

Sunday, June 19, 2005.	
20:00-23:00	REGISTRATION & WELCOME DRINK – reception desk, <i>Hotel Lero</i> , Dubrovnik, Iva Vojnovića 14
Monday, June 20, 2005	
9:00-10:00	REGISTRATION <i>Hotel Lero</i> , Dubrovnik, Iva Vojnovića 14
9:30-9:45	OPENING CEREMONY Dragan PRIMORAC , Minister of Science, Education and Sport of the Republic of Croatia Mladen ŽINIĆ , Director of the Ruđer Bošković Institute, Zagreb Dražen VIKIĆ-TOPIĆ , Counsellor for Science and Education of the IRB, Zagreb Krunoslav PISK , Acting Director General of the Inter-University Centre, Dubrovnik Ante GRAOVAC , Director of the MCC 2005
Morning Session: Session on Proteins (organized by István SIMON) Chairman: Peter F. STADLER	
9:45-10:05	<u><i>Csaba MAGYAR, Michael M GROMIHA, István SIMON</i></u> STABILIZING RESIDUES IN PROTEINS
10:05-10:35	<u><i>Davor JURETIĆ, Paško ŽUPANOVIĆ, Srećko BOTRIĆ</i></u> THE MAXIMUM ENTROPY PRODUCTION PRINCIPLE AS THE GUIDELINE FOR PREDICTING EVOLUTION OF COMPLEX SYSTEMS
10:35-10:50	Coffee Break
Morning Session: Session on Proteins (organized by István SIMON) Chairman: M. RANDIĆ	
10:50-11:10	<u><i>Jiří CZERNEK</i></u> <i>Ab initio</i> STUDIES ON LOW-ENERGY CONFORMERS OF OLIGOPEPTIDES
11:10-11:30	<u><i>Attila G. CSÁSZÁR, Eszter CZINKI</i></u> ON THE USE OF ICS AND CSA NMR DATA FOR PREDICTING SECONDARY STRUCTURES OF PEPTIDES AND PROTEINS
11:30-12:00	<u><i>Nenad JURANIĆ, Franklyn PRENDERGAST, Slobodan MACURA</i></u> <i>De novo</i> DETERMINATION OF PROTEIN SUBSTRUCTURES FROM RESIDUAL DIPOLAR AND HYDROGEN BOND NMR COUPLINGS OF PEPTIDE GROUPS
12:00-12:15	Coffee Break
Morning Session: Session on Proteins (organized by István SIMON) Chairman: D. JURETIĆ	
12:15-12:45	<u><i>Milan RANDIĆ</i></u> (title to be announced)
12:45-13:15	<u><i>Subhash C. BASAK</i></u> USE OF PROTEOMICS BASED BIODESCRIPTORS VERSUS CHEMODESCRIPTORS IN PREDICTING HALOCARBON TOXICITY

Monday, June 20, 2005	
<u>Afternoon Session</u> Chairman: T. ŽIVKOVIĆ	
16:00-16:30	<i>Krishnan BALASUBRAMANIAN</i> RECENT APPLICATIONS OF MATHEMATICAL AND COMPUTATIONAL CHEMISTRY
<u>Course</u>	
16:30-17:10	<i>István SIMON</i> INTRINSICALLY UNSTRUCTURED PROTEINS
18:30	GUIDED CITY TOUR meeting point in front of the Western Gate (PILE GATE) of the Old Town

Tuesday, June 21, 2005	
Morning Session: Session on Bioinformatics (organized by Peter F. STADLER) Chairman: I. SIMON	
8:30-9:10	<i>Guido FRITZSCH, Sonja J. PROHASKA, Peter F. STADLER</i> PARTIAL ORDERS, MOLECULAR PHYLOGENIES, AND MIGRATION
9:10-9:30	<i>Stefan JANSON, Daniel MERKLE</i> A MULTI-OBJECTIVE PARTICLE SWARM OPTIMIZATION ALGORITHM APPLIED TO MOLECULAR DOCKING
9:30-9:50	<i>Matthias BERNT, Daniel MERKLE, Martin MIDDENDORF</i> HEURISTICS FOR THE REVERSAL MEDIAN PROBLEM: HOW TO SELECT GOOD REVERSALS?
9:50-10:10	Coffee Break
Morning Session: Session on Bioinformatics (organized by Peter F. STADLER) Chairman: N. JURANIĆ	
10:10-10:40	<i>Axel MOSIG, Sonja J. PROHASKA, Peter F. STADLER</i> OPTIMIZING BARBECUES AND TANIMOTO SCORES WITH APPLICATIONS IN REGULATORY MOTIF DISCOVERY
10:40-11:00	<i>Matthias KRUSPE, Peter F. STADLER</i> PROGRESSIVE MULTIPLE SEQUENCE ALIGNMENTS FROM TRIPLETS
11:00-11:20	<i>Roman R. STOCSITS, Peter F. STADLER</i> RNA CONSENSUS STRUCTURES IN MOLECULAR MORPHOLOGY
11:20-11:40	Coffee Break
Morning Session: Session on Bioinformatics (organized by Peter F. STADLER) Chairman: D. BUTINA	
11:40-12:00	<i>Kristin MISSAL, Dominic ROSE, Peter F. STADLER</i> COMPUTATIONAL IDENTIFICATION OF ncRNAs IN INVERTEBRATES BY COMPARATIVE GENOMICS
12:00-12:20	<i>Claudia FRIED, Peter F. STADLER</i> TRANSCRIPTION FACTOR TARGET DETECTION IN COMPARATIVE GENOMICS
12:20-12:40	<i>Nikola ŠTAMBUK, Paško KONJEVODA, Nikola GOTOVAC, Biserka POKRIĆ</i> MOLECULAR RECOGNITION OF THE COMPLEMENTARY PEPTIDE STRUCTURES
Morning Session: Clusters Chairman: B. BORŠTNIK	
12:40-13:00	<i>Antonio ŠIBER</i> ICOSAHEDRAL AND CUBOCTAHEDRAL LENNARD-JONES CLUSTERS: GROUND STATE ENERGIES AND VIBRATIONS

Tuesday, June 21, 2005	
Afternoon Session: Session on Bioinformatics (organized by Peter F. STADLER) Chairman: N. ŠTAMBUK	
16:00-16:30	<i>Branko BORŠTNIK, Borut OBLAK, Danilo PUMPERNIK</i> MUTABILITY OF SHORT SEQUENCE REPEATS IN HUMAN GENOME
16:30-17:00	<i>Kirill DEGTYARENKO</i> CHEMICAL ONTOLOGIES FOR BIOINFORMATICS
17:00-17:10	Break
<u>Movie</u> (in Croatian)	
17:10-17:40	<i>Antonio ŠIBER</i> SFERE UNUTAR SFERE

Tuesday, June 21, 2005

Poster Session

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.

Tomislav CVITAŠ, Nenad KEZELE, Leo KLASINC, Matevž POMPE, Marjan VEBER
FREQUENCY ANALYSIS OF PHOTOCHEMICAL POLLUTION DATA

Gergely DEZSŐ, Iván GYÉMÁNT
SPECIAL PROPERTIES OF DENSITY MATRICES DERIVED FROM AN ARBITRARY FULL-CI WAVE FUNCTION

Josipa FRIŠČIĆ, Sonja NIKOLIĆ, Marica MEDIĆ-ŠARIĆ
QSPR STUDY OF FLAVONOID COMPOUNDS

*Jana HERTEL, Claudia FRIED, Manja LINDEMAYER, Kristin MISSAL, Sonja J. PROHASKA,
Andrea TANZER, Christoph FLAMM, Ivo L. HOFACKER, Peter F. STADLER, the students of the bioinform.
compt. labs 2004 and 2005*
THE EVOLUTION OF ANIMAL miRNAs

*Ivana IVANČIĆ-BAĆE, Ignacija VLAŠIĆ, Boris MIHALJEVIĆ, Mirna IMEŠEK, Erika SALAJ-ŠMID, Krunoslav
BRČIĆ-KOSTIĆ*
MECHANISM OF SOS INDUCTION IN *Escherichia coli*: INVOLVEMENT OF RecA LOADING ACTIVITY

Nenad KEZELE, Glenda ŠORGO, Leo KLASINC, William A. PRYOR
GAS PHASE REACTIONS OF AMBIENTAL CO AND SO₂ WITH OZONE

Paško KONJEVODA
DATA MINING AND IDENTIFICATION OF DRUG SIDE-EFFECTS DURING CLINICAL TRIALS

Manuela LINDEMAYER, Peter F. STADLER
snRNA SEARCH WITHOUT A MAGNIFYING GLASS

Vesna MIKUTA-MARTINIS, Lj. MATIJEVIĆ
OSCILLATED PHENOMENA IN BIOSYSTEMS: STATISTICAL APPROACH

Ante MILIČEVIĆ, Nenad RAOS
ESTIMATION OF STABILITY OF DIAMINOETHANE COMPLEXES BY THE OVERLAPPING SPHERES METHOD WITH A
VARIABLE CENTRAL SPHERE RADIUS

Sonja NIKOLIĆ, Ante MILIČEVIĆ, Nenad TRINAJSTIĆ
TOXICITY OF ALIPHATIC ETHERS REVISITED

Borut T. OBLAK, Branko BORŠTNIK
TANDEM REPEATS IN THREE DIMENSIONAL STRUCTURES OF PROTEINS

Sonja J. PROHASKA, Axel MOSIG, Peter F. STADLER
REARRANGEMENT OF REGULATORY ELEMENTS

Milan RANDIĆ, Alexandru T. BALABAN, Dejan PLAVŠIĆ
GRAPHICAL REPRESENTATION OF PROTEINS AS FOUR-COLOR MAPS AND THEIR NUMERICAL REPRESENTATION

Wednesday, June 22, 2005	
Morning Session: Modelling in Chemistry & Biology	
Chairman: L. KLASINC	
8:30-8:50	<i>Željko BAJZER, Yves NOMINE, Georges MER</i> FRACTAL KINETICS AND ITS APPLICATION TO BIACORE BINDING DATA ANALYSIS
8:50-9:10	<i>Urban BREN, Jan FLORIAN</i> DECOMPOSITION OF THE FREE ENERGY USING THE FREE ENERGY PERTURBATION METHOD
9:10-9:30	<i>Dušanka JANEŽIČ, Franci MERZEL, Matej PRAPROTNIK</i> ANALYTICAL TREATMENT OF HYDROGEN VIBRATIONS IN MOLECULAR DYNAMICS SIMULATION
9:30-9:50	<i>Mladen MARTINIS, Vesna MIKUTA-MARTINIS</i> APPLICATION OF RANDOM MATRIX THEORY TO BIO SIGNAL ANALYSIS
9:50-10:10	Coffee Break
Morning Session: Modelling in Chemistry & Biology	
Chairman: N. TRINAJSTIĆ	
10:10-10:30	<i>Markus MERINGER</i> CASE via MS: GENERATION OF MOLECULAR STRUCTURES AND STRUCTURE RANKING BY MASS SPECTRA
10:30-10:50	<i>Robert PONEC</i> MOLECULAR BASIS OF LFER. SIMPLE MODEL FOR THE ESTIMATION OF BRÖNSTED EXPONENT IN ACIDOBASIC CATALYSIS
10:50-11:10	<i>Guillermo RESTREPO</i> THE MEANING OF CLUSTER AND ITS INFORMATION CONTENT
11:10-11:30	Coffee Break
Morning Session: Solid State Chemistry	
Chairman: J. CIOSLOWSKI	
11:30-12:00	<i>Robert GLASER, Itzhak ERGAZ</i> SOLID-STATE AND SOLUTION-STATE CONFORMATIONAL DIFFERENCES AS SHOWN BY SOLUTION-STATE AND ¹³ C CP/MAS NMR STUDIES ON CONFORMATIONAL POLYMORPHIC CRYSTALS ASSISTED BY QUANTUM-MECHANICAL CALCULATIONS OF SHIELDING AND SPIN-SPIN COUPLING CONSTANTS
12:00-12:20	<i>Hrvoj VANČIK</i> MULTIDIMENSIONAL APPROACH TO SOLID STATE REACTION MECHANISMS
Morning Session: Quantum Chemistry	
Chairman: R. PONEC	
12:20-13:00	<i>Jerzy CIOSLOWSKI</i> STUDIES OF HOMOGENEOUS ELECTRON GAS

Wednesday, June 22, 2005	
Afternoon Session: Quantum Chemistry	
	Chairman: D. JANEŽIČ
16:00-16:20	<i>Katarzyna PERNAL</i> AN EFFECTIVE POTENTIAL FOR THE NATURAL SPINORBITALS
16:20-16:40	<i>Patrick BULTINCK, Ana GALLEGOS, Sofie VAN DAMME, Robert PONEC, Ramon CARB-DORCA</i> MOLECULAR QUANTUM SIMILARITY APPROACH TO AROMATICITY
16:40-17:00	<i>Tomislav P. ŽIVKOVIĆ</i> EXACT QUANTUM TREATMENT OF FINITE-DIMENSIONAL SYSTEM IN THE INTERACTION WITH THE KNOWN INFINITE-DIMENSIONAL SYSTEM
17:00-17:20	<i>Ghorban Ali MOGHANI, Ali Reza.ASHRAFI</i> PROPERTIES OF TETRAAMMINE PLATINUM(II) WITH C2V AND C4V POINT GROUPS
21:30	Concert - Guitar Duo: Nataša Klasinc-Lončar & Miroslav Lončar <i>Hotel Lero</i> , Iva Vojnovića 14

Wednesday, June 22, 2005

Poster Session

Posters given below are exhibited from morning of **Wednesday, June 22, 2005**, and are open for discussion between **18:00-19:00**. After that posters should be removed.

Tomislav BILJAN, Zlatko MEIĆ

Yb₃+ AS AN ORIGIN OF THE STRONG ANTI-STOKES LUMINESCENCE IN THE NIR FT-RAMAN SPECTRA OF SOME LANTHANIDE SESQUIOXIDES

Marko BOBEN, Tomaž PISANSKI, Arjana ŽITNIK

I-GRAPHS AND THE CORRESPONDING CONFIGURATIONS

Mircea V. DIUDEA, Monica ŠTEFU, Peter E. JOHN, Ante GRAOVAC

GENERALIZED OPERATIONS ON MAPS

András DALLOS, R. KRESZ

TESTING OF *a priori* VAPOR PRESSURE AND BOILING POINT PREDICTIVE ABILITY OF COSMO^{therm}

Boris HORVAT, Gašper JAKLIČ, Tomaž PISANSKI

ON THE NUMBER OF HAMILTONIAN GROUPS

Edward C. KIRBY

THE CATALOGUING AND ENCODING OF TOROIDAL FULLY RESONANT AZULENOIDS BY THE USE OF TOROIDAL FULLY RESONANT BENZENOID TEMPLATES

Leo KLASINC, Berta KOŠMRLJ, Branka KOVAČ, Boris ŠKET

ELECTRONIC STRUCTURE OF HALOGENATED DIPHENYLMETHANONES

Leo KLASINC, Bogdan KRALJ, Kata MLINARIĆ-MAJERSKI, Marko ROŽMAN, Dunja SRZIĆ, Ines VUJASINOVIĆ, Dušan ŽIGON

METAL COMPLEXATION OF THIACROWN ETHER MACROCYCLES BY MASS SPECTROMETRY IN LIQUID AND GAS PHASE

Alen ORBANIĆ, Tomaž PISANSKI

A CALCULATION AND A REPRESENTATION OF EDGE-TRANSITIVE MAPS OF SMALL ORDER

Wolfgang SCHÖFBERGER, Vilko SMREČKI, Norbert MÜLLER

SOFTWARE IMPLEMENTATION FOR COVARIANCE NMR SPECTROSCOPIC INVESTIGATIONS

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

ALGEBRAIC KEKULÉ STRUCTURES AND BOND ORDERS IN BENZENOIDS

Serge S. TRATCH, Marina S. MOLCHANOVA, Nikolai S. ZEFIROV

ON THE REGULARITY OF STRUCTURAL DEGENERACY: COMPUTER-AIDED DESIGN OF SEMIREGULARLY AND IRREGULARLY DEGENERATE REARRANGEMENTS

Oleg URSU, Mircea V. DIUDEA

MOLECULAR SIMILARITY IN 3D SPACE USING DISTANCE CONSTRAINTS MATRIX

Dražen VIKIĆ-TOPIĆ

DEUTERIUM ISOTOPE EFFECTS IN NMR SPECTRA

Thursday, June 23, 2005	
Morning Session: Session on Spectroscopy Chairman: D. VIKIĆ-TOPIĆ	
8:30-9:00	<u>Gábor KERESZTURY, Krisztina ISTVÁN, Tom SUNDIUS</u> APPLICABILITY OF THE SQM FORCE FIELD METHOD TO THE VIBRATIONAL SPECTRA OF CHARGED SYSTEMS: SODIUM ACETATE
9:00-9:20	<u>Zlatko MEIĆ, Tomislav BILJAN</u> NON-VIBRATIONAL FEATURES IN NIR FT-RAMAN SPECTRA OF LANTHANIDE SESQUIOXIDES
9:20-9:35	<u>Rabah A. KHALIL, Yosif A. SHAHAB</u> A NEW APPROACH TO NMR CHEMICAL SHIFT ADDITIVITY PARAMETERS USING SIMULTANEOUS LINEAR EQUATION METHOD
9:35-9:50	<u>Javad SAFAEI-GHOMI, Zohreh ALISHAHI</u> PREPARATION OF SOME NOVEL INDAZOLE DERIVATIVES BY USING CHALCONES
9:50-10:00	Coffee Break
Morning Session: Polyhedra & Fullerenes Chairman: S. S. TRATCH	
10:00-10:30	<u>Peter E. JOHN, Horst SACHS</u> A 2-PARAMETRIC CLASS OF TRANSFORMATIONS FOR FULLERENES AND OTHER POLYHEDRA
10:30-11:00	<u>Igor PAK</u> CONSTRUCTING CONVEX POLYHEDRA
11:00-11:20	<u>Damir VUKIČEVIĆ, Milan RANDIĆ</u> THE FULLERENE C70 IS ONE OF THE TWO MOST IMPORTANT FULLERENES
11:20-11:30	Coffee Break
Morning Session: Polyhedra & Fullerenes Chairman: H. SACHS	
11:30-11:50	<u>Dragutin SVRTAN</u> INTRINSIC PROOFS FOR AREA AND CIRCUMRADIUS OF CYCLIC HEXAGONS. SOLVING EQUATIONS FOR ARBITRARY CYCLIC POLYGONS
11:50-12:10	<u>Darko VELJAN</u> AREAS OF SOME POLYGONS AND VOLUMES OF FULLERENES
13:00	IUC – RECEPTION, Inter-University Centre , Don Frana Bulića 4

Thursday, June 23, 2005	
Afternoon Session: Graphs in Chemistry	
Chairman: I. PAK	
16:00-16:20	<i>Mustapha AOUCHICHE, Gilles CAPOROSSI, Pierre HANSEN, Marie LAFFAY</i> WHAT CAN THE COMPUTER SAY ABOUT THE RANDIC INDEX
16:20-16:40	<i>Boris HOLLAS</i> THE REDUNDANCY OF TOPOLOGICAL INDICES
16:40-17:00	<i>Matevž POMPE, Milan RANDIĆ</i> VARIABLE TOPOLOGICAL INDICES IN DRUG DESIGN
17:00-17:20	<i>Blaž ZMAZEK, Janez ŽEROVNIK</i> ON GENERALIZATION OF THE HOSOYA-WIENER POLYNOMIAL
17:20-17:30	Break
<u>Course</u>	
17:30-18:10	<i>Josef LEYDOLD</i> AN INTRODUCTION TO NONUNIFORM RANDOM VARIATE GENERATION
21:00	Conference Dinner, YACHT CLUB ORSAN , Ivana Zajca 2

Friday, June 24, 2005	
Morning Session: Mathematics & Statistics with Applications	
	Chairman: D. SVRTAN
9:30-10:00	<i>Serge S. TRATCH, Nikolai S. ZEFIROV</i> THE EASILY CALCULATED GEOMETRY DEVIATION INDICES AND THEIR APPLICATION TO CHARACTERIZATION OF MOLECULAR SYMMETRY
10:00-10:30	<i>Shinsaku FUJITA</i> SPHERICITIES OF CYCLES. WHAT POLYA'S THEOREM IS DEFICIENT IN
10:30-10:50	<i>Matevž BREN, Vladimir BATAGELJ</i> MixeR PACKAGE FOR COMPOSITIONAL DATA ANALYSIS
10:50-11:10	<i>Andrej MRVAR, Vladimir BATAGELJ</i> RELINKING MARRIAGES IN GENEALOGY OF RAGUSAN NOBLE FAMILIES BETWEEN 12 th AND 16 th CENTURY
11:10-11:30	Coffee Break
Morning Session: Modelling of Carbon Structures	
	Chairman: S. FUJITA
11:30-11:50	<i>István LÁSZLÓ</i> GEOMETRIC AND ELECTRONIC STRUCTURE OF CARBON NANOTUBE JUNCTIONS
11:50-12:10	<i>István LUKOVITS</i> ENUMERATION OF KEKULÉ STRUCTURES IN GRAPHITE
Afternoon Session: Einstein's Year	
	Chairman: N. RAOS
16:00-16:30	<i>Krunoslav PISK</i> EINSTEIN: FROM SPECIAL THEORY OF RELATIVITY (1905), THROUGH GENERAL THEORY OF RELATIVITY (1916), UNTIL COSMOLOGICAL TERM (1917)
16:30-17:00	<i>Tomislav ŽIVKOVIĆ</i> (title to be announced)
<u>Book Outline</u>	
17:00-17:20	<i>James SAWYER</i> DE REVOLUTION VII SIX DIMENSIONS
Saturday, June 25, 2005	
	CLOSING OF THE MEETING EXCURSION