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SuChAQuality

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TD-NMR Transfer of Knowledge Report

In SuChAQuality project TD-NMR was covered in 2 partners: METU & RS

METU hosted partners from NUST, SU, UdeC, RS and SGI.

All secondees were trained on basics of TD-NMR.

All secondees learned how to operate the instruments and how to analyze the data.

NUST secondees (ESRs- PhD students at NUST) integrated TD-NMR to their PhD research and conducted experiments accordingly. All NUST researchers, are at the stage of publishing a paper where TD-NMR was used.

Secondees from NUST, SU and UdeC also attended the online graduate level course offered by Dr. Oztop (METU): **Magnetic Resonance in Food**.

One of the most important knowledge transfer activities that took place between **UdeC** and **METU** researchers is the integration of **chemometric techniques** to analyze TD-NMR data. All **UdeC** secondees helped **METU**, **NUST** researchers to use chemometric approaches for their analyzing data.

The activities at **RS** are explained as follows:

Solid State TD-NMR methods: moments of spectra; contribution of different phases into FID; Dependence of T1 and FID shapes on crystallinity; basics of transverse NMR signals processing; fitting of FID shapes by Gaussian, Abragam and Pake functions; sequences Solid Echo (SE), Rhim and Kessemeier - Radiofrequency Optimized Solid-Echo (RK-ROSE), Magic Sandwich Echo (MSE), Saturation-Recovery (SR), Inversion-Recovery (IR), Curr-Purcell-Meiboom-Gill (CPMG), Multi Solid Echo (MTSE), Hahn Echo Decay (HED); Variable sample temperature measurements; fast T1 (one passage) measurement techniques;

Particularly for SU and METU secondees;

Samples preparation, performing experiments, processing data, interpreting results. Together with SU secondee it is developed the Second Moment Approximation approach for characterizing NMR relaxation in solids.

For UdeC Secondee;

Developing experiments strategy for multivariant data analysis, performing experiments, processing data, interpreting results.

All the secondees demonstrated really high motivation, they have acquired firm skills with TD-NMR instrument operation and data processing (filtering, fitting, FFT)

For the next researchers coming to Resonance Systems GmbH, the course will be expanded towards multiple quantum NMR signals and their usage within the Second Moment Approximation technique.

The possible publications that used TD-NMR knowledge in the secondments include;

(1) Formulation Optimization of Hard Candies from Spirulina and Chlorella Algae. Physicochemical, Sensorial and Safety Analysis (**SUBMITTED**)

Authors: Shafia Maryam (NUST); Mecit H. Oztop (METU); Sarper Dođdu (DC); Mehmet Ali Marangoz (DC); Hilmi Eriklioglu (METU); Zeshan Zeshan (NUST); Ramish Riaz (NUST); Waqas Chatta (NUST).

(2) Universal 1H spin-lattice NMR relaxation features of sugar – a step towards quality markers (**SUBMITTED**)

Authors: Hafiz Imran Fakhra (NUST); Karol Kolodziejcki (UWM); Leonid Grunin (RS); Mecit H. Oztop (METU); Muhammad Qasim Hayat (NUST); Hussnain Janjua (NUST); Danuta Kruk (UWM).

(3) Effect of non-centrifugal sugar on low-methoxyl pectin gelation (**1st revision received**)

Authors: Hafiz Imran Fakhra (NUST); Elif Akbas, Muhammad Qasim Hayat (NUST); Hussnain Janjua (NUST); Mecit H. Oztop (METU)

(4) Improvement of techno-functional properties of Chlorella powder via glycation with inulin

Authors: Rabaila Riaz (NUST); Ozan Tas (METU); Mecit H. Oztop (METU); Hussnain Janjua (NUST).

(5) Investigation of the structural changes of starch types stored at different relative humidity by NMR Relaxometry (**Will be submitted**)

Authors: Esmanur Ilhan (METU); Serap Namli (METU); Sahin Namli (METU); Eda Yildiz (METU); Leonid Grunin (RS); Mecit H. Oztop (METU).

(6) Exploring temperature related proton dynamics during gelatinization of starch from roasted wheat (**1st revision received**)

Authors: Jana van Rooyen (SU); Leonid Grunin (RS); Mecit H. Oztop (METU); Marena Manley (SU).

(7) Use of Time-Domain Nuclear Magnetic Resonance (TD-NMR) methodologies for the examination of Feta and Parmesan cheeses (**Will be submitted**)

Authors: Esmanur Ilhan (METU); Ozan Tas (METU); Leonid Grunin (RS); Mecit H. Oztop (METU).

(8) An Alternative Multivariate Strategy for Discriminate Sugar Beet Pectin by Production Methods Based on Time Domain-NMR with Fast Fourier Transform (FFT)

Authors: Esmanur Ilhan (METU), Maria Ivanova (RS), Cristian Fuentes (UdeC), Leonid Grunin (RS), Rosario Castillo (UdeC), Hatice Gul Solmaz (KS), Mecit H. Oztop (METU)