

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY
ORGANIC CHEMISTRY DIVISION
COMMISSION ON NOMENCLATURE OF ORGANIC CHEMISTRY (III.1)

REVISED SECTION F: NATURAL PRODUCTS AND RELATED COMPOUNDS

(IUPAC Recommendations 1999)

Prepared for publication by

P. M. GILES, Jr
Chemical Abstracts Service, Columbus, OH 43210, USA

Membership of the Working Party (1982–1997): J. R. Bull (Republic of South Africa), H. A. Favre (Canada), M. A. C. Kaplan (Brazil), L. Maat (Netherlands), A. D. McNaught (UK), G. P. Moss (UK), W. H. Powell (USA), R. Schoenfeld† (Australia), O. Weissbach (Federal Republic of Germany).

Membership of the Commission on Nomenclature of Organic Chemistry during the preparation of this document was as follows:

Titular Members: O. Achmatowicz (Poland) 1979–1987; J. Blackwood (USA) 1996–1998; H. J. T. Bos (Netherlands) 1987–1995, *Vice-Chairman*, 1991–1995; J. R. Bull (Republic of South Africa) 1987–1993; F. Cozzi (Italy) 1996–; H. A. Favre (Canada) 1989–, *Chairman*, 1991–; P. M. Giles, Jr. (USA) 1989–1995; E. W. Godly (UK) 1987–1993, *Secretary*, 1989–1993; D. Hellwinkel (Federal Republic of Germany) 1979–1987, *Vice-Chairman*, 1981–1987; B. J. Herold (Portugal) 1994–; K. Hirayama (Japan) 1975–1983; M. V. Kisakürek (Switzerland) 1994–, *Vice-Chairman*, 1996–; A. D. McNaught (UK) 1979–1987; G. P. Moss (UK) 1977–1987, *Chairman*, 1981–1987, *Vice-Chairman*, 1979–1981; R. Panico (France) 1981–1991, *Vice-Chairman*, 1989–1991; W. H. Powell (USA), *Secretary*, 1979–1989; J. C. Richer (Canada) 1979–1989, *Vice-Chairman*, 1987–1989; P. A. S. Smith (USA) 1983–1991, *Chairman*, 1987–1991; D. Tavernier (Belgium) 1991–1995; J. G. Traynham (USA) 1991–, *Secretary*, 1994–; O. Weissbach (Federal Republic of Germany) 1987–1991; J. L. Wisniewski (Germany) 1991–.

Associate Members: O. Achmatowicz (Poland) 1987–1989; K. Blaha† (Czech Republic) 1979–1987; H. J. T. Bos (Netherlands) 1983–1987; A. J. Boulton (UK) 1983–1987; J. R. Bull (Republic of South Africa) 1985–1987; F. Cozzi (Italy) 1994–; D. R. Eckroth (USA) 1975–1983; F. Fariña† (Spain) 1989–1994; H. A. Favre (Canada) 1987–1989; J. H. Fletcher (USA) 1975–1983; P. M. Giles, Jr. (USA) 1983–1989; E. W. Godly (UK) 1979–1987; P. Grünanger (Italy) 1987–1993; H. Grünewald, (Federal Republic of Germany) 1989–1991; H. E. Gutmann (Switzerland) 1983–1989; J. Heger (Slovakia) 1985–1989; D. Hellwinkel (Federal Republic of Germany) 1987–1989; K. Hirayama (Japan) 1983–1987; R. L.-R. Hwu (USA; Chemical Society, Taipei) 1989–; M. A. C. Kaplan (Brazil) 1989–; M. V. Kisakürek (Switzerland) 1987–1993; S. R. Klesney (USA) 1979–1985; A. J. Lawson (Federal Republic of Germany) 1991–; W. Liebscher (Federal Republic of Germany) 1989–; K. L. Loening (USA) 1979–1983; N. Lozac’h (France) 1977–1987; A. D. McNaught (UK) 1987–1989; M. Mikolajczyk (Poland) 1989–; G. P. Moss (UK) 1987–1989; J. Nyitrai (Hungary) 1994–; R. Panico (France) 1979–1981; J. Rigaudy (France) 1981–1985; Ch. Schmitz (France) 1989–1993; R. Schoenfeld† (Australia) 1981–1987; H. A. Smith, Jr. (USA) 1994–; P. A. S. Smith (USA) 1979–1983; J. H. Stocker (USA) 1991–; D. Tavernier (Belgium) 1987–1991, 1996–; J. G. Traynham (USA) 1989–1991; F. Vögtle (Federal Republic of Germany) 1972–1983; O. Weissbach (Federal Republic of Germany) 1979–1987.

National Representatives: H. Y. Aboul Enein (Saudi Arabia) 1988–1989; O. Achmatowicz (Poland) 1989–1991; A. T. Balaban (Romania) 1983–1989; R. Bicca de Alencastro (Brazil) 1994–; H. J. T. Bos (Netherlands) 1981–1983; J. R. Bull (Republic of South Africa) 1983–1985; J. R. Cannon (Australia) 1982–1987; K. C. Chan (Malaysia) 1983–1987; S. Chandrasekaran (India) 1994–; Q. Y. Chen (Chinese Chemical Society) 1991–; G. Déak† (Hungary) 1979–1992; F. Fariña† (Spain) 1987–1989; A. A. Formanovsky (Russia) 1996–; M. J. Gasic (Federal Republic of Yugoslavia) 1989–1993; E. W. Godly (UK) 1994–; P. Grünanger (Italy) 1984–1987; B. J. Herold (Portugal) 1991–1993; W.-Y. Huang (Chinese Chemical Society) 1981–1987; S. Ikegami (Japan) 1986–; A. K. Ikizler (Turkey) 1987–; J. Kahovec (Czech Republic) 1989–; M. A. C. Kaplan (Brazil) 1983–1985; P. Kristian (Slovakia) 1994–; G. L’abbé (Belgium) 1981–1985; Eun Lee (Republic of Korea) 1994–; X. T. Liang (Chinese Chemical Society) 1987–1993; L. Maat (Netherlands) 1989–1991, 1996–; G. Mehta (India) 1983–1985; J. Nyitrai (Hungary) 1992–1993; L. J. Porter (New Zealand) 1987–1995; J. A. Retamar (Argentina) 1980–1985; H. Schick (Federal Republic of Germany) 1987–1991; R. Schoenfeld† (Australia) 1980–1981; S. Swaminathan (India) 1985–1987; D. Tavernier (Belgium) 1986–1987; A. Varvoglis (Greece) 1991–1993; M. S. Wadia (India) 1996–.

† Deceased.

Names of countries given after members names are in accord with the *IUPAC Handbook 1996–1997*.

Republication or reproduction of this report or its storage and/or dissemination by electronic means is permitted without the need for formal IUPAC permission on condition that an acknowledgement, with full reference to the source along with use of the copyright symbol ©, the name IUPAC and the year of publication are prominently visible. Publication of a translation into another language is subject to the additional condition of prior approval from the relevant IUPAC National Adhering Organization.

Revised section F: natural products and related compounds (IUPAC Recommendations 1999)

CONTENTS

Preamble	588
Introduction	589
Rules	590
RF-1. Biologically based trivial names	590
RF-2. Semisystematic nomenclature for natural products	591
RF-3. Fundamental parent structures	592
3.1 General guidelines for choice	592
3.2 Structural features allowed	592
3.3 Semisystematic names	592
3.4 Indicated hydrogen	593
3.5 Numbering	593
3.6 Identification of individual rings	593
3.7 Stereochemistry	594
RF-4. Skeletal modification of fundamental parent structures	594
4.1 Removal of skeletal atoms	594
4.2 Addition of skeletal atoms	594
4.3 Bond formation	598
4.4 Bond cleavage	598
4.5 Bond migration	601
4.6 Terminal ring removal	602
4.7 Combinations of operations	602
RF-5. Replacement of skeletal atoms	605
RF-6. Fusion of additional rings	606
RF-7. Bridged parent structures	610
RF-8. Bond order modifications	610
RF-9. Derivatives of parent structures	611
RF-10. Stereochemical modifications	614
References	618

Abstract: The nomenclature of natural products has suffered from much confusion, mostly for historical reasons. The isolation of a new substance, in the early days of the science, generally preceded its characterization by a lengthy period. Thus, these compounds were often assigned trivial names that gave no indication of the structure of the molecule and were often found afterwards to be misleading. Even when the original names were later revised (for example: glycerin to glycerol) the new names often expressed the structure imperfectly and were thus unsuitable for the nomenclatural manipulation that is required to name derivatives or stereoisomers. The result was a proliferation of trivial names that taxed the memory of chemists and obscured important structural relationships.

The resultant disorder in the literature led to the creation of committees of specialists with the task of codifying the naming of compounds in various connected areas of natural-product

chemistry, such as steroids, lipids, and carbohydrates. As far as their recommendations have been followed, their efforts have been successful in eliminating confusing or duplicate nomenclature.

It is the aim of the IUPAC Commission on Nomenclature of Organic Chemistry to unite as far as possible all the specialist reports into a single set of recommendations that can be applied in most areas of natural-product chemistry. Accordingly, provisional recommendations were prepared and published as Section F of the IUPAC Organic Nomenclature Rules, first in 1976 [1], and then in the 1979 edition of the Rules [2].

INTRODUCTION

Section F of these IUPAC Organic Nomenclature Rules is intended to help those working with natural products and related compounds to overcome two difficulties that are encountered frequently in their work:

- a. A new compound has been isolated from a natural source, but its structure may be imperfectly known. To allow ready reference to such a compound, a *trivial* name may be coined for it according to the provisions of Rule RF-1, below.
- b. A new compound has been isolated and its structure determined; its *systematic* name can thus be generated. However, this name may be too cumbersome to be continually inserted into the text of a scientific paper. To overcome this difficulty and show the close similarity to related compounds, a *semisystematic* name can be created in accordance with Rules RF-2 through RF-10.

From the above explanation, three definitions follow:

- i. A *trivial* name is the name given for convenience to a new compound of yet uncertain structure. Such a name carries no (or minimal) structural information and is generally derived from the biological origin of the material. Trivial names should be formed according to the principles of RF-1, which also offers advice on how the change from a trivial to a semisystematic name can be accomplished in such a manner that the literature can still be retrieved without difficulty.
- ii. A *systematic* name is one based on Sections A–E of the IUPAC Organic Nomenclature Rules [1] and on the more recent Guide to IUPAC Organic Nomenclature [3]. It will generally comprise stereo descriptors, followed by prefixes, the ‘parent’, and finally a suffix.
- iii. A *semisystematic* name created according to Rules RF-2 through RF-10, provides a simplified alternative to the systematic name. This is normally achieved by the creation of a ‘semi systematic parent.’ There are two general types of semisystematic parents used for naming natural products and related compounds:
 - (a) *Parent hydrides*, which are structures that do not have terminal hetero atoms or functional groups and therefore consist only of skeletal atoms and hydrogen, for example, in steroid [4], terpene, carotene [5], and alkaloid nomenclature; this type of semisystematic parent can be treated according to the rules in Sections A–D of the IUPAC Organic Nomenclature Rules [2] and the Guide to IUPAC Organic Nomenclature [3], i.e. a suffix and prefixes indicating substituents and modifications to the skeletal structure may be added.
 - (b) *Functional parents*, which are structures that have certain terminal heteroatoms or groups, such as are found in carbohydrates, amino acids, and nucleosides; suffixes are usually not added to this type of semisystematic parent.

Those who wish to name a new compound will obtain the greatest benefit from the present rules if they bear the following in mind:

- i. If the structure is unknown, a trivial name may be formed according to Rule RF-1.

- ii. If the structure is known and not unduly complex, systematic nomenclature should be used [2,3].
- iii. If the structure is known and complex, there are three possibilities:
 - (a). A semisystematic parent name describing most of the skeleton of the compound is already in existence in the literature. This should be used and the new name derived from it by the operations of substitutive nomenclature.
 - (b). The literature does not contain a semisystematic parent name that describes most of the skeleton of the compound, or a structure closely resembling that skeleton. In that case, a new parent name should be created according to Rules RF-2 through RF-7. If necessary, the degree of saturation or unsaturation is indicated according to Rule RF-8; prefixes and suffixes according to Rule RF-9 and stereo descriptors according to Rule RF-10 are added to arrive at the name of the new compound.
 - (c). The literature contains a semisystematic name describing a structure not identical with, but closely resembling the skeleton in question. In that case, a number of 'structure-modifying prefixes' (such as homo, seco) are available under Rule RF-4. Different skeletal atoms, additional rings and bridges can be described according to RF-5 through RF-7. Placed in front of the existing parent name, such prefixes modify the meaning so that it describes the skeletal structure of the new compound. Rules RF-8 through RF-10 are then brought into play to generate the name of the compound itself.

The appendix to this Section lists illustrative semisystematic parent names and the structures they define.

RULES

Rule RF-1. Biologically based trivial names

RF-1.1. When a compound is isolated from a natural source and a trivial name is required, the name should be based whenever possible on the family or genus or species name of the biological material from which the compound has been isolated. (Names based on a presumed metabolic activity of the isolated substance should not be generated.) As far as possible, the name should be selected to reflect the known or the likely distribution of the natural product. For example, a hypothetical species *Paradigma exemplare* (family Beispieliaceae) might yield products named on the basis of beispieliaceae, paradigma, or exemplare. If appropriate, the class or order might also be used as the basis for the name of a compound that occurs in a number of related families.

RF-1.2. The trivial name should not give a false implication as to structure or identity of principal groups present.

RF-1.3. The following groups of letters have significance as terminations in organic chemical nomenclature, and therefore should not be used as terminations to trivial names coined for natural products of unknown structure (except for the special case discussed in Rule RF-1.5 below).

—	—	al	—	am	an	ane	—	—	ate	—
—	—	—	—	—	en	ene	et	—	ete	—
ic	ide	—	ile	—	in	ine	—	—	—	ium
—	—	ol	ole	—	—	one	—	ose	—	—
		olide						oside		
—	yde	yl	—	—	—	yne	—	—	—	—

RF-1.4. As the vowel 'u' does not occur as the first letter in the above list, the ending -une, or where euphony so dictates -iune, has been chosen to indicate that the trivial name it terminates describes a compound of unknown structure (-une can be taken to symbolize *unknown* or the German *unbekannt*).

Such a name implies all substituent groups, including a principal characteristic group; hence, no prefixes or suffixes indicating substituent groups can be used. Thus, products derived from the hypothetical species *Paradigma exemplare* (family Beispieliae) noted above, might be named paradigmune, exemplarune, or beispiefiune.

Note: In the past, the ending -ine has been commonly used for compounds of unknown structure; however, this ending is not recommended under Rule RF-1.3 because of its significance in Hantzsch-Widman ring nomenclature (R-2.3.3).[3]

RF-1.5. Two or more compounds isolated from the same source or obtained by subsequent separation from a substance previously considered as homogeneous may be differentiated by adding a capital letter, e.g. A, B, etc., to a name formed according to RF-1.1 through RF-1.4. Further refinements can be distinguished by the addition of subscript numbers to these letters.

RF-1.6. Names ending in -une or -iune are only temporary in that some unknown function and/or skeleton exists. As soon as the terminal heteroatoms and groups attached to a parent skeletal structure are identified, the ending is changed to -ane, or other suitable ending (see RF-3.3), and the terminal heteroatoms, groups, and other features should be expressed as a suffix and prefixes in the usual manner. For example, the compound paradigmune is found to be fully saturated and have an oxo and two hydroxy substituents; the name then becomes dihydroxyparadigmanone.

RF-1.7. As soon as the structure of a new natural product has been fully determined, if it is relatively simple the trivial name established above in RF-1.4 through 1.6 should be abandoned in favor of a systematic one based on the established principles of organic nomenclature [2,3]. For a more complicated structure, if a previously known parent structure can be easily used to derive a semisystematic name for the new natural product, the trivial name should be abandoned in favor of such a semisystematic name based on the name for the established parent structure. If a previously known parent structure cannot be found, the stem name assigned above becomes that of a new parent which is numbered according to the rules given below.

RF-1.8. If it is subsequently found that the compound is identical with a known natural product structure, the trivial or semisystematic name formed later should be abandoned in favor of the previously recorded one, or a name derived systematically from it. In the latter case, the new name should be as close as possible to the one recorded earlier.

Rule RF-2. Semisystematic nomenclature for natural products

Many naturally occurring compounds belong to well-defined structural classes, each of which can be characterized by a set of parent structures that are closely related structurally, that is, each can be derived from a fundamental structure by one or more well-defined operations.

RF-2.1. A semisystematic name for a naturally occurring compound or a synthetic derivative should be based on the name of an appropriate fundamental parent structure as described in RF-3.

[Examples of fundamental parent structures and names for a variety of natural compound classes are given in the Appendix.]

RF-2.2. To the name of a fundamental parent structure are added affixes denoting: (1) modifications to the skeletal structure (RF-4, 6, and 7); (2) replacement of skeletal atoms (RF-5); (3) changes in the state of hydrogenation implied by the name of the parent structure (RF-8); (4) atoms or groups substituting hydrogen atoms of the parent structure (RF-9); (5) configurations not already implied by the name of the parent structure, or changed from that implied (RF-10). Unless specified otherwise in the rules that follow, methods of construction of the name and the principles of organic nomenclature as given in the IUPAC Organic Nomenclature Rules [2,3] are followed.

Rule RF-3. Fundamental parent structures**RF-3.1. General guidelines for choosing a fundamental parent structure.**

RF-3.1.1. A fundamental parent structure should reflect the basic skeleton (including nonterminal hetero atoms and hetero groups) that is common to most compounds in that class.

RF-3.1.2. Fundamental parent structures should be chosen so that as many related natural products as possible can be derived from each by well-defined operations and principles of organic nomenclature.

RF-3.1.3. A fundamental parent structure should include as much stereochemistry as possible that is common to the relevant class of natural products.

RF-3.2. Structural features allowed for fundamental parent structures:

RF-3.2.1. A fundamental parent structure should only exceptionally include rings that are part of a characteristic group, such as a lactone or cyclic acetal. However, there are a number of widely used names that do include cyclic characteristic groups, for example, spirostan and cardenolide and these are allowed by these rules.

RF-3.2.2. A fundamental parent structure should not contain terminal hetero atoms or groups, except as provided by Rule RF-3.2.5.

RF-3.2.3. A fundamental parent structure should contain acyclic hydrocarbon groups that occur in most of the compounds in the natural product class.

RF-3.2.4. A fundamental parent cyclic structure should be as nearly fully saturated, or fully unsaturated in terms of the maximum number of noncumulative double bonds, as possible, while still representing the level of saturation (or unsaturation) of as many related compounds as possible. This principle should not be applied so rigorously that a large number of unsaturated bonds must be expressed by subtractive suffixes or that a large number of unsaturated bonds must be removed by hydro prefixes.

RF-3.2.5. Certain large classes of natural products, such as carbohydrates, nucleosides and peptides, are characterized by the occurrence of relatively simple but highly functionalized units and their oligomers and polymers. For these classes of compounds, called fundamental functional parents (see Introduction), the provisions of RF-3.2.2 do not apply in that fundamental parent structures may also contain functional groups.

RF-3.3. A semisystematic name for a fundamental parent structure should be derived as far as possible from a trivial name formed according to Rule RF-1. The endings to be used in place of ‘-une’ or ‘-iune’ should follow the following guidelines:

- (a). ‘-an(e)’, if the entire parent structure is saturated;
- (b). ‘-en(e)’, if the cyclic or the main chain of the acyclic part, or both, of the parent structure contain the maximum number of noncumulative double bonds;
- (c). ‘-aran(e)’, if, in an otherwise fully saturated parent structure, there occur one or more individual rings that contain the maximum number of noncumulative double bonds. Most examples of such substances already have names ending in ‘-an’ (see Note 2, below) or are alkaloids whose names end in ‘-ine’, e.g. ergoline, aspidospermidine, and strychnidine.

Note 1: In these rules the final ‘e’ will be used. The omission of this final ‘e’, or the use of a final ‘a’, may occur in languages other than English.

Note 2: The ending ‘-an’ has been used for names of some heterocyclic parent structures having partial unsaturation, e.g. morphinan, rheadan, yohimban. Hence, even though the ending ‘-aran(e)’ has been suggested above for structures of these types, no change to ‘-aran(e)’ is required for names already established. However, for such compounds, the ‘-an(e)’ ending cannot be used to indicate fully saturated analogs, which must be described using hydro prefixes (see RF-6).

RF-3.4. Indicated hydrogen, as described in Rule A-21.6, may be used to describe isomers of fundamental parent structures that have saturated skeletal atoms within a ring system or portion of a ring system having the maximum number of noncumulative double bonds.

RF-3.5. Numbering of fundamental parent structures.

RF-3.5.1. A numbering pattern established among a group of structurally related natural products is used for numbering the skeletal atoms of the fundamental parent structure, providing all skeletal atoms have been included in the numbering system.

RF-3.5.2. If no numbering pattern has become established among the members of a group of structurally related natural products, the fundamental parent structure is numbered according to the following guidelines:

- (a). The skeleton is examined to identify a preferred ring system. This will be the ring system defined as ‘senior’ according to the criteria of Rule C-0.14 [2]. The locant ‘1’ is assigned to the atom of the preferred ring system whose locant would be ‘1’ according to systematic numbering for that particular ring system.
- (b). All skeletal atoms of the preferred ring system are assigned consecutive Arabic numbers, including atoms at fusion positions in fused ring systems, beginning with the locant ‘1’, and following the path prescribed for systematic numbering of that particular type of ring system.
- (c). Acyclic substituents to skeletal atoms of ring components or connecting acyclic structures are numbered each in its entirety, including branches, in order of the increasing value of the locant of the skeletal atom to which each is attached.
- (d). Skeletal atoms of acyclic connections to other rings or ring systems, if any, are numbered consecutively beginning with the atom next to the preferred ring system, followed by the skeletal atoms of the other rings or ring systems as prescribed by (b) above; if two or more acyclic connections to other rings or ring systems are present, the one attached to the preferred ring system at the lowest numbered position is numbered first, then the ring attached to it, followed by the acyclic connector at the next lower numbered position of the preferred ring or ring system, etc.
- (e). Between two groups at a gem-disubstituted position, the larger group, in terms of the number of skeletal atoms, is numbered first; if there is still a choice, the principles of Rule C-15.11(c)–(e) [2] are followed. If the two groups are then identical and attached to a cyclic structure properly drawn (see Appendix) the group stereochemically α is numbered first (see RF-4.5.1); if the two groups are identical and attached to an acyclic structure, the group *trans* to the main chain is numbered first as described in the carotenoid recommendations Rule 12.4

RF-3.6. Identification of individual rings. Certain modifying prefixes for names of fundamental parent structures (see Rule RF-4) have used a ring identifier rather than specific locants of skeletal atoms. Accordingly, the identification of individual rings for some of the more common natural products has become well established. However, since in these recommendations locants of skeletal atoms are used to describe structural modifications instead of letters, except for the rather special case of removal of a terminal ring (see RF-4.6), no attempt has been made here to codify a system for lettering rings. Nevertheless, to provide continuity with the use of this system, names using letters to identify rings are given where appropriate.

RF-3.7. Stereochemical configuration of fundamental parent structures. The name of the fundamental parent structure implies, without further specification, the absolute configuration at all chiral centers and the configuration at double bonds corresponding to the group of natural products from which the parent name was derived, except as specified in these rules, or in rules for specific kinds of natural product compounds. Such stereochemistry for many fundamental parent structures is shown by the drawings in the Appendix. In some instances the configuration at a center is not implied by the parent name and must always be specified.

Rule RF-4. Skeletal modifications of fundamental parent structures.

RF-4.1. Removal of skeletal atoms without affecting the number of rings.

RF-4.1.1. The removal of an unsubstituted skeletal atom, saturated or unsaturated, from a ring or an unsubstituted skeletal atom from an acyclic portion of a fundamental parent structure with its attached hydrogen atom(s) is described by the prefix 'nor-'; the loss of two or more skeletal atoms is indicated by combining an appropriate numerical prefix with 'nor-', e.g. 'dinor ... trinor-', etc.

Note 1: The provisional Section F Rules [1,2] require the skeletal atoms removed to be saturated carbon atoms by using the prefix 'nor' to indicate the removal of methylene groups. The carotenoid recommendations (5(a)) [5] provide that 'nor' be used to indicate the removal of CH groups as well. These revised recommendations are more precise by permitting removal of CH groups only in a ring having the maximum number of noncumulative double bonds; they are also more general by allowing 'nor' to indicate the removal of hetero atoms.

Note 2: The special use of the prefix 'nor-' without multiplying prefixes or locants to indicate the replacement by hydrogen atoms of all methyl groups attached to the ring is discouraged.

The position of the skeletal atom that is removed is denoted in all cases by its locant in the numbering of the parent structure.

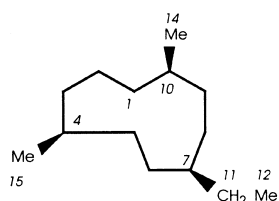
Note: A capital letter, associated with the locant of a skeletal atom where needed, has been used with prefixes such as 'nor-' and 'dinor-' to indicate removal of methylene groups from a particular ring. This system is used in *Chemical Abstracts* index nomenclature, but is not included in Section F because it is not as general as the locant system recommended here.

Although, because the locant of each skeletal atom removed is cited, an unambiguous name can be generated by the removal of any skeletal atom, it is traditional to remove skeletal atoms with the highest possible locant in an atomic connector in a cyclic portion of the skeletal structure. An atomic connector is a chain of homogeneous skeletal atoms of the same element connecting any combination of bridgehead or ring junction atoms, rings or ring systems (i.e. ring assemblies), substituted skeletal atoms in the parent structure, or heteroatoms. In an acyclic portion of a skeletal structure, the skeletal atom removed preferably is the one of an acyclic atomic connector or a terminal segment nearest to the free end of the acyclic part of the structure. (This is done in order to maintain as far as possible traditional numbering of structural features of the compound and of compounds derived from it.) A terminal segment of a skeletal structure is an acyclic segment of homogeneous skeletal atoms connected at only one end by the features of structure that terminate atomic connectors (see above) (Scheme 1, 2).

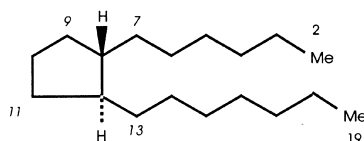
RF-4.1.2 When the removal of an unsaturated skeletal atom from a ring containing the maximum number of noncumulative double bonds in the fundamental parent structure results in the creation of a saturated ring position, this position is described by indicated hydrogen symbolism. When there is a choice, the indicated hydrogen symbol (*H*) is assigned to the lowest numbered nonangular position in the unsaturated portion of the structure (e.g. Scheme 3).

RF-4.2. Addition of skeletal atoms without affecting the number of rings.

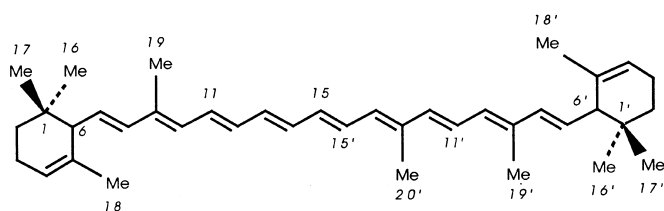
RF-4.2.1. The addition of a methylene ($-\text{CH}_2-$) group between two skeletal atoms of a fundamental parent structure is described by the prefix 'homo-'; the addition of two or more methylene groups is indicated by combining an appropriate numerical prefix with 'homo-', e.g. 'dihomo', 'trihomo-', etc.



13-Norgermacrane

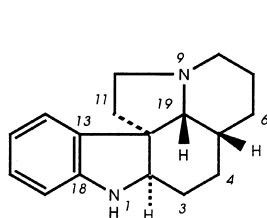


1,20-Dinorpropane

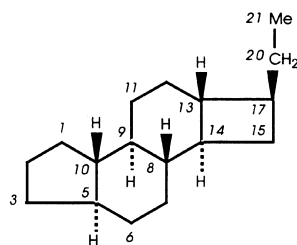


20-Nor-ε,ε-carotene

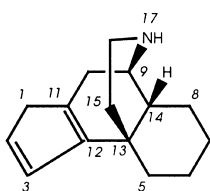
Scheme 1



20,21-Dinoraspidospermidine

4,16,18,19-Tetranor-5α-pregnane
(has been called A,D(15),18,19-Tetranor-5α-pregnane)

Scheme 2



1H-4-Normorphinan

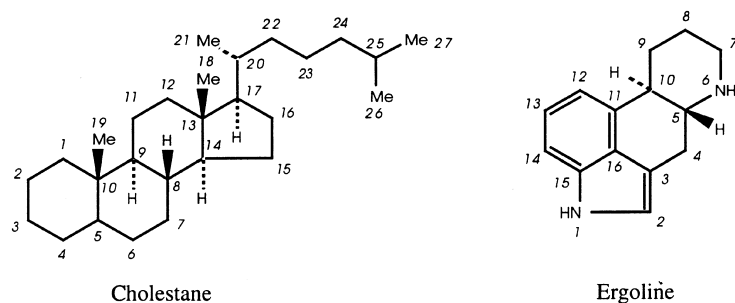
Scheme 3

Positions of inserted methylene groups in the modified fundamental parent structure are indicated by the locants of the added methylene group which are cited in front of the prefixes, 'homo', 'dihomo-', etc.

Note: Capital letters, associated with locants of added methylene groups, where needed, have been used with prefixes such as 'homo-' and 'dihomo-' to indicate insertion of methylene groups into particular rings. This system is used in Chemical Abstracts index nomenclature, but is not included in these Section F recommendations because it is not as general as the locant system recommended here.

The assignment of the locant to an added methylene group depends on whether it is considered to be

inserted into an atomic connector or terminal acyclic segment (see also RF-4.1.1) or into a bond connector. A bond connector is a connection between any combination of bridgehead or ring junction atoms, rings or ring systems (i.e. ring assemblies), substituted skeletal atoms, or heteroatoms. The structures below illustrate atomic connectors, bond connectors, and terminal segments (Scheme 4).



Scheme 4

Atomic connectors:

In cholestane: 1–4, 6–7, 11–12, 15–16 and 22–24.

In ergoline: 2, 4, 7–9 and 12–14.

Terminal segments:

In cholestane: 18, 19, 21, 26 and 27.

In ergoline: None.

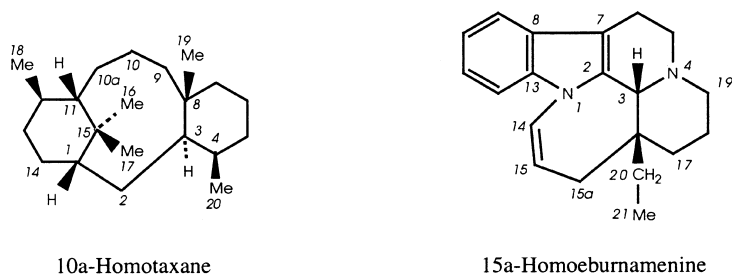
Bond connectors:

In cholestane: 5–10, 8–9, 8–14, 9–10, 13–14, 13–17 and 17–20.

In ergoline: 1–15, 3–16, 5–6, 5–10, 10–11, 11–16 and 15–16.

RF-4.2.2. Numbering of additional skeletal atoms.

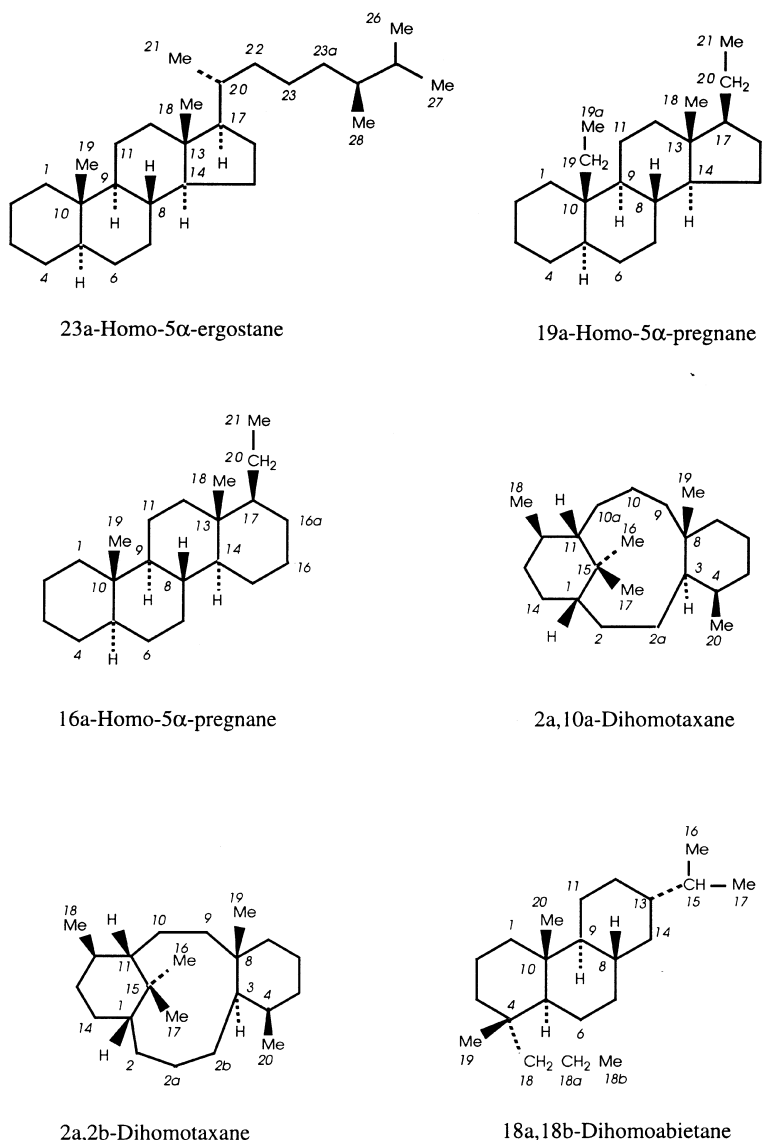
RF-4.2.2.1. Methylene groups inserted into an atomic connector or into a terminal segment are identified by adding a letter 'a', 'b', etc., to the locant of the highest numbered skeletal atom of the atomic connector or terminal segment consistent with the location of double bonds remaining in the structure (compare example 2 below and example 3 under RF-4.2.2.2). If there are equivalent atomic connectors, the highest numbered atomic connector is chosen, and the methylene group is inserted after the highest numbered skeletal atom in that connector (e.g. Schemes 5, 6).



Scheme 5

Note: Addition of acyclic side chains or extension of terminal segments of a side chain already attached to the basic skeleton of a fundamental parent structure may also be done by principles of substitutive nomenclature.

RF-4.2.2.2. Methylene groups inserted into a bond connector are identified by citing both locants of



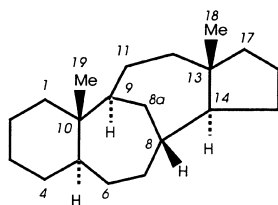
Scheme 6

the skeletal atoms terminating the bond connector enclosing the second (higher) number in parentheses, followed by a letter 'a', 'b', etc. according to the number of methylene groups.

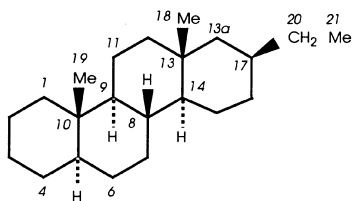
Note: The insertion of a methylene group into a bond connector has been described by combining the capital letter(s) of the expanded ring(s) with the locant of the inserted atom derived by adding a letter 'a', 'b', etc., to one of the locants for the skeletal atoms terminating the ring bond connector (Rule 3S-7.3 [4]) (e.g. Scheme 7).

RF-4.2.3. The insertion of a methylene group into a ring or a ring system of a fundamental parent structure that contains the maximum number of noncumulative double bonds or into a cyclic system of conjugated double bonds may create a saturated ring position that is indicated by 'indicated hydrogen'. The position of the inserted methylene group is prescribed by Rule RF-4.2.2, even though the saturated ring position may be elsewhere in the unsaturated ring system as denoted by the appropriate locant for the indicated hydrogen (e.g Scheme 8).

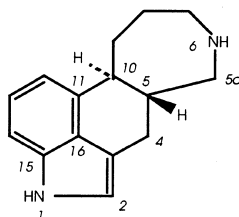
Note 1: Although it would be quite easy to justify the omission of indicated hydrogen when the saturated position is the same as the inserted methylene group, this should not be encouraged.



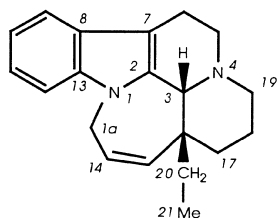
8(9)α-Homo-5α-androstane



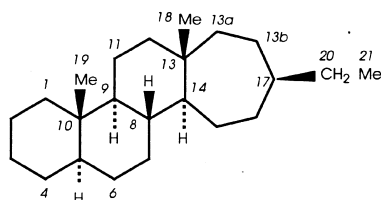
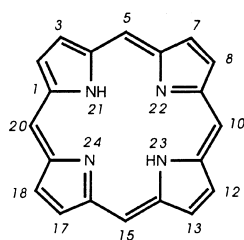
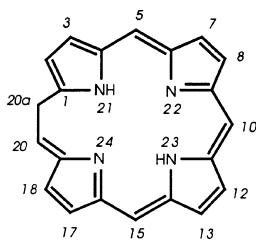
13(17)α-Homo-5α-pregnane



5(6)α-Homoergoline



1(14)α-Homoeburnamenine

13(17)α,13(17)β-Dihomo-5α-pregnane
(has also been called
D(17a,17b)-Dihomo-5α-pregnane)**Scheme 7**Porphyrin (fundamental
parent structure)

20aH-20a-Homoporphyrin

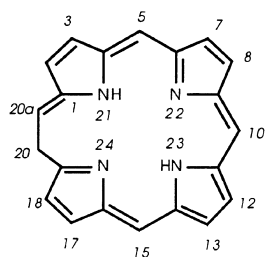
Scheme 8

Note 2: The name 20H-20a-Homoporphyrin describes an alternative tautomeric form shown in Scheme 9.

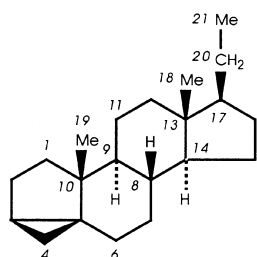
RF-4.3. Bond formation. The creation of an additional ring by means of a direct link between any two atoms of a fundamental parent structure is described by the prefix *cyclo* preceded by the locants of the skeletal atoms so connected. Where necessary, the stereochemical configurations created by the new bond are denoted by α, β, or ξ as described under RF-10 (e.g. Scheme 10, 11).

RF-4.4. Bond cleavage

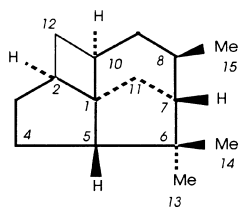
RF-4.4.1. Cleavage of a ring bond (saturated or unsaturated) with addition of the appropriate number



Scheme 9

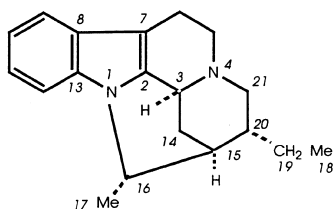


3 α ,5-Cyclo-5 α -pregnane
(note that the cyclo bond in this drawing is α relative to the other three bonds)

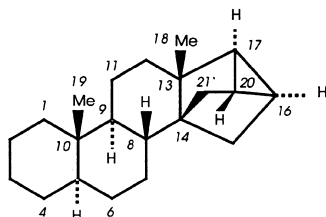


10 β ,12-Cyclocedrane
(note that the locants for the methyl groups at position 6 were reversed in the provisional Section F Rules^{1,2})

Scheme 10



16 β H-1,16-Cyclocorynan
(see RF-4.5.1 for the use of β H)



(20*S*)-14,21:16 β ,20-Dicyclo-5 α ,14 β -pregnane (see RF-10.2.1 for the use of β at position 14)

Scheme 11

of hydrogen atoms at each new terminal group thus created, is indicated by the prefix 'seco-' and the locants of the cleaved bond. The original numbering is retained (e.g. Schemes 12, 14).

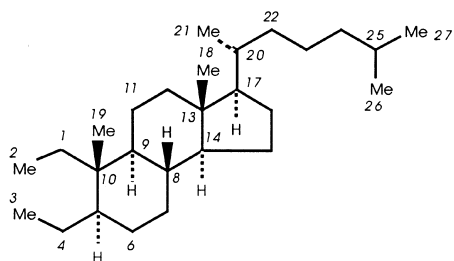
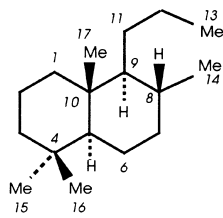
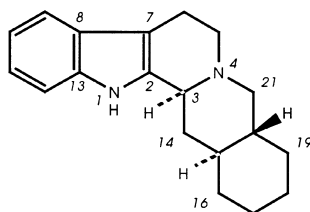
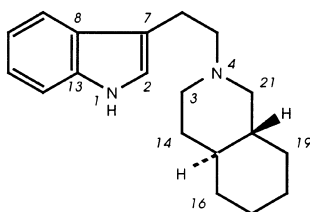
Note: The configuration at positions 15 and 20 of the secoyohimban in Scheme 12 relates to the stereochemistry of the parent structure only if drawn in the same orientation.

Although having the same absolute configuration, the stereochemistry denoted by α - and β - at these positions could be reversed in an alternative orientation as shown in Scheme 13.

This situation has been recognized in the recommendations for naming Vitamin D compounds (9, 10-seco steroids [6]) where sequence rule descriptors (*R/S*) are recommended for describing all configurations in ring A, since these compounds are often drawn in an alternative orientation.

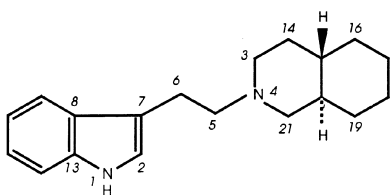
RF-4.4.2. The unitalicized prefix 'apo-' preceded by a locant is used to indicate removal of all of a side chain of a fundamental parent structure beyond the skeletal atom corresponding to that locant. Removal of two or more side chains is indicated by the prefixes 'diapo', 'triapo-', etc., preceded by appropriate locants. Numbering of the skeletal atoms in the parent structure is retained in the resulting fragment.

Note: This procedure has been used only in carotenoid nomenclature (Scheme 15) [5].

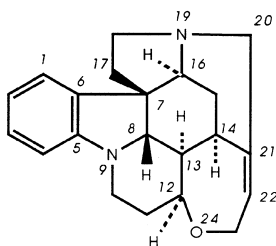
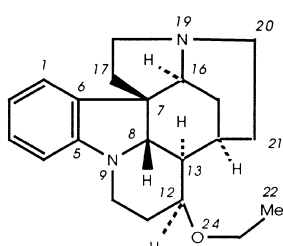
2,3-Seco-5 α -cholestane13,14-Secopodocarpane
(also may be named 8 β -14,15,16-Trinorlabdane by RF-4.1)Yohimban (fundamental
parent structure)

2,3-Secoyohimban

Scheme 12

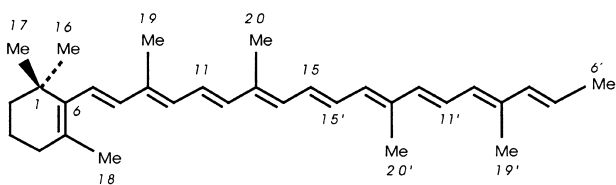


Scheme 13

Strychnidine (fundamental
parent structure)

21,22-Secostrychnidine

Scheme 14

6'-Apo- β -carotene

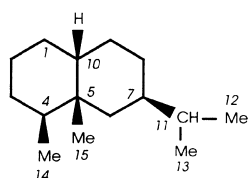
Scheme 15

RF-4.5. Bond migration. Parent structures that are not simple derivatives of accepted fundamental parents, but may be considered to arise from such parents by migration of one or more bonds, may be named by the following methods.

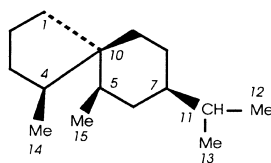
RF-4.5.1. The prefix X(Y→Z)-abeo- designates the migration of one end of a single bond from its original position in a fundamental parent structure to another position. In this prefix, X is the locant of the stationary, i.e. unchanged, end of the migrating bond; Y is the locant of the position of the moving end of the migrating bond in the fundamental parent structure; and Z is the locant of the position of the moving end of the migrating bond in the final structure. The numbering of the fundamental parent structure is retained in the new structure.

Stereochemical configurations of the fundamental parent structure are retained. New stereochemistry of ring atoms having one hydrogen atom still present is indicated by the α/β system, or, if necessary by the Sequence Rule method (R/S). The projection of the hydrogen atom below (α) or above (β) the reference plane of the ring system is indicated by the appropriate symbol and a capital italic letter *H* following the locant of the ring atom in the structure, all enclosed in parentheses, and cited before the 'abeo-' prefix described above.

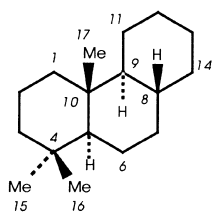
Other new stereochemistry is described by the Sequence Rule System (Scheme 16).



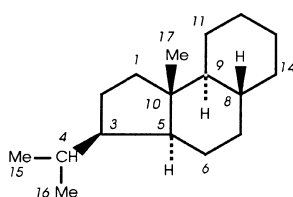
Eremophilane (fundamental parent structure)



(10*R*)-4(5→10)-Abeoeremophilane



Podocarpane (fundamental parent structure)



(3 α *H*)-5(4→3)-Abeopodocarpane

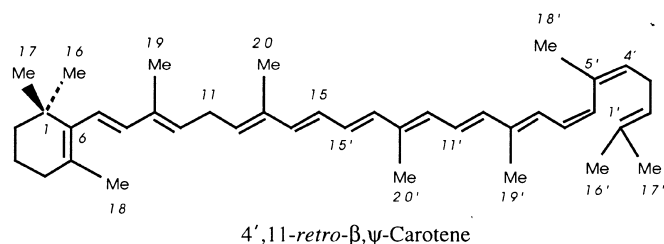
Scheme 16

Note: The prefix 'A-Neo-' has been used to describe the bond migration shown in this last example. However, the 'abeo' operation is preferred because it is general.

RF-4.5.2. The italic prefix '*retro*-' , preceded by a pair of locants is used to indicate a shift, by one position, of all single and double bonds of a conjugated polyene system delineated by the pair of locants that are not part of a system of maximum number of noncumulative double bonds in a ring or ring system. The first locant is the skeletal atom that has lost a hydrogen atom and the second the one that has gained a hydrogen atom. 'Retro' has been used in this manner in the nomenclature of carotenoids (e.g. Scheme 17).

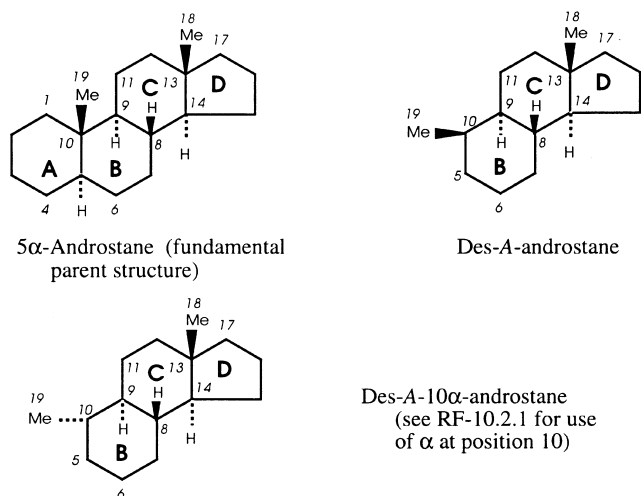
Note 1: The prefix '*retro*-' has been used in steroid nomenclature to indicate a 9 β ,10 α -configuration instead of the implied configuration, but is not recommended.

Note 2: The prefix '*retro*-' is also used to designate a peptide in which the amino acid sequence is the reverse of the sequence of the naturally occurring peptide.



Scheme 17

RF-4.6. Removal of a terminal ring. The removal of a terminal ring from a fundamental parent structure of a natural product with the addition of an appropriate number of hydrogen atoms at each junction with the adjacent ring is indicated by the prefix 'des-' followed by the capital italic letter of the ring removed (see RF-3.6). Stereochemistry implied by the name of the fundamental parent structure remains the same unless otherwise specified. Numbering of skeletal atoms in the parent structure is retained in the modified structure (e.g. Scheme 18).

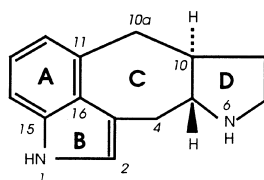


Scheme 18

RF-4.7. Combinations of prefixes for modifying a fundamental parent structure. The modifications to a fundamental parent structure prescribed by the prefixes in the preceding recommendations (RF-4.1 through RF-4.6) may be combined to effect even more drastic changes in structure. The operation indicated by each prefix is applied to the fundamental parent structure sequentially as one 'advances backwards', i.e. moves from right to left, from the name of the fundamental parent structure. The following recommendations are not rigorous rules for choosing a unique name, but are intended to be guidelines for choosing combinations of prefixes and for the order of citation in generating an unambiguous name.

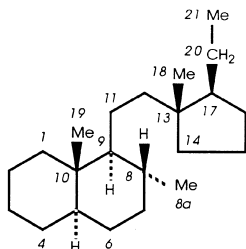
RF-4.7.1. When different combinations of prefixes can be used to effect the same transformation in structure, the combination of choice should express the fewest number of operations. When the number of operations is the same, the combination of homo/nor is preferred to cyclo/seco; choice between other combinations expressing the same number of operations is based on earliest alphabetic order of the prefixes (Scheme 19).

RF-4.7.2. The order of citation of combinations of structure modifying prefixes must avoid improper use of the prefixes as defined above or impossible situations when the corresponding operations are carried out in the manner prescribed above (Scheme 20).



10(11)a-Homo-9-norergoline
(not 5,9-Cyclo-5,10-secoergoline;
also has been called
C(10a)-Homo-D-norergoline)

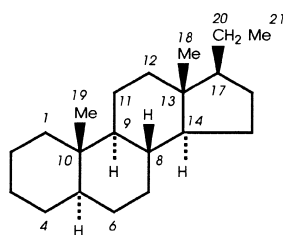
Scheme 19



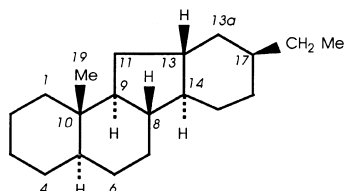
8a,14-Seco-8(14)a-homo-5 α -pregnane
(the ring expansion is followed by
the bond cleavage; a methyl-seco
name might also be used)

Scheme 20

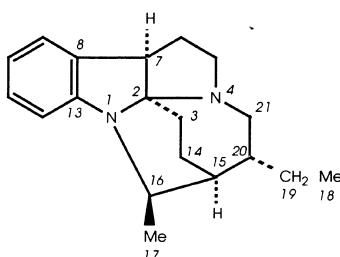
RF-4.7.3. (Alternative to RF-4.7.4). After satisfying RF-4.7.1. and RF-4.7.2., combinations of structure modifying prefixes are cited in alphabetic order from left to right proceeding towards the name of the fundamental structure. Numerical prefixes denoting multiple operations of the same kind do not affect the order (Scheme 21).



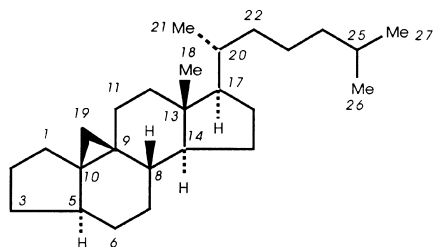
5 α -Pregnane (fundamental parent structure)



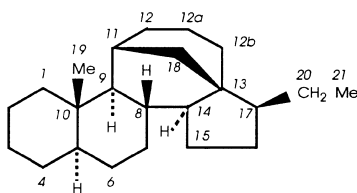
13(17)a-Homo-12,18-dinor-5 α -pregnane



(2*S*,7 α ,16 α H)-7*H*-1,16:2,4-Dicyclo-
3,4-secoecorynan



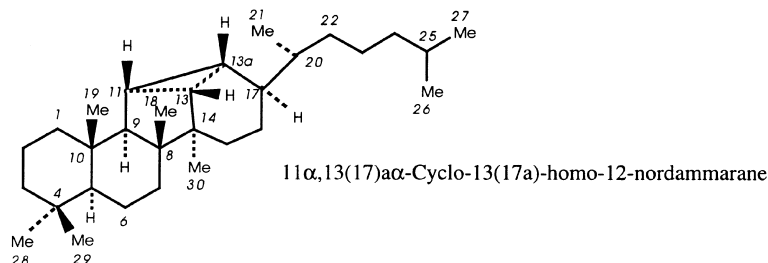
9 β ,19-Cyclo-4-nor-5 α ,9 β -cholestane



11 β ,18-Cyclo-12a,12b-dihomo-
5 α -pregnane

Scheme 21

Note: The cyclodihomopregnane example above can be named in at least two other ways: (1) 11 α ,18b-Cyclo-18a,18b-dihomo-5 α ,13 α -pregnane; (2) 11 α ,13-Propano-18-nor-5 α ,13 α -pregnane. The first name uses the same number of operations, but extends a side chain rather than enlarging a ring (the latter operation seems more usual) resulting in higher locant numbers. The second name uses only one operation of the type discussed in this section, but requires the use of a bridge (see RF-6), which may or may not be considered preferable.

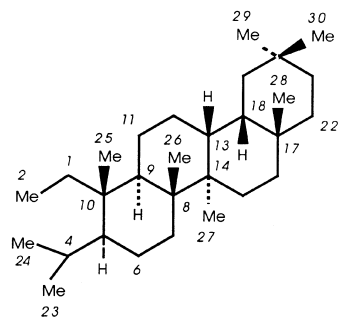


Scheme 22

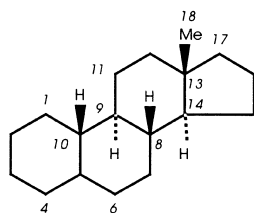
RF-4.7.4. (Alternative to RF-4.7.3). After satisfying RF-4.7.1 and RF-4.7.2., the prefixes that indicate atomic replacement (oxa, aza, etc.) are cited, followed by those showing bond rearrangements (abeo, cyclo, retro, seco, etc.), followed by those that indicate addition or removal of skeletal atoms (apo, de, des, nor). If more than one of any of these operations is needed, they are cited in alphabetic order before the name of the parent structure. Schematically, this order is as follows:

replacement	bond rearrangements	removal/addition of skeletal atoms	parent structure
aza, oxa, etc.	abeo, cyclo, retro, seco	apo, de, des, homo, nor	

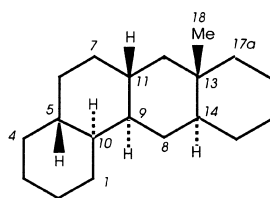
(Examples in Scheme 23)



2,4-Seco-3-noroleanane
(may be named 3-Nor-2,3-secooleanane by RF-4.7.3, above, which is preferable to 24-Nor-2,3-secooleanane or 3-Nor-3,4-secooleanane on the basis of lower locants)



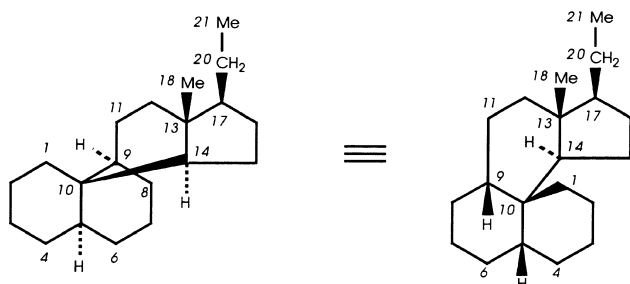
Estrane (fundamental parent structure)



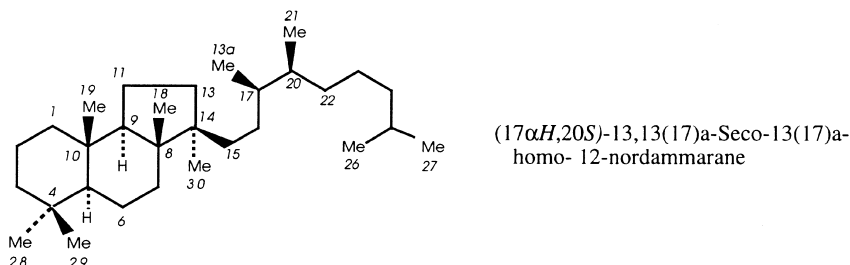
7,11 α -Cyclo-7,8-seco-17a-homo-5 α -estrane
(7,11 α -Cyclo-17a-homo-7,8-seco-5 α -estrane by RF-4.7.3)

Scheme 23

Note. This example can also be named $11\beta H-7(8\rightarrow 11)$ -abeo-17a-homo-5 β ,10 α -estrane, which uses only two operations; however, it requires the use of modified stereochemistry at two implied centers, which may be less preferable.



10,14 β -Cyclo-8,14-seco-19-nor-5 α -pregnane (may also be named 10 β ,14-Cyclo-19-nor-8,14-seco-5 α -pregnane by RF-4.7.3; note the apparent change in configuration in the alternative drawing -- see the note following the third example under RF-4.4.1)



(17 αH ,20 S)-13,13(17) a -Seco-13(17) a -homo-12-nordammarane

Scheme 24

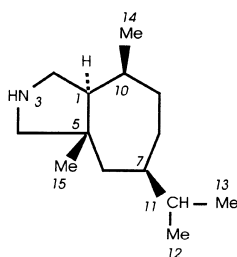
RF-5. Replacement of skeletal atoms in parent structures whose names are formed according to RF-3 and RF-4 above is indicated by extending the principles of organic replacement nomenclature (see rules B-4 [2] and C-0.6 [2]).

RF-5.1. The replacement of a carbon atom in the skeletal system of a parent structure by a heteroatom is described by appropriate replacement 'a' prefixes (see R-9.3 [3]). This procedure is used even though the parent structure may already be a heterocycle. The numbering of the parent structure is retained (e.g. Scheme 25).

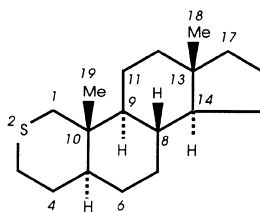
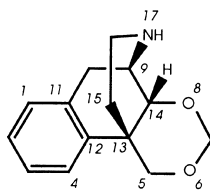
RF-5.2. The replacement of a heteroatom in a parent structure of a natural product by a carbon atom is described by the replacement prefix 'carba'. The original numbering is retained. If the heteroatom in the parent structure is unnumbered, the replacing carbon atom is numbered by affixing the letter 'a' to the locant of the immediately adjacent lower numbered skeletal atom. If the immediately adjacent lower numbered skeletal atom is a 'homo' atom, the letter 'b', 'c', etc., as appropriate is used. Stereochemical configuration at the new carbon skeletal atom is described by methods for specifying additional stereochemistry (see RF-10.2) (e.g. Scheme 26).

RF-5.3. Replacement of a heteroatom in a parent structure by another heteroatom is denoted by the appropriate replacement ('a') prefix (e.g. Scheme 27).

RF-5.4. Indicated Hydrogen. When the replacement of a skeletal atom in a portion of the structure of a fundamental parent structure that contains the maximum number of noncumulative double bonds or an extended conjugated system of double bonds results in the creation of a saturated skeletal position, that position is indicated by the symbolism of indicated hydrogen (e.g. Scheme 28).

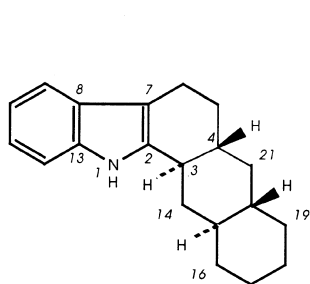
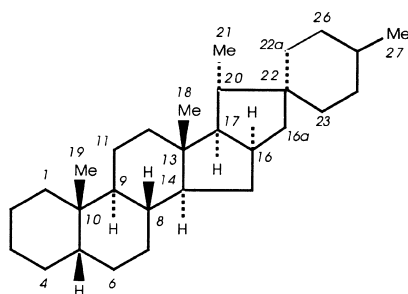


3-Azaambrosane

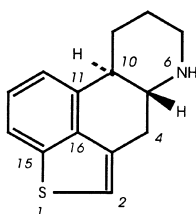
2-Thia-5 α -androstane

6,8-Dioxamorphinan

Scheme 25

(4 β)-1H-4-Carbayohimban16a,22a-Dicarba-5 β -spirostan

Scheme 26

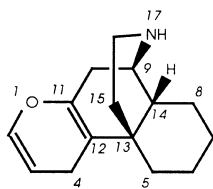


1-Thiaergoline

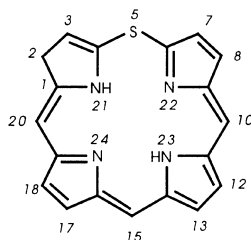
Scheme 27

RF-6. Fusion of additional rings. It is often convenient to retain the advantages of a sernisystematic natural product name, particularly with regard to stereochemistry, for naming structures having rings or ring systems fused to a fundamental parent structure of a natural product.

Since most natural products with cyclic structures have fundamental parent structures that are fully saturated and fusion nomenclature principles are based on the concept of the presence of the maximum number of noncumulative double bonds, adaptations of general fusion nomenclature are necessary. These



4H-1-Oxamorphinan

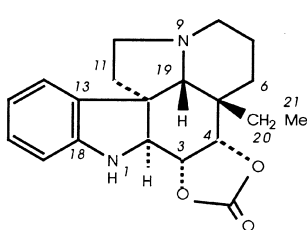
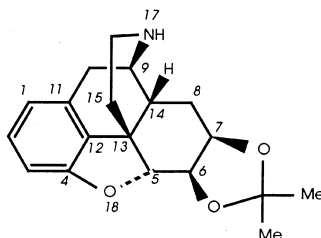
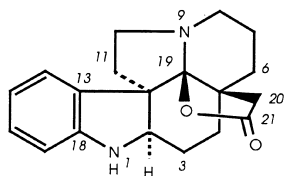


2H-5-Thiaporphyrin (the name porphyrin implies two saturated positions normally shown at 21 and 23)

Scheme 28

adaptations are described in the recommendations that follow. No attempt is made to legislate rigidly or to cover every case. The decision between a fusion-natural product name and a systematic fusion name is left to choice based on particular circumstances in each case.

RF-6.1. Rings or ring systems fused to a fundamental parent structure of a natural product when derived from functional groups, such as lactones or cyclic acetals, are preferably named by the usual methods of organic nomenclature for such cyclic functional groups (see also RF-6.2.2) (e.g. Scheme 29).

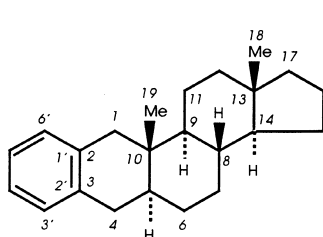
Aspidospermidine-3 α ,4 α -diyl carbonateAcetone 4,5 α -epoxymorphinan-6 β ,7 β -diyl acetal (for use of epoxy as a bridge, see RF-7)21-Noraspidospermidine-20,19-carbolactone
(also named 19-Hydroxyaspidospermidino-21,19-lactone)

Scheme 29

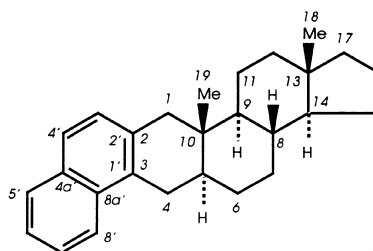
RF-6.2. The fundamental parent structure of the natural product as a component is used in its normal state of saturation or unsaturation. Accordingly, a double bond is not cited in the natural product parent at the fusion site just because the other component contains the maximum number of noncumulative double bonds. Hence, the bonding at a fusion site is governed usually by the non-natural product component; fusion resulting in a quaternary carbon atom at the fusion site also affects the bonding (see RF-6.2.3, below).

RF-6.2.1. A ring or ring system of systematic organic nomenclature [2] (carbocyclic or heterocyclic) fused to a fundamental parent structure is described by its fusion prefix name (see A-21.4 and B-3) [2] prefixed to the name of the fundamental parent structure. The position of the fusion is indicated by sets of locants, as needed, separated by a colon, enclosed in square brackets, and inserted into the name between the components. The skeletal atoms of the natural product are identified by plain

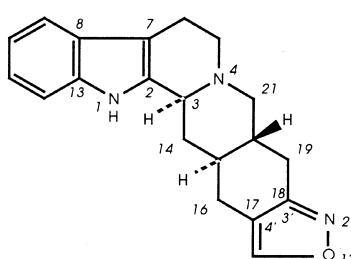
(unprimed) locant numbers and the 'systematic' component by primed locant numbers. Where there is a choice, the locant numbers for the systematic component are as low as possible and are cited in the same direction of numbering as for the natural product component. Terminal vowels of the names of systematic components are not elided when followed by a vowel (this is consistent with the recommendation contained in the fused ring nomenclature report and is a change from previous recommendations) [7] (e.g. Scheme 30).



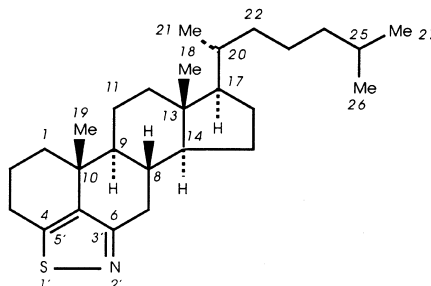
Benzo[2,3]-5 α -androstane
(note that only one set of locants, that of the androstane component, is needed here; the CA Index name is Benz[2,3]androst-2-ene, (5 α -))



Naphtho[2',1':2,3]-5 α -androstane



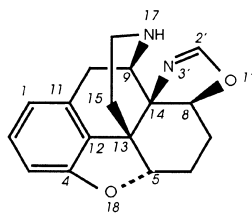
1*H*-Isoxazolo[4',3':17,18]yohimban



Isothiazolo[5',4',3':4,5,6]cholestane

Scheme 30

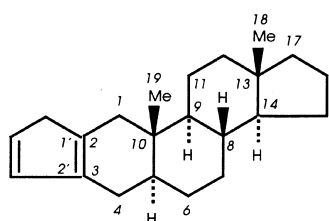
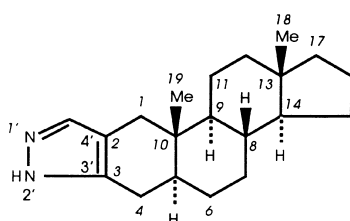
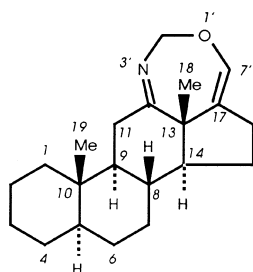
RF-6.2.2. The systematic organic component fused to the fundamental parent component of a natural product structure contains the maximum number of noncumulative double bonds consistent with the bonding requirements at the fusion site. Saturated positions on the systematic component, including the fusion sites, that have at least one hydrogen atom are designated by the indicated hydrogen symbolism (see A-21.6) [2]. Locants of the systematic component are used to identify the position of the indicated hydrogen, where there is a choice (e.g. Scheme 31,32).



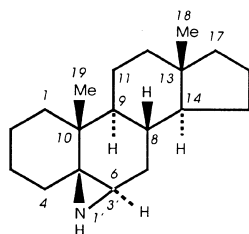
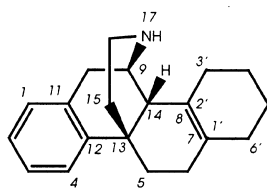
8 α H-4,5 α -Epoxyoxazolo[5',4':8,14]morphinan

Scheme 31

RF-6.2.3. Saturated, or partially saturated, carbocyclic and heterocyclic ring components fused to the fundamental parent structure of a natural product are named using hydro prefixes. Where there is a choice, the unprimed locant numbers of the systematic component are used (e.g. Scheme 33).

5'*H*-Cyclopenta[2,3]-5 α -androstane2'*H*-Pyrazolo[4',3':2,3]-5 α -androstane2'*H*-[1,3]Oxazepino[4',5',6':12,13,17]-5 α -androstane

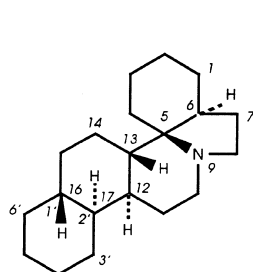
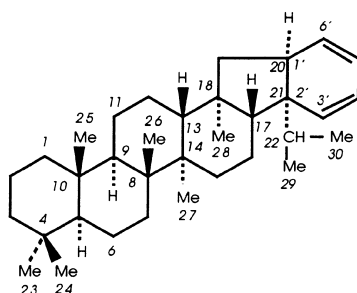
Scheme 32

1',6 α -Dihydroazirino[2',3':5,6]-5 β -androstane

3',4',5',6'-Tetrahydrobenzo[7,8]morphinan

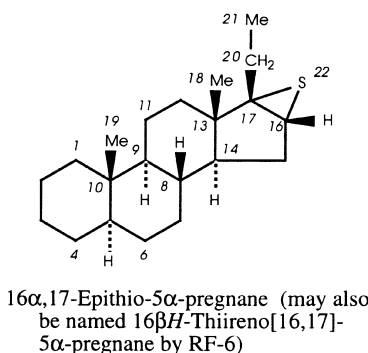
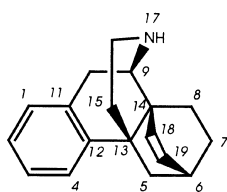
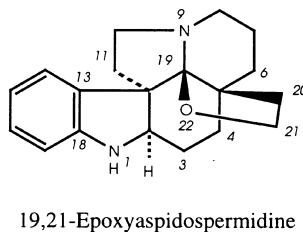
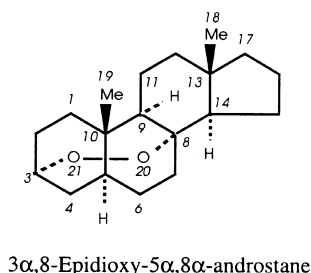
Scheme 33

RF-6.2.4. Stereochemistry in fused rings or hydrogenated derivatives is cited by the α/β symbolism in accordance with its use in the steroid nomenclature recommendations (see 3S-1.4 [4] and RF-10) or by the Sequence Rule method (*R/S*) (see also RF-10) (e.g. Scheme 34).

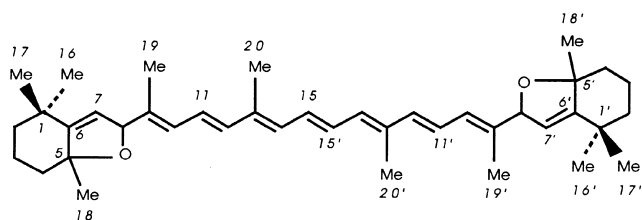
3',4',5',6',12 α ,13 β ,14,15,16 β ,17 α -Decahydrobenzo[16,17]erythrinan20 α *H*-Benzo[20,21]-(21 β *H*)17(22→21)-abeogammacerane (also has been named 1'*H*-Benzo[20,21]-*A'*-neogammacerane)

Scheme 34

RF-7. Bridged fundamental parent structures. Atomic bridges added to fundamental parent structures of natural products may be described by the methods used in systematic organic nomenclature (A-34 [2], B-15.1 [2] and R-9.2 [3]). This method is often used with hetero atom bridges. In fact, this method is often more useful than fusion procedures for describing certain types of heterocyclic rings fused to a fundamental parent structure, for instance, oxireno (epoxy) and thiireno (epithio). Bridge prefixes are always nondetachable (e.g. Schemes 35, 36).



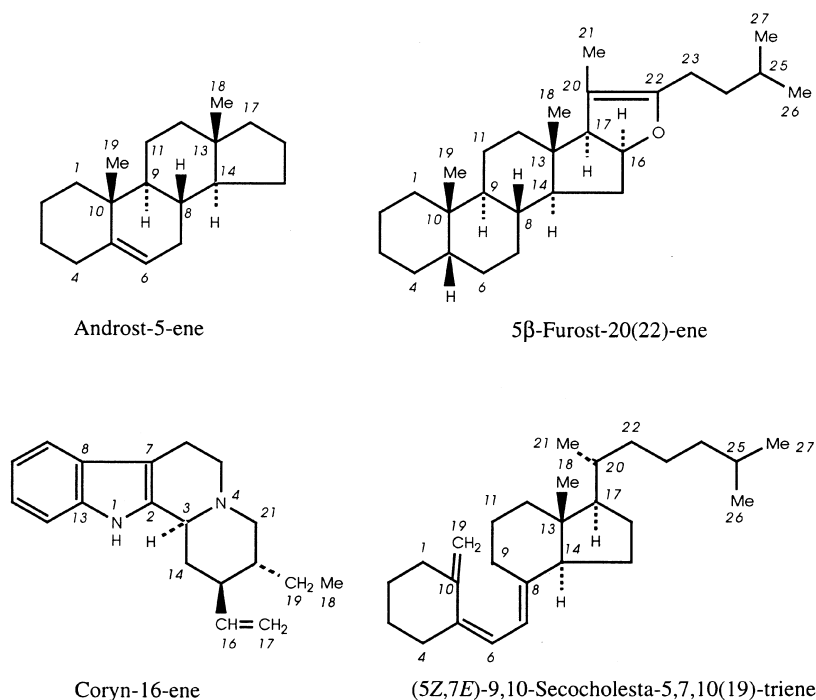
Scheme 35



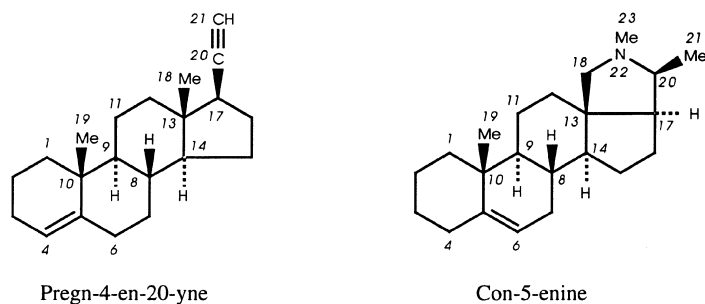
Scheme 36

RF-8. Bond order modification

RF-8.1. Unsaturation in a compound whose parent structure (see RF-3 through RF-7) is fully saturated or in the portion of a parent structure that is otherwise fully saturated and whose name ends in 'an', 'ane', or 'anine' (see 3S-2.5 in the steroid nomenclature recommendations [4]) is indicated by changing -an or -ane to -ene, -adiene, -yne, etc. or -an to -en-, -adien-, -yn-, etc. (Rule RF-3.1.1). Locants (numerals and/or letters) are placed immediately before the part of the name to which they relate (see R-0.1.2 [3]) (Scheme 37, 38).



Scheme 37



Scheme 38

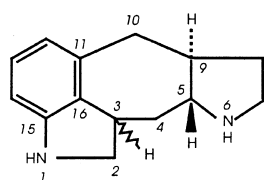
RF-8.2. Saturation of double bonds in a parent structure (see RF-3 through RF-7) whose name implies the presence of isolated double bonds and/or a system of conjugated double bonds is described by the prefix 'hydro-', itself prefixed by an appropriate numerical term (e.g. Scheme 39).

RF-8.3. The introduction of unsaturation additional to any implied in a parent structure (see RF-3 through RF-7) whose name does not end in 'an', 'ane' or 'anine'; the conversion of an implied double bond to a triple bond; and the introduction of an additional double bond with rearrangement of an implied double bond, are denoted by the prefix 'dehydro-', itself prefixed by a numerical term equal to the number of hydrogen atoms removed and the appropriate locants (e.g. Schemes 40, 41).

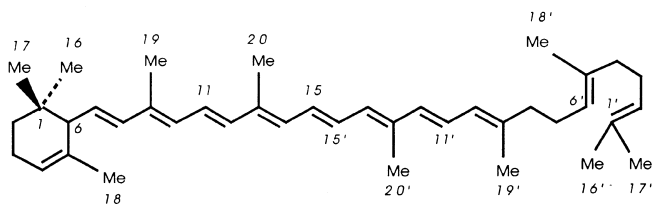
RF-8.4. Rearrangement of a double bond may be indicated by a combination of hydro and dehydro prefixes (e.g. Scheme 42).

RF-9. Derivatives of parent structures are named according to the usual methods of systematic organic nomenclature [2,3] as far as possible.

RF-9.1. The prefixes and suffixes of organic nomenclature are used in the prescribed manner to name atoms and groups that are considered to substitute for hydrogen atoms of parent structures. In naming

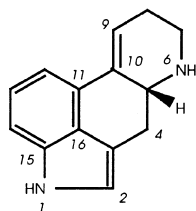


2,3ξ-Dihydro-9αH-5(10→9)-abeoergoline



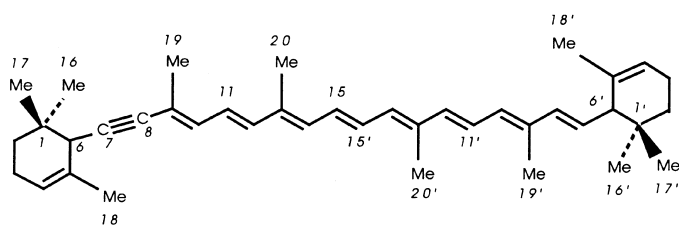
7',8'-Dihydro-ε,ψ-carotene

Scheme 39

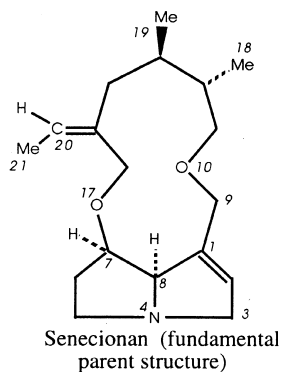


9,10-Didehydroergoline

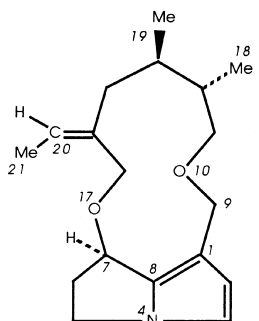
Scheme 40



7,8-Didehydro-ε,ε-carotene

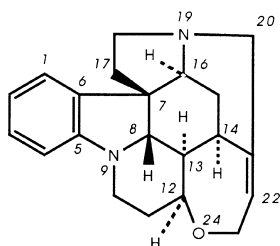


Senecionan (fundamental parent structure)

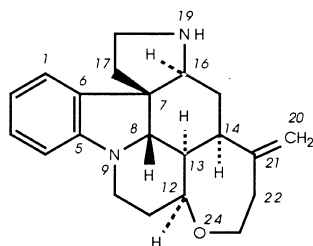


3,8-Didehydrosenecionan

Scheme 41



Strychnidine (fundamental parent structure)

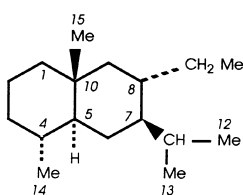
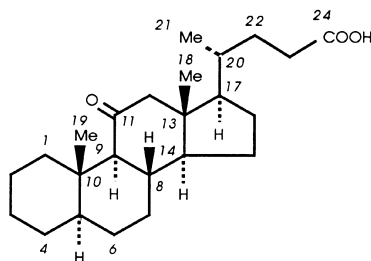
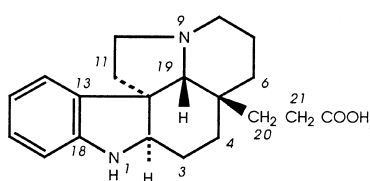


20,21-Didehydro-21,22-dihydro-19,20-secostrychnidine

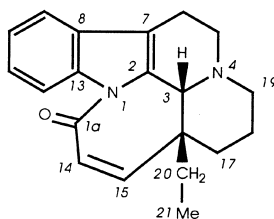
Scheme 42

derived acids and related characteristic groups, unmodified parent structures are used as far as possible (e.g. Scheme 43).

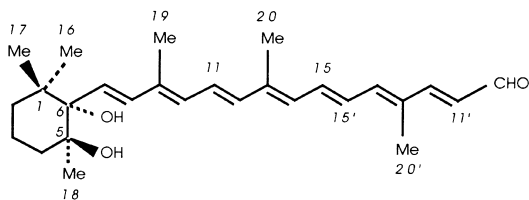
RF-9.2. Modifications to principal characteristic groups, such as esters, acetals, etc., are named by the usual methods of organic nomenclature. Cyclic modifications, such as lactones, cyclic acetals, etc., are named preferably as such rather than as fused ring, bridged, or spiro modified parent structures (see also RF-6.1) (e.g. Scheme 44).

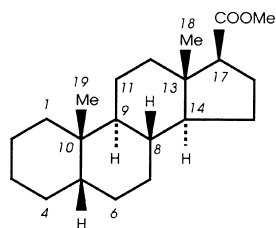
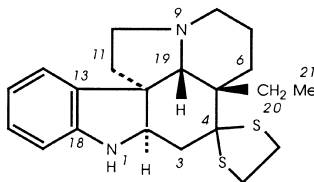
8 α -Ethyleudesmane11-Oxo-5 α -cholan-24-oic acid

Aspidospermidine-21-carboxylic acid



1(14)a-Homoeburnamenin-1(14)a-one

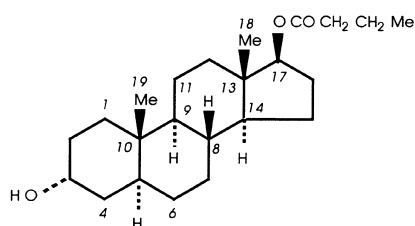
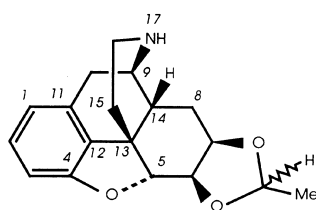
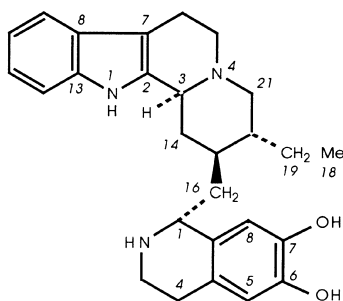
(5*S*,6*S*)-5,6-Dihydroxy-5,6-dihydro-10'-apo- β -caroten-10'-al**Scheme 43**

Methyl 5 β -androstane-17 β -carboxylate

Aspidospermidin-4-one ethylene dithioacetal

Scheme 44

RF-9.3. Substituent prefix names for natural product parent structures may be formed in the usual way by adding a suffix, such as ‘-yl’, ‘-diyl’, ‘-ylidene’, to the name of the parent structure with elision of the final ‘e’, if any, of the parent structure name before ‘y’ (e.g. Scheme 45).

3 α -Hydroxy-5 α -androstan-17 β -yl butyrateAcetaldehyde 4,5 α -epoxy morphinan-6 β ,7 β -diyl acetal1,2,3,4-Tetrahydro-1 α -(17-nor corynan-16-yl)isoquinoline-6,7-diol**Scheme 45**

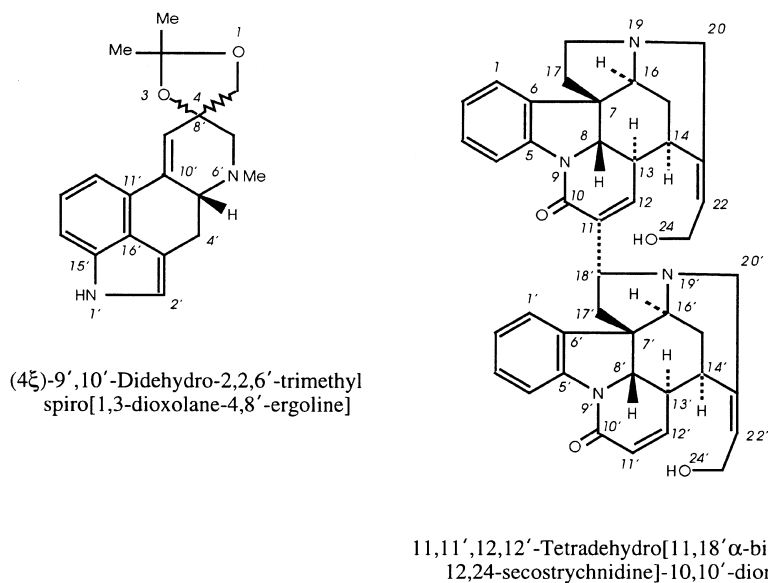
RF-9.4. Ring assemblies and spiro derivatives of parent structures are named in the usual manner [2,3] (e.g. Scheme 46).

Note: In the ring assembly name (dione) in Scheme 46 the hydroxy group is created by the seco operation. To provide for the explicit citation of the hydroxy group as a substituent, the oxygen atom could be removed first using the nor operation; this would be followed by the seco operation and the addition of the prefix ‘hydroxy-’.

RF-10. Stereochemical configuration

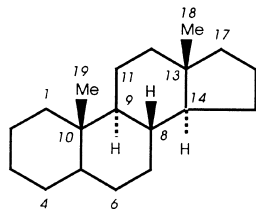
RF-10.1. Names of the fundamental and modified parent structures (see RF-3 through RF-7) imply, without further specification, absolute configuration at all chiral elements as depicted in these recommendations and the following Appendix.

When a planar or quasi-planar system of rings is denoted as a projection on paper, as in these recommendations, an atom or group attached to the ring is called α if it lies below or β if it lies above the plane of the paper. Use of this system requires the orientations of structure as given herein. In the example in Scheme 47,



Scheme 46

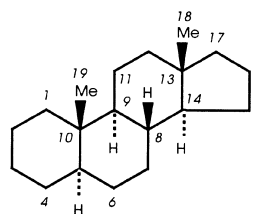
the implied configuration shown defines the attached hydrogen atoms or methyl groups at positions 8, 10 and 13, as β -, and at positions 9 and 14 as α -; here, the hydrogen atom at the chiral position 5 is not known and thus the orientation is ξ (xi). In the case of a racemic compound, that enantiomeric structure drawn should be the one that shows the lowest numbered chiral center in the α - configuration (see also RF-10.4). This may differ from the usual practice, which is to draw the enantiomeric structure having the same absolute configuration as the naturally occurring substance.



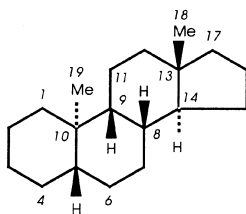
Scheme 47

RF-10.2. Stereochemical configurations that are different from those in the parent structure or that have been generated by substitution, etc.

RF-10.2.1. At chiral centers, the α/β system as described above or by 3S-1.4 in the IUPAC-IUB recommendations for the nomenclature of steroids [4] and Rule E-4.11 of the IUPAC Nomenclature of Organic Chemistry [2] is used (see also Section 2 in the recommendations for the nomenclature of Vitamin D [6]) (Schemes 48, 49).

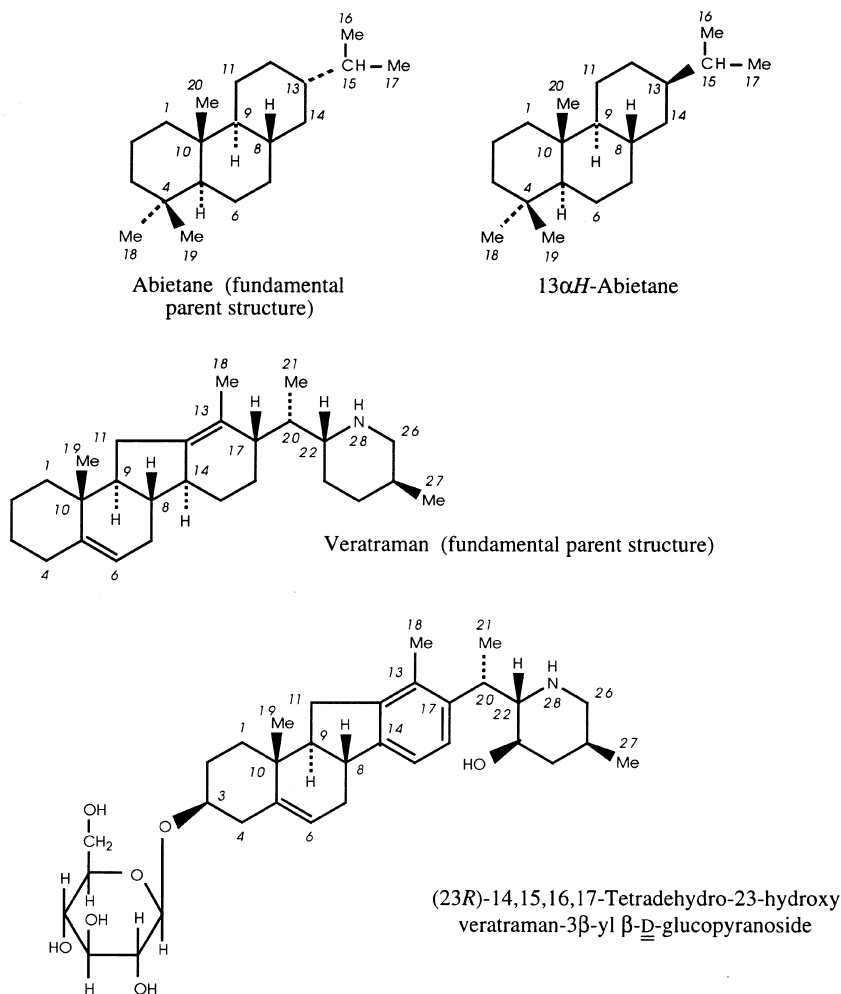


5 α -Androstane (fundamental
parent structure)



5 β ,9 β ,10 α -Androstane

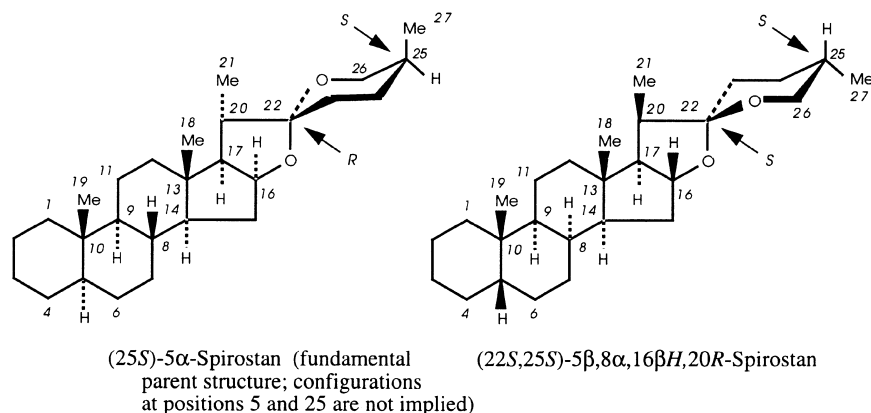
Scheme 48



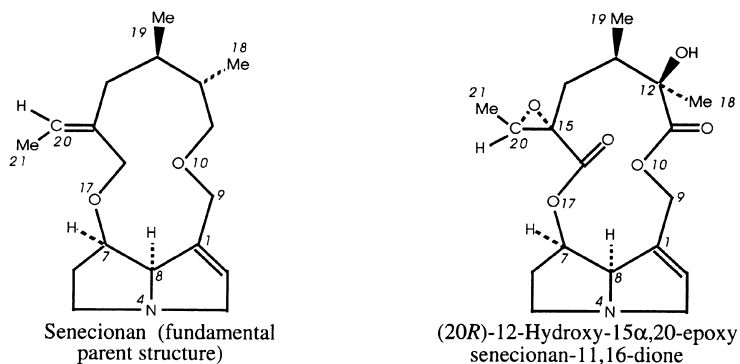
Scheme 49

RF-10.2.2. When the α/β method is not applicable or is not acceptable for the specific natural product class, the *R/S* symbolism of the Sequence Rule System is used (e.g. Schemes 50, 51).

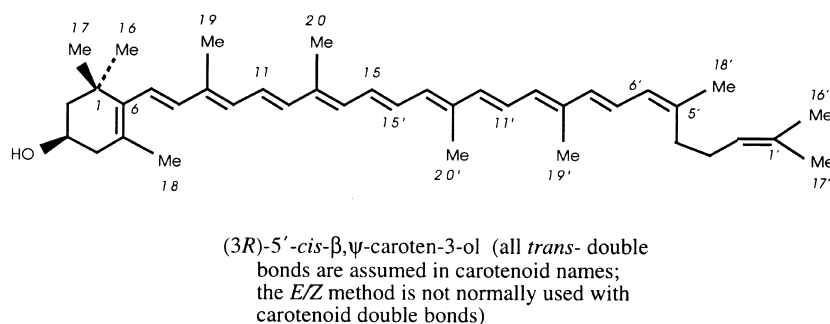
RF-10.2.3. The descriptors *cis/trans* or *E/Z* are used to describe modified or additional stereochemical configurations for double bonds (e.g. Scheme 52).



Scheme 50

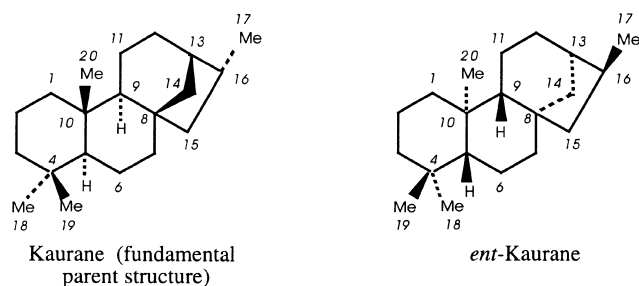


Scheme 51



Scheme 52

RF-10.3. Configurational inversion at all asymmetric centers whose configurations are implied by or stated in the name for the fundamental parent structure is indicated by the italicized prefix *ent*- (a contracted form of *enantio*-) placed in front of the name of the parent structure. (This is a change from that given by 3S-5.1 in the steroid recommendations [3] and by Rule F-6.4 in the provisional Section F recommendations [1,2]) (e.g. Scheme 53, 54).

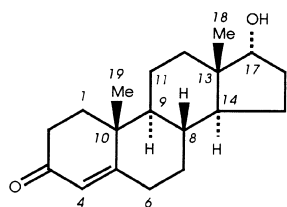
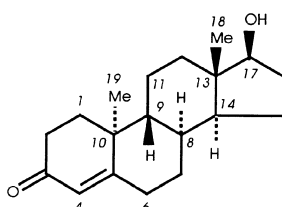


Scheme 53

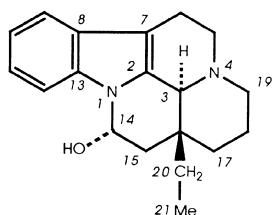
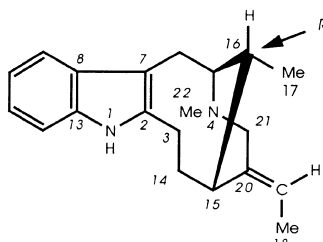
Note: There is confusion in the literature here; some authors (and *Chemical Abstracts*) use Kaurane for the enantiomer called *ent*-Kaurane above.

RF-10.4. Configurational inversion at one asymmetric center whose configuration is implied or stated in the name for the fundamental parent structure can be indicated by the italicized prefix *epi*- (derived from word '*epimer*') placed in front of the name of the parent structure and prefixed by the locant of the affected atom (e.g. Scheme 55).

RF-10.5. Racemates are named by citing the italicized prefix *rac*- (an abbreviation for *racemo*-) in front of the whole name of the compound including the prefix *ent*-, if present. The enantiomer for naming is chosen in accordance with RF-10.1.

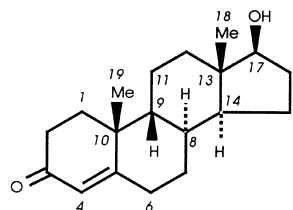
17 α -Hydroxyandrost-4-en-3-one17 β -Hydroxy-*ent*-13 α ,14 β -androst-4-en-3-one
or 17 β -Hydroxy-8 α ,9 β ,10 α -androst-4-en-3-one (see RF-10.2.1) (but not *ent*-17 α -Hydroxy-13 α ,14 β -androst-4-en-3-one)

Scheme 54

3-*epi*-Eburnamin-14 α -ol
(the name Eburnamin
implies a 3 β configuration)16-*epi*-Vobasan (Vobasan
implies a 16 S configuration)

Scheme 55

RF-10.6. When the relative, but not the absolute, configurational relationships among asymmetric centers are known, the symbols R^* and/or S^* are used in accordance with Rule E-4.10 [2]. Alternatively, enantiomers of known relative, but unknown absolute configuration may be distinguished by a prefix (+)-*rel*- or (–)-*rel*-, where the plus and minus sign refer to the direction of rotation of polarized light at the sodium-D line. Hence, the dextrorotatory form of the following structure would be named: (+)-*rel*-17 β -Hydroxy-8 α ,9 β -androst-4-en-3-one (Scheme 56).



Scheme 56

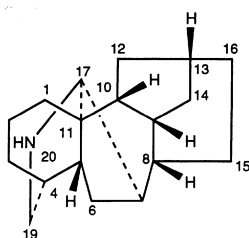
REFERENCES

- 1 International Union of Pure and Applied Chemistry. Nomenclature of Organic Chemistry. Section F—Natural Products and Related Compounds, Recommendations 1976. *IUPAC Information Bulletin Appendices on Tentative Nomenclature, Symbols, Units and Standards*, no. 53, December (1976). [also in: *Eur. J. Biochem.* **86**, 1–8 (1978)].
- 2 International Union of Pure and Applied Chemistry. *Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H*. 1979 edn. Pergamon Press, Oxford (1979).
- 3 International Union of Pure and Applied Chemistry. *A Guide to IUPAC Nomenclature of Organic Compounds*. Blackwell Scientific Publications, Oxford (1993).
- 4 International Union of Pure and Applied Chemistry Joint Commission on Biochemical Nomenclature.

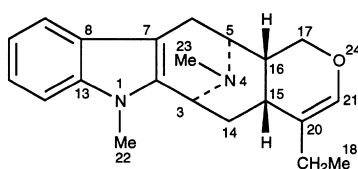
- Nomenclature of steroids. *Pure Appl. Chem.* **61**, 1783–1822 (1989). [also in: *Eur. J. Biochem.* **186**, 429–458 (1989), and in *Dictionary of Steroids* (R. A. Hill, D. X. Kirk, H. L. J. Makin, G. M. Murphy, eds), pp. xxx–lix. Chapman & Hall, London (1991)].
- 5 International Union of Biochemistry, International Union of Pure and Applied Chemistry, Joint Commission on Biochemical Nomenclature. Nomenclature of carotenoids. *Pure Appl. Chem.* **41**, 405–431 (1975).
 - 6 International Union of Biochemistry, International Union of Pure and Applied Chemistry, Joint Commission on Biochemical Nomenclature. Nomenclature of vitamin D. *Pure Appl. Chem.* **54**, 1511–1516 (1982). [also in: *Arch. Biochem. Biophys.* **218**, 342–346 (1982); *Endokrinol. Inf.* **2**, 53–64 (1982); *Eur. J. Biochem.* **124**, 223–227 (1982), and *Mol. Cell. Biochem.* **49**, 177–181 (1982)].
 - 7 International Union of Pure and Applied Chemistry. Nomenclature of fused and bridged fused ring systems. *Pure Appl. Chem.* **70**, 143–216 (1998).

APPENDIX

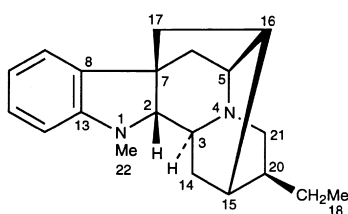
Alkaloids



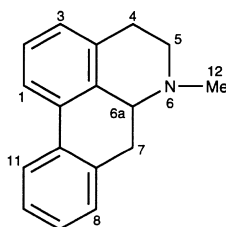
Aconitane



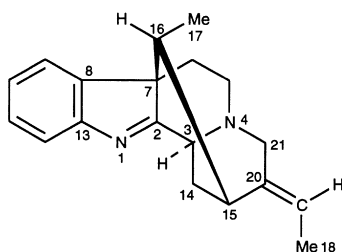
Alstophyllan



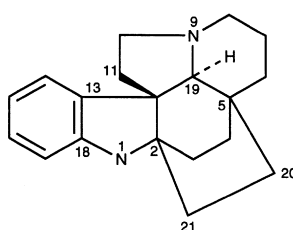
Ajmalan



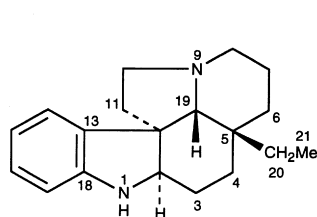
Aporphine



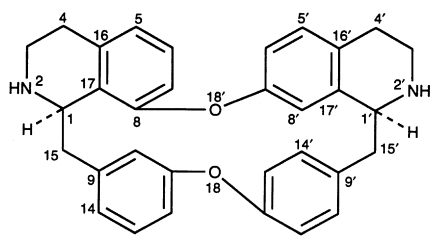
Akuammilan



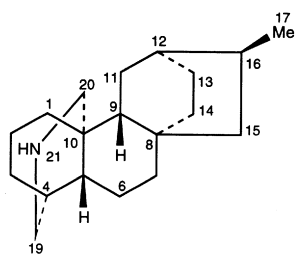
Aspidofractinine



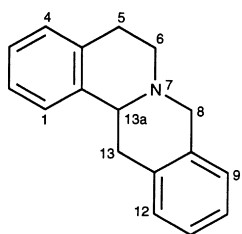
Aspidospermidine



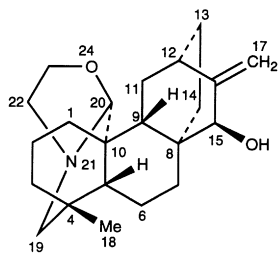
Berbaman



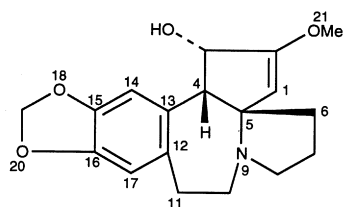
Atidane



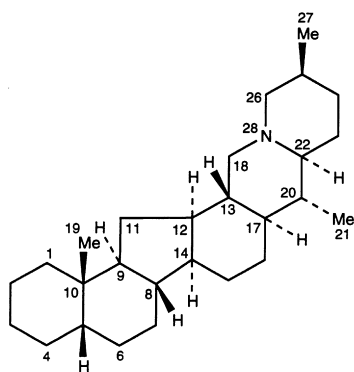
Berbine



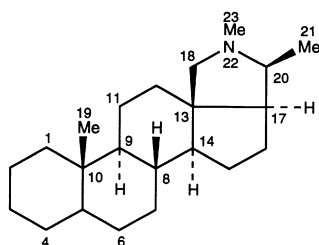
Atisine



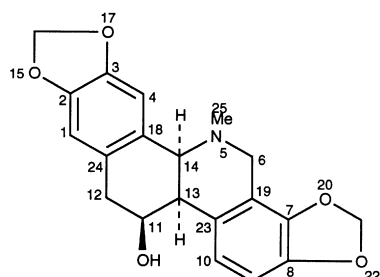
Cephalotaxine



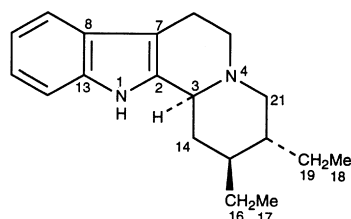
Cevane



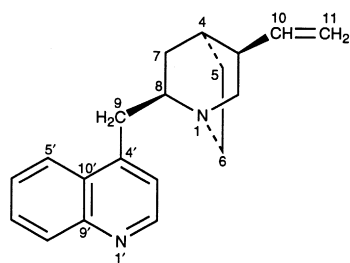
Conanine



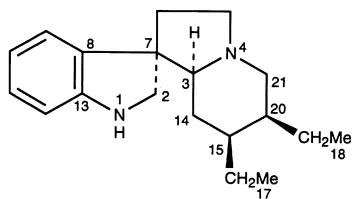
Chelidoniumine



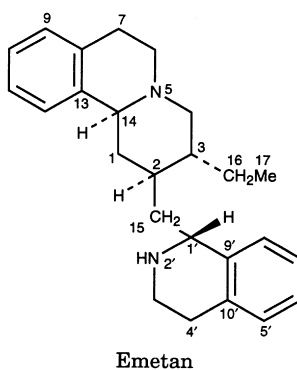
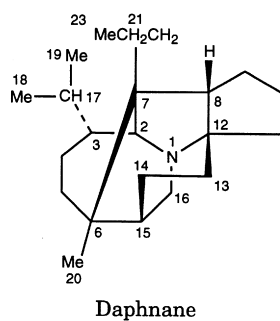
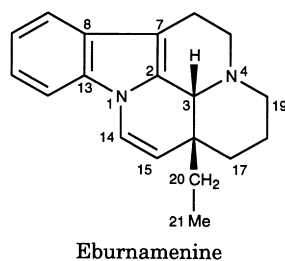
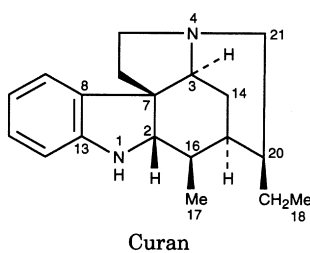
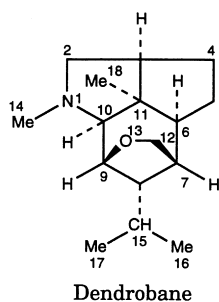
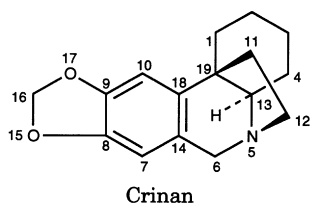
Corynan

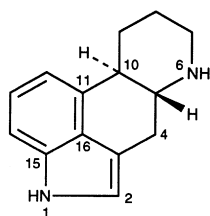


Cinchonan

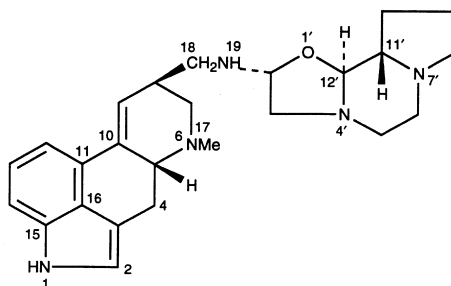


Corynoxan

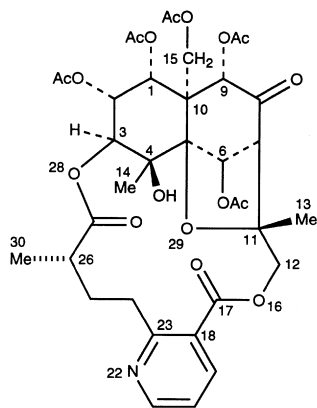




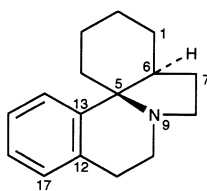
Ergoline



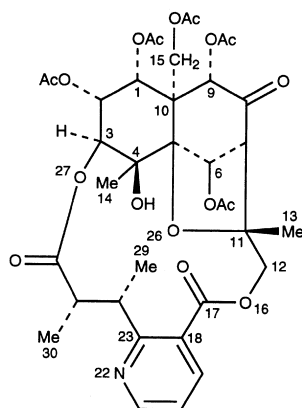
Ergotaman



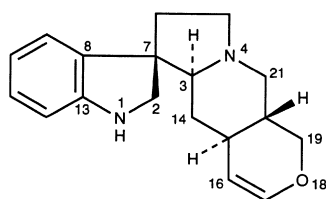
Evonimine



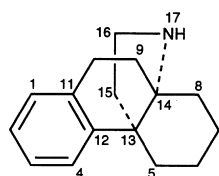
Erythrinan



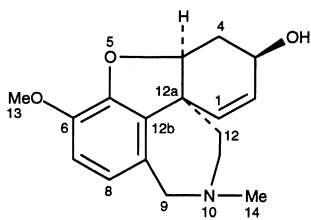
Evonine



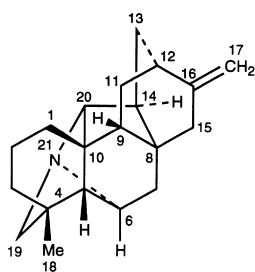
Formosanan



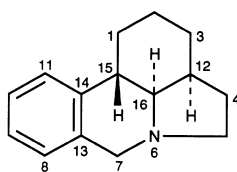
Hasubanan



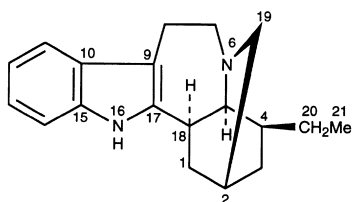
Galanthamine



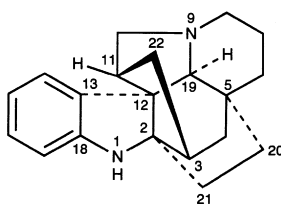
Hetisan



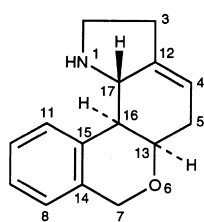
Galanthan



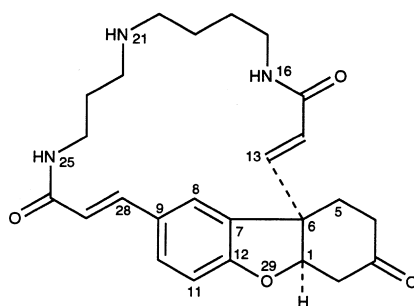
Ibogamine



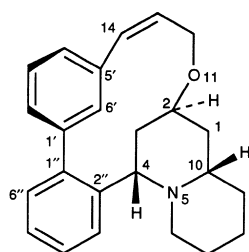
Kopsan



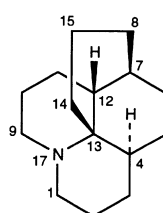
Lycorenan



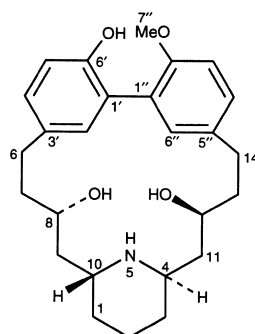
Lunarine



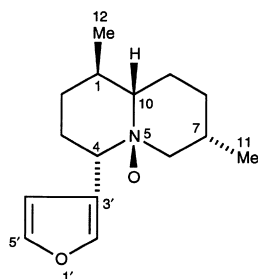
Lythran



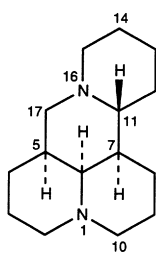
Lycopodane



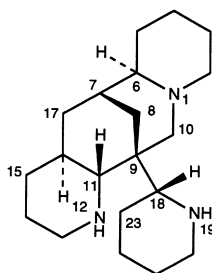
Lythranidine



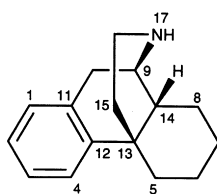
Nupharidine



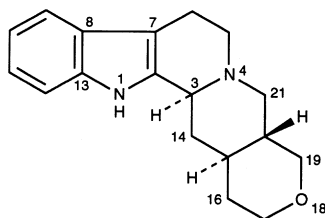
Matridine



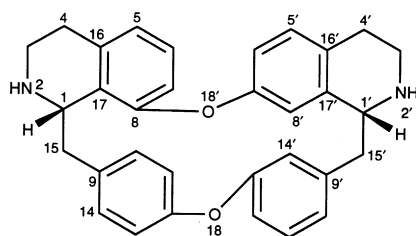
Ormosanine



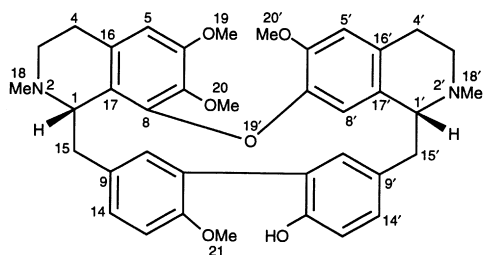
Morphinan



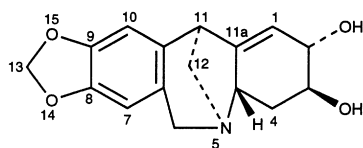
Oxayohimban



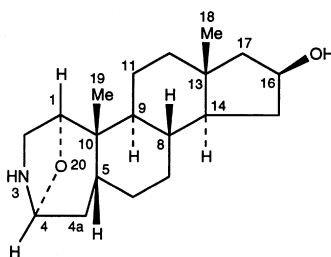
Oxyacanthan



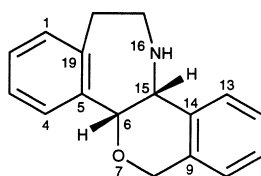
Rodiasine



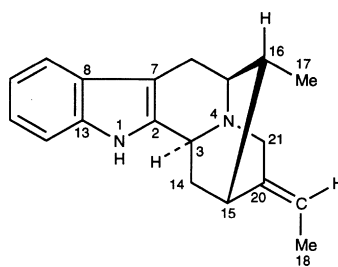
Pancracine



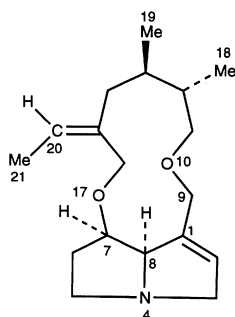
Samandarine



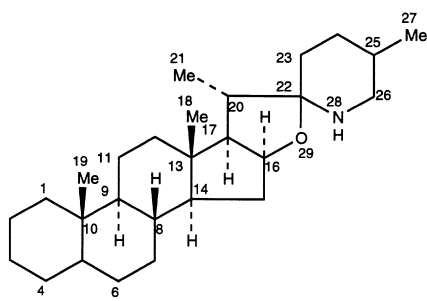
Rheadan



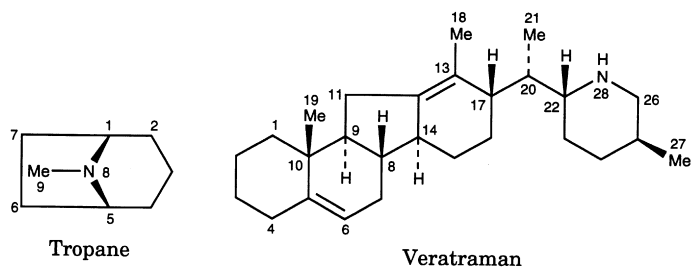
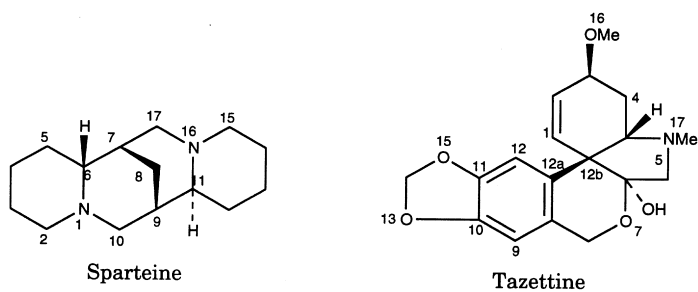
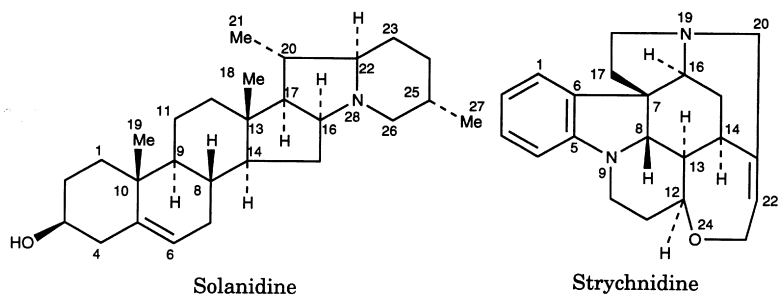
Sarpagan

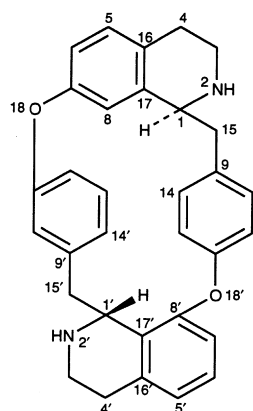


Senecionan

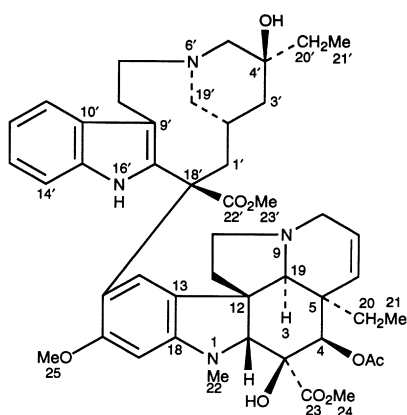


Spirosolane

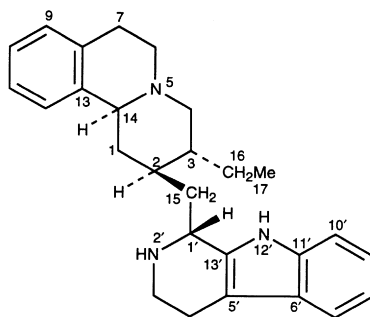




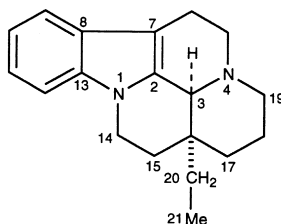
Tubocuraran



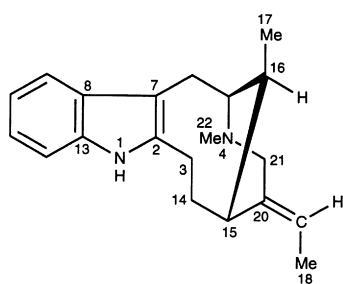
Vincaleukoblastine



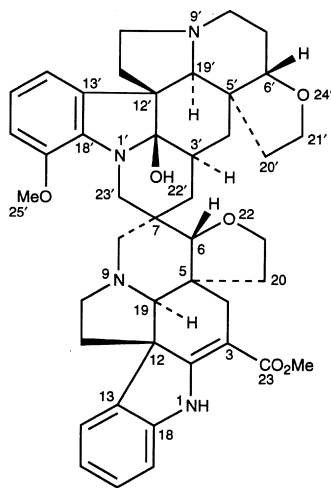
Tubulosan



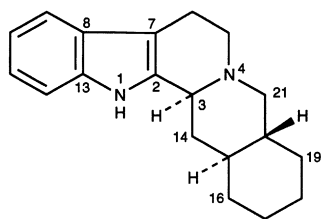
Vincane



Vobasan

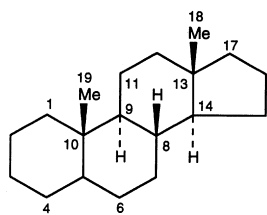


Vobtusine

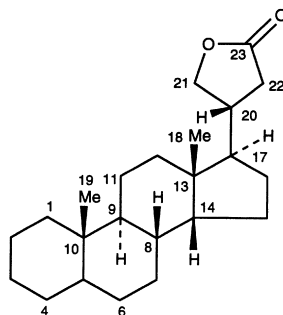


Yohimban

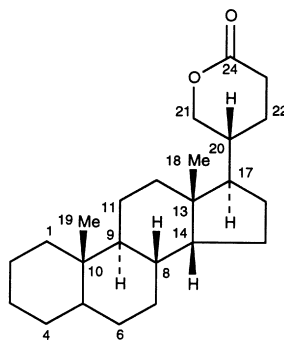
Steroids



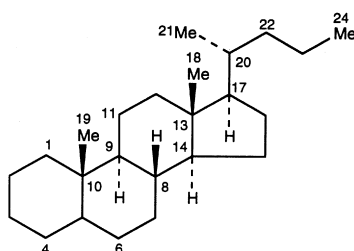
Androstane



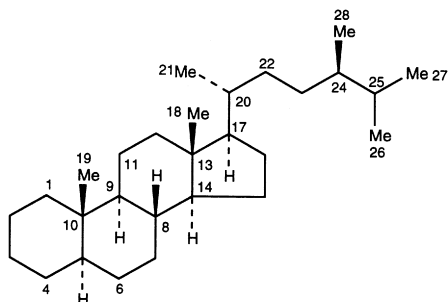
Cardanolide



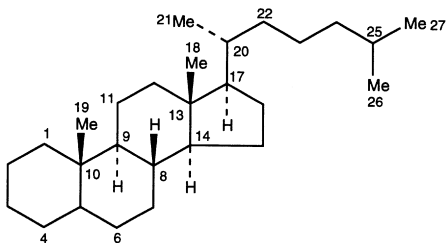
Bufanolide



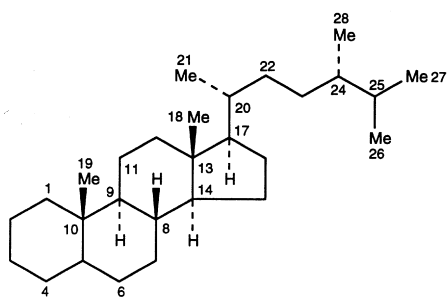
Cholane



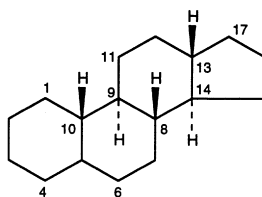
Campestone



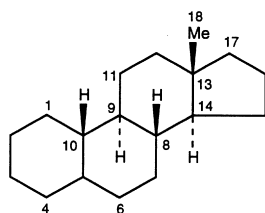
Cholestane



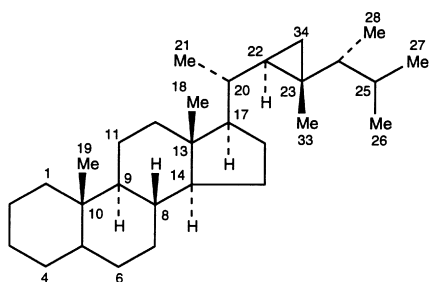
Ergostane



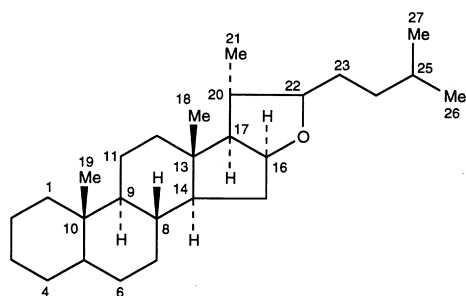
Gonane



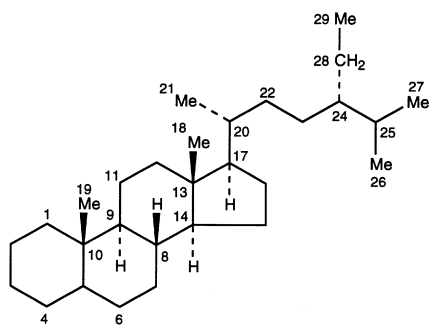
Estrane



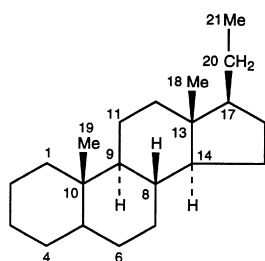
Gorgostane



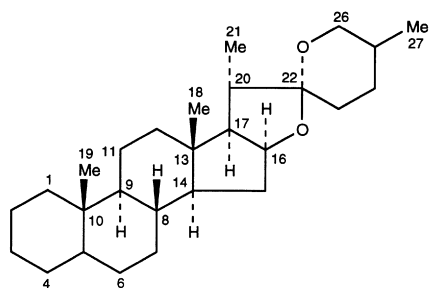
Furostan



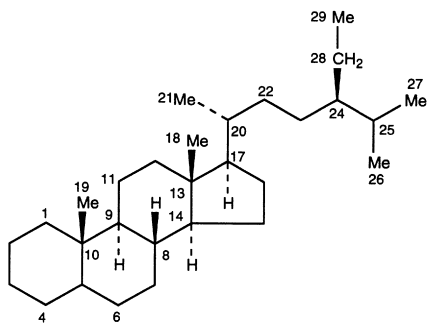
Poriferastane



Pregnane

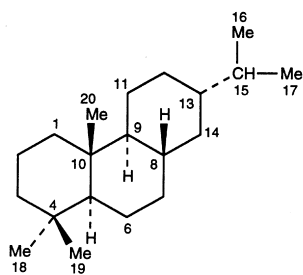


Spirostan

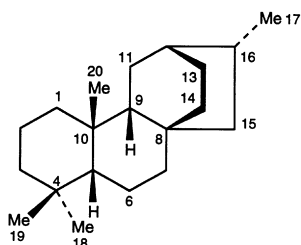


Stigmastane

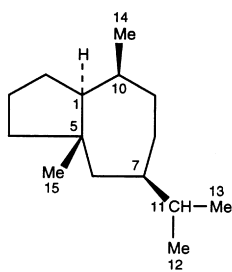
Terpenoids



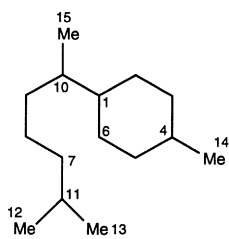
Abietane



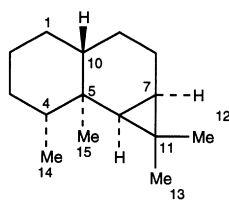
Atisane



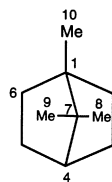
Ambrosane



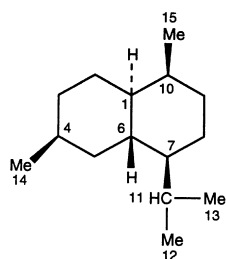
Bisabolane



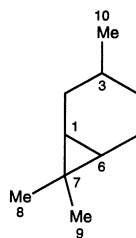
Aristolane



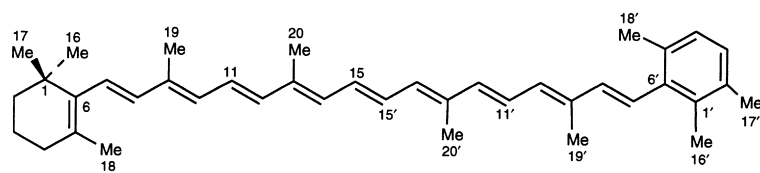
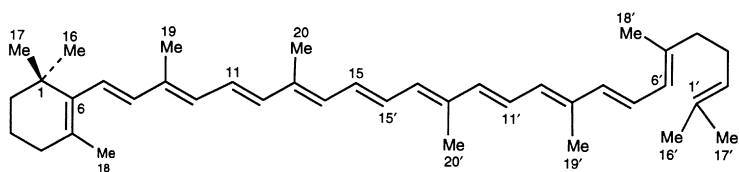
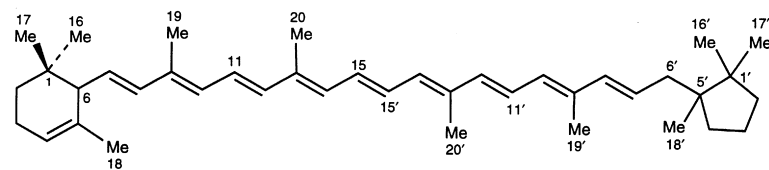
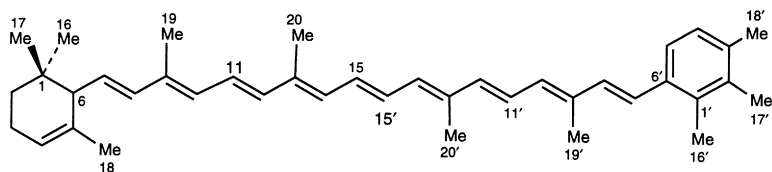
Bornane

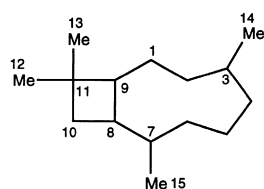


Cadinane

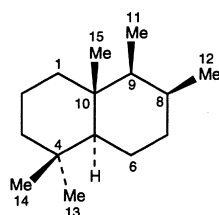


Carane

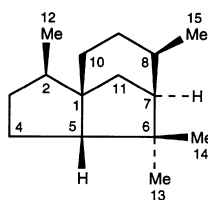
 β,ϕ -Carotene β,ψ -Carotene ϵ,κ -Carotene ϵ,χ -Carotene



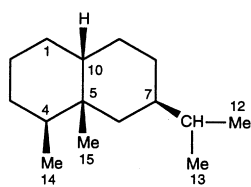
Caryophyllane



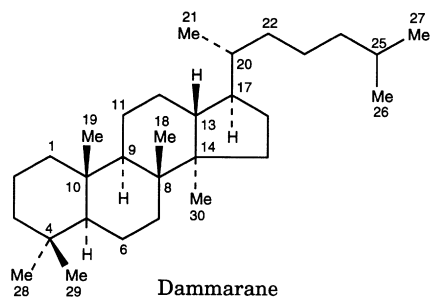
Drimane



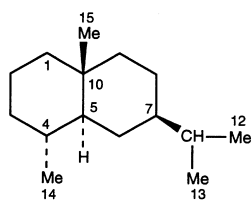
Cedrane



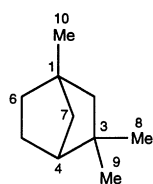
Eremophilane



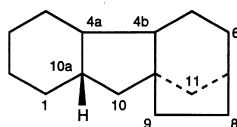
Dammarane



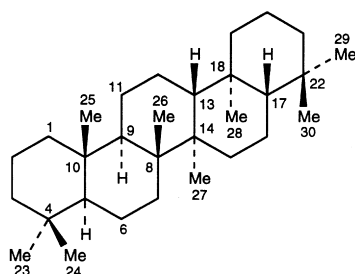
Eudesmane



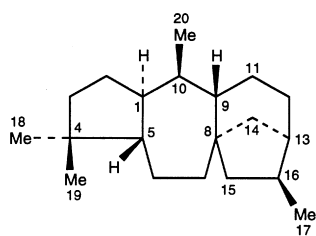
Fenchane



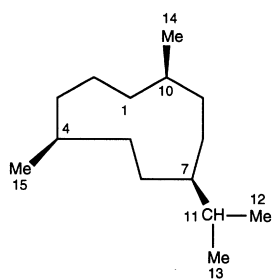
Gibbane



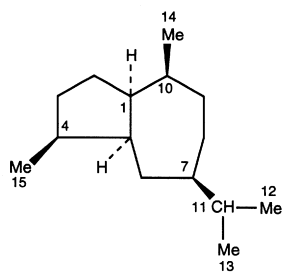
Gammacerane



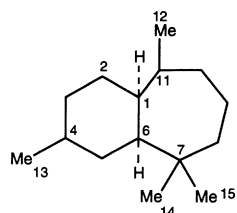
Grayanotoxane



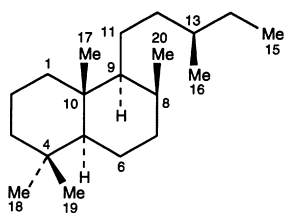
Germacrane



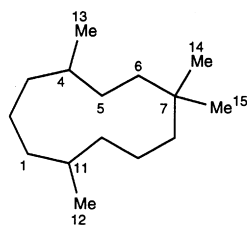
Guaiane



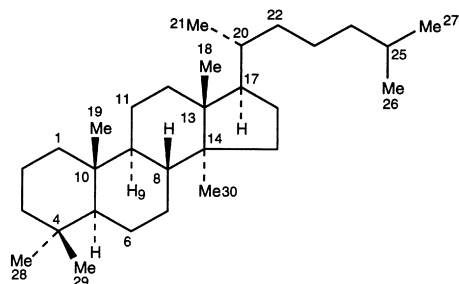
Himachalane



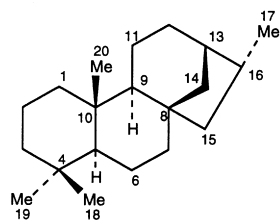
Labdane



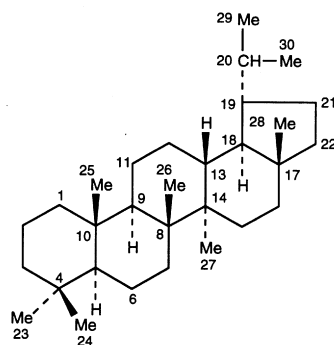
Humulane



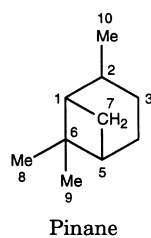
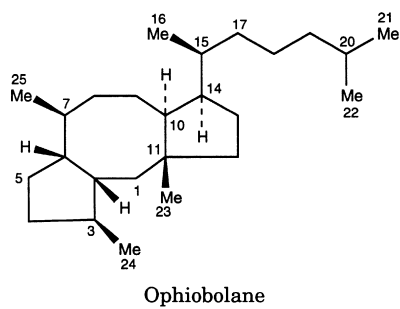
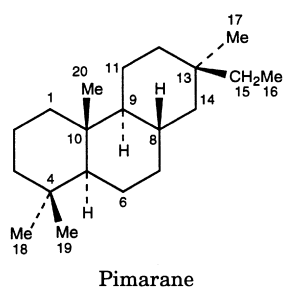
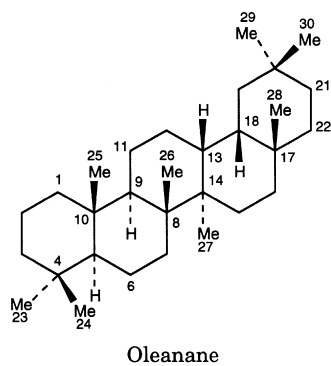
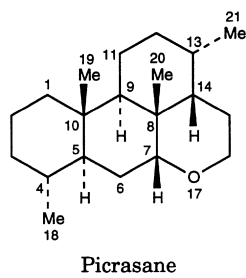
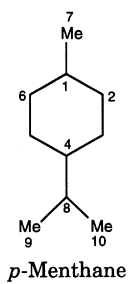
Lanostane

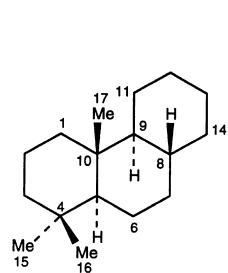


Kaurane

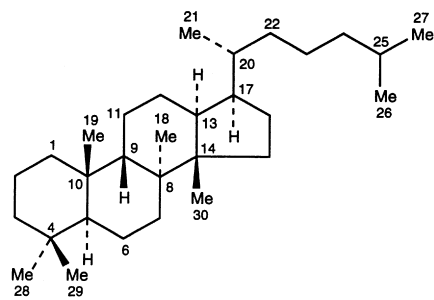


Lupane

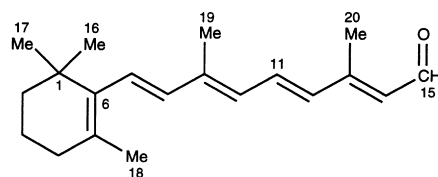




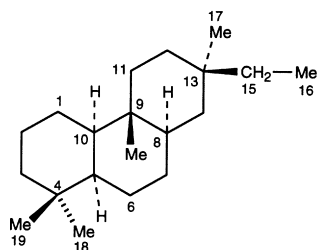
Podocarpane



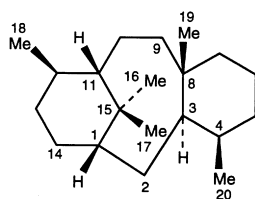
Protostane



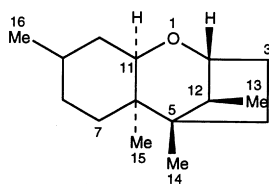
Retinal



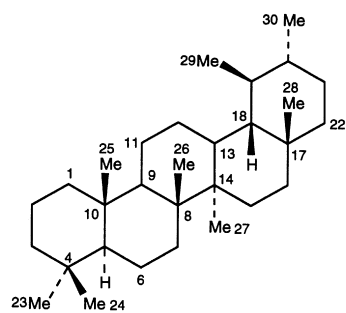
Rosane



Taxane

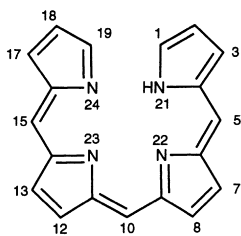


Trichothecane

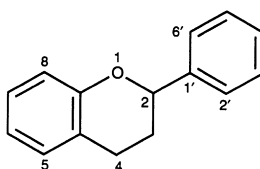


Ursane

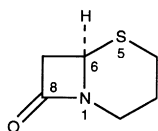
Miscellaneous



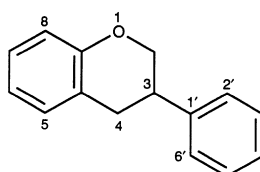
Biline



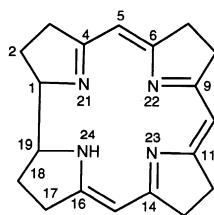
Flavan



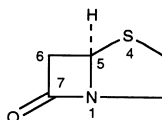
Cepham



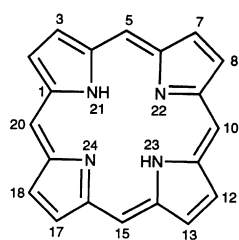
Isoflavan



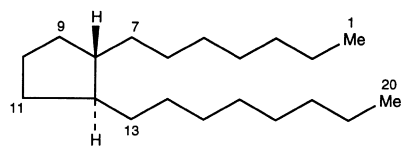
Corrin



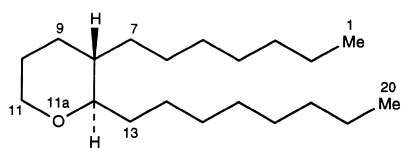
Penam



Porphyrin



Prostane



Thromboxane