

Virtual Laboratory of NMR Spectroscopy

Marcin Lawenda¹, Łukasz Popenda², Norbert Meyer¹, Maciej Stroinski¹, Zofia Gdaniec² and Ryszard W. Adamiak²

¹*Poznań Supercomputing and Networking Center (PSNC)
Z. Noskowskiego 10, 61-704 Poznań, Poland*

²*Institute of Bioorganic Chemistry, Polish Academy of Sciences
Z. Noskowskiego 12/14, 61 704 Poznań, Poland*

Virtual laboratories are now among the front activities of academic research groups and companies, which are working on new solutions for remote access to very expensive laboratory devices. The Virtual Laboratory (VLab) project is being developed by the Poznań Supercomputing and Networking Center in collaboration with the Institute of Bioorganic Chemistry PAS [1,2]. The primary goal of the VLab was to create within grid architecture the VLab of NMR spectroscopy based on access to Bruker Avance 600 MHz and Varian Unity+ 300 MHz spectrometers. This is not only to make remote access to this facilities but, through the VLab broker, to assist researcher in finding necessary basic information for educational purposes (e-learning, digital library, communication), to show details how to run an experiments and how to do experiment using concept of dynamic scenarios. The latter include: pre-processing, executing the experiment, and the post-processing. VLab is giving an unique opportunity to complex visualization tasks. Users would be also allowed to add their own module as a part of the dynamic scenario. Actual stage of our work on the VLab project concerning NMR spectroscopy will presented. All interested are invited to visit an active VLab domain (<http://vlab.psnc.pl>). Currently works are advanced on the VLab project concerning applications of radiotelescope (with A. Kus, Centre for Astronomy, Nicolas Copernicus University, Toruń) and supercomputing (with K. Kulinska, Institute of Bioorganic Chemistry PAS, Poznań).

- [1] KBN project no. 6 T11 0052 2002 C/05836, part of the project co-funded by KBN and SGI: "High Performance Computations and Visualisation for Virtual Laboratory Purposes with the Usage of SGI Cluster" (based on decision number 03282/C.T11-6/2002 of December 9th 2002), WP 3.1 task: Virtual Laboratory and Teleimmersion
- [2] KBN project no. 4 T11 F 010 24: "Building of Universal Architecture for Virtual Laboratory"