

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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CONFORMATIONAL PREFERENCE OF SMALL MOLECULES BY 2D NOESY SPECTROSCOPY AT SUPERCRITICAL PARAMETERS OF STATE

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2D NMR spectroscopy is an extremely useful method for analyzing the structure and dynamics of **small molecules** in liquids and in solid state. Modern 2D NMR approaches allow obtaining direct information about the geometrical configuration of small molecules, which is very important when solving problems of modern physical chemistry of fluids (e.g. micronization of drug substances, polymorphism in pharmaceutical drugs, and supercritical fluid impregnation of polymeric materials). However, the NMR method is utterly problematic when it touches upon experiments at pressures above 100 bar. This report presents the peculiarities of a high-pressure NMR experiment, as well as the effect of the NMR cell on the accurate determination of the conformer distribution at the supercritical condition. In addition, the latest results obtained using the unique high-pressure NMR spectroscopy instrumentation will be presented and discussed together with the development vistas and possibilities of the 2D NOESY method applied at the supercritical condition of state on the example of ibuprofen. Conformation distribution of ibuprofen was determined in supercritical carbon dioxide (scCO₂). A good agreement was found between the NMR and MD results for ibuprofen in scCO₂.

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References: [1] Kolmer, A., Edwards, L.J., Kuprov, I., Thiele, C.M.(2015) Journal of Magnetic Resonance, 261, pp. 101-109. [2] Butts, C.P., Jones, C.R., Towers, E.C., Flynn, J.L., Appleby, L., Barron, N.J.(2011) Organic and Biomolecular Chemistry, 9 (1), pp. 177-184. [3] Khodov, I.A., Efimov, S.V., Klochkov, V.V., Batista De Carvalho, L.A.E., Kiselev, M.G.(2016) Journal of Molecular Structure, 1106, pp. 373-381.

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