**S3 Table. Primary metabolites produced by *S. coelicolor* A3(2) grown in R2YE medium tentatively identified by time-resolved cultivation analyzed by GC-TOF-MS.**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No.** |  | **RTa(min)** | **Tentative Metaboliteb** | **Mass** | **MS Fragment** | **VIP1** | **VIP2** |  **TMS** | **IDd** |
|  | ***Amino acids*** |
| 1  |  | 5.63  | L-Alaninec | 233 | 116 45 117 75 59 | 1.27  | 0.93  | 2 | STD |
| 2  |  | 6.78  | L-Valinec | 261 | 144 45 218 145 100 | 1.35  | 1.06  | 2 | STD |
| 3  |  | 7.32  | L-Leucinec | 275 | 158 45 102 159 74 | 0.98  | 0.73  | 2 | STD |
| 4  |  | 7.54  | L-Isoleucinec | 275 | 158 45 74 75 218 | 1.15  | 0.86  | 2 | STD |
| 5  |  | 7.59  | L-Prolinec | 259 | 142 45 66 74 59 | 0.37  | 1.40  | 2 | STD |
| 6  |  | 7.67  | Glycinec | 291 | 86 174 100 45 59 | 1.52  | 1.09  | 3 | STD |
| 7  |  | 8.40  | L-Threoninec | 335 | 57 117 101 219 45 | 1.59  | 1.36  | 3 | STD |
| 8  |  | 9.52  | Aspartic acidc | 349 | 75 45 61 129 74 | 1.97  | 1.68  | 3 | STD |
| 9  |  | 9.53  | L-Methioninec | 293 | 176 128 61 45 57 | 1.58  | 1.25  | 2 | STD |
| 10  |  | 9.58  | Pidolic acid | 273 | 156 45 157 74 59 | 0.00  | 1.15  | 1 | STD |
| 11  |  | 9.61  | GABA | 319 | 174 86 45 59 175 | 0.85  | 0.71  | 3 | STD |
| 12  |  | 10.30  | Glutamic acidc | 363 | 246 75 128 45 84 | 1.78  | 1.27  | 3 | STD |
| 13  |  | 10.41  | Phenylalaninec | 309 | 218 192 100 45 74 | 1.28  | 0.98  | 2 | STD |
| 14  |  | 11.80  | L-Ornithinec | 420 | 142 174 45 74 89 | 1.16  | 0.83  | 4 | MS |
| 15  |  | 12.52  | L-Lysinec | 434 | 174 156 128 86 59 | 1.78  | 1.41  | 4 | STD |
| 16  |  | 12.65  | L-Tyrosinec | 397 | 218 100 219 45 74 | 1.80  | 1.37  | 3 | STD |
| 17  |  | 14.43  | L-Tryptophanc | 420 | 202 203 45 74 291 | 1.73  | 1.37  | 3 | STD |
|  | ***Sugars and Sugar alcohols*** |
| 18  |  | 7.34  | Glycerolc | 308 | 117 103 45 205 75 | 1.50  | 1.45  | 3 | STD |
| 19  |  | 7.88  | Glyceric acidc | 322 | 189 45 103 102 133 | 1.58  | 1.14  | 3 | MS |
| 20  |  | 9.97  | 2-Deoxy-D-ribosec | 379 | 142 103 45 174 75 | 1.30  | 1.38  | 3 | MS |
| 21  |  | 10.63  | 2-Keto-gluconic acid | 583 | 204 103 117 45 205 | 0.38  | 1.00  | 5 | MS |
| 22  |  | 11.04  | Xylitolc | 512 |  129 45 204 103 217 | 1.63  | 1.57  | 5 | STD |
| 23  |  | 12.25  | Tagatosec | 569 | 103 217 307 218 104 | 1.65  | 1.72  | 5 | STD |
| 24  |  | 12.46  | D-Glucosec | 569 | 205 160 103 319 217 | 1.73  | 1.53  | 5 | STD |
| 25  |  | 13.69  | *myo*-Inositolc | 612 | 217 191 305 103 45 | 1.54  | 1.23  | 6 | STD |
|  | ***Fatty acids*** |
| 26  |  | 6.27  | 2-Hydroxy-2-methylbutyric acid | 262 |  145 75 45 74 146 | 1.01  | 1.00  | 2 | MS |
| 27  |  | 8.48  | Glutaric acid | 276 | 55 75 45 158 97 | 1.04  | 0.88  | 2 | MS |
| 28  |  | 8.60  | 3-Deoxytetronic acid | 336 | 103 219 45 129 55 | 1.24  | 1.04  | 3 | MS |
| 29  |  | 10.38  | Valeric acid, 5-amino- | 333 | 174 82 86 45 175 | 0.95  | 0.94  | 3 | MS |
| 30  |  | 13.50  | Oleanitrile | 263 | 55 69 56 122 83 | 0.37  | 0.97  | 0 | MS |
| 31  |  | 14.26  | Elaidic acid | 326 | 75 117 55 129 67 | 1.24  | 0.89  | 1 | STD |
| 32  |  | 14.39  | Stearic acid | 356 | 117 75 132 129 55 | 1.08  | 0.77  | 1 | STD |
| 33  |  | 15.39  | Oleamide | 353 | 75 131 144 116 128 | 0.80  | 1.08  | 1 | STD |
| 34  |  | 16.28  | 1-Monopalmitin | 474 | 57 55 75 129 71 | 0.95  | 1.09  | 2 | MS |
|  | ***Organic acid*** |
| 35  |  | 5.20  | Lactic acid | 234 | 117 45 66 75 74 | 0.90  | 1.15  | 2 | STD |
| 36  |  | 5.34  | Glycolic acidc | 220 | 66 45 177 148 74 | 1.04  | 1.49  | 2 | MS |
| 37  |  | 6.98  | Ureac | 204 | 171 189 45 66 148 | 1.43  | 1.20  | 2 | MS |
| 38  |  | 7.79  | 2,3-Dihydroxy-2-methylpropanoic acid | 336 | 75 219 129 45 131 | 1.05  | 1.12  | 3 | MS |
| 39  |  | 10.28  | Anthranilic acidc | 281 | 266 45 267 75 118 | 1.56  | 1.36  | 2 | MS |
|  | ***Alcohols*** |
| 40  |  | 4.59  | Propylene glycolc | 220 | 117 66 75 74 59 | 1.34  | 1.55  | 2 | MS |
| 41  |  | 5.84  | 2-Butene-1,4-diol | 232 | 129 66 45 75 69 | 0.87  | 0.62  | 2 | MS |
| 42  |  | 9.45  | Erythritol | 410 | 103 217 117 45 205 | 1.08  | 0.82  | 4 | MS |
|  | ***Others*** |
| 43  |  | 5.76  | Hydroxylamine | 249 | 133 146 119 59 86 | 0.78  | 0.63  | 3 | MS |
| 44  |  | 7.36  | Phosphoric acid | 314 | 45 299 133 74 314 | 0.66  | 1.18  | 3 | STD |
| 45  |  | 7.96  | Uracil | 256 | 99 241 45 113 255 | 1.23  | 0.88  | 2 | MS |
| 46  |  | 13.71  | Uric acid | 456 | 45 74 441 456 100 | 0.33  | 1.18  | 4 | MS |

a Retention time; b Metabolites selected by VIP value > 0.7 based on PLS-DA (S1c Fig); c It was selected by p-value (< 0.05) based on one-way ANOVA analysis; d Identification. MS, mass spectrum was confirmed with the National Institutes of Standards and Technology (NIST) database and in-house libraries; STD, mass spectrum was consistent with that of the standard compounds; TMS, trimethylsilyl.