Synthesis of acibenzolar-S-methyl analogs derived from salicylic acid and 4-hydroxybenzaldehyde: DFT B3LYP computational study and molecular docking against enzymatic targets of biological interest

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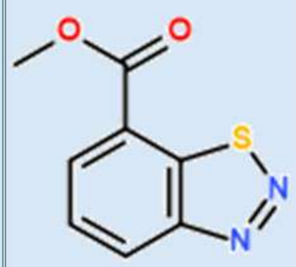
Introduction

One of the primary challenges in Colombian flower exports at the agricultural level is the prevalence of quarantine pests, specifically *Frankliniella occidentalis*.



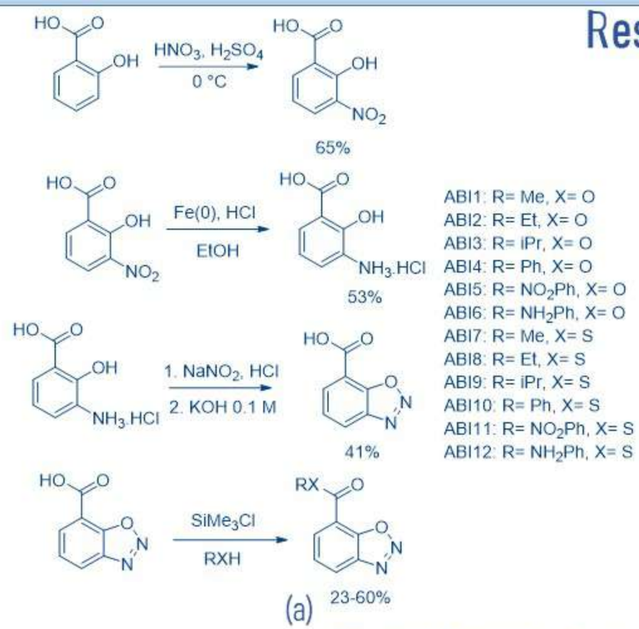
Acibenzolar-S-methyl, is a stimulant for Systemic Acquired Resistance (SAR) in plants.

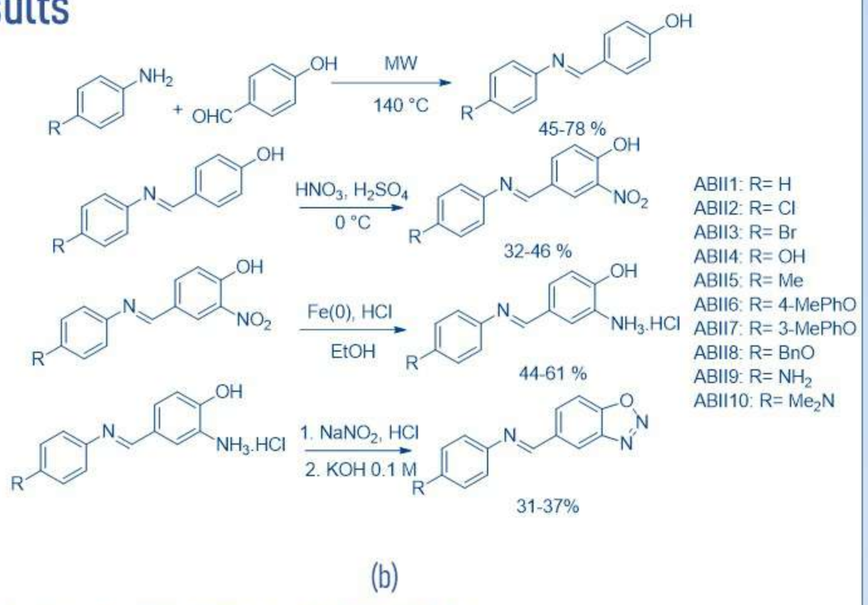
Its efficacy has been substantiated in the treatment of various crops, exhibiting protective properties against fungal, bacterial, viral, and nematode attacks.

Main research findings

The research involved synthesizing two categories of acibenzolar-S-methyl analogs. The first category comprised derivatives of alkyl benzo[*d*][1,2,3]oxadiazole-7-carboxylate ABI1-ABI12 from salicylic acid, and the second category included (*E*)-1-(benzo[*d*][1,2,3] oxadiazol-5-yl)-*N*-arylmethanemine compounds ABII1-ABII10. The synthetic process involved nitration, reduction, diazotization, and intramolecular cyclization, with subsequent purification. The results revealed that specific functional groups influenced interactions with enzymatic targets, enhancing stability and increasing polarizability for favorable ligand interactions and competitive inhibition.

Results





Scheme 1. Chemical synthesis of compounds ABI1-ABI12 (a), and ABII1-ABII10 (b)

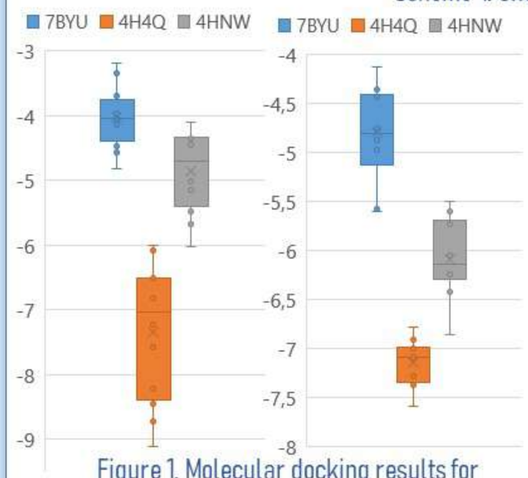


Figure 1. Molecular docking results for compounds ABI1-ABI12, and ABII1-ABII10 against several enzymatic targets

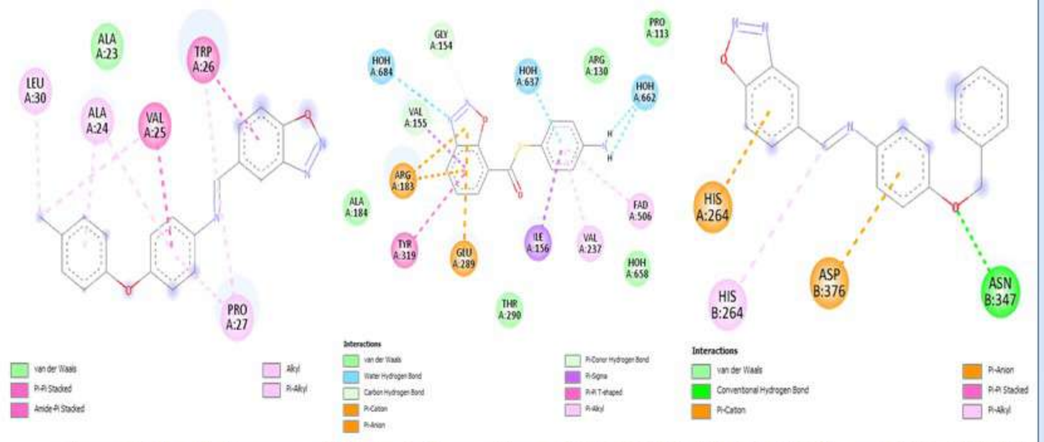


Figure 2. The 2D diagrams of the best-fit complexes ABII6-7BYU (a), ABI12-4H4Q (b), and ABII8-4HNW (c), showing ligand interaction with different amino acid residues of the evaluated enzymatic targets

Conclusions. Our results provides insights into the synthesis, structure, and computational analysis of acibenzolar-S-methyl analogs, emphasizing the impact of specific functional groups on molecular interactions and stability with enzymatic targets.

References

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