

**S3 Table. List of identified polar metabolites of the gas chromatography coupled mass**

**spectrometry approach.** Columns show the substance, the affiliation to natural substance

classes, the mass of quantification, the corresponding retention index and the number of plant

samples per growth form in which the metabolites occur, out of a total of 164 and 140 for grass

and forb species, respectively.

| Metabolite                         | Metabolite class | Quantification mass [m/z] | Retention index [RI] | No. of grass phytometers | No. of forb phytometers |
|------------------------------------|------------------|---------------------------|----------------------|--------------------------|-------------------------|
| Pinitol (260)                      | Alcohol          | 260                       | 1868                 | 120                      | 97                      |
| scyllo-inositol (204)              | Alcohol          | 204                       | 2072                 | 107                      | 124                     |
| scyllo-inositol (305)              | Alcohol          | 305                       | 1995                 | 73                       | 64                      |
| Xylitol (307)                      | Alcohol          | 307                       | 1735                 | 82                       | 89                      |
| Arginine (256)                     | Amino acid       | 256                       | 1843                 | 7                        | 2                       |
| Asparagine (245)                   | Amino acid       | 245                       | 1697                 | 16                       | 8                       |
| beta-Alanine (248)                 | Amino acid       | 248                       | 1473                 | 105                      | 49                      |
| Glutamine (155)                    | Amino acid       | 155                       | 1485                 | 1                        | 1                       |
| Homoserine (218)                   | Amino acid       | 218                       | 1463                 | 49                       | 24                      |
| Lysine (156)                       | Amino acid       | 156                       | 1939                 | 28                       | 21                      |
| Methionine (176)                   | Amino acid       | 176                       | 1532                 | 69                       | 23                      |
| Ornithine / Citrullin (142)        | Amino acid       | 142                       | 1840                 | 85                       | 52                      |
| Tryptophan (202)                   | Amino acid       | 202                       | 2250                 | 47                       | 20                      |
| Tyrosine (218)                     | Amino acid       | 218                       | 1960                 | 116                      | 57                      |
| Digalactosylglycerol (204)         | Lipid            | 204                       | 3218                 | 143                      | 117                     |
| Octadecadienoic acid (337)         | Lipid            | 337                       | 2218                 | 71                       | 44                      |
| Octadecatrienoic acid (335)        | Lipid            | 335                       | 2230                 | 1                        | 2                       |
| sn-Glycerol-3-phosphate (357)      | Lipid            | 357                       | 1797                 | 47                       | 33                      |
| Adenine (264)                      | Nucl. base       | 264                       | 1883                 | 101                      | 77                      |
| Adenosine (236)                    | Nucl. base       | 236                       | 2679                 | 107                      | 77                      |
| 2-Aminoadipate (260)               | Organic acid     | 260                       | 1739                 | 32                       | 13                      |
| 2-Isopropylmalate (275)            | Organic acid     | 275                       | 1600                 | 7                        | 4                       |
| 3-Caffeoyl-trans-quinic acid (345) | Organic acid     | 345                       | 3166                 | 2                        | 2                       |

| Metabolite                                   | Metabolite class | Quantification mass [m/z] | Retention index [RI] | No. of grass phytometers | No. of forb phytometers |
|----------------------------------------------|------------------|---------------------------|----------------------|--------------------------|-------------------------|
| 4-Aminobutanoate [GABA] (174)                | Organic acid     | 174                       | 1543                 | 157                      | 122                     |
| Aminomalonic acid (218)                      | Organic acid     | 218                       | 1483                 | 26                       | 12                      |
| Gluconate (333)                              | Organic acid     | 333                       | 2049                 | 157                      | 137                     |
| Phosphoenol-pyruvate (247)                   | Organic acid     | 247                       | 1623                 | 62                       | 48                      |
| Ribonic_acid-gamma-lactone_like (204) RT1888 | Organic acid     | 204                       | 2784                 | 43                       | 32                      |
| Salicylic acid (267)                         | Organic acid     | 267                       | 1533                 | 11                       | 8                       |
| Shikimate (204)                              | Organic acid     | 204                       | 1841                 | 153                      | 119                     |
| Syringic acid (342)                          | Organic acid     | 342                       | 1912                 | 66                       | 33                      |
| Glucose 6-phosphate (387)                    | Sugar            | 387                       | 2393                 | 14                       | 2                       |
| Lactose (361)                                | Sugar            | 361                       | 2734                 | 48                       | 48                      |
| Melibiose (361)                              | Sugar            | 361                       | 2946                 | 140                      | 112                     |
| Myo-Inositol-1-phosphate (318)               | Sugar            | 318                       | 2487                 | 13                       | 10                      |
| Rhamnose (117)                               | Sugar            | 117                       | 1756                 | 130                      | 115                     |