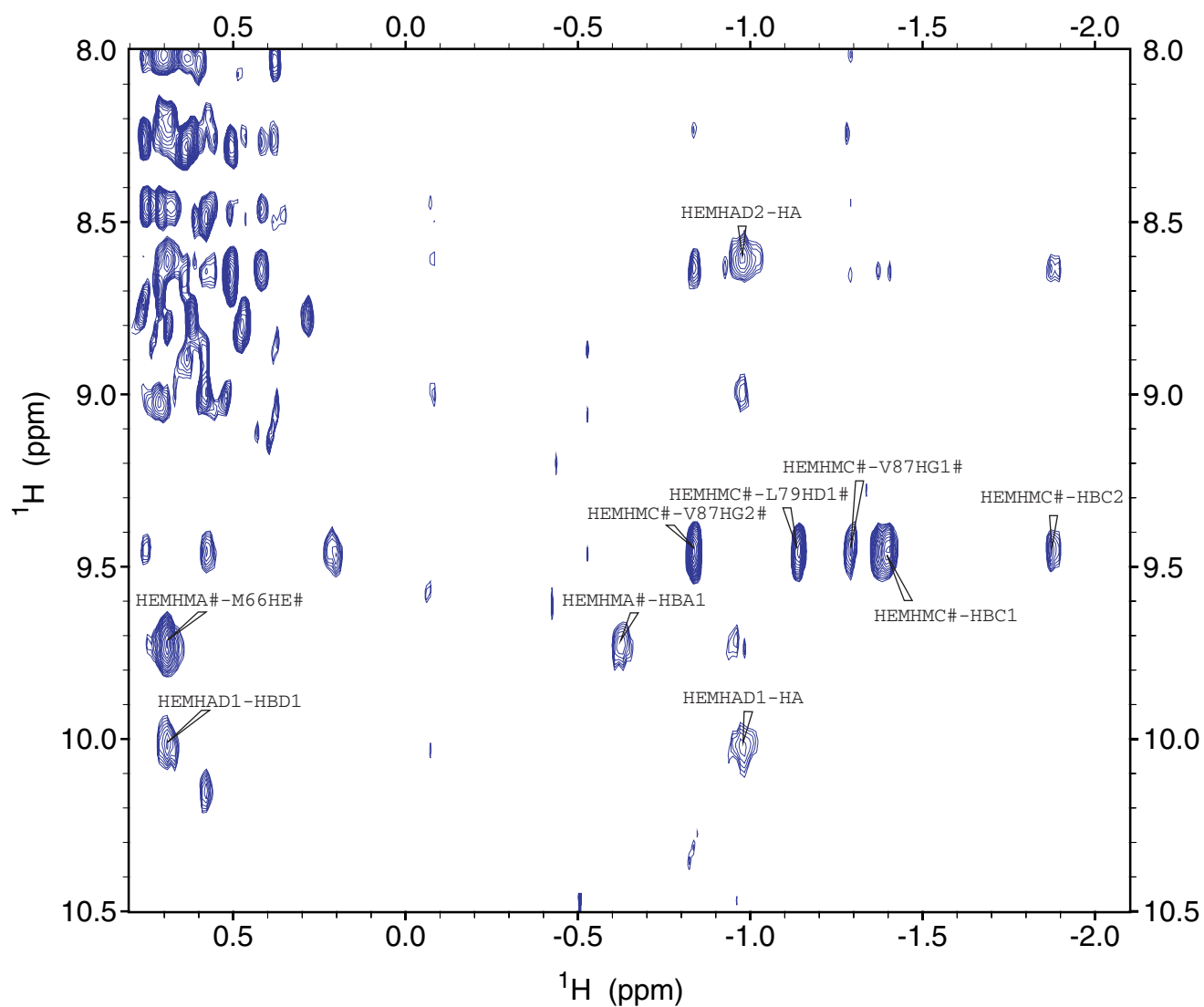


FIGURE S3: Portion of the same NOESY spectrum as in Figure S1. The nomenclature used is that of X-PLOR and the pdb for the heme group [HMA# = 8-CH₃; HAD1 = 6- α -prop; HAD2 = 6- α' -prop; HA = γ -meso; HBD1 = 6- β -prop; HMC# = 3-CH₃; HBA1 = 7- β -prop; HBC1 = 4- β -vinyl (*trans*); HBC2 = 4- β -vinyl (*cis*)]. Each peak is marked with two labels; the first label applies in the indirect dimension. The region contains a number of heme/heme effects

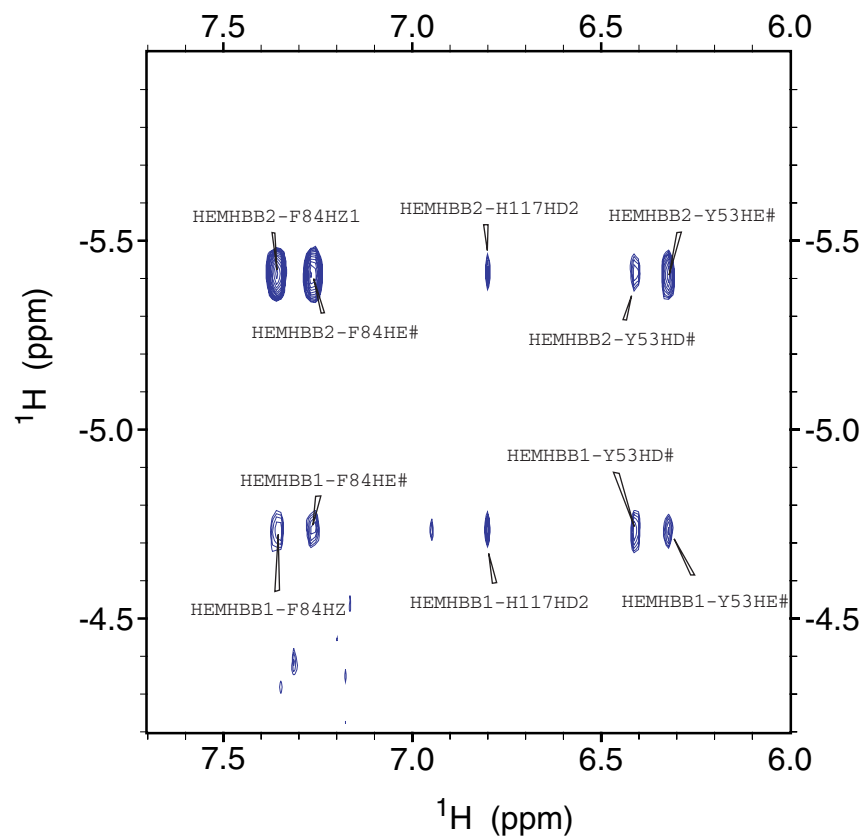


FIGURE S4: Portion of the same NOESY spectrum as in Figure S1. The nomenclature used is that of X-PLOR and the pdb for the heme group [HBB1 = 2- β -vinyl (*trans*); HBB2 = 2- β -vinyl (*cis*)]. Each peak is marked with two labels; the first label applies in the indirect dimension. The region contains 2-vinyl/aromatic effects illustrating the integrity of that environment.