AN EXPLORATORY METHOD FOR IDENTIFYING REACTANT-PRODUCT LIPID PAIRS FROM LIPIDOMIC PROFILES OF WILD-TYPE AND MUTANT LEAVES OF ARABIDOPSIS THALIANA

by

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Abstract

Discerning the metabolic or enzymatic role of a particular gene product, in the absence of information indicating sequence homology to known gene products, is a difficult task. One approach is to compare the levels of metabolites in a wild-type organism to those in an organism with a mutation that causes loss of function of the gene. The goal of this project was to develop an approach to analyze metabolite data on wild-type and mutant organisms for the purpose of identifying the function of a mutated gene.

To develop and test statistical approaches to analysis of metabolite data for identification of gene function, levels of 141 lipid metabolites were measured in leaves of wild-type *Arabidopsis thaliana* plants and in leaves of *Arabidopsis thaliana* plants with known mutations in genes involved in lipid metabolism. The mutations were primarily in fatty acid desaturases, which are enzymes that catalyze reactions in which double bonds are added to fatty acids. When these enzymes are mutated, leaf lipid composition is altered, and the altered levels of specific lipid metabolites can be detected by a mass spectrometry.

A randomization P-Value and other metrics were calculated for all potential reactant-product pairs, which included all lipid metabolite pairs. An algorithm was developed to combine these data and rank the results for each pair as to likelihood of being the actual reactant-product pair. This method was designed and tested on data collected on mutants in genes with known functions, *fad2* (Okuley et al., 1994), *fad3* (Arondel et al., 1992), *fad4*, *fad5* (Mekhedov et al., 2000), *fad6* (Falcone et al., 1994), and *fad7* (Iba et al., 1993 and Gibson et al., 1994). Application of the method to three additional genes produced by random mutagenesis, *sfd1*, *sfd2*, and *sfd3*, indicated that the significant pairs for *fad6* and *sfd3* were similar. Consistent with this, genetic evidence has indicated that *sfd3* is a mutation in the *FAD6* gene.

The methods provide a list of putative reactions for an enzyme encoded by an unknown mutant gene. The output lists for unknown genes and known genes can be compared to provide evidence for similar biochemical activities. However, the strength of the current method is that the list of candidate chemical reactions for an enzyme encoded by a mutant gene can be produced without data other than the metabolite profile of the wild-type and mutant organisms, i.e., known gene analysis is not a requirement to obtain the candidate reaction list.

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Abbreviations Used

DGDG: Digalactosyldiacylglycerol

MGDG: Monogalactosyldiacylglycerol

PC: Phosphatidylcholine

LysoPC: Lyso Phosphatidylcholine

PE: Phosphatidylethanolamine

PG: Phosphatidylglycerol

LysoPG: Lyso Phosphatidylglycerol

PA: Phosphatidic acid

PI: Phosphatidylinositol

PS: Phosphatidylglycerol

Note: DGDG34_6 represents a lipid that has 34 acyl carbons and 6 carbon-carbon double bonds, with a head group like DGDG (Digalactosyldiacylglycerol). Similarly for the others.

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1 Introduction

1.1 Introduction

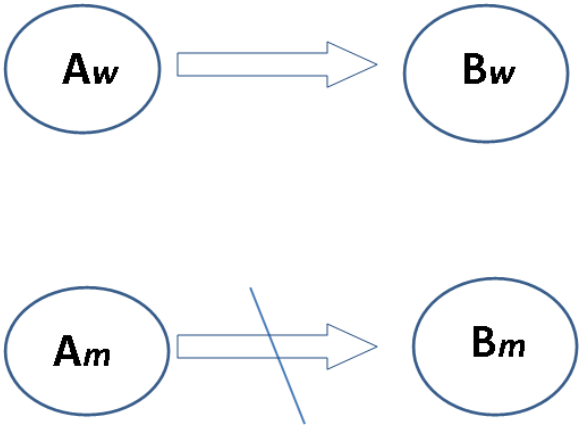
"Omics" technologies allow investigators to study the levels of hundreds or thousands of compounds in an organism simultaneously. Interest is often in the how the levels of a compound vary across tissue type, species type, or in response to a stimulus. Transcriptomics experiments evaluate changes in gene expression, proteomics experiments changes in the expression of proteins, and metabolomics (including lipidomics) changes in metabolite (or lipid) profiles. The latter two involve the study of cellular components downstream from transcription and, thus, experiments can be designed to elucidate the function of genes by the study of their effects on these downstream components (cf., Trethewey, 2001; Holtorf et al., 2002). Knowledge of gene function and downstream components aids in the creation of tools for cataloguing pathways that can be updated as more experiments and results are obtained (cf., Mueller, et al., 2003).

This thesis proposes an exploratory technique to investigate the function of genes potentially involved in metabolism or signaling via the study of the lipidome of *Arabidopsis thaliana*. While the method could be applied to other metabolites, here the lipidome from a mutant plant is compared with that of wild type to determine the loss of function, as revealed by the lipidome associated with the mutated gene. In particular, the levels of lipid pairs were analyzed to screen for candidate reactant-product pairs using a method that exploits the loss of function associated with a mutant genotype. Figure 1 is a simple illustration of the concept. Two lipids are shown, A and B, for two organisms, wild type with lipid concentrations Aw and Bw, and a mutant plant with concentrations Am and Bm.

This figure is a simplification of the biological situation, i.e., it does not take into account that a reaction may be involved in a complex metabolic network of known and/or unknown pathways. However, this figure illustrates the method and ideas proposed herein, which also assume that, to a first approximation, we can obtain information about the function of a particular gene product (enzyme) by looking directly at the levels of its substrate (reactant) and product. If a reactant A is converted into B in wild-type plants but not in mutant plants, then Am concentration should be greater than Aw since the lipid A will build up in the mutant because the reaction does not proceed due to the loss of the function of the gene encoding the enzyme that

catalyzes the reaction. Similarly, the concentration Bw should be greater than Bm. Alterations in metabolite (lipid) concentrations between mutant and wild-type organisms can reveal the role of a genotype that might not otherwise be revealed by easily observable phenotypic characteristics such as "plant height" (e.g., Raamsdonk et al., 2001). In this thesis, plants of nine different mutant genotypes are compared with wild-type plants to identify candidate reactant-product pairs in a targeted lipidomic analysis of *Arabidopsis thaliana* and *I/8E/5*. Data were collected on mutants in genes with known functions, *fad2* (Okuley et al., 1994), *fad3* (Arondel et al., 1992), *fad4*, *fad5* (Mekhedov et al., 2000), *fad6* (Falcone et al., 1994), and *fad7* (Iba et al., 1993 and Gibson et al., 1994) and on mutants with genes produced by random mutagenesis, *sfd1*, *sfd2*, and *sfd3*. Of the nine mutants, information regarding the enzymatic function of the mutated gene product was available initially for six *fad* mutants. Thus the proposed method for identifying candidate reactant-product lipid pairs can, to some degree, be validated by its ability to detect expected reactant-product pairs. The concentrations of 141 lipid species were quantified by mass spectrometry, resulting in an exploration of 141*140 = 19,740 lipid pairs (note, no *a priori* knowledge was assumed as to whether a particular lipid would be a product or a reactant) that were ranked for likelihood of being a "true" reactant-product pair using the proposed method.

Figure 1-1: Two lipids with concentrations Aw and Bw in a wild-type plant and Am and Bm in a mutant. The illustration shows a reactant-product pair when the mutation in a gene encodes an altered enzyme that lacks the ability to catalyze the reaction.



The study of functional genomics via the lipidome or metabolome using high throughput technologies is relatively recent (Last et al., 2007; Wolf and Quinn, 2008), but some methods for analysis and characterization of lipid or metabolite profiles have been proposed. A popular

method involves principal components analysis (PCA) and its extensions. Allen et al. (2003), for example, used PCA and a machine learning technique to classify mutant strains based on metabolomic profiles. The classification is done by clustering strains by the lower dimensional principal component scores. Though useful as a classification tool, such linear combinations from PCA are not always interpretable and are not pursued here since the focus of the proposed screening procedure is on direct detection of candidate reactant-product pairs. Most directly relevant to the method proposed here is the functional analysis by co-response in yeast (FANCY) technique reported in (Raamsdonk et al., 2001). Their method uses a metric that, using our lipid concentration notation above, is of the form,

$$T = \frac{\ln(Am) - \ln(Aw)}{\ln(Rm) - \ln(Rw)}$$

where R was a reference metabolite upstream in the metabolic pathway from the metabolites involved in the reaction catalyzed by the enzyme being analyzed. The metric T was subsequently transformed by arc-tangent to scale it between -90° and 90°. A co-responding metabolite with the reference had a transformed value of T near 45° for a positive co-response and -45° for a negative co-response. Though intuitively appealing, this method is not directly applicable for the analytical objectives for several reasons. Herein, no assumptions are made about an upstream reference. Instead the references are the concentrations of all other lipids. Second, for some lipids, the concentration is zero for all samples in a mutant or wild-type plant. These zero values cannot be ignored because they might be due to the lack of a reaction in the mutant organism (i.e., the product is depleted) or the depletion of a reactant in the wild-type. However, the zero values pose problems for logarithm transformations and for metrics involving certain ratios. Others have computed the correlation between the concentrations of pairs of metabolites and compared these correlation statistics across a control and mutant organism (e.g., Weckwerth et al., 2004). Weckwerth et al., (2004) also used a statistical test comparing the ratio of pairs of metabolites between control and mutant conditions. Considering such metrics herein poses problems again due to the zero values mentioned earlier and the fact that correlation metrics can be misleading as a measure of association in the presence of many tied values, i.e., the usual Pearson's correlation quantifies a *linear association* between two variables. Wu et al. (2005) proposed a conceptual strategy using a quantitative kinetic model relating metabolic fluxes to enzymatic activity and metabolic concentrations, and demonstrated the technique with

an in silicon case study. Approaches involving such kinetic models of fluxes are beyond the scope of the objectives in this thesis.

The method proposed here uses a multi-step procedure to screen a large number of lipid pairs for candidate reactant-product pairs using mutant and wild-type organisms. It can accommodate the zero observations and does not rely on distributional assumptions regarding the data. It is, thus, heuristic in nature and cut-off values in the screening procedure can be "tuned" to produce a larger or smaller number of potential reactant-product pairs for follow-up investigation and verification. A larger candidate reactant-product list may include many irrelevant findings and a smaller list might miss important pairs. In the next section, the data and experimental procedures are discussed. Then the method to screen potential reactant-product pairs is presented, followed by a results section and discussion.

2 Experimental procedures and the data

2.1 Experiment procedures

Electrospray ionization tandem mass spectrometry (ESI-MS/MS) can be used for lipid profiling (Briigger et al., 1997). Here, it was used to provide information for 141 lipids, including lipids unique to plants as function of plant genotype.

Plant material and plant growth: The plants were grown and the lipids were extracted and analyzed by Ashis Nandi and Christen Buseman, working with Jyoti Shah and Ruth Welti, respectively, in the Division of Biology at Kansas State University. The wild-type plants for the first sets of experiments (with the *fad* mutants) were *Arabidopsis thaliana* (Columbia ecotype), while the wild-type plants in the second set of experiments were *1/8E/5*. Surface-sterilized seeds were germinated on agar plates and transferred to soil. Plants were grown in a chamber with a 16-h light/8-h dark cycle, at 23/21°C, under cool fluorescent white light (200 μmol m^{-2} s^{-1}).

Sample preparation: Lipids were extracted according to the procedure of Devaiah et al. (2006) with minor modifications. Briefly, 3 to 5 leaves were quickly immersed in 3 ml isopropanol with 0.01% butylated hydroxytoluene at 75ºC to inactivate lipolytic activity. After 15 minutes, 1.5 ml chloroform and 0.6 ml water were added and the tubes were shaken for 1 h. Thereafter, the extract was removed and replaced with chloroform/methanol (2:1) with 0.01% butylated hydroxytoluene and the tubes were shaken for 30 min. The latter procedure was repeated five times until the leaves of every sample appeared white. The remaining leaf material was dried overnight at 105ºC and weighed. The combined extracts were washed once with 1 ml 1 M KCl and once with 2 ml water, evaporated under nitrogen, and dissolved in 1 ml chloroform.

ESI-MS/MS: An automated electrospray ionization-tandem mass spectrometry approach was used, and data acquisition and analysis and acyl group identification were carried out as described previously (Devaiah et al., 2006).

Unfractionated lipid extracts were introduced by continuous infusion into the ESI source on a triple quadrupole MS/MS (API 4000, Applied Biosystems, Foster City, CA). Samples were introduced using an autosampler (LC Mini PAL, CTC Analytics AG, Zwingen, Switzerland) fitted with the required injection loop for the acquisition time and presented to the ESI needle at 30 μl/min. Scans and data processing were as described by Devaiah et al. (2006).

Nine experiments were conducted, of which, six were used to derive the method while three were used to check its reliability. For each experiment, a control group of 5 samples from wild type plants was obtained and, for a treatment group, 5 samples from mutant plants were obtained. The samples in the first set of experiments included "treated" groups that had *FATTY ACID DESATURASE* point mutations, *fad2*, *fad3*, *fad4*, *fad5*, *fad6* and *fad7*. Other "treated" samples, analyzed in a second set of experiments, included initially unmapped point mutations produced by random mutagenesis, *sfd1, sfd2* and *sfd3*. (Wild-type genes are designated by capital letters, e.g., *FAD2*, while mutant genes are designated by lower case letters, e.g., *fad2*.) The control group (i.e., wild type) was the same for all mutations in the same set of experiments. Each experiment can be thought as a two group comparison where the "treatment" is wild type versus mutant. Levels of 141 different lipids were measured in each sample.

2.2 Description of data

Table 2.2-1 Part of the dataset – *fad2*

lipid	C1	C2	C3	C4	C5	T1	T2	T3	T4	T5
DGDG34_6	2.249	2.175	2.526	1.956	2.212	3.249	2.553	4.058	2.959	2.785
DGDG34_5	0.141	0.103	0.096	0.166	0.061	0.185	0.193	0.074	0.190	0.236
DGDG34_4	0.258	0.194	0.203	0.177	0.226	0.232	0.291	0.316	0.180	0.270
DGDG34_3	4.694	4.329	4.405	3.858	4.026	3.451	3.398	4.164	3.243	3.026
DGDG34_2	1.012	0.951	1.104	0.807	0.794	1.686	1.020	1.771	1.265	1.506
DGDG34_1	0.414	0.398	0.437	0.354	0.396	0.894	0.977	0.935	0.824	0.845
DGDG36_6	14.954	16.683	14.931	14.079	15.010	8.538	8.896	10.074	8.516	8.990
DGDG36_5	0.000	0.000	0.000	0.000	0.000	0.041	0.000	0.000	0.071	0.000
DGDG36_4	0.455	0.458	0.383	0.462	0.427	0.774	0.871	0.941	0.998	0.811
DGDG36_3	0.221	0.178	0.200	0.129	0.155	0.198	0.050	0.189	0.065	0.044
DGDG36_2	0.007	0.000	0.000	0.000	0.000	0.020	0.049	0.022	0.013	0.048
DGDG36_1	0.000	0.000	0.000	0.000	0.000	0.017	0.000	0.000	0.000	0.000
DGDG38_6	0.179	0.224	0.153	0.217	0.156	0.248	0.274	0.329	0.378	0.378
DGDG38_5	0.000	0.000	0.000	0.000	0.000	0.011	0.000	0.000	0.000	0.000
DGDG38_4	0.082	0.000	0.025	0.025	0.045	0.013	0.008	0.000	0.019	0.000
DGDG38_3	0.000	0.009	0.000	0.000	0.000	0.004	0.007	0.017	0.000	0.000

Table 2.2-1 shows partial data (i.e., 16 of the 141 lipid levels) for 10 samples from the *fad2* dataset. The columns show the lipid levels, where C1 to C5 represent the control group (wildtype) and T1 to T5 represent the treated group where the *FAD2* gene is mutated. All the lipids were measured in the unit of nmol/mg dry weight. As can be seen, many zeros appear when lipid levels are either below the detection limit or represent lipids that are not present in the sample; this is partially because zero has been substituted for any values for which the measured intensity is below the limit of detection. For this analysis, zero values will be assumed to mean the lipid is not present in the sample. Imputing values for a lipid, that is present, but below the detection limit, is a topic of further investigation. Lipids that are not present in a sample are important to include in the analysis because their absence may be due to the loss-of-function of the knockout gene. Zero values combined with the relatively small sample sizes create challenges when using usual parametric statistical tests. The other datasets and the remainder of this data set have the same structure and are not shown here. (the whole datasets are listed on Appendix A)

3 Method to analyze the data

The analysis of data from lipidomics experiments is relatively new. This paper proposes a technique that is exploratory in nature and is aimed at identifying metabolites, quantified by mass spectrometry, which are altered when a mutation is present affecting a specific gene. In particular, the goal is to identify compounds that are likely to be substrates (reactants) and products of the affected gene. The method can vet a large number of reactant-product pairs to determine which pairs might be "important" for follow-up analyses. A set of metrics is used to quantify this potential importance and these can be tuned or set by the investigator. Some recommended settings are obtained by analyzing data from the six experiments described earlier using the proposed method, and checking the results against genes with known function to determine if, in fact, the reactant-product pairs identified as "important" are the known reactant-products pairs of the enzymatic activity of the gene product. If a method is proved to be effective on the genes with known functions, it might serve as a method to explore unknown genes' roles. In fact reactions are part of pathways so some lipids not directly associated with a gene product, but in the same pathway or network of pathways, may also be changed by mutation of a particular gene. Thus it is reasonable to expect to pick up some "false" reactant-product pairs, which might provide clues to understand the pathways. Since there are 141 lipid measurements in each sample for the experiments analyzed here, and since we do not assume *a priori* that a particular lipid is a product or reactant, there are a total of 141*140 = 19,740 possible lipid pairs to be evaluated.

3.1 Overview of screening metrics

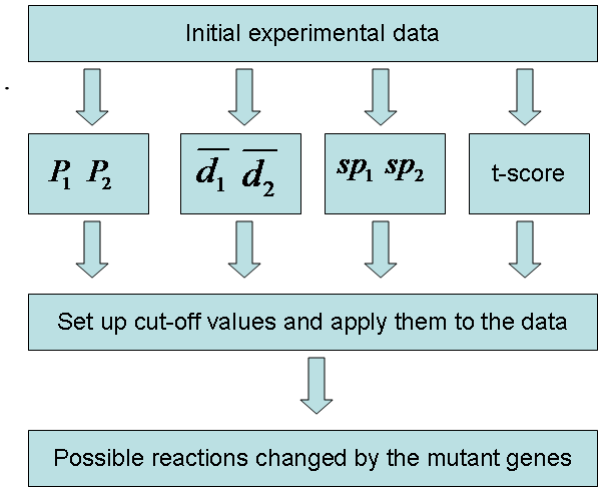
The metrics used to screen candidate reactant-product pairs are described here with details to follow in subsequent subsections. Refer to Figure 1 where two lipids, A (for candidate reactant) and B (for candidate product), are shown with levels denoted by Aw and Bw for the wild-type plant, and Am and Bm for the mutant. First, the levels of Aw and Am (and Bw and Bm) should be "statistically" different. However, usual tests such as the t-test are problematic because of the zeros present for the level of some lipids across samples. Thus, a randomization test is used to assess statistically significant differences between the levels of Aw and Am (and

Bw and Bm). The results are two randomization P-values, P_1 and P_2, for testing Aw versus Am and Bw versus Bm, respectively. This P-value also has a nice intuitive interpretation as a measure of overlap between the values of Aw and Am (and Bw and Bm). The smallest P-values occur when the levels of a mutant lipid are greater than (or less than) the corresponding levels of a wild-type lipid across all samples.

The next set of metrics involves the direction of the differences between levels of Aw and Am (and Bw and Bm). As mentioned in the introduction, the levels of Aw should be less than the levels of Am. We define $\overline{d_1}$ to be the sample mean of Aw values minus the sample mean of Am values. The levels of Bw should be greater than the levels of Bm. Thus we define $\overline{d_2}$ to be the sample mean of Bw values minus the sample mean of Bm values. Moreover, $\overline{d_1}$ should be negative by a distance related to the variability of the sample values of lipid A. So the pooled standard deviation for the candidate reactant lipid is computed and denoted sp_1. Similarly, $\overline{d_2}$ should be positive by a distance related to the variability of the sample values of lipid B. So the pooled standard deviation for the candidate product lipid is computed and denoted sp_2.

Finally, $\overline{d_2} - \overline{d_1}$ should be positive by a sufficient amount to indicate a potential reactant-product pair. Thus we define a t-score to be the standardized difference of $\overline{d_2} - \overline{d_1}$, that is, $tscore = (\overline{d_2} - \overline{d_1}) / SD(\overline{d_2} - \overline{d_1})$ where $SD(\overline{d_2} - \overline{d_1})$ is the estimated standard deviation of the mean difference. The calculation flows are diagramed in Figure 3-1.

Figure 3-1 Calculation flows



In the following subsections, details are provided on each of the above metrics that include formulas used for computation of the values. Then, a subsection describing the selected cut-off values for each metric is provided.

3.2 The randomization p-values

This type of inference involves permutation of observed responses under a specified null hypothesis (Gadbury, 2001). Consider measurements for one lipid, where X denotes lipid levels for wild type (lipid Aw and Bw in previous notation) and Y denotes lipid levels for a mutant (i.e., lipid Am and Bm in previous notation). The null hypothesis is described as a statement: *Ho*: the mutant knockout had no effect on the expression of this lipid. A test statistic, *t*, is computed to represent a difference in gene expression due to treatment.

Suppose that r_j is the lipid level of the jth sample, which represents a value of Y_j or X_j depending on whether that sample is a wild-type or mutant sample. The vector $(r_1,\ldots r_N)$ represents the lipid levels from the experiment for all N samples. The mutant genotype is considered a treatment here with the wild type being a control. A usual randomized experiment would select n samples from N items to receive the "treatment", i.e., mutation. Though this controlled assignment was not possible here, the context of a randomized experiment is useful to assess the change of a particular lipid from wild type to mutant. The null hypothesis, Ho, supposes that a lipid level of a mutant would have been the same if that sample had been wild type. Under *Ho* a randomization distribution of the test statistic is created by randomly choosing n values from $(r_1,\ldots r_N)$ to represent outcomes to mutant with the other m values representing outcomes to wild type. Each time this is done, a test statistic t^*, is computed yielding $t_1^*,\ldots,t_C^*$, where $C = N!/(n!m!)$ is the number of unique treatment assignments and each value of t^* is equally likely under *Ho*. The p-value is then computed as the proportion of t^* that is as extreme as or more extreme than the test statistic *t* observed from the data produced from the actual treatment assignment. The exactness of this p-value depends on an assumption that is sometimes called unit-treatment additivity, meaning, for a sample *j*, $Y_j = X_j + \tau$, where τ is a constant for all *j*; $\tau = 0$ under the null hypothesis of no differential lipid expression and has been called Fishers "sharp null hypothesis" (Rubin, 1990). Note that unit-treatment additivity

necessarily implies that the variances of the two outcome variables Y and X are the same and that the two distribution above, F_Y and F_X, differ only in their location (i.e., their mean).

In this study, the test statistic was a mean difference in lipid levels, that is, $t = \bar{d} = \bar{x} - \bar{y}$. Moreover, N = 10, n = m = 5, C = 252, and the smallest two-tailed P-value is equal to 2/252 = 0.007937. This would represent a lipid for which levels for all samples in the mutant group were either higher or lower than those in the wild-type group. That is, there is no overlap of lipid levels in the two groups. Thus, when selecting potential reactant-product pairs, one might choose to consider only those lipids with a small P-value. The actual mean difference, as mentioned above, is a second criterion that can be used to assess whether a particular lipid is a candidate product or reactant in a pairing. This is discussed next along with the derivation of the t-score for ranking pairs.

3.3 Mean differences and the t-score

Define x_{i1} to be the lipid level of a candidate *reactant* in the *i*th wild-type sample, y_{i1} to be the lipid level of a candidate *reactant* in the ith mutant sample, x_{i2} to be the lipid level of a candidate *product* in the *i*th wild-type sample, and y_{i2} to be the lipid level of a candidate *product* in the ith mutant sample. In this experiment where are n_x wild-type samples and n_y mutant samples. Sample means can be defined as $\bar{x}_1 = (1/n_x)\sum_{i=1}^{n_x} x_{i1}$, $\bar{x}_2 = (1/n_x)\sum_{i=1}^{n_x} x_{i2}$, $\bar{y}_1 = (1/n_y)\sum_{i=1}^{n_y} y_{i1}$ and $\bar{y}_2 = (1/n_y)\sum_{i=1}^{n_y} y_{i2}$. Then mean differences shown in figure 3-1 are $\overline{d_1} = \overline{x_1} - \overline{y_1}$ and $\overline{d_2} = \overline{x_2} - \overline{y_2}$.

Sample variances are then given by,

$$S_{x1}^2 = \frac{1}{n_x - 1}\sum_{i=1}^{n_x}(x_{i1} - \overline{x_1})^2,\ S_{x2}^2 = \frac{1}{n_x - 1}\sum_{i=1}^{n_x}(x_{i2} - \overline{x_2})^2,\ S_{y1}^2 = \frac{1}{n_y - 1}\sum_{i=1}^{n_y}(y_{i1} - \overline{y_1})^2 \text{ and}$$

$$S_{y2}^2 = \frac{1}{n_y - 1}\sum_{i=1}^{n_y}(y_{i2} - \overline{y_2})^2.$$

The pooled standard deviations shown in Figure 3-1 are defined to be,

$$sp_1 = \sqrt{\frac{(n_x - 1) * S_{x1}^2 + (n_y - 1) * S_{y1}^2}{n_x + n_y - 2}} \text{ and } sp_2 = \sqrt{\frac{(n_x - 1) * S_{x2}^2 + (n_y - 1) * S_{y2}^2}{n_x + n_y - 2}} .$$

Finally, the t-score is defined to be,

$$tscore = \frac{\overline{d_2} - \overline{d_1}}{\widehat{SD}(\overline{d_2} - \overline{d_1})}$$

Where, the estimated $\widehat{SD}(\overline{d_2} - \overline{d_1})$ is derived in the following steps.

First,

$$\begin{aligned}
&\text{var}(\overline{d_2} - \overline{d_1}) \\
&= \text{var}(\overline{d_2}) + \text{var}(\overline{d_1}) - 2\,\text{cov}(\overline{d_1}, \overline{d_2}) \\
&= \text{var}(\overline{x_1} - \overline{y_1}) + \text{var}(\overline{x_2} - \overline{y_2}) - 2\,\text{cov}(\overline{x_1} - \overline{y_1}, \overline{x_2} - \overline{y_2}) \\
&= \text{var}(\overline{x_1}) + \text{var}(\overline{y_1}) + \text{var}(\overline{x_2}) + \text{var}(\overline{y_2}) \\
&\quad - 2 * [\text{cov}(\overline{x_1}, \overline{x_2}) - \text{cov}(\overline{y_1}, \overline{x_2}) - \text{cov}(\overline{y_2}, \overline{x_1}) + \text{cov}(\overline{y_1}, \overline{y_2})]
\end{aligned}$$

The estimate of the variance is given by

$$\widehat{\text{var}}(\overline{d_2} - \overline{d_1}) = S_{x1}^2 / n_x + S_{y1}^2 / n_y + S_{x2}^2 / n_x + S_{y2}^2 / n_y - 2\widehat{\text{cov}}(\overline{x_1}, \overline{x_2}) - 2\widehat{\text{cov}}(\overline{y_1}, \overline{y_2}),$$

where, $\widehat{\text{cov}}(\overline{x_1}, \overline{x_2}) = \frac{1}{n_x * (n_x - 1)} \sum_{i=1}^{n_x} (x_{i1} - \overline{x_1})(x_{i2} - \overline{x_2})$, and

$\widehat{\text{cov}}(\overline{y_1}, \overline{y_2}) = \frac{1}{n_y * (n_y - 1)} \sum_{i=1}^{n_y} (y_{i1} - \overline{y_1})(y_{i2} - \overline{y_2})$. Thus, $\widehat{SD}(\overline{d_2} - \overline{d_1}) = \sqrt{\widehat{\text{var}}(\overline{d_2} - \overline{d_1})}$.

Results for all candidate reactant-product pairs are summarized in Table 3.2, which shows criteria used to screen the potential 19,740 possible reactant- product pairs. The description of the criteria and what they represent are below**.**

Table 3.3-1 Example of criteria to evaluate product-reactant pairs

Reaction-name	P_1	P_2	$\overline{d_1}$	$\overline{d_2}$	$\overline{d_1} - \overline{d_2}$	sp_1	sp_2	t-score
DGDG34_1_DGDG34_2								
DGDG34_1_DGDG34_3								
……								
PS44_3_PS44_2								

Reaction-name lists the potential 19740 possible paired reactions (reactant-product). Take the first row as an example, DGDG34_1_DGDG34_2 means the possible reaction from DGDG34_1 to DGDG34_2. P_1 are the randomization p-values for the reactants. In the first row, P_1 are the randomization p-values of lipid DGDG34_1. One may be interested in those candidate reactants that have the smallest P-values. P_2 are the randomization p-values for the products. In the first row, P_2 are the randomization p-values of lipid DGDG34_2. Again one may be interested in P-values close to 0 for the products that are significantly different in the wild type group and in the mutant group. Again, take the first row as an example. The statistic $\overline{x_1}$ represents the mean for DGDG34_1 (reactant) in the wild type group and $\overline{y_1}$ represents the mean for DGDG34_1 (reactant) in the mutant group. Since there would be no (or less) reactions from DGDG34_1 to DGDG34_2 if the critical gene is not functional, $\overline{x_1}$ would be smaller than $\overline{y_1}$. The mean difference $\overline{d_1}$ with the value of $\overline{x_1} - \overline{y_1}$ would be negative. In fact, we may wish to select those pairs with a value of $\overline{d_1}$ less than some negative threshold, δ_1. Similarly, $\overline{x_2}$ represents the mean for DGDG34_2 (product) in the wild type group and $\overline{y_2}$ represents the mean for DGDG34_2 (product) in the mutant group. Since there would be no (or less) reactions from DGDG34_1 to DGDG34_2 if the critical gene is blocked, $\overline{x_2}$ would be bigger than $\overline{y_2}$. The mean difference $\overline{d_2}$ with the value of $\overline{x_2} - \overline{y_2}$ would be positive. We may wish to select those pairs with a value of $\overline{d_2}$ larger than some positive threshold, δ_2. The statistic sp_1 is the estimated pooled standard deviation across the mutant group and the wild-type group and sp_2 is the estimated pooled standard deviation across the mutant group and the wild-type group. The t-score combines the information for a candidate reactant and product and is a summary measure for a reactant-product pair. The interest will be in those pairs with the largest t-scores, i.e., those where $tscore > t.cut$.

3.4 The cut-off values for screening candidate pairs

The rules for the cut-off values are described below.

1. The t-score was computed for each possible pair. The t-score is expected to be a large positive value if the gene mutation prevented the conversion of the candidate reactant to product.

Some t-scores were undefined because the lipid levels for a candidate pair (both reactant and product) were all zero, i.e. the lipids were not detected in any samples for that pair. This number varied by dataset. The top 450 pairs (of 19,740) as ranked by t-score were selected for follow-up screening. This selection produced cutoff values (t.cut) for each experiment of 34.05, 9.34, 9.96, 16.67, 24.65 and 20.30 for *fad2*, *fad3*, *fad4*, *fad5*, *fad6* and *fad7* respectively.

2. Of the 141 lipids that were tested for differential lipid expression across the wild-type versus mutant groups with the randomization test, the smallest possible randomization p-value was 2/252 = 0.00794. Lipids with the smallest possible P-value (i.e., P_1, P_2 in Table 3.2) were chosen as potential candidates for a reactant-product pair.

3. The mean differences described above, $\overline{d_1}$ which is expected to be negative and $\overline{d_2}$ which is expected to be positive, are then considered. A negative cutoff for $\overline{d_1}$ and a positive cutoff for $\overline{d_2}$ were determined as followed. Since multiple lipids are involved some threshold taking into account the simultaneous estimation was needed. A Bonferroni cutoff was chosen for an overall significance level of 0.05, adjusting for the total number of lipids. Since there are 141 lipids, the cutoff is (in terms of standard errors of a mean) $\pm\sqrt{2/5} * qt(0.05/141, 8)$ which gives ±3.36 for the number of pooled standard deviations computed above (in the above the notation *qt* means the quantile from a t-distribution, the degrees of freedom was 8). The cut-off values for $\overline{d_1}$ and $\overline{d_2}$ were $\delta_1 = -3 * sp_1$ and $\delta_2 = 3 * sp_2$, respectively. Thus, $\overline{d_1} < \delta_1 = -3 * sp_1$ and $\overline{d_2} > \delta_2 = 3 * sp_2$ were considered meeting this criterion.

4 Results

The original lists of reactant-product pairs were decreased from 19,740 to a smaller number based on the three selected screening criteria described in section 3. The same cut-off rules for screening criteria were used for every experiment. Application of these rules resulted in a varied number of reactant-product pairs meeting these criteria among experiments.

Results for the experiments of *fad2*, *fad3*, *fad4*, *fad5*, *fad6*, and *fad7* are listed in the following way: the significant reaction pairs detected by this method are presented in Section 4.1 and the biochemically feasible reaction pairs identified among the significant ones is presented in Section 4.2. A comparison of the biochemically feasible pairs with the known substrates and products then follows.

4.1 The significant reactions for *fad*s

This section lists the significant reaction pairs for *fad2*, *fad3*, *fad4*, *fad5*, *fad6*, and *fad7*, respectively. Only t-scores are listed here. More metrics are provided in appendix A.

Table 4.1-1 The significant reactions for *fad2*. Biochemically feasible pairs (see section 4.2) are shown in blue.

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
PE34_1_PE40_2	69.05	PC34_1_LysoPE16_0	45.37	PC36_2_PS44_2	40.09
PE34_1_PS34_2	67.37	PC34_1_LysoPC18_2	45.29	PC36_2_PS36_5	40.09
PE34_1_PS38_2	66.51	PC34_1_PS38_2	45.05	PC36_2_PA36_5	40.04
PE34_1_PC38_5	66.38	PC34_1_LysoPC18_3	45.00	PC36_2_PA34_2	40.01
PE34_1_LysoPE16_0	66.08	PC36_2_PC34_2	44.88	PC36_2_PE34_2	39.93
PE34_1_PI36_3	66.05	PC36_2_PC36_3	44.53	PC36_2_PC36_6	39.80
PE34_1_PS38_3	65.94	PC34_1_PS44_2	44.50	PE34_4_PC38_5	39.76
PE34_1_LysoPE18_2	65.84	PC34_1_PC40_4	44.39	PE36_2_PS34_2	39.04
PE34_1_LysoPC18_3	65.42	PC34_1_PS36_5	44.22	PE36_2_PC38_5	38.78
PE34_1_LysoPC18_2	65.42	PE34_4_PS40_2	43.68	PE36_2_PC38_3	38.77
PE34_1_PC38_3	65.26	PC34_1_PA34_2	42.76	PE36_2_PS42_2	38.55
PE34_1_PS36_5	64.65	PC36_2_PE36_5	42.62	PE36_2_PS38_3	38.51
PE34_1_PI36_5	64.56	PC36_2_PI34_2	42.07	PE36_2_LysoPE18_2	38.42

PE34_1_PE38_5	64.50	PC36_2_PI36_3	42.04	PE36_2_PS40_2	38.36
PE34_1_PC40_4	64.44	PE36_2_PI36_3	41.82	PE36_2_LysoPE16_0	38.08
PE34_1_PS40_2	64.37	PC36_2_PE40_2	41.06	PE36_2_PS38_2	37.99
PE34_1_PS36_3	64.24	PC36_2_PI36_5	41.03	PE36_2_LysoPC18_2	37.90
PE34_1_PS44_2	63.91	PC34_1_PA36_5	41.00	PE36_2_PS36_3	37.90
PE34_1_PS42_2	61.72	PE36_2_PE40_2	40.81	PE36_2_PE38_5	37.89
PE34_1_PA36_5	55.30	PC36_2_PS34_2	40.76	PE36_2_LysoPC18_3	37.63
PE34_1_PA34_2	52.07	PC36_2_PC38_3	40.74	PE36_2_PS36_5	37.33
PC34_1_PI36_3	51.17	PE36_2_PI36_5	40.67	PE36_2_PC40_4	37.32
PC34_1_PI36_5	49.26	PC36_2_PC38_5	40.53	PC36_2_PC34_3	37.27
PC34_1_PE40_2	48.69	PC36_2_PS38_3	40.48	PE36_2_PS44_2	37.25
PC34_1_PS42_2	48.00	PC36_2_PS40_2	40.45	PS42_1_LysoPE16_0	35.67
PC34_1_PC38_3	47.64	PC36_2_LysoPE18_2	40.38	PE36_2_PA34_2	35.60
PC34_1_PC36_3	47.58	PC36_2_PS42_2	40.38	PE36_2_PA36_5	35.59
PC34_1_PS34_2	47.55	PC36_2_LysoPE16_0	40.36	PC36_2_PE34_3	35.48
PC34_1_PS40_2	46.76	PC36_2_PS36_3	40.30	PC34_1_PC34_2	34.87
PC34_1_PC38_5	46.55	PC36_2_PS38_2	40.30	PC38_2_PC38_3	34.72
PC34_1_PS38_3	45.81	PC36_2_PE38_5	40.29	PI34_1_PS34_2	34.34
PC34_1_LysoPE18_2	45.60	PC36_2_LysoPC18_2	40.28	PS42_1_PC40_4	34.27
PC34_1_PE38_5	45.58	PC36_2_LysoPC18_3	40.24	PC38_2_PS34_2	34.11
PC34_1_PS36_3	45.52	PC36_2_PC40_4	40.13		

Table 4.1-2 The significant reactions for *fad3*. Biochemically feasible pairs (see section 4.2) are shown in blue.

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
PC36_4_PE34_3	45.37	PC36_4_PE36_6	12.21	PE36_4_PS34_3	9.95
PE36_4_PE36_5	42.95	PS38_2_LysoPE18_3	12.07	PS38_2_PE34_4	9.93
PC36_4_PC34_3	39.90	PS36_2_PE38_5	12.02	MGDG36_5_PE34_3	9.82
PE36_4_PE34_3	33.99	PS36_2_PE40_3	11.82	PE36_4_PS40_3	9.74
PC36_4_PC36_6	32.60	PS34_2_PS40_3	11.72	PE36_4_PC38_5	9.68
PC36_4_PE36_5	32.13	PS34_2_PE40_3	11.69	PE36_4_PE40_3	9.66
PE36_4_PC36_6	31.88	PS38_2_PC38_6	11.68	PE36_4_PC38_4	9.66
PE36_4_PC34_3	28.32	MGDG36_5_PE36_6	11.63	PE36_4_PE34_4	9.64
PC36_4_PC36_5	28.02	PS34_2_PC38_4	11.61	PE36_4_PS38_3	9.63
PE36_4_PE36_6	20.76	PS34_2_PE36_6	11.27	PS36_2_PC38_6	9.62

PE36_4_PC36_5	16.03	PS36_2_PS38_3	11.15	PE36_4_PS36_3	9.60
PS38_2_PC38_5	14.97	PS36_2_PE42_4	10.98	PE36_4_PE38_5	9.60
PS38_2_PE38_5	14.67	PS36_2_LysoPE16_0	10.90	PS38_2_PS34_3	9.49
PS38_2_PE40_3	14.20	PS34_2_PE38_5	10.60	PE36_4_PE42_4	9.48
PS38_2_PE42_4	13.33	PS38_2_PS40_3	10.59	PE36_4_LysoPE16_0	9.47
PS34_2_PS34_3	13.17	PS38_2_PE36_6	10.57	PE36_4_PC38_6	9.47
PS38_2_PS38_3	12.67	PS36_2_PE36_6	10.50	PE36_4_LysoPE18_3	9.47
PS34_2_PC38_5	12.54	PE36_4_PI36_3	10.40	PE36_4_PS42_4	9.44
PS38_2_PC38_4	12.44	PS36_2_PC38_4	10.39	PE36_4_DGDG36_3	9.38
PS38_2_LysoPE16_0	12.41	PS36_2_PE34_4	10.20	PS36_2_PS40_3	9.36
PS34_2_PS36_3	12.28	PS34_2_PS38_3	10.15	PE36_4_PS36_6	9.36
PS38_2_PS42_4	12.25	PS38_2_PS36_3	10.04	PE36_4_PA36_6	9.35
PS36_2_PC38_5	12.23	PS36_2_PS42_4	10.03		

Table 4.1-3 The significant reactions for *fad4*. Biochemically feasible pairs (see section 4.2) are shown in blue.

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
PG34_3_PG34_4	35.59	PG34_0_PG34_4	24.35	PG34_3_lysoPG18_3	17.80
PG34_3_PG34_2	32.90	PG34_3_PG32_1	21.39	PG34_0_PG32_1	14.26
PG32_0_PG34_4	25.91	PG32_0_PG32_1	19.32	PG32_0_PG34_2	11.62

Table 4.1-4 The significant reactions for *fad5*. Biochemically feasible pairs (see section 4.2) are shown in blue.

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
DGDG34_3_DGDG36_6	34.41	DGDG36_3_DGDG34_2	23.67	DGDG34_3_MGDG34_4	19.72
MGDG36_6_DGDG36_6	33.37	MGDG36_6_MGDG34_2	23.60	MGDG38_4_DGDG36_4	19.38
MGDG36_6_MGDG34_6	30.16	MGDG36_6_DGDG36_4	23.46	MGDG34_3_DGDG34_6	18.56
DGDG36_3_DGDG34_6	30.14	MGDG36_6_DGDG34_1	23.32	MGDG34_3_MGDG34_4	18.50
MGDG38_4_DGDG34_6	28.02	MGDG38_4_MGDG34_6	23.07	DGDG34_3_MGDG36_4	18.37
MGDG34_3_MGDG34_6	27.15	DGDG36_3_MGDG34_6	23.05	DGDG34_3_DGDG34_2	18.07
DGDG34_3_MGDG34_6	26.50	MGDG36_6_PC34_4	22.91	MGDG34_3_DGDG34_2	17.41
MGDG36_6_DGDG34_6	25.40	MGDG36_6_DGDG34_5	22.91	MGDG38_4_DGDG36_6	17.25
DGDG36_3_DGDG34_1	25.07	MGDG36_6_PE34_4	22.88	DGDG34_3_MGDG34_2	17.06
MGDG36_6_MGDG34_4	24.97	LysoPC16_0_MGDG34_6	22.87	MGDG34_3_MGDG34_2	17.05

LysoPC16_0_DGDG34_6	24.50	MGDG38_4_DGDG34_2	20.84	MGDG34_3_MGDG36_4	16.98
MGDG36_6_DGDG34_2	23.98	MGDG34_3_DGDG36_6	20.43	MGDG34_3_DGDG36_4	16.87
MGDG36_6_MGDG36_4	23.70	DGDG34_3_DGDG34_6	20.14	DGDG36_3_DGDG36_6	16.67

Table 4.1-5 The significant reactions for *fad6*. Biochemically feasible pairs (see section 4.2) are shown in blue.

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
MGDG36_4_DGDG34_6	52.78	DGDG36_4_PC38_5	33.97	PG34_1_PG34_4	26.75
PG34_2_PG34_3	49.18	DGDG36_4_PE38_5	33.91	MGDG34_2_DGDG34_3	26.59
PG34_2_PG34_4	45.41	DGDG36_4_PE40_3	33.79	PC36_3_PG34_4	26.48
PG34_2_DGDG34_6	41.98	MGDG34_2_DGDG36_3	33.70	PC34_4_PC38_5	26.47
MGDG34_2_PG34_4	39.74	MGDG34_2_DGDG34_5	33.50	MGDG34_3_DGDG34_6	26.38
DGDG36_4_DGDG34_6	38.72	MGDG34_2_lysoPG18_3	33.46	PE34_4_PC38_5	26.29
PG34_2_PC38_5	37.21	MGDG34_2_PC38_5	33.41	PC34_4_DGDG34_6	26.22
MGDG34_2_DGDG34_6	37.16	MGDG34_2_PE40_3	33.38	PC36_3_PG34_3	25.93
PG34_2_lysoPG18_3	37.12	MGDG34_2_PE38_5	33.38	MGDG34_3_PG34_4	25.76
PG34_2_PE38_5	37.09	DGDG34_1_DGDG34_6	32.40	PC34_4_PE40_3	25.72
PG34_2_DGDG36_3	37.08	DGDG36_4_PG34_3	30.50	PG34_2_MGDG34_6	25.20
PG34_2_PE40_3	37.08	DGDG36_4_PG34_4	29.78	lysoPG18_1_DGDG34_6	24.94
PG34_2_DGDG34_5	37.00	PG34_2_DGDG34_3	28.96	PE34_1_DGDG34_6	24.85
MGDG34_2_PG34_3	35.53	MGDG34_2_MGDG34_6	28.46	DGDG34_1_PG34_4	24.76
DGDG36_4_DGDG34_5	35.40	MGDG36_2_DGDG34_6	27.90	PE34_4_DGDG34_6	24.75
DGDG36_4_DGDG36_3	34.66	MGDG36_4_PG34_4	27.22	PC34_1_PG34_4	24.66
DGDG36_4_lysoPG18_3	34.01	DGDG36_2_DGDG34_6	26.83	PE34_4_PE40_3	24.66

Table 4.1-6 the significant reactions for *fad7*. Biochemically feasible pairs (see section 4.2) are shown in blue.

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
DGDG36_5_MGDG36_6	47.94	DGDG36_4_MGDG36_6	27.92	DGDG36_4_DGDG34_6	23.41
DGDG36_5_DGDG34_6	38.12	DGDG34_5_DGDG34_6	26.69	MGDG34_4_MGDG36_6	22.59
DGDG36_5_DGDG34_3	37.03	DGDG34_2_MGDG36_6	25.95	MGDG34_5_MGDG34_6	22.51
DGDG36_5_DGDG36_3	36.76	MGDG34_5_DGDG36_3	25.76	MGDG36_3_MGDG36_6	21.82
DGDG36_5_lysoPG18_3	34.26	MGDG34_5_lysoPG18_3	25.70	PC34_4_MGDG36_6	21.39
MGDG34_5_MGDG36_6	32.46	DGDG36_5_DGDG36_6	24.77	PE34_4_MGDG36_6	21.35

DGDG34_2_DGDG34_6	32.04	DGDG34_5_MGDG36_6	24.42	LysoPC18_2_MGDG36_6	21.35
MGDG34_5_DGDG36_6	30.99	MGDG36_5_MGDG36_6	24.05	LysoPE18_2_MGDG36_6	21.33
MGDG34_5_DGDG34_3	30.13	DGDG34_4_MGDG36_6	23.76	lysoPG18_2_MGDG36_6	21.32
MGDG34_5_DGDG34_6	28.24	PG34_3_MGDG36_6	23.61	LysoPC18_1_MGDG36_6	21.30
DGDG34_2_DGDG34_3	28.19	DGDG34_5_DGDG34_3	23.51	DGDG36_4_lysoPG18_3	20.76
MGDG34_5_PG34_4	28.12	DGDG36_4_DGDG34_3	23.46		

4.2 The biochemically feasible reactions for *fad* datasets

Since an enzymatic reaction would only be expected to change only one facet of a metabolite's structure, only a few of the determined significant reactions make biochemical sense.

Before further discussion, explanations are needed for the readers with less biology background. For example, lipid PC36_2 (written as PC_36:2 in many cases) has one head group and two fatty acids as tails. "PC" indicates the head group, "36" represents the number of carbons and "2" represents the number of double bonds. So, the lipid PC36_2 is the lipid with "PC" as a head and 36 carbons, and 2 double bonds in two tails. The lipids with names starting with "Lyso" are a little different. LysoPC18_2 has one head and one fatty acid as tail, "PC" represents the head group, "18" represents the number of carbons and "2" represents the number of double bonds. So, LysoPC18_2 is the lipid with "PC" as a head, and 18 carbons and 2 double bonds in one tail.

The following were rules that were used to determine the biochemical feasibility of a particular reactant-product pair, i.e. that the reactant could be converted to the product in a reaction catalyzed by a single enzyme:

1. The change of lipid class. For example, the reaction from PC36_2 to PE36_2 is possible. The other lipid class changes, like MGDG to DGDG, PC to PA, etc. are possible. In this case, neither the carbon number nor the number of the double bonds can be changed.

2. Change of fatty acid tail (acyl chain), i.e. change of the number of double bonds and/or the carbon number. Double bond change cannot be greater than 3, because 0-3 is the range of double bonds in one acyl chain, so a change of more than 3 would require changes in multiple acyl chains. For example, PC_34:1 cannot be changed to PC_34:5 or the reverse, but

PC_34:1 to PC_34:4 is possible, and PC_34:1 to PC_40:4 is also possible. In this case, the head group (lipid class) cannot be changed simultaneously.

3. Addition or subtraction of a fatty acid tail (acyl chain). If change is from X to lyso X, the change can be accomplished by change of one fatty acid. In other words, the double bond number can only be decreased by 0-3 double bonds; the double bond number cannot be increased.

All biochemically feasible reactant-product pairs detected by this method are listed in the following tables from Table 4.2-1 to Table 4.2-6. The reactions known to be catalyzed by the affected gene product are shown in red.

Table 4.2-1 The biochemically feasible reactions for *fad2*

Eighteen biochemically feasible reactions were picked up. According to Somerville et al. (2000), *FAD2* gene product is known to convert an 18:1 chain in PC to 18:2. The chain in the other position may be 16:0, 18:1, 18:2, or 18:3. If the chain in the other position is 16:0, then the "potentially known" reaction would be represented as PC34_1_PC34_2, if both chains are 18:1, the reaction would be represented as PC36_2_PC36_3, if the other chain was 18:2, the reaction would be PC36_3_PC36_4, and if the other chain was 18:3, the reaction would be PC36_4_PC36_5. PC34_1_PC34_2 and PC36_2_PC36_3 appear in the list of biochemically feasible reactions below (red font).

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
PE34_1_PE40_2	69.05	PC34_1_PC40_4	44.39	PE36_2_LysoPE18_2	38.42
PE34_1_LysoPE16_0	66.08	PE36_2_PE40_2	40.81	PE36_2_LysoPE16_0	38.08
PC34_1_PC38_3	47.64	PC36_2_PC38_3	40.74	PE36_2_PE38_5	37.89
PC34_1_PC36_3	47.58	PC36_2_PC38_5	40.53	PC36_2_PC34_3	37.27
PC36_2_PC34_2	44.88	PC36_2_LysoPC18_2	40.28	**PC34_1_PC34_2**	34.87
PC36_2_PC36_3	44.53	PC36_2_PC40_4	40.13	PC38_2_PC38_3	34.72

Table 4.2-2 The biochemically feasible reactions for *fad3*

Twenty-three biochemically feasible pairs were picked up. According to Somerville et al. (2000), *FAD3* gene product is known to convert an 18:2 chain in PC to 18:3. The chain in the other position may be 16:0, 18:1, 18:2, or 18:3. If the chain in the other position is 16:0, then the

"potentially known" reaction would be represented as PC34_2_PC34_3, if the other chain is 18:1, the reaction would be represented as PC36_3_PC36_4, if the other chain is 18:2, then the reaction would be represented as PC36_4_PC36_5, and if the other chain is 18:3, then the reaction would be represented as PC36_5_PC36_6 . PC36_4_PC36_5 appears on the list of biochemically feasible candidate reactions (red font).

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
PE36_4_PE36_5	42.95	PS34_2_PS36_3	12.28	PE36_4_PE40_3	9.66
PC36_4_PC34_3	39.90	PS38_2_PS42_4	12.25	PE36_4_PE34_4	9.64
PE36_4_PE34_3	33.99	PS34_2_PS40_3	11.72	PE36_4_PE38_5	9.60
PC36_4_PC36_6	32.60	PS36_2_PS38_3	11.15	PS38_2_PS34_3	9.49
PC36_4_PC36_5	28.02	PS38_2_PS40_3	10.59	PE36_4_PE42_4	9.48
PE36_4_PE36_6	20.76	PS34_2_PS38_3	10.15	PE36_4_LysoPE18_3	9.47
PS34_2_PS34_3	13.17	PS38_2_PS36_3	10.04	PS36_2_PS40_3	9.36
PS38_2_PS38_3	12.67	PS36_2_PS42_4	10.03		

Table 4.2-3 The biochemically feasible reactions for *fad4*

Seven biochemically feasible pairs were identified for *FAD4*. According to Somerville et al. (2000), *FAD4* gene product is known to convert an 16:0 chain in PG to 16:1. The chain in the other position may be 16:0, 18:1, 18:2, or 18:3. If the chain in the other position is 16:0, then the "potentially known" reaction would be represented as PG32_0_PG32_1, if the chain in the other position is 18:1, then the reaction would be represented as PG34_1_PG34_2, if the chain in the other position is 18:2, then the reaction would be represented as PG34_2_PG34_3, while if the chain in the other position is 18:3, then the reaction would be represented as PG34_3_PG34_4. Both the reactions PG32_0_PG32_1 and PG34_3_PG34_4 appear in the list of biochemically feasible reactions below (red font).

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
PG34_3_PG34_4	35.59	**PG32_0_PG32_1**	19.32	PG32_0_PG34_2	11.62
PG34_3_PG34_2	32.90	PG34_3_lysoPG18_3	17.80		
PG34_3_PG32_1	21.39	PG34_0_PG32_1	14.26		

Table 4.2-4 The biochemically feasible reactions for *fad5*

Sixteen biochemically feasible pairs were detected for *FAD5*. According to Somerville et al. (2000), *FAD5* gene product is known to convert a 16:0 chain in MGDG (or DGDG) to 16:1. The chain in the other position may be 18:1, 18:2, or 18:3. If the chain in the other position is 18:1, then the "potentially known" reaction would be represented as MGDG34_1_MGDG34_2, if the chain in the other position is 18:2, then the reaction would be represented as MGDG34_2_MGDG34_3, while if the chain in the other position is 18:3, then the reaction would be represented as MGDG34_3_MGDG34_4. MGDG34_3_MGDG34_4 appears in the list of biochemically feasible reactions below (red font).

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
DGDG34_3_DGDG36_6	34.41	MGDG36_6_MGDG34_4	24.97	DGDG34_3_DGDG34_2	18.07
MGDG36_6_DGDG36_6	33.37	MGDG36_6_MGDG36_4	23.70	MGDG34_3_MGDG34_2	17.05
MGDG36_6_MGDG34_6	30.16	DGDG36_3_DGDG34_2	23.67	MGDG34_3_MGDG36_4	16.98
DGDG36_3_DGDG34_6	30.14	MGDG38_4_MGDG34_6	23.07	DGDG36_3_DGDG36_6	16.67
MGDG34_3_MGDG34_6	27.15	DGDG34_3_DGDG34_6	20.14		
DGDG36_3_DGDG34_1	25.07	**MGDG34_3_MGDG34_4**	18.50		

Table 4.2-5 The biochemically feasible reactions for *fad6*

Eight biochemically feasible pairs were identified for *FAD6*. According to Somerville et al. (2000), *FAD6* gene product is known to convert 16:1 and 18:1 chains in MGDG (or DGDG) to 16:2 and 18:2, respectively, and to convert an 18:1 chain in PG to 18:2. The chain in the other position in MGDG could be 16:0, 16:1, 16:2, 18:1, 18:2, or 18:3. In PG, the other chain could be 16:0 or 16:1. Thus, the "potentially known" reactions are MGDG34_1_MGDG34_2, MGDG34_2_MGDG34_3, MGDG34_3_MGDG34_4, MGDG34_4_MGDG34_5, MGDG34_5_MGDG34_6, MGDG36_2_MGDG36_3, MGDG36_3_MGDG36_4, MGDG36_4_MGDG36_5, MGDG36_5_MGDG36_6, the corresponding reactions with DGDG, PG34_1_PG34_2, and PG34_2_PG34_3. PG34_2_PG34_3 appears in the list of biochemically feasible reactions below with the highest t-score; DGDG34_4_DGDG34_5 also appears (red font).

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
PG34_2_PG34_3	49.18	**DGDG36_4_DGDG34_5**	35.40	PC34_4_PC38_5	26.47

PG34_2_PG34_4	45.41	DGDG36_4_DGDG36_3	34.66	PE34_4_PE40_3	24.66
DGDG36_4_DGDG34_6	38.72	PG34_1_PG34_4	26.75		

Table 4.2-6 The biochemically feasible reactions for *fad7*

Fourteen biochemically feasible pairs were discovered for *FAD7*. According to Somerville et al. (2000), *FAD7* gene product is known to convert 16:2 and 18:2 chains in MGDG (or DGDG) to 16:3 and 18:3, respectively, and to convert an 18:2 chain in PG to 18:3. The chain in the other position in MGDG could be 16:0, 16:1, 16:2, 18:1, 18:2, or 18:3. In PG, the other chain could be 16:0 or 16:1. The "potentially known" reactions are MGDG34_2_MGDG34_3, MGDG34_3_MGDG34_4, MGDG34_4_MGDG34_5, MGDG34_5_MGDG34_6, MGDG36_2_MGDG36_3, MGDG36_3_MGDG36_4, MGDG36_4_MGDG36_5, MGDG36_5_MGDG36_6, the corresponding reactions with DGDG, PG34_2_PG34_3, and PG34_3_PG34_4. MGDG34_5_MGDG34_6, DGDG34_5_DGDG34_6, MGDG36_5_MGDG36_6 and DGDG36_5_DGDG36_6_appear in the list of biochemically feasible reactions below (red font).

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
DGDG36_5_DGDG34_6	38.12	**DGDG34_5_DGDG34_6**	26.69	DGDG36_4_DGDG34_6	23.41
DGDG36_5_DGDG34_3	37.03	**DGDG36_5_DGDG36_6**	24.77	MGDG34_4_MGDG36_6	22.59
DGDG36_5_DGDG36_3	36.76	**MGDG36_5_MGDG36_6**	24.05	**MGDG34_5_MGDG34_6**	22.51
MGDG34_5_MGDG36_6	32.46	DGDG34_5_DGDG34_3	23.51	MGDG36_3_MGDG36_6	21.82
DGDG34_2_DGDG34_3	28.19	DGDG36_4_DGDG34_3	23.46		

In the six experiments, each list of significant reactions contained at least one reactant-product pair considered to be the true substrates and products of the mutant gene. It can be noted that not all "potentially known" reactions necessarily occur *in vivo*. Next, three more experiments, *sfd1*, *sfd2* and *sfd3*, were used to check the efficiency of this method in Chapter 5.

5 Application of data analysis method to *sfd1, sfd2, and sfd3*

This method is now applied on *sfd1, sfd2* and *sfd3*. These genes were mutated by random mutagenesis and, at the outset of the lipid analysis, the location of the mutations were unknown (from Jyoti Shah's Lab). Later, it was shown that *sfd3* is a mutation in *FAD6* (Nandi et al, 2003). In other words, *sfd3* and *fad6* are different mutations in the same gene.

5.1 The significant reactions for *sfd*s

Table 5.1-1, Table 5.1-2 and Table5.1-3 list the detected significant pairs for *sfd1*, *sfd2*, *sfd3* respectively. The pairs in blue bold are biochemically feasible.

Table 5.1-1 The significant reactions for *sfd1*. Biochemically feasible pairs (see section 5.2) are shown in blue.

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
MGDG36_6_MGDG34_6	27.10	PE34_1_MGDG34_6	15.58	PI34_1_MGDG34_2	12.14
DGDG36_6_MGDG34_6	25.98	PI34_1_MGDG34_6	15.43	PC34_1_DGDG34_6	12.06
PE34_1_MGDG34_2	20.98	PE36_1_MGDG34_6	15.35	MGDG36_6_MGDG34_4	11.94
PI34_1_DGDG34_2	17.68	PA34_1_MGDG34_6	15.35	MGDG36_6_DGDG34_2	11.78
PE34_1_DGDG34_2	17.22	PA34_1_DGDG34_2	14.95	MGDG36_6_MGDG34_2	11.68
PC36_2_MGDG34_6	16.07	PE36_1_DGDG34_2	14.77	PC36_2_DGDG34_6	11.52
PC34_1_MGDG34_6	16.03	MGDG36_6_DGDG34_6	12.94	MGDG36_6_DGDG34_1	11.49

Table 5.1-2 The significant reactions for *sfd2*. Biochemically feasible pairs (see section 5.2) are shown in blue.

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
MGDG36_6_MGDG34_6	21.02	PG34_1_DGDG34_2	12.16	MGDG36_6_PG32_1	9.71
MGDG34_3_MGDG34_6	15.44	PE36_3_DGDG34_6	11.55	MGDG36_6_DGDG34_1	9.58
PG34_1_MGDG34_6	15.03	PE36_2_DGDG34_6	11.26	MGDG34_5_DGDG34_2	9.49
PE36_3_MGDG34_6	15.02	MGDG34_3_DGDG34_6	10.85	PI36_3_DGDG34_6	9.44
PE36_2_MGDG34_6	14.98	MGDG36_6_DGDG34_6	10.59	MGDG34_3_DGDG34_2	9.39
MGDG34_5_MGDG34_6	14.86	PI36_3_DGDG34_1	10.52	PI36_3_DGDG34_2	9.33
PG34_0_MGDG34_6	14.84	PG34_0_DGDG34_2	10.05	PG34_0_DGDG34_1	9.06

PI36_3_MGDG34_6	14.81	MGDG36_6_DGDG34_2	10.05	PE40_3_DGDG34_6	8.96
PE40_3_MGDG34_6	14.79	PG34_0_DGDG34_6	10.00	PE38_3_DGDG34_6	8.90
PE38_3_MGDG34_6	14.78	PE36_2_DGDG34_2	9.88	PE40_3_DGDG34_2	8.72
PE38_5_MGDG34_6	14.77	PE36_3_DGDG34_2	9.87	PE38_5_DGDG34_6	8.70
PG34_0_PG32_1	13.42	MGDG34_5_DGDG34_6	9.75	PE38_3_DGDG34_2	8.68
PG34_1_DGDG34_6	12.57	PG34_1_PG32_1	9.74		

Table 5.1-3 The significant reactions for *sfd3*. Biochemically feasible pairs (see section 5.2) are shown in blue.

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
MGDG34_2_PA36_6	83.15	PE36_4_PG34_4	39.63	PE36_3_MGDG34_6	33.23
MGDG34_2_lysoPG18_3	82.92	PG34_2_MGDG34_6	39.58	PC36_2_MGDG34_6	33.16
MGDG34_2_PG32_1	82.92	DGDG36_4_PG34_3	38.63	PC34_1_MGDG34_6	33.10
MGDG34_2_PC38_5	82.77	MGDG36_6_MGDG34_6	38.33	MGDG34_3_PG34_4	33.00
MGDG34_2_LysoPC18_3	82.63	PC34_2_PG34_4	37.16	PG34_1_PG34_4	32.96
MGDG34_2_PC38_6	82.62	DGDG36_4_PG34_4	36.59	DGDG34_4_MGDG34_6	32.93
MGDG34_2_PG34_3	82.02	DGDG36_4_PE36_6	35.92	PE36_2_MGDG34_6	32.87
MGDG34_2_PE36_6	81.86	PE34_2_MGDG34_6	35.25	MGDG36_2_MGDG34_6	32.85
MGDG34_2_PC36_6	77.14	MGDG36_4_MGDG34_6	34.73	PC34_4_MGDG34_6	32.83
MGDG34_2_DGDG34_6	73.11	PC36_4_MGDG34_6	34.65	PC36_3_PG34_4	32.78
MGDG34_2_PG34_4	67.54	DGDG36_4_MGDG34_6	34.62	PI36_4_MGDG34_6	32.77
PG34_2_PG34_3	65.13	PE36_4_MGDG34_6	34.61	PE42_2_MGDG34_6	32.73
PG34_2_LysoPC18_3	60.05	DGDG36_4_PA36_6	34.58	PE34_4_MGDG34_6	32.73
PG34_2_lysoPG18_3	59.99	MGDG34_3_MGDG34_6	34.55	PE38_2_MGDG34_6	32.73
PG34_2_PC38_5	59.80	MGDG36_4_PG34_4	34.33	PE38_3_MGDG34_6	32.71
PG34_2_PA36_6	59.74	PE36_4_PC36_6	34.27	PI36_2_MGDG34_6	32.71
PG34_2_PC38_6	59.72	DGDG36_4_lysoPG18_3	34.16	PE40_2_MGDG34_6	32.71
PG34_2_PE36_6	59.58	PC34_2_MGDG34_6	34.13	lysoPG18_1_MGDG34_6	32.69
PG34_2_PG32_1	59.14	PG34_1_MGDG34_6	34.09	PC38_3_MGDG34_6	32.69
PG34_2_PG34_4	58.13	PC36_3_MGDG34_6	34.00	PE38_4_MGDG34_6	32.68
PG34_2_PC36_6	56.34	DGDG36_4_LysoPC18_3	33.82	PS42_2_MGDG34_6	32.68
PE34_2_PG34_4	50.04	DGDG36_4_PC38_5	33.74	PC38_2_MGDG34_6	32.68
PG34_2_DGDG34_6	49.57	DGDG36_4_PC38_6	33.56	PI34_4_MGDG34_6	32.67
MGDG34_2_MGDG34_6	42.83	DGDG34_1_MGDG34_6	33.51	PI36_3_MGDG34_6	32.67
PC36_4_PG34_4	40.44	DGDG34_2_MGDG34_6	33.28	PE42_3_MGDG34_6	32.67

5.2 The biochemically feasible reactions for *sfd*s

Table 5.2-1, Table 5.2-2 and Table 5.2-3 list the biochemically feasible reactions for *sfd1*, s*fd2* and s*fd3* respectively.

Table 5.2-1 The biochemically feasible reactions for *sfd1*

Two biochemically feasible pairs were picked up. *SFD1* has been identified as a dihydroxyacetone reductase, which converts dihydroxyacteone to glycerol 3-phosphate. Glycerol 3-phospate is a precursor for plastidic glycerolipid synthesis. The true reactant-product pair is not among the compounds analyzed; the reactions that were picked up are related to indirect effects of the mutation on plastidic glycerolipid synthesis.

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
MGDG36_6_MGDG34_6	27.10	MGDG36_6_MGDG34_4	11.94		

Table 5.2-2 The biochemically feasible reactions for *sfd2*

Five biochemically feasible pairs were observed. *SFD2* has not been mapped or identified as yet.

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
MGDG36_6_MGDG34_6	21.02	MGDG34_5_MGDG34_6	14.86	PG34_1_PG32_1	9.74
MGDG34_3_MGDG34_6	15.44	PG34_0_PG32_1	13.42		

Table 5.2-3 The biochemically feasible reactions for *sfd3*

Seven biochemically feasible pairs were identified. Similar to the *fad6* mutation, PG34_2_PG34_3 is has the highest t-score for *sfd3*. Comparison of Tables 4.2-5 and 5.2-3 for *fad6* and *sfd3*, show additional several similarities.

Reaction-name	t-score	Reaction-name	t-score	Reaction-name	t-score
PG34_2_PG34_3	65.1327	MGDG36_6_MGDG34_6	38.3283	PG34_1_PG34_4	32.9559
PG34_2_PG32_1	59.1446	MGDG36_4_MGDG34_6	34.7344		
PG34_2_PG34_4	58.1266	MGDG34_3_MGDG34_6	34.5495		

5.3 The number of times a reactant appeared in a list

In order to assess how similar the data obtained for allelic mutations, *sfd3* and *fad6* were, in comparison to the similarity of their data to that of other mutations, we assessed the number of times that each reactant lipid appeared in the lists of significant reactions for each mutant. Table 5.3-1 shows how many times a lipid, serving as a reactant, appeared in each of *fad2*, *fad3*, *fad4*, *fad5*, *fad6*, *fad7*, *sfd1*, *sfd2,* and *sfd3* lists. For example, in Table 4.1-1, there were 29 pairs with PC36_2 as a reactant, so in the table below, PC36_2 for *fad2* is 29. The table includes all lipids that appeared as a reactant in at least one of the nine data sets, thus there are several zeros.

Table 5.3-1 The number of times a reactant appeared in a list

	DGDG34_1	DGDG34_2	DGDG34_3	DGDG34_4	DGDG34_5	DGDG34_6	DGDG36_1	DGDG36_2	DGDG36_3	DGDG36_4	DGDG36_5	DGDG36_6	DGDG38_3	DGDG38_4	DGDG38_5	DGDG38_6	LysoPC16_0	LysoPC16_1
fad2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad5	0	0	7	0	0	0	0	0	5	0	0	0	0	0	0	0	2	0
fad6	2	0	0	0	0	0	0	1	0	9	0	0	0	0	0	0	0	0
fad7	0	3	0	1	3	0	0	0	0	4	6	0	0	0	0	0	0	0
sfd1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
sfd2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
sfd3	1	1	0	1	0	0	0	0	0	9	0	0	0	0	0	0	0	0

	LysoPC18_0	LysoPC18_1	LysoPC18_2	LysoPC18_3	LysoPE16_0	LysoPE16_1	LysoPE18_1	LysoPE18_2	LysoPE18_3	lysoPG16_0	lysoPG16_1	lysoPG18_1	lysoPG18_2	lysoPG18_3	MGDG34_1	MGDG34_2	MGDG34_3	MGDG34_4
fad2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8	0
fad6	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	11	2	0
fad7	0	1	1	0	0	0	0	1	0	0	0	0	1	0	0	0	0	1
sfd1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
sfd2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0
sfd3	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	12	2	0

	MGDG34_5	MGDG34_6	MGDG36_1	MGDG36_2	MGDG36_3	MGDG36_4	MGDG36_5	MGDG36_6	MGDG38_3	MGDG38_4	MGDG38_5	MGDG38_6	PA34_1	PA34_2	PA34_3	PA34_4	PA34_6	PA36_2
fad2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad3	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0
fad4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad5	0	0	0	0	0	0	0	12	0	5	0	0	0	0	0	0	0	0
fad6	0	0	0	1	0	2	0	0	0	0	0	0	0	0	0	0	0	0
fad7	8	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0
sfd1	0	0	0	0	0	0	0	6	0	0	0	0	2	0	0	0	0	0
sfd2	3	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0
sfd3	0	0	0	1	0	2	0	1	0	0	0	0	0	0	0	0	0	0

	PA36_3	PA36_4	PA36_5	PA36_6	PC32_0	PC34_1	PC34_2	PC34_3	PC34_4	PC36_1	PC36_2	PC36_3	PC36_4	PC36_5	PC36_6	PC38_2	PC38_3	PC38_4
fad2	0	0	0	0	0	23	0	0	0	0	29	0	0	0	0	2	0	0
fad3	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0
fad4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad6	0	0	0	0	0	1	0	0	3	0	0	2	0	0	0	0	0	0
fad7	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
sfd1	0	0	0	0	0	2	0	0	0	0	2	0	0	0	0	0	0	0
sfd2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
sfd3	0	0	0	0	0	1	2	0	1	0	1	2	2	0	0	1	1	0

	PC38_5	PC38_6	PC40_2	PC40_3	PC40_4	PC40_5	PE34_1	PE34_2	PE34_3	PE34_4	PE36_1	PE36_2	PE36_3	PE36_4	PE36_5	PE36_6	PE38_2	PE38_3
fad2	0	0	0	0	0	0	21	0	0	2	0	21	0	0	0	0	0	0
fad3	0	0	0	0	0	0	0	0	0	0	0	0	0	24	0	0	0	0
fad4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad6	0	0	0	0	0	0	1	0	0	3	0	0	0	0	0	0	0	0
fad7	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
sfd1	0	0	0	0	0	0	3	0	0	0	2	0	0	0	0	0	0	0
sfd2	0	0	0	0	0	0	0	0	0	0	0	3	3	0	0	0	0	3
sfd3	0	0	0	0	0	0	0	2	0	1	0	1	1	3	0	0	1	1

	PE38_4	PE38_5	PE38_6	PE40_2	PE40_3	PE42_2	PE42_3	PE42_4	PG32_0	PG32_1	PG34_0	PG34_1	PG34_2	PG34_3	PG34_4	PI34_1	PI34_2	PI34_3
fad2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
fad3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad4	0	0	0	0	0	0	0	0	3	0	2	0	0	4	0	0	0	0
fad5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

fad6	0	0	0	0	0	0	0	0	0	0	0	1	11	0	0	0	0	0
fad7	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
sfd1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0
sfd2	0	2	0	0	3	0	0	0	0	0	5	4	0	0	0	0	0	0
sfd3	1	0	0	1	0	1	1	0	0	0	0	2	12	0	0	0	0	0

	PI34_4	PI36_1	PI36_2	PI36_3	PI36_4	PI36_5	PI36_6	PS34_1	PS34_2	PS34_3	PS34_4	PS36_1	PS36_2	PS36_3	PS36_4	PS36_5	PS36_6	PS38_1
fad2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad3	0	0	0	0	0	0	0	0	9	0	0	0	12	0	0	0	0	0
fad4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
sfd1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
sfd2	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0
sfd3	1	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0

	PS38_2	PS38_3	PS38_4	PS38_5	PS38_6	PS40_1	PS40_2	PS40_3	PS40_4	PS42_1	PS42_2	PS42_3	PS42_4	PS44_2	PS44_3
fad2	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0
fad3	15	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
fad7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
sfd1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
sfd2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
sfd3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0

5.4 Fisher's exact test for similarity

Fisher's exact test (cf. Conover, 1998) was used to quantify similarity in the lipids appearing as a reactant across two data sets. A null hypothesis is that the reactant counts are independent across two data sets. The alternative hypothesis is that the reactant lists depend on the data set. Thus, rejecting the null hypothesis with a small p-value would indicate two data sets that differ in their reactant lists. The data are formed into a 2 by 2 contingency table with number of columns equal to the total number of lipids in Table 5-3-1 and number of rows equal to 2, one for each of two data sets. Since there are 9 data sets, there are 36 pairs of data sets so 36 hypotheses

are tested. A small P-value indicates evidence for dependence. A large P-value is a metric by which to quantify a similarity of the reactant profiles for two data sets. Fisher's exact test presupposes that row and column totals for the contingency table are fixed, which may be questionable here. However, when this assumption is not met, the test is likely conservative with Type I errors below nominal values. As can be seen in Table 5.4-1 P-values are very small for all pairs except the *fad6*-*sdf3* pairs which show a marked similarity of the reactant profiles indentified in the two data sets. A strength of Fisher's exact test is that it can accommodate the very small counts, and even zero counts appearing in the contingency table (i.e., where a particular lipid did not appear at all as a reactant in a pair of data sets).

With a P-value of 0.957861, the alternative hypothesis that the reactant lists in the *fad6* and *sfd3* datasets are different is not rejected. Thus, the large p-value indicates similarity in the reactant lists. The P-values for the other pairs were as small as 0, which suggests that the feature of the metabolite profiles that is represented by the significant reactants is not similar; this is consistent with the mutations affecting the metabolite profiles being in different genes.

Table 5.4-1 Fisher's exact test for similarity

	fad2	fad3	fad4	fad5	fad6	fad7	sfd1	sfd2_2	sfd3
fad2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
fad3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
fad4	0.000000	0.000000	0.000000	0.000000	0.000000	0.000071	0.000006	0.000040	0.000022
fad5	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000001	0.000000	0.000000
fad6	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	**0.957861**
fad7	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
sfd1	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000002	0.000000
sfd2_2	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
sfd3	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

6 Summary and future work

This report proposed a multi-step exploratory technique to discover reactant-product lipid pairs in mutant/wild-type lipidomics experiments. A numerical screening procedure narrowed a large number of candidate pairs to a much smaller list. This list can then be narrowed further using biochemical knowledge of the genes involved in catalyzing certain reactions. The technique is exploratory and does not discover all pairs that are biochemically feasible nor does it rule out all those that are not. The intent of the method is a screening procedure to simplify follow-on confirmatory work.

Sample sizes were small in these experiments. The role of sample size, as well as sample size requirements for such experiments, is a worthy topic of further research. A larger sample size might improve the detection of likely reactants and possibly allow for other measures of certainty to be computed for each reactant that is discovered. Any method should be vetted by discovering its performance properties. These require analytical investigation or, as is likely the case here, investigation via simulation experiments. How to simulate realistic data from a lipidomics experiment for which some truth is known is another area of future investigation.

Data from lipidomics experiments are relatively new and statistical techniques for such data still evolving. It is hoped that the methods described here are one step forward in the development of statistical technique to deal with the metabolome (lipidome) emerging from mutant/wild-type experiments.

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Appendix A – The original dataset for each experiment

Table A-1 The original dataset for *fad2*

lipid	C1	C2	C3	C4	C5	T1	T2	T3	T4	T5
DGDG34_6	2.25	2.18	2.53	1.96	2.21	3.25	2.55	4.06	2.96	2.79
DGDG34_5	0.14	0.10	0.10	0.17	0.06	0.19	0.19	0.07	0.19	0.24
DGDG34_4	0.26	0.19	0.20	0.18	0.23	0.23	0.29	0.32	0.18	0.27
DGDG34_3	4.69	4.33	4.41	3.86	4.03	3.45	3.40	4.16	3.24	3.03
DGDG34_2	1.01	0.95	1.10	0.81	0.79	1.69	1.02	1.77	1.27	1.51
DGDG34_1	0.41	0.40	0.44	0.35	0.40	0.89	0.98	0.94	0.82	0.85
DGDG36_6	14.95	16.68	14.93	14.08	15.01	8.54	8.90	10.07	8.52	8.99
DGDG36_5	0.00	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.07	0.00
DGDG36_4	0.46	0.46	0.38	0.46	0.43	0.77	0.87	0.94	1.00	0.81
DGDG36_3	0.22	0.18	0.20	0.13	0.16	0.20	0.05	0.19	0.07	0.04
DGDG36_2	0.01	0.00	0.00	0.00	0.00	0.02	0.05	0.02	0.01	0.05
DGDG36_1	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00
DGDG38_6	0.18	0.22	0.15	0.22	0.16	0.25	0.27	0.33	0.38	0.38
DGDG38_5	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
DGDG38_4	0.08	0.00	0.03	0.03	0.05	0.01	0.01	0.00	0.02	0.00
DGDG38_3	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.02	0.00	0.00
MGDG34_6	67.36	73.73	71.54	61.98	58.12	72.07	73.54	70.04	61.64	82.23
MGDG34_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG34_4	2.04	2.69	2.02	2.32	1.86	3.42	3.89	2.81	2.60	3.51
MGDG34_3	0.94	0.72	0.74	0.83	0.70	0.98	0.63	0.83	0.99	1.23
MGDG34_2	0.44	0.80	0.60	0.61	0.49	0.74	1.06	0.92	0.78	1.20
MGDG34_1	0.37	0.00	0.00	1.24	0.00	0.38	1.12	0.00	1.98	0.41
MGDG36_6	11.56	12.24	11.68	10.73	11.68	4.80	5.81	5.59	4.47	5.68
MGDG36_5	0.01	0.04	0.09	0.26	0.03	0.07	0.00	0.05	0.31	0.00
MGDG36_4	1.28	1.18	1.35	0.87	1.17	1.97	1.73	1.76	1.81	1.69
MGDG36_3	0.04	0.11	0.00	0.11	0.00	0.00	0.00	0.04	0.00	0.00
MGDG36_2	0.05	0.00	0.03	0.00	0.01	0.20	0.08	0.14	0.29	0.15
MGDG36_1	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_4	0.04	0.06	0.06	0.00	0.00	0.00	0.00	0.02	0.02	0.02
MGDG38_3	0.00	0.05	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.17
PC32_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PC34_4	0.12	0.12	0.12	0.14	0.16	0.13	0.13	0.14	0.15	0.14
PC34_3	2.45	2.47	2.33	2.81	3.40	1.08	1.07	1.06	1.10	1.00
PC34_2	3.24	3.21	3.12	3.53	4.13	0.44	0.42	0.44	0.45	0.39
PC34_1	0.53	0.50	0.47	0.57	0.67	2.94	2.94	2.93	3.07	2.80
PC36_6	1.71	1.81	1.78	2.18	2.61	0.47	0.53	0.53	0.53	0.48
PC36_5	4.31	4.46	4.35	5.20	6.01	0.31	0.30	0.34	0.33	0.29
PC36_4	3.42	3.33	3.35	3.87	4.52	3.01	3.07	3.30	3.34	3.14
PC36_3	1.43	1.43	1.32	1.57	1.81	0.90	0.94	0.96	0.95	0.91
PC36_2	0.58	0.56	0.51	0.65	0.74	6.98	7.08	7.40	7.90	7.49
PC36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC38_6	0.01	0.01	0.01	0.02	0.02	0.01	0.01	0.01	0.01	0.01
PC38_5	0.05	0.04	0.04	0.05	0.06	0.01	0.00	0.01	0.01	0.01
PC38_4	0.08	0.07	0.07	0.08	0.09	0.06	0.05	0.06	0.07	0.06

PC38_3	0.09	0.08	0.08	0.09	0.09	0.03	0.04	0.04	0.04	0.03
PC38_2	0.05	0.05	0.05	0.05	0.05	0.13	0.12	0.14	0.15	0.13
PC40_5	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC40_4	0.01	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00
PC40_3	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PC40_2	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
LysoPC16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPC16_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
LysoPC18_3	0.01	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01
LysoPC18_2	0.02	0.02	0.02	0.02	0.03	0.00	0.00	0.00	0.00	0.00
LysoPC18_1	0.00	0.00	0.00	0.00	0.01	0.03	0.04	0.03	0.04	0.03
LysoPC18_0	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.01	0.01	0.01
LysoPE16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPE16_0	0.04	0.04	0.04	0.04	0.04	0.02	0.02	0.02	0.02	0.02
LysoPE18_3	0.02	0.02	0.02	0.02	0.03	0.02	0.02	0.02	0.02	0.02
LysoPE18_2	0.04	0.03	0.03	0.04	0.04	0.01	0.01	0.00	0.01	0.01
LysoPE18_1	0.00	0.00	0.00	0.00	0.00	0.04	0.04	0.04	0.04	0.03
PE34_4	0.05	0.05	0.05	0.06	0.06	0.11	0.11	0.11	0.12	0.11
PE34_3	2.74	2.87	2.76	3.33	3.79	1.83	1.80	1.80	1.88	1.80
PE34_2	4.12	4.02	3.89	4.67	5.26	0.53	0.47	0.50	0.54	0.49
PE34_1	0.00	0.00	0.00	0.00	0.00	1.49	1.42	1.52	1.55	1.55
PE36_6	0.75	0.74	0.72	0.92	1.05	0.57	0.56	0.61	0.61	0.57
PE36_5	2.19	2.14	2.13	2.67	2.97	0.36	0.34	0.37	0.38	0.37
PE36_4	2.31	2.28	2.19	2.70	2.95	2.60	2.54	2.67	2.76	2.69
PE36_3	0.59	0.56	0.52	0.66	0.72	0.66	0.64	0.70	0.69	0.71
PE36_2	0.29	0.28	0.26	0.34	0.35	2.28	2.18	2.29	2.46	2.43
PE36_1	0.01	0.01	0.01	0.00	0.01	0.06	0.06	0.05	0.04	0.05
PE38_6	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
PE38_5	0.03	0.03	0.03	0.04	0.04	0.01	0.01	0.01	0.01	0.01
PE38_4	0.05	0.04	0.04	0.05	0.05	0.06	0.06	0.06	0.07	0.06
PE38_3	0.06	0.07	0.06	0.08	0.09	0.07	0.06	0.06	0.06	0.07
PE38_2	0.08	0.09	0.09	0.10	0.11	0.10	0.10	0.10	0.11	0.10
PE40_3	0.05	0.05	0.04	0.05	0.06	0.05	0.05	0.05	0.06	0.05
PE40_2	0.10	0.09	0.09	0.11	0.12	0.03	0.02	0.03	0.03	0.03
PE42_4	0.02	0.02	0.02	0.02	0.03	0.04	0.03	0.03	0.04	0.03
PE42_3	0.09	0.08	0.08	0.09	0.11	0.07	0.07	0.07	0.07	0.07
PE42_2	0.09	0.08	0.08	0.11	0.12	0.12	0.11	0.11	0.12	0.12
PG32_1	0.53	0.60	0.79	0.69	0.81	1.62	1.67	1.51	1.86	1.44
PG32_0	0.23	0.26	0.25	0.41	0.38	0.59	0.62	0.42	0.46	0.56
PG34_4	8.69	9.14	10.46	10.02	10.91	7.87	8.34	8.86	8.17	7.76
PG34_3	2.40	2.58	2.39	2.61	3.16	2.18	2.42	2.37	2.57	2.13
PG34_2	2.03	1.93	2.03	2.16	2.47	1.85	1.96	2.18	1.96	2.16
PG34_1	1.18	1.31	1.22	1.31	1.48	2.74	2.78	3.14	2.84	2.57
PG34_0	0.02	0.00	0.03	0.00	0.04	0.08	0.09	0.07	0.08	0.01
lysoPG16_1	0.01	0.01	0.01	0.01	0.01	0.02	0.01	0.02	0.01	0.02
lysoPG16_0	0.01	0.01	0.01	0.00	0.01	0.01	0.02	0.01	0.01	0.00
lysoPG18_3	0.05	0.04	0.04	0.04	0.04	0.04	0.04	0.03	0.03	0.04
lysoPG18_2	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
lysoPG18_1	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.00
PA34_6	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.00
PA34_4	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA34_3	0.15	0.16	0.28	0.16	0.17	0.08	0.06	0.08	0.09	0.05
PA34_2	0.16	0.18	0.26	0.14	0.21	0.04	0.02	0.02	0.03	0.02
PA34_1	0.11	0.10	0.10	0.06	0.06	0.21	0.16	0.20	0.18	0.16

PA36_6	0.05	0.05	0.08	0.04	0.05	0.02	0.02	0.03	0.03	0.02
PA36_5	0.10	0.09	0.18	0.07	0.11	0.02	0.01	0.01	0.02	0.01
PA36_4	0.11	0.08	0.18	0.09	0.12	0.06	0.05	0.08	0.08	0.05
PA36_3	0.03	0.03	0.06	0.04	0.02	0.03	0.02	0.02	0.03	0.03
PA36_2	0.01	0.01	0.01	0.01	0.01	0.07	0.07	0.09	0.11	0.06
PI34_4	0.02	0.02	0.01	0.02	0.03	0.03	0.02	0.03	0.03	0.02
PI34_3	1.28	1.48	1.45	1.68	2.15	1.19	1.18	1.24	1.15	1.12
PI34_2	1.52	1.64	1.68	1.88	2.35	0.25	0.22	0.27	0.25	0.21
PI34_1	0.00	0.00	0.00	0.00	0.00	1.43	1.26	1.52	1.36	1.35
PI36_6	0.07	0.06	0.08	0.10	0.11	0.04	0.04	0.06	0.05	0.05
PI36_5	0.12	0.11	0.11	0.12	0.15	0.01	0.01	0.00	0.01	0.02
PI36_4	0.14	0.11	0.11	0.16	0.15	0.21	0.17	0.19	0.17	0.17
PI36_3	0.16	0.13	0.15	0.16	0.21	0.08	0.09	0.11	0.10	0.10
PI36_2	0.11	0.11	0.08	0.12	0.13	0.35	0.32	0.34	0.38	0.33
PI36_1	0.01	0.01	0.01	0.01	0.00	0.08	0.08	0.07	0.09	0.07
PS34_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS34_3	0.07	0.07	0.08	0.08	0.10	0.06	0.06	0.06	0.06	0.06
PS34_2	0.08	0.08	0.08	0.08	0.10	0.01	0.01	0.02	0.01	0.01
PS34_1	0.00	0.00	0.00	0.00	0.00	0.05	0.05	0.05	0.06	0.05
PS36_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS36_5	0.01	0.01	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.00
PS36_4	0.01	0.01	0.01	0.01	0.02	0.04	0.03	0.04	0.04	0.05
PS36_3	0.04	0.05	0.04	0.04	0.05	0.02	0.02	0.02	0.02	0.02
PS36_2	0.03	0.03	0.04	0.03	0.03	0.06	0.05	0.06	0.06	0.06
PS36_1	0.00	0.00	0.00	0.00	0.00	0.01	0.03	0.02	0.02	0.02
PS38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_4	0.00	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.02	0.01
PS38_3	0.04	0.04	0.03	0.04	0.05	0.02	0.02	0.02	0.02	0.02
PS38_2	0.04	0.04	0.04	0.04	0.04	0.03	0.03	0.03	0.03	0.03
PS38_1	0.00	0.00	0.00	0.00	0.00	0.01	0.02	0.02	0.02	0.01
PS40_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_3	0.04	0.04	0.04	0.06	0.06	0.04	0.04	0.05	0.05	0.04
PS40_2	0.06	0.05	0.06	0.06	0.07	0.01	0.01	0.01	0.01	0.01
PS40_1	0.00	0.00	0.00	0.00	0.00	0.03	0.03	0.03	0.03	0.03
PS42_4	0.01	0.02	0.02	0.02	0.02	0.01	0.02	0.02	0.02	0.02
PS42_3	0.08	0.07	0.08	0.08	0.11	0.07	0.06	0.08	0.08	0.07
PS42_2	0.07	0.07	0.06	0.08	0.09	0.03	0.03	0.03	0.03	0.03
PS42_1	0.00	0.00	0.00	0.00	0.00	0.04	0.05	0.05	0.05	0.05
PS44_3	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.00	0.00
PS44_2	0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00

Table A-2 The original dataset for *fad3*

lipid	C1	C2	C3	C4	C5	T1	T2	T3	T4	T5
DGDG34_6	2.25	2.18	2.53	1.96	2.21	1.71	2.53	2.29	2.07	1.84
DGDG34_5	0.14	0.10	0.10	0.17	0.06	0.14	0.00	0.21	0.04	0.14
DGDG34_4	0.26	0.19	0.20	0.18	0.23	0.12	0.18	0.17	0.22	0.14
DGDG34_3	4.69	4.33	4.41	3.86	4.03	2.86	3.59	3.31	3.27	2.57
DGDG34_2	1.01	0.95	1.10	0.81	0.79	0.63	0.73	0.64	0.66	0.84
DGDG34_1	0.41	0.40	0.44	0.35	0.40	0.27	0.43	0.35	0.28	0.32
DGDG36_6	14.95	16.68	14.93	14.08	15.01	12.22	13.87	14.07	13.17	11.37
DGDG36_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

DGDG36_4	0.46	0.46	0.38	0.46	0.43	0.56	0.51	0.52	0.55	0.43
DGDG36_3	0.22	0.18	0.20	0.13	0.16	0.10	0.06	0.08	0.08	0.03
DGDG36_2	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.04	0.04
DGDG36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DGDG38_6	0.18	0.22	0.15	0.22	0.16	0.19	0.12	0.20	0.14	0.09
DGDG38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00
DGDG38_4	0.08	0.00	0.03	0.03	0.05	0.00	0.00	0.00	0.00	0.01
DGDG38_3	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG34_6	67.36	73.73	71.54	61.98	58.12	56.92	58.94	79.13	53.16	57.69
MGDG34_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG34_4	2.04	2.69	2.02	2.32	1.86	2.10	1.84	2.58	1.63	1.86
MGDG34_3	0.94	0.72	0.74	0.83	0.70	0.61	0.69	1.16	0.60	0.80
MGDG34_2	0.44	0.80	0.60	0.61	0.49	0.42	0.41	0.40	0.34	0.41
MGDG34_1	0.37	0.00	0.00	1.24	0.00	0.08	0.00	1.27	0.68	0.00
MGDG36_6	11.56	12.24	11.68	10.73	11.68	11.45	11.17	11.03	8.77	9.19
MGDG36_5	0.01	0.04	0.09	0.26	0.03	0.58	0.31	0.37	0.46	0.39
MGDG36_4	1.28	1.18	1.35	0.87	1.17	0.79	0.76	0.71	0.55	0.72
MGDG36_3	0.04	0.11	0.00	0.11	0.00	0.00	0.08	0.16	0.08	0.08
MGDG36_2	0.05	0.00	0.03	0.00	0.01	0.07	0.00	0.00	0.00	0.00
MGDG36_1	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_4	0.04	0.06	0.06	0.00	0.00	0.00	0.00	0.00	0.01	0.00
MGDG38_3	0.00	0.05	0.00	0.02	0.00	0.00	0.00	0.00	0.03	0.14
PC32_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PC34_4	0.12	0.12	0.12	0.14	0.16	0.08	0.10	0.10	0.10	0.10
PC34_3	2.45	2.47	2.33	2.81	3.40	1.24	1.41	1.50	1.42	1.46
PC34_2	3.24	3.21	3.12	3.53	4.13	3.72	4.01	4.04	3.96	3.83
PC34_1	0.53	0.50	0.47	0.57	0.67	0.41	0.50	0.47	0.46	0.53
PC36_6	1.71	1.81	1.78	2.18	2.61	0.59	0.77	0.84	0.77	0.80
PC36_5	4.31	4.46	4.35	5.20	6.01	2.75	3.09	3.16	3.09	3.04
PC36_4	3.42	3.33	3.35	3.87	4.52	5.00	5.36	5.31	5.20	5.07
PC36_3	1.43	1.43	1.32	1.57	1.81	1.61	1.78	1.79	1.75	1.78
PC36_2	0.58	0.56	0.51	0.65	0.74	0.58	0.59	0.59	0.57	0.57
PC36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC38_6	0.01	0.01	0.01	0.02	0.02	0.00	0.00	0.01	0.01	0.00
PC38_5	0.05	0.04	0.04	0.05	0.06	0.02	0.02	0.02	0.02	0.02
PC38_4	0.08	0.07	0.07	0.08	0.09	0.06	0.06	0.06	0.05	0.05
PC38_3	0.09	0.08	0.08	0.09	0.09	0.07	0.07	0.07	0.07	0.07
PC38_2	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.04	0.04
PC40_5	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC40_4	0.01	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00
PC40_3	0.01	0.00	0.01	0.01	0.01	0.00	0.01	0.00	0.00	0.00
PC40_2	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
LysoPC16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPC16_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
LysoPC18_3	0.01	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01
LysoPC18_2	0.02	0.02	0.02	0.02	0.03	0.02	0.03	0.03	0.03	0.03
LysoPC18_1	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.01	0.01
LysoPC18_0	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00
LysoPE16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPE16_0	0.04	0.04	0.04	0.04	0.04	0.03	0.03	0.03	0.03	0.03
LysoPE18_3	0.02	0.02	0.02	0.02	0.03	0.01	0.01	0.01	0.01	0.01
LysoPE18_2	0.04	0.03	0.03	0.04	0.04	0.04	0.05	0.05	0.04	0.05

LysoPE18_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PE34_4	0.05	0.05	0.05	0.06	0.06	0.03	0.03	0.04	0.03	0.03
PE34_3	2.74	2.87	2.76	3.33	3.79	1.22	1.34	1.43	1.34	1.37
PE34_2	4.12	4.02	3.89	4.67	5.26	4.86	5.17	5.15	4.82	4.85
PE34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PE36_6	0.75	0.74	0.72	0.92	1.05	0.15	0.16	0.20	0.17	0.18
PE36_5	2.19	2.14	2.13	2.67	2.97	1.12	1.23	1.29	1.16	1.21
PE36_4	2.31	2.28	2.19	2.70	2.95	3.96	4.14	4.06	3.87	3.80
PE36_3	0.59	0.56	0.52	0.66	0.72	0.58	0.62	0.65	0.61	0.61
PE36_2	0.29	0.28	0.26	0.34	0.35	0.29	0.26	0.26	0.27	0.26
PE36_1	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.01
PE38_6	0.02	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.01	0.01
PE38_5	0.03	0.03	0.03	0.04	0.04	0.01	0.01	0.02	0.01	0.01
PE38_4	0.05	0.04	0.04	0.05	0.05	0.04	0.04	0.03	0.04	0.03
PE38_3	0.06	0.07	0.06	0.08	0.09	0.06	0.05	0.06	0.06	0.05
PE38_2	0.08	0.09	0.09	0.10	0.11	0.10	0.11	0.12	0.10	0.10
PE40_3	0.05	0.05	0.04	0.05	0.06	0.02	0.02	0.02	0.02	0.02
PE40_2	0.10	0.09	0.09	0.11	0.12	0.10	0.10	0.10	0.10	0.10
PE42_4	0.02	0.02	0.02	0.02	0.03	0.01	0.01	0.01	0.01	0.01
PE42_3	0.09	0.08	0.08	0.09	0.11	0.09	0.09	0.09	0.10	0.09
PE42_2	0.09	0.08	0.08	0.11	0.12	0.10	0.10	0.11	0.11	0.10
PG32_1	0.53	0.60	0.79	0.69	0.81	0.47	0.51	0.57	0.46	0.52
PG32_0	0.23	0.26	0.25	0.41	0.38	0.29	0.26	0.25	0.27	0.23
PG34_4	8.69	9.14	10.46	10.02	10.91	8.19	8.20	8.02	7.86	7.27
PG34_3	2.40	2.58	2.39	2.61	3.16	2.60	2.37	2.22	2.34	2.05
PG34_2	2.03	1.93	2.03	2.16	2.47	2.27	2.04	1.94	1.97	1.78
PG34_1	1.18	1.31	1.22	1.31	1.48	1.27	1.18	1.16	1.23	1.08
PG34_0	0.02	0.00	0.03	0.00	0.04	0.04	0.02	0.01	0.01	0.01
lysoPG16_1	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
lysoPG16_0	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.00	0.01
lysoPG18_3	0.05	0.04	0.04	0.04	0.04	0.03	0.04	0.04	0.03	0.03
lysoPG18_2	0.01	0.00	0.00	0.00	0.01	0.01	0.00	0.01	0.00	0.00
lysoPG18_1	0.00	0.01	0.01	0.01	0.00	0.00	0.00	0.01	0.00	0.00
PA34_6	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA34_4	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA34_3	0.15	0.16	0.28	0.16	0.17	0.05	0.06	0.08	0.12	0.08
PA34_2	0.16	0.18	0.26	0.14	0.21	0.14	0.17	0.25	0.33	0.25
PA34_1	0.11	0.10	0.10	0.06	0.06	0.08	0.08	0.08	0.07	0.07
PA36_6	0.05	0.05	0.08	0.04	0.05	0.01	0.01	0.02	0.02	0.02
PA36_5	0.10	0.09	0.18	0.07	0.11	0.03	0.04	0.06	0.08	0.08
PA36_4	0.11	0.08	0.18	0.09	0.12	0.09	0.14	0.18	0.27	0.22
PA36_3	0.03	0.03	0.06	0.04	0.02	0.02	0.03	0.05	0.06	0.03
PA36_2	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.02
PI34_4	0.02	0.02	0.01	0.02	0.03	0.01	0.02	0.01	0.01	0.01
PI34_3	1.28	1.48	1.45	1.68	2.15	0.73	0.94	0.98	0.87	0.83
PI34_2	1.52	1.64	1.68	1.88	2.35	1.99	2.37	2.50	2.24	2.07
PI34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PI36_6	0.07	0.06	0.08	0.10	0.11	0.03	0.05	0.05	0.03	0.04
PI36_5	0.12	0.11	0.11	0.12	0.15	0.06	0.09	0.09	0.08	0.07
PI36_4	0.14	0.11	0.11	0.16	0.15	0.14	0.16	0.18	0.15	0.14
PI36_3	0.16	0.13	0.15	0.16	0.21	0.10	0.11	0.11	0.10	0.10
PI36_2	0.11	0.11	0.08	0.12	0.13	0.11	0.12	0.12	0.10	0.11
PI36_1	0.01	0.01	0.01	0.01	0.00	0.01	0.00	0.01	0.01	0.01
PS34_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

PS34_3	0.07	0.07	0.08	0.08	0.10	0.03	0.04	0.04	0.03	0.03
PS34_2	0.08	0.08	0.08	0.08	0.10	0.13	0.12	0.12	0.12	0.10
PS34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS36_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS36_5	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.01	0.00	0.01
PS36_4	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.01	0.01
PS36_3	0.04	0.05	0.04	0.04	0.05	0.02	0.02	0.03	0.02	0.02
PS36_2	0.03	0.03	0.04	0.03	0.03	0.05	0.04	0.05	0.04	0.04
PS36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_4	0.00	0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00
PS38_3	0.04	0.04	0.03	0.04	0.05	0.01	0.01	0.02	0.02	0.02
PS38_2	0.04	0.04	0.04	0.04	0.04	0.06	0.05	0.05	0.05	0.05
PS38_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_3	0.04	0.04	0.04	0.06	0.06	0.02	0.02	0.02	0.02	0.02
PS40_2	0.06	0.05	0.06	0.06	0.07	0.08	0.08	0.09	0.07	0.09
PS40_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS42_4	0.01	0.02	0.02	0.02	0.02	0.01	0.00	0.01	0.01	0.01
PS42_3	0.08	0.07	0.08	0.08	0.11	0.06	0.06	0.06	0.06	0.06
PS42_2	0.07	0.07	0.06	0.08	0.09	0.09	0.10	0.10	0.09	0.10
PS42_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS44_3	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
PS44_2	0.00	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.00

Table A-3 The original dataset for *fad4*

lipid	C1	C2	C3	C4	C5	T1	T2	T3	T4	T5
DGDG34_6	2.25	2.18	2.53	1.96	2.21	2.35	2.67	2.15	2.21	2.85
DGDG34_5	0.14	0.10	0.10	0.17	0.06	0.24	0.11	0.02	0.11	0.21
DGDG34_4	0.26	0.19	0.20	0.18	0.23	0.22	0.34	0.05	0.22	0.32
DGDG34_3	4.69	4.33	4.41	3.86	4.03	4.40	4.37	3.99	4.03	5.29
DGDG34_2	1.01	0.95	1.10	0.81	0.79	0.71	0.80	0.65	0.75	0.65
DGDG34_1	0.41	0.40	0.44	0.35	0.40	0.52	0.55	0.38	0.45	0.47
DGDG36_6	14.95	16.68	14.93	14.08	15.01	16.82	16.58	16.23	14.62	15.37
DGDG36_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DGDG36_4	0.46	0.46	0.38	0.46	0.43	0.43	0.41	0.47	0.28	0.38
DGDG36_3	0.22	0.18	0.20	0.13	0.16	0.14	0.14	0.12	0.18	0.12
DGDG36_2	0.01	0.00	0.00	0.00	0.00	0.01	0.02	0.04	0.01	0.04
DGDG36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DGDG38_6	0.18	0.22	0.15	0.22	0.16	0.12	0.15	0.13	0.17	0.22
DGDG38_5	0.00	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00
DGDG38_4	0.08	0.00	0.03	0.03	0.05	0.01	0.00	0.01	0.01	0.00
DGDG38_3	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG34_6	67.36	73.73	71.54	61.98	58.12	57.81	64.12	58.41	58.08	58.71
MGDG34_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG34_4	2.04	2.69	2.02	2.32	1.86	1.95	2.19	1.89	1.80	2.12
MGDG34_3	0.94	0.72	0.74	0.83	0.70	0.59	0.71	0.72	0.56	0.66
MGDG34_2	0.44	0.80	0.60	0.61	0.49	0.43	0.52	0.48	0.62	0.44
MGDG34_1	0.37	0.00	0.00	1.24	0.00	0.00	1.09	1.11	0.00	0.00
MGDG36_6	11.56	12.24	11.68	10.73	11.68	13.41	10.71	13.54	10.32	10.84
MGDG36_5	0.01	0.04	0.09	0.26	0.03	0.00	0.00	0.00	0.00	0.00

MGDG36_4	1.28	1.18	1.35	0.87	1.17	1.09	0.87	1.13	0.95	1.58
MGDG36_3	0.04	0.11	0.00	0.11	0.00	0.09	0.07	0.12	0.08	0.00
MGDG36_2	0.05	0.00	0.03	0.00	0.01	0.00	0.00	0.00	0.00	0.00
MGDG36_1	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_4	0.04	0.06	0.06	0.00	0.00	0.05	0.03	0.11	0.01	0.08
MGDG38_3	0.00	0.05	0.00	0.02	0.00	0.04	0.12	0.00	0.00	0.00
PC32_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PC34_4	0.12	0.12	0.12	0.14	0.16	0.12	0.11	0.11	0.12	0.11
PC34_3	2.45	2.47	2.33	2.81	3.40	2.29	2.28	2.30	2.47	2.33
PC34_2	3.24	3.21	3.12	3.53	4.13	2.88	3.08	2.89	3.40	3.22
PC34_1	0.53	0.50	0.47	0.57	0.67	0.52	0.53	0.54	0.59	0.57
PC36_6	1.71	1.81	1.78	2.18	2.61	1.95	1.90	1.88	1.95	1.97
PC36_5	4.31	4.46	4.35	5.20	6.01	4.29	4.42	4.25	4.85	4.62
PC36_4	3.42	3.33	3.35	3.87	4.52	3.32	3.46	3.31	3.84	3.63
PC36_3	1.43	1.43	1.32	1.57	1.81	1.39	1.49	1.38	1.70	1.51
PC36_2	0.58	0.56	0.51	0.65	0.74	0.49	0.54	0.54	0.64	0.59
PC36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC38_6	0.01	0.01	0.01	0.02	0.02	0.01	0.01	0.01	0.01	0.01
PC38_5	0.05	0.04	0.04	0.05	0.06	0.04	0.04	0.04	0.04	0.05
PC38_4	0.08	0.07	0.07	0.08	0.09	0.07	0.06	0.06	0.08	0.09
PC38_3	0.09	0.08	0.08	0.09	0.09	0.07	0.07	0.07	0.09	0.10
PC38_2	0.05	0.05	0.05	0.05	0.05	0.04	0.04	0.04	0.05	0.05
PC40_5	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC40_4	0.01	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00
PC40_3	0.01	0.00	0.01	0.01	0.01	0.01	0.00	0.00	0.01	0.01
PC40_2	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.00
LysoPC16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPC16_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
LysoPC18_3	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
LysoPC18_2	0.02	0.02	0.02	0.02	0.03	0.03	0.03	0.02	0.03	0.03
LysoPC18_1	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01
LysoPC18_0	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.01
LysoPE16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPE16_0	0.04	0.04	0.04	0.04	0.04	0.04	0.03	0.04	0.04	0.04
LysoPE18_3	0.02	0.02	0.02	0.02	0.03	0.03	0.03	0.02	0.02	0.02
LysoPE18_2	0.04	0.03	0.03	0.04	0.04	0.03	0.03	0.04	0.04	0.03
LysoPE18_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PE34_4	0.05	0.05	0.05	0.06	0.06	0.05	0.05	0.05	0.05	0.05
PE34_3	2.74	2.87	2.76	3.33	3.79	2.72	2.76	2.73	2.98	2.85
PE34_2	4.12	4.02	3.89	4.67	5.26	3.72	4.02	3.77	4.21	4.17
PE34_1	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.02	0.02	0.00
PE36_6	0.75	0.74	0.72	0.92	1.05	0.76	0.78	0.76	0.82	0.79
PE36_5	2.19	2.14	2.13	2.67	2.97	2.17	2.19	2.17	2.46	2.36
PE36_4	2.31	2.28	2.19	2.70	2.95	2.19	2.33	2.24	2.60	2.42
PE36_3	0.59	0.56	0.52	0.66	0.72	0.55	0.59	0.55	0.64	0.59
PE36_2	0.29	0.28	0.26	0.34	0.35	0.23	0.26	0.25	0.30	0.29
PE36_1	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.00	0.01
PE38_6	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
PE38_5	0.03	0.03	0.03	0.04	0.04	0.03	0.03	0.03	0.04	0.03
PE38_4	0.05	0.04	0.04	0.05	0.05	0.04	0.04	0.04	0.04	0.05
PE38_3	0.06	0.07	0.06	0.08	0.09	0.05	0.06	0.06	0.07	0.07
PE38_2	0.08	0.09	0.09	0.10	0.11	0.07	0.07	0.07	0.09	0.09

PE40_3	0.05	0.05	0.04	0.05	0.06	0.04	0.04	0.04	0.05	0.05
PE40_2	0.10	0.09	0.09	0.11	0.12	0.08	0.09	0.08	0.10	0.09
PE42_4	0.02	0.02	0.02	0.02	0.03	0.02	0.02	0.02	0.02	0.02
PE42_3	0.09	0.08	0.08	0.09	0.11	0.07	0.08	0.07	0.09	0.08
PE42_2	0.09	0.08	0.08	0.11	0.12	0.07	0.08	0.07	0.09	0.09
PG32_1	0.53	0.60	0.79	0.69	0.81	0.05	0.04	0.02	0.03	0.01
PG32_0	0.23	0.26	0.25	0.41	0.38	0.64	0.66	0.59	0.62	0.56
PG34_4	8.69	9.14	10.46	10.02	10.91	0.07	0.04	0.05	0.05	0.04
PG34_3	2.40	2.58	2.39	2.61	3.16	6.60	6.71	6.24	7.39	6.85
PG34_2	2.03	1.93	2.03	2.16	2.47	1.24	1.21	1.15	1.47	1.39
PG34_1	1.18	1.31	1.22	1.31	1.48	1.55	1.35	1.42	1.64	1.41
PG34_0	0.02	0.00	0.03	0.00	0.04	0.07	0.10	0.11	0.14	0.15
lysoPG16_1	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
lysoPG16_0	0.01	0.01	0.01	0.00	0.01	0.00	0.01	0.01	0.01	0.01
lysoPG18_3	0.05	0.04	0.04	0.04	0.04	0.00	0.00	0.00	0.00	0.00
lysoPG18_2	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
lysoPG18_1	0.00	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00
PA34_6	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA34_4	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA34_3	0.15	0.16	0.28	0.16	0.17	0.13	0.16	0.11	0.13	0.11
PA34_2	0.16	0.18	0.26	0.14	0.21	0.15	0.16	0.15	0.10	0.11
PA34_1	0.11	0.10	0.10	0.06	0.06	0.09	0.05	0.06	0.07	0.09
PA36_6	0.05	0.05	0.08	0.04	0.05	0.05	0.05	0.04	0.04	0.03
PA36_5	0.10	0.09	0.18	0.07	0.11	0.09	0.09	0.07	0.08	0.07
PA36_4	0.11	0.08	0.18	0.09	0.12	0.11	0.09	0.06	0.09	0.08
PA36_3	0.03	0.03	0.06	0.04	0.02	0.03	0.03	0.03	0.03	0.02
PA36_2	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.00	0.01	0.02
PI34_4	0.02	0.02	0.01	0.02	0.03	0.02	0.02	0.02	0.02	0.02
PI34_3	1.28	1.48	1.45	1.68	2.15	1.34	1.45	1.34	1.43	1.51
PI34_2	1.52	1.64	1.68	1.88	2.35	1.40	1.65	1.49	1.61	1.74
PI34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PI36_6	0.07	0.06	0.08	0.10	0.11	0.09	0.07	0.08	0.07	0.08
PI36_5	0.12	0.11	0.11	0.12	0.15	0.11	0.11	0.12	0.12	0.11
PI36_4	0.14	0.11	0.11	0.16	0.15	0.11	0.12	0.11	0.17	0.14
PI36_3	0.16	0.13	0.15	0.16	0.21	0.12	0.17	0.12	0.15	0.14
PI36_2	0.11	0.11	0.08	0.12	0.13	0.08	0.09	0.07	0.10	0.11
PI36_1	0.01	0.01	0.01	0.01	0.00	0.01	0.00	0.01	0.01	0.01
PS34_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS34_3	0.07	0.07	0.08	0.08	0.10	0.08	0.06	0.08	0.08	0.07
PS34_2	0.08	0.08	0.08	0.08	0.10	0.08	0.07	0.08	0.09	0.08
PS34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS36_6	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.00
PS36_5	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PS36_4	0.01	0.01	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.01
PS36_3	0.04	0.05	0.04	0.04	0.05	0.04	0.04	0.04	0.04	0.04
PS36_2	0.03	0.03	0.04	0.03	0.03	0.03	0.03	0.03	0.04	0.04
PS36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_4	0.00	0.01	0.00	0.01	0.01	0.00	0.01	0.01	0.00	0.01
PS38_3	0.04	0.04	0.03	0.04	0.05	0.04	0.03	0.03	0.03	0.04
PS38_2	0.04	0.04	0.04	0.04	0.04	0.04	0.03	0.03	0.04	0.04
PS38_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

PS40_3	0.04	0.04	0.04	0.06	0.06	0.04	0.04	0.05	0.05	0.05
PS40_2	0.06	0.05	0.06	0.06	0.07	0.06	0.06	0.06	0.06	0.06
PS40_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS42_4	0.01	0.02	0.02	0.02	0.02	0.02	0.01	0.01	0.02	0.01
PS42_3	0.08	0.07	0.08	0.08	0.11	0.08	0.07	0.07	0.08	0.08
PS42_2	0.07	0.07	0.06	0.08	0.09	0.07	0.07	0.07	0.08	0.07
PS42_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS44_3	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
PS44_2	0.00	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.01	0.00

Table A-4 The original dataset for *fad5*

lipid	C1	C2	C3	C4	C5	T1	T2	T3	T4	T5
DGDG34_6	2.25	2.18	2.53	1.96	2.21	0.00	0.00	0.01	0.00	0.00
DGDG34_5	0.14	0.10	0.10	0.17	0.06	0.00	0.00	0.00	0.00	0.00
DGDG34_4	0.26	0.19	0.20	0.18	0.23	0.07	0.19	0.11	0.17	0.10
DGDG34_3	4.69	4.33	4.41	3.86	4.03	13.31	13.83	13.53	16.35	13.24
DGDG34_2	1.01	0.95	1.10	0.81	0.79	0.00	0.00	0.00	0.00	0.00
DGDG34_1	0.41	0.40	0.44	0.35	0.40	0.09	0.09	0.07	0.00	0.17
DGDG36_6	14.95	16.68	14.93	14.08	15.01	6.42	6.51	6.58	7.92	6.87
DGDG36_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DGDG36_4	0.46	0.46	0.38	0.46	0.43	0.26	0.03	0.19	0.12	0.16
DGDG36_3	0.22	0.18	0.20	0.13	0.16	0.55	0.53	0.49	0.40	0.49
DGDG36_2	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DGDG36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DGDG38_6	0.18	0.22	0.15	0.22	0.16	0.17	0.24	0.29	0.17	0.30
DGDG38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00
DGDG38_4	0.08	0.00	0.03	0.03	0.05	0.00	0.00	0.01	0.00	0.00
DGDG38_3	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG34_6	67.36	73.73	71.54	61.98	58.12	0.02	0.11	0.02	0.02	0.04
MGDG34_5	0.00	0.00	0.00	0.00	0.00	0.00	0.09	0.00	0.00	0.00
MGDG34_4	2.04	2.69	2.02	2.32	1.86	0.31	0.27	0.27	0.41	0.16
MGDG34_3	0.94	0.72	0.74	0.83	0.70	21.06	19.73	18.05	17.96	14.75
MGDG34_2	0.44	0.80	0.60	0.61	0.49	0.00	0.00	0.00	0.00	0.00
MGDG34_1	0.37	0.00	0.00	1.24	0.00	0.44	0.00	0.00	0.43	0.60
MGDG36_6	11.56	12.24	11.68	10.73	11.68	35.13	31.82	30.26	34.22	34.34
MGDG36_5	0.01	0.04	0.09	0.26	0.03	0.00	0.00	0.00	0.00	0.00
MGDG36_4	1.28	1.18	1.35	0.87	1.17	0.38	0.43	0.49	0.53	0.44
MGDG36_3	0.04	0.11	0.00	0.11	0.00	0.40	0.46	0.12	0.27	0.25
MGDG36_2	0.05	0.00	0.03	0.00	0.01	0.00	0.00	0.02	0.00	0.00
MGDG36_1	0.02	0.00	0.00	0.00	0.00	0.04	0.00	0.06	0.10	0.00
MGDG38_6	0.00	0.00	0.00	0.00	0.00	0.02	0.05	0.00	0.00	0.00
MGDG38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_4	0.04	0.06	0.06	0.00	0.00	0.43	0.22	0.30	0.36	0.33
MGDG38_3	0.00	0.05	0.00	0.02	0.00	0.00	0.00	0.00	0.09	0.00
PC32_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PC34_4	0.12	0.12	0.12	0.14	0.16	0.05	0.05	0.05	0.05	0.04
PC34_3	2.45	2.47	2.33	2.81	3.40	2.26	2.36	2.44	2.18	1.77
PC34_2	3.24	3.21	3.12	3.53	4.13	4.01	3.67	3.96	3.85	2.79
PC34_1	0.53	0.50	0.47	0.57	0.67	0.68	0.65	0.62	0.66	0.51
PC36_6	1.71	1.81	1.78	2.18	2.61	1.61	1.62	1.78	1.56	1.31
PC36_5	4.31	4.46	4.35	5.20	6.01	4.24	3.98	4.30	4.15	3.29
PC36_4	3.42	3.33	3.35	3.87	4.52	4.40	4.08	4.37	4.42	3.29

PC36_3	1.43	1.43	1.32	1.57	1.81	2.03	1.92	1.96	2.06	1.65
PC36_2	0.58	0.56	0.51	0.65	0.74	0.81	0.74	0.75	0.74	0.61
PC36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC38_6	0.01	0.01	0.01	0.02	0.02	0.01	0.01	0.01	0.01	0.01
PC38_5	0.05	0.04	0.04	0.05	0.06	0.06	0.05	0.05	0.05	0.04
PC38_4	0.08	0.07	0.07	0.08	0.09	0.11	0.09	0.10	0.11	0.07
PC38_3	0.09	0.08	0.08	0.09	0.09	0.11	0.09	0.10	0.10	0.08
PC38_2	0.05	0.05	0.05	0.05	0.05	0.07	0.06	0.06	0.07	0.05
PC40_5	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC40_4	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.00	0.00	0.00
PC40_3	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.00	0.01	0.01
PC40_2	0.00	0.00	0.00	0.00	0.01	0.01	0.00	0.01	0.01	0.00
LysoPC16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPC16_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
LysoPC18_3	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.01
LysoPC18_2	0.02	0.02	0.02	0.02	0.03	0.03	0.03	0.03	0.03	0.02
LysoPC18_1	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01
LysoPC18_0	0.00	0.00	0.00	0.01	0.00	0.01	0.01	0.01	0.01	0.01
LysoPE16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPE16_0	0.04	0.04	0.04	0.04	0.04	0.05	0.05	0.05	0.04	0.03
LysoPE18_3	0.02	0.02	0.02	0.02	0.03	0.02	0.02	0.03	0.02	0.02
LysoPE18_2	0.04	0.03	0.03	0.04	0.04	0.05	0.05	0.05	0.05	0.04
LysoPE18_1	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.01
PE34_4	0.05	0.05	0.05	0.06	0.06	0.03	0.03	0.03	0.03	0.02
PE34_3	2.74	2.87	2.76	3.33	3.79	2.78	2.87	2.99	2.75	2.18
PE34_2	4.12	4.02	3.89	4.67	5.26	5.32	5.06	5.13	5.22	3.79
PE34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PE36_6	0.75	0.74	0.72	0.92	1.05	0.63	0.63	0.67	0.58	0.53
PE36_5	2.19	2.14	2.13	2.67	2.97	2.28	2.15	2.36	2.17	1.74
PE36_4	2.31	2.28	2.19	2.70	2.95	3.04	2.84	3.06	3.00	2.25
PE36_3	0.59	0.56	0.52	0.66	0.72	0.85	0.80	0.82	0.75	0.61
PE36_2	0.29	0.28	0.26	0.34	0.35	0.35	0.34	0.34	0.35	0.29
PE36_1	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.01
PE38_6	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
PE38_5	0.03	0.03	0.03	0.04	0.04	0.05	0.04	0.04	0.04	0.03
PE38_4	0.05	0.04	0.04	0.05	0.05	0.08	0.06	0.07	0.07	0.05
PE38_3	0.06	0.07	0.06	0.08	0.09	0.07	0.07	0.07	0.08	0.05
PE38_2	0.08	0.09	0.09	0.10	0.11	0.11	0.11	0.10	0.11	0.09
PE40_3	0.05	0.05	0.04	0.05	0.06	0.05	0.05	0.04	0.04	0.04
PE40_2	0.10	0.09	0.09	0.11	0.12	0.11	0.12	0.11	0.11	0.08
PE42_4	0.02	0.02	0.02	0.02	0.03	0.02	0.02	0.02	0.02	0.01
PE42_3	0.09	0.08	0.08	0.09	0.11	0.10	0.09	0.10	0.10	0.07
PE42_2	0.09	0.08	0.08	0.11	0.12	0.12	0.11	0.11	0.11	0.08
PG32_1	0.53	0.60	0.79	0.69	0.81	0.52	0.59	0.54	0.53	0.42
PG32_0	0.23	0.26	0.25	0.41	0.38	0.25	0.37	0.27	0.26	0.18
PG34_4	8.69	9.14	10.46	10.02	10.91	13.18	11.52	12.40	12.88	8.67
PG34_3	2.40	2.58	2.39	2.61	3.16	2.71	2.94	2.87	2.46	2.18
PG34_2	2.03	1.93	2.03	2.16	2.47	2.04	1.92	1.96	1.91	1.56
PG34_1	1.18	1.31	1.22	1.31	1.48	1.12	1.11	1.12	1.08	0.73
PG34_0	0.02	0.00	0.03	0.00	0.04	0.05	0.03	0.00	0.04	0.00
lysoPG16_1	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.01	0.01	0.02
lysoPG16_0	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.02	0.01	0.01
lysoPG18_3	0.05	0.04	0.04	0.04	0.04	0.05	0.04	0.03	0.06	0.04
lysoPG18_2	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00

lysoPG18_1	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.00	0.00	0.01
PA34_6	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA34_4	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA34_3	0.15	0.16	0.28	0.16	0.17	0.13	0.10	0.12	0.11	0.08
PA34_2	0.16	0.18	0.26	0.14	0.21	0.15	0.10	0.13	0.18	0.08
PA34_1	0.11	0.10	0.10	0.06	0.06	0.15	0.26	0.19	0.10	0.14
PA36_6	0.05	0.05	0.08	0.04	0.05	0.02	0.01	0.03	0.02	0.02
PA36_5	0.10	0.09	0.18	0.07	0.11	0.05	0.04	0.06	0.06	0.04
PA36_4	0.11	0.08	0.18	0.09	0.12	0.06	0.06	0.06	0.08	0.05
PA36_3	0.03	0.03	0.06	0.04	0.02	0.02	0.01	0.03	0.01	0.03
PA36_2	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.00
PI34_4	0.02	0.02	0.01	0.02	0.03	0.00	0.00	0.01	0.01	0.01
PI34_3	1.28	1.48	1.45	1.68	2.15	1.45	1.50	1.34	1.56	1.19
PI34_2	1.52	1.64	1.68	1.88	2.35	1.98	2.15	1.89	2.21	1.56
PI34_1	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
PI36_6	0.07	0.06	0.08	0.10	0.11	0.07	0.12	0.08	0.11	0.07
PI36_5	0.12	0.11	0.11	0.12	0.15	0.10	0.11	0.11	0.11	0.09
PI36_4	0.14	0.11	0.11	0.16	0.15	0.16	0.13	0.14	0.15	0.12
PI36_3	0.16	0.13	0.15	0.16	0.21	0.18	0.19	0.16	0.16	0.14
PI36_2	0.11	0.11	0.08	0.12	0.13	0.13	0.12	0.11	0.12	0.09
PI36_1	0.01	0.01	0.01	0.01	0.00	0.02	0.02	0.01	0.01	0.01
PS34_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS34_3	0.07	0.07	0.08	0.08	0.10	0.08	0.08	0.09	0.08	0.06
PS34_2	0.08	0.08	0.08	0.08	0.10	0.11	0.10	0.11	0.12	0.07
PS34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS36_6	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
PS36_5	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PS36_4	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.01	0.01	0.01
PS36_3	0.04	0.05	0.04	0.04	0.05	0.04	0.04	0.04	0.05	0.04
PS36_2	0.03	0.03	0.04	0.03	0.03	0.04	0.04	0.03	0.04	0.03
PS36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_4	0.00	0.01	0.00	0.01	0.01	0.01	0.00	0.00	0.01	0.00
PS38_3	0.04	0.04	0.03	0.04	0.05	0.04	0.03	0.03	0.04	0.03
PS38_2	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.05	0.03
PS38_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_3	0.04	0.04	0.04	0.06	0.06	0.05	0.04	0.05	0.05	0.04
PS40_2	0.06	0.05	0.06	0.06	0.07	0.06	0.07	0.07	0.07	0.06
PS40_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS42_4	0.01	0.02	0.02	0.02	0.02	0.01	0.01	0.02	0.02	0.01
PS42_3	0.08	0.07	0.08	0.08	0.11	0.08	0.07	0.10	0.08	0.08
PS42_2	0.07	0.07	0.06	0.08	0.09	0.07	0.10	0.09	0.10	0.07
PS42_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS44_3	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
PS44_2	0.00	0.01	0.01	0.00	0.01	0.00	0.01	0.00	0.00	0.00

Table A-5 The original dataset for *fad6*

lipid	C1	C2	C3	C4	C5	T1	T2	T3	T4	T5
DGDG34_6	2.25	2.18	2.53	1.96	2.21	0.01	0.00	0.00	0.00	0.00
DGDG34_5	0.14	0.10	0.10	0.17	0.06	0.01	0.00	0.00	0.01	0.00

DGDG34_4	0.26	0.19	0.20	0.18	0.23	0.52	0.49	0.47	0.43	0.26
DGDG34_3	4.69	4.33	4.41	3.86	4.03	3.35	2.82	3.42	3.14	2.44
DGDG34_2	1.01	0.95	1.10	0.81	0.79	1.24	1.18	1.32	1.18	0.89
DGDG34_1	0.41	0.40	0.44	0.35	0.40	1.29	1.16	1.33	1.11	1.06
DGDG36_6	14.95	16.68	14.93	14.08	15.01	12.61	12.62	12.83	12.07	11.13
DGDG36_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DGDG36_4	0.46	0.46	0.38	0.46	0.43	3.74	3.54	3.53	4.07	3.69
DGDG36_3	0.22	0.18	0.20	0.13	0.16	0.00	0.00	0.00	0.00	0.00
DGDG36_2	0.01	0.00	0.00	0.00	0.00	0.25	0.21	0.26	0.23	0.30
DGDG36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
DGDG38_6	0.18	0.22	0.15	0.22	0.16	0.12	0.14	0.10	0.11	0.11
DGDG38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DGDG38_4	0.08	0.00	0.03	0.03	0.05	0.04	0.07	0.02	0.03	0.06
DGDG38_3	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG34_6	67.36	73.73	71.54	61.98	58.12	0.00	0.00	0.00	0.00	0.00
MGDG34_5	0.00	0.00	0.00	0.00	0.00	0.05	0.06	0.03	0.00	0.04
MGDG34_4	2.04	2.69	2.02	2.32	1.86	1.66	1.30	1.69	1.13	1.48
MGDG34_3	0.94	0.72	0.74	0.83	0.70	3.07	3.18	3.14	3.12	3.82
MGDG34_2	0.44	0.80	0.60	0.61	0.49	16.53	16.55	16.62	16.12	18.84
MGDG34_1	0.37	0.00	0.00	1.24	0.00	0.00	0.00	0.00	0.00	0.00
MGDG36_6	11.56	12.24	11.68	10.73	11.68	14.51	13.60	12.15	12.23	13.63
MGDG36_5	0.01	0.04	0.09	0.26	0.03	0.00	0.00	0.00	0.00	0.00
MGDG36_4	1.28	1.18	1.35	0.87	1.17	3.77	3.66	3.30	3.60	3.50
MGDG36_3	0.04	0.11	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00
MGDG36_2	0.05	0.00	0.03	0.00	0.01	0.27	0.25	0.21	0.21	0.19
MGDG36_1	0.02	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
MGDG38_6	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.00	0.00
MGDG38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_4	0.04	0.06	0.06	0.00	0.00	0.12	0.07	0.07	0.13	0.09
MGDG38_3	0.00	0.05	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00
PC32_0	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.02
PC34_4	0.12	0.12	0.12	0.14	0.16	0.36	0.40	0.38	0.37	0.36
PC34_3	2.45	2.47	2.33	2.81	3.40	2.30	2.43	2.24	2.27	2.24
PC34_2	3.24	3.21	3.12	3.53	4.13	3.48	3.74	3.26	3.51	3.40
PC34_1	0.53	0.50	0.47	0.57	0.67	0.78	0.79	0.79	0.84	0.80
PC36_6	1.71	1.81	1.78	2.18	2.61	1.45	1.49	1.52	1.44	1.39
PC36_5	4.31	4.46	4.35	5.20	6.01	3.83	4.02	3.91	3.89	3.85
PC36_4	3.42	3.33	3.35	3.87	4.52	4.11	4.37	3.87	4.16	4.08
PC36_3	1.43	1.43	1.32	1.57	1.81	1.92	1.98	1.85	2.00	2.08
PC36_2	0.58	0.56	0.51	0.65	0.74	0.68	0.72	0.61	0.67	0.64
PC36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC38_6	0.01	0.01	0.01	0.02	0.02	0.01	0.01	0.01	0.01	0.01
PC38_5	0.05	0.04	0.04	0.05	0.06	0.02	0.03	0.02	0.03	0.02
PC38_4	0.08	0.07	0.07	0.08	0.09	0.06	0.06	0.06	0.06	0.07
PC38_3	0.09	0.08	0.08	0.09	0.09	0.08	0.08	0.07	0.09	0.09
PC38_2	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.06
PC40_5	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC40_4	0.01	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00
PC40_3	0.01	0.00	0.01	0.01	0.01	0.00	0.00	0.01	0.01	0.01
PC40_2	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.00
LysoPC16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPC16_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
LysoPC18_3	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.02
LysoPC18_2	0.02	0.02	0.02	0.02	0.03	0.03	0.03	0.03	0.04	0.03

LysoPC18_1	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01
LysoPC18_0	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
LysoPE16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
LysoPE16_0	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.03	0.04	0.03
LysoPE18_3	0.02	0.02	0.02	0.02	0.03	0.02	0.02	0.02	0.03	0.02
LysoPE18_2	0.04	0.03	0.03	0.04	0.04	0.04	0.05	0.04	0.05	0.04
LysoPE18_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.00
PE34_4	0.05	0.05	0.05	0.06	0.06	0.12	0.13	0.11	0.13	0.12
PE34_3	2.74	2.87	2.76	3.33	3.79	2.60	2.80	2.43	2.66	2.51
PE34_2	4.12	4.02	3.89	4.67	5.26	4.43	4.61	4.01	4.54	4.30
PE34_1	0.00	0.00	0.00	0.00	0.00	0.04	0.04	0.06	0.06	0.05
PE36_6	0.75	0.74	0.72	0.92	1.05	0.61	0.62	0.62	0.62	0.59
PE36_5	2.19	2.14	2.13	2.67	2.97	2.21	2.30	2.06	2.17	2.09
PE36_4	2.31	2.28	2.19	2.70	2.95	2.94	3.01	2.57	2.85	2.79
PE36_3	0.59	0.56	0.52	0.66	0.72	0.74	0.77	0.67	0.74	0.69
PE36_2	0.29	0.28	0.26	0.34	0.35	0.26	0.27	0.20	0.26	0.24
PE36_1	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.02	0.01	0.01
PE38_6	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
PE38_5	0.03	0.03	0.03	0.04	0.04	0.02	0.02	0.02	0.02	0.02
PE38_4	0.05	0.04	0.04	0.05	0.05	0.03	0.04	0.03	0.04	0.04
PE38_3	0.06	0.07	0.06	0.08	0.09	0.07	0.07	0.06	0.07	0.06
PE38_2	0.08	0.09	0.09	0.10	0.11	0.09	0.08	0.08	0.08	0.08
PE40_3	0.05	0.05	0.04	0.05	0.06	0.03	0.04	0.03	0.03	0.03
PE40_2	0.10	0.09	0.09	0.11	0.12	0.08	0.08	0.07	0.08	0.08
PE42_4	0.02	0.02	0.02	0.02	0.03	0.02	0.02	0.02	0.02	0.02
PE42_3	0.09	0.08	0.08	0.09	0.11	0.09	0.09	0.07	0.09	0.09
PE42_2	0.09	0.08	0.08	0.11	0.12	0.09	0.10	0.07	0.10	0.09
PG32_1	0.53	0.60	0.79	0.69	0.81	0.45	0.34	0.47	0.44	0.50
PG32_0	0.23	0.26	0.25	0.41	0.38	0.29	0.31	0.27	0.24	0.21
PG34_4	8.69	9.14	10.46	10.02	10.91	0.33	0.36	0.38	0.42	0.35
PG34_3	2.40	2.58	2.39	2.61	3.16	0.90	0.70	0.87	0.86	0.85
PG34_2	2.03	1.93	2.03	2.16	2.47	11.07	10.63	11.20	12.03	11.42
PG34_1	1.18	1.31	1.22	1.31	1.48	2.55	3.17	2.34	2.77	2.48
PG34_0	0.02	0.00	0.03	0.00	0.04	0.03	0.00	0.00	0.00	0.01
lysoPG16_1	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
lysoPG16_0	0.01	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.00
lysoPG18_3	0.05	0.04	0.04	0.04	0.04	0.00	0.00	0.00	0.00	0.00
lysoPG18_2	0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
lysoPG18_1	0.00	0.01	0.01	0.01	0.00	0.05	0.05	0.05	0.05	0.05
PA34_6	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA34_4	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA34_3	0.15	0.16	0.28	0.16	0.17	0.16	0.12	0.11	0.19	0.13
PA34_2	0.16	0.18	0.26	0.14	0.21	0.23	0.15	0.18	0.29	0.18
PA34_1	0.11	0.10	0.10	0.06	0.06	0.08	0.10	0.06	0.08	0.06
PA36_6	0.05	0.05	0.08	0.04	0.05	0.04	0.03	0.03	0.04	0.04
PA36_5	0.10	0.09	0.18	0.07	0.11	0.09	0.07	0.10	0.13	0.08
PA36_4	0.11	0.08	0.18	0.09	0.12	0.13	0.09	0.10	0.12	0.12
PA36_3	0.03	0.03	0.06	0.04	0.02	0.04	0.02	0.04	0.05	0.03
PA36_2	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PI34_4	0.02	0.02	0.01	0.02	0.03	0.06	0.06	0.05	0.06	0.06
PI34_3	1.28	1.48	1.45	1.68	2.15	1.46	1.53	1.29	1.51	1.35
PI34_2	1.52	1.64	1.68	1.88	2.35	1.91	2.06	1.72	2.07	2.02
PI34_1	0.00	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.02	0.00
PI36_6	0.07	0.06	0.08	0.10	0.11	0.07	0.06	0.07	0.08	0.06

PI36_5	0.12	0.11	0.11	0.12	0.15	0.09	0.10	0.08	0.13	0.08
PI36_4	0.14	0.11	0.11	0.16	0.15	0.18	0.13	0.15	0.16	0.15
PI36_3	0.16	0.13	0.15	0.16	0.21	0.16	0.15	0.16	0.20	0.20
PI36_2	0.11	0.11	0.08	0.12	0.13	0.08	0.10	0.08	0.11	0.08
PI36_1	0.01	0.01	0.01	0.01	0.00	0.02	0.01	0.01	0.01	0.01
PS34_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS34_3	0.07	0.07	0.08	0.08	0.10	0.07	0.08	0.07	0.07	0.07
PS34_2	0.08	0.08	0.08	0.08	0.10	0.09	0.08	0.08	0.10	0.09
PS34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS36_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS36_5	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PS36_4	0.01	0.01	0.01	0.01	0.02	0.01	0.02	0.01	0.02	0.02
PS36_3	0.04	0.05	0.04	0.04	0.05	0.04	0.04	0.03	0.04	0.04
PS36_2	0.03	0.03	0.04	0.03	0.03	0.03	0.03	0.03	0.04	0.03
PS36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_4	0.00	0.01	0.00	0.01	0.01	0.01	0.01	0.00	0.01	0.01
PS38_3	0.04	0.04	0.03	0.04	0.05	0.04	0.04	0.04	0.04	0.03
PS38_2	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04
PS38_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_3	0.04	0.04	0.04	0.06	0.06	0.05	0.05	0.04	0.05	0.05
PS40_2	0.06	0.05	0.06	0.06	0.07	0.06	0.07	0.06	0.06	0.06
PS40_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS42_4	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.01
PS42_3	0.08	0.07	0.08	0.08	0.11	0.09	0.09	0.08	0.10	0.08
PS42_2	0.07	0.07	0.06	0.08	0.09	0.09	0.09	0.08	0.09	0.08
PS42_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS44_3	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
PS44_2	0.00	0.01	0.01	0.00	0.01	0.01	0.01	0.00	0.00	0.00

Table A-6 The original dataset for *fad7*

lipid	C1	C2	C3	C4	C5	T1	T2	T3	T4	T5
DGDG34_6	2.25	2.17	2.53	1.96	2.21	0.72	0.69	0.96	0.45	0.81
DGDG34_5	0.14	0.10	0.10	0.17	0.06	1.88	1.58	2.04	1.38	1.70
DGDG34_4	0.26	0.19	0.20	0.18	0.23	0.99	0.65	0.89	0.81	1.00
DGDG34_3	4.69	4.33	4.40	3.86	4.03	2.37	2.06	2.32	1.77	2.30
DGDG34_2	1.01	0.95	1.10	0.81	0.79	2.42	2.25	2.48	1.82	2.14
DGDG34_1	0.41	0.40	0.44	0.35	0.40	0.37	0.16	0.29	0.30	0.38
DGDG36_6	14.95	16.68	14.93	14.08	15.01	9.39	9.46	9.57	8.30	9.89
DGDG36_5	0.00	0.00	0.00	0.00	0.00	5.90	5.81	5.64	5.62	6.57
DGDG36_4	0.45	0.46	0.38	0.46	0.43	2.45	2.01	2.20	2.06	2.38
DGDG36_3	0.22	0.18	0.20	0.13	0.15	0.00	0.09	0.00	0.00	0.06
DGDG36_2	0.01	0.00	0.00	0.00	0.00	0.10	0.02	0.12	0.12	0.08
DGDG36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
DGDG38_6	0.18	0.22	0.15	0.22	0.16	0.09	0.09	0.02	0.12	0.10
DGDG38_5	0.00	0.00	0.00	0.00	0.00	0.03	0.03	0.01	0.01	0.04
DGDG38_4	0.08	0.00	0.02	0.02	0.05	0.01	0.00	0.02	0.05	0.00
DGDG38_3	0.00	0.01	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.00
MGDG34_6	67.36	73.73	71.54	61.98	58.12	21.02	23.09	20.25	16.03	18.93
MGDG34_5	0.00	0.00	0.00	0.00	0.00	23.51	21.63	21.32	18.85	19.61

MGDG34_4	2.04	2.69	2.02	2.32	1.86	13.08	12.59	9.44	9.49	11.65
MGDG34_3	0.94	0.72	0.74	0.83	0.70	0.66	0.88	0.97	0.90	0.99
MGDG34_2	0.44	0.80	0.60	0.61	0.49	0.85	0.81	0.57	0.64	0.63
MGDG34_1	0.37	0.00	0.00	1.24	0.00	0.00	0.00	0.34	0.17	0.00
MGDG36_6	11.56	12.24	11.68	10.73	11.67	5.16	5.31	4.75	4.63	5.63
MGDG36_5	0.01	0.04	0.09	0.26	0.03	3.98	2.92	3.10	3.68	3.29
MGDG36_4	1.28	1.18	1.35	0.87	1.17	1.35	2.03	1.33	1.57	1.84
MGDG36_3	0.04	0.11	0.00	0.11	0.00	0.24	0.24	0.18	0.39	0.37
MGDG36_2	0.05	0.00	0.03	0.00	0.01	0.05	0.11	0.10	0.03	0.18
MGDG36_1	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.07
MGDG38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_4	0.04	0.06	0.06	0.00	0.00	0.02	0.04	0.00	0.05	0.00
MGDG38_3	0.00	0.05	0.00	0.02	0.00	0.17	0.02	0.12	0.05	0.03
PC32_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PC34_4	0.11	0.11	0.12	0.13	0.16	0.20	0.20	0.21	0.20	0.20
PC34_3	2.45	2.47	2.33	2.81	3.40	1.87	2.02	2.04	1.83	1.94
PC34_2	3.24	3.21	3.12	3.53	4.13	3.80	3.82	3.83	3.63	3.75
PC34_1	0.53	0.50	0.47	0.57	0.66	0.56	0.50	0.48	0.50	0.50
PC36_6	1.71	1.81	1.78	2.18	2.61	1.11	1.34	1.27	1.05	1.17
PC36_5	4.31	4.46	4.35	5.19	6.01	4.34	4.78	4.40	4.18	4.39
PC36_4	3.42	3.33	3.35	3.87	4.52	4.62	4.68	4.44	4.42	4.51
PC36_3	1.43	1.43	1.32	1.57	1.81	1.78	1.70	1.52	1.68	1.67
PC36_2	0.58	0.56	0.51	0.65	0.74	0.61	0.64	0.61	0.63	0.63
PC36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC38_6	0.01	0.01	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.01
PC38_5	0.05	0.04	0.04	0.05	0.06	0.04	0.04	0.04	0.04	0.04
PC38_4	0.08	0.07	0.07	0.08	0.09	0.07	0.08	0.07	0.07	0.08
PC38_3	0.09	0.08	0.08	0.09	0.09	0.08	0.09	0.08	0.08	0.09
PC38_2	0.05	0.05	0.04	0.05	0.05	0.05	0.05	0.05	0.06	0.06
PC40_5	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC40_4	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.01
PC40_3	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.01	0.00
PC40_2	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.01
LysoPC16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPC16_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
LysoPC18_3	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
LysoPC18_2	0.02	0.02	0.02	0.02	0.03	0.03	0.04	0.04	0.04	0.04
LysoPC18_1	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01
LysoPC18_0	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
LysoPE16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPE16_0	0.04	0.03	0.04	0.04	0.04	0.04	0.04	0.05	0.04	0.04
LysoPE18_3	0.02	0.02	0.02	0.02	0.03	0.02	0.03	0.03	0.02	0.02
LysoPE18_2	0.04	0.03	0.03	0.03	0.04	0.05	0.05	0.05	0.05	0.05
LysoPE18_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
PE34_4	0.05	0.05	0.05	0.06	0.06	0.08	0.09	0.08	0.08	0.09
PE34_3	2.74	2.87	2.76	3.33	3.79	2.20	2.57	2.30	2.21	2.28
PE34_2	4.12	4.02	3.89	4.67	5.26	4.87	5.17	4.71	4.76	4.85
PE34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PE36_6	0.75	0.74	0.72	0.92	1.05	0.48	0.62	0.56	0.50	0.52
PE36_5	2.19	2.14	2.13	2.67	2.97	2.14	2.30	2.13	2.02	2.09
PE36_4	2.31	2.28	2.18	2.70	2.95	3.06	3.10	2.91	3.01	2.94
PE36_3	0.59	0.56	0.52	0.66	0.72	0.70	0.69	0.61	0.64	0.64
PE36_2	0.29	0.28	0.26	0.34	0.35	0.31	0.31	0.29	0.31	0.30

PE36_1	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.00	0.01
PE38_6	0.02	0.02	0.01	0.02	0.02	0.01	0.02	0.01	0.01	0.01
PE38_5	0.03	0.03	0.03	0.04	0.04	0.03	0.03	0.03	0.03	0.03
PE38_4	0.05	0.03	0.04	0.05	0.05	0.04	0.05	0.05	0.04	0.04
PE38_3	0.06	0.07	0.06	0.08	0.09	0.05	0.06	0.05	0.06	0.06
PE38_2	0.08	0.09	0.09	0.10	0.11	0.08	0.09	0.10	0.09	0.09
PE40_3	0.05	0.05	0.04	0.05	0.06	0.04	0.05	0.05	0.04	0.04
PE40_2	0.10	0.09	0.09	0.11	0.12	0.11	0.12	0.12	0.12	0.12
PE42_4	0.02	0.02	0.02	0.02	0.03	0.02	0.03	0.02	0.02	0.03
PE42_3	0.09	0.08	0.08	0.09	0.11	0.09	0.11	0.11	0.10	0.10
PE42_2	0.09	0.08	0.07	0.11	0.12	0.13	0.12	0.11	0.12	0.13
PG32_1	0.53	0.60	0.79	0.69	0.80	0.47	0.51	0.51	0.44	0.45
PG32_0	0.23	0.26	0.25	0.41	0.38	0.17	0.21	0.25	0.27	0.22
PG34_4	8.69	9.14	10.46	10.02	10.91	6.83	7.15	6.60	6.37	6.77
PG34_3	2.40	2.58	2.39	2.61	3.16	3.89	4.01	3.45	3.86	3.81
PG34_2	2.02	1.93	2.03	2.16	2.47	2.63	2.39	2.33	2.57	2.54
PG34_1	1.18	1.31	1.22	1.31	1.48	1.34	1.24	1.19	1.32	1.37
PG34_0	0.02	0.00	0.03	0.00	0.04	0.00	0.00	0.00	0.01	0.00
lysoPG16_1	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
lysoPG16_0	0.01	0.01	0.01	0.00	0.01	0.00	0.01	0.01	0.01	0.01
lysoPG18_3	0.05	0.04	0.03	0.04	0.04	0.03	0.02	0.03	0.02	0.03
lysoPG18_2	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.01
lysoPG18_1	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01
PA34_6	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA34_4	0.00	0.01	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA34_3	0.15	0.16	0.28	0.16	0.17	0.12	0.17	0.19	0.13	0.14
PA34_2	0.16	0.18	0.26	0.14	0.21	0.20	0.28	0.26	0.24	0.20
PA34_1	0.11	0.10	0.10	0.06	0.06	0.07	0.07	0.05	0.05	0.07
PA36_6	0.05	0.04	0.08	0.04	0.05	0.03	0.06	0.04	0.03	0.04
PA36_5	0.10	0.09	0.18	0.07	0.11	0.09	0.14	0.12	0.11	0.10
PA36_4	0.10	0.08	0.18	0.09	0.12	0.12	0.18	0.17	0.16	0.15
PA36_3	0.03	0.03	0.06	0.04	0.02	0.03	0.05	0.04	0.03	0.03
PA36_2	0.01	0.01	0.01	0.01	0.01	0.02	0.00	0.02	0.01	0.01
PI34_4	0.02	0.02	0.01	0.02	0.03	0.03	0.03	0.03	0.03	0.03
PI34_3	1.28	1.48	1.45	1.68	2.15	1.15	1.30	1.11	1.25	1.04
PI34_2	1.52	1.64	1.68	1.88	2.35	2.17	2.12	1.84	2.24	2.17
PI34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PI36_6	0.07	0.06	0.08	0.09	0.11	0.06	0.06	0.05	0.05	0.04
PI36_5	0.12	0.11	0.11	0.12	0.15	0.11	0.13	0.13	0.11	0.13
PI36_4	0.14	0.11	0.11	0.16	0.15	0.17	0.16	0.16	0.17	0.15
PI36_3	0.16	0.13	0.15	0.16	0.21	0.14	0.16	0.14	0.13	0.14
PI36_2	0.11	0.11	0.08	0.12	0.13	0.12	0.12	0.11	0.11	0.11
PI36_1	0.01	0.00	0.01	0.01	0.00	0.01	0.02	0.00	0.00	0.03
PS34_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS34_3	0.07	0.07	0.08	0.08	0.10	0.05	0.07	0.06	0.07	0.06
PS34_2	0.08	0.08	0.08	0.07	0.10	0.09	0.10	0.10	0.10	0.11
PS34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS36_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS36_5	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PS36_4	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.01	0.02	0.01
PS36_3	0.04	0.05	0.04	0.04	0.05	0.03	0.05	0.04	0.04	0.04
PS36_2	0.03	0.03	0.03	0.03	0.03	0.03	0.04	0.04	0.04	0.03
PS36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

PS38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_4	0.00	0.01	0.00	0.01	0.01	0.00	0.01	0.01	0.01	0.01
PS38_3	0.04	0.04	0.03	0.04	0.05	0.03	0.04	0.04	0.03	0.04
PS38_2	0.04	0.04	0.04	0.04	0.04	0.04	0.05	0.04	0.05	0.04
PS38_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_3	0.04	0.04	0.04	0.06	0.06	0.04	0.04	0.04	0.04	0.03
PS40_2	0.06	0.05	0.06	0.06	0.07	0.06	0.07	0.06	0.08	0.07
PS40_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS42_4	0.01	0.02	0.02	0.02	0.02	0.01	0.02	0.01	0.01	0.01
PS42_3	0.08	0.07	0.08	0.08	0.11	0.08	0.09	0.08	0.08	0.08
PS42_2	0.07	0.07	0.06	0.08	0.09	0.08	0.09	0.07	0.09	0.10
PS42_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS44_3	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
PS44_2	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00

Table A-7 The original dataset for *sfd1*

lipid	C1	C2	C3	C4	C5	T1	T2	T3	T4	T5
DGDG34_6	2.21	2.71	3.29	2.67	2.32	0.62	0.93	0.84	0.77	0.56
DGDG34_5	0.05	0.00	0.09	0.05	0.05	0.08	0.09	0.12	0.19	0.08
DGDG34_4	0.14	0.17	0.21	0.19	0.15	0.10	0.21	0.14	0.10	0.10
DGDG34_3	3.46	4.28	4.65	4.59	3.59	2.81	3.11	3.04	3.42	2.28
DGDG34_2	0.61	0.66	0.75	0.78	0.57	0.00	0.08	0.00	0.00	0.08
DGDG34_1	0.21	0.35	0.31	0.30	0.25	0.09	0.08	0.09	0.13	0.05
DGDG36_6	11.21	12.35	13.46	14.73	12.38	17.89	22.29	22.04	22.26	16.90
DGDG36_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DGDG36_4	0.31	0.32	0.30	0.37	0.48	0.36	0.51	0.43	0.51	0.41
DGDG36_3	0.10	0.21	0.16	0.17	0.12	0.02	0.11	0.07	0.08	0.10
DGDG36_2	0.05	0.00	0.00	0.00	0.03	0.00	0.01	0.00	0.00	0.00
DGDG36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DGDG38_6	0.17	0.12	0.12	0.14	0.16	0.24	0.24	0.28	0.16	0.26
DGDG38_5	0.00	0.00	0.00	0.01	0.00	0.00	0.02	0.00	0.09	0.00
DGDG38_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.01
DGDG38_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG34_6	51.35	54.56	58.91	60.60	59.56	24.28	29.29	27.36	25.47	23.88
MGDG34_5	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
MGDG34_4	1.50	1.65	1.50	1.96	1.64	0.54	0.54	0.91	0.74	0.69
MGDG34_3	0.49	0.48	0.74	0.60	0.65	0.48	0.60	0.43	0.42	0.20
MGDG34_2	0.34	0.36	0.34	0.40	0.30	0.02	0.18	0.11	0.02	0.03
MGDG34_1	0.64	0.19	0.34	0.00	0.00	0.00	0.74	0.06	0.00	0.00
MGDG36_6	9.11	9.41	9.93	10.51	9.21	24.94	34.51	29.40	31.41	26.42
MGDG36_5	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00
MGDG36_4	0.39	0.43	0.56	0.40	0.56	0.40	0.90	0.74	0.88	0.86
MGDG36_3	0.00	0.04	0.03	0.04	0.00	0.02	0.09	0.03	0.13	0.01
MGDG36_2	0.00	0.00	0.00	0.06	0.00	0.00	0.01	0.00	0.00	0.00
MGDG36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_6	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00
MGDG38_5	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.00	0.00	0.00
MGDG38_4	0.00	0.00	0.03	0.00	0.00	0.03	0.13	0.16	0.00	0.03
MGDG38_3	0.07	0.05	0.00	0.00	0.00	0.00	0.04	0.00	0.07	0.04
PC32_0	0.01	0.01	0.02	0.01	0.01	0.02	0.02	0.01	0.01	0.01
PC34_4	0.11	0.10	0.13	0.12	0.13	0.10	0.16	0.11	0.09	0.09

PC34_3	2.40	2.15	2.71	2.42	2.76	2.06	3.15	2.15	1.90	1.69
PC34_2	2.61	2.44	2.71	2.74	3.02	2.34	3.72	2.67	2.34	2.14
PC34_1	0.55	0.58	0.62	0.61	0.65	1.04	1.47	1.15	0.90	0.96
PC36_6	2.13	1.92	2.54	2.11	2.47	1.85	3.01	1.92	1.73	1.61
PC36_5	4.16	3.82	4.52	4.18	4.90	3.80	6.11	4.24	3.71	3.49
PC36_4	2.96	2.84	3.12	3.15	3.47	3.57	5.57	4.04	3.43	3.46
PC36_3	1.36	1.36	1.46	1.58	1.61	2.45	3.81	2.66	2.33	2.54
PC36_2	0.49	0.52	0.50	0.58	0.59	1.02	1.53	1.13	0.86	1.04
PC36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC38_6	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PC38_5	0.03	0.03	0.03	0.03	0.04	0.03	0.05	0.03	0.03	0.03
PC38_4	0.05	0.05	0.05	0.05	0.05	0.06	0.09	0.06	0.06	0.06
PC38_3	0.05	0.05	0.05	0.06	0.06	0.07	0.10	0.07	0.06	0.07
PC38_2	0.02	0.03	0.03	0.03	0.03	0.04	0.06	0.04	0.03	0.03
PC40_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC40_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00
PC40_3	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.01
PC40_2	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
LysoPC16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPC16_0	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.01	0.01	0.01
LysoPC18_3	0.03	0.03	0.04	0.03	0.04	0.03	0.05	0.03	0.03	0.02
LysoPC18_2	0.03	0.03	0.03	0.03	0.03	0.03	0.05	0.03	0.04	0.03
LysoPC18_1	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.01	0.02
LysoPC18_0	0.00	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00
LysoPE16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPE16_0	0.04	0.04	0.05	0.04	0.04	0.04	0.07	0.04	0.04	0.04
LysoPE18_3	0.04	0.03	0.04	0.03	0.04	0.03	0.06	0.03	0.03	0.03
LysoPE18_2	0.04	0.04	0.04	0.05	0.05	0.05	0.09	0.05	0.04	0.05
LysoPE18_1	0.01	0.01	0.00	0.01	0.01	0.01	0.02	0.01	0.01	0.01
PE34_4	0.05	0.04	0.07	0.06	0.06	0.05	0.08	0.05	0.05	0.04
PE34_3	3.18	2.77	3.75	3.22	3.61	2.92	4.40	2.91	2.70	2.53
PE34_2	3.63	3.31	4.03	3.84	4.21	4.02	5.86	4.10	3.81	3.71
PE34_1	0.07	0.05	0.07	0.04	0.05	0.32	0.47	0.34	0.25	0.29
PE36_6	0.96	0.83	1.19	0.97	1.07	0.83	1.31	0.88	0.75	0.76
PE36_5	2.21	2.01	2.61	2.36	2.57	2.34	3.61	2.53	2.19	2.20
PE36_4	2.04	1.86	2.30	2.20	2.37	2.73	4.17	2.93	2.53	2.56
PE36_3	0.65	0.60	0.76	0.70	0.76	1.16	1.74	1.31	1.02	1.12
PE36_2	0.26	0.23	0.26	0.28	0.30	0.35	0.54	0.35	0.31	0.34
PE36_1	0.01	0.01	0.01	0.01	0.01	0.03	0.03	0.02	0.02	0.02
PE38_6	0.02	0.02	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02
PE38_5	0.02	0.02	0.03	0.03	0.03	0.03	0.04	0.03	0.03	0.03
PE38_4	0.03	0.03	0.03	0.04	0.04	0.05	0.07	0.04	0.04	0.04
PE38_3	0.05	0.06	0.07	0.07	0.07	0.07	0.10	0.07	0.06	0.06
PE38_2	0.07	0.08	0.09	0.09	0.09	0.08	0.13	0.09	0.08	0.08
PE40_3	0.05	0.04	0.05	0.05	0.05	0.04	0.06	0.04	0.03	0.03
PE40_2	0.08	0.07	0.08	0.09	0.09	0.08	0.12	0.08	0.08	0.08
PE42_4	0.02	0.02	0.03	0.02	0.03	0.02	0.03	0.02	0.02	0.02
PE42_3	0.10	0.08	0.09	0.09	0.10	0.08	0.13	0.08	0.09	0.08
PE42_2	0.09	0.08	0.10	0.10	0.11	0.10	0.16	0.11	0.09	0.10
PG32_1	0.61	0.53	0.70	0.69	0.64	0.94	1.30	0.99	0.77	0.88
PG32_0	0.25	0.25	0.34	0.24	0.31	0.28	0.51	0.20	0.25	0.26
PG34_4	7.87	7.53	8.61	8.68	9.31	8.46	11.31	8.03	7.75	7.75
PG34_3	1.74	1.48	1.79	1.76	1.77	1.44	2.14	1.57	1.33	1.40
PG34_2	1.36	1.28	1.33	1.59	1.51	1.36	1.72	1.24	1.15	1.19

PG34_1	0.80	0.74	0.86	0.95	0.97	0.61	0.71	0.49	0.46	0.59
PG34_0	0.03	0.01	0.02	0.00	0.02	0.00	0.00	0.00	0.01	0.02
lysoPG16_1	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
lysoPG16_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
lysoPG18_3	0.04	0.06	0.05	0.05	0.05	0.07	0.07	0.04	0.04	0.04
lysoPG18_2	0.00	0.01	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00
lysoPG18_1	0.00	0.01	0.01	0.00	0.01	0.00	0.01	0.00	0.00	0.00
PA34_6	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
PA34_4	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
PA34_3	0.17	0.14	0.23	0.20	0.24	0.12	0.36	0.21	0.18	0.18
PA34_2	0.18	0.14	0.20	0.21	0.21	0.12	0.37	0.24	0.17	0.16
PA34_1	0.04	0.06	0.05	0.05	0.04	0.10	0.08	0.08	0.07	0.08
PA36_6	0.05	0.07	0.07	0.07	0.07	0.05	0.15	0.08	0.06	0.05
PA36_5	0.12	0.10	0.14	0.13	0.14	0.08	0.25	0.18	0.12	0.13
PA36_4	0.13	0.10	0.12	0.12	0.14	0.10	0.29	0.19	0.15	0.11
PA36_3	0.04	0.04	0.05	0.05	0.06	0.05	0.11	0.08	0.06	0.07
PA36_2	0.01	0.01	0.02	0.01	0.02	0.01	0.04	0.03	0.02	0.02
PI34_4	0.01	0.02	0.02	0.02	0.01	0.01	0.04	0.02	0.01	0.01
PI34_3	1.47	1.36	1.78	1.54	1.66	1.50	2.51	1.55	1.48	1.35
PI34_2	1.33	1.24	1.42	1.47	1.47	1.63	2.76	1.65	1.67	1.52
PI34_1	0.00	0.00	0.02	0.01	0.01	0.11	0.14	0.10	0.08	0.11
PI36_6	0.09	0.09	0.10	0.08	0.09	0.11	0.14	0.09	0.07	0.08
PI36_5	0.09	0.12	0.10	0.10	0.12	0.11	0.20	0.12	0.12	0.11
PI36_4	0.10	0.09	0.12	0.12	0.12	0.17	0.25	0.16	0.13	0.15
PI36_3	0.15	0.15	0.14	0.15	0.15	0.18	0.41	0.19	0.17	0.18
PI36_2	0.08	0.09	0.06	0.09	0.11	0.10	0.15	0.09	0.08	0.11
PI36_1	0.01	0.00	0.00	0.00	0.00	0.02	0.01	0.02	0.01	0.01
PS34_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS34_3	0.08	0.07	0.10	0.09	0.10	0.07	0.13	0.07	0.06	0.06
PS34_2	0.07	0.07	0.07	0.07	0.08	0.08	0.12	0.08	0.08	0.06
PS34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01
PS36_6	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS36_5	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PS36_4	0.01	0.01	0.01	0.01	0.02	0.01	0.02	0.01	0.02	0.01
PS36_3	0.03	0.04	0.04	0.04	0.04	0.03	0.05	0.04	0.03	0.03
PS36_2	0.02	0.02	0.03	0.03	0.03	0.03	0.04	0.03	0.02	0.02
PS36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_4	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.01
PS38_3	0.03	0.03	0.04	0.03	0.04	0.02	0.05	0.03	0.03	0.02
PS38_2	0.03	0.03	0.03	0.03	0.03	0.03	0.05	0.03	0.02	0.03
PS38_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_3	0.05	0.04	0.06	0.05	0.05	0.04	0.08	0.05	0.04	0.04
PS40_2	0.05	0.04	0.05	0.05	0.05	0.05	0.09	0.06	0.05	0.05
PS40_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS42_4	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.01	0.02	0.01
PS42_3	0.08	0.08	0.10	0.08	0.10	0.09	0.15	0.10	0.08	0.09
PS42_2	0.06	0.06	0.07	0.06	0.07	0.08	0.14	0.08	0.08	0.08
PS42_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS44_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS44_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table A-8 The original dataset for *sfd2*

lipid	C1	C2	C3	C4	C5	T1	T2	T3	T4	T5
DGDG34_6	2.72	2.37	3.22	3.62	2.35	0.53	0.73	0.81	0.79	0.64
DGDG34_5	0.25	0.18	0.32	0.52	0.28	0.30	0.36	0.57	0.34	0.57
DGDG34_4	0.18	0.17	0.19	0.23	0.17	0.22	0.21	0.27	0.26	0.26
DGDG34_3	6.26	4.10	5.69	7.68	4.31	5.21	7.39	9.30	8.83	9.10
DGDG34_2	1.45	0.92	1.11	1.60	0.86	0.00	0.00	0.00	0.00	0.00
DGDG34_1	0.22	0.26	0.31	0.38	0.24	0.08	0.10	0.15	0.12	0.09
DGDG36_6	21.92	17.10	19.53	23.71	16.36	16.37	20.05	24.80	18.95	18.18
DGDG36_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DGDG36_4	0.51	0.31	0.40	0.47	0.34	0.39	0.49	0.69	0.65	0.47
DGDG36_3	0.35	0.23	0.24	0.40	0.19	0.43	0.53	0.62	1.38	0.76
DGDG36_2	0.00	0.00	0.01	0.00	0.02	0.02	0.01	0.05	0.00	0.12
DGDG36_1	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.03	0.02	0.05
DGDG38_6	0.18	0.04	0.11	0.07	0.06	0.18	0.36	0.29	0.29	0.29
DGDG38_5	0.00	0.00	0.00	0.00	0.03	0.01	0.00	0.00	0.00	0.00
DGDG38_4	0.04	0.01	0.00	0.04	0.01	0.12	0.04	0.05	0.00	0.14
DGDG38_3	0.00	0.00	0.00	0.00	0.01	0.00	0.04	0.00	0.03	0.00
MGDG34_6	93.22	84.88	98.40	105.88	74.46	9.85	10.22	11.72	12.22	9.07
MGDG34_5	0.00	0.00	0.00	0.00	0.00	0.52	0.44	0.68	0.42	1.09
MGDG34_4	0.58	0.39	0.64	0.83	0.32	0.55	0.50	0.62	0.76	0.39
MGDG34_3	0.62	0.48	0.55	0.54	0.52	3.10	3.34	3.82	5.71	4.94
MGDG34_2	0.09	0.09	0.13	0.10	0.04	0.04	0.00	0.00	0.00	0.00
MGDG34_1	0.45	0.00	0.00	0.00	0.21	0.00	0.00	0.00	0.00	0.18
MGDG36_6	20.26	15.46	18.83	20.41	15.42	35.60	50.50	47.15	50.38	46.60
MGDG36_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG36_4	1.15	0.88	0.79	0.96	1.07	0.91	1.27	1.43	1.86	1.45
MGDG36_3	0.00	0.00	0.00	0.02	0.00	0.20	0.25	0.41	0.99	0.00
MGDG36_2	0.00	0.00	0.00	0.00	0.00	0.01	0.05	0.07	0.12	0.17
MGDG36_1	0.02	0.00	0.01	0.00	0.00	0.00	0.00	0.02	0.00	0.00
MGDG38_6	0.09	0.01	0.02	0.03	0.00	0.04	0.09	0.10	0.11	0.30
MGDG38_5	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.03
MGDG38_4	0.08	0.05	0.02	0.07	0.14	0.32	0.44	0.40	0.66	0.86
MGDG38_3	0.00	0.26	0.06	0.48	0.11	0.00	0.01	0.00	0.00	0.00
PC32_0	0.02	0.02	0.02	0.03	0.02	0.02	0.03	0.04	0.03	0.03
PC34_4	0.17	0.15	0.15	0.17	0.13	0.07	0.11	0.13	0.09	0.11
PC34_3	3.84	3.25	3.58	3.97	2.94	2.60	4.89	6.11	5.75	4.86
PC34_2	3.57	2.89	3.15	3.52	2.64	1.75	3.30	3.64	2.92	3.32
PC34_1	0.18	0.13	0.14	0.22	0.11	0.11	0.14	0.15	0.07	0.17
PC36_6	3.03	2.93	2.89	3.39	2.36	1.87	3.29	3.84	2.77	2.96
PC36_5	5.70	4.80	5.00	5.94	4.16	2.14	4.01	4.54	2.63	3.93
PC36_4	3.52	2.82	2.94	3.58	2.56	1.23	2.31	2.24	1.27	2.28
PC36_3	0.84	0.69	0.74	0.94	0.61	1.25	2.13	2.30	2.86	1.58
PC36_2	0.44	0.35	0.37	0.47	0.32	0.78	1.39	1.43	1.64	0.83
PC36_1	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
PC38_6	0.02	0.01	0.02	0.02	0.01	0.01	0.02	0.03	0.02	0.02
PC38_5	0.04	0.04	0.04	0.04	0.03	0.03	0.06	0.05	0.04	0.05
PC38_4	0.07	0.06	0.05	0.07	0.05	0.05	0.10	0.08	0.09	0.07
PC38_3	0.06	0.05	0.05	0.06	0.05	0.05	0.09	0.08	0.08	0.07
PC38_2	0.03	0.02	0.02	0.03	0.02	0.02	0.04	0.04	0.04	0.03
PC40_5	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.00
PC40_4	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PC40_3	0.01	0.00	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01

PC40_2	0.01	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01
LysoPC16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPC16_0	0.01	0.01	0.01	0.01	0.01	0.02	0.01	0.02	0.03	0.03
LysoPC18_3	0.01	0.02	0.01	0.02	0.01	0.03	0.02	0.02	0.02	0.02
LysoPC18_2	0.01	0.02	0.01	0.02	0.01	0.02	0.01	0.02	0.01	0.03
LysoPC18_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPC18_0	0.00	0.00	0.00	0.00	0.00	0.02	0.02	0.01	0.03	0.01
LysoPE16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPE16_0	0.04	0.03	0.04	0.04	0.02	0.03	0.04	0.05	0.06	0.07
LysoPE18_3	0.01	0.02	0.02	0.02	0.02	0.03	0.02	0.03	0.03	0.03
LysoPE18_2	0.03	0.02	0.03	0.03	0.02	0.03	0.03	0.03	0.04	0.04
LysoPE18_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PE34_4	0.06	0.06	0.06	0.07	0.05	0.04	0.06	0.07	0.06	0.05
PE34_3	3.57	3.24	3.30	3.79	2.71	3.13	4.99	6.42	6.24	5.08
PE34_2	4.69	3.85	4.11	4.58	3.51	3.09	4.95	5.35	4.45	4.65
PE34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PE36_6	0.69	0.72	0.67	0.82	0.54	0.56	1.01	1.25	1.21	0.96
PE36_5	2.28	2.03	2.04	2.44	1.69	1.43	2.47	2.80	2.49	2.35
PE36_4	2.25	1.89	1.98	2.33	1.67	1.26	2.20	2.37	1.96	2.03
PE36_3	0.51	0.41	0.45	0.49	0.36	0.86	1.31	1.53	1.71	0.95
PE36_2	0.37	0.31	0.33	0.38	0.28	0.76	1.19	1.23	1.45	0.68
PE36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PE38_6	0.02	0.02	0.02	0.02	0.02	0.01	0.03	0.03	0.03	0.03
PE38_5	0.03	0.02	0.02	0.03	0.02	0.03	0.05	0.05	0.04	0.04
PE38_4	0.04	0.04	0.04	0.04	0.03	0.04	0.08	0.06	0.06	0.05
PE38_3	0.04	0.04	0.04	0.06	0.04	0.07	0.10	0.09	0.12	0.08
PE38_2	0.06	0.06	0.05	0.06	0.05	0.10	0.13	0.14	0.16	0.07
PE40_3	0.05	0.05	0.05	0.06	0.04	0.08	0.12	0.12	0.14	0.09
PE40_2	0.15	0.12	0.13	0.16	0.12	0.16	0.24	0.24	0.24	0.19
PE42_4	0.04	0.03	0.03	0.04	0.03	0.02	0.04	0.03	0.02	0.03
PE42_3	0.08	0.07	0.08	0.09	0.06	0.05	0.09	0.08	0.09	0.09
PE42_2	0.12	0.11	0.14	0.13	0.11	0.09	0.18	0.13	0.17	0.16
PG32_1	1.03	0.94	0.83	1.02	0.85	0.47	0.57	0.65	0.65	0.68
PG32_0	0.38	0.40	0.38	0.35	0.27	0.48	0.41	0.76	0.63	0.61
PG34_4	17.98	13.78	15.32	15.42	13.36	8.99	12.59	14.22	9.86	10.83
PG34_3	4.09	2.91	3.19	3.31	2.41	3.75	5.36	5.92	4.14	5.77
PG34_2	1.95	1.26	1.44	1.61	1.26	1.83	2.67	2.80	2.62	2.80
PG34_1	0.63	0.31	0.43	0.71	0.44	0.77	1.14	1.42	1.42	1.50
PG34_0	0.02	0.02	0.00	0.00	0.00	0.26	0.27	0.43	0.56	0.45
lysoPG16_1	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.02
lysoPG16_0	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.01	0.00
lysoPG18_3	0.02	0.02	0.02	0.03	0.01	0.03	0.02	0.02	0.00	0.02
lysoPG18_2	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
lysoPG18_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA34_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA34_4	0.02	0.00	0.02	0.00	0.01	0.24	0.02	0.00	0.02	0.21
PA34_3	0.18	0.23	0.19	0.46	0.30	2.49	0.25	0.30	0.33	1.34
PA34_2	0.23	0.21	0.19	0.40	0.25	1.99	0.15	0.19	0.16	1.00
PA34_1	0.00	0.00	0.00	0.00	0.01	0.02	0.04	0.00	0.03	0.06
PA36_6	0.05	0.08	0.06	0.11	0.09	0.80	0.08	0.07	0.08	0.26
PA36_5	0.14	0.13	0.08	0.22	0.18	1.33	0.10	0.09	0.09	0.44
PA36_4	0.09	0.07	0.06	0.17	0.15	0.90	0.08	0.05	0.08	0.29
PA36_3	0.04	0.02	0.02	0.04	0.04	0.52	0.06	0.05	0.08	0.43
PA36_2	0.01	0.00	0.00	0.01	0.02	0.23	0.03	0.03	0.08	0.27

PI34_4	0.00	0.01	0.02	0.02	0.02	0.00	0.01	0.01	0.01	0.01
PI34_3	2.44	2.14	2.17	2.40	2.11	1.99	2.51	2.92	2.56	2.59
PI34_2	2.44	2.02	2.06	2.26	1.95	1.65	2.12	2.17	1.74	2.06
PI34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PI36_6	0.09	0.11	0.14	0.14	0.12	0.09	0.09	0.10	0.06	0.08
PI36_5	0.11	0.11	0.09	0.13	0.09	0.06	0.08	0.07	0.04	0.10
PI36_4	0.09	0.08	0.05	0.08	0.07	0.06	0.04	0.04	0.02	0.07
PI36_3	0.11	0.15	0.11	0.17	0.12	0.25	0.33	0.31	0.36	0.22
PI36_2	0.09	0.09	0.09	0.10	0.10	0.15	0.28	0.23	0.32	0.17
PI36_1	0.01	0.00	0.01	0.04	0.00	0.02	0.00	0.05	0.00	0.06
PS34_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS34_3	0.16	0.14	0.15	0.18	0.13	0.11	0.16	0.21	0.17	0.16
PS34_2	0.16	0.14	0.17	0.19	0.13	0.10	0.15	0.17	0.12	0.14
PS34_1	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
PS36_6	0.01	0.00	0.01	0.01	0.00	0.01	0.01	0.01	0.00	0.00
PS36_5	0.01	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.01	0.01
PS36_4	0.01	0.01	0.02	0.02	0.01	0.01	0.02	0.02	0.01	0.01
PS36_3	0.07	0.06	0.07	0.08	0.05	0.07	0.11	0.11	0.13	0.09
PS36_2	0.06	0.04	0.05	0.06	0.04	0.04	0.07	0.06	0.06	0.06
PS36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_3	0.05	0.04	0.04	0.05	0.04	0.04	0.07	0.07	0.06	0.06
PS38_2	0.05	0.03	0.04	0.05	0.04	0.04	0.05	0.06	0.04	0.05
PS38_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00
PS40_3	0.06	0.05	0.05	0.06	0.04	0.06	0.10	0.11	0.10	0.11
PS40_2	0.08	0.06	0.06	0.07	0.05	0.06	0.10	0.11	0.10	0.08
PS40_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS42_4	0.03	0.02	0.03	0.03	0.02	0.01	0.03	0.03	0.02	0.03
PS42_3	0.16	0.13	0.14	0.15	0.12	0.09	0.15	0.17	0.17	0.19
PS42_2	0.11	0.10	0.12	0.13	0.09	0.08	0.11	0.11	0.14	0.14
PS42_1	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
PS44_3	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.01
PS44_2	0.00	0.01	0.01	0.01	0.00	0.00	0.01	0.01	0.01	0.01

Table A-9 The original dataset for *sfd3*

lipid	C1	C2	C3	C4	C5	T1	T2	T3	T4	T5
DGDG34_6	2.21	2.71	3.29	2.67	2.32	0.00	0.00	0.02	0.00	0.00
DGDG34_5	0.05	0.00	0.09	0.05	0.05	0.00	0.00	0.00	0.00	0.00
DGDG34_4	0.14	0.17	0.21	0.19	0.15	0.59	0.45	0.39	0.32	0.41
DGDG34_3	3.46	4.28	4.65	4.59	3.59	3.31	3.05	2.52	2.66	3.05
DGDG34_2	0.61	0.66	0.75	0.78	0.57	1.37	1.34	1.04	1.06	1.24
DGDG34_1	0.21	0.35	0.31	0.30	0.25	1.96	2.00	1.37	1.44	1.76
DGDG36_6	11.21	12.35	13.46	14.73	12.38	11.60	11.65	11.62	10.69	11.87
DGDG36_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DGDG36_4	0.31	0.32	0.30	0.37	0.48	3.09	3.05	3.28	3.19	3.49
DGDG36_3	0.10	0.21	0.16	0.17	0.12	0.13	0.00	0.01	0.09	0.00
DGDG36_2	0.05	0.00	0.00	0.00	0.03	0.15	0.26	0.18	0.23	0.31
DGDG36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00
DGDG38_6	0.17	0.12	0.12	0.14	0.16	0.16	0.19	0.26	0.18	0.10

DGDG38_5	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
DGDG38_4	0.00	0.00	0.00	0.00	0.00	0.03	0.05	0.03	0.04	0.04
DGDG38_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00
MGDG34_6	51.35	54.56	58.91	60.60	59.56	0.00	0.00	0.00	0.00	0.02
MGDG34_5	0.00	0.00	0.00	0.00	0.00	0.10	0.14	0.00	0.02	0.03
MGDG34_4	1.50	1.65	1.50	1.96	1.64	1.80	1.70	1.49	1.73	1.72
MGDG34_3	0.49	0.48	0.74	0.60	0.65	2.83	2.64	3.25	2.48	3.10
MGDG34_2	0.34	0.36	0.34	0.40	0.30	18.41	18.43	19.41	18.13	18.82
MGDG34_1	0.64	0.19	0.34	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG36_6	9.11	9.41	9.93	10.51	9.21	14.52	13.39	13.56	13.48	13.97
MGDG36_5	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.04
MGDG36_4	0.39	0.43	0.56	0.40	0.56	3.91	3.49	3.36	3.40	4.14
MGDG36_3	0.00	0.04	0.03	0.04	0.00	0.00	0.00	0.00	0.00	0.00
MGDG36_2	0.00	0.00	0.00	0.06	0.00	0.24	0.32	0.13	0.19	0.14
MGDG36_1	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
MGDG38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.02	0.00	0.02
MGDG38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MGDG38_4	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.16
MGDG38_3	0.07	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC32_0	0.01	0.01	0.02	0.01	0.01	0.02	0.02	0.02	0.02	0.02
PC34_4	0.11	0.10	0.13	0.12	0.13	0.37	0.31	0.34	0.33	0.37
PC34_3	2.40	2.15	2.71	2.42	2.76	2.04	1.86	1.97	1.93	2.07
PC34_2	2.61	2.44	2.71	2.74	3.02	3.45	3.09	3.45	3.31	3.36
PC34_1	0.55	0.58	0.62	0.61	0.65	0.95	0.83	0.86	0.85	0.89
PC36_6	2.13	1.92	2.54	2.11	2.47	1.22	1.15	1.22	1.21	1.29
PC36_5	4.16	3.82	4.52	4.18	4.90	3.64	3.45	3.54	3.57	3.72
PC36_4	2.96	2.84	3.12	3.15	3.47	4.31	3.87	4.22	4.23	4.23
PC36_3	1.36	1.36	1.46	1.58	1.61	2.45	2.15	2.29	2.33	2.38
PC36_2	0.49	0.52	0.50	0.58	0.59	1.04	0.90	0.92	0.93	0.97
PC36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC38_6	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PC38_5	0.03	0.03	0.03	0.03	0.04	0.02	0.02	0.03	0.03	0.03
PC38_4	0.05	0.05	0.05	0.05	0.05	0.07	0.07	0.07	0.07	0.07
PC38_3	0.05	0.05	0.05	0.06	0.06	0.11	0.10	0.10	0.10	0.11
PC38_2	0.02	0.03	0.03	0.03	0.03	0.05	0.04	0.05	0.05	0.05
PC40_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC40_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PC40_3	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
PC40_2	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.01	0.01
LysoPC16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LysoPC16_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
LysoPC18_3	0.03	0.03	0.04	0.03	0.04	0.02	0.02	0.02	0.03	0.02
LysoPC18_2	0.03	0.03	0.03	0.03	0.03	0.04	0.04	0.04	0.04	0.04
LysoPC18_1	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
LysoPC18_0	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.01	0.01	0.01
LysoPE16_1	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.01
LysoPE16_0	0.04	0.04	0.05	0.04	0.04	0.05	0.05	0.05	0.04	0.05
LysoPE18_3	0.04	0.03	0.04	0.03	0.04	0.03	0.02	0.03	0.03	0.03
LysoPE18_2	0.04	0.04	0.04	0.05	0.05	0.06	0.06	0.06	0.06	0.08
LysoPE18_1	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01
PE34_4	0.05	0.04	0.07	0.06	0.06	0.14	0.13	0.14	0.13	0.15
PE34_3	3.18	2.77	3.75	3.22	3.61	2.75	2.59	2.59	2.58	2.79
PE34_2	3.63	3.31	4.03	3.84	4.21	4.82	4.58	4.59	4.75	4.86
PE34_1	0.07	0.05	0.07	0.04	0.05	0.08	0.04	0.07	0.04	0.06

PE36_6	0.96	0.83	1.19	0.97	1.07	0.63	0.60	0.63	0.64	0.70
PE36_5	2.21	2.01	2.61	2.36	2.57	2.40	2.22	2.34	2.29	2.42
PE36_4	2.04	1.86	2.30	2.20	2.37	3.46	3.21	3.33	3.26	3.39
PE36_3	0.65	0.60	0.76	0.70	0.76	1.05	0.94	0.95	0.98	0.99
PE36_2	0.26	0.23	0.26	0.28	0.30	0.48	0.45	0.43	0.45	0.44
PE36_1	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.02
PE38_6	0.02	0.02	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02
PE38_5	0.02	0.02	0.03	0.03	0.03	0.02	0.02	0.03	0.02	0.03
PE38_4	0.03	0.03	0.03	0.04	0.04	0.05	0.05	0.05	0.06	0.05
PE38_3	0.05	0.06	0.07	0.07	0.07	0.09	0.08	0.09	0.09	0.08
PE38_2	0.07	0.08	0.09	0.09	0.09	0.12	0.11	0.11	0.10	0.11
PE40_3	0.05	0.04	0.05	0.05	0.05	0.06	0.05	0.05	0.05	0.05
PE40_2	0.08	0.07	0.08	0.09	0.09	0.14	0.12	0.13	0.13	0.13
PE42_4	0.02	0.02	0.03	0.02	0.03	0.02	0.02	0.03	0.02	0.03
PE42_3	0.10	0.08	0.09	0.09	0.10	0.13	0.12	0.12	0.14	0.13
PE42_2	0.09	0.08	0.10	0.10	0.11	0.18	0.17	0.17	0.17	0.16
PG32_1	0.61	0.53	0.70	0.69	0.64	0.50	0.47	0.45	0.41	0.42
PG32_0	0.25	0.25	0.34	0.24	0.31	0.19	0.24	0.26	0.21	0.20
PG34_4	7.87	7.53	8.61	8.68	9.31	0.35	0.33	0.35	0.36	0.39
PG34_3	1.74	1.48	1.79	1.76	1.77	0.63	0.75	0.69	0.73	0.70
PG34_2	1.36	1.28	1.33	1.59	1.51	12.20	11.99	12.86	12.77	12.17
PG34_1	0.80	0.74	0.86	0.95	0.97	2.50	2.13	2.27	2.27	2.06
PG34_0	0.03	0.01	0.02	0.00	0.02	0.00	0.02	0.07	0.00	0.05
lysoPG16_1	0.01	0.01	0.01	0.01	0.01	0.02	0.01	0.01	0.02	0.02
lysoPG16_0	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
lysoPG18_3	0.04	0.06	0.05	0.05	0.05	0.00	0.00	0.00	0.00	0.00
lysoPG18_2	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
lysoPG18_1	0.00	0.01	0.01	0.00	0.01	0.08	0.07	0.08	0.09	0.08
PA34_6	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
PA34_4	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
PA34_3	0.17	0.14	0.23	0.20	0.24	0.18	0.09	0.11	0.17	0.13
PA34_2	0.18	0.14	0.20	0.21	0.21	0.22	0.17	0.16	0.23	0.24
PA34_1	0.04	0.06	0.05	0.05	0.04	0.09	0.06	0.14	0.12	0.07
PA36_6	0.05	0.07	0.07	0.07	0.07	0.04	0.02	0.03	0.02	0.04
PA36_5	0.12	0.10	0.14	0.13	0.14	0.11	0.07	0.07	0.09	0.10
PA36_4	0.13	0.10	0.12	0.12	0.14	0.16	0.09	0.10	0.11	0.15
PA36_3	0.04	0.04	0.05	0.05	0.06	0.06	0.04	0.04	0.05	0.05
PA36_2	0.01	0.01	0.02	0.01	0.02	0.02	0.02	0.00	0.01	0.01
PI34_4	0.01	0.02	0.02	0.02	0.01	0.05	0.04	0.05	0.04	0.05
PI34_3	1.47	1.36	1.78	1.54	1.66	1.28	1.01	1.16	1.16	1.28
PI34_2	1.33	1.24	1.42	1.47	1.47	2.02	1.63	1.79	1.60	1.86
PI34_1	0.00	0.00	0.02	0.01	0.01	0.01	0.00	0.02	0.00	0.01
PI36_6	0.09	0.09	0.10	0.08	0.09	0.07	0.06	0.09	0.07	0.06
PI36_5	0.09	0.12	0.10	0.10	0.12	0.10	0.08	0.09	0.08	0.10
PI36_4	0.10	0.09	0.12	0.12	0.12	0.19	0.14	0.16	0.18	0.17
PI36_3	0.15	0.15	0.14	0.15	0.15	0.21	0.18	0.18	0.19	0.21
PI36_2	0.08	0.09	0.06	0.09	0.11	0.17	0.14	0.14	0.15	0.13
PI36_1	0.01	0.00	0.00	0.00	0.00	0.01	0.03	0.02	0.01	0.00
PS34_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS34_3	0.08	0.07	0.10	0.09	0.10	0.07	0.06	0.06	0.07	0.06
PS34_2	0.07	0.07	0.07	0.07	0.08	0.08	0.07	0.09	0.09	0.08
PS34_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS36_6	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS36_5	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01

PS36_4	0.01	0.01	0.01	0.01	0.02	0.01	0.01	0.01	0.01	0.01
PS36_3	0.03	0.04	0.04	0.04	0.04	0.05	0.04	0.03	0.04	0.04
PS36_2	0.02	0.02	0.03	0.03	0.03	0.03	0.04	0.04	0.04	0.04
PS36_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS38_4	0.00	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.01
PS38_3	0.03	0.03	0.04	0.03	0.04	0.04	0.04	0.04	0.04	0.04
PS38_2	0.03	0.03	0.03	0.03	0.03	0.04	0.04	0.04	0.04	0.04
PS38_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS40_3	0.05	0.04	0.06	0.05	0.05	0.05	0.04	0.05	0.04	0.05
PS40_2	0.05	0.04	0.05	0.05	0.05	0.07	0.06	0.06	0.05	0.06
PS40_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS42_4	0.02	0.02	0.02	0.02	0.02	0.01	0.01	0.01	0.02	0.02
PS42_3	0.08	0.08	0.10	0.08	0.10	0.10	0.10	0.09	0.09	0.10
PS42_2	0.06	0.06	0.07	0.06	0.07	0.11	0.09	0.10	0.10	0.09
PS42_1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS44_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PS44_2	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.00

Appendix B – The significant reactions for each experiment

Table B-10 The significant reactions for *fad2*

Reaction-name	$\overline{d_1}$	$\overline{d_2}$	$\overline{d_1}-\overline{d_2}$	sp_1	sp_2	t-score
PE34_1_PE40_2	**-1.50**	**0.07**	**-1.58**	**0.037**	**0.010**	**69.05**
PE34_1_PS34_2	-1.50	0.07	-1.57	0.037	0.006	67.37
PE34_1_PS38_2	-1.50	0.01	-1.51	0.037	0.002	66.51
PE34_1_PC38_5	-1.50	0.04	-1.55	0.037	0.005	66.38
PE34_1_LysoPE16_0	**-1.50**	**0.02**	**-1.52**	**0.037**	**0.002**	**66.08**
PE34_1_PI36_3	-1.50	0.07	-1.57	0.037	0.021	66.05
PE34_1_PS38_3	-1.50	0.02	-1.52	0.037	0.004	65.94
PE34_1_LysoPE18_2	-1.50	0.03	-1.53	0.037	0.004	65.84
PE34_1_LysoPC18_3	-1.50	0.01	-1.51	0.037	0.002	65.42
PE34_1_LysoPC18_2	-1.50	0.02	-1.52	0.037	0.002	65.42
PE34_1_PC38_3	-1.50	0.05	-1.55	0.037	0.006	65.26
PE34_1_PS36_5	-1.50	0.01	-1.51	0.037	0.001	64.65
PE34_1_PI36_5	-1.50	0.11	-1.62	0.037	0.013	64.56
PE34_1_PE38_5	-1.50	0.02	-1.53	0.037	0.004	64.50
PE34_1_PC40_4	-1.50	0.00	-1.51	0.037	0.000	64.44
PE34_1_PS40_2	-1.50	0.05	-1.56	0.037	0.005	64.37
PE34_1_PS36_3	-1.50	0.02	-1.53	0.037	0.005	64.24
PE34_1_PS44_2	-1.50	0.00	-1.51	0.037	0.001	63.91
PE34_1_PS42_2	-1.50	0.05	-1.55	0.037	0.009	61.72
PE34_1_PA36_5	-1.50	0.10	-1.60	0.037	0.028	55.30
PE34_1_PA34_2	-1.50	0.16	-1.67	0.037	0.034	52.07
PC34_1_PI36_3	-2.39	0.07	-2.46	0.085	0.021	51.17
PC34_1_PI36_5	-2.39	0.11	-2.50	0.085	0.013	49.26
PC34_1_PE40_2	-2.39	0.07	-2.46	0.085	0.010	48.69
PC34_1_PS42_2	-2.39	0.05	-2.43	0.085	0.009	48.00
PC34_1_PC38_3	**-2.39**	**0.05**	**-2.44**	**0.085**	**0.006**	**47.64**
PC34_1_PC36_3	**-2.39**	**0.58**	**-2.97**	**0.085**	**0.134**	**47.58**
PC34_1_PS34_2	-2.39	0.07	-2.46	0.085	0.006	47.55
PC34_1_PS40_2	-2.39	0.05	-2.44	0.085	0.005	46.76
PC34_1_PC38_5	-2.39	0.04	-2.43	0.085	0.005	46.55

PC34_1_PS38_3	-2.39	0.02	-2.41	0.085	0.004	45.81
PC34_1_LysoPE18_2	-2.39	0.03	-2.42	0.085	0.004	45.60
PC34_1_PE38_5	-2.39	0.02	-2.41	0.085	0.004	45.58
PC34_1_PS36_3	-2.39	0.02	-2.41	0.085	0.005	45.52
PC34_1_LysoPE16_0	-2.39	0.02	-2.41	0.085	0.002	45.37
PC34_1_LysoPC18_2	-2.39	0.02	-2.41	0.085	0.002	45.29
PC34_1_PS38_2	-2.39	0.01	-2.40	0.085	0.002	45.05
PC34_1_LysoPC18_3	-2.39	0.01	-2.40	0.085	0.002	45.00
PC36_2_PC34_2	**-6.76**	**3.02**	**-9.78**	**0.267**	**0.292**	**44.88**
PC36_2_PC36_3	**-6.76**	**0.58**	**-7.34**	**0.267**	**0.134**	**44.53**
PC34_1_PS44_2	-2.39	0.00	-2.39	0.085	0.001	44.50
PC34_1_PC40_4	**-2.39**	**0.00**	**-2.39**	**0.085**	**0.000**	**44.39**
PC34_1_PS36_5	-2.39	0.01	-2.39	0.085	0.001	44.22
PE34_4_PS40_2	-0.06	0.05	-0.11	0.006	0.005	43.68
PC34_1_PA34_2	-2.39	0.16	-2.55	0.085	0.034	42.76
PC36_2_PE36_5	-6.76	2.06	-8.82	0.267	0.271	42.62
PC36_2_PI34_2	-6.76	1.58	-8.34	0.267	0.231	42.07
PC36_2_PI36_3	-6.76	0.07	-6.83	0.267	0.021	42.04
PE36_2_PI36_3	-2.02	0.07	-2.09	0.086	0.021	41.82
PC36_2_PE40_2	-6.76	0.07	-6.83	0.267	0.010	41.06
PC36_2_PI36_5	-6.76	0.11	-6.87	0.267	0.013	41.03
PC34_1_PA36_5	-2.39	0.10	-2.48	0.085	0.028	41.00
PE36_2_PE40_2	**-2.02**	**0.07**	**-2.09**	**0.086**	**0.010**	**40.81**
PC36_2_PS34_2	-6.76	0.07	-6.83	0.267	0.006	40.76
PC36_2_PC38_3	**-6.76**	**0.05**	**-6.81**	**0.267**	**0.006**	**40.74**
PE36_2_PI36_5	-2.02	0.11	-2.13	0.086	0.013	40.67
PC36_2_PC38_5	**-6.76**	**0.04**	**-6.80**	**0.267**	**0.005**	**40.53**
PC36_2_PS38_3	-6.76	0.02	-6.78	0.267	0.004	40.48
PC36_2_PS40_2	-6.76	0.05	-6.81	0.267	0.005	40.45
PC36_2_LysoPE18_2	-6.76	0.03	-6.79	0.267	0.004	40.38
PC36_2_PS42_2	-6.76	0.05	-6.81	0.267	0.009	40.38
PC36_2_LysoPE16_0	-6.76	0.02	-6.78	0.267	0.002	40.36
PC36_2_PS36_3	-6.76	0.02	-6.78	0.267	0.005	40.30
PC36_2_PS38_2	-6.76	0.01	-6.77	0.267	0.002	40.30
PC36_2_PE38_5	-6.76	0.02	-6.78	0.267	0.004	40.29
PC36_2_LysoPC18_2	**-6.76**	**0.02**	**-6.78**	**0.267**	**0.002**	**40.28**

PC36_2_LysoPC18_3	-6.76	0.01	-6.77	0.267	0.002	40.24
PC36_2_PC40_4	**-6.76**	**0.00**	**-6.76**	**0.267**	**0.000**	**40.13**
PC36_2_PS44_2	-6.76	0.00	-6.77	0.267	0.001	40.09
PC36_2_PS36_5	-6.76	0.01	-6.77	0.267	0.001	40.09
PC36_2_PA36_5	-6.76	0.10	-6.86	0.267	0.028	40.04
PC36_2_PA34_2	-6.76	0.16	-6.93	0.267	0.034	40.01
PC36_2_PE34_2	-6.76	3.88	-10.65	0.267	0.402	39.93
PC36_2_PC36_6	-6.76	1.51	-8.27	0.267	0.268	39.80
PE34_4_PC38_5	-0.06	0.04	-0.10	0.006	0.005	39.76
PE36_2_PS34_2	-2.02	0.07	-2.09	0.086	0.006	39.04
PE36_2_PC38_5	-2.02	0.04	-2.07	0.086	0.005	38.78
PE36_2_PC38_3	-2.02	0.05	-2.07	0.086	0.006	38.77
PE36_2_PS42_2	-2.02	0.05	-2.07	0.086	0.009	38.55
PE36_2_PS38_3	-2.02	0.02	-2.04	0.086	0.004	38.51
PE36_2_LysoPE18_2	**-2.02**	**0.03**	**-2.05**	**0.086**	**0.004**	**38.42**
PE36_2_PS40_2	-2.02	0.05	-2.07	0.086	0.005	38.36
PE36_2_LysoPE16_0	**-2.02**	**0.02**	**-2.04**	**0.086**	**0.002**	**38.08**
PE36_2_PS38_2	-2.02	0.01	-2.03	0.086	0.002	37.99
PE36_2_LysoPC18_2	-2.02	0.02	-2.04	0.086	0.002	37.90
PE36_2_PS36_3	-2.02	0.02	-2.05	0.086	0.005	37.90
PE36_2_PE38_5	**-2.02**	**0.02**	**-2.04**	**0.086**	**0.004**	**37.89**
PE36_2_LysoPC18_3	-2.02	0.01	-2.03	0.086	0.002	37.63
PE36_2_PS36_5	-2.02	0.01	-2.03	0.086	0.001	37.33
PE36_2_PC40_4	-2.02	0.00	-2.02	0.086	0.000	37.32
PC36_2_PC34_3	**-6.76**	**1.63**	**-8.39**	**0.267**	**0.307**	**37.27**
PE36_2_PS44_2	-2.02	0.00	-2.03	0.086	0.001	37.25
PS42_1_LysoPE16_0	-0.05	0.02	-0.06	0.003	0.002	35.67
PE36_2_PA34_2	-2.02	0.16	-2.19	0.086	0.034	35.60
PE36_2_PA36_5	-2.02	0.10	-2.12	0.086	0.028	35.59
PC36_2_PE34_3	-6.76	1.28	-8.04	0.267	0.322	35.48
PC34_1_PC34_2	**-2.39**	**3.02**	**-5.41**	**0.085**	**0.292**	**34.87**
PC38_2_PC38_3	**-0.08**	**0.05**	**-0.13**	**0.007**	**0.006**	**34.72**
PI34_1_PS34_2	-1.38	0.07	-1.45	0.068	0.006	34.34
PS42_1_PC40_4	-0.05	0.00	-0.05	0.003	0.000	34.27
PC38_2_PS34_2	-0.08	0.07	-0.15	0.007	0.006	34.11

Table B-11 The significant reactions for *fad3*

Reaction-name	$\overline{d_1}$	$\overline{d_2}$	$\overline{d_1}-\overline{d_2}$	sp_1	sp_2	t-score
PC36_4_PE34_3	-1.49	1.76	-3.25	0.375	0.326	45.37
PE36_4_PE36_5	**-1.48**	**1.22**	**-2.70**	**0.250**	**0.275**	**42.95**
PC36_4_PC34_3	**-1.49**	**1.29**	**-2.78**	**0.375**	**0.314**	**39.90**
PE36_4_PE34_3	**-1.48**	**1.76**	**-3.24**	**0.250**	**0.326**	**33.99**
PC36_4_PC36_6	**-1.49**	**1.26**	**-2.76**	**0.375**	**0.276**	**32.60**
PC36_4_PE36_5	-1.49	1.22	-2.71	0.375	0.275	32.13
PE36_4_PC36_6	-1.48	1.26	-2.74	0.250	0.276	31.88
PE36_4_PC34_3	-1.48	1.29	-2.76	0.250	0.314	28.32
PC36_4_PC36_5	**-1.49**	**1.84**	**-3.33**	**0.375**	**0.533**	**28.02**
PE36_4_PE36_6	**-1.48**	**0.66**	**-2.14**	**0.250**	**0.102**	**20.76**
PE36_4_PC36_5	-1.48	1.84	-3.32	0.250	0.533	16.03
PS38_2_PC38_5	-0.01	0.03	-0.04	0.003	0.005	14.97
PS38_2_PE38_5	-0.01	0.02	-0.03	0.003	0.004	14.67
PS38_2_PE40_3	-0.01	0.03	-0.04	0.003	0.004	14.20
PS38_2_PE42_4	-0.01	0.01	-0.03	0.003	0.002	13.33
PS34_2_PS34_3	**-0.04**	**0.04**	**-0.08**	**0.010**	**0.010**	**13.17**
PS38_2_PS38_3	**-0.01**	**0.02**	**-0.04**	**0.003**	**0.004**	**12.67**
PS34_2_PC38_5	-0.04	0.03	-0.06	0.010	0.005	12.54
PS38_2_PC38_4	-0.01	0.02	-0.04	0.003	0.006	12.44
PS38_2_LysoPE16_0	-0.01	0.01	-0.02	0.003	0.002	12.41
PS34_2_PS36_3	**-0.04**	**0.02**	**-0.06**	**0.010**	**0.006**	**12.28**
PS38_2_PS42_4	**-0.01**	**0.01**	**-0.02**	**0.003**	**0.002**	**12.25**
PS36_2_PC38_5	-0.01	0.03	-0.04	0.003	0.005	12.23
PC36_4_PE36_6	-1.49	0.66	-2.16	0.375	0.102	12.21
PS38_2_LysoPE18_3	-0.01	0.01	-0.02	0.003	0.003	12.07
PS36_2_PE38_5	-0.01	0.02	-0.03	0.003	0.004	12.02
PS36_2_PE40_3	-0.01	0.03	-0.04	0.003	0.004	11.82
PS34_2_PS40_3	**-0.04**	**0.03**	**-0.07**	**0.010**	**0.006**	**11.72**
PS34_2_PE40_3	-0.04	0.03	-0.06	0.010	0.004	11.69
PS38_2_PC38_6	-0.01	0.01	-0.02	0.003	0.002	11.68
MGDG36_5_PE36_6	-0.34	0.66	-1.00	0.102	0.102	11.63
PS34_2_PC38_4	-0.04	0.02	-0.06	0.010	0.006	11.61

PS34_2_PE36_6	-0.04	0.66	-0.70	0.010	0.102	11.27
PS36_2_PS38_3	**-0.01**	**0.02**	**-0.04**	**0.003**	**0.004**	**11.15**
PS36_2_PE42_4	-0.01	0.01	-0.02	0.003	0.002	10.98
PS36_2_LysoPE16_0	-0.01	0.01	-0.02	0.003	0.002	10.90
PS34_2_PE38_5	-0.04	0.02	-0.06	0.010	0.004	10.60
PS38_2_PS40_3	**-0.01**	**0.03**	**-0.04**	**0.003**	**0.006**	**10.59**
PS38_2_PE36_6	-0.01	0.66	-0.68	0.003	0.102	10.57
PS36_2_PE36_6	-0.01	0.66	-0.68	0.003	0.102	10.50
PE36_4_PI36_3	-1.48	0.06	-1.54	0.250	0.020	10.40
PS36_2_PC38_4	-0.01	0.02	-0.03	0.003	0.006	10.39
PS36_2_PE34_4	-0.01	0.02	-0.03	0.003	0.005	10.20
PS34_2_PS38_3	**-0.04**	**0.02**	**-0.06**	**0.010**	**0.004**	**10.15**
PS38_2_PS36_3	**-0.01**	**0.02**	**-0.04**	**0.003**	**0.006**	**10.04**
PS36_2_PS42_4	**-0.01**	**0.01**	**-0.02**	**0.003**	**0.002**	**10.03**
PE36_4_PS34_3	-1.48	0.04	-1.52	0.250	0.010	9.95
PS38_2_PE34_4	-0.01	0.02	-0.04	0.003	0.005	9.93
MGDG36_5_PE34_3	-0.34	1.76	-2.09	0.102	0.326	9.82
PE36_4_PS40_3	-1.48	0.03	-1.51	0.250	0.006	9.74
PE36_4_PC38_5	-1.48	0.03	-1.51	0.250	0.005	9.68
PE36_4_PE40_3	**-1.48**	**0.03**	**-1.50**	**0.250**	**0.004**	**9.66**
PE36_4_PC38_4	-1.48	0.02	-1.50	0.250	0.006	9.66
PE36_4_PE34_4	**-1.48**	**0.02**	**-1.50**	**0.250**	**0.005**	**9.64**
PE36_4_PS38_3	-1.48	0.02	-1.50	0.250	0.004	9.63
PS36_2_PC38_6	-0.01	0.01	-0.02	0.003	0.002	9.62
PE36_4_PS36_3	-1.48	0.02	-1.50	0.250	0.006	9.60
PE36_4_PE38_5	**-1.48**	**0.02**	**-1.50**	**0.250**	**0.004**	**9.60**
PS38_2_PS34_3	**-0.01**	**0.04**	**-0.06**	**0.003**	**0.010**	**9.49**
PE36_4_PE42_4	**-1.48**	**0.01**	**-1.49**	**0.250**	**0.002**	**9.48**
PE36_4_LysoPE16_0	-1.48	0.01	-1.49	0.250	0.002	9.47
PE36_4_PC38_6	-1.48	0.01	-1.49	0.250	0.002	9.47
PE36_4_LysoPE18_3	**-1.48**	**0.01**	**-1.49**	**0.250**	**0.003**	**9.47**
PE36_4_PS42_4	-1.48	0.01	-1.49	0.250	0.002	9.44
PE36_4_DGDG36_3	-1.48	0.11	-1.59	0.250	0.032	9.38
PS36_2_PS40_3	**-0.01**	**0.03**	**-0.04**	**0.003**	**0.006**	**9.36**
PE36_4_PS36_6	-1.48	0.00	-1.48	0.250	0.001	9.36
PE36_4_PA36_6	-1.48	0.04	-1.52	0.250	0.013	9.35

Table B-12 The significant reactions for *fad4*

Reaction-name	$\overline{d_1}$	$\overline{d_2}$	$\overline{d_1}-\overline{d_2}$	sp_1	sp_2	t-score
PG34_3_PG34_4	**-4.13**	**9.79**	**-13.92**	**0.371**	**0.648**	**35.59**
PG34_3_PG34_2	**-4.13**	**0.83**	**-4.96**	**0.371**	**0.176**	**32.90**
PG32_0_PG34_4	-0.31	9.79	-10.10	0.064	0.648	25.91
PG34_0_PG34_4	-0.09	9.79	-9.89	0.028	0.648	24.35
PG34_3_PG32_1	**-4.13**	**0.65**	**-4.79**	**0.371**	**0.083**	**21.39**
PG32_0_PG32_1	**-0.31**	**0.65**	**-0.96**	**0.064**	**0.083**	**19.32**
PG34_3_lysoPG18_3	**-4.13**	**0.04**	**-4.17**	**0.371**	**0.003**	**17.80**
PG34_0_PG32_1	**-0.09**	**0.65**	**-0.75**	**0.028**	**0.083**	**14.26**
PG32_0_PG34_2	**-0.31**	**0.83**	**-1.14**	**0.064**	**0.176**	**11.62**

Table B-13 The significant reactions for *fad5*

Reaction-name	$\overline{d_1}$	$\overline{d_2}$	$\overline{d_1}-\overline{d_2}$	sp_1	sp_2	t-score
DGDG34_3_DGDG36_6	**-9.79**	**8.27**	**-18.06**	**0.953**	**0.799**	**34.41**
MGDG36_6_DGDG36_6	**-21.58**	**8.27**	**-29.85**	**1.492**	**0.799**	**33.37**
MGDG36_6_MGDG34_6	**-21.58**	**66.50**	**-88.08**	**1.492**	**4.598**	**30.16**
DGDG36_3_DGDG34_6	**-0.32**	**2.22**	**-2.54**	**0.047**	**0.144**	**30.14**
MGDG38_4_DGDG34_6	-0.29	2.22	-2.52	0.059	0.144	28.02
MGDG34_3_MGDG34_6	**-17.52**	**66.50**	**-84.03**	**1.675**	**4.598**	**27.15**
DGDG34_3_MGDG34_6	-9.79	66.50	-76.29	0.953	4.598	26.50
MGDG36_6_DGDG34_6	-21.58	2.22	-23.80	1.492	0.144	25.40
DGDG36_3_DGDG34_1	**-0.32**	**0.32**	**-0.63**	**0.047**	**0.047**	**25.07**
MGDG36_6_MGDG34_4	**-21.58**	**1.90**	**-23.48**	**1.492**	**0.238**	**24.97**
LysoPC16_0_DGDG34_6	0.00	2.22	-2.23	0.001	0.144	24.50
MGDG36_6_DGDG34_2	-21.58	0.93	-22.51	1.492	0.094	23.98
MGDG36_6_MGDG36_4	**-21.58**	**0.72**	**-22.30**	**1.492**	**0.136**	**23.70**
DGDG36_3_DGDG34_2	**-0.32**	**0.93**	**-1.25**	**0.047**	**0.094**	**23.67**
MGDG36_6_MGDG34_2	-21.58	0.59	-22.17	1.492	0.096	23.60
MGDG36_6_DGDG36_4	-21.58	0.29	-21.86	1.492	0.063	23.46
MGDG36_6_DGDG34_1	-21.58	0.32	-21.89	1.492	0.047	23.32

MGDG38_4_MGDG34_6	**-0.29**	**66.50**	**-66.79**	**0.059**	**4.598**	**23.07**
DGDG36_3_MGDG34_6	-0.32	66.50	-66.82	0.047	4.598	23.05
MGDG36_6_PC34_4	-21.58	0.08	-21.66	1.492	0.014	22.91
MGDG36_6_DGDG34_5	-21.58	0.11	-21.69	1.492	0.029	22.91
MGDG36_6_PE34_4	-21.58	0.03	-21.61	1.492	0.005	22.88
LysoPC16_0_MGDG34_6	0.00	66.50	-66.50	0.001	4.598	22.87
MGDG38_4_DGDG34_2	-0.29	0.93	-1.23	0.059	0.094	20.84
MGDG34_3_DGDG36_6	-17.52	8.27	-25.80	1.675	0.799	20.43
DGDG34_3_DGDG34_6	**-9.79**	**2.22**	**-12.01**	**0.953**	**0.144**	**20.14**
DGDG34_3_MGDG34_4	-9.79	1.90	-11.69	0.953	0.238	19.72
MGDG38_4_DGDG36_4	-0.29	0.29	-0.58	0.059	0.063	19.38
MGDG34_3_DGDG34_6	-17.52	2.22	-19.75	1.675	0.144	18.56
MGDG34_3_MGDG34_4	**-17.52**	**1.90**	**-19.43**	**1.675**	**0.238**	**18.50**
DGDG34_3_MGDG36_4	-9.79	0.72	-10.51	0.953	0.136	18.37
DGDG34_3_DGDG34_2	**-9.79**	**0.93**	**-10.72**	**0.953**	**0.094**	**18.07**
MGDG34_3_DGDG34_2	-17.52	0.93	-18.46	1.675	0.094	17.41
MGDG38_4_DGDG36_6	-0.29	8.27	-8.57	0.059	0.799	17.25
DGDG34_3_MGDG34_2	-9.79	0.59	-10.38	0.953	0.096	17.06
MGDG34_3_MGDG34_2	**-17.52**	**0.59**	**-18.11**	**1.675**	**0.096**	**17.05**
MGDG34_3_MGDG36_4	**-17.52**	**0.72**	**-18.24**	**1.675**	**0.136**	**16.98**
MGDG34_3_DGDG36_4	-17.52	0.29	-17.81	1.675	0.063	16.87
DGDG36_3_DGDG36_6	**-0.32**	**8.27**	**-8.59**	**0.047**	**0.799**	**16.67**

Table B-14 The significant reactions for *fad6*

Reaction-name	$\overline{d_1}$	$\overline{d_2}$	$\overline{d_1}-\overline{d_2}$	sp_1	sp_2	t-score
MGDG36_4_DGDG34_6	-2.39	2.22	-4.62	0.181	0.144	52.78
PG34_2_PG34_3	**-9.15**	**1.79**	**-10.94**	**0.392**	**0.228**	**49.18**
PG34_2_PG34_4	**-9.15**	**9.48**	**-18.62**	**0.392**	**0.649**	**45.41**
PG34_2_DGDG34_6	-9.15	2.22	-11.37	0.392	0.144	41.98
MGDG34_2_PG34_4	-16.35	9.48	-25.82	0.774	0.649	39.74
DGDG36_4_DGDG34_6	**-3.28**	**2.22**	**-5.50**	**0.154**	**0.144**	**38.72**
PG34_2_PC38_5	-9.15	0.02	-9.17	0.392	0.005	37.21
MGDG34_2_DGDG34_6	-16.35	2.22	-18.57	0.774	0.144	37.16
PG34_2_lysoPG18_3	-9.15	0.04	-9.19	0.392	0.003	37.12

PG34_2_PE38_5	-9.15	0.01	-9.16	0.392	0.004	37.09
PG34_2_DGDG36_3	-9.15	0.18	-9.32	0.392	0.026	37.08
PG34_2_PE40_3	-9.15	0.02	-9.16	0.392	0.004	37.08
PG34_2_DGDG34_5	-9.15	0.11	-9.26	0.392	0.029	37.00
MGDG34_2_PG34_3	-16.35	1.79	-18.14	0.774	0.228	35.53
DGDG36_4_DGDG34_5	**-3.28**	**0.11**	**-3.39**	**0.154**	**0.029**	**35.40**
DGDG36_4_DGDG36_3	**-3.28**	**0.18**	**-3.45**	**0.154**	**0.026**	**34.66**
DGDG36_4_lysoPG18_3	-3.28	0.04	-3.32	0.154	0.003	34.01
DGDG36_4_PC38_5	-3.28	0.02	-3.30	0.154	0.005	33.97
DGDG36_4_PE38_5	-3.28	0.01	-3.29	0.154	0.004	33.91
DGDG36_4_PE40_3	-3.28	0.02	-3.29	0.154	0.004	33.79
MGDG34_2_DGDG36_3	-16.35	0.18	-16.52	0.774	0.026	33.70
MGDG34_2_DGDG34_5	-16.35	0.11	-16.46	0.774	0.029	33.50
MGDG34_2_lysoPG18_3	-16.35	0.04	-16.39	0.774	0.003	33.46
MGDG34_2_PC38_5	-16.35	0.02	-16.37	0.774	0.005	33.41
MGDG34_2_PE40_3	-16.35	0.02	-16.36	0.774	0.004	33.38
MGDG34_2_PE38_5	-16.35	0.01	-16.36	0.774	0.004	33.38
DGDG34_1_DGDG34_6	-0.79	2.22	-3.01	0.083	0.144	32.40
DGDG36_4_PG34_3	-3.28	1.79	-5.07	0.154	0.228	30.50
DGDG36_4_PG34_4	-3.28	9.48	-12.75	0.154	0.649	29.78
PG34_2_DGDG34_3	-9.15	1.23	-10.38	0.392	0.369	28.96
MGDG34_2_MGDG34_6	-16.35	66.54	-82.89	0.774	4.598	28.46
MGDG36_2_DGDG34_6	-0.21	2.22	-2.43	0.027	0.144	27.90
MGDG36_4_PG34_4	-2.39	9.48	-11.87	0.181	0.649	27.22
DGDG36_2_DGDG34_6	-0.25	2.22	-2.47	0.022	0.144	26.83
PG34_1_PG34_4	**-1.36**	**9.48**	**-10.84**	**0.242**	**0.649**	**26.75**
MGDG34_2_DGDG34_3	-16.35	1.23	-17.58	0.774	0.369	26.59
PC36_3_PG34_4	-0.45	9.48	-9.93	0.147	0.649	26.48
PC34_4_PC38_5	**-0.24**	**0.02**	**-0.27**	**0.019**	**0.005**	**26.47**
MGDG34_3_DGDG34_6	-2.48	2.22	-4.71	0.232	0.144	26.38
PE34_4_PC38_5	-0.07	0.02	-0.09	0.007	0.005	26.29
PC34_4_DGDG34_6	-0.24	2.22	-2.46	0.019	0.144	26.22
PC36_3_PG34_3	-0.45	1.79	-2.24	0.147	0.228	25.93
MGDG34_3_PG34_4	-2.48	9.48	-11.96	0.232	0.649	25.76
PC34_4_PE40_3	-0.24	0.02	-0.26	0.019	0.004	25.72
PG34_2_MGDG34_6	-9.15	66.54	-75.69	0.392	4.598	25.20

lysoPG18_1_DGDG34_6	-0.04	2.22	-2.27	0.003	0.144	24.94
PE34_1_DGDG34_6	-0.05	2.22	-2.27	0.008	0.144	24.85
DGDG34_1_PG34_4	-0.79	9.48	-10.27	0.083	0.649	24.76
PE34_4_DGDG34_6	-0.07	2.22	-2.29	0.007	0.144	24.75
PC34_1_PG34_4	-0.25	9.48	-9.73	0.056	0.649	24.66
PE34_4_PE40_3	**-0.07**	**0.02**	**-0.08**	**0.007**	**0.004**	**24.66**

Table B-15 The significant reactions for *fad7*

Reaction-name	$\overline{d_1}$	$\overline{d_2}$	$\overline{d_1}-\overline{d_2}$	sp_1	sp_2	t-score
DGDG36_5_MGDG36_6	-5.91	6.48	-12.39	0.273	0.481	47.94
DGDG36_5_DGDG34_6	**-5.91**	**1.50**	**-7.41**	**0.273**	**0.195**	**38.12**
DGDG36_5_DGDG34_3	**-5.91**	**2.10**	**-8.01**	**0.273**	**0.292**	**37.03**
DGDG36_5_DGDG36_3	**-5.91**	**0.15**	**-6.06**	**0.273**	**0.039**	**36.76**
DGDG36_5_lysoPG18_3	-5.91	0.01	-5.92	0.273	0.004	34.26
MGDG34_5_MGDG36_6	**-20.98**	**6.48**	**-27.47**	**1.293**	**0.481**	**32.46**
DGDG34_2_DGDG34_6	-1.29	1.50	-2.78	0.207	0.195	32.04
MGDG34_5_DGDG36_6	-20.98	5.81	-26.79	1.293	0.794	30.99
MGDG34_5_DGDG34_3	-20.98	2.10	-23.08	1.293	0.292	30.13
MGDG34_5_DGDG34_6	-20.98	1.50	-22.48	1.293	0.195	28.24
DGDG34_2_DGDG34_3	**-1.29**	**2.10**	**-3.39**	**0.207**	**0.292**	**28.19**
MGDG34_5_PG34_4	-20.98	3.10	-24.08	1.293	0.680	28.12
DGDG36_4_MGDG36_6	-1.78	6.48	-8.27	0.139	0.481	27.92
DGDG34_5_DGDG34_6	**-1.60**	**1.50**	**-3.10**	**0.183**	**0.195**	**26.69**
DGDG34_2_MGDG36_6	-1.29	6.48	-7.77	0.207	0.481	25.95
MGDG34_5_DGDG36_3	-20.98	0.15	-21.13	1.293	0.039	25.76
MGDG34_5_lysoPG18_3	-20.98	0.01	-21.00	1.293	0.004	25.70
DGDG36_5_DGDG36_6	**-5.91**	**5.81**	**-11.72**	**0.273**	**0.794**	**24.77**
DGDG34_5_MGDG36_6	-1.60	6.48	-8.08	0.183	0.481	24.42
MGDG36_5_MGDG36_6	**-3.30**	**6.48**	**-9.79**	**0.314**	**0.481**	**24.05**
DGDG34_4_MGDG36_6	-0.65	6.48	-7.14	0.105	0.481	23.76
PG34_3_MGDG36_6	-1.18	6.48	-7.66	0.267	0.481	23.61
DGDG34_5_DGDG34_3	**-1.60**	**2.10**	**-3.70**	**0.183**	**0.292**	**23.51**
DGDG36_4_DGDG34_3	**-1.78**	**2.10**	**-3.88**	**0.139**	**0.292**	**23.46**
DGDG36_4_DGDG34_6	**-1.78**	**1.50**	**-3.28**	**0.139**	**0.195**	**23.41**

MGDG34_4_MGDG36_6	**-9.07**	**6.48**	**-15.55**	**1.230**	**0.481**	**22.59**
MGDG34_5_MGDG34_6	**-20.98**	**46.68**	**-67.66**	**1.293**	**4.957**	**22.51**
MGDG36_3_MGDG36_6	**-0.23**	**6.48**	**-6.71**	**0.075**	**0.481**	**21.82**
PC34_4_MGDG36_6	-0.07	6.48	-6.55	0.014	0.481	21.39
PE34_4_MGDG36_6	-0.03	6.48	-6.51	0.006	0.481	21.35
LysoPC18_2_MGDG36_6	-0.02	6.48	-6.50	0.003	0.481	21.35
LysoPE18_2_MGDG36_6	-0.02	6.48	-6.50	0.004	0.481	21.33
lysoPG18_2_MGDG36_6	-0.01	6.48	-6.49	0.002	0.481	21.32
LysoPC18_1_MGDG36_6	0.00	6.48	-6.49	0.001	0.481	21.30
DGDG36_4_lysoPG18_3	-1.78	0.01	-1.80	0.139	0.004	20.76

Table B-16 The significant reactions for *sfd1*

Reaction-name	$\overline{d_1}$	$\overline{d_2}$	$\overline{d_1}-\overline{d_2}$	sp_1	sp_2	t-score
MGDG36_6_MGDG34_6	**-19.70**	**30.94**	**-50.64**	**2.745**	**3.189**	**27.10**
DGDG36_6_MGDG34_6	-7.45	30.94	-38.39	2.099	3.189	25.98
PE34_1_MGDG34_2	-0.28	0.28	-0.55	0.061	0.057	20.98
PI34_1_DGDG34_2	-0.10	0.64	-0.74	0.016	0.071	17.68
PE34_1_DGDG34_2	-0.28	0.64	-0.92	0.061	0.071	17.22
PC36_2_MGDG34_6	-0.58	30.94	-31.52	0.181	3.189	16.07
PC34_1_MGDG34_6	-0.50	30.94	-31.44	0.161	3.189	16.03
PE34_1_MGDG34_6	-0.28	30.94	-31.21	0.061	3.189	15.58
PI34_1_MGDG34_6	-0.10	30.94	-31.04	0.016	3.189	15.43
PE36_1_MGDG34_6	-0.02	30.94	-30.95	0.004	3.189	15.35
PA34_1_MGDG34_6	-0.03	30.94	-30.97	0.010	3.189	15.35
PA34_1_DGDG34_2	-0.03	0.64	-0.68	0.010	0.071	14.95
PE36_1_DGDG34_2	-0.02	0.64	-0.66	0.004	0.071	14.77
MGDG36_6_DGDG34_6	-19.70	1.90	-21.60	2.745	0.318	12.94
PI34_1_MGDG34_2	-0.10	0.28	-0.38	0.016	0.057	12.14
PC34_1_DGDG34_6	-0.50	1.90	-2.40	0.161	0.318	12.06
MGDG36_6_MGDG34_4	**-19.70**	**0.97**	**-20.67**	**2.745**	**0.172**	**11.94**
MGDG36_6_DGDG34_2	-19.70	0.64	-20.35	2.745	0.071	11.78
MGDG36_6_MGDG34_2	-19.70	0.28	-19.98	2.745	0.057	11.68
PC36_2_DGDG34_6	-0.58	1.90	-2.48	0.181	0.318	11.52
MGDG36_6_DGDG34_1	-19.70	0.20	-19.90	2.745	0.046	11.49

Table B-17 The significant reactions for *sfd2*

Reaction-name	$\overline{d_1}$	$\overline{d_2}$	$\overline{d_1}-\overline{d_2}$	sp_1	sp_2	t-score
MGDG36_6_MGDG34_6	**-27.97**	**80.75**	**-108.73**	**4.665**	**8.648**	**21.02**
MGDG34_3_MGDG34_6	**-3.64**	**80.75**	**-84.40**	**0.786**	**8.648**	**15.44**
PG34_1_MGDG34_6	-0.75	80.75	-81.50	0.242	8.648	15.03
PE36_3_MGDG34_6	-0.83	80.75	-81.58	0.264	8.648	15.02
PE36_2_MGDG34_6	-0.73	80.75	-81.48	0.234	8.648	14.98
MGDG34_5_MGDG34_6	**-0.63**	**80.75**	**-81.38**	**0.197**	**8.648**	**14.86**
PG34_0_MGDG34_6	-0.38	80.75	-81.14	0.092	8.648	14.84
PI36_3_MGDG34_6	-0.16	80.75	-80.91	0.045	8.648	14.81
PE40_3_MGDG34_6	-0.06	80.75	-80.81	0.018	8.648	14.79
PE38_3_MGDG34_6	-0.05	80.75	-80.80	0.014	8.648	14.78
PE38_5_MGDG34_6	-0.02	80.75	-80.77	0.006	8.648	14.77
PG34_0_PG32_1	**-0.38**	**0.33**	**-0.71**	**0.092**	**0.090**	**13.42**
PG34_1_DGDG34_6	-0.75	2.16	-2.90	0.242	0.399	12.57
PG34_1_DGDG34_2	-0.75	1.19	-1.93	0.242	0.230	12.16
PE36_3_DGDG34_6	-0.83	2.16	-2.99	0.264	0.399	11.55
PE36_2_DGDG34_6	-0.73	2.16	-2.89	0.234	0.399	11.26
MGDG34_3_DGDG34_6	-3.64	2.16	-5.80	0.786	0.399	10.85
MGDG36_6_DGDG34_6	-27.97	2.16	-30.13	4.665	0.399	10.59
PI36_3_DGDG34_1	-0.16	0.17	-0.34	0.045	0.051	10.52
PG34_0_DGDG34_2	-0.38	1.19	-1.57	0.092	0.230	10.05
MGDG36_6_DGDG34_2	-27.97	1.19	-29.16	4.665	0.230	10.05
PG34_0_DGDG34_6	-0.38	2.16	-2.54	0.092	0.399	10.00
PE36_2_DGDG34_2	-0.73	1.19	-1.91	0.234	0.230	9.88
PE36_3_DGDG34_2	-0.83	1.19	-2.01	0.264	0.230	9.87
MGDG34_5_DGDG34_6	-0.63	2.16	-2.79	0.197	0.399	9.75
PG34_1_PG32_1	**-0.75**	**0.33**	**-1.08**	**0.242**	**0.090**	**9.74**
MGDG36_6_PG32_1	-27.97	0.33	-28.30	4.665	0.090	9.71
MGDG36_6_DGDG34_1	-27.97	0.17	-28.15	4.665	0.051	9.58
MGDG34_5_DGDG34_2	-0.63	1.19	-1.82	0.197	0.230	9.49
PI36_3_DGDG34_6	-0.16	2.16	-2.32	0.045	0.399	9.44
MGDG34_3_DGDG34_2	-3.64	1.19	-4.83	0.786	0.230	9.39

PI36_3_DGDG34_2	-0.16	1.19	-1.35	0.045	0.230	9.33
PG34_0_DGDG34_1	-0.38	0.17	-0.56	0.092	0.051	9.06
PE40_3_DGDG34_6	-0.06	2.16	-2.21	0.018	0.399	8.96
PE38_3_DGDG34_6	-0.05	2.16	-2.21	0.014	0.399	8.90
PE40_3_DGDG34_2	-0.06	1.19	-1.24	0.018	0.230	8.72
PE38_5_DGDG34_6	-0.02	2.16	-2.18	0.006	0.399	8.70
PE38_3_DGDG34_2	-0.05	1.19	-1.24	0.014	0.230	8.68

Table B-18 The significant reactions for *sfd3*

Reaction-name	$\overline{d_1}$	$\overline{d_2}$	$\overline{d_1}-\overline{d_2}$	sp_1	sp_2	t-score
MGDG34_2_PA36_6	-18.29	0.04	-18.33	0.350	0.008	83.15
MGDG34_2_lysoPG18_3	-18.29	0.05	-18.34	0.350	0.004	82.92
MGDG34_2_PG32_1	-18.29	0.18	-18.48	0.350	0.056	82.92
MGDG34_2_PC38_5	-18.29	0.01	-18.30	0.350	0.001	82.77
MGDG34_2_LysoPC18_3	-18.29	0.01	-18.30	0.350	0.003	82.63
MGDG34_2_PC38_6	-18.29	0.00	-18.30	0.350	0.001	82.62
MGDG34_2_PG34_3	-18.29	1.01	-19.30	0.350	0.096	82.02
MGDG34_2_PE36_6	-18.29	0.36	-18.66	0.350	0.098	81.86
MGDG34_2_PC36_6	-18.29	1.02	-19.31	0.350	0.190	77.14
MGDG34_2_DGDG34_6	-18.29	2.64	-20.93	0.350	0.299	73.11
MGDG34_2_PG34_4	-18.29	8.04	-26.34	0.350	0.500	67.54
PG34_2_PG34_3	**-10.98**	**1.01**	**-11.99**	**0.291**	**0.096**	**65.13**
PG34_2_LysoPC18_3	-10.98	0.01	-10.99	0.291	0.003	60.05
PG34_2_lysoPG18_3	-10.98	0.05	-11.03	0.291	0.004	59.99
PG34_2_PC38_5	-10.98	0.01	-10.99	0.291	0.001	59.80
PG34_2_PA36_6	-10.98	0.04	-11.02	0.291	0.008	59.74
PG34_2_PC38_6	-10.98	0.00	-10.99	0.291	0.001	59.72
PG34_2_PE36_6	-10.98	0.36	-11.35	0.291	0.098	59.58
PG34_2_PG32_1	**-10.98**	**0.18**	**-11.17**	**0.291**	**0.056**	**59.14**
PG34_2_PG34_4	**-10.98**	**8.04**	**-19.03**	**0.291**	**0.500**	**58.13**
PG34_2_PC36_6	-10.98	1.02	-12.00	0.291	0.190	56.34
PE34_2_PG34_4	-0.92	8.04	-8.96	0.263	0.500	50.04
PG34_2_DGDG34_6	-10.98	2.64	-13.62	0.291	0.299	49.57
MGDG34_2_MGDG34_6	-18.29	56.99	-75.28	0.350	2.761	42.83

PC36_4_PG34_4	-1.07	8.04	-9.11	0.207	0.500	40.44
PE36_4_PG34_4	-1.18	8.04	-9.22	0.161	0.500	39.63
PG34_2_MGDG34_6	-10.98	56.99	-67.98	0.291	2.761	39.58
DGDG36_4_PG34_3	-2.86	1.01	-3.87	0.135	0.096	38.63
MGDG36_6_MGDG34_6	**-4.15**	**56.99**	**-61.14**	**0.528**	**2.761**	**38.33**
PC34_2_PG34_4	-0.63	8.04	-8.67	0.182	0.500	37.16
DGDG36_4_PG34_4	-2.86	8.04	-10.91	0.135	0.500	36.59
DGDG36_4_PE36_6	-2.86	0.36	-3.22	0.135	0.098	35.92
PE34_2_MGDG34_6	-0.92	56.99	-57.91	0.263	2.761	35.25
MGDG36_4_MGDG34_6	**-3.19**	**56.99**	**-60.18**	**0.252**	**2.761**	**34.73**
PC36_4_MGDG34_6	-1.07	56.99	-58.06	0.207	2.761	34.65
DGDG36_4_MGDG34_6	-2.86	56.99	-59.85	0.135	2.761	34.62
PE36_4_MGDG34_6	-1.18	56.99	-58.17	0.161	2.761	34.61
DGDG36_4_PA36_6	-2.86	0.04	-2.90	0.135	0.008	34.58
MGDG34_3_MGDG34_6	**-2.27**	**56.99**	**-59.26**	**0.236**	**2.761**	**34.55**
MGDG36_4_PG34_4	-3.19	8.04	-11.24	0.252	0.500	34.33
PE36_4_PC36_6	-1.18	1.02	-2.19	0.161	0.190	34.27
DGDG36_4_lysoPG18_3	-2.86	0.05	-2.91	0.135	0.004	34.16
PC34_2_MGDG34_6	-0.63	56.99	-57.62	0.182	2.761	34.13
PG34_1_MGDG34_6	-1.38	56.99	-58.38	0.137	2.761	34.09
PC36_3_MGDG34_6	-0.85	56.99	-57.84	0.114	2.761	34.00
DGDG36_4_LysoPC18_3	-2.86	0.01	-2.87	0.135	0.003	33.82
DGDG36_4_PC38_5	-2.86	0.01	-2.87	0.135	0.001	33.74
DGDG36_4_PC38_6	-2.86	0.00	-2.86	0.135	0.001	33.56
DGDG34_1_MGDG34_6	-1.42	56.99	-58.41	0.209	2.761	33.51
DGDG34_2_MGDG34_6	-0.54	56.99	-57.53	0.126	2.761	33.28
PE36_3_MGDG34_6	-0.29	56.99	-57.28	0.057	2.761	33.23
PC36_2_MGDG34_6	-0.42	56.99	-57.41	0.051	2.761	33.16
PC34_1_MGDG34_6	-0.27	56.99	-57.27	0.043	2.761	33.10
MGDG34_3_PG34_4	-2.27	8.04	-10.31	0.236	0.500	33.00
PG34_1_PG34_4	**-1.38**	**8.04**	**-9.43**	**0.137**	**0.500**	**32.96**
DGDG34_4_MGDG34_6	-0.26	56.99	-57.25	0.074	2.761	32.93
PE36_2_MGDG34_6	-0.18	56.99	-57.17	0.023	2.761	32.87
MGDG36_2_MGDG34_6	-0.19	56.99	-57.18	0.058	2.761	32.85
PC34_4_MGDG34_6	-0.22	56.99	-57.22	0.019	2.761	32.83
PC36_3_PG34_4	-0.85	8.04	-8.89	0.114	0.500	32.78

PI36_4_MGDG34_6	-0.06	56.99	-57.05	0.016	2.761	32.77
PE42_2_MGDG34_6	-0.07	56.99	-57.06	0.009	2.761	32.73
PE34_4_MGDG34_6	-0.08	56.99	-57.07	0.008	2.761	32.73
PE38_2_MGDG34_6	-0.03	56.99	-57.02	0.008	2.761	32.73
PE38_3_MGDG34_6	-0.02	56.99	-57.01	0.006	2.761	32.71
PI36_2_MGDG34_6	-0.06	56.99	-57.05	0.016	2.761	32.71
PE40_2_MGDG34_6	-0.05	56.99	-57.04	0.007	2.761	32.71
lysoPG18_1_MGDG34_6	-0.07	56.99	-57.07	0.006	2.761	32.69
PC38_3_MGDG34_6	-0.05	56.99	-57.04	0.004	2.761	32.69
PE38_4_MGDG34_6	-0.02	56.99	-57.01	0.004	2.761	32.68
PS42_2_MGDG34_6	-0.03	56.99	-57.02	0.007	2.761	32.68
PC38_2_MGDG34_6	-0.02	56.99	-57.01	0.004	2.761	32.68
PI34_4_MGDG34_6	-0.03	56.99	-57.02	0.005	2.761	32.67
PI36_3_MGDG34_6	-0.05	56.99	-57.04	0.010	2.761	32.67
PE42_3_MGDG34_6	-0.04	56.99	-57.03	0.007	2.761	32.67

Appendix C - R Programs used in the study

To make these codes work well, you need to change the file path first. For the convenience of the reader and the possible user, I write all the codes as briefly as I could. All you need to do is just change the file list.

C.1 Calculation of the statistic needed by this method

```
setwd("C:\\lixia document\\My R Files\\ms report\\test");

##the original dataset should be saved as a "*.csv" file.
##if the filename is "fad2.csv", then the the tablename should be "fad2".

tablename <- c("FAD2");

##the sample size for the control group
nc<-5;

##the sample size for the treat group
nt<-5;

############## nothing needs to be changed below ########################

Pval3.rand<-function(data){
#This function does a randomization test for two sample microarray data
#and will be called in the following step
#Version 3 is designed to run faster
pval<-0
k<-dim(data)[1]
N<-dim(data)[2]
n<-N/2
```

```
m <- 2^N
v <- 1:m
mat <- matrix(rep(v - 1, rep(N, m)) %/% 2^(0:(N - 1)) %% 2, ncol = m)
test <- apply(mat, 2, sum)
trt <- mat[, test == (n)]
samps<-dim(trt)[2]
samps<-samps/2
trt<-trt[,1:samps]
trt <<- trt     #trt is the incidence matrix
R.Test<-rep(0,k)

sum1<-0
sum2<-0
for(i in 1:n){
sum1<-data[,i]+sum1
sum2<-data[,(n+i)]+sum2
}
mu1<-sum1/n
mu2<-sum2/n
d.obs<-mu1-mu2
d.obs<-round(d.obs,4)

for(j in 1:samps){
tt<-trt[,j]
x<-data[,tt==1]
y<-data[,tt==0]
sum1a<-0
sum2a<-0
for(i in 1:n){
sum1a<-x[,i]+sum1a
sum2a<-y[,i]+sum2a
```

```
}
mu1a<-sum1a/n
mu2a<-sum2a/n
d.rand<-mu1a-mu2a
d.rand<-round(d.rand,4)
test<-rep(0,k)
test[abs(d.rand)>=abs(d.obs)]<-1
R.Test<-R.Test+test
}
pval<-R.Test/samps
pval<<-pval
return("done, results in pval")
}

## This part call the function Pval3.rand to calculate
## the randomization p-values

filename1<-paste(tablename,".csv",sep="");
filename2<-paste("result_",tablename,".csv",sep="");

a<-read.csv(filename1,row.names=1)[,c(1:(nc+nt))];
x<-apply(a[,c(1:nc)],1,mean);
y<-apply(a[,c((nc+1):(nc+nt))],1,mean);
d<-x-y;

Pval3.rand(a[,1:(nc+nt)]);

rna<-rownames(a);
z<-cbind(d,pval);
rownames(z)<-rna;
```

```
r<-data.frame(z);
write.csv(r,file=filename2,row.names=TRUE,append = FALSE);

## arrange the dataset to a format easily for calculation;
## the data was set in the formation of the reactant_product pairs
## the first five columns are the reactant in the wildtype
## the second five columns are the reatant in the mutant group
## the third five columns are the product in the wildtype
## the forth five columns are the product in the mutant group
## rrx and rry was calculated by the program: pval3rand.r and pval3rand_head.r
## rrx is the randomeration p_values for reactant in wildtype and mutant group
## rry is the randomeration p_values for product in wildtype and mutant group

dat<-read.csv(filename1,header=T,row.names=1)[,c(1:(nc+nt))];
rrdat<-read.csv(filename2,header=T,row.names=1);
lipidname<-rownames(dat);
result=NULL;
for (n1 in 1:141) {
    lipid1 <- lipidname[n1];
    x <- dat[n1,];
    rrx <- rrdat[n1,2];
    for (n2 in 1:141) {
            lipid2 <- lipidname[n2];
            y <- dat[n2,];
            rry <- rrdat[n2,2];
            if (n1 != n2) {
                    lipid12<-paste(lipid1,"_",lipid2,sep="");
                    cresult<-cbind(x,y,lipid1,lipid2,rrx,rry);
                    rownames(cresult)<-lipid12;
                    result<-rbind(result,cresult);
            }
```

```
    }
}

## calculate the tscore;
## x1 is calculated based on the reactant data from the wildtype
## y1 is calculated based on the reactant data from the mutant group
## x2 is calculated based on the product data from the wildtype
## y2 is calculated based on the product data from the mutant group
## x1bar is the mean for the reactant from wildtype
## y1bar is the mean for the reactant from the mutant group
## x2bar is the mean for the product from wildtypd
## y2bar is the mean for the product from mutant group

dat<-result;
lipidname<-rownames(dat);
dat$x1bar<-apply(dat[1:nc],1,mean);
dat$y1bar<-apply(dat[(nc+1):(nc+nt)],1,mean);
dat$x2bar<-apply(dat[(nc+nt+1):(nc+nt+nc)],1,mean);
dat$y2bar<-apply(dat[(nc+nt+nc+1):(nc+nt+nc+nt)],1,mean);
dat$d1bar<-dat$x1bar - dat$y1bar;
dat$d2bar<-dat$x2bar - dat$y2bar;
dat$sx1<-apply(dat[1:nc],1,var);
dat$sy1<-apply(dat[(nc+1):(nc+nt)],1,var);
dat$sx2<-apply(dat[(nc+nt+1):(nc+nt+nc)],1,var);
dat$sy2<-apply(dat[(nc+nt+nc+1):(nc+nt+nc+nt)],1,var);

covx1<-0;
for (i in 1:nc) {
    covx1<-covx1+(dat[i]-dat$x1bar)*(dat[nc+nt+i]-dat$x2bar) ;
}
covx1<-covx1/(nc*(nc-1));
```

```
covy1<-0;
for (i in 1:nt) {
    covy1<-covy1+(dat[nc+i]-dat$y1bar)*(dat[nc+nt+nc+i]-dat$y2bar);
}
covy1<-covy1/(nt*(nt-1));

tscore<-(dat$d2bar-dat$d1bar)/
        sqrt((dat$sx1)/nc+(dat$sy1)/nt+(dat$sx2)/nc+(dat$sy2)/nt-2*covx1-2*covy1);

sp1 <- sqrt(((dat$sx1)*(nc-1) + (dat$sy1)*(nt-1))/(nc+nt-2));
sp2 <- sqrt(((dat$sx2)*(nc-1) + (dat$sy2)*(nt-1))/(nc+nt-2));

a<-dat[,-c(1:(nc+nt+nc+nt))];
a$d1bar_d2bar<-a$d1bar - a$d2bar;
aa<-a[,c(1,2,3,4,9,10,15)];

b<-cbind(tscore,sp1,sp2);
rownames(b)<-lipidname;
colnames(b)<-c("tscore","sp1","sp2");

c<-cbind(aa,b);
write.csv(file=filename2,c,append=F,row.names=T);
```

C.2 Getting the most possible reactions by optimizing cut-off values

```
setwd("C:\\lixia document\\My R Files\\ms report\\test");

/*rank for t-scroe. take NA out of consideration and choose a number 450*/
/*as the cutoff value. then add the number of NA for each dataset to 450*/
```

```
tablename<-c("FAD2");
cut_tscore<-34.053425;
############ nothing needs to be changed below ###############

filename1<-paste("result_",tablename,".csv",sep="");
filename2<-paste("cutoff_",tablename,".csv",sep="");

x<-read.csv(filename1,header=T,row.names=1);
x1<-x[x[,"rrx"]<=.007937,]
x2<-x1[x1[,"rry"]<=.007937,]
x3<-x2[x2[,"d1bar"]<(-3) * x2[,"sp1"],]
x4<-x3[x3[,"d1bar_d2bar"]<0,]
x5<-x4[x4[,"tscore"]>=cut_tscore,]
x6<-x5[x5[,"d2bar"]>3 * x5[,"sp2"],]
m<-x6[order(x6[,"tscore"],decreasing = TRUE),]
write.csv(file=filename2,m,append=F,row.names=T);
```

C.3 Calculate the number of times a lipid appearing as a reactant in each experiment

```
setwd("C:\\lixia document\\My R Files\\ms report");
tablename <- c("FAD2","FAD3","FAD4","FAD5","FAD6","FAD7",
"SFD1","SFD2_2","SFD3");

tmpna<-read.csv('t_nmol_FAD2.csv',header=T)[1:141,1];
tmpno<-rep(0,141);

for (i in 1 : 9) {

    filename1<-paste("cutoff_",tablename[i],".csv",sep="");
```

```
    dat<-read.csv(filename1,header=T,row.names=1);
    lipid1<-dat$lipid1;
    lipid2<-dat$lipid2;
    lipid<-rep(1,nrow(dat));

    reactantna<-c(as.character(tmpna),as.character(lipid1));
    reactantno<-c(tmpno,lipid);
    factor(reactantna);
    reactant<-tapply(reactantno,reactantna,sum);

    productna<-c(as.character(tmpna),as.character(lipid2));
    productno<-c(tmpno,lipid);
    factor(productna);
    product<-tapply(productno,productna,sum);

    if (i==1) {
            tmp_reactant <- reactant
            tmp_product <- product
    }
    else {
            tmp_reactant <- cbind(tmp_reactant,reactant)
            tmp_product <- cbind(tmp_product,product)
    }
}

colnames(tmp_reactant)<-tablename;
write.csv(tmp_reactant,file="single_reactant.csv",append=FALSE)
colnames(tmp_product)<-tablename;
write.csv(tmp_product,file="single_product.csv",append=FALSE)
```

C.4 Permutation test

```
#permutation test  by Gary
#remove zeros, use prob from chisq

setwd("C:\\lixia document\\My R Files\\ms report");

single.reactant <- read.csv("single_reactant.csv",header=TRUE,row.names=1)
x<-as.matrix(single.reactant)
c1<-dim(x)[2]
z<-(1:c1)[apply(x,2,sum)==0]
x2<-x[,-z]

J<-dim(x2)[2]
nam<-unlist(dimnames(x2)[2])
result<-matrix(0,ncol=J,nrow=J)
dimnames(result)[2]<-list(nam)
dimnames(result)[1]<-list(nam)
d<-matrix(0,ncol=J,nrow=J)
dimnames(d)[2]<-list(nam)
dimnames(d)[1]<-list(nam)
pchi<-matrix(0,ncol=J,nrow=J)
dimnames(pchi)[2]<-list(nam)
dimnames(pchi)[1]<-list(nam)
p1<-matrix(0,ncol=J,nrow=J)
dimnames(p1)[2]<-list(nam)
dimnames(p1)[1]<-list(nam)

for(i in 1:(J-1)){
    for(j in (i+1):J){

            y1<-x2[,i]
```

```
            y2<-x2[,j]

            y<-cbind(y1,y2)

            tt<-apply(y,1,sum)

            o1<-y[tt>0,]
            pval<-fisher.test(o1,workspace=2000000)$p.value

            p1[i,j]<-pval

            C<-apply(o1,1,sum)
            n<-apply(o1,2,sum)
            N<-sum(n)
            E<-C%*%t(n)/N

            t1<-(o1-E)^2/E

            r1<-length(n)
            c1<-length(C)
            test<-sum(t1)

            result[i,j]<-test
            df<-dim(o1)[1]-1
            pchi[i,j]<-pchisq(test,df)
            d[i,j]<-df
    }
}
```