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Metabolite Stability in Archived Neonatal Dried Blood Spots Used for Epidemiologic Research.

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Title: Metabolite stability in archived neonatal dried blood spots used for epidemiological research

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Running Head: Metabolite stability in neonatal dried blood spots

Key words: Neonatal blood spots, high-resolution metabolomics, metabolite stability, epidemiological study

Abbreviations: DBS, dried blood spots; HRM, High-resolution metabolomics; GDSP, Genetic Disease Screening Program; HILIC, hydrophilic interaction liquid chromatography; C18, C18 hydrophobic reversed-phase chromatography; ESI, electrospray ionization; m/z, mass-to-charge ratio; HMDB, Human Metabolome Database; KEGG, Kyoto Encyclopedia of Genes and Genomes; LC-MS, liquid chromatography mass spectrometry; LC-MS/MS, liquid chromatography with tandem mass spectrometry.

Abstract

Epidemiologic studies of low-frequency exposures or outcomes using metabolomics analyses of neonatal dried blood spots (DBS) often require assembly of samples with substantial differences in duration of storage. Independent assessment of stability of metabolites in archived DBS will enable improved design and interpretation of epidemiologic research utilizing DBS.

Neonatal DBS routinely collected and stored as part of the California Genetic Disease Screening Program between 1983 and 2011 were used. The study population included 899 children without cancer before age 6 born in California. High-resolution metabolomics with liquid chromatography mass spectrometry (LC-MS) was performed and the relative ion intensities of common metabolites and selected xenobiotic metabolites of nicotine (cotinine and hydroxycotinine) were evaluated.

In total, we detected 26,235 mass spectral features across two separate chromatography methods (C18 and HILIC). For most of the 39 metabolites related to nutrition and health status, we found no statistically significant annual trends across the years of storage. Nicotine metabolites were captured in the DBS with relatively stable intensities.

This study supports the usefulness of DBS stored long-term for epidemiological studies of the metabolome. Omics-based information gained from DBS may also provide a valuable tool for assessing prenatal environmental exposures in child health research.

Keywords: Neonatal blood spots, high-resolution metabolomics, metabolite stability, epidemiological study

Approximately 98% of babies born in the United States participate in newborn screening, a public health program that aims to identify early metabolic and genetic defects to prevent disease and disability.[1] Several US states and other nations store neonatal dried blood spots (DBS) for research purposes.[1,2] Research using DBS continues to increase,[3-6] particularly studies employing metabolomics tools including studies of pediatric leukemia,[7,8] estimating gestational age,[9] and those attempting to assess the early-life exposome.[10] Research targeting rare diseases must often rely on biospecimens that are collected routinely and have been stored for long time periods in order to accumulate a sufficient number of samples to address hypotheses with adequate statistical power. Thus, a key question is whether metabolites are sufficiently stable in DBS over time to produce robust estimates of endogenous or exogenous metabolites (such as those from dietary sources or tobacco use), or whether they degrade, limiting their use for metabolomics research.

In previous studies, the stability of metabolites in DBS was shown to be time-and-temperature dependent with good stability in the short term (a week under all temperature conditions); long-term stability of metabolites in DBS varied with the storage environment, depending on temperature and humidity.[11,12] For example, it has been reported that folate, essential for embryonic development, and hemoglobin concentrations in DBS decreased with storage at warmer temperatures (4°C vs. −80°C), and greater humidity (humid vs. ambient).[12] Others found major alterations in metabolites occurring only at room temperature (21°C), with no attenuation observed in frozen samples (-20°C or −80°C) over a 2-year period.[13] Improved understanding of the stability of metabolites in blood spots that were stored in -20°C for several decades will enhance the value of this important resource for environmental epidemiology research.

High-resolution metabolomics (HRM) is an analytical approach utilizing ultra-high resolution mass spectrometry and data science methods to characterize and quantify small molecules (metabolites) in biological samples.[14,15] Untargeted metabolomics is a hypothesis-free approach that profiles endogenous and exogenous metabolites in biological samples to gain insights into exposures and

pathways underlying disease. Importantly, the development of hybrid approaches to obtain information on identified metabolites without loss of information on un-identified metabolites, considerably enhances translational potential for epidemiologic and model systems research.[16] Untargeted profiling of neonatal DBS has recently been shown to provide a valuable measure of metabolic alterations associated with pediatric disease, including inborn errors of metabolism and the growth in infants associated with breast-feeding.[17-20]

Here, we assess the feasibility of applying untargeted HRM to archived DBS which were selected for a population-based record-linkage study of childhood cancers in California.[21] We comprehensively assessed the stability of metabolites across all study years (1983-2011) and metabolites with confirmed identifications were characterized for stability over increasing storage times.

Methods

Study population

We utilized data from the Smoking and Embryonal Tumor Study, a large population-based case-control study of childhood cancers, which ascertained cancer cases from the California Cancer Registry and included controls from among births in California between 1983 and 2011.[22] Population controls ascertained from California birth rolls were frequency matched (20:1) to cancer cases by year of birth. From this population, we randomly selected 1400 children (501 retinoblastoma cases and 899 controls) for HRM analysis. The demographic, socioeconomic, and gestational characteristics of cases and controls were previously reported.[21,23] Starting 2007, smoking status before and during pregnancy was reported on the birth certificate as responses to the questions about the number of cigarettes smoked per day in the 3 months before pregnancy and during each trimester.

California's newborn screening program, the Genetic Disease Screening Program (GDSP), began in 1966.[2] The GDSP obtained blood samples from babies' heel-sticks between 12 and 48 hours after birth.[24] Blood samples were put on six small circles on a specialized filter paper, dried at room

temperature for at least 3 hours, and shipped to the Neonatal and Prenatal Screening Laboratory within 24 hours of collection.[24] Since 1982, after the routine screening, left-over specimens were packed and stored at -20°C. Additional details concerning dried blood specimen collection and storage are described elsewhere.[25,26] In preparation for shipment, the GDSP anonymized all samples (i.e. none contained information on year sampled) and placed the samples into plastic bags. All bags were loosely put into a box and shipped to the laboratory for HRM analysis. Thus, the samples were 'naturally randomized' as they were tossed together at random in the box for shipment.

High-resolution metabolomics

HRM profiling was completed according to established methods.[27,28] Samples were punched using a 5 mm hole puncher, extracted with 2:1 acetonitrile in water (containing a mixture of stable isotopic internal standards), and then mixed on an orbital shaker in the dark at low speed for 12 hours at 0-4 °C. Samples were then centrifuged to remove any particulate matter and were analyzed in triplicate using liquid chromatography interfaced to an ultra high-resolution mass spectrometer (Thermo Scientific Q-Exactive HF, Waltham, MA).[29] DBS samples along with the NIST 1950 and QSTD (internal quality control) samples were analyzed in batches of 40 study samples using an acetonitrile gradient and two technical columns that include hydrophilic interaction liquid chromatography (HILIC) with positive electrospray ionization (ESI) and C18 hydrophobic reversed-phase chromatography with negative ESI, to enhance the coverage of metabolic feature detection.[30] The NIST 1950 samples were analyzed at the beginning and the end of the entire run and the QSTD samples were analyzed at the beginning, middle, and the end of each batch. Raw data was extracted using apLCMS[31] with modifications by xMSanalyzer,[32] and batch corrected using ComBat.[33] For data analysis, we only included metabolomic features with median coefficients of variation among technical replicates <30% and Pearson correlation coefficients >0.7. Ten samples were considered as outliers and excluded from the analyses, among which 6 were removed from the HILIC positive column and 6 were removed from the C18 negative column (2 overlapping samples). Feature tables of detected signals (referred to as metabolite features) were then

generated with mass-to-charge ratio (*m/z*), retention time, and ion intensity as the unique identifier for each signal.[30]

Statistical analysis

Intensities for each feature were generated based on the median of three replicate measures. If more than 2 out of 3 replicates were missing, the summarized value was represented as a missing value. Metabolite features were then filtered to keep only those metabolites detected in greater than 50% of all samples, with the exception of cotinine and hydroxycotinine. For cotinine and hydroxycotinine, signals were retained even though they were present in less than 50% of samples. Missing values were then imputed by using one-half of the lowest signal intensity in the complete dataset and intensities were log2-transformed before analyses. To control for potential confounders including Hispanic ethnicity and maternal age, we calculated residuals of intensities derived from linear regression against Hispanic ethnicity and maternal age prior to downstream analyses. A total of 894 control subject samples were included in the analysis.

Nutrition and Health Biomarker Assessment

For evaluation of targeted metabolites, we selected a small set of metabolites as examples for the overall quality of the blood spot over 3 decades of storage. We focused on 39 health and nutrition-related metabolites that had previously been assessed in adult serum samples by our team; [34] i.e. a type of sample commonly used to examine metabolites in blood. By focusing on the same set of metabolites that can be found in blood serum in analyses obtained on the same metabolomics platform, we can better understand what we newly see in children's blood samples archived as dried blood spots. We plotted the intensities by year of births using the R (R Core Team 2022, Vienna, Austria) packages "ggplot2" and "cowplot" with LOESS smoothing. To examine the feasibility of using cotinine in long-term stored neonatal DBS as a biomarker to assess maternal smoking status, we also extracted cotinine and hydroxycotinine detected using HILIC with positive ESI.[35] A linear trend test was performed for each selected metabolite to assess

whether there were intensity changes across samples collected over the 29 years such as increasing/decreasing trends.

Endogenous and Exogenous Features

For analysis of untargeted metabolomics data, the detected mass spectral features were matched to the Human Metabolome Database (HMDB), Kyoto Encyclopedia of Genes and Genomes (KEGG), and LipidMaps with a mass error threshold of 10 ppm. Using this approach, metabolite identification is consistent with Level 4 using Schymanski criteria, meaning we have assigned unequivocal molecular formula using spectral information such as *m/z* and adduct, but have insufficient evidence to propose possible structures.[36] We classified the features as endogenous metabolites or having exogenous origin (e.g. food, plant, microbial, drug, cosmetic, or toxin/pollutant) using HMDB matching to *m/z*. For the putative endogenous metabolites, we plotted the intensities by year of births following the same procedure as described above. For the putative exogenous features, we followed the statistical strategy of Bunning et al.[37] and fitted LOESS regression models using the R package "stats" to assess feature intensity according to the year of birth with a default span of 0.75. Then we used the fitted model to obtain the predicted values for the year of birth of each feature and created a matrix of birth years (N=29, 1983-2011) and feature intensities. This matrix was the input for a Fuzzy C-means Clustering analysis (R package "Mfuzz"). We calculated the minimum centroid distance for a range of clusters and selected 10 clusters as the optimal number for the HILIC column and the C18 column.

Results

The demographics of subjects were shown in Table 1. Mothers were mostly white and more than half identified themselves as non-Hispanic. The average maternal and paternal ages at birth were 27.2 and 30.2, respectively. More than half (54.2%) of all mothers were born in the US and the remaining were Mexican-born (26.4%) or other foreign-born (19.4%). Forty-one percent were firstborn children. Only 2 (1.6%) mothers of children born in 2007 and later reported having actively smoked during pregnancy.

In total, we detected 26,235 mass spectral features (15,596 in HILIC and 10,639 in C18), and after filtering out missing values and pre-processing, 21,759 features (12,998 in HILIC column and 8,761 in C18 column) were retained for downstream analyses.

The 39 nutritional and health indicator metabolites detected in DBS (Table 2) included17 amino acids and their metabolites, 2 health indicators (creatine and cholesterol), 4 vitamin coenzymes, 10 fatty acid or lipid metabolites, 4 nucleotide metabolites, and 2 exogenous chemicals (benzoic acid and caffeine). The MS/MS details of the metabolites with annotation level 1 were previously published.[27,38] Their log2-transformed, confounder adjusted residuals of relative intensities over years of birth are shown in Web Figures 1 and 2. Most of the selected metabolites appeared to remain stable across the years 1983-2011, with the exception of methionine, sphingosine, sphinganine, choline, arachidic acid, and caffeine. Stability over the period was seen for 17 out of the 39 selected metabolites with slopes close to zero and no linear trends were detected for the remaining metabolites.

From the untargeted metabolomics data, we selected 1,137 mass spectral features having accurate mass match to endogenous features (547 in HILIC column and 590 in C18 column) and 1,944 with accurate mass match to exogenous features (1,020 in HILIC column and 924 in C18 column). Note that none of these had confirmed identity; the selection strategy was intended to support examination of groups of signals enriched in endogenous metabolites and exogenous chemicals. There was some fluctuation in levels of the endogenous features over time, but the majority (~80%) of these remained stable across samples collected over the years 1983-2011 (Web Table 1, Web Figures 3 & 4). All detectable exogenous features were used as input into clustering analyses and the clustering results are shown in Web Figures 5 & 6. Each feature only contributed to one cluster. No distinct pattern was detected for either of the columns. There were some increasing and some decreasing trends as well as some general fluctuations of features in both columns. The putative exogenous features with cluster IDs are listed in Web Tables 2 & 3.

Residuals of intensities for metabolites of nicotine are shown in Figure 1. Among the 899 subjects, we detected cotinine in 79 (8.8%) and hydroxycotinine in 284 (31.8%) DBS and their intensities were highly correlated (Spearman's rho correlation coefficient = 0.77, Web Figure 7). Overall, we did not observe samples from children born in earlier years to have lower intensity for cotinine or hydroxycotinine compared to those born in the more recent years. A small negative linear trend was seen for hydroxycotinine (beta = -0.04, $P < 0.01$) while a small positive linear trend was seen for cotinine (beta = 0.05, $P = 0.04$).

Discussion

In this study of archived DBS from a large population of children born in California, we found that almost three decades of storage in -20 ˚C freezers did not affect the deterioration of metabolites that reflect the general human physiology or exogenous metabolites that are markers of common lifestyle-related exposures such as cotinine and caffeine. This was true for both the nutritional and health indicator metabolites and some of the exogenous chemicals (Table 2; Web Figures 1 & 2). Our study was conducted in a multi-ethnic California population and our results support the feasibility of future studies that investigate maternal behavior and exposures and rare childhood diseases based on metabolic profiles, such as studies of maternal smoking and caffeine intake, in DBS stored for decades.

There is no gold standard to assess metabolite stability in stored DBS samples. Different studies assessed the stability of various metabolites in DBS with cross-sectionally collected specimens and repeated analysis prospectively conducted over a certain time course. Phosphatidylethanol, a direct ethanol metabolite, remained stable at 4˚C or -80˚C for at least 9 months.[39] In another study, amino acid reference materials degraded after storage for 28 days at ambient temperature in a dry environment and the degradation rate ranged from 3% - 7% per year for several amino acids including alanine, arginine, leucine, methionine, and phenylalanine. An even higher rate of degradation was seen for acylcarnitines such as free carnitine, acetylcarnitine, and propionylcarnitine.[40] However, degradation occurred when DBS were collected between 3-7 days after birth and stored at ambient temperatures and in a dry

environment.[40] Degradation appears to be minimal for amino acids in our samples, likely because California's neonatal blood spots are collected within 12-48 hours after birth, mailed within 24 hours of sampling, and stored at -20°C. Highly unstable metabolites can be expected to be largely lost by the time of storage, so detected metabolites can be expected to be biased towards those that are relatively more stable. There is a possibility that trapping of metabolites within the proteinaceous matrix may stabilize and inhibit degradation, and this could contribute to differences seen compared to amino acid reference materials.

Another targeted metabolomics study found that most of 404 detected metabolites in DBS remained stable for the first month of storage, declined rapidly within 1-3 months of storage, and remained stable for at least one year regardless of the storage conditions (4°C vs. -20°C vs. −80 °C; with/without desiccant; with/without an O_2 scavenger).[41] Phospholipids, sphingolipids, acylcarnitines, amino acids, and steroids were the main chemical groups that degraded by over 30%.[42] However, there were no significant changes in the total number of metabolites detected over a one-year period. Our study assessed the stability of metabolites by examining the patterns of ion intensities in relation to DBS age. We did not measure changes of metabolite intensities over time; i.e. we did not repeatedly test the same sample over time for metabolite levels. However, since we observed a similar number of metabolites in long-term stored DBS in every year this may suggest some general stability in the number of features that can be identified over a very long time in DBS stored at -20 ℃. Palmer employed untargeted metabolomics and examined the stability of metabolites for dried blood spots and dried urine spots over a 12-month period under different storage temperatures (-20, +4, and +21 °C).[43] They found greater instability in polar compounds measured by HILIC in dried blood spots stored at -20 °C. Although the platform they used was not completely comparable to ours, we did observe slightly higher variation with confirmed metabolites identified in the HILICpos column (Web Figure 1) than for those in the C18neg column (Web Figure 2).

Amino acids have been a focus of newborn screening and the most up-to-date quantification platforms can now differentiate isomers.[44] We have found methionine to be the least stable amino acid in our samples, which corresponds to previous findings.[34,40,45] During long-term storage, methionine tends to be slowly oxidized into methionine sulfoxide and methionine sulfone.[34] As an essential amino acid, methionine's carbon skeletons cannot be synthesized by the body and needs to be provided in the diet to meet requirements.[46] Dietary intake of methionine is suspected to affect the fetal genome and pregnancy outcomes and thus has been a target in studies of pregnancy outcomes.[46] Our results suggest that a slight degradation of methionine is common in DBS stored long-term.

We also observed varying intensities across sample years for lipid metabolites such as sphingosine, sphinganine, and choline. Sphingolipid metabolites are lipid mediators that regulate cellular functions such as cell growth, immune cell trafficking, inflammation, and cancer.[34,47] A measurable amount of sphingosine and sphinganine in DBS suggests the possibility of measuring these physiologic parameters and use them to evaluate maternal and child health. Choline was classified as an essential nutrient by the Institute of Medicine in 1998 and both too low and too high levels may cause health concerns.[34,48] Maternal choline supplementation during pregnancy has been suggested to benefit several physiologic systems in the offspring.[49] Therefore, the varying intensities of choline over the past decades in California newborns we observed in the DBS may indicate novel use of choline supplements by pregnant women over time or a major change in diets and/or changes in the underlying distribution of chronic diseases among mothers possibly due to a shift in the age or ethnic/race composition of the population of pregnant women.

The intensities of metabolites measured in neonatal DBS are influenced by many factors including the mother's metabolic status, dietary intake, the maturity of the infant, and maternal behaviors.[40] Pregnancy is frequently a motivator for behavior change, with some women choosing to stop smoking, reducing or eliminating caffeine from the diet, and eating healthier foods.[50] Although the prevalence of caffeine consumption in pregnancy varies by countries and cultures, worldwide 60% to

75% of pregnant women drink caffeine-containing beverages.[51] Caffeine was detected in 737 (82%) of our samples with no significant difference in relative intensities over time in the DBS collected in earlier vs. recent years. The fact that caffeine was detected in a majority of samples possibly indicates breastfeeding-related exposures. The mean half-life of caffeine is 5 hours in adults but 82 hours in newborns.[52] In the US, the rate of breastfeeding initiation was about 60% to 70% in the 1980s to 90s.[53] In 2018, 93.8% of California women reported having initiated breastfeeding.[54] Our DBS represent the child's metabolism affected by maternal behavior in late pregnancy and the newborn's postnatal diet.

Although maternal smoking is of great interest in studies of pregnancy and offspring health, there are concerns about the accuracy of self-reported smoking.[55-57] Thus, cotinine and hydroxycotinine measures in DBS may be more accurate measures compared to self-reported smoking data. Neonatal DBS cotinine is a good biomarker of maternal smoking close to the time of delivery and can predict umbilical cord blood cotinine well ($R^2 = 0.80$) both at room temperature and after long-term freezer storage.[25] As shown in several studies, cotinine of ≥10 ng/ml in neonatal blood spots represents maternal active smoking.[25,58] It has been suggested that the optimal threshold for DBS cotinine to distinguish smokers from nonsmokers is lower than the threshold used in adult blood (3.13-6 ng/mL vs. 10 ng/mL).[59] Cotinine is the primary metabolite of nicotine and half of the cotinine is subsequently metabolized into hydroxycotinine.[60] A study of 13 newborns at San Francisco General Hospital reported an elimination half-life for cotinine and hydroxycotinine of 16.3 hours and 18.8 hours in umbilical cord blood, respectively.[61] Thus, given that the DBS were collected 12-48 hours after birth, it is plausible that we would observe hydroxycotinine (32% in our sample) more frequently than cotinine. However, hydroxycotinine also has other sources including dietary sources such as tomatoes and eggplant.[62] Our study suggests that cotinine and hydroxycotinine remain detectable in DBS after very long-term storage (up to 29 years), which supports the usefulness of cotinine measures to assess maternal smoking status in health studies of pregnancy exposures based on newborn blood.[63,64]

Interpreting our endogenous features plots and the exogenous clustering results will require further investigation. As mentioned above, while the majority of endogenous features remained stable throughout decades of storage some, such as lipid metabolites, appeared to be less stable. Lipids and lipid metabolites are known to be prone to oxidation and hydrolysis.[65,66] Even though lipid profiles derived from DBS are no less reproducible than those from plasma or whole blood, the process of spotting and air drying blood spots might still lead to some level of lipid oxidation and hydrolysis and it is recommended to interpret those results carefully.[66] Clustering analysis allowed us to group putative exogenous features with similar patterns across time of storage. The patterns may suggest differences in maternal lifestyle factors especially diets that may contribute to metabolite changes in newborns over time or reflect environmental exposures that wax and wane. We examined exogenous chemicals such as benzoic acid, caffeine, and cotinine in this study, and our results for mass spectral signals matching exogenous chemicals indicate that further exploration utilizing MS/MS targeted metabolomics platform together with a clustering approach will be useful for environmental epidemiology.

Despite having high specificity, annotation using the combination of *m/z* and retention time is challenging due to the presence of isomers, similar molecular-weight interferences, and in-source degradation products.[64] Metabolites can degrade or interconvert during the process of extraction and the degradation varies from one metabolite to another. During the extraction process, high-energy, high-abundant compounds are more likely to be lost compared to less-abundant, lower-energy ones.[64] This may explain why we did not identify all nutritional and health-related metabolites that were assessed for stability by Accardi et al.[34] Thus, to improve the accuracy of metabolite annotation, it is recommended to conduct an untargeted analysis in parallel with a targeted MS/MS confirmation.[64]

Other than the characteristics of the metabolites, there are other possible reasons why some metabolites that should be detectable were not detected in all samples including instability due to initial handling and storage of the blood spots that were prepared in clinics and labs all over California before being mailed to the California Neonatal Screening program. Specifically, the blood spots were not

collected by one research group but rather for neonatal screening purposes i.e. they represent a public health effort at the community level to collect, transport, extract, and analyze or store these samples. There can be sample-handling issues at every phase of the process, which may cause potential variations that affect sample quality. Thus, it is especially encouraging to find that mostly these samples are of high quality. Nevertheless, limitations include the inability to detect all metabolites that should possibly be detectable in all samples.

In the list below, we summarize the uncontrollable and controllable factors contributing to the quality and consistency of routinely collected neonatal blood spots for epidemiological research. Overall, it is advisable to 1) have enough samples to minimize contributions from factors that may corrupt the sample data and interpretations; 2) design studies with discovery and validation subsets whenever feasible; 3) work towards minimum standards guiding the use of blood spots in targeted and untargeted metabolomics in epidemiologic research; and 4) design a quantification strategy and improve comparability between studies.

- **Uncontrollable**
    - Time and location dependent supplies
    - Site-specific standard operating procedures for collection, processing and delivery
    - Duration of storage
    - Sample-specific differences in lipid content and hematocrit impacting stability of metabolites during blood spot drying and delivery
    - Sample-specific resolubilization of metabolites/loss of metabolites due to free-radical polymerization and protein trapping
- **Controllable**
    - LC-MS-specific variation in operation and analytical drifts
    - Data extraction software-dependent variations in feature identification and intensity determination

This study supports the usefulness of archived DBS in epidemiologic studies of rare diseases in later childhood or life that have to rely on archived routine biospecimens and using an untargeted metabolomics approach. This reflects a strength of California's newborn screening program's use of specific protocols for the collection and storage of DBS, which allowed us to assess the stability of DBS derived metabolites in samples collected in different years.[6] Results from this study support the feasibility of conducting metabolomics studies using archived DBS stored for decades. Utilizing existing biospecimens from statewide newborn screening programs will provide a unique and important resource for future epidemiologic health and environmental exposure studies.

Supplementary data

Supplementary data are available at AJE online.

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Table 1. Demographic characteristics of the control subjects in the study population, selected from births in California from 1983 to 2011

Demographic characteristics	Subjects (n = 899)	
	No.	% [a]
Infant sex		
Male	440	48.9
Female	459	51.1
Ethnicity		
Hispanic	424	47.2
Non-Hispanic	475	52.8
Race		
Native American	5	0.6
Asian	84	9.4
Pacific Islander	31	3.5
Black	57	6.4
White	717	80.2
Missing	5	
Maternal age (years)	27.2 (6.2) [b]	
19 or less	102	11.3
20-24	224	24.9
25-29	240	26.7
30-34	214	23.8
35 and older	119	13.2
Paternal age (years)	30.2 (7.1) [b]	
19 or less	33	3.9
20-24	175	20.7
25-29	215	25.4
30-34	198	23.4
35-39	137	16.2
40+	89	10.5
Missing	52	
Maternal education (years)		
8 or less years	93	11.9
9-11 years	162	20.7
12 years	235	30.1
13 to 15 years	155	19.8
16 more years	136	17.4
Missing	118	
Paternal education (years)		
8 or less years	109	14.9
9-11 years	107	14.6
12 years	229	31.2
13 to 15 years	146	19.9
16 more years	143	19.5
Missing	165	
Mother's place of birth		
Mexico	237	26.4
US	487	54.2
Other foreign	174	19.4
Missing	1	
Parity		
0	374	41.6
1	266	29.6

2	147	16.4
3	72	8
4 or more	39	4.3
Missing	1	
Maternal smoking		
Any smoking during pregnancy (2007+)		
Yes	2	1.6
No	124	98.4
Missing	2	
Any smoking in 3 months before pregnancy (2007+)		
Yes	3	2.4
No	123	97.6
Missing	2	

[a] The percentages may not add up due to rounding them to 1 decimal point.
[b] Values are expressed as mean (standard deviation).

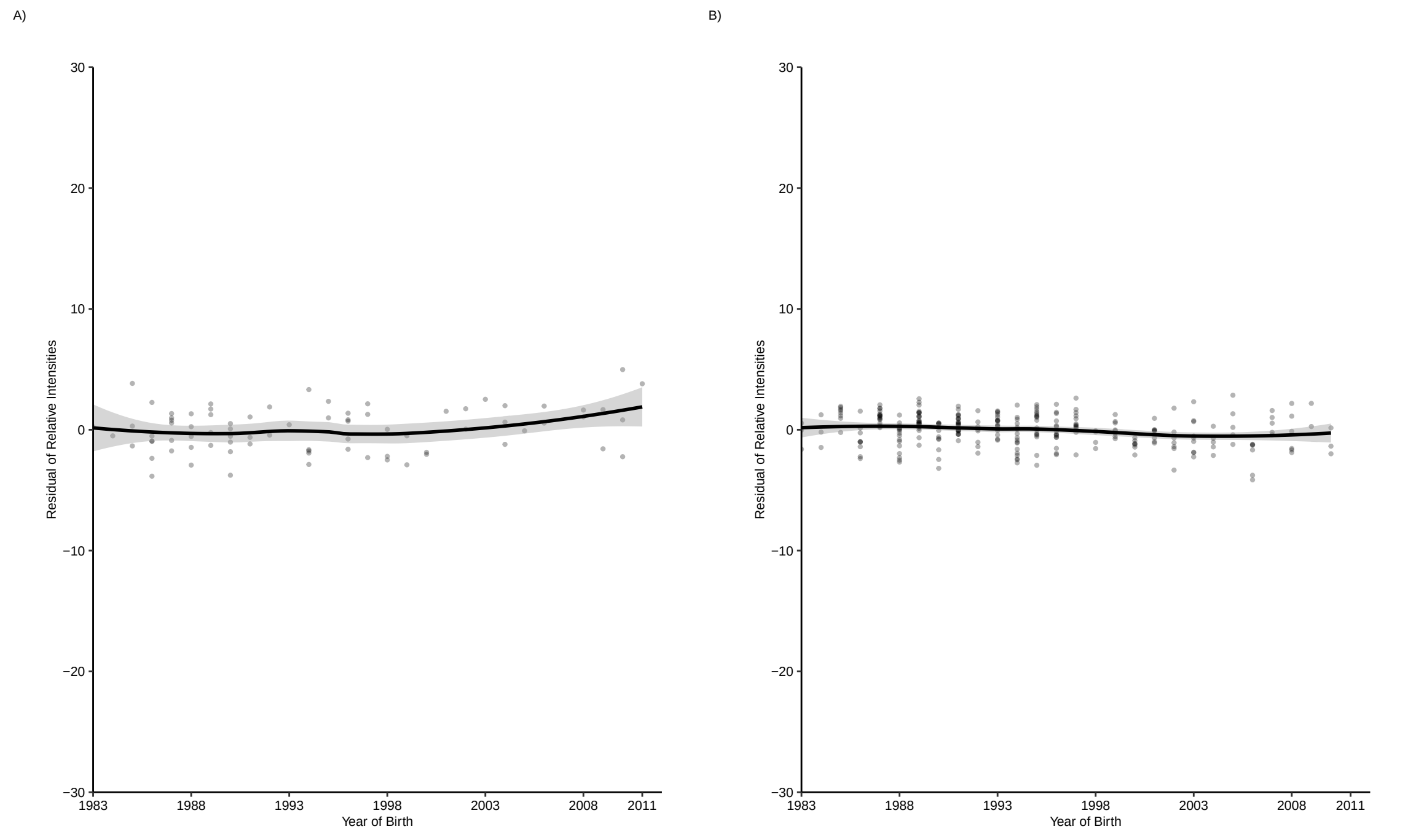
Table 2. Selected nutritional and health indicator metabolites and xenobiotic metabolites of nicotine with identification confidence level [a]

m/z	Time	Metabolite	Classification	Adduct form	Mode	Confidence
90.0550	52.4	Alanine	Amino Acid	M+H	HILIC+	4
116.0707	64.5	Proline	Amino Acid	M+H	HILIC+	1
120.0656	60.6	Threonine	Amino Acid	M+H	HILIC+	4
126.0220	56.1	Taurine	Amino Acid	M+H	HILIC+	1
132.1020	40.8	Leucine/Isoleucine	Amino Acid	M+H	HILIC+	1
145.0982	42.0	Lysine	Amino Acid	M-H	C18-	4
146.0459	19.0	Glutamate	Amino Acid	M-H	C18-	1
154.0623	23.2	Histidine	Amino Acid	M-H	C18-	1
166.0848	45.6	Phenylalanine	Amino Acid	M+H	HILIC+	4
173.1040	124.4	Arginine	Amino Acid	M-H	C18-	4
182.0811	46.0	Tyrosine	Amino Acid	M+H	HILIC+	1
150.0584	48.5	Methionine	Amino Acid	M+H	HILIC+	1
203.0827	21.9	Tryptophan	Amino Acid	M-H	C18-	1
147.0766	77.1	Glutamine	Amino Acid	M+H	HILIC+	1
104.0707	58.8	2-Aminobutyrate	Amino Acid Metabolites	M+H	HILIC+	1
180.0653	44.2	Hippurate	Amino Acid Metabolites	M+H	HILIC+	1
209.0922	51.0	Kynurenine	Amino Acid Metabolites	M+H	HILIC+	1
132.0766	53.7	Creatine	Health Indicators	M+H	HILIC+	1
369.3513	25.3	Cholesterol	Health Indicators	M-H2O+H	HILIC+	1
124.0586	273.2	Niacin	Vitamins Coenzymes	M+H	HILIC+	4
137.0716	48.3	Methylnicotinamide	Vitamins Coenzymes	M+H	HILIC+	4
169.0965	68.4	Pyridoxamine	Vitamins Coenzymes	M+H	HILIC+	1
170.0809	220.7	Pyridoxine	Vitamins Coenzymes	M+H	HILIC+	4
162.1125	41.5	Carnitine	Fatty Acid Metabolism	M+H	HILIC+	4
204.1230	34.3	Acetyl-carnitine	Fatty Acid Metabolism	M+H	HILIC+	4
277.2176	225.5	a-Linolenic acid	Fatty Acid Metabolism	M-H	C18-	1
284.2575	271.0	Oleic acid	Fatty Acid Metabolism	M-H	C18-	4
311.2960	291.3	Arachidic acid	Fatty Acid Metabolism	M-H	C18-	1
258.1091	113.1	sn-Glycero-3-Phosphocholine	Lipid Metabolism	M+H	HILIC+	1
300.2896	21.8	Sphingosine	Lipid Metabolism	M+H	HILIC+	1
302.3053	20.9	Sphinganine	Lipid Metabolism	M+H	HILIC+	1
104.1071	107.9	Choline	Lipid Metabolism	M+H	HILIC+	4
524.3710	27.5	LysoPC(18:0)	Lipid Metabolism	M+H	HILIC+	1
115.0497	264.4	5,6-Dihydrouracil	Nucleotide metabolism	M+H	HILIC+	4
137.0458	40.7	Hypoxanthine	Nucleotide metabolism	M+H	HILIC+	1
167.0208	19.1	Urate	Nucleotide metabolism	M-H	C18-	1
153.0407	246.5	Xanthine	Nucleotide metabolism	M+H	HILIC+	4
121.0294	284.6	Benzoic acid	Exogenous Chemical	M-H	C18-	4
195.0876	31.8	Caffeine	Exogenous Chemical	M+H	HILIC+	1
177.1023	31	Cotinine	Xenobiotic metabolites of nicotine	M+H	HILIC+	1
193.0973	31	Hydroxycotinine	Xenobiotic metabolites of nicotine	M+H	HILIC+	1

Abbreviations: *m/z* (mass-to-charge ratio), hydrophilic interaction liquid chromatography (HILIC), C18 hydrophobic reversed-phase chromatography (C18)

[a] Reference 36: Schymanski EL; Jeon J; Gulde R; Fenner K; Ruff M; Singer HP; Hollender (2014) Identifying Small Molecules via High Resolution Mass Spectrometry: Communicating Confidence. J Environ. Sci. Technol 48: 2097–8

Figure 1. Log2-transformed residual of relative ion intensities of cotinine and hydroxycotinine, adjusted for Hispanic ethnicity and maternal age. A) Cotinine; B) Hydroxycotinine.


A)
B)
30
20
10
0
−10
−20
−30
Residual of Relative Intensities
1983
1988
1993
1998
2003
2008
2011
Year of Birth

Metabolite stability in archived neonatal dried blood spots used for epidemiological research

Di He, Qi Yan, Karan Uppal, Douglas I. Walker, Dean P. Jones, Beate Ritz, Julia E. Heck

Web Materials Table of Contents

Web Table 1. Suggested m/z matches annotation for endogenous features

chemical_ID	mz	time	Name	Mode
HMDB00001	170.0924	67.9	1-Methylhistidine	HILIC+
HMDB00005	103.0397	44.6	2-Ketobutyric acid	HILIC+
HMDB00014	228.0982	197.7	Deoxycytidine	HILIC+
HMDB00017	184.06	43.3	4-Pyridoxic acid	HILIC+
HMDB00022	168.1019	181	3-Methoxytyramine	HILIC+
HMDB00033	227.1155	48.9	Carnosine	HILIC+
HMDB00034	136.0618	280.2	Adenine	HILIC+
HMDB00038	240.1086	87.7	Dihydrobiopterin	HILIC+
HMDB00043	118.0863	53.2	Betaine	HILIC+
HMDB00050	268.1032	131.1	Adenosine	HILIC+
HMDB00056	90.055	52.4	Beta-Alanine	HILIC+
HMDB00061	428.0364	276.5	Adenosine 35-diphosphate	HILIC+
HMDB00062	162.1125	41.5	L-Carnitine	HILIC+
HMDB00064	132.0766	53.7	Creatine	HILIC+
HMDB00068	184.0968	174.9	Epinephrine	HILIC+
HMDB00071	253.0908	107.7	Deoxyinosine	HILIC+
HMDB00073	154.0863	286.5	Dopamine	HILIC+
HMDB00076	115.0497	264.4	Dihydrouracil	HILIC+
HMDB00078	179.0485	213.7	Cysteinylglycine	HILIC+
HMDB00082	483.9936	281.9	Cytidine triphosphate	HILIC+
HMDB00089	244.0927	126.9	Cytidine	HILIC+
HMDB00095	324.0589	252.9	Cytidine monophosphate	HILIC+
HMDB00098	151.0615	231	D-Xylose	HILIC+
HMDB00112	104.0707	58.8	Gamma-Aminobutyric acid	HILIC+
HMDB00114	216.0632	98.5	Glycerylphosphorylethanolamine	HILIC+
HMDB00118	183.0652	176.9	Homovanillic acid	HILIC+
HMDB00122	181.0719	214	D-Glucose	HILIC+
HMDB00124	261.0368	278.5	Fructose 6-phosphate	HILIC+
HMDB00128	118.0611	50.8	Guanidoacetic acid	HILIC+
HMDB00132	152.0567	246.4	Guanine	HILIC+
HMDB00133	284.0989	48.3	Guanosine	HILIC+
HMDB00148	148.0605	58.5	L-Glutamic acid	HILIC+
HMDB00150	179.055	252.9	Gluconolactone	HILIC+
HMDB00158	182.0811	46	L-Tyrosine	HILIC+
HMDB00175	371.036	211.4	Inosinic acid	HILIC+
HMDB00181	198.0755	74	L-Dopa	HILIC+
HMDB00186	343.1236	103.7	Alpha-Lactose	HILIC+

HMDB00187	106.0499	250.9	L-Serine	HILIC+
HMDB00190	91.0396	60.9	L-Lactic acid	HILIC+
HMDB00191	134.0449	73.6	L-Aspartic acid	HILIC+
HMDB00194	241.1311	45.7	Anserine	HILIC+
HMDB00212	222.0972	243.8	N-Acetylgalactosamine	HILIC+
HMDB00216	170.0809	220.7	Norepinephrine	HILIC+
HMDB00224	142.0263	99	O-Phosphoethanolamine	HILIC+
HMDB00225	161.046	124.5	Oxoadipic acid	HILIC+
HMDB00230	310.1131	100.1	N-Acetylneuraminic acid	HILIC+
HMDB00238	238.0921	175.2	Sepiapterin	HILIC+
HMDB00251	126.022	56.1	Taurine	HILIC+
HMDB00262	127.0503	182.2	Thymine	HILIC+
HMDB00263	168.9896	283.7	Phosphoenolpyruvic acid	HILIC+
HMDB00265	651.7911	46.9	Liothyronine	HILIC+
HMDB00267	130.05	224.6	Pyroglutamic acid	HILIC+
HMDB00273	243.0976	56.1	Thymidine	HILIC+
HMDB00288	369.0062	196.1	Uridine 5-monophosphate	HILIC+
HMDB00296	245.0791	59.3	Uridine	HILIC+
HMDB00300	113.0346	208.4	Uracil	HILIC+
HMDB00301	139.0505	33.9	Urocanic acid	HILIC+
HMDB00306	138.0914	175.8	Tyramine	HILIC+
HMDB00310	117.0553	258	Methylacetoacetic acid	HILIC+
HMDB00321	185.042	263.6	2-Hydroxyadipic acid	HILIC+
HMDB00323	115.0867	74.2	3-Amino-2-piperidone	HILIC+
HMDB00325	191.0928	36.8	3-Hydroxysuberic acid	HILIC+
HMDB00329	165.091	24.3	2-Phenylbutyric acid	HILIC+
HMDB00339	160.0966	53.5	2-Methylbutyrylglycine	HILIC+
HMDB00350	219.1243	35.2	3-Hydroxysebacic acid	HILIC+
HMDB00362	187.0003	194	2-Phosphoglyceric acid	HILIC+
HMDB00409	133.0868	222.8	(5R)-5-Hydroxyhexanoic acid	HILIC+
HMDB00421	135.0661	61.1	23-Dihydroxyvaleric acid	HILIC+
HMDB00425	269.0886	47.8	3-Deoxy-D-glycero-D-galacto-2-nonulosonic acid	HILIC+
HMDB00444	113.0228	69.7	3-Furoic acid	HILIC+
HMDB00450	163.1093	217.4	5-Hydroxylysine	HILIC+
HMDB00451	159.1002	185.1	cis-4-Hydroxycyclohexylacetic acid	HILIC+
HMDB00453	115.0758	178.7	Delta-Hexanolactone	HILIC+
HMDB00455	223.0746	156.1	Allocystathionine	HILIC+
HMDB00459	158.0812	255.3	3-Methylcrotonylglycine	HILIC+
HMDB00469	143.0452	208.6	5-Hydroxymethyluracil	HILIC+

HMDB00472	221.0927	52	5-Hydroxy-L-tryptophan	HILIC+
HMDB00473	164.092	61.9	6-Dimethylaminopurine	HILIC+
HMDB00489	336.1399	131.2	Aspartylglycosamine	HILIC+
HMDB00508	153.0748	76.8	Ribitol	HILIC+
HMDB00510	162.076	266.1	Aminoadipic acid	HILIC+
HMDB00532	118.0499	164.4	Acetylglycine	HILIC+
HMDB00536	464.0811	195.8	Adenylsuccinic acid	HILIC+
HMDB00538	508.0076	42.1	Adenosine triphosphate	HILIC+
HMDB00544	157.0608	60.3	5-Hydroxymethyl-4-methyluracil	HILIC+
HMDB00549	87.0441	232.2	Gamma-Butyrolactone	HILIC+
HMDB00557	132.102	40.8	L-Alloisoleucine	HILIC+
HMDB00563	167.0703	51.7	D-Phenyllactic acid	HILIC+
HMDB00567	166.0848	45.6	Cinnamic acid	HILIC+
HMDB00576	133.0496	249.3	Monoethyl malonic acid	HILIC+
HMDB00585	487.2137	199.9	Glucosylgalactosyl hydroxylysine	HILIC+
HMDB00592	171.5523	93.2	Glucosamine 6-sulfate	HILIC+
HMDB00594	295.1288	41.1	Glutamylphenylalanine	HILIC+
HMDB00600	325.1595	202	Galactosylhydroxylysine	HILIC+
HMDB00613	137.0458	40.7	Erythronic acid	HILIC+
HMDB00618	231.0278	250.1	D-Ribulose 5-phosphate	HILIC+
HMDB00623	231.1591	188.6	Dodecanedioic acid	HILIC+
HMDB00630	112.0506	241.7	Cytosine	HILIC+
HMDB00635	159.0652	283.6	Succinylacetone	HILIC+
HMDB00639	211.0462	136.4	Galactaric acid	HILIC+
HMDB00641	147.0766	77.1	L-Glutamine	HILIC+
HMDB00652	476.0704	56.8	Chondroitin 4-sulfate	HILIC+
HMDB00670	189.1336	55.7	Homo-L-arginine	HILIC+
HMDB00679	190.1187	66.1	Homocitrulline	HILIC+
HMDB00684	209.0922	51	L-Kynurenine	HILIC+
HMDB00693	637.9984	257.6	Heparan sulfate	HILIC+
HMDB00701	174.1125	189.9	Hexanoylglycine	HILIC+
HMDB00703	153.0546	134.4	Mandelic acid	HILIC+
HMDB00704	180.0519	202.6	Isoxanthopterin	HILIC+
HMDB00715	190.0503	45.4	Kynurenic acid	HILIC+
HMDB00716	130.0862	67.4	L-Pipecolic acid	HILIC+
HMDB00721	173.0921	207.1	Glycylproline	HILIC+
HMDB00725	132.0656	79.5	4-Hydroxyproline	HILIC+
HMDB00730	146.0811	255.1	Isobutyrylglycine	HILIC+
HMDB00732	225.0879	122.7	Hydroxykynurenine	HILIC+

HMDB00743	743.254	264.1	Hexacarboxylporphyrin I	HILIC+
HMDB00763	192.0646	45.3	5-Hydroxyindoleacetic acid	HILIC+
HMDB00782	315.2529	24.4	Octadecanedioic acid	HILIC+
HMDB00784	189.1122	165.2	Azelaic acid	HILIC+
HMDB00802	164.0564	290.4	Pterin	HILIC+
HMDB00810	591.2981	56.6	Dimethylprotoporphyrin IX dimethyl ester	HILIC+
HMDB00816	156.9902	163.9	Phosphoglycolic acid	HILIC+
HMDB00821	194.0811	111	Phenylacetylglycine	HILIC+
HMDB00832	202.1438	36.8	Capryloylglycine	HILIC+
HMDB00842	174.0548	156.4	Quinaldic acid	HILIC+
HMDB00854	175.0713	212.7	Formiminoglutamic acid	HILIC+
HMDB00857	161.0816	177.9	Pimelic acid	HILIC+
HMDB00870	112.0877	56.5	Histamine	HILIC+
HMDB00872	259.1902	191.5	Tetradecanedioic acid	HILIC+
HMDB00873	125.0597	272.1	4-Methylcatechol	HILIC+
HMDB00881	206.0457	105.4	Xanthurenic acid	HILIC+
HMDB00884	259.0923	101.9	Ribothymidine	HILIC+
HMDB00894	144.0655	234.1	Vinylacetylglycine	HILIC+
HMDB00897	166.0726	39.4	7-Methylguanine	HILIC+
HMDB00898	126.1026	64	1-Methylhistamine	HILIC+
HMDB00902	665.119	273.9	NAD	HILIC+
HMDB00905	332.0739	275.6	Deoxyadenosine monophosphate	HILIC+
HMDB00912	384.1139	156.9	Succinyladenosine	HILIC+
HMDB00913	213.0746	70.8	Vanillactic acid	HILIC+
HMDB00957	111.0441	288.8	Pyrocatechol	HILIC+
HMDB00965	110.0275	66.5	Hypotaurine	HILIC+
HMDB00982	258.1091	113.1	5-Methylcytidine	HILIC+
HMDB00985	208.0815	141.4	Dihydrolipoamide	HILIC+
HMDB00988	356.1609	69.8	S-Adenosylmethioninamine	HILIC+
HMDB00991	160.1332	31.6	DL-2-Aminooctanoic acid	HILIC+
HMDB00992	180.0653	44.2	3-Succinoylpyridine	HILIC+
HMDB01000	389.0151	290.8	dUDP	HILIC+
HMDB01003	214.5174	216.4	Adenosine phosphosulfate	HILIC+
HMDB01004	193.0974	144.5	Oxoamide	HILIC+
HMDB01024	184.9855	262.4	Phosphohydroxypyruvic acid	HILIC+
HMDB01031	215.03	154.8	Deoxyribose 5-phosphate	HILIC+
HMDB01044	392.0341	169.8	2-Deoxyguanosine 5-monophosphate	HILIC+
HMDB01068	291.0481	52.3	D-Sedoheptulose 7-phosphate	HILIC+
HMDB01080	88.0757	259.8	4-Aminobutyraldehyde	HILIC+

HMDB01081	675.2431	259.6	(N-acetylneuraminosyl(a2-6)lactosamine)	HILIC+
HMDB01084	128.0706	115.8	D-1-Piperideine-2-carboxylic acid	HILIC+
HMDB01091	341.185	50.9	3-Hydroxyquinine	HILIC+
HMDB01097	569.3138	31.6	Protoporphyrinogen IX	HILIC+
HMDB01107	299.124	66.5	7-Methylguanosine	HILIC+
HMDB01109	260.0528	251.6	Glucosamine-1P	HILIC+
HMDB01125	485.045	254	Inositol cyclic phosphate	HILIC+
HMDB01127	259.023	82.5	6-Phosphonoglucono-D-lactone	HILIC+
HMDB01132	338.0651	252.3	Nicotinic acid mononucleotide	HILIC+
HMDB01140	129.1274	24.6	Octanal	HILIC+
HMDB01164	113.0602	289.1	trans-12-Dihydrobenzene-12-diol	HILIC+
HMDB01169	110.06	283.3	4-Aminophenol	HILIC+
HMDB01173	298.0989	60.9	5-Methylthioadenosine	HILIC+
HMDB01176	615.1547	225.1	Cytidine monophosphate N-acetylneuraminic acid	HILIC+
HMDB01182	153.0407	246.5	68-Dihydroxypurine	HILIC+
HMDB01184	85.0649	75.1	Methyl propenyl ketone	HILIC+
HMDB01186	245.2334	249.9	N1-Acetylspermine	HILIC+
HMDB01201	444.0272	257	Guanosine diphosphate	HILIC+
HMDB01202	308.0646	222.8	dCMP	HILIC+
HMDB01212	173.0564	62.7	Hydantoin-5-propionic acid	HILIC+
HMDB01216	137.0815	99.2	Tetrahydropteridine	HILIC+
HMDB01240	179.1178	25.2	Pseudooxynicotine	HILIC+
HMDB01248	786.1636	296.5	FAD	HILIC+
HMDB01250	136.0752	41.4	N-Acetylarylamine	HILIC+
HMDB01256	203.2228	292.3	Spermine	HILIC+
HMDB01257	146.1652	230.1	Spermidine	HILIC+
HMDB01265	245.0441	188	Fucose 1-phosphate	HILIC+
HMDB01267	179.082	183.8	4-Oxo-4-(3-pyridyl)-butanamide	HILIC+
HMDB01276	188.1757	34.7	N1-Acetylspermidine	HILIC+
HMDB01280	142.05	227.3	2-Aminomuconic acid semialdehyde	HILIC+
HMDB01301	114.055	237.3	1-Pyrroline-5-carboxylic acid	HILIC+
HMDB01316	277.0317	261.2	6-Phosphogluconic acid	HILIC+
HMDB01325	189.1598	86.9	N6N6N6-Trimethyl-L-lysine	HILIC+
HMDB01366	121.0514	49	Purine	HILIC+
HMDB01379	789.0763	249.9	Diguanosine triphosphate	HILIC+
HMDB01387	152.107	185.7	N-Methylphenylethanolamine	HILIC+
HMDB01397	364.0634	241.1	Guanosine monophosphate	HILIC+
HMDB01405	151.9786	108.5	3-Sulfinylpyruvic acid	HILIC+
HMDB01406	123.0553	274.1	Niacinamide	HILIC+

HMDB01409	309.0481	257.8	dUMP	HILIC+
HMDB01410	535.1328	56.8	2-Amino-4-oxo-6-(12-dioxoprolyl)-78-dihydroxypteridine	HILIC+
HMDB01413	489.1135	268.1	Citicoline	HILIC+
HMDB01416	717.206	253.3	Pantetheine 4-phosphate	HILIC+
HMDB01424	164.071	31.6	4-(3-Pyridyl)-3-butenoic acid	HILIC+
HMDB01431	169.0965	68.4	Pyridoxamine	HILIC+
HMDB01434	212.0918	59.7	3-Methoxytyrosine	HILIC+
HMDB01458	244.1104	203.2	Biotin amide	HILIC+
HMDB01476	154.0497	228.1	3-Hydroxyanthranilic acid	HILIC+
HMDB01487	666.1324	270.6	NADH	HILIC+
HMDB01491	248.0319	235.4	Pyridoxal 5-phosphate	HILIC+
HMDB01494	140.9948	265.7	Acetylphosphate	HILIC+
HMDB01504	262.0677	65	Aminoparathion	HILIC+
HMDB01508	412.0419	293.6	dADP	HILIC+
HMDB01518	279.159	24.1	Alpha-CEHC	HILIC+
HMDB01520	457.1117	146.1	Flavin Mononucleotide	HILIC+
HMDB01526	250.0911	175.2	S-Acetyldihydrolipoamide	HILIC+
HMDB01532	492.011	111.9	Deoxyadenosine triphosphate	HILIC+
HMDB01538	138.055	249.2	3-Pyridylacetic acid	HILIC+
HMDB01539	203.1503	58.5	Asymmetric dimethylarginine	HILIC+
HMDB01542	384.1499	241.9	N-Acetyllactosamine	HILIC+
HMDB01544	157.0048	91.9	m-Chlorobenzoic acid	HILIC+
HMDB01545	168.0655	246.4	Pyridoxal	HILIC+
HMDB01546	404.0255	294.5	CDP	HILIC+
HMDB01563	298.1143	49.9	1-Methylguanosine	HILIC+
HMDB01564	447.0691	235.3	CDP-Ethanolamine	HILIC+
HMDB01587	151.0401	67.6	Phenylglyoxylic acid	HILIC+
HMDB01713	165.0546	50.7	m-Coumaric acid	HILIC+
HMDB01786	276.1078	83.2	Ethenodeoxyadenosine	HILIC+
HMDB01855	178.0866	74.7	5-Hydroxytryptophol	HILIC+
HMDB01867	195.0764	30.5	4-Aminohippuric acid	HILIC+
HMDB01896	192.1026	194	5-Methoxytryptophol	HILIC+
HMDB01904	227.0657	183.3	3-Nitrotyrosine	HILIC+
HMDB01961	312.1321	43.2	17-Dimethylguanosine	HILIC+
HMDB01964	181.0496	98.7	Caffeic acid	HILIC+
HMDB01986	1000.3672	48	Lacto-N-difucopentaose II	HILIC+
HMDB02006	105.0656	67.9	23-Diaminopropionic acid	HILIC+
HMDB02025	177.0768	53.2	23-Dimethyl-3-hydroxyglutaric acid	HILIC+
HMDB02030	180.0867	260.1	Fructosamine	HILIC+

HMDB02038	161.1285	64.6	N(6)-Methyllysine	HILIC+
HMDB02039	86.0601	69.8	2-Pyrrolidinone	HILIC+
HMDB02040	179.0712	212.3	4-Methoxycinnamic acid	HILIC+
HMDB02050	149.0073	54.5	Dihydroxyfumaric acid	HILIC+
HMDB02053	249.1333	30.8	Histidylproline diketopiperazine	HILIC+
HMDB02056	223.0966	39.1	Monoisobutyl phthalic acid	HILIC+
HMDB02074	147.0651	223.5	22-Dimethylsuccinic acid	HILIC+
HMDB02089	288.1181	84.4	N-Ribosylhistidine	HILIC+
HMDB02092	131.0339	52.5	Itaconic acid	HILIC+
HMDB02099	150.0767	63.1	6-Methyladenine	HILIC+
HMDB02127	123.0106	206.5	3-Mercaptolactic acid	HILIC+
HMDB02144	141.0659	210.8	13-Dimethyluracil	HILIC+
HMDB02148	976.3699	48.8	5-Methyltetrahydropteroylpentaglutamate	HILIC+
HMDB02149	163.0394	221.4	3 Hydroxycoumarin	HILIC+
HMDB02160	615.3186	259.7	Harderoporphyrinogen	HILIC+
HMDB02167	101.0606	284	3-Methylbutyrolactone	HILIC+
HMDB02172	287.2441	52.2	N1N12-Diacetylspermine	HILIC+
HMDB02201	176.092	283.8	N-Carboxyethyl-g-aminobutyric acid	HILIC+
HMDB02205	184.0276	136.5	L-Homocysteic acid	HILIC+
HMDB02210	152.0706	281.9	2-Phenylglycine	HILIC+
HMDB02222	151.0752	195.4	3-Methylphenylacetic acid	HILIC+
HMDB02224	242.1136	61.6	5-Methyldeoxycytidine	HILIC+
HMDB02248	262.1415	276.2	Gamma glutamyl ornithine	HILIC+
HMDB02278	366.1385	251.9	2-(acetylamino)-15-anhydro-2-deoxy-3-O-b-D-galactopyranosyl-D-arabino-Hex-1-enitol	HILIC+
HMDB02285	162.0561	33.8	2-Indolecarboxylic acid	HILIC+
HMDB02334	167.0337	25.7	Benzoquinoneacetic acid	HILIC+
HMDB02339	235.1076	48.2	5-Methoxytryptophan	HILIC+
HMDB02894	126.0662	30.8	5-Methylcytosine	HILIC+
HMDB02994	123.0659	123.1	Erythritol	HILIC+
HMDB03012	94.0651	180.8	Aniline	HILIC+
HMDB03033	341.2108	23.3	Canrenone	HILIC+
HMDB03178	617.179	26.3	Heme	HILIC+
HMDB03269	181.0609	229.6	Nicotinuric acid	HILIC+
HMDB03315	99.0805	175.1	Cyclohexanone	HILIC+
HMDB03337	307.081	221.9	Oxidized glutathione	HILIC+
HMDB03357	175.1078	63.5	N-Acetylornithine	HILIC+
HMDB03364	109.0285	249.1	Quinone	HILIC+
HMDB03369	566.0778	291.2	CDP-glucose	HILIC+
HMDB03405	147.1129	75.2	D-Lysine	HILIC+

HMDB03416	175.1189	59.2	D-Arginine	HILIC+
HMDB03417	122.0271	180.5	D-Cysteine	HILIC+
HMDB03419	796.1149	275.9	Formyl-CoA	HILIC+
HMDB03447	162.0914	184.1	Tryptophanol	HILIC+
HMDB03464	146.0924	25.7	4-Guanidinobutanoic acid	HILIC+
HMDB03484	200.0318	247.1	O-Phosphohomoserine	HILIC+
HMDB03536	413.0295	262.9	dIDP	HILIC+
HMDB03539	527.1586	151.8	Levan	HILIC+
HMDB03553	689.2114	241.3	Stachyose	HILIC+
HMDB03556	427.1593	86.4	Chitobiose	HILIC+
HMDB03581	215.1389	40.2	Dethiobiotin	HILIC+
HMDB03584	168.0439	64.7	Taurocyamine	HILIC+
HMDB03601	330.1712	64.4	(S)-Reticuline	HILIC+
HMDB03626	194.1175	17.8	(R)-N-Methylsalsolinol	HILIC+
HMDB03764	219.098	128	Glutamylalanine	HILIC+
HMDB03767	137.0593	189.7	4-Hydroxyphenylacetaldehyde	HILIC+
HMDB03869	276.1553	146.6	Epsilon-(gamma-Glutamyl)-lysine	HILIC+
HMDB03905	111.0553	78.9	Imidazole-4-acetaldehyde	HILIC+
HMDB03950	284.1103	38.9	7-Methylinosine	HILIC+
HMDB03976	275.0148	202.7	D-Glucuronic acid 1-phosphate	HILIC+
HMDB04041	120.0656	60.6	L-Allothreonine	HILIC+
HMDB04045	168.9806	17.4	3-Sulfopyruvic acid	HILIC+
HMDB04051	565.2408	37.2	Aerobactin	HILIC+
HMDB04058	150.055	195.8	56-Dihydroxyindole	HILIC+
HMDB04062	139.039	259	Gentisate aldehyde	HILIC+
HMDB04063	198.1124	204.3	Metanephrine	HILIC+
HMDB04072	121.0648	271.5	4-Hydroxystyrene	HILIC+
HMDB04076	181.0976	40	5-Hydroxykynurenamine	HILIC+
HMDB04094	134.0594	51	Indoxyl	HILIC+
HMDB04113	183.9882	16.8	Se-Methylselenocysteine	HILIC+
HMDB04157	597.3592	26	L-Urobilinogen	HILIC+
HMDB04181	125.071	33.8	Methylimidazole acetaldehyde	HILIC+
HMDB04193	153.0659	232.5	N1-Methyl-2-pyridone-5-carboxamide	HILIC+
HMDB04224	191.112	203.5	N-(o)-Hydroxyarginine	HILIC+
HMDB04230	112.0394	176	Pyrrole-2-carboxylic acid	HILIC+
HMDB04328	225.0997	52.8	Temurin	HILIC+
HMDB04363	85.0397	223	Imidazolone	HILIC+
HMDB04461	122.0595	143.3	Benzamide	HILIC+
HMDB04827	144.1019	54.2	Proline betaine	HILIC+

HMDB05056	303.1591	90.1	Enterodiol	HILIC+
HMDB05765	290.1346	62.4	Ophthalmic acid	HILIC+
HMDB05767	255.1452	53.3	Homoanserine	HILIC+
HMDB05768	338.1828	46.1	Kyotorphin	HILIC+
HMDB05771	457.2473	261.8	Rigin	HILIC+
HMDB05773	611.2916	60.7	Endomorphin-1	HILIC+
HMDB05843	100.0219	210.2	Allyl isothiocyanate	HILIC+
HMDB05874	259.9914	59.5	3-Bromotyrosine	HILIC+
HMDB05923	286.1035	52.9	N4-Acetylcytidine	HILIC+
HMDB06002	358.2769	23.9	Ethyltestosterone	HILIC+
HMDB06005	245.0923	83.6	Indolylacryloylglycine	HILIC+
HMDB06013	321.2787	23	7a17-dimethyl-5b-Androstane-3a17b-diol	HILIC+
HMDB06045	361.1368	37.4	Dityrosine	HILIC+
HMDB06049	262.048	235.6	O-Phosphotyrosine	HILIC+
HMDB06078	162.1357	193.2	Putreanine	HILIC+
HMDB06115	107.0492	269.9	Benzaldehyde	HILIC+
HMDB06239	237.1075	91.2	S-aminomethyldihydrolipoamide	HILIC+
HMDB06348	186.1125	212.8	Pseudoecgonine	HILIC+
HMDB06406	200.1281	267.6	Ecgonine methyl ester	HILIC+
HMDB06456	270.0385	51.9	N-Acetyl-L-glutamyl 5-phosphate	HILIC+
HMDB06462	168.0326	93	Homocysteinesulfinic acid	HILIC+
HMDB06488	174.0762	107.4	N-Acetyl-L-glutamate 5-semialdehyde	HILIC+
HMDB06502	833.0281	260.3	P1P4-Bis(5-adenosyl) tetraphosphate	HILIC+
HMDB06537	708.2562	236	(a-D-mannosyl)2-b-D-mannosyl-N-acetylglucosamine	HILIC+
HMDB06588	966.3373	49.6	Disialosyl galactosyl globoside	HILIC+
HMDB06591	342.1391	271.2	Lactosamine	HILIC+
HMDB06592	546.2021	130.1	Lacto-N-triaose	HILIC+
HMDB06695	229.1183	49.9	Prolylhydroxyproline	HILIC+
HMDB06698	628.2618	275.3	Tri-N-acetylchitotriose	HILIC+
HMDB06744	528.0796	132.3	3-Carboxy-1-hydroxypropylthiamine diphosphate	HILIC+
HMDB06802	216.028	272.6	O-Phospho-4-hydroxy-L-threonine	HILIC+
HMDB06806	404.0944	246.6	Propinol adenylate	HILIC+
HMDB06868	278.1233	74.1	S-(2-Methylpropionyl)-dihydrolipoamide-E	HILIC+
HMDB06902	990.5023	261.1	Cobinamide	HILIC+
HMDB06954	182.045	132.6	2-Methyl-3-hydroxy-5-formylpyridine-4-carboxylate	HILIC+
HMDB10170	355.2478	187.7	111215-TriHETRE	HILIC+
HMDB10200	295.2266	23.1	A-12(13)-EpODE	HILIC+
HMDB10201	313.2372	22.9	1213-DiHODE	HILIC+
HMDB10202	319.2255	33.5	12-HEPE	HILIC+

HMDB10204	337.2375	23.8	1415-DiHETE	HILIC+
HMDB10213	345.2409	22.5	17-HDoHE	HILIC+
HMDB10222	321.2407	42.8	9-HETE	HILIC+
HMDB10319	310.095	206.9	Inodxyl glucuronide	HILIC+
HMDB10328	314.1211	37	Tyramine glucuronide	HILIC+
HMDB10716	313.0285	256.8	Gamma-Glutamyl-Se-methylselenocysteine	HILIC+
HMDB11107	183.0497	91.2	7-Methyluric acid	HILIC+
HMDB11140	234.1812	147.4	Hypusine	HILIC+
HMDB11150	218.1862	111.6	Deoxyhypusine	HILIC+
HMDB11161	261.1091	189.6	L-alpha-glutamyl-L-hydroxyproline	HILIC+
HMDB11162	205.0819	140	L-beta-aspartyl-L-alanine	HILIC+
HMDB11163	249.0717	84.4	L-beta-aspartyl-L-aspartic acid	HILIC+
HMDB11165	191.0665	78.5	L-beta-aspartyl-L-glycine	HILIC+
HMDB11168	203.0672	85.1	L-beta-aspartyl-L-serine	HILIC+
HMDB11169	235.0924	82.8	L-beta-aspartyl-L-threonine	HILIC+
HMDB11170	261.1457	34.4	L-gamma-glutamyl-L-isoleucine	HILIC+
HMDB11174	229.154	43.2	L-isoleucyl-L-proline	HILIC+
HMDB11180	213.1233	139	L-prolyl-L-proline	HILIC+
HMDB11639	212.0542	90.1	Topaquinone	HILIC+
HMDB11648	257.1129	46.6	1-(beta-D-Ribofuranosyl)-14-dihydronicotinamide	HILIC+
HMDB11649	335.0735	285.5	1-(sn-Glycero-3-phospho)-1D-myo-inositol	HILIC+
HMDB11654	272.1478	105	2-(3-Carboxy-3-(methylammonio)propyl)-L-histidine	HILIC+
HMDB11655	257.1246	69.3	2-(3-Carboxy-3-aminopropyl)-L-histidine	HILIC+
HMDB11657	228.0454	51.1	26-Diamino-4-hydroxy-5-N-methylformamidopyrimidine	HILIC+
HMDB11664	130.0651	213.8	3-Methylene-indolenine	HILIC+
HMDB11691	306.0484	255.4	Cytidine 23-cyclic phosphate	HILIC+
HMDB11716	254.1046	29.6	N-Acetylvanilalanine	HILIC+
HMDB11718	123.0441	262.7	4-Hydroxybenzaldehyde	HILIC+
HMDB11737	277.1036	63.4	Gamma Glutamylglutamic acid	HILIC+
HMDB11741	311.1239	54	Gamma-Glutamyltyrosine	HILIC+
HMDB11747	126.0308	65.6	Ciliatine	HILIC+
HMDB11749	100.0757	33	2-Piperidinone	HILIC+
HMDB11750	199.0018	85.9	Dihydroxyacetone Phosphate Acyl Ester	HILIC+
HMDB11751	181.0863	200	3-Methoxybenzenepropanoic acid	HILIC+
HMDB12127	209.0811	87.1	(R)-2-Benzylsuccinate	HILIC+
HMDB12149	175.0612	246.3	2-Isopropyl-3-oxosuccinate	HILIC+
HMDB12150	188.0917	83.9	2-Keto-6-acetamidocaproate	HILIC+
HMDB12153	140.0707	288.9	34-Dihydroxybenzylamine	HILIC+
HMDB12176	117.1023	40.2	5-Aminopentanamide	HILIC+

HMDB12189	160.1808	260.4	Aminopropylcadaverine	HILIC+
HMDB12204	220.1179	29	Cis-zeatin	HILIC+
HMDB12221	391.1174	244.1	Dopaxanthin	HILIC+
HMDB12230	218.1499	60.6	Gamma-glutamyl-L-putrescine	HILIC+
HMDB12234	140.0813	19.9	Histidinal	HILIC+
HMDB12236	221.034	82.5	Imidazole acetol-phosphate	HILIC+
HMDB12246	165.1018	33	Kynuramine	HILIC+
HMDB12254	829.2778	270.9	Maltopentaose	HILIC+
HMDB12267	291.1175	78.8	N-Succinyl-LL-26-diaminopimelate	HILIC+
HMDB12289	172.0604	40.3	Tetrahydrodipicolinate	HILIC+
HMDB12515	419.3155	185.2	11-Carboxy-alpha-chromanol	HILIC+
HMDB12575	414.1598	141.2	13E-Tetranor-16-carboxy-LTE4	HILIC+
HMDB12710	191.0569	30.5	3-Dehydroquinate	HILIC+
HMDB12798	321.2082	29	5-Carboxy-alpha-chromanol	HILIC+
HMDB12799	307.1895	193.5	5-Carboxy-gamma-chromanol	HILIC+
HMDB12815	102.0913	268	5-Aminopentanal	HILIC+
HMDB12848	349.2355	34.3	7-Carboxy-alpha-chromanol	HILIC+
HMDB12850	357.2058	35.4	7-Carboxy-gamma-chromanol	HILIC+
HMDB12851	333.2083	30.1	7-Carboxy-gamma-tocotrienol	HILIC+
HMDB12866	432.3133	24.6	9-Carboxy-alpha-chromanol	HILIC+
HMDB12880	116.0707	64.5	Acetamidopropanal	HILIC+
HMDB12897	169.0758	170.6	Beta-Carboline	HILIC+
HMDB12983	359.2402	36.8	Kinetensin 1-3	HILIC+
HMDB13010	188.1282	39.9	N-Heptanoylglycine	HILIC+
HMDB13019	876.4255	48.8	Neuromedin C 1-8	HILIC+
HMDB13029	167.0571	66.5	Noradrenochrome o-semiquinone	HILIC+
HMDB13034	314.2691	168.8	Palmitoylglycine	HILIC+
HMDB13055	646.335	52.4	S-(11-hydroxy-9-deoxy-delta12-PGD2)-glutathione	HILIC+
HMDB13067	238.1094	57.3	Salsoline-1-carboxylate	HILIC+
HMDB13070	211.0956	185.9	Sinapyl alcohol	HILIC+
HMDB13076	201.1597	35.6	Spermine dialdehyde	HILIC+
HMDB13105	169.1231	253.6	trans-45-epoxy-2(E)-decenal	HILIC+
HMDB13159	169.0595	55.6	23-Diaminosalicylic acid	HILIC+
HMDB13162	201.1727	71.8	2-Hexenoylcholine	HILIC+
HMDB13195	170.0964	28.7	4-Aminobiphenyl	HILIC+
HMDB13204	236.0798	63.4	6-Succinoaminopurine	HILIC+
HMDB13206	257.2334	248.8	9-Decenoylcholine	HILIC+
HMDB13208	341.3316	21.7	9-Hexadecenoylcholine	HILIC+
HMDB13209	276.1345	33.7	Alanyltryptophan	HILIC+

HMDB13225	231.2178	246.3	Capryloylcholine	HILIC+
HMDB13240	304.1319	72.5	Indoleacetyl glutamine	HILIC+
HMDB13243	279.1713	25.9	Leucyl-phenylalanine	HILIC+
HMDB13267	230.175	24.8	N-Decanoylglycine	HILIC+
HMDB13286	244.1905	24.3	N-Undecanoylglycine	HILIC+
HMDB13287	175.1441	66.2	NeNe dimethyllysine	HILIC+
HMDB13327	374.2569	22.1	Dodecanedioylcarnitine	HILIC+
HMDB13328	304.177	35.9	Pimelylcarnitine	HILIC+
HMDB13330	386.2886	22.8	3-Hydroxy-cis-5-tetradecenoylcarnitine	HILIC+
HMDB13333	414.3215	22.4	3-Hydroxy-9-hexadecenoylcarnitine	HILIC+
HMDB13335	412.3048	26.1	3-Hydroxyhexadecadienoylcarnitine	HILIC+
HMDB13336	416.3372	22.7	3-Hydroxyhexadecanoylcarnitine	HILIC+
HMDB13339	442.3516	21.7	3-Hydroxy-11Z-octadecenoylcarnitine	HILIC+
HMDB13593	155.0202	133	14-Dithiothreitol	HILIC+
HMDB13609	205.0972	37.1	D-Tryptophan	HILIC+
HMDB13631	340.2842	24.4	Oleoyl glycine	HILIC+
HMDB13640	1049.3877	285	(S)-Hydroxyoctadecanoyl-CoA	HILIC+
HMDB13674	127.039	256.2	123-Trihydroxybenzene	HILIC+
HMDB13687	219.1743	179.6	Nookatone	HILIC+
HMDB13688	221.1899	257	Nootkatol	HILIC+
HMDB13695	229.0503	79.9	Urolithin A	HILIC+
HMDB13733	121.1012	234.9	124-Trimethylbenzene	HILIC+
HMDB13751	96.0444	231.3	2-Hydroxypyridine	HILIC+
HMDB13804	191.1416	55.6	beta-Damascenone	HILIC+
HMDB13806	163.1481	23	m-Cymene	HILIC+
HMDB13809	127.1117	24.1	(E)-2-octenal	HILIC+
HMDB13813	253.2524	280.2	13-Heptadecyn-1-ol	HILIC+
HMDB13817	221.1525	30.2	26-Di-tert-butylbenzoquinone	HILIC+
HMDB13820	191.1794	23.5	2-Methyl-2-phenyl-undecane	HILIC+
HMDB13825	165.1273	24.2	4-(1133-Tetramethylbutyl)-phenol	HILIC+
HMDB28680	161.0921	62.1	Alanyl-Alanine	HILIC+
HMDB28681	246.154	40.2	Alanyl-Arginine	HILIC+
HMDB28682	204.0977	58.3	Alanyl-Asparagine	HILIC+
HMDB28690	203.1408	32.3	Alanyl-Isoleucine	HILIC+
HMDB28694	237.124	157.7	Alanyl-Phenylalanine	HILIC+
HMDB28695	187.1089	58.2	Alanyl-Proline	HILIC+
HMDB28696	177.087	71.8	Alanyl-Serine	HILIC+
HMDB28697	191.1027	166.6	Alanyl-Threonine	HILIC+
HMDB28704	289.1631	81.6	Arginyl-Asparagine	HILIC+

HMDB28705	290.1455	79.4	Arginyl-Aspartate	HILIC+
HMDB28707	303.1749	59.8	Arginyl-Glutamine	HILIC+
HMDB28709	232.1396	69.3	Arginyl-Glycine	HILIC+
HMDB28712	288.2023	48	Arginyl-Isoleucine	HILIC+
HMDB28714	303.216	26.2	Arginyl-Lysine	HILIC+
HMDB28715	306.161	43.8	Arginyl-Methionine	HILIC+
HMDB28717	272.1716	54.4	Arginyl-Proline	HILIC+
HMDB28718	262.1505	60	Arginyl-Serine	HILIC+
HMDB28719	276.1667	61.5	Arginyl-Threonine	HILIC+
HMDB28722	274.1848	41.1	Arginyl-Valine	HILIC+
HMDB28727	248.0883	89.5	Asparaginyl-Aspartate	HILIC+
HMDB28729	261.1179	97.4	Asparaginyl-Glutamine	HILIC+
HMDB28734	246.1447	44.3	Asparaginyl-Isoleucine	HILIC+
HMDB28736	261.1559	93.6	Asparaginyl-Lysine	HILIC+
HMDB28737	264.0993	259.4	Asparaginyl-Methionine	HILIC+
HMDB28740	220.0929	211.4	Asparaginyl-Serine	HILIC+
HMDB28741	234.108	60.1	Asparaginyl-Threonine	HILIC+
HMDB28742	319.1383	54.1	Asparaginyl-Tryptophan	HILIC+
HMDB28744	232.1293	73.4	Asparaginyl-Valine	HILIC+
HMDB28751	262.1034	99.5	Aspartyl-Glutamine	HILIC+
HMDB28755	271.104	117	Aspartyl-Histidine	HILIC+
HMDB28776	235.076	39.6	Cysteinyl-Hydroxyproline	HILIC+
HMDB28777	259.0834	181.4	Cysteinyl-Histidine	HILIC+
HMDB28784	209.0585	191.5	Cysteinyl-Serine	HILIC+
HMDB28798	260.124	53.1	Glutaminyl-Hydroxyproline	HILIC+
HMDB28799	284.1371	69.7	Glutaminyl-Histidine	HILIC+
HMDB28800	260.1602	34.6	Glutaminyl-Isoleucine	HILIC+
HMDB28802	275.1714	53.4	Glutaminyl-Lysine	HILIC+
HMDB28805	244.1292	86	Glutaminyl-Proline	HILIC+
HMDB28807	248.1242	90.6	Glutaminyl-Threonine	HILIC+
HMDB28832	246.1193	51.9	Glutamyl-Valine	HILIC+
HMDB28843	213.0982	87.8	Glycyl-Histidine	HILIC+
HMDB28846	204.1335	229.6	Glycyl-Lysine	HILIC+
HMDB28848	223.1091	46.4	Glycyl-Phenylalanine	HILIC+
HMDB28850	163.0714	79.3	Glycyl-Serine	HILIC+
HMDB28864	245.1125	63.8	Hydroxyprolyl-Hydroxyproline	HILIC+
HMDB28869	263.1061	86.1	Hydroxyprolyl-Methionine	HILIC+
HMDB28888	269.1603	51.1	Histidinyl-Isoleucine	HILIC+
HMDB28890	284.1717	131.4	Histidinyl-Lysine	HILIC+

HMDB28892	303.1466	41.7	Histidinyl-Phenylalanine	HILIC+
HMDB28893	253.1296	54.7	Histidinyl-Proline	HILIC+
HMDB28910	245.1884	23.8	Isoleucyl-Isoleucine	HILIC+
HMDB28919	295.1657	44	Isoleucyl-Tyrosine	HILIC+
HMDB28920	231.1702	27.7	Isoleucyl-Valine	HILIC+
HMDB28958	294.18	63.2	Lysyl-Phenylalanine	HILIC+
HMDB28959	244.1658	60.9	Lysyl-Proline	HILIC+
HMDB28960	234.1432	273.2	Lysyl-Serine	HILIC+
HMDB28961	248.1597	43	Lysyl-Threonine	HILIC+
HMDB28962	333.1907	41.6	Lysyl-Tryptophan	HILIC+
HMDB28964	246.1812	57.9	Lysyl-Valine	HILIC+
HMDB28985	313.1191	32.7	Methionyl-Tyrosine	HILIC+
HMDB28994	294.1238	87.8	Phenylalanyl-Glutamate	HILIC+
HMDB29006	352.1666	32.4	Phenylalanyl-Tryptophan	HILIC+
HMDB29007	329.1498	55.9	Phenylalanyl-Tyrosine	HILIC+
HMDB29008	265.1572	189.4	Phenylalanyl-Valine	HILIC+
HMDB29164	453.1393	256.4	(-)-epicatechin-3-O-glucuronide	HILIC+
HMDB29171	145.0495	257.3	3-Hydroxyadipic acid 36-lactone	HILIC+
HMDB29174	692.525	50.7	3-Sn-phosphatidylethanolamine	HILIC+
HMDB29176	352.0629	214.8	3-O-Methyl-(-)-epicatechin-5-O-sulphate	HILIC+
HMDB29198	89.071	178.8	Dimethylurea	HILIC+
HMDB29221	662.515	243.9	lysoPC(28:1(5Z))	HILIC+
HMDB41795	347.1841	267	19-Noraldosterone	HILIC+
HMDB41804	153.091	275.8	2-Isopropoxyphenol	HILIC+
HMDB41805	163.9843	156.8	2-Thiothiazolidine-4-carboxylic acid	HILIC+
HMDB41806	182.1177	182.1	34-Dimethoxyphenylethylamine	HILIC+
HMDB41807	215.0692	243.8	3-Phenoxybenzoic acid	HILIC+
HMDB41817	286.0717	257.2	7-Aminoclonazepam	HILIC+
HMDB41849	301.0871	211.3	Carboxytolbutamide	HILIC+
HMDB41887	230.0958	65	Endalin	HILIC+
HMDB41942	221.0593	158.1	N-Acetyl-S-(N-methylcarbamoyl)cysteine	HILIC+
HMDB41946	145.0616	219.2	N-Nitrosoproline	HILIC+
HMDB41953	226.1205	48.8	Nnal-N-oxide	HILIC+
HMDB41993	246.1698	26.3	Pivaloylcarnitine	HILIC+
HMDB41997	351.2527	23.1	Pregnanetriolone	HILIC+
HMDB59978	307.0466	56.1	4-Hydroxy-5-(dihydroxyphenyl)-valeric acid-O-sulphate	HILIC+
HMDB60005	265.0028	221	Methylgallic acid-O-sulphate	HILIC+
HMDB60013	205.0154	215.8	O-methoxycatechol-O-sulphate	HILIC+
HMDB60017	303.0729	57.7	Pyrogallol-2-O-glucuronide	HILIC+

HMDB60029	335.0402	215	5-(345-Trihydroxyphenyl)-gamma-valerolactone-O-methyl-O-sulphate	HILIC+
HMDB00001	168.0777	37.4	1-Methylhistidine	C18-
HMDB00005	101.0243	283.6	2-Ketobutyric acid	C18-
HMDB00008	103.04	20.5	2-Hydroxybutyric acid	C18-
HMDB00012	227.0676	18.7	Deoxyuridine	C18-
HMDB00014	226.0837	269.8	Deoxycytidine	C18-
HMDB00017	218.0233	19.5	4-Pyridoxic acid	C18-
HMDB00026	131.0451	269.2	Ureidopropionic acid	C18-
HMDB00033	225.0993	25.5	Carnosine	C18-
HMDB00034	134.0471	272	Adenine	C18-
HMDB00043	116.0716	288	Betaine	C18-
HMDB00050	266.0896	151.2	Adenosine	C18-
HMDB00054	583.2563	36.9	Bilirubin	C18-
HMDB00056	88.0403	22.9	Beta-Alanine	C18-
HMDB00061	426.023	17.3	Adenosine 35-diphosphate	C18-
HMDB00072	173.0085	20	cis-Aconitic acid	C18-
HMDB00073	152.0717	17.6	Dopamine	C18-
HMDB00076	113.0355	283.5	Dihydrouracil	C18-
HMDB00079	127.0512	287.9	Dihydrothymine	C18-
HMDB00082	481.9784	15.3	Cytidine triphosphate	C18-
HMDB00089	242.0791	289.7	Cytidine	C18-
HMDB00094	191.0197	17.6	Citric acid	C18-
HMDB00095	322.0454	17.4	Cytidine monophosphate	C18-
HMDB00101	250.0938	19.9	Deoxyadenosine	C18-
HMDB00112	102.056	19.6	Gamma-Aminobutyric acid	C18-
HMDB00114	214.05	21.8	Glycerylphosphorylethanolamine	C18-
HMDB00118	181.0512	280.1	Homovanillic acid	C18-
HMDB00122	215.033	20.1	D-Glucose	C18-
HMDB00124	259.0229	17.8	Fructose 6-phosphate	C18-
HMDB00126	171.0066	19.1	Glycerol 3-phosphate	C18-
HMDB00130	167.0352	289.3	Homogentisic acid	C18-
HMDB00131	91.0399	289.6	Glycerol	C18-
HMDB00132	150.0419	291.1	Guanine	C18-
HMDB00133	282.0853	20.1	Guanosine	C18-
HMDB00139	105.0191	193.9	Glyceric acid	C18-
HMDB00148	146.0459	19	L-Glutamic acid	C18-
HMDB00150	177.0406	18.2	Gluconolactone	C18-
HMDB00152	153.0192	289.4	Gentisic acid	C18-
HMDB00156	133.0145	18.7	L-Malic acid	C18-

HMDB00158	180.0667	19.6	L-Tyrosine	C18-
HMDB00174	163.0623	286.7	L-Fucose	C18-
HMDB00175	347.0402	18.1	Inosinic acid	C18-
HMDB00181	196.0617	21.5	L-Dopa	C18-
HMDB00186	341.1089	145.4	Alpha-Lactose	C18-
HMDB00187	104.035	23	L-Serine	C18-
HMDB00190	89.0243	290.2	L-Lactic acid	C18-
HMDB00191	132.0303	20.1	L-Aspartic acid	C18-
HMDB00192	239.0152	28.2	L-Cystine	C18-
HMDB00202	117.0196	289.4	Methylmalonic acid	C18-
HMDB00206	187.1087	26.4	N6-Acetyl-L-lysine	C18-
HMDB00212	220.0841	293.2	N-Acetylgalactosamine	C18-
HMDB00214	131.0826	22.8	Ornithine	C18-
HMDB00216	168.0666	19.3	Norepinephrine	C18-
HMDB00217	743.0716	15.9	NADP	C18-
HMDB00224	140.0118	25.5	O-Phosphoethanolamine	C18-
HMDB00225	159.0305	292.2	Oxoadipic acid	C18-
HMDB00226	155.0097	282.7	Orotic acid	C18-
HMDB00227	147.0673	289.7	Mevalonic acid	C18-
HMDB00230	308.0995	17.9	N-Acetylneuraminic acid	C18-
HMDB00232	166.0144	136.9	Quinolinic acid	C18-
HMDB00238	236.0782	19	Sepiapterin	C18-
HMDB00245	225.088	21.1	Porphobilinogen	C18-
HMDB00251	124.0073	20.6	Taurine	C18-
HMDB00262	125.0355	286.1	Thymine	C18-
HMDB00263	166.9751	16.4	Phosphoenolpyruvic acid	C18-
HMDB00267	128.0353	18.5	Pyroglutamic acid	C18-
HMDB00273	241.084	285.7	Thymidine	C18-
HMDB00285	482.9601	18.5	Uridine triphosphate	C18-
HMDB00286	565.0486	17	Uridine diphosphate glucose	C18-
HMDB00288	323.0294	17.9	Uridine 5-monophosphate	C18-
HMDB00290	606.0765	17.3	Uridine diphosphate-N-acetylglucosamine	C18-
HMDB00291	197.0456	22.1	Vanillylmandelic acid	C18-
HMDB00295	402.9959	17.1	Uridine 5-diphosphate	C18-
HMDB00296	243.0627	284.2	Uridine	C18-
HMDB00300	111.0199	287.3	Uracil	C18-
HMDB00301	137.0355	284.7	Urocanic acid	C18-
HMDB00306	136.0768	18.1	Tyramine	C18-
HMDB00310	115.04	285.4	Methylacetoacetic acid	C18-

HMDB00318	169.0509	287.2	34-Dihydroxyphenylglycol	C18-
HMDB00321	161.0458	265	2-Hydroxyadipic acid	C18-
HMDB00325	189.0777	287.4	3-Hydroxysuberic acid	C18-
HMDB00329	163.0764	288.1	2-Phenylbutyric acid	C18-
HMDB00337	119.0353	289.7	(S)-34-Dihydroxybutyric acid	C18-
HMDB00339	158.0822	286.8	2-Methylbutyrylglycine	C18-
HMDB00350	217.1083	280.8	3-Hydroxysebacic acid	C18-
HMDB00351	117.0556	290	3-Hydroxy-2-methyl-R-(RS)-butanoic acid	C18-
HMDB00362	184.9857	20.1	2-Phosphoglyceric acid	C18-
HMDB00379	205.0354	149.7	2-Methylcitric acid	C18-
HMDB00409	131.0712	285.3	(5R)-5-Hydroxyhexanoic acid	C18-
HMDB00421	133.0517	286.9	23-Dihydroxyvaleric acid	C18-
HMDB00425	267.0739	21.4	3-Deoxy-D-glycero-D-galacto-2-nonulosonic acid	C18-
HMDB00428	129.0187	22.6	3-Hydroxyglutaric acid	C18-
HMDB00434	195.0672	287.3	Homoveratric acid	C18-
HMDB00444	111.0086	289.3	3-Furoic acid	C18-
HMDB00451	157.0869	276.3	cis-4-Hydroxycyclohexylacetic acid	C18-
HMDB00453	113.0607	282.9	Delta-Hexanolactone	C18-
HMDB00459	156.0665	284.5	3-Methylcrotonylglycine	C18-
HMDB00466	130.0675	32	3-Methylindole	C18-
HMDB00469	141.0304	288.1	5-Hydroxymethyluracil	C18-
HMDB00472	219.0778	38.2	5-Hydroxy-L-tryptophan	C18-
HMDB00473	162.0784	289.5	6-Dimethylaminopurine	C18-
HMDB00486	159.1026	285.7	7-Hydroxyoctanoic acid	C18-
HMDB00489	334.1267	21.5	Aspartylglycosamine	C18-
HMDB00497	245.0785	21.8	56-Dihydrouridine	C18-
HMDB00508	151.0609	22.7	Ribitol	C18-
HMDB00510	160.0616	21.1	Aminoadipic acid	C18-
HMDB00512	206.0823	281.1	N-Acetyl-L-phenylalanine	C18-
HMDB00528	157.0254	286.6	45-Dihydroorotic acid	C18-
HMDB00532	116.0352	288	Acetylglycine	C18-
HMDB00536	462.0679	16.7	Adenylsuccinic acid	C18-
HMDB00538	505.9891	15.4	Adenosine triphosphate	C18-
HMDB00539	165.0407	19.4	Arabinonic acid	C18-
HMDB00544	155.0461	285.7	5-Hydroxymethyl-4-methyluracil	C18-
HMDB00549	85.0294	19.6	Gamma-Butyrolactone	C18-
HMDB00557	130.087	172.5	L-Alloisoleucine	C18-
HMDB00559	263.0241	18.7	3-Methoxy-4-hydroxyphenylethyleneglycol sulfate	C18-
HMDB00562	112.0515	279.2	Creatinine	C18-

HMDB00563	165.0556	286.6	D-Phenyllactic acid	C18-
HMDB00565	195.0512	18.8	Galactonic acid	C18-
HMDB00567	147.0448	185.5	Cinnamic acid	C18-
HMDB00572	525.2792	195.9	Desmosine	C18-
HMDB00590	188.0566	17.8	Glutarylglycine	C18-
HMDB00613	135.0303	19.4	Erythronic acid	C18-
HMDB00618	211.0016	17.5	D-Ribulose 5-phosphate	C18-
HMDB00623	229.1444	165.8	Dodecanedioic acid	C18-
HMDB00630	110.0358	287.4	Cytosine	C18-
HMDB00635	157.0511	286.2	Succinylacetone	C18-
HMDB00639	209.0303	26.4	Galactaric acid	C18-
HMDB00641	145.0618	21	L-Glutamine	C18-
HMDB00656	425.0819	18	Cysteineglutathione disulfide	C18-
HMDB00670	187.12	52.2	Homo-L-arginine	C18-
HMDB00671	204.0672	23.1	Indolelactic acid	C18-
HMDB00672	285.2075	276.8	Hexadecanedioic acid	C18-
HMDB00684	207.0778	24.7	L-Kynurenine	C18-
HMDB00701	172.0979	283.6	Hexanoylglycine	C18-
HMDB00703	151.04	286.2	Mandelic acid	C18-
HMDB00704	178.0369	292.5	Isoxanthopterin	C18-
HMDB00715	188.0353	289.4	Kynurenic acid	C18-
HMDB00721	171.0774	283.1	Glycylproline	C18-
HMDB00725	130.0508	290.4	4-Hydroxyproline	C18-
HMDB00726	230.1046	291.5	Isovalerylglutamic acid	C18-
HMDB00730	144.0665	289.3	Isobutyrylglycine	C18-
HMDB00731	199.9691	22.7	Cysteine-S-sulfate	C18-
HMDB00735	208.0619	19.8	Hydroxyphenylacetylglycine	C18-
HMDB00763	190.051	287.7	5-Hydroxyindoleacetic acid	C18-
HMDB00781	300.0408	22.7	N-Acetylgalactosamine 4-sulphate	C18-
HMDB00782	313.239	278.8	Octadecanedioic acid	C18-
HMDB00784	187.0976	287.8	Azelaic acid	C18-
HMDB00788	287.0529	18.4	Orotidine	C18-
HMDB00792	201.1133	284.1	Sebacic acid	C18-
HMDB00797	453.0702	252.5	SAICAR	C18-
HMDB00802	162.042	290.4	Pterin	C18-
HMDB00812	174.0409	17.7	N-Acetyl-L-aspartic acid	C18-
HMDB00816	154.975	26.2	Phosphoglycolic acid	C18-
HMDB00821	192.0666	45.3	Phenylacetylglycine	C18-
HMDB00825	632.2054	17.2	3-Sialyllactose	C18-

HMDB00828	175.0363	18.3	Ureidosuccinic acid	C18-
HMDB00842	172.0404	28.5	Quinaldic acid	C18-
HMDB00851	427.182	27.5	Pyridinoline	C18-
HMDB00854	173.0569	18.3	Formiminoglutamic acid	C18-
HMDB00857	159.067	290	Pimelic acid	C18-
HMDB00872	257.1762	281.9	Tetradecanedioic acid	C18-
HMDB00873	123.0449	168.7	4-Methylcatechol	C18-
HMDB00884	257.0786	18.4	Ribothymidine	C18-
HMDB00888	215.129	290.1	Undecanedioic acid	C18-
HMDB00893	173.0823	287.3	Suberic acid	C18-
HMDB00894	142.0508	278.5	Vinylacetylglycine	C18-
HMDB00897	164.0577	291.5	7-Methylguanine	C18-
HMDB00904	174.0872	21.9	Citrulline	C18-
HMDB00905	330.0615	17.9	Deoxyadenosine monophosphate	C18-
HMDB00912	382.1014	17.1	Succinyladenosine	C18-
HMDB00913	211.0618	294.1	Vanillactic acid	C18-
HMDB00935	579.0279	16.8	Uridine diphosphate glucuronic acid	C18-
HMDB00957	109.0291	128.5	Pyrocatechol	C18-
HMDB00962	204.0516	24.9	Lipoamide	C18-
HMDB00968	360.9719	19.4	1D-Myo-inositol 14-bisphosphate	C18-
HMDB00978	206.0472	24.1	4-(2-Aminophenyl)-24-dioxobutanoic acid	C18-
HMDB00982	256.0948	290.6	5-Methylcytidine	C18-
HMDB00985	206.0684	293.4	Dihydrolipoamide	C18-
HMDB00988	354.1496	178.7	S-Adenosylmethioninamine	C18-
HMDB00992	178.0511	21.2	3-Succinoylpyridine	C18-
HMDB00996	152.0022	286.8	3-Sulfinoalanine	C18-
HMDB01000	387.0018	17.5	dUDP	C18-
HMDB01003	426.0093	24.5	Adenosine phosphosulfate	C18-
HMDB01004	191.0826	29.8	Oxoamide	C18-
HMDB01007	164.0718	26.3	3-Pyridinebutanoic acid	C18-
HMDB01008	581.2414	22.5	Biliverdin	C18-
HMDB01016	298.0673	25	D-4-Phosphopantothenate	C18-
HMDB01024	182.9695	35.1	Phosphohydroxypyruvic acid	C18-
HMDB01030	339.0921	19.2	3-Ketolactose	C18-
HMDB01031	213.0174	19.7	Deoxyribose 5-phosphate	C18-
HMDB01044	346.0565	20	2-Deoxyguanosine 5-monophosphate	C18-
HMDB01049	249.0562	19.4	Gamma-Glutamylcysteine	C18-
HMDB01062	300.0493	18.3	N-Acetyl-D-Glucosamine 6-Phosphate	C18-
HMDB01066	378.099	17.7	S-Lactoylglutathione	C18-

HMDB01067	303.084	18.1	N-Acetylaspartylglutamic acid	C18-
HMDB01068	289.0339	18	D-Sedoheptulose 7-phosphate	C18-
HMDB01084	126.0559	289.3	D-1-Piperideine-2-carboxylic acid	C18-
HMDB01095	588.076	17.2	GDP-L-fucose	C18-
HMDB01109	258.039	18.6	Glucosamine-1P	C18-
HMDB01112	168.9908	18.2	D-Glyceraldehyde 3-phosphate	C18-
HMDB01120	244.9978	291	Dimethylallylpyrophosphate	C18-
HMDB01125	241.0123	18	Inositol cyclic phosphate	C18-
HMDB01127	257.0071	21.6	6-Phosphonoglucono-D-lactone	C18-
HMDB01131	130.0144	289.2	Iminoaspartic acid	C18-
HMDB01132	336.0516	16.9	Nicotinic acid mononucleotide	C18-
HMDB01140	127.1127	23.4	Octanal	C18-
HMDB01142	457.1147	21.4	FMNH2	C18-
HMDB01147	118.0145	290.4	Aminomalonic acid	C18-
HMDB01163	604.071	17.1	Guanosine diphosphate mannose	C18-
HMDB01164	111.045	288.4	trans-12-Dihydrobenzene-12-diol	C18-
HMDB01173	296.0842	29.1	5-Methylthioadenosine	C18-
HMDB01176	613.1434	17.1	Cytidine monophosphate N-acetylneuraminic acid	C18-
HMDB01178	558.0656	16.6	Adenosine diphosphate ribose	C18-
HMDB01182	151.026	292.2	68-Dihydroxypurine	C18-
HMDB01190	158.0608	216.6	Indoleacetaldehyde	C18-
HMDB01191	466.9709	41.8	Deoxyuridine triphosphate	C18-
HMDB01198	624.2926	225.5	Leukotriene C4	C18-
HMDB01200	235.0728	290.1	N-Formylkynurenine	C18-
HMDB01201	442.0178	18.4	Guanosine diphosphate	C18-
HMDB01202	306.05	17.9	dCMP	C18-
HMDB01212	171.0411	279.2	Hydantoin-5-propionic acid	C18-
HMDB01216	135.0672	291.3	Tetrahydropteridine	C18-
HMDB01227	321.0508	25.6	5-Thymidylic acid	C18-
HMDB01228	226.0125	18.7	L-Glutamic acid 5-phosphate	C18-
HMDB01232	138.0195	283.3	4-Nitrophenol	C18-
HMDB01241	156.0302	288.8	2-Aminomuconic acid	C18-
HMDB01250	134.0611	27.7	N-Acetylarylamine	C18-
HMDB01253	192.0304	288.2	56-Dihydroxyindole-2-carboxylic acid	C18-
HMDB01265	243.028	17.9	Fucose 1-phosphate	C18-
HMDB01267	177.0669	34.2	4-Oxo-4-(3-pyridyl)-butanamide	C18-
HMDB01268	199.0235	16.8	4-Fumarylacetoacetic acid	C18-
HMDB01273	521.9841	17.1	Guanosine triphosphate	C18-
HMDB01280	140.0352	288.1	2-Aminomuconic acid semialdehyde	C18-

HMDB01301	112.0403	289.1	1-Pyrroline-5-carboxylic acid	C18-
HMDB01309	212.0121	50.5	m-Chlorohippuric acid	C18-
HMDB01316	275.018	17	6-Phosphogluconic acid	C18-
HMDB01321	199.0016	17.9	D-Erythrose 4-phosphate	C18-
HMDB01330	184.0253	18	2-Amino-3-carboxymuconic acid semialdehyde	C18-
HMDB01346	586.0606	16.7	GDP-4-Dehydro-6-deoxy-D-mannose	C18-
HMDB01352	103.0035	291	Hydroxypyruvic acid	C18-
HMDB01397	362.0517	18	Guanosine monophosphate	C18-
HMDB01406	121.0406	287.7	Niacinamide	C18-
HMDB01424	162.056	44.4	4-(3-Pyridyl)-3-butenoic acid	C18-
HMDB01434	210.0786	292.3	3-Methoxytyrosine	C18-
HMDB01439	365.0513	19.8	Phosphoribosyl formamidocarboxamide	C18-
HMDB01460	169.0079	20.7	Diethylthiophosphate	C18-
HMDB01476	152.0353	40.3	3-Hydroxyanthranilic acid	C18-
HMDB01487	664.1189	16.1	NADH	C18-
HMDB01490	183.0671	289.5	Vanylglycol	C18-
HMDB01494	138.9801	29.6	Acetylphosphate	C18-
HMDB01508	410.0281	16.3	dADP	C18-
HMDB01511	210.0289	17.5	Phosphocreatine	C18-
HMDB01517	337.0551	18.7	AICAR	C18-
HMDB01518	277.1449	252.5	Alpha-CEHC	C18-
HMDB01526	248.0797	289.7	S-Acetyldihydrolipoamide	C18-
HMDB01532	489.9907	27	Deoxyadenosine triphosphate	C18-
HMDB01534	471.1746	50.6	5-Formiminotetrahydrofolic acid	C18-
HMDB01538	136.0401	176.7	3-Pyridylacetic acid	C18-
HMDB01539	201.1357	43.6	Asymmetric dimethylarginine	C18-
HMDB01545	166.0511	23.6	Pyridoxal	C18-
HMDB01546	402.0121	20	CDP	C18-
HMDB01550	334.0724	17	S-Formylglutathione	C18-
HMDB01555	247.0465	21.4	Pyridoxamine 5-phosphate	C18-
HMDB01564	445.0542	20.4	CDP-Ethanolamine	C18-
HMDB01570	303.0374	200.1	Thymidine 35-cyclic monophosphate	C18-
HMDB01587	149.0243	284.9	Phenylglyoxylic acid	C18-
HMDB01713	163.0396	163.8	m-Coumaric acid	C18-
HMDB01786	274.0937	280.4	Ethenodeoxyadenosine	C18-
HMDB01855	176.0715	58.1	5-Hydroxytryptophol	C18-
HMDB01864	129.0556	289.8	2-Ketohexanoic acid	C18-
HMDB01867	193.0619	25.8	4-Aminohippuric acid	C18-
HMDB01890	162.0231	19	Acetylcysteine	C18-

HMDB01931	247.134	199.4	Gamma-CEHC	C18-
HMDB01959	230.149	32.7	Gamma-Aminobutyryl-lysine	C18-
HMDB01964	179.035	286.9	Caffeic acid	C18-
HMDB02005	164.0389	21	Methionine sulfoxide	C18-
HMDB02012	249.1136	290.7	Ubiquinone-1	C18-
HMDB02025	175.0624	291.5	23-Dimethyl-3-hydroxyglutaric acid	C18-
HMDB02030	178.0734	292.1	Fructosamine	C18-
HMDB02034	267.063	292.4	Homolanthionine	C18-
HMDB02038	159.1139	33.8	N(6)-Methyllysine	C18-
HMDB02040	177.0557	289.4	4-Methoxycinnamic acid	C18-
HMDB02053	247.1191	283.4	Histidylproline diketopiperazine	C18-
HMDB02056	221.0821	269.5	Monoisobutyl phthalic acid	C18-
HMDB02070	161.0097	23.3	4-Hydroxy-2-oxoglutaric acid	C18-
HMDB02074	145.0515	289.4	22-Dimethylsuccinic acid	C18-
HMDB02089	286.1051	289.6	N-Ribosylhistidine	C18-
HMDB02099	148.0627	291.3	6-Methyladenine	C18-
HMDB02135	220.0307	27.6	S-(3-oxo-3-carboxy-n-propyl)cysteine	C18-
HMDB02144	139.0511	284.3	13-Dimethyluracil	C18-
HMDB02167	99.045	288.3	3-Methylbutyrolactone	C18-
HMDB02171	284.1259	25.4	Glycylprolylhydroxyproline	C18-
HMDB02201	174.0784	292.3	N-Carboxyethyl-g-aminobutyric acid	C18-
HMDB02203	187.1339	284	3-Hydroxycapric acid	C18-
HMDB02205	182.0118	17.9	L-Homocysteic acid	C18-
HMDB02207	145.0869	288.3	3-Hydroxyisoheptanoic acid	C18-
HMDB02210	150.0557	197.6	2-Phenylglycine	C18-
HMDB02222	149.0607	286.4	3-Methylphenylacetic acid	C18-
HMDB02224	240.0999	291.5	5-Methyldeoxycytidine	C18-
HMDB02243	122.0246	283.6	Picolinic acid	C18-
HMDB02273	160.0252	17.8	4-Hydroxy-L-glutamic acid	C18-
HMDB02277	341.1957	281.8	23-Dinor-6-keto-prostaglandin F1 a	C18-
HMDB02278	364.1241	17.6	2-(acetylamino)-15-anhydro-2-deoxy-3-O-b-D-galactopyranosyl-D-arabino-Hex-1-enitol	C18-
HMDB02285	160.0404	30.9	2-Indolecarboxylic acid	C18-
HMDB02327	243.1604	287.2	111-Undecanedicarboxylic acid	C18-
HMDB02334	165.0191	122.5	Benzoquinoneacetic acid	C18-
HMDB02335	229.0832	19.1	Aspartyl-L-proline	C18-
HMDB02339	233.0934	39.4	5-Methoxytryptophan	C18-
HMDB02372	282.1111	292.5	N-Phenylacetylphenylalanine	C18-
HMDB02455	102.0195	288.4	Pyruvatoxime	C18-
HMDB02511	237.0778	288	345-Trimethoxycinnamic acid	C18-

HMDB02545	193.035	150.4	Galacturonic acid	C18-
HMDB02757	167.9972	287.6	Cysteic acid	C18-
HMDB02818	140.9942	290	Alloxan	C18-
HMDB02894	124.0515	289.4	5-Methylcytosine	C18-
HMDB02916	154.0145	287.8	4-Nitrocatechol	C18-
HMDB02994	121.0518	289.8	Erythritol	C18-
HMDB03033	339.1965	266.5	Canrenone	C18-
HMDB03263	305.0193	22.6	Pelargonidin	C18-
HMDB03269	179.0462	293.8	Nicotinuric acid	C18-
HMDB03315	97.0656	94	Cyclohexanone	C18-
HMDB03331	280.1046	18.5	1-Methyladenosine	C18-
HMDB03337	611.1434	16.7	Oxidized glutathione	C18-
HMDB03357	173.0933	19.3	N-Acetylornithine	C18-
HMDB03362	682.2992	250.1	Chitin	C18-
HMDB03364	107.0148	217.6	Quinone	C18-
HMDB03405	145.0982	42	D-Lysine	C18-
HMDB03416	173.104	124.4	D-Arginine	C18-
HMDB03417	120.0125	20.6	D-Cysteine	C18-
HMDB03426	277.1231	255.8	Pantetheine	C18-
HMDB03431	140.0829	19.3	L-Histidinol	C18-
HMDB03454	164.0352	284.4	4-Pyridoxolactone	C18-
HMDB03484	198.0157	294.7	O-Phosphohomoserine	C18-
HMDB03601	328.1524	18.6	(S)-Reticuline	C18-
HMDB03626	192.1028	201.1	(R)-N-Methylsalsolinol	C18-
HMDB03671	113.0972	19.7	2-Heptanone	C18-
HMDB03764	217.0844	292.7	Glutamylalanine	C18-
HMDB03767	135.045	267.8	4-Hydroxyphenylacetaldehyde	C18-
HMDB03869	274.1402	33.1	Epsilon-(gamma-Glutamyl)-lysine	C18-
HMDB03882	357.0829	174	N1-(5-Phospho-a-D-ribosyl)-56-dimethylbenzimidazole	C18-
HMDB03903	124.9914	19	2-Hydroxyethanesulfonate	C18-
HMDB03905	109.0406	284.3	Imidazole-4-acetaldehyde	C18-
HMDB03933	377.1964	26.3	Pentosidine	C18-
HMDB03974	224.9793	26.7	Oxalosuccinic acid	C18-
HMDB03976	273.0042	17.2	D-Glucuronic acid 1-phosphate	C18-
HMDB04041	118.0507	22.5	L-Allothreonine	C18-
HMDB04058	148.0403	29.8	56-Dihydroxyindole	C18-
HMDB04062	137.0243	282.4	Gentisate aldehyde	C18-
HMDB04063	196.098	289.2	Metanephrine	C18-
HMDB04072	119.0491	287.2	4-Hydroxystyrene	C18-

HMDB04076	179.0827	18.5	5-Hydroxykynurenamine	C18-
HMDB04078	299.0288	17.8	Cinnavalininate	C18-
HMDB04086	251.068	18.6	5-Hydroxy-N-formylkynurenine	C18-
HMDB04157	595.3449	181.9	L-Urobilinogen	C18-
HMDB04181	123.0562	284.6	Methylimidazole acetaldehyde	C18-
HMDB04193	151.0514	285.2	N1-Methyl-2-pyridone-5-carboxamide	C18-
HMDB04195	253.049	18.2	5-L-Glutamyl-taurine	C18-
HMDB04230	110.0246	292.4	Pyrrole-2-carboxylic acid	C18-
HMDB04231	204.1243	271.2	Pantothenol	C18-
HMDB04259	263.1023	20.9	Acetyl-N-formyl-5-methoxykynurenamine	C18-
HMDB04284	137.0606	285.9	Tyrosol	C18-
HMDB04328	223.0825	268.3	Temurin	C18-
HMDB04400	197.0671	22.4	5-Acetylamino-6-amino-3-methyluracil	C18-
HMDB04461	120.0448	291.1	Benzamide	C18-
HMDB04620	215.1147	162.8	N-a-Acetyl-L-arginine	C18-
HMDB04822	213.0712	66.5	Methyl bisnorbiotinyl ketone	C18-
HMDB04823	188.0025	19.6	Lanthionine ketimine	C18-
HMDB04827	142.0872	286.8	Proline betaine	C18-
HMDB05028	323.155	227.2	Escitalopram	C18-
HMDB05765	288.1212	18.6	Ophthalmic acid	C18-
HMDB05766	274.1053	19.3	Norophthalmic acid	C18-
HMDB05768	336.1656	22.9	Kyotorphin	C18-
HMDB05789	371.1531	168.8	Tetrahydrocurcumin	C18-
HMDB05831	261.0391	17.5	Sorbitol-6-phosphate	C18-
HMDB05843	98.0069	21	Allyl isothiocyanate	C18-
HMDB05874	257.9751	243	3-Bromotyrosine	C18-
HMDB05923	284.0897	292.6	N4-Acetylcytidine	C18-
HMDB06002	315.2334	237.9	Ethyltestosterone	C18-
HMDB06012	317.2491	258.7	Epimetendiol	C18-
HMDB06013	319.265	274.2	7a17-dimethyl-5b-Androstane-3a17b-diol	C18-
HMDB06029	187.0725	282.2	N-Acetylglutamine	C18-
HMDB06037	180.053	291.3	8-Hydroxy-7-methylguanine	C18-
HMDB06045	359.1257	18.7	Dityrosine	C18-
HMDB06273	338.037	43	5-amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxylate	C18-
HMDB06348	184.0979	286.4	Pseudoecgonine	C18-
HMDB06355	175.0249	19.9	D-Glucurono-63-lactone	C18-
HMDB06406	198.1136	282.7	Ecgonine methyl ester	C18-
HMDB06409	216.0353	20.8	Tyramine-O-sulfate	C18-
HMDB06488	172.0627	290.1	N-Acetyl-L-glutamate 5-semialdehyde	C18-

HMDB06590	325.1162	293.7	2-O-a-L-Fucopyranosyl-galactose	C18-
HMDB06695	227.1045	290	Prolylhydroxyproline	C18-
HMDB06710	453.2976	261.7	Ubiquinone-4	C18-
HMDB06779	146.0246	268.5	Indole-56-quinone	C18-
HMDB06790	253.0938	166.6	Galactosylglycerol	C18-
HMDB06794	226.036	18.1	5-(2-Carboxyethyl)-46-Dihydroxypicolinate	C18-
HMDB06801	212.9797	51.3	2-Oxo-3-hydroxy-4-phosphobutanoic acid	C18-
HMDB06802	214.013	25.9	O-Phospho-4-hydroxy-L-threonine	C18-
HMDB06834	321.1152	23.8	D-Pantothenoyl-L-cysteine	C18-
HMDB06868	276.1121	22.4	S-(2-Methylpropionyl)-dihydrolipoamide-E	C18-
HMDB06954	180.0307	20.4	2-Methyl-3-hydroxy-5-formylpyridine-4-carboxylate	C18-
HMDB06955	196.0258	20.8	3-Hydroxy-2-methylpyridine-45-dicarboxylate	C18-
HMDB10170	353.2339	25.5	111215-TriHETRE	C18-
HMDB10200	293.2125	221.8	A-12(13)-EpODE	C18-
HMDB10201	311.2233	286.8	1213-DiHODE	C18-
HMDB10213	343.2279	145.7	17-HDoHE	C18-
HMDB10214	361.236	242	1920-DiHDPA	C18-
HMDB10222	319.2282	239.1	9-HETE	C18-
HMDB10319	308.076	18.3	Inodxyl glucuronide	C18-
HMDB10323	296.112	167.7	Phenethylamine glucuronide	C18-
HMDB10328	312.1088	19.7	Tyramine glucuronide	C18-
HMDB10568	744.5526	256.1	PE-NMe2(16:018:1(9Z))	C18-
HMDB10724	185.1183	280	3-Oxodecanoic acid	C18-
HMDB11107	181.0367	291.8	7-Methyluric acid	C18-
HMDB11111	87.0086	289.2	Malonic semialdehyde	C18-
HMDB11142	421.2727	192.3	DHAP(18:0e)	C18-
HMDB11147	385.3326	203.8	DG(18:0e2:00:0)	C18-
HMDB11153	341.3065	266.8	MG(P-18:0e0:00:0)	C18-
HMDB11154	393.2411	179.4	LPA(P-16:0e0:0)	C18-
HMDB11161	259.0943	18	L-alpha-glutamyl-L-hydroxyproline	C18-
HMDB11162	203.0677	18.6	L-beta-aspartyl-L-alanine	C18-
HMDB11163	247.0576	17.5	L-beta-aspartyl-L-aspartic acid	C18-
HMDB11164	261.0736	17.2	L-beta-aspartyl-L-glutamic acid	C18-
HMDB11165	171.0412	18.4	L-beta-aspartyl-L-glycine	C18-
HMDB11166	245.1149	18.1	L-beta-aspartyl-L-leucine	C18-
HMDB11168	219.0629	18.7	L-beta-aspartyl-L-serine	C18-
HMDB11169	233.0783	18.3	L-beta-aspartyl-L-threonine	C18-
HMDB11170	259.1306	18	L-gamma-glutamyl-L-isoleucine	C18-
HMDB11174	227.1402	58.9	L-isoleucyl-L-proline	C18-

HMDB11639	210.0411	18.4	Topaquinone	C18-
HMDB11649	333.0602	18.5	1-(sn-Glycero-3-phospho)-1D-myo-inositol	C18-
HMDB11654	270.1337	20.3	2-(3-Carboxy-3-(methylammonio)propyl)-L-histidine	C18-
HMDB11657	182.0671	21.7	26-Diamino-4-hydroxy-5-N-methylformamidopyrimidine	C18-
HMDB11671	620.0212	17	ADP-ribose 1-2 cyclic phosphate	C18-
HMDB11680	329.0311	16.4	Inosine 23-cyclic phosphate	C18-
HMDB11688	308.9789	16.7	Ribose 15-bisphosphate	C18-
HMDB11691	304.0348	18.4	Cytidine 23-cyclic phosphate	C18-
HMDB11714	209.0459	282.9	Vanilpyruvic acid	C18-
HMDB11716	252.09	165	N-Acetylvanilalanine	C18-
HMDB11718	121.0294	284.6	4-Hydroxybenzaldehyde	C18-
HMDB11719	261.0067	20	Homovanillic acid sulfate	C18-
HMDB11737	275.089	17.5	Gamma Glutamylglutamic acid	C18-
HMDB11745	190.0546	18.8	N-Acetyl-L-methionine	C18-
HMDB11751	179.0713	290	3-Methoxybenzenepropanoic acid	C18-
HMDB12127	207.0678	19.2	(R)-2-Benzylsuccinate	C18-
HMDB12149	173.0463	291	2-Isopropyl-3-oxosuccinate	C18-
HMDB12153	138.0561	19.4	34-Dihydroxybenzylamine	C18-
HMDB12161	231.099	18.5	4-(Glutamylamino) butanoate	C18-
HMDB12182	137.0467	287.3	8-Hydroxypurine	C18-
HMDB12197	291.0933	20.9	Canavaninosuccinate	C18-
HMDB12201	380.1602	23.8	Cis-zeatin-7-N-glucoside	C18-
HMDB12204	218.1037	276.6	Cis-zeatin	C18-
HMDB12221	389.0965	16.6	Dopaxanthin	C18-
HMDB12234	138.0672	281.7	Histidinal	C18-
HMDB12236	219.0158	19	Imidazole acetol-phosphate	C18-
HMDB12240	362.1827	225.5	Isopentenyladenine-9-N-glucoside	C18-
HMDB12243	376.1242	17.1	Kinetin-7-N-glucoside	C18-
HMDB12245	214.0735	293.6	Kinetin	C18-
HMDB12266	288.0741	17.6	N-Succinyl-2-amino-6-ketopimelate	C18-
HMDB12281	373.1047	33	Portulacaxanthin II	C18-
HMDB12285	272.9581	148.1	Ribose-1-arsenate	C18-
HMDB12286	188.0759	289	S-Prenyl-L-cysteine	C18-
HMDB12289	170.0464	290.2	Tetrahydrodipicolinate	C18-
HMDB12518	399.2523	265.9	11-Carboxy-gamma-tocotrienol	C18-
HMDB12575	412.1458	154.7	13E-Tetranor-16-carboxy-LTE4	C18-
HMDB12710	189.0406	19	3-Dehydroquinate	C18-
HMDB12798	319.191	202.1	5-Carboxy-alpha-chromanol	C18-
HMDB12799	305.1762	272.8	5-Carboxy-gamma-chromanol	C18-

HMDB12848	347.2212	245.1	7-Carboxy-alpha-chromanol	C18-
HMDB12849	345.2059	208	7-Carboxy-alpha-tocotrienol	C18-
HMDB12850	333.204	208.6	7-Carboxy-gamma-chromanol	C18-
HMDB12867	385.2366	241.9	9-Carboxy-alpha-tocotrienol	C18-
HMDB12868	375.2524	279.9	9-Carboxy-gamma-chromanol	C18-
HMDB12869	371.221	242.9	9-Carboxy-gamma-tocotrienol	C18-
HMDB12880	114.0559	288.3	Acetamidopropanal	C18-
HMDB12986	570.2793	183.8	Kinetensin 4-7	C18-
HMDB13010	186.1135	281.2	N-Heptanoylglycine	C18-
HMDB13021	503.2916	205.5	Neuromedin N (1-4)	C18-
HMDB13024	406.2316	202	Neurotensin 11-13	C18-
HMDB13034	312.2545	168.3	Palmitoylglycine	C18-
HMDB13055	644.3198	37	S-(11-hydroxy-9-deoxy-delta12-PGD2)-glutathione	C18-
HMDB13067	236.0935	28.3	Salsoline-1-carboxylate	C18-
HMDB13070	209.0814	292.6	Sinapyl alcohol	C18-
HMDB13105	167.1075	67.7	trans-45-epoxy-2(E)-decenal	C18-
HMDB13159	167.0461	289.8	23-Diaminosalicylic acid	C18-
HMDB13204	234.0624	17.9	6-Succinoaminopurine	C18-
HMDB13220	320.0631	16.9	Beta-Citryl-L-glutamic acid	C18-
HMDB13246	326.2701	172.9	Margaroylglycine	C18-
HMDB13250	284.2232	76.8	Myristoylglycine	C18-
HMDB13253	152.0828	291.7	N-Acetylhistamine	C18-
HMDB13267	228.1606	22.8	N-Decanoylglycine	C18-
HMDB13279	214.1447	15.5	N-Nonanoylglycine	C18-
HMDB13286	242.1764	280.1	N-Undecanoylglycine	C18-
HMDB13308	340.2857	191.2	Stearoylglycine	C18-
HMDB13332	382.2633	161.5	3-Hydroxy-5 8-tetradecadiencarnitine	C18-
HMDB13333	412.3071	203.9	3-Hydroxy-9-hexadecenoylcarnitine	C18-
HMDB13336	414.3229	218.1	3-Hydroxyhexadecanoylcarnitine	C18-
HMDB13339	440.3383	174.7	3-Hydroxy-11Z-octadecenoylcarnitine	C18-
HMDB13593	153.0057	19.1	14-Dithiothreitol	C18-
HMDB13609	203.0827	21.9	D-Tryptophan	C18-
HMDB13631	338.2702	175.8	Oleoyl glycine	C18-
HMDB13674	125.024	288	123-Trihydroxybenzene	C18-
HMDB13688	219.1756	236.4	Nootkatol	C18-
HMDB13692	361.1662	177.5	Secoisolariciresinol	C18-
HMDB13696	211.0386	36.3	Urolithin B	C18-
HMDB13751	94.0297	280.8	2-Hydroxypyridine	C18-
HMDB13809	125.0969	160.9	(E)-2-octenal	C18-

HMDB13813	251.2387	275.2	13-Heptadecyn-1-ol	C18-
HMDB13817	219.1389	197.2	26-Di-tert-butylbenzoquinone	C18-
HMDB13825	163.1126	206.6	4-(1133-Tetramethylbutyl)-phenol	C18-
HMDB28680	159.0772	161.5	Alanyl-Alanine	C18-
HMDB28688	201.0884	15.5	Alanyl-Hydroxyproline	C18-
HMDB28690	201.1247	20.3	Alanyl-Isoleucine	C18-
HMDB28695	185.0931	268.3	Alanyl-Proline	C18-
HMDB28696	175.0725	31.7	Alanyl-Serine	C18-
HMDB28697	189.0883	20.1	Alanyl-Threonine	C18-
HMDB28699	251.1054	292.5	Alanyl-Tyrosine	C18-
HMDB28704	287.1449	26.7	Arginyl-Asparagine	C18-
HMDB28727	246.0754	18.2	Asparaginyl-Aspartate	C18-
HMDB28730	259.0829	289.9	Asparaginyl-Glutamate	C18-
HMDB28732	244.0944	20.1	Asparaginyl-Hydroxyproline	C18-
HMDB28734	244.1288	20.2	Asparaginyl-Isoleucine	C18-
HMDB28743	294.1113	293.5	Asparaginyl-Tyrosine	C18-
HMDB28750	235.04	18.1	Aspartyl-Cysteine	C18-
HMDB28751	260.0895	18.1	Aspartyl-Glutamine	C18-
HMDB28773	248.0724	21.1	Cysteinyl-Glutamine	C18-
HMDB28787	283.0738	36.8	Cysteinyl-Tyrosine	C18-
HMDB28796	273.0987	292.6	Glutaminyl-Glutamate	C18-
HMDB28798	258.1094	40.2	Glutaminyl-Hydroxyproline	C18-
HMDB28805	242.1151	24.7	Glutaminyl-Proline	C18-
HMDB28818	273.0736	17.3	Glutamyl-Glutamate	C18-
HMDB28843	211.0835	38.5	Glycyl-Histidine	C18-
HMDB28848	221.0947	26.6	Glycyl-Phenylalanine	C18-
HMDB28850	161.0572	21	Glycyl-Serine	C18-
HMDB28853	237.0897	292	Glycyl-Tyrosine	C18-
HMDB28864	243.1	291.2	Hydroxyprolyl-Hydroxyproline	C18-
HMDB28866	243.1357	19.1	Hydroxyprolyl-Isoleucine	C18-
HMDB28869	261.0926	22.7	Hydroxyprolyl-Methionine	C18-
HMDB28876	229.1199	291.7	Hydroxyprolyl-Valine	C18-
HMDB28887	291.1228	22.3	Histidinyl-Histidine	C18-
HMDB28888	267.1442	284.4	Histidinyl-Isoleucine	C18-
HMDB28892	301.1297	289.3	Histidinyl-Phenylalanine	C18-
HMDB28893	251.1142	288.3	Histidinyl-Proline	C18-
HMDB28896	340.1422	22.7	Histidinyl-Tryptophan	C18-
HMDB28916	217.1205	22.7	Isoleucyl-Serine	C18-
HMDB28920	229.1559	283.3	Isoleucyl-Valine	C18-

HMDB28950	273.1344	182.3	Lysyl-Glutamate	C18-
HMDB28958	292.1639	278.2	Lysyl-Phenylalanine	C18-
HMDB28961	246.1448	25.7	Lysyl-Threonine	C18-
HMDB28980	295.1119	17.6	Methionyl-Phenylalanine	C18-
HMDB28981	245.0969	27.7	Methionyl-Proline	C18-
HMDB28983	249.0893	292.2	Methionyl-Threonine	C18-
HMDB28985	311.1044	31.2	Methionyl-Tyrosine	C18-
HMDB28994	292.1043	291	Phenylalanyl-Glutamate	C18-
HMDB29005	265.1178	187.6	Phenylalanyl-Threonine	C18-
HMDB29007	327.1354	39.2	Phenylalanyl-Tyrosine	C18-
HMDB29027	215.1048	293.3	Prolyl-Threonine	C18-
HMDB29051	267.0992	17.3	Serinyl-Tyrosine	C18-
HMDB29052	185.093	23.2	Serinyl-Valine	C18-
HMDB29094	389.1617	259.6	Tryptophyl-Tryptophan	C18-
HMDB29095	366.1486	20.9	Tryptophyl-Tyrosine	C18-
HMDB29117	343.1307	22.9	Tyrosyl-Tyrosine	C18-
HMDB29164	451.1274	19.7	(-)-epicatechin-3-O-glucuronide	C18-
HMDB29171	143.035	289.6	3-Hydroxyadipic acid 36-lactone	C18-
HMDB29190	397.1111	219.5	5-(34-dihydroxyphenyl)-gamma-valerolactone-3-O-glucuronide	C18-
HMDB41797	218.9635	292.4	24-Dichlorophenoxyacetic acid	C18-
HMDB41804	151.0763	286.7	2-Isopropoxyphenol	C18-
HMDB41806	180.1028	21.5	34-Dimethoxyphenylethylamine	C18-
HMDB41807	213.055	283	3-Phenoxybenzoic acid	C18-
HMDB41820	164.0213	270	8-Oxoguanine	C18-
HMDB41824	319.1555	282.9	alpha-Zearalenol	C18-
HMDB41849	299.0697	26.1	Carboxytolbutamide	C18-
HMDB41900	190.037	18.4	gamma-Carboxyglutamic acid	C18-
HMDB41943	194.082	173.1	N-Acetyldopamine	C18-
HMDB41946	143.0462	18.1	N-Nitrosoproline	C18-
HMDB41947	229.1811	290.3	N1N8-Diacetylspermidine	C18-
HMDB41958	232.1342	200.6	Normeperidine	C18-
HMDB41992	101.0607	269.2	Pivalic acid	C18-
HMDB41997	349.2368	271.5	Pregnanetriolone	C18-
HMDB42033	121.0324	221.9	Thiodiglycol	C18-
HMDB42052	123.9805	54.1	Trimethylselenonium	C18-
HMDB59975	289.0409	24.4	4-Hydroxy-5-(3-hydroxyphenyl)-valeric acid-3-O-sulphate	C18-
HMDB59985	303.0193	24.9	5-(345-Trihydroxyphenyl)-gamma-valerolactone-3-O-sulphate	C18-
HMDB59996	353.0308	17.6	Dihydronaringenin-O-sulphate	C18-
HMDB60013	203.0024	20.5	O-methoxycatechol-O-sulphate	C18-

HMDB60015	172.9916	20.4	Phenol sulphate	C18-
HMDB60017	301.0544	18.5	Pyrogallol-2-O-glucuronide	C18-
HMDB60498	385.1503	20.9	NNAL-N-glucuronide	C18-
HMDB61387	366.9012	27	Triclosan sulfate	C18-

Web Table 2. Exogenous features detected in HILIC column with suggested m/z matches annotation and cluster IDs

mz	time	chemical_ID	Name	cluster
509.3358	33.4	HMDB15057	Buprenorphine	1
680.4134	28.3	HMDB15616	Telaprevir	1
265.0487	246	HMDB36649	Sinalbin B	1
781.5563	24.8	HMDB41454	D8-Merulinic acid A	1
377.1457	93.8	HMDB00244	Riboflavin	1
183.0652	176.9	HMDB00423	34-Dihydroxyhydrocinnamic acid	1
195.0638	71.8	HMDB00954	trans-Ferulic acid	1
315.1501	86.1	HMDB01930	Ranitidine	1
179.1066	264.2	HMDB02043	5-Phenylvaleric acid	1
151.0752	195.4	HMDB02097	4-Ethylbenzoic acid	1
419.2769	24.2	HMDB05007	Simvastatin	1
178.0359	213.5	HMDB05792	Sulforaphane	1
405.2629	26.4	HMDB14372	Lovastatin	1
236.0078	292.2	HMDB14427	Pamidronate	1
373.2736	25.3	HMDB14629	Nabilone	1
307.2239	26.3	HMDB14759	Oxandrolone	1
237.124	157.7	HMDB15444	Hexobarbital	1
282.2214	187.2	HMDB15554	Alverine	1
125.0097	145.3	HMDB15677	Dimercaprol	1
449.2412	55.2	HMDB30421	L-Linalool 3-xylosyl-(1-6)-glucoside	1
561.2494	41.6	HMDB30734	Isomorellic acid	1
235.169	188	HMDB31349	Epiacoronene	1
175.0754	181.7	HMDB32727	4-Methoxy-1-naphthol	1
211.1327	25.2	HMDB32871	Sedanonic acid	1
514.219	65.6	HMDB32880	trans-Zeatin-O-glucoside riboside	1
228.1224	214.8	HMDB32928	2-Amino-348-trimethyl-3H-imidazo45-fquinoxaline	1
226.0848	116.8	HMDB32983	1-Hydroxy-10-methylacridone	1
211.0293	95.8	HMDB33058	1-(Methylsulfinyl)propyl 1-propenyl disulfide	1
239.06	94.7	HMDB33073	1-Propenyl 1-(propylsulfinyl)propyl disulfide	1
275.164	187.2	HMDB33090	6-Dehydroshogaol	1
337.1421	125.6	HMDB33107	Semilepidinoside A	1
100.0219	210.2	HMDB33116	4-Methylthiazole	1
231.1378	127.9	HMDB33235	812-Epoxy-4(15)711-eudesmatrien-1-one	1
276.1228	62.1	HMDB33345	()-Ribaline	1
220.1326	153.3	HMDB33429	Tanakamine	1
127.1117	24.1	HMDB33547	3-Octen-2-one	1
130.0322	68.6	HMDB33561	2-Acetyl-45-dihydrothiazole	1

111.026	71.7	HMDB33746	Benzenethiol	1
182.1177	182.1	HMDB33868	beta-O-Methylynephrine	1
105.074	58.5	HMDB33902	Isopentyl mercaptan	1
239.1278	171.2	HMDB34046	1234-Tetramethoxy-5-(2-propenyl)benzene	1
439.2441	261	HMDB34184	Licorisoflavan A	1
127.039	256.2	HMDB34355	5-Hydroxymethyl-2-furancarboxaldehyde	1
195.1379	273.3	HMDB34450	Neocnidilide	1
133.0689	72.7	HMDB35176	3-Mercapto-2-methylpentanal	1
170.0809	220.7	HMDB35178	6-Acetyl-23-dihydro-2-(hydroxymethyl)-4(1H)-pyridinone	1
407.2772	25.7	HMDB35288	(6b7b13R)-67-Diacetoxy-814-labdadiene-13-ol	1
153.091	275.8	HMDB36169	3-(5-Methyl-2-furanyl)butanal	1
197.1173	177.8	HMDB36226	26-Dimethoxy-4-propylphenol	1
155.1066	163.5	HMDB37276	Octahydro-2H-1-benzopyran-2-one	1
123.1168	240.8	HMDB38140	Santene	1
347.1677	90.7	HMDB38149	Nepetaside	1
104.0707	58.8	HMDB38394	O-Acetylethanolamine	1
323.0716	229.1	HMDB38515	L-gamma-Glutamyl-S-allylthio-L-cysteine	1
117.0378	66.5	HMDB38556	xI-Dihydro-2-methyl-3(2H)-thiophenone	1
165.0821	78.8	HMDB38670	S-Methylmethionine	1
274.1434	44.1	HMDB38834	(2E)-Piperamide-C5:1	1
258.1478	58.4	HMDB39125	Coumaperine	1
133.1081	41.1	HMDB39228	(3-Aminopropoxy)guanidine	1
327.0923	111.5	HMDB39723	3-O-alpha-D-Glucopyranuronosyl-D-xylose	1
119.0167	57.8	HMDB39786	Dihydro-4-mercapto-3(2H)-furanone	1
89.0425	188.6	HMDB39807	cis-23-Dimethylthiirane	1
156.1383	179.7	HMDB39833	3-(1-Pyrrolidinyl)-2-pentanone	1
153.1022	28.7	HMDB40052	2-Isopropyl-5-methoxypyrazine	1
133.0868	222.8	HMDB40409	Ethyl ()-3-hydroxybutyrate	1
900.4326	47.7	HMDB40695	Lyciumin D	1
343.2476	177.4	HMDB40901	13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid	1
270.279	223.9	HMDB40940	Capsiamide	1
205.0697	49.9	HMDB41031	356-Trihydroxy-5-(hydroxymethyl)-2-methoxy-2-cyclohexen-1-one	1
181.0976	40	HMDB41109	(S)-3-Ethylidenehexahydropyrrolo12-apyrazine-14-dione	1
265.13	44.7	HMDB41186	Ilicifolinoside A	1
123.0917	30.8	HMDB41254	2-Ethyl-3-methylpyrazine 9CI	1
389.1801	53.4	HMDB41552	2-4-(3-Hydroxypropyl)-2-methoxyphenoxy-13-propanediol 1-xyloside	1
213.1485	174.4	HMDB41572	3-Ethenyl-4-hydroxy-25-dimethylhex-5-en-2-yl acetate	1
284.1717	131.4	HMDB41845	Cadralazine	1
118.0863	53.2	HMDB00883	L-Valine	2

333.2083	30.1	HMDB02358	Carnosic acid	2
160.1332	31.6	HMDB14375	Pregabalin	2
409.1816	31.3	HMDB14385	Alclometasone	2
241.1547	42.7	HMDB15407	Pirbuterol	2
321.1307	32.4	HMDB33555	Isomugineic acid	2
116.0707	64.5	HMDB34208	Pterolactam	2
178.0241	51.5	HMDB34666	()-2-Hydroxy-2-phenylacetonitrile	2
140.0533	32.2	HMDB37285	24-Dimethyl-5-vinylthiazole	2
307.081	221.9	HMDB38361	(-)-Epigallocatechin	2
266.1222	83.9	HMDB00235	Thiamine	2
661.3406	267.5	HMDB02318	Capsianoside I	2
111.0441	288.8	HMDB02434	Hydroquinone	2
309.1825	49.1	HMDB02720	Gestrinone	2
829.2778	270.9	HMDB03255	Amylopectin	2
611.2025	262.7	HMDB03265	Hesperidin	2
262.1415	276.2	HMDB04987	Alpha-Aspartyl-lysine	2
225.1242	58	HMDB14386	Butalbital	2
532.188	201.2	HMDB14396	Terconazole	2
103.0508	75.4	HMDB14405	Cycloserine	2
381.1289	36.5	HMDB14414	Chlorotrianisene	2
259.023	82.5	HMDB14456	Ethoxzolamide	2
386.2547	26.3	HMDB14633	Buspirone	2
314.1034	271.3	HMDB14683	Amoxapine	2
217.0507	203.3	HMDB14693	Methoxsalen	2
924.4975	40.7	HMDB14819	Amphotericin B	2
254.0273	95.4	HMDB14835	Tizanidine	2
353.2004	43.1	HMDB14909	Clidinium	2
137.1073	26.2	HMDB14918	Phenelzine	2
301.1797	199.2	HMDB15031	Testolactone	2
164.9683	97.5	HMDB15162	Methoxyflurane	2
199.0715	226.4	HMDB15188	Mimosine	2
337.2123	44.3	HMDB15324	Acebutolol	2
161.0816	177.9	HMDB15400	Hydralazine	2
311.0832	69.3	HMDB15413	Sulfadoxine	2
603.4842	258.4	HMDB15431	Pipecuronium	2
279.0927	274.3	HMDB15522	Sulfamethazine	2
209.1033	214.9	HMDB29968	Ethyl beta-D-glucopyranoside	2
115.076	284.1	HMDB31501	3-Hexenoic acid	2
139.1117	273	HMDB31685	24-Nonadienal	2

159.0805	184.4	HMDB32861	2-Methoxynaphthalene	2
97.0284	267.3	HMDB32914	2-Furancarboxaldehyde	2
125.0597	272.1	HMDB32917	1-(2-Furanyl)-2-propanone	2
210.0308	243.4	HMDB32936	4-Chloro-1H-indole-3-acetic acid	2
113.0228	69.7	HMDB32994	3-Hydroxy-2H-pyran-2-one	2
625.1609	246.6	HMDB33005	4-Methyl-6-(34-dihydroxy-E-cinnamoyl)isoorientin	2
323.1447	98.3	HMDB33105	N2-Galacturonyl-L-lysine	2
122.0595	143.3	HMDB33131	3-Acetylpyridine	2
315.1045	95.2	HMDB33137	2-Methoxycarbonylphenyl beta-D-glucopyranoside	2
127.0331	54.7	HMDB33152	2-(Methylthio)pyrazine	2
636.3175	35.7	HMDB33242	Glycylserylprolylmethionylphenylalanylvalinamide	2
129.0548	233.3	HMDB33285	L-erythro-5-(1-Hydroxyethyl)-2(5H)-furanone	2
382.1289	79.7	HMDB33522	Oxopurpureine	2
163.0753	25.5	HMDB33591	Safrole	2
209.1174	193.5	HMDB33778	Elemicin	2
152.0706	281.9	HMDB33903	3alpha477alpha-Tetrahydro-1H-isoindole-13(2H)-dione	2
427.1593	86.4	HMDB34032	6-(2-Carboxyethyl)-7-hydroxy-22-dimethyl-4-chromanone glucoside	2
118.0652	220.1	HMDB34171	Benzeneacetonitrile	2
116.107	249.2	HMDB34203	N-(2-Methylpropyl)acetamide	2
194.0811	111	HMDB34250	Betamipron	2
411.1642	75.3	HMDB34588	Butyl 3-O-caffeoylquinate	2
221.0445	67.5	HMDB35086	Buntansin A	2
939.2093	223.7	HMDB35163	Chestanin	2
309.1433	84	HMDB35173	2-Carboxy-1-5-(2-carboxy-1-pyrrolidinyl)-2-hydroxy-24-pentadienylidenepyrrolidinium	2
183.0917	172.5	HMDB35196	Harman	2
291.2681	22.7	HMDB35276	8alpha-13(16)14-Labdadien-8-ol	2
869.4131	53	HMDB35296	Fevicordin B 2-gentiobioside	2
178.1078	164.3	HMDB35360	N-Methyl-1-deoxynojirimycin	2
353.3427	281.9	HMDB35564	68-Tricosanedione	2
333.2787	182.4	HMDB35677	3-Hydroxy-1-phenyl-1-hexadecanone	2
219.098	128	HMDB36301	N-gamma-L-Glutamyl-D-alanine	2
595.149	144.2	HMDB36303	Epicatechin-(4beta-8)-gallocatechin	2
972.5049	47.1	HMDB36613	Rose bengal	2
144.0841	196.6	HMDB37176	2-Ethyl-25-dihydro-45-dimethylthiazole	2
215.1641	173.3	HMDB37398	4-Acetoxy-2-hexyltetrahydrofuran	2
716.4469	30.3	HMDB37546	2234456-Heptabromodiphenyl ether	2
404.1215	154.7	HMDB37550	24-Dihydroxy-78-dimethoxy-2H-14-benzoxazin-3(4H)-one 2-glucoside	2
259.1692	179.5	HMDB37645	Falcarinolone	2
188.1282	39.9	HMDB37790	Polyethylene glycol	2

233.067	211.6	HMDB37808	Hexahydro-24-dimethylspiro13-dithiolo45-cfuran-23(2H)-furan	2
522.5983	48.9	HMDB37822	Tridodecylamine	2
112.0757	212.1	HMDB37837	2-Ethyl-4-methyloxazole	2
163.0795	57.2	HMDB38084	Ethyl 3-(methylthio)butanoate	2
510.1848	32.5	HMDB38329	Dide-O-methyl-4-O-alpha-D-glucopyranosylsimmondsin	2
260.124	53.1	HMDB38516	Linatine	2
330.0947	207.5	HMDB38575	(Z)-N-Feruloyl-5-hydroxyanthranilic acid	2
408.1429	83.2	HMDB38674	gamma-L-Glutamyl-gamma-L-glutamyl-L-methionine	2
231.0989	63.6	HMDB39110	(2S3S)-alpha-Amino-2-carboxy-5-oxo-1-pyrrolidinebutanoic acid	2
134.0812	55.6	HMDB39499	14-Dideoxy-14-imino-D-ribitol	2
761.1329	241.6	HMDB39717	Samarangenin A	2
342.0517	73	HMDB39757	7-Chloro-6-demethylcepharadione B	2
739.1856	246.1	HMDB39862	3-O-beta-D-Galactopyranosylproanthocyanidin A5	2
264.0993	259.4	HMDB39873	2-Naphthalenol 2-aminobenzoate	2
128.107	278.1	HMDB40030	1-(1-Pyrrolidinyl)-2-propanone	2
151.0615	231	HMDB40056	xi-1-(Propylthio)-1-propanethiol	2
91.0583	54.5	HMDB40576	2-(Methylthio)propane	2
693.3717	47.6	HMDB40773	Bismahanine	2
253.1296	54.7	HMDB40822	23-Butanediol glucoside	2
289.122	83.9	HMDB40915	2-(4-Methyl-13-pentadienyl)anthraquinone	2
853.463	101.3	HMDB41028	Hovenidulcioside A1	2
399.1819	52.3	HMDB41101	Kanzonol M	2
755.1986	251.7	HMDB41357	Kaempferol 3-6-(3-hydroxy-3-methylglutaryl)glucoside-7-glucoside	2
139.0583	207.7	HMDB41361	2-Ethylbenzenethiol	2
321.1111	85.3	HMDB41463	23-Dihydro-23-dihydroxy-4-(4-methoxyphenyl)-1H-phenalen-1-one	2
147.1209	38.6	HMDB41477	2-Ethyl-1-hexanethiol	2
671.1232	148.4	HMDB41851	Cefpimizole	2
201.1597	35.6	HMDB41901	Hexamethylene bisacetamide	2
400.145	179.8	HMDB41970	Oxmetidine	2
343.1236	103.7	HMDB00048	Melibiose	3
339.3261	22.7	HMDB02068	Erucic acid	3
333.1427	45.2	HMDB14698	Zanamivir	3
543.047	260.7	HMDB15423	Cefonicid	3
324.3261	22.4	HMDB34373	N-(14-Methylhexadecanoyl)pyrrolidine	3
642.6867	51.9	HMDB37516	Pentabromodiphenyl ethers	3
294.1553	53.3	HMDB37840	N-(1-Deoxy-1-fructosyl)leucine	3
280.139	60	HMDB37844	N-(1-Deoxy-1-fructosyl)valine	3
220.0817	98.5	HMDB38441	1-Isothiocyanato-7-(methylsulfinyl)heptane	3
355.0587	220.9	HMDB38591	Brassicanal A	3

631.3279	260.1	HMDB39061	(R)-6-O-(4-Geranyloxy-2-hydroxycinnamoyl)-marmin	3
154.0497	228.1	HMDB01972	3-Aminosalicylic acid	3
162.0561	33.8	HMDB03320	Indole-3-carboxylic acid	3
306.1112	104.4	HMDB12226	Entacapone	3
335.1351	178.5	HMDB14450	Mitomycin	3
436.0575	261.7	HMDB14499	Aztreonam	3
325.1885	47.8	HMDB14611	Quinine	3
274.0919	265.9	HMDB14883	Modafinil	3
417.2616	69.3	HMDB14940	Alfentanil	3
310.2739	186.3	HMDB14942	Dicyclomine	3
195.0876	31.8	HMDB14962	Enprofylline	3
138.0662	235.1	HMDB15086	Isoniazid	3
390.1098	261.5	HMDB15281	Cefprozil	3
628.3252	271.8	HMDB15641	Dabigatran etexilate	3
528.1614	133.5	HMDB15653	Lumefantrine	3
328.0115	197.9	HMDB15684	Diloxanide	3
376.1106	168.1	HMDB15685	Azidocillin	3
101.0606	284	HMDB31178	Dihydro-2-methyl-3(2H)-furanone	3
191.1066	229.1	HMDB32064	(S)-3-Butyl-1(3H)-isobenzofuranone	3
181.1222	273.5	HMDB32468	2-Phenylpropionaldehyde dimethyl acetal	3
889.4572	44.9	HMDB32711	Pectenotoxin 7	3
163.0256	200.5	HMDB32750	S-2-Propenyl 1-propenesulfinothioate	3
142.1226	257.9	HMDB33364	Conhydrinone	3
431.1008	202.4	HMDB33587	Coumestrin	3
127.0754	170.9	HMDB33629	xi-4-Hydroxy-4-methyl-2-cyclohexen-1-one	3
281.08	77.9	HMDB33743	Neodunol	3
123.0799	232.2	HMDB33944	2-Phenylethanol	3
537.0974	259.2	HMDB34035	Sagecoumarin	3
505.0951	263.5	HMDB34271	Hypericin	3
173.0564	62.7	HMDB34322	L-alpha-Amino-5-oxo-2(5H)-isoxazolepropanoic acid	3
241.2161	33.1	HMDB34455	Exaltolide	3
453.1393	256.4	HMDB34753	7-Hydroxybutylidenephthalide 7-(6-malonylglucoside)	3
140.107	184.3	HMDB34884	1234-Tetrahydro-6-propanoylpyridine	3
179.962	105	HMDB34895	3-(Dichloromethylene)-25-pyrrolidinedione	3
435.1989	83.3	HMDB34899	11-Ethylidenebistryptophan	3
335.1251	278.9	HMDB34937	Cappariloside A	3
433.3673	22.3	HMDB35194	beta-Tocopheryl quinone	3
571.3585	30.7	HMDB35292	Ganodermic acid P2	3
531.2964	259.1	HMDB35325	Ganoderic acid N	3

452.2756	31.8	HMDB35366	Cytochalasin Opho	3
311.2943	23.6	HMDB35572	68-Icosanedione	3
110.06	283.3	HMDB35882	2-Acetylpyrrole	3
141.091	277.4	HMDB37167	3-Ethyl-5-methyl-12-cyclopentanedione	3
771.2348	145.1	HMDB37748	Isorhamnetin 3-rutinoside 4-rhamnoside	3
457.1117	146.1	HMDB37945	Epicatechin 3-O-(3-O-methylgallate)	3
860.2252	278.5	HMDB37981	Cyanidin 3-(malonylsophoroside) 5-glucoside	3
693.6009	63.4	HMDB38059	Glycerol 1-(9Z-octadecenoate) 2-octanoate 3-tetradecanoate	3
427.361	22.4	HMDB38063	Stigmast-4-ene-36-dione	3
717.2828	278	HMDB38229	Bn-NCC-1	3
347.076	106.9	HMDB38466	5678-Tetrahydroxy-34-dimethoxyflavone	3
259.1284	102	HMDB38614	gamma-L-Glutamyl-L-pipecolic acid	3
194.0315	240.2	HMDB38669	S-(Allylthio)-L-cysteine	3
897.3812	24.4	HMDB38673	Lyciumin B	3
295.1139	116.4	HMDB38752	Distichonic acid A	3
631.2006	263.4	HMDB39041	(R)-Rutaretin 1-(6-sinapoylglucoside)	3
293.1177	96.5	HMDB39096	N-gamma-Glutamyl-S-propylcysteine	3
107.9937	202.3	HMDB39221	Methylcarbamodithioic acid K salt	3
539.1144	37.6	HMDB39523	Isomelitric acid A	3
674.2711	271.7	HMDB39640	Ustiloxin A	3
594.0855	230	HMDB39936	Cyanidin 3-(6-dioxalylglucoside)	3
203.0547	66.4	HMDB40275	Ethyl aconitate	3
831.3218	278.7	HMDB40282	6-HMG SDG	3
393.1597	93.6	HMDB40776	11-Bis(2-hydroxy-3-methylcarbazole)	3
456.1883	37.9	HMDB40825	Tryptophol xylosyl-(1-6)-glucoside	3
873.4864	38.9	HMDB40959	Capsicoside C2	3
111.1169	24	HMDB40966	13-Octadiene	3
436.2457	259.2	HMDB40979	14alpha-Hydroxy-4beta-deoxypaxilline	3
537.3018	48.9	HMDB41137	Corchorosol A	3
435.1776	74.7	HMDB41166	Cycloartocarpin	3
743.2048	257.6	HMDB41412	Quercetin 3-(2Gal-apiosylrobinobioside)	3
633.2534	28.6	HMDB41423	Mulberrofuran E	3
207.1499	23.4	HMDB41445	Agrocybenine	3
176.0658	40.8	HMDB00172	L-Isoleucine	4
413.3776	23.8	HMDB00937	Stigmasterol	4
423.166	45.9	HMDB14816	Losartan	4
454.2927	25.6	HMDB41085	Sambutoxin	4
429.3736	23	HMDB41112	(3alpha5alpha7alpha)-14-Methylergosta-9(11)24(28)-dien-37-diol	4
151.0227	73.8	HMDB00956	Tartaric acid	4

137.0593	189.7	HMDB02340	2-Methylbenzoic acid	4
581.187	247.9	HMDB02927	Naringin	4
303.1591	90.1	HMDB14325	Masoprocol	4
411.1976	58.2	HMDB14368	Diflorasone	4
310.2162	188.5	HMDB14477	Methadone	4
390.2143	55.8	HMDB14490	Alfuzosin	4
210.1363	23	HMDB14494	Minoxidil	4
169.9989	93	HMDB14500	Chlorzoxazone	4
290.1725	35.7	HMDB14568	Hyoscyamine	4
657.1687	136.7	HMDB14587	Teniposide	4
453.2095	46.2	HMDB14729	Fluocinolone Acetonide	4
415.2114	22.9	HMDB14838	Eplerenone	4
241.1434	181.1	HMDB14862	Imiquimod	4
358.202	53.6	HMDB14982	Nalbuphine	4
335.109	43.7	HMDB15186	Penicillin G	4
366.1099	94.4	HMDB15193	Amoxicillin	4
399.3614	22.9	HMDB15203	Dihydrotachysterol	4
179.082	183.8	HMDB15253	Phenacemide	4
405.1297	30.6	HMDB15269	Sulfinpyrazone	4
280.1713	35.5	HMDB15273	Doxepin	4
877.4532	271.6	HMDB15332	Rifapentine	4
171.1128	59.3	HMDB15333	Levetiracetam	4
311.2005	191	HMDB15446	Mestranol	4
400.1751	43.7	HMDB15466	Colchicine	4
325.1126	244	HMDB15527	Prazepam	4
283.069	115	HMDB15573	Niflumic Acid	4
507.2894	51.5	HMDB15593	Ixabepilone	4
391.0901	37.8	HMDB15604	Permethrin	4
259.0391	85.4	HMDB15606	Lofexidine	4
383.2195	45.1	HMDB29488	Farnesiferol A	4
133.0496	249.3	HMDB29884	2-C-Methyl-14-erythrono-D-lactone	4
271.104	117	HMDB29955	D-erythro-L-galacto-Nonulose	4
223.0966	39.1	HMDB30725	Dillapiol	4
129.0911	171.5	HMDB31174	4-Methyl-5-hexanolide	4
129.1274	24.6	HMDB31296	(E)-2-Octen-1-ol	4
335.0062	260.4	HMDB32721	2-Methyl-14-naphthalenediol bis(dihydrogen phosphate)	4
260.1133	96.9	HMDB32769	Osmaronin	4
406.1457	91.1	HMDB32809	4-Hydroxyphenylacetonitrile triacetylrhamnoside	4
130.9993	216	HMDB32939	3-(Methylthio)thiophene	4

305.1102	90.5	HMDB32943	Diazinon	4
237.0419	97.3	HMDB33062	2-Propenyl 1-(2-propenylsulfinyl)propyl disulfide	4
331.2267	185.1	HMDB33126	10-Dehydroshogaol	4
430.0408	285.3	HMDB33147	Cloransulam-methyl	4
575.1458	241	HMDB33185	Anigorootin	4
179.0712	212.3	HMDB33248	Di-alpha-furfuryl ether	4
429.1918	60.1	HMDB33332	Garcinone D	4
165.0697	27.5	HMDB33518	S-(2-Aminoethyl)-L-cysteine	4
141.1274	175.3	HMDB33554	2-Methyl-2-octenal	4
207.1022	185.9	HMDB33594	Cuelure	4
434.1211	265.6	HMDB33682	Pelargonidin 3-galactoside	4
169.1231	253.6	HMDB33700	(-)-(Z)-Tetrahydro-6-(2-pentenyl)-2H-pyran-2-one	4
182.045	132.6	HMDB33733	24-Dihydroxy-2H-14-benzoxazin-3(4H)-one	4
268.1296	38.9	HMDB33758	L-Agaritine	4
119.0524	185.6	HMDB33856	S-Propyl thioacetate	4
121.0648	271.5	HMDB33910	Acetophenone	4
137.0961	271.9	HMDB33962	3-Phenyl-1-propanol	4
433.1145	59.6	HMDB33982	Isogenistein 7-glucoside	4
229.0107	246.5	HMDB34228	Thiolutin	4
425.1409	73.6	HMDB34231	Apterin	4
175.1078	63.5	HMDB34365	L-Theanine	4
546.3065	56	HMDB34441	Americine	4
399.2	64.8	HMDB34575	3-Hydroxy-T2-triol	4
403.0667	82.6	HMDB34589	Shoyuflavone B	4
295.0593	69.6	HMDB34765	Wasalexin A	4
194.1175	17.8	HMDB35072	2-Methylpropyl 2-aminobenzoate	4
367.1787	28.1	HMDB35104	Diacetoxyscirpenol	4
455.3516	31.1	HMDB35247	Isomasticadienonic acid	4
425.3777	22.4	HMDB35265	Anhydrosophoradiol	4
379.2841	199.7	HMDB35273	1-Acetoxy-2-hydroxy-51215-heneicosatrien-4-one	4
251.2004	177.2	HMDB35293	Norambreinolide	4
441.3729	23	HMDB35314	Ganoderol B	4
219.1743	179.6	HMDB35835	Furanoeremophilane	4
211.0818	189.1	HMDB36431	139-Trimethyluric acid	4
439.2072	120.1	HMDB36597	1-Hydroxy-367-trimethoxy-28-diprenylxanthone	4
397.1836	63.6	HMDB36608	Pteroside P	4
614.1223	155.9	HMDB36939	Glucosinalbin 4-(4-acetylrhamnoside)	4
221.1184	178.7	HMDB37492	Ethyl methyl-p-tolylglycidate	4
219.1059	56.4	HMDB37764	S-1-2-(Acetyloxy)ethylbutyl ethanethioate	4

99.0917	41.2	HMDB37787	xi-45-Dihydro-24(5)-dimethyl-1H-imidazole	4
643.1498	119.6	HMDB37850	Myricetin 33-digalactoside	4
431.352	22	HMDB37914	(2beta3alpha9alpha24R)-Ergosta-722-diene-239-triol	4
788.2104	242.6	HMDB37987	Cyanidin 3-(6-ferulylglucoside) 5-glucoside	4
628.1609	256.7	HMDB38006	Delphinidin 3-gentiobioside	4
195.1743	22.9	HMDB38026	Dihydro-alpha-ionone	4
463.1977	102.1	HMDB38159	Retrocalamin	4
514.1818	25.9	HMDB38599	Acrimarine H	4
551.2139	105.7	HMDB38718	Scorzonoside	4
330.1712	64.4	HMDB38724	xi-Anomuricine	4
103.0575	286	HMDB38892	1-(Methylthio)-1-butene	4
327.1173	78.7	HMDB39123	Humilixanthin	4
173.101	194.7	HMDB39467	Allyl thiohexanoate	4
463.378	264.7	HMDB39713	(3beta22R23R24S)-32223-Trihydroxystigmastan-6-one	4
160.1154	186.3	HMDB40057	()-2-Pentylthiazolidine	4
223.9721	37.1	HMDB40147	2-Bromo-1H-indole-3-carboxaldehyde	4
302.1001	37.5	HMDB40515	gamma-Glutamyl-beta-(isoxazolin-5-on-2-yl)alanine	4
385.0752	34.6	HMDB40571	2-O-Feruloylhydroxycitric acid	4
505.3479	28.8	HMDB40772	Isothankunic acid	4
421.1197	122.1	HMDB40774	Bismurrayaquinone A	4
421.1569	180.6	HMDB40789	Bikoeniquinone A	4
341.185	50.9	HMDB40799	11-Hydroxytubotaiwine	4
621.3637	62.1	HMDB41049	Physagulin D	4
857.2694	274.3	HMDB41211	Sesaminol glucosyl-(1-2)-glucosyl-(1-6)-glucoside	4
486.2849	29.3	HMDB41421	Sarcodon scabrosus Depsipeptide	4
260.0877	92.4	HMDB41934	Mizoribine	4
178.0975	113.7	HMDB41940	N-nitrosonornicotine	4
166.0848	45.6	HMDB00159	L-Phenylalanine	5
120.0656	60.6	HMDB00167	L-Threonine	5
156.0768	72.5	HMDB00177	L-Histidine	5
205.0972	37.1	HMDB00929	L-Tryptophan	5
183.5382	206.7	HMDB14665	Metolazone	5
557.1414	231.6	HMDB33488	Aurasperone D	5
465.0441	212.4	HMDB35145	Chrycolide	5
265.2524	26.5	HMDB37543	()-(Z)-2-(5-Tetradecenyl)cyclobutanone	5
145.1223	24.5	HMDB01877	Valproic acid	5
168.1019	181	HMDB02182	Phenylephrine	5
271.263	158.8	HMDB02259	Heptadecanoic acid	5
223.0746	156.1	HMDB03075	Flavone	5

459.0876	51.9	HMDB03153	Epigallocatechin gallate	5
89.0597	25.8	HMDB03243	Acetoin	5
106.0863	37.4	HMDB04437	Diethanolamine	5
359.9624	42.8	HMDB14377	Methyclothiazide	5
213.1233	139	HMDB14382	Butabarbital	5
286.0717	257.2	HMDB14387	Cladribine	5
112.0877	56.5	HMDB14417	Betazole	5
339.0202	58.6	HMDB14455	Chlorthalidone	5
144.0655	234.1	HMDB14491	Trimethadione	5
560.1378	232.7	HMDB14735	Gadoteridol	5
225.0879	122.7	HMDB14787	Stavudine	5
405.2346	54.9	HMDB14905	Benzquinamide	5
385.2401	33.7	HMDB14961	Ethynodiol Diacetate	5
150.0584	48.5	HMDB14997	Penicillamine	5
489.2238	64.2	HMDB15000	Vardenafil	5
804.4961	48.4	HMDB15002	Tacrolimus	5
313.2031	24.9	HMDB15026	Granisetron	5
485.1206	226.1	HMDB15289	Bretylium	5
269.1056	47	HMDB15302	Moclobemide	5
417.1307	34.6	HMDB15318	Iophendylate	5
218.085	219.6	HMDB15328	Captopril	5
310.201	22.7	HMDB15334	Nadolol	5
298.1143	49.9	HMDB15401	Nelarabine	5
466.1606	45	HMDB15540	Bacampicillin	5
405.21	69	HMDB15589	Flunarizine	5
199.1692	23.8	HMDB31683	xi-Dihydro-5-octyl-2(3H)-furanone	5
137.0088	127.8	HMDB32744	S-Methyl 2-propene-1-sulfinothioate	5
164.092	61.9	HMDB32862	2-Amino-4-ethoxy-3-hydroxybutanoic acid	5
155.0535	216	HMDB32935	1-(2-Thienyl)-1-butanone	5
98.0601	202.5	HMDB32968	24-Dimethyloxazole	5
315.2178	24.6	HMDB32995	2-Undecyl-4(1H)-quinolinone N-oxide	5
266.0801	107.1	HMDB33060	Piperolactam A	5
385.1689	44.3	HMDB33063	23-Butanediol apiosylglucoside	5
249.1333	30.8	HMDB33064	(E)-2-Methyl-2-buten-1-ol O-beta-D-Glucopyranoside	5
135.0921	38.2	HMDB33154	5678-Tetrahydroquinoxaline	5
167.143	23.9	HMDB33546	25-Undecadienal	5
181.0362	53	HMDB33556	25-Dimethyl-14-dithiane-25-diol	5
101.0421	67.4	HMDB33564	23-Dihydro-2-methylthiophene	5
169.1587	184.7	HMDB33577	10-Undecen-2-one	5

435.1311	87.7	HMDB33739	Floribundoside	5
213.0746	70.8	HMDB33835	Propyl gallate	5
88.0757	259.8	HMDB33870	Butyramide	5
101.071	69.4	HMDB33952	Gyromitrin	5
118.1227	205.5	HMDB33971	2-Diethylaminoethanol	5
399.1446	96.9	HMDB34030	Dulxanthone E	5
405.1584	94.4	HMDB34117	(E)-4-Methylresveratrol 3-glucoside	5
176.092	283.8	HMDB34252	2-Aminoheptanedioic acid	5
277.1296	30.7	HMDB34263	Triethyl citrate	5
237.1483	27.8	HMDB34462	Heptyl 4-hydroxybenzoate	5
647.2347	26	HMDB34634	3-Prenylapigenin 7-rhamnosyl-(1-6)-glucoside	5
126.0912	174.7	HMDB34883	34-Dihydro-5-propanoyl-2H-pyrrole	5
458.1683	49.6	HMDB35030	Amygdalin	5
475.378	22	HMDB35326	Ganoderiol A	5
552.207	74.9	HMDB35475	Simmondsin 2-ferulate	5
367.3568	22.4	HMDB35559	1012-Tetracosanedione	5
325.31	190.9	HMDB35570	68-Heneicosanedione	5
387.2755	23.1	HMDB36015	Mangalkanyl glucoside	5
201.1493	30.7	HMDB36029	Clarycet	5
210.1851	28.9	HMDB36031	Labienoxime	5
347.1841	267	HMDB36474	Verimol G	5
190.1075	195.3	HMDB36604	N-Methylcalystegine B2	5
281.1761	122.1	HMDB36979	6b-Hydroxy-8a-methoxy-7(11)-eremophilen-128-olide	5
172.1154	219.4	HMDB37159	25-Dihydro-45-dimethyl-2-(2-methylpropyl)thiazole	5
671.1863	253	HMDB37469	Spinacetin 3-gentiobioside	5
547.0573	37.6	HMDB37522	Orange B	5
475.2696	62.1	HMDB37610	Lucidenic acid B	5
147.0847	71	HMDB37621	4-Methyl-4-(methylthio)-2-pentanone	5
491.3733	22.3	HMDB37783	Ganoderiol H	5
212.2009	23.4	HMDB37834	Ethyl menthane carboxamide	5
800.168	258	HMDB37999	Delphinidin 35-di(6-O-malonylglucoside)	5
640.1789	268.7	HMDB38012	Malvidin 3-(6-coumaroylglucoside)	5
292.0986	256.4	HMDB38956	Avenalumin III	5
419.3155	185.2	HMDB39317	Hexadecyl ferulate	5
395.1563	61.1	HMDB39952	1-(3-Methyl-2-butenoyl)-6-apiosylglucose	5
99.0441	253.4	HMDB40145	5-Hydroxy-4-pentenoic acid d-lactone	5
147.0477	29	HMDB40237	Dihydro-2-methoxy-2-methyl-3(2H)-thiophenone	5
197.1011	64.4	HMDB40241	1-(2-Thienyl)-1-heptanone	5
257.1384	186.4	HMDB40352	2-4-(3-Hydroxypropyl)-2-methoxyphenoxy-13-propanediol	5

197.1284	48.2	HMDB40551	L-alpha-Amino-1H-pyrrole-1-hexanoic acid	5
229.1183	49.9	HMDB40573	Tetraacetylethylenediamine	5
441.2992	41.1	HMDB40748	2-Acetoxy-3-geranylgeranyl-14-dihydroxybenzene	5
366.2043	39.9	HMDB40775	Aegle marmelos Alkaloid C	5
447.3459	26.5	HMDB40999	Secasterone	5
545.3429	28.7	HMDB41027	Hovenidulcigenin A	5
459.181	47.2	HMDB41045	Valechlorin	5
282.0294	217.4	HMDB41052	Ajocysteine	5
465.3581	19.5	HMDB41135	2-Deoxybrassinolide	5
197.19	182.3	HMDB41404	2-Methylcyclododecanone	5
264.8525	52.4	HMDB41974	Pentachlorophenol	5
279.2317	23.9	HMDB01388	Alpha-Linolenic acid	6
151.1117	24.5	HMDB01878	Thymol	6
135.1168	23.7	HMDB03450	(-)-trans-Carveol	6
193.1586	24.1	HMDB37390	Tsibulin 1	6
263.2368	25.6	HMDB37519	2-(58-Tetradecadienyl)cyclobutanone	6
316.0791	85.7	HMDB38576	Avenanthramide C	6
167.0703	51.7	HMDB00375	3-(3-Hydroxyphenyl)propanoic acid	6
207.1378	28.2	HMDB01925	Ibuprofen	6
306.2064	187.8	HMDB02227	Capsaicin	6
237.1848	37.5	HMDB02352	Capsidiol	6
305.2109	184.4	HMDB03956	7a-Hydroxytestosterone	6
137.1325	23.9	HMDB04321	()-Limonene	6
313.2162	230.2	HMDB04626	Tetrahydrogestrinone	6
199.0947	28.3	HMDB04998	Guaifenesin	6
165.091	24.3	HMDB05802	Isoeugenol	6
135.1168	247.5	HMDB05805	p-Cymene	6
245.1125	63.8	HMDB14336	Carbidopa	6
352.1307	71.8	HMDB14686	Adinazolam	6
376.1424	94.2	HMDB15042	Tiagabine	6
146.0811	255.1	HMDB15127	Methyl aminolevulinate	6
162.1357	193.2	HMDB15154	Bethanechol	6
184.1332	186.9	HMDB15239	Methyprylon	6
489.2528	51.1	HMDB15262	Prednicarbate	6
251.1632	36.1	HMDB15371	Gemfibrozil	6
243.0976	56.1	HMDB15394	Telbivudine	6
403.2097	46.3	HMDB15459	Cortisone acetate	6
266.1749	185	HMDB15520	Oxprenolol	6
184.0968	174.9	HMDB15652	Levonordefrin	6

224.1644	178.1	HMDB29875	Tigloidine	6
197.1535	33.1	HMDB31030	6-Heptyl-56-dihydro-2H-pyran-2-one	6
164.0564	290.4	HMDB31187	Thialdine	6
113.0962	176.2	HMDB31487	(E)-4-Hepten-2-one	6
181.0863	200	HMDB32174	Benzaldehyde glyceryl acetal	6
167.1178	25.6	HMDB32933	2-Methoxy-3-(1-methylpropyl)pyrazine	6
141.0705	201.4	HMDB32948	5-Phenyl-13-pentadiyne	6
206.0457	105.4	HMDB32963	Zeanic acid	6
186.0583	67.3	HMDB32986	5-(2-Hydroxyethyl)-4-methylthiazole acetate	6
191.0696	215.3	HMDB32991	7-Methoxy-6-methyl-2H-1-benzopyran-2-one	6
203.0903	113	HMDB33092	3-(1-Hydroxymethyl-1-propenyl)pentanedioic acid	6
125.0961	26.4	HMDB33238	2-Isopropyl-5-methylfuran	6
309.2057	23.7	HMDB33243	Corchorifatty acid D	6
193.1222	27.8	HMDB33380	3-Methylbutyl benzoate	6
555.1245	250.5	HMDB33390	CI Acid Green 50	6
295.1657	44	HMDB33464	Sinapoylputrescine	6
261.1582	30.2	HMDB33481	Baptifoline	6
285.1695	175.1	HMDB33483	67-Dihydro-4-(hydroxymethyl)-2-(p-hydroxyphenethyl)-7-methyl-5H-2-pyrindinium	6
232.1696	221.3	HMDB33530	(2E4E6Z)-246-Decatrienoic acid dehydropiperidide	6
279.2681	22.4	HMDB33609	2-Pentadecylfuran	6
332.1327	56.2	HMDB33665	N-Hydroxyneosaxitoxin	6
135.0805	23.3	HMDB33716	3-Phenylpropanal	6
130.0651	213.8	HMDB33731	Quinoline	6
177.091	225.7	HMDB33834	Ethyl cinnamate	6
367.121	97.1	HMDB33882	Glycyrol	6
175.1317	181.5	HMDB34040	246-Triethyl-135-trioxane	6
239.2368	176.8	HMDB34181	3-Methylcyclopentadecanone	6
105.0699	23.3	HMDB34240	Styrene	6
173.0804	287.4	HMDB34851	Ethyl 24-dioxohexanoate	6
135.0843	56.6	HMDB34878	3-Mercapto-2-methylpentanol	6
149.1069	68.3	HMDB34892	3-Ethyl-5-methyl-2-vinylpyrazine	6
165.1018	33	HMDB34900	2-(12-Diamino-1-propenyl)phenol	6
179.143	24.7	HMDB35055	11-Methyl-7-oxatetracyclo6310160411dodecane	6
420.1073	246.6	HMDB35174	3-1-Formyl-2-(2-furanyl)ethenyl-2-(2-furanyl)-5-(2-furanylmethylene)-45-dihydro-a-methyl-4-oxo-1H-pyrrole-1-acetic acid 9CI	6
177.1263	40.8	HMDB36021	Rhubafuran	6
124.0758	193.2	HMDB36058	1-Ethyl-1H-pyrrole-2-carboxaldehyde	6
183.1379	25.1	HMDB36191	4-Hydroxy-4-methyl-7-decenoic acid gamma-lactone	6
173.1173	25.1	HMDB36213	cis-3-Hexenyl lactate	6
249.1847	24.3	HMDB36221	2-(Dimethoxymethyl)-1-heptenylbenzene	6

189.1122	165.2	HMDB36233	Butyl ethyl malonate	6
159.0652	283.6	HMDB36380	xi-23-Dihydro-35-dihydroxy-6-methyl-4H-pyran-4-one	6
159.1002	185.1	HMDB36395	2-Methylpropyl 3-oxobutanoate	6
367.2111	25.1	HMDB37062	Sporotrichiol	6
142.0682	71	HMDB37140	2-(1-Methylpropyl)thiazole	6
267.2681	26	HMDB37517	2-Tetradecylcyclobutanone	6
763.15	138.3	HMDB37648	3-Galloylprodelphinidin B2	6
219.1382	251.8	HMDB37704	Isoamyl cinnamate	6
291.2317	186.7	HMDB37711	4-Methylphenyl dodecanoate	6
221.1525	30.2	HMDB37714	Hexyl phenylacetate	6
169.0859	276.7	HMDB37729	2-Furanylmethyl butanoate	6
125.1325	175.2	HMDB37777	2-Isopropyl-14-hexadiene	6
85.0649	75.1	HMDB37788	xi-23-Dihydro-3-methylfuran	6
168.1383	183.8	HMDB37864	4-Ethyl-5-pentyloxazole	6
253.1797	179.1	HMDB37969	Urodiolenone	6
293.2109	252.5	HMDB38035	Panaquinquecol 1	6
217.1584	202.5	HMDB38147	Isogermafurene	6
269.1747	191.8	HMDB38153	1-(3-Furanyl)-67-dihydroxy-48-dimethyl-1-nonanone	6
140.0707	288.9	HMDB38174	5-Acetyl-24-dimethyloxazole	6
171.101	278.4	HMDB38276	cis-3-Hexenyl pyruvate	6
204.0867	248.8	HMDB38440	1-Isothiocyanato-7-(methylthio)heptane	6
460.1583	125.1	HMDB38598	Narceinone	6
176.0706	140.3	HMDB38628	Hydroxymethyl indol-3-yl ketone	6
222.0972	243.8	HMDB38751	Avenic acid B	6
124.956	274.4	HMDB39433	124-Trithiolane	6
138.0914	175.8	HMDB39657	123456-Hexahydro-7H-cyclopentabpyridin-7-one	6
150.0913	216.8	HMDB39662	2367-Tetrahydrocyclopentbazepin-8(1H)-one	6
197.9258	105.4	HMDB39853	356-Trichloro-2-pyridinol	6
162.0914	184.1	HMDB40028	1-(23-Dihydro-1H-pyrrolizin-5-yl)-2-propen-1-one	6
125.071	33.8	HMDB40141	2-Methoxy-5-methylpyrazine	6
111.0805	177	HMDB40277	2-Propylfuran	6
357.1551	273.4	HMDB40558	Zingerone glucoside	6
381.2251	26.1	HMDB40568	6-Gingerdiol 35-diacetate	6
349.2355	34.3	HMDB40641	8-Paradyl acetate	6
227.1274	24.9	HMDB40705	Allixin	6
245.0923	83.6	HMDB40734	Haematopodin	6
311.1642	22.8	HMDB40742	23-Dehydrosalvipisone	6
269.2473	281.2	HMDB40888	24-Heptadecanedione	6
257.211	177.9	HMDB40904	Ipomeatetrahydrofuran	6

202.1438	36.8	HMDB41540	N-(5-Methyl-3-oxohexyl)alanine	6
262.0854	214.9	HMDB41895	Flumequine	6
127.0727	249.9	HMDB41922	Melamine	6
115.5516	64.7	HMDB03045	Ergothioneine	7
505.1758	143.8	HMDB03213	Raffinose	7
148.0605	58.5	HMDB03339	D-Glutamic acid	7
229.0875	140.4	HMDB03747	Resveratrol	7
319.2255	33.5	HMDB06027	Oxymesterone	7
134.0449	73.6	HMDB11753	Iminodiacetic acid	7
329.2118	24	HMDB14495	Megestrol	7
137.0458	40.7	HMDB14581	Allopurinol	7
255.1102	43.7	HMDB14789	Dyphylline	7
305.2474	23.8	HMDB14996	Drostanolone	7
417.3362	22.7	HMDB15046	Paricalcitol	7
372.0537	152.3	HMDB15093	Carboplatin	7
383.3307	23.7	HMDB15504	Alfacalcidol	7
267.2106	22.6	HMDB15655	Methyltestosterone	7
429.3358	22.6	HMDB15694	Nandrolone decanoate	7
335.0735	285.5	HMDB33014	Hovenitin I	7
144.0808	38.8	HMDB33115	6-Methylquinoline	7
569.3138	31.6	HMDB34101	Adouetine Y	7
86.0965	46.5	HMDB34301	Piperidine	7
200.0926	62.8	HMDB35177	2-Acetyl-1567-tetrahydro-6-hydroxy-7-(hydroxymethyl)-4H-azepine-4-one	7
205.195	23.3	HMDB35199	Sesquisabinene hydrate	7
638.403	27.4	HMDB35264	Avenestergenin A1	7
335.2214	26.5	HMDB35286	Crispanone	7
689.2114	241.3	HMDB35323	Fagopyritol B3	7
415.357	22.2	HMDB35586	1-Phenyl-13-docosanedione	7
317.2109	24	HMDB36147	Furanojaponin	7
136.0752	41.4	HMDB37071	2-Acetyl-4-methylpyridine	7
510.3132	32.8	HMDB37802	2-46-Bis(24-dimethylphenyl)-135-triazin-2-yl-5-(octyloxy)phenol	7
135.0304	54.3	HMDB38974	33-Dimethyl-12-dithiolane	7
147.0441	50.4	HMDB41592	Coumaric acid	7
550.1273	234.5	HMDB41668	4-Methyl-(-)-epigallocatechin 3-(4-methyl-gallate)	7
301.216	23	HMDB41925	Metandienone	7
220.1179	29	HMDB00210	Pantothenic acid	7
191.1027	166.6	HMDB01370	Diaminopimelic acid	7
123.0441	262.7	HMDB01870	Benzoic acid	7
138.055	249.2	HMDB01891	m-Aminobenzoic acid	7

345.2409	22.5	HMDB01939	Medroxyprogesterone	7
254.1127	72.7	HMDB01940	Triamterene	7
149.096	23.4	HMDB02214	Cuminaldehyde	7
285.1847	267.4	HMDB03422	Boldione	7
133.0648	24.4	HMDB03441	Cinnamaldehyde	7
417.2395	49.5	HMDB14324	Ramipril	7
255.1354	58.2	HMDB14356	Midodrine	7
249.0717	84.4	HMDB14395	Dapsone	7
245.1281	30.5	HMDB14437	Etomidate	7
158.1175	229.5	HMDB14447	Tranexamic Acid	7
227.1401	180.9	HMDB14457	Pentobarbital	7
433.2395	43.1	HMDB14498	Buclizine	7
298.1231	54.9	HMDB14619	Duloxetine	7
353.1276	65.7	HMDB14650	Triflupromazine	7
142.0863	257.3	HMDB14731	Ethosuximide	7
342.1718	53.3	HMDB14842	Naltrexone	7
441.2402	38.5	HMDB14913	Tirofiban	7
369.2277	33.5	HMDB14920	Propantheline	7
332.2176	26.6	HMDB14924	Marimastat	7
252.0291	79.9	HMDB14929	Uracil mustard	7
276.1747	44.7	HMDB15060	Cyclobenzaprine	7
383.2789	177.3	HMDB15064	Misoprostol	7
206.152	91.3	HMDB15072	Diethylpropion	7
582.2777	54.7	HMDB15214	Streptomycin	7
280.18	34.1	HMDB15237	Sibutramine	7
347.1236	34.8	HMDB15247	Nifedipine	7
270.185	24.3	HMDB15304	Orphenadrine	7
267.1854	171.5	HMDB15307	Cyclizine	7
232.1293	73.4	HMDB15322	Dexfenfluramine	7
277.0885	115.6	HMDB15477	Clenbuterol	7
340.0589	214.5	HMDB15484	Cefacetrile	7
301.2526	27.3	HMDB15500	Allylestrenol	7
413.3049	22.9	HMDB15567	Calcipotriol	7
277.1796	276.4	HMDB15586	Cyclandelate	7
241.0487	190.9	HMDB29752	Dantron	7
207.0662	76.5	HMDB30818	Scoparone	7
607.494	21.9	HMDB30940	Squamocin L	7
192.0867	82.5	HMDB31346	Calystegine C1	7
209.1308	28	HMDB31821	12-Diphenylcyclobutane	7

183.1014	43.6	HMDB32607	()-threo-Anethole glycol	7
238.1094	57.3	HMDB32775	3-Hydroxy-carbofuran	7
119.0492	50.1	HMDB32929	Benzofuran	7
151.1229	25.4	HMDB32946	35-Diethyl-2-methylpyrazine	7
95.0604	68.7	HMDB33112	Methylpyrazine	7
303.1952	180.4	HMDB33125	8-Dehydroshogaol	7
235.142	53.2	HMDB33461	4-Coumaroylputrescine	7
178.0866	74.7	HMDB33482	Plantagonine	7
99.0805	175.1	HMDB33549	(E)-4-Hexenal	7
187.144	29.4	HMDB33553	3-(3-Methylbutyl)nitrosoamino-2-butanone	7
243.1723	30.5	HMDB33693	Falcarinone	7
248.1123	71.8	HMDB33699	Linamarin	7
162.076	266.1	HMDB33747	()-22-Iminobispropanoic acid	7
179.0928	241.8	HMDB33789	2-O-Methyl-L-fucose	7
347.2575	24.4	HMDB33897	Ginkgoic acid	7
305.1321	83.2	HMDB33909	2-Deoxymugineic acid	7
283.0461	101.8	HMDB34034	Bikojic acid	7
333.0802	142.1	HMDB34051	6-Galloylglucose	7
167.086	240.9	HMDB34294	1311-Tridecatriene-579-triyne	7
191.112	203.5	HMDB34326	L-erythro-4-Hydroxyarginine	7
167.0571	66.5	HMDB34394	S-Propyl 1-propanesulfinothioate	7
155.0855	24.3	HMDB34437	Biphenyl	7
251.1497	56	HMDB34750	Isopentyl beta-D-glucoside	7
307.1895	193.5	HMDB34780	Capsiate	7
328.1685	70.6	HMDB35218	Cinereain	7
239.2004	277.8	HMDB35287	Daucol	7
326.8593	46.8	HMDB35290	Bis(m-methanethiolato)tetranitrosyldiiron	7
311.2213	274.7	HMDB35337	Sterebin A	7
512.2992	32.2	HMDB35368	Cytochalasin Ppho	7
331.263	181.3	HMDB35581	1-Phenyl-13-hexadecanedione	7
217.097	37.1	HMDB35665	L-1234-Tetrahydro-beta-carboline-3-carboxylic acid	7
677.2437	42.5	HMDB35961	Artonin D	7
253.1435	178.6	HMDB36047	3alpha-Hydroxyoreadone	7
233.1525	31	HMDB36110	(S)-Bilobanone	7
341.1579	52.9	HMDB36157	15-Deacetylneosolaniol	7
441.209	49	HMDB36162	3-Hydroxy-HT2 toxin	7
172.1695	24.2	HMDB36195	N23-Trimethyl-2-(1-methylethyl)butanamide	7
247.1691	188.2	HMDB36207	alpha-Amylcinnamyl acetate	7
571.2856	39.1	HMDB36360	Pipercyclobutanamide A	7

201.1638	185	HMDB36451	(S)-gamma-Calacorene	7
213.1294	45	HMDB36454	Pyrocurzerenone	7
102.055	66.2	HMDB36458	1-Aminocyclopropanecarboxylic acid	7
150.9657	270.7	HMDB36577	Trifluoromethanesulfonic acid	7
201.1121	267.5	HMDB36715	Matsutakic acid A	7
255.1452	53.3	HMDB37180	(S)-Argpyrimidine	7
435.2952	187.7	HMDB37183	Polysorbate 60	7
225.1484	274.8	HMDB37726	Octyl 2-furoate	7
253.216	281.4	HMDB37805	D6-Ambrettolide	7
369.3146	22.2	HMDB37826	(E)-2627-Dinorergosta-422-dien-3-one	7
263.2004	178.8	HMDB37832	Vetiveryl acetate	7
318.1309	90.7	HMDB37839	N-(1-Deoxy-1-fructosyl)histidine	7
238.0921	175.2	HMDB37848	N-(1-Deoxy-1-fructosyl)glycine	7
203.1793	23.3	HMDB38125	149-Cadinatriene	7
197.1325	23.2	HMDB38162	Lactarazulene	7
112.0394	176	HMDB38175	2-Acetyloxazole	7
321.2407	42.8	HMDB38520	2-Hydroxy-6-tridecylbenzoic acid	7
169.1012	23.1	HMDB38754	(EEE)-13511-Tridecatetraene-79-diyne	7
329.2478	24	HMDB38908	(ZZ)-2-Methyl-5-(81114-pentadecatrienyl)-13-benzenediol	7
569.1823	287.5	HMDB39384	Piceatannol 34-diglucoside	7
185.1161	266.9	HMDB39710	1-Acetylcyclohexyl acetate	7
341.2487	21.7	HMDB39762	11-111-Undecanediylbis(oxy)bisbenzene	7
165.1385	26.8	HMDB39979	25-Diethyl-36-dimethylpyrazine	7
163.123	34.5	HMDB39982	Trimethyl-2-propenylpyrazine	7
139.0866	38.3	HMDB40054	3-Ethyl-2-methoxypyrazine	7
235.2054	279.2	HMDB40179	26-Di-tert-butyl-4-ethylphenol	7
173.1324	22.7	HMDB40284	12-Dihydro-116-trimethylnaphthalene	7
313.1191	32.7	HMDB40435	Dictyoquinazol A	7
329.1498	55.9	HMDB40441	Dictyoquinazol B	7
271.1903	180.8	HMDB40459	Ethylene brassylate	7
303.1466	41.7	HMDB40462	Garcinia lactone dibutyl ester	7
401.122	99.3	HMDB40556	5-Hydroxyflavone	7
289.1786	216.6	HMDB40864	O-Geranylvanillin	7
395.3307	22.5	HMDB41050	(3beta22E24R)-Ergosta-468(14)22-tetraen-3-ol	7
589.4826	20.9	HMDB41092	Tripoxyrollin	7
453.1925	48.3	HMDB41323	Heteroartonin A	7
255.2106	24.2	HMDB41371	18-Nor-4(19)81113-abietatetraene	7
195.1126	42.2	HMDB41440	Laccarin	7
319.0955	67.1	HMDB41451	Musanolone F	7

254.1046	29.6	HMDB41725	Dihydroferuloylglycine	7
358.2769	23.9	HMDB04627	Calusterone	8
309.0884	214.9	HMDB14548	Alprazolam	8
325.1595	202	HMDB14716	Valaciclovir	8
310.3103	22.4	HMDB32740	N-Hexadecanoylpyrrolidine	8
149.0588	47.8	HMDB32947	Di-2-furanylmethane	8
121.0148	202.8	HMDB33052	Ethyl vinyl disulfide	8
308.0904	210.3	HMDB33247	Aristolodione	8
188.0702	40	HMDB33249	6-Chloro-N-(1-methylethyl)-135-triazine-24-diamine	8
359.221	24.1	HMDB33443	Sorgoleone 358	8
316.1351	48.4	HMDB33664	N-Hydroxysaxitoxin	8
137.0716	48.3	HMDB33947	2-Aminobenzamide	8
100.0757	33	HMDB34587	1-Pyrrolidinecarboxaldehyde	8
177.0768	53.2	HMDB00402	2-Isopropylmalic acid	8
278.1233	74.1	HMDB01495	Queuine	8
441.1668	42	HMDB01833	Aminopterin	8
181.0496	98.7	HMDB01879	Aspirin	8
431.3915	20.9	HMDB01893	Alpha-Tocopherol	8
295.1288	41.1	HMDB01894	Aspartame	8
319.083	163.8	HMDB01941	Brompheniramine	8
147.0651	223.5	HMDB02173	Solerol	8
569.4354	21.9	HMDB02789	Zeaxanthin	8
451.3612	21.7	HMDB03555	Vitamin K1	8
425.255	44.6	HMDB05022	Pravastatin	8
295.1881	71.7	HMDB05783	Gingerol	8
181.0719	214	HMDB06088	Scyllitol	8
255.2317	180.2	HMDB12328	Palmitelaidic acid	8
268.1032	131.1	HMDB14340	Vidarabine	8
445.1624	38.5	HMDB14399	Doxycycline	8
180.1382	178.4	HMDB14523	Mexiletine	8
393.209	32.1	HMDB14586	Betamethasone	8
271.0302	75.6	HMDB14715	Sulfamethizole	8
847.444	245.4	HMDB14753	Rifabutin	8
457.2051	236.6	HMDB14843	Delavirdine	8
200.1756	34.4	HMDB14849	Diethylcarbamazine	8
369.2395	42	HMDB14928	Perindopril	8
190.086	172.4	HMDB14970	Phensuximide	8
248.0701	93.4	HMDB15047	Tinidazole	8
443.1452	30.4	HMDB15066	Methacycline	8

615.3186	259.7	HMDB15129	Neomycin	8
358.1746	47.6	HMDB15147	Cinacalcet	8
494.1468	36.7	HMDB15151	Glyburide	8
303.216	26.2	HMDB15216	Emedastine	8
537.2789	258.8	HMDB15254	Ambenonium	8
500.1725	69.7	HMDB15349	Halofantrine	8
211.1073	248.7	HMDB15441	Aprobarbital	8
292.227	200.6	HMDB15447	Penbutolol	8
455.0104	284.8	HMDB15629	Sitaxentan	8
386.1324	76.6	HMDB15657	Nilvadipine	8
326.9944	57.6	HMDB15679	Niclosamide	8
349.2094	47.3	HMDB15695	Roxatidine acetate	8
313.1429	189.8	HMDB30600	4-(3-Methyl-1-butenyl)-3345-tetrahydroxystilbene	8
225.1123	179.4	HMDB30680	Diplosporin	8
147.0804	231.2	HMDB31619	2-Phenyl-2-butenal	8
183.1743	183.9	HMDB32279	2-Ethyl-133-trimethyl-2-norbornanol	8
235.0827	38	HMDB32438	1-Isopropyl citrate	8
153.1638	182.8	HMDB32712	14-Undecadiene	8
136.0394	204.4	HMDB32931	2-Benzoxazolol	8
97.0648	279.2	HMDB32965	24-Dimethylfuran	8
109.0761	54.1	HMDB32971	23-Dimethylpyrazine	8
150.038	105.2	HMDB33001	2-Methylbenzothiazole	8
155.0022	193.7	HMDB33047	Ethyl (methylthio)methyl disulfide	8
370.1633	37	HMDB33084	7-Hydroxydehydroglaucine	8
127.0203	58.7	HMDB33133	2-Acetylthiophene	8
111.0553	78.9	HMDB33156	Methoxypyrazine	8
157.1222	275.2	HMDB33167	Ethyl cyclohexanecarboxylate	8
134.0713	240	HMDB33172	3-Methylpyrrolo12-apyrazine	8
171.1379	28.5	HMDB33203	6-Decanolide	8
620.3173	254.5	HMDB33241	Glycylalanylprolylmethionylphenylalanylvalinamide	8
331.08	86.7	HMDB33268	135-Trihydroxy-67-dimethoxy-2-methylanthraquinone	8
681.2405	269.1	HMDB33369	Hydroxypropyl methyl cellulose	8
381.1823	48.7	HMDB33466	Di-4-coumaroylputrescine	8
438.239	32.7	HMDB33469	N1N10-Dicoumaroylspermidine	8
163.0974	166.8	HMDB33532	Dimethicone	8
192.1026	194	HMDB33560	(E)-5-(3456-Tetrahydro-3-pyridylidenemethyl)-2-furanmethanol	8
113.0602	289.1	HMDB33569	Syoyualdehyde	8
307.2995	22.3	HMDB33608	2-Heptadecylfuran	8
537.1655	182.9	HMDB33706	Salviaflaside methyl ester	8

211.0956	185.9	HMDB33798	3-Methyl-1-(246-trihydroxyphenyl)-1-butanone	8
87.0269	36.7	HMDB33875	23-Dihydrothiophene	8
137.0815	99.2	HMDB33919	2-Deoxy-D-ribitol	8
147.0305	229.2	HMDB33966	Di-2-propenyl disulfide 9CI	8
349.0712	168.5	HMDB34067	Maclurin 3-C-(2-galloyl-6-p-hydroxybenzoyl-glucoside)	8
403.2298	50.3	HMDB34159	Acetyl tributyl citrate	8
93.0699	273.2	HMDB34168	Toluene	8
195.1015	249.6	HMDB34206	Ethyl 4-methylphenoxyacetate	8
211.144	178.8	HMDB34276	LL-Cyclo(leucylprolyl)	8
217.1328	85	HMDB34292	Nb-Methyltetrahydroharmol	8
235.0243	215.3	HMDB34453	4-22-Bithiophen-5-yl-3-butyn-1-ol	8
289.1898	45.8	HMDB34554	Sakacin A	8
154.1226	175.6	HMDB34580	psi-Pelletierine	8
107.0703	29.8	HMDB34778	(2R3R)-123-Butanetriol	8
168.0655	246.4	HMDB34887	3alpha457alpha-Tetrahydro-5-hydroxy-1H-isoindole-13(2H)-dione	8
383.1722	29	HMDB35201	48-Diacetyl-T2-tetrol	8
163.0537	54	HMDB35400	1-Tridecene-357911-pentayne	8
523.1106	47.8	HMDB35462	Myricetin 3-(6-acetylgalactoside)	8
192.0646	45.3	HMDB35514	xi-23-Dihydro-2-oxo-1H-indole-3-acetic acid	8
516.4751	255.4	HMDB35517	11-(14-Dihydro-4-nonyl-35-pyridinediyl)bis1-decanone	8
234.0973	86.9	HMDB35923	Hirsutin	8
96.0444	231.3	HMDB36057	1H-Pyrrole-2-carboxaldehyde	8
299.15	28.8	HMDB36159	Toxin T2 tetrol	8
609.1179	256.2	HMDB36336	Prodelphinidin A1	8
115.0577	33	HMDB36491	Di-2-propenyl sulfide	8
422.9867	272.2	HMDB36699	Chlorophenol red	8
193.0686	62	HMDB37166	2-(Methylthiomethyl)-3-phenyl-2-propenal	8
175.1117	229.6	HMDB37281	4-Methyl-2-phenyl-2-pentenal	8
114.0914	30.4	HMDB37293	2-Acetylpyrrolidine	8
591.1546	254.8	HMDB37655	Proanthocyanidin A2	8
519.4044	22	HMDB37781	Ganoderiol C	8
191.0569	30.5	HMDB37815	5-(Methylthio)-2-(methylthio)methyl-2-pentenal	8
344.1339	73	HMDB37845	N-(1-Deoxy-1-fructosyl)tyrosine	8
213.1849	24.3	HMDB37907	261010-Tetramethyl-1-oxaspiro45decan-6-ol	8
774.2037	281.7	HMDB37983	Cyanidin 3-(6-caffeoylglucoside) 5-glucoside	8
337.2733	189.6	HMDB38105	Isolinderanolide	8
127.1482	194.4	HMDB38191	Isopropylcyclohexane	8
394.0317	217.6	HMDB38408	2-(Methylthio)ethyl glucosinolate	8
231.0278	250.1	HMDB38430	5-(1-Propynyl)-5-vinyl-22-bithiophene	8

479.1727	53.2	HMDB38714	Kelampayoside A	8
220.0608	137.9	HMDB39387	Methyl 26-dihydroxy-4-quinolinecarboxylate	8
161.046	124.5	HMDB39447	2-Methyl-4-oxopentanedioic acid	8
152.107	185.7	HMDB39659	123456-Hexahydro-6-methyl-7H-cyclopentabpyridin-7-one	8
450.2355	267.2	HMDB39857	Cadabicine methyl ether	8
641.3295	280.5	HMDB39962	N1N5N10-Tris-trans-p-coumaroylspermine	8
191.0928	36.8	HMDB40220	Diethyl L-malate	8
483.1131	230.5	HMDB40622	3-(2-Galloylglucosyl)-phloroacetophenone	8
355.1354	70.4	HMDB40797	Methyl helianthenoate F glucoside	8
559.1398	232.3	HMDB40862	Piceatannol 4-galloylglucoside	8
839.4361	88.5	HMDB40957	Talinumoside I	8
505.538	57.3	HMDB41033	17-Pentatriacontadien-11-ol	8
511.2726	42.8	HMDB41047	Physagulin A	8
235.2419	180.4	HMDB41082	(5Z8Z)-158-Heptadecatriene	8
160.0254	82.7	HMDB41083	(E)-Raphanusanin	8
381.2975	278.9	HMDB41103	Persin	8
818.2247	79.2	HMDB41154	Alatanin 1	8
583.4339	267.3	HMDB41180	Hericene B	8
231.1242	30.1	HMDB41448	Dicyclohexyl disulfide	8
195.0466	86.4	HMDB41503	Bis(2-furanylmethyl) sulfide	8
413.1384	40.5	HMDB41623	N6-Carbamoyl-L-threonyladenosine	8
185.108	88.7	HMDB41835	Benzidine	8
406.1998	61.2	HMDB41907	Imidapril	8
437.1329	249.2	HMDB42038	Tianeptine	8
149.0233	24.1	HMDB02107	Phthalic acid	9
303.0473	275.5	HMDB05794	Quercetin	9
321.0208	211.2	HMDB14332	Lorazepam	9
429.2402	42.2	HMDB15163	Irbesartan	9
290.0345	206.7	HMDB15420	Quinethazone	9
315.1953	23.9	HMDB35200	Yucalexin B5	9
615.1691	230.4	HMDB35435	Cinchonain Id 7-glucoside	9
308.9837	177.1	HMDB38142	58-Dihydro-6-(4-methyl-3-pentenyl)-1234-tetrathiocin	9
539.1311	224.9	HMDB38508	Rheidin C	9
546.2021	130.1	HMDB39750	Lacto-N-triose I	9
191.1794	23.5	HMDB39884	2-Cyclotetradecen-1-one	9
277.0317	261.2	HMDB40924	2-Carboxyarabinitol 5-phosphate	9
153.0546	134.4	HMDB00020	p-Hydroxyphenylacetic acid	9
139.039	259	HMDB01895	Salicylic acid	9
323.0341	212.3	HMDB02708	Cyanidin	9

155.143	176.2	HMDB04043	Alpha-Terpineol	9
155.0702	290.1	HMDB05784	Hydroxytyrosol	9
274.0686	237.4	HMDB14468	Tolcapone	9
286.1435	200.8	HMDB14472	Hydromorphone	9
187.054	211.4	HMDB14533	Carbimazole	9
261.1828	52.4	HMDB14539	Carisoprodol	9
384.0445	245.2	HMDB15427	Ceftizoxime	9
368.2193	41.1	HMDB15478	Bambuterol	9
192.1383	186.4	HMDB15519	Phendimetrazine	9
301.06	206.2	HMDB15544	Tazobactam	9
256.0194	290.3	HMDB15619	Sulfathiazole	9
185.1536	29	HMDB32308	(E)-3-Heptenyl 2-methylpropanoate	9
225.1849	22.8	HMDB32524	Terpinyl isobutyrate	9
109.0148	55.6	HMDB32912	Ethyl methyl disulfide	9
143.0339	290.7	HMDB32923	Kojic acid	9
279.159	24.1	HMDB33244	Dibutyl phthalate	9
455.2462	56.3	HMDB33370	Ethyl cellulose	9
148.0969	180.7	HMDB33453	Fagomine	9
357.1002	256.3	HMDB33659	Dihydrohydroxy-O-methylsterigmatocystin	9
245.0791	59.3	HMDB33735	Graveolone	9
611.3157	266	HMDB33749	Isoliensinine	9
221.1899	257	HMDB33826	26-Di-tert-butyl-4-methylphenol	9
87.0441	232.2	HMDB33977	Methyl acrylate	9
121.1012	234.9	HMDB34029	Isopropylbenzene	9
117.091	27.3	HMDB34163	3-Methylbutyl formate	9
209.0811	87.1	HMDB34315	3-(34-Dimethoxyphenyl)-2-propenoic acid	9
193.05	200.2	HMDB34344	Scopoletin	9
209.1535	248.7	HMDB34672	(5alpha8beta9beta)-59-Epoxy-36-megastigmadien-8-ol	9
161.096	25.1	HMDB35207	2-Phenyl-4-pentenal	9
167.1068	31.4	HMDB35235	247-Decatrienoic acid	9
207.1743	23.2	HMDB35245	1-(266-Trimethyl-2-cyclohexen-1-yl)-1-penten-3-one	9
143.1067	181.6	HMDB35422	4-Butyl-gamma-butyrolactone	9
297.2787	23.2	HMDB35575	46-Nonadecanedione	9
275.2004	23.2	HMDB35579	1-Phenyl-13-dodecanedione	9
487.2137	199.9	HMDB35590	15-Acetoxyscirpene-34-diol 4-O-a-D-glucopyranoside	9
198.1124	204.3	HMDB36074	Tenuazonic acid	9
191.1416	55.6	HMDB36178	2-(3-Phenylpropyl)tetrahydrofuran	9
289.2154	26.8	HMDB36205	alpha-Amylcinnamyl isovalerate	9
779.2481	275.7	HMDB36321	(7E7R8R)-e-Viniferin 35-diglucoside	9

142.0322	217.4	HMDB37168	2-Propanoylthiazole	9
347.1096	245.5	HMDB37250	Muscomin	9
219.2106	275.2	HMDB37740	12-Dimethyl-4-(6-methyl-4-heptenyl)-13-cyclohexadiene	9
466.1068	225	HMDB37997	Delphinidin 3-glucoside	9
369.2997	196.6	HMDB38073	Octadecyl fumarate	9
170.1175	260.4	HMDB38321	Homoarecoline	9
371.604	250.7	HMDB38822	Malvidin 3-(6-malonylglucoside) 5-glucoside	9
937.1009	203.1	HMDB39244	1-O-Galloylpedunculagin	9
321.2082	29	HMDB39276	8-Gingerdione	9
664.1141	271.5	HMDB39421	Fenugreekine	9
164.1069	182.7	HMDB39661	2367-Tetrahydro-7-methylcyclopentbazepin-8(1H)-one	9
107.0524	280.5	HMDB40185	3-Mercapto-2-butanol	9
258.0805	204.1	HMDB40288	2-(Ethylsulfonylmethyl)phenyl methylcarbamate	9
217.1213	198.9	HMDB40833	3-4-Hydroxy-3-(3-methyl-2-butenyl)phenyl-2-propenal	9
897.4883	38.2	HMDB41020	Momordin Ie	9
357.2266	41.5	HMDB41044	57-Megastigmadien-9-ol glucoside	9
451.0843	205.3	HMDB41635	Myricetin 3-arabinoside	9
146.975	262.4	HMDB41971	P-Dichlorobenzene	9
109.0637	47.7	HMDB02055	o-Cresol	10
476.3065	29.1	HMDB15090	Netilmicin	10
299.1021	59.9	HMDB15160	Amlexanox	10
361.1368	37.4	HMDB15187	Nitrendipine	10
191.0665	78.5	HMDB15673	Carglumic acid	10
186.0871	50.7	HMDB34912	(S)-N-(45-Dihydro-1-methyl-4-oxo-1H-imidazol-2-yl)alanine	10
160.0966	53.5	HMDB36384	Calystegine A7	10
369.2627	20.9	HMDB37961	gamma-Eudesmol rhamnoside	10
144.1019	54.2	HMDB38949	3beta6beta-Dihydroxynortropane	10
258.1091	113.1	HMDB39229	Pyro-L-glutaminyl-L-glutamine	10
330.2638	22.2	HMDB40900	()-(E)-13-Hydroxy-10-oxo-11-octadecenoic acid	10
337.1532	108	HMDB41519	Nb-Feruloyltryptamine	10
147.1129	75.2	HMDB00182	L-Lysine	10
95.0491	286.2	HMDB00228	Phenol	10
272.2007	180.6	HMDB01920	Dextromethorphan	10
166.1226	187.5	HMDB01943	Pseudoephedrine	10
153.0748	76.8	HMDB02917	D-Xylitol	10
88.0393	80.2	HMDB03609	2-Aminoacrylic acid	10
172.1332	197.9	HMDB05015	Gabapentin	10
264.1956	197.7	HMDB14339	Tramadol	10
311.2367	23.5	HMDB14449	Desogestrel	10

266.1643	51.8	HMDB14514	Mirtazapine	10
285.1417	69.2	HMDB14564	Promazine	10
199.1068	182.6	HMDB14606	Metharbital	10
158.0812	255.3	HMDB14755	Paramethadione	10
222.1122	186.7	HMDB14798	Metaxalone	10
212.1281	182.5	HMDB14861	Methoxamine	10
130.0862	67.4	HMDB15212	Vigabatrin	10
585.2887	31.7	HMDB15224	Ouabain	10
357.1256	70.1	HMDB15264	Pioglitazone	10
364.0989	252.2	HMDB15271	Cefadroxil	10
370.1844	109.8	HMDB15288	Trimetrexate	10
399.2195	60.3	HMDB15397	Sunitinib	10
354.2674	30.8	HMDB15562	Isopropamide	10
265.1572	189.4	HMDB15568	Vorinostat	10
231.1591	188.6	HMDB30143	Talaromycin A	10
151.0401	67.6	HMDB32612	34-Methylenedioxybenzaldehyde	10
177.0538	41.7	HMDB32883	145-Naphthalenetriol	10
387.3253	177.3	HMDB32925	1-Phenyl-13-eicosanedione	10
163.0502	180.2	HMDB32927	Quindoxin	10
136.0215	270	HMDB32930	Benzothiazole	10
108.0808	172.6	HMDB32972	26-Dimethylpyridine	10
223.0637	160.3	HMDB33041	1-(1-Propenylthio)propyl propyl disulfide	10
367.1521	49.5	HMDB33108	Semilepidinoside B	10
127.0584	235.4	HMDB33160	2-Propylthiophene	10
205.1217	275.3	HMDB33379	cis-3-Hexenyl benzoate	10
272.0462	75.6	HMDB33602	Brassica oleracea Alkaloid	10
339.1567	78.5	HMDB33671	2-O-Methylglabridin	10
435.091	76.3	HMDB33795	Quercetin 3-arabinoside	10
299.2369	193	HMDB33862	3-(81114-Pentadecatrienyl)phenol	10
141.054	265.6	HMDB34246	Furfuryl acetate	10
128.0354	69.5	HMDB34368	Hydroxyminaline	10
152.0163	76.8	HMDB34413	12-Benzisothiazol-3(2H)-one	10
117.0553	258	HMDB34466	Acetoxyacetone	10
227.2005	25.3	HMDB34561	Houttuynin	10
212.0542	90.1	HMDB34864	24-Dihydroxy-7-methoxy-2H-14-benzoxazin-3(4H)-one	10
289.0937	80.1	HMDB35589	Phlorin	10
223.1691	23.6	HMDB37820	Acetaldehyde butyl phenethyl acetal	10
492.1299	40.2	HMDB37971	Cyanidin 3-(4-acetylglucoside)	10
181.1587	23.5	HMDB38108	cis-Quinceoxepane	10

198.0755	74	HMDB38336	2-Hydroxy-3-(34-dihydroxyphenyl)propanamide	10
266.1518	48.3	HMDB38838	Lansiumamide C	10
374.1948	111.6	HMDB39503	N-Jasmonoyltyrosine	10
355.2639	24.7	HMDB39760	11-112-Dodecanediylbis(oxy)bisbenzene	10
199.0563	90.7	HMDB40164	4-Methyldibenzothiophene	10
375.1393	100.6	HMDB40912	N-(5-Hydroxy-2-pyridinyl)methyladenosine	10
417.1744	57.8	HMDB41274	Phenylethyl primeveroside	10
163.9843	156.8	HMDB41280	Raphanusamic acid	10

Web Table 3. Exogenous features detected in C18 column with suggested m/z matches annotation and cluster IDs

mz	time	chemical_ID	Name	cluster
145.0515	289.4	HMDB02173	Solerol	1
566.3107	167.8	HMDB14365	Nelfinavir	1
190.0734	291.1	HMDB31346	Calystegine C1	1
418.0939	17.5	HMDB35174	3-1-Formyl-2-(2-furanyl)ethenyl-2-(2-furanyl)-5-(2-furanylmethylene)-45-dihydro-a-methyl-4-oxo-1H-pyrrole-1-acetic acid 9CI	1
636.3882	208.8	HMDB35264	Avenestergenin A1	1
181.0512	280.1	HMDB00423	34-Dihydroxyhydrocinnamic acid	1
779.4188	185.4	HMDB01917	Digoxin	1
311.296	291.3	HMDB02212	Arachidic acid	1
87.045	28.6	HMDB03243	Acetoin	1
197.0821	286.3	HMDB04998	Guaifenesin	1
153.0556	284.8	HMDB05784	Hydroxytyrosol	1
163.0764	288.1	HMDB05802	Isoeugenol	1
197.0317	293.5	HMDB14480	Nitrofurazone	1
142.0508	278.5	HMDB14491	Trimethadione	1
371.2594	195.5	HMDB14629	Nabilone	1
156.0665	284.5	HMDB14755	Paramethadione	1
266.1162	292	HMDB14852	Apomorphine	1
239.1292	287.4	HMDB14862	Imiquimod	1
272.0757	21.4	HMDB14883	Modafinil	1
248.1656	194	HMDB15004	Alprenolol	1
235.0822	174.4	HMDB15037	Didanosine	1
204.1243	271.2	HMDB15050	Phenformin	1
170.0571	289.2	HMDB15052	Metronidazole	1
293.1402	286.8	HMDB15104	Alosetron	1
144.0665	289.3	HMDB15127	Methyl aminolevulinate	1
190.037	18.4	HMDB15155	Isosorbide Mononitrate	1
355.1102	200.9	HMDB15264	Pioglitazone	1
669.3818	176.3	HMDB15362	Saquinavir	1
249.1513	289.1	HMDB15371	Gemfibrozil	1
415.2117	247.6	HMDB15389	Desonide	1
301.0544	18.5	HMDB15513	Fludiazepam	1
207.0882	280.6	HMDB29968	Ethyl beta-D-glucopyranoside	1
197.1545	171.8	HMDB31683	xi-Dihydro-5-octyl-2(3H)-furanone	1
103.0219	148	HMDB31982	3-Mercapto-2-butanone	1
183.139	270.5	HMDB32308	(E)-3-Heptenyl 2-methylpropanoate	1
189.0968	23.2	HMDB32427	(S)-3-Methylthiohexyl acetate	1
179.1076	58.9	HMDB32468	2-Phenylpropionaldehyde dimethyl acetal	1

181.087	288.9	HMDB32607	()-threo-Anethole glycol	1
204.0672	23.1	HMDB32755	Methyl 1-methoxy-1H-indole-3-carboxylate	1
134.0243	47.7	HMDB32931	2-Benzoxazolol	1
259.095	291.9	HMDB32953	7-Methoxy-5-prenyloxycoumarin	1
106.0661	40.2	HMDB32972	26-Dimethylpyridine	1
111.0086	289.3	HMDB32994	3-Hydroxy-2H-pyran-2-one	1
221.0483	20.7	HMDB33041	1-(1-Propenylthio)propyl propyl disulfide	1
167.0019	289.1	HMDB33042	Methyl 1-(methylthio)propyl disulfide	1
163.0623	286.7	HMDB33050	Butyl isopropyl disulfide	1
209.0126	293.2	HMDB33058	1-(Methylsulfinyl)propyl 1-propenyl disulfide	1
182.9969	289.7	HMDB33075	Methyl 1-(methylsulfinyl)propyl disulfide	1
120.0448	291.1	HMDB33131	3-Acetylpyridine	1
109.0406	284.3	HMDB33156	Methoxypyrazine	1
193.035	150.4	HMDB33245	6-(Hydroxymethyl)-24(1H3H)-pteridinedione	1
251.1054	292.5	HMDB33317	(1Z4Z)-15-bis(4-hydroxyphenyl)-14-pentadiene	1
125.0969	160.9	HMDB33547	3-Octen-2-one	1
141.0556	288.9	HMDB33551	5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone	1
139.1127	288	HMDB33554	2-Methyl-2-octenal	1
205.0731	287.8	HMDB33584	Diethyl tartrate	1
205.0867	292.8	HMDB33594	Cuelure	1
247.134	199.4	HMDB33707	Heliannuol E	1
119.0491	287.2	HMDB33910	Acetophenone	1
135.0672	291.3	HMDB33919	2-Deoxy-D-ribitol	1
292.1043	291	HMDB34085	(3R)-34-Dihydroxy-3-(hydroxymethyl)butanenitrile 4-glucoside	1
236.0567	36.7	HMDB34251	N-Benzoylaspartic acid	1
191.0358	26.7	HMDB34344	Scopoletin	1
125.024	288	HMDB34355	5-Hydroxymethyl-2-furancarboxaldehyde	1
158.0468	290.4	HMDB34442	L-trans-alpha-Amino-2-carboxycyclopropaneacetic acid	1
169.0656	187.8	HMDB34446	Diphenyl ether	1
239.202	290.4	HMDB34455	Exaltolide	1
115.04	285.4	HMDB34466	Acetoxyacetone	1
327.181	284.2	HMDB34579	8-O-Methyloblongine	1
160.0515	289	HMDB34888	4-Acetylimidazo45-cpyridine	1
198.0785	286.7	HMDB35177	2-Acetyl-1567-tetrahydro-6-hydroxy-7-(hydroxymethyl)-4H-azepine-4-one	1
407.1863	183.4	HMDB35255	3-Geranyl-2344-tetrahydroxychalcone	1
591.3673	208.7	HMDB35266	Avenestergenin B2	1
492.2731	167.5	HMDB35367	Cytochalasin Npho	1
381.1904	38.6	HMDB35396	T2 Triol	1
209.0459	282.9	HMDB35484	3-(34-Dihydroxy-5-methoxy)-2-propenoic acid	1

401.3427	183.4	HMDB35681	3-Hydroxy-1-phenyl-1-heneicosanone	1
251.1295	291.2	HMDB36047	3alpha-Hydroxyoreadone	1
196.098	289.2	HMDB36074	Tenuazonic acid	1
181.1235	25.9	HMDB36191	4-Hydroxy-4-methyl-7-decenoic acid gamma-lactone	1
158.0822	286.8	HMDB36384	Calystegine A7	1
204.0889	291.4	HMDB36394	N-Methylcalystegine C1	1
100.0403	284.5	HMDB36458	1-Aminocyclopropanecarboxylic acid	1
199.0976	283.8	HMDB36715	Matsutakic acid A	1
305.1605	191.1	HMDB37107	N1-trans-Feruloylagmatine	1
119.0613	289.5	HMDB37134	(1-Methylethenyl)pyrazine	1
219.1029	187.2	HMDB37492	Ethyl methyl-p-tolylglycidate	1
261.2226	246.6	HMDB37519	2-(58-Tetradecadienyl)cyclobutanone	1
264.1007	293.2	HMDB37594	Eduleine	1
211.1704	291.6	HMDB37907	261010-Tetramethyl-1-oxaspiro45decan-6-ol	1
113.0972	19.7	HMDB38052	1-Ethoxy-3-methyl-2-butene	1
215.1048	293.3	HMDB38239	Sakacin P	1
202.0734	289.1	HMDB38440	1-Isothiocyanato-7-(methylthio)heptane	1
257.1148	23	HMDB38614	gamma-L-Glutamyl-L-pipecolic acid	1
296.0901	295.3	HMDB38723	(S)-Annocherine A	1
159.0305	292.2	HMDB39447	2-Methyl-4-oxopentanedioic acid	1
770.4241	204.6	HMDB40136	beta-D-Glucosyloxydestruxin B	1
201.1133	284.1	HMDB40196	Oxalic acid dibutyl ester	1
361.1662	177.5	HMDB40759	3-Oxo-6b-angeloyloxy-8b-hydroxy-7(11)-eremophilen-128-olide	1
503.3389	210.3	HMDB40772	Isothankunic acid	1
311.2233	286.8	HMDB40900	()-(E)-13-Hydroxy-10-oxo-11-octadecenoic acid	1
649.3908	187.1	HMDB40941	Arjunolic acid 3-glucoside	1
203.057	284.5	HMDB41031	356-Trihydroxy-5-(hydroxymethyl)-2-methoxy-2-cyclohexen-1-one	1
355.2122	188.3	HMDB41044	57-Megastigmadien-9-ol glucoside	1
463.3433	295.5	HMDB41135	2-Deoxybrassinolide	1
294.1113	293.5	HMDB41245	7-Hydroxyheptaphylline	1
165.0781	287.8	HMDB41500	1-Deoxy-D-glucitol	1
367.3587	271.6	HMDB02003	Tetracosanoic acid	2
264.0595	24.6	HMDB03045	Ergothioneine	2
297.2803	291.7	HMDB04085	Tuberculostearic acid	2
311.2023	218.6	HMDB04626	Tetrahydrogestrinone	2
347.2442	231.3	HMDB14364	Oxyphenonium	2
297.1847	169.4	HMDB14855	Norethindrone	2
301.2059	182.7	HMDB15216	Emedastine	2
233.1547	211.8	HMDB31349	Epiacoronene	2

177.0781	288.1	HMDB33789	2-O-Methyl-L-fucose	2
205.1597	227.2	HMDB35245	1-(266-Trimethyl-2-cyclohexen-1-yl)-1-penten-3-one	2
309.2803	291.2	HMDB35572	68-Icosanedione	2
251.2018	199.5	HMDB37805	D6-Ambrettolide	2
513.3022	204.4	HMDB39150	Flavidulol C	2
267.2334	257.8	HMDB40888	24-Heptadecanedione	2
151.04	286.2	HMDB00020	p-Hydroxyphenylacetic acid	2
116.0716	288	HMDB00883	L-Valine	2
153.0192	289.4	HMDB01856	Protocatechuic acid	2
121.0294	284.6	HMDB01870	Benzoic acid	2
329.1761	208.2	HMDB02121	Carnosol	2
135.045	267.8	HMDB02340	2-Methylbenzoic acid	2
315.2334	237.9	HMDB04627	Calusterone	2
243.1	291.2	HMDB14336	Carbidopa	2
629.3362	178.7	HMDB14357	Remikiren	2
403.2518	269.7	HMDB14372	Lovastatin	2
286.8538	47.4	HMDB14575	Lindane	2
313.2185	228.8	HMDB14613	Dronabinol	2
302.0466	17.6	HMDB14769	Clofarabine	2
339.1818	293.7	HMDB14876	Pentamidine	2
212.0943	291.3	HMDB15506	Phenazopyridine	2
314.1846	43.1	HMDB15634	Saxagliptin	2
99.045	288.3	HMDB31178	Dihydro-2-methyl-3(2H)-furanone	2
149.0243	284.9	HMDB32612	34-Methylenedioxybenzaldehyde	2
129.0919	268.2	HMDB32874	Hexyl formate	2
382.1291	189.3	HMDB32878	13-Oxocryptopine	2
347.1863	173.5	HMDB32895	3b-Hydroxy-6b-angeloyloxy-7(11)-eremophilen-128b-olide	2
147.0448	185.5	HMDB32947	Di-2-furanylmethane	2
169.0509	287.2	HMDB32966	Furaneol acetate	2
98.0069	21	HMDB33116	4-Methylthiazole	2
301.181	205.6	HMDB33125	8-Dehydroshogaol	2
345.132	24.3	HMDB33290	Junosmarin	2
463.2081	230.6	HMDB33316	Garcinone E	2
161.083	290.4	HMDB33532	Dimethicone	2
275.0547	20.9	HMDB33649	O-Demethylfonsecin	2
173.0823	287.3	HMDB33838	Diethyl succinate	2
297.2228	222.7	HMDB33862	3-(81114-Pentadecatrienyl)phenol	2
135.0562	285.8	HMDB33947	2-Aminobenzamide	2
173.1182	286.2	HMDB34040	246-Triethyl-135-trioxane	2

226.9966	17.7	HMDB34228	Thiolutin	2
174.0784	292.3	HMDB34252	2-Aminoheptanedioic acid	2
275.114	289.5	HMDB34263	Triethyl citrate	2
171.0667	287.1	HMDB34851	Ethyl 24-dioxohexanoate	2
217.0621	26.6	HMDB34911	(S)-3-(Cyanophenylmethyl)amino-3-oxopropanoic acid	2
183.0671	289.5	HMDB35056	1-(3-Hydroxy-4-methoxyphenyl)-12-ethanediol	2
200.0942	290.7	HMDB35170	12-Dihydro-11-dimethyl-2-oxo-44-bipyridinium(1)	2
393.3744	266.1	HMDB35215	Ximenic acid	2
405.2649	29.3	HMDB35288	(6b7b13R)-67-Diacetoxy-814-labdadiene-13-ol	2
345.2813	281.7	HMDB35678	3-Hydroxy-1-phenyl-1-heptadecanone	2
94.0297	280.8	HMDB36057	1H-Pyrrole-2-carboxaldehyde	2
315.1966	203.6	HMDB36147	Furanojaponin	2
195.1025	176.7	HMDB36226	26-Dimethoxy-4-propylphenol	2
217.0844	292.7	HMDB36301	N-gamma-L-Glutamyl-D-alanine	2
157.0511	286.2	HMDB36380	xi-23-Dihydro-35-dihydroxy-6-methyl-4H-pyran-4-one	2
188.0941	290.7	HMDB36604	N-Methylcalystegine B2	2
361.0402	24.1	HMDB36932	2-O-Galloylgalactaric acid	2
276.0213	17.1	HMDB37131	()-Furilazole	2
139.0763	286.9	HMDB37167	3-Ethyl-5-methyl-12-cyclopentanedione	2
289.2177	223.5	HMDB37711	4-Methylphenyl dodecanoate	2
167.0712	290.7	HMDB37729	2-Furanylmethyl butanoate	2
221.1545	251	HMDB37820	Acetaldehyde butyl phenethyl acetal	2
251.1654	211.3	HMDB37969	Urodiolenone	2
110.0246	292.4	HMDB38175	2-Acetyloxazole	2
299.1137	24.9	HMDB38332	2-(3-Hydroxyphenyl)ethanol 1-glucoside	2
319.2282	239.1	HMDB38520	2-Hydroxy-6-tridecylbenzoic acid	2
142.0872	286.8	HMDB38949	3beta6beta-Dihydroxynortropane	2
443.3015	228.7	HMDB39225	2-Stearyl citrate	2
117.0196	289.4	HMDB39324	xi-3-Hydroxy-2-oxobutanoic acid	2
132.0666	21.2	HMDB39499	14-Dideoxy-14-imino-D-ribitol	2
123.0562	284.6	HMDB40141	2-Methoxy-5-methylpyrazine	2
189.0777	287.4	HMDB40220	Diethyl L-malate	2
109.0657	118.6	HMDB40277	2-Propylfuran	2
89.0427	160.2	HMDB40576	2-(Methylthio)propane	2
341.2339	173.5	HMDB40901	13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid	2
375.2184	24.8	HMDB40955	9alpha-(Angeloyloxy)-4S-hydroxy-10(14)-oplopen-3-one 4-acetate	2
404.1856	241	HMDB41907	Imidapril	2
369.1756	21.3	HMDB41918	Lorcainide	2
122.0246	283.6	HMDB41950	Nitrobenzene	2

449.1927	202.2	HMDB42013	Sofalcone	2
164.0718	26.3	HMDB00159	L-Phenylalanine	3
277.2176	225.5	HMDB01388	Alpha-Linolenic acid	3
151.0609	22.7	HMDB02917	D-Xylitol	3
379.1911	44.9	HMDB14825	Fludrocortisone	3
136.0518	22.9	HMDB15086	Isoniazid	3
397.205	238.8	HMDB15397	Sunitinib	3
301.2182	234.1	HMDB15655	Methyltestosterone	3
349.2368	271.5	HMDB33616	(S)-10-Gingerol	3
331.2648	267.5	HMDB35677	3-Hydroxy-1-phenyl-1-hexadecanone	3
389.127	19.7	HMDB36294	(E)-2-Glucosyl-345-trihydroxystilbene	3
345.2059	208	HMDB36624	4-Deoxyhumulone	3
157.0128	22.7	HMDB37759	2-Methylene-4-oxopentanedioic acid	3
388.1212	20.4	HMDB39896	xi-8-Acetonyldihydrosanguinarine	3
105.0378	24.7	HMDB40185	3-Mercapto-2-butanol	3
379.2112	31.4	HMDB40568	6-Gingerdiol 35-diacetate	3
347.2212	245.1	HMDB40641	8-Paradyl acetate	3
369	16.6	HMDB41831	Azosemide	3
152.0352	289.6	HMDB01972	3-Aminosalicylic acid	3
294.1713	227.5	HMDB14333	Esmolol	3
262.1814	209	HMDB14339	Tramadol	3
257.0071	21.6	HMDB14456	Ethoxzolamide	3
308.1503	160.8	HMDB14484	Metixene	3
317.0908	168.3	HMDB14620	Chlorpromazine	3
140.0717	18	HMDB14731	Ethosuximide	3
228.0396	19.9	HMDB14732	Amiloride	3
314.0184	47.3	HMDB14763	Efavirenz	3
194.082	173.1	HMDB14903	Metyrosine	3
439.2252	171.9	HMDB14913	Tirofiban	3
308.2588	257.5	HMDB14942	Dicyclomine	3
243.0186	17.6	HMDB15099	Apraclonidine	3
405.2415	196.3	HMDB15119	Nandrolone phenpropionate	3
386.1826	240.9	HMDB15293	Terazosin	3
335.2047	232	HMDB15316	Fluoxymesterone	3
166.9937	51.4	HMDB15320	Desflurane	3
398.1517	24.3	HMDB15686	Pipazethate	3
233.0672	17.9	HMDB32438	1-Isopropyl citrate	3
161.0097	23.3	HMDB32750	S-2-Propenyl 1-propenesulfinothioate	3
162.0784	289.5	HMDB32862	2-Amino-4-ethoxy-3-hydroxybutanoic acid	3

340.1422	22.7	HMDB32864	Mycotoxin T 2	3
152.9862	286.4	HMDB33047	Ethyl (methylthio)methyl disulfide	3
368.1515	21.6	HMDB33084	7-Hydroxydehydroglaucine	3
125.0068	20.7	HMDB33133	2-Acetylthiophene	3
428.0273	17.7	HMDB33147	Cloransulam-methyl	3
132.0566	289.5	HMDB33172	3-Methylpyrrolo12-apyrazine	3
277.0118	21.7	HMDB33209	Fenthion	3
447.1985	29.5	HMDB33273	Cubebinin	3
111.045	288.4	HMDB33569	Syoyualdehyde	3
337.1431	18.2	HMDB33671	2-O-Methylglabridin	3
133.0656	221.7	HMDB33716	3-Phenylpropanal	3
117.0378	23.8	HMDB33856	S-Propyl thioacetate	3
114.0559	288.3	HMDB34208	Pterolactam	3
171.0411	279.2	HMDB34322	L-alpha-Amino-5-oxo-2(5H)-isoxazolepropanoic acid	3
557.2	19.5	HMDB34402	Physalin I	3
377.2104	243.4	HMDB34566	Neotame	3
263.0776	21.2	HMDB34681	3-Hydroxy-4-butanolide	3
451.1274	19.7	HMDB34753	7-Hydroxybutylidenephthalide 7-(6-malonylglucoside)	3
433.1899	183	HMDB34899	11-Ethylidenebistryptophan	3
309.2076	290.2	HMDB35337	Sterebin A	3
273.1863	214.7	HMDB35579	1-Phenyl-13-dodecanedione	3
287.2019	225.3	HMDB36205	alpha-Amylcinnamyl isovalerate	3
263.2384	256.2	HMDB37543	()-(Z)-2-(5-Tetradecenyl)cyclobutanone	3
291.1228	22.3	HMDB37774	Coriandrone A	3
261.1862	229.8	HMDB37832	Vetiveryl acetate	3
216.0878	27.7	HMDB38447	1-Isothiocyanato-8-(methylthio)octane	3
138.9705	288.2	HMDB38891	Ethyl methyl trisulfide	3
243.0517	17.4	HMDB39177	1-O-Galloylglycerol	3
662.1028	17.4	HMDB39421	Fenugreekine	3
229.0363	18.4	HMDB39670	33-Dithiobis45-dihydro-2-methylfuran	3
149.0456	18.9	HMDB40056	xi-1-(Propylthio)-1-propanethiol	3
269.1764	290.3	HMDB40459	Ethylene brassylate	3
401.1802	26.5	HMDB40729	D-Linalool 3-(6-malonylglucoside)	3
309.1733	282.6	HMDB40756	3-Hydroxy-68-dimethoxy-7(11)-eremophilen-128-olide	3
397.1696	182	HMDB41101	Kanzonol M	3
289.0528	18.2	HMDB41121	2-(4-Hydroxyphenyl)naphthalic anhydride	3
484.2666	289.1	HMDB41421	Sarcodon scabrosus Depsipeptide	3
381.1388	20.2	HMDB05000	Loratadine	4
215.033	20.1	HMDB06088	Scyllitol	4

648.74	50.1	HMDB14416	Diatrizoate	4
135.0303	19.4	HMDB14581	Allopurinol	4
421.1553	183	HMDB14816	Losartan	4
482.1044	18.3	HMDB14837	Nicergoline	4
415.3214	245.1	HMDB15046	Paricalcitol	4
308.187	248.3	HMDB15334	Nadolol	4
528.1776	194.2	HMDB15595	Nilotinib	4
232.0595	18.7	HMDB33349	Casimiroin	4
173.0085	20	HMDB33717	(1R2R)-Isocitric acid	4
231.0518	18.4	HMDB37808	Hexahydro-24-dimethylspiro13-dithiolo45-cfuran-23(2H)-furan	4
385.1503	20.9	HMDB39570	Methylsyringin	4
445.3328	221	HMDB40999	Secasterone	4
367.1594	21.2	HMDB41255	(2S)-2-Butanol O-b-D-Apiofuranosyl-(1-6)-b-D-glucopyranoside	4
154.0623	23.2	HMDB00177	L-Histidine	4
453.2714	256.1	HMDB01850	Verapamil	4
136.0401	176.7	HMDB01891	m-Aminobenzoic acid	4
311.1336	21.4	HMDB05012	Olanzapine	4
293.1763	270.5	HMDB05783	Gingerol	4
247.0757	18	HMDB14350	Pyrimethamine	4
612.3524	222.7	HMDB14369	Indinavir	4
356.0668	16.9	HMDB14473	Indomethacin	4
270.9867	16.8	HMDB14543	Zoledronate	4
337.206	285.1	HMDB14727	Lisuride	4
316.9483	37.5	HMDB14786	Mitotane	4
474.286	183.3	HMDB14907	Hydrocortamate	4
148.0438	22.4	HMDB14997	Penicillamine	4
331.1483	29.6	HMDB15055	Spectinomycin	4
505.0428	19.5	HMDB15199	Cefditoren	4
382.0312	21.8	HMDB15427	Ceftizoxime	4
356.0579	16.9	HMDB15533	Cinolazepam	4
313.079	272.1	HMDB15667	Sulfaphenazole	4
195.1391	285.6	HMDB31030	6-Heptyl-56-dihydro-2H-pyran-2-one	4
94.0662	17.9	HMDB32973	25-Dimethyl-1H-pyrrole	4
313.2026	285.2	HMDB32995	2-Undecyl-4(1H)-quinolinone N-oxide	4
187.1339	284	HMDB33201	9-Hydroxydecanoic acid	4
169.1233	287.9	HMDB33203	6-Decanolide	4
129.0556	289.8	HMDB33286	Sherry lactone	4
273.039	18.3	HMDB33326	BR-Xanthone B	4
176.0715	58.1	HMDB33482	Plantagonine	4

555.1283	20.3	HMDB33488	Aurasperone D	4
97.0656	94	HMDB33549	(E)-4-Hexenal	4
121.0158	20.6	HMDB33552	()-13-Butanedithiol	4
429.0841	17.3	HMDB33587	Coumestrin	4
176.039	18.4	HMDB33592	(R)C(S)S-Alliin	4
314.1227	99.2	HMDB33664	N-Hydroxysaxitoxin	4
160.0616	21.1	HMDB33747	()-22-Iminobispropanoic acid	4
211.0618	294.1	HMDB33835	Propyl gallate	4
280.099	17.3	HMDB33954	Juzirine	4
85.0294	19.6	HMDB33977	Methyl acrylate	4
115.0763	256.3	HMDB34163	3-Methylbutyl formate	4
207.0678	19.2	HMDB34315	3-(34-Dimethoxyphenyl)-2-propenoic acid	4
173.0933	19.3	HMDB34365	L-Theanine	4
165.0407	19.4	HMDB34394	S-Propyl 1-propanesulfinothioate	4
193.1232	194.8	HMDB34450	Neocnidilide	4
210.0411	18.4	HMDB34864	24-Dihydroxy-7-methoxy-2H-14-benzoxazin-3(4H)-one	4
124.0768	17.5	HMDB34883	34-Dihydro-5-propanoyl-2H-pyrrole	4
166.0511	23.6	HMDB34887	3alpha457alpha-Tetrahydro-5-hydroxy-1H-isoindole-13(2H)-dione	4
231.012	98.3	HMDB35145	Chrycolide	4
471.3488	238.8	HMDB35258	Azukisapogenol	4
377.2725	249.3	HMDB35273	1-Acetoxy-2-hydroxy-51215-heneicosatrien-4-one	4
333.204	208.6	HMDB35286	Crispanone	4
249.1862	203.3	HMDB35293	Norambreinolide	4
473.3644	262.2	HMDB35326	Ganoderiol A	4
385.2605	290.1	HMDB36015	Mangalkanyl glucoside	4
171.1026	269.9	HMDB36213	cis-3-Hexenyl lactate	4
739.4266	192.1	HMDB36248	Schidigerasaponin D5	4
113.0438	18.4	HMDB36491	Di-2-propenyl sulfide	4
164.0352	284.4	HMDB36582	6-Methoxy-2(3H)-benzoxazolone	4
134.0611	27.7	HMDB37071	2-Acetyl-4-methylpyridine	4
623.1588	232.9	HMDB37085	Isorhamnetin 3-O-b-D-glucopyranosyl-(1-2)-a-L-rhamnopyranoside	4
664.3471	175.3	HMDB37300	Jubanine C	4
639.1526	212	HMDB37358	Ranupenin 3-rutinoside	4
637.1746	232.2	HMDB37462	Tricin 7-neohesperidoside	4
186.1135	281.2	HMDB37790	Polyethylene glycol	4
189.0406	19	HMDB37815	5-(Methylthio)-2-(methylthio)methyl-2-pentenal	4
280.1046	18.5	HMDB37843	N-(1-Deoxy-1-fructosyl)threonine	4
367.2492	248.4	HMDB37961	gamma-Eudesmol rhamnoside	4
295.1551	186.4	HMDB38120	Ovalicin	4

267.1595	280.9	HMDB38153	1-(3-Furanyl)-67-dihydroxy-48-dimethyl-1-nonanone	4
373.2781	237	HMDB38522	2-(10-Heptadecenyl)-6-hydroxybenzoic acid	4
378.1788	31.1	HMDB38642	Fumitremorgin C	4
328.1524	18.6	HMDB38724	xi-Anomuricine	4
249.1136	290.7	HMDB38804	34-Dihydro-6-hydroxy-2578-tetramethyl-2H-1-benzopyran-2-carboxylic acid	4
218.0437	20.8	HMDB39164	L-Oxalylalbizziine	4
240.9291	25	HMDB39459	Di-2-propenyl pentasulfide	4
365.1427	19.6	HMDB39610	Curcumin II	4
221.9558	82.3	HMDB40147	2-Bromo-1H-indole-3-carboxaldehyde	4
461.1228	16.5	HMDB40533	Artomunoxanthentrione epoxide	4
353.0529	201	HMDB40570	2-O-p-Coumaroylhydroxycitric acid	4
397.3694	292	HMDB40909	2-Hydroxy-22-methyltetracosanoic acid	4
736.4924	265.8	HMDB40991	Ternatin	4
277.06	258.7	HMDB41200	Dehydroxymethylflazine	4
441.1603	21	HMDB41225	b-D-Xylopyranosyl-(1-4)-a-L-rhamnopyranosyl-(1-2)-D-fucose	4
340.0714	17	HMDB41247	Alkaloid A6	4
317.0818	172.4	HMDB41451	Musanolone F	4
163.0396	163.8	HMDB41592	Coumaric acid	4
128.01	291.7	HMDB41861	Cyanuric acid	4
131.0357	292	HMDB29884	2-C-Methyl-14-erythrono-D-lactone	5
220.0501	20.2	HMDB34912	(S)-N-(45-Dihydro-1-methyl-4-oxo-1H-imidazol-2-yl)alanine	5
447.2757	236	HMDB40993	(ent-2b4S9a)-249-Trihydroxy-10(14)-oplopen-3-one 2-(2-methylbutanoate) 9-(3-methyl-2E-pentenoate)	5
130.087	172.5	HMDB00172	L-Isoleucine	5
218.1037	276.6	HMDB00210	Pantothenic acid	5
193.0505	22.2	HMDB00954	trans-Ferulic acid	5
143.1076	255.6	HMDB01877	Valproic acid	5
179.035	286.9	HMDB01879	Aspirin	5
107.05	284.5	HMDB02055	o-Cresol	5
109.0293	20.8	HMDB02434	Hydroquinone	5
160.0404	30.9	HMDB03320	Indole-3-carboxylic acid	5
151.1128	21	HMDB03450	(-)-trans-Carveol	5
169.0129	51.6	HMDB05807	Gallic acid	5
156.1029	274.4	HMDB14447	Tranexamic Acid	5
297.1711	288.3	HMDB14943	Minaprine	5
193.0731	290.8	HMDB14962	Enprofylline	5
211.0192	18.6	HMDB15045	Zonisamide	5
197.0573	292.3	HMDB15188	Mimosine	5
278.1485	285.5	HMDB15228	Oxamniquine	5
220.147	265.3	HMDB15299	Procarbazine	5

352.2252	265.5	HMDB15358	Levomethadyl Acetate	5
281.0559	20	HMDB15573	Niflumic Acid	5
678.4005	199.4	HMDB15616	Telaprevir	5
283.1192	290	HMDB29819	2-Phenylethyl beta-D-glucopyranoside	5
239.0771	20	HMDB29954	D-glycero-L-galacto-Octulose	5
127.1127	23.4	HMDB31296	(E)-2-Octen-1-ol	5
113.0607	282.9	HMDB31501	3-Hexenoic acid	5
253.1087	291.4	HMDB32796	Methyl 3-(23-dihydroxy-3-methylbutyl)-4-hydroxybenzoate	5
226.1092	291.5	HMDB32928	2-Amino-348-trimethyl-3H-imidazo45-fquinoxaline	5
247.1191	283.4	HMDB33064	(E)-2-Methyl-2-buten-1-ol O-beta-D-Glucopyranoside	5
201.077	281.3	HMDB33092	3-(1-Hydroxymethyl-1-propenyl)pentanedioic acid	5
357.2073	206.7	HMDB33443	Sorgoleone 358	5
117.0457	293.1	HMDB33576	7-Azaindolizine	5
325.0928	127.3	HMDB33581	trans-o-Coumaric acid 2-glucoside	5
125.0607	288.6	HMDB33629	xi-4-Hydroxy-4-methyl-2-cyclohexen-1-one	5
137.0606	285.9	HMDB34241	4-Methoxybenzyl alcohol	5
150.0016	178.9	HMDB34413	12-Benzisothiazol-3(2H)-one	5
235.1347	290	HMDB34462	Heptyl 4-hydroxybenzoate	5
225.1862	286.4	HMDB34561	Houttuynin	5
168.0666	19.3	HMDB35178	6-Acetyl-23-dihydro-2-(hydroxymethyl)-4(1H)-pyridinone	5
165.092	41.8	HMDB35235	247-Decatrienoic acid	5
141.092	287.5	HMDB35422	4-Butyl-gamma-butyrolactone	5
171.1389	263.1	HMDB35595	trans-p-Menthane-18-diol	5
195.0672	287.3	HMDB35721	(S)-Batatic acid	5
151.0763	286.7	HMDB36169	3-(5-Methyl-2-furanyl)butanal	5
187.0976	287.8	HMDB36233	Butyl ethyl malonate	5
569.2706	176	HMDB36360	Pipercyclobutanamide A	5
143.0712	284.5	HMDB36594	Botryodiplodin	5
221.1182	81.3	HMDB36819	Dehydrovomifoliol	5
153.092	284.6	HMDB37276	Octahydro-2H-1-benzopyran-2-one	5
209.1548	290	HMDB37390	Tsibulin 1	5
219.1389	197.2	HMDB37714	Hexyl phenylacetate	5
287.2232	260.2	HMDB37798	(S)-1016-Dihydroxyhexadecanoic acid	5
609.5106	255.4	HMDB38058	Glycerol 1-dodecanoate 2-tetradecanoate 3-octanoate	5
335.2595	226.2	HMDB38105	Isolinderanolide	5
241.0724	289.8	HMDB38126	Genipinic acid	5
263.0065	21.9	HMDB38142	58-Dihydro-6-(4-methyl-3-pentenyl)-1234-tetrathiocin	5
169.0869	287.2	HMDB38276	cis-3-Hexenyl pyruvate	5
239.0928	20.4	HMDB38627	Ethyl 345-trimethoxybenzoate	5

175.0363	18.3	HMDB38668	L-3-Amino-2-(oxalylamino)propanoic acid	5
267.1241	283.2	HMDB38935	Kamahine C	5
173.1012	291.1	HMDB39466	Hexanethioic acid S-propyl ester	5
183.1026	282.4	HMDB39710	1-Acetylcyclohexyl acetate	5
339.2358	252.5	HMDB39762	11-111-Undecanediylbis(oxy)bisbenzene	5
117.0748	86.6	HMDB39806	1-Hexanethiol	5
144.9792	48.5	HMDB39828	4-Mercapto-5-methyl-3(2H)-thiophenone	5
185.1547	270.4	HMDB40171	Heptyl 2-methylpropanoate	5
201.0405	277.3	HMDB40275	Ethyl aconitate	5
131.0712	285.3	HMDB40409	Ethyl ()-3-hydroxybutyrate	5
301.1297	289.3	HMDB40462	Garcinia lactone dibutyl ester	5
255.1972	287.3	HMDB40904	Ipomeatetrahydrofuran	5
479.3385	286.8	HMDB41130	24-Epibrassinolide	5
225.0782	291.6	HMDB41560	246-Trimethoxyphenyl acetate	5
276.0083	25.4	HMDB41893	Fenitrothion	5
299.202	289.6	HMDB41925	Metandienone	5
235.1704	203.3	HMDB02352	Capsidiol	6
253.2177	236.7	HMDB12328	Palmitelaidic acid	6
368.1628	21.4	HMDB15633	Amisulpride	6
453.2328	21.3	HMDB33370	Ethyl cellulose	6
321.2085	207.5	HMDB33615	(S)-8-Gingerol	6
309.0406	17.3	HMDB33657	De-O-methylsterigmatocystin	6
219.1756	236.4	HMDB33826	26-Di-tert-butyl-4-methylphenol	6
247.1706	227.4	HMDB36221	2-(Dimethoxymethyl)-1-heptenylbenzene	6
227.2018	289.9	HMDB38034	Nonyl isovalerate	6
585.4868	272.3	HMDB38713	Erythrinasinate A	6
361.236	242	HMDB39226	(Z)-24-Dihydroxy-6-(8-pentadecenyl)benzoic acid	6
233.1913	241.9	HMDB40179	26-Di-tert-butyl-4-ethylphenol	6
395.1895	25.4	HMDB40305	(S)-(E)-2-(36-Dimethyl-2-heptenyl)-347-trihydroxyflavanone	6
405.1911	49.7	HMDB41091	1-(4-Hydroxy-35-dimethoxyphenyl)-7-(4-hydroxy-3-methoxyphenyl)-35-heptanediol	6
145.0982	42	HMDB00182	L-Lysine	6
149.0094	220.3	HMDB00956	Tartaric acid	6
149.0969	204.3	HMDB01878	Thymol	6
205.1232	197.9	HMDB01925	Ibuprofen	6
197.0456	22.1	HMDB02085	Syringic acid	6
176.0201	18	HMDB05792	Sulforaphane	6
266.0896	151.2	HMDB14340	Vidarabine	6
240.0886	18.1	HMDB14567	Methocarbamol	6
655.1478	192.5	HMDB14587	Teniposide	6

197.0932	289.6	HMDB14606	Metharbital	6
450.1757	186.7	HMDB14728	Doxazosin	6
331.0623	22.5	HMDB14831	Fluorescein	6
413.1959	195.4	HMDB14838	Eplerenone	6
389.1787	22	HMDB14875	Meclizine	6
198.0418	292.2	HMDB14904	Clavulanate	6
311.1864	200.4	HMDB15026	Granisetron	6
311.1765	233.7	HMDB15191	Praziquantel	6
413.1249	19.8	HMDB15310	Podofilox	6
232.0843	293.6	HMDB15337	Lomustine	6
244.1707	216.4	HMDB15340	Dezocine	6
416.2195	20.9	HMDB15433	Cilazapril	6
410.1708	22.7	HMDB15439	Tasosartan	6
288.1139	17.1	HMDB15585	Chlophedianol	6
379.1572	237.1	HMDB15613	Ecabet	6
410.2706	198.8	HMDB15648	Fesoterodine	6
325.0541	180.5	HMDB29199	Fertaric acid	6
229.1444	165.8	HMDB30143	Talaromycin A	6
221.0821	269.5	HMDB30725	Dillapiol	6
181.1595	192.4	HMDB32279	2-Ethyl-133-trimethyl-2-norbornanol	6
449.0442	211.4	HMDB32738	CI Food Red 6	6
209.1184	284.9	HMDB32871	Sedanonic acid	6
161.0458	265	HMDB32873	Diethyl dicarbonate	6
95.0138	25.9	HMDB32914	2-Furancarboxaldehyde	6
211.0386	36.3	HMDB32997	2-Hydroxyxanthone	6
225.054	22.1	HMDB32998	2-Methoxyxanthone	6
347.1718	219.9	HMDB33009	Foeniculoside VIII	6
185.1183	280	HMDB33010	(1S2S4S5R)-18-Epoxy-p-menthane-25-diol	6
343.1405	29.1	HMDB33066	(-)-erythro-Anethole glycol 1-glucoside	6
142.0662	22.9	HMDB33115	6-Methylquinoline	6
186.0561	23.1	HMDB33249	6-Chloro-N-(1-methylethyl)-135-triazine-24-diamine	6
313.1655	288.5	HMDB33347	Lotusine	6
310.1057	294.5	HMDB33361	Norisodomesticine	6
191.1076	207.3	HMDB33380	3-Methylbutyl benzoate	6
99.0276	21.3	HMDB33564	23-Dihydro-2-methylthiophene	6
281.0454	17.5	HMDB33588	9-O-Methylcoumestrol	6
265.1178	187.6	HMDB33598	N5-(4-Methoxybenzyl)glutamine	6
209.0814	292.6	HMDB33798	3-Methyl-1-(246-trihydroxyphenyl)-1-butanone	6
279.0888	17.2	HMDB33884	Gravolenic acid	6

135.0812	206.1	HMDB33962	3-Phenyl-1-propanol	6
145.0143	17.3	HMDB33966	Di-2-propenyl disulfide 9CI	6
325.1079	276.9	HMDB34015	16-Dihydroxy-3-methoxy-2-prenylxanthone	6
297.1515	282.7	HMDB34054	Auraptene	6
118.0145	290.4	HMDB34259	Bovinocidin	6
304.0622	17.9	HMDB34364	Cepharadione A	6
289.0875	284	HMDB34688	23-Dihydro-23-dihydroxy-9-phenyl-1H-phenalen-1-one	6
365.1208	178.3	HMDB34752	7-beta-D-Glucopyranosyloxybutylidenephthalide	6
177.1282	205.1	HMDB35055	11-Methyl-7-oxatetracyclo6310160411dodecane	6
192.1028	201.1	HMDB35072	2-Methylpropyl 2-aminobenzoate	6
607.1643	259.5	HMDB36009	Physcion 8-gentiobioside	6
231.1389	204.9	HMDB36110	(S)-Bilobanone	6
433.2813	290.3	HMDB37183	Polysorbate 60	6
171.0562	42.5	HMDB37296	3-Acetyl-27-naphthyridine	6
669.1639	192.3	HMDB37469	Spinacetin 3-gentiobioside	6
636.5294	257.6	HMDB37515	Hexabromodiphenyl ethers	6
177.0058	18.5	HMDB37553	SS-Ethylidene dithioacetate	6
223.1339	178.6	HMDB37726	Octyl 2-furoate	6
691.5889	288.5	HMDB38059	Glycerol 1-(9Z-octadecenoate) 2-octanoate 3-tetradecanoate	6
258.1099	290	HMDB38516	Linatine	6
174.0558	193.5	HMDB38628	Hydroxymethyl indol-3-yl ketone	6
101.0429	24.4	HMDB38892	1-(Methylthio)-1-butene	6
145.0869	288.3	HMDB39407	Methyl ()-3-hydroxyhexanoate	6
597.4217	251.5	HMDB39594	Hericenone G	6
262.9364	100.8	HMDB39734	23579-Pentathiadecane 22-dioxide	6
273.0827	22.3	HMDB39877	Charine	6
175.0442	18.3	HMDB40003	Methylthio 2-(propanoyloxy)propanoate	6
289.1246	25.4	HMDB40916	2-(4-Methyl-3-pentenyl)anthraquinone	6
379.2867	258.5	HMDB41103	Persin	6
248.9395	159.8	HMDB41188	Bis(methylsulfonylmethyl) disulfide	6
335.1395	21.9	HMDB41519	Nb-Feruloyltryptamine	6
258.0738	290	HMDB41934	Mizoribine	6
286.0682	17.7	HMDB14445	Tenofovir	7
387.1639	259.3	HMDB14909	Clidinium	7
285.2232	240.8	HMDB14996	Drostanolone	7
389.1617	259.6	HMDB15464	Yohimbine	7
435.1035	203	HMDB15561	Zuclopenthixol	7
577.3744	203.2	HMDB30046	Asparagoside A	7
403.1394	194.8	HMDB34117	(E)-4-Methylresveratrol 3-glucoside	7

385.1281	247.1	HMDB34629	(7R8S)-Methyl 47-epoxy-38-bilign-7-ene-49-dihydroxy-35-dimethoxy-9-oate	7
401.1237	218.3	HMDB35415	334568-Hexamethoxyflavone	7
291.1941	219.5	HMDB38035	Panaquinquecol 1	7
387.2866	163.7	HMDB38523	Methyl 2-(10-heptadecenyl)-6-hydroxybenzoate	7
419.1743	259.4	HMDB40787	Murrastifoline F	7
241.2176	250.8	HMDB40998	7(14)-Farnesene-912-diol	7
401.1422	191.3	HMDB41190	Benzyl beta-primeveroside	7
341.1089	145.4	HMDB00048	Melibiose	7
276.1121	22.4	HMDB01495	Queuine	7
137.0243	282.4	HMDB01895	Salicylic acid	7
149.0607	286.4	HMDB02097	4-Ethylbenzoic acid	7
165.0191	122.5	HMDB02107	Phthalic acid	7
595.3815	190.4	HMDB02204	Astaxanthin	7
323.155	227.2	HMDB05038	Citalopram	7
301.0739	28.3	HMDB05782	Hesperetin	7
205.0354	149.7	HMDB06471	Methylisocitric acid	7
411.1954	221	HMDB14355	Adapalene	7
445.199	182.3	HMDB14420	Olmesartan	7
519.2131	172.4	HMDB14538	Beclometasone dipropionate	7
351.0615	37.4	HMDB14544	Griseofulvin	7
436.1642	259.4	HMDB14761	Fluphenazine	7
183.0603	140.7	HMDB14815	Isoflurophate	7
235.0534	26.8	HMDB14882	Zileuton	7
367.2268	287	HMDB14928	Perindopril	7
210.0885	289.6	HMDB15078	Zalcitabine	7
356.1623	284.6	HMDB15147	Cinacalcet	7
389.2109	256.2	HMDB15180	Lubiprostone	7
272.0158	25.5	HMDB15309	Chlormezanone	7
423.1684	259.7	HMDB15321	Clindamycin	7
546.2296	163.7	HMDB15393	Darunavir	7
288.0195	25.1	HMDB15420	Quinethazone	7
309.1394	186.8	HMDB15583	Bifonazole	7
703.3896	285.5	HMDB15597	Voacamine	7
384.1217	20.1	HMDB15657	Nilvadipine	7
427.3222	278.7	HMDB15694	Nandrolone decanoate	7
349.0242	24.8	HMDB32902	Sodium 6-hydroxy-5-(phenylazo)-2-naphthalenesulfoniate	7
161.0356	288.7	HMDB32927	Quindoxin	7
423.0919	16.3	HMDB33145	Azimsulfuron	7
166.0144	136.9	HMDB33161	26-Pyridinedicarboxylic acid	7

263.1299	284.3	HMDB33227	Curcolonol	7
277.1449	252.5	HMDB33244	Dibutyl phthalate	7
334.0724	17	HMDB33367	Oxonantenine	7
321.086	22.3	HMDB33457	Flazine methyl ether	7
179.0207	18.2	HMDB33556	25-Dimethyl-14-dithiane-25-diol	7
270.0367	24	HMDB33602	Brassica oleracea Alkaloid	7
167.1075	67.7	HMDB33700	(-)-(Z)-Tetrahydro-6-(2-pentenyl)-2H-pyran-2-one	7
160.0252	17.8	HMDB33764	Erucin	7
150.0557	197.6	HMDB33903	3alpha477alpha-Tetrahydro-1H-isoindole-13(2H)-dione	7
433.1268	204.1	HMDB34021	Artobiloxanthone	7
116.0505	22.7	HMDB34171	Benzeneacetonitrile	7
193.0878	286.6	HMDB34206	Ethyl 4-methylphenoxyacetate	7
126.0196	25.7	HMDB34368	Hydroxyminaline	7
417.0487	37.4	HMDB34590	Shoyuflavone C	7
157.1233	262	HMDB34606	Hexyl propionate	7
337.0551	18.7	HMDB34621	2-O-Acetyl-trans-coutaric acid	7
437.1452	259.7	HMDB34698	7-Hydroxy-5-(4-hydroxy-2-oxopentyl)-2-methylchromone 7-glucoside	7
291.1606	270	HMDB34738	Isotrichodermin	7
353.0918	19.2	HMDB34854	Flumioxazin	7
287.1042	35	HMDB34881	3-Carboxy-2349-tetrahydro-1H-pyrido34-bindole-1-propanoic acid	7
333.1101	20.4	HMDB34937	Cappariloside A	7
485.3274	185.3	HMDB35259	28-Hydroxyglycyrrhetic acid	7
413.3436	200.5	HMDB35586	1-Phenyl-13-docosanedione	7
389.1423	251.1	HMDB35876	Mesuagin	7
122.0611	18.3	HMDB36058	1-Ethyl-1H-pyrrole-2-carboxaldehyde	7
295.1212	17	HMDB36156	Deoxynivalenol	7
209.0666	155.8	HMDB36431	139-Trimethyluric acid	7
240.0497	17.7	HMDB37548	24-Dihydroxy-67-dimethoxy-2H-14-benzoxazin-3(4H)-one	7
145.0696	131.2	HMDB37621	4-Methyl-4-(methylthio)-2-pentanone	7
487.3433	185.7	HMDB37782	Ganoderiol D	7
236.0782	19	HMDB37848	N-(1-Deoxy-1-fructosyl)glycine	7
429.338	293.2	HMDB37914	(2beta3alpha9alpha24R)-Ergosta-722-diene-239-triol	7
390.0513	33.8	HMDB38418	Glucoconringiin	7
262.1236	20	HMDB38573	Lansiumamide B	7
220.0841	293.2	HMDB38751	Avenic acid B	7
174.0409	17.7	HMDB39163	D-N-(Carboxyacetyl)alanine	7
375.2524	279.9	HMDB39278	12-Gingerdione	7
148.0767	26.9	HMDB39662	2367-Tetrahydrocyclopentbazepin-8(1H)-one	7
130.0683	146.4	HMDB40058	()-2-Propylthiazolidine	7

360.1222	17.5	HMDB40546	Pyriminobac-methyl	7
196.9763	15.2	HMDB40585	()-Sulfobutanedioic acid	7
339.1965	266.5	HMDB40635	Piperochromenoic acid	7
117.0556	290	HMDB40735	Ethyl lactate	7
280.0135	17.6	HMDB41052	Ajocysteine	7
179.0827	18.5	HMDB41109	(S)-3-Ethylidenehexahydropyrrolo12-apyrazine-14-dione	7
385.1174	21.9	HMDB41175	1-O-Sinapoylglucose	7
397.1111	219.5	HMDB41285	Picraquassioside A	7
459.0611	252	HMDB41341	Flupoxam	7
377.1001	17.4	HMDB41441	11-Methylgerberinol	7
229.1084	281.8	HMDB41448	Dicyclohexyl disulfide	7
256.06	20.7	HMDB41468	135-Trihydroxy-10-methylacridone	7
335.1565	227.8	HMDB41541	N2-Fructopyranosylarginine	7
163.0513	291.8	HMDB42006	Ricinine	7
129.0187	22.6	HMDB00426	Citramalic acid	8
269.2491	285.8	HMDB02259	Heptadecanoic acid	8
146.0459	19	HMDB03339	D-Glutamic acid	8
310.121	175.5	HMDB14977	Tolazamide	8
345.1099	20.3	HMDB15247	Nifedipine	8
189.0519	18.6	HMDB15673	Carglumic acid	8
133.0145	18.7	HMDB32872	Velcorin	8
306.0772	17.8	HMDB33247	Aristolodione	8
379.1177	16.9	HMDB33883	3-O-Methylglycyrol	8
203.1038	19	HMDB33891	N6-Acetyl-5S-hydroxy-L-lysine	8
345.2435	166.9	HMDB33897	Ginkgoic acid	8
273.1252	20.3	HMDB34885	Imazamethabenz	8
271.1093	43.8	HMDB35191	(2S4R)-4-(9H-Pyrido34-bindol-1-yl)-124-butanetriol	8
295.2646	290.4	HMDB35575	46-Nonadecanedione	8
367.2856	223.7	HMDB38073	Octadecyl fumarate	8
138.0561	19.4	HMDB38174	5-Acetyl-24-dimethyloxazole	8
305.0685	17.5	HMDB38361	(-)-Epigallocatechin	8
461.3644	281.2	HMDB39713	(3beta22R23R24S)-32223-Trihydroxystigmastan-6-one	8
175.0249	19.9	HMDB00044	Ascorbic acid	8
167.0352	289.3	HMDB00484	Vanillic acid	8
189.0883	20.1	HMDB01370	Diaminopimelic acid	8
344.1103	17.3	HMDB01913	Omeprazole	8
343.2279	145.7	HMDB01939	Medroxyprogesterone	8
252.1002	290	HMDB01940	Triamterene	8
119.0353	289.7	HMDB02649	Erythrose	8

191.0574	290.4	HMDB03072	Quinic acid	8
469.2572	172.8	HMDB03218	Withanolide	8
250.0938	19.9	HMDB03254	Muramic acid	8
253.049	18.2	HMDB03312	Daidzein	8
132.0303	20.1	HMDB11753	Iminodiacetic acid	8
217.1205	22.7	HMDB14515	Meprobamate	8
296.112	167.7	HMDB14619	Duloxetine	8
206.1038	22.4	HMDB14634	Miglitol	8
165.05	260.8	HMDB14747	Ethionamide	8
431.2803	173.6	HMDB14792	Latanoprost	8
220.0982	18	HMDB14798	Metaxalone	8
415.2468	201	HMDB14940	Alfentanil	8
383.2225	223.2	HMDB14961	Ethynodiol Diacetate	8
188.0715	74.7	HMDB14970	Phensuximide	8
366.0319	40.3	HMDB14971	Cefaclor	8
227.0676	18.7	HMDB15023	Pemirolast	8
555.3877	210.8	HMDB15079	Demecarium	8
237.0887	17.8	HMDB15084	Felbamate	8
370.0391	16.9	HMDB15093	Carboplatin	8
477.2645	176.3	HMDB15220	Iloprost	8
199.0016	17.9	HMDB15366	Sevoflurane	8
263.0612	17.6	HMDB15521	Sulfamerazine	8
299.0474	42	HMDB15544	Tazobactam	8
275.1783	171.8	HMDB15555	Molindone	8
411.2908	224.8	HMDB15567	Calcipotriol	8
505.2755	212.9	HMDB15593	Ixabepilone	8
319.0443	17.9	HMDB30835	trans-334557-Hexahydroxyflavanone	8
127.0763	286.7	HMDB31174	4-Methyl-5-hexanolide	8
163.0249	17.8	HMDB32741	S-2-Propenyl 1-propanesulfinothioate	8
236.0935	28.3	HMDB32775	3-Hydroxy-carbofuran	8
282.1111	292.5	HMDB32845	2-Methyl(3-phenylpropanoyl)aminobenzoic acid	8
141.0193	25.2	HMDB32923	Kojic acid	8
259.0829	289.9	HMDB32924	3-Furanmethanol glucoside	8
95.0502	15.7	HMDB32965	24-Dimethylfuran	8
217.0489	20.6	HMDB32989	4-Methylumbelliferyl acetate	8
333.0602	18.5	HMDB33014	Hovenitin I	8
321.1313	20.1	HMDB33105	N2-Galacturonyl-L-lysine	8
335.127	17.8	HMDB33107	Semilepidinoside A	8
125.0179	21.3	HMDB33152	2-(Methylthio)pyrazine	8

218.0825	37.3	HMDB33436	Nigellimine N-oxide	8
146.0823	21.6	HMDB33453	Fagomine	8
238.0845	294.3	HMDB33519	N-Ornithyl-L-taurine	8
518.2868	182.3	HMDB33617	Vignatic acid B	8
277.0549	20.3	HMDB33626	D-Erythroascorbic acid 1-a-D-xylopyranoside	8
330.1184	28	HMDB33665	N-Hydroxyneosaxitoxin	8
180.0307	20.4	HMDB33733	24-Dihydroxy-2H-14-benzoxazin-3(4H)-one	8
207.1025	182.4	HMDB33778	Elemicin	8
375.1207	17.5	HMDB33932	Cinnatriacetin A	8
335.0896	17.6	HMDB34027	Sojagol	8
321.1152	23.8	HMDB34173	Phaseollin	8
237.2232	264.8	HMDB34181	3-Methylcyclopentadecanone	8
130.0675	32	HMDB34236	Benzenepropanenitrile	8
192.0666	45.3	HMDB34250	Betamipron	8
201.0884	15.5	HMDB34266	L-Coprine	8
245.0439	19.2	HMDB34312	Isopimpinellin	8
393.1331	19.2	HMDB34436	Rotenone	8
275.018	17	HMDB34454	5-(4-Acetoxy-1-butynyl)-22-bithiophene	8
397.1862	24.6	HMDB34575	3-Hydroxy-T2-triol	8
176.0941	291.7	HMDB35360	N-Methyl-1-deoxynojirimycin	8
510.2871	174.6	HMDB35368	Cytochalasin Ppho	8
352.1044	17.7	HMDB35502	Sambucus nigra Degraded cyanogenic glycosides (2-Epimer)	8
323.2959	259.5	HMDB35570	68-Heneicosanedione	8
251.068	18.6	HMDB35993	N5-(34-Dioxo-15-cyclohexadien-1-yl)-L-glutamine	8
119.0541	25.1	HMDB36149	3-Mercapto-3-methyl-1-butanol	8
164.0389	21	HMDB37057	Ethiin	8
187.0246	31.2	HMDB37157	2-Methyl-3-(propyldithio)furan	8
364.0828	17	HMDB37475	4beta-(2-Aminoethylthio)catechin	8
129.0387	18.3	HMDB37493	S-2-Propenyl propanethioate	8
228.0645	23.7	HMDB37614	Pteleine	8
517.3903	262.4	HMDB37781	Ganoderiol C	8
316.1158	18	HMDB37839	N-(1-Deoxy-1-fructosyl)histidine	8
342.1186	20.8	HMDB37845	N-(1-Deoxy-1-fructosyl)tyrosine	8
511.3055	193	HMDB38189	Carindone	8
196.0617	21.5	HMDB38336	2-Hydroxy-3-(34-dihydroxyphenyl)propanamide	8
102.056	19.6	HMDB38394	O-Acetylethanolamine	8
497.1029	16.7	HMDB38458	NN-Bis(gamma-glutamyl)cystine	8
204.0516	24.9	HMDB38461	1-Isothiocyanato-6-(methylsulfinyl)hexane	8
512.1686	17.5	HMDB38599	Acrimarine H	8

293.0784	24.1	HMDB38613	gamma-L-Glutamyl-L-methionine sulfoxide	8
187.0511	32.4	HMDB38633	(-)-3-Cyanomethyl-3-hydroxy-1H-indol-2(3H)-one	8
230.1187	20	HMDB38839	1-(m-Methoxycinnamoyl)pyrrolidine	8
331.1122	102.8	HMDB39002	Mytilin A	8
260.0785	19.2	HMDB39127	Pisatoside	8
136.0768	18.1	HMDB39657	123456-Hexahydro-7H-cyclopentabpyridin-7-one	8
355.0889	17.8	HMDB39722	2-O-beta-D-Glucopyranuronosyl-D-mannose	8
339.0921	19.2	HMDB39725	4-O-(4-O-Methyl-alpha-D-glucopyranuronosyl)-L-arabinose	8
471.1746	50.6	HMDB39741	alpha-L-Rhamnopyranosyl-(1-3)-alpha-D-galactopyranosyl-(1-3)-L-fucose	8
213.0601	18.2	HMDB40055	Ethyl 3-(2-furanylmethyl)thiopropanoate	8
190.0723	18.6	HMDB40332	Dihydro-6-isopropyl-24-dimethyl-4H-135-dithiazine	8
377.1372	18.5	HMDB40350	611-Dihydroxy-3-methyl-3-(4-methyl-3-pentenyl)-3H7H-pyrano23-cxanthen-7-one	8
133.0331	22.2	HMDB40410	Ethyl 3-mercaptopropanoic acid	8
311.1044	31.2	HMDB40435	Dictyoquinazol A	8
327.1354	39.2	HMDB40441	Dictyoquinazol B	8
300.0851	17.7	HMDB40515	gamma-Glutamyl-beta-(isoxazolin-5-on-2-yl)alanine	8
176.0353	41	HMDB40612	4-Acetyl-2(3H)-benzoxazolone	8
319.0996	21.7	HMDB41463	23-Dihydro-23-dihydroxy-4-(4-methoxyphenyl)-1H-phenalen-1-one	8
298.0917	56.8	HMDB41517	beta-D-Glucopyranosyl anthranilate	8
302.1231	31.7	HMDB41989	Pipemidic acid	8
466.3105	285.8	HMDB42042	Tiropramide	8
197.0224	20.5	HMDB14693	Methoxsalen	9
389.0763	202.3	HMDB36935	Dimethyl 2-galloylgalactarate	9
165.0556	286.6	HMDB00375	3-(3-Hydroxyphenyl)propanoic acid	9
175.0624	291.5	HMDB00402	2-Isopropylmalic acid	9
404.2157	192.2	HMDB01938	Lisinopril	9
285.0983	291.3	HMDB03546	Salicin	9
86.0239	31.7	HMDB03609	2-Aminoacrylic acid	9
101.0355	291.4	HMDB14405	Cycloserine	9
752.3974	174.3	HMDB14454	Vindesine	9
286.2152	263.7	HMDB14531	Procyclidine	9
232.1342	200.6	HMDB14566	Methylphenidate	9
507.1222	232.8	HMDB14596	Clomocycline	9
342.2153	170.8	HMDB14668	Dibucaine	9
228.0097	25.7	HMDB14714	Clonidine	9
393.1719	171.4	HMDB14758	Triamcinolone	9
277.1293	190.8	HMDB14944	Pentoxifylline	9
268.156	289.1	HMDB15088	Rizatriptan	9
373.2037	195.5	HMDB15094	Methylprednisolone	9

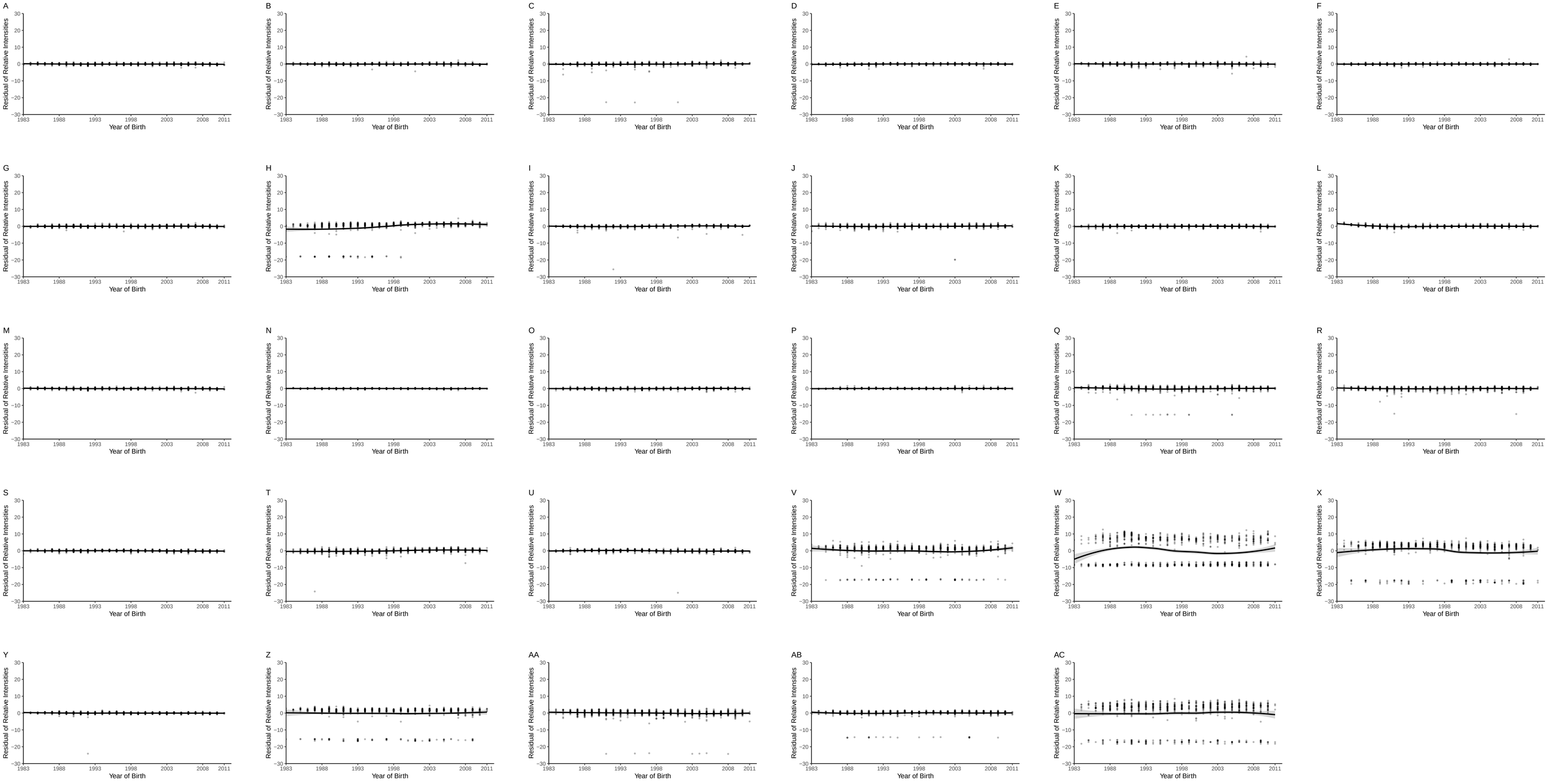
290.1764	203.8	HMDB15114	Cyclopentolate	9
384.9722	34.3	HMDB15142	Tioconazole	9
222.1134	195.7	HMDB15168	Cerulenin	9
267.0902	291.6	HMDB15302	Moclobemide	9
169.0981	291.1	HMDB15333	Levetiracetam	9
314.0784	198.2	HMDB15369	Chlorprothixene	9
211.966	44.5	HMDB15373	Chloroxine	9
241.084	285.7	HMDB15394	Telbivudine	9
212.0568	18.7	HMDB15627	Droxidopa	9
223.0977	17.1	HMDB30680	Diplosporin	9
101.0607	269.2	HMDB31175	Tetrahydro-2-furanmethanol	9
162.042	290.4	HMDB31187	Thialdine	9
191.071	293.5	HMDB31623	Ethyl phenylglycidate	9
407.2207	199	HMDB32021	cis-Methylbixin	9
179.0713	290	HMDB32174	Benzaldehyde glyceryl acetal	9
223.1705	280.2	HMDB32524	Terpinyl isobutyrate	9
258.0995	294.2	HMDB32769	Osmaronin	9
181.0176	291.4	HMDB32825	Dipropyl trisulfide	9
305.0821	193.7	HMDB32848	23-Dihydro-23-dihydroxy-4-(4-hydroxyphenyl)-1H-phenalen-1-one	9
491.1923	177.9	HMDB32906	Isolariciresinol 9-O-alpha-L-arabinofuranoside	9
118.9985	16.2	HMDB33052	Ethyl vinyl disulfide	9
211.0283	290.9	HMDB33061	1-(Methylsulfinyl)propyl propyl disulfide	9
237.0996	288.3	HMDB33065	(x)-12-Propanediol 1-O-b-D-glucopyranoside	9
239.0599	254.7	HMDB33071	Propyl 1-(propylsulfinyl)propyl disulfide	9
237.0442	290	HMDB33073	1-Propenyl 1-(propylsulfinyl)propyl disulfide	9
182.0721	186.7	HMDB33141	2-Amino-a-carboline	9
155.1076	286	HMDB33167	Ethyl cyclohexanecarboxylate	9
618.3128	37.4	HMDB33241	Glycylalanylprolylmethionylphenylalanylvalinamide	9
177.0557	289.4	HMDB33248	Di-alpha-furfuryl ether	9
277.1086	281.7	HMDB33262	Solanolone	9
127.0401	286.3	HMDB33285	L-erythro-5-(1-Hydroxyethyl)-2(5H)-furanone	9
296.1265	294	HMDB33435	()-Aegeline	9
275.1505	292.3	HMDB33460	4-Hydroxycinnamoylagmatine	9
496.2487	290.4	HMDB33471	N1N10-Diferuloylspermidine	9
246.0999	294.8	HMDB33699	Linamarin	9
180.1028	21.5	HMDB33868	beta-O-Methylynephrine	9
103.0586	21.3	HMDB33902	Isopentyl mercaptan	9
273.1107	293.7	HMDB33921	3-(11-Dimethyl-2-propenyl)-78-dimethoxy-2H-1-benzopyran-2-one	9
285.1105	294.6	HMDB34024	Isosativan	9

123.028	289	HMDB34448	Methyl phenyl sulfide	9
207.1391	287.5	HMDB34672	(5alpha8beta9beta)-59-Epoxy-36-megastigmadien-8-ol	9
305.1762	272.8	HMDB34780	Capsiate	9
147.0921	58.7	HMDB34892	3-Ethyl-5-methyl-2-vinylpyrazine	9
307.1555	287	HMDB35724	15-Deacetylcalonectrin	9
199.134	273.3	HMDB36029	Clarycet	9
431.1901	18.4	HMDB36131	S-Furanopetasitin	9
297.1347	287.1	HMDB36159	Toxin T2 tetrol	9
157.0869	276.3	HMDB36395	2-Methylpropyl 3-oxobutanoate	9
521.3339	294.1	HMDB37182	Polysorbate 20	9
138.0389	293	HMDB37285	24-Dimethyl-5-vinylthiazole	9
473.107	175.8	HMDB37341	Apigenin 7-O-(2-O-acetylglucoside)	9
913.4901	196.6	HMDB37926	Tragopogonsaponin L	9
345.1551	36.7	HMDB38149	Nepetaside	9
161.0221	36.5	HMDB38379	1-Piperazinecarbodithioic acid	9
128.0529	289.1	HMDB38433	1-Isothiocyanatopentane	9
218.0684	293	HMDB38441	1-Isothiocyanato-7-(methylsulfinyl)heptane	9
251.0929	292.1	HMDB38551	Methyl 345-trimethoxycinnamate	9
891.5199	215.6	HMDB38578	Chlorophyll a	9
725.1894	46.6	HMDB38767	Camelliaside B	9
249.0778	292.1	HMDB38926	Samin	9
229.0839	291.8	HMDB39110	(2S3S)-alpha-Amino-2-carboxy-5-oxo-1-pyrrolidinebutanoic acid	9
224.0942	294.5	HMDB39238	Cytokinin B	9
319.191	202.1	HMDB39276	8-Gingerdione	9
302.1355	23.2	HMDB39423	N5-Acetyl-N2-gamma-L-glutamyl-L-ornithine	9
171.0855	290.7	HMDB39467	Allyl thiohexanoate	9
137.0719	291.4	HMDB40054	3-Ethyl-2-methoxypyrazine	9
97.0294	288.9	HMDB40145	5-Hydroxy-4-pentenoic acid d-lactone	9
145.0331	20.9	HMDB40237	Dihydro-2-methoxy-2-methyl-3(2H)-thiophenone	9
225.1134	288.4	HMDB40705	Allixin	9
251.1142	288.3	HMDB40822	23-Butanediol glucoside	9
158.0095	290	HMDB41083	(E)-Raphanusanin	9
263.1137	182.1	HMDB41186	Ilicifolinoside A	9
726.1858	182.8	HMDB41261	Cyanidin 3-(6-p-coumarylsambubioside)	9
137.0436	49.2	HMDB41361	2-Ethylbenzenethiol	9
151.0341	294.4	HMDB41565	57-Dihydro-2-methylthieno34-dpyrimidine	9
211.1341	291.4	HMDB41572	3-Ethenyl-4-hydroxy-25-dimethylhex-5-en-2-yl acetate	9
176.0829	292.4	HMDB41940	N-nitrosonornicotine	9
103.04	20.5	HMDB00729	Alpha-Hydroxyisobutyric acid	10

387.1949	242.8	HMDB14800	Trimethobenzamide	10
585.2684	25.8	HMDB14900	Irinotecan	10
329.0311	16.4	HMDB14910	Malathion	10
359.1257	18.7	HMDB15187	Nitrendipine	10
177.0669	34.2	HMDB15253	Phenacemide	10
264.1609	237.8	HMDB15520	Oxprenolol	10
371.221	242.9	HMDB32784	5-Ethoxysorgoleone 358	10
487.0315	250	HMDB34113	34-Hexahydroxydiphenoylarabinose	10
450.2627	192.7	HMDB35366	Cytochalasin Opho	10
329.249	252.7	HMDB35581	1-Phenyl-13-hexadecanedione	10
357.2809	268.1	HMDB35583	1-Phenyl-13-octadecanedione	10
359.2963	293.4	HMDB35680	3-Hydroxy-1-phenyl-1-octadecanone	10
651.4483	293.2	HMDB38016	Ginsenoside Rh5	10
571.371	213.8	HMDB38564	3-N-Acetyl-4-O-(14-methylpentadecanoyl)fusarochromanone	10
327.2335	234.9	HMDB38908	(ZZ)-2-Methyl-5-(81114-pentadecatrienyl)-13-benzenediol	10
455.0856	250.9	HMDB41883	Doripenem	10
118.0507	22.5	HMDB00167	L-Threonine	10
93.0344	46.2	HMDB00228	Phenol	10
203.0827	21.9	HMDB00929	L-Tryptophan	10
177.092	256.8	HMDB02043	5-Phenylvaleric acid	10
747.5087	261.3	HMDB14352	Azithromycin	10
210.0687	26.6	HMDB14380	Milrinone	10
251.0813	179.8	HMDB14397	Phenytoin	10
370.1421	20.3	HMDB14415	Isradipine	10
457.1147	21.4	HMDB14438	Raltitrexed	10
398.1734	21	HMDB14516	Thiethylperazine	10
253.0938	166.6	HMDB14789	Dyphylline	10
370.0923	16	HMDB14854	Nedocromil	10
466.2933	212.3	HMDB15057	Buprenorphine	10
424.1557	183.4	HMDB15315	Domperidone	10
311.169	268.9	HMDB32549	N-Undecylbenzenesulfonic acid	10
371.1531	168.8	HMDB32733	(8R8R9S)-9-Hydroxy-34-dimethoxy-34-methylenoxy-99-epoxylignan	10
261.0746	291.4	HMDB32838	Dorsteniol	10
195.0777	20.6	HMDB32852	2-(Ethylamino)-45-dihydroxybenzamide	10
123.0449	168.7	HMDB32917	1-(2-Furanyl)-2-propanone	10
224.0739	21.6	HMDB32983	1-Hydroxy-10-methylacridone	10
289.0946	252.6	HMDB32992	Furaneol 4-glucoside	10
93.0458	21.1	HMDB33112	Methylpyrazine	10
259.0587	19.4	HMDB33265	2-Methoxystypandrone	10

229.0509	18.6	HMDB33329	Coriandrin	10
403.0916	24.5	HMDB33343	Mollicellin D	10
554.0206	36.9	HMDB33384	CI Direct Red 45	10
283.1557	289.9	HMDB33483	67-Dihydro-4-(hydroxymethyl)-2-(p-hydroxyphenethyl)-7-methyl-5H-2-pyrindinium	10
228.1378	271.1	HMDB33531	2468-Decatetraenoic acid dehydropiperidide	10
523.101	176.1	HMDB34318	Sennidin C	10
632.1733	44.9	HMDB35420	Pyranocyanin A	10
190.051	287.7	HMDB35514	xi-23-Dihydro-2-oxo-1H-indole-3-acetic acid	10
231.0296	19.8	HMDB36628	9-Hydroxy-4-methoxypsoralen	10
213.1497	285.4	HMDB37398	4-Acetoxy-2-hexyltetrahydrofuran	10
477.1627	18.7	HMDB38714	Kelampayoside A	10
569.1713	211	HMDB39040	Apiumoside	10
256.0948	290.6	HMDB39229	Pyro-L-glutaminyl-L-glutamine	10
272.9008	155.9	HMDB39460	Di-2-propenyl hexasulfide	10
87.027	148.7	HMDB39807	cis-23-Dimethylthiirane	10
325.1162	293.7	HMDB40154	6-O-b-D-Fructofuranosyl-2-deoxy-D-glucose	10
87.0086	289.2	HMDB40261	Glucosereductone	10
276.8537	64.5	HMDB40450	23456-Pentachlorobenzyl alcohol	10
227.1045	290	HMDB40573	Tetraacetylethylenediamine	10
329.0223	16.8	HMDB40599	()-Fenarimol	10
423.4213	292.6	HMDB40885	10-Octacosene-112-diol	10
185.0458	285.7	HMDB41026	Erinapyrone C	10
452.2787	207.6	HMDB41085	Sambutoxin	10
535.2864	190.1	HMDB41137	Corchorosol A	10
252.09	165	HMDB41725	Dihydroferuloylglycine	10
347.9156	26	HMDB41856	Chlorpyrifos	10
287.0979	250.5	HMDB42029	Tetrazepam	10
409.1705	21.6	HMDB42040	Tipredane	10
394.1783	18.8	HMDB42059	Vesnarinone	10

Web Figure 1. Log2-transformed residual of relative ion intensities of selected metabolites detected in HILIC column, adjusted for Hispanic ethnicity and maternal age. A) Alanine; B) Proline; C) Threonine; D) Taurine; E) Leucine/Isoleucine; F) Phenylalanine; G) Tyrosine; H) Methionine; I) Glutamine; J) 2-Aminobutyrate; K) Hippurate; L) Kynurenine; M) Creatine; N) Cholesterol; O) Niacin; P) Methylnicotonic acid; Q) Pyridoxamine; R) Pyridoxine; S) Carnitine; T) Acetyl-carnitine; U) sn-glycero-3-Phosphocholine; V) Sphingosine; W) Sphinganine; X) Choline; Y) LysoPC(18:0); Z) 5,6-Dihydrouracil; AA) Hypoxanthine; AB) Xanthine; AC) Caffeine.


A
B
C
D
E
F
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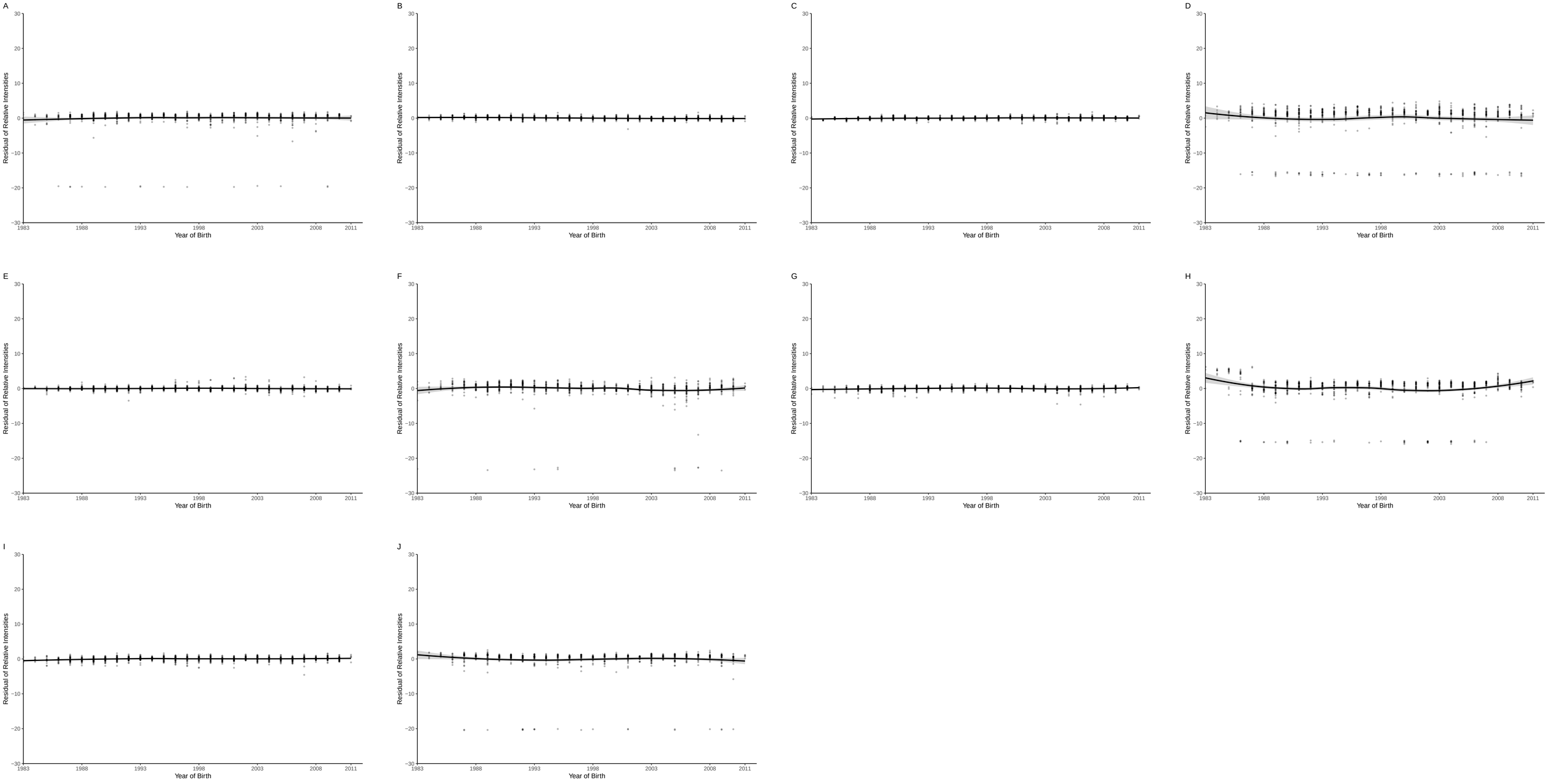
H
I
J
K
L
M
N
O
P
Q
R
S
T
U
V
W
X
Y
Z
AA
AB
AC
Residual of Relative Intensities
Year of Birth
30
20
10
0
−10
−20
−30
1983
1988
1993
1998
2003
2008
2011

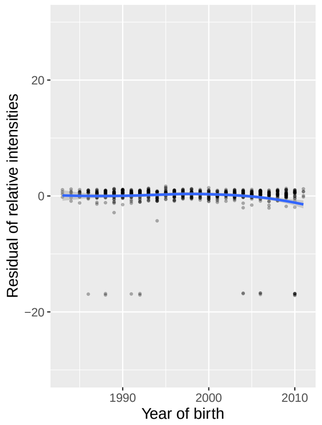
Web Figure 2. Log2-transformed residual of relative ion intensities of selected metabolites detected in C18 column, adjusted for Hispanic ethnicity and maternal age. A) Lysine; B) Glutamate; C) Histidine; D) Arginine; E) Tryptophan; F) a-Linolenic acid; G) Oleic acid; H) Arachidic acid; I) Urate; J) Benzoic acid.

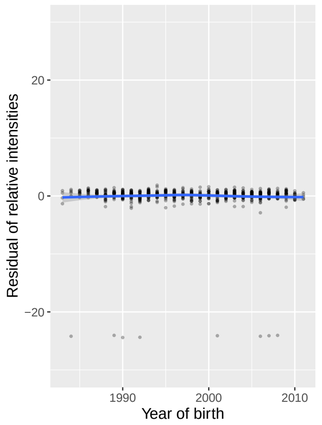

A
B
C
D
E
F
G
H
I
J
Residual of Relative Intensities
Year of Birth
30
20
10
0
−10
−20
−30
1983
1988
1993
1998
2003
2008
2011

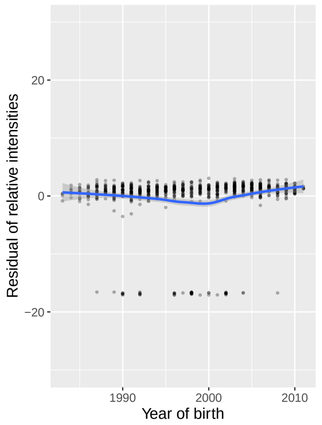
Web Figure 3. Endogenous Features in HILIC column with suggested m/z matches annotation

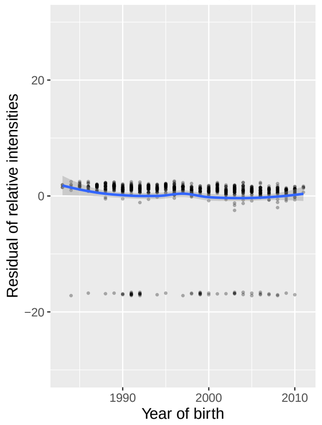
1−Methylhistidine
2−Ketobutyric acid
Deoxycytidine
4−Pyridoxic acid
3−Methoxytyramine
Carnosine
Adenine
Dihydrobiopterin
Betaine
Adenosine
Beta−Alanine
Adenosine 35−diphosphate
L−Carnitine
Creatine
Epinephrine
Deoxyinosine
Dopamine
Dihydrouracil
Cysteinylglycine
Cytidine triphosphate
Cytidine
Cytidine monophosphate
D−Xylose
Gamma−Aminobutyric acid
Glycerylphosphorylethanolamine
Homovanillic acid
D−Glucose
Fructose 6−phosphate
Guanidoacetic acid
Guanine
Guanosine
L−Glutamic acid
Gluconolactone
L−Tyrosine
Inosinic acid
L−Dopa
Alpha−Lactose
L−Serine
L−Lactic acid
L−Aspartic acid
Anserine
N−Acetylgalactosamine
Norepinephrine
O−Phosphoethanolamine
Oxoadipic acid
N−Acetylneuraminic acid
Sepiapterin
Taurine
Thymine
Phosphoenolpyruvic acid

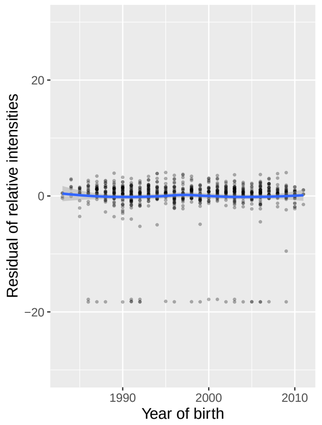
Residual of relative intensities
Year of birth

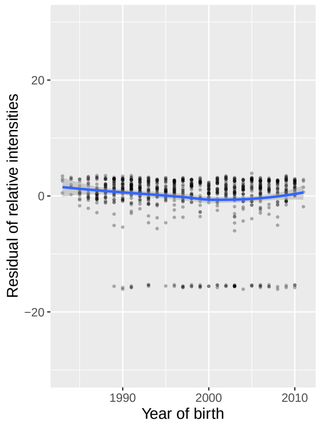
Liothyronine


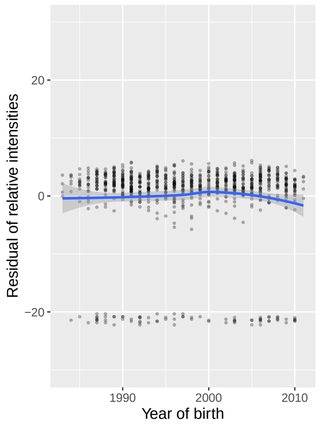
Pyroglutamic acid


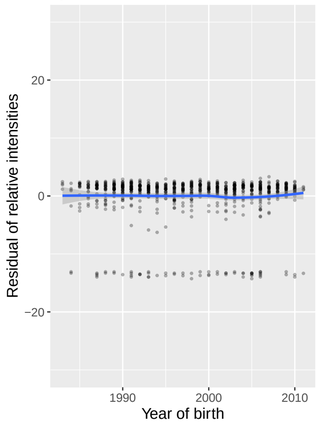
Thymidine


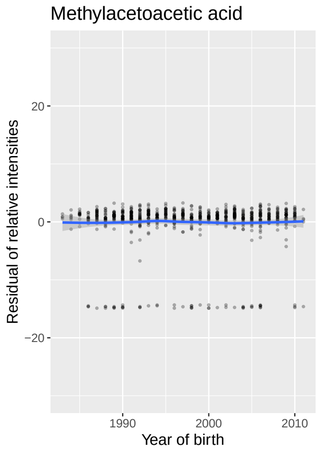
Uridine 5−monophosphate


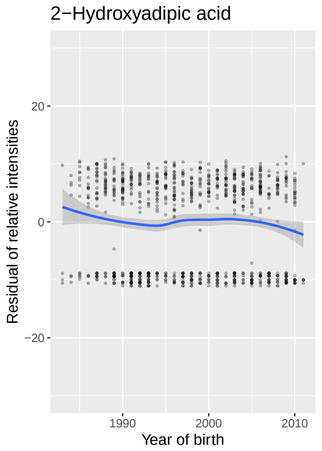
Uridine


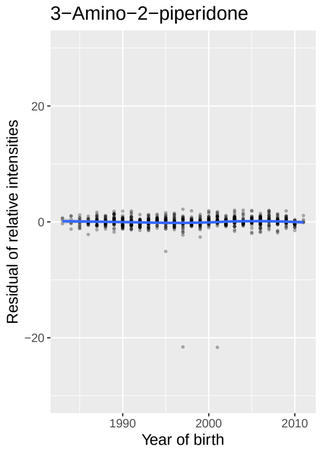
Uracil


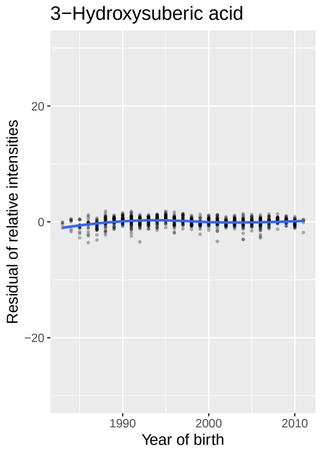
Urocanic acid


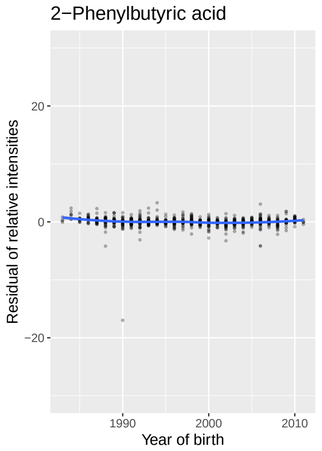
Tyramine


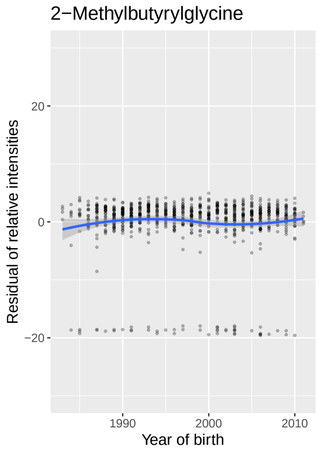
Methylacetoacetic acid


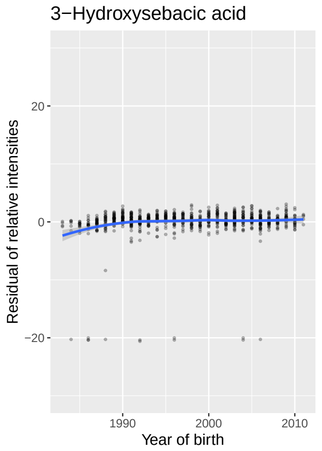
2−Hydroxyadipic acid


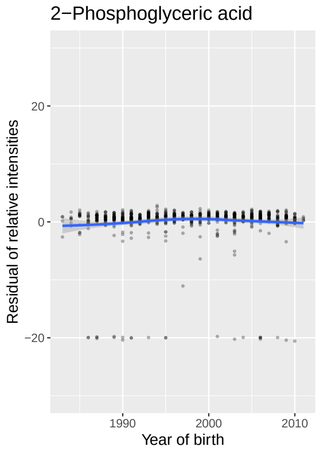
3−Amino−2−piperidone


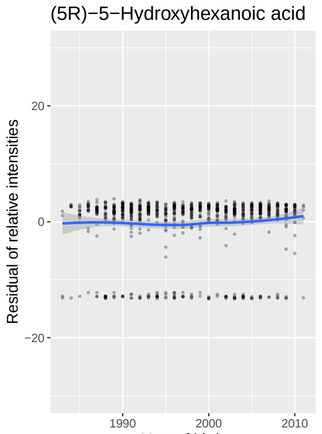
3−Hydroxysuberic acid


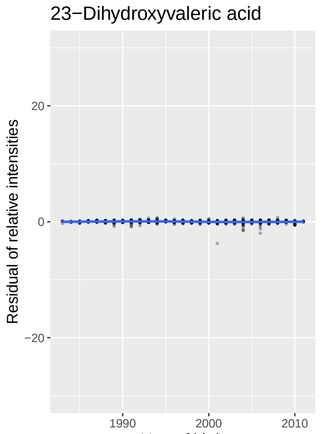
2−Phenylbutyric acid


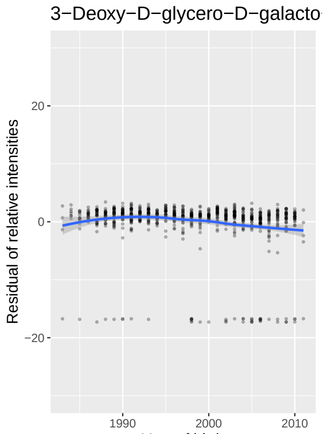
2−Methylbutyrylglycine


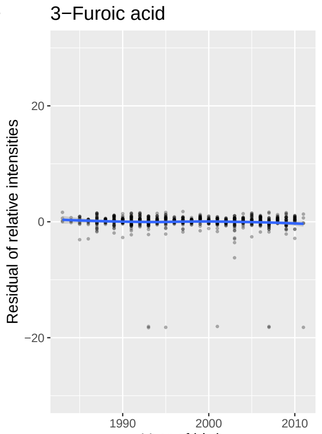
3−Hydroxysebacic acid


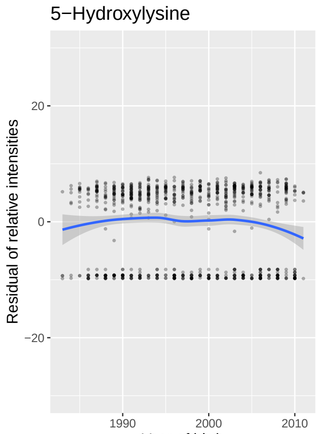
2−Phosphoglyceric acid


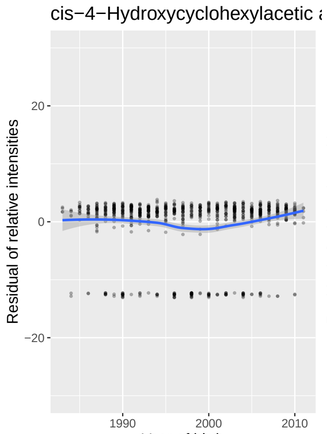
(5R)−5−Hydroxyhexanoic acid


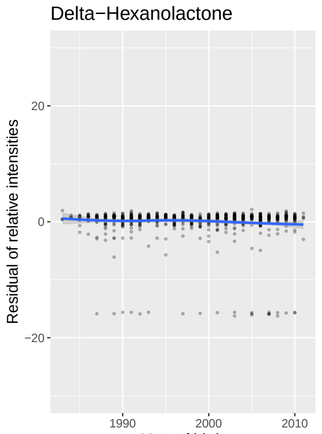
23−Dihydroxyvaleric acid


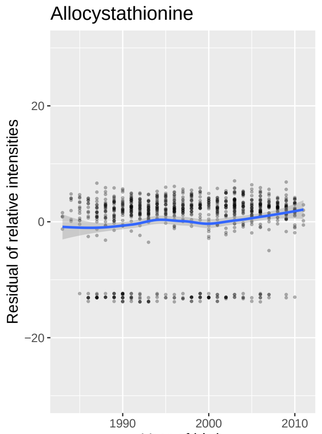
3−Deoxy−D−glycero−D−galacto


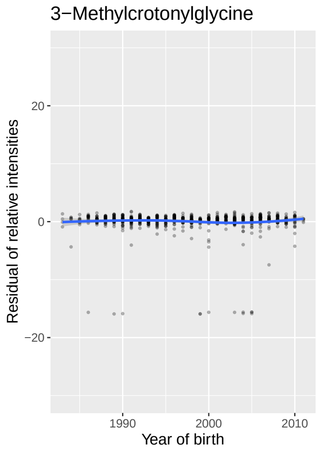
3−Furoic acid


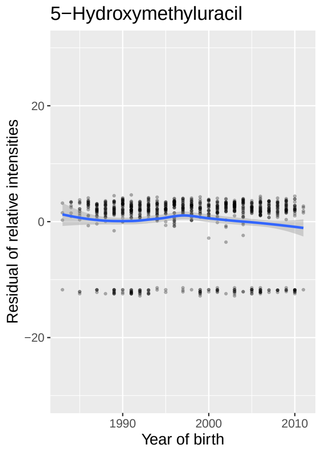
5−Hydroxylysine


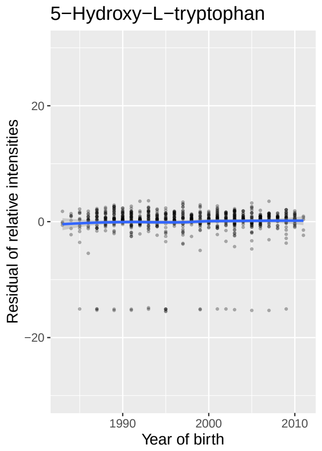
cis−4−Hydroxycyclohexylacetic a


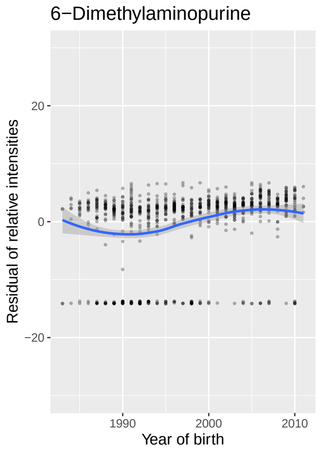
Delta−Hexanolactone


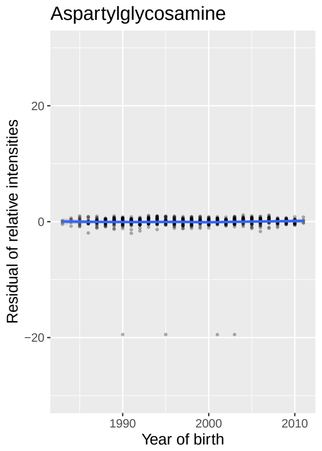
Allocystathionine


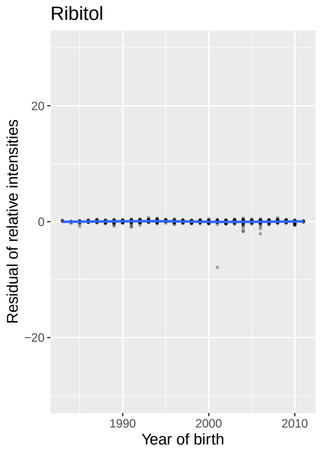
3−Methylcrotonylglycine


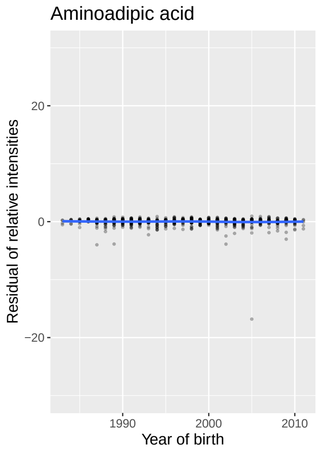
5−Hydroxymethyluracil


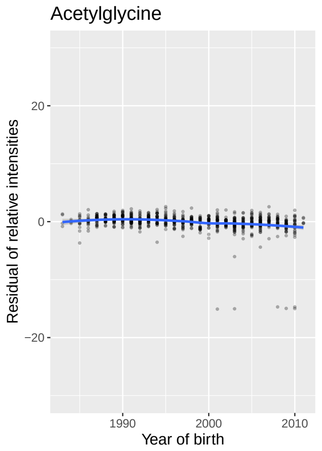
5−Hydroxy−L−tryptophan


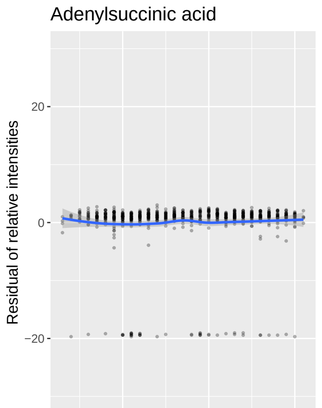
6−Dimethylaminopurine


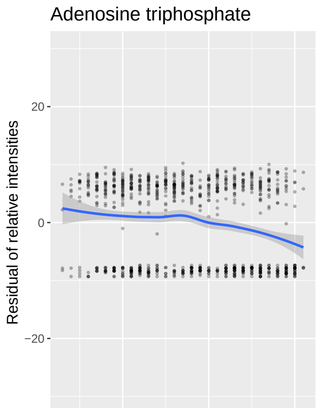
Aspartylglycosamine


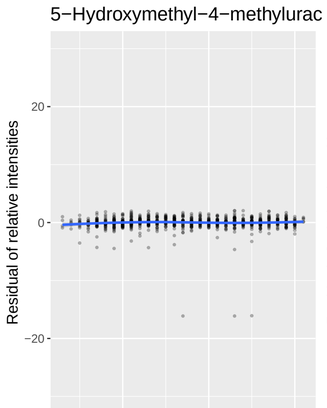
Ribitol


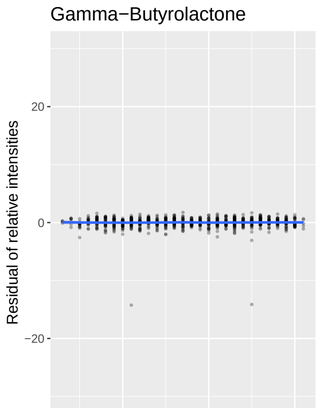
Aminoadipic acid


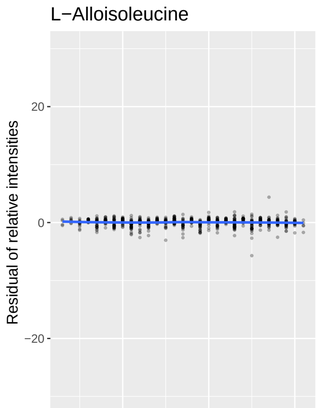
Acetylglycine


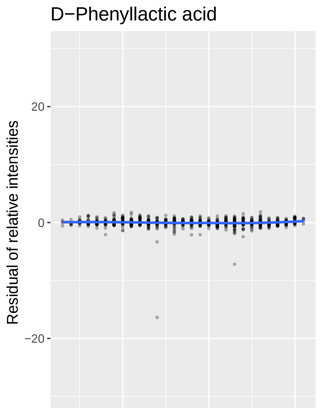
Adenylsuccinic acid


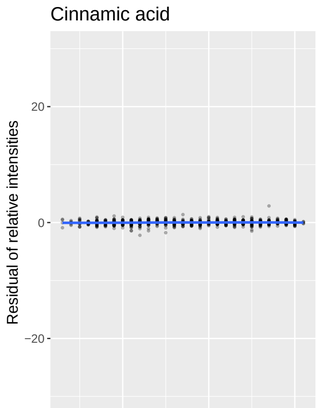
Adenosine triphosphate


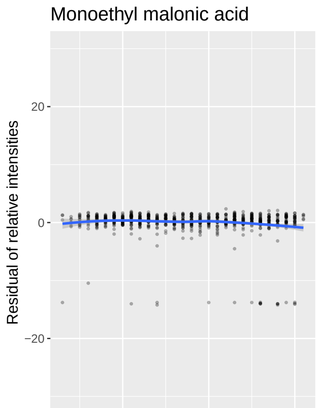
5−Hydroxymethyl−4−methylurac


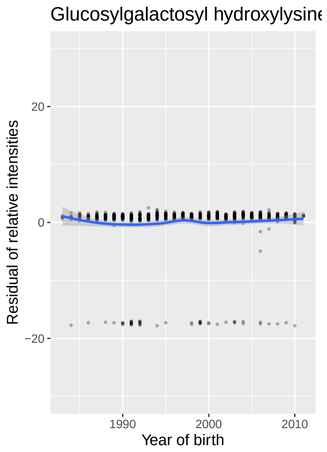
Gamma−Butyrolactone


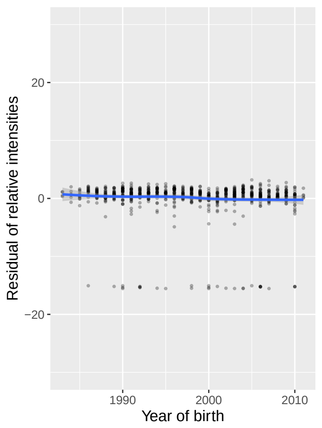
L−Alloisoleucine


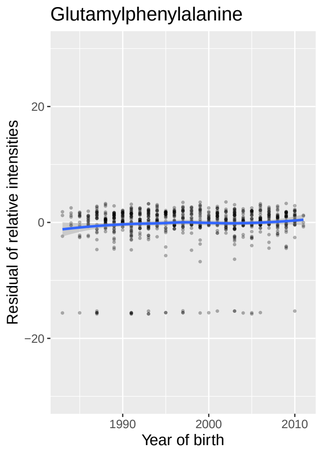
D−Phenyllactic acid


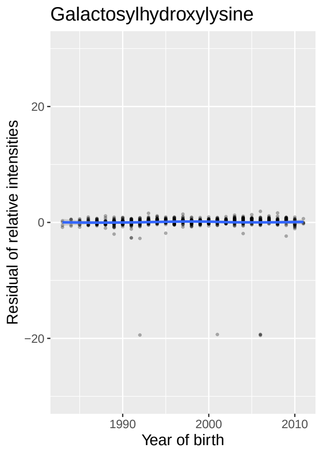
Cinnamic acid


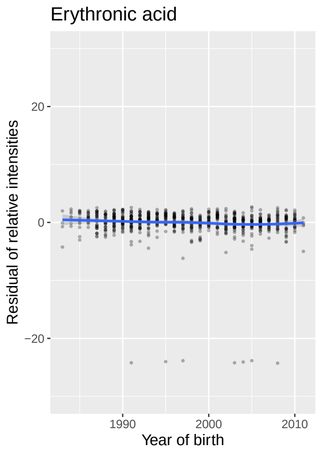
Monoethyl malonic acid


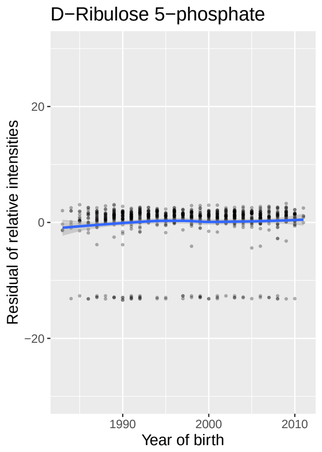
Glucosylgalactosyl hydroxylysine


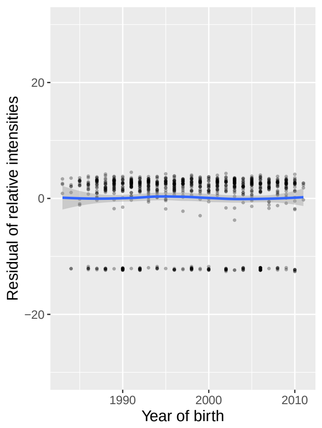
Glucosamine 6−sulfate


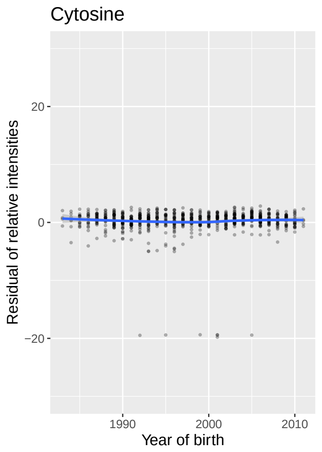
Glutamylphenylalanine


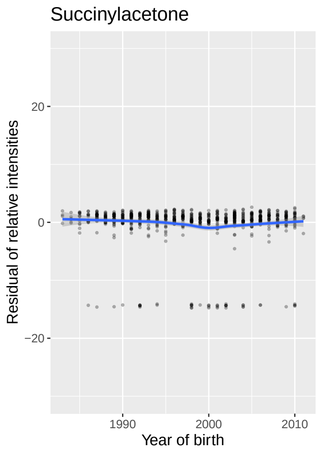
Galactosylhydroxylysine


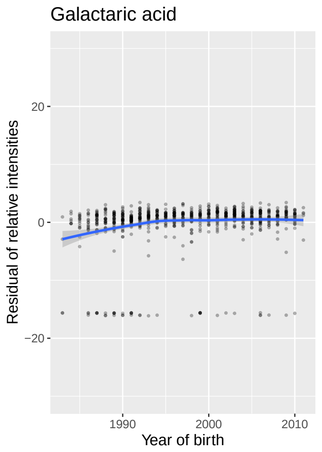
Erythronic acid


D−Ribulose 5−phosphate


Dodecanedioic acid


Cytosine


Succinylacetone


Galactaric acid


L−Glutamine

Chondroitin 4−sulfate

Homo−L−arginine

Homocitrulline

L−Kynurenine

Heparan sulfate

Hexanoylglycine

Mandelic acid

Isoxanthopterin

Kynurenic acid

L−Pipecolic acid

Glycylproline

4−Hydroxyproline

Isobutyrylglycine

Hydroxykynurenine

Hexacarboxylporphyrin I

5−Hydroxyindoleacetic acid

Octadecanedioic acid

Azelaic acid

Pterin

Dimethylprotoporphyrin IX dimet

Phosphoglycolic acid

Phenylacetylglycine

Capryloylglycine

Quinaldic acid

Formiminoglutamic acid

Pimelic acid

Histamine

Tetradecanedioic acid

4−Methylcatechol

Xanthurenic acid

Ribothymidine

Vinylacetylglycine

7−Methylguanine

1−Methylhistamine

NAD

Deoxyadenosine monophosphat

Succinyladenosine

Vanillactic acid

Pyrocatechol

Hypotaurine

5−Methylcytidine

Dihydrolipoamide

S−Adenosylmethioninamine

DL−2−Aminooctanoic acid

3−Succinoylpyridine

dUDP

Adenosine phosphosulfate

Oxoamide

Phosphohydroxypyruvic acid

Residual of relative intensities

Year of birth

Deoxyribose 5−phosphate
2−Deoxyguanosine 5−monopho
D−Sedoheptulose 7−phosphate
4−Aminobutyraldehyde
(N−acetylneuraminosyl(a2−6)lac
D−1−Piperideine−2−carboxylic a
3−Hydroxyquinine
Protoporphyrinogen IX
7−Methylguanosine
Glucosamine−1P
Inositol cyclic phosphate
6−Phosphonoglucono−D−lacton
Nicotinic acid mononucleotide
Octanal
trans−12−Dihydrobenzene−12−(
4−Aminophenol
5−Methylthioadenosine
Cytidine monophosphate N−ace
68−Dihydroxypurine
Methyl propenyl ketone
N1−Acetylspermine
Guanosine diphosphate
dCMP
Hydantoin−5−propionic acid
Tetrahydropteridine
Pseudooxynicotine
FAD
N−Acetylarylamine
Spermine
Spermidine
Fucose 1−phosphate
4−Oxo−4−(3−pyridyl)−butanamic
N1−Acetylspermidine
2−Aminomuconic acid semialdel
1−Pyrroline−5−carboxylic acid
6−Phosphogluconic acid
N6N6N6−Trimethyl−L−lysine
Purine
Diguanosine triphosphate
N−Methylphenylethanolamine
Guanosine monophosphate
3−Sulfinylpyruvic acid
Niacinamide
dUMP
2−Amino−4−oxo−6−(12−dioxopr
Citicoline
Pantetheine 4−phosphate
4−(3−Pyridyl)−3−butenoic acid
Pyridoxamine
3−Methoxytyrosine

Residual of relative intensities
Year of birth

Biotin amide

3−Hydroxyanthranilic acid

NADH

Pyridoxal 5−phosphate

Acetylphosphate

Aminoparathion

dADP

Alpha−CEHC

Flavin Mononucleotide

S−Acetyldihydrolipoamide

Deoxyadenosine triphosphate

3−Pyridylacetic acid

Asymmetric dimethylarginine

N−Acetyllactosamine

m−Chlorobenzoic acid

Pyridoxal

CDP

1−Methylguanosine

CDP−Ethanolamine

Phenylglyoxylic acid

m−Coumaric acid

Ethenodeoxyadenosine

5−Hydroxytryptophol

4−Aminohippuric acid

5−Methoxytryptophol

3−Nitrotyrosine

17−Dimethylguanosine

Caffeic acid

Lacto−N−difucopentaose II

23−Diaminopropionic acid

23−Dimethyl−3−hydroxyglutaric

Fructosamine

N(6)−Methyllysine

2−Pyrrolidinone

4−Methoxycinnamic acid

Dihydroxyfumaric acid

Histidylproline diketopiperazine

Monoisobutyl phthalic acid

22−Dimethylsuccinic acid

N−Ribosylhistidine

Itaconic acid

6−Methyladenine

3−Mercaptolactic acid

13−Dimethyluracil

5−Methyltetrahydropteroylpentag

3 Hydroxycoumarin

Harderoporphyrinogen

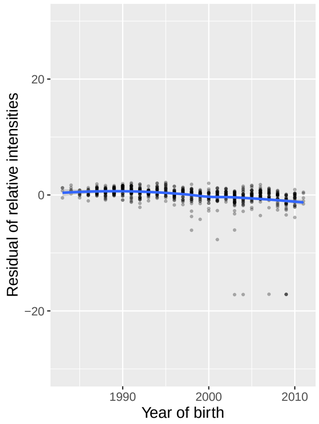
3−Methylbutyrolactone

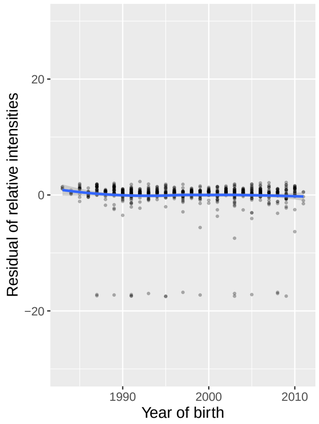
N1N12−Diacetylspermine

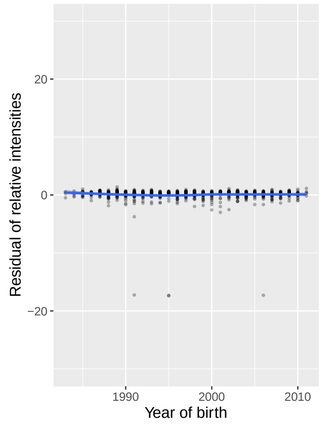
N−Carboxyethyl−g−aminobutyric acid

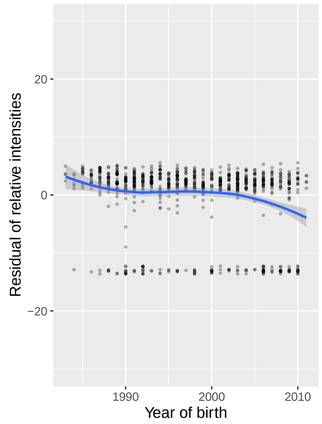
Residual of relative intensities

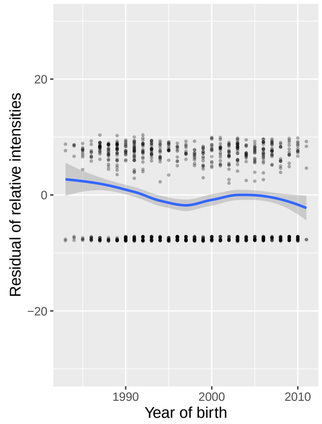
Year of birth

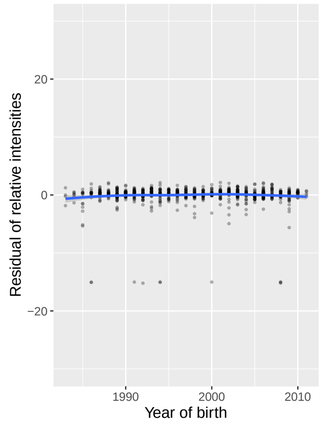
L−Homocysteic acid


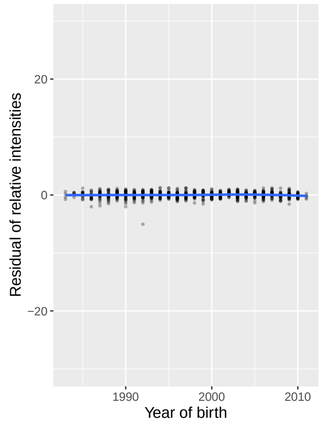
2−Phenylglycine


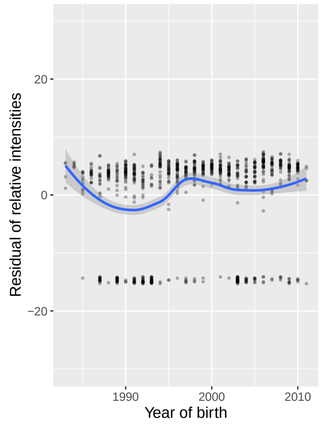
3−Methylphenylacetic acid


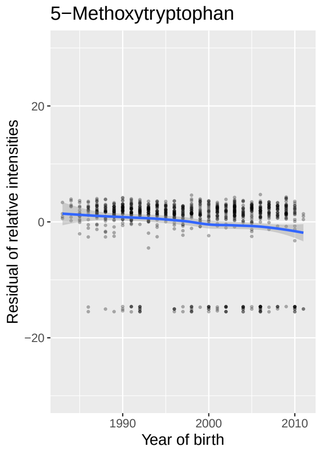
5−Methyldeoxycytidine


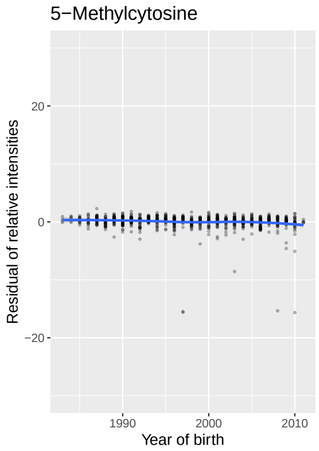
Gamma glutamyl ornithine


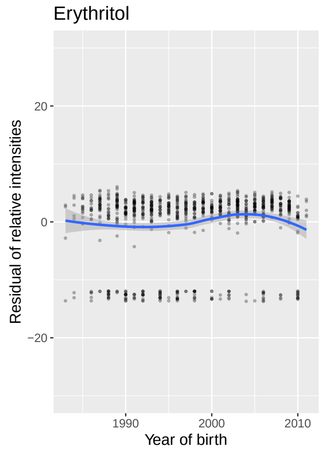
2−(acetylamino)−15−anhydro−2


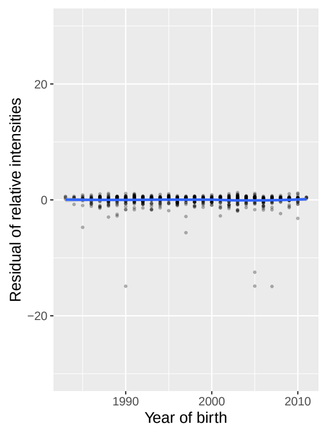
2−Indolecarboxylic acid


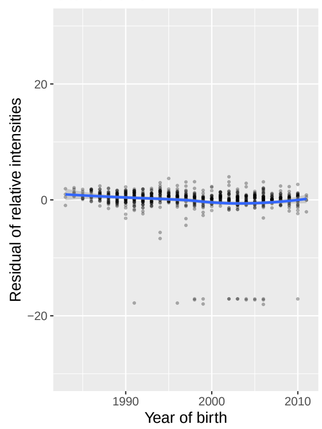
Benzoquinoneacetic acid


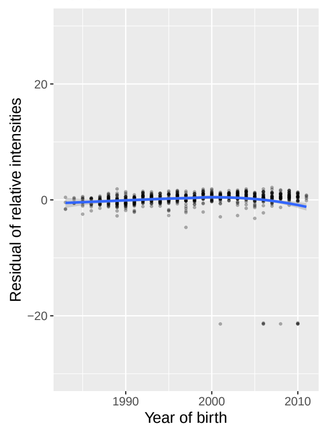
5−Methoxytryptophan


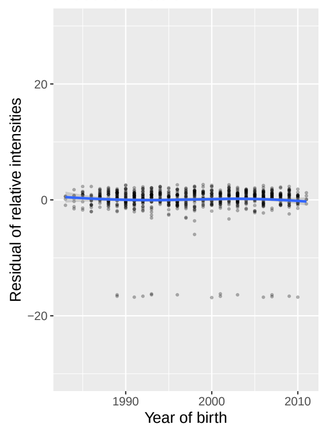
5−Methylcytosine


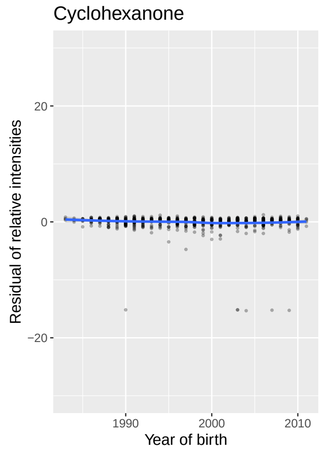
Erythritol


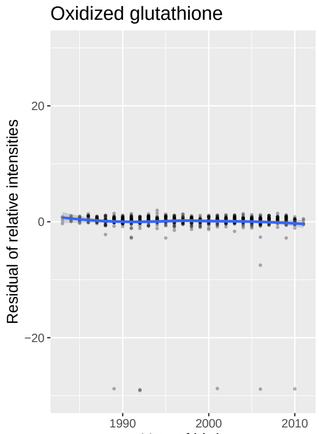
Aniline


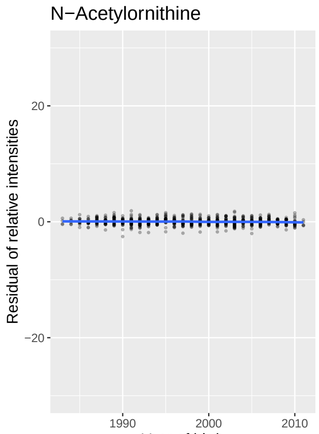
Canrenone


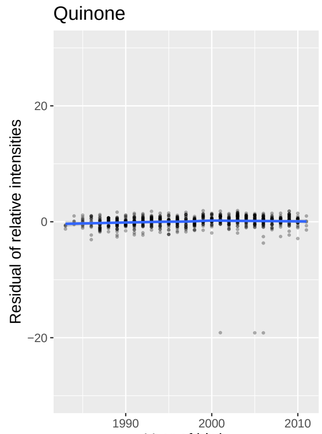
Heme


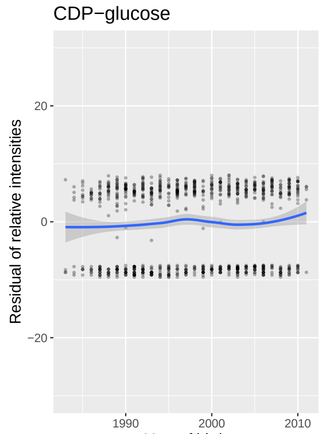
Nicotinuric acid


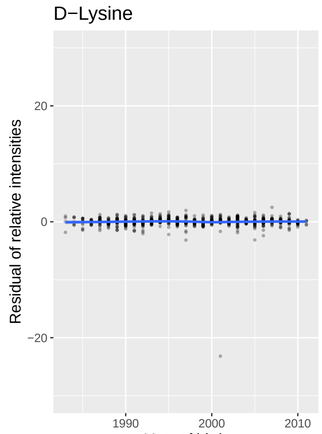
Cyclohexanone


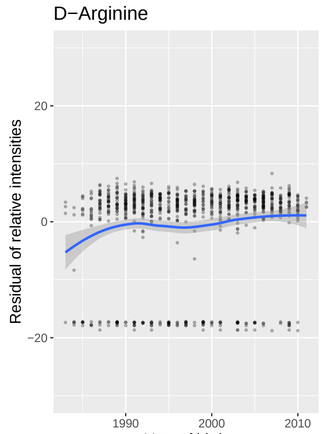
Oxidized glutathione


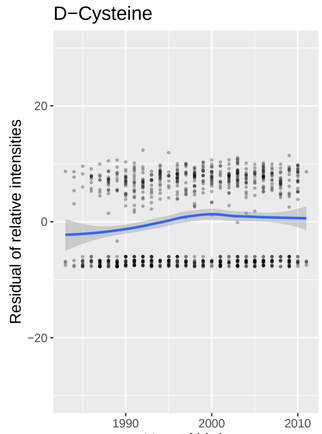
N−Acetylornithine


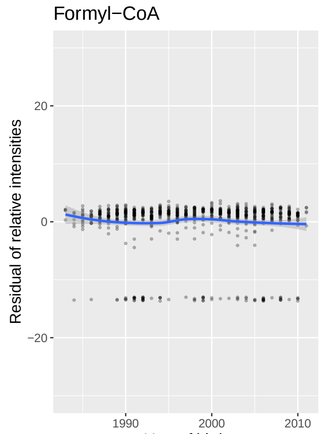
Quinone


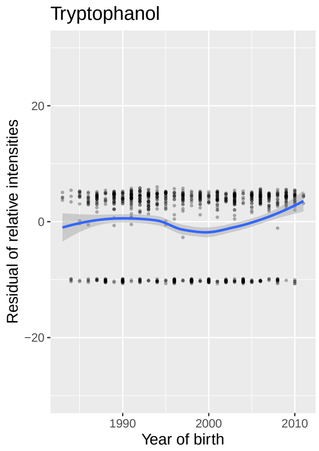
CDP−glucose


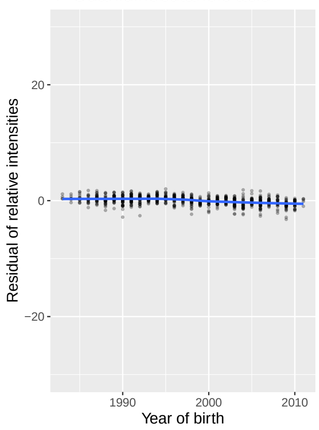
D−Lysine


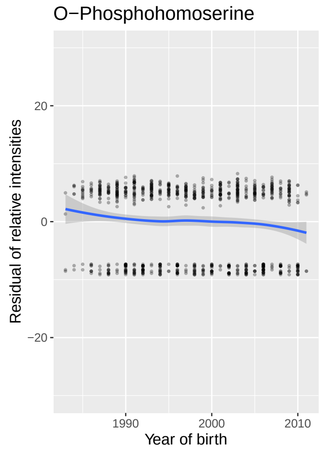
D−Arginine


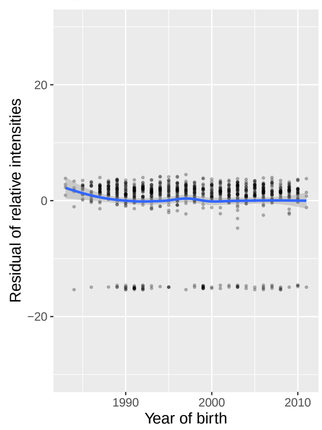
D−Cysteine


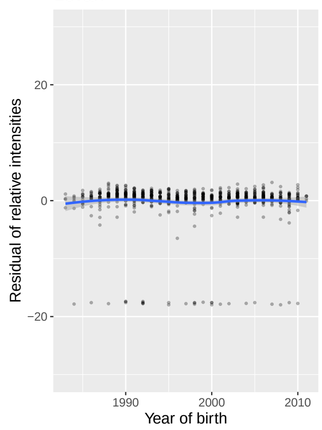
Formyl−CoA


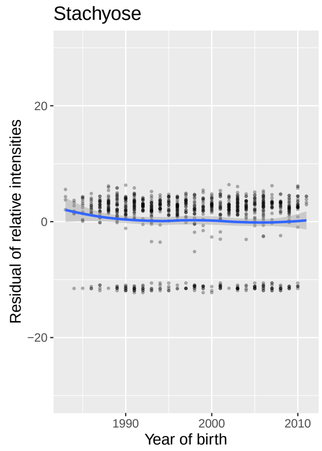
Tryptophanol


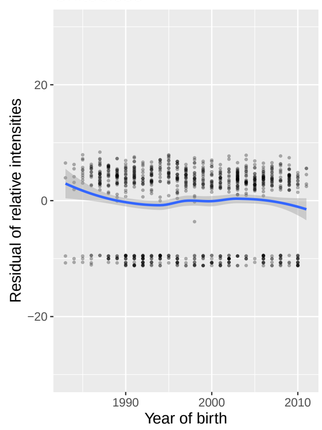
4−Guanidinobutanoic acid


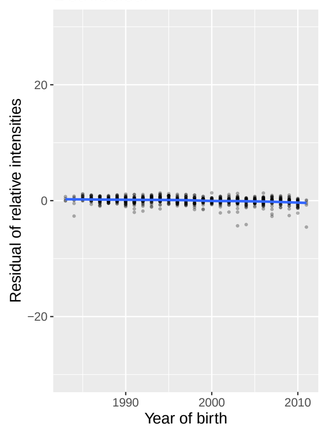
O−Phosphohomoserine


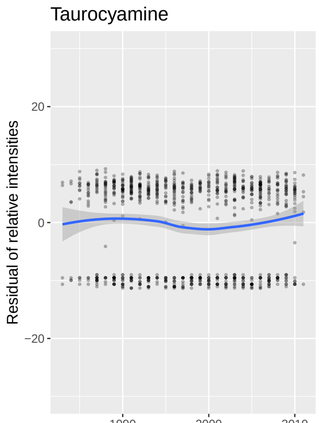
dIDP


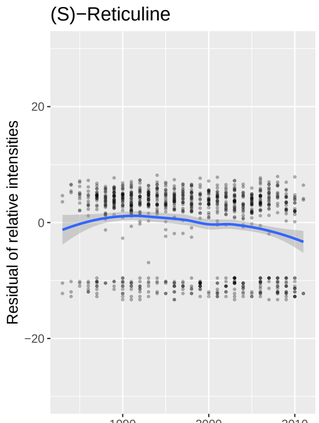
Levan


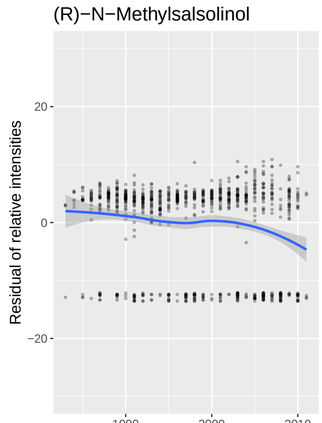
Stachyose


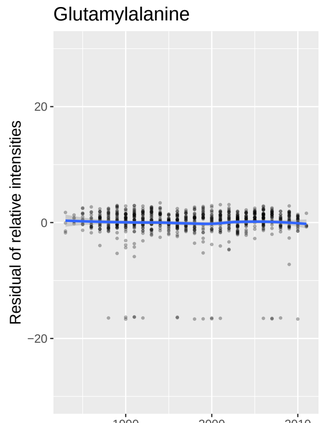
Chitobiose


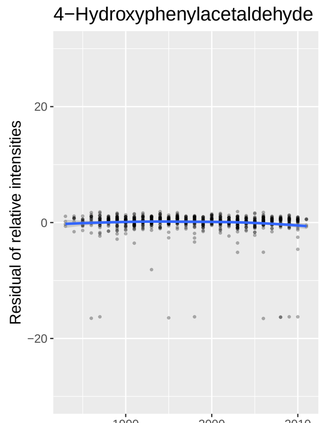
Dethiobiotin


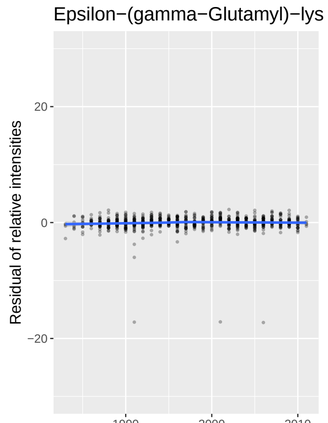
Taurocyamine


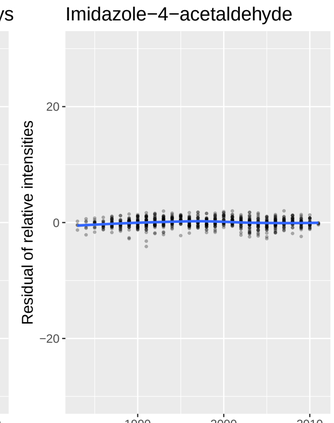
(S)−Reticuline


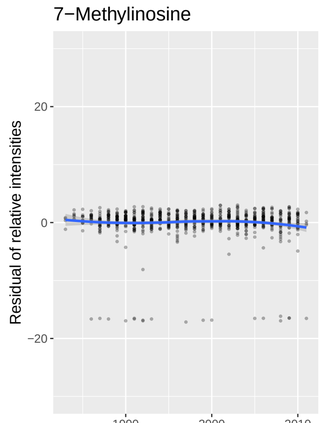
(R)−N−Methylsalsolinol


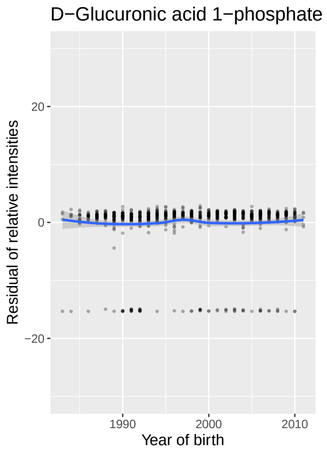
Glutamylalanine


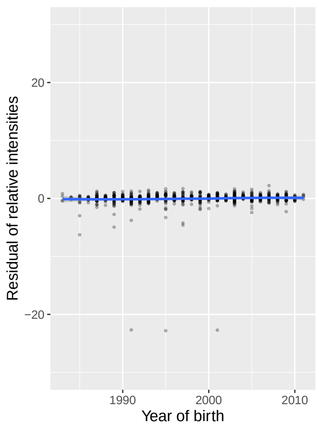
4−Hydroxyphenylacetaldehyde


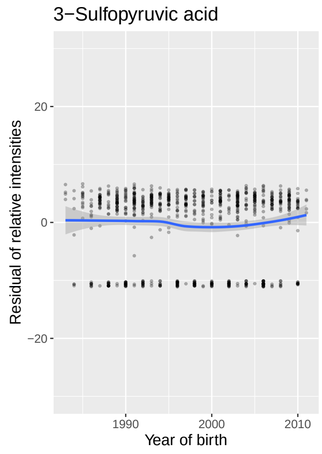
Epsilon−(gamma−Glutamyl)−lys


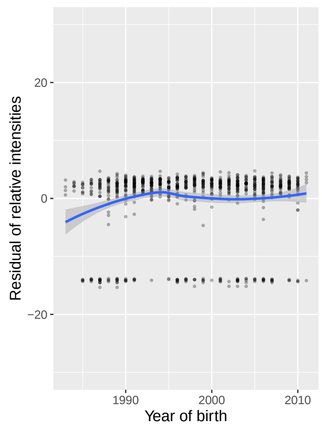
Imidazole−4−acetaldehyde


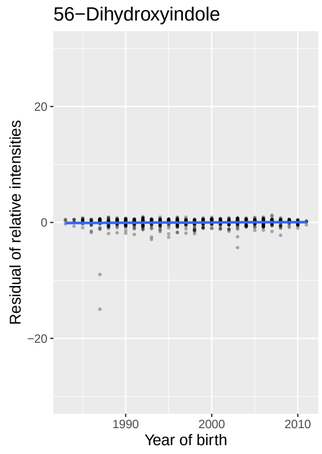
7−Methylinosine


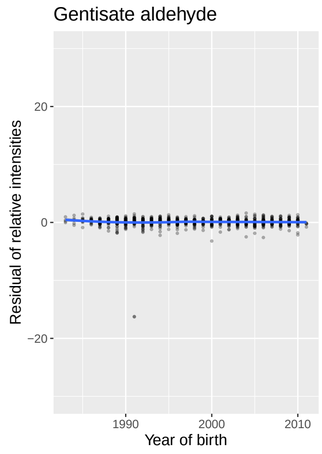
D−Glucuronic acid 1−phosphate


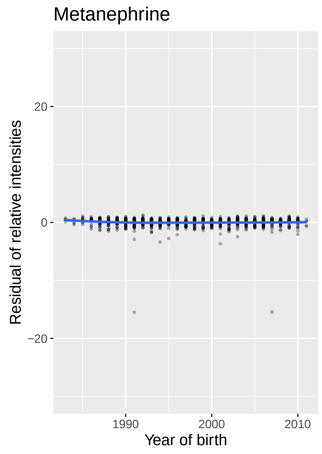
L−Allothreonine


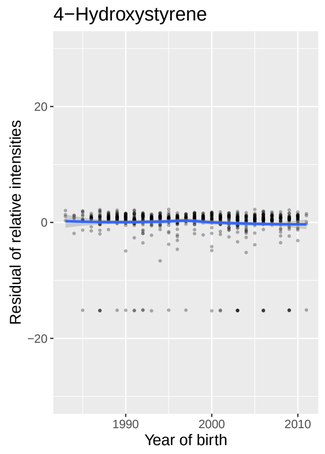
3−Sulfopyruvic acid


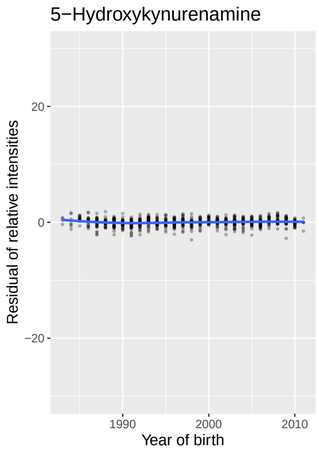
Aerobactin


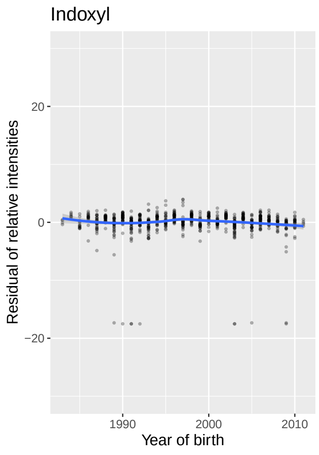
56−Dihydroxyindole


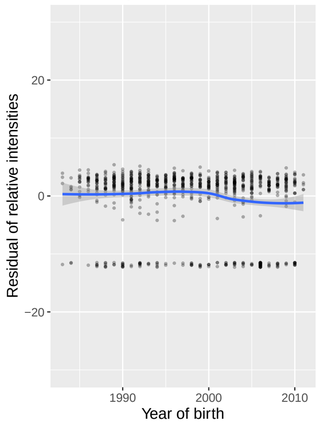
Gentisate aldehyde


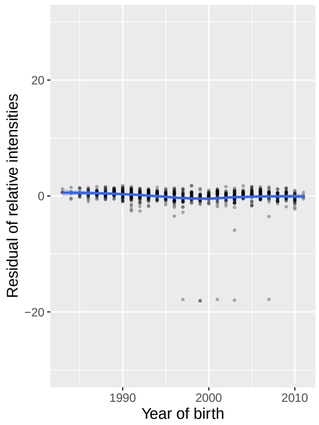
Metanephrine


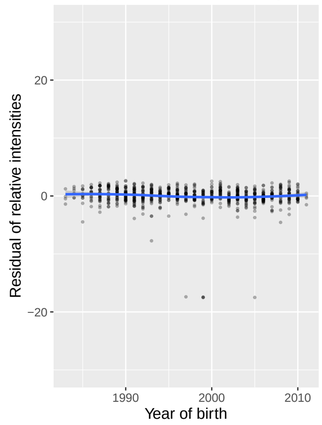
4−Hydroxystyrene


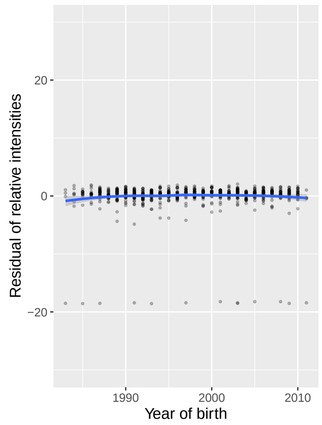
5−Hydroxykynurenamine


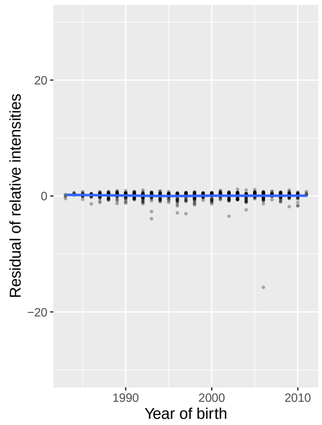
Indoxyl


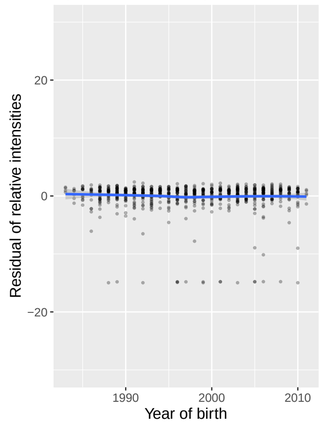
Se−Methylselenocysteine


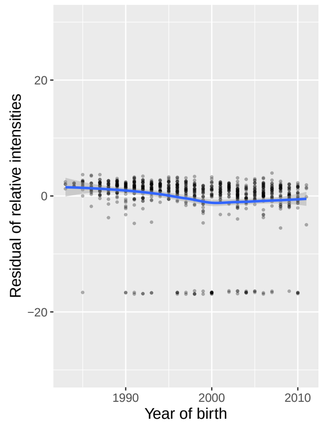
L−Urobilinogen


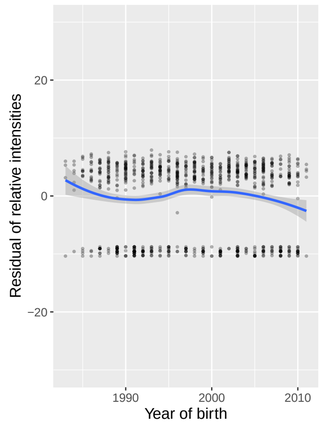
Methylimidazole acetaldehyde


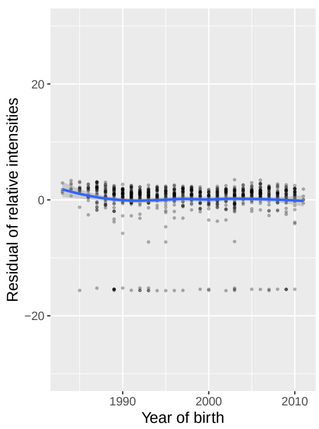
N1−Methyl−2−pyridone−5−carbo


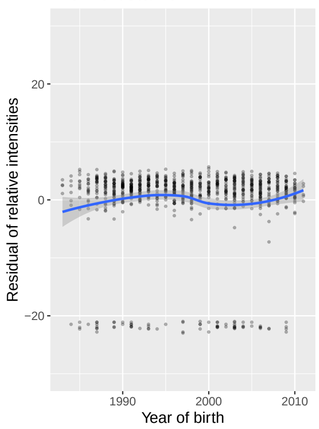
N−(o)−Hydroxyarginine


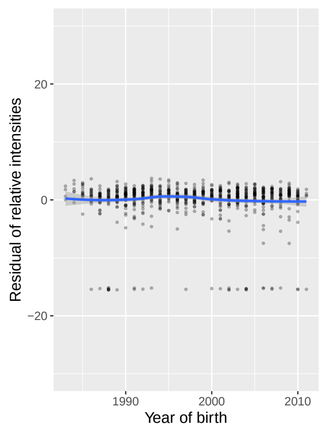
Pyrrole−2−carboxylic acid


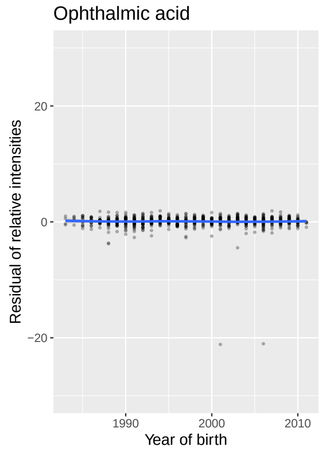
Temurin


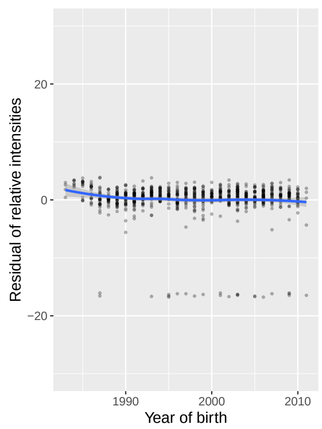
Imidazolone


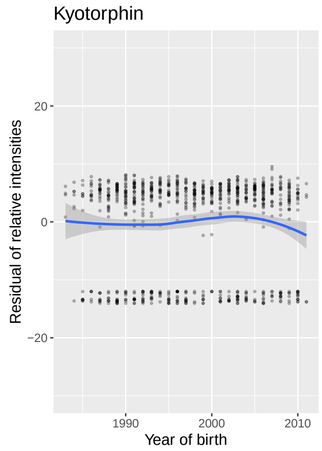
Benzamide


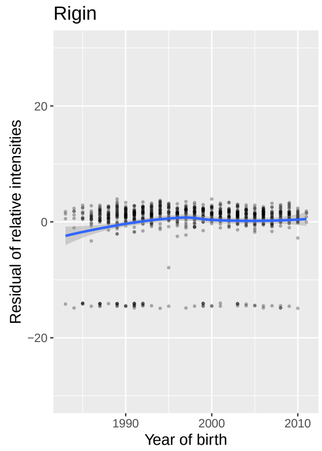
Proline betaine


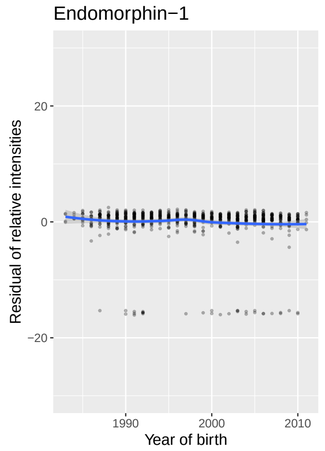
Enterodiol


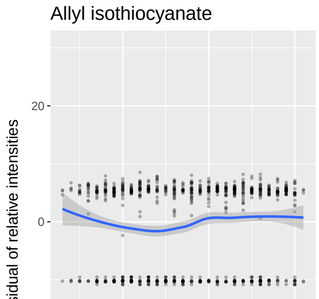
Ophthalmic acid


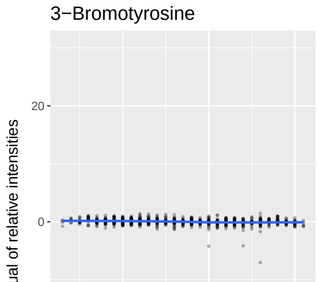
Homoanserine


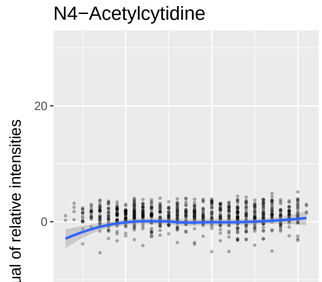
Kyotorphin


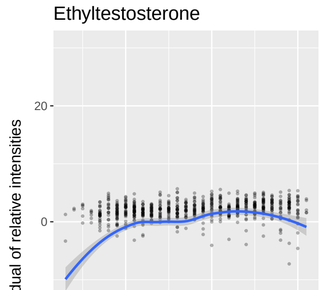
Rigin


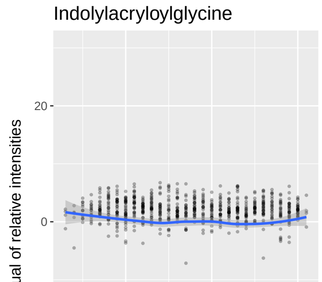
Endomorphin−1


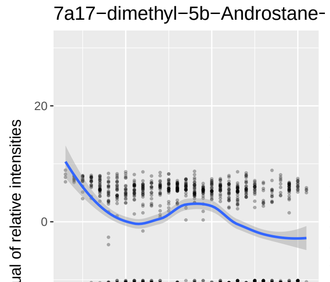
Allyl isothiocyanate


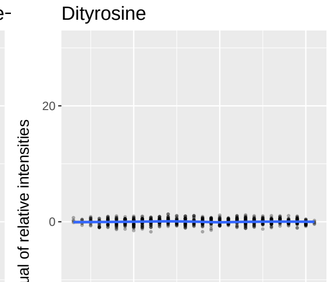
3−Bromotyrosine


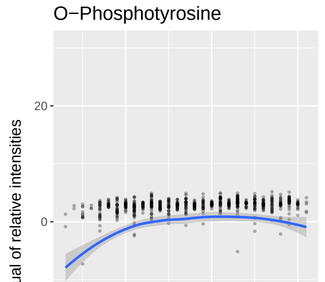
N4−Acetylcytidine


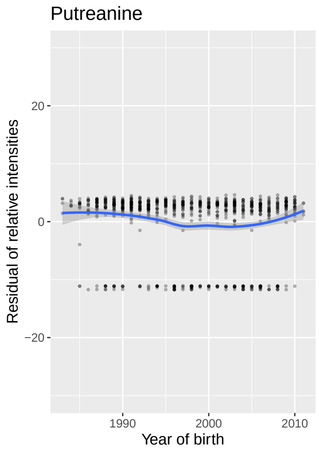
Ethyltestosterone


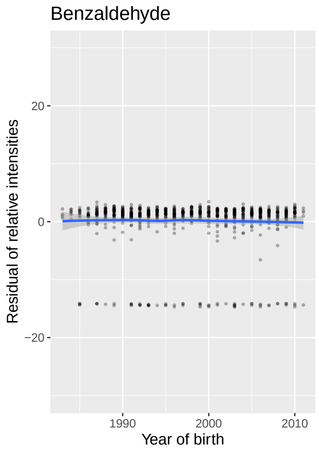
Indolylacryloylglycine


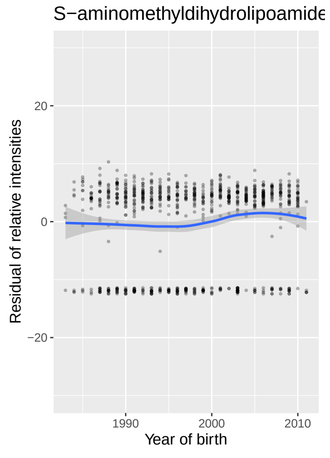
7a17−dimethyl−5b−Androstane−


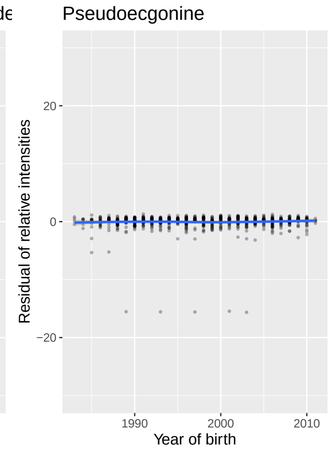
Dityrosine


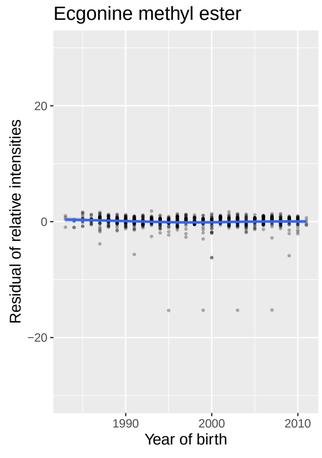
O−Phosphotyrosine


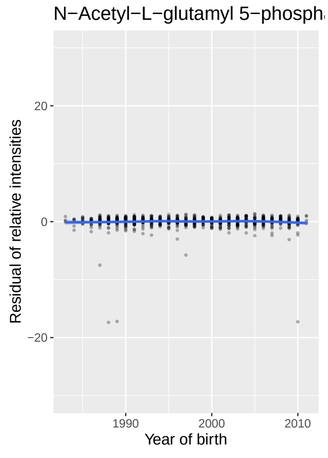
Putreanine


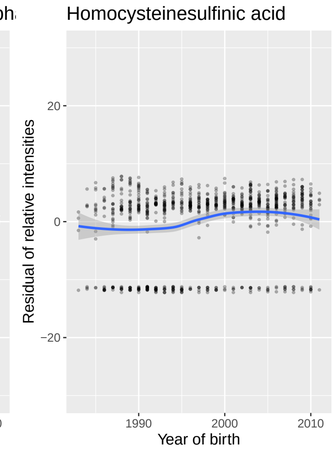
Benzaldehyde


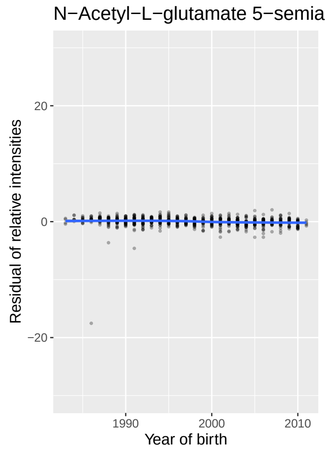
S−aminomethyldihydrolipoamide


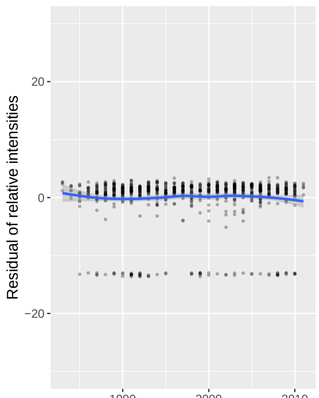
Pseudoecgonine


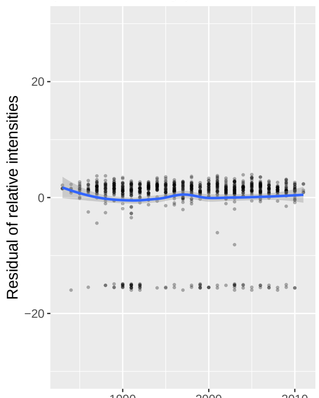
Ecgonine methyl ester


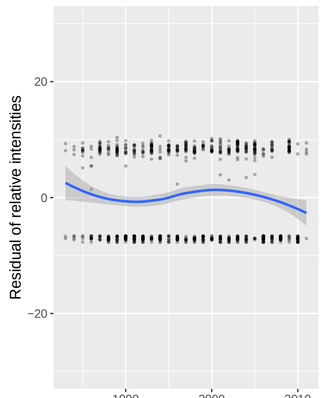
N−Acetyl−L−glutamyl 5−phosph


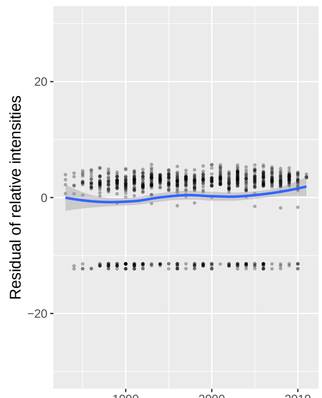
Homocysteinesulfinic acid


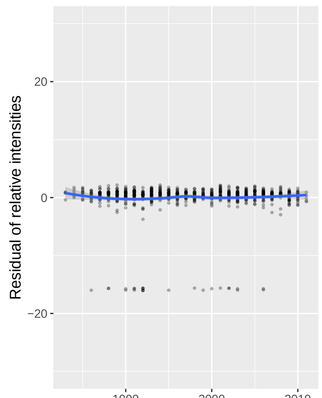
N−Acetyl−L−glutamate 5−semia


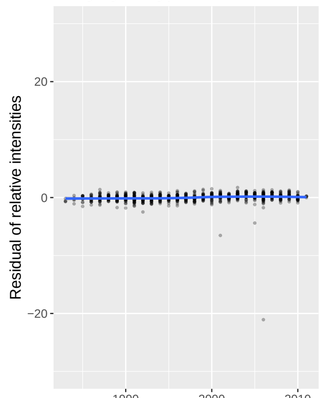
P1P4−Bis(5−adenosyl) tetrapho


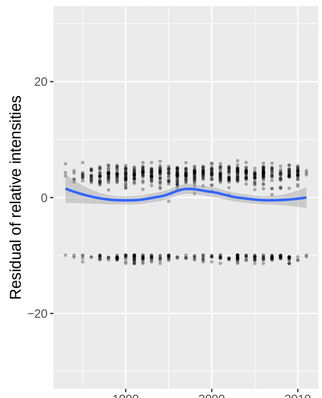
(a−D−mannosyl)2−b−D−mannos


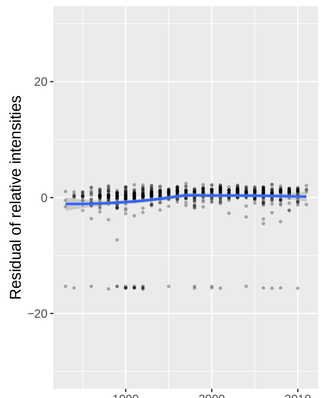
Disialosyl galactosyl globoside


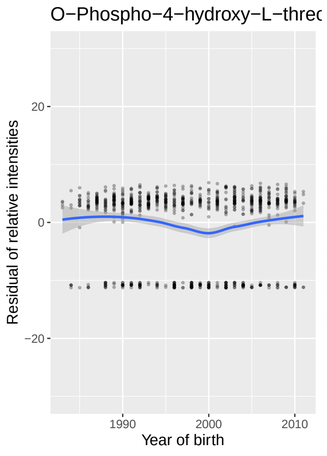
Lactosamine


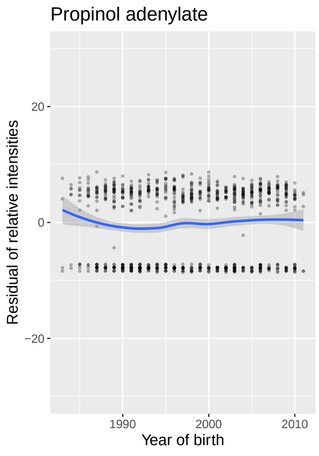
Lacto−N−triaose


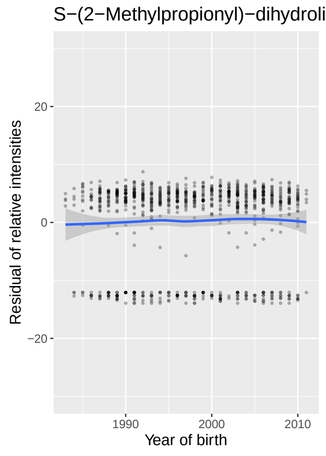
Prolylhydroxyproline


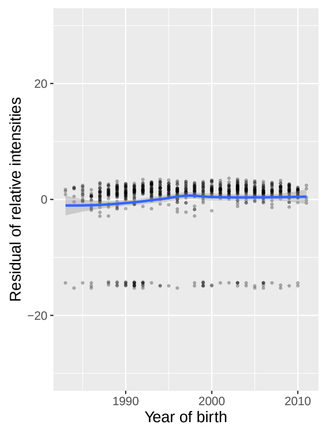
Tri−N−acetylchitotriose


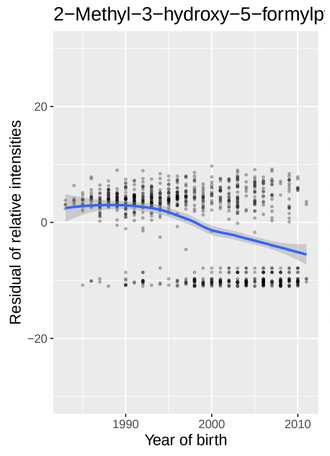
3−Carboxy−1−hydroxypropylthia


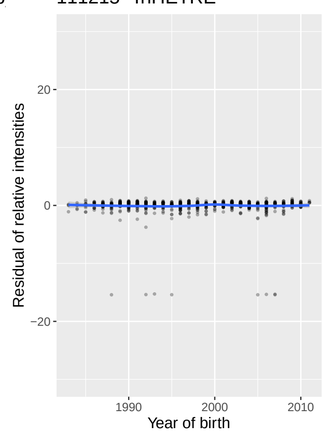
O−Phospho−4−hydroxy−L−threo


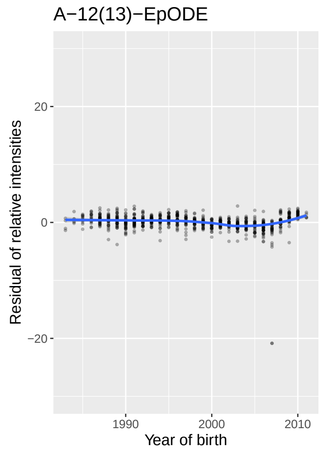
Propinol adenylate


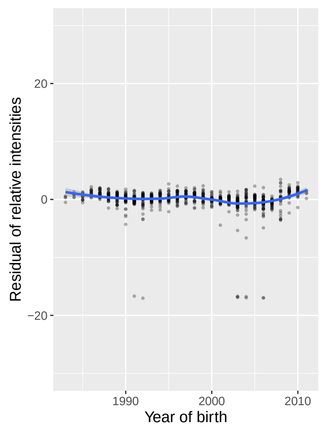
S−(2−Methylpropionyl)−dihydroli


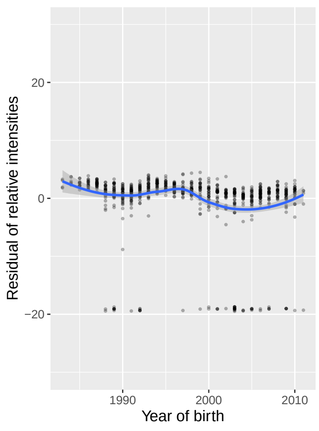
Cobinamide


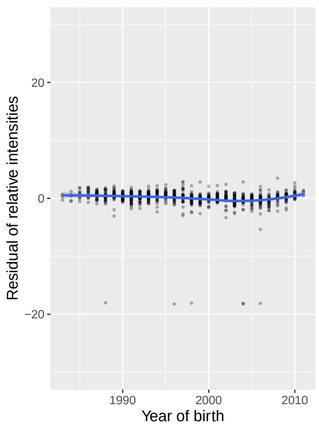
2−Methyl−3−hydroxy−5−formylp


111215−TriHETRE


A−12(13)−EpODE


1213−DiHODE


12−HEPE


1415−DiHETE


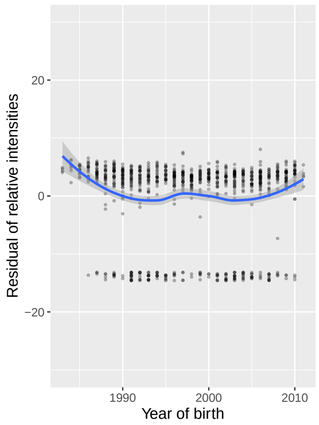
17−HDoHE
9−HETE
Inodxyl glucuronide
Tyramine glucuronide
Gamma−Glutamyl−Se−methylse
7−Methyluric acid
Hypusine
Deoxyhypusine
L−alpha−glutamyl−L−hydroxypro
L−beta−aspartyl−L−alanine
L−beta−aspartyl−L−aspartic acid
L−beta−aspartyl−L−glycine
L−beta−aspartyl−L−serine
L−beta−aspartyl−L−threonine
L−gamma−glutamyl−L−isoleucin
L−isoleucyl−L−proline
L−prolyl−L−proline
Topaquinone
1−(beta−D−Ribofuranosyl)−14−(
1−(sn−Glycero−3−phospho)−1D
2−(3−Carboxy−3−(methylammoi
2−(3−Carboxy−3−aminopropyl)−
26−Diamino−4−hydroxy−5−N−m
3−Methylene−indolenine
Cytidine 23−cyclic phosphate
N−Acetylvanilalanine
4−Hydroxybenzaldehyde
Gamma Glutamylglutamic acid
Gamma−Glutamyltyrosine
Ciliatine
2−Piperidinone
Dihydroxyacetone Phosphate Ac
3−Methoxybenzenepropanoic ac
(R)−2−Benzylsuccinate
2−Isopropyl−3−oxosuccinate
2−Keto−6−acetamidocaproate
34−Dihydroxybenzylamine
5−Aminopentanamide
Aminopropylcadaverine
Cis−zeatin
Dopaxanthin
Gamma−glutamyl−L−putrescine
Histidinal
Imidazole acetol−phosphate
Kynuramine
Maltopentaose
N−Succinyl−LL−26−diaminopim
Tetrahydrodipicolinate
11−Carboxy−alpha−chromanol
13E−Tetranor−16−carboxy−LTE4

Residual of relative intensities
Year of birth

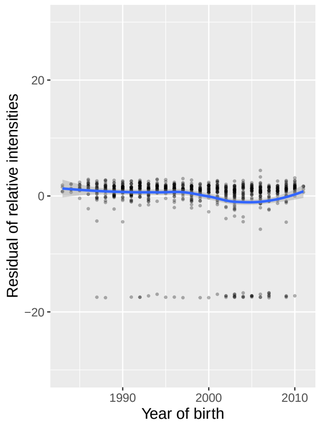
3−Dehydroquinate
5−Carboxy−alpha−chromanol
5−Carboxy−gamma−chromanol
5−Aminopentanal
7−Carboxy−alpha−chromanol
7−Carboxy−gamma−chromanol
7−Carboxy−gamma−tocotrienol
9−Carboxy−alpha−chromanol
Acetamidopropanal
Beta−Caroline
Kinetensin 1−3
N−Heptanoylglycine
Neuromedin C 1−8
Noradrenochrome o−semiquinor
Palmitoylglycine
S−(11−hydroxy−9−deoxy−delta1
Salsoline−1−carboxylate
Sinapyl alcohol
Spermine dialdehyde
trans−45−epoxy−2(E)−decenal
23−Diaminosalicylic acid
2−Hexenoylcholine
4−Aminobiphenyl
6−Succinoaminopurine
9−Decenoylcholine
9−Hexadecenoylcholine
Alanyltryptophan
Capryloylcholine
Indoleacetyl glutamine
Leucyl−phenylalanine
N−Decanoylglycine
N−Undecanoylglycine
NeNe dimethyllysine
Dodecanedioylcarnitine
Pimelylcarnitine
3−Hydroxy−cis−5−tetradecenoyl
3−Hydroxy−9−hexadecenoylcarı
3−Hydroxyhexadecadienoylcarn
3−Hydroxyhexadecanoylcarnitin
3−Hydroxy−11Z−octadecenoylca
14−Dithiothreitol
D−Tryptophan
Oleoyl glycine
(S)−Hydroxyoctadecanoyl−CoA
123−Trihydroxybenzene
Nookatone
Nootkatol
Urolithin A
124−Trimethylbenzene
2−Hydroxypyridine

Residual of relative intensities
Year of birth

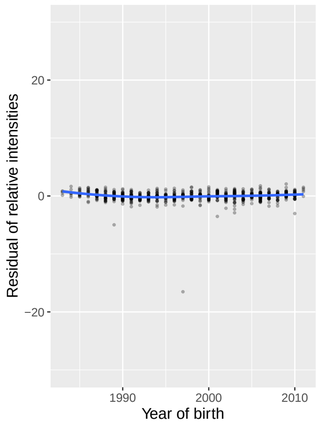
beta−Damascenone



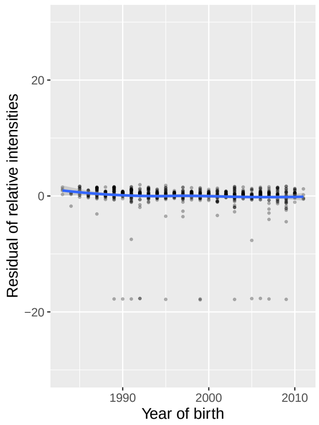
m−Cymene



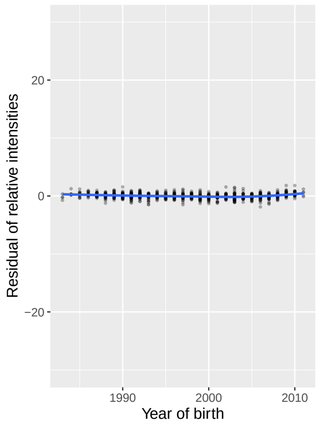
(E)−2−octenal



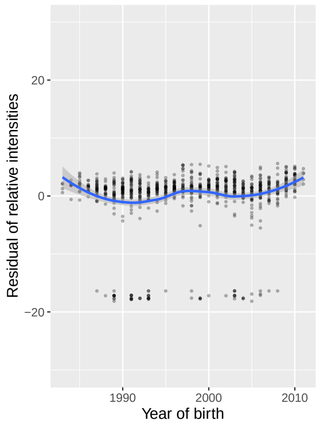
13−Heptadecyn−1−ol



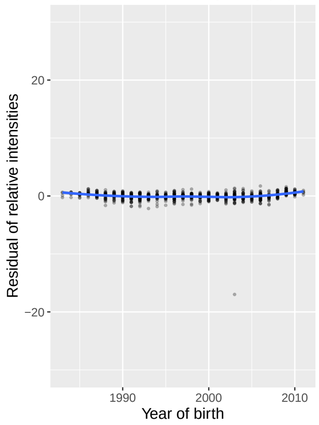
26−Di−tert−butylbenzoquinone



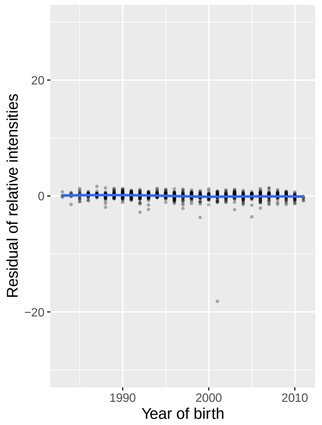
2−Methyl−2−phenyl−undecane



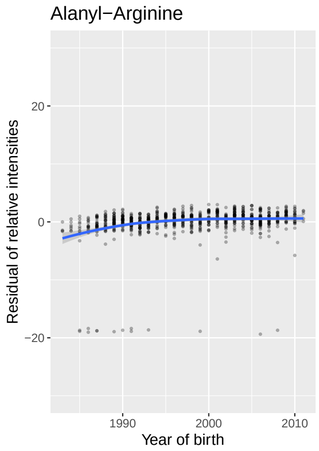
4−(1133−Tetramethylbutyl)−phe



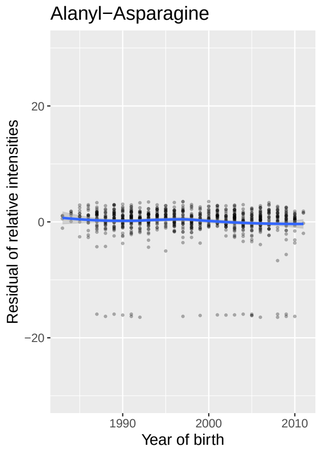
Alanyl−Alanine



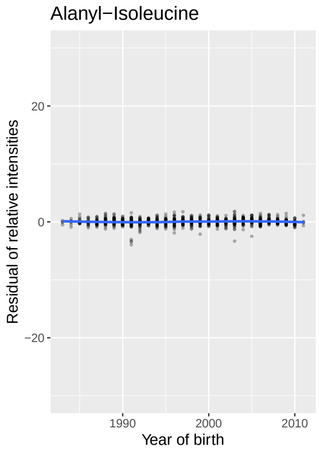
Alanyl−Arginine



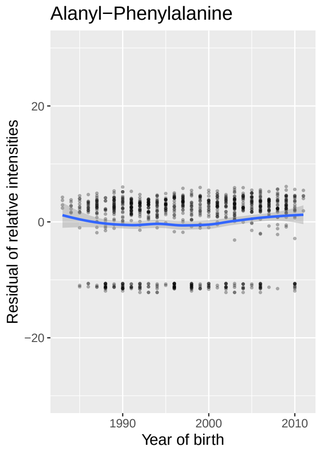
Alanyl−Asparagine



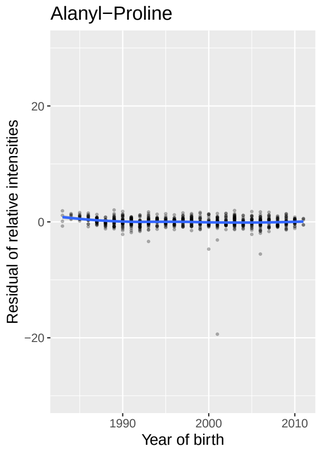
Alanyl−Isoleucine



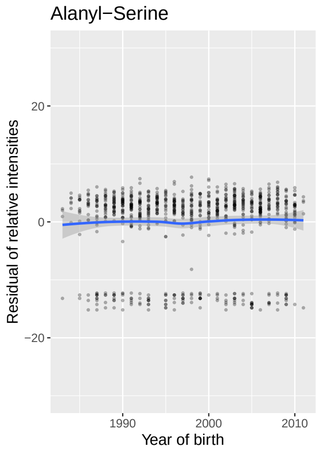
Alanyl−Phenylalanine



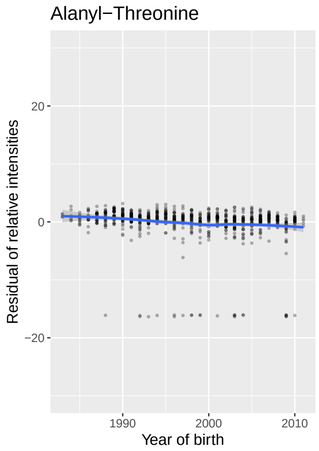
Alanyl−Proline



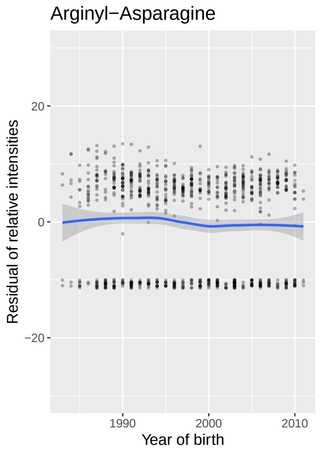
Alanyl−Serine



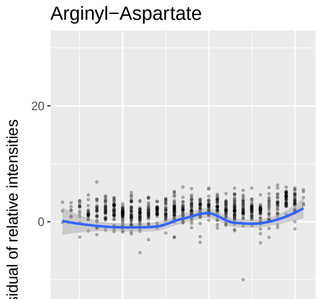
Alanyl−Threonine



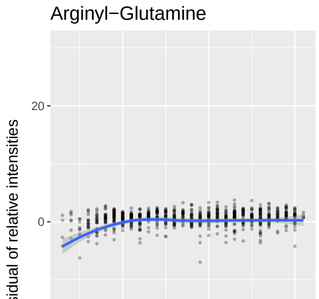
Arginyl−Asparagine



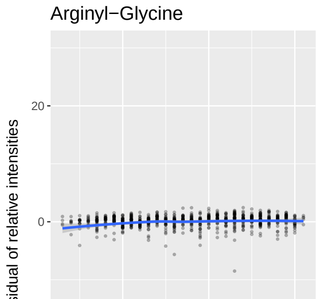
Arginyl−Aspartate



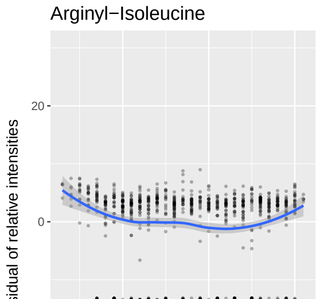
Arginyl−Glutamine



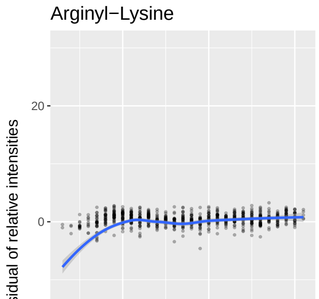
Arginyl−Glycine



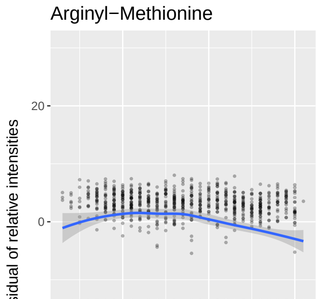
Arginyl−Isoleucine



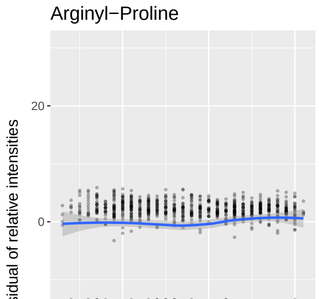
Arginyl−Lysine



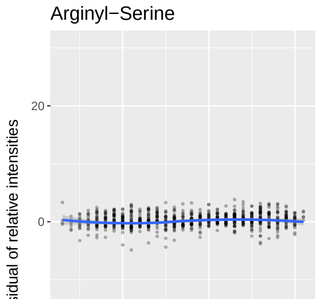
Arginyl−Methionine



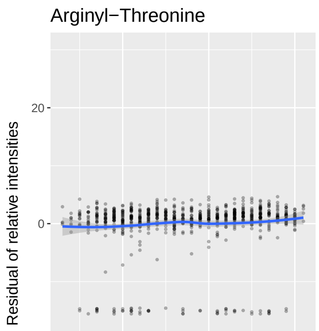
Arginyl−Proline



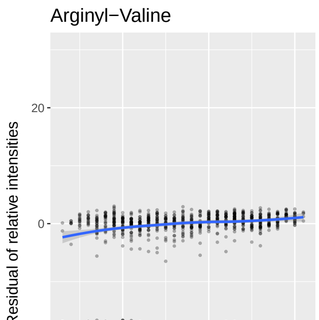
Arginyl−Serine



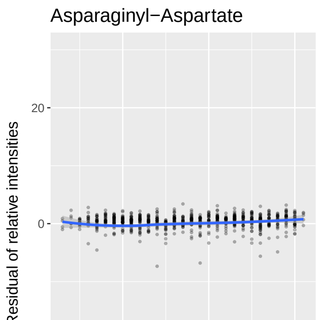
Arginyl−Threonine



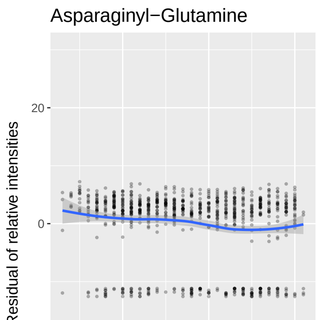
Arginyl−Valine



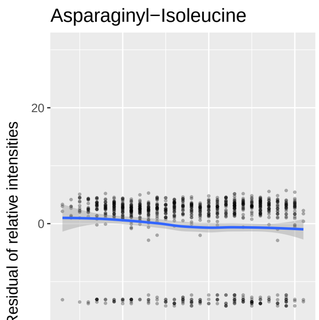
Asparaginyl−Aspartate



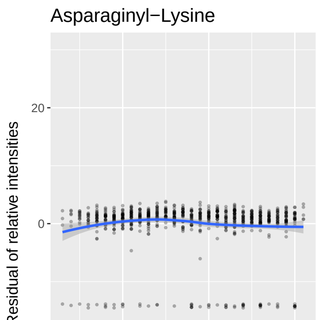
Asparaginyl−Glutamine



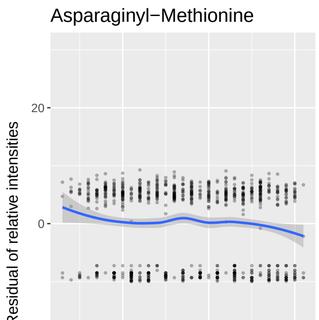
Asparaginyl−Isoleucine



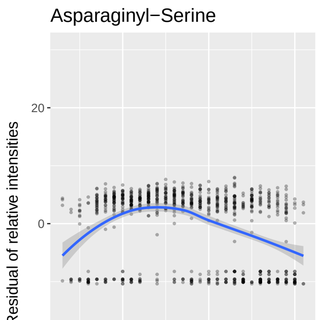
Asparaginyl−Lysine



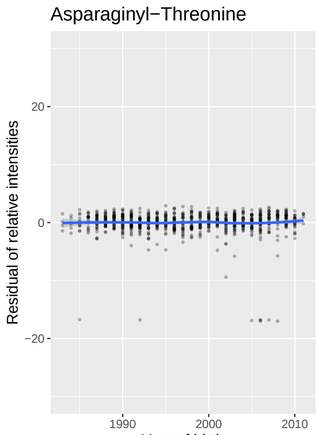
Asparaginyl−Methionine



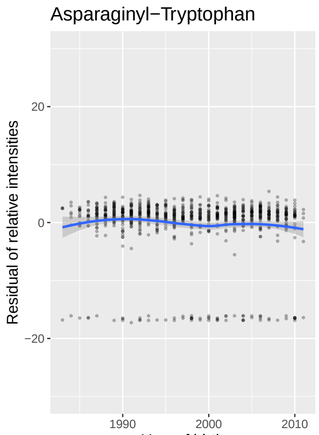
Asparaginyl−Serine



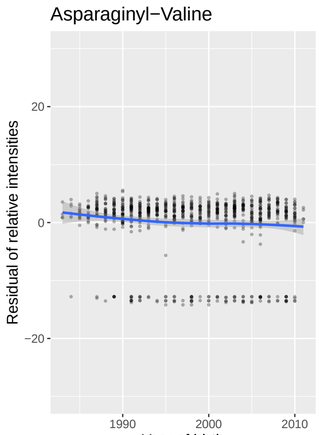
Asparaginyl−Threonine



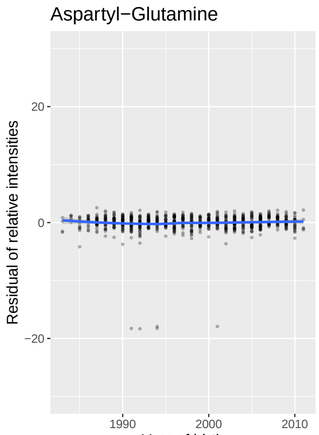
Asparaginyl−Tryptophan



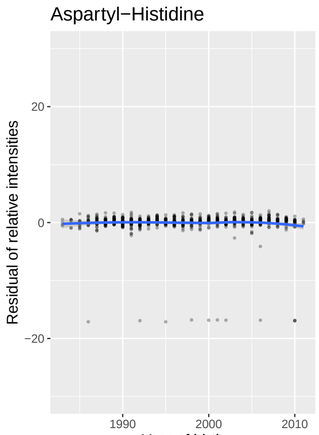
Asparaginyl−Valine



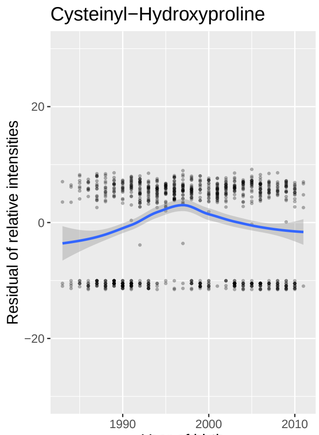
Aspartyl−Glutamine



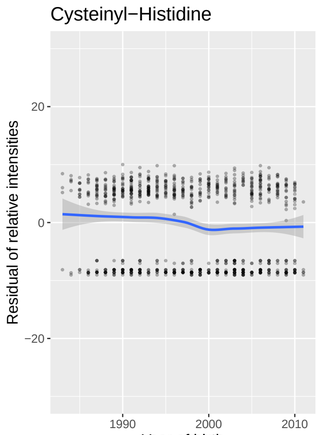
Aspartyl−Histidine



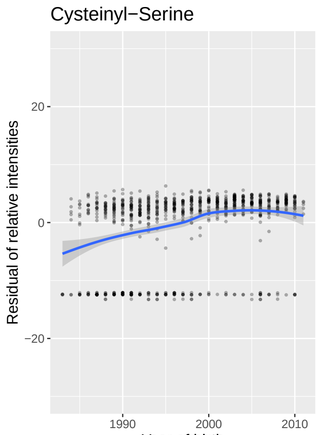
Cysteinyl−Hydroxyproline



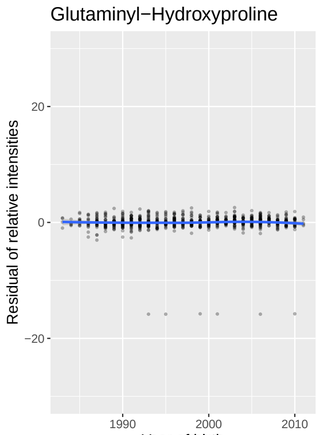
Cysteinyl−Histidine



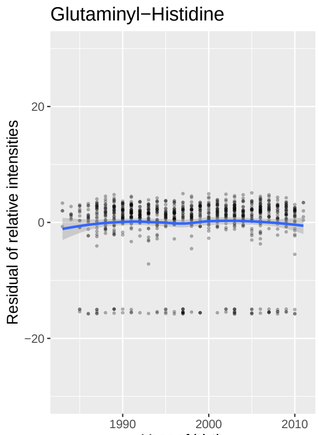
Cysteinyl−Serine



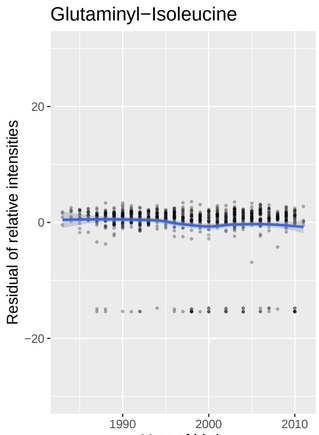
Glutaminyl−Hydroxyproline



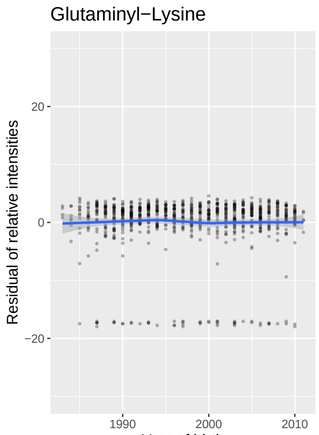
Glutaminyl−Histidine



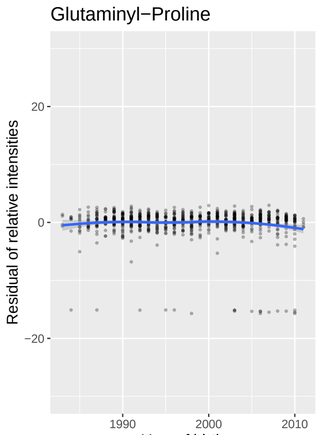
Glutaminyl−Isoleucine



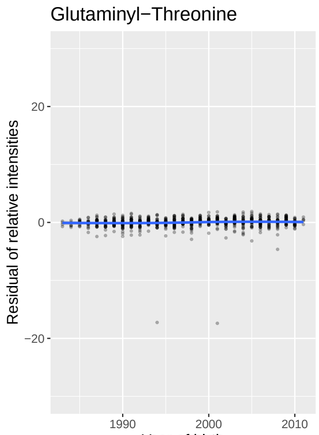
Glutaminyl−Lysine



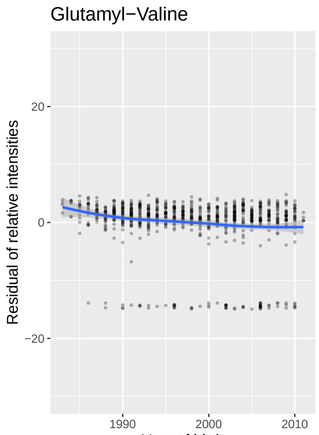
Glutaminyl−Proline



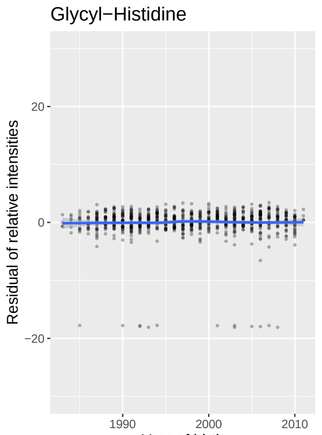
Glutaminyl−Threonine



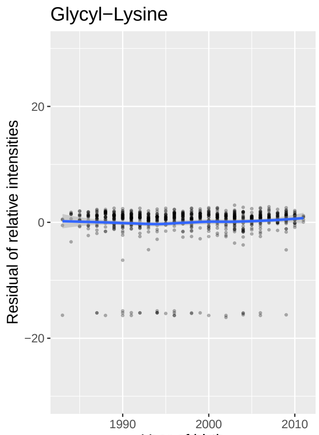
Glutamyl−Valine



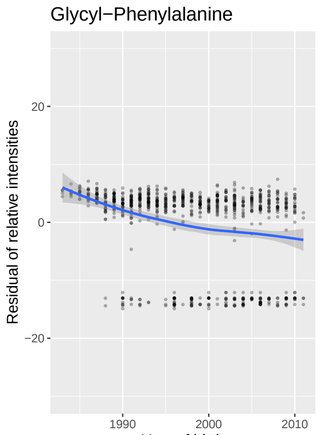
Glycyl−Histidine



Glycyl−Lysine



Glycyl−Phenylalanine



Glycyl−Serine
Hydroxyprolyl−Hydroxyproline
Hydroxyprolyl−Methionine
Histidinyl−Isoleucine
Histidinyl−Lysine
Histidinyl−Phenylalanine
Histidinyl−Proline
Isoleucyl−Isoleucine
Isoleucyl−Tyrosine
Isoleucyl−Valine
Lysyl−Phenylalanine
Lysyl−Proline
Lysyl−Serine
Lysyl−Threonine
Lysyl−Tryptophan
Lysyl−Valine
Methionyl−Tyrosine
Phenylalanyl−Glutamate
Phenylalanyl−Tryptophan
Phenylalanyl−Tyrosine
Phenylalanyl−Valine
(−)−epicatechin−3−O−glucuronide
3−Hydroxyadipic acid 36−lactone
3−Sn−phosphatidylethanolamine
3−O−Methyl−(−)−epicatechin−5−O−sı
Dimethylurea
lysoPC(28:1(5Z))
19−Noraldosterone
2−Isopropoxyphenol
2−Thiothiazolidine−4−carboxylic acid
34−Dimethoxyphenylethylamine
3−Phenoxybenzoic acid
7−Aminoclonazepam
Carboxytolbutamide
Endalin
N−Acetyl−S−(N−methylcarbamoyl)cys
N−Nitrosoproline
Nnal−N−oxide
Pivaloylcarnitine
Pregnanetriolone
4−Hydroxy−5−(dihydroxyphenyl)−vale
Methylgallic acid−O−sulphate
O−methoxycatechol−O−sulphate
Pyrogallol−2−O−glucuronide
5−(345−Trihydroxyphenyl)−gamma−valerolactone−O−methyl−O−sulphate

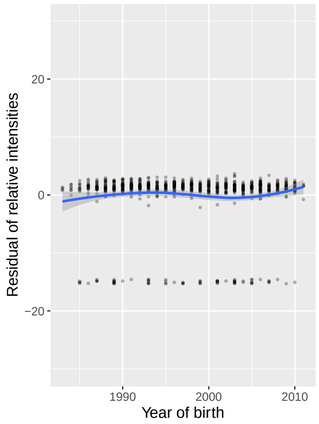
Residual of relative intensities
Year of birth

Web Figure 4. Endogenous Features in C18 column with suggested m/z matches annotation

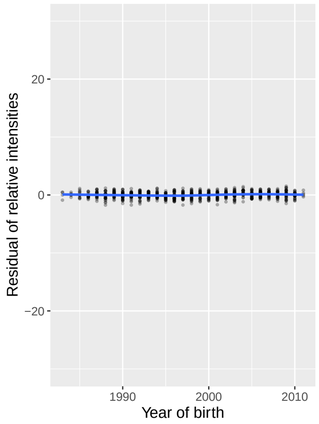
1−Methylhistidine
2−Ketobutyric acid
2−Hydroxybutyric acid
Deoxyuridine
Deoxycytidine
4−Pyridoxic acid
Ureidopropionic acid
Carnosine
Adenine
Betaine
Adenosine
Bilirubin
Beta−Alanine
Adenosine 35−diphosphate
cis−Aconitic acid
Dopamine
Dihydrouracil
Dihydrothymine
Cytidine triphosphate
Cytidine
Citric acid
Cytidine monophosphate
Deoxyadenosine
Gamma−Aminobutyric acid
Glycerylphosphorylethanolamine
Homovanillic acid
D−Glucose
Fructose 6−phosphate
Glycerol 3−phosphate
Homogentisic acid
Glycerol
Guanine
Guanosine
Glyceric acid
L−Glutamic acid
Gluconolactone
Gentisic acid
L−Malic acid
L−Tyrosine
L−Fucose
Inosinic acid
L−Dopa
Alpha−Lactose
L−Serine
L−Lactic acid
L−Aspartic acid
L−Cystine
Methylmalonic acid
N6−Acetyl−L−lysine
N−Acetylgalactosamine

Residual of relative intensities
Year of birth

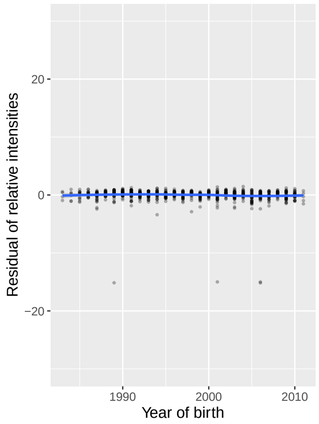
Ornithine



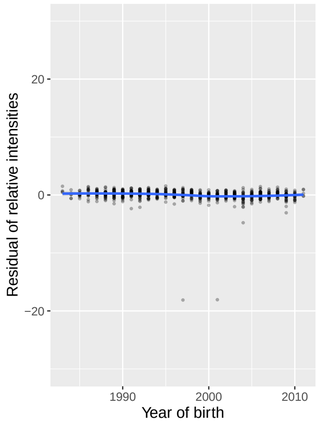
Norepinephrine



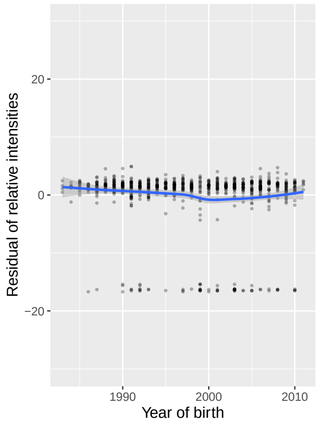
NADP



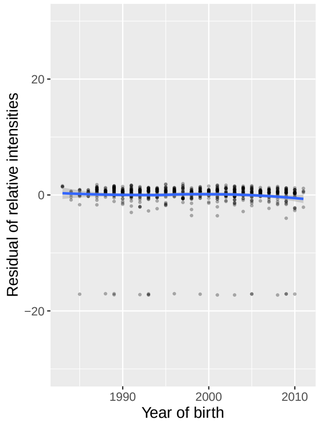
O−Phosphoethanolamine



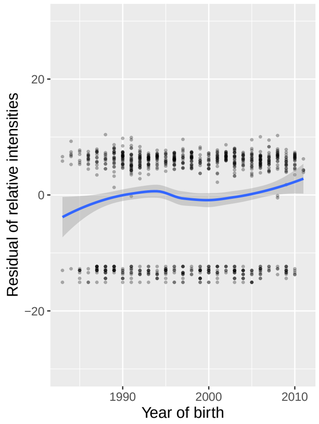
Oxoadipic acid



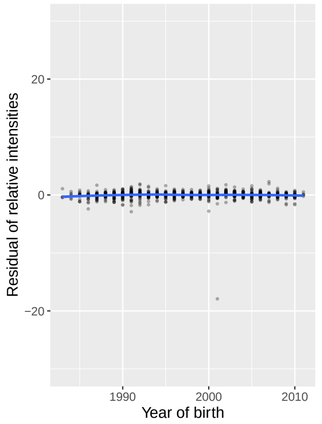
Orotic acid



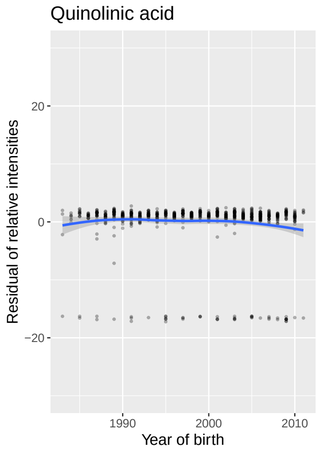
Mevalonic acid



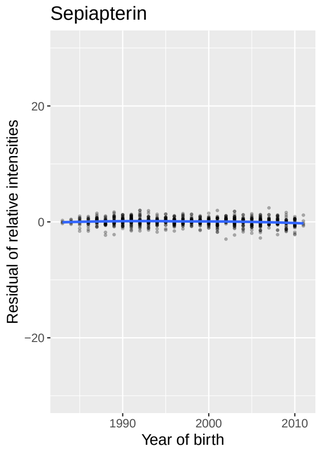
N−Acetylneuraminic acid



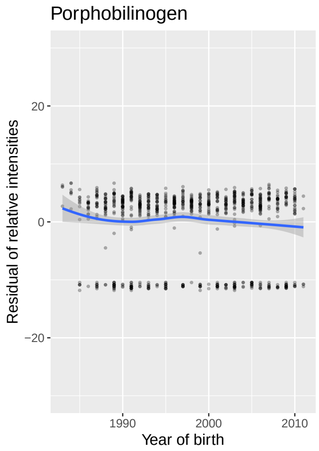
Quinolinic acid



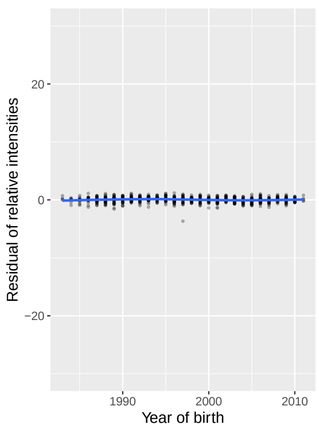
Sepiapterin



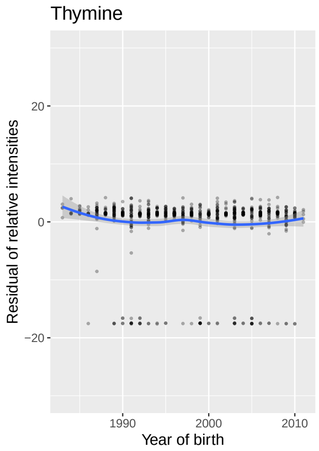
Porphobilinogen



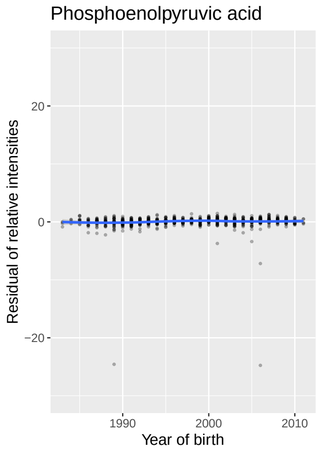
Taurine



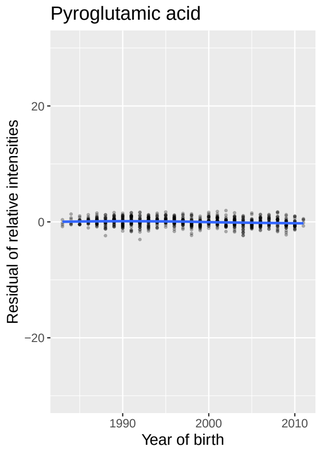
Thymine



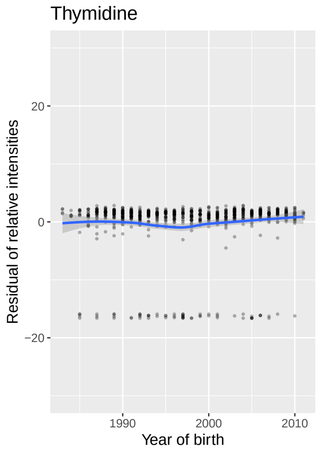
Phosphoenolpyruvic acid



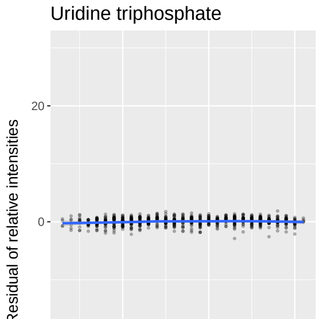
Pyroglutamic acid



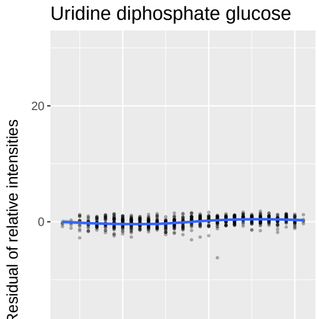
Thymidine



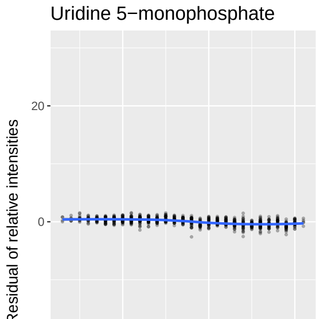
Uridine triphosphate



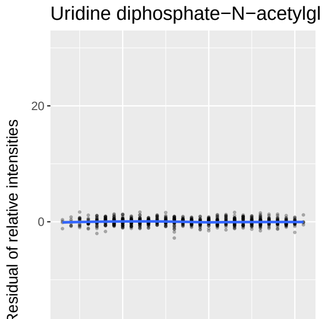
Uridine diphosphate glucose



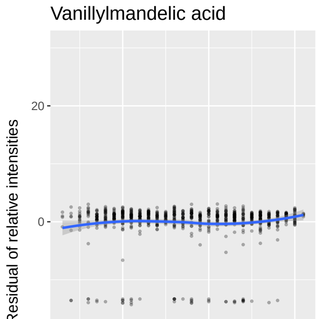
Uridine 5−monophosphate



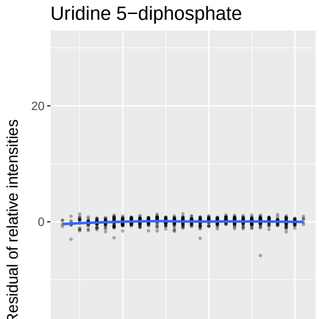
Uridine diphosphate−N−acetylgl



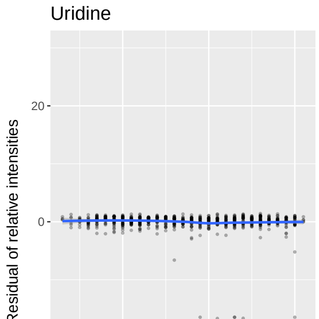
Vanillylmandelic acid



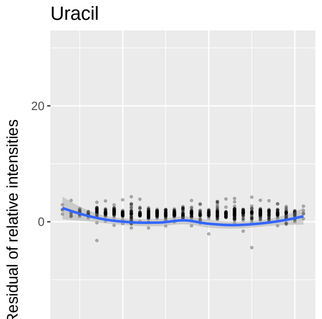
Uridine 5−diphosphate



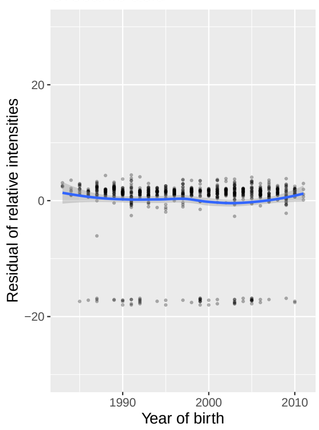
Uridine



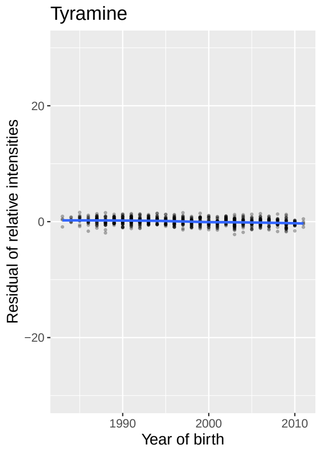
Uracil



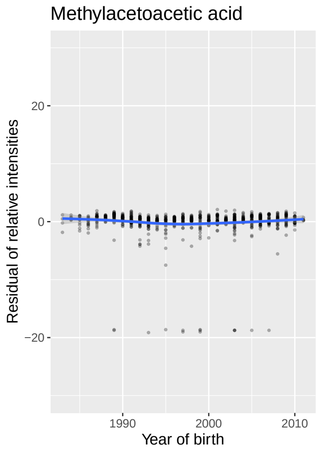
Urocanic acid



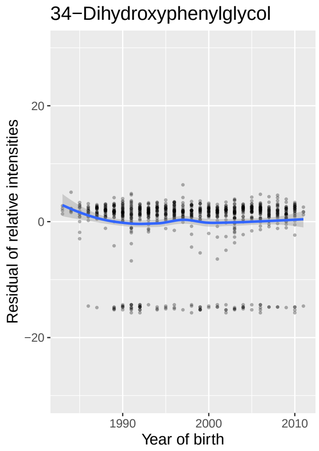
Tyramine



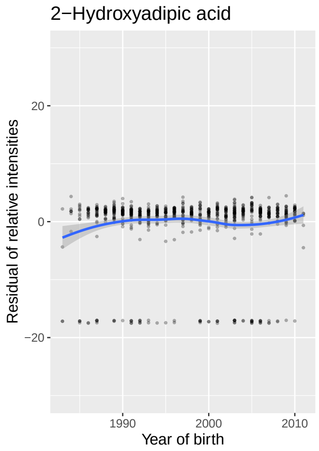
Methylacetoacetic acid



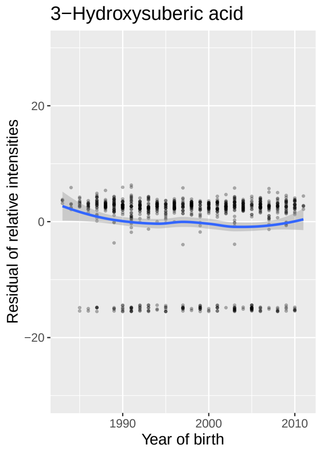
34−Dihydroxyphenylglycol



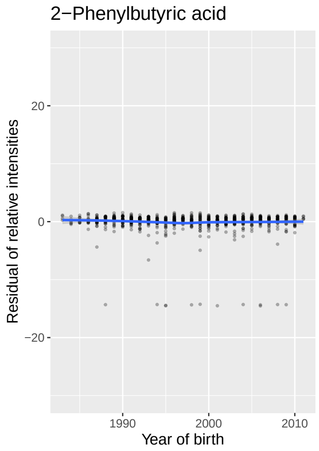
2−Hydroxyadipic acid



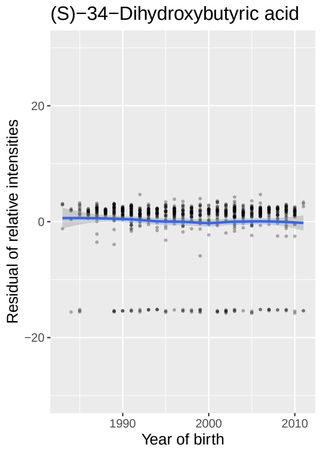
3−Hydroxysuberic acid



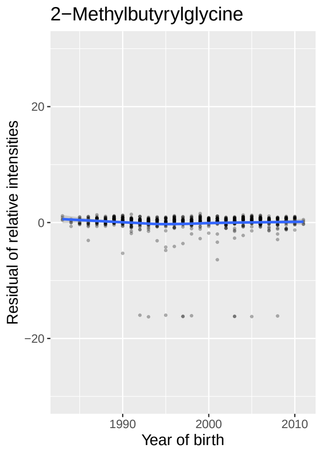
2−Phenylbutyric acid



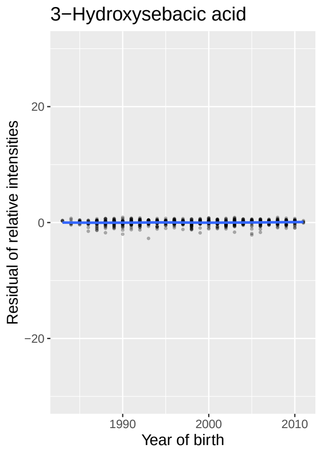
(S)−34−Dihydroxybutyric acid



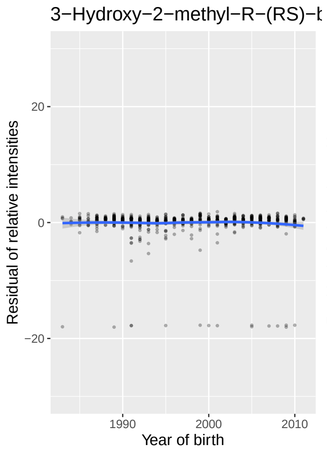
2−Methylbutyrylglycine



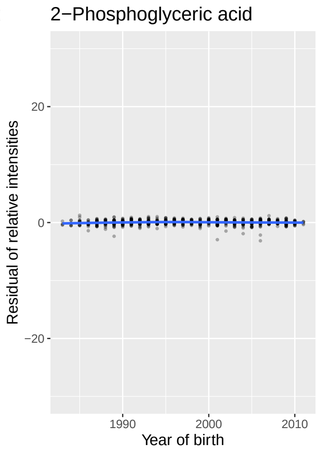
3−Hydroxysebacic acid



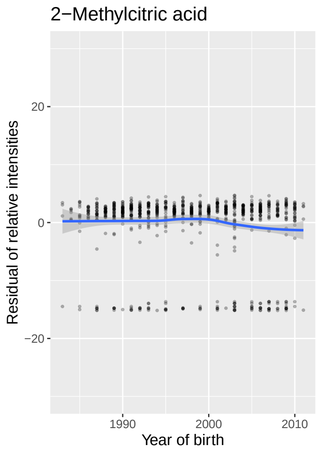
3−Hydroxy−2−methyl−R−(RS)−b



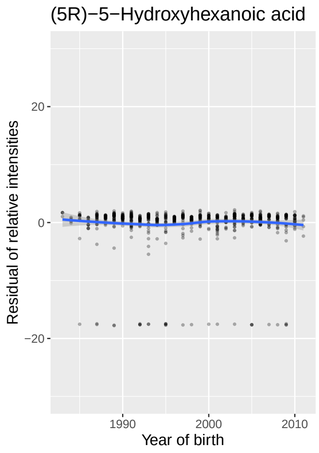
2−Phosphoglyceric acid



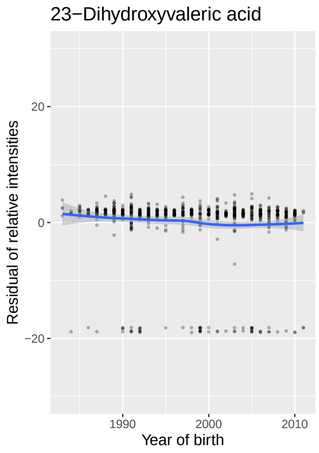
2−Methylcitric acid



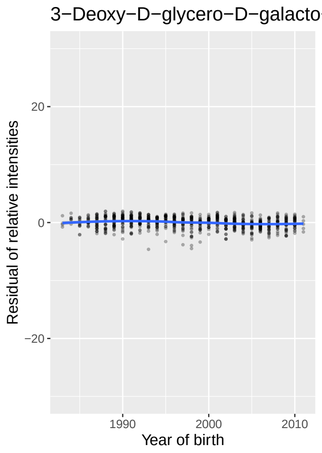
(5R)−5−Hydroxyhexanoic acid



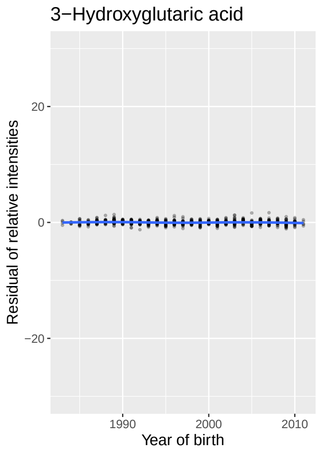
23−Dihydroxyvaleric acid



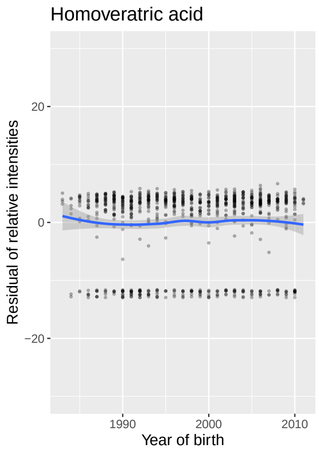
3−Deoxy−D−glycero−D−galacto



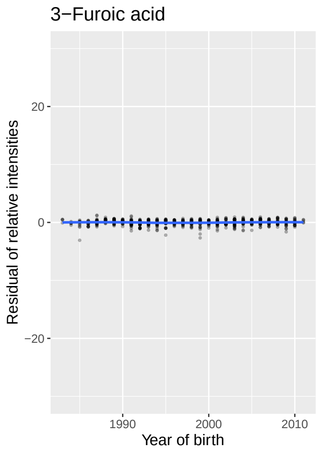
3−Hydroxyglutaric acid



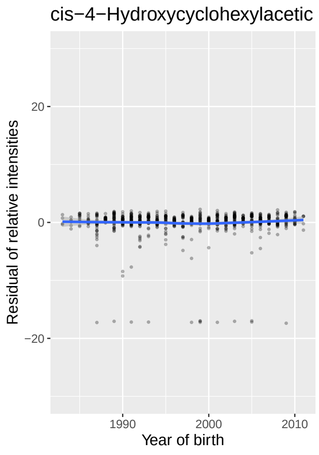
Homoveratric acid



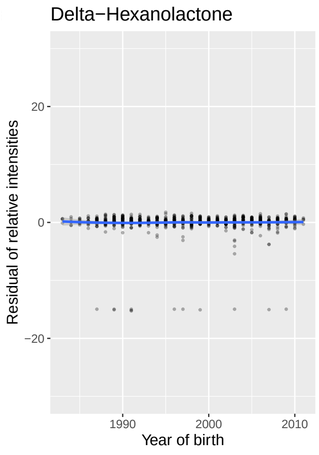
3−Furoic acid



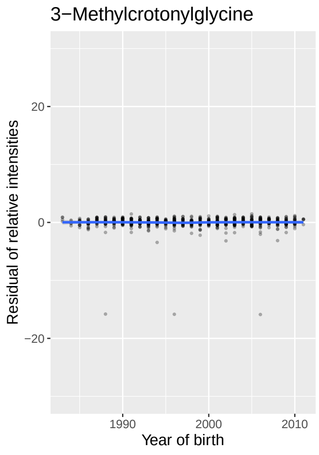
cis−4−Hydroxycyclohexylacetic a



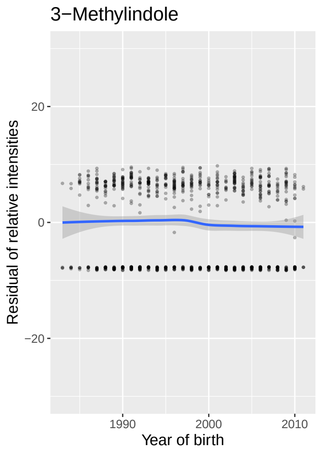
Delta−Hexanolactone



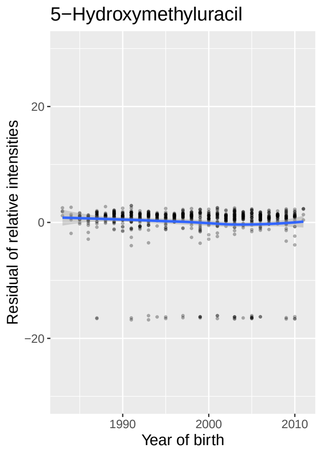
3−Methylcrotonylglycine



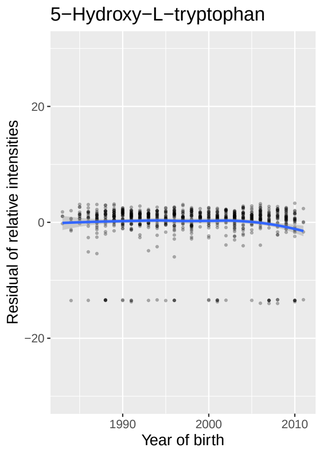
3−Methylindole



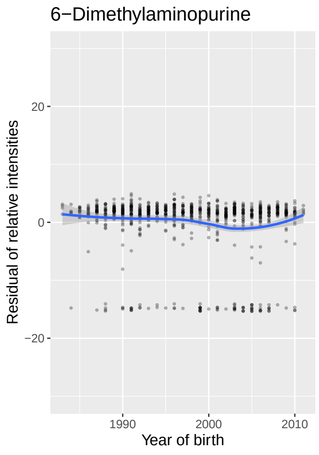
5−Hydroxymethyluracil



5−Hydroxy−L−tryptophan



6−Dimethylaminopurine



7−Hydroxyoctanoic acid
Aspartylglycosamine
56−Dihydrouridine
Ribitol
Aminoadipic acid
N−Acetyl−L−phenylalanine
45−Dihydroorotic acid
Acetylglycine
Adenylsuccinic acid
Adenosine triphosphate
Arabinonic acid
5−Hydroxymethyl−4−methylurac
Gamma−Butyrolactone
L−Alloisoleucine
3−Methoxy−4−hydroxyphenyleth
Creatinine
D−Phenyllactic acid
Galactonic acid
Cinnamic acid
Desmosine
Glutarylglycine
Erythronic acid
D−Ribulose 5−phosphate
Dodecanedioic acid
Cytosine
Succinylacetone
Galactaric acid
L−Glutamine
Cysteineglutathione disulfide
Homo−L−arginine
Indolelactic acid
Hexadecanedioic acid
L−Kynurenine
Hexanoylglycine
Mandelic acid
Isoxanthopterin
Kynurenic acid
Glycylproline
4−Hydroxyproline
Isovalerylglutamic acid
Isobutyrylglycine
Cysteine−S−sulfate
Hydroxyphenylacetylglycine
5−Hydroxyindoleacetic acid
N−Acetylgalactosamine 4−sulph
Octadecanedioic acid
Azelaic acid
Orotidine
Sebacic acid
SAICAR

Residual of relative intensities
Year of birth
20
0
−20
1990
2000
2010

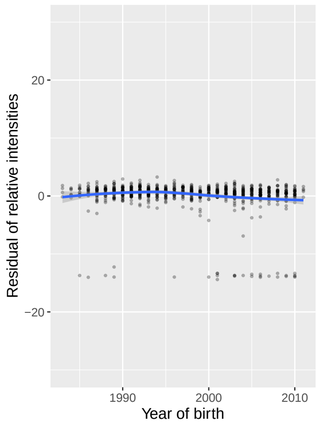
Pterin
N−Acetyl−L−aspartic acid
Phosphoglycolic acid
Phenylacetylglycine
3−Sialyllactose
Ureidosuccinic acid
Quinaldic acid
Pyridinoline
Formiminoglutamic acid
Pimelic acid
Tetradecanedioic acid
4−Methylcatechol
Ribothymidine
Undecanedioic acid
Suberic acid
Vinylacetylglycine
7−Methylguanine
Citrulline
Deoxyadenosine monophosphat
Succinyladenosine
Vanillactic acid
Uridine diphosphate glucuronic a
Pyrocatechol
Lipoamide
1D−Myo−inositol 14−bisphospha
4−(2−Aminophenyl)−24−dioxobu
5−Methylcytidine
Dihydrolipoamide
S−Adenosylmethioninamine
3−Succinoylpyridine
3−Sulfinoalanine
dUDP
Adenosine phosphosulfate
Oxoamide
3−Pyridinebutanoic acid
Biliverdin
D−4−Phosphopantothenate
Phosphohydroxypyruvic acid
3−Ketolactose
Deoxyribose 5−phosphate
2−Deoxyguanosine 5−monopho
Gamma−Glutamylcysteine
N−Acetyl−D−Glucosamine 6−Ph
S−Lactoylglutathione
N−Acetylaspartylglutamic acid
D−Sedoheptulose 7−phosphate
D−1−Piperideine−2−carboxylic a
GDP−L−fucose
Glucosamine−1P
D−Glyceraldehyde 3−phosphate

Residual of relative intensities
Year of birth

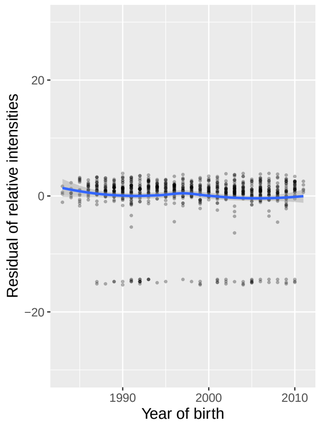
Dimethylallylpyrophosphate
Inositol cyclic phosphate
6−Phosphonoglucono−D−lacton
Iminoaspartic acid
Nicotinic acid mononucleotide
Octanal
FMNH2
Aminomalonic acid
Guanosine diphosphate mannos
trans−12−Dihydrobenzene−12−(
5−Methylthioadenosine
Cytidine monophosphate N−ace
Adenosine diphosphate ribose
68−Dihydroxypurine
Indoleacetaldehyde
Deoxyuridine triphosphate
Leukotriene C4
N−Formylkynurenine
Guanosine diphosphate
dCMP
Hydantoin−5−propionic acid
Tetrahydropteridine
5−Thymidylic acid
L−Glutamic acid 5−phosphate
4−Nitrophenol
2−Aminomuconic acid
N−Acetylarylamine
56−Dihydroxyindole−2−carboxyl
Fucose 1−phosphate
4−Oxo−4−(3−pyridyl)−butanami
4−Fumarylacetoacetic acid
Guanosine triphosphate
2−Aminomuconic acid semialdel
1−Pyrroline−5−carboxylic acid
m−Chlorohippuric acid
6−Phosphogluconic acid
D−Erythrose 4−phosphate
2−Amino−3−carboxymuconic ac
GDP−4−Dehydro−6−deoxy−D−r
Hydroxypyruvic acid
Guanosine monophosphate
Niacinamide
4−(3−Pyridyl)−3−butenoic acid
3−Methoxytyrosine
Phosphoribosyl formamidocarbc
Diethylthiophosphate
3−Hydroxyanthranilic acid
NADH
Vanylglycol
Acetylphosphate

Residual of relative intensities
Year of birth

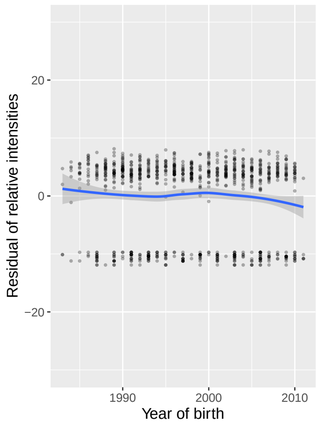
dADP



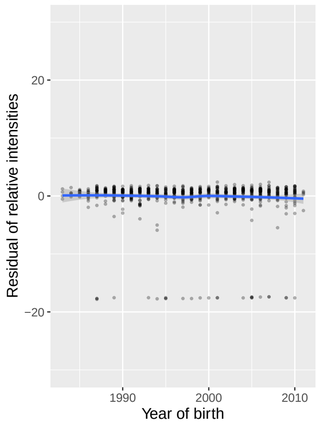
Phosphocreatine



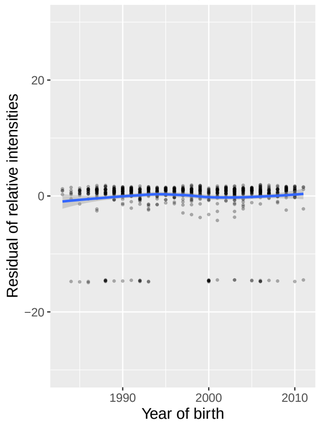
AICAR



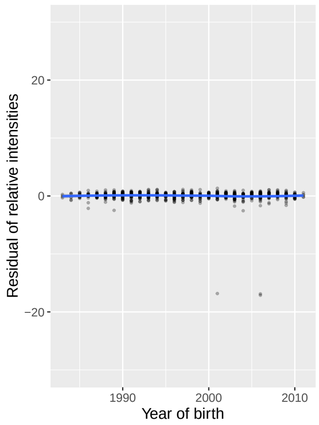
Alpha−CEHC



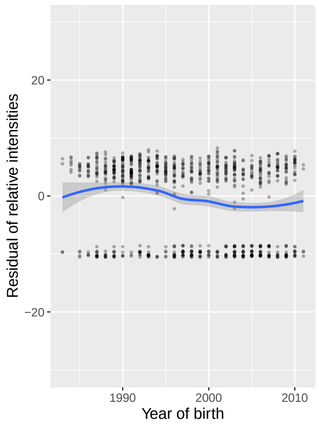
S−Acetyldihydrolipoamide



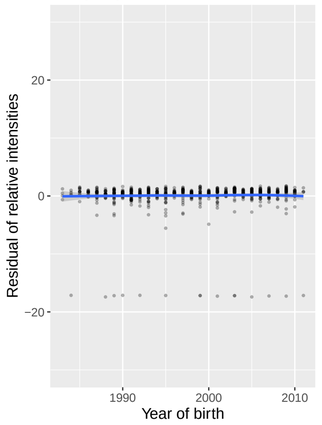
Deoxyadenosine triphosphate



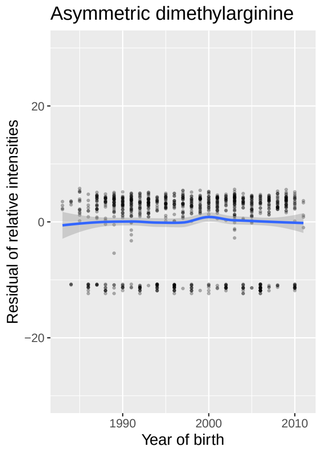
5−Formiminotetrahydrofolic acid



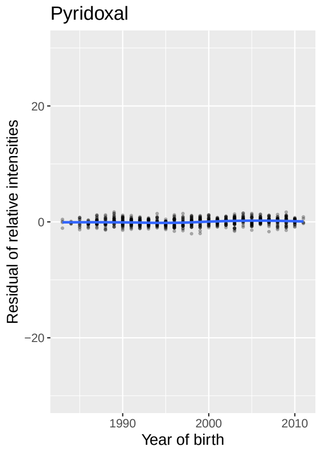
3−Pyridylacetic acid



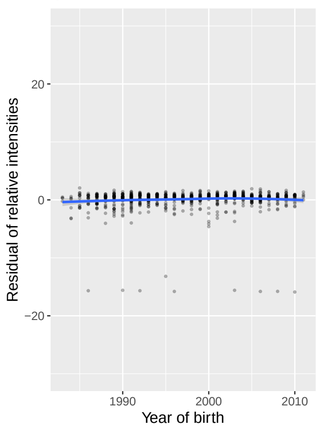
Asymmetric dimethylarginine



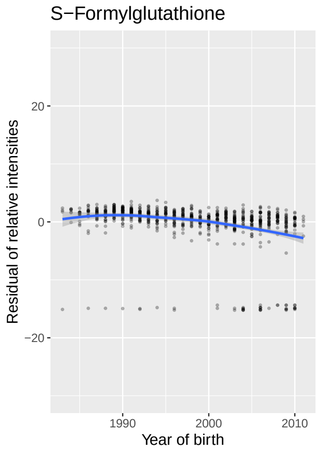
Pyridoxal



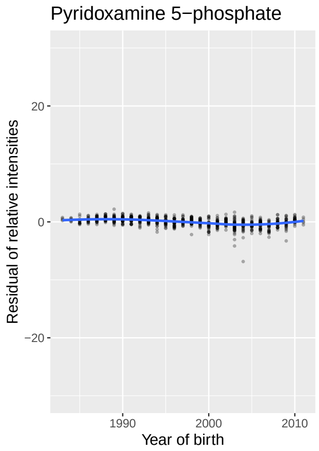
CDP



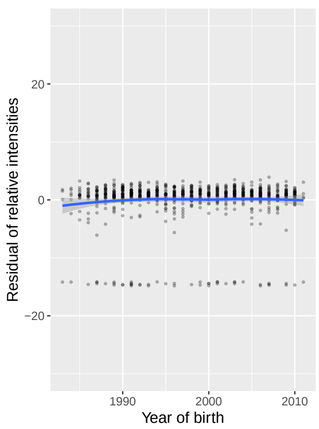
S−Formylglutathione



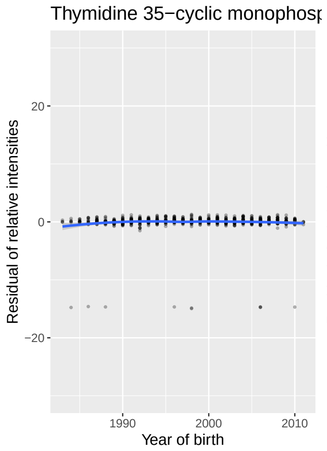
Pyridoxamine 5−phosphate



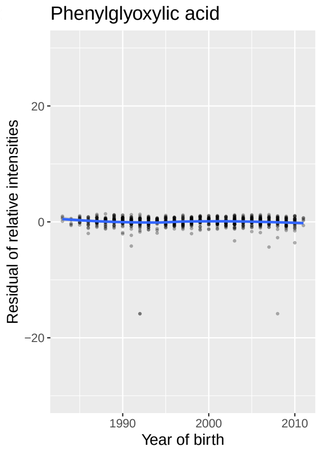
CDP−Ethanolamine



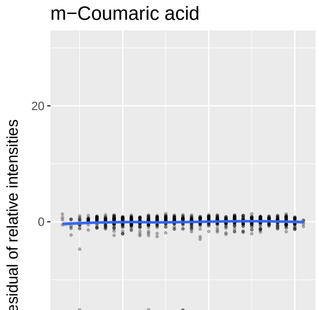
Thymidine 35−cyclic monophosp



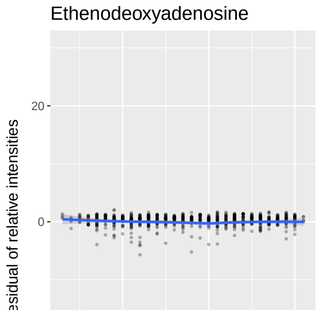
Phenylglyoxylic acid



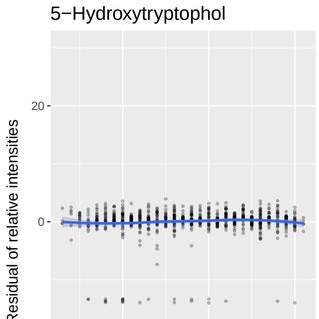
m−Coumaric acid



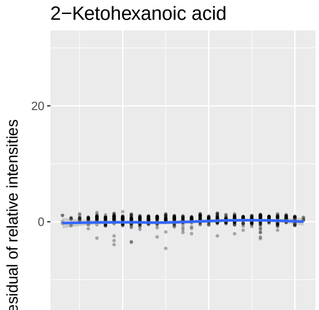
Ethenodeoxyadenosine



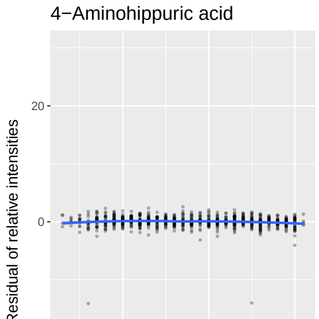
5−Hydroxytryptophol



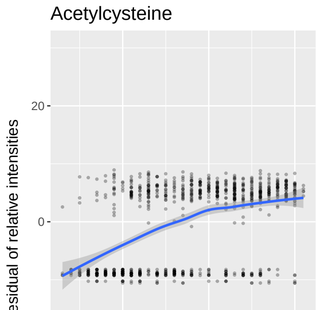
2−Ketohexanoic acid



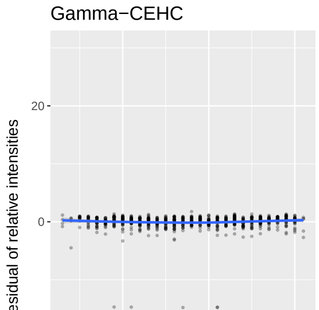
4−Aminohippuric acid



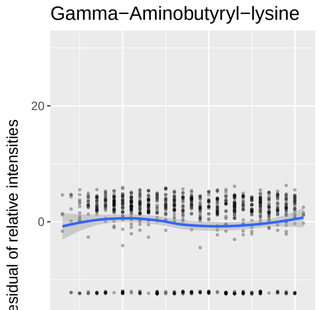
Acetylcysteine



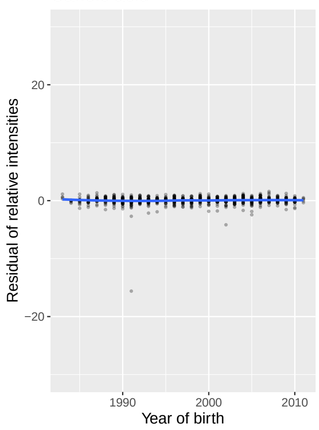
Gamma−CEHC



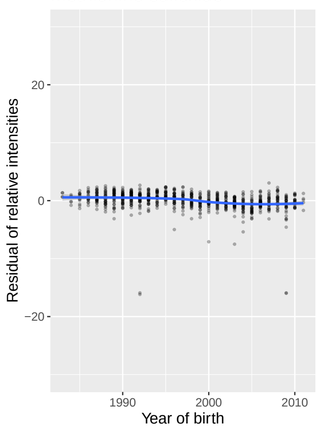
Gamma−Aminobutyryl−lysine



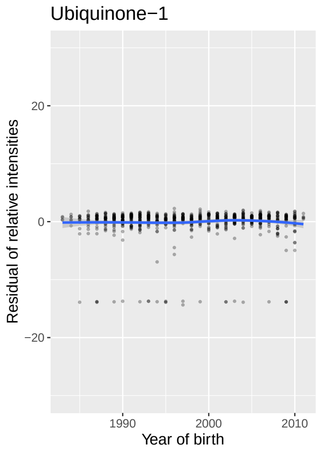
Caffeic acid



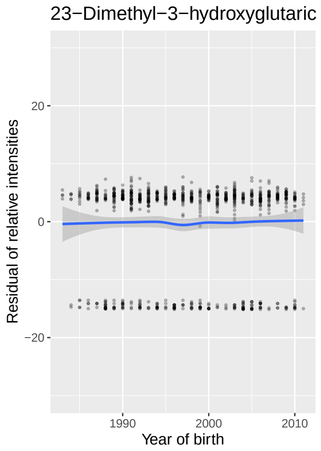
Methionine sulfoxide



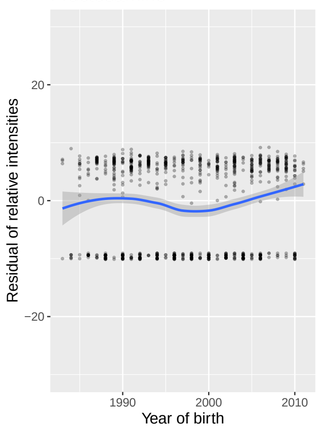
Ubiquinone−1



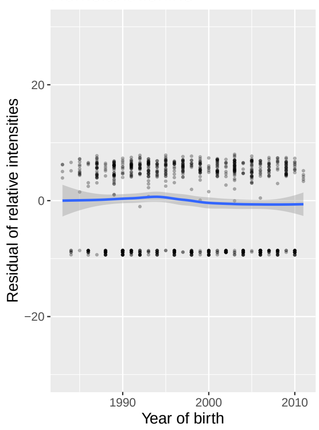
23−Dimethyl−3−hydroxyglutaric



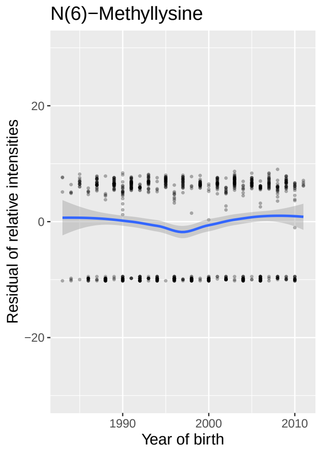
Fructosamine



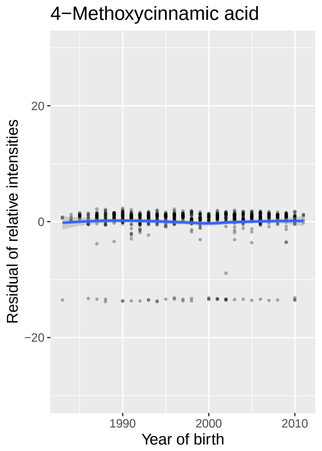
Homolanthionine



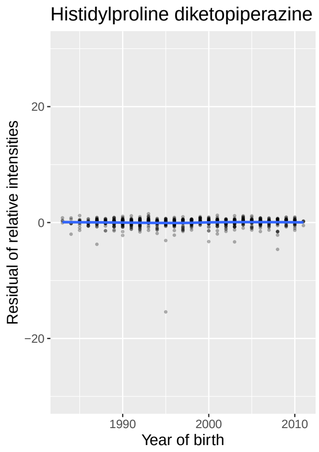
N(6)−Methyllysine



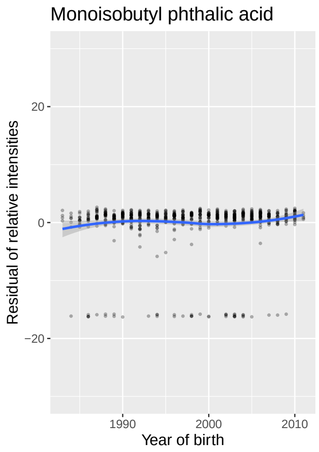
4−Methoxycinnamic acid



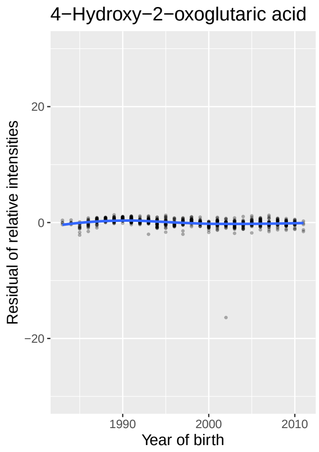
Histidylproline diketopiperazine



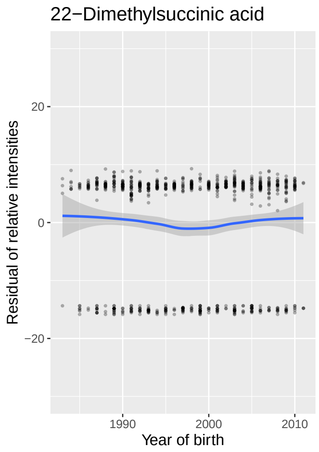
Monoisobutyl phthalic acid



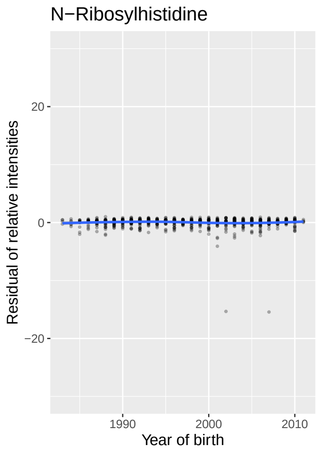
4−Hydroxy−2−oxoglutaric acid



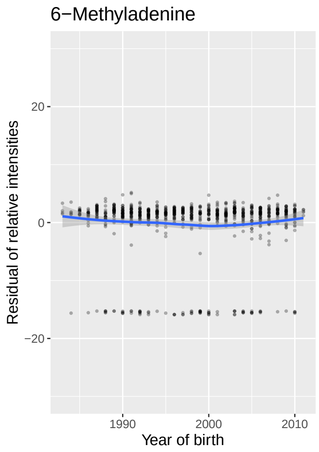
22−Dimethylsuccinic acid



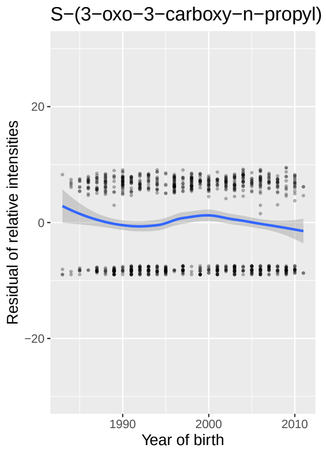
N−Ribosylhistidine



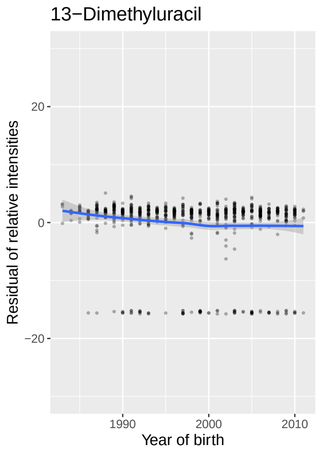
6−Methyladenine



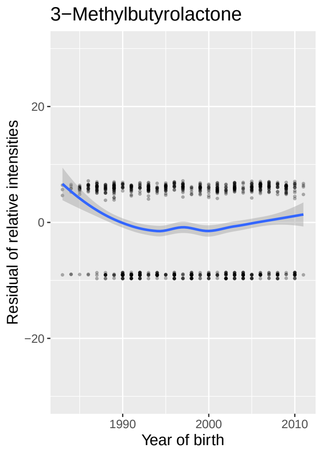
S−(3−oxo−3−carboxy−n−propyl)



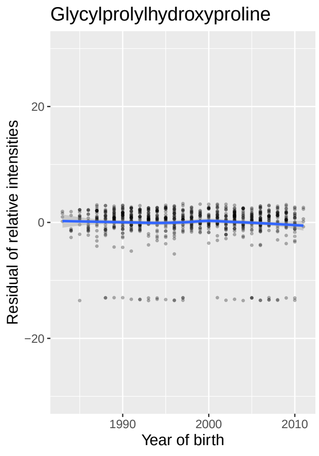
13−Dimethyluracil



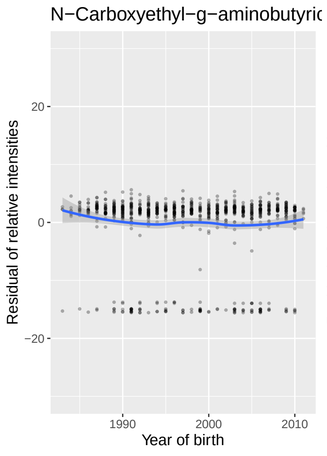
3−Methylbutyrolactone



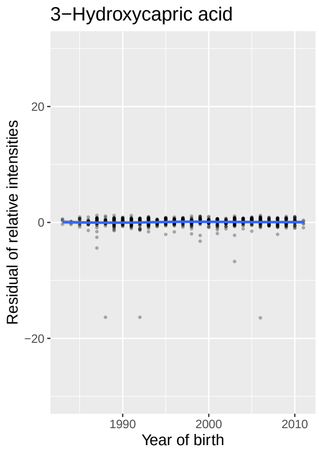
Glycylprolylhydroxyproline



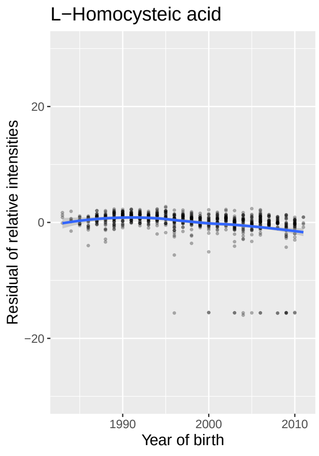
N−Carboxyethyl−g−aminobutyric



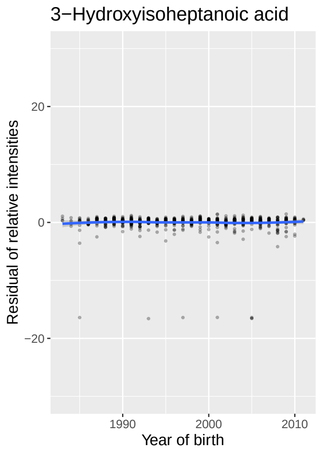
3−Hydroxycapric acid



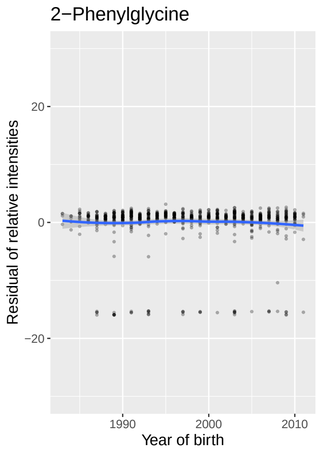
L−Homocysteic acid



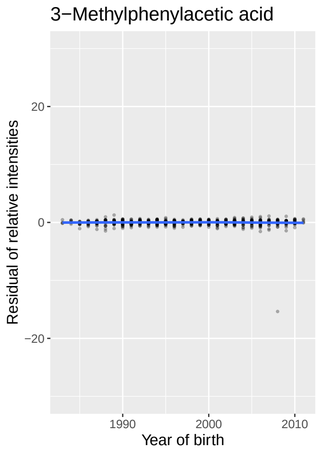
3−Hydroxyisoheptanoic acid



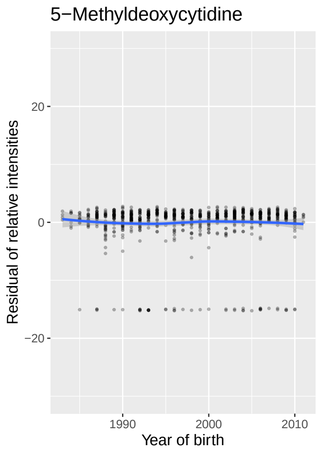
2−Phenylglycine



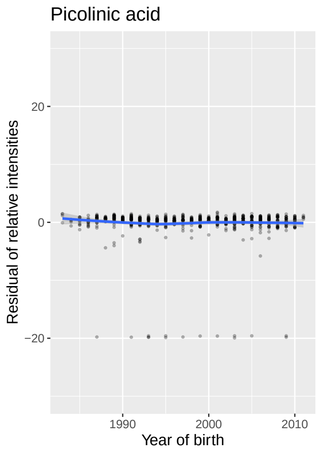
3−Methylphenylacetic acid

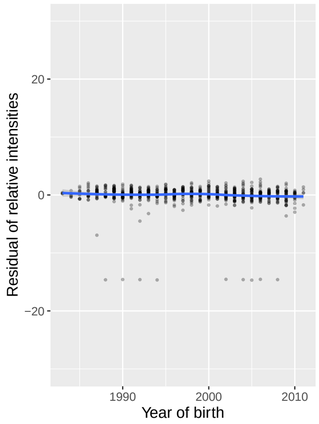


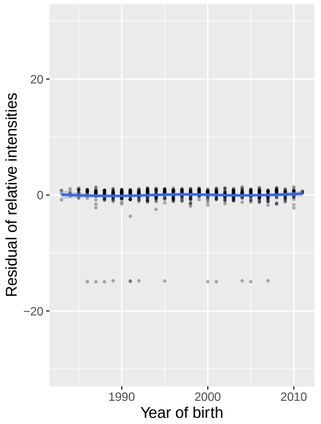
5−Methyldeoxycytidine

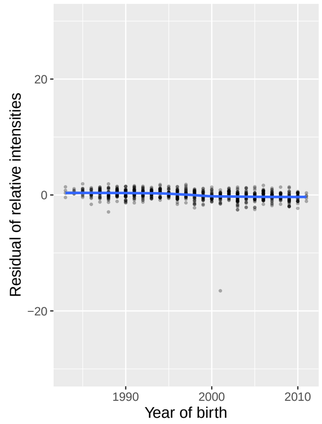


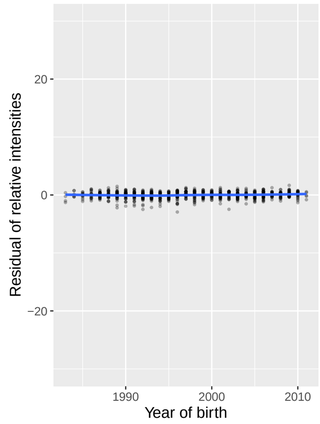
Picolinic acid

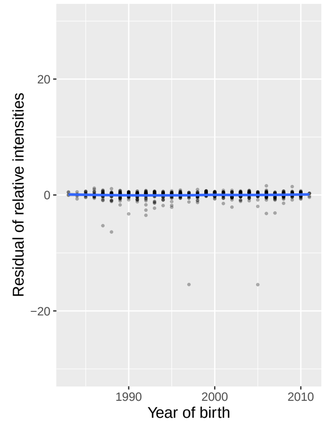


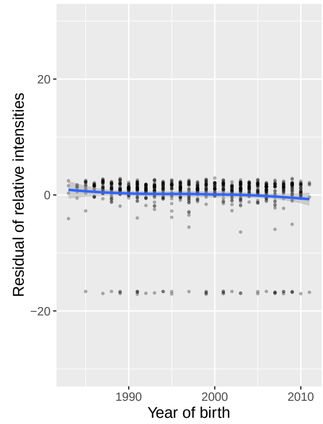
4−Hydroxy−L−glutamic acid


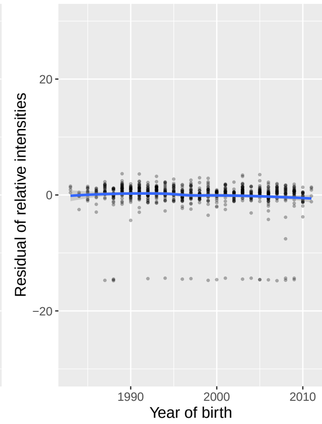
23−Dinor−6−keto−prostaglandin


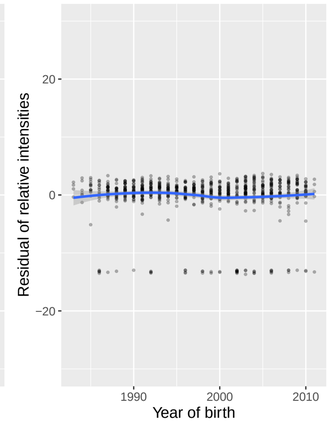
2−(acetylamino)−15−anhydro−2


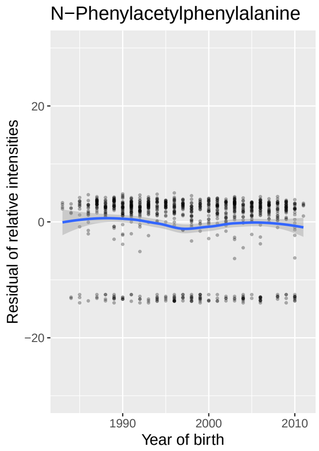
2−Indolecarboxylic acid


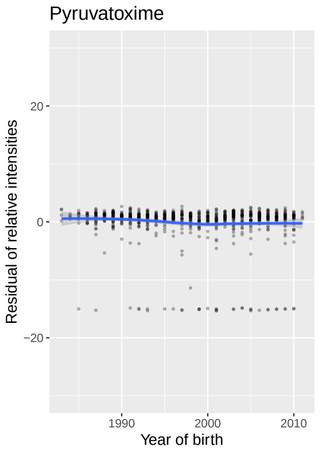
111−Undecanedicarboxylic acid


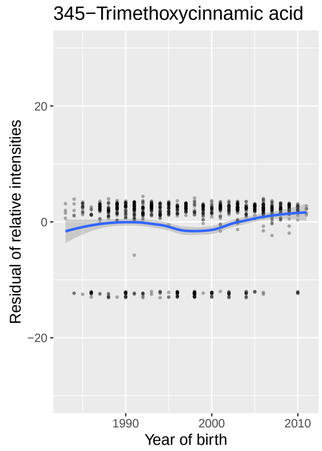
Benzoquinoneacetic acid


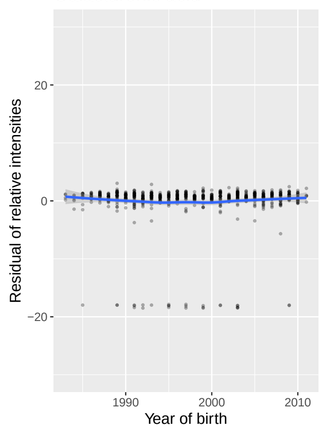
Aspartyl−L−proline


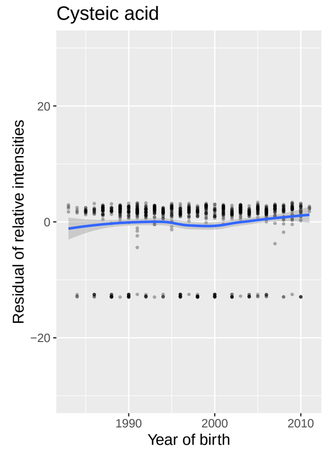
5−Methoxytryptophan


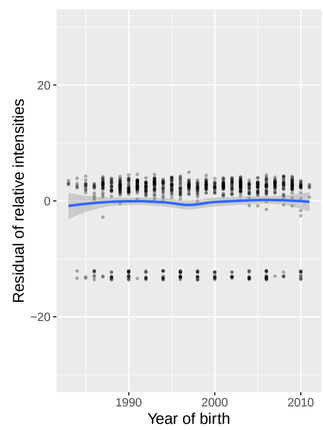
N−Phenylacetylphenylalanine


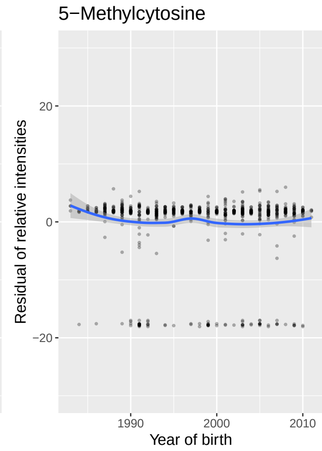
Pyruvatoxime


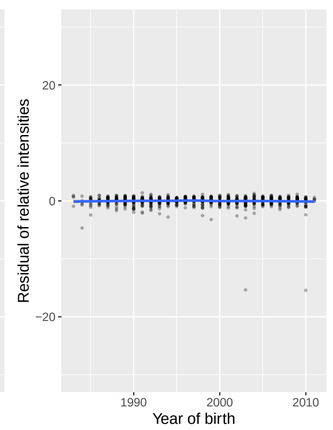
345−Trimethoxycinnamic acid


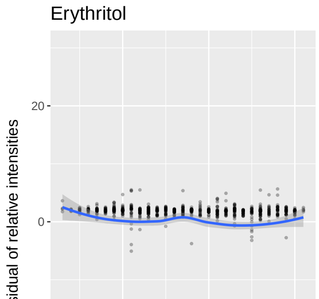
Galacturonic acid


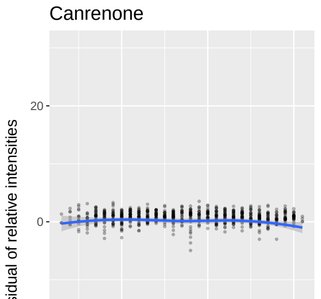
Cysteic acid


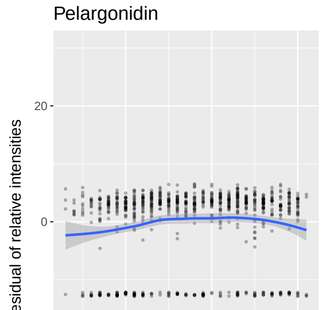
Alloxan


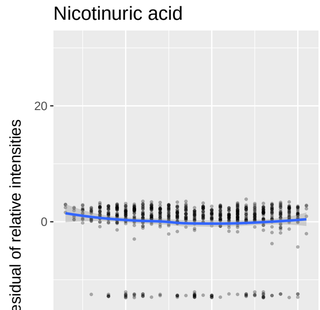
5−Methylcytosine


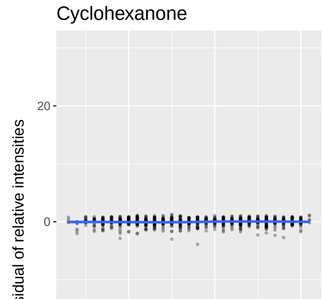
4−Nitrocatechol


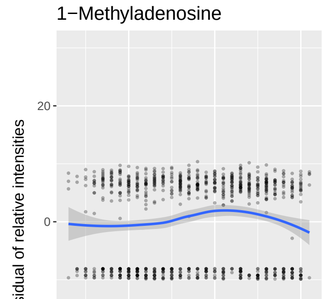
Erythritol


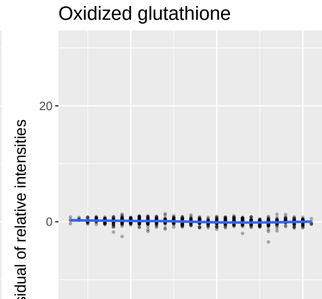
Canrenone


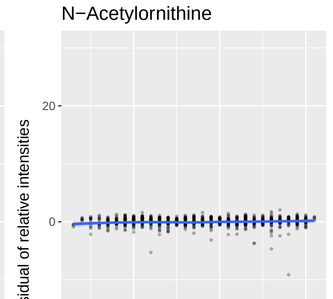
Pelargonidin


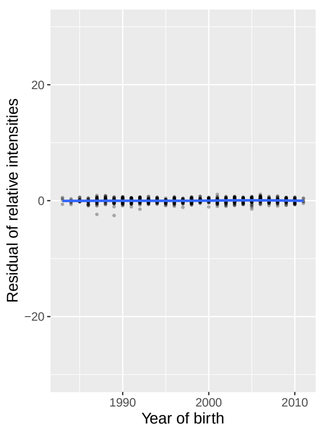
Nicotinuric acid


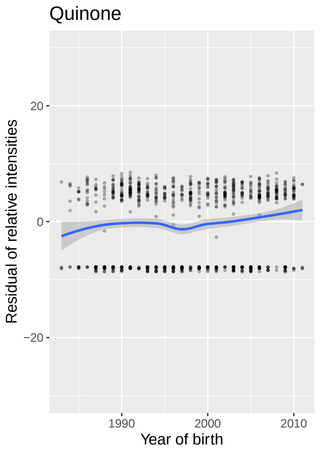
Cyclohexanone


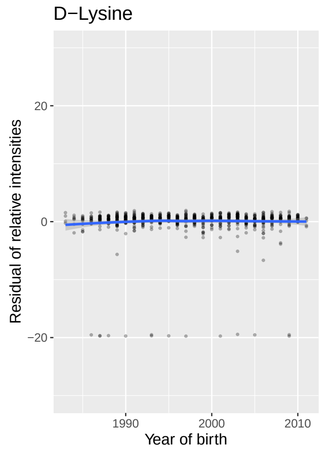
1−Methyladenosine


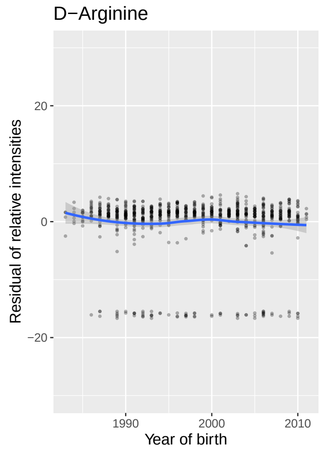
Oxidized glutathione


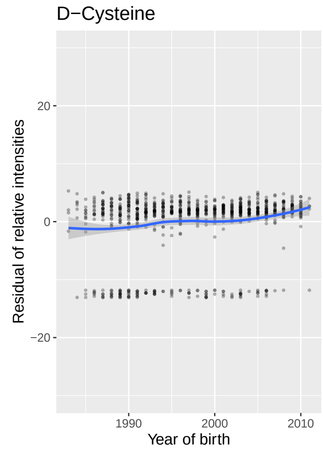
N−Acetylornithine


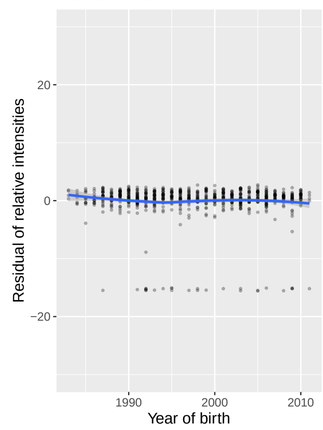
Chitin


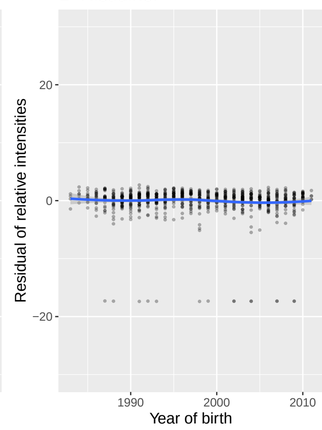
Quinone


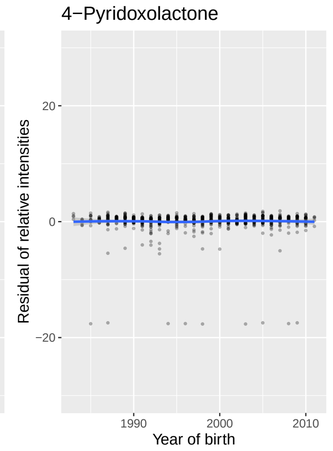
D−Lysine


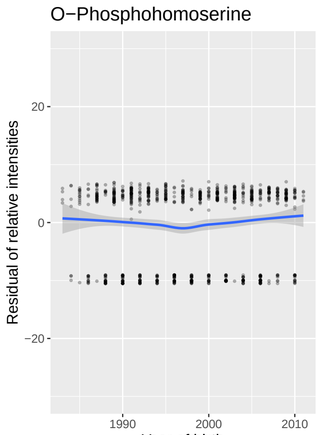
D−Arginine


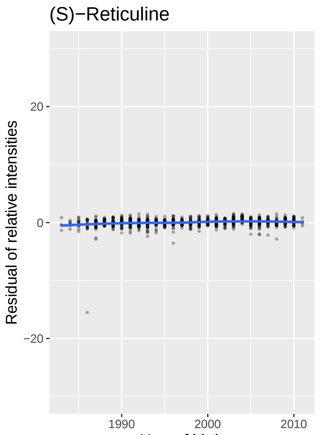
D−Cysteine


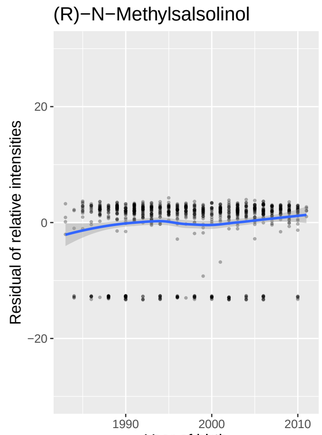
Pantetheine


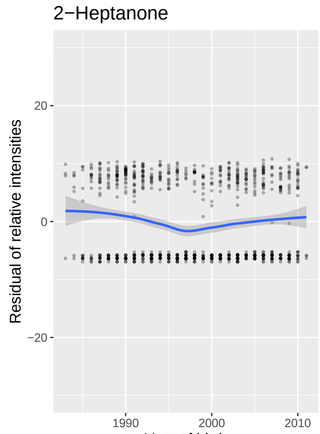
L−Histidinol


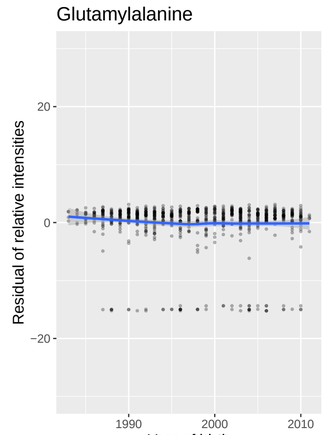
4−Pyridoxolactone


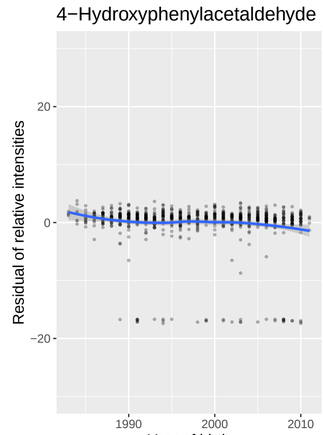
O−Phosphohomoserine


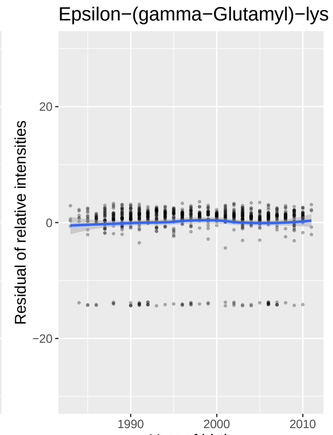
(S)−Reticuline


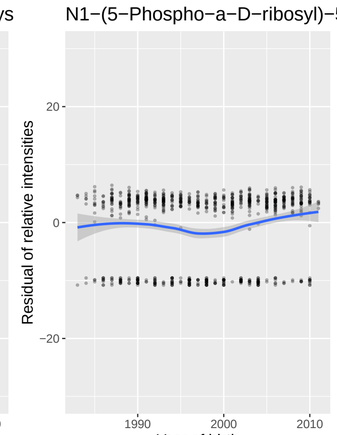
(R)−N−Methylsalsolinol


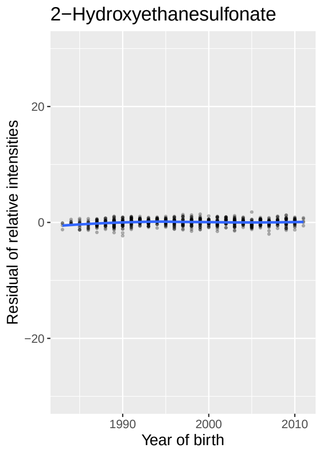
2−Heptanone


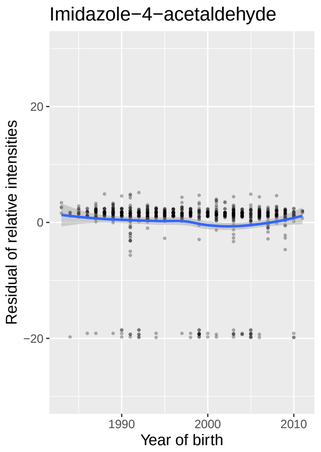
Glutamylalanine


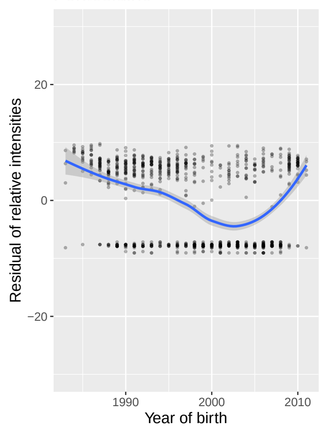
4−Hydroxyphenylacetaldehyde


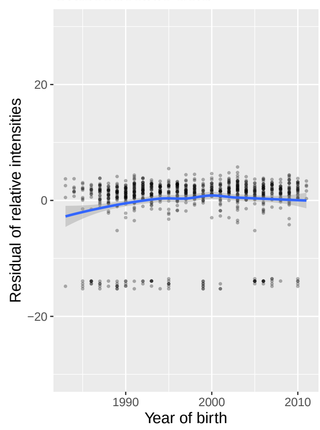
Epsilon−(gamma−Glutamyl)−lys


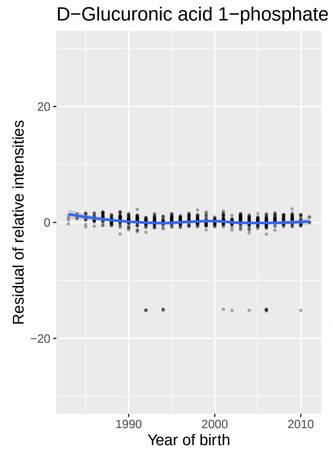
N1−(5−Phospho−a−D−ribosyl)−5


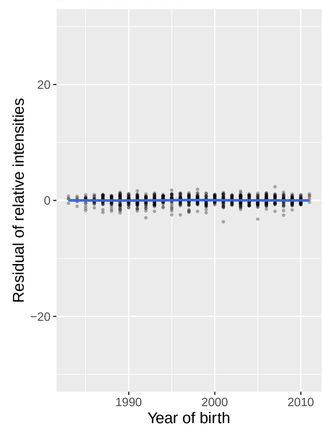
2−Hydroxyethanesulfonate


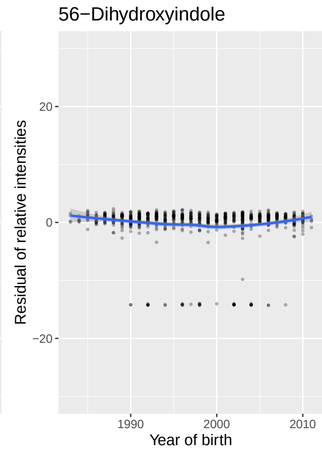
Imidazole−4−acetaldehyde


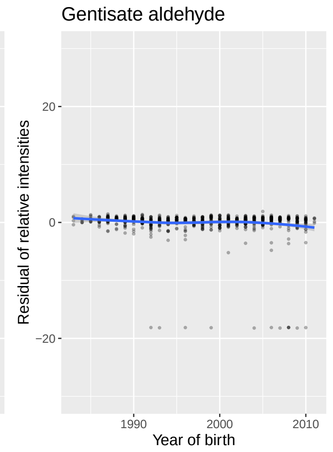
Pentosidine


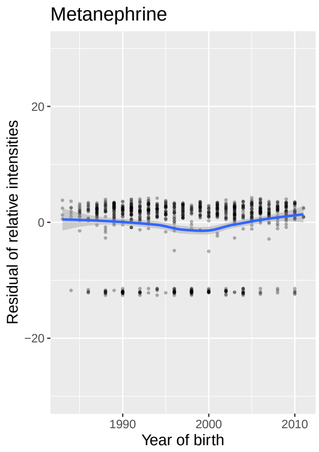
Oxalosuccinic acid


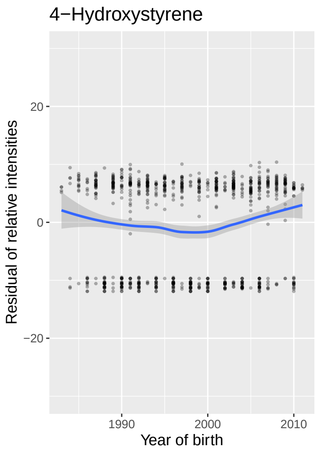
D−Glucuronic acid 1−phosphate


L−Allothreonine


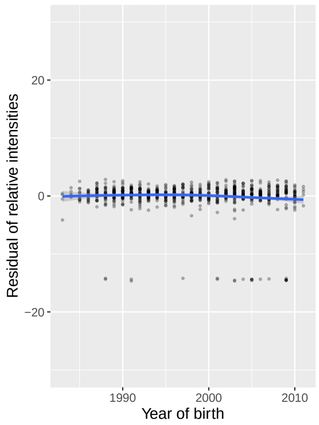
56−Dihydroxyindole


Gentisate aldehyde


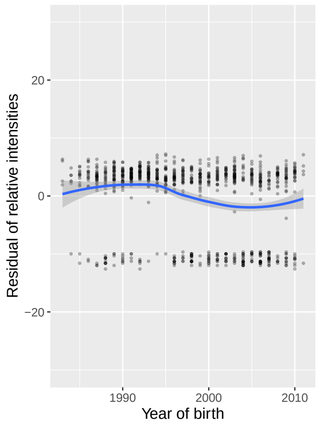
Metanephrine


4−Hydroxystyrene


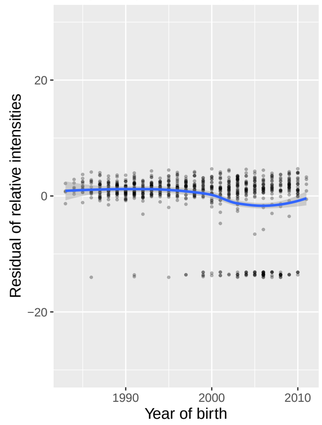
5−Hydroxykynurenamine



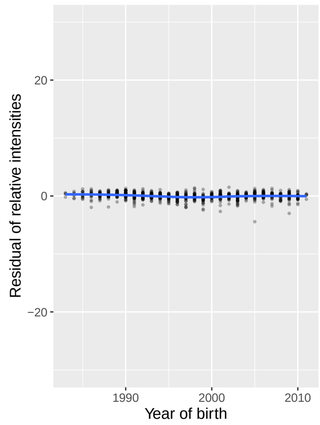
Cinnavalininate



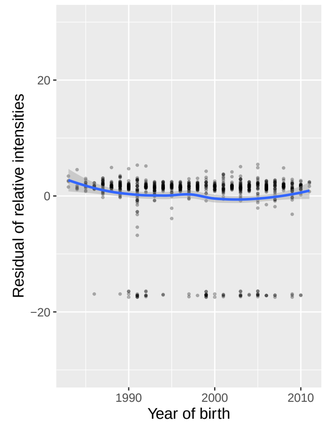
5−Hydroxy−N−formylkynurenine



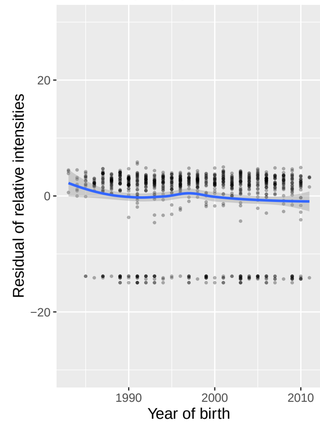
L−Urobilinogen



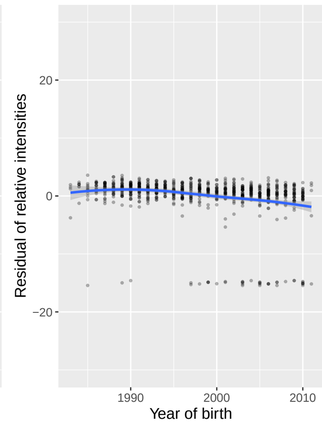
Methylimidazole acetaldehyde



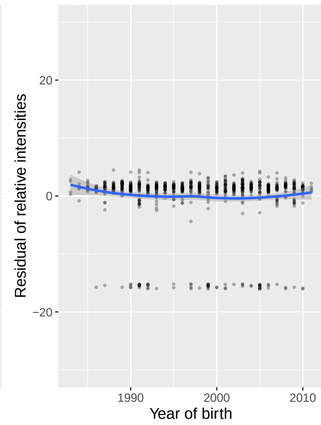
N1−Methyl−2−pyridone−5−carbo



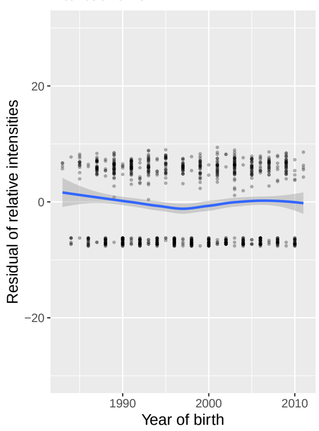
5−L−Glutamyl−taurine



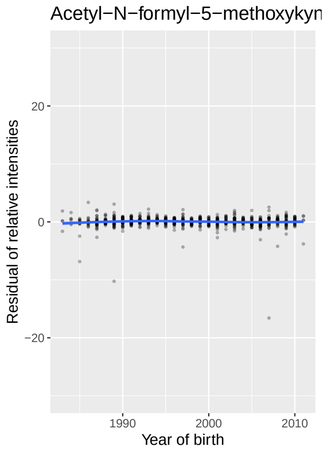
Pyrrole−2−carboxylic acid



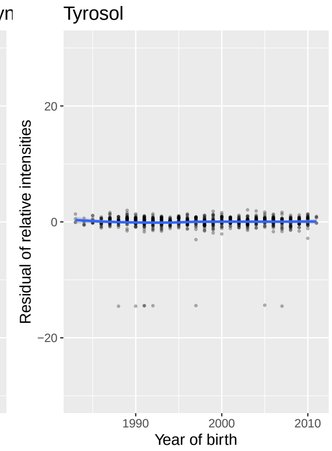
Pantothenol



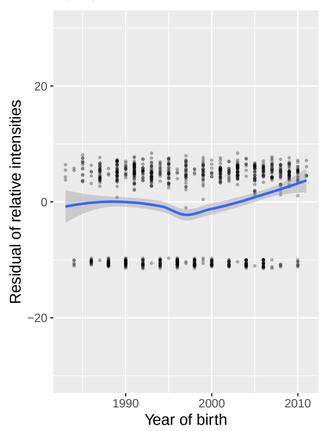
Acetyl−N−formyl−5−methoxykyn



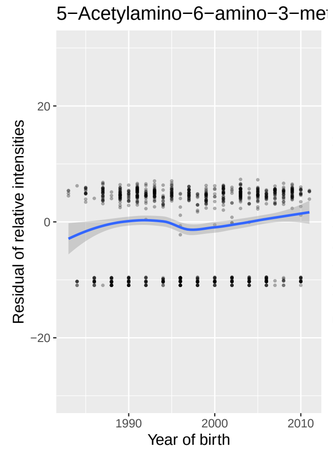
Tyrosol



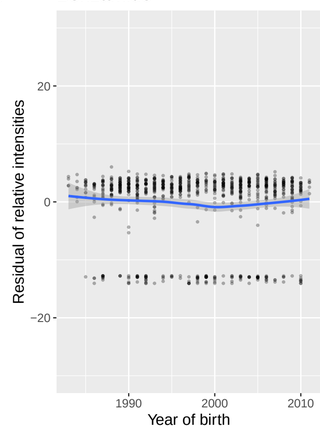
Temurin



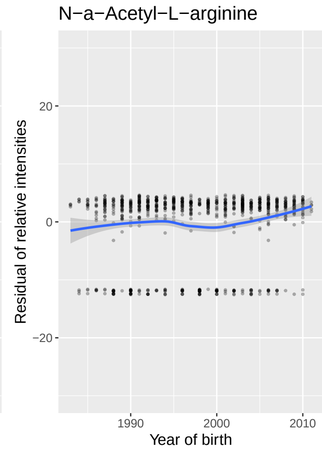
5−Acetylamino−6−amino−3−me



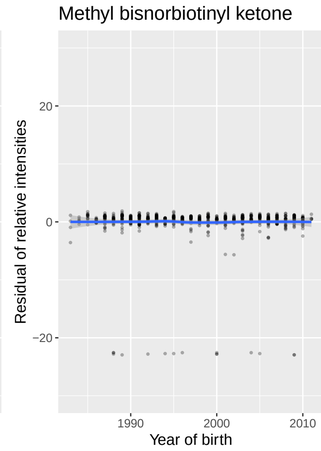
Benzamide



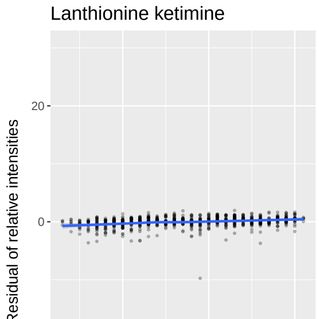
N−a−Acetyl−L−arginine



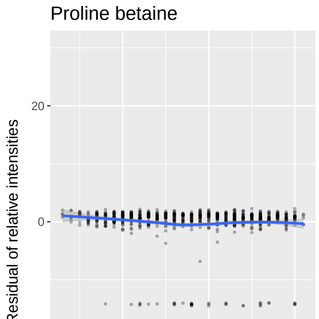
Methyl bisnorbiotinyl ketone



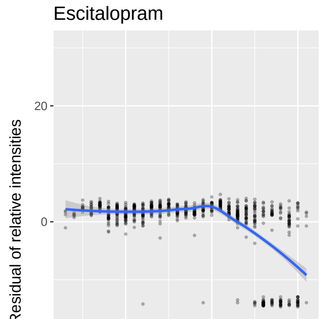
Lanthionine ketimine



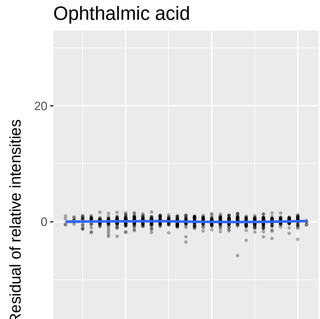
Proline betaine



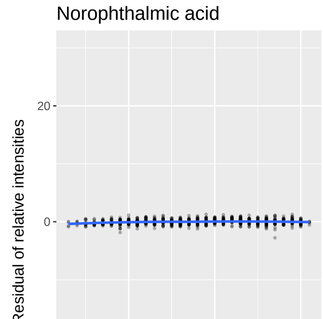
Escitalopram



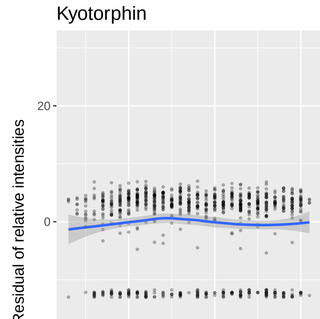
Ophthalmic acid



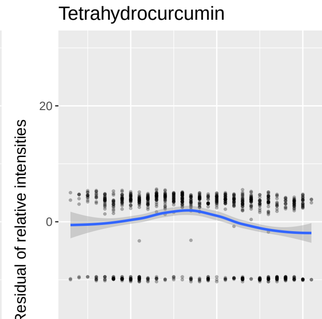
Norophthalmic acid



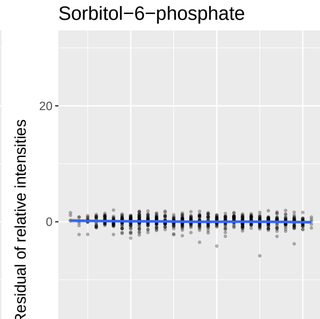
Kyotorphin



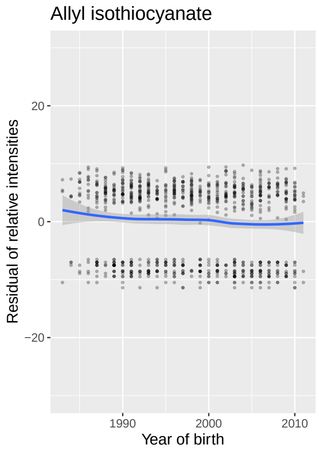
Tetrahydrocurcumin



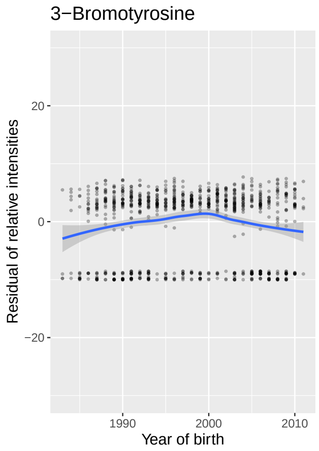
Sorbitol−6−phosphate



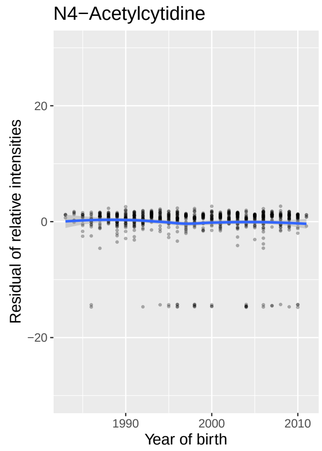
Allyl isothiocyanate



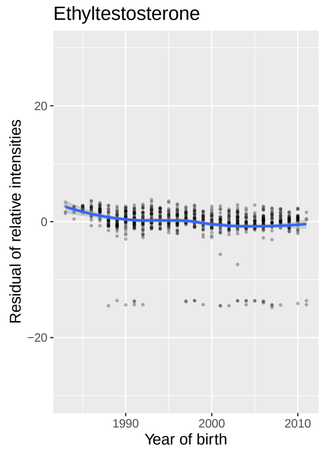
3−Bromotyrosine



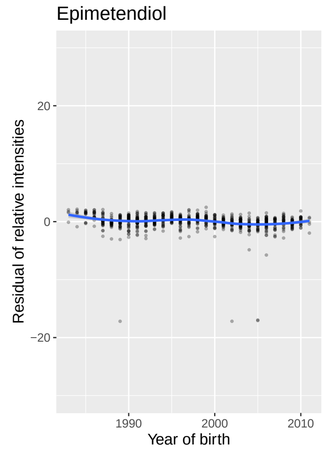
N4−Acetylcytidine



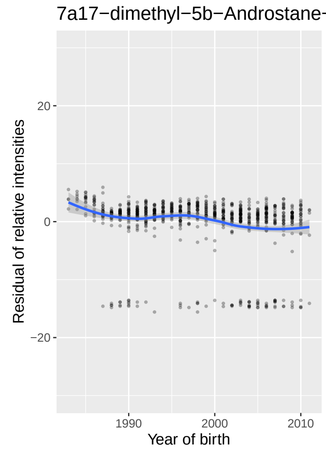
Ethyltestosterone



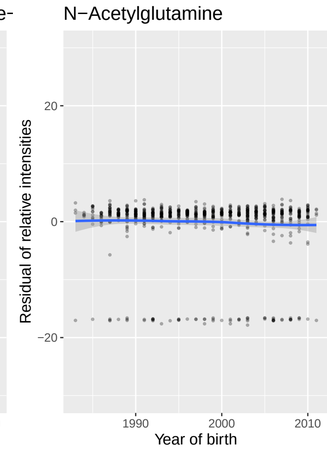
Epimetendiol



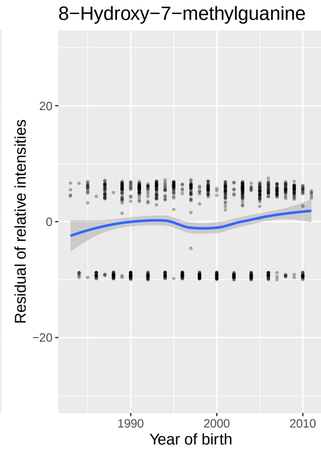
7a17−dimethyl−5b−Androstane−



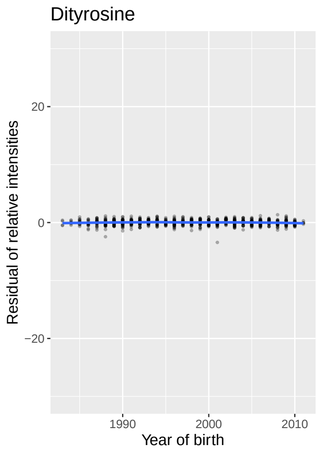
N−Acetylglutamine



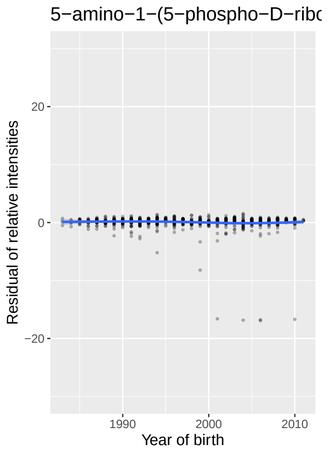
8−Hydroxy−7−methylguanine



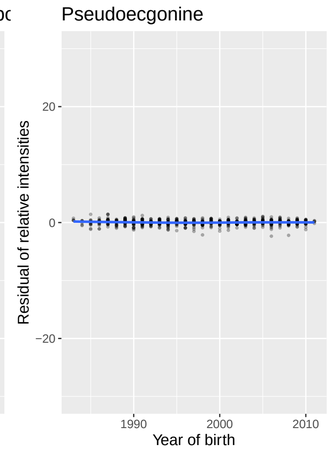
Dityrosine



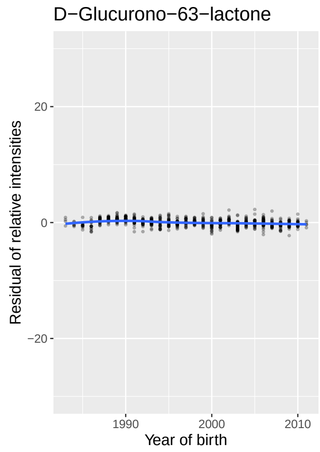
5−amino−1−(5−phospho−D−ribo



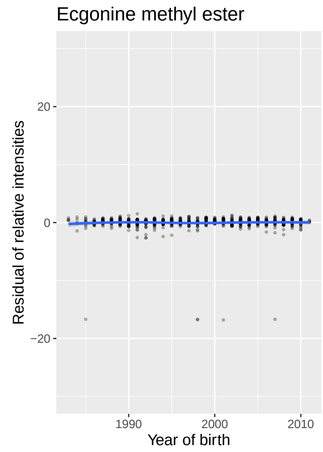
Pseudoecgonine



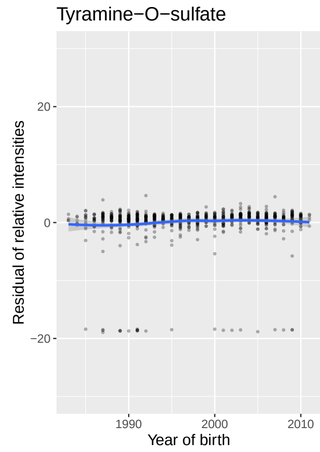
D−Glucurono−63−lactone



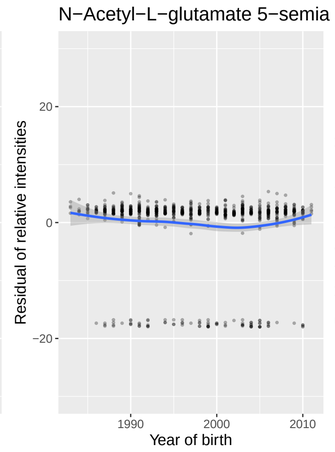
Ecgonine methyl ester



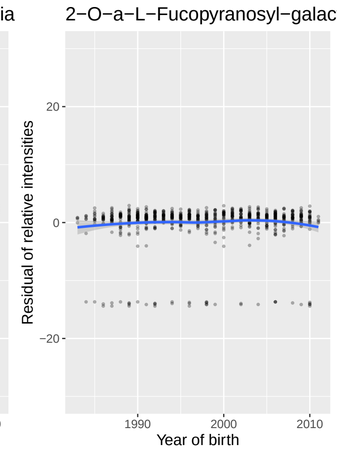
Tyramine−O−sulfate



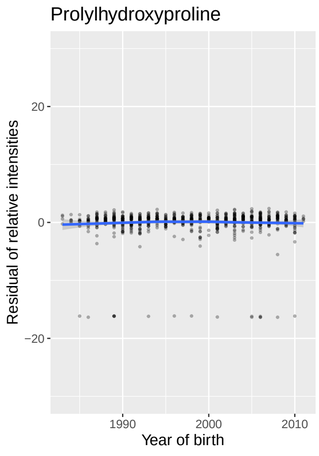
N−Acetyl−L−glutamate 5−semia



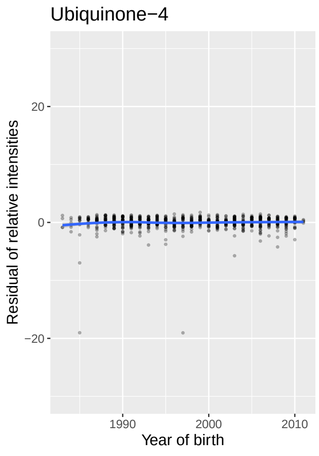
2−O−a−L−Fucopyranosyl−galac



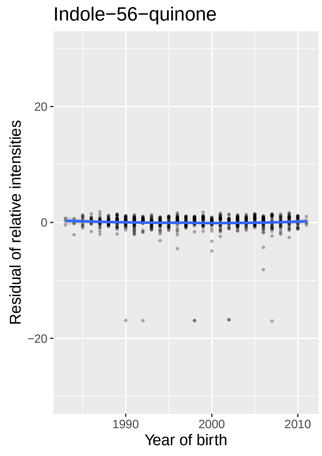
Prolylhydroxyproline



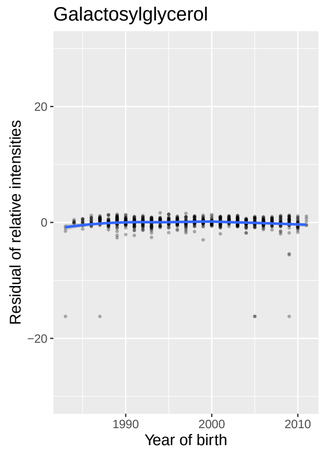
Ubiquinone−4



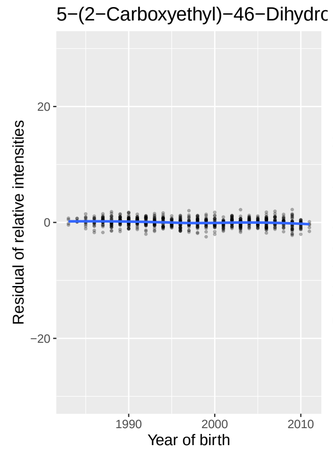
Indole−56−quinone



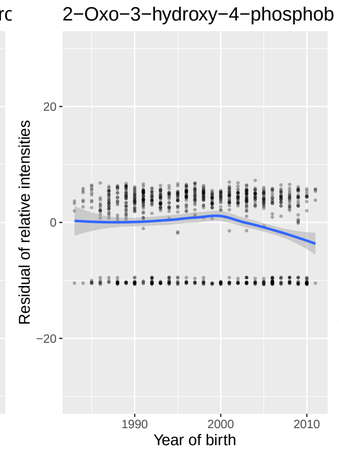
Galactosylglycerol



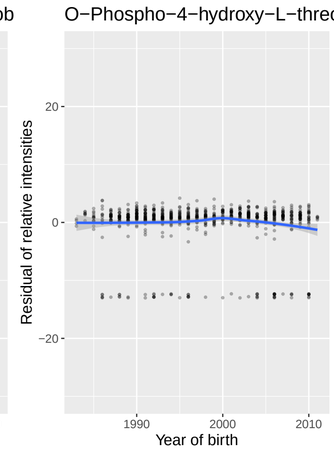
5−(2−Carboxyethyl)−46−Dihydrc



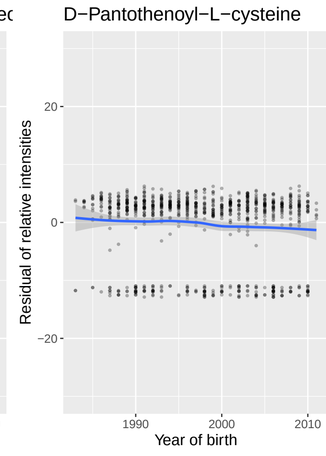
2−Oxo−3−hydroxy−4−phosphob



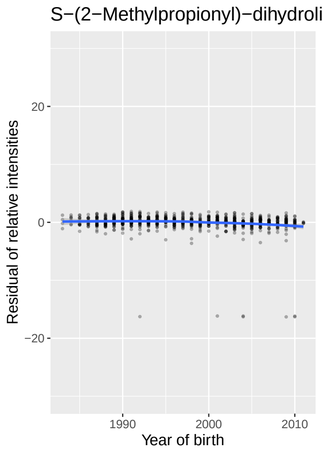
O−Phospho−4−hydroxy−L−threo



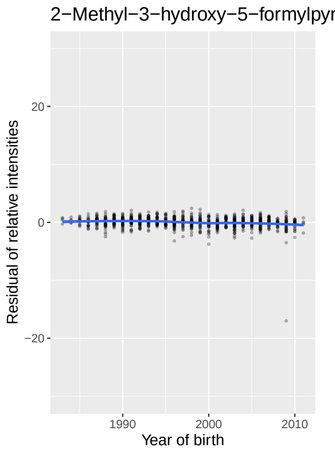
D−Pantothenoyl−L−cysteine

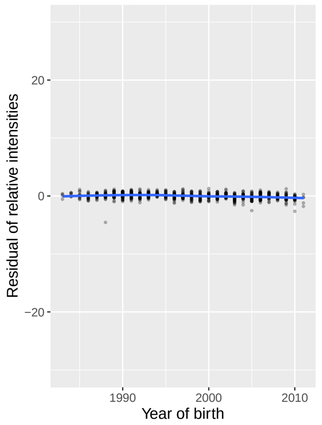


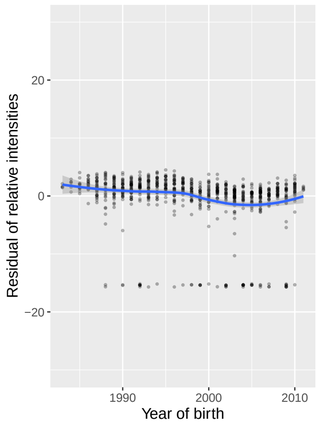
S−(2−Methylpropionyl)−dihydroli

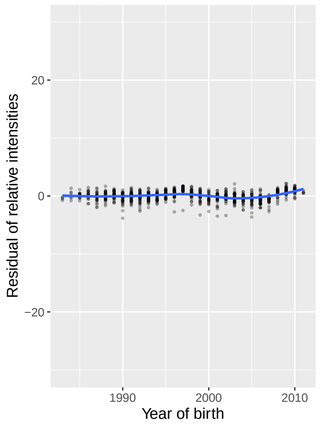


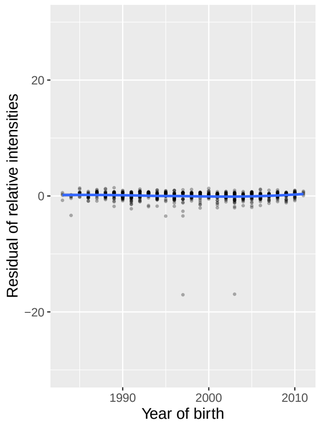
2−Methyl−3−hydroxy−5−formylpyridine−4−carboxylate

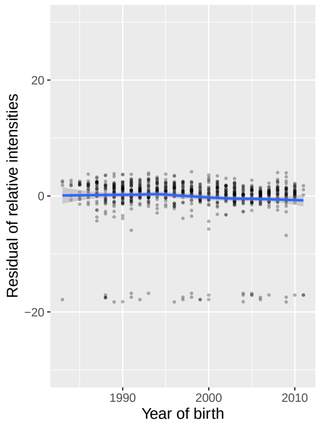


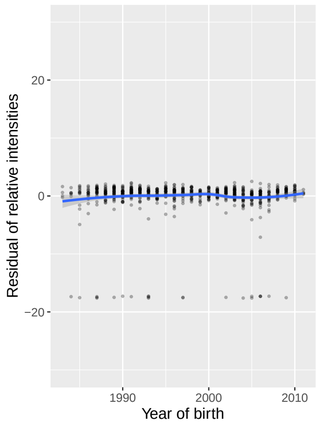
3−Hydroxy−2−methylpyridine−4S


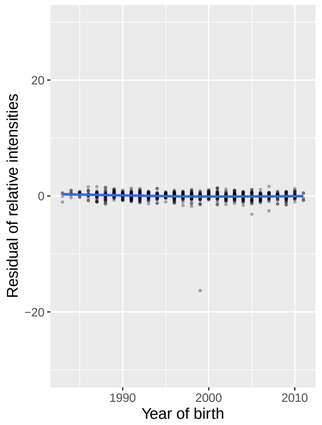
111215−TriHETRE


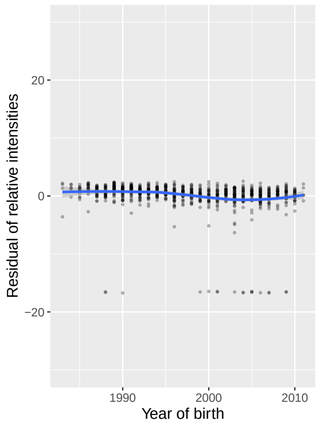
A−12(13)−EpODE


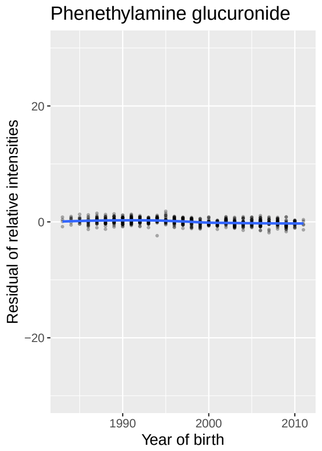
1213−DiHODE


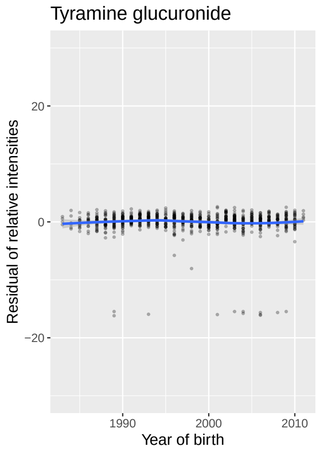
17−HDoHE


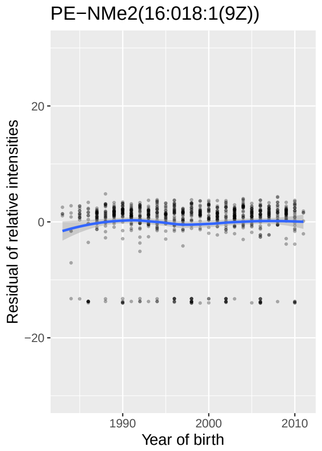
1920−DiHDPA


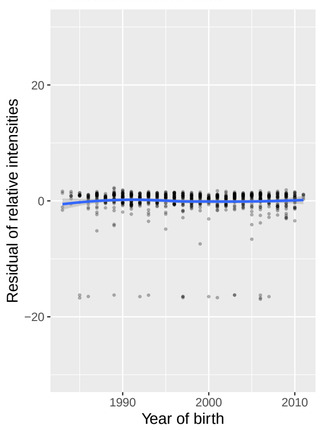
9−HETE


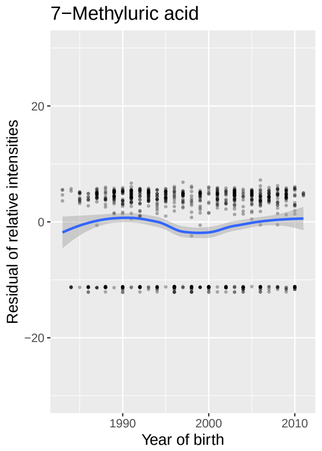
Inodxyl glucuronide


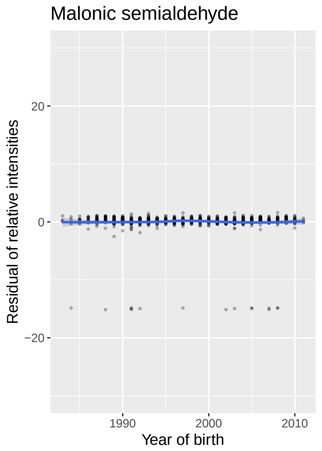
Phenethylamine glucuronide


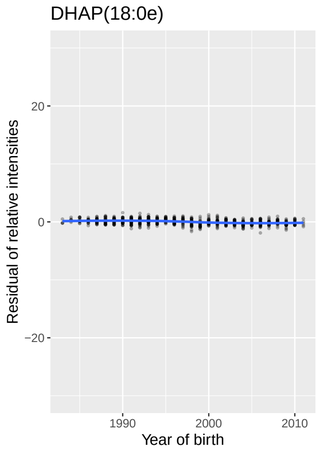
Tyramine glucuronide


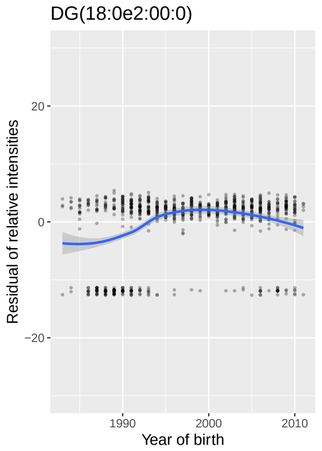
PE−NMe2(16:018:1(9Z))


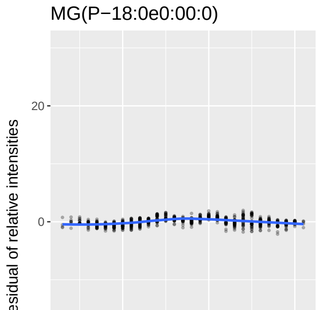
3−Oxodecanoic acid


7−Methyluric acid


Malonic semialdehyde


DHAP(18:0e)


DG(18:0e2:00:0)


MG(P−18:0e0:00:0)


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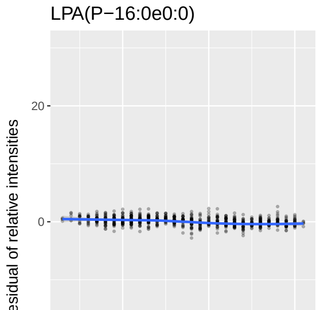
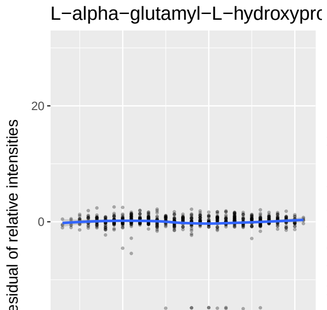
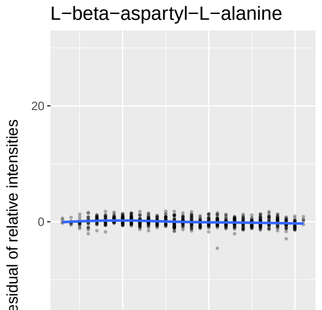
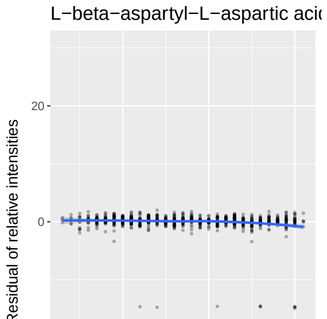
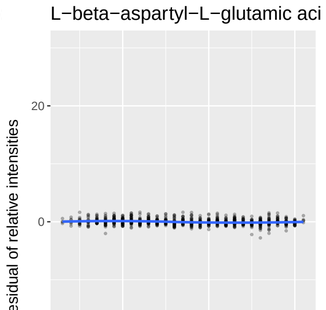
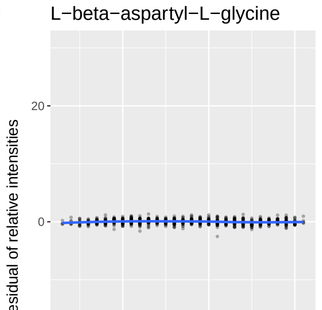


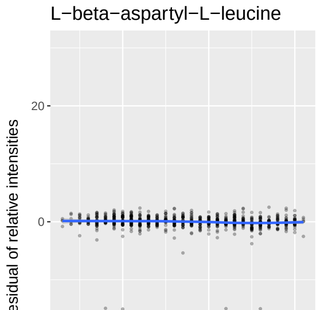
L−alpha−glutamyl−L−hydroxypro


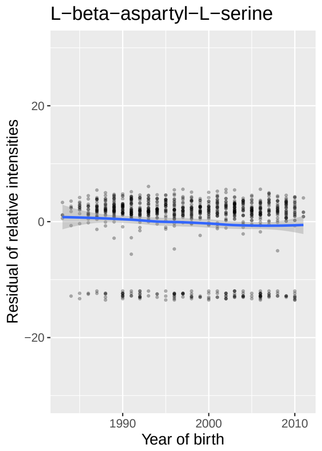
L−beta−aspartyl−L−alanine


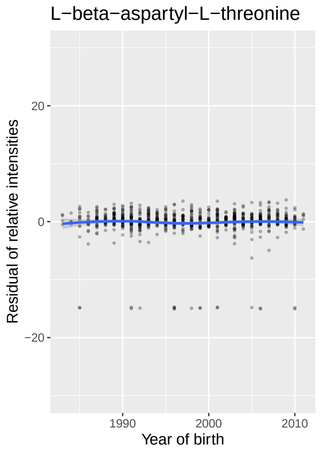
L−beta−aspartyl−L−aspartic aci


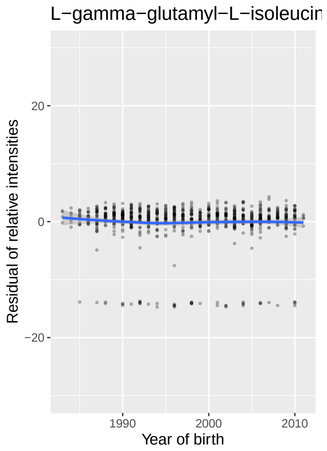
L−beta−aspartyl−L−glutamic aci


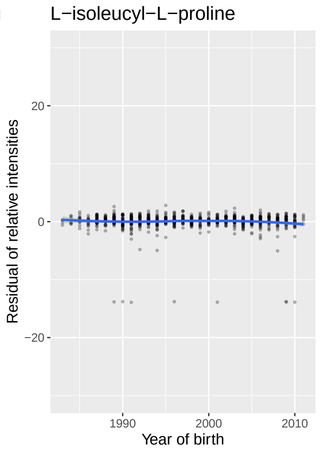
L−beta−aspartyl−L−glycine


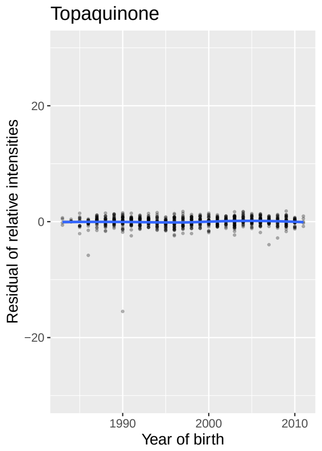
L−beta−aspartyl−L−leucine


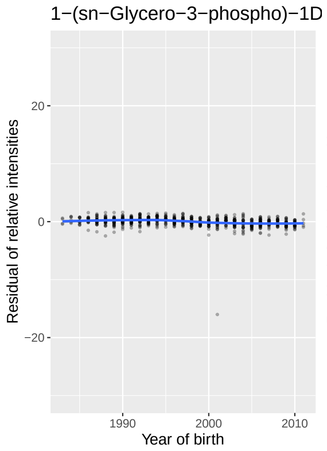
L−beta−aspartyl−L−serine


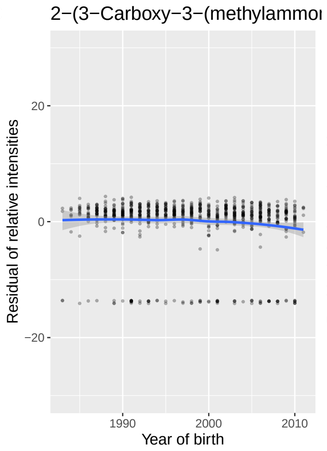
L−beta−aspartyl−L−threonine


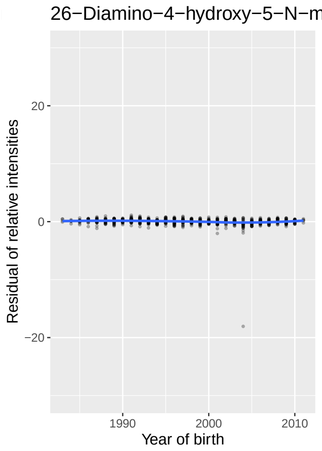
L−gamma−glutamyl−L−isoleucin


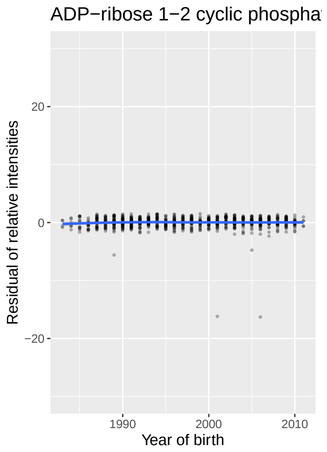
L−isoleucyl−L−proline


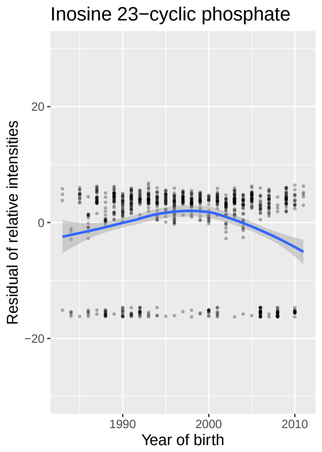
Topaquinone


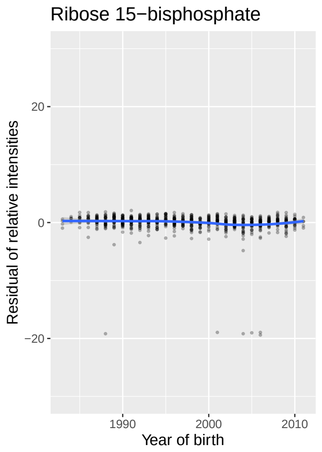
1−(sn−Glycero−3−phospho)−1D


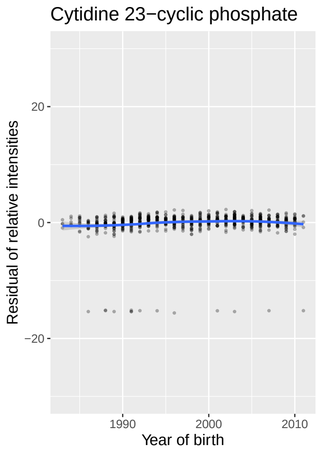
2−(3−Carboxy−3−(methylammoı


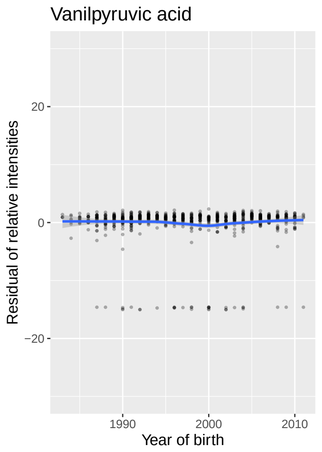
26−Diamino−4−hydroxy−5−N−m


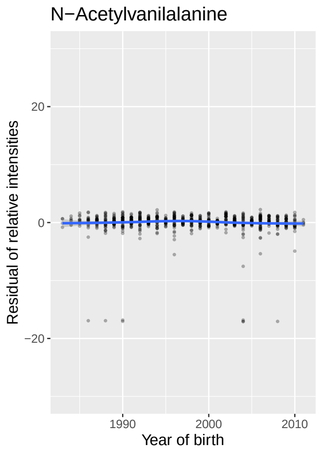
ADP−ribose 1−2 cyclic phospha


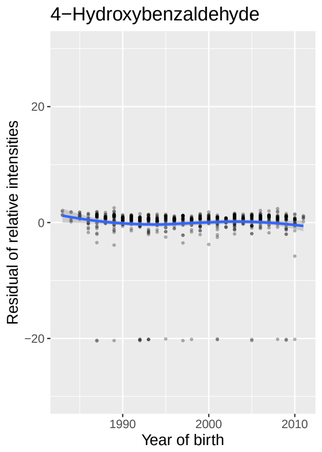
Inosine 23−cyclic phosphate


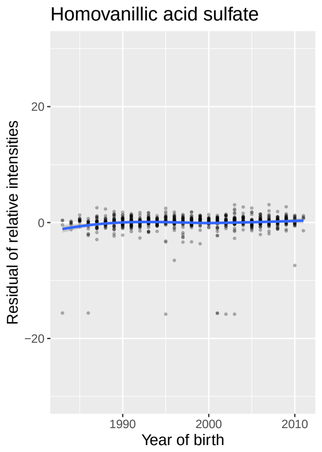
Ribose 15−bisphosphate


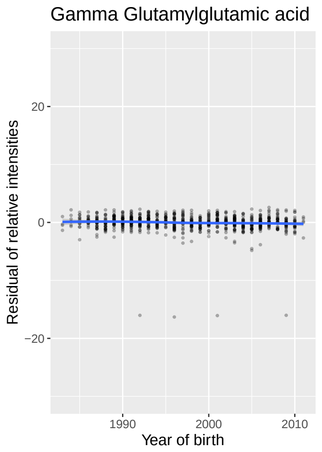
Cytidine 23−cyclic phosphate


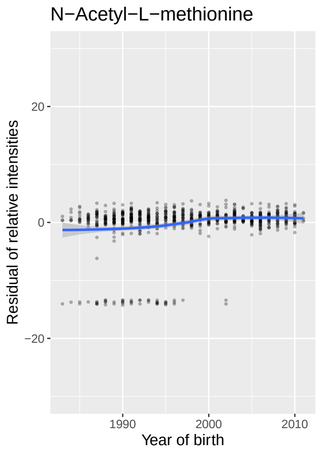
Vanilpyruvic acid


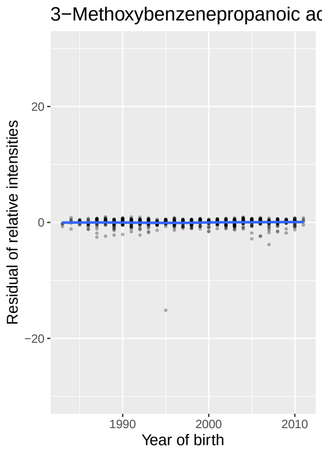
N−Acetylvanilalanine


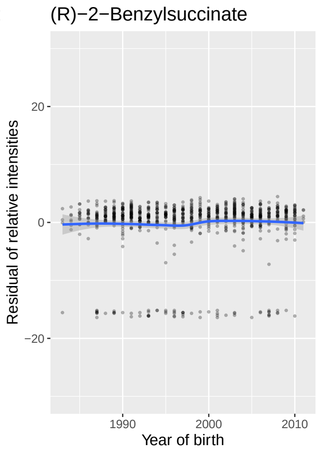
4−Hydroxybenzaldehyde


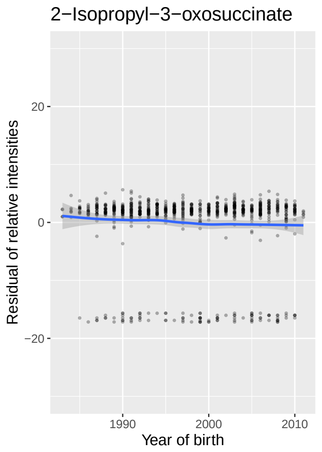
Homovanillic acid sulfate


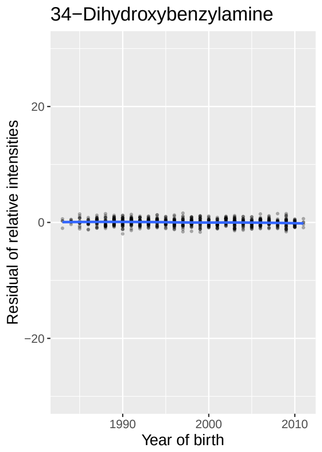
Gamma Glutamylglutamic acid


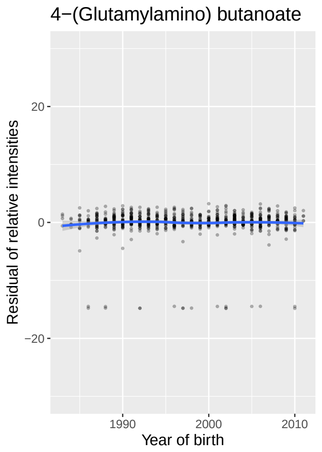
N−Acetyl−L−methionine


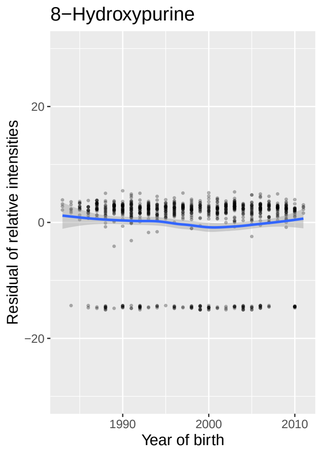
3−Methoxybenzenepropanoic ac


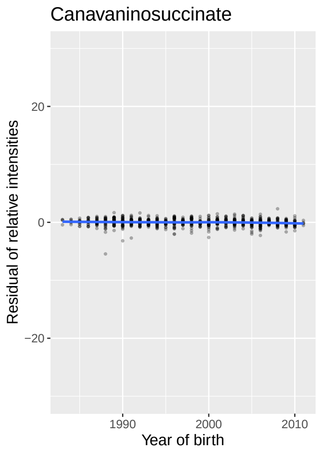
(R)−2−Benzylsuccinate


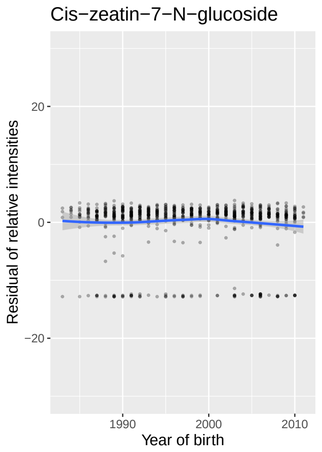
2−Isopropyl−3−oxosuccinate


34−Dihydroxybenzylamine


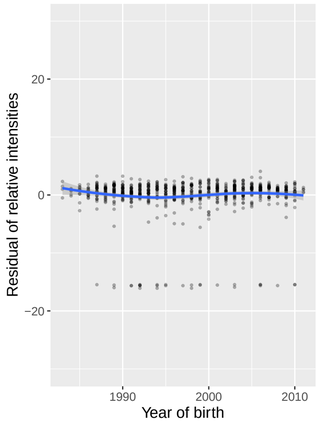
4−(Glutamylamino) butanoate


8−Hydroxypurine


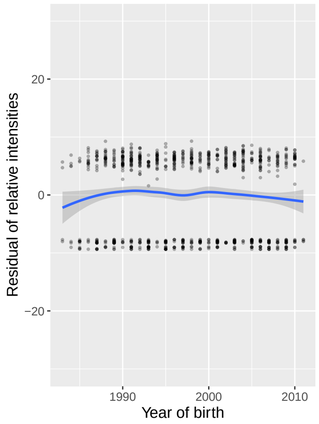
Canavaninosuccinate


Cis−zeatin−7−N−glucoside


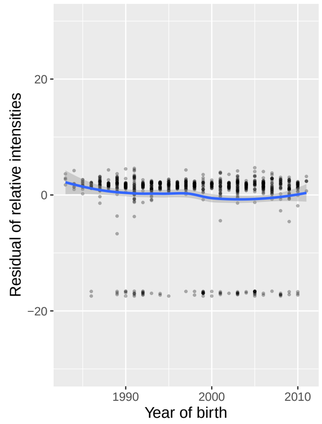
Cis−zeatin



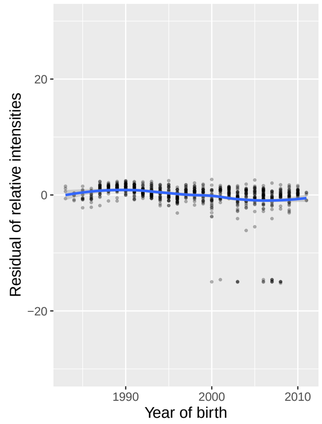
Dopaxanthin



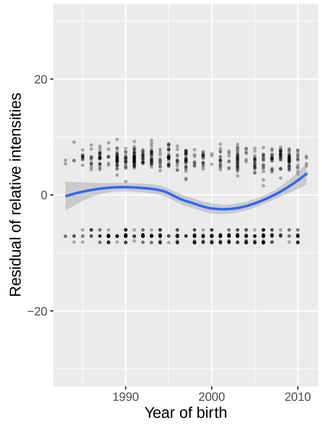
Histidinal



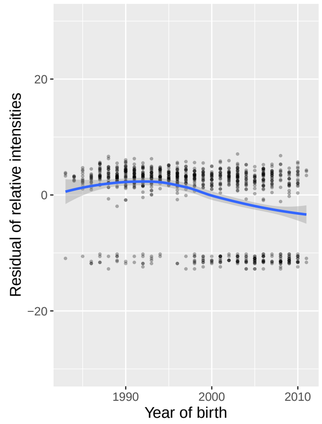
Imidazole acetol−phosphate



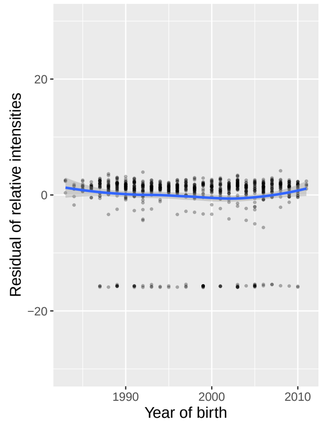
Isopentenyladenine−9−N−glucos



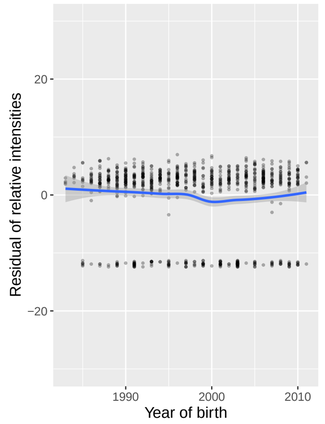
Kinetin−7−N−glucoside



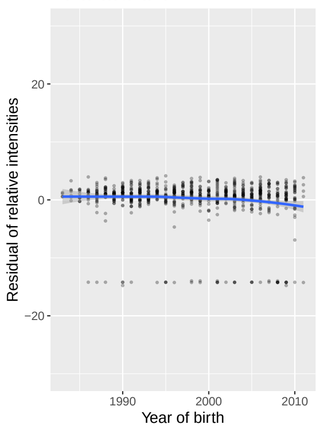
Kinetin



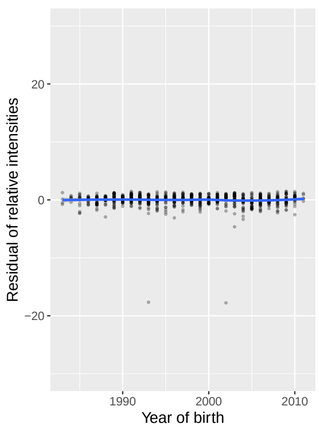
N−Succinyl−2−amino−6−ketopi



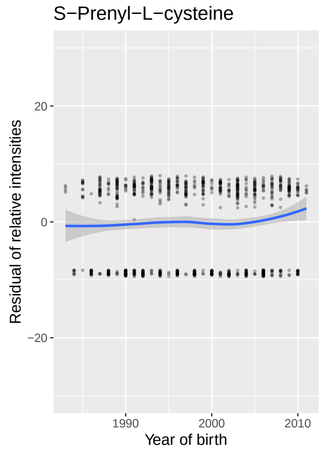
Portulacaxanthin II



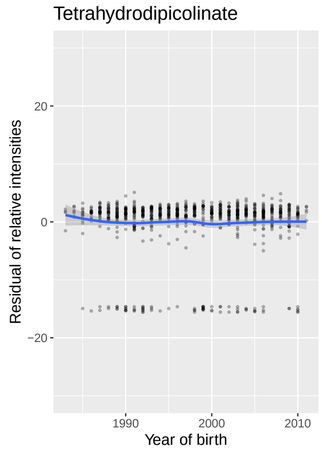
Ribose−1−arsenate



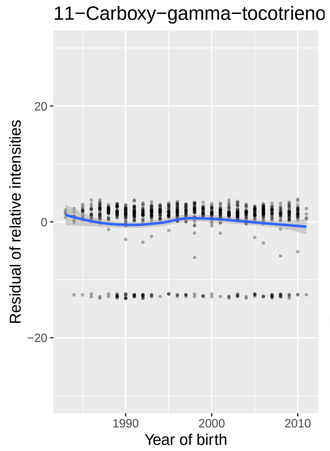
S−Prenyl−L−cysteine



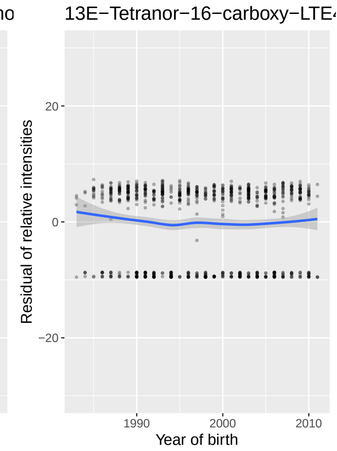
Tetrahydrodipicolinate



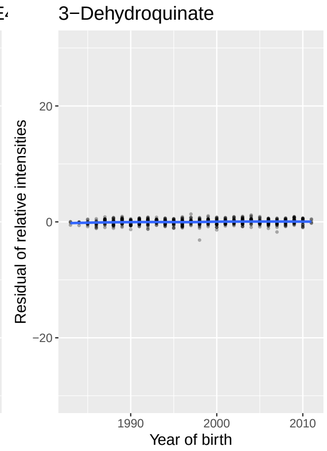
11−Carboxy−gamma−tocotrieno



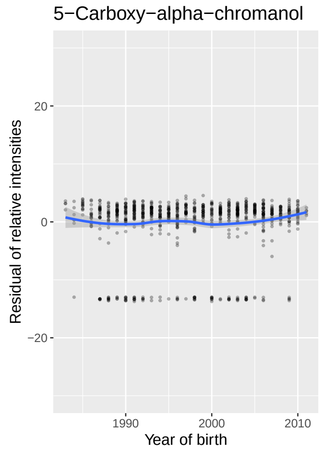
13E−Tetranor−16−carboxy−LTE



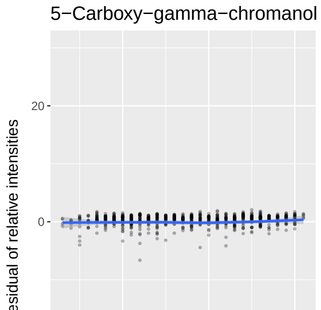
3−Dehydroquinate



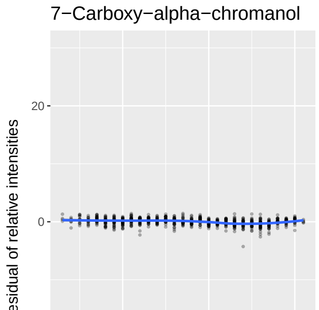
5−Carboxy−alpha−chromanol



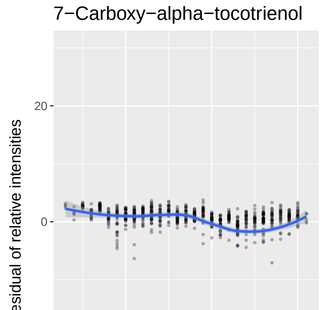
5−Carboxy−gamma−chromanol



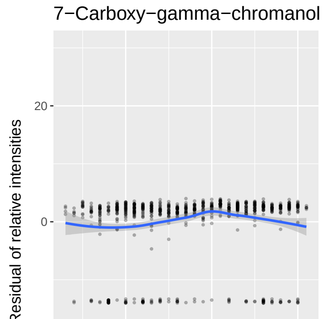
7−Carboxy−alpha−chromanol



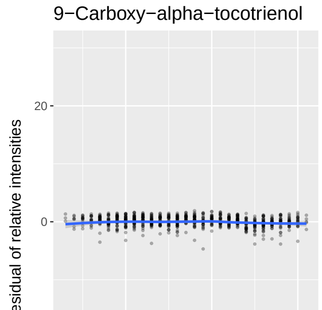
7−Carboxy−alpha−tocotrienol



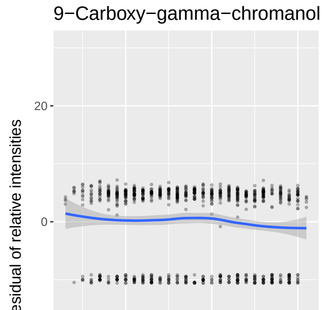
7−Carboxy−gamma−chromanol



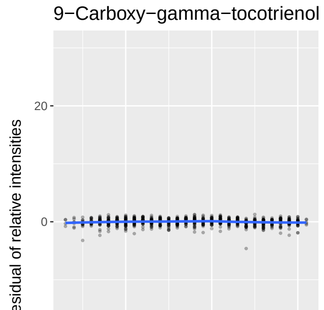
9−Carboxy−alpha−tocotrienol



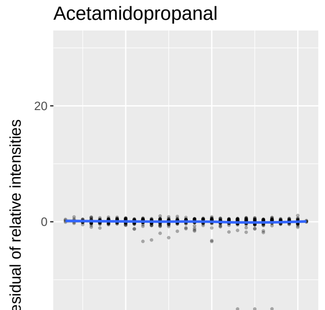
9−Carboxy−gamma−chromanol



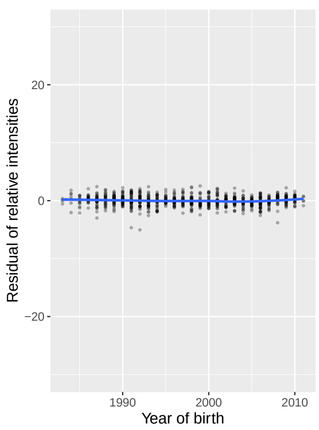
9−Carboxy−gamma−tocotrienol



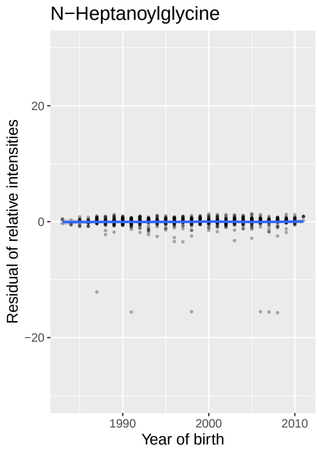
Acetamidopropanal



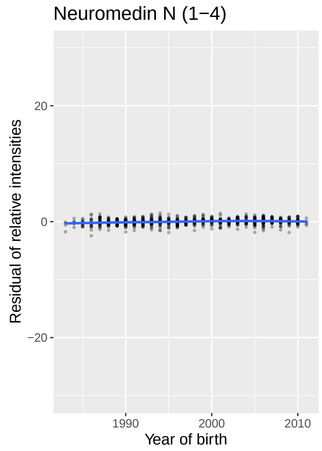
Kinetensin 4−7



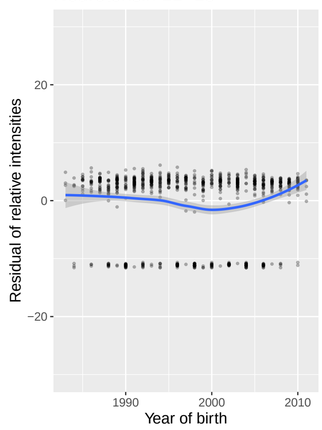
N−Heptanoylglycine



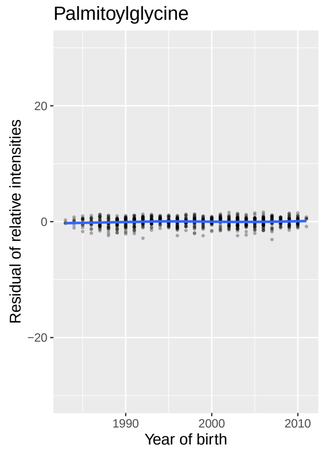
Neuromedin N (1−4)



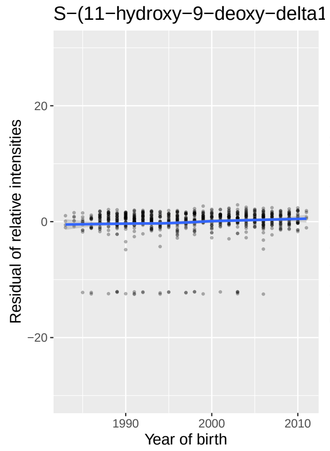
Neurotensin 11−13



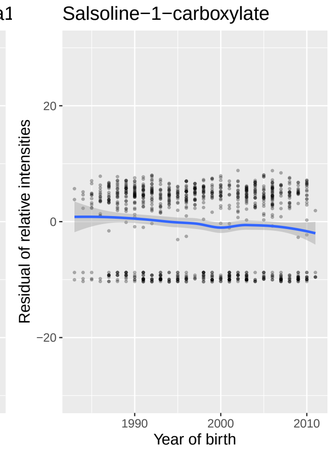
Palmitoylglycine



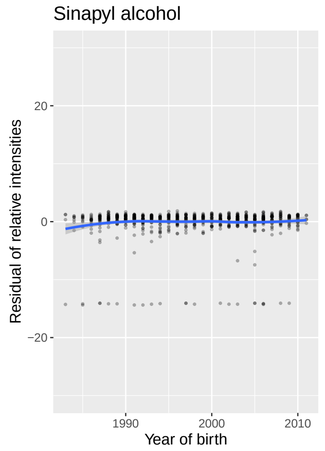
S−(11−hydroxy−9−deoxy−delta1



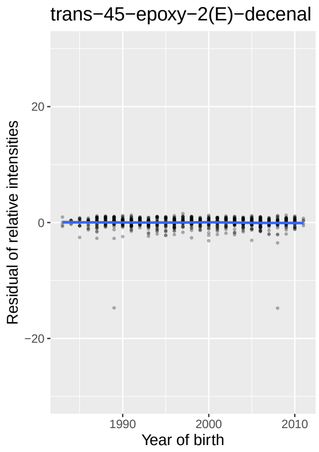
Salsoline−1−carboxylate



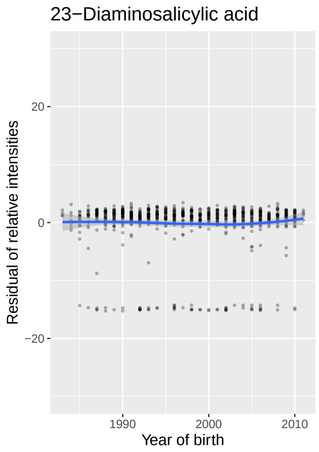
Sinapyl alcohol



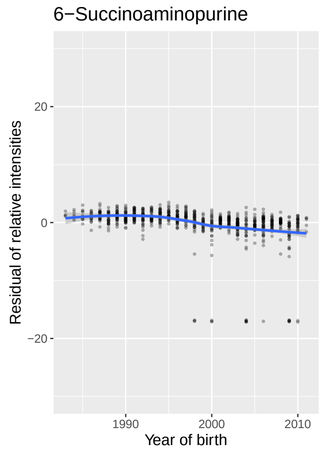
trans−45−epoxy−2(E)−decenal



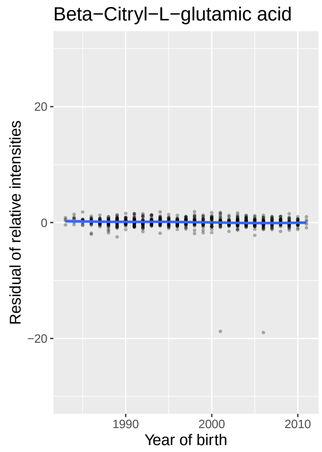
23−Diaminosalicylic acid



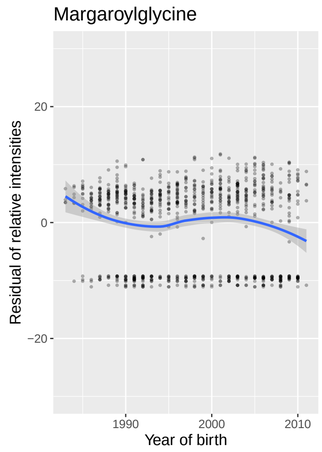
6−Succinoaminopurine



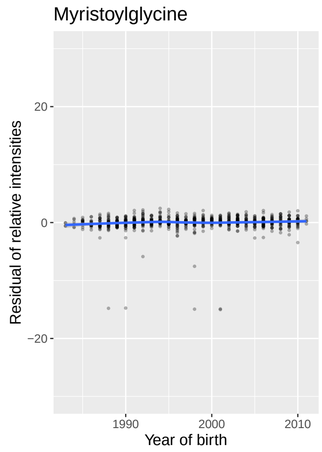
Beta−Citryl−L−glutamic acid



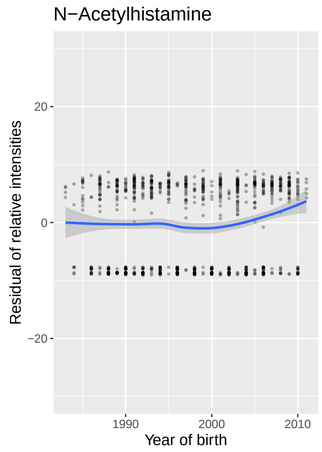
Margaroylglycine



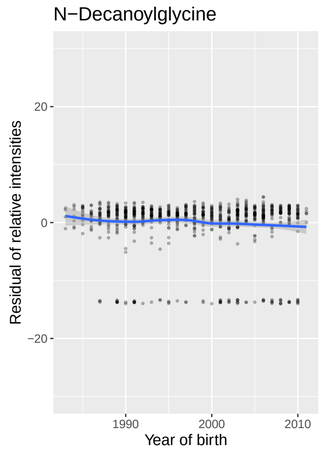
Myristoylglycine



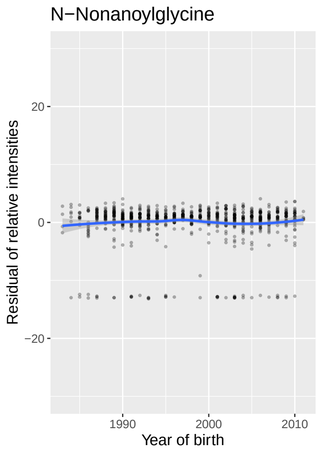
N−Acetylhistamine



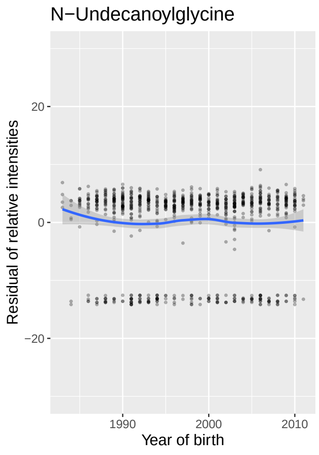
N−Decanoylglycine



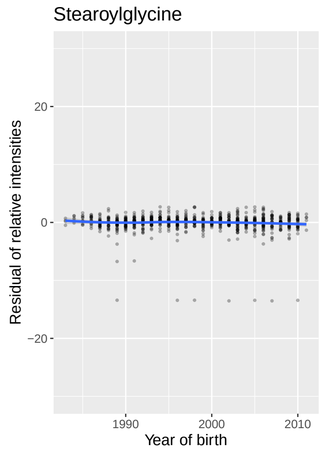
N−Nonanoylglycine



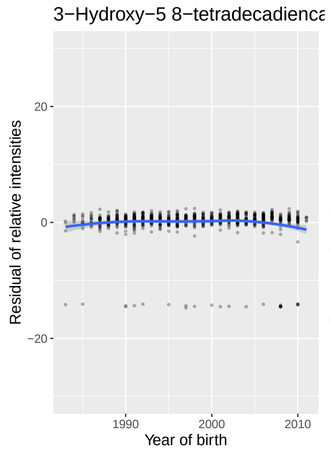
N−Undecanoylglycine



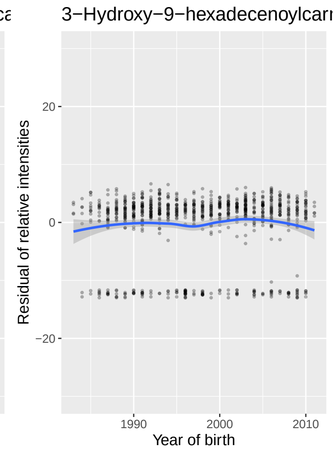
Stearoylglycine



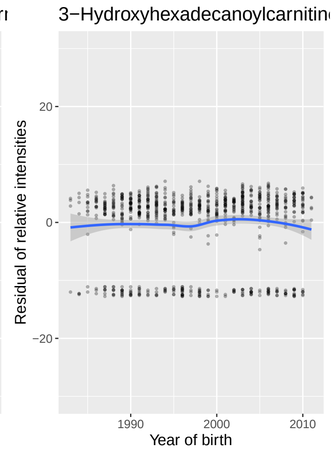
3−Hydroxy−5 8−tetradecadienca



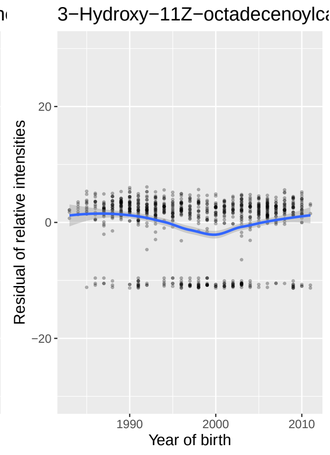
3−Hydroxy−9−hexadecenoylcarı



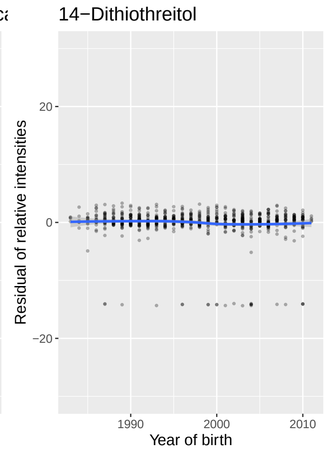
3−Hydroxyhexadecanoylcarnitin



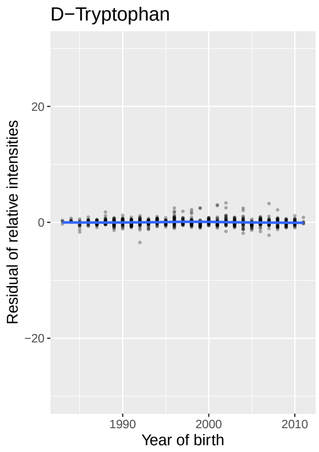
3−Hydroxy−11Z−octadecenoylca



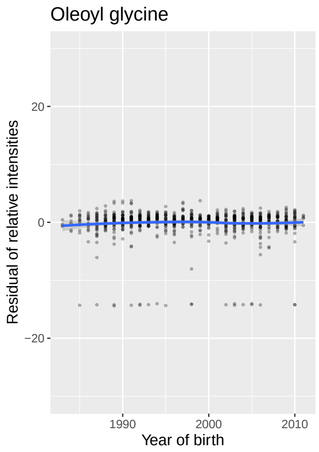
14−Dithiothreitol



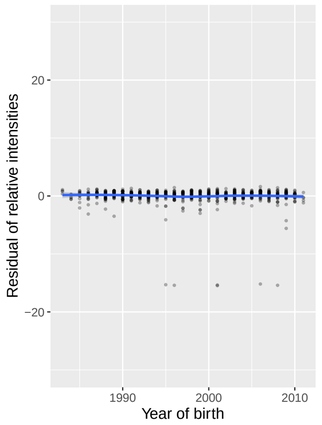
D−Tryptophan



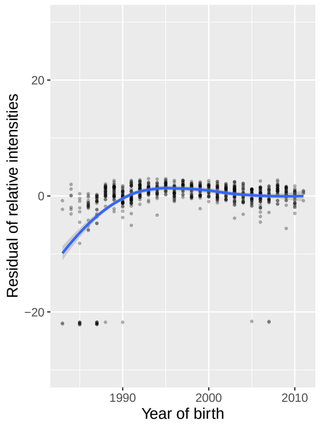
Oleoyl glycine



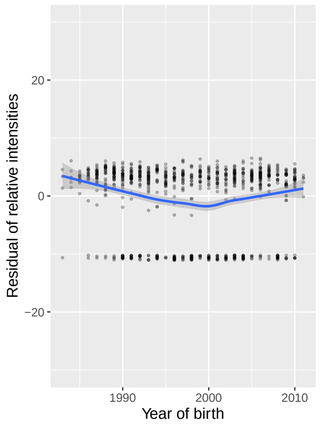
123−Trihydroxybenzene



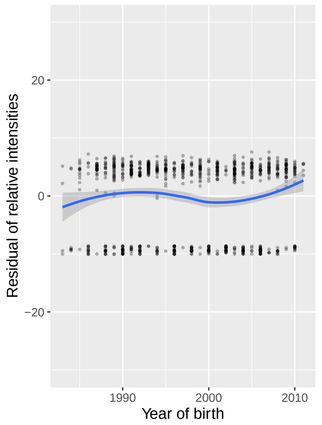
Nootkatol



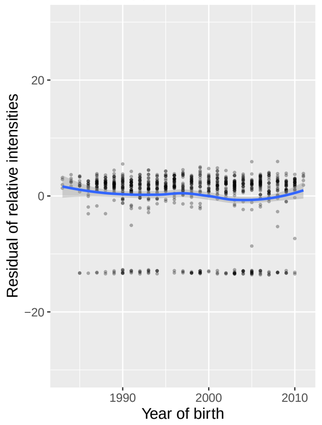
Secoisolariciresinol



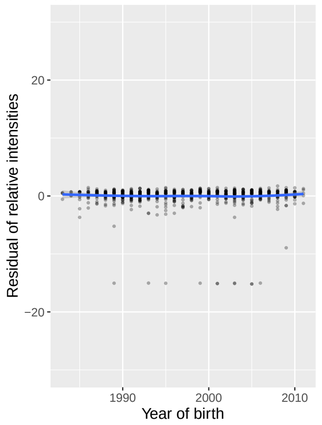
Urolithin B



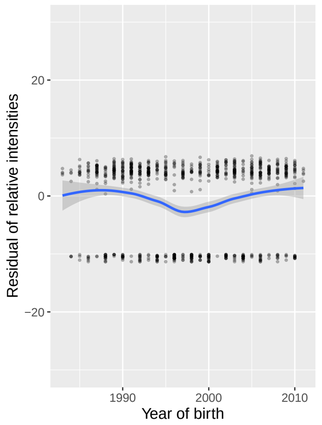
2−Hydroxypyridine



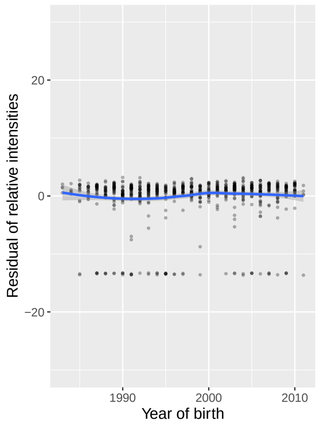
(E)−2−octenal



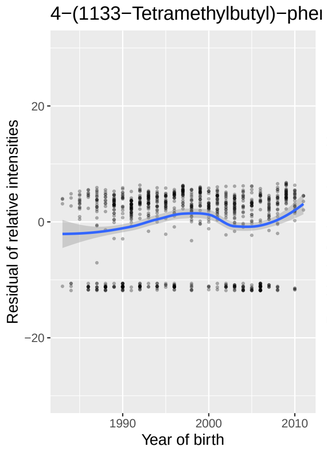
13−Heptadecyn−1−ol



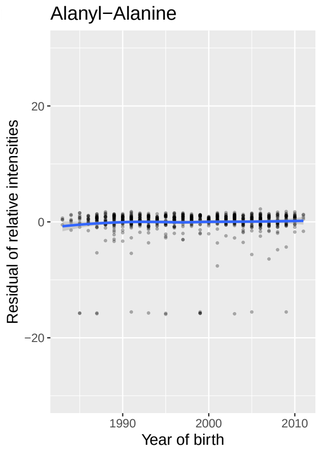
26−Di−tert−butylbenzoquinone



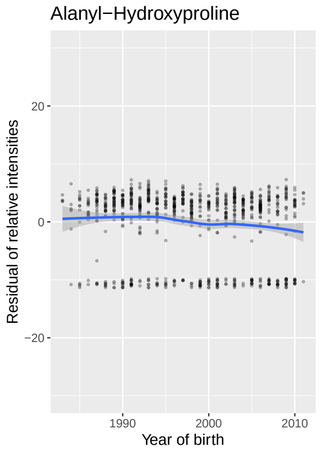
4−(1133−Tetramethylbutyl)−phe



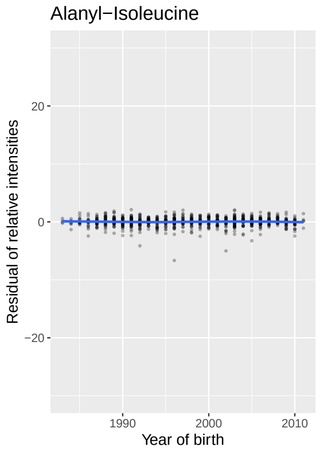
Alanyl−Alanine



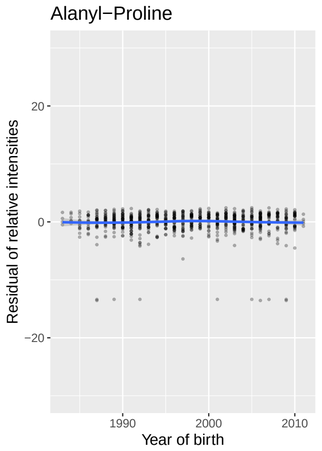
Alanyl−Hydroxyproline



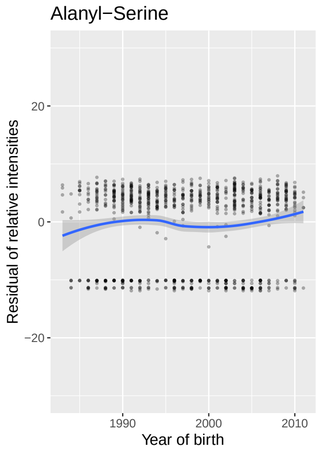
Alanyl−Isoleucine



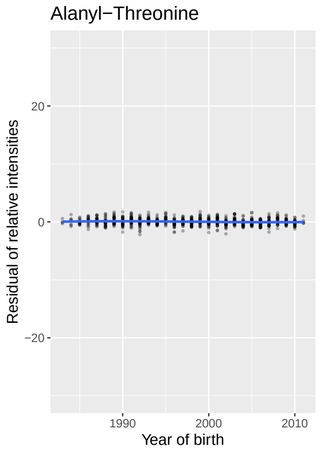
Alanyl−Proline



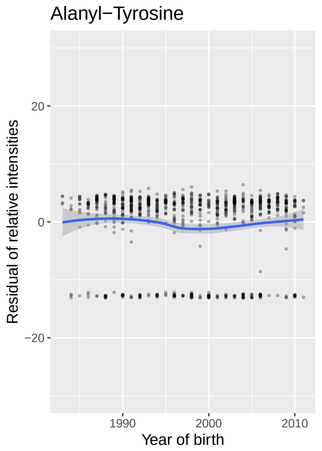
Alanyl−Serine



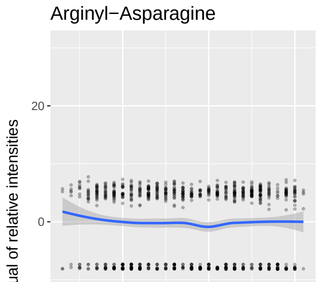
Alanyl−Threonine



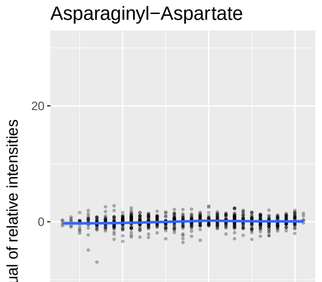
Alanyl−Tyrosine



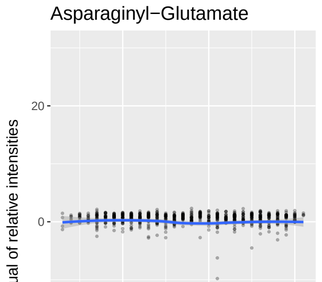
Arginyl−Asparagine



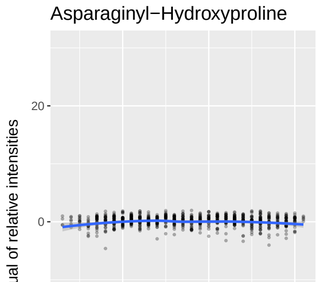
Asparaginyl−Aspartate



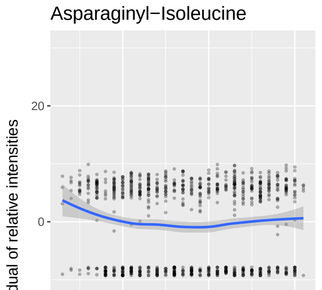
Asparaginyl−Glutamate



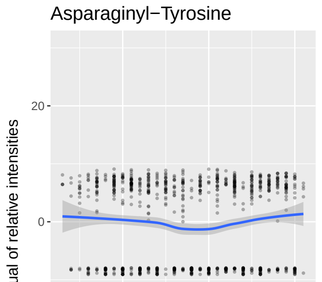
Asparaginyl−Hydroxyproline



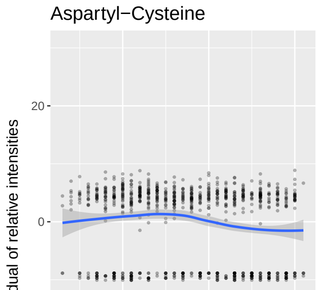
Asparaginyl−Isoleucine



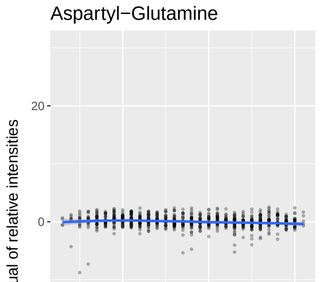
Asparaginyl−Tyrosine



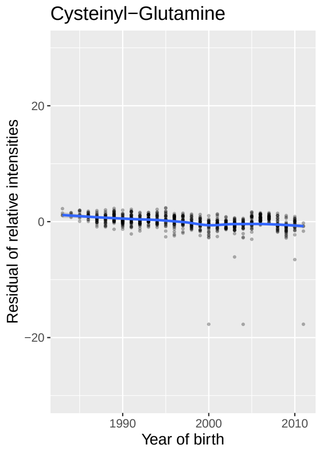
Aspartyl−Cysteine



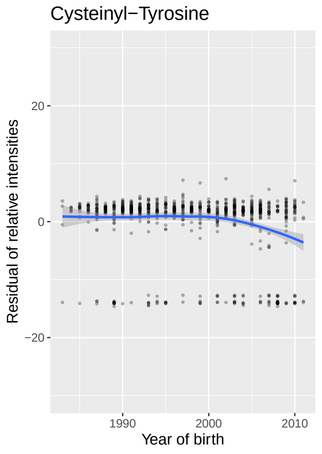
Aspartyl−Glutamine



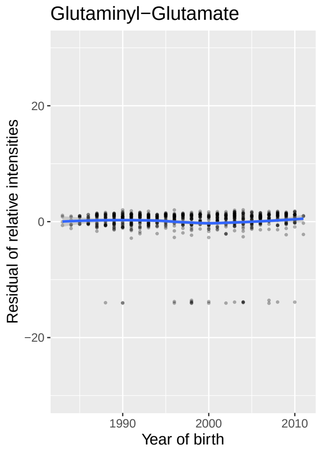
Cysteinyl−Glutamine



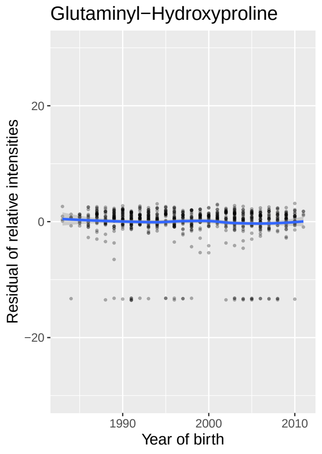
Cysteinyl−Tyrosine



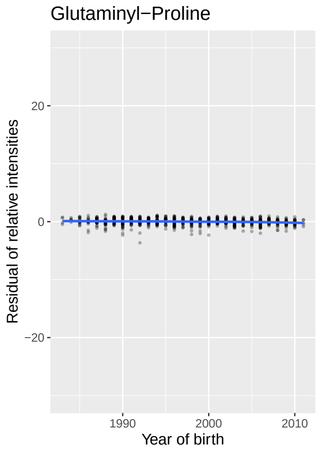
Glutaminyl−Glutamate



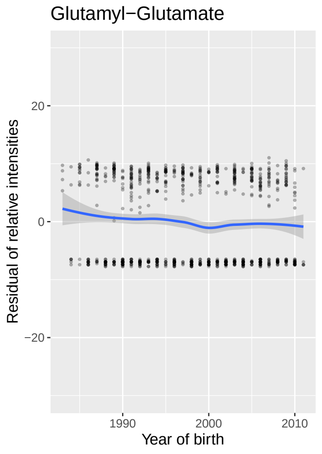
Glutaminyl−Hydroxyproline



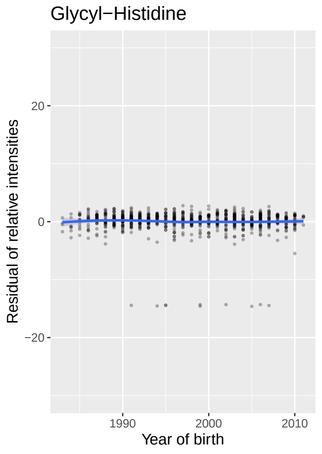
Glutaminyl−Proline



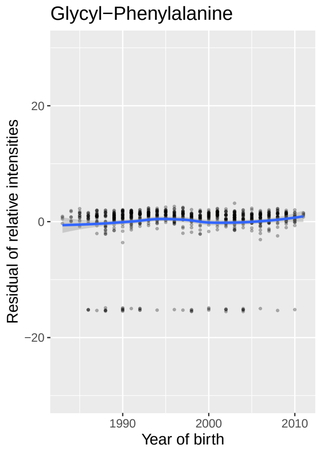
Glutamyl−Glutamate



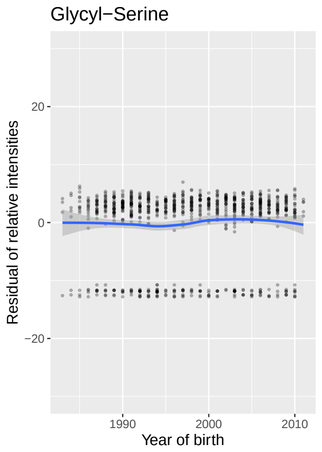
Glycyl−Histidine



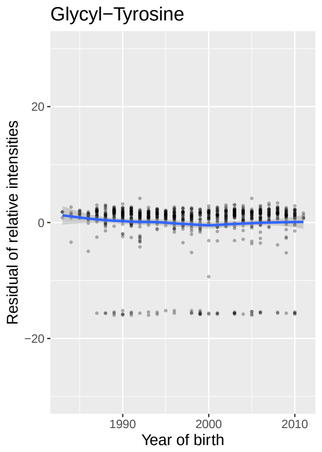
Glycyl−Phenylalanine



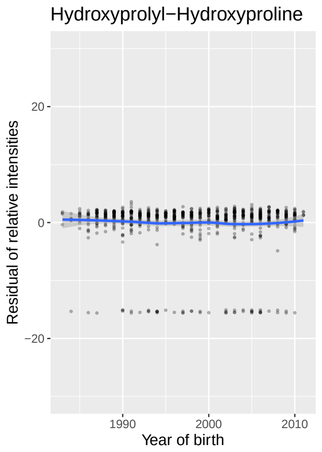
Glycyl−Serine



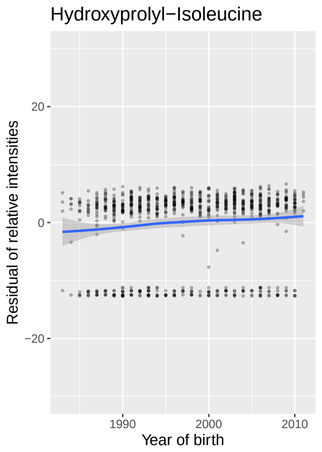
Glycyl−Tyrosine



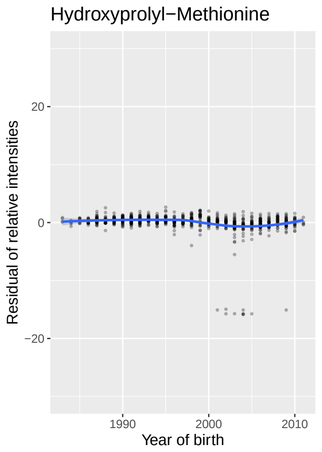
Hydroxyprolyl−Hydroxyproline



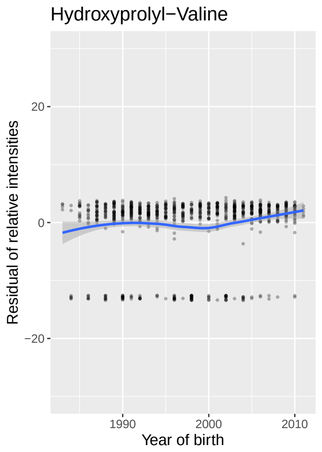
Hydroxyprolyl−Isoleucine



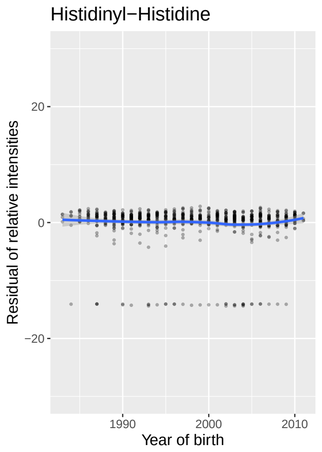
Hydroxyprolyl−Methionine



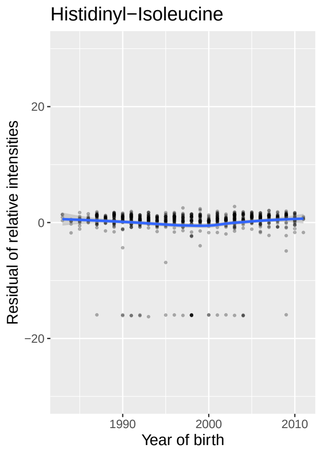
Hydroxyprolyl−Valine



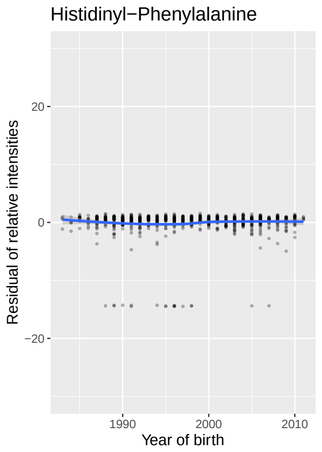
Histidinyl−Histidine



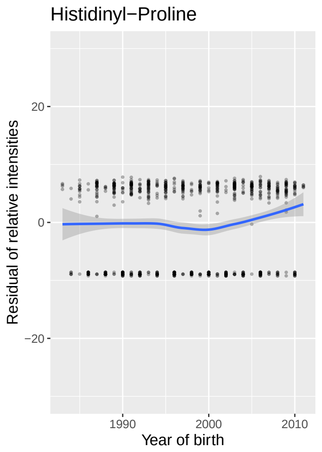
Histidinyl−Isoleucine



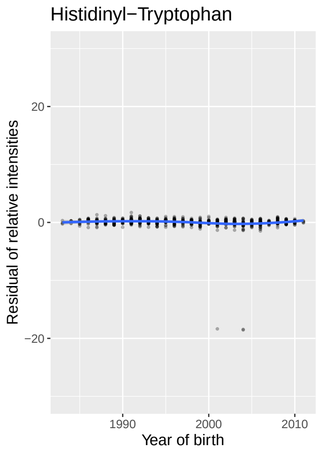
Histidinyl−Phenylalanine



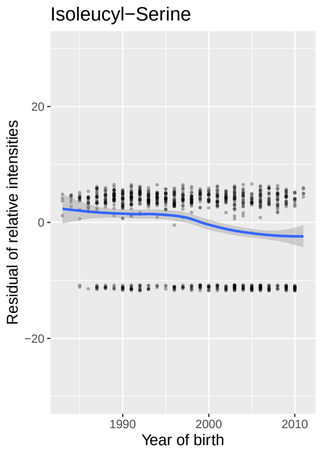
Histidinyl−Proline



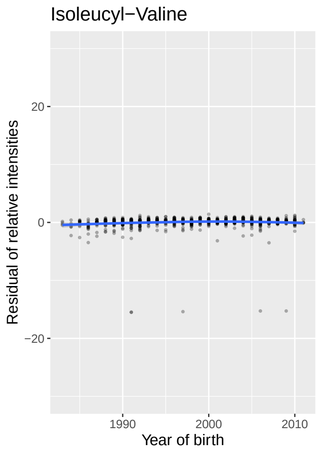
Histidinyl−Tryptophan



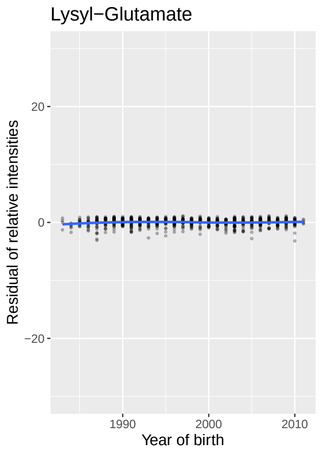
Isoleucyl−Serine



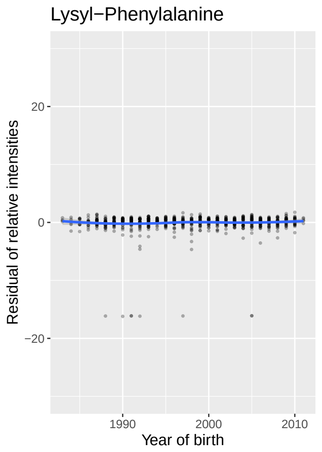
Isoleucyl−Valine



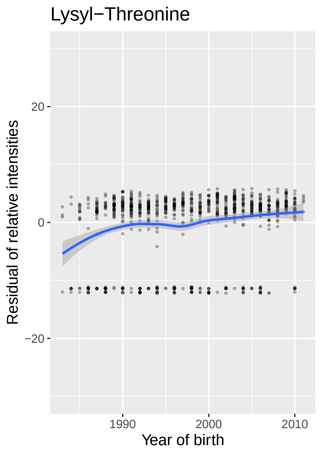
Lysyl−Glutamate



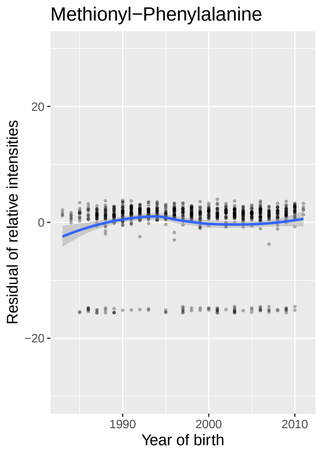
Lysyl−Phenylalanine



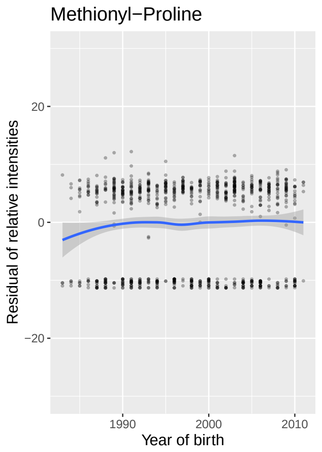
Lysyl−Threonine

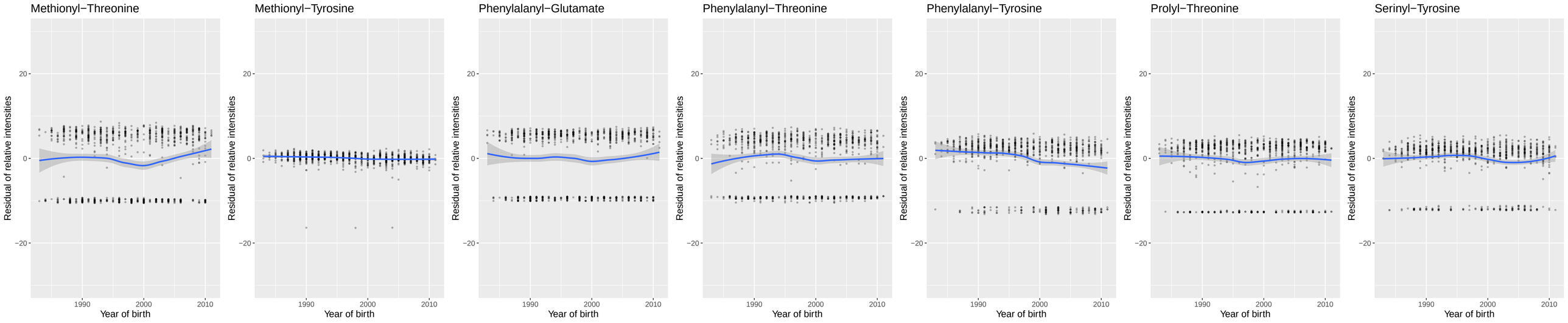


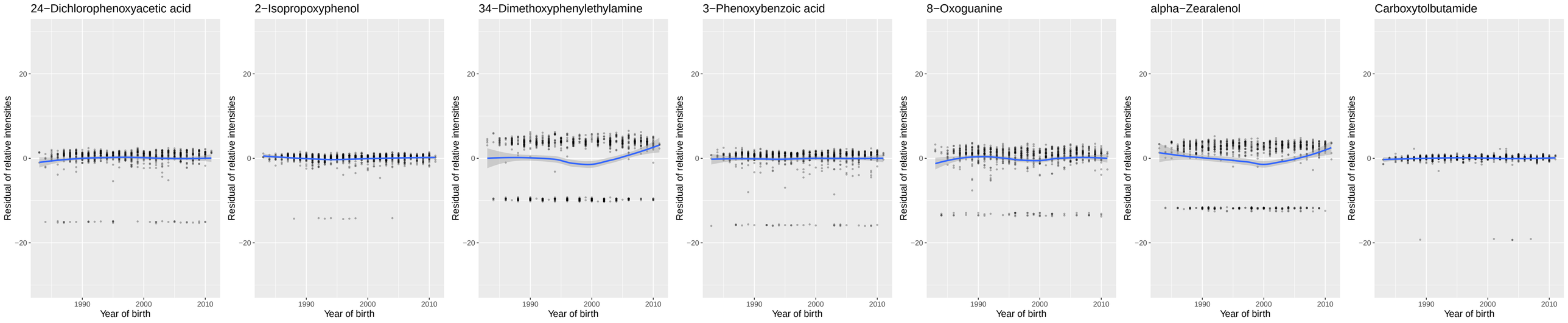
Methionyl−Phenylalanine



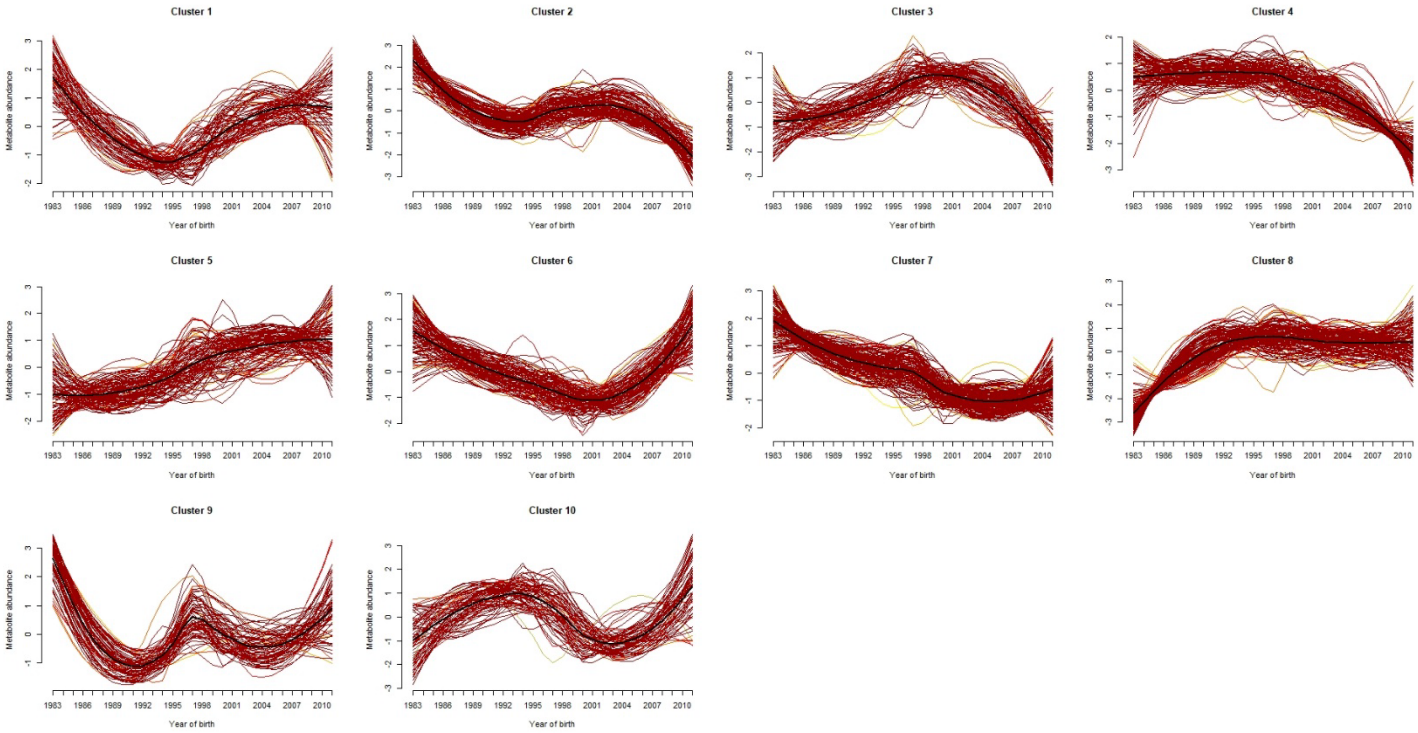
Methionyl−Proline



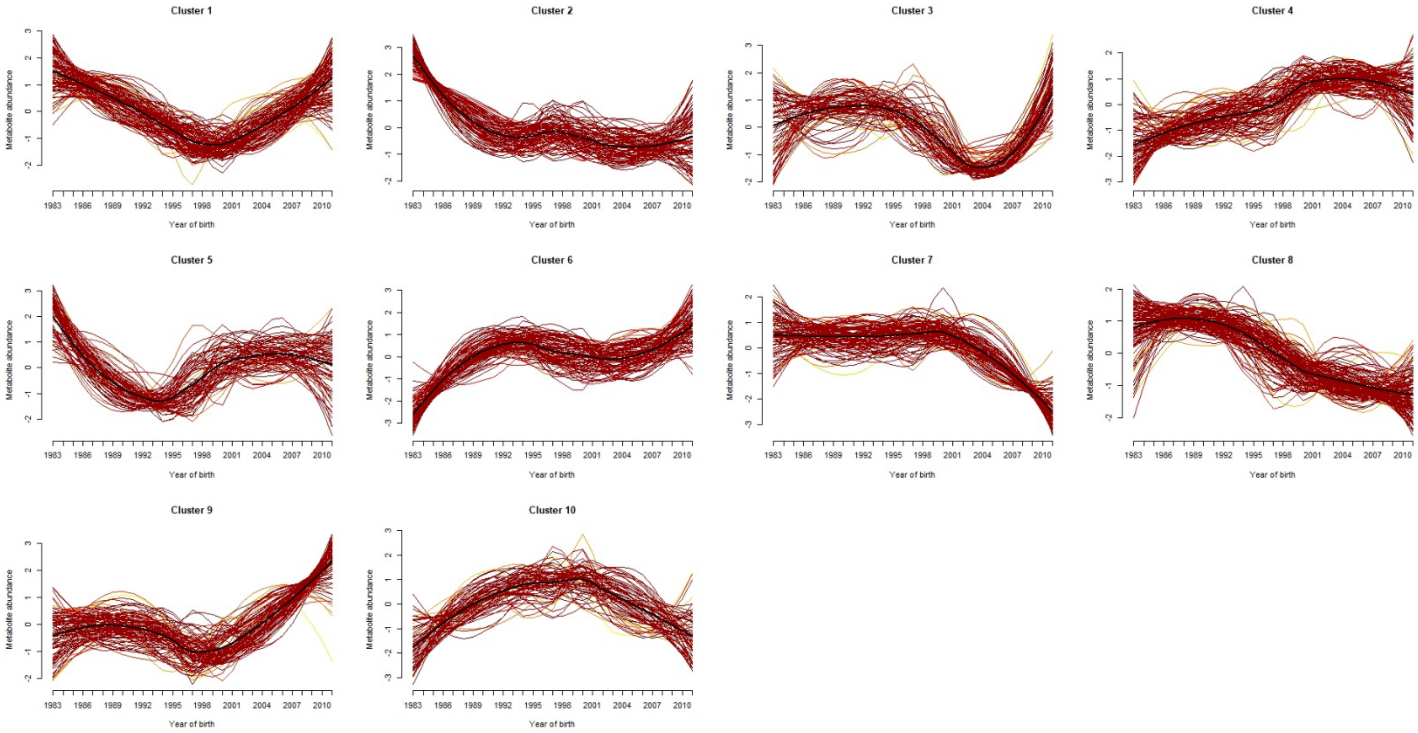

Methionyl−Threonine
Methionyl−Tyrosine
Phenylalanyl−Glutamate
Phenylalanyl−Threonine
Phenylalanyl−Tyrosine
Prolyl−Threonine
Serinyl−Tyrosine
Serinyl−Valine
Tryptophyl−Tryptophan
Tryptophyl−Tyrosine
Tyrosyl−Tyrosine
(−)−epicatechin−3−O−glucuronide
3−Hydroxyadipic acid 36−lactone
5−(34−dihydroxyphenyl)−gamma−vale
Residual of relative intensities
Year of birth


24−Dichlorophenoxyacetic acid
2−Isopropoxyphenol
34−Dimethoxyphenylethylamine
3−Phenoxybenzoic acid
8−Oxoguanine
alpha−Zearalenol
Carboxytolbutamide
gamma−Carboxyglutamic acid
N−Acetyldopamine
N−Nitrosoproline
N1N8−Diacetylspermidine
Normeperidine
Pivalic acid
Pregnanetriolone
Residual of relative intensities
Year of birth

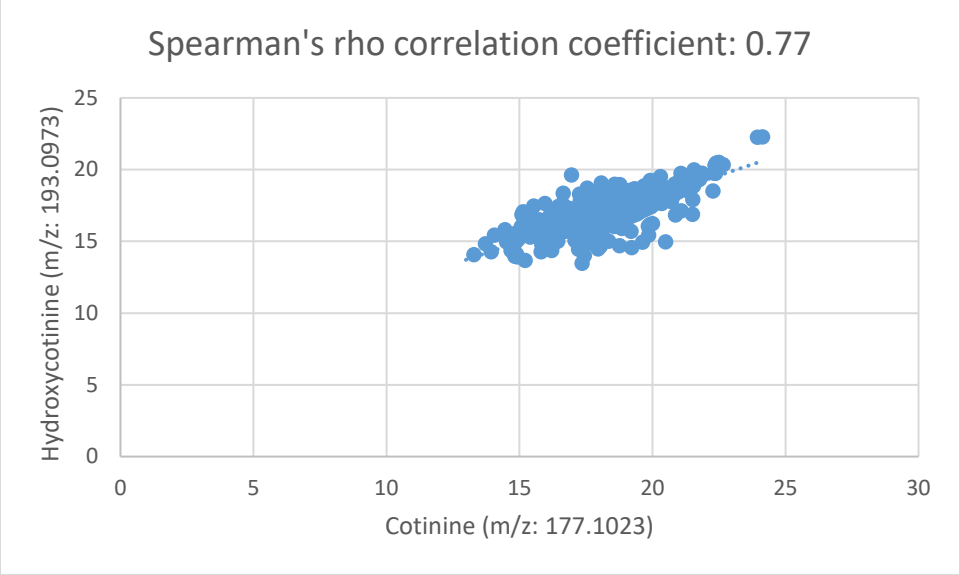
Thiodiglycol
Trimethylselenonium
4−Hydroxy−5−(3−hydroxyphenyl)−val
5−(345−Trihydroxyphenyl)−gamma−va
Dihydronaringenin−O−sulphate
O−methoxycatechol−O−sulphate
Phenol sulphate
Pyrogallol−2−O−glucuronide
NNAL−N−glucuronide
Triclosan sulfate
Residual of relative intensities
Year of birth



Web Figure 5 FCM clustering for exogenous features in HILIC column. Features were fitted to a loess curve and Z-score scaled (red lines), adjusted for Hispanic ethnicity and maternal age, as a function of birth year. Averaged trend is shown in black lines.



Web Figure 6 FCM clustering for exogenous features in C18 column. Features were fitted to a loess curve and Z-score scaled (red lines), adjusted for Hispanic ethnicity and maternal age, as a function of birth year. Averaged trend is shown in black lines.



Web Figure 7: Spearman's rho correlation of log2-transformed cotinine and hydroxycotinine detected in the DBS