Computer Software Reviews

KaleidaGraph: Graphing and Data Analysis. Version 3.5 for Windows. Synergy Software, 2457 Perkiomen Ave., Reading, PA 19606-2049. www.Synergy.com. $155.00

KaleidaGraph is a data analysis and graphing program for use with the Windows and Macintosh platforms. A PC with 192 MB of RAM with a Pentium III 700 MHz processor running Windows 98 was used for the present evaluation. The minimum requirements are a 486 processor, 16 MB RAM, Windows 95, and 4 MB free hard disk space.

KaleidaGraph comes with a 10-minute quick start guide that shows the user everything needed to get started. Included in this guide are data import options that facilitate data entry for plotting. The plotting capabilities are standard. Data analysis allows for basic statistics, basic curve fitting, and simple calculations as well as dynamic links to Microsoft Excel. To augment these data analysis capabilities, user-defined curve fits and macros can be written and implemented within KaleidaGraph. Complete and flexible page layouts containing plots, tables, and text can be created. Overall, this product provides a cost-effective way of creating presentation/publication-quality figures.

Data can be imported from Microsoft Excel, from a text file or a binary file, but was difficult from an ASCII file. Data analysis includes nine standard curve-fit types, such as linear, polynomial, and exponential. Additionally, an extensive user-defined curve-fit library exists with functions such as erf and erfc. Equations can be displayed on the graph and/or exported to perform further analysis. Basic statistics can be performed on a set of data to return mean, root-mean-square, standard deviation, variance, skewness, and kurtosis. In addition, a Student's *t*-test can be used to compare sets of data, and results can be sent directly to the clipboard to paste elsewhere or to save. Several useful macros exist, such as numerical integration and differentiation. The user can also add macros to perform specific tasks. Last, unlike some graphing programs, simple algebraic manipulations can be done directly in the data worksheet using the formula entry window.

After the data are loaded and analyzed, plotting options are routine. A variety of line and scatter plots exist that allow for double *x*, double *y*, and double *xy* plots. Adding multiple traces to a plot was especially straightforward, although it was not possible to offset the traces to allow the reader to view all data clearly. Other types of plots include statistical, polar, bar, pie, function, and text. The program allows the user to control nearly all features of the graph. For example, subscripts and superscripts can be used in the text labels. No contour or 3-D graphing options are available, however.

Page layouts allow the user to display plots, tables, and text in a suitable manner for publication or presentation. Multiple graphs can be placed on a single page layout to allow for multiple panels in a figure, and inset plots can be made by resizing and overlaying the graphs within the page layout window. Page layouts can be printed, exported as TIF, BMP, PICT, JPEG, GIF, etc., or pasted into other applications. Exporting plots is similar to page layout export. Plots can be exported as TIF, BMP, PICT, JPEG, GIF, etc. and then pasted into other applications. Last, EPS files can be created from plots using the print driver.

Additional features include scripting and template graphing. These two commands are similar and allow the user to automatically create graphs with new data in the form of a pre-existing graph. This feature should be useful in scientific or engineering work where the same type of data is collected and plotted frequently. The data can simply be imported into KaleidaGraph, and the template plot or script creates new plots without user interaction. Error bars, curve fits, axis labels, and formats are automatically reproduced from the script or the template graph.

Overall, KaleidaGraph provides a cost-effective way for basic data analysis and graphing. KaleidaGraph interfaces well with other applications, is easy to use, and creates publication/presentation-quality output.

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Book Reviews *

Topological Indices and Related Descriptors in QSAR and QSPR. Edited by James Devillers (Centre de Traitement de l'Information Scientifique, Rilleux La Pape, France) and Alexandru T. Balaban (Polytechnic University Bucharest, Romania). Gordon and Breach Science Publishers: Amsterdam. x + 811 pp. $198.00. ISBN 90-5699-239-2

This is an excellent book that covers a controversial topic for investigators in the field of quantitative structure activity relationships (QSAR) and quantitative structure property relationships (QSPR), namely how best to describe a chemical structure numerically. For this, one typically uses physicochemical descriptors (partition coefficient, molar refraction, dipole moments, quantum chemical indices, van der Waal radii, etc.) or topological indices (Wiener index, Hosoya index, Zagreb group indices, centric indices, Randic and Kier-Hall molecular connectivity indices and their derivatives, etc).

There is repetition in the 17 chapters of this lengthy book because most authors provide overviews of various techniques, particularly the first generation of topological indices that lay the foundation for the particular method described in the chapter. The repetition is welcome, however, as it allows the reader to treat each chapter as a separate review. Moreover, several of the authors have written more than one chapter, which results in more continuity than one normally expects in a multiauthored book. Taken together, this compilation is very comprehensive.

The editors have done a good job of selecting the authors and arranging the chapters in a logical order. The opening chapter presents a historical overview and can be thought of as an abstract for the entire book. This is followed by four chapters on different aspects of graph theory. The next three chapters focus on molecular connectivity descriptors that are the most common of the topological indices used in QSAR and QSPR. How topological indices can be used to indicate shape and electronic environment is the focus of Chapters 10−12, whereas specialized approaches, like DARC and neural networks (which are also used with physicochemical descriptors), are emphasized in Chapters 13−16. The book's final chapter presents an overview of relevant algorithms and software; importantly, most methods for obtaining topological indices can be done using a desktop computer and fairly inexpensive software.

Several authors emphasize that the impetus for development and subsequent refining of topological indices comes from the demand in the pharmaceutical and agricultural chemical industries for ways to screen and predict activity rapidly. Moreover, the development of combinatorial chemistry has added to the need for building diversity into chemical libraries and "mining" large chemical databases for compounds with specific characteristics. Topological descriptors are relevant to this because they are an easy way to describe a molecule in numerical form. Topological indices, on the other hand, do not require carefully measured physicochemical descriptors, nor do they present the problem of reproducibility between laboratories.

Nearly every chapter points out that a molecule can be treated as a graph with atoms (points) interconnected by paths or edges. Refinements for developing graphs are presented that differentiate between elements, note the hybridization of atoms and presence of nonbonding electrons, recognize degrees of unsaturation, and acknowledge conformational properties. Also, while the final QSAR and QSPR equations are given in some chapters, there is minimal discussion describing how the equations are developed and evaluated. This is important because many of the algorithms generate large amounts of data, and collinearity can be a problem.

*Unsigned book reviews are by the Book Review Editor.

Some of the authors address the problem that topological descriptors provide little information that would help the chemist understand what structural components determine activity. It is very difficult—some say impossible—to design new molecules based on a QSAR equation that only uses topological indices for descriptors. Because of the aforementioned ability of algorithms to generate large amounts of data, some of the authors use principal component analysis to reduce the dimensionality or cluster the indices leading to some type of hierarchal treatment.

The book has a good index, and all of its chapters have extensive bibliographies that span the era from when a technique was first introduced to the late 1990s. Whether or not a chemist uses topological indices, all who use QSAR or QSPR should consider purchasing this book. It definitely is a resource that belongs in libraries.

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Biosynthesis: Aromatic Polyketides, Isoprenoids, Alkaloids. Topics in Current Chemistry. Vol. 209. Edited by Finian J. Leeper (University of Cambridge) and John C. Vederas (University of Alberta). Springer-Verlag: Berlin, Heidelberg, New York. 2000. viii + 247 pp. $159.00. ISBN 3-540-66573-0.

This is the second of two volumes emphasizing the powerful combination of molecular biology, stable isotopes, and NMR spectroscopy to study biosynthetic pathways leading to aromatic polyketides, terpenoids and alkaloids. Each chapter constitutes a critical review written by an active researcher in the field.

In Chapter 1, Shen reviews the genes encoding aromatic polyketide synthases (PKSs) in bacteria, fungi, and plants. A very detailed and useful discussion of the enzymology of selected synthases is provided, and the chapter concludes with an up-to-date account (including references to works published in 1999) of the mixing and matching of PKS genes leading to novel products and the concept of combinatorial biosynthesis.

In Chapter 2, Davis and Croteau discuss terpene synthases including mono-, sesqui-, and diterpene cyclases. The enzymology and mechanistic details are well covered, though this is such a rapidly expanding field that many discoveries have been made during the last year and could not be included.

The remaining three chapters—somewhat more specialized—are concerned with alkaloids and begin with a review by Williams et al. on prenylated tryptophan-derived compounds. In this particular field of biosynthesis, the molecular biology has not yet been developed, so that most of the results come from feeding experiments rather than enzymology.

This is also the case for the tropane alkaloids reviewed by Hemscheidt and is largely true for the final chapter on pyrrolizidine alkaloids by Hartmann and Ober, although some gene sequences are now emerging for this class, and we can expect similar progress for the other alkaloid families reviewed in Chapters 3 and 4.

Overall, the authors have covered their chosen areas in considerable depth while retaining the critical outlook necessary for interpretation of biosynthetic mechanisms based on incorporation. Together with the first volume, which covers the biosynthesis of enzyme cofactors, vitamin B_{12}, and reduced polyketides, the editors Leeper and Vederas have provided the general and specialist reader alike with nearly current coverage of natural product biosynthesis. It is hoped that several further volumes covering other vistas of the natural product landscape will emerge in due course.

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JA0047626

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Spectral Data for Highly Ionized Atoms: Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr, and Mo. Journal of Physical and Chemical Reference Data. Monograph No. 8. By T. Shirai, J. Sugar, A. Musgrove, W. L. Wiese (National Institute of Standards and Technology). American Institute of Physics: Melville, NY. 2000. iv + 632 pp. $145.00. ISBN 1-56396-934-3.

This book is a compilation of spectroscopic data on energy levels, wavelengths, ionization energies, and oscillator strengths for ionized forms of the title elements. Each chapter begins with introductory comments for each atom being investigated, and these are followed by tables of spectral data and an extensive list of references.

JA004794T

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Seminars in Organic Synthesis. XXV Summer School "A. Corbella", June 12−16, 2000, Palazzo Feltrinelli, Università degli Studi di Milano, Gargnano (BS). Società Chimica Italiana, Divisione di Chimica Organica: Rome. 2000. 584 pp. ISBN 88-86208-15-4

This book presents the extended lectures given by invited speakers of the 25th summer A. Corbella summer school. The topics are organized under the following headings: New Classes of Pharmaceutically Active Compounds; Recent Advances in the Field of Organometallic Chemistry; Recent Advances in the Field of Radical Reactions; Stereoselective Synthesis of Natural Products; and Critical Surveys Covering the Year 1999.

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Chemistry in the Marine Environment. Issues in Environmental Science and Technology. Edited by R. E. Hester (University of York) and Roy M. Harrison (Univeristy of Birmingham). Royal Society of Chemistry: Cambridge. 2000. xiv + 98 pp. $49.00. ISBN 0-85404-260-1

The five chapters of this book provide a multidisciplinary approach to addressing some of the special issues currently facing marine chemistry. In its Introduction and Overview are discussed the unique challenges of applying fundamental chemical principles to the vast and compositionally complex subject represented by the ocean. It is within this context that the remaining chapters of the book—The Oceans and Climate; The Use of U−Th Series Radionuclides and Transient Traces in Oceanography: an Overview; Pharmaceuticals from the Sea; and Contamination and Pollution in the Marine Environments—are presented. The book contains references that are current to the late 1990s and should appeal to a variety of environmental scientists and policymakers.

JA0047828

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Houben-Weyl. Organo-Fluorine Compounds. Workbook Edition E10a. Edited by Bernd Baasner (Leverkusen), Hermann Hagemann (Leverkusen), and John C. Tatlow (Birmingham). Georg Thieme Verlag: Stuttgart. 2000. xviii + 746 pp. $199.00. ISBN 3-13-116664-9

This paperback edition of the Houben-Weyl E10 series serves as an introduction to organofluorine compounds and includes articles on their history, nomenclature, physical and physicochemical properties, elemental analysis, structure determination, toxicity, and applications. It also includes several articles on various fluorinating agents that are used to make C−F bonds.

JA004789P

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