

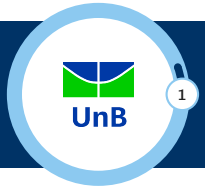


UnB

In silico reconstruction of *Copaifera multijuga* Hayne terpenoids network

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Outline

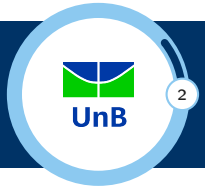


Introduction

- Terpenoid metabolism
- Sesquiterpene cyclases
- Copaifera multijuga* Hayne

Method

Preliminary results



Terpenoid metabolism

Metabolism

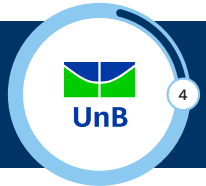
Set of metabolic reactions and physicochemical processes occurring in a live organism.

- ▶ Primary metabolism
- ▶ **Secondary metabolism**
 - ▶ polyketides (PKS)
 - ▶ non-ribosomal peptides (NRP)
 - ▶ alkaloids
 - ▶ **terpenoids**

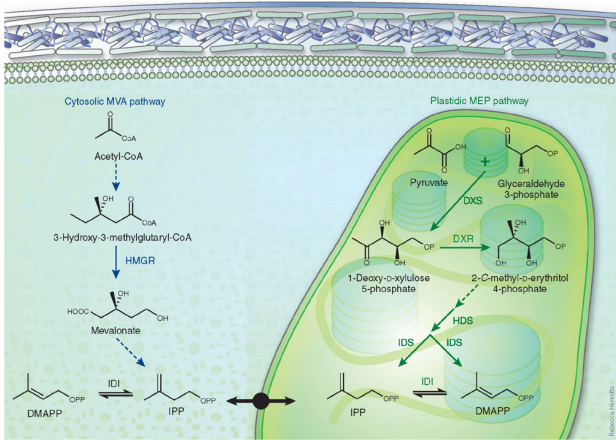
Terpenoids



- ▶ hydrocarbons resulting from the combination of several isoprene units
- ▶ interact as signal molecules for:
 - ▶ communication intra/inter species
 - ▶ attracting pollinating insects
- ▶ act as a defense against herbivores and microbes
- ▶ vast applicability in medicine and biotechnology

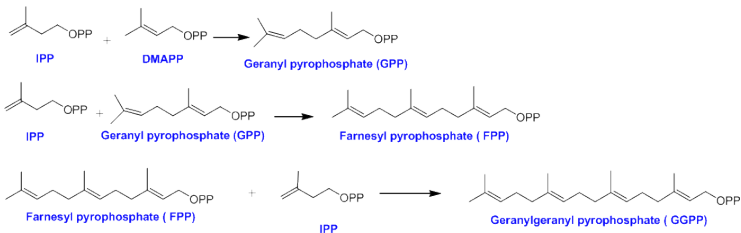


Terpenoid biosynthesis



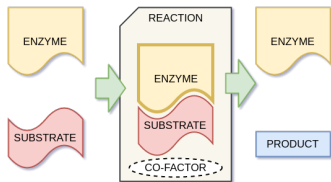
Compartmentalized biosynthesis of IPP and DMAPP [3].

Terpenoid biosynthesis





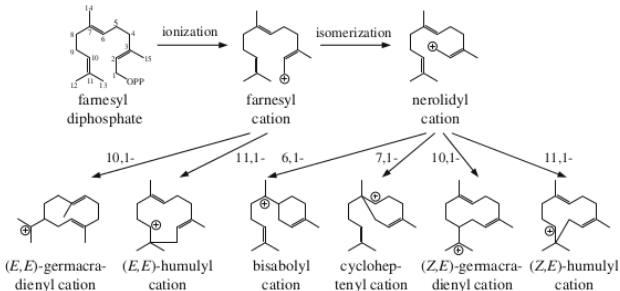
Cyclization mechanisms



- ▶ C – C bonds formation
- ▶ cationic intermediates
- ▶ hydride, methyl, and allyl shifts
- ▶ Wagner-Meerwein rearrangements
- ▶ carbocation capture by water



Cyclization mechanisms



Initial cyclization mechanisms for sesquiterpenes biosynthesis [2] [1].

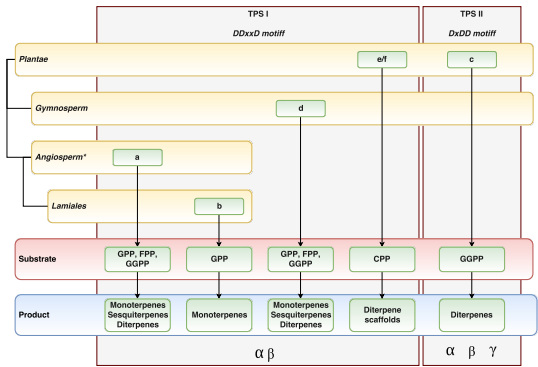
Sesquiterpene cyclases



- ▶ 500–580 amino acids
- ▶ aspartate-rich region, DDxxD
- ▶ often a second motif, NSE/DTE
- ▶ product specificity:
 - ▶ dependent on the amino acid residues, and
 - ▶ constraints of the active site



Cyclases classification



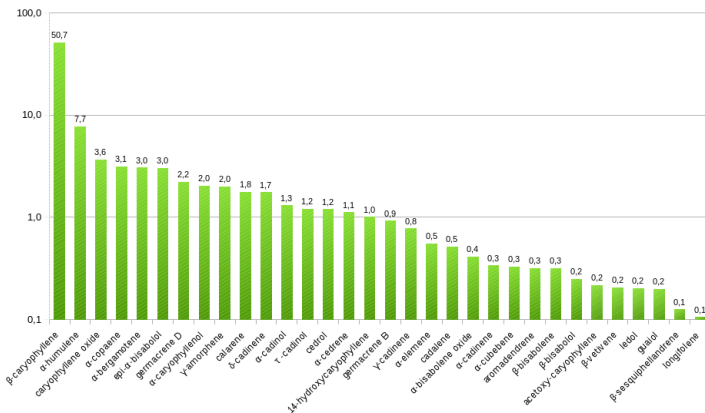
Sesquiterpene cyclases classification.

Copaifera multijuga Hayne



Area of occurrence of *Copaifera multijuga* Hayne in Brazil.

Copaifera multijuga Hayne



Percent amount of sesquiterpenes in *C. multijuga* Hayne's oil-resin.

Method



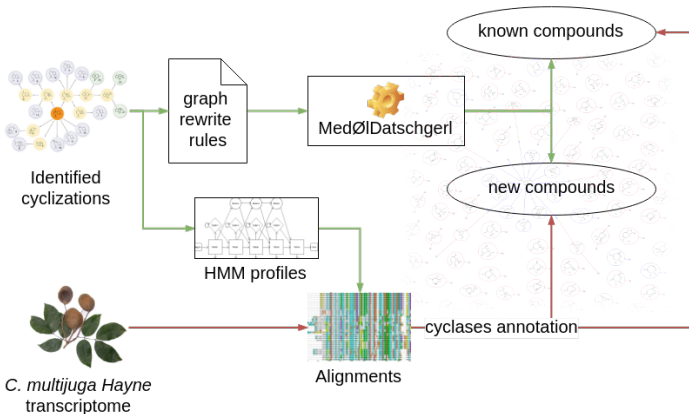
For the 42 known sesquiterpenes of *Copaiba*:

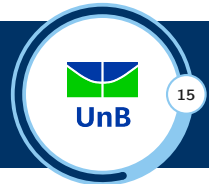
- ▶ Can we confirm the literature reported cyclizations?
- ▶ Can we propose new predicted cyclizations?

For the transcriptome of *Copaiba*:

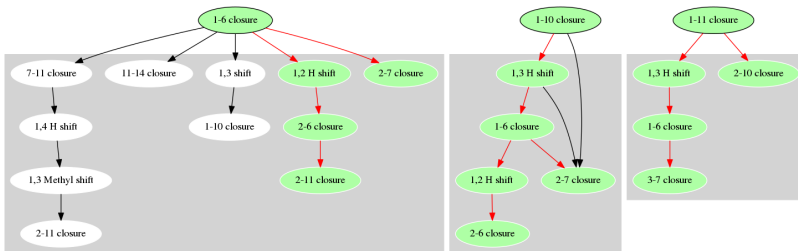
- ▶ Can we use a cyclization family based HMM profile to annotate the enzymes?

Method



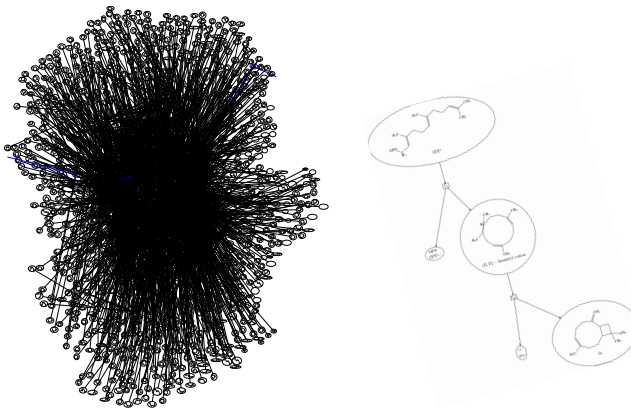


Method



Cyclizations identified in the literature for *Copaifera multijuga* Hayne compounds.

Preliminary results



Unfiltred and filtered results for β -caryophyllene cyclization experiment.

Next steps



- ▶ Update 2Path database to a new level of details;

[A terpenoid metabolic network modelled as graph database](#)

by Waldeyr Mendes Cordeiro Da Silva; Danilo José Vilar; Daniel Da Silva Souza; Maria Emilia Machado Telles Walter; Maristela Terto De Holanda; Marcelo De Macêdo Brígido
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- ▶ Expand source sequences for the HMM profiles;
- ▶ Make available pathway searches from submitted sequences.



Acknowledgements



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References



- [1] David W. Christianson. Structural and Chemical Biology of Terpenoid Cyclases. *Chemical Reviews*, 117(17):11570–11648, 2017.
- [2] Jörg Degenhardt, Tobias G Köllner, and Jonathan Gershenzon. Monoterpene and sesquiterpene synthases and the origin of terpene skeletal diversity in plants. *Phytochemistry*, 70(15-16):1621–1637, 2009.
- [3] Susan C Roberts. Production and engineering of terpenoids in plant cell culture. *Nature chemical biology*, 3(7):387, 2007.