

## 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

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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.

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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