



# Math/Chem/Comp 2017

## 29<sup>th</sup> MC<sup>2</sup> Conference

Inter University Centre Dubrovnik

19 – 24 June 2017

### CONFERENCE PROGRAM

#### MONDAY, 19 June

08:30–9:30 Registration (IUC, Don Frane Bulića 4, Dubrovnik)

9:30–10:00 **H. Vancik** and **J. Cioslowski** *Conference opening*  
**B. Lučić**, *few words in honour of Professor Ivan Gutman*

10:00–11:00 **I. Gutman**, *The total  $\pi$ -electron energy saga*

--- [coffee break] ---

11:30–12:15 **R. B. Mallion**, *Ring-current properties of bispentalenes – comparison of ab initio and Hückel-London-Pople-McWeeny (HLPM) “topological” calculations*

12:15–13:00 **B. Lučić**, *The outcome of reasoning based on models greatly depends on the procedure used for their validation*

13:00–13:45 **D. Svrtan**, *Finding Largest small polygons via symbolic computations*

13:45–14:30 **B. Furtula**, *Structural dependence of extended energy*

**TUESDAY, 20 June**

**9:00–9:45** **J. Cioslowski**, *One-electron densities of freely rotating Wigner molecules*

**9:45–10:30** **D. Fijan**, *Thermodynamic anomalies and network topology in liquids*

--- [coffee break] ---

**11:00–11:45** **I. László**, *Molecular dynamics simulation of carbon structures inside nanochambers*

**11:45–12:30** **U. Bren**, *Microwave effects on model aqueous solutions*

**13:00 IUC RECEPTION**

**WEDNESDAY, 21 June**

**9:00–9:45** **H. A. Witek**, *Zhang-Zhang polynomials of benzenoid structures and their application to geometry optimization of molecular crystals*

**9:45–10:30** **A. Ali**, *On the  $n$ -vertex bicyclic graphs with minimum reduced reciprocal Randić index*

**10:30–11:15** **J. Langer**, *Interface theory of benzenoid structures*

**11:15–12:00** **A. R. Ashrafi**, *Symmetry-based topological indices of molecular graphs*

**14:00 CONFERENCE TRIP**

**THURSDAY, 22 June**

**9:00–9:45** **M. Solà**, *The aromaticity in low-lying excited states*

**9:45–10:30** **H. U. Siehl**, *Quantum chemical calculation of amino-substituted but-2-yne dications. Distonic and gitonic character?*

**10:30–11:15** **A. Amic**, *The role of guaiacyl moiety in radical scavenging by 3,5-dihydroxy-4-methoxybenzyl alcohol*

--- [coffee break] ---

**11:45–13:45** **T. Hrenar**, *Workshop: Advanced statistical analysis of molecular dynamics data*

**FRIDAY, 23 June**

**9:00–9:45** **J. Đorović**, *Examination of antioxidant activity of phenolic functionalized piperidine*

**9:45–10:30** **K. Varga**, *Behaviour of 2-nitrosopyridines in solution and in solid state*

--- [coffee break] ---

**11:15–12:00** **J. Tošović**, *Antioxidative activity of chlorogenic acid: DFT study*

**12:00–12:45** **K. Héberger**, *Bootstrap-like validation for sum of ranking differences*

--- [lunch break] ---

**16:00–18:00** **H. Vančík**, *Workshop: Basic ideas in philosophy of chemistry*

**SATURDAY, 24 June**

**9:00–11:00 Poster session**

**11:00 Conference summary / discussions / closing**