

Sunday, June 10, 2007	
20:00–22:00	REGISTRATION & WELCOME DRINK – reception desk, <i>Hotel Lero</i> , Dubrovnik, I. Vojnovića 14
Monday, June 11, 2007	
8:30–9:00	REGISTRATION – reception desk, <i>Hotel Lero</i> , Dubrovnik, I. Vojnovića 14
Lectures – <i>Hotel Lero</i>, I. Vojnovića 14	
9:00–9:30	OPENING CEREMONY - ADDRESSES <i>Dražen VIKIĆ-TOPIĆ</i> , State Secretary for Science and Technology of the Republic of Croatia <i>Ante GRAOVAC</i> , Director of the MCC 2007 <i>Krunoslav PISK</i> , Director General of the Inter-University Centre, Dubrovnik ON LIFE AND WORK OF ACADEMICIAN IVAN SUPEK <i>Nenad TRINAJSTIĆ</i> , Academician ON LIFE AND WORK OF DR. ISTVÁN LUKOVITS
THEORY OF CHEMICAL BONDING	
Chairman: Milan RANDIĆ	
9:45–10:30	<i>Klaus RUEDENBERG, Michael W. SCHMIDT</i> WHY DOES ELECTRON SHARING LEAD TO COVALENT BONDING? A VARIATIONAL ANALYSIS
10:30- 11:00	<i>Patrick BULTINCK, Ramon CARBÓ-DORCA</i> THE HIRSHFELD ATOM IN THE MOLECULE CRITICALLY EXAMINED
11:00-11:15	Coffee Break
Chairman: Haruo HOSOYA	
11:15 -11:35	<i>Ramanathan NATARAJAN, Subhash C. BASAK</i> NMR-SPECTRAL INVARIANTS
11:35-11:55	<i>Robert PONEC</i> CHEMICAL STRUCTURES FROM THE ANALYSIS OF DOMAIN AVERAGED FERMI HOLES. PECULIARITIES OF METAL-METAL BONDING
11:55-12:15	<i>Tomislav ŽIVKOVIĆ</i> EXACT TREATMENT OF OPEN QUANTUM SYSTEMS
Course – Inter-University Centre - IUC, Don F. Bulića 4	
17:00 – 17:45 18:00 – 18:45	<i>Subhash C. BASAK</i> CHEMODESCRIPTORS AND BIODESCRIPTORS: MATHEMATICAL BASIS AND APPLICATIONS
19:00	GUIDED CITY TOUR meeting point in front of the Western Gate (PILE GATE) of the Old Town

Tuesday, June 12, 2007	
Lectures – <i>Hotel Lero</i>, I. Vojnovića 14	
STUDIES OF MOLECULES OF BIOLOGICAL INTEREST	
Chairman: Subhash C. BASAK	
9:00-9:30	<i>Milan RANDIĆ</i> CANONICAL CODES
9:30-9:45	<i>Gašper JAKLIČ, Tomaž PISANSKI, Milan RANDIĆ</i> LINE DISTANCE MATRICES IN BIOINFORMATICS
9:45-10:00	<i>Igor PESEK, Janez ŽEROVNIK</i> SOME NEW NUMERICAL CHARACTERIZATIONS OF MODIFIED HAMORI CURVE REPRESENTATION OF DNA SEQUENCES
10:00-10:20	Coffee Break
Chairman: Tomaž PISANSKI	
10:20-10:40	<i>Subhash C. BASAK, Brian D. GUTE, Ramanathan NATARAJAN, Denise MILLS</i> USE OF ARBITRARY AND TAILORED MOLECULAR SIMILARITY METHODS IN THE ESTIMATION OF PROPERTY/BIOACTIVITY OF CHEMICALS
10:40-10:55	<i>Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI</i> GROWTH INHIBITION ACTIVITY ANALYSIS OF TAXOIDS: INTEGRATION OF STRUCTURE INFORMATION
10:55-11:10	<i>Urban BREN, Matevž BREN</i> REACTION BETWEEN GUANINE AND THE POTENT CARCINOGEN AFLATOXIN B1
11:10-11:25	<i>Sorana D. BOLBOACĂ, Lorentz JÄNTSCHI</i> FROM STRUCTURAL CHEMISTRY TO STRUCTURAL BIOLOGY THROUGH INFORMATION SCIENCE STUDY ON COLLAGEN
11:25-11:40	<i>Mladen MARTINIS, Vesna MIKUTA-MARTINIS</i> LIGHT POLLUTION AND CANCER
11:40-12:00	Coffee Break
BENZENOIDS & RELATED SYSTEMS – Part 1	
Chairman: Tomislav P. ŽIVKOVIĆ	
12:00-12:40	<i>Alexandru T. BALABAN, Milan RANDIĆ</i> RECENT GRAPH-THEORETICAL INVESTIGATIONS ON POLYCYCLIC AROMATIC HYDROCARBONS
12:40-13:20	<i>Jerzy CIOSŁOWSKI, Eduard MATITO, Miquel SOLÀ</i> PROPERTIES OF AROMATICITY INDICES BASED ON THE ONE-ELECTRON DENSITY MATRIX
Course – Inter-University Centre - IUC, Don F. Bulića 4	
17:00 – 17:45	<i>István SIMON</i> BIOINFORMATICS OF INTRINSICALLY UNSTRUCTURED PROTEINS
21:30	Concert - Guitar Duo: Nataša Klasinc-Lončar & Miroslav Lončar <i>Hotel Lero</i>, I. Vojnovića 14

Tuesday, June 12, 2007
Poster Session – Inter-University Centre , Don F. Bulića 4
<p>Moderator: Damir VUKIČEVIĆ</p> <p>Posters given below are exhibited from 18:00, and are open for discussion between 18:30-19:30. After that posters should be removed.</p>
<p><u>MOHAMMAD ESMAIEL AFZALPOUR</u>, REZA GHARAKHANLOU, ABBAS ALI GAEINI, ALI SEGHTOL ESLAMI RELATIONSHIPS AMONG PARAOXONASE/ARYLESTERASE ENZYME ACTIVITY AND SERUM LIPID INDICES</p>
<p><u>Mohammad Mazloum ARDAKANI</u>, Shahram LOTFI, Jahanbakhsh GHASEMI, Alahdad SHABABI, Mohammad NOROOZI SPECTROPHOTOMETRIC DETERMINATION OF ACIDITY CONSTANTS OF CALCON IN WATER AND MIXED WATER-ORGANIC SOLVENTS WITH DATAN ANALYSIS PROGRAM</p>
<p>Gábor JÁRVÁS, Anett KONDOR, <u>András DALLOS</u> COMPUTER SIMULATION OF EVAPORATION AND TRANSPORT OF MULTICOMPONENT MIXTURES IN AIR USING COMSOL MULTIPHYSICS AND COSMOTHERM</p>
<p><u>Siavash DASTMANESH</u>, Rahman SOORI, Mohamad Reza ASAD EFFECT OF CARBOHYDRATE-PROTEIN SUPPLEMENT TIMING ON EXERCISE INDUCED MUSCLE DAMAGE</p>
<p>Takayoshi ISHIMOTO, Masanori TACHIKAWA, Yuichi INADOMI, Hiroaki UMEDA, Toshio WATANABE, Umpei NAGASHIMA DEVELOPMENT OF PROTONIC AND DEUTERONIC BASIS FUNCTIONS BASED ON MULTI-COMPONENT MOLECULAR ORBITAL METHOD</p>
<p><u>Mika ITO</u>, Kaori FUKUZAWA, Yuji MOCHIZUKI, Tatsuya NAKANO, Shigenori TANAKA Ab Initio FRAGMENT MOLECULAR ORBITAL STUDY OF MOLECULAR INTERACTIONS BETWEEN LIGANDED RETINOID X RECEPTOR AND ITS COACTIVATOR</p>
<p>Gábor JÁRVÁS, Anett KONDOR, <u>András DALLOS</u> COMPUTER SIMULATION OF EVAPORATION AND TRANSPORT OF MULTICOMPONENT MIXTURES IN AIR USING COMSOL MULTIPHYSICS AND COSMOTHERM</p>
<p><u>Junko KAMBE</u>, Umpei NAGASHIMA, Eiko NAKAYAMA, Tomoo AOYAMA ANALYSIS OF AIR POLLUTANT: SPM AND NO_x, AN EXAMPLE OF METROPOLIS OF TOKYO AND CHIBA PREFECTURE, JAPAN</p>
<p>Peter Ige KEHINDE COMPUTATIONAL ANALYSIS IN THE MARKETING POINTS</p>
<p>Igor NOVAK, <u>Branka KOVAČ</u> ELECTRONIC STRUCTURE OF METAL β-DIKETONATO COMPLEXES</p>
<p>Vesna MIKUTA-MARTINIS THE CIRCADIAN RHYTHMS OF SOME BODY FUNCTIONS: STATISTICAL APPROACH</p>
<p><u>Mohammad Javad POURVAGHAR</u>, Rahman SOORI A SURVEY OF SODIUM AND POTASSIUM ALTERATIONS DURING REST TIME AFTER AEROBIC ACTIVITIES IN ATHLETES</p>
<p><u>Mehrdad SAMET</u>, Ali MOGHANI SOME PSYCHOPHYSICAL EXPERIMENTS AND SIMULATION IN COLOR CATEGORIZATION</p>
<p><u>Olivera ŠAUPERL</u>, Karin STANA-KLEINSCHKEK, Miran BREZOČNIK CROSSLINKING EFFICIENCY OF COTTON CELLULOSE MONITORED BY DIFFERENT PHYSICAL-CHEMICAL METHODS AND GENETIC PROGRAMMING</p>
<p><u>Nikola ŠTAMBUK</u>, Paško KONJEVODA, Dražen VIKIĆ-TOPIC, Biserka POKRIĆ MODELLING OF EPIPEPE-PARAPEPE INTERACTION USING MOLECULAR RECOGNITION THEORY</p>
<p><u>Farnaz TORABI</u>, Rahman SOORI, Ahmad FAROKHI THE EFFECTS OF SLOW AND FAST CLASSICAL MUSIC ON THE AMOUNT OF PHYSICAL AND MENTAL FATIGUE IN NONATHLETE GIRL STUDENTS</p>
<p><u>Sofie VAN DAMME</u>, Robert PONEC MOLECULAR BASIS OF LFER: THEORETICAL STUDY OF POLAR SUBSTITUENT EFFECT IN ALIPHATIC SERIES</p>

Wednesday, June 13, 2007	
Lectures – <i>Hotel Lero</i>, I. Vojnovića 14	
SESSION ON QSAR & SIMILAR RELATIONSHIPS	
Chairman: István SIMON	
9:00-9:40	<i>Ramon CARBÓ-DORCA, Sofie VAN DAMME</i> QUANTUM QUANTITATIVE STRUCTURE-PROPERTIES RELATIONSHIPS (QQSPR)
9:40-9:55	<i>Kimito FUNATSU, Masamoto ARAKAWA</i> APPLICATION OF THE NOVEL MOLECULAR ALIGNMENT METHOD USING THE HOPFIELD NEURAL NETWORK TO 3D-QSAR
9:55-10:10	<i>Kunal ROY, Gopinath GHOSH</i> QSTR WITH EXTENDED TOPOCHEMICAL ATOM (ETA) INDICES. COMPARATIVE QSAR FOR THE TOXICITY OF DIVERSE FUNCTIONAL ORGANIC COMPOUNDS TO <i>CHLORELLA VULGARIS</i> USING CHEMOMETRIC TOOLS
10:10-10:25	<i>Christoph RÜCKER, Gerta RÜCKER, Markus MERINGER</i> Y-RANDOMIZATION AND ITS VARIANTS IN QSPR/QSAR
10:25-10:40	Coffee Break
Chairman: Ramon CARBÓ-DORCA	
10:40-11:00	<i>Mira GRDIŠA</i> DRUG DELIVERY BY TAT-TECHNOLOGY
11:00-11:20	<i>Željko JERIČEVIĆ</i> GENERALIZED FOSSE'S METHOD FOR RESOLVING A SUM OF EXPONENTIALS
Workshop – <i>Hotel Lero</i>, I. Vojnovića 14	
11:20-12:00	<i>Darko BUTINA</i> QSAR, ADMET AND STATISTICS
13:00	EXCURSION, meeting point Gruž Harbor do not forget your ticket

Thursday, June 14, 2007	
<i>Lectures – Hotel Lero, I. Vojnovića 14</i>	
CHEMISTRY & SPECTROSCOPY	
Chairman: Sean P. McGLYNN	
9:00-9:20	<i>Tibor FURTENBACHER, Attila G. CSÁSZÁR</i> MARVELOUS WATER
9:20-9:50	<i>Jiří CZERNEK</i> SELECTING THE METHOD FOR A RELIABLE DESCRIPTION OF INTERMOLECULAR POTENTIALS: THE C_{2h}-SYMMETRIC SF₂ DIMER AS A TEST CASE
9:50-10:10	<i>Hrvoj VANČIK</i> CONCEPT FOR THE SOLID STATE REACTION MECHANISM
10:10-10:30	Coffee Break
Chairman: Leo KLASINC	
10:30-10:50	<i>Serge S. TRATCH, Marina S. MOLCHANOVA, Nikolai S. ZEFIROV</i> ON THE LEVELS OF MULTIPLE DEGENERACY: INTRINSIC MULTIPLICITY EXEMPLIFIED BY THE SIMPLEST SEMIREGULARLY AND IRREGULARLY DEGENERATE REARRANGEMENTS
10:50-11:10	<i>Ray HEFFERLIN</i> SIMPLIFICATIONS OF THE VECTOR INDEX
11:10-11:30	<i>Salih CINAKLI, Mustafa BÖYÜKATA, Jadson C. BELCHIOR</i> MOLECULAR-DYNAMICS SIMULATIONS OF ACTINIDE-SERIES METAL CLUSTERS
11:30-11:45	Coffee Break
FULLERENES & NANOTUBES	
Chairman: Ivan GUTMAN	
11:45-12:00	<i>István LÁSZLÓ</i> CHIRALITY OF FULLERENES AND NANOTUBES
12:00-12:15	<i>Peter E. JOHN, Horst SACHS</i> EIGENVALUES OF TOROIDAL FULLERENES
12:15-12:30	<i>Zdenka KOLAR-BEGOVIĆ, Ružica KOLAR-ŠUPER</i> AFFINE FULLERENE IS COMPLETELY GOLDEN
12:30-12:45	<i>Jelena SEDLAR, Klavdija KUTNAR, Damir VUKIČEVIĆ</i> ON THE ANTI-KEKULÉ NUMBER OF LEAP-FROG FULLERENES
Course – Inter-University Centre, Don F. Bulića 4	
17:00 – 17:30	<i>Ivan GUTMAN</i>
17:45 – 18:15	AN INVITATION TO CHEMICAL GRAPH THEORY WITH EXAMPLES AND EXERCISES – Part 1
21:00	Conference Dinner, YACHT CLUB ORSAN, I. Zajca 2 do not forget your ticket

Thursday, June 14, 2007
Poster Session – Inter-University Centre, Don F. Bulića 4
<p>Moderator: Paško KONJEVODA</p> <p>Posters given below are exhibited from 18:30, and are open for discussion between 19:00-20:00. After that posters should be removed.</p>
<p><i>Tissaoui ANIS</i> A SELF-STABILIZING ALGORITHM FOR THE MINIMAL COLOUR SUM OF A GRAPH</p>
<p><i>Marina DEKHTYAR, Viktor ROZENBAUM</i> A TOPOLOGY-BASED METHOD FOR CALCULATION OF GROUND-TO-EXCITED STATE CHANGE IN DIPOLE MOMENT</p>
<p><i>Modjtaba GHORBANI, Ali Reza ASHRAFI</i> NON-RIGID GROUP AND SYMMETRY OF TMTB MOLECULE</p>
<p><i>Gašper JAKLIČ, Klemen BERGANT, Jernej BODLAJ, Nataša GRLJ, Boris HORVAT, Peter OGRINC, Gorazd POBERAJ, Milan RANDIĆ, Franc SOLINA, Smiljana ŠKVARČ, Aleš ZALOŽNIK, Marko ZGONIK, Igor POBERAJ, Tomaž PISANSKI</i> ANALYSIS OF LIDAR BACKSCATTERING CURVE BY LINE DISTANCE MATRICES</p>
<p><i>Maryam JALALI, Modjtaba GHORBANI</i> ON OMEGA INDEX OF SOME NANOTUBES</p>
<p><i>Dušana JANEŽIČ, Ante MILIČEVIĆ, Sonja NIKOLIĆ, Nenad TRINAJSTIĆ, Damir VUKIČEVIĆ</i> ZAGREB INDICES: EXTENSION TO WEIGHTED GRAPHS REPRESENTING MOLECULES CONTAINING HETEROATOMS</p>
<p><i>Sanjeev KUMAR, Ravendra SINGH</i> SYMMETRY AND NUMERICAL SOLUTIONS FOR SYSTEMS OF NON-LINEAR REACTION DIFFUSION EQUATIONS</p>
<p><i>Umpei NAGASHIMA, Takatoshi HIGUCHI, Tomoo AOYAMA</i> HIGH-SPEED PSEUDO-ORTHOGONALIZATION FOR THE CAR-PARRINELLO METHOD</p>
<p><i>Sonja NIKOLIĆ, Nenad TRINAJSTIĆ, Damir VUKIČEVIĆ</i> ON THE PATH-ZAGREB MATRICES</p>
<p><i>Milan RANDIĆ, Marjana NOVIČ, Dražen VIKIĆ-TOPIĆ, Dejan PLAVŠIĆ</i> ON ¹³C CHEMICAL SHIFT SUMS IN NONANES</p>
<p><i>Nenad RAOS, Nenad JUDAŠ, Ante MILIČEVIĆ</i> OVERLAPPING SPHERES VOLUMES AND APICAL COORDINATION</p>
<p><i>Hosein SABAGHIAN, Gholam Reza VAKILI-NEZHAAD, Mehdi VAHIDIPOUR</i> PREDICTION OF THE NUMBER OF CARBON ATOMS IN DIFFERENT NANOSTRUCTURES BY USING GEOMETRICAL APPROACH</p>
<p><i>Hiroaki UMEDA, Yuichi INADOMI, Toshio WATANABE, Takayoshi ISHIMOTO, Umpei NAGASHIMA</i> GRID-ENABLED PARALLEL FOCK MATRIX CONSTRUCTION</p>
<p><i>Mehdi VAHIDIPOUR, Hosein SABAGHIAN-BIDOLI, Gholam Reza VAKILI-NEZHAAD</i> GENERATING OF THE FIGURES OF SOME FULLERENES BY USING L-SYSTEM</p>
<p><i>Aniela E. VIZITIU, Simona CHIGER, Margareta S. FLORESCU, Mircea V. DIUDEA</i> THE TRUE FAMILY OF C₆₀</p>
<p><i>Damir VUKIČEVIĆ, Sarah Michele RAJTMAJER</i> TREES WITH MAXIMAL ZAGREB INDEX AND PRESCRIBED NUMBERS OF VERTICES OF GIVEN DEGREE</p>
<p><i>Igor G. ZENKEVICH</i> RECURRENT APPROXIMATION OF PHYSICO-CHEMICAL PROPERTIES OF HOMOLOGUES OF ORGANIC COMPOUNDS. ANALOGY WITH RECURSIVE NUMERICAL SEQUENCES</p>

Friday, June 15, 2007	
Lectures – <i>Hotel Lero</i>, I. Vojnovića 14	
MATHEMATICS WITH APPLICATIONS	
Chairman: Alexandru T. BALABAN	
9:00-9:20	<i>Dragutin SVRTAN</i> A PROGRESS ON ATIYAH-SUTCLIFFE GEOMETRIC CONJECTURES
9:20-9:35	<i>Darko VELJAN</i> NONEUCLIDEAN GEOMETRY-FACTS, FEATURES AND FUNS
9:35-9:50	<i>Ali Reza ASHRAFI, Modjtaba GHORBANI</i> COMPUTING MARKARACTER TABLE AND USCI TABLE OF FINITE GROUPS
9:50-10:10	Coffee Break
Chairman: Dragutin SVRTAN	
10:10-10:25	<i>Ali MOGHANI</i> A COMPUTATIONAL MODEL FOR FUZZY COLOR NAMING
10:25-10:40	<i>Ali MOGHANI, Soroor NAGHDI</i> DATA SET FOR DISCRETE MODEL IN COLOR CATEGORIZATION
10:40-10:55	<i>Nenad KEZELE, Leo KLASINC, Sean P. McGLYNN, Matevž POMPE, Marjan VEBER</i> A FREQUENCY ANALYSIS EVALUATION OF SOME OZONE MONITORING STATIONS
10:55-11:10	<i>Jernej BODLAJ, Tomaž PISANSKI, Franc SOLINA, Boris HORVAT, Igor POBERAJ</i> EYE SAFE LIDAR WITH COMPUTER CONTROL AND ASSISTANCE
11:10-11:25	Coffee Break
BENZENOIDS & RELATED SYSTEMS – Part 2	
Chairman: Dejan PLAVŠIĆ	
11:25-11:40	<i>Boris FURTULA, Ivan GUTMAN</i> KEKULÉ STRUCTURE BASIS OF PHENYLENES AND THEIR CONGENERS
11:40-11:55	<i>Primož LUKŠIČ, Tomaž PISANSKI</i> GROWTH IN CATACONDENSED BENZENOID GRAPHS
11:55-12:10	<i>Petra ŽIGERT</i> HAMILTONICITY AND THE CATACONDENSED BENZENOID GRAPHS
13:00	IUC – RECEPTION, <i>Hotel Lero</i>, I. Vojnovića 14
Course – Inter-University Centre, Don F. Bulića 4	
17:00 – 17:30 17:45 – 18:15	<i>Ivan GUTMAN</i> AN INVITATION TO CHEMICAL GRAPH THEORY WITH EXAMPLES AND EXERCISES – <i>Part 2</i>

Saturday, June 16, 2007	
<i>Lectures - Hotel Lero, I. Vojnovića 14</i>	
GRAPH THEORY IN CHEMISTRY	
Chairman: Nenad TRINAJSTIĆ	
9:00-9:30	<i>Roberto TODESCHINI</i> K OPERATOR: A NEW APPROACH TO DERIVE MOLECULAR DESCRIPTORS FROM GRAPH THEORETICAL MATRICES
9:30-9:45	<i>Slavko RADENKOVIĆ, Ivan GUTMAN</i> CALCULATING THE ESTRADA INDEX
9:45-10:00	<i>Ante GRAOVAC</i> ON THE ESTRADA INDEX
10:00-10:15	Coffee Break
Chairman: Jerzy CIOSLOWSKI	
10:15-10:30	<i>Damir VUKIČEVIĆ, Ivan GUTMAN</i> ON THE VALENCE CONNECTIVITY IN TREES
10:30-10:45	<i>Boris HORVAT, Tomaž PISANSKI</i> THE CONFIGURATION SPACE OF SMALL UNIT DISTANCE GRAPHS
10:45-11:00	<i>Sonja STANKOVIĆ, Ivan GUTMAN</i> SOME CHEMICAL APPLICATIONS OF THE ZHANG-ZHANG POLYNOMIAL
11:00-11:20	Coffee Break
Chairman: Roberto TODESCHINI	
11:20-11:35	<i>Guillermo RESTREPO, Héber MESA, Eugenio J. LLANOS</i> TOPOLOGICAL RELATIONS OF THE CHEMICAL ELEMENTS
11:35-11:50	<i>Dušanka JANEŽIČ, Ante MILIČEVIĆ, Sonja NIKOLIĆ, Nenad TRINAJSTIĆ</i> GRAPH-THEORETICAL MATRICES IN CHEMISTRY
11:50-12:00	CLOSING OF THE MEETING
12:00	FAREWELL DRINK, <i>Hotel Lero</i>, I. Vojnovića 14