New Methods of NMR Spectroscopy

HEAD:

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GROUP MEMBERS:

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RESEARCH PROFILE:

Our group works mostly on methodological aspects of NMR spectroscopy. The aim of this work is faster and more accurate determination of structurally important NMR parameters, and their application in chemistry and biochemistry. Recently we focus on the development of new approaches for acquisition of multidimensional NMR spectra necessary in the studies of biomolecules.

Most important topics include: development of new pulse sequences for faster or more accurate determination of spectral parameters, methods of fast acquisition of multidimensional spectra, determination of scalar and residual dipolar couplings, chiral recognition.
Currently our work focuses on the following tasks:

- Acquisition of high dimensional NMR spectra (4-7D) and new strategies of resonance assignment in biomolecules.
- Application of new methods for the studies of intrinsically disordered proteins (IDP).
- Development of methods for cleaning spectra from artefacts which are result of sparse sampling. This would allow analysis of spectra featuring high dynamic range of peak amplitudes, as for example heteronuclear edited 4D NOESY.
- Development of NMR methods exploring the new possibilities of random sampling for the accurate and precise determination of scalar and residual dipolar couplings from 3 and 4D NMR spectra.
- Protein structure elucidation and protein interaction studies.
- Peptide structure elucidation.
- NMR resonance assignment, structure determination and dynamics of biomolecules in the solid-state.

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CURRENT RESEARCH ACTIVITIES:

Creating and developing new methods for measuring and processing multidimensional NMR spectra and their application in the study of semi- unstructured proteins. These achievements represent a breakthrough in NMR multidimensional spectroscopy and its applications, especially in biomolecule research.

SELECTED PUBLICATIONS:

1. K. Grudziąż, A. Zawadzka-Kazimierczuk, W. Koźmiński, High-dimensional NMR methods for intrinsically disordered proteins studies, Methods. 148 (2018) 81-87.
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3. M. Nowakowski, S. Saxena, J. Stanek, S. Żerko, W. Koźmiński, Applications of high dimensional experiments in biomolecular NMR, Prog. Nucl. Mag. Res. Sp. 90-91 (2015) 49-73.
4. M. Urbańczyk, W. Koźmiński, K. Kazimierczuk, Accelerating Diffusion-Ordered NMR Spectroscopy by Joint Sparse Sampling of Diffusion and Time Dimensions, Angewandte Chemie Int. Ed. Engl. 53 (2014) 6464–6467.
5. J. Stanek, S. Saxena, L. Geist, R. Konrat, W. Koźmiński, Probing of Local Backbone Geometries in Intrinsically Disordered Proteins by Cross-Correlated NMR Relaxation, Angewandte Chemie Int. Ed. Engl. 52 (2013) 4604–4606.
6. K. Kazimierczuk, J. Stanek, A. Zawadzka-Kazimierczuk, W. Koźmiński, High-dimensional NMR spectra for structural studies of biomolecules, ChemPhysChem. 14 (2013) 3015–3025.
7. K. Kazimierczuk, M. Misiak, J. Stanek, A. Zawadzka-Kazimierczuk, W. Koźmiński, Generalized Fourier transform for non-uniform sampled data, Topics in Current Chemistry. 316 (2012) 79–124.
8. K. Kazimierczuk, J. Stanek, A. Zawadzka-Kazimierczuk, W. Koźmiński, Random sampling in multidimensional NMR spectroscopy, Prog. Nucl. Mag. Res. Sp. 57 (2010) 420–434.
9. K. Kazimierczuk, A. Zawadzka, W. Koźmiński, I. Zhukov, Determination of spin-spin couplings from ultrahigh resolution 3D NMR spectra obtained by optimized random sampling and Multidimensional Fourier ransformation, J. Am. Chem. Soc. 130 (2008) 5404-5405.
10. K. Kazimierczuk, W. Koźmiński, I. Zhukov, Two-dimensional Fourier transform of arbitrarily sampled NMR data sets, J. Magn. Reson. 179 (2006) 323-328.