

DICTIONARY OF  
MARINE NATURAL  
PRODUCTS  
with CD-ROM



Edited by  
JOHN W. BLUNT  
MURRAY H. G. MUNRO

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 Chapman & Hall/CRC  
Taylor & Francis Group  
Boca Raton London New York

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10 9 8 7 6 5 4 3 2 1

International Standard Book Number-13: 978-0-8493-8216-1 (Hardcover)

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**Library of Congress Cataloging-in-Publication Data**

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Dictionary of marine natural products with CD-ROM / editors, John Blunt and Murray H. G. Munro.  
p. cm.  
Includes bibliographical references and indexes.  
ISBN 978-0-8493-8216-1 (alk. paper)  
1. Marine natural products--Dictionaries. I. Blunt, John, 1942- II. Munro, Murray H. G. III. Title.

QD415.A25D529 2008  
615'.303--dc22

2007028673

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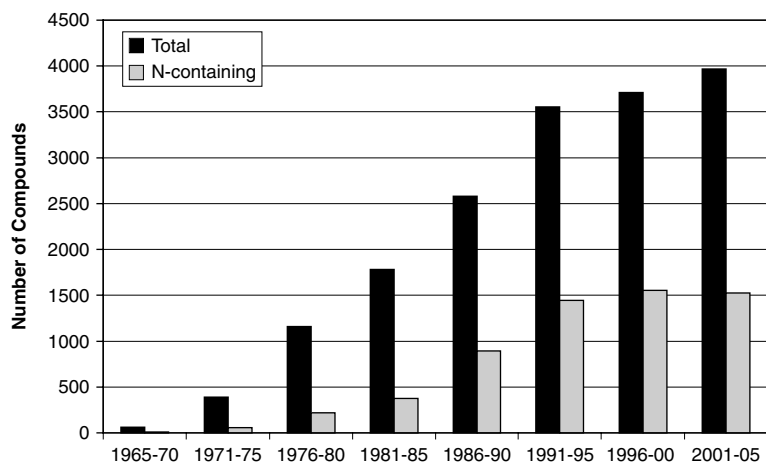
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# Preface

This production of the *Dictionary of Marine Natural Products* has been made in response to the growing importance of marine natural products (MNPs) as a subset of all natural product studies. Whilst the study of natural products has been a major focus of the discipline of chemistry for well over a century, most of the effort has been on those derived from terrestrial sources. This emphasis began to change after the 1950s when the impact and significance of Werner Bergmann's pioneering work on natural products from the marine environment was recognised. Bergmann started his work on MNPs in 1933 and published the 50<sup>th</sup> article in his "Marine Product" series in 1961. The work for which he is widely recognised was the isolation and characterisation in the early 1950s of the non-ribose nucleosides, spongthymidine and spongouridine, from the Caribbean sponge *Cryptotethia crypta*. Within a decade of these discoveries the biomedical importance of non-ribose nucleosides was being realised and the development of drugs such as Ara-C, Ara-A and AZT can be traced directly back to Bergmann's work. The delayed onset of more extensive research into MNPs was partly a consequence of the relatively limited access that biologists and chemists had to that part of the marine environment beyond the sub-tidal zones. This was remedied by the popularisation of SCUBA which dramatically enhanced the ability to collect in the aquatic environment as well as opening up possibilities for marine environmental chemistry. SCUBA was followed in turn by the use of ROVs and various submersibles that have allowed access to very much deeper water. Along with the enhanced collecting opportunities came the recognition that most of the biodiversity on earth was actually present in the oceans.

From the recognition of the importance of marine natural products in the 1950s the field progressed steadily with the next champion, Paul Scheuer, who played a dominant role from the mid-1960s until recently. Joining Scheuer as leaders in the field from the 1970s onwards were Ken Rinehart and John Faulkner (sadly, all three recently deceased). Further MNP studies from the 1970s onwards were assisted by advances in spectroscopic methods and separation science that allowed for the rapid isolation and characterisation of many new structural types. Since then the number of groups undertaking research in the area has grown rapidly, as reflected by the rapid increase in MNP publications and the establishment of MNPs as a separate focal point for conferences. Currently, studies on MNPs are carried out by a wide range of research groups (in excess of 150) scattered across at least 40 countries, but with many of the current leaders of the field able to trace an academic ancestry back to having worked for, or with, Scheuer, Rinehart or Faulkner. Over the years the number of new compounds reported has been rising steadily and is shown graphically below from 1965 until 2005. In 2006 814 new compounds were reported in 302 refereed publications. The total number of MNPs is now approximately 18,000.



Early investigations focussed on the diversity of chemical structures elaborated by marine organisms readily accessible to collectors, notably algae, sponges, tunicates and other invertebrates. The best illustration of this approach was the degree of attention that was focused on halogenated metabolites available from red algae (Rhodophycota). Genera such as *Plocamium* and *Laurencia* were readily available by shore wading, could be collected in relatively large amounts and the metabolites present were relatively non-polar and could be readily



extracted and separated by the conventional separation techniques available at that time (1970s). However, by the 1980s the focus of attention was switching to the role of these diverse structures in ecological interactions and especially to the potential of compounds of marine origin as pharmaceutical agents. Considering the dramatic start that Bergmann's discovery of the non-ribose nucleosides had on the biomedical role of MNPs some 20 years earlier, this preoccupation with non-polar non-nitrogenous compounds was a distraction. In John Faulkner's first review on marine metabolites (1977) covering the period 1974-6 only 10% of the metabolites covered were nitrogenous. However, for the period 1977-85 this figure had almost doubled to 19.5% with 332 out of 1706 metabolites containing at least one N. Long before Lipinski's "rule of five" had been enunciated it was well recognised that nitrogen was an important structural feature in bioactive compounds. Fortunately, rapid advances in chromatographic techniques and phases were occurring at this time that dramatically eased the problems of working on the (usually) more polar bioactive compounds. This move towards searching for bioactive compounds was a major driving force for the expansion of interest in MNPs and continues to provide a strong rationale for new discovery programmes. Structural elucidation aspects of MNPs continue as a core activity. With the advent of more sensitive NMR techniques, the mass requirements for obtaining good 1D- and 2D-NMR data have been reduced by two orders of magnitude. The effects of this have been two-fold. Firstly, it is easier to examine and characterise the very minor metabolites. Secondly, these advances have had a distinct influence on the mass requirements for field collections - smaller samples are possible as well as the opening up of a whole new range of marine organisms that are only ever available in small amounts.

Also dating back to the 1980s was the move towards the study of marine microorganisms. A continuing leader in this field is William Fenical. Initially, Fenical and his group focused on bacteria, especially those colonising the surfaces of marine algae and invertebrates, but in time changed their emphasis more towards marine fungi. This focus is now a major preoccupation of many of the marine research groups. For the literature on marine microorganisms, 45% of the total citations over the 1965 to 2005 period have been published since 2001. A significant find has been the discovery of new obligate marine actinomycete genera that produce unique metabolites. Accompanying the study of marine microorganisms has been the recognition that many of the MNPs described in the literature may well be of microbial origin and produced by microorganisms that are symbiotic, commensal or dietary components of the host invertebrate species. Modern developments in the tools of molecular biology are making the studies of these relationships more accessible. There has been a hiatus in the use or development of compounds of marine origin as pharmaceuticals. The recent licensing of Prialt, from the toxin of a *Conus* species, for the treatment of intractable pain comes some 50 years since the introduction of Ara-A and Ara-C and is the first direct drug from a marine invertebrate. It is likely that others, such as Yondelis for the treatment of cancer, will now soon follow.

No matter what the role or the source of MNPs might be, or what the focus of the research, the type of assays or analytical techniques that are directing the purification, chemists need to quickly establish the novelty of compounds that they are working on (dereplication), and to explore the relatedness of new compounds to others in the same class of structural types. The dereplication process in a modern context relies heavily on UV libraries (from HPLC data), mass spectrometry (from LC-MS data) and NMR pattern recognition (from cryoprobe or capillary probe NMR spectroscopy). The scale of such operations is now at the  $\mu\text{g}$  level and effectively telescopes the traditional process of several steps (crude extract evaluation, isolation, dereplication and characterisation) into just one process. The dereplication of MNPs relies heavily on access to appropriate collections of data, especially those with substructure searching capability, MW and UV data, that enable researchers to rapidly distinguish unique molecules from known compounds.

Such collections of data include the *Dictionary of Natural Products* (DNP) which is an all-encompassing compilation of natural product compound information from all sources including compound data, taxonomy and key references to structural, synthetic, ecological and biological activity studies. DNP was first published in 1992, and since that time has been continually updated by a team of specialist contributors and republished every six months in electronic form (CD-ROM, and more recently also as a web product). The *Dictionary of Marine Natural Products* is a specialist subset of the DNP. During 2004 to 2006, all entries in the DNP database referring to marine natural products were extracted, reviewed and where necessary expanded with reference to specialist literature sources such as MarinLit, and with the input of further levels of expertise from the marine natural specialists (John Blunt and Murray Munro).

The resulting *Dictionary of Marine Natural Products* in printed/CD-ROM format consists of approximately one-sixth of the DNP database, specially enhanced with new types of information particularly relevant to the marine environment. In particular, during the compilation, Type of Organism codes were added to the (whole) database for the first time, allowing the data to be searched by broad taxonomic criteria in parallel with other

parameters. This information, along with the MS, MF and UV data, can be directly searched in the CD-ROM version of *Dictionary of Marine Natural Products* and can give a rapid, unambiguous answer on the novelty of any metabolite isolated or partially characterised.

It is intended that the *Dictionary of Marine Natural Products* will be republished periodically, probably in CD-ROM format only. Users can obtain access to more frequent updates of the whole DNP database (including new marine information) by subscription. This first compilation of the *Dictionary of Marine Natural Products* will be of significant value to the growing number of investigators in the field of marine natural products. The efforts of John Buckingham and Steve Walford, coordinating a team of contributors (principally Keith Baggaley, Bob Hill and Andy Roberts) will be greatly appreciated.

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June 2007



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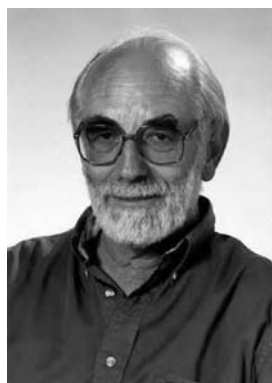
Additional data collected by contributors to the *Chapman & Hall Chemical Database*.



# Biography



John Blunt obtained his BSc (Hons) and PhD degrees from the University of Canterbury, followed by postdoctoral appointments in Biochemistry at the University of Wisconsin-Madison, and with Sir Ewart Jones at Oxford University. He took up a lectureship at the University of Canterbury in 1970, where he is now a Professor. His research interests are with natural products, and the application of NMR techniques to structural problems.



Murray Munro, University of Canterbury, Christchurch New Zealand, has worked on natural products, mainly of New Zealand origin, right through his career. Following a sabbatical with Ken Rinehart at the University of Illinois in 1973 interest in marine natural products developed with a particular focus on bioactive compounds. In recent years his research interests have widened to include terrestrial and marine fungi and actinomycetes as well as marine invertebrates.



# Introduction

## 1. COVERAGE

The *Dictionary of Marine Natural Products* is a comprehensive database containing over 30,000 compounds. It is a subset of the *Dictionary of Natural Products* (DNP) database. DNP is an ongoing project based on a 25-year review of the natural product literature. For the present project, the subset of DNP entries referring to marine natural products were carefully checked and reviewed and enhanced with a considerable amount of additional information relating to their natural occurrence. Several careful reviews were also carried out to ensure that the coverage of marine natural products in the finished publication was as complete as possible.

The compounds present in the Dictionary have been classified under the following major headings, which are described in more in the **Structural Types** section below. (There are obvious overlaps between the categories.)

- Aliphatic natural products
- Carbohydrates
- Oxygen heterocycles
- Simple aromatic natural products
- Terpenoids
- Steroids
- Aminoacids and peptides
- Alkaloids
- Polypyrroles

Biosynthetic information on these compound classes can also be found in the Structural Types section. Taxonomic information on the organisms and their metabolites is covered in the **Classification of Organisms** section.

In compiling the printed version and the CD-ROM, the primary literature has been reviewed up to mid-2006.

The definition of a marine natural product is imprecise. The coverage of this Dictionary in terms of 'mainstream' natural products is intended to be comprehensive and as far as can be determined by various cross-checks carried out in the later stages of compilation, it comes extremely close to achieving that aim. Natural products which may be considered marginal are present to a great extent, but to include every compound that might be found somewhere in the sea would be an unrealistic target. In particular, compounds of the following type may not necessarily be present:

- (1) Biochemicals endogenous to the higher marine animals, e.g. bile acids of marine mammals, endocrine hormones of crustaceans.
- (2) Microbial products isolated from organisms that are widespread on both sea and land and have in fact been isolated from a marine-related source, e.g. an antibiotic from *Streptomyces* harvested from driftwood.
- (3) Natural products of a 'terrestrial' type isolated from plants and animals in marginal environments, e.g. mangrove saltmarshes, may not be fully covered.
- (4) Widespread polysaccharides, e.g. Amylose, Amylopectin.

All of these are included in the parent database *Dictionary of Natural Products*, available on DVD or online from CRC Press.

The coverage of lipids is extensive but not completely comprehensive. Numerous homologous series of fatty acids with different unsaturation patterns occur in both terrestrial and marine organisms, and there may not be an individual entry for every minor congener.

### 1.1 NATURAL PRODUCTS IN THE MARINE ENVIRONMENT; GENERAL OBSERVATIONS

The marine environment is an extremely complex one, showing immense biodiversity. Marine organisms produce all of the main type of natural product found among their terrestrial counterparts, but with a very different range of chemodiversity, so that, for example, the range of terpenoid skeletons includes some not found on land. Conversely, there are large groups of natural product found in some higher plants (e.g. many terpenoid skeletons; large categories of alkaloids) for which the enzymatic pathways have not evolved among marine organisms; higher plants are essentially absent from the sea.



### 1.1.1 Elemental composition

Many marine natural products contain the elements nitrogen, sulfur and halogens available in seawater, but with very uneven distribution across the phyla. A few compounds containing other elements such as arsenic and boron are also known, and also metal complexes (Ni, V, Zn). Vanadium bromoperoxidases are involved in the production of brominated marine natural products (but chlorinated metabolites arise by a different route). The proportion of nitrogenous compounds is much higher in cyanobacteria, bryozoans and ascidians, and the proportion of halogenated compounds is very high in the red algae (in marked contradistinction to the brown algae). More details are given in the sections below describing these organisms.

Kornprobst, J.M. *et al*, *Comp. Biochem. Physiol. B*, 1998, **119**, 1–51 (*rev, sulfates*)

Jiménez, C., *Stud. Org. Chem.*, 2001, **25**, 811-917 (*rev, sulfur-containing marine natural products*)

Butler, A. *et al*, *Nat. Prod. Rep.*, 2004, **21**, 180-188 (*vanadium bromoperoxidases*)

### 1.1.2 Interspecific interactions

It is now clear that, whilst many marine natural products are located in the tissues of the larger marine animals and plants, and are thus genuine natural products of those organisms, many others are produced by associated endo- and epibiotic microorganisms. Most marine microorganisms have not yet been successfully cultured, and definitive proof of origin is in most cases currently lacking. These products produced by symbiotic or epiphytic microorganisms appear in many cases to play a role in chemical defence mechanisms.

In the past five years, however, much progress has been made in assigning a definite microbial origin to many natural products. For example, in the case of **Swinholide A**, originally isolated from the sponge *Theonella swinhoei*, centrifugation of macerated cell samples from the sponge showed that the alkaloid was located within heterotrophic unicellular bacterial cells, was absent from the sponge cells themselves, but was also in the cells of the co-occurring cyanobacterium *Aphanocapsa feldmanni* also present. More recently, however, Swinholide A has been found in some cyanobacteria, and it has been speculated that it may be produced by one component of this symbiont system, and stored by another. In the case of the isocyano- and related metabolites found in marine invertebrate extracts, the isocyano group, possibly derived from cyanide ion, may be produced by an associated microorganism, while the terpenoid component derives from the animal. Genomic techniques are now being used; for example to show that **Patellamides A** and **C** are biosynthesised by a cyanobacterial symbiont of the originally cited source. Other natural products isolated from the higher marine organisms, however, have a known dietary origin, while a definite *de novo* biosynthesis of some mollusc products has been demonstrated.

It may be true in some cases that although a particular type of metabolite isolated from a higher animal has not yet been found among the lower forms such as cyanophytes forming part of the same ecosystem, this is merely an accident of the search process.

Haygood, M.G. *et al*, *J. Mol. Microbiol. Biotechnol.*, 1999, **1**, 33–43 (*rev, microbial symbionts*)

Paul, V.J. *et al*, *Nat. Prod. Rep.*, 2004, **21**, 189–209 (*rev, chemical mediation of interorganism interactions*)

Salomon, C.E. *et al*, *Nat. Prod. Rep.*, 2004, **21**, 105–121 (*rev, microbial genetics and chemical diversity*)

Hildebrand, M. *et al*, *Nat. Prod. Rep.*, 2004, **21**, 122–142 (*rev, symbiont genetics*)

Proksch, P. *et al*, *BIOforum Eur.*, 2004, **8**, 44

Moore, B.S., *Nat. Prod. Rep.*, 2005, **22**, 580–593; 2006, **23**, 615–629 (*rev, biosynth*)

## 2. ORGANISATION OF ENTRIES

The Dictionary is arranged alphabetically by entry name. Every entry is numbered to assist ready location. Many compounds are included as derivatives of main entry compounds but important derivatives have their own individual cross-referenced entries. Use of the CD-ROM indexes enables the rapid location of all compounds in the Dictionary by name or compound type, regardless of their location. Entries may sometimes contain data on natural products which are not of marine origin, but this is obvious from the context and may provide valuable links to relationships between marine and terrestrial sources. This is especially true of entries dealing with fungal metabolites (see the section dealing with fungi, below).

A representative dictionary entry is shown in **Figure 1**.

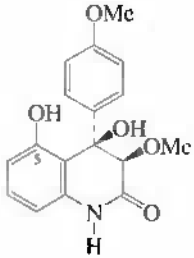
Entry Name	→ 3,4-Dihydro-4,5-dihydroxy-3-methoxy-4-(4-methoxyphenyl)-2(1H)-quinolinone	D-528	← Entry Number
CAS Registry Number	→ [184046-65-9]		
Structural formula and stereochemical descriptor	→ 	Relative Configuration	
Molecular formula	→ C <sub>17</sub> H <sub>17</sub> NO <sub>5</sub> 315.325	←	Molecular weight
	Prod. by <i>Penicillium</i> sp. NTC-47 and <i>Penicillium</i> cf. <i>simplicissimum</i> . Prisms (MeOH). Mp 208-210°. [ $\alpha$ ] <sub>D</sub> <sup>20</sup> -55 (c. 0.02 in MeOH). $\lambda_{max}$ 225 ( $\epsilon$ 35000); 280 ( $\epsilon$ 7000); 296 ( $\epsilon$ 8400).		
Derivative heading	→ 5-Deoxy: 3,4-Dihydro-4-hydroxy-3-methoxy-4-(4-methoxyphenyl)-2(1H)-quinolinone [183854-01-5] C <sub>17</sub> H <sub>17</sub> NO <sub>4</sub> 299.326	←	Derivative synonym
	Prod. by <i>Penicillium</i> sp. NTC-47, <i>Penicillium</i> cf. <i>simplicissimum</i> and a marine-derived <i>Penicillium janczewskii</i> . Needles (MeOH). Mp 76-79°. [ $\alpha$ ] <sub>D</sub> <sup>20</sup> -62 (c. 0.3 in MeOH). $\lambda_{max}$ 229 ( $\epsilon$ 11000); 254 ( $\epsilon$ 6500); 281 ( $\epsilon$ 2800) (MeOH)	←	Physical data
Biological source and other information	→ 5-Deoxy, O <sup>1</sup> -de-Me: 3,4-Dihydro-3,4-dihydroxy-4-(4-methoxyphenyl)-2(1H)-quinolinone C <sub>16</sub> H <sub>15</sub> NO <sub>4</sub> 285.299 Prod. by a marine-derived <i>Penicillium janczewskii</i> . Amorph. solid. [ $\alpha$ ] <sub>D</sub> <sup>25</sup> -4.2 (c. 0.5 in MeOH)		
	3-Epimer, 5-deoxy, O <sup>1</sup> -de-Me: C <sub>16</sub> H <sub>15</sub> NO <sub>4</sub> 285.299 Prod. by a marine-derived <i>Penicillium janczewskii</i> . Amorph. solid. [ $\alpha$ ] <sub>D</sub> <sup>25</sup> -12.9 (c. 0.7 in MeOH).		
Bibliographic references	→ Hayashi, H. et al., <i>Biosci., Biotechnol., Biochem.</i> , 1997, 61, 914-916 (isol. uv, ir, pmr, cmr)	←	Reference tags
	Kusano, M. et al., <i>Biosci., Biotechnol., Biochem.</i> , 2000, 64, 2559-2568 (isol. uv, pmr, cmr, ms)		
	Hu, J. et al., <i>J. Nat. Prod.</i> , 2005, 68, 1397-1399 (isol. pmr, cmr)	←	

FIGURE 1

## 2.1 CHEMICAL NAMES AND SYNONYMS

The Dictionary contains a wide range of synonyms which may be (a) those found in the primary literature, (b) *Chemical Abstracts* names, or (c) names added editorially to achieve as much consistency as possible with other closely related substances. Names corresponding to those used by CAS during the 9<sup>th</sup> and subsequent Collective Index periods (1973) are labelled 9CI Names. All important derivatives embedded within entries are named (but see comment on CAS nomenclature below). If a compound cannot be located immediately in the main body of the entries, it is important to use the indexes. The CD-ROM version of the Dictionary is much more highly indexed than the printed version.

The most authoritative current statement of good practice on natural product nomenclature is the document *IUPAC Recommendations 1999 (Pure Appl. Chem., 1999, 71, 587-643)* the full text of which can be read on the *Dictionary of Marine Natural Products on CD-ROM* (access from the Windows<sup>®</sup> Start menu item or via the Help menu in the main program).

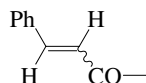
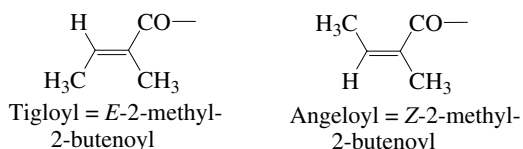
Some marine natural products have been given trivial names which duplicate those already in the literature, or which are simultaneously published for two or more non-identical substances. Where such a duplication is noticed this is indicated by the dagger symbol (‡) immediately following the name. Borderline cases, especially as between presence or absence of terminal e or suffix A or 1, are considered to constitute duplicates for this purpose.

### 2.1.1 Nomenclature

It is expected that this Dictionary will be used by a wide variety of scientists, not all of whom will be specialist organic chemists. Therefore compounds have been named so as to facilitate access to their factual data by keeping the nomenclature as simple as possible, whilst still adhering to good practice as determined by IUPAC (the International Union of Pure and Applied Chemistry). A great deal of care has been taken to achieve this aim as nearly as possible.

A much fuller description of the detailed nomenclature of individual classes of marine natural product is given in the **Structural Types** section. The following notes are of general applicability throughout the Dictionary.

1. There are many examples in the primary literature of compounds being named in ways which are violations of good IUPAC practice, e.g. where the substituents are ordered non-alphabetically. These are not reported in their incorrect form but have been corrected.
2. The number of trivial names used for acylating substituents has been kept to a minimum but the following are used throughout the Dictionary.



Cinnamoyl = 3-phenyl-2-propenoyl

3. Many other trivial appellations have from time to time appeared in the literature for other acyl groups (e.g. Seneciroyl = 3-methyl-2-butenoyl, Feruloyl = 3-(4-hydroxy-3-methoxyphenyl)-2-propenoyl or 4-hydroxy-3-methoxycinnamoyl).

The term **prenyl** for the common 3-methyl-2-butenyl substituent,  $(\text{H}_3\text{C})_2\text{C}=\text{CHCH}_2-$ , is used throughout the Dictionary. Several other names for this substituent have from time to time been used and appear in the primary literature including the following:

3-Methyl-2-butenyl (systematic)  
 $\gamma,\gamma$ -Dimethylallyl  
3,3-Dimethylallyl  
3,3-Dimethylpropenyl  
Dimethallyl  
Isoprenyl  
Isopentenyl  
 $\beta,\beta$ -Dimethylacrylyl

### 2.2 CAS REGISTRY NUMBERS

CAS numbers are identifying numbers allocated to each distinctly definable chemical substance indexed by CAS since 1965 (plus some retrospective allocation of numbers by CAS to compounds from earlier index periods). The numbers have no chemical significance but they provide a label for each substance independent of any system of nomenclature. They are extensively used for exchanging information between individuals and databases. The numbers take the form NNNNNN-NN-R, where the total number of digits is five or more and R is a check digit.

For practical purposes, CAS numbers have certain shortcomings arising from their free allocation, resulting in one substance having more than one potential number. Duplication may arise for one of several reasons to do with the detailed chemistry of the substance, for example tautomerism, solvent formation, partially unspecified stereochemistry. There are also replaced numbers. For this reason, Dictionary entries will often contain one or more *Additional CAS numbers* which may help the user to obtain further information about the substance, especially by online searching.

Clearly, the additional CAS numbers given in this Dictionary have to be used with care. Their inclusion in the entry is the result of an editorial decision by the Dictionary contributor that they refer to what is essentially the same substance, but this decision may be a subjective one. Care has been taken to ensure that the main CAS number given in this Dictionary for each substance is the correct one.

Further information on CAS number allocation policy can be obtained from CAS indexes or *The Organic Chemist's Desk Reference* (Chapman & Hall, 1995).

### 2.3 STRUCTURAL FORMULAE

Every attempt has been made to present the structures of chemical substances as accurately as possible according to best current practice and recommendations of IUPAC. As much consistency as possible has aimed at between closely-related structures. For example, all sugars are shown as Haworth formulae, and whenever possible in complex structures the rings are oriented in the standard Haworth convention so that structural comparisons can be quickly made.

### 2.4 MOLECULAR FORMULA AND MOLECULAR WEIGHT

The elements in the molecular formula are given according to the Hill convention (C, H, then other elements in alphabetical order). The molecular weights given are formula weights (or more strictly, molar masses in daltons) and are rounded to three places in decimals. In the case of some high molecular mass substances, such as proteins, the value quoted may be that taken from an original literature source and may be an aggregate molar mass.

### 2.5 PHYSICAL DATA

The Dictionary gives the following physical characteristics of substances, when available: appearance, melting point, boiling point, optical rotation, density, refractive index, solubility, p*K*<sub>a</sub>. All of these fields are searchable by numerical value (including range searching) in the CD-ROM version of the Dictionary.

#### 2.5.1 Appearance

Organic compounds are considered to be colourless unless otherwise stated. Where the compound contains a chromophore which would be expected to lead to visible colour, but no colour is mentioned in the literature, the Dictionary entry will mention this fact if it has been noticed by the contributor. An indication of crystal form and recrystallisation solvent is often given but these are imprecise items of data; most compounds can be crystallised from several solvent systems and the crystal form often varies. In the case of the small number of compounds where crystal behaviour has been intensively studied (e.g. pharmaceuticals), it is found that polymorphism is a very common phenomenon and there is no reason to believe that it is not widespread among organic compounds generally.

#### 2.5.2 Melting Points and Boiling Points

The policy followed in the case of conflicting data is as follows:

- a. Where the literature melting points are closely similar, only one figure (the highest or most probable) is quoted
- b. Where two or more melting points are recorded and differ by several degrees (the most likely explanation being that one sample was impure) the lower figure is given in parentheses, thus Mp 139° (134–135°)
- c. Where quoted figures differ widely and some other explanation such as polymorphism or incorrect identity seems the most likely explanation, both figures are quoted without parentheses, thus Mp 142°, Mp 205–206°
- d. Known cases of polymorphism or double melting points are noted

Boiling point determination is less precise than that of melting points and conflicting boiling point data are not usually reported except when there appears to be a serious discrepancy between the different authors.

#### 2.5.3 Optical rotations

These are given wherever possible, and normally refer to what the Dictionary contributor believes to be the best characterised sample of highest chemical and optical purity. Where available an indication of the optical purity