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Metabolomics Approach using LC-Orbitrap High Resolution Mass Spectrometry and Chemometrics for Authentication of Beef Meats from Different Origins in Indonesia

(Pendekatan Metabolomik menggunakan Spektrometri Jisim Resolusi Tinggi LC-Orbitrap dan Kemometrik untuk Pengesahan Daging Lembu daripada Asalan Berbeza di Indonesia)

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ABSTRACT

Beef is one of the favourite meats consumed by people worldwide due to its high nutrition value needed by human development. It is highly susceptible for the adulteration practice by substituting beef with lower price meats by unethical meat traders due to the economic reasons. Therefore, the authenticity of beef meat (BM) is important because it is also related to halal status of meat which is required for certain religions. This research aimed to differentiate metabolites of BM from different origins using liquid chromatography-high resolution mass spectrometry (LC-HRMS) combined with chemometrics for the authentication purposes. Various metabolites mostly amino acids and lipids could be detected using methanol extraction. Principal component analysis (PCA), partial least square-discriminant analysis (PLS-DA) and sparse PLS-DA were successfully used to discriminate BMs from different origins. Fifty potential metabolite markers which are important for discrimination have been identified using variable importance projection (VIP) value extracted from PLS-DA analysis. Metabolites of (*4S)-4-{[(9Z*)-3-Hydroxy-9-hexadecenoyl] oxy}-4-(trimethylammonio)butanoate, *N,N*-Diisopropylethylamine (DIPEA), D-sphingosine, (*2E,4Z*)-*N*-Isobutyl-2,4-octadecadienamide, 1-(14-methylhexadecanoyl)pyrrolidine, linoleic acid, 12-HAS, dodecylamine1, myristamide, and tributyl phosphate had high responsibility in discriminating BMs from different origins (VIP value > 2.0). It can be concluded that LC-HRMS based untargeted metabolomics combined with chemometrics could be used for authentication of BMs from different regions.

Keywords: Beef meat; *halal* authentication; LC- HRMS; PLS-DA; untargeted metabolomics

ABSTRAK

Daging lembu ialah salah satu daging kegemaran yang dimakan di seluruh dunia kerana nilai pemakanannya yang tinggi yang diperlukan oleh tumbesaran manusia. Ia sangat terdedah kepada amalan pemalsuan dengan menggantikan daging lembu dengan harga daging yang lebih rendah oleh peniaga daging yang tidak beretika atas sebab ekonomi. Oleh itu, keaslian daging lembu (BM) adalah penting kerana ia juga berkaitan dengan status halal daging yang dituntut bagi agama tertentu. Penyelidikan ini bertujuan untuk membezakan metabolit BM daripada punca yang berbeza menggunakan spektrometri jisim resolusi tinggi kromatografi cecair (LC-HRMS) digabungkan dengan kemometrik untuk tujuan pengesahan. Pelbagai metabolit kebanyakannya asid amino dan lipid boleh dikesan menggunakan pengekstrakan metanol. Analisis komponen utama (PCA), analisis diskriminasi kuasa dua terkecil separa (PLS-DA) dan jarang PLS-DA berjaya digunakan untuk mendiskriminasi BM daripada punca yang berbeza. Lima puluh penanda

metabolit berpotensi yang penting untuk diskriminasi telah dikenal pasti menggunakan nilai unjuran kepentingan berubah (VIP) yang diekstrak daripada analisis PLS-DA. Metabolit (4S)-4-{[(9Z)-3-Hidroksi-9-heksadesenoil] oksi}-4-(trimetilammonio)butanoate, N,N-Diisopropylethylamine (DIPEA), D-sphingosine, (2E,4Z) -N-Isobutyl-2,4-octadecadienamide, 1-(14-metilheksadesenoil)pyrrolidine, asid linoleik, 12-HAS, dodecylamine1, myristamide dan tributil fosfat mempunyai tanggungjawab yang tinggi dalam mendiskriminasi BM daripada punca yang berbeza (nilai VIP > 2.0). Dapat disimpulkan bahawa metabolomik tidak disasarkan berasaskan LC-HRMS digabungkan dengan kemometrik boleh digunakan untuk pengesahan BM dari kawasan yang berbeza.

Kata kunci: Daging lembu; pengesahan halal; LC- HRMS; PLS-DA; metabolomik tidak disasarkan

Introduction

Food authenticity is an important issue due to the increased reports of mislabelling, substitution, and adulteration in the food products. The main objective of these fraudulent practices is for economic reasons to gain more profits, for instance, high quality foods are often adulterated using lower price foods (Böhme et al. 2019). However, the adulteration is obviously associated with some negative impacts that could affect the quality and safety of food products (Schieber 2018). In addition, the adulteration using non-halal components such as in meat and meat-based food products is also a serious concern because several religions such as Muslim and Jewish have strict rule to avoid the consumption of non-halal meats (Martuscelli et al. 2020). The consumption of meat and meat products has increased every year which makes the increasing demand on meats. However, meat is susceptible for the adulteration practice because it is easy to blend high quality meat with other meats from other species without any significant change in visual appearance (Owolabi & Olayinka 2021). Beef meat (BM) is consumed worldwide due to its nutrition values which are benefits for the human health. Due to its high price of high-quality BM, BM is subjected to be adulterated using lower price and non-halal meats such as pork (Pranata et al. 2021). Therefore, the authentication of BM is required to ensure its authenticity, quality, and safety.

Numerous analytical methods could be used for the authentication of BM such as chromatographic-based methods including gas chromatography coupled with flame ionization and mass spectrometer detectors and liquid chromatography hyphenated with various detectors including UV-Vis, fluorescence, photodiode array, and mass spectrometer (Häfner, Kalkhof & Jira 2021; Perez-Palacios et al. 2022; Von Bargen, Brockmeyer & Humpf 2014). Rapid methods based on vibrational spectroscopic techniques such as Fourier transform infrared (FTIR) (Rohman et al. 2016), near infrared (NIR) (Leng et al. 2020), and Raman spectroscopy combined with chemometrics (Motoyama et al. 2018) have been used for the meat authentication using their fingerprint spectra. Currently, analytical methods for metabolomics approach such as nuclear magnetic resonance spectrometry (NMR) (Wang et al. 2020), gas chromatography mass spectrometry (GC-MS) (Trimigno et al. 2018), liquid chromatography mass spectrometry (LC-MS) (Jia et al. 2021) have been developed for food authentication including meat and meat products. Liquid chromatography high resolution mass spectrometry using time of flight (TOF) and Orbitrap mass analyser provides high resolving power associated to high sensitivity and high specificity for analysis of food products (Chan et al. 2021; Panseri et al. 2022). Powerful statistical analysis such as chemometrics or multivariate data analysis has been employed for treating big data analysis coming from instrumental responses obtained from metabolomics studies. Chemometrics is capable of processing and handling the vast number of data becoming more interpretable (Callao & Ruisánchez 2018).

The authentication of BM from different geographical origins (Australia, Korea, New Zealand, and United States) has been performed by metabolomics approach using NMR spectroscopy combined with principal component analysis (PCA) and orthogonal projections to latent structures-discriminant analysis (OPLS-DA) (Jung et al. 2010). Metabolomics analysis for authentication of BF from Japan, United States, and Australia has been successfully carried out by using LC-HRMS and GC-MS. The detailed chemical compositions could be obtained using these approaches which are important for BF differentiation (Man et al. 2021). In addition, lipidomics approaches using DART-QTOF (direct analysis in real time-quadrupole time of flight) and LC-ESI-QTOF (liquid chromatography-electrospray ionization-quadrupole time of flight) have been applied for differentiation of

BMs from six different countries, namely Argentina, Brazil, Canada, Australia, New Zealand and Uruguay. PCA and support vector machine (SVM) were applied for metabolite discrimination (Wang et al. 2021).

However, to the best of our knowledge, reports on the authentication study of BMs from different origins in Indonesia are still lacking. Therefore, this research was conducted to apply an LC-HRMS technique for metabolomics analysis in combination with PCA, PLS-DA, and sparse PLS-DA for authentication of BMs from different origins in Indonesia. Therefore, this study was important to ensure the authenticity of BMs which are related to the quality, safety, as well as halal status of beef meats to protect consumers from product's mislabelling and adulteration practices.

Materials and Methods

CHEMICALS

The solvents of methanol and water (LC-MS grade) were purchased from Thermo Fisher (Thermo Scientific, USA). HPLC grade methanol and formic acid analytical grade were obtained from Merck (Darmstadt, Germany). The calibration solution for both ESI positive and ESI negative calibration was purchased from Thermo Fisher (Thermo Scientific, USA).

BEEF MEAT COLLECTION AND PREPARATION

Beef meats (BMs) were purchased from ten different regions in Indonesia; namely Borobudur (B1), Muntilan (B2), Tempel (B3), Klaten (B4), Gunungkidul (B5), Yogyakarta (B6), Bantul 1 (B7), Gamping (B8), Godean (B9), and Bantul 2 (B10). The BMs were obtained from three bovines (*Bos taurus*) from the loin part for each region. Samples were stored in the freezer (-20 °C) prior being used for extraction.

SAMPLES EXTRACTION

The BM samples from each different region were ground using a meat grinder (Tummy, China). Amount of 100 ± 5 mg sample was weighed using an analytical balance and placed into a 2 mL centrifuge tube. Sample was added with 1 mL of LC-MS grade methanol for metabolite extraction. Subsequently, the sample was vortexed (Nemco, Velp Scientifica, Italy) at room temperature (25 °C) for 2 min. After that, ultrasonication (Elmasonic S 60 H, Elma, Germany) was performed for deeper extraction of the metabolites at room temperature for 30 min. Centrifugation (Megafuge 8R, Thermo Scientific, USA) at 5000 rpm for 10 min was performed to separate pellet and supernatant. The supernatant was pipetted from each tube and a PTFE filter (0.22 µm) was used to filter the supernatant into a clear HPLC glass vial.

UNTARGETED METABOLOMICS USING LC-HRMS

A liquid chromatography (UHPLC Vanquish, Thermo Scientific, USA) connected with a mass spectrometer with high resolution (Q-Exactive, Orbitrap, Thermo Scientific, USA) was used for metabolomics analysis. The method used was according to previous method by Windarsih et al. (2022) with modification. Metabolite separation from methanol extract of meats was performed using an analytical column Accucore C18 (10 mm × 2.1 mm ID × 2.6 um). The mobile phase used was water (A) and methanol (B), both containing 0.1% formic acid. Samples were injected at 10 µL and eluted with flow of 0.3 mL/min. The elution used was gradient mode as follows: 0-5 min (5% B), 5-16 min (5% B – 90% B), 16-20 min (90% B), 20-25 min (95% B – 5% B). The parameters for MS condition such as capillary temperature was set at 320 °C, sheath gas flow rate was 32 AU, and auxiliary gas flow rate was 8 AU. The spray voltage was 3.5 kV with collision energy of 10 NCE. Analysis was performed both in full MS and dd-MS2 with resolution of 70,000 and 17,500, respectively. Scanning was performed either using positive and negative ionization modes.

DATA ANALYSIS

The total ion chromatogram (TIC) was exported using XCalibur (Thermo Scientific, USA). Compound Discoverer software (Thermo Scientific, USA) was used for data processing such as peak alignment, peak integration, baseline correction, and background correction. The identification of metabolites from TIC used untargeted metabolomics workflow. The metabolites were identified against databases of MzCloud (https://www.mzcloud.org/) and ChemSpider (http://www.chemspider.com/). Metabolites which have full match with MzCloud and ChemSpider were selected. The resulted compounds were filtered according to MS2 of DDA for preferred ion, mass tolerance of 5 ppm, and retention time tolerance of 0.2 min.

CHEMOMETRICS ANALYSIS

Data pre-processing was carried out using MetaboAnalyst 5.0 prior to chemometrics analysis including normalization and data scaling. The metabolites and their peak area were used as variables during the chemometrics modelling.

Sum area was chosen for data normalization whereas auto-scaling was selected for data scaling. Chemometrics analysis was performed using MetaboAnalyst 5.0. Principal component analysis (PCA) was initially used to identify pattern of BM from different origins. Then, partial least square-discriminant analysis (PLS-DA) and sparse PLS-DA (sPLS-DA) was applied for the discrimination and classification of samples. The discriminating metabolites having important roles in meat differentiation among origins was observed from the PLS-DA model using variable importance for projections (VIP) value.

Results and Discussions

LC-Orbitrap HRMS based metabolomics

The metabolites of BMs from different origins in Indonesia was successfully analysed using LC-Orbitrap HRMS. A total of 208 metabolites was annotated from both positive and negative ionization modes (Table S1). Various metabolites include amino acids, peptides, nucleotides, and lipids were found in BM extracted using methanol indicating high coverage of extraction using methanol. It has been reported that methanol become the most common extraction solvent used for the metabolomics analysis in plasma and tissue samples due to its high coverage to extract compounds (Zeki et al. 2020).

The amino acids contained in BMs obtained from this study were varied such as DL-lysine, L-histidine, N6,N6,N6-trimethyl-L-lysine, DL-alanine, D-(+)-Proline, L-glutamic acid, DL-glutamine, L-pyroglutamic acid, L-(-)-threonine, L-(-)-methionine, L-isoleucine, L-tyrosine, L-norleucine, alanyltyrosine, L-phenylalanine, DL-tryptophan, and leucylproline. Some lipids compound from different lipid classes were also found in BMs such as palmitoyl sphingomyelin, PC(o-18:0/18:2(9Z,12Z)), 1-stearoylglycerol, 1-oleoyl-2-hydroxy-sn-glycero-3-PE, lysoPC(18:3(9Z,12Z,15Z)), and fatty acids (oleic acid, linoleic acid, γ-linolenic acid, palmitoleic acid, 8Z,11Z,14Z-eicosatrienoic acid, 3-(Icosanoyloxy)-4-(trimethylammonio) butanoate, 3-[(12-hydroxyoctadecanoyl)oxy]-4-(trimethylammonio)butanoate, (4S)-4-[(9Z,12Z,15Z)-9,12,15-octadecatrienoyloxy]-4-(trimethylammonio) butanoate, and (4S)-4-{[(9Z)-3-hydroxy-9-hexadecenoyl]oxy}-4-(trimethylammonio)butanoate). The amino acids and lipids varied among BMs from different origins as shown by the variation in the peak area. Therefore, the information on the metabolite compositions is important for differentiation and discrimination of BM from the different origins. Moreover, the metabolites composition could be further used for developing the discrimination and classification models using chemometrics analysis.

Previous research on the metabolomics analysis for differentiation of BM obtained from Australia, Korea, New Zealand, and United States using ^{1}H-NMR technique demonstrated that the signals of carnosine and anserine were dominant in all samples. In addition, various amino acids such as glutamine, glutamate, tyrosine, phenylalanine, methionine, valine, leucine, isoleucine, and alanine were also found (Jung et al. 2010). Another study on the metabolomics analysis for differentiation of BM from Japan, Australia, and United States using a modified Bligh and Dyer extraction method showed different metabolites either polar such as amino acids and non-polar such as lipids in BM (Man et al. 2021). In the present study, the use of methanol as extraction solvent could extract various metabolites from polar to semi polar.

Analysis using principal component analysis (PCA)

PCA was applied to identify pattern of BM from different origins. Five principal components (PC) from PCA were successfully used to differentiate beef meat from different regions as depicted in the PCA score plot (Figure 1). BMs were clustered into four main clusters. The first cluster consist of beef B1, B4, B5, B6, and B7 which appeared in one tight cluster. Secondly, BMs of B8 and B9 are grouped into the similar area. Meanwhile BF of B2 appeared in one cluster close to the first cluster. The last, BM of B10 appeared in a different region far from the other clusters. Based on PCA's loading plots, the metabolites of hypaphorine, acetyl methyl choline, 3-Methylsulfolene, and inosine-5-monophosphate were responsible for differentiation of BM B10 (Bantul 2) among others. These compounds were significantly found in high peak area in B10, as shown in the Box-plot (Figure 2).

Samples which appeared close to each other in PCA score plot indicated their high similarity in their metabolite compositions, whereas samples which observed far from other samples indicated the high dissimilarity meaning the more differences in their

metabolite compositions. PCA is an unsupervised pattern recognition of qualitative chemometrics analysis to recognize pattern by reducing the vast number of variables into principal components (PC) (Worley & Powers 2016). It has been widely used as the first step in metabolomics analysis to identify pattern without time consuming. Previous study reported that PCA could be used to differentiate BM from six countries (Argentina, Australia, Brazil, Canada, New Zealand, and Uruguay) using the lipid compounds (Wang et al. 2021). In addition, PCA has also been successfully used in other meat research such as differentiation of concentrate-fed and pasture-fed of goat meat (Wang et al. 2021), and differentiation of normally slaughtered and dead-on chicken meat (Sidwick et al. 2017).

The information in PCA analysis is essential to know the metabolite compositions of beef meat from different origins. The PCA analysis is very useful for differentiation of beef meats from different origins based on the similarity and dissimilarity of their metabolite compositions. It can be very helpful when choosing beef meat with certain metabolites target by using PCA. The PCA analysis is also important to authenticate beef meat from each origin that support the halal authentication to ensure the halal authenticity of beef meats obtained from different origins.

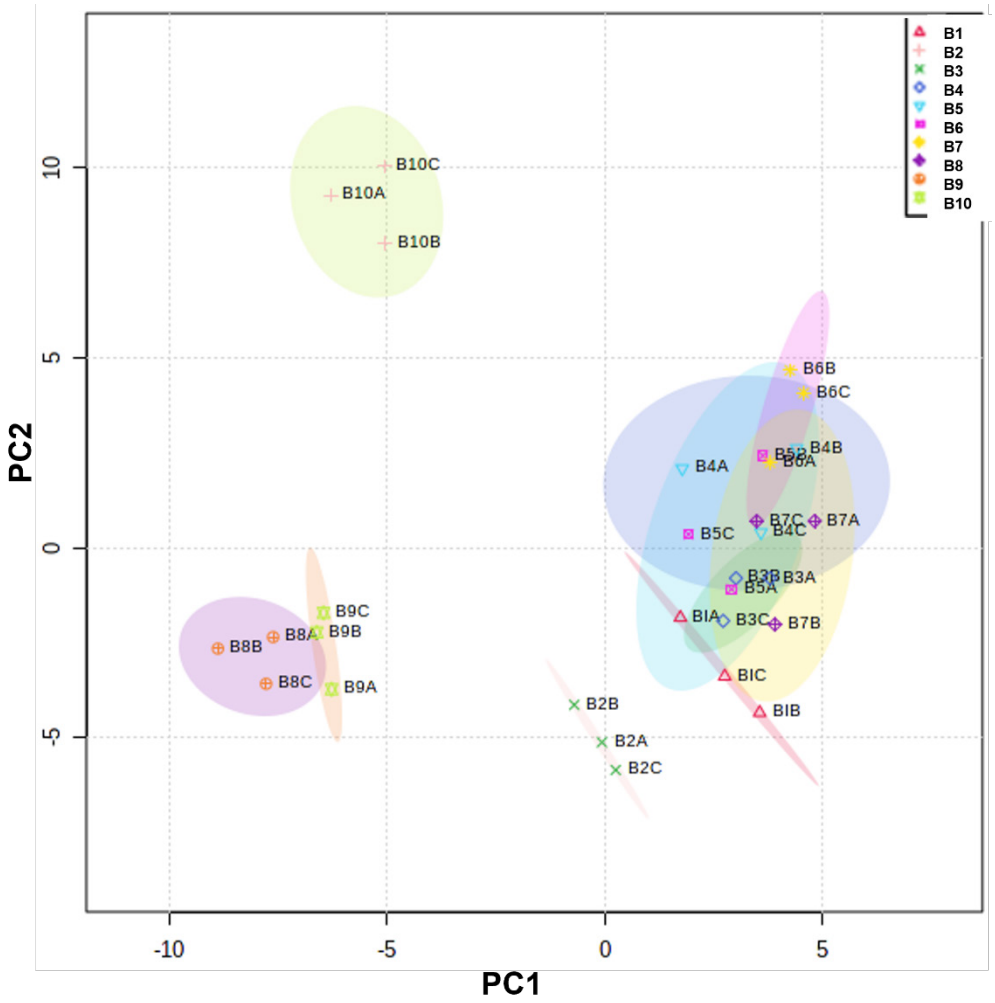

FIGURE 1. Principal component analysis (PCA) of beef meat obtained from different origins in Indonesia (B1=Borobudur, B2=Muntilan, B3=Tempel, B4=Klaten, B5=Gunungkidul, B6=Yogyakarta, B7=Bantul 1, B8=Gamping, B9=Godean, and B10=Bantul 2; each region was measured in three replicates)

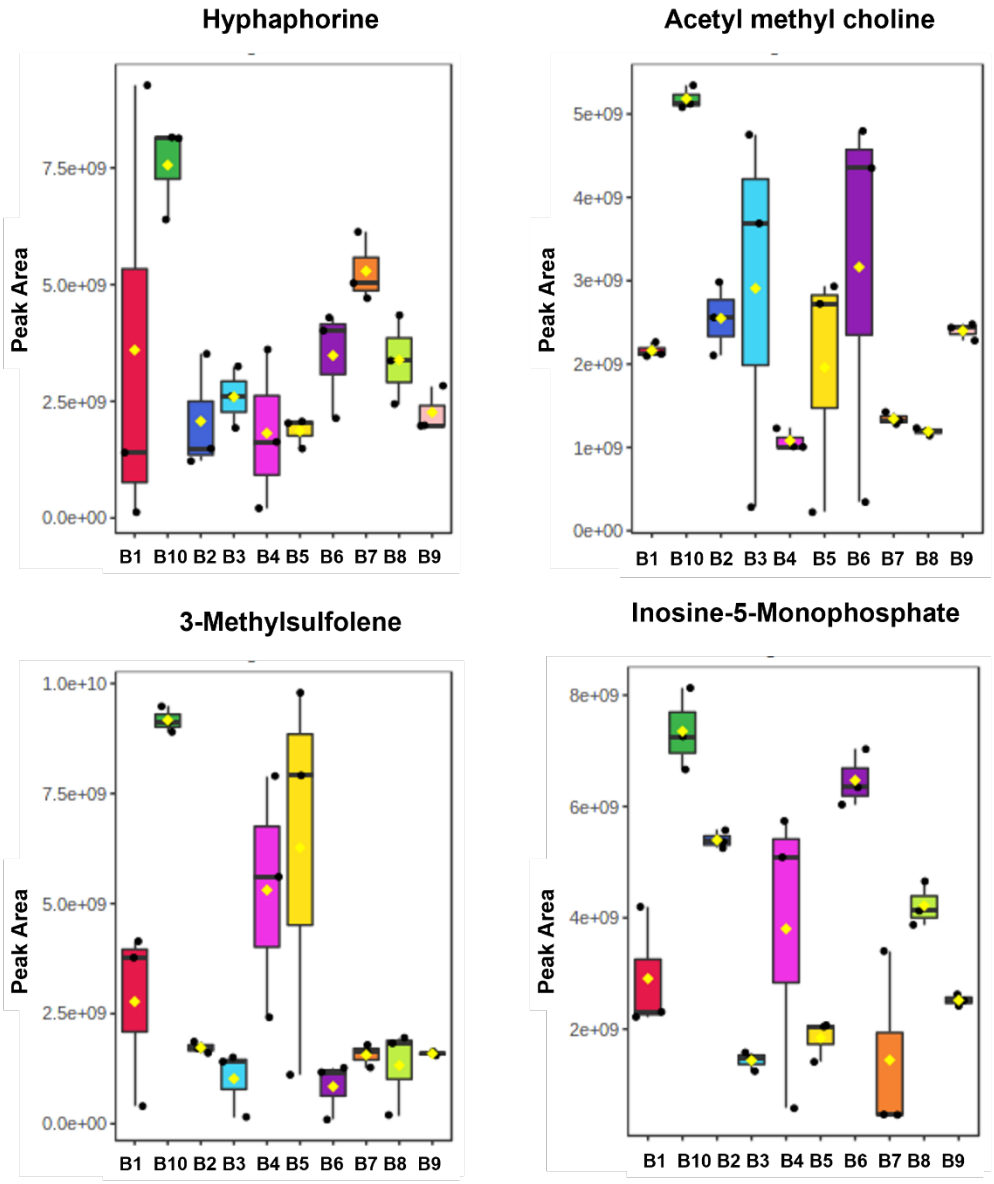

FIGURE 2. Box-plot of metabolites from PCA loading plot responsible for differentiation of beef meat B10 (B1=Borobudur, B2=Muntilan, B3=Tempel, B4=Klaten, B5=Gunungkidul, B6=Yogyakarta, B7=Bantul 1, B8=Gamping, B9=Godean, and B10=Bantul 2)

CLASSIFICATION USING SUPERVISED PATTERN RECOGNITIONS

Analysis using PLS-DA was successfully used for discrimination and classification of BMs from different origins. The result differs from the differentiation result obtained from PCA analysis. PLS-DA could maximize the variation in the dataset resulting better separation. Each class appeared in the separate cluster except in BF samples of B3 and B4 (Figure 3). PLS-DA search the latent variables among the datasets than only principal components. The latent variables are capable of searching the relationship between x-matric and y-predicted to maximize the variation. The variables having high responsibility in discrimination of each class were observed using variable importance for projections (VIP) value. The value of VIP which is more than 1 is known for its big role in discrimination, thus potential to be identified as potential markers (Paul, De & Harrington 2021). Table 1 shows 50 metabolites obtained from VIP value more than 1, which were responsible in classification of BM samples from ten different origins. The metabolites are from fatty acids, lipids, and peptides class. Among those variables, 10 metabolites were found to have VIP value more than 2.0 such as (4S)-4-{[(9Z)-3-Hydroxy-9-hexadecenoyl]oxy}-4-(trimethylammonio)butanoate, N,N-Diisopropylethylamine (DIPEA), D-Sphingosine, (2E,4Z)-N-Isobutyl-2,4-octadecadienamide, 1-(14-methylhexadecanoyl)pyrrolidine, linoleic acid, 12-HAS, dodecylamine, myristamide, and tributyl phosphate. This indicated their crucial role of VIP in BM differentiation because the higher the VIP value of metabolites, the more the role of metabolites for discrimination. The distribution of these variables among BM from ten different origins were demonstrated in the Box-plot (Figure 4). The use of PLS-DA has been successfully proven to discriminate beef from Japan, Australia, and United States by previous researchers resulting better differentiation result than using PCA. Amino acids and their derivatives as well as lipids such as PC (phosphatidylcholine) and LysoPE (Lyso phosphatidylethanolamine) were found as potential biomarkers (Man et al. 2021). The differences in metabolites might be a result from the differences in bovine husbandry practices in each origin (Saleem et al. 2012).

Apart from PLS-DA, sparse PLS-DA was also applied for differentiation of BM from different origins. The result showed that the classification pattern had more similar overview (Figure 3) with the PCA result. However, B2 did not appear as a single class like in PCA. Only BM of B10 appeared in a single class far from other classes. Sparse PLS-DA is similar to PLS-DA; however, it has one step procedure in variable selection and classification. The contribution of irrelevant variables could be reduced; therefore, it could maximize the role of important variables to build the latent components which contributed to the most discrimination variables among BM samples (Jiménez-Carvelo et al. 2021). The metabolites important for discrimination in sPLS-DA observed using the loading plots were compiled in Table 2. The present study showed that PLS-DA resulted better discrimination of BM samples from different origins compared to sPLS-DA. It might be the simultaneous step of variable selection and classification does not always provide a better discrimination as in PLS-DA (Paul, De & Harrington 2021).

Supervised methods such as PLS-DA and sPLS-DA are susceptible for model overfitting. To avoid the negative effect of model overfitting, validation test is carried out to evaluate the developed PLS-DA and sPLS-DA models. The PLS-DA was validated using cross validation employing leave one out technique and permutation test. The cross-validation technique using 3 components (Q2) confirmed the PLS-DA model validity with R2Y value of 0.9960 and Q2 value of 0.5746. Meanwhile, permutation test also confirmed the validity through the significant p value (p value < 0.05). The observed p-value from 1000 permutation was 0.031. The cross validation and permutation test results were supplemented in Figure S1 (supplementary files). Validation of sPLS-DA model using leave one out cross validation technique also confirmed the model validity. Therefore, both models had high accuracy and predictivity and were free from model overfitting. Validation techniques such as cross validation and permutation test have been widely used to validate supervised pattern recognition techniques such as PLS-DA, sPLS-DA, and OPLS-DA applied for discrimination of various types of samples. The results of validation test could warrant the performance of those models (Paul, De & Harrington 2021).

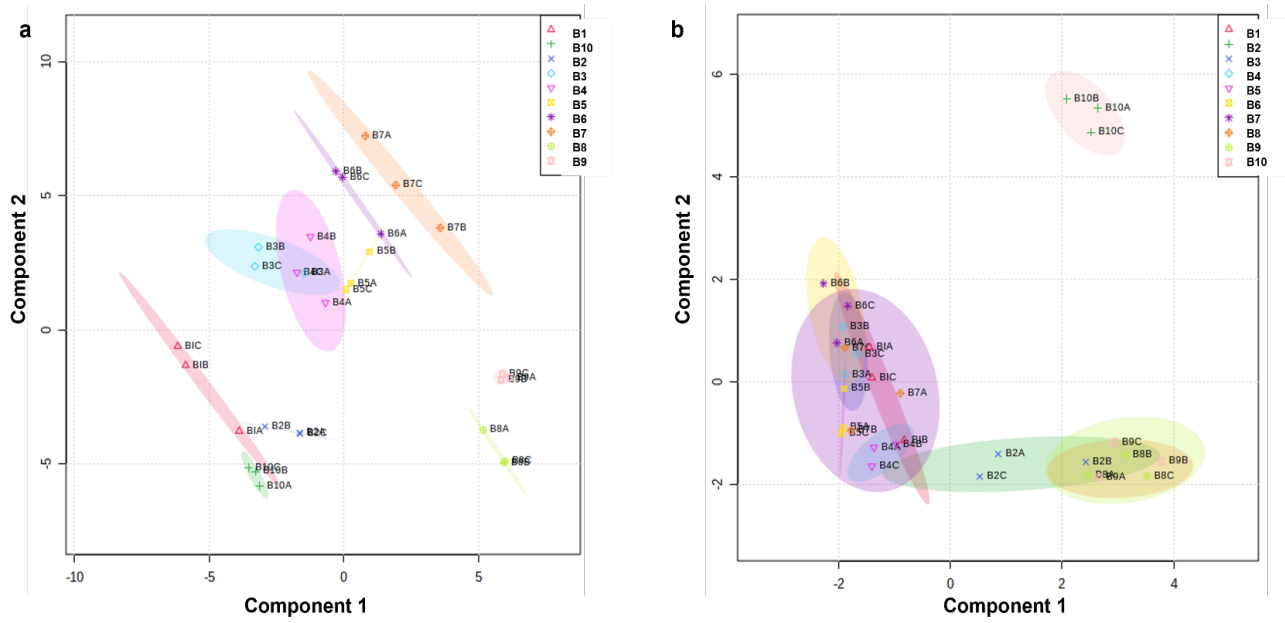

FIGURE 3. Partial least square-discriminant analysis (A) and sparse partial least square-discriminant analysis (B) for discrimination and classification of beef meats from different origins in Indonesia (B1=Borobudur, B2=Muntilan, B3=Tempel, B4=Klaten, B5=Gunungkidul, B6=Yogyakarta, B7=Bantul 1, B8=Gamping, B9=Godean, and B10=Bantul 2; each region was measured in three replicates)

TABLE 1. Potential metabolite markers to differentiate beef meats from different origins in Indonesia obtained from variable importance for projections (VIP) value analysis

No.	Compounds	VIP Value
1.	(4S)-4-{[(9Z)-3-Hydroxy-9-hexadecenoyl]oxy}-4-(trimethylammonio)butanoate	2.96
2.	N,N-Diisopropylethylamine (DIPEA)	2.71
3.	D-Sphingosine	2.37
4.	(2E,4Z)-N-Isobutyl-2,4-octadecadienamide	2.32
5.	1-(14-methylhexadecanoyl)pyrrolidine	2.30
6.	Linoleic acid	2.28
7.	12-HSA	2.25
8.	Dodecylamine.1	2.19
9.	Myristamide	2.12
10.	Tributyl phosphate	2.00
11.	cis-5-Tetradecenoylcarnitine	1.99
12.	3-Methylhistidine	1.98
13.	1-Heptanethiol	1.89
14.	4-Dodecylbenzenesulfonic acid	1.85
15.	1-Linoleoyl-2-Hydroxy-sn-glycero-3-PC	1.82

16.	(2E)-hexadecenoylcarnitine	1.80
17.	3-hydroxyhexadecanoylcarnitine	1.73
18.	Hexanoylcarnitine	1.73
19.	Ebelactone B	1.69
20.	Platelet-activating factor	1.63
21.	2-(2-amino-3-methylbutanamido)-3-phenylpropanoic acid	1.61
22.	1-(6-Nonyl-3-pyridinyl)-1-decanone	1.61
23.	4-Undecylbenzenesulfonic acid	1.59
24.	Octacosyl (2E)-3-(3-hydroxy-4-methoxyphenyl)acrylate	1.58
25.	Nicotinamide	1.57
26.	ACPC	1.52
27.	3-Methylsulfolene	1.51
28.	Biacetyl	1.50
29.	3-BHA	1.50
30.	D-ribose 5-phosphate	1.50
31.	O-heptanoylcarnitine	1.47
32.	N,N-Dimethyldecylamine N-oxide	1.47
33.	Propionylcarnitine	1.47
34.	Inosine	1.45
35.	Dodecyl sulfate	1.45
36.	Decanoylcarnitine	1.44
37.	Acetyl-methylcholine	1.37
38.	11(Z),14(Z)-Eicosadienoic acid	1.35
39.	N6,N6,N6-Trimethyl-L-lysine	1.35
40.	3-Hydroxy-3-[(3-methylbutanoyl)oxy]-4-(trimethylammonio)butanoate	1.32
41.	Leu-Leu	1.32
42.	8Z,11Z,14Z-Eicosatrienoic acid	1.30
43.	Urolithin B	1.30
44.	O-heptadecanoylcarnitine	1.30
45.	5-hydroxy-4-methoxy-5,6-dihydro-2H-pyran-2-one	1.28
47.	(+)-Nootkatone	1.28
47.	4-Acetamidobenzoic acid	1.26
48.	27-Norcholestane-3,7,12,24,25,26-hexol, (3Î±,5Î²,7Î±,12Î±)	1.25
49.	Benzoic acid	1.25
50.	2,2’-Methylenebis(4-methyl-6-tert-butylphenol)	1.22

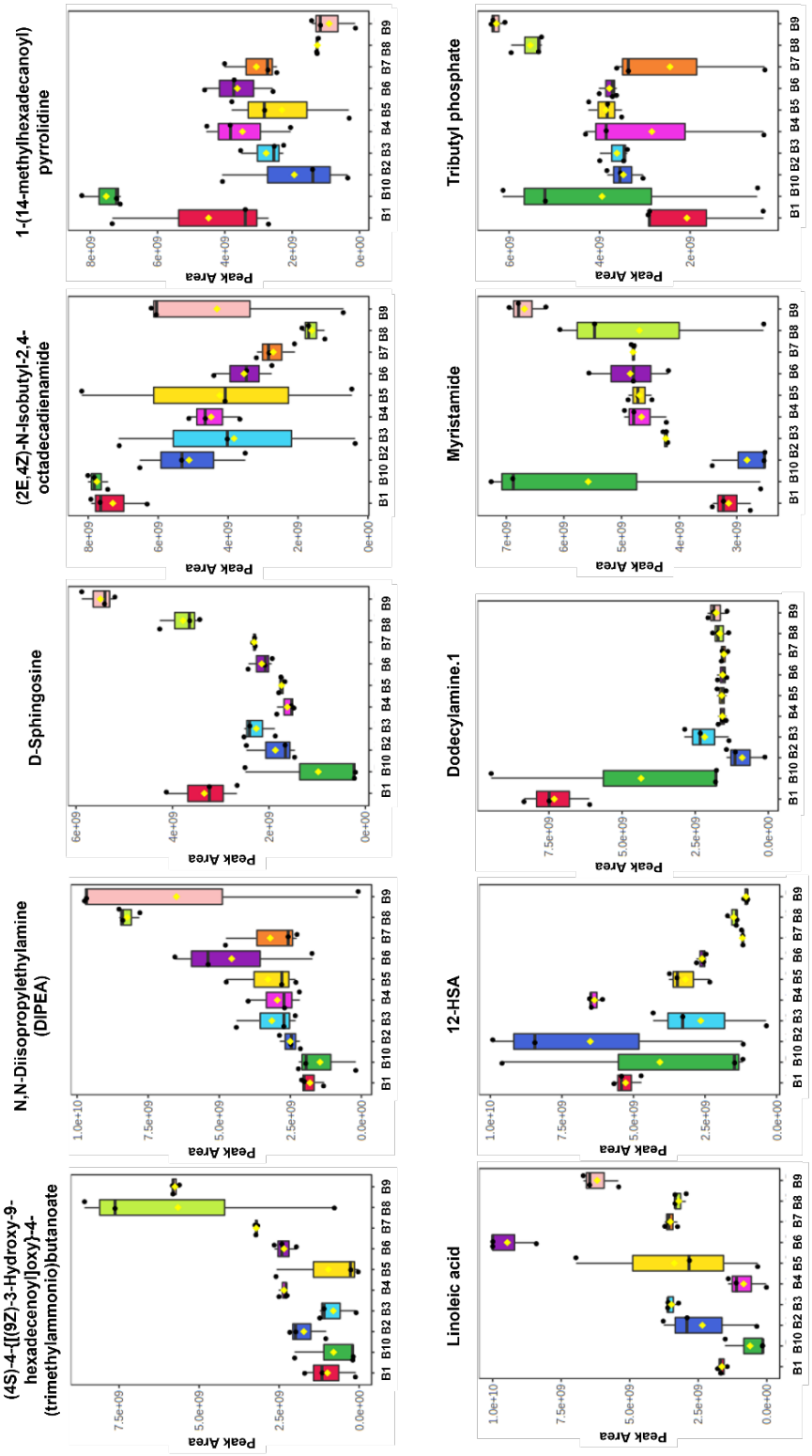

FIGURE 4. Box-plot of metabolites which have high responsibility for discrimination in PLS-DA model with VIP (variable importance for projections value) more than 2.0 (B1=Borobudur, B2=Muntilan, B3=Tempel, B4=Klaten, B5=Gunungkidul, B6=Yogyakarta, B7=Bantul 1, B8=Gamping, B9=Godean, and B10=Bantul 2)

TABLE 2. Responsible metabolites for classification using sparse partial least square-discriminant analysis through loading 1 and loading 2

No.	Compounds	
	Loading 1	Loading 2
1.	Bis(2-ethylhexyl) amine	Xanthine
2.	2,2'-Methylenebis(4-methyl-6-tert-butylphenol)	Octacosyl (2E)-3-(3-hydroxy-4-methoxyphenyl)acrylate
3.	D-ribose 5-phosphate	1-(14-methylhexadecanoyl)pyrrolidine
4.	Octadecanamine	2-(2-amino-3-methylbutanamido)-3-phenylpropanoic acid
5.	D-Panthothenic acid	N,N-Dimethyldecylamine N-oxide
6.	DL-Carnitine	Acetyl-?-methylcholine
7.	Butopyronoxyl	Tiglylcarnitine
8.	Stearic acid	hypaphorine
9.	Navenone A	Uric acid
10.	1-(2-Furyl)-N-({(2R,4S,5R)-5-[1-methyl-3-(2-naphthyl)-1H-pyrazol-5-yl]-1-azabicyclo[2.2.2]oct-2-yl}methyl) methanamine	Creatinine

CONCLUSIONS

The authenticity of beef meat is important to warrant that the products are free from mislabelling, substitution, and adulteration. Metabolomics approach using LC-HRMS and chemometrics analyses demonstrated good capability for authentication of beef meats from different origins in Indonesia. Principal component analysis successfully identified separation of beef meats from different origins based on the metabolite compositions. The discrimination and classification beef meats from ten different origins could be obtained using PLS-DA. Metabolites of (4S)-4-{[(9Z)-3-Hydroxy-9-hexadecenoyl]oxy}-4-(trimethylammonio)butanoate, N,N-Diisopropylethylamine (DIPEA), D-Sphingosine, (2E,4Z)-N-Isobutyl-2,4-octadecadienamide, 1-(14-methylhexadecanoyl)pyrrolidine, linoleic acid, 12-HAS, dodecylamine, myristamide, and tributyl phosphate were identified as important metabolites for discrimination and classification of beef meats from ten different origins. Sparse partial least square-discriminant analysis allowed for classification of beef meats and the responsible metabolites for classification both in loading 1 and loading 2 could be observed. Among the chemometrics used, PLS-DA provided the best discrimination result for differentiation of BM from different origins. It can be summarized that metabolomics approach using LC-HRMS and chemometrics is a reliable analytical technique that can be used for beef meats authentication from different origins.

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SUPPLEMENTARY FILES

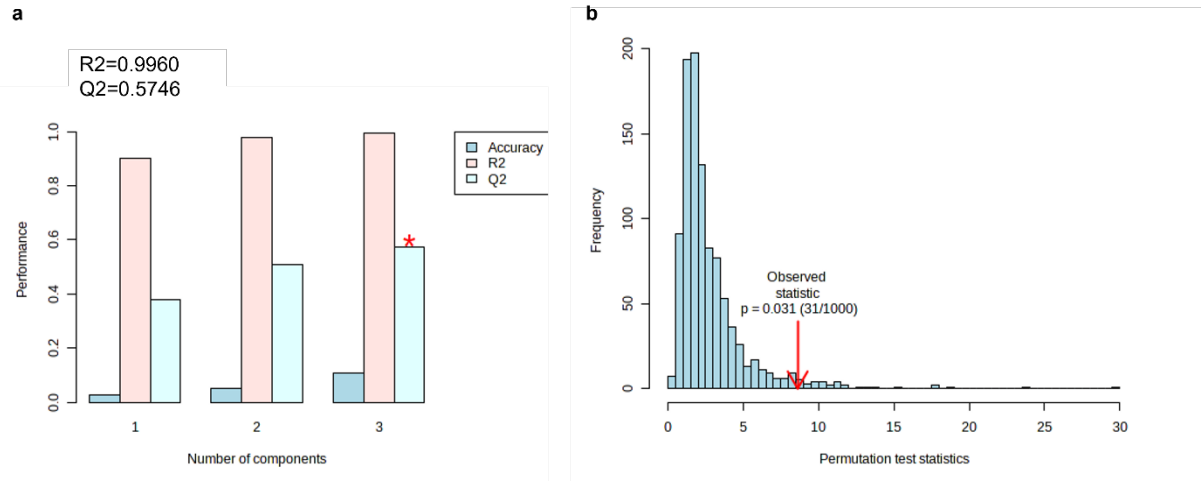

FIGURE S1. The graphic of cross validation (a) and permutation test (b) of the partial least square-discriminant analysis model to discriminate beef meats from different origins

SUPPLEMENTARY TABLE

Name	Formula	Annot. DeltaMass [ppm]	Calculated MW	RT [min]	Peak Area																								
					B1A	B1B	B1C	B2A	B2B	B2C	B3A	B3B	B3C	B4A	B4B	B4C	B5A	B5B	B5C	B6A	B6B	B6C	B7A	B7B	B7C	B8A	B8B	B8C	B9A	B9B	B9C	B10A	B10B	B10C
Gly-Lys	C8H17N3O3	-1.92	203.1266	0.61	66770.3435	67977.9918	106183.014	116243.038	61252.0616	138175.844	139218.599	199335.523	258076.996	79537.7158	66481.7561	104560.121	6648559.77	10975378.8	5947469.86	67783.0617	54096.2894	103115.298	1508263.15	1705339.27	113120.13	49989.3468	56240.4033	39318.6049	73893.5824	77088.7905	41987.1767	74029.4597	117853.452	113427.95
DL-Lysine	C6H14N2O2	-1.11	146.1053 6	0.636	17394142.5	20429570.3	20893582.6	42203274.8	24269307.4	31549577.2	9003966.47	5247224.57	9227099.92	32782305.8	25577078.6	25711470.5	8426329.27	7896656.22	1522706.07	2932 1863.1	5040115 0.7	38598079.5	46020824	47634701.9	52649883.3	12592463.3	15008053.5	17418516.6	27104828.4	2266011 0.4	2332105 0	26606466.5	32100026.1	26211465.5
3-Mercapto-3-methylbutan-1-ol	C5H12OS	1.86	120.0611 1	0.643	15868417 2	26707617 87	39553563 2	23668 9469	21291885 0	21185608 5	41481664 2	33102926 6	33683239 9	18735583 0	17219258 9	24601145 1	64969255 .1	72666353	14644513 7	22172765 1	20443043 9	26170098 3	27858475 7	22895344 1	22403943 5	10215387 4	13747345 8	13022931 8	19397017 8	16880270 2	20452169 2	11338955 6	14634799 1	12144690 1
N,pi.-Methyl-L-histidine	C7H11N3O2	-1.08	169.0849 4	0.644	16798949 4	18455611 0	19464068 8	40368304 8	24705099 9	21204200 2	23102604 1	26613411 0	23191867 4	21121143 1	19469539 8	20991190 4	10973779 5	13644079 0	14202637 9	22171796 0	23655938 7	31576103 1	24194566 7	22868580 7	20601592 3	13974021 5	17267650 4	17917321 5	22355272 6	18487765 2	18241429 6	15522903 2	19241272 52	16585861 1
2-Amino-4-methylpyrimidine	C5H7N3	0.25	109.0640 2	0.646	18249343 1	20123038 7	23291276 1	46887870 0	37590166 2	52134283 8	13023335 3	21279911 4	20309970 5	32680555 9	29522142 1	25547521 8	10031668 8	19460857 4	11210308 2	31331720 8	40123542 7	44193994 8	19980885 0	20715235 7	22686273 8	28783780 6	23599149 0	31478869 6	27868753 0	24158980 4	23226881 0	23007772 8	28866196 7	21978997 4
L-Histidine	C6H9N3O2	-1.95	155.0691 7	0.646	53317462 5	59853150 0	81574673 2	12788218 03	75812258 5	69833393 2	44539618 5	47490004 79	42830885 1	58099109 1	65023549 7	58301343 7	34937487 3	29980909 0	30182930 8	75165980 3	79028326 2	92616980 7	48354332 7	92769010 0	53209281 0	48021732 7	61755684 6	54218236 6	54322059 4	43846525 4	46217356 8	44988011 1	63931083 8	47438018 9
N6,N6,N6-Trimethyl-L-lysine	C9H20N2O2	-1.88	188.1521 2	0.677	31102977 9	27384955 .8	29540124 .2	37175327 .6	40991810 .1	39403770 .7	23436521 .7	15485991 .4	29367938 .5	21622547	31600292 .1	29601524 .9	20819783 0	23762496 4	26453081 6	37823080 .4	39373589	35226360 .6	10238901 0	12032486 6	12588584 1	21003150 .5	19242739	22262156 .3	13691967 .8	15634239 .1	13517177 .7	49318769 .2	59014187 .2	54695863 .8
Carnosine	C9H14N4O3	-2.24	226.1060 8	0.68	89790421 03	97005919 96	89930091 75	1.6779E+10	1.4354E+10	1.3584E+10	75004946 14	71900507 11	77101258 25	1.1157E+10	1.0933E+10	1.0284E+10	32802446 07	35470778 71	37034915 79	1.3E+10	1.5308E+10	1.466E+10	72033930 15	77765765 58	83665895 09	85854409 80	85034709 54	1.0031E+10	74401611 05	72385076 00	75688675 07	73385750 50	78291044 68	74173205 0.5
D-(-)-Fructose	C6H12O6	-3.87	180.0626 9	0.707	7194613.48	52160 52.71	50417 20.78	41435898 .3	29308134 .4	40628677 .9	4562413 .22	4428485 .04	17995 27.37	18550203 .6	25258695 .1	20194282 .4	7902891 .07	13049766 .5	12070434 .6	27717028 .2	21500856	20456279 .4	14040997 .3	18395892 .1	15966535 .9	29348453 .1	25999064 .4	21126953 .9	30030885 .8	32581561 .5	24567104 .7	18224498 .2	15309294 .1	17043277
DL-Carnitine	C7H15NO3	-1.98	161.1048 7	0.718	94394842 77	1.2223E+10	98623812 02	75096361 88	64201884 32	80502526 19	1.533E+10	1.1747E+10	1.3473E+10	1.7037E+10	1.9992E+10	1.6653E+10	1.4531E+10	1.8846E+10	1.6331E+10	1.739E+10	1.6101E+10	1.5802E+10	1.1653E+10	1.3523E+10	1.2039E+10	79979231 73	76018914 58	78633614 67	81063795 87	80422505 60	85116187 43	1.0706E+10	1.0763E+10	1.1428E+10
Acetylcholine	C7H15NO2	-1.64	145.1100 4	0.72	19386425 34	28139478 19	26784652 39	30879790 73	25974681 0	28425511 4	37700016 8	37387103 7	41968097 7	47258506 9	37228625 7	42054181 8	26788815 5	36103972 5	27087369 5	36135659 1	45807686 2	37897600 7	47728698 2	57366604 5	57686083 3	21371191 1	23899175 5	19482726 8	33123414 1	32062166 0	33981410 9	49443730	52888574 1	52874147 1
Acetyl-β-methylcholine	C8H17NO2	-0.13	159.1259 1	0.722	21216859 5	20696278 4	22649494 5	29834222 9	25600572 .5	21025718 6	28480114 7	47514709 2	36872847 4	10053478 27	10093666 38	12278223 54	22287765 4	29301730 8	27227402 .52	34566545	43514449 2	47949431 4	12798418 33	14244959 275	13244622 01	12000232	11440965 5	12317366 2	22809919 5	24355682 1	24789012 9	53447263 7	51216049 2	50810950 6
Anhinosylhypoxanthine	C10H12N4O5	-0.42	268.0806 6	0.724	55488814 .9	23390021 .9	33564447 .2	24357599 .3	39914077 .8	56895800 .5	30754036 .8	15974077	29029633 .9	28839170 .7	34293931 .6	33513001 .3	27068558 .9	20562491 .1	15905058 .8	28419629 .2	17493345 .1	30758788 .5	22662849 .2	29750118 .1	38184527 .8	31639314 .9	32636535 .6	49641657 .7	62521146 .9	47512612 .3	36305810 .6	17804233 .8	18293945 .8	15998404 .6
3-Hydroxy-3-[(3-methylbutanoyl)oxy]-4-(trimethylammonio)butanoate	C12H23NO5	-1.49	261.1572 3	0.726	27820538 7	26087829 7	24829261 6	55673938 .6	43061122 .4	46852187 .9	13439837 5	13832554 2	14196366 5	12012704 8	11446366 1	99236272 .4	9373823 2	90375086 .1	89112793 .8	15684220	16188191 5	16512043 1	82883732 .3	73045684 .8	89029174 .5	36314793 .1	37997765 .2	38106687 .7	95807289 .8	96044741 .5	10973283 6	11301464 0	10947627 2	11062778 0
Acetyl-L-carnitine	C9H17NO4	-2.59	203.1152 3	0.727	30559219 05	25947165 95	20228054 27	1.2676E+10	1.0462E+10	1.3986E+10	87312474 15	96962572 84	86815614 24	37538197 48	41653228 07	43721685 91	60110958 54	71044127 23	75638673 71	85608295 77	92634071 83	83626435 70	81012662 94	1.1442E+10	92078260 08	91533049 63	1.1093E+10	62669268 2	25749478 46	73961910 12	76659818 88	72767381 65	80755634 18	85430340 38
(R)-3-hydroxybutyrylcarnitine	C11H21NO5	-1.73	247.1415 4	0.73	23190338 6	29471890 9	77605144 1	74058487 7	65256987 4	52656000 5	40033209 1	50608880 3	25123097 6	17223041 6	24716943 9	26553278 2	43182845 1	81677070 8	77076564 3	10220514 5	10488905 0	28591071 8	17077543 6	12015849 4	17027249 0	56995292 4	42555174 2	39503876 3	47944558 8	20281985 6	56003963 9	34632929 8	36881851 6	39426120 6
Creatinine	C4H7N3O	-0.39	113.0588 7	0.73	11950766 48	11879557 41	12053251 95	10770421 90	10525686 45	12480241 13	12497087 9	88837279 4	12903206 64	13487758 15	39833181 6	11487529 97	55565020 2	65328366	12496353 82	79501467 2	10985869 92	78396510 6	83465874 5	10885341 14	10983375 34	98538668 2	11349089 069	10575299 73	12938300 50	15142889 98	12019846 86	66175591 0	90191118 2	70405286 0
Propionylcarnitine	C10H19NO4	-1.52	217.1310 8	0.733	77056625 9	76410422 .3	49821155 .9	25737951 3	17211852 5	19467602 0	21884542 6	40448907 6	31457252 0	16167157 2	20463381 6	15549429 3	52422045 1	95775352 6	74733086 6	21378055 1	22927779 0	20424647 7	41671565 9	35198250 6	41150363 2	10589794 1	97331010 .2	84450332 .9	96637720 .8	13928565 5	99813080 .8	15002444 5	14495288 7	16740956 7
gamma-Aminobutyric acid	C4H9NO2	0.93	103.0634 2	0.734	74817545 .4	80972779 .5	95099190 .4	10882629 .9	11212823 .1	98492887 1	16199710 .5	15011683 .4	18733065 .4	10482549	11116900 .4	12757619 .4	11278749 .1	10163520 .9	11898864 .8	11089922 .5	92309 73.4	10405031 .8	88589 65.01	84710 55.29	10486511 .7	98695 79.95	13910999 .5	90514917 .5	26487762 .3	12020680 .9	14485466 .7	15924871 .4	14549531	17666370 .6
Betaine	C5H11NO2	-0.58	117.0789 1	0.744	60798256 90	61065414 50	52719099 92	91146054 1	81797404 6	97672509 0	18549900 54	18599278 57	18216835 73	13594434 01	11887558 18	13868922 00	95529159 9	10742312 51	98496455 4	16172258 20	18311588 68	19096915 88	13520667 03	13882937 13	15820385 92	84692549 2	91233384	85443250 7	25994726 57	29227018 83	26896931 89	20317623 58	23543834 47	20876410 684
Creatine	C4H9N3O2	-1.75	131.0692 5	0.744	3.3867E+10	3.3512E+10	3.4325E+10	3.5049E+10	3.0986E+10	3.483E+10	3.2483E+10	3.1892E+10	3.1766E+10	3.8E+10	3.8161E+10	4.5245E+10	3.037E+10	3.0701E+10	3.5456E+10	3.3756E+10	4.3543E+10	3.8347E+10	3.248 1E+10	3.3657E+10	3.4291E+10	2.9952E+10	3.1699E+10	2.9744E+10	3.0092E+10	3.0714E+10	3.2358E+10	3.3924E+10	3.5721E+10	3.4836E+10
Prolylleucine	C11H20N2O3	-1.92	228.1469 6	0.745	34299363 8	22677958 2	20056584 59	25480896 3	25063228 3	25113953 5	15244064 0	13279551 7	16756593 8	32214004 6	48762908 7	31593254 1	80332779 .5	92362039	98811010 .1	17309927 2	18826151 6	17607916 5	10172644 7	10982130 3	12012993 5	23622300 1	22374119 0	21660712 1	46068703 6	32282327 7	45173883 0	17869205	36132754 3	18653081 4
Dihydrothymine	C5H8N2O2	0.86	128.0586 9	0.748	19559560 5	19794661 8	20518400 1	57094666 8	44289889 9	48597947 3	25434377 5	22877393 3	32676931 5	23722185 0	27765398 5	29576509 1	19145178 8	23582604 2	22258212 8	15998736 5	17761017 3	20130647 0	39084035 4	37359935 6	33760501 1	11699293 1	10917657 1	16726076 0	93231970 .1	17574753 3	16358364 6	11484523 6	13601706 5	12166673 6
DL-Alanine	C3H7NO2	2.12	89.0478 7	0.761	48849787 6	63192474 2	51208306 2	29079488 4	34230803 2	34580863 2	45768078 9	51913578 3	52132902 5	40241785 8	40346789 8	37378459 6	65251405 6	72258009 5	58915234 5	30696326 4	41498864 4	39365821 9	43707716 8	59882540 3	45750784 8	38724694 4	36284771 0	33725682 4	49351621 8	42154885 8	45684231 2	54478566 3	48373102 8	57374203 3
N-Acetyl-L-histidine	C8H11N3O3	-2.15	197.0796 2	0.762	52519681 8	39298321 4	66709381 2	90012066 8	55362380 3	12608552 82	57491043 5	67820288 7	23681225 6	42708097 0	43616987 9	98479319 0	31747755 5	36378835 0	32805606 8	63617729 0	10515824 48	49728815 1	68594053 4	82670042 6	24700536	59144575 0	48738317 8	65316823 3	56452239 8	50448471 0	47360005 1	59473134 7	77035984 0	65986358 9
D-Gluconic acid	C6H12O7	-3.92	196.0575 3	0.769	20478049 6	21684615 3	22437652 1	43517795 .2	41350709 .5	42203473 .3	12718128 2	13491696 7	14059406 .77	11564928 .7	14374558 .2	11743559 .3	3573950 .45	3008401 .11	3125641 .15	8917002 .62	11708221 .4	11118948 .2	12232425 .7	10049829 .5	11192455 .6	2353 1146	24441411 .1	24774157 .1	47921257 .4	48403 258	49915342	12077829 .5	12476725 .7	12385109 .6
D-(+)-Proline	C5H9NO2	-0.41	115.0632 8	0.77	22094748 2	22925289	22091793	97997518 .2	96987540 .5	11803258 5	18219473 7	17529186 8	18016971 5	13154994 7	14063412 3	14562785 1	19216665 2	19402545 4	20251925 0	69093335 .8	88170402 .1	91790099 .9	14155712 4	18578590 5	16587671 0	10770644 2	11340755 2	94226735 .5	23060580 9	16103950 7	16159175 7	15063308 9	18098961 8	22595417 9
L-Glutamic acid	C5H9NO4	-3.26	147.0526 8	0.773	66176465 4	79973584 4	70307702 5	54309050 3	44477428 2	69312766 8	78115819 6	91457476 5	90638920 3	45378796 0	42129745 3	36110600 8	12802221 73	13896962 98	13653309 62	18195990 90	23983910 3	21538938 1	99102831 2	10552386 75	90997532 1	38800569 7	39004822 1	41342080 7	48049341 2	35864906 0	48654690	24074526 9	26087413 6	24828816 1
DL-Glutamine	C5H10N2O3	-0.41	146.0690 8	0.774	40105888 7	45007181 7	36056573 6	10242242 84	87543486 1	10674494 00	92109233 1	96236930 0	11068317 43	94395572 8	89343790 3	86527216 5	32630660 18	34446057 57	35821485 26	30516337 6	36374814 7	34721726 0	23451293 34	25327586 07	23506291 22	51180818 2	50061627 3	51808328 5	36756744 5	41121636 5	40438554 7	34952792 8	35277400 6	35303367 6
L-Pyroglutamic acid	C5H7NO3	-0.16	129.0425 7	0.775	29592941 0	34577365 1	25540788 0	59536688 0	49638014 5	60763791 9	75103548 9	82620007 1	87031415 4	72766335 5	63509415 4	61415423 6	28065307 29	29822924 77	31502565 38	22933263 5	27941667 4	26392281 6	19202915 02	21144364 54	19075072 95	37486790 6	37039720 7	38736050 2	28477487 4	31874221 1	31443175 3	27396671 3	27539177 8	28364710 4
L-(-)-Threonine	C4H9NO3	0.99	119.0583 6	0.777	49342163 .5	47524201 .8	52837090 .6	25053341 .4	24947262 .1	28661538 .3	26013782 .5	23490641 .1	33498580 .5	30143838 .3	29646696	31064506 .7	27297559 .6	29652462 .3	35197552 .4	25775707 .4	29677029 .3	27228123 .7	30954418 .8	40792493	30256354 .2	95585117 .8	24338066 .3	33082974 .3	30995859 .9	30862873 .7	29710344 .4	31022323 .7	19590474 .3	24729137 .4
L-alpha-Glycerylphosphorylcholine	C8H20NO6P	-1.35	257.1024 8	0.777	57401748 .4	57830270 .1	49624272 .6	45991128	46346470 .3	43873562 .4	95829100 .2	98950089 .9	10450790 9	70066982 .6	50488200	41474749 .8	15213954 1	22896552 4	21836389 3	20181833 1	20879368 2	21164817 7	53469774 .5	66723021 .5	39840995 .9	86539638 .2	10176346 5	10584309 4	86796935 .7	84482133 .9	89295489 .7	29732945 .5	34114249	29666665 .1
Uric acid	C5H4N4O3	-4.74	168.0275 4	0.787	57170417 3	37118797 .7	55330138 .9	12911034 .4	16063315	14217444 .8	43718913 .4	46595233 .41	38671555 .33	12159120 .7	12037026 .3	12716125 .2	62734349 .2	51507961 .1	47661487 .4	85518325 .6	87087605 1	88627760 .7	21255547 .3	22466361 .3	68590888 .73	17743329 .3	16030598 .1	75320226 .16	14117195 .5	16946827 .6	17980600 .4	99363289	93510233 .36	94291905
3-Methylhistidine	C7H11N3O2	-1.35	169.0849	0.788	10972292 3	10093380 7	10961523 1	20541072 9	17326364 9	15469908 5	14747828 6	18290469 4	15329372 0	14793171 1	15331909 1	15026496 5	56027559 .5	32540530 .7	10411078 8	17826741 7	20797561 9	17353994 7	91606225 .9	15787674 1	17281400 9	87537222 .1	67636924 .4	97337967 .3	69797792 .9	13452808 7	13452621 9	39506713 .2	74284900 .1	13814520 8
D-Glucose 6-phosphate	C6H13O9P	-1.03	260.0294 5	0.797	88800 15.13	10195471 .6	90073 97.26	10279044 89	10631913 86	10334166 67	80334 99.31	89622 56.58	10439350 .1	85715 3457	78073 0909	77783 2342	86656 69.24	12399001 .3	10879658 .4	78025 9599	92419 2136	88751 3067	26573 8388	32768 9565	32929 8182	73305 9456	72704 2349	80969 3410	52296 3173	53529 3519	55980 97.53	60207 7301	55586 2904	49395 6373

Citric acid	C6H8O7	-4.33	192.02617	0.799	7684467	8749594.95	6369617.9	1586386 4.1	1408818 5.9	2104591 3.8	6950144 5.2	5419488 4	1895536 3.9	3131811 .29	2535868 .72	2760477 .47	1611635 5.2	1322942 3.9	2818381 7.9	4711123 .34	4074115 .68	4711053 .36	1020039 5.3	1345680 7	6937351 .8	4559036 .9	3267690 3.1	5674572 7.2	3097102 9	3219427 7.9	3293839	1595018 9.9	1716037 9.4	1663288 0.7
4-Hydroxyprolylleucine	C11H20N2O4	-1.92	244.14184	0.802	5192338 9.3	7374582 2.6	7473627 5.1	3775705 9.1	5703296 2.6	3316066 4.7	3351269 3.4	6155613 0.2	8378429 2.3	46186000	3914918 9.8	1921391 3.9	2643912 40	2086588 37	9237015 0.6	2954221 0.8	1815848 0.2	1937697 0.8	7248554 2.8	1106788 39	3390445 2.8	3165802 2.8	4287703 9.1	2987434 8.8	4785821 1.6	5641027 3.5	6082911 8.9	1272112 3.1	1788469 8.3	1143091 2.6
D-ribose 5-phosphate	C5H11O8P	-1.87	230.01872	0.806	2414505 3.8	1668159 8.5	1658516 2.5	5116312 4.1	5817188 4.1	5643916 5.6	2564824 9.3	1608427 7.5	2243759 0	4240003 0.6	4451048 .4	4274255 4.2	3211454 6.8	2867082 1.7	2177495 2.5	3072638 9	4048712 9	3570823 6.8	2030956 .9	2334309 .4	2290863 2.6	7093395 5.5	7559428 2.8	9353954 6.9	6240013 4.9	6682961 4.5	6980786 8.3	5905603 5.6	5557741 0.8	4658833 6.9
ACPC	C4H7NO2	0.81	101.04776	0.838	2297752 6.3	2617422 8.1	2653952 6.7	1887972 9.7	1162879 2.4	1392944 1.4	2018199 4.5	1713525 5.4	2733610 3.1	1234988 0.9	9222432 .01	1202939 2.1	3794914 8.8	4089204 2.3	3841503 0.2	6195498 .64	463016 9.4	4736263 .67	2388910 2.8	2618193 2.5	339325 08	9456266 9.9	1755956 .5	3438681 2.3	2660336 4.6	2004821 4.5	3141137 5.7	2008917 7.7	2299159 1.7	2290994 9.4
Uridine monophosphate (UMP)	C9H13N2O9P	-1.86	324.03526	0.838	3117 54.193	301918 .357	304393 .376	4373352 .29	4493419 .77	4292844 .23	720901 .715	628247 .808	825552 .258	8437550 .61	8279350 .95	7705295 .63	2118152 .57	2938267 .04	2660630 .07	1077073 1.9	1031587 2.3	9184040 .14	4018668 .24	4706493 .65	4155304 .68	3630274 .51	3726001 .52	4407945 .18	2307429 .56	3052758 .69	3204242 .79	1388126 0.8	1278262 0.5	1240544 8.8
Nicotinic acid	C6H5NO2	-1.03	123.0319	0.839	1664283 252	1731335 107	1623417 019	6670619 7.7	9469646 5.8	8868735 2.4	1812162 965	1968930 603	2086273 998	2241774 87	1358416 46	2411428 17	2987354 0	1980268 7.1	1428772 0.7	5267432 .53	7462651 .21	5378465 .01	3566756 4.2	2880206 3.6	3831966 5.3	1190849 66	1225821 56	1259610 99	7595023 0.1	8590476 1.7	7350835 0.2	7336090 .31	6715647 .64	7631444 .66
L-(-)-Methionine	C5H11NO2S	-1.76	149.05079	0.854	3268803 08	3368328 49	3294342 60	1505742 41	1637000 877	1347970 66	1253228 42	1126924 35	1345806 28	7119115 9.7	5597665 2.4	4884437 1.7	6672563 0.7	9835801 2.8	9131841 1.8	7118370 7	1049498 80	9871470 2.2	1333300 17	1462189 86	1081784 69	1651725 07	1588773 25	1639756 66	1353641 21	1302072 43	1329027 55	7648784 2.8	8136092 4.1	7721534 3.4
3-Methylsulfolene	C5H8O2S	-1.78	132.02426	0.86	4011137 59	4147215 28	3774037 13	7119891 4	1866726 81	1606200 56	1505592 25	1407890 36	1559859 31	7899326 9.2	2418969 6.6	5609157 6.8	7910386 0.2	1111369 62	9788669 4.2	9153696 2	1270560 17	1169233 19	1625302 81	1790567 95	1277071 99	1964049 15	1828837 57	1950646 55	1592357 76	1550423 73	1636893 41	8902045 6.6	9480415 4.5	9121441 4.6
L-Glutathione (reduced)	C10H17N3O6S	-1.68	307.08329	0.87	9640632 0.5	8223124 0.2	1235915 82	3148724 48	3733625 09	3754713 14	1195610 3	1040702 32	1315415 34	3263723 84	3678296 43	3532520 86	7748532 68	7258636 65	8012755 59	4511208 65	3751140 13	3369374 58	5996854 12	6159331 96	5641656 77	2172111 825	2363221 98	2661626 37	3111640 71	3129132 84	3036161 62	6248605 02	6665019 95	6013687 94
4-Hydroxy-5-methylfuran-3(2H)-one	C5H6O3	-1.35	114.03154	0.885	6084612 .67	6417394 .13	6147475 .99	7264040 .58	6501462 .99	6290300 .39	5830952 .4	6729205 .11	7306610 .37	7650453 .03	6985128 .31	7177799 .58	6239231 .09	7119179 .68	7445760 .88	6619580 .82	8097052 .59	6759115 .3	5548548 .8	6384554 .46	7214050 .64	1739987 5.7	3767484 6	3430825 4.8	4682556 2.7	4986631 2.7	3799484 4	1443491 6.1	1389927 2.2	1347883 4.9
Nicotinamide	C6H6N2O	-0.99	122.04789	0.923	5279233 .03	5645190 .21	6843491 .59	1623436 341	1765517 471	2052976 429	1659801 .4	6895797 .33	7245426 .02	2016497 785	2196129 162	2083506 880	1102305 412	1171944 892	7925471 56	1973749 73	2050334 390	1822112 540	1148835 216	1309899 713	1304077 341	2518718 941	2493535 359	2792231 268	1806938 669	1820802 138	1916872 634	2363254 783	2633521 994	2436300 600
Phosphoric acid	H3O4P	1.53	97.97704	0.923	1325592 60	2288425 88	1379986 06	9318560 5.6	1070770 53	1075273 22	1672266 72	2507430 85	2447778 45	1158025 48	1076294 92	6320933 4.3	1277619 82	1281647 25	5667761 03	4886543 6.8	1918072 55	1029289 32	1278945 10	2464822 04	1571657 81	9589842 3.7	1285637 10	1365538 94	1742934 47	2096698 49	2447431 44	2183013 44	2136338 91	2017807 27
Inosine-5'-monophosphate (IMP)	C10H13N4O8P	-1.63	348.04653	0.925	2306636 .78	2219964 .15	4199860 .4	5251561 07	5369596 64	5573823 43	1487533 78	1577478 95	1247770 32	5808071 76	5738129 50	5089762 10	1411510 51	2046190 07	2072826 11	6033664 14	6346546 47	7031833 71	3404851 64	4679872 08	4613300 09	3873901 06	4126352 41	4657111 85	2516468 58	2415983 66	2625650 77	7257458 72	8130696 31	6665324 33
Hypoxanthine	C5H4N4O	-2.53	136.03817	0.933	3760362 270	3779001 120	3789813 769	2117719 297	2036482 643	2214905 493	4121157 476	4530827 071	4954717 049	1543912 960	1563806 355	1527942 463	2337889 094	2186594 767	2194263 475	9593416 14	1038348 606	1044296 726	1803406 409	2057363 657	2034956 861	2158551 908	2248213 729	2492683 654	3399208 869	3688180 506	3598183 790	1591987 888	1254139 488	1660221 489
L-Isoleucine	C6H13NO2	-3.06	131.09423	0.934	7754546 00	3380034 06	3306958 41	3153277 50	5347613 76	2952836 93	2267289 49	1972868 0.4	3543660 7.1	2074890 30	1884986 4.9	5312245 7.3	5267968 4.6	3856421 8.9	2389013 39	1314960 17	6421689 .95	1154802 1	1304947 99	1730977 69	9021997 8.5	1018465 77	3773752 94	3592745 46	5482908 18	1231125 06	2816188 54	3234349 51	2451059 61	3132345 89
4-Hydroxy-6-methyl-2-pyrone	C6H6O3	-2.22	126.03141	0.938	4921878 .97	5092905 .5	4660567 .88	2250677 7.1	2101584 0.4	1930567 3.4	5489462 .43	5255153 .47	5204925 .75	9565953 .19	1002918 3.4	1211707 29.9	5142645 .22	5555514 .25	4905651 .94	2141393 4.8	1698434 4.4	1180040 5.9	5792375 .82	5316560 .7	5429624 .56	1066336 03	1129190 469	1354636 499	9554518 78	4296869 58	6333790 11	8366974 49	8103468 66	8023574 62
5-hydroxy-4-methoxy-5,6-dihydro-2H-pyran-2-one	C6H8O4	-2.58	144.04189	0.99	6715349 .11	1116657 5.3	6358819 .57	3045628 2.9	8282445 .88	1171896 0.9	7489752 .76	7170066 .4	7101534 .53	7816449 .51	1215446 0.2	9127837 .03	7016559 .77	7579873 .03	5413224 .21	1783771 6.2	1078237 3.9	7623788 .54	7903043 .94	7253847 .84	1103074 6.5	4088479 11	4417090 69	6652156 41	6479477 26	5588721 30	6292693 55	3184436 59	5094558 894	4912610 25
Acetophenone	C8H8O	-0.11	120.0575	1.004	1677135 62	1632274 89	1927307 03	5303175 .74	6534857	7827648 .2	3036398 4.2	2603448 0.5	3678743 4.3	6290057 .23	5363498 .89	8882546 .66	8339443 .31	1168764 .37	1081041 .2	7074086 .83	5448569 14	5316319 72	6111056 .3	9387905 .23	1031463 .36	2616935 .73	2490276 .77	2755144 .53	2329553 .31	2438964 .03	2957421 .2	1597216 .26	1513935 .23	1670944 .35
Furfurano1	C5H6O2	0.57	98.03683	1.016	3214742 .2	4483652 9.9	4599854 1.4	4082282 2.4	3234180 3.7	3556211 3	4597717 0.4	3838799 3.2	9040455 8.3	2234810 4.7	9538311 1.1	4181753 3.9	3053631 9.8	5500266 3.3	8037253 0.9	5618853 9.1	9098630 .5	4780491 8.4	7921381 0.8	3636647 0.3	2367832 9.3	1059637 23	1311795 20	1313845 89	1042818 76	1318431 71	1507540 97	1128799 80	9747201 2.1	1020196 30
Xanthine	C5H4N4O2	-2.93	152.03298	1.024	3461549 43	3886459 27	4087228 04	1800155 18	1635370 96	1802171 94	5768212 48	5242166 92	5422403 50	1366460 76	1496256 96	1463280 08	3728107 16	3102783 93	2688515 14	8711390 7.8	8724040 4.6	8715516 5	3226818 62	3552157 95	3557870 22	2072391 53	1947081 25	2165826 70	2837627 30	2842992 42	3150622 08	8797819 5.4	9008602 7.5	8616131 8.4
Acetanilide	C8H9NO	-0.9	135.06829	1.053	2304926 4.7	1523686 4.8	1836526 1.9	4340755 6.4	3687821 8.1	3739242 0.9	1928205 .44	1614085 .01	2318016 .17	3379520 5.7	2720434 9.1	2228219 9.3	2272806 6	1934731 5.3	1909583 4.6	3721891 1	4020163 5.5	2793287 1.6	3624053 3.5	2866100 9.8	2975072 9.2	2303033 0.6	2762735 7	2776271 4.8	2512942 4.5	2690405 5.8	3048370 2.1	2187598 7	2349618 3.9	2524259 7.5
L-Tyrosine	C9H11NO3	-0.91	181.07373	1.06	1017547 49	7375252 6.4	9022219 8.5	1796705 04	1735437 67	1670321 97	1119688 8.4	8282054 .25	1227451 9.6	1198675 02	1156193 87	1176819 28	1003197 69	9263139 8.1	8586730 6.2	1303059 83	1442507 24	1342883 09	1431884 83	1423441 66	1624035 12	1091558 24	1226440 08	1370186 85	1201105 57	1260539 11	1372041 00	1061166 49	1088820 06	1150341 72
Benzoic acid	C7H6O2	3.71	122.03723	1.066	5531329 .71	3632957 .89	4974643 .69	1119176 9.8	1044246 7.1	6961163 .05	759775 .087	287391 .123	1421193 .41	4969636 .08	5724654 .33	4849166 .71	6540707 .06	5304312 .55	5009981 .07	7170148 .05	5992746 .88	556980 1.2	8347284 .62	8139335 .26	6547498 .05	3261211 .09	3115083 .52	2660090 .55	4297579 .67	5172291 .59	5692802 .06	2271586 .78	2304622 .67	3315051 .87
D-(+)-Proline	C5H9NO2	-0.87	115.06323	1.068	2636343 7.2	3942483 6.5	4188207 8.5	3708811 0.3	2726250 4.7	2965444 2.6	4110178 1.5	3416606 8.6	6673911 2.8	1795825 8.6	4684092 7.5	3619390 4.4	2645432 6	3115572 7	5586886 0.1	5090035 3.5	2444798 9.2	3868195 8.5	7253885 7.9	3154484 6.8	1971079 1.1	2678378 8.5	6376722 1.6	5952572 3.7	3009277 1.2	4396429 7.1	8687310 2.9	6555040 5.5	4527671 6.9	5292995 0.3
Biacetyl	C4H6O2	2.13	86.03696	1.073	9194070 .13	9665490 .89	1300574 9	2571716 9.6	2358093 9.1	1666186 4.3	1383414 4.2	1402317 1	1462355 4.7	8227113 .12	7741478 .58	7166451 .91	2485510 2.7	2502920 1.3	3073753 9.9	2040753 5.1	2116490 4.5	1958539 3.5	1111366 2.9	1183042 1.9	1082549	2512303 8.2	2460983 3.1	3046561 3.5	3016088 5	2283936 0.6	2223293 0.9	2142262 8.8	3027163 8.1	2703600 9.9
1-Heptanethiol	C7H16S	2.08	132.09755	1.165	1236575 87	1213315 95	1285969 89	8121831 8.8	8937334 4.9	9905803 7.6	4270691 .6	3874129 1	4369147 4.1	6435326 0	6726225 5.2	6223782 1.6	6003305 4	7556633 0.9	6839355 7.8	7738367 6.9	7333696 7.4	8119553 9.1	8354475 4.9	9644305 2.3	7940820 1.5	5385084 2.5	7423668 4.9	7419768 7.2	7820252 0.4	6602382 1.2	8292112 9.2	5400995 4.1	6524268 3	5089041 9.4
L-Norleucine	C6H13NO2	-4.15	131.09408	1.18	1700411 343	1497745 426	2212065 099	1340748 204	1270345 782	1505921 444	6544959 63	6762359 82	8408593 44	1116552 519	7836811 62	9207570 38	1242079 071	1438968 97	9496453 53	1299581 577	9599717 23	1106855 039	1031582 177	1341153 706	1147550 28	8018373 68	8153650 74	9366493 37	8574581 78	1185680 432	1441011 927	7153640 77	7498702 68	7627895 05
4-Ethyl-2-methoxyphenyl hydrogen sulfate	C9H12O5S	-4.04	232.03961	1.226	2689537 0.5	2842736 0.7	3008544 1.6	1251321 .58	1412526 .24	1174227 .45	4097960 7.5	5452606 9.2	3789642 8.1	8920199 .851	1684810 .71	2212037 .05	3377075 38	2593223 .313	4147206 .52	1511961 .64	2985070 93	8194790 07	6956089 .61	2005371 3	5016201 .7	8844996 .57	1166874 .92	6695724 65	1612497 .45	1282643 .6	1147569 .91	7829086 96	1166023 .53	1033698 .3
Isobutyraldehyde	C4H8O	4.83	72.05786	1.255	3870674 89	4024031 04	3868873 94	1628137 9.3	1022726 4	2035370 06	5525363 82	3271896 78	4455570 11	1907259 6.6	1782492 6.7	2130522 8	1677392 1	1844857 2.3	1065680 2.2	1870268 47	7267250 .75	1864576 03	1875973 98	1782664 12	1010003 7.8	7614816 .1	9129341 .12	5921372 .29	1103769 6.8	1842305 6.5	2269355 4.9	9686659 .59	6956839 .33	5656351 .2
Furaneol	C6H8O3	0.83	128.04745	1.295	8881498 .84	1126891 6.9	7290590 .31	2323127 2.2	1315414 8.4	1330566 9.2	9583078 .91	6782415 .05	1000974 9.2	1116136 9.4	9645794 .7	9482192 .76	2444026 5.6	2083168 4.5	1817591 6.6	2276353 2.6	1719078 5.3	2328410 2.9	7206754 .24	6744869 .01	7364530 .38	7236326 .71	8470930 .29	9117951 .7	8956099 .19	7103700 .2	7332097 .07	6392990 .08	6177675 .7	5279029 .99
Inosine	C10H12N4O5	-0.59	268.08061	1.318	5955612 12	4691025 83	5107967 35	6502392 35	5721682 42	6088988 56	3860777 88	2490031 21	3749629 38	5437456 12	5167561 18	5632951 33	2637683 11	2658941 10	2661144 14	3430610 08	3672220 01	3338378 63	6477051 73	6899779 05	6818197 71	5955223 87	5746310 87	6428206 92	6572230 39	6628859 60	7151045 18	2759983 27	2763946 31	2982349 08
Alanyltyrosine	C12H16N2O4	0.15	252.11104	1.389	1163296 .01	4974372 06	1281981 .18	3206621 .69	2961819 .89	3214624 .7	1450814 14	1642749 19	1261986 51	4409405 .12	3954471 .72	4499904 .87	5118914 07	8831434 22	7824656 74	1735198 3.4	2048987 4.3	1779031 7.9	1097211 3.18	1227636 .05	1577606 .49	5618693 .53	4100656 .63	4540644 .63	2217059 .62	3052639 .78	2657575 .52	3526560 .67	5588375 .25	6160457 .53
4-Hydroxy-6-methyl-2-pyrone	C6H6O3	-1.69	126.03148	1.45	2094629 98	1663561 07	1455273 .89	8134980 .67	7757147 .46	7946754 .28	2656731 .08	2810909 .59	2239796 59	7271242 .15	8918849 .15	3298327 .14	4046506 .86	3289006 .07	3610172 .16	5548573 .91	7821251 .94	3840690 .75	6796160 .1	5997693 .8	5964079 .42	2849877 82	5185467 9.7	8968632 0.5	6385724 1.2	3196145 09	3053545 7.8	3007466 4.8	3348274 0.7	2526776 0.1
L-Phenylalanine	C9H11NO2	-0.79	165.07885	1.852	1180506 805	1083349 622	2562646 191	1488447 563	1425301 802	1664734 730	1118814 199	5256047 33	1006677 197	4340985 50	4347975 39	4707420 78	5648188 03	1237681 939	5136495 99	1079454 009	1343086 322	5217431 31	6724789 38	9965293 81	6348695 67	3804161 68	6504364 20	5045781 98	1168869 369	1017608 286	6178900 54	8528069 88	3678393 32	3991757 54
N-(tert-Butoxycarbonyl)-L-leucine	C11H21NO4	-1.99	231.1466	2.078	8113904 62	5057620 24	4513590 61	9402712 90	1912020 958	1005915 009	1863777 783	1988850 564	3599773 420	1893139 092	1102585 842	9373378 69	7246911 83	1935316 868	9779082 46	1161480 285	2715513 003	1302610 880	4163706 689	4548935 034	3921032 434	2377262 206	1117283 717	2769503 973	1074652 226	1135186 642	1328292 172	1094624 538	1017519 101	1283858 777
asp-leu	C10H18N2O5	-1.11	246.1213	2.483	1756014 .66	1520343 .52	2703954 .74	2491937 9.2	2101109 4.7	5497893 .4	6151562 26	243089 .85	245464 .794	1519163 .32	2356717 .94	1783580 .43	9904652 .72	8977449 .36	6721385 .28	7871620 .33	9562698 .73	8801952 .59	2074029 8.3	2140368 6.1	1883047 3.2	3289700 0.1	1196281 9.2	2172617 8.1	1154982 1	1221399 6.9	1116231 9	2545858 .22	2701836 .55	3147998 .15

D-PANTOTHENIC ACID	C9H17NO5	0	219.11067	2.829	12677346.3	21041837.8	20688480.6	8566768.14	7864758	9195271.32	10417102.9	9979590.35	12349505.6	20166151.7	29844239.1	21882470.2	38584553.8	29481336.2	30338701.9	16941533.9	22748735.2	10425097.4	23936989.8	16498269.4	27092767.4	4699622.43	4869520.19	5489251.64	9005467.24	9073725.05	9110924.52	9163574.51	10862301.6	9758992.51
Hydroxyhexanoycarnitine	C13H25NO5	0.02	275.17328	3.01	7164067.59	8522567.34	9223969.35	11873264.1	10092532.3	11259467.5	42225210.6	22622438.5	25081283.7	3030334.86	3172203.78	3740668.83	30767665.4	33239702.2	28311617.5	43543367.6	39677684.4	41458291.6	34584580.4	40619601.2	33710582.2	10262117.8	9195525.62	9061221	7733657.9	7905219.48	8537629.09	2035324.01	2204970.52	2044181.89
DL-Tryptophan	C11H12N2O2	-1.35	204.0896	3.136	13809288.9	210381302	47036897.9	41559135.7	8616134.84	21889995.7	7914928.7	4995864.98	4929921.1	6946516.2	9845389.81	41544130	4514879.28	6173824.91	9213623.9	14165153.9	9476960.64	11202424.7	13586485.4	19285184.1	60600870.3	94070858.8	6619017.95	6773497	7286104.23	38055025	79053775	85442206.6	5401554.06	14991597.7
Leucylasparagine	C10H19N3O4	0.29	245.13763	3.311	5713756.35	9772371.35	6213324.15	705234.317	508380.883	502004.646	50523269.5	52249580.8	61958748.5	2043185.88	2098374.23	2322426.1	43345.6852	42874.2297	45844.563	126222.679	78556.0931	117719.955	48505.9283	41551.8606	82324.7028	40929.7572	42796.3117	43160.7954	92613.2503	39047.9893	39858.4992	37160.3015	39400.1292	40466.1688
2-Naphthylamine	C10H9N	0.2	143.07353	3.326	26156003.8	27803265.8	27575533.4	1608912.09	1343237.9	1419189.08	3399454.66	2747104.78	3692980.71	1044362.34	874973.485	1302051.98	855479.666	1063082.89	160746.02	1118211.67	1249073.83	1137522.88	297801.034	1221909.98	1399833.46	834876.297	1124358.78	897455.163	675140.145	625235.018	779385.973	729509.171	711534.533	716967.481
trans-3-Indoleacrylic acid	C11H9NO2	-0.98	187.06314	3.363	358701453	366201490	260361535	227317075	241865828	230824339	172381359	150959261	163240664	198575536	219964594	243544157	216961134	216615788	179155963	232038361	263388895	222416727	147069684	18990339.9	292236342	137646996	203785483	233503202	141278679	98649395.2	166917486	175964172	187346506	162068056
Leucylproline	C11H20N2O3	-1.03	228.14716	3.449	9044761.79	1761112.07	3982472.65	18628904.9	20843285.2	76252118.3	1921909.25	1517336.01	887169.392	10563571.2	17934561.4	13066571.1	36082803.4	31616152.8	10161301.9	9975908.44	10138044.5	8713649.41	13481352.2	5372604.37	16565417.7	4647132.2	12963729.9	35210324.2	21720983.9	50054890.2	45651358.9	10248071	12800807.3	13786818.9
Tiglylcarnitine	C12H21NO4	0.12	243.14709	3.78	16320291.7	10169440.2	14895996.4	21294982.1	13229587.2	22040146.1	37404480.5	44479108.6	50130613.7	10941929.5	13664414.4	13172372.3	47292280.1	41496535.3	38096250.9	32946170.6	39914720.3	44730925.5	31718590.3	44845340.3	49104132.4	24583914.5	27250392.3	19848223.8	18181310.3	16568747.7	23158477.2	9304565.66	8981766.21	10654616.6
hypaphorine	C14H18N2O2	0.18	246.13687	3.948	926918.114	1248221.38	1402580.75	121995.185	148537.258	351504.578	1928905.41	2608728.03	3249120.18	163106.889	210307.214	361053.315	14878954.7	20676813.7	20340946.8	213809.057	42922.049	40150.6626	6128794.38	5032586.49	4708854.3	2442409.89	4345205.14	3369099.07	197477.961	283208.013	198546.243	813234.814	639252.542	815431.646
2-methylbutyrylcarnitine	C12H23NO4	0.01	245.16271	4.109	96465607.9	123234190	114981918	108315521	109989925	139087899	230063654	204641991	225672361	94296700.2	108461013	123999323	316423327	300634231	280276602	114762393	150418546	130601419	238341489	191785166	189147999	56882486.8	59726697.7	54926389.1	150917941	163956852	160869115	70590119.6	74058616.8	80395947.6
Isopropyl beta-D-galactopyranoside	C9H18O6	-0.18	222.1103	4.294	56170048.6	52465620.1	47805539.9	82120569.2	55078324.8	110247594	55277896.2	62422714.6	90444561.5	53137331.4	80809902	84623225.4	57261567.2	101740309	87977127.6	117856371	80136336.6	86984108.8	92280037.5	92486879.7	102037185	52222736.1	68301932.6	71867556.4	66876364	68362152.9	51972074.2	75743007	70514522.7	86743023.4
N,N-Diisopropylethylamine (DIPEA)	C8H19N	0.27	129.15178	4.393	20002778.4	13295374.7	21047694.5	21508203.8	24755216.7	28867488.3	27248356.8	43942562.2	23299777	39788016.8	21847658.7	27069104.6	47493369.2	27971059.8	23038120.2	65650295.2	53871568.6	173616913	25720220.1	22694954.6	47768759.3	7792493.91	8388998.92	8528337.43	9668622.51	9739151.35	11157911.8	19597829.1	19210208.9	22149557.1
4-Acetamidobenzoic acid	C9H9NO3	-4.8	179.05738	4.527	714207.327	792084.335	642188.63	7558594.29	7501291.26	7686231.42	1173439.25	1120858.26	1198829.96	1991602.94	2164368.58	2188888.15	9296594.75	10764710.6	10362614.1	876729.513	681344.977	785219.045	2087640.49	2006737.78	2208989.44	2993501.74	4198531.64	4296092.47	2382771.56	2215128.36	2808737.36	15205756	9980720.01	16421944.9
Z-Leu-OH	C14H19NO4	0.03	265.13142	4.677	4671121.69	4444321.66	3567780.29	20487544	18435048.1	28106170.6	10173655.9	7082783.3	7518375.82	6362873.25	7170026.76	4764383.28	70917389	101704787	97056113.4	23281278.6	2057795.26	16187906.5	59852282	25210123.9	130163534	55294459.5	58257655.4	56371495.2	4338830.95	3139322.24	3608412	8251471.7	7538145.26	12169309.4
2-(2-amino-3-methylbutanamido)-3-phenylpropanoic acid	C14H20N2O3	0.17	264.14744	5.282	3274762.32	1449095	3534428.57	25901412.3	14468165.4	13804161.4	237276.733	276105.381	310518.184	2184614.37	3683657.38	3426991.73	975220.727	1140760.62	1290794.77	37973331.5	26153268.2	24168038.2	5835636.52	1136920.54	5600530.1	16367728.7	18252225.3	17645857.5	17388000.3	13319833.6	12477644.7	5743318.32	9721895.44	7157377.42
2-Hexenoylcarnitine	C13H23NO4	0.74	257.1629	5.474	67194.3964	41709.5782	70772.2229	402835.781	618493.028	540999.321	688397.019	573989.904	728795.029	300711.979	240001.286	212429.065	8990561.85	12888283.7	11540847	1415431.46	1091673.18	1203420.73	1012706.12	1162375.79	1147468.52	457610.127	667416.287	477092.736	817128.363	736901.805	740555.788	576498.427	578985.792	447696.721
p-Cresylsulfate	C7H8O4S	-3.24	188.01372	5.725	670604.382	651327.337	618591.945	173126.193	25953.1872	2069503.46	404632.846	5297450.92	5882578.77	3020562.85	3100235	3383047.18	13107219.4	18608908.5	9699274.44	2529083.32	3238018.94	2698408.27	3741814.36	4145370.75	4336524.23	9391567.28	9273254.97	10442610.7	7921617.89	8473971.49	8365753.55	10498234.8	65718.4363	9657689.94
Leu-Leu	C12H24N2O3	0.39	244.17879	5.815	200463.008	146016.037	302537.219	421838.138	453675.629	314578.713	820694.252	1033195.6	1012838.69	11796693.9	14266484.9	14346863.7	3797597.84	5575845.46	5297162.58	62741814.9	55481842.5	57669027.1	5869842.24	4840621.33	6343182.65	599877.034	22627626.8	582319.472	16867330.3	285467.581	18784350.3	18637380.7	394761.056	16311040.1
2-Hydroxyquinoline	C9H7NO	-0.46	145.0527	6.243	622899.922	846756.43	738140.278	669877.377	858620.496	705688.188	7551272.42	7262291.77	7614584.07	1032584.66	1222394.28	1371366.32	173569.495	146599.801	125762.035	105653.499	130535.814	78838.0677	611876.009	536876.352	550134.146	61534.301	502957.134	611485.631	692352.616	609745.502	546451.801	1613142.82	1638733.07	1312726.87
Hexanoylcarnitine	C13H25NO4	0.04	259.17837	6.622	43051129.2	31544330.4	28329846.9	67982214.1	73511937.8	90078777.6	381652787	407957040	435718085	47964038.8	41081630.9	39934989.1	116997511	169055044	163839344	207871121	221225822	198678951	475030281	461642608	480710956	5559189.34	223334229	205995886	402124957	296669926	313411036	70308707.9	75858383.2	56614792.3
D(+)-Phenyllactic acid	C9H10O3	-4.3	166.06228	6.947	40762337.8	51653343.2	46853212.7	1581387.28	2451949.27	1454715.29	28685009.9	40471283.3	27932961.1	1921239.86	2230147.32	1866647.85	114355.621	102450.812	81384.9277	479709.227	407297.552	387718.663	144774.178	195326.513	157524.628	917062.601	640213.532	714892.299	1984602.75	2460676.85	2105817.15	56188.9537	244024.845	263910.728
Dibenzylamine	C14H15N	-1.1	197.12023	7.167	4195358.99	3244141.3	3606065.43	3673370.6	7053368.22	5136508.26	7849902.94	2682465.4	196277296	3048431.68	377137422	326105851	294458659	376287372	83014744.9	373514485	303439748	379256088	358423367	450859995	324155235	2118789.6	3867431.25	3170527.29	3918929.27	5926012.37	225497580	190552412	182632336	185324106
3-hydroxyoctanoylcarnitine	C15H29NO5	-0.31	303.20448	7.374	607649.121	93514.5029	110783.83	8610057.58	8709610.03	9818296.74	19224682	18070763	19305195.5	1050186.24	1156680.15	1117122.16	33543512.5	34999920.5	28610748.4	11177594.8	12100720.2	10998187.3	1597647.62	1564719.66	1026803.14	10130362.4	8350279.12	9013488.27	9618285.28	13670551.2	10242582	2022409.08	2355991.81	2349092.39
4-Indolecarbaldehyde	C9H7NO	-1.35	145.05257	7.59	13477541.4	25911830.1	19248025.4	894193.379	962037.734	803551.316	55104685.5	63971470	46305086.1	571973.774	753480.779	640289.295	756137.218	756470.1	1234077.19	677448.935	733837.89	810134.689	1398886.5	1471612.29	1133626.3	239526.962	340117.428	293864.441	373814.701	303381.998	338271.551	189416.9	111448.083	144148.136
O-heptanoylcarnitine	C14H27NO4	0.76	273.19421	8.185	261174.6	332996.958	373877.834	270996.13	389230.808	385468.176	3899245.23	3759431.71	2224726.15	600016.965	3420238.19	3633799.29	15340660.2	19288201.2	16467215.2	24206589.2	26640288	23748855.5	15841806.4	19853366.9	19978146	1522736.92	1604459.49	1276231.58	3011843.64	5312248.49	1181443.39	2280271.72	2238465.88	1194613.1
12-Aminododecanoic acid	C12H25NO2	0.76	215.18869	8.832	751869.517	804562.288	971734.559	426135.152	944499.564	757965.881	365097.926	522695.093	50570622.5	1093043.69	48922123.2	46137604.3	41463578.8	48723405.5	71525110.7	53098529.7	71216342	73236061.9	35524267.6	45222668.1	50445064.7	454790.532	421325.074	468674.8	809192.041	39498309.1	497797.371	404734.686	723724.889	519913.201
Azelaic acid	C9H16O4	-3.79	188.10415	9.607	459786.493	62293.2331	529915.016	3944645.34	4298963.17	7814880.11	8467461.1	7820867.18	506344.215	3360946.93	344531.333	901755.485	1152872.48	271624.439	530718.12	375076.532	295245.87	266729.189	708424.388	3139354.61	595940.464	10424713.1	25853741.8	27281013.8	31285525.6	12992581.1	37080856.1	22799283.8	6636692.98	13016618.9
3-[(3-Hydroxydecanoyl)oxy]-4-(trimethylammonio)butanoate	C17H33NO5	-0.52	331.2357	10.842	35098.5259	30059.5215	35842.0347	28024.948	581394.806	27298.3565	80739.4888	132259.872	1012581.69	634474.608	748524.168	767994.661	50244828	63632715	56674388.4	4482399.85	3937933.97	4537457.27	5202538.57	5091360.28	4970029.65	795833.148	960093.318	2183841.23	2100524.28	2459301.42	2691021.75	2178706.53	3837520.31	5048461.89
trans-geranic acid	C10H16O2	1.07	168.11521	11.482	1463151.35	1833514.23	5103188.46	10288960.1	9678863.2	7844931.76	8050077.7	7811112.87	8131639.8	10226867.9	11722915.4	11097792.3	10978340.2	13228124.6	14763255.8	18843369.9	23446006	23811908.7	20530489.5	20651492.5	27082471.9	605040.085	1373108.48	1215775.23	984199.97	6546888.85	10574546.2	1760360.82	11502962.8	10960852.2
Benzyl butyrate	C11H14O2	-0.58	178.09928	11.623	174011.141	890020.608	2103685.22	4081455.78	4864068.99	3345998.05	7310571.63	7365674.9	9400901.95	10106670.6	10677026.8	13064857.1	9705744.93	12527585.1	15208171.4	17969778.7	17063557.1	21192432.2	17745238	20910369	21790914.1	535266.815	814156.784	736405.434	5032642.8	10734189.3	20301145.3	1073154.59	27563029.8	26237923.7
Urolithin B	C13H8O3	-2.76	212.04676	11.695	10774.2094	11230.7433	10929.9039	11370.9593	11172.1133	11200.1219	11347.8458	11373.2948	11321.7026	11585.3113	11441.6626	11393.7583	11390.8666	10978.3796	11746.2917	11334.3833	11583.1556	11361.7387	11271.8733	11346.1837	11270.4836	6304830.29	6144308.81	7491755.74	19060.6852	11518.0434	11836.0493	11424.6059	11783.787	11512.0146
Myristamide	C14H29NO	-1.45	227.22459	11.843	276579.233	323164.381	342496.971	252640.208	251258.053	342614.955	4279165.68	4197492.83	4223191.21	4948511.1	4785845.49	4222962.4	4472163.5	4712962.9	4886435.61	4795155.16	5566384.41	4186344.05	4780287.89	4785533.09	4832938.96	5466969.67	6069863.01	253223.693	6950116.8	6312512.36	6791446.55	258607.457	7261882.32	6887396.68
N,N-Dimethyldecylamine N-oxide	C12H27NO	-1.18	201.20903	11.982	96557492.2	80445185.2	100753929	86504611.3	95116041	82381372.5	63679789.4	78593851.3	67922826.2	100346422	79483981.5	78407074.3	87079244.5	95846051.6	94528251	81634483	100220626	109952719	67093660.2	70025705.3	78717869.2	66843275.2	72834180.9	77487938.7	91848437	98669389.2	91669340.5	121882220	95464809.3	105817680
DG6650000	C7H4Cl2O2	-4.29	189.95802	12.054	574255.087	947541.494	1358924.73	796702.03	1258009.4	12935958.8	915982.447	906395.158	598252.397	450078.332	933396.126	1536606	1762331.58	1053506.07	3233183.78	271112.018	506141.209	824754.055	808117.575	447020.368	791358.508	880151.65	2025049.94	14402.0722	3799978.05	5441740.17	27788462.5	14575.6716	11132215.7	13277753.9
3-BHA	C11H16O2	-1.14	180.11482	12.457	4115166.53	2797931.77	2382868.56	7417050.29	5646030.28	2128370.67	57397.3906	16905290	9957467.39	902625.634	581772.321	661135.704	2996194.37	1460842.71	1298348.53	430443.527	226272.974	301820.129	1289104.99	1787891.56	2020349.58	4550555.3	4956830.32	4391730.4	2197721.39	2192946.44	2327021.69	541632.047	388350.943	374029.045
hymecromone	C10H8O3	-0.42	176.04727	12.495	2583693.24	2222580.98	2527461.03	2308676.94	2374197.59	2377053.18	11407506.3	12439900.2	10202032.2	2173360.31	2536905.26	2569767.29	2811273.32	2183657.01	3034130.82	2046620.94	2056791.41	2372034.44	2075135.54	2200928.96	2954774.78	1988477.33	1903156.8	1751721.09	1799361.01	1858998.04	1768438.63	2233704.63	1422000.11	1634764.69

Diethyl phthalate	C12H14O4	-0.5	222.0891	12.496	17408442.8	23205185.6	22744873.5	18494835.6	17292325.5	20716972.6	77314767	83557397.9	66348392.5	30122296.6	28045138.8	28313181.8	23396110	20943431.2	26735222.3	30067607.7	27439929.1	31584328.7	33048233.3	23333689	28127048.7	19964447.4	20799606.6	20329076.4	22640634.5	29159125	23497885.6	34109684.9	22873809.3	30713762.3
Cxa-10	C18H33NO4	0.11	327.24099	12.717	89440.8469	78123.5444	107657.813	34213.6191	208651.028	288824.49	1245499.53	1332716.58	1215667.06	567819.938	744809.771	834585.7	4203634.89	4543632.26	4218298.44	20129814.9	19880937.1	19433039	2054806.77	1594329.48	1702535.76	5408927.82	5842439.68	30446.881	409482.311	31151.6491	1013317.42	5284798.97	3853021.46	4431757.78
Decanoylcarnitine	C17H33NO4	-0.2	315.2409	12.767	165431.879	7215749.52	9675987.38	946399.621	868576.617	1027538.57	11714288.7	9685504.8	10645537.9	2161591.72	1925515.22	2103408.14	13506399.3	18687223.4	18885515.7	33185813.9	42565178.8	38219624.2	15271001.7	11685807.5	13206917.1	4443550.43	3938853.25	21708.3773	110486.376	23514035.9	24138229.6	8475068.56	5965281.06	7658639.5
2,2,6,6-Tetramethyl-1-piperidinol (TEMPO)	C9H19NO	0.35	157.14672	12.798	18314405.6	22610998.4	20349074.2	22091503	18568789.5	21700536.9	19465786.9	23870891.3	31265636.6	14773028.2	16959046.5	16708364.2	15366355.2	15970293.6	15822393.4	28091143.8	22937442.7	37344080.1	21544591.5	17162121.1	17729671.9	3980413.49	4889586.76	716600.632	4554275.61	4300577.98	4373394.64	5604013.61	4197001.08	5001870.84
Cyprodenate	C13H25NO2	-1.25	227.18825	13.144	106823.337	63491.6591	66673.576	61490.856	26032551.7	127119.872	103956.387	151445.249	25516687.9	65218.3403	98177.1819	53569.2785	121410.594	86119.9452	141874.292	67269.7501	72553.9834	54212.5679	75027.204	65568.0926	101476.728	24842831.8	26944880.8	30028845.1	29707325.4	29693661.7	27620978.1	127645.653	25134517	29995903
3-hydroxydodecanoylcarnitine	C19H37NO5	-0.56	359.26697	13.175	195948.529	37528.0419	191489.831	45081.5386	35026.3447	33550.8075	151761.533	161553.726	57329.9025	378268.969	457424.344	412040.547	47693751	53531642.3	54012074.3	3217156.09	2669748.32	3440543.92	3310146.06	3470246.84	3663822.81	617916.015	1066659.87	977114.497	2066569.66	210653.097	357495.764	2977297.58	324648.79	3016546.26
navenone A	C15H15NO	-0.74	225.1152	13.439	488674862	338889213	311981375	254724759	360166972	352987525	306300491	338650540	240618683	326106845	374368956	366170113	318847793	379913315	276094817	396215033	298807335	353897067	362984372	376439680	372410403	209660398	226698598	168071135	351470.554	257682514	239556635	250341099	219330259	225114486
6-Pentyl-2H-pyran-2-one	C10H14O2	0.52	166.09947	13.604	5752324.21	4712629.83	5828791.84	1593975.94	2530573.8	1917338.1	1825910.68	2641788.33	4098086.14	1597496.16	2008716.84	1677156.49	7793764.56	7325516.82	5612836.94	3611220.21	2832655.69	9059193.01	8974984.89	5985543.04	4959558.27	787609.688	128868.262	938512.571	116794.438	1728509.97	1677804.87	1083274.56	219249.959	1203141.82
N,N-Diethyldodecanamide	C16H33NO	-1.2	255.25591	13.744	45456944.2	42532925.6	44151706.1	42040018.4	35356244.3	35621827.9	37444349.7	37548802	41749665.5	43102723.4	51620237.4	41101603.9	46491767.8	46464012.2	41963678.8	46403789	45098631.6	39007477.5	43368083.9	41410167.3	44521482.6	55190653.3	57570639.2	67482362.2	61997739.9	55669927.4	55227264.6	51151017.6	43093626.4	53269016.2
2-Amino-1,3,4-octadecanetriol	C18H39NO3	-1.78	317.29243	13.839	2870837.66	3467604.56	5555462.88	371902328	331522963	356556525	355869700	314164171	346115337	338760437	402387389	430990751	406213669	433492332	418802043	473369081	479672144	399098139	410221629	451812915	466891496	568777769	686145757	721231544	663096096	561218730	556122088	527749609	472231532	573104733
1-Tetradecylamine	C14H31N	-0.94	213.24545	13.896	15774484	11333024.2	14680995.4	13171068.8	14772559.8	13983417	15548104.5	14945195.7	15482559.6	13676789.1	16558685.4	14712828	16838020.6	14870007.1	16795723.3	18192031.9	17082580.5	17004172.4	16675912.5	16984671.1	17474904.9	19670632.6	19180498.6	18872203.4	22495407.4	23677134.7	21741972.4	21730310.8	20195955.4	19943529.9
Dodecylamine	C12H27N	-0.33	185.21429	14.086	15171625.1	15900011	13853396.1	19362539.3	13136260.6	12734956.1	13607700.3	14627633.9	15374210.1	14409350.2	15629638.8	17117898.1	14420891	17489588.3	15778683.9	15289941.9	17362194.2	14196120.7	15773170.2	13822637.3	16026593.7	17186263.4	20156594.2	19042449	19996963.8	20630683.2	18729832.5	18038580.2	17277581.4	17714122.3
S-3-oxodecanoyl cysteamine	C12H23NO2S	0.23	245.14501	14.143	780495.106	409101.68	463604.811	446863.173	512687.657	349976.928	1156584.6	1027888.43	1046850.71	247320.144	251630.237	190798.816	12007363.5	5413169.31	4510912.97	721243.351	701708.906	1168430.11	1696166.62	1531765.77	1569396.86	426430.096	513917.508	31396.4431	34277.7872	1680086.16	1528783.67	3118972.94	37752.7372	3922303.5
Dodecylamine	C12H27N	-0.27	185.2143	14.254	61085.9013	74937.0924	83551.1853	116042.214	112694.498	143079.066	134476.338	232275.738	285677.157	14409350.2	15629638.8	17117898.1	14420891	17489588.3	15778683.9	15289941.9	17362194.2	14196120.7	15773170.2	13822637.3	16026593.7	17186263.4	135447.436	19042449	140942.917	20630683.2	18729832.5	18038580.2	94767.1654	17714122.3
3, 5-Tetradecadiencarnitine	C21H37NO4	-1.11	367.27185	14.367	6123568.96	6103332.4	6670331.87	32767.6259	102361.312	612858.251	75405.3413	20791.9777	723108.779	628251.118	610093.62	470960.898	14856185.2	18314882.5	20133990.9	1418560.32	1476674.87	2130107.07	1649811.25	1681656.11	1586960.35	735965.979	55450.3206	750186.843	16944551.5	1447416.59	14398571.7	992549.492	144932.559	1061312.74
3-hydroxytetradecanoylcarnitine	C21H41NO5	-0.37	387.29833	14.844	361599.378	405585.212	510190.072	284564.264	299987.028	32779.9304	2708181.11	51993.147	29884.5714	231377.038	269539.451	206615.719	52243924.6	57058115.4	54755012.7	1685186.59	2052525.05	1669017.69	2812736.03	2496306.7	2380232.34	73054.6575	45019.8112	59169.3907	75721.0386	125297.105	66461.3226	2167491.46	80225.4176	1935299.05
sphinganine	C18H39NO2	-0.45	301.29795	15.267	392322.693	606467.787	601815.917	1783379.02	995074.749	67734639.1	51403798.8	55599015.7	67523118.5	54111556.4	54523080.8	58804986.5	51949072.5	51846528.4	61321290.6	59783922.7	69347581.9	52417238.3	49207851.4	55476406.2	49978507.1	95937123	167544718	100080259	101954674	101324003	111285172	80177581.2	101619012	104116942
(4S)-4-{[(9Z)-3-Hydroxy-9-hexadecenoyl]oxy}-4-(trimethylammonio)butanoate	C23H43NO5	-0.32	413.31399	15.423	169528.659	114968.617	115730.608	103935.502	216293.887	197557.819	1229454.1	1095985.75	877313.84	250336.962	224676.438	228672.248	25758739.7	25937371.7	25235228	2653383.38	2413832.47	1964094.95	3168137.68	3221372.09	3251908.72	768297.466	858314.745	763212.299	5822396.81	5618547.97	5832579.22	1926373.03	2011145.12	1814218.97
(4S)-4-[(9Z,12Z,15Z)-9,12,15-Octadecatrienoyloxy]-4-(trimethylammonio)butanoate	C25H43NO4	-0.08	421.31917	16.037	342906.465	328360.405	418462.162	1167493.01	1050054.24	1352109.16	663175.983	690733.484	794577.764	843394.883	950170.551	1164691.77	16334511	16149722.9	16315491.6	2815886.84	2360517	2774280.5	9303809.04	11758709.4	7836756.59	1851422.08	2217272.05	2166504.41	5764309.2	5519952.3	5988942.67	1833225.68	1668952.7	1765132.07
3-hydroxyhexadecanoylcarnitine	C23H45NO5	-0.69	415.32949	16.121	639470.822	678349.899	713123.711	580644.861	437189.163	530532.155	4566459.96	5826590.97	93766.9873	528051.651	329849.314	594676.28	85066146.2	114344166	38786075.8	3976893.32	4432071.09	4293718.34	8878004.85	8005034.89	11445775.4	2333019.29	2745994.31	2304197.49	10780845.8	10035620.4	11281428.7	2939776.48	3431493.99	2440982.08
D-Sphingosine	C18H37NO2	-0.57	299.28226	16.195	265735.923	323932.995	412550.1	246812.443	14708888.3	16628244.6	18701557.2	23991040.4	25190054.9	15362214.6	14857356.1	18381698.9	16709216.1	17956277.3	17499135.8	20833100.3	24346573	19334048.5	23408110.4	22882797.4	22974847.3	34383660.8	42638304.9	36447683.4	54099551.8	51963425.5	58809919	24955376.7	21038205.7	22950692.3
(2E)-hexadecenoylcarnitine	C23H43NO4	-0.89	397.31885	16.235	1009190.64	1263823.31	834724.918	622742.465	683405.479	306643.649	2387306.1	9653325.75	9690947	7899063.3	6045566.77	6948661.65	106095319	158012701	156878190	46756089.6	70024228.8	53669917.7	39488552.4	36951921.8	47140424.9	5185936.53	10088348.2	8929767.16	160488610	154837245	173111919	79621222.8	41300959.5	55636902.7
O-pentadecanoylcarnitine	C22H43NO4	-1.11	385.31878	16.237	432955.69	375376.778	410805.352	309013.521	231757.927	313311.245	1692042.66	632743.551	426491.648	1157937.54	1068364.13	1326724.49	22675857.3	30961750.1	33479894.1	11388850.5	13377534.9	12236248	7076717.13	7046204.82	7482929.38	4774776.93	5890459.86	5789685.41	13447379.2	15168919.4	20066431.4	3984537.77	3223558.42	3817310.38
Tributyl phosphate	C12H27O4P	-0.61	266.16453	16.319	28951445.7	29302564.9	38666785.2	35409635.8	38385123.4	30410602.3	34689569.9	39956316.1	33860992.2	43107871.9	37115235.7	38543158.6	38216694.3	35123597.3	42395419.9	40093833.8	36258291.5	37152864.4	34925502.3	33620449.2	36219348	5284615.17	5953621.21	5351139.96	6092158.04	6394943.9	6355854.05	5197261.01	5096294.93	6131345.92
Linoleyl carnitine	C25H45NO4	-0.8	423.33452	16.546	12199706.4	11829929.5	11820098	1662795.41	2128319.66	2185266.12	878636.817	2047713.57	2373603.34	3681482.92	4875636.9	4841357.43	131125976	132279489	121646412	11179728.1	9997143.52	12944346.1	131118866	161617384	151228383	4091439.89	4950371	4115946.51	46255042.9	37869477.7	46244004.9	7815622.28	5334757.82	14347859.1
N-Stearoyltyrosine	C27H45NO4	-0.51	447.33463	16.555	581679.35	701593.45	488612.276	1099761.56	1044910.99	1695289.08	223184.52	457288.331	572593.473	823948.91	1149989.37	1253793.84	40755451.9	32317190.3	27044097.7	2455753.88	1720279.64	1906998.83	28080011.3	31260900.8	27924391.5	2263676.05	2019844.16	1959928.76	3556911.87	3225160.48	3642662.48	2119002	1437226.64	1985913.14
Bis(2-ethylhexyl) amine	C16H35N	-0.17	241.27691	16.613	195255.013	287487.908	229988.201	341592.636	6943561.64	4997216.63	15088296.6	15247980.9	16599242.3	15520436.3	29754586.2	28319093.5	15084126.7	12812032.8	23060765	10266169	12928341.8	11998520.7	33917306.6	30594100.8	22187910.1	5377662.64	6324459.09	6481731.58	5839675.02	7271942.35	7449021.89	6427601.81	6203735.36	5494235.64
Palmitoylcarnitine	C23H45NO4	-1.54	399.33424	16.918	25576513.3	20227745.5	21576067.4	6653527.16	5970928.6	8034505.05	52069672.4	6540028.05	64797909.1	21496340.3	19422570.6	21731730.7	358672943	487379265	460391615	243320549	339162522	242737000	255089298	244757766	228237428	55253274	60615972.5	57726510.1	482232425	392962581	413037562	118853088	131859014	121584024
(+)-Nootkatone	C15H22O	-0.04	218.16706	17.055	852366.243	992119.884	798332.816	673163.837	736304.391	804147.739	1097982.86	724313.754	1028887.01	882020.116	850690.405	923915.456	1057405.77	946297.707	137963532	69766632	978621.886	91373114.7	1118991.61	1588279.58	153990888	1772250.64	1432199.18	1950663.96	2071403.73	2063789.78	1860783.36	1649354.18	1533114.17	1338068.09
3-[(12-Hydroxyoctadecanoyl)oxy]-4-(trimethylammonio)butanoate	C25H49NO5	-0.59	443.36081	17.112	15165572.3	13014520.9	9464130.74	9019537.57	5241200.76	9798429.01	20922836.1	19916814.7	24614299.7	16817993.7	15333589.3	20138824.4	228092398	297191499	417772518	208357744	289239065	285475203	246492337	168322597	204957671	30396916	31608806.6	27370217.5	303135417	317342903	313087722	150146907	165305211	201173587
α-Eleostearic acid	C18H30O2	-1.14	278.22426	17.2	16107982.3	23215588.9	16163538.8	1549352.7	1698229.55	1232425.32	3630969.55	7842082.79	4221002.03	659690.808	573173.378	583737.097	2150214.79	840738.582	1233467.39	493460.011	779390.652	1104243.25	4036261.79	2849384.87	2815477.95	1827352.37	2115750.8	2184225.65	1976521.11	2203283.8	2506227.06	1412616.78	1318265.78	974567.137
O-heptadecanoylcarnitine	C24H47NO4	-1.31	413.34997	17.209	3123452.06	884078.266	1880257.05	417756.879	836248.888	1078711.18	2797864.52	8406274.5	9879871.15	3099058.59	2387191.25	2496890.75	54527609.5	66315060	62223922.7	12708165.1	16314730.2	15572052.4	18129094.4	15350435.5	14336543.4	4428499.15	4902047.92	2953403.5	22285840.9	19783624.1	21075657.5	6342160.27	4506748.52	4774340.74
1-(2-Furyl)-N-({(2R,4S,5R)-5-[1-methyl-3-(2-naphthyl)-1H-pyrazol-5-yl]-1-azabicyclo[2.2.2]oct-2-yl}methyl)methanamine	C27H30N4O	-2.51	426.24089	17.404	12662545.5	14462265.1	15106670.9	13839936.7	12464386.2	6343143.27	14693530.9	13318864.3	17567402.8	15613357.1	13758960	17976575	17124443.1	17172060.9	14332108.3	16732823.4	20245936.6	16937888.1	17793451.6	14988766	16369536.3	31627894.1	31812588.8	32456872.3	29526147.3	26519735.5	27605561.9	36626026.7	32325080.7	25759374.1
Octadecanamine	C18H39N	-0.33	269.30816	17.444	410674.806	454812.809	262500.329	8107733.21	7690238.56	4678315.5	12744158.8	13730590.2	14725871.2	11485023.6	22690227.9	19429885.7	13011345.1	10957285.3	19608669.4	10368837.3	11672715.1	10679580.1	27740745.6	36304135.4	19533002.3	7225262.21	8144464	6555534.44	7147895.28	8787759.37	9880559.62	7379148.64	8659069.34	7552056.68
Leupeptin Ac-LL	C20H38N6O4	3.89	426.29711	17.491	78972444.9	73864184.6	83486231.3	85822367.1	57006044.5	93993988.8	93420194.4	72494140.9	79711835.8	107325285	81056647.2	90371341.8	94145146.3	108467942	97265175.2	115312035	82410772.6	97201554.5	99759311.8	80647052.9	115402288	133926572	187893754	169737392	158068377	140563287	171008723	186410414	192816005	195689800
12-HSA	C18H36O3	3.63	300.26753	17.547	5679417.25	4732826.74	5414982.84	1166945.75	844413.168	991762.846	3557980.81	3278395.75	4313886.21	608193.812	653576.08	647346.981	233364.563	374432.641	348036.424	246376.418	279811.007	255117.906	1175312.64	1184878.54	1226272.79	1380386.85	1714434.54	1408281.36	10443614.1	10092850.2	11477864.7	117763.204	146446.082	95929.3089

LysoPC(18:3(9Z,12Z,15Z))	C26H48NO7P	-2.48	517.31555	17.579	9768328	12847206.5	12186388	175358647	94828389.8	118955797	71186877.2	70530926.3	49823754	31475052.4	35315907.2	21835364.3	99841462	86248731.8	92842389.3	63825626.9	58287210.3	55204167.6	52190557.5	74153082.1	46784424.3	133973873	281344119	195665391	81358822.8	86325030.2	100654223	43054251.3	39041771.7	42924434
mephenesin	C10H14O3	-1.46	182.09403	17.897	21946379.1	25349871.5	17110590.9	23877829.2	12615288.9	26758898	20575663.9	19098871.1	24405551.1	23056441.5	19154112.1	17803857.3	22247529.3	21058918	18987808.9	24030290.1	25029245.1	18007580.8	23804252	21493144.7	19390715.3	28563226.5	30901499.2	28829164.3	18056557.2	27152277.1	30060382.9	24736095.1	20968345	23802525.4
Ebelactone B	C21H36O4	-3.57	352.2601	17.944	2839709535	2483533471	2624728164	2929434545	2255456109	2749952628	3013360049	2155633101	2830793068	3206138397	2110206049	3007788275	2795639800	2953690572	3073384350	2621251060	3095186283	2966181646	3321667499	3054830699	2708773351	3117905004	3268798601	3393942503	2878861381	2971077146	3110380223	3266559119	3236462228	3206094298
cis-5-Tetradecenoylcarnitine	C21H39NO4	-1.91	369.2872	17.946	195746249	142977449	129143538	123502073	95662115.5	99151824.6	115981842	82341515.4	93998022.4	110640217	85267143.3	82053595	76366626	97138174.4	86482735.4	91927809.9	89758099.5	91324803.6	96192588.2	86096913.7	74128698.8	84186260.9	75807537.6	73654838.5	58212296.1	62693301.3	53456641.9	54323113.5	53726474.4	52747063.5
Butopyronoxyl	C12H18O4	-3	226.11983	17.953	83864672.4	89615786.5	72875604.4	88642765.6	59035961.5	75088360.1	92062875.4	72356547.3	85700835.9	95227374.8	72250457.7	90254095.5	89680102.3	87584974.9	85148060.8	93154457.8	104230483	87920279.9	110474141	88749448.9	76578468.3	136454560	140790340	134018363	142630602	142938765	148941126	150992814	147221452	147437327
1-Linoleoyl-2-Hydroxy-sn-glycero-3-PC	C26H50NO7P	-1.53	519.33169	18.164	1217602852	1554098404	1415603143	785961714	670320180	532558297	350340953	395020545	355284862	274403978	332774966	291713731	876446986	957090145	843858929	421870924	351137075	377906097	891007228	914188457	884379894	845057634	936217229	873011647	837312320	812444769	1065481135	302606231	405036183	362396857
27-Norcholestane-3,7,12,24,25,26-hexol, (3Î±,5Î²,7Î±,12Î±)-	C26H46O6	-2.27	454.32841	18.35	355929938	326629394	349285113	333763934	273090956	306606704	341455342	303184773	354252049	399343990	303730273	331529984	236125604	380344279	366112186	352800993	382125097	387673983	380579027	370332921	419437572	571187041	624625515	669323735	665739546	769051343	630991183	753817343	770482475	365544789
Dodecyl sulfate	C12H26O4S	-0.89	266.15494	18.356	100074.639	108878.093	110844.223	116366.74	114930.027	111666.381	113800.284	119002.814	106956.63	129744.457	108728.353	115525.937	95522.5233	116329.58	117502.061	142328.366	132184.175	135123.031	127367.926	91083.4471	112115.393	53646068.1	62229646.5	63547421.6	68634067.3	78356563.7	94789568.6	83887134.2	86202846.5	83477951.2
3-(Icosanoyloxy)-4-(trimethylammonio)butanoate	C27H53NO4	-1.74	455.39667	18.443	28473006	26664814.8	29246761	12008061.2	7293567.86	8084857.52	121237585	92815717	121772467	34978409.5	36603707.4	42440853.5	243315880	350579861	301043050	103270454	126810464	108164293	160374333	150190855	140473397	70580646.6	103811041	106673204	444713045	611127700	493876951	110421125	87095984.3	90493240.8
D-Arginyl-L-histidyl-D-prolyl-D-tyrosine	C26H37N9O6	2.16	571.28792	18.486	602100.326	938306.616	924979.133	1308518.22	1057251.13	1088475.17	1409570.64	1493736.18	1766852.43	1003171.09	1426505.78	1623795.96	1782739.36	1813960.01	2171648.3	1671496.94	1750459.81	1537194.23	917595.813	914157.765	999007.99	4632670.11	5297624.32	5900107.9	4351065.03	4976810.1	4449406.92	6441928.18	5848820.61	5998838.13
(2R)-1-{[(2-Aminoethoxy)(hydroxy)phosphoryl]oxy}-3-hydroxy-2-propanyl (7Z,10Z,13Z,16Z)-7,10,13,16-docosatetraenoate	C27H48NO7P	-2.87	529.31532	18.867	19519092.1	20995116.3	22728150.8	6805841.45	4636854.08	6294694.26	18858520.9	12728381.9	19353057.6	9371028.37	11896166.7	13049329.5	15986631.7	12730330	10367834.8	14823213.5	17808559.1	12644872.4	16528998.2	20214575.2	14933013.2	37872246.2	28084410.6	36686582.7	42235658	41561825.5	34135685.1	36601888	37116217.8	33749238.6
Choline	C5H13NO	0.64	103.09978	18.908	47139482.6	36276102.2	41157175.3	37397224.1	32393607.7	34423013.7	37369224	40717678.2	30982548.8	25303162.4	18910489.1	25125224.7	39502697.2	39587533.9	40530527.3	21446067.7	19221404.9	16346066.5	21746349.7	22200192.4	22811578.4	62137919	48365193.5	44285986.1	40413471.6	21897482.3	47811260.4	28930640.4	25292065.4	18631484
2,2'-Methylenebis(4-methyl-6-tert-butylphenol)	C23H32O2	-0.77	340.23997	18.91	371327245	425679798	264970273	128106041	364874046	307300405	224874720	366084556	108557899	222023994	232859508	239633617	172496183	263018960	114636355	180948243	111046665	164006709	174493175	207780067	172873077	930613570	856751461	808288529	842503285	846151565	862961248	737104460	776157135	801662035
1-Oleoyl-2-hydroxy-sn-glycero-3-PE	C23H46NO7P	1.06	479.3017	18.959	36775437.9	31420220.3	31758212.6	10903691.8	10428452.9	10251566.3	16156475.7	23568853.1	35520586.4	9441949.3	6692024.43	7952328.79	11256283.5	13717369.9	15376124.2	13713988.6	16103124.4	14613564.7	8010061.93	10376141	8231659.06	19368174.5	24653798.2	14089005.6	29259278.7	24695905.8	25977113.3	13942633.4	13119089.9	16024435.7
γ-Linolenic acid	C18H30O2	-2.25	278.22395	18.988	133092800	99926594.7	91445935.5	249882012	190533960	226950202	119717746	168850433	134030346	35064203.4	32401497.7	30839976.1	116196395	89165720.7	115130747	26725166.1	25757836.8	28526853.9	76778935.7	73744708.2	69802965.1	249312411	230037382	202788794	228439219	204122422	210960133	31891458.3	33238849.5	30766257.9
Palmitoleic acid	C16H30O2	-0.19	254.22453	19.236	9257906.33	10008077.8	12501440.2	13566029.5	9621212.38	14524045.9	21075966	18751673.9	20313520.3	10101785	8508780.21	8590656.56	23052861.4	19662100.2	19698750.4	9645327.99	6879061.12	8518181.06	14799417.3	12017948.3	13153763.8	2954431.22	2951296.16	3008543.42	5932513.03	5820917.28	5749096.68	3534135.03	2447221.96	2616744.79
Oleamide	C18H35NO	-0.43	281.27174	19.367	101768475	163138442	99014387.1	1092626454	906794352	1195847895	431592361	776633320	546112658	37161605.7	40337944.5	39748871.4	29780207.9	34725979.1	32697677.2	35252692.7	511510797	34681605.7	205935865	84429505.1	34361124	94725597.4	108949776	77316883.9	1401710869	1363412032	1471060944	94657271.1	101253231	75918342.4
4-Undecylbenzenesulfonic acid	C17H28O3S	-0.7	312.1757	19.397	167370.533	201268.769	218245.708	285040.416	211884.41	37459.4252	291375.749	225917.576	241273.842	331342.587	287956.823	294663.677	527166.727	441920.407	481192.619	682364.186	316537.195	275493.705	405343.389	285059.048	305081.149	39994664.7	44563350.3	47461582.8	34303597.1	36146620.5	50456335.9	48709584.6	47858475.5	53801942.6
3,6-Anhydro-1-O-palmitoylhexitol	C22H42O6	-0.1	402.2981	19.445	18929880.1	13100995.3	17670013.8	9375044.33	8717300.63	9632686.93	19427083.5	21874860.2	14217656.5	14713906.6	15392221.4	16891465	3711949.37	5247462.25	3682398.08	30198695.9	32016877	26839945.2	22086086.8	20826325.1	22570503.7	10658209.6	11519498.4	10468315.2	16847368.4	16029221.3	17974105	16316830.2	17768901.9	15965511.8
1-(1Z-hexadecenyl)-2-arachidonoyl-sn-glycero-3-phosphoethanolamine	C41H74NO7P	-4.31	723.51717	19.497	5709951.09	6406580.27	4449182.76	3476516.91	10828436.5	1424194.71	7372444.77	1526176.94	4711539.47	1308070.52	2704670.56	2406910.94	1195316.08	5201839.44	2401531.22	5635692.73	5617686.05	1091453.09	6078217.72	1009372.64	1150941.22	2310829.8	2619802.6	321727543	335904492	391862309	570766932	451785153	213423538	288386782
1-heptadecanoyl-sn-glycero-3-phosphocholine	C25H52NO7P	-2.7	509.34676	19.507	6516322.84	12346112.4	5686290.06	17478190.6	12306899.3	13234561.9	7078053.57	10909310.1	11132102.3	3709311.52	4110961.21	1791652.95	16345142.9	12672800	8499897.32	5396881.48	3122092.55	3636599.81	2684046.91	6725132.03	4231927.96	40692622.7	37560779.8	42269631.3	24716179.7	26319659.2	26578527	7284184.41	12480990.6	7777128.33
Linoleic acid	C18H32O2	-0.21	280.24017	19.627	179535160	144436206	167585404	37774869.3	29064524.3	36444193.6	35998114.4	36144729.6	32168626.4	11164904.7	14188532	14056729.8	69632512.8	33487073.5	28215963.1	8405209.42	9993394.43	9998253.61	35881544.9	37192261.3	32593070.3	29400991.7	33443481.5	33464639.7	54043582.3	6464876.39	66955550.7	16003842.3	15312407.8	15165717.2
Monoolein	C21H40O4	-1.1	356.29227	19.656	419465571	548579673	422657371	125285279	124093938	54575037.5	202576936	271688832	227023926	157541095	152116292	166304299	82311429	153668719	140215007	321339491	140392805	265646920	412918678	347261244	367643319	219125985	196525032	162898543	167691119	187010875	177516441	113151001	98878945.1	179972513
PC	C44H84NO8P	-3.44	785.59075	19.683	1520387.24	1477069.25	2941137.48	17620473.4	23413630.4	22718668	33801385.7	73738831.7	57568326.8	89369569.4	94488747.3	103446453	113037671	265665316	83581295.9	45170199.8	50539208.8	69803663.3	121474423	99504810.2	93390957.2	1217276.99	1514236.21	1504329.47	98493392.2	59970569.8	150510937	56919516.3	48554306.1	62120932.6
1-hexadecanoyl-2-[(7Z,10Z,13Z,16Z,19Z)-docosapentaenoyl]-sn-glycero-3-phosphocholine	C46H82NO8P	-4.88	807.57387	19.744	681496.137	2262440.44	7654898.06	13220199.1	3066252.75	74229830.1	48562552.2	65866885.7	89583639.1	149312682	118779868	97924400.4	67389031.3	142507138	81126007.9	144142244	86546061	78510379.3	94189533.9	112453194	58839007.1	480412.042	583867.831	66026782.3	146330664	53580370	52860125.5	96719403.6	91331530.8	92573916.3
Cyclopamine	C27H41NO2	-1.83	411.31297	19.797	4592827.3	3670451.1	3315212.99	2073985.84	5101266.03	3328574.45	3437847.71	4108275.27	1674878.45	2723922.49	3722779.57	3834549.29	2126193.9	3818132.95	3032989.9	3464208.41	2322404.74	3100870.72	2954342.27	2623539.66	2582691.05	4684100.65	5703964.89	5748616	5878995.37	5195093.22	5204952.58	4395906.94	5811833.64	5138518.96
1-Stearoyl-2-hydroxy-sn-glycero-3-PE	C23H48NO7P	-1.08	481.31632	19.897	258805675	104877833	74854697.3	39273539	36064819.1	42446669.3	54917028	65460309.5	64773448.1	28405959	30969024.7	28111846.6	374207136	102367591	110014653	46095394	42602303.5	33985681.9	64450127.2	60677742	53063476.1	298485657	328357802	276141385	438720384	427666461	355111655	146168016	135387272	117764920
8Z,11Z,14Z-Eicosatrienoic acid	C20H34O2	-0.11	306.25585	20.071	19093359.1	22192416	24174253.3	22886137.6	17220647.9	19963247.3	32815492.7	28468736.8	27117060.1	11462831.7	11072555.2	9771905.66	22916648.3	19232937.3	15947357.7	13216815.3	12540129.5	16032373.3	11677103.6	9820891.06	10783740.8	9901301.21	12359860.8	17606940.7	40599115.8	45773001.3	46526012.4	12267401.9	11420560.2	15389656.8
Platelet-activating factor	C26H54NO7P	-1.54	523.36299	20.218	110886551	86194763.4	55568960.6	59553184.3	49589600.3	50831122.1	69046893.1	85451633.3	70327222.8	25820892.2	25217730	26437346.4	121570665	101788896	82040299	19523594.3	20027389.5	17974807	40480269.9	34025421.5	39017569	194892350	149993935	131087695	250314233	248869868	260965294	43190297.8	33405906	44648481.6
Stearamide	C18H37NO	-2.71	283.28675	20.23	1407808038	1409213536	1159871086	883964534	1520423444	1142123861	968010762	1204607600	861546638	1036565087	1264575163	1246608776	1093945276	1283387735	1013612634	1253789782	944198624	1202153551	1189758885	1232978244	1133743538	1700479142	2002373197	1679228146	2050221201	1836424605	2058251178	2094359156	2100283877	1967592049
Ethyl myristate	C16H32O2	-0.31	256.24015	20.305	44116640.4	37981555.2	39290745.8	24555692.7	20483533	24960580.4	33341417.1	36518312.5	35225871.4	21353417.4	19560760.8	21059164.2	33399223.3	31494743.7	34153593.1	20586877.9	24143482.3	19262021.9	23984236.6	29640908	28149392	11982077.9	12584679.7	14626603.4	18400501.4	18784778.5	25639897.2	10919681.2	10378605.5	9845264.4
(3?)-androsta-5,16-dieno(17,16-b)quinolin-3-ol	C26H31NO	-1.53	373.23999	20.355	14852884.3	25229215.8	21978788.6	12249229.8	23223213.7	15415393.4	15444007.8	23977193.6	11445345.2	18515781.7	17381377.1	19063639.1	13389641.2	22318114.5	9165319.74	13820385.1	3747917.5	10623442.5	9603512	14259835.7	13902301.1	18198957.6	18592739.5	17496402.1	36904.2618	20414011.5	19097675.2	18624920	18656172.9	20190804
Octacosyl (2E)-3-(3-hydroxy-4-methoxyphenyl)acrylate	C38H66O4	-4.69	586.49336	20.514	2904836.93	2585827.28	2244467.94	1362325.69	1233016.05	1084539.84	3043613.62	3205036.65	3082549.12	1156499.9	1126568.81	1343699.98	5560570.81	4176687.96	4018412.73	1336951.16	1707015.61	1639483.58	3120682.13	2970117.87	2956050.64	605538.518	1628303.4	1342097.28	2134117.49	2067890.37	2038056.41	941444.053	895182.19	888396.578
Oleic acid	C18H34O2	-0.22	282.25582	20.517	89146895.9	82442592.1	88003042.8	66115275.1	57812027.5	48624446.8	104406546	103091257	106072444	58130415.2	59465612.9	54853834.3	163358578	133905341	129995670	65005886.5	76853155.8	69836524.8	113084846	107371303	103996890	65940533.6	69820163.6	53524764.2	84758809.3	91484875	89556805.9	46949134.9	51132742.4	47887169.8
PC(o-18:1(9Z)/18:2(9Z,12Z))	C44H84NO7P	-4.11	769.59538	20.517	62140.7045	55792.3774	76766.2466	695890.637	1223926.09	1175700.59	2816623.49	3667621.56	6562477.86	659680.756	1277271.17	1259797.81	2627270.35	6824804.93	1276919.19	695562.227	2434499.07	1810656.41	3280902.5	3046000.1	2883569.65	90799.6646	92263.3588	113471.963	14541537.2	42444922.7	44463676.9	54259997.4	58032927.1	54098645.8
Adrenic acid	C22H36O2	0.6	332.27173	20.594	9277905.34	8004797.71	8952294.42	2371865.98	1996006.76	2317009.3	5472103.56	6061459.87	6096614.46	2925391.54	2786930.05	3151816.19	7140576.02	5845566.07	5818266.15	3809828.33	4020900.63	3162165.74	6638482.46	6880057.97	6095667.83	4026689.88	4436228.28	4745247.63	10880049.6	11231661.3	11348261.8	3492237.2	3663661.4	4030051.91

Di(2-ethylhexyl) phthalate	C24H38O4	-2.16	390.27617	20.71	278944105	247358617	314629125	228654880	228906242	215514214	590387440	582090315	431426766	274377054	234371063	220210919	334400337	235645520	85143653.2	241591839	224984170	238846685	104889061	232078145	250908804	404319174	426209093	415245713	367948588	377474016	348482502	418125029	411866994	367427055
1-Stearoylglycerol	C21H42O4	-2.99	358.30724	20.861	2073172228	1934359390	1759910013	1374681391	1397483292	1083634593	1181507922	1232405921	1427057109	1250713068	1288743861	1518479224	1512224473	1536110279	1250336906	1436153241	984220812	1185876064	1203941293	1332482042	1371392679	2234547655	2389864722	1708722677	1705913103	1727172163	1754497295	1405350383	1291749628	1166092514
(3S,5R,10R,12S,14S,15R,16R)-3,5,10,14,15-Pentahydroxy-12,16-dimethyl-2-icosanone	C22H44O6	-0.27	404.31368	20.863	20789689.6	20402278.8	21022874.2	19403290.7	17605006.6	17412161.5	17148584.6	18241865.5	20035072.8	19708786.1	17381611.2	21849576.6	20740422.6	21302072.7	18634932.7	19667727.7	14005189.6	17931761.5	33435976.6	19122485.9	21668779.6	9088076.62	10048404.2	9098600.48	10643871.9	11363023.8	10769687.4	8422835.91	8399796.06	8777230.27
11(Z),14(Z)-Eicosadienoic acid	C20H36O2	0.39	308.27165	20.992	3153341.42	3453374.07	5783433.19	786685.797	748743.074	777292.924	1202301.55	1898115.23	268466.041	1211050.59	919159.103	939562.102	3433993.56	2827043.08	3374519.49	1735906.74	921693.979	368039.202	1825669.95	2227613.66	1835403.11	322968.278	617336.175	1249744.65	1672494.15	1454043.45	1287062.83	3230828.22	2995379.16	3324027.41
1-(6-Nonyl-3-pyridinyl)-1-decanone	C24H41NO	-4.19	359.31731	21.026	1295067.84	4121699.9	4291086.89	3355022.08	4997715.76	988923.326	3850255.72	1296660.05	4222123.53	3261806.99	2123590.16	3436776.51	2746685.67	1739469.06	3729767.76	5523860.46	2789601.37	3394036.51	4072959.76	2830689.75	1766308.16	16802367.3	17506209.7	1861964.62	2166334.25	5404346.74	2514266.59	768070.136	734339.359	622411.9
(2E,4Z)-N-Isobutyl-2,4-octadecadienamide	C22H41NO	-2.02	335.31814	21.13	76584227.7	79269694.1	63051145	35075612.4	65205623	53200174.6	40128788.1	71167996.6	35775574.4	46553833.5	51331980.7	36666374.9	40781142.9	81758673.3	46536413.6	44081391.6	34802439.3	27470128.2	31910017.4	20914213.7	28397143.3	187880141	170774146	123732362	70345643.6	60481134.4	62009338.2	78192367.6	79976536.2	74374800.6
Margaric acid	C17H34O2	0.57	270.25603	21.145	1991885.41	2378333.85	3890419.58	3294174.41	2359468.57	3130200.02	5691565.43	5868991.65	4700142.67	1669331.92	1524503.53	1553827.3	7773509.65	5449258.09	6311906.36	2898894.73	3342556.76	2630788.59	3488447.54	3873588.4	3332006.76	788546.439	1211240.5	2105397.15	2738036.55	2903266.3	2821122.03	1200471.15	1382486.51	1212664.83
4-Dodecylbenzenesulfonic acid	C18H30O3S	0.96	326.19188	21.461	985562.568	992843.865	949320.656	948673.568	863575.089	1042938.44	1219813.88	3578603.37	4274830.17	5828191.77	4575518.26	1340183.78	1348056.53	7676876.48	3483597.63	64047884.3	54696411.8	57117435.2	60730485	66243962	75380599.3	2166754.5	1939740.13	2982966.92	1824463.38	2047970.75	1604085.37	2009321.21	2059395.18	1824002.16
1-(14-methylhexadecanoyl)pyrrolidine	C21H41NO	-2.21	323.3181	21.588	73517830.4	27050021.3	33919581.1	13954573.9	40687855	34698682.4	35302506.3	22488288.8	25345154.6	20452146.1	38461361.7	45386890.9	30815712.1	28186421.3	37903611.5	37239761.1	45954911.2	25655595.5	24579600.9	40103754.4	27233810.3	127074118	122152293	125778039	123765693	115951728	142233973	71044408	72174265.1	82511143
(2E,4E,16Z)-1-(1-Piperidinyl)-2,4,16-icosatrien-1-one	C25H43NO	-3.38	373.3332	22.137	37962947.4	27365342.1	22332039.4	18112918.6	30727223.5	12114099.5	20875954.5	12480456	12010583.6	20252816.9	22266535.7	21906292.8	11637271.2	14203260.1	19821227.1	20815345.8	10761269.1	15046369.2	15927021.3	20680915.3	11365784.5	70954331.9	62594231.8	35888567.8	36820224	36134431.7	35603560.6	33901299.3	27456976.8	31866051.9
Stearic acid	C18H36O2	0.02	284.27154	22.172	41284609.4	45799747.6	49716123.9	34063009.6	27100829.5	33174089.6	52943103.5	50841662.2	50709623.9	34047263.5	35029025.9	34754618.9	59424129.1	51167329.5	54618487.4	36569466.3	37231421.4	34330193.3	42365585.2	41272437.4	40110666.8	13323245.6	17328314.1	17808890.6	21386129.1	22776807.2	24016276.7	17527594	16163367.6	15848752.6
PC(o-18:0/18:2(9Z,12Z))	C44H86NO7P	-2.85	771.61199	22.177	315487.419	239420.549	300582.231	504480.455	2603716.21	11243326.7	4526130.83	4880116.29	4577395.28	6607879.98	7943475.54	9967001.49	37187929.4	62135349.3	16531685.1	7104737.2	7514000.49	2177789.14	10841601.3	15699820.2	12794576.5	341275.104	340510.451	370222.481	2538223.58	3481742.07	3480047.11	4251644.69	3663590.27	4280085.08
Myristyl sulfate	C14H30O4S	0.18	294.18653	22.205	284214.12	235898.43	245857.562	228169.525	261330.688	290399.333	266223.62	271448.311	292269.274	327322.426	301182.894	47412601.8	67655963.6	67025842.7	4844482.21	3764697.37	2070332.48	985883.031	842651.985	158628.913	2131108.57	588536.095	573925.958	528196.543	547171.352	532605.591	507253.773	499290.457	506217.728	783121.769
1-(1Z-hexadecenyl)-2-linoleoyl-sn-glycero-3-phosphoethanolamine	C39H74NO7P	-2.94	699.51823	22.209	160448.5	278420.736	85540998.7	40153802.4	42224661	14975403.2	9158331.19	15248972	23215838.6	16353489.4	20812135.2	17826258.2	21967734.7	196974.027	14474852.4	20583588.1	35120775.3	9378314.8	7708929.12	9572245.09	25258364.7	183095.664	324870.611	1622628.41	1269061.57	1307375.48	1741144.8	1541515.08	1297821.51	1803766.07
Erucamide	C22H43NO	-3.66	337.33323	22.532	3235550277	3247892532	3192712925	1964443328	2601290144	2837113624	2022034327	2984011319	2262752642	2364762614	2270894816	1698592598	1592110813	2551255922	2086098644	1963496696	1626668347	1247215063	1227447819	951614497	1105633447	6069654869	5957099272	4309867116	2383692758	2526078786	2574162734	2326437723	2532436110	2395281110
Palmitoyl sphingomyelin	C39H79N2O6P	-3.02	702.56545	23.359	338659.869	2392077.27	854774.34	1539845.67	618736.34	669325.565	840263.952	1120404.06	962122.054	810821.756	668121.125	717543.884	441055.6	1198949.23	1227057.26	868523.114	543091.778	716856.797	856941.419	1156418.5	989075.618	389458.571	113732941	498544783	441446569	456282104	543746261	381208022	239542956	250037751
1-(1Z-hexadecenyl)-2-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphocholine	C42H80NO7P	-2.87	741.56511	24.239	144794.786	174447.019	483674351	569978902	1098900158	9422420.55	12027041.9	17629975.7	22686089.9	12002243.5	20434135.1	9810795.57	8261330.07	1052048.19	12444527.4	357924195	27717842.3	19461896.4	11344401.2	72518643.2	55360227.3	177890.329	250616.822	86847300.3	193148758	73557771.3	66146570.5	116981402	118876968	219309065
(3beta,24R,24'R)-fucosterol epoxide	C29H48O2	-2	428.36457	25.417	77673074.9	48550733.8	37966808.4	47184039	35548604.3	39204795.4	30549553.9	33339436.6	37270720	17651711.6	17901284.1	20092643.8	79690951.9	90617956.1	68153132.4	27183826.6	29010529.9	26248326.4	67826254.5	62474820.2	63778234.6	158974549	152745680	111594686	75846587	74133746.8	70206267.2	43196844.1	46862471.3	55742946.3
Docosanamide	C22H45NO	-3.05	339.34908	25.544	41130409.6	30933361.7	19548786.4	10332847.9	17751820.7	18963455.4	11298547.3	22359841.4	15678858.6	21484667.3	22252953.3	13713885.3	15231966.5	33243567.6	19550640.3	16106055.2	13430155.9	11892363.5	9626700.72	6431547.16	7737673.19	116226797	109019641	61254438.7	26407705.3	25962020	24351205	21798392.8	22223540.9	22971906.8
1-tetradecanoyl-2-[(9Z)-octadecenoyl]-sn-glycero-3-phosphocholine	C40H78NO8P	-3.58	731.54388	27.032	171772.98	211427.286	294300.642	329600.598	363448.035	377291.336	370161.399	421602.072	1034029.81	2675122.32	1153195.45	301693.406	377420.809	368671.233	451722.132	1016683.74	2031572.69	3129626.84	2048487.96	1203401.35	805926.566	191513.877	2269786.12	304571201	269094444	148167558	161909124	83548875.9	488340456	244041074
1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine	C42H82NO8P	-1.36	759.57677	28.91	98606.4072	113524.449	20792499.9	38995595	44637844.7	33902438.1	1866118.8	4207584.24	400685181	203232772	22367376.4	438402741	403406527	2135169.75	310816106	329587346	582239880	417331245	408103160	406656185	127653863	98236.2283	185195.126	482631191	438530605	222324260	389771986	273138326	336513073	490852140
Progesterone	C21H30O2	-2.89	314.22367	30.78	78011642.4	11103887.2	12304227.8	10200062.1	18842167.7	21148791.5	24625017.7	22192272.3	22830801.6	22486149.6	16484473.9	19548727.5	19228581.5	27754543	14954225.7	25236029.7	18406194.4	21962614	19247248	24040346.5	18541651.6	175174777	73180344.1	67450772.8	55106989.9	53136366.9	48103704.7	246805.7	56707622.6	59248229.4
1-oleoyl-2-linoleyl-sn-glycero-3-phosphoethanolamine	C41H76NO8P	-2.79	741.52879	31.073	221180.175	52945074.6	43425674.4	50463688.9	19429561.6	16049271.8	15004569	11278535.5	7319713.25	7089258.03	12531849	10719227.3	321104.343	12785757.3	11201935.7	11607147.5	14759558.7	15511530.7	14901612.6	17110670.7	15725349.4	183036.774	5843006.8	3763373.91	2987105.49	2746589.83	3032066.77	4553799.27	3239443.22	2624872.89
N-[(2S,3R,4E)-1-{[4-O-(beta-D-Galactopyranosyl)-beta-D-glucopyranosyl]oxy}-3-hydroxy-4-octadecen-2-yl]dodecanamide	C42H79NO13	2.38	805.55705	31.971	594899.874	2025132.6	2426154.62	885537.988	2214503.55	553314.468	1095953.76	279044.538	677703.545	2929859.56	2270876.51	1728568.54	443728.694	1879082.22	1067329.91	2110921.16	1325147.45	1710162.63	1945831.01	1338888.48	1953915.81	204710.117	3530033.66	8008522.58	4069929.38	25113760.6	11208394.7	297364440	25965831	878166.159
1-oleoyl-2-linoleoyl-sn-glycero-3-phosphocholine	C44H82NO8P	-4.02	783.57465	32.261	841785.769	3606625.56	2851340.92	2290519.44	4562258.53	837962.136	701064.377	1065463.41	3651207.67	914949.019	3276151.79	2509898.07	640839.667	1046881.35	2712226.63	2749239.55	2115661.99	2208905.32	1804248.64	1404626.92	798863.155	822859.897	101643335	225551940	276631427	503848465	650020519	28649151.6	459554464	142130411
1-stearoyl-2-arachidonoyl-sn-glycero-3-phosphoethanolamine	C43H78NO8P	-2.39	767.54467	32.293	404500.538	4745127.77	149310016	86577719.1	100108236	115856224	111145681	104941444	92336519.1	100683354	83322070.1	80597416.5	69797988.5	723236.067	138644249	162447080	141411085	91053100.1	78381670	69661314.4	86066015.4	295301.85	10879881.1	28007409.3	15468526	16421135.7	14604848.7	16785622.9	7733266.84	10571978.4
1-(1Z-hexadecenyl)-2-(9Z-hexadecenoyl)-sn-glycero-3-phosphocholine	C40H78NO7P	-3.92	715.54878	32.525	724036.808	769001.94	812663.607	959938.67	802553.27	1028746.79	763398.566	1002370.41	1300060.35	2012783.5	1563990.34	754891.723	843043.398	2255425.71	1079152.95	1077876.18	790291.656	1245169.99	1438150.46	1056693.02	812992.331	450683.286	58140774.8	78116018.7	49081650.3	23680528.6	70868908.3	3627671.02	89660472.3	122056127
(~224~Ra)Radium	[224]Ra	-4.09	224.01929	32.904	2914056.62	12616764.7	4910364.52	2627353.77	8189440.68	13690668.5	1938785.18	9218846.59	7704557.66	3185829.59	8140830.78	22775851.3	85073983.8	6847539.08	10917684.2	5131831.03	7949536.16	3951267.98	17586595.3	8545922.57	2152990.52	37078888.9	43988516.5	40023523.8	40766697.2	44801713.2	54483061.9	1707839.96	54088952.3	53584254.8
Barbituric acid	C4H4N2O3	3.62	128.02266	32.975	421467587	216542090	529106989	461477962	358607083	379638432	433652580	424772751	182096919	429392796	330813115	238586497	321249534	376489888	298290839	362177340	505096262	469643131	514752829	463707505	379743909	1516505765	1729779700	1697916722	1628972710	1658062759	2151047327	166144984	1498264842	824641518

B1=Borobudur
B2=Muntilan
B3=Tempel
B4=Klaten
B5=Gunungkidul
B6=Yogyakarta
B7=Bantul 1
B8=Gamping
B9=Godean
B10=Bantul 2