

A Molecular Dynamics Examination on Mutation Induced Catalase Activity in Coral Allene Oxide Synthase.

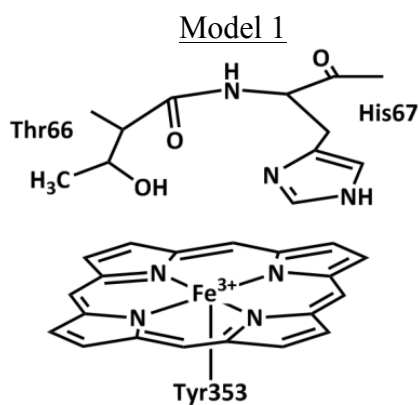
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Canada

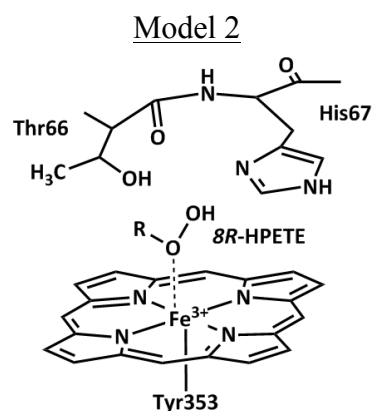
Supplementary Information

(**Figures S1** and **S2**, and full citation for reference 24; 5 pages in total)

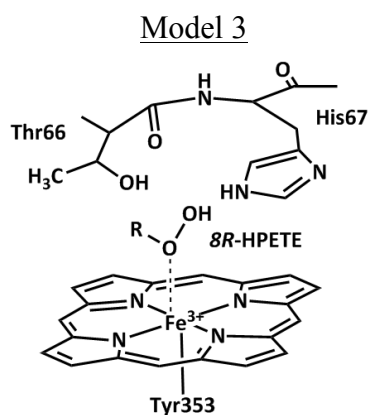
Figure S1. Schematic representations of the active site residues for all molecular dynamics simulations performed.



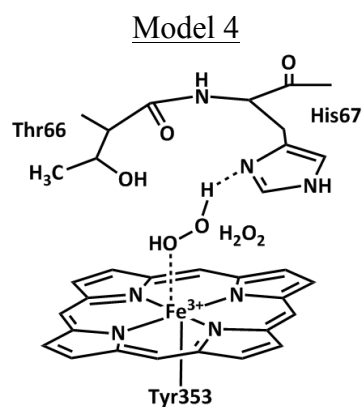
A. WT cAOS with no substrate bound.



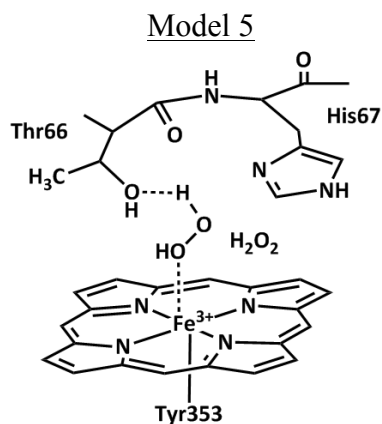
B. WT cAOS with 8R-HPETE bound.



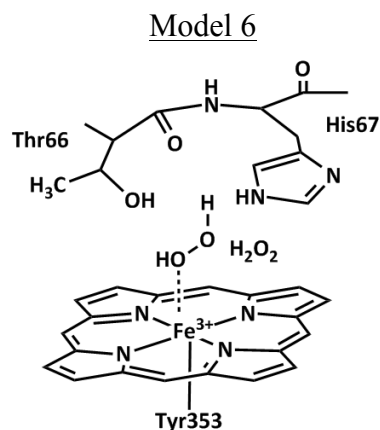
C. WT cAOS with 8R-HPETE bound and a rotated His67.



D. WT cAOS with H_2O_2 bound and initial orientation H-bonded to His67.

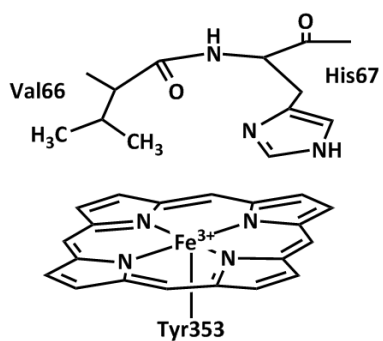


E. WT cAOS with H_2O_2 bound and initial orientation H-bonded to Thr66.



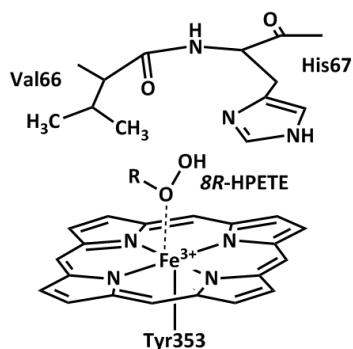
F. WT cAOS with H_2O_2 bound and rotated His67.

Model 7



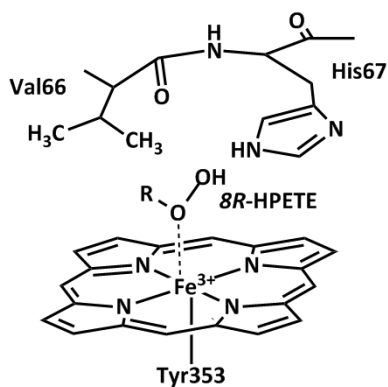
G. T66V cAOS with no substrate bound.

Model 8



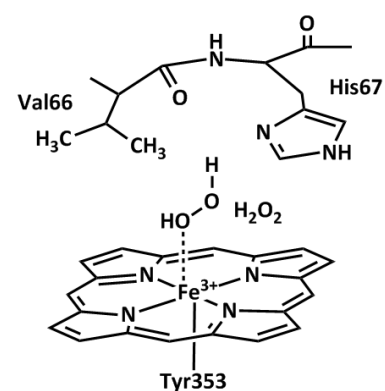
H. T66V cAOS with 8R-HPETE bound.

Model 9



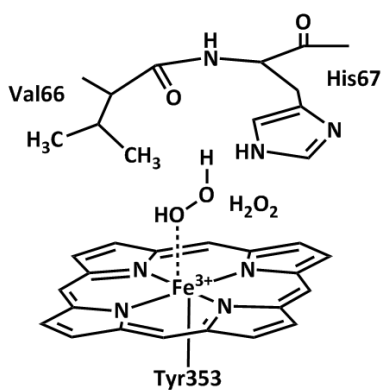
I. T66V cAOS with 8R-HPETE bound and a rotated His67.

Model 10



J. T66V cAOS with H₂O₂ bound.

Model 11



K. T66V with H₂O₂ bound.

Figure S2A. Heme RMSDs with respect to time for the 10 ns MD simulations of all WT cAOS models 1-6.

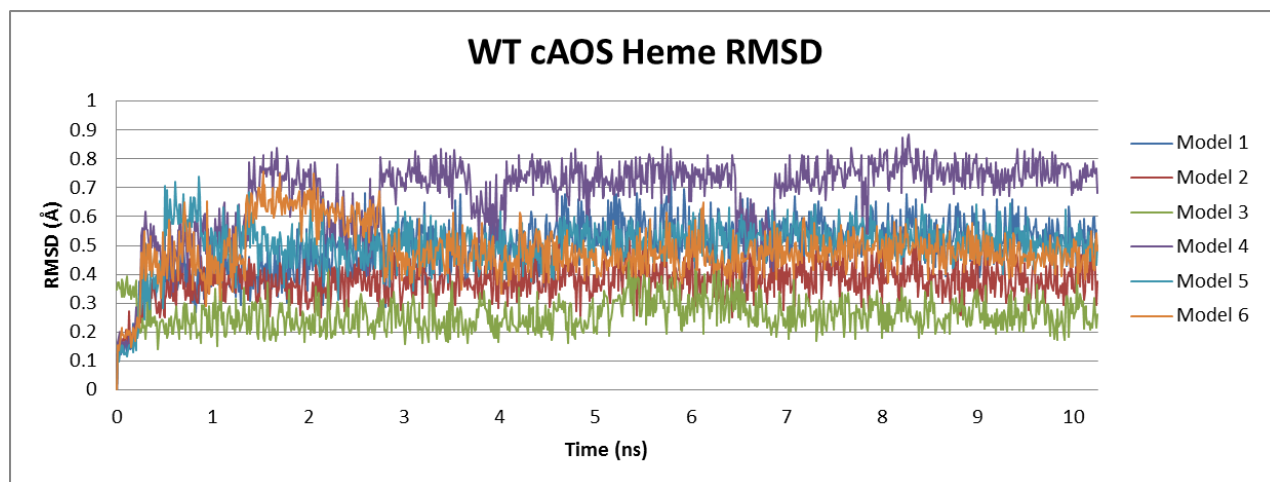
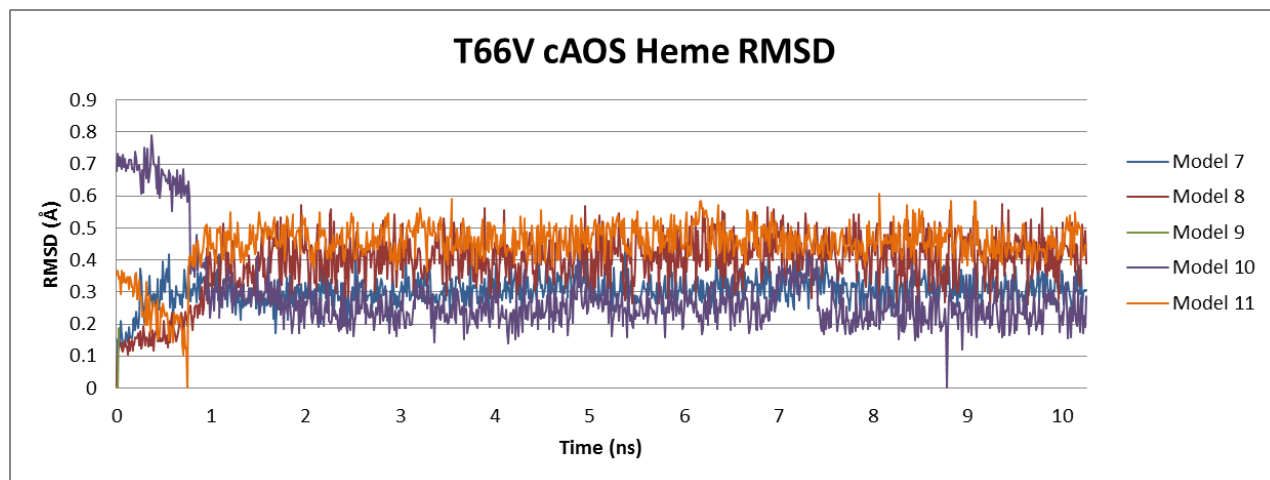


Figure S2B. Heme RMSDs with respect to time for the 10 ns MD simulations of all T66V cAOS models 7-11.



Full citation for Reference 24:

Bhandarkar, M.; Bhatele, A.; Bohm, E.; Brunner, R.; Buelens, F.; Chipot, C.; Dalke, A.; Dixit, S.; Fiorin, G.; Freddolino, P.; Grayson, P.; Gullingsrud, J.; Gursoy, A.; Hardy, D.; Harrison, C.; Hénin, J.; Humphrey, W.; Hurwitz, D.; Krawetz, N.; Kumar, S.; Kunzman, D.; Lai, J.; Lee, C.; McGreevy, R.; Mei, C.; Nelson, M.; Phillips, J.; Sarood, O.; Shinozaki, A.; Tanner, D.; Wells, D.; Zheng, G.; Zhu, F.; NAMD User's Guide Version 2.7 b1. **2009**.