

QSAR & Combinatorial Science

Volume 22, Number 1/2003

April 2003

Pages 1 – 180

WITH ABSTRACT SERVICE

Papers/News Section

- | | | |
|-----|--|--|
| 3 | R. Breton, G. Schüürmann
and R. Purdy | Preface |
| 5 | S. Dimitrov, Y. Koleva, M. Lewis,
R. Breton, G. Veith and O. Mekenyan | Modeling mode of action of industrial chemicals: Application using
chemicals on Canada's Domestic Substances List (DSL) |
| 18 | Kun Gao, Bo Tao Fan, Nadia El Fassi,
Krystyna Zakrzewska, Zhongjian Jia,
Rongliang Zheng, Annick Panaye,
T. Couesnon and Jean-Pierre Doucet | Comparative Study of Activities between Verbascoside and Rutin
by Docking Method |
| 29 | Xiaojun Yao, Botao Fan, J. P. Doucet,
A. Panaye, Mancang Liu,
Ruisheng Zhang, Xiaoyun Zhang and
Zhide Hu | Quantitative structure property relationship models for the prediction
of liquid heat capacity |
| 49 | Lars Carlsen and John D. Walker | QSARs for Prioritizing PBT Substances to Promote Pollution
Prevention |
| 58 | Sabcho D. Dimitrov,
Nadezhda C. Dimitrova,
John D. Walker, Gilman D. Veith and
Ovanes G. Mekenyan | Bioconcentration potential predictions based on molecular attributes –
an early warning approach for chemicals found in humans, birds, fish
and wildlife |
| 69 | Alexander Tropsha, Paola Gramatica
and Vijay K. Gombar | The Importance of Being Earnest: Validation is the Absolute Essential
for Successful Application and Interpretation of QSPR Models |
| 78 | Kelly P. Coleman, William A. Toscano,
Jr. and Thomas E. Wiese | QSAR Models of the <i>in vitro</i> Estrogen Activity of Bisphenol A
Analogues |
| 89 | John D. Walker, Hong Fang,
Roger Perkins and Weida Tong | QSARs for Endocrine Disruption Priority Setting Database 2:
The Integrated 4-Phase Model |
| 106 | Don Mackay, Jennifer Hubbarde and
Eva Webster | The role of QSARs and fate models in chemical hazard and risk
assessment
Paper prepared for Quantitative Structure-Activity Relationships
(QSAR) Proceedings of the QSAR 2002 Conference, Ottawa May 2002 |
| 113 | Aynur O. Aptula, Ralph Kühne, Ralf-
Uwe Ebert, Mark T. D. Cronin,
Tatiana I. Netzeva and Gerrit
Schüürmann | Modeling Discrimination between Antibacterial and Non-Antibacterial
Activity based on 3D Molecular Descriptors |