**S4 Table. Secondary metabolites produced by *S. coelicolor* A3(2) grown in R2YE medium tentatively identified by time-resolved cultivation analyzed by UPLC-Q-TOF-MS.**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **No.** | **Rta (min)** | **Tentative Metaboliteb** | **UPLC-Q-TOF-MS** | | | | | |  | **UHPLC-LTQ-IT-MS/MS** | | | | **IDd** |
| **[M+H]+** | **[M-H]-** | **M.W.** | **M.F.** | **Error (mDa)** | **i-Fit (norm)** |  | **MSn fragment ions** | **UV max (nm)** | **VIP1** | **VIP2** |
| ***Prodiginines*** | | | | | | | | | | | | | |  |
| 1 | 7.70 | 4-Keto-2-undecylpyrrolinec | 238.2171 | - | 237 | C15H27NO | 0.9 | - |  | 238>196>179 | 223 | 2.16 | 1.66 | Ref[S1], CCD |
| 2 | 8.05 | 23-Hydroxyundecylprodiginine | 410.2808 | 408.2651 | 409 | C25H35N3O2 | 1.2 | 0.997 |  | 410>392>377>278 | 276 533 | 0.99 | 0.80 | Ref[S2], CCD |
| 3 | 8.18 | Streptorubin Bc | 392.2702 | - | 391 | C25H33N3O | -0.6 | 0.334 |  | 392>377>252 | 280 533 | 0.94 | 1.25 | Ref[S3] |
| 4 | 9.02 | Undecylprodigiosin | 394.2858 | 392.2702 | 393 | C25H35N3O | -3.1 | 0.112 |  | 394>379>251>237 | 270 366 524 | 0.96 | 0.93 | Ref[S3] |
| ***Indoles*** | | | | | | | | | | | | | |  |
| 5 | 4.09 | Indole-3-acetic acidc | 176.0712 | 174.0555 | 175 | C10H9NO2 | 1.6 | - |  | 176>157>129>117 | 240 257 298 | 2.36 | 1.73 | Ref[S4] |
| 6 | 5.45 | Oxopropaline Dc | 271.1103 | 269.0926 | 270 | C15H14N2O3 | -0.1 | - |  | 271>257>239>211>169 | 225 291 | 0.41 | 1.40 | CCD |
| ***Germicidins*** | | | | | | | | | | | | | |  |
| 7 | 5.02 | Germicidin Bc | 183.1021 | 181.0766 | 182 | C10H14O3 | -1.1 | 0.02 |  | 183>155>137>109 | 207 288 | 0.95 | 1.66 | Ref[S5], BioCyc |
| 8 | 5.54 | Germicidin Ac | 197.1178 | 195.1021 | 196 | C11H16O3 | 1 | - |  | 197>168>151>123>97 | 204 291 | 1.46 | 1.74 | Ref[S6] |
| ***Other antibiotics*** | | | | | | | | | | | | | |  |
| 9 | 4.03 | Phaeochromycin Gc | 217.0854 | - | 216 | C13H12O3 | 0.1 | - |  | 217>174>162 | 240 291 | 1.47 | 1.40 | Ref[S7] |
| 10 | 5.95 | Antibiotic KF 77AG6c | 366.1777 | - | 365 | C16H23N5O5 | -2 | 1.192 |  | 366>348>321>226 | 218 284 301 | 2.34 | 1.79 | CCD |
| 11 | 6.23 | Violapyrone Jc | 211.1334 | - | 210 | C12H18O3 | -0.6 | 0.125 |  | 211>183>155>138 | 220 275(sh) | 1.92 | 1.76 | Ref[S8] |
| ***Diketopiperazines*** | | | | | | | | | | | | | |  |
| 12 | 3.94 | Gancidin Wc | 211.1370 | - | 210 | C11H18N2O2 | -0.4 | - |  | 211>183>154 | 268 | 1.09 | 1.74 | HMDB, CCD |
| 13 | 4.28 | Tryptophandehydrobutyrine diketopiperazine | 284.1399 | - | 283 | C16H17N3O2 | 1 | 0.008 |  | 284>267>130 | 250 282 | 0.80 | 0.90 | CCD |
| 14 | 4.95 | Cyclo(leucylphenylalanyl) | 261.1603 | - | 260 | C15H20N2O2 | 1.3 | 0.004 |  | 261>133>188>120 | 225 290 | 1.10 | 0.91 | Ref[S9], CCD |
| 15 | 5.99 | Cyclo(phenylalanyl-N-methyltryptophyl) | 348.1712 | - | 347 | C21H21N3O2 | 1.7 | 0.971 |  | 348>320>303>264 | 219 270(sh) | 2.27 | 1.72 | CCD |

a Retention time; b Metabolites selected by VIP value > 0.7 based on PLS-DA (S1d Fig); c It was selected by p-value (< 0.05) based on one-way ANOVA analysis. d Identification. CCD, *The Dictionary of Natural Products* (version 16:2, 2007, Chapman & Hall, USA); BioCys, Identification of metabolites was carried out using BioCyc Database Collection (https://biocyc.org/); HMDB, Identification of metabolites was carried out using the Human Metabolome Database (HMDB; http://www.hmdb.ca/).

**Supplementary references**

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