

**Table A.** Above ground biomass, grain yield and yield components at maturity of durum wheat grown in the field. Wheat with natural arbuscular mycorrhizal inoculum (NAT), inoculated with AM fungi spores (AMF), or inoculated with both AMF and plant growth-promoting rhizobacteria (AMF+PGPR). Yield components are number of spikes per square meter, number of kernels per spike, and 1000-kernel weight.

	Above ground biomass	Grain yield	Spikes per m <sup>-2</sup>	Kernels per spike	1000-kernel weight
	Mg ha <sup>-1</sup>	Mg ha <sup>-1</sup>			g
NAT	9.0 ± 0.21	3.8 ± 0.12	255 ± 9.8	31.5 ± 1.72	47.1 ± 0.39
AMF	9.2 ± 0.25	3.8 ± 0.15	266 ± 13.0	32.4 ± 3.83	45.7 ± 3.25
AMF+PGPR	9.0 ± 0.25	3.7 ± 0.09	252 ± 12.4	31.3 ± 1.84	47.3 ± 0.98
<i>P-value</i>	<i>0.806</i>	<i>0.834</i>	<i>0.673</i>	<i>0.935</i>	<i>0.837</i>

**Table B.** Enrichment metabolomic analysis for Pathways as displayed in MBRole.

<b>Pathways (set: 73 background: 3327)</b>	<b>P- value</b>	<b>Adjusted P-value*</b>	<b>In background</b>	<b>In set</b>	<b>%**</b>	<b>Compounds</b>
Alanine aspartate and glutamate metab.	0.000	0.000	24	10	13.7	C00334 C00022 C00122 C00064 C00041 C00026 C00152 C00025 C00042 C00049
Aminoacyl-tRNA bios.	0.000	0.000	75	11	15.1	C00047 C00079 C00082 C00152 C00188 C00041 C00049 C00078 C00064 C00407 C00025
Citrate cycle (TCA cycle)	0.000	0.000	20	6	8.2	C00122 C00149 C00026 C00022 C00158 C00042
Metabolic pathways	0.000	0.000	1455	51	69.9	C00198 C00026 C00064 C00116 C06427 C00025 C00085 C00811 C00156 C00099 C05437 C00158 C00134 C00077 C00259 C00122 C00042 C05422 C00093 C00188 C00009 C00095 C00208 C00257 C01595 C00212 C00047 C00089 C00249 C00041 C00152 C00180 C00049 C00379 C00189 C00092 C00181 C01694 C00387 C00031 C00334 C00474 C00149 C00078 C00407 C00186 C00022 C00408 C00079 C00082 C00493
Phenylalanine metab.	0.000	0.000	46	8	11	C00082 C00022 C00811 C00042 C00156 C00180 C00122 C00079
Butanoate metab.	0.000	0.000	40	7	9.6	C00025 C00042 C00026 C00022 C01384 C00334 C00122
Fatty acid bios.	0.000	0.001	49	7	9.6	C00712 C00249 C06424 C08362 C01530 C01571 C02679
Starch and sucrose metab.	0.000	0.001	50	7	9.6	C00089 C00185 C00095 C00208 C00181 C00092 C00031
Carbon fixation in photosynthetic organisms	0.000	0.001	23	5	6.8	C00049 C00041 C00149 C00022 C00085
Pentose and glucuronate interconversions	0.000	0.001	53	7	9.6	C00085 C00181 C00379 C00474 C00259 C00022 C01904
Nitrogen metab.	0.000	0.001	26	5	6.8	C00049 C00064 C00152 C00025 C00192
Galactose metab.	0.000	0.001	41	6	8.2	C00089 C01235 C00031 C05401 C00095 C00116
Phenylalanine tyrosine and tryptophan bios.	0.000	0.001	27	5	6.8	C00078 C00296 C00493 C00082 C00079
Arginine and proline metab.	0.000	0.002	82	8	11	C00025 C00077 C00134 C00122 C00022 C00334 C00064 C00049
Pentose phosphate pathway	0.001	0.002	32	5	6.8	C00022 C00198 C00257 C00031 C00121
Bios. of unsaturated fatty acids	0.001	0.004	54	6	8.2	C06427 C01595 C00712 C00249 C06425 C01530
Glutathione metab.	0.001	0.005	38	5	6.8	C00025 C01879 C00077 C05422 C00134
Glyoxylate and dicarboxylate metab.	0.002	0.009	44	5	6.8	C00042 C00022 C00026 C00149 C00158
Glycolysis / Gluconeogenesis	0.004	0.014	31	4	5.5	C01451 C00022 C00186 C00031
Glycerolipid metab.	0.005	0.014	32	4	5.5	C00093 C00116 C02457 C05401
Oxidative phosphorylation	0.005	0.014	16	3	4.1	C00009 C00122 C00042
Nicotinate and nicotinamide metab.	0.015	0.042	44	4	5.5	C00022 C01384 C00122 C00049
Tropane piperidine and pyridine alkaloid bios.	0.016	0.043	68	5	6.8	C00408 C00407 C00134 C00047 C00079
Ascorbate and aldarate metab.	0.019	0.048	47	4	5.5	C00022 C00026 C00259 C05422
Pantothenate and CoA bios.	0.020	0.050	27	3	4.1	C00049 C00022 C00099
Glycine serine and threonine metab.	0.021	0.051	49	4	5.5	C00049 C00188 C00078 C00022
Valine leucine and isoleucine bios.	0.022	0.051	28	3	4.1	C00022 C00188 C00407
Steroid bios.	0.025	0.054	51	4	5.5	C01753 C05437 C05442 C01694
beta-Alanine metab.	0.029	0.062	31	3	4.1	C00099 C00049 C00334

C5-Branched dibasic acid metab.	0.032	0.062	32	3	4.1	C00022 C00026 C00025
Lysine bios.	0.032	0.062	32	3	4.1	C00026 C00047 C00049
Pyruvate metab.	0.032	0.062	32	3	4.1	C00149 C00022 C00186
Cysteine and methionine metab.	0.033	0.062	56	4	5.5	C00049 C00022 C02989 C00041
Propanoate metab.	0.043	0.079	36	3	4.1	C00099 C00042 C00186
Cyanoamino acid metab.	0.060	0.106	41	3	4.1	C00082 C00152 C00049
Histidine metab.	0.071	0.119	44	3	4.1	C00025 C00026 C00049
Taurine and hypotaurine metab.	0.070	0.119	20	2	2.7	C00041 C00022
Bios. of secondary metabolites	0.074	0.120	1038	29	39.7	C00047 C00122 C00180 C00082 C00134 C00025 C00493 C00149 C00156 C00257 C00408 C00811 C00407 C00026 C00092 C01753 C00042 C00049 C00158 C00079 C00198 C00186 C05442 C00031 C00078 C00077 C00022 C00152 C00188
Tyrosine metab.	0.084	0.133	76	4	5.5	C00122 C00022 C00082 C00042
Thiamine metab.	0.110	0.171	26	2	2.7	C00022 C00082
Phenylpropanoid bios.	0.119	0.179	55	3	4.1	C00082 C00079 C00811
Vitamin B6 metab.	0.155	0.229	32	2	2.7	C00022 C00026
Ubiquinone and other terpenoid-quinone bios.	0.232	0.335	76	3	4.1	C00082 C00811 C00156
Glycerophospholipid metab.	0.268	0.377	46	2	2.7	C00093 C00189
Lysine degradation	0.276	0.380	47	2	2.7	C00047 C00408
Amino sugar and nucleotide sugar metab.	0.298	0.402	87	3	4.1	C00181 C00259 C00031
Purine metab.	0.328	0.433	92	3	4.1	C00212 C00064 C00387
Pyrimidine metab.	0.373	0.482	59	2	2.7	C00064 C00099
Tryptophan metab.	0.536	0.678	81	2	2.7	C05659 C00078
Porphyrin and chlorophyll metab.	0.772	0.957	126	2	2.7	C00188 C00025
alpha-Linolenic acid metab.	1.000	1.000	40	1	1.4	C06427
Biotin metab.	1.000	1.000	11	1	1.4	C00047
Fatty acid metab.	1.000	1.000	50	1	1.4	C00249
Fructose and mannose metab.	1.000	1.000	48	1	1.4	C00095
Inositol phosphate metab.	1.000	1.000	39	1	1.4	C00092
Isoquinoline alkaloid bios.	1.000	1.000	94	1	1.4	C00082
Methane metab.	1.000	1.000	34	1	1.4	C00085
Photosynthesis	1.000	1.000	11	1	1.4	C00009
Riboflavin metab.	1.000	1.000	21	1	1.4	C00474
Selenoamino acid metab.	1.000	1.000	30	1	1.4	C00041
Terpenoid backbone bios.	1.000	1.000	33	1	1.4	C00022
Valine leucine and isoleucine degradation	1.000	1.000	41	1	1.4	C00407

Compounds with no annotations (10): C08240 C01389 C01601 C00503 C08243 C16537 C01018 C08374 C02112 C01725

\* *P*-value of annotation adjusted for multiple testing using false discovery rate according to Benjamini & Hochberg (1995) doi:10.2307/2346101.

\*\* In set for the present background comparing total Kegg assigned compounds.

**Table C.** Enrichment metabolomic analysis for Enzyme interactions as displayed in MBRole.

Enzyme interactions (set: 38 background: 729)	<i>P</i> - value	Adjusted <i>P</i> -value*	In background	In set	%**	Compounds
alanine transaminase	0.000	0.005	5	4	10.5	C00022 C00025 C00026 C00041
anthranilate synthase	0.001	0.032	5	3	7.9	C00025 C00064 C00022
asparagine synthase (glutamine-hydrolysing)	0.001	0.032	9	4	10.5	C00064 C00152 C00025 C00049
aspartate transaminase	0.001	0.032	5	3	7.9	C00049 C00026 C00025
phenylalanine/tyrosine ammonia-lyase	0.001	0.032	5	3	7.9	C00811 C00082 C00079
tyrosine transaminase	0.001	0.032	5	3	7.9	C00082 C00025 C00026
glucose-6-phosphate isomerase	0.003	0.060	2	2	5.3	C00092 C00085
asparaginyl-tRNA synthase (glutamine-hydrolysing)	0.004	0.070	7	3	7.9	C00009 C00025 C00064
glutamyl-tRNA synthase (glutamine-hydrolysing)	0.004	0.070	7	3	7.9	C00025 C00064 C00009
phosphoribosylformylglycinamide synthase	0.006	0.097	8	3	7.9	C00025 C00009 C00064
(R)-3-amino-2-methylpropionate---pyruvate transaminase	0.015	0.098	4	2	5.3	C00041 C00022
carbamoyl-phosphate synthase (glutamine-hydrolysing)	0.009	0.098	9	3	7.9	C00064 C00025 C00009
fructokinase	0.015	0.098	4	2	5.3	C00085 C00095
fructose-2, 6-bisphosphate 2-phosphatase	0.015	0.098	4	2	5.3	C00085 C00009
fructose-bisphosphatase	0.015	0.098	4	2	5.3	C00085 C00009
fumarate hydratase	0.008	0.098	3	2	5.3	C00149 C00122
glutamate decarboxylase	0.015	0.098	4	2	5.3	C00334 C00025
glutamate N-acetyltransferase	0.015	0.098	4	2	5.3	C00025 C00077
glutamate---ammonia ligase	0.012	0.098	10	3	7.9	C00009 C00025 C00064
glycerol kinase	0.015	0.098	4	2	5.3	C00093 C00116
ornithine carbamoyltransferase	0.015	0.098	4	2	5.3	C00077 C00009
ornithine decarboxylase	0.015	0.098	4	2	5.3	C00134 C00077
phosphorylase	0.009	0.098	9	3	7.9	C00009 C00198 C00092
sucrose synthase	0.015	0.098	4	2	5.3	C00089 C00095
glutamate synthase (ferredoxin)	0.016	0.103	11	3	7.9	C00025 C00064 C00026
alanine---glyoxylate transaminase	0.024	0.119	5	2	5.3	C00022 C00041
branched-chain-amino-acid transaminase	0.024	0.119	5	2	5.3	C00025 C00026
histidinol-phosphate transaminase	0.024	0.119	5	2	5.3	C00025 C00026
L-lactate dehydrogenase	0.024	0.119	5	2	5.3	C00022 C00186
malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+)	0.024	0.119	5	2	5.3	C00149 C00022
serine---pyruvate transaminase	0.024	0.119	5	2	5.3	C00041 C00022
threonine synthase	0.024	0.119	5	2	5.3	C00188 C00009
adenylosuccinate synthase	0.035	0.142	6	2	5.3	C00049 C00009
amidophosphoribosyltransferase	0.035	0.142	6	2	5.3	C00064 C00025
phosphoribosylaminoimidazolesuccinocarboxamide synthase	0.035	0.142	6	2	5.3	C00009 C00049
phosphoserine transaminase	0.035	0.142	6	2	5.3	C00025 C00026
pyruvate & phosphate dikinase	0.035	0.142	6	2	5.3	C00022 C00009
succinate---CoA ligase (ADP-forming)	0.035	0.142	6	2	5.3	C00009 C00042
succinate---CoA ligase (GDP-forming)	0.035	0.142	6	2	5.3	C00042 C00009
aspartate carbamoyltransferase	0.047	0.178	7	2	5.3	C00009 C00049
ATP citrate synthase	0.047	0.178	7	2	5.3	C00158 C00009
glutamate---cysteine ligase	0.047	0.178	7	2	5.3	C00009 C00025
procollagen-proline dioxygenase	0.061	0.220	8	2	5.3	C00042 C00026
succinate dehydrogenase (ubiquinone)	0.061	0.220	8	2	5.3	C00122 C00042

glutamate dehydrogenase [NAD(P)+]	0.076	0.261	9	2	5.3	C00025 C00026
GMP synthase (glutamine-hydrolysing)	0.076	0.261	9	2	5.3	C00064 C00025
1-deoxy-D-xylulose-5-phosphate synthase	1.000	1.000	4	1	2.6	C00022
3'(2'),5'-bisphosphate nucleotidase	1.000	1.000	4	1	2.6	C00009
3-dehydroquinase synthase	1.000	1.000	4	1	2.6	C00009
3-deoxy-7-phosphoheptulonase synthase	1.000	1.000	6	1	2.6	C00009
3-deoxy-8-phosphooctulonase synthase	1.000	1.000	5	1	2.6	C00009
4-nitrophenylphosphatase	1.000	1.000	4	1	2.6	C00009
5'-nucleotidase	1.000	1.000	4	1	2.6	C00009
6-phosphofructokinase	1.000	1.000	6	1	2.6	C00085
acetolactate synthase	1.000	1.000	9	1	2.6	C00022
acetyl-CoA carboxylase	1.000	1.000	8	1	2.6	C00009
acetylornithine deacetylase	1.000	1.000	4	1	2.6	C00077
acireductone synthase	1.000	1.000	5	1	2.6	C00009
aconitate hydratase	1.000	1.000	7	1	2.6	C00158
acylphosphatase	1.000	1.000	3	1	2.6	C00009
adenosine deaminase	1.000	1.000	6	1	2.6	C00212
adenosylhomocysteinase	1.000	1.000	4	1	2.6	C00212
adenosylmethionine decarboxylase	1.000	1.000	3	1	2.6	C00022
adenylosuccinate lyase	1.000	1.000	5	1	2.6	C00122
alanine---tRNA ligase	1.000	1.000	6	1	2.6	C00041
alpha,alpha-trehalase	1.000	1.000	3	1	2.6	C00031
alpha,alpha-trehalose-phosphate synthase (UDP-forming)	1.000	1.000	4	1	2.6	C00092
amino-acid N-acetyltransferase	1.000	1.000	4	1	2.6	C00025
arginase	1.000	1.000	4	1	2.6	C00077
argininosuccinate lyase	1.000	1.000	3	1	2.6	C00122
argininosuccinate synthase	1.000	1.000	6	1	2.6	C00049
arsenite-transporting ATPase	1.000	1.000	5	1	2.6	C00009
asparagine---tRNA ligase	1.000	1.000	6	1	2.6	C00152
aspartate kinase	1.000	1.000	4	1	2.6	C00049
aspartate-semialdehyde dehydrogenase	1.000	1.000	6	1	2.6	C00009
aspartate---tRNA ligase	1.000	1.000	6	1	2.6	C00049
biotin carboxylase	1.000	1.000	6	1	2.6	C00009
Ca2+-transporting ATPase	1.000	1.000	6	1	2.6	C00009
Cd2+-exporting ATPase	1.000	1.000	5	1	2.6	C00009
CDP-diacylglycerol---glycerol-3-phosphate 3-phosphatidyltransferase	1.000	1.000	4	1	2.6	C00093
chorismate synthase	1.000	1.000	3	1	2.6	C00009
citrate (Si)-synthase	1.000	1.000	5	1	2.6	C00158
CTP synthase	1.000	1.000	6	1	2.6	C00009
Cu2+-exporting ATPase	1.000	1.000	5	1	2.6	C00009
cyanoalanine nitrilase	1.000	1.000	4	1	2.6	C00049
cystathionine beta-lyase	1.000	1.000	6	1	2.6	C00022
cysteine desulfurase	1.000	1.000	4	1	2.6	C00041
diaminopimelate decarboxylase	1.000	1.000	4	1	2.6	C00047
dihydrodipicolinate synthase	1.000	1.000	4	1	2.6	C00022
diphosphomevalonate decarboxylase	1.000	1.000	6	1	2.6	C00009
fumarylacetoacetase	1.000	1.000	4	1	2.6	C00122
gluconokinase	1.000	1.000	4	1	2.6	C00257
glucose-6-phosphate dehydrogenase	1.000	1.000	6	1	2.6	C00092
glutamate 5-kinase	1.000	1.000	4	1	2.6	C00025
glutamate-5-semialdehyde dehydrogenase	1.000	1.000	6	1	2.6	C00009
glutamate---tRNA ligase	1.000	1.000	6	1	2.6	C00025

glutamine---tRNA ligase	1.000	1.000	6	1	2.6	C00064
glutathione synthase	1.000	1.000	7	1	2.6	C00009
glyceraldehyde-3-phosphate dehydrogenase (phosphorylating)	1.000	1.000	6	1	2.6	C00009
glycerol-3-phosphate dehydrogenase	1.000	1.000	4	1	2.6	C00093
glycerol-3-phosphate dehydrogenase (NAD+)	1.000	1.000	5	1	2.6	C00093
glycerol-3-phosphate O-acyltransferase	1.000	1.000	4	1	2.6	C00093
glycerophosphodiester phosphodiesterase	1.000	1.000	4	1	2.6	C00093
H+-transporting two-sector ATPase	1.000	1.000	5	1	2.6	C00009
indole-3-glycerol-phosphate synthase	1.000	1.000	5	1	2.6	C00022
inorganic diphosphatase	1.000	1.000	4	1	2.6	C00009
inositol-3-phosphate synthase	1.000	1.000	3	1	2.6	C00092
inositol-phosphate phosphatase	1.000	1.000	4	1	2.6	C00009
isocitrate dehydrogenase (NADP+)	1.000	1.000	7	1	2.6	C00026
isoleucine---tRNA ligase	1.000	1.000	6	1	2.6	C00407
L-aspartate oxidase	1.000	1.000	5	1	2.6	C00049
lysine---tRNA ligase	1.000	1.000	6	1	2.6	C00047
magnesium chelatase	1.000	1.000	8	1	2.6	C00009
malate dehydrogenase	1.000	1.000	5	1	2.6	C00149
malate synthase	1.000	1.000	5	1	2.6	C00149
mannitol-1-phosphate 5-dehydrogenase	1.000	1.000	5	1	2.6	C00085
mannose-6-phosphate isomerase	1.000	1.000	3	1	2.6	C00085
methionine adenosyltransferase	1.000	1.000	6	1	2.6	C00009
methylcrotonoyl-CoA carboxylase	1.000	1.000	7	1	2.6	C00009
microtubule-severing ATPase	1.000	1.000	4	1	2.6	C00009
N4-(beta-N-acetylglucosaminyl)-L-asparaginase	1.000	1.000	4	1	2.6	C00049
Na+/K+-exchanging ATPase	1.000	1.000	9	1	2.6	C00009
N-acetyl-gamma-glutamyl-phosphate reductase	1.000	1.000	6	1	2.6	C00009
oleoyl-[acyl-carrier-protein] hydrolase	1.000	1.000	4	1	2.6	C00712
ornithine aminotransferase	1.000	1.000	5	1	2.6	C00077
oxoglutarate dehydrogenase (succinyl-transferring)	1.000	1.000	4	1	2.6	C00026
pantoate---beta-alanine ligase	1.000	1.000	6	1	2.6	C00099
phenylalanine---tRNA ligase	1.000	1.000	6	1	2.6	C00079
phosphatidylserine decarboxylase	1.000	1.000	5	1	2.6	C00022
phosphoenolpyruvate carboxylase	1.000	1.000	5	1	2.6	C00009
phosphoglycerate dehydrogenase	1.000	1.000	7	1	2.6	C00026
phospholipid-translocating ATPase	1.000	1.000	5	1	2.6	C00009
phosphoprotein phosphatase	1.000	1.000	12	1	2.6	C00009
phosphoribosylamine---glycine ligase	1.000	1.000	6	1	2.6	C00009
phosphoserine phosphatase	1.000	1.000	5	1	2.6	C00009
polynucleotide 3'-phosphatase	1.000	1.000	4	1	2.6	C00009
polynucleotide 5'-phosphatase	1.000	1.000	4	1	2.6	C00009
polyribonucleotide nucleotidyltransferase	1.000	1.000	3	1	2.6	C00009
protein-synthesizing GTPase	1.000	1.000	4	1	2.6	C00009
protein-tyrosine-phosphatase	1.000	1.000	4	1	2.6	C00009
pyruvate dehydrogenase (acetyl-transferring)	1.000	1.000	4	1	2.6	C00022
pyruvate kinase	1.000	1.000	5	1	2.6	C00022
ribokinase	1.000	1.000	4	1	2.6	C00121
selenocysteine lyase	1.000	1.000	6	1	2.6	C00041
shikimate dehydrogenase	1.000	1.000	5	1	2.6	C00493
shikimate kinase	1.000	1.000	3	1	2.6	C00493
spermidine synthase	1.000	1.000	3	1	2.6	C00134
succinate-semialdehyde dehydrogenase [NAD(P)+]	1.000	1.000	8	1	2.6	C00042
sucrose-phosphate synthase	1.000	1.000	4	1	2.6	C00085

threonine aldolase	1.000	1.000	4	1	2.6	C00188
threonine ammonia-lyase	1.000	1.000	4	1	2.6	C00188
transaldolase	1.000	1.000	4	1	2.6	C00085
trans-cinnamate 4-monooxygenase	1.000	1.000	8	1	2.6	C00811
trehalose-phosphatase	1.000	1.000	4	1	2.6	C00009
tryptophan synthase	1.000	1.000	7	1	2.6	C00078
tryptophan--tRNA ligase	1.000	1.000	5	1	2.6	C00078
tyrosine---tRNA ligase	1.000	1.000	6	1	2.6	C00082
xylose isomerase	1.000	1.000	2	1	2.6	C00181
Zn2+-exporting ATPase	1.000	1.000	5	1	2.6	C00009

Compounds with no annotations (45): C05659 C08240 C01389 C01601 C00408 C00180 C08243  
C06427 C00259 C00185 C00189 C08362 C01725 C05437 C00503 C01571 C06425 C01451  
C01530 C01018 C01384 C06424 C00474 C00156 C00192 C00208 C05442 C00296 C01694  
C16537 C01904 C01595 C08374 C00249 C01879 C01235 C00379 C05422 C02989 C01753  
C05401 C00387 C02679 C02112 C02457

\* *P*-value of annotation adjusted for multiple testing using false discovery rate according to Benjamini & Hochberg (1995) doi:10.2307/2346101.

\*\* In set for the present background comparing total Kegg assigned compounds.

**Table D.** Enrichment metabolomic analysis for Biological role as displayed in MBRole.

Biological role (set: 44 background: 1117)	P-value	Adjusted P-value*	In background	In set	%**	Compounds
Common amino acids	0.000	0.000	20	11	25	C00041 C00078 C00049 C00152 C00064 C00082 C00188 C00407 C00047 C00025 C00079
Peptides	0.000	0.000	54	16	36.4	C00407 C00152 C00077 C00025 C00082 C00064 C00041 C00079 C00099 C00188 C00334 C00189 C00134 C00049 C00047 C00078
Amino acids	0.000	0.000	45	14	31.8	C00152 C00025 C00049 C00077 C00099 C00078 C00407 C00334 C00188 C00079 C00041 C00047 C00082 C00064
Fatty acids	0.000	0.000	25	9	20.5	C06425 C00249 C01595 C06427 C02679 C06424 C00712 C01571 C01530
FA0101 Straight chain fatty acids	0.000	0.000	13	6	13.6	C01571 C06424 C06425 C00249 C02679 C01530
Saturated fatty acids	0.000	0.000	13	6	13.6	C01530 C06425 C01571 C06424 C02679 C00249
FA01 Fatty Acids and Conjugates	0.000	0.000	62	11	25	C00249 C00712 C01530 C08362 C06427 C01571 C06424 C02679 C01595 C00334 C06425
Carbohydrates	0.000	0.000	43	9	20.5	C00089 C00208 C00185 C00095 C00031 C00121 C00257 C00259 C00181
Lipids	0.000	0.000	67	11	25	C01571 C01595 C00712 C00116 C02679 C00249 C06427 C06425 C01694 C06424 C01530
Aldoses	0.000	0.001	9	4	9.1	C00181 C00259 C00031 C00121
Amines	0.001	0.002	11	4	9.1	C00134 C00189 C00099 C00334
Biogenic amines	0.001	0.002	11	4	9.1	C00134 C00334 C00189 C00099
Disaccharides	0.001	0.004	6	3	6.8	C00185 C00089 C00208
Oligosaccharides	0.001	0.004	6	3	6.8	C00185 C00089 C00208
Monosaccharides	0.002	0.008	37	6	13.6	C00181 C00257 C00121 C00259 C00095 C00031
FA0103 Unsaturated fatty acids	0.003	0.010	17	4	9.1	C01595 C06427 C08362 C00712
ST0105 Fungal sterols and derivatives	0.004	0.013	3	2	4.5	C01694 C05437
Ribonucleosides	0.009	0.023	4	2	4.5	C00387 C00212
Neurotransmitters	0.010	0.023	12	3	6.8	C00334 C00049 C00025
Unsaturated fatty acids	0.010	0.023	12	3	6.8	C06427 C01595 C00712
Monounsaturated fatty acids	0.014	0.032	5	2	4.5	C00712 C08362
ST01 Sterols	0.014	0.032	25	4	9.1	C05442 C01753 C05437 C01694
ST0103 Phytosterols and derivatives	0.037	0.076	8	2	4.5	C01753 C05442
Nucleosides	0.046	0.092	9	2	4.5	C00387 C00212
Other amino acids	0.072	0.138	25	3	6.8	C00334 C00099 C00077
Polyunsaturated fatty acids	0.078	0.144	12	2	4.5	C01595 C06427
FA Fatty acyls	0.128	0.228	195	11	25	C00249 C06424 C02679 C08362 C01530 C00334 C01571 C06427 C00712 C01595 C06425
Hormones and transmitters	0.156	0.258	35	3	6.8	C00334 C00049 C00025
Sterols and steroids	0.156	0.258	18	2	4.5	C01753 C05442
Triterpenoids (C30) and related compounds	0.214	0.342	22	2	4.5	C01753 C05442
ST Sterol Lipids	0.233	0.360	63	4	9.1	C01753 C01694 C05442 C05437
Nucleic acids	0.562	0.844	47	2	4.5	C00212 C00387
Alkaloids	1.000	1.000	200	1	2.3	C00408



Alkaloids derived from lysine	1.000	1.000	18	1	2.3	C00408
Biogenic amines	1.000	1.000	8	1	2.3	C00334
FA0110 Amino fatty acids	1.000	1.000	8	1	2.3	C00334
Fats	1.000	1.000	4	1	2.3	C00116
Glycerols	1.000	1.000	1	1	2.3	C00116
Ketoses	1.000	1.000	9	1	2.3	C00095
Monolignols	1.000	1.000	37	1	2.3	C00811
Phenylpropanoids and related compounds	1.000	1.000	140	1	2.3	C00811
Piperidine alkaloids	1.000	1.000	15	1	2.3	C00408
ST03 Secosteroids	1.000	1.000	6	1	2.3	C01694
ST0301 Vitamin D2 and derivatives	1.000	1.000	3	1	2.3	C01694
Steroids	1.000	1.000	4	1	2.3	C01694
Sterols	1.000	1.000	2	1	2.3	C01694
Terpenoids	0.993	1.000	165	2	4.5	C05442 C01753
Uronic acids	1.000	1.000	8	1	2.3	C00257

Compounds with no annotations (39): C05659 C08240 C01389 C01601 C00026 C00180

C08243 C00186 C01725 C00503 C00085 C00149 C01451 C01384 C01018 C00042

C00022 C00493 C00474 C00156 C00192 C00296 C01904 C16537 C08374 C00198

C01879 C01235 C00379 C02989 C05422 C05401 C00158 C00092 C00093 C00122

C02112 C00009 C02457

\* *P*-value of annotation adjusted for multiple testing using false discovery rate according to Benjamini & Hochberg (1995) doi:10.2307/2346101.

\*\* In set for the present background comparing total Kegg assigned compounds.

**Table E.** Enrichment metabolomic analysis for Chemical groups as displayed in MBRole.

Chemical groups (set: 64 background: 2902)	P-value	Adjusted P-value*	In background	In set	%**	Compounds
carboxylicacid	0.000	0.000	1084	41	64.1	C00712 C06425 C00077 C00079 C00064 C00078 C00186 C02989 C06424 C00022 C00249 C00408 C00047 C00180 C01879 C00158 C00152 C00188 C00122 C00049 C00041 C00156 C08362 C02679 C06427 C00493 C00026 C01595 C00334 C01384 C00407 C01571 C00811 C01530 C00149 C00042 C00082 C00099 C00257 C00025 C00296
alpha-aminoacid	0.000	0.001	200	14	21.9	C00041 C00025 C00078 C00049 C00064 C00077 C00082 C00407 C00047 C00188 C00408 C02989 C00152 C00079
prim.aliphatic.amine	0.000	0.004	354	18	28.1	C00047 C00152 C00064 C00188 C00077 C00099 C00025 C00189 C05659 C02989 C00049 C00082 C00079 C00407 C00134 C00041 C00334 C00078
prim.alcohol	0.025	0.164	439	16	25	C00116 C05422 C00198 C01451 C00089 C05401 C01904 C00474 C01235 C02457 C00093 C00257 C00387 C00212 C00379 C00189
alpha-hydroxyacid	0.067	0.351	100	5	7.8	C00296 C00158 C00149 C00186 C00257
1;2-aminoalcohol	0.559	1.000	84	2	3.1	C00189 C00188
1;2-diol	0.306	1.000	631	16	25	C01235 C00379 C00093 C00387 C00212 C00116 C00474 C01451 C05401 C00296 C00089 C00257 C00198 C05422 C01904 C00493
acetal	0.747	1.000	226	4	6.2	C05401 C00089 C01235 C01451
alkene	0.998	1.000	989	12	18.8	C08362 C01694 C00712 C00493 C00811 C01753 C00122 C05437 C01595 C05442 C01384 C06427
alkylarylether	1.000	1.000	202	1	1.6	C05659
aromaticcompound	1.000	1.000	1406	10	15.6	C00387 C00079 C00082 C00156 C05659 C00212 C01451 C00180 C00078 C00811
carboxylicacidester	0.964	1.000	224	2	3.1	C00198 C05422
heterocycliccompound	1.000	1.000	1417	12	18.8	C00387 C05659 C01235 C00212 C01451 C00078 C00089 C05422 C05401 C00198 C01879 C00408
hydroxylamine	1.000	1.000	11	1	1.6	C00192
iminoheterarene	1.000	1.000	111	1	1.6	C00387
ketone	1.000	1.000	605	3	4.7	C00026 C00022 C05422
lactone	0.559	1.000	84	2	3.1	C00198 C05422
phenol	1.000	1.000	763	4	6.2	C00082 C00156 C00387 C00811
phosphoricacid	1.000	1.000	1	1	1.6	C00009
phosphoricacidderiv.	1.000	1.000	625	2	3.1	C00093 C00009
phosphoricacidester	1.000	1.000	607	1	1.6	C00093
prim.aromat.amine	1.000	1.000	254	1	1.6	C00212
sec.alcohol	0.927	1.000	1278	23	35.9	C01694 C01235 C00493 C05401 C01451 C00379 C00149 C01904 C01753 C00474 C00198 C00257 C05442 C00212 C00296 C00093 C00089 C00188 C00387 C05437 C00116 C00186 C05422

sec.aliphat.amine	1.000	1.000	77	1	1.6	C00408
sulfoxide	1.000	1.000	1	1	1.6	C02989
tert.alcohol	0.940	1.000	198	2	3.1	C00158 C00296

Compounds with no annotations (19): C08240 C01389 C01601 C00181 C08243 C00208  
C00259 C00185 C16537 C08374 C01725 C00503 C00085 C00095 C00031 C00092  
C01018 C00121 C02112

\* *P*-value of annotation adjusted for multiple testing using false discovery rate according to Benjamini & Hochberg (1995)  
doi:10.2307/2346101.

\*\* In set for the present background comparing total Kegg assigned compounds.

**Table F.** Enrichment metabolomic analysis for Other interactions as displayed in MBRole.

Other interactions (set: 28 background: 224)	P-value	Adjusted P-value*	In background	In set	%**	Compounds
ABC Transporters, Prokaryotic Type	0.000	0.000	69	21	75	C00031 C00134 C00049 C00185 C00208 C00009 C00093 C00079 C00181 C00188 C00064 C00089 C00121 C00025 C00047 C00041 C00259 C00077 C05401 C00407 C00095
Phosphate and amino acid transporters	0.000	0.001	21	10	35.7	C00079 C00047 C00077 C00064 C00407 C00009 C00049 C00188 C00025 C00041
Simple sugar transporters	0.000	0.004	9	6	21.4	C00031 C00095 C05401 C00181 C00121 C00259
Metabotropic glutamate family	0.001	0.016	15	7	25	C00077 C00041 C00334 C00047 C00025 C00078 C00064
D-Xylose transporter	0.015	0.111	2	2	7.1	C00121 C00181
Glucose/arabinose transporter	0.015	0.111	5	3	10.7	C00181 C00031 C00095
Glutamate (ionotropic), non-NMDA	0.015	0.111	2	2	7.1	C00025 C00049
Glutamate/aspartate transporter	0.015	0.111	2	2	7.1	C00025 C00049
GPRC6A, G protein-coupled receptor, family C, group 6, member A	0.010	0.111	8	4	14.3	C00047 C00077 C00041 C00064
GRIA, glutamate receptor, ionotropic, AMPA	0.015	0.111	2	2	7.1	C00025 C00049
GRIK, glutamate receptor, ionotropic, kainate	0.015	0.111	2	2	7.1	C00025 C00049
Orphan GPCR6	0.010	0.111	8	4	14.3	C00047 C00064 C00077 C00041
Basic organic compound transporters	0.023	0.154	37	9	32.1	C00185 C00089 C00093 C00208 C00095 C00134 C00031 C00259 C00181
alpha-Glucoside transporter	0.042	0.202	3	2	7.1	C00208 C00089
Fructose transporter	0.042	0.202	3	2	7.1	C00121 C00095
Lysine/arginine/ornithine transporter	0.042	0.202	3	2	7.1	C00047 C00077
Methyl-galactoside transporter	0.042	0.202	3	2	7.1	C00031 C05401
Multiple sugar transporter	0.044	0.202	7	3	10.7	C00181 C00031 C00259
Trehalose/maltose transporter	0.042	0.202	3	2	7.1	C00089 C00208
Neutral amino acid transporter	0.064	0.281	8	3	10.7	C00041 C00064 C00079
Branched-chain amino acid transporter	0.119	0.436	5	2	7.1	C00188 C00407
Glutamate (ionotropic), NMDA	0.119	0.436	5	2	7.1	C00025 C00049
Glutamate-gated cation channels	0.119	0.436	5	2	7.1	C00025 C00049
GRIN, glutamate receptor, ionotropic, N-methyl D-aspartate	0.119	0.436	5	2	7.1	C00049 C00025
GLRA1/4, glycine receptor, alpha 1/4	0.165	0.517	6	2	7.1	C00334 C00099
GLRA2, glycine receptor, alpha 2	0.165	0.517	6	2	7.1	C00334 C00099
GLRA3, glycine receptor, alpha 3	0.165	0.517	6	2	7.1	C00099 C00334
Glycine	0.165	0.517	6	2	7.1	C00334 C00099
GABA-A	0.321	0.943	16	3	10.7	C00099 C00334 C00212
GABRA, gamma-aminobutyric acid (GABA) A receptor, alpha	0.321	0.943	16	3	10.7	C00099 C00212 C00334
ABC-2 type and other transporters	1.000	1.000	7	1	3.6	C00134
Adenosine	1.000	1.000	3	1	3.6	C00212
ADORA1, adenosine A1 receptor	1.000	1.000	3	1	3.6	C00212
ADORA2A, adenosine A2a receptor	1.000	1.000	3	1	3.6	C00212
ADORA2B, adenosine A2b receptor	1.000	1.000	1	1	3.6	C00212
ADORA3, adenosine A3 receptor	1.000	1.000	1	1	3.6	C00212

Antibiotic transporter	1.000	1.000	4	1	3.6	C00134
Arginine/ornithine transporter	1.000	1.000	2	1	3.6	C00077
CASR, calcium-sensing receptor	1.000	1.000	3	1	3.6	C00078
Cellobiose transporter	1.000	1.000	2	1	3.6	C00185
CYP2 family	1.000	1.000	23	1	3.6	C02679
CYP2E subfamily	1.000	1.000	12	1	3.6	C02679
CYP2E1	1.000	1.000	12	1	3.6	C02679
CYP4 family	1.000	1.000	16	1	3.6	C02679
CYP4A subfamily	1.000	1.000	4	1	3.6	C02679
CYP4A1	1.000	1.000	3	1	3.6	C02679
CYP4A11	1.000	1.000	3	1	3.6	C02679
CYP4A2	1.000	1.000	1	1	3.6	C02679
Cys-loop superfamily	0.716	1.000	28	3	10.7	C00099 C00334 C00212
D-Allose transporter	1.000	1.000	1	1	3.6	C00121
Extracellular calcium-sensing	1.000	1.000	3	1	3.6	C00078
GABA-B	1.000	1.000	1	1	3.6	C00334
GABBR1, gamma-aminobutyric acid (GABA) B receptor	1.000	1.000	1	1	1	C00334
Glutamate (metabotropic)	1.000	1.000	3	1	3.6	C00025
Glutamate transporter	1.000	1.000	1	1	3.6	C00025
Glutamine transporter	1.000	1.000	1	1	3.6	C00064
GRM1, glutamate receptor, metabotropic 1	1.000	1.000	2	1	3.6	C00025
GRM2, glutamate receptor, metabotropic 2	1.000	1.000	1	1	3.6	C00025
GRM3, glutamate receptor, metabotropic 3	1.000	1.000	1	1	3.6	C00025
GRM4, glutamate receptor, metabotropic 4	1.000	1.000	2	1	3.6	C00025
GRM5, glutamate receptor, metabotropic 5	1.000	1.000	2	1	3.6	C00025
GRM6, glutamate receptor, metabotropic 6	1.000	1.000	2	1	3.6	C00025
GRM7, glutamate receptor, metabotropic 7	1.000	1.000	2	1	3.6	C00025
GRM8, glutamate receptor, metabotropic 8	1.000	1.000	2	1	3.6	C00025
Inward rectifier channel (Kir)	1.000	1.000	8	1	3.6	C00134
K+ channel, KCNB, Kv2.x (Shab)	1.000	1.000	1	1	3.6	C01595
K+ channel, KCNK, K2px.x	1.000	1.000	7	1	3.6	C01595
KCNB1, potassium voltage-gated channel, Shab-related subfamily B, member 1	1.000	1.000	1	1	3.6	C01595
KCNJ2, potassium inwardly-rectifying channel, subfamily J, member 2	1.000	1.000	4	1	3.6	C00134
KCNK10, potassium channel, subfamily K, member 10	1.000	1.000	6	1	3.6	C01595
Lactose/L-arabinose transporter	1.000	1.000	2	1	3.6	C00259
L-Arabinose transporter	1.000	1.000	1	1	3.6	C00259
Maltose/maltodextrin transporter	1.000	1.000	2	1	3.6	C00208
Mas proto-oncogene & Mas-related (MRGs)	1.000	1.000	1	1	3.6	C00099
MRGPRD, MAS-related GPR, member D	1.000	1.000	1	1	3.6	C00099
Phosphate transporter	1.000	1.000	1	1	3.6	C00009
Purine / pyrimidine	1.000	1.000	15	1	3.6	C00042
Putrescine transporter	1.000	1.000	1	1	3.6	C00134
Related to inward rectifier K+channels	1.000	1.000	8	1	3.6	C00134

Related to voltage-gated cation channels	1.000	1.000	23	1	3.6	C00212
Rhodopsin family: other receptors	0.853	1.000	35	3	10.7	C00042 C00099 C00212
Ribose transporter	1.000	1.000	1	1	3.6	C00121
Ryanodine receptor (RYP)	1.000	1.000	10	1	3.6	C00212
RYP, ryanodine receptor	1.000	1.000	10	1	3.6	C00212
sn-Glycerol 3-phosphate transporter	1.000	1.000	1	1	3.6	C00093
Spermidine/putrescine transporter	1.000	1.000	2	1	3.6	C00134
SUCNR1, GPR91, succinate receptor 1	1.000	1.000	1	1	3.6	C00042
Voltage-gated cation channels	1.000	1.000	14	1	3.6	C01595

Compounds with no annotations (55): C00408 C00116 C00180 C00257 C00189 C00186

C01725 C08362 C00503 C00085 C00082 C01451 C00149 C00493 C00152 C00156

C00192 C01694 C00296 C01904 C16537 C08374 C00249 C00198 C01753 C05422

C02989 C00811 C00387 C00158 C00092 C08240 C05659 C01389 C01601 C00026

C08243 C06427 C00712 C05437 C01571 C06425 C01530 C06424 C01384 C01018

C00022 C00474 C05442 C01879 C01235 C00379 C02112 C00122 C02457

\* *P*-value of annotation adjusted for multiple testing using false discovery rate according to Benjamini & Hochberg (1995) doi:10.2307/2346101.

\*\* In set for the present background comparing total Kegg assigned compounds.

**Table G.** Group means  $\pm$  S.E. across standardised data for identified GC peaks grouped per biological group.

<b>Class of compounds</b>	<b>Subclass</b>	<b>n*</b>	<b>P</b>	<b>NAT</b>	<b>AMF</b>	<b>AMF+PGPR</b>
Carbohydrates	Annotated	38	0.44	0.04 $\pm$ 0.18	-0.15 $\pm$ 0.12	0.11 $\pm$ 0.15
	Unannotated	10	0.22	0.18 $\pm$ 0.27	-0.35 $\pm$ 0.15	0.17 $\pm$ 0.17
Lipids	Total	27	0.10	0.41 $\pm$ 0.17	-0.37 $\pm$ 0.30	-0.04 $\pm$ 0.20
	Sterols	4	0.45	0.38 $\pm$ 0.21	-0.19 $\pm$ 0.44	-0.19 $\pm$ 0.26
	Total FA&E	20	0.08	0.44 $\pm$ 0.23	-0.42 $\pm$ 0.29	-0.02 $\pm$ 0.23
	Unsaturated FA&E	7	0.31	0.31 $\pm$ 0.29	-0.45 $\pm$ 0.27	0.14 $\pm$ 0.37
	Saturated FA&E	13	0.05	0.50 $\pm$ 0.28	-0.40 $\pm$ 0.31	-0.10 $\pm$ 0.16
Peptides	Total	27	0.04	0.33 $\pm$ 0.19	-0.44 $\pm$ 0.19	0.11 $\pm$ 0.28
	Amino acids	21	0.04	0.41 $\pm$ 0.23	-0.54 $\pm$ 0.18	0.13 $\pm$ 0.35
	Amines	6	0.62	0.03 $\pm$ 0.12	-0.10 $\pm$ 0.25	0.08 $\pm$ 0.11
Others	Organic acids	24	0.85	0.01 $\pm$ 0.10	-0.08 $\pm$ 0.26	0.06 $\pm$ 0.19
	P-containing Compounds	5	1.00	-0.02 $\pm$ 0.41	0.01 $\pm$ 0.35	0.01 $\pm$ 0.35
	Other Compounds	3	0.46	0.36 $\pm$ 0.18	-0.21 $\pm$ 0.43	-0.14 $\pm$ 0.37
All Compounds		127	0.01	0.19 $\pm$ 0.05	-0.25 $\pm$ 0.15	0.06 $\pm$ 0.15

\* n indicates the number of compounds contributing to the relative mean, and *P* is the *P*-value of the ANOVA for that group. Carbohydrates were analysed separately according to KEGG annotation. All compounds include both annotated and unannotated compounds. GC was run with methanol:chloroform:water (5:2:2) extracts from roots of durum wheat grown in the field with natural arbuscular mycorrhizal inoculum (NAT), inoculation with AM fungi (AMF), or inoculation with both AMF and plant growth-promoting rhizobacteria (PGPR). FA&E, fatty acids and their esters.

**Table H.** HILIC-Q-TOF MS identified compounds. Wheat with natural arbuscular mycorrhizal inoculum (NAT), inoculated with AM fungi spores (AMF), or inoculated with both AMF and plant growth-promoting rhizobacteria (AMF+PGPR).

Row m/z	Row retention time	Assigned name	Assigned molecular formula	NAT		AMF		AMF+PGPR	
				mean	S.E.	mean	S.E.	mean	S.E.
162.111331832826	8.14	Carnitine C0:0	C7H15NO3	1297050	140113	1100170	139212	1140694	67595
204.125360147688	7.53	Carnitine C2:0	C9H17NO4	2178796	104815	1885182	230832	2007212	156289
218.138724154545	7.10	Carnitine C3:0	C10H19NO4	408000	54723	317415	84814	380358	79845
232.152469696014	6.68	Carnitine C4:0	C11H21NO4	622782	72449	497447	124801	527594	105178
246.166521744862	6.36	Carnitine C5:0	C12H23NO4	563282	73084	346432	57413	379545	52015
258.111401912647	8.82	Glycerophosphocholine	C8H20NO6P	203782	44361	171368	41524	195655	32477
496.342041358028	5.19	LPC 16:0	C24H50NO7P	83658	8661	59478	8663	65430	8940
520.342671800083	4.99	LPC 18:2	C26H50NO7P	60394	11194	73237	14355	58032	7886
518.324927309940	5.22	LPC 18:3	C26H48NO7P	31185	7346	22340	2410	22056	1796
542.324614903292	4.98	LPC 20:5	C28H48NO7P	48229	6946	50413	9412	37268	4153
454.291432778278	3.82	LPE 16:0	C21H44NO7P	89413	5742	71313	10735	77703	9202
478.292971167064	3.68	LPE 18:2	C23H44NO7P	80665	6390	69313	7858	69636	6451
476.279116547599	3.85	LPE 18:3	C23H42NO7P	30825	2498	27455	2162	26688	932
732.550394519425	3.80	PC 32:1	C40H78NO8P	83396	15219	68438	11726	93101	7376
730.539874881159	3.83	PC 32:2	C40H76NO8P	74009	9768	66575	9727	80698	5943
728.531098806654	3.84	PC 32:3	C40H74NO8P	17088	2396	15823	1755	15766	1200
744.559122955340	3.78	PC 33:2	C41H78NO8P	345765	55456	335022	29798	361659	40240
742.547053951094	3.76	PC 33:3	C41H76NO8P	135692	30928	127711	12656	122462	10798
758.568223571777	3.75	PC 34:2	C42H80NO8P	3728031	456719	3841986	343719	4075886	358470
756.553636600625	3.77	PC 34:3	C42H78NO8P	1976427	240899	1933897	215946	2015736	101951
754.533900546512	3.75	PC 34:4	C42H76NO8P	109454	25134	76399	13605	98631	11812
752.521186909934	3.76	PC 34:5	C42H74NO8P	33321	11286	20275	4364	31797	6777
772.579167569223	3.72	PC 35:2	C43H82NO8P	94015	15304	79975	6294	84955	5128
770.569566527624	3.72	PC 35:3	C43H80NO8P	94741	6008	86198	9214	83416	2992
768.558704555256	3.71	PC 35:4	C43H78NO8P	61051	5841	61806	5351	52765	2171
766.537849329832	3.76	PC 35:5	C43H76NO8P	31394	2272	32670	1566	27548	1617
786.596162070884	3.70	PC 36:2	C44H84NO8P	332301	42679	307935	39582	333267	20787
782.567459651066	3.71	PC 36:4	C44H80NO8P	2442170	230717	2443472	321903	2597066	264984
780.552364267460	3.73	PC 36:5	C44H78NO8P	1801435	143097	1816263	210965	1840443	118984
778.536872623506	3.76	PC 36:6	C44H76NO8P	615909	62108	570081	75612	544640	33033
816.617546364734	3.75	PC 38:1	C46H90NO8P	370028	49389	378721	31241	402435	33614
814.609608776092	3.74	PC 38:2	C46H88NO8P	170861	21879	168594	17393	177590	6470
812.607672459073	3.66	PC 38:3	C46H86NO8P	33816	3434	33485	5520	33813	1988
808.57777539906	3.68	PC 38:5	C46H82NO8P	93830	17590	86470	15658	96364	15413
804.553135052820	3.69	PC 38:7	C46H78NO8P	105577	5994	116680	8859	124027	7277
840.616675153823	3.71	PC 40:3	C48H90NO8P	191708	21357	193632	25555	206604	20337
828.554322797146	3.66	PC 40:9	C48H78NO8P	16717	3602	15871	2887	17249	3531
868.668537596606	3.60	PC 42:3	C50H94NO8P	9894	1698	10663	2419	10827	946
676.490970354433	2.68	PE 31:1	C36H70NO8P	42668	3456	48001	4044	52411	6710



690.503581521432	2.69	PE 32:1	C37H72NO8P	65849	7826	71288	5757	78890	10126
688.495405505980	2.69	PE 32:2	C37H70NO8P	57528	6789	62587	4655	69485	7575
716.523574554207	2.63	PE 34:2	C39H74NO8P	296988	38023	328520	33041	331272	22326
714.510715576371	2.64	PE 34:3	C39H72NO8P	117803	15327	118849	11532	118259	3881
730.535156162020	2.62	PE 35:2	C40H76NO8P	11546	972	11594	907	12597	1496
740.523546134838	2.60	PE 36:4	C41H74NO8P	262333	30123	261533	24895	278279	28690
738.507977207778	2.62	PE 36:5	C41H72NO8P	161674	18883	167705	16070	166551	9539

Data were acquired in positive mode. Adduct was [M+H+].