

# QSAR & Combinatorial Science

Volume 23, Number 1/2004  
February 2004  
Pages 1–72

[www.interscience.wiley.com/journal/qsar-combsci](http://www.interscience.wiley.com/journal/qsar-combsci)

## Editorial

- 3 Ferenc Darvas, C. Oliver Kappe, Gisbert Schneider, Michael Wiese *QSAR & Combinatorial Science – Facing the Challenges*

## QSAR Section

- 5 Ovanes Mekenyan, Nina Nikolova, Patricia Schmieder and Gilman Veith **Full Paper:** COREPA-M: A Multi-Dimensional Formulation of COREPA
- 19 Uli Fechner, Gisbert Schneider **Full Paper:** Optimization of a Pharmacophore-based Correlation Vector Descriptor for Similarity Searching
- 23 J. Thomas Leonard and Kunal Roy **Full Paper:** Classical QSAR Modeling of HIV-1 Reverse Transcriptase Inhibitor 2-Amino-6-arylsulfonylbenzotrioles and Congeners
- 36 Haifeng Chen, Qiang Li, Xiaojun Yao, BoTao Fan, Shengang Yuan, A. Panaye, J. P. Doucet **Full Paper:** CoMFA/CoMSIA/HQSAR and Docking Study of the Binding Mode of Selective Cyclooxygenase (COX-2) Inhibitors

# QSAR & Combinatorial Science


www.interscience.wiley.com/journal/qsar-combsci

Volume 23, Number 2–3/2004  
April 2004  
Pages 73–204

## QSAR Section

- 75 John C. Dearden,  
Elaine H. Y. Wong and John D. Walker **Full Paper:** Molecular Connectivity: Polarity Correction to Improve Correlation with Hydrophobicity
- 80 Huabei Zhang, Chunping Liu, Hua Li **Full Paper:** CoMFA and CoMSIA Studies of nAChRs Ligands: Epibatidine Analogues
- 89 Isabel Dorronsoro, Antonio Chana,  
M Inés Abasolo, Ana Castro,  
Carmen Gil, Manfred Stud,  
Ana Martinez **Full Paper:** CODES/Neural Network Model: a Useful Tool for in Silico Prediction of Oral Absorption and Blood-Brain Barrier Permeability of Structurally Diverse Drugs
- 99 Kunal Roy and Gopinath Ghosh **Full Paper:** QSTR with Extended Topochemical Atom Indices. 3. Toxicity of Nitrobenzenes to *Tetrahymena pyriformis*

## Combinatorial Section

- 109 Caspar Christensen,  
Christian W. Tornøe, Morten Meldal **Full Paper:** Pyrazines on Solid Support from Peptides by Periodinane Oxidation of Threonine Side-Chains. A Quantitative Chemical Transformation (QCT) for Combinatorial Chemistry
- 117 Juan M. Benito and Morten Meldal **Full Paper:** Bicyclic Organo-Peptides as Selective Carbohydrate Receptors: Design, Solid-phase Synthesis, and on-bead Binding Capability 
- 130 F. Diness, J. Beyer, Morten Meldal **Full Paper:** Synthesis of 3-Boc-(1,3)-oxazinane-Protected Amino Aldehydes from Amino Acids and Their Conversion into Urea Precursors. Novel Building Blocks for Combinatorial Synthesis
- 145 Francesc Yraola, Rubén Ventura,  
Marc Vendrell, Aina Colombo, Joan-  
Carles Fernández, Natalia de la  
Figuera, Dolors Fernández-Fórner,  
Miriam Royo, Pilar Fornés, Fernando  
Albericio **Full Paper:** A Re-evaluation of the Use of Rink, BAL, and PAL Resins and Linkers

# QSAR & Combinatorial Science


www.interscience.wiley.com/journal/qsar-combsci

Volume 23, Number 4/2004

June 2004

Pages 205 – 292

## QSAR Section

- 207** Alexander Böcker, Gisbert Schneider, Andreas Teckentrup **Review:** Status of HTS Data Mining Approaches
- 214** Anne Tromelin, Elisabeth Guichard **Full Paper:** 2D- and 3D-QSAR Models of Interaction between Flavor Compounds and beta-Lactoglobulin Using Catalyst and Cerius<sup>2</sup>
- 234** Yenamandra S. Prabhakar, V. Raja Solomon, Ravindra K. Rawal, Manish K. Gupta, S. B. Katti **Full Paper:** CP-MLR/PLS Directed Structure-Activity Modeling of the HIV-1 RT Inhibitory Activity of 2,3-Diaryl-1,3-thiazolidin-4-ones 

## Combinatorial Section

- 254** Jacqueline T. Bork, Jae Wook Lee, and Young-Tae Chang **Full Paper:** The Combinatorial Synthesis of Purine, Pyrimidine and Triazine-based Libraries

# QSAR & Combinatorial Science

Volume 23, Number 5/2004

June 2004

Pages 293–384

[www.interscience.wiley.com/journal/qsar-combsci](http://www.interscience.wiley.com/journal/qsar-combsci)

## QSAR Section

- 295** M. R. Hodjmohammadi, P. Ebrahimi, F. Pourmorad **Full Paper:** Quantitative Structure-Retention Relationships (QSRR) of Some CNS Agents Studied on DB-5 and DB-17 Phases in Gas Chromatography
- 303** Anneli Nordqvist, Jonas Nilsson, Tuulikki Lindmark, Alf Eriksson, Per Garberg and Mats Kihlén **Full Paper:** A General Model for Prediction of Caco-2 Cell Permeability
- 311** Holger Fröhlich, Jörg K. Wegner, Andreas Zell **Full Paper:** Towards Optimal Descriptor Subset Selection with Support Vector Machines in Classification and Regression
- 319** Andrzej Persona, Barbara Marczevska, Zygmunt Fekner, Bogdan Senczyna, Joanna Matysiak, Andrzej Niewiadomy **Full Paper:** Dynamic Method of Determination of Octanol-Water Partition Coefficient of 2,4-Dihydroxythiobenzanilides in QSAR Studies
- 327** Oleg A. Raevsky, Olga E. Raevskaja and Klaus-Jürgen Schaper **Full Paper:** Analysis of Water Solubility Data on the Basis of HYBOT Descriptors. Part 3. Solubility of Solid Neutral Chemicals and Drugs
- 344** Thomas Hoeg-Jensen **Full Paper:** Preparation and Screening of Diboronate Arrays for Identification of Carbohydrate Binders

# QSAR & Combinatorial Science

www.interscience.wiley.com/journal/qsar-combsci

Volume 23, Number 6/2004

July 2004

Pages 385–492

## QSAR Section

- 387** J. Thomas Leonard and Kunal Roy **Full Paper:** Classical QSAR Modeling of CCR5 Receptor Binding Affinity of Substituted Benzylpyrazoles
- 399** Miha Kotnik, Marko Oblak, Jan Humljan, Stanislav Gobec, Uros Urleb and Tom Solmajer **Full Paper:** Quantitative Structure-Activity Relationships of *Streptococcus pneumoniae* MurD Transition State Analogue Inhibitors
- 406** Michael C. Hutter and Rolf W. Hartmann **Full Paper:** QSAR of Human Steroid 5 $\alpha$ -Reductase Inhibitors: Where are the differences between isoenzyme type 1 and 2?
- 416** G. Absalan, B. Hemmateenejad, M. Soleimani, M. Akhond and R. Miri **Full Paper:** Quantitative Structure–Micellization Relationship Study of Gemini Surfactants Using Genetic-PLS and Genetic-MLR
- 426** Mark Rogers-Evans, Alexander I. Alanine, Konrad H. Bleicher, Dagmar Kube, Gisbert Schneider **Full Paper:** Identification of novel cannabinoid receptor ligands *via* evolutionary de novo design and rapid parallel synthesis
- 431** Sanjay Bajaj, S. S. Sambhi and A. K. Madan **Full Paper:** Prediction of Carbonic Anhydrase Activation by Tri-/Tetrasubstituted-pyridinium-azole Compounds: A Computational Approach Using Novel Topochemical Descriptor

## Combinatorial Section

- 440** Markus M. Vögtle and Andreas L. Marzinzik **Full Paper:** Synthetic Approaches Towards Quinazolines, Quinazolinones and Quinazolinones on Solid Phase

# QSAR & Combinatorial Science


www.interscience.wiley.com/journal/qsar-combsci

Volume 23, Number 7/2004  
September 2004  
Pages 493–600

## QSAR Section

- 495 Catherine J. Williford,  
Erland P. Stevens **Full Paper:** Strain Energies as a Steric Descriptor in QSAR Calculations
- 506 Sanjay Bajaj, S. S. Sambhi and  
A. K. Madan **Full Paper:** Prediction of Carbonic Anhydrase Activation by Tri-/Tetrasubstituted-pyridinium-azole Compounds: A Computational Approach using Novel Topochemical Descriptor
- 515 Matthew J. Walker **Full Paper:** Training ACD/LogP with Experimental Data
- 521 Watze de Wolf, Paul H. Lieder and  
John D. Walker **Full Paper:** Application of QSARs: Correlation of Acute Toxicity in the Rat Following Oral or Inhalation Exposure
- 526 Kunal Roy and Gopinath Ghosh **Full Paper:** QSTR with Extended Topochemical Atom Indices. 4. Modeling of the Acute Toxicity of Phenylsulfonyl Carboxylates to *Vibrio fischeri* using Principal Component Factor Analysis and Principal Component Regression Analysis
- 536 Magdalena J. Ślusarz, Rafał Ślusarz,  
Robert Meadows, Jerzy Trojnar and  
Jerzy Ciarkowski **Full Paper:** Molecular Dynamics of Complexes of Atosiban with Neurohypophyseal Receptors in the Fully Hydrated Phospholipid Bilayer

## Combinatorial Section

- 546 Menno C. F. Monnee, Arwin J.  
Brouwer and Rob M. J. Liskamp **Full Paper:** Synthesis, Screening and Evaluation of a Combined Library of Tweezer- and Tripodal Synthetic Receptors 

# QSAR & Combinatorial Science


www.interscience.wiley.com/journal/qsar-combsci

Volume 23, Number 8/2004  
October 2004  
Pages 601–706

## QSAR Section

- 603 HaiFeng Chen, Xiaojun Yao, Michel Petitjean, Hairong Xia, JianHua Yao, A. Panaye, J. P. Doucet and BoTao Fan  
**Full Paper:** Insight into the Bioactivity and Metabolism of Human Glucagon Receptor Antagonists from 3D-QSAR Analyses
- 621 Sivaprakasam Prasanna, Elangovan Manivannan and Subash Chandra Chaturvedi  
**Full Paper:** QSAR Analysis of 2,3-Diaryl Benzopyrans/Pyrans as Selective COX-2 Inhibitors Based on Semiempirical AM1 Calculations
- 629 Irina G. Tsygankova  
**Full Paper:** Combination of Fragmental and Topological Descriptors for QSPR Estimations of Boiling Temperature
- 637 Kwan Hoon Hyun, Do Young Lee, Bon-Su Lee and Chan Kyung Kim  
**Full Paper:** Receptor-based 3D QSAR Studies on PPAR<sub>γ</sub> Agonists using CoMFA and CoMSIA Approaches
- 650 Chongli Zhong, Jingtao He, Zhiqiang Xia and Yajun Li  
**Full Paper:** Modeling of Activity of Efavirenz with the Mutant of HIV Reverse Transcriptase using Variable Connectivity Indices

## Combinatorial Section

- 655 Saman Sandanayake, Senake Perera and Nicholas J. Ede  
**Full Paper:** A Convenient Solid Phase Synthesis of Disubstituted Guanidines
- 662 Michael Roice, Ib Johannsen and Morten Meldal  
**Full Paper:** High Capacity Poly(ethylene glycol) Based Amino Polymers for Peptide and Organic Synthesis 

# QSAR & Combinatorial Science

www.interscience.wiley.com/journal/qsar-combsci

Volume 23, Number 9/2004  
October 2004  
Pages 707–822

## QSAR Section

- 709** S. H. Hilal and S. W. Karickhoff **Full Paper:** Prediction of the Solubility, Activity Coefficient and Liquid/Liquid Partition Coefficient of Organic Compounds
- 721** John D. Walker, Ingrid Gerner, Etje Hulzebos and Kerstin Schlegel **Full Paper:** (Q)SARs for Predicting Skin Irritation and Corrosion: Mechanisms, Transparency and Applicability of Predictions
- 726** Ingrid Gerner, Kerstin Schlegel, John D. Walker, and Etje Hulzebos **Full Paper:** Use of Physicochemical Property Limits to Develop Rules for Identifying Chemical Substances with no Skin Irritation or Corrosion Potential
- 734** Mojtaba Shamsipur, Raof Ghavami, Bahram Hemmateenejad and Hashem Sharghi **Full Paper:** Highly Correlating Distance-Connectivity-Based Topological Indices. 2: Prediction of 15 Properties of a Large Set of Alkanes Using a Stepwise Factor Selection-Based PCR Analysis
- 754** Akash Khandelwal, Viera Lukacova, Daniel M. Kroll, Dogan Çömez, Soumyendu Raha, and Stefan Balaz **Full Paper:** Simulation-Based Predictions of Binding Affinities of Matrix Metalloproteinase Inhibitors
- 767** L. Baumes, D. Farrusseng, M. Lengliz, and C. Mirodatos **Full Paper:** Using Artificial Neural Networks to boost high-throughput discovery in heterogeneous catalysis
- 779** Simon Spycher, Monika Nendza, and Johann Gasteiger **Full Paper:** Comparison of Different Classification Methods Applied to a Mode of Toxic Action Data Set

## Abstracts of QSAR-related Publications

- |            |  |            |                                 |
|------------|--|------------|---------------------------------|
| <b>795</b> | Classical QSAR: Review                     | <b>808</b> | Combinatorial Library           |
| <b>796</b> | Classical QSAR: Theoretical Papers         | <b>809</b> | Multivariate Analysis           |
| <b>799</b> | Classical QSAR: Pharmacology               | <b>814</b> | Quantum Chemistry               |
| <b>801</b> | Classical QSAR: Organic Chemistry          | <b>816</b> | Data Base and Virtual Screening |
| <b>804</b> | Classical QSAR: Toxicology and Environment | <b>818</b> | Molecular Graphics              |
| <b>806</b> | 3D QSAR                                    | <b>820</b> | Peptides                        |



## Editorial

- 825 Erik Van der Eycken, Johan Van der Eycken  
Microwaves in Combinatorial and High-Throughput Synthesis

## Combinatorial Section

- 827 Yimin Lu, Wei Zhang  
**Full Paper:** Microwave-assisted Synthesis of a 3-Aminoimidazo[1,2-*a*]-pyridine/pyrazine Library by Fluorous Multicomponent Reactions and Subsequent Cross-coupling Reactions
- 836 N. Mont, L. Fernández-Megido, J. Teixidó, C. O. Kappe, J. I. Borrell  
**Full Paper:** A Diversity-Oriented, Microwave-Assisted Synthesis of 4-oxo and 4-chloropyrido[2,3-*d*]pyrimidin-7(8*H*)-ones
- 850 Aurélie Berthault, Sabine Berteina-Raboin, Adriana Finaru, Gérald Guillaumet  
**Full Paper:** Solid Phase Synthesis of 2-substituted Melatonin Derivatives *via* Palladium-mediated Coupling Reactions using Microwave Irradiation
- 854 Blanca Martinez-Teipel, Rosalyn C. Green and Roland E. Dolle  
**Full Paper:** Microwave-assisted Synthesis of Di- and trisubstituted Ureas from Thiophenoxy Carbamate Resins
- 859 Mark C. Bagley, David D. Hughes, M. Caterina Lubinu, Eleanor A. Merritt, Paul H. Taylor and Nicholas C. O. Tomkinson  
**Full Paper:** Microwave-Assisted Synthesis of Pyrimidine Libraries
- 868 Sang Hyun Park, Hui Jeong Gwon, Jeong Sook Park, Kyung Bae Park  
**Full Paper:** Synthesis and Radiochemical Labeling of *N*-(2,6-Diisopropylacetanilido)-Iminodiacetic Acid and Its Analogues under Microwave Irradiation: A Hepatobiliary Imaging Agent
- 875 Lin Bai, Yumei Zhang and Jin-Xian Wang  
**Full Paper:** Rapid Microwave-Promoted Cross-Coupling Reaction of Aryl Bromides with Aryl Boronic Acids and Sodium Tetraphenylborate Catalyzed by a Reusable Polymer-Supported Palladium Complex
- 883 Stephen Patterson, Christiane Lorenz, Alexandra M. Z. Slawin, Nicholas J. Westwood  
**Full Paper:** Rapid Access to a Pentacyclic Library Core Structure: A Microwave Assisted Approach
- 891 Yuhong Ju, Chao-Jun Li and Rajender S. Varma  
**Full Paper:** Microwave-assisted Cu (I) Catalyzed Solvent-free Three Component Coupling of Aldehyde, Alkyne and Amine
- 895 Heiko Leutbecher, Jürgen Conrad, Iris Klaiber and Uwe Beifuss  
**Short Communication:** Microwave Assisted Domino Knoevenagel Condensation/ $6\pi$ -electron Electrocyclization Reactions for the Rapid and Efficient Synthesis of Substituted 2*H*.5*H*-pyrano[4,3-*b*]pyran-5-ones and Related Heterocycles