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INTEGRATED *IN VITRO* AND *IN SILICO* APPROACHES FOR THE ECOTOXICOLOGICAL ASSESSMENT OF FUNGICIDES: A CASE STUDY ON DIFENOCONAZOLE, PROTHIOCONAZOLE, AND MEFENTRIFLUCONAZOLE

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• Introduction

Triazole fungicides may pose environmental risks to aquatic ecosystems, highlighting the need for integrated approaches that combine experimental ecotoxicity assessments with computational predictions.

• Material and method

The proposed approach combines OECD 221 growth inhibition testing of difenoconazole, prothioconazole, and mefentrifluconazole on *Lemna minor* with morphometric and biochemical analyses, complemented by physicochemical and toxicological information retrieved from PPDB and PubChem and *in silico* toxicity predictions obtained using ADMETlab 3.0 and admetSAR 3.0.

• Results and discussions

The proposed approach enables the characterization of concentration-dependent phytotoxic effects, physiological and biochemical responses, and predicted toxicity profiles, supporting the identification of potential biological effects and risks to non-target organisms (Figure 1).

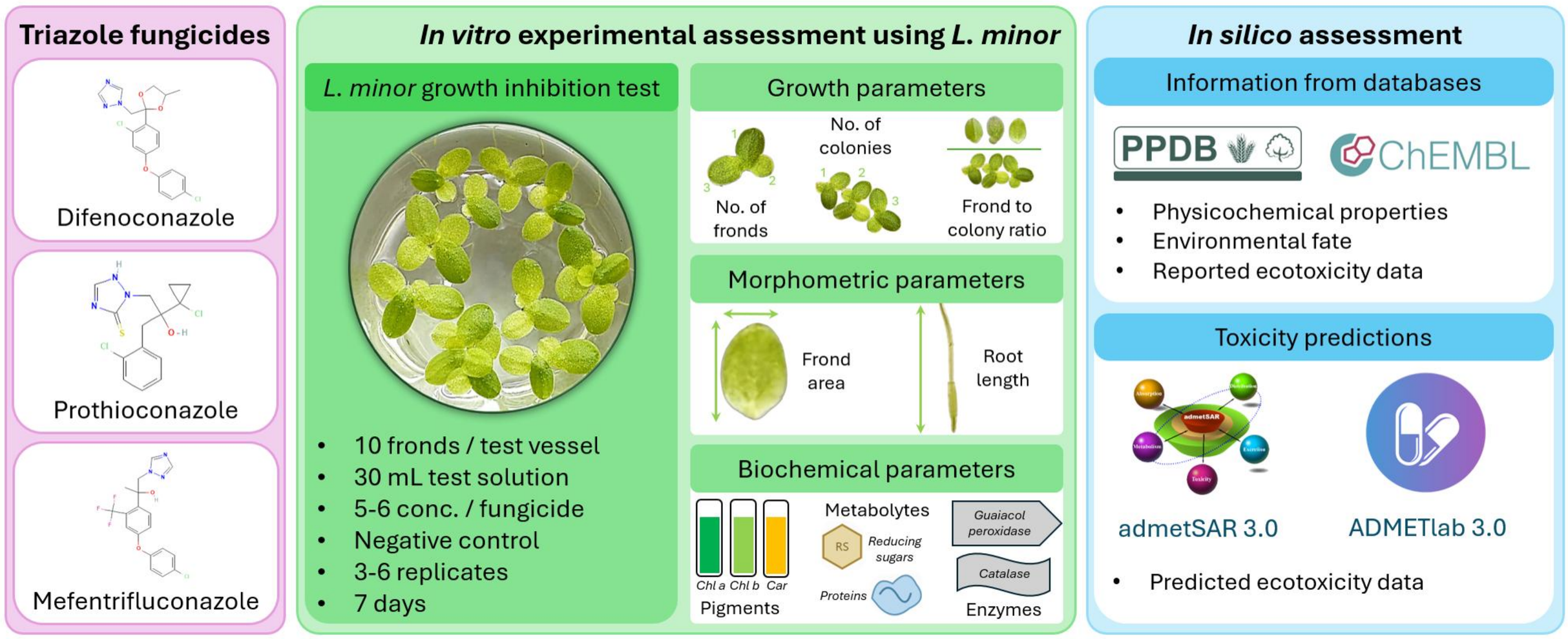


Figure 1. Integrated assessment of the ecotoxicological profiles of three triazole fungicides using *in vitro* experimental and *in silico* approaches

• Conclusions

Integrating experimental and computational approaches may provide a more comprehensive understanding of triazole fungicide ecotoxicity and support improved environmental risk assessment.

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