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The new dimensions of Quantum Mechanical Spectral Analysis (QMSA)

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The coupled nuclear spins floating in sea of molecular electrons obey the laws of quantum mechanics so that frequencies of complex 1H NMR spectra can be calculated within experimental accuracy from chemical shifts and coupling constants. When the effects of molecular environment are added to the model, even the smallest spectral details can be interpreted. This forms the basics of computerized QMSA, pioneered by the computer programs like LAOCOON and NUMARIT. The potential of quantitative QMSA (qQMSA) has been recently realized and several groups work on novel software tools. The bottleneck of QMSA, that the computation time grow steeply with the size of spin-system is not a serious problem anymore. For example, our ChemAdder software allows simulation of testosterone or urine spectra (with >210 metabolites and >1000 spin-particles) in < 1 sec, on standard desktop and their complete iterative fitting demands typically < 1 min. In this presentation the two examples are discussed. Other topics are the Field Independent Adaptive Spectral Libraries (FIASL), qQMSA of isotopomer 2D HSQC spectra, the multispectral QMSA (simultaneous fitting of different types of spectra like real and imaginary), and the holistic QMSA which takes advantage from prior knowledge about populations and chemical shift variations (a common nuisance) so that the current and accumulated results of analyses are consistent – approaching the case that all the spectra were fitted simultaneously. With novel graphical tools, the analysis of even a large spectral set demands from samples to results (mg/mL), just a few clicks.

Biography

Reino Laatikainen since late 1980's he worked as the Professor of Chemistry in University of Kuopio, which now-a-days is a part of University of Eastern Finland (UEF). From 2015 he continued his work as Emeritus Professor, focusing to qQMSA. He has published 125 papers on computerized NMR and Structural Chemistry. A general trend has been his interest in flexible and fuzzy systems, including flexible small molecules, drug molecules, proteins and represented also by the 4D NMR spectral parameter prediction and qQMSA of complex NMR spectra.

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