

## 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-001-S85

### THE BLANCHAE CLINICAL CASE STUDIES

Contributor: Professor M. C. Blanchae, Department of Biochemistry, University of Manitoba, Canada

Brief description: Simulations for the Apple II which recreate typical syndromes:

SYDNEY has aspirin poisoning, so his acid-base problems and toxic symptoms are of interest to physiology, pharmacology and biochemistry students as well as those studying medicine.

MARK has diabetes and his biochemistry endocrinology and physiology all need investigating.

WALTER has oedema caused by lowered serum albumin. The simulation includes use of radioisotopes to measure body fluid compartments and turnover of compounds: relevant to a wide range of students.

DINAH is obese; exploring her problem is of importance to most biomedical disciplines including nutrition.

CHARLEY, ELSIE AND LISA have specific biochemical defects (metabolic block at glycogen phosphorylase, defective cystathionine synthetase, phenylketonuria, respectively) but the implications of their illness spread far and wide in biology and medicine.

The simulations are complete and self-contained and require no additional work from the teacher. Students are assumed to have background knowledge and to know where other information can be found.

Reductions are available for bulk purchases from colleges.

Potential users: Students of medicine, nursing, nutrition and biological sciences.

Fields of interest: Biochemistry, endocrinology, physiology, nutrition.

§ This application program in the area of clinical biochemistry has been developed for Apple IIe. It is available on 5-1/4", single-sided, double-density floppy diskette. Required memory is 64K.

§ Distributed by Elsevier-Biosoft.

§ No user training is required. There is extensive external documentation. Source code is available if purchaser owns the Apple<sup>R</sup> "Author" diskette.

§ The package is fully operational. It has been in use at many sites for approximately 18 months.

Software package BP-002-S85

## STATSTREAM

Contributor: A. Bangham, University of East Anglia, Department of Biology, Norwich, Norfolk, UK

Brief description: STATSTREAM has 76 procedures including: enter and edit data, draw and annotate graphs, open or close text window, display and disk file data, find the mean of a column of data, statistical tests, fit a non-linear function to data and generate pseudodata, etc. These can be used very simply by:

Calling the user-friendly, menu-driven Statpack, which enables a variety of parametric and non-parametric tests to be performed after a single entry of data.

Using the 32 demonstration programs designed to teach the user all about statistics and fitting functions to data.

Writing straightforward BASIC programs to incorporate the desired procedures.

Command features include: mean, standard deviation, standard error and confidence interval, Student's t test, ANOVA 1-way, ANOVA 2-way, F test, Linear regression, correlation;  $\chi^2$  (chi-squared) test, contingency tables; Median, non-parametric confidence interval; Signtest, Wilcoxon signed ranks test, Mann-Whitney, Kruskal Wallis, Friedman t-test, Ftest; Pseudodata generators for Gaussian, skewed noise, etc; Minimization routines for non-linear function fitting and solving equations. Other command procedures can be added. STATSTREAM can be used to analyze data in pre-existing Apple data files and also has a routine for using Visicalc files.

Potential users: Beginner to statistics and computing to professional statistician or research worker; teachers.

Fields of interest: Statistics/biosciences.

§ This application program in the area of statistics/curve fitting has been developed for Apple II in (structured) BASIC to run under DOS 3.3. It is available on 5-1/4", single-sided, double-density floppy diskette. Required memory is 48K.

§ Distributed by Elsevier-Biosoft.

§ The minimum hardware configuration required is 48K Apple II. No user training is required. There is extensive external documentation. Source code is available.

§ The package is fully operational. It has been in use at many sites for approximately 6 months.

Software package BP-003-S85

## ALLOCATE

Contributor: Dr. R. Hammond, Morganville, USA

Brief description: ALLOCATE rapidly assigns clinical or experimental subjects to treatment groups. It functions iteratively to allocate subjects randomly on the basis of a relevant measurement such as body weight. After each iteration the program automatically performs statistical tests to assess uniformity of group means (F ratio) and homogeneity of variances between groups (percent difference between standard errors). Iterations proceed until statistical criteria set by the investigator have been fulfilled or until the 'best allocation so far' is accepted. Then full details of groups and statistical results can be displayed on screen and printed out. Unequal group sizes are catered for and an optional cull facility enables deletion of outliers. ALLOCATE is fully menu-driven and comprehensively documented. The disk contains a working example.

Potential users: Scientific/medical research workers.

Fields of interest: Pharmacology, psychology, medicine, etc.

- § This application program in the area of research where subjects need random allocation to groups has been developed for IBM-PC in BASIC to run under DOS 2.0 and succeeding versions only. It is available on 5-1/4", single-sided, double-density floppy diskette. Required memory is 128K.
- § Distributed by Elsevier-Biosoft.
- § 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 multiple sites for approximately six months.

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Software package BP-004-S85

ENZYME ACTION

Contributors: C. Mueller and T. Spencer, Department of Biochemistry, Queens University, Kingston, Ontario, Canada

Brief description: ENZYME ACTION is a tutorial for the Apple II computer on the basic nature and function of enzymes. It is intended as an aid to understanding and revision by students in the first year of their biochemistry studies. ENZYME ACTION is interactive and has excellent graphics throughout. The program is divided into two parts: 1) A program which gives a general overview of enzyme structures, mechanism of action, kinetics and classification. This includes quizzes to reinforce learning. 2) A program which details chymotrypsin synthesis, storage, site of action and mechanism of action. Quizzes are included and the program features an animated graphics representation of chymotrypsin cleaving a peptide bond on the carbonyl side of a phenylalanine residue in a typical protein.

Potential users: Students of biochemistry.

- § This application program in the area of biochemistry has been developed for Apple II in Compiled BASIC to run under a standard operating system. It is available on 5-1/4", dual-sided, double-density floppy diskette. Required memory is 48K.
- § Distributed by Elsevier-Biosoft.
- § No user training is required. There is minimal documentation. Source code not available.
- § The package is fully operational. It has been in use at 1 site for approximately 1 year.

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Software package BP-005-S85

ENZLAB

Contributors: Drs. J. Garratt and P. Groves, Department of Chemistry, University of York, England

Brief description: ENZLAB computer program simulates exercises in designing and carrying out enzyme kinetics experiments. It randomly selects characteristics of an enzyme from a repertoire of 150,000 different combinations and gives sufficient data to get started. You make choices about pH, substrate concentration, amount of enzyme to use, etc. The results are subject to realistic degrees of experimental imprecision. You can pause to analyze the results obtained so far and the program will calculate the best estimates for the enzyme's kinetic characteristics. ENZLAB will be available for the IBM-PC, Apple II and BBC B microcomputers.

Potential users: Students of medicine, pharmacy and biological sciences.

Fields of interest: Biochemistry.

- § This application program in the area of teaching biochemistry has been developed for Apple II, IBM-PC, BBC B in BASIC to run under a standard operating system. It is available on 5-1/4", single-sided, double-density floppy diskette. Required memory is standard (Apple-48K).
- § Distributed by Elsevier-Biosoft.
- § The minimum hardware configuration required is graphics card for IBM-PC. No user training is required. There is extensive external documentation. Source code is available.
- § The package is fully operational. It has been in use at 1 site for approximately 2 years.

Software package BP-006-S85

## ENZPACK

**Contributor:** Professor P. A. Williams, Department of Biochemistry and Soil Science, University College of N. Wales, Bangor, Gwynedd, Wales

**Brief description:** ENZPACK explores single substrate enzyme kinetics according to the Michaelis-Menten equation for  $K_M$  and  $V_{max}$  values selected by the user. The program can also be used to derive  $K_M$  and  $V_{max}$  values from experimental data and provide graphical representation of the results. Using high resolution graphics, ENZPACK displays velocity/substrate curves plus the major linear derivative plots (Lineweaver-Burk, Hanes-Woolf and Eadie-Hofstee). It also shows the effects of experimental error on the basic and derivative plots, demonstrating the different properties of the plots and how they are not all equally suitable for extrapolating kinetic parameters. In addition, the program illustrates the effects of various types of inhibition on the results obtained, and how the shapes of the different derivative plots are affected. It demonstrates the derivation of the Direct Linear plot and how  $K_M$  and  $V_{max}$  are extrapolated from it. Manual gives full theoretical basis of the calculations used, plus exercises to demonstrate all the program features.

**Potential users:** Students of medicine and biochemistry.

§ This application program in the area of biochemistry has been developed for Apple II, IBM-PC and BBC B in BASIC to run under a standard operating system. It is available on 5-1/4", single-sided, double-density floppy diskette. Required memory is standard (Apple-48K).

§ Distributed by Elsevier-Biosoft.

§ The minimum hardware configuration required is a graphics card (for IBM version.) No user training is required. There is extensive external documentation. Source code is available.

§ The package is fully operational. It has been in use at many sites for approximately 6 months.

Software package BP-007-S86

## ULTRAMASTER

**Contributor:** Ambrose O'Halloran, Pharmacology Department, University College, Galway, Ireland

**Brief description:** ULTRAMASTER'S various modules allow the entry, storage and manipulation of clinical or scientific data which may be numeric or alphanumeric. Data may subsequently be printed in report form, edited, updated or analyzed using a range of relevant statistical tests. In addition the program modules also allow for selective sorting of the data by up to 40 criteria.

**Potential users:** Doctors, research scientists, pharmaceutical companies.

**Fields of interest:** Clinical trials/scientific research data analysis.

§ This application program in the area of database for scientific and clinical data 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 128K.

§ Distributed by Ruby Computer Systems, Surrey, England.

§ The minimum hardware configuration required is dual disk drive. No user training is required. There is minimal documentation. Source code not available.

§ The package is fully operational. It has been in use at 3 sites for approximately 1 year.

Software package BP-008-S86

DOSE-EFFECT ANALYSIS WITH MICROCOMPUTERS:  
Quantitation of ED<sub>50</sub>, LD<sub>50</sub>, Synergism,  
Antagonism, Low-Dose Risk, Receptor Ligand  
Binding and Enzyme Kinetics

Contributor: Ting-Chao Chou, Ph.D., Laboratory of Pharmacology, Memorial Sloan-Kettering Cancer Center, 1275 York Avenue, New York, NY 10021

Brief description: DOSE-EFFECT ANALYSIS WITH MICROCOMPUTERS is a thoroughly documented series of programs for the quantitation of ED<sub>50</sub> and LD<sub>50</sub>, synergism, antagonism, low-dose risk, receptor ligand binding and enzyme kinetics using the IBM-PC and Apple II microcomputers. This manual/disk combination contains the theoretical background, worked examples and full program listings for a variety of analytical techniques in the pharmacology, toxicology, oncology and biochemistry fields. Contents include:

- 1) Michaelis-Menten Kinetics: double reciprocal plot; calculation of  $K_m$ ,  $V_{max}$ ,  $K_i$ ; diagnosis of type of inhibitions, etc.
- 2) Multiple Drug Effect Analysis: determination of the median-effect dose (ED<sub>50</sub>, etc.); relative potency; sigmoidicity of dose-effect curves; isobolograms; combination index; graphical and tabular representations of synergism; antagonism and summation at different effect levels; statistical parameters.
- 3) Effect or Risk Assessment: risk assessment for carcinogens; dose required to produce a given risk, risk assessment for radiation.
- 4) Therapeutic and Safety Indexes: therapeutic index and safety margin.
- 5) Scatchard Plot.
- 6) Calculation of Receptor  $K_i$ .

Price: \$60.00, including disk and manual.

Potential users: Pharmacologists, biochemists, toxicologists, oncologists.

Fields of interest: LD<sub>50</sub>, ED<sub>50</sub>, Synergism/Antagonism, Isobologram, Scatchard.

§ This application program in the area of analysis and graphics for LD<sub>50</sub>, ED<sub>50</sub>, Synergism/Antagonism, Isobologram, Lineweaver-Burk plot, Scatchard plot and Therapeutic Index has been developed for IBM-PC and Apple II in BASIC to run under DOS 2.1 (IBM-PC) and DOS 3.3 (Apple). It is available on 5-1/4", single-sided, single- or double-density floppy diskette. Required memory is 64K.

§ Distributed by Elsevier-Biosoft.

§ 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 100 sites for approximately 1 year. The contributor is available for user inquiries.

NAME OF JOURNAL BIOCHEMICAL PHARMACOLOGYP E R G A M O N P R E S S  
SOFTWARE DESCRIPTION FORMTitle 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 ☐ NoDocumentation: ☐ None ☐ Minimal ☐ Self-documenting  
☐ Extensive external documentationSource code available: ☐ Yes ☐ NoLevel of development: ☐ Design complete ☐ Coding complete  
☐ Fully operational ☐ Collaboration would be welcomedIs software being used currently? ☐ Yes ☐ No  
If yes, how long? \_\_\_\_\_ If yes, how many sites? \_\_\_\_\_Contributor is available for user inquiries: ☐ Yes ☐ No

Return completed form to:

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

(continued)

[This Software Description Form may be photocopied without permission]

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] \_\_\_\_\_

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[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]