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INTERNATIONAL UNION OF BIOCHEMISTRY AND MOLECULAR BIOLOGY  
JOINT COMMISSION ON BIOCHEMICAL NOMENCLATURE\*

# NOMENCLATURE OF LIGNANS AND NEOLIGNANS

## (IUPAC Recommendations 2000)

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## Nomenclature of lignans and neolignans (IUPAC Recommendations 2000)

*Abstract:* Lignans and neolignans are a large group of natural products characterized by the coupling of two  $C_6C_3$  units. For nomenclature purposes the  $C_6C_3$  unit is treated as propylbenzene and numbered from 1 to 6 in the ring, starting from the propyl group, and with the propyl group numbered from 7 to 9, starting from the benzene ring. With the second  $C_6C_3$  unit the numbers are primed. When the two  $C_6C_3$  units are linked by a bond between positions 8 and 8' the compound is referred to and named as a lignan. In the absence of the C-8 to C-8' bond, and where the two  $C_6C_3$  units are linked by a carbon-carbon bond it is referred to and named as a neolignan. The linkage with neolignans may include C-8 or C-8'. Where there are no direct carbon-carbon bonds between the  $C_6C_3$  units and they are linked by an ether oxygen atom the compound is named as an oxyneolignan. The nomenclature provides for the naming of additional rings and other modifications following standard organic nomenclature procedures for naming natural products. Provision is included to name the higher homologues. The sesquieolignans have three  $C_6C_3$  units, and dineolignans have four  $C_6C_3$  units.

### CONTENTS

#### LG-0. INTRODUCTION

- 0.1 Previous proposals
- 0.2 General principles

#### LG-1. FUNDAMENTAL PARENT STRUCTURES

- 1.1 Lignane
- 1.2 Neolignane
- 1.3 Indicated hydrogen
- 1.4 Oxyneolignane
- 1.5 Numbering of lignane, neolignane, and oxyneolignane skeletons

#### LG-2. MODIFICATION OF THE FUNDAMENTAL PARENT STRUCTURE

- 2.1 Additional carbocyclic rings (the prefix cyclo-)
- 2.2 Ring cleavage (the prefix seco-)
- 2.3 Removal of skeletal atoms (the prefix nor-)
- 2.4 Addition of skeletal atoms (the prefix homo-)
- 2.5 Replacement of skeletal atoms (the prefix oxa-, etc.)
- 2.6 Bridged parent structures (the prefix epoxy-, etc.)
- 2.7 Bond migration (the prefix *abeo*-)
- 2.8 Combination of prefixes

#### LG-3. CHANGES IN HYDROGENATION LEVEL

- 3.1 Unsaturation in the side chain
- 3.2 Reduction of the aromatic ring
- 3.3 Double bonds between the aromatic ring and side chain

#### LG-4. LIGNANE, NEOLIGNANE, AND OXYNEOLIGNANE DERIVATIVES

- 4.1 Carboxylic acids
- 4.2 Lactones
- 4.3 Esters
- 4.4 Ketones

- 4.5 Alcohols or phenols
- 4.6 Ethers and alcohol or phenol derivatives
- LG-5. STEREOCHEMISTRY
  - 5.1 Orientation of formulae
  - 5.2 Configuration symbols
  - 5.3 Absolute configuration
  - 5.4 Relative configuration
  - 5.5 Racemate
  - 5.6 Enantiomers
- LG-6. TRIMERS OF THE  $C_6C_3$  UNIT AND HIGHER ANALOGUES
  - 6.1 Sesquiolignans
  - 6.2 Dineolignans
- LG-7. SUMMARY

## LG-0. INTRODUCTION

The lignans comprise a class of natural plant products which are derived from cinnamic acid derivatives and which are related biochemically to phenylalanine metabolism. They fall into five major subgroups, and the nomenclature in use is neither consistent between the groups or even within a subgroup.

Many lignans show physiological activity, such as the tumor-inhibiting podophyllotoxins. This specific activity leads to interference with cell division by two different mechanisms in animals including humans. Some are active in suppressing the central nervous system and inhibiting cyclic-AMP phosphodiesterase, while others act as fish poisons or germination inhibitors. In Chinese traditional medicine lignans are used for treatment of viral hepatitis and protection of the liver.

The growing interest in the lignans and neolignans and the increasing number of variations of their skeletons make a rational system for naming them a necessity.

### LG-0.1 Previous proposals

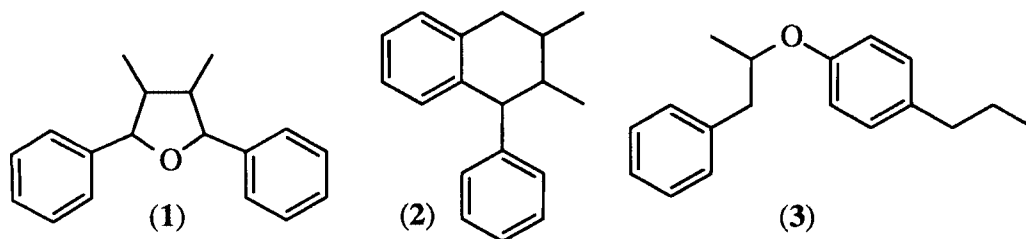
Robinson [1] recognized in 1927 a common feature of many natural products was a  $C_6C_3$  unit (i.e., a propylbenzene skeleton) perhaps derived from cinnamyl units. In a review of natural resins Haworth [2] proposed that the class of compounds derived from two  $C_6C_3$  units  $\beta,\beta'$ -linked should be called lignans (his original spelling was lignane but the "e" was deleted in subsequent publications). The nomenclature of the diverse range of structures classified as lignans depended largely on trivial names and if necessary the appropriate numbering derived from the systematic name. This resulted sometimes in alternative numbering systems for closely related compounds with potential ambiguity in the naming of analogues. For example, in the aryl-naphthalenes (**2**) (2,7'-cyclo-lignane, see Table 1 and LG-2.1), the aryl group might be attached to the naphthalene at C-1 or C-4 depending on the location of functional groups.

In an extensive review by Hearon and MacGregor [3] the different skeletal types were consistently numbered although there was no correlation between them. Freudenberg and Weinges [4] proposed in 1961 that the  $C_6C_3$  unit be numbered from 1 to 9 and the second unit from 1' to 9' to provide a consistent numbering system. Thus, the lignans all had an 8-8' linkage. In addition, they proposed the term cyclo-lignans for lignans with an additional ring. This system was discussed in more detail by Weinges *et al.* in 1978 [5].

The term neolignan was defined by Gottlieb [6] as including the lignans and also related compounds where the two  $C_6C_3$  units are joined by other bonds (e.g., 3-3' instead of 8-8'). In addition, he included compounds where an oxygen atom provides the link between the two  $C_6C_3$  units. With the aryl-naphthalenes the additional ring was formed between 7 and 2' rather than 7 and 6' as proposed by Weinges [4].

The inclusion of the lignans as a type of neolignan has not been generally accepted. Whiting [7] in his review separated the lignans (i.e., with an 8-8' linkage) from the neolignans and highlighted their unsatisfactory nomenclature. The anomalies that have accrued in describing the stereochemistry of the podophyllotoxin group of lignans were reviewed by Dewick and Jackson [8].

Some of the differences between the various proposed nomenclature systems are shown by the three skeletal types illustrated by (1) to (3). Table 1 shows some of the ways these sub-classes of lignans have been described.



**Table 1** Comparison of nomenclature proposals.

Skeleton e.g. (1)	Skeleton e.g. (2)	Skeleton e.g. (3)	Reference
7,7'-epoxylignane	2,7'-cyclooctylidene	8,4'-oxyneolignane	This paper
2,5-diaryltetrahydrofuran	4-aryl-1,2,3,4-tetrahydronaphthalene	–	[3]
7,7'-epoxylignane	cyclooctylidene	–	[4]
7.O.7',8,8'-lignan	8.8',7.2'-lignan	8.O.4'-lignan	[6]
2,5-diaryl-3,4-dimethyltetrahydrofuran	1-aryltetralin	(8-O-4')-neolignan	[7]

This nomenclature problem is further complicated by the retrieval problem as the Chemical Abstracts index name of lignans and neolignans uses systematic nomenclature. Table 2 illustrates this problem with the aryl-naphthalene skeleton (2) where the index heading parent depends on the location of the preferred substituent (if any) which is cited as a suffix, or the preferred ring system.

## LG-0.2 General principles

The recommendations in this document are based on the general IUPAC recommendations for naming natural products [9,12]. Existing trivial names for lignans and neolignans may still be used, but it is recommended that the semisystematic name for the lignan or neolignan also be quoted in a paper when first encountered. It should be noted that several different numbering systems are in use so that it must be clear with a modified trivial name which system is being used.

## LG-1. FUNDAMENTAL PARENT STRUCTURES

The lignans and neolignans are a class of natural products derived from two  $C_6C_3$  molecules (4) by coupling. The term lignan was introduced by Haworth [2] for the structures where the two units are  $\beta,\beta'$ -linked. When the two are coupled in other ways ( $m,m'$ ;  $\gamma,\gamma'$ ;  $\beta,m'$ ; etc.) they are called neolignans. This group is also considered to include examples where the two units are joined by an ether oxygen atom which for nomenclature purposes is treated as a linking oxygen of an assembly.

*Note:* (1) The class names lignan and neolignan are spelled in the conventional way without a terminal "e". The parent structures below are spelled with a terminal "e" to indicate a saturated side chain unless modified to show unsaturation (see LG-3.1).

(2) For the purposes of numbering the various parent structures, the  $C_6C_3$  unit (4) is numbered 1 to 9 where the  $\alpha$  position is 9,  $\beta$  is 8, and  $\gamma$  is 7.

**Table 2** Variation of numbering of aryl/naphthalene lignans.

The locant columns are headed by those used in this document [see LG-2.1(a) for 2,7'-cyclo lignane (5)] compared with the Chemical Abstracts Service (CAS) index heading parent numbering. Primed numbers refer to the aryl group attached to the index heading parent. An asterisk refers to a carboxy group.

CAS Index	Heading Parent	1	2	3	4	5	6	7	8	9	1'	2'	3'	4'	5'	6'	7'	8'	9'	Example
5H-benzol[k]bis[1,3]dioxolo- [4,5-b:4',5'-g]xanthen-5-one	5a	14b	14a	3a	4	5	6	7	7	-	8b	9	9a	12a	13	13a	8a	8	-	carpanone
1,3-benzodioxole	4a'	8a'	8'	7'	6'	5'	4'	3'	-	5	4	3a	3a	7a	7	6	1'	2'	-	isogalcatin
furo[3,4':6,7]naphtho[2,3-d]- -1,3-dioxole-5,8-dione	4a	9a	10	10a	3a	4	5	5a	6	1'	2'	3'	3'	4'	5'	6'	9	8a	8	isopicro- podophyllone
furo[3,4':6,7]naphtho[2,3-d]- -1,3-dioxol-6(8H)-one	4a	9a	10	10a	3a	4	5	5a	6	5'	4'	3a'	3a'	7a'	7'	6'	9	8a	8	justicidin D
furo[3,4':6,7]naphtho[2,3-d]- -1,3-dioxol-6(5aH)-one	9a	4a	4	3a	10a	10	9	8a	8	1'	2'	3'	3'	4'	5'	6'	5	5a	6	podophyllotoxin
furo[3,4':6,7]naphtho[2,3-d]- -1,3-dioxol-6(8H)-one	9a	4a	4	3a	10a	10	9	8a	8	5'	4'	3a'	3a'	7a'	7'	6'	5	5a	6	justicidin F
furo[3,4':6,7]naphtho[1,2-d]- -1,3-dioxol-7(9H)-one	5a	10a	10b	3a	4	5	6	6a	7	5'	4'	3a'	3a'	7a'	7'	6'	10	9a	9	justicimol
naphthalene	4a	8a	8	7	6	5	4	3	-	1'	2'	3'	3'	4'	5'	6'	1	2	-	galbulin
2-naphthalenecarboxylic acid	4a	8a	8	7	6	5	4	3	-	1'	2'	3'	3'	4'	5'	6'	1	2	*	plicatic acid
"	8a	4a	5	6	7	8	1	2	*	1'	2'	3'	3'	4'	5'	6'	4	3	-	thomasic acid
2,3-naphthalenedicarboxylic acid	4a	8a	8	7	6	5	4	3	*	1'	2'	3'	3'	4'	5'	6'	1	2	*	thomasideoic acid
2,3-naphthalenedimethanol	4a	8a	8	7	6	5	4	3	α	1'	2'	3'	3'	4'	5'	6'	1	2	α	isoolivil
2,3-naphthalenediol	8a	4a	4	3	2	1	8	7	-	1'	2'	3'	3'	4'	5'	6'	5	6	-	norisoguaiacin
2-naphthalenol	4a	8a	1	2	3	4	5	6	-	1'	2'	3'	3'	4'	5'	6'	8	7	-	guaiacin
"	4a	8a	1	2	3	4	5	6	-	5'	4'	3a'	3a'	7a'	7'	6'	8	7	-	otobaphenol
naphtho[1,2-d]-1,3-dioxole	5a	9a	9b	3a	4	5	6	7	-	5'	4'	3a'	3a'	7a'	7'	6'	9	8	-	otobain
"	8a	4a	4	3a	9a	9	8	7	-	1'	2'	3'	3'	4'	5'	6'	5	6	-	galcatin

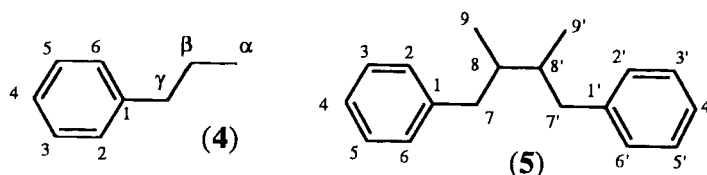
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Table 2 Continued

CAS Index	Heading Parent	1	2	3	4	5	6	7	8	9	1'	2'	3'	4'	5'	6'	7'	8'	9'	Example
"		9a	5a	5	4	3a	9b	9	8	-	1'	2'	3'	4'	5'	6'	6	7	-	hypophyllanthin
	naphtho[1,2- <i>d</i> ]-1,3-dioxol-9-ol	5a	9a	9b	3a	4	5	6	7	-	5'	4'	3a'	7a'	7'	6'	9	8	-	hydroxyotobain
	naphtho[1,2- <i>d</i> ]-1,3-dioxol-6(7 <i>H</i> )-one	5a	9a	9b	3a	4	5	6	7	-	5'	4'	3a'	7a'	7'	6'	9	8	-	otobanone
	naphtho[2,3- <i>c</i> ]furan-1(3 <i>H</i> )-one	4a	8a	8	7	6	5	4	3a	3	1'	2'	3'	4'	5'	6'	9	9a	1	sikkimotoxin
"		4a	8a	8	7	6	5	4	3a	3	5'	4'	3a'	7a'	7'	6'	9	9a	1	collinusin
"		8a	4a	5	6	7	8	9	9a	1	1'	2'	3'	4'	5'	6'	4	3a	3	conidendrin
"		8a	4a	5	6	7	8	9	9a	1	5'	4'	3a'	7a'	7'	6'	4	3a	3	justicidin C
	phenol	8a'	4a'	4'	3a'	9a'	9'	8'	7'	-	4	3	2	1	6	5	5'	6'	-	attenuol

**LG-1.1 Lignane**

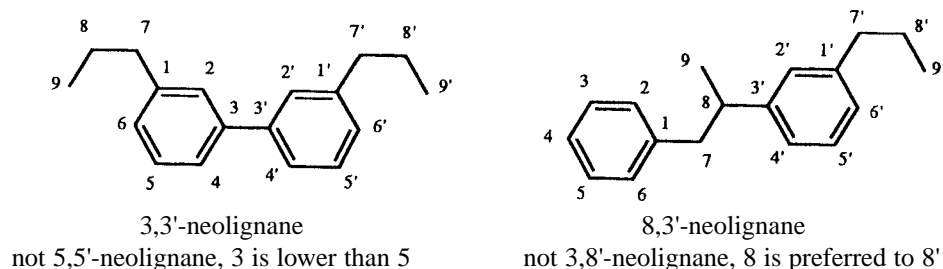
If the two  $C_6C_3$  units (4) are linked by a  $\beta,\beta'$ -bond the parent structure lignane (5) is used as the basis for naming the lignan.

**LG-1.2 Neolignane**

If the two  $C_6C_3$  units (4) are linked by a bond other than a  $\beta,\beta'$ -bond the parent structure, neolignane, is used as the basis for naming the neolignan. The locants of the bond linking the two units are cited in front of the name and with the second number primed. Where there is a choice of locants, preference is made in the order:

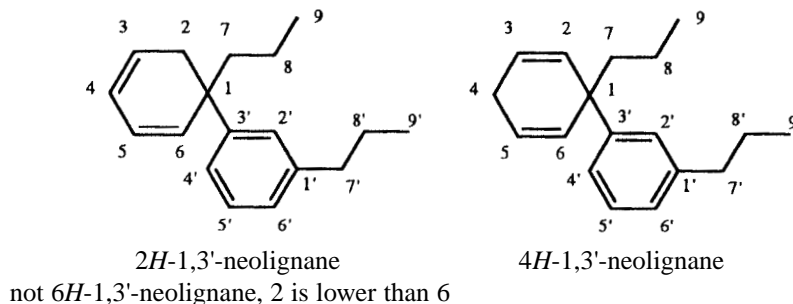
- position 8
- lower unprimed numbers
- lower primed numbers

Examples:



If the bond linking the two  $C_6C_3$  units (4) of a neolignan involves position 1 (or 1') the corresponding phenyl ring cannot be aromatic. The maximum number of noncumulative double bonds is two, and there must be one position (other than C-1 or C-1') which is saturated in the parent hydrocarbon. This position is indicated by means of the locant of this position and an uppercase italic *H* (or underlined type) that is, indicated hydrogen (see rule A-21.6 [10], R-1.3 [13]). Where there is a choice, lower locants are selected.

Examples:

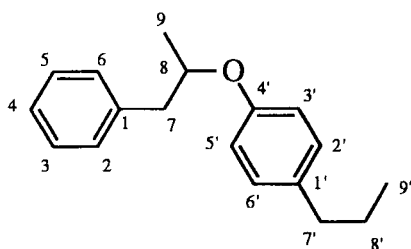


**LG-1.4 Oxyneolignane**

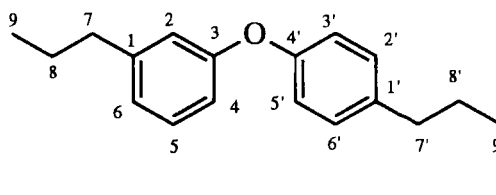
If the two  $C_6C_3$  units (**4**) are linked by an ether oxygen atom and not directly bonded together the parent structure, oxyneolignane, is used as the basis for naming the neolignan. The locants of the two positions linked by the ether oxygen are cited in front of the name with the second number primed. Where there is a choice of locants, preference is made in order to:

- position 8
- lower unprimed numbers
- lower primed numbers

*Examples:*



8,4'-oxyneolignane  
not 4,8'-oxyneolignane, 8 is preferred to 8'



3,4'-oxyneolignane  
not 5,4'- or 4,3'- or 4,5'-oxyneolignane

**LG-1.5 Numbering of lignane, neolignane, and oxyneolignane skeletons**

The parent skeletons illustrated in LG-1.1, 1.2, 1.3, and 1.4 also show the appropriate numbering. If there is still a choice of numbering, preference is made in order to:

- lower locants required to identify modifications of the parent structure (see LG-2)
- lower locants required to identify indicated hydrogen (see LG-1.3)
- lower locants required to identify the principal functional group expressed as a suffix (see LG-4)
- lower locants required to identify double bonds in the side chain (see LG-3.1)
- lower locants required to identify substituents expressed as a prefix when the locants are considered as a set (e.g., see balanophonin in LG-5.4; the methoxy is at 3 not 5)
- lower locants required to identify substituents expressed as a prefix when considered in the order of citation (e.g., see second example in LG-5.4; the methoxy is at 3 not 5)

These criteria follow the established procedures for systematic nomenclature [10,13].

**LG-2. MODIFICATION OF THE FUNDAMENTAL PARENT STRUCTURE**

Modification of the fundamental parent structure (see LG-1) which results in additional rings and/or addition or removal of carbon atoms to that structure (i.e., not treated as a substituent) are indicated by the prefixes described below. These prefixes are always cited next to the parent structure rather than mixed with the other substituent prefixes (see LG-4) (i.e., they are nondetachable).

**LG-2.1 Additional carbocyclic rings (the prefix cyclo-)**

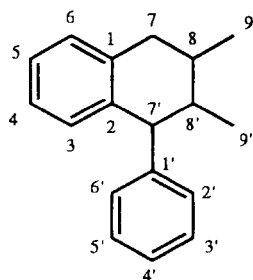
- Cyclo**lignane. If the carbon skeleton of a lignan has an additional carbocyclic ring which is formed by direct bonding between two atoms of the lignane skeleton this is indicated by the pre-



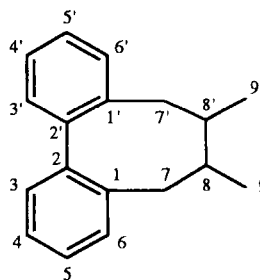
fix cyclo- and the two locants which identify the relevant bond (see rule F-4.1 [9], rule RF-4.3 [12], rule R-1.2.6.1 [13]). If there is a choice of locants, lower numbers are preferred in the order:

- (i) unprimed numbers
- (ii) primed numbers

Examples:



2,7'-cyclo-lignane  
not 2',7-, 6,7'-, or 6',7-cyclo-lignane

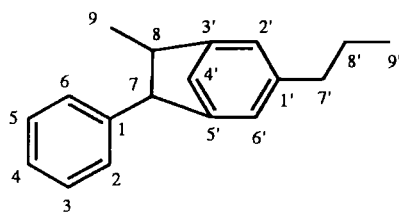


2,2'-cyclo-lignane  
not 6,6'-cyclo-lignane

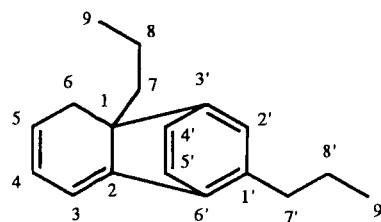
- (b) **Cycloneolignane.** If the carbon skeleton of a neolignan with the two  $C_6C_3$  units (4) directly bonded has an additional carbocyclic ring which is formed by direct bonding between two atoms of the neolignane skeleton this is indicated by the prefix cyclo- and the two locants which identify the relevant bond (see rule F-4.1 [9], rule RF-4.3 [12], rule R-1.2.6.1 [13]). If there is a choice, lower numbers are preferred in the order:

- (i) unprimed numbers for cyclo
- (ii) primed numbers for cyclo
- (iii) indicated hydrogen

Examples:



5',7'-cyclo-8,3'-neolignane  
not 3,8'-cyclo-5,7'-neolignane  
nor 3',7-cyclo-8,5'-neolignane  
8,3'-neolignane is the preferred parent



6H-2,6'-cyclo-1,3'-neolignane  
not 6H-2,2'-cyclo-1,5'-neolignane  
1,3'-neolignane is the preferred parent

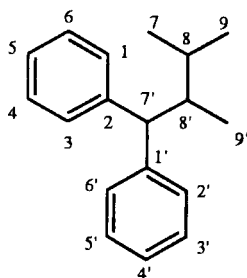
*Note:* These parent structures do not exist but are required for naming hydrogenated or partially hydrogenated compounds (see, for example, LG-4.4 example 2).

### LG-2.2 Ring cleavage (the prefix *seco*-)

Cleavage of a ring bond with addition of the appropriate number of hydrogen atoms is indicated by the prefix *seco*- and the locants of the bond cleaved (see rule F-4.7 [9], rule RF-4.4.1 [12], rule R-1.2.6.2 [13]). The original numbering of the system is retained. If there is a choice of locants, lower numbers are preferred in the order:

- (a) unprimed numbers  
 (b) primed numbers

Example:



1,7-seco-2,7'-cyclo-lignane

Note that strict application of the rules for this example gives 1,7-seco-1,7'-cyclo-lignane, which would result in a different numbering of ring C1-C6. However, the probable relationship with 2,7'-cyclo-lignane is best illustrated by the name shown. Another possible name is 1(7→7')-abeo-lignane (see LG-2.7).

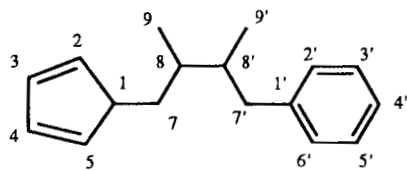
### LG-2.3 Removal of skeletal atoms (the prefix nor-)

If the parent structure is derived from lignane, neolignane, or oxyneolignane by the loss of one or more carbon atoms this is expressed by the prefix nor- (or dinor-, etc.) (see rule F-4.2 and F-4.4 [9], rule RF-4.1.1 [12]). If there is a choice of locations for the removal of the carbon atom, preference is made in the order:

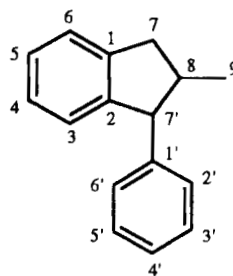
- (a) unprimed number  
 (b) higher number

This number is cited with the prefix nor- while the numbers of all other atoms are unchanged. If necessary, double bond locations are identified by indicated hydrogen (see LG-1.3).

Examples:

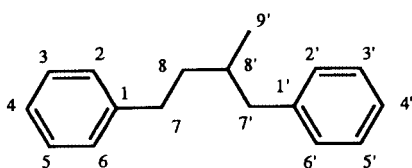


1H-6-norlignane  
 not 1'H-6'-norlignane (6 is preferred to 6')

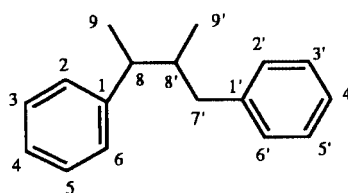


8',9'-dinor-2,7'-cyclo-8,7'-neolignane  
 8,9-dinor-2',7'-cyclo-7,8'-neolignane  
 (8,7' preferred to 7,8')

Note: In the second example the two modifying prefixes are cited in alphabetical order (see rule F-4.7 [9], rule RF-4.7 [12])



9-norlignane  
not 8'-nor-8,9'-neolignane  
(for both lignane is the preferred parent)



7-norlignane  
not 9'-nor-8,7'-neolignane

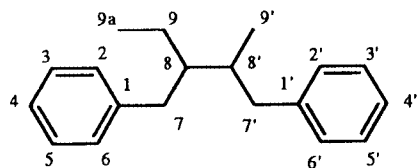
### LG-2.4 Addition of skeletal atoms (the prefix homo-)

If the parent structure is derived from lignane, neolignane, or oxyneolignane by the addition of one or more carbon atoms this is expressed by the prefix homo- (or diho-, etc.) (see rule F-4.5 [9], rule RF-4.2 [12]). The additional carbon atom(s) are numbered by adding a letter "a" (then "b", "c", etc.) to the locant of the appropriate atom. If there is a choice for the location of the extra carbon atom, preference is made in the order:

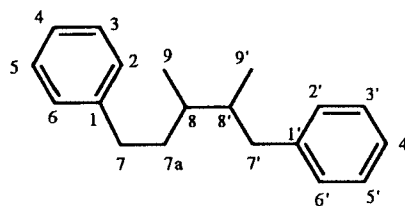
- unprimed numbers
- higher number

If necessary, double bond locations are identified by indicated hydrogen (see LG-1.3).

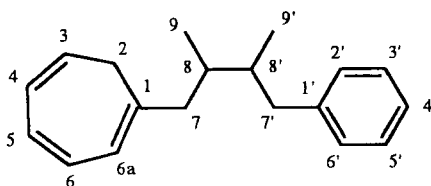
Examples:



9a-homolignane



7a-homolignane  
not 9a'-homo-8,9'-neolignane (lignane preferred)



2H-6a-homolignane  
not 2'H-6a'-homolignane (6a preferred to 6a')

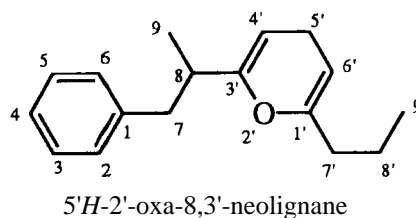
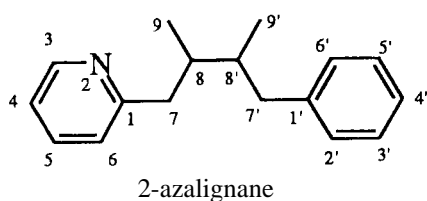
### LG-2.5 Replacement of skeletal atoms (the prefix oxa, etc)

When a carbon atom of a lignane, neolignane, or oxyneolignane is replaced by a heteroatom the replacement ("oxa-aza") system of nomenclature is used (see rule B-4 [10], rule F-4.11 [9], rule RF-5 [12], rule R-1.2.2 [13]). If there is a choice of locants, preference is made in order to:

- unprimed numbers
- lower numbers

If necessary, indicated hydrogen (see LG-1.3) should be used to identify double bond positions.

Examples:



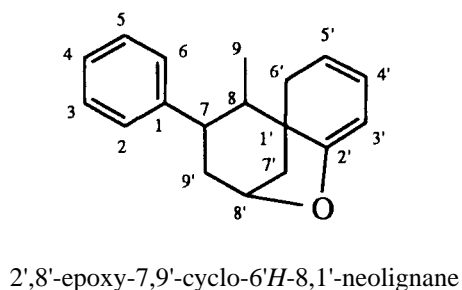
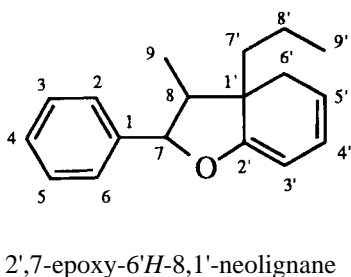
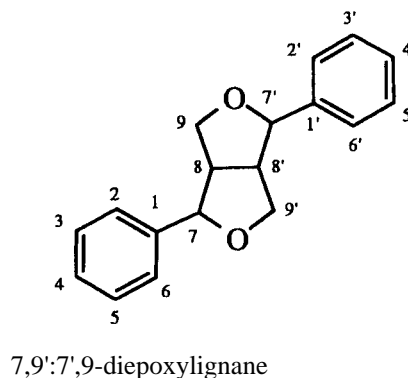
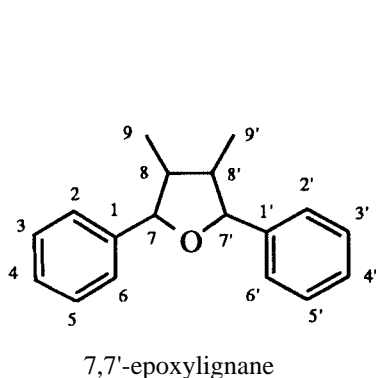
### LG-2.6 Bridged parent structure (the prefix epoxy, etc.)

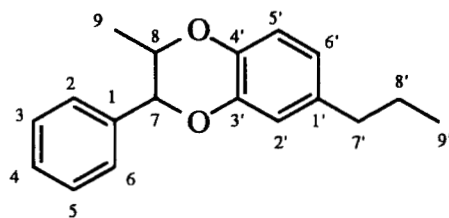
Additional rings created by bridging two positions of a lignane, neolignane, or oxyneolignane by an atom or appropriate group are indicated by the name of the bridging atom or group as a prefix with the appropriate locants. The most common examples of such additional rings are the furanoid or furanofuranoid lignanes. In these cases the bridging oxygen atom is indicated by the prefix epoxy. If there is a choice of locants, preference is made in the order to:

- unprimed numbers
- lower numbers

If there is more than one identical bridge each pair of locants is cited in order, separated by colons. If necessary, double bond locations are identified by indicated hydrogen (see LG-1.3).

Examples:



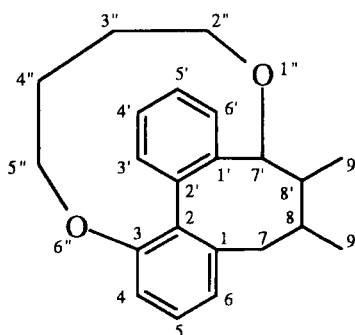


3',7'-epoxy-8,4'-oxyneolignane

not 4',8'-epoxy-7,3'-oxyneolignane (8,4'-oxyneolignane is the preferred parent)

Composite bridges are named by a combination of simple bridges and are cited within round brackets. If the bridge is further substituted the bridge is numbered starting from the highest numbered attachment position. Each atom in the bridge is numbered starting with 1'' as it is necessary to distinguish between it and the unprimed and single primed numbers of the main skeleton.

Example:

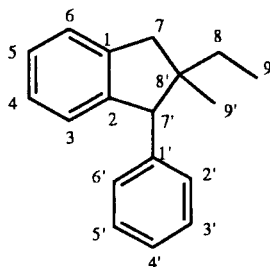


3,7'-(epoxybutanoxy)-2,2'-cyclo lignane

### LG-2.7 Bond migration (the prefix *abeo*-)

A parent structure that does not possess an accepted skeleton but may be considered in a formal sense to arise from one by migration of one or more bonds may be named by the prefix  $x(y \rightarrow z)$ *abeo*- (see rule F-4.9 [9], rule RF-4.5.1 [12], rule R-1.2.7.1 [13]). This designates the migration of the group terminating in the atom numbered  $x$  from position  $y$  to position  $z$ .

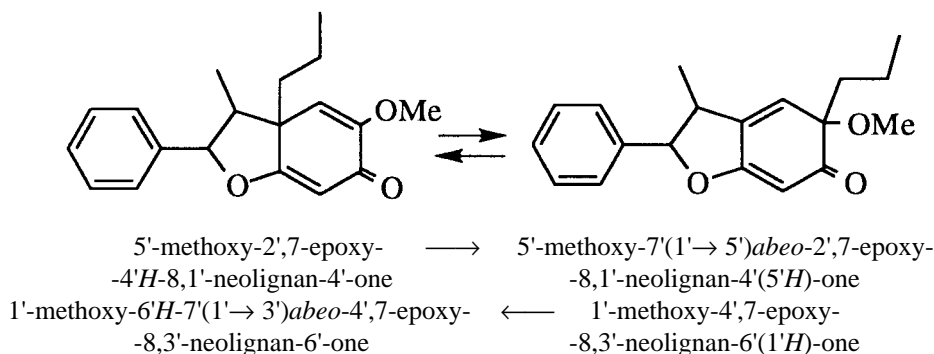
Example:

7(8→8')*abeo*-2,7'-cyclo lignane

The above example might also be called 7'(8'→8)*abeo*-2,7'-cyclo lignane, 8'(7'→8)*abeo*-2,7'-cyclo-8,7'-neolignane, or 8'(7'→8)*abeo*-2,7'-cyclo-8,7'-neolignane if it was required to show the relationship to the corresponding unrearranged neolignane skeletons. A more systematic name for this example is 8-ethyl-

2,7'-cyclo-8',9'-dinor-8,7'-neolignane (see LG-2.3 example 4). The prefix *abeo-* may also be used to show the relationship between two lignans, neolignans, or oxyneolignans.

Example:



Note: In the rearrangement above, the double bond locations are identified by indicated hydrogen (LG-1.3) with the names of the left-hand structure and by added hydrogen (LG-4.4) with the names of the right-hand structure. This is because of the difference between the hypothetical parents.

### LG-2.8 Combination of prefixes

If more than one modifying prefixes is used the effect on the parent is applied sequentially from right to left “advancing backwards” (see rule F-4.7). When there is a choice of operations the minimum number of changes should be used. Prefixes are cited as far as possible in alphabetical order from left to right. The order must avoid improper use of the prefixes or impossible situations. For example, LG-2.2 is illustrated with 1,7-seco-2,7'-cyclo-lignane. The alternative name 2,7'-cyclo-1,7-secolignane is not permitted as it would require “1,7-secolignane” to form it and this is not possible.

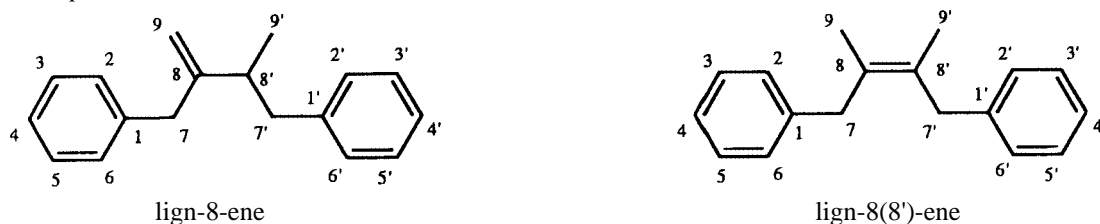
### LG-3. CHANGES IN HYDROGENATION LEVEL

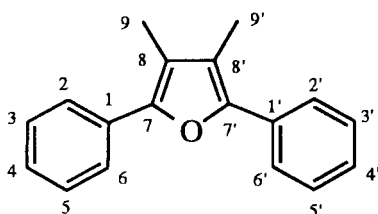
The parent structures described in LG-1 and LG-2 have the maximum number of noncumulative double bonds in the rings corresponding to C-1 to C-6 and C-1' to C-6', and saturated side chains. Methods for describing changes from this skeletal oxidation level depend on the location of the modification.

#### LG-3.1 Unsaturation in the side chain

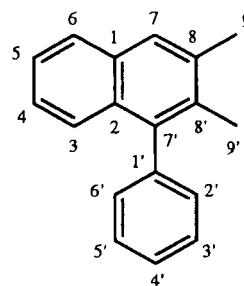
The presence of a double bond (or triple bond) in the side chain (i.e., C-7 to C-9 and C-7' to C-9') of the lignane, neolignane, or epoxyneolignane skeleton is indicated by changing the -ane ending to -ene (or -yne) with a locant to indicate the position of the double bond. If there are two double bonds then the -ane ending is changed to -diene with retention of the “a”.

Examples:

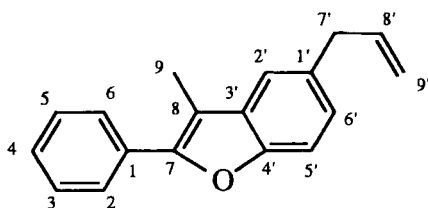




7,7'-epoxyligna-7,7'-diene



2,7'-cycloigna-7,7'-diene

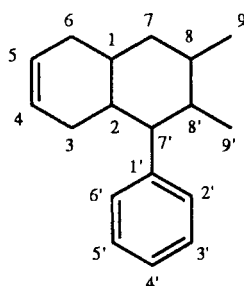


4',7'-epoxy-8,3'-neoligna-7,8'-diene

### LG-3.2 Reduction of the aromatic ring

If an aromatic ring is reduced the location of the additional hydrogen atoms is indicated by the prefix dihydro (or tetrahydro, etc.) with the appropriate locants. See also LG-4 for saturation due to the presence of a ketone.

*Example:*

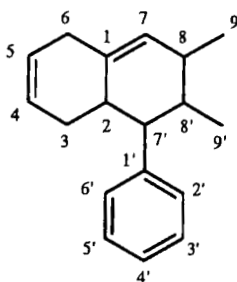


1,2,3,6-tetrahydro-2,7'-cycloignane

### LG-3.3 Double bonds between the aromatic ring and side chain

Isomerization of a double bond from the aromatic ring to the adjacent atom in the side chain is indicated by reduction of the aromatic ring using dihydro (or tetrahydro), see LG-3.2, followed by didehydro with the appropriate locants of the new double bond.

*Example:*



1,7-didehydro-1,2,3,6-tetrahydro-2,7'-cyclo lignane

#### LG-4. LIGNANE, NEOLIGNANE, AND OXYNEOLIGNANE DERIVATIVES

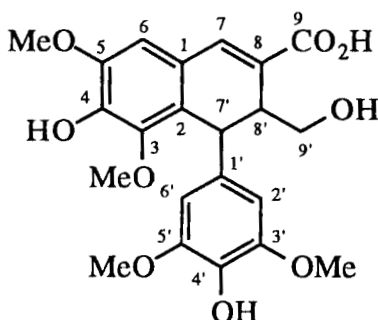
Functional groups and other substituents are expressed as in the general recommendations for organic compounds. Where possible, the preferred group is cited as a suffix and all other groups are expressed by means of prefixes. For the more commonly encountered functional groups the order of preference as a suffix is carboxylic acid, lactone, ester, ketone, and alcohol. When the suffix starts with a vowel the "e" of lignane is elided. All groups other than that expressed as a suffix are cited as prefixes which are quoted in alphabetical order ignoring multiplying affixes such as di-, tri-, tetra-, etc. If there is a choice of locations for a functional group, preference is given in the order:

- unprimed numbers
- lower numbers for principal functional group (i.e., the group named by a suffix)
- lower numbers for locants for prefixes when the locants are considered as a set
- lower numbers for locants for prefixes in the order of citation

##### LG-4.1 Carboxylic acids

When a methyl group of a lignan or neolignan is converted into a carboxy group this is indicated by the suffix -oic acid with the locant of this position.

*Example:*



4,4',9'-trihydroxy-3,3',5,5'-tetramethoxy-2,7'-cyclo lign-7-en-9-oic acid

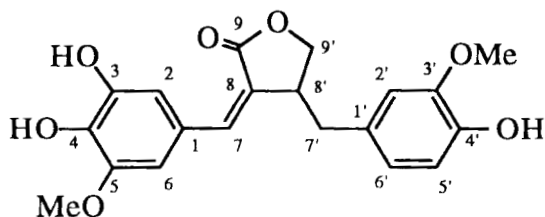
##### LG-4.2 Lactones

Lactones are named by changing the ending -ic acid of the corresponding acid to -lactone preceded by the locant of the acid group and then the locant of the hydroxy group which forms the lactone in that

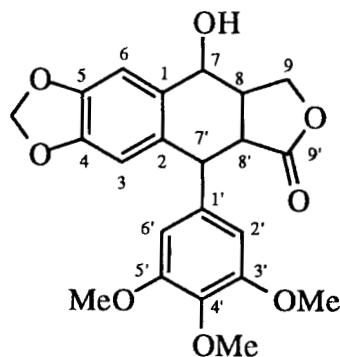


order. The preference for the carbonyl group to be unprimed is contrary to common practice with symmetric skeletons [e.g., steganone (see LG-5.3) and enterolactone (see LG-5.5)]. The preference for the unprimed number assists comparison with related compounds, such as other carboxylic acid derivatives and stereochemistry (see LG-5.3). When the lactone group is part of a bridge [e.g., gonisin D (see LG-5.3)] one of the oxygen atoms is included in the bridge and the other oxygen atom of the carbonyl group is treated as a “ketone” (see LG-4.4).

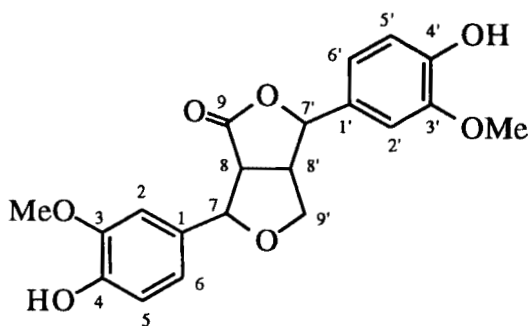
Examples:



3,4,4'-trihydroxy-3',5-dimethoxylign-7-eno-9,9'-lactone



7-hydroxy-3',4',5'-trimethoxy-4,5-methylenedioxy-2,7'-cyclo lignano-9,9'-lactone

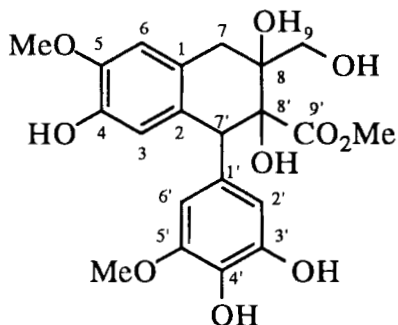


4,4'-dihydroxy-3,3'-dimethoxy-7,9'-epoxylignano-9,7'-lactone

### LG-4.3 Esters

Esterification of a carboxylic acid (see LG-4.1) is indicated by changing the suffix -oic acid to -oate and adding the name of the alkyl group in front of the name.

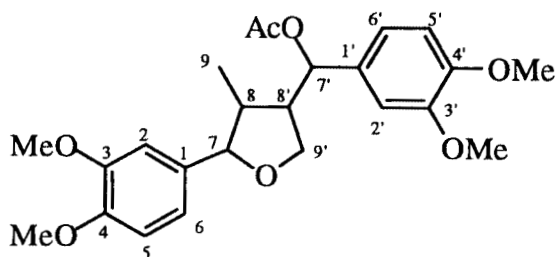
Example:



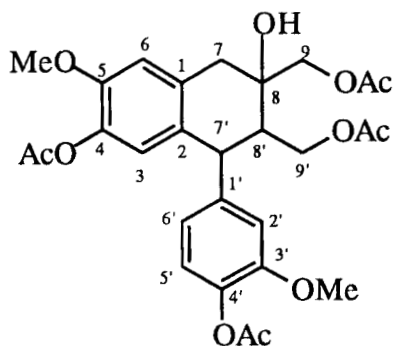
methyl 3',4,4',8,8',9-hexahydroxy-5,5'-dimethoxy-2,7'-cyclo lignan-9'-oate

Esterification of an alcoholic or phenolic hydroxy group (see LG-4.5) is indicated by replacing the terminal -e of lignane, neolignane, or oxyneolignane by -yl, (or by the prefix -diyl, -triyl, etc.) with the locant of the associated position and the anionic form of the acyloxy group. If there is a preferred group such as a carboxylic acid, lactone, or ester of a carboxy group the esterified hydroxy group is indicated by an acyloxy prefix.

Examples:



3,3',4,4'-tetramethoxy-7,9'-epoxylignan-7'-yl acetate

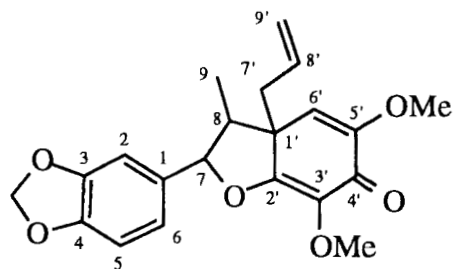


8-hydroxy-3',5-dimethoxy-2,7'-cyclo lignane-4,4',9,9'-tetrayl tetraacetate

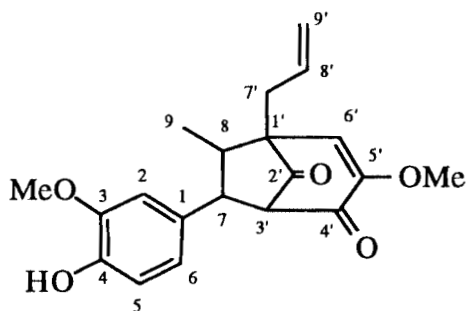
#### LG-4.4 Ketones

Ketones are named by the suffix -one (or the prefix oxo-, if a preferred group is used as a suffix). If the ketone is cited as a suffix at one of the ring atoms C-2 to C-6, and it is necessary to identify double bond locations, this is shown by added hydrogen atoms cited in brackets after the locant of the ketone.

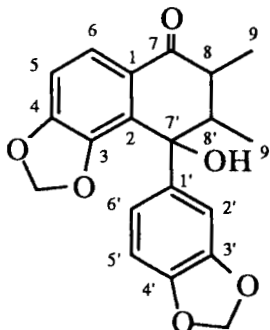
Examples:



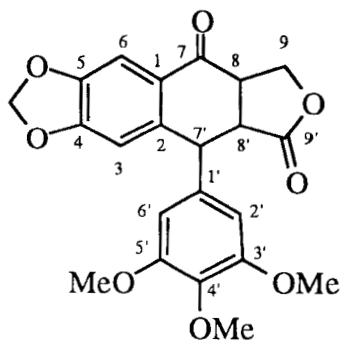
3',5'-dimethoxy-3,4-methylenedioxy-2',7-epoxy-4'H-8,1'-neolign-8'-en-4'-one



4-hydroxy-3,5'-dimethoxy-3',7-cyclo-8,1'-neolign-8'-ene-2',4'(3'H)-dione



7'-hydroxy-3,4:3',4'-bis(methylenedioxy)-2,7'-cyclo-8,1'-neolign-8'-ene-2',4'(3'H)-dione

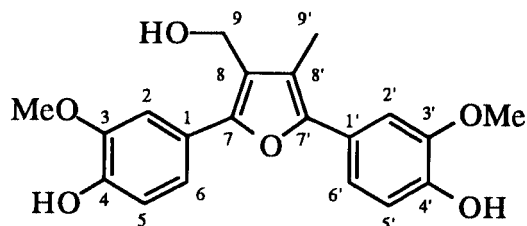


3',4',5'-trimethoxy-4,5-methylenedioxy-7-oxo-2,7'-cyclo-8,1'-neolign-8'-ene-2',4'(3'H)-lactone

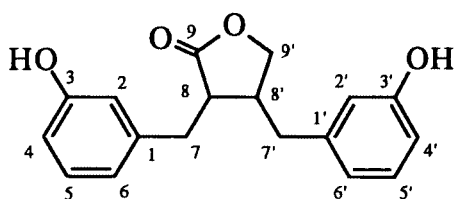
**LG-4.5 Alcohols or phenols**

Alcohols or phenols are named by the suffix -ol; or by the prefix hydroxy- if there is a preferred group used as a suffix.

*Examples:*



3,3'-dimethoxy-7,7'-epoxyligna-7,7'-diene-4,4',9-triol  
(trivial name: furoguaiacidin)

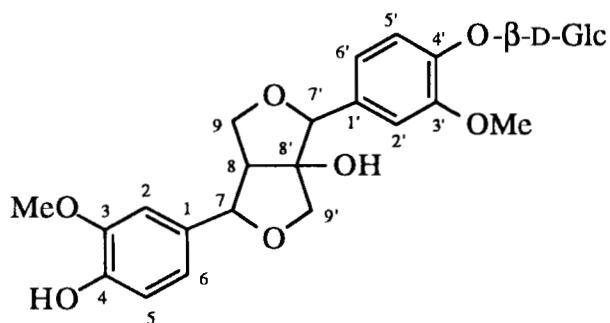


3,3'-dihydroxylignano-9,9'-lactone

**LG-4.6 Ethers and alcohol or phenol derivatives**

Ethers can only be named by means of an alkoxy prefix. Sugar derivatives are named by a glycosyloxy prefix. Esters of alcoholic or phenolic lignanes, neolignanes, or oxyneolignanes are considered in LG-4.3.

*Example:*

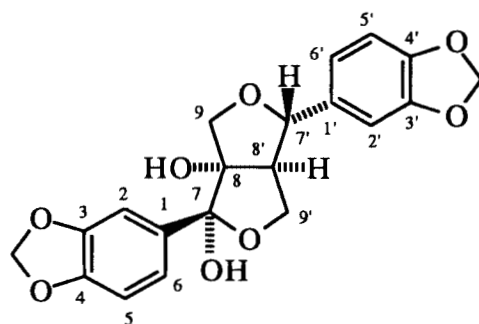


4'-(β-D-glucopyranosyloxy)-3,3'-dimethoxy-7,9':7',9-diepoxylygnane-4,8'-diol

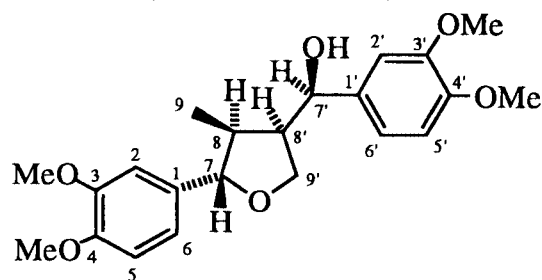
**LG-5. STEREOCHEMISTRY**

Most natural lignans or neolignans are optically active. In order to indicate the absolute or relative configuration, and to readily compare related structures, it is convenient to use a standard orientation of the molecule.

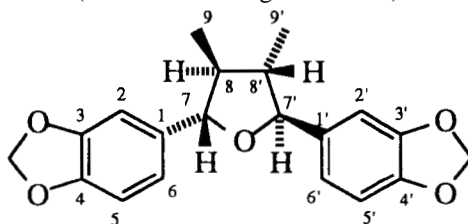




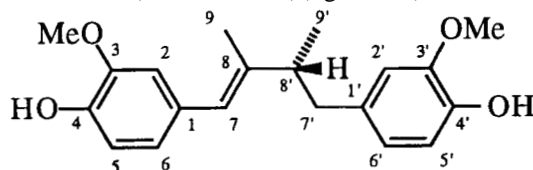
(7 $\beta$ ,7' $\alpha$ ,8 $\alpha$ ,8' $\alpha$ )-3,4:3',4'-bis(methylenedioxy)-7,9':7',9-diepoxyignane-7,8-diol  
(trivial name: arboreol)



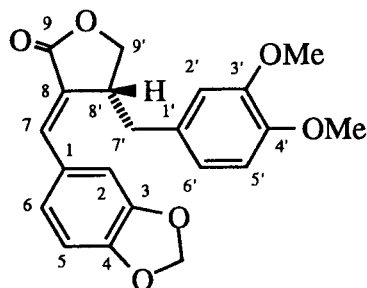
(7'*R*)-(7 $\alpha$ ,8 $\beta$ ,8' $\beta$ )-3,3',4,4'-tetramethoxy-7,9'-epoxyignan-7'-ol  
(trivial name: magnostellin A)



(7 $\alpha$ ,7' $\beta$ ,8 $\beta$ ,8' $\alpha$ )-3,4:3',4'-bis(methylenedioxy)-7,7'-epoxyignane  
(trivial name: (-)-galbacin)

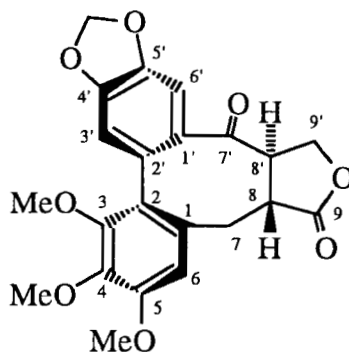


(7*E*)-(8'*R*)-3,3'-dimethoxyign-7-ene-4,4'-diol  
(trivial name: (-)-guaiaretic acid)



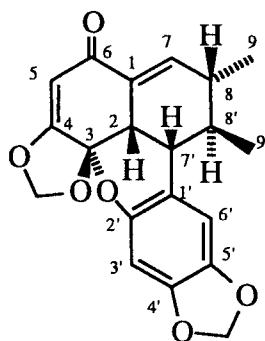
(7*E*)-(8' $\alpha$ )-3',4'-dimethoxy-3,4-methylenedioxyign-7-eno-9,9'-lactone

Note: The two preceding structures are both *7E* due to the priority rules [14,15].

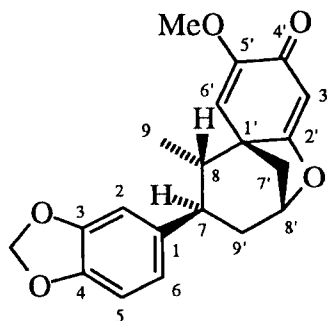


( $2R_a$ )-(8 $\beta$ ,8' $\alpha$ )-3,4,5-trimethoxy-4',5'-methylenedioxy-7'-oxo-2,2'-cyclo[1,2]lignano-9,9'-lactone  
(trivial name: (-)-steganone)

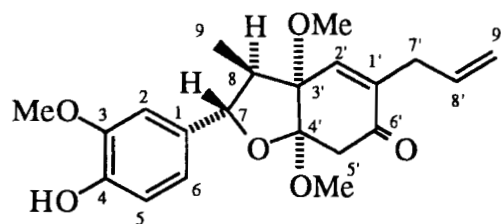
Note:  $2R_a$  refers to the axial chiral biphenyl unit (see ref 15 for details).



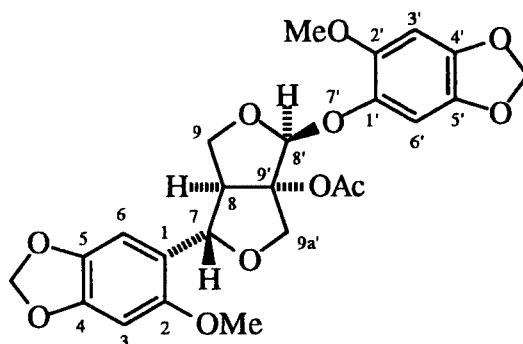
( $3R$ )-(2 $\beta$ ,7' $\beta$ ,8 $\alpha$ ,8' $\beta$ )-1,7-didehydro-1,2,3,6-tetrahydro-2',3'-epoxy-3,4:4',5'-bis(methylenedioxy)-  
2,7'-cyclo[1,2]lignan-6-one  
(trivial name: carpanone)



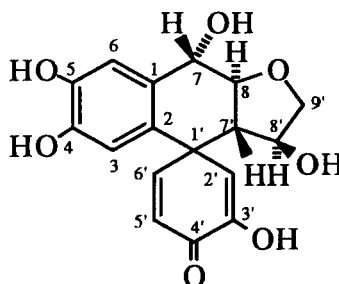
(1' $\beta$ ,7 $\beta$ ,8 $\alpha$ ,8' $\beta$ )-5'-methoxy-3,4-methylenedioxy-2',8'-epoxy-7,9'-cyclo-4'*H*-8,1'-neolignan-4'-one  
(trivial name: futoenone)



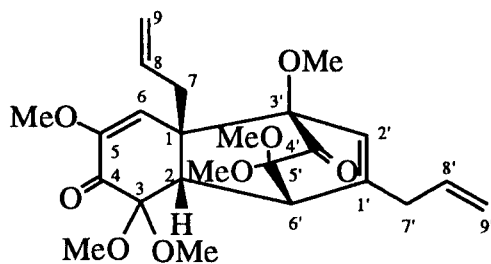
(3' $\alpha$ ,4' $\alpha$ ,7 $\alpha$ ,8 $\beta$ )-4',5'-dihydro-4-hydroxy-3,3',4'-trimethoxy-4',7-epoxy-8,3'-neolign-8'-en-6'(3'*H*)-one  
(trivial name: liliflone)



(7 $\alpha$ ,8 $\alpha$ ,8' $\beta$ ,9' $\alpha$ )-2,2'-dimethoxy-4,5:4',5'-bis(methylenedioxy)-7,9a':8',9'-diepoxy-7'-oxa-9a'-homo--8,9'-neolignan-9'-yl acetate  
(trivial name: phrymarolin I)

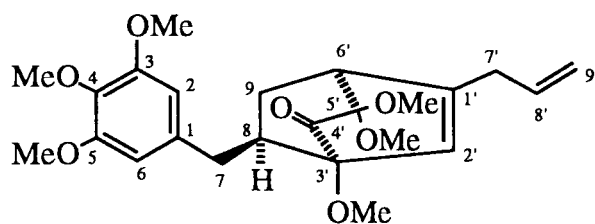


(1' $\xi$ ,7 $\alpha$ ,7' $\beta$ ,8 $\alpha$ ,8' $\beta$ )-3',4,5,7,8'-pentahydroxy-8,9'-epoxy-1',2-cyclo-9-nor-8,7'-neolignan-4'-one  
(trivial name: hydroxyathrotaxin)

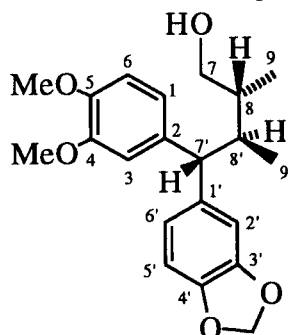


(3'*R*,6'*S*)-(1 $\beta$ ,2 $\beta$ )-2,3,5,6'-tetrahydro-3,3,3',5,5',5'-hexamethoxy-2,6'-cyclo-1,3'-neoligna-8,8'-diene-4,4'(3'*H*)-dione  
(trivial name: asatone)



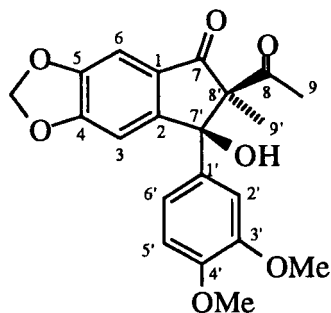


(3'*S*,6'*S*,8*R*)-5',6'-dihydro-3,3',4,5,5',5'-hexamethoxy-6',9-cyclo-8,3'-neolign-8'-en-4'(3'*H*)-one  
(trivial name: heterotropanone)

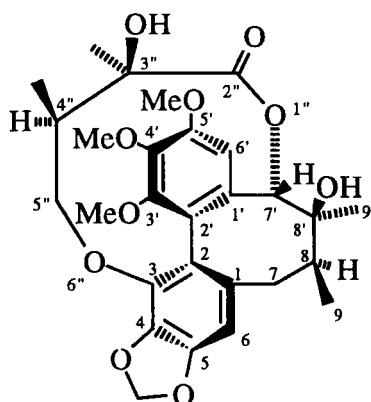


(7'*S*,8*R*,8'*S*)-4,5-dimethoxy-3',4'-methylenedioxy-1,7-seco-2,7'-cyclo lignan-7-ol

*Note:* Due to the acyclic nature of 7', 8, and 8' the *R/S*-system is used rather than  $\alpha/\beta$ . Also, see note to LG-2.2.



(8'*R*)-(7' $\alpha$ )-7'-hydroxy-3',4'-dimethoxy-4,5-methylenedioxy-7(8 $\rightarrow$ 8')abeo-2,7'-cyclo lignane-7,8-dione



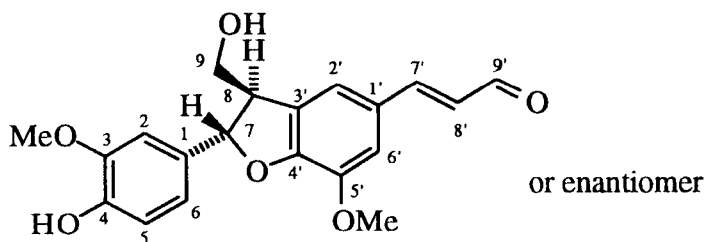
(2*S*<sub>a</sub>,3''*R*,4''*R*)-(7' $\alpha$ ,8 $\beta$ ,8' $\alpha$ )-3'',8'-dihydroxy-3',4',5'-trimethoxy-3'',4''-dimethyl-4,5-methylenedioxy--3,7'-(epoxybutanoxy)-2,2'-cyclo lignan-2''-one  
(trivial name: gomisin D)

Note that although the principal functional group is a lactone one of the oxygen atoms is included in the bridge so that the oxygen atom of the carbonyl group is treated as a “ketone”.

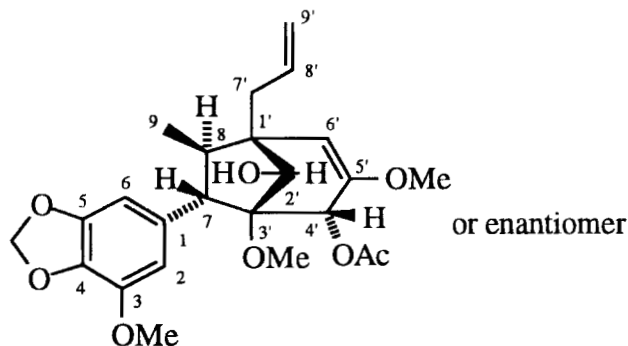
### LG-5.4 Relative configuration

When the relative, but not the absolute, configuration is known this is shown by prefixing the name of one enantiomer with *rel-* (see rule E-4.10(b) [14], rule RF-10.6 [12]). If known, the sign of rotation of polarized light (+) or (–) may be added. If *R* or *S* is needed to describe the stereochemistry then **all** chiral centers will need to be described using *R*\* or *S*\* (see rule E-4.10 (a) [14], rule R-7.2.2 [13], F-6.7 [9], rule RF-10.6 [12]).

Examples:



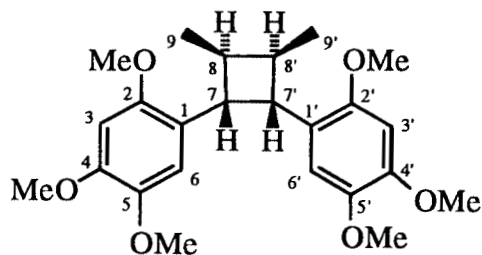
*rel*-(7*E*)-(7 $\alpha$ ,8 $\beta$ )-4,9-dihydroxy-3,5'-dimethoxy-4',7-epoxy-8,3'-neolign-7'-en-9'-al  
(trivial name: balanophonin)



*rel*-(2'*R*)-(1' $\beta$ ,3' $\beta$ ,4' $\alpha$ ,7 $\alpha$ ,8 $\beta$ )-3',4'-dihydro-2'-hydroxy-3,3',5'-trimethoxy-4,5-methylenedioxy-2'*H*-3',7-cyclo-8,1'-neolign-8'-en-4'-yl acetate

The relative configuration of an achiral lignan, neolignan, or oxyneolignan is specified by the configuration symbols (LG-5.2) in the same way as before (LG-5.3).

Example:

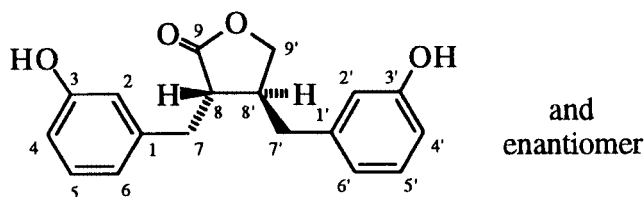


(7 $\alpha$ ,7' $\alpha$ ,8 $\beta$ ,8' $\beta$ )-2,2',4,4',5,5'-hexamethoxy-7,7'-cyclo lignane  
(trivial name: heterotropan)

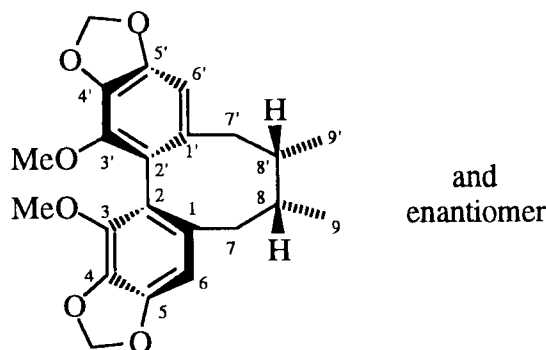
**LG-5.5 Racemate**

Racemates are named by citing the italicized prefix *rac*- in front of the whole name for the enantiomer with the lowest numbered chiral center in the  $\alpha$  form (see rule F-6.6 [9], rule RF-10.5 [12]).

Examples:



*rac*-(8 $\alpha$ ,8' $\beta$ )-3,3'-dihydroxylignano-9,9'-lactone  
(trivial name: enterolactone)

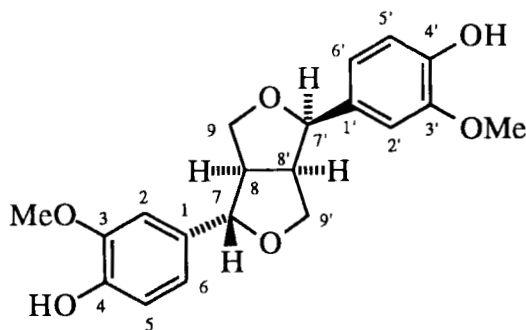


*rac*-(8 $\alpha$ ,8' $\alpha$ )-3,3'-dimethoxy-4,5:4',5'-bis(methylenedioxy)-2,2'-cyclo lignane  
(trivial name: ( $\pm$ )-wuweizisu C)

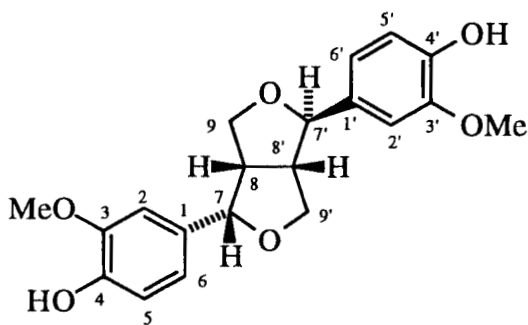
**LG-5.6 Enantiomers**

The stereochemistry of enantiomers are in general clearly indicated by the procedure of LG-5.3. If it is necessary to indicate an enantiomeric relationship between two lignans or neolignans where only the relative configuration is known, or if not even the relative configuration is known, then the italicized prefix *ent*- may be used to show this relationship (see rule F-6.5 [9], rule RF-10.3 [12]). The prefix *ent*- is more commonly used to show the relationship using trivial names.

Examples:



(7 $\alpha$ ,7' $\beta$ ,8 $\alpha$ ,8' $\alpha$ )-3,3'-dimethoxy-7,9':7',9'-diepoxylignane-4,4'-diol  
(trivial name: (+)-epipinoresinol or *ent*-symplocosigenol)



(7 $\alpha$ ,7' $\beta$ ,8 $\beta$ ,8' $\beta$ )-3,3'-dimethoxy-7,9':7',9'-diepoxylignane-4,4'-diol  
(trivial name: (-)-epipinoresinol or symplocosigenol)

## LG-6. TRIMERS OF THE C<sub>6</sub>C<sub>3</sub> UNIT AND HIGHER ANALOGUES

Higher analogues of the lignans and neolignans are composed of three or more C<sub>6</sub>C<sub>3</sub> units. By analogy with the terpenoids these have been referred to as sesquieolignans, dineolignans, etc. They may be named by an analogous way to the lignans and neolignans. The unprimed numbers are assigned to one of the terminal units and the other units are primed serially. Where there is a choice of locants, preference is made in order to:

- less primed numbers
- position 8
- lower numbers

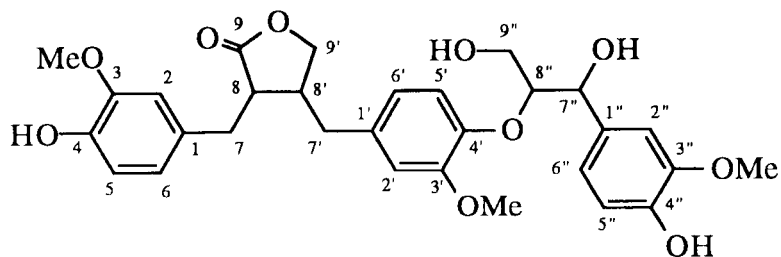
If there is an oxy linkage (see LG-1.4) this is quoted separate from and in front of the direct C–C linkages. If there is more than one oxylinkage then bis-, tris-, etc. is used. The number of C<sub>6</sub>C<sub>3</sub> units is indicated by the appropriate prefix and neolignane:

- three C<sub>6</sub>C<sub>3</sub> units      sesquieolignane
- four C<sub>6</sub>C<sub>3</sub> units      dineolignane
- five C<sub>6</sub>C<sub>3</sub> units      sesterneolignane

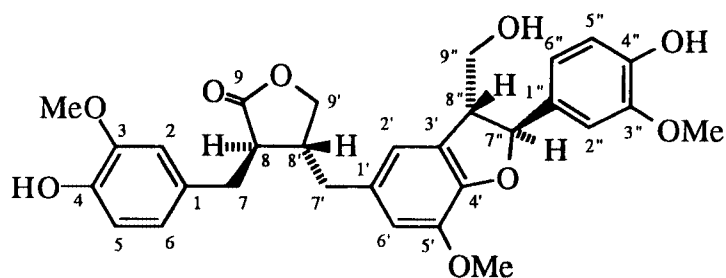
### LG-6.1 Sesquieolignans

Derivatives of the sesquieolignane skeleton are named following the recommendations of LG-2 to LG-5. If there is a choice the same criteria apply. In addition to unprimed numbers being preferred to primed, less primed numbers are preferred to ones with more primes.

*Examples:*



4,4'',7'',9''-tetrahydroxy-3,3',3''-trimethoxy-4',8''-oxy-8,8'-sesquieolignano-9,9'-lactone  
(trivial name: lappaol E)

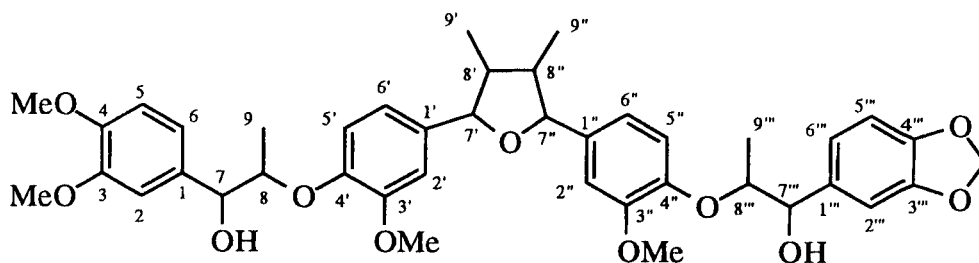


(7'' $\beta$ ,8 $\beta$ ,8' $\alpha$ ,8'' $\alpha$ )-4,4'',9''-trihydroxy-3,3'',5''-trimethoxy-4',7''-epoxy-  
-8,8':3',8''-sesquielignano-9,9''-lactone  
(trivial name: lappaol A)

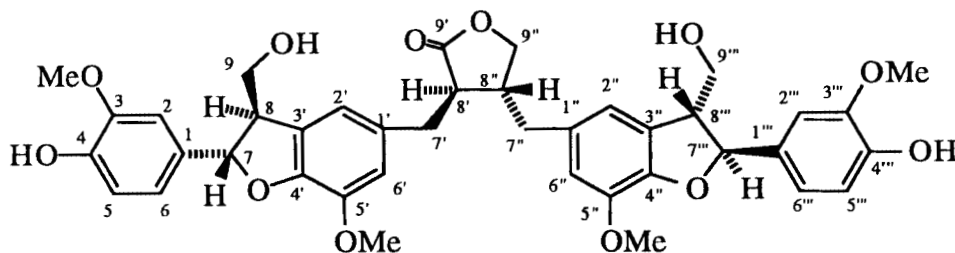
### LG-6.2 Dineolignans

Dineolignans are named in a similar way to sesquielignans. The locants for the additional C<sub>6</sub>C<sub>3</sub> unit are triple primed.

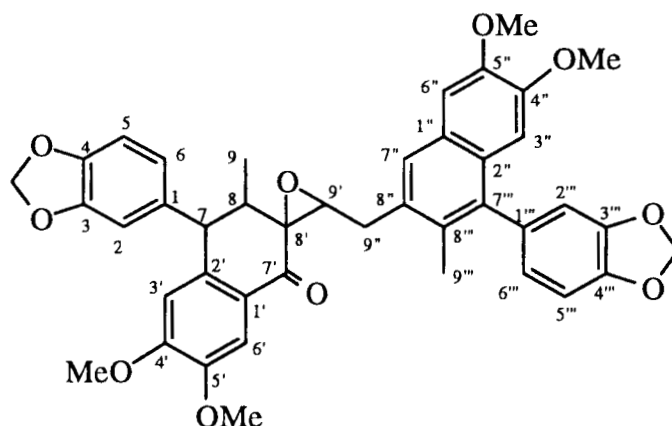
Examples:



7,7'''-dihydroxy-3,3',3'',4-tetramethoxy-3''',4'''-methyleneedioxy-7',7''-epoxy-8,4':4'',8'''-bisoxo-  
-8',8''-dineolignane  
(trivial name: manassantin B)



(7 $\alpha$ ,7''' $\beta$ ,8 $\beta$ ,8' $\beta$ ,8'' $\alpha$ ,8''' $\alpha$ )-4,4''',9,9'''-tetrahydroxy-3,3''',5''-tetramethoxy-4',7:4'',7'''-  
-diepoxy-8,3':8',8''':3'',8'''-dineolignano-9,9'''-lactone  
(trivial name: lappaol F)



4',4'',5',5''-tetramethoxy-3,4:3''',4''''-bis(methylenedioxy)-8',9'-epoxy-2',7:2'',7''''-dicyclo-  
-8,8':9',9'':8'',8''''-dineoligna-7'',7''''-dien-7'-one

### LG-7. SUMMARY

To generate a semisystematic name for a lignan, neolignan, oxyleneolignan, or higher homologue the following stages should be applied in order:

- Identify the  $C_6C_3$  units.
- Identify the preferred link(s) between the units with  $\beta, \beta'$  (LG-1.1) preferred to other carbon-carbon links (LG-1.2), and oxygen-linked units (LG-1.4) least preferred. Homologues are considered similarly (LG-6).
- Identify parent lignane, neolignane, oxyleneolignane, or higher homologue, with indicated hydrogen (LG-1.3) if needed.
- Identify any additional rings present (LG-2.1), cleaved rings (LG-2.2), removed skeletal atoms (LG-2.3), added skeletal atoms (LG-2.4), replaced skeletal atoms (LG-2.5), bridges such as epoxy (LG-2.6), or rearranged skeletons (LG-2.7). In each case, identify any indicated hydrogen if required (LG-1.3).
- Identify any side-chain double bonds (LG-3.1).
- Identify, if present, the principal functional group named as a suffix (LG-4.1 to LG-4.5) with added hydrogen if appropriate (LG-4.4).
- Identify any further changes in hydrogenation level, such as reduction of the aromatic ring (LG-3.2) or a double bond between an aromatic ring and side chain (LG-3.3).
- Identify any other functional groups (excluding the principal functional group) that are named as a prefix (LG-4.3 to LG-4.6).
- Orientate the structural formula to indicate stereochemistry (LG-5.1).
- Identify the stereochemistry present (LG-5.3 to LG-5.6) with appropriate configuration symbols (LG-5.2).
- Number the skeleton by application of the selection rules cited above, applied in the same order until a unique numbering system is obtained (see also LG-1.5).
- Construct the name in the order of stereochemistry (j above), detachable prefixes in alphabetical order ignoring multiplicative prefixes (g and h above), nondetachable prefixes in order *abeo-* to *cyclo-* (i.e., reverse of order identified; d above), parent (c above), side-chain double bonds (e above) and principal functional group (f above). Indicated or added hydrogen is included where appropriate.

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