

Sevastyan Rabdano

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Education

2014 – Master of Science, Saint-Petersburg State University (SPbSU), Department of Physics.

Area of specialization: Quantum Radiophysics.

2011 – Bachelor of Applied Mathematics and Physics, Saint-Petersburg State University (SPbSU), Department of Physics.

Area of specialization: Computer and Tomography Technology.

Projects

2014 – Master thesis: The study of hydration properties of functional groups of glycine and beta-alanine amino acids by nuclear magnetic resonance and quantum chemical calculation. (grade: excellent).

2014 – Research project: RNA-recognition motif RRM2 in TDP-43: oxidative stress leads to conformational change, proteolysis, formation of inclusion bodies, and neurodegenerative disease. (in progress).

2012 – Bachelor thesis: Study of microstructure of β -alanine hydration shells by NMR relaxation and quantum chemistry methods. (grade: excellent).

Experience

2013 – Researcher at the laboratory of biomolecular NMR, St. Petersburg State University. Principal investigator: N.R. Skrynnikov.

2012-2013 – Specialist at the Research Center for Magnetic Resonance, St. Petersburg State University.

Scientific research experience

NMR

- Work on the NMR spectrometers: Bruker SXP and Avance III series.
- NMR methods for labeled proteins. Protein backbone and sidechain chemical shifts assignment based on 3-dimensional and triple resonance NMR experiments. Bruker pulse programming. Use of selective pulses; selective excitation; broadband, adiabatic and selective decoupling; cross-polarization. (Certificate from Bruker).
- Measurement of the relaxation times and diffusion coefficients with different pulse sequences for small and large molecules. Writing of pulse sequences for diffusion and relaxation measurements. Diffusion ordered NMR spectroscopy (DOSY) on different nuclei. Applying of advanced techniques for elimination of eddy currents and convection flows artifacts. Gradient calibration. Tuning of gradient preemphasis. (Certificate from Bruker).
- Routine 1D NMR experiments, homonuclear 2D NMR experiments like COSY, NOESY, TOCSY, ROESY, and heteronuclear 2D NMR experiments like HSQC, HMQC, HMBC. Dynamic NMR, studies of reaction kinetics. Work with automation software IconNMR.
- Modification of NMR probes (manufacturing of adoptive coils for registering of the signal from different nuclei).
- Tuning of temperature control system in range $-150 \div +150^{\circ}\text{C}$. Experience of working with cryo liquids (nitrogen, helium).
- Experience of preparing of liquid samples with different concentrations by gravimetric method. Preparation of samples from high purity materials.

- Experience in writing of programs for analyzing NMR experiment data.

Computer modeling methods

- Performing of quantum-chemical calculations in programs GAMESS, Gaussian on supercomputer (up to 100 CPUs).
- Calculation of geometry, energy and electronic structure parameters of molecular ion complexes with Hartree Fock and DFT methods. Model systems consisting of organic molecules and solvent. Performed Morokuma, RVS and LMO energy decomposition analysis.
- Molecular dynamics modeling experience. Development of software for MD modeling in Matlab.

Mechanics

- Theoretical and practical solving of problems in the area of aerodynamics.
- Developing of software for numerical solution of problems in aerodynamics area on example of investigation of boomerang flight.

Teaching experience

- Curator of course works on first and second courses of Department of Physics, SPbSU (field of study: Applied Mathematics and Physics).
- Participation in student seminars as a lector. Topic: studies of microstructure of solutions containing organic molecules.

Theoretical knowledge

Knowledge of the structure and the physical principles of the hardware in the field of NMR. When training at the Physics faculty passed examinations in the following subjects:

- The basics of magnetic resonance,
- Automation of the experiment,
- Experimental methods for nuclear magnetic resonance,
- Quantum radio-electronics,
- Numerical methods,
- Computer equipment and systems,
- Applications of magnetic resonance spectroscopy,
- Computer modeling in quantum radiophysics,
- The basics of electronic paramagnetic resonance,
- Correlation methods in 2D NMR spectroscopy,
- Application of correlation methods in NMR for elucidation of structure and conformation of organic molecules,
- Experimental and mathematical methods in MRI and CT,
- Nuclear quadrupole resonance spectroscopy,
- High-resolution NMR in solids,
- NMR in the magnetic field of Earth

Research interests

- NMR technology.
- Hydrophilic and hydrophobic effects.
- Hydration of organic molecules in aqueous solutions.

- Spin relaxation. Diffusion.
- Proteins.
- Quantum-chemical calculations, the quadrupole coupling constants.
- Study of the microstructure of solutions based on an integrated approach: NMR studies and quantum-chemical calculations.

Additional knowledge and interests

- Foreign language: English, intermediate level.
- Advanced computer skills.
- Experience in the preparation of scientific papers in the system LaTeX.
- Knowledge of programs for data processing (TopSpin, ACDLabs, iNMR, Matlab, SAGE, Mathematica), office applications (Microsoft Office, iWork). Excellent typing skills.
- Visualization of molecular structures, writing of animation scripts, capturing of HD video and images of molecules and clusters.
- Programming languages: C, Objective-C, Java, FORTRAN, PHP, Python, JavaScript, Matlab, LabView, Tcl/Tk.
- Markup languages: HTML, CSS.
- Knowledge of writing and supporting software workflow.

Honors

Award "for the best oral report" at the International Symposium and Summer School in Saint Petersburg "Nuclear Magnetic Resonance in Condensed Matter". Saint-Petersburg, July, 2013.

Student/Post Doc grant at the EUROMAR 2013 conference, Hersonissos, Crete, Greece, 2013.

Award "for the best oral report" at the 9th Conference Spinus "Magnetic resonance and its applications", Saint Petersburg, December, 2012.

Award "for the best oral report" at the International Student Conference «Science and Progress», Saint Petersburg, November, 2011.

Special Prize at the 8th Conference Spinus "Magnetic resonance and its applications", Saint Petersburg, December, 2011.

Highlights

1. Excellent academic achievements scholarship of SPbSU in 2011-2014.
2. Experience of speaking in English at international conferences.
3. II level in basketball in 2008 for the second place in regional competitions in Vologda, Russia.

Interests

Bicycle, Basketball.

Publications & conferences

1. Rabdano S.O., Donets A.V. The study of hydration properties of functional groups of glycine and beta-alanine amino acids by nuclear magnetic resonance and quantum chemical calculations // Book of abstracts of International Symposium and Summer School in St. Petersburg "Nuclear Magnetic Resonance in Condensed Matter." Saint Petersburg, 2014.
2. Rabdano S.O. The study of hydration properties of functional groups of glycine and beta-alanine by nuclear magnetic resonance and quantum-chemical calculations: Master thesis. St. Petersburg: SPbSU, 2014. (Only in Russian)
3. Rabdano S.O., Donets A.V. Properties of hydration of distinct functional groups of organic molecules // Abstracts of the youth conference-school "Physical-chemical methods of analysis in organic chemistry". St. Petersburg, 2013. (Only in Russian)
4. Rabdano S.O. Microstructure and mobility in water solutions of amino acids as studied by NMR and quantum chemistry. // Proceedings of the 10th winter youth conference "Magnetic resonance and its applications". St. Petersburg, 2013. (Only in Russian)
5. Rabdano S.O. Hydration of distinct functional groups of protein-like molecules // Materials of scientific online conference "Spectrometric analysis techniques". Kazan, 2013. (Only in Russian)
6. Rabdano S.O., Donets A.V. Hydrophobic and hydrophilic effects in aqueous solutions of organic molecules // Book of abstracts International Symposium and Summer School in St. Petersburg "Nuclear Magnetic Resonance in Condensed Matter." St. Petersburg, 2013.
7. Rabdano S.O., Donets A.V. Hydration properties of functional groups of organic molecules in aqueous solutions // Proceedings of EUROMAR 2013. Hersonissos, Greece, 2013.
8. Rabdano S.O. Temperature features of hydrophobic and hydrophilic interactions // Proceedings of Interdisciplinary International Student Conference "Science and Progress." St. Petersburg, 2013.
9. Rabdano S.O., Donets A.V. Hydration of functional groups of glycine and beta-alanine // Proceedings of the 9th winter youth conference "Magnetic resonance and its applications". St. Petersburg, 2012. (Only in Russian)
10. Rabdano S.O. Properties of hydration of beta-alanine: the study by of NMR-relaxation and quantum chemistry methods // Abstracts of VII conference "Mendeleev-2012". St. Petersburg, 2012. (Only in Russian)
11. Rabdano S.O. Study of microstructure of β -alanine hydration shells by NMR relaxation and quantum chemistry methods: Bachelor thesis. St. Petersburg: SPbSU, 2012. 45 p. (Only in Russian)
12. Rabdano S.O., Donets A.V. β -alanine hydration shells in aqueous

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solution studied by NMR relaxation method and quantum chemistry // Book of abstracts International Symposium and Summer School in St. Petersburg "Nuclear Magnetic Resonance in Condensed Matter." Saint-Petersburg, 2012.

13. Rabdano S.O., Donets A.V. Hydration properties of organic molecules functional groups as studied by NMR-relaxation and quantum chemical calculations // Proceedings of XV International Youth Scientific School "Actual problems of magnetic resonance and its application." Kazan, 2012.
14. Rabdano S.O., Donets A.V. Hydration properties of biological nanostructures in complex solutions // Proceedings of Interdisciplinary International Student Conference "Science and Progress." Saint-Petersburg, 2012.
15. Rabdano S.O., Donets A.V. The microstructure of β -alanine hydration environment in water solutions // Proceedings of the 8th winter youth conference "Magnetic resonance and its applications". St. Petersburg, 2012. (Only in Russian)
16. Rabdano S.O., Donets A.V. Hydration of Alanine in aqueous solution as studied by NMR-relaxation and quantum-chemical methods // Book of abstracts International Symposium and Summer School in St. Petersburg "Nuclear Magnetic Resonance in Condensed Matter." St. Petersburg, 2011.
17. Rabdano S.O. β -alanine hydration shells in aqueous solutions studied by NMR relaxation method and quantum chemistry // Proceedings of Interdisciplinary International Student Conference "Science and Progress". St. Petersburg, 2011.
18. Donets A.V., Rabdano S.O. Microstructure of complex solutions with organic molecules // Proceedings of EUROMAR 2011. Frankfurt am Main, Germany, 2011.
19. Rabdano S.O. New puzzles of the boomerang // Proceedings of Interdisciplinary International Student Conference "Science and Progress". St. Petersburg, 2009. (Only in Russian)
20. Rabdano S.O., Donets A.V. Study of double and triple systems by NMR-relaxation // Proceedings of the 6th winter youth conference "Magnetic resonance and its applications". St. Petersburg: St. Petersburg State University, 2009.