OPEN ACCESS

Scientific Letters

III 1H-TOXRUN
International Congress 2024
02-03 May, 2024 | Porto, Portugal

Poster 43

Prediction of fenpyroximate affinity to the NADH-ubiquinone oxidoreductase protein from complex I, for different bee species

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Abstract

Background: Pesticide usage has several beneficial impacts on agricultural production. However, it also has negative environmental impacts on soil, water, and non-target species, which can potentially cause a decrease in biodiversity. A good example is the decline of bee populations due to pesticide use. Fenpyroximate (FEN) is a fungicide that acts by inhibiting mitochondrial complex I electron transport, focusing on the translocation of protons from NADH to ubiquinone oxidoreductase. It is among those detected in Caatinga crops and was already reported to have negative impacts on bees [1,2]. **Objective:** The main objective of this study is to understand the sensibility of different species of bees from the Caatinga biome to FEN using *in silico* analysis. **Methods:** A protein-ligand analysis was used to determine FEN's affinity and binding sites to the NADH-ubiquinone oxidoreductase complex I protein (NADH) for 26 bee species inhabiting the Caatinga biome. A phylogenetic tree was performed to determine the similarity and position of similar binding sites and pockets, and the protein-ligand docking was performed with Autodock (v4.2.6). **Results:** NADH sequences for the 26 bee species had a length between 438 and 566 bp, sharing 79% of pairwise residues for all sequences. Results show that the binding energy of FEN to NADH was between -8.39 and -10.28kcal/mol, inhibition constants between 28.98 and 713 nM, and ligand efficiency between 0.27 and 0.32. For all species, a minimum of 3 and a maximum of 10 ligand aminoacids were found. **Conclusions:** This bioinformatics analysis pipeline is a useful complementary tool to animal testing, giving important insights for determining the mechanisms underlying toxicity of pesticides in non-target bee species. Additionally, it was possible to determine a rank of species sensitivity to FEN that can be used as a policy-maker tool.

Keywords: fenperoxymate; native bees; bioinformatics; protein-ligand docking

Acknowledgments

Pedro Rodrigues was supported by a research contract (BEESNESS – DOI:10.54499/CIRCNA/BRB/0293/2019). Nuno Gonçalo Ferreira was supported by FCT through 2021.02111.CEECIND (DOI: 10.54499/2021.02111.CEECIND/CP1665/CT0003). FCT also supported this study within the scope of UIDB/04423/2020, UIDP/04423/2020 and Project BEESNESS (DOI:10.54499/CIRCNA/BRB/0293/2019).

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