

Sunday, September 8th, 2024

15.00 – 17.00 Check-In (In case you arrive later than 5pm, please let me know per email in advance !)

18.00 - 19.00 Dinner

19:30-19:35 Opening remarks

19.35 – 20.35 **Norbert Müller**: NMR, what else?

Monday, September 9th, 2024

9.00 - 10.15 **Klaus Zangger**: Introduction into 1D- and 2D-NMR Spectroscopy

10.40 - 11.55 **Herbert Kogler**: Deriving Structural Information from NMR spectral data

13.00 - 14.00 **Lothar Brecker**: Tutorial "Basics of NMR-Spectroscopy - Part 1"

The list of exercises and tutorials will be changed according to the needs of the participants – the titles given below should give you a flavor of what is planned !

14.15 - 16.00 **Exercises**:

Group 1: **Lothar Brecker**: Interpretation of 1D- and 2D-NMR Spectra (Part 1 Interpretation)

Group 2: **Wolfgang Schöfberger**: From Spectra to Structures

Group 3: **Herbert Kogler**: Assignment and structure elucidation using realistic spectra

Group 4: **Klaus Zangger**: Interpretation of 1D- and 2D-NMR Spectra (Part 1)

Group 5: **Harald Maid**: 1D- and 2D-NMR Interpretation

16.30 – 17.55 **Lothar Brecker**: Tutorial "Basics of NMR-Spectroscopy – (Part 2 Theory)"

19.00 - 20.00 Meeting of the Working Party "NMR-Spectroscopy" within the Austrian Chemical Society

20.00 - ? Informal get-together

Tuesday, September 10th, 2024

9.00 - 10.15 **Wolfgang Holzer**: Techniques for Heteronuclear Correlations

10.40 - 11.55 **Norbert Müller**: Description of NMR-Experiments using Product Operator Formalism

14.00 - 16.00 **Exercises**:

Group 1: **Lothar Brecker**: Interpretation of 1D- and 2D-NMR Spectra (Part 2)

Group 2: **Norbert Müller**: Product Operator Formalism

Group 3: **Herbert Kogler**: Assignment and structure elucidation using realistic spectra

Group 4: **Wolfgang Schöfberger**: From Spectra to Structure

16.30 - 17.55 **Norbert Müller**: Phase Cycles and Gradients

19.00 – open end **Exercises:**

Group 1: **Wolfgang Robien:** Spectrum Prediction, Structure Verification and fully Automatic Structure Revisions (own laptop strongly recommended)

Group 2: **Norbert Müller:** Product Operator Formalism and Phase Cycles

Group 3: **Wolfgang Holzer:** Interpretation of 2D-Correlation Spectra

Group 4: **Harald Maid:** 1D- and 2D-NMR Interpretation

Wednesday, September 11th, 2024

9.00 - 10.15 **Lothar Brecker:** Relaxation and Nuclear Overhauser Effect

10.40 - 11.55 **TBA**

13:00 - 14:15 **Reinhard Wimmer:** Gradients in NMR-Spectroscopy

14.30 - 16.00 **Exercises:**

Group 1: **Lothar Brecker:** Interpretation of 1D- and 2D-NMR Spectra (Part 3)

Group 2: **TBA**

Group 3: **Klaus Zangger:** Interpretation of 1D- and 2D-NMR Spectra (Part 2)

16.30 – 17.45: **Reinhard Wimmer:** Metabolomics by NMR - a Rapidly Emerging Field

19.00 – open end **Exercises:**

Group 1: **Herbert Kogler:** Assignment and structure elucidation using realistic spectra

Group 2: **Harald Maid:** 1D- and 2D-NMR Interpretation

Thursday, September 12th, 2024

9.00 - 10.15 **Daniel Mathieu:** Assignment Strategies for Peptides and Proteins

10.40 - 11.55 **Mario Schubert:** Assignment Strategies for Oligosaccharides

14.00 - 16.00 **Exercises:**

Group 1: **Daniel Mathieu:** Exercises to "Assignment Strategies for Peptides and Proteins" on paper

Group 2: **Reinhard Wimmer:** CARA - A Program for Assigning Protein Spectra (own laptop strongly recommended)

Group 3: **Mario Schubert:** Assigning spectra of oligosaccharides (own laptop strongly recommended)

16.30 - 17.55 **Daniel Mathieu:** Tutorial "Fast Data Acquisition in NMR-Spectroscopy"

19.30 – 20.30: **TBA**

Friday, September 13th, 2024

Please check out BEFORE 9am! The luggage can be stored in a dedicated place.

9.00 – 10.15: **Tobias Madl:** Calculating molecular structures from NMR data

10.40- 11.55: **Wolfgang Robien:** Computer Application during the Structure Elucidation Process

12.00 Lunch and Closing Remarks