

Supplementary Materials

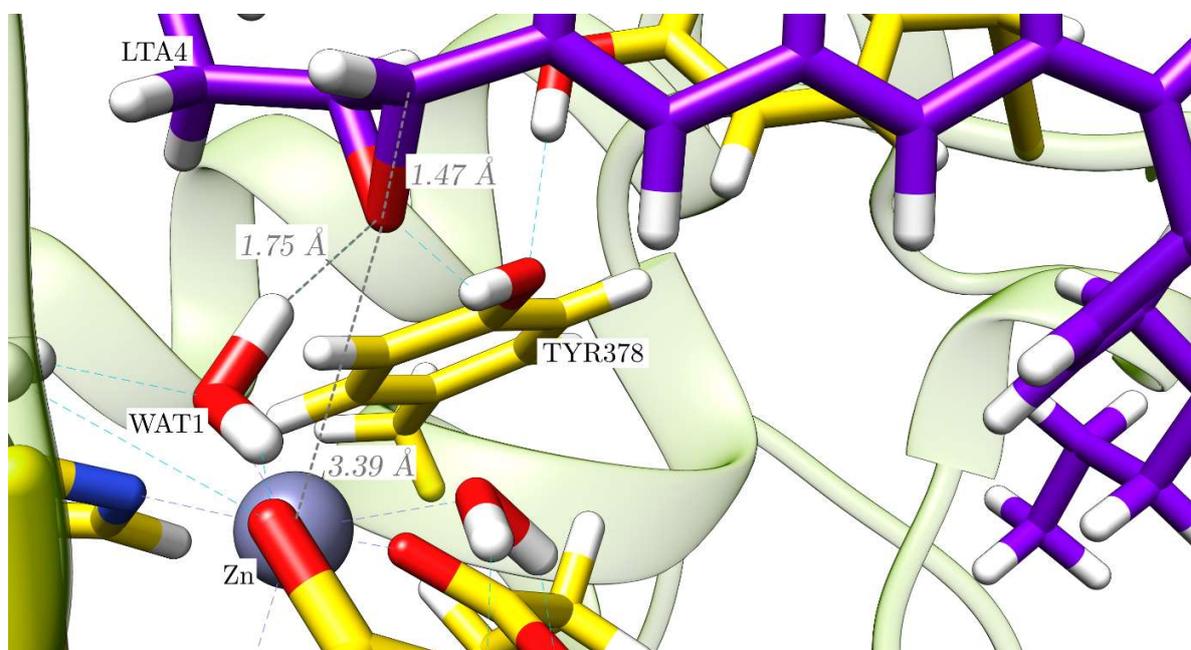
Theoretical Characterization of the Step-By-Step Mechanism of Conversion of Leukotriene A₄ to Leukotriene B₄ Catalysed by the Enzyme Leukotriene A₄ Hydrolase

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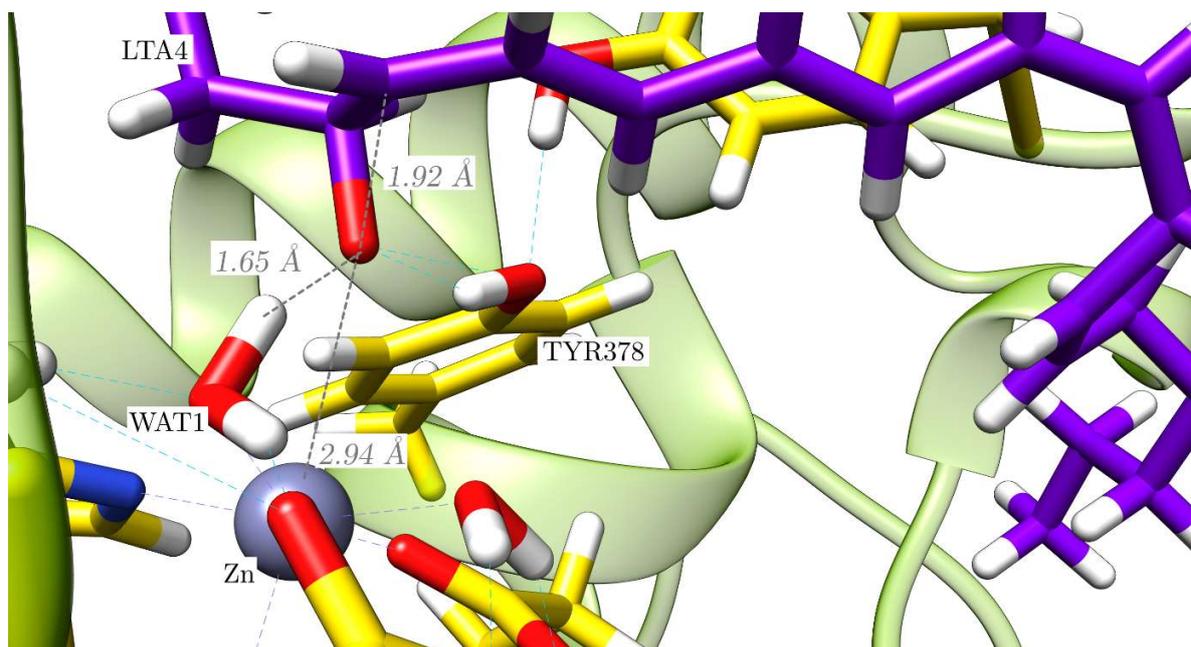
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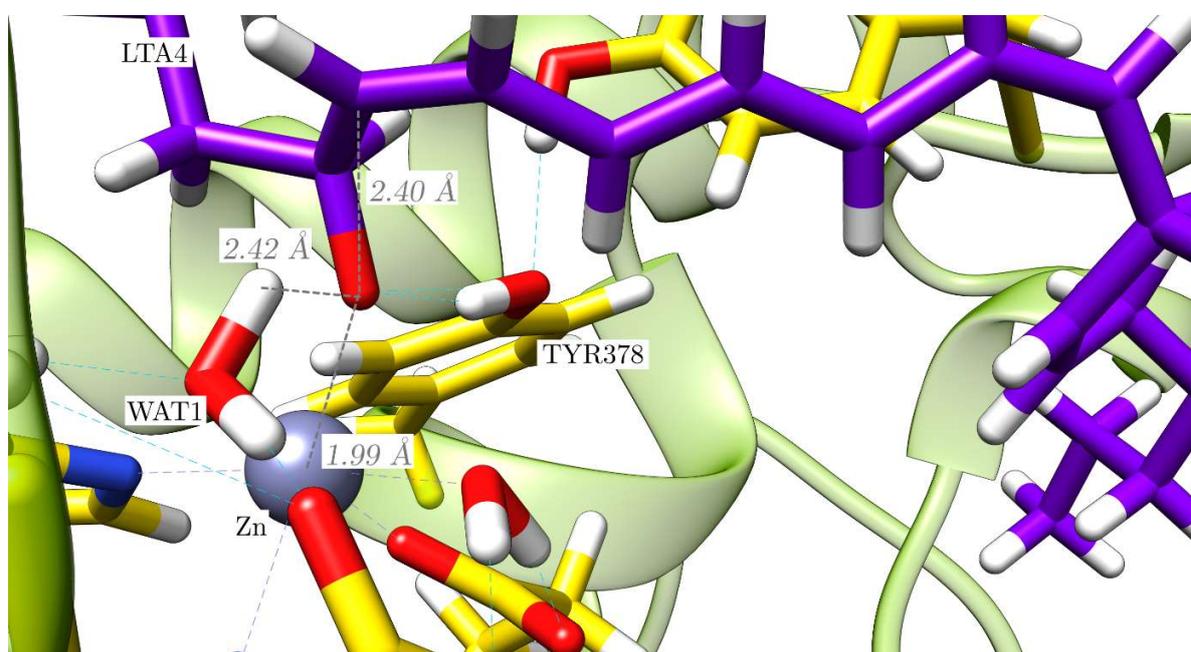
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R

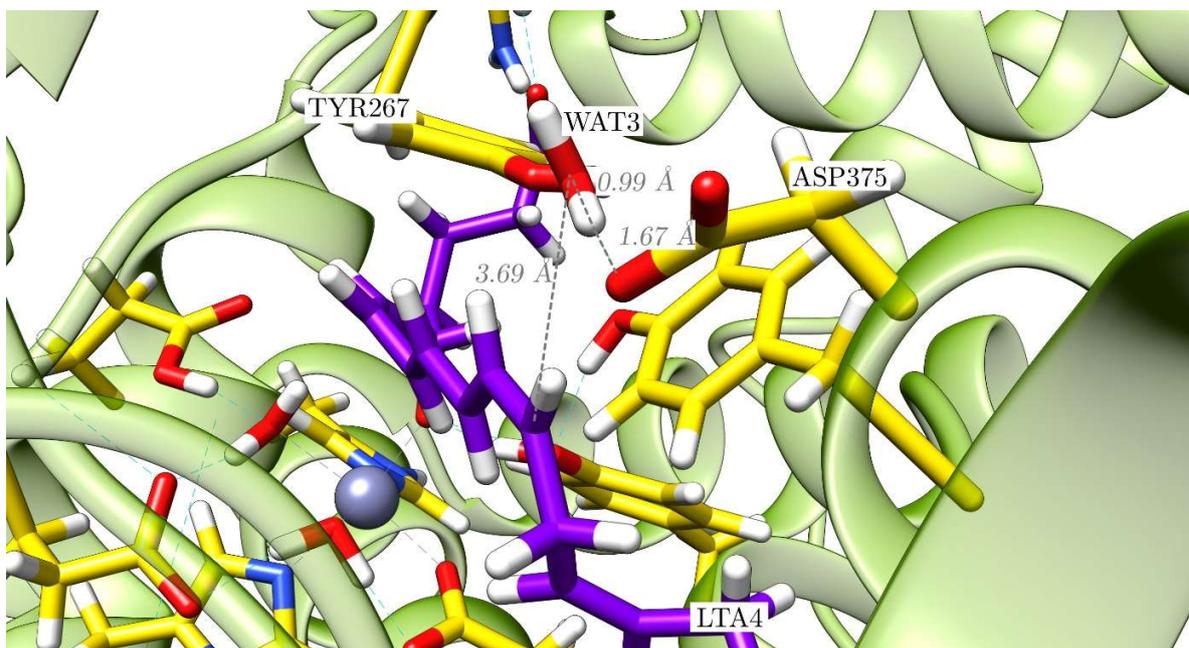


TS1cis

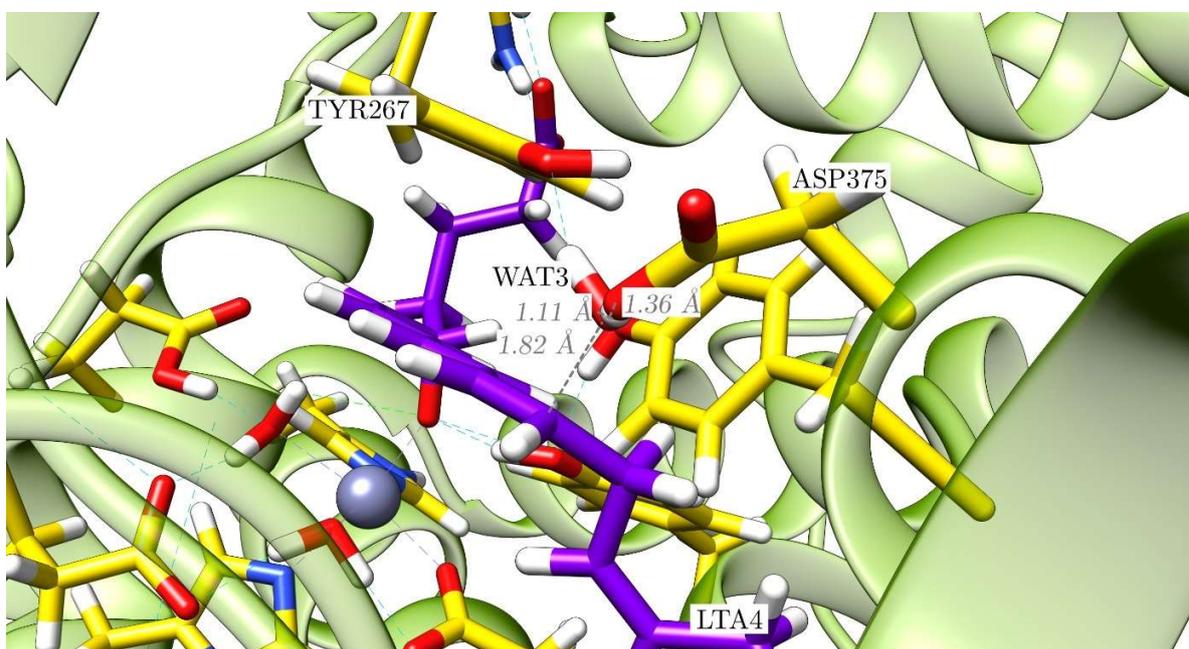


INT1cis

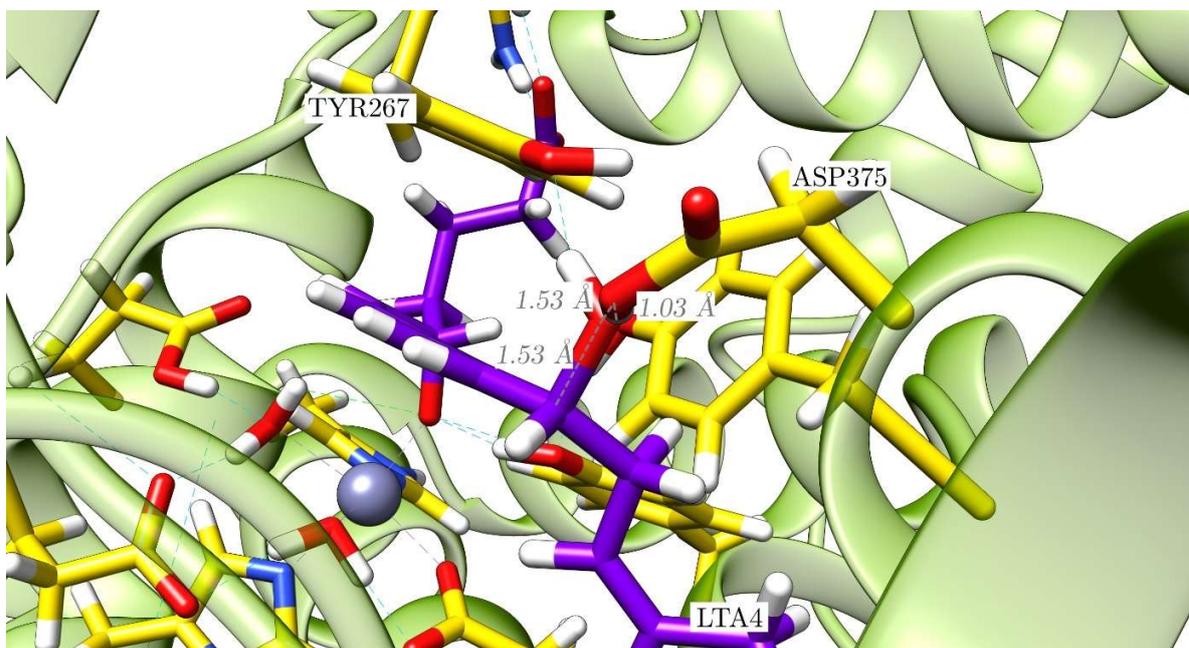
Figure S1. Representation of the stationary structures R, TS1cis and INT1cis focused on the region corresponding to the epoxide ring opening.



INT1cis

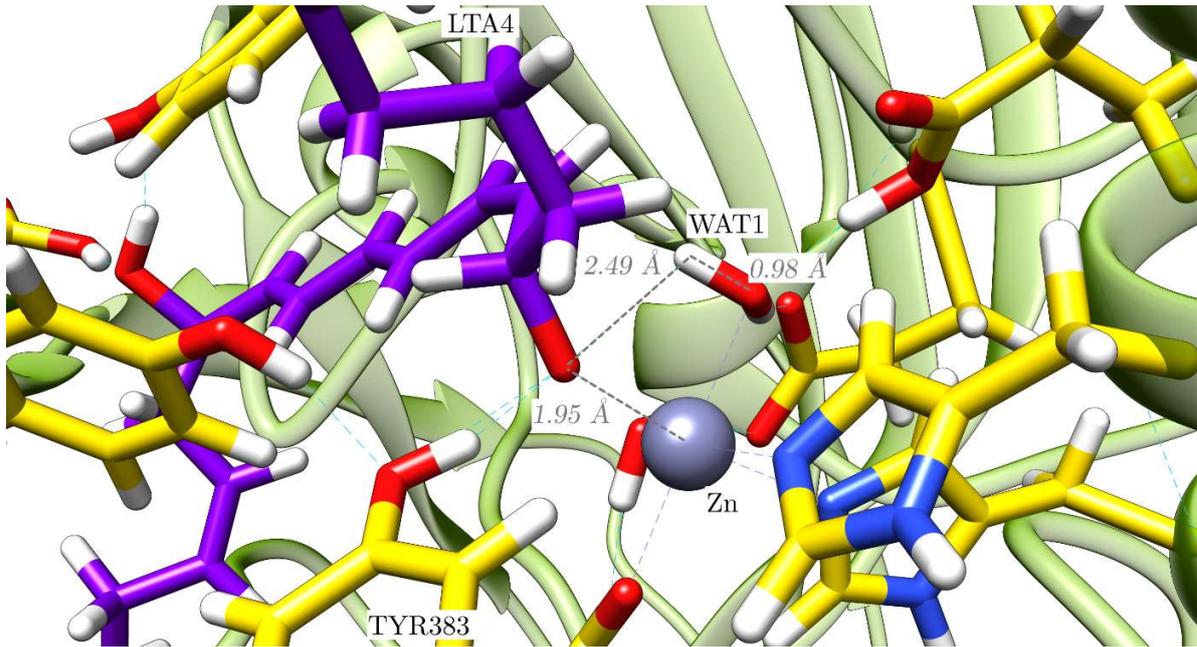


TS2cis

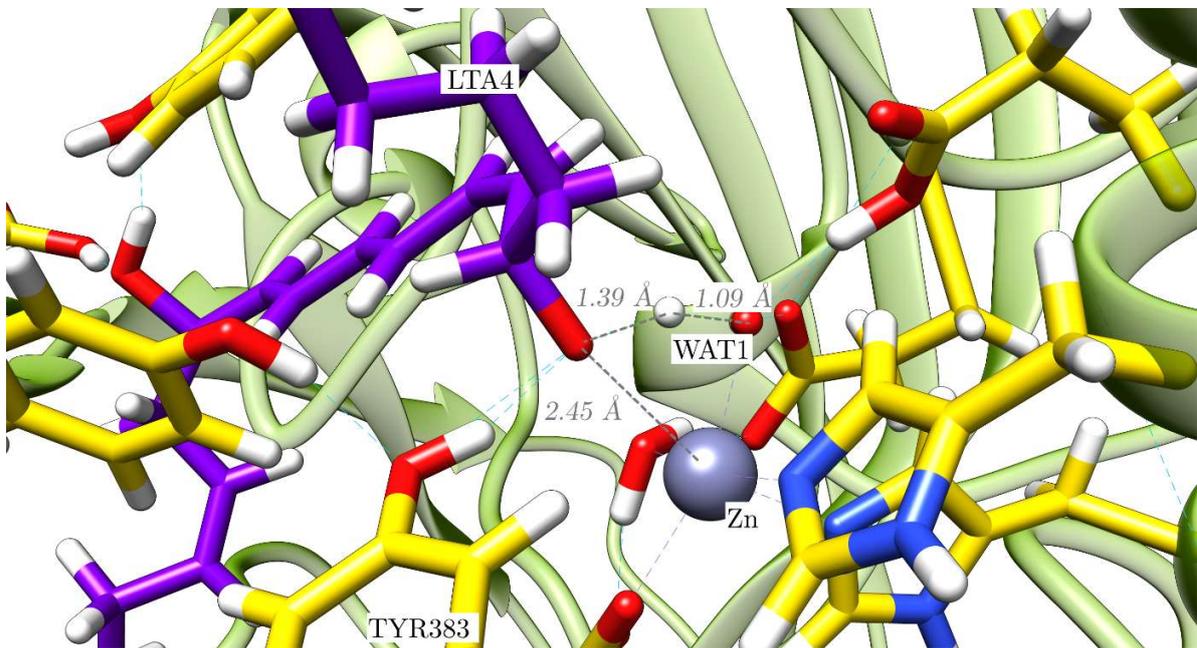


INT2cis

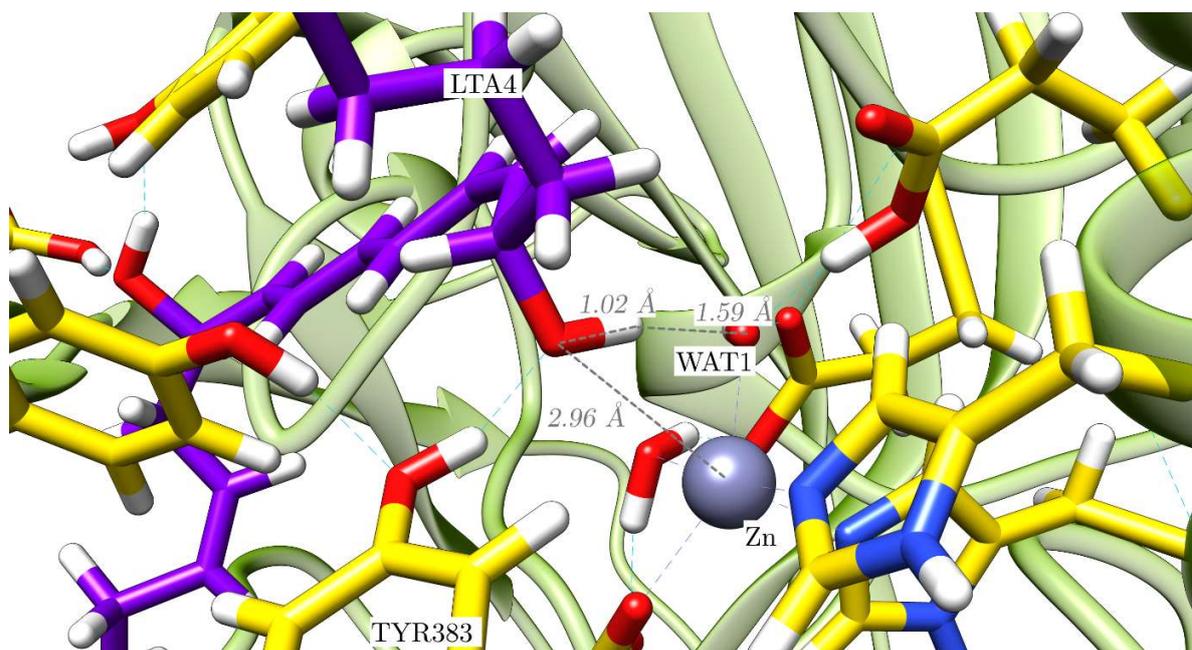
Figure S2. Representation of the stationary structures INT1cis, TS2cis and INT2cis focused on the region corresponding to the addition of WAT3 to C₁₂ of the substrate.



INT2cis

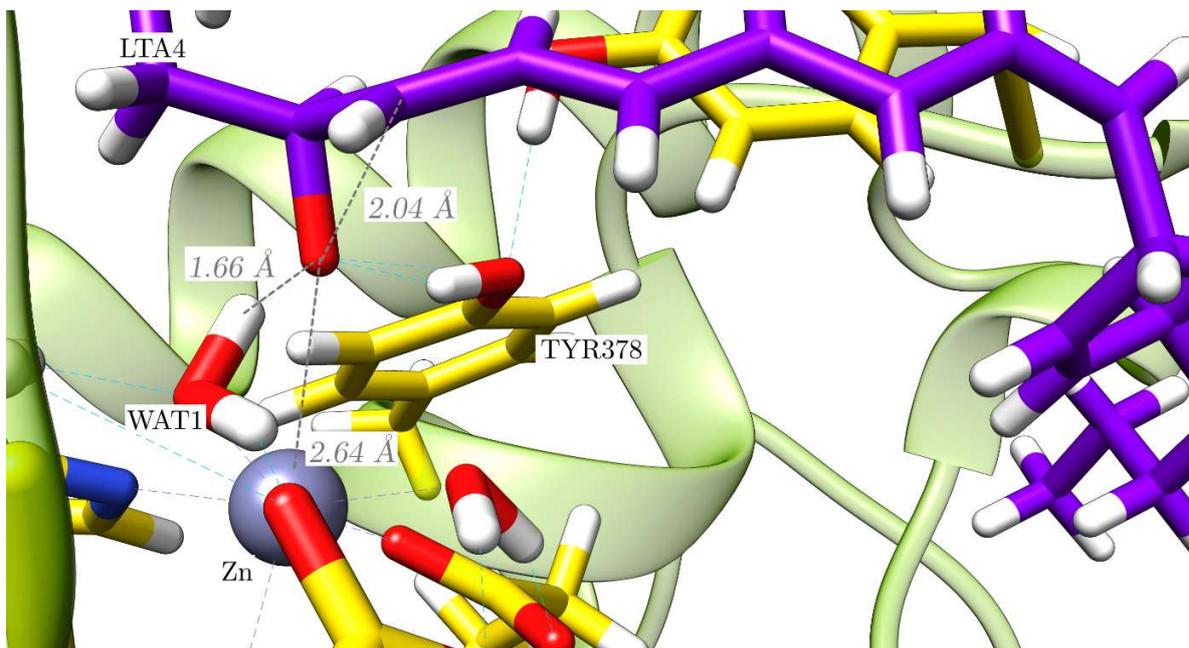


TS3cis

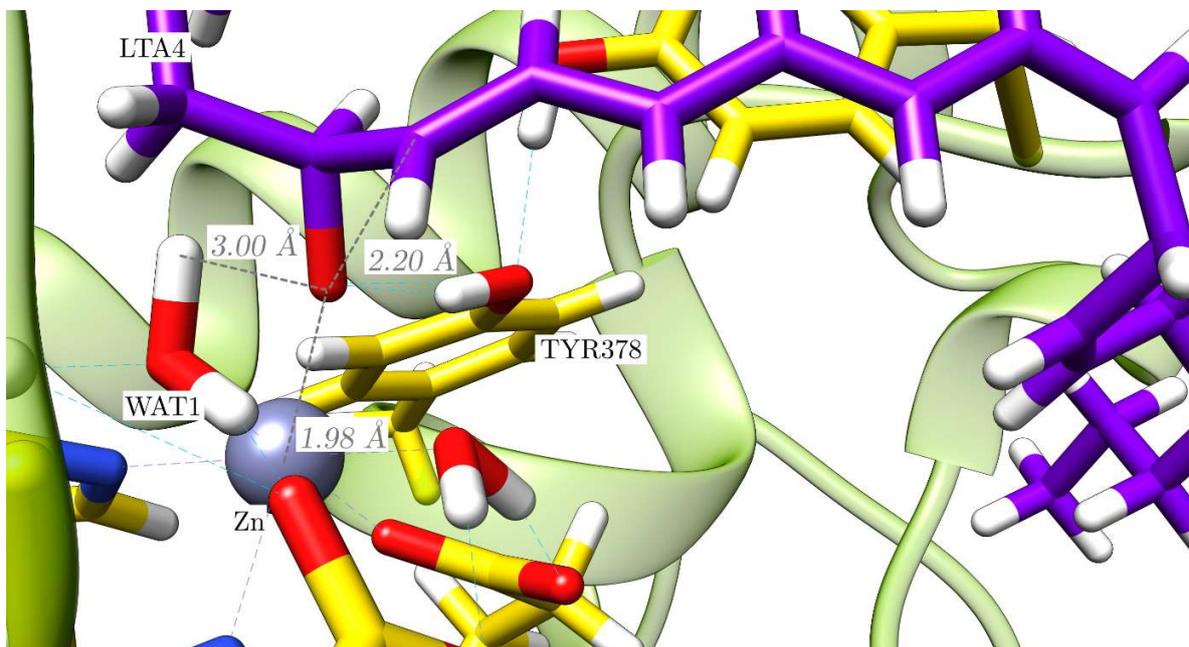


Pcis

Figure S3. Representation of the stationary structures INT2cis, TS3cis and Pcis focused on the region corresponding to the final protonation of the oxygen atom bonded to C₆ (the former oxygen atom of the epoxide).

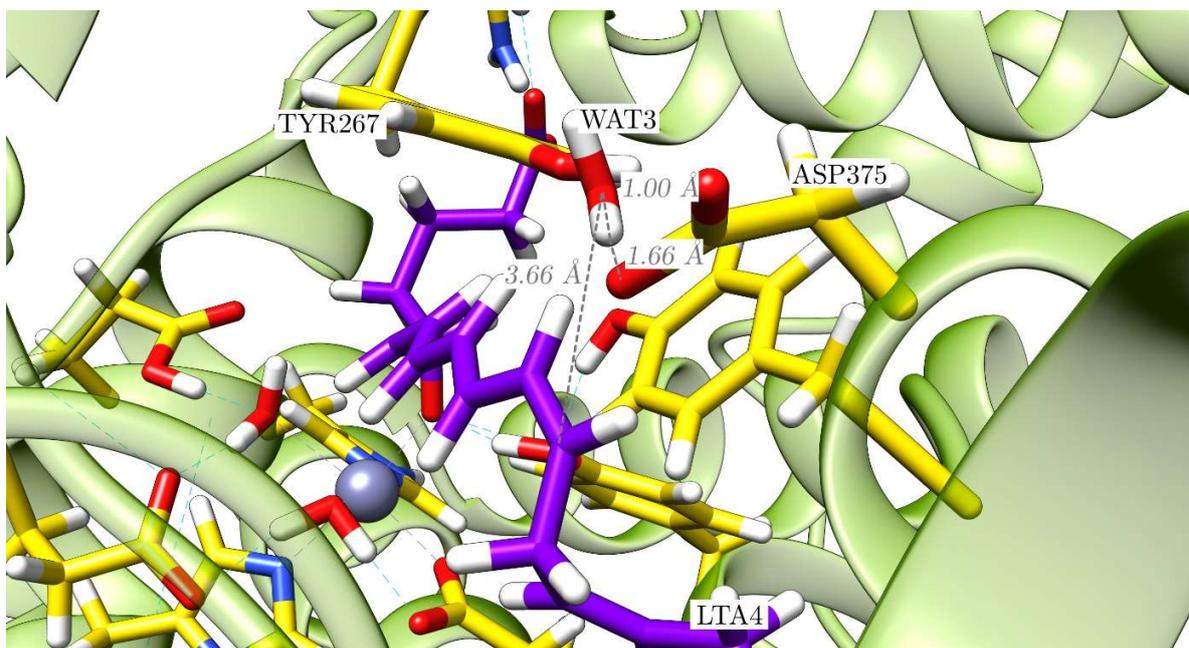


TS1trans

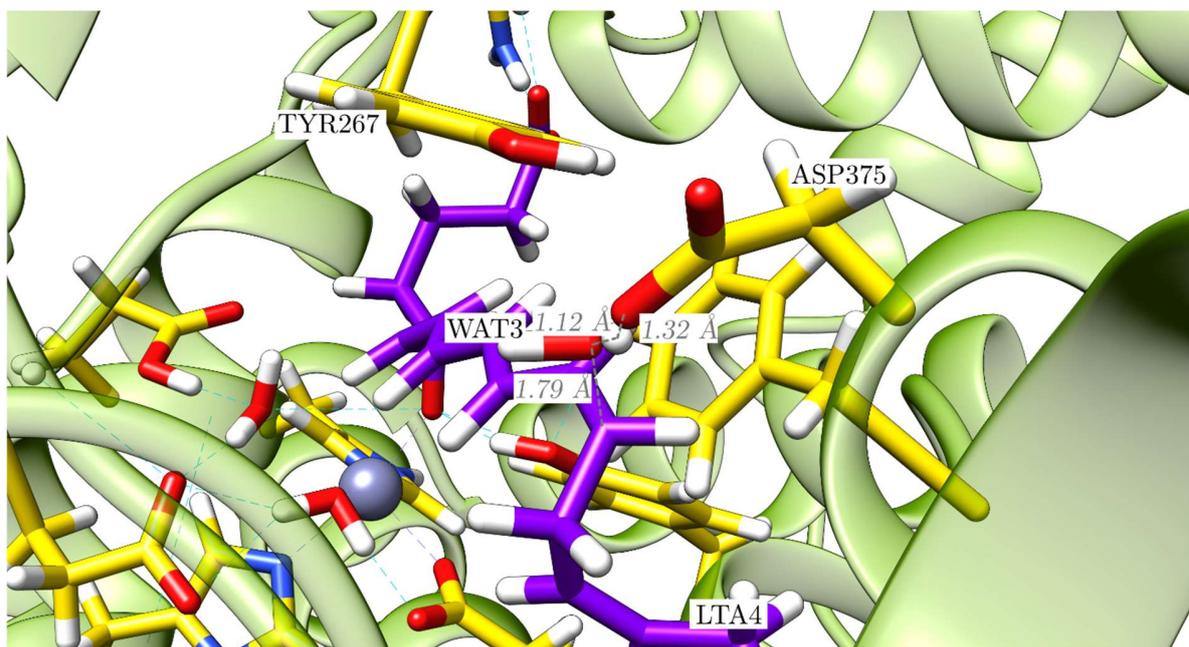


INT1trans

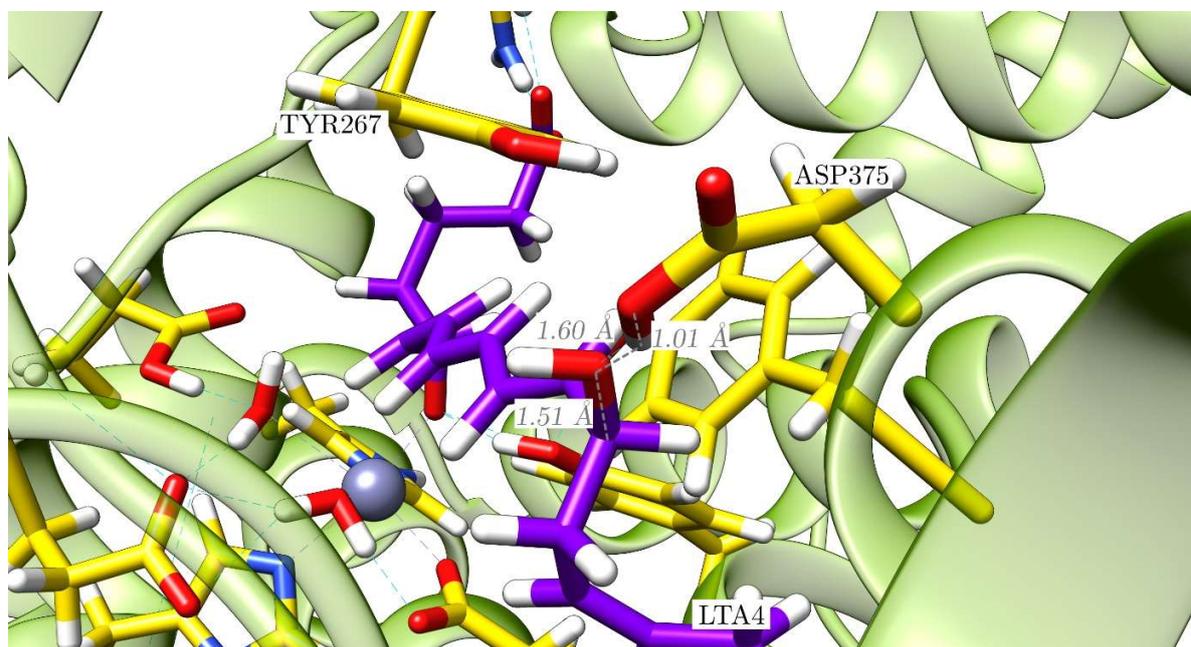
Figure S4. Representation of the stationary structures TS1trans and INT1trans focused on the region corresponding to the epoxide ring opening.



INT1trans

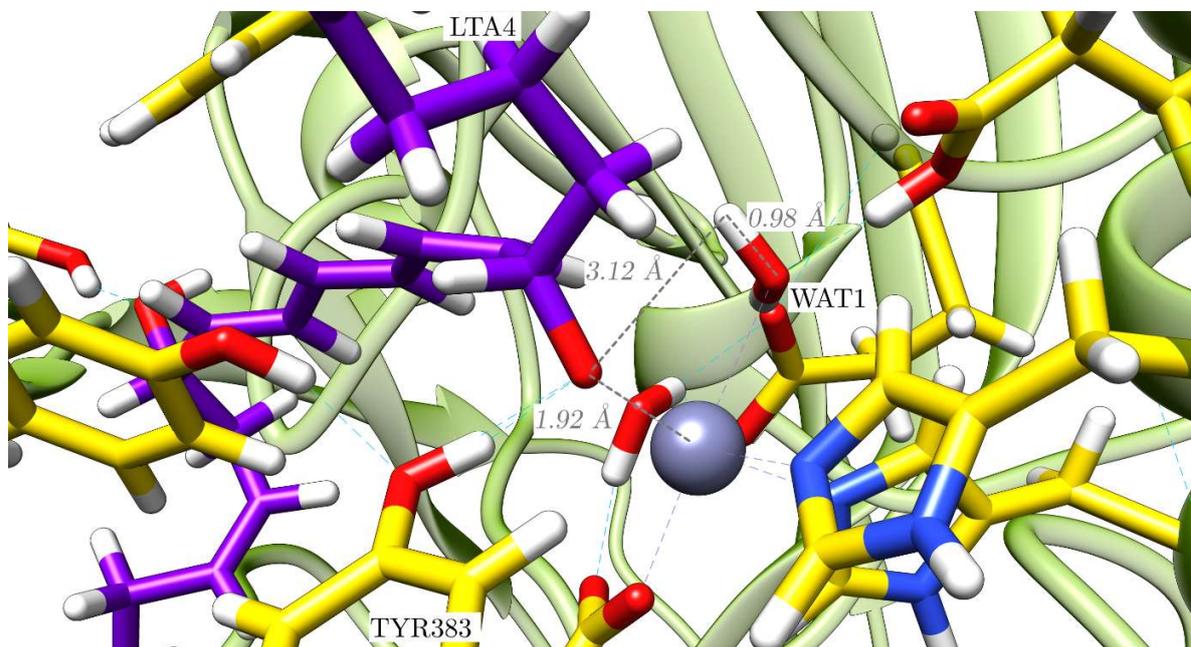


TS2trans

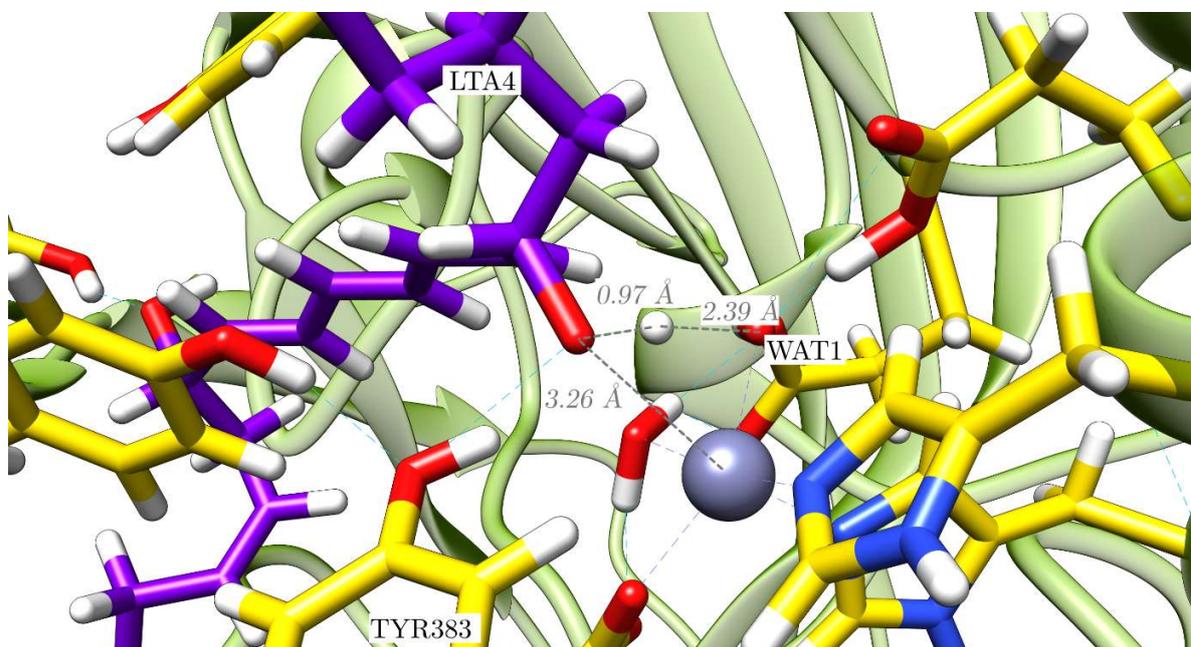


INT2trans

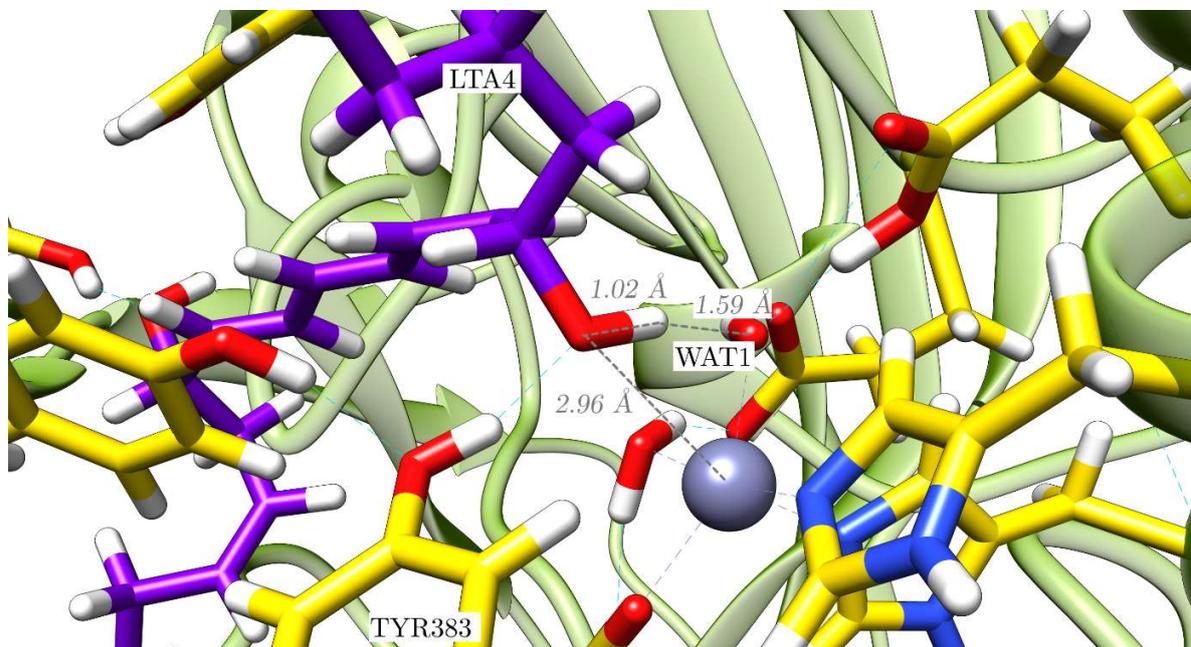
Figure S5. Representation of the stationary structures INT1trans, TS2trans and INT2trans focused on the region corresponding to the addition of WAT3 to C₁₂ of the substrate.



INT2trans



TS3trans



Ptrans

Figure S6. Representation of the stationary structures INT2trans, TS3trans and Ptrans focused on the region corresponding to the final protonation of the oxygen atom bonded to C₆ (the former oxygen atom of the epoxide).