

Biomolecular NMR: Advanced Tools, AI perspective

An advanced hands-on PhD workshop (equivalent to 3 ECTS)

Dates: 28 Sep - 2 Oct.

Venue & Address:

- Swedish NMR Centre, University of Gothenburg,
[Medicinaregatan 5C, 41390 Gothenburg](#)
- Getting there:
From/To Landvetter Airport. Landvetter Airport bus <https://www.flygbussarna.se/en/landvetter>
To plan your trip and buy bus/tram tickets in Gothenburg use mobile App "Västtrafik To Go"
- Zoom webinars: BioNMR 2026
<https://gu-se.zoom.us/j/64250722497?pwd=OoC6D0qBsvdjYvwWwfoY9bim77ZZ06.1>
Passcode: 016119

Target group: PhD students and researchers with projects involving protein characterization by NMR

Format: Lectures, discussions, and practical hands-on exercises.

Organizers and Contacts: Vladislav Orekhov; Chemistry & Molecular Biology & Swedish NMR Centre, University of Gothenburg, Sweden

Contact: e-mail: bionmr.snc@gmail.com

Registration: the course is free; send your contact info and a motivation to attend the course (max 1 page) to [vladislav.orekhov \[at\] nmr.gu.se](mailto:vladislav.orekhov[at]nmr.gu.se) deadline – 12 August 2026; number of participants for the hands-on sessions is limited.

Registration for NMRbox (only for the students registered for the tutorial hands on sessions)

Since this course will use NMRbox for the tutorial sessions, you need to set up an account at [NMRbox.org](https://nmrbox.org). Then, please register for the course at <https://nmrbox.nmrhub.org/events>. You find an intro about NMRbox by Dr. Adam Schuyler at <https://api.nmrhub.org/files/120/326/nmrbox22-2-NMRbox-intro-schuyler.mp4>

Information:

at <https://www.gu.se/en/nmr/workshops-courses-and-conferences>

Course Certificates and ECTS credit points:

In order to fully accomplish the course, the student should attend all tutorial lectures and practical sessions. For every tutorial session a short report should be submitted as outlined by the session instructors. After acceptance of the lab reports by the instructors, the course certificate can be requested by e-mail to bionmr.snc@gmail.com.

Program

Course teachers

BMB	Björn Marcus Burmann (University of Gothenburg)
VH	Vicky Higman (University of Leicester, UK)
SH	Sebastian Hiller (University Basel, Switzerland)
ES	Elsa Stern (University Basel, Switzerland)
JM	Jalil Mahdizadeh (University of Gothenburg)
MM	Maksim Mayzel (Buker Biospin, Switzerland)
VO	Vladislav Orekhov,
AJ	Amir Jahangiri (University of Gothenburg)
KP	Konstantin Pervushin (Nanyang Technological University, Singapore)
XQ	Xiaobo Qu (Xiamen University, China)
TQ	Tianyu Qiu (Xiamen University of Technology)

Schedule overview

date	9:00 am – 12 am	1:30 pm – 5 pm
M, 28	Intro, student presentations, BMB	VO, AJ
Tu, 29	SH, ES	KP
W, 30	JM, VH	VH
Th, 1	Mini conference	MM
Fr, 2	XQ, TQ	Reports and clean ups

Topics:

- Automated Assignment and Structure
- AI in NMR spectra processing
- Agentic AI in NMR workflows
- Python tools in TopSpin
- NMR with automated protein production
- CCPN software toolbox for NMR data analysis
- AI in drug discovery

Time (CEST)¹ Title Type Teachers

Monday Sep 28 Vladislav Orekhov, Björn Marcus Burmann, Amir Jahangiri

8.40 – 9.00	(on-site only) Registration.		
9.00 – 10.45	Welcome, information & student presentations (5 min/student)		VO, BMB
10.45 – 11.00	Coffee break		
11.00 – 11.30	continued student presentations (5 min/student)		
11.30 – 12.10	???	Lecture	BMB
12.30 – 13.30	Lunch		
13.30 – 14.20	Next generation spectra processing with AI	Lecture	VO
14.20 – 14.40	Coffee break		
14.40 – 17:30	Next generation spectra processing with AI	hands-on	VO, AJ
18:00– 19.30	(on-site only) Get-together	SNC	

Tuesday Sep 29 Sebastian Hiller, Konstantin Pervushin

09.00 – 09.40	NMR with automated protein production	Lecture	SH
09.40 – 12.20	NMR with automated protein production	hands-on	SH, ES
10.10 – 10.30	Coffee break		

¹ Central European Summer Time (CEST). Lectures and hands-on sessions will be recorded and shared with the participants. Use the recordings, if you cannot attend the sessions, e.g. because of the time zone difference.

12.30 – 13.30	Lunch		
13.30 – 14.30	Use of AI agents for the next generation NMR spectroscopy	Lecture	KP
14.30 – 14.50	Coffee break		
14.50 – 17.00	NMR AI agent performs protein NMR experiments	hands-on	KP

Wednesday Sep 30 Jalil Mahdizadeh, Vicky Higman

09.00 – 09.50	AI in drug discovery	Lecture	JM
09.50 – 10.10	Coffee break		
10.10 – 11.30	Introduction to CcpNmr Analysis	Lecture & hands-on	VH
11.30 – 12.30	Protein NMR Assignment and Structure Validation	Lecture	VH
12.30 – 14.00	Lunch		
14.00 – 14.50	Validation of AlphaFold structures against NMR data	hands-on,	VH
14.50 – 15.10	Coffee break		
15.10 – 17.10	Validating and correcting Artina assignments	hands-on,	VH

Thursday Oct 1

Min-conference. NMR and AI in structural biology (TBA)

Chair: Göran Karlsson (Swedish NMR Centre, University of Gothenburg, Sweden)

08.30 – 09.00	Coffee		
9.00 – 9.30	NMR as a video game played by AI agents Konstantin Pervushin (Nanyang Technological University, Singapore)		
9.30 – 10.00	What have data formats ever done for us? Vicky Higman (University of Leicester, UK)		
10.00 – 10.30	Exponential Functions for Physical Intelligence Magnetic Resonance Xiaobo Qu (Xiamen University, China)		
10.30– 11.00	AI in NMR and Structural Biology Vladislav Orekhov (University of Gothenburg, Sweden)		
11.00– 11.30	???		
	Björn Marcus Burmann (University of Gothenburg)		
11.30– 12.00			
12.00– 12.30			
12.30 – 13.30	Lunch		
13.30 – 14.40	Poster session		

Course continues at the Swedish NMR center, Maksim Mayzel

13.50– 14:40	Python in TopSpin: From Data Analysis and Spectrometer Control to Custom NMR Workflows	Lecture	
	MM		
14.40 – 15.00	Coffee break		
15.00 – 17:30	Developing Practical NMR Applications Using the TopSpin Python API	hands-on	MM

Friday Oct 2 Xiaobo Qu & Tianyu Qiu

09.00 – 09.50	Physical Intelligence Design for Fast NMR	Lecture	XQ
09.50 – 10.10	Coffee break		
10.10 – 12.20	NUS Reconstruction with Physical Intelligence NMR	hands-on	XQ, TQ
12.30 – 13.30	Lunch		
13.40 – 16:00	Cleaning up hands-on reports		