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A new computational approach to graphically highlight regulation relationships in metabolic systems from chromatographic data

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A new computational approach was developed to highlight some metabolic order by statistically exploring the variability between and within chromatographic profiles representing different states in the studied population. The approach consisted in combining metabolic variability of chromatographic profiles initially classified into metabolic trends (MbTrs). Illustration was based on 248 profiles of plasmatic L-dopa and its metabolites (3-OMD, DOPAC and HVA) analysed at different times (after L-dopa administration) in 34 patients suffering from Parkinson disease. After statistical classification of the population into different MbTrs, classified profiles were iteratively combined *in silico* by applying a Scheffé's mixture design. To take into account the variability within and between MbTrs, the mixture design was iterated k times by bootstrap leading to k response matrices that were averaged to obtain a complete set of smoothed profiles representing gradual regulations between metabolites. Smoothed response data were used to graphically analyse backbone of the metabolic system. The results highlighted MbTr-dependent relationships between metabolites, revealing high metabolic flexibility. Apart from this static application, the same iterative algorithm was applied to separate data subsets corresponding to different sampling times. From 3-D plots (time t, metabolite x, metabolite y), smoothed results highlighted a counter-clock hysteresis between a precursor (DOPAC) and its derivative (HVA) suggesting a lag between metabolic regulations; such a process was compatible with the metabolic pathways.

Biography

Nabil Semmar is specialized in computational biology focusing his scientific researches on analysis of regulation laws of structural diversity and functional variability in biosystems. He is a multidisciplinary biologist with a long academic itinerary including Master's in Environmental Sciences (marine and terrestrial), a PhD in Phytochemistry and Post-doctoral researches in Pharmacometrics and Pharmacokinetic Modeling (1988-2004). In his PhD (Lyon, 2000), he developed an original simplex approach helping to statistically highlight multidirectional (flexible) relationships between biological components of polymorphic systems. His finding concerning simplex control of complex biosystems was appreciated by IAEA who invited him as consultant and speaker for conference in scientific program on plant and animal resources management (Vienna, 2008). More recently, he showed the ability of simplex approach to extract hysteretic regulation laws between drug metabolites in pharmacokinetic populations (2010). Moreover, his statistical contributions in pharmacometrics and population pharmacokinetics modeling were appreciated by Biomedical Simulations Resource Group (California) who invited him as speaker for a conference (Los Angeles, 2007). In pedagogy, he is the author of three books on statistics, computational metabolomics and chemotaxonomy in addition to several book chapters published in different international publishers (since 2009). He is Associate Professor at the University of Tunis (ISSBAT) (Tunisia) where he teaches these fundamental and specialization fields in different licenses and masters of biological sciences.

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