Supplementary Information for

Multi-omics analysis on an agroecosystem reveals the significant role of organic nitrogen to increase agricultural crop yield

Yasunori Ichihashi, Yasuhiro Date, Amiu Shino, Tomoko Shimizu, Arisa Shibata, Kie Kumaishi, Fumiaki Funahashi, Kenji Wakayama, Kohei Yamazaki, Akio Umezawa, Takumi Sato, Makoto Kobayashi, Mayu Kamimura, Miyako Kusano, Fang-Sik Che, Keitaro Tanoi, Makoto Hayashi, Ryuhei Nakamura, Ken Shirasu, Jun Kikuchi, Naoto Nihei

Yasunori Ichihashi
Email: yasunori.ichihashi@riken.jp

Naoto Nihei
Email: anaoto@mail.ecc.u-tokyo.ac.jp

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Other supplementary materials for this manuscript include the following:

Dataset S1
Figure S1. Environmental sensor data for soil solarization (SS). (A, B) Time course of soil temperature (A) and oxidation-reduction potential (B) at a depth of 10 in SS soils.
Figure S2. Weed coverage and insect damage after seeding of *B. rapa* var. *perviridis*. (A) number of monocots weeds. (B) number of eudicots weed. (C) insect damage. SS, soil solarization; NS, non-solarization; Che, chemical fertilizer; Org, organic compost.
Figure S3. Crop yield in the 2nd year. Shoot fresh weight (kg/m²) of B. rapa var. perviridis were measured as crop yield. *P* value, calculated by the unequal variance *t*-test between SS and NS, are shown.
Figure S4. Annotation for NMR analysis. (A, B) $^1$H NMR spectra derived from one-dimensional skyline projection of two-dimensional $J$-resolved NMR measurements for soil (A) and plant (B). 1, acetic acid; 2, acetylcholine; 3, alanine; 4, asparagine; 5, aspartic acid; 6, betaine; 7, choline; 8, citric acid; 9, formic acid; 10, fructose; 11, fumaric acid; 12, GABA; 13, glucose; 14, glutamic acid; 15, glutamine; 16, glycine; 17, isoleucine; 18, lactic acid; 19, leucine; 20, malic acid; 21, methanol; 22, N-methylglycine; 23, phenylalanine; 24, proline; 25, succinic acid; 26, sucrose; 27, tyrosine; 28, valine.
Figure S5. $^1$H NMR spectra derived from one-dimensional skyline projection of two-dimensional $J$-resolved NMR measurements for soil with or without reference standards to validate the metabolic annotations of choline and acetylcholine. Red and blue dashed lines indicate the peaks derived from choline (corresponding to No. 7 in Fig. S4) and acetylcholine (corresponding to No. 2 in Fig. S4), respectively.
Figure S6. Rhizosphere that underwent SS are enriched and depleted for specific bacteria. (A, B) Enrichment and depletion of the rhizosphere bacteria at SS treatment in phylum (A) and family levels (B). The logarithms of the fold change (log FC) of individual OTU are plotted against the negative logarithm of their FDR. Negative and positive log FC values represent enrichment and depletion at SS treatment, respectively. Red dots represent differentially abundant OTUs with an FDR <0.05. Taxon in parentheses were unclassified at family level. As an outlier, phylum FCPU426 is not shown because it had an extremely high log FC (24.23) with an FDR <0.05. (C) Abundance of OTUs belonging to plant growth promoting rhizobacteria, such as the genera Paenibacillus and Pseudomonas. P values, calculated by the unequal variance t-test between SS and NS, are shown.
Figure S7. PCA of the integrated data. Principal component 1 and 2 explains 18.9% and 14.1%, respectively, of the variance. Omics data of plant phenome, plant metabolome, soil metabolome, soil ionome and rhizosphere microbiome were used. SS, soil solarization; NS, non-solarization; Che, chemical fertilizer; Org, organic compost.
Figure S8. Soil $\text{NO}_3^-\text{N}$ module. Heatmap visualization of M6 module. Soil inorganic nitrogen positively correlates with sugar content in the plant but not with plant yield.
Figure S9. Organic nitrogen affects root biomass. (A, B) Evaluation of organic nitrogen as a nitrogen source (A) and as a supplemental application (B) for plant root biomass using the *in vitro* germ-free *B. rapa* var. *perviridis* system. The growth conditions were the same with that of Figure 4A and B. \( n = 4 \) plant culture boxes (3 plants grown in each plant culture box). * and ** indicate \( P < 0.05 \) and \( P < 0.01 \), respectively, as analyzed by unequal variance t-test compared with mock and ammonium nitrate for (A) and (B), respectively.
Figure S10. Effect of choline acetate on plant growth. (A, B) Evaluation of different concentration of choline acetate for shoot biomass (A) and for root biomass (B) using the in vitro germ-free B. rapa var. perviridis system. Different letters indicate significant differences determined by one-way ANOVA followed by Tukey’s test ($P < 0.05$). $n = 5$ plant culture boxes (3 plants grown in each plant culture box). Although choline is a cation that forms various salts, we observed that choline chloride (Fig.4) and choline acetate (Fig.S10) showed similar effects on plant growth.
Figure S11. $^{13}$C-$^{13}$C coupling patterns at alanine, succinic acid, glutamine and proline derived from the dual-labelled alanine treated in the *B. rapa* var. *periridis* root. These coupling patterns are detected by $^1$H-$^{13}$C heteronuclear single quantum coherence NMR spectroscopy. The x-axis and the y-axis indicate $^1$H and $^{13}$C chemical shifts, respectively. $^{1}$J$^{13}$C values are shown by blue letter. Deducible $^{13}$C-$^{13}$C bondomers are indicated by red lines, and unconfirmed positions of $^{13}$C label are indicated by black dot.
Figure S12. Time series for $^{14}$C-Alanine images. (A-C) Photograph (upper) and autoradiograph (lower) of the *B. rapa* var. *perviridis* seedlings at 1 hour (A), 3 hours (B) and 6 hours (C) after absorbing $^{14}$C-Alanine. Scale bar beside the image indicates 1 cm.
Figure S13. PCA of NMR-based soil metabolome data. (A) Principal component 1, 2 and 3 explains 51.8%, 24.2%, and 13.3%, respectively, of the variance. SS, soil solarization; NS, non-solarization; Che, chemical fertilizer; Org, organic compost. (B) PCA loading plot of PC3 with annotations for higher contributed metabolites.
### Table S1. Abundance test comparing solarization treatments for phenotypic traits.

| Phenotypic_traits                  | Metabolite_annotation  | FDR      | log2FC(NS/S S)   |
|------------------------------------|------------------------|----------|------------------|
| shoot.dry.weight(mg)               | NA                     | 0.0078345| -0.769047004     |
| Met_Plant_ROI.P83                  | unannotated metabolite | 0.0372864| 0.440822311      |
| Met_Plant_ROI.P108                 | unannotated metabolite | 0.0412850| 0.445243908      |
| Met_Plant_ROI.P112                 | unannotated metabolite | 0.0589385| 0.283444014      |
| Met_Plant_ROI.P76                  | unannotated metabolite | 0.0652176| 0.45841855       |
| Met_Plant_ROI.P72                  | unannotated metabolite | 0.0777469| -1.054057983     |
| Met_Plant_ROI.P54                  | Fructose/Sucrose       | 0.0899222| -0.216020471     |
| K(extracted with ammonium acetate) | NA                     | 0.0922004| -0.189749174     |
| Carbon                             | NA                     | 0.0931629| 0.027454141      |
| Hydrogen                           | NA                     | 0.0940419| 0.035565303      |
| Vitamin.C(mg/100g)_shoot          | NA                     | 0.0966079| 0.242207656      |
| Met_Plant_ROI.P39                  | unannotated metabolite | 0.1144354| -0.610392641     |
| Met_Plant_ROI.P118                 | unannotated metabolite | 0.1144354| 0.486681963      |
| Met_Plant_ROI.P89                  | Fumaric acid           | 0.1257947| -0.397536944     |
| Met_Plant_ROI.P84                  | unannotated metabolite | 0.1257947| 0.525509957      |
| Met_Plant_ROI.P67                  | Sucrose                | 0.1408048| -0.380163823     |
| Taste.indexShoot                  | NA                     | 0.1408048| 0.222392421      |
| Met_Plant_ROI.P114                 | unannotated metabolite | 0.1408048| 0.501018249      |
| Met_Plant_ROI.P70                  | Sucrose                | 0.1521489| -0.413739509     |
| Met_Plant_ROI.P44                  | Methanol               | 0.1524019| -0.143784698     |
| No.of.leaves                      | NA                     | 0.1532685| -0.138873822     |
| Met_Plant_ROI.P115                 | unannotated metabolite | 0.1569596| 0.509132697      |
| Shoot.height(mm)                  | NA                     | 0.1814622| -0.09050489      |
| Feature                                    | Value          |
|--------------------------------------------|----------------|
| SPAD                                       | 0.1814622      |
| Leaf.length (mm)                           | 0.1863847      |
| Met_Plant_ROI.P75 Sucrose                  | 0.1882296      |
| Met_Plant_ROI.P80 unannotated metabolite   | 0.2008759      |
| Met_Plant_ROI.P78 unannotated metabolite   | 0.2219930      |
| Antioxidation (TE mg/100g) shoot           | 0.2744062      |
| Met_Plant_ROI.P117 unannotated metabolite  | 0.2876417      |
| Met_Plant_ROI.P91 unannotated metabolite   | 0.3113966      |
| Brix (%)_shoot                             | 0.3286469      |
| Met_Plant_ROI.P97 unannotated metabolite   | 0.3302579      |
| Met_Plant_ROI.P119 Formic acid             | 0.3353540      |
| Met_Plant_ROI.P106 unannotated metabolite  | 0.3374191      |
| Leaf.dry.weight (mg)                       | 0.3437258      |
| Met_Plant_ROI.P31 Aspartic acid            | 0.3545502      |
| Met_Plant_ROI.P86 unannotated metabolite   | 0.3613337      |
| Met_Plant_ROI.P100 unannotated metabolite  | 0.3631327      |
| Met_Plant_ROI.P87 unannotated metabolite   | 0.3869238      |
| Met_Plant_ROI.P11 Acetic acid              | 0.4044417      |
| Met_Plant_ROI.P40 Glucose                  | 0.4044417      |
| Met_Plant_ROI.P35 unannotated metabolite   | 0.4750425      |
| Met_Plant_ROI.P90 Tyrosine                 | 0.4824168      |
| Met_Plant_ROI.P81 unannotated metabolite   | 0.4851813      |
| Met_Plant_ROI.P92 unannotated metabolite   | 0.5301702      |
| Met_Plant_ROI.P107 unannotated metabolite  | 0.5377726      |
| Met_Plant_ROI.P38 Choline                  | 0.5451830      |
| Met_Plant_ROI.P85 unannotated metabolite   | 0.5451830      |
| Metabolite                             | Value    | p-value  |
|---------------------------------------|----------|----------|
| Mg (extracted with ammonium acetate)  | NA       | 0.5480575 |
| Met_Plant_ROI.P14 Proline             | 0.5480575 | 0.202538261 |
| Na (extracted with ammonium acetate)  | NA       | 0.5487526 |
| Met_Plant_ROI.P104 Phenylalanine      | 0.5487526 | -0.179735998 |
| Met_Plant_ROI.P68 Fructose            | 0.5487526 | -0.081482491 |
| Met_Plant_ROI.P101 unannotated metabolite | 0.5487526 | 0.072062458 |
| Met_Plant_ROI.P21 Malic acid          | 0.5487526 | 0.086337408 |
| Met_Plant_ROI.P94 unannotated metabolite | 0.5727481 | -0.129125733 |
| Met_Plant_ROI.P19 GABA                | 0.5745912 | 0.082682044 |
| Met_Plant_ROI.P93 unannotated metabolite | 0.5745912 | -0.039483081 |
| Met_Plant_ROI.P16 Proline             | 0.5751660 | 0.190503551 |
| Met_Plant_ROI.P13 Proline             | 0.5814373 | 0.18930558 |
| Met_Plant_ROI.P53 unannotated metabolite | 0.5881350 | -0.073407492 |
| Ca (extracted with ammonium acetate)  | NA       | 0.5981051 |
| Met_Plant_ROI.P99 unannotated metabolite | 0.6010108 | 0.056456732 |
| Met_Plant_ROI.P43 Proline             | 0.6010819 | 0.123490092 |
| Met_Plant_ROI.P12 Proline             | 0.6064216 | 0.179138468 |
| Met_Plant_ROI.P41 unannotated metabolite | 0.6088020 | 0.035722414 |
| Met_Plant_ROI.P116 unannotated metabolite | 0.6088521 | -0.075332922 |
| Met_Plant_ROI.P50 Fructose            | 0.6088521 | -0.074588916 |
| Met_Plant_ROI.P18 Glutamic acid/Glutamine | 0.6088521 | 0.064188546 |
| Brix (%) leaf                        | NA       | 0.6088521 |
| Met_Plant_ROI.P28 Aspartic acid       | 0.6088521 | 0.110323415 |
| Met_Plant_ROI.P73 Glucose            | 0.6185709 | 0.130123708 |
| Met_Plant_ROI.P25 Glutamine          | 0.6185709 | 0.069903837 |
| Met_Plant_ROI.P5 | Isoleucine | 0.6187799 | 3 | -0.124303026 |
| Met_Plant_ROI.P69 | unannotated metabolite | 0.6187799 | 3 | -0.083737409 |
| Met_Plant_ROI.P2 | Leucine | 0.6346704 | 2 | -0.153977045 |
| Met_Plant_ROI.P7 | Isoleucine | 0.6383147 | 7 | -0.126474604 |
| Met_Plant_ROI.P52 | Fructose | 0.6435283 | 6 | -0.058505194 |
| Met_Plant_ROI.P4 | Valine | 0.6449586 | 4 | -0.097896661 |
| Leaf.width(mm) | NA | 0.6512770 | 7 | 0.04231118 |
| Met_Plant_ROI.P56 | Fructose | 0.6581298 | 7 | -0.055017893 |
| Met_Plant_ROI.P23 | Glutamine | 0.6581298 | 7 | 0.058398186 |
| Met_Plant_ROI.P65 | Fructose | 0.6661231 | 7 | -0.062678123 |
| Met_Plant_ROI.P1 | Isoleucine | 0.6666031 | 9 | -0.103809448 |
| Met_Plant_ROI.P49 | Glucose | 0.6666031 | 9 | -0.056560799 |
| Met_Plant_ROI.P64 | unannotated metabolite | 0.6696464 | 9 | -0.047919796 |
| Met_Plant_ROI.P111 | unannotated metabolite | 0.6707571 | 7 | 0.089699281 |
| Met_Plant_ROI.P8 | Lactic acid | 0.6724131 | 7 | -0.062560812 |
| Met_Plant_ROI.P3 | Leucine | 0.6786996 | 4 | -0.13496833 |
| Met_Plant_ROI.P6 | Valine | 0.6786996 | 4 | -0.085782805 |
| Fv/Fm | NA | 0.6900512 | 9 | 0.007387797 |
| Met_Plant_ROI.P98 | Tyrosine | 0.6910523 | 5 | -0.133165658 |
| Met_Plant_ROI.P77 | unannotated metabolite | 0.6964519 | 2 | 0.070848292 |
| Met_Plant_ROI.P110 | unannotated metabolite | 0.7001223 | 7 | 0.051699428 |
| Met_Plant_ROI.P48 | Glucose/Sucrose | 0.7001394 | 4 | -0.049267227 |
| Met_Plant_ROI.P45 | Glucose | 0.7036121 | 1 | -0.050764195 |
| Met_Plant_ROI.P113 | unannotated metabolite | 0.7115500 | 3 | 0.04142542 |
| Met_Plant_ROI.P27 | Citric acid/Malic acid | 0.7143593 | 2 | 0.057621122 |
| Met_Plant_ROI.P96     | unannotated metabolite | 0.71573105 | -0.047568353|
|----------------------|------------------------|------------|--------------|
| Met_Plant_ROI.P22    | Succinic acid          | 0.72032237 | -0.083062569|
| Met_Plant_ROI.P66    | Fructose               | 0.72032237 | -0.046905974|
| Met_Plant_ROI.P79    | unannotated metabolite | 0.72859178 | 0.041540659  |
| Met_Plant_ROI.P51    | Fructose               | 0.73069532 | -0.04101782  |
| C/N                  | NA                     | 0.73069532 | 0.015819994  |
| Met_Plant_ROI.P15    | Glutamic acid          | 0.73069532 | 0.081592046  |
| Met_Plant_ROI.P103   | Phenylalanine          | 0.73239448 | -0.105162565|
| Met_Plant_ROI.P105   | unannotated metabolite | 0.74047178 | 0.073091751  |
| Met_Plant_ROI.P24    | Glutamine              | 0.74296177 | 0.057376021  |
| Met_Plant_ROI.P109   | unannotated metabolite | 0.76536718 | -0.048478993|
| Met_Plant_ROI.P59    | Alanine/Glutamine      | 0.76536718 | 0.039356594  |
| Nitrogen             | NA                     | 0.76954095 | 0.01060793   |
| Met_Plant_ROI.P36    | GABA                   | 0.76969746 | -0.063773927|
| Met_Plant_ROI.P26    | Citric acid            | 0.77073514 | 0.071613503  |
| Met_Plant_ROI.P32    | unannotated metabolite | 0.78569961 | 0.018313597  |
| Met_Plant_ROI.P57    | Glucose                | 0.79958918 | -0.038311226|
| Leaf.index(length/width)| NA               | 0.82125133 | 0.023925253  |
| Met_Plant_ROI.P58    | Glucose/Sucrose        | 0.83074347 | -0.038406548|
| Met_Plant_ROI.P17    | Glutamic acid/Glutamine| 0.83187516 | -0.118352873|
| Met_Plant_ROI.P10    | GABA                   | 0.83187516 | -0.054579708|
| Met_Plant_ROI.P9     | Alanine                | 0.83187516 | -0.024259867|
| Met_Plant_ROI.P29    | unannotated metabolite | 0.83187516 | 0.008758043  |
| Met_Plant_ROI.P82    | unannotated metabolite | 0.83187516 | 0.023048195  |
| Met_Plant_ROI.P34    | Asparagine             | 0.83187516 | 0.035098796  |
| Metabolite                          | Annotation              | Root.length (mm) | Leaf.area (mm^2) | Y(II)          | NO3(mg/l)_shoot | Met_Plant_ROI.P37  | Met_Plant_ROI.P63 | Met_Plant_ROI.P95 | Met_Plant_ROI.P20  | Met_Plant_ROI.P60 | Met_Plant_ROI.P30 | Met_Plant_ROI.P47  | Met_Plant_ROI.P71 | Met_Plant_ROI.P61  | Met_Plant_ROI.P74 | Met_Plant_ROI.P62 | Met_Plant_ROI.P102 | Met_Plant_ROI.P55  | Met_Plant_ROI.P88  | Met_Plant_ROI.P42  | Met_Plant_ROI.P46  | Met_Plant_ROI.P33 |
|-----------------------------------|-------------------------|------------------|-------------------|----------------|----------------|-------------------|-------------------|-------------------|--------------------|-------------------|------------------|----------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| Met_Plant_ROI.P37                 | unannotated metabolite  | 0.8334767 9      | 0.8352314 2       | NA              | 0.8505841 5     | 0.8352314 2       | 0.8352630 3       | 0.8734444 5       | 0.8734444 5       | 0.8770995 4       | 0.8781787 8       | 0.8984332 7     | 0.9095594 4       | 0.9221619 1       | 0.9221619 1       | 0.9406968 1       | 0.9695369 2       | 0.9769652 1       | 0.9896747 3       | 0.9927417 4       | 0.9975501 2       | 0.038035162       |
| Met_Plant_ROI.P63                 | Serine                  | 9                | 2                 | 3               | 0.02217731      | 0.020403847       | 0.02217731        | 0.016120712       | 0.02724843        | 0.024837433      | 0.089087894      | 0.01008473       | 0.018870885       | 0.022136964       | 0.020864994       | 0.016425877       | 0.038035162       | 0.001765466       | 0.00246927        | 0.015482944       | 0.004021218       |
| Soil_metabolite&ion     | Sampling stage | Metabolite_annotation     | FDR   | log2FC(N/S/SS)  |
|------------------------|----------------|---------------------------|-------|----------------|
| Met_Soil_Oct_ROI.OS57  | Seeding        | unannotated metabolite    | 0.001978 001 | 1.2130167 74 |
| Met_Soil_Dec_ROI.DS3   | Harvest        | Isoleucine                | 0.005571 899 | 1.1318155 55 |
| Met_Soil_Dec_ROI.DS42  | Harvest        | Valine                    | 0.009215 042 | - 0.8415328 96 |
| Met_Soil_Oct_ROI.OS56  | Seeding        | Choline                   | 0.009215 042 | 1.5134711 24 |
| Met_Soil_Dec_ROI.DS7   | Harvest        | Isoleucine                | 0.009248 302 | - 1.1641896 23 |
| Met_Soil_Dec_ROI.DS29  | Harvest        | N-Methylglycine           | 0.018302 423 | - 0.6061203 65 |
| Met_Soil_Dec_ROI.DS6   | Harvest        | Valine                    | 0.023108 774 | - 1.0947869 61 |
| Met_Soil_Dec_ROI.DS5   | Harvest        | Leucine                   | 0.026338 069 | - 0.9471578 3 |
| Met_Soil_Dec_ROI.DS4   | Harvest        | Leucine                   | 0.029677 536 | - 1.0459503 42 |
| Met_Soil_Oct_ROI.OS55  | Seeding        | unannotated metabolite    | 0.029840 799 | 1.3622903 3 |
| Met_Soil_Dec_ROI.DS28  | Harvest        | unannotated metabolite    | 0.032766 989 | 0.6516325 33 |
| Met_Soil_Dec_ROI.DS8   | Harvest        | Valine                    | 0.037286 484 | - 1.0514274 38 |
| Met_Soil_Oct_ROI.OS17  | Seeding        | unannotated metabolite    | 0.037816 763 | 1.2730838 02 |
| Met_Soil_Oct_ROI.OS59  | Seeding        | Betaine                   | 0.040792 74  | 0.8187720 58 |
| Nitrogen               | Seeding        | NA                        | 0.050971 823 | 0.1688635 13 |
| Met_Soil_Oct_ROI.OS22  | Seeding        | unannotated metabolite    | 0.050971 823 | 1.2842413 42 |
| Met_Soil_Dec_ROI.DS46  | Harvest        | Leucine                   | 0.051066 566 | - 0.9231571 97 |
| Met_Soil_Dec_ROI.DS32  | Harvest        | unannotated metabolite    | 0.056591 437 | 0.4425949 62 |
| Met_Soil_Oct_ROI.OS88  | Seeding        | Betaine                   | 0.059275 025 | 0.9227567 71 |
| Sample Name                   | Sample Type | Metabolite       | Value 1     | Value 2     |
|-------------------------------|-------------|------------------|-------------|-------------|
| Met_Soil_Oct_ROI.OS87         | Seeding     | Glucose          | 0.059275    | 1.347376    |
| Met_Soil_Dec_ROI.DS31         | Harvest     | unannotated metabolite | 0.061023    | 1.092355    |
| Met_Soil_Dec_ROI.DS41         | Harvest     | Glycine          | 0.070368    | 0.564027    |
| Met_Soil_Oct_ROI.OS86         | Seeding     | unannotated metabolite | 0.073689    | 1.285522    |
| Met_Soil_Oct_ROI.OS100        | Seeding     | Glucose          | 0.073689    | 1.319633    |
| Met_Soil_Dec_ROI.DS33         | Harvest     | unannotated metabolite | 0.074266    | 0.632594    |
| Met_Soil_Oct_ROI.OS58         | Seeding     | Glucose          | 0.074266    | 1.082330    |
| Met_Soil_Dec_ROI.DS21         | Harvest     | Alanine          | 0.074537    | 0.771963    |
| Met_Soil_Oct_ROI.OS79         | Seeding     | Glucose          | 0.074537    | 1.252812    |
| Met_Soil_Oct_ROI.OS78         | Seeding     | unannotated metabolite | 0.077746    | 1.215862    |
| Met_Soil_Oct_ROI.OS68         | Seeding     | Glucose          | 0.077746    | 1.250531    |
| Met_Soil_Oct_ROI.OS64         | Seeding     | Glucose          | 0.077746    | 1.287439    |
| Met_Soil_Oct_ROI.OS69         | Seeding     | Glucose          | 0.079703    | 1.199992    |
| Met_Soil_Oct_ROI.OS67         | Seeding     | Glucose          | 0.081915    | 1.183913    |
| Met_Soil_Oct_ROI.OS27         | Seeding     | unannotated metabolite | 0.089922    | 0.885571    |
| Met_Soil_Dec_ROI.DS19         | Harvest     | Lactic acid      | 0.091628    | 0.695188    |
| Met_Soil_Oct_ROI.OS75         | Seeding     | unannotated metabolite | 0.093118    | 1.119140    |
| K(extracted with ammonium acetate) | Seeding | NA               | 0.093162    | 0.443786    |
| Met_Soil_Oct_ROI.OS102        | Seeding     | unannotated metabolite | 0.093162    | 1.329623    |
| Met_Soil_Oct_ROI.OS66         | Seeding     | Glucose          | 0.093424    | 1.172141    |
| Met_Soil_Dec_ROI.DS44         | Harvest     | Isoleucine       | 0.095095    | 0.450465    |
| Met_Soil_Dec_ROI.DS34         | Harvest     | Choline          | 0.105986    | 0.850156    |
| Sample Name                        | Sample Type | Metabolite | C/N Value | C/N Standard Deviation | Glucose Value | Glucose Standard Deviation |
|-----------------------------------|-------------|------------|-----------|------------------------|---------------|---------------------------|
| Met_Soil_Oct_ROI.OS82             | Seeding     | Glucose    | 0.114095  | 0.078407               | 1.314220     | 0.789724                  |
| C/N                               | Seeding     | NA         | 0.116836  | 0.789724               | 0.942143     | 0.574999                  |
| Met_Soil_Oct_ROI.OS93             | Seeding     | unannotated metabolite | 0.124684  | 0.574999               | 0.693914     | 0.378511                  |
| Met_Soil_Oct_ROI.OS77             | Seeding     | unannotated metabolite | 0.182819  | 0.378511               | 0.691183     | 0.473931                  |
| Met_Soil_Oct_ROI.OS85             | Seeding     | Glucose    | 0.140804  | 0.473931               | 1.080399     | 0.789724                  |
| Met_Soil_Oct_ROI.OS65             | Seeding     | unannotated metabolite | 0.152148  | 0.789724               | 1.087751     | 0.574999                  |
| Met_Soil_Oct_ROI.OS101            | Seeding     | Glucose    | 0.166511  | 0.789724               | 1.156742     | 0.378511                  |
| Met_Soil_Dec_ROI.DS22             | Harvest     | unannotated metabolite | 0.181312  | 0.378511               | 0.831381     | 0.473931                  |
| Met_Soil_Oct_ROI.OS74             | Seeding     | unannotated metabolite | 0.208696  | 0.473931               | 0.696118     | 0.473931                  |
| Carbon                            | Seeding     | NA         | 0.232424  | 0.378511               | 0.088547     | 0.473931                  |
| Ca(extracted with ammonium acetate)| Harvest     | NA         | 0.235533  | 0.473931               | 0.097631     | 0.473931                  |
| Met_Soil_Oct_ROI.OS84             | Seeding     | unannotated metabolite | 0.254764  | 0.473931               | 1.044006     | 0.378511                  |
| Met_Soil_Oct_ROI.OS42             | Seeding     | unannotated metabolite | 0.274406  | 0.473931               | 2.109996     | 0.473931                  |
| Mn(extracted with nitric acid)    | Harvest     | NA         | 0.281999  | 0.473931               | 0.086943     | 0.473931                  |
| NH4(mg/100g)                      | Seeding     | NA         | 0.283739  | 0.473931               | 0.378511     | 0.473931                  |
| Cu(extracted with nitric acid)    | Harvest     | NA         | 0.300182  | 0.473931               | 0.072484     | 0.473931                  |
| Met_Soil_Oct_ROI.OS42             | Seeding     | unannotated metabolite | 0.311396  | 0.473931               | 0.783067     | 0.473931                  |
| Met_Soil_Oct_ROI.OS53             | Seeding     | unannotated metabolite | 0.325664  | 0.473931               | 0.410033     | 0.473931                  |
| Met_Soil_Dec_ROI.DS11             | Harvest     | unannotated metabolite | 0.328646  | 0.473931               | 0.408921     | 0.473931                  |
| NO3(mg/100g)                      | Seeding     | NA         | 0.328646  | 0.473931               | 0.473931     | 0.473931                  |
| Met_Soil_Oct_ROI.OS52             | Seeding     | N-Methylglycine | 0.337419  | 0.473931               | 0.448823     | 0.473931                  |
| Met_Soil_Oct_ROI.OS48             | Seeding     | unannotated metabolite | 0.340004  | 0.473931               | 1.157951     | 0.473931                  |
| Met_Soil_Oct_ROI.OS12             | Seeding     | unannotated metabolite | 0.352982  | 0.473931               | 0.574999     | 0.473931                  |
| Substance                        | Sample Type | Metabolite Type                | Value1   | Value2   |
|---------------------------------|-------------|--------------------------------|----------|----------|
| Cr(extracted with nitric acid)  | Harvest     | NA                             | 0.361333 | 706      |
|                                 | Seeding     | unannotated metabolite         | 0.371567 | 296      |
| Met_Soil_Oct_ROI.OS90           | Seeding     | unannotated metabolite         | 0.382234 | 954      |
| Fe(extracted with nitric acid)  | Harvest     | NA                             | 0.384851 | 29       |
| Met_Soil_Oct_ROI.OS92           | Seeding     | unannotated metabolite         | 0.386455 | 444      |
| Met_Soil_Oct_ROI.OS60           | Seeding     | unannotated metabolite         | 0.387189 | 504      |
| Met_Soil_Oct_ROI.OS30           | Seeding     | Acetic acid                    | 0.388428 | 099      |
| Met_Soil_Dec_ROI.DS9            | Harvest     | unannotated metabolite         | 0.398399 | 738      |
| Met_Soil_Dec_ROI.DS13           | Harvest     | unannotated metabolite         | 0.404441 | 763      |
| C/N                             | Harvest     | NA                             | 0.426787 | 679      |
| Met_Soil_Oct_ROI.OS51           | Seeding     | unannotated metabolite         | 0.429345 | 93       |
| Met_Soil_Oct_ROI.OS96           | Seeding     | unannotated metabolite         | 0.429345 | 93       |
| Na(extracted with ammonium acetate) | Seeding     | NA                             | 0.441143 | 664      |
| Met_Soil_Oct_ROI.OS89           | Seeding     | Serine                         | 0.443139 | 729      |
| Met_Soil_Oct_ROI.OS31           | Seeding     | unannotated metabolite         | 0.443139 | 729      |
| Met_Soil_Oct_ROI.OS23           | Seeding     | unannotated metabolite         | 0.445879 | 27       |
| Met_Soil_Oct_ROI.OS72           | Seeding     | unannotated metabolite         | 0.449129 | 721      |
| Hydrogen                        | Seeding     | NA                             | 0.451455 | 583      |
| Met_Soil_Oct_ROI.OS10           | Seeding     | unannotated metabolite         | 0.519904 | 374      |
| Met_Soil_Oct_ROI.OS91           | Seeding     | unannotated metabolite         | 0.521161 | 518      |
| Met_Soil_Oct_ROI.OS35           | Seeding     | unannotated metabolite         | 0.525542 | 791      |
| Met_Soil_Oct_ROI.OS61           | Seeding     | unannotated metabolite         | 0.527645 | 535      |

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| Sample ID                  | Type       | Description                      | Value    | P-value   |
|---------------------------|------------|----------------------------------|----------|-----------|
| Met_Soil_Oct_ROI.OS103    | Seeding    | Formic acid                      | 0.535774 | 0.5670193 |
| Met_Soil_Oct_ROI.OS49     | Seeding    | unannotated metabolite           | 0.537772 | 0.3245885 |
| S(extracted with nitric   | Harvest    | NA                               | 0.540119 | 0.0768599 |
| Met_Soil_Dec_ROI.DS14     | Harvest    | unannotated metabolite           | 0.545183 | 0.2031469 |
| Ca(extracted with nitric  | Harvest    | NA                               | 0.548752 | 0.0667608 |
| Co(extracted with nitric  | Harvest    | NA                               | 0.548752 | 0.0450401 |
| Met_Soil_Dec_ROI.DS36     | Harvest    | Betaine                          | 0.548752 | 0.2451138 |
| Met_Soil_Oct_ROI.OS62     | Seeding    | unannotated metabolite           | 0.548752 | 0.7149614 |
| Met_Soil_Oct_ROI.OS3      | Seeding    | unannotated metabolite           | 0.548752 | 0.5133214 |
| Li(extracted with nitric  | Harvest    | NA                               | 0.548752 | 0.0625988 |
| Met_Soil_Oct_ROI.OS16     | Seeding    | unannotated metabolite           | 0.548752 | 0.3742238 |
| NH4(mg/100g)              | Harvest    | NA                               | 0.571730 | 0.1468413 |
| Met_Soil_Oct_ROI.OS39     | Seeding    | unannotated metabolite           | 0.572748 | 0.5109489 |
| Met_Soil_Oct_ROI.OS34     | Seeding    | unannotated metabolite           | 0.574311 | 0.2078375 |
| Met_Soil_Dec_ROI.DS48     | Harvest    | Betaine                          | 0.577214 | 0.2278950 |
| Met_Soil_Oct_ROI.OS29     | Seeding    | unannotated metabolite           | 0.577214 | 0.2738947 |
| Met_Soil_Oct_ROI.OS50     | Seeding    | unannotated metabolite           | 0.606421 | 0.2529064 |
| Met_Soil_Oct_ROI.OS97     | Seeding    | unannotated metabolite           | 0.608802 | 0.3069465 |
| Sc(extracted with nitric  | Harvest    | NA                               | 0.608852 | 0.0318093 |
| Met_Soil_Oct_ROI.OS45     | Seeding    | unannotated metabolite           | 0.608852 | 0.2770902 |
| Met_Soil_Oct_ROI.OS99     | Seeding    | unannotated metabolite           | 0.608852 | 0.3332925 |
| Substance                        | Type     | Source/Stage | Metabolite                      | Value 1   | Value 2   |
|---------------------------------|----------|--------------|---------------------------------|-----------|-----------|
| K(extracted with nitric acid)    | Harvest  | NA           | unannotated metabolite          | 0.623099  | 0.0882800 |
| Met_Soil_Oct_ROI.OS54           | Seeding  | unannotated metabolite | 0.624465  | 0.2074181 |
| V(extracted with nitric acid)    | Harvest  | NA           | unannotated metabolite          | 0.629356  | 0.0520789 |
| Ba(extracted with nitric acid)   | Harvest  | NA           | unannotated metabolite          | 0.634670  | 0.3708393 |
| Met_Soil_Oct_ROI.OS38           | Seeding  | unannotated metabolite | 0.643528  | 0.0882800 |
| Met_Soil_Oct_ROI.OS41           | Seeding  | unannotated metabolite | 0.643528  | 0.6856005 |
| Met_Soil_Dec_ROI.DS18           | Harvest  | unannotated metabolite | 0.643811  | 0.1073452 |
| Met_Soil_Dec_ROI.DS49           | Harvest  | Serine       | 0.644958  | 0.2671518 |
| NO3(mg/100g)                    | Harvest  | NA           | unannotated metabolite          | 0.646225  | 0.2313255 |
| Met_Soil_Dec_ROI.DS27           | Harvest  | unannotated metabolite | 0.646225  | 0.1446290 |
| Met_Soil_Oct_ROI.OS81           | Seeding  | unannotated metabolite | 0.661864  | 0.4036995 |
| Met_Soil_Oct_ROI.OS28           | Seeding  | unannotated metabolite | 0.666603  | 0.1510532 |
| Met_Soil_Oct_ROI.OS11           | Seeding  | unannotated metabolite | 0.669646  | 0.1643896 |
| Met_Soil_Dec_ROI.DS15           | Harvest  | unannotated metabolite | 0.670757  | 0.1400736 |
| Met_Soil_Dec_ROI.DS17           | Harvest  | unannotated metabolite | 0.672413  | 0.0657524 |
| Met_Soil_Dec_ROI.DS23           | Harvest  | unannotated metabolite | 0.678699  | 0.1072926 |
| Ce(extracted with nitric acid)   | Harvest  | NA           | unannotated metabolite          | 0.678699  | 0.0351415 |
| Ca(extracted with ammonium acetate) | Seeding | NA           | unannotated metabolite          | 0.678699  | 0.0578274 |
| Met_Soil_Oct_ROI.OS26           | Seeding  | Alanine      | 0.678699  | 0.3270801 |
| Ti(extracted with nitric acid)   | Harvest  | NA           | unannotated metabolite          | 0.694996  | 0.0268900 |
| Met_Soil_Dec_ROI.DS30           | Harvest  | unannotated metabolite | 0.703612  | 0.1560220 |
| Sample Name                          | Process     | Metabolite                     | p1 Value | p2 Value |
|-------------------------------------|-------------|--------------------------------|----------|----------|
| Mg(extracted with ammonium acetate) | Seeding     | NA                             | 0.703612 | 0.082046 |
| Met_Soil_Dec_ROI.DS45               | Harvest     | Glucose                        | 0.703612 | 0.229023 |
| Met_Soil_Oct_ROI.OS70               | Seeding     | Glycine                        | 0.703612 | 0.384673 |
| Met_Soil_Dec_ROI.DS10               | Harvest     | unannotated metabolite         | 0.704014 | -        |
| P(extracted with nitric acid)       | Harvest     | NA                             | 0.704014 | 0.035271 |
| Met_Soil_Oct_ROI.OS44               | Seeding     | unannotated metabolite         | 0.720322 | 0.371237 |
| Met_Soil_Oct_ROI.OS25               | Seeding     | unannotated metabolite         | 0.730695 | 0.549517 |
| Met_Soil_Oct_ROI.OS105              | Seeding     | unannotated metabolite         | 0.730695 | 0.258441 |
| Met_Soil_Oct_ROI.OS106              | Seeding     | unannotated metabolite         | 0.730695 | 0.307342 |
| Met_Soil_Dec_ROI.DS20               | Harvest     | unannotated metabolite         | 0.736534 | 0.148471 |
| Met_Soil_Dec_ROI.DS54               | Harvest     | unannotated metabolite         | 0.742961 | 0.078560 |
| Met_Soil_Oct_ROI.OS7                | Seeding     | Valine                         | 0.742961 | 0.274039 |
| Met_Soil_Oct_ROI.OS9                | Seeding     | Valine                         | 0.749167 | 0.273109 |
| Met_Soil_Oct_ROI.OS24               | Seeding     | Lactic acid                    | 0.754998 | 0.296834 |
| Met_Soil_Dec_ROI.DS16               | Harvest     | unannotated metabolite         | 0.756334 | 0.084136 |
| Met_Soil_Oct_ROI.OS80               | Seeding     | Leucine                        | 0.764491 | 0.232075 |
| Sr(extracted with nitric acid)      | Harvest     | NA                             | 0.769697 | -        |
| K(extracted with ammonium acetate)  | Harvest     | NA                             | 0.769697 | 0.043180 |
| Met_Soil_Dec_ROI.DS51               | Harvest     | Glucose                        | 0.774684 | 0.361576 |
| Carbon                              | Harvest     | NA                             | 0.778592 | -        |
| Met_Soil_Oct_ROI.OS37               | Seeding     | unannotated metabolite         | 0.778592 | 0.150536 |
| Sample Name                  | Experiment | Metabolite Type          | Conc. (mg/g) | SD (mg/g) |
|------------------------------|------------|--------------------------|--------------|-----------|
| Met_Soil_Dec_ROI.DS25        | Harvest    | unannotated metabolite   | 0.782903     | 0.0025781 |
| Met_Soil_Oct_ROI.OS43        | Seeding    | unannotated metabolite   | 0.785231     | 0.2854033 |
| Met_Soil_Oct_ROI.OS40        | Seeding    | unannotated metabolite   | 0.805167     | 0.3711468 |
| Met_Soil_Oct_ROI.OS94        | Seeding    | unannotated metabolite   | 0.807637     | 0.0054250 |
| Met_Soil_Dec_ROI.DS1         | Harvest    | unannotated metabolite   | 0.812187     | 0.0451844 |
| Met_Soil_Oct_ROI.OS83        | Seeding    | unannotated metabolite   | 0.822900     | 0.188582  |
| Met_Soil_Dec_ROI.DS50        | Harvest    | Glucose                  | 0.823528     | 0.2889510 |
| Met_Soil_Dec_ROI.DS38        | Harvest    | unannotated metabolite   | 0.828728     | 0.0219733 |
| Met_Soil_Dec_ROI.DS12        | Harvest    | unannotated metabolite   | 0.828728     | 0.0696333 |
| Met_Soil_Oct_ROI.OS63        | Seeding    | unannotated metabolite   | 0.831875     | 0.2543583 |
| Met_Soil_Oct_ROI.OS20        | Seeding    | unannotated metabolite   | 0.831875     | 0.1288389 |
| Yb(extracted with nitric acid)| Harvest    | NA                       | 0.831875     | 0.0136349 |
| Zr(extracted with nitric acid)| Harvest    | NA                       | 0.831875     | 0.0154941 |
| Na(extracted with ammonium acetate) | Harvest    | NA                       | 0.831875     | 0.0216411 |
| Met_Soil_Oct_ROI.OS98        | Seeding    | unannotated metabolite   | 0.831875     | 0.1397478 |
| Met_Soil_Oct_ROI.OS6         | Seeding    | Leucine                  | 0.831875     | 0.1865185 |
| Met_Soil_Dec_ROI.DS47        | Harvest    | Glucose                  | 0.831875     | 0.2355137 |
| Met_Soil_Oct_ROI.OS47        | Seeding    | unannotated metabolite   | 0.831875     | 0.6229827 |
| Met_Soil_Oct_ROI.OS1         | Seeding    | unannotated metabolite   | 0.832975     | 0.2473823 |
| Hydrogen                     | Harvest    | NA                       | 0.835141     | 0.0359584 |
| Mg(extracted with ammonium acetate) | Harvest    | NA                       | 0.835141     | 0.0302368 |
| Sample ID                  | Type      | Metabolite                  | Score   | P-Value  |
|---------------------------|-----------|----------------------------|---------|----------|
| Met_Soil_Dec_ROI.DS37     | Harvest   | unannotated metabolite     | 0.835141699 | 0.127440345 |
| Met_Soil_Dec_ROI.DS43     | Harvest   | unannotated metabolite     | 0.835680852 | 0.242231921 |
| La(extracted with nitric acid) | Harvest   | NA                         | 0.851529888 | 0.009805521 |
| Met_Soil_Dec_ROI.DS53     | Harvest   | unannotated metabolite     | 0.863856037 | 0.225643136 |
| Met_Soil_Dec_ROI.DS26     | Harvest   | unannotated metabolite     | 0.877099498 | 0.024784117 |
| Met_Soil_Dec_ROI.DS2      | Harvest   | unannotated metabolite     | 0.87817878  | 0.145775894 |
| Met_Soil_Oct_ROI.OS5      | Seeding   | Leucine                    | 0.87817878  | 0.17029735 |
| Met_Soil_Dec_ROI.DS40     | Harvest   | Glucose                    | 0.88219046  | 0.1767868 |
| Met_Soil_Oct_ROI.OS15     | Seeding   | unannotated metabolite     | 0.882596404 | 0.013931535 |
| Met_Soil_Oct_ROI.OS14     | Seeding   | unannotated metabolite     | 0.88405186  | 0.078299455 |
| Met_Soil_Oct_ROI.OS8      | Seeding   | Isoleucine                 | 0.886795027 | 0.175287864 |
| Met_Soil_Oct_ROI.OS71     | Seeding   | unannotated metabolite     | 0.891809182 | 0.260959946 |
| Met_Soil_Oct_ROI.OS46     | Seeding   | unannotated metabolite     | 0.898433271 | 0.064718422 |
| Met_Soil_Oct_ROI.OS36     | Seeding   | unannotated metabolite     | 0.898643577 | 0.039664036 |
| Met_Soil_Dec_ROI.DS39     | Harvest   | Glucose                    | 0.90036439  | 0.05425666 |
| Met_Soil_Oct_ROI.OS21     | Seeding   | unannotated metabolite     | 0.907213579 | 0.012322893 |
| Met_Soil_Oct_ROI.OS4      | Seeding   | Isoleucine                 | 0.909559439 | 0.144084963 |
| Mg(extracted with nitric acid) | Harvest   | NA                         | 0.919935793 | 0.03288141 |
| Met_Soil_Oct_ROI.OS13     | Seeding   | unannotated metabolite     | 0.922161906 | 0.125647202 |
| Met_Soil_Dec_ROI.DS35     | Harvest   | unannotated metabolite     | 0.922161906 | 0.138773737 |
| Met_Soil_Dec_ROI.DS24     | Harvest   | Acetic acid                | 0.934359058 | 0.045025114 |
| Nitrogen                  | Harvest   | NA                         | 0.939808422 | 0.005673646 |
| Sample ID                        | Event    | Compound     | Annotation   | Score     | P-value  
|---------------------------------|----------|--------------|-------------|----------|---------
| Met_Soil_Oct_ROI.OS104          | Seeding  | unannotated  | 0.950741    | 0.0960598| 22      
| Al(extracted with nitric acid)  | Harvest  | NA           | 0.954322    | 0.0028963| 58      
| Met_Soil_Oct_ROI.OS18           | Seeding  | unannotated  | 0.959153    | 0.3354278| 76      
| Si(extracted with nitric acid)  | Harvest  | NA           | 0.959533    | 0.0027843| 47      
| Met_Soil_Oct_ROI.OS33           | Seeding  | unannotated  | 0.963328    | -        | 0.4925426| 69      
| Zn(extracted with nitric acid)  | Harvest  | NA           | 0.975630    | 0.0064731| 12      
| Met_Soil_Oct_ROI.OS2            | Seeding  | unannotated  | 0.977219    | 0.0019784| 23      
| Y(extracted with nitric acid)   | Harvest  | NA           | 0.985801    | -        | 0.0025580| 54      
| Na(extracted with nitric acid)  | Harvest  | NA           | 0.985801    | 0.0092107| 77      
| Met_Soil_Dec_ROI.DS52           | Harvest  | unannotated  | 0.988676    | 0.0864981| 47      
| Met_Soil_Oct_ROI.OS19           | Seeding  | unannotated  | 0.989674    | -        | 0.0025504| 16      
| Met_Soil_Oct_ROI.OS73           | Seeding  | Valine       | 0.996748    | 0.1181168| 99      
| Met_Soil_Oct_ROI.OS76           | Seeding  | Isoleucine   | 0.998386    | 0.1396163| 84      |
Table S3. List of nodes in the nine major modules of the integrated network.

| Node                                      | Sample_type    | Metabolite_annotation                  | Module |
|-------------------------------------------|----------------|----------------------------------------|--------|
| Na(extracted with ammonium acetate)       | Plant_harvest  | NA                                     | 1      |
| Met_Plant_ROI.P31                         | Plant_harvest  | Aspartic acid                          | 1      |
| Met_Plant_ROI.P92                         | Plant_harvest  | unannotated metabolite                 | 1      |
| Acidobacteria.Acidobacteria-6.iii1-15.mb2424 | Rhizosphere microbe | NA                                     | 1      |
| Acidobacteria.Solibacteres.Solibacterales.Other | Rhizosphere microbe | NA                                     | 1      |
| Actinobacteria.Actinobacteria.Actinomycetales.Cellulomonadaceae | Rhizosphere microbe | NA                                     | 1      |
| Actinobacteria.Actinobacteria.Actinomycetales.Mycobacteriaceae | Rhizosphere microbe | NA                                     | 1      |
| Actinobacteria.Actinobacteria.Actinomycetales.Nocardioidaceae | Rhizosphere microbe | NA                                     | 1      |
| Actinobacteria.Actinobacteria.Actinomycetales.Promicomonosporaceae | Rhizosphere microbe | NA                                     | 1      |
| Actinobacteria.Other.Other.Other          | Rhizosphere microbe | NA                                     | 1      |
| Actinobacteria.Thermoleophilia.Solirubrobacterales.Solirubrobacteraceae | Rhizosphere microbe | NA                                     | 1      |
| Bacteroidetes.[Saprospirae].[Saprospirales].Saprospiraceae | Rhizosphere microbe | NA                                     | 1      |
| BRC1.PRR-11.unidentified.unidentified    | Rhizosphere microbe | NA                                     | 1      |
| Chlorobi.BSV26.A89.unidentified          | Rhizosphere microbe | NA                                     | 1      |
| Cyanobacteria.Chloroplast.Stramenopiles.unidentified | Rhizosphere microbe | NA                                     | 1      |
| Cyanobacteria.Other.Other.Other          | Rhizosphere microbe | NA                                     | 1      |
| Cyanobacteria.Synechococcophycideae.Pseudanabenales.unidentified | Rhizosphere microbe | NA                                     | 1      |
| Gemmatimonadetes.Gemm-5.unidentified.unidentified | Rhizosphere microbe | NA                                     | 1      |
| Planctomycetes.C6.MVS-107.unidentified   | Rhizosphere microbe | NA                                     | 1      |
| Proteobacteria.Alphaproteobacteria.Rhizobiales.Bruccellaceae | Rhizosphere microbe | NA                                     | 1      |
| Proteobacteria.Alphaproteobacteria.Rhizobiales.Rhizobiaceae | Rhizosphere microbe | NA                                     | 1      |
| Proteobacteria.Deltaproteobacteria.Myxococcales.Myxococccaceae | Rhizosphere microbe | NA                                     | 1      |
| Proteobacteria.Deltaproteobacteria.Myxococcales.OOM27 | Rhizosphere microbe | NA                                     | 1      |
| Proteobacteria.Gammaproteobacteria.Legionellales.Other | Rhizosphere microbe | NA                                     | 1      |
| Species                                   | Sample Type   | Extraction Method         | Metabolite         | Count |
|------------------------------------------|---------------|---------------------------|--------------------|-------|
| Verrucomicrobia.Verrucomicrobiae.Verrucomicrobiales.Verrucomicrobiaceae | Rhizosphere microbe | NA                        | 1                  |
| Ca(extracted with nitric acid)           | Soil_harvest  | NA                        | 1                  |
| Mg(extracted with nitric acid)           | Soil_harvest  | NA                        | 1                  |
| Mg(extracted with ammonium acetate)      | Soil_harvest  | NA                        | 1                  |
| Na(extracted with nitric acid)           | Soil_harvest  | NA                        | 1                  |
| Na(extracted with ammonium acetate)      | Soil_harvest  | NA                        | 1                  |
| Met_Soil_Dec_ROI.DS18                    | Soil_harvest  | unannotated metabolite    | 1                  |
| Met_Soil_Dec_ROI.DS27                    | Soil_harvest  | unannotated metabolite    | 1                  |
| Sr(extracted with nitric acid)           | Soil_harvest  | NA                        | 1                  |
| Met_Soil_Oct_ROI.OS11                    | Soil_seeding  | unannotated metabolite    | 1                  |
| Met_Soil_Oct_ROI.OS13                    | Soil_seeding  | unannotated metabolite    | 1                  |
| Met_Soil_Oct_ROI.OS16                    | Soil_seeding  | unannotated metabolite    | 1                  |
| Met_Soil_Oct_ROI.OS2                     | Soil_seeding  | unannotated metabolite    | 1                  |
| Met_Soil_Oct_ROI.OS21                    | Soil_seeding  | unannotated metabolite    | 1                  |
| Met_Soil_Oct_ROI.OS24                    | Soil_seeding  | Lactic acid               | 1                  |
| Met_Soil_Oct_ROI.OS26                    | Soil_seeding  | Alanine                   | 1                  |
| Met_Soil_Oct_ROI.OS29                    | Soil_seeding  | unannotated metabolite    | 1                  |
| Met_Soil_Oct_ROI.OS37                    | Soil_seeding  | unannotated metabolite    | 1                  |
| Met_Soil_Oct_ROI.OS39                    | Soil_seeding  | unannotated metabolite    | 1                  |
| Met_Soil_Oct_ROI.OS4                     | Soil_seeding  | Isoleucine                | 1                  |
| Met_Soil_Oct_ROI.OS41                    | Soil_seeding  | unannotated metabolite    | 1                  |
| Met_Soil_Oct_ROI.OS43                    | Soil_seeding  | unannotated metabolite    | 1                  |
| Met_Soil_Oct_ROI.OS46                    | Soil_seeding  | unannotated metabolite    | 1                  |
| Met_Soil_Oct_ROI.OS47                    | Soil_seeding  | unannotated metabolite    | 1                  |
| Met_Soil_Oct_ROI.OS49                    | Soil_seeding  | unannotated metabolite    | 1                  |
| Met_Soil_Oct_ROI.OS5                     | Soil_seeding  | Leucine                   | 1                  |
| Met_Soil_Oct_ROI.OS50                    | Soil_seeding  | unannotated metabolite    | 1                  |
| Sample ID            | Process Type     | Description      | Abundance |
|----------------------|------------------|------------------|-----------|
| Met_Soil_Oct_ROI.OS51| Soil_seeding     | unannotated metabolite | 1         |
| Met_Soil_Oct_ROI.OS52| Soil_seeding     | N-Methylglycine  | 1         |
| Met_Soil_Oct_ROI.OS59| Soil_seeding     | Betaine          | 1         |
| Met_Soil_Oct_ROI.OS6 | Soil_seeding     | Leucine          | 1         |
| Met_Soil_Oct_ROI.OS61| Soil_seeding     | unannotated metabolite | 1         |
| Met_Soil_Oct_ROI.OS7 | Soil_seeding     | Valine           | 1         |
| Met_Soil_Oct_ROI.OS70| Soil_seeding     | Glycine          | 1         |
| Met_Soil_Oct_ROI.OS71| Soil_seeding     | unannotated metabolite | 1         |
| Met_Soil_Oct_ROI.OS73| Soil_seeding     | Valine           | 1         |
| Met_Soil_Oct_ROI.OS76| Soil_seeding     | Isoleucine       | 1         |
| Met_Soil_Oct_ROI.OS8 | Soil_seeding     | Isoleucine       | 1         |
| Met_Soil_Oct_ROI.OS80| Soil_seeding     | Leucine          | 1         |
| Met_Soil_Oct_ROI(OS81)| Soil_seeding     | unannotated metabolite | 1         |
| Met_Soil_Oct_ROI.OS83| Soil_seeding     | unannotated metabolite | 1         |
| Met_Soil_Oct_ROI.OS89| Soil_seeding     | Serine           | 1         |
| Met_Soil_Oct_ROI.OS9  | Soil_seeding     | Valine           | 1         |
| Met_Soil_Oct_ROI.OS90 | Soil_seeding     | unannotated metabolite | 1         |
| Met_Soil_Oct_ROI.OS91 | Soil_seeding     | unannotated metabolite | 1         |
| Met_Soil_Oct_ROI.OS92 | Soil_seeding     | unannotated metabolite | 1         |
| Met_Soil_Oct_ROI.OS93 | Soil_seeding     | unannotated metabolite | 1         |
| Met_Soil_Oct_ROI.OS94 | Soil_seeding     | unannotated metabolite | 1         |
| Met_Soil_Oct_ROI.OS95 | Soil_seeding     | unannotated metabolite | 1         |
| Met_Soil_Oct_ROI.OS96 | Soil_seeding     | unannotated metabolite | 1         |
| Met_Soil_Oct_ROI.OS97 | Soil_seeding     | unannotated metabolite | 1         |
| Mg(extracted with ammonium acetate) | Plant_harvest | NA               | 2         |
| Met_Plant_ROI.P99  | Plant_harvest    | unannotated metabolite | 2         |
| Met_Plant_ROI.P100 | Plant_harvest    | unannotated metabolite | 2         |
| Sample ID          | Harvest Type     | Metabolite Type          | Value |
|-------------------|------------------|--------------------------|-------|
| Met_Plant_ROI.P101 | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P102 | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P105 | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P106 | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P107 | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P110 | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P111 | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P114 | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P115 | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P117 | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P118 | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P11  | Plant_harvest    | Acetic acid              | 2     |
| Met_Plant_ROI.P15  | Plant_harvest    | Glutamic acid            | 2     |
| Met_Plant_ROI.P17  | Plant_harvest    | Glutamic acid/Glutamine  | 2     |
| Met_Plant_ROI.P29  | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P38  | Plant_harvest    | Choline                  | 2     |
| Met_Plant_ROI.P44  | Plant_harvest    | Methanol                 | 2     |
| Met_Plant_ROI.P77  | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P78  | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P79  | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P80  | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P81  | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P84  | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P85  | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P86  | Plant_harvest    | unannotated metabolite   | 2     |
| Met_Plant_ROI.P87  | Plant_harvest    | unannotated metabolite   | 2     |
| Sample Name | Harvest Type | Metabolite | Occurrence Count |
|-------------|--------------|------------|-----------------|
| Met_Plant_ROI.P89 | Plant harvest | Fumaric acid | 2 |
| Met_Plant_ROI.P97 | Plant harvest | unannotated metabolite | 2 |
| Armatimonadetes.Armatimonadia.Armatimonadales.Armatimonadaceae | Rhizosphere microbe | NA | 2 |
| Chloroflexi.P2-11E.unidentified.unidentified | Rhizosphere microbe | NA | 2 |
| Chloroflexi.TK10.AKYG885.5B-12 | Rhizosphere microbe | NA | 2 |
| Gemmatimonadetes.Gemmatimonadetes.N1423WL.unidentified | Rhizosphere microbe | NA | 2 |
| OD1.SM2F11.unidentified.unidentified | Rhizosphere microbe | NA | 2 |
| Planctomycetes.BD7-11.unidentified.unidentified | Rhizosphere microbe | NA | 2 |
| TM6.SBRH58.unidentified.unidentified | Rhizosphere microbe | NA | 2 |
| S(extracted with nitric acid) | Soil harvest | NA | 2 |
| Met_Soil_Oct_ROI.OS33 | Soil seeding | unannotated metabolite | 2 |
| Met_Plant_ROI.P22 | Plant harvest | Succinic acid | 3 |
| Met_Plant_ROI.P72 | Plant harvest | unannotated metabolite | 3 |
| [Thermi].Deinococci.Deinococcales.Deinococcaceae | Rhizosphere microbe | NA | 3 |
| Actinobacteria.Actinobacteria.Actinomycetales.Micrococccaceae | Rhizosphere microbe | NA | 3 |
| Actinobacteria.Other.Other.Other | Rhizosphere microbe | NA | 3 |
| Bacteroidetes.Flavobacteriia.Flavobacteriales.Cryomorphaceae | Rhizosphere microbe | NA | 3 |
| Bacteroidetes.Flavobacteriia.Flavobacteriales.Flavobacteriaceae | Rhizosphere microbe | NA | 3 |
| Bacteroidetes.Sphingobacteriia.Sphingobacteriales.Sphingobacteriaceae | Rhizosphere microbe | NA | 3 |
| Bacteroidetes.Sphingobacteriia.Sphingobacteriales.unidentified | Rhizosphere microbe | NA | 3 |
| Chloroflexi.Anaerolineae.SBR1031.SHA-31 | Rhizosphere microbe | NA | 3 |
| Chloroflexi.C0119.unidentified.unidentified | Rhizosphere microbe | NA | 3 |
| Chloroflexi.Thermomicrobia.AKYG1722.unidentified | Rhizosphere microbe | NA | 3 |
| Firmicutes.Bacilli.Other.Other | Rhizosphere microbe | NA | 3 |
| Firmicutes.Clostridia.Halanaerobiaes.Halanaerobiacaeae | Rhizosphere microbe | NA | 3 |
| Firmicutes.Clostridia.OPB54.unidentified | Rhizosphere microbe | NA | 3 |
| Kingdom                  | Phylum                        | Class                          | Rhizosphere microbe | Plant_harvest | Carbon | Brix(%)_leaf | Acidobacteria.Solibacteres.Solibacterales.MVS-65 | Actinobacteria.Actinobacteria.Actinomycetales.Sporichthyaecae | Actinobacteria.Thermoleophilia.Gaiellales.Other | Bacteroidetes.Cytophagia.Cytophagales.Other | Chloroflexi.Anaerolineae.envOPS12.unidentified | Chloroflexi.Ktedonobacteria.TK10.unidentified | Cyanobacteria.Synechococcophycideae.Pseudanabenaenales.Pseudanabaenaceae | Elusimicrobia.Elusimicrobia.MVP-88.unidentified | Firmicutes.Other.Other.Other | Gemmatimonadetes.Gemmatimonadetes.C114.unidentified | Gemmatimonadetes.Other.Other.Other | OD1.unidentified.unidentified.unidentified | Proteobacteria.Deltaproteobacteria.FAC87.unidentified | Proteobacteria.Deltaproteobacteria.Myxococcales.unidentified | Proteobacteria.Deltaproteobacteria.Other.Other | Spirochaetes.Spirochaetes.Spirochaetales.Spirochaetaceae |
|-------------------------|-------------------------------|--------------------------------|---------------------|---------------|-------|-------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|--------------------------------|--------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|-------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|------------------------------------------------|
| Gemmatimonadetes        | Gemmatimonadetes              | Gemmatimonadales.Other         | Rhizosphere microbe | NA            | 3     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Other                   | Other                         | Other                          | Rhizosphere microbe | NA            | 3     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Planctomycetes          | Planctomycetalia              | Gemmatimonadales.Gemmatimonadetes | Rhizosphere microbe | NA            | 3     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Proteobacteria          | Alphaproteobacteria           | Caulobacteriales               | Rhizosphere microbe | NA            | 3     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Proteobacteria          | Alphaproteobacteria           | Rhizobiales.Rhodobiaceae       | Rhizosphere microbe | NA            | 3     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Proteobacteria          | Deltaproteobacteria           | Bdellovibrionales.Bacteriovoraceae | Rhizosphere microbe | NA            | 3     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Proteobacteria          | Deltaproteobacteria           | MIZ46.unidentified             | Rhizosphere microbe | NA            | 3     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Proteobacteria          | Gammaproteobacteria           | Pseudomonadales.Pseudomonadaceae | Rhizosphere microbe | NA            | 3     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Carbon                  |                               |                                | Plant_harvest       | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Brix(%)_leaf            |                               |                                | Plant_harvest       | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Acidobacteria           | Solibacteres.Solibacterales.MVS-65 |                              | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Actinobacteria          | Actinobacteria.Actinomycetales.Sporichthyaecae |              | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Actinobacteria          | Thermoleophilia.Gaiellales.Other |                              | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Bacteroidetes           | Cytophagia.Cytophagales.Other |                               | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Chloroflexi             | Anaerolineae.envOPS12.unidentified |                             | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Chloroflexi             | Ktedonobacteria.TK10.unidentified |                             | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Cyanobacteria           | Synechococcophycideae.Pseudanabenaenales.Pseudanabaenaceae | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Elusimicrobia           | Elusimicrobia.MVP-88.unidentified |                             | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Firmicutes              | Other                         | Other                          | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Gemmatimonadetes        | Gemmatimonadetes              | C114.unidentified              | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Gemmatimonadetes        | Other                         | Other                          | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| OD1.unidentified        | unidentified.unidentified.unidentified |                       | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Proteobacteria          | Deltaproteobacteria           | FAC87.unidentified             | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Proteobacteria          | Deltaproteobacteria           | Myxococcales.unidentified      | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Proteobacteria          | Deltaproteobacteria           | Other.Other                    | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Spirochaetes            | Spirochaetes.Spirochaetales.Spirochaetaceae |                             | Rhizosphere microbe | NA            | 4     |             |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                         |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |                                                |
| Dataset | Category | Microbe | Annotation | Metabolite | Value |
|---------|----------|---------|------------|------------|-------|
| TM7.SC3.unidentified.unidentified | Rhizosphere microbe | NA | 4 |
| Verrucomicrobia.[Pedosphaerae].Other.Other | Rhizosphere microbe | NA | 4 |
| Verrucomicrobia.[Spartobacteria].[Chthoniobacterales].Other | Rhizosphere microbe | NA | 4 |
| Verrucomicrobia.Opitutae.Opitutales.Opitutaceae | Rhizosphere microbe | NA | 4 |
| Verrucomicrobia.Opitutae.Other.Other | Rhizosphere microbe | NA | 4 |
| Verrucomicrobia.Opitutae.Other.unidentified | Rhizosphere microbe | NA | 4 |
| Met_Soil_Oct_ROI.OS100 | Soil_seeding | Glucose | 4 |
| Met_Soil_Oct_ROI.OS101 | Soil_seeding | Glucose | 4 |
| Met_Soil_Oct_ROI.OS102 | Soil_seeding | unannotated metabolite | 4 |
| Met_Soil_Oct_ROI.OS17 | Soil_seeding | unannotated metabolite | 4 |
| Met_Soil_Oct_ROI.OS55 | Soil_seeding | unannotated metabolite | 4 |
| Met_Soil_Oct_ROI.OS56 | Soil_seeding | Choline | 4 |
| Met_Soil_Oct_ROI.OS57 | Soil_seeding | unannotated metabolite | 4 |
| Met_Soil_Oct_ROI.OS58 | Soil_seeding | Glucose | 4 |
| Met_Soil_Oct_ROI.OS64 | Soil_seeding | Glucose | 4 |
| Met_Soil_Oct_ROI.OS65 | Soil_seeding | unannotated metabolite | 4 |
| Met_Soil_Oct_ROI.OS66 | Soil_seeding | Glucose | 4 |
| Met_Soil_Oct_ROI.OS67 | Soil_seeding | Glucose | 4 |
| Met_Soil_Oct_ROI.OS68 | Soil_seeding | Glucose | 4 |
| Met_Soil_Oct_ROI.OS69 | Soil_seeding | Glucose | 4 |
| Met_Soil_Oct_ROI.OS72 | Soil_seeding | unannotated metabolite | 4 |
| Met_Soil_Oct_ROI.OS74 | Soil_seeding | unannotated metabolite | 4 |
| Met_Soil_Oct_ROI.OS75 | Soil_seeding | unannotated metabolite | 4 |
| Met_Soil_Oct_ROI.OS77 | Soil_seeding | unannotated metabolite | 4 |
| Met_Soil_Oct_ROI.OS78 | Soil_seeding | unannotated metabolite | 4 |
| Met_Soil_Oct_ROI.OS79 | Soil_seeding | Glucose | 4 |
| Met_Soil_Oct_ROI.OS82 | Soil_seeding | Glucose | 4 |
| Study ID                | Treatment     | Metabolite       | Sample Size |
|------------------------|---------------|------------------|-------------|
| Met_Soil_Oct_ROI.OS85  | Soil_seeding  | Glucose          | 4           |
| Met_Soil_Oct_ROI.OS86  | Soil_seeding  | unannotated metabolite | 4 |
| Met_Soil_Oct_ROI.OS87  | Soil_seeding  | Glucose          | 4           |
| Met_Soil_Oct_ROI.OS88  | Soil_seeding  | Betaine          | 4           |
| Met_Soil_Oct_ROI.OS99  | Soil_seeding  | unannotated metabolite | 4 |
| C/N                    | Plant harvest | NA               | 5           |
| Nitrogen               | Plant harvest | NA               | 5           |
| Actinobacteria.Acidimicrobia.Acidimicrobiales. Other | Rhizosphere microbe | NA | 5 |
| Actinobacteria.Actinobacteria.Actinomycetales. Micro monosporaceae | Rhizosphere microbe | NA | 5 |
| Actinobacteria.Actinobacteria.Actinomycetales.Nakamuraellaceae | Rhizosphere microbe | NA | 5 |
| Actinobacteria.Actinobacteria.Actinomycetales.Nocardiosporaceae | Rhizosphere microbe | NA | 5 |
| Actinobacteria.Nitriliruptoria.Euzebyales.Euzebyaceae | Rhizosphere microbe | NA | 5 |
| Bacteroidetes. Other. Other. Other | Rhizosphere microbe | NA | 5 |
| Firmicutes.Clostridia.Clostridiales.[Tissierellaceae] | Rhizosphere microbe | NA | 5 |
| Firmicutes.Clostridia.Clostridiales.Peptococcaceae | Rhizosphere microbe | NA | 5 |
| Firmicutes.Clostridia.Clostridiales.Ruminococcaceae | Rhizosphere microbe | NA | 5 |
| OD1.ZB2.unidentified.unidentified | Rhizosphere microbe | NA | 5 |
| OP3.koll11.unidentified.unidentified | Rhizosphere microbe | NA | 5 |
| Planctomycetes.Pla4.unidentified.unidentified | Rhizosphere microbe | NA | 5 |
| Planctomycetes.Planctomycetia.Planctomycetales.Planctomycetaceae | Rhizosphere microbe | NA | 5 |
| Proteobacteria.Alphaproteobacteria.Rhizobiales.Xanthobacteraceae | Rhizosphere microbe | NA | 5 |
| Proteobacteria.Alphaproteobacteria.Rhodobacterales.Hyphomonaaceae | Rhizosphere microbe | NA | 5 |
| Proteobacteria.Deltaproteobacteria.Myxococcales.Polyangiaceae | Rhizosphere microbe | NA | 5 |
| Proteobacteria.Gammaproteobacteria.Xanthomonadales.Sinobacteraceae | Rhizosphere microbe | NA | 5 |
| TM7.TM7-3.EW055.unidentified | Rhizosphere microbe | NA | 5 |
| WS3.PRR-12.LD1-PA13.unidentified | Rhizosphere microbe | NA | 5 |
| Sample Name                  | Sample Type       | Annotation       | Metabolite Type |
|-----------------------------|-------------------|------------------|-----------------|
| Met_Soil_Dec_ROI.DS9        | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS10       | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS12       | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS14       | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS15       | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS16       | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS17       | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS20       | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS23       | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS25       | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS1        | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS37       | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS2        | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS38       | Soil_harvest      | unannotated      | metabolite      |
| Met_Soil_Dec_ROI.DS49       | Soil_harvest      | Serine           | 5               |
| Met_Soil_Oct_ROI.OS84       | Soil_seeding      | unannotated      | metabolite      |
| Met_Plant_ROI.P109          | Plant_harvest     | unannotated      | metabolite      |
| Met_Plant_ROI.P113          | Plant_harvest     | unannotated      | metabolite      |
| Met_Plant_ROI.P119          | Plant_harvest     | Formic acid      | 6               |
| Met_Plant_ROI.P39           | Plant_harvest     | unannotated      | metabolite      |
| Met_Plant_ROI.P45           | Plant_harvest     | Glucose          | 6               |
| Met_Plant_ROI.P46           | Plant_harvest     | unannotated      | metabolite      |
| Met_Plant_ROI.P47           | Plant_harvest     | Glucose          | 6               |
| Met_Plant_ROI.P48           | Plant_harvest     | Glucose/Sucrose  | 6               |
| Met_Plant_ROI.P49           | Plant_harvest     | Glucose          | 6               |
| Met_Plant_ROI.P50           | Plant_harvest     | Fructose         | 6               |
| Met_Plant_ROI.P51   | Plant_harvest | Fructose      | 6 |
|--------------------|---------------|---------------|---|
| Met_Plant_ROI.P52   | Plant_harvest | Fructose      | 6 |
| Met_Plant_ROI.P53   | Plant_harvest | unannotated metabolite | 6 |
| Met_Plant_ROI.P55   | Plant_harvest | Fructose      | 6 |
| Met_Plant_ROI.P56   | Plant_harvest | Fructose      | 6 |
| Met_Plant_ROI.P57   | Plant_harvest | Glucose       | 6 |
| Met_Plant_ROI.P58   | Plant_harvest | Glucose/Sucrose | 6 |
| Met_Plant_ROI.P60   | Plant_harvest | Fructose      | 6 |
| Met_Plant_ROI.P61   | Plant_harvest | Glucose/Sucrose | 6 |
| Met_Plant_ROI.P62   | Plant_harvest | Fructose/Glucose/Sucrose | 6 |
| Met_Plant_ROI.P68   | Plant_harvest | Fructose      | 6 |
| Met_Plant_ROI.P69   | Plant_harvest | unannotated metabolite | 6 |
| Met_Plant_ROI.P73   | Plant_harvest | Glucose       | 6 |
| Met_Plant_ROI.P74   | Plant_harvest | Glucose       | 6 |
| Met_Plant_ROI.P95   | Plant_harvest | unannotated metabolite | 6 |
| Met_Plant_ROI.P96   | Plant_harvest | unannotated metabolite | 6 |
| Actinobacteria.MB-A2-108.0319-7L14.unidentified | Rhizosphere microbe | NA | 6 |
| Firmicutes.Clostridia.Clostridiales.Other | Rhizosphere microbe | NA | 6 |
| NO3(mg/100g)       | Soil_harvest  | NA            | 6 |
| No.of.leaves       | Plant_harvest | NA            | 7 |
| PheShoot.dry.weight(mg) | Plant_harvest | NA | 7 |
| [Thermi].Deinococci.Thermales.Thermaceae | Rhizosphere microbe | NA | 7 |
| Acidobacteria.Acidobacteria-5.unidentified.unidentified | Rhizosphere microbe | NA | 7 |
| Acidobacteria.Acidobacteria-6.CCU21.unidentified | Rhizosphere microbe | NA | 7 |
| Acidobacteria.Acidobacteria-6.iii1-15.RB40 | Rhizosphere microbe | NA | 7 |
| Acidobacteria.Acidobacteria-6.iii1-15.unidentified | Rhizosphere microbe | NA | 7 |
| Acidobacteria.Other.Other.Other | Rhizosphere microbe | NA | 7 |
| Phylum                                  | Taxonomy                                      | Location  | Replicates |
|-----------------------------------------|-----------------------------------------------|-----------|------------|
| Acidobacteria                          | Acidobacteria.Solibacteres.Solibacteraceae    | Rhizosphere| NA         |
|                                        | Acidobacteria.Solibacteres.Solibacteraceae    | Rhizosphere| NA         |
|                                        | Acidobacteria.Solibacteres.unidentified      | Rhizosphere| NA         |
|                                        | Actinobacteria.Actinomycetales.Geodermatophilaceae | Rhizosphere| NA         |
|                                        | Actinobacteria.Actinomycetales.Strptomosporangiaceae | Rhizosphere| NA         |
|                                        | Actinobacteria.Thermoleophilia.Solirubrobacterales.Conexibacteraceae | Rhizosphere| NA         |
|                                        | Armatimonadetes.[Fimbriimonadia].[Fimbriimonadaceae] | Rhizosphere| NA         |
|                                        | Bacteroidetes.[Saprospirae].[Saprospirales].Chitinophagaceae | Rhizosphere| NA         |
|                                        | Chlorobi.BSV26.C20.unidentified              | Rhizosphere| NA         |
|                                        | Chlorobi.unidentified.unidentified           | Rhizosphere| NA         |
|                                        | Chloroflexi.Anaerolineae.H39.unidentified     | Rhizosphere| NA         |
|                                        | Chloroflexi.Anaerolineae.SBR1031.A4b          | Rhizosphere| NA         |
|                                        | Chloroflexi.Anaerolineae.SBR1031.oc28         | Rhizosphere| NA         |
|                                        | Chloroflexi.Ktedonobacteria.unidentified.unidentified | Rhizosphere| NA         |
|                                        | Chloroflexi.Other.Other.Other                 | Rhizosphere| NA         |
|                                        | Chloroflexi.Thermomicrobia.Other.Other       | Rhizosphere| NA         |
|                                        | Cyanobacteria.Chloroplast.Chlorophyta.Chlamydomonadaece | Rhizosphere| NA         |
|                                        | Cyanobacteria.Chloroplast.Chlorophyta.unidentified | Rhizosphere| NA         |
|                                        | Elusimicrobia.Elusimicrobia.IIb.unidentified | Rhizosphere| NA         |
|                                        | Elusimicrobia.Elusimicrobia.unidentified.unidentified | Rhizosphere| NA         |
|                                        | Firmicutes.Bacilli.Bacillales.Paenibacillaceae | Rhizosphere| NA         |
|                                        | Gemmatimonadetes.Gemmatimonadetes.Ellin5290.unidentified | Rhizosphere| NA         |
|                                        | Gemmatimonadetes.Gemmatimonadetes.KD8-87.unidentified | Rhizosphere| NA         |
|                                        | Nitrospirae.Nitrospira.Nitrospirales.Nitrospiraceae | Rhizosphere| NA         |
| Taxonomy | Rhizosphere microbe | Origin | Cpm |
|----------|---------------------|--------|-----|
| OD1.Other.Other.Other | Rhizosphere microbe | NA | 7 |
| Planctomycetes.Other.Other.Other | Rhizosphere microbe | NA | 7 |
| Planctomycetes.Planctomycetia.Gemmatales.Isosp haeracea | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Alphaproteobacteria.Ellin329.unidentifed | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Alphaproteobacteria.Other.Other | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Alphaproteobacteria.Rhizobiales.Phy llobacteriaceae | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Alphaproteobacteria.Rickettsiales.mитochondria | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Alphaproteobacteria.Sphingomonad ales.Sphingomonadaceae | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Betaproteobacteria.A21b.EB1003 | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Betaproteobacteria.IS-44.unidentified | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Betaproteobacteria.Methylphilales. Methylphilaceae | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Betaproteobacteria.Nitrosomonadale s.Nitrosomonadaceae | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Betaproteobacteria.SC-I-84.unidentified | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Deltaproteobacteria.Myxococcales.H aliangiaceae | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Deltaproteobacteria.Myxococcales.O ther | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Gammaproteobacteria.unidentified.unidentified | Rhizosphere microbe | NA | 7 |
| Proteobacteria.Gammaproteobacteria.Xanthomonad ales.Other | Rhizosphere microbe | NA | 7 |
| Spirochaetes.[Leptospirae].[Leptospirales].Leptospir aceae | Rhizosphere microbe | NA | 7 |
| Verrucomicrobia.[Methylacidiphilae].S-BQ2-57.unidentified | Rhizosphere microbe | NA | 7 |
| Verrucomicrobia.[Pedosphaerae].[Pedosphaerales]. auto67_4W | Rhizosphere microbe | NA | 7 |
| Verrucomicrobia.[Pedosphaerae].[Pedosphaerales]. Other | Rhizosphere microbe | NA | 7 |
| Verrucomicrobia.[Pedosphaerae].[Pedosphaerales]. unidentified | Rhizosphere microbe | NA | 7 |
| WS2.SHA-109.unidentified.unidentified | Rhizosphere microbe | NA | 7 |
| WS3.PRR-12.Sediment-1.PRR-10 | Rhizosphere microbe | NA | 7 |
| Ca(extracted with ammonium acetate) | Soil_harvest | NA | 7 |
| Met_Soil_Dec_ROI.DS8 | Soil_harvest | Valine | 7 |
| Sample Name                  | Harvest Type     | Metabolite Description                  | Value |
|-----------------------------|------------------|----------------------------------------|-------|
| Met_Soil_Dec_ROI.DS19       | Soil_harvest     | Lactic acid                            | 7     |
| Met_Soil_Dec_ROI.DS21       | Soil_harvest     | Alanine                                | 7     |
| Met_Soil_Dec_ROI.DS28       | Soil_harvest     | unannotated metabolite                 | 7     |
| Met_Soil_Dec_ROI.DS29       | Soil_harvest     | N-Methylglycine                         | 7     |
| Met_Soil_Dec_ROI.DS33       | Soil_harvest     | unannotated metabolite                 | 7     |
| Met_Soil_Dec_ROI.DS34       | Soil_harvest     | Choline                                | 7     |
| Met_Soil_Dec_ROI.DS41       | Soil_harvest     | Glycine                                | 7     |
| Met_Soil_Dec_ROI.DS42       | Soil_harvest     | Valine                                 | 7     |
| Met_Soil_Dec_ROI.DS44       | Soil_harvest     | Isoleucine                             | 7     |
| Met_Soil_Dec_ROI.DS3         | Soil_harvest     | Isoleucine                             | 7     |
| Met_Soil_Dec_ROI.DS4         | Soil_harvest     | Leucine                                | 7     |
| Met_Soil_Dec_ROI.DS5         | Soil_harvest     | Leucine                                | 7     |
| Met_Soil_Dec_ROI.DS6         | Soil_harvest     | Valine                                 | 7     |
| Met_Soil_Dec_ROI.DS7         | Soil_harvest     | Isoleucine                             | 7     |
| K(extracted with ammonium acetate) | Soil_seeding     | NA                                     | 7     |
| Met_Soil_Oct_ROI.OS22       | Soil_seeding     | unannotated metabolite                 | 7     |
| Met_Soil_Oct_ROI.OS48       | Soil_seeding     | unannotated metabolite                 | 7     |
| Met_Soil_Oct_ROI.OS60       | Soil_seeding     | unannotated metabolite                 | 7     |
| Taste.indexShoot            | Plant_harvest    | NA                                     | 8     |
| Acidobacteria.Acidobacteriia.Acidobacteriales.Koribacteraceae | Rhizosphere microbe | NA                                     | 8     |
| Acidobacteria.DA052.Ellin6513.unidentified | Rhizosphere microbe | NA                                     | 8     |
| Acidobacteria.Holophagae.Holophagales.Holophagaceae | Rhizosphere microbe | NA                                     | 8     |
| Acidobacteria.S035.unidentified.unidentified | Rhizosphere microbe | NA                                     | 8     |
| Actinobacteria.Actinobacteria.Actinomycetales.Actinoosynnemataceae | Rhizosphere microbe | NA                                     | 8     |
| Actinobacteria.Actinobacteria.Actinomycetales.Glycomycetaceae | Rhizosphere microbe | NA                                     | 8     |
| Actinobacteria.Actinobacteria.Actinomycetales.Nocardia | Rhizosphere microbe | NA                                     | 8     |
| Armatimonadetes.[Fimbriimonadaceae].[Fimbriimonadales].undefined | Rhizosphere microbe | NA                                     | 8     |
| Armatimonadetes.Armatimonadetes.FW68.unidentified | Rhizosphere microbe | NA | 8 |
| Armatimonadetes.Chthonomonadetes.SJA-22.unidentified | Rhizosphere microbe | NA | 8 |
| Chlorobi.BSV26.VC38.unidentified | Rhizosphere microbe | NA | 8 |
| Chloroflexi.Ktedonobacteria.B10-SB3A.unidentified | Rhizosphere microbe | NA | 8 |
| Cyanobacteria.4C0d-2.SM1D11.unidentified | Rhizosphere microbe | NA | 8 |
| Cyanobacteria.Nostocophycideae.Nostocales.Nostocaceae | Rhizosphere microbe | NA | 8 |
| Cyanobacteria.Nostocophycideae.Other.Other | Rhizosphere microbe | NA | 8 |
| FCPU426.unidentified.unidentified.unidentified | Rhizosphere microbe | NA | 8 |
| Firmicutes.Clostridia.Clostridiales.Symbiobacteriaceae | Rhizosphere microbe | NA | 8 |
| Firmicutes.Clostridia.Other.Other | Rhizosphere microbe | NA | 8 |
| Gemmatimonadetes.Gemm-1.unidentified.unidentified | Rhizosphere microbe | NA | 8 |
| GN02.GKS2-174.unidentified.unidentified | Rhizosphere microbe | NA | 8 |
| OP11.OP11-3.unidentified.unidentified | Rhizosphere microbe | NA | 8 |
| Proteobacteria.Alphaproteobacteria.Rhizobiales.Met hylocystaceae | Rhizosphere microbe | NA | 8 |
| Proteobacteria.Alphaproteobacteria.Rhizobiales.unidentified | Rhizosphere microbe | NA | 8 |
| Proteobacteria.Betaproteobacteria.Methylophilales.Other | Rhizosphere microbe | NA | 8 |
| Proteobacteria.Betaproteobacteria.MND1.unidentified | Rhizosphere microbe | NA | 8 |
| Proteobacteria.Betaproteobacteria.unidentified.unidentified | Rhizosphere microbe | NA | 8 |
| Proteobacteria.Deltaproteobacteria.Syntrophobacter ales.Syntrophobacteraceae | Rhizosphere microbe | NA | 8 |
| Spirochaetes.Spirochaetes.Other.Other | Rhizosphere microbe | NA | 8 |
| WS3.PRR-12.Sediment-1.Other | Rhizosphere microbe | NA | 8 |
| Met_Soil_Dec_ROI.DS22 | Soil_harvest | unannotated metabolite | 8 |
| Carbon | Soil_seeding | NA | 8 |
| Nitrogen | Soil_seeding | NA | 8 |
| Met_Soil_Oct_ROI.OS27 | Soil_seeding | unannotated metabolite | 8 |
| Met_Soil_Oct_ROI.OS31 | Soil_seeding | unannotated metabolite | 8 |
| File_Name            | Harvest_Type       | Metabolite            | Sample_Number |
|----------------------|--------------------|-----------------------|---------------|
| Met_Plant_ROI.P103   | Plant_harvest      | Phenylalanine         | 9             |
| Met_Plant_ROI.P104   | Plant_harvest      | Phenylalanine         | 9             |
| Met_Plant_ROI.P10    | Plant_harvest      | GABA                  | 9             |
| Met_Plant_ROI.P18    | Plant_harvest      | Glutamic acid/Glutamine | 9 |
| Met_Plant_ROI.P1     | Plant_harvest      | Isoleucine            | 9             |
| Met_Plant_ROI.P19    | Plant_harvest      | GABA                  | 9             |
| Met_Plant_ROI.P23    | Plant_harvest      | Glutamine             | 9             |
| Met_Plant_ROI.P24    | Plant_harvest      | Glutamine             | 9             |
| Met_Plant_ROI.P25    | Plant_harvest      | Glutamine             | 9             |
| Met_Plant_ROI.P2     | Plant_harvest      | Leucine               | 9             |
| Met_Plant_ROI.P33    | Plant_harvest      | Asparagine            | 9             |
| Met_Plant_ROI.P34    | Plant_harvest      | Asparagine            | 9             |
| Met_Plant_ROI.P35    | Plant_harvest      | unannotated metabolite | 9 |
| Met_Plant_ROI.P36    | Plant_harvest      | GABA                  | 9             |
| Met_Plant_ROI.P3     | Plant_harvest      | Leucine               | 9             |
| Met_Plant_ROI.P41    | Plant_harvest      | unannotated metabolite | 9 |
| Met_Plant_ROI.P4     | Plant_harvest      | Valine                | 9             |
| Met_Plant_ROI.P5     | Plant_harvest      | Isoleucine            | 9             |
| Met_Plant_ROI.P59    | Plant_harvest      | Alanine/Glutamine     | 9             |
| Met_Plant_ROI.P6     | Plant_harvest      | Valine                | 9             |
| Met_Plant_ROI.P7     | Plant_harvest      | Isoleucine            | 9             |
| Met_Plant_ROI.P8     | Plant_harvest      | Lactic acid           | 9             |
| Met_Plant_ROI.P90    | Plant_harvest      | Tyrosine              | 9             |
| Met_Plant_ROI.P98    | Plant_harvest      | Tyrosine              | 9             |
| Actinobacteria.Acidimicrobiia.Acidimicrobiales.AKIW 874 | Rhizosphere microbe | NA | 9 |
| Actinobacteria.Actinobacteria.Actinomycetales.Corynebacteriaceae | Rhizosphere microbe | NA | 9 |
| Bacteroidetes.Cytophagia.Cytophagaes.Cytophagaceae | Rhizosphere microbe | NA | 9 |
| Cyanobacteria.Chloroplast.Streptophyta.unidentified | Rhizosphere microbe | NA | 9 |
| Firmicutes.Bacilli.Bacillales.Staphylococcaceae | Rhizosphere microbe | NA | 9 |