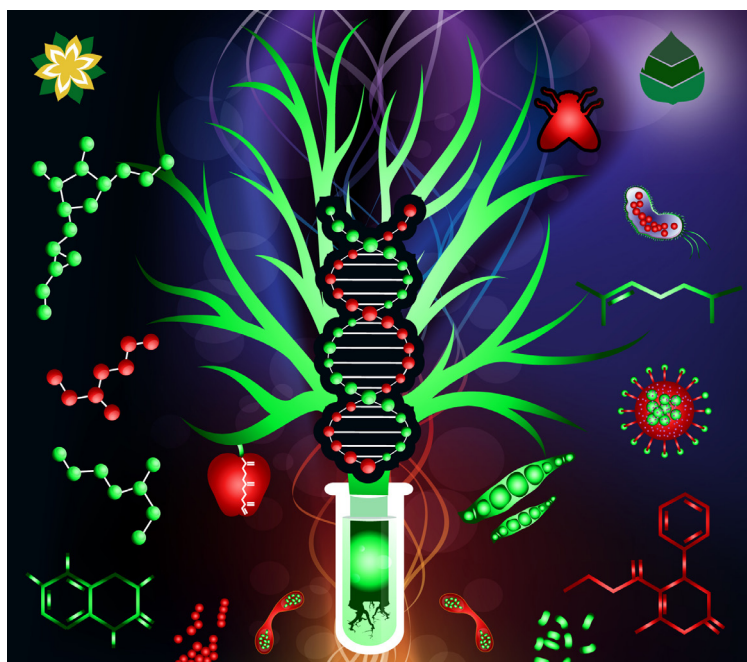


Cover Picture



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

- 1319 **5th BCNP and XXXI RESEM: a Tribute to Biodiversity**
Anita Jocelyne Marsaioli

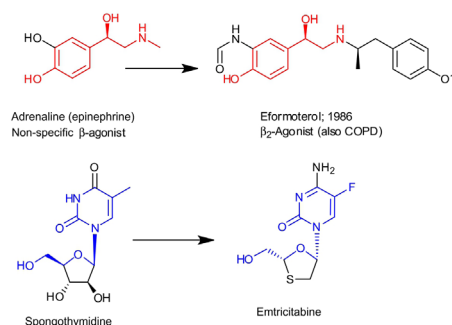
Reviews

1320 Natural Product-Derived Drugs Based on β -Adrenergic Agents and Nucleosides

David J. Newman

Graphical Abstract

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

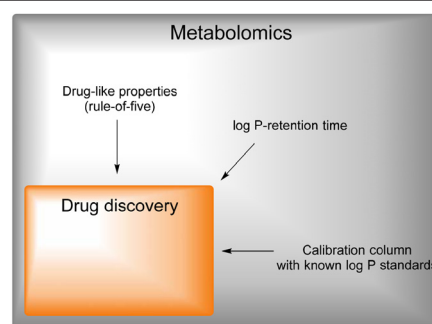


1334 Turning Metabolomics into Drug Discovery

Asmaa Boufridi and Ronald J. Quinn

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).

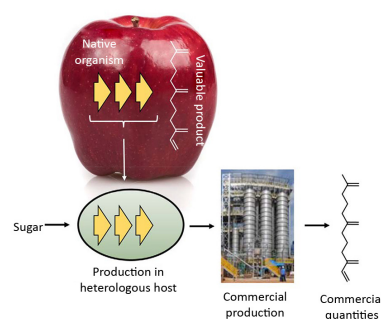


1339 Developing Commercial Production of Semi-Synthetic Artemisinin, and of β -Farnesene, an Isoprenoid Produced by Fermentation of Brazilian Sugar

Kirsten R. Benjamin, Iris R. Silva, João P. Cherubim,
Derek McPhee and Chris J. Paddon

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. Copyright © 2016 Amyris, inc. All rights reserved.

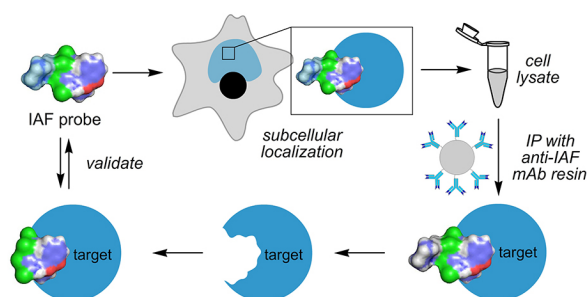


1346 Elucidating the Mode of Action of Marine Natural Products through an Immunoaffinity Fluorescent (IAF) Approach

James J. La Clair, William Fenical and Leticia V. Costa-Lotufo

Graphical Abstract

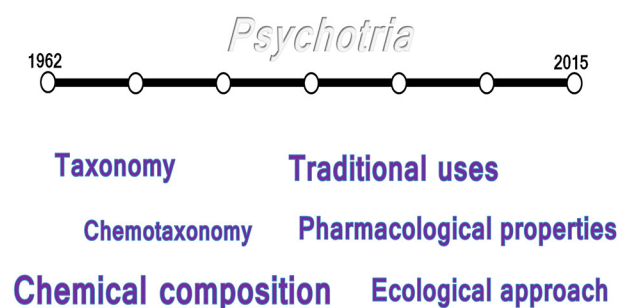
Elucidating the mode of action (MOA) and associated biomolecular targets of a natural product is often one of the bottlenecks in the drug discovery process. We present an overview of recent developments on an immunoaffinity fluorescent (IAF) approach that unites cellular microscopy with immunoaffinity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



- 1355 The Genus *Psychotria*: Phytochemistry, Chemotaxonomy, Ethnopharmacology and Biological Properties**
 Nivea O. Calixto, Meri Emili F. Pinto, Suelem D. Ramalho, Marcela C. M. Burger, Antonio F. Bobey, Maria Claudia Marx Young, Vanderlan S. Bolzani and Angelo C. Pinto

Graphical Abstract

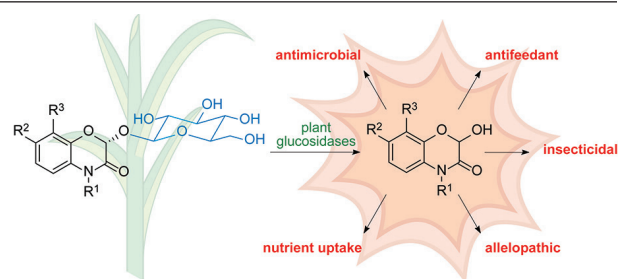
Highlighting the relevant literature from 1962 until 2015, on taxonomy, chemotaxonomy, traditional uses, pharmacological properties, chemical composition and ecological approach from *Psychotria* genus.



- 1379 Benzoxazinoids: Reactivity and Modes of Action of a Versatile Class of Plant Chemical Defenses**
 Felipe C. Wouters, Jonathan Gershenzon and Daniel G. Vassão

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.

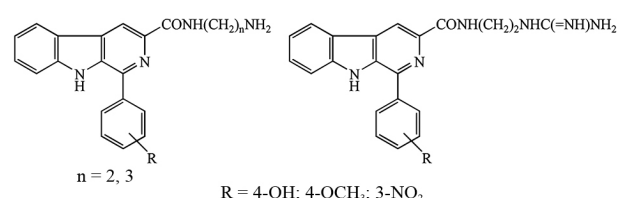


Articles

- 1398 Synthesis, *in vitro* Antiproliferative and Anti-*Mycobacterium tuberculosis* Activities of Novel β -Carboline Derivatives**
 Flora M. F. Moreira, Julio Croda, Maria H. Sarragiotto, Mary A. Foglio, Ana L. T. G. Ruiz, João E. Carvalho and Anelise S. N. Formagio



SI online



Graphical Abstract

Novel 1-substituted-phenyl- β -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.

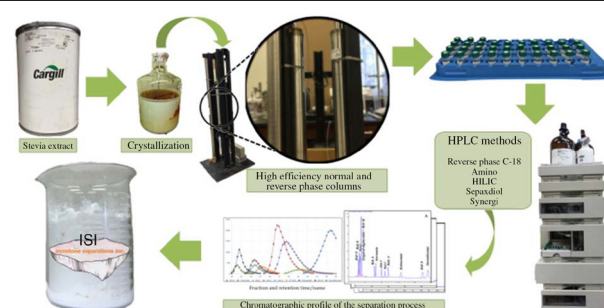
- 1406 Development of HPLC Analytical Techniques for Diterpene Glycosides from *Stevia rebaudiana* (Bertoni) Bertoni: Strategies to Scale-Up**
 Douglas L. Rodenburg, Kamilla Alves, Wilmer H. Perera, Taylor Ramsaroop, Raquel Carvalho and James D. McChesney



SI online

Graphical Abstract

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

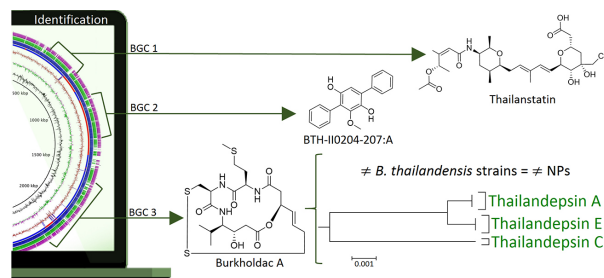


1413 An Insight Into the Intraspecific Variation of Biosynthetic Gene Clusters Between Strains of *Burkholderia thailandensis* spp.

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.

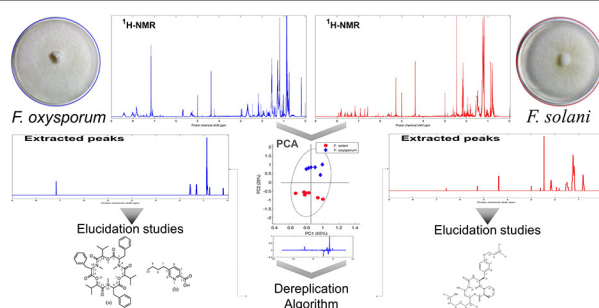


1421 New Dereplication Method Applied to NMR-Based Metabolomics on Different *Fusarium* Species Isolated from Rhizosphere of *Senna spectabilis*

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

Graphical Abstract

Workflow of the dereplication method: ^1H NMR data from *F. oxysporum* 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 ^1H 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.

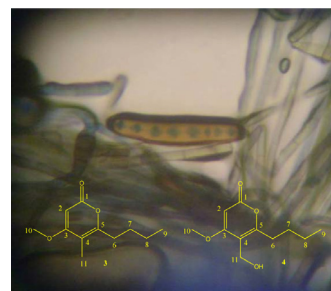


1432 Annularins I and J: New Metabolites Isolated from Endophytic Fungus *Exserohilum rostratum*

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.



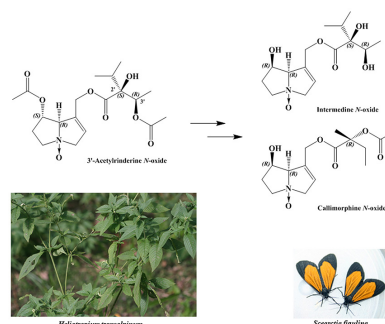
Exserohilum rostratum

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

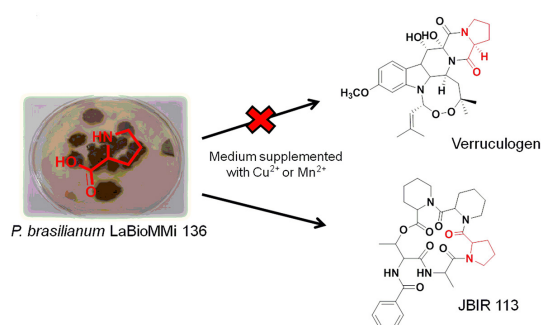
The pericopine moth *Scearctia figulina* transforms pyrrolizidine alkaloids from their host plant *Heliotropium transalpinum*.



1444 Copper and Manganese Cations Alter Secondary Metabolism in the Fungus *Penicillium brasilianum*

http://
Taícia Pacheco Fill, Heloisa Fassina Pallini, Luciana da Silva Amaral, José Vinicius da Silva, Danielle Lazzarin Bidóia, Francieli Peron, Francielle Pelegrin Garcia, Celso Vataru Nakamura and Edson Rodrigues-Filho

SI online



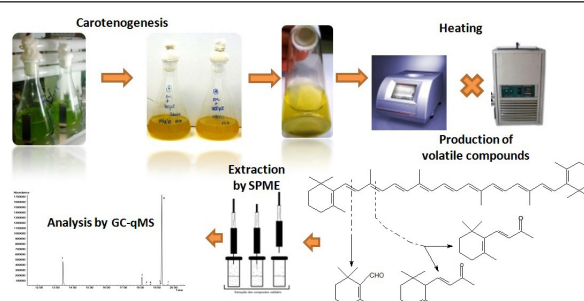
Graphical Abstract

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

1452 Generation of Volatile Compounds from Carotenoids of *Dunaliella bardawil* Algae by Water Bath Heating and Microwave Irradiation

http://
Natália A. B. Tinoco, Thais M. Uekane, Anna Tsukui, Paula F. de Aguiar, Cláudia M. L. L. Teixeira and Claudia M. Rezende

SI online



Graphical Abstract

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

1459 (E)-4-Oxo-2-hexenal Dimers in the Scent Glands of the Bark Bug *Phloea subquadrata* (Heteroptera, Phloeidae)

http://
Francine S. A. da Fonseca, Marília Medeiros, Adriana T. Salomão, João Vasconcellos-Neto and Anita J. Marsaioli

SI online



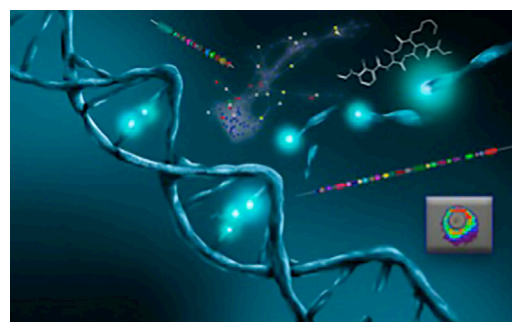
Graphical Abstract

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

1465 Genome Mining of Endophytic *Streptomyces wadayamensis* Reveals High Antibiotic Production Capability

http://
Célio F. F. Angolini, Ana B. Gonçalves, Renata Sigríst, Bruno S. Paulo, Markiyan Samborsky, Pedro L. R. Cruz, Adriana F. Vivian, Eduardo M. Schmidt, Marcos N. Eberlin, Wellington L. Araújo and Luciana G. de Oliveira

SI online



Graphical Abstract

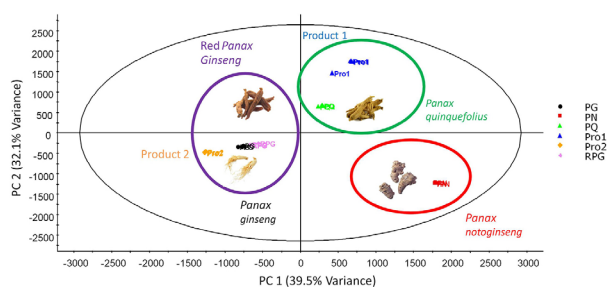
Mining DNA coupled with networking and analytical tools is a new-fashioned strategy to guide dereplication and finding for new therapeutic targets.

1476 Chemical Profiling of Ginseng Species and Ginseng Herbal Products Using UPLC/QTOF-MS

Jimmy Yuk, Dhaval Kumar N. Patel, Giorgis Isaac, Kerri Smith, Mark Wrona, Hernando J. Olivos and Kate Yu

Graphical Abstract

Classification of authentic and commercial ginseng using multivariate statistical analysis with ultra-performance liquid chromatography (UPLC)-quadrupole time-of-flight (QTOF)-mass spectrometry.

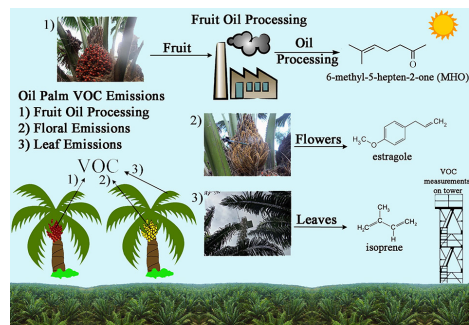


1484 Diurnal Pattern of Leaf, Flower and Fruit Specific Ambient Volatiles above an Oil Palm Plantation in Pará State, Brazil

Kolby J. Jardine, Bruno O. Gimenez, Alessandro C. Araújo, Roberto L. Cunha, Juliana Feitosa Felizzola, Luani R. Piva, Jeffrey Q. Chambers and Niro Higuchi

Graphical Abstract

Tissue specific volatile organic compounds (VOC) emissions from Oil Palm plantations into the atmosphere during fruit oil processing resulting in emissions of 6-methyl-5-hepten-2-one (MHO) as an oxidation biomarker of lycopene; pollinator attraction resulting in floral emissions of estragole, and leaf photosynthesis resulting in leaf emissions of isoprene. Individual tissue measurements of VOC emissions were made using plant enclosure methods while diurnal concentrations of ambient VOCs were made on a walkup flux tower at the plantation scale near Belém, Brazil.

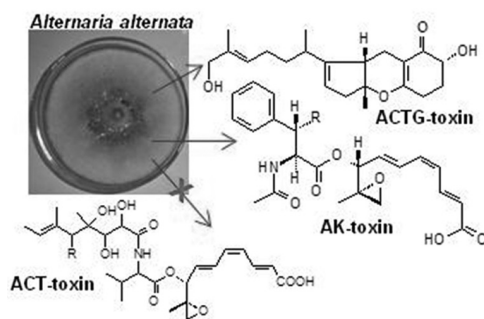


1493 Rapid Detection of ACTG- and AK-Toxins in *Alternaria alternata* by LC-ESI-MS/MS Analysis and Antifungal Properties of *Citrus* Compounds

Kátia R. Prieto, Livia S. de Medeiros, Marsele M. Isidoro, Leonardo Toffano, Maria Fátima G. F. da Silva, João B. Fernandes, Paulo C. Vieira, Moacir R. Forim, Edson Rodrigues-Filho, Rodrigo M. Stuart and Marcos A. Machado

Graphical Abstract

Using LC-ESI-MS/MS analysis, five toxins ACTG-C, D, E and F, and AK-toxin II were identified in *A. alternata*, ACT-toxins appear to be absent.

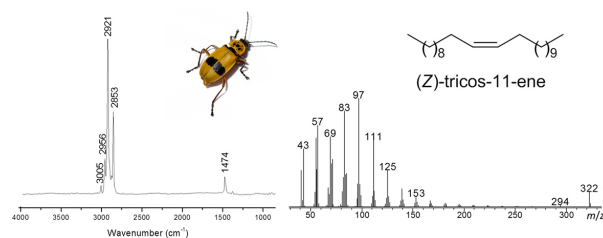


1506 Identification and Synthesis of the Male-Produced Sex Pheromone of the Soldier Beetle *Chauliognathus fallax* (Coleoptera: Cantharidae)

Diogo M. Vidal, Carla F. Fávoro, Matheus M. Guimarães and Paulo H. G. Zarbin

Graphical Abstract

This paper describes the structure elucidation of the male-produced sex pheromone of the soldier beetle *Chauliognathus fallax* through GC-EAD, GC-MS and GC-FTIR analyses, microderivatization and synthesis. The natural compound was identified as (Z)-tricos-11-ene.



1512 Urease Inhibitors of Agricultural Interest Inspired by Structures of Plant Phenolic Aldehydes

Livia P. Horta, Yane C. C. Mota, Gisele Maria Barbosa, Taniris C. Braga, Ivanildo E. Marriel, Ângelo de Fátima and Luzia V. Modolo

Graphical Abstract

Hybrids of plant phenolic natural products protocatechuic aldehyde, syringaldehyde or vanillin with (thio)urea were obtained and investigated for the potential as urease inhibitors of agricultural interest.

