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Supplementary Information

Article

Theoretical Studies of Cyanophycin Dipeptides as Inhibitors of Tyrosinases

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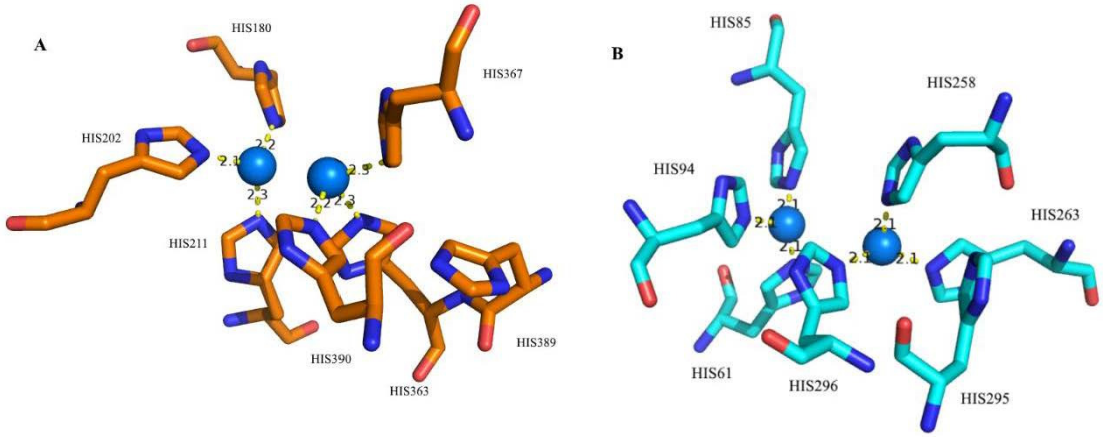

Figure S1. The distances between copper atoms at (**A**) TYR and (**B**) abTYR.

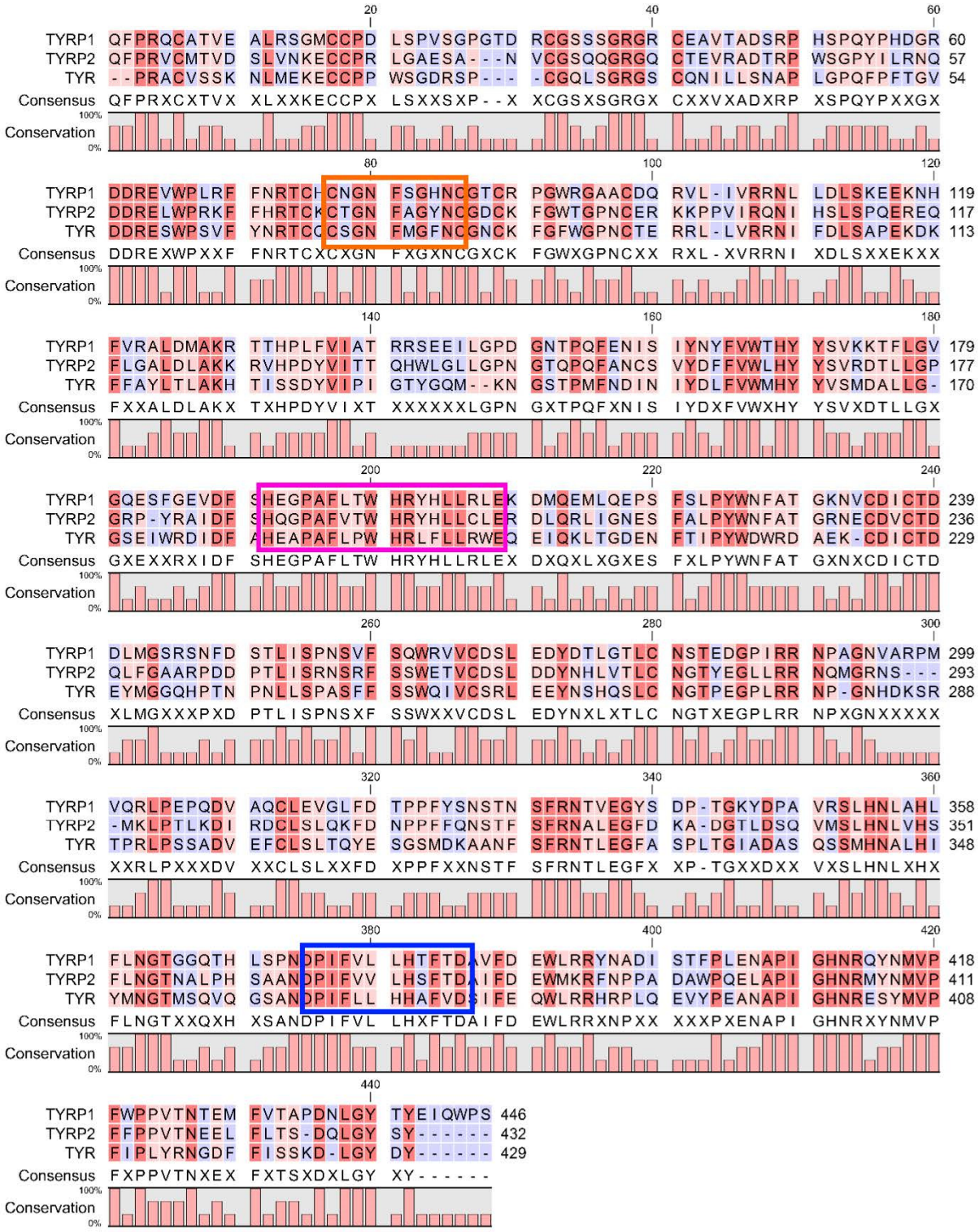

Figure S2. Multiple Sequence Alignment of TYR, TYRP1 and TYRP2. Magenta—CuA binding pattern, blue—CuB binding pattern, orange EFG pattern.

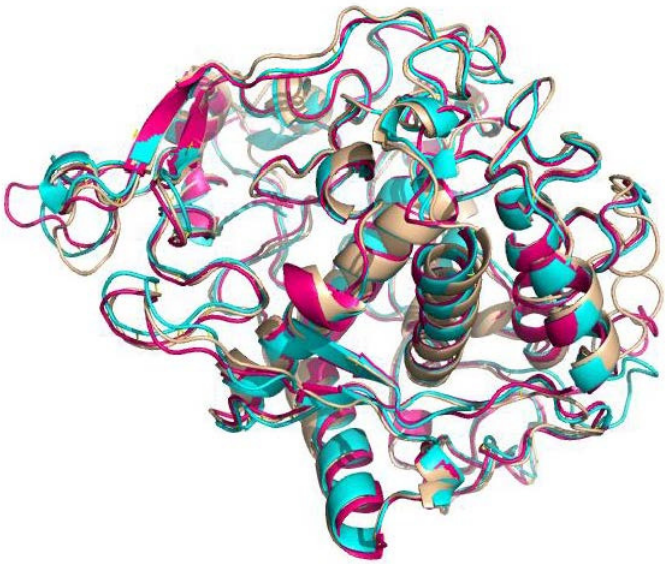

Figure S3. Alignment of TYR (wheat), TYRP1(magenta) and TYRP2 (cyan).

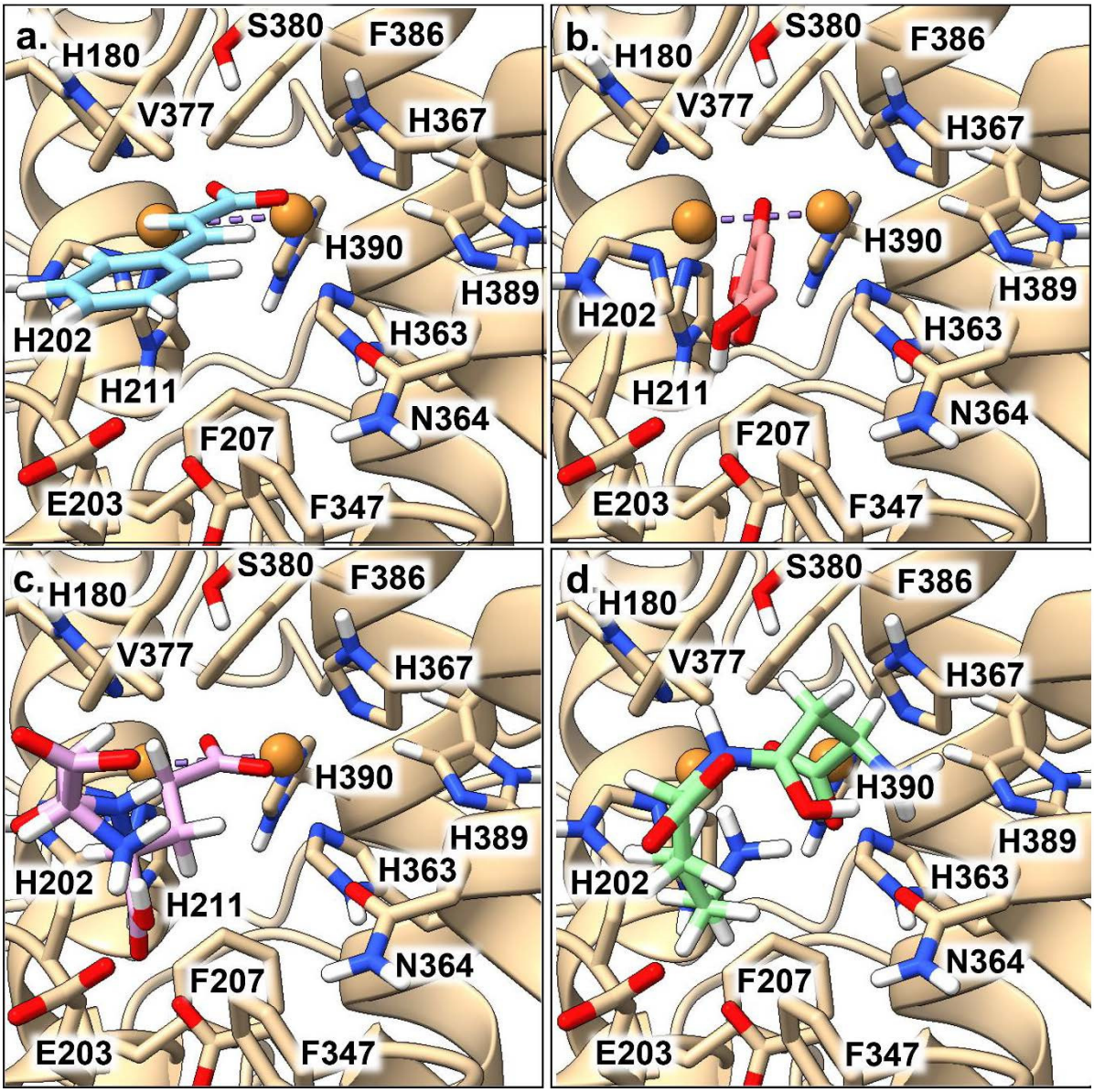

Figure S4. Ribbon representation of the TYR active site with two copper atoms (orange balls) in complex with (**a**) cinnamic acid, (**b**) kojic acid, (**c**) aspartate-glutamate (lig2), and (**d**) aspartate-lysine (lig4). Key amino acids that create interactions with ligands are labeled in black.

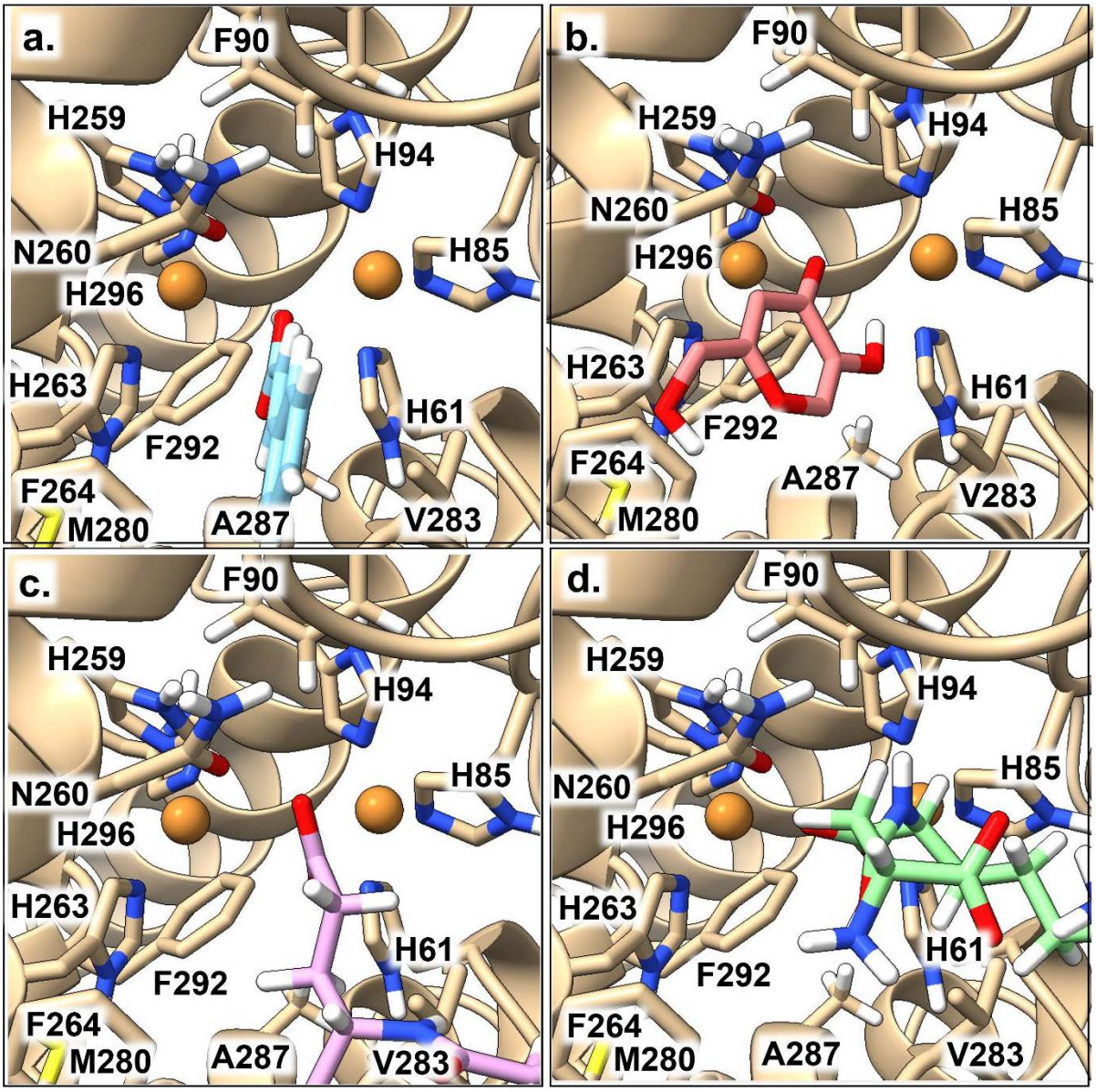

Figure S5. Ribbon representation of the abTYR active site with two copper atoms (orange balls) in complex with (**a**) cinnamic acid, (**b**) kojic acid, (**c**) aspartate-glutamate (lig2), and (**d**) aspartate-lysine (lig4). Key amino acids that create interactions with ligands are labeled in black.

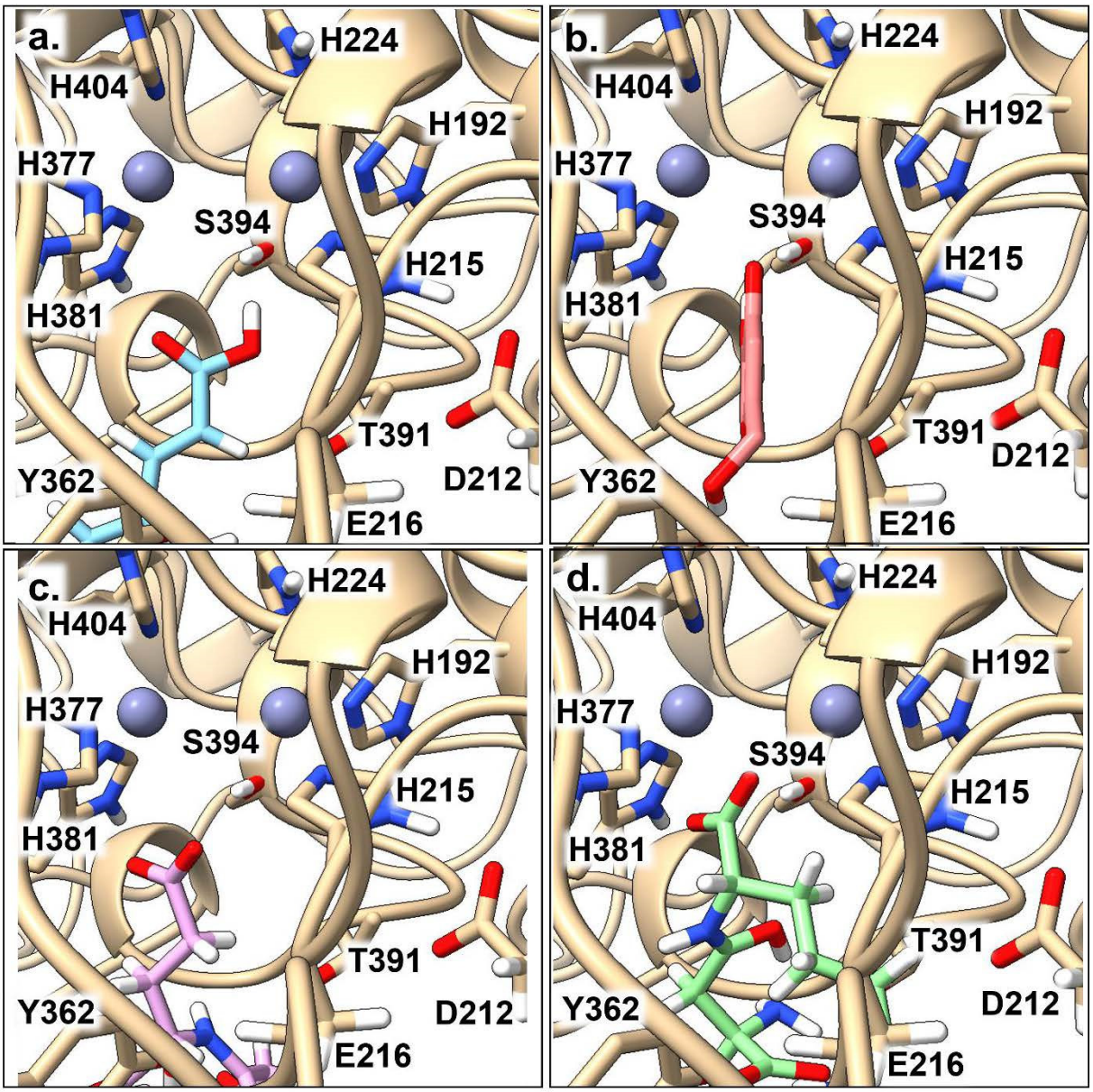

Figure S6. Ribbon representation of the TYRP1 active site with two zinc atoms (blue balls) in complex with (**a**) cinnamic acid, (**b**) kojic acid, (**c**) aspartate-glutamate (lig2), and (**d**) aspartate-lysine (lig4). Key amino acids that create interactions with ligands are labeled in black.

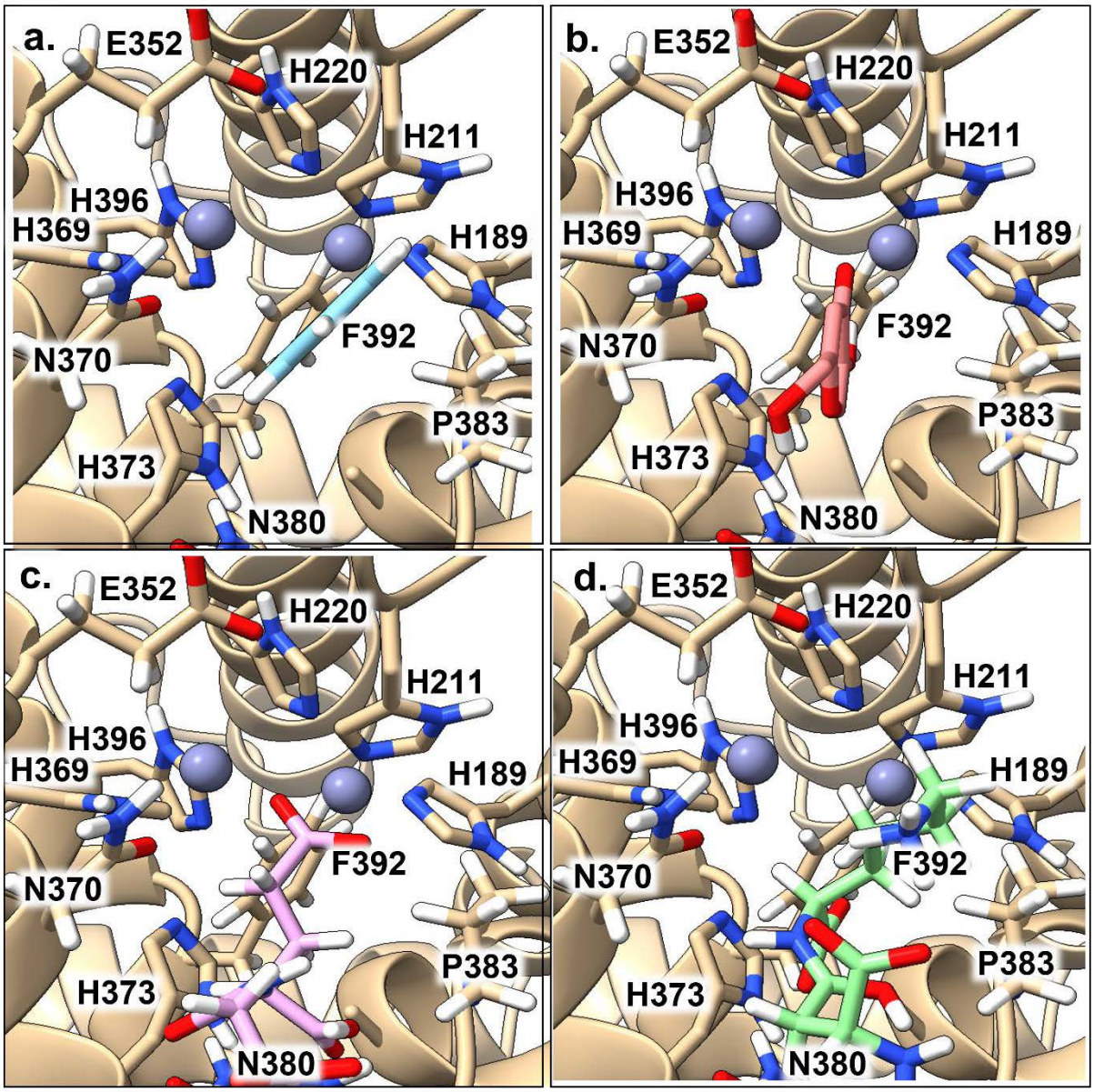

Figure S7. Ribbon representation of the TYRP2 active site with two zinc atoms (blue balls) in complex with (**a**) cinnamic acid, (**b**) kojic acid, (**c**) aspartate-glutamate (lig2), and (**d**) aspartate-lysine (lig4). Key amino acids that create interactions with ligands are labeled in black.