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Professor Ulrich Günther

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Teaching

Metabolism and Biochemistry, Biomolecular NMR.

Research

Structural Biology and Biomarkers

Research Activity

My main research interest has always been in Biomolecular NMR with a primary focus on protein interactions. This work included the development of line shape analysis as a tool to study protein ligand interactions.

More recently I started to work on metabolic analysis, mainly in the context of cancer. I am developing this work in the direction of metabolic flux analysis. Much of the recent work about metabolomics of AML cell lines was done in collaboration with **Chris Bunce (/staff/profiles/biosciences/bunce-chris.aspx)** and **Mark Viant (/staff/profiles/biosciences/viant-mark.aspx)** .

Another field of research has been in Dynamic Nuclear Polarization (DNP) which has great potential in the context of metabolic flux analysis but also opens new avenues for NMR as it can boost its sensitivity by several orders of magnitude. My DNP research has been focussed on low temperature ex situ polarization. Recent work highlights quantum tunnelling as an additional polarisation mechanism at low temperatures.

I am also part of the at the Systems Science for Health scheme funded by the University of Birmingham, a new research initiative at the University of Birmingham focussed on Systems Science in a medical context with applications in cancer, inflammation and obesity.

I am part of serval EU programmes and coordinator of the EU projetcs WW-NMR and METAFLUX.

Other activities

Scientific Director of the Henry Wellcome Building for Biomolecular NMR.

Publications

Metabolomics

D.V. Rubtsov, H. Jenkins, C. Ludwig, J. Easton, M. R. Viant, U. Günther, J.L. Griffin and Nigel Hardy. 'Proposed reporting requirements for the description of NMR-based metabolomics experiments'. *Metabolomics*, 3(3), 223-229 (2007).

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MR Viant, C Ludwig, S Rhodes, UL Günther and D Allaway. 'Validation of a urine metabolome fingerprint in dog for phenotypic classification'. *Metabolomics* 3(4), 453-463 (2007).

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S.Tiziani, V. Lopes, U.L. Günther. 'Metabolic profiling of head and neck cancer from human blood serum using 1H NMR spectroscopy'. *Neoplasia* 11(3), 1-8 (2009).

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DNP

Emwas A-H, Saunders M, Ludwig C, and Günther UL. 'terminants for Optimal Enhancement in ex situ DNP Experiments'. *Applied Magn Reson*, 34, 483-494 (2008).

Saunders MG, Ludwig C, and Günther UL. 'Optimizing the Signal Enhancement In Cryogenic ex situ DNP-NMR'. J *Am Chem Soc*, 130, 6914-5 (2008).

Ludwig C, Marin-Montesinos I, Sauners MG and Günther UL. 'Optimizing the Polarization Matrix for ex Situ Dynamic Nuclear Polarization'. *J Am Chem Soc* 132(8), 2508-9 (2010).

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Ludwig C, Marin-Montesinos I, Günther UL. 'Rapid two-dimensional NMR Spectra for ex situ Dynamic Nuclear Polarization'. *PCCP*, in press.n

Binding Properties and Structures of Proteins

U. L. Günther, Y. Liu, D. Sanford, W.W. Bachovchin, and B. Schaffhausen. 'NMR analysis of interactions of a PI-3 kinase SH2 domain with phosphotyrosine peptides reveals interdependence of major binding sites'. *Biochemistry* 35, 15570-15581 (1996).

T. Weber; B. Schaffhausen; Y. Liu; U. Günther. 'Structure of p85 N-SH2 complexed with a doubly phosphorylated peptide reveals second phosphotyrosine binding site'. *Biochemistry*, 39, 15860 (2000)

UL Günther, B Schaffhausen. 'NMRKIN: Simulating lineshapes derived from two-dimensional spectra of proteins'. *J. Biomol. NMR*. 22(3), 201-209 (2002)

U. Gunther, T. Mittag, B. Schaffhausen. 'Probing SH2 Domain Ligand Interactions by Differential Line Broadening'. *Biochemistry*, 41(39), 11658-11669 (2002)

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T. Mittag, B. Schaffhausen and U. Günther. 'Tracing structural intermediates in ligand binding'. *E. Biophys. J.* 32(3), 243 (2003)

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Ludwig, C, Michiels, PJA Wu, X, Kavanagh, KL, Pilka, E, Jansson, A, Oppermann, U, Günther, UL. 'SALMON: Solvent Accessibility, Ligand binding and Mapping of ligand Orientation by NMR spectroscopy'. *J Med Chem*, 51(1), 1-3 (2007) (Rated 'must read' by Faculty1000Biology).

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