Biochemical Pharmacology, Vol. 37, pp. I-IV, 1988
0006-2952/88 $3.00 + .00 Printed in Great Britain

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-015-S87 — Molecules: Presentation of Chemical Structures

Contributor: Rainer Paape, Paschenburgstr. 67, 2800 Bremen 1, West Germany

Brief description: Molecule: Construction, presentation and animation of chemical structures. You can design your own molecules via Z-matrices or cartesian coordinates. Coordinate input is possible by keyboard (built-in editor) or by results from other calculations (eg. MOPAC, GAUSS80, MM2P, etc.). Own input definition is possible. Data from x-ray analysis can be transformed to cartesian coordinates. The bindings are automatically computed by the program. The molecules are shown as stick, ball or stick, and ball models with atomic, van der Waals or ionic radii. High and medium graphic resolution is supported. On a color monitor even a presentation of a stereo picture consisting of a red and green halfpicture is possible. The colors can be adjusted to your own glasses. The molecule can rotate around any axis. The number of pictures for an animation depends on the free memory (about 30 pictures/1MB RAM). Size and orientation of a molecule is freely selectable. The documentation on disk (1ST-Word and text file) is in German.

Potential users: Chemists, teachers, biologists.
Fields of interest: Chemical structures.

§ This application program in the area of chemical structures has been developed for Atari to run under GEM. It is available on 3-1/2", dual-sided floppy diskette. Required memory is 1MB.
§ No user training is required. It is self-documenting with documentation on disk in German. Source code not available.
§ The package is fully operational. It has been in use at 40 sites for approximately 6 months.

JOURNAL NAME BIOCHEMICAL PHARMACOLOGY

P E R G A M O N
SOFTWARE DESCRIPTION FORM

Title of software program: _____

_____

Type of program: [ ] Application [ ] Utility [ ] Other_____

Category: _____ (ie. Psychological assessment, statistics, thermodynamics, etc.)

Developed for (name of computer/s): _____

in (language/s):_____

to run under (operating system): _____

available on: [ ] Floppy disk/diskette. Specify:

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

[ ] Magnetic tape. Specify:

Size _____ Density _____ Character set _____

Hardware required: _____

Memory required: _____ User training required: [ ] Yes [ ] No

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

Source code available: [ ] Yes [ ] No

Stage of development: [ ] Design complete [ ] Coding complete
[ ] Fully operational [ ] Collaboration welcomed

Is program in use? [ ] Yes How long? _____ How many sites? _____
[ ] No

Is the contributor available for user inquiries: [ ] Yes [ ] No

Distributed by: _____

Cost of program: _____

Demonstration disk available? [ ] Yes Cost: _____
[ ] 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

IV Software Survey Section

Description of what software does [maximum: 200 words]:

Potential users: _____

Field/s 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