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-023-S90

Scatchard Analysis

Contributor: Biosoft, 22 Hills Road, Cambridge CB2 1JP, UK

<u>Brief Description:</u> Scatchard Analysis is a user-friendly package for the rapid analysis and storage of ligand-binding data. It analyses radioligand binding data according to the modified Scatchard equation. The program is designed to provide easy entry of data and other values necessary for the calculations. A summary of results, a graph of the Scatchard plot and the Kd and Bmax are displayed, and can be printed out on Epson-compatible printers. Scatchard Analysis has its own straightforward data editor, but data can also be entered using any editor which can download ASCII files, including spreadsheets like Lotus 1-2-3.

<u>Potential Users:</u> Pharmacologists, biochemists, toxicologists, oncologists. <u>Fields of Interest:</u> Radioligand binding.

- ** This utility program in the area of radioligand binding has been developed for IBM PC in Compiled Pascal to run under DOS 2.0+. It is available on 5-1/4" and 3-1/2" floppy diskette. Required memory is 256K.
- ** Distributed by contributor.
- ** User training is not required. There is extensive external documentation.
- ** The package is fully operational. The publisher is available for user inquiries.

Software Package BP-024-S90

OSAR-PC

Contributor: Dr. R.A. Coburn, University of Buffalo, Buffalo, NY

Brief Description: QSAR-PC is a series of programs which enable an investigator to search conveniently for correlations between biological or chemical properties and physicochemical property variations produced by structural changes in a series of congenetic drugs. These quantitative correlations are employed in the optimization of drug structure and in the elucidation of molecular mechanisms of action. This method, which has been popularized by Corwin Hansch, is one of the most widely used techniques in the rational design of biologically active molecules. It is an extrathermodynamic method which makes use of multiple linear regression analyses. QSAR-PC is largely menu driven and minimizes user entry of data.

<u>Potential Users:</u> Medicinal or pharmaceutical chemists, organic chemists, chemical pharmacologists, pharmacologists, graduate students in medicinal chemistry or pharmacology.

- ** This program in the area of chemistry has been developed for IBM PCs and compatibles in Quick BASIC 3. It is available on 5-1/4" and 3-1/2" floppy diskette. Required memory is 256K.
- ** Distributed by Biosoft.
- ** User training is not required. There is extensive external documentation.
- ** The package is fully operational. It is in use at 50 sites.

Software Package BP-025-S90

MultiStat

Contributor: Biosoft, 22 Hills Road, Cambridge CB2 1JP, UK

Brief Description: MultiStat is based around "columns" of data--up to 30 on screen at one time, each with up to 1000 data items. It will generate random numbers from four different distributions -- Uniform, Normal, Poisson, Exponential -- making it ideal for educational and simulation purposes. column can be transformed in a large number of ways including linear, logarithmic, square root, cube root, reciprocal and absolute value transformations. Trigonometric transformation is also provided and a column can be sorted or ranked. Any number of columns can be appended to create a larger column and data can be moved to and from EXCEL. MultiStat provides descriptive statistics and a comprehensive range of analytic statistics, both parametric and non-parametric, including t-test, linear regression and correlation, multiple linear regression, and analysis of variance. Kruskal-Wallis and Friedman analysis of variance by ranks is provided, also tests of proportion and contingency table tests. MultiStat also provides Fisher's exact test, McNemar's test, Wilcoxon's signed ranks test, the Mann-Whitney U test, and Spearman's and Kendall's rank correlation procedures. MultiStat has a range of graphics capabilities including histograms, bar charts, pie charts, line graphs and scatter graphs.

- ** This application program in the area of statistics has been developed for Macintosh Plus/SE/II. It is available on 3-1/2" floppy diskette.
- ** Distributed by Biosoft
- ** User training not required. There is extensive external documentation.
- ** The package is fully operational.

Software Package BP-026-S90

DisFree

Contributor: Biosoft, 22 Hills Road, Cambridge CB2 1JP, UK

<u>Brief Description:</u> The program is based on the book, "Distribution-free Statistics--An Application-oriented Approach" by Joachim Krauth (Elsevier 1988). DisFree has a superb user interface, with hierarchical menus, excellent data editing and storage facilities and comprehensive printout of results. The 25 most complex tests have built-in simulations for training purposes. All tests have separate versions for large and small sample sizes. Tests included are: Two-sample tests of heterogeneity; Two-sample tests of dependence; tests for heterogeneity for three or more samples.

- ** This program in the area of statistics has been developed for IBM PC in Compiled BASIC to run under DOS 2.0+. It is available on 5-1/4" and 3-1/2" floppy diskette. Required memory is 256K.
- ** Distributed by Biosoft.
- * User training not required. There is extensive external documentation.
- ** The package is fully operational.

| JOURNAL NAME | BIOCHEMICAL PHARMACOLOGY |
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| | PERGAMON PRESS |
| | SOFTWARE DESCRIPTION FORM |
| Title of Software Pro | gram: |
| | |
| Contributor: | |
| Institution: | |
| Address: | |
| | Telephone: |
| | |
| Type of program: [] | Application [] Utility [] Other |
| Category: | (ie., Psychological Assessment, |
| statisti | cs, thermodynamics, etc.) |
| | |
| Field/s of interest: | |
| Developed for (name o | f computer/s): |
| <pre>in (language/s):</pre> | |
| to run under (ope | rating system): |
| available on: [|] Floppy 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: [] N | one [] Minimal [] Self-documenting |
| ı |] 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 av | ailable for user inquiries?: [] Yes [] No |
| Distributed by: | |
| Cost of program: | |
| Demonstration dis | k available? [] Yes Cost: |

[] No

Description of what software does (maximum of 200 words):

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

| Reference | number | |
|-----------|--------|----------------------|
| | | (assigned by Editor) |

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