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

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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:**

|  |  |
| --- | --- |
| **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** | |  |  | |  |  | |  |  | |  |  | | 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 | |  | | | | | |

**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 |

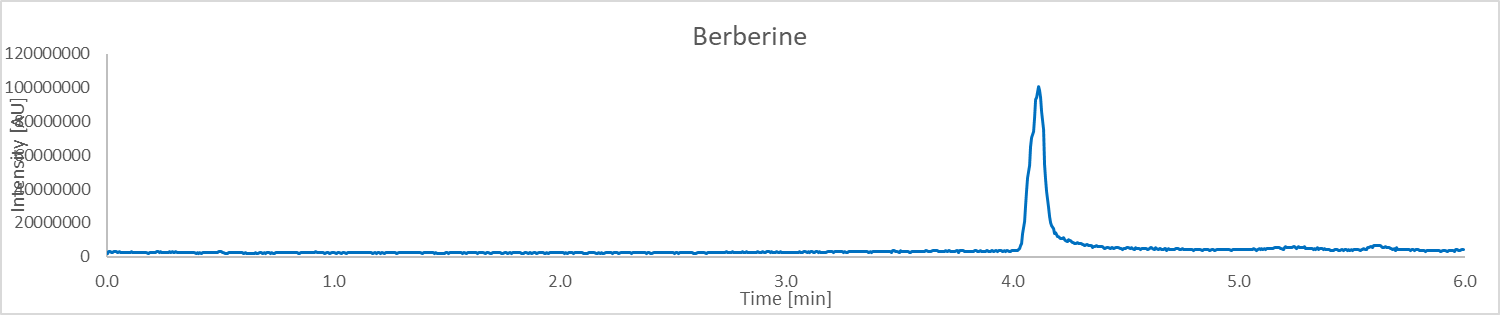
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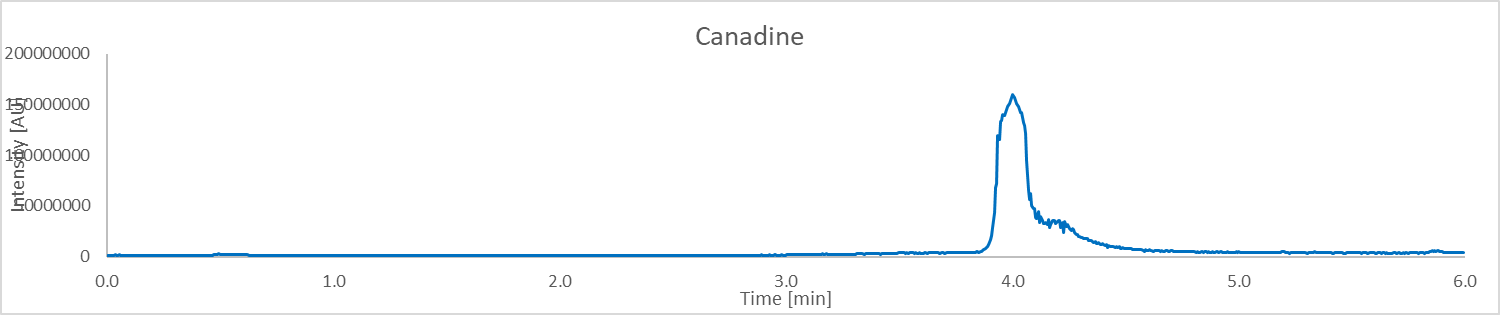
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| --- | --- | --- | --- | --- | --- |
| **Name** | **Supplier** | **CAS Number** | **Catalog number** | **Purity %** | **Batch/Lot number** |
| **Berberine** | USP | 2086-83-1 | 1065210 | >98% | R04130 |
| **Canadine** | Phytolab | 522-97-4 | 80378-10mg | >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 |

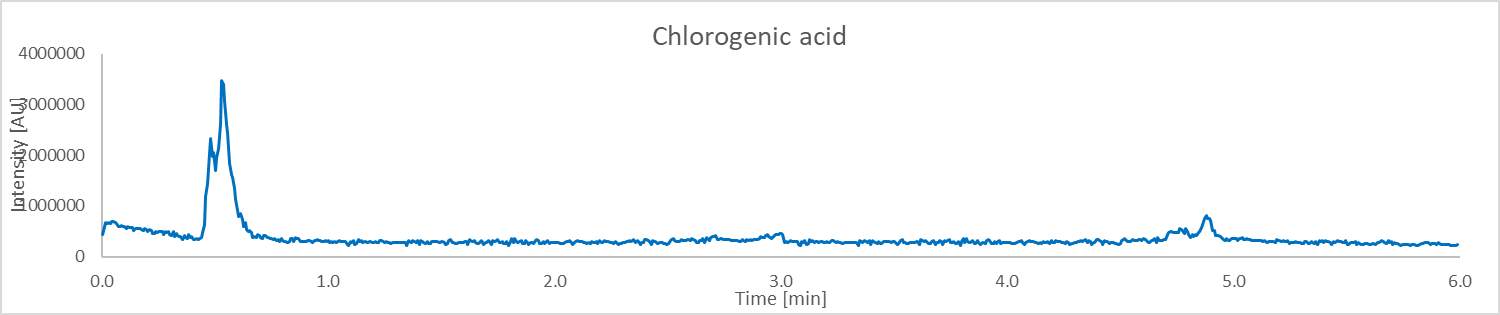
**Chemical structures of standards used for quantitative analysis**

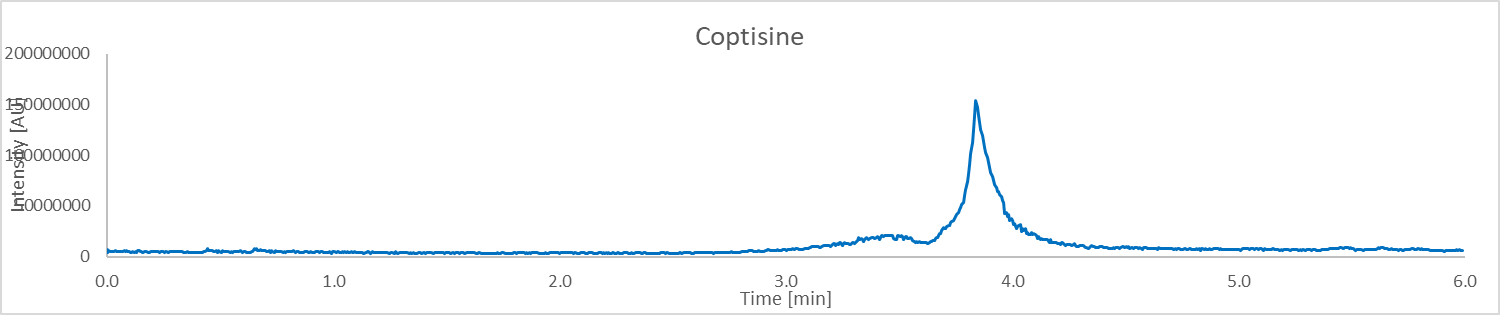


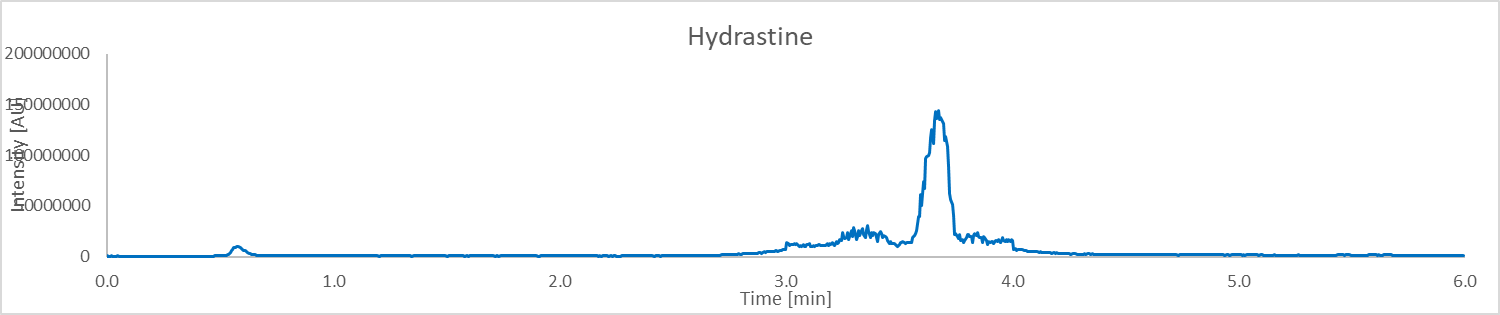
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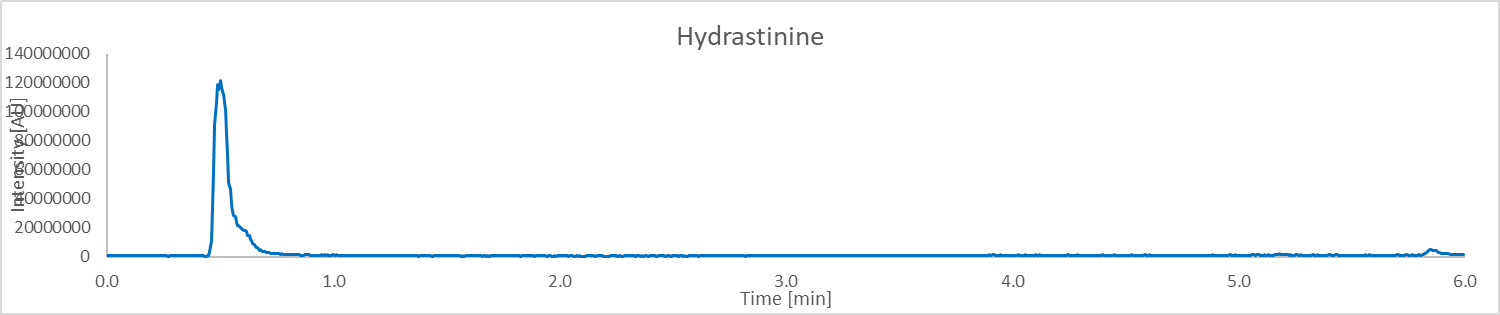
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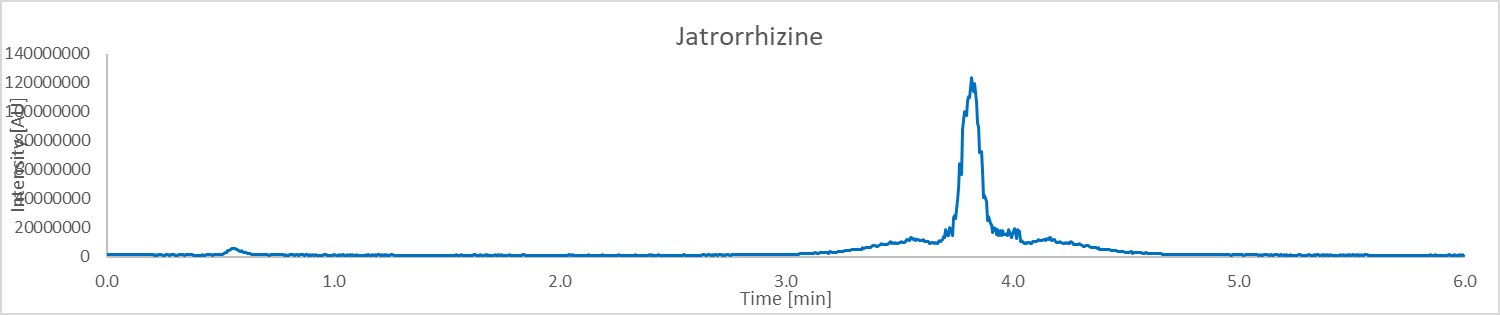
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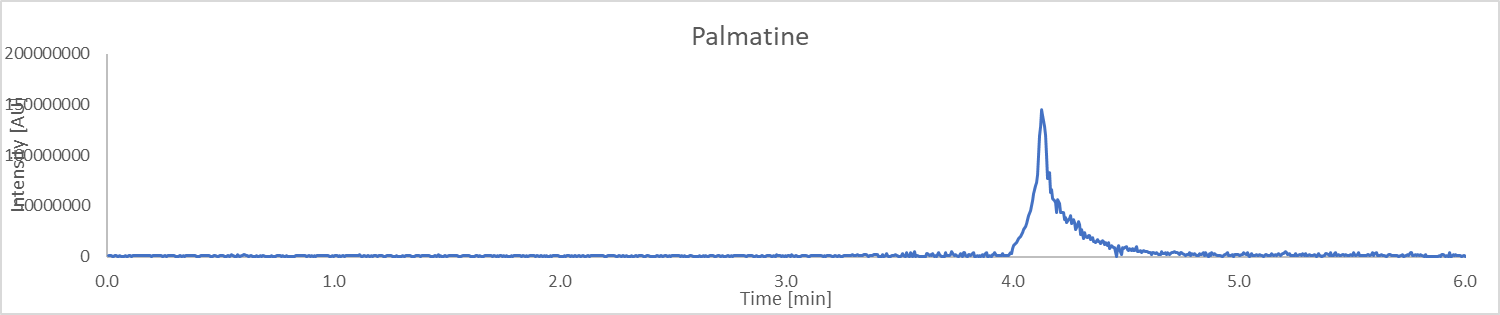
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**Calibration**

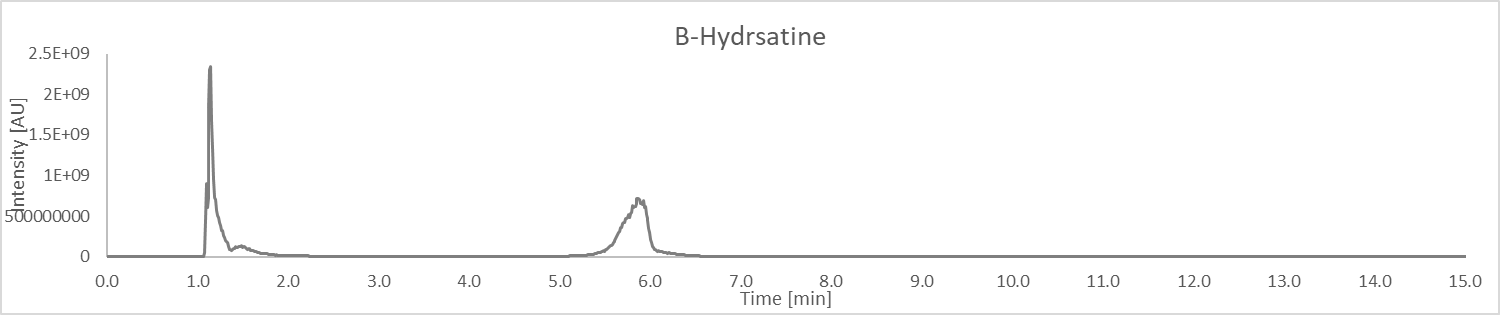
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| --- | --- | --- | --- | --- | --- |
| Compound | Lower limit of quantitation (LLOQ) **ug/mL** | Calibration range (**ug/mL**) | Number of Calibration Points | R2 | Concentration  mg/g **in extract** (n = 3) |
| **Berberine** | 0.001 | 0.001 – 0.243 | 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 |

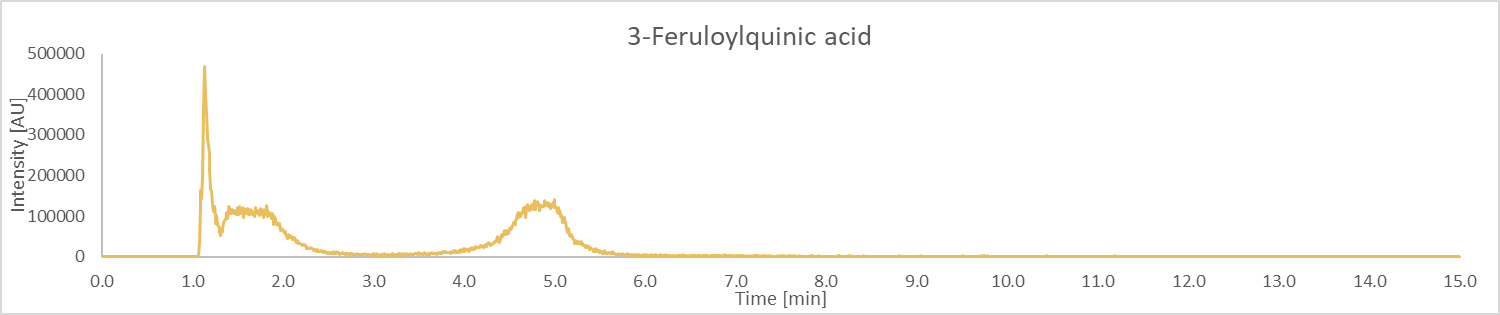
Untargeted Analysis

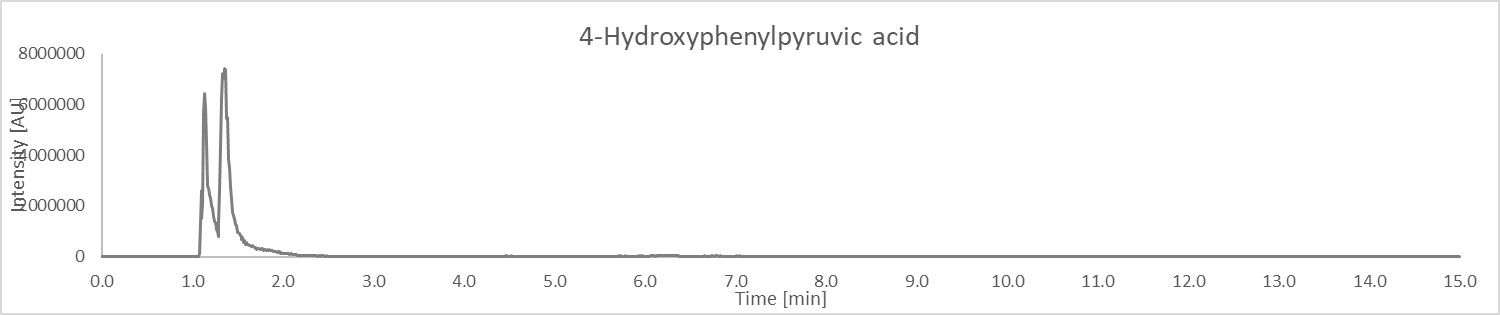
|  |  |
| --- | --- |
|  | |
| UHPLC conditions | Mass spectrometer conditions |
| System: Thermo Vanquish  Column: Waters Acquity Ultra C18 (1.7 um, 1.0 x 150 mm)  Mobile phase A: H2O w/ 0.1% FA  Mobile phase B: ACN w/ 0.1% FA  Flow rate: 0.100 mL/min  Column temperature: 55℃  Gradient:   |  |  | | --- | --- | | Time (min) | Mobile phase B (%) | | 0 | 5 | | 1 | 5 | | 12.5 | 98 | | 13.5 | 98 | | 12.6 | 5 | | 15 | 5 | | System: Thermo Orbitrap Fusion Lumos  Mode: ESI  Polarity: positive/negative  Main-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 |

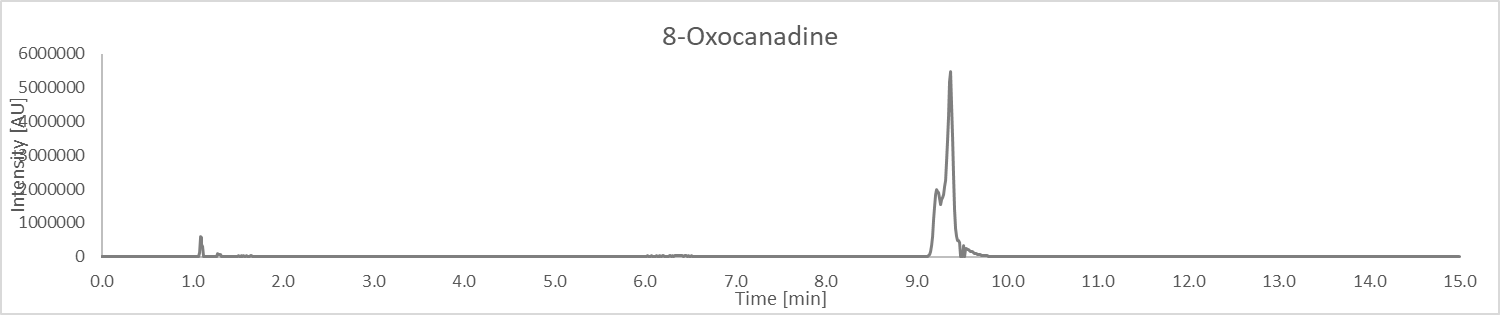
|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Table 1: Proposed identification of constituents of Goldenseal** | | | | | |
| Peak No. | RT (min) | Exp. *m/z* | Mass accuracy  (ppm) | Proposed ID’s  (Confirmed with Std in **green**)  (Structure with correlated MS2 spectra in **orange**)  (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 |

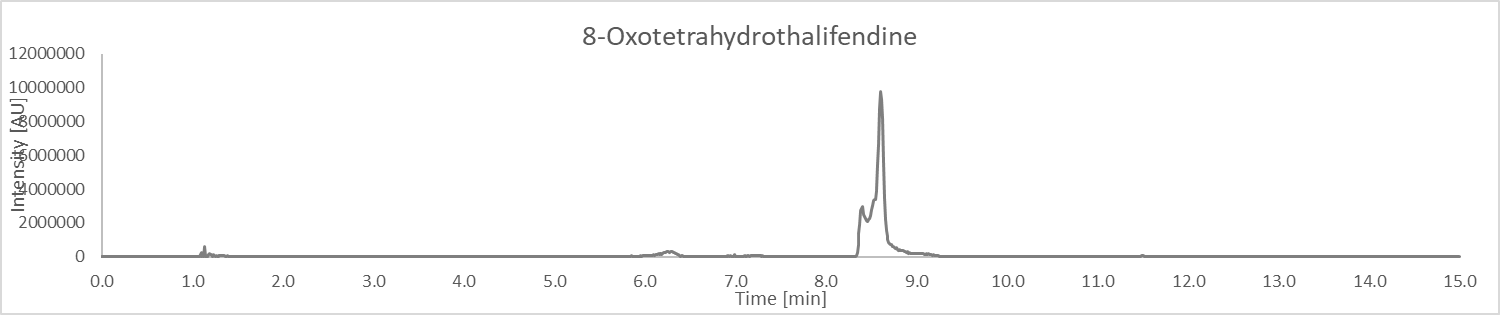
Figure 1: Chromatograms

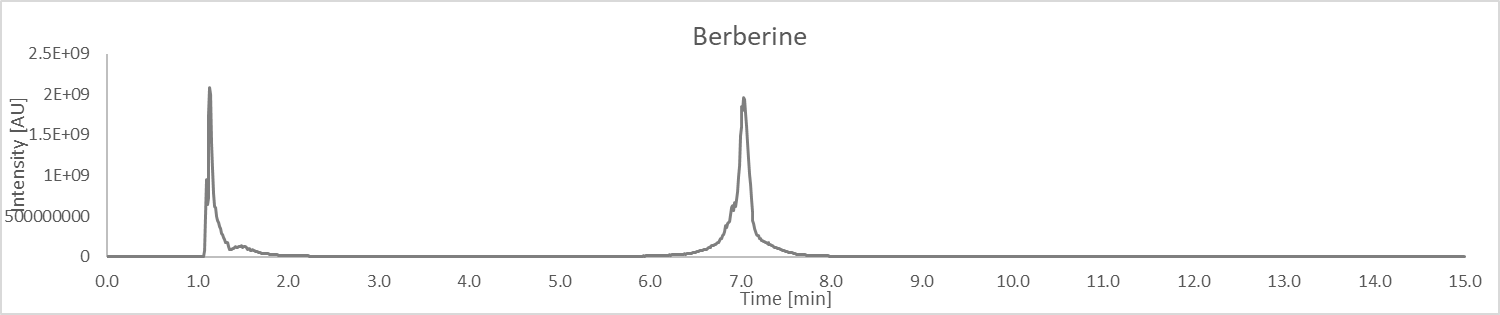


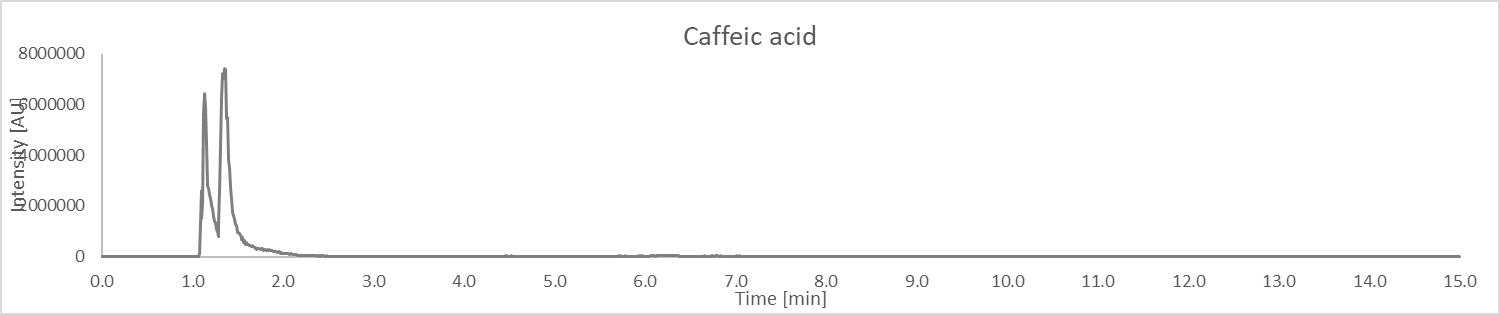


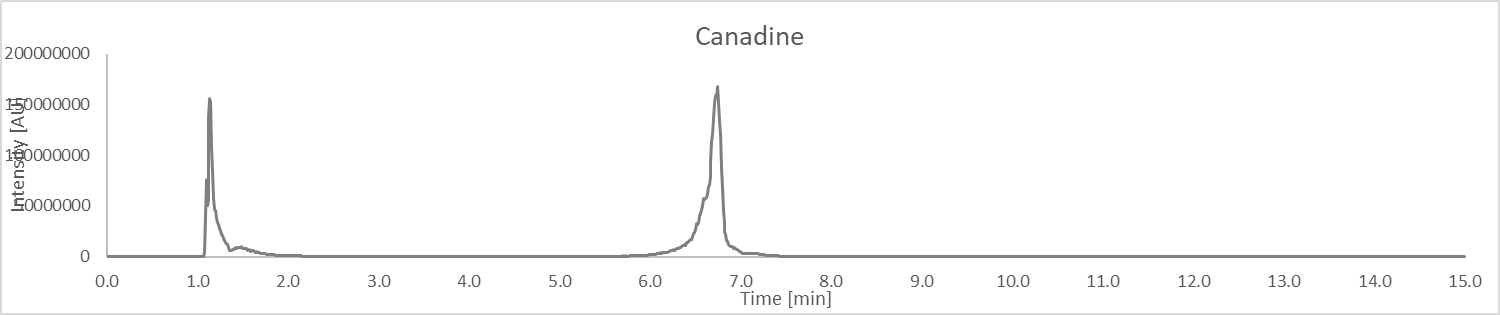


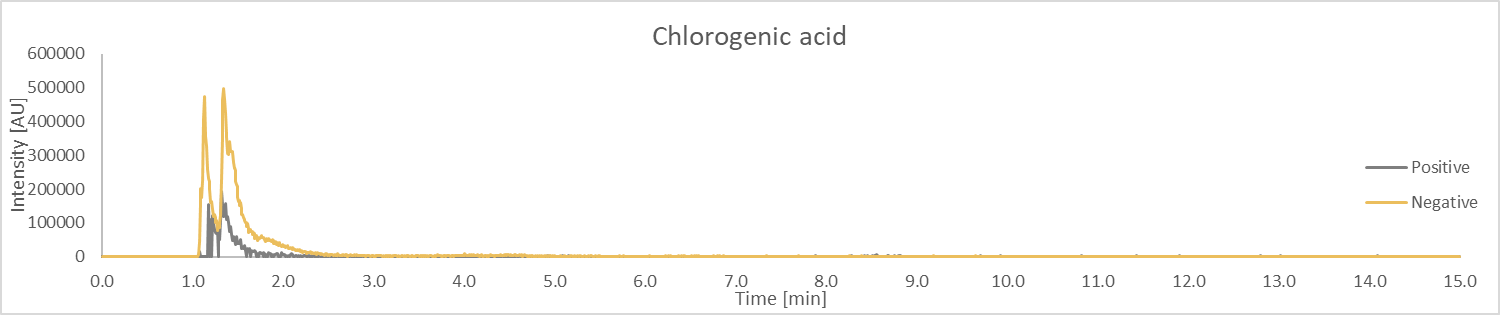


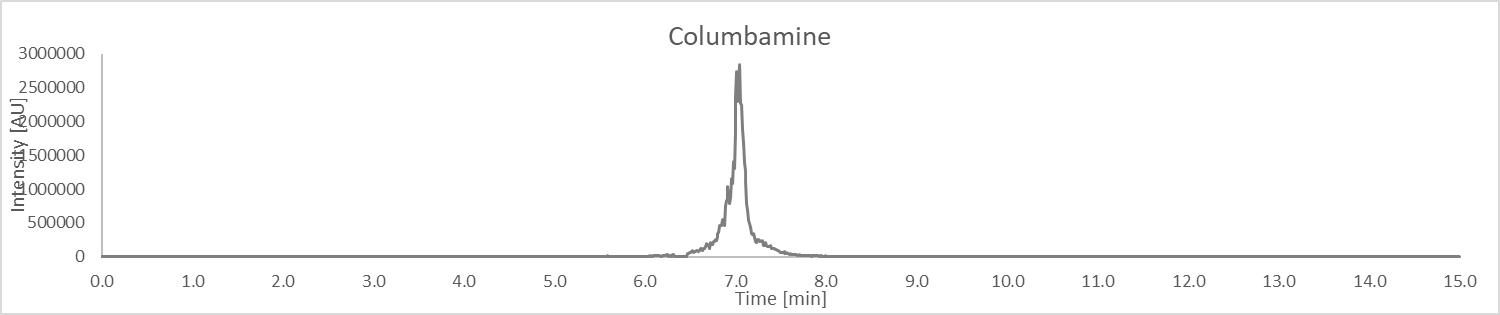


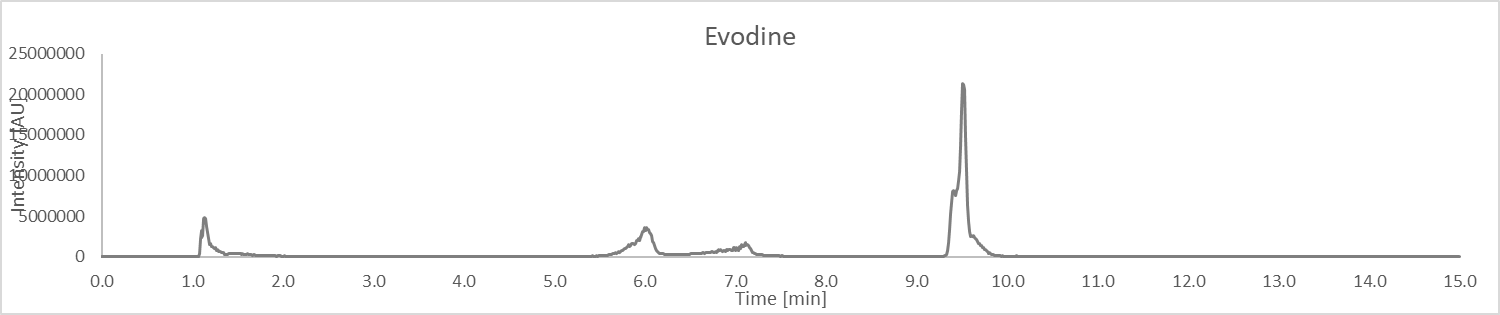


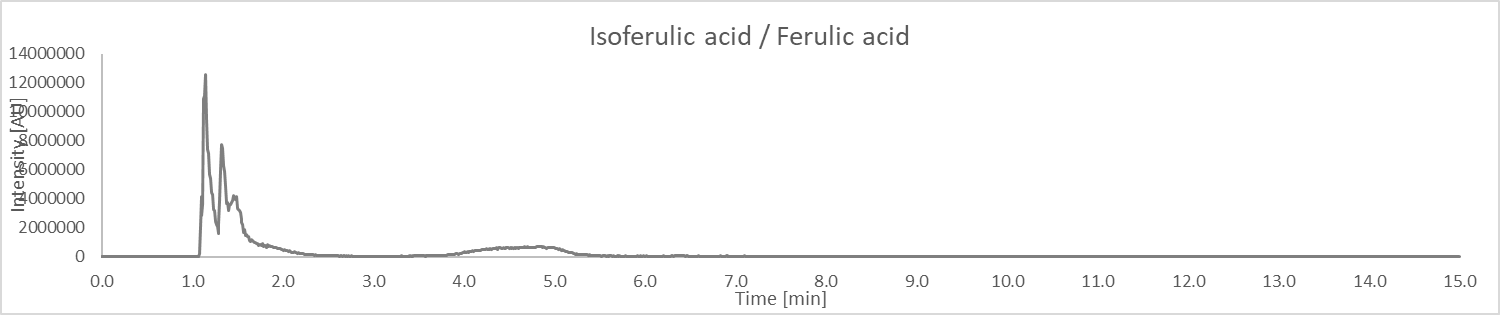


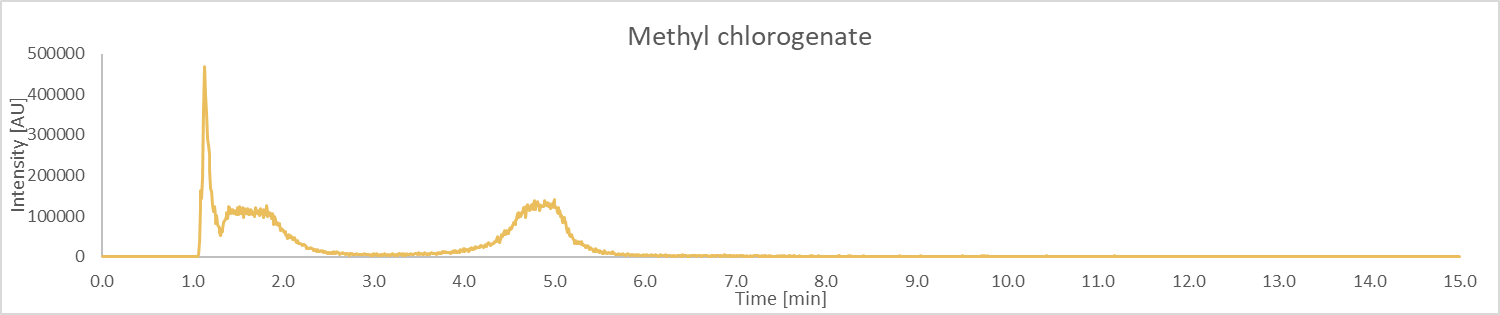


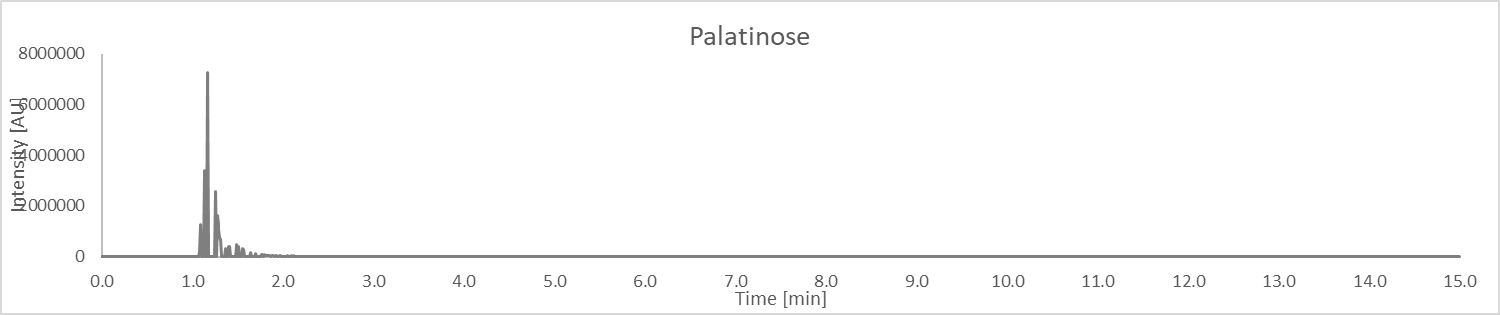


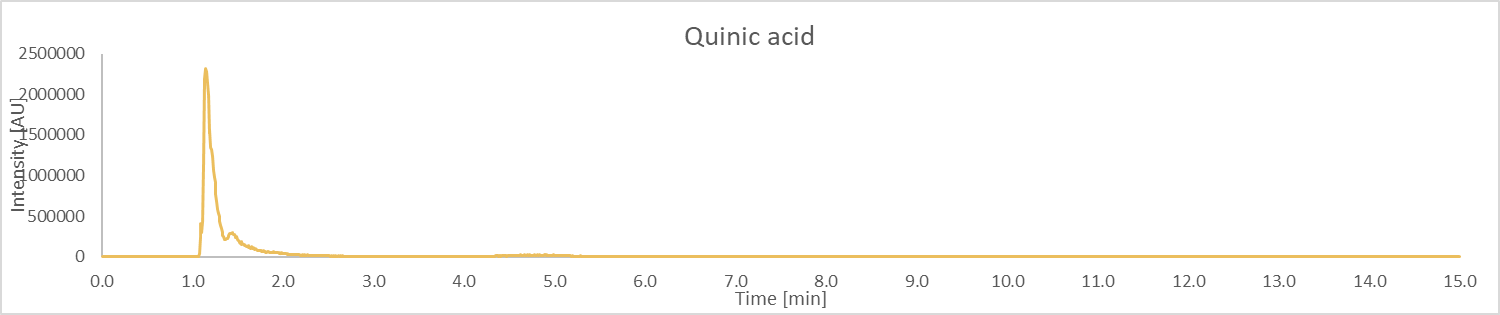


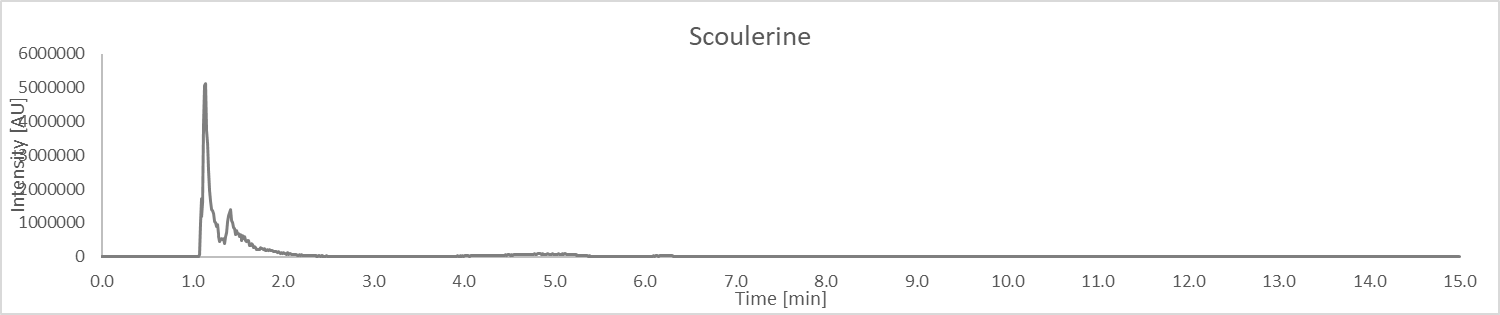


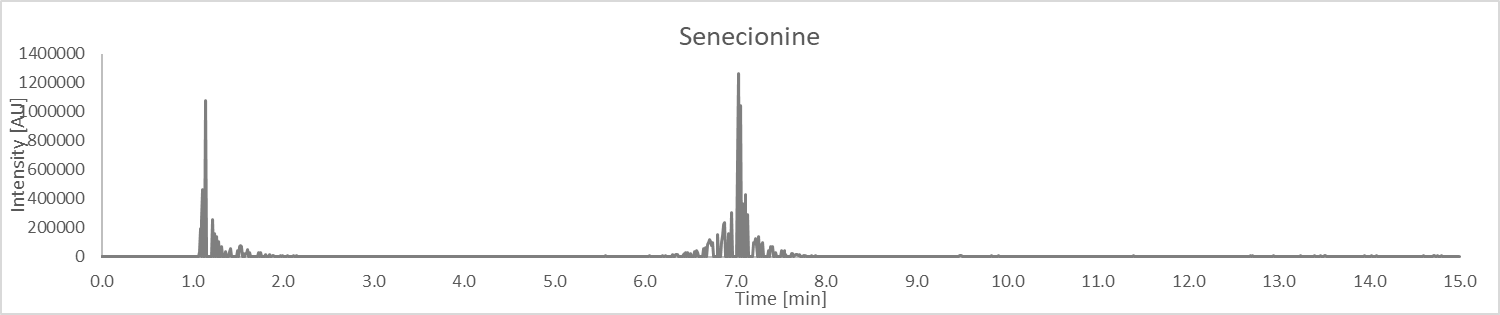


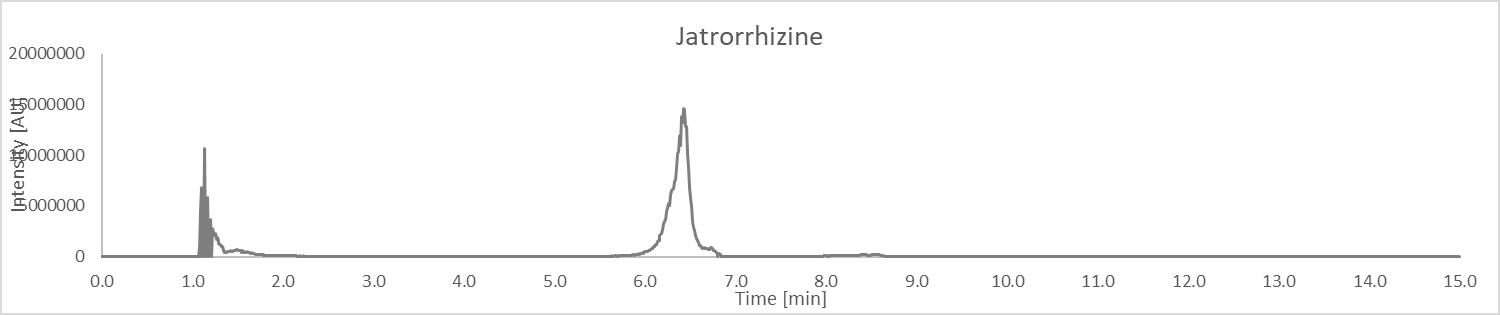


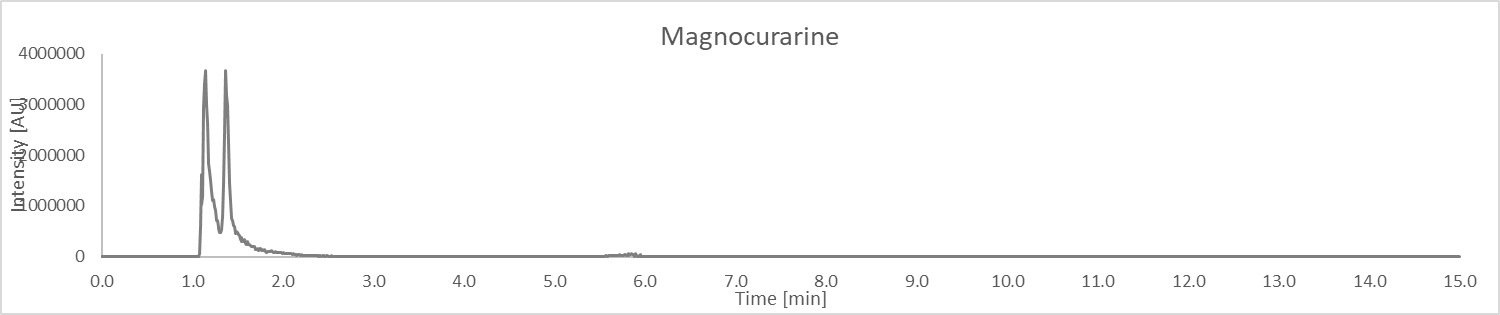


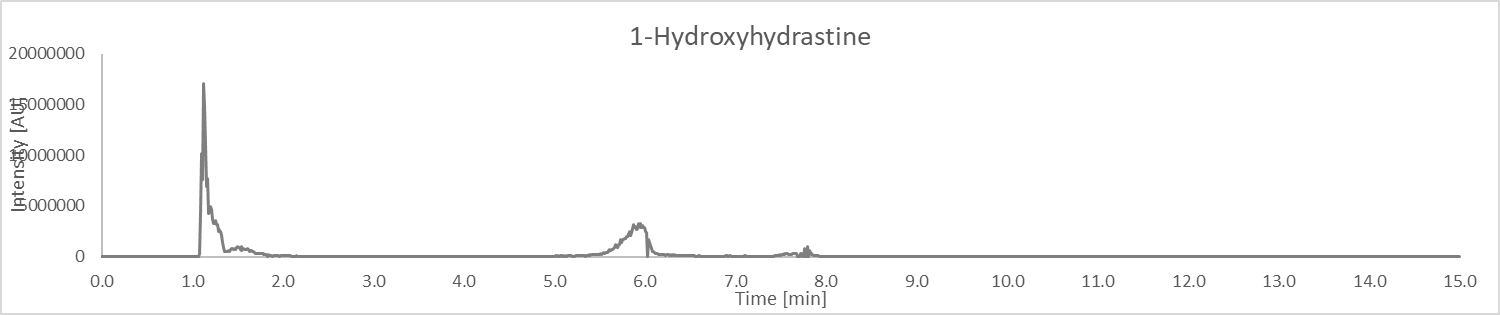


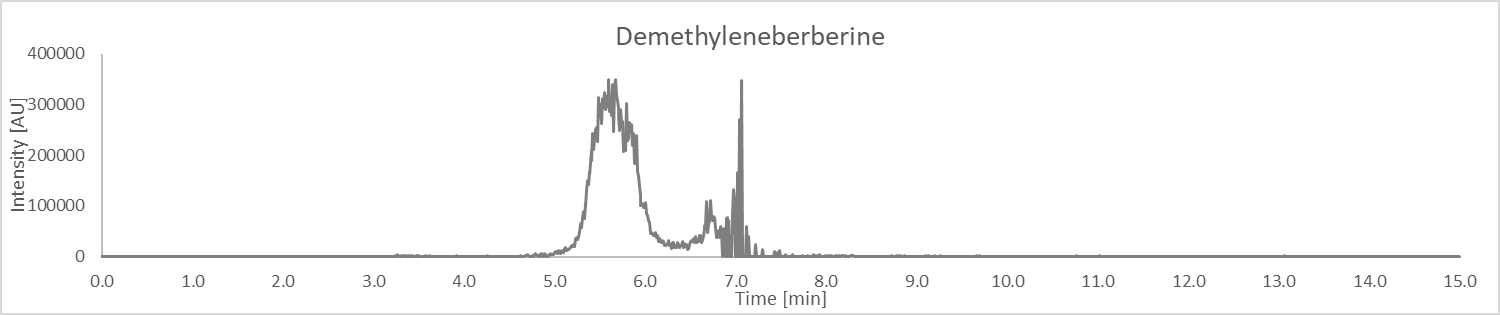


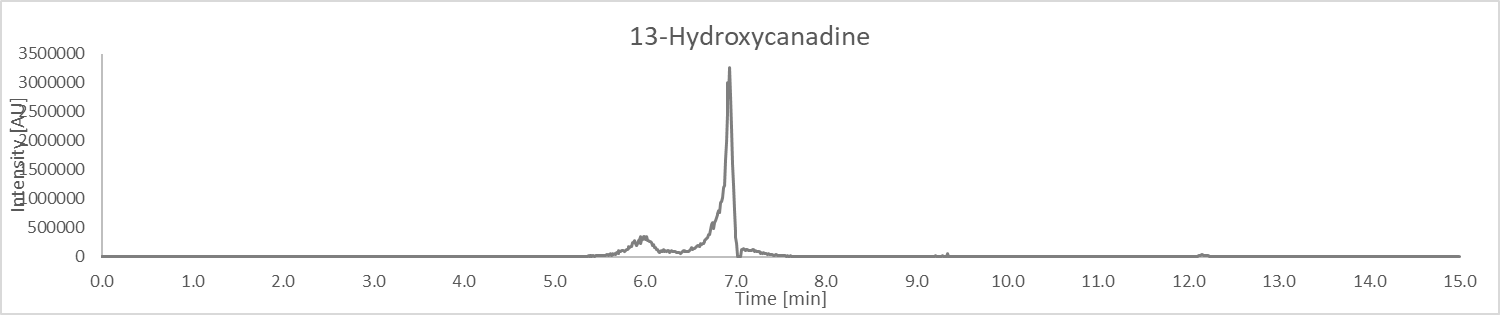


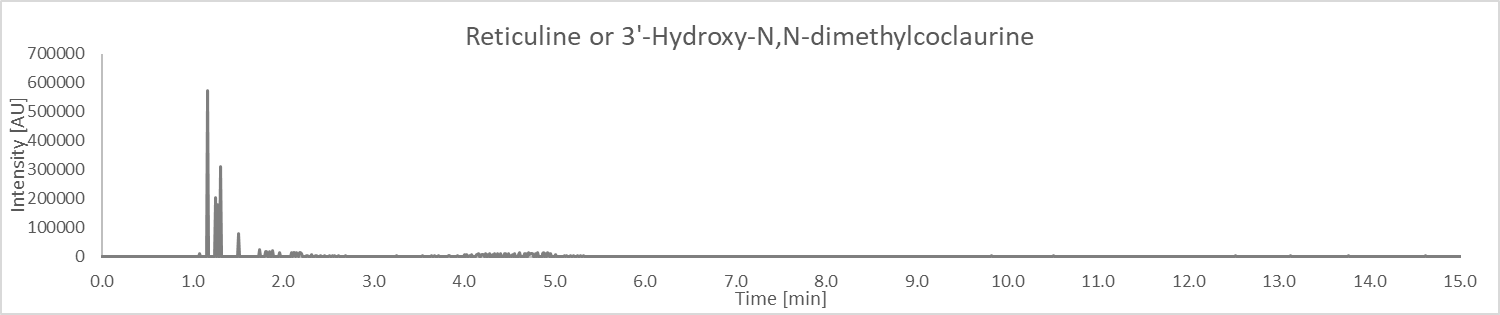


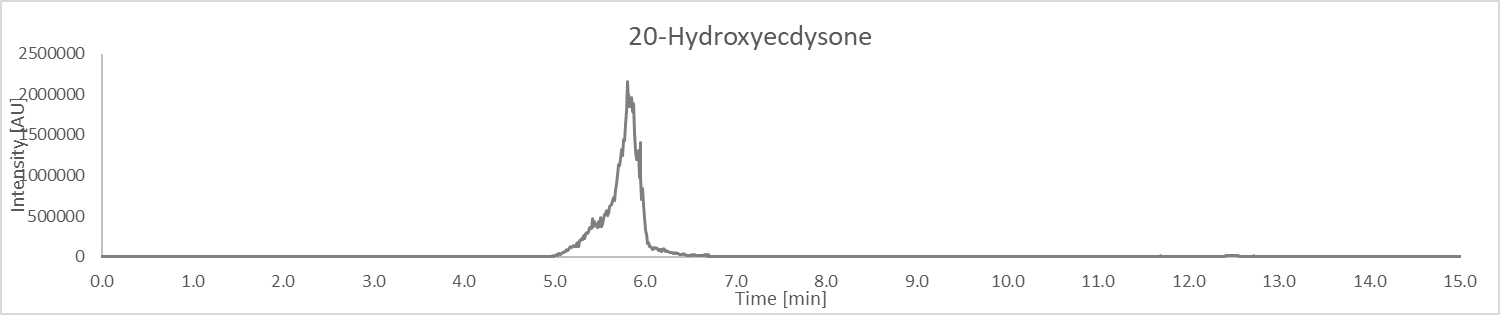


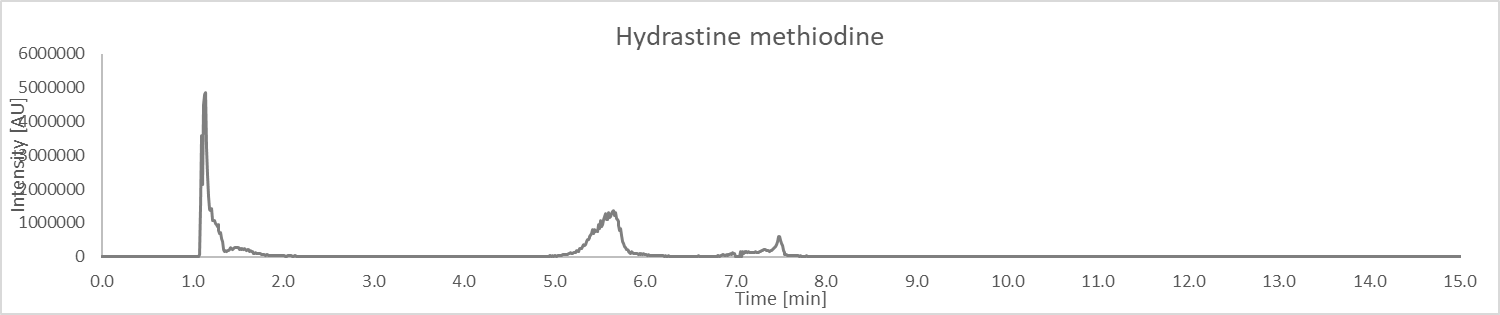


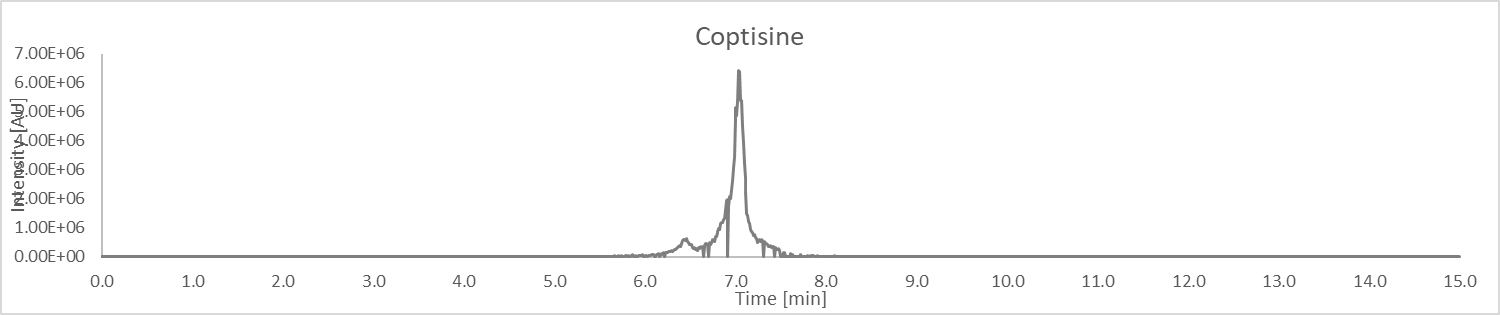


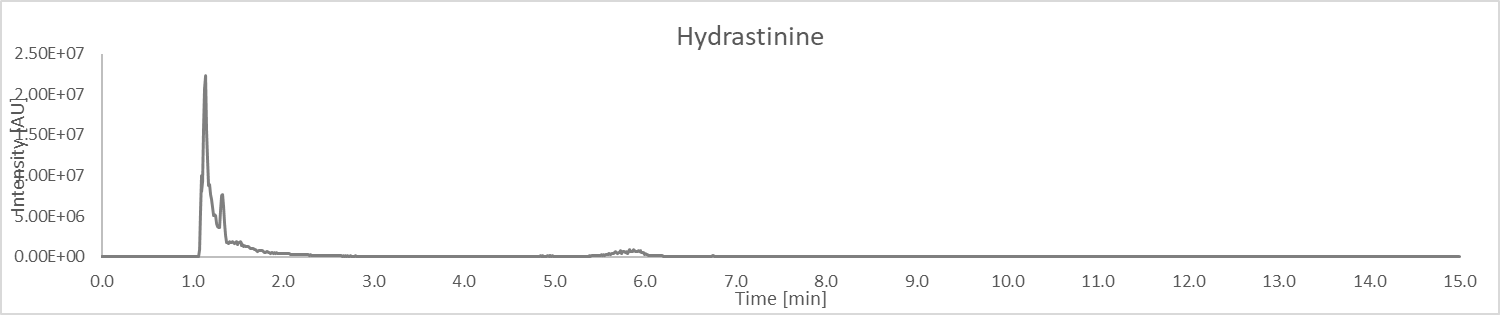


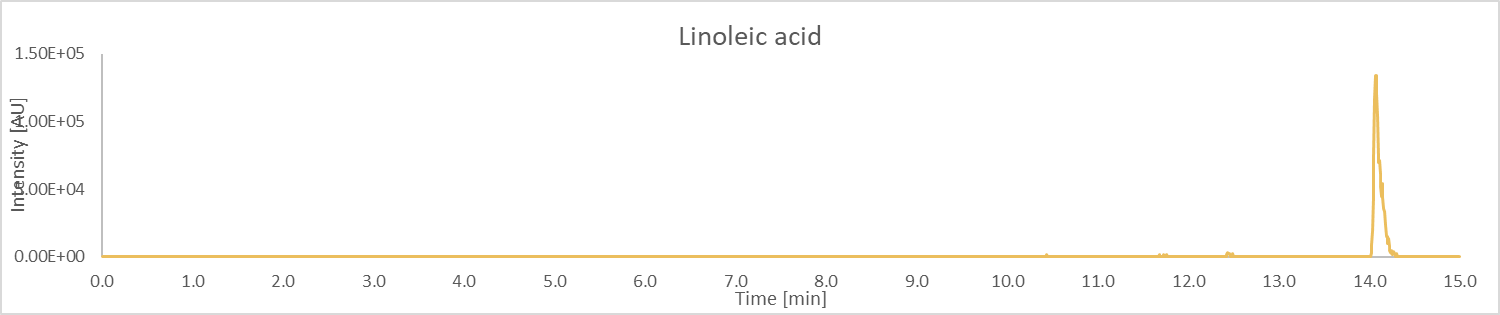


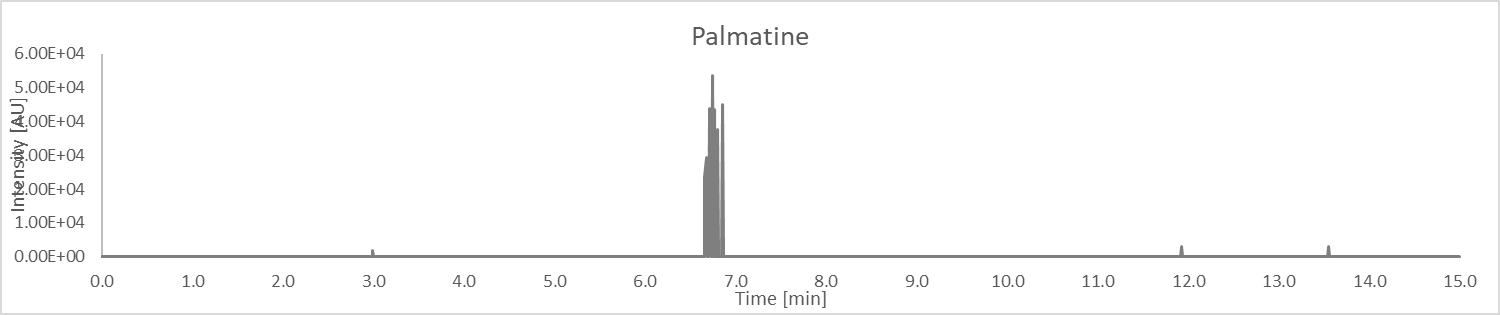


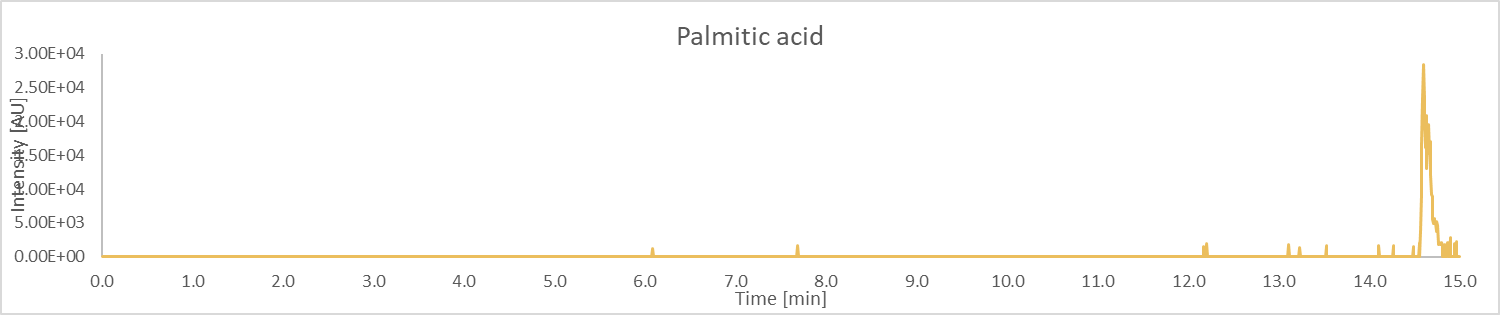


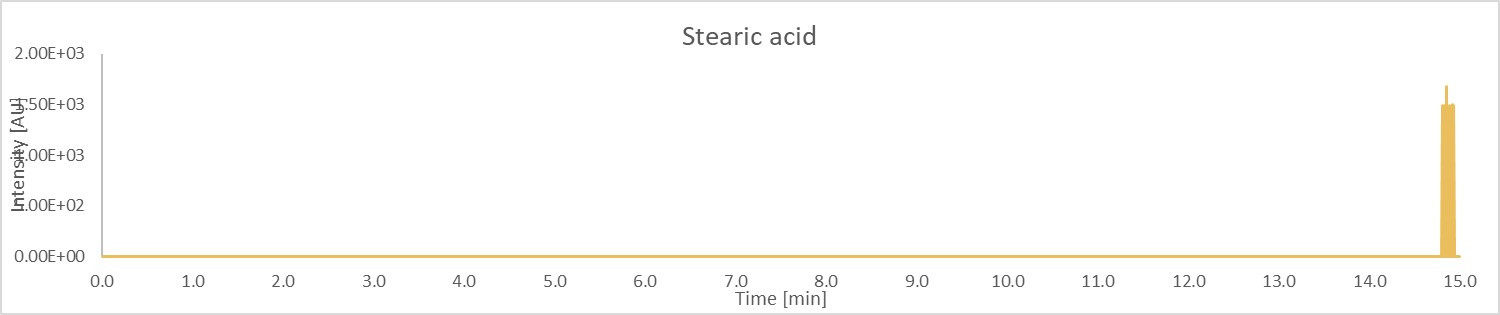












Structures of compounds in Table 1



|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **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 |