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Bioinformatics tool towards GC-MS data analysis, with extraction, classification, standardization, visualization and management features

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The software platform “Isotopo” quantifies the population of isotopomers in mixtures of ¹³C-labelled amino acids. It estimates mass values, and predicts relative intensities with respect to the used mass to charge ratios, natural abundances, relative abundances and fractional molar abundances of each fragment derived from the compound under study. The platform is user-friendly and robust and includes facile data management of multiple experiments. Relative intensities are calculated applying a partial least square method and, furthermore, iterative refinement on the data is done for optimal resolution of the isotopologue data. Using the new platform, isotopologue patterns can be easily calculated from MS data, visualized and compared for metabolic flux modelling in an effort to provide an easy-to-use user platform of isotopologue profiling and metabolic flux analysis. Isotopo provides a database and third party independent file based experimental data management system. Furthermore it offers user friendly graphical interface towards automatic isotopomer data extraction from different file formats, with classification, standardization and management, using a newly proposed special purpose data classifier based on supervised machine learning principles. Isotopo implementation follows the principles of one newly proposed software engineering paradigm i.e. *Butterfly*, ‘V-Model’ software development life cycle, integrating formal unified modelling language to scheme from different perspectives, and incorporating human computer interaction guidelines, principles and patterns. Looking at the future perspectives and focusing own scientific system requirements, Isotopo is programmed in C#, Microsoft Visual Studio Dot Net Framework.

Biography

Zeeshan Ahmed works at the University of Wuerzburg with a strong interest in scientific software solution design and development. He is Post Doc. and Scientific Software Engineer and in the central computation support project of the collaborative research center SFB 1047 at the Biocenter, Department of Neurobiology and Genetics. He did Ph.D. in Bioinformatics from the University of Wuerzburg Germany in collaboration with Technical University of Munich Germany. Furthermore, he is also the alumni (pre. Doctoral research and degree course work) of Vienna University of Technology Austria, Fraunhofer Institute for Experimental Software Engineering Germany and Blekinge Institute of Technology Sweden.