Core Facility NMR-spectroscopy

Peter Schmieder

Overview



Aims

The NMR facility is organized as a core facility to allow a better administration of the many requests from inside and outside the FMP for the use of the NMR machines or the utilization of NMR as a technique. This eased the participation in the European i-NEXT network as well as the German DFG-funded G-NMR network of facilities. The NMR core facility also serves as a platform for the use of NMR spectrometers by nondepartmental groups. These include for example FMP groups that perform chemical synthesis and, thus, heavily rely on continuous NMR support as well as groups studying the interaction of proteins with peptides or small molecules that benefit from the strength of NMR to detect weak proteinligand interactions. In addition, there are requests from groups outside the FMP for access to the NMR facility, including access to the DNP spectrometer. These other groups from Berlin and the whole of Germany use the equipment of the facility if comparable resources are not available at their own sites.

Group Members

Peter Schmieder, Senior Scientist Nils Trieloff, Technician (3/4)

Monika Beerbaum, Scientist (3/4) Matthias Herreira-Glomm, Scientist (1/2)

Veniamin Chevelkov, Scientist (1/2)

Brigitte Schlegel, Technician

Probes

		Г	
	Magnets [MHz]	Probes	Observable nuclei
Solution NMR	300 (SB)	5 mm QNP, z-gradient 5 mm BBFO, z-gradient	¹ H, ¹³ C, ¹⁹ F, ³¹ P ¹ H, ¹⁹ F, ⁿ X
	3 x 600 (SB)	5 mm QXI, z-Gradient 5mm BBFO, z-Gradient 5 mm TCI Cryoprobe, z-Gradient 5 mm QCI Cryoprobe, z-Gradient 5 mm TXI, xyz-Gradient 5 mm TXI, z-Gradient 5 mm TXI, z-Gradient 8 mm TXI, z-Gradient	1H, 13C, 15N, 31P 1H, 19F, nX 1H, 13C, 15N 1H, 13C, 15N, 31P 1H, 13C, 15N 1H, 13C, 15N 1H, 13C, 15N 1H, nX 1H, 13C, 15N
	750 (SB)	5 mm TCl Cryoprobe, z-Gradient 5 mm TXI, z-Gradient 8 mm TXI, z-Gradient	¹ H, ¹³ C, ¹⁵ N ¹ H, ¹³ C, ¹⁵ N ¹ H, ¹³ C, ¹⁵ N
	900 (SB)	5 mm TXI, z-Gradient 5 mm TCI Cryoprobe, z-Gradient	¹H, ¹³C, ¹⁵N
Solid state NMR		0.7, 1.3 and 1.9 mm HCND 3.2 and 4.0 mm HCN	¹ H, ¹³ C, ¹⁵ N
	800 (WB)	1.3 mm HCND 3.2 and 4.0 mm Efree HCN 1.9 mm low temp. (DNP)	¹ H, ¹³ C, ¹⁵ N
	700 (WB)	0.7, 1.3 and 1.9 mm HCND 3.2 mm Efree HCN 3.2 and 4 mm HXY	¹ H, ¹³ C, ¹⁵ N, (³¹ P)
	600 (WB)	1.3 and 1.9 mm HXY 3.2 and 4.0 mm HXY	¹ H, ¹³ C/ ³¹ P, ¹⁵ N
	400 (WB)	3.2 mm low temp. (DNP) 3.2 mm HXY	¹ H, ¹³ C, ¹⁵ N, (³¹ P)
Imaging	400 (WB)	Live mouse imaging Spin exchange optical pumping (Xe polarizer)	Double resonance probes

Participation in G-NMR and iNEXT



Development of teaching standardization of spectrometer tools, german NMR summer school.



Infrastructure for NMR, EM and X-rays for Translational Research

Spectrometers































Open access automation



A basic NMR service providing 1D (1H, 13C, 31P, 19F) and simple 2D (COSY, TOCSY, HMQC, HMBC) spectra is available on dedicated open-access 300 and 600 MHz spectrometer.

Collaborations

Internal

Dorothea Fiedler Christian Hackenberger Volker Haucke Ronald Kühne Adam Lange Marc Nazaré Hartmut Oschkinat Leif Schröder Johannes Broichhagen Han Sun Adam Lange Michael Krauss

External

Christoph Rademacher, MPI Golm Christian Freund, FU Berlin Alexander Weng, FU Berlin Timo Niedermayer, Universität Halle Thomas Müller, Universität Würzburg Katharina Koschek, IFAM Bremen Robert Brinson, NIST Theresa Carlomagno, Hannover Erich Wanker, MDC Harald Schwalbe, Universität Frankfurt/Main Ricardo Pires, Federal University of Rio de Janeiro Vera Meyer, TU Berlin

Companies

Fa. EMP biotec (Berlin-Buch) Fa. Celares (Berlin-Buch) Fa. S&V (Hennigsdorf)

Fa. Evotec (Hamburg) Fa. PentixaPharm (Berlin-Buch) Fa. OctreoPharm (Berlin-Buch)

