Math/Chem/Comp 2016
28th MC² Conference
Interuniversity Centre Dubrovnik (IUC)
20 – 25 June 2016

CONFERENCE PROGRAM

SUNDAY, 19 June

18:00-20:00 Registration (IUC, Don Frana Bulića 4, Dubrovnik)

MONDAY, 20 June

8:30-9:00 Registration (IUC)
9:00-9:30 H. Vančík and J. Cioslowski Conference opening and few words in honour to Professor Nenad Trinajstić

9:30-10:15 N. Trinajstić, How Math/Chem/Comp meetings started

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10:45-11:30 R. B. Mallion, What Kirchhoff really did concerning spanning trees in electrical networks and its relationship to modern graph-theoretical work


13:00 IUC RECEPTION

TUESDAY, 21 June

9:00-9:45 D. K. Sunko, Beyond Slater determinants: A general scheme to construct realistic wave functions
9:45–10:30 J. Cioslowski, Robust validation of approximate 1-matrix functionals with few-electron harmonium atoms

10:30–11:15 A. G. Csaszar, Spectroscopic networks: small molecules as complex systems

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11:45–12:15 D. Vikić-Topić, Harold Kroto, In Memoriam

12:15–13:00 B. Lućić, Optimization, interpretation, and selection of molecular descriptors in structure–property models
13:00–13:45 D. Janežič, Graph-Theoretical Approaches in Drug Discovery
13:45–14:30 I. László, Topological coordinates for bar polyhex carbon structures

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17:00–17:45 S. Feretić, Enumeration of diagonally convex polyominoes
17:45–18:30 A. Amić, Free radical scavenging potency of phloretic acid: thermodynamisc of 2H+/2e-processes

WEDNESDAY, 22 June
Sub-conference

NMR: From Theory to Biomolecules
Chair: Predrag Novak

9:00–9:45 W. Kozminski, New high dimensionality experiments for intrinsically disordered proteins
9:45–10:30 H.-U. Siehl, From Superacid Chemistry to 'in silico' Chemistry
10:30–11:15 K. Zangger, Enhancing the resolution of NMR spectra by interrupted acquisition

11:15–11:45 coffee break

11:45–12:30 J. Plavec, NMR studies of tetrahelical G-rich DNA structures
12:30-13:15 S. Valić, Deuterium NMR – a powerful tool in studying molecular order
13:15-14:00 N. Fujii and S. Sakurai, Introduction of new triple resonance system for analysis of fluorine molecules  
JEOL comp. presentation

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17:00-17:45 V. Smrečki, DOSY NMR technique in studies of ionic-liquid gels and aggregation of asphaltenes
17:45-18:30 M. Vazdar, Molecular dynamics simulations in biologically relevant systems
18:30- Poster section (posters can be retained till the end of the Conference)

THURSDAY 23 June

9:00-9:45 M. Sola, A walk through several rules of aromaticity
9:45-10:30 J. Djorović, UV-VIS spectra of some phenolic Schiff bases: experimental and theoretical study
10:30-11:15 I. Kodrin, The role of the amino acid chirality as the potential promoter of different types of turns in ferrocene peptides
11:15-12:00 I. Rončević, Modelling the structure and reactivity of organic compounds using a new cluster-continuum solvation method
13:00 Conference trip and dinner

FRIDAY 24 June

9:00-9:45 J. Tosović, Structural and antioxidative features of chlorogenic acid
9:45-10:30 Ž. Kurtanjek, Molecular extended graph signatures and descriptors QSAR of ionic liquid toxicity
10:30-11:15 U. Bren, Computer simulations of urethane-induced carcinogenesis

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11:45–14:00 T. Hrenar (The course in molecular dynamics)

SATURDAY

9:00–9:45 I. Biljan, Aromatic C-nitroso compounds as building blocks for new supramolecular assemblies
9:45–10:30 H. Vančik, Ontological status of molecular formulas
11:00–11:30 Conference closing (Vančik/Cioslowski)