Computer Software Reviews

TGRAF-07; Version 2.0.07, Grafpoint: 4340 Stevens Creek Blvd. No. 270, San Jose, CA 95129. (408)-249-7951.

TGRAF-07 is a graphics terminal emulation package for DOS computer systems. TGRAF-07 allows the PC to effectively replace a Tektronix 4107 graphics terminal. Emulation modes for the Tektronix 4105, Tektronix 4010, DEC VT52, and DEC VT100 are also included. TGRAF-07 is designed to run on any IBM PC compatible system with a minimum of 256 kB memory, an RS-232 serial port or a built-in modem, and a compatible color graphics card and monitor. Options are available within the software for use with several printers and cursor input devices. TGRAF-07 is copy protected. The emulation files can be copied onto a hard disk as backup files, but the initiation of the emulation still requires the floppy diskette, which contains a "fingerprint", to be in drive A. This "fingerprint" can supposedly be transferred to the hard disk, but the version of TGRAF on which this review is based did not contain the file needed for such a transfer.

This program contains a number of parameters providing several options each. The numerous combinations of these options permit the user to configure the program to meet a variety of needs. However, the use of some of these parameters necessitates a working knowledge of the terminal to be emulated. The documentation provided with the program gives a basic description of each parameter, but it does not indicate the proper settings necessary to most closely emulate the above listed terminals. Many of the parameters are simply equated to the corresponding command on the Tektronix 4107. Some of the descriptions are lacking in other details, as well. For example, the Background Index and the Line Index parameters determine the color of the background and lines, respectively. The choices for these parameters are 0 through 7 and 0 through 15, respectively. However, the specific color determined by each number is not given. This lack of detailed documentation makes it difficult to determine the source of problems when the emulation program interacts with software with which it is not totally compatible. One section of the documentation involves the commands to which TGRAF responds. This is helpful for the development of computer programs with which TGRAF could be utilized.

This software was studied with use of an IBM PC/AT equipped with an RS-232 serial port, an IBM Enhanced Graphics Monitor or an IBM Professional Graphics Monitor, an IBM color printer, and a MouseSystems PCMouse. This review is limited to the interaction of the emulation software with MacroModel,[1] a powerful molecular modeling and graphics package. The documentation for MacroModel includes a section on terminal setups in which the parameter settings for several emulation programs are discussed. Following these directions provides sufficient emulation of a Tektronix 4107 using the above hardware.

There is a significant difference in resolution between the Enhanced Color Monitor and the Professional Graphics Monitor. The Enhanced Color Monitor (with an EGA card) is sufficient for small molecules, but larger molecules, such as enzymes or large polypeptides, are much more difficult to distinguish. Also, the selection buttons on the side of the screen are not sufficiently defined. They can be read, but not easily. These problems are not apparent with the Professional Graphics Monitor.

There is a problem involving the optical mouse (MouseSystems PCMouse) which was used. If the mouse is moved slightly as a button is pressed, the crosshairs disappear, but no legible signal is sent. The carriage return must be pressed several times very quickly in order to regain control of the crosshairs. The cursor arrows on the keyboard of the IBM can be used in place of a mouse, but drawing complex molecules using this method becomes very tedious due to the limitations of the arrows, i.e., unidirectional and finite increments of movement.

The printer utilized in this review is not one of the listed printer options for the emulation program. Thus, use of the ⟨PrtSc⟩ key, the ⟨alt⟩ a command, or the ⟨alt⟩ g command is not successful in the Tek Mode. However, in the VT100 mode, the ⟨PrtSc⟩ key produces a hardcopy of the text on the screen. The MacroModel software contains a plotting subroutine which uses Versatec and Zeta-8 Plotters. If the plotter is connected between the Vax computer on which MacroModel resides and the IBM, a plot of the graphics window from MacroModel should be successfully obtained via the software in MacroModel.

Overall, TGRAF-07 has a great capacity for further extending the use of the PC into a graphics terminal. Its interaction with MacroModel gives the chemist a reasonably inexpensive entrance into an extremely versatile and productive molecular modeling program.

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pdVIEWER, Version 1.03, Biotechnology Center, University of Illinois, 901 S. Mathews Street, Urbana, IL 61801. (217)-333-1695. $150.00.

pdViewer is a drawing package for students and researchers to visualize in three dimensions the structure of molecules. It requires an IBM PC, PC-AT or PS/2 computer or compatible with a CGA, EGA or VGA display adapter and display. The program requires 384K or memory but 512–640K is recommended to display a large number of atoms. A hard disk is not required but is highly recommended. An EGA or VGA (in EGA mode) has significant advantages and added functions and is also highly recommended. It requires DOS 2.0 or later and is not copy protected. pdViewer is written in Microsoft QuickBasic V 3.0 and includes the source code and instructions for compiling. Since the program is intended for educational purposes, registered users are encouraged to explore and modify the program to suit their needs. This program is *not* placed in the public domain so that modified or unmodified copies may not be distributed.

pdViewer consists of two main programs: pdViewer and SPHERE. The latter provides shaded spherical display of the molecules and requires a PGA display adapter and display (640 × 480 with 256 colors). A PGA adapter was not available to this reviewer so my comments are confined to pdViewer.

pdViewer requires a set of known atomic coordinates usually obtained by diffraction X-ray analysis and uses the Brookhaven National Laboratory Protein Data Bank format for reading and writing data. Information on how one can obtain several hundred protein structures is provided. The three-dimensional effect is achieved by drawing the structure twice: first in red rotated 3° to the right and then in green rotated 3° to the left. A pair of glasses with one lens red and the other green gives a three-dimensional image. The 3-D effect is not immediately apparent and requires a "learning" process that takes a few minutes.

pdViewer has the following features: The images of molecules leap from the screen in a way that this reviewer has never seen before. pdViewer can highlight heteroatoms, amino acids, prosthetic groups, water molecules, or hydrogen bonds. pdViewers can center the image and with use of a control panel, the size, shape, and orientation of the molecule can be adjusted. pdViewer can display a view along any axis or show any portion of the molecule while keeping the 3-D effect. The use of the control panel is not simple and not interactive and requires practice to achieve the desired results. pdViewer can use a cursor to measure distances from one residue to another or to identify the residue. The best feature may be the ability to draw two different images and to switch between them rapidly. This gives a better 3-D effect and some motion to otherwise static displays. Finally, pdViewer can plot the 3-D images on a plotter that uses the HP-GL compatible format. pdViewer does not claim that the plotted images will show a 3-D effect but I had no difficulty in seeing the 3-D images of DNA and cytochrome *c* on paper after plotting them in green and red.

The program is easy to start but it is difficult to run. All of the commands are given by pressing the function keys by themselves or in conjunction with shift, alt, or ctrl keys. There seems to be no simple plan and therefore the keys were very difficult to memorize. One needed to refer to the manual almost all of the time. There was no simple and complete command summary that one could use. I had to keep turning the pages to find the command that I needed. After striking a key one does not get immediate feedback on the result. One needs to press the F10 key to redraw the 3-D image on the screen to see if anything has happened. This saves time if one is familiar with all of the commands and can strike several keys before a single redraw, but during the learning process the lack of feedback is a significant hindrance.

The manual (36 pages) has 6 lessons on the use of pdVIEWER and a number of sample structures. The structures are highly useful during the learning process. Otherwise the manual is difficult and incomplete. Plotting is not explained in any lesson and the instructions on the screen are not clear. The use of the cursor is barely mentioned in the manual. The instructions for recompiling the program are almost nonexistent. One of the major reasons for recompiling is to include coprocessor support so that the calculations would be faster. On a 8 MHz PC-AT an increase in performance of about 10% was observed.

(1) This program was graciously provided by Prof. Clark Still, Columbia University.

Other products that may serve some of the same functions are Molecular Graphics (V 2.0 review: *J. Am. Chem. Soc.* **1986**, *108*, 7882), Sterochimica on the Mac (review: *J. Am. Chem. Soc.* **1987**, *109*, 956), ChemCad (review: *J. Am. Chem. Soc.* **1987**, *109*, 2229), Visual Molecules V 1.0 (review: *J. Am. Chem. Soc.* **1987**, *109*, 5056), and Alchemy V 1.0 (review: *J. Am. Chem. Soc.* **1988**, *110*, 325).

Summary: If you need to view 3-D images of biological molecules that include several thousand atoms, pdViewer may be what you seek. It gives you the source code to change the program to do some special things that are currently not possible. The input files are in ascii and can be modified with appropriate filters. pdViewer is not outstanding in any respect such as speed, ease of use, ease of learning, or convenience of a wide variety of output options, but it does give excellent 3-D images.

Joseph V. Paukstelis, *Kansas State University*

WIMP, Version 6.0, By H. W. Whitlock. Aldrich Chemical Co., 940 West St. Paul Ave., Milwaukee, WI 53233. List Price: $250. No educational discount. Optional Structure-Template Database, Wimplates $95.00. Optional Glassware and Apparatus Database, WIMP Lab Gallery, $75.00.

WIMP (Wisconsin Interactive Molecule Processor) is a molecule drawing program designed for the production of two-dimensional structures and reaction schemes on an IBM Personal Computer and many compatibles (see specifications). Two databases are available, a structure-template database with over 400 structure backbones, functional groups and specialty items such as circle arrows, equilibrium double arrows, etc., and a glassware and apparatus database with more than 230 templates of apparatus and fragments of apparatus.

Specifications: WIMP has very exacting hardware specifications. The software is designed to operate on an IBM PC, PC XT, PC AT, PS/2 or compatible with MS DOS or PC DOS 3.0 or higher. A minimum of 512 K RAM is required as well as an 8087 or 80287 math coprocessor chip. A minimum of 1 floppy disk drive is required (ds-dd) although a hard disk is strongly recommended. Additional hardware required includes a mouse (Microsoft or Mouse Systems mouse recommended), a color graphics adapter, and a color monitor. Structures may be drawn to either an HP 7000 series plotter with serial interface or printers which use the Adobe Postscript standard such as the Apple LaserWriter. It is also possible to use a HP Laserjet printer if the user purchases the driver program (Laser Plotter program, $150 from Aldrich). Plotter and mouse installation instructions are clearly described in the manual.

Upon startup of WIMP the user is presented with the main menu which provides for (1) editing a previously created file, (2) starting a new structure, (3) fetching a structure from disk, (4) saving a structure, (5) changing operating parameters (baud rate, default directory for files, printer communication port), and (6) exiting the program. There is no provision for deleting structures and this must be done at the DOS level. Also, backup files of structures are made but they may only be retrieved by exiting to DOS and changing the extension of the backup file to the WIMP readable extension.

The molecule editor of WIMP requires some effort to learn how to use since the commands for editing and drawing structures are not available in pull down menus and the commands are not displayed on the screen as they are in another similar molecule-drawing program (see: *J. Am. Chem. Soc.* **1987**, *109*, 3177). Nonetheless, the commands are relatively easy to learn and an on-line help is available. Upon entering the edit mode for making a new structure, the cursor coordinates and the drawing status are displayed in the upper left hand corner of the screen. The cursor may be controlled either by the mouse or the numeric keypad. The cursor may also be moved standard bond lengths at various angles specified by a grid command. This is particularly useful for rapidly drawing ring structures. WIMP allows structures up to 1000 atoms and/or 1000 bonds in size.

Features of the drawing mode are similar to those of other similar drawing programs. A rubber band mode for drawing exists as well as point-to-point drawing. There is also a hide-bond feature. Simple keystroke commands allow the bond type to be selected; choices include double, triple, hatched, long and short wedge, and jagged bonds. The hatched bond does not vary the length of the hatch marks along the bond. Commands also exist for drawing arcs, circles, and ovals (with a 2:1 aspect ratio). Bonds and points are edited independently with keystroke commands (i.e., to erase a portion of a drawing, the bonds must be erased and the remaining unconnected points are subsequently erased with a separate key).

Three template menus are built into WIMP with 22 ring structures, arrows, a circle, and the various bond types described above. The templates include 7 different cyclohexane configurations, 3- to 9-membered rings, and 4 perspective drawings of benzene. The templates are retrieved from a pull-down menu of figures and are conveniently attached to existing structures allowing structures such as adamantanes and steroids to be easily prepared. Templates improperly placed in a drawing can be readily removed with a single command. Templates may be retrieved from one of the databases (i.e., Wimplates) by using the fetch command in the drawing mode. The user must look up the file name of the template in the database manual for entry with the fetch command (of course the user can change the names of templates frequently used to make retrieving templates more convenient).

Addition of labels and captions to structures or reaction schemes can be accomplished easily with a single keystroke to invoke the text mode. Positioning of text with the rubber band command is straightforward. Text input is unique. For example, numbers are automatically subscripted; to suppress subscripting a "$" must be entered before each number. Also, titles and text must be preceeded by "$$" as an identifier, thus "$" cannot be used as a character within text. One nice feature is the left label option in which the text typed begins at the cursor and flows to the left. Superscripts and subscripts can be added to text. WIMP does not have a Greek character set.

Complete or partial structures or reactions may be moved, erased, zoomed, copied, inverted, or rotated by encapsulating the desired screen segment in a box. Unlike other drawing programs the box is not displayed as it is being drawn (i.e., in a rubber band mode). As a result, boxes must occasionally be redrawn to capture a portion of a structure which is close to other structural features which are meant to be outside the box. The box-editing modes, particularly zoom, copy, and invert (mirror image), are very useful. Also, the contents of a box may be saved to disk.

The reviewer used an HP 7475 plotter for drawing figures. WIMP is designed to be used in conjunction with word processors by inserting figures onto a page that already contains text. Thus the printing and plotting software is designed to position and size the figure on the page. Plotting commands (for HP plotters) allow selection of pen speed, lettering type for labels, and caption and picture positioning and sizing. Figures may also be plotted from DOS by using the separate WIMPlot (what else?) program. Use of Postscript output is considerably different. Preliminary figures may be sent from the molecule editor within WIMP directly to the printer but final figures for documents must be prepared by using one of two off-line programs. A program (COMPOSER) is included for positioning and printing up to twenty WIMP files on a single page.

WIMP can create disk files in HPGL plot language or Postscript. Both Encapsulated Postscript and HPGL files can be incorporated into *PageMaker*, a desktop publishing program. One other feature of WIMP is that a program is included which will translate files from the three-dimensional molecular modeling program MACROMODEL into WIMP files which can be printed.

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PROSTAT, By Charles Ward and James Reeves (The University of North Carolina, Wilmington, NC). Price: $125. ISBN 0-88720-287-X. Copyright (1986) and published by COMPress Division of Wadsworth Inc.: P.O. Box 102, Wentworth, NH 03282 (Phone: 603-764-5831/5225).

PROSTAT is a set of statistical programs and data-file manipulation utilities for routine analysis of laboratory data. Data used by the program are read from simple ASCII files and thus interfacing is relatively simple. A large choice of statistical operations is available, selectable from a menu: (a) Data manipulation including a simple spreadsheet. (b) Descriptive statistics: means, variances, modes, skewness, frequency distributions and histograms. (c) Linear regression and correlation: weighted and unweighted, reduced axis regression and back calculation. (d) Curve fitting and nonlinear regression: polynomials, power, exponential and logarithmic. (e) T tests. (f) Multiple linear regression. (g) Analysis of variance: one way ANOVA with and without repreated measures, two-way ANOVA. (h) Numerical analysis: a rather ingenious graphic display with displayed and calculated first and second derivatives, maxima and minima, smoothing, areas, etc. The data selected can be chosen from a larger set by zooming and cursor controls.

Features: The program is stated to require an IBM-PC or compatible with 256K RAM, two floppy disc drives or one floppy and a hard disc, a monochrome or color graphics adapter, and a graphics monitor. To print the screen, an IBM compatible graphics printer is required. The program was tested on two IBM-PC-ATs, one with a CGA adapter and one with an EGA, and in both cases it worked as expected. The printers used were an Epson FX-80 and an Epson LQ-850 and both produced satisfactory output. The program was also run on a KAYPRO-PC clone with a monochrome graphics monitor and two floppy discs. The program ran at both the standard (4 MHz) and high speed (8 MHz) of the KAYPRO and the speed of calculation was especially satisfactory at high speed. The printout of the screens was inadequate with an OKIDATA-92 printer (an unmodified version with the original ROM). It seems that

close compatibility with the IBM graphics standard is required in the printer. The program is reasonably fast but it is regrettable that it is incapable of recognizing and using the coprocessors with which all three computers were equipped (80287 and 8087-2). There also is no option to use a plotter and such an interface would be most desirable for production of publication quality output.

At its reasonable price, PROSTAT is a worthwhile purchase and the manual is adequate. The program passes my personal test for user-friendliness in that the manual is hardly used at all after initial tests. In fact one of my colleagues has used the program for months without the manual. Nonetheless, the lack of an index is a real nuisance. Another irritation is cursor movement since it is necessary to retrain oneself to use function and letter keys rather than arrow keys. The addition of optional arrow keys and also a mouse interface, both for cursors and menu selection, would much facilitate the use of the program. There are more general programs but, for its stated purpose and for its price, PROSTAT can be recommended both for research and applied chemistry.

The manual has a few typographical errors, none of them serious although the use of the word data is sometimes a little inexact. There are limitations and omissions which one would like to see dealt with in a future version. The ability to temporarily return to DOS and the addition of messages like "Press any key to go on" at several points would be appreciated. A fairly major limitation lies in the small choice of least-squares weights: an expansion of the choices or, better, the ability to define a weighting function or to use a precalculated weight vector would be appreciated. The ability to experiment with different orders of fitted polynomials is very useful and it is possible to go back from a higher polynomial to a lower when the addition of extra terms proves unnecessary, but the menu option, Review last equation, is confusing. One could perhaps wish for some expansion of the explanations of statistical tests but it must be admitted that is probably unreasonable to expect the authors to write a statistical textbook as well as a program manual.

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Enzfitter, A Non-Linear Regression Data Analysis Program for the IBM PC, By Robin J. Leatherbarrow. BIOSOFT: P.O. Box 580, Milltown, NJ 08850. $249.

Enzfitter is a nonlinear regression program that fits nonlinear functions of the form $y = F(x)$ by use of Marquart's algorithm. Simple linear regression is also supported. It requires an "IBM PC or compatible computer with a minimum of 384K memory". A graphics display adapter is required and the choice of adapters is complete (Hercules monochrome, CGA, or EGA). Printer support is not extensive, comprising the Epson FX80 and the Hewlett Packard Laserjet (and their compatibles or emulators), and a simple daisy wheel printer mode in which no control codes are passed. Two types of plots are supported, medium and high resolution. High-resolution plots require 512K of RAM and it is claimed that a resolution of 1920 × 1600 can obtained. The absence of plotter support is a significant omission.

Enzfitter is supplied on two 5.5 in. floppy diskettes, and the program is not copy protected. Source code is not provided. Math coprocessor support is not claimed, nor does it appear to be provided. The installation instructions are very clear and should be easily followed by a novice. A 91-page spiral-bound manual *without* an index or a separate listing of command functions is provided. This omission is a major annoyance for the casual user who needs detailed information about the program during a session.

Enzfitter is supplied with a number of canned routines presumably of immediate interest to biological scientists. These include programs to fit experimental data to Michaelis-Menton kinetics, first-order rate equations, pK_a determinations, ligand binding to one and two sites, and various exponential decay expressions. Provision is made for defining other functions, directly entering experimental data, or importing ASCII files with a space as the delimiter. Keyboard entry of data is supported.

Initial starting values must be supplied unless a linearized form of the function can be obtained and programmed. In that case, the Enzfitter uses the linearized form to calculate the initial values needed for the nonlinear regression. A number of preprogrammed linear transformations are provided, including Scatchard, Eadie, Lineweaver-Burk, semi-logarithmic, and linearly transformed pK_a plots.

This program has some very nice features. It is reasonably user friendly and operates either from the command line of from a main menu system which branches to either of two submenus. Pop-up help screens which describe the various menu choices are always available by pressing F1. Within an hour or two after first using Enzfitter, one can easily churn out the results of the regression analysis in tabular form and produce high quality graphics using the canned programs. Only a brief reading of the manual supplied with the program is required for using the program at this level.

It is possible to add to the list of functions that can be subjected to nonlinear regression analysis. The syntax is superficially BASIC-like and the usual algebraic and square, square root, exponential, logarithmic, and circular functions are supported. Inverse circular functions and hyperbolic functions are not supported. However, the procedure for defining a new function is an unfamiliar one to me. Unfortunately, the manual explains how to proceed with use of a single example, which makes the learning process unduly painful. The explanation of the various terms used is, at times, obscure and best deduced, as the author recommends, by examining the various example programs, a procedure which unnecessarily increases the difficulty of learning how to add new functions. Be prepared to invest a fair amount of time learning how to add custom functions.

The on-screen plots produced within the program are visual gems with an EGA monitor, and Enzfitter's "print screen" function produces high-quality plots with a laser printer. It is easy to insert text into plots and change plotting symbols, colors, and the line characteristics of the regression plot. Three methods of controlling plotting ranges are provided: axis ranges supplied by the user, automatic scaling to display only over the range of the data, and automatic scaling from 0 to the maximum value of the data. My only reservation about the graphs that result arises from the lack of user control in the placing of tick marks on the axes. An especially nice feature is provision for adding complete smaller plots with labeled axes within the boundaries of the large plot. This permits displaying other data related to the main plot, such residuals versus either variable or a linear transformation of the data set.

The program was tested on an IBM AT (80286, 7 MHz), a NEC ABC IV (AT compatible, 8 MHz), a PC Designs compatible (8088, ~ 8 MHz), and a IBM PC (8088, 4.77 MHz). All had EGA monitors. No difficulties were discovered. A 24 pin dot matrix printer emulating an IBM Graphics printer (Toshiba P351), an Epson F86 18 pin dot matrix printer, and a laser printer emulating a HP Laser Jet were used to produce plots from the screen display of regression results using the program's "print screen" function. While the laser copy was superior, the dot matrix product was also quite good. The time to print the screen display is about 50 s on both the AT-class machines mentioned above for either printer. The laser output produces a medium quality plot, which is acceptable for most purposes. High-resolution plots were made by using the laser jet emulation of the HP Laser Jet and a Epson F86. A special plotting program, which must be entered after exiting the main program, must be used. The time for the high-resolution plot was 9 min on the IBM AT and a laser printer and 35–37 min on a 4.77 MHz PC and dot matrix printers. The time required for output appears to be processor, not printer speed, controlled. Error messages seemingly unrelated to actual errors appeared several times during the high-resolution plotting mode. This required manual intervention to continue the plotting procedure. The quality of the high-resolution laser plots was superb, and the dot matrix output was excellent.

The tabular output of the regression equation is also well-organized, providing the values of the regression coefficients, their standard error, and the input data and the calculated value of the dependent variable. Chi squared is available only from the screen display. Data are rounded to the fifth decimal place. The few comparisons I made of results obtained with ENZFITTER in the nonlinear fitting mode to treat linear regression problems with a conventional linear regression program agreed at this level. The advertising claim that Enzfitter is "The ultimate curve-fitting package for the IBM PC" is hyperbola. The fundamental framework for such a program exists but has not been implemented. It is unfortunate that polynomial regression and multilinear regression is not supported, as is the ability to plot a data set without assuming a specific functional form. If this were possible, Enzfitter would provide, within a single program, a comprehensive solution to obtaining publication quality graphs for all the commonly occurring plotting situations. Overall, Enzfitter is a very nice program for fitting and plotting experimental data with nonlinear regression, although it is a bit expensive.

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