Dr. Krzysztof Kazimierczuk
University of Warsaw
Centre of New Technologies
Laboratory of NMR Spectroscopy
ul. Banacha 2C
02-089 Warszawa

Summary of scientific achievements in relation to habilitation procedure

Warsaw, Tuesday 17th May, 2016

1 Name and surname: Krzysztof Kazimierczuk

2 Education:

(a) **PhD in chemistry (thesis with honours)**, Faculty of Chemistry, University of Warsaw, 10.06.2009, Supervisor: prof. Wiktor Koźmiński, title of the thesis: ""Methods of fast acquisition of NMR spectra for structural studies"

(b) **MSc in physics (note:excellent)**, Faculty of Physics, University of Warsaw, 5.04.2007, Supervisor: prof. Ryszard Stolarski and prof. Wiktor Koźmiński, title of the thesis: "Fourier Transform of two variables in three-dimensional NMR spectra"

(c) **MSc in chemsitry (note: very good, thesis with honours)**, Faculty of Chemistry, University of Warsaw, 16.06.2005, Supervisor: prof. Wiktor Koźmiński, title of the thesis: "Active stabilization of magnetic field in high-resolution NMR spectrometers"

3 Information on academic employment

(a) 1.11.2012-now - University of Warsaw, Centre of New Technologies (assistant professor, head of the laboratory of NMR spectroscopy)

(b) 1.02.2010 - 15.04.2011 - Post-doc at Swedish NMR Centre, University of Gothenburg, Sweden.

(c) 1.11.2009-1.11.2012 - University of Warsaw, Faculty of Chemistry (assistant professor)

4 Identification of achievement pursuant to Art.16(2) of the Act of 14 March 2003 on scientific degrees and artistic titles (Journal of Laws no. 65, item 595 as amended) setting the basis for the habilitation proceedings

(a) **Title of scientific achievement:** "Sparse and nearly-sparse representations in problems of NMR spectroscopy"

(b) **List of scientific publications setting the basis for habilitation proceedings:**

(1) K. Kazimierczuk and V.Yu. Orekhov. Accelerated NMR spectroscopy by using compressed sensing. *Angewandte Chemie - International Edition*, 50(24):5556–5559, 2011

My contribution to this work was to implement IRLS and IST algorithms in MATLAB, perform simulations, process the data from NMR experiments and perform statistical analysis. I also wrote a part of the manuscript. Author's contribution: 70%. **IF(2011)=13,455 number of citations=90**

(2) K. Kazimierczuk and V.Yu. Orekhov. A comparison of convex and non-convex compressed sensing applied to multidimensional NMR. *J. Magn. Reson.*, 223:1–10, 2012

My contribution to this work was to formulate a research hypothesis, run simulations, process data from the NMR experiments and perform statistical analysis. I have also written 50 % of the manuscript. I have coordinated the IUVENTUS PLUS project from which the study was co-financed. I am the corresponding author of the paper . Author's contribution: 80%. **IF(2012)=2,300 number of citations=13**

(3) M. Misiak, W. Koźmiński, K. Chmurski, and K. Kazimierczuk. Study of near-symmetric cyclodextrins by compressed sensing 2D NMR. *Magnetic Resonance in Chemistry*, 51(2):110–115, 2013

My contribution to this work was to formulate part of the concept of work (use of CS in 2D NMR to enhance resolution), perform experiments, data processing and analysis of the effectiveness of methods. I have also written a part of the manuscript. I have coordinated the IUVENTUS PLUS project from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 40%. **IF(2013)=1,528 number of citations=3**

(4) M. Urbańczyk, D. Bernin, W. Koźmiński, and K. Kazimierczuk. Iterative thresholding algorithm for multiexponential decay applied to PGSE NMR data. *Analytical Chemistry*, 85(3):1828–1833, 2013

My contribution to this work was to formulate the research hypothesis (the idea of using sparse regularization) and perform part of the analysis of the effectiveness of the method. I have also written a part of the manuscript. I have coordinated the IUVENTUS PLUS project from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 30%. **IF(2013)=5,825 number of citations=2**

(5) K. Kazimierczuk, O. Lafon, and P. Lesot. Criteria for sensitivity enhancement by compressed sensing: Practical application to anisotropic NAD 2D-NMR spectroscopy. *Analyst*, 139(11):2702–2713, 2014 My contribution to the work was the theoretical part, simulations as well as processing and analysis of experimental data. I have coordinated the IUVENTUS PLUS and SONATA BIS 2 projects from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 60 %. **IF(2014)=4,107 number of citations=8**

(6) Mateusz Urbańczyk and Krzysztof Kazimierczuk. A method for joint sparse sampling of time and gradient domains in diffusion-ordered NMR spectroscopy. In *Signal Processing Symposium (SPS), 2013*, pages 1–6. IEEE, 2013

My contribution to this work was to formulate the research hypothesis (the idea of using sparse regularization) and perform a part of the analysis of the effectiveness of the method. I also wrote a part of the manuscript. I have coordinated the HARMONIA and SONATA BIS 2 projects from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 50%. **IF(2013)=0 number of citations=0**

(7) M. Urbańczyk, W. Koźmiński, and K. Kazimierczuk. Accelerating diffusion-ordered NMR spectroscopy by joint sparse sampling of diffusion and time dimensions. *Angewandte Chemie - International Edition*, 53(25):6464–6467, 2014 My contribution to this work was to formulate the research hypothesis (the idea of using sparse regularization)

and perform half of the experiments and a part of the analysis of the effectiveness of the method. I also wrote a part of the manuscript. I have coordinated the HARMONIA and SONATA BIS 2 projects from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 35%. **IF(2014)=11,261 number of citations=2**

(8) W. Bermel, R. Dass, K.-P. Neidig, and K. Kazimierczuk. Two-dimensional NMR spectroscopy with temperature-sweep. *ChemPhysChem*, 15(11):2217–2220, 2014

My contribution to this work was to develop a research concept, perform simulations and prepare the data processing algorithms. I also wrote a part of the manuscript. I have coordinated the IUVENTUS PLUS and SONATA BIS 2 projects from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 70%. **IF(2014)=3,419 number of citations=2**

(9) M. Mayzel, K. Kazimierczuk, and V.Yu. Orekhov. The causality principle in the reconstruction of sparse NMR spectra. *Chemical Communications*, 50(64):8947–8950, 2014

My contribution to this work was to develop part of the theory, run and analyse simulations and prepare data processing algorithms for the part of work on compressed sensing. I have coordinated the IUVENTUS PLUS and SONATA BIS 2 projects from which the study was co-financed. Author's contribution: 40%. **IF(2014)=6,834 number of citations=8**

(10) K. Kazimierczuk and P. Kasprzak. Modified OMP algorithm for exponentially decaying signals. *Sensors (Switzerland)*, 15(1):234–247, 2014

My contribution to this work was to develop part of the theory of direct NMR spectroscopy, and the execution and analysis of experimental data. I also wrote a part of the manuscript. I am the corresponding author of the paper. Author's contribution: 50%. **IF(2014)=2,245 number of citations=2**

(11) Rupashree Dass, Wiktor Kozminski, and Krzysztof Kazimierczuk. Analysis of complex reacting mixtures by time-resolved 2D NMR. *Analytical Chemistry*, 87(2):1337–1343, 2015

My contribution to this work was to develop a concept of research, perform a part of the experiments and prepare some of data processing algorithms. I also wrote a part of the manuscript. I have coordinated the IUVENTUS PLUS and SONATA BIS 2 projects from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 50%.

IF(2014)=5,636 number of citations=3

(12) A. Piai, L. Gonnelli, I. C. Felli, R. Pierattelli, K. Kazimierczuk, K. Grudziąż, W. Koźmiński, and A. Zawadzka-Kazimierczuk. Amino acid recognition for automatic resonance assignment of intrinsically disordered proteins. *Journal of Biomolecular NMR*, pages 1–15, 2016

My contribution to this work was to carry out a series of reconstruction of NMR spectra using CS algorithms. Author's contribution: 10%. **IF(2014)=3,141 number of citations=0**

(13) R. Dass, P. Kasprzak, W. Koźmiński, and K. Kazimierczuk. Artifacts in time-resolved NUS: A case study of NOE build-up curves from 2D NOESY. *Journal of magnetic*

resonance, 265:108–116, 2016

My contribution to this work was to develop a concept of research, perform a part of the experiments and prepare some of data processing algorithms. I also wrote a part of the manuscript. I have coordinated the SONATA BIS 2 project from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 40%. **IF(2014)=2,51 number of citations=0**

(14) M. Urbańczyk, D. Bernin, A. Czuroń, and K. Kazimierczuk. Monitoring polydispersity by NMR diffusometry with tailored norm regularisation and moving-frame processing. *The Analyst*, 141(5):1745–1752, 2016

My contribution to this work was to formulate an idea of the paper (use of "smoothing regularizations"). I also wrote a part of the manuscript. I have coordinated the HARMONIA and SONATA BIS 2 projects from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 30%. **IF(2014)=4,107 number of citations=0**

Total impact factor of papers listed above according to the list from Journal Citation Reports: 59,534

(c) **Summary of the scientific goals and major results of presented publications**

Throughout my scientific career I have studied at the University of Warsaw (UW) and worked in its laboratories of NMR spectroscopy. Master studies at the College of Inter-faculty Studies in Mathematics and Natural Sciences allowed me to gain knowledge and skills from the fields of chemistry and physics.

In 2005 at the Faculty of Chemistry of UW, I defended a thesis concerning the development of a device stabilizing the magnetic field in high-resolution NMR spectrometers (supervisor: prof . Wiktor Koźmiński). Later it proved useful not only in the NMR laboratory at the Faculty of Chemistry, but also in several other laboratories in Europe, including the one at the Technical University in Bratislava, Pasteur Institute in Paris, the Institute of Organic Chemistry in Madrid and application laboratory of Varian company in Darmstadt. Finally, in 2013 the Agilent company bought the technology.

In 2007 I defended a thesis in the field of biophysics (Faculty of Physics, UW) on the properties of the Fourier transform of non-uniformly sampled NMR signals (supervisors: prof. Ryszard Stolarski and prof. Wiktor Koźmiński).

In 2009, at the Faculty of Chemistry, UW I defended my doctoral thesis in the field of physical chemistry on methods of rapid NMR spectroscopy in structural studies (supervisor: prof. Dr hab. Wiktor Koźmiński). The work described a way to speed up the time-consuming NMR experiments based on under-sampling of a signal in indirectly detected dimensions of a multidimensional experiment. The study included: working out a theoretical relationship between the shape of the spectral lines and sampling schedules such as spiral, radial, concentric and random; optimization of the latter; development of high-dimensional techniques based on random sampling and their use in protein research. A particularly impressive example of the application, published in *JACS*, was a method of measuring small coupling constants in proteins using HNCO-C_α-coupled technique.

With hindsight one can say, that works conducted at that time in the group of prof. Koźminski (including my work), made the UW a recognized centre of the development of NMR methodology.

After defending my PhD dissertation in May 2009, I got hired as an assistant professor at the Faculty of Chemistry of the University of Warsaw and began to look for a postdoc position. In February 2010, I went to the Swedish NMR Centre in Gothenburg, where I started working in the group of prof. Vladislav Orekhov. My stay was initially funded by a grant from Bruker company (manufacturer of NMR spectrometers) and then by the KOLUMB program of the Foundation for Polish Science.

The work that I conducted in Sweden established a basis for a series of studies that make up the *scientific achievement* presented here. That work concerned the possibility of using in NMR spectroscopy the approach referred to as compressed sensing (CS). The idea of CS is to exploit the compressibility of an object at the stage of its measurement (sampling), not only at the stage of storing data. This idea can be best exemplified using the case of digital photography. The digital camera samples an image using the CCD matrix containing millions of pixels, which results in a fairly large set of data (min. few MB). However, photography is rarely stored in a raw format, but rather compressed to the *png* or *jpg* file, which contains only the most important components of the image processed using some transform (e.g. wavelet) and usually does not exceed hundreds of kilobytes. Compressed sensing in photography reduces the measurement data set to a size similar to the size of the compressed object. The measurement is performed by an optical system performing mixing of a signal (light) coming from randomly selected points of the measured object, and the detector, which may be similar to the standard one, but consisting of a single pixel (M. F. Duarte et al. IEEE Signal Processing Magazine (2008)).

In NMR spectroscopy, one also deals with compressible objects as the spectrum can be usually described sufficiently well by providing peak coordinates, sometimes also their heights and half-widths. The number of peaks is usually not higher than a few hundred, and therefore the information content of the spectra is not larger than several kB, while the raw signal (FID or a spectrum) are datasets of size from a few up to hundreds megabytes. During my studies, it also turned out that compression can be used in so-called *diffusion-ordered spectroscopy* (DOSY), or be improved to better match the properties of the NMR spectra.

The works included into the *scientific achievement* described here are focused on the implementation of solutions from the field of CS into NMR spectroscopy and can be divided into five groups: (i) direct use of CS methods known from other fields (works (1) and (2)), (ii) the application of solutions developed during the chemical studies (3),(12), (iii) the use of compressibility of the spectra in the measurement of diffusion (4),(6),(7),(14), (iv) development of new CS methods for NMR spectrum (5),(9),(10), (v) time-resolved techniques based on the data processing using CS (8),(11),(13).

The main goals of my research were as follows:

- Examine the possibility of implementing some of the CS algorithms that assume the existence of strictly sparse signal representation, known from other areas, into NMR spectroscopy. The answer whether it is possible or not was not obvious, because the NMR spectrum is not exactly sparse (perfect compressible).

- Develop customized CS algorithms adapted to NMR spectra, by strengthening the sparsity of the spectrum, matching the density of the sampling to the relaxation of NMR signal (and define the limits of applicability of this treatment in the case of CS) and employing the assumption of Lorentzian peak shape.
- Exploit the compressibility of a spectrum from diffusion experiments by introducing sparse regularization of the inverse Laplace transform, its modification adapting it to the samples of polydispersed polymers and combined Fourier and inverted Laplace transform for three-dimensional experiments with diffusion dimension.
- Elaborate the theory and practice of time-resolved techniques based on non-uniform random sampling combined with CS reconstruction. Transfer the idea to diffusion experiments.

The magnetic properties of nuclei with non-zero spin (eg. ^{1}H, ^{13}C, ^{15}N, ^{31}P) are the basis of NMR spectroscopy. In a classic NMR experiment nuclear spins are polarized with high, static magnetic field and excited with electromagnetic irradiation of radio frequency. Signal often referred to as Free Induction Decay (FID) is emitted during the return to equilibrium. The FID signal is a sum of decaying oscillations corresponding to the number of groups of nuclei with different electron environment (i.e. shielding). Therefore, the analysis of the NMR spectrum allows one to draw information about the molecular structure. The FID signal is measured in a discrete manner, i.e. it is sampled by analog-to-digital converter. A result of measurement is a vector of samples $\mathbf{s}$, while its spectrum $\mathbf{S}$ is a solution to the following system of equations:

$$\hat{\mathbf{F}}\mathbf{S} = \mathbf{s} \tag{1}$$

where $\hat{\mathbf{F}}$ is an inverse Fourier transform matrix, $\mathbf{s}$ is an FID signal, and $\mathbf{S}$ is its spectrum.

System of equations 1 has a unique solution only when $\hat{\mathbf{F}}$ is a full-rank matrix, which corresponds to sampling consistent with the sampling theorem formulated independently by Nyquist, Shannon, Kotelnikov and others. The theorem says that the signal is perfectly represented by a finite discrete set of spectral samples, if the sampling rate is greater than or equal to twice the highest frequency of the signal. The second condition is that the number of equations has to be equal to the number of unknowns. This condition binds the resolution of the spectrum with the length of the vector $\mathbf{s}$ (the number of sampling points).

Studying complex mixtures of macromolecules using NMR became possible in 1970's, after introducing the concept of multidimensional spectroscopy. In such experiments the multidimensional signal is recorded, that originates from pairs (2D), triplets (3D) etc. of nuclei linked by some physical interaction (e.g., dipolar or scalar coupling). Additional dimensions increase resolution of the spectrum - each peak therein corresponds to at least a pair of frequency coordinates (2D), making peak position more unique than in 1D spectrum.

The introduction of additional dimensions leads to significant increase in the experimental time, because every point in indirectly measured dimensions costs a few seconds of "real time". As a result, the time spent on the experiment is associated with the resolution of the recorded spectrum. This relation is sometimes called the Fourier uncertainty

principle. As a result, despite very long (hours, days) experiments, the spectral resolution is far from being determined purely by relaxation.

Since the mid-eighties of the XX century, a number of methods known as *fast* NMR spectroscopy has been developed. The methods allow to accelerate the multidimensional experiments. The most commonly used approach is called non-uniform sampling (NUS), also known as random or sparse sampling. The idea of NUS is to omit a large fraction of sampling points and reconstruct them afterwards using sophisticated mathematical methods.

The methods described within the presented series of works are based on NUS and data processing using the most modern group of NUS reconstruction algorithms, known as compressed sensing (CS). An important feature of the approach is a solid mathematical theory that distinguishes CS from many formerly used semi-empirical NUS methods.

The main theorem of CS states that a perfect reconstruction of the omitted signal points is possible from much smaller set of data than specified in a classic sampling theorem and that NUS is the optimal way to obtain these data. To enable the reconstruction using CS, the signal must have *sparse* representation, i.e. representation consisting mostly of zeros. NMR spectrum, as an object compressible to the list of peaks, is such a representation of the FID signal.

One of the ways in which CS can be understood is considering the system of equations 1 with a vector $\mathbf{s}$ being a set of samples of indirectly measured dimensions of N-dimensional FID signal. In NUS approach, the number of equations is smaller than the number of unknowns (elements of $\mathbf{S}$), and thus the number of solutions to 1 is infinite. Choosing one of them is possible under additional assumptions. The CS theory shows, that the assumption, that $\mathbf{S}$ has a minimal ℓ_1-norm [1] is equivalent to the assumption, that spectrum is sparse (i.e. it has also minimum ℓ_0-norm, whose direct minimization is a complex combinatorial task). In the CS method, spectrum $\mathbf{S}$ is thus found by minimizing the functional:

$$\min_{\mathbf{S}} \; ||\hat{\mathbf{F}} \cdot \mathbf{S} - \mathbf{s}||_{\ell_2} + \lambda \cdot ||\mathbf{S}||_{\ell_p} \tag{2}$$

Norm in the second term is usually ℓ_1-norm and then the minimized function has one global minimum. Using the standard ℓ_p-norm ($0 < p < 1$) theoretically allows for the reconstruction from a smaller number of samples, but minimized function becomes non-convex.

In my first paper on the use of CS in NMR spectroscopy (1) I verified the applicability of the method for several cases of two-dimensional spectra of the proteins: ubiquitin and azurin. The used techniques were: 2D ^{15}N HSQC, 2D DQF COSY and 2D NOESY. The first of them, giving the most compressible spectrum (containing smallest number of peaks) allowed to verify the behaviour of the algorithm for very low sampling level and comparing the effectiveness of popular algorithms: minimizing the ℓ_1-norm (*iterative soft thresholding*, *IST*) and the ℓ_p-norm (*iteratively re-weighted least squares IRLS*). For such a simple spectrum, both methods gave similar results. In the case of 2D NOESY spectrum, significant difference in the convergence was observed, with IRLS being superior method. NOESY spectrum, characterized by a large range of peak intensities is a big

[1] ℓ_p-norm in a space of coordinates is a following function: $|\mathbf{x}|_p = (|x|_1^p + |x|_2^p + \ldots + |x|_n^p)^{\frac{1}{p}}$

challenge for the methods of *fast* NMR. Accuracy analysis of the reproducibility of peak intensities, which are the most important data obtained from NOESY spectra, showed good agreement with the results obtained from the full sampling. 2D DQF COSY spectrum served as an example of NMR measurement of unusually shaped signal (starting from zero) and the complex spectral lines (multiplets in antiphase). IRLS method perfectly coped with the reconstruction from about 30 % of the data.

Paper (1) was a short communication and constituted only a starting point to the further work. It became clear that one should more accurately analyse performance of the tested algorithms, improve their speed, extend them to the spectra of higher dimensionality and check the effectiveness for more or less standard cases. It is worth noting, that work with almost identical title (*Fast Multidimensional NMR Spectroscopy Using Compressed Sensing*) was sent by a group of Daniel Holland from Cambridge to the same journal, just 3 days after ours (18.01.2011 vs. 15.01.2011). This shows how hot topic was the use of CS at the time.

After the success of the first paper and my coming back to Poland, I decided to apply for IUVENTUS PLUS grant for the development of the method. I got the funding and implemented the grant from 2011 to 2014.

The second work of the series concerned the extended performance analysis of IST and IRLS algorithms, that is, two approaches to the CS problem - one based on the minimization of a functional with one global minimum (standard ℓ_1-norm IST algorithm) and with many local minima (ℓ_p-norm IRLS algorithm). In addition, it contained a comparison of CS with completely different NUS method known as multidimensional decomposition (MDD). The analysis was conducted based on the following spectra: a) 2D 15^{N} HSQC, b) 3D 15^{N}-edited NOESY-HSQC c) 3D HNCO, and noiseless simulated spectra having different (similarly to the mentioned experimental spectra) distribution of spectral magnitude (DoSM). The spectrum a) characterized by a wide DoSM gave similar result from IST and IRLS (which was in line with the observations made in other areas than NMR), and the small compressibility (sparsity) of 2D spectra did not allow to reach the low levels of sampling. In the case b), characterized by a narrow DoSM, but a large range of peak intensities, IRLS has beaten IST, both in terms of quality and convergence as a result of the low sampling rate, but still MDD method gave better results. For spectra from example c), with a narrow DoSM and low intensity of peaks, IRLS proved to be the best available method of data processing, beating IST in both the convergence and reconstruction quality at low sampling levels. The conclusion from the work made it possible to choose the optimal algorithm for future applications. It was the IRLS, except for the cases of large 3D data sets, where it proved to be too computationally demanding.

In November 2012, after publishing paper (2), I started working at the Centre of New Technologies, University of Warsaw.

Conclusions from work (2) were used in studies of chemically modified cyclodextrin, described in the paper (3). The test compound, mono-(6-deoxy-6-(1-1,2,3-triazol-4-yl)-1-propane-3-O-(phenyl))-β-CD, was obtained by a chemical modification (functionalization) of one of the sugar residues in the cyclodextrin ring. The molecule was "almost-symmetrical", ie. breaking its perfect symmetry by the attached "tail" had only a little impact on the otherwise completely degenerated chemical shifts characteristic for non-functionalised β-CD. Therefore, the assignment of the spectrum of such molecule requires

very high resolution that can be achieved only in very long (20 h) acquisition of 2D ^{13}C HSQC, and equally long 2D ^{13}C HSQC-TOCSY and 2D ^{13}C HSQC-NOESY. The reasons are purely mathematical - requirement of dense sampling due to large spectral range for ^{13}C, and of "reaching" far into ^{13}C evolution time space due to overlap of peaks. Both lead to the necessity of measuring 10 000 points in the ^{13}C dimension. The study showed that the CS reconstruction with just 512 points gives equally good results, allowing one to carry out the necessary measurements in one night, instead of 60 hours. In addition to analysing the linearity of the reproduced peak intensities, I conducted the analysis of the fidelity of the peak intensity reconstruction.

In May 2013 I obtained SONATA BIS 2 grant for establishing a team developing the theory and applications of CS-NMR, in particular for the adaptation of the method to specific features of NMR spectra (e.g. the fact, that they are not strictly sparse).

Paper (4) opened a new direction in the applications of sparse regularization, i.e. its use in the processing of data from diffusion and "diffusion-resolved" spectroscopy (DOSY). Such experiments contain diffusion dimension where the signal decays exponentially at the rate proportional to the rate of self-diffusion of a given molecule in the sample. The method is sometimes used to measure the diffusion coefficient, but more often to split the spectrum of the mixture of compounds into the individual sub-spectra. The problem is, however, decoding of the exponential decay rate. Inverse Laplace transform (ILT), which is used for this purpose, is a procedure that is numerically very unstable and requires regularization. The paper (4) proposed to use here the sparsity-promoting variant of Tikhonov regularization in order to turn the solved the problem into a form similar to the one given by Equation 2:

$$\min_{A} \ \|\Phi\mathbf{A} - \Psi\|_{\ell_2}^2 + \tau\|\mathbf{A}\|_{\ell_1} \tag{3}$$

where $\mathbf{A}$ is the distribution of diffusion coefficients, Φ - ILT operator and Ψ - the measured signal. The problem can be solved using algorithms identical to those used for Fourier transform and NUS. The method was implemented and compared with other approaches by mgr Mateusz Urbańczyk, the first author of the paper (4). These and other results of Mateusz Urbańczyk are present in his doctoral dissertation and I am an auxiliary supervisor of his work. Experimental tests were conducted on samples of polymers of polyethylene oxide with different molecular weights. The conclusions from the work were promising - FISTA algorithm (faster variant of IST) gave better reproduction of the relative peak heights in the diffusion dimension than the previously used ℓ_2-norm regularization or maximum entropy method. The only disadvantage was the possible presence of false peaks for polydisperse samples, i.e. those characterized by a wide profile of the diffusion coefficient distribution. This problem was addressed later in the work (14).

Another publication was made in collaboration with the French team, which I established at the NMR symposium organized at the Institute of Organic Chemistry, PAS. It concerned the often-discussed aspect of NUS, namely the possibility of improving the sensitivity of measurement by relaxation-matched sampling of the signal, i.e. denser in its initial part. There was a number of studies showing the effect (e.g. Rovnyak et al., Magn. Reson. Chem., 2011), but they did not consider the limitations of reconstruction

algorithms applied to sampling of varying density. In the work (5) I used the elements of the CS theory to formalize these restrictions. The theory shows that the most effective sampling is purely random and any deviation from it, such as sampling rate decaying along with the signal, can cause problems with the reconstruction. Feature of sub-sampled matrix $\hat{\mathbf{F}}$ known as *restricted isometry property* (RIP) allows to assess whether the sampling gives a chance for accurate reproduction of all K-sparse vectors $\mathbf{S}$. The smaller the isometric constants δ_K^{min} and δ_K^{max} in an inequality fulfilled for such vectors:

$$\left(1-\delta_K^{min}\right)||\mathbf{S}||_{\ell_2}^2 \leq ||\hat{\mathbf{F}}\cdot\mathbf{S}||_{\ell_2}^2 \leq (1+\delta_K^{max})\,||\mathbf{S}||_{\ell_2}^2 \tag{4}$$

the greater the chance of accurate reconstruction using CS methods. Chance of perfect reconstruction of all K-sparse vectors is very low because it requires $(4\sqrt{2}-3)\delta_{2K}^{min}+\delta_{2K}^{max} < 4(\sqrt{2}-1)$. However, even if this condition is not met, the values of constants well reflect the "quality" of the sampling. Calculating them can be difficult, but it is possible by using advanced algorithms. One of them was used in the work to show that the sampling patterns with strong decay result in high isometric constant values. I also showed the reconstruction errors resulting from such a sampling (false peak splittings in the spectrum) and how to find an optimum between gain in signal-to-noise ratio and imperfections of the reconstruction. The optimal sampling was used in the two-dimensional autocorrelation experiments in which the co-authors of the paper recorded a deuterium signal of chiral compounds dissolved in a chiral liquid crystal PBLG in order to separate the spectra of the enantiomers. Experiments featured low sensitivity, because they were conducted on the natural abundance of deuterium. Using an optimum NUS schedule and CS reconstruction, the obtained spectra were better than those obtained with a classical, full sampling.

In July 2013 I obtained HARMONIA grant for the cooperation with Dr. Diana Bernin from Swedish NMR Centre in Gothenburg. The goal of the project was to study the possibility of implementing methods of sparsity-regularized DOSY in studies of mixtures of metabolites.

In papers (6) and (7) I dealt with the implementation of a concept of a joint non-uniform sampling of a signal in diffusion and evolution time dimensions. A glance at the equations 2 and 3 allows to suggest the following functional, whose minimization will quickly and accurately lead to a spectrum in experiments such as 3D HSQC-DOSY:

$$\min_{\mathbf{Q}} \ \|\mathbf{PQ}-\mathbf{q}\|_{\ell_2}^2 + \tau\|\mathbf{Q}\|_{\ell_1}$$

where $\mathbf{P}$ is a combined FT-ILT operator:

$$\mathbf{P} = \mathbf{F}\otimes\mathbf{\Phi}$$

$\mathbf{q}$ is a vector of samples of an indirect dimension of a signal:

$$q(t_1,g) = \sum_{i=1}^{N} s_i(t_1)\otimes\Psi_i(g)$$

and $\mathbf{Q}$ is its spectrum.

Publication (6) was a communication at the IEEE conference on signal processing, presented with the hope that the concept may find wider application outside NMR. The paper (7) showed the applications of the method for obtaining the spectrum of a three-dimensional signal with indirectly measured diffusion and time dimensions (3D-HSQC iDOSY) where combined gradient and evolution time space were non-uniformly sampled. I tested the fidelity of a reconstruction of a spectrum of four-component mixture involving compounds which are common metabolites (citrate, taurine, alanine, 2,4,6-trimethyloalanine) and two-component sample of quercetin and rutin that, due to the similarity of these compounds, featured degeneration of the ^{1}H resonance frequencies and only higher-dimensional spectrum could separate them. Quite surprisingly, the precision of reconstructed diffusion coefficients was well above the classical approach based on a uniform sampling of the evolution time repeated for several values of diffusion-encoding gradient. The presented method gave better results than even 2.5× longer classic experiment. The analogical method based on combined NUS and FT-ILT is currently being implemented in the relaxation measurements of proteins.

Publication (8) was the first of a series of works discussing the theory and possible applications of time-resolved non-uniform sampling with CS processing. The basis of the method is to carry out NUS of two or more indirectly measured dimensions in parallel to certain process (chemical or physical) occurring in the sample and influencing the spectrum. Since the sampling scheme is "shuffled", it can be divided into equivalent, overlapping subsets and each of them can be reconstructed with CS. The result is a set of spectra resembling frames of a movie and forming a temporal pseudo-dimension that shows changes of the sample.

In the work (8), which consisted of research conducted in collaboration with Bruker Biospin company, we presented the method to monitor the process of thermal unfolding of a protein. In parallel to random sampling of indirectly measured signal in the 2D ^{15}N HSQC experiment, we changed the temperature of the sample at a rate of about 1 K/min (slow enough to avoid significant gradients of temperature). The division of data into subsets provides almost continuous picture of changes of chemical shifts and intensities of peaks arising from changes in the structure of the protein within a wide range of temperatures (293 K $\rightarrow$ 338 K). The data obtained for the human ubiquitin protein and SH3 domain of spectrin protein from chicken brain well coincided with the spectra from a series of conventionally sampled 2D ^{15}N HSQC experiments carried out at constant temperatures. Accordance was almost ideal for chemical shifts, but slightly worse in the case of peak intensities. This effect, caused by additional artefacts in time-resolved NUS, was examined in more details in the work (13). The publication described the problems that may be associated with the wrong choice of the size of a subset of data, i.e. "a frame". If frames are too small, then obtained spectrum has a low signal-to-noise ratio or artefacts from the NUS reconstruction. If frames are too large, the problem may be the averaging of the studied effects (peak shifts and changes in their intensities) over the time needed to acquire a single subset.

Adaptation of CS methods to NMR spectra is necessary, due to the fact that the NMR spectrum is not perfectly compressible. It consists of Lorentzian-shaped peaks, so even a single peak is, strictly speaking, infinitely broad (in particular its dispersion part). The idea of optimizing the CS performance, based on the elimination of the imaginary part

of the spectrum by combining an FID signal with its own *Virtual Echo* (VE), i.e. the conjugate reflection, has been tested and developed in collaboration with prof. Vladislav Orekhov from University of Gothenburg. I took care of its implementation in CS methods and the explanation of its mechanism based on the concept of sparse minimization. The results are described in the publication (9). The use of VE significantly improved the efficiency of CS methods and related SIFT method (also based on a concept of sparsity, but with strictly defined regions free of peaks, see Matsuki et al. JACS, 2009, (13) 4648–4656), in particular for low sampling levels. This is consistent with the CS theory, which connects the number of sampling points required for perfect reconstruction with a number of significant points of the spectrum, where "significant" means high value of their ℓ_p-norm. Using VE has one limitation, namely, it requires knowledge of a possible phase error of a signal in the dimensions in which VE is used. However, for indirectly measured dimensions, phase is always well-known, if only the pulse sequence is properly implemented. Interestingly, the concept of VE helped to explain the effect that I noticed during the first tests of CS algorithms, namely, that the quality of the reconstruction is much better, if the input FID signal is zero-filled twice in each of the reconstructed dimensions. It turns out that each of the sparse reconstruction algorithms which has in the minimized functional the term $||\mathbf{S}||_{\ell_p}$ (and thus contains both Re and Im parts) attempts to zero the imaginary part by "constructing" VE. Therefore, it seems reasonable to add VE to the signal before the reconstruction in order to reduce the number of unknowns. VE has yet another advantage - in the case of spectra with three and more dimensions, it allows the reconstruction of all quadrature modulations (e.g..cosine-cosine, sine-cosine, sine-cosine and sine-sine for 3D) in one minimization procedure, i.e. they can all be reconstructed from the corresponding components of VE. In the case of classical processing and use of programming libraries of complex numbers (not hypercomplex), one has to perform the processing of 3D signal in two steps, reconstructing separately cosine and sine signal in one of the dimensions.

Publication (10) also described the adaptation of one of the most classic CS methods, namely, the greedy algorithm of *orthogonal matching pursuit* (OMP) to the specific case of decaying signal, such as FID signal. The most standard variant of OMP starts the reconstruction from a spectrum obtained by the direct FT of NUS data. Then each iteration finds the highest point of such a vector and subtracts from it the convolution of that point with *point spread function* (PSF), i.e. FT of a sampling scheme. The point itself is added to the output vector. The approach is slightly different from the method known in NMR spectroscopy as CLEAN algorithm (Högböm, Astron. Astrophys. Suppl., 1974; Barna et al., Journ. Magn. Reson., 1988) by the orthogonalization of the components found in each iteration. Both CLEAN and OMP are not particularly effective in the case of the NMR signals. Numerous optimizations of CLEAN can be found in the literature, but they are not based on the CS formalism (specifically, on the mathematical description of OMP). In our work, we proposed a modification of OMP adapting the method to NMR spectra. An additional step was added into the algorithm, where the optimal peak width is found and the convolution is performed not only with the PSF, but also with an appropriate Lorentzian curve. The algorithm of Lorentzian Peak Matching Pursuit (LPMP), developed by co-author of the paper, Dr. Paweł Kasprzak and adapted by me to NMR spectra was compared by us with other CS methods, e.g. IST, StOMP, COSAMP, OMP. All of them provided worse reconstruction quality for the

spectra consisting of Lorentzian peaks.

Work (11) was the second publication (after (8)) on the applications of time-resolved CS. This time, we explored the possibility of monitoring multiple reactions occurring at once in natural mixtures of fermenting milk and flour, using time-resolved 2D ^{13}C HSQC spectra. The case of naturally occurring chemical reactions differs from the case discussed in (8) where the process was enforced by varying temperature. The reactions cannot be easily stopped in order to perform classical experiment. In this situation, the multidimensional NUS/CS measurement is the only alternative to a series of one-dimensional spectra, which, however, (as shown in (11)) do not have sufficient resolution to follow even the main products of reactions. The paper showed, that the intensities of the peaks in a time-resolved spectrum accurately reflect the reaction progress. The fact, that time profiles of peak intensities of the molecules belonging to the same reaction are correlated, allows the separation of the spectrum of a mixture into "sub-spectra" of individual components. Therefore, this approach may be a good alternative to DOSY. What is needed, is only an adaptation of the tools of statistical correlation spectroscopy (STOCSY), so that one can efficiently process large data sets. For this purpose it is planned to create STOCSY algorithms operating on peak intensities not on the points of the spectrum. The development of time-resolved spectroscopy based on NUS/CS is the main goal of OPUS 9 project entitled "Time-resolved N-dimensional spectroscopy for monitoring of physical and chemical processes", which will be implemented in years 2016-2018.

Publication (12) is an example of effective use of CS, that is different from the one shown in (3), as here CS is applied to the spectra of disordered proteins. It is also the case where CS is particularly effective because of the good compressibility of spectra. Two-dimensional techniques presented in the paper are used to effectively excite only the nuclei of selected amino acid residues. As a result, the number of peaks in a spectrum is very small (comparing to non-selective techniques) and they can be successfully restored from the small set of data.

In work (13) I took up the problem of artefacts present in the time-resolved spectra processed with CS. The artefacts resemble thermal noise, and they appear due to a change of signal parameters during the measurement. This effect was already thoroughly discussed for the classically sampled spectra, where it lead to a peak shape convolved with the FT of a function describing the change. In the case of "shuffled" sampling, the function (and its FT) take up a form of noise, independently of their original shape. In the paper, I presented the theory that allows to predict the ratio between the peak height and the level of noise (artefacts). To verify the theory, I chose the 2D NOESY spectrum in which the faithful reproduction of peak intensities is particularly important, because they carry information on the distances between the correlated nuclei. In the presented NOESY technique with time-resolved CS, the evolution delay t_1 was subjected to shuffled NUS and the length of mixing time varied linearly. In this way, each subset of the data corresponded to some average mixing time and the peak intensity as a function of that time formed a curve showing a build-up of a nuclear Overhauser effect (*nOe build-up curve*). In the classical approach, the curve is obtained by measuring at least two 2D NOESY experiments with full sampling, each with a different mixing time (but fixed for a given experiment). Slope of the line fitted to peak intensity vs mixing time plot, allows

to determine the distance between the interacting nuclei. The problem may be, however, deviations from linearity due to spin diffusion and relaxation. If the data set consists of only two points, such a deviation can be difficult to grasp. Therefore, the proposed CS experiment allows to obtain more complete data in a short time. It was demonstrated, that the internuclear distances were reconstructed with a good accuracy using the number of sampling points significantly less than that corresponding to the two spectra with full sampling. For example, the 2D NOESY experiment with time-resolved NUS carried out on a sample of strychnine in $CDCl_3$ with the change of mixing time from 300 ms to 700 ms and sampling using only 340 points allowed to determine internuclear distance with over three times smaller error than two classic experiments with constant mixing time of 300 and 700 ms (512 points). The reason could be the fact that 700 ms was in the non-linear part of nOe curve. The use of classical spectra with mixing time of 300 and 600 ms made it possible to achieve the result of a quality comparable to that obtained with NUS. This proves that the proposed measurement method has low inherent errors and is also less prone to mistakes in experimental design, such as a overestimation of the length of linear region in nOe build-up curve. Nevertheless, the main achievement of the work (13) was not to present a novel NOESY method, but to verify theoretical predictions concerning the artefact level in time-resolved NUS. As it turned out, the theoretically calculated trend binding the signal-to-artefact ratio with the rate of peak intensity change within a "frame" was well confirmed by the experiments.

The last publication in the present series (14) described the analysis of the possibility of controlled "depart" from the sparse regularization in the spectra in which peaks are characterized by a substantial width. Although these problems can also be found in the frequency dimensions (e.g. in experiments carried out in solid state), we decided to develop a solution for the inverse Laplace transform (ILT) used in the diffusion spectra due to the issues with which we are dealing in the research carried out together with cooperating groups. From the previous work on sparsely regularized ILT (4), I knew that the method might cause problems with the artificial splitting of peaks in the case of spectra of polydisperse samples, i.e. those characterized by a broad (and unknown) distribution of diffusion coefficients associated with a wide range of molecular weights. The study (14) recalled a mathematical proof showing that the use of norms higher than 1 in the regularization term in equation 3 leads to a "smoothing" of a result. Thus, in the case of polydisperse samples using such a regularization may allow more accurate reconstruction of the spectrum. Of course, if the actual distribution of diffusion coefficients is not known, then unknown is also an optimal ℓ_p ($1 \leq p \leq 2$). We proposed a simple but effective method of finding it by repeating reconstruction for different values of p and choosing the one that gave the best fit on the side of the signal.

Two experimental tests have shown the performance of the new solution. First was based on the measurement of spectra of a series of synthetic samples of polymers of polyethylene oxide each having different diffusion profiles - both the medium value and the width of the distribution. It turned out that the value of p correlates well with the latter parameter. The second test consisted of carrying out the reaction which changed the polydispersity of the sample, and its monitoring by an experiment similar to time-resolved NUS, but containing shuffled sampling of diffusion-encoding gradient. In the experiment, high molecular weight heparin underwent hours-long decomposition reaction

by the enzyme heparinase. This resulted in smaller fragments that were quite random in size, and thus in a change of average diffusion coefficient (going down), as well as the width of the distribution (increasing). The study showed that the rates of change of these two values are similar, as well as the rate of increase of peak intensity of another reaction product i.e. uronic acid.

Summary of the main achievements connected with the presented series of papers:

- Proof of the possibility of application of the CS algorithms in the reconstruction of NMR spectra from incomplete data; demonstration of a such possibility in studies of small and large molecules
- Modyfing the CS methods in order to adapt them to NMR signal - sampling matched with the relaxation (defining the limits of applicability), *virtual echo*, *LPMP* algorithm
- Application of sparse regularization in diffusion experiments and joint gradient/time sampling in FT/ILT
- Development of theory and time-resolved techniques for homo- and heteronuclear correlation experiments as well as diffusion spectroscopy.

The significance of the achievements for the field of NMR spectroscopy and beyond:

- The developed algorithms are implemented in the free software MddNMR and constitute a NUS module of TopSpin software that drives the spectrometers of Bruker company, the biggest NMR vendor in the world.
- They are used by hundreds of NMR labs in the world. The most spectacular examples of use of the program are:
  - T. Wauer, M. Simicek, A. Schubert, and D. Komander. Mechanism of phospho-ubiquitin-induced parkin activation. *Nature*, 524(7565):370–374, 2015
  - T. Didenko, A. Proudfoot, S.K. Dutta, P. Serrano, and K. Wüthrich. Non-Uniform Sampling and J-UNIO Automation for Efficient Protein NMR Structure Determination. *Chemistry - A European Journal*, 21(35):12363–12369, 2015
  - J. Saurí, N. Marcó, R.T. Williamson, G.E. Martin, and T. Parella. Extending long-range heteronuclear NMR connectivities by HSQMBC-COSY and HSQMBC-TOCSY experiments. *Journal of Magnetic Resonance*, 258:25–32, 2015
  - Christina M Thiele and Wolfgang Bermel. Speeding up the measurement of one-bond scalar (1J) and residual dipolar couplings (1D) by using non-uniform sampling (NUS). *J Magn Reson*, 216:134–143, 2012
- I have established a team at the Centre of New Technologies, which is involved in the development of dedicated NMR solutions for chemical and biological groups cooperating with us.
- I have established a spin-off company with the contribution from UW - Spektrino Sp. z o.o., where I am a chairman of the board. The activity of the company focuses on the commercialization of the developed solutions, e.g. currently it is participating

in establishing a computational server for NUS processing with user-friendly web interface.

5 Summary of other scientific achievements

After completing my doctoral studies, I was involved for some time in the development of the method based on the direct Fourier transform of the NUS signal, which I have described in my PhD dissertation. This method, in contrast to the CS, does not attempt to reconstruct the omitted signal points, but assumes that they are equal to zero. The advantage of this method is high computational efficiency, making it suitable for use in large data sets, for example high-dimensional spectra (4D+). The disadvantage are the noise-like artefacts, the source of which is in mentioned coarse assumption about the points omitted during measurement of the signal. Each peak in the spectrum is convolved with the artifact pattern (point spread function).

The resulting artefacts resemble noise, not only in their shape, but also properties. For example, the ratio between the height of a single peak and artefacts convolved with it, scales with the square root of a number of sampling points (see the paper (i)). This means, that such a simple processing method as direct FT is often quite sufficient for high-dimensional experiments where, due to the poor sensitivity, one has to collect a huge number of sampling points. An exception are NOESY or TOCSY spectra, where one deals with a large range of peak intensities. However, for spectra serving for e.g. assignment of signals to the protein backbone nuclei, direct Fourier transformation provides many opportunities. New experiments of this type were described in papers (i, v, vi). In addition, due to the fact that the method does not try to reconstruct the full signal, one can limit the spectrum to the areas in which peaks are expected. The method of Sparse Multidimensional Fourier Transform (SMFT) based on such a principle was described in paper (iii).

Besides the works on the development of multidimensional techniques, I was a co-author of several reviews concerning new methods of NMR signal processing based on sparse sampling (iv,vii,ix,xi,xii). Also, I have run standard NMR experiments, for instance described in work (viii).

During my employment at the Centre of New Technologies UW, I have been free of teaching duties, but I was given a task of organizing the NMR lab, i.e. finding the funding for a team, instrumentation maintenance, planning the rooms in a newly constructed building and re-installation of Varian 700 MHz spectrometer working before at the Faculty of Chemistry, UW. All these tasks were completed with success. My team includes currently 6 persons financed from grants. The lab will be soon equipped with a new bench-top mini-spectrometer.

Dr. Krzysztof Kazimierczuk
University of Warsaw
Centre of New Technologies
Laboratory of NMR Spectroscopy
ul. Banacha 2C
02-089 Warszawa

List of published scientific papers or professional creative works and information on teaching achievements, scientific collaborations and popularization of science

Warsaw, Tuesday 17th May, 2016

1 List of published scientific papers or professional creative works and information on teaching achievements, scientific collaborations and popularization of science

(a) **Identification of achievement pursuant to Art.16(2) of the Act of 14 March 2003 on scientific degrees and artistic titles (Journal of Laws no. 65, item 595 as amended) setting the basis for the habilitation proceedings**

(A) **Title of scientific achievement: "Sparse and nearly-sparse representations in problems of NMR spectroscopy"**

(B) **List of scientific publications setting the basis for habilitation proceedings:**

(1) K. Kazimierczuk and V.Yu. Orekhov. Accelerated NMR spectroscopy by using compressed sensing. *Angewandte Chemie - International Edition*, 50(24):5556–5559, 2011

My contribution to this work was to implement IRLS and IST algorithms in MATLAB, perform simulations, process the data from NMR experiments and perform statistical analysis. I also wrote a part of the manuscript. Author's contribution: 70%. **IF(2011)=13,455 number of citations=90**

(2) K. Kazimierczuk and V.Yu. Orekhov. A comparison of convex and non-convex compressed sensing applied to multidimensional NMR. *J. Magn. Reson.*, 223:1–10, 2012

My contribution to this work was to formulate a research hypothesis, run simulations, process data from the NMR experiments and perform statistical analysis. I have also written 50 % of the manuscript. I have coordinated the IUVENTUS PLUS project from which the study was co-financed. I am the corresponding author of the paper . Author's contribution: 80%. **IF(2012)=2,300 number of citations=13**

(3) M. Misiak, W. Koźmiński, K. Chmurski, and K. Kazimierczuk. Study of near-symmetric cyclodextrins by compressed sensing 2D NMR. *Magnetic Resonance in Chemistry*, 51(2):110–115, 2013

My contribution to this work was to formulate part of the concept of work (use of CS in 2D NMR to enhance resolution), perform experiments, data processing and analysis of the effectiveness of methods. I have also written a part of the manuscript. I have coordinated the IUVENTUS PLUS project from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 40%. **IF(2013)=1,528 number of citations=3**

(4) M. Urbańczyk, D. Bernin, W. Koźmiński, and K. Kazimierczuk. Iterative thresholding algorithm for multiexponential decay applied to PGSE NMR data. *Analytical Chemistry*, 85(3):1828–1833, 2013

My contribution to this work was to formulate the research hypothesis (the idea of using sparse regularization) and perform part of the analysis of the effectiveness of the method. I have also written a part of the manuscript. I have coordinated the IUVENTUS PLUS project from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 30%. **IF(2013)=5,825 number of citations=2**

(5) K. Kazimierczuk, O. Lafon, and P. Lesot. Criteria for sensitivity enhancement by compressed sensing: Practical application to anisotropic NAD 2D-NMR spectroscopy. *Analyst*, 139(11):2702–2713, 2014 My contribution to the work was the theoretical part, simulations as well as processing and analysis of experimental data. I have coordinated the IUVENTUS PLUS and SONATA BIS 2 projects from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 60 %. **IF(2014)=4,107 number of citations=8**

(6) Mateusz Urbańczyk and Krzysztof Kazimierczuk. A method for joint sparse sampling of time and gradient domains in diffusion-ordered NMR spectroscopy. In *Signal Processing Symposium (SPS), 2013*, pages 1–6. IEEE, 2013

My contribution to this work was to formulate the research hypothesis (the idea of using sparse regularization) and perform a part of the analysis of the effectiveness of the method. I also wrote a part of the manuscript. I have coordinated the HARMONIA and SONATA BIS 2 projects from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 50%. **IF(2013)=0 number of citations=0**

(7) M. Urbańczyk, W. Koźmiński, and K. Kazimierczuk. Accelerating diffusion-ordered NMR spectroscopy by joint sparse sampling of diffusion and time dimensions. *Angewandte Chemie - International Edition*, 53(25):6464–6467, 2014 My contribution to this work was to formulate the research hypothesis (the idea of using sparse regularization) and perform half of the experiments and a part of the analysis of the effectiveness of the method. I also wrote a part of the manuscript. I have coordinated the HARMONIA and SONATA BIS 2 projects from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 35%. **IF(2014)=11,261 number of citations=2**

(8) W. Bermel, R. Dass, K.-P. Neidig, and K. Kazimierczuk. Two-dimensional NMR spectroscopy with temperature-sweep. *ChemPhysChem*, 15(11):2217–2220, 2014

My contribution to this work was to develop a research concept, perform simulations and prepare the data processing algorithms. I also wrote a part of the manuscript. I have coordinated the IUVENTUS PLUS and SONATA BIS 2 projects from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 70%. **IF(2014)=3,419 number of citations=2**

(9) M. Mayzel, K. Kazimierczuk, and V.Yu. Orekhov. The causality principle in the reconstruction of sparse NMR spectra. *Chemical Communications*, 50(64):8947–8950, 2014

My contribution to this work was to develop part of the theory, run and analyse simulations and prepare data processing algorithms for the part of work on compressed sensing. I have coordinated the IUVENTUS PLUS and SONATA BIS 2 projects from which the study was co-financed. Author's contribution: 40%. **IF(2014)=6,834 number of citations=8**

(10) K. Kazimierczuk and P. Kasprzak. Modified OMP algorithm for exponentially decaying signals. *Sensors (Switzerland)*, 15(1):234–247, 2014

My contribution to this work was to develop part of the theory of direct NMR spectroscopy, and the execution and analysis of experimental data. I also wrote a part of the manuscript. I am the corresponding author of the paper. Author's contribution:

50%. **IF(2014)=2,245 number of citations=2**

(11) Rupashree Dass, Wiktor Kozminski, and Krzysztof Kazimierczuk. Analysis of complex reacting mixtures by time-resolved 2D NMR. *Analytical Chemistry*, 87(2):1337–1343, 2015

My contribution to this work was to develop a concept of research, perform a part of the experiments and prepare some of data processing algorithms. I also wrote a part of the manuscript. I have coordinated the IUVENTUS PLUS and SONATA BIS 2 projects from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 50%.

IF(2014)=5,636 number of citations=3

(12) A. Piai, L. Gonnelli, I. C. Felli, R. Pierattelli, K. Kazimierczuk, K. Grudziąż, W. Koźmiński, and A. Zawadzka-Kazimierczuk. Amino acid recognition for automatic resonance assignment of intrinsically disordered proteins. *Journal of Biomolecular NMR*, pages 1–15, 2016

My contribution to this work was to carry out a series of reconstruction of NMR spectra using CS algorithms. Author's contribution: 10%. **IF(2014)=3,141 number of citations=0**

(13) R. Dass, P. Kasprzak, W. Koźmiński, and K. Kazimierczuk. Artifacts in time-resolved NUS: A case study of NOE build-up curves from 2D NOESY. *Journal of magnetic resonance*, 265:108–116, 2016

My contribution to this work was to develop a concept of research, perform a part of the experiments and prepare some of data processing algorithms. I also wrote a part of the manuscript. I have coordinated the SONATA BIS 2 project from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 40%. **IF(2014)=2,51 number of citations=0**

(14) M. Urbańczyk, D. Bernin, A. Czuroń, and K. Kazimierczuk. Monitoring polydispersity by NMR diffusometry with tailored norm regularisation and moving-frame processing. *The Analyst*, 141(5):1745–1752, 2016

My contribution to this work was to formulate an idea of the paper (use of "smoothing regularizations"). I also wrote a part of the manuscript. I have coordinated the HARMONIA and SONATA BIS 2 projects from which the study was co-financed. I am the corresponding author of the paper. Author's contribution: 30%. **IF(2014)=4,107 number of citations=0**

Total impact factor of papers listed above according to the list from Journal Citation Reports: 59,534

2 List of other scientific publications (not included in point IB) and research and scientific achievement indices

A **Publications indexed in JCR database**

Paper published before PhD thesis defence:

i. K. Kazimierczuk and W. Koźmiński. Efficient compensation of low-frequency magnetic field disturbances in NMR with fluxgate sensors. *Journal of Magnetic Resonance*, 174(2):287–291, 2005

My contribution was to elaborate part of the concepts of the study and implement the solution described. Author's contribution: 50%. **IF(2005)=2,418 number of citations=13**

ii. K. Kazimierczuk, W. Koźmiński, and I. Zhukov. Two-dimensional Fourier transform of arbitrarily sampled NMR data sets. *Journal of Magnetic Resonance*, 179(2):323–328, 2006 My contribution was to create the idea of the processing method and implement it as a program used in the study. Author's contribution: 40%. **IF(2006)=2,076 number of citations=96**

iii. K. Kazimierczuk and W. Koźmiński. On the influence of low-frequency magnetic field disturbances on basic high resolution NMR experiments. *Polish Journal of Chemistry*, 80(7):1119–1124, 2006 My contribution was to describe part of the observations made during the implementation of the solution described in a paper (i). Author's contribution: 40%. **IF(2006)=0,491 number of citations=0**

iv. K. Kazimierczuk, A. Zawadzka, W. Koźmiński, and I. Zhukov. Random sampling of evolution time space and Fourier transform processing. *Journal of Biomolecular NMR*, 36(3):157–168, 2006

My contribution was to create the idea of the processing method and implement it as a program used in the study. Author's contribution: 35%. **IF(2006)=1,791 number of citations=73**

v. K. Kazimierczuk, A. Zawadzka, W. Koźmiński, and I. Zhukov. Lineshapes and artifacts in Multidimensional Fourier Transform of arbitrary sampled NMR data sets. *Journal of Magnetic Resonance*, 188(2):344–356, 2007

My contribution was to create part of the ideas of the method, perform part of the experiments and participate in the development of programs used for data processing. Author's contribution: 35%. **IF(2007)=2,253 number of citations=52**

vi. K. Kazimierczuk, M. Misiak, A. Zawadzka, and W. Koźmiński. Progress in structural studies of proteins by nmr spectroscopy. *Polimery/Polymers*, 52(10):736–744, 2007 My contribution was to describe methods of the reconstruction of under-sampled NMR spectra. Also, I wrote a part of a manuscript. Author's contribution: 25%.**IF(2007)=1,376 number of citations=2**

vii. K. Kazimierczuk, A. Zawadzka, W. Koźmiński, and I. Zhukov. Determination of spin-spin couplings from ultrahigh resolution 3D NMR spectra obtained by optimized random sampling and multidimensional Fourier transformation. *Journal of the American Chemical Society*, 130(16):5404–5405, 2008

My contribution was to create part of the ideas of the method, perform part of the experiments and participate in the development of programs used for data processing. Author's contribution: 25%. **IF(2008)=8,091 number of citations=24**

viii. K. Kazimierczuk, A. Zawadzka, and W. Koźmiński. Optimization of random time domain sampling in multidimensional NMR. *Journal of Magnetic Resonance*, 192(1):123–130, 2008

My contribution was to create part of the ideas of the method, perform part of the experiments and participate in the development of programs used for data processing. . Author's contribution: 45%. **IF(2008)=2,438 number of citations=55**

ix. K. Kazimierczuk, A. Zawadzka, and W. Koźmiński. Narrow peaks and high dimensionalities: Exploiting the advantages of random sampling. *Journal of Magnetic*

Resonance, 197(2):219–228, 2009

My contribution was to create part of the ideas of the method, perform part of the experiments and participate in the development of programs used for data processing. Author's contribution: 45%. **IF(2009)=2,531 number of citations=37**

Papers published after defence of PhD thesis:

i. A. Zawadzka-Kazimierczuk, K. Kazimierczuk, and W. Koźmiński. A set of 4D NMR experiments of enhanced resolution for easy resonance assignment in proteins. *Journal of Magnetic Resonance*, 202(1):109–116, 2010

My contribution was to create part of the ideas of the method, perform part of the experiments and participate in the development of programs used for data processing. Author's contribution: 35%. **IF(2010)=2,333 number of citations=21**

ii. K. Kazimierczuk, A. Zawadzka-Kazimierczuk, and W. Koźmiński. Non-uniform frequency domain for optimal exploitation of non-uniform sampling. *Journal of Magnetic Resonance*, 205(2):286–292, 2010

My contribution was to create part of the ideas of the method, perform part of the experiments and participate in the development of programs used for data processing. Author's contribution: 30%. **IF(2010)=2,333 number of citations=40**

iii. K. Kazimierczuk, J. Stanek, A. Zawadzka-Kazimierczuk, and W. Koźmiński. Random sampling in multidimensional NMR spectroscopy. *Progress in Nuclear Magnetic Resonance Spectroscopy*, 57(4):420–434, 2010

My contribution was to describe the method of multidimensional decomposition used in reconstruction of undersampled NMR spectra. Author's contribution: 25%. **IF(2010)=4,933 number of citations=47**

iv. V. Motáčková, J. Nováček, A. Zawadzka-Kazimierczuk, K. Kazimierczuk, L. Žídek, H. Šanderová, L. Krásný, W. Koźmiński, and V. Sklenář. Strategy for complete NMR assignment of disordered proteins with highly repetitive sequences based on resolution-enhanced 5D experiments. *Journal of Biomolecular NMR*, 48(3):169–177, 2010

My contribution was to create programs used for data processing. Author's contribution: 10%.**IF(2010)=3,047 number of citations=56**

v. D. Lozhko, J. Stanek, K. Kazimierczuk, A. Zawadzka-Kazimierczuk, W. Kozminski, I. Zhukov, and A. Kornelyuk. ^{1}H, ^{13}C, and ^{15}N chemical shifts assignments for human endothelial monocyte-activating polypeptide EMAP II. *Biomolecular NMR Assignments*, pages 1–5, 2012

My contribution was to create programs used for data processing. Author's contribution: 10%. **IF(2012)=0,82 number of citations=1**

vi. K. Kazimierczuk, Misiak M., J. Stanek, A. Zawadzka-Kazimierczuk, and Koźmiński W. Generalized Fourier transform for non-uniform sampled data. *Top Curr Chem*, 316:79–124, 2012

My contribution was to describe the method of generalized Fourier transform used in reconstruction of undersampled NMR spectra. Author's contribution: 25%.**IF(2012)=8,456 number of citations=14**

vii. L. Wu, A. Reymer, C. Persson, K. Kazimierczuk, T. Brown, P. Lincoln, B. Nordén, and M. Billeter. Initial DNA interactions of the binuclear threading intercalator Λ,Λ-[μ-bidppz(bipy)4Ru2]4+: An NMR study with [d(CGCGAATTCGCG)]2. *Chemistry - A European Journal*, 19(17):5401–5410, 2013

My contribution was to perform NOESY experiments and write a part of the manuscript. Author's contribution: 10%.**IF(2012)=5,696 number of citations=6**

viii. K. Kazimierczuk, J. Stanek, A. Zawadzka-Kazimierczuk, and W. Koźmiński. High-dimensional NMR spectra for structural studies of biomolecules. *ChemPhysChem*, 14(13):3015–3025, 2013 My contribution was to describe the methods of signal processing used in reconstruction of under-sampled multidimensional NMR spectra. Author's contribution: 25%. **IF(2013)=3,36 number of citations=13**

ix. Philippe Lesot, Krzysztof Kazimierczuk, Julien Trébosc, Jean-Paul Amoureux, and Olivier Lafon. Fast acquisition of multidimensional NMR spectra of solids and mesophases using alternative sampling methods. *Magnetic resonance in chemistry : MRC*, 53(11):927–39, nov 2015

My contribution was to describe the methods of sparse reconstruction in NMR. Also, I wrote a part of manuscript. I coordinated the SONATA BIS 2 project, from which the study was co-financed. Author's contribution: 10%.**IF(2014)=1,179 number of citations=0**

x. Krzysztof Kazimierczuk and Vladislav Orekhov. Non-uniform sampling: post-Fourier era of NMR data collection and processing. *Magnetic resonance in chemistry : MRC*, 53(11):921–6, dec 2015 My contribution was to review and describe the methods of NUS reconstruction in NMR in the context of possible gain on signal-to-noise and signal-to-artifact ratios. Also, I wrote half of the manuscript. I coordinated the SONATA BIS 2 project, from which the study was co-financed. Author's contribution: 50%.**IF(2014)=1,179 number of citations=1**

Total impact factor of papers listed above according to the list from Journal Citation Reports: 61.104

B Inventions and industrial/craft patterns subjected to protection and presented at international or domestic exhibitions:

NONE

C Monographs, scientific publications in international and domestic journals other than included in point IB:

NONE

D Collective works, collection catalogs, documentation of research, expert analyses, artistic works

E Total Impact Factor according to the JCR list: **120,638**

F Total rumen of citations according to Web of Science (WoS): **593** (without self-citations); **703** (with self-citations)

G Hirsch index Web of Science (WoS): **15** (with self-citations); **13**(without self-citations)

H Managing and participation in international and domestic research projects:

Own-managed projects:

- KOLUMB stipend of Foundation for Polish Science for the postdoc project "NMR toolbox for studying intrinsically disordered proteins“ (2011)

- IUVENTUS PLUS (no. IP2011 023171) grant from Polish Ministry of Science and Higher Education, project: "Reconstruction of NMR spectra from incomplete data with compressed sensing algorithms" (2012-2014)
- SONATA-BIS 2 (no. 2012/07/E/ST4/01386) grant from National Centre of Science, project: "Sparse and approximately-sparse representations in problems of NMR spectroscopy" (2013-2018)
- HARMONIA (no. 2013/08/M/ST4/00975) grant from National Centre of Science, project: "Regularization algorithms for the processing of NMR spectra of metabolite mixtures" (2013-2014)
- "Inkubator Innowacyjności" grant by Ministry of Science and Higher Education, project: "Statusino - mobile application for monitoring status of NMR spectrometers"
- OPUS (no. 2015/17/B/ST4/04221) grant from National Centre of Science, project: "Time-resolved N-dimensional spectroscopy for monitoring of physical and chemical processes " (2016-2018)

Participation in projects

- N301 071/312159 "Development of new methods of NMR spectroscopy for structural studies of proteins", grant of Polish Ministry of Science for 2006-2009.
- Polish-Slovenian bilateral cooperation 2008-2009 (National Institute of Chemistry, Ljubljana)
- "New applications of NMR spectroscopy In chemistry, biology, pharmacy and medicine" scientific network granted by Polish Ministry of Science for 2008-2009.
- "Towards new applications of NMR spectroscopy in chemical and biomolecular structural studies" TEAM project of the Foundation for Polish Science for 2010-2014.
- EAST NMR, "Enhancing Access and Services To East European users towards an efficient and coordinated pan-European pool of NMR capacities to enable global collaborative research and boost technological advancements". Combination of a Collaborative Project & Coordination and Support Action. (Proj. 228461) FP7-Infrastructure project funded by the European Commission (2009-2013).

I International and domestic awards for scientific or artistic activity:

- 2005 - First Award in Poster Session presenting MSc. results
- 2007 - Antoni Grabowski Award for PhD student in Chemistry
- 2008 - Stipend of the Foundation for Polish Science (START programme). Prolongation for 2009.
- 2009 - Nominated as a "Young Researcher" for Nobel Laureates Meeting in Lindau
- 2009 - PhD Thesis "Methods of fast acquisition of NMR spectra for structural studies" honoured by Faculty Council of the Faculty of Chemistry, University of Warsaw.
- 2010 - PhD Thesis "Methods of fast acquisition of NMR spectra for structural studies" awarded with Kolos Prize
- 2010 - Postdoc stipend funded by the Foundation for Polish Science (KOLUMB programme).
- 2010 - PhD Thesis "Methods of fast acquisition of NMR spectra for structural studies" awarded by Prime Minister of Poland Award for PhD Thesis.

- 2014 - Wojciech Świętosławski award of the 2nd grade by the Polish Chemical Society
- 2015 - Wiley Award for the best lecture in NMR spectroscopy: “Dynamic non-uniform sampling”

J Oral presentations at international and domestic scientific conferences:

i. 20-22 Sep 2007 NMR in Chemistry, Biology and Medicine, Warszawa, Poland (lecture, 1st Award in Young Scientist Contest) "Practical aspects of Multidimensional Fourier Transform.” K. Kazimierczuk
ii. 18-23 May 2008, Computational Aspects - Biomolecular NMR Il Ciocco, Italy (lecture)” What can Multidimensional Fourier Transform do?” K. Kazimierczuk
iii. 2 Jun 2008, NMR School, Łódź, Poland (invited lecture) "Wprowadzenie do mechaniki kwantowej układów spinowych. Reguły ewolucji” K. Kazimierczuk
iv. 11-15 Feb 2009 "Magnetic Moments in Central Europe”, Otočec, Slovenia , (lecture) " Narrow peaks and high dimensionalities: Exploiting the advantages of random sampling.” K. Kazimierczuk, A. Zawadzka, W. Koźmiński
v. 3-7.05.2010, 24-28.05.2010 Fundamentals of Protein NMR, A hands-on PhD course on protein NMR Göteborg, Sweden (invited lecture & organizacja) "From FID signal to NMR spectrum” Krzysztof Kazimierczuk
vi. 1.20-23.09.2010 Advanced Course on New Methods of Data Acquisition and Analysis in Biomolecular NMR Göteborg, Sweden (invited lecture & organizacja) "How to (and how not to) apply Fourier transform to non-uniformly sampled NMR signals” Krzysztof Kazimierczuk
vii. 17-28.01.2011. Workshop "Advanced protein NMR: structure and dynamics”, University of Gothenburg, invited lecture: "Non-uniform sampling – basic concepts” Krzysztof Kazimierczuk.
viii. 27.01.2011, "Advances in biomolecular NMR”, University of Gothenburg, invited lecture "Accelerated NMR with compressed sensing” Krzysztof Kazimierczuk, Vladislav Orekhov.
ix. 27-30.04.2011 „Bio-NMR Workshop: Acquisition and processing of sparsely sampled NMR data”, Warsaw, invited lecture: "Introduction to sparse sampling” Krzysztof Kazimierczuk i hands-on "Determination of coupling constants”.
x. 4-7.10.2011, Bio-NMR workshop, Vilnius, Lithuania, invited lecture & hands-on ”NMR signal processing“, Krzysztof Kazimierczuk
xi. 26-28 Sep 2012 NMR in Chemistry, Biology and Medicine, Warszawa , Poland . lecture: ”Compressed sensing in NMR spectroscopy“. K. Kazimierczuk, M. Misiak, K. Chmurski, W. Koźmiński, V.Yu. Orekhov
xii. 20-23 Nov 2012 Biomolecular NMR with Non-Uniform Sampling, Gothenburg, Sweden. invited lecture i hands-on ”CS in NMR spectroscopy“. K. Kazimierczuk
xiii. 21 Nov 2012 Workshop on Fast Methods in NMR, Gothenburg, Sweden. lecture: ”Compressed sensing in NMR spectroscopy“. K. Kazimierczuk, M. Misiak, K. Chmurski, W. Koźmiński, V.Yu. Orekhov
xiv. 5-7 Jun 2013 Signal Processing Symposium, Jachranka, Poland, lecture: ”A combined sparse sampling of time-gradient domain for NMR diffusometry and relaxometry“. M. Urbańczyk, K. Kazimierczuk

xv. 5 May - 8 May 2014 – The 4th Bio-NMR Annual User Meeting, Warsaw, Poland, invited lecture: ”Sparse sampling in Non-frequency dimensions“. K. Kazimierczuk

xvi. 24-26 September 2014, 8th symposium on Nuclear Magnetic Resonance in Chemistry, Physics and Biological Sciences, Warszawa, lecture: ”2D NMR with temperature-sweep“. W. Bermel, R. Dass, K. Neidig, K. Kazimierczuk

xvii. 20-23 November 2014, II Ogólnopolskie Sympozjum Interdyscyplinarne Inter-Mix 2014, invited lecture: ”Oszczędna spektroskopia NMR“, K. Kazimierczuk

xviii. 25 Feb - 1 Mar 2015 "Magnetic Moments in Central Europe”, Krynica Zdrój , Poland, invited lecture "Sparsity in NMR and around” K. Kazimierczuk

xix. 14-20 Jun 2015 AMPERE XII NMR School, Zakopane, Poland invited lecture "Sparsity in NMR spectroscopy” K. Kazimierczuk

xx. 5-10 Jul 2015 EUROMAR – Magnetic Resonance Meeting, Prague, Czech Republic, lecture: "Dynamic non-uniform sampling”Krzysztof Kazimierczuk, Rupashree Dass, Wiktor Koźmiński, Wolfgang Bermel, Klaus-Peter Neidig, Wojciech Bocian, Jerzy Sitkowski, Michał Nowakowski

xxi. 20-24 Sep 2015 SMASH NMR, Baveno, Italy, lecture: "Dynamic non-uniform sampling” Krzysztof Kazimierczuk, Rupashree Dass, Wiktor Koźmiński

xxii. 18-19 Jan 2016 Danish NMR meeting, Aarhus, Denmark, invited lecture: "Sparse representations in NMR spectroscopy” Krzysztof Kazimierczuk

xxiii. 18-21 Feb 2016 22nd Conference of National NMR Society of India, invited lecture: "Sparse representations in NMR spectroscopy” Krzysztof Kazimierczuk

3 Teaching and popularization achievements and information on international collaborations of the applicant

(A) **Participation in European, other international and domestic programs:** NONE

(B) **Active participation in international and domestic scientific conferences:** Beside the talks listed in point II J, I participated in the following scientific conferences and presented the results as a poster presentation:

i. 1-2 Dec 2004 XXXVII Ogólnopolskie Seminarium Zastosowań NMR, Kraków, Poland. Poster: "Aktywna stabilizacja pola magnetycznego w spektrometrach NMR wysokiej zdolności rozdzielczej” K. Kazimierczuk, W. Koźmiński

ii. 5-10 Jun 2005 AMPERE XII NMR School, Zakopane, Poland. Poster: "Efficient compensation of magnetic field disturbances in high resolution NMR spectrometers” K. Kazimierczuk, W. Koźmiński

iii. 8-10 Sep 2005 NMR in Chemistry, Biology and Medicine, Warszawa , Poland . Poster: "Efficient compensation of magnetic field disturbances in high resolution NMR spectrometers” K. Kazimierczuk, W. Koźmiński

iv. 1-2 Dec 2005 XXXVIII Ogólnopolskie Seminarium Zastosowań NMR, Kraków, Poland, Poster: „Uogólniona wielowymiarowa transformata Fouriera” K. Kazimierczuk, W. Koźmiński

v. 20-25 Aug 2006 International Conference on Magnetic Resonance in Biological Systems, Goettingen , Germany. Poster: " Multidimensional Fourier Transform of arbitrarily sampled multidimensional data sets." K. Kazimierczuk, A. Zawadzka, W. Koźmiński

vi. 11-13 Nov 2006 NMR in Chemistry, Biology and Medicine, Warszawa, Poland Poster: "New flavours of old Fourier transform", K. Kazimierczuk, A. Zawadzka, W. Koźmiński, I. Zhukov

vii. 1-6 Jul 2007 EUROMAR – Magnetic Resonance Meeting, Tarragona, Spain .Poster:" Lineshapes and artefacts in Multidimensional Fourier Transform of arbitrarily sampled NMR data sets." K. Kazimierczuk, A. Zawadzka, W. Koźmiński, I. Zhukov

viii. 6-11 Jul 2008 EUROMAR – Magnetic Resonance Meeting, St. Petersburg, Russia Poster: " Optimization of random time domain sampling in multidimensional NMR" K. Kazimierczuk, A. Zawadzka, W. Koźmiński

ix. 24-26 Sep 2008 „Nuclear Magnetic Resonance in Chemistry, Physics and Biological Sciences" Warszawa, Poland, Poster: " Optimization of random time domain sampling in multidimensional NMR" K. Kazimierczuk, A. Zawadzka, W. Koźmiński

x. 27-29 Oct 2008 "Extend-NMR Meeting" Joachimsthal, Germany. Poster: "Multidimensional NMR Spectroscopy beyond sampling limitations." K. Kazimierczuk, A. Zawadzka, W. Koźmiński

xi. 23-25 Oct 2009, 5th symposium on Nuclear Magnetic Resonance in Chemistry, Physics and Biological Sciences, Warszawa (poster presentation), Poland. Poster: " "Fast NMR" or "Accurate NMR¿' Towards New applications of random sampling." K. Kazimierczuk, A. Zawadzka, W. Koźmiński

xii. 11-14 Jun 2010, The 14th annual Structural Biology Net Meeting, Tällberg, Sweden Poster: "Non-uniform frequency domain for optimal exploitation of non-uniform sampling." Krzysztof Kazimierczuk, Anna Zawadzka-Kazimierczuk, Wiktor Koźmiński

xiii. 4-9 Jul 2010, Joint Euromar 2010 and 17th ISMAR conference „A Worldwide Magnetic Resonance Conference", Florence, Italy. Poster: "Non-uniform frequency domain for optimal exploitation of non-uniform sampling." Krzysztof Kazimierczuk, Anna Zawadzka-Kazimierczuk, Wiktor Koźmiński

xiv. 10-15.04.2011 52nd Experimental NMR Conference Pacific Grove, California, USA (poster) "Accelerated NMR with compressed sensing" Krzysztof Kazimierczuk, Vladislav Orekhov.

xv. 25-30.06.2011 "FEBS Congress: Biochemistry for Tomorrow's Medicine", Torino, Italy, poster: "New high-dimensionality NMR experiments for efficient structural studies of proteins in solution" Krzysztof Kazimierczuk, Maria Misiak, Jan Stanek, Anna Zawadzka-Kazimierczuk, Wiktor Koźmiński, Rafał Augustyniak, Lukaš Žídek, Vladimir Sklenář, Libor Krásný

xvi. 29 Jul - 1 Jul 2012 EUROMAR – Magnetic Resonance Meeting, Dublin, Ireland. Poster:"A comparison of convex and non-convex compressed sensing applied in multidimensional NMR" K. Kazimierczuk, V.Yu. Orekhov

xvii. 19-24 Aug 2012 International Conference on Magnetic Resonance in Biological Systems, Lyon, France. Poster:"A comparison of convex and non-convex compressed sensing applied in multidimensional NMR" K. Kazimierczuk, V.Yu. Orekhov

xviii. 10-13 Jun 2013 The 3rd Bio-NMR Annual User Meeting, Budapest, Hungary, Poster: "A combined sparse sampling of time-gradient domain for NMR diffusometry and relaxometry". M. Urbańczyk M. Nowakowski W. Koźmiński K. Kazimierczuk

xix. 30 Jun -5 Jul 2013 EUROMAR – Magnetic Resonance Meeting, Hersonissos, Greece, Poster: "Combination of Non-uniform Sampling and Compressed Sensing: An Efficient Way for enhancing Sensitivity of Natural Abundance Deuterium 2D-NMR Spectroscopy in Oriented Solvents". K. Kazimierczuk, O. Lafon, P. Lesot

xx. 29 Jun - 3 Jul 2014 EUROMAR – Magnetic Resonance Meeting, Zurich, Switzerland, Poster: "Sparse sampling in Non-frequency dimensions". M. Urbańczyk, W. Bermel, R. Dass, W. Koźmiński, K. Neidig, K. Kazimierczuk

(C) **Participation in organizing committees of international and domestics scientific conferences** I participated or participate in the committees of the following conferences:

- The 4th BioNMR Annual User Meeting, Warsaw, Poland
- Magnetic Moments in Central Europe, Krynica Zdrój , Poland,
- EUROMAR 2017, Warsaw, Poland
- Minisymposia of the NMR section of Polish Chemical Society: 2014 i 2015.

(D) **Awards and distinctions other than listed in point II H**
NONE

(E) **Participation in research networks and consortia:**

- Polish-Slovenian bilateral cooperation 2008-2009 (National Institute of Chemistry, Ljubljana)
- "New applications of NMR spectroscopy In chemistry, biology, pharmacy and medicine" scientific network granted by Polish Ministry of Science for 2008-2009.

(F) **Managing in projects realized with cooperation with scientists from other Polish and international sites, as well as in cooperation with private companies**
NONE

(G) **Participation in editorial committees and editorial boards of scientific journals**
NONE

(H) **Participation in international and domestics organisations and scientific societies** Member of Polish Chemical Society

(I) **Teaching achievements and achievements in popularization of science or art** ***List of courses:***

- Introductory seminars in molecular spectroscopy
- Laboratory courses in molecular spectroscopy, physics and physical chemistry
- Popular science: lecture and laboratory practice for high-school students etc.
- International courses in biomolecular NMR spectroscopy organized in Swedish NMR Centre, at the University of Warsaw, Vilnius (Spronk NMR Consultancy AB), and in the Polish Academy of Sciences in Łodź

New lab exercises, manuals etc.

- I have set-up a new student lab exercises "EPR spectra of hydrochinone derivatives" at Faculty of Chemistry, UW.

Supervising master works:

- Application of compressed sensing method in double-sparse NMR spectra, Agata Jarzębowska

Reviewing master and bachelor works:

- Bachelor degree: "Compressive sensing methods in nuclear magnetic resonance", Krzysztof Lis
- Master degree: "Implementation of the signal separation algorithm for five-dimensional NMR spectra", Krzysztof Kosiński

Popularization of science:

- NMR lab for the foundation "Przyszłość w nauce", 2011
- NMR lab Young Chemist School, 2011, Stowarzyszenie Klatrat
- Promoting Faculty of Chemistry together with journal "Perspektywy", 2011
- NMR lab on the open-doors day of Ochota Campus, 2016

I was invited to participate in the broadcast on Polish Public Radio (twice).

(J) **Scientific assistance to PhD students**

- Auxiliary supervisor: "Application of the sparse regularization in NMR Diffusometry measurements" Mateusz Urbańczyk (will be defended in the second half of 2016)

(K) **Interships in international and domestic academic or research centres**

Post-doc at the Swedish NMR Centre, University of Gothenburg, Sweden. 15 months, 2010-2011

(L) **Expert opinions or other contracted studies**

NONE

(M) **Participation in expert panels and juries**

NONE

(N) **Reviewing international and domestic research projects**

- National Science Centre, 1 project
- Swiss National Science Foundation, 1 project

(O) **Reviewing scientific papers in domestic and international journals**

- Journal of Magnetic Resonance, **IF**=, 2 papers
- Journal of Biomolecular NMR, **IF**=, 3 papers
- Magnetic Resonance in Chemistry, **IF**=, 1 paper
- ChemPhysChem, **IF**=, 1 papers
- Digital Signal Processing, **IF**=, 1 paper
- Acta Physica Polonica, **IF**=, 1 paper

(P) **Other achievements**

I created and currently manage the spin-off company Spektrino, implementing the achievements of the scientific team.