**Table S2. KEGG pathways and annotated compounds in the comparison group SD3 vs. CP**

| Kegg_pathway | ko_ID | Sig_compound | compound | Sig_compound_all | compound_all | IndexList | CIDList | Pathway |
|---|---|---|---|---|---|---|---|---|
| Tyrosine metabolism | ko00350 | 10 | 11 | 63 | 94 | mws0180;Lmbn001981;pme1292;pme1002;pme2598;Zmpp000906;MWS4301;mws2368;pme1439;Ymjm000148 | C00628+C05585+C00544+C00483+C01161+C00547+C05593+C06044+C00811+C06046 | https:\\www.genome.jp\dbget-bin\www_bget?map00350 |
| Metabolic pathways | ko01100 | 47 | 66 | 63 | 94 | mws0180;Lmmn001643;mws2212;pme3083;Lmbn001981;mws0628;mws0183;pme1292;Lmgn001670;MWSHY0163;Lmbn002648;pme1002;pme2598;mws0458;Lmbn002644;mws0467;mws0704;mws0749;MWSmce248;Zmpp000906;pme1841;MWS4301;mws1358;MWSmce118;MWSmce548;MA10107783;pmb0501;Cmmn012997;mws0982;pme1137;Lmbp000728;mws1346;pme2292;MWSslk106;pmb1096;MWSmce466;NK10264324;pmb0764;mws0005;Lmbn002737;mws2368;pmb0819;pme1439;mws4085;Lmrn003000;Ymjm000148;MWS20194 | C00628+C01772+C01197+C05653+C05585+C00633+C00230+C00544+C00805+C00974+C02763+C00483+C01161+C00755+C06758+C01744+C00346+C00156+C12621+C00547+C01672+C05593+C00090+C02835+C00719+C20772+C00179+C06087+C05127+C01020+C20782+C00956+C00134+C05332+C00463+C10700+C02183+C04294+C00398+C07209+C06044+C02938+C00811+C00482+C05607+C06046+C00423 | https:\\www.genome.jp\dbget-bin\www_bget?map01100 |
| Phenylalanine metabolism | ko00360 | 8 | 9 | 63 | 94 | Lmmn001643;Lmbn002648;MWSmce248;MWS4301;ML10179289;MWSslk106;Lmrn003000;MWS20194 | C01772+C02763+C12621+C05593+C05853+C05332+C05607+C00423 | https:\\www.genome.jp\dbget-bin\www_bget?map00360 |
| Biosynthesis of various plant secondary metabolites | ko00999 | 7 | 8 | 63 | 94 | Lmmn001643;Zmln002252;pmb0501;pmb1096;Zmpn003044;mws1014;MWS20194 | C01772+C22007+C00179+C00463+C09315+C09265+C00423 | https:\\www.genome.jp\dbget-bin\www_bget?map00999 |
| Biosynthesis of secondary metabolites | ko01110 | 28 | 40 | 63 | 94 | Lmmn001643;mws2212;mws0639;mws0183;Lmgn001670;MWSHY0163;Zmln002252;pme1002;mws0458;mws0749;pme1841;MA10107783;pmb0501;Cmmn012997;mws1346;pme2292;pmb1096;mws0005;pmp000509;Zmpn003044;mws1014;pme1439;mws1574;mws4085;Lmrn003000;MWSCX015;pmb3074;MWS20194 | C01772+C01197+C00196+C00230+C00805+C00974+C22007+C00483+C00755+C00156+C01672+C20772+C00179+C06087+C00956+C00134+C00463+C00398+C11918+C09315+C09265+C00811+C11673+C00482+C05607+C10945+C12208+C00423 | https:\\www.genome.jp\dbget-bin\www_bget?map01110 |
| Isoquinoline alkaloid biosynthesis | ko00950 | 3 | 3 | 63 | 94 | Hmgn001653;pme1002;pme1439 | C16700+C00483+C00811 | https:\\www.genome.jp\dbget-bin\www_bget?map00950 |
| Phenylpropanoid biosynthesis | ko00940 | 8 | 11 | 63 | 94 | mws2212;mws0011;Lhhp120814;pme1439;mws4085;MWSCX015;pmb3074;MWS20194 | C01197+C01533+C10453+C00811+C00482+C10945+C12208+C00423 | https:\\www.genome.jp\dbget-bin\www_bget?map00940 |
| Tryptophan metabolism | ko00380 | 7 | 7 | 63 | 94 | pme3083;Zmtn001624;NK10253223;pmb0818;pmb1096;mws0005;pmb0819 | C05653+C02172+C05831+C05660+C00463+C00398+C02938 | https:\\www.genome.jp\dbget-bin\www_bget?map00380 |
| Phenylalanine, tyrosine and tryptophan biosynthesis | ko00400 | 2 | 2 | 63 | 94 | mws0183;pmb1096 | C00230+C00463 | https:\\www.genome.jp\dbget-bin\www_bget?map00400 |
| Isoflavonoid biosynthesis | ko00943 | 1 | 2 | 63 | 94 | mws0894 | C16195 | https:\\www.genome.jp\dbget-bin\www_bget?map00943 |
| Ubiquinone and other terpenoid-quinone biosynthesis | ko00130 | 5 | 5 | 63 | 94 | pme1292;mws0749;MA10107783;pme1439;MWS20194 | C00544+C00156+C20772+C00811+C00423 | https:\\www.genome.jp\dbget-bin\www_bget?map00130 |
| Biosynthesis of cofactors | ko01240 | 5 | 6 | 63 | 94 | pme1292;pme1002;mws0749;MA10107783;pmb0764 | C00544+C00483+C00156+C20772+C04294 | https:\\www.genome.jp\dbget-bin\www_bget?map01240 |
| Biosynthesis of various alkaloids | ko00996 | 3 | 3 | 63 | 94 | Lmgn001670;mws0458;MWS20194 | C00805+C00755+C00423 | https:\\www.genome.jp\dbget-bin\www_bget?map00996 |
| Plant hormone signal transduction | ko04075 | 1 | 1 | 63 | 94 | Lmgn001670 | C00805 | https:\\www.genome.jp\dbget-bin\www_bget?map04075 |
| Flavonoid biosynthesis | ko00941 | 2 | 4 | 63 | 94 | MWSHY0163;pmb3074 | C00974+C12208 | https:\\www.genome.jp\dbget-bin\www_bget?map00941 |
| Glycosylphosphatidylinositol (GPI)-anchor biosynthesis | ko00563 | 1 | 1 | 63 | 94 | mws0704 | C00346 | https:\\www.genome.jp\dbget-bin\www_bget?map00563 |
| Glycerophospholipid metabolism | ko00564 | 1 | 2 | 63 | 94 | mws0704 | C00346 | https:\\www.genome.jp\dbget-bin\www_bget?map00564 |
| Sphingolipid metabolism | ko00600 | 1 | 1 | 63 | 94 | mws0704 | C00346 | https:\\www.genome.jp\dbget-bin\www_bget?map00600 |
| Folate biosynthesis | ko00790 | 1 | 1 | 63 | 94 | mws0749 | C00156 | https:\\www.genome.jp\dbget-bin\www_bget?map00790 |
| Lysine degradation | ko00310 | 2 | 2 | 63 | 94 | pme1841;mws1346 | C01672+C00956 | https:\\www.genome.jp\dbget-bin\www_bget?map00310 |
| D-Amino acid metabolism | ko00470 | 2 | 2 | 63 | 94 | pme1841;pme2292 | C01672+C00134 | https:\\www.genome.jp\dbget-bin\www_bget?map00470 |
| Glutathione metabolism | ko00480 | 2 | 4 | 63 | 94 | pme1841;pme2292 | C01672+C00134 | https:\\www.genome.jp\dbget-bin\www_bget?map00480 |
| Tropane, piperidine and pyridine alkaloid biosynthesis | ko00960 | 3 | 6 | 63 | 94 | pme1841;pme2292;Lmrn003000 | C01672+C00134+C05607 | https:\\www.genome.jp\dbget-bin\www_bget?map00960 |
| Histidine metabolism | ko00340 | 2 | 4 | 63 | 94 | MWSmce118;mws0982 | C02835+C05127 | https:\\www.genome.jp\dbget-bin\www_bget?map00340 |
| Glycine, serine and threonine metabolism | ko00260 | 1 | 1 | 63 | 94 | MWSmce548 | C00719 | https:\\www.genome.jp\dbget-bin\www_bget?map00260 |
| ABC transporters | ko02010 | 2 | 4 | 63 | 94 | MWSmce548;pme2292 | C00719+C00134 | https:\\www.genome.jp\dbget-bin\www_bget?map02010 |
| Arginine and proline metabolism | ko00330 | 2 | 7 | 63 | 94 | pmb0501;pme2292 | C00179+C00134 | https:\\www.genome.jp\dbget-bin\www_bget?map00330 |
| Diterpenoid biosynthesis | ko00904 | 1 | 2 | 63 | 94 | Cmmn012997 | C06087 | https:\\www.genome.jp\dbget-bin\www_bget?map00904 |
| Nicotinate and nicotinamide metabolism | ko00760 | 1 | 2 | 63 | 94 | pme1137 | C01020 | https:\\www.genome.jp\dbget-bin\www_bget?map00760 |
| Lysine biosynthesis | ko00300 | 1 | 1 | 63 | 94 | mws1346 | C00956 | https:\\www.genome.jp\dbget-bin\www_bget?map00300 |
| 2-Oxocarboxylic acid metabolism | ko01210 | 1 | 1 | 63 | 94 | mws1346 | C00956 | https:\\www.genome.jp\dbget-bin\www_bget?map01210 |
| Biosynthesis of amino acids | ko01230 | 1 | 2 | 63 | 94 | mws1346 | C00956 | https:\\www.genome.jp\dbget-bin\www_bget?map01230 |
| Benzoxazinoid biosynthesis | ko00402 | 1 | 1 | 63 | 94 | pmb1096 | C00463 | https:\\www.genome.jp\dbget-bin\www_bget?map00402 |
| Thiamine metabolism | ko00730 | 1 | 1 | 63 | 94 | pmb0764 | C04294 | https:\\www.genome.jp\dbget-bin\www_bget?map00730 |
| Indole alkaloid biosynthesis | ko00901 | 1 | 1 | 63 | 94 | mws0005 | C00398 | https:\\www.genome.jp\dbget-bin\www_bget?map00901 |
| Polyketide sugar unit biosynthesis | ko00523 | 1 | 1 | 63 | 94 | pmp000509 | C11918 | https:\\www.genome.jp\dbget-bin\www_bget?map00523 |
| Monoterpenoid biosynthesis | ko00902 | 1 | 1 | 63 | 94 | mws1574 | C11673 | https:\\www.genome.jp\dbget-bin\www_bget?map00902 |
| Stilbenoid, diarylheptanoid and gingerol biosynthesis | ko00945 | 1 | 1 | 63 | 94 | pmb3074 | C12208 | https:\\www.genome.jp\dbget-bin\www_bget?map00945 |

**Table S2. KEGG pathways and annotated compounds in the comparison group SD6 vs. SD3**

| Kegg_pathway | ko_ID | Sig_compound | compound | Sig_compound_all | compound_all | IndexList | CIDList | Pathway |
|---|---|---|---|---|---|---|---|---|
| Phenylpropanoid biosynthesis | ko00940 | 5 | 12 | 34 | 99 | mws2212;HJN003;mws0014;pme1439;mws4085 | C01197+C01175+C01494+C00811+C00482 | https:\\www.genome.jp\dbget-bin\www_bget?map00940 |
| Metabolic pathways | ko01100 | 25 | 70 | 34 | 99 | mws2212;MWSHY0163;Lmlp003161;mws0704;mws0014;Zmpp000906;pme1841;mws1358;mws0059;pmb0501;Cmmn012997;pmb0490;mws0346;mws0982;pme1137;pme2292;pmb1096;NK10264324;pmb0764;pmb0819;pme1439;mws4085;pme2693;MWSHY0017;mws0044 | C01197+C00974+C10497+C00346+C01494+C00547+C01672+C00090+C05625+C00179+C06087+C18326+C11457+C05127+C01020+C00134+C00463+C02183+C04294+C02938+C00811+C00482+C02714+C00509+C01617 | https:\\www.genome.jp\dbget-bin\www_bget?map01100 |
| Biosynthesis of secondary metabolites | ko01110 | 18 | 44 | 34 | 99 | mws2212;MWSHY0163;Zmln002252;HJN003;mws0014;pme1841;mws0059;pmb0501;Cmmn012997;Lmsn003297;pme2292;pmb1096;pmp000509;Zmpn003044;pme1439;mws4085;MWSHY0017;mws0044 | C01197+C00974+C22007+C01175+C01494+C01672+C05625+C00179+C06087+C16408+C00134+C00463+C11918+C09315+C00811+C00482+C00509+C01617 | https:\\www.genome.jp\dbget-bin\www_bget?map01110 |
| Flavonoid biosynthesis | ko00941 | 5 | 7 | 34 | 99 | MWSHY0163;Lmsn003297;Zbsp007084;MWSHY0017;mws0044 | C00974+C16408+C09614+C00509+C01617 | https:\\www.genome.jp\dbget-bin\www_bget?map00941 |
| Biosynthesis of various plant secondary metabolites | ko00999 | 4 | 8 | 34 | 99 | Zmln002252;pmb0501;pmb1096;Zmpn003044 | C22007+C00179+C00463+C09315 | https:\\www.genome.jp\dbget-bin\www_bget?map00999 |
| Arginine and proline metabolism | ko00330 | 5 | 7 | 34 | 99 | Lmlp003161;pmb0501;pmb0490;pme2292;pme2693 | C10497+C00179+C18326+C00134+C02714 | https:\\www.genome.jp\dbget-bin\www_bget?map00330 |
| Glycosylphosphatidylinositol (GPI)-anchor biosynthesis | ko00563 | 1 | 1 | 34 | 99 | mws0704 | C00346 | https:\\www.genome.jp\dbget-bin\www_bget?map00563 |
| Glycerophospholipid metabolism | ko00564 | 1 | 2 | 34 | 99 | mws0704 | C00346 | https:\\www.genome.jp\dbget-bin\www_bget?map00564 |
| Sphingolipid metabolism | ko00600 | 1 | 1 | 34 | 99 | mws0704 | C00346 | https:\\www.genome.jp\dbget-bin\www_bget?map00600 |
| Tyrosine metabolism | ko00350 | 2 | 11 | 34 | 99 | Zmpp000906;pme1439 | C00547+C00811 | https:\\www.genome.jp\dbget-bin\www_bget?map00350 |
| Lysine degradation | ko00310 | 1 | 2 | 34 | 99 | pme1841 | C01672 | https:\\www.genome.jp\dbget-bin\www_bget?map00310 |
| D-Amino acid metabolism | ko00470 | 2 | 2 | 34 | 99 | pme1841;pme2292 | C01672+C00134 | https:\\www.genome.jp\dbget-bin\www_bget?map00470 |
| Glutathione metabolism | ko00480 | 2 | 4 | 34 | 99 | pme1841;pme2292 | C01672+C00134 | https:\\www.genome.jp\dbget-bin\www_bget?map00480 |
| Tropane, piperidine and pyridine alkaloid biosynthesis | ko00960 | 2 | 6 | 34 | 99 | pme1841;pme2292 | C01672+C00134 | https:\\www.genome.jp\dbget-bin\www_bget?map00960 |
| Tryptophan metabolism | ko00380 | 3 | 7 | 34 | 99 | pmb0818;pmb1096;pmb0819 | C05660+C00463+C02938 | https:\\www.genome.jp\dbget-bin\www_bget?map00380 |
| Flavone and flavonol biosynthesis | ko00944 | 3 | 5 | 34 | 99 | mws0059;MWSmce498;mws1434 | C05625+C12627+C01714 | https:\\www.genome.jp\dbget-bin\www_bget?map00944 |
| Diterpenoid biosynthesis | ko00904 | 1 | 2 | 34 | 99 | Cmmn012997 | C06087 | https:\\www.genome.jp\dbget-bin\www_bget?map00904 |
| Phenylalanine metabolism | ko00360 | 1 | 10 | 34 | 99 | mws0346 | C11457 | https:\\www.genome.jp\dbget-bin\www_bget?map00360 |
| Histidine metabolism | ko00340 | 1 | 4 | 34 | 99 | mws0982 | C05127 | https:\\www.genome.jp\dbget-bin\www_bget?map00340 |
| Nicotinate and nicotinamide metabolism | ko00760 | 1 | 2 | 34 | 99 | pme1137 | C01020 | https:\\www.genome.jp\dbget-bin\www_bget?map00760 |
| ABC transporters | ko02010 | 1 | 4 | 34 | 99 | pme2292 | C00134 | https:\\www.genome.jp\dbget-bin\www_bget?map02010 |
| Phenylalanine, tyrosine and tryptophan biosynthesis | ko00400 | 1 | 2 | 34 | 99 | pmb1096 | C00463 | https:\\www.genome.jp\dbget-bin\www_bget?map00400 |
| Benzoxazinoid biosynthesis | ko00402 | 1 | 1 | 34 | 99 | pmb1096 | C00463 | https:\\www.genome.jp\dbget-bin\www_bget?map00402 |
| Thiamine metabolism | ko00730 | 1 | 1 | 34 | 99 | pmb0764 | C04294 | https:\\www.genome.jp\dbget-bin\www_bget?map00730 |
| Biosynthesis of cofactors | ko01240 | 1 | 6 | 34 | 99 | pmb0764 | C04294 | https:\\www.genome.jp\dbget-bin\www_bget?map01240 |
| Polyketide sugar unit biosynthesis | ko00523 | 1 | 1 | 34 | 99 | pmp000509 | C11918 | https:\\www.genome.jp\dbget-bin\www_bget?map00523 |
| Ubiquinone and other terpenoid-quinone biosynthesis | ko00130 | 1 | 5 | 34 | 99 | pme1439 | C00811 | https:\\www.genome.jp\dbget-bin\www_bget?map00130 |
| Isoquinoline alkaloid biosynthesis | ko00950 | 1 | 3 | 34 | 99 | pme1439 | C00811 | https:\\www.genome.jp\dbget-bin\www_bget?map00950 |
| Isoflavonoid biosynthesis | ko00943 | 1 | 3 | 34 | 99 | MWSHY0017 | C00509 | https:\\www.genome.jp\dbget-bin\www_bget?map00943 |

**Table S2. KEGG pathways and annotated compounds in the comparison group SD9 vs. SD6**

| Kegg_pathway | ko_ID | Sig_compound | compound | Sig_compound_all | compound_all | IndexList | CIDList | Pathway |
|---|---|---|---|---|---|---|---|---|
| Phenylalanine metabolism | ko00360 | 4 | 10 | 28 | 96 | Lmmn001643;Lmbn002648;MWSmce248;MWS4301 | C01772+C02763+C12621+C05593 | https:\\www.genome.jp\dbget-bin\www_bget?map00360 |
| Biosynthesis of various plant secondary metabolites | ko00999 | 3 | 8 | 28 | 96 | Lmmn001643;pmb0501;Zmpn003044 | C01772+C00179+C09315 | https:\\www.genome.jp\dbget-bin\www_bget?map00999 |
| Metabolic pathways | ko01100 | 18 | 68 | 28 | 96 | Lmmn001643;pme3083;Lmbn001981;Lmbn002648;Lmlp003161;Lmbn002644;mws0749;MWSmce248;MWS4301;MWSmce548;MA10107783;pmb0501;pme2292;Lmbn002737;pme1439;pme2693;pme2122;Ymjm000148 | C01772+C05653+C05585+C02763+C10497+C06758+C00156+C12621+C05593+C00719+C20772+C00179+C00134+C07209+C00811+C02714+C00388+C06046 | https:\\www.genome.jp\dbget-bin\www_bget?map01100 |
| Biosynthesis of secondary metabolites | ko01110 | 12 | 43 | 28 | 96 | Lmmn001643;mws0749;MA10107783;pmb0501;Lmsn003297;pme2292;Zmpn003044;pme1439;mws1574;MWSCX015;pmb3074;pme2122 | C01772+C00156+C20772+C00179+C16408+C00134+C09315+C00811+C11673+C10945+C12208+C00388 | https:\\www.genome.jp\dbget-bin\www_bget?map01110 |
| Isoquinoline alkaloid biosynthesis | ko00950 | 2 | 3 | 28 | 96 | Hmgn001653;pme1439 | C16700+C00811 | https:\\www.genome.jp\dbget-bin\www_bget?map00950 |
| Tryptophan metabolism | ko00380 | 1 | 5 | 28 | 96 | pme3083 | C05653 | https:\\www.genome.jp\dbget-bin\www_bget?map00380 |
| Tyrosine metabolism | ko00350 | 4 | 11 | 28 | 96 | Lmbn001981;MWS4301;pme1439;Ymjm000148 | C05585+C05593+C00811+C06046 | https:\\www.genome.jp\dbget-bin\www_bget?map00350 |
| Arginine and proline metabolism | ko00330 | 4 | 7 | 28 | 96 | Lmlp003161;pmb0501;pme2292;pme2693 | C10497+C00179+C00134+C02714 | https:\\www.genome.jp\dbget-bin\www_bget?map00330 |
| Ubiquinone and other terpenoid-quinone biosynthesis | ko00130 | 3 | 5 | 28 | 96 | mws0749;MA10107783;pme1439 | C00156+C20772+C00811 | https:\\www.genome.jp\dbget-bin\www_bget?map00130 |
| Folate biosynthesis | ko00790 | 1 | 1 | 28 | 96 | mws0749 | C00156 | https:\\www.genome.jp\dbget-bin\www_bget?map00790 |
| Biosynthesis of cofactors | ko01240 | 2 | 6 | 28 | 96 | mws0749;MA10107783 | C00156+C20772 | https:\\www.genome.jp\dbget-bin\www_bget?map01240 |
| Glycine, serine and threonine metabolism | ko00260 | 1 | 1 | 28 | 96 | MWSmce548 | C00719 | https:\\www.genome.jp\dbget-bin\www_bget?map00260 |
| ABC transporters | ko02010 | 2 | 4 | 28 | 96 | MWSmce548;pme2292 | C00719+C00134 | https:\\www.genome.jp\dbget-bin\www_bget?map02010 |
| Flavonoid biosynthesis | ko00941 | 2 | 7 | 28 | 96 | Lmsn003297;pmb3074 | C16408+C12208 | https:\\www.genome.jp\dbget-bin\www_bget?map00941 |
| D-Amino acid metabolism | ko00470 | 1 | 2 | 28 | 96 | pme2292 | C00134 | https:\\www.genome.jp\dbget-bin\www_bget?map00470 |
| Glutathione metabolism | ko00480 | 1 | 4 | 28 | 96 | pme2292 | C00134 | https:\\www.genome.jp\dbget-bin\www_bget?map00480 |
| Tropane, piperidine and pyridine alkaloid biosynthesis | ko00960 | 1 | 6 | 28 | 96 | pme2292 | C00134 | https:\\www.genome.jp\dbget-bin\www_bget?map00960 |
| Phenylpropanoid biosynthesis | ko00940 | 5 | 12 | 28 | 96 | mws0011;Lhhp120814;pme1439;MWSCX015;pmb3074 | C01533+C10453+C00811+C10945+C12208 | https:\\www.genome.jp\dbget-bin\www_bget?map00940 |
| Monoterpenoid biosynthesis | ko00902 | 1 | 1 | 28 | 96 | mws1574 | C11673 | https:\\www.genome.jp\dbget-bin\www_bget?map00902 |
| Stilbenoid, diarylheptanoid and gingerol biosynthesis | ko00945 | 1 | 1 | 28 | 96 | pmb3074 | C12208 | https:\\www.genome.jp\dbget-bin\www_bget?map00945 |
| Histidine metabolism | ko00340 | 1 | 4 | 28 | 96 | pme2122 | C00388 | https:\\www.genome.jp\dbget-bin\www_bget?map00340 |
| Flavone and flavonol biosynthesis | ko00944 | 2 | 4 | 28 | 96 | MWSmce498;mws1434 | C12627+C01714 | https:\\www.genome.jp\dbget-bin\www_bget?map00944 |