Biochemical Pharmacology, Vol. 37, pp. I-VI 1988 0006-2952/88 \$3.00 + .00 Printed in Great Britain Copyright (c) 1988 Pergamon Press plc All Rights Reserved

#### SOFTWARE SURVEY SECTION

<u>Editor's Note:</u> 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-016-S87

ChemText

<u>Contributor:</u> Lise M. Dumont, Science Writer, Molecular Design Limited, 2132 Farallon Drive, San Leandro, CA 94577

<u>Brief description:</u> ChemText is a chemical word processor that allows researchers to create complete chemical documents at a personal computer and to then print the final presentation-quality document. ChemText provides multiple fonts for both text and images. Boldface, italics and underscore features serve to add emphasis. Full word processing functions make text editing easier. With a mouse, chemists can draw any molecule on the computer screen with no limit on bond angle. A clean function standardizes bond lengths. Wedges indicate stereochemistry. Reaction centers can be highlighted. ChemText understands chemistry and will signal if a chemically impossible structure is drawn. Straight and curved reaction arrows, boxes, circles and frams are available. A complete set of math fonts ensures that any equation is possible. Chemists can move around and resize all components of an image making it easy to draw complex chemical schemes, tables, flowcharts and process diagrams. ChemText will accept any ASCII text file. Documents can include molfiles from Molecular Design Limited's MACCS-II, CHEMLAB-II and ChemBase, as well as reaction files from REACCS and ChemBase. ChemText will accept data and graphs of data from analytical instruments; images created in other software packages; any HPGL format files; and other file types. ChemText can combine any of the images either created in ChemText or incorporated from outside ChemText and can incorporate them right in the text.

Potential users: All scientists--especially chemists.

- § This application program in the area of chemical word processing has been developed for IBM PC/XT/AT and 100% compatibles in C to run under PC-DOS and MS-DOS. It is available on 5-1/4", dual-sided, double-density floppy diskette. Required memory is 640K.
- § Distributed by Molecular Design Limited.
- § The minimum hardware configuration required is Hercules Graphic Card, IBM Color Card or IBM enhanced graphics memory; mouse; two floppy drives or floppy/hard disk combination; interface card for mouse. 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 150 sites for approximately one year. The contributor is available for user inquiries.

Software package BP-017-S87

GRANT TRACKER<sup>tm</sup>

<u>Contributor:</u> Dr. Kendric C. Smith, President, KCS Software, 927 Mears Court, Stanford, CA 94305

Brief description: GRANT TRACKER is a simple, common-sense bookkeeping program that keeps track of the financial status of your grants, with up-to-the-minute displays of funds awarded, expense-to-date, commitments and balances, and information on all personnel. You enter the information from your grant award statement, salaries and information on your employees, all items of expense as they occur (eg., purchase orders, store orders, etc.), expenses-to-date from the monthly expenditure statement from your institution and the computer automatically calculates your commitments and balances and saves the data. You can also do "what-if" calculations that are not saved, unless you want them to be. The search routine allows you to list and total your expenses in any particular category (eg., travel, reprints, photography, service contracts, etc.); to find a given purchase order by number; to search for orders that are closed or open (ie., paid for or not); to search for specific items ordered, or to search for a specific vendor.

Price: \$149.00 plus \$5.00 postage and handling (prepaid).

<u>Potential users:</u> All people who receive grants of any type. <u>Fields of interest:</u> All.

- § This application program in the area of administration of grants has been developed for IBM PC and compatibles in Compiled BASIC to run under MS-DOS. It is available on 5-1/4", dual-sided floppy diskette. Required memory is 256K.
- § Distributed by KCS Software.
- § 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 19 sites for approximately 2 years. The contributor is available for user inquiries.

### Software package BP-018-S88

AssayZap

Contributor: P.L. Taylor, West Markam, East Lothian, Scotland

Brief description: AssayZap not only offers the familiar regression fit to the logistic equation for calculating RIAs, ELISAs and IRMAs, but also includes a unique interactive visual curve fitting technique which permits all standard curves to be fitted, whatever their shape. Least squares minimization routines for two-parameter log-logit fitting, plus unweighted and weighted four-parameter fit are included. AssayZap maintains a record of all previous assays processed, and permits the current standard curve to be compared with this and if necessary adjusted. Large assays (up to 2000 samples) can be handled, and each assay may include up to four standard curves. Assay drift may be compensated for by interpolation of results between the standard curves. AssayZap conforms completely to the conventions of the Macintosh interface, making full use of the mouse, windows and pull-down menus and, despite its power, is extremely easy to use. It was designed to integrate with a Macintosh-based laboratory data processing system, and includes communication routines which permit the Macintosh to be connected directly to data sources. All data and results may be printed, stored on disk or passed on to other programs for further processing.

<u>Potential users:</u> Laboratory. <u>Fields of interest:</u> Clinical, immunology, etc.

- § This assay calculator program has been developed for the Apple Macintosh. It is available on 3-1/2" floppy diskette. Required memory is 512K.
- § Distributed by Biosoft.
- § No user training is required. There is extensive external documentation. Source code not available.
- § The package is fully operational. It will be available in February, 1988. The Publisher is available for user inquiries.

### Software package BP-019-S88

**AUTOBIBLIO** 

<u>Contributor:</u> J.R. Florini, Syracuse University, Department of Biology, Syracuse, NY 13210

<u>Brief description:</u> AUTOBIBLIO stores references and enables their selection, recall and printing in required formats. You can create your own database of literature references and automatically incorporate those cited in your papers in the bibliography listing. AUTOBIBLIO Modules are as follows:

FindCite searches your manuscript disk and prepares alphabetized or number-order lists of references which it finds cited as "name, year" or "name(year)" in the text. It can read Text and ASCII files and also text prepared with Microsoft Word. The lists are stored on disks as a Text file and can be edited by wordprocessors.

MakeBiblio prepares the final bibliography in the format required by any chosen journal. You can create formulas to suit your own requirements. The bibliography is stored on disk as a text file and can be incorpoated directly into a paper with a wordprocessor. You can store on disk the formats required by your favorite journals.

EditRef prepares the database of references. It can cope with authors who write several papers each year, and with book references. References can be of any size and you can move records from one file to another. There is a search facility enabling you to find references containing any given term, author, year, etc. in your database.

<u>Potential users:</u> Scientists and other authors. <u>Fields of interest:</u> Bibliographic storage.

- § This application program in the area of bibliographic storage and retrieval has been developed for Apple Macintosh. It is available on 3-1/2" floppy diskette. Required memory is 512K.
- § Distributed by Biosoft.
- § The minimum hardware configuration required is two, single-sided 400K drives or one double-sided (800K) drive. 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 50 sites for approximately 2 months. The contributor is available for user inquiries.

JOURNAL	NAME	BIOCHEMICA	AL PHARMACOLOGY	

## PERGAMON PRESS 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?
Is the contributor available for user inquiries: [ ] Yes [ ] No
Distributed by:
Cost of program:
Demonstration disk available? [ ] Yes Cost:
(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
[This Software Description Form may be photocopied without permission]