

Competition notice

Competition within the research project: New dimensions in NMR spectroscopy for better chemical analysis - from small molecules to proteins, OPUS 18 NCN, project leader: Prof. Krzysztof Kazimierczuk, CeNT UW.

The main goal of the project is to develop new approaches to tackle the problem of ambiguities occurring in a chemical analysis based on Nuclear Magnetic Resonance Spectroscopy (NMR). The first step in an analysis of an NMR spectrum is its assignment, i.e. linking particular frequencies ("peaks") to atomic nuclei. Through an analysis of two-dimensional (2D) spectra, the "topology" of the molecule, i.e. connections between atoms, can be determined. The proper identification of structure is crucial, e.g., if it is a starting point for the development of a new drug. Too often, however, the assignment is wrong, because the data on the connections between atoms are ambiguous. Reasons may be different, e.g., two nuclei may have similar resonant frequencies, and thus their peaks overlap in the spectrum. Also, the inter-nuclear transfer exploited in 2D spectra may be suppressed. Finally, the sensitivity may be low, causing spectral peaks to disappear under the noise. The current project aims at proposing solutions to increase the uniqueness of spectral information by exploiting the fact that NMR spectra depend on temperature and solvent.

This fact, although known for a long time, was used mostly in an ad hoc manner, not as a basis of a systematical solution.

The project verifies four main research hypotheses:

1. By slightly varying the temperature of a studied sample, one can generate a new "spectral dimension" and get new information about the sample.
2. Controlled changes of solvent composition can be used in a similar way to form a "spectral dimension" and resolve peaks.
3. Both temperature and solvent effects can be roughly modelled by classical molecular dynamics (MD) and used to assist spectral assignment
4. The approach is general and can be applied to various classes of chemical compounds

The specific practical goal of the project is to create widely available data acquisition and processing protocols to exploit approaches invented while testing the above hypotheses.

Tool-box resulting from the project should involve new experimental and data processing protocols for:

1. Structure elucidation of natural and synthetic products. Temperature and solvent effects can be used to select structures among the ones fitting to the data acquired using standard sets of 2D spectra and generated automatically using Computer-Assisted Structure Elucidation approaches (CASE).
2. Identification of mixture components exploiting temperature- and solvent-induced effects on chemical shifts. In particular, easily accessible metabolite mixtures like urine will be tested, where variable-temperature ¹H spectra will be added to a standard set of "stationary" ¹H data and 2D TOCSY.
3. New tools for the temperature-resolved analysis of peptides and proteins, including peak assignment of intrinsically disordered proteins.

Requirement

- A master degree in physics or chemistry
- Basic knowledge of NMR spectroscopy theory
- Practical skills in NMR spectroscopy

- Basic programming skills
- Interest in interdisciplinary research

Discipline: Chemical Sciences

Admission limit: 1

Recruitment schedule

- registration in the Internet Registration of Candidates, referred to as “IRK”, submitting an application to the IRK: 23.11.2020 – 10.12.2020
- qualification procedure: 14.12.2020-17.12.2020
- announcement of the ranking list: until 21.12.2020
- accepting documents from qualified candidates: 22.12.2020-27.01.2021
- announcement of the list of accepted candidates: until 31.01.2021

Recruitment fee

150 PLN

Form of the selection procedure

Evaluation of the following elements shall be taken into account in the selection process:

- 1) the research project proposed by the candidate;
- 2) scientific activity of the candidate based on a CV or resumé, documented with scans of materials attached to the application for admission to the School;
- 3) interview with the candidate.

Language of the selection process, including the interview

The interview shall be carried out in Polish or English – in accordance with the candidate’s preferences presented in IRK. If the Polish language is selected, the interview may include parts in English.

Required documents

The candidate shall submit the application for admission to the School only in IRK. It shall include:

- 1) the application for admission to the Doctoral School;
- 2) scan of a diploma of completion of the long-cycle Master’s degree programme or second-cycle programme or an equivalent diploma obtained under separate regulations or –in the case of candidates pursuing education within the European Higher Education Areas –a declaration that the diploma or certificate of obtaining a Master’s degree shall be provided by 27 January 2021, in the case of holding a diploma equivalent to the diploma of completion of the long-cycle Master’s degree programme or second-cycle programme, the candidate shall justify this equivalence;
- 3) a description of the initial research project proposal in English, which comprises no more than 6,000 characters including spaces; the description shall contain the bibliography that is not included in the character limit;
- 4) a resumé or curriculum vitae containing information about scientific activities, including scientific interests and scientific achievements during five calendar years preceding the submission of the application, subject to § 18 s. 5, in particular publications, research and

organisational work in scientific associations, participation in scientific conferences, participation in research projects, awards, distinctions, research internships, completed training courses on research skills, science popularisation activities, activities in bodies representing scientific societies, professional career;

- 5) scans of materials confirming scientific activities referred to in the resumé or CV;
- 6) a document confirming the command of English at least at B2 level or declaration about the command of English to the extent enabling the education in the school;
- 7) a scan of the declaration of the supervisor candidate about their willingness to be the candidate's supervisor and the number of doctoral students, for whom they are appointed as the supervisor, in accordance with the template determined by the Rector; additionally, the candidate can enclose a scan of the opinion of the supervisor candidate and opinions of other academic staff on the candidate and their scientific activities or the proposed research project;
- 8) one photograph of the candidate's face, allowing their identification;
- 9) declaration whether the candidate is or was a doctoral student or participant of doctoral studies, and if yes – title of doctoral dissertation or the research project prepared by the candidate, as well as first name and surname of the academic tutor or the supervisor;
- 10) declaration on familiarising themselves with the content of the Resolution, as well as Article 40 and Article 41 of the Code of Administrative Procedure;
- 11) scans of transcripts of records of the first and second cycle programmes, the long-cycle Master's degree programme or equivalent documents (e.g. diploma supplement);
- 12) abstract of the master's thesis or draft master's thesis in English (up to 3,000 characters with spaces);
- 13) other documents in form of scans: letter of recommendation from a scientist who knows the candidate;

Evaluation criteria

While ranking candidates, following criteria are taken into account:

1. Preliminary evaluation of the research project proposal (0-5 points);
2. Assessment of experience necessary to work in a research project, including scientific achievements (0-35 points) ;
3. Interview (0-60 points)
 - Checking the candidate's knowledge and skills in the discipline of Chemical Sciences;
 - conversation about the research project, candidate's understanding of the research topic;
 - a series of short questions about the presented scientific achievements and questions about the course of studies;
 - questions pertaining to information included in letter of recommendations, including nature and results of cooperation of the candidate with authors of these letters;
 - questions pertaining to the other information included in the documentation submitted by the candidate;

Education program

The education lasts 4 years. It includes obligatory classes (no more than 300 hours in total during the whole period of education) and the implementation of an individual research program, carried out under the supervision of a supervisor. Beginning of education - March 1, 2021.

Scholarships

During the four years of study, the PhD student receives a scholarship in the amount of PLN 4 750 gross-gross for the first two years of studies (before the mid-term evaluation) and PLN 5 000 gross-gross in the next two years after the mid-term evaluation.