

A substrate of the ABC transporter PEN3 stimulates bacterial flagellin (flg22)-induced callose deposition in *Arabidopsis thaliana*

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Supporting Information

Supporting Figure S1: CID spectra of 4-methoxyindol-3-yl methanol and S-(4-methoxy-indol-3-ylmethyl) cysteine.

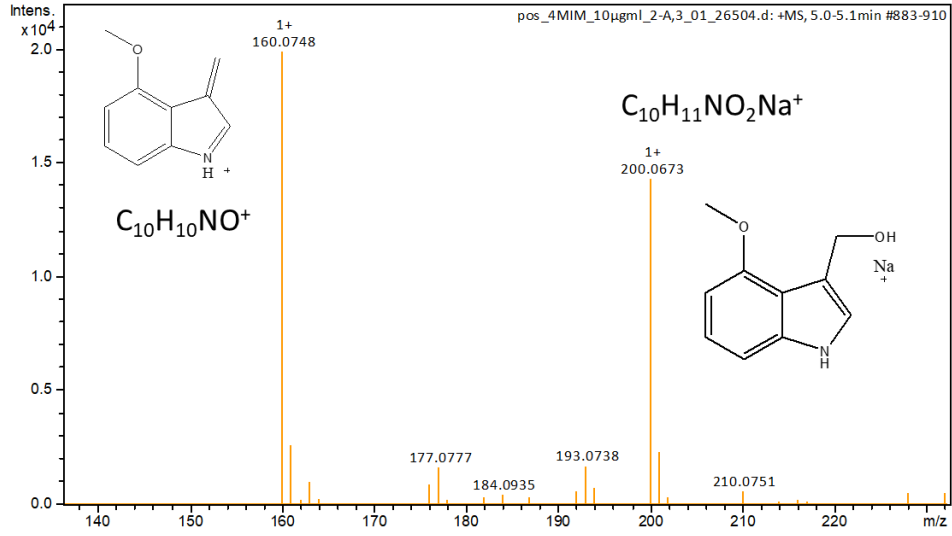
Supporting Figure S2: Scatter plots of the data shown in Fig. 3

Supporting Figure S3: Scatter plots of the data shown in Fig. 4

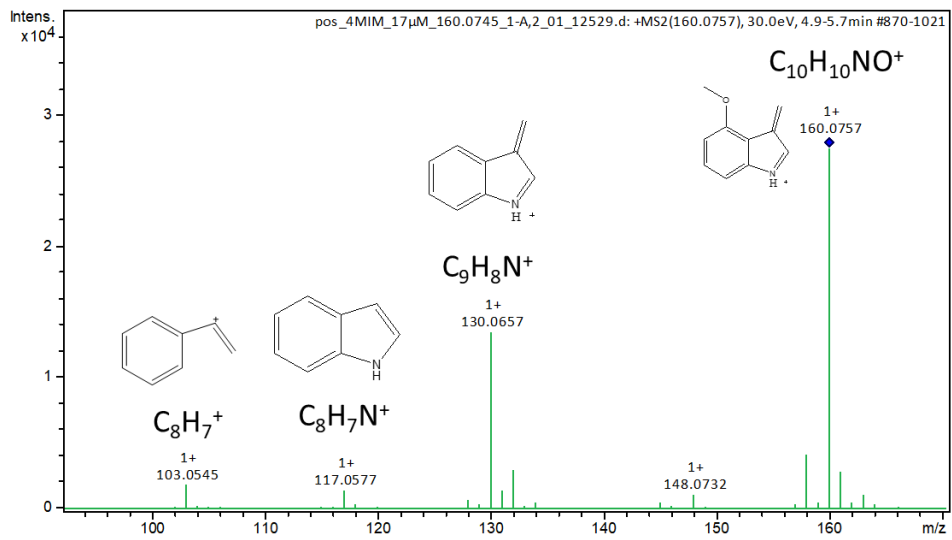
Table S1: Tentatively annotated features that were detected in the spore suspension without contact to leaves.

Table S2: Tentatively annotated features that accumulated to significantly higher levels in spore suspension droplets recollected from *pen3* mutants compared to WT.

A



B



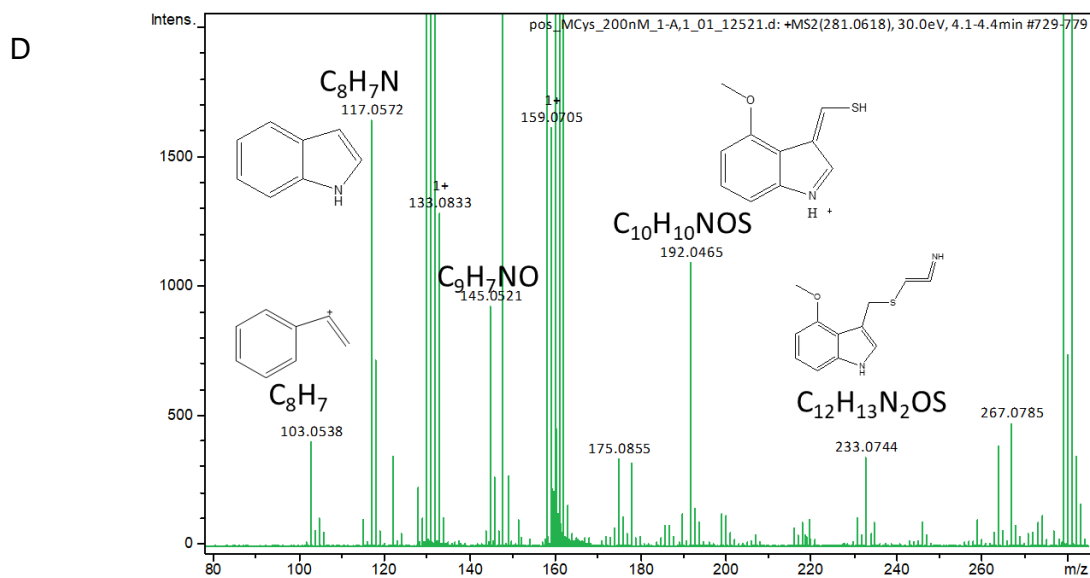
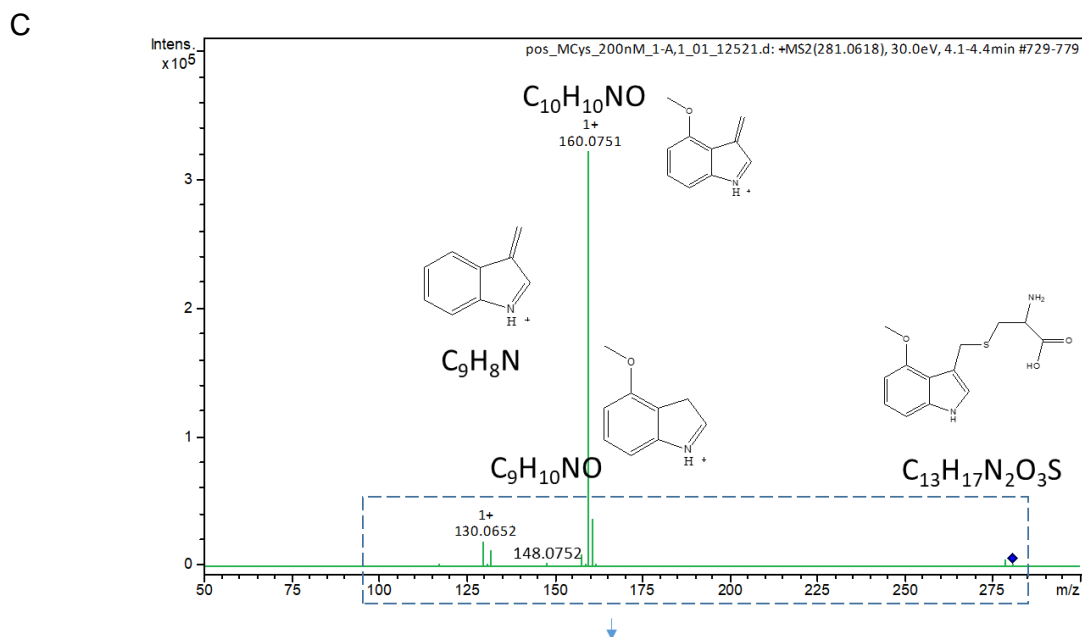


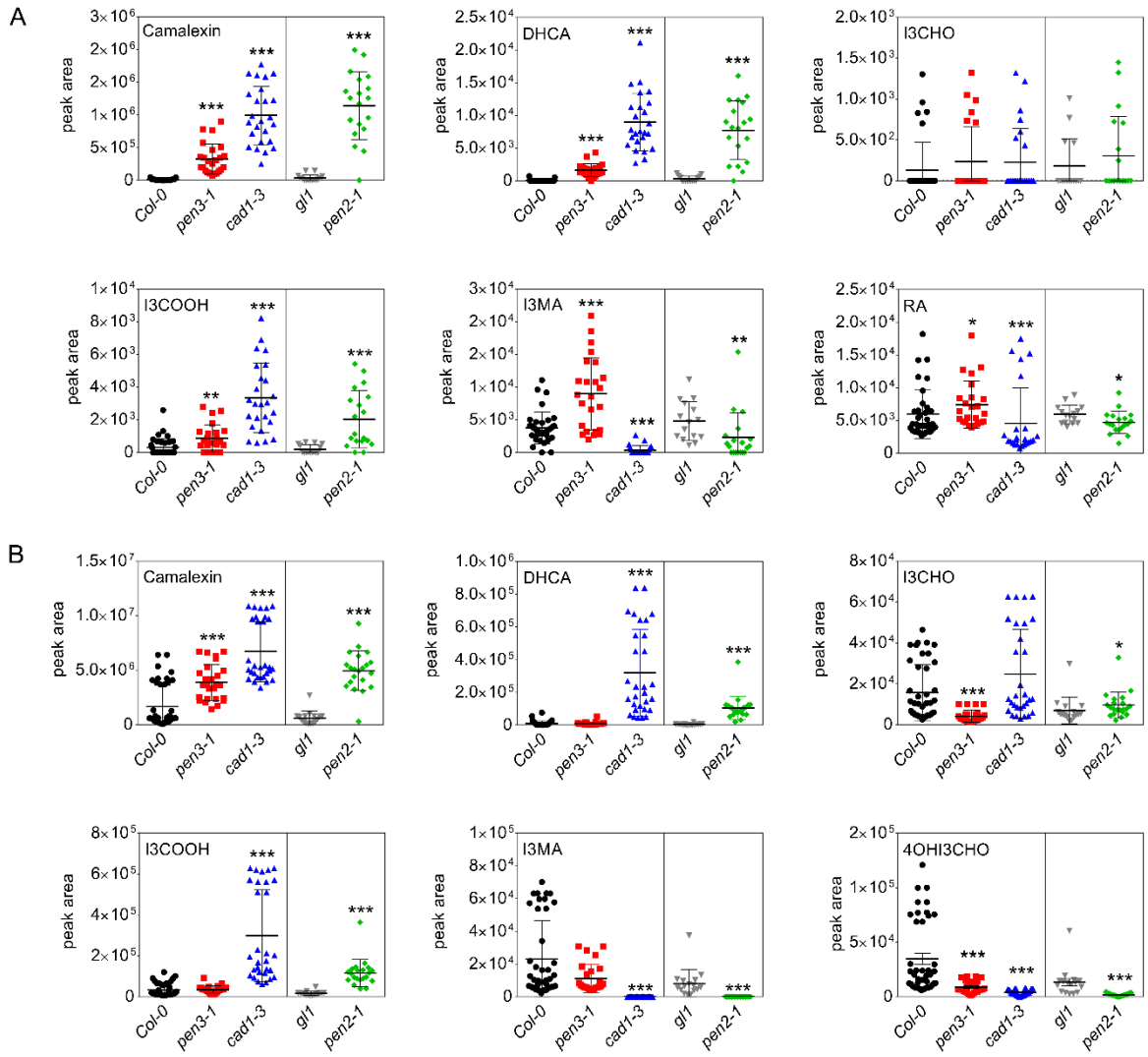
Figure S1: Mass spectrum of 4-methoxy-indol-3-yl methanol.

A, MS adducts and fragments

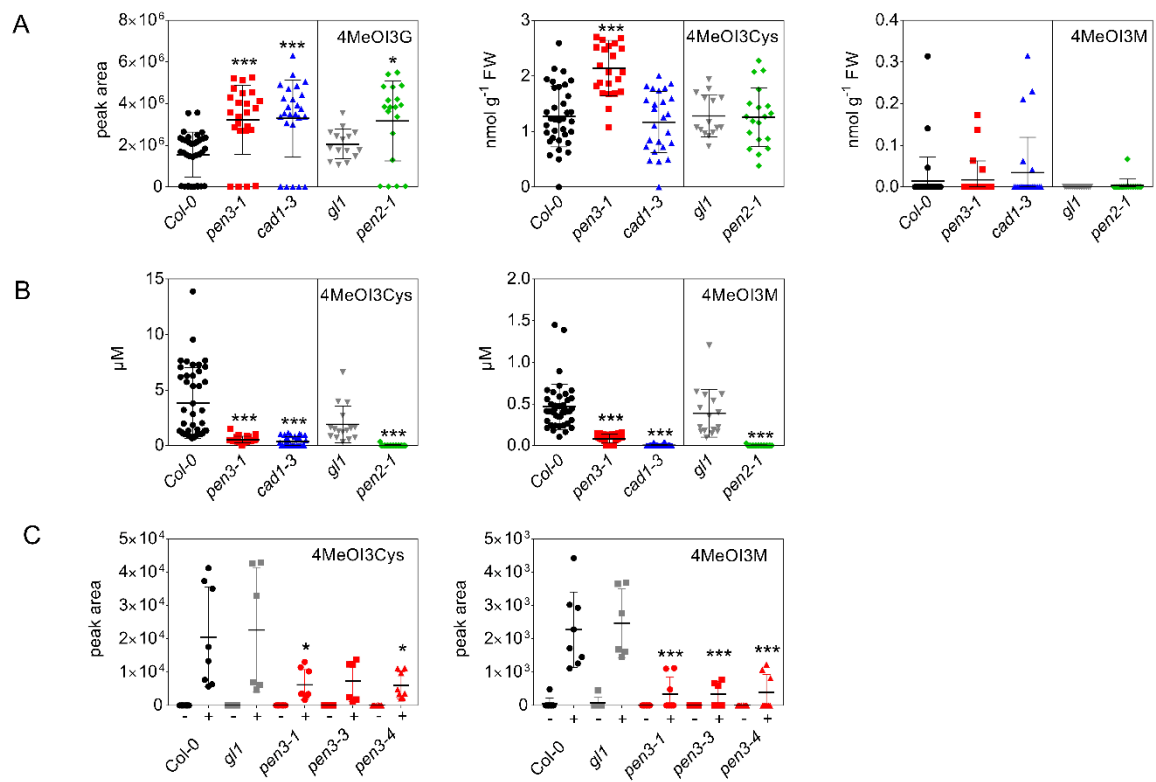
B, MS2 of quantifier ion (MRM mode)

C, Fragmentation pattern (MRM mode) and possible fragments of S-(4-methoxy-indol-3-ylmethyl)cysteine

D, magnification of C



Supporting Figure S2: Scatter plots of the data shown in Fig. 3



Supporting Figure S3: Scatter plots of the data shown in Fig. 4

Table S1: Tentatively annotated features that were detected in the spore suspension without contact to leaves. Annotation according to an in-house analyte list using m/z ratio and retention time. Allowed deviation: 15mDa, RT 0.2min. The feature table was acquired from the merged four repetitions containing measurements of 4 spore suspension samples. All features with a summed up intensity ≥ 2000 in the four spore suspension samples were taken into consideration.

feature	m/z meas.	M meas.	RT [min]
L-arginine	175.11808	174.1108	0.4
D-glucose-6-phosphate RT1	283.03293	282.02565	0.41
D-glucurono-3,6-lactone, adduct	184.04966	366.08476	0.43
shikimic acid (dimer)	175.05054	348.08653	0.43
D-galacturonic acid, dimer	411.06729	410.06002	0.43
D-xylitol, xylite	175.05609	174.04882	0.43
L-aspartic acid, dimer	156.04064	310.06672	0.44
fructose, dimer	383.11141	382.10413	0.44
ureidosuccinic acid, dimer RT1	375.08929	374.08201	0.44
myo-inositol	219.02651	180.06327	0.44
betaine, trimethylglycine; dimer	235.16428	234.157	0.46
D-(+)-raffinose	543.13193	504.16826	0.46
D-sucrose	365.10357	364.09629	0.46
L-valine	118.08387	117.07659	0.46
L-proline	138.05346	115.06265	0.47
L-cysteine, dimer	263.02117	262.01389	0.48
pipecolic acid	130.08402	129.07674	0.48
cytidine RT1	244.09146	243.08418	0.48
L-methionine, dimer	321.09147	320.08419	0.48
D-galacturonic acid, dimer	206.02689	410.03975	0.49
nicotinic acid - dimer	247.07374	246.06646	0.49
adduct of ascorbic acid, charge 2+	230.99011	192.02729	0.49
L-proline + H2O	130.04975	129.04247	0.49
uridine RT1	245.07036	244.06308	0.49
L-(+)-glutamic acid	148.05935	147.05207	0.49
D-(-)-ribose, adduct	265.08538	264.0781	0.49
3-hydroxy-3-methylglutaric acid	163.05979	162.05251	0.5
L-methionine, dimer	321.09121	320.08393	0.52
D-sucrose	343.1219	342.11462	0.56
D-gluconic acid, dimer	208.04233	414.07011	0.57
L-aspartic acid, dimer	267.07034	266.06306	0.58
L-glutamic acid, dimer	170.02877	338.04299	0.59
ureidosuccinic acid; dimer RT2	353.09132	352.08404	0.6
alpha-ketoglutaric acid	147.03136	146.02408	0.62
D-sucrose RT2	325.11249	342.11607	0.62
uridine RT2	245.07147	244.06419	0.62
D-sucrose RT2	343.12374	342.11646	0.62
ureidosuccinic acid	199.03734	198.03007	0.63
cytidine 5'-monophosphate	324.06385	323.05658	0.63

D-galacturonic acid, dimer	206.02738	410.0402	0.63
cytosine	112.04865	111.04137	0.63
D-glucose 6-phosphate RT2	261.03338	260.0261	0.63
uric acid	169.03559	168.02831	0.64
citric acid	230.99024	192.02691	0.64
nicotinic acid, niacin	124.03673	123.02946	0.64
cytidine RT2	244.0919	243.08462	0.64
adenosine 5'-monophosphate (AMP), RT2	348.0686	347.06133	0.65
xanthine, 2,6-dihydroxypurine	153.03921	152.03194	0.65
glutathione	308.09017	307.08289	0.65
uracil	113.03346	112.02618	0.66
L-proline + H2O	130.04903	129.04175	0.66
nicotinic acid - dimer	247.07443	246.06715	0.66
uridine RT2	245.07771	244.07043	0.66
L-tyrosine, peak 2, -NH2	165.05419	164.04691	0.68
L-tyrosine	182.0808	181.07353	0.68
adenosine, peak 2	268.10326	267.09598	0.69
3,4-dihydroxyphenylalanine, L-DOPA, RT2	198.07287	197.0656	0.7
hypoxanthine	137.04486	136.03759	0.76
guanosine	284.0993	283.09203	0.76
inosine	269.09146	268.08419	0.78
L-leucine	132.10024	131.09297	0.78
cis-aconitic acid	175.02604	174.01877	0.81
hypoxanthine; 6-hydroxypurine, dimer	295.07341	294.06614	0.84
2-O-methyladenosine	282.11743	281.11015	1.01
phenylalanine, in-source fragment	120.07876	119.07149	1.23
L-phenylalanine	166.08518	165.07791	1.24
D-pantothenic acid	220.11746	219.11019	1.57
D-panthenol	206.13806	205.13078	1.59
H-Leu-Pro-OH, leucyl-proline	229.15413	228.14685	2.51
H-Phe-Val-OH, phenylalanyl-valine	265.14299	264.13571	2.97
kinetin (internal standard)	216.08761	215.08034	3
beta-carbocine-3-carboxylic acid	217.09601	216.08873	3.1
Ile-Phe, isoleucyl-phenylalanine, in-source fragment phenylalanine	166.0853	165.07803	3.81
N-phenylacetyl-aspartic acid	252.08647	251.0792	4.1
trans-sinapic acid	207.06756	224.06954	4.52
3,4-dimethoxyhydrocinnamic acid	211.09379	210.08651	5.15
herniarin, 7-methoxycoumarin	177.05472	176.04744	6.01
IAA-valine; IAA-Val; Indole-3-acetyl-valine (internal standard)	297.12012	274.13108	6.22
apigenin	271.05889	270.05161	6.79
corchorifatty acid F	351.21336	328.22396	7.11
9,12,13-trihydroxyoctadec-10-enoic acid	353.22862	330.23908	7.38
biochanin (Na-Addukt) (internal standard)	307.05667	284.06706	8.82
biochanin A, 5,7-dihydroxy-4'-methoxyisoflavone (internal standard)	285.07504	284.06777	8.82

oxo-phytodienoic acid 12-OPDA	293.21004	292.20271	10.26
L-alpha-lecithin, in-source fragment	454.29081	453.28354	11.2
lauric acid, n-dodecanoic acid	201.18387	200.1766	12.11
eicosapentaenoic acid	303.23051	302.22068	13.69
myristic acid, tetradecanoic acid	229.21506	228.20735	13.78
linoleic acid	281.24635	280.23882	14.64

Table S2: Tentatively annotated features that accumulated to significantly higher levels in spore suspension droplets recollected from *pen3* mutants compared to WT. Annotation according to an in-house analyte list using m/z ratio and retention time. Allowed deviation: 15mDa, RT 0.2min. The feature table was acquired from four repetitions containing measurements of 4 spore suspension samples each.

feature	m/z meas.	M meas.	RT [min]	fold change <i>pen3/Col-0</i>
acetylglutamine	173.13945	172.13217	0.48	5.0
3,3 dimethylglutaric acid	161.07041	160.06314	3.48	2.3
1-O-sinapoyl-beta-glucose	189.04766	206.05231	3.52	10.3
kaempferol 3-O-Rha(1-2)Glc 7-O-Rha	741.21924	740.21197	3.79	2.6
5-hydroxycamalexin	217.0428	216.03544	3.85	4.8
beta-d-glucosyl indole-3-carboxylate	306.09651	323.0984	4	2.8
scopoletin	193.04282	192.03555	4.29	5.2
kaempferol deoxyhex Hex	595.16563	594.15836	4.33	2.0
unknown camalexin metabolite #1	217.04267	234.04616	4.43	14.7
kaempferitrin, kaempferol 3,7-di-O-alpha-Rha	579.16939	578.16211	4.7	3.2
1-methylindole-3-carboxylic acid (1Me-I3COOH)	176.07081	175.06353	5.91	2.4
8-methylsulphonyloctyl	266.12397	265.11667	5.95	10.6
2-formamidophenyl-2'-thiazolylketone	233.03819	232.03055	6.00	3.2
(-)-jasmonic acid	211.13333	210.12587	6.74	7.5