Tropane alkaloids and terpenes synthase genes of *Datura stramonium* (Solanaceae)

BACKGROUND

Plants have evolved physical-chemical defenses to prevent/diminish damage by their enemies. The TRI, TRII, PMT, H6H, and the terpene synthase genes (TPSs) are involved in the production of tropane alkaloids and terpenoids, respectively, that help to protect plants against herbivores and pathogens. **In our study we analyze the evolutionary history of these genes within the Solanaceae family and in two draft genomes of the poisonous and medicinal plant, *Datura stramonium*.**

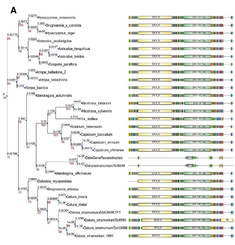
METHODS

Using bioinformatic tools **we analyze gene divergence of tropane alkaloids (TAs) and terpene synthases (TPSs) in *Datura stramonium*** and other species of Solanaceae. We also compared TAs and TPSs' gene and amino acid sequences, cDNA and Viridiplantae proteins sequences.

RESULTS

For TAs, we detected an expansion event in the tropinone reductase II (TRII). The ratio synonymous/nonsynonymous substitutions indicated positive selection. In contrast, a contraction event and negative selection was detected in tropinone reductase I (TRI). **In Hyoscyamine 6-b-hydroxylase** (H6H), an enzyme involved in the production of tropane alkaloids atropine and scopolamine, **the synonymous/non-synonymous substitution ratio indicated that there is positive selection.**

PHYLOGENY OF GENE H6H

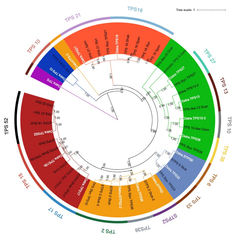


Two copies of the gene are present in the two sequenced genomes of *D. stramonium* (Tic and Teo).

Alignment of protein H6H sequences with the conserved zones highlighted. In the terminal carboxyl, the DIOX-N dominion is duplicated in TIC8550.

For terpenes (TPS), we found 18 DsTPS in *D. stramonium* and 7 in *D. metel*; evolutionary analyses detected positive selection in TPS10.1 and TPS10.2 of *D. stramonium* and *D. metel*. Comparison of TPSs copies in *D. stramonium* detected variation among them in the binding site. **Compared to other Solanaceae, duplication events and differentiation of *D. stramonium's* TAs and TPSs suggest that they are possibly involved in the adaptive evolution of defense against herbivores.**

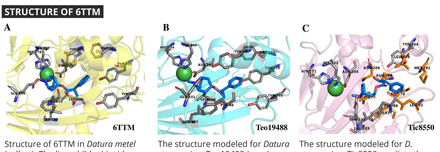
PHYLOGENY OF TPS



18 TPSs were found in *D. stramonium* (white letters) and Solanaceae and other angiosperms.

The protein modeling and docking of *D. stramonium* DsH6H from Teo19488 (B) and Tic8550 (C) suggest high similarity of Teo19488 with the reference structure 6TTM from *Datura metel* (A).

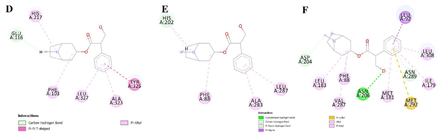
STRUCTURE OF 6TTM



Structure of 6TTM in *Datura metel* (yellow). The ligand (blue) inside the BP is surrounded by amino acids (gray).

The structure modeled for *Datura stramonium* Teo19488 (cyan) contains the same amino acids in the BP as in the structure of 6TTM.

The structure modeled for *D. stramonium* Tic8550 predicts the interactions of some different amino acids (orange) in the BP as compared to 6TTM of *D. metel*.



The interactions between the predicted residues of the BP and the ligand Hy-o.

CONCLUSION

Our results indicate that there are differences in the number of gene copies involved in tropane alkaloids synthesis between the two *D. stramonium* genomes from Mexican populations. More copies of genes related to the synthesis of tropane alkaloids (TRI, TRII, H6H, PMT-10) are found in *D. stramonium* as compared to Viridiplantae. Likewise, for terpene synthases (TPS), TPS-10 is duplicated in *D. stramonium* and *D. metel*. Further studies should be directed to experimentally assess the gain (overexpression) or loss (silencing) of the function of duplicated genes.

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