LXIX JCET LECTURE, 28.09.2015, 9.00

Time-resolved FTIR of proteins and vibrational imaging of cells and tissue

Prof. Klaus Gerwert, PhD
Ruhr-University Bochum, Department of Biophysics, Bochum, Germany

Integration of time-resolved ns-step-scan FTIR-spectroscopy and biomolecular QM/MM simulations provides detailed spatiotemporal resolved reaction mechanisms of proteins. The proton pump mechanism of bacteriorhodospsin (bR) is elucidated thereby in detail as reviewed in (1). Especially the crucial role of protein bound water molecules for proton transfer is shown (2,3).Also the light-activated opening of the optogenetic tool channelrhodospsin 2 is elaborated by this approach (4). Using photolabile caged GTP the GAP catalyzed reaction mechanism of Ras is elucidated at molecular detail (5). Oncogenic mutations of Ras disturb protein network interaction in cells resulting in cancer in tissue.

For cells and tissue Infrared, Raman and CARS imaging are emerging tools for marker--free, non-invasive classification (6). Thereby, the histopathological annotation of tissue and cytopathological annotation of cells is performed with high sensitivity and specificity. For tissues of colon, bladder and lung cancer data bases are established to characterize these tissues in an automated bioinformatics workflow with sensitivity and specificity of over 90% respectively (7,8). Even subclasses of lung cancer adenocarcinoma are identified (9). While IR provides much faster annotation of larger tissue sections, Raman allows a 10 times higher spatial resolution as compared to IR. As a result, erythrocytes, lymphocytes and even single cell nuclei are resolved in tissue sections by Raman imaging (10). Raman imaging of cancer cell lines furthermore allows monitoring of drug response *in vitro* as shown for a kinase inhibitor and a monoclonal antibody against the EGF receptor (11,12).

In summary: Vibrational spectroscopy provides a deep in sight in the dynamics of proteins and their interactions at different scales from recombinant proteins up to tissue.

Most relevant publications:

(1) Gerwert, K.; Freier, E.; Wolf, S. *BBA-Bioenergetics* **2014**, *1837*, 606.

(2) Garczarek, F.; Gerwert, K. *Nature* **2005**, *439*, 109.

(3) Freier, E.; Wolf, S.; Gerwert, K. *Proc. Natl. Acad. Sci. USA* **2011**, *108*, 11435.

(4) Kuhne, J.; Eisenhauer, K.; Ritter, E.; Hegemann, P.; Gerwert, K.; Bartl, F. *Angewandte Chemie Int. Ed.* **2015**, 54, 4953-4957.

(5) Koetting, C. Gerwert, K. *Biol. Chem.* **2015;** 396(2): 131–144

(6) Gerwert, K.; Großerüschkamp, F.; Ollesch, J. *SPIE Newsroom* **2014**, DOI: 10.1117/2.1201-312.005297.

(7) Mavarani, L.; Petersen, D.; El-Mashtoly, S.F.; Mosig, A.; Tannapfel, A.; Kötting, C.; Gerwert, K. *Analyst* **2013**, 138(14), 4035-9.

(8) Kallenbach-Thieltges, A.; Großerüschkamp, F.; Mosig, A.; Diem, M.; Tannapfel, A.; Gerwert, K. *J. Biophotonics* **2013**, 6(1), 88-100.

(9) Großerüschkamp, F., Kallenbach-Thieltges, A., Behrens, T., Brüning, T., Altmayer, M., Stamatis, G., Theegarten, D., Gerwert, K. *Analyst*. **2015** ,140(7):2114-20

(10) El-Mashtoly, S.F.; Niedieker, D.; Petersen, D.; Krauss, S.D.; Freier, E.; Mosig, A.; Kötting, C.; Hahn, S.; Gerwert, K. *Biophys J.* **2014**, 106(9), 1910-20.

(11) El-Mashtoly, S.F.; Petersen, D.; Yosef, H.K.; Mosig, A.; Reinacher-Schick, A.; Kötting, C.; Gerwert, K. *Analyst* **2013**,139(5), 1155-1161.

(12) El-Mashtoly, S.F., Yosef, H.K., Petersen, D., Mavarani, L., Maghnouj, A., Hahn, S.A., Kötting, C. and Gerwert, K. *Anal. Chem.* 87 **(2015)** 7297-7304

Curriculum Vitae

Name:	Klaus Gerwert, Professor Dr. rer. nat.
Citizenship:	German
Address:	Department of Biophysics,
	Ruhr-University Bochum
	44801 Bochum,
	Germany
	Email: gerwert@bph.ruhr-uni-bochum.de

Professional Experience:

2015	Founding Director of ProDi (Protein-Diagnostics-Research-Institute)
2008 – 2013	Director at the CAS (Chinese Academy of Sciences)-MPG (Max Planck Society) Partner institute for Computational Biology (PICB), Shanghai, China (dual appointment)
Since 1993	Professor (W3) and chairman of the Department for Biophysics, Faculty for Biology and Biotechnology, Ruhr University Bochum, Germany
1990 – 1993	Heisenberg-fellow, Deutsche Forschungsgemeinschaft, Scripps Research Institute, La Jolla, USA, Molecular Biology Department and MPI-Dortmund
1986-1990	Researcher, Max-Planck-Institute, Dortmund
1985	Doctoral thesis in Biophysical Chemistry at the University of Freiburg, Germany.
1980	Diploma in Physics, University of Muenster

Honours, Awards:

Since 2009	Fellow of the Max-Planck-Society
Since 2008	Member of the North Rhine-Westphalian Academy of Sciences, Humanities and the Art
2006	Innovation Award Ruhr 2006, Award of the prime minister of North Rhine-Westphalia, Alfried Krupp von Bohlen and Halbach foundation
1992	Karl Arnold Jansen Award 1992 of the Rhine-Westphalian Academy of Sciences
1990-1993	Heisenberg-Fellow of the Deutsche Forschungsgemeinschaft