

## **Linoleic acid induces metabolic stress in the intestinal microorganism *Bifidobacterium breve***

**DSM 20213**

Alice Senizza<sup>1</sup>, Gabriele Rocchetti<sup>1</sup>, Maria Luisa Callegari<sup>1,2</sup>, Luigi Lucini<sup>1</sup>, Lorenzo Morelli<sup>1</sup>

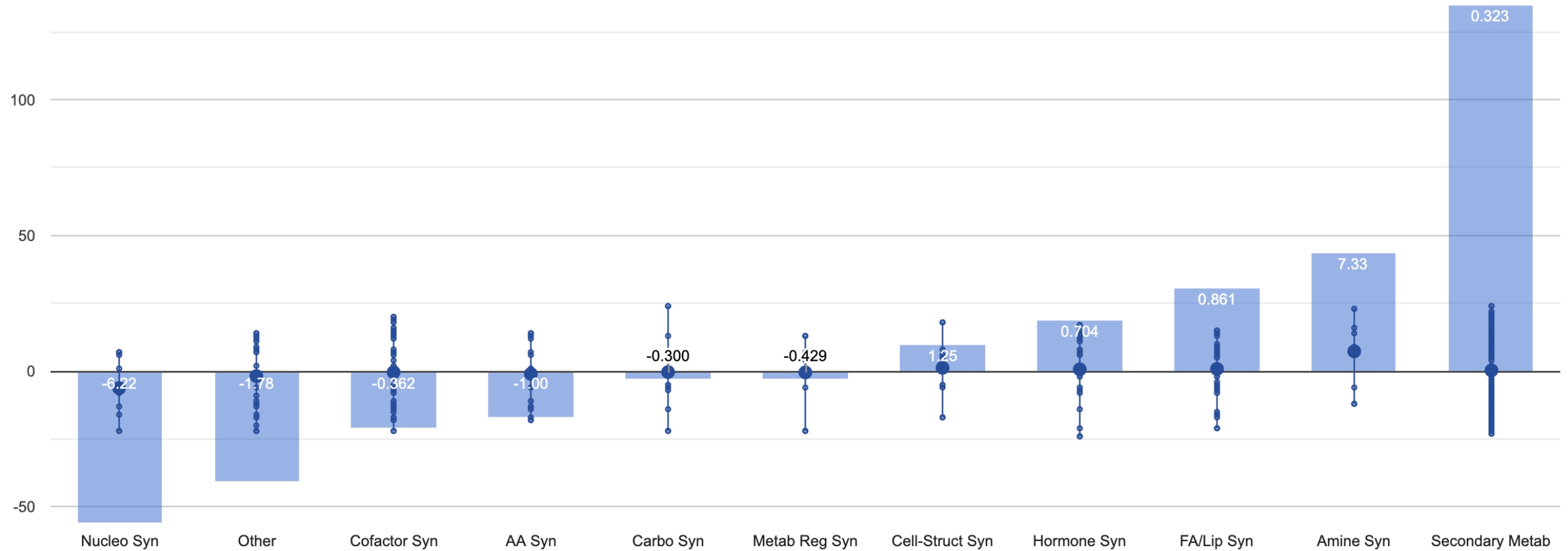
<sup>1</sup>*Department for Sustainable Food Process, Università Cattolica del Sacro Cuore, via Emilia Parmense 84, 29122 Piacenza, Italy*

<sup>2</sup>*Centre for Research on Biotechnology (CRB), Università Cattolica del Sacro Cuore, via Milano 24, 26100 Cremona, Italy*

### ***SUPPLEMENTARY MATERIAL:***

**Supplementary File 2.** Bar plot considering *B. breve* DSM 20213 + LA vs. *B. breve* DSM metabolic pathways from the Pathway Tools Omics Dashboard of MetaCyc ([www.metacyc.org](http://www.metacyc.org)).

**Supplementary File 3.** VIP markers identified by OPLS-DA multivariate analysis of UHPLC-ESI-QTOF mass spectrometry data gained from *B. breve* DSM 20213 + LA and *B. breve* DSM 20213, as imported into MetaCyc omic viewer. LogFC values for each marker at different stages of the bacterial growth curve are also provided.



## Metabolite changes, lag and log phases

| Biochemical class                      | Metacyc code          | Compound name                                   | fold-change                      |                                  |
|----------------------------------------|-----------------------|-------------------------------------------------|----------------------------------|----------------------------------|
|                                        |                       |                                                 | LA-treated vs control, lag phase | LA-treated vs control, log phase |
| Amino Acid Biosynthesis                | VAL                   | L-valine                                        | 0                                | -18                              |
| Amino Acid Biosynthesis                | LEU                   | L-leucine                                       | 0                                | 0                                |
| Amino Acid Biosynthesis                | HIS                   | L-histidine                                     | 0                                | -18                              |
| Amino Acid Biosynthesis                | PHE                   | L-phenylalanine                                 | 0                                | -16                              |
| Amino Acid Biosynthesis                | L-HISTIDINOL-P        | L-histidinol phosphate                          | 2                                | 2                                |
| Amino Acid Biosynthesis                | NADH                  | NADH                                            | 17                               | 0                                |
| Amino Acid Biosynthesis                | ILE                   | L-isoleucine (ile)                              | 0                                | -20                              |
| Amino Acid Biosynthesis                | PAPS                  | 3'-phosphoadenylyl-sulfate (PAPS)               | 15                               | -2                               |
|                                        |                       |                                                 |                                  |                                  |
| Nucleoside and Nucleotide Biosynthesis | GUANINE               | guanine                                         | -2                               | -20                              |
| Nucleoside and Nucleotide Biosynthesis | DATP                  | dATP                                            | 15                               | 0                                |
| Nucleoside and Nucleotide Biosynthesis | DUTP                  | dUTP                                            | 17                               | 0                                |
| Nucleoside and Nucleotide Biosynthesis | TTP                   | dTTP                                            | 0                                | -17                              |
| Nucleoside and Nucleotide Biosynthesis | DCTP                  | dCTP                                            | 15                               | -2                               |
| Nucleoside and Nucleotide Biosynthesis | NADH                  | NADH                                            | 17                               | 0                                |
|                                        |                       |                                                 |                                  |                                  |
| Fatty Acid and Lipid Biosynthesis      | CHOLINE               | choline                                         | 0                                | -18                              |
| Fatty Acid and Lipid Biosynthesis      | CPD-5441              | N-dimethylethanolamine phosphate                | 0                                | 8                                |
| Fatty Acid and Lipid Biosynthesis      | LINOLEIC_ACID         | linoleate                                       | 22                               | 3                                |
| Fatty Acid and Lipid Biosynthesis      | CPD-8477              | petroselinate                                   | 18                               | 2                                |
| Fatty Acid and Lipid Biosynthesis      | OLEATE-CPD            | oleate                                          | 20                               | 2                                |
| Fatty Acid and Lipid Biosynthesis      | STEARIC_ACID          | stearate                                        | -1                               | -19                              |
| Fatty Acid and Lipid Biosynthesis      | 18-OXOOLEATE          | 18-oxo-oleate                                   | 19                               | 2                                |
| Fatty Acid and Lipid Biosynthesis      | DEOXYCHOLATE          | deoxycholate                                    | -21                              | -36                              |
| Fatty Acid and Lipid Biosynthesis      | CPD-481               | sphingosylphosphorylcholine                     | -21                              | -18                              |
| Fatty Acid and Lipid Biosynthesis      | GLYCOCHOLIC_ACID      | glycocholate                                    | -1                               | -18                              |
| Fatty Acid and Lipid Biosynthesis      | CPD-7283              | taurochenodeoxycholate                          | 0                                | -18                              |
| Fatty Acid and Lipid Biosynthesis      | CPD-3743              | taurocholate                                    | 0                                | 0                                |
| Fatty Acid and Lipid Biosynthesis      | CPD-10538             | digiproside                                     | 18                               | -37                              |
| Fatty Acid and Lipid Biosynthesis      | CPD-18694             | C36-phenolphthiodiolone A                       | 17                               | -1                               |
| Fatty Acid and Lipid Biosynthesis      | CPD-18658             | C37-phenolphthiocerol A                         | -1                               | -29                              |
| Fatty Acid and Lipid Biosynthesis      | CPD-465               | presqualene diphosphate                         | 16                               | -18                              |
| Fatty Acid and Lipid Biosynthesis      | NADH                  | NADH                                            | 17                               | 0                                |
| Fatty Acid and Lipid Biosynthesis      | CPD-18625             | (behenoyl)adenylate                             | 0                                | -18                              |
| Fatty Acid and Lipid Biosynthesis      | CPD1G-69              | D-mannopyranosyl-1-phosphoheptaprenol           | 0                                | -17                              |
| Fatty Acid and Lipid Biosynthesis      | CPD-8078              | 1-18:3-2-16:2-monogalactosyldiacylglycerol      | 0                                | -1                               |
| Fatty Acid and Lipid Biosynthesis      | CPD-8086              | 1-linoleoyl-2-palmitoyl-phosphatidylglycerol    | 15                               | -18                              |
| Fatty Acid and Lipid Biosynthesis      | CPD-2190              | 1-18:3-2-16:3-monogalactosyldiacylglycerol      | 15                               | 0                                |
| Fatty Acid and Lipid Biosynthesis      | CPD-2183              | 1-oleoyl-2-palmitoyl-phosphatidylglycerol       | 15                               | 0                                |
| Fatty Acid and Lipid Biosynthesis      | CPD-8079              | 1-18:1-2-16:3-monogalactosyldiacylglycerol      | 16                               | 0                                |
| Fatty Acid and Lipid Biosynthesis      | CPD-8076              | 1-18:3-2-16:1-monogalactosyldiacylglycerol      | 4                                | 0                                |
| Fatty Acid and Lipid Biosynthesis      | CPD-8167              | 1-18:3-2-18:2-monogalactosyldiacylglycerol      | 18                               | 2                                |
| Fatty Acid and Lipid Biosynthesis      | CPD-2188              | 1-18:1-2-16:1-monogalactosyldiacylglycerol      | 18                               | 2                                |
| Fatty Acid and Lipid Biosynthesis      | CPD-8165              | 1-18:2-2-18:2-monogalactosyldiacylglycerol      | 0                                | -19                              |
| Fatty Acid and Lipid Biosynthesis      | CPD-2187              | 1-18:1-2-16:0-monogalactosyldiacylglycerol      | 0                                | -19                              |
| Fatty Acid and Lipid Biosynthesis      | CPD-8158              | 1-palmitoyl-2-linoleoyl-phosphatidylcholine     | 9                                | 0                                |
| Fatty Acid and Lipid Biosynthesis      | CPD-12644             | 1-palmitoyl-2-vernoloyl-phosphatidylcholine     | 0                                | 8                                |
| Fatty Acid and Lipid Biosynthesis      | CPD-8162              | 1-18:3-2-16:0-digalactosyldiacylglycerol        | 17                               | 0                                |
| Fatty Acid and Lipid Biosynthesis      | CPD-8081              | 1-18:3-2-18:3-digalactosyldiacylglycerol        | 10                               | -1                               |
| Fatty Acid and Lipid Biosynthesis      | CPD-8082              | 1-18:2-2-18:2-digalactosyldiacylglycerol        | 18                               | 0                                |
| Fatty Acid and Lipid Biosynthesis      | Vernolates            | vernolate                                       | 19                               | 2                                |
| Fatty Acid and Lipid Biosynthesis      | PAPS                  | 3'-phosphoadenylyl-sulfate (PAPS)               | 15                               | -2                               |
|                                        |                       |                                                 |                                  |                                  |
| Amine and Polyamine Biosynthesis       | CHOLINE               | choline                                         | 0                                | -18                              |
| Amine and Polyamine Biosynthesis       | BETAINE               | glycine betaine                                 | 0                                | -18                              |
| Amine and Polyamine Biosynthesis       | TYRAMINE              | tyramine                                        | 0                                | -17                              |
| Amine and Polyamine Biosynthesis       | CREATINE              | creatine                                        | 16                               | -11                              |
| Amine and Polyamine Biosynthesis       | HIS                   | L-histidine                                     | 0                                | -18                              |
| Amine and Polyamine Biosynthesis       | CPD-5441              | N-dimethylethanolamine phosphate                | 0                                | 8                                |
| Amine and Polyamine Biosynthesis       | NADH                  | NADH                                            | 17                               | 0                                |
|                                        |                       |                                                 |                                  |                                  |
| Secondary Metabolite Biosynthesis      | CPD-11528             | 3-oxo-2-(cis-2'-pentenyl)-cyclopentane-1-(3-oxo | 17                               | 0                                |
| Secondary Metabolite Biosynthesis      | CPD-2482              | D-cycloserine                                   | 0                                | -17                              |
| Secondary Metabolite Biosynthesis      | CPD-6361              | indolin-2-one                                   | -18                              | -18                              |
| Secondary Metabolite Biosynthesis      | CPD-8853              | 2-descarboxy-cyclo-dopa                         | 0                                | -18                              |
| Secondary Metabolite Biosynthesis      | BACIMETHRIN           | bacimethrin                                     | 0                                | -18                              |
| Secondary Metabolite Biosynthesis      | CPD-10211             | furaneol (enol form)                            | 0                                | 8                                |
| Secondary Metabolite Biosynthesis      | CPD-2205              | (E)-(4-hydroxyphenyl)acetaldehyde oxime         | -18                              | -18                              |
| Secondary Metabolite Biosynthesis      | CPD-8914              | (1H-indol-3-yl)-N-methylmethanamine             | 0                                | -19                              |
| Secondary Metabolite Biosynthesis      | 1-7-DIMETHYLYXANTHINE | paraxanthine                                    | 2                                | 2                                |
| Secondary Metabolite Biosynthesis      | CPD-18776             | (R)-4-deoxygadusol                              | 0                                | -16                              |
| Secondary Metabolite Biosynthesis      | D-GLUCARATE           | D-glucarate                                     | -17                              | -18                              |
| Secondary Metabolite Biosynthesis      | CPD-6963              | dihydrodiposylvlin                              | 0                                | -18                              |
| Secondary Metabolite Biosynthesis      | CPD-18032             | fusarinolate                                    | 0                                | -7                               |
| Secondary Metabolite Biosynthesis      | CPD-9940              | harmine                                         | 0                                | -7                               |
| Secondary Metabolite Biosynthesis      | INDOLE_PYRUVATE       | (indol-3-yl)pyruvate                            | 2                                | 2                                |
| Secondary Metabolite Biosynthesis      | 6-AMINOPENICILLANATE  | 6-aminopenicillanate                            | 0                                | -7                               |
| Secondary Metabolite Biosynthesis      | CPD-398               | (R)-3-(indol-3-yl)-2-oxobutanoate               | 0                                | -7                               |
| Secondary Metabolite Biosynthesis      | CPD-17043             | cyclo(L-phenylalanyl-L-seryl)                   | -22                              | -18                              |
| Secondary Metabolite Biosynthesis      | CPD-13616             | pentalen-13-ol                                  | 0                                | -18                              |
| Secondary Metabolite Biosynthesis      | CPD-4744              | 3-hydroxylubimin                                | -17                              | -19                              |
| Secondary Metabolite Biosynthesis      | CPD-14471             | elymoclavine aldehyde                           | 0                                | 0                                |
| Secondary Metabolite Biosynthesis      | CPD-4742              | 2-dehydrolubimin                                | -17                              | -19                              |
| Secondary Metabolite Biosynthesis      | CPD-19419             | norcraugsodine                                  | 0                                | -1                               |
| Secondary Metabolite Biosynthesis      | CPD-9366              | (-)-vestitol                                    | 18                               | -18                              |
| Secondary Metabolite Biosynthesis      | CPD-13619             | pentalenolactone                                | -22                              | -18                              |
| Secondary Metabolite Biosynthesis      | CPD-12973             | demethyldehydrophos                             | -21                              | 0                                |

|                                   |                           |                                                 |     |     |
|-----------------------------------|---------------------------|-------------------------------------------------|-----|-----|
| Secondary Metabolite Biosynthesis | CPD-12674                 | salinosporamide A                               | -21 | 0   |
| Secondary Metabolite Biosynthesis | CPD-17539                 | dapdiamide A                                    | -1  | -19 |
| Secondary Metabolite Biosynthesis | CPD-19429                 | hemanthamine                                    | -1  | -19 |
| Secondary Metabolite Biosynthesis | CPD-13541                 | kauralexin A3                                   | 19  | 3   |
| Secondary Metabolite Biosynthesis | CPD-14815                 | protoemetine                                    | 17  | -9  |
| Secondary Metabolite Biosynthesis | CPD-1777                  | coniferin                                       | -1  | -19 |
| Secondary Metabolite Biosynthesis | CPD-18058                 | prefusarin                                      | -19 | 0   |
| Secondary Metabolite Biosynthesis | CPD-17992                 | equisetin                                       | -19 | 0   |
| Secondary Metabolite Biosynthesis | CPD-12949                 | UWM6                                            | 0   | 0   |
| Secondary Metabolite Biosynthesis | CPD-15906                 | aurachin RE                                     | -4  | -20 |
| Secondary Metabolite Biosynthesis | CPD-14629                 | spinosyn tricyclic macrolactone                 | -17 | -18 |
| Secondary Metabolite Biosynthesis | CPD-17334                 | preandiloid B                                   | -1  | -18 |
| Secondary Metabolite Biosynthesis | CPD-12600                 | 2-arachidonoylglycerol                          | -1  | 0   |
| Secondary Metabolite Biosynthesis | CPD-19790                 | adlupulone                                      | -11 | -27 |
| Secondary Metabolite Biosynthesis | CPD-7110                  | lupulone                                        | -21 | -38 |
| Secondary Metabolite Biosynthesis | CPD-14627                 | 15-oxo spinosyn macrolactone                    | -1  | -18 |
| Secondary Metabolite Biosynthesis | CPD-16743                 | 13-desoxypaxilline                              | -1  | -18 |
| Secondary Metabolite Biosynthesis | CPD-17361                 | notoamide D                                     | 17  | 0   |
| Secondary Metabolite Biosynthesis | CPD-7973                  | bixin dimethyl ester                            | 0   | -17 |
| Secondary Metabolite Biosynthesis | CPD-18646                 | furostanol-26-alcohol                           | -24 | -18 |
| Secondary Metabolite Biosynthesis | CPD-16956                 | terpendole E                                    | -1  | -18 |
| Secondary Metabolite Biosynthesis | CPD-14818                 | 7'-O-demethylcephaeline                         | 0   | -1  |
| Secondary Metabolite Biosynthesis | CPD-17192                 | terpendole F                                    | 16  | -1  |
| Secondary Metabolite Biosynthesis | CPD-18332                 | lyngbyatoxin C                                  | -22 | 0   |
| Secondary Metabolite Biosynthesis | CPD-13830                 | 10-deoxymethymycin                              | -23 | -18 |
| Secondary Metabolite Biosynthesis | CPD-14502                 | steviolmonoside                                 | 10  | -2  |
| Secondary Metabolite Biosynthesis | CPD-9470                  | gypsogenin                                      | -21 | 0   |
| Secondary Metabolite Biosynthesis | CPD-14206                 | gentamicin A                                    | 7   | -9  |
| Secondary Metabolite Biosynthesis | TTP                       | dTTP                                            | 0   | -17 |
| Secondary Metabolite Biosynthesis | CPD-18226                 | guadinomine B                                   | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-14215                 | JI-20A                                          | -1  | -18 |
| Secondary Metabolite Biosynthesis | CPD-15998                 | novamethymycin                                  | -1  | -18 |
| Secondary Metabolite Biosynthesis | CPD-16839                 | fusicoccin P                                    | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-17431                 | prochaetoglobosin IV                            | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-10076                 | 3'-keto-3'-dehydroATP                           | 0   | -17 |
| Secondary Metabolite Biosynthesis | CPD-16963                 | aflatrem                                        | -1  | -18 |
| Secondary Metabolite Biosynthesis | CPD-9483                  | medicagenate                                    | -3  | -19 |
| Secondary Metabolite Biosynthesis | CPD-9474                  | gypsogenate                                     | 5   | -17 |
| Secondary Metabolite Biosynthesis | CPD-14817                 | emetine                                         | -1  | -18 |
| Secondary Metabolite Biosynthesis | CPD-13835                 | pikromycin                                      | -1  | -18 |
| Secondary Metabolite Biosynthesis | CPD-14214                 | gentamicin X2                                   | -1  | -18 |
| Secondary Metabolite Biosynthesis | CPD-17429                 | cytoglobosin D                                  | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-13834                 | narbomycin                                      | 18  | 0   |
| Secondary Metabolite Biosynthesis | CPD-17197                 | terpendole J                                    | 0   | -17 |
| Secondary Metabolite Biosynthesis | CPD-14630                 | rhamnosyl tricyclic spinosyn pseudoaglycone     | 8   | 0   |
| Secondary Metabolite Biosynthesis | CPD-14631                 | rhamnosyl tetracyclic spinosyn pseudoaglycone   | -2  | -19 |
| Secondary Metabolite Biosynthesis | CPD-13825                 | L-oleandrosyl-oleandolide                       | -1  | -18 |
| Secondary Metabolite Biosynthesis | CPD-9635                  | hyperforin                                      | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-12232                 | hordatine A                                     | -1  | -18 |
| Secondary Metabolite Biosynthesis | UDP-APIOSE                | UDP-D-apiose                                    | 0   | -17 |
| Secondary Metabolite Biosynthesis | CPD-14520                 | 2-methylbacteriohopanetetrol                    | 17  | -1  |
| Secondary Metabolite Biosynthesis | CPD-21021                 | acinetoferin                                    | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-15996                 | novapikromycin                                  | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-3764                  | desferrioxamine B                               | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-15033                 | nostoxanthin                                    | -1  | -18 |
| Secondary Metabolite Biosynthesis | CPD-20680                 | diadinoxanthin                                  | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-15032                 | caloxanthin                                     | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-17660                 | 2-hydroxycanthaxanthin                          | 16  | 0   |
| Secondary Metabolite Biosynthesis | CPD-465                   | presqualene diphosphate                         | 16  | -18 |
| Secondary Metabolite Biosynthesis | CPD-17731                 | linoleyl-AMP                                    | -1  | 0   |
| Secondary Metabolite Biosynthesis | CPD-17665                 | 2-hydroxyastaxanthin                            | 0   | -1  |
| Secondary Metabolite Biosynthesis | CPD-20691                 | amarouciaxanthin A                              | 0   | 0   |
| Secondary Metabolite Biosynthesis | CPD-20690                 | fucoxanthinol                                   | 17  | 0   |
| Secondary Metabolite Biosynthesis | CPD-14142                 | neomycin B                                      | 0   | -1  |
| Secondary Metabolite Biosynthesis | CPD-17204                 | lolitriol                                       | 0   | -1  |
| Secondary Metabolite Biosynthesis | CPD-14177                 | paromomycin                                     | 0   | -1  |
| Secondary Metabolite Biosynthesis | CPD-17957                 | apicidin                                        | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-9472                  | gypsogenin-28-beta-D-glucoside                  | 17  | 0   |
| Secondary Metabolite Biosynthesis | CPD-9475                  | gypsogenate-28-beta-D-glucoside                 | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-20679                 | fucoxanthin                                     | 0   | 0   |
| Secondary Metabolite Biosynthesis | CPD-14522                 | adenosyl hopane                                 | 18  | 1   |
| Secondary Metabolite Biosynthesis | CPD-9477                  | 16-alpha-hydroxygypsogenate-28-beta-D-glucoside | 0   | -1  |
| Secondary Metabolite Biosynthesis | CPD-13823                 | mycinamicin VI                                  | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-12803                 | fusicoccin A                                    | 0   | -1  |
| Secondary Metabolite Biosynthesis | CPD-17202                 | lolitrem B                                      | 0   | 0   |
| Secondary Metabolite Biosynthesis | CPD-8658                  | amaranthin                                      | 0   | -1  |
| Secondary Metabolite Biosynthesis | CPD-17500                 | decarboxy-dehydroxy-demycosaminyl-nystatin      | 0   | -17 |
| Secondary Metabolite Biosynthesis | CPD-13805                 | erythromycin B                                  | 0   | -1  |
| Secondary Metabolite Biosynthesis | CPD-464                   | prephytoene diphosphate                         | 0   | -17 |
| Secondary Metabolite Biosynthesis | CPD-15297                 | lampranthin II                                  | 0   | -1  |
| Secondary Metabolite Biosynthesis | CPD-17498                 | demycosaminyl-nystatin                          | -3  | -19 |
| Secondary Metabolite Biosynthesis | CPD-9916                  | staphyloxanthin                                 | 0   | -18 |
| Secondary Metabolite Biosynthesis | CPD-16625                 | monodeglucosyl des-acyl avenacin A              | 0   | -17 |
| Secondary Metabolite Biosynthesis | CPD-12680                 | 4-chloro-crotonyl-CoA                           | 19  | 2   |
| Secondary Metabolite Biosynthesis | TRANS-3-METHYL-GLUTACONYL | 3-methylglutaconyl-CoA                          | 18  | -1  |
| Secondary Metabolite Biosynthesis | CPD-12675                 | chloroethylmalonyl-CoA                          | 18  | 1   |
| Secondary Metabolite Biosynthesis | CPD-514                   | 3-oxo-3-phenylpropanoyl-CoA                     | 16  | 0   |
| Secondary Metabolite Biosynthesis | CPD-9772                  | 4-(1-methyl-2-pyrrolidinyl)-3-oxobutanoyl-CoA   | 0   | 0   |
| Secondary Metabolite Biosynthesis | CPD-12180                 | feruloylacyetyl-CoA                             | 8   | 0   |
| Secondary Metabolite Biosynthesis | P-COUMAROYL-COA           | (E)-4-coumaroyl-CoA                             | 16  | 0   |
| Secondary Metabolite Biosynthesis | CPDQT-35                  | 2-[(7'-methylsulfanyl)heptyl]malate             | -19 | -18 |

|                                   |                             |                                               |     |     |
|-----------------------------------|-----------------------------|-----------------------------------------------|-----|-----|
| Secondary Metabolite Biosynthesis | PAPS                        | 3'-phosphoadenylyl-sulfate (PAPS)             | 15  | -2  |
| Secondary Metabolite Biosynthesis | CPD-4663                    | 3-deoxycapsidiol                              | 0   | -18 |
| Secondary Metabolite Biosynthesis | MI-HEXAKISPHOSPHATE         | phytate (Ins(1,2,3,4,5,6)                     | 18  | 0   |
| Secondary Metabolite Biosynthesis | CPD-8728                    | isopimara-7,15-dienal                         | -1  | -28 |
| Secondary Metabolite Biosynthesis | AMINO-RIBOSYLAMINO-1H-3H-f  | 5-amino-6-(D-ribitylamino)uracil (ARP)        | -19 | -18 |
| Cofactor                          | CPD-15779                   | 2-(2-methylpyridin-3-yl)ethanol               | 0   | -17 |
| Cofactor                          | TYRAMINE                    | tyramine                                      | 0   | -17 |
| Cofactor                          | 2-DEHYDROPANTOYL-LACTONE    | 2-dehydropantolactone                         | 0   | 8   |
| Cofactor                          | CPD-13577                   | formylaminopyrimidine                         | 0   | -17 |
| Cofactor                          | CPD-7323                    | methanophenazine                              | -1  | -18 |
| Cofactor                          | CPD-8124                    | thio-molybdenum cofactor                      | 0   | -17 |
| Cofactor                          | 2-HEXAPRENYL-3-METHYL-5-HYC | 3-demethylubiquinol-6                         | 0   | -18 |
| Cofactor                          | UBIQUINOL-30                | ubiquinol-6                                   | 0   | 0   |
| Cofactor                          | CPD-9852                    | 3-heptaprenyl-4-hydroxybenzoate               | 0   | -1  |
| Cofactor                          | CPDQT-400                   | ADP-5-ethyl-4-methylthiazole-2-carboxylate    | 0   | 0   |
| Cofactor                          | CPD-12117                   | demethylmenaquinol-7                          | 16  | 0   |
| Cofactor                          | NADH                        | NADH                                          | 17  | 0   |
| Cofactor                          | DEAMIDO-NAD                 | nicotinate adenine dinucleotide               | 17  | 0   |
| Cofactor                          | CPD-17070                   | Fe-coproporphyrin III                         | 0   | 0   |
| Cofactor                          | 3-OCTAPRENYL-4-HYDROXYBENZ  | 3-octaprenyl-4-hydroxybenzoate                | 17  | 1   |
| Cofactor                          | NONAPRENYL-4-HYDROXYBENZ    | 3-nonaprenyl-4-hydroxybenzoate                | 0   | -1  |
| Cofactor                          | CPD-12118                   | demethylmenaquinol-9                          | 17  | 0   |
| Cofactor                          | AMINO-RIBOSYLAMINO-1H-3H-f  | 5-amino-6-(D-ribitylamino)uracil (ARP)        | -19 | -18 |
| Cofactor                          | PAPS                        | 3'-phosphoadenylyl-sulfate (PAPS)             | 15  | -2  |
| Cofactor                          | CPD-15190                   | 3-all trans-hexaprenyl-4-aminobenzoate        | 15  | -7  |
| Cofactor                          | CPD-15191                   | 3-all trans-hexaprenyl-4-amino-5-hydroxybenzo | 0   | -18 |
| Cell Structure Biosynthesis       | CHOLINE                     | choline                                       | 0   | -18 |
| Cell Structure Biosynthesis       | TYRAMINE                    | tyramine                                      | 0   | -17 |
| Cell Structure Biosynthesis       | PHE                         | L-phenylalanine                               | 0   | -16 |
| Cell Structure Biosynthesis       | 18-HYDROXYOLEATE            | 18-hydroxyoleate                              | 22  | 3   |
| Cell Structure Biosynthesis       | OLEATE-CPD                  | oleate                                        | 20  | 2   |
| Cell Structure Biosynthesis       | CPD-17640                   | 18-hydroxystearate                            | 19  | 1   |
| Cell Structure Biosynthesis       | STEARIC_ACID                | stearate                                      | -1  | -19 |
| Cell Structure Biosynthesis       | 18-OXOLEATE                 | 18-oxo-oleate                                 | 19  | 2   |
| Cell Structure Biosynthesis       | NADH                        | NADH                                          | 17  | 0   |
| Cell Structure Biosynthesis       | P-COUMAROYL-COA             | (E)-4-coumaroyl-CoA                           | 16  | 0   |
| Metabolic Regulator Biosynthesis  | HIS                         | L-histidine                                   | 0   | -18 |
| Metabolic Regulator Biosynthesis  | CREATINE                    | creatine                                      | 16  | -11 |
| Metabolic Regulator Biosynthesis  | NADH                        | NADH                                          | 17  | 0   |
| Metabolic Regulator Biosynthesis  | CARNITINE                   | L-carnitine                                   | 0   | -18 |
| Metabolic Regulator Biosynthesis  | GDP-TP                      | pppGpp                                        | 17  | -1  |

## Metabolite changes, stationary phase

| Biochemical class                      | Metacyc code                         | Compound name                                         | fold-change                             |
|----------------------------------------|--------------------------------------|-------------------------------------------------------|-----------------------------------------|
|                                        |                                      |                                                       | LA-treated vs control, stationary phase |
| Amino Acid Biosynthesis                | CYS                                  | L-cysteine                                            | 13                                      |
| Amino Acid Biosynthesis                | ACETYL-COA                           | acetyl-CoA                                            | -6                                      |
| Amino Acid Biosynthesis                | 2-AMINOACRYLATE                      | 2-aminoprop-2-enoate                                  | -17                                     |
| Amino Acid Biosynthesis                | O-SUCCINYL-L-HOMOSERINE              | O-succinyl-L-homoserine                               | 6                                       |
| Amino Acid Biosynthesis                | MET                                  | L-methionine                                          | 7                                       |
| Amino Acid Biosynthesis                | HISTIDINOL                           | histidinol                                            | -1                                      |
| Amino Acid Biosynthesis                | IMIDAZOLE-ACETOL-P                   | 3-(imidazol-4-yl)-2-oxopropyl phosphate               | -2                                      |
| Amino Acid Biosynthesis                | D-ERYTHRO-IMIDAZOLE-GLYCEROL-P       | D-erythro-1-(imidazol-4-yl)-glycerol 3-phosphate      | -2                                      |
| Amino Acid Biosynthesis                | IMIDAZOLE-LACTATE                    | imidazole-lactate                                     | -14                                     |
| Amino Acid Biosynthesis                | CPD-31                               | (R)-citramalate                                       | -13                                     |
| Amino Acid Biosynthesis                | SUC-COA                              | succinyl-CoA                                          | 7                                       |
| Amino Acid Biosynthesis                | CPD-68                               | 1-aminocyclopropane-1-carboxylate                     | 7                                       |
| Amino Acid Biosynthesis                | SHIKIMATE-5P                         | shikimate 3-phosphate                                 | -11                                     |
| Amino Acid Biosynthesis                | TYR                                  | L-tyrosine                                            | 14                                      |
| Amino Acid Biosynthesis                | CARBOXYPHENYLAMINO-DEOXYRIBULOSE-P   | 1-(2-carboxyphenylamino)-1-deoxy-D-ribose 5-phospha   | -18                                     |
| Amino Acid Biosynthesis                | TRP                                  | L-tryptophan (trp)                                    | 12                                      |
| Amino Acid Biosynthesis                | INDOLE                               | indole                                                | 1                                       |
|                                        |                                      |                                                       |                                         |
| Nucleoside and Nucleotide Biosynthesis | XANTHINE                             | xanthine                                              | -8                                      |
| Nucleoside and Nucleotide Biosynthesis | XANTHOSINE                           | xanthosine                                            | 7                                       |
| Nucleoside and Nucleotide Biosynthesis | INOSINE                              | inosine                                               | -13                                     |
| Nucleoside and Nucleotide Biosynthesis | PHOSPHORIBOSYL-FORMAMIDO-CARBOXAMIDE | 5-formamido-1-(5-phospho-D-ribosyl)-imidazole-4-carbo | -6                                      |
| Nucleoside and Nucleotide Biosynthesis | GTP                                  | GTP                                                   | -22                                     |
| Nucleoside and Nucleotide Biosynthesis | TTP                                  | dTTP                                                  | 1                                       |
| Nucleoside and Nucleotide Biosynthesis | TDP                                  | dTDP                                                  | -5                                      |
| Nucleoside and Nucleotide Biosynthesis | UMP                                  | UMP                                                   | 6                                       |
| Nucleoside and Nucleotide Biosynthesis | OROTATE                              | orotate                                               | -16                                     |
|                                        |                                      |                                                       |                                         |
| Fatty Acid and Lipid Biosynthesis      | ACETYL-COA                           | acetyl-CoA                                            | -6                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-10512                            | 16-oxo-palmitate                                      | -6                                      |
| Fatty Acid and Lipid Biosynthesis      | TDP                                  | dTDP                                                  | -5                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-12644                            | 1-palmitoyl-2-vernoloyl-phosphatidylcholine           | 2                                       |
| Fatty Acid and Lipid Biosynthesis      | DODECANOATE                          | laurate                                               | 8                                       |
| Fatty Acid and Lipid Biosynthesis      | CPD-7836                             | myristate                                             | 13                                      |
| Fatty Acid and Lipid Biosynthesis      | ARACHIDONIC_ACID                     | arachidonate                                          | -2                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-9245                             | palmitoleate                                          | -16                                     |
| Fatty Acid and Lipid Biosynthesis      | CPD-8073                             | 1-18:2-2-16:0-monogalactosyldiacylglycerol            | 9                                       |
| Fatty Acid and Lipid Biosynthesis      | CPD-8075                             | 1-18:2-2-16:1-monogalactosyldiacylglycerol            | -7                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-8163                             | 1-16:0-2-18:2-digalactosyldiacylglycerol              | 15                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-8168                             | 1-18:3-2-18:3-monogalactosyldiacylglycerol            | 14                                      |
| Fatty Acid and Lipid Biosynthesis      | UMP                                  | UMP                                                   | 6                                       |
| Fatty Acid and Lipid Biosynthesis      | GLYCEROL                             | glycerol                                              | 5                                       |
| Fatty Acid and Lipid Biosynthesis      | CPD0-1812                            | 2-oleoylglycerol                                      | 9                                       |
| Fatty Acid and Lipid Biosynthesis      | CPD-18709                            | (palmitoyl)adenylate                                  | -8                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-18617                            | p-HBAD-I                                              | -4                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-18623                            | 17-(4-hydroxyphenyl)heptadecanoate                    | 14                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-18655                            | C34-phenolphthiodiolone A                             | 9                                       |
| Fatty Acid and Lipid Biosynthesis      | CPD-18654                            | C34-phenolphthiotriol A                               | -8                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-18670                            | C35-phenolcarboxyphthiodiolenone                      | 7                                       |
| Fatty Acid and Lipid Biosynthesis      | CPD-18671                            | C37-phenolcarboxyphthiodiolenone                      | 1                                       |
| Fatty Acid and Lipid Biosynthesis      | CPD-18660                            | C36-phenolphthiodiolenone A                           | 10                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-18659                            | 19-(4-hydroxyphenyl)nonadecanoyl adenylate            | -7                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-8086                             | 1-linoleoyl-2-palmitoyl-phosphatidylglycerol          | 15                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-8091                             | 1-oleoyl-2-linoleoyl-phosphatidylcholine              | 1                                       |
| Fatty Acid and Lipid Biosynthesis      | CPD-2182                             | 1-linoleoyl-2-linoleoyl-phosphatidylcholine           | -15                                     |
| Fatty Acid and Lipid Biosynthesis      | CPD-18629                            | C33-phthiodiolone A                                   | -6                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-18630                            | C33-phthiotriol A                                     | 13                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-13611                            | icosasphinganine                                      | 7                                       |
| Fatty Acid and Lipid Biosynthesis      | SPHINGOSINE                          | sphingosine                                           | 15                                      |
| Fatty Acid and Lipid Biosynthesis      | CPD-14901                            | poriferst-7-enol                                      | -16                                     |
| Fatty Acid and Lipid Biosynthesis      | CPD-3743                             | taurocholate                                          | 8                                       |
| Fatty Acid and Lipid Biosynthesis      | CPD-7283                             | taurochenodeoxycholate                                | -17                                     |
| Fatty Acid and Lipid Biosynthesis      | CPD-707                              | campesterol                                           | -21                                     |
| Fatty Acid and Lipid Biosynthesis      | CPD-4181                             | cycloartanol                                          | -1                                      |
| Fatty Acid and Lipid Biosynthesis      | 3-OXO-5-BETA-CHOLANATE               | 3-dehydrolithocholate                                 | 8                                       |
|                                        |                                      |                                                       |                                         |
| Amine and Polyamine Biosynthesis       | BETAINE-ALDEHYDE-HYDRATE             | betaine aldehyde hydrate                              | -12                                     |
| Amine and Polyamine Biosynthesis       | ACETYL-COA                           | acetyl-CoA                                            | -6                                      |
| Amine and Polyamine Biosynthesis       | CPD-9995                             | carboxynorspermidine                                  | 16                                      |
| Amine and Polyamine Biosynthesis       | TYR                                  | L-tyrosine                                            | 14                                      |
| Amine and Polyamine Biosynthesis       | CPD-58                               | octopamine                                            | 9                                       |
| Amine and Polyamine Biosynthesis       | CPD-10012                            | carboxyspermidine                                     | 23                                      |
|                                        |                                      |                                                       |                                         |
| Carbohydrate Biosynthesis              | L-SORBOSONE                          | L-sorbose                                             | -14                                     |
| Carbohydrate Biosynthesis              | UMP                                  | UMP                                                   | 6                                       |
| Carbohydrate Biosynthesis              | TDP                                  | dTDP                                                  | -5                                      |
| Carbohydrate Biosynthesis              | ACETYL-COA                           | acetyl-CoA                                            | -6                                      |
| Carbohydrate Biosynthesis              | GTP                                  | GTP                                                   | -22                                     |
| Carbohydrate Biosynthesis              | DPG                                  | 3-phospho-D-glyceroyl phosphate (13-DPG)              | 13                                      |
| Carbohydrate Biosynthesis              | CPD-464                              | prephytoene diphosphate                               | -7                                      |
| Carbohydrate Biosynthesis              | MET                                  | L-methionine                                          | 7                                       |
| Carbohydrate Biosynthesis              | TTP                                  | dTTP                                                  | 1                                       |
| Carbohydrate Biosynthesis              | CPD-17206                            | GDP-mycosamine                                        | 24                                      |
|                                        |                                      |                                                       |                                         |
| Secondary Metabolite Biosynthesis      | CPD-17074                            | (-)-microperfurane                                    | 16                                      |
| Secondary Metabolite Biosynthesis      | TRP                                  | L-tryptophan (trp)                                    | 12                                      |
| Secondary Metabolite Biosynthesis      | SUC-COA                              | succinyl-CoA                                          | 7                                       |
| Secondary Metabolite Biosynthesis      | CPD-7901                             | 2-tridecanone                                         | 7                                       |
| Secondary Metabolite Biosynthesis      | CPD-10227                            | 1-deoxy-1-imino-D-erythrose 4-phosphate               | 4                                       |
| Secondary Metabolite Biosynthesis      | STERIGMATOCYSTIN                     | sterigmatocystin                                      | -20                                     |
| Secondary Metabolite Biosynthesis      | CPD-16743                            | 13-desoxyxaxilline                                    | 15                                      |
| Secondary Metabolite Biosynthesis      | CPD-16963                            | afatrem                                               | -9                                      |
| Secondary Metabolite Biosynthesis      | CPD-17337                            | andilesin D                                           | -14                                     |
| Secondary Metabolite Biosynthesis      | ACETYL-COA                           | acetyl-CoA                                            | -6                                      |
| Secondary Metabolite Biosynthesis      | CPD-16792                            | rhizoctin B                                           | 6                                       |
| Secondary Metabolite Biosynthesis      | OLEANDOMYCIN                         | oleandomycin                                          | 15                                      |

|                                   |                       |                                                         |     |
|-----------------------------------|-----------------------|---------------------------------------------------------|-----|
| Secondary Metabolite Biosynthesis | CPD-13826             | L-oliviosyl-oleandolide                                 | 8   |
| Secondary Metabolite Biosynthesis | CPD-13827             | oleandolide                                             | 22  |
| Secondary Metabolite Biosynthesis | DEMETHYLMACROCIN      | demethylmacrocin                                        | 7   |
| Secondary Metabolite Biosynthesis | TYLOSIN               | tylosin                                                 | 20  |
| Secondary Metabolite Biosynthesis | CPD-16508             | L-(4-hydroxyphenyl)glycine                              | -18 |
| Secondary Metabolite Biosynthesis | CPD-9418              | nocardicin G                                            | -6  |
| Secondary Metabolite Biosynthesis | CPD-14209             | G-418                                                   | -14 |
| Secondary Metabolite Biosynthesis | CPD-14213             | gentamicin C1                                           | 15  |
| Secondary Metabolite Biosynthesis | CPD-14212             | gentamicin C2a                                          | 8   |
| Secondary Metabolite Biosynthesis | CPD-15229             | 3'-phospho-JI-20A                                       | -7  |
| Secondary Metabolite Biosynthesis | CPD-17208             | 18-hydroxy candicidinolide                              | 6   |
| Secondary Metabolite Biosynthesis | CPD-17193             | candicidinolide                                         | 5   |
| Secondary Metabolite Biosynthesis | CPD-19834             | 8-demethyl-8-(methylamino)riboflavin                    | -7  |
| Secondary Metabolite Biosynthesis | CPD-12847             | pyocyanin                                               | 7   |
| Secondary Metabolite Biosynthesis | CPD-17531             | L-dihydroanticapsin                                     | 9   |
| Secondary Metabolite Biosynthesis | CPD-17508             | bacilysin                                               | 1   |
| Secondary Metabolite Biosynthesis | CPD-10013             | bialaphos                                               | -7  |
| Secondary Metabolite Biosynthesis | CPD-18284             | sch210971                                               | 8   |
| Secondary Metabolite Biosynthesis | CPD-13831             | 10-deoxymethynolide                                     | -7  |
| Secondary Metabolite Biosynthesis | CPD-13830             | 10-deoxymethymycin                                      | 1   |
| Secondary Metabolite Biosynthesis | CPD-13619             | pentalenolactone                                        | 7   |
| Secondary Metabolite Biosynthesis | CPD-13622             | pentalenolactone F                                      | -22 |
| Secondary Metabolite Biosynthesis | CPD-20141             | 6'-chloromelleolide F                                   | 15  |
| Secondary Metabolite Biosynthesis | CPD-12952             | dehydrorabelomycin                                      | -5  |
| Secondary Metabolite Biosynthesis | CPD-14187             | 6'''-hydroxyparomomycin                                 | 1   |
| Secondary Metabolite Biosynthesis | CPD-14188             | 6'''-oxoparomomycin                                     | -14 |
| Secondary Metabolite Biosynthesis | CPD-15934             | protomycinolide IV                                      | -14 |
| Secondary Metabolite Biosynthesis | CPD-13820             | mycinamicin III                                         | -8  |
| Secondary Metabolite Biosynthesis | CPD-13822             | mycinamicin II                                          | -7  |
| Secondary Metabolite Biosynthesis | CPD-13821             | mycinamicin IV                                          | 8   |
| Secondary Metabolite Biosynthesis | CPD-17541             | dapdiamide C                                            | 9   |
| Secondary Metabolite Biosynthesis | CPD-17540             | dapdiamide B                                            | 16  |
| Secondary Metabolite Biosynthesis | CPD-15965             | 2-oxo-4-phosphonobutanoate                              | -16 |
| Secondary Metabolite Biosynthesis | CPD-17786             | griseofulvin                                            | 18  |
| Secondary Metabolite Biosynthesis | CPD-11755             | dichloro-arcyriaflavin A                                | -16 |
| Secondary Metabolite Biosynthesis | CPD-11754             | dichlorochromopyrrolate                                 | -6  |
| Secondary Metabolite Biosynthesis | CPD-17957             | apicidin                                                | 4   |
| Secondary Metabolite Biosynthesis | CPD-15531             | 5-hydroxymethylcytosine                                 | 1   |
| Secondary Metabolite Biosynthesis | CPD0-2021             | bacimethrin pyrophosphate                               | 13  |
| Secondary Metabolite Biosynthesis | CPDMETA-13642         | neopentalenoketolactone                                 | -10 |
| Secondary Metabolite Biosynthesis | CPD-16513             | saframycin A                                            | 1   |
| Secondary Metabolite Biosynthesis | CPD-16512             | 3-hydroxy-5-methyl-L-tyrosine                           | -13 |
| Secondary Metabolite Biosynthesis | CPD-18559             | 3-hydroxyquinaldate adenylate                           | 6   |
| Secondary Metabolite Biosynthesis | STREPTOMYCIN          | streptomycin                                            | 2   |
| Secondary Metabolite Biosynthesis | CPD-12972             | [1-(2-amino-4-methylpentanamido)ethenyl]phosphonate     | -4  |
| Secondary Metabolite Biosynthesis | CPD-17787             | griseophenone C                                         | -20 |
| Secondary Metabolite Biosynthesis | CPD-17799             | desmethyl-dehydro-dechlorogriseofulvin                  | -14 |
| Secondary Metabolite Biosynthesis | CPD-17800             | dechloro-dehydrogriseofulvin                            | -7  |
| Secondary Metabolite Biosynthesis | CPD-11887             | K252a                                                   | 4   |
| Secondary Metabolite Biosynthesis | CPD-11889             | K252b                                                   | 13  |
| Secondary Metabolite Biosynthesis | CPD-17158             | arginomycin                                             | 6   |
| Secondary Metabolite Biosynthesis | CPD-17164             | L-leucyl-arginomycin                                    | 1   |
| Secondary Metabolite Biosynthesis | CPD-13894             | 4-propyl-L-proline                                      | 20  |
| Secondary Metabolite Biosynthesis | CPD-13835             | pikromycin                                              | -2  |
| Secondary Metabolite Biosynthesis | CPD-18203             | 4-amino-2-(methanethioyl)-5-oxo-3-sulfanylpyrrolidine-2 | -11 |
| Secondary Metabolite Biosynthesis | CPD-17948             | holothin                                                | 13  |
| Secondary Metabolite Biosynthesis | CPD-15467             | 3-dimethylallyl-4-hydroxyphenylpyruvate                 | -12 |
| Secondary Metabolite Biosynthesis | TYR                   | L-tyrosine                                              | 14  |
| Secondary Metabolite Biosynthesis | CPD-18932             | 2-(phosphinatomethylidene)butanedioate                  | -16 |
| Secondary Metabolite Biosynthesis | CPD-10011             | demethyl-L-phosphinothricin                             | 1   |
| Secondary Metabolite Biosynthesis | CPD-18977             | pseudomonate C                                          | 8   |
| Secondary Metabolite Biosynthesis | CPD-7733              | aurachin C                                              | 15  |
| Secondary Metabolite Biosynthesis | CPD-15912             | aurachin B epoxide                                      | -15 |
| Secondary Metabolite Biosynthesis | CPD-15909             | aurachin D                                              | 17  |
| Secondary Metabolite Biosynthesis | CPD-16638             | 12-demethyl-elloramycin                                 | -6  |
| Secondary Metabolite Biosynthesis | CPD-13100             | toyocamycin phosphate                                   | -17 |
| Secondary Metabolite Biosynthesis | ANHYPOTETRACYCLINE    | anhydrotetracycline                                     | -6  |
| Secondary Metabolite Biosynthesis | CPD0-1414             | tetracycline                                            | 5   |
| Secondary Metabolite Biosynthesis | CPD-17874             | 5-hydroxy-desmethylantrhothainin                        | 11  |
| Secondary Metabolite Biosynthesis | CPD-17871             | previridatum toxin                                      | -1  |
| Secondary Metabolite Biosynthesis | CPD-11909             | dTDP-L-ristosamine                                      | 16  |
| Secondary Metabolite Biosynthesis | CPD-11789             | K-252c                                                  | -14 |
| Secondary Metabolite Biosynthesis | CPD-11786             | chromopyrrolate                                         | 1   |
| Secondary Metabolite Biosynthesis | CYS                   | L-cysteine                                              | 13  |
| Secondary Metabolite Biosynthesis | CPD-18437             | 3-hydroxy-4-methyl-anthranilate pentapeptide lactone    | 9   |
| Secondary Metabolite Biosynthesis | CPD-18448             | 3-hydroxy-4-methylantranilyl-adenylate                  | -11 |
| Secondary Metabolite Biosynthesis | CPD-17739             | echinocandin D                                          | 18  |
| Secondary Metabolite Biosynthesis | CPD-17711             | echinocandin B                                          | 12  |
| Secondary Metabolite Biosynthesis | CPD-17212             | nystatin A1                                             | 13  |
| Secondary Metabolite Biosynthesis | CPD-17206             | GDP-mycosamine                                          | 24  |
| Secondary Metabolite Biosynthesis | CPD-12966             | mevalomycin A                                           | 7   |
| Secondary Metabolite Biosynthesis | CPD-13951             | erythromycin C                                          | 8   |
| Secondary Metabolite Biosynthesis | TTP                   | dTTP                                                    | 1   |
| Secondary Metabolite Biosynthesis | CPD-14156             | 2'-deamino-2'-hydroxy-6'-dehydroparomamine              | -14 |
| Secondary Metabolite Biosynthesis | CPD-14127             | 2'-deamino-2'-hydroxyparomamine                         | -7  |
| Secondary Metabolite Biosynthesis | CPD-15254             | 2'-dehydrokanamycin A                                   | -15 |
| Secondary Metabolite Biosynthesis | CPD-4822              | kanamycin B                                             | 15  |
| Secondary Metabolite Biosynthesis | GTP                   | GTP                                                     | -22 |
| Secondary Metabolite Biosynthesis | CPD-18787             | GDP-valienol                                            | 7   |
| Secondary Metabolite Biosynthesis | CPD-18790             | validamycin B                                           | 8   |
| Secondary Metabolite Biosynthesis | CPD-18226             | guadinomine B                                           | 8   |
| Secondary Metabolite Biosynthesis | CPD-15729             | methyl aknanonate                                       | 5   |
| Secondary Metabolite Biosynthesis | CPD-15733             | 13-deoxydaunorubicin                                    | -13 |
| Secondary Metabolite Biosynthesis | CPD-15735             | 13-dihydrodaunorubicin                                  | 4   |
| Secondary Metabolite Biosynthesis | CPD-15736             | 13-dihydrocarminomycin                                  | 6   |
| Secondary Metabolite Biosynthesis | AMIDINOPROCLAVAMINATE | amidinoproclavaminat                                    | -15 |
| Secondary Metabolite Biosynthesis | CPD-17169             | L-leucyl-demethyl-blasticidin S                         | 2   |
| Secondary Metabolite Biosynthesis | CPD-17168             | L-leucyl-blasticidin S                                  | 8   |
| Secondary Metabolite Biosynthesis | CPD-10236             | rifamycin SV                                            | 9   |

|                                   |                             |                                               |     |
|-----------------------------------|-----------------------------|-----------------------------------------------|-----|
| Secondary Metabolite Biosynthesis | CPD-16644                   | tetracenomycin B3                             | 1   |
| Secondary Metabolite Biosynthesis | UMP                         | UMP                                           | 6   |
| Secondary Metabolite Biosynthesis | CPD-398                     | (R)-3-(indol-3-yl)-2-oxobutanoate             | 6   |
| Secondary Metabolite Biosynthesis | CPD-18934                   | indolmycenate                                 | 16  |
| Secondary Metabolite Biosynthesis | CPD0-920                    | indolmycin                                    | 8   |
| Secondary Metabolite Biosynthesis | CPD-14167                   | 6'''-deamino-6'''-oxoneomycin C               | 8   |
| Secondary Metabolite Biosynthesis | CPD-10151                   | 2-deoxystreptamine                            | 7   |
| Secondary Metabolite Biosynthesis | TDP                         | dTDP                                          | -5  |
| Secondary Metabolite Biosynthesis | CPD-428                     | 6-deoxyerythronolide B                        | 13  |
| Secondary Metabolite Biosynthesis | CPD-9122                    | penicillin K                                  | 7   |
| Secondary Metabolite Biosynthesis | DPG                         | 3-phospho-D-glyceroyl phosphate (13-DPG)      | 13  |
| Secondary Metabolite Biosynthesis | CPD-18237                   | zwittermicin A                                | 8   |
| Secondary Metabolite Biosynthesis | MET                         | L-methionine                                  | 7   |
| Secondary Metabolite Biosynthesis | CPD-12430                   | 5-guanidino-3-methyl-2-oxopentanoate          | -5  |
| Secondary Metabolite Biosynthesis | CPD-824                     | 5-guanidino-2-oxopentanoate                   | 1   |
| Secondary Metabolite Biosynthesis | INDOLE                      | indole                                        | 1   |
| Secondary Metabolite Biosynthesis | CPD-8686                    | 9-oxononanoate                                | -13 |
| Secondary Metabolite Biosynthesis | CPD-5923                    | 5'-deoxy-5'-fluoroadenosine                   | -7  |
| Secondary Metabolite Biosynthesis | CPD-18772                   | gadusol                                       | -11 |
| Secondary Metabolite Biosynthesis | CPD-17453                   | dithiolgliotoxin                              | 6   |
| Secondary Metabolite Biosynthesis | CPD-17053                   | bis(methylsulfanyl)gliotoxin                  | 12  |
| Secondary Metabolite Biosynthesis | CPD-17455                   | mono(methylsulfanyl)gliotoxin                 | 6   |
| Secondary Metabolite Biosynthesis | CPD-17043                   | cyclo(L-phenylalanyl-L-seryl)                 | -13 |
| Secondary Metabolite Biosynthesis | CPD-9700                    | hypoglycin B                                  | -7  |
| Secondary Metabolite Biosynthesis | CPD-9699                    | hypoglycin A                                  | 16  |
| Secondary Metabolite Biosynthesis | CPD-10525                   | indigo                                        | -14 |
| Secondary Metabolite Biosynthesis | CPD-14625                   | spinosyn macrolactone                         | 14  |
| Secondary Metabolite Biosynthesis | CPD-14629                   | spinosyn tricyclic macrolactone               | 8   |
| Secondary Metabolite Biosynthesis | CPD-13385                   | spinosyn A                                    | -10 |
| Secondary Metabolite Biosynthesis | CPD-463                     | L-nicotianamine                               | -6  |
| Secondary Metabolite Biosynthesis | CPD-18328                   | lyngbyatoxin A                                | 7   |
| Secondary Metabolite Biosynthesis | BENZOATE                    | benzoate                                      | 8   |
| Secondary Metabolite Biosynthesis | CAPSAICIN                   | capsaicin                                     | 9   |
| Secondary Metabolite Biosynthesis | CPD-9329                    | 8-methyl-6-nonenoate                          | -13 |
| Secondary Metabolite Biosynthesis | O-UREIDOHOMOSERINE          | O-ureido-L-homoserine                         | 15  |
| Secondary Metabolite Biosynthesis | CANAVANINOSUCCINATE         | canavaninosuccinate                           | 1   |
| Secondary Metabolite Biosynthesis | L-CANALINE                  | L-canaline                                    | 13  |
| Secondary Metabolite Biosynthesis | BENZYL-DESULFOGLUCOSINOLATE | desulfoglucotropaeolin                        | 13  |
| Secondary Metabolite Biosynthesis | CPD-8001                    | calystegine A3                                | -7  |
| Secondary Metabolite Biosynthesis | CPD-17697                   | tomatidine                                    | -8  |
| Secondary Metabolite Biosynthesis | CPD-18641                   | tomatidine galactoside                        | 1   |
| Secondary Metabolite Biosynthesis | CPD-8935                    | feruloylserotonin                             | -7  |
| Secondary Metabolite Biosynthesis | CPD-8987                    | senecionine N-oxide                           | 8   |
| Secondary Metabolite Biosynthesis | CPD-1103                    | taxiphyllin                                   | -14 |
| Secondary Metabolite Biosynthesis | CPD-11852                   | dehydrocoulerine                              | -13 |
| Secondary Metabolite Biosynthesis | CPD-8658                    | amaranthin                                    | -6  |
| Secondary Metabolite Biosynthesis | CPD-17338                   | peramine                                      | -1  |
| Secondary Metabolite Biosynthesis | CPD-16985                   | ardeemin                                      | -14 |
| Secondary Metabolite Biosynthesis | INDOLEYL-CPD                | (indole-3-yl)acetonitrile                     | -7  |
| Secondary Metabolite Biosynthesis | 2-AMINO-4-CARBOXYPYRIMIDINE | 2-amino-4-carboxypyrimidine                   | 1   |
| Secondary Metabolite Biosynthesis | N-EE-PIPEROYL-PIPERIDINE    | piperine                                      | -1  |
| Secondary Metabolite Biosynthesis | CPDQT-418                   | 7-(methylsulfanyl)heptyl-desulfoglucosinolate | -6  |
| Secondary Metabolite Biosynthesis | CPD-9217                    | solanidine                                    | -7  |
| Secondary Metabolite Biosynthesis | CPD-8941                    | cinnamoyltyramine                             | -7  |
| Secondary Metabolite Biosynthesis | CPD-8943                    | p-coumaroyltyramine                           | -15 |
| Secondary Metabolite Biosynthesis | VINORINE                    | vinorine                                      | 13  |
| Secondary Metabolite Biosynthesis | CPD-14751                   | ajmaline                                      | -8  |
| Secondary Metabolite Biosynthesis | CPD-4243                    | sarpagine                                     | 14  |
| Secondary Metabolite Biosynthesis | CPD-2748                    | normicotine                                   | 13  |
| Secondary Metabolite Biosynthesis | CPD-10277                   | lotaustralin                                  | 14  |
| Secondary Metabolite Biosynthesis | CPD-18646                   | furostanol-26-alcohol                         | 8   |
| Secondary Metabolite Biosynthesis | CPD-19447                   | 11-hydroxyvittatine                           | -14 |
| Secondary Metabolite Biosynthesis | CPD-19438                   | lycorine                                      | -8  |
| Secondary Metabolite Biosynthesis | CPD-12600                   | 2-arachidonoylglycerol                        | -1  |
| Secondary Metabolite Biosynthesis | CPD-446                     | N-glucosylnicotinate                          | -13 |
| Secondary Metabolite Biosynthesis | PYRIDOXINE                  | pyridoxine                                    | -7  |
| Secondary Metabolite Biosynthesis | PYRIDOXAL_PHOSPHATE         | pyridoxal 5'-phosphate (PLP)                  | 18  |
| Secondary Metabolite Biosynthesis | CPD-12421                   | 2-benzoyloxy-3-butenylglucosinolate           | 5   |
| Secondary Metabolite Biosynthesis | CPDQT-274                   | 4-hydroxybutylglucosinolate                   | 17  |
| Secondary Metabolite Biosynthesis | CPD-17022                   | asperlicin D                                  | -3  |
| Secondary Metabolite Biosynthesis | CPD-17021                   | asperlicin C                                  | -15 |
| Secondary Metabolite Biosynthesis | CPD-16970                   | fumiquinazoline A                             | 1   |
| Secondary Metabolite Biosynthesis | CPD-16899                   | (R)-benzodiazepinedione                       | 1   |
| Secondary Metabolite Biosynthesis | CPD-9936                    | (S)-magnoflorine                              | 8   |
| Secondary Metabolite Biosynthesis | CPD-17881                   | fumiquinazoline F-indoline-3'-ol              | 7   |
| Secondary Metabolite Biosynthesis | CPD-17886                   | deoxynortryptoquialanone                      | -2  |
| Secondary Metabolite Biosynthesis | CPD-17888                   | tryptoquialanol                               | -12 |
| Secondary Metabolite Biosynthesis | 3-URACIL-1-YL-L-SERINE      | L-willardiine                                 | -7  |
| Secondary Metabolite Biosynthesis | XANTHOSINE                  | xanthosine                                    | 7   |
| Secondary Metabolite Biosynthesis | 7-METHYLYXANTHOSINE         | 7-methylxanthosine                            | -14 |
| Secondary Metabolite Biosynthesis | 7-METHYLYXANTHINE           | 7-methylxanthine                              | -6  |
| Secondary Metabolite Biosynthesis | CPD-8919                    | 17-oxosparteine                               | 9   |
| Secondary Metabolite Biosynthesis | CPD-18299                   | 4'-methoxycyclopeptine                        | 9   |
| Secondary Metabolite Biosynthesis | XANTHINE                    | xanthine                                      | -8  |
| Secondary Metabolite Biosynthesis | CPD-15260                   | fumitremorgin B                               | -8  |
| Secondary Metabolite Biosynthesis | CPD-15261                   | fumitremorgin A                               | -2  |
| Secondary Metabolite Biosynthesis | CPD-12232                   | hordatine A                                   | 15  |
| Secondary Metabolite Biosynthesis | CPD-8757                    | betaxanthin                                   | 2   |
| Secondary Metabolite Biosynthesis | CPDQT-419                   | 8-(methylsulfanyl)octyl-desulfoglucosinolate  | 9   |
| Secondary Metabolite Biosynthesis | RICININE                    | ricinine                                      | 6   |
| Secondary Metabolite Biosynthesis | CPD-9941                    | harmol                                        | 2   |
| Secondary Metabolite Biosynthesis | 6-O-METHYLNORLAUDANOSOLINE  | (S)-6-O-methylnorlaudanosoline                | -5  |
| Secondary Metabolite Biosynthesis | CPD-8659                    | miraxanthin V                                 | 5   |
| Secondary Metabolite Biosynthesis | CPD-15267                   | demethoxyfumitremorgin C                      | 2   |
| Secondary Metabolite Biosynthesis | CPD-15262                   | tryprostatin A                                | 7   |
| Secondary Metabolite Biosynthesis | CPD-17361                   | notoamide D                                   | 7   |
| Secondary Metabolite Biosynthesis | CPDQT-417                   | 6-(methylsulfanyl)hexyl-desulfoglucosinolate  | -18 |
| Secondary Metabolite Biosynthesis | CPD-17389                   | glandicoline A                                | -7  |
| Secondary Metabolite Biosynthesis | CPD-17390                   | glandicoline B                                | 7   |

|                                   |                                        |                                       |     |
|-----------------------------------|----------------------------------------|---------------------------------------|-----|
| Secondary Metabolite Biosynthesis | CPD-17393                              | roquefortine F                        | 7   |
| Secondary Metabolite Biosynthesis | CPD-9788                               | O-methylandrocybine                   | 14  |
| Secondary Metabolite Biosynthesis | S-NORLAUDANOSOLINE                     | (S)-norlaudanoline                    | -13 |
| Secondary Metabolite Biosynthesis | 17-O-DEACETYLVINDOLINE                 | 17-O-deacetylvindoline                | 8   |
| Secondary Metabolite Biosynthesis | CPD-7858                               | vinblastine                           | -1  |
| Secondary Metabolite Biosynthesis | CPD-9981                               | 7-deoxyloganate                       | -6  |
| Secondary Metabolite Biosynthesis | LOGANIN                                | loganin                               | 7   |
| Secondary Metabolite Biosynthesis | PROTOPINE                              | protopine                             | -14 |
| Secondary Metabolite Biosynthesis | CPD-9893                               | chelirubine                           | 7   |
| Secondary Metabolite Biosynthesis | BERBAMUNINE                            | berbamunine                           | -22 |
| Secondary Metabolite Biosynthesis | CPD-8851                               | dopamine quinone                      | 6   |
| Secondary Metabolite Biosynthesis | CPD-14816                              | cephaeline                            | 8   |
| Secondary Metabolite Biosynthesis | CPD-460                                | 4-(3-methylbut-2-enyl)-L-tryptophan   | -14 |
| Secondary Metabolite Biosynthesis | CPD-12352                              | 4-(3-methylbut-2-enyl)-L-abrine       | -12 |
| Secondary Metabolite Biosynthesis | CPD-12356                              | chanoclavine-I                        | -19 |
| Secondary Metabolite Biosynthesis | CPD-12363                              | ergotamine                            | -7  |
| Secondary Metabolite Biosynthesis | CPD-12357                              | agroclavine                           | 8   |
| Secondary Metabolite Biosynthesis | AMINO-ETCETERA-PYRIDIN-1-YL-PROPANOATE | L-mimosine                            | 20  |
| Secondary Metabolite Biosynthesis | CPD-19480                              | 2-[(2'-methylsulfanyl)hexyl]maleate   | 1   |
| Secondary Metabolite Biosynthesis | CPDQT-35                               | 2-[(7'-methylsulfanyl)heptyl]malate   | -7  |
| Secondary Metabolite Biosynthesis | CPDQT-277                              | L-hexahomomethionine                  | 14  |
| Secondary Metabolite Biosynthesis | CPDQT-404                              | L-trihomomethionine                   | 14  |
| Secondary Metabolite Biosynthesis | CPDQT-28                               | 7-(methylsulfanyl)-2-oxoheptanoate    | -13 |
| Secondary Metabolite Biosynthesis | CPDQT-29                               | 8-(methylsulfanyl)-2-oxooctanoate     | -4  |
| Secondary Metabolite Biosynthesis | CPD-17378                              | histidyltryptophyldiketopiperazine    | -21 |
| Secondary Metabolite Biosynthesis | CPD-15265                              | brevianamide F                        | 4   |
| Secondary Metabolite Biosynthesis | CPD-7996                               | littorine                             | -7  |
| Secondary Metabolite Biosynthesis | SCOPOLAMINE                            | scopolamine                           | -22 |
| Secondary Metabolite Biosynthesis | CPD-16844                              | didemethylasterriquinone D            | 6   |
| Secondary Metabolite Biosynthesis | CPD-16846                              | terrequinone A                        | 6   |
| Secondary Metabolite Biosynthesis | CPD-14465                              | dihydrochanoclavine-I aldehyde        | 10  |
| Secondary Metabolite Biosynthesis | CPD-14469                              | fumigaclavine C                       | -7  |
| Secondary Metabolite Biosynthesis | BERBERINE                              | berberine                             | -7  |
| Secondary Metabolite Biosynthesis | CODEINONE                              | codeinone                             | -7  |
| Secondary Metabolite Biosynthesis | CODEINE                                | codeine                               | -13 |
| Secondary Metabolite Biosynthesis | R-RETICULINE                           | (R)-reticuline                        | 15  |
| Secondary Metabolite Biosynthesis | DOPAQUINONE                            | dopaquinone                           | -6  |
| Secondary Metabolite Biosynthesis | CPD-9835                               | cinchonidine                          | -13 |
| Secondary Metabolite Biosynthesis | CPD-9851                               | corynantheal                          | -6  |
| Secondary Metabolite Biosynthesis | CPD-9848                               | quinidinone                           | -7  |
| Secondary Metabolite Biosynthesis | CPD-9846                               | quinidine                             | 8   |
| Secondary Metabolite Biosynthesis | 3-HYDROXY-L-KYNURENINE                 | 3-hydroxy-L-kynurenine                | 13  |
| Secondary Metabolite Biosynthesis | LICODIONE                              | licodione                             | 1   |
| Secondary Metabolite Biosynthesis | CPD-1962                               | (+)-afzelechin                        | 1   |
| Secondary Metabolite Biosynthesis | CPD-9711                               | dalcocinin                            | 8   |
| Secondary Metabolite Biosynthesis | CPD-17599                              | (-)-bursehernin                       | -8  |
| Secondary Metabolite Biosynthesis | CPD-18755                              | (-)-5'-demethylatein                  | 12  |
| Secondary Metabolite Biosynthesis | CPD-9588                               | maysin                                | 12  |
| Secondary Metabolite Biosynthesis | CPD-14619                              | atromentin                            | -2  |
| Secondary Metabolite Biosynthesis | 6-METHOXYMELLEIN                       | 6-methoxymellein                      | 13  |
| Secondary Metabolite Biosynthesis | CPD-10256                              | 5-pentadecatrienyl resorcinol         | -8  |
| Secondary Metabolite Biosynthesis | CPD-12348                              | methoxydihydrosorgoleone              | -4  |
| Secondary Metabolite Biosynthesis | CPD-10258                              | dihydrosorgoleone                     | 14  |
| Secondary Metabolite Biosynthesis | CPD-8949                               | tellimagrandin II                     | 12  |
| Secondary Metabolite Biosynthesis | CPD-7119                               | xanthohumol                           | -7  |
| Secondary Metabolite Biosynthesis | CPD-7075                               | hesperidin                            | -1  |
| Secondary Metabolite Biosynthesis | CPD-14960                              | kaempferide triglycoside              | 12  |
| Secondary Metabolite Biosynthesis | CPD-9318                               | 3-geranyl-4-hydroxybenzoate           | 19  |
| Secondary Metabolite Biosynthesis | CPD-9320                               | 3"-hydroxy-geranylhdroquinone         | 10  |
| Secondary Metabolite Biosynthesis | SULOCHRIN                              | sulochrin                             | -6  |
| Secondary Metabolite Biosynthesis | CPD-12037                              | hispidol                              | -16 |
| Secondary Metabolite Biosynthesis | CPD-14848                              | genistin 7-gentiobioside              | 21  |
| Secondary Metabolite Biosynthesis | CPD-6964                               | pinosylvin monomethylether            | 14  |
| Secondary Metabolite Biosynthesis | PHENYLACETALDEHYDE                     | phenylacetaldehyde                    | -23 |
| Secondary Metabolite Biosynthesis | CPD-9561                               | protohypericin                        | 14  |
| Secondary Metabolite Biosynthesis | CPD-6602                               | curcumin                              | 13  |
| Secondary Metabolite Biosynthesis | CPD-9536                               | 5'-hydroxy-rot-2'-enonate             | 7   |
| Secondary Metabolite Biosynthesis | CPD-7026                               | afformosin                            | 13  |
| Secondary Metabolite Biosynthesis | CPD-9534                               | rot-2'-enonate                        | 8   |
| Secondary Metabolite Biosynthesis | CPD-16749                              | 5'-demethoxy-6-methoxypodophyllotoxin | 2   |
| Secondary Metabolite Biosynthesis | CPD-19955                              | butyl benzoate                        | -15 |
| Secondary Metabolite Biosynthesis | CPD-18998                              | propyl acetate                        | 9   |
| Secondary Metabolite Biosynthesis | KIEVITONE-CPD                          | kievitone                             | 5   |
| Secondary Metabolite Biosynthesis | MYRICETIN                              | myricetin                             | -19 |
| Secondary Metabolite Biosynthesis | CPD-11530                              | dihydroconiferyl aldehyde             | -6  |
| Secondary Metabolite Biosynthesis | CPD-17703                              | coniferyl alcohol 9-methyl ester      | 1   |
| Secondary Metabolite Biosynthesis | CPD-7252                               | kaempferide                           | 1   |
| Secondary Metabolite Biosynthesis | CPD-79                                 | sinapaldehyde glucoside               | -13 |
| Secondary Metabolite Biosynthesis | CPD-8921                               | (+)-piperitol                         | -13 |
| Secondary Metabolite Biosynthesis | CPD-18761                              | coniferyl alcohol radical             | 7   |
| Secondary Metabolite Biosynthesis | CPD-13494                              | 6-gingerol                            | 7   |
| Secondary Metabolite Biosynthesis | CPD-8184                               | chrysin                               | -16 |
| Secondary Metabolite Biosynthesis | CPD-6991                               | (2S)-pinocembrin                      | 1   |
| Secondary Metabolite Biosynthesis | CPD-20014                              | vicenin-2                             | 22  |
| Secondary Metabolite Biosynthesis | PHLORETIN                              | phloretin                             | 1   |
| Secondary Metabolite Biosynthesis | 574-TRIHIDROXY-3-METHOXYFLAVONE        | chrysoeriol                           | -12 |
| Secondary Metabolite Biosynthesis | SINAPATE                               | sinapate                              | -12 |
| Secondary Metabolite Biosynthesis | CPD-6481                               | eugenol                               | -14 |
| Secondary Metabolite Biosynthesis | CPD-4885                               | (-)-phaseollidin                      | -1  |
| Secondary Metabolite Biosynthesis | CPD-13543                              | kauralexin B2                         | 7   |
| Secondary Metabolite Biosynthesis | CPD-13544                              | kauralexin B3                         | -8  |
| Secondary Metabolite Biosynthesis | INDOLE-CARBOXY-HYDRO-THIAZOLE          | (R)-dihydrocamalexate                 | 1   |
| Secondary Metabolite Biosynthesis | CPD-4745                               | rishitin                              | -1  |
| Secondary Metabolite Biosynthesis | CPD-4746                               | 3-hydroxy-15-dihydrolubimin           | 8   |
| Secondary Metabolite Biosynthesis | CPD-18574                              | 3-hydroxy-5-methoxybiphenyl           | -2  |
| Secondary Metabolite Biosynthesis | CPD-4461                               | plumbagin                             | -15 |
| Secondary Metabolite Biosynthesis | CPD-12673                              | 5-chloro-5-deoxy-D-ribonate           | 8   |
| Secondary Metabolite Biosynthesis | CPD-11020                              | 5-chloro-4-hydroxy-2-oxopentanoate    | 2   |
| Secondary Metabolite Biosynthesis | CPD-12679                              | 4-chloro-3-hydroxybutyryl-CoA         | -14 |

|                                   |                                    |                                      |     |
|-----------------------------------|------------------------------------|--------------------------------------|-----|
| Secondary Metabolite Biosynthesis | CPD-12680                          | 4-chloro-crotonyl-CoA                | 6   |
| Secondary Metabolite Biosynthesis | CPD-12684                          | L-3-cyclohex-2'-enylalanine          | -1  |
| Secondary Metabolite Biosynthesis | CPD-12201                          | anigorufone                          | 1   |
| Secondary Metabolite Biosynthesis | CPD-18211                          | 6-hydroxy-norbikaverin               | -16 |
| Secondary Metabolite Biosynthesis | CPD-18032                          | fusarinolate                         | 6   |
| Secondary Metabolite Biosynthesis | CPD-18034                          | methyl fusarate                      | 1   |
| Secondary Metabolite Biosynthesis | CPD-18031                          | fusarate                             | 13  |
| Secondary Metabolite Biosynthesis | CPD-10679                          | flaviolin                            | -16 |
| Secondary Metabolite Biosynthesis | CPD-11587                          | chrysophanol anthrone                | -6  |
| Secondary Metabolite Biosynthesis | CPD-18255                          | YWA1                                 | -18 |
| Secondary Metabolite Biosynthesis | CPD-18244                          | dimeric 9-hydroxyrubrofusarin        | 12  |
| Secondary Metabolite Biosynthesis | CPD-6801                           | aloesone                             | -2  |
| Secondary Metabolite Biosynthesis | CPD-12180                          | feruloylacetyl-CoA                   | 15  |
| Secondary Metabolite Biosynthesis | CPD-17133                          | desmethylbassianin                   | -2  |
| Secondary Metabolite Biosynthesis | CPD-17131                          | predesmethylbassianin A              | 8   |
| Secondary Metabolite Biosynthesis | CPD-20577                          | norbaeocystin                        | 7   |
| Secondary Metabolite Biosynthesis | CPD-20579                          | baeocystin                           | 13  |
| Secondary Metabolite Biosynthesis | CPD-20104                          | dihydrorhizobitoxine                 | -16 |
| Secondary Metabolite Biosynthesis | CPD-18452                          | cylindropermopsin                    | 13  |
| Secondary Metabolite Biosynthesis | CPD-21113                          | felinine                             | 6   |
| Secondary Metabolite Biosynthesis | L-CYSTEATE                         | L-cysteate                           | 12  |
| Secondary Metabolite Biosynthesis | CPD-12491                          | phenylmethanesulfenate               | -7  |
| Secondary Metabolite Biosynthesis | 2-AMINOACRYLATE                    | 2-aminoprop-2-enoate                 | -17 |
| Secondary Metabolite Biosynthesis | CPD-18776                          | (R)-4-deoxygadusol                   | 5   |
| Secondary Metabolite Biosynthesis | CPD-3764                           | desferrioxamine B                    | 8   |
| Secondary Metabolite Biosynthesis | CPD0-2241                          | ferrichrome                          | -16 |
| Secondary Metabolite Biosynthesis | CPD-9990                           | anguibactin                          | 8   |
| Secondary Metabolite Biosynthesis | CPD-11965                          | pre-putrebactin                      | -4  |
| Secondary Metabolite Biosynthesis | CPD-9985                           | petrobactin                          | 11  |
| Secondary Metabolite Biosynthesis | CPD-11968                          | alcaligin                            | 8   |
| Secondary Metabolite Biosynthesis | CPD-7836                           | myristate                            | 13  |
| Secondary Metabolite Biosynthesis | CPD-12313                          | schizokinen                          | -7  |
| Secondary Metabolite Biosynthesis | CPD-20999                          | pseudomonine                         | -22 |
| Secondary Metabolite Biosynthesis | CPD-21000                          | pre-pseudomonine                     | -2  |
| Secondary Metabolite Biosynthesis | CPD-21009                          | baumannoferrin A                     | 16  |
| Secondary Metabolite Biosynthesis | CPD-7228                           | 3"-deamino-3"-oxonicotianamine       | -7  |
| Secondary Metabolite Biosynthesis | CPD-11970                          | bisucaberin                          | -7  |
| Secondary Metabolite Biosynthesis | CPD-9986                           | achromobactin                        | 6   |
| Secondary Metabolite Biosynthesis | CPD-7289                           | 3-epihydroxymugineate                | -14 |
| Secondary Metabolite Biosynthesis | CPD-7291                           | 3-epihydroxy-2'-deoxymugineate       | 7   |
| Secondary Metabolite Biosynthesis | CPD-12151                          | D-histidine                          | 7   |
| Secondary Metabolite Biosynthesis | CPD-10176                          | versicolorin A                       | 6   |
| Secondary Metabolite Biosynthesis | CPD-12930                          | neurospoxanthin                      | -7  |
| Secondary Metabolite Biosynthesis | CPD-9481                           | hederagenin                          | 1   |
| Secondary Metabolite Biosynthesis | CPD-9482                           | soyasapogenol E                      | 1   |
| Secondary Metabolite Biosynthesis | CPD-7968                           | bixin aldehyde                       | 14  |
| Secondary Metabolite Biosynthesis | CPD-7972                           | bixin                                | 9   |
| Secondary Metabolite Biosynthesis | CPD-8662                           | crocetin                             | -19 |
| Secondary Metabolite Biosynthesis | CPD-8668                           | picrocrocin                          | 7   |
| Secondary Metabolite Biosynthesis | CPD-14499                          | erythrodial                          | -8  |
| Secondary Metabolite Biosynthesis | CPD-20690                          | fucoxanthinol                        | 1   |
| Secondary Metabolite Biosynthesis | CPD-14485                          | glycyrrhetaldehyde                   | 16  |
| Secondary Metabolite Biosynthesis | CPD-18415                          | 3-acetyl T-2 toxin                   | 12  |
| Secondary Metabolite Biosynthesis | CPD-10662                          | C30 botryococcene                    | -12 |
| Secondary Metabolite Biosynthesis | CPD-14289                          | C33 botryococcene                    | -15 |
| Secondary Metabolite Biosynthesis | CPD-9528                           | desoxyhemigossypol-6-methyl ether    | -13 |
| Secondary Metabolite Biosynthesis | CPD-17204                          | lolitriol                            | 7   |
| Secondary Metabolite Biosynthesis | CPD-17196                          | terpendole I                         | -8  |
| Secondary Metabolite Biosynthesis | CPD-16667                          | cyclooctat-9-en-7-ol                 | 7   |
| Secondary Metabolite Biosynthesis | CPD-17660                          | 2-hydroxycanthaxanthin               | 9   |
| Secondary Metabolite Biosynthesis | CPD-17662                          | 2-hydroxyadonixanthin                | -16 |
| Secondary Metabolite Biosynthesis | CPD-14505                          | rubusoside                           | -15 |
| Secondary Metabolite Biosynthesis | CPD-7003                           | tetrahydrogeranylgeranyl diphosphate | 4   |
| Secondary Metabolite Biosynthesis | CPD-7002                           | dihydrogeranylgeranyl diphosphate    | 7   |
| Secondary Metabolite Biosynthesis | CPD-17491                          | astaxanthin dirhamnoside             | 5   |
| Secondary Metabolite Biosynthesis | CPD-14519                          | bacteriohopanetetrol                 | 8   |
| Secondary Metabolite Biosynthesis | CPD-14521                          | aminobacteriohopanetriol             | 8   |
| Secondary Metabolite Biosynthesis | CPD-14517                          | 2-methyltetrahymanol                 | -7  |
| Secondary Metabolite Biosynthesis | CPD-18508                          | hydroxysqualene                      | 8   |
| Secondary Metabolite Biosynthesis | CPD-17304                          | okenone                              | -1  |
| Secondary Metabolite Biosynthesis | CPD-9525                           | hemigossypol                         | 7   |
| Secondary Metabolite Biosynthesis | CPD-9744                           | heliocide H4                         | -7  |
| Secondary Metabolite Biosynthesis | BACCATIN-III                       | baccatin III                         | -7  |
| Secondary Metabolite Biosynthesis | 10-DEACETYL-2-DEBENZOYLACCATIN-III | 10-deacetyl-2-debenzoylbaccatin III  | -8  |
| Secondary Metabolite Biosynthesis | CPD-11442                          | botrydial                            | -13 |
| Secondary Metabolite Biosynthesis | CPD-18554                          | stellatic alcohol                    | 8   |
| Secondary Metabolite Biosynthesis | CPD-16861                          | 2-hydroxyspirilloxanthin             | 8   |
| Secondary Metabolite Biosynthesis | CPD-12615                          | spirilloxanthin                      | -8  |
| Secondary Metabolite Biosynthesis | CPD-9758                           | geranyl acetate                      | -1  |
| Secondary Metabolite Biosynthesis | CPD-7559                           | dihydroartemisinin                   | -7  |
| Secondary Metabolite Biosynthesis | CPD-18410                          | 15-decalonectrin                     | -21 |
| Secondary Metabolite Biosynthesis | CPD-464                            | prephytoene diphosphate              | -7  |
| Secondary Metabolite Biosynthesis | CPD-18005                          | dihydroisopentenyldehydrohodopin     | -9  |
| Secondary Metabolite Biosynthesis | CPD-18004                          | bacterioruberin                      | -1  |
| Secondary Metabolite Biosynthesis | CPD-18021                          | monoanhydrobacterioruberin           | 1   |
| Secondary Metabolite Biosynthesis | CPD-20624                          | isorenieratene                       | -8  |
| Secondary Metabolite Biosynthesis | CPD-11469                          | methoxyneurosporene                  | -17 |
| Secondary Metabolite Biosynthesis | CPD-11464                          | demethylspheroidene                  | 8   |
| Secondary Metabolite Biosynthesis | CPD-8723                           | dehydroabietadiene-diol              | -8  |
| Secondary Metabolite Biosynthesis | CPD-8722                           | dehydroabietadienol                  | 15  |
| Secondary Metabolite Biosynthesis | CPD-8721                           | abietatriene                         | 6   |
| Secondary Metabolite Biosynthesis | CPD-10307                          | arabidial                            | 16  |
| Secondary Metabolite Biosynthesis | CPD-9475                           | gypsogenate-28-beta-D-glucoside      | 8   |
| Secondary Metabolite Biosynthesis | CPD-9474                           | gypsogenate                          | 8   |
| Secondary Metabolite Biosynthesis | CPD-14495                          | ursolic aldehyde                     | -15 |
| Secondary Metabolite Biosynthesis | ALL-TRANS-PENTAPRENYL-DIPHOSPHATE  | geranylarnesyl diphosphate (GFPP)    | 7   |
| Secondary Metabolite Biosynthesis | CPD-707                            | campesterol                          | -21 |
| Secondary Metabolite Biosynthesis | CPD-7850                           | echinenone                           | -15 |
| Secondary Metabolite Biosynthesis | CPD-16623                          | des-acyl avenacin A                  | 6   |

|                                   |                                    |                                                 |     |
|-----------------------------------|------------------------------------|-------------------------------------------------|-----|
| Secondary Metabolite Biosynthesis | CPD-11505                          | olivetoI                                        | 8   |
| Secondary Metabolite Biosynthesis | CPD-9635                           | hyperforin                                      | 1   |
| Secondary Metabolite Biosynthesis | CPD-7110                           | lupulone                                        | -22 |
| Secondary Metabolite Biosynthesis | CPD-19790                          | adlupulone                                      | 2   |
| Secondary Metabolite Biosynthesis | CPD-1086                           | 5-amino-6-(5-phospho-D-ribitylamino)uracil      | 19  |
| Secondary Metabolite Biosynthesis | AMINO-RIBOSYLAMINO-1H-3H-PYR-DIONE | 5-amino-6-(D-ribitylamino)uracil (ARP)          | -7  |
| Secondary Metabolite Biosynthesis | CPD-10171                          | versiconal                                      | -6  |
| Secondary Metabolite Biosynthesis | CPD-14318                          | deoxyviolacein                                  | 7   |
| Secondary Metabolite Biosynthesis | CPD-14323                          | deoxyviolaceinate                               | 6   |
| Secondary Metabolite Biosynthesis | CPD-14322                          | prodeoxyviolacein                               | -2  |
| Secondary Metabolite Biosynthesis | CPD-14319                          | protoviolaceinate                               | 13  |
| Secondary Metabolite Biosynthesis | CPD-264                            | 3-hydroxybenzoyl-CoA                            | 8   |
| Cell Structure Biosynthesis       | GLYCEROL                           | glycerol                                        | 5   |
| Cell Structure Biosynthesis       | UMP                                | UMP                                             | 6   |
| Cell Structure Biosynthesis       | TDP                                | dTDP                                            | -5  |
| Cell Structure Biosynthesis       | CPD-11591                          | 16-feruloyloxypalmitate                         | 1   |
| Cell Structure Biosynthesis       | DODECANOATE                        | laurate                                         | 8   |
| Cell Structure Biosynthesis       | CPD-17645                          | 2-(8-hydroxy-2-oxotridecyl)-6-oxopyran-4-olate  | 18  |
| Cell Structure Biosynthesis       | CPD-10512                          | 16-oxo-palmitate                                | -6  |
| Cell Structure Biosynthesis       | CPD-12247                          | D-alanyl-D-lactate                              | -17 |
| Metabolic Regulator Biosynthesis  | CPD-10470                          | dimethylsulfonio-2-hydroxybutanoate             | -6  |
| Metabolic Regulator Biosynthesis  | MET                                | L-methionine                                    | 7   |
| Metabolic Regulator Biosynthesis  | CPD-16905                          | monacolin L acid                                | 4   |
| Metabolic Regulator Biosynthesis  | CPD-16924                          | lovastatin acid                                 | 7   |
| Metabolic Regulator Biosynthesis  | ACETYL-COA                         | acetyl-CoA                                      | -6  |
| Metabolic Regulator Biosynthesis  | GTP                                | GTP                                             | -22 |
| Metabolic Regulator Biosynthesis  | DPG                                | 3-phospho-D-glyceroyl phosphate (13-DPG)        | 13  |
| Other Biosynthesis                | ACETYL-COA                         | acetyl-CoA                                      | -6  |
| Other Biosynthesis                | CPD-10793                          | hydroxypyruvaldehyde phosphate                  | 2   |
| Other Biosynthesis                | CPD-10791                          | 6-deoxy-5-ketofructose 1-phosphate              | 7   |
| Other Biosynthesis                | CPD-15467                          | 3-dimethylallyl-4-hydroxyphenylpyruvate         | -12 |
| Other Biosynthesis                | CPD-10600                          | 3-(4-hydroxyphenyl)-3-oxo-propanoyl-CoA         | 9   |
| Other Biosynthesis                | TYR                                | L-tyrosine                                      | 14  |
| Other Biosynthesis                | CPD-205                            | pimelate                                        | -13 |
| Other Biosynthesis                | BENZOATE                           | benzoate                                        | 8   |
| Other Biosynthesis                | SHIKIMATE-5P                       | shikimate 3-phosphate                           | -11 |
| Other Biosynthesis                | DIPHTHAMIDE                        | a diphthamide-[translation elongation factor 2] | -16 |
| Other Biosynthesis                | GTP                                | GTP                                             | -22 |
| Other Biosynthesis                | CPD-16457                          | aurodrosoperin                                  | 13  |
| Other Biosynthesis                | DOPAQUINONE                        | dopaquinone                                     | -6  |
| Other Biosynthesis                | MET                                | L-methionine                                    | 7   |
| Other Biosynthesis                | CPD-20340                          | ophthalmate                                     | -20 |
| Other Biosynthesis                | NAPHTHOL                           | 1-naphthol                                      | -6  |
| Other Biosynthesis                | CYS                                | L-cysteine                                      | 13  |
| Other Biosynthesis                | CPD-20554                          | pentabromopseudilin                             | -9  |
| Other Biosynthesis                | CPD-20571                          | (L-prolyl)adenylate                             | -6  |
| Other Biosynthesis                | 2-AMINOACRYLATE                    | 2-aminoprop-2-enoate                            | -17 |
| Other Biosynthesis                | SELENOHOMOCYSTEINE                 | seleno-L-homocysteine                           | 11  |
| Other Biosynthesis                | CPD-20564                          | spongiadioxin C                                 | 7   |
| Other Biosynthesis                | TRP                                | L-tryptophan (trp)                              | 12  |