

University of Groningen

## Crystal Structure of *Agaricus bisporus* Mushroom Tyrosinase

Ismaya, Wangsa T.; Rozeboom, Henriette J.; Weijn, Amrah; Mes, Jurriaan J.; Fusetti, Fabrizia; Wichers, Harry J.; Dijkstra, Bauke W.

*Published in:*  
 Biochemistry

*DOI:*  
[10.1021/bi200395t](https://doi.org/10.1021/bi200395t)

**IMPORTANT NOTE:** You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

*Document Version*  
 Publisher's PDF, also known as Version of record

*Publication date:*  
 2011

[Link to publication in University of Groningen/UMCG research database](#)

### *Citation for published version (APA):*

Ismaya, W. T., Rozeboom, H. J., Weijn, A., Mes, J. J., Fusetti, F., Wichers, H. J., & Dijkstra, B. W. (2011). Crystal Structure of *Agaricus bisporus* Mushroom Tyrosinase: Identity of the Tetramer Subunits and Interaction with Tropolone. *Biochemistry*, 50(24), 5477-5486. <https://doi.org/10.1021/bi200395t>

### **Copyright**

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

### **Take-down policy**

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

*Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.*

Supplementary Information belonging to

Wangsa T. Ismaya, Henriëtte J. Rozeboom, Amrah Weijn, Jurriaan J. Mes, Fabrizia Fusetti, Harry J. Wichers and Bauke W. Dijkstra. Crystal structure of *Agaricus bisporus* mushroom tyrosinase - Identity of the tetramer subunits and interaction with tropolone.

Fig. S1. *A. bisporus* tyrosinase tetramer in the asymmetric unit of a) space group  $P2_12_12$  (dimensions  $\sim 139 \times 97 \times 59 \text{ \AA}$ ), and b) space group  $P2_1$  (dimensions  $\sim 107 \times 87 \times 84 \text{ \AA}$ ). The H subunits are coloured red and green, and the L subunits are in light blue and purple. The black balls represent the positions of the bound holmium ions (see main text for explanation).

a)

b)

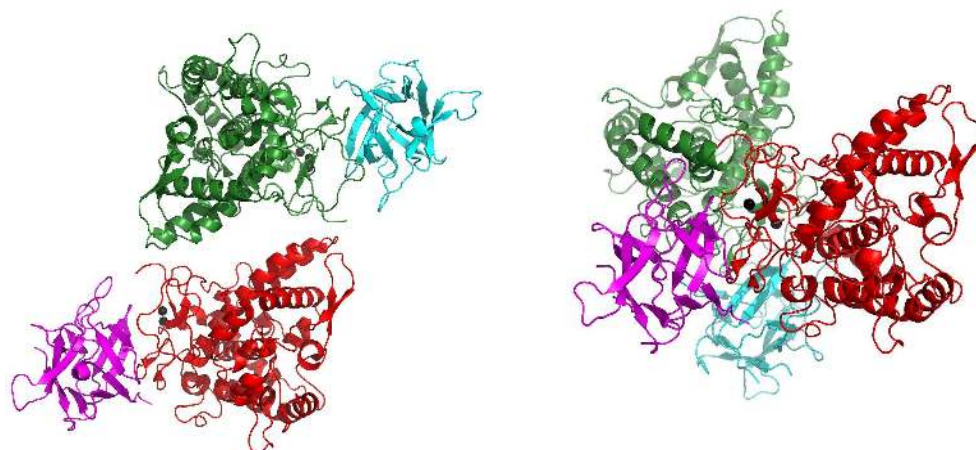


Fig. S2. Structure-based sequence alignment of tyrosinase-related type 3 copper proteins. The aligned structures and PDB database accession numbers are *AbTyr*, *A. bisporus* tyrosinase (PPO3, this article; PDB 2y9w); *BmTyr*, *B. megaterium* tyrosinase (PDB 3nm8 (1)); *ScTyr*, *S. castaneoglobisporus* tyrosinase (PDB 1wx2 (2)); *IbCox*, *I. batata* catechol oxidase (PDB 1bt1 (3)) and *Odhecy*, *Octopus dofleini* hemocyanin (PDB 1js8 (4)). Structural alignment was performed using the DALI server. The secondary structure elements are shown as squiggles ( $\alpha$ -helix and  $3_{10}$ -helix), black arrows ( $\beta$ -strands) and strict  $\beta$ -turns as **TT** letters at the top of

the alignment. Residues involved in copper binding are shown in cyan. Cysteines involved in the thioether bond are shown in purple. The fully conserved residues are shown in white on red background. Numbers indicate the residue numbers of *AbTyr*. The figure was prepared with ESPript (5).

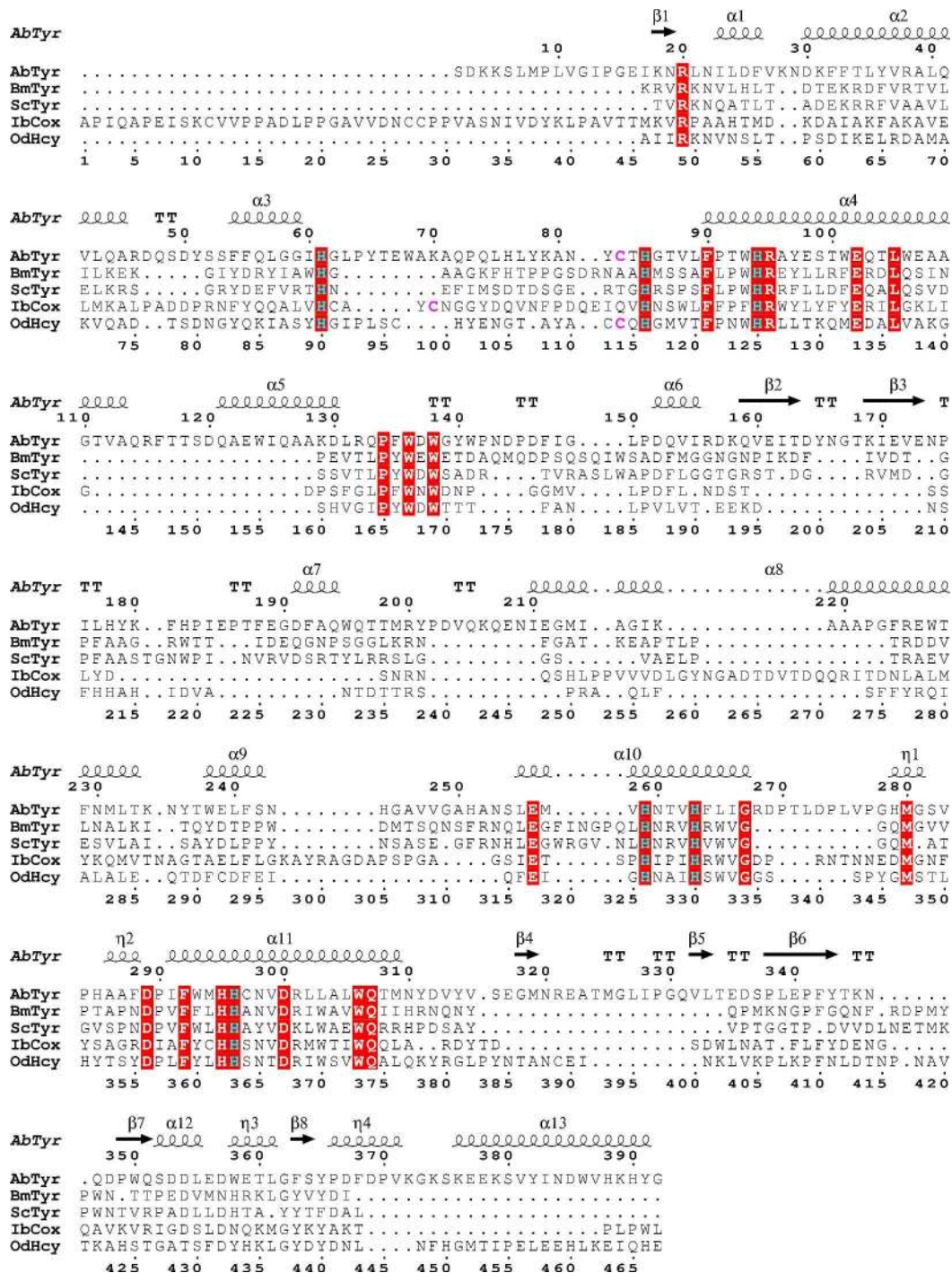


Fig. S3. Stereo figure of a superposition of *A. bisporus* tyrosinase (green; PDB 2y9w (this article)), *B. megaterium* tyrosinase (orange; PDB 3nq1 (1)), *S. castaneoglobisporus* tyrosinase (magenta; PDB 1wx2 (2)). Copper ions are in light brown and the inhibitor kojic acid from the *B. megaterium* tyrosinase structure is shown in orange.

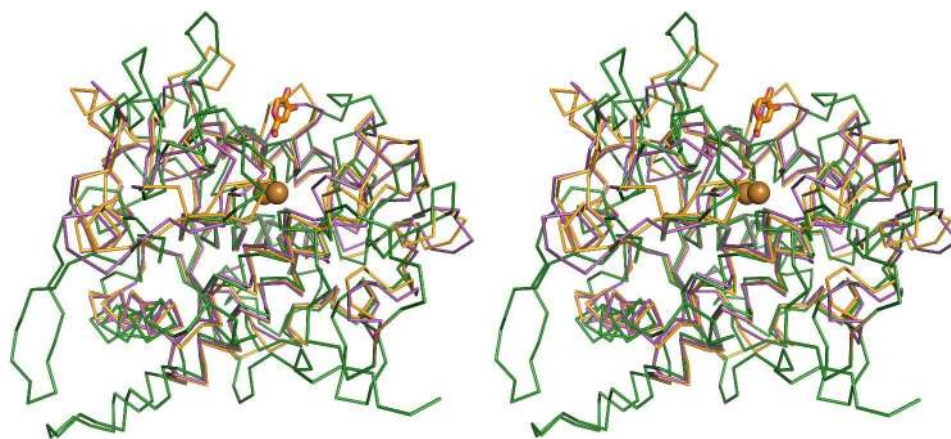
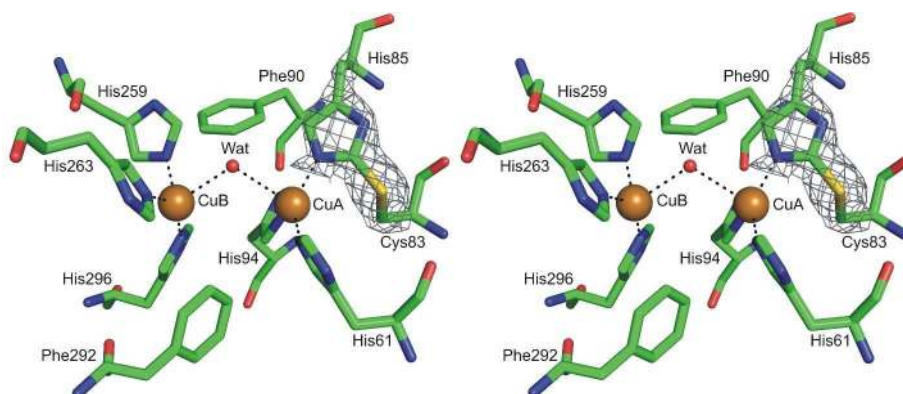


Fig. S4. Stereo figure of the geometry of the binuclear copper-binding site in space group  $P2_12_12$ . The ligands are colored according to atom type (green, blue, red, yellow for carbon, nitrogen, oxygen, sulfur, respectively). The brown spheres are the Cu-A and Cu-B copper ions, and the red sphere is a bound water molecule/hydroxyl ion. The electron density for the covalent thioether bond between the Cys83  $S\gamma$  and His85  $C\epsilon 1$  atoms is contoured at  $2.0 \sigma$  and is shown in black mesh.



## REFERENCES

1. Sendovski, M., Kanteev, M., Shuster Ben-Yosef, V., Adir, N., and Fishman, A. (2011) First structures of an active bacterial tyrosinase reveal copper plasticity, *J. Mol. Biol.* 405, 227–237.
2. Matoba, Y., Kumagai, T., Yamamoto, A., Yoshitsu, H., and Sugiyama, M. (2006) Crystallographic evidence that the dinuclear copper center of tyrosinase is flexible during catalysis, *J. Biol. Chem.* 281, 8981-8990.
3. Klabunde, T., Eicken, C., Sacchettini, J. C., and Krebs, B. (1998) Crystal structure of a plant catechol oxidase containing a dicopper center, *Nat. Struct. Biol.* 5, 1084-1090.
4. Cuff, M. E., Miller, K. I., van Holde, K. E., and Hendrickson, W. A. (1998) Crystal structure of a functional unit from *Octopus* hemocyanin, *J. Mol. Biol.* 278, 885-870.
5. Gouet, P., Robert, X., and Courcelle, E. (2003) ESPript/ENDscript: extracting and rendering sequence and 3D information from atomic structures of proteins, *Nucleic Acids Res.* 31, 3320-3323.