Table S1 The components of extracts from the whole plants of *Galinsoga parviflora* Cav.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Noa | Name | Type | Formula | CAS | Fragmentation Score | *t*R(min) |
| 1 | 1,4-Cyclohexanedicarboxylic acid | Dicarboxylic acid | C8H12O4 | 1076-97-7 | 80.9 | 6.88 |
| 2 | Trehalose | Disaccharide | C12H22O11 | 99-20-7 | 96.6 | 0.79 |
| 3 | Gossypin | Flavonoid | C21H20O13 | 540-25-4 | 97.3 | 5.34 |
| 4 | α，β-Trehalose | Disaccharide | C12H22O11 | 585-91-1 | 67.2 | 0.79 |
| 5 | Adenosine | Nucleoside | C10H13N5O4 | 58-61-7 | 90.4 | 1.43 |
| 6 | Cyclohexanecarboxylic acid | Aromatic acid | C16H18O9 | 630-21-3 | 76.9 | 4.66 |
| 7 | 3,4-Dicaffeoylquinic acid | Hydroxycinnamic acid ester | C25H24O12 | 14534-61-3 | 79.6 | 6.17 |
| 8 | Succinic acid | Dicarboxylic acid | C4H6O4 | 110-15-6 | 60.8 | 1.20 |
| 9 | Raffinose | Trisaccharide | C18H32O16 | 512-69-6 | 95.5 | 0.79 |
| 10 | *D*-Tryptophan | Amino acid | C11H12N2O2 | 1756-70-5 | 85.7 | 3.64 |
| 11 | 3,5-Dicaffeoylquinic acid | Hydroxycinnamic acid derivative | C25H24O12 | 2450-53-5 | 77.5 | 6.07 |
| 12 | Verbascose | Tetrasaccharide | C30H52O26 | 585-83-9 | 73.9 | 0.83 |
| 13 | Spiraeoside | Flavonoid glycoside | C21H20O12 | 20249-74-3 | 98.3 | 5.72 |
| 14 | 5,7,3'-Trihydroxy-6,4',5'-Trimethoxyflavone | Flavonoid | C18H16O8 | 78417-26-2 | 69.6 | 8.41 |
| 15 | 4-Methylphthalic anhydride | Anhydride | C9H6O3 | 1124-11-4 | 63.5 | 4.66 |
| 16 | Laricitrin 3-galactoside | Flavonoid glycoside | C22H22O13 | 93219-26-2 | 80.7 | 5.97 |
| 17 | Syringetin-3-O-galactoside | Flavonoid glycoside | C23H24O13 | 55025-56-4 | 84.7 | 6.18 |
| 18 | Myricetin-3-O-galactoside | Flavonoid glycoside | C21H20O13 | 15648-86-9 | 85 | 5.35 |
| 19 | Mucicacid | Organic acid | C6H10O8 | 526-99-8 | 66.3 | 7.35 |
| 20 | 1-O-(3-Hydroxy-4,5-dimethoxybenzoyl) hexopyranose | Glycoside | C15H20O10 | - | 78.9 | 3.66 |
| 21 | Loliolide | Lactone | C11H16O3 | 59889-61-3 | 67 | 6.40 |
| 22 | Maleic acid | Dicarboxylic acid | C4H4O4 | 110-16-7 | 72.5 | 1.63 |
| 23 | 9*S*,10*S*,11*R*-trihydroxy-12*Z*-octadecenoic acid | Fatty acid | C18H34O5 | 339186-36-6 | 52.4 | 8.06 |
| 24 | 3 Hydroxycoumarin | Coumarin | C9H6O3 | 939-19-5 | 83.6 | 8.80 |
| 25 | *(R)*-Camphor | Terpenoid | C10H16O | 464-48-2 | 73 | 3.04 |
| 26 | Uridine | Nucleoside | C9H12N2O6 | 58-96-8 | 81.8 | 1.03 |
| 27 | *D*-phenylalanine | Amino acid | C9H11NO2 | 673-06-3 | 85.3 | 1.90 |
| 28 | *D*-threo-Isocitric acid | Organic acid | C6H8O7 | 3634-58-4 | 55.3 | 0.88 |
| 29 | Quercetin 3-O-beta-glucopyranosyl-6'-acetate | Flavonoid glycoside | C23H22O13 | 54542-51-7 | 79.5 | 6.15 |
| 30 | PC(18:2/0:0) | Phosphatidylcholine | C26H50NO7P | 22252-07-9 | 90 | 10.79 |
| 31 | 1-[3-[(4-fluorophenyl)methyl]-4-oxothieno[3,2-d]pyrimidin-2-yl]-N-propylpiperidine-4-carboxamide | Heterocyclic compound | C22H25FN4O2S | 1021418-53-0 | 77.1 | 7.04 |
| 32 | PC(18:3/0:0) | Phosphatidylcholine | C26H48NO7P | 67270-42-2 | 88.8 | 10.19 |
| 33 | Dihydroactinidiolide | Lactone | C11H16O2 | 17092-92-1 | 56.7 | 8.85 |
| 34 | Quercetin 3-O-glucuronide | Flavonoid glucuronide | C21H18O13 | 22688-79-5 | 61 | 6.15 |
| 35 | N-Methylisoleucine | Amino acid derivative | C7H15NO2 | 4125-98-8 | 75.8 | 2.30 |
| 36 | Citrate | Tricarboxylic acid | C6H8O7 | 77-92-9 | 55.3 | 1.23 |
| 37 | GPSer(22:6/18:0) | Glycerophosphoserine | C46H78NO10P | - | 96.6 | 11.40 |
| 38 | Quercetin 3-O-malonylglucoside | Flavonoid glycoside | C24H22O15 | 96862-01-0 | 95.6 | 6.16 |
| 39 | 6-Hydroxyluteolin 6,3'-dimethyl ether 7-glucoside | Flavonoid glycoside | C23H24O12 | 54300-65-1 | 85.7 | 6.60 |
| 40 | Quercetin-3-O-glucoside | Flavonoid glycoside | C21H20O12 | 5169-21-5 | 93 | 5.72 |
| 41 | Quercetin | Flavonoid | C15H10O7 | 117-39-5 | 89.7 | 5.76 |
| 42 | (*E*)-5-(1,2,4a,5-tetramethyl-7-oxo-3,4,8,8a-tetrahydro-2H-naphthalen-1-yl)-3-methylpent-2-enoic acid | Organic acid | C20H30O3 | - | 59 | 10.20 |
| 43 | Piperidine | Alicyclic amine | C5H11N | 110-89-4 | 61.2 | 1.03 |
| 44 | Quercetin-3,4'-O-di-beta-glucoside | Flavonoid glycoside | C27H30O17 | 29125-80-2 | 82.5 | 5.23 |
| 45 | PC(16:0/0:0) | Phosphatidylcholine | C24H50NO7P | 17364-16-8 | 87 | 11.24 |
| 46 | Protocatechuic acid | Phenolic acid | C7H6O4 | 99-50-3 | 91.8 | 3.66 |
| 47 | Isorhamnetin-3-galactoside | Flavonoid glycoside | C22H22O12 | 6743-92-6 | 93.1 | 6.23 |
| 48 | N-Methylthreonine | Amino acid derivative | C5H11NO3 | 2634-33-3 | 70.5 | 0.81 |
| 49 | Kaempferol 3-O-gentiobioside | Flavonoid glycoside | C27H30O16 | 22149-35-5 | 94.6 | 5.47 |
| 50 | Malate | Organic acid | C4H6O5 | 96-01-1 | 79.3 | 0.91 |
| 51 | Rutin | Flavonoid glycoside | C27H30O16 | 153-18-4 | 94.6 | 5.57 |
| 52 | N-acetylphenylalanine | Amino acid derivative | C11H13NO3 | 156-88-1 | 74.9 | 5.91 |
| 53 | Kaempferol | Flavonoid | C15H10O6 | 520-18-3 | 90.4 | 5.47 |
| 54 | N-Acetyl-leucine | Amino acid derivative | C8H15NO3 | 1188-21-2 | 75.8 | 5.47 |
| 55 | Azelaic acid | Dicarboxylic acid | C9H16O4 | 123-99-9 | 72.9 | 6.48 |
| 56 | *D*-(-)-Gulono-gamma-lactone | Hexonic acid lactone | C6H10O6 | 90-80-2 | 59.6 | 0.86 |
| 57 | Phthalic acid | Organic acid | C8H6O4 | 88-99-3 | 68.2 | 5.40 |
| 58 | Isorhamnetin-3-O-glucoside | Flavonoid glycoside | C22H22O12 | 5041-82-7 | 60.4 | 6.21 |
| 59 | Isoeugenol | Phenolic compound | C10H12O2 | 93-28-7 | 75.6 | 7.06 |
| 60 | 3,5-Di-O-caffeoylquinic acid | Hydroxycinnamic acid ester | C25H24O12 | 89919-62-0 | 82.3 | 6.07 |
| 61 | Esculetin | Coumarin. | C9H6O4 | 92-10-6 | 64.9 | 5.09 |
| 62 | γ-Aminobutyric acid | Amino acid | C4H9NO2 | 56-12-2 | 55.4 | 0.81 |
| 63 | Guanine | Purine base | C5H5N5O | 73-40-5 | 73.3 | 1.34 |
| 64 | 2-Aminoacetophenone | Aromatic ketone | C8H9NO | 551-87-9 | 66 | 3.63 |
| 65 | 5-O-Methylbiochanin A | Isoflavone | C17H14O5 | 34086-51-6 | 64.9 | 7.02 |
| 66 | Glu Arg Tyr | Amino acid mixture | C20H30N6O7 | - | 74.9 | 8.16 |
| 67 | Val Tyr | Amino acid dipeptide | C14H20N2O4 | 72-18-4 | 50.8 | 1.65 |
| 68 | 4-(4-benzyl-2,3-dioxopiperazin-1-yl)-N-(2,5-dimethoxyphenyl)piperidine-1-carboxamide | Heterocyclic compound | C25H30N4O5 | 39178-60-4 | 69.4 | 7.81 |
| 69 | Xanthosine | Purine nucleoside | C10H12N4O6 | 146-80-5 | 76.7 | 1.57 |
| 70 | Diethyloxalpropionate | Beta-lactone | C9H14O5 | 10601-80-6 | 53.7 | 4.76 |
| 71 | 13*S*-Hydroperoxy-9*Z*,11*E*,15*Z*-octadecatrienoic acid | Fatty acid | C18H30O4 | 67597-26-6 | 69.2 | 10.87 |
| 72 | Pantothenic acid | Vitamin (B5) | C9H17NO5 | 83-89-6 | 80.2 | 2.52 |
| 73 | Cynaroside | Flavonoid glycoside | C21H20O11 | 520-27-4 | 98.5 | 6.17 |
| 74 | 2,6-Dihydroxynaphthalene | Aromatic compound | C10H8O2 | 575-25-9 | 62.5 | 4.62 |
| 75 | Irigenol | Flavonoid | C15H10O8 | - | 63.2 | 6.13 |
| 76 | Curcumenol | Sesquiterpenoid | C15H22O2 | 19431-84-6 | 80.2 | 8.58 |
| 77 | 9-Hydroxy-10,12-octadecadienoic acid | Fatty acid | C18H32O4 | 73543-67-6 | 89.5 | 9.77 |
| 78 | Flavin mononucleotide | Flavin | C17H20N4O6 | 146-78-7 | 94 | 5.05 |
| 79 | Centaureidin | Flavonoid | C18H16O8 | 17313-52-9 | 94.7 | 7.09 |
| 80 | 2'-O-Methyladenosine | Nucleoside | C11H15N5O4 | 2438-59-5 | 88.1 | 2.58 |
| 81 | Caffeic acid | Phenolic acid | C9H8O4 | 1732-08-1 | 82 | 4.21 |
| 82 | Guanosine | Nucleoside | C10H13N5O5 | 118-00-3 | 84.2 | 1.03 |
| 83 | Phenylpyruvic acid | Keto acid | C9H8O3 | 156-06-1 | 51.7 | 6.11 |
| 84 | 4-(3,4-Dihydroxyphenyl)-7-hydroxy-2-oxo-2H-chromen-5-yl 6-O-*D*-xylopyranosyl-beta-*D*-glucopyranoside | Flavonoid glycoside | C26H28O15 | - | 58.8 | 5.10 |
| 85 | Tricetin | Flavonol | C15H10O7 | 529-44-8 | 68.6 | 7.27 |
| 86 | N,N-Dimethyldodecylamine N-oxide | Amine oxide | C14H31NO | 1643-20-5 | 70.4 | 7.92 |
| 87 | Cumic alcohol | Phenolic compound | C10H14O | 536-60-7 | 77.3 | 6.43 |
| 88 | 4(15)-Selinene-11,12-diol | Sesquiterpene | C15H26O2 | - | 53.2 | 6.74 |
| 89 | Luteolin 4'-glucoside | Flavonoid glycoside | C21H20O11 | 6920-38-3 | 95.4 | 5.47 |
| 90 | Syringic acid | Phenolic acid | C9H10O5 | 530-57-4 | 92.1 | 3.67 |
| 91 | N-Acetyl-proline | Amino acid derivative | C7H11NO3 | 68-95-1 | 61.6 | 2.27 |
| 92 | Vanillin | Organic compound | C8H8O3 | 121-33-5 | 87.7 | 5.85 |
| 93 | *L*-Tyrosine | Amino acid | C9H11NO3 | 60-18-4 | 71.9 | 1.03 |
| 94 | 9-Oxo-10*E*,12*Z*-octadecadienoic acid | Fatty acid | C18H30O3 | 54232-59-6 | 71.3 | 11.69 |
| 95 | Feruloyl allylamine | Amide | C13H15NO3 | 66648-44-0 | 72.1 | 4.98 |
| 96 | PE(18:2/0:0) | Phosphatidylethanolamine | C23H44NO7P | 89576-29-4 | 91.7 | 10.75 |
| 97 | Malonyltryptophan | Amino acid derivative | C14H14N2O5 | 29399-11-9 | 51.8 | 6.33 |
| 98 | *L*-Pyroglutamic acid | Amino acid | C5H7NO3 | 372-58-9 | 72.8 | 1.19 |
| 99 | Indole-3-acetamide | Indole derivative | C10H10N2O | 578-54-1 | 74 | 3.63 |
| 100 | Cytidine | Nucleoside | C9H13N3O5 | 65-46-3 | 95.6 | 0.82 |
| 101 | P-Hydroxybenzoic acid | Benzoic acid | C7H6O3 | 99-96-7 | 85.7 | 6.69 |
| 102 | 2-Hydroxy-3,4-Dimethoxybenzoic Acid | Phenolic acid | C9H10O5 | 5653-46-3 | 83.6 | 3.94 |
| 103 | Olivil 4'-O-Glucoside | Flavonoid glycoside | C26H34O12 | 76880-93-8 | 71.9 | 5.65 |
| 104 | *(R)*-2-Hydroxycaprylic acid | Fatty acid | C8H16O3 | 2835-39-4 | 55.6 | 6.53 |
| 105 | Vanillic acid | Phenolic acid | C8H8O4 | 121-34-6 | 80.5 | 5.10 |
| 106 | 4-Methylcoumarin | Coumarin | C10H8O2 | 5839-66-5 | 69 | 8.92 |
| 107 | Costunolide | Sesquiterpene lactone | C15H20O2 | 553-21-9 | 63.6 | 7.60 |
| 108 | 4-Hydroxy-3,5-dimethoxybenzyl -D-glucopyranoside | Glycoside | C15H22O9 | 530-56-3 | 84.1 | 3.46 |
| 109 | Kaempferol 3-glucuronoside | Flavonoid glycoside | C21H18O12 | 22688-78-4 | 89.5 | 6.30 |
| 110 | Cordycepin | Nucleoside | C10H13N5O3 | 73-03-0 | 73.8 | 1.53 |
| 111 | Quercetin 3-(6-O-acetyl-beta-glucoside) | Flavonoid glycoside | C23H22O13 | - | 87.5 | 5.69 |
| 112 | Cyanidin 3-(6''-acetylglucoside) | Anthocyanin | C23H22O12 | 7084-24-4 | 60.4 | 5.01 |
| 113 | Sinapaldehyde | Aldehyde | C11H12O4 | 104-54-1 | 77.2 | 5.61 |
| 114 | Dipteryxin | Flavonoid | C17H14O6 | - | 55.8 | 6.60 |
| 115 | Lactarorufin B | Flavonoid | C15H22O5 | 52483-05-3 | 63.2 | 5.23 |
| 116 | 4-Hydroxybenzaldehyde | Aromatic aldehyde | C7H6O2 | 123-08-0 | 60.1 | 1.03 |
| 117 | Perilla alcohol | Terpene alcohol | C10H16O | 536-59-4 | 61.9 | 6.40 |
| 118 | Scutellarein | Flavonoid | C15H10O6 | 529-52-2 | 50.1 | 4.83 |
| 119 | 1,3,5-Trihydroxybenzene | Aromatic compound | C6H6O3 | 108-61-2 | 59.5 | 1.36 |
| 120 | Esculin | Glycosyl compounds | C15H16O9 | 5321-75-9 | 81.9 |  |
| 121 | N-methyl-N-(2-(pyridin-2-yl)ethyl)-2-(2,3,5-trimethyl-7-oxo-7H-furo[3,2-g]chromen-6-yl)acetamide | Acetamide derivative | C24H24N2O4 | 942195-80-4 | 61.5 | 5.14 |
| 122 | PE(18:3/0:0) | Phosphatidylethanolamine | C23H42NO7P | 67270-42-2 | 91.5 | 10.14 |
| 123 | Syringaldehyde | Aldehyde | C9H10O4 | 536-36-1 | 83.1 | 5.98 |
| 124 | Swainsonine | Indolizidine alkaloid | C8H15NO3 | 21675-39-6 | 60.4 | 0.85 |
| 125 | Dehydroascorbic acid | Vitamin C derivative | C6H6O6 | 490-85-5 | 51.2 | 0.88 |
| 126 | (+)-Abscisic acid | Plant hormone | C15H20O4 | 21293-29-8 | 73 | 7.16 |
| 127 | GPSer(22:6/20:3) | Glycerophosphoserine | C48H76NO10P | - | 81 | 14.81 |
| 128 | Pyrocatechol | Aromatic compound | C6H6O2 | 120-80-9 | 65.9 | 3.65 |
| 129 | Jaceosidin | Flavonoid | C17H14O7 | 18085-97-7 | 92.2 | 6.60 |
| 130 | Leu Glu Val | Amino acid tripeptide | C16H29N3O6 | 61-90-5 | 51 | 4.60 |
| 131 | (2*E*,4*E*)-12-hydroxy-13-(hydroxymethyl)-3,5,7-trimethyltetradeca-2,4-dienedioic acid | Organic acid | C18H30O6 | - | 61.1 | 8.13 |
| 132 | 3',5'-cyclic GMP | Cyclic nucleotide | C10H12N5O7P | 58-63-9 | 73 | 1.90 |
| 133 | Myricetin | Flavonol | C15H10O8 | 529-44-8 | 71.9 | 6.15 |
| 134 | Isoferulic Acid | Organic acid | C10H10O4 | 537-73-5 | 57.4 | 5.84 |
| 135 | Leu Pro | Amino acid dipeptide | C11H20N2O3 | 61-90-5 | 60.6 | 3.81 |
| 136 | 4-Hydroxy-3,5-dimethoxybenzaldehyde | Organic compound | C9H10O4 | 136-62-7 | 65.9 | 5.98 |
| 137 | 1-Hydroxy-4(15),11(13)-eudesmadien-12,6-olide | Sesquiterpenoid | C15H20O3 | - | 55.9 | 8.27 |
| 138 | Thr Arg Tyr | Amino acid mixture. | C19H30N6O6 | 114495-97-5 | 59.1 | 6.66 |
| 139 | Honokiol | Lignan | C18H18O2 | 35156-17-1 | 59.1 | 5.27 |
| 140 | Nordihydroguaiaretic acid | Lignan | C18H22O4 | 500-38-9 | 53.3 | 10.79 |
| 141 | N-Acetyl-*D*-Glucosamine | Amino sugar | C8H15NO6 | 7512-17-6 | 80.5 | 0.83 |
| 142 | PC(18:1/0:0) | Phosphatidylcholine | C26H52NO7P | 17420-57-6 | 82.4 | 11.58 |
| 143 | Indoleacetic acid | Auxin (Plant hormone) | C10H9NO2 | 87-51-4 | 50.5 | 5.99 |
| 144 | PC(15:1/0:0) | Phosphatidylcholine | C23H46NO7P | 3355-27-9 | 71.1 | 10.15 |
| 145 | Glucodistylin | Flavonoid | C21H22O12 | 27297-45-6 | 50.3 | 4.31 |
| 146 | [4-(4-chlorophenyl)piperazin-1-yl]-(5,6,7,8-tetrahydroimidazo[1,2-a]pyridin-2-yl)methanone | Heterocyclic compound | C18H21ClN4O | - | 52.3 | 6.31 |
| 147 | Leu Val Leu | Peptide | C17H33N3O4 | 13588-95-9 | 59.3 | 5.16 |
| 148 | Isorhamnetin | Flavonoid | C16H12O7 | 480-19-3 | 90.3 | 8.00 |
| 149 | Phe Pro | Amino acid dipeptide | C14H18N2O3 | 63-91-2 | 61.4 | 4.74 |
| 150 | Cytosine | Pyrimidine base | C4H5N3O | 71-30-7 | 67.4 | 0.82 |
| 151 | 1,2,4-Trideoxy-3-C-methyl-4-{[(2*E*,4*E*)-2-methyl-2,4-hexadienoyl]amino}pentitol | Amino sugar derivative | C13H23NO3 | - | 67.3 | 5.76 |
| 152 | 4-Guanidinobutanoic acid | Amino acid derivative | C5H11N3O2 | 463-00-3 | 59.8 | 0.84 |
| 153 | Tyr Leu | Amino acid dipeptide | C15H22N2O4 | 60-18-4 | 56.9 | 4.32 |
| 154 | 4-Oxododecanedioic acid | Dicarboxylic acid | C12H20O5 | 2421-62-7 | 79.9 | 6.44 |
| 155 | Kynurenic acid | Amino acid metabolite | C10H7NO3 | 327-65-6 | 52.2 | 5.10 |
| 156 | Tulipalin A | Sesquiterpene lactone | C5H6O2 | 547-65-9 | 86.1 | 0.84 |
| 157 | Hemiphloin | Lignan | C21H22O10 | 71963-94-5 | 95.3 | 5.50 |
| 158 | Gentiobiose | Disaccharide | C12H22O11 | 585-86-4 | 55.3 | 0.82 |
| 159 | Sphinganine | Sphingolipid | C18H39NO2 | 10357-83-2 | 67.7 | 8.71 |
| 160 | Gamma-Glutamylleucine | Amino acid dipeptide | C11H20N2O5 | 2566-39-4 | 62.1 | 4.23 |
| 161 | PC(14:0/0:0) | Phosphatidylcholine | C22H46NO7P | 20559-16-4 | 77.1 | 10.04 |
| 162 | 3-O-Methylquercetin | Flavonoid | C16H12O7 | 1486-70-0 | 87.3 | 7.49 |
| 163 | 2',4',6'-Trihydroxydihydrochalcone | Flavonoid | C15H14O4 | 1088-08-0 | 73.3 | 8.55 |
| 164 | Caryophyllene epoxide | Sesquiterpene | C15H24O | 1139-30-6 | 65.6 | 8.37 |
| 165 | N-[4-(dimethylsulfamoyl)phenyl]-2-(4-fluorophenyl)acetamide | Amide | C16H17FN2O3S | 692762-37-1 | 58.2 | 4.70 |
| 166 | N-cyclohexyl-4-[4-(1,2-dihydroacenaphthylen-3-ylsulfonyl)piperazin-1-yl]-6-methylpyrimidin-2-amine | Heterocyclic compound | C27H33N5O2S | - | 58.1 | 7.32 |
| 167 | Val Thr Leu | Amino acid tripeptide | C15H29N3O5 | 72-18-4 | 57.8 | 4.41 |
| 168 | Val Leu Phe | Tripeptide | C20H31N3O4 | 3918-90-9 | 63.9 | 5.40 |
| 169 | Phenethylamine | Aromatic amine | C8H11N | 64-04-0 | 65.6 | 2.36 |
| 170 | *(E)*-Cinnamic acid | Aromatic acid | C9H8O2 | 104-55-2 | 64.9 | 4.74 |
| 171 | Altrenogest | Progestin | C21H26O2 | 96569-55-8 | 65.9 | 9.23 |
| 172 | 2-Hexenal | Aldehyde | C6H10O | 6728-26-3 | 53.4 | 6.22 |
| 173 | Gln Ile | Amino acid dipeptide | C11H21N3O4 | 56-85-9 | 69.5 | 1.69 |
| 174 | Acetyl-Valine | Amino acid derivative | C7H13NO3 | 96-81-1 | 54.9 | 0.84 |
| 175 | 6-Methylcoumarin | Coumarin | C10H8O2 | 92-48-8 | 58.9 | 5.95 |
| 176 | Ser Val Leu | Amino acid tripeptide | C14H27N3O5 | 56-45-1 | 55 | 4.46 |
| 177 | 9-Oxo-12,13-Epoxy-10-Octadecenoic acid | Fatty acid | C18H30O4 | 79741-28-9 | 88 | 10.61 |
| 178 | N-Cyclohexyl-2-benzothiazol-amine | Heterocyclic compound | C13H16N2S | 28291-75-0 | 80 | 9.87 |
| 179 | α-guaiaconic acid | Organic acid | C20H20O5 | 526-75-0 | 73.3 | 6.92 |
| 180 | 3-O-Feruloylquinic acid | Hydroxycinnamic acid derivative | C17H20O9 | 1899-29-2 | 76.9 | 5.39 |
| 181 | Inosine | Nucleoside | C10H12N4O5 | 58-63-9 | 66.2 | 1.34 |
| 182 | Indole-3-acetyl-L-leucine | Amino acid derivative | C16H20N2O3 | 36838-63-8 | 55.4 | 5.89 |
| 183 | PE(16:0/0:0) | Phosphatidylethanolamine | C21H44NO7P | 53862-35-4 | 89.4 | 11.16 |
| 184 | 3'-AMP | Nucleotide | C10H14N5O7P | 360-95-6 | 71.7 | 0.89 |
| 185 | 9*S*-Hydroperoxy-10*E*,12*Z*,15*Z*-octadecatrienoic acid | Fatty acid derivative | C18H30O4 | 89886-42-0 | 59.8 | 8.57 |
| 186 | Coniferaldehyde | Organic acid | C10H10O3 | 530-57-4 | 91.4 | 5.53 |
| 187 | Isodemethylwedelolactone | Lactone | C15H8O7 | 350681-33-3 | 70.2 | 5.76 |
| 188 | Alpha-Calacorene | Sesquiterpene | C15H20 | 21391-99-1 | 63.1 | 8.85 |
| 189 | Naringenin 5-O-beta-D-glucopyranoside | Flavonoid glycoside | C21H22O10 | 19253-00-0 | 74.8 | 5.56 |
| 190 | Quinic acid | Organic acid | C7H12O6 | 77-90-1 | 79.9 | 0.91 |
| 191 | 2,4-Dichlorophenoxyacetic acid | Herbicide | C8H6Cl2O3 | 94-75-7 | 91.2 | 8.80 |
| 192 | Val Asn Ile | Amino acid tripeptide | C15H28N4O5 | 72-18-4 | 51.5 | 4.40 |
| 193 | P-Synephrine | Alkaloid | C9H13NO2 | 94-07-5 | 62.1 | 6.55 |
| 194 | 1-(4-oxo-4h-chromen-3-yl)-2,3,4,9-tetrahydro-1h-beta-carboline-3-carboxylic acid | Beta-carboline derivative | C21H16N2O4 | - | 59.8 | 6.39 |
| 195 | Muurolladie-3-One | Sesquiterpene | C15H22O | 3481-69-4 | 57.3 | 11.53 |
| 196 | Cinnamaldehyde | Aldehyde | C9H8O | 104-55-2 | 57.1 | 5.46 |
| 197 | Leu Val Val | Amino acid tripeptide | C16H31N3O4 | 61-90-5 | 52.3 | 4.78 |
| 198 | Ile Asn Ile | Amino acid tripeptide | C16H30N4O5 | 73-32-5 | 65.3 | 4.94 |
| 199 | 7-oxodehydroabietic acid | Organic acid | C20H26O3 | 18684-55-4 | 57.9 | 11.22 |
| 200 | 9,10-Dihydroxy-12*Z*-octadecenoic acid | Fatty acid | C18H34O4 | 263399-34-4 | 81.3 | 10.95 |
| 201 | *(5R)*-trans-1,7-diphenyl-5-hydroxy-6-hepten-3-one | Phenylheptanoid | C19H20O2 | - | 85.8 | 5.71 |
| 202 | N2,N2-Dimethylguanosine | Nucleoside | C12H17N5O5 | 2140-67-2 | 83.7 | 3.60 |
| 203 | Alanine | Amino acid | C3H7NO2 | 56-41-7 | 55.7 | 0.81 |
| 204 | Celastrol | Quinone | C29H38O4 | 35661-16-2 | 77.5 | 10.60 |
| 205 | PC(15:0/0:0) | Phosphatidylcholine | C23H48NO7P | 25037-45-0 | 64.5 | 10.61 |
| 206 | Skimmin | Coumarin | C15H16O8 | 93-39-0 | 53.6 | 5.18 |
| 207 | Asp Val Leu | Amino acid tripeptide | C15H27N3O6 | 56-84-8 | 68 | 4.87 |
| 208 | Ethyl syringate | Ester | C11H14O5 | 3943-80-4 | 51.2 | 5.22 |
| 209 | Ile Tyr | Amino acid dipeptide | C15H22N2O4 | 73-32-5 | 62.3 | 2.93 |
| 210 | 6-Methoxyluteolin | Flavonoid | C16H12O7 | 520-11-6 | 59.4 | 7.50 |
| 211 | 15,16-Dihydrotanshinone I | Quinone | C18H14O3 | 87205-99-0 | 54.3 | 6.82 |
| 212 | 7-Acetoxy-2-methylisoflavone | Isoflavone | C18H14O4 | 3211-63-0 | 51.8 | 7.17 |
| 213 | 2,6-dihydroxy-7-methoxy-1,1,4a-trimethyl-3,4,10,10a-tetrahydro-2H-phenanthren-9-one | Phenanthrenone | C18H24O4 | - | 61.6 | 7.83 |
| 214 | Atractylenolide III | Sesquiterpene lactone | C15H20O3 | 73030-71-4 | 75.3 | 10.53 |
| 215 | Uridine 5'-monophosphate | Nucleotide | C9H13N2O9P | 58-97-9 | 71 | 0.86 |
| 216 | Gly Phe | Amino acid dipeptide | C11H14N2O3 | 56-40-6 | 50.7 | 2.63 |
| 217 | Biotin | Vitamin | C10H16N2O3S | 58-85-5 | 60.8 | 5.17 |
| 218 | Jaceidin | Flavonoid | C18H16O8 | 10173-01-0 | 91.7 | 7.35 |
| 219 | 3-Hydroxymandelic acid | Phenolic acid | C8H8O4 | 501-52-0 | 65.2 | 3.18 |
| 220 | IAA-Val | Auxin-amino acid conjugate | C15H18N2O3 | 87-51-4 | 80.5 | 5.45 |
| 221 | 2,2'-(3-Methylcyclohexane-1,1-diyl)diacetic acid | Dicarboxylic acid | C11H18O4 | 5345-12-0 | 58.9 | 7.55 |
| 222 | Rhamnetin | Flavonoid | C16H12O7 | 90-19-7 | 57.1 | 7.99 |
| 223 | 6-Methoxy-4-methylcoumarin | Coumarin | C11H10O3 | 2198-59-2 | 59.4 | 6.09 |
| 224 | 3,7-Di-O-methylquercetin | Flavonoid | C17H14O7 | 2068-02-2 | 68.7 | 7.91 |
| 225 | Jasmonic acid | Plant hormone | C12H18O3 | 112-26-5 | 61.5 | 8.67 |
| 226 | Gln Val Leu | Amino acid tripeptide | C16H30N4O5 | 56-85-9 | 67.2 | 4.34 |
| 227 | Melilotoside | Flavonoid glycoside | C15H18O8 | 618-67-7 | 74.5 | 4.26 |
| 228 | Gardenin B | Flavonoid | C19H18O7 | 2798-20-1 | 78.4 | 10.80 |
| 229 | Tyr Asp Ile | Tripeptide | C19H27N3O7 | 60-18-4 | 52.6 | 5.05 |
| 230 | Acetyl-Tyrosine | Amino acid derivative | C11H13NO4 | 556-03-6 | 60.2 | 4.38 |
| 231 | 3'-O-Methylguanosine | Nucleoside | C11H15N5O5 | 10300-27-3 | 64.5 | 1.92 |
| 232 | Scoparone | Quinoline | C11H10O4 | 512-24-1 | 53.1 | 7.37 |
| 233 | 2-Hyroxybiphenyl | Biphenyl | C12H10O | 90-43-7 | 73.3 | 10.08 |
| 234 | Indole-3-acetyl-L-phenylalanine | Amino acid derivative | C19H18N2O3 | 57105-50-7 | 50.9 | 6.43 |
| 235 | 14-Deoxyandrographolide | Diterpenoid | C20H30O4 | 4176-97-0 | 58.9 | 9.80 |
| 236 | N-Acetyl-L-glutamic acid | Amino acid derivative | C7H11NO5 | 1188-37-4 | 74.6 | 1.03 |
| 237 | Arecoline hydrobromide | Alkaloid | C8H14BrNO2 | 63-76-1 | 53.3 | 15.03 |
| 238 | N-Acetyl-tryptophan | Amino acid derivative | C13H14N2O3 | 2525-71-7 | 84 | 6.14 |
| 239 | 5*(S)*-HpEPE | Eicosapentaenoic acid derivative | C20H30O4 | 143292-98-2 | 59 | 8.13 |
| 240 | Glutamylleucine | Dipeptide | C11H20N2O5 | 2566-39-4 | 50.2 | 5.19 |
| 241 | Hydroxykynurenine | Tryptophan metabolite | C10H12N2O4 | 484-78-6 | 61.3 | 4.67 |
| 242 | Glu Phe | Amino acid dipeptide | C14H18N2O5 | 56-86-0 | 55 | 3.55 |
| 243 | O-Methylbenzhydrol | Phenol | C14H14O | 5472-13-9 | 75 | 11.49 |
| 244 | 4-(butan-2-yl)phenyl 2-(acetylamino)-2-deoxy-beta-D-glucopyranoside | Glycoside | C18H27NO6 | - | 85.4 | 6.75 |
| 245 | 4-(4-chlorophenoxy)-N-[5-methyl-4-(4-methylphenyl)-1,3-thiazol-2-yl]butanamide | Amide | C21H21ClN2O2S | - | 50.5 | 4.70 |
| 246 | *(S)*-α-Amino-beta-phenylpropionicacid | Amino acid | C9H11NO2 | 156-07-4 | 62.4 | 1.89 |
| 247 | Campestrinoside | Steroid glycoside | C20H24O10 | 84458-87-7 | 73.8 | 8.26 |
| 248 | Threonine | Amino acid | C4H9NO3 | 72-19-5 | 55.4 | 0.77 |
| 249 | 5,7,3',4'-Tetrahydroxy-6,8-dimethoxyflavone | Flavonoid | C17H14O8 | 57093-50-2 | 90.3 | 7.55 |
| 250 | 4-Methylumbelliferone | Coumarin | C10H8O3 | 92-49-7 | 54 | 8.18 |
| 251 | Pinoresinol | Lignan | C20H22O6 | 526-42-5 | 68 | 6.49 |
| 252 | Trifluoromethanesulfonic acid | Sulfonic acid | CHF3O3S | 1493-13-6 | 51.4 | 4.78 |
| 253 | Asp Ile Ile | Tripeptide | C16H29N3O6 | 121377-67-1 | 66.8 | 5.53 |
| 254 | NAlpha-Acetyl-L-glutamine | Amino acid derivative | C7H12N2O4 | 1188-37-4 | 60.2 | 0.90 |
| 255 | 7,8-Dihydroxycoumarin | Coumarin | C9H6O4 | 119-84-6 | 57.1 | 1.07 |
| 256 | N6-Methyladenosine | Nucleoside | C11H15N5O4 | 2004-33-3 | 79.8 | 3.74 |
| 257 | Gallic acid | Organic acid | C7H6O5 | 149-91-7 | 68.7 | 12.78 |
| 258 | Clemaphenol A | Flavonoid | C20H22O6 | 83-45-4 | 57.1 | 4.59 |
| 259 | Gentiopicroside | Iridoid glycoside | C16H20O9 | 536-47-9 | 52.3 | 5.60 |
| 260 | 1-Methylpseudouridine | Nucleoside | C10H14N2O6 | 13860-38-3 | 58.6 | 1.54 |
| 261 | Methoxyeugenol | Phenolic compound | C11H14O3 | 93-28-7 | 53.1 | 7.01 |
| 262 | 7-O-Prenylscopoletin | Flavonoid | C15H16O4 | 13544-37-1 | 52.2 | 8.31 |
| 263 | 9-(2,3-Dihydroxypropoxy)-9-oxononanoic acid | Organic acid | C12H22O6 | 109421-77-4 | 77.1 | 6.59 |
| 264 | Ile Leu Glu | Amino acid tripeptide | C17H31N3O6 | 73-32-5 | 67.5 | 4.17 |
| 265 | ferulic acid | Phenolic acid | C10H10O4 | 537-93-3 | 73.7 | 8.08 |
| 266 | (2-methoxyphenyl)-[2-(5-methyl-1,2-oxazol-3-yl)pyrrolidin-1-yl]methanone | Heterocyclic compound | C16H18N2O3 | - | 50.8 | 9.34 |
| 267 | Morroniside | Iridoid glycoside | C17H26O11 | 25406-64-8 | 55 | 4.74 |
| 268 | 2-Nitrophenol | Phenol | C6H5NO3 | 88-75-5 | 51.9 | 7.01 |
| 269 | L-glutamic acid | Amino acid | C5H9NO4 | 56-86-0 | 57.1 | 0.72 |
| 270 | Asp Phe | Amino acid dipeptide | C13H16N2O5 | 56-84-8 | 90.5 | 3.97 |
| 271 | Pechueloic Acid | Organic acid | C15H20O3 | 75-98-9 | 66.4 | 7.79 |
| 272 | β-Myrcene | Terpene | C10H16 | 123-35-3 | 60.1 | 7.92 |
| 273 | 13-Hydroxy-9*Z*,11*E*-octadecadienoic acid | Fatty acid | C18H32O3 | 29623-28-7 | 55.5 | 10.77 |
| 274 | MDL 72832 HCL | Phosphodiesterase inhibitor | C22H30N2O4 | 113777-40-5 | 72.1 | 9.10 |
| 275 | DL-2-Aminooctanoic acid | Amino acid | C8H17NO2 | 22328-10-7 | 50.8 | 4.47 |
| 276 | Isopsoralidin | Coumarin | C20H16O5 | 3564-61-2 | 91.5 | 8.48 |
| 277 | Glutamylphenylalanine | Amino acid dipeptide | C14H18N2O5 | 7432-24-8 | 85.6 | 4.53 |
| 278 | [3-[2-(4-fluoroanilino)pyrimidin-4-yl]piperidin-1-yl]-(5-methylthiophen-2-yl)methanone | Heterocyclic compound | C21H21FN4OS | 900449-54-9 | 77.7 | 5.81 |
| 279 | 16,16-dimethyl-PGE1 | Prostaglandin | C22H38O5 | 41692-15-3 | 63 | 11.77 |
| 280 | 4-Hydroxycinnamic acid | Organic acid | C9H8O3 | 501-98-4 | 74.4 | 5.77 |
| 281 | 1a,1b-dihomo PGF2Alpha | Prostaglandin | C22H38O5 | 57944-39-5 | 61.6 | 11.60 |
| 282 | Brevicarine | Indole alkaloid | C17H21N3 | 35706-60-4 | 52.8 | 6.38 |
| 283 | Ile Leu Thr | Amino acid tripeptide | C16H31N3O5 | 73-32-5 | 71.7 | 4.27 |
| 284 | Pro Val Val | Amino acid tripeptide | C15H27N3O4 | 2854-40-2 | 55.3 | 3.94 |
| 285 | Farnesyl acetone | Sesquiterpene | C18H30O | 1117-52-8 | 53 | 10.39 |
| 286 | 5,9-dihydroxy-5,7,7-trimethyl-4,5a,6,8,8a,9-hexahydro-1H-azuleno[5,6-c]furan-3-one | Azulene derivative | C15H22O4 | - | 56.4 | 10.10 |
| 287 | Alanylisoleucine | Amino acid derivative | C9H18N2O3 | 817204-32-3 | 51.3 | 1.79 |
| 288 | Scopoletin | Coumarin | C10H8O4 | 92-61-5 | 69.1 | 9.67 |
| 289 | Ser Leu Val | Amino acid tripeptide | C14H27N3O5 | 56-45-1 | 60.8 | 3.73 |
| 290 | 2-Indolecarboxylic acid | Amino acid derivative | C9H7NO2 | 1477-55-0 | 69.2 | 6.37 |
| 291 | Gliocladic acid | Organic acid | C14H22O4 | 82425-48-7 | 62.2 | 8.93 |
| 292 | linolenic acid | Essential fatty acid | C18H30O2 | 463-40-1 | 65.2 | 11.38 |
| 293 | N-Ethyl-N-Methylcathinone | Stimulant | C12H17NO | 2872-55-9 | 67.2 | 14.79 |
| 294 | Monoethyl phthalate | Ester | C10H10O4 | 2306-33-4 | 50.5 | 9.59 |
| 295 | L-Arginine | Amino acid | C6H14N4O2 | 74-79-3 | 59.9 | 14.87 |
| 296 | Vitexin | Flavone glycoside | C21H20O10 | 84-51-5 | 87.8 | 5.67 |
| 297 | Indolelactic acid | Indole derivative | C11H11NO3 | 1821-52-9 | 78.8 | 5.36 |
| 298 | 1-Naphthylmethanol | Phenolic compound | C11H10O | 5329-66-4 | 50.5 | 10.08 |
| 299 | Corymboside | Flavonoid glycoside | C26H28O14 | 73543-87-0 | 89.4 | 5.19 |
| 300 | 2',5'-Dihydroxy-4-methoxychalcone | Chalcone | C16H14O4 | 6342-92-3 | 55.8 | 7.53 |
| 301 | Isoorientin | Flavone | C21H20O11 | 4261-42-1 | 92.6 | 5.29 |
| 302 | 2-hydroxyhexadecanoic acid | Fatty acid | C16H32O3 | 156-33-3 | 65.7 | 13.41 |
| 303 | L-aspartic acid | Amino acid | C4H7NO4 | 56-84-8 | 54.8 | 0.71 |
| 304 | γ-Cadinene | Sesquiterpene | C15H24 | 465-15-4 | 54.3 | 12.48 |
| 305 | 3,6-Dimethoxyapigenin | Flavone | C17H14O7 | 22697-65-0 | 75.8 | 7.89 |
| 306 | Coniferyl ferulate | Phenolic compound | C20H20O6 | 63644-62-2 | 53.7 | 7.99 |
| 307 | Trans-Zeatin-o-glucoside | Cytokinin | C16H23N5O6 | 87-85-4 | 80.5 | 4.13 |
| 308 | Cl-Amidine | Heterocyclic compound | C14H19ClN4O2 | 1043444-18-3 | 71.2 | 14.78 |
| 309 | Corylin | Flavonoid | C20H16O4 | 53947-92-5 | 66 | 7.86 |
| 310 | Tiglic acid | Unsaturated fatty acid | C5H8O2 | 499-36-7 | 55.1 | 16.64 |
| 311 | 3-Isochromanone | Isochromanone | C9H8O2 | 4170-30-3 | 52.9 | 6.35 |
| 312 | 4-Pyridoxic acid | Vitamin B6 derivative | C8H9NO4 | 108-53-4 | 50.1 | 4.66 |
| 313 | Acaciin | Flavonoid. | C28H32O14 | 480-36-4 | 99.4 | 6.82 |

aNo, Substances are ranked according to their content in the whole plant of *G. parviflora*.

“-” indicates that there is no CAS for the substance.