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. Vančik 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*

--- [coffee break] ---

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*

11:30-12:15 J.von Knop, *Chemistry 4.0: Challenges and Solutions for the Digital Transformation.*

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*

--- [coffee break] ---

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

12:15-13:00 B. Lučić, *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*

--- [lunch break] ---

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*

--- [lunch break] ---

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-**
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*

--- [coffee break] ---

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 supramoleculaf assemblies*
9:45-10:30 H. Vančik, *Ontological status of molecular formulas*
11:00-11:30 Conference closing (Vančik/Cioslowski)