Colloquium

Topic: ***Time-resolved FTIR of proteins and vibrational imaging of cells and tissue***

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Place: ***ISAS - Room 218***
Schwarzschildstr.8
12489 Berlin-Adlershof

Time: ***Wednesday, 08.07.2015***
14:00 hrs s.t.

Mitglied der Leibniz-Gemeinschaft

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

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Integration of time-resolved ns-step-scan FTIR-technique 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 (chR2) is elaborated by this approach. Especially the role of E90 as crucial for the central gate opening is revealed (4).

For cells and tissue Infrared, Raman and CARS imaging are furthermore emerging tools for label-free, non-invasive classification (5). 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 data bases are established to characterize these tissues in an automated bioinformatics workflow with sensitivity and specificity of over 90% respectively (6, 7). 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 (8). 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 (9).

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

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