Computer Software Reviews

ChemPrep. Institute for Scientific Information: 3501 Market Street, Philadelphia, PA 19104. Telephone: 1-800-336-4474. Fax: 215-386-6362. http://www.Isinet.Com. List Price for 1985−1997 databases: \$11 750 (1 user) and \$21 500 (2−5 users). 1998 subscription price \$2450 (1 user) and \$4250 (2−5 users).

ChemPrep is a database set for Windows containing new synthetic methods, heralded by ISI as “a reaction database and current literature awareness tool”. The current complete package consists of five separate CD-ROM’s (one each for 1985−1989, 1990−1992, 1993−1994, 1995−1996, and 1997), and a subscription can be taken for updates. Each database can either be installed on a hard drive (1.8 GB for all five), for faster access, or read directly from the CDs after installing minimized database files (60 MB for all five). The database is updated quarterly. At the present time, ISI has no concrete plans for additional pre-1985 databases.

Once installed, the program is user-friendly. Each menu and option is explained in the detailed online manual. The manual uses graphical examples to demonstrate each point, which is a considerable aid for the novice user. The reviewers had no difficulty in performing successful searches within 15 min of installing the software.

The first search option is “article search”, which allows the user to query each database by author, author institution or address, publication year, article title, reaction descriptor, author keywords (available 1992 to the present), and ISI’s expanded “keywords plus” (also available 1992 to the present). However, in our own search for relevant articles published by one of the authors of this review in one review period, we found two missing that we felt were highly relevant (out of nine that were absent).

The “keywords plus” field expands upon the keywords provided by the article author by abstracting keywords from the article titles, not always relevant, listed as references for the article (using data from another ISI product: *The Science Citation Index*), providing a much wider listing. To obtain the highest number of hits, one should search both the “author keywords” and “keywords plus” fields for the same terms simultaneously using the provided “or” operator. Most of the search fields have a “phrase” option, which allows the user to quickly scan the relevant terms alphabetically for faster access. Once the desired fields are identified, the actual search is very fast, even in reading from the CD-ROMs. Keyword searches of “article titles” as well as searches of the “author keywords” and “keywords plus” fields can be performed by using truncated words (denoted with an asterisk), which greatly simplifies the use of this program.

The second text search option is “reaction search”, which allows for query of the database by specific reaction conditions such as catalyst, solvent, temperature, time, yield, pressure, and reaction key phrases (e.g., erythro selective). The “catalyst symbol” field is somewhat of a misnomer, as it encompasses all of the reagents used for a given transformation. Again, most fields have a “phrase” option that aids in finding specific reagents quickly. Unfortunately, the nonuniform abbreviation of reagents in the literature has translated into the ChemPrep abstracting as well (e.g., titanium isopropoxide is notated as $Ti(OiPr)_4$, $Ti(OPr)_4$, and $Ti(OPr\text{-}i)_4$), so one must be careful to consider all possible variations in denoting a reagent or compound to be certain of the best search results. This potential problem can be averted by using the “phrase” option to identify multiple search terms for the same field. The “reaction search” option can be combined with the “article search” option to form the “entire data search” option, which the reviewers found to be the most useful method for text based searches.

To complement the text search fields, ChemPrep also contains a “structure search” mode that allows for searches by exact structure (for finding a specific compound) or by partial structure (for finding related compounds). The desired structure is entered through a separate drawing module, similar to other available chemical drawing programs. The drawing module is quite intuitive, and contains predrawn functional groups and simple rings for added speed. Additionally, any atom in the structure may be variably defined (X for halogens, M for metals, A for all atoms other than hydrogen, and Q for all atoms other than carbon or hydrogen). While the structure search module is more time-consuming, an average structure search requires only 2 to 5 min per database.

Once a search is completed, the results are displayed in a split screen format with the author, title, and other bibliographic information in one window and the synthetic schemes in a second window. Key steps are highlighted with detailed conditions and yields. References to relay procedures are also provided where appropriate. Some reagents are abbreviated in a less than obvious manner, but this seems to be another undesirable carryover from the chemical literature. When a search yields multiple results, a control at the bottom of the screen advances from article to article manually, or another control advances between articles automatically. Results of the search can be printed, either article by article or as an entire search. The bibliographic text can be adjusted (font and size) to suit the user. Unfortunately, the text and graphics of the synthetic schemes are not adjustable and are quite small.

Additionally, the option to browse the database by journal title and issue from quarterly updates effectively gives the user an online version of another more widespread ISI product: *Current Contents*.

All in all, ChemPrep represents a powerful tool for both searching and keeping up with the current literature. In many ways, ChemPrep resembles the Beilstein database, but is more accessible (albeit less comprehensive) since the ChemPrep user owns the database files, rather than accessing them through a network or modem connection. In addition, the ChemPrep database is smaller, since it concentrates only on synthetic methods, rather than providing all data and properties for compounds as the Beilstein database is designed to do.

Brant J. Chapman and Michael P. Doyle, *University of Arizona*

JA985632O

S0002-7863(98)05632-7

Book Reviews

Humic and Fulvic Acids: Isolation, Structure and Environmental Role. Edited by Jeffrey S. Gaffney and Nancy A. Marley (Argonne National Laboratory) and Sue B. Clark (Washington State University). American Chemical Society: Washington, DC. 1996. \$109.95. xii + 338 pp. ISBN 0-8412-3468-X.

Humic and fulvic acids are predominant forms of organic matter in natural waters and have important environmental consequences and impacts. This large and complex class of compounds is a major organic carbon pool in terrestrial and aquatic ecosystems. Although humic substances have been intensively studied during the last century, much is unclear about their chemical structure and reactivity. The symposium volume reviewed here presents recent results from internationally recognized experts summarizing advances in the elucidation of the structure and chemical reactivity of humic and fulvic acids.

Chapters are divided into themes following the subheading in the title, which are (1) Overview, (2) Chemical Characterization and Structural Determination, (3) Metal Binding, and (4) Organic Pollutant Interactions. Several chapters summarize results of recent or long-term research efforts. Others examine application of sophisticated analytical procedures to isolate, identify, and characterize humic and fulvic acids. Comprehensive overviews of specific characterization techniques are given and are integrated with past work. Chapters are well illustrated with excellent quality figures and tables. There are three indexes: an author index, an affiliation index, and a thorough subject index. References are timely; most chapters have references up to about 1993, with some to 1995.

A theme of the monograph is the importance of humic and fulvic acid reactivity in understanding radionuclide migration in the environment. This research topic has lacked reference materials for intercomparison of different characterization methods. However, several researchers in this monograph use reference materials recently made available through the International Humic Substances Society (IHSS).

The first chapter presents a brief overview of humic and fulvic acids and colloidal organic materials in the environment. The following two chapters examine the nature of humic colloids and use of hollow-fiber ultrafilters for humic and fulvic acid isolation. Hollow-fiber ultrafilters are reported to minimize humic and fulvic acid isolation problems associated with use of XAD-resins or sodium hydroxide processing. Use of hollow-fiber ultrafilters is recommended by the authors for isolation and size fractionation of humic and fulvic acids in surface water and groundwater. However, the authors point out that this method assumes a spherical structure for humic and fulvic acids for the separation cutoffs and is, therefore, an empirical approach.

The following eight chapters summarize chemical characterization and structural determination techniques. Procedures described include nuclear magnetic resonance (NMR), reflectance infrared spectroscopy, fluorescence spectroscopy, and liquid chromatography. These chapters are noteworthy for the wide range of approaches used to characterize the chemical nature of humic substances. Six subsequent chapters examine the importance of humic substances−metal binding reactivity, including transport of radionuclides (Chapter 16). Methods presented include UV-scanning ultracentrifugation to determine humic and fulvic acid molecular weights and to investigate changes in aggregation brought about by metal ion complexation. Metal binding affinity varies among humic substance fractions.

Some interesting presentations include Chapters 13 and 14. Chapter 13 summarizes trivalent ion−humic substance interaction kinetics. Humic acid−metal binding kinetics involve a range of reaction rates, with more rapid reaction rates associated with lower molecular weight fractions. Similar kinetic results were observed for size-fractionated humic acids and poly(acrylic acid). Chapter 14 examines humic material characterization using isotopic techniques to determine the significance of groundwater colloids in the transport of radionuclides. The authors report that differences between humic acid and fulvic acid fractions suggest different sources of the two organic carbon fractions. Two subsequent chapters also address questions of radionuclide migration in the environment.

The final two chapters examine humic acid and fulvic acid interactions with organic pollutants. Chapter 19 describes use of ^{15}N NMR to study aniline covalent binding to humic substances. Aniline incorporation into natural organic matter is reported to resemble noncatalyzed nucleophilic addition reactions. These investigations are important because there is concern that aromatic amines may be released by incomplete industrial waste treatment. Use of ^{15}N NMR may have broad utility for investigations of aromatic amine covalent reactivity with organic matter in the environment.

The monograph is recommended for scientists studying humic and fulvic acid mediated reactions in the environment. It may also serve as an auxiliary text in an upper undergraduate or graduate level course dealing with the structure and reactivity of natural organic matter.

Michael M. Reddy, *U.S. Geological Survey*

JA9756782

S0002-7863(97)05678-3

Prolyl Hydroxylase, Protein Disulfide Isomerase, and Other Structurally Related Proteins. Edited by Norberto Guzman (The R.W. Johnson Pharmaceutical Research Institute). Marcel Dekker, Inc.: New York, Basel, and Hong Kong. 1998. xvii + 530 pp. $185. ISBN 0-8247-9831-7.

Protein disulfide isomerase (PDI) was discovered over 30 years ago; however, it is only recently that this protein has received substantial attention. Over the past several years, this protein has assumed a high profile as a result of its role in assisting in protein folding occurring in the endoplasmic reticulum by catalysis of disulfide rearrangements in these proteins. This role for PDI has been shown to be essential to the viability of yeast cells. This book intends to provide an overview of the current state of knowledge in the field of PDI-related biochemistry. The contributors are acknowledged experts in their fields and provide, for the most part, clear understandable explanations for those not intimately involved in the field.

As the title of the book implies, the coverage spans PDI and the proteins prolyl hydroxylase and microsomal triglyceride transfer protein which have been shown to have PDI as a subunit. The first five chapters focus on prolyl hydroxylase, and Chapter 16 focuses on microsomal triglyceride transfer protein. Although these represent excellent accounts of the properties of these proteins, the connection to the remainder of the volume is unclear. The exact role of PDI in these enzymes is not clear, and the relevance to PDI's role as a protein disulfide isomerase or as a chaperone has not been established. The focus and organization of the book would have been better served by focusing only on PDI and its role as a protein disulfide isomerase and as a chaperone.

The remainder of the volume presents a wide range of articles on the biochemical properties and functions of PDI. Although no grouping of articles has been utilized, the remainder of the articles in this book can be loosely grouped in several categories on the basis of their focus. Chapters 7 and 18 provide a basic introduction to the family of protein disulfide oxidoreductases and PDI, in particular. The relationship between thioredoxin and PDI, in particular the redox chemistry catalyzed by both, is well-covered in Chapters 11 and 21 by A. Holmgren and R. Raines. The role of PDI in protein folding is discussed in Chapter 13 by H. Gilbert, which, along with Chapter 21 by Raines, presents outstanding descriptions of the redox chemistry involved and the role of PDI in protein folding. These should be required reading for anyone working in the field of protein disulfide oxidoreductases. Chapters 12 and 14 provide a provocative discussion of PDI's interaction with peptides and potential role as a chaperone for protein folding. Chapters 15 and 20 provide a discussion of the possible role of PDI as a storage protein for calcium. Chapters 8−10 provide coverage of novel regulation behavior of PDI. Chapters 6, 17, and 19 cover unrelated topics involving plant PDI, the role of PDI in viral entry into cells, and a PDI-related protein involved in cell signaling. The final chapter, 22, provides a useful overview of the applications of PDI for enhancing the production of recombinant proteins.

An index is provided which is helpful in identifying specific areas of interest. All of the articles provide detailed sets of references which make the book a very useful reference guide to lead one into this area. A clearer organization of the articles to group them according to focus and an effort to reduce duplication among the articles would have provided an even better presentation. For both the neophyte and the experienced investigator, this book provides an excellent review of current research regarding PDI and a very useful reference guide.

John Bushweller, *Dartmouth College*

JA975674X

S0002-7863(97)05674-6

Methods in Enzymology Volume 284. Lipases: Part A, Biotechnology. Edited by B. Rubin (Lipomed) and E. A. Dennis (University of California−San Diego). Academic Press: San Diego. 1997. xxxi + 408 pp. $99.00. ISBN 0-12-182185-4.

Lipases constitute a large and broad group of esterases that act on lipidic substrates that do not disperse as monomers in aqueous solutions. In spite of physiological, pharmacological, and industrial importance of interfacial enzymes, basic understanding of these enzymes has lagged compared to those of their cousins that act on monodisperse substrates in aqueous solutions. The knowledge gap has narrowed in recent years, and the subject has been reviewed in numerous edited books.

The scope of this volume is limited to some of the better characterized primary and tertiary structural features of selected triglyceride lipases. The individual articles are written by experts in the field with emphasis on isolation, assay, cloning, and expression. The volume could be useful for beginners who wish to find procedures and references for specific manipulations. The results reported in these articles have limited value because such procedures are notoriously specific for a particular enzyme and substrate used under a specific set of assay conditions. With the appreciation of such a limitation most articles do not even try to identify a general trend.

Mahendra Kumar Jain, *University of Delaware*

JA9756679

S0002-7863(97)05667-9