Programme 25-29 Sep 2017

Course: **Biomolecular NMR: modern tools for data processing and interpretation dynamics (up to 3 ECTS)**

Address: Swedish NMR Centre, University of Gothenburg
Medicinaregatan 5C, 41390 Gothenburg, Sweden

Info: http://www.nmr.gu.se/english/courses/

Course teachers

MB	Billeter Martin	Prof.,	University of Gothenburg, Sweden
AG	Gutmanas Aleksandras	Dr.	PDB Europe, EMBL-EBI
JH	Hoch Jeffrey	Prof.	UConn Health, USA
SK	Kazemi Sina	Dr.	Goethe-University, Frankfurt, Germany
KK	Kazimierczuk Krzysztof	Prof.	University of Warsaw, Poland
MM	Maciejewski Mark	Prof.	UConn Health, USA
M	Maxim Mayzel	Dr.	University of Gothenburg, Sweden
VO	Orekhov Vladislav	Prof.,	University of Gothenburg, Sweden
YP	Pustovalova Yulia	Dr.	University of Gothenburg, Sweden
AS	Schuyler Adam	Prof.	UConn Health, USA
JW	Würz Julia	Dr.	Goethe-University, Frankfurt, Germany

Time	Title	Type	Place	Teachers
Monday Sep 25				
8.40 – 9.00	Registration and Coffee			
9.00 – 10.00	Welcome, information & student presentations (3-5 min/student)			
10.00 – 11.20	Quantitative NMR with Non-Uniform Sampling		Lecture	VO
11.20 – 12.30	Non-uniform sampling for high dimensionality		Lecture	KK
12.45 – 14.00	Lunch			
14.00 – 17.30	NMR signal processing		*Lab*	VO, M, MB
17.30 – 19.00	Get-together	Entry hall		
Tuesday Sep 26				
9.00 – 12.30	High dimensional spectra		Lab	KK,YP,VO
10.00 – 10.20	Coffee Break			
12.40 – 14.00	Lunch			
14.00 – 17.30	Tools for validation of NMR structures and experimental data		Lecture & Lab	AG
15.30 – 16.00	Coffee Break			
Wednesday Sep 27 – NMR Box				
9.15 – 16.30	NMR Box	Lecture & Lab	JH,MM, AS (via video)	
9.00 – 9.15	Introduction to the NMRbox Platform		JH	

9.15 – 10.00	Introduction to NMRbox VM		MM
10.00 – 10.30	Coffee Break		
10.30 – 11:45	Introduction to RNMRTK		MM
11:45 – 12:30	Overview of Spectral Reconstruction Methods		JH
12.30 – 13.30	Lunch		
13.30 – 14.15	Fundamentals of nonuniform sampling: a reprise		AS (via video)
14.15 – 15.00	MaxEnt and NMRfx reconstruction workflows for NUS experiments		MM
15.00 – 15.20	Coffee Break		
16.30 – 17.30	**Round Table**		Moderated by JH & MB

Thursday Sep 28

9.00 – 9.40	State of automated NMR structure calculations	Lecture	MB
9.40 – 10.20	Automated assignment and structure calculations	Lecture	SK,JW
10.20 – 10.40	Coffee Break		
10.40 – 12.30	Automated assignment	Lab	SK,JW
12.30 – 13.30	Lunch		
13.30 – 17.30	Automated assignment (cont.)	Lab	SK,JW
15.00 – 15.30	Coffee Break		

Friday Sep 29

9.00 – 12.20	Automated NMR structure calculations	Lab	SK,JW
10.30 – 10.50	Coffee Break		
12.00 – 13.00	Lunch		
13.00 – 15.00	*Wrap-up*	*Lab*	*VO,M, MB*
15.00 – 16.00	Discussions and report wrap-ups	Lect. Room	MB, VO, YP, M, SK, JW