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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 EJCCO-037-S87 — 2600 Chromatography Software for the IBM PC and Compatibles

Contributor: Barry Giordano, Nelson Analytical, Inc., 205 Robin Road, Paramus, NJ 07652

Brief description: Data acquisition and report generation of up to fifteen chromatographic detectors simultaneously and a single PC. Extensive use of graphics aid the analyst to develop methods interactively. Multi-level calibration, autosampler rack and vial reading, and sequence control available. Supports enhanced graphics color and is mouse-driven. Comparison and ratio/difference overlay of spectra are standard. Software supported on IBM Token-Ring and PC Networks.

Potential users: Pharmaceutical QA and R&D.
Fields of interest: Analytical chemistry.

§ This application program in the area of chromatography has been developed for IBM PC/AT and compatibles in Compiled BASIC to run under DOS 2.2 or later. It is available on 5-1/4", dual-sided, low density, floppy diskette. Required memory is 640K.
§ Distributed by Nelson Analytical, Inc.
§ The minimum hardware configuration required is Hercules Graphics Card. No user training is required. There is extensive external documentation. Some source code is available.
§ The package is fully operational. It has been in use at 800+ sites for approximately 5 years. The contributor is available for user inquiries.

Software package EJCCO-038-S87 — CALS PEAKPRO

Contributor: Dr. Robert B. Janney, Beckman/CIS, 160 Hopper Avenue, Waldwick, NJ 07463

Brief description: CALS PEAKPRO is a powerful Chromatographic Data Acquisition Analysis and Reporting program. It provides for control of various autosamplers and automatic collection of data from a wide variety of gas and liquid chromatographs. Powerful algorithms analyze each raw chromatogram (or data file) and detect peaks, set baselines, compute peak areas and heights, without user interaction. If methods require modification the analyst communicates graphically with the analytical method, using a mouse driven cursor. Colored multiplots are available for comparison of chromatograms, and several report formats are available. A unique catalog

function allows searches and retrievals on all chromatographic results, raw data files and methods. An optional System Suitability program is available for determination of system performance.

Potential users: Laboratory technicians, analysts, chromatographers.
Fields of interest: Pharmaceutical R&D and QC, analytical chemists.

§ This application program has been developed for HP1000A in FORTRAN 77 to run under RTE-A, RTE-6/VM. It is available on magnetic tape. Required memory is at least 1MB.
§ Distributed by Beckman Instruments, Inc.
§ The minimum hardware configuration required is Micro 24 or Micro 26. User training is required. There is extensive external documentation. Source code is available.
§ The package is fully operational. It has been in use at 20+ sites for approximately 1 year. The contributor is available for user inquiries.

Software package EJCCO-039-S87 CALS LAB MANAGER

Contributor: Peter G. Berthrong, Beckman,CIS, 160 Hopper Avenue, Waldwick, NJ 07463

Brief description: CALS LAB MANAGER is a highly developed, field tested Laboratory Information Management System (LIMS), especially suited for laboratories subject to GLP or GMP compliance. Highly configurable and supportable to meet the individual laboratory needs either by Beckman staff or the customer. Data can be entered manually through customer modifiable screens or online from laboratory instruments connected to the computer. Provides sample log-in, testing, validation, approval, reporting and archiving. Can provide worklists by technician, instrument, priority, etc., sample status, test status, and trend analysis. Used to automate QC labs, drug metabolism departments, stability studies.

Potential users: Laboratory technicians, supervisors, managers.
Fields of interest: Pharmaceutical R&D and QC, analytical labs.

§ This application program has been developed for DEC VAX, HP1000A, IBM 43XX, IBM 30XX in FORTRAN 77 to run under VMS, RTE-A, MVS/TSO. It is available on magnetic tape.
§ Distributed by Beckman Instruments, Inc.
§ The minimum hardware configuration required varies with application. User training is required. There is extensive external documentation. Source code is available.
§ The package is fully operational. It has been in use at 160+ sites for approximately 5-6 years. The contributor is available for user inquiries.

Software package EJCCO-040-S87 ILEUM ver. 2.0

Contributor: Dr. I. Hughes, OIDATA, Leeds, United Kingdom

Brief description: ILEUM accurately simulates laboratory experiments which investigate the effects of drugs on the vitro guinea-pig ileum. The in vitro guinea-pig ileum preparation is commonly used to demonstrate and quantitate the actions of drugs on intestinal smooth muscle. It has the advantage of retaining its responsiveness for many hours, of having relatively little spontaneous activity and of containing a great variety of receptor types. Thus the actions of many different drugs can be demonstrated on this tissue and simulated on ILEUM. Drugs available for the ILEUM simulation include a dozen familiar agonists, which will contract the muscle, together with blockers of various sorts. It is possible to mimic experiments to identify

"an unknown compound." For this the computer can select at random one of the 20 "unknowns," some of which do not appear in the regular program runs, although a key is given in the manual allowing deductions about the compound(s) to be checked. Random elements are incorporated into ILEUM to simulate the inherent biological variability in the response to the same dose of agonist. ILEUM has the great advantage over the animal preparation that the time between additions of drug can be reduced to seconds, so an entire series of test can be carried out in a short time, rather than hours normally required. However, good experimental design is still essential. ILEUM can be used quantitatively or qualitatively and a permanent record of output can be produced on a normal printer in the form of a "chart trace" which can then be measured and processed using the usual statistical procedures.

Potential users: Students
Fields of interest: Pharmacology/physiology.

§ This application program in the area of pharmacology/physiology has been developed for Apple II, IBM PC, BBC B in BASIC. It is available on 5-1/4", double-sided, double-density floppy diskette.
§ Distributed by Elsevier-Biosoft.
§ The minimum hardware configuration required is a printer. No user training is required. There is exensive external documentation. Source code is available.
§ The package is fully operational. The publisher is available for user inquiries.

Software package EJCCO-041-S87 CARDIOLAB

Contributor: Dr. I. Hughes, PIDATA, Leeds, United Kingdom

Brief description: CARDIOLAB costs less than a single dog yet can be used repeatedly to simulate the chart recorder outputs of experiments on anaesthetized (normal or reserpinized) animals and pithed animals. The simulated heart rate and blood pressure traces can be made on almost any printer. The program allows "administration" of many agonist/antagonist drugs and can mimic stimulation of vagal and sympathetic cardiac nerves. Effects of blockers "wear off" at a rate corresponding to their $t_{1/2}$. "Overdoses" with agonists or blockers will "kill" the preparation. Responses are subject to "biological variation" and are influenced by cardiac compensatory reflexes if appropriate. Tachyphylaxis is seen with relevant agonists. CARDIOLAB simulates the slow deterioration of a preparation which may "die" unexpectedly after six hours of "preparation time" (responses each take about 10s to be printed but represent about 3 minutes of "preparation time"). CARDIOLAB provides "unknown" drugs for characterization by students.

Potential users: Students.
Fields of interest: Physiology/pharmacology/medical.

§ This application program in the area of pharmacology/physiology/medical has been developed for IBM PC, Apple II, BBC B. It is available on 5-1/4", double-sided, double-density floppy diskette. Required memory is 128K (IBM PC), 48K (Apple II).
§ Distributed by Elsevier-Biosoft.
§ The minimum hardware configuration required is a printer. No user training is required. There is extensive external documentation. Source code is available.
§ The package is fully operational. The publisher is available for user inquiries.

Software package EJCCO-042-S87 Compudex

Contributor: Dorte Jensen, Compudex, Inc., 5612 Spruce Tree Avenue, Bethesda, MD 20814

Brief description: Compudex is a software program which allows fast, full text searching and retrieval of information. Although the software was developed for searching the Code of Federal Regulations, Compudex may be used to search any documents (for example, standard company reports, correspondence, etc.). No keywording or abstracting is required. Compudex allows single term, multiple term, adjacency, proximity, and Boolean searches. Results of searches may be filled, edited, or sent to word processing files. Documents currently available include Titles 7/9/21/29/40 of the Code of Federal Regulations (CFR) as well as the Federal Register.

Potential users: Scientists, professionals, etc. working in regulated industry.
Fields of interest: Food, pharmaceutical, chemical, environmental.

§ This application program in the area of government regulations has been developed for IBM PC/AT, DEC/VAX in C language to run under DOS 2.0 or higher. It is available on 5-1/4" floppy diskette, Bernoulli cartridge, magnetic tape. Required memory is 640K.
§ Distributed by Compudex, Inc.
§ The minimum hardware configuration required is 20MB hard disk. User training is required. It is self-documenting. Source code not available.
§ The package is fully operational. It has been in use at 10 sites for approximately 1 year. The contributor is available for user inquiries.

Software package EJCCO-043-S87 CAMSEQ/M Molecular Modeling System

Contributor: H.J.R. Weintraub, Ph.D., Weintraub Software Design Associates, Inc., P.O. Box 42577, Cincinnati, OH 45242

Brief description: CAMSEQ/M is a full featured, menu driven, PC-based molecular modeling system. Capabilities include:

1. Molecular Sketchpad providing conversions from user drawn structures to idealized 3D molecules. Templates may be incorporated into structures.
2. Various display renditions including stick, ball and stick, space filling and "Ortep."
3. Full structure inquiry features.
4. Dynamic, interactive bond rotations.
5. Molecular comparisons and overlays.
6. Conformational searching (unique to CAMSEQ/M on a PC).
7. Molecular Librarian to assist in organizing structure files.
8. Interface to other modeling packages, including MM2 and SYBYL.

CAMSEQ/M is layered on a device-independent graphics interface to protect your hardware investment. The software supports most existing displays, input and hardcopy devices and will support new hardware as it is developed.

Potential users: Chemists, biochemists, MD's, students.
Fields of interest: Chemistry/agricultural products/biochemistry/medicine.

§ This application program in the area of molecular modeling has been developed for IBM PC/AT/XT and compatibles and PS/2 in FORTRAN 77 and C to run under MS-DOS and PC-DOS. It is available on 5-1/4", dual-sided, double-density floppy diskettes. Required memory is 640K.

§ Distributed by AIMS.
§ The minimum hardware configuration required is EGA/CGA/Hercules Graphics 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 15 sites for approximately 1 year. The contributor is available for user inquiries.

Software package EJCCO-044-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.

Potential users: Laboratory.
Fields of interest: 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 has been available since February, 1988. The Publisher is available for user inquiries.

Software package EJCCO-045-S88 AUTOBIBLIO

Contributor: J.R. Florini, Syracuse University, Department of Biology, Syracuse, NY 13210

Brief description: 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 the 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.

Potential users: Scientists and other authors.
Fields of interest: 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.

Software package EJCCO-046-S88 CLIN-TEAMS/PCS™ V1.1
(Product Complaint System)

Contributor: Jeanne L. Oliver, R.R.A., Technical Evaluation and Management Systems, Inc., 5151 Beltline Road, Suite 1110, Dallas, TX 75240

Brief description: CLIN-TEAMS/PCS™ is a system of programs designed to facilitate the collection, organization, analysis and reporting of information about product complaints and adverse drug experiences as required by the FDA. The system is designed to permit capture of information on a wide variety of communications about pharmaceutical products that can be categorized under the term "complaint." The reports can be divided generally into two categories which may be described by the terms "pharmaceutical complaints" and "medical complaints." The system also permits controlling access to this information about complaints in each category on a need-to-know basis and permits recording certain information about complaints which involve litigation. The portion of the system concerned with adverse drug experiences has been designed to be consistent with the FDA's "Draft Guidelines for Postmarketing Reporting of Adverse Drug Reactions." The CLIN-TEAMS/PCS system consists of four modules: 1) Data Collector, 2) Report Generator, 3) Data Display, and 4) Utilities.

Potential users: Pharmaceutical Q&A and R&D.
Fields of interest: Clinical trials/products complaint.

§ This application program in the area of product complaints/ADR reporting was developed for Digital-VAX to run under VMS. It is available on 600', 1600bpi, VAX BU FMT character set magnetic tape. Required memory is 4MB.
§ Distributed by Technical Evaluation and Management Services, Inc.
§ The minimum hardware configuration required is Microvax II with RA81. 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 2 years. The contributor is available for user inquiries.

JOURNAL NAME **EUROPEAN JOURNAL OF CANCER & CLINICAL ONCOLOGY**

P 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 [ ] 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:

Professor H. Tagnon
Institut Jules Bordet
Centre des Tumeurs
1 rue Heger-Bordet
B-1000 Bruxelles, Belgium

VIII 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