**Table S1.** Untargeted metabolomics profiling of *P. triticisoli* BJ-18

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Comp. | Formula | Molecular | RT | ChemSpider | mzCloud | mzVault |
| Weight | [min] | Results | Results | Results |
| Carbohydrate and derivatives | | | | | | |
| Glyceraldehyde | C3H6O3 | 90.0316 | 1.293 | Full match | No results | No results |
| erythrose | C4H8O4 | 120.0421 | 1.289 | Full match | No results | No results |
| D-(-)-Fructose | C6H12O6 | 180.0633 | 1.221 | Not the top hit | Full match | No results |
| Sucrose | C12H22O11 | 342.11583 | 1.327 | Full match | Full match | Full match |
| Glucose 1-phosphate | C6H13O | 260.02928 | 1.18 | Not the top hit | Full match | No results |
| α-D-Glucose-1,6-bisphosphate | C6H14O12P2 | 339.99553 | 1.114 | Not the top hit | Full match | No results |
| trehalose 6-phosphate | C12H23O14P | 422.08226 | 1.18 | Full match | No results | No results |
| Amino acids and peptides | | | | | | |
| L-(+)-Alanine | C3H7NO2 | 89.04774 | 1.3 | Full match | No results | No results |
| L-(+)-Aspartic acid | C4H7NO4 | 133.03744 | 1.161 | Full match | No results | No results |
| L-(-)-Threonine | C4H9NO3 | 119.05808 | 1.303 | Full match | No results | No results |
| L-(+)-Lysine | C6H14N2O2 | 146.10544 | 1.343 | Full match | No results | No results |
| valeramide | C5H11NO | 101.08396 | 1.378 | Partial match | No results | Full match |
| D-(-)-Glutamine | C5H10N2O3 | 146.06901 | 1.248 | Full match | Full match | Full match |
| D-(+)-Proline | C5H9NO2 | 115.06307 | 8.79 | Full match | Full match | No results |
| D-(+)-Pyroglutamic Acid | C5H7NO3 | 129.04213 | 1.77 | Full match | No results | No results |
| L-Pyroglutamic acid | C5H7NO3 | 129.04213 | 1.418 | Full match | Full match | No results |
| 4-Oxoproline | C5H7NO3 | 129.04242 | 1.282 | Partial match | Full match | No results |
| Betaine | C5H11NO2 | 117.07862 | 1.324 | Partial match | Full match | No results |
| N-Acetyl-L-aspartic acid | C6H9NO5 | 175.0472 | 1.653 | Full match | No results | No results |
| D/L-Arginine | C6H14N4O2 | 174.11086 | 1.286 | Full match | Full match | No results |
| Prolylglycine | C7H12N2O3 | 172.08472 | 1.292 | Full match | No results | No results |
| N2-Acetylornithine | C7H14N2O3 | 174.10026 | 1.299 | Partial match | Full match | No results |
| L-Theanine | C7H14N2O3 | 174.0997 | 8.024 | Full match | No results | No results |
| Tyramine | C8H11NO | 137.08348 | 10.754 | Full match | No results | No results |
| Ne-Acetyllysine | C8H16N2O3 | 188.11589 | 1.295 | Full match | No results | No results |
| N2-succinyl-L-ornithine | C9H16N2O5 | 232.10571 | 1.236 | Full match | No results | No results |
| Capryloylglycine | C10H19NO3 | 201.1364 | 8.833 | No results | Full match | No results |
| Spermine | C10H26N4 | 202.2148 | 1.088 | Full match | No results | No results |
| L-Ala-Gamma-D-Glu-Meso-Diaminopimelic Acid | C15H26N4O8 | 390.175 | 1.168 | Full match | No results | No results |
| L-Saccharopine | C11H20N2O6 | 276.13191 | 1.181 | Full match | Full match | No results |
| (+/-)-pantetheine | C11H22N2O4S | 278.12997 | 7.213 | Full match | No results | No results |
| N-Acetylneuraminic acid | C11H19NO9 | 309.10585 | 1.266 | Full match | No results | No results |
| D-Sphingosine | C18H37NO2 | 299.28107 | 12.053 | No results | Full match | No results |
| Alcohols, aldehydes, ketones, fatty acids and lipids | | | | | | |
| Methylglyoxal | C3H4O2 | 72.02104 | 1.336 | Full match | No results | No results |
| D-(+)-Glyceric acid | C3H6O4 | 106.02643 | 1.22 | Full match | No results | No results |
| Succinic acid | C4H6O4 | 118.02653 | 1.232 | Full match | Full match | No results |
| 5-Aminovaleric acid | C5H11NO2 | 117.07883 | 1.379 | Partial match | Full match | No results |
| (+/-)-2-Hydroxyglutaric acid | C5H8O5 | 148.03706 | 1.219 | Full match | No results | No results |
| Aminolevulinic acid | C5H9NO3 | 131.05811 | 1.295 | Full match | No results | No results |
| 2,3-Dihydroxy-3-methyl-butanoic acid | C5H10O4 | 134.0578 | 1.29 | Full match | No results | No results |
| Hexanoic acid | C6H12O2 | 116.08368 | 7.445 | Full match | Full match | No results |
| Histidinol | C6H11N3O | 141.08962 | 1.063 | Full match | No results | No results |
| 4-Aminobenzoic acid | C7H7NO2 | 137.04714 | 1.356 | Full match | No results | No results |
| Caprylic acid | C8H16O2 | 144.11481 | 10.757 | Full match | Full match | No results |
| 8-Amino-7-oxononanoic acid | C9H17NO3 | 187.11997 | 9.62 | Full match | No results | No results |
| Decanoic acid | C10H20O2 | 172.14606 | 12.252 | Full match | Full match | No results |
| 4-Methoxycinnamaldehyde | C10H10O2 | 162.06734 | 13.257 | No results | Full match | No results |
| 3-Hydroxydecanoic acid | C10H20O3 | 188.14104 | 11.095 | No results | Full match | No results |
| Undecanoic acid | C11H22O2 | 186.16176 | 12.648 | No results | Full match | No results |
| Jasmonic acid | C12H18O3 | 210.12555 | 11.39 | No results | Full match | No results |
| 12-Hydroxydodecanoic acid | C12H24O3 | 216.17238 | 11.665 | No results | Full match | No results |
| Tridecylic acid | C13H26O2 | 214.19305 | 13.48 | No results | Full match | No results |
| 3,5-Tetradecadienoic acid | C14H24O2 | 224.17655 | 12.628 | Full match | No results | No results |
| Pentadecanoic acid | C15H30O2 | 242.22409 | 14.056 | No results | Full match | No results |
| Palmitoleic acid | C16H30O2 | 254.2242 | 14.013 | Full match | Full match | No results |
| α-Humulene | C15H24 | 204.1868 | 13.828 | No results | No results | Full match |
| (-)-Caryophyllene oxide | C15H24O | 220.18171 | 13.451 | No results | Full match | No results |
| Tetradecanedioic acid | C14H26O4 | 258.18297 | 10.665 | No results | Full match | No results |
| 7Z-heptadecenoic acid | C17H32O2 | 268.23982 | 14.283 | Full match | No results | No results |
| Margaric acid | C17H34O2 | 270.25539 | 14.519 | Full match | No results | No results |
| 16-Hydroxyhexadecanoic acid | C16H32O3 | 272.23482 | 13.802 | No results | Full match | No results |
| Diosmetin | C16H12O6 | 300.06404 | 1.119 | No results | Full match | No results |
| Elaidolinolenic acid | C18H30O2 | 278.22421 | 13.933 | Full match | No results | No results |
| Oleic acid | C18H34O2 | 282.25552 | 14.483 | Full match | Full match | No results |
| Hexadecanedioic acid | C16H30O4 | 286.21419 | 11.779 | No results | Full match | No results |
| 9-hydroxy-10,12-octadecadienoic acid | C18H32O3 | 296.235 | 13.008 | No results | No results | Full match |
| 8Z,11Z,14Z-Eicosatrienoic acid | C20H34O2 | 306.25553 | 14.385 | No results | Full match | No results |
| Arachidic acid | C20H40O2 | 312.30256 | 14.882 | No results | No results | Full match |
| 20-Oxoleukotriene B4 | C20H30O5 | 350.20881 | 13.389 | Full match | No results | No results |
| Tetrahydrocurcumin | C21H24O6 | 372.15759 | 6.929 | Full match | No results | No results |
| Deoxycholic acid | C24H40O4 | 392.29234 | 13.047 | Full match | Full match | Full match |
| Cholic acid | C24H40O5 | 408.28724 | 12.308 | Partial match | Full match | Full match |
| Glycocholic acid | C26H43NO6 | 465.30833 | 12.038 | No results | Full match | Full match |
| Dipalmitoylphosphatidic acid | C35H69O8P | 648.4723 | 15.965 | Full match | No results | No results |
| Dilauroyl phosphatidylglycerol | C30H59O10P | 610.38399 | 14.888 | Full match | No results | No results |
| Nucleic acids | | | | | | |
| Guanine | C5H5N5O | 151.04869 | 1.347 | Full match | No results | No results |
| Xanthine | C5H4N4O2 | 152.03325 | 1.302 | Full match | Full match | No results |
| Dihydrothymine | C5H8N2O2 | 128.05801 | 1.336 | Full match | No results | No results |
| 2'-Deoxycytidine | C9H13N3O4 | 227.08967 | 1.31 | Full match | No results | No results |
| Uridine | C9H12N2O6 | 244.06923 | 1.3 | Full match | Full match | Full match |
| 5-aminoimidazole ribotide | C8H14N3O7P | 295.05718 | 1.262 | Full match | No results | No results |
| Vitamins | | | | | | |
| Nicotinic acid | C6H5NO2 | 123.0316 | 1.555 | Full match | Full match | Full match |
| Nicotinamide | C6H6N2O | 122.04761 | 1.454 | Partial match | Full match | Full match |
| (+)-Dethiobiotin | C10H18N2O3 | 214.13164 | 1.324 | Full match | No results | No results |
| Biotin | C10H16N2O3S | 244.08702 | 7.932 | Full match | No results | No results |
| Biotin l-Sulfoxide | C10H16N2O4S | 260.08179 | 6.665 | Full match | No results | No results |
| Flavin mononucleotide | C17H21N4O9P | 456.10451 | 7.032 | Full match | Full match | No results |
| Riboflavin | C17H20N4O6 | 376.138 | 7.927 | Full match | Full match | Full match |
| Choline | C5H13NO | 103.09966 | 1.282 | No results | Full match | No results |
| Cyclics | | | | | | |
| 8-Hydroxyquinoline | C9H7NO | 145.05213 | 12.814 | Full match | Full match | Full match |
| 2-hydroxyquinoline | C9H7NO | 145.05264 | 8.945 | Partial match | No results | Full match |
| Indole | C8H7N | 117.05731 | 6.349 | Full match | Full match | No results |
| Skatole | C9H9N | 131.07288 | 6.356 | No results | Full match | No results |
| 6-Methylquinoline | C10H9N | 143.07289 | 7.359 | No results | Full match | No results |
| lumichrome | C12H10N4O2 | 242.07921 | 9.882 | No results | No results | Full match |
| Indirubin | C16H10N2O2 | 262.07317 | 11.351 | No results | Full match | No results |
| Coproporphyrin III | C36H38N4O8 | 654.26604 | 12.468 | Full match | No results | No results |
| Alkaloids | | | | | | |
| Trigonelline | C7H7NO2 | 137.04708 | 14.241 | Partial match | Full match | No results |
| Acetylcarnitine | C9H17NO4 | 203.11563 | 6.98 | Full match | No results | No results |
| Oxymatrine | C15H24N2O2 | 264.1825 | 11.473 | No results | Full match | No results |
| Luotonin A | C18H11N3O | 285.08891 | 12.303 | No results | Full match | No results |