

The Effects of the Fungicide Myclobutanil on Soil Enzyme Activity

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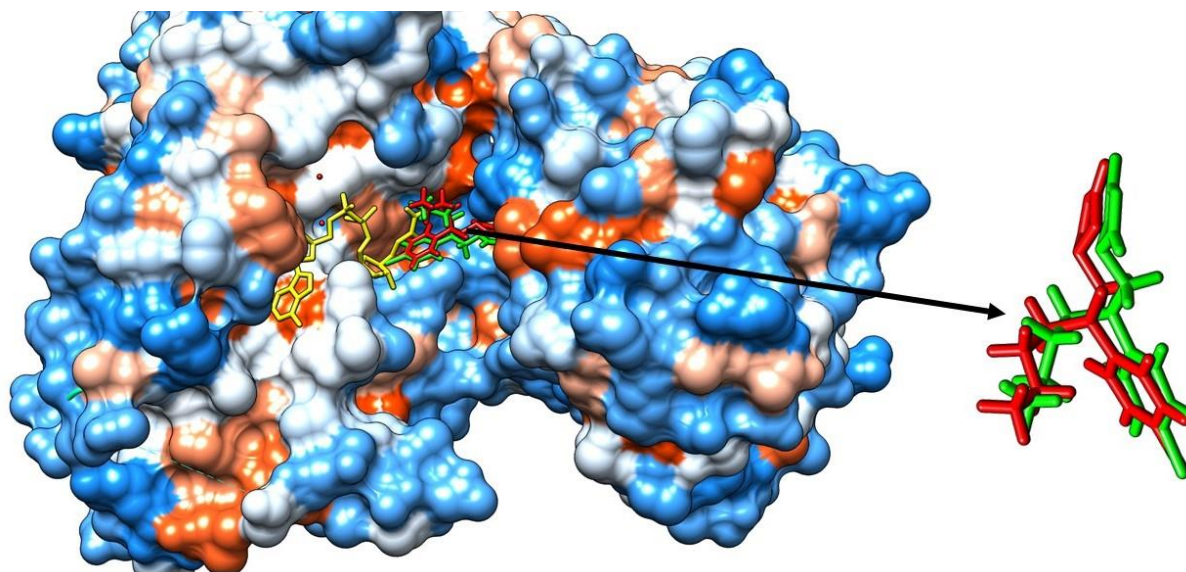


Figure S1. Binding of (*R*)-myclobutanil (red sticks) and of (*S*)-myclobutanil (green sticks) to the active site of *Aspergillus fumigatus* dehydrogenase (PDB ID 7RK5) (solid hydrophobicity surface, blue regions are hydrophilic and orange regions are hydrophobic). The substrate 1,4-dihydronicotinamide adenine dinucleotide (yellow sticks) illustrates the position of the active site.

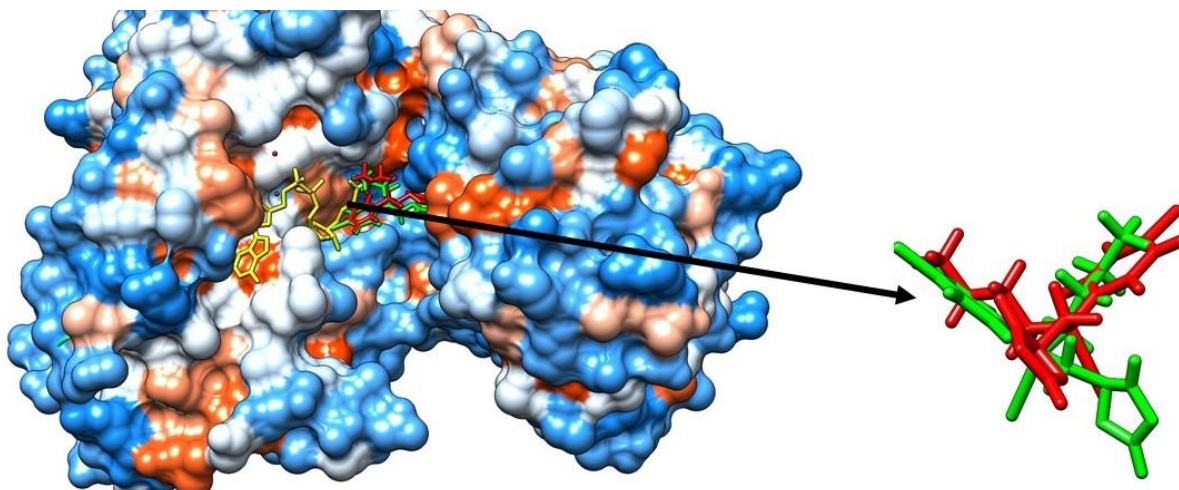


Figure S2. Binding of (*R*)-myclobutanil (red sticks) and of (*S*)-myclobutanil (green sticks) to the active site of *Rhizobium leguminosarum* dehydrogenase (PDB ID 8C54) (solid hydrophobicity surface, blue regions are hydrophilic and orange regions are hydrophobic). The substrate 1,4-dihydronicotinamide adenine dinucleotide (yellow sticks) illustrates the position of the active site.

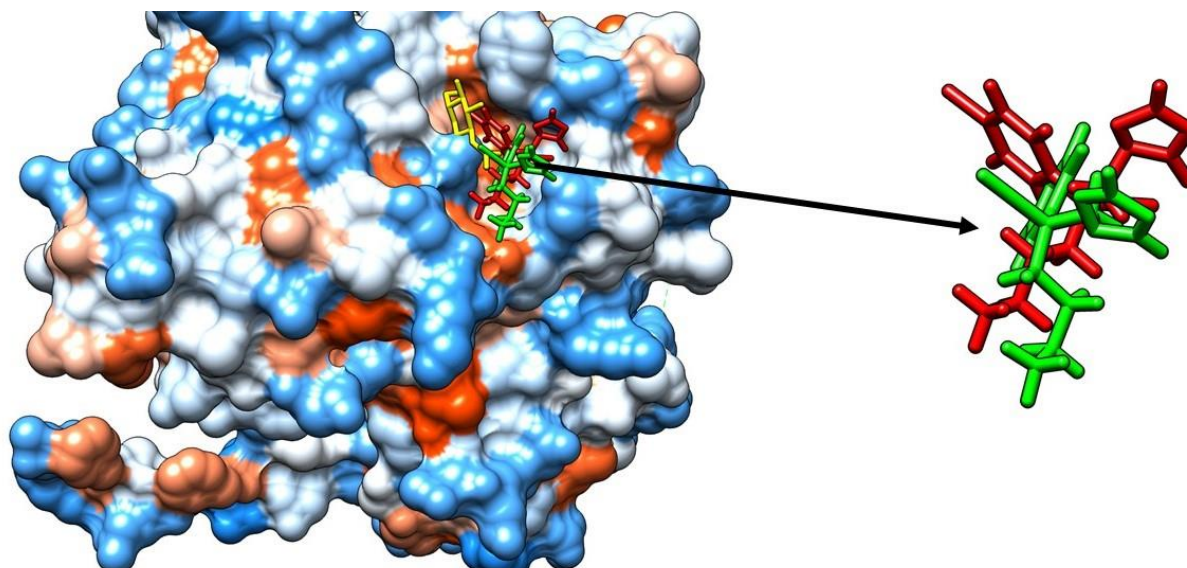


Figure S3. Binding of (*R*)-myclobutanil (red sticks) and of (*S*)-myclobutanil (green sticks) to the active site of *Aspergillus niger* phosphatase (PDB ID 1QFX) (solid hydrophobicity surface, blue regions are hydrophilic and orange regions are hydrophobic). The substrate 2-acetamido-2-deoxy-beta-D-glucopyranose (yellow sticks) illustrates the position of the active site.

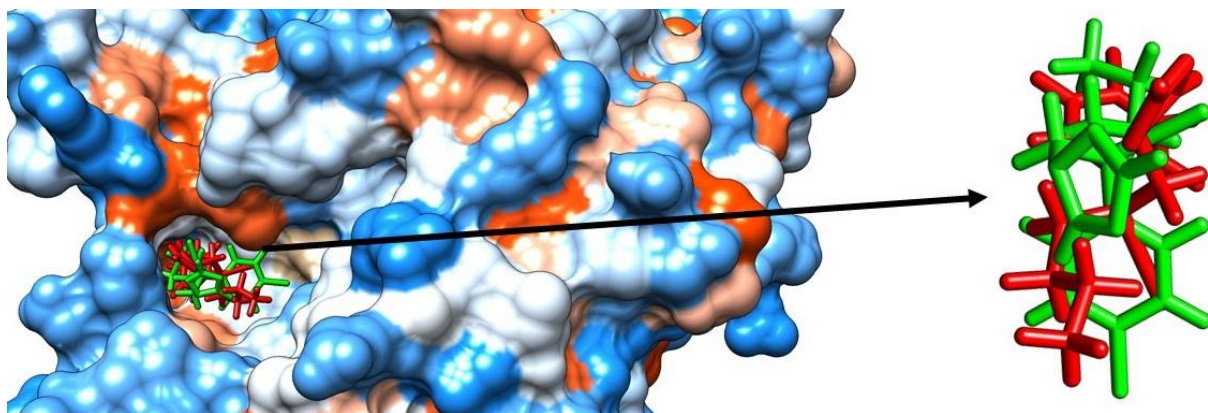


Figure S4. Binding of (*R*)-myclobutanil (red sticks) and of (*S*)-myclobutanil (green sticks) to the active site of *Rhizobium leguminosarum* phosphatase (PDB ID 2VQR) (solid hydrophobicity surface, blue regions are hydrophilic and orange regions are hydrophobic). The active site was found taking into consideration the position of the Ca^{2+} and Mn^{2+} ions (not shown).

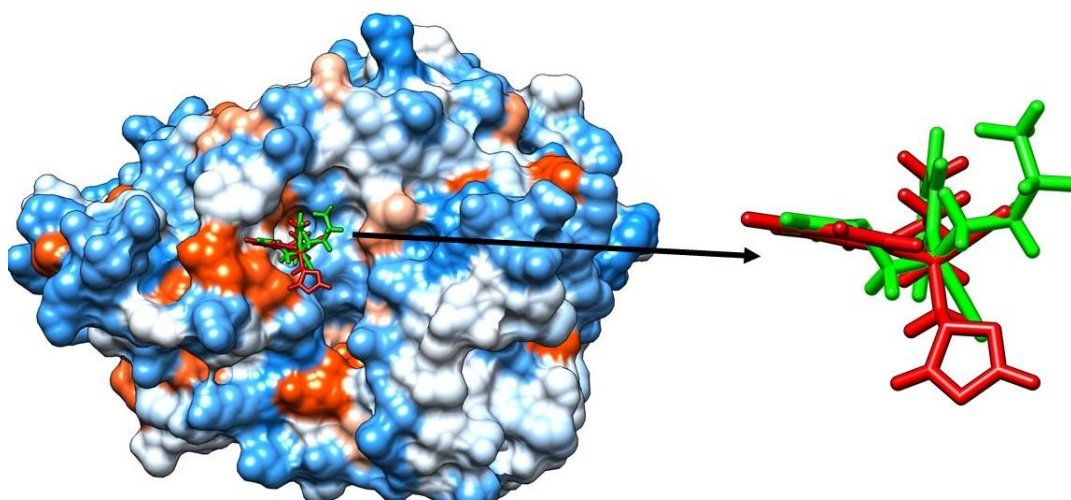


Figure S5. Binding of (*R*)-myclobutanil (red sticks) and of (*S*)-myclobutanil (green sticks) to the active site of *Aspergillus clavatus* protease (PDB ID 7Z6T) (solid hydrophobicity surface, blue regions are hydrophilic and orange regions are hydrophobic). The active site was found taking into consideration the position of the Ca^{2+} and Zn^{2+} ions (not shown).

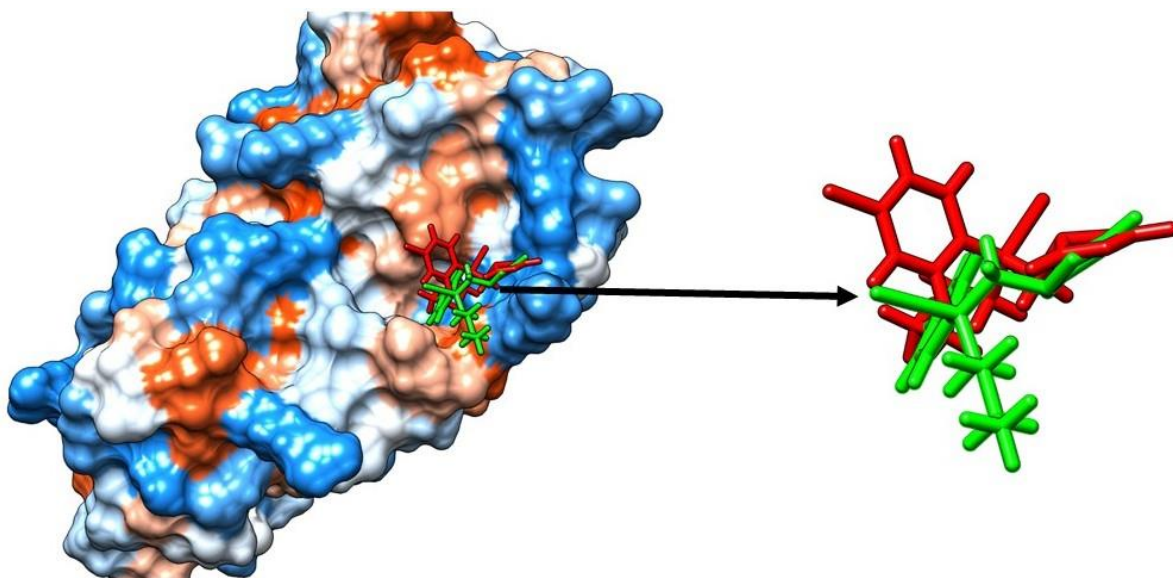


Figure S6. Best binding modes of (*R*)-myclobutanil (red sticks) and of (*S*)-myclobutanil (green sticks) to the active site of *Rhizobium leguminosarum* protease (AF-A0A0Q7ALB8-F1) (solid hydrophobicity surface, blue regions are hydrophilic and orange regions are hydrophobic).

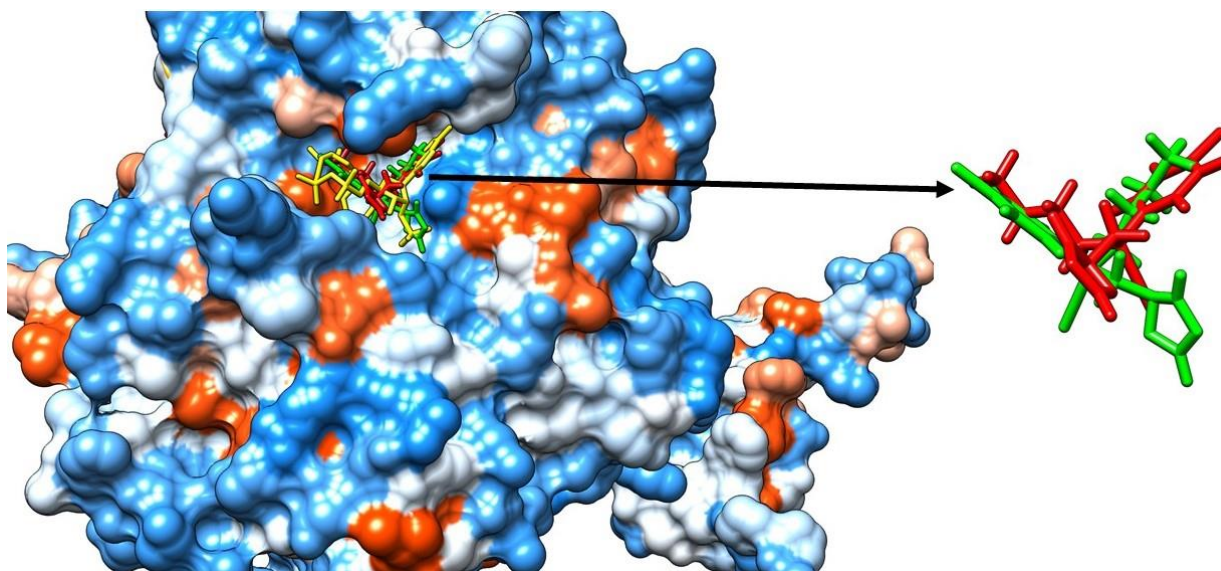


Figure S7. Binding of (*R*)-myclobutanil (red sticks) and of (*S*)-myclobutanil (green sticks) to the active site of *Komagataella pastoris* catalase (solid hydrophobicity surface, blue regions are hydrophilic and orange regions are hydrophobic). The substrate dihydropyridine-nicotinamide-adenine dinucleotide phosphate (yellow sticks) illustrates the position of the active site.

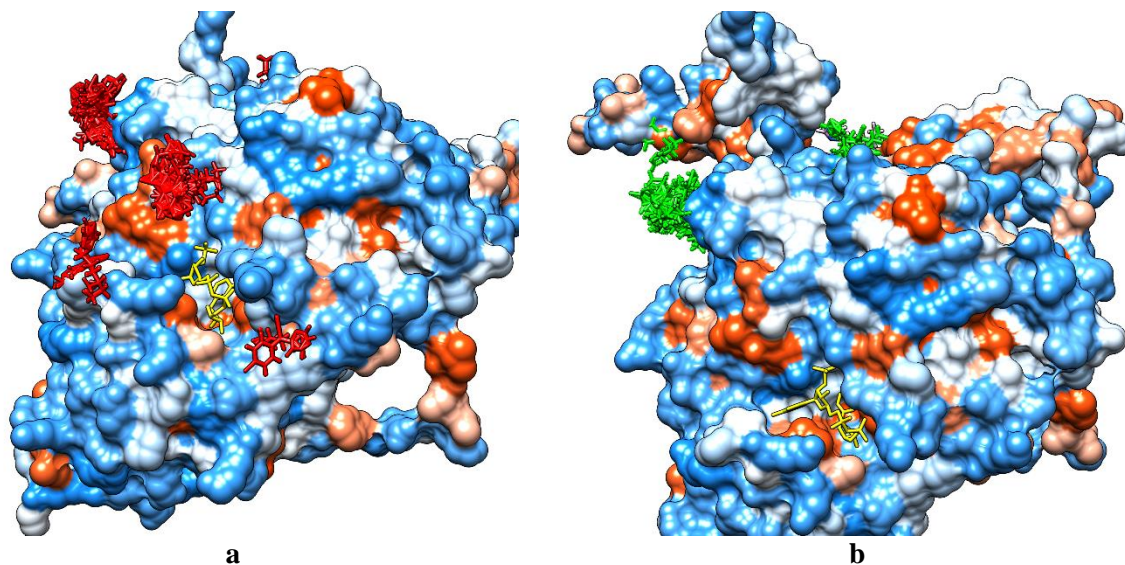


Figure S8. Binding of (*R*)-myclobutanil (red sticks) (a) and of (*S*)-myclobutanil (green sticks) (b) to site of *Rhizobium meliloti* catalase (solid hydrophobicity surface, blue regions are hydrophilic and orange regions are hydrophobic). The position substrate dihydronicotinamide-adenine dinucleotide phosphate (yellow sticks) illustrates the active site by superposing the structures of *Rhizobium meliloti* and *Komagataella pastoris* catalases.

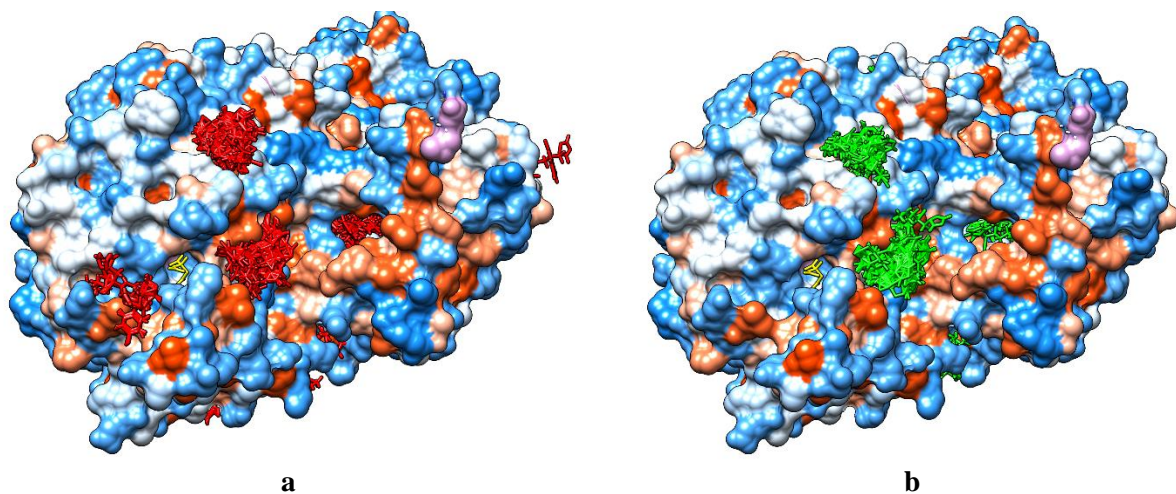


Figure S9. Binding of (*R*)-myclobutanil (red sticks) (a) and of (*S*)-myclobutanil (green sticks) (b) to *Aspergillus fumigatus* (AF-Q6A3P9-F1) urease (solid hydrophobicity surface, blue regions are hydrophilic and orange regions are hydrophobic). The myclobutanil enantiomers do not bind to the active site, those position is illustrated by the citrate ion (yellow sticks).

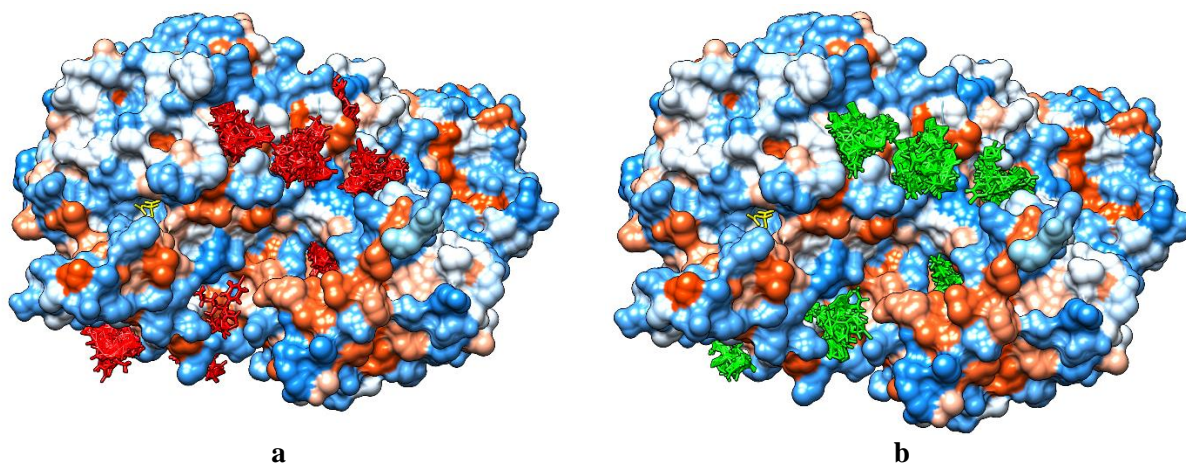


Figure S10. Binding of (*R*)-myclobutanil (red sticks) (a) and of (*S*)-myclobutanil (green sticks) (b) to *Rhizobium leguminosarum* (AF-Q1MCV9-F1, solid hydrophobicity surface, blue regions are hydrophilic and orange regions are hydrophobic). The myclobutanil enantiomers do not bind to the active site, those position is illustrated by the citrate ion (yellow sticks).