|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Supplementary Table 3. Metabolic pathway enrichment scores (PES) for discriminating metabolites between rice bran varieties** | | | | | | | | | | | | | | | | | | |
| **Rice Cultivar** | | **Kenya – Basmati 217** | **Kenya – Basmati 370** | **Mali – Gambiaka** | **Mali – Shwetasoke** | **Mali – DM-16** | **Mali – Khao Gaew** | **Nicaragua – Dorado** | **Nepal – Sawa Mahsuli** | **India – Chennula** | **India – Njavara** | **USA – Calrose** | **USA – RBT 300** | **USA – Jasmine 85** | **USA – IAC 600** | **USA – LTH** | **USA – SHZ-2** | **Cambodia – Rang Jey** |
| **Chemical class** | **Metabolic Pathway** |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| **Amino acid** | **Aromatic amino acid metabolism (PEP derived)** | 1.0 | 1.0 | 1.0 | 1.0 | **24.8** | 1.0 | 1.0 | 1.0 | 1.0 | **1.7** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **2.4** |
| **Aspartate family (OAA derived)** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **1.6** | 1.0 | **1.2** | **3.9** | **1.1** | 1.0 | 1.0 | 1.0 | **1.5** | 1.0 | 1.0 | 1.0 |
| **Glutamate family (alpha-ketoglutarate derived)** | 1.0 | 1.0 | **6.9** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **0.9** | **2.1** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| **Serine family (phosphoglycerate derived)** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **6.0** | 1.0 | **2.9** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| **Carbohydrate** | **Amino sugar and nucleotide sugar** | **2.9** | 1.0 | 1.0 | 1.0 | 1.0 | **20.3** | 1.0 | 1.0 | 1.0 | **0.7** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| **TCA cycle** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **9.9** | **7.4** | 1.0 | 1.0 | **6.8** | 1.0 | 1.0 | **1.2** |
| **Cofactors & vitamins** | **Tocopherol metabolism** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **9.6** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| **Lipids** | **Free fatty acid** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **2.5** | 1.0 | 1.0 | **3.1** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| **Glycerolipids (diacyl)** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **1.2** | 1.0 | 1.0 | **12.8** | **4.1** | 1.0 | 1.0 | 1.0 | **2.1** |
| **Glycerolipids (monoacyl)** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **3.6** | 1.0 | 1.0 | **5.7** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| **Lyso-phospholipids** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **3.6** |
| **Oxylipins** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **6.5** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| **Phospholipid Metabolism** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **4.6** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| **Nucleotide** | **Purine metabolism** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **1.1** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **1.4** | 1.0 | 1.0 | 1.0 | 1.0 | **2.7** |
| **Secondary metabolism** | **Benzenoids** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **3.2** | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | **4.3** |
| PES greater or less than 1.0 is notable (bolded) and it indicates that the metabolic pathway contains at least 1 metabolite with significant Z-score (Z-score > **|**2.0**|)**, i.e., level of expression for that metabolite is different from the rest of cultivars for the same metabolites across the metabolic pathway. | | | | | | | | | | | | | | | | | | |