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### Title

Correction for Chreifi et al., Crystal structure of the pristine peroxidase ferryl center and its relevance to proton-coupled electron transfer

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### Authors

Chreifi, Georges  
Baxter, Elizabeth L  
Doukov, Tzanko  
[et al.](#)

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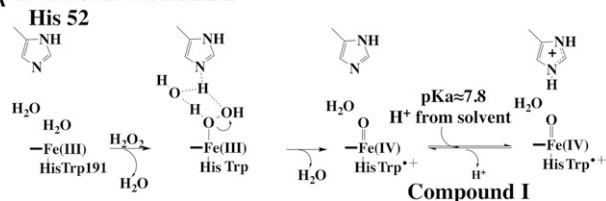
# Correction

## BIOPHYSICS AND COMPUTATIONAL BIOLOGY

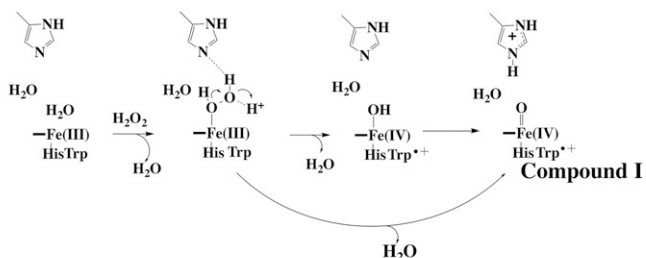
Correction for “Crystal structure of the pristine peroxidase ferryl center and its relevance to proton-coupled electron transfer,” by Georges Chreifi, Elizabeth L. Baxter, Tzanko Doukov, Aina E. Cohen, Scott E. McPhillips, Jinhu Song, Yergalem T. Mehareenna, S. Michael Soltis, and Thomas L. Poulos, which appeared in issue 5, February 2, 2016, of *Proc Natl Acad Sci USA* (113:1226–1231; first published January 19, 2016; 10.1073/pnas.1521664113).

The authors note that Fig. 1 appeared incorrectly. The corrected figure and its legend appear below.

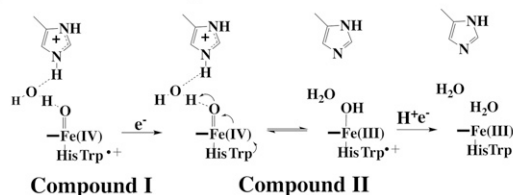
### A Traditional Mechanism



### B Modified Mechanism Based on Neutron Diffraction



### C Reduction of Compounds I and II



**Fig. 1.** Peroxidase mechanism. (A) Traditional “water-modified” mechanism of Cmpl formation. In this mechanism, peroxide first coordinates with the heme iron, followed by proton transfer to the distal peroxide O atom via an ordered water molecule and the distal His. The protonation state of the distal His depends on the His pK<sub>a</sub>. Our computational experiments indicate that the pK<sub>a</sub> substantially increases in Cmpl. (B) Modified mechanism based on the observation that His52 in CCP Cmpl is protonated in the neutron diffraction structure (8). Going from the initial peroxide complex to Cmpl proceeds via two possible routes, one of which involves the Fe(IV)-OH intermediate. (C) Mechanism of CmplI reduction, which includes a proton-coupled electron transfer event resulting in a net transfer of a proton from the distal His to the ferryl O atom.

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