

Sunday, June 18, 2006	
20:00–22:00	REGISTRATION & WELCOME DRINK – reception desk, <i>Hotel Lero</i> , Dubrovnik, Iva Vojnovića 14
Monday, June 19, 2006	
9:00-10:00	REGISTRATION <i>Hotel Lero</i> , Dubrovnik, Iva Vojnovića 14
9:30-10:00	OPENING CEREMONY Dražen VIKIĆ-TOPIĆ , State Secretary for Science and Technology of the Republic Croatia Krunoslav PISK , Director General of the Inter-University Centre, Dubrovnik Ante GRAOVAC , Director of the MCC 2006
<u>Morning Session:</u> Session Dedicated to Professor Hosoya Chairman: A. T. BALABAN	
10:00-10:40	<i>Haruo HOSOYA</i> MATHEMATICAL IMPORTANCE OF MY Z-INDEX
10:40-10:50	Coffee Break
<u>Morning Session:</u> Session Dedicated to Professor Hosoya Chairman: H. HOSOYA	
10:50-11:10	<i>Duškanka JANEŽIČ, Sonja NIKOLIĆ, Ante MILIČEVIĆ, Nenad TRINAJSTIĆ</i> ON HOSOYA MATRICES
11:10-11:30	<i>Blaž ZMAZEK, Janez ŽEROVNIK</i> THE HOSOYA-WIENER POLYNOMIAL ON WEIGHTED TREES
11:30-11:45	Coffee Break
<u>Morning Session:</u> Session Dedicated to Professor Hosoya Chairman: N. TRINAJSTIĆ	
11:45-12:15	<i>Antonio ŠIBER</i> CARBON sp^2 SHAPES, VIRUSES AND THEORY OF ELASTICITY
12:15-12:35	<i>Ali Reza ASHRAFI</i> COMPUTING THE WIENER INDEX OF SOME NANOTORI
12:35-12:55	<i>Abdolhamid BAMONIRI, Ali Reza ASHRAFI</i> ON USE OF THE TOPOLOGICAL INDICES FOR STUDYING OF ALKANES

Monday, June 19, 2006	
Afternoon Session: Mathematical Chemistry Chairman: R. A. HEFFERLIN	
16:00-16:30	<i>Shinsaku FUJITA</i> SPHERICITIES OF ORBITS, CYCLES, AND DOUBLE COSETS. THEIR APPLICATIONS TO COMBINATORIAL ENUMERATION OF STEREOISOMERS
16:30-16:45	<i>Antoaneta KLOBUČAR</i> K-DOMINATING SETS ON THE ASSOCIATIVE AND COMMUTATIVE PRODUCTS OF TWO PATHS
16:45-17:00	<i>Peter E. JOHN</i> AN EIGENVALUE CONJECTURE OF P. C. MÜLLER (UNIVERSITY OF WUPPERTAL)
17:00-17:20	Break
Afternoon Session: Mathematical Chemistry Chairman: D. SVRTAN	
17:20-17:50	<i>Ray HEFFERLIN, Ken LUK, Rebecca CHUNG</i> MOLECULAR IDENTIFICATION FROM GRAPHS
17:50-18:10	<i>Damir VUKIČEVIĆ</i> THORNY GRAPH CALCULATOR
18:10-18:30	<i>Ralf GUGISCH</i> CONFORMATIONAL ANALYSIS <i>via</i> CHIROTOPE GENERATION
18:30-18:50	<i>Nenad RAOS, Ante MILIČEVIĆ</i> THE INFLUENCE OF THE FORM OF MOLECULAR GRAPH ON THE SUCCESS OF ESTIMATION OF STABILITY CONSTANTS OF COORDINATION COMPOUNDS
18:50-19:10	<i>Gholam Reza VAKILI-NEJAD</i> INVESTIGATION OF THE ROLE OF COORDINATION NUMBER IN THE LENNARD-JONES-DEVONSHIRE THEORY
19:10-19:30	<i>Mohammad Reza JALALI</i> CALCULATION OF CONFINED FLUID MEAN DENSITY WITH INTERACTION OF YUKAWA
18:30	GUIDED CITY TOUR meeting point in front of the Western Gate (PILE GATE) of the Old Town

Tuesday, June 20, 2006	
Morning Session: Mathematics of Nanostructures Chairman: K. NAKADA	
8:30-9:00	<i>Mircea V. DIUDEA, Monica ȘTEFU, Alexandru E. VIZITIU, Csaba L. NAGY, Damir VUKIČEVIĆ, Ante GRAOVAC</i> STRANGE FULLEROIDS BY MAP OPERATIONS
9:00-9:30	<i>István LÁSZLÓ</i> CONSTRUCTION OF CARBON NANOTUBE JUNCTIONS
9:30-9:50	<i>Tomislav DOŠLIĆ, Damir VUKIČEVIĆ</i> COMPUTING BIPARTITE EDGE FRUSTRATION OF FULLERENE GRAPHS
9:50-10:10	Coffee Break
Morning Session: Mathematics of Nanostructures Chairman: M. V. DIUDEA	
10:10-10:50	<i>Kyoko NAKADA, Kei KUWABARA, Kota DAIGOKU, Takazumi KAWAI, Susumu OKADA</i> ELECTRONIC AND MAGNETIC STRUCTURES OF CARBON NANOTUBES WITH TOPOLOGICAL LINE DEFECTS
10:50-11:20	<i>István LUKOVITS, Franciska H. KÁRMÁN, Peter M. NAGY, Erika KÁLMÁN</i> AROMATICITY OF CARBON NANOTUBES
11:20-11:40	<i>Masood HAMADANIAN, Modjtaba GHORBANI, Ali Reza ASHRAFI</i> COUNTING THE NUMBER OF HETERO FULLERENES $C_{n-k}X_k$, FOR $n = 180, 240, 260, 320, 540$
11:40-12:00	<i>Ghorban Ali MOGHANI, A. R. MIRHABIBI, Hamid MESGARANI</i> Q-CONJUGACY CHARACTER TABLES OF SOME FULLERENS AND MOLECULES: AN APPLICATION OF COMBINATORIAL ENUMERATION OF ISOMERS
12:00-12:20	<i>Morteza YAVARI, Ali Reza ASHRAFI</i> ON THE SYMMETRY OF A POLYHEX CARBON TORUS

Tuesday, June 20, 2006	
<u>Afternoon Session:</u>	
16:00-16:45	<i>Jerzy CIOŚŁOWSKI</i> A COURSE ON EXACTLY SOLVABLE MODELS IN QUANTUM CHEMISTRY – <i>Part I</i>
16:45-17:00	Break
17:00-17:45	<i>Jerzy CIOŚŁOWSKI</i> A COURSE ON EXACTLY SOLVABLE MODELS IN QUANTUM CHEMISTRY – <i>Part II</i>
18:00-19:00	POSTER DISCUSSION
21:30	Concert - Guitar Duo: Nataša Klasinc-Lončar & Miroslav Lončar <i>Hotel Lero</i> , Iva Vojnoviča 14

Tuesday, June 20, 2006

Poster Session

Moderator: I. LUKOVITS

Posters given below are exhibited from morning of **Tuesday, June 21**, and are open for discussion between **18:00-19:00**. After that posters should be removed.

Ljiljana ARAMBAŠIĆ

FRAMES FOR HILBERT SPACES AND HILBERT C^* -MODULES

Ahmad GHOLAMI

SOME RESULTS ON SYMMETRY AND NON-TRANSITIVE CHEMICAL GRAPHS

Dužanka JANEŽIČ, Sonja NIKOLIĆ, Ante MILIČEVIĆ, Nenad TRINAJSTIĆ

THE CONSTRUCTION OF HOSOYA MATRICES

Mohammad MAZLOUM ARDEKANI, Jahanbakhsh GHASEMI, S. LOTFI

APPLICATION OF CHEMOMETRICS METHODS IN DIMERIZATION REACTION OF A DYE IN WATER AND WATER-NON AQUEOUS SOLVENTS MIXTURE

Seyed Nezamoddin MIRSATTARI, Mirabdullah Sed SADJAD

Ab-initio RHF & DENSITY FUNCTIONAL THEORY STUDIES OF SOME CYCLIC ORGANODIBORANES

Chizuru MUGURUMA, Yuko OKAMOTO

NEW APPROACHES TO THE LIQUID-SOLID PHASE TRANSITION OF LENNARD-JONES FLUIDS. II. MONTE CARLO SIMULATION IN THE ISOBARIC-MULTITHERMAL ENSEMBLE

Umpei NAGASHIMA, Yuichi INADOMI, Hiroaki UMEDA, Toshio WATANABE, Takayoshi ISHIMOTO, Tetsuya SAKURAI

MOLECULAR ORBITAL CALCULATION FOR LARGE MOLECULE WITH SAKURAI-SUGIURA METHOD ON GRID COMPUTING ENVIRONMENT

Ghorban Ali MOGHANI, Soroor NAGHDI

SOME COMPUTATIONAL METHODS FOR CALCULATING ISOMERS OF FULLERENES AND MONSTER MOLECULES

Sarah RAJTMAJER, Nenad TRINAJSTIĆ

ON THE DISTANCE MATRICES OF POLYCYCLIC GRAPHS AND THEIR SPANNING TREES

Zahra SADEGH, Javad SAFARI

alpha-PHENYLHYDRAZATION OF HETEROCYCLIC SYSTEMS UNDER SOLVENT FREE CONDITIONS

Masoud SALAVATI-NIASARI, Masood HAMADANIAN, Elham ZAMANI

THERMODYNAMIC THEORETICAL CALCULATION, SYNTHESIS AND LIQUID PHASE OXIDATION OF CYCLOHEXANOL USING *tert*-BUTYLHYDROPEROXIDE OVER HOST/GUEST NANOCOMPOSITE MATERIALS

Lech P. SCHULZ, Jacek KOMASA

FUZZY SET BASED ALGORITHMS AND EFFICIENCY IN THE OPTIMIZATION OF NON-LINEAR PARAMETERS FOR MANY-ELECTRON EXPONENTIALLY CORRELATED GAUSSIAN FUNCTIONS

Jelena SEDLAR, Ivana ANDELIĆ, Ivan GUTMAN, Damir VUKIČEVIĆ,

Ante GRAOVAC

VINDICATING THE PAULING-BOND-ORDER CONCEPT

Wednesday, June 21, 2006	
Morning Session: Session on Modelling of Bioactive Molecules (organized by Darko BUTINA & Dejan PLAVŠIĆ) Chairman: D. BUTINA	
8:30-9:10	<i>Subhash C. BASAK, Denise MILLS, Brian D. GUTE</i> PREDICTION OF TISSUE PARTITION COEFFICIENTS USING MATHEMATICAL STRUCTURAL DESCRIPTORS VERSUS EXPERIMENTAL PROPERTIES
9:10-9:30	<i>Urban BREN, Janez MAVRI</i> CHEMICAL REACTIVITY AS A TOOL TO STUDY CARCINOGENICITY
9:30-9:50	<i>Ramanathan NATARAJAN, Subhash C. BASAK, Jessica J. KRAKER, Douglas M. HAWKINS</i> DESCRIPTOR THINNING AND PROPER CROSS-VALIDATION IN QSAR
9:50-10:10	Coffee Break
Morning Session: Session on Modelling of Bioactive Molecules (organized by Darko BUTINA & Dejan PLAVŠIĆ) Chairman: S. C. BASAK	
10:10-10:40	<i>Darko BUTINA</i> HIGH THROUGHPUT <i>in silico</i> SCREENING IN PHARMACEUTICAL INDUSTRY
10:40-11:00	<i>Branimir BERTOŠA, Sanja TOMIĆ</i> MOLECULAR DYNAMICS AND RANDOM EXPULSION MOLECULAR DYNAMICS SIMULATIONS OF AUXIN BINDING PROTEIN1 AND ITS AUXIN COMPLEXES
11:00-11:15	<i>Vjera BUTKOVIĆ, Saša P. KAZAZIĆ, Nenad KEZELE, Leo KLASINC, William A. PRYOR</i> PROBLEMS IN QUANTIFICATION OF FLAVONOID ACTIVITY
11:15-11:35	<i>Ali IRANMANESH, B. SOLEIMANI</i> SOME TOPOLOGICAL INDICES OF $TUC_4C_8(R)$ NANOTUBES
11:35-12:00	Coffee Break
12:00-13:00	Workshop on QSAR/ADME and Statistics (organized by Darko BUTINA)

Wednesday, June 21, 2006	
Afternoon Session: Session on Proteomics Chairman: P. KONJEVODA	
16:00-16:20	<i>Milan RANDIĆ</i> ON CHARACTERIZATION OF 2-D MAPS
16:20-16:40	<i>Sol BOBST, Milan RANDIĆ, Marjana NOVIČ, Marjan VRAČKO</i> ON NUMERICAL CHARACTERIZATION OF PROTEOMIC DATA
16:40-17:00	<i>Andrea MAURI, Viviana CONSONNI, Roberto TODESCHINI</i> CHARACTERIZATION AND SIMILARITY/DIVERSITY STUDY OF PROTEOMIC MAPS
17:00-17:20	Break
Afternoon Session: Session on Proteomics Chairman: M. RANDIĆ	
17:20-17:40	<i>Matevž POMPE, Gregor ARH</i> MODELING OF BIOTRANSFER FACTORS OF ORGANOCHLORINE COMPOUNDS
17:40-18:00	<i>Nikola ŠTAMBUK, Paško KONJEVODA, Nikola GOTOVAC, Biserka POKRIĆ</i> MOLECULAR RECOGNITION OF THE ANTISENSE PEPTIDES
18:00-18:20	<i>Ali BENVIDI, Shah Nawaz LANJWANI, Zhifeng DING</i> PROTON TRANSFER ASSISTED BY 2-ACETYLPIRIDINE-4-PHENYL-3-THIOSEMICARBAZONE ACROSS WATER/1,2-DICHLOROETHANE INTERFACE
18:30-19:30	POSTER DISCUSSION

Wednesday, June 22, 2006

Poster Session

Moderator: I. LÁSZLÓ

Posters given below are exhibited from morning of **Wednesday, June 22**, and are open for discussion between **18:30-19:30**. After that posters should be removed.

Sachiko AIDA-HYUGAJI, Hiroshi NAKAGAWA, Jumma NOMURA, Minoru SAKURAI, Umpei NAGASHIMA, Toshihisa ISHIKAWA

MOLECULAR MODELING TO CIRCUMVENT CANCER DRUG RESISTANCE ASSOCIATED WITH ABCG2

Vladimir BLAGAIĆ, Nikola ŠTAMBUK, Paško KONJEVODA, Alenka BOBAN-BLAGAIĆ, Biserka POKRIĆ

MOLECULAR RECOGNITION AND SECONDARY STRUCTURE OF ACTH (1-24) AND ITS ANTISENSE PEPTIDES

Edgar E. DAZA C., Clara I. BERMÚDEZ S., Johan F. GALINDO C.

A MODEL OF tRNA STRUCTURE FROM A GRAPH AND QUANTUM THEORETICAL PERSPECTIVE

Vedran ČORIĆ, Paško KONJEVODA, Davor MILIČIĆ, Nikola ŠTAMBUK

THE BRAIN NATRIURETIC PEPTIDE (BNP) AND OPERATIVE RISK ASSESSMENT IN PATIENTS WITH CORONARY ARTERY BYPASS GRAFTING

Petra GALER, Leo KLASINC, Berta KOŠMRLJ, Branka KOVAČ, Boris ŠKET

ELECTRONIC STRUCTURE OF 2-HALOSUBSTITUTED 1,2-DIPHENYLETHANONES

Masood HAMADANIAN, Mohsen BEHPOUR, Gholam Reza VATANKHAH

NEW SCHIFF BASES AS CORROSION INHIBITOR FOR COPPER OBJECTS TO ASSIST CURATORS IN TREATMENTS OF RELATED ARTWORKS: THEORETICAL STUDIES

Leo KLASINC, Bogdan KRALJ, Marko ROŽMAN, Dunja SRZIĆ, Dušan ŽIGON

GAS PHASE INTERACTION OF TEMPO-RADICALS WITH Cr⁺ AND Fe⁺ IONS

Janez KONC, Dušanka JANEŽIČ

PREDICTING PROTEIN INTERACTIONS WITH SURFACE DESCRIPTORS

Vesna MIKUTA-MARTINIS, Ljubica MATIJEVIĆ-MAŠIĆ

RELATIONSHIP BETWEEN THE INTERNAL BODY CLOCK AND SOME BODY FUNCTIONS: STATISTICAL APPROACH

Katarina PIČULJAN, Predrag NOVAK, Tomislav BILJAN, Tomica HRENAR, Mirta RUBČIĆ, Marina CINDRIĆ, Zlatko MEIĆ

EXPERIMENTAL AND DFT STUDIES OF HYDROGEN BONDS IN SALICYLALDEHYDE-4-PHENYLTHIOSEMICARBAZONE

Milan RANDIĆ, Marjana NOVIĆ, Dražen VIKIĆ-TOPIC, Dejan PLAVŠIĆ

ON NUMERICAL REPRESENTATION OF DNA AND PROTEINS

Sofie VAN DAMME, Wilfried LANGENAEKER, Patrick BULTINCK

QUANTUM CHEMICAL PREDICTION OF ADME-Tox PROPERTIES

Thursday, June 22, 2006	
<u>Morning Session: Session on Remote Sensing and GIS</u> (organized by Anita ŠIMIĆ & Marjan SIKORA) Chairman: J. E. MILLER	
8:30-9:10	<i>Jing M. CHEN</i> SATELLITE IMAGERY FOR MAPPING TERRESTRIAL CARBON SOURCE AND SINK DISTRIBUTIONS: METHODOLOGIES AND A CASE STUDY IN CANADA
9:10-9:30	<i>Anita ŠIMIĆ, Jing CHEN, David GOODENOUGH</i> HYPERSPETRAL ALGORITHMS FOR FORESTRY APPLICATIONS
9:30-9:50	Coffee Break
<u>Morning Session: Session on Remote Sensing and GIS</u> (organized by Anita ŠIMIĆ & Marjan SIKORA) Chairman: J. M. CHEN	
9:50-10:30	<i>John E. MILLER</i> RETRIEVAL OF BIOPHYSICAL/STRUCTURAL CANOPY PROPERTIES FOR AGRICULTURE AND FORESTRY APPLICATIONS USING AIRBORNE IMAGING SPECTROMETRY
10:30-10:50	<i>Marjan SIKORA</i> HYBRID HATCHING-SHADING METHOD FOR DEPICTING OF RELIEF IN MODERN MAPS
12:00 19:00-22:00	EXCURSION to Ston by bus including Conference Dinner, [KORUNA] Restaurant, Mali Ston meeting point: <i>Hotel Lero</i> do not forget your ticket

Friday, June 23, 2006	
<u>Morning Session</u> Chairman: A. R. ASHRAFI	
8:00-8:15	<i>Masoud KAVOSH TEHRANI</i> THE STUDY OF LASER ABLATION EFFECTS ON PMMA AND POLYCARBONATE POLYMERS
8:15-8:30	<i>Masood HAMADANIAN, Mohsen OFTADEH, Reza HABIBPOUR</i> INVESTIGATION OF EXPLOSIVE PERFORMANCE OF MONO-, BI- AND TRI-CYCLIC NITRAMINES BY <i>ab-initio</i> COMPUTATIONAL METHODS
8:30-8:45	<i>Nahid TAVAKOLI</i> CESIUM ION-SELECTIVE ELECTRODE BASED ON DIBENZOPYRIDINO-18-CROWN-6
8:45-9:00	<i>Mohammad Taghi SALEHI</i> AN IMPROVED MNEMONIC DIAGRAM FOR THERMODYNAMIC RELATIONSHIPS
9:00-9:20	Coffee Break
<u>Morning Session</u> Chairman L. KLASINC	
9:20-10:00	<i>Jürgen ECKERT</i> SUPPORTED METHYLTRIOXORHENIUM AS A CATALYST FOR OLEFIN METATHESIS
10:00-10:30	<i>Ivan HALASZ, Ernest MEŠTROVIĆ, Hrvoj VANČIK</i> RATIONALIZATIONS OF THE SOLID-STATE REACTION MECHANISMS
10:30-10:50	<i>Veljko ZLATIĆ</i> STRONGLY CORRELATED THERMOELECTRICS
10:50-11:00	Coffee Break
<u>Morning Session</u> Chairman N. JURANIĆ	
11:00-11:30	<i>Zlatko BAČIĆ</i> (HCl) ₂ AND (HF) ₂ IN SMALL HELIUM CLUSTERS: QUANTUM SOLVATION OF HYDROGEN-BONDED DIMERS
11:30-11:50	<i>Haruo HOSOYA, Fuyuko KIDO, Sumio TOKITA</i> A NEW VIEW OF HYBRIDIZED ATOMIC ORBITALS FROM <i>n</i> -DIMENSIONAL WORLD
11:50-12:10	<i>Matevž BREN, Urban BREN</i> THIELE CUMULANTS AND THE FREE ENERGY DECOMPOSITION
12:10-12:30	<i>Mladen MARTINIŠ, Vesna MIKUTA-MARTINIŠ</i> ENTROPY PRODUCTION IN A SYSTEM OF COUPLED NONLINEAR DRIVEN OSCILLATORS
13:15	IUC – RECEPTION, Inter-University Centre, Don Frana Bulića 4

Friday, June 23, 2006	
Afternoon Session: Session on NMR Chairman: T. P. ŽIVKOVIĆ	
16:00-16:30	<i>Hiroko SATOH</i> NUMERICAL REPRESENTATION OF STEREOCHEMICAL ENVIRONMENTS BY USING FRAU
16:30-16:50	<i>Nenad JURANIĆ, Slobodan MACURA, Alan R. PENHEITER, Keith A. JONES, John H. STREIFF</i> VOLATILE ANESTHETIC-PROTEIN INTERACTION: NMR STRUCTURE OF CaM/HALOTHANE COMPLEX IN SOLUTION
16:50-17:20	<i>Predrag NOVAK</i> FREE AND RIBOSOME-BOUND STRUCTURES OF MACROLIDE ANTIBIOTICS: THE ROLE OF NMR AND CONFORMATIONAL ANALYSIS IN LIGAND DESIGN
17:20-17:30	Break
Afternoon Session: Session on Mathematics Chairman P. E. JOHN	
17:30-18:00	<i>Tomislav P. ŽIVKOVIĆ</i> HOW TO OPTIMISE USEFULL INFORMATION DERIVED FROM EXPERIMENTAL DATA?
18:00-18:30	<i>Željko JERIČEVIĆ</i> APPROXIMATE SOLUTION OF LINEAR SYSTEM
18:30-19:00	<i>Dragutin SVRTAN</i> EXPLICIT CIRCUMRADIUS EQUATIONS FOR CYCLIC HEPTAGONS AND OCTAGONS

Saturday, June 24, 2006	
<u>Morning Session: Session on Topics of General Interest</u> Chairman: R. B. MALLION	
9:00-9:20	<i>Krunoslav PISK</i> EINSTEIN: FROM SPECIAL THEORY OF RELATIVITY (1905), THROUGH GENERAL THEORY OF RELATIVITY (1916), UNTIL COSMOLOGICAL TERM (1917)
9:20-9:40	<i>Lech P. SCHULZ</i> COMPLEX SYSTEMS AND MEASUREMENTS OF VAGUE AFFINITIES
9:40-10:00	<i>Ghorban Ali MOGHANI</i> SOME MATHEMATICAL METHODS FOR COMBINATORIAL ENUMERATIONS
10:00-10:20	Coffee Break
<u>Morning Session: Session on Topics of General Interest</u> Chairman: K. PISK	
10:20-10:40	<i>Book Outline</i> <i>Jim SAWYER</i> DE REVOLUTION VII SIX DIMENSIONS
10:40-11:20	<i>Roger B. MALLION</i> THE SIX (OR SEVEN) BRIDGES OF KALININGRAD: A PERSONAL EULERIAN WALK, 2006
11:20-11:50	<i>LECTURE TO BE PRESENTED BY IBM REPRESENTATIVE</i>
12:00	CLOSING OF THE MEETING FAREWELL DRINK