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SOFTWARE SURVEY SECTION

Editor's Note: The following Software Descriptions have been submitted by our readers in response to our call for an open exchange of information on software programs. They are offered without review or comment to provide a rapidly published, easily accessible avenue of communication. Other readers with relevant software packages are invited to complete and submit a Software Description Form (found at the end of this section).

Software package BP-012-S87 — MOLGRAF - Molecular Graphics for Microcomputers

Contributors: Dr. R.B. Barlow, Department of Pharmacology, University of Bristol, Bristol, UK and, Mr. C. O'Donnell, Elsevier-Biosoft, 68 Hills Road, Cambridge CB2 1LA, UK

Brief description: MOLGRAF is a comprehensive package to display, examine and experiment with three-dimensional maps of chemical compounds. It is suitable for teaching and research purposes wherever it is desirable to visualise a molecular structure. Features include: entry of new compounds using crystallographic coordinates and saving the data to disk; the ability to check, add, delete and correct data; calculation of bond lengths, bond angles and torsion angles. It also provides on disk an atlas consisting of data for more than 200 structures, including many common pharmaceuticals. MOLGRAF displays structures in high resolution graphics which may be rotated, expanded and moved across the screen. The images may be printed using a screen dump program or a plotter. Images of different compounds may be superimposed. Also included is a routine called LECTURE which displays a sequence of images which can be prepared in advance by the user. These may then be used to illustrate a talk or presentation. MOLGRAF also incorporates DIY which helps the user to build a compound by specifying only atom names, bond lengths, bond angles and torsion angles. The coordinates are calculated by the program and may subsequently be visualised using the main program.

Potential users: Pharmacologists, chemists, biochemists.
Fields of interest: Crystallography, three-dimensional structure.

§ This application program in the area of molecular graphics has been developed for IBM PC, Apple II series in BASIC to run under PC-DOS (2.1) and DOS 3.3. It is available on 5-1/4", dual-sided, double-density floppy diskette. Required memory is 256K (IBM PC); 64K (Apple).
§ Distributed by Elsevier-Biosoft.
§ The minimum hardware configuration required is IBM-PC color card. No user training is required. There is extensive external documentation. Source code not available.
§ The package is fully operational. The contributor is available for user inquiries.

NAME OF JOURNAL BIOCHEMICAL PHARMACOLOGY

P E R G A M O N
SOFTWARE DESCRIPTION FORM

Title of software package: _____

_____

_____

It Is: [ ]Application program [ ]Utility [ ]Other_____

Specific area _____ (e.g. Thermodynamics, Inventory Control)

Software developed for [name of computer(s)] _____

in [language(s)] _____

to run under [operating system] _____

and is available in the following media:

[ ]Floppy disk/diskette. Specify:

Size _____ Density _____ [ ]Single-sided [ ]Dual-sided

[ ]Magnetic tape. Specify:

Size _____ Density _____ Character set _____

Distributed by:_____

Minimum hardware configuration required: _____

Required memory: _____ User training required: [ ]Yes [ ]No

Documentation: [ ]None [ ]Minimal [ ]Self-documenting
[ ]Extensive external documentation

Source code available: [ ]Yes [ ]No

Level of development: [ ]Design complete [ ]Coding complete
[ ]Fully operational [ ]Collaboration would be welcomed

Is software being used currently? [ ]Yes [ ]No
If yes, how long? _____ If yes, how many sites? _____

Contributor is available for user inquiries: [ ]Yes [ ]No

(continued)

RETURN COMPLETED FORM TO:

Dr. David Stagg
Department of Pharmacology
Yale University School of Medicine
333 Cedar Street
P.O. Box 3333
New Haven, CT 06510

Description of what software does [200 words]:

Potential users: _____

Fields of interest: _____

# # # # # # #

Name of contributor: _____

Institution: _____

Address: _____

_____

Telephone number:_____

# # # # # # #

Reference No. [Assigned by Journal Editor]_____

- -

[The information below is not for publication.]

Would you like to have your program:

Reviewed? [ ]Yes [ ]No [ ]Not at this time

Marketed and distributed? [ ]Yes [ ]No [ ]Not at this time