

# **EUROISMAR2019**

## **Joint Conference**

GDCh Fachgruppe MR Discussion Meeting  
Berlin, August 25th – 30th

## Welcome to EUROISMAR2019

The sculpture Molecule Man by Jonathan Borofsky shows three persons coming together at the meeting point of three former districts of Berlin, right in the river Spree, originally symbolizing the interaction of humans from East and West, and now from all over the world. The principle of interaction is carried forward in the microstructure of the sculpture, the holes representing ‘the molecules of all human beings coming together to create our existence’.

This nicely symbolizes the aim of EUROISMAR2019, the combined ISMAR, EUROMAR and GDCh 2019 conferences, devoted to delivering an exciting display of NMR, MRI and EPR state-of-the-art progress and describing such interactions, extending into all fields of Chemistry, Biology and Medicine.

Both venues of EUROISMAR2019 are on the campus of the Freie Universität/Max Planck Society in Berlin-Dahlem. The Henry Ford Building of the Free University as well as the Harnack House of the Max Planck Society captivate with a green splendid environment characteristic for the Southwest of Berlin, and architectural simplicity in midst a historical site.

On behalf of the Local Organizing Committee, let me cordially welcome you to the EUROISMAR2019 in Berlin.

Hartmut Oschkinat  
Chairman

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**Different variants of cyclosporin studied by NMR:  
Molecular structure and conformational flexibility**

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Cyclosporin A, well known as an immunosuppressive agent, is one of a family of congeners synthesised in certain soil fungi. Three natural variants of cyclosporin (B, C, D) were studied by high resolution NMR spectroscopy in chloroform and dimethyl formamide. CsB has alanine in position 2 instead of  $\alpha$ -aminobutyric acid (Abu2) found in CsA, in CsC this residue is replaced by threonine, and in CsD, by valine.

In general, obtained spectra of the peptides are alike. However, there are some differences seen in  $^1\text{H}$  and 2D  $^1\text{H}, ^{13}\text{C}$ -HSQC spectra. For instance, the OH proton of residue Thr2 in CsC is visible in  $\text{CDCl}_3$  at 298 K, as well as the OH proton of Bmt1 in CsD. In CsA and CsB, however, hydroxyl protons were not observed directly due to the exchange. CsD was also found to have negligible signals of the minor conformer, while it is clearly seen in the spectra of other three compounds.

Structural data were obtained from ROESY spectra, which allowed building model structures of the investigated molecules.

The case of chemical exchange was considered on the example of CsC in DMF. The pattern of exchange resembles that observed for CsA in polar media such as DMSO. Signals of the NH protons were assigned, and temperature behaviour of their chemical shifts was analysed. It was found that most of the observed conformers have lost their intramolecular H-bonds. Cis-trans isomerisation of the peptide bonds was suggested to be the reason of the conformational exchange.

The work was funded by the Russian Science Foundation (project no. 18-73-10088).

**References:** [1] Survase S.A., Kagliwal L.D., Annapure U.S., Singhal R.S.: Biotechnol. Adv. 2011, 29, 418-435. [2] Efimov S.V., Zgadzay Yu.O., Darwish S., Klochkov V.V.: BioNanoScience. 2019, 10.1007/s12668-019-00641-z.

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