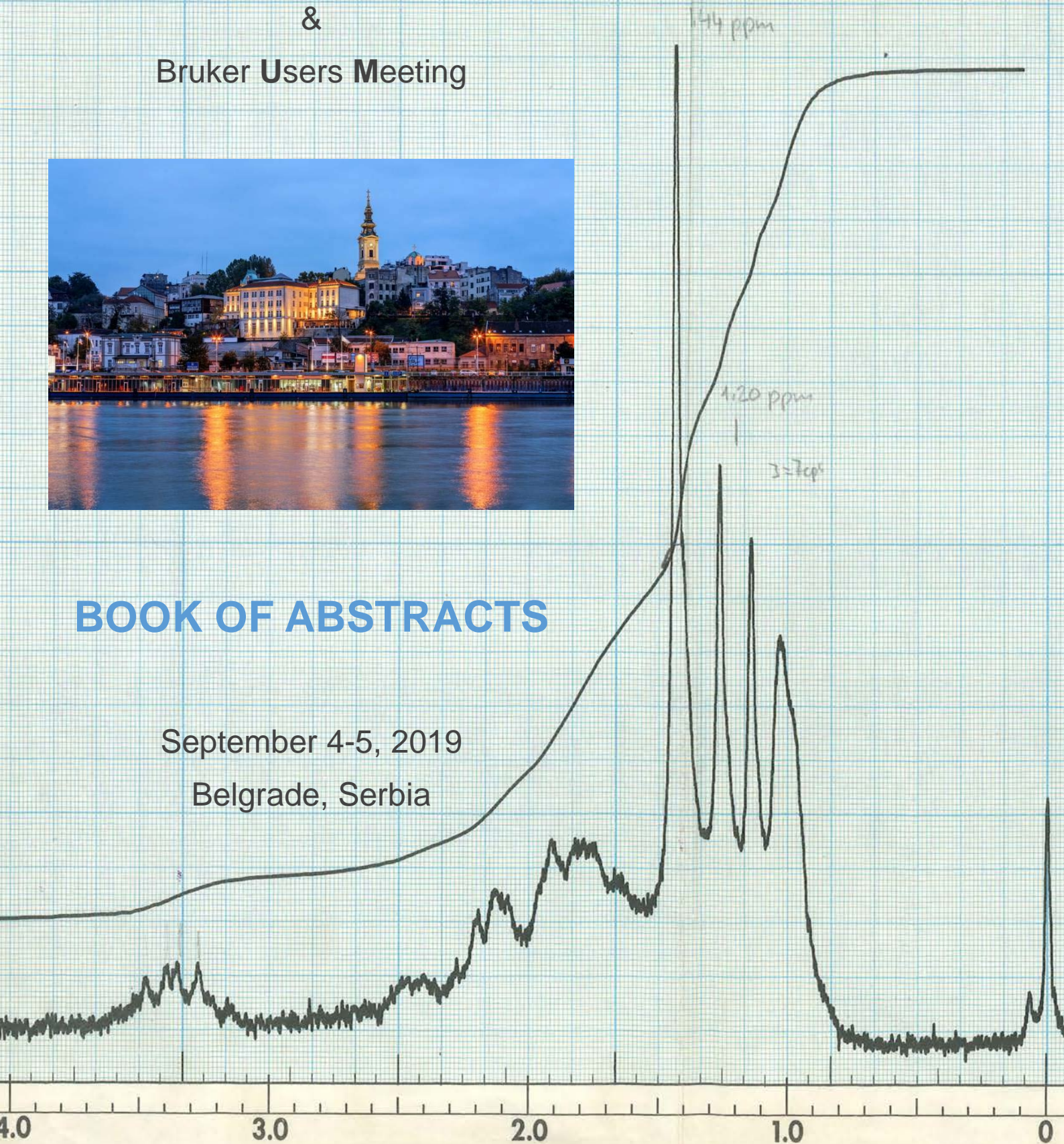# 21st CEUM

21st Central European NMR Symposium
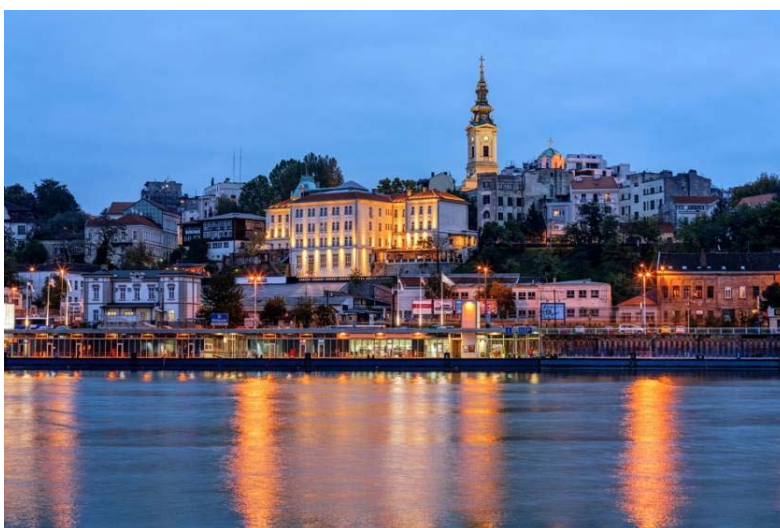
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Bruker Users Meeting

BOOK OF ABSTRACTS

September 4-5, 2019

Belgrade, Serbia

21st CEUM

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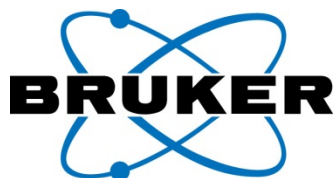
The organization of the 21th Central European NMR Symposium and Bruker users meeting at the University of Belgrade - Faculty of Chemistry was possible due to the support of **University of Belgrade - Faculty of Chemistry, Institute of Chemistry, Technology and Metallurgy, National Institute, University of Belgrade, Serbia, Bruker BioSpin Rheinstetten Gmbh, Germany, Bruker Italia srl, Milano, Italy** as well **DonauLab, Belgrade, Serbia.**
We are very grateful to main sponsor Bruker BioSpin for the financial and professional support and to Donau Lab (Bruker partner in Serbia) for helping in the organization.

Preface

The 21st Central European NMR Symposium & Bruker users meeting (CEUM) is an important scientific and professional event for all NMR users in Central Europe.

It has already a long history and has travelled along many counties in Europe.

It has always been an important occasion to share experience and know-how inside the community and meet scientists working mainly in the close countries (but not only!) in order to built up a stronger NMR community and have also a vision on new applications of NMR and new developments in the Magnetic Resonance Technology.

We are sincerely grateful to the lectures and guests coming from Greece, Bulgaria, Romania, Moldovia, Croatia, Slovenia, Bosnia and Herzegovina, Hungary, the Netherlands, US and from different cities from Serbia to have jointed this meeting.

He sincerely hope that all our effort will be lead also this year in this very nice city to a interesting and successful conference.

Editor in chief

Angrlo Ripamonti

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EVALUATION OF THE UNIVERSALITY OF NMR METABOLIC FINGERPRINTS OF SCHIZOPHRENIA

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Schizophrenia (SCZ) is a very disabling mental disorder whose molecular basis is a combination of many factors still not completely understood, with a diagnosis based on observed behavior, the person's reported experiences and reports of others that are familiar with the person, with no objective test. Also, up to date, there are no reliable markers for monitoring the SCZ. NMR-metabolomics [1] reported in 2017 bring some of the possible markers from blood serum of SCZ individuals linked strongly with known dopamine, glutamate and GABA dysfunction in SCZ. As to verify if these findings are universal, we have compared the SCZ patients from geographically different environments and cited interesting SCZ characteristics.

The first set of samples was collected in Belgrade, Serbia. 14 mental health patients (50% male) with 52.86 ± 7.27 years of age had a confirmed diagnosis of SCZ. The control group of 13 healthy individuals (69% male) had none of psychotic disorders, and individuals were 23.07 ± 2.79 years of age. Blood serum samples were collected and prepared for the analysis following the published methodology [1, 2]. NMR spectra were measured on a Bruker AVANCE III spectrometer (500.26 MHz for ^{1}H). The spectra were acquired at 298 K with 128 scans and 32 k. The serum samples were prepared and measured as triplicates.

On the other side, the group of individuals from Brazil that was matched in number, age, gender and history of mental illness with individuals from Serbia was previously described [1].

^{1}H NMR spectra were phase and baseline corrected using MestreNova and the lactate doublet was used as the chemical shift reference. The data were binned (0.005 ppm) in a spectral range 0.50 - 9.00 ppm, while the residual HDO peak (4.50-5.00 ppm) was excluded. Then, the data were normalized by the sum equal to 1000, the variables were mean centered and PCA and PLS-DA were performed using MATLAB.

It was shown that the mental health patients have clearly different blood serum metabolites when compared to the healthy ones independently from where the samples were obtained with almost identical marker set. Also, it was shown that the samples are different metabolically when Brazilian and Serbian samples were compared.

REFERENCES

[1] L. Tasic et al., *Schizophrenia Research* **2017**, *185*, 182.

[2] J. Pontes *et al.*, *Analytical Methods* **2017**, *9*, 1078.