**Analysis of Goldenseal Extract Using UPLC-MS/MS**

Josh Kellogg, Teal Jordan

Pennsylvania State University

325 Huck Life Sciences Building

Pennsylvania State University

University Park, PA 16802

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| --- | --- | --- | --- | --- |
| Common Botanical Name | CAS No. | Lot No. | Container ID | Net Weight |
| Goldenseal |  |  |  |  |

|  |
| --- |
| Sample storage condition until analysis |
| -80 ℃ |

**Quantitative/Targeted method:**

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| --- |
| **UPLC-MS Method** |
| UHPLC conditions | Mass spectrometry |
| System: **Waters Acquity**Column: **Waters Acquity Ultra C18 (2.1 x 100 mm, 1.7 um)**Mobile phase A: **H2O + 0.1% FA**Mobile phase B: **CH3CN + 0.1% FA**Flow rate: **0.3 mL/min**Column temperature: **50 ℃**Gradient

|  |  |
| --- | --- |
| Time (min) | Mobile phase B (%) |
| **0** | **3** |
| **1.0** | **3** |
| **5.0** | **75** |
| **5.5** | **75** |
| **6.0** | **3** |
|  |  |
|  |  |
|  |  |
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 | System: **Waters TQS**Ionization: **Electrospray (ESI)**Polarity: **Positive**Main Interface: · Nebulizing gas flow: **150 L/hr** · Heating gas flow: **500 L/hr** · Interface temperature: **150 ℃** · Capillary voltage: **2.5 kV** · Cone voltage: **50 V**Ion guide: · Drying gas flow: **0.15 mL/min** · Desolvation line temperature: **500 ℃**  · Heat block temperature: SRM dwell time:

|  |
| --- |
| Selected Reaction Monitoring (SRM) events |
| Compound | Precursor ion (*m/z*) | Product ion (*m/z*) | Collision energy (V) | Retention time (min) |
| **Hydrastine** | 384.14 | - | 45 | 3.60 |
| **Canadine** | 340.15 | - | 45 | 4.02 |
| **Coptisine** | 320.09 | - | 45 | 3.90 |
| **Hydrastinine** | 190.08 | - | 45 | 0.48 |
| **Jatrorrhizine** | 338.14 | - | 45 | 3.95 |
| **Palmatine** | 352.15 | - | 45 | 4.14 |
| **Berberine** | 336.12 | - | 45 | 4.15 |
| **Chlorogenic acid** | 163.04 | - | 45 | 5.25 |
|  |

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**Quantitative results**

|  |  |
| --- | --- |
| **Compound** | **Concentration in extract (mg/g)** |
| **Berberine** | 8.12 ± 0.20 |
| **Canadine** | 0.197 ± 0.025 |
| **Chlorogenic acid** | 0.6987 ± 0.0061 |
| **Coptisine** | 0.1800 ± 0.0093 |
| **Hydrastine** | 7.26 ± 0.38 |
| **Hydrastinine** | 0.0875 ± 0.0046 |
| **Jatrorrhizine** | 0.0773 ± 0.0121 |
| **Palmatine** | 0.0813 ± 0.0066 |

**Standards**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Name** | **Supplier** | **CAS Number** | **Catalog number** | **Purity %** | **Batch/Lot number** |
| **Berberine** | USP | 2086-83-1 | 1065210 | >98% | R04130 |
| **Canadine** | Phytolab | 522-97-4 | 80378-10mg | >98% | 97763836 |
| **Chlorogenic acid** | USP | 202650-88-2 | 11155545 | >98% | R001C0 |
| **Coptisine** | Sigma | 6020-18-4 | SMB00314-25mg | >98% | SLCC9042 |
| **Hydrastine** | Phytolab | 118-08-1 | 89511-50mg | >98% | 85963619 |
| **Hydrastinine** | Sigma |  | 5438308-10mg | >98% | B02666596 |
| **Jatrorrhizine** | Phytolab | 6681-15-8 | 89530-10mg | >98% | 117270386 |
| **Palmatine** | Phytolab | 10605-02-4 | 89490-25mg | >98% | 78339594 |

**Chemical structures of standards used for quantitative analysis**



**Chromatograms**

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**Calibration**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Compound | Lower limit of quantitation (LLOQ) **ug/mL** | Calibration range (**ug/mL**) | Number of Calibration Points | R2 | Concentration mg/g **in extract** (n = 3) |
| **Berberine** | 0.001 | 0.001 – 0.243 | 6 | 0.9984 | 8.12 ± 0.20 |
| **Canadine** | 0.001 | 0.001 – 0.243 | 6 | 0.9986 | 0.197 ± 0.025 |
| **Chlorogenic acid** | 0.001 | 0.001 – 0.243 | 6 | 0.9967 | 0.6987 ± 0.0061 |
| **Coptisine** | 0.001 | 0.001 – 0.243 | 6 | 0.9990 | 0.1800 ± 0.0093 |
| **Hydrastine** | 0.001 | 0.001 – 0.243 | 6 | 0.9996 | 7.26 ± 0.38 |
| **Hydrastinine** | 0.001 | 0.001 – 0.243 | 6 | 0.9982 | 0.0875 ± 0.0046 |
| **Jatrorrhizine** | 0.001 | 0.001 – 0.729 | 7 | 0.9979 | 0.0773 ± 0.0121 |
| **Palmatine** | 0.001 | 0.001 – 0.243 | 6 | 0.9990 | 0.0813 ± 0.0066 |

Untargeted Analysis

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| --- |
|  |
| UHPLC conditions | Mass spectrometer conditions |
| System: Thermo VanquishColumn: Waters Acquity Ultra C18 (1.7 um, 1.0 x 150 mm)Mobile phase A: H2O w/ 0.1% FAMobile phase B: ACN w/ 0.1% FAFlow rate: 0.100 mL/minColumn temperature: 55℃Gradient:

|  |  |
| --- | --- |
| Time (min) | Mobile phase B (%) |
| 0 | 5 |
| 1 | 5 |
| 12.5 | 98 |
| 13.5 | 98 |
| 12.6 | 5 |
| 15 | 5 |

 | System: Thermo Orbitrap Fusion LumosMode: ESIPolarity: positive/negativeMain-Interface: · Interface voltage: 3500/2500 · Nebulizing gas flow: 25 · Heating gas flow: 5 · Interface temperature: 325 ℃ · Desolvation temperature: 350 ℃Ion guide: · Drying gas flow: 1 · DL temperature: 350 ℃ · Heat block temperature |

|  |
| --- |
| **Table 1: Proposed identification of constituents of Goldenseal** |
| Peak No. | RT (min) | Exp. *m/z* | Mass accuracy (ppm) | Proposed ID’s (Confirmed with Std in **green**)(Structure with correlated MS2 spectra in **orange**)(Most probable ID is **blue**) | Molecular Formula |
| 1 | 7.28 | 384.1442 | -1.30 | **Hydrastine** | C21H21NO6 |
| 2 | 1.12 | 367.1035 | 1.63 | **3-Feruloylquinic acid** | C17H20O9 |
| 3 | 1.14 | 163.0390 | 6.13 | **4-Hydroxyphenylpyruvic acid** | C9H8O4 |
| 4 | 9.16 | 354.1338 | 2.26 | **8-oxocanadine**  | C20H19NO5 |
| 5 | 8.53 | 340.1176 | -2.65 | **8-oxotetrahydrothalifendine**  | C19H17NO5 |
| 6 | 5.93 | 337.1270 | -13.05 | **Berberine** | C20H18NO4+ |
| 7 | 1.14 | 163.0390 | 0.00 | **Caffeic acid** | C9H8O4 |
| 8 | 1.09 | 340.1543 | -1.47 | **Canadine** | C20H21NO4 |
| 9 | 1.10 | 353.0877 | 1.42 | **Chlorogenic acid** | C16H18O9 |
| 10 | 6.32 | 339.1324 | -20.05 | **Columbamine** | C20H20NO4 |
| 11 | 1.13 | 352.1178 | 22.15 | **Evodine** | C18H19NO5 |
| 12 | 1.12 | 177.0546 | 3.39 | **Ferulic aid** | C10H10O4 |
| 13 | 9.51 | 274.2740 | 0.00 | **Lauryldiethanolamine** | C16H35NO2 |
| 14 | 5.19 | 367.1035 | 1.36 | **Methyl chlorogenate** | C17H20O9 |
| 15 | 1.17 | 360.1500 | 0.00 | **Palatinose** | C12H22O11 |
| 16 | 1.1 | 191.0560 | 2.62 | **Quinic acid** | C7H12O6 |
| 17 | 1.16 | 328.1544 | 1.22 | **Scoulerine** | C19H21NO4 |
| 18 | 6.65 | 336.1814 | 4.16 | **Senecionine** | C18H25NO5 |
| 19 | 7.56 | 338.1410 | 5.32 | **Jatrorrhizine** | C20H20NO4 |
| 20 | 1.17 | 314.1750 | -0.32 | **Magnocurarine** | C19H24NO3+ |
| 21 | 1.11 | 400.1389 | -0.50 | **1-Hydroxyhydrastine** | C21H21NO7 |
| 22 | 5.24 | 324.1232 | 0.62 | **Demethyleneberberine** | C19H18NO4+ |
| 23 | 6.9 | 356.1494 | -1.12 | **13-Hydroxycanadine** | C20H21NO5 |
| 24 | 1.13 | 330.1702 | -0.91 | **3'-Hydroxy-N,N-dimethylcoclaurine** | C19H24NO4+ |
| 25 | 5.75 | 481.3159 | -0.21 | **20-Hydroxyecdysone** | C27H44O7 |
| 26 | 1.14 | 385.1595 | -2.34 | **Hydrastine methiodine** | C22H24NO6+ |
| 27 | 1.14 | 370.1648 | -0.27 | **Canadaline** | C21H23NO5 |
| 28 | 1.26 | 355.1024 | 0.00 | Neochlorogenic acid | C16H18O9 |
| 29 | 1.1 | 354.1695 | -1.41 | **13-Methylcanadine** | C21H23NO4 |
| 30 | 6.45 | 352.1180 | 0.28 | **8-Oxoberberine** | C20H17NO5 |
| 31 | 1.13 | 350.1388 | -1.14 | **13-Methylberberine** | C21H20NO4+ |
| 32 | 6.98 | 344.1856 | -1.74 | **Tembetarine** | C20H26NO4+ |
| 33 | 5.10 | 342.1696 | -2.63 | **Magnoflorine** | C20H24NO4+ |
| 34 | 1.11 | 342.1699 | -0.29 | **Isocorypalmine** | C20H23NO4 |
| 35 | 5.80 | 336.1236 | 0.30 | **Epiberberine** | C20H18NO4+ |
| 36 | 1.16 | 328.1544 | -1.22 | **1,2-dehydroreticuline** | C19H22NO4+ |
| 37 | 9.86 | 329.1021 | 0.30 | **6,8-C-Dimethylluteolin-7-methyl ether** | C18H16O6 |
| 38 | 5.24 | 327.0872 | -0.61 | **Dehydrodiscretamine** | C19H18NO4+ |
| 39 | 1.29 | 324.1231 | -1.12 | **Thalinfendin** | C19H16NO4+ |
| 40 | 6.51 | 315.0865 | -1.55 | **6-C-Methylluteolin-7-methyl ether** | C17H14O6 |
| 41 | 6.94 | 313.0718 | 0.63 | **1,2-Dihydronorreticuline** | C18H19NO4 |
| 42 | 10.66 | 314.1385 | 0.32 | **Sideroxylin** | C18H16O5 |
| 43 | 1.13 | 313.1069 | -0.64 | **N-methylcocluarine / canelilline** | C18H22NO3+ |
| 44 | 9.98 | 311.0924 | -0.32 | **Desmethyl-sideroxylin** | C17H14O5 |
| 45 | 7.04 | 320.0918 | -1.25 | **Coptisine** | C19H14NO4+ |
| 46 | 1.11 | 190.0864 | -2.10 | **Hydrastinine** | C11H13NO3 |
| 47 | 14.08 | 279.2329 | 0.00 | **Linoleic acid** | C18H32O2 |
| 48 | 6.74 | 352.1539 | -1.14 | **Palmatine** | C21H22NO4+ |
| 49 | 14.60 | 255.2329 | 0.00 | **Palmitic acid** | C16H32O2 |
| 50 | 14.80 | 283.2643 | 0.35 | **Stearic acid** | C18H36O2 |

Figure 1: Chromatograms































































Structures of compounds in Table 1



|  |
| --- |
| **Table 3: HRMS product ions for the peaks of the botanical extract** |
| Peak No. | RT (min) | *m/z* | Proposed ID’s (Confirmed with Std in **green**)(Structure with correlated MS2 spectra in **orange**)(Most probable ID is **blue**)CAS ID | Product Ions*m/z* Rel. Int.. |
| 1 | 7.28 | 384.1442 | **Hydrastine** |

|  |  |
| --- | --- |
| 91.0537 | 4 |
| 97.4632 | 3 |
| 119.0484 | 5 |
| 142.2554 | 3 |
| 149.059 | 19 |
| 165.0579 | 3 |
| 174.0556 | 4 |
| 176.0711 | 11 |
| 188.0706 | 4 |
| 189.078 | 11 |
| 190.0862 | 100 |
| 193.0504 | 11 |
| 206.0816 | 4 |
| 237.0897 | 4 |
| 247.0777 | 4 |
| 250.063 | 6 |
| 260.0459 | 3 |
| 263.0705 | 5 |
| 265.0858 | 31 |
| 267.1037 | 4 |
| 277.0929 | 5 |
| 278.0555 | 7 |
| 279.0627 | 6 |
| 280.0744 | 10 |
| 282.0897 | 8 |
| 291.065 | 10 |
| 292.0741 | 21 |
| 293.0814 | 88 |
| 294.0874 | 10 |
| 295.0966 | 24 |
| 302.0598 | 9 |
| 304.0771 | 11 |
| 305.0765 | 4 |
| 307.0613 | 3 |
| 308.0697 | 11 |
| 320.0706 | 14 |
| 322.0891 | 11 |
| 323.0919 | 62 |
| 335.0929 | 5 |
| 336.1235 | 4 |
| 338.1125 | 5 |

 |
| 2 | 1.12 | 367.1035 | **3-Feruloylquinic acid** |

|  |  |
| --- | --- |
| 61.7852 | 1 |
| 67.0191 | 3 |
| 83.0506 | 2 |
| 85.029 | 4 |
| 85.3573 | 1 |
| 87.0086 | 7 |
| 93.0344 | 20 |
| 111.0449 | 5 |
| 117.0346 | 11 |
| 134.0369 | 100 |
| 149.0606 | 7 |
| 155.0343 | 3 |
| 173.0444 | 6 |
| 191.0551 | 30 |
| 191.0895 | 2 |
| 193.0498 | 24 |

 |
| 3 | 1.14 | 163.039 | **4-Hydroxyphenylpyrucid acid** |

|  |  |
| --- | --- |
| 51.0227 | 0 |
| 53.0385 | 0 |
| 55.0176 | 1 |
| 57.0335 | 1 |
| 63.0227 | 5 |
| 69.0333 | 2 |
| 77.0384 | 7 |
| 79.054 | 7 |
| 85.0284 | 1 |
| 89.0384 | 100 |
| 91.0539 | 1 |
| 93.2065 | 0 |
| 95.0489 | 5 |
| 103.0544 | 1 |
| 105.0447 | 2 |
| 107.0491 | 4 |
| 115.0545 | 2 |
| 117.0336 | 19 |
| 117.0702 | 2 |
| 120.1275 | 0 |
| 135.0442 | 9 |
| 159.0427 | 0 |
| 162.0473 | 1 |
| 163.0544 | 4 |

 |
| 4 | 9.16 | 354.1338 | **8-Oxocanadine** |

|  |  |
| --- | --- |
| 61.0151 | 4 |
| 67.6876 | 4 |
| 93.0339 | 4 |
| 110.0371 | 4 |
| 117.656 | 4 |
| 125.0593 | 4 |
| 136.0523 | 8 |
| 164.0474 | 46 |
| 172.0397 | 5 |
| 174.0549 | 13 |
| 176.0712 | 100 |
| 176.104 | 6 |
| 190.0507 | 23 |
| 244.5497 | 4 |
| 339.1139 | 6 |
| 354.1369 | 14 |

 |
| 5 | 8.53 | 340.1176 | **8-Oxotetrahydrothalifendine** |

|  |  |
| --- | --- |
| 66.5769 | 25 |
| 105.6166 | 23 |
| 176.0714 | 100 |
| 268.9152 | 25 |
| 310.0732 | 91 |
| 325.0962 | 36 |

 |
| 6 | 5.93 | 337.1270 | **Berberine** |

|  |  |
| --- | --- |
| 74.9383 | 2 |
| 75.5677 | 2 |
| 87.5868 | 2 |
| 143.688 | 3 |
| 259.908 | 3 |
| 261.2167 | 3 |
| 276.0958 | 10 |
| 279.0843 | 11 |
| 292.0967 | 15 |
| 293.1021 | 97 |
| 305.1016 | 23 |
| 306.0811 | 7 |
| 307.0818 | 36 |
| 320.0914 | 5 |
| 321.0974 | 100 |
| 322.1053 | 45 |
| 337.1293 | 17 |

 |
| 7 | 1.14 | 163.039 | **Caffeic acid** |

|  |  |
| --- | --- |
| 51.0227 | 0 |
| 53.0385 | 0 |
| 55.0176 | 1 |
| 57.0335 | 1 |
| 63.0227 | 5 |
| 69.0333 | 2 |
| 77.0384 | 7 |
| 79.054 | 7 |
| 85.0284 | 1 |
| 89.0384 | 100 |
| 91.0539 | 1 |
| 93.2065 | 0 |
| 95.0489 | 5 |
| 103.0544 | 1 |
| 105.0447 | 2 |
| 107.0491 | 4 |
| 115.0545 | 2 |
| 117.0336 | 19 |
| 117.0702 | 2 |
| 120.1275 | 0 |
| 135.0442 | 9 |
| 159.0427 | 0 |
| 162.0473 | 1 |
| 163.0544 | 4 |

 |
| 8 | 1.09 | 340.1543 | **Canadine** |

|  |  |
| --- | --- |
| 91.0545 | 2 |
| 119.0494 | 3 |
| 149.0601 | 9 |
| 150.0679 | 2 |
| 151.0756 | 1 |
| 165.0914 | 3 |
| 174.0555 | 2 |
| 176.071 | 100 |
| 189.0789 | 1 |
| 292.1026 | 1 |
| 324.1219 | 1 |
| 340.1543 | 2 |

 |
| 9 | 1.10 | 353.0877 | **Chlorogenic acid** |

|  |  |
| --- | --- |
| 85.029 | 12 |
| 93.0338 | 4 |
| 135.0441 | 60 |
| 135.0655 | 5 |
| 173.0441 | 4 |
| 178.3094 | 3 |
| 179.0329 | 13 |
| 191.054 | 100 |
| 235.9413 | 3 |

 |
| 10 | 6.32 | 339.1324 | **Columbamine** |

|  |  |
| --- | --- |
| 178.3113 | 3 |
| 257.0621 | 2 |
| 278.111 | 10 |
| 280.091 | 20 |
| 281.1003 | 10 |
| 293.1034 | 3 |
| 294.1103 | 15 |
| 295.1151 | 78 |
| 306.1075 | 3 |
| 307.1152 | 20 |
| 308.0891 | 8 |
| 309.0947 | 46 |
| 322.1037 | 5 |
| 323.1102 | 100 |
| 324.1181 | 47 |
| 339.1405 | 15 |

 |
| 11 | 1.13 | 352.1178 | **Evodine** |

|  |  |
| --- | --- |
| 108.3074 | 1 |
| 117.5906 | 1 |
| 263.3792 | 1 |
| 269.3829 | 1 |
| 278.0826 | 3 |
| 279.0851 | 2 |
| 280.0999 | 3 |
| 290.0872 | 2 |
| 291.0904 | 12 |
| 292.1001 | 4 |
| 294.0792 | 10 |
| 306.0782 | 5 |
| 307.0854 | 6 |
| 308.0944 | 98 |
| 309.0994 | 2 |
| 318.0843 | 1 |
| 319.0847 | 1 |
| 320.0944 | 24 |
| 321.1035 | 4 |
| 322.0742 | 38 |
| 336.0895 | 100 |
| 337.097 | 47 |
| 352.1213 | 25 |

 |
| 12 | 1.12 | 177.0546 | **Isoferulic acid / Ferulic acid** |

|  |  |
| --- | --- |
| 55.9343 | 2 |
| 63.0229 | 3 |
| 65.0383 | 1 |
| 72.937 | 2 |
| 77.0385 | 2 |
| 78.0462 | 13 |
| 79.0537 | 1 |
| 89.0385 | 100 |
| 91.0542 | 5 |
| 95.0491 | 3 |
| 103.0542 | 2 |
| 105.0332 | 2 |
| 105.0459 | 1 |
| 106.0412 | 7 |
| 117.0336 | 42 |
| 124.0521 | 1 |
| 134.0365 | 9 |
| 135.0444 | 1 |
| 145.0288 | 2 |
| 149.0602 | 4 |

 |
| 13 | 9.51 | 274.2740 | **Lauryldiethanolamine** |

|  |  |
| --- | --- |
| 57.0697 | 67 |
| 58.0656 | 7 |
| 70.065 | 78 |
| 71.085 | 18 |
| 73.5135 | 7 |
| 88.0756 | 100 |
| 102.0912 | 22 |
| 106.0864 | 48 |
| 178.2883 | 7 |
| 190.1865 | 9 |
| 256.2643 | 13 |
| 274.2755 | 22 |
| 279.0829 | 8 |

 |
| 14 | 5.19 | 367.1035 | **Methyl chlorogenate** |

|  |  |
| --- | --- |
| 61.3372 | 14 |
| 67.0187 | 16 |
| 87.0094 | 17 |
| 93.0344 | 72 |
| 104.6632 | 15 |
| 134.0363 | 37 |
| 191.0552 | 100 |
| 193.0466 | 26 |
| 294.2483 | 18 |

 |
| 15 | 1.17 | 360.1500 | **Palatinose** |

|  |  |
| --- | --- |
| 69.0333 | 4 |
| 72.6721 | 1 |
| 73.0281 | 1 |
| 85.0282 | 91 |
| 85.3258 | 1 |
| 97.0282 | 32 |
| 99.044 | 3 |
| 109.0281 | 2 |
| 115.0389 | 1 |
| 127.039 | 81 |
| 145.0498 | 100 |
| 162.0749 | 1 |
| 163.0606 | 9 |
| 163.8879 | 1 |
| 180.0869 | 14 |
| 180.1206 | 1 |
| 198.0979 | 7 |
| 211.0609 | 1 |
| 247.4641 | 1 |
| 259.0822 | 3 |
| 271.0834 | 1 |
| 289.0932 | 6 |
| 307.1062 | 1 |
| 325.115 | 5 |
| 360.1493 | 1 |

 |
| 16 | 1.10 | 191.0560 | **Quinic acid** |

|  |  |
| --- | --- |
| 54.6171 | 5 |
| 57.0342 | 5 |
| 58.9589 | 11 |
| 59.0137 | 24 |
| 67.0187 | 5 |
| 71.0139 | 9 |
| 81.0345 | 7 |
| 83.0498 | 6 |
| 85.0294 | 100 |
| 87.0084 | 16 |
| 93.0347 | 28 |
| 109.0291 | 9 |
| 127.0404 | 7 |
| 178.3156 | 13 |
| 191.0554 | 9 |

 |
| 17 | 1.16 | 328.1544 | **Scoulerine** |

|  |  |
| --- | --- |
| 91.0538 | 2 |
| 95.0494 | 1 |
| 119.0488 | 2 |
| 137.0594 | 1 |
| 151.0752 | 7 |
| 163.0629 | 6 |
| 164.0706 | 8 |
| 176.0714 | 2 |
| 178.0864 | 100 |
| 191.0935 | 1 |
| 233.0611 | 1 |
| 265.0882 | 1 |
| 296.1285 | 1 |
| 312.1217 | 1 |
| 313.1316 | 1 |
| 328.1554 | 1 |

 |
| 18 | 6.65 | 336.1814 | **Senecionine** |

|  |  |
| --- | --- |
| 67.0355 | 1 |
| 79.1607 | 1 |
| 92.9701 | 1 |
| 118.306 | 1 |
| 275.0958 | 10 |
| 278.0832 | 12 |
| 291.0904 | 5 |
| 292.0987 | 100 |
| 304.099 | 22 |
| 306.0784 | 37 |
| 320.0941 | 95 |
| 321.102 | 39 |
| 336.1254 | 16 |

 |
| 19 | 7.56 | 338.1410 | **Jatrorrhizine** |

|  |  |
| --- | --- |
| 96.894 | 3 |
| 129.5885 | 3 |
| 277.0977 | 7 |
| 278.0759 | 4 |
| 280.0886 | 8 |
| 292.0977 | 11 |
| 293.0991 | 16 |
| 294.103 | 81 |
| 304.1021 | 4 |
| 306.1034 | 20 |
| 307.0792 | 5 |
| 308.0825 | 32 |
| 321.0977 | 10 |
| 322.0984 | 100 |
| 323.1055 | 40 |
| 338.1314 | 16 |
| 345.779 | 3 |

 |
| 20 | 1.17 | 314.175 | **Magnocurarine** |

|  |  |
| --- | --- |
| 58.0649 | 100 |
| 89.9815 | 1 |
| 91.0543 | 1 |
| 97.0283 | 1 |
| 103.1647 | 1 |
| 107.0491 | 35 |
| 115.0549 | 2 |
| 117.0699 | 1 |
| 119.0499 | 1 |
| 121.0649 | 7 |
| 131.049 | 1 |
| 136.0624 | 3 |
| 137.06 | 4 |
| 143.0498 | 4 |
| 145.033 | 1 |
| 145.0649 | 4 |
| 147.0806 | 1 |
| 149.06 | 1 |
| 151.0755 | 3 |
| 152.0714 | 1 |
| 160.0524 | 2 |
| 163.0766 | 2 |
| 164.0684 | 1 |
| 175.0759 | 6 |
| 176.0798 | 1 |
| 176.6842 | 1 |
| 181.1017 | 1 |
| 191.0847 | 1 |
| 192.1022 | 3 |
| 193.109 | 1 |
| 209.0962 | 3 |
| 211.1147 | 2 |
| 237.0925 | 4 |
| 239.1068 | 1 |
| 254.0945 | 1 |
| 269.12 | 1 |
| 298.1095 | 4 |
| 299.1162 | 2 |

 |
| 21 | 1.11 | 400.1389 | **1-Hydroxyhydrastine** |

|  |  |
| --- | --- |
| 118.2722 | 1 |
| 149.0588 | 1 |
| 176.0713 | 2 |
| 178.0876 | 1 |
| 188.0699 | 5 |
| 190.0861 | 13 |
| 193.0486 | 4 |
| 206.0808 | 5 |
| 265.0859 | 1 |
| 279.0672 | 1 |
| 281.0856 | 1 |
| 292.0959 | 5 |
| 293.0813 | 3 |
| 296.0699 | 1 |
| 302.0529 | 1 |
| 305.0782 | 1 |
| 306.0774 | 2 |
| 308.0727 | 1 |
| 311.0937 | 3 |
| 320.0879 | 6 |
| 321.0997 | 21 |
| 322.0934 | 1 |
| 323.0928 | 3 |
| 334.0975 | 1 |
| 336.1234 | 100 |
| 337.1274 | 2 |
| 338.1348 | 2 |
| 339.0848 | 1 |

 |
| 22 | 5.24 | 324.1232 | **Demethyleneberberine** |

|  |  |
| --- | --- |
| 81.106 | 32 |
| 97.8473 | 31 |
| 100.9352 | 38 |
| 294.0756 | 52 |
| 309.1021 | 100 |

 |
| 23 | 6.90 | 356.1494 | **13-Hydroxycanadine** |

|  |  |
| --- | --- |
| 91.0542 | 4 |
| 118.0772 | 4 |
| 121.0654 | 5 |
| 132.0436 | 5 |
| 133.0639 | 4 |
| 134.072 | 8 |
| 135.0434 | 8 |
| 135.0804 | 12 |
| 136.0884 | 3 |
| 147.0799 | 5 |
| 149.0596 | 84 |
| 150.0674 | 32 |
| 161.0853 | 5 |
| 162.056 | 4 |
| 163.0751 | 21 |
| 164.0833 | 100 |
| 165.0552 | 12 |
| 165.091 | 65 |
| 165.1204 | 5 |
| 174.0553 | 31 |
| 175.063 | 11 |
| 176.0712 | 17 |
| 183.102 | 3 |
| 189.0794 | 5 |
| 190.0863 | 3 |
| 192.066 | 98 |
| 192.1029 | 13 |
| 289.5709 | 3 |
| 294.1132 | 3 |
| 304.1013 | 7 |
| 308.1306 | 12 |
| 322.1109 | 10 |
| 338.1426 | 51 |
| 356.1475 | 4 |

 |
| 24 | 1.13 | 330.1702 | **Reticuline / 3'-Hydroxy-N,N-dimethylcoclaurine** | n/a |
| 25 | 5.75 | 481.3159 | **20-Hydroxyecdysone** | n/a |
| 26 | 1.14 | 385.1595 | **Hydrastine methiodine** | n/a |
| 27 | 1.14 | 370.1648 | **Canadaline** |

|  |  |
| --- | --- |
| 145.0278 | 7 |
| 190.0869 | 100 |
| 251.069 | 11 |
| 279.067 | 22 |
| 281.0853 | 10 |
| 298.9464 | 6 |
| 309.0789 | 20 |

 |
| 28 | 1.26 | 355.1024 | **Neochlorogenic acid** |

|  |  |
| --- | --- |
| 89.0385 | 5 |
| 117.0333 | 7 |
| 135.0441 | 20 |
| 145.0282 | 22 |
| 163.0393 | 100 |
| 190.0856 | 3 |
| 191.0904 | 4 |

 |
| 29 | 6.45 | 354.1695 | **13-Methylcanadine** |

|  |  |
| --- | --- |
| 61.019 | 17 |
| 140.981 | 16 |
| 181.7687 | 17 |
| 190.0872 | 100 |
| 320.0554 | 23 |
| 339.0992 | 18 |

 |
| 30 | 1.13 | 352.1180 | **8-Oxoberberine** |

|  |  |
| --- | --- |
| 108.3074 | 1 |
| 117.5906 | 1 |
| 263.3792 | 1 |
| 269.3829 | 1 |
| 278.0826 | 3 |
| 279.0851 | 2 |
| 280.0999 | 3 |
| 290.0872 | 2 |
| 291.0904 | 12 |
| 292.1001 | 4 |
| 294.0792 | 10 |
| 306.0782 | 5 |
| 307.0854 | 6 |
| 308.0944 | 98 |
| 309.0994 | 2 |
| 318.0843 | 1 |
| 319.0847 | 1 |
| 320.0944 | 24 |
| 321.1035 | 4 |
| 322.0742 | 38 |
| 336.0895 | 100 |
| 337.097 | 47 |
| 352.1213 | 25 |

 |
| 31 | 6.98 | 350.1388 | **13-Methylberberine** |

|  |  |
| --- | --- |
| 247.5166 | 100 |

 |
| 32 | 5.10 | 344.1856 | **Tembetarine** | n/a |
| 33 | 1.11 | 342.1696 | **Magnoflorine** |

|  |  |
| --- | --- |
| 91.0542 | 2 |
| 95.049 | 1 |
| 119.0493 | 2 |
| 136.0523 | 1 |
| 149.06 | 2 |
| 150.066 | 4 |
| 151.0753 | 8 |
| 163.0636 | 6 |
| 165.0912 | 4 |
| 166.0932 | 1 |
| 176.0712 | 16 |
| 177.0746 | 18 |
| 178.0863 | 100 |
| 190.0855 | 1 |
| 191.0909 | 1 |
| 192.1029 | 6 |
| 207.0822 | 1 |
| 222.0665 | 1 |
| 237.0914 | 1 |
| 265.0883 | 2 |
| 282.0916 | 1 |
| 294.0945 | 1 |
| 297.1127 | 1 |
| 326.1398 | 1 |
| 342.1689 | 3 |

 |
| 34 | 5.80 | 342.1699 | **Isocorypalmine** |

|  |  |
| --- | --- |
| 128.7082 | 2 |
| 150.0671 | 6 |
| 151.0749 | 9 |
| 158.5845 | 2 |
| 163.062 | 4 |
| 165.0908 | 14 |
| 169.0445 | 2 |
| 176.0702 | 6 |
| 177.0753 | 7 |
| 178.0863 | 100 |
| 178.3134 | 2 |
| 190.0877 | 2 |
| 192.1022 | 46 |

 |
| 35 | 1.08 | 336.1236 | **Epiberberine** |

|  |  |
| --- | --- |
| 263.0953 | 1 |
| 275.0955 | 11 |
| 276.1032 | 1 |
| 278.0829 | 11 |
| 291.0909 | 5 |
| 292.0985 | 100 |
| 304.099 | 23 |
| 305.1061 | 1 |
| 306.0783 | 35 |
| 318.0811 | 1 |
| 320.0938 | 91 |
| 321.102 | 38 |
| 336.1256 | 15 |

 |
| 36 | 1.16 | 328.1544 | **1,2-Dehydroreticuline** |

|  |  |
| --- | --- |
| 91.0538 | 2 |
| 95.0494 | 1 |
| 119.0488 | 2 |
| 137.0594 | 1 |
| 151.0752 | 7 |
| 163.0629 | 6 |
| 164.0706 | 8 |
| 176.0714 | 2 |
| 178.0864 | 100 |
| 191.0935 | 1 |
| 233.0611 | 1 |
| 265.0882 | 1 |
| 296.1285 | 1 |
| 312.1217 | 1 |
| 313.1316 | 1 |
| 328.1554 | 1 |

 |
| 37 | 9.86 | 329.1021 | **6,8-C-Dimethylluteolin-7-methyl ether** | n/a |
| 38 | 5.24 | 324.1231 | **Dehydrodiscretamine** |

|  |  |
| --- | --- |
| 81.106 | 32 |
| 97.8473 | 31 |
| 100.9352 | 38 |
| 294.0756 | 52 |
| 309.1021 | 100 |

 |
| 39 | 1.19 | 322.1074 | **Thalinfendin** |

|  |  |
| --- | --- |
| 100.9064 | 6 |
| 113.0107 | 5 |
| 145.0039 | 6 |
| 151.9779 | 10 |
| 161.9604 | 6 |
| 177.0366 | 6 |
| 279.0901 | 13 |
| 293.1007 | 14 |
| 305.0992 | 9 |
| 307.0857 | 100 |
| 321.0983 | 23 |
| 322.1099 | 15 |

 |
| 40 | 6.51 | 315.0865 | **6-C-Methylluteolin-7-methyl ether** |

|  |  |
| --- | --- |
| 154.2853 | 45 |
| 178.2729 | 80 |
| 201.1571 | 44 |
| 224.7724 | 38 |
| 299.056 | 50 |
| 300.0638 | 100 |

 |
| 41 | 6.94 | 314.1385 | **1,2-Dihydronorreticuline** |

|  |  |
| --- | --- |
| 93.0697 | 26 |
| 102.4157 | 32 |
| 121.0649 | 100 |
| 132.6369 | 24 |
| 145.0285 | 90 |
| 177.0548 | 45 |

 |
| 42 | 10.66 | 313.1069 | **Sideroxylin** | n/a |
| 43 | 1.13 | 300.1595 | **N-methylcocluarine / canelilline** |

|  |  |
| --- | --- |
| 79.0543 | 1 |
| 91.0541 | 1 |
| 93.0699 | 1 |
| 95.0489 | 1 |
| 103.0541 | 1 |
| 107.0491 | 100 |
| 115.0544 | 5 |
| 117.0699 | 2 |
| 119.0494 | 2 |
| 121.0649 | 9 |
| 131.0494 | 3 |
| 133.0651 | 1 |
| 137.06 | 8 |
| 143.0495 | 13 |
| 144.0575 | 1 |
| 145.0651 | 7 |
| 147.0807 | 1 |
| 149.0604 | 1 |
| 151.0754 | 2 |
| 155.0611 | 1 |
| 160.0524 | 3 |
| 163.0757 | 2 |
| 164.0707 | 1 |
| 165.0719 | 1 |
| 175.076 | 10 |
| 175.1097 | 1 |
| 178.0864 | 2 |
| 179.0873 | 1 |
| 180.1028 | 1 |
| 181.0658 | 1 |
| 181.1024 | 2 |
| 182.0735 | 1 |
| 191.0869 | 3 |
| 192.1027 | 2 |
| 194.0734 | 2 |
| 195.0804 | 1 |
| 197.0971 | 6 |
| 207.0829 | 1 |
| 209.0971 | 9 |
| 209.1404 | 1 |
| 211.1124 | 1 |
| 219.0824 | 2 |
| 225.0926 | 2 |
| 237.0923 | 7 |
| 238.0999 | 1 |
| 254.0947 | 2 |
| 269.1196 | 2 |

 |
| 44 | 9.98 | 299.0916 | **Desmethyl-sideroxylin** |

|  |  |
| --- | --- |
| 79.9387 | 47 |
| 80.5415 | 46 |
| 133.8388 | 44 |
| 178.3192 | 73 |
| 194.8692 | 45 |
| 284.0692 | 100 |

 |
| 45 | 7.04 | 320.0918 | **Coptisine** |

|  |  |
| --- | --- |
| 66.0495 | 1 |
| 85.2445 | 1 |
| 127.6488 | 1 |
| 149.0857 | 1 |
| 169.0817 | 1 |
| 178.2759 | 2 |
| 218.0732 | 1 |
| 262.0836 | 7 |
| 264.106 | 2 |
| 274.0699 | 6 |
| 277.0553 | 8 |
| 288.0689 | 1 |
| 290.0807 | 13 |
| 291.0708 | 2 |
| 292.0965 | 9 |
| 303.0509 | 2 |
| 305.0699 | 4 |
| 318.0759 | 100 |
| 320.0917 | 93 |

 |
| 46 | 1.11 | 190.0864 | **Hydrastinine** |

|  |  |
| --- | --- |
| 82.4169 | 3 |
| 91.0535 | 8 |
| 103.0536 | 11 |
| 117.0575 | 6 |
| 119.0489 | 9 |
| 131.0491 | 18 |
| 131.069 | 4 |
| 132.0808 | 29 |
| 134.0974 | 4 |
| 135.0446 | 3 |
| 137.2301 | 2 |
| 147.068 | 4 |
| 149.0594 | 12 |
| 159.0439 | 5 |
| 160.0761 | 22 |
| 161.0596 | 5 |
| 174.0541 | 5 |
| 175.0629 | 35 |
| 190.0865 | 100 |

 |
| 47 | 14.08 | 279.2329 | **Linoleic acid** |

|  |  |
| --- | --- |
| 74.367 | 8 |
| 80.7718 | 9 |
| 85.0036 | 9 |
| 86.9123 | 8 |
| 128.0099 | 100 |
| 134.7439 | 10 |
| 181.6503 | 7 |
| 196.9125 | 12 |
| 235.5706 | 8 |
| 258.3408 | 9 |

 |
| 48 | 6.74 | 352.1539 | **Palmatine** | n/a |
| 49 | 14.56 | 255.2329 | **Palmitic acid** |

|  |  |
| --- | --- |
| 67.3201 | 100 |
| 75.7724 | 95 |
| 85.2747 | 84 |
| 229.6982 | 95 |

 |
| 50 | 14.80 | 283.2643 | **Stearic acid** | n/a |