Future Papers

Prediction of p*K* Values, Half-Lives, and Electronic Spectra of Flavylium Salts from Molecular Structure. *Dragan Amić, Dušanka Davidović-Amić, Drago Bešlo, Bono Lučić, and Nenad Trinajstić*, The Josip Juraj Strossmayer University, Osijek, and The Rugjer Bošković Institute, Zagreb, The Republic of Croatia.

Prediction of Hydroxyl Radical Rate Constants from Molecular Structure. *Gregory A. Bakken and Peter C. Jurs*, The Pennsylvania State University, University Park, PA.

Name=Struct: A Practical Approach to the Sorry State of Real-Life Chemical Nomenclature. *Jonathan S. Brecher*, CambridgeSoft Corporation, Cambridge, MA.

Comment on "Exhaustive Generation of Organic Isomers. 5. Unsaturated Optical and Geometrical Stereoisomers and a New CIP Subrule". *Jonathan S. Brecher*, CambridgeSoft Corporation, Cambridge, MA.

Response to Comment on "Exhaustive Generation of Organic Isomers. 5. Unsaturated Optical and Geometrical Stereoisomers and a New CIP Subrule". *M. L. Contreras, G. M. Trevisiol, J. Alvarez, G. Arias, and R. Rozas*, University of Santiago de Chile, Casilla, Santiago, Chile.

On Molecular Polarizability: 2. Relationship to the Boiling Point of Alkanes and Alcohols. *Chenzhong Cao, Shusheng Liu, and Zhiliang Li*, Xiangtan Normal University, Xiangtan, Hunan University, Changsha, Guilin Institute of Technology, Guilin, and Chongqing University, Chongqing, People's Republic of China.

Discrimination and Molecular Design of New Theoretical Hypolipaemic Agents Using the Molecular Connectivity Functions. *Rosa Ana Cercos del Pozo, Facundo Perez-Gimenez, M. Teresa Salabert-Salvador, and Francisco J. Garcia-March*, Universitat de Valencia, Valencia, Spain.

Substituent Effects on Thermochemical Properties of C-, N-, O-, and S-Centered Radicals. Physical Interpretation of Substituent Effects. *Artem Cherkasov and Mats Jonsson*, Royal Institute of Technology, Stockholm, Sweden.

Development of Quantitative Structure−Property Relationships (QSPR) Using Calculated Descriptors for the Prediction of the Physico-Chemical Properties (nD, p, bp, s and Tq) of a Series of Organic Solvents. *Marina Cocchi, Pier Giuseppe De Benedetti, Renato Seeber, Lorenzo Tassi, and Alessandro Ulrici*, University of Modena, Modena, Italy.

Hierarchical Neural Network Modeling for Infrared Spectra Interpretation of Modified Starches. *Ludmila Dolmatova, Valery Tchistiakov, Cyril Ruckebusch, Nathalie Dupuy, Jean-Pierre Huvenne, and Pierre Legrand*, Russian Academy of Sciences, Chernogolovka, Russia, and Université des Sciences et Technologies de Lille, Villeneuve d'Ascq Cedex, France.

XyM Markup Language (XyMML) for Electronic Communication of Chemical Documents Containing Structural Formulas and Reaction Schemes. *Shinsaku Fujita*, Kyoto Institute of Technology, Kyoto, Japan.

XyM Notation for Electronic Communications of Organic Chemical Structures. *Shinsaku Fujita and Nobuya Tanaka*, Kyoto Institute of Technology, Kyoto, Japan.

Predictive Carcinogenicity: A Model for Aromatic Compounds, with Nitrogen-Containing Substituents, Based on Molecular Descriptors Using an Artificial Neural Network. *Giuseppina Gini, Marco Lorenzini, Emilio Benfenati, Paola Grasso, and Maurizio Bruschi*, Politecnico di Milano, and Istituto di Ricerche Famacologiche "Mario Negri", Milano, Italy.

Construction of a Virtual High Throughput Screen by 4D-QSAR Analysis: Application to a Combinatorial Library of Glucose Inhibitors of Glycogen Phosphorylase *b*. *Anton J. Hopfinger, Andrea Reaka, Prabha Venkatarangan, José S. Duca, and Shen Wang*, The University of Illinois at Chicago, Chicago, IL.

Prediction of Ligand−Receptor Binding Free Energy by 4D-QSAR Analysis: Application to a Set of Glucose Analogue Inhibitors of Glycogen Phosphorylase. *Prabha Venkatarangan and Anton J. Hopfinger*, University of Illinois at Chicago, Chicago, IL.

The CIP System Again: Respecting Hierarchies Is Always a Must. *Paulina Mata*, Universidade Nova de Lisboa, Monte de Caparica, Portugal.

Comparing 3D Pharmacophore Triplets and 2D Fingerprints for Selecting Diverse Compound Subsets. *Hans Matter and Thorsten Pötter*, Tripos GmbH, München, Germany, and Bayer AG, Monheim, Germany.

Quantum Chemical AM1 Treatment of the Circumscribing Algorithm: Fullerene Growth Mechanism. *Rama K. Mishra, Ying-Ting Lin, and Shyi-Long Lee*, National Chung-Cheng University, Ming-Hsiung, Chia-Yi, Taiwan.

Chemical Markup, XML, and the Worldwide Web. 1. Basic Principles. *Peter Murray-Rust and Henry S. Rzepa*, University of Nottingham, U.K., and Imperial College of Science, Technology and Medicine, London, U.K.

Development of Pharmacophore Alignment Models as Input for Comparative Molecular Field Analysis of a Diverse Set of Azole Antifungal Agents. *Tanaji T. Talele, Santosh S. Kulkarni, and Vithal M. Kulkarni*, University of Mumbai, India.

Simulated Annealing Search Algorithm for the Determination of Activation Energies and Arrhenius Prefactors from Limited Experimental Kinetic Data. *David B. Terry, Jessica L. Bader, and Michael Messina*, University of North Carolina at Wilmington, Wilmington, NC.

Self-Configuring Radial Basis Function Neural Networks for Chemical Pattern Recognition. *Chuanhao Wan and Peter de B. Harrington*, Ohio University, Athens, OH.

Structural Features of Toxic Chemicals for Specific Toxicity. *Jiansuo Wang, Luhua Lai, and Youqi Tang*, Peking University, Beijing, People's Republic of China.

Predicting the Entropy of Boiling for Organic Compounds. *Luwei Zhao, Ping Li, and Samuel H. Yalkowsky*, The University of Arizona, Tucson, AZ.