Bibliography for molecular graphics 1983/84

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This is the second bibliography on molecular graphics. It mainly covers years 1983/4. However, there are some papers included which should have appeared in the earlier bibliography (MORF83a) but which were overlooked. The bibliography follows the same format as the previous one, including an author index and keyword index.

INTRODUCTION

This bibliography has been compiled over the last two years. The caveats mentioned in the previous introduction also apply here, namely, that the compiler was bound to fail to find every reference and the bibliography should only be considered as a comprehensive guide.

The previous bibliography contained about 140 references covering the period 1966 to 1982. This bibliography shows that about 100 references have been found for the two years it covers, another indication of the increase in interest in molecular graphics.

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BOOK REVIEWS

Stimulus to new methods of molecular description

Logical and combinatorial algorithms for drug design, V E Golender and A B Rozenblit, Research Studies Press, UK (1983) £31.00, 289 pp

Any book that originates from eastern Europe is bound to excite interest since it may provide a different view from that of western scientists. In that respect at least, this volume does not disappoint, and the series editor, David Bawden, must be congratulated in adding yet another novel example to his chemometrics series.

The authors have provided a text that discusses the 'logico-structural' approach to drug design. Use is made of combinatorial methods in the implementation of similarity algorithms, as graph theoretical and matrix methods are employed for the description of molecular structure. Logical analysis of structure-activity data is employed, with the aim of revealing relationships between compounds by elucidating the structural features that establish their biological activity.

The first half of the book includes a discussion of the theory underlying this approach, followed by a description of the methods used for encoding chemical structures and of the principles involved in determining features responsible for the manifestation of activity. A program that reads in and encodes structural formulae is described, and algorithms for the solution of problems caused by the choice of graph theoretical forms of molecular representation are provided. The remainder of the book is largely taken up by a description of three software packages, Strac, Oracle and Toplog, which attempt to rationalize and predict biological activities of compounds by the previously defined approach.

The authors' interpretation of the term 'chemical structure' is, to say the least, unusual:

> 'Both local (presence of particular functional groups, certain values of substituent constants) and global characteristics of compounds (partition coefficient, dipole moment, ionisation potential, etc.) can be useful to describe chemical structure.'

The most questionable statement in the book is:

> 'The development of an adequate chemical structure description language appears to be the main