

# QSAR

WITH ABSTRACT SERVICE

## Papers/News Section

- 457 Benjamin G. Tehan, Edward J. Lloyd, Margaret G. Wong, Will R. Pitt, John G. Montana, David T. Manallack and Emanuela Gancia Estimation of  $pK_a$  Using Semiempirical Molecular Orbital Methods. Part 1: Application to Phenols and Carboxylic Acids.
- 473 Benjamin G. Tehan, Edward J. Lloyd, Margaret G. Wong, Will R. Pitt, Emanuela Gancia and David T. Manallack Estimation of  $pK_a$  Using Semiempirical Molecular Orbital Methods. Part 2: Application to Amines, Anilines and Various Nitrogen Containing Heterocyclic Compounds.
- 486 Shijin Ren Use of Molecular Descriptors in Separating Phenols by Three Mechanisms of Toxic Action
- 493 Eugen Deretey, Miklos Feher and Jonathan M. Schmidt Rapid Prediction of Human Intestinal Absorption
- 507 Knut Baumann Distance Profiles (DiP): A translationally and rotationally invariant 3D structure descriptor capturing steric properties of molecules

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