**Supplementary Table S4:** Differential accumulation of metabolites at stages 2-5 compared to stage 1.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Metabolite** | **Ratio 2vs1** | **Ratio 3vs1** | **Ratio 4vs1** | **Ratio 5vs1** |
| *Monoterpenoids* |  |  |  |  |
| Free linalool | 6.04 | 51.72 | 71.34 | 44.79 |
| Bound linalool | 4.03 | 41.09 | 125.88 | 197.81 |
| Free geraniol | 3.89 | 5.21 | 3.84 | 6.01 |
| Bound geraniol | 1.65NS | 5.54 | 7.46 | 9.67 |
| Free nerol | 7.55 | 19.90 | 13.55 | 22.88 |
| Bound nerol | 3.65 | 16.11 | 22.52 | 26.47 |
| Free *trans*-8-hydroxy-linalool | 1.29NS | 9.31 | 8.41 | 6.64 |
| Bound *trans*-8-hydroxy-linalool | 0.86NS | 1.58NS | 2.31 | 3.89 |
| Free *cis*-8-hydroxy-linalool | 14.12 | 22.44 | 7.37 | 6.70 |
| Bound *cis*-8-hydroxy-linalool | 1.43NS | 3.05 | 3.24 | 4.12 |
| Free *trans-*furan linalool oxide | 0.77NS | 0.60NS | 0.81NS | 0.79NS |
| Bound *trans-*furan linalool oxide | 1.58NS | 2.31 | 3.17 | 3.62 |
| Free *cis*-furan linalool oxide | 0.33 | 0.54NS | 0.64NS | 0.47 |
| Bound *cis*-furan linalool oxide | 0.89NS | 0.86NS | 0.66NS | 0.66NS |
| Free *trans*-pyran linalool oxide | 0.78NS | 0.92NS | 1.18NS | 1.12NS |
| Bound *trans*-pyran linalool oxide | 1.28NS | 1.31NS | 1.48NS | 2.15 |
| Free *cis*-pyran linalool oxide | 0.45 | 0.93NS | 1.03NS | 0.64NS |
| Bound *cis*-pyran linalool oxide | 0.98NS | 1.31NS | 1.44NS | 1.72NS |
| Free *trans*-geranic acid | 3.46 | 6.24 | 2.99 | 3.39 |
| Bound *trans*-geranic acid | 1.09NS | 1.59NS | 1.49NS | 1.84NS |
| Free 7-hydroxy-geraniol | 2.81 | 5.89 | 3.43 | 2.30 |
| Bound 7-hydroxy-geraniol | 0.93NS | 0.75NS | 0.55NS | 0.83NS |
| Free 7-hydroxy-nerol | 1.24NS | 2.37 | 1.00NS | 1.75NS |
| Bound 7-hydroxy-nerol | 0.24 | 0.79NS | 0.56NS | 1.06NS |
| Free citronellol | 1.94NS | 2.45 | 1.37NS | 1.79NS |
| Bound citronellol | 0.58NS | 1.74NS | 2.16 | 2.06 |
| Free 7-hydroxy-citronellol | 2.10 | 4.79 | 1.81NS | 1.72NS |
| Bound 7-hydroxy-citronellol | 0.84NS | 0.69NS | 0.41 | 0.60NS |
| Free α-terpineol | 0.44 | 1.65NS | 1.84NS | 1.74NS |
| Bound α-terpineol | 1.15NS | 1.59NS | 1.37NS | 2.13 |
| Free 4-terpineol | 0.66NS | 0.69NS | 0.64NS | 0.65NS |
| Bound 4-terpineol | 1.12NS | 1.13NS | 0.77NS | 1.42NS |
| Free hydroxy-diendiol I | 0.35 | 0.34 | 0.28 | 0.20 |
| Bound hydroxy-diendiol I | 2.03 | 3.98 | 6.58 | 8.32 |
| Free hydroxy-diendiol II | 1.17NS | 13.75 | 24.66 | 32.24 |
| Bound hydroxy-diendiol II | 1.42NS | 5.43 | 9.54 | 23.09 |
| Free hydroxy-trienol | 0.24 | 0.37 | 0.20 | 0.12 |
| Bound hydroxy-trienol | 1.97NS | 1.07NS | 0.81NS | 1.53NS |
| Free rose oxide I | 0.64NS | 1.43NS | 1.38NS | 1.31NS |
| Bound rose oxide I | 1.02NS | 1.44NS | 2.27 | 2.30 |
| Free rose oxide II | 1.00NS | 1.39NS | 1.22NS | 1.13NS |
| Bound rose oxide II | 1.00NS | 1.11NS | 1.35NS | 1.43NS |
| *C13-norisoprenoids* |  |  |  |  |
| Free 3-hydroxy-β-damascone | 1.64NS | 1.47NS | 1.00NS | 0.99NS |
| Bound 3-hydroxy-β-damascone | 2.62 | 0.68NS | 0.42 | 0.58NS |
| Free 3-oxo-α-ionol | 2.01 | 2.20 | 0.96NS | 0.53NS |
| Bound 3-oxo-α-ionol | 2.80 | 3.88 | 2.82 | 3.16 |
| Free 6-methyl-5-hepten-2-one | 0.62NS | 0.46 | 0.57NS | 0.69NS |
| Bound 6-methyl-5-hepten-2-one | 1.00NS | 0.79NS | 0.70NS | 0.73NS |
| *Phenylpropanoids/Benzenoids* |  |  |  |  |
| Free phenol | 1.19NS | 1.54NS | 0.92NS | 0.81NS |
| Bound phenol | 1.00NS | 1.60NS | 1.09NS | 1.27NS |
| Free benzyl alcohol | 1.95NS | 2.10 | 1.52NS | 1.90NS |
| Bound benzyl alcohol | 1.45NS | 1.62NS | 2.01 | 1.99NS |
| Free benzaldehyde | 0.65NS | 0.79NS | 0.59NS | 0.47 |
| Bound benzaldehyde | 0.88NS | 1.26NS | 1.16NS | 1.07NS |
| Free 2-phenylethanol | 1.80NS | 2.68 | 1.45NS | 2.14 |
| Bound 2-phenylethanol | 1.24NS | 1.37NS | 1.48NS | 1.60NS |
| Free methyl salicylate | 0.82NS | 0.73NS | 0.62NS | 0.57NS |
| Bound methyl salicylate | 3.65 | 2.65 | 4.06 | 2.70 |
| *C6 aliphatic compounds* |  |  |  |  |
| Free hexanol | 1.54NS | 1.99NS | 2.23 | 1.83NS |
| Bound hexanol | 3.05 | 4.86 | 6.74 | 6.80 |
| Free *trans*-3-hexen-1-ol | 1.34NS | 2.03 | 1.45NS | 2.00 |
| Bound *trans*-3-hexen-1-ol | 1.13NS | 1.38NS | 1.28NS | 1.38NS |
| Free *cis*-3-hexen-1-ol | 1.47NS | 1.26NS | 0.84NS | 0.55NS |
| Bound *cis*-3-hexen-1-ol | 3.65 | 4.81 | 3.81 | 2.05 |

NS = not significant (the significance is achieved with a 2-fold change between time points).