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Compound Identification of Small Molecules

Guest Editor:

Dr. Tobias Kind
UC Davis Genome Center, University of California, Davis, CA, USA

Deadline for manuscript submissions:
closed (31 January 2020)

Message from the Guest Editor

Compound identification in the environmental sciences, drug research and metabolomics is still a challenging topic. Complex matrices contain 5,000 to 10,000 metabolites. Currently, combinations of multiple platforms and analytical techniques can annotate around 1,200 compounds in total. Without the annotation of these unknown metabolites, biological interpretations are impossible.

This Special Issue will deal with a diverse array of methods for structure elucidation, preferably those that can elucidate multiple compounds at once. This can include classical structure elucidation approaches such as NMR, but more importantly those that can perform compound replication based on hyphenated technologies such as GC-MS/MS or LC-MS/MS. Techniques that describe the modelling of physical parameters such as CSS values from ion mobility or retention time and retention index modelling are also invited, even if they are just a gateway to full compound annotation. Chemical derivatization strategies and isotopic labelling strategies are also welcome for this Special Issue, if they can at least elucidate parts of a compound structure or the full structure.

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Editor-in-Chief

Dr. Amedeo Lonardo

1. Formerly Director of the Simple Operating Unit "Metabolic Syndrome", Azienda Ospedaliero-Universitaria, 41126 Modena, Italy
2. Formerly Professor of Internal Medicine, School of Specialization of Allergology and Clinical Immunology, University of Modena and Reggio Emilia, 41121 Modena, Italy

Message from the Editor-in-Chief

The metabolome is the result of the combined effects of genetic and environmental influences on metabolic processes. Metabolomic studies can provide a global view of metabolism and thereby improve our understanding of the underlying biology. Advances in metabolomic technologies have shown utility for elucidating mechanisms which underlie fundamental biological processes including disease pathology. *Metabolites* is proud to be part of the development of metabolomics and we look forward to working with many of you to publish high quality metabolomic studies.

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Contact Us

Metabolites Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/metabolites
metabolites@mdpi.com
𝕏@MetabolitesMDPI