
19th Dubrovnik International Course & Conference
MATH / CHEM / COMP 2004
Dubrovnik
June 21–26, 2004

FOREWORD

Ante Graovac, Biserka Pokrić, and Dražen Vikić-Topić

Croat. Chem. Acta 78 (2005) XXI

EDWARD CAMERON KIRBY – curriculum vitae

Ante Graovac

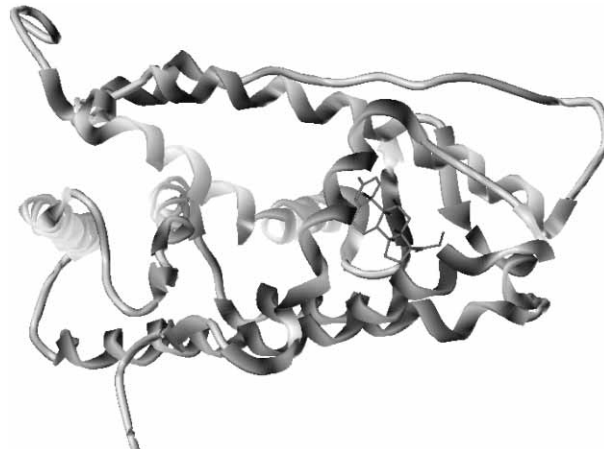
Croat. Chem. Acta 78 (2005) XXIII–XXIV

FEATURE ARTICLE

CCA-2989

Combined *in silico* and *in vitro* Approach to Drug Screening

Donatella Verbanac, Dubravko Jelić, Višnja Stepanić,
Iva Tatić, Dinko Žihner, and Sanja Koštrun



Croat. Chem. Acta 78 (2005) 133–139

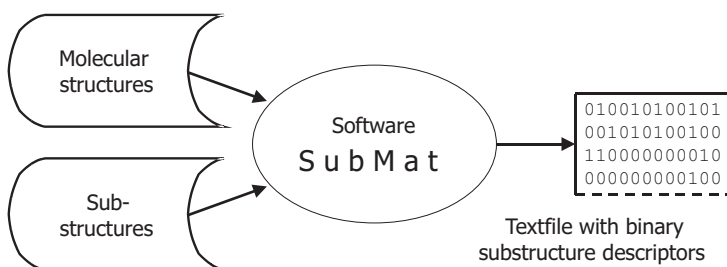
ORIGINAL SCIENTIFIC PAPERS

CCA-2990

Binary Substructure Descriptors for Organic Compounds

Kurt Varmuza, Wilhelm Demuth,
Manfred Karlovits, and Heinz Scsibrany

Croat. Chem. Acta 78 (2005) 141–149



CCA-2991

Annotation of Transmembrane Segments of Experimentally Solved Bacterial Porins and Adhesins

Damir Zucić

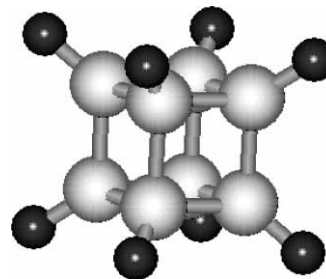
Croat. Chem. Acta **78** (2005) 151–158

ASP	ASP	ASP	ASP	GLU	ASP	ASP	ASP	P3
ASN	VAL	ILE	HIS	GLY	MET	ILE	ALA	P2
ASP	THR	ASP	LYS	ASP	GLU	LYS	GLN	P1
ALA	TYR	LEU	ALA	ALA	GLN	GLU	GLU	P0
ILE	TYR	VAL	TYR	TYR	LEU	TYR	MET	P-1
GLY	GLY	GLN	GLY	TYR	GLU	GLY	ALA	P-2
GLY	LEU	VAL	LEU	ALA	LEU	LEU	VAL	P-3
VAL	GLY	TYR	SER	LYS	ALA	GLY	ALA	P-4
ILE	ALA	GLY	VAL	VAL	ALA	VAL	ALA	P-5
SER	SER	GLY	ASP	ASN	ILE	THR	ALA	P-6
ALA	TYR	VAL	SER	THR	ALA	TYR	TYR	P-7

CCA-2992

Symmetry Properties of Some Chemical Graphs

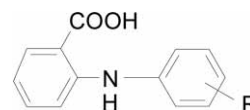
Ali Reza Ashrafi and Masood Hamadianian

Croat. Chem. Acta **78** (2005) 159–163

CCA-2993

Prediction of Anti-Inflammatory Activity of *N*-Arylanthranilic Acids: Computational Approach Using Refined Zagreb Indices

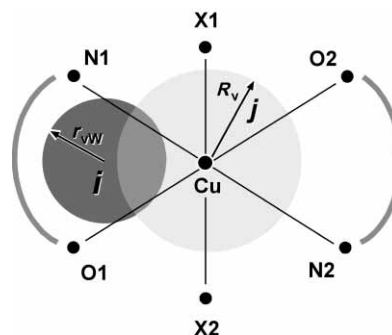
Sanjay Bajaj, S. Singh Sambi, and Anil Kumar Madan

Croat. Chem. Acta **78** (2005) 165–174

CCA-2994

Estimation of Stability Constants of Copper(II) Chelates with Amino Acids by Overlapping Spheres Method

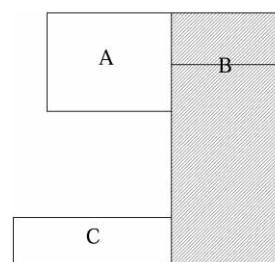
Nenad Raos

Croat. Chem. Acta **78** (2005) 175–180

CCA-2995

Is the Stationary Current Distribution in a Linear Planar Electric Network Determined by the Principle of Maximum Entropy Production?

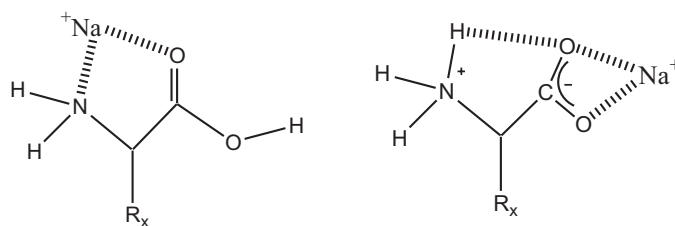
Srećko Botrić, Paško Županović, and Davor Juretić

Croat. Chem. Acta **78** (2005) 181–184*Croat. Chem. Acta* **78** (2) XI–XVII (2005)

CCA-2996

Gas Phase Structure of Sodiated Amino Acids Probed by H/D Exchange Reactions

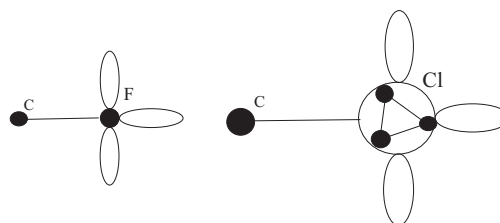
Marko Rožman

Croat. Chem. Acta **78** (2005) 185–188

CCA-2997

A Chemical Graph Model Study of The Partition Coefficient of Halogenated Carbocompounds

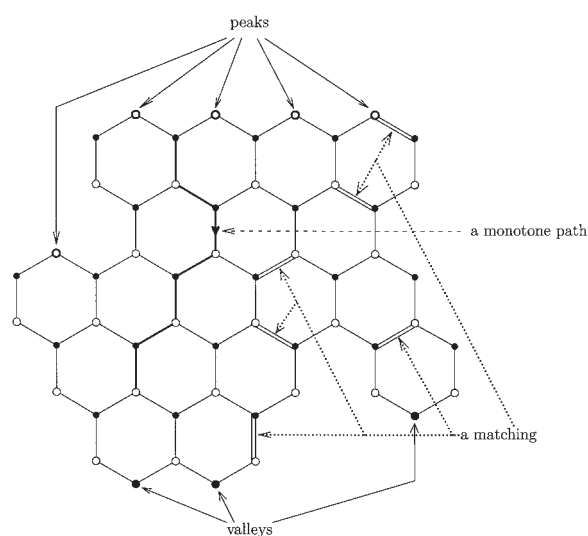
Lionello Pogliani

Croat. Chem. Acta **78** (2005) 189–194

CCA-2998

On Maximum Matchings and Eigenvalues of Benzenoid Graphs

Siemion Fajtlowicz, Peter E. John, and Horst Sachs

Croat. Chem. Acta **78** (2005) 195–201

CCA-2999

Compact Valence Sequences for Molecules with Single, Double and Triple Covalent Bonds

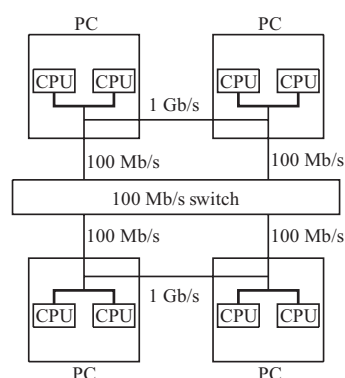
Damir Vukičević and Ante Graovac

Croat. Chem. Acta **78** (2005) 203–209

CCA-3000

Fast Parallel Molecular Simulations

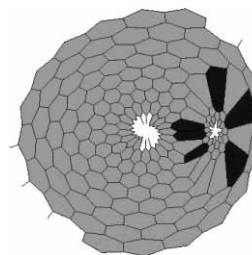
Urban Borštnik, Milan Hodošček, and Dušanka Janežič

Croat. Chem. Acta **78** (2005) 211–216

CCA-3001

Topological Description and Construction of Single Wall Carbon Nanotube Junctions

István László

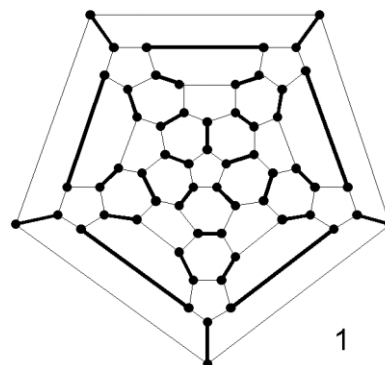


Croat. Chem. Acta **78** (2005) 217–221

CCA-3002

Atlas of Kekulé Valence Structures of Buckminsterfullerene

Damir Vukičević, Harry W. Kroto, and Milan Randić

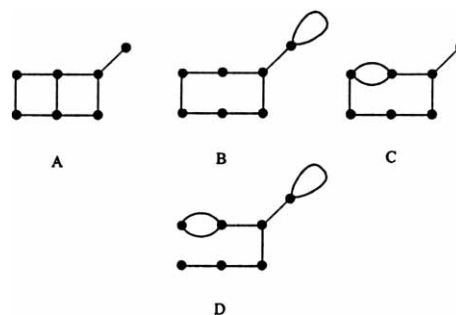


Croat. Chem. Acta **78** (2005) 223–234

CCA-3003

Comparison of the Hosoya Z-Indices for Simple and General Graphs of the Same Size

Damir Vukičević and Nenad Trinajstić

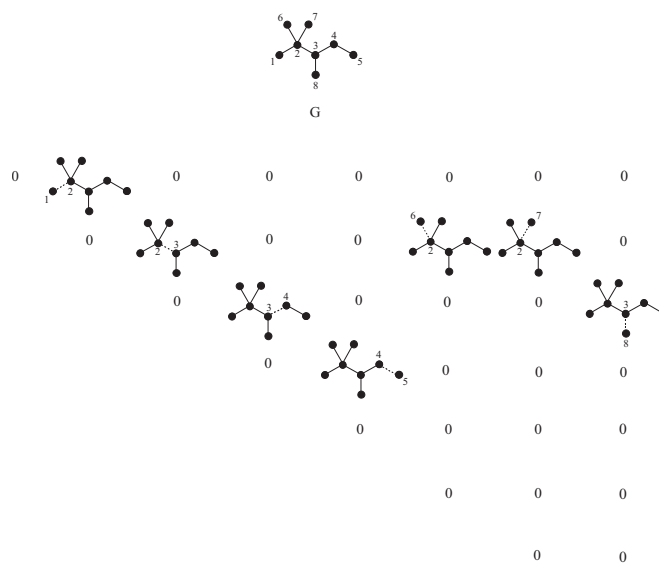


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CCA-3004

Graphical Matrices in Chemistry

Sonja Nikolić, Ante Miličević, and Nenad Trinajstić

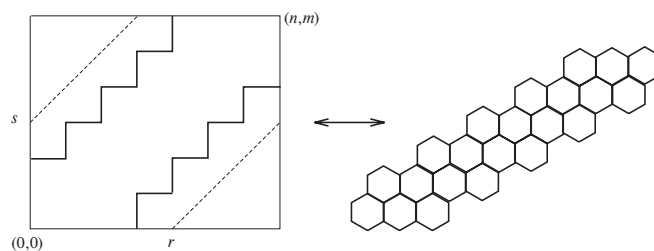


Croat. Chem. Acta **78** (2005) 241–250

CCA-3005

Perfect Matchings in Lattice Animals and Lattice Paths with Constraints

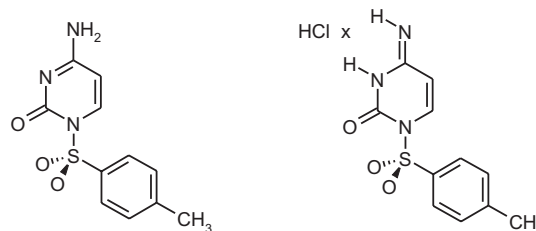
Tomislav Došlić

Croat. Chem. Acta **78** (2005) 251–259

CCA-3006

Synthesis, Spectroscopic Characterization and Biological Activity of *N*-1-Sulfonylcytosine Derivatives

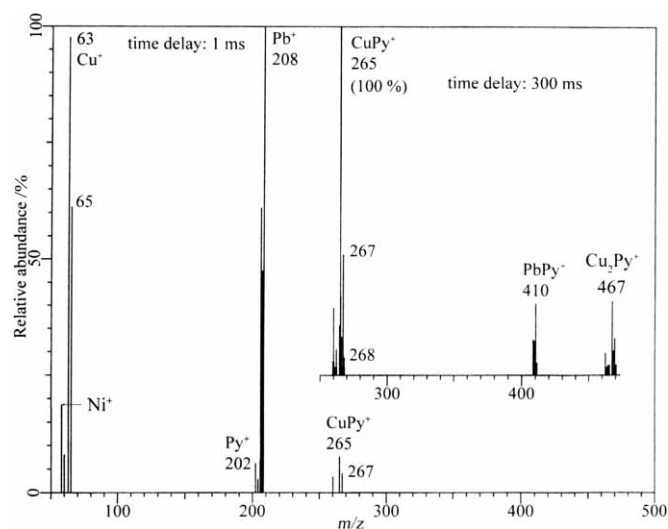
Jelena Kašnar-Šamprec, Ljubica Glavaš-Obrovac,
Marina Pavlak, Ivica Mihaljević, Vladimir Mrljak,
Nikola Štambuk, Paško Konjevoda, and Biserka Žinić

Croat. Chem. Acta **78** (2005) 261–267

CCA-3007

Gas Phase Ligation Kinetics of Metal Monocations with Pyrene

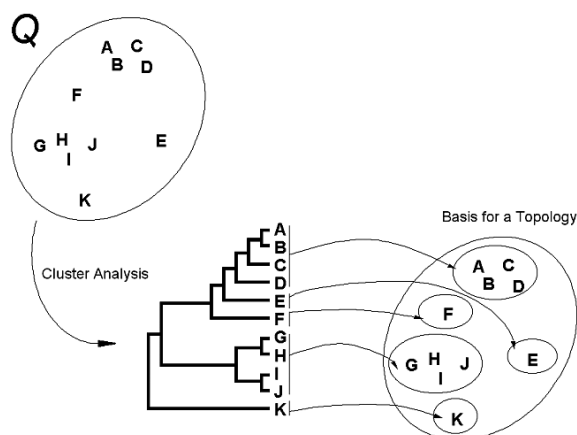
Saša Kazazić, Snježana P. Kazazić, Leo Klasinc,
Marko Rožman, and Dunja Srzić

Croat. Chem. Acta **78** (2005) 269–274

CCA-3008

From Trees (Dendrograms and Consensus Trees) to Topology

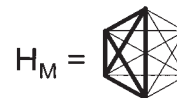
Guillermo Restrepo and José L. Villaveces

Croat. Chem. Acta **78** (2005) 275–281

CCA-3009

Simplified Computation of Matchings in Polygraphs

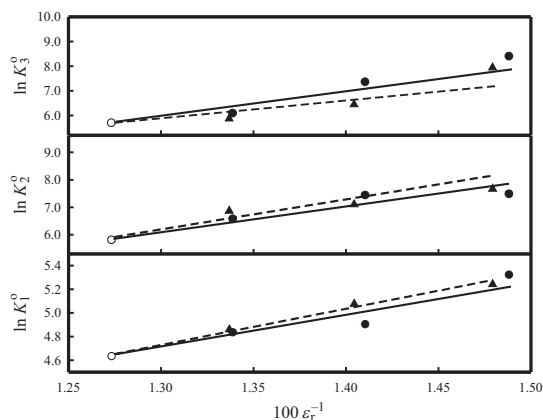
Ante Graovac, Damir Vukičević, Damir Ježek, and Janez Žerovnik

Croat. Chem. Acta **78** (2005) 283–287**ORDINARY CCA PAPERS****ORIGINAL SCIENTIFIC PAPERS**

CCA-3010

Complexation of Cd²⁺ and Cl⁻ Ions in Aqueous Mixtures of 2-Butanol

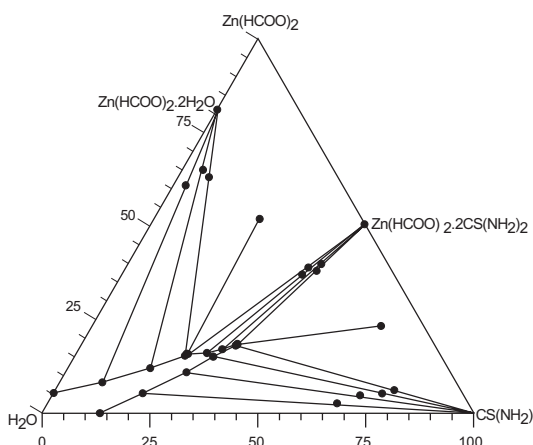
Renato Tomaš, Ivo Tominić, Marija Višić, and Vesna Sokol

Croat. Chem. Acta **78** (2005) 289–294

CCA-3011

Formation and Characterization of Bisthiourea Zinc Formate

Violeta Z. Vassileva and Petranka P. Petrova

Croat. Chem. Acta **78** (2005) 295–299

CCA-3012

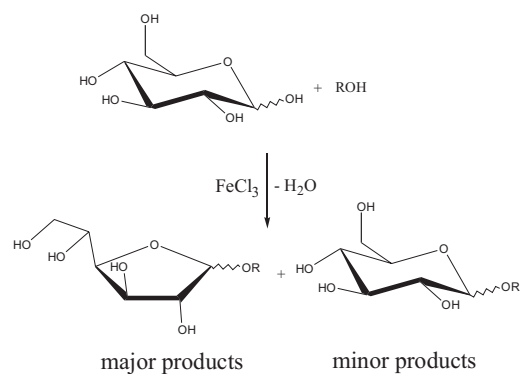
3-O-Acyl Derivatives of Bridged-15-Membered Azalides: Synthesis, Structural Determination and Antibacterial Activity

Andrea Fajdetić, Gabrijela Kobrehel, Gorjana Lazarevski, Vlado Štimac, and Stjepan Mutak

Croat. Chem. Acta **78** (2005) 301–312

	R1	R2	R1	R2
	H	CH ₃	Me	
H		Et		
H		H		
H		Me		
H		Et		
H				

CCA-3013

**GC-MS Characterization of Acetylated *O*-glucofuranosides:
Direct Glucosylation of Volatile Alcohols
from Unprotected Glucose**Igor Jerković, Josip Mastelić, Ivica Blažević,
Marija Šindler-Kulyk, and Dražen Vikić-Topić*Croat. Chem. Acta* **78** (2005) 313–318**APPENDIX****BOOK REVIEWS**Nenad Trinajstić
Štefica HorvatA3
A5