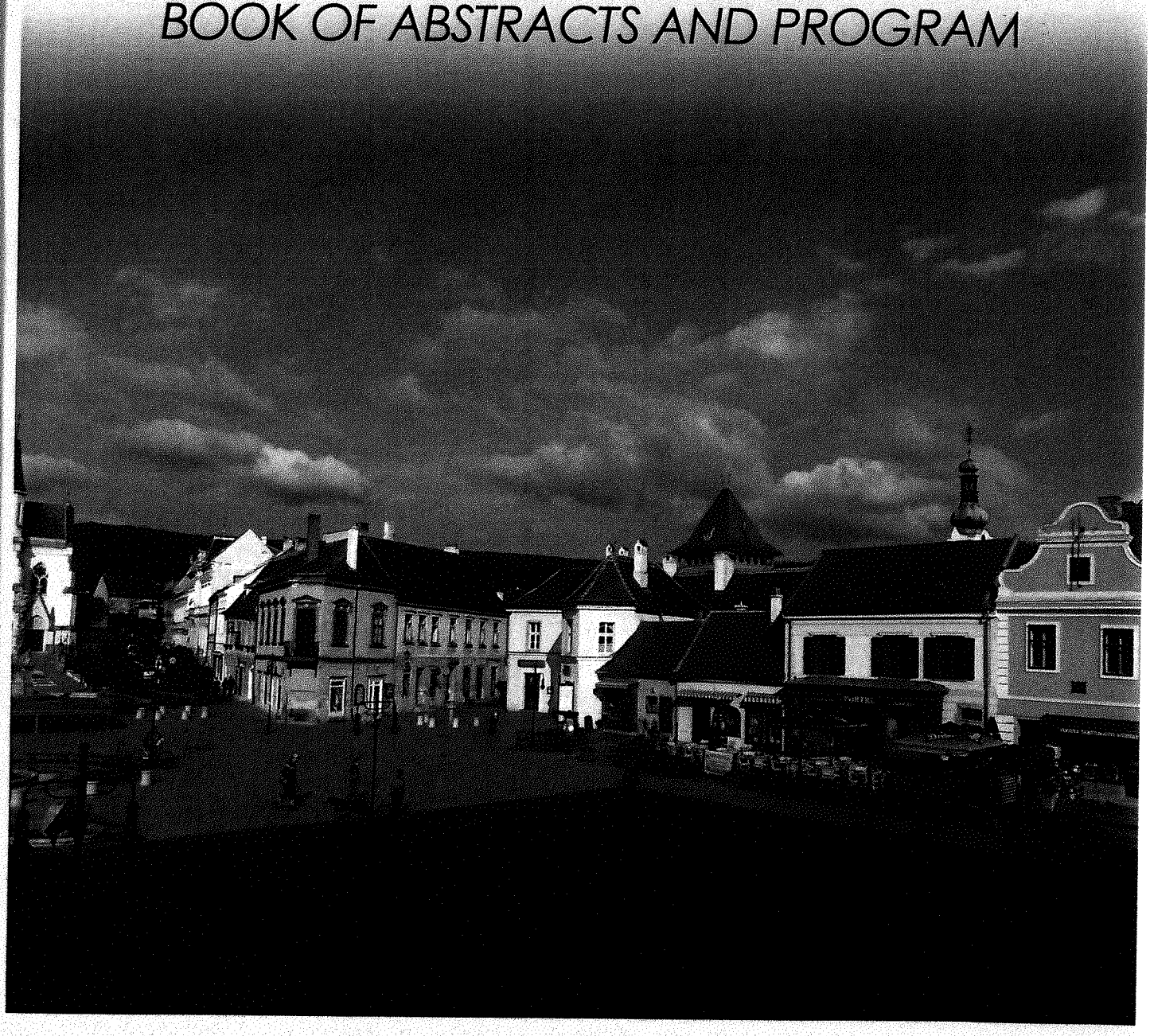
36TH INFORMAL MEETING ON MASS SPECTROMETRY

BOOK OF ABSTRACTS AND PROGRAM



6TH–9TH MAY, 2018,
KŐSZEG, HUNGARY

36th INFORMAL MEETING ON MASS SPECTROMETRY

6th - 9th May, 2018 Kőszeg, HUNGARY

organized by:

MS Proteomics Research Group of RCNS, Hungarian Academy of Sciences, Budapest, Hungary

Division of Mass Spectrometry of the Italian Chemical Society

Working Committee on Separation Sciences of the Hungarian Academy of Sciences

ORGANIZING COMMITTEE

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Venue:
Hotel Írottkő, Fő tér 4., Kőszeg, Hungary

EXPERIMENTAL EVIDENCES OF THE PRESENCE OF BIMOLECULAR CAFFEINE/CATECHIN COMPLEXES IN GREEN TEA EXTRACTS

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A hypothesis on the peculiar pharmacological behavior of biologically active natural compounds is based on the occurrence of molecular interactions originating from the high complexity of the natural matrix following the rules of supramolecular chemistry. In this frame, some investigations were performed to establish unequivocally the presence of catechin/caffeine complexes in green tea extracts (GTEs). ^{1}H NMR was utilized to compare profiles from GTEs with catechin/caffeine mixtures in different molar ratios, showing that peaks related to caffeine in GTEs are generally upfield shifted compared to those of free caffeine. On the other hand, ESI-MS experiments performed on GTE by means of precursor ion scan and neutral loss scan methods, the presence of caffeine/catechin complexes was unequivocally proved. Further experiments were performed by LC-MS method operating in high resolution conditions. The reconstructed ion chromatograms of the exact mass ions corresponding to the caffeine/catechin complexes have been obtained, showing the presence of the complexes of caffeine with gallate-type catechins. By this approach it was possible to put in evidence the presence of the same bimolecular complex having different structures and thus exhibiting different retention times. Both "All Ions" and "Target" methods confirm the nature of caffeine/cathechin complexes of the detected ions.