

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-020-S88

WAALSURF

Contributor: Dr. Han van de Waterbeemd, Softarts-Actimol, Chemin de Maillefer 37, CH-1052 Le Mont/Lausanne, Switzerland

Brief description: WAALSURF is a high-quality, low-cost molecular structure display program to be used in teaching and research. It allows you to display and manipulate a molecule of up to 2500 atoms each. The program can represent molecules in ball-and-stick representation, as Dreiding models or as space-filled Van der Waals surfaces. You have access to powerful colorcoding and can make a sequence of images for lectures/demonstrations. WAALSURF allows you to upgrade an IBM PC/AT to a powerful graphics station.

Potential users: Chemists/medicinal chemists/biologists/crystallographers.

Fields of interest: Molecular design.

- § This application program in the area of molecular design has been developed for IBM PC/AT or Olivetti PE24/PE28 in Pascal to run under MS-DOS 3.2 or higher. It is available on 5-1/4" floppy diskettes. Required memory is 640K.
- § Distributed by Softwarts-Actimol.
- § The minimum hardware configuration required is PGA card. No user training is required. There is extensive external documentation. Source code not available.
- § The package is fully operational. It has been in use at 2 sites for approximately 1 year.

JOURNAL NAME BIOCHEMICAL PHARMACOLOGYP E R G A M O N P R E S S
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 ☐ NoDocumentation: ☐ None ☐ Minimal ☐ Self-documenting
☐ Extensive external documentationSource code available: ☐ Yes ☐ NoStage of development: ☐ Design complete ☐ Coding complete
☐ Fully operational ☐ Collaboration welcomedIs program in use? ☐ Yes How long? _____ How many sites? _____
☐ NoIs 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

[This Software Description Form may be photocopied without permission]

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