

PHENOLIC COMPOUNDS OF PLANTS OF THE *Scutellaria* L. GENUS. DISTRIBUTION, STRUCTURE, AND PROPERTIES

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Information on flavones, flavanones, flavanonols, flavonols, chalcones, isoflavones, biflavonoids, lignoflavonoids, and lignane glycosides and stilbenes isolated from plants of the Scutellaria L. genus was systematized and reviewed. A list of 208 phenolic compounds was given according to flavonoid type with an indication of the plant sources, structures, and physicochemical properties and citations of the original articles.

Key words: *Scutellaria* (Lamiaceae), flavones, flavanones, flavanonols, flavonols, chalcones, isoflavones, biflavonoids, lignoflavonoids, lignane glycosides and stilbenes (formula, physicochemical constants, spectral data).

Plants of the *Scutellaria* L. (Lamiaceae) genus are widely distributed over the world and are represented by 360 species. The territory of the CIS contains 148 species; the flora of Uzbekistan, 32 species of skullcap [1-3]. Many *Scutellaria* species are economically significant and have been thoroughly studied. Essential oils, organic alcohols (derivatives of phenylethanol) and acids (esters and glycosides of vanillic, coumaric, syringic, and ferulic acids), iridoid sesquiterpenes, clerodane diterpenoids, steroids, cardenolides, coumarins, tanning agents, and flavonoids have been isolated from these plants [4, 5].

Flavonoids are the most widely distributed and common of the aforementioned classes of natural compounds [6, 7]. This can be seen using plants of the *Scutellaria* genus as examples. Many species of this genus and the phenolic compounds isolated from them are widely used in folk and conventional medicine. Flavonoids possessing P-vitamin, inhibitory, cytotoxic, antimetastatic, antibacterial, and other activities have been isolated from plants of this genus [5].

Tibetan medicine includes 42 known recipes that include *S. baicalensis* in addition to other plants [8]. Japanese researchers showed special interest in plants of this genus and demonstrated the relationship of many biological properties to the presence of several flavonoids in them [9]. Therefore, the high physiological activity of flavonoids indicates that they are important to the vitality of both plants and animals.

The phenolic compounds of *Scutellaria* plants include phenylpropanoid glycosides, chalcones, flavones, flavanones, isoflavones, biflavones, and lignoflavones. These compounds are known to contain reactive phenolic hydroxyls and carbonyls. These groups of compounds are certainly interrelated and undergo mutual transformations [6]. Owing to this and the ability to transform into chalcones and to form quinones, flavonoids are considered to be highly physiologically active compounds with a wide spectrum of pharmacological activity.

Therefore, phenolic compounds from *Scutellaria* plants are constantly at the center of attention of many researchers. A huge volume of literature has been accumulated worldwide on the isolation, identification, structure determination, and biological activity of flavonoids from various skullcap species. Therefore, the collection into one place of the dispersed information on phenolic compounds from *Scutellaria* plants is of definite scientific interest.

Another equally important consideration is that flavonoids are the most numerous group of natural phenolic compounds. The number of natural flavonoids of established structure that have been described in the literature is increasing at a rapid pace and at present is apparently approaching 6000 [7, 10]. Information on these compounds is scattered over many monographs and reviews [11] and is difficult to reference. The structure of a newly isolated flavonoid can be determined much quicker than it can be identified by analyzing volumes of chemical and spectral data.

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TABLE 1. Studied *Scutellaria* Species and Number of Isolated Phenolic Compounds

Plant	Number of compounds	Plant	Number of compounds
1. <i>S. adenostegia</i> Briq.	15	30. <i>S. orientalis</i> L.	6
2. <i>S. adsurgens</i> M. Pop.	14	31. <i>S. ovata</i> Hill.	7
3. <i>S. alpina</i> L.	20	32. <i>S. oxystegia</i> Juz.	3
4. <i>S. altaica</i> Fisch. ex. Sweet	1	33. <i>S. peregrina</i> Ldb.	1
5. <i>S. altissima</i> L.	11	34. <i>S. phyllostachya</i> Juz.	3
6. <i>S. amoena</i> C. H. Wright.	16	35. <i>S. planipes</i> L.	13
7. <i>S. araxensis</i> Grossh.	5	36. <i>S. polyodon</i> Juz.	13
8. <i>S. baicalensis</i> Georgi.	62	37. <i>S. prilipkoana</i> Grossh.	1
9. <i>S. barbata</i> D. Don.	1	38. <i>S. prostrata</i> Jacq. et Benth.	30
10. <i>S. columnae</i> L. (All)	2	39. <i>S. przewalskii</i> Juz.	18
11. <i>S. comosa</i> Juz.	14	40. <i>S. pycnoclada</i> Juz.	16
12. <i>S. cretica</i> Juz.	14	41. <i>S. ramosissima</i> M. Pop.	11
13. <i>S. discolor</i> Colebr.	23	42. <i>S. rehderiana</i> Diels.	7
14. <i>S. epilobiiifolia</i> A. Hamilt.	10	43. <i>S. repens</i> Buch-Ham, ex D. Don	14
15. <i>S. galericulata</i> L.	23	44. <i>S. rivularis</i> Wall.	28
16. <i>S. glabrata</i> Vved.	7	45. <i>S. scandens</i> Buch-Ham. ex D. Don.	16
17. <i>S. granulosa</i> Juz.	2	46. <i>S. scordifolia</i> Fisch. ex Schrank	14
18. <i>S. grossa</i> Wall.	19	47. <i>S. sedelmeyeria</i> Juz.	3
19. <i>S. ikonnikovii</i> Juz.	7	48. <i>S. sevanensis</i> Sosn.	19
20. <i>S. immaculata</i> Nevski	8	49. <i>S. squarrosa</i> Nevski	6
21. <i>S. incona</i> Spreng.	1	50. <i>S. strigillosa</i> Hemsl	15
22. <i>S. indica</i> L.	33	51. <i>S. supina</i> L.	19
23. <i>S. iskanderi</i> Juz.	10	52. <i>S. tenax</i> W. W. Smith.	5
24. <i>S. karjaginii</i> Grossh	3	53. <i>S. tournefortii</i> Benth.	4
25. <i>S. lateriflora</i> L.	1	54. <i>S. transiliensis</i> Juz.	6
26. <i>S. litwinowii</i> Bornm. Et. Sint.	10	55. <i>S. ussuriensis</i> (Regel) Kubo	2
27. <i>S. nepetoides</i> M. Pop.	4	56. <i>S. virularis</i> Wall	2
28. <i>S. ocellata</i> Juz.	7	57. <i>S. viscidulla</i> Bunge	7
29. <i>S. oreophila</i> Grossh.	5		

We have attempted to collect information about phenolic compounds from *Scutellaria* plants into a single reference.

Thus, the data that we present can serve as a reference for specialists working on the chemistry of flavonoids, their distribution in natural sources, and their physicochemical properties. The composition, melting point, specific rotation, UV-, IR-, and mass-spectra, and ^1H and ^{13}C NMR spectra are given for every compound in several groups. The list includes information on unsubstituted flavone, 3-hydroxyflavone (flavonol), and flavanone, the cores of the corresponding groups of compounds, although they are not found in the studied samples. We feel that the data presented for these compounds can be useful for comparative studies of this type of compounds.

Phenolic compounds from 65 skullcap species have been studied (Table 1). Of these, 8 (*S. abider*, *S. karatschaica*, *S. mesostegia*, *S. grindiflora*, *S. oligodonta*, *S. platustegia*, *S. sosnowskyi*, *S. woronowii*) have been studied only preliminarily by observing flavonoids in them [12-14]. A total of 208 substances has been isolated and identified from all plant species. These include: chalcones and stilbenes, 11; flavones, 119; flavanones, 48; flavonols, 6; isoflavones, 4; biflavones, 1; lignoflavones, lignane glycosides, and stilbenes, 19.

In addition to the aforementioned compounds, certain *Scutellaria* species afforded compounds (>10) that are glycosides and esters of derivatives of phenylethanol and coumaric and ferulic acids. The last two, so-called phenylpropanoids, are biogenetic precursors of flavonoids.

The research results showed that Baikal skullcap, from which 62 compounds have been isolated, is apparently the most common and, therefore, the most thoroughly studied in all respects. After it follow *S. indica*, 33; *S. prastrata*, 30; *S. rivularis*, 28; and *S. discolor* and *S. galericulata*, from which 23 flavonoids have been isolated. Only one compound (scutellarein) was

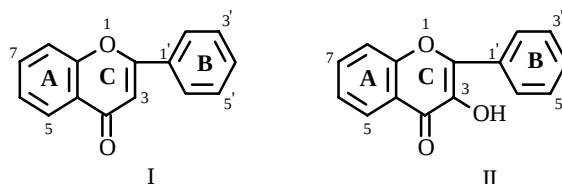
found in six species of plants from this genus.

Therefore, the flavonoid scutellarein is typical of *Scutellaria* plants although it was first isolated in 1890 from *Oroxylum indicum* [15].

METHODS FOR ESTABLISHING FLAVONOID STRUCTURES

As noted above, flavonoids are physiologically active compounds that are widely distributed in plants and possess great scientific and practical interest. The study of flavonoid structures is important for resolving issues connected with chemotaxonomy and the search for new physiologically active compounds.

The isolation, chemical transformations, synthesis, and biological conversions in addition to information about the physiological activity of natural phenolic compounds have been reviewed in monographs and articles [16-23]. Therefore, we considered it advisable to include brief data regarding the use of spectral methods to establish the structures of flavonoids using flavone (I) and flavonol (II) derivatives as examples.



Significant success has been achieved in this area in the last decades owing to the appearance of new effective instrumental research methods. Important questions about the biogenesis and structure of flavonoids have been answered by the wide use of IR-, UV-, mass-, and NMR-spectroscopies.

The information value, quickness of analysis, and ability to obtain spectra practically without destroying the compound and with a minimal amount of sample favorably distinguish physical methods of research from others.

IR-spectroscopy. The carbonyl group of unsubstituted flavone absorbs in the IR spectrum at 1650 cm^{-1} . Introducing a hydroxyl group on C-3 lowers the C=O stretching vibration to 1619 cm^{-1} whereas placing it on C-5 raises the frequency to 1655 cm^{-1} . The double-bond stretching vibration appears as several strong bands at $1600\text{--}1470\text{ cm}^{-1}$.

The skeletal vibrations of the benzene rings of flavonoids include two main absorption bands at 1600 and 1500 cm^{-1} . An additional one or two bands appear at $1580\text{--}1550\text{ cm}^{-1}$. These bands in flavones are shifted to lower frequencies. The band at 1580 cm^{-1} almost disappears for flavones with an intramolecular H-bond between C=O and the C-5 hydroxyl [6, 20, 24].

Phenolic hydroxyls absorb at $3500\text{--}3600\text{ cm}^{-1}$. Hydroxyl groups in phenolic glycosides are most commonly involved in intermolecular and intramolecular H-bonds. Therefore, they appear at lower frequencies. Several bands typical of the sugar component are found at $840\text{--}890$ and $1000\text{--}1100\text{ cm}^{-1}$.

UV-spectroscopy. UV spectra of many flavonoids contain two absorption maxima, one of which is located at $240\text{--}285\text{ nm}$ (band II), the other of which appears at $300\text{--}400\text{ nm}$ (band I) [6, 16-18].

The long-wavelength band in the spectra of flavones and flavonols is situated at $304\text{--}350$ and $352\text{--}385\text{ nm}$, respectively. Thus, the type of flavonoid can be determined from the position of this band.

Flavonoids with a higher degree of oxidation absorb at longer wavelengths compared with less oxidized flavonoids:

3,5,7-trihydroxyflavone	$359\lambda_{\text{max}},\text{ nm}$
3,5,7,4'-tetrahydroxyflavone	$367\lambda_{\text{max}},\text{ nm}$
3,5,7,3',4'-pentahydroxyflavone	$370\lambda_{\text{max}},\text{ nm}$
3,5,7,3',4',5'-hexahydroxyflavone	$374\lambda_{\text{max}},\text{ nm}$

The spectra of 3',4'-dihydroxyflavones contain in the region of band II two maxima or a main peak and a shoulder whereas those of 4'-hydroxyflavones have only one maximum.

The position of the main maximum of band II is greatly influenced by the degree of oxidation of ring A. This can be seen from the following data:

Flavone	250 λ_{max} nm
7-hydroxyflavone	252 λ_{max} nm
5,7-dihydroxyflavone	268 λ_{max} nm
5,6,7-trihydroxyflavone	274 λ_{max} nm
5,7,8-trihydroxyflavone	281 λ_{max} nm

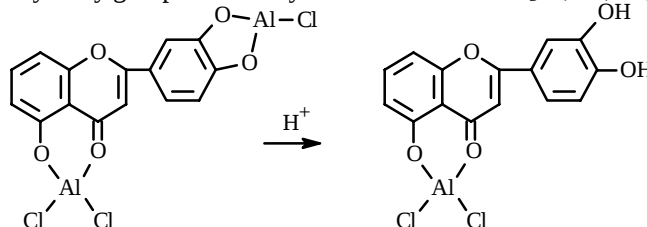
Methylation or glycosylation of hydroxyl groups at the 3-, 5-, and 4'-positions of the flavone core causes a hypsochromic shift of the bands [25]. The magnitude of this shift is 3-10 nm (band I) for substitution of the 4'-OH, 5-15 nm (bands I and II) for substitution of the 5-OH, and 12-17 nm for substitution of the 3-OH. Substitution of OH groups in other positions does not significantly affect the UV spectrum.

Various reagents that affect the chromophore system of flavonoids are commonly used to determine the position of the hydroxyl groups [25-27]. Sodium methoxide or ethoxide ionize flavonoid hydroxyl groups.

The presence of a free C-4' hydroxyl on flavones and flavonols causes a bathochromic shift of band I by 40-65 nm without decreasing the intensity. A C-3 hydroxyl on flavonols without a C-4' hydroxyl also causes a bathochromic shift of band I by 50-60 nm but with a decrease of intensity. Flavonols containing hydroxyls in the 3'- and 4'-positions are oxidized by sodium methoxide and give spectra in which the absorption maxima decrease in intensity with time.

Flavones and flavonols containing a C-7 hydroxyl experience a bathochromic shift of band II by 5-20 nm. The presence of groups sensitive to base (5,6,7-, 5,7,8-, and 3,3',4'-trihydroxy groups) cause the absorption maxima to disappear over time.

A mixture of sodium acetate and boric acid enables an *ortho*-dihydroxy group to be determined in all positions of the flavone core except C-5,6. Flavones and flavonols containing this group in ring B show a bathochromic shift by 12-30 nm. Flavones and flavonols containing C-3 or C-5 hydroxyls form complexes with aluminum chloride that are stable to acid. Complexes formed by an *ortho*-dihydroxy group are destroyed in acidic medium [17, 25, 26].



The bathochromic shift of band I in 5-hydroxyflavones caused by adding $\text{AlCl}_3 + \text{HCl}$ is 35-55 nm. A shift of only 17-20 nm indicates the presence of hydroxyl or methoxyl on C-6 [28]. Flavonols and $\text{AlCl}_3 + \text{HCl}$ cause a bathochromic shift of band I by 50-60 nm. Using ZrOCl_2 and citric acid instead of AlCl_3 can determine the presence of a 3-hydroxy group in the presence of a 5-hydroxy group [27]. Reaction with AlCl_3 causes a bathochromic shift of 30-40 nm if the phenyl substituent contains a dihydroxy group.

A study of the spectra of several flavonoids containing a prenyl group on C-6 found that the UV spectra do not experience a bathochromic shift with AlCl_3 even if there is a free OH on C-5 [28]. This was explained by steric factors, i.e., hindrance to complex formation owing to the presence of a bulky substituent in the position *ortho* to the hydroxyl group [29].

^1H and ^{13}C NMR Spectroscopy. PMR spectroscopy (^1H NMR) was widely used in structural studies of several flavonoids [6, 25, 30]. Many natural flavonoids are insoluble in deuteriochloroform and carbon tetrachloride. Therefore, spectra are often recorded in deuterated dimethylsulfoxide and deuteropyridine.

Flavonoids can be made much more soluble by preparing various derivatives such as trimethylsilyl esters, acetates, methyl esters, etc. The signals in PMR spectra of flavonoids are located at 0-9 ppm.

Signals of Ring A Protons. The signals of C-6 and C-8 protons in spectra of 5,7-dihydroxy flavones and flavonols appear at 5.7-6.9 ppm as doublets with a spin-spin coupling constant (SSCC) of 2.5 Hz. The H-6 signal usually resonates at stronger field than that of H-8. Glycosylation of the 7-OH shifts both signals to weak field.

Certain natural flavonoids do not contain a 5-OH. The spectra of these compounds contain at weak field (about 8 ppm) a doublet from H-5 with SSCC 8.5-9.0 Hz owing to deshielding by the C-4 carbonyl. In this instance the H-6 (quartet, $J = 9$ Hz, $J_2 = 2.5$ Hz) and H-8 (doublet, $J = 2.5$ Hz) signals usually appear at weaker field compared with the 5,7-dihydroxyflavonoid.

Signals of Ring B Protons. The C-2', 3', 5', and 6' protons in 4'-hydroxyflavones appear as two 2H doublets with

SSCC 8.5 Hz at 6.5-7.9 ppm. The H-3',5' doublet is usually located at stronger field than that of H-2',6'. The H-2',6' chemical shift depends on the degree of oxidation of ring C and is δ 7.7-7.9 ppm in spectra of flavones and 7.9-8.1 ppm in spectra of flavonols.

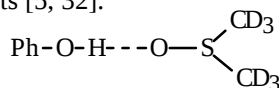
The signal for the C-5' proton in spectra of 3',4'-dihydroxyflavonoids resonates as a doublet at 6.7-7.1 ppm ($J = 8.5$ Hz). Protons on C-2' (doublet, $J = 2.5$ Hz) and C-6' (quartet, $J_1 = 8.5$ Hz, $J_2 = 2.5$ Hz) give signals at 7.2-7.9 ppm.

Methylation or glycosylation of one of these hydroxyls changes the spectrum because of redistribution of electron density on ring B.

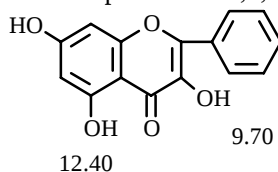
The signal of H-3 in spectra of flavones usually appears as a 1H singlet at 6.3 ppm. However, many flavonoids contain a single proton in ring A (5,6,7- or 5,7,8-trisubstituted) that resonates in the same region as H-3. In such situations it is difficult to make an unambiguous assignment of the H-3, H-6, and H-8 signals. Comparison of the spectra of fully and partially (with the C-5 hydroxyl unsubstituted) trimethylsilylated (TMS) flavonoids can distinguish these signals [31].

The H-3 signal in the spectrum of the partial TMS ester shifts to weak field by 0.15 ppm compared with the full TMS ester whereas the H-8 signal undergoes a diamagnetic shift of the same magnitude. The position of the H-6 signal is unchanged.

Deuterated DMSO is often used as the solvent to record spectra of flavonoids. Protons of hydroxyl groups in DMSO- d_6 form H-bonds to the solvent and appear as singlets [5, 32].



The chemical shifts of phenolic hydroxyls in the spectrum of 3,5,7-trihydroxyflavone recorded in DMSO- d_6 have the following values (δ , ppm):



Unfortunately, DMSO has several drawbacks as a solvent. These include its hygroscopicity, high boiling point, reaction with certain flavonoids, etc. [25].

The anomeric proton (H-1'') in PMR spectra of monoglycosides appears at weaker field than other protons of the carbohydrate moiety. The chemical shift of this proton provides some information about the site of glycosylation and the nature of the sugar. For example, the H-1'' signal in the spectra of flavonol-3-O-glucosides appears at 5.7-6.0 ppm and differs significantly from that in the corresponding 5,7- and 4'-O-glucosides of flavonoids, which usually resonates at 4.8-5.2 ppm.

Furthermore, the chemical shift of H-1'' in flavonol 3-O-glucosides differs from that in 3-O-rhamnosides, the anomeric proton of which resonates at 5.0-5.1 ppm [6, 25].

The H-1''—H-2'' SSCC in flavonoid β -glycosides is 7 Hz and is due to diaxial coupling [33]. The H-1''—H-2'' diequatorial coupling in natural α -rhamnosides is only 2-2.5 Hz [34]. The presence of rhamnose in flavonoids is easily demonstrated by the characteristic signals of the methyl group, which resonates at 0.8-1.2 ppm as a 3H doublet with SSCC 6.0-6.5 Hz or as a multiplet [25]. The anomeric proton in flavonoid biosides is observed at much stronger field. It was also found that the chemical shift of this proton depends on the site of attachment of the terminal sugar. Thus, the anomeric proton of L-rhamnose in rutinoides [-O- α -L-rhamnopyranosyl-(1 $\rightarrow$ 6)-O- β -D-glucopyranosides] resonates at 4.2-4.4 ppm whereas it is found at 4.9-5.0 ppm for neohesperidosides [-O- α -L-rhamnopyranosyl-(1 $\rightarrow$ 2)-O- β -D-glucopyranosides]. The aforementioned glycosides can also be distinguished by the chemical shifts of the protons, which are 0.7-1.0 and 1.1-1.3 ppm, respectively [35].

The sequence of binding of the sugars can in certain instances also be determined by studying the PMR spectra of the permethylates and peracetates of flavonoid biosides.

Signals of flavonoid methoxy protons appear at 3.5-4.1 ppm. The effect of solvents on the position of PMR signals of methoxyflavonoids was studied on going from chloroform to benzene [36].

It was found that the shift [$\Delta\delta = \delta(\text{CDCl}_3) - \delta(\text{C}_6\text{H}_6)$] depends on the location of the methoxy group in the flavone core. The largest shift is found for CH_3O groups occupying the C-5, C-7, and C-4' positions. The presence of hydroxy and methoxy groups in the position *ortho* to the observed CH_3O group decreases the shift [6, 25].

A study of the ^{13}C NMR spectrum of flavone was published in 1974 [37]. The review contains spectra of several flavonoids [38]. Comparison of spectra recorded with partial and full ^{13}C — ^1H decoupling, measurement of the SSCC, and the study of model compounds greatly facilitate the interpretation of the ^{13}C NMR spectra. The location of various substituents on

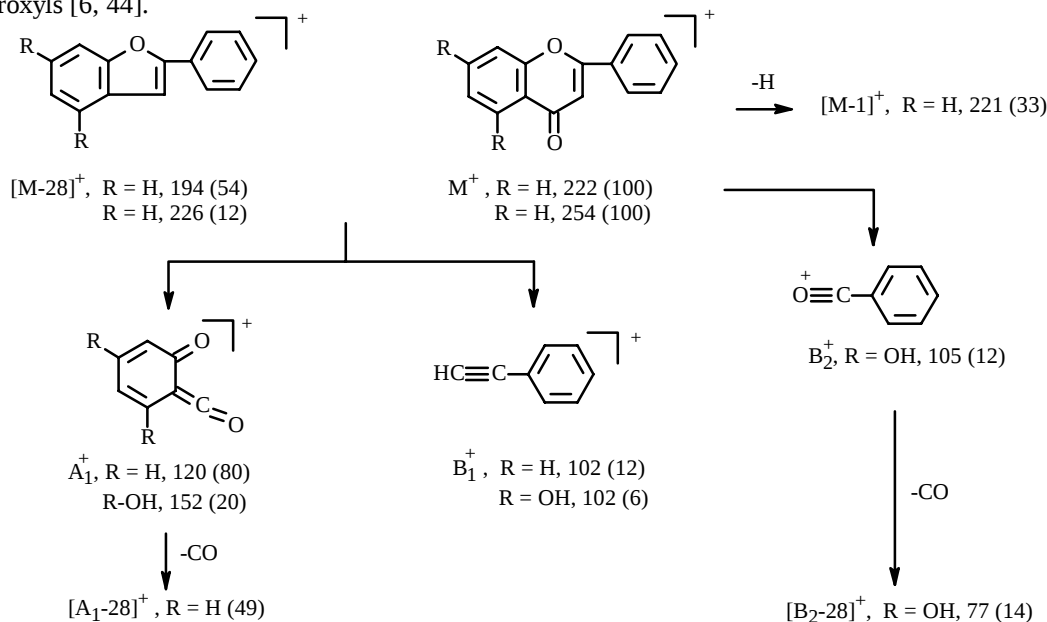
the flavonoid core [39], the location and sequence of sugar binding in glycosides, and the determination of the position of acyl groups in acylated flavonoids [38, 40] can be found using this method. The chemical shifts of C atoms in certain flavonoids are given below.

Mass Spectroscopy. Electron-impact mass spectrometry is an informative method [6, 41] for studying flavonoids and glycosides.

Mass spectrometry can produce valuable structural data and determine the molecular weight of flavonoids. Many flavonoids give a base or sufficiently strong peak for the molecular ion.

Electron impact fragments them to form $[M - H]^+$, $[M - CH_3]^+$ (for methoxyflavones), $[M - CO]^+$, and other ions. Ions formed by retrodiene decomposition of the flavone core are very interesting for structural investigations [6, 42-44].

Unsubstituted flavone gives peaks for $[M - H]^+$, $[M - CO]^+$, $[A_1]^+$, $[A_1 - CO]^+$, and $[B_1]^+$ in addition to a peak for the molecular ion (Scheme 1). Substitution in rings A and B increases correspondingly the values of $[A_1]^+$ and $[B_1]^+$. The intensity of peaks from ions formed by retrodiene decomposition is insignificant in the spectra of flavones containing four and more phenolic hydroxyls [6, 44].



The first fragmentation of 6- or 8-methoxyflavones involves loss of $-CH_3$ radical to form a strong peak for the $[M - CH_3]^+$ ion, which in turn converts to $[M - 43]^+$ by losing CO [6, 19, 22, 41, 45].

Spectra of 2'-hydroxyflavones contain a rather strong peak for the $[M - 17]^+$ ion [22].

In exceptional instances, the peak for the molecular ion in mass spectra of flavonols is the base peak. Furthermore, peaks of the fragment ions $[M - H]^+$, $[M - CH_3]^+$, and $[M - CH_3 - CO]^+$ and very weak peaks of the corresponding fragments $[A_1]^+$, $[A_1 + H]^+$, and $[B_2]^+$ are present. The main fragmentation pattern of flavonols containing 6-OR or 8-OR groups is a process leading to the $[M - R]^+$ ion [19, 45]. In contrast with flavones, not all 6- or 8-methoxyflavonols give a peak for the $[M - 15]^+$ ion, although the spectra of these compounds contain a strong peak for the $[M - CH_3 - CO]^+$ ion, i.e., $[M - 43]^+$ (Scheme 2).

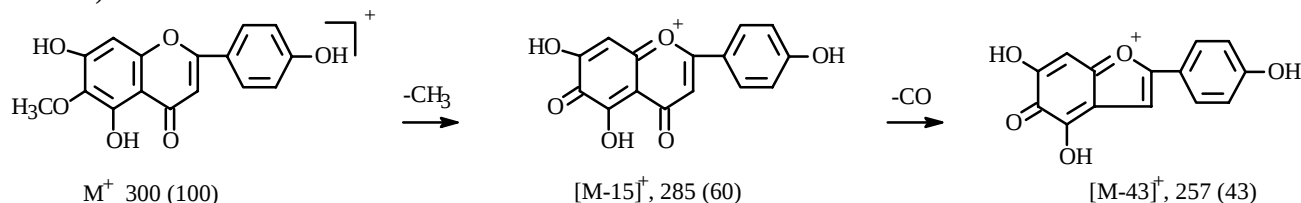
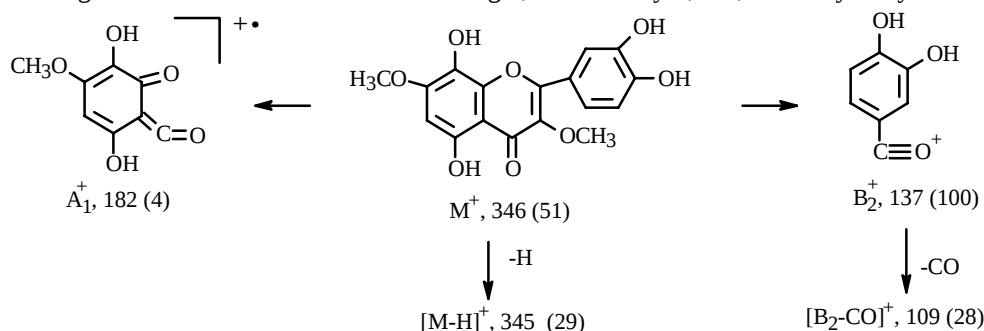


TABLE 2. Mass Spectra of Flavones

Flavones	Substituents					M		M-1		M-15		M-18	
	5	6	7	8	4'	m/z	%	m/z	%	m/z	%	m/z	%
Oroxylin A	OH	OMe	OH			284	100	283	5	269	53	266	27
Wogonin	OH		OH	OMe		284	73			269	100		
Pectolinarigenin	OH	OMe	OH		OMe	314	100	313	6	299	52	296	31
5,7-Dihydroxy-8-methoxyflavone	OH		OH	OMe		314	73			299	100		

The typical fragmentation of flavonols is shown using 3,7-dimethoxy-5,8-3',4'-tetrahydroxyflavone as an example:



Comparison of the mass spectra of a series of 3-, 6-, and 8-methoxylated flavones and flavonols found that the relative intensities of the $[\text{M}]^+$, $[\text{M} - 1]^+$, and $[\text{M} - 15]^+$ peaks and the presence or absence of a peak for the $[\text{M} - 18]^+$ ion can differentiate 6-methoxylated from 8-methoxylated compounds (Table 2) [46].

It can be seen that the base peak in the spectra of 6-methoxyflavones is the $[\text{M}]^+$ ion. Peaks are also present for the $[\text{M} - 1]^+$ and $[\text{M} - 18]^+$ ions. The base peak for 8-methoxyflavones is the $[\text{M} - 15]^+$ ion. Peaks for the $[\text{M} - 1]^+$ and $[\text{M} - 18]^+$ ions are absent.

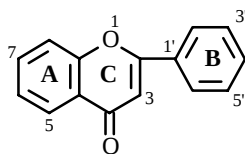
Mass spectra of TMS esters and acetates of flavonoid glycosides also provide valuable information about the structure of the sugar part [47-49].

FLAVONES

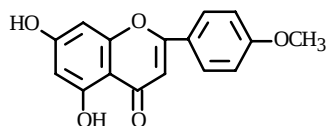
Flavones are the principal phenolic compounds in *Scutellaria* plants (119 compounds isolated) according to quantitative content and distribution in nature. Their molecules contain a conjugated chromophore and are yellow in color. Their fluorescent properties depend on the pH of the medium, the solution concentration, and the nature of the substituents [50]. They are also represented among natural food and textile dyes. Flavone itself has been found in certain *Primula* and *Dionysia* species [51]. Monosubstituted flavones (5-OH, 6-OCH₃, 7-OCH₃, 2'-OH-flavones) were isolated from plants of the *Daphnopsis*, *Primula*, *Pinus*, and *Oroxylum* genera [51, 52].

The disubstituted flavone derivatives chrysin (found in 27 species), wogonin (27), and oroxylin (19); the trisubstituted derivatives baicalin (34) and apigenin (19); and the tetrasubstituted derivatives scutellarein (26) and luteolin (16) are characteristic and most widely distributed among *Scutellaria* plants.

The variety of flavones is due to the nature, quantity, and mutual location of substituents.



It can be concluded based on the literature data that baicalin, wogonin, oroxylin, scutellarein, chrysin, and their glucuronides are compounds typical of *Scutellaria* plants. The C-methyl and C-prenyl derivatives have not yet been observed in plants of this genus.



Acacetin (5,7-dihydroxy-4'-methoxyflavone)

Scutellaria polyodon [53], *S. sevanensis* [54]

$C_{16}H_{12}O_5$: 284

mp: 261-263°C

$[\alpha]_D^{20}$ -64.5°

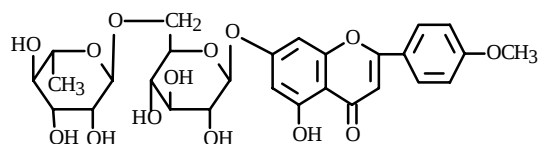
UV: 271, 328; +NaOMe, 278, 368; +NaOAc, 280, 300, 342; +CH₃COONa/H₃BO₃, 272, 340; +AlCl₃, 278, 350; +AlCl₃/HCl, 278, 345

IR: 3170(OH), 2940 (OCH₃), 1660 (C=O γ pyrone)

PMR (Py-d₅): 3.70 (s, OCH₃), 6.64 (d, J = 2.5, H-8), 6.72 (d, J = 2.5, H-6), 6.84 (s, H-3), 7.02 (d, J = 9, H-3',5'), 7.92 (d, J = 9, H-2',6')

¹³C NMR (DMSO-d₆) [54]:

C-2	164.6	C-8	92.9	C-4'	161.8
3	103.4	9	161.8	5'	116.3
4	182.3	10	105.0	6'	128.8
5	157.7	1'	121.6	OCH ₃	55.5
6	98.2	2'	128.8		
7	165.6	3'	116.3		



Acacetin 7-O-rutinoside (linarin)

S. polyodon [55]

$C_{28}H_{32}O_{14}$: 592

mp: 267-269°C

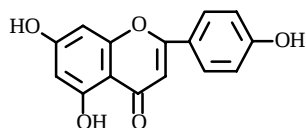
$[\alpha]_D^{20}$ -120° (c 0.65, formamide)

UV: 270, 330; +CH₃ONa, 282, 372; +CH₃COONa, 278, 342; +CH₃COONa/H₃BO₃, 270, 330; +AlCl₃/HCl, 315, 345

PMR (TMS ester): 3.40-3.90 (10H, glucose and rhamnose), 4.36 (s, H-1'', rhamnose), 5.00 (d, J = 7, H-1'', glucose), 6.24 (d, J = 2.5, H-8), 6.56 (d, J = 2.5, H-6), 6.45 (s, H-3), 6.74 (d, J = 9, H-3',5'), 7.74 (d, J = 9, H-2',6')

¹³C NMR (DMSO-d₆) [38]:

C-2	163.2	C-7	164.4	C-2'	128.1
3	104.3	8	95.1	3'	113.0
4	182.4	9	161.6	4'	162.9
5	157.4	10	105.8	5'	115.0
6	100.8	1'	123.1	6'	128.8



Apigenin (5,7,4'-trihydroxyflavone)

S. adenostegia [56, 57], *S. adsurgens* [58, 59], *S. alpina* [60], *S. comosa* [61], *S. cretica* [62], *S. discolor* [63], *S. galericulata* [64-66], *S. indica* [67], *S. iskanderi* [68], *S. karjaginii* [69], *S. ocellata* [185], *S. orietalis* [69], *S. ovata* [70], *S. polyodon* [53], *S. przewalskii* [71], *S. pycnoclada* [57], *S. rivularis* [72, 73], *S. scordiifolia* [74], *S. sevanensis* [54], *S. supina* [57]

$C_{15}H_{10}O_5$: 270

mp: 346-347°C

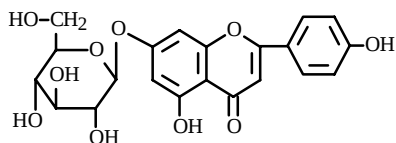
UV: 270, 340; +CH₃COONa, 275, 385; ZrOCl₂, 305, 395; +NaOH, 395

PMR (Py-d₅): 6.62 (d, J = 2.0, H-6), 6.71 (d, J = 2.0, H-8), 6.80 (s, H-3), 7.09 (d, J = 9.0, H-3',5'), 7.84 (d, J = 9, H-2',6'), 13.68 (br.s, 5-OH)

Mass: [M]⁺ 270, 242, 213, 153, 152, 123, 111, 96, 89, 69

^{13}C NMR (DMSO- d_6 — D_2O , 2:1) [38, 40]:

C-2	164.1	C-7	164.9	C-2'	129.8
3	104.3	8	95.6	3'	117.3
4	183.2	9	158.7	4'	161.8
5	162.0	10	105.1	5'	117.3
6	100.3	1'	122.7	6'	129.8



Apigenin 7-O-glucoside (cosmosiin)

S. adenostegia [57], *S. adsurgens* [59], *S. cretica* [62], *S. galericulata* [66], *S. immaculata* [186], *S. przewalskii* [71]

$\text{C}_{21}\text{H}_{20}\text{O}_{10}$: 432

mp: 203–205°C

$[\alpha]_D^{20}$ -52.8° (c 0.91, DMF)

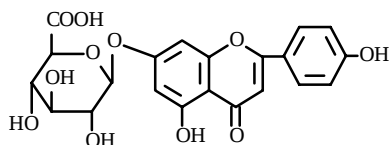
UV: 269, 338; + CH_3COONa , 268, 338, 400; + AlCl_3 , 279, 301, 343; + CH_3ONa , 268, 398 [71]

IR: 3320 (OH), 1660 (C=O), 1595, 1500, (C_6H_5), 1460, 1420, 1078, 1058, 1035, 1000, 910, 750, 680

PMR (Py- d_5): 4.12 (6H, m, H-2''—H-6'', glucose), 5.73 (1H, d, J = 8.0, H-1'', glucose), 6.65 (1H, d, J = 2.5, H-6), 6.80 (1H, s, H-3), 6.98 (1H, d, J = 2.5, H-8), 7.13 (2H, d, J = 8.0, H-3',5'), 7.80 (2H, d, J = 8.0, H-2',6')

^{13}C NMR (DMSO- d_6 — D_2O , 2:1) [38, 40]:

C-2	163.3	C-7	164.6	C-2'	128.8
3	103.3	8	95.1	3'	116.3
4	182.3	9	161.9	4'	161.3
5	152.2	10	105.6	5'	116.3
6	99.7	1'	121.1	6'	128.8



Apigenin 7-O-glucuronide

S. adenostegia [57], *S. adsurgens* [59], *S. alpina* [60], *S. galericulata* [64, 65], *S. indica* [67], *S. iskanderi* [68], *S. nepetoides* [185], *S. polydon* [53], *S. przewalskii* [71], *S. pycnoclada* [57], *S. scordiifolia* [74], *S. supina* [57]

$\text{C}_{21}\text{H}_{18}\text{O}_{11}$: 446

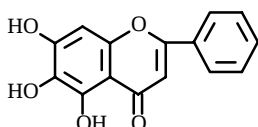
mp: 173–176°C

$[\alpha]_D$ -115.0°

UV: 270, 335; + ZrOCl_2 , 295, 390

IR: 3400 (OH), 1730 (COOH), 1650 (C=O γ -pyrone), 1600, 1580 (C=C aromatic)

PMR (Py- d_5): 4.00–4.65 (m, H-2'',3'',4''), 4.83 (d, J = 8.5, H-5''), 5.87 (d, J = 6.5, H-1''), 6.70 (d, J = 2, H-6), 6.76 (s, H-3), 6.95 (d, J = 2, H-8), 7.15–7.32 (m, H-3',5'), 7.50–7.72 (m, H-2',6') [185]



Baicalin (5,6,7-trihydroxyflavone)

S. adenostegia [56, 57], *S. adsurgens* [59], *S. alpina* [60], *S. altissima* [75, 76], *S. amoena* [77], *S. araxensis* [78], *S. baicalensis* [79–87], *S. comosa* [88], *S. cretica* [62], *S. epilobiifolia* [89], *S. galericulata* [64–66, 90], *S. grossa* [91], *S. iskanderi* [68], *S. litwinowii* [76], *S. oreophila* [92], *S. phyllostachya* [93], *S. polyodon* [53, 94], *S. prostrata* [95], *S. pycnoclada* [57], *S. rehderiana* [96], *S. rivularis* [73], *S. scandens* [97], *S. scordifolia* [74], *S. sevanensis* [54], *S. squarrosa* [98], *S. strigillosa* [188], *S. supina* [57], *S. tenax* [99], *S. viscidula* [100]

C₁₅H₁₀O₅: 270

mp: 260-262°C

UV: 275, 325; +CH₃COONa, 260, 375; +ZrOCl₂, 290, 360; +NaOH, 255, 370; +CH₃COONa/H₃BO₃, 260, 365

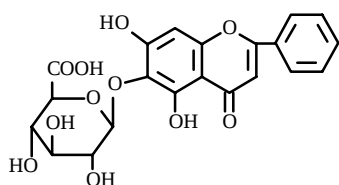
IR: 3540-3220 (OH), 1660 (C=O γ-pyrone)

Mass: [M]⁺ 270, 254, 242, 225, 213, 196, 179, 168, 155, 153, 141, 129, 128, 122, 115, 111, 105, 98, 97, 95, 93, 89, 77, 75, 67, 63

PMR (Py-d₅): 6.65 (1H, s, H-3), 7.49 (1H, s, H-8), 7.55 (3H, m, H-3',4',5'), 7.85 (2H, m, H-2',6')

¹³C NMR (DMSO-d₆): [73]

C-2	162.9	C-7	153.6	C-2'	126.2
3	104.4	8	94.1	3'	129.0
4	182.1	9	149.8	4'	131.7
5	147.0	10	104.3	5'	129.0
6	129.3	1'	130.9	6'	126.2



Baicalein 6-O-β-D-glucuronide

S. baicalensis [101], *S. grossa* [91]

C₂₁H₁₈O₁₁: 446

mp: 197°C (dec.) (CH₃OH)

[α]_D³¹ -55° (c 0.11, CH₃OH)

UV: 245 sh (4.03), 272 (4.42), 309 (4.16); +AlCl₃, 250 sh (4.01), 284 (4.40), 333 (4.24)

IR: 3400 (OH), 1734 (COOH), 1658 (C=O γ-pyrone), 1624, 1588 (C=C aromatic)

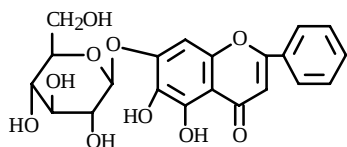
EI-MS *m/z* (%): 270 (C₁₅H₁₀O₅; 100)

FAB-MS *m/z* (%): 447 [M + 1]⁺ (10)

PMR (DMSO-d₆): 3.26-3.64 (m, sugar protons), 4.94 (1H, d, J = 7.7, anomeric proton of glucuronic acid H-1''), 6.64 (1H, s, H-8), 6.97 (1H, s, H-3), 7.58 (3H, m, H-3',4',5'), 8.07 (2H, dd, J = 1.3 and 8.2, H-2',6'), 10.62 (1H, s, 7-OH), 13.05 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆) [91]:

C-2	163.2	C-9	153.1	C-6'	126.4
3	104.7	10	104.1	1''	103.7
4	182.3	1'	130.7	2''	73.5
5	152.6	2'	126.4	3''	75.3
6	128.1	3'	129.1	4''	71.3
7	157.8	4'	132.0	5''	75.6
8	94.5	5'	129.1	6''	170.1



Baicalein 7-O-β-D-glucopyranoside

S. baicalensis [101, 102, 183], *S. glabrata* [103], *S. immaculata* [186]

C₂₁H₂₀O₁₀: 432

mp: 206-207°C (dec.)

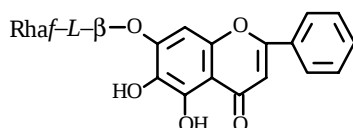
UV: 279, 314; +AlCl₃, 290, 341

IR: 3385 (OH), 1660 (C=O γ-pyrone), 1622, 1584 (C=C aromatic)

PMR (DMSO-d₆): 5.23 (1H, d, J = 7.5, anomeric glucose proton), 6.97 (1H, s, H-3), 7.07 (1H, s, H-8), 7.58 (3H, m, H-3',4',5'), 8.02 (2H, m, H-2',6'), 12.75 (1H, s, 5-OH) [101, 102]

¹³C NMR (DMSO-d₆) [183]:

C-2	163.7	C-9	149.4	C-6'	126.5
3	104.8	10	106.2	1''	101.1
4	182.8	1'	130.8	2''	73.2
5	146.7	2'	126.5	3''	75.9
6	131.0	3'	129.3	4''	69.8
7	151.8	4'	132.2	5''	77.4
8	94.3	5'	129.3	6''	60.7



Baicalein 7-O-β-L-rhamnofuranoside (galeroside)

S. galericulata [64, 66, 90]

C₂₁H₂₀O₉: 416

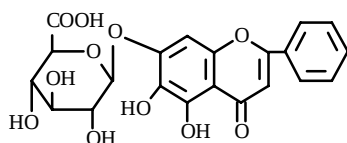
mp: 189-190°C

[α]_D -56° (c 0.1, ethanol)

UV: 280, 315; +CH₃COONa, 280, 315; +CH₃COONa/H₃BO₃, 280, 315; +C₂H₅ONa, 270, 350; +ZrOCl₂, 295, 350

IR: 3380 (OH), 1662 (C=O γ-pyrone), 1620, 1580, 1518 (C=C aromatic)

[M]_D^{KE} = -133° compared with the phenyl rhamnosides ([M]_D of the phenyl-β-L-rhamnofuranoside, -90°) and difference spectrum (two absorption bands at 1010-1100 cm⁻¹)



Baicalin (baicalein-7-O-glucuronide)

S. adenostegia [57], *S. adsurgens* [59], *S. alpina* [60], *S. altissima* [75, 104, 105],

S. amoena [77], *S. araxensis* [78], *S. baicalensis* [79-82, 84-87, 101, 102, 106],

S. columnae [107], *S. comosa* [88], *S. cretica* [62], *S. galericulata* [64-66, 90],

S. grossa [91], *S. ikonnikovii* [108], *S. iskanderi* [68], *S. litwinowii* [76], *S. ocellata* [185], *S. oreophila* [92], *S. polyodon* [53, 94], *S. prostrata* [95], *S. przewalskii* [109], *S. pryncoclada* [57], *S. rivularis* [110], *S. scandens* [97], *S. scordifolia* [74], *S. squarrosa* [98], *S. strigillosa* [188], *S. supina* [57]

C₂₁H₁₈O₁₁: 446

mp: 220-222°C

UV: 245 (3.96), 277 (4.41), 313 (4.15); +CH₃COONa (no shifts observed); +AlCl₃, 289 (4.35), 340 (4.23)

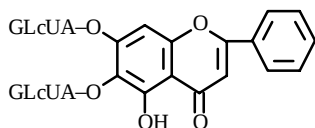
IR: 3390 (OH), 1729 (COOH), 1662 (C=O γ-pyrone), 1612 (C=C aromatic)

FAB-MS: m/z 447 [M + H]⁺

PMR (DMSO-d₆): 5.24 (1H, d, J = 7.1, anomeric proton of glucuronic acid H-1''), 6.98 (1H, s, H-3), 7.09 (1H, s, H-8), 7.6 (3H, m, H-3',4',5'), 8.0 (2H, m, H-2',6'), 12.70 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆) [108]:

C-2	163.9	C-9	149.3	C-6'	126.1
3	104.1	10	106.0	1''	99.8
4	182.4	1'	130.3	2''	72.7
5	146.5	2'	126.1	3''	75.3
6	130.1	3'	129.1	4''	71.4
7	150.9	4'	132.1	5''	75.1
8	93.7	5'	129.1	6''	170.7



Baicalein 6,7-di-O- β -glucuranopyranoside

S. baicalensis [101]

$C_{27}H_{26}O_{17}$: 622

mp: >300°C

$[\alpha]_D^{22}$ -96.1° (c 0.5, H₂O)

UV: 244 sh (3.93), 273 (4.38), 306 (4.10); +CH₃COONa (no shifts observed), +AlCl₃, 280 (5.34), 327 (4.08)

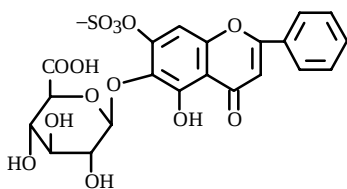
IR: 3431 (OH), 1749 (COOH), 1658 (C=O γ -pyrone), 1625 (C=C aromatic)

FAB-MS m/z 623 [M + H]⁺, 447 [MH - glucuronic acid]⁺

PMR (DMSO- d_6): 5.00 (1H, d, J = 7.5, C6, H-1''), 5.29 (1H, d, J = 7.6, C7, H-1'''), 7.06 (1H, s, H-3), 7.12 (1H, s, H-8), 7.6 (3H, m, H-3',4',5'), 8.0 (2H, m, H-2',6'), 12.89 (1H, s, 5-OH)

¹³C NMR (DMSO- d_6):

C-2	163.8	C-1'	130.5	C-4''	71.3
3	105.1	2'	126.4	5''	75.2
4	182.5	3'	129.1	6''	169.9
5	152.9	4'	132.1	(C-7)-1'''	100.5
6	129.1	5'	129.1	2'''	73.8
7	155.6	6'	126.4	3'''	75.8
8	94.8	(C-6)-1''	103.3	4'''	71.3
9	152.6	2''	72.9	5'''	75.5
10	106.3	3''	75.6	6'''	169.8



Baicalein 6-O- β -glucoronopyranosyl-7-O-sulfate

S. baicalensis [101]

$C_{21}H_{17}O_{14}S$: 525

mp: 191-193°C

UV: 275 (4.37), 3.06 sh (4.07); +CH₃COONa (no shifts observed); +AlCl₃, 247 sh (3.88), 287 (4.37), 329 (4.16)

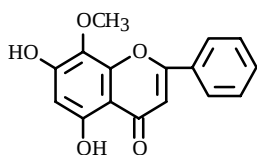
IR: 3449 (OH), 1718 (COOH), 1653 (C=O γ -pyrone), 1621 (C=C aromatic)

FAB-MS m/z : 547 [M + Na - H]⁻, 525 [M - H]⁻, 445 [M - SO₃H]⁻

PMR (DMSO- d_6): 5.08 (1H, br. s, H-1''), 7.04 (1H, s, H-3), 7.33 (1H, s, H-8), 7.60 (3H, m, H-3',4',5'), 8.0 (2H, m, H-2',6')

¹³C NMR (DMSO- d_6):

C-2	163.8	C-9	151.8	C-6'	126.5
3	104.8	10	106.4	(C-6)-1''	103.5
4	182.4	1'	130.5	2''	73.6
5	152.3	2'	126.5	3''	76.0
6	129.7	3'	129.1	4''	71.5
7	151.7	4'	132.1	5''	76.0
8	98.9	5'	129.1	6''	171.1



Wogonin (5,7-dihydroxy-8-methoxyflavone)

S. alpina [60], *S. altissima* [75, 104], *S. amoena* [77], *S. baicalensis* [79-84, 103], *S. comosa* [61], *S. discolor* [63, 111], *S. epilobiifolia* [89], *S. galericulata* [63, 65], *S. glabrata* [112], *S. grossa* [91], *S. indica* [113, 114], *S. iskanderi* [68], *S. ocellata*

[185], *S. polyodon* [94], *S. prostrata* [95], *S. ramosissima* [115], *S. rehderiana* [96], *S. rivularis* [72, 116, 117], *S. scandens* [97], *S. scorifolia* [74], *S. sevanensis* [54], *S. squarrosa* [98], *S. strigillosa* [188], *S. supina* [57], *S. tenax* [99], *S. viscidula* [100]

C₁₆H₁₂O₆: 284

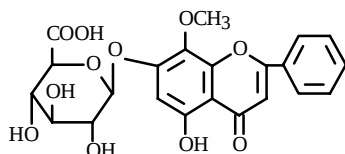
mp: 202°C

UV: 245, 275, 315; +CH₃COONa, 290, 395; +NaOH, 295, 400; +CH₃COONa/H₃BO₃, 275, 315; +ZrOCl₂, 295, 335, 415

IR: 3450 (OH), 2930 (OCH₃), 1660 (C=O γ-pyrone), 1612, 1585 (C=C aromatic)

Mass: 284 [M]⁺, 269 [M - CH₃]⁺ (100), 241 [M - CH₃ - CO]⁺, 167, 139, 105, 102

PMR (Py-d₅): 3.85 (3H, s, OCH₃), 6.70 (1H, s, H-3), 6.90 (1H, s, H-6), 7.41 (3H, m, H-3',4',5'), 7.98 (2H, m, H-2',6'), 13.12 (br.s, 5-OH) [185, 188]



Wogonoside (wogonin-7-O-glucuronide)

S. alpina [60], *S. altissima* [75, 104], *S. amoena* [77], *S. baicalensis* [79, 82, 84, 106], *S. comosa* [61, 88], *S. discolor* [111], *S. galericulata* [64, 65], *S. grossa* [91], *S. immacullata* [186], *S. indica* [113], *S. iskanderi* [68], *S. ocellata* [185], *S. polyodon* [94], *S. prostrata* [95], *S. rivularis* [110], *S. scandens* [97], *S. scorifolia* [74], *S. strigillosa* [188], *S. supina* [57]

C₂₂H₂₀O₁₁: 460

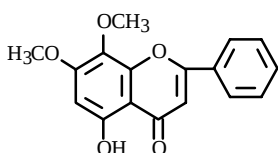
mp: 194-196°C

[α]_D -15° (c 1, DMF)

UV: 275, 345; +ZrOCl₂, 415; +NaOH, 310 (dec.)

IR: 3454 (OH), 1735 (COOH), 1659 (C=O γ-pyrone), 1614 (C=C aromatic)

PMR (DMSO-d₆): 3.78 (3H, s, 8-OCH₃), 5.32 (1H, d, J = 7, H-1''), 7.06 (1H, s, H-3), 7.12 (1H, s, H-6), 7.60 (3H, m, H-3',4',5'), 8.00 (2H, m, H-2',6'), 12.79 (1H, s, 5-OH)



5-Hydroxy-7,8-dimethoxyflavone (7-O-methylwogonin)

S. baicalensis [83, 84, 184], *S. rivularis* [99, 116]

C₁₇H₁₄O₅: 298

mp: 183-184°C (hexane)

UV: 274 (4.52), 315 (3.85), 346 (3.78)

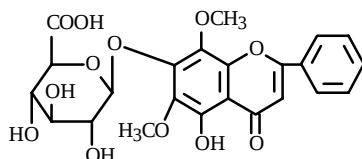
IR: 3450 (OH), 1668 (C=O γ-pyrone), 1592, 1450, 1375, 1122

Mass: 298 [M]⁺ (C₁₇H₁₄O₅)

PMR (CDCl₃): 3.95 (6H, s, OCH₃), 6.43 (1H, s, H-6), 6.66 (1H, s, H-3), 7.4-7.7 (3H, m, H-3',4',5'), 7.93 (2H, dd, J = 2.2 and 7.4, H-2',6'), 12.55 (1H, s, 5-OH)

¹³C NMR (CDCl₃) [83, 84]:

C-2	163.9	C-8	129.1	C-4'	131.9
3	105.4	9	157.6	5'	129.1
4	182.7	10	105.0	6'	126.4
5	158.7	1'	131.4	OCH ₃	56.3
6	95.9	2'	126.4	OCH ₃	61.7
7	157.6	3'	129.1		



5-Hydroxy-6,8-dimethoxy-7-O-β-D-glucuronidopyranosylflavone

S. repens [187]

C₂₃H₂₂O₁₂: 490

mp: 149°C (dec.) (MeOH)

[α]_D²⁷ +36.3° (c 0.08, MeOH)

UV: 280 (4.52), 315 sh (4.01), 350 sh (3.66); +CH₃ONa, 280 (4.47), 327 sh (3.65), 395 (3.62); +AlCl₃, 300 (4.48), 329 sh (4.16), 416 (3.62); +AlCl₃/HCl, 300 (4.52), 329 sh (4.16), 416 (6.63); +CH₃COONa, 279 (4.52), 375 sh (3.50); +CH₃COONa/H₃BO₃, 278 (4.56), 315 sh (4.04), 353 sh (3.75)

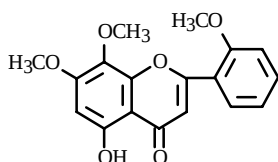
IR: 3424 (OH), 1720 (COOH), 1650 (C=O γ -pyrone), 1612 (C=C aromatic)

FAB-MS *m/z* (%): 491 [M + H]⁺ (29)

PMR (DMSO-d₆): 3.31 (1H, m, H-3''), 3.33 (1H, m, H-2''), 3.38 (1H, t, J = 9.5, H-4''), 3.57 (1H, d, J = 9.5, H-5''), 3.82 (3H, s, 6-OCH₃), 3.94 (3H, s, 8-OCH₃), 5.32 (1H, d, J = 7.3, H-1''), 7.08 (1H, s, H-3), 7.63 (3H, m, H-3',4',5'), 8.09 (2H, m, H-2',6'), 12.60 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	163.7	C-9	145.4	C-6'	126.4
3	105.0	10	107.0	1''	102.6
4	182.8	1'	130.6	2''	73.7
5	148.5	2'	126.4	3''	75.8
6	136.0	3'	129.3	4''	71.5
7	149.0	4'	132.3	5''	75.5
8	132.9	5'	129.3	6''	170.1
				OCH ₃	60.4
				OCH ₃	61.8



5-Hydroxy-7,8,2'-trimethoxyflavone

S. baicalensis [118], *S. grossa* [91]

C₁₈H₁₆O₆: 328

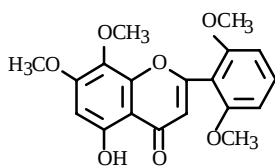
mp: 190-191°C (ethylacetate)

UV: 273, 330; +AlCl₃ or AlCl₃/HCl, 283, 296 sh, 342, 410

IR: 1660 (C=O γ -pyrone), 1615 (methoxylated aromatic ring)

Mass: 328 [M]⁺ (67) C₁₈H₁₆O₆; 313 (100) C₁₇H₁₃O₆, 285 (10) C₁₆H₁₃O₅, 181 (19) C₈H₅O₅, 153 (23) C₇H₅O₄, 135 (2) C₈H₇O₂

PMR (CDCl₃): 3.92, 3.95 (3H, 6H, s, 3×OCH₃), 6.43 (1H, s, H-3), 7.05 (1H, s, H-6), and other aromatic protons H-3', H-4', H-5', and H-6'



5-Hydroxy-7,8,2',6'-tetramethoxyflavone (altisin)

S. altissima [75, 104], *S. grossa* [91]

C₁₉H₁₈O₇: 358

mp: 199°C (dec.) (MeOH)

UV: 266 (4.48), 338 (3.84)

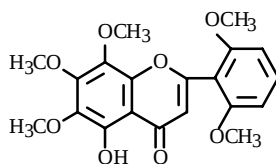
IR: 3400 (OH), 1650 (C=O γ -pyrone), 1600, 1580 (C=C aromatic)

EI-MS *m/z* (%): 358 [M]⁺ (46), 346 [M - CH₃]⁺ (100)

PMR (DMSO-d₆): 3.70, 3.92 (3H each, s, 2×OCH₃), 3.80 (6H, s, 2',6'-OCH₃), 6.32 (1H, s, H-3), 6.62 (1H, s, H-6), 6.83 (2H, d, J = 8.3, H-3',5'), 7.52 (1H, t, J = 8.3, H-4'), 12.63 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆) [91]:

C-2	161.7	C-9	149.9	C-6'	158.3
3	112.2	10	104.1	2'-OCH ₃	56.2
4	182.2	1'	110.2	6'-OCH ₃	56.2
5	157.0	2'	158.3	7-OCH ₃	56.5
6	96.2	3'	104.6	8-OCH ₃	61.0
7	158.7	4'	133.1		
8	128.6	5'	104.6		



5-Hydroxy-6,7,8,2',6'-pentamethoxyflavone

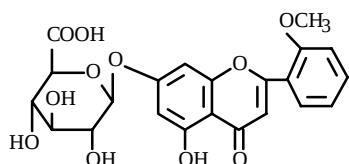
S. baicalensis [119]

$C_{20}H_{20}O_8$: 388

UV: 272, 330

IR: 3520 (OH), 2930 (OCH_3), 1660 ($C=O$ γ -pyrone), 1615, 1575 ($C=C$ aromatic)

Mass: 388 $[M]^+$, 373 $[M - OCH_3]^+$ (100)



5-Hydroxy-2'-methoxy-7-O-glucuronylflavone

(2'-methoxychrysin-7-O-glucuronide)

S. granulosa [120], *S. prostrata* [95]

$C_{22}H_{20}O_{11}$: 460

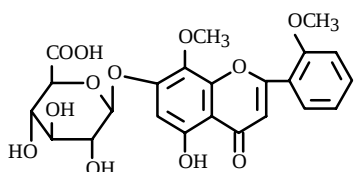
mp: 200-202°C

$[\alpha]_D^{20}$ -75° (ethanol)

UV: 270, 330 sh; +NaOH, 380; +ZrOCl₂, 290, 390

IR: 3540 (OH), 1730 (COOH), 1665 ($C=O$ γ -pyrone), 1612, 1572 ($C=C$ aromatic), 1093, 1080, 1018 ($C-O$ glycosides)

PMR (TMS-ester) (CCl_4): 3.3-3.4 (4H, m, sugar protons), 5.0 (1H, d, $J = 7$, H-1'') [120]



5-Hydroxy-8,2'-dimethoxy-7-O- β -glucuronylflavone

S. indica [113]

$C_{23}H_{22}O_{12}$: 490

mp: 247°C (dec.) (MeOH)

$[\alpha]_D^{14}$ -45.9° (c 0.04, MeOH)

UV: 275 (4.41), 333 (4.04); +CH₃ONa, 276 (4.39), 283 sh (4.37), 320 sh (4.33), 380 (3.74); +AlCl₃, 255 (3.94), 286 (4.37), 295 sh (4.34), 345 (4.07), 404 (3.84); +AlCl₃/HCl, 284 (4.36), 295 sh (4.31), 342 (4.07), 405 (3.78); +CH₃COONa, 275 (4.40), 333 (4.03); +CH₃COONa/H₃BO₃, 275 (4.40), 333 (4.03)

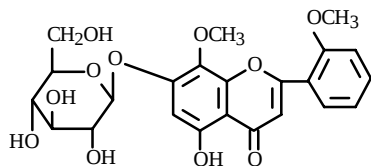
IR: 3500 (OH), 1714 (COOH), 1653 ($C=O$ γ -pyrone), 1607, 1565 ($C=C$ aromatic)

Mass: 314 (100) $C_{17}H_{14}O_6$, 299 (70) $C_{16}H_{11}O_6$

PMR (DMSO- d_6): 3.86, 3.91 (3H, s, each 2 $\times$ OCH_3), 5.29 (1H, br.s, anomeric proton of glucuronic acid H-1''), 6.90 (1H, s, H-3), 6.70 (1H, s, H-6), 7.15 (1H, br.t, $J = 7.6$, H-5'), 7.22 (1H, br.d, $J = 7.9$, H-3'), 7.57 (1H, br.t, $J = 7.9$, H-4'), 7.86 (1H, dd, $J = 7.6$ and 12, H-6'), 12.54 (1H, s, 5-OH)

¹³C NMR (DMSO- d_6):

C-2	161.9	C-10	105.4	C-2''	73.1
3	109.8	1'	119.5	3''	75.5
4	182.5	2'	158.1	4''	71.4
5	156.2	3'	112.8	5''	75.9
6	98.7	4'	133.5	6''	170.2
7	156.2	5'	121.1	2''-OCH ₃	56.0
8	129.5	6'	129.1	8-OCH ₃	61.5
9	149.5	1''	99.9		



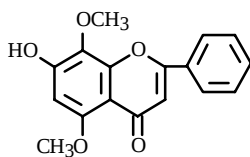
5-Hydroxy-8,2'-dimethoxy-7-O- β -glucopyranosylflavone

S. rivularis [110]

$C_{23}H_{24}O_{11}$: 476

UV: 275, 335; +CH₃COONa, 276, 335

IR: 3450 (OH), 2930 (OCH₃), 1650 (C=O γ -pyrone), 1610, 1570 (C=C aromatic)



7-Hydroxy-5,8-dimethoxyflavone

S. discolor [121], *S. rivularis* [73]

$C_{17}H_{14}O_5$: 298

mp: 290°C (MeOH)

UV: 244, 281, 345; +CH₃ONa, 243, 283, 370; +AlCl₃, 272, 332; +AlCl₃/HCl, 265 sh, 273, 332 sh; +CH₃COONa, 281, 360

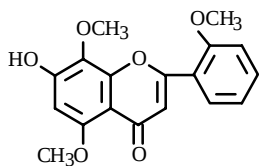
IR: 3400 (OH), 1630 (C=O γ -pyrone), 1610, 1570 (C=C aromatic)

Mass: 298 [M]⁺, 283 [M - CH₃]⁺

PMR (DMSO-d₆): 3.89, 3.81 (3H, s, each 2×OCH₃), 6.52 (1H, s, H-6), 6.79 (1H, s, H-3), 7.61 (3H, m, H-3',4',5'), 8.06 (2H, m, H-2',6'), 10.62 (1H, s, 7-OH)

¹³C NMR (DMSO-d₆) [73]:

C-2	159.4	C-8	129.0	C-4'	131.5
3	108.0	9	152.0	5'	129.3
4	175.9	10	107.6	6'	125.9
5	155.2	1'	131.3	8-OCH ₃	61.0
6	96.9	2'	125.9	2'-OCH ₃	55.9
7	155.6	3'	129.3		



7-Hydroxy-5,8,2'-trimethoxyflavone

S. discolor [121]

$C_{18}H_{16}O_6$: 328

mp: 249°C (dec.) (MeOH)

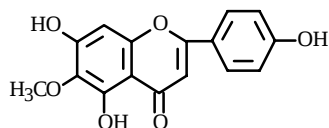
UV: 225 sh (4.35), 270 (4.42), 331 (4.11); +CH₃ONa, 230 sh (4.37), 280 (4.50), 320 (4.02), 370 (4.02); +AlCl₃, 225 sh (4.41), 270 (4.47), 331 (4.19); +AlCl₃/HCl, 225 sh (4.40), 270 (4.45), 299 sh (4.15), 331 (4.15) (4.16); +CH₃COONa, 279 (4.47), 320 (3.99), 370 (4.00); +H₃BO₃/CH₃COONa, 273 (4.42), 327 (4.06)

IR: 3100 (OH), 1630 (C=O γ -pyrone), 1600, 1580 (C=C aromatic)

PMR (DMSO-d₆): 3.78, 3.82, 3.93 (3H, s, each 3×OCH₃), 10.55 (1H, br.s, 7-OH), 6.66 (1H, s, H-3), 6.48 (1H, s, H-6), 7.86 (1H, dd, J = 7.6 and 1.7, H-6'), 7.48-7.65 (1H, m, H-4'), 7.24 (1H, br.d, J = 7.8, H-3'), 7.08-7.24 (1H, m, H-5')

¹³C NMR (DMSO-d₆):

C-2	157.7	C-8	129.0	C-4'	132.6
3	112.7	9	152.1	5'	121.0
4	176.0	10	107.4	6'	128.7
5	155.1	1'	120.0	8-OCH ₃	60.9
6	96.8	2'	157.5	5-OCH ₃	55.9
7	155.6	3'	112.6	2'-OCH ₃	55.9



Hispidulin (5,7,4'-trihydroxy-6-methoxyflavone)

S. alpina [60], *S. amoena* [77], *S. baicalensis* [112], *S. cretica* [62], *S. litwinowii* [76], *S. orientalis* [69], *S. przewalskii* [71], *S. repens* [187], *S. rivularis* [72]
 $C_{16}H_{12}O_6$: 300

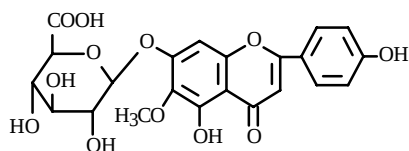
mp: 288-290°C (EtOH)

UV: 335, 274; +NaOCH₃, 394, 326, 276; +AlCl₃, 363, 302, 282 sh, 264 sh; +AlCl₃/HCl, 356, 300, 284 sh, 262 sh; +CH₃COONa, 389, 329, 306, 274; +CH₃COONa/H₃BO₃, 340, 272 [174]

IR: 3350-3530 (OH), 2930 (OCH₃), 1665 (C=O γ -pyrone), 1614, 1573, 1517 (C=C aromatic)

Mass: 300 [M]⁺, 282 [M - H₂O]⁺, 271, 254, 167, 153, 139, 128, 119, 93

PMR (TMS): 6.36 (1H, s, H-3), 6.55 (1H, s, H-8), 7.73 (1H, d, J = 9.0, H-2'), 6.85 (1H, d, J = 9.0, H-3'), 6.85 (1H, d, J = 9.0, H-5'), 7.73 (1H, d, J = 9.0, H-6') [174]



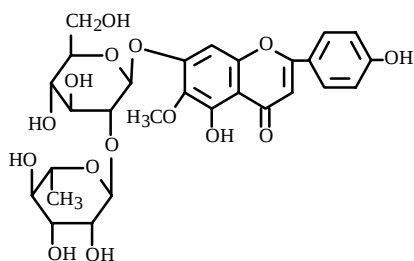
Hispidulin 7-O-glucuronide (hispiduloside)

S. cretica [62], *S. litwinowii* [76]

$C_{22}H_{20}O_{12}$: 476

UV: 275, 336; +CH₃COONa, 276, 237

IR: 3340-3550 (OH), 2930 (OCH₃), 1720 (COOH), 1660 (C=O γ -pyrone), 1612, 1570, 1515 (C=C aromatic)



Hispidulin 7-O-glucobioside (hispidulin 7-O-neohesperidoside)

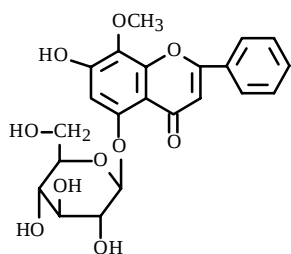
S. przewalskii [71]

$C_{26}H_{32}O_{15}$: 584

UV: 280, 335; +CH₃COONa, 275, 335; +C₂H₅ONa, 275, 370;

+Zr(NO₃)₂, 305, 335

IR: 3340 (OH), 2930 (OCH₃), 1665 (C=O γ -pyrone), 1615, 1575, 1519 (C=C aromatic), 1092, 1065, 1020 (C-O glycosides)



Wogonin 5-O- β -D-glucoside

S. baicalensis [123]

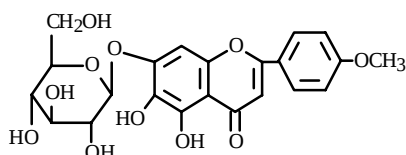
$C_{22}H_{22}O_{10}$: 446

mp: 165°C (MeOH)

UV: 268 (4.42), 310 sh (4.04); +CH₃ONa, 241 (4.30), 279 (4.54), 372 (3.92); +CH₃COONa, 242 (4.24), 278 (4.47), 330 sh (3.82); +AlCl₃, 268 (4.38), 304 sh (4.13); +AlCl₃/HCl, 272 sh (4.28), 285 (4.30), 295 sh (4.29), 330 sh (3.95) [123]

IR: 1625 (C=O γ -pyrone)

PMR (DMSO-d₆): 3.40-3.83 (6H, m, sugar protons), 3.93 (3H, s, OCH₃), 4.80 (1H, d, J = 6.0, H-1''), 6.82 (1H, s, H-6), 6.95 (1H, s, H-3), 7.58-7.72 (3H, m, H-3',4',5'), 7.97-8.13 (2H, m, H-2',6')



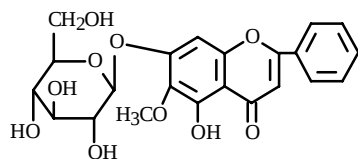
Dinatin 7-O-glucoside

S. przewalskii [71]

$C_{22}H_{22}O_{11}$: 462

UV: 275, 325; +CH₃COONa, 270, 325; +C₂H₅ONa, 260, 365; +Zr(NO₃)₂, 290, 360

IR: 3350-3540 (OH), 1660 (C=O γ -pyrone), 1620, 1580, 1510 (C=C aromatic), 1089, 1060, 1015 (C–O glycosides)



Oroxylin A 7-O-glucoside

S. cretica [62], *S. ovata* [70]

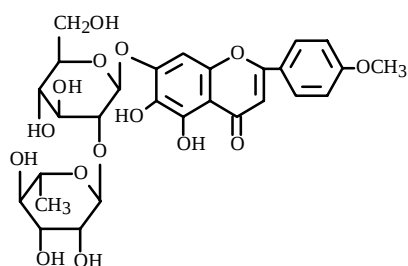
C₂₂H₂₂O₁₀: 446

mp: 162°C

UV: 271, 310; +CH₃COONa, 272, 311

IR: 3450 (OH), 2930 (OCH₃), 1665 (C=O γ -pyrone), 1615, 1575, 1510 (C=C aromatic)

PMR (CDCl₃): 7.86-7.79 (2H, H-2',6'), 7.53-7.44 (3H, m, H-3',4',5'), 6.65 (1H, s, H-8), 6.57 (1H, s, H-3), 5.26 (1H, s, H-1'' glucose), 3.75 (3H, s, 6-OCH₃), 3.5-3.4 (6H, s, sugar protons)



Dinatin 7-O-glucobioside (dinatin 7-O-neohesperidoside)

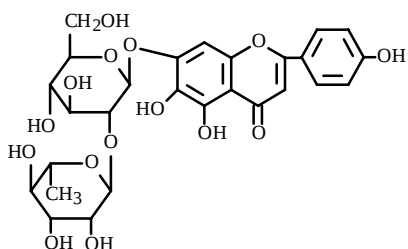
S. przewalskii [71]

C₂₈H₃₂O₁₅: 608

UV: 275, 325; +CH₃COONa, 270, 325; +C₂H₅ONa, 260, 365;

+Zr(NO₃)₂, 290, 360

IR: 3340-3550 (OH), 2930 (OCH₃), 1665 (C=O γ -pyrone), 1618, 1578, 1512 (C=C aromatic), 1090, 1062, 1020 (C–O glycosides)



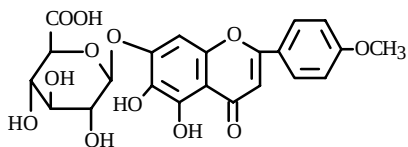
Scutellarein 7-O-glucobioside (scutellarein 7-O-neohesperidoside)

S. przewalskii [71]

C₂₇H₃₀O₁₅: 594

UV: 280, 335; +CH₃COONa, 285, 335; +C₂H₅ONa, 270; +Zr(NO₃)₂, 303, 365

IR: 3450 (OH), 1665 (C=O γ -pyrone), 1620, 1580, 1515 (C=C aromatic), 1095, 1065, 1018 (C–O glycosides)



Dinatin 7-O-glucuronide

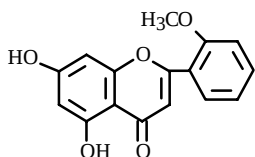
S. przewalskii [71]

C₂₂H₂₀O₁₂: 476

UV: 275, 325; +CH₃COONa, 270, 325; +C₂H₅ONa, 260, 365;

+Zr(NO₃)₂, 290, 360

IR: 3450 (OH), 2930 (OCH₃), 1730 (COOH), 1660 (C=O γ -pyrone), 1620, 1575, 1515 (C=C aromatic)



5,7-Dihydroxy-2'-methoxyflavone (2'-methoxychrysin)

S. adenostegia [56], *S. epilobiifolia* [89], *S. granulosa* [120], *S. phyllostachya* [93],

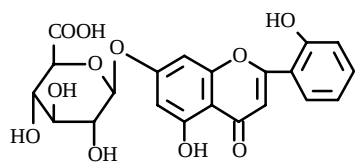
S. prostrata [95], *S. sevanensis* [54], *S. strigillosa* [188]

C₁₆H₁₂O₅: 284

mp: 288-290°C

UV: 267, 330; +CH₃COONa, 385; +NaOH, 380; +ZrOCl₂, 390

PMR (DMSO- d_6): 3.94 (3H, s, OCH₃), 6.20 (1H, d, $J = 2.5$, H-6), 6.46 (1H, d, $J = 2.5$, H-8), 6.84 (1H, s, H-3), 7.14 (1H, m, $J_1 = J_2 = 8$, $J_3 = 2$, H-5'), 7.23 (1H, t, $J_1 = 8$, $J_2 = 2$, H-3'), 7.60 (1H, m, $J_1 = J_2 = 8$, $J_3 = 2$, H-4'), 7.88 (1H, q, $J_1 = 8$, $J_2 = 2$, H-6'), 10.85 (1H, s, 7-OH), 12.84 (1H, s, 5-OH) [120]



**5,2'-Dihydroxy-7-O-glucuronylflavone
(7-O-glucuronyl-2'-hydroxychrysin)**

S. comosa [88], *S. ikonnikovii* [108], *S. pycnoclada* [57], *S. tournefortii* [124]

$C_{21}H_{18}O_{11}$: 446

mp: 230-235°C

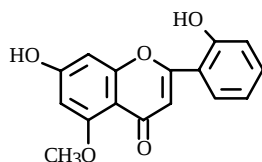
$[\alpha]_D -140.0^\circ$ (EtOH)

UV: 270, 330; +ZrOCl₂, 290, 390; +NaOH, 405

PMR (DMSO- d_6): 5.23 (1H, d, $J = 6.9$, H-1''), 6.44 (1H, d, $J = 2.2$, H-6), 6.82 (1H, d, $J = 2.2$, H-8), 6.98 (1H, t, H-5'), 7.07 (1H, d, $J = 8.0$, H-3'), 7.13 (1H, s, H-3), 7.39 (1H, t, H-4'), 7.83 (1H, d, $J = 8.0$, H-6'), 12.86 (1H, s, 5-OH)

^{13}C NMR (DMSO- d_6) [108]:

C-2	163.07	C-9	157.34	C-6'	128.25
3	105.34	10	109.12	1''	99.45
4	182.20	1'	117.35	2''	72.96
5	161.00	2'	157.08	3''	74.11
6	99.37	3'	116.82	4''	71.89
7	161.73	4'	132.84	5''	76.32
8	94.69	5'	119.13	6''	172.02



7,2'-Dihydroxy-5-methoxyflavone

S. planipes [125]

$C_{16}H_{12}O_5$: 284

mp: 282-284°C (MeOH)

UV: 261 (4.37), 276 (4.10), 333 (3.85)

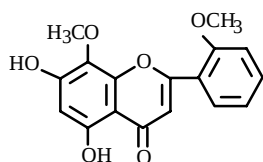
IR: 3436 (OH), 1632 (C=O γ -pyrone), 1594, 1562 (C=C aromatic)

EI-MS m/z (%): 284 [M]⁺ (100), 283 (47.7), 255 (30.7), 253 (3.7), 238 (43.3), 137 (29.0), 118 (11.7)

PMR (DMSO- d_6): 3.80 (s, 5-OCH₃), 6.37 (1H, d, $J = 2.2$, H-6), 6.50 (1H, d, $J = 2.2$, H-8), 6.83 (s, H-3), 6.98 (1H, dd q, $J = 7.9$, 7.2, and 1.2, H-5'), 7.03 (1H, dd, $J = 8.2$ and 1.2, H-3'), 7.35 (1H, dd q, $J = 8.2$, 7.2, and 1.7, H-4'), 7.82 (1H, dd, $J = 7.9$ and 1.7, H-6')

^{13}C NMR (DMSO- d_6):

C-2	160.5	C-7	162.4	C-2'	156.2
3	112.3	8	95.1	4'	131.9
4	175.7	9	159.1	3'	116.8
5	157.3	10	107.1	5'	119.3
6	96.3	1'	117.5	6'	128.1
				5-OCH ₃	55.8



5,7-Dihydroxy-8,2'-dimethoxyflavone

S. discolor [63, 111], *S. indica* [113, 114], *S. rivularis* [72, 73], *S. strigillosa* [188], *S. virularis* [73]

$C_{17}H_{14}O_6$: 314

mp: 231°C (MeOH)

UV: 278, 328; +CH₃ONa, 264 sh, 285, 325 sh, 370; +AlCl₃, 255 sh, 285, 296 sh, 346; +AlCl₃/HCl, 255 sh, 285, 296 sh, 345; +CH₃COONa, 264 sh, 284, 323 sh, 370; +CH₃COONa/H₃BO₃, 279, 328

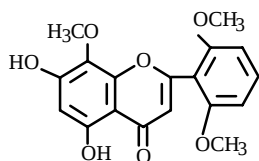
IR: 3450, 3000 (OH), 1640 (C=O γ -pyrone), 1610, 1570 (C=C aromatic)

Mass: 314 [M]⁺, 299 [M - CH₃]⁺

PMR (DMSO-d₆): 3.84, 3.95 (3H, s, each 2×OCH₃), 6.32 (1H, s, H-6), 6.86 (1H, s, H-3), 7.18 (1H, br.t, J = 7.6, H-5'), 7.26 (1H, br.d, J = 7.9, H-3'), 7.60 (1H, ddd, J = 7.9, 7.6, and 1.5, H-4'), 7.88 (1H, dd, J = 7.6 and 1.5, H-6'), 10.80 (1H, br.s, 7-OH), 12.53 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆) [73]:

C-2	161.3	C-8	127.8	C-4'	132.2
3	109.6	9	149.9	5'	121.0
4	182.1	10	103.7	6'	129.1
5	156.4	1'	119.7	8-OCH ₃	61.0
6	99.1	2'	158.0	2'-OCH ₃	55.9
7	157.4	3'	112.7		



5,7-Dihydroxy-8,2',6'-trimethoxyflavone

S. discolor [63, 121]

C₁₈H₁₆O₇: 344

mp: 206°C (dec.) (MeOH)

UV: 267 (4.42), 310 sh (3.92), 350 sh (3.72); +CH₃ONa, 277 (4.48), 335 sh (3.86), 360 (3.90); +AlCl₃, 277 sh (4.40), 300 sh (4.10), 326 (3.93), 395 (3.72); +AlCl₃/HCl, 278 sh (4.41), 300 sh (4.11), 324 (3.91), 395 (3.72); +CH₃COONa, 277 (4.45), 330 sh (3.84), 360 (3.88); +H₃BO₃/CH₃COONa, 270 (4.37), 341 (3.78)

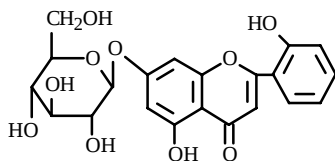
IR: 3300, 3100 (OH), 1650 (C=O γ -pyrone), 1610, 1580 (C=C aromatic)

Mass: 344 [M]⁺ (48), 329 [M - CH₃]⁺ (100)

PMR (DMSO-d₆): 3.72 (3H, s, 8-OCH₃), 3.80 (6H, s, 2',6'-OCH₃), 12.51 (1H, s, 5-OH), 10.50 (1H, br.s, 7-OH), 6.28 (1H, s, H-6), 6.34 (1H, s, H-3), 7.52 (1H, t, J = 8.3, H-4'), 6.83 (2H, d, J = 8.3, H-3',5')

¹³C NMR (DMSO-d₆):

C-2	161.2	C-8	127.8	C-4'	133.0
3	112.2	9	150.6	5'	104.5
4	182.0	10	103.8	6'	158.3
5	156.5	1'	110.3	8-OCH ₃	60.9
6	99.2	2'	158.3	2'-OCH ₃	56.1
7	157.4	3'	104.5	6'-OCH ₃	56.1



5,2'-Dihydroxy-7-O- β -D-glucopyranosylflavone

S. ramosissima [126]

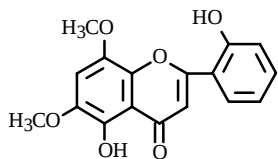
C₂₁H₂₀O₁₀: 432

mp: 280-281°C (MeOH)

UV: 269, 325; +CH₃COONa, 268, 327

IR: 3550-3260 (OH), 1665 (C=O γ -pyrone), 1615, 1565 (C=C aromatic), 1100-1000 (C-O glycosides)

PMR (Py-d₅): 3.88-4.43 (sugar protons), 5.63 (d, J = 6.5, H-1''), 6.59 (d, J = 2.0, H-6), 6.65 (d, J = 2.0, H-8), 6.93-7.07 (m, H-3',5'), 7.08 (s, H-3), 7.28 (dt, J = 2.0 and 8.0, H-4'), 7.72 (dd, J = 2.0 and 8.0, H-6'), 13.48 (br.s, 5-OH)



5,2'-Dihydroxy-6,8-dimethoxyflavone

S. baicalensis [127, 190]

$C_{17}H_{14}O_6$: 314

mp: 251°C (benzene)

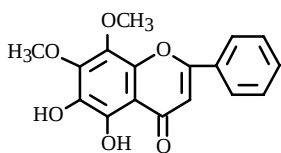
UV: 287 (3.7), 330 (3.4); +AlCl₃, 292 sh, 307, 364

Mass: 314 [M]⁺, 299 [M - 15]⁺ (100)

PMR (DMSO-d₆): 3.91, 3.15 (3H, s, each 2×OCH₃), 6.89-7.99 (6H, m) [190]

¹³C NMR (DMSO-d₆ + D₂O) [170]:

C-2	161.6	C-8	141.7	C-4'	132.4
3	108.4	9	139.2	5'	119.2
4	183.0	10	107.5	6'	128.0
5	141.1	1'	119.2	8-OCH ₃	57.2
6	139.2	2'	156.4	6-OCH ₃	56.8
7	116.8	3'	116.8		



5,6-Dihydroxy-7,8-dimethoxyflavone

S. ramosissima [115]

$C_{17}H_{14}O_6$: 314

mp: 182-184°C (CHCl₃)

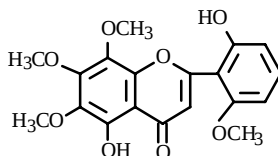
UV: 249, 272, 321

Mass: 314 [M]⁺ (56), 299 [M - CH₃]⁺ (100), 284 (47), 269 (78), 241 (28), 202 (25), 197 (28), 164 (44), 149 (56), 105 (56)

PMR (Py-d₅): 3.92, 4.08 (3H, s, each 2×OCH₃), 6.88 (1H, s, H-3), 7.39 (3H, m, H-3',4',5'), 7.91 (2H, m, H-2',6'), 13.08 (br.s, 5-OH)

¹³C NMR (CDCl₃ + CD₃OD):

C-2	164.2	C-8	133.2	C-4'	131.8
3	104.7	9	142.2	5'	129.0
4	183.0	10	106.6	6'	126.1
5	142.9	1'	131.2	OCH ₃	61.2
6	133.8	2'	126.1	OCH ₃	61.9
7	147.4	3'	129.0		



5,2'-Dihydroxy-6,7,8,6'-tetramethoxyflavone

S. baicalensis [127]

$C_{19}H_{18}O_8$: 370

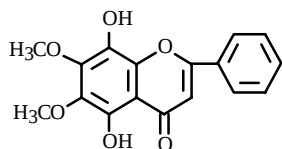
mp: 180-181°C

UV: 275, 350

IR: 3380 (OH), 2930 (OCH₃), 1650 (C=O γ-pyrone), 1615, 1580 (C=C aromatic)

¹³C NMR (DMSO-d₆ + D₂O) [170]:

C-2	162.1	C-8	132.7	C-4'	132.2
3	111.7	9	148.2	5'	101.9
4	182.2	10	118.9	6'	158.1
5	146.0	1'	108.6	7,8-OCH ₃	61.4
6	135.5	2'	156.4	6-OCH ₃	60.2
7	152.7	3'	106.1	6'-OCH ₃	55.8



5,8-Dihydroxy-6,7-dimethoxyflavone

S. baicalensis [128, 129]

$C_{17}H_{14}O_6$, 314

mp: 235-236°C (MeOH)

UV: 250 sh, 279, 322; +CH₃COONa, 270, 286 sh, 375; +AlCl₃, 255 sh, 295, 347

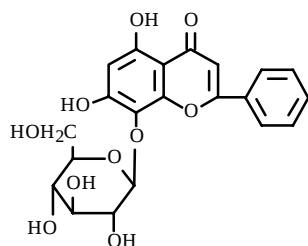
IR: 3420 (OH), 1650 (C=O γ -pyrone), 1615, 1600, 1580 (C=C aromatic)

Mass: 314 [M]⁺ (84.2), 299 (100)

PMR (DMSO-d₆): 3.87 (3H, s, OCH₃), 3.77 (3H, s, OCH₃), 6.95 (1H, s, H-3), 7.95-8.10 (2H, m, H-2',6'), 7.50-7.65 (3H, m, H-3',4',5'), 12.60 (1H, br.s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	163.4	C-8	128.5	C-4'	132.1
3	104.9	9	148.5	5'	129.3
4	182.6	10	103.6	6'	126.4
5	145.8	1'	131.2	OCH ₃	60.3
6	132.1	2'	126.4	OCH ₃	61.3
7	151.3	3'	129.3		



5,7-Dihydroxy-8-O- β -D-glucopyranosylflavone (norwogonin 8-O-glucoside)

S. ikonnikovii [108]

$C_{21}H_{20}O_{10}$: 434

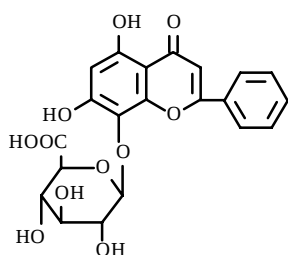
UV: 278, 350

IR: 3540 (OH), 1665 (C=O γ -pyrone), 1620, 1580, 1520 (C=C aromatic), 1095, 1065, 1015 (C-O glycosides)

PMR (DMSO-d₆): 4.65 (1H, d, J = 7.7, anomeric proton of glucose H-1''), 6.23 (1H, s, H-6), 6.99 (1H, s, H-3), 7.08-7.59 (3H, m, H-3',4',5'), 8.29 (2H, d, J = 6.2, H-2',6'), 12.66 (br.s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	162.89	C-9	149.40	C-6'	126.84
3	106.66	10	102.87	1''	104.45
4	181.63	1'	130.57	2''	74.03
5	157.18	2'	126.84	3''	75.99
6	99.43	3'	128.90	4''	69.02
7	159.03	4'	131.83	5''	77.22
8	125.67	5'	128.90	6''	60.40



5,7-Dihydroxy-8-O- β -D-glucuronylflavone (norwogonin 8-O-glucuronide)

S. discolor [63], *S. ikonnikovii* [108]

$C_{21}H_{18}O_{11}$: 446

mp: 212°C (dec.) (MeOH)

$[\alpha]_D^{14}$ +23.7° (c 0.07, MeOH)

UV: 279 (4.39), 346 (3.68); +CH₃ONa, 240 sh (4.13), 265 sh (4.31), 284 (4.42), 370 (3.78); +AlCl₃, 255 (3.53), 287 sh (4.32), 295 (4.34), 334 (3.90), 405 (3.64); +AlCl₃/HCl, 257 (4.10), 287 (4.32), 295 (4.34), 332 (3.87), 405 (3.59); +CH₃COONa, 265 sh (4.20), 284 (4.40), 370 (3.79); +CH₃COONa/H₃BO₃, 265 sh (4.21), 283 (4.39), 370 (3.73)

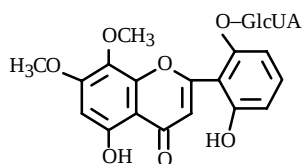
IR: 3400 (OH), 1730 (COOH), 1650 (C=O γ -pyrone), 1600, 1580 (C=C aromatic)

EI-MS m/z (%): 270 (100) $C_{15}H_{10}O_5$, 168 (95) $C_7H_4O_5$

PMR (DMSO- d_6): 3.00-4.20 (sugar protons), 4.82 (1H, d, $J = 7.4$, anomeric proton of glucuronic acid H-1''), 6.30 (1H, s, H-6), 7.01 (1H, s, H-3), 7.58 (3H, m, H-3',4',5'), 8.19 (2H, m, H-2',6'), 12.65 (1H, s, 5-OH)

^{13}C NMR (DMSO- d_6):

C-2	163.4	C-9	149.6	C-6'	126.8
3	104.8	10	103.7	1''	106.4 $J = 162.5$
4	182.0	1'	130.6	2''	73.8
5	157.5	2'	126.8	3''	75.3
6	99.2	3'	129.9	4''	71.5
7	157.6	4'	132.1	5''	76.2
8	125.4	5'	129.2	6''	170.2



5,6'-Dihydroxy-7,8-dimethoxy-2'-O- β -D-glucuronidopyranosylflavone

S. rivularis [110]

$C_{23}H_{22}O_{13}$: 506

mp: 276-277°C (dec.) (MeOH)

$[\alpha]_D^{25} +42.6^\circ$ (c 0.5, pyridine)

UV: 266 (4.34), 310 sh (3.77), 340 (3.71); + CH_3ONa , 265 (4.35), 3.70 (3.90); + $AlCl_3$, 277 (4.34), 297 sh (4.08), 323 (3.81), 404 (3.66); + $AlCl_3/HCl$, 277 (4.33), 297 sh (4.06), 322 sh (3.80), 404 (3.66); + CH_3COONa , 266 (4.43), 310 sh (3.86), 345 (3.84); + H_3BO_3/CH_3COONa , 264 sh (4.45), 347 (3.86)

IR: 3454 (OH), 1736 (COOH), 1662 (C=O γ -pyrone), 1616, 1575 (C=C)

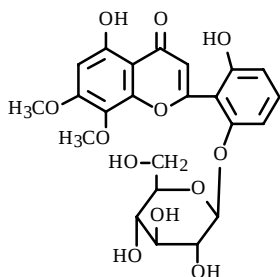
FAB-MS m/z (%): 507 $[M + 1]^+$ (3), 154 $[C_9H_8O_5 - CO - CH_3 + 1]$ (100)

EI-MS m/z (%): 330 $[C_{17}H_{14}O_7$ (aglycone)] (57), 315 [aglycone - CH_3] (100)

PMR (DMSO- d_6): 3.73, 3.92 (3H, d, each $2 \times OCH_3$), 6.32 (1H, s, H-6), 6.61 (1H, s, H-3), 6.68 (1H, d, $J = 8.4$, H-3' or H-5'), 6.73 (1H, d, $J = 8.4$, H-3' or H-5'), 7.31 (1H, t, $J = 8.4$, H-4'), 3.08-3.35 (3H, m, H-2'',3'',4''), 3.90 (1H, d, $J = 9.5$, H-5''), 5.11 (1H, d, $J = 8.0$, H-1''), 10.20 (1H, s, 6'-OH), 12.75 (1H, s, 5-OH)

^{13}C NMR (DMSO- d_6):

C-2	161.5	C-10	104.2	C-2''	72.8
3	112.1	1'	110.1	3''	75.7
4	182.1	2'	156.6	4''	71.1
5	156.6	3'	105.1	5''	75.3
6	95.7	4'	132.1	6''	169.9
7	158.1	5'	109.7	7-OCH ₃	56.4
8	128.3	6'	155.6	8-OCH ₃	61.0
9	149.8	1''	99.6 (d, $J = 162.7$)		



5,6'-Dihydroxy-7,8-dimethoxy-2'-O- β -D-glucopyranosylflavone

S. baicalensis [130]

$C_{23}H_{24}O_{12}$: 492

mp: 238-239°C (dec.) (MeOH) [130]

$[\alpha]_D^{25} -45.2^\circ$ (c 0.02, MeOH)

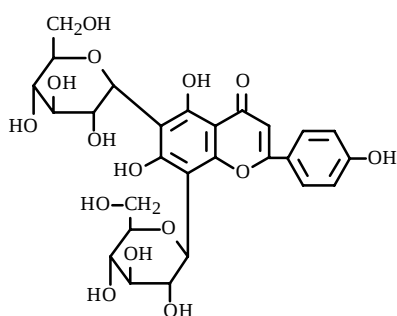
UV: 263 (4.23), 305 sh (3.69), 335 (3.61); + CH_3ONa , 263 (4.20), 365 (3.67); + $AlCl_3$, 273 (4.22), 295 sh (3.93), 321 (3.74), 392 (3.58); + $AlCl_3/HCl$, 255 (4.16), 263 (4.20), 273 (4.22), 295 sh (3.93), 321 (3.73), 392 (3.55)

IR: 3424 (OH), 1658 (C=O γ -pyrone), 1614, 1578 (C=C aromatic)

PMR (DMSO- d_6): 3.71 (1H, s, 8-OCH₃), 3.91 (3H, s, 7-OCH₃), 3.06 (1H, m, H-2''), 3.08 (1H, m, H-4''), 3.19 (1H, m, H-3''), 3.23 (1H, m, H-5''), 3.48 (1H, m, H-6''), 3.68 (1H, br.dd, J = 5.8 and 12.0, H-6''), 4.54 (1H, t, J = 5.8, 6''-OH), 4.91 (1H, d, J = 7.7, H-1''), 6.31 (1H, s, H-3), 6.60 (1H, s, H-6), 6.65 (1H, d, J = 8.4, H-5'), 6.72 (1H, d, J = 8.4, H-3'), 7.29 (1H, t, J = 8.4, H-4'), 10.14 (1H, br.s, 6'-OH), 12.75 (1H, s, 5-OH)

¹³C NMR (DMSO- d_6):

C-2	161.7	C-10	104.2	C-2''	73.1
3	112.2	1'	110.1	3''	76.5
4	182.2	2'	156.6	4''	69.6
5	156.7	3'	105.4	5''	77.1
6	95.8	4'	132.2	6''	60.7
7	158.2	5'	109.5	7-OCH ₃	56.4
8	128.4	6'	156.2	8-OCH ₃	61.1
9	149.9	1''	100.2		



6,8-C-Diglycosideapigenin

S. supina [57]

C₂₇H₃₀O₁₅: 594

mp: 225-227°C

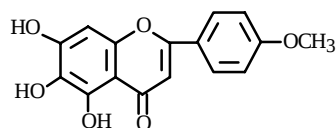
[α]_D²⁰ +54.0° (c 1.0, DMF)

UV: 275, 335; +CH₃COONa, 285, 395; +ZrOCl₂, 290, 395; +NaOH, 285, 410

IR: 3540, 3345 (OH), 1660 (C=O γ-pyrone), 1625, 1580, 1515 (C=C aromatic), 1090, 1040, 1005 (C-O glycosides)

¹³C NMR (DMSO- d_6 —D₂O, 2:1) [38, 40]:

C-2	163.9	C-7	161.4	C-2'	129.0
3	102.6	8	103.7	3'	115.9
4	182.2	9	161.3	4'	158.7
5	155.0	10	105.3	5'	115.9
6	107.6	1'	121.5	6'	129.0



Dinatin (5,6,7-trihydroxy-4'-methoxyflavone)

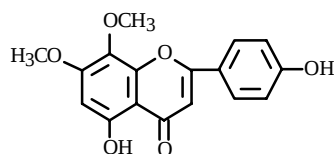
S. ovata [70], *S. przewalskii* [71], *S. sevanensis* [54], *S. ussuriensis* [124]

C₁₆H₁₂O₆: 300

mp: 273-275°C

UV: 275, 325; +CH₃COONa, 270, 360; +C₂H₅ONa, 260, 370; +Zr(NO₃)₂, 290, 360

PMR (CD₃OD): 7.86-7.75 (2H, dd, J = 8, H-2',6'), 6.96-6.85 (2H, dd, J = 8.2, H-3',5'), 6.52 (1H, s, H-8), 6.48 (1H, s, H-3), 3.86 (3H, s, 4'-OCH₃)



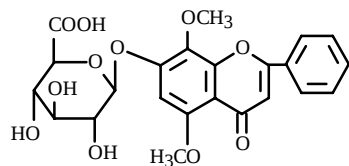
7,8-Dimethoxyisoscutearein

S. sevanensis [54]

C₁₇H₁₄O₆: 314

UV: 280, 335

IR: 3450 (OH), 2930 (OCH₃), 1655 (C=O γ-pyrone), 1618, 1570, 1515 (C=C aromatic)



5,8-Dimethoxy-7-O- β -D-glucuronidopyranosylflavone

S. rivularis [110]

$C_{23}H_{22}O_{11}$: 474

mp: 205°C (MeOH)

$[\alpha]_D^{20}$ -77.7° (c 0.04, MeOH)

UV: 272 (4.37), 332 (3.79); +CH₃ONa, 272 (4.37), 332 (3.79); +AlCl₃, 271 (4.35), 330 (3.82); +CH₃COONa, 271 (4.43), 332 (3.88)

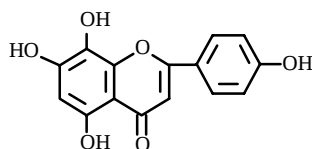
IR: 3424 (OH), 1720 (COOH), 1643 (C=O γ -pyrone), 1601, 1580 (C=C)

FAB-MS m/z (%): 475 [M + 1]⁺ (30), 299 [C₁₇H₁₄O₅ (aglycone) + 1] (100)

PMR (DMSO-d₆): 3.84, 3.91 (3H, s, each 2×OCH₃), 3.40-4.00 (m, sugar protons), 5.40 (1H, d, J = 5.9, H-1''), 6.81 (1H, s, H-3,6), 7.5-7.7 (3H, m, H-3',4',5'), 7.9-8.1 (2H, m, H-2',6')

¹³C NMR (DMSO-d₆):

C-2	159.9	C-10	109.7	C-2''	73.1
3	108.2	1'	131.2	3''	75.5
4	176.1	2'	126.1	4''	71.3
5	155.4	3'	129.4	5''	76.2
6	96.9	4'	131.7	6''	170.2
7	154.1	5'	129.4	5-OCH ₃	56.2
8	131.2	6'	126.1	8-OCH ₃	61.4
9	151.6	1''	100.3 (J = 165.5)		



Isoscutellarein (5,7,8,4'-tetrahydroxyflavone)

S. baicalensis [131], *S. indica* [67], *S. pycnoclada* [57], *S. sevanensis* [54]

$C_{15}H_{10}O_6$: 286

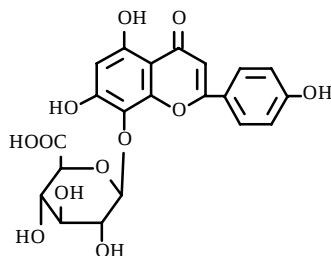
mp: 340-342°C

UV: 282, 308, 328 sh, 366 sh

IR: 1650 (C=O γ -pyrone), 1615, 1590, 1585, 1510 (C=C aromatic) [175]

Mass: 286 [M]⁺ (100), 258, 257, 168 (100), 140 (25), 129 (12), 121 (8), 119 (12), 118 (8), 112 (17), 84 (8), 69 (11). Metastable peaks: 233 (186→268), 116.6 (168→140), 98.6 (286→168), 89.6 (140→112), 63 (112→84) [175]

PMR (CD₃OD): 6.19 (1H, s, H-6), 6.43 (1H, s, H-3), 6.80 (2H, dd, J = 8.5 and 2.5, H-3',5'), 7.80 (2H, dd, J = 8.5 and 2.5, H-2',6') [175]



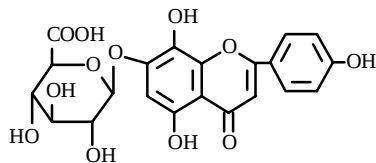
Isoscutellarein 8-O-glucuronide

S. indica [67]

$C_{21}H_{18}O_{12}$: 462

UV: 271, 332; +CH₃ONa, 279, 329 sh, 397; +CH₃COONa, 278, 310 sh, 389; +CH₃COONa/H₃BO₃, 277, 318, 345 sh, 412 sh; +AlCl₃, 277, 306, 346, 386; +AlCl₃/HCl, 278, 305, 345, 386 [178]

IR: 3560 (OH), 1730 (COOH), 1660 (C=O γ -pyrone), 1620, 1575, 1518 (C=C aromatic), 1090, 1050, 1005 (C-O glycosides)



Isoscutellarin (Isoscutellarein 7-O-glucuronide)

S. pycnoclada [57]

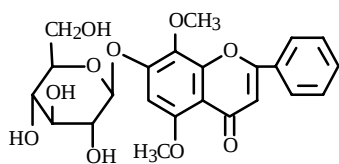
$C_{21}H_{18}O_{12}$: 462

mp: 220°C (dec.)

$[\alpha]_D^{20}$ -152.0° (c 1.0, DMF)

UV: 280, 335; +ZrOCl₂, 365, 430; +NaOH, 400

IR: 3550 (OH), 1730 (COOH), 1665 (C=O γ -pyrone), 1618, 1578, 1515 (C=C aromatic), 1092, 1065, 1005 (C–O glycosides)



Immaculoside (5,8-dimethoxy-7-O- β -D-glucopyranosylflavone)

S. immaculata [186]

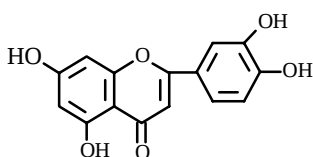
$C_{23}H_{24}O_{10}$: 460

mp: 197-199°C

UV: 270, 331; +CH₃COONa, 271, 332

IR: 3445 (OH), 2930 (OCH₃), 1664 (C=O γ -pyrone), 1619, 1578, 1516 (C=C aromatic), 1072, 1022, 1009 (C–O glycosides)

PMR (Py-d₅): 3.85, 3.92 (3H, s, each 2×OCH₃), 3.38-4.00 (sugar protons), 5.44 (1H, d, J = 6.5, H-1''), 6.72 (1H, s, H-6), 6.81 (1H, s, H-3), 7.52-7.74 (3H, m, H-3',4',5'), 7.92-8.15 (2H, m, H-2',6')



Luteolin (5,7,3',4'-tetrahydroxyflavone)

S. adenostegia [57], *S. adsurgens* [58, 59], *S. araxensis* [78], *S. cretica* [62], *S. discolor* [63], *S. galericulata* [64, 65], *S. grossa* [91], *S. indica* [67], *S. iskanderi* [68], *S. oreophila* [92], *S. ovata* [70], *S. przewalskii* [71], *S. pycnoclada* [57], *S. rivularis* [72], *S. scordiifolia* [74], *S. sevanensis* [54], *S. supina* [57]

$C_{15}H_{10}O_6$: 286

mp: 328-331°C (dec.)

UV: 260, 274 sh, 356; +CH₃COONa, 272, 362; +CH₃COONa/H₃BO₃, 262, 373; +AlCl₃, 275, 406; +AlCl₃/HCl, 274, 388; +CH₃ONa, 271, 404

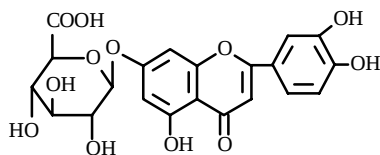
IR: 3450-3300 (OH), 1658 (C=O γ -pyrone), 1612, 1584 (C=C aromatic)

Mass: 286 [M]⁺, 258, 229, 213, 153, 149, 137, 134, 129, 109, 107, 91, 81, 69

PMR (Py-d₅): 6.58 (1H, d, J = 2.0, H-6), 6.67 (1H, d, J = 2.0, H-8), 6.79 (1H, s, H-3), 7.08 (1H, d, J = 8.0, H-5'), 7.51 (br.s, H-2'), 7.56 (dd, J = 2.0 and 8.0, H-6')

¹³C NMR (DMSO-d₆—D₂O, 2:1) [38, 40]:

C-2	165.1	C-7	164.3	C-2'	114.4
3	103.9	8	94.9	3'	146.0
4	182.6	9	158.2	4'	149.8
5	161.6	10	104.8	5'	117.0
6	99.9	1'	123.1	6'	120.1



Luteolin 7-O-glucuronide

S. galericulata [64, 65], *S. iskanderi* [68], *S. przewalskii* [71], *S. pycnoclada* [57], *S. scordiifolia* [74], *S. supina* [57]

$C_{21}H_{18}O_{12}$: 462

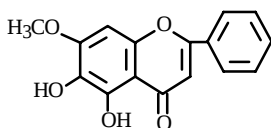
mp: 192-195°C

$[\alpha]_D^{20}$ -98.0° (c 1.0, DMF)

UV: 256 sh, 350; +ZrOCl₂, 415; +NaOH, 400; +CH₃COONa/H₃BO₃, 390

¹³C NMR (DMSO-d₆) [176]:

C-2	165.2	C-8	98.2	C-4'	149.0
3	103.1	9	157.0	5'	116.0
4	182.0	10	105.6	6'	119.5
5	161.0	1'	123.2	COOH	172.5
6	100.2	2'	113.5		
7	163.0	3'	145.5		



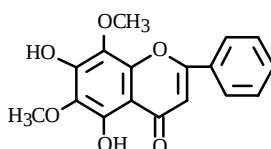
7-Methoxybaicalein (5,6-dihydroxy-7-methoxyflavone)

S. baicalensis [83]

C₁₆H₁₂O₅: 284

UV: 275, 340; +CH₃COONa, 275, 340; +NaOH, 410; +CH₃COONa/H₃BO₃, 275, 340; +ZrOCl₂, 380

IR: 3540-3250 (OH), 1660 (C=O γ-pyrone), 1630, 1580, 1515 (C=C aromatic)



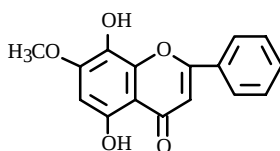
6-Methoxywogonin (5,7-dihydroxy-6,8-dimethoxyflavone)

S. repens [187], *S. sevanensis* [54]

C₁₇H₁₄O₆: 314

UV: 275, 318

IR: 3450 (OH), 2930 (OCH₃), 1660 (C=O γ-pyrone), 1615, 1580 (C=C aromatic)



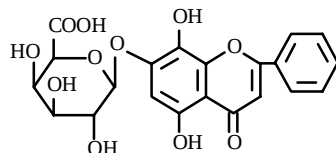
7-Methoxynorwogonin (5,8-dihydroxy-7-methoxyflavone)

S. baicalensis [83], *S. strigillosa* [188]

C₁₆H₁₂O₅: 284

UV: 275, 340; +CH₃COONa, 275, 340; +NaOH, 415; +CH₃COONa/H₃BO₃, 275, 340; +ZrOCl₂, 410

IR: 3450, 3230 (OH), 1655 (C=O γ-pyrone), 1615, 1580, 1525 (C=C aromatic)



Nepetosite A (5,8-dihydroxy-7-O-β-D-galacturonidopyranosylflavone)

S. nepetoides [185]

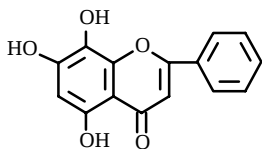
C₂₁H₁₈O₁₁: 446

mp: 204-206°C

UV: 277, 314; +CH₃COONa, 275, 315

IR: 3358 (OH), 1729 (COOH), 1664 (C=O γ-pyrone), 1612, 1575, 1492 (C=C aromatic), 1070, 1038 (C-O glycosides)

PMR (Py-d₅): 4.00-4.70 (3H, m, H-2'',3'',4''), 4.87 (1H, d, J = 8.5, H-5''), 5.95 (1H, d, J = 7.0, H-1''), 6.77 (1H, s, H-6), 6.85 (1H, s, H-3), 7.39 (3H, m, H-3',4',5'), 7.70 (2H, m, H-2',6'), 12.85 (1H, br.s, 5-OH)



Norwogonin (5,7,8-trihydroxyflavone)

S. alpina [60], *S. baicalensis* [83, 184], *S. comosa* [88], *S. discolor* [111], *S. epilobiifolia* [89], *S. grossa* [91], *S. prostrata* [95], *S. ramosissima* [115], *S. scandens* [97], *S. strigillosa* [188], *S. supina* [57], *S. ussuriensis* [124]

$C_{15}H_{10}O_5$: 270

mp: 250-252°C (dec.)

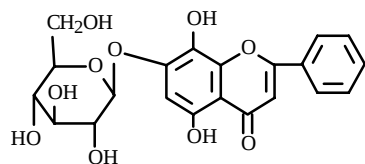
UV: 246, 285, 357 sh; +AlCl₃, 228, 249, 290 sh, 319, 360; +CH₃COONa, 240, 287 sh, 304, 345 sh; +CH₃COONa/H₃BO₃, 292, 412 sh [184]

IR: 3250, 3000 (OH), 1640 (C=O γ -pyrone), 1600 (C=C aromatic)

PMR (DMSO-d₆): 6.95 (1H, s, H-3), 6.31 (1H, s, H-6), 8.13-8.23 (2H, m, H-2',6'), 7.57-7.64 (3H, m, H-3',4',5') [184]

¹³C NMR (DMSO-d₆) [184]:

C-2	163.2	C-7	153.9	C-2'	126.7
3	104.7	8	125.2	3'	129.2
4	182.4	9	153.3	4'	132.1
5	145.8	10	103.7	5'	129.2
6	98.9	1'	131.1	6'	126.7



Norwogonin 7-O- β -D-glucopyranoside

S. discolor [121], *S. baicalensis* [184], *S. immaculata* [186]

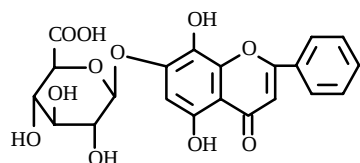
$C_{21}H_{20}O_{10}$: 432

mp: 278-280°C

UV: 279, 350; +CH₃COONa, 280, 351

IR: 3450 (OH), 1660 (C=O γ -pyrone), 1618, 1575, 1517 (C=C aromatic), 1075, 1024, 1005 (C-O glycosides)

PMR (Py-d₅): 3.98-4.74 (sugar protons), 5.62 (1H, d, J = 7.0, H-1''), 6.38 (1H, s, H-6), 6.52 (1H, s, H-3), 7.45-7.62 (3H, m, H-3',4',5'), 7.82-8.00 (2H, m, H-2',6'), 12.78 (1H, br.s, 5-OH) [186]



Norwogonin 7-O-glucuronide (norwogonoside)

S. epilobiifolia [89], *S. grossa* [91], *S. ikonnikovii* [108], *S. nepetoides* [185]

$C_{21}H_{18}O_{11}$: 446

mp: 230-235°C

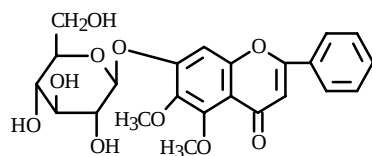
$[\alpha]_D$ -152.0°

UV: 280, 350; +ZrOCl₂, 310, 440; +NaOH, 315, 330

PMR (DMSO-d₆): 5.02 (1H, d, J = 7.3, H-1''), 6.65 (1H, s, H-6), 7.01 (1H, s, H-3), 7.58-7.64 (3H, m, H-3',4',5'), 8.10-8.15 (2H, m, H-2',6'), 12.20 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	163.56	C-9	144.71	C-6'	126.58
3	105.03	10	105.57	1''	101.23
4	182.62	1'	130.91	2''	72.98
5	151.45	2'	126.58	3''	74.63
6	99.16	3'	129.21	4''	71.83
7	152.17	4'	132.18	5''	75.54
8	127.51	5'	129.21	6''	172.01



Ovatin (5,6-dimethoxy-7-O-glucopyranosylflavone)

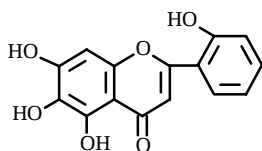
S. ovata [70]

$C_{23}H_{24}O_{10}$: 460

mp: 149°C (dec.)

UV: 310, 265; +AlCl₃, 310, 290 sh, 262; +AlCl₃/HCl, 310, 290 sh, 263; +CH₃ONa, 360, 268, 240 sh

PMR (CD₃OD): 7.88-7.56 (2H, m, H-2',6'), 7.53-7.48 (3H, m, H-3',4',5'), 6.81 (1H, s, H-3), 6.63 (1H, s, H-8), 5.24 (1H, d, J = 7.0, H-1''), 3.91 (3H, s, 5-OCH₃), 3.89 (3H, s, 6-OCH₃), 3.95-4.05 (6H, sugar protons)



2'-Hydroxybaicalein (5,6,7,2'-tetrahydroxyflavone)

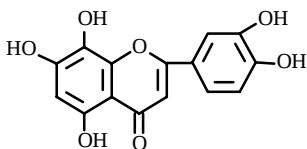
S. sevanensis [54]

$C_{15}H_{10}O_6$: 286

mp: 306°C

UV: 278, 327

IR: 3545-3235 (OH), 1660 (C=O γ -pyrone), 1618, 1578, 1519 (C=C aromatic)



8-Hydroxyluteolin (5,7,8,3',4'-pentahydroxyflavone)

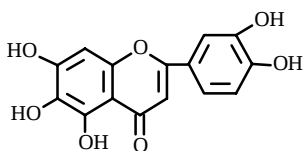
S. sevanensis [54]

$C_{15}H_{10}O_7$: 302

mp: 198-199°C

UV: 235 sh, 248 sh, 280, 354

IR: 3450-3250 (OH), 1660 (C=O γ -pyrone), 1612, 1585, 1514 (C=C aromatic)



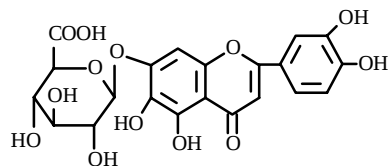
6-Hydroxyluteolin (5,6,7,3',4'-pentahydroxyflavone)

S. galericulata [64, 65], *S. sevanensis* [54]

$C_{15}H_{10}O_7$: 302

UV: 234 sh, 245 sh, 283, 349; +CH₃COONa, 246 sh, 302 sh, 396; +CH₃COONa/H₃BO₃, 253, 289, 368; +AlCl₃, 250 sh, 271, 306, 416; +AlCl₃/HCl, 238 sh, 258, 296, 372; +CH₃ONa, 248, 306 sh, 342, 391

IR: 3440-3210 (OH), 1660 (C=O γ -pyrone), 1615, 1580, 1520 (C=C aromatic)



6-Hydroxyluteolin 7-O-glucuronide

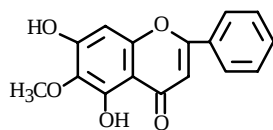
S. galericulata [64, 65]

$C_{21}H_{18}O_{13}$: 478

mp: amorph.

UV: 275, 350

IR: 3540 (OH), 1730 (COOH), 1665 (C=O γ -pyrone), 1620, 1575 (C=C aromatic), 1095, 1020 (C-O glycosides)



Oroxylin A (5,7-dihydroxy-6-methoxyflavone)

S. alpina [60], *S. altissima* [75, 104], *S. amoena* [132], *S. baicalensis* [80, 83, 84, 103], *S. cretica* [62], *S. galericulata* [64, 65], *S. grossa* [91], *S. iskanderi* [68], *S. litwinowii* [76], *S. ocellata* [185], *S. oxystegia* [4], *S. prostrata* [95], *S. ramosissima* [115], *S. rehderiana* [96], *S. scandens* [97], *S. scordifolia* [74], *S. sevanensis* [54], *S. squarrosa* [98], *S. strigillosa* [188], *S. supina* [57], *S. tenax* [99], *S. viscidula* [100]

$C_{16}H_{12}O_5$: 284

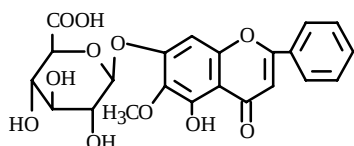
mp: 218-219°C (benzene—hexane)

UV: 270, 320; +CH₃COONa, 375; +NaOH, 377; +CH₃COONa/H₃BO₃, 320; +ZrOCl₂, 367

IR: 3460-3350 (OH), 2930 (OCH₃), 1665 (C=O γ -pyrone), 1615, 1580 (C=C aromatic)

Mass: 284 [M]⁺, 269, 254, 241, 226, 202, 167, 142, 124, 113, 103, 77, 69

PMR (Py-d₅): 3.85 (3H, s, OCH₃), 6.78 (1H, s, H-3), 6.85 (1H, s, H-8), 7.36 (2H, m, H-2',6'), 13.56 (1H, br.s, 5-OH)



Oroxyloside (oroxylin A 7-O-glucuronide)

S. alpina [60], *S. altissima* [64, 65], *S. baicalensis* [79, 101], *S. comosa* [61], *S. cretica* [62], *S. galericulata* [64, 65], *S. grossa* [91], *S. immaculata* [186], *S. iskanderi* [68], *S. litwinowii* [76], *S. prostrata* [95], *S. scordifolia* [74], *S. squarrosa* [98], *S. supina* [57]

$C_{22}H_{20}O_{11}$: 460

mp: 192-194°C

UV: 245 sh (4.03), 272 (4.42), 309 (4.16); +AlCl₃, 250 sh (4.01), 284 (4.40), 333 (4.24); +CH₃COONa (no shifts observed)

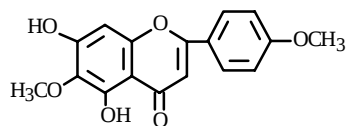
IR: 3456 (OH), 1735 (COOH), 1658 (C=O γ -pyrone), 1612 (C=C aromatic)

FAB-MS *m/z*: 461 [M + H]⁺, 285 [MH - glcUA]⁺

PMR (DMSO-d₆): 3.78 (3H, s, 6-OCH₃), 5.34 (1H, d, J = 7.0, anomeric proton of glucuronic acid H-1''), 7.06 (1H, s, H-3), 7.13 (1H, s, H-8), 7.6 (3H, m, H-3',4',5'), 8.0 (2H, m, H-2',6'), 12.82 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	163.7	C-10	106.1	C-2''	72.8
3	104.9	1'	130.6	3''	75.8
4	182.4	2'	126.4	4''	71.1
5	152.5	3'	129.1	5''	169.9
6	132.6	4'	132.1	6-OCH ₃	60.2
7	156.2	6'	126.4		
9	152.2	1''	99.4		



Pectolinarigenin (5,7-dihydroxy-6,4'-dimethoxyflavone)

S. polyodon [53], *S. przewalskii* [71]

$C_{17}H_{14}O_6$: 314

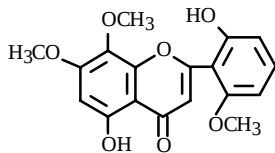
mp: 217-219°C (EtOH)

UV: 275, 331; +CH₃COONa, 276, 295 sh, 367; +CH₃COONa/H₃BO₃, 276, 298 sh, 336; +AlCl₃, 262 sh, 294, 302, 356; +AlCl₃/HCl, 262 sh, 294, 301, 305; +CH₃ONa, 276, 296 sh, 370

IR: 3560-3350 (OH), 2932 (OCH₃), 1658 (C=O γ -pyrone), 1612, 1583 (C=C aromatic)

Mass: 314 [M]⁺, 300, 299, 297, 296, 272, 271, 167, 157, 153, 139, 135, 133, 132 [172]

PMR (DMSO-d₆): 3.77 (3H, s, OCH₃), 3.86 (3H, s, OCH₃), 6.63 (1H, s, H-3), 6.86 (1H, s, H-8), 7.12 (2H, d, J = 9.0, H-3',5'), 8.03 (2H, d, J = 9.0, H-2',6'), 13.00 (1H, s, 5-OH) [172]



Rivularin (5,2'-dihydroxy-7,8,6'-trimethoxyflavone)

S. glabrata [133], *S. indica* [113], *S. ramosissima* [126], *S. rivularis* [72, 116, 117],
S. virularis [134]

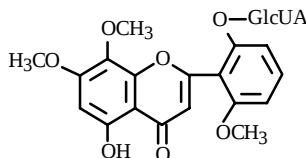
$C_{18}H_{16}O_7$: 344

mp: 259°C

UV: 270, 340

IR: 3530-3350 (OH), 2935 (OCH₃), 1664 (C=O γ -pyrone), 1617, 1583 (C=C aromatic)

Mass: 344 [M]⁺ (73), 329 [M - 15]⁺ (100), 221, 183, 149, 121, 111, 97, 91, 83, 69



Rivularin 2'-O-glucuronide

(5-hydroxy-7,8,6'-trimethoxy-2'-O- β -D-glucuronidopyranosylflavone)

S. rivularis [110]

$C_{24}H_{24}O_{13}$

mp: 186-188°C (dec.) (MeOH)

$[\alpha]_D^{30} +32.7^\circ$ (c 0.2, pyridine)

UV: 266 (4.28), 310 sh (3.69), 340 (3.61); +CH₃ONa, 270 (4.25), 376 (3.79); +AlCl₃, 277 (4.39), 320 sh (3.84), 400 (3.67); +AlCl₃/HCl, 270 (4.38), 320 sh (3.83), 400 (3.68); +CH₃COONa, 265 (4.39), 310 sh (3.83), 340 (3.71); +H₃BO₃/CH₃COONa, 265 (4.38), 310 sh (3.81), 340 (3.71)

IR: 3456 (OH), 1735 (COOH), 1660 (C=O γ -pyrone), 1618, 1588 (C=C aromatic)

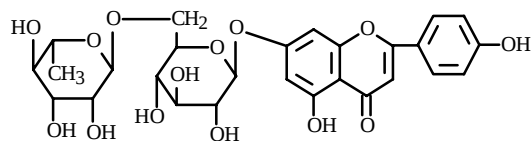
FAB-MS m/z (%): 521 [M + 1]⁺ (22)

EI-MS m/z (%): 344 [$C_{18}H_{16}O_7$ (aglycone)] (54), 329 [aglycone - CH₃] (100), 181 [$C_9H_8O_5$ - CH₃] (26), 153 [$C_9H_8O_5$ - CH₃ - CO] (31)

PMR (DMSO- d_6): 3.70, 3.78, 3.91 (3H, s, each 3 $\times$ OCH₃), 6.32 (1H, s, H-6), 6.61 (1H, s, H-3), 6.88 (1H, d, J = 8.4, H-3' or H-5'), 6.92 (1H, d, J = 8.4, H-3' or H-5'), 7.50 (1H, d, J = 8.4, H-4'), 3.06-3.86 (3H, m, H-2'', 3'', 4''), 3.84 (1H, d, J = 9.1, H-5''), 5.11 (1H, d, J = 7.7, H-1''), 12.69 (1H, s, 5-OH)

¹³C NMR (DMSO- d_6):

C-2	161.0	C-10	104.2	C-2''	72.8
3	112.3	1'	111.3	3''	75.8
4	182.1	2'	155.6	4''	71.3
5	156.7	3'	107.4	5''	75.2
6	95.9	4'	132.7	6''	170.1
7	158.3	5'	105.5	OCH ₃	56.2
8	128.4	6'	158.1	OCH ₃	56.5
9	149.8	1''	99.8	8-OCH ₃	61.1



Roifolin (apigenin 7-O-rutinoside)

S. polyodon [53, 55]

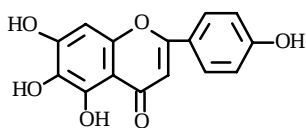
$C_{27}H_{30}O_{14}$: 578

mp: 261-262°C (EtOH)

$[\alpha]_D^{20} -92.0^\circ$ (c 0.1, DMF)

UV: 269, 334

IR: 3550-3340 (OH), 1665 (C=O γ -pyrone), 1615, 1578, 1510 (C=C aromatic), 1092, 1058, 1005 (C-O glycosides)



Scutellarein (5,6,7,4'-tetrahydroxyflavone)

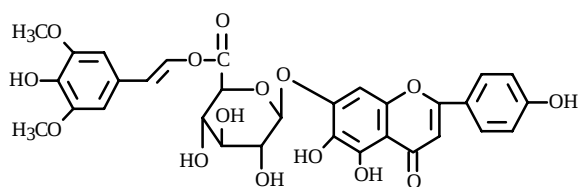
S. adenostegia [57], *S. adsurgens* [59], *S. alpina* [60], *S. altissima* [75, 104], *S. baicalensis* [81], *S. cretica* [62], *S. galericulata* [64, 65], *S. grossa* [91], *S. indica* [67], *S. litwinowii* [76], *S. polyodon* [53, 135], *S. przewalskii* [71], *S. pycnoclada* [57], *S. scordilifolia* [74], *S. sevanensis* [54], *S. supina* [57], *S. tournefortii* [136]

$C_{15}H_{10}O_6$: 286

mp: >340°C

UV: 284, 336; +CH₃COONa, 264 sh, 278, 302, 384; +CH₃COONa/H₃BO₃, 289, 344; +AlCl₃, 304, 375; +AlCl₃/HCl, 302, 361; +CH₃ONa, 279 sh, 308, 334, 384

IR: 3450 (OH), 1665 (C=O γ -pyrone), 1615, 1580, 1515 (C=C aromatic)



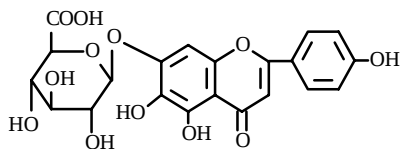
Scutellarein 7-O- β -D-glucuronidesinapoyl

S. polyodon [135]

$C_{31}H_{28}O_{15}$: 640

UV: 285, 336; +CH₃COONa, 286, 338

IR: 3384 (OH), 1740 (C=O ester), 1665 (C=O γ -pyrone), 1615, 1584, 1510 (C=C aromatic), 834 (4'-substituent)



Scutellarin (scutellarein 7-O-glucuronide)

S. adenostegia [57], *S. adsurgens* [59], *S. alpina* [60], *S. altaica* [137], *S. altissima* [75, 104, 105], *S. baicalensis* [107], *S. barbata* [138], *S. columnae* [107], *S. cretica* [62], *S. galericulata* [64, 65], *S. grossa* [91], *S. ikonnikovii* [108], *S.*

ikona [105], *S. indica* [67], *S. karjagii* [69], *S. lateriflora* [105], *S. litwinowii* [76], *S. nepetoides* [185], *S. orientalis* [69], *S. peregrina* [105], *S. polyodon* [53, 135], *S. prilipkoana* [12], *S. przewalskii* [71], *S. pycnoclada* [57], *S. scordiifolia* [74], *S. supina* [57], *S. tournefortii* [136]

$C_{21}H_{18}O_{12}$: 462

mp: 220°C (dec.)

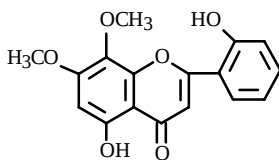
$[\alpha]_D$ -102.0°

UV: 285, 335; +ZrOCl₂, 305, 375; +NaOH, 375

PMR (DMSO-d₆): 5.17 (1H, d, J = 7.3, H-1'), 6.80 (1H, s, H-8), 6.94 (2H, d, J = 8.4, H-3',5'), 6.99 (1H, s, H-3), 7.91 (2H, d, J = 8.4, H-2',6'), 12.73 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆) [108]:

C-2	164.05	C-9	151.06	C-6'	128.29
3	102.35	10	105.80	1''	100.30
4	182.25	1'	121.09	2''	72.79
5	146.74	2'	128.29	3''	75.03
6	130.46	3'	115.92	4''	71.49
7	148.91	4'	161.24	5''	75.36
8	93.77	5'	115.92	6''	170.68



Skullcapflavone I (5,2'-dihydroxy-7,8-dimethoxyflavone)

S. alpina [60], *S. baicalensis* [84], *S. glabrata* [112], *S. prostrata* [95],

S. rivularis [74]

$C_{17}H_{14}O_6$: 314

mp: 259-260°C

UV: 272, 343

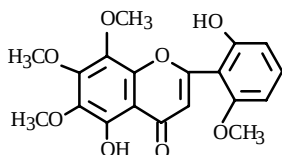
IR: 3500-3350 (OH), 2932 (OCH₃), 1665 (C=O γ -pyrone), 1615, 1583 (C=C aromatic)

Mass: 314 [M]⁺, 299 [M - CH₃]⁺ (100), 271 [M - CH₃ - CO]⁺, 181, 153, 121, 113

PMR (DMSO-d₆): 3.75, 3.84 (3H, s, each 2×OCH₃), 6.56 (1H, s, H-3), 6.97 (1H, s, H-6), 6.87-7.91 (4H, m, H-3',4',5',6'), 12.91 (br.s, 5-OH)

¹³C NMR (DMSO-d₆+D₂O) [170]:

C-2	161.2	C-8	127.8	C-4'	132.3
3	108.6	9	156.1	5'	119.1
4	181.8	10	103.6	6'	128.7
5	148.6	1'	117.1	8-OCH ₃	60.6
6	95.4	2'	156.4	7-OCH ₃	56.1
7	157.9	3'	116.4		



Skullcapflavone II (5,2'-dihydroxy-6,7,8,6'-tetramethoxyflavone)

S. amoena [139], *S. baicalensis* [79-82, 84, 85, 140]

$C_{18}H_{16}O_7$: 344

mp: 180-181°C (ethylacetate)

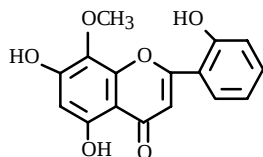
UV: 270 (4.46)

IR: 3200-3100 (OH), 1650 (C=O γ -pyrone), 1600, 1560 (C=C aromatic)

PMR (DMSO-d₆): 3.76, 3.80, 3.82, 4.00 (3H, s, each 4×OCH₃), 6.22 (1H, s, H-3), 6.56 (2H, d, J = 8.0, H-3',5'), 7.24 (1H, t, J = 8.0, H-4'), 10.0 (1H, br.s, 2'-OH), 12.67 (1H, s, 5-OH) [84]

¹³C NMR (DMSO-d₆+D₂O) [170]:

C-2	162.1	C-8	132.2	C-4'	132.2
3	111.7	9	148.2	5'	101.9
4	182.2	10	118.9	6'	158.1
5	146.0	1'	108.6	7,8-OCH ₃	61.4
6	135.5	2'	156.4	6-OCH ₃	60.2
7	152.2	3'	106.1	6'-OCH ₃	55.8



Scutevulin (5,7,2'-trihydroxy-8-methoxyflavone)

S. alpina [60], *S. baicalensis* [127, 141, 181], *S. discolor* [111], *S. indica* [113],

S. prostrata [95], *S. rivularis* [72, 117, 181]

$C_{16}H_{12}O_6$: 300

mp: 278°C (dec.) (MeOH) [181]

UV: 234 sh, 263 sh, 281, 330, 380 sh; +CH₃ONa, 240, 282, 327 sh, 414; +AlCl₃, 256 sh, 284, 296 sh, 359, 400 sh; +AlCl₃/HCl, 255 sh, 285, 296 sh, 356, 410 sh; +CH₃COONa, 266 sh, 284, 410 sh

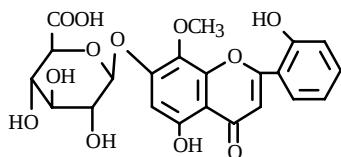
IR: 3350 (OH), 1650 (C=O γ -pyrone), 1600, 1570 (C=C aromatic)

Mass: 300 [M]⁺, 285 [M - CH₃]⁺

PMR (DMSO-d₆): 3.83 (3H, s, OCH₃), 6.30 (1H, s, H-6), 7.08 (1H, s, H-3), 7.87 (1H, dd, J = 7.9 and 1.5, H-6'), 7.43 (1H, br.t, J = 7 and 9, H-4'), 7.00-7.10 (2H, m, H-3',5'), 12.85 (1H, s, 5-OH) [181]

¹³C NMR (DMSO-d₆) [181]:

C-2	161.3	C-8	127.8	C-4'	133.0
3	109.0	9	149.8	5'	119.6
4	182.2	10	103.5	6'	128.3
5	156.3	1'	117.5	8-OCH ₃	61.0
6	99.0	2'	157.1		
7	157.6	3'	117.3		



Scutevulin 7-O-glucuronide

(5,2'-dihydroxy-8-methoxy-7-O-β-D-glucopyranosylflavone)

S. prostrata [95]

C₂₂H₂₀O₁₂: 476

mp: 257-259°C (dec.)

[α]_D³¹ -101° (c 0.04, MeOH)

UV: 275 (4.26), 342 (3.93); +CH₃ONa, 233 sh (4.24), 261 sh (4.19), 272 (4.22), 387 (4.07); +AlCl₃, 284 (4.25), 297 (4.22), 353 (4.00), 382 sh (3.81); +AlCl₃/HCl, 284 (4.26), 298 (4.21), 350 (4.10), 383 sh (3.80); +CH₃COONa, 213 (4.62), 218 sh (4.61), 275 (4.38), 341 (4.04); +CH₃COONa/H₃BO₃, 214 (4.64), 219 sh (4.63), 275 (4.33), 345 (4.00)

IR: 3456 (OH), 1736 (COOH), 1654 (C=O γ-pyrone), 1616 (C=C aromatic)

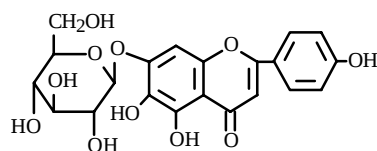
EI-MS *m/z* (%): 300 C₁₆H₁₂O₆ (50), 285 C₁₅H₉O₆ (100)

FAB-MS *m/z* (%): 477 [M + 1]⁺ (35), 301 [C₁₆H₁₂O₆ + 1] (100)

PMR (DMSO-d₆): 3.85 (3H, s, 8-OCH₃), 3.31-3.98 (sugar protons), 5.25 (1H, d, J = 7.3, anomeric proton of glucuronic acid H-1''), 6.69 (1H, s, H-6), 7.14 (1H, s, H-3), 7.04 (1H, br.t, J = 7.4, H-5'), 7.08 (1H, dd, J = 1.5 and 8.1, H-6'), 12.61 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	161.7	C-10	105.1	C-2''	72.9
3	109.0	1'	117.2	3''	75.2
4	182.4	2'	157.1	4''	71.4
5	155.9	3'	117.1	5''	75.9
6	98.4	4'	133.1	6''	170.4
7	155.9	5'	119.6	8-OCH ₃	61.4
8	129.2	6'	128.3		
9	149.2	1''	99.7		



Scutellarein 7-O-β-D-glucopyranoside

S. immaculata [186], *S. indica* [67], *S. przewalskii* [71]

C₂₁H₂₀O₁₁: 448

mp: 194-195°C (dec.) (MeOH)

[α]_D¹⁸ -73.5° (c 0.07, MeOH)

UV: 287 (4.30), 337 (4.40); +CH₃ONa, 314 (4.18), 382 (4.51); +AlCl₃, 292 sh (4.22), 305 (4.33), 370 (4.47); +AlCl₃/HCl, 290 sh (4.23), 303 (4.33), 360 (4.44); +CH₃COONa, 295 (4.20), 350 (4.25), 385 (4.21); +CH₃COONa/H₃BO₃, 295 (4.39), 331 (4.35)

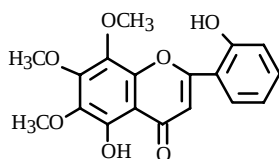
IR: 3350 (OH), 1660 (C=O γ-pyrone), 1605 (C=C aromatic)

Mass: 448 [M]⁺ (tr.), 286 [C₁₅H₁₀O₆] (100), 168 [C₇H₄O₅] (60)

PMR (DMSO-d₆): 5.08 (1H, d, J = 5.9, anomeric proton of glucose H-1''), 6.83 (1H, s, H-3), 6.97 (2H, d, J = 8.8, H-3',5'), 7.04 (1H, s, H-8), 7.95 (2H, d, J = 8.8, H-2',6'), 8.56 (1H, s, 6-OH), 10.40 (1H, s, 4'-OH), 12.75 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	164.3	C-9	151.5	C-6'	128.5
3	102.6	10	106.0	1''	101.2
4	182.6	1'	121.5	2''	73.3
5	146.8	2'	128.5	3''	76.0
6	130.6	3'	116.1	4''	69.8
7	149.2	4'	161.4	5''	77.4
8	94.3	5'	116.1	6''	60.8



Tenaxin I (5,2'-dihydroxy-6,7,8-trimethoxyflavone)

S. baicalensis [184, 127, 142], *S. tenax* [99]

C₁₈H₁₆O₇: 344

mp: 234-235°C (MeO) [184]

UV: 277, 336; +AlCl₃, 250 sh, 285, 358; +CH₃COONa, 276, 418

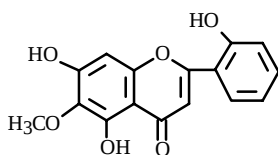
IR: 3300, 3000 (OH), 1640 (C=O γpyrone), 1620, 1590 (C=C aromatic)

Mass: 344 [M]⁺, 118 [C₈H₆O]

PMR (DMSO-d₆): 3.84, 3.91, 4.04 (3H, s, each 3×OCH₃), 7.12 (1H, s, H-3), 7.87 (1H, dd, J = 8.1 and 7.1, H-6'), 6.96-7.12 (2H, m, H-3',5'), 7.36-7.51 (1H, m, H-4'), 12.56 (1H, s, 5-OH) [184]

¹³C NMR (DMSO-d₆) [184]:

C-2	162.1	C-8	132.9	C-4'	133.3
3	108.9	9	148.6	5'	119.7
4	183.0	10	106.3	6'	128.4
5	145.6	1'	117.3	6-OCH ₃	60.6
6	135.9	2'	157.3	7-OCH ₃	61.5
7	152.8	3'	117.3	8-OCH ₃	61.9



Tenaxin II (5,7,2'-trihydroxy-6-methoxyflavone)

S. amoena [139], *S. baicalensis* [127, 184], *S. viscidula* [143]

C₁₆H₁₂O₆: 300

mp: 270-272°C (methanol)

UV: 249, 271, 339; +AlCl₃, 256, 278 sh, 286, 362; +CH₃COONa, 268, 378 [184]

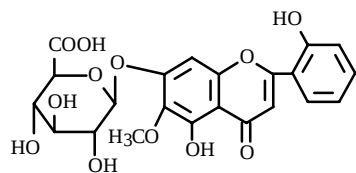
IR: 3500 (OH), 1650 (C=O γpyrone), 1610, 1570 (C=C aromatic)

Mass: 300 [M]⁺, 285 [M - CH₃]⁺, 118 [C₈H₆O]

PMR (DMSO-d₆): 3.78 (3H, s, OCH₃), 7.07 (1H, s, H-3), 6.60 (1H, s, H-8), 7.88 (1H, dd, J = 8.3 and 1.5, H-6'), 6.93-7.11 (2H, m, H-3',5'), 7.33-7.50 (1H, m, H-4'), 13.02 (1H, s, 5-OH) [184]

¹³C NMR (DMSO-d₆) [184]:

C-2	161.5	C-8	94.3	C-4'	132.5
3	108.6	9	152.8	5'	119.5
4	182.5	10	104.2	6'	128.6
5	152.8	1'	117.4	OCH ₃	60.0
6	131.4	2'	156.9		
7	157.7	3'	117.2		



Tenaxin II 7-O-glucuronide

S. baicalensis [144]

$C_{22}H_{20}O_{12}$: 476

mp: 269°C

$[\alpha]_D^{25}$ -68.4° (c 0.07, MeOH)

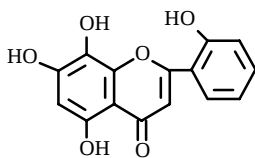
UV: 270 (4.40), 333 (4.21); +CH₃ONa, 275 (4.36), 400 (4.32); +AlCl₃, 275 sh (4.36), 285 (4.42), 358 (4.25); +AlCl₃/HCl, 275 sh (4.36), 284 (4.43), 351 (4.25); +CH₃COONa, 269 (4.34), 300 sh (4.02), 405 (3.90); +CH₃COONa/H₃BO₃, 270 (4.49), 336 (4.34)

IR: 3452 (OH), 1741 (COOH), 1645 (C=O γ -pyrone), 1608 (C=C aromatic)

PMR (DMSO-d₆): 3.77 (3H, s, 6-OCH₃), 7.07 (1H, s, H-8), 7.12 (1H, s, H-3), 7.03 (1H, br.t, J = 8.1, H-5'), 7.07 (1H, br.d, J = 7.7, H-3'), 7.23 (1H, dt, J = 1.5 and 8.1, H-4'), 7.90 (1H, dd, J = 1.5 and 8.1, H-6''), 3.35 (2H, m, H-2'',3''), 3.43 (1H, t, J = 9.5, H-4''), 4.05 (1H, d, J = 9.5, H-5''), 5.33 (1H, d, J = 7.3, H-1''), 5.29 (1H, d, J = 4.7, 3''-OH), 5.57 (1H, d, J = 5.1, 2''-OH), 10.88 (1H, s, 2'-OH), 12.88 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	161.9	C-9	152.4	C-6'	128.5
3	108.8	10	105.9	1''	99.3
4	182.5	1'	117.1	2''	72.8
5	152.5	2'	156.8	3''	75.9
6	132.4	3'	117.1	4''	71.2
7	156.2	4'	133.0	5''	75.4
8	93.9	5'	119.4	6''	170.0
				6-OCH ₃	60.3



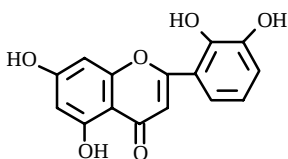
5,7,8,2'-Tetrahydroxyflavone (2'-hydroxynorwogonin)

S. cretica [62], *S. litwinowii* [76]

$C_{15}H_{10}O_6$: 286

UV: 281, 354

IR: 3540, 3250 (OH), 1655 (C=O γ -pyrone), 1610, 1580 (C=C aromatic)



5,7,2',3'-Tetrahydroxyflavone

S. baicalensis [127, 141, 181]

$C_{15}H_{10}O_6$: 286

mp: >360°C (MeOH) [181]

UV: 235 sh, 269, 277 sh, 295 sh, 348; +CH₃ONa, 239 sh, 274, 301 sh, 400; +AlCl₃, 227 sh, 252 sh, 274, 290, 300, 349, 380, 420 sh; +AlCl₃/HCl, 254 sh, 278, 285 sh, 295 sh, 334, 380; +CH₃COONa, 274, 303 sh, 400; +CH₃COONa/H₃BO₃, 269, 297, 378 sh

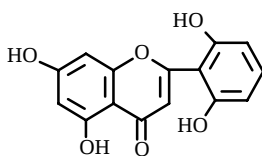
IR: 3350 (OH), 1650 (C=O γ -pyrone), 1610 (C=C aromatic)

Mass: 286 [M]⁺, 134 [C₈H₆O₂]

PMR (DMSO-d₆): 7.06 (1H, s, H-3), 6.23 (1H, d, J = 1.9, H-6), 6.47 (1H, d, J = 1.9, H-8), 7.02 (1H, br.d, J = 7.4, H-4'), 6.83 (1H, br.t, J = 7.4, H-5'), 7.33 (1H, br.d, J = 7.4, H-6'), 12.95 (1H, s, 5-OH) [181]

¹³C NMR (DMSO-d₆) [56, 170]:

C-2	161.9	C-7	164.5	C-2'	145.7
3	109.1	8	93.9	3'	146.1
4	182.1	9	157.7	4'	117.9
5	161.6	10	103.9	5'	119.3
6	98.8	1'	117.9	6'	118.6



5,7,2',6'-Tetrahydroxyflavone

S. baicalensis [103, 127, 128]

C₁₅H₁₀O₆: 286

mp: >360°C (MeOH) [128]

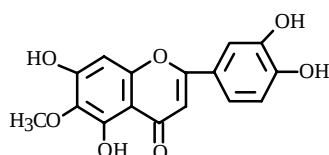
UV: 261, 310; +CH₃COONa, 268, 340; +AlCl₃, 269, 290 sh, 325, 370; +CH₃ONa, 269, 352; +CH₃COONa/H₃BO₃, 261, 310

IR: 3450, 3100 (OH), 1650 (C=O γ-pyrone), 1610, 1580 (C=C aromatic)

PMR (DMSO-d₆): 6.20 (1H, s, H-3), 6.23 (1H, d, J = 2.4, H-6), 6.36 (1H, d, J = 2.4, H-8), 6.43 (2H, d, J = 8.5, H-3',5'), 7.14 (1H, t, J = 8.5, H-4'), 12.90 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	162.5	C-7	164.3	C-2'	156.8
3	108.7	8	94.0	3'	106.9
4	182.0	9	161.8	4'	131.9
5	158.4	10	104.2	5'	106.9
6	98.8	1'	112.1	6'	156.8



5,7,3',4'-Tetrahydroxy-6-methoxyflavone (6-methoxyluteolin)

S. ovata [70]

C₁₆H₁₂O₇: 316

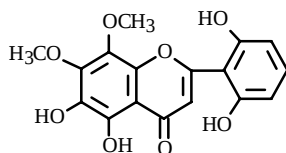
mp: 299°C

UV: 253 (4.23), 272 (4.17), 346 (4.30)

IR: 3410 (OH), 1662 (CO)

Mass: 316 [M]⁺, 302 (8), 301 (50), 299 (4), 288 (25), 297 (2), 287 (2.5), 274 (2.5), 273 (28), 270 (4), 167 (6), 153 (2), 139 (13), 137 (3.5), 135 (10) [172]

PMR (CD₃OD): 7.37-7.32 (2H, m, H-2',6'), 6.94-6.83 (1H, d, J = 9, H-5'), 6.51, 5.87 (1H, s, H-3), 6.43-6.41 (1H, d, J = 2, H-8), 6.21-6.18 (1H, s, J = 2, H-6), 3.88 (3H, s, 6-OCH₃) [70]



5,6,2',6'-Tetrahydroxy-7,8-dimethoxyflavone

S. prostrata [95]

C₁₇H₁₄O₈: 346

mp: 274-275°C (dec.)

UV: 231 sh (4.26), 278 (4.30), 318 sh (3.93), 372 sh (3.47); +CH₃ONa, 245 sh (4.20), 288 (4.03), 349 (3.83), 380 sh (3.70); +AlCl₃, 232 sh (4.31), 295 (4.28), 345 (4.08), 420 (3.45); +AlCl₃/HCl, 292 (4.29), 335 (4.05), 420 (3.41); +CH₃COONa, 278 (4.27), 321 sh (3.89); +CH₃COONa/H₃BO₃, 279 (4.33), 326 (3.73), 387 sh (3.37)

IR: 3388 (OH), 1662 (C=O γ-pyrone), 1626 (C=C aromatic)

EI-MS *m/z* (%): 346 [M]⁺ (80), 331 [M - CH₃]⁺ (100), 197 [C₈H₅O₆] (65)

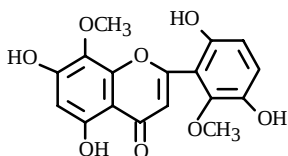
Gives a positive qualitative reaction with SrCl₂

PMR (DMSO-d₆): 3.82, 3.95 (3H, s, each 2×OCH₃), 6.27 (1H, s, H-3), 6.45 (1H, d, J = 8.2, H-3',5'), 7.14 (1H, t, J = 8.2, H-4'),

9.90 (2H, s, 2',6'-OH), 9.05 (1H, s, 6-OH), 12.45 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	162.6	C-8	132.7	C-4''	132.7
3	111.2	9	142.8	5''	106.5
4	182.5	10	106.1	6''	156.5
5	142.9	1'	108.2	OCH ₃	60.8
6	133.8	2'	156.6	OCH ₃	61.6
7	147.9	3'	106.5		



5,7,2',5'-Tetrahydroxy-8,6'-dimethoxyflavone

S. baicalensis [102, 183], *S. viscidula* [143]

C₁₇H₁₄O₈: 346

mp: 255°C (MeOH) [183]

UV: 273 (4.42), 343 (4.17); +AlCl₃, 278 (4.49), 326 (4.22), 378 (4.22); +AlCl₃/HCl, 277 (4.46), 320 (4.20), 370 (4.20); +CH₃COONa, 278 (4.44), 364 (4.19); +CH₃COONa/H₃BO₃, 268 (4.42), 347 (4.15)

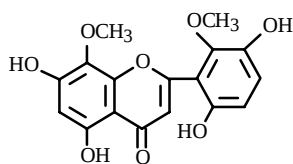
IR: 3250 (OH), 1650 (C=O γ-pyrone), 1610, 1580 (C=C aromatic)

Mass: 346 [M]⁺, 331 [M - CH₃]⁺, 164 [C₉H₈O₃]

PMR (DMSO-d₆): 3.74, 3.77 (3H, s, each 2×OCH₃), 6.31 (1H, s, H-6), 6.35 (1H, s, H-3), 6.60 (1H, d, J = 8.8, H-3'), 6.93 (1H, d, J = 8.8, H-4'), 12.58 (1H, s, 5-OH) [183]

¹³C NMR (DMSO-d₆) [183]:

C-2	162.0	C-7	157.5	C-3'	111.4
3	111.8	8	127.9	4'	120.1
4	182.1	9	148.5	5'	142.7
5	156.6	10	103.9	6'	146.3
6	93.3	1'	115.1	6'-OCH ₃	60.6
		2'	150.7	8-OCH ₃	61.0



5,7,3',6'-Tetrahydroxy-8,2'-dimethoxyflavone (viscidulin III)

S. baicalensis [80-82, 103, 127, 142], *S. rehderiana* [145]

C₁₇H₁₄O₈: 346

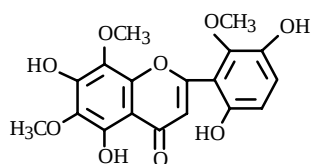
mp: 255-256°C (MeOH)

UV: 264, 338

IR: 3500-3360 (OH), 2934 (OCH₃), 1662 (C=O γ-pyrone), 1614, 1575 (C=C aromatic)

Mass: 346 [M]⁺ (67), 331 [M - CH₃]⁺ (100), 316, 303, 288, 167, 139

PMR (Py-d₅): 3.75 (3H, s, OCH₃), 3.97 (3H, s, OCH₃), 6.66 (1H, s, H-3), 6.76 (1H, s, H-6), 6.84 (1H, d, J = 7.5, H-5'), 7.19 (1H, d, J = 7.5, H-4'), 13.20 (br.s, 5-OH)



5,7,3',6'-Tetrahydroxy-6,8,2'-trimethoxyflavone

S. planipes [125]

C₁₈H₁₆O₉: 376

mp: 243-245°C (dec.) (MeOH)

UV: 267, 311 (4.38, 3.98)

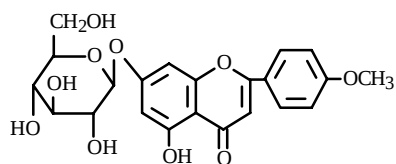
IR: 3360 (OH), 1664 (C=O γ-pyrone), 1626, 1594 (C=C aromatic)

EI-MS m/z (%): 376 $[M]^+$ (89.1), 361 (100), 197 (3.48), 169 (22.8)

PMR (DMSO- d_6) ppm: 3.73 (3H, s, 2'-OCH₃), 3.74 (3H, s, 8-OCH₃), 3.79 (3H, s, 6-OCH₃), 6.27 (1H, s, H-3), 6.57 (1H, d, $J = 8.8$, H-5'), 6.88 (1H, d, $J = 8.8$, H-4')

¹³C NMR (DMSO- d_6):

C-2	161.7	C-8	127.8	C-4'	119.8
3	111.13	9	145.9	5'	111.06
4	182.1	10	103.0	6'	148.3
5	148.2	1'	114.8	6-OCH ₃	60.1
6	131.6	2'	146.3	8-OCH ₃	61.0
7	151.0	3'	142.4	2'-OCH ₃	60.4



Tilianin (5-hydroxy-4'-methoxy-7-O- β -D-glucopyranosylflavone)

S. polyodon [53, 135]

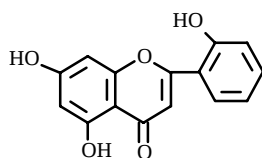
$C_{22}H_{22}O_{10}$: 446

mp: 234-236°C

UV: 270, 325; +CH₃ONa, 290, 370; +CH₃COONa, 278, 342; +CH₃COONa/H₃BO₃,

270, 325; +AlCl₃ and AlCl₃/HCl, 278, 348, 390

PMR (Py- d_5): 7.86 (2H, d, $J = 9$, H-2',6'), 7.04 (2H, d, $J = 9$, H-3',5'), 7.00 (1H, d, $J = 2.5$, H-6), 6.85 (s, H-3), 6.76 (1H, d, $J = 2.5$, H-8), 5.70 (1H, d, $J = 7.0$, H-1''), 3.00-6.00 (6H glucose), 3.75 (s, 4-OCH₃)



5,7,2'-Trihydroxyflavone (2'-hydroxychrysin)

S. adsurgens [59], *S. alpina* [60], *S. baicalensis* [102, 127, 183], *S. prostrata* [95], *S. pycnoclada* [57], *S. sevanensis* [54], *S. tournefortii* [124]

$C_{15}H_{10}O_5$: 270

mp: 284°C (MeOH) [183]

UV: 268 (4.33), 342 (4.04); +AlCl₃, 254 (4.06), 277 (4.34), 287 sh (4.30), 356 (4.12), 390 sh (4.06); +CH₃COONa, 274 (4.39), 325 sh (3.77), 380 (3.95)

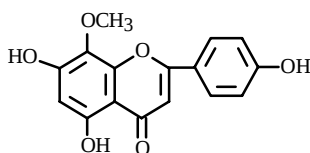
IR: 3350 (OH), 1650 (C=O γ -pyrone), 1610, 1580 (C=C aromatic)

Mass: 270 $[M]^+$, 118 $[C_8H_6O]$

PMR (DMSO- d_6): 6.22 (1H, d, $J = 1.7$, H-6), 6.49 (1H, d, $J = 1.7$, H-8), 6.93-7.49 (3H, m, H-3',4',5'), 7.06 (1H, s, H-3), 7.87 (1H, dd, $J = 7.9$ and 1.5, H-6'), 12.90 (1H, s, 5-OH) [183]

¹³C NMR (DMSO- d_6) [183]:

C-2	161.6	C-7	164.5	C-2'	156.8
3	109.2	8	94.0	3'	117.1
4	182.1	9	157.7	4'	132.9
5	161.6	10	103.9	5'	119.6
6	98.8	1'	117.4	6'	128.7



5,7,4'-Trihydroxy-8-methoxyflavone (4'-hydroxywogonin)

S. alpina [60], *S. baicalensis* [67, 128], *S. discolor* [63, 121], *S. indica* [113], *S. prostrata* [95], *S. rivularis* [72]

$C_{16}H_{12}O_6$: 300

mp: 300-302°C (dec.) (MeOH) [128]

UV: 277, 303 sh, 328, 360 sh; +CH₃COONa, 284, 310 sh, 396; +AlCl₃, 264 sh, 284, 312, 353, 400; +CH₃ONa, 284, 330 sh, 400

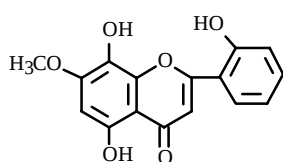
IR: 3430, 3200 (OH), 1660 (C=O γ -pyrone), 1610, 1580 (C=C aromatic)

Mass: 300 [M]⁺ (55.6), 285 (100), 118 (19.4)

PMR (DMSO-d₆): 3.82 (3H, s, OCH₃), 6.20 (1H, s, H-6), 6.68 (1H, s, H-3), 6.87 (2H, d, J = 9, H-3',5'), 7.81 (2H, d, J = 9, H-2',6'), 12.35 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆) [128]:

C-2	163.8	C-8	127.9	C-4'	161.5
3	102.9	9	156.5	5'	116.3
4	182.1	10	103.7	6'	128.5
5	149.7	1'	121.5	OCH ₃	61.1
6	99.1	2'	128.5		
7	157.2	3'	116.3		



5,8,2'-Trihydroxy-7-methoxyflavone

S. baicalensis [128, 129, 191]

C₁₆H₁₂O₆: 300

mp: 270-272°C

UV: 271 (4.39), 338 (4.27); +CH₃ONa, 238 sh (4.49), 272 (4.35), 290 sh (3.97), 4.64 (4.33); +CH₃COONa, 270 (4.41), 340 (4.23); +AlCl₃, 256 (4.14), 280 sh (4.38), 286 (4.41), 360 (4.31); +AlCl₃/HCl, 254 (4.11), 280 sh (4.37), 285 (4.39), 354 (4.28) [191]

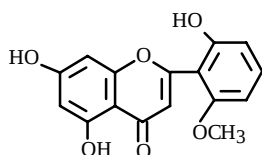
IR: 3450 (OH), 1660 (C=O γ -pyrone)

Mass: 300 [M]⁺, 118 [C₈H₆O]

PMR (DMSO-d₆): 3.82 (3H, s, OCH₃), 6.62 (1H, s, H-6), 7.07 (1H, s, H-3), 7.0-7.9 (4H, m, H-3',4',5',6'), 12.53 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆) [191]:

C-2	161.5	C-8	131.4	C-4'	132.6
3	108.6	9	152.6	5'	119.4
4	182.2	10	104.2	6'	128.5
5	152.6	1'	117.5	OCH ₃	59.9
6	94.2	2'	156.5		
7	157.3	3'	117.0		



5,7,2'-Trihydroxy-6'-methoxyflavone

S. baicalensis [127, 141, 181]

C₁₆H₁₂O₆: 300

mp: 256-257°C (dec.) (MeOH) [181]

UV: 263, 323; +CH₃ONa, 269, 342; +AlCl₃, 269, 293 sh, 321, 372; +AlCl₃/HCl, 270, 291 sh, 318, 372; +CH₃COONa, 269, 340

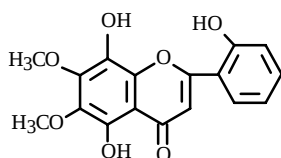
IR: 3350 (OH), 1650 (C=O γ -pyrone), 1610, 1570 (C=C aromatic)

Mass: 300 [M]⁺, 148 [C₉H₈O₂]

PMR (DMSO-d₆): 3.74 (3H, s, OCH₃), 6.19 (1H, s, H-3), 6.20 (1H, d, J = 1.7, H-6), 6.32 (1H, d, J = 1.7, H-8), 6.58 (2H, br.d, J = 8.3, H-3',5'), 7.29 (1H, br.t, J = 8.3, H-4'), 12.75 (1H, s, 5-OH) [181]

¹³C NMR (DMSO-d₆) [181]:

C-2	161.9	C-7	164.5	C-3'	108.8
3	112.1	8	93.9	4'	132.3
4	181.9	9	158.4	5'	102.2
5	161.8	1'	104.0	6'	158.5
6	98.9	2'	156.7	6'-OCH ₃	55.9



5,8,2'-Trihydroxy-6,7-dimethoxyflavone

S. baicalensis [129, 146, 191]

C₁₇H₁₄O₇: 330

mp: 282-283°C

UV: 277 (4.42), 338 (4.19); +CH₃ONa, 238 (4.45), 279 (4.37), 410 (4.30); +CH₃COONa, 276 (4.39), 349 (4.06); +AlCl₃, 257 (4.08), 290 (4.39), 360 (4.24); +AlCl₃/HCl, 255 (4.06), 289 (4.37), 355 (4.21) [191]

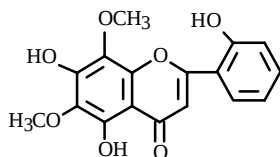
IR: 3350 (OH), 1660 (C=O γ-pyrone)

Mass: 330 [M]⁺, 118 [C₈H₆O]

PMR (DMSO-d₆): 3.83 (3H, s, OCH₃), 3.90 (3H, s, OCH₃), 7.08 (1H, s, H-3), 7.17-7.90 (4H, m, H-3',4',5',6'), 12.76 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆) [191]:

C-2	161.5	C-8	128.2	C-4'	132.6
3	108.7	9	148.2	5'	119.6
4	182.4	10	103.2	6'	128.3
5	145.6	1'	117.8	OCH ₃	61.2
6	131.7	2'	156.7	OCH ₃	60.1
7	150.8	3'	117.3		



5,7,2'-Trihydroxy-6,8-dimethoxyflavone

S. repens [187]

C₁₇H₁₄O₇: 330

mp: 262-263°C (MeOH)

UV: 275 (4.14), 336 (4.18); +CH₃ONa, 278 (4.37), 340 sh (3.82), 409 (4.29); +AlCl₃, 289 (4.41), 358 (4.25), 398 sh (3.89); +AlCl₃/HCl, 288 (4.40), 354 (4.26), 398 sh (3.82); +CH₃COONa, 267 (4.36), 2.78 (4.36), 323 sh (3.92), 380 (4.10); +CH₃COONa/H₃BO₃, 274 (4.37), 338 (4.03)

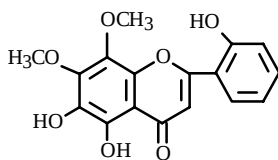
IR: 3456 (OH), 1658 (C=O γ-pyrone), 1610, 1578 (C=C aromatic)

Mass: 330 [M]⁺ (78), 315 [C₁₆H₁₁O₇] (100)

PMR (DMSO-d₆): 3.79 (3H, s, 6-OCH₃), 3.85 (3H, s, 8-OCH₃), 7.04 (1H, br.t, J = 8.0, H-4'), 7.06 (1H, s, H-3), 7.07 (1H, br.d, J = 8.0, H-3'), 7.42 (1H, dt, J = 1.5 and 8.0, H-5'), 7.86 (1H, dd, J = 1.5 and 8.0, H-6'), 10.42, 10.85 (1H, s, each 7,2'-OH), 12.73 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	161.2	C-8	127.9	C-4'	132.9
3	108.6	9	145.6	5'	119.6
4	182.4	10	103.0	6'	128.2
5	148.2	1'	117.4	6-OCH ₃	61.2
6	131.4	2'	156.8	8-OCH ₃	60.2
7	151.0	3'	117.1		



5,6,2'-Trihydroxy-7,8-dimethoxyflavone

S. glabrata [13], *S. grossa* [91], *S. rivularis* [73]

$C_{17}H_{14}O_7$: 330

mp: 249-250°C (MeOH)

UV: 247 sh (3.98), 283 (4.38), 340 (4.16); +CH₃ONa, 258 sh (4.15), 291 (4.27), 305 sh (4.18), 404 (4.17); +AlCl₃, 255 sh (3.99), 294 (4.38), 370 (4.28); +AlCl₃/HCl, 255 (4.01), 292 (4.34), 305 sh (4.23), 360 (4.24); +CH₃COONa, 285 (4.32), 320 sh (4.06), 347 sh (4.01), 410 (3.89); +CH₃COONa/H₃BO₃, 250 sh (4.02), 285 (4.39), 337 (4.14), 390 sh (3.47) [73]

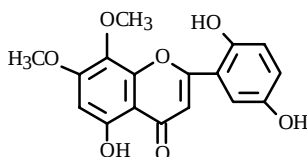
IR: 3468 (OH), 1664 (C=O γ -pyrone), 1612 (C=C aromatic) [73]

EI-MS m/z (%): 330 [M]⁺ (65), 315 [M - CH₃]⁺ (100) [73]

PMR (DMSO-d₆): 3.90, 3.96 (3H each, s, each 2×OCH₃), 7.09 (1H, s, H-3), 7.04 (2H, m, H-3',5'), 7.42 (1H, dt, J = 1.8 and 7.9, H-4'), 7.87 (1H, dd, J = 1.5 and 8.1, H-6'), 9.11 (1H, s, 6-OH), 10.84 (1H, s, 2'-OH), 12.43 (1H, s, 5-OH) [73]

¹³C NMR (DMSO-d₆) [73]:

C-2	161.1	C-8	132.9	C-4'	133.0
3	108.5	9	142.1	5'	119.7
4	182.8	10	106.1	6'	128.3
5	142.4	1'	117.4	OCH ₃	60.9
6	134.1	2'	156.8	OCH ₃	61.8
7	148.2	3'	117.2		



5,2',5'-Trihydroxy-7,8-dimethoxyflavone (rehderianin I)

S. rehderiana [145]

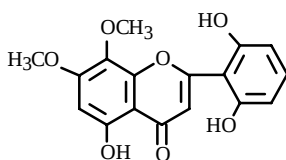
$C_{17}H_{14}O_7$: 330

mp: 265°C (ethylacetate—hexane)

UV: 277 (3.5), 374 (3.1); +CH₃ONa, 270, 350, 420; +AlCl₃, 280, 296 sh, 330 sh, 416; +AlCl₃/HCl, 280, 290 sh, 330 sh, 410; +CH₃COONa, 273, 375; +CH₃COONa/H₃BO₃, 273, 375

Mass: 330 [M]⁺ (56), 315 (100), 287 (5), 181 (35), 165 (7), 158 (14), 153 (27), 125 (8)

PMR (DMSO-d₆): 3.83 (3H, s, OCH₃), 3.89 (3H, s, OCH₃), 6.49 (1H, s, H-6), 6.83-6.87 (2H, m, H-3',4'), 7.11 (1H, s, H-3), 7.30 (1H, d, J = 2, H-6'), 9.09 (1H, s, OH), 12.64 (1H, s, 5-OH)



5,2',6'-Trihydroxy-7,8-dimethoxyflavone (viscidulin II)

S. adenostegia [56], *S. adsurgens* [58, 59], *S. baicalensis* [127, 181], *S. glabrata* [112], *S. indica* [113]

$C_{17}H_{14}O_7$: 330

mp: 286°C (dec.) (MeOH)

UV: 224 sh, 267, 313 sh, 345 sh; +CH₃ONa, 266, 299 sh, 374; +AlCl₃, 227 sh, 275, 300 sh, 330, 375; +AlCl₃/HCl, 227 sh, 275, 300 sh, 330, 375; +CH₃COONa, 265, 293 sh, 345

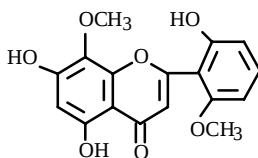
IR: 3500-3380 (OH), 1665 (C=O γ -pyrone), 1615, 1583 (C=C aromatic)

Mass: 330 [M]⁺, 315 [M - CH₃] (100), 138, 134

PMR (DMSO-d₆): 3.73, 3.91 (3H, s, each 2×OCH₃), 6.28 (1H, s, H-3), 6.60 (1H, s, H-6), 6.44 (2H, d, J = 8.0, H-3',5'), 7.14 (1H, t, J = 8.0, H-4'), 12.75 (1H, br.s, 5-OH) [181]

¹³C NMR (DMSO-d₆) [56, 170]:

C-2	162.8	C-8	128.4	C-4'	132.2
3	111.8	9	149.9	5'	106.7
4	182.3	10	104.1	6'	156.9
5	146.0	1'	108.2	8-OCH ₃	61.1
6	95.9	2'	156.9	7-OCH ₃	56.5
7	158.3	3'	106.7		



5,7,2'-Trihydroxy-8,6'-dimethoxyflavone

S. baicalensis [66, 183, 127], *S. discolor* [121]

C₁₇H₁₄O₇: 330

mp: 266°C (MeOH) [183]

UV: 267 (4.69), 350 (4.39); +AlCl₃, 277 (4.68), 298 sh (4.51), 327 (4.42); +CH₃COONa, 276 (4.75), 362 (4.34); +CH₃COONa/H₃BO₃, 270 (4.66), 355 (4.29)

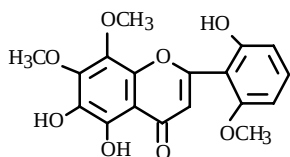
IR: 3500, 3250 (OH), 1650, 1630 (C=O γ-pyrone), 1610, 1570 (C=C aromatic)

Mass: 330 [M]⁺, 315 [M - CH₃]⁺, 148 [C₉H₈O₂]

PMR (DMSO-d₆): 3.78, 3.79 (3H, s, each 2×OCH₃), 6.32 (1H, s, H-6), 6.38 (1H, s, H-3), 6.63 (1H, d, J = 7.8, H-3'), 6.67 (1H, d, J = 8.3, H-5'), 7.34 (1H, dd, J = 7.8 and 8.3, H-4'), 12.61 (1H, s, 5-OH) [183]

¹³C NMR (DMSO-d₆) [183]:

C-2	161.9	C-8	127.8	C-4'	132.6
3	112.2	9	150.8	5'	102.4
4	182.1	10	103.9	6'	158.6
5	156.5	1'	109.3	6'-OCH ₃	56.0
6	99.2	2'	156.9	8-OCH ₃	61.0
7	157.3	3'	109.0		



5,6,2'-Trihydroxy-7,8,6'-trimethoxyflavone (6-hydroxyrivularin)

S. prostrata [95]

C₁₈H₁₆O₈: 360

mp: 224-225°C (dec.)

UV: 277 (4.27), 317 sh (3.88), 368 sh (3.44); +AlCl₃, 293 (4.20), 346 (3.96), 418 sh (3.43); +AlCl₃/HCl, 292 (4.22), 338 (3.96), 430 (3.31); +CH₃COONa, 276 (4.21), 368 sh (3.58); +CH₃COONa/H₃BO₃, 277 (4.30), 368 sh (3.44)

IR: 3384 (OH), 1662 (C=O γ-pyrone), 1622 (C=C aromatic)

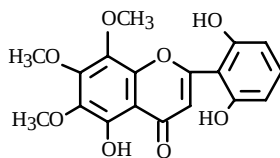
EI-MS *m/z* (%): 360 [M]⁺ (70), 345 [M - CH₃]⁺ (100), 197 [C₈H₅O₆] (50)

Gives a positive qualitative reaction with SrCl₂

PMR (DMSO-d₆): 3.75, 3.80, 3.95 (3H, s, each 3×OCH₃), 6.28 (1H, s, H-3), 6.62 (2H, d, J = 8.2, H-3',5'), 7.32 (1H, t, J = 8.2, H-4'), 9.13 (1H, br.s, 6-OH), 10.13 (1H, s, 2'-OH), 12.40 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	162.0	C-8	132.8	C-4'	132.3
3	111.4	9	142.8	5'	102.2
4	182.4	10	106.1	6'	158.2
5	143.0	1'	109.0	6'-OCH ₃	55.8
6	134.0	2'	156.6	7-OCH ₃	60.9
7	148.0	3'	108.7	8-OCH ₃	61.9



5,2',6'-Trihydroxy-6,7,8-trimethoxyflavone

S. adenostegia [56], *S. alpina* [60], *S. ramosissima* [115]

$C_{18}H_{16}O_8$: 360

mp: 246-247°C (dec.)

UV: 270 (4.34), 315 (3.95), 355 sh (3.91); +CH₃COONa, 240 sh (4.37), 265 (4.29), 360 (4.01); +CH₃ONa, 240 sh (4.37), 265 (4.29), 360 (4.01); +AlCl₃/HCl, 280 (4.30), 295 sh (4.23), 330 (3.97), 406 (3.65); +CH₃COONa, 269 (4.38), 315 (3.99), 355 sh (3.94)

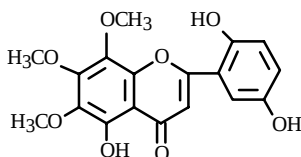
IR: 3250, 3150 (OH), 1665 (C=O γ -pyrone), 1600 (C=C aromatic)

Mass: 360 [M]⁺ (80), 345 [M - CH₃]⁺ (100), 211 [C₉H₇O₆] (40)

PMR (DMSO-d₆): 3.84 (6H, s, 2×OCH₃), 4.02 (3H, s, OCH₃), 6.35 (1H, s, H-3), 6.46 (2H, d, J = 8.0, H-3',5'), 7.16 (1H, t, J = 8.0, H-4'), 9.99 (2H, s, OH-2',6'), 12.73 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆) [60]:

C-2	162.9	C-8	132.8	C-4'	132.3
3	119.9	9	146.5	5'	106.8
4	182.8	10	106.5	6'	157.0
5	146.7	1'	108.2	OCH ₃	60.7
6	135.9	2'	157.0	OCH ₃	61.5
7	152.7	3'	106.8	OCH ₃	61.8



5,2',5'-Trihydroxy-6,7,8-trimethoxyflavone

S. baicalensis [102, 183, 127]

$C_{18}H_{16}O_8$: 360

mp: 268°C (dec.) (MeOH) [183]

UV: 283 (4.39), 376 (4.08); +AlCl₃, 296 (4.41), 334 (4.00), 414 (4.17); +CH₃COONa, 282 (4.37), 382 (4.02); +CH₃COONa/H₃BO₃, 282 (4.39), 380 (4.10)

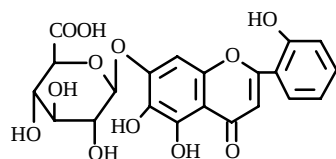
IR: 3400 (OH), 1650, 1635 (C=O), 1590 (C=C aromatic)

Mass: 360 [M]⁺, 345 [M - CH₃]⁺, 134 [C₈H₆O₂]

PMR (DMSO-d₆): 3.82, 3.92, 4.03 (3H, s, each 3×OCH₃), 6.90 (2H, br.s, H-3',4'), 7.19 (1H, s, H-3), 7.33 (1H, br.s, H-6), 12.70 (1H, s, 5-OH) [183]

¹³C NMR (DMSO-d₆) [183]:

C-2	162.0	C-8	132.8	C-4'	120.9
3	108.8	9	145.5	5'	150.1
4	183.0	10	106.3	6'	113.3
5	148.6	1'	118.3	6-OCH ₃	60.6
6	135.9	2'	150.1	7-OCH ₃	61.5
7	152.7	3'	117.0	8-OCH ₃	62.0



5,6,2'-Trihydroxy-7-O-glucuronylflavone (ikonnikoside I)

S. ikonnikovii [108]

$C_{21}H_{18}O_{11}$: 446

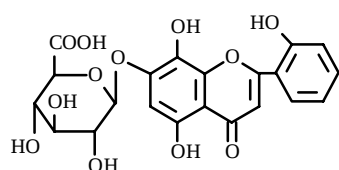
mp: 175-176°C (MeOH)

UV: 275, 330; +CH₃COONa, 275, 334

PMR (DMSO-d₆): 5.15 (1H, d, J = 7.3, anomeric proton of glucuronic acid, H-1''), 6.97, 7.01 (1H, m, H-5'), 6.98 (1H, s, H-8), 7.06 (1H, s, H-3), 7.06 (1H, d, J = 7.7, H-3'), 7.37-7.40 (1H, m, H-4'), 7.85 (1H, dd, J = 6.6 and 1.4, H-6'), 12.65 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	161.69	C-9	151.20	C-6'	128.40
3	108.54	10	105.81	1''	100.06
4	182.45	1'	117.30	2''	72.76
5	146.40	2'	156.63	3''	75.17
6	130.32	3'	117.05	4''	71.34
7	149.20	4'	132.72	5''	75.27
8	93.62	5'	119.32	6''	170.20



5,8,2'-Trihydroxy-7-O-glucuronidopyranosylflavone

S. rivularis [110]

C₂₁H₁₈O₁₂: 462

mp: 174°C (dec.) (MeOH)

[α]_D²⁰ -75.9° (c 0.03, methanol)

UV: 279 (4.20), 336 (3.80); +CH₃ONa, 258 sh (3.92), 286 (4.03), 330 (3.50), 400 (3.83); +AlCl₃, 287 (4.19), 300 (4.18), 355 (3.95), 426 (3.54); +AlCl₃/HCl, 286 (4.20), 298 sh (4.18), 351 (3.94), 426 (3.54); +CH₃COONa, 281 (4.34), 330 (4.07), 400 (3.64); +H₃BO₃/CH₃COONa, 279 (4.35), 336 (3.7)

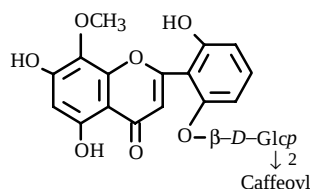
IR: 3426 (OH), 1735 (COOH), 1663 (C=O γ-pyrone), 1620, 1585 (C=C aromatic)

FAB-MS *m/z* (%): 463 [M + 1]⁺ (33), 287 [C₁₅H₁₀O₆ (aglycone) + 1] (100)

PMR (DMSO-d₆): 3.4-4.0 (m, sugar protons), 5.18 (1H, d, J = 6.4, anomeric sugar proton, H-1''), 6.64 (1H, s, H-6), 7.14 (1H, s, H-3), 6.96-7.12 (2H, m, H-3',5'), 7.30 (1H, ddd, J = 7.8, 7.6, and 1.5, H-4'), 7.99 (1H, dd, J = 7.8 and 1.5, H-6'), 8.74, 10.88 (each 1H, br.s, 2×OH), 12.31 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	161.9	C-9	145.2	C-6'	128.9
3	109.2	10	105.5	1''	100.8 (J = 164.7)
4	183.0	1'	117.5	2''	73.1
5	151.2	2'	157.2	3''	75.3
6	98.4	3'	117.4	4''	71.5
7	152.5	4'	133.2	5''	75.6
8	127.2	5'	119.8	6''	170.3



5,7,6'-Trihydroxy-8-methoxy-2'-O-β-D-(2-O-caffeoyl)-glucopyranosylflavone

S. discolor [63]

C₃₁H₂₈O₁₅: 640

UR: 267 (4.23), 305 sh (3.97), 332 (3.99); +CH₃ONa, 277 (4.30), 278 (4.61); +AlCl₃, 275 (4.24), 295 sh (3.98), 325 sh (3.85), 370 (3.99); +AlCl₃/HCl, 257 (4.25), 279 (4.23), 330 (4.00); +CH₃COONa, 276 (4.23), 340 (3.92), 380 sh (3.87); +CH₃COONa/H₃BO₃, 264 (4.25), 305 sh (3.86), 353 (4.00)

IR: 3400 (OH), 1700 (C=O ester), 1650 (C=O γ-pyrone), 1610 (C=C aromatic)

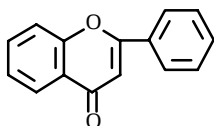
EI-MS *m/z* (%): 316 [C₁₆H₁₂O₇] (65), 301 [C₁₅H₉O₇] (100)

FAB-MS *m/z* (%): 641 [M + 1]⁺ (26), 317 [C₁₆H₁₂O₇ + 1] (75)

PMR (DMSO-d₆): (caffeic acid, c.a.), 3.66 (3H, s, 8-OCH₃), 3.00-4.00 (m, sugar protons), 5.13 (1H, d, J = 8.3, anomeric glucose proton H-1''), 5.94 (1H, d, J = 15.6, c.a. α-H), 5.95 (1H, s, 3-H), 6.28 (1H, s, H-6), 6.65 (1H, d, J = 8.8, c.a. 5-H), 6.72 (2H, d, J = 8.3, H-3',5'), 6.75 (1H, d, J = 8.8, c.a. 6-H), 6.92 (1H, s, c.a. 2+H), 7.10 (1H, d, J = 16.1, c.a. β-H), 7.30 (1H, t, J = 8.3, H-4'), 9.40 (2H, br.s, 2×OH), 10.10, 10.50 (1H, br.s, each 2×OH), 12.63 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

Aglycon		Caffeic acid		Glucose	
C-2	160.6	CO	165.1	C-1	98.4 J = 161.0
3	111.9	C-a	115.0	2	73.7
4	182.0	b	145.2	3	72.9
5	56.4	1	15.7	4	70.0
6	98.4	2	113.4	5	77.3
7	156.8	3	145.8	6	60.5
8	127.5	4	148.2		
9	150.8	5	115.7		
10	104.0	6	121.2		
1'	110.2				
2'	156.2				
3'	105.4				
4'	132.2				
5'	110.0				
6'	156.0				
8-OCH ₃	60.8				



Flavone

C₁₅H₁₀O₂: 222

mp: 95-96°C (hexane)

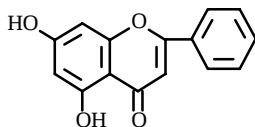
UV: 294, 250, 206

IR: 1644, 1567, 1370

Mass: 222 [M]⁺, 165, 149, 120, 102, 97, 92, 64, 50 [147]

¹³C NMR (CDCl₃) [148]:

C-2	163.0	C-7	133.5	C-2'	126.0
3	107.3	8	117.9	3'	128.8
4	178.0	9	156.0	4'	131.3
5	125.4	10	123.7	5'	128.8
6	124.9	1'	131.5	6'	126.0



Chrysin (5,7-dihydroxyflavone)

S. adenostegia [56], *S. adsurgens* [58, 59], *S. alpina* [60], *S. amoena* [139],

S. araxensis [78], *S. baicalensis* [79-82], *S. comosa* [61], *S. discolor* [63],

S. galericulata [64, 65], *S. glabrata* [112], *S. grossa* [91], *S. indica* [67],

S. orientalis [69], *S. ovata* [70], *S. oxystegia* [4], *S. phyllostachya* [93], *S. polyodon* [53], *S. prostrata* [95], *S. pycnoclada* [57],

S. scandens [97], *S. scordiifolia* [74, 120], *S. sevanensis* [54], *S. squarrosa* [98], *S. strigillosa* [188], *S. supina* [57]

C₁₅H₁₀O₄: 254

mp: 290-292°C

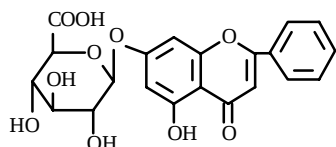
UV: 270, 310 sh; +CH₃COONa, 375; +NaOH, 380; +ZrOCl₂, 290, 340, 390

Mass: 254 [M]⁺, 152, 102

PMR (DMSO-d₆): 6.22 (1H, d, J = 2.0, H-6), 6.52 (1H, d, J = 2.5, H-8), 6.93 (1H, s, H-3), 7.58 (3H, m, H-3',4',5'), 8.30 (2H, m, H-2',6'), 10.90 (1H, s, 7-OH), 12.83 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆) [38]:

C-2	163.4	C-7	164.4	C-2'	128.2
3	103.6	8	94.2	3'	114.6
4	181.1	9	157.5	4'	162.4
5	161.7	10	104.0	5'	114.6
6	99.1	1'	122.9	6'	128.2



Chrysin 7-O-glucuronide

S. adsurgens [59], *S. alpina* [60], *S. comosa* [88], *S. discolor* [63], *S. galericulata* [64, 65, 136], *S. glabrata* [112], *S. grossa* [91], *S. ikonnikovii* [108], *S. immaculata* [186], *S. indica* [67], *S. orientalis* [69], *S. polyodon* [53], *S. prostrata* [95], *S. pycnoclada* [57], *S. ramosissima* [149], *S. scandens* [97], *S. scordiifolia* [74, 120], *S. supina* [57]

C₂₁H₁₈O₁₁: 430

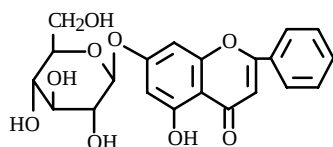
mp: 219-221°C (MeOH)

UV: 270, 305; +CH₃COONa, 268, 308; +AlCl₃, 250, 282, 329, 378

PMR (DMSO-d₆): 5.18 (1H, br.s, H-1''), 6.48 (1H, br.s, H-6), 6.90 (1H, br.s, H-8), 7.06 (1H, s, H-3), 7.50-7.60 (3H, m, H-3',4',5'), 8.00-8.11 (2H, m, H-2',6'), 12.60 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	163.80	C-9	157.20	C-6'	126.58
3	105.54	10	105.71	1''	99.76
4	182.25	1'	130.67	2''	72.93
5	161.18	2'	126.58	3''	74.72
6	99.51	3'	129.25	4''	71.65
7	163.11	4'	132.27	5''	76.14
8	94.94	5'	129.25	6''	171.00



Chrysin 7-O-β-D-glucoside

S. baicalensis [144], *S. orientalis* [69]

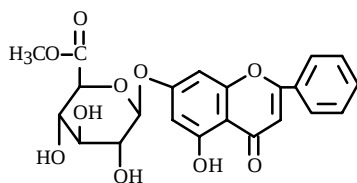
C₂₁H₂₀O₉: 416

mp: 189-192°C

[α]_D -65.7° (c 0.3, formamide)

UV: 269, 306

IR: 3540-3260 (OH), 1660 (C=O γ-pyrone), 1620, 1578, 1512 (C=C aromatic), 1090, 1065, 1005 (C-O glycosides)



Chrysin 7-O-methylglucuronide

S. comosa [61]

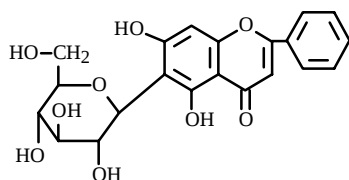
C₂₂H₂₀O₁₀: 444

mp: 184-186°C (MeOH)

UV: 270, 305

IR: 3510-3320 (OH), 1660 (C=O γ-pyrone), 1728 (C=O ester)

PMR (Py-d₅): 3.48 (3H, s, COOCH₃), 4.00-4.67 (3H, m, H-2'',3'',4''), 4.84 (1H, d, J = 8.5, H-5''), 5.88 (1H, d, J = 6.5, H-1''), 6.70 (1H, d, J = 2, H-6), 6.78 (1H, s, H-3), 6.97 (1H, d, J = 2, H-8), 7.15-7.33 (3H, m, H-3',4',5'), 7.51-7.73 (2H, m, H-2',6'), 12.49 (1H, br.s, 5-OH)



Chrysin 6-C- β -D-glucopyranoside

S. baicalensis [144]

$C_{21}H_{20}O_9$: 416

mp: 180°C

$[\alpha]_D^{25} +20.0^\circ$ (c 0.04, methanol)

UV: 247 (4.13), 270 (4.40), 314 (4.00); +CH₃ONa, 262 sh (4.32), 279 (4.37), 370 (3.91); +AlCl₃, 253 (4.11), 283 (4.38), 331 (4.06), 382 (3.76); +AlCl₃/HCl, 253 (4.10), 283 (4.39), 328 (4.03), 382 (3.73); +CH₃COONa, 262 sh (4.32), 278 (4.37), 370 (3.90); +CH₃COONa/H₃BO₃, 262 sh (4.32), 271 (4.38), 328 (3.85)

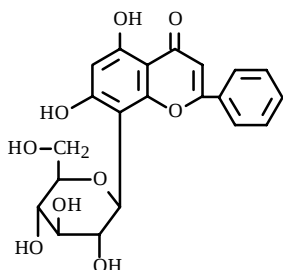
IR: 3404 (OH), 1653 (C=O γ -pyrone), 1620, 1587 (C=C aromatic)

Mass: 416 [M]⁺ (1), 268 [M - 148]⁺ (92), 267 [M - 149]⁺ (100)

PMR (DMSO-d₆): 6.55 (1H, s, H-8), 6.98 (1H, s, H-3), 7.60 (3H, m, H-3',4',5'), 8.18 (2H, br.d, J = 7.0, H-2',6'), 3.19, 3.21, 3.41, 3.47 (1H, m, each H-5'',3'',4'',6''), 3.69 (1H, br.d, J = 11.0, H-6''), 4.05 (1H, br.t, J = 8.7, H-2''), 4.60 (1H, d, J = 9.9, H-1''), 4.62 (1H, t, J = 4.5, 6''-OH), 4.84 (3H, br.s, 2'',3'',4''-OH), 10.75 (1H, br.s, 7-OH), 13.32 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	164.0	C-9	156.4	C-6'	126.4
3	105.1	10	103.5	1''	73.1
4	182.0	1'	130.7	2''	70.6
5	160.7	2'	126.4	3''	78.9
6	109.1	3'	129.2	4''	70.2
7	162.9	4'	132.0	5''	81.6
8	93.8	5'	129.2	6''	61.5



Chrysin 8-C- β -D-glucopyranoside

S. baicalensis [144]

$C_{21}H_{20}O_9$: 416

mp: 206°C

$[\alpha]_D^{25} -25.9^\circ$ (c 0.07, methanol)

UV: 247 (4.10), 270 (4.44), 314 (4.01); +CH₃ONa, 261 sh (4.33), 279 (4.36), 365 (3.96); +AlCl₃, 253 (4.05), 281 (4.41), 330 (4.09), 385 (3.76); +AlCl₃/HCl, 253 (4.04), 281 (4.41), 327 (4.06), 385 (3.79); +CH₃COONa, 261 sh (4.31), 278 (4.42), 365 (3.94); +CH₃COONa/H₃BO₃, 271 (4.42), 320 (3.91)

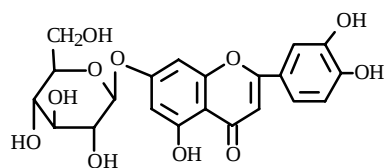
IR: 3468 (OH), 1652 (C=O γ -pyrone), 1616, 1582 (C=C aromatic)

Mass: 416 [M]⁺ (2), 268 [M - 148]⁺ (20), 267 [M - 149]⁺ (100)

PMR (DMSO-d₆): 6.32 (1H, s, H-6), 6.99 (1H, s, H-3), 7.55 (3H, br.t, J = 7.3, H-3',5'), 7.63 (1H, br.t, J = 7.3, H-4'), 8.19 (2H, br.d, J = 7.3, H-2',6'), 3.26, 3.28, 3.41, 3.57 (1H, m, each, H-5'',3'',4'',6''), 3.79 (1H, br.dd, J = 4.5 and 11.2, H-6''), 3.86 (1H, br.t, J = 8.6, H-2''), 4.72 (1H, d, J = 9.9, H-1''), 4.64 (1H, t, J = 4.5, 6''-OH), 4.92 (1H, br.s, 2''-OH), 4.99 (1H, d, J = 3.7, 3''-OH), 5.00 (1H, d, J = 5.1, 4''-OH), 10.95 (1H, br.s, 7-OH), 13.04 (1H, s, 5-OH)

¹³C NMR (DMSO-d₆):

C-2	163.4	C-9	156.2	C-6'	126.9
3	104.7	10	104.3	1''	73.4
4	182.2	1'	131.1	2''	70.8
5	160.4	2'	126.9	3''	78.6
6	98.4	3'	129.0	4''	70.5
7	162.9	4'	132.0	5''	81.9
8	104.8	5'	129.0	6''	61.3



Cinaroside (luteolin-7-O-glucoside)

S. araxensis [78], *S. cretica* [62], *S. ocellata* [185], *S. oreophila* [92],

S. przewalskii [71]

$C_{21}H_{20}O_{11}$: 448

mp: 240-242°C

$[\alpha]_D$ -27.6° (pyridine)

UV: 255, 267 sh, 348; +CH₃COONa, 259, 266 sh, 365 sh, 405; +CH₃COONa/H₃BO₃, 259, 372; +AlCl₃, 274, 298 sh, 329, 432; +AlCl₃/HCl, 273, 294 sh, 358, 387; +CH₃ONa, 263, 300 sh, 394

IR: 3480-3300 (OH), 1665 (C=O γ -pyrone), 1560, 1510 (C=C aromatic), 1095, 1030, 900 (C–O glycosides)

PMR (Py-d₅): 3.90-4.05 (6H, sugar protons), 5.66 (1H, d, J = 7.0, H-1''), 6.67 (1H, d, J = 2.5, H-6), 6.77 (1H, s, H-3), 6.84 (1H, d, J = 2.5, H-8), 7.13 (1H, d, J = 8.0, H-5'), 7.38 (1H, dd, J = 8.0 and 2.5, H-6'), 7.74 (1H, d, J = 2.5, H-2')

¹³C NMR (DMSO-d₆+D₂O, 2:1) [38, 40]:

C-2	164.5	C-7	162.9	C-2'	113.7
3	103.2	8	94.9	3'	145.7
4	181.6	9	156.9	4'	149.7
5	161.1	10	105.5	5'	116.0
6	99.7	1'	121.6	6'	119.0