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

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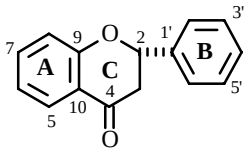
## FLAVANONES AND FLAVANONOLS (DIHYDROFLAVONOLS)

Flavanones, 2-phenylbenzopyran-4-ones, are colorless compounds that contain one asymmetric carbon atom. Flavanone itself has not yet been found in nature. The first representative of this group of natural compounds, 7-hydroxyflavanone, was first observed in plants of the Leguminosae family [6]. Flavanones, isoflavanones, and flavonols can act as intermediates in the synthesis (microbiological transformations) of phenolic compounds [147].




Flavanones that have been described in the literature are OH, $OCH_3$, C–$CH_3$, C–Pr, C–*i*-Pr, and O-glucoside derivatives of 2-phenylbenzopyran-4-one. The substituents were located on the A and B rings. Therefore, the structures of flavanones were established by determining the nature, number, and relative location of the substituents. Both chemical and spectral methods were used to resolve these issues [6, 150, 151].

The absolute configuration of the C-2 chiral center of flavanones was determined mainly by studying circular dichroism spectra [97].

Flavanones are rather widely distributed among plants of the *Scutellaria* genus.

A total of 48 flavanones were isolated from 19 species of skullcap. The simplest representative of this group, 5,7-dihydroxyflavanone or pinocembrin, was found in plants of the *Scutellaria* genus. The next compounds were OH and $OCH_3$ derivatives of flavanone and its glycosides. The sugar component of the glycosides was glucose, rhamnose, and in most instances D-glucuronic acid.

The chemical structures of flavanonols include 3-hydroxyflavanones or dihydroflavonols. They contain two asymmetric carbon atoms and can theoretically have four optical isomers: 2*S*,3*S*, 2*R*,3*R*; 2*R*,3*S*; and 2*S*,3*R*, and two racemates [6, 152].

Flavanonols differed from flavanones by the presence of strong peaks in their mass spectra. It was demonstrated that flavanonols exhibit a base peak for the $[M - 57]^+$ ion whereas a peak for the $[M - 43]^+$ ion was typical of flavanones [153].

The structures and stereochemistry of flavanonols were established using traditional chemical methods [6] and PMR, $^{13}C$ NMR, and circular dichroism [154, 155].

It should be noted that an alcohol solution of flavanonols at room temperature can undergo *cis—trans* epimerization according to the scheme below [156] to form a new isomeric compound.

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*Continued from *Khim. Prir. Soedin.*, No. 4, 358 (2002).

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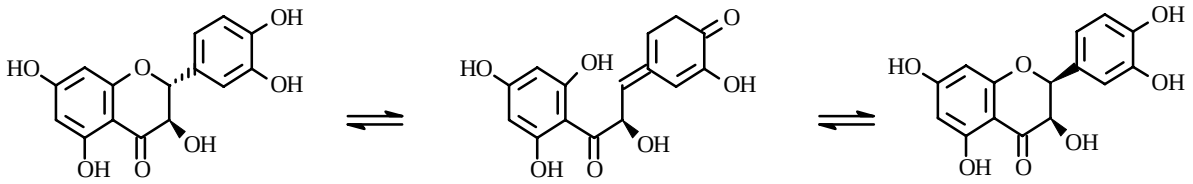
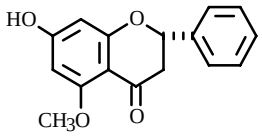
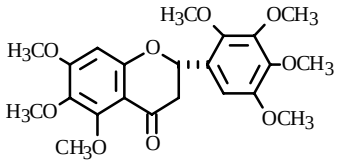



**Alpinetin (7-hydroxy-5-methoxyflavanone)**

*S. indica* [113]
$C_{16}H_{14}O_4$: 270
**mp**: 222°C

**UV**: 286 (4.26)
**IR**: 3540 (OH), 1650 (C=O γ-pyrone), 1585 (C=C aromatic)
**PMR**: (DMSO-$d_6$): 3.75 (3H, s, $OCH_3$), 2.49 (1H, dd, J = 17.1 and 3.2, H-3eq), 3.90 (1H, dd, J = 17.1 and 13.7, H-3ax), 5.92 (1H, dd, J = 13.7 and 3.2, H-2), 6.20 (1H, d, J = 2.5, H-6), 6.42 (1H, d, J = 2.5, H-8), 7.05-7.56 (3H, m, H-3′,4′,5′), 8.27 (2H, d, J = 6.2, H-2′,6′)

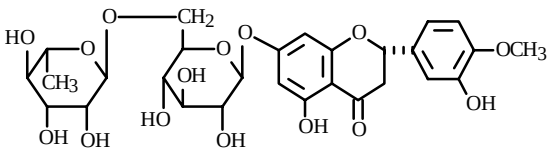



**5,6,7,2′,3′,4′,5′-Heptamethoxyflavanone**

*S. indica* [67]
$C_{22}H_{26}O_9$: 434
**mp**: 108-109°C (dec.) (MeOH)
**UV**: 280 (4.09), 325 (3.52)

**IR**: 1680 (C=O γ-pyrone), 1605 (C=C aromatic)
**Mass**: 434 (40) $[M]^+$, 403 (100) $C_{21}H_{23}O_8$, 224 (90) $C_{12}H_{16}O_4$, 211 (25) $C_{10}H_{11}O_5$, 210 (20) $C_{11}H_{14}O_4$, 209 (40) $C_{11}H_{13}O_4$, 195 (40) $C_9H_7O_5$
**CD** (*c* 0.005, MeOH) $[\theta]^{25}$ (nm): -6986 (275) (negative maximum)
**PMR** (DMSO-$d_6$): 3.70, 3.77, 3.82 (3H, s, each 3×$OCH_3$), 3.80, 3.86 (6H, s, each 4×$OCH_3$), 2.55 (1H, dd, J = 16.3 and 2.4, H-3eq), 3.25 (1H, dd, J = 16.3 and 13.4, H-3ax), 5.69 (1H, dd, J = 13.4 and 2.4, H-2), 6.53 (1H, s, H-8), 7.00 (1H, s, H-2′)
**$^{13}$C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 73.7 | C-10 | 108.8 | $OCH_3$ | 56.3 |
| 3 | 43.9 | 1′ | 126.4 | $OCH_3$ | 56.3 |
| 4 | 188.9 | 2′ | 144.9 | $OCH_3$ | 60.7 |
| 5 | 153.8 | 3′ | 146.7 | $OCH_3$ | 60.9 |
| 6 | 137.2 | 4′ | 143.2 | $OCH_3$ | 60.9 |
| 7 | 159.2 | 5′ | 149.7 | $OCH_3$ | 61.4 |
| 8 | 96.9 | 6′ | 105.8 | $OCH_3$ | 61.6 |
| 9 | 159.7 | | | | |



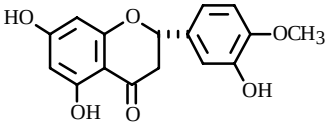

**Hesperidin (hesperitin-7-O-rutinoside)**

*S. baicalensis* [79]
$C_{28}H_{34}O_{15}$: 610
**mp**: 260°C

**UV**: 283, 326; +$CH_3COONa$, 284, 328; +$CH_3COONa/H_3BO_3$, 284, 326; +$AlCl_3$, 308, 383; +$AlCl_3$/HCl, 306, 379

**IR**: 3450 (OH), 1665 (C=O γ-pyrone), 1615, 1572 (C=C aromatic), 1097, 1058, 1025 (C–O glycoside)
$^{13}$**C NMR** (DMSO-$d_6$):

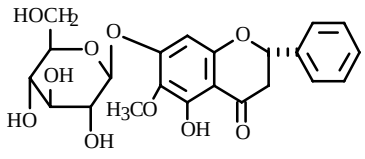
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 78.4 | C-1′ | 131.2 | C-4″ | 69.9 |
| 3 | 42.0 | 2′ | 114.3 | 5″ | 75.8 |
| 4 | 196.7 | 3′ | 146.7 | 6″ | 66.4 |
| 5 | 163.0 | 4′ | 148.1 | 1″ | 100.7 |
| 6 | 96.7 | 5′ | 112.7 | 2″ | 70.6 |
| 7 | 165.2 | 6′ | 117.8 | 3‴ | 71.0 |
| 8 | 95.8 | 1″ | 99.8 | 4‴ | 72.4 |
| 9 | 162.5 | 2″ | 73.3 | 5‴ | 68.6 |
| 10 | 103.5 | 3″ | 76.6 | 6‴ | 18.2 |
| | | | | $OCH_3$ | 56.0 |




**Hesperetin (5,7,3′-trihydroxy-4′-methoxyflavanone)**

*S. baicalensis* [79]
$C_{16}H_{14}O_6$: 302
**mp**: 224°C
**UV**: 289, 330 sh
**IR**: 3380 (OH), 2930 ($OCH_3$), 1660 (C=O γ-pyrone), 1610, 1580 (C=C aromatic)
$^{13}$**C NMR** ($CDCl_3$ + DMSO-$d_6$) [177]:

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 78.61 | C-8 | 95.44 | C-4′ | 147.88 |
| 3 | 42.80 | 9 | 162.93 | 5′ | 111.53 |
| 4 | 195.0 | 10 | 102.20 | 6′ | 117.66 |
| 5 | 163.99 | 1′ | 131.28 | $OCH_3$ | 55.87 |
| 6 | 96.44 | 2′ | 113.64 | | |
| 7 | 166.90 | 3′ | 146.56 | | |

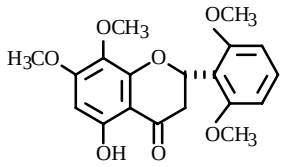



**2(*S*)-5-Hydroxy-6-methoxy-7-O-glucopyranosylflavanone (dihydrooroxylin A-7-O-glucopyranoside)**

*S. baicalensis* [130]
$C_{22}H_{24}O_{10}$: 448
**mp**: 230-231°C (dec.) (MeOH)
$[\alpha]_D^{25}$ -116.5° (*c* 0.02, MeOH)
**UV**: 285 (4.25), 344 (3.50); +$CH_3ONa$, 242 (4.18), 288 (4.17), 3.71 (3.76); +$AlCl_3$, 312 (4.37), 403 (3.43); +$AlCl_3$, 285 sh (3.78), 310 (4.35), 403 (3.51)
**IR**: 3408 (OH), 1648 (C=O γ-pyrone), 1580 (C=C aromatic)
**CD** (*c* 0.006, MeOH) $[\theta]^{25}$ (nm): +7419 (338) (positive maximum), -36310 (286) (negative maximum)
**PMR** (DMSO-$d_6$): 3.68 (3H, s, 6-$OCH_3$), 2.82 (1H, br.dd, J = 3.2 and 17.2, H-3eq), 3.33 (1H, dd, J = 13.4 and 17.2, H-3ax), 5.62 (1H, dd, J = 3.2 and 13.4, H-2), 3.16-3.42 (5H, m, H-2″,3″,4″,5″,6″), 3.66 (1H, br.dd, J = 6.0 and 10.6, H-6″), 4.54 (1H, t, J = 6.0, 6″-OH), 5.01 (1H, d, J = 7.0, H-1″), 6.36 (1H, s, H-8), 7.37-7.46 (3H, m, H-3′,4′,5′), 7.53 (2H, m, H-2′,6′), 11.95 (1H, s, 5-OH)

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

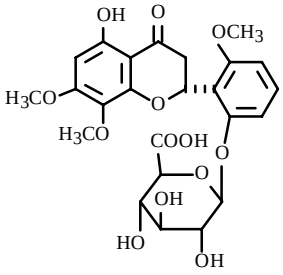
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 78.7 | C-10 | 103.3 | C-2″ | 73.1 |
| 3 | 42.3 | 1′ | 138.5 | 3″ | 76.6 |
| 4 | 197.4 | 2′ | 126.7 | 4″ | 69.5 |
| 5 | 154.5 | 3′ | 128.6 | 5″ | 77.1 |
| 6 | 130.3 | 4′ | 128.7 | 6″ | 60.5 |
| 7 | 158.6 | 5′ | 128.6 | 6-$OCH_3$ | 60.3 |
| 8 | 94.6 | 6′ | 126.7 | | |
| 9 | 157.8 | 1″ | 99.8 | | |



**2(*S*)-5-Hydroxy-7,8,2′,6′-tetramethoxyflavanone**

*S. grossa* [91]
$C_{19}H_{20}O_7$: 360
**mp**: 137°C (MeOH)
**UV**: 286 (3.87), 342 (3.26); +$CH_3ONa$, 286 (3.85), 366 (3.49); +$AlCl_3$, 310 (3.98), 395 (3.27); +$AlCl_3$/HCl, 309 (3.96), 395 (3.27); +$CH_3COONa$, 286 (3.87), 342 (3.26)
**IR**: 3400 (OH), 1638 (C=O γ-pyrone), 1599 (C=C aromatic)
**EI-MS** *m/z* (%): 360 (80) $[M]^+$, 196 (100) $C_9H_8O_5$
**CD** (*c* $8.3\times10^{-5}$) (MeOH) $[\theta]^{31}$ (nm): 5225 (307) (positive maximum), -13933 (279) (negative maximum)
**PMR** (DMSO-$d_6$): 3.52, 3.84 (each 3H, 2×$OCH_3$), 3.78 (6H, s, 2′,6′-$OCH_3$), 2.57 (1H, dd, J = 3.3 and 17.2, H-3eq), 3.80 (1H, dd, J = 13.2 and 17.2, H-3ax), 5.98 (1H, dd, J = 3.3 and 13.2, H-2), 6.22 (1H, s, H-6), 6.74 (2H, d, J = 8.4, H-3′,5′), 7.37 (1H, t, J = 8.4, H-4′), 12.12 (1H, s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 71.1 | C-8 | 128.5 | C-4′ | 131.0 |
| 3 | 39.2 | 9 | 154.3 | 5′ | 104.8 |
| 4 | 197.7 | 10 | 102.1 | 6′ | 158.9 |
| 5 | 159.1 | 1′ | 112.8 | 2′- $OCH_3$ | 56.0 |
| 6 | 92.6 | 2′ | 158.9 | 6′- $OCH_3$ | 56.0 |
| 7 | 160.8 | 3′ | 104.8 | 7-$OCH_3$ | 56.3 |
| | | | | 8-$OCH_3$ | 60.2 |

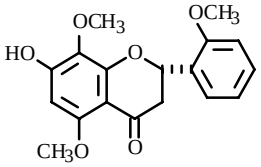


**2(*S*)-5-Hydroxy-7,8,6′-trimethoxy-2′-O-β-D-glucuronylflavanone**

*S. indica* [113]
$C_{24}H_{26}O_{13}$: 522
**mp**: 143°C (dec.)
$[\alpha]_D^{14}$ -71.8° (*c* 0.03, MeOH)
**UV**: 241 sh (3.97), 289 (4.19), 347 (3.55); +$CH_3ONa$, 350 sh (4.14), 287 (4.18), 370 (3.84); +$AlCl_3$, 280 sh (3.72), 3.14 (4.30), 404 (3.58); +$AlCl_3$/HCl, 280 sh (3.74), 312 (4.29), 400 (3.60); +$CH_3COONa$, 289 (4.17), 349 (3.53); +$CH_3COONa/H_3BO_3$, 289 (4.17), 346 (3.54)
**IR**: 3452 (OH), 1740 (COOH), 1637 (C=O γ-pyrone), 1603 (C=C aromatic)
**Mass**: 346 (67) $C_{18}H_{18}O_7$, 328 (50) $C_{18}H_{16}O_6$, 313 (100) $C_{17}H_{13}O_6$
**EI-MS** *m/z* (%): 360 (80) $[M]^+$, 196 (100) $C_9H_8O_5$
**CD** (*c* 0.005, MeOH) $[\theta]^{14}$ (nm): +6812 (309) (positive maximum), -34058 (285) (negative maximum)

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

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 71.5 | C-10 | 102.5 | C-2″ | 73.2 |
| 3 | 39.4 | 1′ | 114.8 | 3″ | 75.7 |
| 4 | 198.2 | 2′ | 156.8 | 4″ | 71.4 |
| 5 | 159.3 | 3′ | 108.6 | 5″ | 75.9 |
| 6 | 92.6 | 4′ | 131.0 | 6″ | 170.3 |
| 7 | 161.1 | 5′ | 106.4 | 6′-$OCH_3$ | 56.2 |
| 8 | 129.2 | 6′ | 159.0 | 7-$OCH_3$ | 56.4 |
| 9 | 154.8 | 1″ | 101.1 | 8-$OCH_3$ | 60.6 |

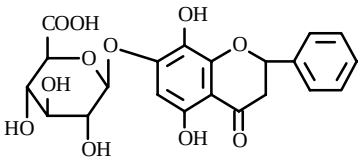


**2(*S*)-7-Hydroxy-5,8,2′-trimethoxyflavanone**

*S. baicalensis* [74], *S. discolor* [111]
$C_{18}H_{18}O_6$: 330
**mp**: 214°C (dec.) (MeOH)

**UV**: 240 sh (4.05), 287 (4.23), 329 (3.89); +$CH_3ONa$, 255 (3.97), 330 (4.42); +$AlCl_3$, 238 (4.24), 287 (4.32), 326 (3.95), 370 sh (3.69); +$AlCl_3$/HCl, 238 sh (4.28), 287 (4.33), 322 (3.99), 370 sh (3.74); +$CH_3COONa$, 254 sh (3.96), 329 (4.39); +$CH_3COONa/H_3BO_3$, 291 (4.08), 329 (4.17)
**IR**: 3150 (OH), 1640 (C=O γ-pyrone), 1580 (C=C aromatic)
**Mass**: 330 (38) $[M]^+$, 196 (100) $C_9H_8O_5$, 181 (47) $C_8H_5O_5$
**CD** (*c* 0.005, MeOH) $[\theta]^{25}$ (nm): +5390 (330) (positive maximum), -26940 (280) (negative maximum)
**PMR** (DMSO-$d_6$): 3.65, 3.73, 3.83 (3H, s, each 3×$OCH_3$), 2.59 (1H, dd, J = 16.4 and 3.4, H-3eq), 2.95 (1H, dd, J = 16.4 and 12.2, H-3ax), 5.68 (1H, dd, J = 12.2 and 3.4, H-2), 6.17 (1H, s, H-6), 6.97-7.12 (1H, m, H-5′), 7.08 (1H, br.s, J = 7.3, H-3′), 7.30 (1H, m, H-4′), 7.55 (1H, br.d, J = 7.3, H-6′), 10.33 (1H, s, 7-OH)
$^{13}$**C NMR** (DMSO-$d_6$) [111]:

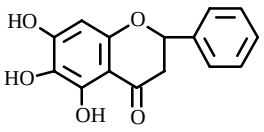
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 73.8 | C-8 | 129.3 | C-4′ | 129.7 |
| 3 | 43.8 | 9 | 156.7 | 5′ | 120.7 |
| 4 | 188.1 | 10 | 104.8 | 6′ | 126.5 |
| 5 | 157.0 | 1′ | 127.1 | 8- $OCH_3$ | 55.6 |
| 6 | 93.5 | 2′ | 156.2 | 5- $OCH_3$ | 55.6 |
| 7 | 157.3 | 3′ | 111.3 | 2′-$OCH_3$ | 60.4 |



**Dihydronorwogonin-7-O-glucoronide**

*S. galericulata* [64, 65]
$C_{21}H_{20}O_{11}$: 448
**mp**: amorph.
$[\alpha]_D^{20}$ -10.0° (EtOH)

**IR**: 3540 (OH), 1735 (COOH), 1665 (C=O γ-pyrone), 1618, 1576, 1572 (C=C aromatic)

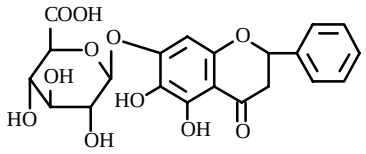


**Dihydrobaicalein (5,6,7-trihydroxyflavanone)**

*S. epilobiifolia* [89], *S. baicalensis* [184],
*S. galericulata* [64, 65], *S. scandens* [97]
$C_{15}H_{12}O_5$: 272

**mp**: 146°C (dec.) (MeOH) [184]
**UV**: 245 sh, 290, 375 sh; +$AlCl_3$, 250 sh, 330, 385 sh; +$CH_3COONa/H_3BO_3$, 250 sh, 305, 370

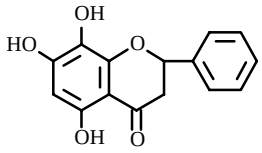
**IR**: 3450 (OH), 1660 (C=O γ-pyrone), 1625 (C=C aromatic)
**Mass**: 272 $[M]^+$, 104 $C_8H_8$ [184]



**Dihydrobaicalin (dihydrobaicalein-7-O-glucoronide)**

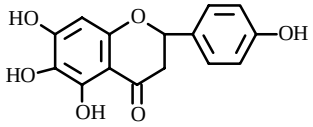
*S. epilobiifolia* [89], *S. baicalensis* [184],
*S. galericulata* [64, 65], *S. scandens* [97]
$C_{21}H_{20}O_{11}$: 448
**mp**: 155-156°C (dec.) (MeOH) [184]
**UV**: 242, 289, 363; +$AlCl_3$, 240 sh, 255 sh, 318, 370; +$CH_3COONa/H_3BO_3$, 253 sh, 288, 380
**IR**: 3450 (OH), 1740 (COOH), 1640 (C=O γ-pyrone), 1610, 1580 (C=C aromatic)
**PMR** (DMSO-$d_6$): 5.54 (1H, dd, J = 12.0 and 3.2, H-2), 2.78 (1H, dd, J = 16.8 and 3.2, H-3eq), 3.21 (1H, dd, J = 16.8 and 12.0, H-3ax), 6.26 (1H, s, H-8), 5.01 (1H, anomeric H), 11.73 (1H, s, 5-OH), 7.37-7.47 (5H, m, H-2′,3′,4′,5′,6′) [184]
$^{13}$**C NMR** (DMSO-$d_6$) [184]:

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 78.7 | C-10 | 103.6 | C-2″ | 72.8 |
| 3 | 42.6 | 1′ | 138.8 | 3″ | 75.1 |
| 4 | 197.7 | 2′ | 126.7 | 4″ | 71.2 |
| 5 | 149.6 | 3′ | 128.6 | 5″ | 75.3 |
| 6 | 128.0 | 4′ | 128.6 | 6″ | 169.3 |
| 7 | 154.5 | 5′ | 128.6 | | |
| 8 | 93.9 | 6′ | 126.7 | | |
| 9 | 153.6 | 1″ | 99.6 | | |



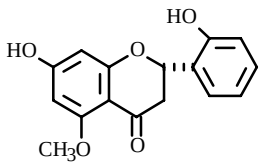
**Dihydronorwogonin (5,7,8-trihydroxyflavanone)**

*S. amoena* [132], *S. galericulata* [64], *S. sevanensis* [54]
$C_{15}H_{12}O_5$: 272
**mp**: amorph.
**UV**: 244 sh, 292, 365
**IR**: 3540 (OH), 1655 (C=O γ-pyrone), 1610, 1585 (C=C aromatic)



**Dihydroscutellarein (carthamidin-5,6,7,4′-tetrahydroxyflavanone)**

*S. adenostegia* [57], *S. baicalensis* [131, 180], *S. pycnoclada* [57],
*S. sevanensis* [54], *S. supina* [57]
$C_{15}H_{12}O_6$: 288
**mp**: 221-223°C
**UV**: 295, 360; +$CH_3COONa$, 270, 330; +$ZrOCl_2$, 275, 320; +NaOH, 320, 325; +$CH_3COONa/H_3BO_3$, 260
**IR**: 3450, 3250 (OH); 1660 (C=O γ-pyrone), 1615, 1582 (C=C aromatic)
**Mass**: 288 (100), 168 (60) $C_7H_4O_5$ [180]

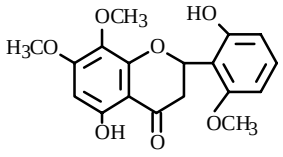


**2(*S*)-7,2′-Dihydroxy-5-methoxyflavanone**

*S. strigillosa* [188]
$C_{16}H_{14}O_5$: 286
**mp**: 133-134°C (dec.)

$[\alpha]_D^{25}$ -65.8° (*c* 0.09, MeOH)
**UV**: 282 (4.40), 315 sh (3.92); +$CH_3ONa$, 318 (4.59); +$AlCl_3$, 282 (4.35); +$AlCl_3$/HCl, 282 (4.35); +$CH_3COONa$, 319 (4.48); +$CH_3COONa/H_3BO_3$, 282 (4.28), 315 sh (4.02)
**IR**: 3290 (OH), 1658 (C=O γ-pyrone), 1612, 1585 (C=C aromatic)
**CD** (*c* $8.3\times10^{-5}$, MeOH) $[\theta]^{25}$ (nm): +13430 (332) (positive maximum), -28170 (279) (negative maximum)
**EI-MS** *m/z* (%): 286 (45) $[M]^+$, 268 (100), 167 (50)
**PMR** (DMSO-$d_6$): 2.57 (1H, dd, J = 3.0 and 16.0, H-3eq), 2.90 (1H, dd, J = 12.6 and 16.0, H-3ax), 5.62 (1H, dd, J = 3.0 and 12.6, H-2), 3.74 (3H, s, 5-$OCH_3$), 6.00 (1H, d, J = 2.0, H-6), 6.08 (1H, d, J = 2.0, H-8), 6.85 (1H, br.t, J = 7.6, H-5′), 6.86 (1H, br.d, J = 7.6, H-3′), 7.17 (1H, dt, J = 1.8 and 7.6, H-4′), 7.40 (1H, dd, J = 1.8 and 7.6, H-6′), 9.76 (1H, s, 2′-OH), 10.54 (1H, s, 7-OH)
**$^{13}$C NMR** (DMSO-$d_6$):

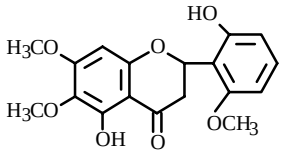
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 73.5 | C-7 | 164.5 | C-2′ | 154.1 |
| 3 | 43.8 | 8 | 95.6 | 3′ | 115.4 |
| 4 | 187.8 | 9 | 164.5 | 4′ | 129.1 |
| 5 | 162.2 | 10 | 104.3 | 5′ | 119.1 |
| 6 | 93.3 | 1′ | 125.2 | 6′ | 126.7 |
| | | | | 5-$OCH_3$ | 55.6 |




**(±)-5,2′-Dihydroxy-7,8,6′-trimethoxyflavanone**

*S. discolor* [111], *S. indica* [113]
$C_{18}H_{18}O_7$: 346
**mp**: 202°C (dec.) (MeOH)
**UV**: 241 sh (3.98), 290 (4.18), 347 (3.65); +$CH_3ONa$, 241 sh (4.27), 292 (4.21), 360 (3.93); +$AlCl_3$, 222 sh (4.45), 315 (4.36), 390 (3.85); +$AlCl_3$/HCl, 223 sh (4.43), 313 sh (4.36), 374 (3.89); +$CH_3COONa$, 290 (4.16), 350 (3.63); +$CH_3COONa/H_3BO_3$, 290 (4.06), 350 (3.48)
**IR**: 3150, 3350 (OH), 1620 (C=O γ-pyrone), 1590 (C=C aromatic)
**Mass**: 346 (63) $[M]^+$, 328 (47) $C_{18}H_{16}O_6$, 313 (100) $C_{17}H_{13}O_6$, 181 (42) $C_8H_5O_5$
**PMR** (DMSO-$d_6$): 3.54, 3.76, 3.85 (3H, s, each 3×$OCH_3$), 2.55 (1H, dd, J = 17.1 and 3.2, H-3eq), 3.90 (1H, dd, J = 17.1 and 13.5, H-3ax), 5.94 (1H, dd, J = 13.5 and 3.2, H-2), 6.22 (1H, s, H-6), 6.55 (2H, br.d, J = 8.3, H-3′,5′), 7.19 (1H, br.t, J = 8.3, H-4′), 9.87 (1H, s, 2′-OH), 12.14 (1H, s, 5-OH) [111]
**$^{13}$C NMR** (DMSO-$d_6$) [113]:

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 71.5 | C-8 | 129.0 | C-4′ | 130.5 |
| 3 | 39.3 | 9 | 154.6 | 5′ | 102.8 |
| 4 | 198.1 | 10 | 102.2 | 6′ | 159.4 |
| 5 | 159.2 | 1′ | 111.5 | $OCH_3$ | 56.2 |
| 6 | 92.6 | 2′ | 157.3 | $OCH_3$ | 56.2 |
| 7 | 160.9 | 3′ | 109.1 | 8-$OCH_3$ | 60.2 |

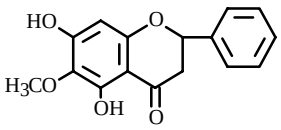



**(±)-5,2′-Dihydroxy-6,7,6′-trimethoxyflavanone**

*S. comosa* [61], *S. discolor* [111], *S. indica* [113]
$C_{18}H_{18}O_7$: 346
**mp**: 221°C (dec.) (MeOH)
**UV**: 240 sh (4.16), 290 (4.24), 346 (3.53); +$CH_3ONa$, 238 sh (4.34), 292 (4.24), 352 (3.71); +$AlCl_3$, 225 sh (4.46), 316 (4.40), 374 (3.82); +$AlCl_3$/HCl, 227 sh (4.47), 315 sh (4.41), 370 (3.85); +$CH_3COONa$, 290 (4.23), 347 (3.54); +$CH_3COONa/H_3BO_3$, 289 (4.11), 345 (3.41)
**IR**: 3200, 3400 (OH), 1630 (C=O γ-pyrone), 1590 (C=C aromatic)

**Mass**: 346 (51) $[M]^+$, 328 (43) $C_{18}H_{16}O_6$, 313 (100) $C_{17}H_{13}O_6$, 181 (63) $C_8H_5O_5$
**PMR** (DMSO-$d_6$): 3.64, 3.75, 3.81 (3H, s, each 3×$OCH_3$), 2.51 (1H, dd, J = 17.1 and 3.2, H-3eq), 3.93 (1H, dd, J = 17.1 and 13.7, H-3ax), 5.95 (1H, dd, J = 13.7 and 3.2, H-2), 6.23 (1H, s, H-8), 6.52 (2H, br.d, J = 8.3, H-3′,5′), 7.17 (1H, br.t, J = 8.3, H-4′), 9.87 (1H, s, 2′-OH), 12.06 (1H, s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$) [113]:

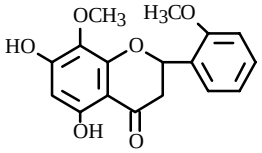
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 71.4 | C-8 | 91.9 | C-4′ | 130.5 |
| 3 | 38.9 | 9 | 154.4 | 5′ | 102.6 |
| 4 | 198.5 | 10 | 102.4 | 6′ | 159.6 |
| 5 | 159.3 | 1′ | 111.2 | $OCH_3$ | 55.7 |
| 6 | 129.5 | 2′ | 157.2 | $OCH_3$ | 56.2 |
| 7 | 160.6 | 3′ | 108.9 | 6-$OCH_3$ | 60.0 |




**Dihydrooroxylin A (5,7-dihydroxy-6-methoxyflavanone)**

*S. baicalensis* [191], *S. scandens* [97]
$C_{16}H_{14}O_5$: 286
**mp**: 165-167°C [191]
**UV**: 294 (4.14), 334 (3.88); +$CH_3COONa$, 295 (4.04), 334 (4.12); +$AlCl_3$, 313 (4.28), 390 (3.39)
**IR**: 3300 (OH), 1630 (C=O γ-pyrone)
**Mass**: 286 $[M]^+$
**CD** (*c* 0.001, $CHCl_3$) [θ] (nm): +17288 (257) (positive maximum), -20062 (296) (negative maximum)
**PMR** ($CDCl_3$): 2.88 (1H, d, J = 5.0, H-3eq), 2.97 (1H, d, J = 11.0, H-3ax), 3.95 (1H, s, $OCH_3$), 5.40 (1H, dd, J = 11.0 and 5.0, H-2), 6.13 (1H, s, H-8), 7.45 (5H, br.s, H-2′,3′,4′,5′,6′), 12.18 (1H, s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 78.1 | C-8 | 94.9 | C-4′ | 128.1 |
| 3 | 42.0 | 9 | 157.5 | 5′ | 128.2 |
| 4 | 196.1 | 10 | 101.7 | 6′ | 126.2 |
| 5 | 154.8 | 1′ | 138.5 | $OCH_3$ | 59.7 |
| 6 | 129.0 | 2′ | 126.2 | | |
| 7 | 159.3 | 3′ | 128.2 | | |

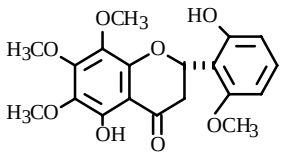



**2(*S*)-5,7-Dihydroxy-8,2′-dimethoxyflavanone**

*S. discolor* [111], *S. indica* [114], *S. strigillosa* [188]
$C_{17}H_{16}O_6$: 316
**mp**: 208°C (dec.) (MeOH)
**UV**: 241 (3.94), 293 (4.29), 342 (3.75); +$CH_3ONa$, 253 sh (3.85), 280 (3.61), 332 (4.49); +$AlCl_3$, 242 sh (4.13), 280 sh (3.84), 317 (4.50), 390 (3.84); +$AlCl_3$/HCl, 242 sh (4.18), 280 sh (3.90), 314 (4.50), 380 (3.86); +$CH_3COONa$, 255 sh (3.84), 280 (3.63), 332 (4.47); +$CH_3COONa/H_3BO_3$, 293 sh (4.07), 333 (4.28)
**IR**: 3150 (OH), 1630 (C=O γ-pyrone), 1600 (C=C aromatic)
**Mass**: 316 (79) $[M]^+$, 182 (100) $C_8H_6O_5$, 167 (53) $C_7H_3O_5$
**CD** (*c* 0.005, MeOH) $[\theta]^{25}$ (nm): +15502 (310) (positive maximum), -59623 (288) (negative maximum)
**PMR** (DMSO-$d_6$): 3.65, 3.83 (3H, s, each 2×$OCH_3$), 2.74 (1H, dd, J = 17.0 and 3.3, H-3eq), 3.22 (1H, dd, J = 17.0 and 12.4, H-3ax), 5.77 (1H, dd, J = 12.4 and 3.3, H-2), 6.00 (1H, s, H-6), 6.98-7.13 (1H, m, H-5′), 7.09 (1H, br.d, J = 7.4, H-3′), 7.32-7.49 (1H, m, H-4′), 7.56 (1H, br.d, J = 7.3, H-6′), 10.68 (1H, s, 7-OH), 11.91 (1H, s, 5-OH)

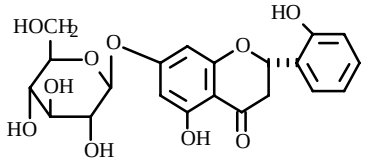
$^{13}$**C NMR** (DMSO-$d_6$) [111]:

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 74.0 | C-8 | 128.7 | C-4′ | 129.9 |
| 3 | 41.1 | 9 | 154.7 | 5′ | 120.7 |
| 4 | 196.6 | 10 | 101.8 | 6′ | 126.8 |
| 5 | 158.8 | 1′ | 126.6 | 2′- $OCH_3$ | 55.7 |
| 6 | 96.0 | 2′ | 156.4 | 8- $OCH_3$ | 60.4 |
| 7 | 160.1 | 3′ | 111.4 | | |



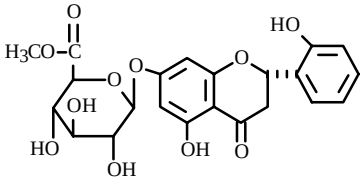
**(-)-5,2′-Dihydroxy-6,7,8,6′-tetramethoxyflavanone**

*S. comosa* [61], *S. oxystegia* [4]
$C_{19}H_{20}O_8$: 376
**mp**: 148-149°C
**UV**: 289, 358; +$AlCl_3$, 316, 372
**IR**: 3450-3260 (OH), 2930 ($OCH_3$), 1662 (C=O γ-pyrone), 1615, 1575 (C=C aromatic)
**Mass**: 376 $[M]^+$, 358 [M - $H_2O$], 343 [M - $H_2O$ - $CH_3$], 315, 226 $[a]^+$, 211, 183, 131, 119, 83, 69 (100)
**PMR** ($CDCl_3$): 2.73 (1H, dd, J = 3.1 and 17.5, H-3eq), 3.17 (1H, dd, J = 13.5 and 17.5, H-3ax), 3.71, 3.74, 3.87, and 4.03 (3H, s, each 4×$OCH_3$), 6.01 (1H, d, J = 3.1 and 13.5, H-2), 6.36 (br.d, J = 8.2, H-5′), 6.50 (br.d, J = 7.8, H-3′), 7.10 (1H, dd, J = 7.8 and 8.2, H-4′), 11.82 (1H, br.s, 5-OH) [61]



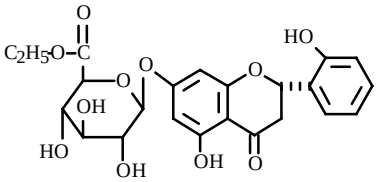
**2(*S*)-5,2′-Dihydroxy-7-O-β-D-glucopyranosylflavanone**

*S. ramosissima* [115]
$C_{21}H_{22}O_{10}$: 434
**mp**: 209-210°C
**UV**: 289, 330; +$CH_3COONa$, 288, 332
**Mass** (hexaacetate), *m/z*: 686 $[M]^+$, 644, 331, 284, 271, 169
**PMR** (Py-$d_5$): 2.78-3.13 (2H, m, 2H-3), 3.75-4.56 (sugar protons), 5.37 (1H, d, J = 7.0, H-1″), 6.15 (1H, dd, J = 7.0 and 10.0, H-2), 6.25 (1H, d, J = 2.0, H-6), 6.33 (1H, d, J = 2.0, H-8), 6.98 (1H, dd, J = 7.5 and 7.5, H-5′), 7.08 (1H, dd, J = 7.5 and 2.0, H-3′), 7.19 (1H, ddd, J = 7.5, 7.5, and 2.0, H-4′), 7.62 (1H, dd, J = 7.5 and 2.0, H-6′), 12.75 (1H, br.s, 5-OH)



**2(*S*)-5,2′-Dihydroxy-7-O-β-D-methylglucuronidopyranosylflavanone**

*S. ramosissima* [149]
$C_{22}H_{22}O_{11}$: 462
**mp**: 141-142°C (MeOH)
$[\alpha]_D$ -98.0° (*c* 0.62, DMF)
**UV**: 213 (3.99), 225.5 (3.86), 284 (3.81), 331 (3.19)
**IR**: 3480-3330 (OH), 1724 (C=O ester), 1643 (C=O γ-pyrone), 1620, 1580 (C=C), 1097, 1057, 1045, 1026 (C–O glycoside)
**Mass**: 462 (8) $[M]^+$, 444 (4) [M - $H_2O$], 273 (33), 272 (76), 255 (43), 254 (100) [272 - $H_2O$], 253 (79), 153 (83), 152 (16), 120 (12)
**PMR** (Py-$d_5$): 2.82-3.26 (m, 2H-3), 3.48 (3H, s, $OCH_3$), 4.05-4.50 (3H, m, H-2″,3″,4″), 4.65 (1H, d, J = 8.5, H-5″), 5.72 (1H, d, J = 6.5, H-1″), 5.92 (1H, dd, J = 5.3 and 10.0, H-2), 6.43 (1H, s, H-6), 6.43 (1H, s, H-8), 6.83 (1H, dd, J = 7.5 and 7.3, H-5′), 6.93 (1H, d, J = 7.3, H-3′), 7.12 (1H, dd, J = 7.5 and 7.3, H-4′), 7.51 (1H, d, J = 7.3, H-6′), 12.32 (1H, br.s, 5-OH)

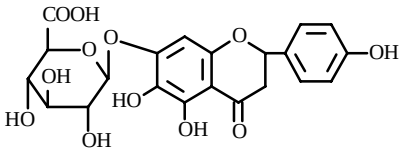


**2(*S*)-5,2′-Dihydroxy-7-O-$\beta$-D-ethylglucuronidopyranosylflavanone**

*S. ramosissima* [149]
$C_{23}H_{24}O_{11}$: 476
**mp**: 130-132°C (MeOH)
$[\alpha]_D$ -115.8° (*c* 0.48, MeOH)

**UV**: 211.5 (4.39), 224 sh (4.25), 283 (4.22), 330 sh (3.59)
**IR**: 3560-3220 (OH), 1740 (C=O ester), 1650 (C=O $\gamma$-pyrone), 1635, 1587, 1510 (C=C), 1100, 1078, 1050 (C–O glucoside)
**Mass**: 476 (3) $[M]^+$, 458 (3.5) [M - $H_2O$], 273 (24), 272 (64), 255 (58), 254 (100) [272 - $H_2O$], 253 (69), 226 (8), 153 (92), 152 (28), 120 (17)
**PMR** (Py-$d_5$): 0.92 (3H, t, J = 7.0, -$CH_3$), 2.75-3.27 (m, 2H-3), 3.97 (2H, q, J = 7.0, $CH_2$), 4.10-4.50 (3H, m, H-2″,3″,4″), 4.61 (1H, d, J = 8.7, H-5″), 5.69 (1H, d, J = 6.5, H-1″), 5.90 (1H, dd, J = 5.5 and 10.0, H-2), 6.42 (1H, s, H-6), 6.42 (1H, s, H-8), 6.82 (1H, dd, J = 7.5 and 7.5, H-5′), 6.92 (1H, d, J = 7.4, H-3′), 7.10 (1H, dd, J = 7.5 and 7.4, H-4′), 7.49 (1H, d, J = 7.5, H-6′), 12.30 (1H, br.s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 74.6 | C-10 | 103.9 | C-2″ | 73.1 |
| 3 | 41.3 | 1′ | 124.9 | 3″ | 75.6 |
| 4 | 197.8 | 2′ | 154.9 | 4″ | 71.7 |
| 5 | 163.6 | 3′ | 116.0 | 5″ | 75.6 |
| 6 | 97.0 | 4′ | 130.2 | 6″ | 169.3 |
| 7 | 165.3 | 5′ | 119.9 | $OCH_2$ | 61.4 |
| 8 | 95.7 | 6′ | 127.6 | $CH_3$ | 14.5 |
| 9 | 163.6 | 1″ | 99.5 | | |

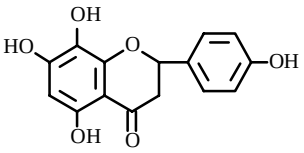


**Isocarthamidin-7-O-glucuronide (dihydroscutellarein-7-O-glucuronide)**

*S. adenostegia* [57], *S. baicalensis* [180], *S. rivularis* [110, 157], *S. supina* [57]
$C_{21}H_{20}O_{12}$: 464
**mp**: 201°C (dec.) (MeOH + $H_2O$) [180]
$[\alpha]_D^{15}$ -98.0° (*c* 0.08, MeOH)

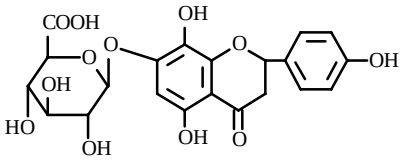
**UV**: 248 sh (4.08), 286 (4.13), 362 (3.60); +$CH_3ONa$, 246 (4.17), 288 (3.96), 388 (4.15); +$AlCl_3$, 255 sh (3.85), 314 (4.32), 423 (3.67); +$AlCl_3$/HCl, 255 sh (3.93), 313 (4.29), 414 (3.66); +$CH_3COONa$, 297 (4.98), 344 (4.11); +$CH_3COONa/H_3BO_3$, 247 sh (4.19), 285 (4.21), 366 (3.64)
**IR**: 3376 (OH), 1737 (COOH), 1662 (C=O $\gamma$-pyrone), 1622, 1598 (C=C aromatic)
**CD** (*c* 0.0001, MeOH) $[\theta]^{15}$ (nm): +1853 (335) (positive maximum), -27791 (284) (negative maximum)
**PMR** (DMSO-$d_6$): 2.71 (1H, br.d, J = 16.9, H-3eq), 3.40 (m, H-3ax), 5.50 (1H, br.d, J = 10.0, H-2), 3.3-4.1 (m, sugar protons), 5.16 (1H, br.s, glucuronic acid anomeric proton), 6.81 (2H, d, J = 8.0, H-3′,5′), 7.35 (2H, d, J = 8.0, H-2′,6′), 6.36 (1H, s, H-8), 11.85 (1H, s, 5-OH) [180]
$^{13}$**C NMR** (DMSO-$d_6$) [180]:

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 78.8 | C-9 | 154.8 | C-6′ | 128.5 |
| 3 | 42.5 | 10 | 103.6 | 1″ | 99.9 |
| 4 | 198.3 | 1′ | 129.1 | 2″ | 72.9 |
| 5 | 153.2 | 2′ | 128.5 | 3″ | 75.2 |
| 6 | 128.1 | 3′ | 115.3 | 4″ | 71.4 |
| 7 | 149.7 | 4′ | 157.9 | 5″ | 75.4 |
| 8 | 94.2 | 5′ | 115.3 | 6″ | 170.2 |



**Carthamidin (5,7,8,4′-tetrahydroxyflavanone, dihydroisoscutellarein)**

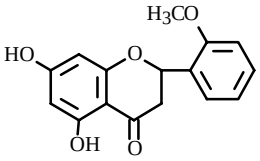
*S. baicalensis* [131, 180]
$C_{15}H_{12}O_6$: 288
**mp**: 216-218°C
**Mass**: 288 (100), 168 (65) $C_7H_4O_5$ [180]



**Carthamidin-7-O-glucuronide**

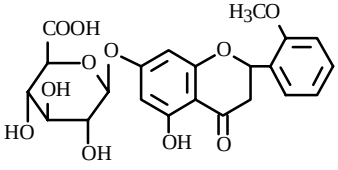
*S. rivularis* [110, 157, 180]
$C_{21}H_{20}O_{12}$: 464
**mp**: 208°C (dec.) (MeOH—$H_2O$) [180]
$[\alpha]_D^{15}$ -117° (*c* 0.08, MeOH)
**UV**: 244 sh (4.02), 285 (4.08), 365 (3.57); +$CH_3ONa$, 246 (4.12), 290 (2.92), 390 (4.10); +$AlCl_3$, 256 sh (3.80), 314 (4.28), 425 (3.64); +$AlCl_3$/HCl, 255 sh (3.89), 312 (4.26), 420 (3.63); +$CH_3COONa$, 306 (4.22), 317 sh (4.23), 344 (4.27); +$CH_3COONa/H_3BO_3$, 247 sh (4.15), 266 (3.64), 285 (4.16)
**IR**: 3400 (OH), 1731 (COOH), 1650 (C=O γ-pyrone), 1610 (C=C aromatic)
**CD** (*c* 0.0001, MeOH) $[\theta]^{15}$ (nm): +1920 (311) (positive maximum), -45112 (284) (negative maximum)
**PMR** (DMSO-$d_6$): 2.71 (1H, br.d, J = 16.9, H-3eq), 3.40 (m, H-3ax), 5.50 (1H, br.d, J = 10.0, H-2), 3.3-4.1 (m, sugar protons), 5.16 (1H, br.s, glucuronic acid anomeric proton), 6.81 (2H, d, J = 8.0, H-3′,5′), 7.35 (2H, d, J = 8.0, H-2′,6′), 6.29 (1H, s, H-6), 11.70 (1H, s, 5-OH) [180]
$^{13}$**C NMR** (DMSO-$d_6$) [180]:

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 78.8 | C-9 | 149.2 | C-6′ | 128.5 |
| 3 | 42.5 | 10 | 103.7 | 1″ | 99.9 |
| 4 | 198.0 | 1′ | 129.1 | 2″ | 72.9 |
| 5 | 153.8 | 2′ | 128.5 | 3″ | 75.2 |
| 6 | 95.1 | 3′ | 115.4 | 4″ | 71.4 |
| 7 | 155.1 | 4′ | 158.0 | 5″ | 75.4 |
| 8 | 127.4 | 5′ | 115.4 | 6″ | 170.2 |

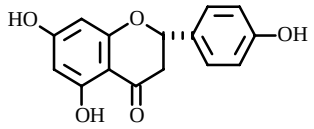


**2′-Methoxydihydrochrysin (5,7-dihydroxy-2′-methoxyflavanone)**

*S. epilobiifolia* [89]
$C_{15}H_{14}O_6$: 286
**UV**: 285, 328
**IR**: 3540 (OH), 2930 ($OCH_3$), 1665 (C=O γ-pyrone), 1618, 1575 (C=C aromatic)



**2′-Methoxydihydrochrysin-7-O-glucuronide**
*S. epilobiifolia* [89]
$C_{22}H_{22}O_{11}$: 462
**UV**: 286, 330
**IR**: 3560 (OH), 1730 (COOH), 1665 (C=O γ-pyrone), 1620, 1580 (C=C aromatic), 1090, 1065, 1015 (C–O glycoside)

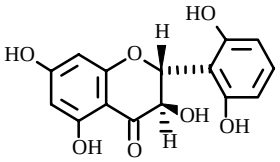


**Naringenin (5,7,4′-trihydroxyflavanone)**

*S. baicalensis* [79], *S. rivularis* [72], *S. strigillosa* [188]
$C_{15}H_{12}O_5$: 272
**mp**: 248-250°C

**UV**: 289, 326 sh; +$CH_3COONa$, 284 sh, 323; +$CH_3COONa/H_3BO_3$, 290, 332 sh; +$AlCl_3$, 312, 375; +$AlCl_3$/HCl, 311, 371
**PMR** (Py-$d_5$): 2.66 (1H, dd, J = 14.0 and 4.0, H-3eq), 3.20 (1H, dd, J = 14.0 and 12.0, H-3ax), 5.46 (1H, dd, J = 12.0 and 4.0, H-2), 5.94 (2H, s, H-6,8), 6.82 (2H, d, J = 8.5, H-3′,5′), 7.37 (2H, d, J = 8.5, H-2′,6′), 11.83 (br.s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

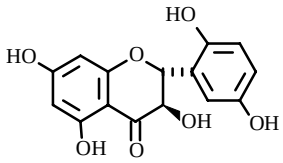
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 78.8 | C-7 | 166.9 | C-2′ | 128.5 |
| 3 | 42.8 | 8 | 95.4 | 3′ | 115.6 |
| 4 | 196.4 | 9 | 163.1 | 4′ | 157.9 |
| 5 | 163.7 | 10 | 102.1 | 5′ | 115.6 |
| 6 | 96.3 | 1′ | 129.1 | 6′ | 128.5 |



**(2*R*,3*R*)-3,5,7,2′,6′-Pentahydroxyflavanone**

*S. amoena* [132], *S. baicalensis* [81, 103, 158]
$C_{15}H_{12}O_7$: 304
**mp**: 221-225°C (dec.) (MeOH)

**UV**: 292 (4.38), 326 sh (3.66); +$AlCl_3$, 316, 376; +$CH_3COONa$, 296 sh, 329
**IR**: 3460, 3250 (OH), 1640 (C=O γ-pyrone), 1615, 1510 (C=C aromatic)
**CD** (*c* 0.16, MeOH) $[\theta]^{20}$ (nm): -8000 (277), -1800 (299), +11000 (327)
**Mass**: 304.0567 $C_{15}H_{12}O_7$ $[M]^+$
**PMR** (DMSO-$d_6$): 5.31, 5.62 (1H, d, each, J = 12.0, H-2,3), 5.19-5.98 (1H, br.s, 3-OH), 5.83, 5.90 (1H, d, each, J = 1.5, aromatic proton), 6.34 (2H, d, J = 8.5, aromatic 2×H), 6.96 (1H, t, J = 8.5, aromatic H), 9.58 (2H, br.s, 2×OH), 10.73 (1H, br.s, OH), 12.11 (1H, s, 5-OH) [158]

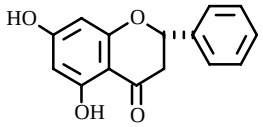


**(2*R*,3*R*)-3,5,7,2′,5′-Pentahydroxyflavanone**

*S. planipes* [125]
$C_{15}H_{12}O_7$: 304
**mp**: 242-244°C (dec.) (MeOH)
$[\alpha]_D^{28}$ 120.0° (*c* 0.10, DMSO)

**UV**: 211, 292 (4.46, 4.38)
**IR**: 3508 (OH), 1658 (C=O γ-pyrone), 1590, 1508 (C=C aromatic)
**EI-MS** *m/z* (%): 304 (24.9) $[M]^+$, 153 (90.0), 152 (8.5)
**CD** (*c* 1.583) $[\theta]_{286}^{29}$ (nm):-22510, $[\theta]_{318}^{29}$ +10628
**PMR** (DMSO-$d_6$): 4.62 (1H, dd, J = 10.2 and 3.9, H-3), 5.43 (1H, d, J = 10.2, H-2), 5.87 (1H, d, J = 2.1, H-6), 5.91 (1H, d, J = 2.1, H-8), 6.60 (1H, dd, J = 8.8 and 2.9, H-4′), 6.68 (1H, d, J = 8.8, H-3′), 6.73 (1H, d, J = 2.9, H-6′), 11.86 (s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

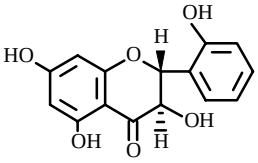
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 77.8 | C-7 | 166.8 | C-2′ | 149.6 |
| 3 | 70.3 | 8 | 94.8 | 3′ | 116.3 |
| 4 | 197.3 | 9 | 162.6 | 4′ | 116.2 |
| 5 | 163.3 | 10 | 100.3 | 5′ | 148.1 |
| 6 | 95.9 | 1′ | 123.0 | 6′ | 114.6 |



**Pinocembrin (5,7-dihydroxyflavanone)**

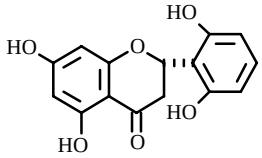
*S. discolor* [121]
$C_{15}H_{12}O_4$: 256
**mp**: 195-196°C
**UV**: 289, 325 sh; +$CH_3COONa$, 253 sh, 323; +$CH_3COONa/H_3BO_3$, 291, 320 sh; +$AlCl_3$, 331, 375; +$AlCl_3$/HCl, 309, 373
**Mass**: 256 (88) $[M]^+$, 179 (100), 152 (79), 124 (51), 104 (24), 96 (30), 78 (39), 77 (31)
**PMR** (Py-$d_5$): 2.63 (1H, dd, J = 4.5 and 16.5, H-3eq), 3.02 (1H, dd, J = 12.0 and 16.5, H-3ax), 5.31 (1H, dd, J = 4.5 and 12.0, H-2), 6.17 (1H, d, J = 2.0, H-6), 6.26 (1H, d, J = 2.0, H-8), 7.05-7.48 (5H, m, -$C_6H_5$)
$^{13}$**C NMR** (DMSO-$d_6$) [38]:

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 78.4 | C-7 | 166.6 | C-2′ | 126.5 |
| 3 | 42.2 | 8 | 95.1 | 3′ | 128.5 |
| 4 | 195.8 | 9 | 162.7 | 4′ | 128.5 |
| 5 | 163.6 | 10 | 101.9 | 5′ | 128.5 |
| 6 | 96.1 | 1′ | 138.0 | 6′ | 126.5 |



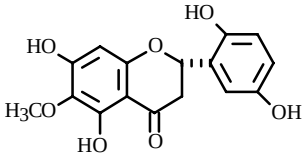
**(2*R*,3*R*)-3,5,7,2′-Tetrahydroxyflavanone**

*S. amoena* [132]
$C_{15}H_{12}O_6$: 288
**UV**: 288, 338 sh
**IR**: 3400 (OH), 1650 (C=O γ-pyrone), 1620, 1575 (C=C aromatic)



**2(*S*)-5,7,2′,6′-Tetrahydroxyflavanone**

*S. baicalensis* [81, 84, 103, 158]
$C_{15}H_{12}O_6$: 288
**mp**: 240°C (dec.) (*n*-hexane—ethylacetate)
$[\alpha]_D^{20}$ +6.13° (*c* 1.012, MeOH)
**UV**: 289 (4.21)
**IR**: 3450, 3200 (OH), 1640 (C=O γ-pyrone), 1610, 1517 (C=C aromatic)
**CD** (*c* 0.126, MeOH) $[\theta]^{25}$ (nm): -29000 (284), +7800 (306), +9400 (327)
**Mass**: 288 $[M]^+$
**PMR** (DMSO-$d_6$): 2.35 (1H, d, J = 4.0, H-3), 3.40 (1H, q, J = 14.0 and 17.0, H-3), 5.83, 5.87 (1H, d, each, J = 2.5, aromatic proton), 5.84 (1H, q, J = 14.0 and 4.0, H-2), 6.32 (2H, d, J = 9.0, aromatic proton), 6.98 (1H, m, J = 9.0, aromatic proton), 9.48 (2H, s, 2×OH), 12.24 (1H, s, 5-OH) [84]

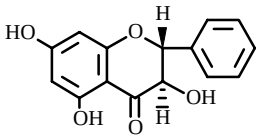


**2(*S*)-5,7,2′,5′-Tetrahydroxy-6-methoxyflavanone**

*S. scandens* [97]
$C_{16}H_{14}O_7$: 318
**mp**: 122°C (dec.) (MeOH-$H_2O$)
**UV**: 295 (4.07), 340 sh (3.26); +$CH_3ONa$, 248 (3.84), 323 (4.26), 334 sh (4.21), 410 sh (3.13); +$AlCl_3$, 297 sh (4.05), 305 (4.07), 316 sh (4.04), 392 (2.91); +$AlCl_3$/HCl, 312 (4.18), 392 (3.06); +$CH_3COONa$, 254 sh (3.59), 330; +$CH_3COONa/H_3BO_3$, 298 (4.02), 330 (3.90)
**IR**: 3400 (OH), 1640 (C=O γ-pyrone), 1600 (C=C aromatic)
**EI-MS** *m/z* (%): 318 (85) $[M]^+$, 300 (50) $C_{16}H_{12}O_6$, 285 (100) $C_{15}H_9O_6$, 183 (68) $C_8H_7O_5$, 136 (20) $C_8H_8O_2$

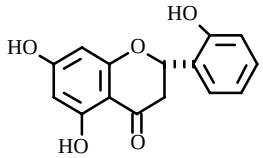
**CD** (*c* 0.0001, MeOH) $[\theta]^{15}$ (nm): +7337 (330) (positive maximum), -47165 (285) (negative maximum)
**PMR** (DMSO-$d_6$): 3.68 (3H, s, 6-$OCH_3$), 2.70 (1H, dd, J = 17.2 and 3.3, H-3eq), 3.12 (1H, dd, J = 17.2 and 12.5, H-3ax), 5.61 (1H, dd, J = 12.5 and 3.3, H-2), 6.02 (1H, s, 8-H), 6.58 (1H, dd, J = 8.3 and 2.5, H-4′), 6.70 (1H, d, J = 8.3, H-3′), 6.84 (1H, d, J = 2.5, H-6′), 8.84, 9.09 (1H, s, each, 5,2′-OH), 10.73 (1H, br.s, 7-OH), 12.16 (1H, s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 74.2 | C-8 | 95.1 | C-4″ | 115.9 |
| 3 | 41.3 | 9 | 158.4 | 5″ | 150.1 |
| 4 | 197.2 | 10 | 101.9 | 6″ | 113.2 |
| 5 | 155.4 | 1′ | 125.6 | 6-$OCH_3$ | 60.1 |
| 6 | 129.2 | 2″ | 146.6 | | |
| 7 | 159.7 | 3″ | 116.4 | | |



**(2*R*,3*R*)-3,5,7-Trihydroxyflavanone**

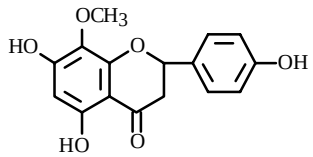
*S. amoena* [139]
$C_{15}H_{12}O_5$: 272
**UV**: 289, 337
**IR**: 3450 (OH), 1660 (C=O γ-pyrone), 1620, 1585 (C=C aromatic)



**2(*S*)-5,7,2′-Trihydroxyflavanone**

*S. indica* [113]
$C_{15}H_{12}O_5$: 272
**mp**: 202°C (MeOH—$H_2O$)
**UV**: 239 sh (3.83), 290 (4.23), 330 sh (3.56); +$CH_3ONa$, 241 sh (4.11), 325 (4.40); +$AlCl_3$, 339 sh (3.81), 275 sh (3.54), 313 (4.35), 380 (3.53); +$AlCl_3$/HCl, 239 sh (3.83), 275 sh (3.62), 311 (4.32), 379 (3.53); +$CH_3COONa$, 253 (3.69), 278 sh (3.59), 326 (4.32); +$CH_3COONa/H_3BO_3$, 291 (4.16), 232 sh (3.90)
**IR**: 3428 (OH), 1639 (C=O γ-pyrone), 1597 (C=C aromatic)
**Mass**: 272 (60) $[M]^+$, 254 (94) $C_{15}H_{10}O_4$, 153 (100) $C_6H_1O_5$
**CD** (*c* 0.005, MeOH) $[\theta]^{14}$ (nm): +9301 (309) (positive maximum), -62006 (283) (negative maximum)
**PMR** (DMSO-$d_6$): 2.71 (1H, dd, J = 17.1 and 3.4, H-3eq), 3.23 (1H, dd, J = 17.1 and 12.7, H-3ax), 5.72 (1H, dd, J = 12.7 and 3.4, H-2), 5.91 (1H, d, J = 2.0, H-6), 5.94 (1H, d, J = 2.0, H-8), 6.87 (1H, dd, J = 7.8 and 7.6, H-5′), 6.89 (1H, br.d, J = 7.8, H-3′), 7.21 (1H, dd, J = 7.8 and 7.6, H-4′), 7.44 (1H, d, J = 7.8, H-6′), 12.15 (1H, s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 74.0 | C-7 | 166.8 | C-2′ | 154.4 |
| 3 | 41.1 | 8 | 95.1 | 3′ | 115.6 |
| 4 | 196.5 | 9 | 163.4 | 4′ | 129.5 |
| 5 | 163.7 | 10 | 101.8 | 5′ | 119.2 |
| 6 | 95.9 | 1′ | 124.9 | 6′ | 127.1 |

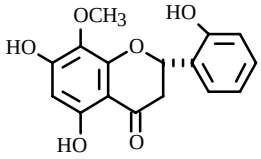


**5,7,4′-Trihydroxy-8-methoxyflavanone**

*S. repens* [187], *S. rivularis* [72, 182], *S. strigillosa* [188]
$C_{16}H_{14}O_6$: 302
**mp**: 183°C (MeOH) [182]
**UV**: 293 (4.19), 342 (3.63); +$CH_3ONa$, 247 (4.33), 331 (4.39); +$AlCl_3$, 317 (4.35), 400 (3.60); +$AlCl_3$/HCl, 314 (4.31), 398 (3.59); +$CH_3COONa$, 255 sh (3.83), 331 (4.38); +$CH_3COONa/H_3BO_3$, 296 (4.01), 333 (4.07)

**IR**: 3240 (OH), 1660 (C=O γ-pyrone), 1620 (C=C aromatic)
**Mass**: 302 (78) $[M]^+$, 182 (100) $C_8H_6O_5$
**PMR** (DMSO-$d_6$): 3.62 (3H, s, $OCH_3$), 2.72 (1H, dd, J = 17.1 and 2.7, H-3eq), 3.27 (1H, dd, J = 17.1 and 12.4, H-3ax), 5.47 (1H, dd, J = 12.4 and 2.7, H-2), 5.99 (1H, s, H-6), 6.84 (2H, d, J = 8.3, H-3′,5′), 7.36 (2H, d, J = 8.3, H-2′,6′), 9.62 (1H, s, 4′-OH), 10.64 (1H, s, 7-OH), 11.96 (1H, s, 5-OH) [182]
$^{13}$**C NMR** (DMSO-$d_6$):

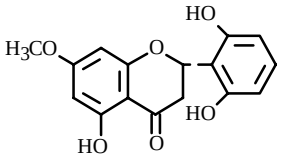
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 78.8 | C-7 | 160.1 | C-2′ | 128.3 |
| 3 | 42.0 | 8 | 128.6 | 3′ | 115.4 |
| 4 | 196.7 | 9 | 154.5 | 4′ | 158.0 |
| 5 | 158.8 | 10 | 101.9 | 5′ | 115.4 |
| 6 | 95.9 | 1′ | 129.1 | 6′ | 128.3 |
| | | | | 8-$OCH_3$ | 60.4 |




**2(*S*)-5,7,2′-Trihydroxy-8-methoxyflavanone**

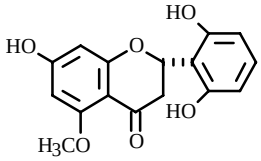
*S. indica* [113, 114]
$C_{16}H_{14}O_6$: 302
**mp**: 197°C (dec.)
**UV**: 240 sh (3.82), 291 (4.21), 342 (3.63); +$CH_3ONa$, 241 sh (4.12), 329 (4.36); +$AlCl_3$, 240 sh (3.91), 277 sh (3.56), 316 (4.34), 400 (3.60); +$AlCl_3$/HCl, 240 sh (3.91), 313 (4.31), 398 (3.58); +$CH_3COONa$, 253 sh (3.74), 283 (3.59), 330 (4.35); +$CH_3COONa/H_3BO_3$, 292 (4.10), 333 (4.01)
**IR**: 3488 (OH), 1641 (C=O γ-pyrone), 1614 (C=C aromatic)
**Mass**: 302 (70) $[M]^+$, 269 (100) $C_{15}H_9O_5$, 167 (73) $C_7H_3O_5$
**CD** (*c* 0.005, MeOH) $[\theta]^{14}$ (nm): +16717 (309) (positive maximum), -59554 (288) (negative maximum)
**PMR** (DMSO-$d_6$): 3.67 (3H, s, $OCH_3$), 2.76 (1H, dd, J = 17.0 and 3.2, H-3eq), 3.23 (1H, dd, J = 17.0 and 12.3, H-3ax), 5.76 (1H, dd, J = 12.3 and 3.2, H-2), 6.01 (1H, s, H-6), 6.89 (1H, dd t, J = 7.5, H-5′), 6.92 (1H, br.d, J = 7.9, H-3′), 7.23 (1H, dd, J = 7.9 and 7.5, H-4′), 7.48 (1H, d, J = 7.5, H-6′), 9.6 (1H, br.s, 2′-OH), 10.8 (1H, br.s, 7-OH), 11.93 (1H, s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 74.3 | C-8 | 128.5 | C-3′ | 151.6 |
| 3 | 41.1 | 9 | 154.6 | 4′ | 129.4 |
| 4 | 196.4 | 10 | 101.8 | 5′ | 119.1 |
| 5 | 158.6 | 1′ | 124.9 | 6′ | 126.8 |
| 6 | 95.9 | 2′ | 154.3 | 8-$OCH_3$ | 60.4 |
| 7 | 159.9 | | | | |




**2(*S*)-5,2′,6′-Trihydroxy-7-methoxyflavanone (scuteamoenin)**

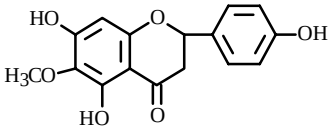
*S. amoena* [139]
$C_{16}H_{14}O_6$: 302
**UV**: 241 sh, 290, 340
**IR**: 3460 (OH), 1645 (C=O γ-pyrone), 1620 (C=C aromatic)



**2(*S*)-7,2′,6′-Trihydroxy-5-methoxyflavanone**

*S. baicalensis* [127, 141, 181]
$C_{16}H_{14}O_6$: 302
**mp**: 211°C (dec.) (MeOH) [181]

**UV**: 252 sh, 290, 323; +$CH_3ONa$, 243, 323, 325 sh, 430; +$AlCl_3$, 230, 285, 320 sh, 363; +$CH_3COONa$, 255 sh, 323
**IR**: 3400 (OH), 1650 (C=O γ-pyrone), 1600, 1570 (C=C aromatic)
**Mass**: 302 $[M]^+$
**CD** (*c* 0.005, MeOH) $[\theta]^{25}$ (nm): +1813 (325) (positive maximum), -3141 (285) (negative maximum)
**PMR** (DMSO-$d_6$): 3.74 (3H, s, $OCH_3$), 5.77 (1H, dd, J = 14.0 and 2.5, H-2), 3.75 (1H, dd, J = 17.0 and 14.0, H-3ax), 2.22 (1H, dd, J = 17.0 and 2.5, H-3eq), 5.91 (1H, d, J = 2.0, H-6), 6.04 (1H, d, J = 2.0, H-8), 6.33 (2H, d, J = 8.3, H-3′,5′), 6.96 (1H, t, J = 8.3, H-4′) [181]

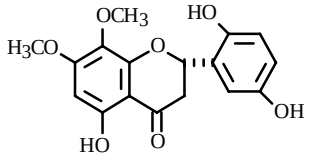


**5,7,4′-Trihydroxy-6-methoxyflavanone**

*S. baicalensis* [191], *S. repens* [187], *S. rivularis* [72]
$C_{16}H_{14}O_6$: 302
**mp**: 228-230°C

**UV**: 293 (4.23), 331 (3.68); +$CH_3ONa$, 247 (4.30), 329 (4.44); +$CH_3COONa$, 294 (4.07), 330 (4.19); +$AlCl_3$, 225 (4.42), 300 sh (4.12), 316 (4.21), 394 (3.41); +$AlCl_3$/HCl, 225 (4.47), 314 (4.32), 394 (3.41) [191]
**IR**: 3500 (OH), 1640 (C=O γ-pyrone)
**Mass**: 302 $[M]^+$, 120 $C_8H_8O$
**CD** (*c* 0.001, MeOH) [θ] (nm): -10744 (300) (negative maximum), +13358 (268) (positive maximum)
**PMR** (DMSO-$d_6$): 2.80 (1H, dd, J = 4.0, H-3eq), 3.10 (1H, d, J = 12.0, H-3ax), 3.72 (3H, s, $OCH_3$), 5.42 (1H, dd, J = 12.0 and 4.0, H-2), 6.00 (1H, s, H-8), 6.83 (2H, d, J = 9.0, H-3′,5′), 7.34 (2H, d, J = 9.0, H-2′,6′), 12.20 (1H, s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 78.4 | C-8 | 95.1 | C-4′ | 157.9 |
| 3 | 42.1 | 9 | 157.6 | 5′ | 115.2 |
| 4 | 196.8 | 10 | 102.0 | 6′ | 127.9 |
| 5 | 155.0 | 1′ | 129.0 | $OCH_3$ | 59.9 |
| 6 | 129.0 | 2′ | 127.9 | | |
| 7 | 159.4 | 3′ | 115.2 | | |



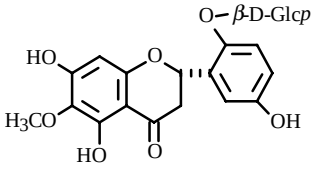
**2(*S*)-5,2′,5′-Trihydroxy-7,8-dimethoxyflavanone**

*S. indica* [113, 114]
$C_{17}H_{16}O_7$: 332
**mp**: 192°C (MeOH—$H_2O$)

**UV**: 240 sh (3.89), 2.92 (4.13); +$CH_3ONa$, 243 (4.11), 288 (4.00), 315 sh (3.76), 390 (3.75); +$AlCl_3$, 314 (4.22), 404 (3.56); +$AlCl_3$/HCl, 310 (4.21), 396 (3.49); +$CH_3COONa$, 292 (4.10), 345 (3.48); +$CH_3COONa/H_3BO_3$, 292 (4.11), 345 (3.50)
**IR**: 3400 (OH), 1639 (C=O γ-pyrone), 1580 (C=C aromatic)
**Mass**: 332 (58) $[M]^+$, 299 (100) $C_{16}H_{11}O_6$, 136 (25) $[C_8H_8O_2]^+$
**CD** (*c* 0.005, MeOH) $[\theta]^{14}$ (nm): +9501 (308) (positive maximum), -54292 (285) (negative maximum)
**PMR** (DMSO-$d_6$): 3.66, 3.87 (each 3H, s, each 2×$OCH_3$), 2.80 (1H, dd, J = 19.0 and 3.9, H-3eq), 3.18 (1H, dd, J = 19.0 and 12.9, H-3ax), 5.70 (1H, dd, J = 12.9 and 3.9, H-2), 6.25 (1H, s, H-6), 6.62 (1H, dd, J = 9.3 and 2.0, H-4′), 6.75 (1H, d, J = 9.3, H-3′), 6.92 (1H, d, J = 2.0, H-6′), 8.87, 9.11 (1H, s, each 5′ and 2′-OH), 12.03 (1H, s, 5-OH)

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

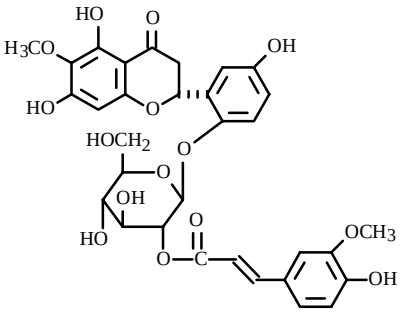
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 74.5 | C-8 | 129.3 | C-4′ | 115.9 |
| 3 | 41.5 | 9 | 153.9 | 5′ | 150.1 |
| 4 | 197.1 | 10 | 102.4 | 6′ | 113.2 |
| 5 | 159.0 | 1′ | 125.5 | 7-$OCH_3$ | 56.3 |
| 6 | 93.0 | 2′ | 146.5 | 8-$OCH_3$ | 60.5 |
| 7 | 161.1 | 3′ | 116.4 | | |




**2(*S*)-5,7,5′-Trihydroxy-6-methoxy-2′-O-$\beta$-D-glucopyranosylflavanone**

*S. scandens* [97]
$C_{22}H_{24}O_{12}$: 480
**mp**: 255°C (dec.) (MeOH—$H_2O$)
$[\alpha]_D^{15}$ -146° (*c* 0.04, MeOH)
**UV**: 294 (4.29), 334 (3.53); +$CH_3ONa$, 242 sh (4.17), 330 (4.46); +$AlCl_3$, 299 (4.16), 315 (4.15), 396 (3.15); +$AlCl_3$/HCl, 314 (4.26), 396 (3.23); +$CH_3COONa$, 253 sh (3.75), 290 sh (3.77), 330 (4.39); +$CH_3COONa/H_3BO_3$, 295 (4.17), 332 (3.99)
**IR**: 3400 (OH), 1640 (C=O γ-pyrone), 1605, 1580 (C=C aromatic)
**EI-MS** *m/z* (%): 318 (70) $C_{16}H_{14}O_7$, 285 (100) $C_{15}H_9O_6$
**FAB-MS** *m/z* (%): 481 (75) $[M + 1]^+$, 319 (100) $[C_{16}H_{14}O_7 + 1]$
**CD** (*c* 0.0001, MeOH) $[\theta]^{15}$ (nm): +6287 (330) (positive maximum), -52096 (285) (negative maximum)
**PMR** (DMSO-$d_6$): 3.68 (3H, s, 6-$OCH_3$), 2.71 (1H, dd, J = 17.0 and 3.3, H-3eq), 3.03 (1H, dd, J = 17.0 and 12.0, H-3ax), 3.0-3.8 (m, sugar protons), 4.58 (1H, d, J = 6.0, glucose anomeric proton H-1″), 5.90 (1H, dd, J = 12.0 and 3.3, H-2), 6.03 (1H, s, H-8), 6.70 (1H, dd, J = 8.8 and 2.9, H-4′), 6.95 (1H, d, J = 2.9, H-6′), 7.05 (1H, d, J = 8.8, H-3′), 9.25 (1H, s, 5′-OH), 10.48 (1H, br.s, 7-OH), 12.20 (1H, s, 5-OH)
**$^{13}$C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 73.8 | C-10 | 102.2 | C-2″ | 73.5 |
| 3 | 42.1 | 1′ | 129.8 | 3″ | 76.4 |
| 4 | 197.3 | 2′ | 147.0 | 4″ | 70.0 |
| 5 | 155.4 | 3′ | 117.8 | 5″ | 77.2 |
| 6 | 129.3 | 4′ | 115.7 | 6″ | 61.1 |
| 7 | 159.7 | 5′ | 152.8 | $OCH_2$ | 60.2 |
| 8 | 95.2 | 6′ | 112.8 | | |
| 9 | 158.4 | 1″ | 103.2 J = 160.3 | | |

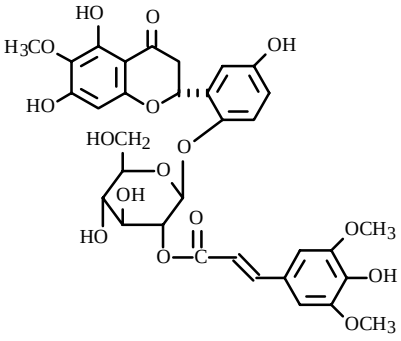



**2(*S*)-5,7,5′-Trihydroxy-6-methoxy-2′-O-$\beta$-D-(2-O-feruloyl)-glucopyranosylflavanone**

*S. scandens* [97]
$C_{32}H_{32}O_{15}$: 656
**mp**: 176°C (dec.) (MeOH—$H_2O$)
$[\alpha]_D^{15}$ -116.9° (*c* 0.03, MeOH)
**UV**: 295 (4.38), 335 (4.19); +$CH_3ONa$, 245 sh (4.27), 332 (4.44), 382 (4.35); +$AlCl_3$, 296 sh (4.32), 318 (4.41), 345 sh (4.10); +$AlCl_3$/HCl, 313 (4.44), 343 sh (4.11); +$CH_3COONa$, 253 sh (4.11), 293 sh (4.11), 328 (4.51), 396 sh (3.75); +$CH_3COONa/H_3BO_3$, 297 (4.37), 332 (4.33)
**IR**: 3400 (OH), 1700 (C=O), 1630 (C=O γ-pyrone), 1590 (C=C aromatic)
**EI-MS** *m/z* (%): 318 (100) $C_{16}H_{14}O_7$, 300 (80) $C_{16}H_{12}O_6$, 177 (60) $C_{10}H_9O_3$

**FAB-MS** *m/z* (%): 657 (35) $[M + 1]^+$, 319 (70) $[C_{16}H_{14}O_7 + 1]$
**CD** (*c* 0.0001, MeOH) $[\theta]^{15}$ (nm): +19172 (382) (positive maximum), -89469 (285) (negative maximum)
**PMR** (DMSO-$d_6$): (f = ferulic acid) 3.66 (3H, s, 6-$OCH_3$), 3.79 (3H, s, f3-$OCH_3$), 2.69 (1H, br.d, J = 17.2, H-3eq), 2.93 (1H, dd, J = 17.2 and 11.2, H-3ax), 3.1-3.8 (m, sugar protons), 4.90 (1H, d, J = 5.9, glucose anomeric proton H-1″), 5.33 (1H, br.d, J = 11.2, H-2), 5.84 (1H, s, H-8), 6.31 (1H, d, f$\alpha$-H, J = 15.6), 6.69 (1H, dd, J = 9.1 and 2.5, H-4′), 6.74 (2H, s, f5, f6-H), 6.89 (1H, d, J = 2.5, H-6′), 7.06 (1H, d, J = 9.1, H-3′), 7.13 (1H, s, f2′-H), 7.25 (1H, d, J = 15.6, $\beta$-H), 9.27 (1H, s, 5′-OH), 9.57 (1H, s, f4-OH), 10.57 (1H, s, 7-OH), 12.22 (1H, s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| Aglycon | | Ferulic acid | | Glucose | |
|---|---|---|---|---|---|
| C-2 | 73.8 | CO | 166.2 | C-1″ | 100.3 |
| 3 | 41.5 | C-$\alpha$ | 114.1 | 2″ | 73.8 |
| 4 | 196.4 | $\beta$ | 145.7 | 3″ | 73.5 |
| 5 | 155.3 | 1 | 125.4 | 4″ | 70.1 |
| 6 | 129.3 | 2 | 110.8 | 5″ | 77.4 |
| 7 | 159.6 | 3 | 148.0 | 6″ | 60.7 |
| 8 | 94.9 | 4 | 149.5 | | |
| 9 | 157.8 | 5 | 115.5 | | |
| 10 | 101.7 | 6 | 123.3 | | |
| 1′ | 129.3 | 3-$OCH_3$ | 55.9 | | |
| 2′ | 146.2 | | | | |
| 3′ | 117.3 | | | | |
| 4′ | 115.5 | | | | |
| 5′ | 153.0 | | | | |
| 6′ | 112.6 | | | | |
| 6-$OCH_3$ | 59.9 | | | | |

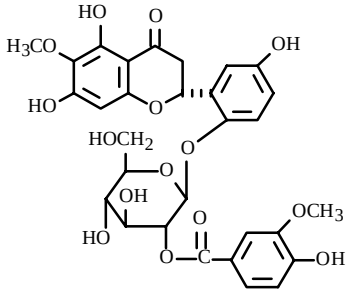



**2(*S*)-5,7,5′-Trihydroxy-6-methoxy-2′-O-$\beta$-D-(2-O-sinapoyl)-glucopryanosylflavanone**

*S. scandens* [97]
$C_{33}H_{34}O_{16}$: 686
**mp**: 172°C (dec.) (MeOH—$H_2O$)
$[\alpha]_D^{15}$ -136.1° (*c* 0.05, MeOH)
**UV**: 295 (4.23), 337 (4.08); +$CH_3ONa$, 242 (4.19), 265 sh (4.01), 320 sh (4.01), 370 (4.33), 400 sh (4.24); +$AlCl_3$, 297 sh (4.33), 317 (4.45), 345 sh (4.21); +$AlCl_3$/HCl, 314 (4.48), 343 sh (4.20); +$CH_3COONa$, 247 sh (4.27), 328 (4.55), 400 sh (3.70); +$CH_3COONa/H_3BO_3$, 298 (4.36), 332 (4.33)
**IR**: 3400 (OH), 1700 (C=O), 1630 (C=O $\gamma$-pyrone), 1600 (C=C aromatic)
**FAB-MS** *m/z* (%): 687 (10) $[M + 1]^+$, 319 (30) $[C_{16}H_{14}O_7 + 1]$
**CD** (*c* 0.0001, MeOH) $[\theta]^{15}$ (nm): +20079 (327) (positive maximum), -100395 (290) (negative maximum)
**PMR** (DMSO-$d_6$): (s = sinapic acid) 3.62 (3H, s, 6-$OCH_3$), 3.79 (6H, s, $OCH_3$-3,$OCH_3$-5), 2.70 (1H, br.d, J = 17.3, H-3eq), 2.94 (1H, dd, J = 17.3 and 11.2, H-3ax), 3.1-3.8 (m, sugar protons), 4.90 (1H, d, J = 6.1, glucose anomeric proton H-1″), 5.35 (1H, br.d, J = 11.2, H-2), 5.87 (1H, s, H-8), 6.38 (1H, d, s$\alpha$-H, J = 15.6), 6.69 (1H, dd, J = 8.8 and 2.9, H-4′), 6.80 (2H, s, s2,s6-H), 6.90 (1H, d, J = 2.9, H-6′), 7.06 (1H, d, J = 8.8, H-3′), 7.30 (1H, d, J = 15.6, s$\beta$-H), 8.91 (1H, s, s4-OH), 9.27 (1H, s, 5′-OH), 10.55 (1H, s, 7-OH), 12.21 (1H, s, 5-OH)

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

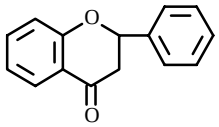
| Aglycon | | Sinapic acid | | Glucose | |
|---|---|---|---|---|---|
| C-2 | 73.8 | CO | 166.1 | C-1″ | 100.3 |
| 3 | 41.6 | C-$\alpha$ | 114.6 | 2″ | 73.7 |
| 4 | 196.4 | $\beta$ | 146.0 | 3″ | 73.5 |
| 5 | 155.2 | 1 | 124.3 | 4″ | 70.1 |
| 6 | 129.2 | 2 | 106.2 | 5″ | 77.4 |
| 7 | 159.5 | 3 | 148.1 | 6″ | 60.8 |
| 8 | 94.9 | 4 | 138.5 | | |
| 9 | 157.8 | 5 | 148.1 | | |
| 10 | 101.7 | 6 | 106.2 | | |
| 1′ | 129.4 | 3-$OCH_3$ | 56.0 | | |
| 2′ | 146.2 | 5-$OCH_3$ | 56.0 | | |
| 3′ | 117.4 | | | | |
| 4′ | 115.5 | | | | |
| 5′ | 153.0 | | | | |
| 6′ | 112.7 | | | | |
| 6-$OCH_3$ | 59.9 | | | | |




**2(*S*)-5,7,5′-Trihydroxy-6-methoxy-2′-O-$\beta$-D-(2-O-vanilloyl)-glucopyranosylflavanone**

*S. scandens* [97]
$C_{30}H_{30}O_{15}$: 630
**mp**: 202°C (dec.) (MeOH—$H_2O$)
$[\alpha]_D^{15}$ -97.9° (*c* 0.03, MeOH)
**UV**: 270 sh (4.12), 293 (4.27), 335 (3.40); +$CH_3ONa$, 320 (4.54); +$AlCl_3$, 270 (4.08), 297 (4.20), 320 sh (4.02), 380 (3.28); +$AlCl_3$/HCl, 270 (4.06), 301 (4.20), 317 sh (4.08), 380 (3.22); +$CH_3COONa$, 325 (4.35); +$CH_3COONa/H_3BO_3$, 274 (4.07), 294 (4.18), 332 (3.86)
**IR**: 3400 (OH), 1700 (C=O), 1630 (C=O $\gamma$-pyrone), 1600 (C=C aromatic)
**FAB-MS** *m/z* (%): 631 (25) $[M + 1]^+$, 653 (20) $[M + Na]^+$, 669 (10) $[M + K]^+$
**CD** (*c* 0.0001, MeOH) $[\theta]^{15}$ (nm): +6427 (330) (positive maximum), -47561 (285) (negative maximum)
**PMR** (DMSO-$d_6$): (v = vanillic acid) 3.68 (3H, s, 6-$OCH_3$), 3.71 (3H, s, v3-$OCH_3$), 2.62 (1H, br.d, J = 17.2, H-3eq), 2.86 (1H, dd, J = 17.2 and 11.0, H-3ax), 3.1-3.8 (m, sugar protons), 4.97 (1H, d, J = 6.3, glucose anomeric proton H-1″, 5.25 (1H, dd, J = 11.0 and 3.9, H-2), 5.81 (1H, s, H-8), 6.68 (2H, br.d, 4′,v5-H, J = 8.8), 6.87 (1H, d, J = 3.0, H-6′), 7.07 (1H, d, J = 8.8, H-3′), 7.25 (1H, br.d, J = 8.8, v6-H), 12.15 (1H, s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

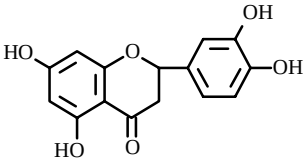
| Aglycon | | Vanillic acid | | Glucose | |
|---|---|---|---|---|---|
| C-2 | 73.8 | CO | 165.2 | C-1″ | 100.5 |
| 3 | 41.7 | 1 | 120.4 | 2″ | 74.0 |
| 4 | 195.9 | 2 | 112.7 | 3″ | 73.7 |
| 5 | 155.2 | 3 | 147.4 | 4″ | 70.2 |
| 6 | 129.5 | 4 | 151.8 | 5″ | 77.5 |
| 7 | 160 | 5 | 115.1 | 6″ | 60.9 |
| 8 | 95.2 | 6 | 123.7 | | |
| 9 | 157.8 | 3-$OCH_3$ | 55.5 | | |
| 10 | 101.4 | | | | |
| 1′ | 129.6 | | | | |
| 2′ | 146.2 | | | | |
| 3′ | 117.7 | | | | |
| 4′ | 115.5 | | | | |
| 5′ | 153.1 | | | | |
| 6′ | 112.7 | | | | |
| 6-$OCH_3$ | 60.0 | | | | |



**Flavanone**

$C_{15}H_{12}O_2$: 224
**mp**: 76-78°C (hexane)
**IR**: 1690, 1606, 1574, 1452, 1369, 1324, 1304, 1228, 1146, 1112, 1067, 1025, 983, 911, 862, 967, 703, 491
**Mass**: 224 $[M]^+$, 147, 120, 104, 92, 77, 63, 51, 40
**PMR** ($CDCl_3$): 7.293 (1H, d, H-5, J = 10), 7.43 (7H, m, H-6 and H-8, ring B protons), 7.035 (1H, d, H-6), 5.46 (1H, q, H-2), 3.07 (1H, q, H-3eq), 2.873 (1H, q, H-3ax)
$^{13}$**C NMR** ($CDCl_3$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 79.49 | C-7 | 135.95 | C-2′ | 126.05 |
| 3 | 44.57 | 8 | 118.00 | 3′ | 128.73 |
| 4 | 191.53 | 9 | 161.50 | 4′ | 126.96 |
| 5 | 128.73 | 10 | 121.00 | 5′ | 128.73 |
| 6 | 121.52 | 1′ | 138.82 | 6′ | 126.05 |



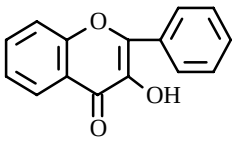
**Eriodictyol (5,7,3′,4′-tetrahydroxyflavanone)**

*S. rivularis* [72]
$C_{15}H_{12}O_6$: 288
**mp**: 267°C
**UV**: 289, 324 sh; +$CH_3COONa$, 289 sh, 325; +$CH_3COONa/H_3BO_3$, 289, 333; +$AlCl_3$, 310, 378; +$AlCl_3$/HCl, 309, 373
$^{13}$**C NMR** (DMSO-$d_6$):

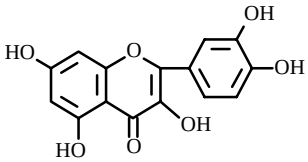
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 83.1 | C-7 | 166.8 | C-2′ | 155.3 |
| 3 | 71.7 | 8 | 95.1 | 3′ | 144.9 |
| 4 | 197.1 | 9 | 162.5 | 4′ | 145.7 |
| 5 | 163.3 | 10 | 100.6 | 5′ | 115.3 |
| 6 | 96.1 | 1′ | 128.9 | 6′ | 119.2 |

## FLAVONOLS

Six representatives of this group of flavanoids were found in plants of the *Scutellaria* genus (*S. baicalensis*, *S. amoena*).



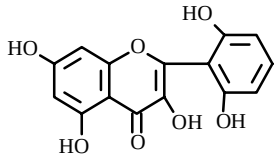
**Quercetin (3,5,7,3′,4′-pentahydroxyflavone)**



*S. baicalensis* [79]
$C_{15}H_{10}O_7$: 302
**mp**: 313-315°C
$[\alpha]_D^{20}$ +70.4° (*c* 0.69, $CHCl_3$—MeOH)
**UV**: 257, 268, 371; +$CH_3COONa$, 270, 405; +$ZrOCl_2$, 275, 440; +NaOH, 330; +$CH_3COONa/H_3BO_3$, 270, 405
**IR**: 3320 (OH), 1660 (C=O γ-pyrone), 1620, 1580, 1510 (C=C aromatic)
**Mass**: 302 $[M]^+$, 273, 262, 153, 141, 137, 128, 110, 95, 69, 57
**PMR** (Py-$d_5$): 6.56 (1H, d, J = 2.5, H-6), 6.63 (1H, d, J = 2.5, H-8), 7.24 (1H, d, J = 8.5, H-5′), 7.94 (1H, dd, J = 8.5 and

2.5, H-6′), 8.47 (1H, d, J = 2.5, H-2′), 11.75 (1H, br.m, 3-OH), 13.81 (1H, br.m, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

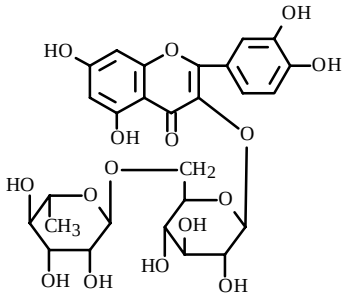
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 147.1 | C-7 | 164.2 | C-2′ | 115.5 |
| 3 | 136.0 | 8 | 93.9 | 3′ | 145.3 |
| 4 | 176.0 | 9 | 160.9 | 4′ | 147.9 |
| 5 | 160.9 | 10 | 103.4 | 5′ | 116.0 |
| 6 | 98.7 | 1′ | 122.4 | 6′ | 120.0 |



**3,5,7,2′,6′-Pentahydroxyflavone (viscidulin I)**

*S. baicalensis* [127, 141, 181], *S. menax* [99], *S. viscidula* [100, 127]
$C_{15}H_{10}O_7$: 302
**mp**: 293°C (dec.) (MeOH) [181]
**UV**: 225, 265, 376; +$CH_3ONa$, 275, 390; +$AlCl_3$, 263, 297 sh, 326, 396; +$AlCl_3$/HCl, 264, 296 sh, 323, 394; +$CH_3COONa$, 273, 305 sh, 386
**IR**: 3250 (OH), 1630 (C=O γ-pyrone), 1590, 1560 (C=C aromatic)
**Mass**: 302 $[M]^+$, 285 $[M - 17]^+$, 137 $C_7H_5O_3$
**PMR** (DMSO-$d_6$): 6.20 (1H, d, J = 2.0, H-6), 6.32 (1H, d, J = 2.0, H-8), 6.38 (2H, d, J = 8.1, H-3′,5′), 7.10 (1H, t, J = 8.1, H-4′), 12.45 (1H, br.s, 5-OH) [181]
$^{13}$**C NMR** (DMSO-$d_6$) [181]:

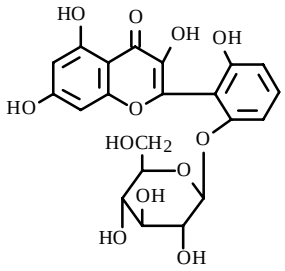
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 147.9 | C-7 | 163.8 | C-2′ | 157.3 |
| 3 | 140.7 | 8 | 93.4 | 3′ | 107.1 |
| 4 | 177.5 | 9 | 157.3 | 4′ | 131.4 |
| 5 | 160.8 | 10 | 104.2 | 5′ | 107.1 |
| 6 | 98.1 | 1′ | 107.5 | 6′ | 157.3 |



**Rutin**

*S. baicalensis* [79]
$C_{27}H_{30}O_{16}$: 610
**mp**: 189-191°C (EtOH)
$[\alpha]_D$ -33.5° (*c* 0.2, MeOH)
**UV**: 259, 267 sh, 362; +$CH_3COONa$, 270, 391; +$CH_3COONa/H_3BO_3$, 261, 385; +$AlCl_3$, 274, 431; +$AlCl_3$/HCl, 271, 400; +$CH_3ONa$, 273, 412
**PMR** (Py-$d_5$): 1.34 (3H, br.s, $CH_3$), 3.80-4.10 (10 carbohydrate protons), 5.14 (1H, s, H-1‴), 5.78 (1H, d, J = 7.5, H-1″), 6.53 (2H, br.s, H-6 and H-8), 7.17 (1H, d, J = 8.5, H-5′), 7.90 (1H, dd, J = 8.5 and 2.5, H-6′), 8.13 (br.s, H-2′)
$^{13}$**C NMR** (DMSO-$d_6$):

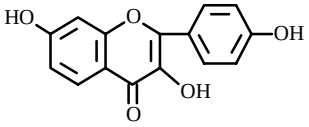
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 156.6 | C-1′ | 121.4 | C-4″ | 70.3 |
| 3 | 133.5 | 2′ | 115.4 | 5″ | 76.1 |
| 4 | 177.4 | 3′ | 144.8 | 6″ | 67.3 |
| 5 | 161.3 | 4′ | 148.5 | 1‴ | 100.9 |
| 6 | 99.0 | 5′ | 116.5 | 2‴ | 70.6 |
| 7 | 164.0 | 6′ | 121.5 | 3‴ | 70.6 |
| 8 | 93.9 | 1″ | 101.4 | 4‴ | 72.1 |
| 9 | 156.8 | 2″ | 74.3 | 5‴ | 68.5 |
| 10 | 104.2 | 3″ | 76.6 | 6‴ | 18.0 |



**3,5,7,6′-Tetrahydroxy-2′-O-$\beta$-D-glucopyranosylflavone (viscidulin I-2′-O-$\beta$-D-glucopyranoside)**

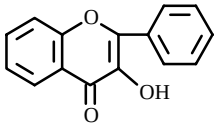
*S. baicalensis* [130]
$C_{21}H_{20}O_{12}$: 464
**mp**: 240-242°C (dec.) (MeOH—$H_2O$)
$[\alpha]_D^{25}$ -27.6° (c 0.02, MeOH)
**UV**: 254 (3.75), 290 sh (3.44), 338 (3.31); +$CH_3ONa$, 272 (3.83), 315 sh (3.45), 385 (3.48); +$AlCl_3$, 261 (3.97), 316 (3.52), 388 (3.48); +$AlCl_3$/HCl, 256 (4.10), 261 (4.09), 316 (3.56), 388 (3.42); +$CH_3COONa$, 267 (3.81), 325 (3.44), 379 (3.63); +$CH_3COONa/H_3BO_3$, 264 (3.85), 310 (3.48), 352 (3.91)
**IR**: 3408 (OH), 1640 (C=O $\gamma$-pyrone), 1604 (C=C aromatic)
**FAB-MS** *m/z* (%): 465 (3) $[M + H]^+$, 487 (4) $[M + Na]^+$
**PMR** (DMSO-$d_6$): 3.08-3.68 (5H, m, H-2″,3″,4″,5″,6″), 4.91 (1H, d, J = 7.5, H-1″), 6.02 (1H, d, J = 1.8, H-6), 6.27 (1H, d, J = 1.8, H-8), 6.32 (1H, d, J = 8.0, H-5′), 6.42 (1H, d, J = 8.0, H-3′), 7.06 (1H, t, J = 8.0, H-4′), 10.30 (1H, br.s, 7-OH), 9.80 (1H, br.s, 6′-OH), 13.63 (1H, s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 147.8 | C-9 | 156.9 | C-6′ | 156.4 |
| 3 | 141.2 | 10 | 104.1 | 1″ | 99.9 |
| 4 | 178.2 | 1′ | 110.8 | 2″ | 73.4 |
| 5 | 161.2 | 2′ | 156.4 | 3″ | 76.8 |
| 6 | 97.0 | 3′ | 102.8 | 4″ | 69.7 |
| 7 | 162.8 | 4′ | 130.4 | 5″ | 77.0 |
| 8 | 93.0 | 5′ | 111.9 | 6″ | 60.7 |



**3,7,4′-Trihydroxyflavone**

*S. ocellata* [185]
$C_{15}H_{10}O_5$: 270
**mp**: 203-205°C
**UV**: 267, 364
**IR**: 3540 (OH), 1660 (C=O $\gamma$-pyrone), 1605, 1575, 1515 (C=C aromatic)
**PMR** (Py-$d_5$): 8.35 (3H, d, J = 9.7, H-5, 2′,6′), 7.15 (1H, br.s, 3-OH), 7.45 (4H, m, aromatic protons)



**Flavonol**

$C_{15}H_{10}O_3$: 238
**mp**: 170°C (hexane)
**UV**: 343, 305, 238, 204
**IR**: 3213, 1628, 1607, 1562, 1481, 1471, 1417, 1351, 1308, 1287, 1212, 1131, 1078, 1036, 992, 902, 780, 759, 701, 688, 471, 437
**Mass**: 238 $[M]^+$, 237, 210, 209, 181, 152, 105, 104, 118, 89, 77, 63, 50
**PMR** ($CDCl_3$): 8.267 (3H, d, H-5, H-2′, H-6′, J = 9.64), 7.707 (1H, t, H-7), 7.5 (5H, m, aromatic protons), 7.11 (3-OH) [147]

**$^{13}$C NMR** ($CDCl_3$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 142.972 | C-7 | 133.648 | C-2′ | 127.817 |
| 3 | 138.504 | 8 | 118.350 | 3′ | 128.660 |
| 4 | 174.000 | 9 | 156.000 | 4′ | 130.249 |
| 5 | 125.529 | 10 | 129.724 | 5′ | 128.660 |
| 6 | 124.585 | 1′ | 131.138 | 6′ | 127.817 |

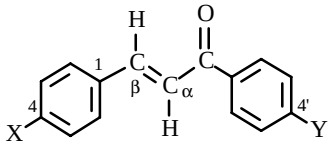
**$^{13}$C NMR** ($DMSO\text{-}d_6$) [159]:

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 145.20 | C-7 | 133.65 | C-2′ | 127.63 |
| 3 | 139.03 | 8 | 118.34 | 3′ | 128.46 |
| 4 | 172.96 | 9 | 154.59 | 4′ | 129.82 |
| 5 | 124.75 | 10 | 121.28 | 5′ | 128.660 |
| 6 | 124.5 | 1′ | 131.29 | 6′ | 127.63 |

## CHALCONES AND STILBENES

Chalcones are plant pigments owing to the presence in them of a conjugated chromophore. Research on these natural compounds began approximately in 1960. At present, the number of newly discovered compounds is increasing at a rapid rate.

X-ray structure analysis showed that chalcone has the *trans*-configuration [160]. The chemical shifts and spin—spin coupling constants of the corresponding protons in the PMR and $^{13}$C NMR spectra of series of 4,4′-substituted chalcones also were consistent with the *trans*-configuration [161].




**PMR** ($CDCl_3$) of chalcone (X,Y = H) [161]:

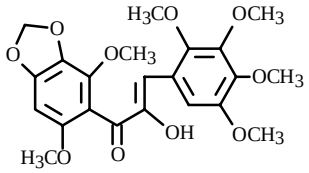
| | | | | | |
|---|---|---|---|---|---|
| H-$\alpha$ | 7.32 | | H-4 | 7.40 |
| $\beta$ | 7.809 | (J = 15.6 ) | 2′, 6′ | 8.021 |
| 2, 6 | 6.36 | | 3′, 5′ | 7.496 |
| 3, 5 | 7.41 | | 4′ | 7.574 |

$^{13}$C NMR ($DMSO\text{-}d_6$) [38, 171]:

| | | | |
|---|---|---|---|
| C-$\alpha$ | 121.9 | C-6′ | 130.3 |
| $\beta$ | 144.4 | 1 | 134.9 |
| CO | 190.0 | 2 | 128.7 |
| C-1′ | 138.1 | 3 | 128.7 |
| 2′ | 130.3 | 4 | 128.7 |
| 3′ | 130.3 | 5 | 128.7 |
| 4′ | 132.6 | 6 | 128.7 |
| 5′ | 130.3 | | |

Chalcones and stilbenes are precursors of flavanones and flavones according to biogenesis [7] and chemical properties [162].

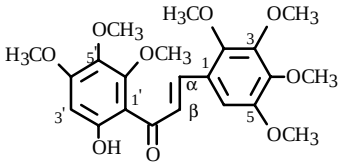
Chalcones have been observed in three species of the *Scutellaria* genus: *S. baicalensis*, *S. discolor*, and *S. indica*. All are polysubstituted compounds, i.e., they contain from five to eight substituents (OH, $OCH_3$, O–$CH_2$–O) in rings A and B. Stilbenes have been found only in *S. scandens* [192].



**2,3,4,5,2′,6′-Hexamethoxy-4′,5′-methylenedioxychalcone**

*S. indica* [67]
$C_{22}H_{24}O_9$: 432
**mp**: 229°C (dec.) (MeOH)
**UV**: 314 (4.22), 355 (4.11)
**IR**: 1650 (C=O), 1620 (C=C aromatic)
**Mass**: 432 (10) $[M]^+$, 401 (100) $C_{19}H_{17}O_8$
**PMR** (DMSO-$d_6$): 3.65, 3.66, 3.80, 3.81, 3.85 (3H, s, each 6×$OCH_3$), 6.03 (2H, s, $OCH_2O$), 6.64 (1H, s, H-3′), 7.01 (1H, d, J = 16.4, $\alpha$-H), 7.16 (1H, s, H-6), 7.41 (1H, d, J = 16.4, $\beta$-H)
$^{13}$**C NMR** (DMSO-$d_6$):

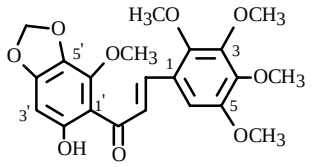
| | | | | | |
|---|---|---|---|---|---|
| C-$\beta$ | 138.5 | C-1′ | 114.3 | $OCH_3$ | 56.1 |
| $\alpha$ | 128.7 | 1 | 122.2 | $OCH_3$ | 56.5 |
| C=O | 192.9 | 2 | 146.8 | $OCH_3$ | 59.6 |
| 2′ | 152.0 | 3 | 146.5 | $OCH_3$ | 60.6 |
| 3′ | 89.8 | 4 | 145.0 | $OCH_3$ | 60.9 |
| 4′ | 149.9 | 5 | 149.6 | $OCH_3$ | 61.6 |
| 5′ | 129.9 | 6 | 104.8 | $OCH_2O$ | 101.3 |
| 6′ | 140.0 | | | | |



**2′-Hydroxy-2,3,4,5,4′,5′,6′-heptamethoxychalcone**

*S. indica* [67]
$C_{22}H_{26}O_9$
**mp**: 88°C (dec.) (MeOH)
**UV**: 262 sh (3.80), 320 sh (4.20), 376 (4.34); +$CH_3ONa$, 250 sh (4.16), 317 (4.23), 345 sh (4.17), 410 sh (3.74); +$AlCl_3$, 270 sh (3.76), 335 sh (4.08), 406 (4.35), 440 sh (4.34); +$AlCl_3$/HCl, 265 sh (3.78), 335 sh (4.13), 386 (4.33), 430 (4.24); +$CH_3COONa$, 262 sh (3.80), 320 sh (4.20), 376 (4.33); +$CH_3COONa/H_3BO_3$, 262 sh (3.87), 320 sh (4.20), 376 (4.33)
**IR**: 3200 (OH), 1630 (C=O), 1610 (C=C aromatic)
**Mass**: 434 (40) $[M]^+$, 403 (100) $C_{21}H_{23}O_8$, 224 (75) $C_{12}H_{16}O_4$, 211 (30) $C_{10}H_{11}O_5$, 210 (20) $C_{10}H_{10}O_5$, 209 (30) $C_{11}H_{13}O_4$, 195 (35) $C_9H_7O_5$
**PMR** (DMSO-$d_6$): 3.73, 3.79 (3H, s, each 2×$OCH_3$), 3.85 (6H, s, 2×$OCH_3$), 3.87 (9H, s, 3×$OCH_3$), 6.41 (1H, s, H-3′), 7.12 (1H, s, H-6), 7.59 (1H, d, J = 16.9, $\alpha$-H), 7.82 (1H, d, J = 16.9, $\beta$-H), 12.24 (1H, s, 2′-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-$\beta$ | 137.8 | C-6′ | 153.5 | $OCH_3$ | 56.2 |
| $\alpha$ | 127.5 | 1 | 122.9 | $OCH_3$ | 56.2 |
| C=O | 193.1 | 2 | 147.6 | $OCH_3$ | 60.7 |
| 1′ | 110.6 | 3 | 147.1 | $OCH_3$ | 60.8 |
| 2′ | 158.5 | 4 | 145.1 | $OCH_3$ | 61.1 |
| 3′ | 96.6 | 5 | 149.9 | $OCH_3$ | 61.7 |
| 4′ | 158.5 | 6 | 105.4 | $OCH_3$ | 61.7 |
| 5′ | 134.8 | | | | |

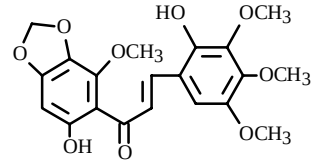


**2′-Hydroxy-2,3,4,5,6′-pentamethoxy-4′,5′-methylenedioxychalcone**

*S. indica* [67]
$C_{21}H_{20}O_9$: 418
**mp**: 110°C (dec.) (MeOH)

**UV**: 265 sh (3.820), 320 sh (4.15), 380 (4.23); +$CH_3ONa$, 318 (4.19), 345 sh (4.13), 435 (3.68); +$AlCl_3$, 275 sh (3.75), 335 sh (4.04), 397 (4.28), 460 (4.19); +$AlCl_3$/HCl, 275 sh (3.79), 335 sh (4.10), 384 (4.27), 452 (4.12); +$CH_3COONa$, 265 sh (3.85), 320 sh (4.17), 370 (4.25); +$CH_3COONa/H_3BO_3$, 265 sh (3.86), 320 sh (4.15), 370 (4.25)
**IR**: 3200 (OH), 1620 (C=C aromatic)
**Mass**: 418 (40) $[M]^+$, 387 (100) $C_{20}H_{19}O_8$, 224 (80) $C_{12}H_{16}O_4$, 209 (40) $C_{11}H_{13}O_4$, 195 (20) $C_9H_7O_5$, 194 (20) $C_9H_6O_5$
**PMR** (DMSO-$d_6$): 3.75, 3.82, 3.99 (each 3H, s, 3×$OCH_3$), 3.84 (6H, s, 2×$OCH_3$), 6.03 (2H, s, $OCH_2O$), 6.32 (1H, s, H-3′), 7.10 (1H, s, H-6), 7.48 (1H, d, J = 15.8, $\alpha$-H), 7.74 (1H, d, J = 15.8, $\beta$-H), 12.35 (1H, s, 2′-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-$\beta$ | 137.3 | C-6′ | 141.9 | C-6 | 105.3 |
| $\alpha$ | 127.7 | 1′ | 109.8 | $OCH_3$ | 56.1 |
| C=O | 192.7 | 1 | 122.7 | $OCH_3$ | 59.9 |
| 2′ | 158.3 | 2 | 147.4 | $OCH_3$ | 60.7 |
| 3′ | 92.8 | 3 | 146.9 | $OCH_3$ | 61.0 |
| 4′ | 153.2 | 4 | 145.1 | $OCH_3$ | 61.7 |
| 5′ | 129.7 | 5 | 199.7 | $OCH_2O$ | 101.6 |

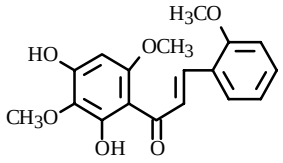


**2,2′-Dihydroxy-3,4,5,6′-tetramethoxy-4′,5′-methylenedioxychalcone**

*S. indica* [67]
$C_{20}H_{20}O_9$: 404
**mp**: 188°C (dec.) (MeOH)

**UV**: 272 (3.73), 327 (4.15), 405 (4.07); +$CH_3ONa$, 260 sh (3.81), 325 (3.83), 465 (3.68); +$AlCl_3$, 282 (3.65), 330 sh (3.90), 368 (3.97), 472 (4.14); +$AlCl_3$/HCl, 278 sh (3.75), 330 sh (3.98), 360 (4.05), 460 (4.18); +$CH_3COONa$, 272 (3.84), 327 (3.93), 405 (4.08); +$CH_3COONa/H_3BO_3$, 272 (3.90), 327 (4.08), 405 (422)
**IR**: 3400 (OH), 1640 (C=O), 1620 (C=C aromatic)
**Mass**: 404 (20) $[M]^+$, 386 (100) $C_{20}H_{18}O_8$, 210 (40) $C_{11}H_{14}O_4$, 195 (70) $C_9H_7O_5$
**PMR** (DMSO-$d_6$): 3.77, 3.80, 3.84, 3.99 (3H, s, each 4×$OCH_3$), 6.03 (2H, s, $OCH_2O$), 6.30 (1H, s, H-3′), 7.00 (1H, s, H-6), 7.55 (1H, d, J = 16.1, $\alpha$-H), 7.80 (1H, d, J = 16.1, $\beta$-H), 9.66 (1H, s, 2-OH), 11.60 (1H, s, 2′-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-$\beta$ | 138.0 | C-6′ | 141.7 | C-6 | 106.3 |
| $\alpha$ | 126.0 | 1′ | 109.7 | $OCH_3$ | 56.1 |
| C=O | 192.7 | 1 | 116.3 | $OCH_3$ | 59.8 |
| 2′ | 157.7 | 2 | 145.1 | $OCH_3$ | 60.5 |
| 3′ | 92.7 | 3 | 141.5 | $OCH_3$ | 60.9 |
| 4′ | 152.7 | 4 | 144.9 | $OCH_2O$ | 101.4 |
| 5′ | 129.6 | 5 | 145.9 | | |



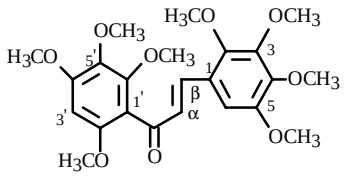
**2′,4′-Dihydroxy-2,3′,6′-trimethoxychalcone**

*S. discolor* [111]
$C_{18}H_{18}O_6$: 330
**mp**: 134°C (dec.) (MeOH)

**UV**: 250 sh (3.89), 315 sh (4.13), 368 (4.44); +$CH_3ONa$, 298 (4.00), 398 (4.46); +$AlCl_3$, 252 sh (4.08), 320 sh (4.06), 400

(4.55); +$AlCl_3$/HCl, 251 sh (4.16), 320 sh (4.10), 396 (4.54); +$CH_3COONa$, 253 (3.94), 301 (4.01), 396 (4.45); +$CH_3COONa/H_3BO_3$, 258 sh (3.87), 280 (3.90), 322 (3.95), 418 (4.47)
**IR**: 3300 (OH), 1650 (C=O), 1610, 1580 (C=C aromatic)
**Mass**: 330 (67) $[M]^+$, 196 (100) $C_9H_8O_5$, 181 (55) $C_8H_5O_5$
**PMR** (DMSO-$d_6$): 3.68, 3.87, 3.91 (3H, s, each 3×$OCH_3$), 6.10 (1H, s, H-5′), 6.96-7.11 (1H, m, H-5), 7.11 (1H, br.d, J = 7.3, H-3), 7.36-7.53 (1H, m, H-4), 7.70 (1H, dd, J = 7.8 and 1.5, H-6), 7.96 (2H, s, $\alpha,\beta$-H), 10.47 (1H, br.s, 4′-OH), 14.04 (1H, s, 2′-OH)
**$^{13}$C NMR** (DMSO-$d_6$):

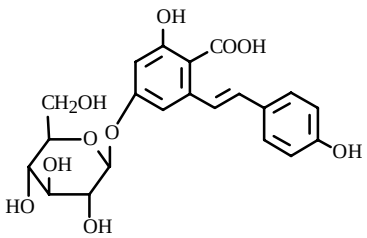
| | | | | | |
|---|---|---|---|---|---|
| C-1 | 123.4 | C-1′ | 105.5 | C-$\alpha$ | 127.8 |
| 2 | 158.1 | 2′ | 157.4 | $\beta$ | 137.4 |
| 3 | 111.9 | 3′ | 129.2 | (>C=O) | 192.7 |
| 4 | 132.1 | 4′ | 158.5 | $OCH_3$ | 55.7 |
| 5 | 121.0 | 5′ | 91.6 | $OCH_3$ | 56.0 |
| 6 | 129.0 | 6′ | 159.1 | 3-$OCH_3$ | 59.9 |




**2,3,4,5,2′,4′,5′,6′-Octamethoxychalcone**

*S. indica* [67]
$C_{23}H_{28}O_9$: 448
**mp**: 205°C (dec.) (MeOH)
**UV**: 314 (4.03), 355 sh (3.91)
**IR**: 1650 (C=O), 1610, 1580 (C=C aromatic)
**Mass**: 448 (20) $[M]^+$, 417 (100) $C_{22}H_{25}O_8$
**PMR** (DMSO-$d_6$): 3.64, 3.71, 3.72, 3.74, 3.83, 3.89 (each 3H, s, 6×$OCH_3$), 3.80 (6H, s, 2×$OCH_3$), 6.59 (1H, s, H-3′), 7.04 (1H, d, J = 16.1, $\alpha$-H), 7.16 (1H, s, 6-H), 7.40 (1H, d, J = 16.1, $\beta$-H)
**$^{13}$C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-$\beta$ | 138.6 | C-1′ | 115.7 | $OCH_3$ | 56.0 |
| $\alpha$ | 128.7 | 1 | 122.2 | $OCH_3$ | 56.1 |
| C=O | 193.1 | 2 | 146.8 | $OCH_3$ | 60.5 |
| 2′ | 152.3 | 3 | 146.5 | $OCH_3$ | 60.5 |
| 3′ | 93.3 | 4 | 144.9 | $OCH_3$ | 60.9 |
| 4′ | 154.4 | 5 | 149.6 | $OCH_3$ | 61.3 |
| 5′ | 135.3 | 6 | 104.8 | $OCH_3$ | 61.6 |
| 6′ | 150.5 | $OCH_3$ | 56.0 | | |

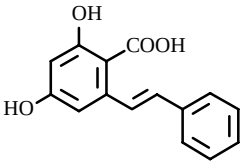



**5-($\beta$-D-Glucosyloxy)-3-hydroxy-*trans*-stilbene-2-carboxylic acid (gaylussacin)**

*S. scandens* [192]
$C_{21}H_{22}O_9$: 418
**mp**: 236°C (dec.) (MeOH—$H_2O$)
$[\alpha]_D^{22}$ -85.9° (*c* 0.04, MeOH)
**UV**: 252 (4.25), 300 (4.18); +$CH_3ONa$, 249 (4.23), 303 (4.20); +$AlCl_3$, 257 (4.18), 303 (4.20)
**IR**: 3550 (OH), 3100, 1630 (COOH), 1600 (C=C aromatic)
**EI-MS** *m/z* (%): 374 (10) $C_{20}H_{22}O_7$, 212 (100) $C_{14}H_{12}O_2$
**FAB-MS** *m/z* (%): 419 (40) $[M + 1]^+$, 257 (100) $[C_{15}H_{12}O_4 + 1]$
**PMR** (DMSO-$d_6$): 3.0-4.0 (m, sugar protons), 4.99 (1H, d, J = 5.9, glucose anomeric proton), 6.55 (1H, d, J = 2.0, H-4),

6.92 (1H, d, J = 2.0, H-6), 7.09 (1H, d, J = 16.1, H-$\alpha$), 7.62 (1H, d, J = 16.1, H-$\alpha'$), 7.26-7.54 (5H, m, H-2′,3′,4′,5′,6′)
$^{13}$**C NMR** (DMSO-$d_6$):

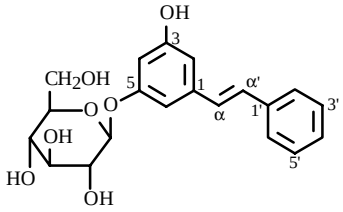
| | | | | | |
|---|---|---|---|---|---|
| C-1 | 140.3 | C-2′ | 126.8 | C-1″ | 100.4 |
| 2 | 110.0 | 3′ | 129.0 | 2″ | 73.4 |
| 3 | 161.3 | 4′ | 128.0 | 3″ | 76.8 |
| 4 | 103.4 | 5′ | 129.0 | 4″ | 70.1 |
| 5 | 160.7 | 6′ | 126.8 | 5″ | 77.5 |
| 6 | 106.3 | $\alpha$ | 131.0 | 6″ | 61.0 |
| 1′ | 137.3 | $\alpha'$ | 128.2 | COOH | 171.7 |




**3,5-Dihydroxy-*trans*-stilbene-2-carboxylic acid**

*S. scandens* [192]
$C_{15}H_{12}O_4$: 256
**mp**: 165°C (dec.) (MeOH—$H_2O$)
**UV**: 253 (4.26), 303 (4.24); +$CH_3ONa$, 269 (4.44), 313 (4.21); +$AlCl_3$, 262 (4.26), 303 (4.21)
**IR**: 3400 (OH), 3000, 1630 (COOH), 1600 (C=C aromatic)
**EI-MS** *m/z* (%): 256 (60) $[M]^+$, 212 (100) $C_{14}H_{12}O_2$
**PMR** (DMSO-$d_6$): 6.27 (1H, d, J = 2.0, H-4), 6.58 (1H, d, J = 2.0, H-6), 6.91 (1H, d, J = 16.1, H-$\alpha$), 7.69 (1H, d, J = 16.1, H-$\alpha'$), 7.31-7.58 (5H, m, H-2′,3′,4′,5′,6′), 10.26 (1H, br.s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

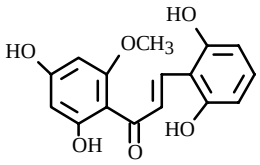
| | | | | | |
|---|---|---|---|---|---|
| C-1 | 141.7 | C-6 | 106.7 | C-5′ | 128.9 |
| 2 | 105.5 | 1′ | 137.3 | 6′ | 126.6 |
| 3 | 163.1 | 2′ | 126.6 | $\alpha$ | 130.0 |
| 4 | 102.2 | 3′ | 128.9 | $\alpha'$ | 129.3 |
| 5 | 161.8 | 4′ | 127.9 | COOH | 172.4 |




**Pinosylvin-3-O-$\beta$-D-glucopyranoside**

*S. scandens* [192]
$C_{20}H_{22}O_7$: 374
**mp**: 191°C (dec.) (MeOH—$H_2O$)
$[\alpha]_D^{20}$ -79.8° (*c* 0.04, MeOH)
**UV**: 300 (4.18), 310 (4.18); +$CH_3ONa$, 261 (3.88), 310 (4.15); +$AlCl_3$, 300 (4.18), 310 (4.17)
**IR**: 3350 (OH), 1600, 1585 (C=C aromatic)
**FAB-MS** *m/z* (%): 375 (20) $[M + 1]^+$, 213 (100) $[C_{14}H_{12}O_2 + 1]$
**PMR** (DMSO-$d_6$): 3.0-4.0 (m, sugar protons), 4.86 (1H, d, J = 6.4, glucose anomeric proton), 6.43 (1H, br.t, J = 1.7, H-4), 6.67 (1H, br.s, H-2), 6.84 (1H, br.s, H-6), 7.15 (2H, br.s, H-$\alpha,\alpha'$), 7.26-7.64 (5H, m, H-2′,3′,4′,5′,6′), 9.51 (1H, s, 5-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-1 | 139.1 | C-2′ | 126.7 | C-1″ | 100.9 |
| 2 | 105.4 | 3′ | 128.9 | 2″ | 73.5 |
| 3 | 158.7 | 4′ | 127.9 | 3″ | 76.9 |
| 4 | 103.6 | 5′ | 128.9 | 4″ | 70.0 |
| 5 | 159.2 | 6′ | 126.7 | 5″ | 77.3 |
| 6 | 107.9 | $\alpha$ | 128.8 | 6″ | 60.9 |
| 1′ | 137.1 | $\alpha'$ | 128.8 | | |

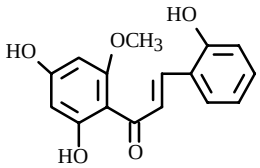


**2,6,2′,4′-Tetrahydroxy-6′-methoxychalcone**

*S. baicalensis* [127, 141, 181]
$C_{16}H_{14}O_6$: 302
**mp**: 165°C (dec.) (MeOH)

**UV**: 380; +$CH_3ONa$, 410; +$AlCl_3$, 247 sh , 330, 378, 416 sh; +$CH_3COONa$, 320 sh, 390
**IR**: 3400 (OH), 1650 (CO), 1610 (C=C aromatic)
**PMR** (DMSO-$d_6$): 3.83 (3H, s, $OCH_3$), 5.91 (1H, d, J = 1.9, H-3′), 5.99 (1H, d, J = 1.9, H-5′), 6.38 (2H, d, J = 8.1, H-3,5), 7.00 (1H, t, J = 8.1, H-4), 8.09 (1H, d, J = 15.6, $\alpha$-H), 8.40 (1H, d, J = 15.6, $\beta$-H), 14.18 (1H, s, 2′-OH) [181]
$^{13}$**C NMR** (DMSO-$d_6$) [181]:

| | | | | | |
|---|---|---|---|---|---|
| C-1 | 110.3 | C-1′ | 105.4 | C=O | 193.5 |
| 2 | 158.9 | 2′ | 162.7 | C-$\alpha$ | 128.1 |
| 3 | 106.7 | 3′ | 95.9 | $\beta$ | 135.1 |
| 4 | 131.4 | 4′ | 164.5 | 6′-$OCH_3$ | 55.7 |
| 5 | 106.7 | 6′ | 166.6 | | |
| 6 | 158.9 | | | | |



**2,2′,4′-Trihydroxy-6′-methoxychalcone**

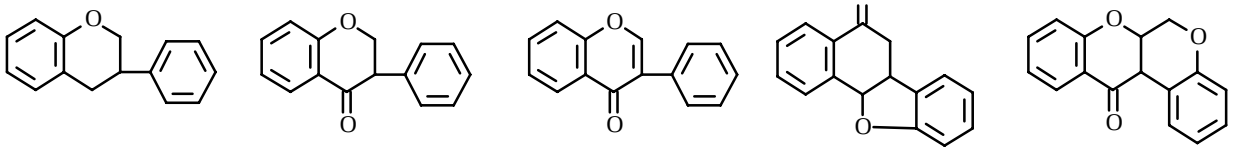
*S. strigillosa* [188]
$C_{16}H_{14}O_5$: 286
**mp**: 182-183°C (dec.)

**UV**: 300 sh (4.12), 364 (4.47); +$CH_3ONa$, 424 (4.45); +$AlCl_3$, 315 sh (4.01), 403 (4.58); +$AlCl_3$/HCl, 315 sh (4.02), 392 (4.55); +$CH_3COONa$, 285 (4.02), 385 (4); +$CH_3COONa/H_3BO_3$, 315 sh (4.05), 410 (4.43)
**IR**: 3535 (OH), 1640 (C=O $\gamma$-pyrone), 1616 (C=C aromatic)
**PMR** (DMSO-$d_6$): 3.86 (3H, s, 6′-$OCH_3$), 5.92 (1H, d, J = 1.8, H-3′), 6.01 (1H, d, J = 1.8, H-5′), 6.87 (1H, br.t, J = 8.0, H-5), 6.93 (1H, br.d, J = 8.0, H-3), 7.25 (1H, dt, J = 1.6 and 8.0, H-4), 7.59 (1H, dd, J = 1.6 and 8.0, H-6), 7.90 (1H, d, J = 16.0, H-$\beta$ or $\alpha$), 7.93 (1H, d, J = 16.0, H-$\alpha$ or $\beta$), 10.24 (1H, s, 2-OH), 10.62 (1H, s, 4′-OH), 13.84 (1H, s, 2′-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-1 | 121.7 | C-1′ | 105.2 | C-$\beta$ | 137.9 |
| 2 | 157.1 | 2′ | 162.6 | $\alpha$ | 126.7 |
| 3 | 116.3 | 3′ | 95.8 | CO | 192.2 |
| 4 | 131.6 | 4′ | 164.8 | 6-$OCH_3$ | 55.9 |
| 5 | 119.5 | 5′ | 91.6 | | |
| 6 | 128.8 | 6′ | 166.2 | | |

## ISOFLAVONES

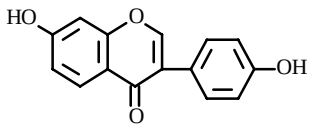
Isoflavanoids, which are similar in chemical structure and biogenetic origin to flavonoids, are also formed in plants. Like flavonoids, they are subdivided depending on the structure into isoflavanes (I), isoflavanones (II), isoflavones (III), pterocarpanes (IV), and rotenoids (V).



I II III IV V

Isoflavones such as daidzein, formononetin, genistein, and others are the most common of these groups of phenolic compounds [6].

Only *S. baicalensis* of plants of the *Scutellaria* genus have yielded compounds that were identified as the isoflavones daidzein, daidzin, formononetin, and puerarin [79].

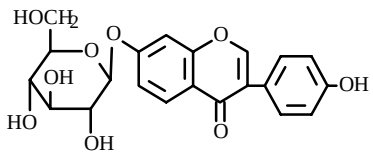


**Daidzein (7,4′-dihydroxyisoflavone)**

*S. baicalensis* [79]
$C_{15}H_{10}O_4$: 254
**mp**: 276-277°C

**UV**: 238 sh, 249, 259 sh, 303 sh; +$CH_3COONa$, 253, 272 sh, 310, 330 sh; +$CH_3COONa/H_3BO_3$, 261 sh, 240, 303 sh, 300 sh; +$AlCl_3$, 249 sh, 240, 240, 260 sh; +$AlCl_3$/HCl, 249, 262 sh, 302 sh; +$CH_3ONa$, 259, 289, 328
**Mass**: 254 $[M]^+$, 213, 202, 185, 149, 143, 137, 129, 118, 111, 97 [79]
**PMR** (DMSO-$d_6$): 8.22 (1H, s, H-2), 7.94 (1H, d, J = 9.0, H-5), 6.90 (1H, dd, J = 9.0 and 2.0, H-6), 6.83 (1H, d, J = 2, H-8), 7.36 (2H, d, J = 9.0, H-2′,6′), 6.79 (2H, d, J = 9.0, H-3′,5′) [79]
$^{13}$**C NMR** (DMSO-$d_6$) [79]:

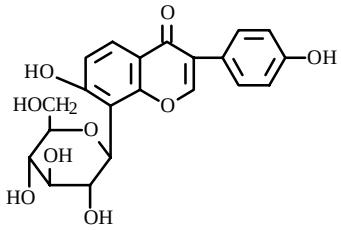
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 152.2 | C-7 | 162.6 | C-2′ | 129.9 |
| 3 | 122.6 | 8 | 102.1 | 3′ | 115.0 |
| 4 | 178.5 | 9 | 157.6 | 4′ | 147.3 |
| 5 | 127.1 | 10 | 116.8 | 5′ | 115.0 |
| 6 | 115.0 | 1′ | 123.9 | 6′ | 129.9 |



**Daidzin (daidzein-7-O-glucoside)**

*S. baicalensis* [79]
$C_{21}H_{20}O_9$: 416
**mp**: 235-236°C

**UV**: 256, 313 sh; +$CH_3COONa$, 256, 322 sh; +$CH_3COONa/H_3BO_3$, 254, 318 sh; +$AlCl_3$, 258, 304 sh; +$AlCl_3$/HCl, 257, 303 sh, 362; +$CH_3ONa$, 256, 272 sh, 320 sh
**PMR** (Py-$d_5$): 3.90-4.55 (sugar protons), 5.63 (1H, d, J = 6.5, H-1″), 7.04 (1H, d, J = 2.0, H-8), 7.18 (1H, dd, J = 8.0 and 2.0, H-6), 7.93 (1H, s, H-2), 8.18 (1H, d, J = 8, H-5)

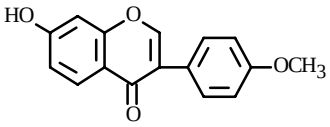


**Puerarin (7,4′-dihydroxy-8-C-glucosylisoflavone)**

*S. baicalensis* [79]
$C_{21}H_{20}O_9$: 416
**mp**: 187°C (dec.)
**UV**: 243 sh, 251 sh, 309; +$CH_3OH$/NaOH, 213, 265, 292 sh, 336; +$CH_3OH/CH_3COONa$, 260, 242
**PMR** (DMSO-$d_6$): 8.21 (1H, s, H-2), 7.82 (1H, d, J = 8.8, H-5), 6.85 (1H, d, J = 8.8, H-6), 7.40 (2H, d, J = 8.5, H-2′,6′), 6.80 (2H, d, J = 8.5, H-3′,5′), 4.82 (1H, d, J = 9.3, H-1 sugar) [179]

$^{13}$C NMR (DMSO-$d_6$) [179]:

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 152.0 | C-9 | 157.1 | C-6′ | 130.1 |
| 3 | 123.1 | 10 | 117.4 | 1″ | 74.1 |
| 4 | 174.8 | 1′ | 122.9 | 2″ | 70.8 |
| 5 | 125.8 | 2′ | 130.1 | 3″ | 79.2 |
| 6 | 114.3 | 3′ | 115.1 | 4″ | 70.5 |
| 7 | 166.4 | 4′ | 157.3 | 5″ | 81.6 |
| 8 | 111.9 | 5′ | 115.1 | 6″ | 61.3 |




**Formononetin (7-hydroxy-4′-methoxyflavone)**

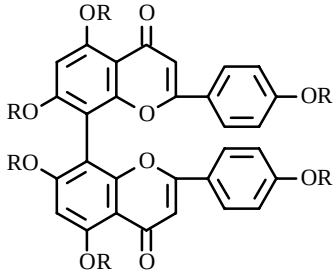
*S. baicalensis* [79]
$C_{16}H_{12}O_4$: 268
**mp**: 260-261°C
**UV**: 240 sh, 248, 259 sh, 311; +$CH_3COONa$, 254, 312 sh, 334; +$CH_3COONa/H_3BO_3$, 264 sh, 303; +$AlCl_3$, 239 sh, 248, 261 sh, 301; +$AlCl_3$/HCl, 240 sh, 261 sh; +$CH_3ONa$, 249, 255, 301, 273 sh
**IR**: 3150 (OH), 1641 (C=O γ-pyrone), 1624, 1613-1600, 1573, 1518 (C=C)
**Mass**: 268 (100) $[M]^+$, 267 (34), 253 (22), 239 (3), 225 (12), 197 (5), 136 (5), 132 (70), 117 (20), 108 (10), 89 (27)
**PMR** (Py-$d_5$): 3.57 (3H, s, $OCH_3$), 6.99 (2H, d, J = 9.0, H-3′,5′), 7.07 (br.s, H-8), 7.14 (1H, dd, J = 9.0 and 2.0, H-6), 7.72 (1H, d, J = 9.0, H-2′,6′), 8.10 (1H, s, H-2), 8.40 (1H, d, J = 9.0, H-5)
**$^{13}$C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 152.2 | C-7 | 162.7 | C-2′ | 130.0 |
| 3 | 124.4 | 8 | 102.3 | 3′ | 113.6 |
| 4 | 175.1 | 9 | 157.7 | 4′ | 159.2 |
| 5 | 127.2 | 10 | 117.0 | 5′ | 113.6 |
| 6 | 115.1 | 1′ | 123.8 | 6′ | 130.0 |

## BIFLAVONOIDS

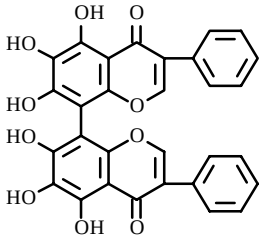
Bibaicalein is the first and as yet only representative of biflavonoids found in skullcap plants. Keeping in mind the formation scheme of bimolecular compounds [6], it seems likely that the number of this type of phenolic compounds may be several times greater. Therefore, research in this area of the chemistry of natural compounds is developing rapidly.

According to the proposed classification [6], bibaicalein belongs to the cupressiflavone group of bimolecular compounds.




Dimeric compounds consisting of flavone—flavone, flavone—flavanone, isoflavone—flavanone, isoflavone—isoflavone, chalcone—flavanone, and other components are known. The dimers can be formed through C–C or C–O–C bonds of C atoms at various positions (rings A, B, and C) [6].

The bimolecular nature of the compounds was determined using PMR and mass spectral data [163]. The nature and sequence of bonds were established by comparing $^{13}$C NMR spectra, which gave unambiguous results [164].



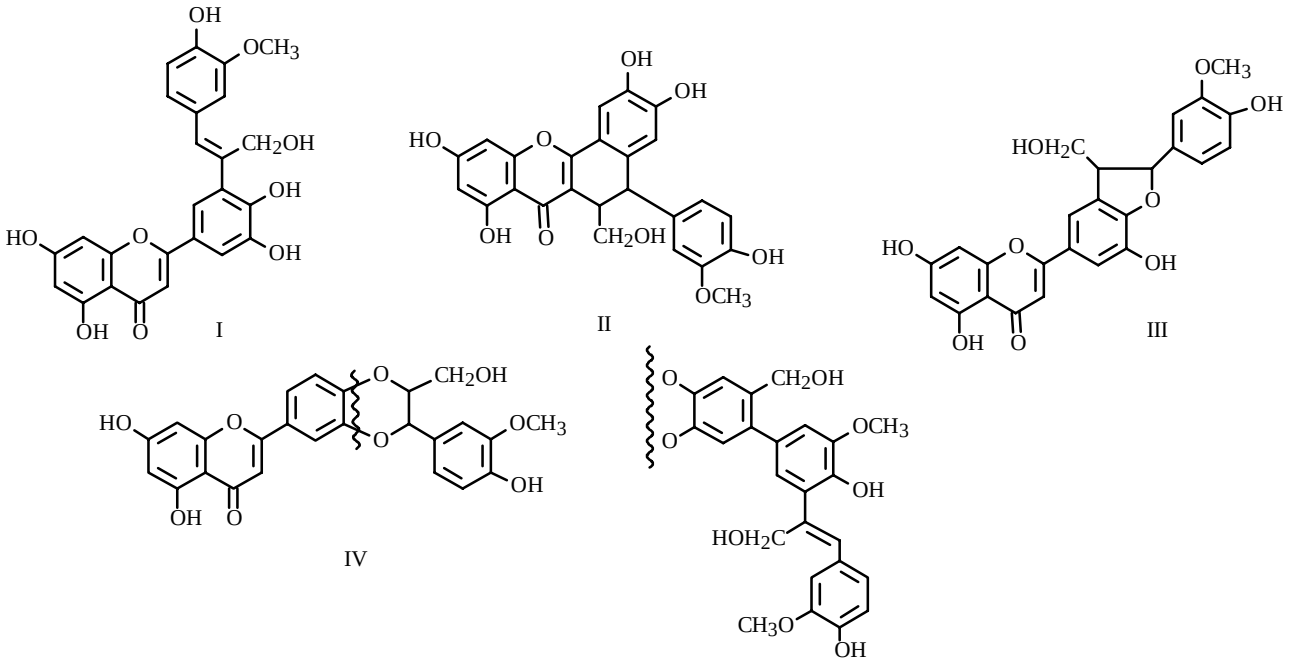
**8,8″-Bibaicalein (5,5″,6,6″,7,7″-hexahydroxy-8,8″-biflavone)**

*S. alpina* [60]
$C_{30}H_{18}O_{10}$: 583
**mp**: >350°C
**UV**: 221 (4.62), 241 (4.61), 285 (4.56), 326 (4.28); +$CH_3ONa$, 261 (4.64), 376 (4.19); +$AlCl_3$, 228 (4.58), 253 (4.54), 275 (4.55), 295 sh (4.41), 320 (4.23). 388 (4.37); +$AlCl_3$/HCl, 228 (4.58), 247 (4.62), 301 (4.47), 350 (4.35); +$CH_3COONa$, 261 (4.72), 376 (4.26); +$H_3BO_3$/$CH_3COONa$, 261 (4.66), 376 (4.24)
**IR**: 3450 (OH), 1650 (C=O γ-pyrone), 1610, 1580 (C=C aromatic)
**PMR** (DMSO-$d_6$): 6.95 (2H, s, H-3/3″), 7.38 (4H, t, J = 7.3, H-3′,5′/3‴,5‴), 7.47 (2H, t, J = 7.3, H-4′/4‴), 7.61 (4H, d, J = 7.3, H-2′,6′/2‴,6‴), 9.26 (2H)
**$^{13}$C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2/2″ | 162.7 | C-7/7″ | 152.8 | C-2′/2‴ | 125.7 |
| 3/3″ | 104.3 | 8/8″ | 98.5 | 3′/3‴ | 128.9 |
| 4/4″ | 182.3 | 9/9″ | 147.8 | 4′/4‴ | 131.7 |
| 5/5″ | 146.5 | 10/10″ | 103.9 | 5′/5‴ | 128.9 |
| 6/6″ | 129.0 | 1′/1‴ | 130.8 | 6′/6‴ | 125.7 |

## LIGNOFLAVONOIDS AND LIGNANIC GLYCOSIDES

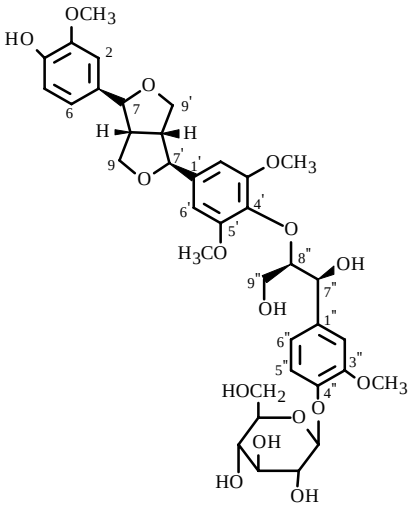
Lignoflavonoids include a large group of phenolic compounds that are similar to biflavonoids in biogenetic origin and chemical structure. They are condensation products of a flavonoid unit with derivatives of (*n*)-phenylpropanol in 1:1, 1:2, etc., ratios that form acyclic (I), cyclic (II), and heterocyclic compounds of the tetrahydrofuran (III) and morpholine (IV) series [165].



The structures of lignoflavonoids have been found using chemical methods [166] such as PMR and $_{13}$C NMR spectra [165, 167] and mass-spectral fragmentation patterns of the components [168].

This group of compounds is represented in plants of the *Scutellaria* genus by scutellaprostins A-F (six compounds), all of which were isolated from *S. prostrata* [169]. The structural formulas show that the phenylpropanol moiety in these compounds is fused to the flavonoid at ring A to form a morpholine ring that incorporates C-7—C-8 and C-6—C-7. Three new

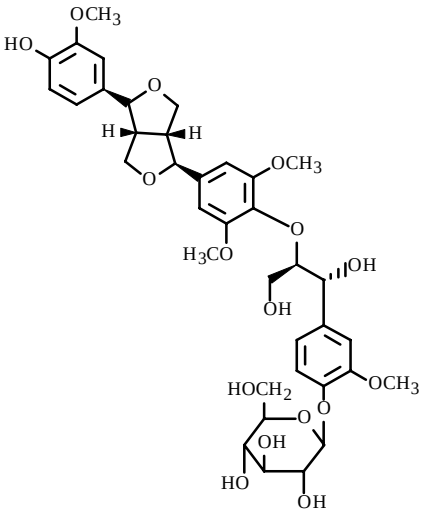
lignan glycosides were recently isolated from *S. baicalensis*. These were derivatives of 2,6-diaryl-3,7-dioxabicyclo-[3,3,0]-octane (eudesmane).



**Hediotol C-4″-O-*β*-D-glucopyranoside**

*S. baicalensis* [189]
$C_{37}H_{46}O_{16}$: 746
**mp**: amorph.
$[\alpha]_D^{25}$ -11.3° (*c* 0.02, MeOH)
**UV**: 207 (4.82), 230 sh (4.37), 276 (3.86)
**IR**: 3460 (OH), 1608 (C=C aromatic)
**EI-MS** *m/z* (%): 536 (74), 388 (100), 181 (60), 151 (60), 137 (80)
**FAB-MS** *m/z* (%): 769 (2) $[M + Na]^+$
**PMR** (DMSO-$d_6$): 3.03 (2H, m, H-8,8′), 3.14 (1H, t, J = 9.0, H-4‴), 3.24 (2H, m, H-2‴,3‴), 3.28 (1H, m, H-5‴), 3.37 (1H, dd, J = 4.0 and 11.4, H-9″), 3.43 (1H, dd, J = 5.6 and 11.2, H-6‴), 3.64 (1H, br.d, J = 11.2, H-6‴′), 3.68 (1H, dd, J = 4.5 and 11.4, H-9″), 3.74 (3H, s, $OCH_3$), 3.75 (3H, s, each 3×$OCH_3$), 3.77 (2H, dd, J = 3.0 and 9.0, H-9,9″), 4.11 (1H, q, J = 5.0, H-8″), 4.15 (2H, br.t, J = 8.0, H-9,9″), 4.60 (1H, d, J = 5.0, H-7), 4.65 (1H, d, J = 5.0, H-7′), 4.82 (1H, d, J = 5.0, H-7″), 4.86 (1H, d, J = 7.0, H-1‴), 6.63 (2H, s, H-2′,6′), 6.72 (1H, d, J = 8.0, H-5), 6.75 (1H, dd, J = 1.8 and 8.0, H-6), 6.83 (1H, dd, J = 1.8 and 8.0, H-6″), 6.88 (1H, d, J = 1.8, H-2), 6.97 (1H, d, J = 1.8, H-2″), 7.01 (1H, d, J = 8.0, H-5″)
**$^{13}$C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-1 | 132.4 | C-4′ | 137.1 | C-7″ | 72.0 |
| 2 | 110.6 | 5′ | 152.8 | 8″ | 86.1 |
| 3 | 147.6 | 6′ | 103.4 | 9″ | 59.8 |
| 4 | 145.9 | 7′ | 85.3 | 1‴ | 100.3 |
| 5 | 115.2 | 8′ | 53.6 | 2‴ | 73.2 |
| 6 | 118.8 | 9′ | 71.4 | 3‴ | 76.7 |
| 7 | 85.3 | 1″ | 136.3 | 4‴ | 69.7 |
| 8 | 53.9 | 2″ | 111.4 | 5‴ | 77.0 |
| 9 | 71.2 | 3″ | 148.5 | 6‴ | 60.7 |
| 1′ | 134.8 | 4″ | 145.5 | 2×$OCH_3$ | 55.8 |
| 2′ | 103.4 | 5″ | 114.9 | 2×$OCH_3$ | 56.1 |
| 3′ | 152.8 | 6″ | 119.3 | | |



**Hediotol D-4″-O-*β*-D-glucopyranoside**

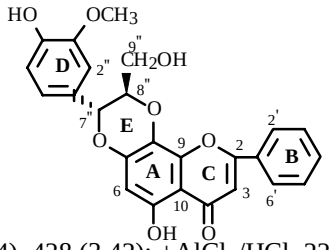
*S. baicalensis* [189]
$C_{37}H_{46}O_{16}$: 746
**mp**: amorph.
$[\alpha]_D^{25}$ -7.4° (*c* 0.02, MeOH)
**UV**: 207 (4.79), 228 sh (4.36), 376 (3.90)
**IR**: 3450 (OH), 1596 (C=C aromatic)
**EI-MS** *m/z* (%): 536 (95), 388 (100), 181 (55), 151 (55), 137 (70)
**FAB-MS** *m/z* (%): 769 (2) $[M + Na]^+$
**PMR** (DMSO-$d_6$): 3.03 (2H, m, H-8,8′), 3.14 (1H, t, J = 9.0, H-4‴), 3.19 (1H, dd, J = 4.5 and 11.0, H-9″), 3.25 (2H, m, H-2‴,3‴), 3.28 (1H, m, H-5‴), 3.43 (1H, dd, J = 5.6 and 11.2, H-6‴), 3.62 (1H, dd, J = 4.5 and 11.0, H-9″), 3.65

(1H, br.d, J = 11.2, H-6‴), 3.73 (3H, s, $OCH_3$), 3.74 (3H, s, each 2×$OCH_3$), 3.76 (3H, s, $OCH_3$), 3.77 (2H, dd, J = 3.0 and 9.0, H-9,9′), 4.00 (1H, q, J = 5.0, H-8″), 4.15 (2H, m, H-9,9′), 4.60 (1H, d, J = 5.0, H-7), 4.65 (1H, d, J = 5.0, H-7′), 4.86 (1H, d, J = 7.0, H-1‴), 4.87 (1H, d, J = 5.0, H-7″), 6.62 (2H, s, H-2′,6′), 6.72 (1H, d, J = 8.0, H-5), 6.75 (1H, dd, J = 1.8 and 8.0, H-6), 6.88 (1H, d, J = 1.8, H-2), 6.89 (1H, dd, J = 1.8 and 8.0, H-6″), 7.00 (1H, d, J = 8.0, H-5″), 7.03 (1H, d, J = 1.8, H-2″)

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

| | | | | | |
|---|---|---|---|---|---|
| C-1 | 132.5 | C-4′ | 137.3 | C-7″ | 71.2 |
| 2 | 110.6 | 5′ | 152.7 | 8″ | 86.9 |
| 3 | 147.7 | 6′ | 103.4 | 9″ | 60.2 |
| 4 | 145.9 | 7′ | 85.3 | 1‴ | 100.3 |
| 5 | 115.3 | 8′ | 53.7 | 2‴ | 73.3 |
| 6 | 118.9 | 9′ | 71.4 | 3‴ | 76.8 |
| 7 | 85.3 | 1″ | 136.0 | 4‴ | 69.8 |
| 8 | 54.0 | 2″ | 111.3 | 5‴ | 77.0 |
| 9 | 71.4 | 3″ | 148.4 | 6‴ | 60.8 |
| 1′ | 135.3 | 4″ | 145.5 | 2×$OCH_3$ | 55.8 |
| 2′ | 103.4 | 5″ | 114.8 | 2×$OCH_3$ | 56.2 |
| 3′ | 152.7 | 6″ | 119.1 | | |

## Scutellaprostin A




*S. prostrata* [169]

$C_{25}H_{20}O_8$: 448

**mp**: 221-222°C (dec.) (MeOH)

$[\alpha]_D^{20}$ ±0° (*c* 0.05, MeOH)

**UV**: 234 (4.24), 286 (4.45), 370 (3.40); +$CH_3ONa$, 253 (4.27), 289 (4.44), 394 (3.27); +$AlCl_3$, 221 (4.35), 236 (4.31), 290 (4.34), 310 (4.38), 346 sh (3.74), 428 (3.42); +$AlCl_3$/HCl, 221 (4.36), 238 (4.29), 290 (4.33), 309 (4.38), 346 sh (3.63), 440 (3.44); +$CH_3COONa$, 285 (4.44), 360 (3.40)

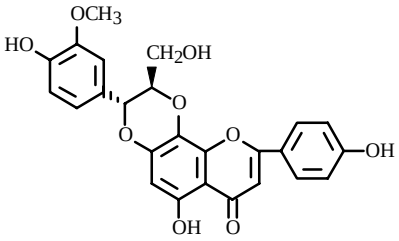
**IR**: 3460 (OH), 1664 (C=O γ-pyrone), 1616 (C=C aromatic)

**EI-MS** *m/z* (%): 448 (100) $[M]^+$, 270 (89) $C_{15}H_{10}O_5$, 180 (72) $C_{10}H_{12}O_5$, 168 (40) $C_7H_4O_5$, 137 (97) $C_8H_9O_2$, 124 (52) $C_7H_8O_2$, 105 (27) $C_7H_5O$

**PMR** (DMSO-$d_6$): 7.10 (s, H-3), 6.43 (s, H-6), 8.13 (1H, br.dd, J = 8.2 and 1.7, H-2′), 7.53-7.65 (3H, m, H-3′,4′,5′), 8.13 (3H, br.dd, J = 8.2 and 1.7, H-6′), 7.06 (1H, d, J = 1.8, H-2″), 6.83 (1H, d, J = 8.4, H-5″), 6.90 (1H, dd, J = 8.4, and 1.8, H-6″), 5.16 (1H, d, J = 7.7, H-7″), 4.31 (1H, ddd, J = 7.7, 4.4, and 2.6, H-8″), 3.39 (1H, ddd, J = 12.5, 5.5, and 4.4, H-9″), 3.65 (1H, ddd, J = 12.5, 5.5, and 2.6, H-9″), 3.79 (3H, s, $OCH_3$), 12.25 (1H, s, 5-OH), 9.20 (1H, s, Ar-OH), 5.09 (1H, m, J = 5.5, 9″-OH)

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

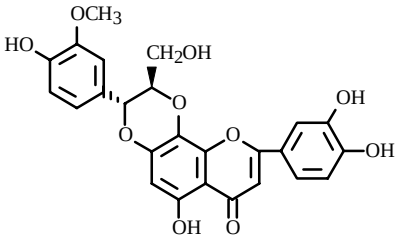
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 163.1 | C-1′ | 130.5 | C-4″ | 147.2 |
| 3 | 105.3 | 2′ | 126.4 | 5″ | 115.3 |
| 4 | 182.2 | 3′ | 129.2 | 6″ | 120.5 |
| 5 | 153.0 | 4′ | 132.2 | 7″ | 77.1 |
| 6 | 99.0 | 5′ | 129.2 | 8″ | 77.6 |
| 7 | 149.6 | 6′ | 126.4 | 9″ | 60.0 |
| 8 | 124.6 | 1″ | 126.6 | $OCH_3$ | 55.7 |
| 9 | 144.5 | 2″ | 111.7 | | |
| 10 | 104.9 | 3″ | 147.6 | | |



**Scutellaprostin B**

*S. prostrata* [169]
$C_{25}H_{20}O_9$: 464
**mp**: 255-256°C (dec.) (MeOH)
$[\alpha]_D^{20}$ ±0° (*c* 0.05, MeOH)
**UV**: 229 (4.45), 285 (4.41), 303 sh (4.32), 310 sh (4.31), 332 sh (4.27); $+CH_3ONa$, 233 sh (4.49), 258(4.49), 281 (4.51), 303 sh (4.31), 400 (4.54); $+AlCl_3$, 237 (4.46), 290 (4.36), 323 (4.34), 357 (4.35), 424 (3.94); $+AlCl_3$/HCl, 236 (4.46), 290 (4.36), 322 (4.38), 353 (4.34), 422 (3.82); $+CH_3COONa$, 230 sh (4.49), 283 (4.39), 310 sh (4.23), 333 (4.17), 396 (4.11)
**IR**: 3457 (OH), 1667 (C=O γ-pyrone), 1612 (C=C aromatic)
**EI-MS** *m/z* (%): 464 (26) $[M]^+$, 286 (100) $C_{15}H_{10}O_6$, 180 (55), $C_{10}H_{12}O_3$, 168 (81) $C_7H_4O_5$, 137 (90) $C_8H_9O_9$, 124 (48) $C_7H_8O_2$, 121 (20) $C_7H_5O_2$
**PMR** (DMSO-$d_6$): 6.84 (1H, s, H-3), 6.36 (1H, s, H-6), 7.96 (1H, d, J = 8.8, H-2′), 6.94 (1H, d, J = 8.8, H-3′), 6.94 (1H, d, J = 8.8, H-4′,5′), 7.96 (1H, d, J = 8.8, H-6′), 7.05 (1H, d, J = 1.7, H-2″), 6.83 (1H, d, J = 8.2, H-5″), 6.89 (1H, dd, J = 8.2 and 1.7, H-6″), 5.12 (1H, d, J = 7.9, H-7″), 4.26 (1H, ddd, J = 7.9, 4.9, and 2.8, H-8″), 3.45 (1H, ddd, J = 12.1, 5.5, and 2.8, H-9″), 3.66 (1H, ddd, J = 12.1, 5,5, and 4.9, H-9″), 3.80 (3H, s, $OCH_3$), 12.38 (1H, s, 5-OH), 9.16 (1H, s, Ar-OH), 10.36 (1H, s, Ar-OH), 5.03 (1H, m, J = 5.5, 9″-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 163.6 | C-1′ | 121.0 | C-3″ | 147.5 |
| 3 | 102.9 | 2′ | 128.4 | 4″ | 147.1 |
| 4 | 181.8 | 3′ | 115.9 | 5″ | 115.3 |
| 5 | 152.9 | 4′ | 161.2 | 6″ | 120.5 |
| 6 | 98.6 | 5′ | 115.9 | 7″ | 77.0 |
| 7 | 149.3 | 6′ | 128.4 | 8″ | 77.6 |
| 8 | 124.4 | 1″ | 126.7 | 9″ | 60.0 |
| 9 | 144.3 | 2″ | 111.8 | $OCH_3$ | 55.7 |
| 10 | 104.6 | | | | |

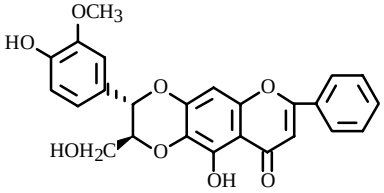


**Scutellaprostin C**

*S. prostrata* [169]
$C_{25}H_{20}O_{10}$: 480
**mp**: 150-151°C (dec.) (MeOH)
$[\alpha]_D^{20}$ ±0° (*c* 0.05, MeOH)
**UV**: 230 sh (4.82), 283 (4.74), 304 sh (4.48), 348 (4.74); $+CH_3ONa$, 234 sh (4.75), 270 (4.81), 282 sh (4.77), 304 sh (4.47), 416 (4.75); $+AlCl_3$, 235 sh (4.87), 290 (4.77), 318 sh (4.40), 444 (4.75); $+AlCl_3$/HCl, 235 sh (4.82), 290 (4.70), 317 sh (4.50), 366 (4.63); $+CH_3COONa$, 282 (4.73), 410 (4.52); $+CH_3COONa/H_3BO_3$, 270 sh (4.73), 283 (4.73), 307 (4.32), 384 (4.65)
**IR**: 3424 (OH), 1664 (C=O γ-pyrone), 1612 (C=C aromatic)
**EI-MS** *m/z* (%): 302 (20) $C_{15}H_{10}O_7$, 180 (45) $C_{10}H_{12}O_3$, 168 (21) $C_7H_4O_5$, 137 (100) $C_8H_9O_2$, 120 (74) $C_7H_8O_2$
**FAB-MS** *m/z* (%): 481 (8) $[M + 1]^+$, 154 (100)
**PMR** (DMSO-$d_6$): 6.77 (1H, s, H-3), 6.38 (1H, s, H-6), 7.45 (1H, d, J = 2.2, H-2′), 6.91 (1H, d, J = 8.2, H-4′,5′), 7.48 (1H, dd, J = 8.2 and 2.2, H-6′), 7.05 (1H, br.t, J = 7.4, H-5′), 7.08 (1H, dd, J = 1.5 and 8.1, H-6′), 12.61 (1H, d, J = 1.8, H-2″), 6.82 (1H, d, J = 8.0, H-5″), 6.89 (1H, dd, J = 8.0 and 1.8, H-6″), 5.15 (1H, d, J = 7.7, H-7″), 4.30 (1H, ddd, J = 7.76, 4.8, and 3.0, H-8″), 3.44 (1H, ddd, J = 13.2, 5.5, and 4.8, H-9″), 3.70 (1H, ddd, J = 13.2, 5.5, and 3.0, H-9″), 3.78 (3H, s, $OCH_3$), 12.43 (1H, s, 5-OH), 9.44 (1H, s, Ar-OH), 10.02 (1H, s, Ar-OH), 5.05 (1H, m, J = 5.5, 9″-OH)

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

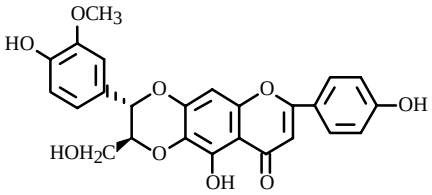
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 163.9 | C-1′ | 121.4 | C-3″ | 147.6 |
| 3 | 103.1 | 2′ | 113.6 | 4″ | 147.2 |
| 4 | 181.9 | 3′ | 145.7 | 5″ | 115.4 |
| 5 | 153.1 | 4′ | 150.0 | 6″ | 120.6 |
| 6 | 98.8 | 5′ | 116.0 | 7″ | 77.0 |
| 7 | 149.4 | 6′ | 119.2 | 8″ | 77.6 |
| 8 | 124.5 | 1″ | 126.8 | 9″ | 60.1 |
| 9 | 144.5 | 2″ | 111.8 | $OCH_3$ | 55.7 |
| 10 | 104.8 | | | | |



**Scutellaprostin D**

*S. prostrata* [169]
$C_{25}H_{20}O_8$ 448
**mp**: 234-235°C (dec.) (MeOH)
$[\alpha]_D^{20}$ ±0° (*c* 0.05, MeOH)
**UV**: 219 (4.58), 239 sh (4.31), 280 (4.49), 320 (4.27); +$CH_3ONa$, 233 sh (4.50), 256 (4.43), 205 (4.49), 400 (3.46); +$AlCl_3$, 223 (4.55), 287 (4.49), 297 sh (4.44), 348 (4.35), 402 sh (3.58); +$AlCl_3$/HCl, 225 (4.56), 287 (4.47), 297 sh (4.43), 345 (4.33), 402 sh (3.58); +$CH_3COONa$, 280 (4.49), 321 (4.26)
**IR**: 3280 (OH), 1664 (C=O γ-pyrone), 1622 (C=C aromatic)
**EI-MS** *m/z* (%): 448 (59) $[M]^+$, 270 (100) $C_{15}H_{10}O_5$, 180 (23) $C_{10}H_{12}O_3$, 168 (11) $C_7H_4O_5$, 137 (40) $C_8H_9O_2$, 124 (21) $C_7H_8O_2$
**PMR** (DMSO-$d_6$): 7.00 (1H, s, H-3), 6.85 (1H, s, H-8), 8.09 (1H, br.d, J = 6.7, H-2′), 7.53-7.62 (1H, m, H-3′,4′,5′), 8.09 (1H, br.d, J = 6.7, H-6′), 7.05 (1H, d, J = 1.8, H-2″), 6.84 (1H, d, J = 8.2, H-5″), 6.91 (1H, dd, J = 8.1 and 1.8, H-6″), 5.13 (1H, d, J = 8.1, H-7″), 4.23 (1H, ddd, J = 8.1, 4.1, and 2.1, H-8″), 3.39 (1H, ddd, J = 12.4, 5.3, and 2.1, H-9″), 3.65 (1H, ddd, J = 12.4, 5.3, and 4.1, H-9″), 3.79 (3H, s, $OCH_3$), 12.94 (1H, s, 5-OH), 9.18 (1H, s, Ar-OH), 5.02 (1H, m, J = 5.3, 9″-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 163.5 | C-1′ | 130.6 | C-3″ | 147.5 |
| 3 | 104.4 | 2′ | 126.3 | 4″ | 147.2 |
| 4 | 182.5 | 3′ | 129.0 | 5″ | 115.3 |
| 5 | 147.8 | 4′ | 132.0 | 6″ | 120.5 |
| 6 | 128.0 | 5′ | 129.0 | 7″ | 76.9 |
| 7 | 150.1 | 6′ | 126.3 | 8″ | 77.4 |
| 8 | 94.7 | 1″ | 126.6 | 9″ | 59.8 |
| 9 | 149.7 | 2″ | 111.8 | $OCH_3$ | 55.6 |
| 10 | 104.9 | | | | |



**Scutellaprostin E**

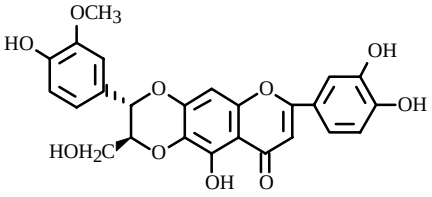
*S. prostrata* [169]
$C_{25}H_{20}O_9$: 464
**mp**: 240-241°C (dec.) (MeOH)
$[\alpha]_D^{20}$ ±0° (*c* 0.05, MeOH)
**UV**: 220 (4.52), 236 sh (4.38), 340 (4.40); +$CH_3ONa$, 218 (4.61), 255 (4.37), 293 (4.30), 374 (4.39); +$AlCl_3$, 224 (4.51), 239 sh (4.41), 290 sh (4.24), 309 sh (4.28), 373 (4.45); +$AlCl_3$/HCl, 224 (4.51), 238 sh (4.42), 292 sh (4.28), 307 sh (4.31), 364 (4.44); +$CH_3COONa$, 223 (4.59), 284 (4.27), 344 (4.29), 408 sh (4.06)
**IR**: 3440 (OH), 1664 (C=O γ-pyrone), 1610 (C=C aromatic)

**EI-MS** *m/z* (%): 464 (26) $[M]^+$, 286 (100) $C_{15}H_{10}O_6$, 180 (55) $C_{10}H_{12}O_3$, 168 (81) $C_7H_4O_5$, 137 (90) $C_8H_9O_2$, 124 (48) $C_7H_8O_2$, 121 (20) $C_7H_5O$

**PMR** (DMSO-$d_6$): 6.80 (1H, s, H-3), 6.77 (1H, s, H-8), 7.93 (1H, d, J = 8.8, H-2′), 6.93 (1H, d, J = 8.8, H-3′), 6.93 (1H, d, J = 8.8, H-4′,5′), 7.93 (1H, d, J = 8.8, H-6′), 7.04 (1H, d, J = 1.8, H-2″), 6.82 (1H, d, J = 8.1, H-5″), 6.89 (1H, dd, J = 8.1 and 1.8, H-6″), 5.11 (1H, d, J = 7.7, H-7″), 4.21 (1H, ddd, J = 7.7, 4.1, and 2.6, H-8″), 3.37 (1H, br.dd, J = 12.5 and 4.1, H-9″), 3.67 (1H, ddd, J = 12.5 and 2.6, H-9″), 3.79 (3H, s, $OCH_3$), 13.09 (1H, s, 5-OH), 9.16 (1H, s, Ar-OH), 10.33 (1H, s, Ar-OH), 5.00 (1H, br.s, 9″-OH)

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

| | | | | | |
|---|---|---|---|---|---|
| C-2 | 164.0 | C-1′ | 121.1 | C-3″ | 147.5 |
| 3 | 102.1 | 2′ | 128.4 | 4″ | 147.1 |
| 4 | 182.3 | 3′ | 115.8 | 5″ | 115.3 |
| 5 | 147.8 | 4′ | 161.1 | 6″ | 120.5 |
| 6 | 127.9 | 5′ | 115.8 | 7″ | 76.9 |
| 7 | 149.8 | 6′ | 128.4 | 8″ | 77.3 |
| 8 | 94.4 | 1″ | 126.6 | 9″ | 59.8 |
| 9 | 149.5 | 2″ | 111.8 | $OCH_3$ | 55.6 |
| 10 | 104.5 | | | | |




**Scutellaprostin F**

*S. prostrata* [169]

$C_{25}H_{20}O_{10}$: 480

**mp**: 204-205°C (dec.) (MeOH)

$[\alpha]_D^{20}$ ±0° (*c* 0.05, MeOH)

**UV**: 220 sh (4.61), 237 sh (4.40), 261 (4.12), 284 (4.28), 352 (4.39); +$CH_3ONa$, 258 (4.40), 294 (4.28), 394 (4.32); +$AlCl_3$, 224 (4.58), 258 (4.26), 311 sh (4.05), 433 (4.46); +$AlCl_3$/HCl, 224 (4.56), 240 sh (4.36), 265 (4.05), 290 (4.24), 302 sh (4.20), 376 (4.40); +$CH_3COONa$, 282 (4.23), 354 (4.19), 414 (4.06); +$CH_3COONa/H_3BO_3$, 266 (4.27), 282 (4.23), 378 (4.37)

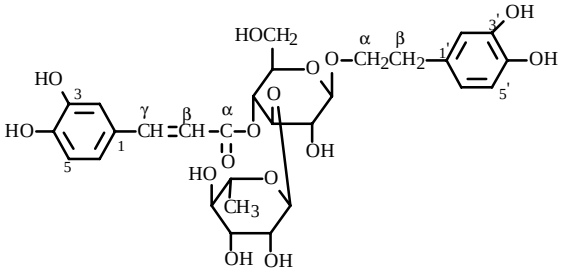
**IR**: 3428 (OH), 1664 (C=O γ-pyrone), 1610 (C=C aromatic)

**EI-MS** *m/z* (%): 480 (3) $[M]^+$, 302 (77) $C_{15}H_{10}O_7$, 180 (63) $C_{10}H_{12}O_3$, 168 (28) $C_7H_4O_5$, 137 (100) $C_8H_9O_2$, 124 (61) $C_7H_8O_2$

**PMR** (DMSO-$d_6$): 6.68 (1H, s, H-3), 6.71 (1H, s, H-8), 7.40 (1H, d, J = 2.2, H-2′), 6.89 (2H, d, J = 8.1, H-4′,5′), 7.41 (1H, dd, J = 8.1 and 2.2, H-6′), 7.04 (1H, d, J = 1.7, H-2″), 6.83 (1H, d, J = 8.1, H-5″), 6.89 (1H, dd, J = 8.1 and 1.7, H-6″), 5.08 (1H, d, J = 8.1, H-7″), 4.02 (1H, br.d, J = 8.1, H-8″), 3.36 (1H, br.dd, J = 12.3 and 3.9, H-9″), 3.63 (1H, br.d, J = 12.3, H-9″), 3.79 (3H, s, $OCH_3$), 13.12 (1H, s, 5-OH), 9.20 (1H, br.s, Ar-OH), 9.45 (1H, br.s, Ar-OH), 9.95 (1H, br.s, Ar-OH), 5.03 (1H, br.s, 9″-OH)

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

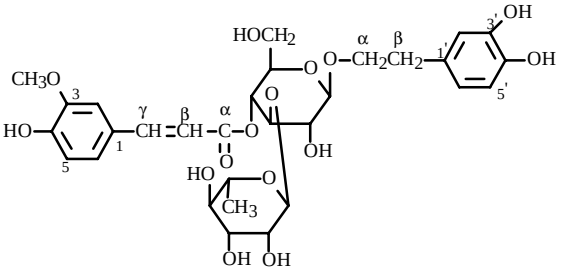
| | | | | | |
|---|---|---|---|---|---|
| C-2 | 164.4 | C-1′ | 121.5 | C-3″ | 147.7 |
| 3 | 102.3 | 2′ | 113.4 | 4″ | 147.3 |
| 4 | 182.3 | 3′ | 145.8 | 5″ | 115.4 |
| 5 | 148.0 | 4′ | 149.8 | 6″ | 120.7 |
| 6 | 128.0 | 5′ | 116.0 | 7″ | 77.1 |
| 7 | 149.9 | 6′ | 119.1 | 8″ | 77.5 |
| 8 | 94.5 | 1″ | 126.8 | 9″ | 60.0 |
| 9 | 149.7 | 2″ | 111.9 | $OCH_3$ | 55.7 |
| 10 | 104.8 | | | | |



**Acteoside**

*S. baicalensis* [144], *S. prostrata* [95], *S. repens* [187]
$C_{29}H_{36}O_{15}$: 624
**mp**: amorph.
**UV**: 246 (3.98), 290 (4.11), 330 (4.27)
**IR**: 3380 (OH), 1695, 1628, 1602, 1515 (aromatic ring)
**PMR** ($CD_3OD$): 1.10 (3H, d, J = 6, $CH_3$), 2.78 (2H, t, J = 7, Ar-$CH_2$), 4.36 (1H, d, J = 8, H-1 glucose), 5.17 (1H, s, H-1 rhamnose), 6.28 (1H, d, J = 15, Ar–C=CH), 6.4-7.1 (6H, aromatic protons), 7.57 (1H, d, J = 15, Ar–CH=C)
$^{13}$**C NMR** ($CD_3OD$):

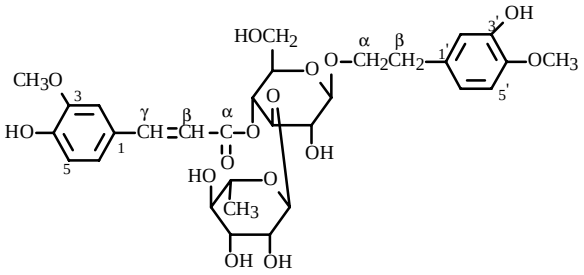
| Aglycon | | Caffeic acid | | Glucos | | Rhamnose | |
|---|---|---|---|---|---|---|---|
| C-1 | 131.4 | C-1 | 127.4 | C-1 | 103.7 | C-1 | 102.6 |
| 2 | 116.3 | 2 | 114.5 | 2 | 75.4 | 2 | 71.9 |
| 3 | 144.0 | 3 | 149.1 | 3 | 81.5 | 3 | 71.9 |
| 4 | 145.5 | 4 | 146.2 | 4 | 70.1 | 4 | 73.6 |
| 5 | 117.0 | 5 | 116.3 | 5 | 75.7 | 5 | 70.1 |
| 6 | 121.2 | 6 | 123.1 | 6 | 62.1 | 6 | 18.2 |
| $\alpha$ | 71.9 | $\alpha$ | 168.2 | | | | |
| $\beta$ | 36.1 | $\beta$ | 115.3 | | | | |
| | | $\gamma$ | 147.8 | | | | |



**Leucoceptoside A**

*S. baicalensis* [144], *S. prostrata* [95], *S. repens* [187]
$C_{30}H_{38}O_{15}$: 638
**mp**: amorph.
$[\alpha]_D^{19}$ -42.5° (*c* 1.59, MeOH)
**UV**: 246 sh (4.00), 289 (4.14), 327 (4.31)
**IR**: 3400 (OH), 1700, 1625, 1600, 1590, 1515
**PMR** ($CD_3OD$): 1.10 (3H, d, J = 6, $CH_3$), 2.78 (2H, t, J = 7, Ar–$CH_2$), 3.89 (3H, s, $OCH_3$), 4.38 (1H, d, J = 8, H-1 glucose), 5.23 (1H, s, H-1 rhamnose), 6.36 (1H, d, J = 15, Ar–C=CH), 6.5-7.3 (6H, aromatic protons), 7.67 (1H, d, J = 15, Ar–CH=C)
$^{13}$**C NMR** ($CD_3OD$):

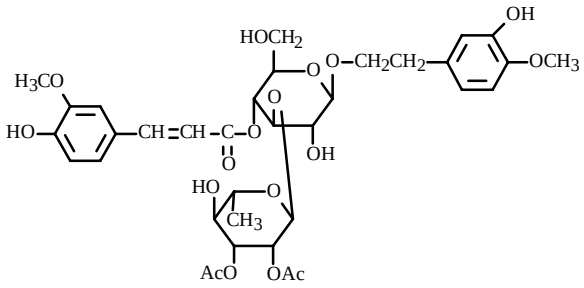
| Aglycon | | Ferulic acid | | Glucose | | Rhamnose | |
|---|---|---|---|---|---|---|---|
| C-1 | 131.5 | C-1 | 127.6 | C-1 | 104 | C-1 | 102.8 |
| 2 | 116.5 | 2 | 111.9 | 2 | 75.8 | 2 | 72.1 |
| 3 | 144.4 | 3 | 150.6 | 3 | 81.4 | 3 | 72.1 |
| 4 | 145.9 | 4 | 149.2 | 4 | 70.3 | 4 | 73.7 |
| 5 | 117.7 | 5 | 116.3 | 5 | 76.0 | 5 | 70.6 |
| 6 | 121.3 | 6 | 124.2 | 6 | 62.3 | 6 | 18.4 |
| $\alpha$ | 72.1 | $\alpha$ | 168.2 | | | | |
| $\beta$ | 36.4 | $\beta$ | 115.0 | | | | |
| | | $\gamma$ | 147.8 | | | | |
| | | $OCH_3$ | 56.5 | | | | |



**Martinoside**

*S. prostrata* [95], *S. repens* [187]
$C_{31}H_{40}O_{15}$: 652
**mp**: amorph.
**UV**: 246 sh (4.11), 287 (4.16), 327 (4.33)
**IR**: 3400, 1704, 1626, 1590, 1510
**PMR** ($CD_3OD$): 1.09 (3H, d, J = 6, $CH_3$), 2.81 (2H, t, J = 7, Ar–$CH_2$), 3.80, 3.88 (3H, s, each 2×$OCH_3$), 4.35 (1H, d, J = 8, H-1 glucose), 5.17 (1H, s, H-1 rhamnose), 6.34 (1H, d, J = 15, Ar–CH=CH), 6.5-7.2 (6H, aromatic protons), 7.64 (1H, d, J = 15, Ar–CH=C)
$^{13}$**C NMR** ($CD_3OD$):

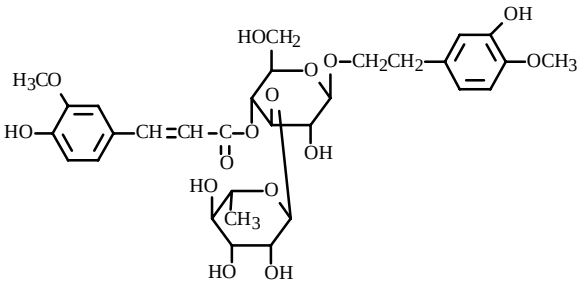
| Aglycon | | Ferulic acid | | Glucose | | Rhamnose | |
|---|---|---|---|---|---|---|---|
| C-1 | 132.7 | C-1 | 127.5 | C-1 | 104.0 | C-1 | 102.8 |
| 2 | 117.0 | 2 | 111.9 | 2 | 75.9 | 2 | 72.2 |
| 3 | 147.1 | 3 | 150.4 | 3 | 81.5 | 3 | 72.2 |
| 4 | 147.2 | 4 | 149.1 | 4 | 70.3 | 4 | 73.7 |
| 5 | 112.8 | 5 | 116.6 | 5 | 75.9 | 5 | 70.6 |
| 6 | 121.1 | 6 | 124.2 | 6 | 62.4 | 6 | 18.4 |
| $\alpha$ | 72.2 | $\alpha$ | 168.1 | | | | |
| $\beta$ | 36.4 | $\beta$ | 115.1 | | | | |
| $OCH_3$ | 56.5 | $\gamma$ | 147.8 | | | | |
| | | $OCH_3$ | 56.5 | | | | |



**O-2-(3-Hydroxy-4-methoxyphenyl)ethyl-O-2,3-di-O-acetyl-$\alpha$-L-rhamnopyranosyl-(1→3)-(4-O-*trans*-feruloyl)-$\beta$-D-glucopyranoside**

*S. repens* [187]
$C_{35}H_{44}O_{17}$: 736
**mp**: amorph.
$[\alpha]_D^{27}$ -67.1°
**PMR** (DMSO-$d_6$): 6.68 (1H, d, J = 2.2, H-2), 6.81 (1H, d, J = 8.1, H-5), 6.63 (1H, dd, J = 2.2 and 8.1, H-6), 3.61 (1H, m, H-$\alpha$), 3.89 (1H, m, H-$\alpha$), 2.73 (1H, br.t, J = 6.6, H-$\beta$), 7.30 (1H, d, J = 1.8, H-2′), 6.79 (1H, d, J = 8.1, H-5′), 7.11 (1H, dd, J = 1.8 and 8.1, H-6′), 6.44 (1H, d, J = 16.1, H-$\beta$′), 5.56 (1H, d, J = 16.1, H-$\gamma$′), 4.36 (1H, d, J = 7.7, H-1″), 3.33 (1H, m, H-2″), 3.75 (1H, t, J = 9.5, H-3″), 4.81 (1H, t, J = 9.5, H-4″), 3.49 (1H, m, H-5″), 3.42 (1H, m, H-6″), 5.11 (1H, br.s, H-1‴), 5.18 (1H, dd, J = 1.8 and 3.3, H-2‴), 4.71 (1H, dd, J = 3.3 and 9.9, H-3‴), 3.26 (1H, dt, J = 5.1 and 9.7, H-4‴), 3.57 (1H, m, H-5‴), 1.04 (1H, d, J = 5.9, H-6‴), 8.80 (1H, br.s, 3-OH), 9.62 (1H, br.s, 4′-OH), 5.64 (1H, d, J = 5.5, 2″-OH), 4.75 (1H, t, J = 5.5, 6″-OH), 5.21 (1H, d, J = 5.1, 4‴-OH), 3.72 (3H, s, 4-$OCH_3$), 3.80 (3H, s, 3′-$OCH_3$), 1.90 (3H, s, $OCOCH_3$), 2.04 (3H, s, $OCOCH_3$)
$^{13}$**C NMR** (DMSO-$d_6$):

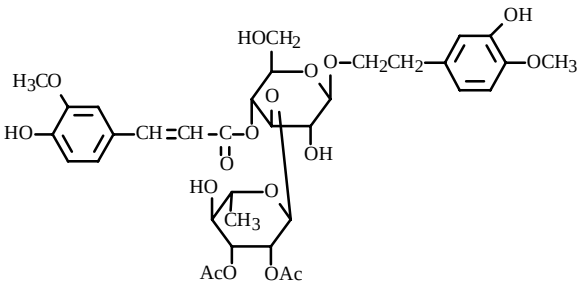
| Aglycon | | Ferulic acid | | Glucose | | Rhamnose | |
|---|---|---|---|---|---|---|---|
| C-1 | 131.0 | C-1 | 125.5 | C-1 | 102.2 | C-1 | 98.2 |
| 2 | 116.6 | 2 | 111.1 | 2 | 74.3 | 2 | 69.4 |
| 3 | 146.3 | 3 | 147.9 | 3 | 79.7 | 3 | 71.4 |
| 4 | 146.1 | 4 | 149.4 | 4 | 68.8 | 4 | 68.8 |
| 5 | 112.3 | 5 | 115.5 | 5 | 74.4 | 5 | 68.8 |
| 6 | 119.4 | 6 | 123.2 | 6 | 60.7 | 6 | 17.8 |
| $\alpha$ | 70.1 | $\alpha$ | 165.7 | $O\underline{C}OCH_3$ | 169.5; 169.7 | | |
| $\beta$ | 34.9 | $\beta$ | 113.9 | $OCO\underline{C}H_3$ | 20.6; 20.7 | | |
| $OCH_3$ | 55.6 | $\gamma$ | 145.8 | | | | |
| | | $OCH_3$ | 55.7 | | | | |



**O-2-(3-Hydroxy-4-methoxyphenyl)ethyl-O-$\alpha$-L-rhamnopyranosyl-(1→3)-(4-O-*cis*-feruloyl)-$\beta$-D-glucopyranoside**

*S. repens* [187]
$C_{31}H_{40}O_{15}$: 652
**mp**: amorph.
**UV**: 218 (4.25), 228 sh (4.17), 246 sh (3.97), 287 (4.04), 302 sh (4.06), 329 (4.25)
**IR**: 3432 (OH), 1698 (ester), 1630 (C=C) 1594, 1512 (C=C aromatic)
**PMR** (DMSO-$d_6$): 6.69 (1H, br.s, H-2), 6.80 (1H, d, J = 8.1, H-5), 6.62 (1H, br.d, J = 8.1, H-6), 3.60 (1H, m, H-$\alpha$), 3.89 (1H, m, H-$\alpha$), 2.72 (1H, m, H-$\beta$), 7.71 (1H, d, br.s, H-2′), 6.69 (1H, d, J = 8.4, H-5′), 7.16 (1H, br.d, J = 8.4, H-6′), 5.62 (1H, d, J = 12.8, H-$\beta$′), 6.85 (1H, d, J = 12.8, H-$\gamma$′), 4.35 (1H, d, J = 7.7, H-1″), 3.21 (1H, m, H-2″), 3.69 (1H, m, H-3″), 4.68 (1H, t, J = 9.5, H-4″), 3.43 (1H, m, H-5″), 3.36 (1H, m, H-6″), 5.03 (1H, br.s, H-1‴), 3.69 (1H, m, H-2‴), 3.32 (1H, m, H-3‴), 3.14 (1H, dt, J = 4.4 and 9.5, H-4‴), 3.38 (1H, m, H-5‴), 1.04 (1H, d, J = 6.2, H-6‴), 8.77 (1H, s, 3-OH), 9.55 (1H, s, 4′-OH), 5.51 (1H, d, J = 5.9, 2″-OH), 4.69 (1H, t, J = 5.5, 6″-OH), 4.61 (1H, d, J = 4.0, 2‴-OH), 4.47 (1H, br.d, J = 5.5, 3‴-OH), 4.56 (1H, d, J = 4.4, 4‴-OH), 3.72 (3H, s, 4-$OCH_3$), 3.75 (3H, s, 3′-$OCH_3$)
$^{13}$**C NMR** (DMSO-$_6$):

| Aglycon | | Ferulic acid | | Glucose | | Rhamnose | |
|---|---|---|---|---|---|---|---|
| C-1 | 131.0 | C-1 | 128.3 | C-1 | 102.3 | C-1 | 101.3 |
| 2 | 116.3 | 2 | 112.7 | 2 | 74.5 | 2 | 70.5 |
| 3 | 146.1 | 3 | 147.3 | 3 | 79.2 | 3 | 70.4 |
| 4 | 146.4 | 4 | 148.6 | 4 | 68.9 | 4 | 71.7 |
| 5 | 112.3 | 5 | 115.1 | 5 | 74.5 | 5 | 68.6 |
| 6 | 119.2 | 6 | 126.5 | 6 | 60.8 | 6 | 18.0 |
| $\alpha$ | 70.1 | $\alpha$ | 164.9 | | | | |
| $\beta$ | 34.9 | $\beta$ | 114.5 | | | | |
| $OCH_3$ | 55.4 | $\gamma$ | 146.0 | | | | |
| | | $OCH_3$ | 55.4 | | | | |

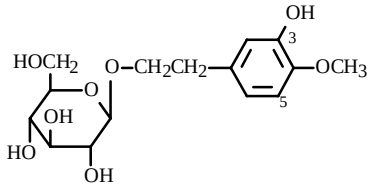


**O-2-(3-Hydroxy-4-methoxyphenyl)ethyl-O-2,3-di-O-acetyl-$\alpha$-L-rhamnopyranosyl-(1→3)-(4-O-*cis*-feruloyl)-$\beta$-D-glucopyranoside**

*S. repens* [187]
$C_{35}H_{44}O_{17}$: 736
**mp**: amorph.
**PMR** (DMSO-$d_6$): 6.67 (1H, d, J = 2.2, H-2), 6.80 (1H, d, J = 8.1, H-5), 6.62 (1H, dd, J = 2.2 and 8.1, H-6), 3.59 (1H, m, H-$\alpha$), 3.89 (1H, m, H-$\alpha$), 2.72 (1H, br.t, J = 7.7, H-$\beta$), 7.72 (1H, d, J = 1.8, H-2′), 6.75 (1H, d, J = 8.1, H-5′), 7.16 (1H, dd, J = 1.8 and 8.1, H-6′), 5.71 (1H, d, J = 13.2, H-$\beta$′), 6.92 (1H, d, J = 13.2, H-$\gamma$′), 4.35 (1H, d, J = 7.7, H-1″), 3.35 (1H, br.t, J = 8.4, H-2″), 3.77 (1H, t, J = 9.5, H-3″), 4.79 (1H, t, J = 9.5, H-4″), 3.48 (1H, dd, J = 4.8 and 9.5, H-5″), 3.43 (1H, m, H-6″), 5.11 (1H, br.s, H-1‴), 5.19 (1H, dd, J = 1.8 and 3.3, H-2‴), 4.75 (1H, dd, J = 3.3 and 9.9, H-3‴), 3.27 (1H, t, J = 9.7, H-4‴), 3.61 (1H, m, H-5‴), 1.09 (1H, d, J = 6.2, H-6‴), 8.80 (1H, br.s, 3-OH), 9.60 (1H, br.s, 4′-OH), 5.61 (1H, br.s, 2″-OH), 4.75 (1H, t, J = 6.6, 6″-OH), 5.24 (1H, br.s, 4‴-OH), 3.72 (3H, s, 4-$OCH_3$), 3.75 (3H, s, 3′-$OCH_3$), 1.91 (3H, s, $OCOCH_3$), 2.05 (3H, s, $OCOCH_3$)

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

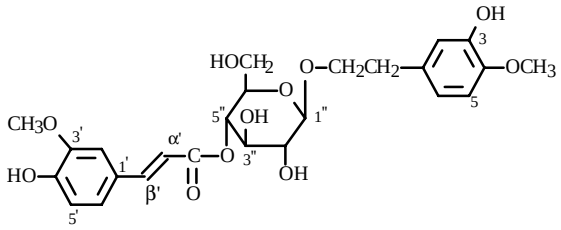
| Aglycon | | Ferulic acid | | Glucose | | Rhamnose | |
|---|---|---|---|---|---|---|---|
| C-1 | 131.0 | C-1 | 128.1 | C-1 | 101.0 | C-1 | 98.3 |
| 2 | 116.3 | 2 | 113.0 | 2 | 74.2 | 2 | 69.3 |
| 3 | 146.3 | 3 | 147.9 | 3 | 79.7 | 3 | 71.5 |
| 4 | 146.1 | 4 | 148.6 | 4 | 68.8 | 4 | 68.7 |
| 5 | 112.3 | 5 | 114.8 | 5 | 74.2 | 5 | 68.8 |
| 6 | 119.4 | 6 | 125.9 | 6 | 60.2 | 6 | 17.1 |
| $\alpha$ | 70.1 | $\alpha$ | 164.7 | | | $O\underline{C}OCH_3$ | 169.5; 169.7 |
| $\beta$ | 34.9 | $\beta$ | 114.1 | | | $OCO\underline{C}H_3$ | 20.6; 20.6 |
| $OCH_3$ | 55.7 | $\gamma$ | 146.7 | | | | |
| | | $OCH_3$ | 55.7 | | | | |



**2-(3-Hydroxy-4-methoxyphenyl)ethyl-1-O-$\beta$-D-glucopyranoside**

*S. prostrata* [95]
$C_{15}H_{22}O_8$: 330
**mp**: amorph.
$[\alpha]_D^{31}$ -12.9° (*c* 0.33, MeOH)
**UV**: 219 sh (4.30), 280 sh (3.93)
**IR**: 3460 (OH), 1596 (C=C aromatic)
**EI-MS** *m/z* (%): 330 (2) $[M]^+$, 137 (100) $C_8H_9O_2$
**FAB-MS** *m/z* (%): 353 (23) $[M + Na]^+$, 331 (20) $[M + 1]^+$
**PMR** (DMSO-$d_6$): 2.70 (2H, m, $\beta$-H), 2.92-3.49 (m, sugar protons), 3.55 (1H, d, t, J = 6.6 and 9.2, $\alpha$-H), 3.71 (3H, s, 4-$OCH_3$), 3.87 (1H, d, t, J = 7.0 and 9.2, $\alpha$-H), 4.16 (1H, d, J = 8.1, glucose anomeric proton H-1′), 6.60 (1H, br.d, J = 8.1, H-6), 6.68 (1H, d, J = 1.8, H-2), 6.79 (1H, d, J = 8.1, H-5), 8.43 (1H, br.s, 3-OH)
$^{13}$**C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-1 | 131.3 | C-6 | 119.3 | C-3″ | 76.9 |
| 2 | 116.3 | $\alpha$ | 69.8 | 4″ | 70.1 |
| 3 | 146.4 | $\beta$ | 35.1 | 5″ | 76.8 |
| 4 | 146.1 | 1″ | 102.8 | 6″ | 61.1 |
| 5 | 112.9 | 2″ | 73.5 | 4-$OCH_3$ | 55.7 |



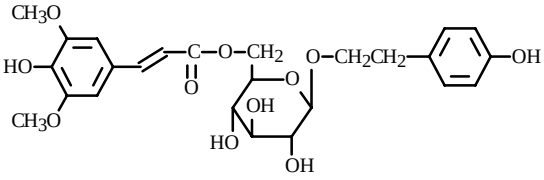
**2-(3-Hydroxy-4-methoxyphenyl)ethyl-1-O-$\beta$-D-(4-O-feruloyl)glucopyranoside**

*S. prostrata* [95]
$C_{25}H_{30}O_{11}$: 506
**mp**: amorph.
$[\alpha]_D^{31}$ -31.2° (*c* 0.33, MeOH)
**UV**: 220 sh (4.11), 231 sh (4.03), 291 sh (3.90), 330 (4.06)
**IR**: 3470 (OH), 1703 ($\alpha$, $\beta$, C=O), 1600 (C=C aromatic)
**EI-MS** *m/z* (%): 207 (66) $C_7H_{11}O_7$, 150 (100) $C_9H_{10}O_2$, 137 (40) $C_8H_9O_2$
**FAB-MS** *m/z* (%): 529 (8) $[M + Na]^+$, 507 (15) $[M + 1]^+$
**PMR** (DMSO-$d_6$): 2.74 (2H, m, $\beta$-H), 3.35-3.48 (m, sugar protons), 3.62 (1H, dt, J = 7.0 and 9.6, $\alpha$-H), 3.73 (3H, s, 4-$OCH_3$), 3.82 (3H, s, 3′-$OCH_3$), 3.91 (1H, dt, J = 7.3 and 9.6, $\alpha$-H), 4.30 (1H, d, J = 7.7, glucose anomeric proton H-1″), 4.60 (1H, t, J = 9.0, H-4″), 6.47 (1H, d, J = 15.8, $\alpha$′-H), 6.63 (1H, dd, J = 1.8 and 8.1, H-6), 6.69 (1H, d, J = 1.8, H-2), 6.80 (1H, d, J = 8.1,

H-5′), 6.81 (1H, d, J = 8.1, H-5), 7.12 (1H, dd, J = 1.8 and 8.1, H-6″), 7.33 (1H, d, J = 1.8, H-2′), 7.55 (1H, d, J = 15.8, $\beta'$-H), 8.78 (1H, s, 3-OH), 9.58 (1H, s, 4′-OH)

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

| Aglycon | | Glucose | | Ferulic acid | |
|---|---|---|---|---|---|
| C-1 | 131.1 | C-1″ | 102.8 | C-1′ | 125.6 |
| 2 | 116.3 | 2″ | 73.6 | 2′ | 11.1 |
| 3 | 146.3 | 3″ | 74.1 | 3′ | 147.9 |
| 4 | 146.1 | 4″ | 71.3 | 4′ | 149.4 |
| 5 | 112.3 | 5″ | 74.7 | 5′ | 115.5 |
| 6 | 119.4 | 6″ | 60.9 | 6′ | 123.2 |
| $\alpha$ | 70.0 | | | $\beta'$ | 145.3 |
| $\beta$ | 35.0 | | | $\alpha'$ | 114.5 |
| | | | | CO | 166.0 |
| | | | | 4-$OCH_3$ | 55.7 |
| | | | | 3′-$OCH_3$ | 55.7 |



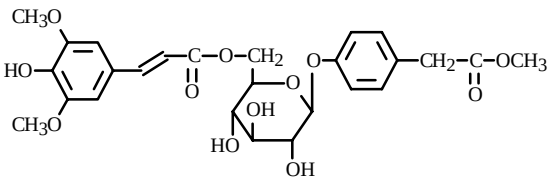
**2-(4-Hydroxyphenyl)ethyl-6′-O-sinapoyl-$\beta$-D-glucopyranoside**

*S. scandens* [193]
$C_{25}H_{30}O_{10}$: 490
**mp**: amorph.
$[\alpha]_D^{26}$ -26.0° (*c* 0.36, MeOH)

**UV**: 328 (4.27), 237 sh (4.20), 225 (4.32), 206 (4.22)
**IR**: 3464, 2928, 1718, 1640, 1614, 1520, 1464, 1382, 1340, 1292, 1120, 1084
**EI-MS**: 506 (2) $[M]^+$, 293 (3), 224 (8) $[C_{11}H_{12}O_5]^+$, 207 (12) $[C_{11}H_{11}O_4]^+$, 121 (100) $[C_8H_9O]^+$
**PMR** (DMSO-$d_6$): 2.73 (2H, m, $H_2$-7), 3.61, 3.81 (1H, m, each $H_2$-8), 3.79 (6H, s, $OCH_3$), 4.23 (1H, dd, J = 6.2 and 12.0, H-6′), 6.57 (1H, d, J = 15.8, H-8″), 6.61 (2H, d, J = 8.4, H-3, 5), 7.01 (2H, d, J = 8.4, H-2, 6), 7.02 (2H, s, H-2″, 6″), 7.57 (1H, d, J = 15.8, H-7″), 8.95, 9.13 (1H, br.s, each 4-OH, 4″-OH)

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

| Aglycon | | Glucose | | Sinapic acid | |
|---|---|---|---|---|---|
| C-1 | 128.5 | C-1′ | 103.0 | C-1″ | 124.4 |
| 2 | 129.7 | 2′ | 73.0 | 2″ | 106.3 |
| 3 | 115.0 | 3′ | 76.5 | 3″ | 148.0 |
| 4 | 155.6 | 4′ | 70.0 | 4″ | 138.3 |
| 5 | 115.0 | 5′ | 73.7 | 5″ | 140.0 |
| 6 | 129.7 | 6′ | 63.7 | 6″ | 106.3 |
| 7 | 34.9 | | | 7″ | 145.6 |
| 8 | 70.2 | | | 8″ | 114.7 |
| | | | | 9″ | 166.7 |
| | | | | $OCH_3$ | 56.0 |

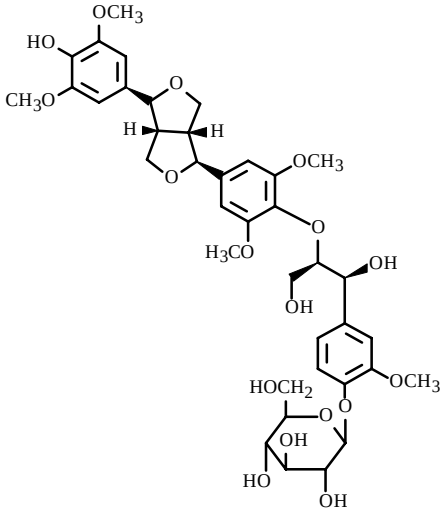


**4-Methoxycarbonylmethylphenyl-6′-O-sinapoyl-$\beta$-D-glucopyranoside**

*S. scandens* [193]
$C_{26}H_{30}O_{12}$: 534
**mp**: amorph.

$[\alpha]_D^{22}$ -30.3° (*c* 0.97, MeOH)
**UV**: 329 (4.17), 327 (4.17), 236 sh (4.11), 224 (4.20)
**IR**: 3465, 2978, 1741, 1721, 1644, 1621, 1528, 1468, 1440
**FAB-MS**: 535 (0.3) $[M + H]^+$, 369 (1.5) $[M + C_9H_9O_3]^+$, 277 (8), 241 (2), 185 (100), 149 (15) $[C_9H_9O_2]^+$
**PMR** (DMSO-$d_6$): 3.48, 3.53 (1H, d, each J = 16.0, $H_2$-7), 3.54 (3H, s, $CO_2CH_3$), 3.81 (6H, s, 2×$OCH_3$), 4.25 (1H, dd, J = 6.2 and 12.0, H-6′), 4.39 (1H, dd, J = 1.8 and 12.0, H-6′), 5.21 (1H, d, J = 4.4, OH), 5.31 (1H, d, J = 5.1, OH), 5.39 (1H, d, J = 4.8, OH), 6.55 (1H, d, J = 15.8, H-8″), 6.86 (2H, d, J = 8.4, H-2, 6), 7.03 (2H, s, H-2″, 6″), 7.13 (2H, d, J = 8.4, H-3, 5), 7.56 (1H, d, J = 15.8, H-7″), 8.97 (1H, br.s, 4″-OH)
**$^{13}$C NMR** (DMSO-$d_6$):

| Aglycon | | Glucose | | Sinapic acid | |
|---|---|---|---|---|---|
| C-1 | 156.2 | C-1′ | 100.4 | C-1″ | 124.4 |
| 2 | 116.2 | 2′ | 73.2 | 2″ | 106.2 |
| 3 | 130.3 | 3′ | 76.4 | 3″ | 148.0 |
| 4 | 127.7 | 4′ | 69.8 | 4″ | 138.4 |
| 5 | 130.3 | 5′ | 73.8 | 5″ | 148.0 |
| 6 | 116.2 | 6′ | 63.2 | 6″ | 106.2 |
| 7 | 40.1 | | | 7″ | 145.5 |
| 8 | 171.1 | | | 8″ | 114.7 |
| $OCH_3$ | 51.6 | | | 9″ | 166.5 |
| | | | | $OCH_3$ | 56.1 |



**Erythro-guaiacylglycerol-*β*-syringaresinol ether 4″-O-*β*-D-glucopyranoside**

*S. baicalensis* [189]
$C_{38}H_{48}O_{17}$: 776
**mp**: amorph.
$[\alpha]_D^{25}$ -13.2° (*c* 0.02, MeOH)
**UV**: 208 (4.96), 230 sh (4.33), 376 (3.90)
**IR**: 3480 (OH), 1602 (C=C aromatic)
**EI-MS** *m/z* (%): 566 (40), 418 (95), 181 (100), 167 (78), 137 (60)
**FAB-MS** *m/z* (%): 799 (5) $[M + Na]^+$
**PMR** (DMSO-$d_6$): 3.04 (2H, m, H-8, 8′), 3.14 (1H, t, J = 9.0, H-4‴), 3.24 (2H, m, H-2‴, 3‴), 3.28 (1H, m, H-5‴), 3.37 (1H, dd, J = 4.5 and 11.4, H-9″), 3.43 (1H, dd, J = 5.6 and 11.2, H-6‴), 3.64 (1H, br.d, J = 11.2, H-6‴), 3.68 (1H, dd, J = 4.5 and 11.4, H-9″), 3.75 (3H, s, each 5×$OCH_3$), 3.79 (2H, dd, J = 3.0 and 9.0, H-9, 9′), 4.10 (1H, q, J = 5.0, H-8″), 4.17 (2H, m, H-9, 9′), 4.61 (1H, d, J = 5.0, H-7), 4.65 (1H, d, J = 5.0, H-7′), 4.82 (1H, d, J = 5.0, H-7″), 4.86 (1H, d, J = 7.0, H-1‴), 6.59 (2H, s, H-6, 2), 6.63 (2H, s, H-2′, 6′), 6.83 (1H, dd, J = 1.8 and 8.0, H-6″), 6.97 (1H, d, J = 1.8, H-2″), 7.01 (1H, d, J = 8.0, H-5″)
**$^{13}$C NMR** (DMSO-$d_6$):

| | | | | | |
|---|---|---|---|---|---|
| C-1 | 131.4 | C-4′ | 136.9 | C-7″ | 71.9 |
| 2 | 103.6 | 5′ | 152.6 | 8″ | 86.1 |
| 3 | 147.9 | 6′ | 103.3 | 9″ | 59.7 |
| 4 | 134.8 | 7′ | 85.3 | 1‴ | 100.2 |
| 5 | 147.9 | 8′ | 53.6 | 2‴ | 73.2 |
| 6 | 103.6 | 9′ | 71.2 | 3‴ | 76.9 |
| 7 | 85.6 | 1″ | 136.2 | 4‴ | 69.7 |
| 8 | 53.7 | 2″ | 111.3 | 5‴ | 77.0 |
| 9 | 71.1 | 3″ | 148.4 | 6‴ | 60.6 |
| 1′ | 134.7 | 4″ | 145.4 | $OCH_3$ | 55.6 |
| 2′ | 103.3 | 5″ | 114.7 | 4×$OCH_3$ | 56.0 |
| 3′ | 152.6 | 6″ | 119.1 | | |

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