

# 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**.

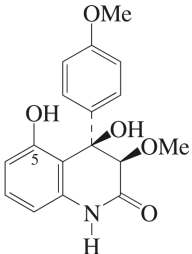
Entry Name	→	<b>3,4-Dihydro-4,5-dihydroxy-3-methoxy-4-(4-methoxyphenyl)-2(1H)-quinolinone</b>	D-528	←	Entry Number
CAS Registry Number	→	[184046-65-9]			
Structural formula and stereochemical descriptor	→		Relative Configuration		
Molecular formula	→	C <sub>17</sub> H <sub>17</sub> NO <sub>5</sub> 315.325			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). $\lambda_{\text{max}}$ 225 ( $\epsilon$ 35000); 280 ( $\epsilon$ 7000); 296 ( $\epsilon$ 8400).			
Derivative heading	→	<b>5-Deoxy: 3,4-Dihydro-4-hydroxy-3-methoxy-4-(4-methoxyphenyl)-2(1H)-quinolinone</b> [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). $\lambda_{\text{max}}$ 229 ( $\epsilon$ 11000); 254 ( $\epsilon$ 6500); 281 ( $\epsilon$ 2800) (MeOH).			Physical data
Biological source and other information	→	<b>5-Deoxy, O<sup>3</sup>-de-Me: 3,4-Dihydro-3,4-dihydroxy-4-(4-methoxyphenyl)-2(1H)-quinolinone</b> 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>15</sup> -4.2 (c, 0.5 in MeOH).			
		<b>3-Epimer, 5-deoxy, O<sup>3</sup>-de-Me:</b> 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>15</sup> -12.9 (c, 0.7 in MeOH).			
Bibliographic references	→	Hayashi, H. <i>et al.</i> , <i>Biosci., Biotechnol., Biochem.</i> , 1997, <b>61</b> , 914-916 ( <i>isol, uv, ir, pmr, cmr</i> ) Kusano, M. <i>et al.</i> , <i>Biosci., Biotechnol., Biochem.</i> , 2000, <b>64</b> , 2559-2568 ( <i>isol, uv, pmr, cmr, ms</i> ) He, J. <i>et al.</i> , <i>J. Nat. Prod.</i> , 2005, <b>68</b> , 1397-1399 ( <i>isol, pmr, cmr</i> )			Reference tags

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® Start menu item or via the Help menu in the main program).

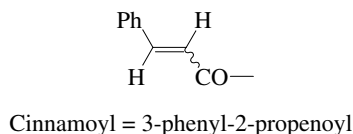
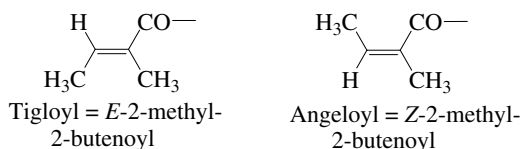
Some marine natural products have been given trivial names which duplicate those already in the literature, or which are simultaneously published for two or more non-identical substances. Where such a duplication is noticed this is indicated by the dagger symbol (‡) immediately following the name. Borderline 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.



3. Many other trivial appellations have from time to time appeared in the literature for other acyl groups (e.g. Senecioyl = 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:

- Where the literature melting points are closely similar, only one figure (the highest or most probable) is quoted
- 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°)
- 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°
- 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

(op) or enantiomeric excess (ee) of the sample measured follows the specific rotation value. For a recent discussion of the validity and applicability of these terms, see Gawley, R.E., *J. Org. Chem.*, 2006, **71**, 2411–2416.

Specific rotations are dimensionless numbers and the degree sign which was formerly universal in the literature has been discontinued.

## 2.6 SPECTROSCOPIC DATA

Many Dictionary entries include ultraviolet spectra which are presented in the format:

[neutral]  $\lambda_{\max}$  198(log  $\epsilon$  1.55); 224 (sh) (log  $\epsilon$  0.61); 241 (sh) (log  $\epsilon$  0.55)(H<sub>2</sub>O)(Berdy)

where  $\epsilon$  is the absorption coefficient for a given UV maxima value ( $\lambda_{\max}$ ). A description of the solvent conditions used, if reported in the literature, is listed at the beginning and end of the UV data in parentheses. All peak absorptions cited are maxima unless otherwise described, e.g. shoulder/inflection (sh) and end absorption (end). In addition, UV data may be followed by the term 'Berdy' or 'DEREP' indicating from which database the data originated. The absence of these terms implies that the data were abstracted from the primary literature.

On the CD-ROM, all the  $\lambda_{\max}$  values are indexed in the UV Maxima field and can be searched for numerically including range searching. Similarly, the solvent data associated with the UV data are indexed in the UV Solvent field.

## 2.7 HAZARD AND TOXICITY INFORMATION

### 2.7.1 General

Toxicity and hazard information is highlighted by the symbol and has been selected to assist in risk assessments for experimental, manufacturing and manipulative procedures with chemicals.

The Publishers cannot be held responsible for any inaccuracies in the reported information, neither does the omission of hazard data in the Dictionary imply an absence of this data from the literature. Widely recognised hazards are included, however, and where possible key toxicity reviews are identified in the references. Further advice on the storage, handling and disposal of chemicals is given in *The Organic Chemist's Desk Reference*.

### 2.7.2 RTECS<sup>®</sup> Accession Numbers\*

Many entries in this Dictionary contain one or more RTECS<sup>®</sup> Accession Numbers. Possession of these numbers allows users to locate toxicity information on relevant substances from the NIOSH *Registry of Toxic Effects of Chemical Substances*, which is a compendium of toxicity data extracted from the scientific literature.

## 2.8 BIBLIOGRAPHIC REFERENCES

The selection of references is made with the aim of facilitating entry into the literature for the user who wishes to locate more detailed information about a particular compound. The contents of most references are indicated by reference tags (suffixes) indicating their content and in particular the stereoisomers and derivatives of the parent compound which they document. The number of references cited does not indicate the relative importance of a compound; one key recent citation may supersede a number of older ones.

Journal abbreviations generally follow the practice of the Chemical Abstracts Service Source Index (CASSI), except for a short list of very well known journals where the Dictionary gives shorter abbreviations to save space (e.g. *J.A.C.S.* instead of *J. Am. Chem. Soc.*)

### 2.8.1 Further References

Further useful information on a variety of topics concerned with the structure, description, stereochemistry and nomenclature of organic compounds can be found in the *Organic Chemist's Desk Reference*.

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\*RTECS<sup>®</sup> Accession Numbers are compiled and distributed by the National Institute for Occupational Safety and Health Service of the U.S. Department of Health and Human Services of The United States of America. All rights reserved (1996)

### 3. INDEXES

There are three printed indexes:

1. **Name Index** which lists every compound name and synonym in the Dictionary
2. **Type of Compound index** listing all compounds given in the Dictionary organised by structural type
3. **Type of Organism index** listing all compounds according to the species from which they have been isolated.

The indexes refer to the entry number. Searches on all text and numerical indexes, as well as structure and substructure searching can be carried out on the CD-ROM version of the Dictionary. For information on the Type of Compound codes used in the Type of Compound Index, please see the **Structural Types** section.

### 4. ABBREVIATIONS

The following is a selection of the most common Database abbreviations used:

Abbreviation	Name
[ $\alpha$ ]	specific rotation
abs config	absolute configuration
Ac	acetyl
acc	according
AcOH	acetic acid
Ac <sub>2</sub> O	acetic anhydride
alk	alkaline
amorph	amorphous
amt	amount
anal	analytical applications, analysis of detection
anhyd	anhydrous
aq	aqueous
BAN	British Approved Name
bibl	bibliography
biosynth	biosynthesis
Bp	boiling point
c	concentration
ca	( <i>circa</i> ) about
cd	circular dichroism
CAS	Chemical Abstracts Service
chromatog	chromatography
cmr	carbon ( <sup>13</sup> C) nuclear magnetic resonance
CNS	central nervous system
col	colour, coloration
coml	commercial(ly)
compd	compound
conc	concentrated
config	configuration
conformn	conformation
constit	constituent
cryst struct	X-ray crystal structure determination
d	density
dec	decomposes, decomposition
degradn	degradation
deg	degree
deriv(s)	derivative(s)
detn	detection, determination
dil	dilute, dilution
dimorph	dimorphic

diss	dissolves, dissolved
dist(n)	distil, distillation
DMF	dimethylformamide
DMSO	dimethyl sulfoxide
ee	enantiomeric excess
epr	electron paramagnetic (spin) resonance
equilib	equilibrium
esp	especially
Et	ethyl
EtOAc	ethyl acetate
EtOH	ethanol
EtOH aq	aqueous ethanol
exp	experimental
FEMA	Flavor and Extract Manufacturers' Association
fl p	flash point
fluor	fluoresces, fluorescence
formn	formation
Fp	freezing point
g	gram
glc	gas liquid chromatography
Glc	$\beta$ -D-glucopyranosyl
GRAS	Generally Recognised As Safe
ham	hamster
haz	hazard
hplc	high performance liquid chromatography
hydrol	hydrolyses, hydrolysed, hydrolysis
ihl	inhalation
ims	intramuscular
INN	International Nonproprietary Name
intermed	intermediate
ipr	intraperitoneal
ir	infra-red spectrum
isol(n)	isolation, isolated
isom	isomerism, isomers, isomerises
ivn	intravenous
JAN	Japanese Accepted Name
JMAF	Japanese Ministry for Agriculture, Forestry and Fisheries
LC	lethal concentration
LD	lethal dose: LD <sub>50</sub> , a dose which is lethal to 50% of the animals tested
M	molecular weight (formula weight)
manuf	manufacturer, manufactured
max	maximum
Me	methyl
MeOH	methanol
Me <sub>2</sub> CO	acetone
MEL	maximum exposure limit
metab	metabolite, metabolism
misc	miscible
mixt	mixture
mod	moderately
Mp	melting point
ms	mass spectrum
mus	mouse
<i>n</i>	index of refraction, e.g. $n_D^{20}$ for 20° and sodium light
nmr	nuclear magnetic resonance spectrum (general)
obt	obtained



oc	open cup
occup	occupational
OES	Occupational Exposure Standard
op	optical purity
ord	optical rotatory dispersion
orl	oral
Ph	phenyl (C <sub>6</sub> H <sub>5</sub> )
pharmacol	pharmacology
pmr	proton ( <sup>1</sup> H) nuclear magnetic resonance
polarog	polarography
polym	polymerises, polymer
ppd	precipitated
ppm	parts per million
props	properties
purifn	purification
Py	pyridine
rbt	rabbit
ref	reference
resoln	resolution
rev	review
rt	room temperature
scu	subcutaneous
sepn	separation
skn	skin
sl	slightly
sol	soluble
soln	solution
solv	solvent
sp	species (singular)
spar	sparingly
spp	species (plural)
ssp	subspecies
subl	sublimation, sublimates
synth	synthesis
tautom	tautomerism
THF	tetrahydrofuran
tlc	thin layer chromatography
TLV	Threshold Limit Value
tox	toxicity
unsatd	unsaturated
USAN	United States Adopted Name
uv	ultraviolet spectrum
v	very
var	variety
vis	visible
vol	volume

#### 4.1 REFERENCE TAGS

The following is a selection of the most common Reference Tag abbreviations used:

Abbreviation	Name
abs config	absolute configuration
anal	analysis
bibl	bibliography
biosynth	biosynthesis

cd	circular dichroism
chromatog	chromatography
cmr	<sup>13</sup> C nuclear magnetic resonance spectrum
config	configuration
conformn	conformation
cryst struct	X-ray crystal structure determination
deriv(s)	derivative(s)
detn	determination, detection
dta	differential thermal analysis
glc	gas-liquid chromatography
hplc	high performance liquid chromatography
ir	infrared spectrum
isol	isolation
isom	isomerism
manuf	manufacture
metab	metabolism
ms	mass spectrum
nmr	nuclear magnetic resonance spectrum
occur	occurrence
ord	optical rotatory dispersion
pharmacol	pharmacology
pmr	proton ( <sup>1</sup> H) nuclear magnetic resonance spectrum
props	properties (chemical or physical)
Raman	Raman spectrum
resoln	resolution
rev	review
sepn	separation
struct	structure
synth	synthesis
tautom	tautomerism
tlc	thin layer chromatography
tox	toxicity
trans	transition(s)
uv	ultraviolet spectrum
uv-vis	ultraviolet visible spectrum

## 5. THE DICTIONARY OF MARINE NATURAL PRODUCTS ON CD-ROM

The *Dictionary of Marine Natural Products* is published together with a fully searchable CD-ROM. Space considerations have precluded the inclusion of indexes other than the Name, the Type of Compound and the Type of Organism indexes in the hard-copy version. By contrast, the CD-ROM contains searchable indexes on the following 35 fields:

Accurate Mass	Chemical Name	Molecular Weight	Supplier
All Entries	Density	Optical Rotation	Type of Compound
All Text	Development Status	Partition Coefficient (Calc.)	Type of Compound Words
Biological Source	Dissociation Constant	Percent Composition	Type of Organism
Biological Use/Importance	Hazard & Toxicity	References	Type of Organism Words
Boiling Point	Hazard Flag	Refractive Index	Use/Importance
Boiling Point Pressure	Ion Charge	Rotation Conditions	UV Maxima
CAS Registry Number	Melting Point	RTECS Accession No.	UV Solvent
Chapman & Hall Number	Molecular Formula	Source/Synthesis	

In addition to searching the above text fields, it is possible to search on structure and substructure.

Once installed, a Help file providing additional information on data content and guide to searching is available from the Chapman & Hall\_CRC folder in the Start Menu and from the Help menu on the CD-ROM.

When accessing the *Dictionary of Marine Natural Products on CD-ROM* the first screen that is obtained is the Search Form window (**Figure 2**).

The Search Form window is divided into three main panes. The top pane contains search criteria fields: a text input, a dropdown for 'Chemical Name', and a counter '0'. Below this are four rows of search criteria, each with an 'AND' dropdown, a text input, a dropdown for the field name, and a counter '0'. The fields are: 'CAS Registry No', 'All Text', and 'Molecular Formula'. The bottom pane contains an 'Add Term' button, a text input with 'brevetoxin', and a dropdown for 'OR'. Below this is a list of hits for 'Chemical Name (255897 items)'. The list has two columns: 'Hits' and 'Index'. The hits are: BREVETOXIN 1, BREVETOXIN 2, BREVETOXIN 3, BREVETOXIN A, and BREVETOXIN B. The right pane is empty and contains the text '<No structure>'. The window has a standard Windows-style title bar and a toolbar with icons for search, previous, exact, view hits, and other functions.

Hits	Index
1	BREVETOXIN 1
1	BREVETOXIN 2
1	BREVETOXIN 3
1	BREVETOXIN A
1	BREVETOXIN B

**FIGURE 2**

The Search Form window is split in to three panes:

1. Structure Search pane – allowing structure and substructure searching
2. Search Terms pane – search from one or more of the 35 available data/text fields
3. Index pane – displays the indexed terms within a selected field

From the Search Form window design your search profile using text, structure or text/structure searching. Once your search has been performed the resultant hits are listed alphabetically by chemical name in the Hit List screen. Clicking on any one of the hits in the hit list screen will result in that entry being displayed in the Entry Display screen (**Figure 3**).

Dictionary of Marine Natural Products on CD-ROM

File Edit Display Search HitList View Window Help

Search Form Hit List Entry Display


Hit List Item 1 of 9257

Name	UKEY	SUBS	Type Code
<input type="checkbox"/> Aaptamine	00013886- -000	K0	ZW05
<input type="checkbox"/> Aaptamine; O <sup>3</sup> -De-Me	00013886- -002	K0	ZW05
<input type="checkbox"/> Aaptamine; O <sup>3</sup> -De-Me, N <sup>1</sup> -Me	00013886- -003	K0	VX760
<input type="checkbox"/> Aaptamine; Di-O-de-Me	00013886- -004	K0	VX760
<input type="checkbox"/> Aaptosine	00015725- -000	K0	VX760
<input type="checkbox"/> 15(4→3)-Abeo-1,3,9-cadinatrien-8-ol	00010004- -000		
<input type="checkbox"/> 15(4→3)-Abeo-1,3,9-cadinatrien-8-ol; (6β, 7β, 8α)-form	00010004- A-000		VS229
<input type="checkbox"/> 13(11→10)-Abeo-2,7(14),11-chamigatrien-4-one	00222861- -000	K0 V10	ZW65
<input type="checkbox"/> 14(7→6)-Abeo-2,7-cuparadiene	00228594- -000	V12	
<input type="checkbox"/> 14(7→6)-Abeo-2,7-cuparadiene; (R)-form	00228594- A-000	V12	VS179
<input type="checkbox"/> 12(11→10)-Abeo-1,3,5,10-cuparatetraen-2-ol	00253842- -000	K0 V20	VS179
<input type="checkbox"/> 14(7→6)-Abeo-4-cuparen-3-ol	00026552- -000		VS179
<input type="checkbox"/> 7(8→9)-Abeo-8,13-dinor-11-oxo-6-eremophilen-15-olc acid	00185489- -000		
<input type="checkbox"/> 14(5→6)-Abeo-5,7,9,11-eremophilatetraen-9-ol	00008604- -000		VS218
<input type="checkbox"/> 14(10→1)-Abeo-5,11-eudesmadiene	00253838- -000	K0 V20	
<input type="checkbox"/> 14(10→1)-Abeo-5,11-eudesmadiene; (1β, 4β, 7α, 10α)-form	00253838- A-000	K0 V20	ZW10
<input type="checkbox"/> 14(10→1)-Abeo-11-eudesmen-1-ol	00185161- -000		
<input type="checkbox"/> 14(10→1)-Abeo-11-eudesmen-1-ol; (1α, 4β)-form	00185161- A-000		ZQ37
<input type="checkbox"/> 14(5→6)-Abeo-5,9-furanoeremophiladien-1-one	00230008- -000	V99	VS218
<input type="checkbox"/> 14(5→6)-Abeo-1,3,5(10),6(14)-furanoeremophilatetraen-9-one	00008344- -000		ZQ17
<input type="checkbox"/> 14(5→6)-Abeo-1,5,9-furanoeremophilatriene	00330341- -000		ZQ18
<input type="checkbox"/> 14(5→6)-Abeo-1,5,9-furanoeremophilatrien-9-ol	00023769- -000		
<input type="checkbox"/> 5(1→10)-Abeo-15-nor-3-patchoulen-1-ol	00338121- -000		VS266
<input type="checkbox"/> 5(1→10)-Abeo-1-patchoulanol	00007545- -000	M0 R84	ZQ37
<input type="checkbox"/> 11(1→10)-Abeo-1(5)-patchoulene	00007542- -000	W0	W150

Entry Item 1 of 9257

Aaptamine

>> Entry Name: Aaptamine  
 Synonym(s): 8,9-Dimethoxy-1*H*-benzo[*de*]1,6)naphthyridine, sci



Chapman & Hall Number: CFH28-Z  
 CAS Registry Number: 85547-22-4  
 Type of Compound Code(s): ZW0500 VX7600

Molecular Formula: C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>  
 Molecular Weight: 228.25  
 Accurate Mass: 228.089878  
 Percentage Composition: C 68.41%; H 5.30%; N 12.27%; O 14.02%  
 Biological Source: Alkaloid from the marine sponge *Aaptos aaptos*  
 Biological Use/Importance: α-Adrenoreceptor blocker. Antineoplastic agent  
 Physical Description: Brilliant green cryst; bright yellow cryst. (MeOH/Me<sub>2</sub>CO) (as hydrochloride)  
 Melting Point: Mp 110-113° (107°) (hydrochloride)  
 Solubility: Sol. MeOH, CHCl<sub>3</sub>  
 UV: [neutral] λ<sub>max</sub> 215 (ε 13700); 236 (ε 14700); 255 (ε 17900); 309 (ε 3640); 350 (ε 3750); 380 (ε 5000); 394 (ε 4570) (H<sub>2</sub>O) (Derep) [neutral] λ<sub>max</sub> 220 (ε 8900); 239 (ε 11750); 257 (ε 13200); 274 (ε 9700); 312 (ε 3160); 354 (ε 3300); 384 (ε 5620) (MeOH) (Berdy) [neutral] λ<sub>max</sub> 214 (ε 13700); 236 (ε 14700); 255 (ε 17900); 309 (ε 3640); 352 (ε 3750); 381 (ε 300); 394 (ε 4570) (H<sub>2</sub>O) (Berdy)  
 RTECS Accession Number: DI2410500

Derivative: N<sup>4</sup>-Me  
 Synonym(s): N<sup>4</sup>-Methylaaptamine  
 Chapman & Hall Number: MCH41-J  
 Type of Compound Code(s): ZW0500 VX7600  
 Molecular Formula: C<sub>14</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>  
 Molecular Weight: 242.277  
 Accurate Mass: 242.105528  
 Percentage Composition: C 69.41%; H 5.82%; N 11.56%; O 13.21%  
 Biological Source: Alkaloid from *Aaptos* sp.

Total Hits: 9257

FIGURE 3

Any comments and suggestions for inclusion may be sent to:

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