

Metabolomics fingerprinting in clinical study of multiple sclerosis disease

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The composition of biofluids carries invaluable information about the biochemical status of a living organism. Cerebrospinal Fluid (CSF) is the biofluid, which is in closest interaction with the Central Nervous System (CNS). It is therefore the biofluid that best mirrors the biochemical status and processes in brain and CNS. The chemical composition of CSF may thus provide insights about metabolic pathways in the CNS. The comprehensive analysis of CSF may define the fingerprint of neurological diseases such as the Multiple Sclerosis (MS).

Our objective is to detect molecular biomarkers for MS in CSF. For this we used ^1H Nuclear Magnetic Resonance (^1H -NMR) spectroscopy and Gas Chromatography coupled with Mass Spectrometry (GC-MS) in combination with chemometric analysis.

The research results we will present are obtained from a clinical study on MS. We examined the human CSF metabolomics profile of MS group. It was then compared to group representing the early stage of MS, i.e. clinically isolated syndrome of demyelination (CIS). This human dataset is very complex, because the biological variations and environmental variations are comparable in size or larger than the variance of interest. The challenge is then to still extract the relevant variances, which requires special, more sophisticated approaches. For this purpose we have applied a kernel-PLS-DA for fused NMR and GC-MS datasets in kernel space. In addition we implemented variable selection procedure which is based on SVM Recursive Feature Elimination for nonlinear kernel function. Using this approach we obtained discrimination between MS group and CIS group with high prediction accuracy for class memberships. Variables importance in kernel space was achieved by applying the pseudo-samples concept, recently introduced in our group.

Biography

Agnieszka Smolinska completed her Msc in Chemistry in Poland (Silesian University in Katowice). Currently she is a PhD student in The Netherlands (Radboud University in Nijmegen). She is investigating metabolic profiles of autoimmune disease, especially Multiple Sclerosis.