IUPAC Recommendations

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Nomenclature of flavonoids (IUPAC Recommendations 2017)

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Abstract: Flavonoid structures, found in nature or obtained by synthesis, may be very complex. These Recommendations provide a guide for flavonoid aglycone names. This will also allow the construction of the names for their polyglycosylated species with clarity and conciseness. A joint working party of IUPAC/IUBMB members has prepared these recommendations, which establish rules for the general nomenclature of flavonoids, providing examples of acceptable trivial names, and names derived from trivial names, together with semi-systematic and fully systematic names that follow the published IUPAC recommendations.

Keywords: flavonoid; nomenclature; semi-systematic name.

CONTENTS

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Flv-1 Introduction

Flavonoids, including the parent cyclic structures and their *O*- and *C*-glycosylated derivatives, are a group of structurally diverse natural or synthetic compounds, many of them exhibiting biological activity [1–5]. They are cited in the literature by researchers in diverse specialized areas, including natural product chemistry, organic synthesis, medicinal and food chemistry, biology, toxicology, and biochemistry. Different workers have used a variety of alternative names and naming systems for such compounds, and trivial names are commonly used. Semi-systematic names derived from parent structures (unsubstituted skeletal structures) are very useful for naming flavonoids, and have been widely used to simplify complex systematic names, but they often lead to misunderstandings. There is an urgent need to avoid ambiguity in the naming of flavonoids by clarifying acceptable usage and limiting the variety of options to a reasonable extent.

In IUPAC nomenclature, three levels of nomenclature are accepted in the field of natural products [6–9]: (a) the trivial name, given for convenience to a new compound, carrying no (or minimal) structural information, and often derived from the biological origin of the material; (b) the systematic name, describing the full structure that comprises the skeleton, the characteristic groups, and the substituent groups; (c) the semi-systematic name, providing a simplified alternative to the systematic name, which often becomes too cumbersome to be continually inserted into the text of a publication. The semi-systematic name is normally achieved by the creation of one of the two possible 'semi-systematic parents': (a) the parent hydride or parent structure, which does not have terminal hetero atoms or functional groups and therefore consists only of skeletal atoms and hydrogen; (b) the functional parent, which is a structure that has certain terminal heteroatoms or groups. When applied, the Preferred IUPAC Name (PIN) [6] is also given. The PIN is a name assigned to a chemical substance and preferred among two or more names generated from two or more IUPAC recommendations, including the many synonyms that have been coined and used over the years. These recommendations establish rules for the general nomenclature of flavonoids, providing examples of acceptable trivial, semi-systematic, and fully systematic names that follow the published IUPAC recommendations, *e.g.* references [6–11]. Class names for flavonoids, their parent structures, and the order of citation of primed or unprimed locants are revisited and clarified. Names of *O*- and *C*-glycosylated derivatives follow established carbohydrate nomenclature [11]. Semi-systematic names are based on the parent structures or their functional parents. These are presented and illustrative examples are provided to avoid ambiguous interpretations.

Flv-2 Flavonoids – Definition and conventions

The term "flavonoid" includes natural and synthetic products and is applied to: (1) compounds whose structural feature is based on derivatives of a phenyl-substituted propylbenzene (in the literature commonly termed 1-phenylpropane) possessing a C15 skeleton; (2) compounds having a C16 skeleton that are phenyl-substituted propylbenzene derivatives (rotenoids); (3) flavonolignans, whose structure is based on derivatives of phenyl-substituted propylbenzene condensed with C6-C3 lignan [12] precursors.

The following carbon frameworks characterize the various flavonoid classes.

Flv-2.1 Flavonoid classes with a C_6-C_3-C_6 carbon framework

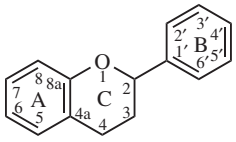
The term flavonoid is also used in a restricted sense as comprising only those compounds with a C_6-C_3-C_6 carbon framework exhibiting the structure of a chromane or that of a 1-benzopyran (PIN) (chromene), in which the fused benzene ring is designated as ring A and the 3,4-dihydro-2*H*-pyran or the pyran as ring C, along with a (substituted) phenyl group (ring B) on ring C.

Depending on the position of the linkage of ring B to the chromane/1-benzopyran (chromene) moiety, three different classes can be assigned: flavonoids (Flv-2.1.1), isoflavonoids (Flv-2.1.2) and neoflavonoids (Flv-2.1.3).

The other flavonoid classes that have a structure with a C_6-C_3-C_6 carbon framework are the chalcones (Flv-2.1.4), the aurones (Flv-2.1.5), and the pterocarpans and their 3,4-didehydro derivatives (coumestans) (Flv-2.1.6).

Flv-2.1.1 Flavonoids (in restricted sense)

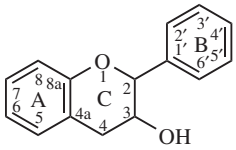
Flavonoids (in restricted sense) include flavans (**1**) as well as compounds of type **1** with one or two additional double bonds, and carbonyl or hydroxy groups or both in ring C, used to classify flavonoids into different categories, such as flavones, flavonols, and anthocyanidins.



1

Flv-2.1.1.1 Flavans

Flavans are compounds with a 2-phenyl-3,4-dihydro-2*H*-1-benzopyran skeleton **1**, that may be substituted, and include flavan-3-ols (compounds derived from 2-phenyl-3,4-dihydro-2*H*-1-benzopyran-3-ol skeleton **2**) and flavan-4-ones (compounds derived from 2-phenyl-2,3-dihydro-4*H*-1-benzopyran-4-one skeleton **3**), which are generically designated as flavanols and flavanones, respectively. Compounds derived from 2-phenyl-3,4-dihydro-2*H*-1-benzopyran-3,4-diol skeleton **4** are flavan-3,4-diols, designated leukoanthocyanidins because these colourless compounds have their structure derived from that of an anthocyanidin (see Flv-2.1.1.3), specifically they are dehydronated 3,4-dihydroxy-1,2,3,4-tetrahydroanthocyanidins.



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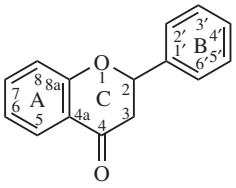

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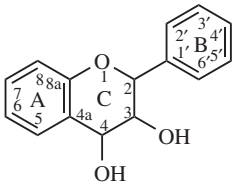
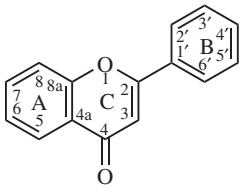


4

Flv-2.1.1.2 Flavones and 3-hydroxyflavones (flavonols)

Flavones and 3-hydroxyflavones (flavonols) are compounds with a 2-phenyl-4*H*-1-benzopyran-4-one (2-phenyl-4*H*-chromen-4-one) skeleton **5**. The term "flavonol" is used as a class name for compounds with a 3-hydroxy-2-phenyl-4*H*-1-benzopyran-4-one (3-hydroxy-2-phenyl-4*H*-chromen-4-one) skeleton **6**.



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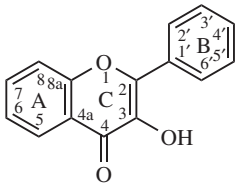
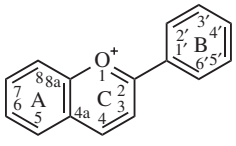


6

Flv-2.1.1.3 Anthocyanidins/anthocyanins (anthocyanidin 3-glycosides)

Anthocyanidins are compounds derived from a flavylium (2-phenyl-1λ^4-benzopyran-1-ylium or 2-phenylchromenylium) ion **7**. Anthocyanidins display colours from red to purple and, together with the 3-glycosides of anthocyanidin, the anthocyanins, represent a large group of plant pigments.



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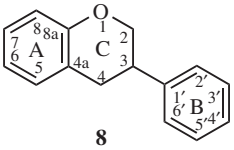
Flv-2.1.2 Isoflavonoids

The isoflavonoids are compounds derived from the parent structure 3-phenyl-3,4-dihydro-2*H*-1-benzopyran (**8**).



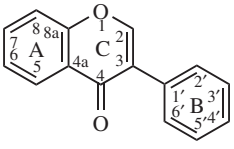
8

Flv-2.1.2.1 Isoflavans

Isoflavans are compounds with a 3-phenyl-3,4-dihydro-2*H*-1-benzopyran skeleton **8**. They may be substituted.

Flv-2.1.2.2 Isoflavones

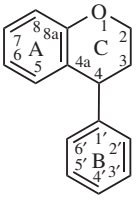
Isoflavones are compounds with a 3-phenyl-4*H*-1-benzopyran-4-one (3-phenyl-4*H*-chromen-4-one) skeleton **9**. They may be substituted.



9

Flv-2.1.3 Neoflavonoids

The neoflavonoids are compounds with a 4-phenyl-3,4-dihydro-2*H*-1-benzopyran parent structure **10**.



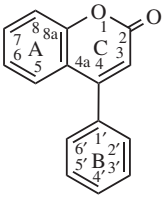
10

Flv-2.1.3.1 Neoflavans

Neoflavans are compounds with a 4-phenyl-3,4-dihydro-2*H*-1-benzopyran skeleton **10**. They may be substituted.

Flv-2.1.3.2 Neoflavones

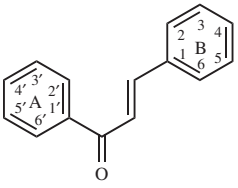
Neoflavones are compounds with a 4-phenyl-2*H*-1-benzopyran-2-one (4-phenyl-2*H*-chromen-2-one) skeleton **11**. They may be substituted. Neoflavones are also known as 4-phenylcoumarins.



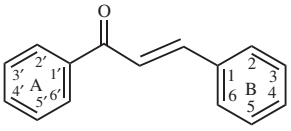
11

Flv-2.1.4 Chalcones and dihydrochalcones

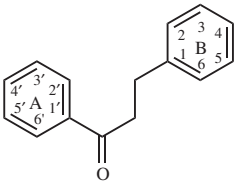
Chalcones are compounds derived from (2*E*)-1,3-diphenylprop-2-en-1-one [chalcone (PIN), structure depicted as in **12a**, **12b**]. Some of them are intermediates in the biosynthesis of flavonoids, in which the pyran ring C has not yet been formed, and are therefore biogenetically and structurally related to them. Dihydrochalcones are compounds derived from 1,3-diphenylpropan-1-one (PIN, compound **13**).



12a



12b

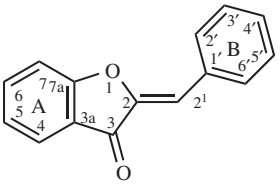


13

Note – The chalcone structure is depicted in **12a** as in the IUPAC recommendations [6], appearing in the literature mostly depicted as in **12b.**

Flv-2.1.5 Aurones

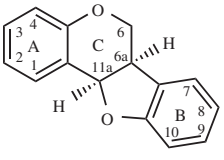
Aurones are compounds derived from (2*Z*)-2-benzylidene-1-benzofuran-3(2*H*)-one [alternative name: (2*Z*)-2-(phenylmethylidene)-1-benzofuran-3(2*H*)-one] (aurone, compound **14**).



14

Flv-2.1.6 Pterocarpans and their 3,4-didehydro derivatives (coumestans)

Pterocarpans are compounds derived from (6a*R*,11a*R*)-6a,11a-dihydro-6*H*-[1]benzofuro[3,2-*c*][1]benzopyran (**15**), and their 6a,11a-didehydro derivatives **16** are named coumestans. They are numbered systematically following the numbering rules for fused ring systems (see P-25.3.3 [6] and FR-5 [10]).



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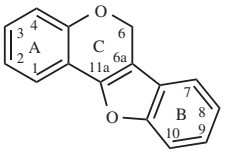
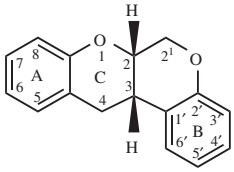


16

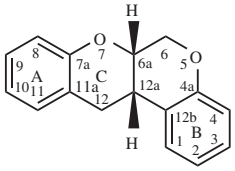
Flv-2.2 Rotenoids

Rotenoids comprise rotenanes, which are compounds with a (6a*S*,12a*S*)-6,6a,12,12a-tetrahydro[1]-benzopyrano[3,4-*b*][1]benzopyran skeleton **17b**, and rotenones, with a (6a*S*,12a*S*)-6a,12a-dihydro[1]-benzopyrano[3,4-*b*][1]benzopyran-12(6*H*)-one skeleton **18.** They may be substituted. Since the name rotenone

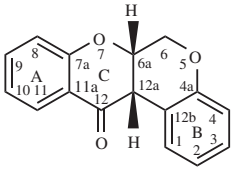
has been used not only for the functional parent **18**, but also for a more substituted specific compound (see Example **56** in Flv-3.6.6), names based on rotenone are no longer acceptable. Rotenoids are numbered as in **17a** when named as rotenane derivatives, but when named systematically, the numbering rules for fused ring systems apply, as in **17b** (see P-25.3.3 [6] and FR-5 [10]).



17a



17b



18

Flv-2.3 Flavonolignans

Flavonolignans have structures based on flavonoids condensed with C_6-C_3 lignan precursors (see Flv-3.7).

Flv-2.4 Biflavonoids and other flavonoid oligomers

Biflavonoid and other flavonoid oligomers, which occur widely in nature, are exemplified and named in Flv-3.8.

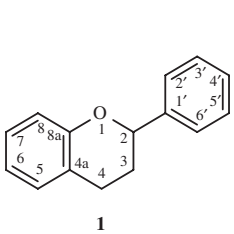
Flv-3 Guide to the construction of semi-systematic names

This section illustrates the construction of semi-systematic names. Examples are given, with trivial names, if known, and the systematic names are added.

Locant sets are arranged in ascending order, *i.e.* primed locants are placed immediately after the corresponding unprimed locants (P-14.3.5 in [6] and R-0.2.4.2 in [7]). Example: 2′,3,4,4′,6,7 (not 3,4,6,7,2′,4′).

Flv-3.1 Flavans, isoflavans, neoflavans and compounds derived from them

Names of flavans, isoflavans, and neoflavans can be derived from the name of the respective parent hydride (Fig. 1). The presence of a characteristic group is denoted by a prefix or by a suffix attached to the parent name. The suffix is used for the principal characteristic group(s) according to the priority order given in R-4.1 [7], and P-33 and P-41 [6].



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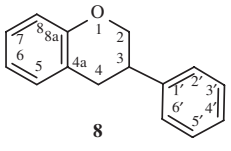

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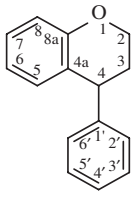

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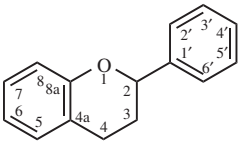
Fig. 1: Parent hydrides flavan (**1**), isoflavan (**8**), and neoflavan (**10**).

Flv-3.1.1 Flavans

Flv-3.1.1.1 Flavan aglycones

Example 1:



Semi-systematic name

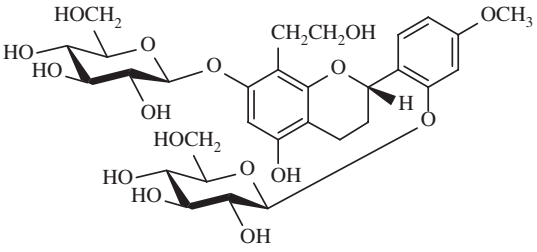
flavan

Systematic names

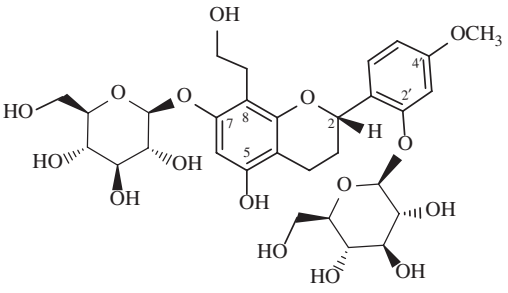
2-phenyl-3,4-dihydro-2*H*-1-benzopyran
2-phenylchromane
2-phenyl-3,4-dihydro-2*H*-chromene

Flv-3.1.1.2 Flavan glycosides

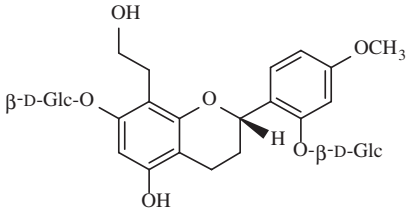
Example 2:



(a)



(b)



(c)

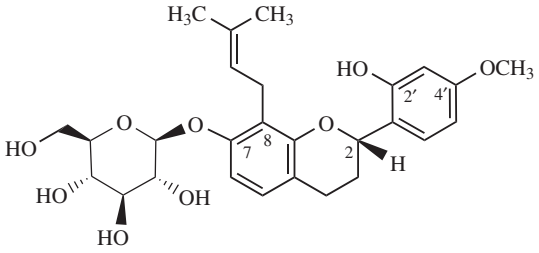
Note – Carbohydrate moieties are shown in conformational form (a), in Mills depiction (b), and in abbreviated form (c) [11].

Semi-systematic name

(2*S*)-2′,7-bis(β-D-glucopyranosyloxy)-8-(2-hydroxyethyl)-4′-methoxyflavan-5-ol

Systematic names
2-[(2*S*)-7-(β-D-glucopyranosyloxy)-5-hydroxy-8-(2-hydroxyethyl)-3,4-dihydro-2*H*-1-benzopyran-2-yl]-5-methoxyphenyl β-D-glucopyranoside
2-[(2*S*)-7-(β-D-glucopyranosyloxy)-5-hydroxy-8-(2-hydroxyethyl)-3,4-dihydro-2*H*-chromen-2-yl]-5-methoxyphenyl β-D-glucopyranoside
(2*S*)-7-(β-D-glucopyranosyloxy)-2-[2-(β-D-glucopyranosyloxy)-4-methoxyphenyl]-8-(2-hydroxyethyl)-3,4-dihydro-2*H*-1-benzopyran-5-ol
(2*S*)-7-(β-D-glucopyranosyloxy)-2-[2-(β-D-glucopyranosyloxy)-4-methoxyphenyl]-8-(2-hydroxyethyl)-chroman-5-ol
(2*S*)-7-(β-D-glucopyranosyloxy)-2-[2-(β-D-glucopyranosyloxy)-4-methoxyphenyl]-8-(2-hydroxyethyl)-3,4-dihydro-2*H*-chromen-5-ol

Example 3:

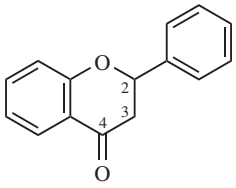


Semi-systematic names
(2*S*)-7-(β-D-glucopyranosyloxy)-4′-methoxy-8-(3-methylbut-2-en-1-yl)flavan-2′-ol
(2*S*)-2′-hydroxy-4′-methoxy-8-(3-methylbut-2-en-1-yl)flavan-7-yl β-D-glucopyranoside

Systematic names
(2*S*)-2-(2-hydroxy-4-methoxyphenyl)-8-(3-methylbut-2-en-1-yl)-3,4-dihydro-2*H*-1-benzopyran-7-yl β-D-glucopyranoside
(2*S*)-2-(2-hydroxy-4-methoxyphenyl)-8-(3-methylbut-2-en-1-yl)chroman-7-yl β-D-glucopyranoside
(2*S*)-2-(2-hydroxy-4-methoxyphenyl)-8-(3-methylbut-2-en-1-yl)-3,4-dihydro-2*H*-chromen-7-yl β-D-glucopyranoside
2-[(2*S*)-7-(β-D-glucopyranosyloxy)-8-(3-methylbut-2-en-1-yl)-3,4-dihydro-2*H*-1-benzopyran-2-yl]-5-methoxyphenol
2-[(2*S*)-7-(β-D-glucopyranosyloxy)-8-(3-methylbut-2-en-1-yl)chroman-2-yl]-5-methoxyphenol
2-[(2*S*)-7-(β-D-glucopyranosyloxy)-8-(3-methylbut-2-en-1-yl)-3,4-dihydro-2*H*-chromen-2-yl]-5-methoxyphenol

Flv-3.1.1.3 Flavanones

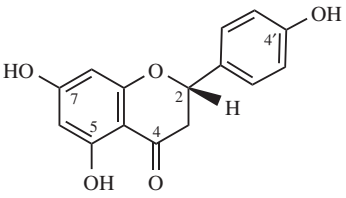
Example 4:



Semi-systematic name
flavan-4-one

Systematic names
2-phenyl-2,3-dihydro-4*H*-1-benzopyran-4-one
2-phenylchroman-4-one
2-phenyl-2,3-dihydro-4*H*-chromen-4-one

Example 5:

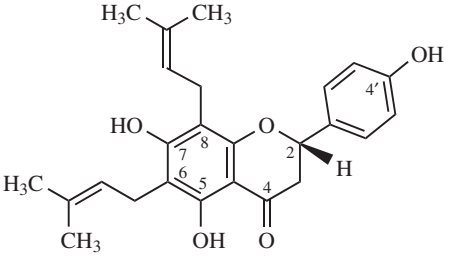


Semi-systematic name
(2*S*)-4′,5,7-trihydroxyflavan-4-one

Trivial name
naringenin

Systematic names
(2*S*)-5,7-dihydroxy-2-(4-hydroxyphenyl)-2,3-dihydro-4*H*-1-benzopyran-4-one
(2*S*)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one
(2*S*)-5,7-dihydroxy-2-(4-hydroxyphenyl)-2,3-dihydro-4*H*-chromen-4-one

Example 6:

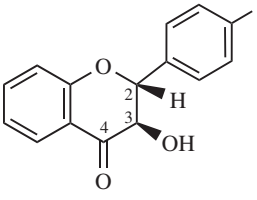


Semi-systematic name
(2*S*)-4′,5,7-trihydroxy-6,8-bis(3-methylbut-2-en-1-yl)flavan-4-one

Trivial names
6,8-bis(3-methylbut-2-en-1-yl)naringenin, 6,8-diprenylnaringenin, lonchocarpol A, senegalensin
Note – The trivial name "senegalensin" is used in the Dictionary of Flavonoids [4] and is kept as such in the present recommendations. In the literature, the incorrect spelling "senegalensein" is found in some instances.

Systematic names
(2*S*)-5,7-dihydroxy-2-(4-hydroxyphenyl)-6,8-bis(3-methylbut-2-en-1-yl)-2,3-dihydro-4*H*-1-benzopyran-4-one
(2*S*)-5,7-dihydroxy-2-(4-hydroxyphenyl)-6,8-bis(3-methylbut-2-en-1-yl)chroman-4-one
(2*S*)-5,7-dihydroxy-2-(4-hydroxyphenyl)-6,8-bis(3-methylbut-2-en-1-yl)-2,3-dihydro-4*H*-chromen-4-one

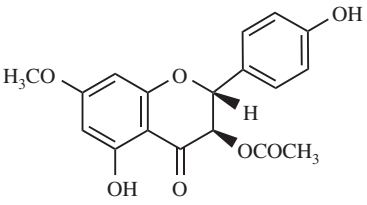
Example 7:



Semi-systematic name
(2*R*,3*R*)-3-hydroxyflavan-4-one
Not: flavanon-3-ol (see P-41, table 4.1 in the 2013 IUPAC recommendations [6], R-4.1, table 10 in [7] and C-0.0 (2) (b) in the 1979 recommendations [8]).

Systematic names
(2*R*,3*R*)-3-hydroxy-2-phenyl-2,3-dihydro-4*H*-1-benzopyran-4-one
(2*R*,3*R*)-3-hydroxy-2-phenylchroman-4-one
(2*R*,3*R*)-3-hydroxy-2-phenyl-2,3-dihydro-4*H*-chromen-4-one

Example 8:



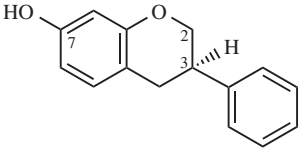
Semi-systematic name
(2*R*,3*R*)-4′,5-dihydroxy-7-methoxy-4-oxoflavan-3-yl acetate
Not: (2*R*,3*R*)-4′,5-dihydroxy-7-methoxyflavanone 3-acetate

Trivial names
7-*O*-methylaromadendrin 3-acetate
Not: 3-*O* acetyl-7-*O*-methylaromadendrin

Systematic names
(2*R*,3*R*)-5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-4-oxo-3,4-dihydro-2*H*-1-benzopyran-3-yl acetate
(2*R*,3*R*)-5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-4-oxochroman-3-yl acetate
(2*R*,3*R*)-5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-4-oxo-3,4-dihydro-2*H*-chromen-3-yl acetate

Flv-3.1.2 Isoflavans

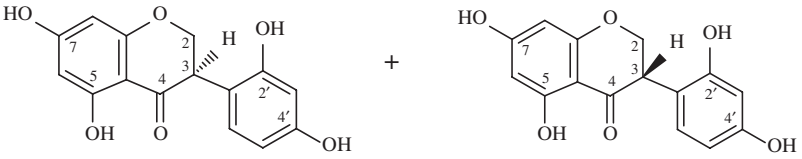
Example 9:



Semi-systematic name
(3*R*)-isoflavan-7-ol

Systematic names
(3*R*)-3-phenyl-3,4-dihydro-2*H*-1-benzopyran-7-ol
(3*R*)-3-phenylchroman-7-ol
(3*R*)-3-phenyl-3,4-dihydro-2*H*-chromen-7-ol

Example 10:



(1:1)

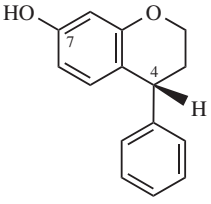
Semi-systematic name
rac-2′,4′,5,7-tetrahydroxyisoflavan-4-one

Trivial name
dalbergioidin

Systematic names
rac-3-(2,4-dihydroxyphenyl)-5,7-dihydroxy-2,3-dihydro-4*H*-1-benzopyran-4-one
rac-3-(2,4-dihydroxyphenyl)-5,7-dihydroxychroman-4-one
rac-3-(2,4-dihydroxyphenyl)-5,7-dihydroxy-2,3-dihydro-4*H*-chromen-4-one

Flv-3.1.3 Neoflavans

Example 11:



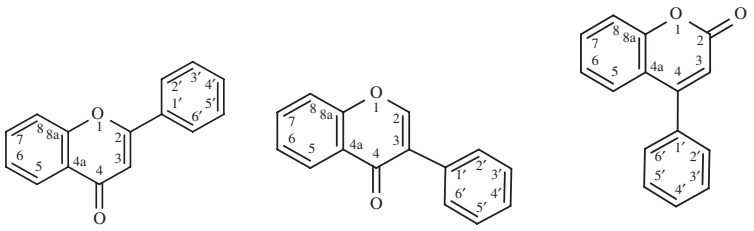
Semi-systematic name
(4*R*)-neoflavan-7-ol

Systematic names
(4*R*)-4-phenyl-3,4-dihydro-2*H*-1-benzopyran-7-ol
(4*R*)-4-phenylchroman-7-ol
(4*R*)-4-phenyl-3,4-dihydro-2*H*-chromen-7-ol

Flv-3.2 Flavones, isoflavones, neoflavones and compounds derived from them

Names of flavones, isoflavones, and neoflavones can be derived from the names of the respective functional parents (Fig. 2), which already contain one carbonyl group as an implied suffix. When substituents are among those characteristic groups with a lower priority than ketones, they have to be cited as prefixes, according to table 10, Section R-4.1 [7].

When the principal characteristic group has a higher priority than a ketone, according to table 10, Section R-4.1 [7] (see also table 3.3 in P-33.2 and table 4.1 in P-41 [6]), names of flavones, isoflavones, and neoflavones are derived from the respective flavan, isoflavan, or neoflavan parent hydride. Such groups are radicals, ions, acids, acid derivatives (anhydrides, esters, acyl halides, amides), nitriles, aldehydes, and chalcogen analogues of aldehydes.



5 **9** **11**

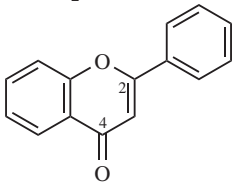
Fig. 2: Functional parents flavone (**5**), isoflavone (**9**), and neoflavone (**11**).

Flavones, isoflavones, and neoflavones containing a substructure with more than one carbonyl group are named systematically on the basis of the respective parent hydride modified by the appropriate suffix, *i.e.* -dione, -trione, *etc.*

Flv-3.2.1 Flavones

Flv-3.2.1.1 Flavone aglycones

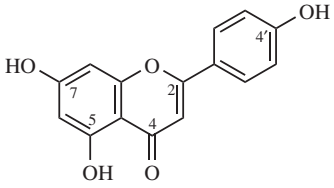
Example 12:



Semi-systematic name
flavone

Systematic names
2-phenyl-4*H*-1-benzopyran-4-one
2-phenyl-4*H*-chromen-4-one

Example 13:

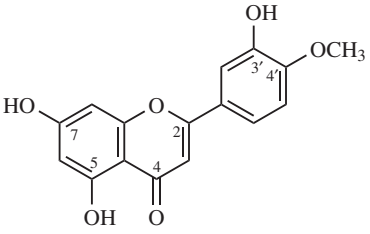


Semi-systematic name
4′,5,7-trihydroxyflavone

Trivial name
apigenin

Systematic names
5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one
5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-chromen-4-one

Example 14:

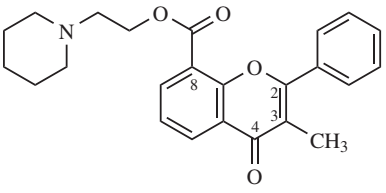


Semi-systematic name
3′,5,7-trihydroxy-4′-methoxyflavone

Trivial name
diosmetin

Systematic names
5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4*H*-1-benzopyran-4-one
5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-4*H*-chromen-4-one

Example 15:



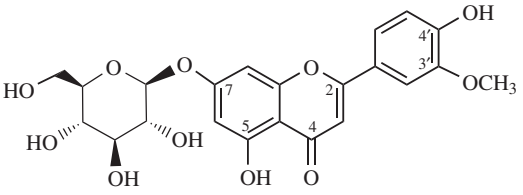
Semi-systematic name
2-(piperidin-1-yl)ethyl 3-methyl-4-oxoflav-2-ene-8-carboxylate
Not: 2-(piperidin-1-yl)ethyl 3-methyl-4-oxo-2,3-didehydroflavan-8-carboxylate (RF-8.1 [9]).

Trivial name
flavoxate
Note – Flavoxate is the International Nonproprietary Name (INN) for the anticholinergic drug.

Systematic names
2-(piperidin-1-yl)ethyl 3-methyl-4-oxo-2-phenyl-4*H*-1-benzopyran-8-carboxylate
2-(piperidin-1-yl)ethyl 3-methyl-4-oxo-2-phenyl-4*H*-chromene-8-carboxylate

Flv-3.2.1.2 Flavone glycosides

Example 16:

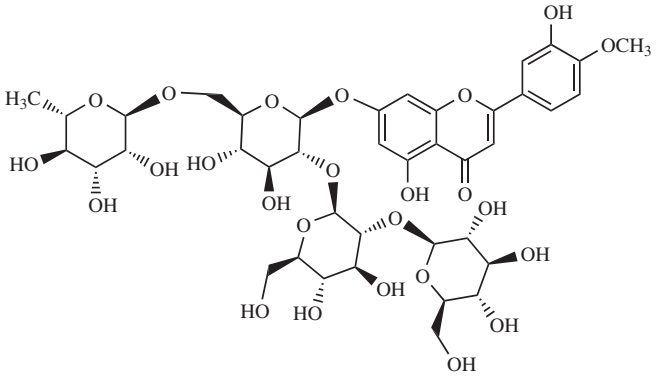


Semi-systematic name
7-(β-D-glucopyranosyloxy)-4′,5-dihydroxy-3′-methoxyflavone

Trivial name
7-*O*-(β-D-glucopyranosyl)chrysoeriol

Systematic names
5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-4-oxo-4*H*-1-benzopyran-7-yl β-D-glucopyranoside
5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-4-oxo-4*H*-chromen-7-yl β-D-glucopyranoside
7-(β-D-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-4*H*-1-benzopyran-4-one
7-(β-D-glucopyranosyloxy)-5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-4*H*-chromen-4-one

Example 17:

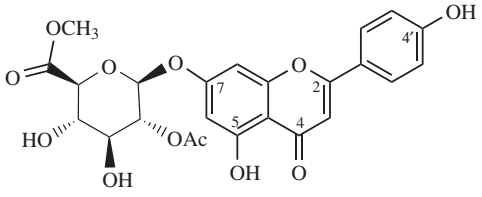


Semi-systematic name
7-{β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranosyloxy}-3′,5-dihydroxy-4′-methoxyflavone

Trivial name
7-*O*-{β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranosyl}diosmetin
Not: diosmetin 7-{β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)-[α-L-rhamnopyranosyl-(1→6)]-β-D-glucopyranoside} (because it specifies the oxygen atom at position 7 twice as diosmetin has a 7-OH and the term glucopyranoside includes both oxygen atoms of the anomeric acetal function.

Systematic names
5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-4-oxo-4*H*-1-benzopyran-7-yl 6-deoxy-α-L-mannopyranosyl-(1→6)-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside
5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-4-oxo-4*H*-chromen-7-yl 6-deoxy-α-L-mannopyranosyl-(1→6)-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)]-β-D-glucopyranoside
7-{6-deoxy-α-L-mannopyranosyl-(1→6)-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)]-β-D-glucopyranosyloxy}-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-4*H*-1-benzopyran-4-one
7-{6-deoxy-α-L-mannopyranosyl-(1→6)-[β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→2)]-β-D-glucopyranosyloxy}-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-4*H*-chromen-4-one

Example 18:



Semi-systematic name
methyl (4′,5-dihydroxy-4-oxoflav-2-en-7-yl 2-*O*-acetyl-β-D-glucopyranosid)uronate
Not: methyl (4′,5-dihydroxy-4-oxo-2,3-didehydroflavan-7-yl 2-*O*-acetyl-β-D-glucopyranosid)uronate (RF-8.1 in [9])
Not: methyl (4′,5-dihydroxyflavon-7-yl 2-*O*-acetyl-β-D-glucopyranosid)uronate (rule C-0.0 (2) (b) in the 1979 recommendations [8]).

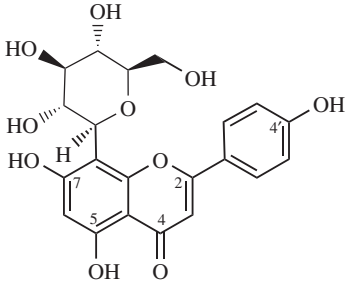
Trivial name
7-*O*-(methyl 2-*O*-acetyl-β-D-glucopyranosyluronate)apigenin
Not: methyl [apigenin 7-(2-*O*-acetyl-β-D-glucopyranosiduronate)] (because it specifies the oxygen atom at position 7 twice)
Note – The general rule that a name cannot contain two suffixes can be sometimes infringed in carbohydrate nomenclature, such as with "yluronate" in the trivial name (see 2-Carb-22 in [11]).

Systematic names
methyl [5-hydroxy-2-(4-hydroxyphenyl)-4-oxo-4*H*-1-benzopyran-7-yl 2-*O*-acetyl-β-D-glucopyranosid]uronate
methyl [5-hydroxy-2-(4-hydroxyphenyl)-4-oxo-4*H*-chromen-7-yl 2-*O*-acetyl-β-D-glucopyranosid]uronate

Flv-3.2.1.3 *C*-Glycosyl substituted flavones

Compounds arising formally from the elimination of water from the anomeric hydroxy group and a hydrogen atom bound to a carbon atom (thus creating a C–C bond) are named using the appropriate glycosyl group [11]. In the past they have been frequently named as flavonoid *C*-glycosides, but this terminology is not recommended (2-Carb-33.7 [11]).

Example 19:

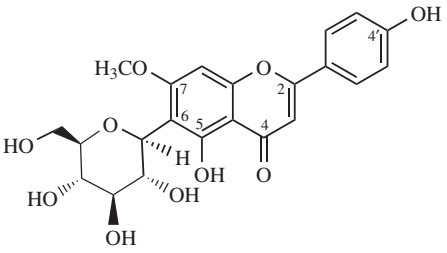


Semi-systematic name
8-(β-D-glucopyranosyl)-4′,5,7-trihydroxyflavone

Trivial names
vitexin
8-(β-D-glucopyranosyl)apigenin
Not: 8-*C*-(β-D-glucopyranosyl)apigenin, because the substituent 'β-D-glucopyranosyl' is linked directly from its anomeric carbon to C-8 of the aglycone, and the use of *C* to reinforce this C–C bond is not necessary.

Systematic names
8-(β-D-glucopyranosyl)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one
8-(β-D-glucopyranosyl)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-chromen-4-one
(1*S*)-1,5-anhydro-1-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4*H*-1-benzopyran-8-yl]-D-glucitol
(1*S*)-1,5-anhydro-1-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4*H*-chromen-8-yl]-D-glucitol
Note – In general organic-chemical nomenclature, the prefix anhydro is treated as nondetachable, but in carbohydrate nomenclature it has traditionally been detachable, *i.e.* alphabetized amongst the substituent prefixes (see 2-Carb-26 [11] and P-102.4 [6]).

Example 20:

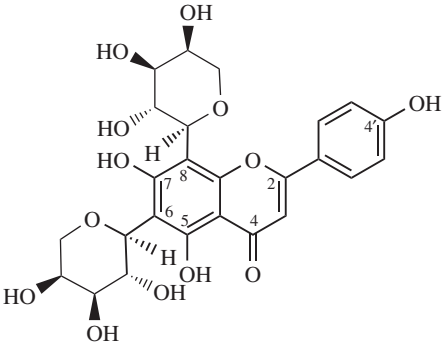


Semi-systematic name
6-(β-D-glucopyranosyl)-4′,5-dihydroxy-7-methoxyflavone

Trivial name
6-(β-D-glucopyranosyl)-7-*O*-methylapigenin

Systematic names
6-(β-D-glucopyranosyl)-5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-4*H*-1-benzopyran-4-one
6-(β-D-glucopyranosyl)-5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-4*H*-chromen-4-one
(1*S*)-1,5-anhydro-1-[5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-4-oxo-4*H*-1-benzopyran-6-yl]-D-glucitol
(1*S*)-1,5-anhydro-1-[5-hydroxy-2-(4-hydroxyphenyl)-7-methoxy-4-oxo-4*H*-chromen-6-yl]-D-glucitol
Note – See note to Example 19.

Example 21:

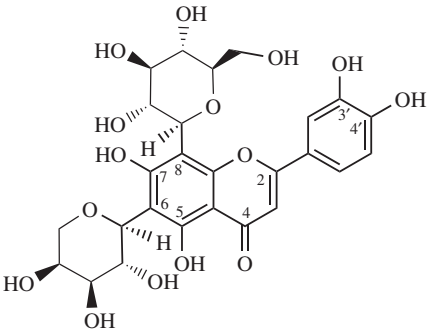


Semi-systematic name
6,8-di-(α-L-arabinopyranosyl)-4′,5,7-trihydroxyflavone

Trivial name
6,8-di-(α-L-arabinopyranosyl)apigenin
Not: apigenin 6,8-di-*C*-α-L-arabinopyranoside, because an α-L-arabinopyranosyl substituent is linked by the anomeric carbon atom to C-6 and to C-8 an of apigenin. The anomeric carbon is not linked to an oxygen atom, but to a carbon atom, and it is incorrect to name this compound as a pyranoside that includes both oxygen atoms of the anomeric acetal function [11].

Systematic names
6,8-di-(α-L-arabinopyranosyl)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one
6,8-di-(α-L-arabinopyranosyl)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-chromen-4-one

Example 22:

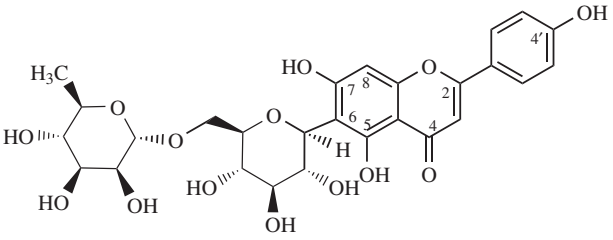


Semi-systematic name
6-(α-L-arabinopyranosyl)-8-(β-D-glucopyranosyl)-3′,4′,5,7-tetrahydroxyflavone

Trivial names
isocarlinoside
6-(α-L-arabinopyranosyl)-8-(β-D-glucopyranosyl)luteolin
Not: 6-*C*-(α-L-arabinopyranosyl)luteolin 8-β-D-glucopyranoside (since it specifies an oxygen atom linked to position 8, because the term glucopyranoside includes both oxygen atoms of the anomeric acetal function).

Systematic names
6-(α-L-arabinopyranosyl)-2-(3,4-dihydroxyphenyl)-8-(β-D-glucopyranosyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one
6-(α-L-arabinopyranosyl)-2-(3,4-dihydroxyphenyl)-8-(β-D-glucopyranosyl)-5,7-dihydroxy-4*H*-chromen-4-one

Example 23:



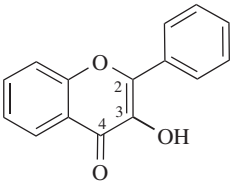
Semi-systematic name
4′,5,7-trihydroxy-6-[α-D-rhamnopyranosyl-(1→6)-β-D-glucopyranosyl]flavone

Trivial names
dulcinoside
6-[α-D-rhamnopyranosyl-(1→6)-β-D-glucopyranosyl]apigenin
Not: 6-*C*-[6″-*O*-(α-D-rhamnopyranosyl)-β-D-glucopyranosyl]apigenin, see the IUPAC Recommendations for Carbohydrate Nomenclature [11]. Apigenin does not have any hydroxy group at position 6, thus the anomeric carbon atom is linked to position 6 by a C–C bond and this should not be specified twice.

Systematic names
6-[6-deoxy-α-D-mannopyranosyl-(1→6)-β-D-glucopyranosyl]-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one
6-[6-deoxy-α-D-mannopyranosyl-(1→6)-β-D-glucopyranosyl]-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-chromen-4-one
(1*S*)-1,5-anhydro-6-*O*-(6-deoxy-α-D-mannopyranosyl)-1-[5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4*H*-1-benzopyran-6-yl]-D-glucitol

Flv-3.2.1.4 Flavonols and flavonol glycosides

Example 24:



Semi-systematic name

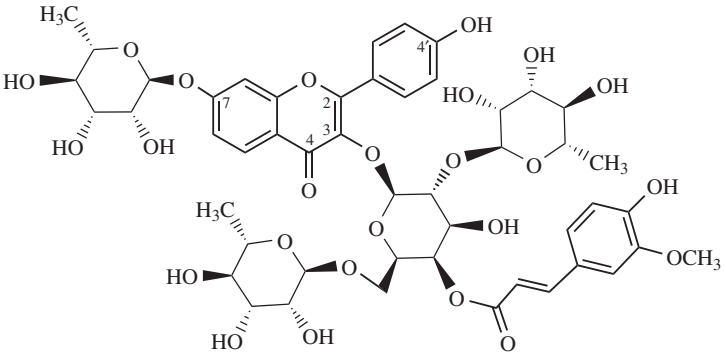
3-hydroxyflavone

Systematic name

3-hydroxy-2-phenyl-4*H*-1-benzopyran-4-one

3-hydroxy-2-phenyl-4*H*-chromen-4-one

Example 25:



Semi-systematic name

4′-hydroxy-3-{4-*O*-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]-[α-L-rhamnopyranosyl-(1→2)]-[α-L-rhamnopyranosyl-(1→6)]-β-D-galactopyranosyloxy}-7-(α-L-rhamnopyranosyloxy)flavone

Systematic names

7-(6-deoxy-α-L-mannopyranosyloxy)-2-(4-hydroxyphenyl)-4-oxo-4*H*-1-benzopyran-3-yl [6-deoxy-α-L-mannopyranosyl-(1→2)]-[6-deoxy-α-L-mannopyranosyl-(1→6)]-4-*O*-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)-prop-2-enoyl]-β-D-galactopyranoside

7-(6-deoxy-α-L-mannopyranosyloxy)-2-(4-hydroxyphenyl)-4-oxo-4*H*-chromen-3-yl [6-deoxy-α-L-mannopyranosyl-(1→2)]-[6-deoxy-α-L-mannopyranosyl-(1→6)]-4-*O*-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)-prop-2-enoyl]-β-D-galactopyranoside

{7-(6-deoxy-α-L-mannopyranosyloxy)-2-(4-hydroxyphenyl)-4-oxo-4*H*-1-benzopyran-3-yl 4-deoxy-[6-deoxy-α-L-mannopyranosyl-(1→2)]-[6-deoxy-α-L-mannopyranosyl-(1→6)]-β-D-galactopyranosid-4-yl} (2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate

{7-(6-deoxy-α-L-mannopyranosyloxy)-2-(4-hydroxyphenyl)-4-oxo-4*H*-chromen-3-yl 4-deoxy-[6-deoxy-α-L-mannopyranosyl-(1→2)]-[6-deoxy-α-L-mannopyranosyl-(1→6)]-β-D-galactopyranosid-4-yl} (2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate

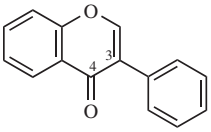
3-{[6-deoxy-α-L-mannopyranosyl-(1→2)]-[6-deoxy-α-L-mannopyranosyl-(1→6)]-4-*O*-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]-β-D-galactopyranosyloxy}-7-(6-deoxy-α-L-mannopyranosyloxy)-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one

3-{[6-deoxy-α-L-mannopyranosyl-(1→2)]-[6-deoxy-α-L-mannopyranosyl-(1→6)]-4-*O*-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]-β-D-galactopyranosyloxy}-7-(6-deoxy-α-L-mannopyranosyloxy)-2-(4-hydroxyphenyl)-4*H*-chromen-4-one

Flv-3.2.2 Isoflavones and isoflavone glycosides

Flv-3.2.2.1 Isoflavone aglycones

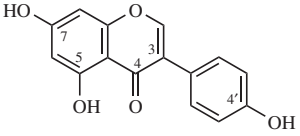
Example 26:



Semi-systematic name
isoflavone

Systematic name
3-phenyl-4*H*-1-benzopyran-4-one
3-phenyl-4*H*-chromen-4-one

Example 27:



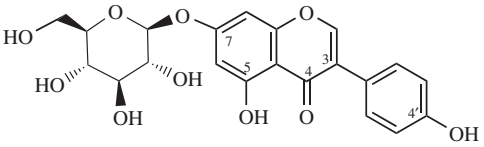
Semi-systematic name
4′,5,7-trihydroxyisoflavone

Trivial name
genistein

Systematic names
5,7-dihydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one
5,7-dihydroxy-3-(4-hydroxyphenyl)-4*H*-chromen-4-one

Flv-3.2.2.2 Isoflavone glycosides

Example 28:



Semi-systematic name
7-(β-D-glucopyranosyloxy)-4′,5-dihydroxyisoflavone

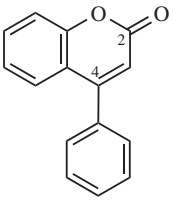
Trivial names
genistin
7-*O*-(β-D-glucopyranosyl)genistein

Systematic names
5-hydroxy-3-(4-hydroxyphenyl)-4-oxo-4*H*-1-benzopyran-7-yl β-D-glucopyranoside
5-hydroxy-3-(4-hydroxyphenyl)-4-oxo-4*H*-chromen-7-yl β-D-glucopyranoside
7-(β-D-glucopyranosyloxy)-5-hydroxy-3-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one
7-(β-D-glucopyranosyloxy)-5-hydroxy-3-(4-hydroxyphenyl)-4*H*-chromen-4-one

Flv-3.2.3 Neoflavones and neoflavone glycosides

Flv-3.2.3.1 Neoflavone aglycones

Example 29:

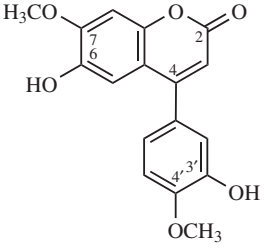


Semi-systematic name
neoflavone

Trivial name
4-phenylcoumarin

Systematic names
4-phenyl-2*H*-1-benzopyran-2-one
4-phenyl-2*H*-chromen-2-one

Example 30:



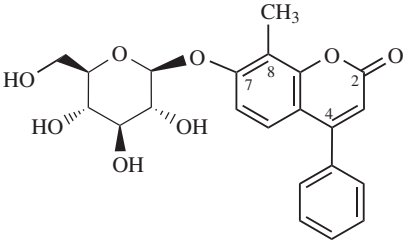
Semi-systematic name
3′,6-dihydroxy-4′,7-dimethoxyneoflavone

Trivial name
melannein

Systematic names
6-hydroxy-4-(3-hydroxy-4-methoxyphenyl)-7-methoxy-2*H*-1-benzopyran-2-one
6-hydroxy-4-(3-hydroxy-4-methoxyphenyl)-7-methoxy-2*H*-chromen-2-one

Flv-3.2.3.2 Neoflavone glycosides

Example 31:



Semi-systematic name
7-(β-D-glucopyranosyloxy)-8-methylneoflavone

Trivial name
7-(β-D-glucopyranosyloxy)-8-methyl-4-phenylcoumarin

Systematic names
8-methyl-2-oxo-4-phenyl-2*H*-1-benzopyran-7-yl β-D-glucopyranoside
8-methyl-2-oxo-4-phenyl-2*H*-chromen-7-yl β-D-glucopyranoside
7-(β-D-glucopyranosyloxy)-8-methyl-4-phenyl-2*H*-1-benzopyran-2-one
7-(β-D-glucopyranosyloxy)-8-methyl-4-phenyl-2*H*-chromen-2-one

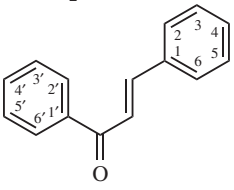
Flv-3.3 Chalcones and dihydrochalcones

There is ambiguity in the literature concerning the numbering of the carbon atoms in chalcone. Most authors, following IUPAC rule C-313.2 [8] as applied with alkyl aryl ketones such as acetophenone, have assigned primed numbers to atoms in the phenyl ring attached to the carbonyl group, and unprimed numbers to atoms in the other phenyl group. Atoms of the ethene-1,2-diyl linker have been designated α and β. Some authors have used a reverse system, assigning unprimed numbers to the ring attached to the carbonyl group and primed numbers to the other phenyl ring. [The latter usage correlates with the numbering in the flavan parent structure (Flv-2.1.1.1) that arises biosynthetically from a chalcone].

Because of this ambiguity, the term chalcone has been restricted since 1993 to its use as a retained name of "Type 3, no substitution" (R-9.1, table 27a [7]), and individual substituted chalcones are named systematically, based usually on (2*E*)-prop-2-en-1-one.

The Dictionary of Flavonoids [4] and other standard sources [1], for example, adhere consistently to the numbering of chalcones according to IUPAC rule C-313.2 [8], and the alternative usage has been largely abandoned. Since the use of Greek letters as locants has been restricted, it is now proposed that the term chalcone as a functional parent be retained as a "Type 2, limited substitution" name (P-64.2.1.1 [6]). This allows substitution in the phenyl rings, except where a substituent has priority over the carbonyl group, in which situation a fully systematic name is required (Examples 34, and 35). For the same reason, dihydrochalcones are named systematically (Example 36).

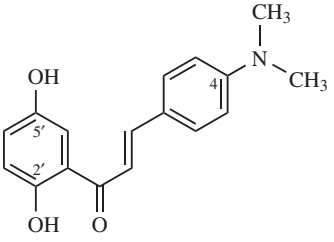
Example 32:



Semi-systematic name
chalcone (PIN)

Systematic name
(2*E*)-1,3-diphenylprop-2-en-1-one

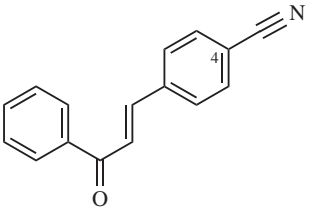
Example 33:



Semi-systematic name
4-(dimethylamino)-2′,5′-dihydroxychalcone (PIN)

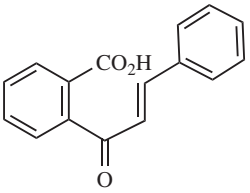
Systematic name
(2*E*)-1-(2,5-dihydroxyphenyl)-3-[4-(dimethylamino)phenyl]prop-2-en-1-one

Example 34:



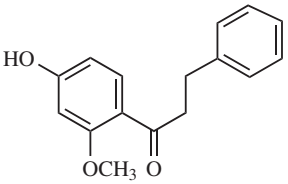
Systematic name
4-[(1*E*)-3-oxo-3-phenylprop-1-en-1-yl]benzonitrile (PIN)

Example 35:



Systematic name
2-[(2*E*)-3-phenylprop-2-enoyl]benzoic acid (PIN)

Example 36:

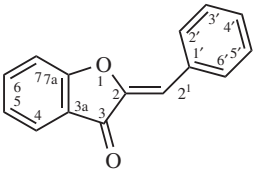


Systematic name
1-(4-hydroxy-2-methoxyphenyl)-3-phenylpropan-1-one (PIN)

Flv-3.4 Aurones

Flv-3.4.1 Aurone aglycones

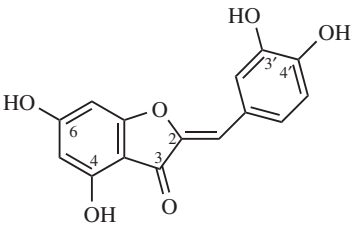
Example 37:



Semi-systematic name
aurone

Systematic name
(2*Z*)-2-benzylidene-1-benzofuran-3(2*H*)-one
(2*Z*)-2-(phenylmethylidene)-1-benzofuran-3(2*H*)-one

Example 38:



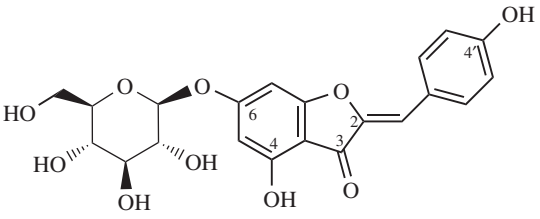
Semi-systematic name
3′,4,4′,6-tetrahydroxyaurone

Trivial name
aureusidin

Systematic name
(2*Z*)-2-[(3,4-dihydroxyphenyl)methylidene]-4,6-dihydroxy-1-benzofuran-3(2*H*)-one
(2*Z*)-2-(3,4-dihydroxybenzylidene)-4,6-dihydroxy-1-benzofuran-3(2*H*)-one

Flv-3.4.2 Aurone glycosides

Example 39:



Semi-systematic name
6-(β-D-glucopyranosyloxy)-4,4′-dihydroxyaurone

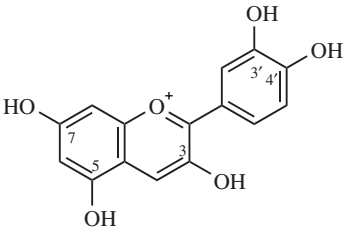
Systematic name
(2*Z*)-6-(β-D-glucopyranosyloxy)-4-hydroxy-2-(4-hydroxybenzylidene)-1-benzofuran-3(2*H*)-one
(2*Z*)-6-(β-D-glucopyranosyloxy)-4-hydroxy-2-[(4-hydroxyphenyl)methylidene]-1-benzofuran-3(2*H*)-one

Flv-3.5 Anthocyanidins and anthocyanidin 3-glycosides (anthocyanins)

Flv-3.5.1 Anthocyanidins

Anthocyanidins contain a flavylium (2-phenyl-1λ⁴-benzopyran-1-ylium, 2-phenylchromenylium) ion as a parent structure.

Example 40:



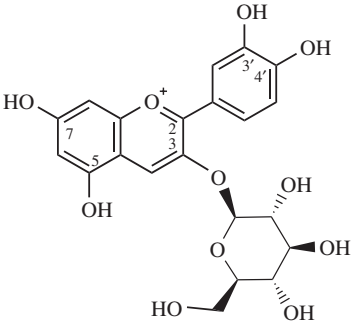
Semi-systematic name
3,3′,4′,5,7-pentahydroxyflavylium (also accepted as a retained name – see P-73.3.2, table 7.5 in [6])

Trivial name
cyanidin

Systematic names
2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-1λ⁴-benzopyran-1-ylium
2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxychromenylium

Flv-3.5.2 Anthocyanins

Example 41:

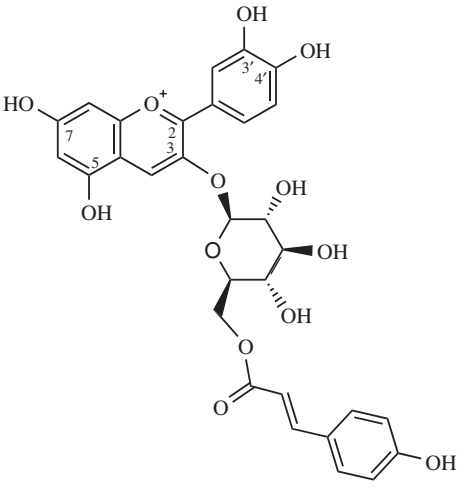


Semi-systematic name
3-(β-D-glucopyranosyloxy)-3′,4′,5,7-tetrahydroxyflavylium (also accepted as a retained name – see P-73.3.2, table 7.5 in [6])

Trivial name
3-*O*-(β-D-glucopyranosyl)cyanidin

Systematic names
2-(3,4-dihydroxyphenyl)-3-(β-D-glucopyranosyloxy)-5,7-dihydroxy-1λ⁴-benzopyran-1-ylium
2-(3,4-dihydroxyphenyl)-3-(β-D-glucopyranosyloxy)-5,7-dihydroxychromenylium

Example 42:



Semi-systematic name

3′,4′,5,7-tetrahydroxy-3-{6-*O*-[(*E*)-3-(4-hydroxyphenyl)prop-2-enoyl]-β-D-glucopyranosyloxy}flavylium (also accepted as a retained name – see P-73.3.2, table 7.5 in [6])

Trivial name

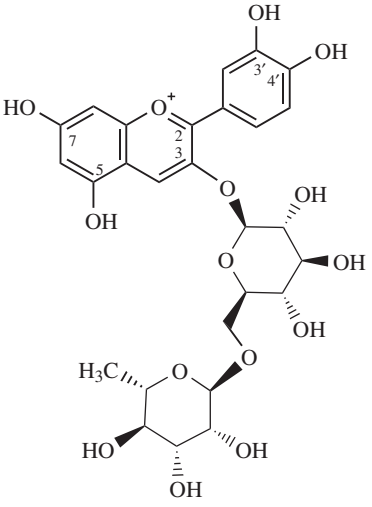
3-*O*-{6-*O*-[(*E*)-3-(4-hydroxyphenyl)prop-2-enoyl]-β-D-glucopyranosyl}cyanidin

Systematic names

2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-{6-*O*-[(2*E*)-3-(4-hydroxyphenyl)prop-2-enoyl]-β-D-glucopyranosyloxy}-1λ⁴-benzopyran-1-ylium

2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-{6-*O*-[(2*E*)-3-(4-hydroxyphenyl)prop-2-enoyl]-β-D-glucopyranosyloxy}-chromenylium

Example 43:



Semi-systematic name

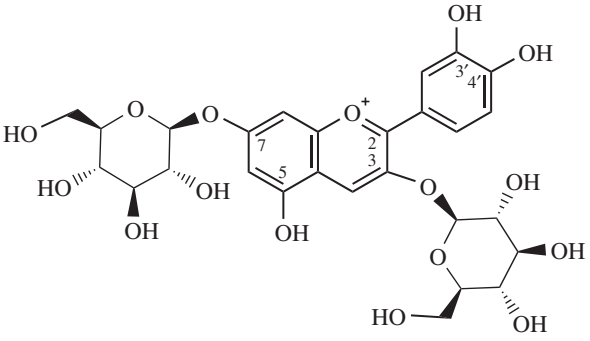
3′,4′,5,7-tetrahydroxy-3-[α-L-rhamnopyranosyl-(1→6)-β-D-glucopyranosyloxy]flavylium

Trivial name

3-*O*-β-rutinosylcyanidin

Systematic names
3-[6-deoxy-α-L-mannopyranosyl-(1→6)-β-D-glucopyranosyloxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-1λ⁴-benzopyran-1-ylium
3-[6-deoxy-α-L-mannopyranosyl-(1→6)-β-D-glucopyranosyloxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxychromenylium

Example 44:



Semi-systematic name
3,7-bis(β-D-glucopyranosyloxy)-3′,4′,5-trihydroxyflavylium

Trivial name
3,7-di-*O*-(β-D-glucopyranosyl)cyanidin
Note – The multiplicative prefix "di" is used with non-substituted substituents, but with substituted substituents "bis" must be used (P-14.2 in [6], R-0.1.4 in [7]).

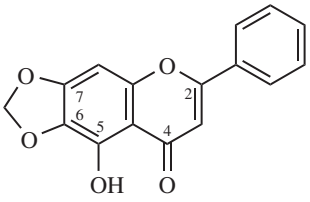
Systematic names
2-(3,4-dihydroxyphenyl)-3,7-bis(β-D-glucopyranosyloxy)-5-hydroxy-1λ⁴-benzopyran-1-ylium
2-(3,4-dihydroxyphenyl)-3,7-bis(β-D-glucopyranosyloxy)-5-hydroxychromenylium

Flv-3.6 Flavonoids containing additional fused/spiro rings in their structures

Locants for additional rings must be double primed to prevent confusion with those for the phenyl ring, which are already single primed.

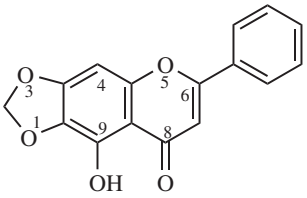
Flv-3.6.1 Flavones

Example 45:



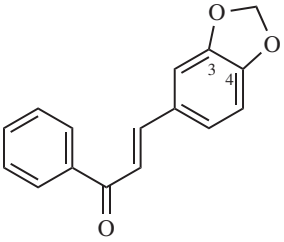
Semi-systematic name
5-hydroxy-6,7-[methylenebis(oxy)]flavone

Systematic names
9-hydroxy-6-phenyl-8*H*-[1,3]dioxolo[4,5-*g*][1]benzopyran-8-one
9-hydroxy-6-phenyl-8*H*-[1,3]dioxolo[4,5-*g*]chromen-8-one
Note – Systematic numbering is given below:



Flv-3.6.2 Chalcones

Example 46:

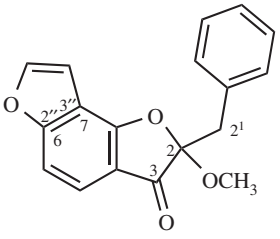


Semi-systematic name
3,4-[methylenebis(oxy)]chalcone

Systematic names
(2*E*)-3-(1,3-benzodioxol-5-yl)-1-phenylprop-2-en-1-one

Flv-3.6.3 Aurones

Example 47:

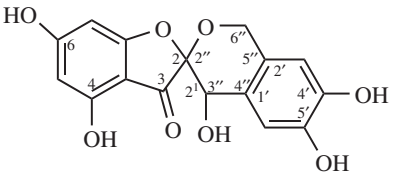


Semi-systematic name
(+)-2-methoxy-2,2¹-dihydrofuro[2″,3″:6,7]aurone

Trivial name
castillene A

Systematic name
(+)-2-benzyl-2-methoxybenzo[1,2-*b*:3,4-*b*′]difuran-3(2*H*)-one

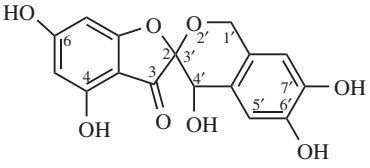
Example 48:



Semi-systematic name
2^1,4,4′,5′,6-pentahydroxy-2^1,6″-dihydropyrano[2″,3″,4″,5″:2,2^1,1′,2′]aurone

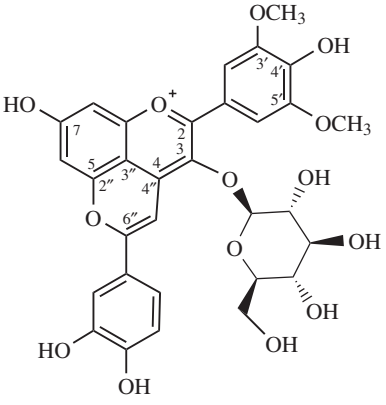
Trivial name
crombenin

Systematic names
4,4′,6,6′,7′-pentahydroxy-1′,4′-dihydro-3*H*-spiro[[1]benzofuran-2,3′-[2]benzopyran]-3-one
4,4′,6,6′,7′-pentahydroxy-3*H*-spiro[[1]benzofuran-2,3′-isochroman]-3-one
Note – Systematic numbering is given below:



Flv-3.6.4 Anthocyanidins/Anthocyanins

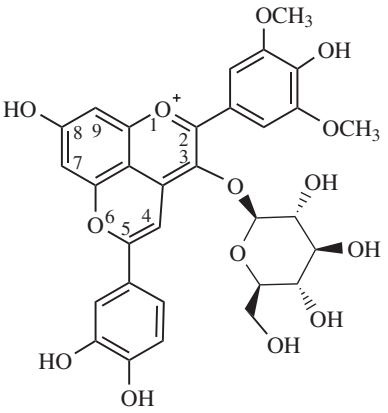
Example 49:



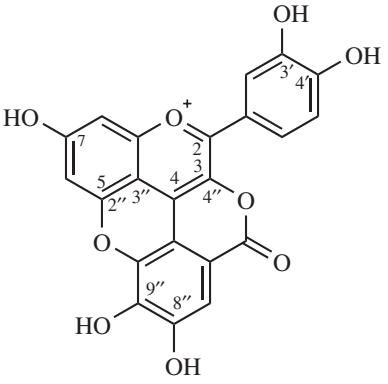
Semi-systematic name
6″-(3,4-dihydroxyphenyl)-3-(β-D-glucopyranosyloxy)-4′,7-dihydroxy-3′,5′-dimethoxypyrano[4″,3″,2″:4,5]-flavylium

Systematic names
5-(3,4-dihydroxyphenyl)-3-(β-D-glucopyranosyloxy)-8-hydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-$1\lambda^4$-pyrano[4,3,2-*de*][1]benzopyran-1-ylium
5-(3,4-dihydroxyphenyl)-3-(β-D-glucopyranosyloxy)-8-hydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-pyrano[4,3,2-*de*]chromenylium

Note – Systematic numbering [6,10] is given below:



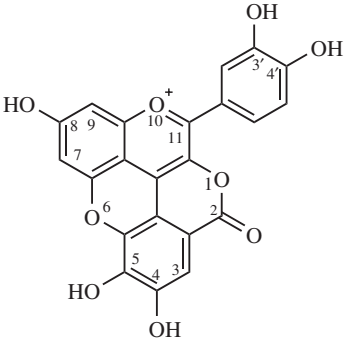
Example 50:



Semi-systematic name
3′,4′,7,8″,9″-pentahydroxy-6″-oxo-6″*H*-1″,5″-dioxaphenaleno[4″,3″,2″:3,4,5]flavylium

Trivial name
rosacyanin B

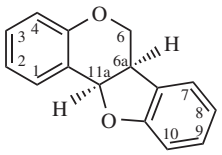
Systematic name
11-(3,4-dihydroxyphenyl)-4,5,8-trihydroxy-2*H*-1,6-dioxa-10-oxoniabenzo[*cd*]pyren-2-one
Note – Systematic numbering [6,10] is given below:



Flv-3.6.5 Pterocarpans

Although simple pterocarpans are ring-closure products of isoflavonoids, systematic numbering is used [6,10].

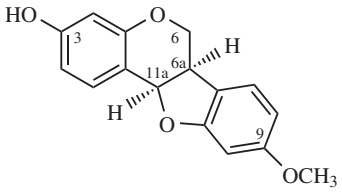
Example 51:



Semi-systematic name
pterocarpan

Systematic names
(6a*R*,11a*R*)-6a,11a-dihydro-6*H*-[1]benzofuro[3,2-*c*][1]benzopyran
(6a*R*,11a*R*)-6a,11a-dihydro-6*H*-[1]benzofuro[3,2-*c*]chromene

Example 52:

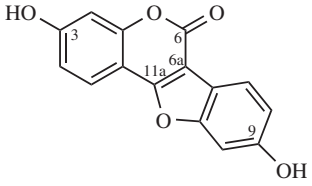


Semi-systematic name
9-methoxypterocarpan-3-ol

Trivial name
(–)-medicarpin

Systematic names
(6a*R*,11a*R*)-9-methoxy-6a,11a-dihydro-6*H*-[1]benzofuro[3,2-*c*][1]benzopyran-3-ol
(6a*R*,11a*R*)-9-methoxy-6a,11a-dihydro-6*H*-[1]benzofuro[3,2-*c*]chromen-3-ol

Example 53:



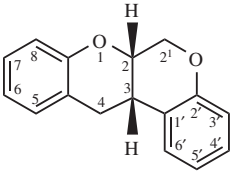
Semi-systematic names
3,9-dihydroxypterocarp-6a(11a)-en-6-one
3,9-dihydroxycoumestan-6-one
Not: 3,9-dihydroxy-6a,11a-didehydropterocarpan-6-one, because of rule RF-8.1 on introduction of unsaturation in parent names ending with 'an' [9].

Trivial name
coumestrol

Systematic names
3,9-dihydroxy-6*H*-[1]benzofuro[3,2-*c*][1]benzopyran-6-one
3,9-dihydroxy-6*H*-[1]benzofuro[3,2-*c*]chromen-6-one

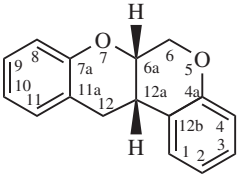
Flv-3.6.6 Rotenoids

Example 54:

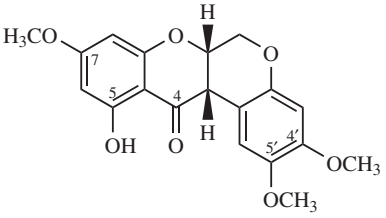


Semi-systematic name
Rotenane

Systematic names
(6a*S*,12a*S*)-6,6a,12,12a-tetrahydro[1]benzopyrano[3,4-*b*][1]benzopyran
(6a*S*,12a*S*)-6,6a,12,12a-tetrahydrochromeno[3,4-*b*]chromene
Note – Systematic numbering [6,10] is given below:



Example 55:

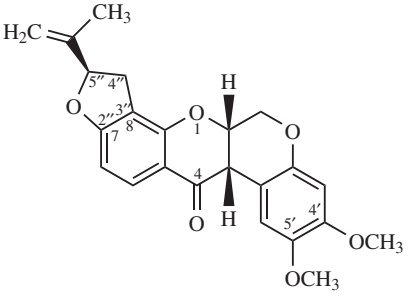


Semi-systematic name
5-hydroxy-4′,5′,7-trimethoxyrotenan-4-one

Trivial name
sermundone

Systematic names
(6a*S*,12a*S*)-11-hydroxy-2,3,9-trimethoxy-6a,12a-dihydro[1]benzopyrano[3,4-*b*][1]benzopyran-12(6*H*)-one
(6a*S*,12a*S*)-11-hydroxy-2,3,9-trimethoxy-6a,12a-dihydrochromeno[3,4-*b*]chromen-12(6*H*)-one

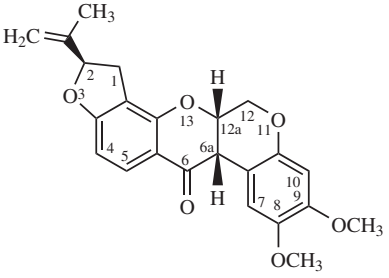
Example 56:



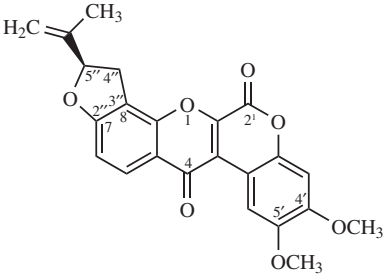
Semi-systematic name
(5″*R*)-4′,5′-dimethoxy-5″-(prop-1-en-2-yl)-4″,5″-dihydrofuro[2″,3″:7,8]rotenan-4-one

Trivial name
Not: rotenone
Note – Since the name rotenone is identical to that of the functional parent **18** (see Flv-2.2) its use is no longer recommended.

Systematic names
(2*R*,6a*S*,12a*S*)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydro[1]benzopyrano[3,4-*b*]furo[2,3-*h*]-[1]benzopyran-6(6a*H*)-one
(2*R*,6a*S*,12a*S*)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrochromeno[3,4-*b*]furo[2,3-*h*]-chromen-6(6a*H*)-one
Note – Systematic numbering [6,10] is given below:

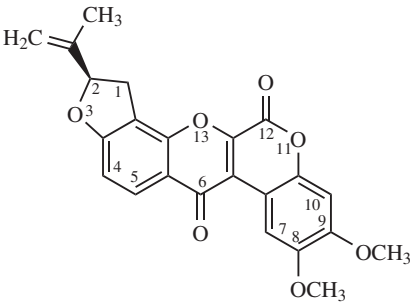


Example 57:

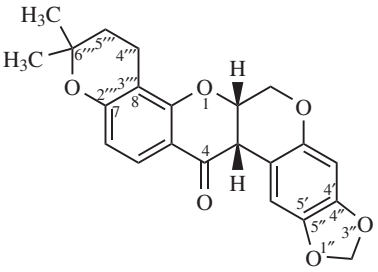


Semi-systematic name
(5″*R*)-4′,5′-dimethoxy-5″-(prop-1-en-2-yl)-4″,5″-dihydrofuro[2″,3″:7,8]roten-2-ene-2^{1},4-dione
Not: (5″*R*)-4′,5′-dimethoxy-5″-(prop-1-en-2-yl)-2,3-didehydro-4″,5″-dihydrofuro[2″,3″:7,8]rotenane-2^{1},4-dione, because of rule RF-8.1 on introduction of unsaturation in parent names ending with 'an' [9].

Systematic names
(2*R*)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2-dihydro[1]benzopyrano[3,4-*b*]furo[2,3-*h*][1]benzopyran-6,12-dione
(2*R*)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2-dihydrochromeno[3,4-*b*]furo[2,3-*h*]chromene-6,12-dione
Note – Systematic numbering [6,10] is given below:

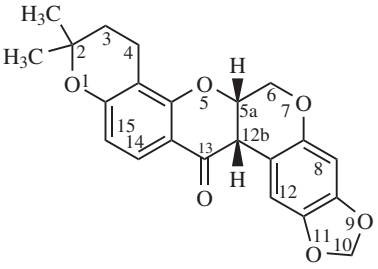


Example 58:



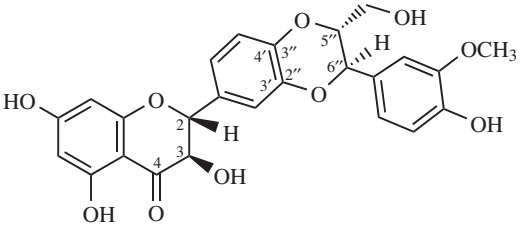
Semi-systematic name
6‴,6‴-dimethyl-5‴,6‴-dihydro-4‴*H*-[1,3]dioxolo[4″,5″:4′,5′]pyrano[2‴,3‴:7,8]rotenan-4-one

Systematic names
(5a*S*,12b*S*)-2,2-dimethyl-3,4,5a,12b-tetrahydro-2*H*-[1,3]dioxolo[4,5-*g*]pyrano[2,3-*c*:6,5-*f*′]bis-([1]benzopyran)-13(6*H*)-one
(5a*S*,12b*S*)-2,2-dimethyl-3,4,5a,12b-tetrahydro-2*H*-[1,3]dioxolo[4,5-*g*]pyrano[2,3-*c*:6,5-*f*′]dichromen-13(6*H*)-one]
Note – Systematic numbering [6,10] is given below:



Flv-3.7 Flavonolignans

Example 59:



Semi-systematic name
(2*R*,3*R*,5″*R*,6″*R*)-3,5,7-trihydroxy-6″-(4-hydroxy-3-methoxyphenyl)-5″-(hydroxymethyl)-5″,6″-dihydro-[1,4]dioxino[2″,3″:3′,4′]flavan-4-one

Trivial names
silibinin, also called silybin

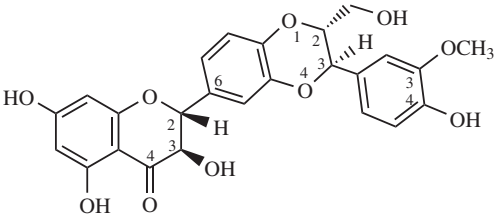
Systematic names

(2*R*,3*R*)-3,5,7-trihydroxy-2-[(2*R*,3*R*)-3-(4-hydroxy-3-methoxyphenyl)-2-(hydroxymethyl)-2,3-dihydro-1,4-benzodioxin-6-yl]-2,3-dihydro-4*H*-1-benzopyran-4-one

(2*R*,3*R*)-3,5,7-trihydroxy-2-[(2*R*,3*R*)-3-(4-hydroxy-3-methoxyphenyl)-2-(hydroxymethyl)-2,3-dihydro-1,4-benzodioxin-6-yl]chroman-4-one

(2*R*,3*R*)-3,5,7-trihydroxy-2-[(2*R*,3*R*)-3-(4-hydroxy-3-methoxyphenyl)-2-(hydroxymethyl)-2,3-dihydro-1,4-benzodioxin-6-yl]-2,3-dihydro-4*H*-chromen-4-one

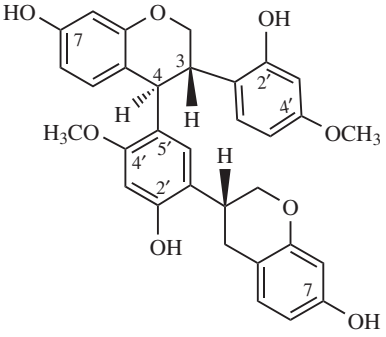
Note – Systematic numbering [6,10] is given below:



Flv-3.8 Biflavonoids and other flavonoid oligomers

Biflavonoids and other flavonoid oligomers have been widely reported in the flavonoid literature [13–19] and are also included in the present recommendations. The recommended semi-systematic names consider the terminal flavonoid first in alphabetical order as the preferred one, that is substituted by the other components. If the terminal flavonoid components are identical, the one with the lower attachment locant is cited first in the name.

Example 60:



Semi-systematic name

[(3*S*,4*R*)-4′-methoxyisoflavan-2′,7-diol]-(4→5′)-[(3*R*)-4′-methoxyisoflavan-2′,7-diol]

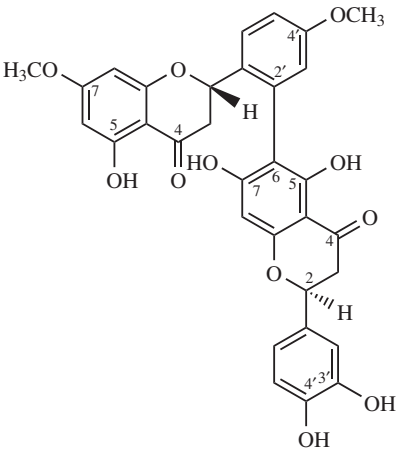
Systematic names

(3*S*,4*R*)-4-{4-hydroxy-5-[(3*R*)-7-hydroxy-3,4-dihydro-2*H*-1-benzopyran-3-yl]-2-methoxyphenyl}-3-(2-hydroxy-4-methoxyphenyl)-3,4-dihydro-2*H*-1-benzopyran-7-ol

(3*S*,4*R*)-4-{4-hydroxy-5-[(3*R*)-7-hydroxychroman-3-yl]-2-methoxyphenyl}-3-(2-hydroxy-4-methoxyphenyl)-chroman-7-ol

(3*S*,4*R*)-4-{4-hydroxy-5-[(3*R*)-7-hydroxy-3,4-dihydro-2*H*-chromen-3-yl]-2-methoxyphenyl}-3-(2-hydroxy-4-methoxyphenyl)-3,4-dihydro-2*H*-chromen-7-ol

Example 61:

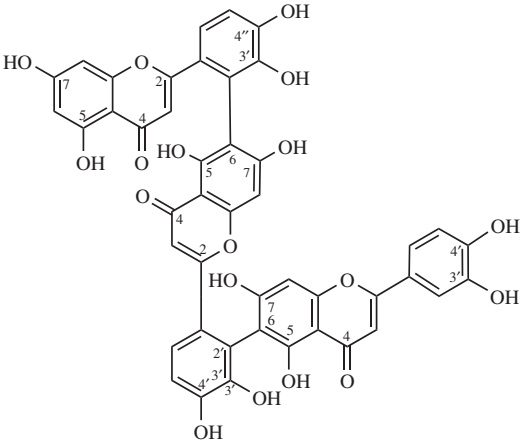


Semi-systematic name
[(2*S*)-5-hydroxy-4′,7-dimethoxyflavan-4-one]-(2′→6)-[(2*S*)-3′,4′,5,7-tetrahydroxyflavan-4-one]

Trivial name
[(2*S*)-4′,7-di-*O*-methylnaringenin]-(2′→6)-[(2*S*)-3′-hydroxynaringenin]

Systematic names
(2*S*)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-{2-[(2*S*)-5-hydroxy-7-methoxy-4-oxo-3,4-dihydro-2*H*-1-benzopyran-2-yl]-5-methoxyphenyl}-2,3-dihydro-4*H*-1-benzopyran-4-one
(2*S*)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-{2-[(2*S*)-5-hydroxy-7-methoxy-4-oxochroman-2-yl]-5-methoxyphenyl}chroman-4-one
(2*S*)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-{2-[(2*S*)-5-hydroxy-7-methoxy-4-oxo-3,4-dihydro-2*H*-chromen-2-yl]-5-methoxyphenyl}-2,3-dihydro-4*H*-chromen-4-one

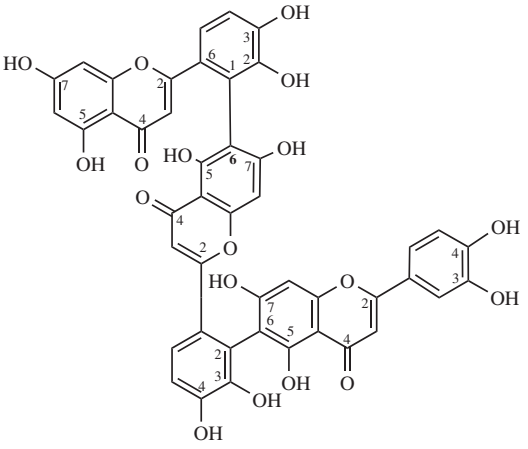
Example 62:



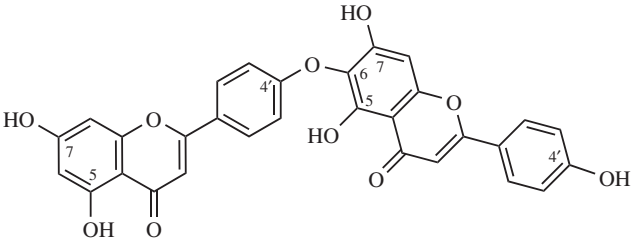
Semi-systematic name
(3′,4′,5,7-tetrahydroxyflavone)-(2′→6)-(3′,4′,5,7-tetrahydroxyflavone)-(2′→6)-(3′,4′,5,7-tetrahydroxyflavone)

Systematic names
6-(6-{6-[6-(5,7-dihydroxy-4-oxo-4*H*-1-benzopyran-2-yl)-2,3-dihydroxyphenyl]-5,7-dihydroxy-4-oxo-4*H*-1-benzopyran-2-yl}-2,3-dihydroxyphenyl)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4*H*-1-benzopyran-4-one

6-(6-{6-[6-(5,7-dihydroxy-4-oxo-4*H*-chromen-2-yl)-2,3-dihydroxyphenyl]-5,7-dihydroxy-4-oxo-4*H*-chromen-2-yl}-2,3-dihydroxyphenyl)-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4*H*-chromen-4-one
Note – Systematic numbering [6,10] is given below:



Example 63:

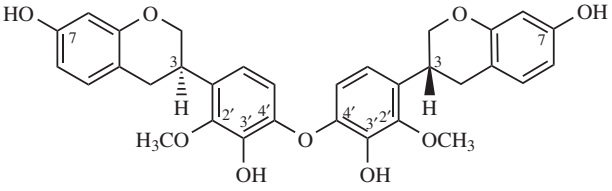


Semi-systematic name
(5,7-dihydroxyflavone)-(4′-oxy-6)-(4′,5,7-trihydroxyflavone)

Trivial name
hinokiflavone

Systematic names
6-[4-(5,7-dihydroxy-4-oxo-4*H*-1-benzopyran-2-yl)phenoxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-1-benzopyran-4-one
6-[4-(5,7-dihydroxy-4-oxo-4*H*-chromen-2-yl)phenoxy]-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-chromen-4-one

Example 64:



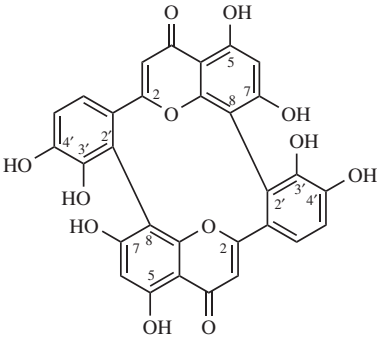
Semi-systematic name
[(3*R*)-2′-methoxyisoflavan-3′,7-diol]-(4′-oxy-4′)-[(3*R*)-2′-methoxyisoflavan-3′,7-diol]

Trivial name
biscyclolobin

Systematic names

3,3′-[oxybis(3-hydroxy-2-methoxy-4,1-phenylene)]bis[(3*R*)-3,4-dihydro-2*H*-1-benzopyran-7-ol]
3,3′-[oxybis(3-hydroxy-2-methoxy-4,1-phenylene)]bis[(3*R*)-chroman-7-ol]
3,3′-[oxybis(3-hydroxy-2-methoxy-4,1-phenylene)]bis[(3*R*)-3,4-dihydro-2*H*-chromen-7-ol]

Example 65:



Semi-systematic name

(3′,4′,5,7-tetrahydroxyflavone)-(2′→8,8→2′)-(3′,4′,5,7-tetrahydroxyflavone)

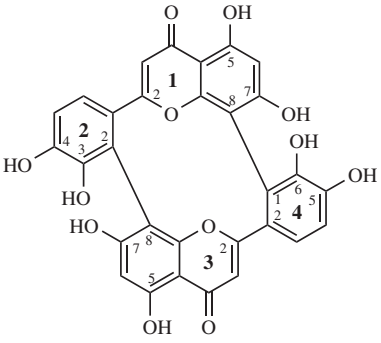
Trivial name

anhydrobartramiaflavone

Systematic names

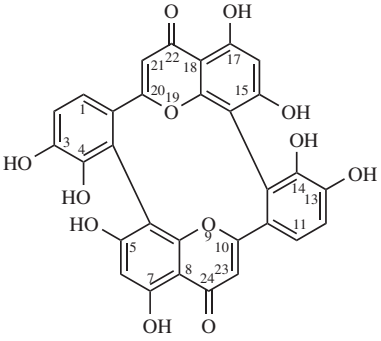
1^5,1^7,2^3,2^4,3^5,3^7,4^5,4^6-octahydroxy-1^4H,3^4H-1(2,8),3(8,2)-bis([1]benzopyrana)-2,4(1,2)-dibenzenacyclotetraphane-1^4,3^4-dione

Note – Structure numbering [6] is given below:



3,4,5,7,13,14,15,17-octahydroxy-8,10:18,20-di(ethanylylidene)tetrabenzo[*b*,*d*,*h*,*j*][1,7]dioxacyclododecine-22,24-dione

Note – Structure numbering [6,10] is given below:



Membership of sponsoring bodies

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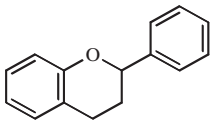
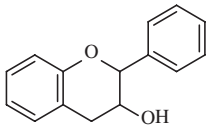
Annex 1. Flavonoid class names and characteristic structures



Flavan



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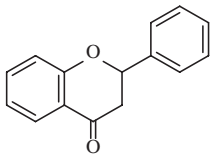

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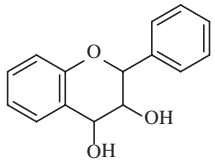

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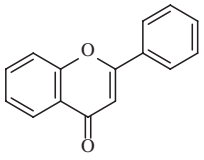

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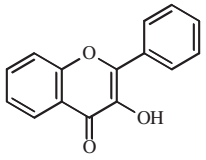

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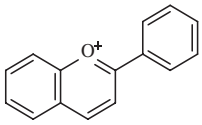

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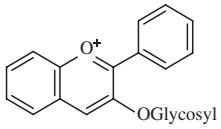

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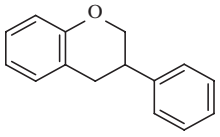

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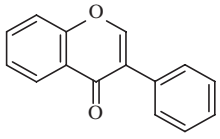

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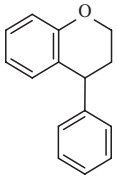

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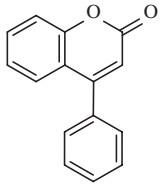

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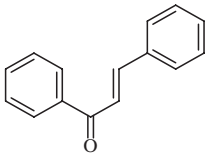

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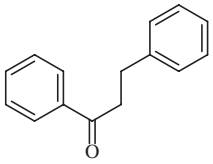

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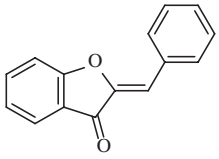

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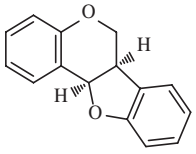

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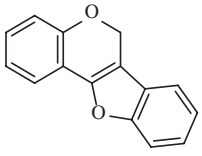
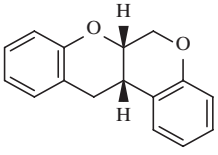


Coumestan



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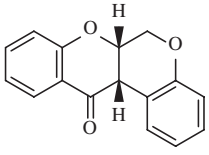

Rotenone

Annex 2. InChIs and InChIKeys for the flavonoids given as examples

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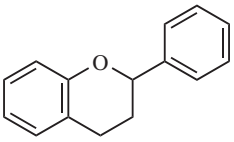

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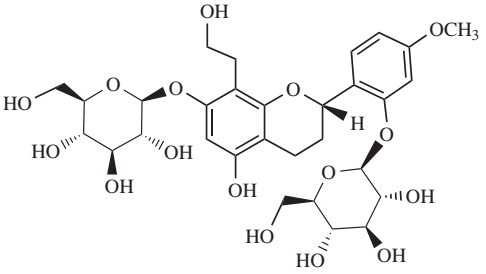
InChI=1S/C15H14O/c1-2-6-12(7-3-1)15-11-10-13-8-4-5-9-14(13)16-15/h1-9,15H,10-11H2

Example 2:



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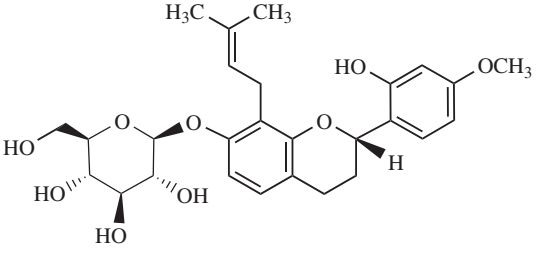
Example 3:



InChIKey GSRJVBMXUGFHSJ-RIDQRPLBSA-N
InChI=1S/C27H34O9/c1-14(2)4-8-18-21(35-27-25(32)24(31)23(30)22(13-28)36-27)11-6-15-5-10-20(34-26(15)18)17-9-7-16(33-3)12-19(17)29/h4,6-7,9,11-12,20,22-25,27-32H,5,8,10,13H2,1-3H3/t20-,22+,23+,24-,25+,27+/m0/s1

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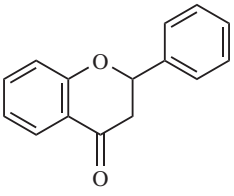

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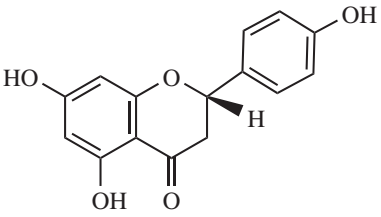

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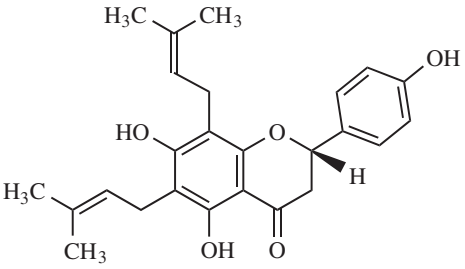
Example 6:



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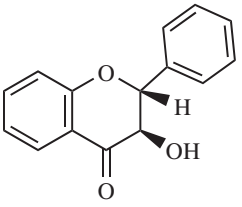
Example 7:



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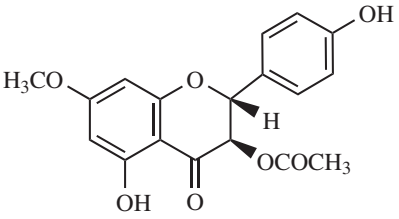
Example 8:



InChIKey MXFVIYRBYOWKKJ-MSOLQXFVSA-N
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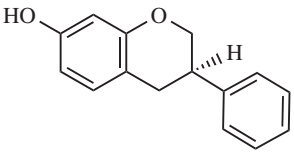

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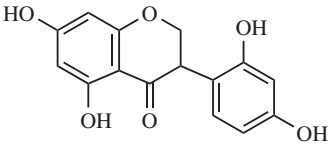
Example 10:



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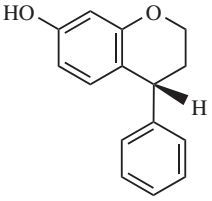

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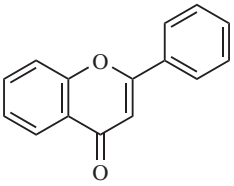

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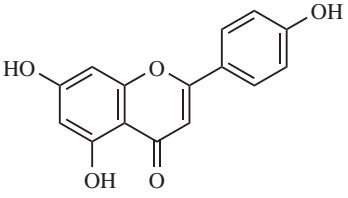
Example 13:



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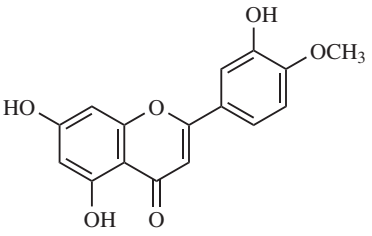

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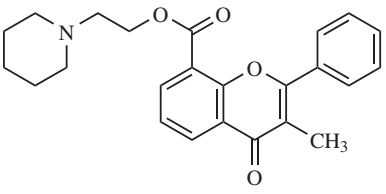

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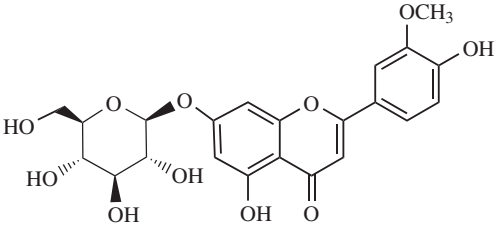
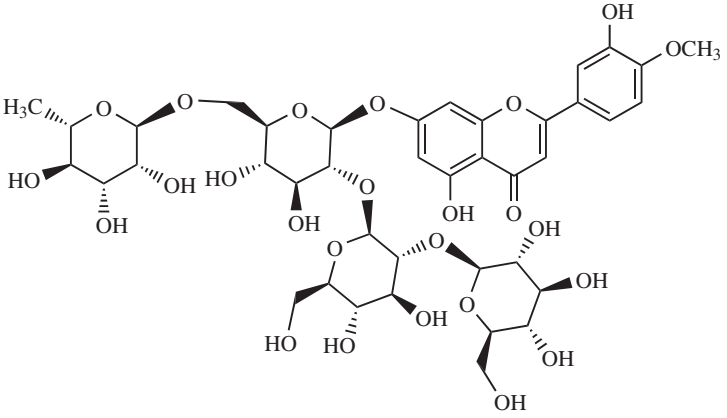
InChI=1S/C24H25NO4/c1-17-21(26)19-11-8-12-20(23(19)29-22(17)18-9-4-2-5-10-18)24(27)28-16-15-25-13-6-3-7-14-25/h2,4-5,8-12H,3,6-7,13-16H2,1H3

Example 16



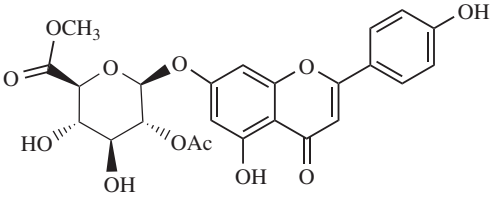
InChIKey GAMYVSCDDLXAQW-MIUGBVLSSA-N
InChI=1S/C22H22O11/c1-30-15-4-9(2-3-11(15)24)14-7-13(26)18-12(25)5-10(6-16(18)32-14)31-22-21(29)20(28)19(27)17(8-23)33-22/h2-7,17,19-25,27-29H,8H2,1H3/t17-,19-,20+,21-,22-/m1/s1

Example 17:



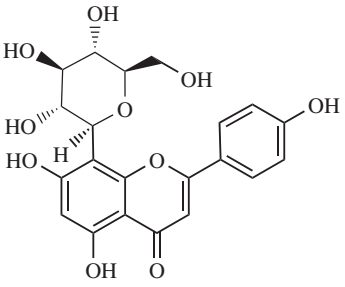
InChIKey WOECZRXKNFBVRD-MLKODYMUSA-N
InChI=1S/C40H52O25/c1-12-25(46)29(50)33(54)37(58-12)57-11-23-28(49)32(53)35(65-40-36(31(52)27(48)22(10-42)62-40)64-38-34(55)30(51)26(47)21(9-41)61-38)39(63-23)59-14-6-16(44)24-17(45)8-19(60-20(24)7-14)13-3-4-18(56-2)15(43)5-13/h3-8,12,21-23,25-44,46-55H,9-11H2,1-2H3/t12-,21+,22+,23+,25-,26+,27+,28+,29+,30-,31-,32-,33+,34+,35+,36+,37+,38-,39+,40-/m0/s1

Example 18:



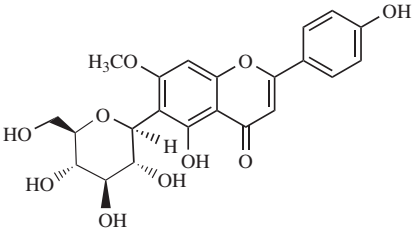
InChIKey UIAVWDXUPQFAJB-VZGLXOSZSA-N
InChI=C24H22O12/c1-10(25)33-22-20(30)19(29)21(23(31)32-2)36-24(22)34-13-7-14(27)18-15(28)9-16(35-17(18)8-13)11-3-5-12(26)6-4-11/h3-9,19-22,24,26-27,29-30H,1-2H3/t19-,20-,21-,22+,24+/m0/s1

Example 19:



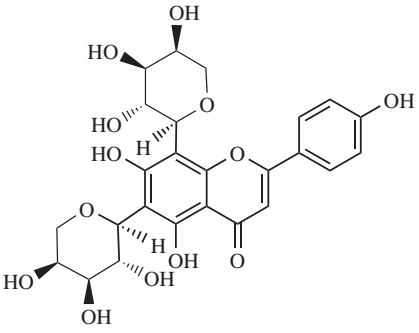
InChIKey SGEWCQFRYRRZDC-VPRICQMDSA-N
InChI=1S/C21H20O10/c22-7-14-17(27)18(28)19(29)21(31-14)16-11(25)5-10(24)15-12(26)6-13(30-20(15)16)8-1-3-9(23)4-2-8/h1-6,14,17-19,21-25,27-29H,7H2/t14-,17-,18+,19-,21+/m1/s1

Example 20:



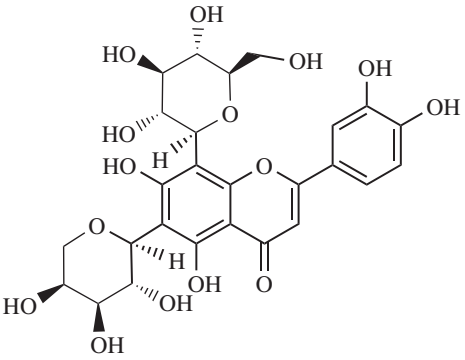
InChIKey ABRULANJVVJLFI-DGHBBABESA-N
InChI=1S/C22H22O10/c1-30-13-7-14-16(11(25)6-12(31-14)9-2-4-10(24)5-3-9)19(27)17(13)22-21(29)20(28)18(26)15(8-23)32-22/h2-7,15,18,20-24,26-29H,8H2,1H3/t15-,18-,20+,21-,22+/m1/s1

Example 21:



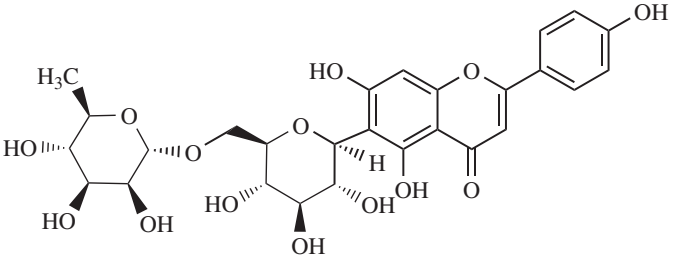
InChIKey LDVNKZYMYPZDAI-LTZKYNCBSA-N
InChI=1S/C25H26O13/c26-9-3-1-8(2-4-9)13-5-10(27)14-19(32)15(24-21(34)17(30)11(28)6-36-24)20(33)16(23(14)38-13)25-22(35)18(31)12(29)7-37-25/h1-5,11-12,17-18,21-22,24-26,28-35H,6-7H2/t11-,12-,17-,18-,21+,22+,24-,25-/m0/s1

Example 22:



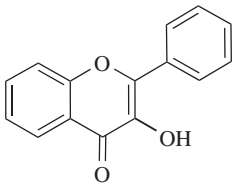
InChIKey WYYFCTVKFALPQV-VYUBKLCTSA-N
InChI=1S/C26H28O15/c27-5-13-18(33)21(36)23(38)26(41-13)16-20(35)15(25-22(37)17(32)11(31)6-39-25)19(34)14-10(30)4-12(40-24(14)16)7-1-2-8(28)9(29)3-7/h1-4,11,13,17-18,21-23,25-29,31-38H,5-6H2/t11-,13+,17-,18+,21-,22+,23+,25-,26-/m0/s1

Example 23:



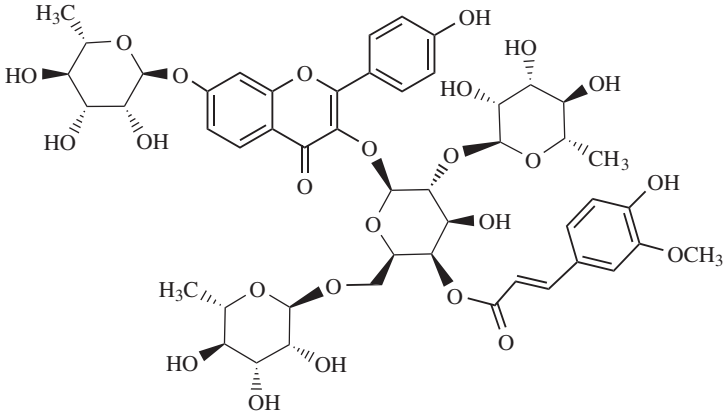
InChIKey FESGFDALJOTSAP-ALOWIAECSA-N
InChI=1S/C27H30O14/c1-9-19(31)22(34)25(37)27(39-9)38-8-16-20(32)23(35)24(36)26(41-16)18-13(30)7-15-17(21(18)33)12(29)6-14(40-15)10-2-4-11(28)5-3-10/h2-7,9,16,19-20,22-28,30-37H,8H2,1H3/t9-,16-,19-,20-,22+,23+,24-,25+,26+,27+/m1/s1

Example 24:



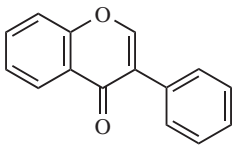
InChIKey HVQAJTFOCKOKIN-UHFFFAOYSA-N
InChI=1S/C15H10O3/c16-13-11-8-4-5-9-12(11)18-15(14(13)17)10-6-2-1-3-7-10/h1-9,17H

Example 25:



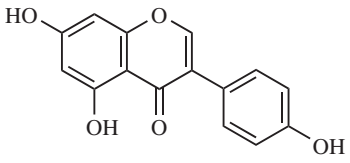
InChIKey KLHFSBCOSGENOE-TZZWOYRASA-N
InChI=1S/C49H58O25/c1-18-31(53)35(57)38(60)46(66-18)65-17-29-43(72-30(52)14-6-21-5-13-26(51)28(15-21)64-4)41(63)45(74-48-40(62)37(59)33(55)20(3)68-48)49(71-29)73-44-34(56)25-12-11-24(69-47-39(61)36(58)32(54)19(2)67-47)16-27(25)70-42(44)22-7-9-23(50)10-8-22/h5-16,18-20,29,31-33,35-41,43,45-51,53-55,57-63H,17H2,1-4H3/b14-6+/t18-,19-,20-,29+,31-,32-,33-,35+,36+,37+,38+,39+,40+,41-,43-,45+,46+,47-,48-,49-/m0/s1

Example 26:



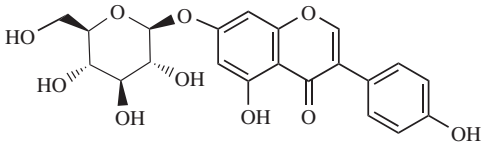
InChIKey GOMNOOKGLZYEJT-UHFFFAOYSA-N
InChI=1S/C15H10O2/c16-15-12-8-4-5-9-14(12)17-10-13(15)11-6-2-1-3-7-11/h1-10H

Example 27:



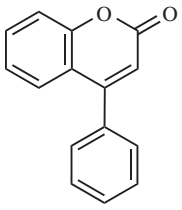
InChIKey TZBJGXHYKVUXJN-UHFFFAOYSA-N
InChI=1S/C15H10O5/c16-9-3-1-8(2-4-9)11-7-20-13-6-10(17)5-12(18)14(13)15(11)19/h1-7,16-18H

Example 28:



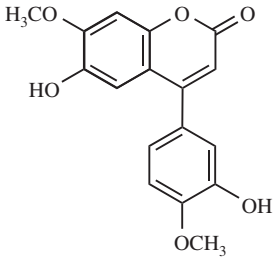
InChIKey ZCOLJUOHXJRHDI-CMWLGVBASA-N
InChI=1S/C21H20O10/c22-7-15-18(26)19(27)20(28)21(31-15)30-11-5-13(24)16-14(6-11)29-8-12(17(16)25)9-1-3-10(23)4-2-9/h1-6,8,15,18-24,26-28H,7H2/t15-,18-,19+,20-,21-/m1/s1

Example 29:



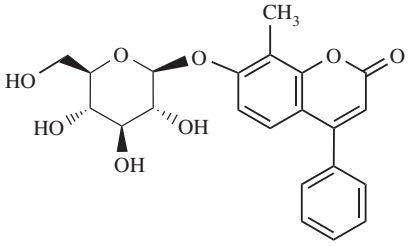
InChIKey SAZHWFFOFMSQPA-UHFFFAOYSA-N
InChI=1S/C15H10O2/c16-15-10-13(11-6-2-1-3-7-11)12-8-4-5-9-14(12)17-15/h1-10H

Example 30:



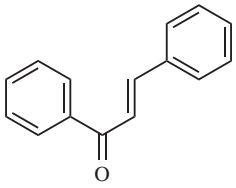
InChIKey XZOXEPMJIGHPMG-UHFFFAOYSA-N
InChI=1S/C17H14O6/c1-21-14-4-3-9(5-12(14)18)10-7-17(20)23-15-8-16(22-2)13(19)6-11(10)15/h3-8,18-19H,1-2H3

Example 31:



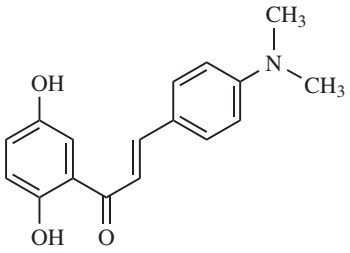
InChIKey RHTBSKLRGSELHW-QKYBYQKWSA-N
InChI=1S/C22H22O8/c1-11-15(28-22-20(27)19(26)18(25)16(10-23)29-22)8-7-13-14(9-17(24)30-21(11)13)12-5-3-2-4-6-12/h2-9,16,18-20,22-23,25-27H,10H2,1H3/t16-,18-,19+,20-,22-/m1/s1

Example 32:



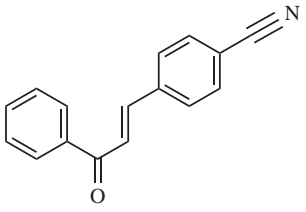
InChIKey DQFBYFPFKXHELB-VAWYXSNFSA-N
InChI=1S/C15H12O/c16-15(14-9-5-2-6-10-14)12-11-13-7-3-1-4-8-13/h1-12H/b12-11+

Example 33:



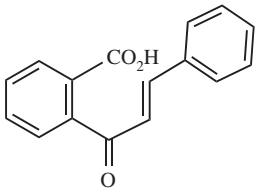
InChIKey MHVFCVMAJIDJMY-WEVVVXLNSA-N
InChI=1S/C17H17NO3/c1-18(2)13-6-3-12(4-7-13)5-9-16(20)15-11-14(19)8-10-17(15)21/h3-11,19,21H,1-2H3/b9-5+

Example 34:



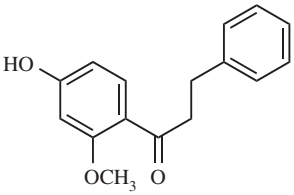
InChIKey CAHMJFODGBXCBM-ZHACJKMWSA-N
InChI=1S/C16H11NO/c17-12-14-8-6-13(7-9-14)10-11-16(18)15-4-2-1-3-5-15/h1-11H/b11-10+

Example 35:



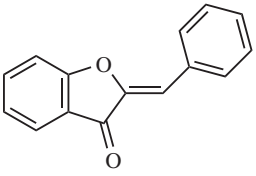
InChIKey XHISZGCLMMMERP-ZHACJKMWSA-N
InChI=1S/C16H12O3/c17-15(11-10-12-6-2-1-3-7-12)13-8-4-5-9-14(13)16(18)19/h1-11H,(H,18,19)/b11-10+

Example 36:



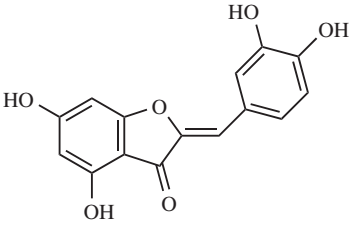
InChIKey CSEOFFVAVSWEAR-UHFFFAOYSA-N
InChI=1S/C16H16O3/c1-19-16-11-13(17)8-9-14(16)15(18)10-7-12-5-3-2-4-6-12/h2-6,8-9,11,17H,7,10H2,1H3

Example 37:



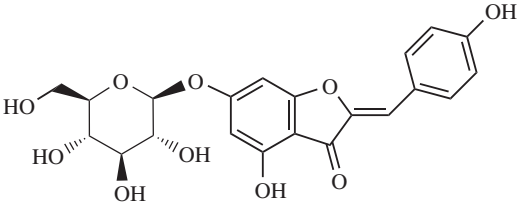
InChIKey OMUOMODZGKSORV-UVTDQMKNSA-N
InChI=1S/C15H10O2/c16-15-12-8-4-5-9-13(12)17-14(15)10-11-6-2-1-3-7-11/h1-10H/b14-10-

Example 38:



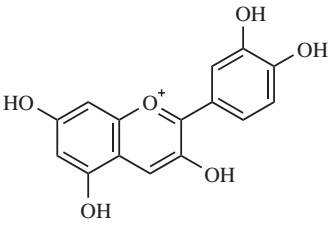
InChIKey FJNPIZYWMKBHNJ-REVZYDSWSA-N
InChI=1S/C15H10O6/c16-8-5-11(19)14-12(6-8)21-13(15(14)20)4-7-1-2-9(17)10(18)3-7/h1-6,16-19H/b13-4-

Example 39:



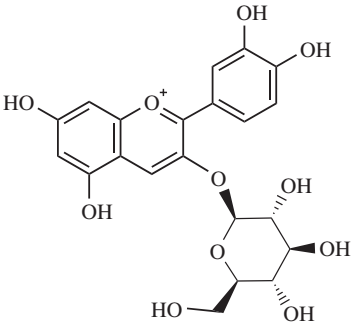
InChIKey RPVWXHFOBGSJNJ-AMBNHXPHSA-N
InChI=1S/C21H20O10/c22-8-15-18(26)19(27)20(28)21(31-15)29-11-6-12(24)16-13(7-11)30-14(17(16)25)5-9-1-3-10(23)4-2-9/h1-7,15,18-24,26-28H,8H2/b14-5-/t15-,18-,19+,20-,21-/m1/s1

Example 40:



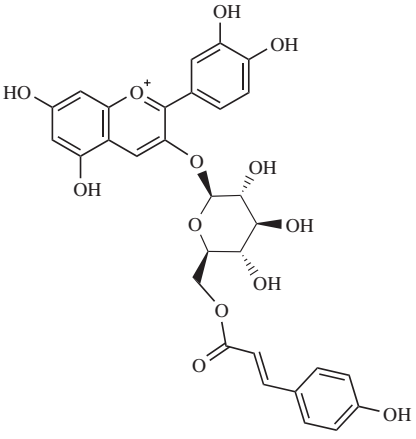
InChIKey VEVZSMAEJFVWIL-UHFFFAOYSA-O
InChI=1S/C15H10O6/c16-8-4-11(18)9-6-13(20)15(21-14(9)5-8)7-1-2-10(17)12(19)3-7/h1-6H,(H4-,16,17,18,19,20)/p+1

Example 41:



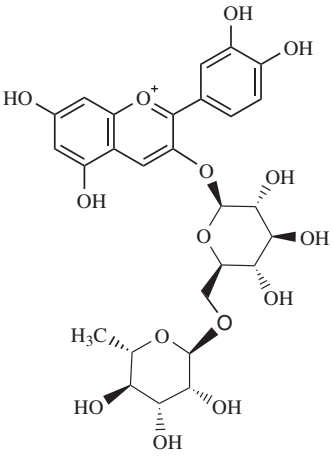
InChIKey FSJHYQBGKVHBDZ-UBNZBFALSA-O
InChI=1S/C21H20O11/c22-7-16-17(27)18(28)19(29)21(32-16)31-15-6-10-12(25)4-9(23)5-14(10)30-20(15)8-1-2-11(24)13(26)3-8/h1-6,16-19,21-22,27-29H,7H2,(H3-,23,24,25,26)/p+1/t16-,17-,18+,19-,21-/m1/s1

Example 42:



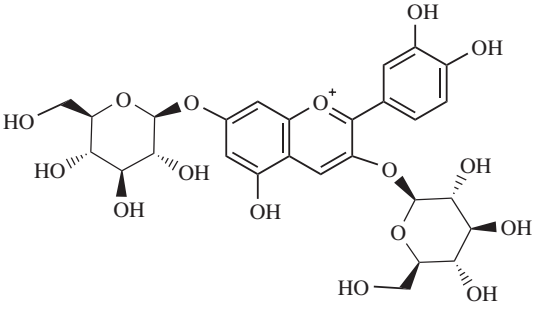
InChIKey QAOBEOXFSUJDJL-SHPGVJHPSA-O
InChI=1S/C30H26O13/c31-16-5-1-14(2-6-16)3-8-25(36)40-13-24-26(37)27(38)28(39)30(43-24)42-23-12-18-20(34)10-17(32)11-22(18)41-29(23)15-4-7-19(33)21(35)9-15/h1-12,24,26-28,30,37-39H,13H2,(H4-,31,32,33,34,35,36)/p+1/t24-,26-,27+,28-,30-/m1/s1

Example 43:



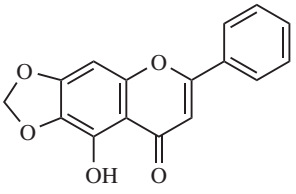
InChIKey USNPULRDBDVJAO-FXCAAIILSA-O
InChI=1S/C27H30O15/c1-9-19(32)21(34)23(36)26(39-9)38-8-18-20(33)22(35)24(37)27(42-18)41-17-7-12-14(30)5-11(28)6-16(12)40-25(17)10-2-3-13(29)15(31)4-10/h2-7,9,18-24,26-27,32-37H,8H2,1H3,(H3-,28,29,30,31)/p+1/t9-,18+,19-,20+,21+,22-,23+,24+,26+,27+/m0/s1

Example 44:



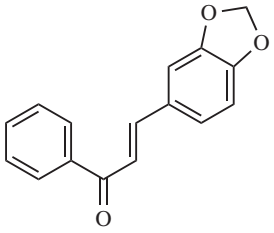
InChIKey ULXBEUBSYSSVTP-ZOTFFYTFSA-O
InChI=1S/C27H30O16/c28-7-17-19(33)21(35)23(37)26(42-17)39-10-4-13(31)11-6-16(41-27-24(38)22(36)20(34)18(8-29)43-27)25(40-15(11)5-10)9-1-2-12(30)14(32)3-9/h1-6,17-24,26-29,33-38H,7-8H2,(H2-,30,31,32)/p+1/t17-,18-,19-,20-,21+,22+,23-,24-,26-,27-/m1/s1

Example 45:



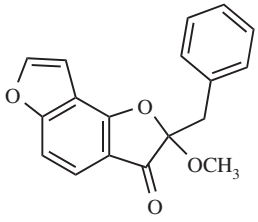
InChIKey NJIUXIXNVAHRDW-UHFFFAOYSA-N
InChI=1S/C16H10O5/c17-10-6-11(9-4-2-1-3-5-9)21-12-7-13-16(20-8-19-13)15(18)14(10)12/h1-7,18H,8H2

Example 46:



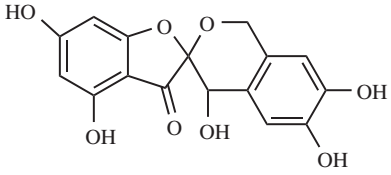
InChIKey ATKADZVINWFQOE-SOFGYWHQSA-N
InChI=1S/C16H12O3/c17-14(13-4-2-1-3-5-13)8-6-12-7-9-15-16(10-12)19-11-18-15/h1-10H,11H2/b8-6+

Example 47:



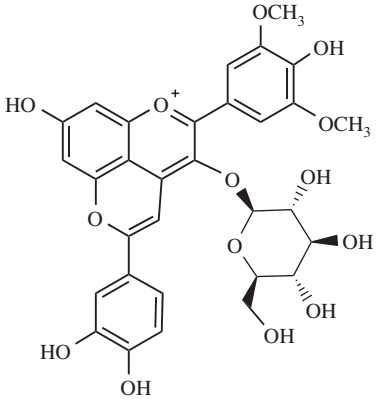
InChIKey ZDPDYRQJYGVUMW-UHFFFAOYSA-N
InChI=1S/C18H14O4/c1-20-18(11-12-5-3-2-4-6-12)17(19)14-7-8-15-13(9-10-21-15)16(14)22-18/h2-10H,11H2,1H3

Example 48:



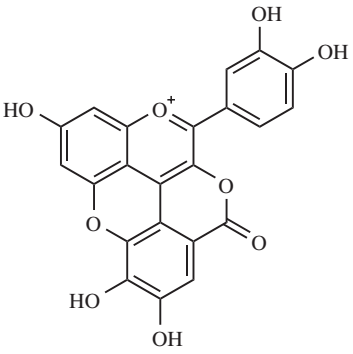
InChIKey AZXDUXHNBXWISJ-UHFFFAOYSA-N
InChI=1S/C16H12O8/c17-7-2-11(20)13-12(3-7)24-16(15(13)22)14(21)8-4-10(19)9(18)1-6(8)5-23-16/h1-4,14,17-21H,5H2

Example 49:



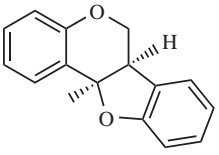
InChIKey RFTHDRVOYDHSOC-BGXVWEPQSA-O
InChI=1S/C31H28O14/c1-40-21-6-13(7-22(41-2)25(21)36)29-30(45-31-28(39)27(38)26(37)23(11-32)44-31)15-10-18(12-3-4-16(34)17(35)5-12)42-19-8-14(33)9-20(43-29)24(15)19/h3-10,23,26-28,31-32,37-39H,11H2,1-2H3,(H3-,33,34,35,36)/p+1/t23-,26-,27+,28-,31+/m1/s1

Example 50:



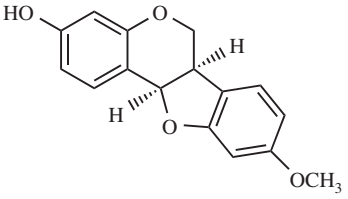
InChIKey DKOQTUOFLKDZKY-UHFFFAOYSA-O
InChI=1S/C22H10O9/c23-8-4-13-16-14(5-8)30-20-15-9(6-12(26)18(20)27)22(28)31-21(17(15)16)19(29-13)7-1-2-10(24)11(25)3-7/h1-6H,(H4-,23,24,25,26,27,28)/p+1

Example 51:



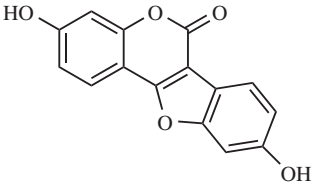
InChIKey LZEPVVDVBJUKSG-WFASDCNBSA-N
InChI=1S/C15H12O2/c1-4-8-14-10(5-1)12-9-16-13-7-3-2-6-11(13)15(12)17-14/h1-8,12,15H,9H2/t12-,15-/m0/s1

Example 52:



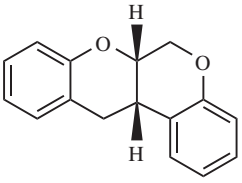
InChIKey NSRJSISNDPOJOP-BBRMVZONSA-N
InChI=1S/C16H14O4/c1-18-10-3-5-11-13-8-19-14-6-9(17)2-4-12(14)16(13)20-15(11)7-10/h2-7,13,16-17H,8H2,1H3/t13-,16-/m0/s1

Example 53:



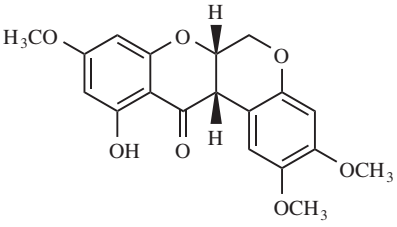
InChIKey ZZIALNLLNHEQPJ-UHFFFAOYSA-N
InChI=1S/C15H8O5/c16-7-1-3-9-11(5-7)19-14-10-4-2-8(17)6-12(10)20-15(18)13(9)14/h1-6,16-17H

Example 54:



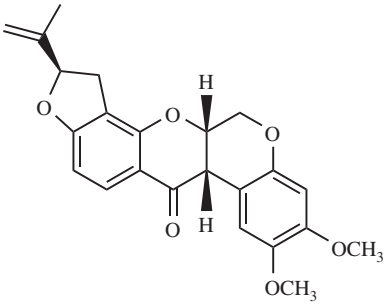
InChIKey VRMJETRWSYBVKR-XJKSGUPXSA-N
InChI=1S/C16H14O2/c1-3-7-14-11(5-1)9-13-12-6-2-4-8-15(12)17-10-16(13)18-14/h1-8,13,16H,9-10H2/t13-,16+/m0/s1

Example 55:



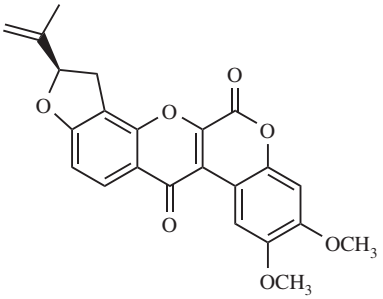
InChIKey BCRQIJDETOPQBA-SJORKVTESA-N
InChI=1S/C19H18O7/c1-22-9-4-11(20)18-15(5-9)26-16-8-25-12-7-14(24-3)13(23-2)6-10(12)17(16)19(18)21/h4-7,16-17,20H,8H2,1-3H3/t16-,17+/m1/s1

Example 56:



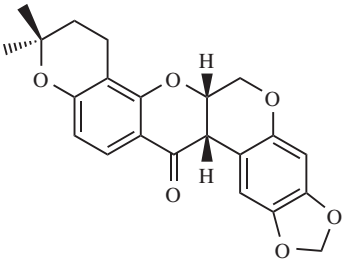
InChIKey JUVIOZPCNVVQFO-HBGVWJBISA-N
InChI=1S/C23H22O6/c1-11(2)16-8-14-15(28-16)6-5-12-22(24)21-13-7-18(25-3)19(26-4)9-17(13)27-10-20(21)29-23(12)14/h5-7,9,16,20-21H,1,8,10H2,2-4H3/t16-,20-,21+/m1/s1

Example 57:



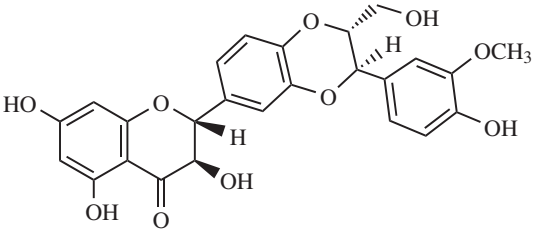
InChIKey CWZIPBGXMLRVIC-OAHLLOKOSA-N
InChI=1S/C23H18O7/c1-10(2)15-8-13-14(28-15)6-5-11-20(24)19-12-7-17(26-3)18(27-4)9-16(12)29-23(25)22(19)30-21(11)13/h5-7,9,15H,1,8H2,2-4H3/t15-/m1/s1

Example 58:



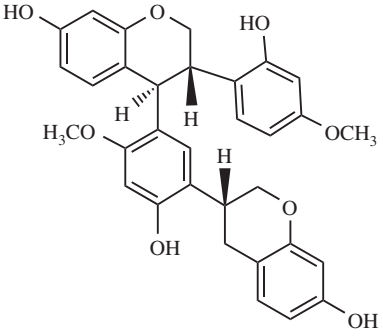
InChIKey IAFATVLPBBJEBM-MOPGFXCFSA-N
InChI=1S/C22H20O6/c1-22(2)6-5-11-14(28-22)4-3-12-20(23)19-13-7-16-17(26-10-25-16)8-15(13)24-9-18(19)27-21(11)12/h3-4,7-8,18-19H,5-6,9-10H2,1-2H3/t18-,19+/m1/s1

Example 59:



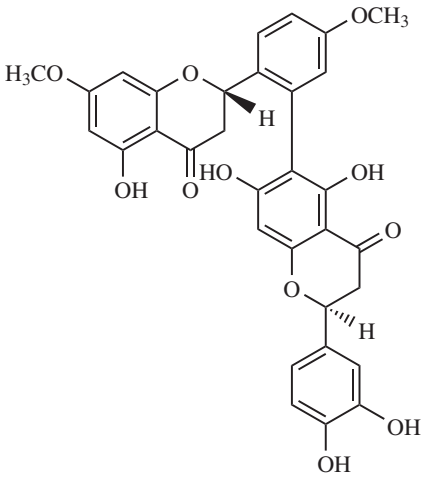
InChIKey SEBFKMXJBCUCAI-HKTJVKLFSA-N
InChI=1S/C25H22O10/c1-32-17-6-11(2-4-14(17)28)24-20(10-26)33-16-5-3-12(7-18(16)34-24)25-23(31)22(30)21-15(29)8-13(27)9-19(21)35-25/h2-9,20,23-29,31H,10H2,1H3/t20-,23+,24-,25-/m1/s1

Example 60:



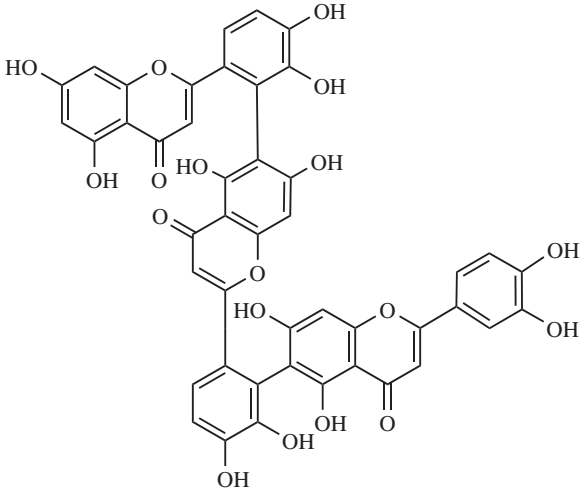
InChIKey GMRYHQZTHKNHAY-ZHWNBNGFSA-N
InChI=1S/C32H30O8/c1-37-21-6-8-22(27(35)12-21)26-16-40-31-11-20(34)5-7-23(31)32(26)25-13-24(28(36)14-30(25)38-2)18-9-17-3-4-19(33)10-29(17)39-15-18/h3-8,10-14,18,26,32-36H,9,15-16H2,1-2H3/t18-,26+,32+/m0/s1

Example 61:



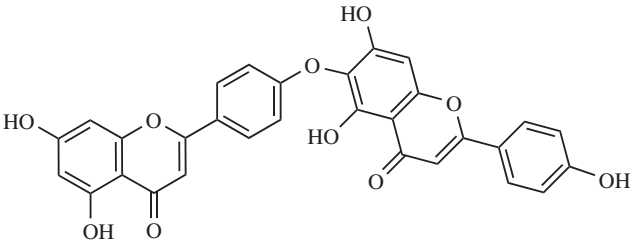
InChIKey FCYBLXOWPSBBJH-UIOOFZCWSA-N
InChI=1S/C32H26O11/c1-40-15-4-5-17(26-12-23(37)30-21(35)9-16(41-2)10-27(30)43-26)18(8-15)29-22(36)13-28-31(32(29)39)24(38)11-25(42-28)14-3-6-19(33)20(34)7-14/h3-10,13,25-26,33-36,39H,11-12H2,1-2H3/t25-,26-/m0/s1

Example 62:



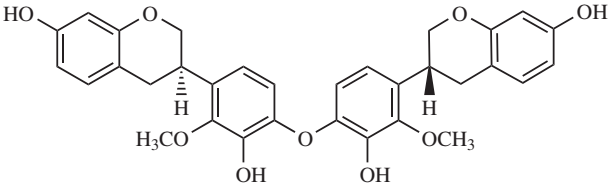
InChIKey AOKUQXYGIOWNDM-UHFFFAOYSA-N
InChI=1S/C46H28O18/c47-18-9-25(52)38-27(54)13-32(64-33(38)10-18)20-3-6-23(50)44(59)37(20)42-30(57)14-34-39(46(42)61)26(53)11-19(62-34)7-17-2-5-22(49)43(58)36(17)41-29(56)15-35-40(45(41)60)28(55)12-31(63-35)16-1-4-21(48)24(51)8-16/h1-6,8-15,47-52,56-61H,7H2

Example 63:



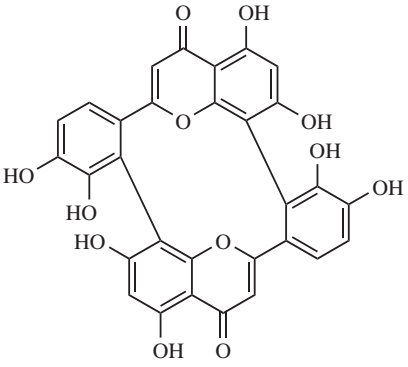
InChIKey WTDHMFBJQJSTMH-UHFFFAOYSA-N
InChI=1S/C30H18O10/c31-16-5-1-14(2-6-16)24-12-21(35)28-26(40-24)13-22(36)30(29(28)37)38-18-7-3-15(4-8-18)23-11-20(34)27-19(33)9-17(32)10-25(27)39-23/h1-13,31-33,36-37H

Example 64:



InChIKey YNSOGFXHKXTWBP-PMACEKPBSA-N
InChI=1S/C32H30O9/c1-37-31-23(19-11-17-3-5-21(33)13-27(17)39-15-19)7-9-25(29(31)35)41-26-10-8-24(32(38-2)30(26)36)20-12-18-4-6-22(34)14-28(18)40-16-20/h3-10,13-14,19-20,33-36H,11-12,15-16H2,1-2H3/t19-,20-/m0/s1

Example 65:



InChIKey TUTVHJWUONTOOJ-UHFFFAOYSA-N
InChI=1S/C30H16O12/c31-11-3-1-9-19-7-17(37)23-14(34)6-16(36)26(30(23)41-19)22-10(2-4-12(32)28(22)40)20-8-18(38)24-13(33)5-15(35)25(29(24)42-20)21(9)27(11)39/h1-8,31-36,39-40H