

CALL FOR PAPERS SPECIAL ISSUE

MOLECULAR DIVERSITY Topological Description in Drug Design & Modeling Studies

Submission Topics:

- 1. Applications of chemical graph theory
- 2. Introduction and evaluation of novel topological descriptors
- 3. Topological descriptors in Quantitative Structure-Activity Relationships (QSAR)
- 4. Topological descriptors in modeling physicochemical properties
- 5. Topological descriptors in Quantitative Structure-Toxicity Relationships (QSTR)
- 6. Topological descriptors in modeling ADME parameters
- 7. Topological descriptors in classification analyses
- 8. Use of topological descriptors in combinatorial library design
- 9. Recent advances in the use of topological indices in the lead discovery process
- 10. Atom level topological indices.

SUBMISSIONS DUE JANUARY 1, 2004 Special Instructions for QSAR/QSPR/QSTR papers

- 1. All mathematical equations should be entered using equation editor available in Word.
- 2. The statistical quality of the multiple regression equations should be checked by explained variance (Ra2), variance ratio (F) and standard error of estimate (s). The 95% confidence intervals (or standard errors) of all regression coefficients should be mentioned. In addition, all the QSAR/QSPR/QSTR models should be cross-validated by "leave-one-out" and/or "leave-many-out" techniques and the cross-validated R2 (Q2) should be mentioned.
- 3. Intercorrelation among the predictor variables should be checked.
- 4. The calculated and residual activity/property/toxicity values for all the compounds should be given.
 Compounds not used in deriving a model should be clearly mentioned.
- 5. For new/relatively new descriptors, methods of calculations should be illustrated with examples.
- 6. The references of the original data sets should be clearly mentioned.
- 7. The values of all descriptors for all compounds should be supplied as supplementary material if these are not already present in the paper.
- 8. The software(s) used for all calculations should be mentioned.

The manuscripts prepared in MS WORD 97/2000 should be sent by email to:

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