# Supporting Information

# *In vitro* metabolization of six C-glycosidic flavonoids from *Passiflora incarnata* L.

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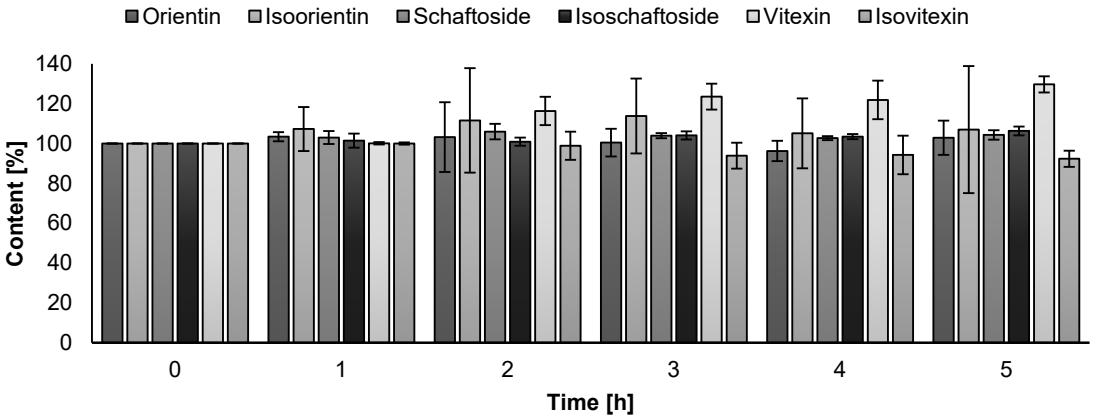


**Figure S1.** Stability testing of O, IO, S, IS, V and IV diluted in HBSS (pH 6.0; 10 µM) in an atmosphere of 5% $CO_2$ and 90% of relative humidity at 37 °C (n = 3). Data are presented as mean +/- SD.

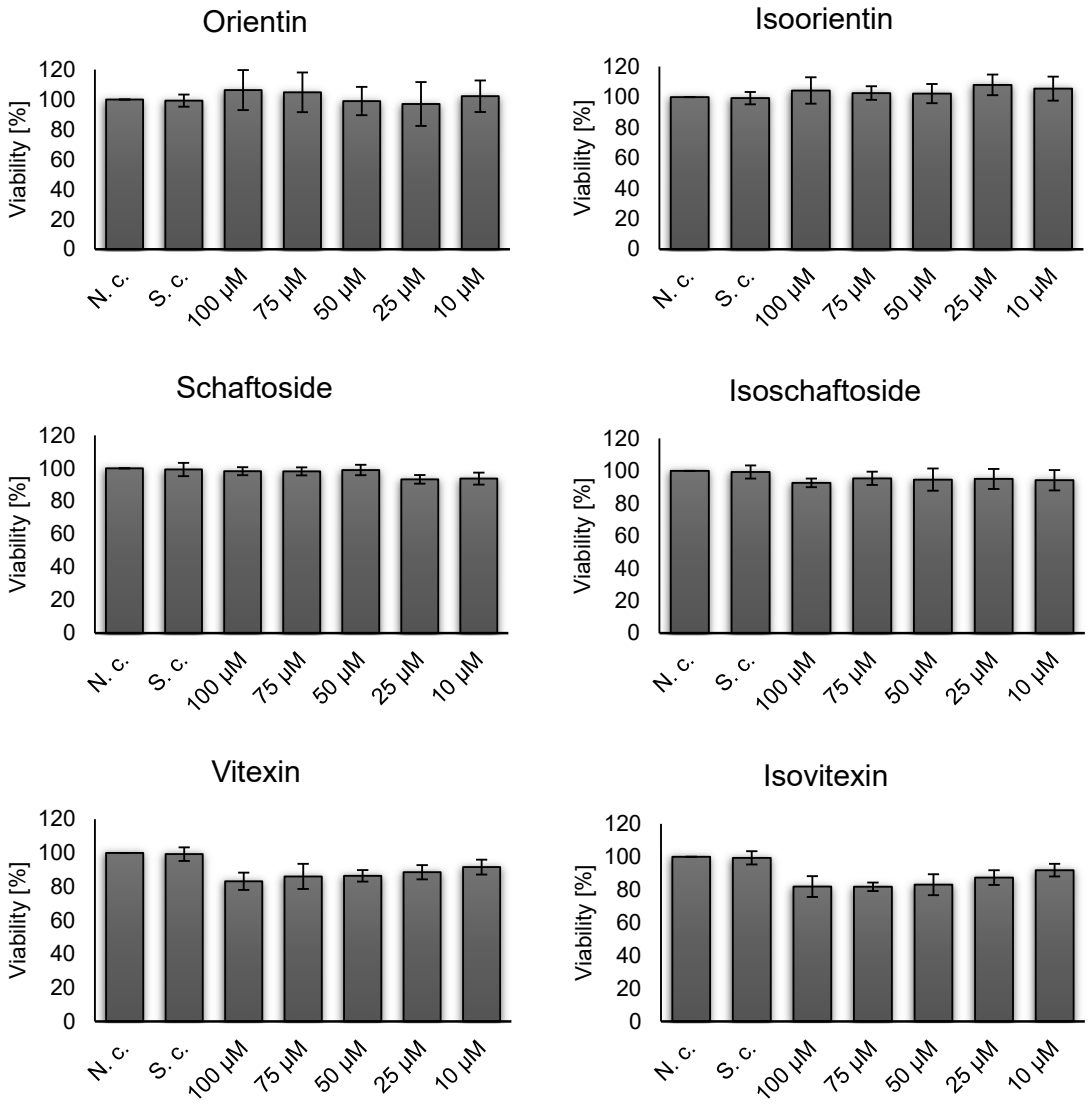


**Figure S2.** Results of the MTT assay under metabolization conditions. N.c.: negative control (HBSS); S.c.: solvent control (0.5% DMSO in HBSS); n = 3. Data are presented as mean +/- SD.

**Table S1**.: Compound library of orientin.

| Molecular formula | Exact mass | Compound |
|---|---|---|
| $C_{21}H_{20}O_{11}$ | 448.1006 | Orientin |
| $C_{15}H_{10}O_6$ | 286.0477 | Luteolin |
| $C_7H_8O_2$ | 124.0524 | Dihydroxy-toluene |
| $C_7H_6O_3$ | 138.0317 | Hydroxy-benzoic acid |
| $C_8H_8O_3$ | 152.0473 | Hydroxy-phenylacetic acid |
| $C_8H_8O_4$ | 168.0423 | Dihydroxy-phenylacetic acid |
| $C_9H_{10}O_4$ | 182.0579 | Hydroxy-methoxy-phenylacetic acid |
| $C_6H_6O_3$ | 126.0317 | Phloroglucinol |
| $C_6H_6O_6S$ | 205.9885 | Phloroglucinol-sulfate |
| $C_{12}H_{14}O_9$ | 302.0638 | Phloroglucinol-glucuronide |
| $C_7H_8O_3$ | 140.0473 | Methyl-phloroglucinol |
| $C_8H_8O_6S$ | 232.0042 | Hydroxy-phenylacetic acid-sulfate |
| $C_{14}H_{16}O_9$ | 328.0794 | Hydroxy-phenylacetic acid-glucuronide |
| $C_{10}H_{11}NO_4$ | 209.0688 | Hydroxy-phenylacetic acid-glycine conjugate |
| $C_{11}H_{11}NO_4$ | 223.0845 | Hydroxy-phenylpropionic acid-glycine conjugate |
| $C_9H_{10}O_6S$ | 246.0198 | Hydroxy-phenylpropionic acid-sulfate |
| $C_{15}H_{18}O_9$ | 342.0951 | Hydroxy-phenylpropionic acid-glucuronide |
| $C_{15}H_{16}O_9$ | 340.0794 | Hydroxy-cinnamic acid-glucuronide |
| $C_9H_8O_6S$ | 244.0042 | Hydroxy-cinnamic acid-sulfate |
| $C_9H_8O_4$ | 180.0423 | Caffeic acid |
| $C_9H_8O_7S$ | 259.9991 | Caffeic acid-sulfate |
| $C_{15}H_{16}O_{10}$ | 356.0743 | Caffeic acid-glucuronide |
| $C_{10}H_{10}O_4$ | 194.0579 | Ferulic acid |
| $C_{10}H_{10}O_7S$ | 274.0147 | Ferulic acid-sulfate |
| $C_{16}H_{18}O_{10}$ | 370.0900 | Ferulic acid-glucuronide |
| $C_9H_{10}O_4$ | 182.0597 | Dihydroxy-phenylpropionic acid |
| $C_9H_{10}O_3$ | 166.0630 | Hydroxy-phenylpropionic acid |
| $C_9H_8O_3$ | 164.0473 | Hydroxy-phenylacrylic acid |
| $C_{10}H_{12}O_4$ | 196.0736 | Hydroxy-methoxy-phenylpropionic acid |
| $C_{16}H_{12}O_6$ | 300.0634 | Methoxy-luteolin |
| $C_{15}H_{10}O_7$ | 302.0427 | Hydroxy-luteolin |
| $C_{16}H_{12}O_7$ | 316.0583 | Hydroxy-methoxy-luteolin |
| $C_{17}H_{14}O_6$ | 314.0790 | Dimethoxy-luteolin |
| $C_{18}H_{16}O_6$ | 328.0947 | Trimethoxy-luteolin |
| $C_{17}H_{14}O_7$ | 330.0740 | Hydroxy-dimethoxy-luteolin |
| $C_{18}H_{16}O_7$ | 344.0896 | Hydroxy-trimethoxy-luteolin |
| $C_{21}H_{18}O_{12}$ | 462.0798 | Luteolin-glucuronide |
| $C_{15}H_{10}O_9S$ | 366.0046 | Luteolin-sulfate |
| $C_{27}H_{26}O_{18}$ | 638.1119 | Luteolin-diglucuronide |
| $C_{15}H_{10}O_{12}S_2$ | 445.9614 | Luteolin-disulfate |
| $C_{21}H_{18}O_5S$ | 542.0366 | Luteolin-glucuronide-sulfate |
| $C_{15}H_{10}O_{10}S$ | 381.9995 | Hydroxy-luteolin-sulfate |
| $C_{21}H_{18}O_{13}$ | 478.0747 | Hydroxy-luteolin-glucuronide |
| $C_{22}H_{20}O_{13}$ | 492.0904 | Hydroxy-methoxy-luteolin-glucuronide |

| | | |
|---|---|---|
| $C_{27}H_{26}O_{19}$ | 654.1068 | Hydroxy-luteolin-diglucuronide |
| $C_{21}H_{10}O_{13}S_2$ | 461.9563 | Hydroxy-luteolin-disulfate |
| $C_{21}H_{18}O_{16}S$ | 558.0316 | Hydroxy-luteolin-glucuronide-sulfate |
| $C_{16}H_{12}O_{10}S$ | 396.0151 | Hydroxy-methoxy-luteolin-sulfate |
| $C_{16}H_{12}O_{9}S$ | 380.0202 | Methoxy-luteolin-sulfate |
| $C_{22}H_{20}O_{12}$ | 476.1955 | Methoxy-luteolin-glucuronide |
| $C_{21}H_{20}O_{12}$ | 464.0955 | Hydroxy-orientin |
| $C_{22}H_{22}O_{12}$ | 478.1111 | Hydroxy-methoxy-orientin |
| $C_{22}H_{22}O_{11}$ | 462.1162 | Methoxy-orientin |
| $C_{21}H_{20}O_{14}S$ | 528.0574 | Orientin-sulfate |
| $C_{21}H_{20}O_{15}S$ | 544.0523 | Hydroxy-orientin-sulfate |
| $C_{27}H_{28}O_{18}$ | 640.1276 | Hydroxy-orientin-glucuronide |
| $C_{27}H_{28}O_{17}$ | 624.1326 | Orientin-glucuronide |
| $C_{22}H_{22}O_{14}S$ | 542.0730 | Methoxy-orientin-sulfate |
| $C_{28}H_{30}O_{17}$ | 638.1483 | Methoxy-orientin-glucuronide |
| $C_{28}H_{30}O_{18}$ | 654.1432 | Hydroxy-methoxy-orientin-glucuronide |
| $C_{22}H_{22}O_{15}S$ | 558.0679 | Hydroxy-methoxy-orientin-sulfate |
| $C_{27}H_{28}O_{21}S$ | 720.0844 | Hydroxy-orientin-glucuronide-sulfate |
| $C_{27}H_{28}O_{20}S$ | 704.0895 | Orientin-glucuronide-sulfate |
| $C_{33}H_{36}O_{23}$ | 800.1647 | Orientin-diglucuronide |
| $C_{21}H_{20}O_{17}S_2$ | 608.0142 | Orientin-disulfate |
| $C_{33}H_{36}O_{24}$ | 816.1597 | Hydroxy-orientin-diglucuronide |
| $C_{21}H_{20}\ O_{18}S_2$ | 624.0091 | Hydroxy-orientin-disulfate |

**Table S2**.: Compound library of isoorientin.

| Molecular formula | Exact mass | Compound |
|---|---|---|
| $C_{21}H_{20}O_{11}$ | 448.1006 | Isoorientin |
| $C_{15}H_{10}O_6$ | 286.0477 | Luteolin |
| $C_7H_8O_2$ | 124.0524 | Dihydroxy-toluene |
| $C_7H_6O_3$ | 138.0317 | Hydroxy-benzoic acid |
| $C_8H_8O_3$ | 152.0473 | Hydroxy-phenylacetic acid |
| $C_8H_8O_4$ | 168.0423 | Dihydroxy-phenylacetic acid |
| $C_9H_{10}O_4$ | 182.0579 | Hydroxy-methoxy-phenylacetic acid |
| $C_6H_6O_3$ | 126.0317 | Phloroglucinol |
| $C_6H_6O_6S$ | 205.9885 | Phloroglucinol-sulfate |
| $C_{12}H_{14}O_9$ | 302.0638 | Phloroglucinol-glucuronide |
| $C_7H_8O_3$ | 140.0473 | Methyl-phloroglucinol |
| $C_8H_8O_6S$ | 232.0042 | Hydroxy-phenylacetic acid-sulfate |
| $C_{14}H_{16}O_9$ | 328.0794 | Hydroxy-phenylacetic acid-glucuronide |
| $C_{10}H_{11}NO_4$ | 209.0688 | Hydroxy-phenylacetic acid-glycine conjugate |
| $C_{11}H_{11}NO_4$ | 223.0845 | Hydroxy-phenylpropionic acid-glycine conjugate |
| $C_9H_{10}O_6S$ | 246.0198 | Hydroxy-phenylpropionic acid-sulfate |
| $C_{15}H_{18}O_9$ | 342.0951 | Hydroxy-phenylpropionic acid-glucuronide |
| $C_{15}H_{16}O_9$ | 340.0794 | Hydroxy-cinnamic acid-glucuronide |
| $C_9H_8O_6S$ | 244.0042 | Hydroxy-cinnamic acid-sulfate |
| $C_9H_8O_4$ | 180.0423 | Caffeic acid |
| $C_9H_8O_7S$ | 259.9991 | Caffeic acid-sulfate |
| $C_{15}H_{16}O_{10}$ | 356.0743 | Caffeic acid-glucuronide |
| $C_{10}H_{10}O_4$ | 194.0579 | Ferulic acid |
| $C_{10}H_{10}O_7S$ | 274.0147 | Ferulic acid-sulfate |
| $C_{16}H_{18}O_{10}$ | 370.0900 | Ferulic acid-glucuronide |
| $C_9H_{10}O_4$ | 182.0597 | Dihydroxy-phenylpropionic acid |
| $C_9H_{10}O_3$ | 166.0630 | Hydroxy-phenylpropionic acid |
| $C_9H_8O_3$ | 164.0473 | Hydroxy-phenylacrylic acid |
| $C_{10}H_{12}O_4$ | 196.0736 | Hydroxy-methoxy-phenylpropionic acid |
| $C_{16}H_{12}O_6$ | 300.0634 | Methoxy-luteolin |
| $C_{15}H_{10}O_7$ | 302.0427 | Hydroxy-luteolin |
| $C_{16}H_{12}O_7$ | 316.0583 | Hydroxy-methoxy-luteolin |
| $C_{17}H_{14}O_6$ | 314.0790 | Dimethoxy-luteolin |
| $C_{18}H_{16}O_6$ | 328.0947 | Trimethoxy-luteolin |
| $C_{17}H_{14}O_7$ | 330.0740 | Hydroxy-dimethoxy-luteolin |
| $C_{18}H_{16}O_7$ | 344.0896 | Hydroxy-trimethoxy-luteolin |
| $C_{21}H_{18}O_{12}$ | 462.0798 | Luteolin-glucuronide |
| $C_{15}H_{10}O_9S$ | 366.0046 | Luteolin-sulfate |
| $C_{27}H_{26}O_{18}$ | 638.1119 | Luteolin-diglucuronide |
| $C_{15}H_{10}O_{12}S_2$ | 445.9614 | Luteolin-disulfate |
| $C_{21}H_{18}O_5S$ | 542.0366 | Luteolin-glucuronide-sulfate |
| $C_{15}H_{10}O_{10}S$ | 381.9995 | Hydroxy-luteolin-sulfate |
| $C_{21}H_{18}O_{13}$ | 478.0747 | Hydroxy-luteolin-glucuronide |
| $C_{22}H_{20}O_{13}$ | 492.0904 | Hydroxy-methoxy-luteolin-glucuronide |

| | | |
|---|---|---|
| $C_{27}H_{26}O_{19}$ | 654.1068 | Hydroxy-luteolin-diglucuronide |
| $C_{21}H_{10}O_{13}S_2$ | 461.9563 | Hydroxy-luteolin-disulfate |
| $C_{21}H_{18}O_{16}S$ | 558.0316 | Hydroxy-luteolin-glucuronide-sulfate |
| $C_{16}H_{12}O_{10}S$ | 396.0151 | Hydroxy-methoxy-luteolin-sulfate |
| $C_{16}H_{12}O_{9}S$ | 380.0202 | Methoxy-luteolin-sulfate |
| $C_{22}H_{20}O_{12}$ | 476.1955 | Methoxy-luteolin-glucuronide |
| $C_{21}H_{20}O_{12}$ | 464.0955 | Hydroxy-orientin |
| $C_{22}H_{22}O_{12}$ | 478.1111 | Hydroxy-methoxy-orientin |
| $C_{22}H_{22}O_{11}$ | 462.1162 | Methoxy-orientin |
| $C_{21}H_{20}O_{14}S$ | 528.0574 | Orientin-sulfate |
| $C_{21}H_{20}O_{15}S$ | 544.0523 | Hydroxy-isoorientin-sulfate |
| $C_{27}H_{28}O_{18}$ | 640.1276 | Hydroxy-isoorientin-glucuronide |
| $C_{27}H_{28}O_{17}$ | 624.1326 | Isoorientin-glucuronide |
| $C_{22}H_{22}O_{14}S$ | 542.0730 | Methoxy-isoorientin-sulfate |
| $C_{28}H_{30}O_{17}$ | 638.1483 | Methoxy-isoorientin-glucuronide |
| $C_{28}H_{30}O_{18}$ | 654.1432 | Hydroxy-methoxy-isoorientin-glucuronide |
| $C_{22}H_{22}O_{15}S$ | 558.0679 | Hydroxy-methoxy-isoorientin-sulfate |
| $C_{27}H_{28}O_{21}S$ | 720.0844 | Hydroxy-isoorientin-glucuronide-sulfate |
| $C_{27}H_{28}O_{20}S$ | 704.0895 | Isoorientin-glucuronide-sulfate |
| $C_{33}H_{36}O_{23}$ | 800.1647 | Isoorientin-diglucuronide |
| $C_{21}H_{20}O_{17}S_2$ | 608.0142 | Isoorientin-disulfate |
| $C_{33}H_{36}O_{24}$ | 816.1597 | Hydroxy-isoorientin-diglucuronide |
| $C_{21}H_{20}\ O_{18}S_2$ | 624.0091 | Hydroxy-isoorientin-disulfate |

**Table S3.**: Compound library of schaftoside.

| Molecular formula | Exact mass | Compound |
|---|---|---|
| $C_{26}H_{28}O_{14}$ | 564.1479 | Schaftoside |
| $C_{15}H_{10}O_5$ | 270.528 | Apigenin |
| $C_7H_8O_2$ | 124.0524 | Dihydroxy-toluene |
| $C_7H_6O_3$ | 138.0317 | Hydroxy-benzoic acid |
| $C_8H_8O_3$ | 152.0473 | Hydroxy-phenylacetic acid |
| $C_8H_8O_4$ | 168.0423 | Dihydroxy-phenylacetic acid |
| $C_9H_{10}O_4$ | 182.0579 | Hydroxy-methoxy-phenylacetic acid |
| $C_6H_6O_3$ | 126.0317 | Phloroglucinol |
| $C_6H_6O_6S$ | 205.9885 | Phloroglucinol-sulfate |
| $C_{12}H_{14}O_9$ | 302.0638 | Phloroglucinol-glucuronide |
| $C_7H_8O_3$ | 140.0473 | Methyl-phloroglucinol |
| $C_8H_8O_6S$ | 232.0042 | Hydroxy-phenylacetic acid-sulfate |
| $C_{14}H_{16}O_9$ | 328.0794 | Hydroxy-phenylacetic acid-glucuronide |
| $C_{10}H_{11}NO_4$ | 209.0688 | Hydroxy-phenylacetic acid-glycine conjugate |
| $C_{11}H_{11}NO_4$ | 223.0845 | Hydroxy-phenylpropionic acid-glycine conjugate |
| $C_9H_{10}O_6S$ | 246.0198 | Hydroxy-phenylpropionic acid-sulfate |
| $C_{15}H_{18}O_9$ | 342.0951 | Hydroxy-phenylpropionic acid-glucuronide |
| $C_{15}H_{16}O_9$ | 340.0794 | Hydroxy-cinnamic acid-glucuronide |
| $C_9H_8O_6S$ | 244.0042 | Hydroxy-cinnamic acid-sulfate |
| $C_9H_8O_4$ | 180.0423 | Caffeic acid |
| $C_9H_8O_7S$ | 259.9991 | Caffeic acid-sulfate |
| $C_{15}H_{16}O_{10}$ | 356.0743 | Caffeic acid-glucuronide |
| $C_{10}H_{10}O_4$ | 194.0579 | Ferulic acid |
| $C_{10}H_{10}O_7S$ | 274.0147 | Ferulic acid-sulfate |
| $C_{16}H_{18}O_{10}$ | 370.0900 | Ferulic acid-glucuronide |
| $C_9H_{10}O_4$ | 182.0597 | Dihydroxy-phenylpropionic acid |
| $C_9H_{10}O_3$ | 166.0630 | Hydroxy-phenylpropionic acid |
| $C_9H_8O_3$ | 164.0473 | Hydroxy-phenylacrylic acid |
| $C_{10}H_{12}O_4$ | 196.0736 | Hydroxy-methoxy-phenylpropionic acid |
| $C_{16}H_{12}O_5$ | 284.0685 | Methoxy-apigenin |
| $C_{17}H_{14}O_5$ | 298.0841 | Dimethoxy-apigenin |
| $C_{15}H_{10}O_6$ | 286.477 | Hydroxy-apigenin |
| $C_{16}H_{12}O_6$ | 300.0634 | Hydroxy-methoxy-apigenin |
| $C_{17}H_{14}O_6$ | 314.0790 | Hydroxy-dimethoxy-apigeninr |
| $C_{18}H_{16}O_6$ | 328.0947 | Hydroxy-trimethoxy-apigeninr |
| $C_{15}H_{10}O_8S$ | 350.0096 | Apigenin-sulfate |
| $C_{21}H_{18}O_{11}$ | 446.0849 | Apigenin-glucuronide |
| $C_{27}H_{26}O_{17}$ | 622.1170 | Apigenin-diglucuronide |
| $C_{15}H_{10}O_{11}S_2$ | 429.9665 | Apigenin-disulfate |
| $C_{21}H_{18}O_{14}S$ | 526.0417 | Apigenin-glucuronide-sulfate |
| $C_{15}H_{10}O_9S$ | 366.0046 | Hydroxy-apigenin-sulfate |
| $C_{16}H_{12}O_8S$ | 364.0253 | Methoxy-apigenin-sulfate |
| $C_{16}H_{12}O_9S$ | 380.0202 | Hydroxy-methoxy-apigenin-sulfate |
| $C_{22}H_{20}O_{11}$ | 460.1006 | Methoxy-apigenin-glucuronide |

| | | |
|---|---|---|
| $C_{21}H_{18}O_{12}$ | 462.0798 | Hydroxy-apigenin-glucuronide |
| $C_{22}H_{20}O_{12}$ | 476.0955 | Hydroxy-methoxy-apigenin-glucuronide |
| $C_{15}H_{10}O_{12}S_2$ | 445.9614 | Hydroxy-apigenin-disulfate |
| $C_{27}H_{28}O_{18}$ | 638.1119 | Hydroxy-apigenin-diglucuronide |
| $C_{21}H_{18}O_{15}S$ | 542.0366 | Hydroxy-apigenin-glucuronide-sulfate |
| $C_{27}H_{30}O_{14}$ | 578.1636 | Methoxy-schaftoside |
| $C_{27}H_{30}O_{15}$ | 594.1585 | Hydroxy-methoxy-schaftoside |
| $C_{26}H_{28}O_{15}$ | 580.1428 | Hydroxy-schaftoside |
| $C_{28}H_{32}O_{14}$ | 592.1792 | Dimethoxy-schaftoside |
| $C_{28}H_{32}O_{15}$ | 608.1741 | Hydroxy-dimethoxy-schaftoside |
| $C_{26}H_{28}O_{17}S$ | 644.1047 | Schaftoside-sulfate |
| $C_{26}H_{28}O_{20}S_2$ | 724.0618 | Schaftoside-disulfate |
| $C_{26}H_{28}O_{21}S_2$ | 740.0564 | Hydroxy-schaftoside-disulfate |
| $C_{32}H_{36}O_{20}$ | 740.1800 | Schaftoside-glucuronide |
| $C_{32}H_{26}O_{23}S$ | 820.1368 | Schaftoside-glucuronide-sulfate |
| $C_{38}H_{44}O_{26}$ | 916.2121 | Schaftoside-diglucuronide |
| $C_{32}H_{36}O_{24}S$ | 836.1317 | Hydroxy-schaftoside-glucuronide-sulfate |
| $C_{38}H_{44}O_{27}$ | 932.2070 | Hydroxy-schaftoside-diglucuronide |
| $C_{33}H_{38}O_{20}$ | 754.1956 | Methoxy-schaftoside-glucuronide |
| $C_{32}H_{36}O_{21}$ | 756.1749 | Hydroxy-schaftoside-glucuronide |
| $C_{33}H_{38}O_{21}$ | 770.1906 | Hydroxy-methoxy-schaftoside-glucuronide |
| $C_{27}H_{30}O_{17}S$ | 658.1204 | Methoxy-schaftoside-sulfate |
| $C_{26}H_{28}O_{18}S$ | 660.0996 | Hydroxy-schaftoside-sulfate |
| $C_{27}H_{30}O_{18}S$ | 674.1153 | Hydroxy-methoxy-schaftoside-sulfate |
| $C_{22}H_{22}O_{10}$ | 446.1213 | Methoxy-apigenin-8-C-riboside |
| $C_{22}H_{22}O_{11}$ | 462.1162 | Hydroxy-methoxy-apigenin-8-C-riboside |
| $C_{21}H_{20}O_{11}$ | 448.1006 | Hydroxy-apigenin-8-C-riboside |
| $C_{23}H_{24}O_{10}$ | 460.1369 | Dimethoxy-apigenin-8-C-riboside |
| $C_{23}H_{24}O_{11}$ | 476.1319 | Hydroxy-dimethoxy-apigenin-8-C-riboside |
| $C_{21}H_{20}O_{13}S$ | 512.0625 | Apigenin-8-C-riboside-sulfate |
| $C_{21}H_{20}O_{16}S_2$ | 592.0193 | Apigenin-8-C-riboside-disulfate |
| $C_{21}H_{20}O_{17}S_2$ | 608.0142 | Hydroxy-apigenin-8-C-riboside-disulfate |
| $C_{27}H_{28}O_{16}$ | 608.1377 | Apigenin-8-C-riboside-glucuronide |
| $C_{27}H_{28}O_{19}S$ | 688.0945 | Apigenin-8-C-riboside-glucuronide-sulfate |
| $C_{33}H_{36}O_{22}$ | 784.1698 | Apigenin-8-C-riboside-diglucuronide |
| $C_{27}H_{28}O_{20}S$ | 704.0895 | Hydroxy-apigenin-8-C-riboside-glucuronide-sulfate |
| $C_{33}H_{36}O_{23}$ | 800.1647 | Hydroxy-apigenin-8-C-riboside-diglucuronide |
| $C_{28}H_{30}O_{16}$ | 622.1534 | Methoxy- apigenin-8-C-riboside-glucuronide |
| $C_{27}H_{28}O_{17}$ | 624.1326 | Hydroxy-apigenin-8-C-riboside-glucuronide |
| $C_{28}H_{30}O_{17}$ | 638.1483 | Hydroxy-methoxy- apigenin-8-C-riboside-glucuronide |
| $C_{22}H_{22}O_{13}S$ | 526.0781 | Methoxy- apigenin-8-C-riboside-sulfate |
| $C_{21}H_{20}O_{14}S$ | 528.0574 | Hydroxy-apigenin-8-C-riboside-sulfate |
| $C_{22}H_{22}O_{14}S$ | 542.0730 | Hydroxy-methoxy-apigenin-8-C-riboside-sulfat |
| $C_{21}H_{20}O_9$ | 416.1107 | Methoxy-apigenin-6-C-glucoside |
| $C_{21}H_{20}O_{10}$ | 432.1056 | Hydroxy-methoxy- apigenin-6-C-glucoside |
| $C_{20}H_{18}O_{10}$ | 418.0900 | Hydroxy-apigenin-6-C-glucoside |
| $C_{22}H_{22}O_9$ | 430.1264 | Dimethoxy-apigenin-6-C-glucoside |

| | | |
|---|---|---|
| $C_{20}H_{20}O_{10}$ | 446.1213 | Hydroxy-dimethoxy-apigenin-6-C-glucoside |
| $C_{20}H_{18}O_{12}S$ | 482.0519 | Apigenin-6-C-glucoside-sulfate |
| $C_{20}H_{18}O_{15}S_2$ | 562.0087 | Apigenin-6-C-glucoside-disulfate |
| $C_{20}H_{18}O_{16}S_2$ | 578.0036 | Hydroxy-apigenin-6-C-glucoside-disulfate |
| $C_{26}H_{26}O_{15}$ | 578.1272 | Apigenin-6-C-glucoside-glucuronide |
| $C_{26}H_{26}O_{18}S$ | 658.0840 | Apigenin-6-C-glucoside-glucuronide-sulfate |
| $C_{33}H_{34}O_{21}$ | 754.1593 | Apigenin-6-C-glucoside-diglucuronide |
| $C_{26}H_{26}O_{19}S$ | 674.0789 | Hydroxy-apigenin-6-C-glucoside-glucuronide-sulfate |
| $C_{32}H_{34}O_{22}$ | 770.1542 | Hydroxy-apigenin-6-C-glucoside-diglucuronide |
| $C_{27}H_{28}O_{15}$ | 592.1428 | Methoxy- Apigenin-6-C-glucoside-glucuronide |
| $C_{26}H_{26}O_{16}$ | 594.1221 | Hydroxy-apigenin-6-C-glucoside-glucuronide |
| $C_{27}H_{28}O_{16}$ | 608.1377 | Hydroxy-methoxy-apigenin-6-C-glucoside-glucuronide |
| $C_{21}H_{20}O_{12}S$ | 496.0675 | Methoxy-apigenin-6-C-glucoside-sulfate |
| $C_{20}H_{18}O_{13}S$ | 498.0468 | Hydroxy-apigenin-6-C-glucoside-sulfate |
| $C_{21}H_{20}O_{13}S$ | 512.0625 | Hydroxy-methoxy-apigenin-6-C-glucoside-sulfate |

**Table S4**.: Compound library of isoschaftoside.

| Molecular formula | Exact mass | Compound |
|---|---|---|
| $C_{26}H_{28}O_{14}$ | 564.1479 | Isoschaftoside |
| $C_{15}H_{10}O_5$ | 270.528 | Apigenin |
| $C_7H_8O_2$ | 124.0524 | Dihydroxy-toluene |
| $C_7H_6O_3$ | 138.0317 | Hydroxy-benzoic acid |
| $C_8H_8O_3$ | 152.0473 | Hydroxy-phenylacetic acid |
| $C_8H_8O_4$ | 168.0423 | Dihydroxy-phenylacetic acid |
| $C_9H_{10}O_4$ | 182.0579 | Hydroxy-methoxy-phenylacetic acid |
| $C_6H_6O_3$ | 126.0317 | Phloroglucinol |
| $C_6H_6O_6S$ | 205.9885 | Phloroglucinol-sulfate |
| $C_{12}H_{14}O_9$ | 302.0638 | Phloroglucinol-glucuronide |
| $C_7H_8O_3$ | 140.0473 | Methyl-phloroglucinol |
| $C_8H_8O_6S$ | 232.0042 | Hydroxy-phenylacetic acid-sulfate |
| $C_{14}H_{16}O_9$ | 328.0794 | Hydroxy-phenylacetic acid-glucuronide |
| $C_{10}H_{11}NO_4$ | 209.0688 | Hydroxy-phenylacetic acid-glycine conjugate |
| $C_{11}H_{11}NO_4$ | 223.0845 | Hydroxy-phenylpropionic acid-glycine conjugate |
| $C_9H_{10}O_6S$ | 246.0198 | Hydroxy-phenylpropionic acid-sulfate |
| $C_{15}H_{18}O_9$ | 342.0951 | Hydroxy-phenylpropionic acid-glucuronide |
| $C_{15}H_{16}O_9$ | 340.0794 | Hydroxy-cinnamic acid-glucuronide |
| $C_9H_8O_6S$ | 244.0042 | Hydroxy-cinnamic acid-sulfate |
| $C_9H_8O_4$ | 180.0423 | Caffeic acid |
| $C_9H_8O_7S$ | 259.9991 | Caffeic acid-sulfate |
| $C_{15}H_{16}O_{10}$ | 356.0743 | Caffeic acid-glucuronide |
| $C_{10}H_{10}O_4$ | 194.0579 | Ferulic acid |
| $C_{10}H_{10}O_7S$ | 274.0147 | Ferulic acid-sulfate |
| $C_{16}H_{18}O_{10}$ | 370.0900 | Ferulic acid-glucuronide |
| $C_9H_{10}O_4$ | 182.0597 | Dihydroxy-phenylpropionic acid |
| $C_9H_{10}O_3$ | 166.0630 | Hydroxy-phenylpropionic acid |
| $C_9H_8O_3$ | 164.0473 | Hydroxy-phenylacrylic acid |
| $C_{10}H_{12}O_4$ | 196.0736 | Hydroxy-methoxy-phenylpropionic acid |
| $C_{16}H_{12}O_5$ | 284.0685 | Methoxy-apigenin |
| $C_{17}H_{14}O_5$ | 298.0841 | Dimethoxy-apigenin |
| $C_{15}H_{10}O_6$ | 286.4770 | Hydroxy-apigenin |
| $C_{16}H_{12}O_6$ | 300.0634 | Hydroxy-methoxy-apigenin |
| $C_{17}H_{14}O_6$ | 314.0790 | Hydroxy-dimethoxy-apigeninr |
| $C_{18}H_{16}O_6$ | 328.0947 | Hydroxy-trimethoxy-apigeninr |
| $C_{15}H_{10}O_8S$ | 350.0096 | Apigenin-sulfate |
| $C_{21}H_{18}O_{11}$ | 446.0849 | Apigenin-glucuronide |
| $C_{27}H_{26}O_{17}$ | 622.1170 | Apigenin-diglucuronide |
| $C_{15}H_{10}O_{11}S_2$ | 429.9665 | Apigenin-disulfate |
| $C_{21}H_{18}O_{14}S$ | 526.0417 | Apigenin-glucuronide-sulfate |
| $C_{15}H_{10}O_9S$ | 366.0046 | Hydroxy-apigenin-sulfate |
| $C_{16}H_{12}O_8S$ | 364.0253 | Methoxy-apigenin-sulfate |
| $C_{16}H_{12}O_9S$ | 380.0202 | Hydroxy-methoxy-apigenin-sulfate |
| $C_{22}H_{20}O_{11}$ | 460.1006 | Methoxy-apigenin-glucuronide |

| | | |
|---|---|---|
| $C_{21}H_{18}O_{12}$ | 462.0798 | Hydroxy-apigenin-glucuronide |
| $C_{22}H_{20}O_{12}$ | 476.0955 | Hydroxy-methoxy-apigenin-glucuronide |
| $C_{15}H_{10}O_{12}S_2$ | 445.9614 | Hydroxy-apigenin-disulfate |
| $C_{27}H_{28}O_{18}$ | 638.1119 | Hydroxy-apigenin-diglucuronide |
| $C_{21}H_{18}O_{15}S$ | 542.0366 | Hydroxy-apigenin-glucuronide-sulfate |
| $C_{27}H_{30}O_{14}$ | 578.1636 | Methoxy-isoschaftoside |
| $C_{27}H_{30}O_{15}$ | 594.1585 | Hydroxy-methoxy-isoschaftoside |
| $C_{26}H_{28}O_{15}$ | 580.1428 | Hydroxy-isoschaftoside |
| $C_{28}H_{32}O_{14}$ | 592.1792 | Dimethoxy-isoschaftoside |
| $C_{28}H_{32}O_{15}$ | 608.1741 | Hydroxy-dimethoxy-isoschaftoside |
| $C_{26}H_{28}O_{17}S$ | 644.1047 | Isoschaftoside-sulfate |
| $C_{26}H_{28}O_{20}S_2$ | 724.0618 | Isoschaftoside-disulfate |
| $C_{26}H_{28}O_{21}S_2$ | 740.0564 | Hydroxy-isoschaftoside-disulfate |
| $C_{32}H_{36}O_{20}$ | 740.1800 | Isoschaftoside-glucuronide |
| $C_{32}H_{26}O_{23}S$ | 820.1368 | Isoschaftoside-glucuronide-sulfate |
| $C_{38}H_{44}O_{26}$ | 916.2121 | Isoschaftoside-diglucuronide |
| $C_{32}H_{36}O_{24}S$ | 836.1317 | Hydroxy-isoschaftoside-glucuronide-sulfate |
| $C_{38}H_{44}O_{27}$ | 932.2070 | Hydroxy-isoschaftoside-diglucuronide |
| $C_{33}H_{38}O_{20}$ | 754.1956 | Methoxy-isoschaftoside-glucuronide |
| $C_{32}H_{36}O_{21}$ | 756.1749 | Hydroxy-isoschaftoside-glucuronide |
| $C_{33}H_{38}O_{21}$ | 770.1906 | Hydroxy-methoxy-isoschaftoside-glucuronide |
| $C_{27}H_{30}O_{17}S$ | 658.1204 | Methoxy-isoschaftoside-sulfate |
| $C_{26}H_{28}O_{18}S$ | 660.0996 | Hydroxy-isoschaftoside-sulfate |
| $C_{27}H_{30}O_{18}S$ | 674.1153 | Hydroxy-methoxy-isoschaftoside-sulfate |
| $C_{22}H_{22}O_{10}$ | 446.1213 | Methoxy-apigenin-6-C-riboside |
| $C_{22}H_{22}O_{11}$ | 462.1162 | Hydroxy-methoxy-apigenin-6-C-riboside |
| $C_{21}H_{20}O_{11}$ | 448.1006 | Hydroxy-apigenin-6-C-riboside |
| $C_{23}H_{24}O_{10}$ | 460.1369 | Dimethoxy-apigenin-6-C-riboside |
| $C_{23}H_{24}O_{11}$ | 476.1319 | Hydroxy-dimethoxy-apigenin-6-C-riboside |
| $C_{21}H_{20}O_{13}S$ | 512.0625 | Apigenin-6-C-riboside-sulfate |
| $C_{21}H_{20}O_{16}S_2$ | 592.0193 | Apigenin-6-C-riboside-disulfate |
| $C_{21}H_{20}O_{17}S_2$ | 608.0142 | Hydroxy-apigenin-6-C-riboside-disulfate |
| $C_{27}H_{28}O_{16}$ | 608.1377 | Apigenin-6-C-riboside-glucuronide |
| $C_{27}H_{28}O_{19}S$ | 688.0945 | Apigenin-6-C-riboside-glucuronide-sulfate |
| $C_{33}H_{36}O_{22}$ | 784.1698 | Apigenin-6-C-riboside-diglucuronide |
| $C_{27}H_{28}O_{20}S$ | 704.0895 | Hydroxy-apigenin-6-C-riboside-glucuronide-sulfate |
| $C_{33}H_{36}O_{23}$ | 800.1647 | Hydroxy-apigenin-6-C-riboside-diglucuronide |
| $C_{28}H_{30}O_{16}$ | 622.1534 | Methoxy- apigenin-6-C-riboside-glucuronide |
| $C_{27}H_{28}O_{17}$ | 624.1326 | Hydroxy-apigenin-6-C-riboside-glucuronide |
| $C_{28}H_{30}O_{17}$ | 638.1483 | Hydroxy-methoxy- apigenin-6-C-riboside-glucuronide |
| $C_{22}H_{22}O_{13}S$ | 526.0781 | Methoxy- apigenin-6-C-riboside-sulfate |
| $C_{21}H_{20}O_{14}S$ | 528.0574 | Hydroxy-apigenin-6-C-riboside-sulfate |
| $C_{22}H_{22}O_{14}S$ | 542.0730 | Hydroxy-methoxy-apigenin-6-C-riboside-sulfat |
| $C_{21}H_{20}O_9$ | 416.1107 | Methoxy-apigenin-8-C-glucoside |
| $C_{21}H_{20}O_{10}$ | 432.1056 | Hydroxy-methoxy- apigenin-8-C-glucoside |
| $C_{20}H_{18}O_{10}$ | 418.0900 | Hydroxy-apigenin-8-C-glucoside |
| $C_{22}H_{22}O_9$ | 430.1264 | Dimethoxy-apigenin-8-C-glucoside |

| | | |
|---|---|---|
| $C_{20}H_{20}O_{10}$ | 446.1213 | Hydroxy-dimethoxy-apigenin-8-C-glucoside |
| $C_{20}H_{18}O_{12}S$ | 482.0519 | Apigenin-8-C-glucoside-sulfate |
| $C_{20}H_{18}O_{15}S_2$ | 562.0087 | Apigenin-8-C-glucoside-disulfate |
| $C_{20}H_{18}O_{16}S_2$ | 578.0036 | Hydroxy-apigenin-8-C-glucoside-disulfate |
| $C_{26}H_{26}O_{15}$ | 578.1272 | Apigenin-8-C-glucoside-glucuronide |
| $C_{26}H_{26}O_{18}S$ | 658.0840 | Apigenin-8-C-glucoside-glucuronide-sulfate |
| $C_{33}H_{34}O_{21}$ | 754.1593 | Apigenin-8-C-glucoside-diglucuronide |
| $C_{26}H_{26}O_{19}S$ | 674.0789 | Hydroxy-apigenin-8-C-glucoside-glucuronide-sulfate |
| $C_{32}H_{34}O_{22}$ | 770.1542 | Hydroxy-apigenin-8-C-glucoside-diglucuronide |
| $C_{27}H_{28}O_{15}$ | 592.1428 | Methoxy- Apigenin-8-C-glucoside-glucuronide |
| $C_{26}H_{26}O_{16}$ | 594.1221 | Hydroxy-apigenin-8-C-glucoside-glucuronide |
| $C_{27}H_{28}O_{16}$ | 608.1377 | Hydroxy-methoxy-apigenin-8-C-glucoside-glucuronide |
| $C_{21}H_{20}O_{12}S$ | 496.0675 | Methoxy-apigenin-8-C-glucoside-sulfate |
| $C_{20}H_{18}O_{13}S$ | 498.0468 | Hydroxy-apigenin-8-C-glucoside-sulfate |
| $C_{21}H_{20}O_{13}S$ | 512.0625 | Hydroxy-methoxy-apigenin-8-C-glucoside-sulfate |

**Table S5**.: Compound library of vitexin.

| Molecular formula | Exact mass | Compound |
|---|---|---|
| $C_{21}H_{20}O_{10}$ | 432.1056 | Vitexin |
| $C_{15}H_{10}O_5$ | 270.528 | Apigenin |
| $C_7H_8O_2$ | 124.0524 | Dihydroxy-toluene |
| $C_7H_6O_3$ | 138.0317 | Hydroxy-benzoic acid |
| $C_8H_8O_3$ | 152.0473 | Hydroxy-phenylacetic acid |
| $C_8H_8O_4$ | 168.0423 | Dihydroxy-phenylacetic acid |
| $C_9H_{10}O_4$ | 182.0579 | Hydroxy-methoxy-phenylacetic acid |
| $C_6H_6O_3$ | 126.0317 | Phloroglucinol |
| $C_6H_6O_6S$ | 205.9885 | Phloroglucinol-sulfate |
| $C_{12}H_{14}O_9$ | 302.0638 | Phloroglucinol-glucuronide |
| $C_7H_8O_3$ | 140.0473 | Methyl-phloroglucinol |
| $C_8H_8O_6S$ | 232.0042 | Hydroxy-phenylacetic acid-sulfate |
| $C_{14}H_{16}O_9$ | 328.0794 | Hydroxy-phenylacetic acid-glucuronide |
| $C_{10}H_{11}NO_4$ | 209.0688 | Hydroxy-phenylacetic acid-glycine conjugate |
| $C_{11}H_{11}NO_4$ | 223.0845 | Hydroxy-phenylpropionic acid-glycine conjugate |
| $C_9H_{10}O_6S$ | 246.0198 | Hydroxy-phenylpropionic acid-sulfate |
| $C_{15}H_{18}O_9$ | 342.0951 | Hydroxy-phenylpropionic acid-glucuronide |
| $C_{15}H_{16}O_9$ | 340.0794 | Hydroxy-cinnamic acid-glucuronide |
| $C_9H_8O_6S$ | 244.0042 | Hydroxy-cinnamic acid-sulfate |
| $C_9H_8O_4$ | 180.0423 | Caffeic acid |
| $C_9H_8O_7S$ | 259.9991 | Caffeic acid-sulfate |
| $C_{15}H_{16}O_{10}$ | 356.0743 | Caffeic acid-glucuronide |
| $C_{10}H_{10}O_4$ | 194.0579 | Ferulic acid |
| $C_{10}H_{10}O_7S$ | 274.0147 | Ferulic acid-sulfate |
| $C_{16}H_{18}O_{10}$ | 370.0900 | Ferulic acid-glucuronide |
| $C_9H_{10}O_4$ | 182.0597 | Dihydroxy-phenylpropionic acid |
| $C_9H_{10}O_3$ | 166.0630 | Hydroxy-phenylpropionic acid |
| $C_9H_8O_3$ | 164.0473 | Hydroxy-phenylacrylic acid |
| $C_{10}H_{12}O_4$ | 196.0736 | Hydroxy-methoxy-phenylpropionic acid |
| $C_{16}H_{12}O_5$ | 284.0685 | Methoxy-apigenin |
| $C_{17}H_{14}O_5$ | 298.0841 | Dimethoxy-apigenin |
| $C_{15}H_{10}O_6$ | 286.477 | Hydroxy-apigenin |
| $C_{16}H_{12}O_6$ | 300.0634 | Hydroxy-methoxy-apigenin |
| $C_{17}H_{14}O_6$ | 314.0790 | Hydroxy-dimethoxy-apigenin |
| $C_{18}H_{16}O_6$ | 328.0947 | Hydroxy-trimethoxy-apigenin |
| $C_{15}H_{10}O_8S$ | 350.0096 | Apigenin-sulfate |
| $C_{21}H_{18}O_{11}$ | 446.0849 | Apigenin-glucuronide |
| $C_{27}H_{26}O_{17}$ | 622.1170 | Apigenin-diglucuronide |
| $C_{15}H_{10}O_{11}S_2$ | 429.9665 | Apigenin-disulfate |
| $C_{21}H_{18}O_{14}S$ | 526.0417 | Apigenin-glucuronide-sulfate |
| $C_{15}H_{10}O_9S$ | 366.0046 | Hydroxy-apigenin-sulfate |
| $C_{16}H_{12}O_8S$ | 364.0253 | Methoxy-apigenin-sulfate |
| $C_{16}H_{12}O_9S$ | 380.0202 | Hydroxy-methoxy-apigenin-sulfate |
| $C_{22}H_{20}O_{11}$ | 460.1006 | Methoxy-apigenin-glucuronide |

| | | |
|---|---|---|
| $C_{21}H_{18}O_{12}$ | 462.0798 | Hydroxy-apigenin-glucuronide |
| $C_{22}H_{20}O_{12}$ | 476.0955 | Hydroxy-methoxy-apigenin-glucuronide |
| $C_{15}H_{10}O_{12}S_2$ | 445.9614 | Hydroxy-apigenin-disulfate |
| $C_{27}H_{28}O_{18}$ | 638.1119 | Hydroxy-apigenin-diglucuronide |
| $C_{21}H_{18}O_{15}S$ | 542.0366 | Hydroxy-apigenin-glucuronide-sulfate |
| $C_{22}H_{22}O_{10}$ | 446.1213 | Methoxy-vitexin |
| $C_{23}H_{24}O_{10}$ | 460.1369 | Dimethoxy-vitexin |
| $C_{21}H_{20}O_{11}$ | 448.1006 | Hydroxy-vitexin |
| $C_{21}H_{20}O_{12}$ | 464.0955 | Dihydroxy-vitexin |
| $C_{22}H_{22}O_{11}$ | 462.1162 | Hydroxy-methoxy-vitexin |
| $C_{23}H_{24}O_{11}$ | 476.1319 | Hydroxy-dimethoxy-vitexin |
| $C_{22}H_{22}O_{12}$ | 478.1111 | Dihydroxy-methoxy-vitexin |
| $C_{23}H_{24}O_{12}$ | 492.1268 | Dihydroxy-dimethoxy-vitexin |
| $C_{21}H_{20}O_{13}S$ | 512.0625 | Vitexin-sulfate |
| $C_{22}H_{22}O_{13}S$ | 526.0781 | Methoxy-vitexin-sulfate |
| $C_{21}H_{20}O_{14}S$ | 528.0574 | Hydroxy-vitexin-sulfate |
| $C_{22}H_{20}O_{14}S$ | 542.0730 | Hydroxy-methoxy-vitexin-sulfate |
| $C_{21}H_{20}O_{16}S_2$ | 592.0193 | Vitexin-disulfate |
| $C_{27}H_{28}O_{16}$ | 608.1377 | Vitexin-glucuronide |
| $C_{28}H_{30}O_{16}$ | 622.1534 | Methoxy-vitexin-glucuronide |
| $C_{27}H_{28}O_{17}$ | 624.1326 | Hydroxy-vitexin-glucuronide |
| $C_{28}H_{30}O_{17}$ | 638.1483 | Hydroxy-methoxy-vitexin-glucuronide |
| $C_{33}H_{36}O_{22}$ | 784.1698 | Vitexin-diglucuronide |
| $C_{27}H_{28}O_{19}S$ | 688.0945 | Vitexin-glucuronide-sulfate |
| $C_{27}H_{28}O_{20}S$ | 704.0895 | Hydroxy-vitexin-glucuronide-sulfate |
| $C_{21}H_{20}O_{17}S_2$ | 608.0142 | Hydroxy-vitexin-disulfate |
| $C_{33}H_{36}O_{23}$ | 800.1647 | Hydroxy-vitexin-diglucuronide |

**Table S6**.: Compound library of isovitexin.

| Molecular formula | Exact mass | Compound |
|---|---|---|
| $C_{21}H_{20}O_{10}$ | 432.1056 | Isovitexin |
| $C_{15}H_{10}O_5$ | 270.528 | Apigenin |
| $C_7H_8O_2$ | 124.0524 | Dihydroxy-toluene |
| $C_7H_6O_3$ | 138.0317 | Hydroxy-benzoic acid |
| $C_8H_8O_3$ | 152.0473 | Hydroxy-phenylacetic acid |
| $C_8H_8O_4$ | 168.0423 | Dihydroxy-phenylacetic acid |
| $C_9H_{10}O_4$ | 182.0579 | Hydroxy-methoxy-phenylacetic acid |
| $C_6H_6O_3$ | 126.0317 | Phloroglucinol |
| $C_6H_6O_6S$ | 205.9885 | Phloroglucinol-sulfate |
| $C_{12}H_{14}O_9$ | 302.0638 | Phloroglucinol-glucuronide |
| $C_7H_8O_3$ | 140.0473 | Methyl-phloroglucinol |
| $C_8H_8O_6S$ | 232.0042 | Hydroxy-phenylacetic acid-sulfate |
| $C_{14}H_{16}O_9$ | 328.0794 | Hydroxy-phenylacetic acid-glucuronide |
| $C_{10}H_{11}NO_4$ | 209.0688 | Hydroxy-phenylacetic acid-glycine conjugate |
| $C_{11}H_{11}NO_4$ | 223.0845 | Hydroxy-phenylpropionic acid-glycine conjugate |
| $C_9H_{10}O_6S$ | 246.0198 | Hydroxy-phenylpropionic acid-sulfate |
| $C_{15}H_{18}O_9$ | 342.0951 | Hydroxy-phenylpropionic acid-glucuronide |
| $C_{15}H_{16}O_9$ | 340.0794 | Hydroxy-cinnamic acid-glucuronide |
| $C_9H_8O_6S$ | 244.0042 | Hydroxy-cinnamic acid-sulfate |
| $C_9H_8O_4$ | 180.0423 | Caffeic acid |
| $C_9H_8O_7S$ | 259.9991 | Caffeic acid-sulfate |
| $C_{15}H_{16}O_{10}$ | 356.0743 | Caffeic acid-glucuronide |
| $C_{10}H_{10}O_4$ | 194.0579 | Ferulic acid |
| $C_{10}H_{10}O_7S$ | 274.0147 | Ferulic acid-sulfate |
| $C_{16}H_{18}O_{10}$ | 370.0900 | Ferulic acid-glucuronide |
| $C_9H_{10}O_4$ | 182.0597 | Dihydroxy-phenylpropionic acid |
| $C_9H_{10}O_3$ | 166.0630 | Hydroxy-phenylpropionic acid |
| $C_9H_8O_3$ | 164.0473 | Hydroxy-phenylacrylic acid |
| $C_{10}H_{12}O_4$ | 196.0736 | Hydroxy-methoxy-phenylpropionic acid |
| $C_{16}H_{12}O_5$ | 284.0685 | Methoxy-apigenin |
| $C_{17}H_{14}O_5$ | 298.0841 | Dimethoxy-apigenin |
| $C_{15}H_{10}O_6$ | 286.477 | Hydroxy-apigenin |
| $C_{16}H_{12}O_6$ | 300.0634 | Hydroxy-methoxy-apigenin |
| $C_{17}H_{14}O_6$ | 314.0790 | Hydroxy-dimethoxy-apigenin |
| $C_{18}H_{16}O_6$ | 328.0947 | Hydroxy-trimethoxy-apigenin |
| $C_{15}H_{10}O_8S$ | 350.0096 | Apigenin-sulfate |
| $C_{21}H_{18}O_{11}$ | 446.0849 | Apigenin-glucuronide |
| $C_{27}H_{26}O_{17}$ | 622.1170 | Apigenin-diglucuronide |
| $C_{15}H_{10}O_{11}S_2$ | 429.9665 | Apigenin-disulfate |
| $C_{21}H_{18}O_{14}S$ | 526.0417 | Apigenin-glucuronide-sulfate |
| $C_{15}H_{10}O_9S$ | 366.0046 | Hydroxy-apigenin-sulfate |
| $C_{16}H_{12}O_8S$ | 364.0253 | Methoxy-apigenin-sulfate |
| $C_{16}H_{12}O_9S$ | 380.0202 | Hydroxy-methoxy-apigenin-sulfate |
| $C_{22}H_{20}O_{11}$ | 460.1006 | Methoxy-apigenin-glucuronide |

| | | |
|---|---|---|
| $C_{21}H_{18}O_{12}$ | 462.0798 | Hydroxy-apigenin-glucuronide |
| $C_{22}H_{20}O_{12}$ | 476.0955 | Hydroxy-methoxy-apigenin-glucuronide |
| $C_{15}H_{10}O_{12}S_2$ | 445.9614 | Hydroxy-apigenin-disulfate |
| $C_{27}H_{28}O_{18}$ | 638.1119 | Hydroxy-apigenin-diglucuronide |
| $C_{21}H_{18}O_{15}S$ | 542.0366 | Hydroxy-apigenin-glucuronide-sulfate |
| $C_{22}H_{22}O_{10}$ | 446.1213 | Methoxy-isovitexin |
| $C_{23}H_{24}O_{10}$ | 460.1369 | Dimethoxy-isovitexin |
| $C_{21}H_{20}O_{11}$ | 448.1006 | Hydroxy-isovitexin |
| $C_{21}H_{20}O_{12}$ | 464.0955 | Dihydroxy-isovitexin |
| $C_{22}H_{22}O_{11}$ | 462.1162 | Hydroxy-methoxy-isovitexin |
| $C_{23}H_{24}O_{11}$ | 476.1319 | Hydroxy-dimethoxy-isovitexin |
| $C_{22}H_{22}O_{12}$ | 478.1111 | Dihydroxy-methoxy-isovitexin |
| $C_{23}H_{24}O_{12}$ | 492.1268 | Dihydroxy-dimethoxy-isovitexin |
| $C_{21}H_{20}O_{13}S$ | 512.0625 | Isovitexin-sulfate |
| $C_{22}H_{22}O_{13}S$ | 526.0781 | Methoxy-isovitexin-sulfate |
| $C_{21}H_{20}O_{14}S$ | 528.0574 | Hydroxy-isovitexin-sulfate |
| $C_{22}H_{20}O_{14}S$ | 542.0730 | Hydroxy-methoxy-isovitexin-sulfate |
| $C_{21}H_{20}O_{16}S_2$ | 592.0193 | Isovitexin-disulfate |
| $C_{27}H_{28}O_{16}$ | 608.1377 | Isovitexin-glucuronide |
| $C_{28}H_{30}O_{16}$ | 622.1534 | Methoxy-isovitexin-glucuronide |
| $C_{27}H_{28}O_{17}$ | 624.1326 | Hydroxy-isovitexin-glucuronide |
| $C_{28}H_{30}O_{17}$ | 638.1483 | Hydroxy-methoxy-isovitexin-glucuronide |
| $C_{33}H_{36}O_{22}$ | 784.1698 | Isovitexin-diglucuronide |
| $C_{27}H_{28}O_{19}S$ | 688.0945 | Isovitexin-glucuronide-sulfate |
| $C_{27}H_{28}O_{20}S$ | 704.0895 | Hydroxy-isovitexin-glucuronide-sulfate |
| $C_{21}H_{20}O_{17}S_2$ | 608.0142 | Hydroxy-isovitexin-disulfate |
| $C_{33}H_{36}O_{23}$ | 800.1647 | Hydroxy-isovitexin-diglucuronide |

**Table S7.**: Detected metabolites of orientin with an initial concentration of 10 µM and an incubation time of three hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| **K** | **RT [min]** | **$[M-H]^-$ (*m/z*) found** | **$[M-H]^-$ (*m/z*) calculated** | **Molecular formula** | **Possible metabolite** |
|---|---|---|---|---|---|
| **A** | 3.146 | 527.0494 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Orientin-sulfate |
| **B** | 3.209 | 527.0500 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Orientin-sulfate |
| **A** | 8.516 | 477.1035 | 477.1038 | $C_{22}H_{22}O_{12}$ | Hydroxy-methoxy-orientin |
| **B** | 8.539 | 477.1035 | 477.1038 | $C_{22}H_{22}O_{12}$ | Hydroxy-methoxy-orientin |
| **A** | 9.597 | 461.1086 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-orientin |

**Table S8.**: Detected metabolites of orientin with an initial concentration of 100 µM and an incubation time of three hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 3.204 | 527.0499 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Orientin-sulfate |
| **B** | 3.162 | 527.0493 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Orientin-sulfate |
| **A** | 4.402 | 463.0870 | 463.0882 | $C_{21}H_{20}O_{12}$ | Hydroxy-orientin |
| **A** | 5.134 | 477.0675 | 477.0675 | $C_{21}H_{18}O_{13}$ | Hydroxy-luteolin-glucuronide |
| **A** | 6.073 | 299.0559 | 299.0561 | $C_{16}H_{12}O_6$ | Methoxy-luteolin |
| **A** | 8.497 | 477.1034 | 477.1038 | $C_{22}H_{22}O_{12}$ | Hydroxy-methoxy-orientin |
| **A** | 9.578 | 461.1089 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-orientin |

**Table S9.**: Detected metabolites of orientin with an initial concentration of 10 µM and an incubation time of five hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 3.007 | 527.0507 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Orientin-sulfate |
| **A** | 9.459 | 461.1091 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-orientin |

**Table S10.**: Detected metabolites of orientin with an initial concentration of 100 µM and an incubation time of five hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 3.001 | 527.0501 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Orientin-sulfate |
| **A** | 4.184 | 463.0846 | 463.0882 | $C_{21}H_{20}O_{12}$ | Hydroxy-orientin |
| **A** | 5.044 | 477.0657 | 477.0675 | $C_{21}H_{18}O_{13}$ | Hydroxy-luteolin-glucuronide |
| **A** | 8.340 | 477.1029 | 477.1038 | $C_{22}H_{22}O_{12}$ | Hydroxy-methoxy-orientin |
| **A** | 9.450 | 461.1085 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-orientin |
| **C** | 9.382 | 461.1088 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-orientin |

**Table S11.**: Detected metabolites of isoorientin with an initial concentration of 10 µM and an incubation time of three hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 2.514 | 527.0500 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **A** | 5.107 | 527.0497 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **B** | 2.439 | 527.0500 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **A** | 4.044 | 463.0880 | 463.0882 | $C_{21}H_{20}O_{12}$ | Hydroxy-isoorientin |
| **A** | 5.476 | 461.0723 | 461.0725 | $C_{21}H_{18}O_{12}$ | Luteolin-glucuronide |
| **A** | 5.467 | 477.0672 | 477.0675 | $C_{21}H_{18}O_{13}$ | Hydroxy-luteolin-glucuronide |
| **A** | 8.290 | 477.1034 | 477.1038 | $C_{22}H_{22}O_{12}$ | Hydroxy-methoxy-isoorientin |
| **B** | 8.284 | 477.1046 | 477.1038 | $C_{22}H_{22}O_{12}$ | Hydroxy-methoxy-isoorientin |
| **A** | 9.890 | 461.1089 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-isoorientin |
| **A** | 10.479 | 461.1089 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-isoorientin |

**Table S12.**: Detected metabolites of isoorientin with an initial concentration of 100 µM and an incubation time of three hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 2.494 | 527.0501 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **A** | 5.069 | 527.0505 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **B** | 2.491 | 527.0498 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **B** | 5.008 | 527.0499 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **C** | 5.116 | 527.0495 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **A** | 4.031 | 463.0883 | 463.0882 | $C_{21}H_{20}O_{12}$ | Hydroxy-isoorientin |
| **A** | 5.739 | 541.0654 | 541.0657 | $C_{22}H_{22}O_{14}S$ | Methoxy-isoorientin-sulfate |
| **A** | 6.503 | 541.0655 | 541.0657 | $C_{22}H_{22}O_{14}S$ | Methoxy-isoorientin-sulfate |
| **A** | 5.393 | 461.0723 | 461.0725 | $C_{21}H_{18}O_{12}$ | Luteolin-glucuronide |
| **A** | 5.427 | 477.0674 | 477.0675 | $C_{21}H_{18}O_{13}$ | Hydroxy-luteolin-glucuronide |
| **A** | 6.204 | 299.0550 | 299.0561 | $C_{16}H_{12}O_6$ | Methoxy-luteolin |
| **A** | 8.232 | 477.1040 | 477.1038 | $C_{22}H_{22}O_{12}$ | Hydroxy-methoxy-isoorientin |
| **B** | 8.252 | 477.1042 | 477.1038 | $C_{22}H_{22}O_{12}$ | Hydroxy-methoxy-isoorientin |
| **A** | 9.843 | 461.1087 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-isoorientin |
| **A** | 10.457 | 461.1088 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-isoorientin |
| **B** | 10.441 | 461.1089 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-isoorientin |
| **C** | 10.566 | 461.1084 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-isoorientin |

**Table S13.**: Detected metabolites of isoorientin with an initial concentration of 10 µM and an incubation time of five hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 2.332 | 527.0505 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **A** | 4.673 | 527.0507 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **A** | 6.221 | 477.1034 | 477.1038 | $C_{22}H_{22}O_{12}$ | Hydroxy-methoxy-isoorientin |
| **A** | 9.474 | 461.1085 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-isoorientin |
| **A** | 10.079 | 461.1080 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-isoorientin |

**Table S14.**: Detected metabolites of isoorientin with an initial concentration of 100 µM and an incubation time of five hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 2.308 | 527.0493 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **A** | 4.644 | 527.0500 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **B** | 2.296 | 527.0496 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **B** | 4.682 | 527.0500 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **C** | 4.692 | 527.0521 | 527.0501 | $C_{21}H_{20}O_{14}S$ | Isoorientin-sulfate |
| **A** | 4.178 | 463.0885 | 463.0882 | $C_{21}H_{20}O_{12}$ | Hydroxy-isoorientin |
| **A** | 5.206 | 541.0654 | 541.0657 | $C_{21}H_{22}O_{14}S$ | Methoxy-isoorientin-sulfate |
| **A** | 5.972 | 541.0649 | 541.0657 | $C_{21}H_{22}O_{14}S$ | Methoxy-isoorientin-sulfate |
| **A** | 5.181 | 461.0717 | 461.0725 | $C_{21}H_{18}O_{12}$ | Luteolin-glucuronide |
| **A** | 5.232 | 477.0665 | 477.0675 | $C_{21}H_{18}O_{13}$ | Hydroxy-luteolin-glucuronide |
| **A** | 9.496 | 461.1089 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-isoorientin |
| **A** | 10.106 | 461.1090 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-isoorientin |
| **C** | 10.178 | 461.1107 | 461.1089 | $C_{22}H_{22}O_{11}$ | Methoxy-isoorientin |

**Table S15.**: Detected metabolites of schaftoside with an initial concentration of 10 µM and an incubation time of three hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 7.732 | 593.1509 | 593.1512 | $C_{27}H_{30}O_{15}$ | Hydroxy-methoxy-schaftoside |

**Table S16.**: Detected metabolites of schaftoside with an initial concentration of 100 µM and an incubation time of three hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 5.804 | 579.1350 | 579.1355 | $C_{26}H_{28}O_{15}$ | Hydroxy-schaftoside |
| **A** | 7.716 | 593.1506 | 593.1512 | $C_{27}H_{30}O_{15}$ | Hydroxy-methoxy-schaftoside |
| **B** | 7.744 | 593.1507 | 593.1512 | $C_{27}H_{30}O_{15}$ | Hydroxy-methoxy-schaftoside |

**Table S17.**: Detected metabolites of schaftoside with an initial concentration of 10 µM and an incubation time of five hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 7.383 | 593.1513 | 593.1512 | $C_{27}H_{30}O_{15}$ | Hydroxy-methoxy-schaftoside |

**Table S18.**: Detected metabolites of schaftoside with an initial concentration of 100 µM and an incubation time of five hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 5.524 | 579.1349 | 579.1355 | $C_{26}H_{28}O_{15}$ | Hydroxy-schaftoside |
| **A** | 7.549 | 593.1512 | 593.1512 | $C_{27}H_{30}O_{15}$ | Hydroxy-methoxy-schaftoside |

**Table S19.**: Detected metabolites of isoschaftoside with an initial concentration of 10 µM and an incubation time of three hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 8.720 | 593.1511 | 593.1512 | $C_{27}H_{30}O_{15}$ | Hydroxy-methoxy-isoschaftoside |

**Table S20.**: Detected metabolites of isoschaftoside with an initial concentration of 100 µM and an incubation time of three hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 8.705 | 593.1499 | 593.1512 | $C_{27}H_{30}O_{15}$ | Hydroxy-methoxy-isoschaftoside |
| **B** | 8.710 | 593.1513 | 593.1512 | $C_{27}H_{30}O_{15}$ | Hydroxy-methoxy-isoschaftoside |
| **A** | 10.712 | 577.1565 | 577.1563 | $C_{27}H_{30}O_{14}$ | Methoxy-isoschaftoside |
| **A** | 11.597 | 607.1668 | 607.1668 | $C_{28}H_{32}O_{15}$ | Hydroxy-dimethoxy-isoschaftoside |

**Table S21.**: Detected metabolites of isoschaftoside with an initial concentration of 100 µM and an incubation time of five hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 8.469 | 593.1456 | 593.1512 | $C_{27}H_{30}O_{15}$ | Hydroxy-methoxy-isoschaftoside |
| **A** | 11.464 | 607.1668 | 607.1668 | $C_{28}H_{32}O_{15}$ | Hydroxy-dimethoxy-isoschaftoside |

**Table S22.**: Detected metabolites of vitexin with an initial concentration of 100 µM and an incubation time of three hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 9.615 | 461.1091 | 461.1089 | $C_{22}H_{22}O_{11}$ | Hydroxy-methoxy-vitexin |
| **B** | 9.646 | 461.1092 | 461.1089 | $C_{22}H_{22}O_{11}$ | Hydroxy-methoxy-vitexin |

**Table S23.**: Detected metabolites of vitexin with an initial concentration of 100 µM and an incubation time of five hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 5.695 | 447.0934 | 447.0933 | $C_{21}H_{20}O_{11}$ | Hydroxy-vitexin |

**Table S24.**: Detected metabolites of isovitexin with an initial concentration of 10 µM and an incubation time of three hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 8.491 | 447.0934 | 447.0933 | $C_{21}H_{20}O_{11}$ | Hydroxy-isovitexin |
| **A** | 8.912 | 445.1140 | 445.1140 | $C_{22}H_{22}O_{10}$ | Methoxy-isovitexin |
| **A** | 9.468 | 461.1093 | 461.1089 | $C_{22}H_{22}O_{11}$ | Hydroxy-methoxy-isovitexin |
| **A** | 11.658 | 364.9978 | 364.9973 | $C_{15}H_{10}O_9S$ | Hydroxy-apigenin-sulfate |
| **A** | 11.909 | 379.0133 | 379.0129 | $C_{16}H_{12}O_9S$ | Hydroxy-methoxy-apigenin-sulfate |
| **A** | 11.910 | 299.0564 | 299.0561 | $C_{16}H_{12}O_6$ | Hydroxy-methoxy-apigenin |

**Table S25.**: Detected metabolites of isovitexin with an initial concentration of 100 µM and an incubation time of three hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 8.501 | 447.0928 | 447.0933 | $C_{21}H_{20}O_{11}$ | Hydroxy-isovitexin |
| **A** | 8.905 | 445.1144 | 445.1140 | $C_{21}H_{22}O_{10}$ | Methoxy-isovitexin |
| **A** | 9.451 | 461.1098 | 461.1089 | $C_{22}H_{22}O_{11}$ | Hydroxy-methoxy-isovitexin |
| **A** | 11.648 | 364.9978 | 364.9973 | $C_{15}H_{10}O_9S$ | Hydroxy-apigenin-sulfate |
| **A** | 11.651 | 475.1251 | 475.1246 | $C_{23}H_{24}O_{11}$ | Hydroxy-dimethoxy-isovitexin |
| **B** | 11.654 | 475.1248 | 475.1246 | $C_{23}H_{24}O_{11}$ | Hydroxy-dimethoxy-isovitexin |
| **A** | 11.900 | 299.0562 | 299.0561 | $C_{16}H_{12}O_6$ | Hydroxy-methoxy-apigenin |
| **A** | 11.957 | 379.0135 | 379.0129 | $C_{16}H_{12}O_9S$ | Hydroxy-methoxy-apigenin-sulfate |
| **B** | 11.903 | 379.0131 | 379.0129 | $C_{16}H_{12}O_9S$ | Hydroxy-methoxy-apigenin-sulfate |

**Table S26.**: Detected metabolites of isovitexin with an initial concentration of 10 µM and an incubation time of five hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 8.569 | 447.0937 | 447.0933 | $C_{21}H_{20}O_{11}$ | Hydroxy-isovitexin |
| **A** | 9.564 | 461.1093 | 461.1089 | $C_{22}H_{22}O_{11}$ | Hydroxy-methoxy-isovitexin |
| **A** | 11.681 | 475.1248 | 475.1246 | $C_{23}H_{24}O_{11}$ | Hydroxy-dimethoxy-isovitexin |
| **A** | 11.702 | 364.9976 | 364.9973 | $C_{15}H_{10}O_9S$ | Hydroxy-apigenin-sulfate |
| **A** | 11.953 | 379.0133 | 379.0129 | $C_{16}H_{12}O_9S$ | Hydroxy-methoxy-apigenin-sulfate |

**Table S27.**: Detected metabolites of isovitexin with an initial concentration of 100 µM and an incubation time of five hours in the Caco-2 cell metabolization assay. K: Compartment, RT: retention time, A: apical compartment, B: basolateral compartment, C: cell lysate

| K | RT [min] | $[M-H]^-$ (*m/z*) found | $[M-H]^-$ (*m/z*) calculated | Molecular formula | Possible metabolite |
|---|---|---|---|---|---|
| **A** | 8.514 | 447.0932 | 447.0933 | $C_{21}H_{20}O_{11}$ | Hydroxy-isovitexin |
| **A** | 8.951 | 445.1145 | 445.1140 | $C_{21}H_{22}O_{10}$ | Methoxy-isovitexin |
| **A** | 9.478 | 461.1099 | 461.1089 | $C_{22}H_{22}O_{11}$ | Hydroxy-methoxy-isovitexin |
| **A** | 11.655 | 364.9984 | 364.9973 | $C_{15}H_{10}O_9S$ | Hydroxy-apigenin-sulfate |
| **A** | 11.656 | 475.1252 | 475.1246 | $C_{23}H_{24}O_{11}$ | Hydroxy-dimethoxy-isovitexin |
| **A** | 11.906 | 299.0566 | 299.0561 | $C_{16}H_{12}O_6$ | Hydroxy-methoxy-apigenin |
| **A** | 11.960 | 379.0131 | 379.0129 | $C_{16}H_{12}O_9S$ | Hydroxy-methoxy-apigenin-sulfate |
| **B** | 11.908 | 379.0132 | 379.0129 | $C_{16}H_{12}O_9S$ | Hydroxy-methoxy-apigenin-sulfate |