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THE EFFECTS OF TRIAZOLE FUNGICIDES ON COMMON DUCKWEED ENZYMES. A MOLECULAR DOCKING APPROACH

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Abstract: Triazole fungicides are applied to various crops for the treatment of fungal diseases. This enables these fungicides to reach the aquatic environment, being able to exert ecotoxic effects on the present aquatic organisms. The aquatic macrophyte, *Lemna minor*, also known as the common duckweed, is such an organism. It can interact with triazole fungicides by uptake, which can thus exert various effects on some plant enzymes at a molecular level. For the assessment of these potential effects, three model protein sequences with available 3D structures were considered in this study: ribulose-1,5-bisphosphate carboxylase/oxygenase (RuBisCo), glutathione peroxidase (GPX) and glutathione S-transferase (GST). Flutriafol, metconazole, myclobutanil, tebuconazole, tetraconazole and triticonazole were the studied fungicides, their effects on the selected enzymes being studied through molecular docking using SwissDock program. Results showed that not all six fungicides bound in the active site of all three protein sequences. GST was the only enzyme in the active site of which all six studied fungicides could bind. Regarding GPX, only the fungicides flutriafol, myclobutanil and tetraconazole could bind in the active site, while in the case of RuBisCo, only tetraconazole could bind in the active site of this enzyme. Tetraconazole was the only studied triazole fungicide that could bind in the active site of all three assessed enzymes. The studied triazole fungicides can thus influence the interaction of the respective enzymes with their specific substrates, potentially leading to the inhibition of their enzymatic activity. Experimental studies are to be carried out to confirm/deny the predictions of the modeling made in this study.

• Introduction

Triazole fungicides may reach the **aquatic environment** as they are used on plants to treat fungal diseases. This allows these fungicides to exert potential **ecotoxicological effects** on aquatic organisms present.

One such organism is *Lemna minor*, an aquatic macrophyte. This plant **takes up triazole fungicides** from the aquatic environment, allowing them to exert various **effects at the molecular level on plant enzymes**.

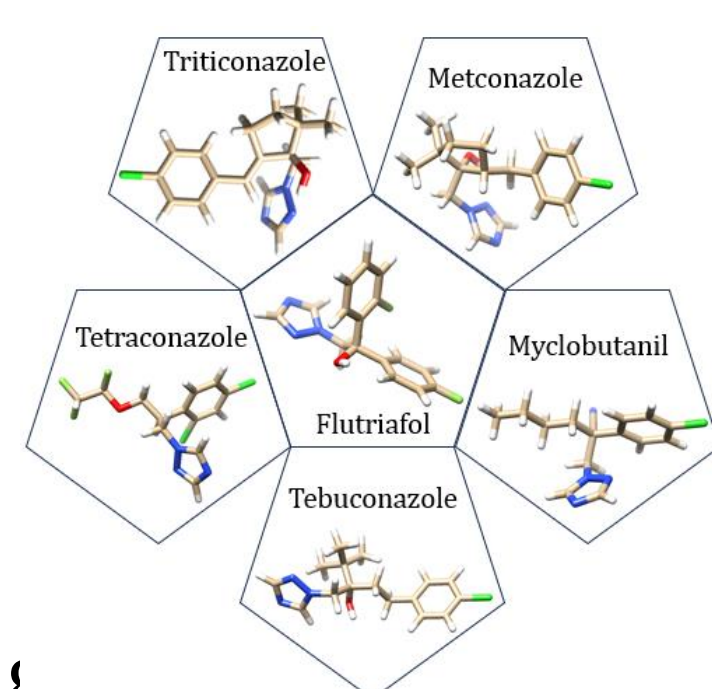
• Material and method

Three **model protein** sequences with available 3D structures were considered in this study:

- Ribulose-1,5-bisphosphate carboxylase/oxygenase (RuBisCo)
- Glutathione peroxidase (GPX)
- Glutathione S-transferase (GST)

The effect of **six triazole fungicides** on the enzymes of interest was investigated:

- Flutriafol
- Metconazole
- Myclobutanil
- Tebuconazole
- Tetraconazole
- Triticonazole



The effect of the selected fungicides on the enzymes of interest was studied by **molecular docking** performed with **SwissDock** software.

• Conclusions

Not all six fungicides bound in the active site of all three protein sequences.

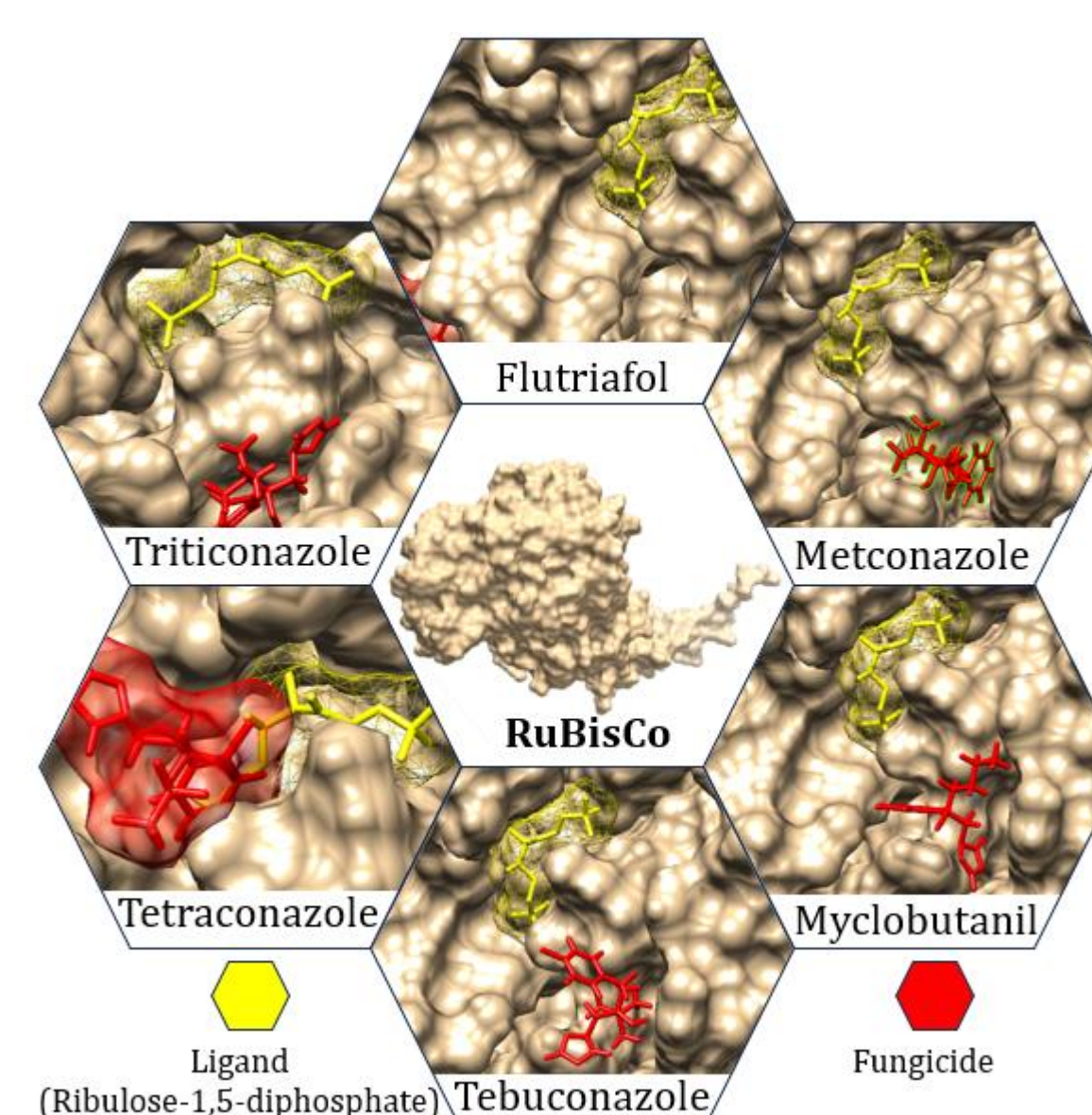
All analyzed fungicides can bind in the active site of only **glutathione transferase**.

Tetraconazole was the only studied triazole fungicide that could bind in the active site of all three assessed enzymes.

The studied triazole fungicides can influence the interaction of the respective enzymes with their specific substrates, potentially leading to the inhibition of their enzymatic activity.

Experimental studies are to be carried out to confirm/deny the predictions of the modeling made in this study.

• Results and discussions

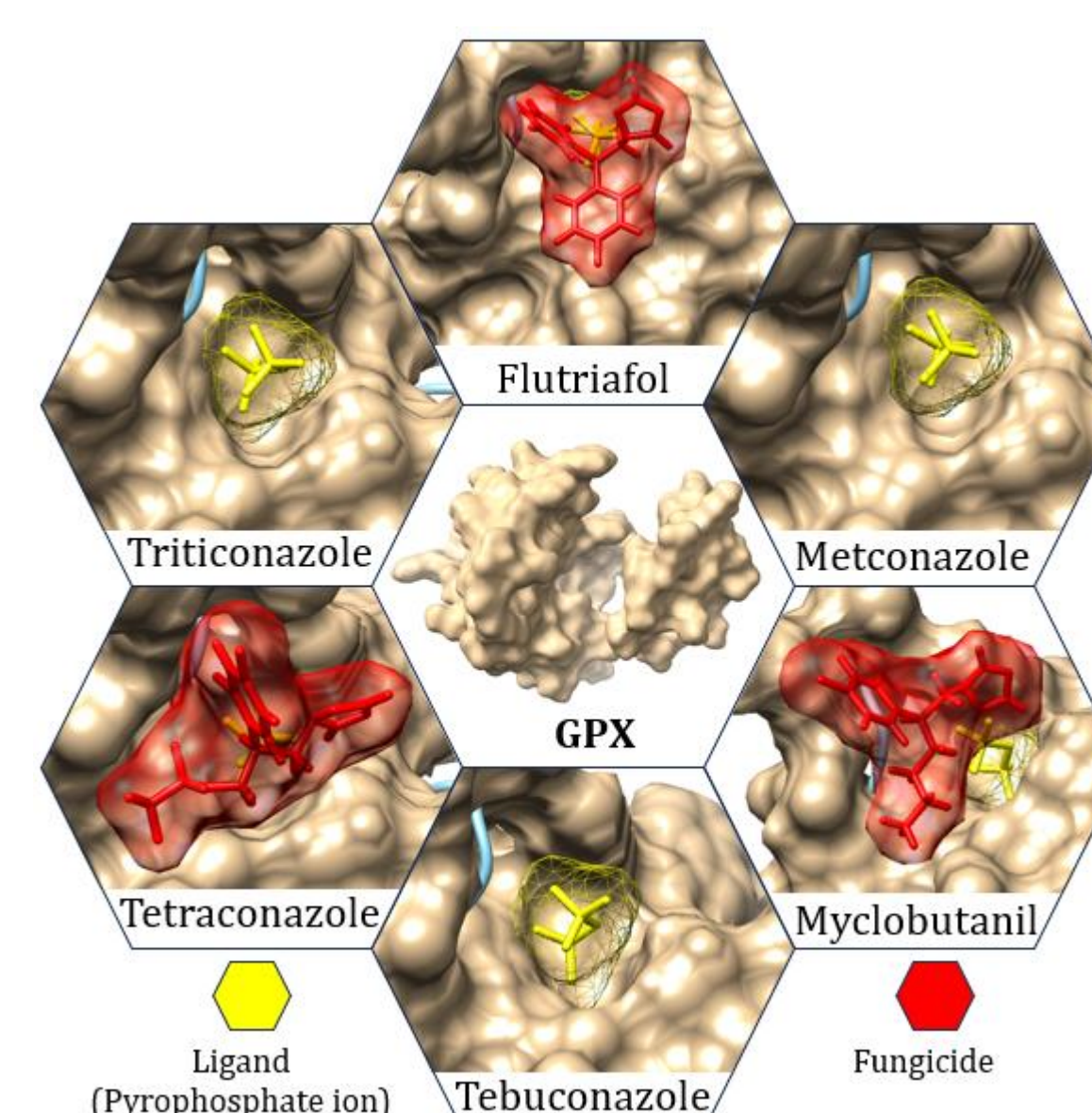


Only tetraconazole could bind in the active site of RuBisCo (Figure 1).

Figure 1. Molecular docking results for RuBisCo and the six analyzed triazole fungicides.

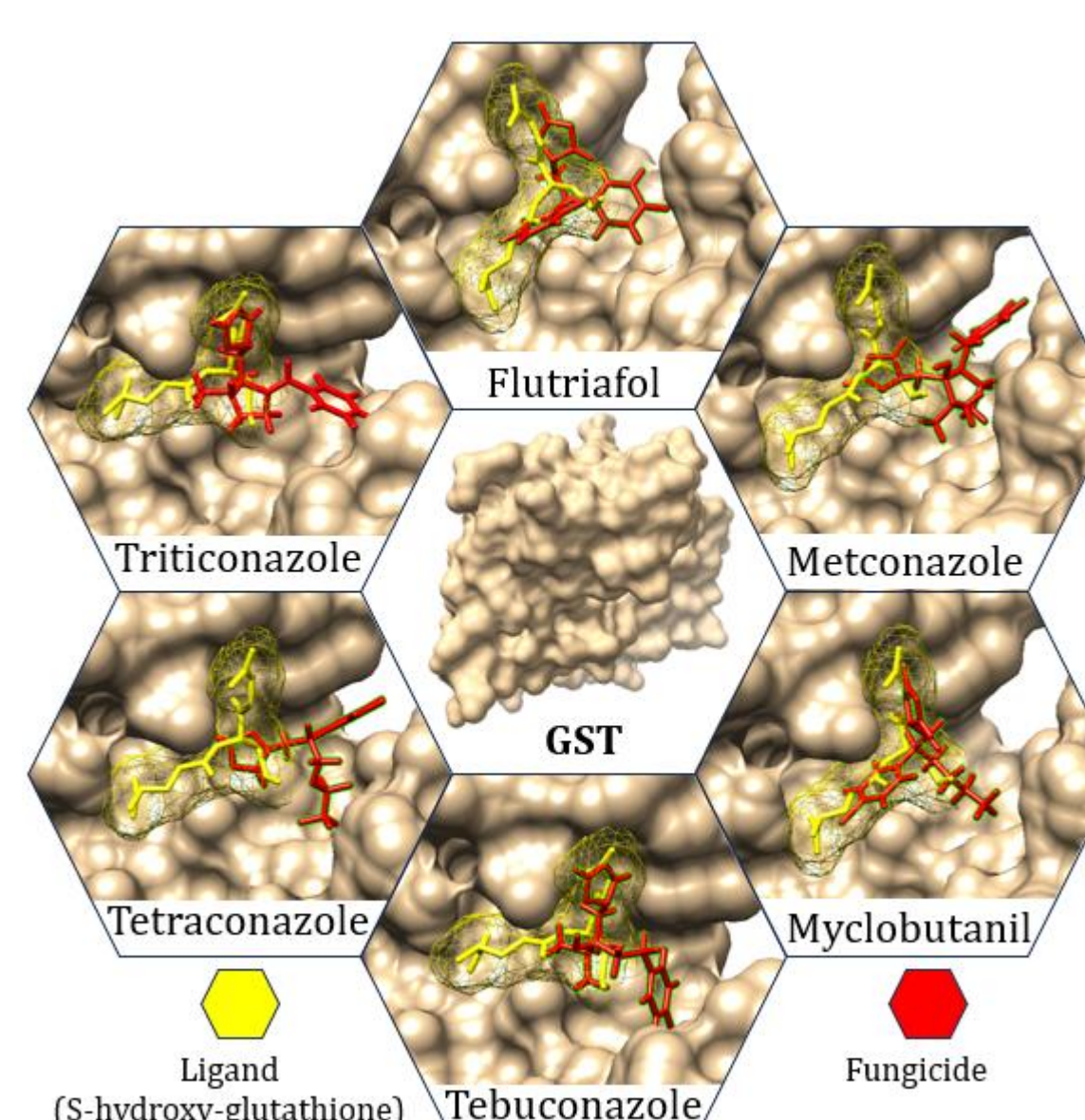
Only flutriafol, myclobutanil and tetraconazole could bind in the active site of GPX (Figure 2).

Figure 2. Molecular docking results for GPX and the six analyzed triazole fungicides.



All six fungicides could bind in the active site of GST (Figure 3).

Figure 3. Molecular docking results for GST and the six analyzed triazole fungicides.



• Acknowledgement

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