

Special Issue

Cheminformatics of Natural Products Chemistry

Message from the Guest Editor

The identification of natural products has experienced a dramatic increase in the last few years, thanks to important advances in numerical methods. New chemical entities have been reported using computer-assisted methods, in the first steps of isolation and purification, for the identification of the planar structure or for the determination of their relative and absolute configurations. Recent publications regarding the targeted isolation of new compounds are paving the way for a paradigm shift in natural product chemistry, which is guiding researchers towards previously undescribed computer-generated natural products. This Special Issue of *Molecules* is dedicated to original research, review, and opinion articles that deal with numerical methods, their application, or the development of new methods.

Guest Editor

Dr. Grégory Genta-Jouve

USR mixte LEEISA (CNRS, Université de Guyane, Ifremer), C-TAC, UMR CNRS 8038 CITCoM (CNRS, Université Paris Descartes), France

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Molecules
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
molecules@mdpi.com

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About the Journal

Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt

Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Corrensstrasse 48, D-48149 Münster, Germany

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