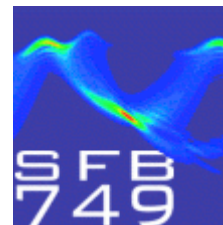


**8<sup>th</sup> SFB 749 workshop at Kloster Irsee, Allgäu**  
**02.10.- 04.10.2017**



**Monday, 02.10.2017**



- 10:00 departure of the bus from Großhadern,  
Butenandtstraße / Feodor-Lynen-Straße
- 12:00 Lunch**
- 13:55 welcome  
*Thomas Carell*
- 14:00 Christian Ochsenfeld (C07): Quantum-chemical studies of  
biochemical processes
- 14:30 Philip Tinnefeld: Manipulating and Visualizing Single-molecule  
reaction by DNA nanotech
- 15:00 Iris Antes (C08): Computational investigations of enzyme-substrate  
recognition
- 15:30 Anja Hoffmann-Röder (A11): Photoswitchable Peptidomimetics
- 16:00 – 16:45 Coffee break**  
*Dorian Didier*
- 16:45 Alois Bräuer (A10 Groll): Biosynthetic megaenzymes: Crystal  
structures of a minimal PKS type II system
- 17:15 Lena Daumann: The impact of different rare earth elements on the  
mechanism and activity of the XoxF-type methanol dehydrogenase  
from *Methylacidiphilum fumariolicum*
- 17:45 Roland Wilcken (B05 Riedle): Microfluidic Mixer for Ultrafast  
Spectroscopy of Unstable Compounds
- 18:05 Short presentation of posters part I ( A3, A4 (3x), A10, A12 (2x), A13,  
B1 (3x), B2 )
- 18:45 end
- 19:00 dinner**

## Tuesday, 03.10.2017

*Herbert Mayr*

- 9:00 Thomas Carell (A04): Deformylations in the genome  
9:30 Oliver Trapp: Self-Amplification of Chirality in Catalysis and Beyond  
10:00 Martin Zacharias (C05): DNA-Flexibility and Recognition studied by Molecular Dynamics Simulations

### **10:30 – 11:15 Coffee break**

*Armin Ofial*

- 11:15 Qi Hu (B05 Riedle): Mechanistic studies of photoredox organocatalysis  
11:35 Short presentation of posters part II (AK Kellner, B5, B11,C2 (3x), C5 (2x), C6, C7 (2x), C8 (2x))

### **12:05-14:00 Lunch**

- 14:00 free time  
15:15 Mitgliederversammlung  
15:45 Oliver Trapp – Ideen zum neuen SFB in der Chemie

### **16:15-17:00 coffee break**

*Eberhard Riedle*

- 17:00 Rasmus Linser (A13): Complete solid-state NMR shift assignments of a 29 kDa enzyme as an access to site-resolved enzyme dynamics  
17:30 Daniel Keefer (C02 de Vivie-Riedle): Photostability of Uracil: From Quantum Control on the Isolated Nucleobase to Environmental Effects in RNA  
18:00 Stefanie Kellner: Biosynthetic isotope labeling in nucleic acid modification research  
18:30 end  
**19:00-20:00 dinner**  
20:00-21:30 Poster Session

**Wednesday, 04.10.2017**

*Stephan Sieber*

9:00 Dorian Didier: Selective sequences towards four-membered carbo- and heterocycles

9:30 Armin Ofial (B01) & Harish Jangra (C06 Zipse): Concertedness in (3+2)-Cycloadditions of Diazoalkanes

- Theory and Experiment -

**10:15 – 11:00 coffee break**

*Regina de Vivie-Riedle*

11:00 Varvara Morozova (B02 Knochel): A General Preparation of Optically Enriched Acyclic Molecules Using Chiral Secondary Alkyl-Lithium and -Copper Reagents

11:20 Marthe Ketels (B02 Knochel): In-Situ-Trapping Halogen–Lithium Exchange in Continuous Flow

11:40 Stephan Sieber (A03): Small molecule proteome mining

**12:10-14:00 Lunch**

14:30 departure

- the bus leaves at 14:30 from Kloster Irsee -

## Poster SFB749 meeting 2017

### Area A

#### A03 Sieber

- 1) Mathias Hackl: Empirical methods for the validation of QM/MM-based simulations of ClpP inhibition by lactone-based compounds

#### A04 Carell

- 2) Antony Crisp: Peptides in an RNA world: Synthesis of Poly-aaRNA
- 3) Eva Korytiakova: Investigation of active Demethylation of 5-Methyl-2'-Deoxycytidine
- 4) Christina Schneider: Ubiquitous non-canonical RNA nucleosides are vestiges of the early Earth

#### A10 Groll

- 5) Alois Bräuer: Biosynthetic megaenzymes: Crystal structures of a minimal PKS type II system

#### A12 Dube

- 6) Stefan Thumser: Hemiindigo a Forgotten Chromophore - Highly Bistable Photoswitching in the Red Part of the Visible Spectrum
- 7) Christian Petermayer: Indigoid Photoswitches and Their Applications

#### A13 Linser

- 8) Alexander Klein: A suite of pulse sequences for fast small molecule analysis using UTOPIA NMR

### Area B

#### B01 Ofial/Mayr

- 9) Patrick Jüstel: Concurrent  $S_N1$  and  $S_N2$  Mechanisms in Solvolysis Reactions
- 10) Robert Mayer: Can Peroxide Anion Reactivities Be Applied To Weitz-Scheffer Epoxidations?
- 11) Daria Timofeeva: Nucleophilic Reactivity and Lewis Basicity of Deoxybenzoin-Derived Enamines

#### B02 Knochel

- 12) Dorothée Ziegler: Magnesium Alkoxides

B05 Riedle

13) Christina Leonardo: Shedding new light on DNA base dynamics

B11 Magauer

14) Johannes Feierfeil: Ring Expansion for the de nova synthesis of indoles and indazoles

### **Area C**

C02 de Vivie-Riedle

15) Franziska Schüppel: Dynamical studies on the photodissociation of diphenylmethyl bromide

16) Matthias Roos: Quantum Dynamical and Semi-classical Studies of Pyrene

17) Florian Rott: Quantum chemical studies of a hemithioindigo-based photodriven molecular motor

C05 Zacharias

18) Korbinian Liebl: Impact of methyl-sugar clashes on fine structure and deformability of DNA

19) Christina Frost: Converged Chignolin Folding Landscape from Molecular Dynamics Simulations

C06 Zipse

20) Harish Jangra: Electrostatic Effects on The Stability of Peptide Radicals

C07 Ochsenfeld

21) Andrea Kreppel: A Quantum-Chemical Study of the DNA Base-Excision Repair of 8-Oxoguanine

22) Eli Naydenova: QM size sensitivity in the QM/MM investigations of the hUNG2 reaction mechanism

C08 Antes

23) Okke Melse: Combining molecular docking and QM/MM methods for studying ligand binding to metalloproteins.

24) Chen Zheng: Applications of QM/MM methods to protein/ligand binding

### **Associated**

25) Stefanie Kellner: Observing the fate of tRNA and its modifications by nucleic acid isotope labeling mass spectrometry: NAIL-MS