Supporting Information

Identification and Characterization of a Redox Sensor Phosphodiesterase from *Ferrovum* sp. PN-J185 Containing Bacterial Hemerythrin and HD-GYP Domains

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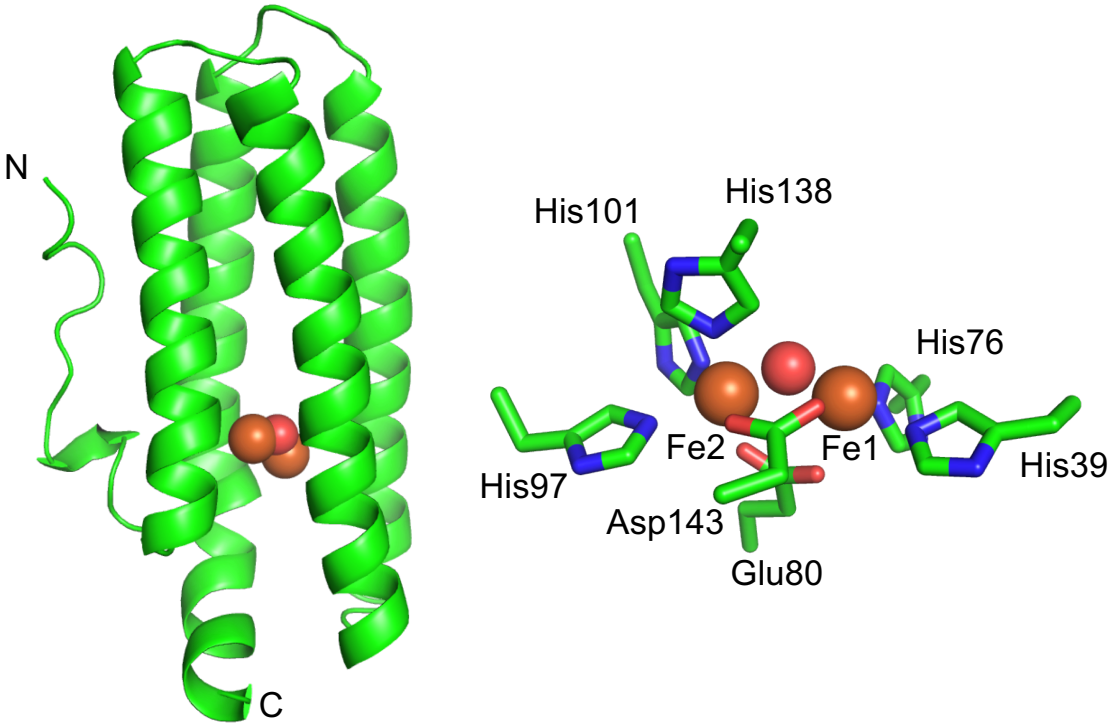

Figure S1. Modeled structure of the hemerythrin domain of Bhr-HD-GYP.

The homology model was generated by SWISS-MODEL[1] using the crystal structure of the hemerythrin domain of DcrH (PDB entry 3AGT)[2] as a template for the sequence of the hemerythrin domain (residues 18-154) of Bhr-HD-GYP. Iron atoms and bridging oxo from 3AGT coordinates are shown as orange and red spheres, respectively. Iron-coordinating residues are indicated in stick representation. It is assumed that His39, His76, Glu80 and Asp143 coordinate Fe1 in Bhr-HD-GYP, whereas His97, His101, His138, Glu80 and Asp143 coordinate Fe2, and Glu80 and Asp143 bridge both iron ions. Ligands such as oxygen and azide can bind to one (Fe1) of the two irons in the five-coordinated iron.

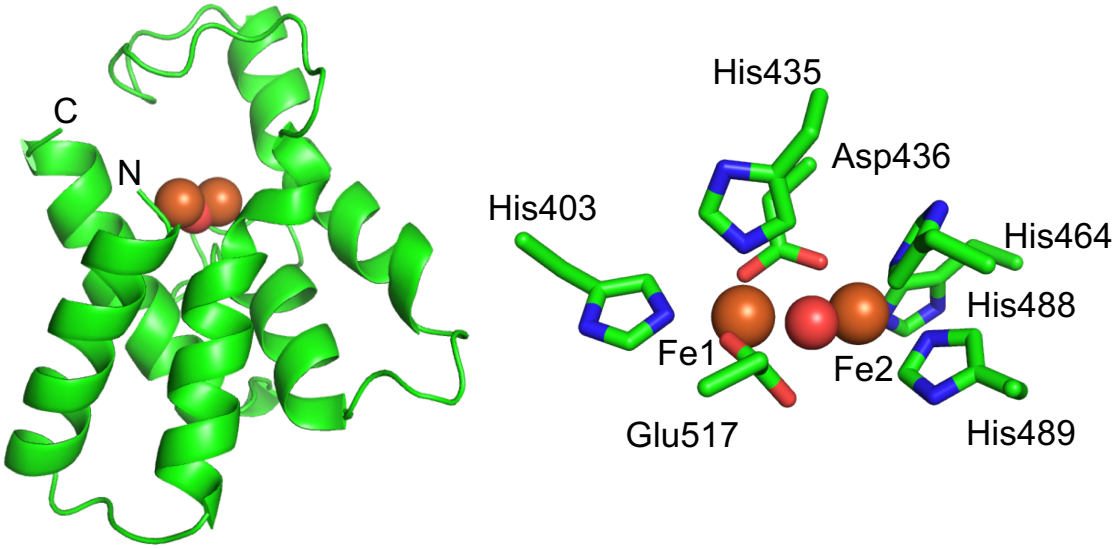

Figure S2. Modeled structure of the HD-GYP domain of Bhr-HD-GYP.

The homology model was generated by SWISS-MODEL[1] using the crystal structure of *B. bacteriovorus* Bd1817 (PDB entry 3TM8)[3] as a template for the sequence of the HD-GYP domain (residues 403-524) of Bhr-HD-GYP. Iron atoms and bridging oxo from 3TM8 coordinates are shown as orange and red spheres, respectively. Iron-coordinating residues are indicated in stick representation. It is assumed that His403, His435, Asp436 and Glu517 coordinate Fe1 in Bhr-HD-GYP, whereas His464, His488, His489, Asp436 and Glu517 coordinate Fe2, and Asp436 and Glu517 bridge both iron ions. Azide can bind to one (Fe1) of the two irons in the five-coordinated iron.

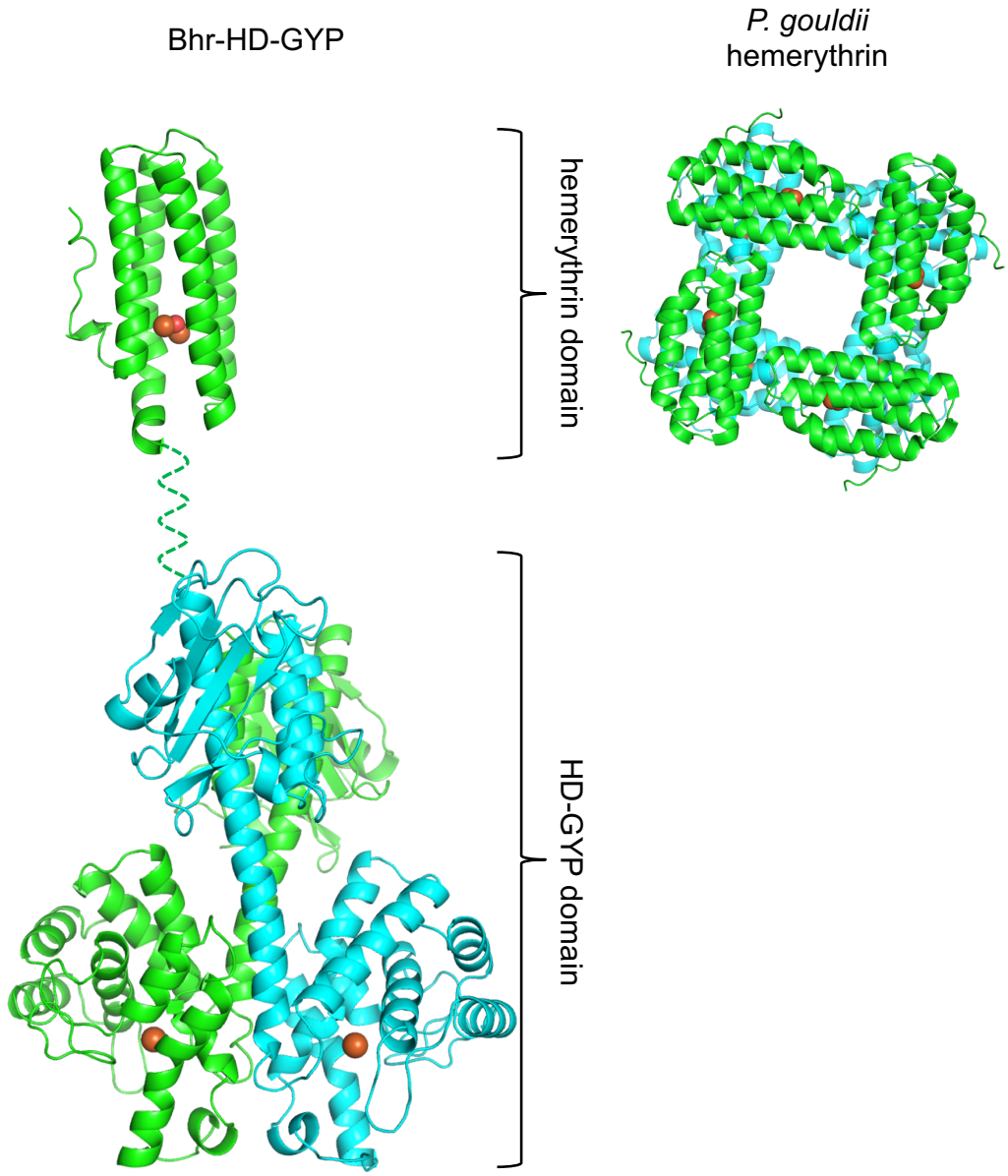

Figure S3. Modeled structure of full-length Bhr-HD-GYP.

The structure was created using the crystal structures of the hemerythrin sensor domain of DcrH (PDB entry 3AGT)[2] and HD-GYP domain of *P. marina* PmGH (PDB entry 4MCW)[4] as templates. The respective monomers are shown in green and cyan. A dashed line denotes the putative signaling helix between the hemerythrin and HD-GYP domains with an unmodeled structure. For comparison, the crystal structure of *P. gouldii* hemerythrin (PDB entry 1I4Y)[5] is shown.

References

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(2) Onoda, A., Okamoto, Y., Sugimoto, H., Shiro, Y., and Hayashi, T. (2011) Crystal structure and spectroscopic studies of a stable mixed-valent state of the hemerythrin-like domain of a bacterial chemotaxis protein. *Inorg. Chem. 50*, 4892–4899.

(3) Lovering, A. L., Capeness, M. J., Lambert, C., Hobley, L., and Sockett, R. E. (2011) The structure of an unconventional HD-GYP protein from *Bdellovibrio* reveals the roles of conserved residues in this class of cyclic-di-GMP phosphodiesterases. *mBio 2*, e00163-11.

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(5) Farmer, C. S., Kurtz, D. M., Jr., Liu, Z. J., Wang, B. C., Rose, J., Ai, J., and Sanders-Loehr, J. (2001) The crystal structures of *Phascolopsis gouldii* wild type and L98Y methemerythrins: Structural and functional alterations of the O_2 binding pocket. *J. Biol. Inorg. Chem. 6*, 418–429.