Metabolomic characterization of the possible involvement of a Cytochrome P450, CYP81F4, in the biosynthesis of indolic glucosinolate in *Arabidopsis*
[Plant Biotechnol. 28(4): 379-385 (2011)]

Supplemental Table 1. Numbers of metabolite pairs as substrates and products of known enzyme reactions in the KNApSAcK databse.

Reaction	Difference[a]	Number
Monooxygenation	O	2383
Methylation	CH_2	2055
Dehydrogenation	H_2	1262
Glycosylation	$C_6H_{10}O_5$	
Glycosylation	$C_6H_{10}O_4$	200
Glycosylation	$C_6H_{10}O_3$	7
Glycosylation	$C_5H_8O_4$	100
Phosphorylation	HO_3P	97
Pyrophosphorylation	$H_2O_6P_2$	10
CoA thioester formation	$C_{21}H_{34}N_7O_{15}P_3S$	162
Acetylation	C2H2O	402
Malonylation	$C3H2O_3$	76
Benzoylation	C_7H_4O	8
Amination	HN	13
Amidation	CHON	7
Cylation	indefinite[b]	71
Methoxy formation	CH_2O	685

Substrate and product pairs were searched in the KNApSAcK database, and classified according to the catalytic properties. Only the substrate and product pairs found within the same organisms were listed.

[a] Differences in the elemental compositions from the enzyme reactions.

[b] Metabolite pairs as acyltransferase reactions explained by either the reaction of "R_1–COOH+R_2–OH→R_1–COO–R_2+H_2O" or "R_1–COOH+R_2–NH_2→R_1–CONH–R_2+H_2O."

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Supplemental Table 2. The *m*/*z* values contributed to separate the wild-type from *cyp81f4* mutant lines in the principal component analysis shown in Figure 4.

No.	Score[a]	*m*/*z* (observed)	Predicted molecular formula	Difference[b] (ppm)	Candidate metabolites[c]
1	0.974	447.0444	—	—	—
2	0.963	447.0606	—	—	—
3	0.961	447.0308	—	—	—
4	0.959	449.0497	—	—	—
5	0.959	447.0541	$C_{16}H_{20}N_2O_9S_2$	0.90	indol-3-ylmethylglucosinolate
6	0.930	448.0574	—	—	—
7	0.903	463.0487	$C_{16}H_{20}N_2O_{10}S_2$	0.081	4-hydroxyindol-3-yl-methylglucosinolate, etc.
8	0.902	485.0100	—	—	—
9	0.864	447.0373	—	—	—
10	0.763	484.9983	—	—	—
11	0.698	341.1089	$C_{12}H_{22}O_{11}$	0.014	sucrose, maltose, melibiose, etc.
12	0.665	462.0835	—	—	—
13	0.640	439.0764	—	—	—
14	0.637	565.0477	$C_{15}H_{24}N_2O_{17}P_2$	0.13	UDP-D-glucose, UDP-D-galactose
15	0.623	448.0496	—	—	—
16	0.598	447.0227	—	—	—
17	0.590	462.0936	$C_{15}H_{29}NO_9S_3$	0.91	7-methylthioheptylglucosinolate
18	0.587	707.1135	—	—	—
19	0.583	548.0055	—	—	—
20	0.578	593.1512	$C_{27}H_{30}O_{15}$	0.076	quercetin-3,7-dirhamnoside, etc.
⋮	⋮	⋮	⋮	⋮	⋮
334	-0.867	477.0952	—	—	—
335	-0.870	479.0461	—	—	—
336	-0.871	477.0718	—	—	—
337	-0.880	477.0241	—	—	—
338	-0.908	611.1501	—	—	—
339	-0.929	446.0149	—	—	—
340	-0.933	478.0757	—	—	—
341	-0.936	478.0489	—	—	—
342	-0.937	550.9968	—	—	—
343	-0.942	477.0849	—	—	—
344	-0.947	577.9974	—	—	—
345	-0.947	650.9436	—	—	—
346	-0.948	552.9941	—	—	—
347	-0.949	446.0398	—	—	—
348	-0.951	446.0345	—	—	—
349	-0.951	446.0462	—	—	—
350	-0.951	446.0292	—	—	—
351	-0.952	447.0503	—	—	—

No.	Score[a]	*m*/*z* (observed)	Predicted molecular formula	Difference[b] (ppm)	Candidate metabolites[c]
352	-0.952	446.0530	—	—	—
353	-0.953	446.0233	—	—	—

[a] List of the principal component scores. Positive and negative values correspond to those contributing to form the *cyp81f4-1* type metabolome and wild-type metabolome, respectively.
[b] Differences in the *m*/*z* values between the observed values and the theoretical values from the predicted molecular formulas.
[c] Metabolite candidates found in the KNApSAcK database within the *m*/*z* analytical errors of 2 ppm.
— For these analytes, candidate metabolites were not found in the KNApSAcK database with an *m*/*z* error allowance within 2 ppm.