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In silico* structural analysis of peroxidase in *Theobroma cacao*, a potential alternative of *Rhapanus sativus

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Class III peroxidases are widely distributed and conserved catalytic enzymes in plants. *Rhapanus sativus* peroxidase has been extensively studied,¹ mainly due to its antioxidant properties, great stability, commercial use, applications in immunochemical techniques and simplicity to detect it. However, the extraction process yields low active protein, thus, there is a need to search for alternative peroxidases that could be used in natural antioxidant products and enzymes. *Theobroma cacao* is an abundant native crop in Guatemala, and it could be of commercial interest for a more stable peroxidase with similar or better catalytic properties than *Rhapanus sativus* peroxidase. Structural analysis by 3D protein models and homology modelling were performed. The peroxidase sequence of *Theobroma cacao* was obtained from UniprotKB-A0A061ET.² A search was performed on Protein Data Bank, ModBase and ModIDB to obtain the 3-dimensional protein. Homology modeling was performed using Swiss-Model software, and 4A5G-PDB template corresponding to *Rhapanus sativus*. Software UCSF Chimera was used to obtain the percent of identity and root-mean-square deviation (RMSD). An alignment with the Smith-Waterman algorithm was also performed with the existing data-bases in NCBI. The sequence was obtained from Uniprot. The values for QMEAN -3.24 and 0.65 QMQE validate the model.^{3,4} Chimera USFC Software was used to compare both *Theobroma cacao* and *Rhapanus sativus* peroxidases, with RMSD value of 0.33 and 33.67 percentage of identity. The comparative sequences of peroxidase and *Theobroma cacao* differ in a high percentage, however a low RMSD explains a conserved structure of the class III peroxidases. Both peroxidases share similarities in their glycosylation sites and the central position of the Hemo group. The QMEAN and QMQE values confirm the quality of the model, as well as the Ramachandran plots show an acceptable model with residues within the defined theoretical spaces. The *Theobroma cacao* peroxidase structure is very similar to that of *Rhapanus sativus* (RMSD 0.33 Å^o), particularly, with the 4A5G.PDB. This warrants further research to verify if the *in vitro* activity of this enzyme may be similar or superior to *Rhapanus sativus*.

Keywords: peroxidase, oxidoreductase, homology modeling

References

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