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HETEROCOVARIANCE A NEW TOOL FOR THE EFFICIENT DETECTION OF BIOACTIVE COMPOUNDS IN COMPLEX MIXTURES

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Spectral data reflect concentration variations of the components of an extract and can correlate statistically with measurable dose-dependent properties such as bioactivity. A carefully planned fractionation of plant material can generate a concentration variance of the components and can be reflected on the corresponding spectroscopic data. Correlation of these data with bioactivity would result to the identification of active constituents in the complex extract or fraction mixtures prior to any purification step. Examples of the fractionation procedure using the Centrifugal Partition Chromatography technique (CPC) and the correlation of NMR and MS data with bioactivity to identify the active constituents through the heterocovariance statistical analysis will be discussed. This highly innovative activity-based-metabolite-profiling can dramatically accelerate the discovery of active natural products challenging global biodiversity and chemo-diversity.



Biography

Emmanuel Mikros is Professor of Pharmaceutical Chemistry at University of Athens. He completed his PhD in Chemistry at Université Paris-Sud (Paris XI) in 1988 and then he joined University of Athens. He is a Research Fellow at Universität zu Lübeck, (Germany), and at INRA, Nantes, (France). He was awarded the DAAD (Germany, 1996) and Marie Curie (European 1994) Fellowships. He is co-author of 115 peer reviewed scientific publications. He has participated in over 20 funded research and projects. He is President of Hellenic Society of Medicinal Chemistry; invited speaker in more than 40 conferences and universities; he has also participated in the organizing committee of seven international and national scientific congresses. He leads a research group focused on NMR spectroscopy; NMR based metabolomics drug discovery and structure based drug design.

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