

# QSAR

WITH ABSTRACT SERVICE

## Papers/News Section

- 115 Edgar Jacoby A Novel Chemogenomics Knowledge-Based Ligand Design Strategy-Application to G Protein-Coupled Receptors
- 124 Irini Doytchinova, Iva Valkova and Roumiana Natcheva CoMFA Study on Adenosine A<sub>2a</sub> Receptor Agonists
- 130 Ilza K. Pajeva and Michael Wiese Human P-Glycoprotein Pseudoreceptor Modeling: 3D-QSAR Study on Thioxanthene Type Multidrug Resistance Modulators
- 139 You-Min Sun, Xiu-Li Wang, Hong-Yu Zhang and De-Zhan Chen Short Communication: Theoretical Elucidation of Structure-Antioxidant Activity Relationships for Thiazolidinone Derivatives
- 143 Keigo Gohda, Daisaku Ohta, Akiko Kozaki, Ko Fujimori, Ichiro Mori and Takeshi Kikuchi Identification of Novel Potent Inhibitors for ATP-Phosphoribosyl Transferase Using Three-Dimensional Structural Database Search Technique
- 148 Hong-Yu Zhang, You-Min Sun and De-Zhan Chen O–H Bond Dissociation Energies of Phenolic Compounds are Determined by Field/Inductive Effect or Resonance Effect? A DFT Study and Its Implication
- 153 Future Events

## Abstracts of QSAR related Publications

- |     |  |     |  |
|-----|--|-----|--|
| 157 | Review   | 175 | 3D QSAR  |
| 158 | Classical QSAR: Theoretical Papers                   | 183 | DB Search & Similarity                                 |
| 163 | Classical QSAR: Pharmacology                         | 184 | Multivariate Analysis and Neural Network               |
| 166 | Classical QSAR: Agricultural                         | 187 | Combinatorial Library Design and Diversity Calculation |
| 168 | Classical QSAR: Organic Chemistry                    | 191 | Quantum Chemistry                                      |
| 171 | Classical QSAR: Chromatography                       | 192 | Molecular Graphics, X-ray, NMR                         |
| 171 | Classical QSAR: Toxicology and Environmental Science | 207 | Protein, Peptides                                      |
| 173 | Classical QSAR: Disposition                          | 208 | Programs, Algorithms, Data Bases                       |