Supporting Information for the Manuscript:
Catalytic Reaction Mechanism of Oxalate Oxidase (Germin). A Hybrid DFT Study.

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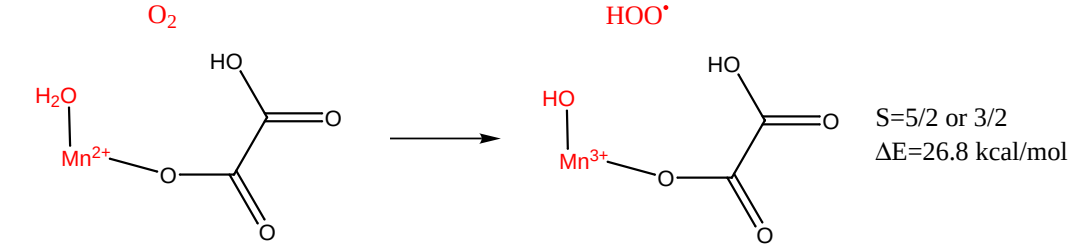
Scheme S 1: The alternative mechanisms for Oxalate Oxidase catalytic reaction investigated in this study. A. The mechanism with the hydrogen atom transfer to unbound dioxygen. B. The PCET on the sextet PES. C. The mechanism with the hydrogen atom transfer to Mn-bound dioxygen. D. The mechanism with the peroxo-bridged intermediate. E. The mechanism with one histidine dissociating from Mn and HOO radical attacking on oxalate. F. The mechanism with one histidine dissociating from Mn and the electron transfer from oxalate to Mn^{4+}.

A



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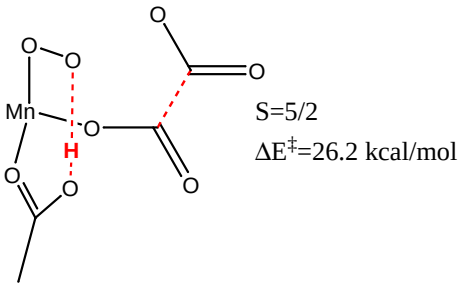

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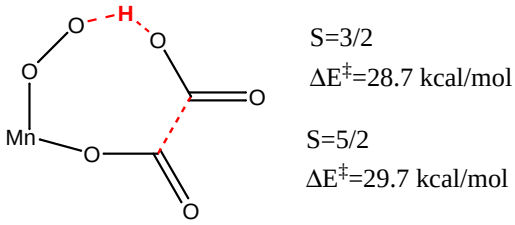

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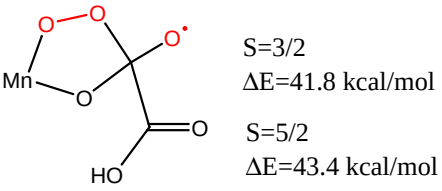

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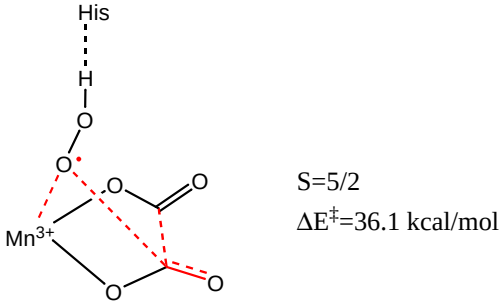

F