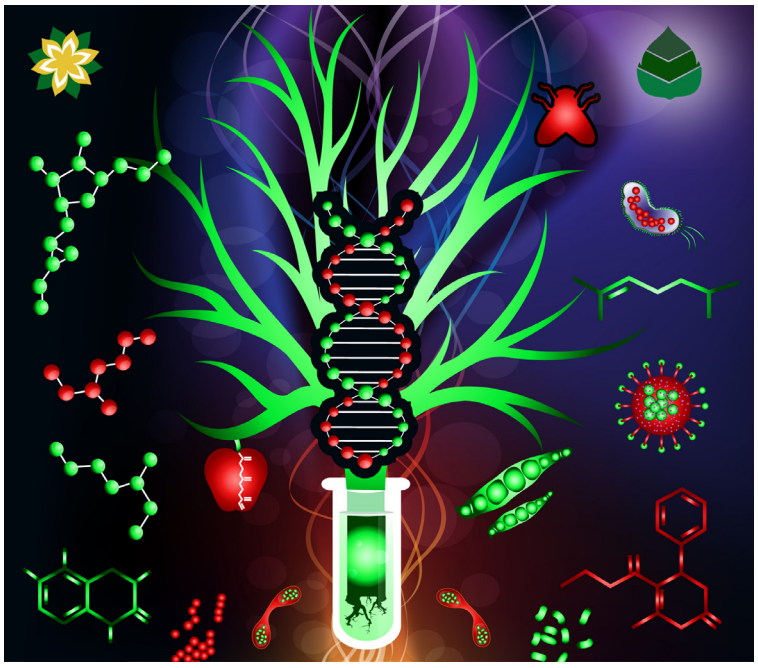
JBCS

Journal of the Brazilian Chemical Society

ISSN 0103-5053

Vol. 27, No. 8, August, 2016

Cover Picture

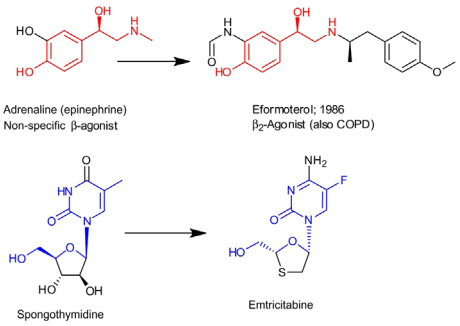


This special issue covers all aspects of the research on natural products such as isolation, structural, elucidation, bioactivities displayed in 6 reviews and 15 articles, focusing the chemistry and biosynthesis of plants, microorganisms and others. Contributions from Brazil and from all over the world is assessed by reading this JBSC issue, enjoy!

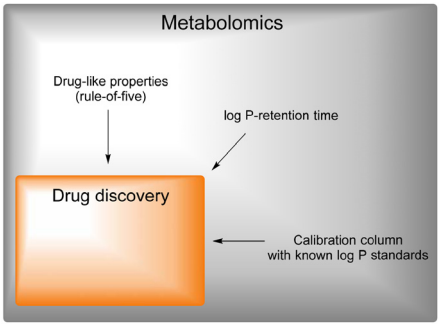
Contents

Editorial

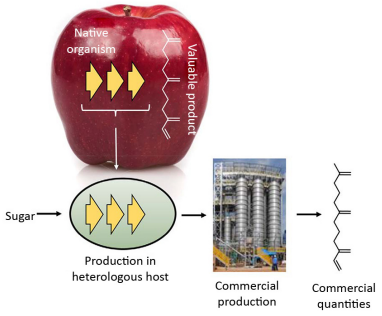
Reviews



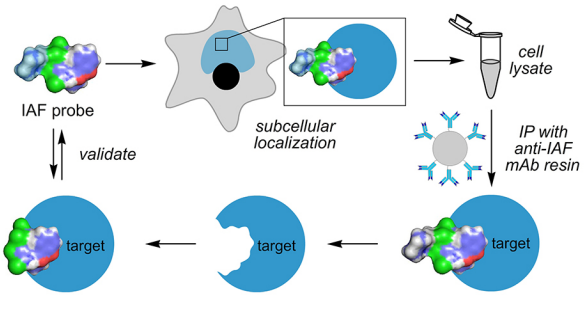
Graphical Abstract
The influence of natural products on ß-agonists/antagonists, anti-tumor and antiviral agents.



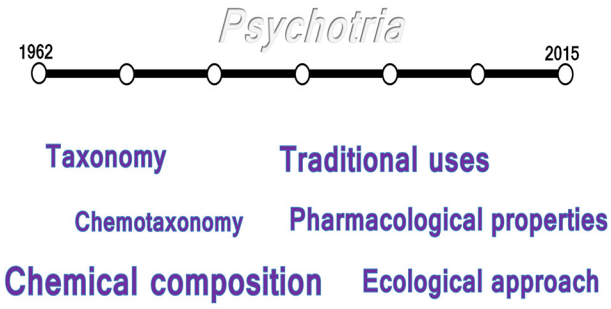
Graphical Abstract
Limit metabolome space to drug space. Drug-like properties - Lipinski's rule-of-five. Use standards with known physicochemical properties to calibrate the column. Correlate log P to retention time (t_R).



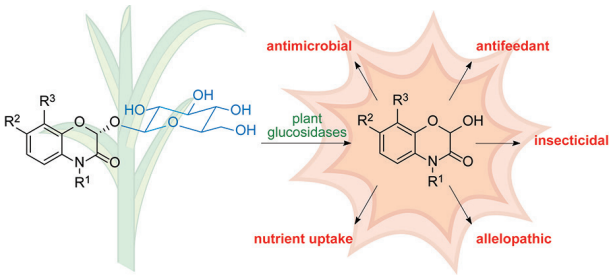
Graphical Abstract
Genes encoding the biosynthetic pathway for production of a valuable product (e.g., farnesene) in a native organism are expressed in a heterologous microbial host (e.g., yeast). The engineered yeast produces farnesene by commercial fermentation.



Graphical Abstract
Elucidating the mode of action (MOA) and associated biomolecular targets of a natural product is often one of the bottlenecks in the drug discovery process. We present an overview of recent developments on an immunoaffinity fluorescent (IAF) approach that unites cellular microscopy with immunoaffinity target identification to rapidly characterize and subsequently validate the targets and cellular activity of natural products.

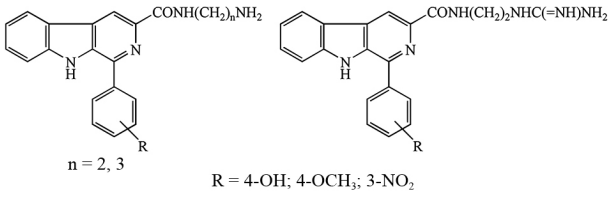


Graphical Abstract
Highlighting the relevant literature from 1962 until 2015, on taxonomy, chemotaxonomy, traditional uses, pharmacological properties, chemical composition and ecological approach from *Psychotria* genus.

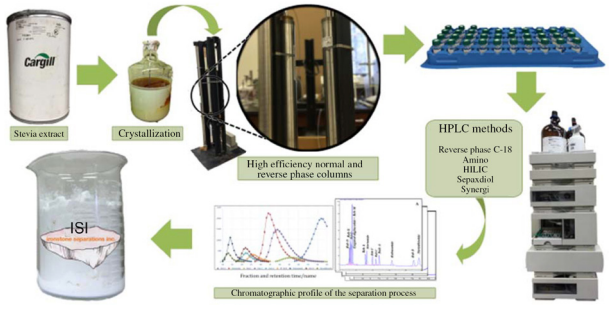


Graphical Abstract
Benzoxazinoids constitute a diverse family of plant secondary metabolites with defensive roles against herbivores, pathogens, and competing plants. Their chemical properties and possible modes of action are discussed in the context of their biological activities.

Articles



Graphical Abstract
Novel 1-substituted-phenyl-ß-carbolines with an amino or guanidinium group-terminated side chain at C-3 were evaluated for *in vitro* anti-tuberculosis, antiproliferative properties and through *in silico* study.



Graphical Abstract
Large scale purification process for steviol glycosides from a commercial crude extract of *Stevia rebaudiana*.

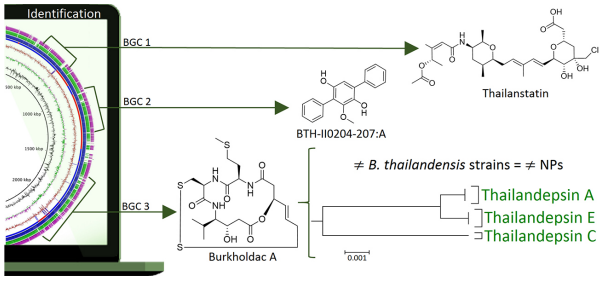
1413 An Insight Into the Intraspecific Variation of Biosynthetic Gene Clusters Between Strains of *Burkholderia thailandensis* spp.

SI online

João Luiz Baldim and Marisi Gomes Soares

Graphical Abstract

Replicons of *Burkholderia thailandensis* strains related to the production of three natural products (NPs). The biosynthetic gene clusters (BGCs) related to burkholdac were further analyzed and their side chain differentiation were tracked according to their genomes explaining the side chains modifications for this NP.



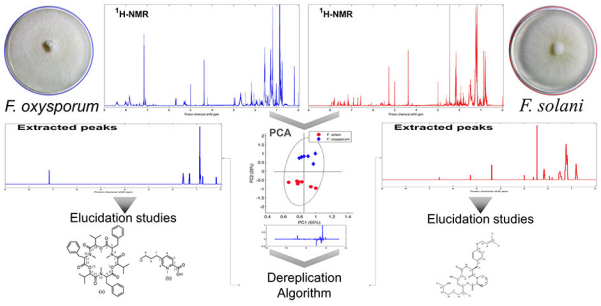
1421 New Dereplication Method Applied to NMR-Based Metabolomics on Different *Fusarium* Species Isolated from Rhizosphere of *Senna spectabilis*

SI online

Denise M. Selegato, Rafael T. Freire, Alberto Tannús and Ian Castro-Gamboa

Graphical Abstract

Workflow of the dereplication method: ^{1}H NMR data from *F. oxyporum* and *F. solani* extracts were subjected to principal component analysis (PCA) for the selection of important chemical shifts region (loading values), followed by dereplication algorithm that extracts real ^{1}H NMR peaks from the selected loading regions, enabling, through the comparison with an *in-house* NMR libraries and online databases, the identification of important bioactive metabolites in complex mixture.



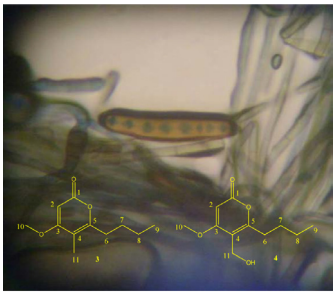
1432 Annularins I and J: New Metabolites Isolated from Endophytic Fungus *Exserohilum rostratum*

SI online

Eduardo A. A. Pinheiro, Fabio C. Borges, Jeferson R. S. Pina, Leila R. S. Ferreira, Jorgeffson S. Cordeiro, Josiwander M. Carvalho, André O. Feitosa, Francinete R. Campos, Andersson Barison, Afonso D. L. Souza, Patrícia S. B. Marinho and Andrey M. R. Marinho

Graphical Abstract

This paper describes the isolation of the compounds ergosterol peroxide, monocerin, annularin I and annularin J of the biomass extracts of *Exserohilum rostratum*. The compounds annularin I and annularin J are new natural products.



Exserohilum rostratum

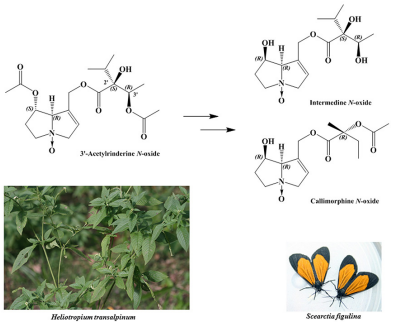
1437 Pyrrolizidine Alkaloids in the Pericopine Moth *Scearctia figulina* (Erebidae: Arctiinae): Metabolism and Chemical Defense

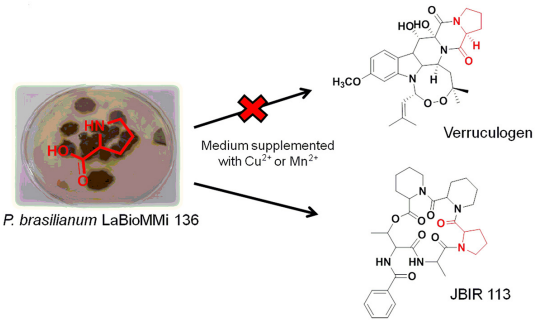
SI online

Carlos H. Z. Martins and José R. Trigo

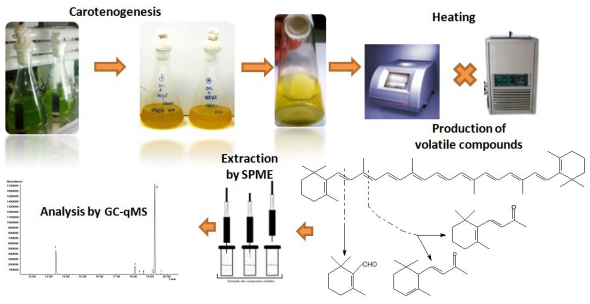
Graphical Abstract

The pericopine moth *Scearctia figulina* transforms pyrrolizidine alkaloids from their host plant *Heliotropium transalpinum*.

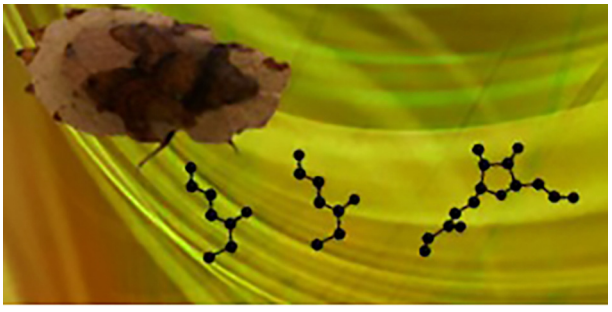




Graphical Abstract
Medium composition modification locked verruculogen biosynthesis and addressed proline to the production of the cyclodepsipeptide JBIR 113 by the fungus *P. brasilianum*.



Graphical Abstract
Volatiles from *Dunaliella bardawil* carotenoids produced by microwave irradiation and water bath controlled heating.



Graphical Abstract
Phloea subquadrata (Heteroptera, Phloeidae) and two molecules of (*E*)-4-oxo-2-hexenal which dimerize in the scent gland.

Graphical Abstract
Mining DNA coupled with networking and analytical tools is a new-fashioned strategy to guide dereplication and finding for new therapeutic targets.