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A new computational approach to analysis the variability and regulation processes in drug metabolic systems based on iterative combinations of metabolic profiles

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Metabolic regulation processes of drug metabolites can be statistically analysed from the variability between and within chromatographic profiles representing different subjects' states along time. To analyse such regulation processes, a new metabolomic approach was developed by combining *in silico* metabolic profiles representing different biochemical regulation states. Illustration was based on 248 profiles of L-dopa and its metabolites (3-OMD, DOPAC and HVA) analysed at different times (from L-dopa administration) in 34 patients suffering from Parkinson disease. After statistical classification of population into different metabolic trends (MbTrs), the separated profiles were iteratively combined *in silico* by applying a Scheffé's mixture design. Taking into account the variability within and between MbTrs, the mixture design was iterated several times to calculate a complete set of average profiles from which gradual regulations between metabolites were graphically analysed to understand the functional aspect of the studied metabolic system. The results highlighted MbTr-dependent relationships between metabolites, revealing high metabolic flexibility. Apart from this static application, the mixture design was applied at the different sampling times. Results visualizations on 3-D plots (time *t*, metabolite *x*, metabolite *y*) highlighted a counter-clock hysteresis between precursor (DOPAC) and product (HVA) suggesting metabolic regulation lag between them that was revealed to be compatible with metabolic network.