**Uncovering Taste-Active Metabolites in Chili Sauce Fermentation Through Metabolomics and Web-based Computing Tools Analysis**

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**Table S1.** Taxonomic Profiling of Fermentation-Annotated Metabolites and Their Dynamic Content Analysis.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Compounds** | **Classes** | **Dynamic Content Analysis using Mass Spectral Peak Area Quantification** | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| **0day-1** | **0day-2** | **0day-3** | | **0day-4** | | **0day-5** | | **3day-1** | | **3day-2** | | **3day-3** | | **3day-4** | | **3day-5** | | **5day-1** | | **5day-2** | | **5day-3** | | **5day-4** | | **5day-5** | |
| Acetylleucine | Amino acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 5.00E+05 | | 4.90E+05 | | 3.74E+05 | | 4.33E+05 | | 5.11E+05 | | 4.62E+05 | | 4.80E+05 | | 3.80E+05 | | 4.51E+05 | | 8.50E+05 |
| Arginine | Amino acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.25E+06 | | 1.23E+06 | | 6.21E+05 | | 1.82E+06 | | 1.23E+06 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Cyclo(proline-leucine) | Amino acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.25E+05 | | 8.86E+05 | | 5.05E+05 | | 5.06E+05 | | 5.05E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| D-Alloisoleucine | Amino acids | 1.92E+06 | 2.13E+06 | | 1.92E+06 | | 1.70E+06 | | 1.92E+06 | | 4.31E+06 | | 5.01E+06 | | 3.30E+06 | | 4.13E+06 | | 5.59E+06 | | 1.39E+06 | | 3.78E+06 | | 2.58E+06 | | 2.58E+06 | | 2.58E+06 |
| Glutamine | Amino acids | 6.24E+06 | 6.24E+06 | | 6.24E+06 | | 6.15E+06 | | 6.32E+06 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 7.96E+05 | | 7.96E+05 | | 8.35E+05 | | 7.57E+05 | | 7.97E+05 |
| Isoleucine | Amino acids | 8.47E+06 | 5.99E+06 | | 3.38E+06 | | 5.99E+06 | | 6.12E+06 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 3.05E+06 | | 3.05E+06 | | 3.41E+06 | | 2.70E+06 | | 3.05E+06 |
| L-5-Oxoproline | Amino acids | 3.26E+06 | 3.35E+06 | | 3.08E+06 | | 3.63E+06 | | 3.41E+06 | | 7.88E+06 | | 7.68E+06 | | 8.02E+06 | | 7.93E+06 | | 7.24E+06 | | 1.10E+07 | | 1.01E+07 | | 1.02E+07 | | 9.95E+06 | | 6.48E+06 |
| L-Gln | Amino acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.91E+05 | | 1.71E+05 | | 3.37E+05 | | 3.60E+05 | | 2.95E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| L-Leucine | Amino acids | 1.60E+07 | 1.40E+07 | | 1.24E+07 | | 9.37E+06 | | 1.24E+07 | | 2.24E+07 | | 1.73E+07 | | 2.07E+07 | | 5.82E+06 | | 1.82E+07 | | 3.45E+06 | | 1.98E+07 | | 2.08E+07 | | 2.13E+07 | | 1.11E+07 |
| M-Tyrosine | Amino acids | 3.28E+04 | 4.38E+04 | | 3.82E+04 | | 3.84E+04 | | 3.84E+04 | | 1.20E+06 | | 9.76E+05 | | 1.22E+06 | | 1.39E+06 | | 1.20E+06 | | 3.17E+05 | | 3.15E+05 | | 7.70E+04 | | 7.12E+04 | | 8.01E+05 |
| Phenylalanine | Amino acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 5.60E+06 | | 7.52E+06 | | 9.46E+06 | | 7.53E+06 | | 7.53E+06 | | 8.53E+06 | | 9.41E+06 | | 9.83E+06 | | 9.35E+06 | | 5.51E+06 |
| Proline | Amino acids | 5.10E+05 | 5.44E+05 | | 5.11E+05 | | 5.29E+05 | | 4.59E+05 | | 3.43E+05 | | 1.84E+05 | | 2.75E+05 | | 5.69E+05 | | 3.43E+05 | | 6.70E+04 | | 2.54E+05 | | 4.38E+05 | | 2.53E+05 | | 2.52E+05 |
| Tryptophan | Amino acids | 4.38E+06 | 3.90E+06 | | 3.86E+06 | | 4.62E+06 | | 3.77E+06 | | 4.89E+06 | | 3.48E+06 | | 3.58E+06 | | 3.60E+06 | | 3.11E+06 | | 2.38E+06 | | 2.72E+06 | | 2.49E+06 | | 2.58E+06 | | 3.00E+06 |
| Tyrosine | Amino acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 4.57E+05 | | 4.57E+05 | | 5.25E+05 | | 3.89E+05 | | 4.57E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Valine | Amino acids | 9.51E+05 | 9.45E+05 | | 9.46E+05 | | 9.45E+05 | | 9.40E+05 | | 6.74E+05 | | 6.74E+05 | | 5.44E+05 | | 8.25E+05 | | 6.53E+05 | | 5.91E+05 | | 5.92E+05 | | 4.88E+05 | | 6.95E+05 | | 5.92E+05 |
| (E)-1-(4-hydroxy-3-methoxyphenyl)dodec-4-en-3-one | Phenolics | 4.09E+05 | 3.42E+05 | | 3.43E+05 | | 3.45E+05 | | 3.34E+05 | | 3.16E+05 | | 3.23E+05 | | 2.55E+05 | | 2.20E+05 | | 2.40E+05 | | 1.91E+05 | | 2.22E+05 | | 2.09E+05 | | 1.97E+05 | | 1.88E+05 |
| 3,4-Dihydroxybenzoic acid | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.76E+05 | | 2.78E+05 | | 2.76E+05 | | 2.71E+05 | | 2.81E+05 | | 3.06E+05 | | 2.84E+05 | | 2.98E+05 | | 3.35E+05 | | 3.06E+05 |
| 3-Hydroxycinnamic acid | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.70E+05 | | 8.25E+04 | | 1.17E+05 | | 1.00E+05 | | 1.18E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| 4-ACETOXYPHENOL | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.79E+05 | | 2.90E+05 | | 2.13E+05 | | 2.15E+05 | | 2.35E+05 | | 2.83E+05 | | 2.27E+05 | | 2.11E+05 | | 2.12E+05 | | 2.08E+05 |
| 4-Coumaric acid | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 9.27E+04 | | 9.49E+04 | | 9.25E+04 | | 9.26E+04 | | 9.05E+04 |
| 4-Hydroxybenzoylcholine | Phenolics | 1.10E+05 | 9.19E+04 | | 8.54E+04 | | 8.12E+04 | | 7.56E+04 | | 1.12E+05 | | 9.64E+04 | | 9.19E+04 | | 9.29E+04 | | 9.65E+04 | | 1.84E+05 | | 8.16E+04 | | 9.84E+04 | | 9.33E+04 | | 1.26E+05 |
| 4-Methyldaphnetin | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.34E+04 | | 2.83E+04 | | 2.16E+04 | | 2.19E+04 | | 2.32E+04 | | 3.52E+04 | | 2.54E+04 | | 2.69E+04 | | 2.46E+04 | | 2.80E+04 |
| 4-Nitrophenol | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.24E+05 | | 1.21E+05 | | 1.16E+05 | | 1.17E+05 | | 1.05E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| 6,7-Dihydroxycoumarin | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 6.00E+06 | | 5.73E+06 | | 6.28E+06 | | 6.03E+06 | | 5.98E+06 | | 5.29E+06 | | 6.12E+06 | | 6.11E+06 | | 6.00E+06 | | 5.88E+06 |
| 6-Shogaol | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 7.78E+04 | | 7.24E+04 | | 5.88E+04 | | 2.61E+04 | | 5.89E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Aloe-emodin | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.29E+05 | | 1.49E+05 | | 8.39E+04 | | 1.48E+05 | | 2.33E+05 | | 2.49E+05 | | 1.21E+06 | | 1.11E+05 | | 1.06E+05 | | 4.36E+06 |
| Angelol A | Phenolics | 3.07E+04 | 2.22E+04 | | 2.04E+04 | | 2.51E+04 | | 2.10E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| CAPSAICIN | Phenolics | 6.08E+06 | 5.48E+06 | | 5.03E+06 | | 5.07E+06 | | 5.07E+06 | | 5.54E+06 | | 7.99E+06 | | 4.48E+06 | | 4.03E+06 | | 4.19E+06 | | 5.08E+06 | | 3.98E+06 | | 3.62E+06 | | 3.75E+06 | | 4.02E+06 |
| Catechol | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 3.62E+06 | | 4.49E+06 | | 6.05E+04 | | 2.11E+06 | | 2.60E+05 | | 3.94E+06 | | 2.16E+06 | | 5.65E+04 | | 2.16E+06 | | 2.48E+06 |
| Convolidine | Phenolics | 4.43E+05 | 4.57E+05 | | 4.43E+05 | | 4.29E+05 | | 4.43E+05 | | 3.88E+05 | | 2.95E+05 | | 4.07E+05 | | 3.65E+05 | | 3.93E+05 | | 4.33E+05 | | 3.72E+05 | | 3.89E+05 | | 3.60E+05 | | 3.88E+05 |
| Darutigenol | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.28E+06 | | 1.14E+06 | | 1.57E+05 | | 1.56E+05 | | 3.91E+05 | | 1.16E+06 | | 1.65E+05 | | 2.32E+05 | | 2.21E+05 | | 2.45E+06 |
| Gastrodin | Phenolics | 2.92E+05 | 2.24E+05 | | 2.42E+05 | | 2.28E+05 | | 2.23E+05 | | 9.80E+04 | | 9.80E+04 | | 8.73E+04 | | 1.09E+05 | | 9.78E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Monnieriside G | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 6.24E+04 | | 6.25E+04 | | 6.60E+04 | | 5.90E+04 | | 6.25E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| N-Vanillylnonanamide | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 5.16E+05 | | 4.66E+05 | | 4.16E+05 | | 4.66E+05 | | 4.66E+05 |
| P-Coumaric acid | Phenolics | 7.98E+05 | 6.97E+05 | | 4.49E+05 | | 8.53E+05 | | 8.65E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Salicylic acid | Phenolics | 4.95E+04 | 4.20E+04 | | 4.28E+04 | | 5.74E+04 | | 3.83E+04 | | 1.93E+05 | | 2.08E+05 | | 1.03E+05 | | 1.01E+05 | | 1.10E+05 | | 1.45E+05 | | 1.27E+05 | | 1.15E+05 | | 1.28E+05 | | 1.68E+05 |
| Trans-4-Coumaric acid | Phenolics | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.21E+06 | | 1.35E+06 | | 1.36E+06 | | 1.36E+06 | | 1.50E+06 |
| 3-hydroxyPuerarin | Flavonoids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 4.40E+04 | | 3.84E+04 | | 4.13E+04 | | 4.12E+04 | | 4.12E+04 | | 3.72E+04 | | 3.45E+04 | | 2.90E+04 | | 3.30E+04 | | 3.34E+04 |
| afzelin | Flavonoids | 2.33E+05 | 1.75E+05 | | 1.73E+05 | | 1.91E+05 | | 1.59E+05 | | 2.84E+05 | | 2.59E+05 | | 2.24E+05 | | 2.16E+05 | | 2.17E+05 | | 2.53E+05 | | 2.14E+05 | | 1.85E+05 | | 1.93E+05 | | 2.22E+05 |
| Ambocin | Flavonoids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.87E+06 | | 1.87E+06 | | 1.87E+06 | | 2.26E+06 | | 1.49E+06 |
| Apigenin | Flavonoids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 3.79E+05 | | 4.17E+05 | | 2.83E+05 | | 3.99E+05 | | 3.03E+05 | | 3.93E+05 | | 4.02E+05 | | 4.13E+05 | | 3.63E+05 | | 3.93E+05 |
| apigenin 6,8-digalactoside | Flavonoids | 3.28E+05 | 3.23E+05 | | 3.27E+05 | | 3.40E+05 | | 3.21E+05 | | 3.04E+05 | | 2.63E+05 | | 3.50E+05 | | 3.35E+05 | | 3.20E+05 | | 2.09E+05 | | 3.33E+05 | | 3.00E+05 | | 3.00E+05 | | 2.86E+05 |
| apigetrin | Flavonoids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.50E+05 | | 1.68E+05 | | 1.50E+05 | | 1.50E+05 | | 1.33E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Apiin | Flavonoids | 4.71E+04 | 3.66E+04 | | 3.54E+04 | | 3.98E+04 | | 3.97E+04 | | 6.89E+04 | | 6.89E+04 | | 6.80E+04 | | 6.98E+04 | | 6.89E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Genistein | Flavonoids | 4.76E+04 | 3.23E+04 | | 6.01E+04 | | 4.34E+04 | | 5.53E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.40E+05 | | 1.17E+05 | | 1.09E+05 | | 1.09E+05 | | 6.86E+04 |
| Isoshaftoside | Flavonoids | 6.88E+04 | 4.62E+04 | | 4.64E+04 | | 3.82E+04 | | 3.17E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 6.54E+04 | | 5.96E+04 | | 6.64E+04 | | 7.02E+04 | | 6.53E+04 |
| Kaempferol | Flavonoids | 6.87E+04 | 4.97E+04 | | 4.99E+04 | | 5.04E+05 | | 1.68E+05 | | 8.90E+04 | | 7.88E+04 | | 7.88E+04 | | 7.44E+04 | | 7.29E+04 | | 5.95E+04 | | 1.88E+05 | | 5.85E+05 | | 6.92E+04 | | 3.82E+04 |
| Kaempferol-7-O-deoxyhexoside | Flavonoids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.60E+06 | | 2.38E+06 | | 2.38E+06 | | 2.16E+06 | | 2.38E+06 | | 2.15E+06 | | 2.06E+06 | | 2.06E+06 | | 1.97E+06 | | 2.06E+06 |
| Luteolin | Flavonoids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 6.37E+05 | | 6.87E+05 | | 6.04E+05 | | 6.36E+05 | | 6.18E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Naringenin | Flavonoids | 7.76E+05 | 6.84E+05 | | 7.49E+05 | | 6.71E+05 | | 5.77E+05 | | 2.48E+05 | | 2.66E+05 | | 2.40E+05 | | 2.55E+05 | | 2.64E+05 | | 3.11E+05 | | 2.13E+05 | | 2.44E+05 | | 2.08E+05 | | 2.44E+05 |
| tiliroside | Flavonoids | 6.79E+04 | 5.01E+04 | | 5.03E+04 | | 5.61E+04 | | 5.61E+04 | | 6.62E+04 | | 7.20E+04 | | 6.43E+04 | | 6.38E+04 | | 6.46E+04 | | 5.61E+04 | | 6.60E+04 | | 6.06E+04 | | 5.79E+04 | | 6.26E+04 |
| 1-Methyladenosine | Alkaloids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 3.56E+04 | | 3.58E+04 | | 3.59E+04 | | 4.65E+04 | | 2.50E+04 | | 2.18E+04 | | 2.17E+04 | | 2.16E+04 | | 2.70E+04 | | 1.65E+04 |
| Calycanthine | Alkaloids | 5.57E+04 | 6.31E+04 | | 3.31E+04 | | 1.19E+05 | | 3.26E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| canthin-6-one | Alkaloids | 1.27E+06 | 1.34E+06 | | 1.26E+06 | | 1.17E+06 | | 1.36E+06 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Coptisine | Alkaloids | 2.73E+04 | 2.38E+04 | | 2.26E+04 | | 2.14E+04 | | 2.37E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Corynoxeine | Alkaloids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.48E+04 | | 1.48E+04 | | 1.53E+04 | | 1.48E+04 | | 1.43E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Denudatine | Alkaloids | 3.85E+04 | 3.69E+04 | | 4.71E+04 | | 3.53E+04 | | 3.95E+04 | | 1.17E+05 | | 9.07E+04 | | 8.86E+04 | | 8.81E+04 | | 1.01E+05 | | 1.23E+05 | | 1.21E+05 | | 7.18E+04 | | 8.21E+04 | | 1.09E+05 |
| dihydrocapsaicin | Alkaloids | 1.83E+06 | 1.69E+06 | | 1.59E+06 | | 1.63E+06 | | 1.71E+06 | | 1.85E+06 | | 1.46E+06 | | 1.38E+06 | | 1.31E+06 | | 1.32E+06 | | 1.72E+06 | | 1.49E+06 | | 1.28E+06 | | 1.49E+06 | | 1.48E+06 |
| feruloyltyramine | Alkaloids | 5.19E+04 | 3.80E+04 | | 4.42E+04 | | 4.65E+04 | | 4.11E+04 | | 8.69E+04 | | 8.07E+04 | | 5.53E+04 | | 5.81E+04 | | 6.07E+04 | | 1.36E+05 | | 9.03E+04 | | 6.30E+04 | | 5.66E+04 | | 1.06E+05 |
| gelsemine | Alkaloids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 7.14E+04 | | 3.08E+04 | | 5.10E+04 | | 5.10E+04 | | 5.10E+04 | | 2.23E+05 | | 1.33E+05 | | 1.33E+05 | | 1.33E+05 | | 4.27E+04 |
| Harmane | Alkaloids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.63E+05 | | 1.16E+05 | | 7.04E+04 | | 1.17E+05 | | 1.17E+05 |
| hydroquinidine | Alkaloids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.97E+05 | | 1.60E+05 | | 1.60E+05 | | 1.34E+05 | | 1.50E+05 | | 1.37E+05 | | 1.26E+05 | | 1.16E+05 | | 1.26E+05 | | 1.26E+05 |
| Lonicerin | Alkaloids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.55E+04 | | 2.56E+04 | | 2.48E+04 | | 2.55E+04 | | 2.63E+04 | | 2.40E+04 | | 2.41E+04 | | 2.40E+04 | | 2.21E+04 | | 2.57E+04 |
| Macamide B | Alkaloids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.38E+05 | | 1.51E+05 | | 1.51E+05 | | 1.92E+05 | | 1.24E+05 |
| Mesaconine | Alkaloids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.12E+04 | | 2.39E+04 | | 2.39E+04 | | 2.56E+04 | | 2.47E+04 | | 1.83E+04 | | 2.64E+04 | | 1.05E+04 | | 1.84E+04 | | 1.82E+04 |
| Nordihydrocapsaicin | Alkaloids | 6.19E+05 | 5.11E+05 | | 5.00E+05 | | 5.05E+05 | | 4.88E+05 | | 4.79E+05 | | 5.63E+05 | | 4.79E+05 | | 4.16E+05 | | 4.59E+05 | | 4.29E+05 | | 4.22E+05 | | 4.29E+05 | | 3.89E+05 | | 4.75E+05 |
| Norharman | Alkaloids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 6.16E+04 | | 3.33E+04 | | 1.22E+05 | | 1.16E+05 | | 9.66E+04 | | 1.53E+05 | | 1.69E+05 | | 1.83E+05 | | 1.64E+05 | | 1.04E+05 |
| Pilocarpine | Alkaloids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 9.49E+04 | | 9.46E+04 | | 9.47E+04 | | 6.73E+04 | | 1.22E+05 | | 5.60E+04 | | 2.02E+04 | | 5.55E+04 | | 5.60E+04 | | 9.19E+04 |
| quinine | Alkaloids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.69E+05 | | 7.47E+04 | | 1.22E+05 | | 1.22E+05 | | 1.22E+05 | | 9.24E+05 | | 4.35E+04 | | 4.33E+04 | | 4.15E+04 | | 2.34E+05 |
| Sinapine | Alkaloids | 8.55E+04 | 7.70E+04 | | 7.28E+04 | | 7.01E+04 | | 7.51E+04 | | 6.53E+04 | | 6.47E+04 | | 5.62E+04 | | 5.02E+04 | | 6.16E+04 | | 6.78E+04 | | 5.45E+04 | | 4.90E+04 | | 4.64E+04 | | 5.44E+04 |
| Theophylline | Alkaloids | 1.59E+07 | 1.56E+07 | | 1.25E+07 | | 1.39E+07 | | 9.56E+06 | | 4.51E+06 | | 6.47E+06 | | 6.79E+06 | | 7.29E+06 | | 7.29E+06 | | 2.48E+06 | | 7.32E+06 | | 2.92E+06 | | 6.59E+06 | | 4.83E+06 |
| Vinpocetine | Alkaloids | 3.17E+04 | 2.87E+04 | | 2.87E+04 | | 2.71E+04 | | 2.73E+04 | | 5.21E+04 | | 2.27E+04 | | 5.25E+04 | | 8.20E+04 | | 5.27E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| 2-Hydroxy-4-methylpentanoic acid | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 8.94E+06 | | 8.77E+06 | | 2.72E+06 | | 4.03E+06 | | 4.29E+06 | | 1.30E+07 | | 3.94E+06 | | 3.88E+06 | | 3.84E+06 | | 6.16E+06 |
| 3,4-Dihydroxyphenylacetic acid | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.51E+05 | | 1.52E+05 | | 1.67E+05 | | 1.51E+05 | | 1.36E+05 | | 1.45E+05 | | 1.45E+05 | | 1.34E+05 | | 1.56E+05 | | 1.45E+05 |
| 3-Hydroxyvaleric acid | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 3.38E+06 | | 3.27E+06 | | 6.93E+05 | | 7.28E+05 | | 1.15E+06 | | 5.29E+06 | | 7.10E+05 | | 6.72E+05 | | 6.85E+05 | | 3.21E+06 |
| 3-Phenyllactic acid | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 5.38E+06 | | 5.18E+06 | | 4.18E+06 | | 4.41E+06 | | 3.97E+06 | | 6.32E+06 | | 3.57E+06 | | 3.99E+06 | | 4.22E+06 | | 4.83E+06 |
| 5-Methoxysalicylic acid | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.21E+05 | | 4.22E+04 | | 1.31E+05 | | 1.31E+05 | | 1.31E+05 |
| Aconitic Acid | acids | 3.25E+05 | 3.16E+05 | | 2.98E+05 | | 3.26E+05 | | 3.16E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Azelaic acid | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 4.72E+05 | | 2.23E+05 | | 3.14E+05 | | 2.49E+05 | | 3.14E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| CAFFEIC ACID | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.21E+05 | | 9.49E+04 | | 9.11E+04 | | 8.89E+04 | | 7.91E+04 | | 2.30E+04 | | 6.13E+04 | | 5.18E+04 | | 3.01E+04 | | 1.02E+05 |
| Citric acid | acids | 5.36E+06 | 5.36E+06 | | 4.53E+06 | | 5.93E+06 | | 5.61E+06 | | 5.92E+06 | | 5.91E+06 | | 6.70E+06 | | 6.63E+06 | | 4.41E+06 | | 5.91E+06 | | 5.93E+06 | | 5.91E+06 | | 5.90E+06 | | 5.91E+06 |
| dihydroferulic acid | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.29E+06 | | 1.09E+06 | | 7.06E+05 | | 6.55E+05 | | 6.18E+05 | | 1.60E+06 | | 5.41E+05 | | 4.77E+05 | | 5.04E+05 | | 1.87E+06 |
| D-sorbosonic acid | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 4.07E+05 | | 1.36E+06 | | 8.85E+05 | | 8.86E+05 | | 8.85E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Ferulic Acid | acids | 1.88E+05 | 1.88E+05 | | 1.64E+05 | | 2.11E+05 | | 1.88E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Ganoderic Acid F | acids | 2.02E+04 | 1.28E+04 | | 2.62E+04 | | 2.97E+04 | | 2.21E+04 | | 4.38E+05 | | 2.16E+05 | | 1.35E+05 | | 2.47E+05 | | 2.17E+05 | | 2.32E+05 | | 2.46E+05 | | 9.22E+04 | | 1.77E+05 | | 1.38E+05 |
| Phenylpyruvic acid | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.19E+06 | | 1.24E+06 | | 1.33E+06 | | 1.31E+06 | | 1.29E+06 | | 1.23E+06 | | 1.22E+06 | | 1.21E+06 | | 1.26E+06 | | 1.23E+06 |
| Vanillic acid | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 4.21E+04 | | 4.21E+04 | | 3.84E+04 | | 4.21E+04 | | 4.57E+04 | | 5.73E+04 | | 5.68E+04 | | 5.70E+04 | | 3.88E+04 | | 7.52E+04 |
| Gluconic acid | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 5.45E+06 | | 7.88E+06 | | 6.67E+06 | | 6.67E+06 | | 6.67E+06 | | 4.92E+06 | | 4.28E+06 | | 4.28E+06 | | 4.28E+06 | | 3.65E+06 |
| Lactic acid | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.55E+07 | | 1.26E+07 | | 3.88E+07 | | 3.74E+07 | | 2.61E+07 | | 6.03E+06 | | 1.65E+07 | | 3.33E+07 | | 1.65E+07 | | 1.03E+07 |
| 3-(4-Hydroxyphenyl)lactic acid | acids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 3.30E+06 | | 2.45E+06 | | 1.50E+06 | | 1.60E+06 | | 1.66E+06 | | 1.92E+06 | | 1.70E+06 | | 1.55E+06 | | 1.52E+06 | | 2.92E+06 |
| Gentiobiose | Sugars | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 8.59E+05 | | 8.59E+05 | | 7.01E+05 | | 8.32E+05 | | 1.04E+06 | | 3.10E+05 | | 8.12E+05 | | 4.87E+05 | | 7.81E+05 | | 5.97E+05 |
| Indolelactic acid | Sugars | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.89E+06 | | 1.22E+06 | | 8.48E+05 | | 7.59E+05 | | 8.37E+05 | | 4.29E+06 | | 7.72E+05 | | 6.34E+05 | | 6.63E+05 | | 1.03E+06 |
| Isomaltulose | Sugars | 2.19E+05 | 2.19E+05 | | 2.08E+05 | | 1.60E+05 | | 2.89E+05 | | 5.95E+05 | | 6.51E+05 | | 6.24E+05 | | 6.24E+05 | | 6.23E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Melezitose | Sugars | 1.03E+05 | 8.80E+04 | | 8.79E+04 | | 7.25E+04 | | 8.82E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Melibiose | Sugars | 3.81E+05 | 2.04E+05 | | 1.47E+05 | | 2.31E+05 | | 1.88E+05 | | 3.22E+05 | | 3.24E+05 | | 3.71E+05 | | 4.07E+05 | | 3.56E+05 | | 1.00E+05 | | 4.06E+05 | | 3.10E+05 | | 3.87E+05 | | 1.54E+05 |
| 8-Acetylharpagide | Terpenoids | 2.77E+05 | 2.41E+05 | | 2.90E+05 | | 3.00E+05 | | 2.77E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| andrograpanin | Terpenoids | 2.81E+04 | 3.99E+04 | | 5.16E+04 | | 3.98E+04 | | 3.98E+04 | | 2.80E+05 | | 3.32E+05 | | 2.51E+05 | | 2.24E+05 | | 2.20E+05 | | 1.10E+05 | | 2.35E+05 | | 3.28E+05 | | 2.40E+05 | | 2.45E+05 |
| Atractylenolide III | Terpenoids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 5.80E+04 | | 2.78E+04 | | 5.23E+04 | | 9.44E+04 | | 5.85E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Cafestol | Terpenoids | 1.70E+05 | 1.21E+05 | | 1.11E+05 | | 1.31E+05 | | 1.13E+05 | | 8.93E+04 | | 9.42E+04 | | 9.16E+04 | | 9.19E+04 | | 9.17E+04 | | 1.01E+05 | | 1.01E+05 | | 1.05E+05 | | 9.68E+04 | | 1.01E+05 |
| Cryptotanshinone | Terpenoids | 1.05E+05 | 9.40E+04 | | 9.49E+04 | | 8.86E+04 | | 9.55E+04 | | 5.73E+04 | | 5.73E+04 | | 5.73E+04 | | 5.84E+04 | | 5.62E+04 | | 5.64E+04 | | 5.64E+04 | | 5.86E+04 | | 5.42E+04 | | 5.64E+04 |
| Daphylloside | Terpenoids | 1.91E+04 | 1.90E+04 | | 1.90E+04 | | 2.29E+04 | | 1.52E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Darutoside | Terpenoids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.30E+04 | | 2.36E+04 | | 2.39E+04 | | 2.35E+04 | | 2.35E+04 |
| Gentiopicrin | Terpenoids | 2.16E+05 | 1.71E+05 | | 1.73E+05 | | 1.64E+05 | | 1.74E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Ingenol | Terpenoids | 1.94E+05 | 6.36E+04 | | 1.03E+05 | | 8.26E+04 | | 7.05E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.46E+05 | | 8.44E+04 | | 8.44E+04 | | 6.90E+04 | | 3.87E+04 |
| Lathyrol | Terpenoids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 3.60E+04 | | 2.92E+04 | | 3.14E+04 | | 3.23E+04 | | 5.10E+04 |
| Lucidenic acid D | Terpenoids | 1.45E+04 | 1.44E+04 | | 1.52E+04 | | 1.44E+04 | | 1.36E+04 | | 2.03E+04 | | 2.03E+04 | | 2.32E+04 | | 2.14E+04 | | 2.18E+04 | | 2.45E+04 | | 2.45E+04 | | 2.64E+04 | | 2.27E+04 | | 2.45E+04 |
| neoandrographolide | Terpenoids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.30E+05 | | 2.12E+04 | | 2.22E+04 | | 2.00E+04 | | 6.30E+04 |
| Ophiopogonoside A | Terpenoids | 4.96E+04 | 4.76E+04 | | 4.58E+04 | | 4.53E+04 | | 4.71E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.59E+04 | | 2.59E+04 | | 2.54E+04 | | 2.63E+04 | | 2.58E+04 |
| roseoside | Terpenoids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.20E+05 | | 2.37E+05 | | 2.22E+05 | | 2.00E+05 | | 2.20E+05 | | 1.29E+05 | | 2.05E+05 | | 1.67E+05 | | 1.67E+05 | | 1.67E+05 |
| (1S,2R,9R,10S,12S)-12-hydroxy-7,15-diazatetracyclo[7.7.1.0^{2,7}.0^{10,15}]heptadecan-6-one | Ketones | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 7.23E+04 | | 9.87E+04 | | 9.86E+04 | | 9.88E+04 | | 1.25E+05 |
| (4R,4aS,6R)-6-isopropenyl-4,4a-dimethyl-4,4a,5,6,7,8-hexahydro-2(3H)-naphthalenone | Ketones | 2.10E+05 | 2.47E+05 | | 2.06E+05 | | 2.06E+05 | | 1.61E+05 | | 1.62E+05 | | 1.62E+05 | | 1.31E+05 | | 1.63E+05 | | 1.94E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| (E)-5-hydroxy-3-isobutyl-6-(3-methylbenzylidene)-1,6-dihydropyrazin-2(3H)-one | Ketones | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.63E+05 | | 1.52E+05 | | 1.58E+05 | | 1.57E+05 | | 1.58E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| 1-(4-methoxyphenyl)ethanone | Ketones | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 4.93E+04 | | 2.80E+04 | | 4.92E+04 | | 4.94E+04 | | 7.02E+04 |
| 1,10a-dihydroxy-4,4,7,11b-tetramethyl-1,2,3,4a,5,6,6a,7,11,11a-decahydronaphtho[2,1-f][1]benzofuran-9-one | Ketones | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 4.20E+05 | | 3.34E+05 | | 3.35E+05 | | 3.34E+05 | | 2.49E+05 |
| 1,2,3,4-tetrahydro-6-methoxy-1-oxo-beta-carboline | Ketones | 1.01E+05 | 7.50E+04 | | 7.78E+04 | | 7.21E+04 | | 6.34E+04 | | 5.98E+04 | | 4.18E+04 | | 6.31E+04 | | 6.11E+04 | | 5.52E+04 | | 5.58E+04 | | 6.14E+04 | | 5.89E+04 | | 5.98E+04 | | 5.86E+04 |
| 1,3,8-trihydroxy-6-methylanthra-9,10-quinone | Ketones | 6.63E+04 | 6.98E+04 | | 6.65E+04 | | 6.65E+04 | | 6.31E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| 2-(2-hydroxybut-3-en-2-yl)-3a,6,6,9a-tetramethyl-2,4,5,5a,7,8,9,9b-octahydro-1H-benzo[e][1]benzofuran-4,5-diol | Ketones | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 3.38E+05 | | 3.38E+05 | | 3.48E+04 | | 4.10E+04 | | 9.38E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| 2-Butanone, 4-[3-(beta-D-glucopyranosyloxy)-4-hydroxy-2,6,6-trimethyl-1-cyclohexen-1-yl]- | Ketones | 2.65E+05 | 2.47E+05 | | 2.38E+05 | | 2.34E+05 | | 2.32E+05 | | 8.43E+04 | | 6.72E+04 | | 1.27E+05 | | 1.30E+05 | | 1.15E+05 | | 9.17E+04 | | 1.13E+05 | | 5.21E+04 | | 1.10E+05 | | 9.18E+04 |
| 3-Buten-2-one, 4-[4-(beta-D-glucopyranosyloxy)-2-hydroxy-2,6,6-trimethylcyclohexylidene]- | Ketones | 4.04E+05 | 3.60E+05 | | 3.53E+05 | | 3.26E+05 | | 3.31E+05 | | 1.91E+05 | | 1.50E+05 | | 2.54E+05 | | 2.35E+05 | | 2.27E+05 | | 1.16E+05 | | 2.29E+05 | | 2.02E+05 | | 2.23E+05 | | 7.47E+04 |
| (-)-Riboflavin | Vitamins | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.26E+05 | | 9.62E+04 | | 6.66E+04 | | 6.89E+04 | | 7.18E+04 | | 2.10E+05 | | 6.82E+04 | | 6.53E+04 | | 6.32E+04 | | 1.25E+05 |
| (2R)-2,5,7,8-tetramethyl-2-[(4R,8R)-4,8,12-trimethyltridecyl]-3,4-dihydro-2H-chromen-6-ol | Vitamins | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 5.27E+04 | | 7.92E+04 | | 6.57E+04 | | 6.59E+04 | | 6.61E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| ADENINE | Vitamins | 2.25E+06 | 1.98E+06 | | 1.60E+06 | | 1.88E+06 | | 1.53E+06 | | 3.31E+05 | | 1.16E+06 | | 1.70E+06 | | 1.41E+06 | | 1.20E+06 | | 4.96E+05 | | 1.42E+06 | | 1.42E+06 | | 1.50E+06 | | 3.01E+05 |
| ASCORBIC ACID | Vitamins | 7.12E+05 | 9.44E+05 | | 6.18E+05 | | 1.31E+06 | | 1.14E+06 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Pantothenate | Vitamins | 2.91E+05 | 2.73E+05 | | 2.90E+05 | | 2.90E+05 | | 3.08E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| 9Z,12Z-Linoleic acid | Lipids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.84E+05 | | 1.09E+05 | | 1.84E+05 | | 2.64E+05 | | 1.79E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Cinobufagin | Lipids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 5.96E+04 | | 5.83E+04 | | 6.07E+04 | | 5.96E+04 | | 5.96E+04 |
| Dihydrosphingosine | Lipids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.62E+07 | | 1.11E+07 | | 1.37E+07 | | 1.36E+07 | | 1.37E+07 | | 4.60E+07 | | 2.95E+07 | | 2.95E+07 | | 2.95E+07 | | 1.30E+07 |
| FA 18:1+3O | Lipids | 2.69E+06 | 3.07E+06 | | 2.89E+06 | | 2.89E+06 | | 2.90E+06 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| FA 18:2+2O | Lipids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.10E+05 | | 2.10E+05 | | 3.00E+05 | | 1.20E+05 | | 2.10E+05 |
| FA 18:4+1O | Lipids | 1.55E+06 | 1.30E+06 | | 1.39E+06 | | 1.62E+06 | | 1.32E+06 | | 1.60E+06 | | 1.45E+06 | | 3.23E+06 | | 3.27E+06 | | 2.96E+06 | | 9.96E+05 | | 3.14E+06 | | 2.98E+06 | | 3.06E+06 | | 9.12E+05 |
| Heptadecanoic acid | Lipids | 4.49E+05 | 5.10E+05 | | 4.91E+05 | | 5.10E+05 | | 5.92E+05 | | 2.82E+06 | | 2.82E+06 | | 2.78E+06 | | 2.82E+06 | | 2.87E+06 | | 3.04E+06 | | 3.03E+06 | | 3.05E+06 | | 3.04E+06 | | 3.04E+06 |
| hexadecanedioic acid | Lipids | 5.84E+04 | 6.24E+04 | | 5.25E+04 | | 7.09E+04 | | 4.65E+04 | | 4.66E+05 | | 4.97E+05 | | 2.50E+05 | | 2.77E+05 | | 2.94E+05 | | 2.77E+05 | | 3.58E+05 | | 2.50E+05 | | 2.76E+05 | | 2.40E+05 |
| Myristic acid | Lipids | 3.56E+06 | 4.13E+06 | | 3.16E+06 | | 2.49E+06 | | 2.64E+06 | | 5.85E+06 | | 4.53E+06 | | 4.06E+06 | | 3.07E+06 | | 2.78E+06 | | 1.10E+07 | | 2.82E+06 | | 2.91E+06 | | 2.48E+06 | | 4.45E+06 |
| Palmitic Acid | Lipids | 1.31E+05 | 2.19E+05 | | 4.99E+05 | | 6.28E+04 | | 1.77E+05 | | 3.79E+05 | | 3.65E+05 | | 2.44E+05 | | 3.00E+05 | | 2.11E+05 | | 4.44E+05 | | 3.53E+05 | | 2.71E+05 | | 2.58E+05 | | 3.31E+05 |
| Pentadecanoic acid | Lipids | 1.81E+06 | 1.74E+06 | | 1.53E+06 | | 1.36E+06 | | 6.38E+05 | | 1.34E+06 | | 5.08E+05 | | 4.77E+05 | | 4.13E+05 | | 6.84E+05 | | 2.35E+06 | | 4.07E+05 | | 4.40E+05 | | 3.54E+05 | | 7.99E+05 |
| Phytosphingosine | Lipids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 8.44E+06 | | 6.77E+06 | | 9.01E+06 | | 9.02E+06 | | 8.51E+06 | | 4.71E+06 | | 8.44E+06 | | 7.07E+06 | | 7.59E+06 | | 5.61E+06 |
| Stearic acid | Lipids | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 4.61E+04 | | 4.81E+04 | | 4.40E+04 | | 4.60E+04 | | 4.60E+04 |
| 2-(4-oxoquinazolin-3(4H)-yl)ethyl isobutyrate | Esters | 1.75E+05 | 1.53E+05 | | 1.45E+05 | | 1.46E+05 | | 1.32E+05 | | 1.47E+05 | | 1.43E+05 | | 1.15E+05 | | 1.20E+05 | | 1.09E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| 2-hydroxy-3-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}propyl (9Z,12Z,15Z)-octadeca-9,12,15-trienoate | Esters | 8.10E+05 | 3.95E+05 | | 4.90E+05 | | 7.00E+05 | | 3.83E+05 | | 2.33E+05 | | 1.72E+05 | | 5.12E+05 | | 7.06E+05 | | 1.72E+05 | | 6.92E+04 | | 8.76E+05 | | 8.13E+05 | | 7.92E+05 | | 1.91E+05 |
| 9,12,15-Octadecatrienoic acid, 3-(hexopyranosyloxy)-2-hydroxypropyl ester, (9Z,12Z,15Z)- | Esters | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.41E+06 | | 1.41E+06 | | 1.41E+06 | | 1.41E+06 | | 1.41E+06 |
| C12-AE1S | Esters | 2.38E+05 | 3.19E+05 | | 3.20E+05 | | 3.52E+05 | | 3.69E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.09E+05 | | 2.58E+05 | | 2.69E+05 | | 1.70E+05 | | 1.38E+05 |
| C12-AS | Esters | 5.33E+05 | 5.58E+05 | | 6.34E+05 | | 8.11E+05 | | 6.34E+05 | | 4.13E+05 | | 4.13E+05 | | 4.22E+05 | | 4.22E+05 | | 3.95E+05 | | 5.27E+05 | | 6.74E+05 | | 5.42E+05 | | 4.26E+05 | | 5.42E+05 |
| Dioctyl Phthalate | Esters | 3.17E+05 | 1.98E+05 | | 1.57E+05 | | 1.30E+05 | | 2.01E+05 | | 1.00E+05 | | 8.10E+04 | | 8.79E+04 | | 8.20E+04 | | 5.91E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Propamocarb | Esters | 2.91E+06 | 2.42E+06 | | 2.44E+06 | | 2.23E+06 | | 2.39E+06 | | 1.84E+06 | | 1.34E+06 | | 1.73E+06 | | 1.53E+06 | | 1.60E+06 | | 2.70E+06 | | 1.63E+06 | | 1.61E+06 | | 1.55E+06 | | 2.05E+06 |
| Propyl gallate | Esters | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 4.50E+04 | | 4.50E+04 | | 4.68E+04 | | 4.32E+04 | | 4.49E+04 |
| Pyraclostrobin | Esters | 5.58E+05 | 5.16E+05 | | 4.49E+05 | | 4.27E+05 | | 4.43E+05 | | 2.78E+05 | | 2.89E+05 | | 2.52E+05 | | 2.57E+05 | | 2.33E+05 | | 1.95E+05 | | 2.43E+05 | | 2.30E+05 | | 2.43E+05 | | 1.77E+05 |
| (2R,3R,4S,5R)-2-(6-amino-9H-purin-9-yl)-5-(hydroxymethyl)tetrahydrofuran-3,4-diol | Others | 1.40E+05 | 1.35E+05 | | 1.12E+05 | | 1.35E+05 | | 1.53E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| (2R,3R,4S,5S,6R)-2-[6-hydroxy-3-[(E)-3-hydroxybut-1-enyl]-2,4,4-trimethylcyclohexyl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol | Others | 1.19E+05 | 1.06E+05 | | 1.06E+05 | | 1.01E+05 | | 1.00E+05 | | 5.58E+04 | | 5.58E+04 | | 5.80E+04 | | 5.78E+04 | | 5.14E+04 | | 5.23E+04 | | 5.08E+04 | | 5.27E+04 | | 5.34E+04 | | 5.23E+04 |
| (3aS,3a1S,10bR,13S)-3a-ethyl-5-(methoxycarbonyl)-1,2,3,3a,3a1,4,6,11,12,13-decahydroindolizino[8,1-cd]carbazol-13-ium iodide | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.45E+05 | | 1.16E+05 | | 1.16E+05 | | 1.16E+05 | | 8.69E+04 |
| (3R,4S,5S,6R)-2-(6-hydroxy-2,6-dimethylocta-2,7-dienoxy)-6-(hydroxymethyl)oxane-3,4,5-triol | Others | 8.04E+04 | 7.79E+04 | | 7.60E+04 | | 6.84E+04 | | 7.31E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| (3S)-5-[(1S,8aR)-2,5,5,8a-tetramethyl-4-oxo-4a,6,7,8-tetrahydro-1H-naphthalen-1-yl]-3-methylpentanoic acid | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 6.81E+05 | | 1.31E+06 | | 1.21E+05 | | 1.18E+05 | | 5.55E+05 | | 5.81E+05 | | 7.19E+05 | | 1.27E+05 | | 1.12E+05 | | 2.06E+06 |
| (4-chlorophenyl)(7,8-dimethoxy-3-methyl-2,3-dihydro-1H-benzo[d]azepin-4-yl)methanone | Others | 7.25E+05 | 7.00E+05 | | 6.34E+05 | | 6.75E+05 | | 6.84E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.89E+05 | | 1.89E+05 | | 1.87E+05 | | 1.88E+05 | | 1.94E+05 |
| (E)-3-[4-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyphenyl]prop-2-enoic acid | Others | 1.71E+06 | 1.92E+06 | | 1.31E+06 | | 1.77E+06 | | 2.01E+06 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| (E)-4-[(1R,2S,3S,4R,8aS)-2,3,4-trihydroxy-2,5,5,8a-tetramethyl-3,4,4a,6,7,8-hexahydro-1H-naphthalen-1-yl]but-3-en-2-one | Others | 2.04E+05 | 1.86E+05 | | 1.82E+05 | | 1.70E+05 | | 1.66E+05 | | 1.65E+05 | | 1.82E+05 | | 1.48E+05 | | 1.65E+05 | | 1.65E+05 | | 1.46E+05 | | 1.26E+05 | | 1.46E+05 | | 1.46E+05 | | 1.66E+05 |
| (E)-5-(1,2,4a,5-tetramethyl-7-oxo-3,4,8,8a-tetrahydro-2H-naphthalen-1-yl)-3-methylpent-2-enoic acid | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 5.83E+04 | | 5.03E+04 | | 5.04E+04 | | 5.03E+04 | | 4.23E+04 | | 2.10E+04 | | 2.09E+04 | | 2.09E+04 | | 2.11E+04 | | 2.09E+04 |
| 1-[4,5-bis(hydroxymethyl)-3-methoxy-2-methylphenoxy]-3-methylbutane-2,3-diol | Others | 1.12E+05 | 1.09E+05 | | 1.05E+05 | | 1.08E+05 | | 9.89E+04 | | 2.35E+04 | | 2.53E+04 | | 5.98E+04 | | 5.31E+04 | | 5.31E+04 | | 4.42E+04 | | 4.70E+04 | | 4.07E+04 | | 4.49E+04 | | 4.42E+04 |
| 2-(3,5-difluorophenyl)-N-(((1S,9aR)-octahydro-1H-quinolizin-1-yl)methyl)acetamide | Others | 6.84E+05 | 1.19E+06 | | 1.03E+06 | | 8.51E+05 | | 1.00E+06 | | 1.13E+06 | | 8.42E+05 | | 1.33E+06 | | 1.31E+06 | | 1.38E+06 | | 7.71E+05 | | 1.39E+06 | | 1.20E+06 | | 1.31E+06 | | 5.28E+05 |
| 2-(4-(3,4-dihydro-2H-benzo[b][1,4]dioxepin-7-yl)-3-methyl-1H-pyrazol-5-yl)-5-methoxyphenol | Others | 4.59E+04 | 4.60E+04 | | 4.60E+04 | | 4.81E+04 | | 4.39E+04 | | 8.68E+04 | | 4.90E+04 | | 6.80E+04 | | 6.77E+04 | | 6.80E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| 2-[4a-methyl-8-methylidene-4-(3-methylpentanoyloxy)-1,2,3,4,5,6,7,8a-octahydronaphthalen-2-yl]prop-2-enoic acid | Others | 1.23E+05 | 8.46E+04 | | 1.34E+05 | | 1.94E+05 | | 1.33E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| 2-Methylindole | Others | 6.23E+04 | 6.13E+04 | | 6.22E+04 | | 6.32E+04 | | 6.23E+04 | | 7.46E+04 | | 6.10E+04 | | 6.13E+04 | | 6.10E+04 | | 4.78E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| 2-Pentenoic acid, 3-[(acetyloxy)methyl]-5-[(1R,4aR,8aR)-decahydro-5,5,8a-trimethyl-2-methylene-1-naphthalenyl]-, methyl ester, (2Z)- | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.36E+04 | | 1.38E+04 | | 1.37E+04 | | 1.35E+04 | | 1.37E+04 |
| 2-Phenylethyl 2-O-[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)tetrahydro-2-furanyl]-beta-D-glucopyranoside | Others | 1.92E+05 | 1.34E+05 | | 1.92E+05 | | 2.49E+05 | | 1.91E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| 3-(sec-butyl)-2-hydroxy-3H-benzo[e][1,4]diazepin-5(4H)-one | Others | 2.43E+04 | 2.53E+04 | | 2.33E+04 | | 2.43E+04 | | 2.43E+04 | | 2.93E+04 | | 2.51E+04 | | 2.50E+04 | | 2.07E+04 | | 2.50E+04 | | 2.43E+04 | | 2.05E+04 | | 1.93E+04 | | 2.43E+04 | | 3.26E+04 |
| 4-((3S,5S,10R,13R,14S,17S)-3-(((2R,4S,5S,6R)-4,5-dihydroxy-6-methyltetrahydro-2H-pyran-2-yl)oxy)-5,14-dihydroxy-10-(hydroxymethyl)-13-methylhexadecahydro-1H-cyclopenta[a]phenanthren-17-yl)furan-2(5H)-one | Others | 1.39E+04 | 1.24E+04 | | 1.48E+04 | | 1.46E+04 | | 1.40E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| 4-(3,4-dihydroxyphenyl)-7-hydroxy-5-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-2-one | Others | 4.16E+04 | 3.31E+04 | | 3.31E+04 | | 2.95E+04 | | 2.83E+04 | | 4.56E+04 | | 4.61E+04 | | 4.50E+04 | | 4.56E+04 | | 4.56E+04 | | 6.53E+04 | | 4.40E+04 | | 5.46E+04 | | 5.45E+04 | | 5.48E+04 |
| 4-epivulgarin | Others | 5.38E+04 | 4.95E+04 | | 5.17E+04 | | 5.17E+04 | | 5.17E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 9.78E+04 | | 6.11E+04 | | 4.23E+04 | | 4.33E+04 | | 6.13E+04 |
| 4-Hydroxyquinoline | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.35E+05 | | 1.05E+05 | | 6.95E+04 | | 6.98E+04 | | 8.02E+04 | | 1.51E+05 | | 9.76E+04 | | 9.13E+04 | | 9.52E+04 | | 3.18E+05 |
| 5-(1,2,4a,5-tetramethyl-7-oxo-3,4,8,8a-tetrahydro-2H-naphthalen-1-yl)-3-methylpentanoic acid | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 3.97E+06 | | 3.92E+06 | | 2.21E+05 | | 3.11E+05 | | 2.84E+06 | | 4.06E+06 | | 5.17E+05 | | 4.98E+05 | | 4.18E+05 | | 3.88E+06 |
| 5,7-dihydroxy-2-(4-hydroxyphenyl)-4H-chromen-4-one | Others | 1.01E+05 | 8.21E+04 | | 6.46E+04 | | 8.10E+04 | | 8.24E+04 | | 1.53E+05 | | 2.72E+05 | | 1.23E+05 | | 3.30E+05 | | 8.96E+04 | | 1.50E+05 | | 2.30E+05 | | 1.06E+05 | | 1.07E+05 | | 6.83E+04 |
| 5,7-dihydroxy-2-(4-hydroxyphenyl)-8-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]-6-(3,4,5-trihydroxyoxan-2-yl)chromen-4-one | Others | 1.39E+06 | 1.37E+06 | | 1.08E+06 | | 3.26E+05 | | 1.31E+06 | | 1.23E+06 | | 1.03E+06 | | 1.14E+06 | | 1.11E+06 | | 1.05E+06 | | 9.13E+05 | | 1.32E+06 | | 9.18E+05 | | 9.90E+05 | | 3.48E+05 |
| 5-[(8aS)-2,5,5,8a-tetramethyl-3-oxo-4a,6,7,8-tetrahydro-4H-naphthalen-1-yl]-3-methylpentanoic acid | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.45E+06 | | 2.51E+06 | | 2.51E+06 | | 2.51E+06 | | 2.56E+06 |
| 5-O-methylvisammioside | Others | 4.18E+04 | 3.58E+04 | | 3.02E+04 | | 3.51E+04 | | 3.46E+04 | | 1.75E+04 | | 1.90E+04 | | 1.74E+04 | | 2.26E+04 | | 1.74E+04 | | 5.86E+04 | | 1.84E+04 | | 1.53E+04 | | 8.96E+04 | | 4.55E+04 |
| 7-[3-[3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl]oxy-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-5-hydroxy-2-(4-hydroxyphenyl)chromen-4-one | Others | 1.89E+06 | 1.32E+06 | | 1.40E+06 | | 1.46E+06 | | 1.52E+06 | | 3.52E+06 | | 3.12E+06 | | 2.47E+06 | | 2.87E+06 | | 2.37E+06 | | 3.32E+06 | | 2.48E+06 | | 2.37E+06 | | 2.72E+06 | | 2.72E+06 |
| Adenosine | Others | 4.17E+06 | 3.17E+06 | | 3.28E+06 | | 3.01E+06 | | 3.02E+06 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 8.52E+04 | | 1.92E+05 | | 1.92E+05 | | 4.07E+05 | | 8.19E+04 |
| Anileridine | Others | 1.03E+06 | 1.03E+06 | | 1.03E+06 | | 8.10E+05 | | 1.25E+06 | | 4.56E+06 | | 2.36E+06 | | 9.52E+05 | | 2.62E+06 | | 2.62E+06 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Arabinofuranosyluracil | Others | 7.83E+05 | 7.93E+05 | | 7.84E+05 | | 7.84E+05 | | 7.74E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| bonactin | Others | 6.80E+04 | 8.31E+04 | | 7.41E+04 | | 6.88E+04 | | 7.51E+04 | | 3.10E+04 | | 6.54E+04 | | 9.21E+04 | | 7.40E+04 | | 6.44E+04 | | 6.69E+04 | | 7.23E+04 | | 6.14E+04 | | 6.68E+04 | | 6.68E+04 |
| brucine | Others | 4.10E+05 | 3.93E+05 | | 3.85E+05 | | 3.65E+05 | | 3.75E+05 | | 3.92E+04 | | 6.10E+04 | | 7.74E+04 | | 6.67E+04 | | 6.08E+04 | | 5.93E+04 | | 6.85E+04 | | 5.04E+04 | | 5.89E+04 | | 5.93E+04 |
| Choline | Others | 4.66E+06 | 3.88E+06 | | 2.92E+06 | | 3.66E+06 | | 3.52E+06 | | 3.57E+06 | | 3.26E+06 | | 2.56E+06 | | 2.83E+06 | | 2.70E+06 | | 2.03E+06 | | 2.57E+06 | | 2.32E+06 | | 2.37E+06 | | 1.46E+06 |
| cordycepin | Others | 6.92E+05 | 2.59E+05 | | 2.76E+05 | | 4.59E+05 | | 1.70E+05 | | 5.96E+04 | | 3.03E+04 | | 1.89E+04 | | 1.34E+04 | | 3.06E+04 | | 2.47E+04 | | 2.23E+04 | | 1.83E+04 | | 1.97E+04 | | 2.12E+04 |
| Cyanidin | Others | 6.13E+05 | 4.57E+05 | | 4.51E+05 | | 5.24E+04 | | 4.21E+05 | | 7.73E+05 | | 7.81E+04 | | 7.07E+04 | | 5.92E+05 | | 3.78E+05 | | 7.03E+05 | | 8.63E+04 | | 4.83E+05 | | 5.36E+05 | | 6.05E+05 |
| Cyanidin-3-O-galactoside | Others | 2.83E+04 | 2.89E+04 | | 2.77E+04 | | 2.83E+04 | | 2.83E+04 | | 1.10E+05 | | 5.12E+04 | | 6.20E+04 | | 4.27E+04 | | 4.39E+04 | | 3.90E+04 | | 3.89E+04 | | 4.19E+04 | | 3.77E+04 | | 3.73E+04 |
| Cytarabine | Others | 6.46E+04 | 6.54E+04 | | 6.45E+04 | | 6.46E+04 | | 6.37E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Difenoconazole | Others | 1.66E+05 | 1.66E+05 | | 1.46E+05 | | 1.55E+05 | | 1.42E+05 | | 1.33E+05 | | 1.24E+05 | | 1.04E+05 | | 9.62E+04 | | 9.74E+04 | | 9.10E+04 | | 9.12E+04 | | 7.39E+04 | | 7.77E+04 | | 8.43E+04 |
| Dihydromethysticin | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.29E+05 | | 7.63E+04 | | 5.05E+04 | | 4.91E+04 | | 7.58E+04 |
| Dimethomorph | Others | 5.64E+04 | 5.65E+04 | | 5.84E+04 | | 6.12E+04 | | 4.98E+04 | | 7.43E+04 | | 5.49E+04 | | 4.51E+04 | | 5.28E+04 | | 5.02E+04 | | 6.46E+04 | | 4.86E+04 | | 5.32E+04 | | 4.69E+04 | | 5.27E+04 |
| Guanosine | Others | 3.35E+05 | 7.17E+05 | | 4.58E+05 | | 8.62E+05 | | 6.66E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| haplamine | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.45E+05 | | 2.71E+05 | | 2.45E+05 | | 2.45E+05 | | 2.19E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Hetisine | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 4.34E+05 | | 3.76E+05 | | 4.34E+05 | | 4.92E+05 | | 4.34E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Hydroxybutorphanol | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 1.08E+05 | | 1.23E+05 | | 9.28E+04 | | 1.08E+05 | | 1.08E+05 |
| Indole-3-acetyl-L-valine | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 7.17E+04 | | 6.52E+04 | | 6.53E+04 | | 6.52E+04 | | 5.87E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Isoproturon | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 8.82E+04 | | 5.60E+04 | | 5.66E+04 | | 5.64E+04 | | 2.42E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Lagochilin | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 4.07E+04 | | 3.42E+04 | | 2.76E+04 | | 3.41E+04 | | 3.41E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| LTD4 | Others | 5.41E+04 | 4.93E+04 | | 4.93E+04 | | 5.58E+04 | | 3.80E+04 | | 7.83E+04 | | 7.72E+04 | | 6.61E+04 | | 5.40E+04 | | 5.56E+04 | | 2.35E+05 | | 1.10E+05 | | 5.57E+04 | | 5.20E+04 | | 9.48E+04 |
| N-(3-(dimethylamino)propyl)-2-((3,4,8,8-tetramethyl-2-oxo-2,8,9,10-tetrahydropyrano[2,3-f]chromen-5-yl)oxy)acetamide | Others | 5.36E+04 | 5.16E+04 | | 5.35E+04 | | 5.53E+04 | | 5.34E+04 | | 6.59E+04 | | 4.56E+04 | | 4.55E+04 | | 3.64E+04 | | 3.40E+04 | | 4.37E+04 | | 3.88E+04 | | 7.30E+04 | | 3.76E+04 | | 2.52E+04 |
| N,N-dimethyl-7H-purin-6-amine | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 4.13E+04 | | 3.43E+04 | | 3.44E+04 | | 2.60E+04 | | 3.57E+04 | | 2.29E+05 | | 2.51E+04 | | 2.25E+04 | | 2.38E+04 | | 5.05E+04 |
| N,N-Dimethyldodecylamine N-oxide | Others | 1.50E+06 | 1.61E+06 | | 1.22E+06 | | 1.26E+06 | | 1.40E+06 | | 8.21E+05 | | 7.17E+05 | | 8.21E+05 | | 9.26E+05 | | 8.21E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| N6-benzyl-7H-purine-2,6-diamine | Others | 7.44E+04 | 7.83E+04 | | 7.40E+04 | | 8.37E+04 | | 6.08E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Phosphocholine | Others | 3.97E+05 | 4.20E+05 | | 3.03E+05 | | 4.64E+05 | | 4.12E+05 | | 8.91E+04 | | 8.92E+04 | | 8.91E+04 | | 8.74E+04 | | 9.07E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Pyridoxamine | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 5.12E+04 | | 6.22E+04 | | 5.13E+04 | | 5.13E+04 | | 4.03E+04 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| PYRIDOXINE | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 4.67E+05 | | 3.39E+05 | | 3.39E+05 | | 3.39E+05 | | 2.11E+05 | | 5.44E+05 | | 3.63E+05 | | 3.63E+05 | | 1.53E+05 | | 3.91E+05 |
| Spiroxamine | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.73E+04 | | 2.74E+04 | | 2.65E+04 | | 2.80E+04 | | 2.73E+04 |
| Tebufenozide | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 2.90E+05 | | 2.90E+05 | | 2.94E+05 | | 2.85E+05 | | 2.90E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 |
| Thiamine | Others | 1.48E+05 | 1.74E+05 | | 1.67E+05 | | 1.74E+05 | | 2.08E+05 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 6.95E+04 | | 7.70E+04 | | 6.97E+04 | | 6.22E+04 | | 6.96E+04 |
| Tramadol | Others | 0.00E+00 | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 0.00E+00 | | 9.67E+04 | | 1.52E+05 | | 8.12E+04 | | 1.23E+05 | | 6.64E+04 | | 1.30E+05 | | 1.00E+05 | | 7.44E+04 | | 1.37E+05 | | 9.04E+04 |

**Table S2.** The most representative round-rectangle nodes based on the FBMN databases.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Cluster Index | Compounds | Formula | Rt (min) | Identified *m/z* (Da) | Standard *m/z* (Da) | Delta ppm value | Adduct | Characteristic MS2  ions (*m/z*) | Standard MS2  ions (*m/z*) |
| ESI+ |  |  |  |  |  |  |  |  |  |  |
| Fig.1A. | 5748 | Linoleic acid | C18H32O2 | 11.76 | 281.2468 | 281.2475 | 2.4911 | [M+H]+ | 81.0693  95.0855  83.0846 | 81.0694  95.0851  83.0854 |
| Fig.1B. | 7344 | Phytosphingosine | C18H39NO3 | 12.94 | 318.2981 | 318.3003 | 6.9182 | [M+H]+ | 60.0435  282.2790  318.2980 | 60.0474  282.2796  318.3020 |
| Fig.1D. | 7635 | N-Fructosyl phenylalanine | C15H21NO7 | 5.13 | 328.1374 | 328.1388 | 4.2683 | [M+H]+ | 310.1280  292.1180  97.0278 | 310.12982  292.11557  97.02886 |
| Fig.1E. | 1913 | L-Phenylalanine | C9H11NO2 | 3.70 | 166.0849 | 166.0863 | 8.4337 | [M+H]+ | 77.0384  103.0540  91.0543 | 77.03862  103.05475  91.05425 |
| Fig.1F. | 12940 | Isoschaftoside | C26H28O14 | 7.20 | 565.1530 | 565.1553 | 4.0708 | [M+H]+ | 409.0910  427.1020  511.1270 | 409.0924  427.1029  511.1238 |
| ESI- |  |  |  |  |  |  |  |  |  |  |
| Fig.1H. | 5031 | FA(18:1; 3O) | C18H34O5 | 8.59 | 329.2247 | 329.2332 | 25.8359 | [M-H]- | 329.23  171.102 | 329.23273  171.10077 |
| Fig.1I. | 6772 | Afzelin | C21H20O10 | 8.22 | 431.0870 | 431.0984 | 26.4501 | [M-H]- | 285.038  284.031  431.095 | 285.0396  284.0316  431.0975 |



(B)

(C)

(F)

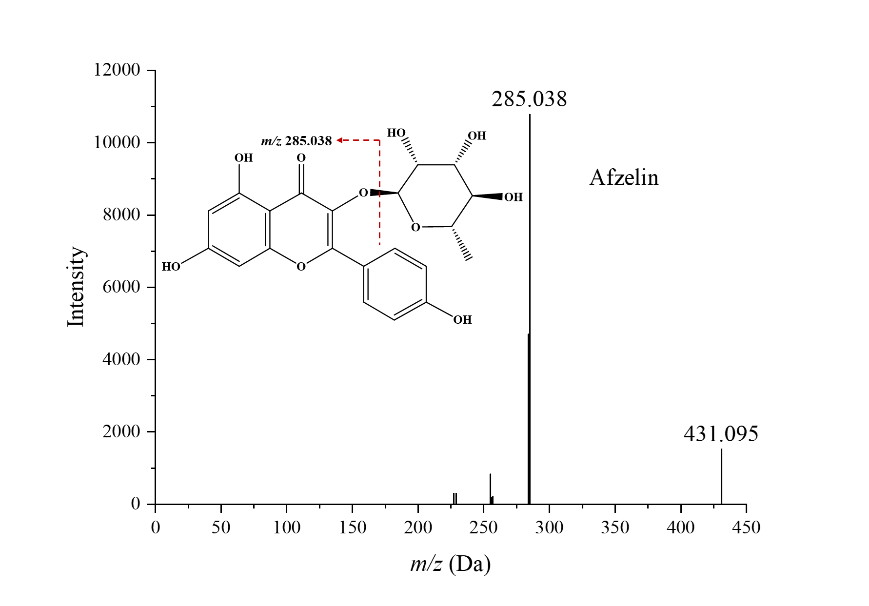
(E)

(D)

(A)



**Figure S1.** Dynamic UHPLC-QTOF Total Ion Chromatography (TIC) Profiling of Metabolites in Chili Sauce: Comparing ESI Positive and Negative Modes at 0, 3, and 5 Days. Panels (A)-(C) Displaying ESI Positive TIC, Panels (D)-(F) Displaying ESI Negative TIC.

C:\Users\Juses\Desktop\图片111111111111111111111111111111.tifC:\Users\Juses\Desktop\图片111111.tif

(A)

(B)

(C)

**Figure S2.** Molecular family and structure deduction based on MS2 spectrometry. (A) Phytosphingosine; (B) L-Phenylalanine; (C) Afzelin.