



# Math/Chem/Comp 2019

## 31<sup>st</sup> MC<sup>2</sup> Conference

Inter University Centre Dubrovnik (IUC)

11 – 14 June 2019

### Conference program

#### MONDAY, 10 June

17:00–19:00 Registration

#### TUESDAY, 11 June

9:00–9:30 Conference opening  
H. Vančik and J. Cioslowski  
S. Tomić: To the memory of Dr. Edward C. Kirby

Session chairman: H.-U. Siehl

9:30–10:30 D. Svrtan: A new algorithm for finding largest small polygons  
10:30–11:30 J. Cioslowski: Unoccupied natural orbitals in atoms and molecules  
11:30–12:30. H. Vančik: Concept of thermal solid-state reaction mechanisms

13:00 IUC Reception

#### WEDNESDAY, 12 June

Session chairman: J. Cioslowski

9:30–10:30 H.-U. Siehl: 1, 3-H-shift – A new route to static bicyclobutonium ions  
10:30–13:30 Course: F. Pratnicki: Explicitly correlated wavefunctions in quantum chemistry

14:00 CONFERENCE TRIP

**THURSDAY, 13 June**

Session chairman: H. Vančik

9:30-10:30 U. Bren: Inverse molecular docking as a powerful new approach in discerning promiscuous mode of action of natural compounds

10:30-11:30 B. Lučić: Classification of fungicides based on the mode of action (MOA) with extension to DrugBank molecules

11:30-12:30 S. Tomić: Interdisciplinary Study of Dipeptidyl Peptidase III – Keap1 Interactions

**FRIDAY, 14 June**

9:30-12:30 Poster session

13:00 Conference summary / discussions / closing