Book Reviews*

Combinatorial and High-Throughput Discovery and Optimization of Catalysts and Materials. Edited by R. A. Potyrailo and W. F. Maier. CRC Press, Taylor and Francis Group: Boca Raton, FL, U.S.A. 2007. £115 (hard back). 467 pp. ISBN 978-0-8493-3669-0.

This book is a series of monographs in molecular diversity and combinatorial chemistry, high-throughput and associated technologies. The general conclusion is that high-throughput screening approaches can assist in rapid advancement in many areas of materials science, covering topics as diverse as heterogeneous catalysis to aid in combustion of waste gases to phosphors for flat screen displays.

The book has limited appeal for organic process research and development chemists but does give interesting insights into the diversity of materials under investigation for many applications joined by the common theme of using combinatorial approaches and high-throughput experimentation. Each of the 23 chapters is well written with an informative introduction, an outline of the techniques applied, and a conclusion.

The lack of colour diagrams and illustrations is a weakness in the book, with some chapters referring to the (absent) colours within a diagram.

John Knight

Scientific Update LLP, Maycroft Place, Stone Cross, Mayfield TN20 6EW, U.K.

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Microwaves in Organic Synthesis, Volumes 1 and 2. Edited by André Loupy. Wiley-VCH, Verlag GmbH and Co. KGaA: Weinheim. 2006. \$375. Vol 1, 517 pp, Vol 2, 466 pp. Hard back. ISBN 978-3-527-31452-2.

This two-volume series is an updated and expanded version of the initially prepared series, with the addition of eight new fields of application. It is clear from the concluding remarks in many of the monographs that, whilst there has been significant expansion in the interest and application of microwaves across many sectors of the chemical industry, the field is still developing and movement from laboratory-scale utilisation to larger-scale operation remains to be adequately addressed.

Overall the two volumes cover a wide array of chemistry and areas of application.

Volume 1 (Chapters 1-10) starts with the history of microwaves and their pre-WWII discovery through to some

commercial applications and an overview of the theory of microwaves and their impact on molecules. For many organic chemists, the theory may be too extensive, and such depth or detail may not be warranted. However, later chapters in both volumes provide more basic outlines of the basis for microwave interaction with molecules at which point the information contained in Chapter 1 becomes more relevant and helpful.

Chapter 2 is very useful in outlining the development of commercial systems, including larger-scale options. It comments that, owing largely to the depth of penetration of microwaves being less than decimetres in classic reaction solvents such as water and alcohols, the application of microwave technology to batch reactors of several thousand liters capacity is not likely. Instead, continuous flow is required, and currently applications are best found in product drying.

Chapters 3–5 then follow to (a) discuss organic chemistry in pressurised reactors, (b) the cases where the impact of microwaves is not simply thermal (the chapter presents many different reaction types wherein microwave enhancements are noted in rate/yield which can be ascribed to the impact derived from the presence of polar transition state), and (c) reviews of selectivity and provides a series of examples from a broad array of reaction types where the microwave-assisted chemistry has behaved differently.

Having provided the basis for microwaves, their application in chemistry, and how microwave irradiation can influence reaction rate and selectivity, the remaining five chapters of Volume 1 and subsequent 12 chapters of Volume 2 present up-to-date overviews of the major areas where microwave synthesis is being applied to a wide range of research interests in organic chemistry.

The chapters are well written with many examples in each to illustrate the impact of microwave irradiation in organic synthesis. The recurrent theme is one of faster reactions, lower side-product liability, and reduction in energy consumption. Presently there are only limited examples of significant upscaling of chemical reactions under microwave assistance so a conclusion of many of the chapters is that, with an ever-increasing array of chemical applications and the need to improve speed to market coupled with waste/ energy minimisation, there is an obvious driver to design and develop the tools to enable larger-scale applicability. There are several chapters likely to be of particular interest to process development chemists, including phase transfer catalysis, heterocyclic chemistry, cycloadditions, catalysis, transition-metal catalysed cross-coupling reactions, and multicomponent reactions. Other chapters are also very informative and equally well written, providing interesting insights into preparation and use of ionic liquids, combinatorial and

high throughput applications, solid-phase peptide synthesis, and extraction of essential oils.

Overall, each of the 22 chapters is well written with an informative introduction, an outline of the techniques applied, and a conclusion, providing clear explanations to newcomers on the use of microwaves in organic synthesis as well as details and theory for the more experienced user of this technique. A key challenge for development chemistry is how best to assist in advancing the tools required for scaling up the technique as it looks set to be a standard laboratory-based operation applied to the synthesis of targets that subsequently demand production at larger scale.

John Knight

Scientific Update LLP, Maycroft Place, Stone Cross, Mayfield TN20 6EW, U.K.

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Pharmaceutical Substances, Syntheses, Patents, Applications. By A. Kleeman, J. Engel, B. Kutscher and D. Reichert. Online version 3.0. Price on application.

Pharmaceutical Substances is a compendium of more than 2300 of the most significant pharmaceutical compounds of industrial interest. It has been available in hard copy printed form for a number of years. The latest edition (4th) was published in 2001. It is now available in an online version accessible through the Internet as a web-based system (www.thieme-chemistry.com) and is updated on a regular basis (this version 3.0, updated in June 2007, is the seventh update since its launch in November 2003). The online version is the result of a project developed by Thieme Chemistry in collaboration with FIZ Chemie GmbH and InfoChem. According to the Web site, the online version of Pharmaceutical Substance confers many advantages over its print incarnation, making use of the latest developments in information technology. The stated aim of the electronic version of the product is to provide the user with a data source that can be accessed anywhere, at any time, using a standard browser interface. Further, it is reported on the Web site that not only is this product easy to access, it also provides the user with search facilities that allow them to rapidly screen the data for salient entries.

All of the information in the hard copy is provided in the online version. So for each drug the following information can be accessed: chemical structure, synthetic route, intermediates, nomenclature (INN standard, trivial names, synonyms), CAS registry number, ATC codes, medical applications/therapeutic category, toxicological data, patent information (number, origin, holder, and application date),

commercial information, bibliographic information (including CASSI codes). Furthermore, newly approved substances are added biannually. The bibliographic information provided is good, but the references would be much more useful if the titles of the papers and patents were also included.

As part of the review process the following aspects were examined:

- Getting started.
- Structure searching using the in-built Java Applet drawing package.
- Substructure searching, which included searching smaller fragments for intermediates contained within the reported routes of synthesis.
- Searching using other fields such as molecular weight, EINECS number, structural type (e.g., diazepines), pharmacological area (e.g., 5-HT, etc.)
 - Searches for salt counterions were also conducted.

First, getting started was simple with clear guidance, a good help section, and FAQs. The program is quite intuitive, so little use of the "getting started" notes is likely to be actually required.

In all cases the searches were very rapid and located appropriate hits based on the search. There are useful buttons to help scroll through multiple pages of data efficiently. However, it should be noted that text searching is less successful than structure or substructure searching; it is important to consider a number of ways to enter the text search, and use of the wildcard (*) is particularly helpful to maximise the chances of finding the contained references. For instance, a search for "polymorph" yielded only two hits, while "polymorphic" yielded four (different) hits and "polymorphism" two (different again) hits. A search using "polymor*" found 19 hits, which included all of the hits covered by the previous "full word" searches. Similarly, searching for "mesilate" or "mesylate" gave different results, but searching for "mes*late" covers the search more effectively.

Overall, the stated aims of the online version are met, although the text searching aspect was notably weaker and required a little effort to devise successful strategies. It is generally very user friendly and provides a useful reference source for those working in the pharmaceutical industry. I found the ability to search on a good variety of field types very encouraging (for example, to check for the use of napadisilate salts). If you already use and are familiar with the paper version, I think you will find the online version is a genuine advance.

John Knight

Scientific Update LLP, Maycroft Place, Stone Cross, Mayfield TN20 6EW, U.K.

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