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REGULAR ARTICLE

Differential olive grove management regulates the levels of primary metabolites in xylem sap

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Abstract
Aims The conventional management adopted in many Mediterranean olive orchards makes them more vulnerable to climate change and attacks by pathogens, due to the decreased chemical plant defenses. In this scenario, a metabolomic analysis was carried out on the xylem sap (X_{sap}) of olive plants (*Olea europaea* L.) grown in the Salento peninsula (Italy).
Methods Trials were carried out in two olive groves, one organically and one conventionally managed (controls), successively both converted to sustainable management (i.e. frequent light pruning, soil and foliar fertilization, cover crops). The X_{sap} was extracted from the shoots of olive plants using a Scholander pressure chamber pressurized with N_2 and gas chromatography-mass spectrometry metabolite profiling was performed in the X_{sap}.
Results An untargeted gas chromatography mass spectrometry (GC-MS) based metabolomic analysis of primary metabolites (including underivatized volatiles) of the X_{sap} revealed relative abundances of 153 identified metabolites and 336 unknown features across the 12 samples from four groups of samples. Among them, more than half were involved in the primary metabolism. Many of the compounds with increased levels under sustainable management (such as amino acids, soluble sugars, sugar alcohols) have a well-known role as osmoprotectants or are involved in plant defense, growth and development during stress or recovery stages.
Conclusions Sustainable management in olive groves can increase the ability of plants to overcome environmental stressors and enhance ecosystem balance.

Keywords metabolomic profiling · olive xylem sap · plant defense · plant-soil interactions · sustainable soil management

Abbreviations

GC/MS	gas chromatography/mass spectrometry
PCA	principal component analysis
S_{ctrl}	Squinzano control plot
S_{sust}	Squinzano sustainable plot
V_{ctrl}	Vernole control plot
V_{sust}	Vernole sustainable plot
X_{sap}	xylem sap

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Introduction

The olive tree (*Olea europaea* L.) represents the main crop in the Salento peninsula (Apulia region, southern Italy), which is ranked first in terms of areas suitable for olive cultivation (379,910 hectares, about 32.6% of the overall areas at the national level) and olive oil production (about 26% of the national production) (Palese et al. 2013; Lardo et al. 2018).

For many years, the Salento landowners widely applied on dry-farmed olive groves an approach based on low-cost management techniques (i.e. minimum tillage of the soil) coupled with chemical weed control or they abandoned them, making olive trees more vulnerable to the effects of climate change and to the attacks by pathogens, as in the case of the pest *Xylella fastidiosa* in the recent years (Castellini et al. 2020). By applying sustainable agronomic practices, such as no-tillage, fertigation and internal C-inputs (spontaneous cover crops and pruning residues), light and annual pruning and/or fertigation with treated wastewater, it is possible to obtain benefits in terms of climate change mitigation and increase of soil organic carbon (Lardo et al. 2018), faster C and N turnover (Pascazio et al. 2018) and improvement of soil structure and water storage (Palese et al. 2014). Many studies highlighted that sustainable management of olive grove could have positive effects on environmental impact (water cycle, soil microbiological fertility, biodiversity, productivity, and product quality) (Palese et al. 2013) and natural defense of plants to biotic and abiotic stresses (Bragard et al. 2019; Sofo et al. 2019a). It was revealed that olive groves sustainably managed present a higher microbial diversity and complexity both in the soil and in the phyllosphere compared to conventional management (Sofo et al. 2014; Pascazio et al. 2015). It was also showed that sustainable management affects the composition of soil bacterial communities, favoring those with physiological and protective functions for the plants (Fausto et al. 2018).

Many studies were focused on the key role of some metabolites in a) plant defense responses and plant-pathogen interactions, b) plant tolerance to environmental stresses, and c) the capacity of plants to cope with nutrient deficiencies (López-Bucio et al. 2000; Bolton 2009; Kangasjärvi et al. 2012). Among the primary metabolites, sugars play an important role in the process of olive ripening, as they provide energy for metabolic changes and serve as a source for the biosynthesis of fatty acids (Marsilio et al. 2001). Višnjevec et al. (2018) confirmed that the content of oleuropein, sugars and sugar alcohols in leaves and fruits of olive trees ultimately depend on various factors, and not just on drought stress. Furthermore, 76 metabolites were identified in three different tissues of olive, mostly corresponding to distinct types of primary metabolism, with some of them involved in secondary metabolism pathways (Rao et al. 2017).

Primary metabolism has been investigated in studies on olive fruit and leaves under particular agronomic management or specific stress. Martinelli et al. (2012) tested the effects of irrigation on metabolic changes in olive. Their metabolomic analysis by gas chromatography-mass spectrometry (GC-MS) allowed to identify several hundred metabolites in ripe olive mesocarp, 46 of which showed significantly different contents in the rain-fed and irrigated samples. Some of these compounds, involved in primary metabolism (carbohydrates, amino acids, organic acids), appeared to be more abundant when irrigation was performed. A similar study (Martinelli et al. 2013) examined 57 compounds, among which 19 metabolites (organic acids, fatty acids, soluble sugars and terpenes) accumulated differently in the two sets of the sample (pulp + skin) of ripe olives grown under water-stress and irrigated conditions, applied during the last part of the fruit developmental cycle. A reduction in soluble sugars and unsaturated fatty acids was detected in water-stressed samples, suggesting an acceleration of the ripening process.

Despite the tremendous importance of metabolites for the plant, primary metabolism remains poorly characterized, particularly in the xylem sap (X_{sap}). The importance of X_{sap} lives in the fact that, besides transporting water, nutrients, and metabolites, xylem is also involved in long-distance signaling in response to pathogens, symbionts, and environmental stresses (Xylogiannis et al. 2020). While the characterization of compounds of the primary metabolism in olive leaves and fruit has been examined, what happens in the X_{sap} and how compounds change in response to different management remains still a matter of debate (Sofo et al. 2019a). We hypothesize that sustainable olive grove management could influence the primary metabolites present in the X_{sap} regulating the levels of those involved in plant defense and abiotic stress tolerance. We adopted a sustainable management in two different olive orchards and, through a metabolomic approach, the metabolic profile and natural metabolite variations in

the X_{sap} of olive trees were investigated. The aim of this study is providing new insights into the understanding of compounds that could have an important role in the physiological and developmental processes of olive plants under differential management practices.

Materials and methods

Description of the field sites and their agricultural management

The trial has been carried out from 2017 to 2019 at two olive orchards: an organic olive grove in Squinzano municipality (site 1) and a conventional olive grove in Vernole municipality (site 2), in the Salento peninsula of Apulia region (southern Italy). Both areas have a warm and temperature climate, annual precipitation of approximately 742 mm (mean 2017-2019), a mean annual temperature of 16.9 °C, and a mean annual relative humidity of 0.77%. Details on the two sites are reported in Table 1. Olive trees belonging to 'Ogliarola di Lecce' cultivar were selected for sampling within each site to be of similar age and to be growing with agronomic practices specific for each management. Over the three years, phytosanitary treatments had been carried out by the farmers, according to EU Decision 2015/789 (http://data.europa.eu/eli/dec_impl/2015/789/oj), including the control of the insect vector of *X. fastidiosa* (*Philaenus spumarius*) and the removal of wild plant hosts.

In site 1 (Squinzano), organic management includes the following practices: light plowing one time a year, weed mowing two times a year, spontaneous cover crops, organic fertilization (compost, 2 q ha^{-1}) once a year distributed on the soil surface. Pruning was not carried out for at least ten years and when the trees used to be pruned, the pruning residues were burned. Pyrethrum and copper were used for pest and disease control following the recommendations for organic crop production according to EU Regulation 2018/848 (http://data.europa.eu/eli/reg/2018/848/oj) relating to organic production and labeling of organic products.

The site 2 (Vernole) was managed according to conventional agronomic practices: severe pruning carried out every 3-4 years with the removal of pruning residues from the field, harrowing one time a year, weed mowing two times a year, spontaneous cover crops, empirical soil fertilization carried out in winter using nitrogen fertilizer and foliar nitrogen fertilization in summer once per year. Pest management was performed with copper and fly control with traps.

Application of sustainable management protocols

Within each site (Squinzano and Vernole), a 0.5-ha plot with 20 treated plants and 10 control plants was selected. The control plants included the olive trees managed organically (site 1, Squinzano; S_{ctrl}) and conventionally (site 2, Vernole; V_{ctrl}) for site 1 and 2, respectively, whereas the treated plants represented the olive tree subjected to sustainable management (site 1, Squinzano;

Table 1 Details of the olive orchard sites and agronomic practices applied. a.s.l. = above sea level

Parameter	Unit	Site 1	Site 2
Variety	–	Cellina di Nardò, Ogliarola di Lecce	Cellina di Nardò, Ogliarola di Lecce, Leccino
Age of trees	(years)	50–60	70–80
Training system	–	Vase	Vase
Layout	(m)	12 × 12	10 × 10
Planting density	(trees ha^{-1})	70	100
Location	–	N 40° 18′ 59.02 " E 18° 16′ 17.97"	N 40° 27′ 9.65″ E 18° 3′ 4.84"
Elevation	(m a.s.l.)	35	37
Soil texture (USDA)	–	sandy with coarse-texture	loamy-sand with coarse-texture
pH	–	7.9	7.4
Soil management type	–	minimum tillage	minimum tillage
Coverage	–	grass cover	grass cover
Irrigation method	–	none	none

S_{sust}; and site 2. Vernole, V_{sust}). In each sustainably treated plot (S_{sust} and V_{sust}), a severe pruning was carried out at the beginning of the experimental plan in February 2017. Subsequently, plants were lightly pruned twice a year in winter and summer to get a uniform distribution of light in all parts of the canopy and to facilitate air circulation and prevent the increase in relative humidity. Pruning residues were cut and burned, harrowing and weed mowing were carried out twice per year according to EU Decision 2015/789 to prevent the widespread of the infection. In addition, spontaneous vegetation crops were left grown on the ground during the growing season.

Historical information on the nutritional management of plants was also asked to farmers, and soil analyses were carried out in both experimental plots. Considering the results of the soil analyses and the information collected, the fertilization plan was determined for S_{sust} and V_{sust}. Therefore, 30 t ha^{-1} $year^{-1}$ of compost were distributed to the soil of S_{sust} and V_{sust} in winter, and 30 nitrogen units (26% ammonium sulfate) per hectare were distributed once in V_{sust}.

In V_{sust}, it was performed a foliar treatment based on biostimulants Kendal® and Megafol® (Valagro, Atessa, Chieti, Italy) that was distributed with a dose of about 250-300 mL for the first two years, while during the third year Activo Rame (Eno Advance S.r.l., Poggibonsi, Siena, Italy) was used, an amino acid complex (mainly glycine, proline, and alanine) containing polypeptides and 5% (w/w) copper. For pest management the insecticide Decis® (Bayer CropScience S.r.l., Filago, Bergamo, Italy) two times a year and Activo Rame three times a year were applied.

No irrigation was carried out because of the unavailability of wells or nearby water supplies in both plots.

Soil sampling and chemical analyses

At the beginning (February 2017) and at the end of the trial (October 2019), soil samples were collected randomly from 10 different points at 0-30 cm depth (7-cm-diameter cores). After plant debris, roots, and stones were removed, they were mixed thoroughly in a clean pail without sieving to give a composite sample. Three composite soil samples were collected in the field for each experimental plot (n = 3). Each composite sample was divided into two parts, a field-moist sample and an air-dried one. The field-moist samples were refrigerated at 4 °C before biochemical analyses, whereas the air-dried samples were used to determine chemical and physical parameters.

Chemical analyses were carried out following the official methods of DM 13/09/1999 SO n. 185, GU n. 248 21/10/1999. Met II.6 and the enzymatic activities of some enzymes involved in the main biogeochemical cycles, such as acid and alkaline phosphatase (Eivazi and Tabatabai 1977), β-glucosidase (Eivazi and Tabatabai 1988) expressed as μg p-nitrophenol g^{-1} dry soil h^{-1}, and urease (Tabatabai and Bremner 1972) expressed as μg NH_4^+-N g^{-1} dry soil h^{-1}, were measured. The enzyme activities were expressed as units per g of dry soil (units g^{-1} soil).

Plant material and xylem sap extraction

The X_{sap} was collected from shoots of olive trees in October 2019 from three control plants and three treated plants for each plot (n = 3). To avoid border interferences, plants in the central part of each plot and far each other, were randomly chosen.

The X_{sap} was extracted using a Scholander pressure chamber (Model 600, PMS Instruments, Corvallis, OR) pressurized with N_2. Two shoots with a length of approximately 15-20 cm were taken from each of the four cardinal points per plant using sterile cutting shears. The plant material was put in plastic bags, transported to the laboratory, and stored at 4 °C before use. For each shoot, a 1-cm wide bark strip was removed in the proximal part with a sharp knife sterilized with 75% ethanol, to prevent external contamination. The cut end of the stem was placed in the pressure chamber facing out. The foliage of the cutting was placed in the pressure chamber and the lid was locked down. Then, high pressure was applied (approximately from 5.0 to 7.0 MPa, *i.e.* 50-70 bar) to exude the X_{sap} from the tissue at the proximal end of the cutting. After discarding the first drops, 400-500 μL of sap were collected into Eppendorf tubes for 15-20 min per shoot and kept at –80 °C until metabolomic analysis was performed.

Metabolomic analysis

Sample derivatization and GC/MS analysis

Samples extraction, derivatization, and analysis were performed using a modified version of the protocol proposed by Lisec et al. (2006). In particular, 400 μL of X_{sap}, for each sample and replicate, were collected and immediately lyophilized at –40°C. After lyophilization, the samples were newly suspended in 1.4 mL of

methanol (at –20°C) and vortexed for 5 min. Then, 60 μL ribitol (0.2 mg mL^{-1} stock in ddH_2O) were added as internal quantitative standard. Samples were shaken for 10 min at 950 rpm in a thermomixer (at 70 °C) and then centrifuged for 10 min at 11,000 g to avoid the eventual presence of debris. After supernatant collection, 750 μL of $CHCl_3$ (–20 °C) and 1500 μL of ultrapure H_2O (4 °C) were added. Samples were then emulsified by vortexing the vials for 30 sec and successively centrifuged for 15 min at 2,200 g.

The upper polar phase (300 μL for each sample and replicate) were collected, transferred in a 2 mL vial and dried in a speed vacuum at room temperature. To the dried samples, 40 μL methoxyamine hydrochloride (20 mg mL^{-1} in pyridine) were added. Samples were incubated at 37 °C for 2 h in a thermomixer (950 rpm). After methoxyamation, the samples were silylated by adding 70 μL of MSTFA, and then the mixture incubated at 37 °C for 60 min (950 rpm).

The derivatized samples were injected in a gas chromatograph apparatus (Thermo Fisher Scientific; G-Trace 1310) coupled with a single quadrupole mass spectrometer (Thermo Fisher Scientific, ISQ LT). A MEGA-5MS capillary column (30 m × 0.25 mm × 0.25 μm + 10 m of precolumn) was used. Both injectors and sources were settled at a temperature of 250 °C and 260 °C, respectively. Samples (1 μL) were injected in a splitless mode with a helium flow of 1 mL min^{-1} using the following temperature gradient: isothermal 5 min at 70 °C followed by a 5 °C min^{-1} ramp to 350 °C and a final 5-min heating at 330 °C. Mass spectra were recorded in full scan using a 40-600 m/z range with a scan time of 0.2 sec and a solvent delay settled at 9 min. n-Alkane standards (C8-C40, all even), blank solvents, and pooled samples (quality control - QCs) were injected at scheduled intervals for monitoring instrumental performance, shifts in retention indices (RI) and tentative identification.

GC/MS analysis and data acquisition

Data analysis (raw peaks extraction, baseline filtering and calibration, peak alignment, deconvolution, peak identification, and integration) was carried out using the open-source software MS-DIAL, version 4.16 (Tsugawa et al. 2015). The software parameters for data collection, peak detection, deconvolution, alignment, and filtering were settled as successively reported. A minimum peak height of 1,000 amplitudes was applied for peak detection, and a sigma window value of 0.5, EI spectra cut-off of 10 amplitudes was implemented for deconvolution. The linear weighted moving average was used as a smoothing method with a smoothing level of 3 scans and an average peak width of 20 scans. The identification settings were settled as following: retention time tolerance = 0.5 min, RI tolerance = 30, m/z tolerance = 0.5 Da. Both the EI similarity cut-off and the identification score cut-off was settled at 70%. In the alignment parameters setting process, the retention time tolerance was 0.075 min, with an EI similarity tolerance of 70%, and both retention time factor and EI similarity factor settled at 0.5.

Data annotation was carried out in MS-DIAL using publicly available libraries. Compounds identification was based on the mass spectral pattern as compared to EI spectral libraries such as the MoNA (Mass Bank of North America, http://mona.fiehnlab.ucdavis.edu/), the Mass Bank, the MSRI spectral libraries from Golm Metabolome Database (Horai et al. 2010). Metabolite annotation and assignment of the EI-MS spectra were achieved following the guidelines for metabolomics standards initiative for compounds identification, i.e. Level 2: identification was based on spectral database (match factor > 80%) and Level 3: only compound groups were known, e.g. specific ions and RT regions of metabolites (Sansone et al. 2007). Additional annotation of unknown EI-MS features that did not match with the existing spectral libraries were annotated using MS-FINDER version 3.44 (Lai et al. 2018).

Statistical analysis

Experiments were carried out using a randomized design with three replications (n = 3), that is three soil composite samples and three plants for X_{sap} extraction. Means of the values of soil chemical data were separated according to Fisher's LSD test at $p \leq 0.01$.

Metabolomic data were analyzed using the software Metaboanalyst 4.0 (Chong et al. 2019). Metabolomics data were normalized using the internal standard and QCs for LOESS based normalization functions available in the MS-DIAL software for batch correction procedures.

Internal standard normalized dataset, obtained as MS-DIAL output, were log2 normalized and square root transformed. Data were then classified through principal component analysis (PCA), where the output comprised score plots to visualize the contrast between different

samples and loading plots to explain the cluster separation. To highlight statistical differences among single metabolites and treatments, data were then analysed through the univariate analysis to yield volcano plots that demonstrated the significantly differential metabolites with a p value ≤0.05 and the following fold-change cut-off: FC >1.2 and FC <0.8.

Raw data sharing

The raw datasets and the metadata associated with the GC-MS-based metabolomics efforts are deposited at the Mendeley database (DOI: 10.17632/5yxhmnxmks.1, https://data.mendeley.com/datasets/5yxhmnxmks/1) and are freely available for download from 01 March 2021.

Results

Chemical and enzymatic analyses

The soil management practice and the supply of carbon and energy sources provided by compost to the soil have produced an increase in soil organic C in S_{sust} and V_{sust}, compared to S_{ctrl} and V_{ctrl} (Table 2), and an increase in soil C (more than the double in V_{sust}, compared to V_{ctrl}) (Table 2). The content of soil total N in the treated plots (S_{sust} and V_{sust}) (Table 2) was higher than in the controls (S_{ctrl} and V_{ctrl}). Instead, low values of pH and available-P in S_{sust} and V_{sust} than in S_{ctrl} and V_{ctrl} were found (Table 2). The activity of β-glucosidase was significantly higher in the treated plots (S_{sust} and V_{sust}) compared to the controls (S_{ctrl} and V_{ctrl}) (Table 3). The acid/alkaline phosphatase and urease activities were higher in S_{sust} and V_{sust} than in S_{ctrl} and V_{ctrl} (Table 3).

Metabolomic analysis

Untargeted metabolomic analysis of xylem sap using gas chromatography mass spectrometry (GC-MS) revealed individual and grouped metabolites that discriminated samples.

Using an untargeted GC-MS based metabolomics approach, we obtained identification and relative abundances of 153 annotated metabolites and 336 unknowns EI-MS features shared between all 4 sample groups. The processed data from MS-DIAL are provided for identified metabolites (Supplementary Table S1) and unknown features (Supplementary Table S2), displaying their retention times, quant mass, signal/ noise (S/N), EI-spectrum, and relative abundances. Further, using MS-FINDER, we tentatively assigned annotations to 41 EI-MS features as well (Supplementary Table S3). A KEGG-based metabolic pathway enrichment analysis revealed enrichment of taurine and hypotaurine metabolism, aminoacyl-tRNA biosynthesis, arginine biosynthesis, phenylalanine, tyrosine and tryptophan biosynthesis, galactose metabolism, glutathione metabolism, pentose and glucuronate interconversions, D-glutamine and D-glutamate metabolism, nitrogen metabolism, thiamine metabolism, among others (Supplementary Table S4). Most of these annotated metabolites belonged to flavonoids, and lipids, and mostly plant specialized metabolites. The normalized relative abundances (Supplementary Table S5) were used to calculate the fold changes between control and treatment samples (Supplementary Table S6).

A 4-way Venn diagram (Fig. 1) revealed 9 metabolites that were shared and significantly (p-value < 0.05) increased for S_{sust} and V_{sust} samples, such as ribose-5-phosphate, trehalose, fumarate, 2-phosophoglycerate, taurine, and others (Supplementary Table S7). Eight

Table 2 Soil chemical analysis in site 1 (control S_{ctrl} and treated S_{sust}) and in site 2 (control V_{ctrl} and treated V_{sust})

Treatment	Soil organic C (% w/w)	Soil total C (g kg^{-1})	Soil total N (g kg^{-1})	Soil available P (mg kg^{-1})	Soil pH
S_{ctrl}	2.1 b	12.0 ab	1.4 b	5.0 b	7.9 a
S_{sust}	2.5 a	14.2 a	2.1 a	0.9 c	6.7 d
V_{ctrl}	1.3 c	7.0 b	0.3 c	9.0 a	7.4 b
V_{sust}	2.7 a	15.4 a	2.4 a	0.9 c	7.1 c

For each plot, the average of three replicates ($n = 3$) at a depth of 0–30 cm is presented. Values followed by different letters are statistically different ($p \leq 0.01$) within columns, according to Fisher's LSD test. The values were validated following the Eurachem guidelines (www.eurachem.org) respecting the validation parameters: LOD (limit of detection), LOQ (limit of quantification), RL (repeatability limit) and MS (measuring range). The Soil organic C was derivated from the formula Soil organic C = Soil total C × 1.724

Table 3 Enzymatic activity analysis in site 1 (control S_{ctrl} and treated S_{sust}) and in site 2 (control V_{ctrl} and treated V_{sust})

Treatment	β-glucosidase (units g^{-1} soil)	Acid phosphatase (units g^{-1} soil)	Alkaline phosphatase (units g^{-1} soil)	Urease (units g^{-1} soil)
S_{ctrl}	38.67 ± 0.72 c	26.97 ± 3.38 c	59.64 ± 3.51 d	16.92 ± 4.40 d
S_{sust}	242.75 ± 29.69 b	172.12 ± 34.28 b	430.28 ± 79.23 b	20.94 ± 0.61 c
V_{ctrl}	25.89 ± 2.06 c	38.69 ± 1.61 c	83.95 ± 5.52 c	30.50 ± 0.21 b
V_{sust}	309.69 ± 31.49 a	298.86 ± 14.19 a	628.11 ± 39.61 a	46.08 ± 1.01 a

For each plot, the average of three replicates ($n = 3$) ± standard deviation at a depth of 0–30 cm is presented. Values followed by different letters are statistically different ($p \leq 0.01$) within columns, according to Fisher's LSD test

metabolites that significantly (p-value < 0.05) increased in S_{sust} were ribose, UDP-N-acetylglucosamine, urea, 5,6-dihydrouracil, octadecylglycerol and others. Fourteen metabolites significantly (p-value < 0.05) increased in V_{sust} samples were pantothenic acid, gluconolctone, lactic acid, tyrosine, glutamine, maltotriose, xylulose, cystamine and others. Significantly (p-value < 0.05) decreased metabolites in V_{sust} included ureidopropionate, urocanic acid, cysteinylglycine, benzoic acid, tryptamine, and others (Supplementary Figure 1).

An ANOVA analysis identified 75 significantly differential metabolites mainly belonged to chemical classes of the amino acids, polyamines, organic acids, sugars, volatiles, and sugar alcohols differentially produced in olive xylem sap of control (S_{ctrl} and V_{ctrl}) and treated (S_{sust} and V_{sust}) plots (Supplementary Table S8). ANOVA analysis revealed significantly differential metabolites belonging to organic acids (succinic acid, alpha-ketoglutaric acid, fumaric acid: that belong to the TCA cycle, and pyruvic acid, lactic acid, 2-phosphoglyceric acid, 3-hydroxyphenylacetic acid, 4-hydroxybenzoic acid, and glycolic acid), amino acids (asparagine, aspartate, beta-alanine, homocysteine, glutamine, tyrosine, and histidine), and sugars (ribose, xylulose, trehalose, and melibiose) and sugar alcohols (palatinitol) (Fig. 2).

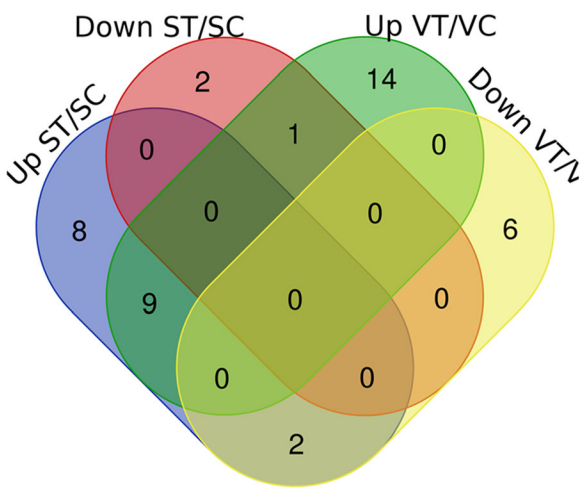

Fig. 1 A 4-way Venn diagram showing the significantly (p-value = 0.05) increased and decreased metabolites in S_{sust} (ST) and V_{sust} (VT) samples, as compared to S_{ctrl} (SC) and V_{ctrl} (VC), respectively (n = 3)

Besides, data with a FC < 0.8, FC > 1.2 and a p-value of 0.05 were presented as volcano plot highlighting the significantly altered metabolites (up or down accumulated) by the field management (Fig. 3 and Supplementary Table S6). As shown in Fig. 3a in the treatment S_{sust}/S_{ctrl} three compounds (isobutyl acetate; tagetone<dihydro-> and 4-hydroxybenzoic acid) were down-accumulated in the X_{sap} as a consequence of soil management, whereas other 21 compounds (trehalose, 2-phosphoglycerate, D-ribose, 5-phosphate, fumaric acid, linalool<tetrahydro->, taurine, encecalin, oxamic acid, nootkatinol, UDP-N-acetylglucosamine, senecioic acid, ribose, cyclohexadecanolide, palatinitol, hexadienol, butanoate<2E,4E->, octadecylglycerol, 5,6-dihydrouracil, urea, hexanal dimethyl acetal) were significantly accumulated.

Concerning the treatment V_{sust}/V_{ctrl}, were reduced (tryptamine, urocanic acid, cysteinylglycine, 2-oxoglutaric acid, palatinitol, benzoic acid, ureidopropionate, hexadienol butanoate<2E,4E->), whereas 23 significantly accumulated (glutamine; 4-hydroxybenzoic acid; xylulose; octane<n->; maltotriose; trehalose; 2-phosphoglycerate; D-ribose 5-phosphate; cystamine; fumaric acid; tyrosine; penten-3-ol<1->; linalool<tetrahydro->; ethyl ether; taurine; encecalin; lavandulyl acetate<tetrahydro->; oxamic acid; gluconolactone; N-formylkynurenine; lactic acid; pantothenic acid; nootkatinol) (Fig. 3b and Supplementary Table S6). Principal Component

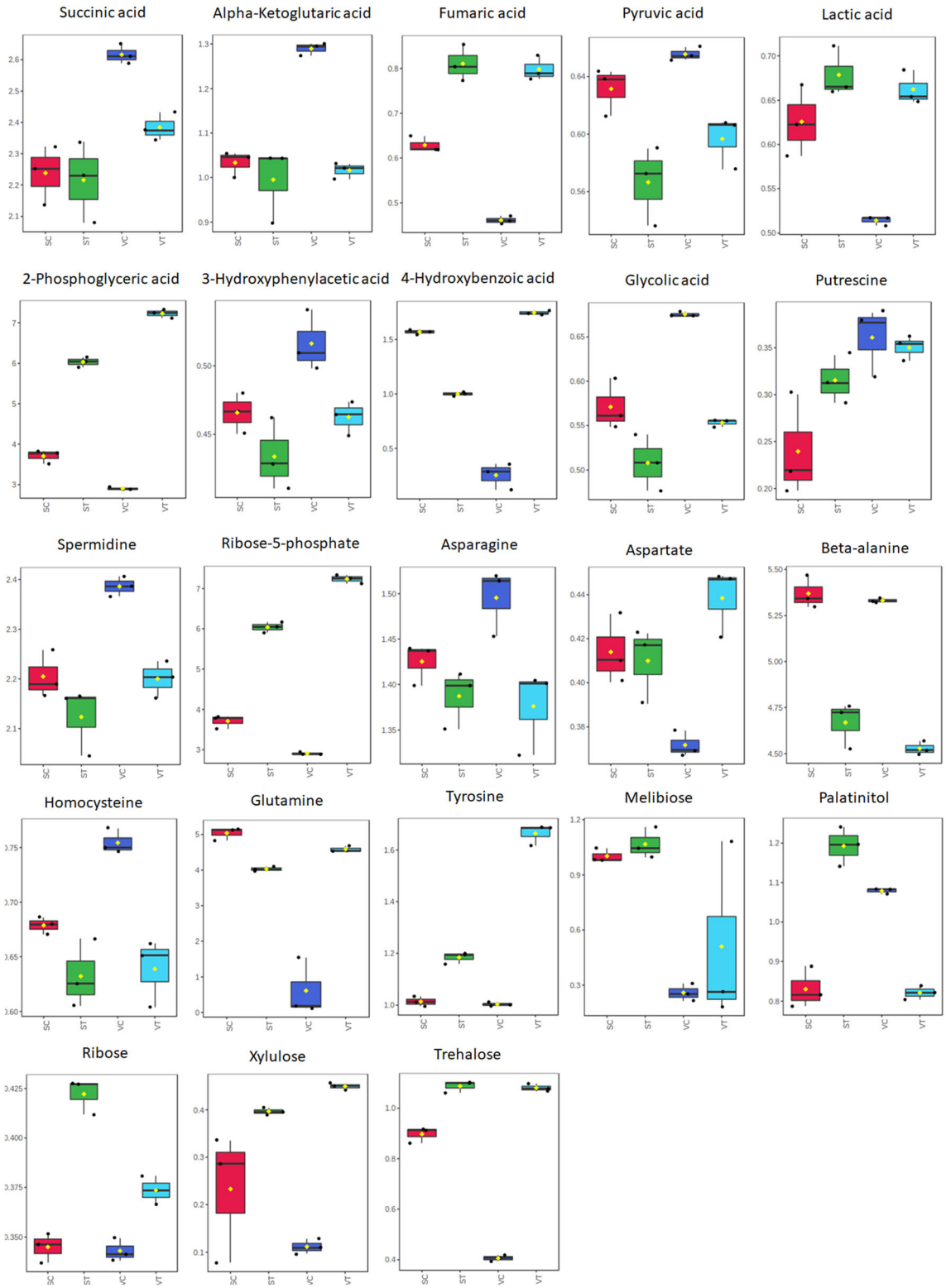

Fig. 2 Significantly differential metabolites accumulated in S_{ctrl} (SC), S_{sust} (ST), V_{ctrl} (VC), and V_{sust} (VT) samples as analyzed using a 3-way ANOVA. Chemical metabolites classes point to amino acids, organic acids, sugars, volatiles and specialized metabolites, and other such as polyamine (n = 3)

Fig. 3 Volcano plot analysis showing the metabolites significantly up or down accumulated by the field management in the treatment S_{sust}/S_{ctrl} (ST/SC) **(a)** and in the treatment V_{sust}/V_{ctrl} (VT/VC) **(b)** (n = 3)

Analysis (PCA) was carried out on all samples analyzed using GC-MS, such as blanks, pooled quality controls (QCs) and all four sample groups together to demonstrate the system suitability. The PCA score plot, revealed a good discrimination of sample groups against QCs and blanks (Supplementary Figure 2). Similarly, a

Pearson correlation analysis among samples based on the relative metabolite abundances revealed clustering of samples within the group (Supplementary Figure 3).

Both unsupervised PCA run on identified metabolites (Supplementary Figure 4a) and unassigned/unidentified features (Supplementary Figure 4b) revealed discrimination of sample groups. Further, both supervised PCA analysis (Fig. 4a) and unsupervised partial least squares discriminant analysis (PLS-DA) conducted on annotated metabolites (Fig. 4b) demonstrated group separation with the first 2 principal components (PCs) explaining 63.4% variance for PCA and 53.6% variance in PLS-DA score plots. PLS-DA derived variable importance of projection (VIP) scores revealed 3-nitro-tyrosine, 2-phosophoglycerate, ribose-5-phosphate, octadecylglycerol as the ones with the highest VIP scores for the four sample groups (Fig. 4c). A random forest analysis revealed octadecylglycerol, glutamine, farnesol, lavandulyl acetate with the highest mean decrease accuracy for the four sample groups (Fig. 4d).

A hierarchical clustering analysis (HCA) run on the samples of both identified and unknown/unassigned metabolites reveals clustering of the sample groups and the pooled QCs (Supplementary Figure 4c, d and Supplementary Table S9).

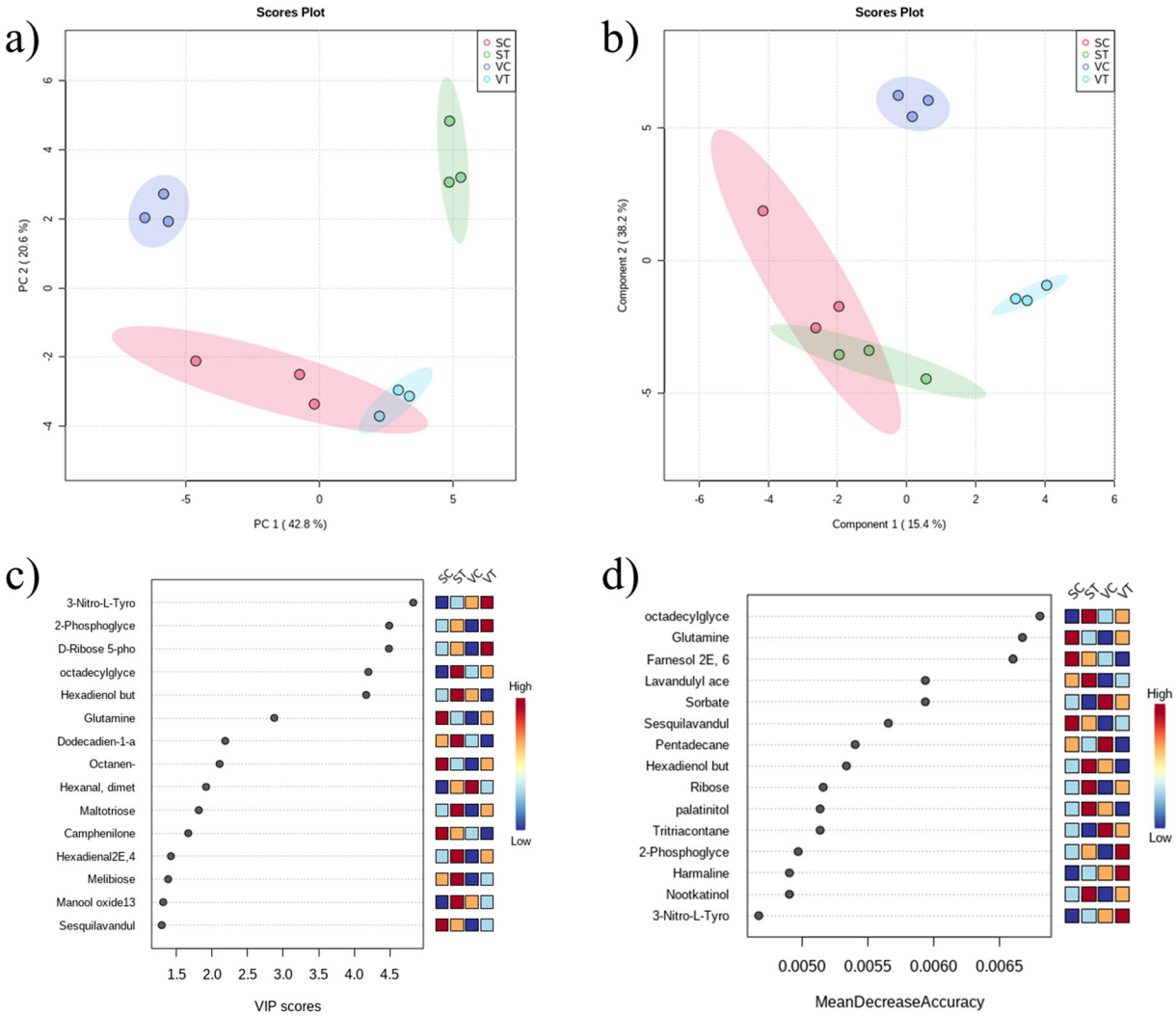

Fig. 4 **(a)** Principal component analysis showing score plots discriminating S_{ctrl} (SC), S_{sust} (ST), V_{ctrl} (VC), and V_{sust} (VT) groups by virtue of the first 2 PCs. **(b)** Partial least square discriminant analysis (PLS-DA) showing discrimination of S_{ctrl}, S_{sust}, V_{ctrl}, V_{sust} groups by virtue of the first 2 components. **(c)** PLS-DA derived analysis variable importance of projection (VIP) features for the groups, and **(d)** random forest (RF) analysis displaying the mean decrease accuracies (n = 3)

Discussions

Soil management practices

The weed control, fertilization, frequent pruning, and pruning residues management have influenced the ecosystem of both olive groves managed organically (site 1) and conventionally (site 2). The balanced and rational nutrition provided by treated organic material recycling and additional fertilizers to the experimental plots has induced effective olive trees' effective responses. The chemical properties of soils subjected to sustainable management for three years were significantly improved (Tables 2 and 3). Similarly, Ebabu et al. (2020) found that after three years of sustainable land management practices in three contrasting agro-ecological zones, most soil parameters (such as bulk density, soil organic carbon, total nitrogen, available phosphorus, and potassium) were optimal for supporting plant production.

Comparing the control plots (S_{ctrl} and V_{ctrl}) to the treated plots (S_{sust} and V_{sust}) (Table 2) we confirm that the adoption of sustainable management (aimed mainly at increasing the C inputs) can favour an increase of soil C stock (Fiore et al. 2018). In our study, three years of sustainable management were enough to reveal an increase in soil C (Table 2), showing that soil chemical properties can be at least partially recovered also after disturbances over a longer time (García-Gil et al. 2000). A conceivable explanation of N content differences between treated (S_{sust} and V_{sust}) and control plots (S_{ctrl} and V_{ctrl}) (Table 2) is a higher activity of the microbial nitrifying population, which is affected by different fertilizer applications (Chao et al. 1996).

The lower values of pH and available-P in treated (S_{sust} and V_{sust}) than in control (S_{ctrl} and V_{ctrl}) plots (Table 2) could mainly be because of the continuous cropping system and to the long term use of mineral nitrogen fertilizers, which substantially decrease the amounts of exchangeable base cations (mostly Ca^{2+} and Mg^{2+}) but on the other side, they increase the H^{+} concentration (Schroder et al. 2011).

Some soil management practices, such as no-tillage or reduction in tillage frequency, increase the activity of β-glucosidase because of improvement in microbial biomass, more substrate availability, and reduced soil disturbance (Sofo et al. 2014). The high β-glucosidase activity occurring in S_{sust} and V_{sust}, compared to S_{ctrl} and V_{ctrl} (Table 3) was significantly related to the increase of soil organic carbon (SOC) (Table 2). The activity of this enzyme has been found to be higher in fertilization treatments with compost than in those without compost, as well as those with synthetic fertilizers and herbicides (Crecchio et al. 2004; Meyer et al. 2015).

Low levels of soil P and pH influence the production of phosphatases in the ecosystem (Acosta-Martínez and Tabatabai 2000). In our analysis, a decrease in pH in S_{sust} and V_{sust} (Table 2) corresponded to a rise of acid phosphatase activity (see S_{sust} and V_{sust}; Table 3). The increase of acid phosphatase is more marked in the V_{sust}, compared to S_{sust}, likely because the difference between the two plots (organic vs sustainable and conventional vs sustainable) was more defined. The increase in phosphatase activity (both acid and alkaline) in soils amended with organic materials (as in S_{sust} and V_{sust}; Table 3) can be attributed to the stimulation of microbial growth and soil organic matter enrichment (Adetunji et al. 2017).

Urease expression is under N regulation, and its production is activated in the presence of urea or alternative N sources (Mobley et al. 1995). The increase of urease activity in S_{sust} and V_{sust} (Table 3) were related to the higher soil total N in sustainable plots compared to controls (Table 2).

Metabolomic profile in olive xylem sap under different management

The established role of X_{sap} is to transfer and distribute, through the xylem vessels, the minerals, and water absorbed by roots to the aerial parts of the plant (Shi et al. 2002). In the past, X_{sap} was thought to be mainly composed of inorganic compounds and water, but relatively recent studies highlighted that X_{sap} also contains a wide range of small, water-soluble, organic substances. These include many primary metabolites, such as polyols and simple sugars, amino acids, organic acids, plant hormones, and secondary metabolites, which play a pivotal role in plant growth and resistance to stresses (Lowe-Power et al. 2018; Sofo et al. 2019b). Several studies recently showed that X_{sap} composition could be influenced by a large variety of factors, such as changes in climatic conditions, biotic issues, and changes in crop management (Sofo et al. 2019a).

In our study, to get more insights into X_{sap} metabolic changes in olive groves under different management in the two sites, a GC/MS-driven untargeted-metabolomic analysis was carried out.

The multivariate analysis, carried out on both annotated and unknown compounds, pointed out a clear separation among all groups (S_{ctrl}, S_{sust}, V_{ctrl}, and V_{sust}), suggesting that either the location or soil management had a significant influence on xylem sap composition. Also, the univariate analysis allowed to identify those metabolites significantly changed in response to the treatments.

As reported in the Venn diagram, and supported by the ANOVA analysis, in the xylem sap of both organically managed fields have been identified 9 common metabolites significantly up-regulated by the treatment. In particular, has been observed an up-regulation of trehalose, fumaric acid, taurine, encecalin, linalool and nootkatinol, which are known mainly to play a pivotal role in protecting plants from both biotic and abiotic stress.

The osmoprotectants and reactive oxygen species (ROS) scavenger role of trehalose has largely been described (Kosar et al. 2019). Kaplan et al. (2004) reported that in plants exposed for few hours to heat stress, trehalose content was increasing two times, whereas in chilled plants, it was eightfold higher than control after a few days of exposition to stress. A microarray analysis pointed out that during abiotic stresses (e.g., cold, UV, salinity) most of the genes involved in trehalose metabolism were significantly activated, supporting the hypothesis that trehalose levels change in response to abiotic environmental fluctuations (Iordachescu and Imai 2008). As well as trehalose, also taurine has been shown to act as a ROS scavenger since it has been reported that this amino acid promotes plant growth and development, improves the efficiency of the photosynthetic machinery, and protects cell membranes from lipid peroxidation (Hao et al. 2004).

In the X_{sap} of plants, cropped through sustainable management, was also observed an increment in pyruvate and fumaric acid (two Krebbs cycle intermediates), which could be connected to the increment in 2-phosphoglyceric acid. In fact, this metabolite serves as the substrate, during glycolysis, for the conversion of glucose to pyruvate. The increase in both fumaric acid and pyruvate could be extremely useful for plants during hypothetical stress. In fact, both metabolites are metabolized under stresses to generate energy and carbon skeletons to produce other compounds (Rhodes et al. 1986; Chia et al. 2000). In particular, fumaric acid could help to maintain cellular pH and turgor pressure and be metabolically accessible as a transient storage form of fixed carbon (Fernie and Martinoia 2009). Similarly, it has been reported that high content in pyruvate is important in helping plants during water stress (Rhodes et al. 1986).

Concerning the three specialized metabolites, the chromene encecalin, the tropolone nootkatinol, and the terpenoid linalool, several reports showed that these metabolites have antimicrobial, insecticidal, antifungal, and broad antimicrobial activity (Isman and Proksch 1985; Saniewski et al. 2007; Herman et al. 2016). Encecalin is a chromene characterized by antifeedant and insecticidal properties reducing larval growth and decreasing survivorship of neonate larvae (Isman and Proksch 1985), whereas linalool is largely known for its repellent activity versus various insect species (Lawal et al. 2014; Pajaro-Castro et al. 2017).

The presence of these three secondary metabolites is extremely interesting in olive trees. In the last years in Apulia, olive has been strongly attacked by a xylematic bacteria (*X. fastidiosa*), which is decimating the population of centuries-old olive trees. This pathogen is spread through different insect vectors belonging to the family Aphrophoridae (*Philaenus spumarius, Philaenus italosignus, Neophilaenus campestris,* among others) (Saponari et al. 2019). Therefore, we could speculate that encecalin, nootkatinol and linalool could increase sustainably managed plants' ability to cope with this biotic stress.

Since xylem vessels are formed by non-metabolically active cells, it should be assumed that controlled uptake and secretion by neighboring protoxylem, sugar-rich phloem cells, and parenchyma cells could deplete or enrich X_{sap} with specific metabolites which will be distributed through the aerial parts (Shi et al. 2002). Therefore, it is expected that the composition of X_{sap} could represent a signature of the root status, whose health and activity are strongly influenced by soil management and fertilization. Youssefi et al. (2000) highlighted that a positive correlation exists between N fertilization and amino acid content in X_{sap}. Interestingly, as reported in both ANOVA and volcano plot analysis, in V_{sust} fields, which received a higher amount of fertilizer and amino acid-based bio-stimulants treatments, a higher amount of several amino acids (ornithine, putrescine, spermidine, among others) has been observed compared to S_{sust} (Supplementary Table S6). The increment of these compounds could play a pivotal role in ameliorating plants' ability to cope with both biotic and abiotic stress typical of semi-arid environments where olive is cultivated.

It has been largely reported that both polyamines and amino acids, such as ornithine, putrescine, asparagine, and spermidine, play a pivotal role in protecting plants recovery from environmental stresses (Kuznetsov and Shevyakova 2007; Bown and Shelp 2016). Polyamines, particularly putrescine, spermidine and ornithine, can protect plants from several environmental adverse conditions, such as salt, osmotic, chilling, and oxidative stress (Kuznetsov and Shevyakova 2007). Also, several amino acids (e.g., alanine, asparagine, etc.) and soluble sugars (e.g., ribose, trehalose, etc.) and sugar alcohols (e.g., palatinitol), all of them stimulated by the treatments, could alleviate plant stress, acting as osmoprotectants (Singh et al. 2015; Lu et al. 2020). Pagliarani et al. (2019) showed that during drought conditions, similarly to the semi-arid climate in our experiment, there is an alteration between starch and soluble sugars partitioning. In particular, under such type of stress, an increase of soluble sugars is observable in poplar trees, because of starch degradation, and a drop of xylem pH that induces an accumulation of soluble sugars (sucrose, fructose, glucose, etc.). These latter are pivotal for plant protection and for repairing xylem functionality during drought. Soluble sugars could also be a source of carbon for plant maintenance, growth, and development during stresses or recovery stages (Chaves et al. 2002). Besides, biotic factors and/or soil management type could take part in increasing the sugar alcohol concentration (e.g. galactinol and palatinitol) in the X_{sap} of several tree species (Noiraud et al. 2001).

Concerning palatinitol, a sugar alcohol which significantly accumulated in X_{sap} of S_{sust} treated plants, several manuscripts reported its role and/or its involvement in protecting plants from stress (Lu et al. 2020; Lee et al. 2016). It is known that sugar alcohols could serve as energy conservation compounds allowing plants sustainment during stress (Sasse et al. 2018).

Besides amino acids, sugars, polyols and polyamine accumulation in response to soil management, also the increase in organic acids, observed in S_{sust} and V_{sust} fields, could play an important role in improving plants performances, and their production seems to be more stimulated in V_{sust} fields than in S_{sust} ones (Supplementary Table S6). Glucose, organic acids, such as fumaric and succinic acids, which are components of the tricarboxylic acid (TCA) cycle, can be metabolized by stressed plants to generate energy and carbon skeletons for the biosynthesis of other metabolites playing an important role in stress defense (López-Bucio et al. 2000). Ashrafi et al. (2018) found that, in the shrubby species thyme subjected to drought, the tricarboxylic acid intermediates have a prominent role in activating drought tolerance mechanisms. The transport of organic acid along the transpiration stream has also been connected and correlated with the transport of micronutrients. It has been found that the formation of metal-citrate complexes increased copper transport through the excised stem of *Papyrus*, iron in several dicotyledonous, zinc in *Pinus radiata*, and aluminium in *Fagopyrum esculentum* (López-Bucio et al. 2000; Ma and Hiradate 2000). In the X_{sap}, these complexes are more efficiently transported, as they are subjected to a reduction of lateral escape and lower adsorption to the negatively-charged vessel walls.

Conclusions

From the general analysis of the results we can affirm that, compared to classical management, the sustainable soil management of olive orchards had a positive impact on the chemical and biochemical soil properties, improving total C, N levels, the content of available nutrients, as well as regulating soil microbial activities. In this study, a significant change in X_{sap} composition was observed in response to soil management. In the X_{sap} of sustainably managed olive orchards, it was observed the up-regulation of several primary and specialized metabolites (such as amino acids, soluble sugars, sugar alcohols, among others) involved in plant defense against biotic and abiotic stresses.

In conclusion, we suggest that the transition from the low-input traditional management model to an alternative, sustainable and multifunctional one, could be a solution for maintaining soil fertility and increase plant defenses in these agricultural systems. The sustainably managed olive groves could better face the environmental challenges related to climate change, including the consequent lack of resources (particularly water and nutrients). In this scenario, the adoption of sustainable agronomic practices could increase both the resistance and resilience to biotic and abiotic stresses in this important tree crop, with clear environmental, economic, social and cultural benefits.

Limitations of the study

Our study has several limitations. The first limitation is connected with the hypothesis that the increase of X_{sap}

metabolites with osmoprotectants and defense roles could really increase plant defense and recovery. To confirm this hypothesis plants must be stressed in order to understand if they can effectively increase plant resistance and resilience. Moreover, other analytical techniques such as liquid chromatography-mass-spectrometry, characterized by a less complex sample manipulation and preparations steps (liquid-liquid separation, drying and derivatization) and with wider metabolic coverage, could hallow in the identification and relative quantification of various primary and specialized metabolites belonging to more numbers of pathways and involved in plant stress metabolic responses.

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Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

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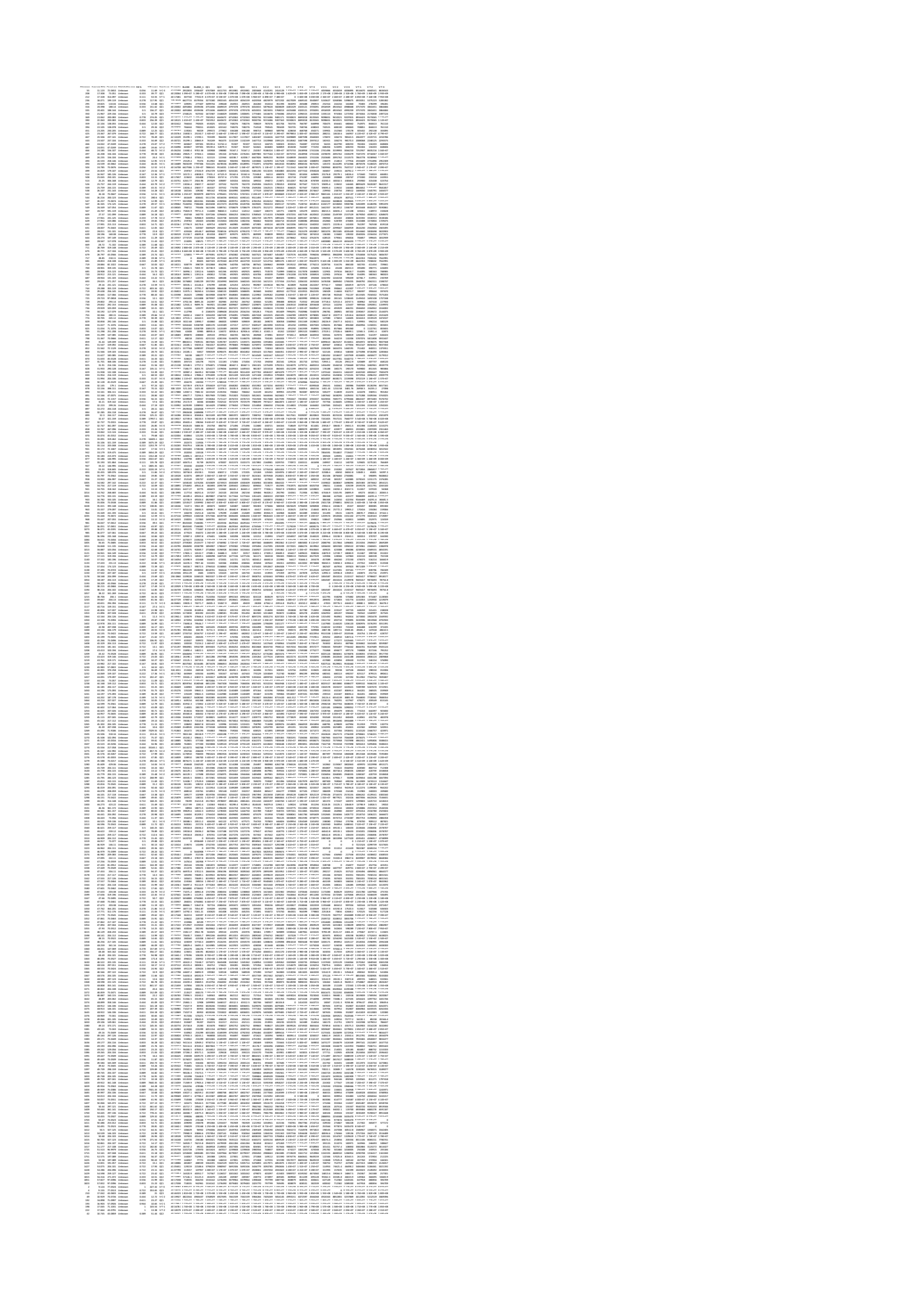
Alignment	Average R	Quant ma	Metabolite name	Fill %	Formula	INCHIKEY	SMILES	RT similar	Total spec	Dot produ	Reverse d	S/N avera	Spectrum	EI spectru	BLANK	BLANK 1	QC1	QC2	QC3	QC4	S-C-1	S-C-2	S-C-3	S-T-1	S-T-2	S-T-3	V-C-1	V-C-2	V-C-3	V-T-1	V-T-2	V-T-3
955	33.83	81.09885	Manool oxide<13-epi->	1	C20H34O			null	98.2	98	98.1	1057.38	S-T-3	40.19645:	3427095	4831913	333823.2	750876.1	211111.3	211111.3	213241.7	131359.6	268857	1.78E+07	9.95E+07	6.40E+08	289197.9	222142.8	223950.9	164237.9	244761.9	316944.2
353	21.655	57.0893	Hexacosane	0.944	C26H54			null	95.6	95.1	95.5	3.38	S-T-3	40.19094:	1.18E+07	1.23E+07	1.26E+07	1.20E+07	1.16E+07	1.16E+07	1.41E+07	1.33E+07	1.21E+07	1.42E+07	1.36E+07	1.34E+07	1.10E+07	1.09E+07	1.14E+07	1.30E+07	1.36E+07	1.47E+07
973	34.252	55.07444	Manool oxide	0.722	C20H34O			null	95.3	94.8	94.5	6.31	S-T-3	40.19857:	1695836	3980274	1217931	1284369	3847088	3847088	1712843	5333852	4973911	2340224	6284227	2.50E+07	1546370	1649796	0	3590366	4292164	323470.4
14	9.54	43.0874	Decane<n->	0.944	C10H22			null	93.8	93.2	91.6	3.27	S-T-1	40.19896:	9564978	9514564	8335736	8025497	7663438	7663438	8790844	8188943	7725276	8356076	9088289	1.20E+07	6977395	7552978	8291921	6794572	8401298	6921703
35	10.34	152.069	2-Hydroxypyridine	0.889	C5H5NO	UBQKCCH	Oc(c1)ncc	53.7	92.8	87.7	96.7	468.43	V-T-3	42.06466:	1.40E+07	1.79E+07	2.87E+07	3.60E+07	3.77E+07	3.77E+07	3.11E+07	3.80E+07	3.51E+07	4.67E+07	5.33E+07	4.63E+07	2.48E+07	2.43E+07	2.41E+07	5.28E+07	5.56E+07	5.20E+07
166	15.564	73.06283	Cytidine	1				16.5	91.9	90.1	90.6	80	V-T-3	40.20778:	1.03E+08	1.01E+08	3.46E+07	3.16E+07	3.40E+07	3.40E+07	5.91E+07	5.91E+07	7.36E+07	5.34E+07	8.44E+07	7.81E+07	9.01E+07	9.21E+07	9.40E+07	9.37E+07	9.37E+07	8.38E+07
221	17.793	69.07942	Tetradecene<1->	1	C14H28			null	91.8	90.5	89.7	27.78	QC2	40.17607:	2.84E+07	2.77E+07	2.74E+07	2.65E+07	2.60E+07	2.60E+07	2.71E+07	2.60E+07	2.64E+07	2.85E+07	2.81E+07	2.45E+07	2.01E+07	2.00E+07	2.06E+07	2.14E+07	2.20E+07	2.26E+07
442	23.432	69.08123	Hexadecene<1->	0.944	C16H32			null	91.6	90.4	90.3	9.42	BLANK 1	40.19298:	1.42E+07	1.41E+07	1.40E+07	1.33E+07	1.28E+07	1.28E+07	1.42E+07	1.42E+07	1.41E+07	2.04E+07	1.98E+07	1.95E+07	1.22E+07	1.21E+07	1.19E+07	1.41E+07	1.48E+07	1.57E+07
207	17.301	57.09255	Hexadecane	0.667	C16H34			null	91.1	89.8	92.4	41.71	QC1	40.20278:	3.18E+07	3.18E+07	3.34E+07	2.11E+07	3.99E+07	3.99E+07	4.07E+07	4.22E+07	4.30E+07	0	6.70E+07	5.68E+07	3.34E+07	3.37E+07	3.38E+07	5.31E+07	5.52E+07	5.63E+07
97	12.421	147.0911	Hydroxylamine	1	H3NO	AVXURJPC	NO	30.9	90.6	85	94.4	83.36	V-C-2	40.19265:	1.31E+08	1.34E+08	9.11E+07	7.87E+07	1.01E+08	1.01E+08	8.14E+07	9.67E+07	9.55E+07	9.07E+07	1.01E+08	1.07E+08	1.12E+08	1.14E+08	1.20E+08	1.07E+08	1.19E+08	1.19E+08
956	33.861	43.06534	Cedroxyde	0.667	C15H24O			null	90.5	91	89	5.31	S-T-3	40.1943:6	0	1.16E+07	8967424	7142532	214226.4	214226.4	1.09E+07	1.02E+07	1.05E+07	2.97E+07	0	4.08E+08	0	0	0	3645183	1.33E+07	1.30E+07
131	13.837	86.05521	Sorbate	1				27.8	90	91.5	87.4	538.15	BLANK	40.17815:	9.16E+07	9.15E+07	7.09E+07	7.23E+07	7.57E+07	7.57E+07	8.32E+07	8.68E+07	8.78E+07	8.70E+07	9.25E+07	8.34E+07	8.76E+07	8.67E+07	8.81E+07	8.73E+07	9.07E+07	9.43E+07
12	9.419	70.11008	Undecane<n->	1	C11H24			null	89.2	91	84.8	4.64	QC3	40.18431:	3400237	3113623	2787040	3024930	2984511	2984511	2108381	2573219	3042089	2252825	2560121	1741940	2270257	2056265	1871318	1552906	1840952	1577115
407	22.831	57.07927	Heptacosane	0.889	C27H56			null	88.3	84.5	91.4	4.61	V-T-1	40.20053:	9911477	1.13E+07	1.13E+07	1.05E+07	1.01E+07	1.01E+07	1.21E+07	1.20E+07	1.32E+07	1.20E+07	1.14E+07	0	1.07E+07	9909668	1.02E+07	1.06E+07	1.18E+07	1.22E+07
859	31.704	73.07033	Hexadienol butanoate<2E,4E->	1	C10H16O2			null	88.1	94.2	74.9	5.06	V-T-2	40.18664:	5317813	1850949	3171365	2855434	3205247	3205247	6244475	7374193	7398148	3.72E+09	3.78E+09	1.54E+09	1.34E+07	1.41E+07	1.61E+07	816851.1	625998.9	1033274
339	20.429	174.1172	Gly-Gly	1	C4H8N2O	YMAWOP	NCC(=O)N	48.5	87.9	80.9	92.3	6947.36	S-C-1	40.17814:	2.35E+08	2.39E+08	2.34E+08	2.37E+08	2.35E+08	2.35E+08	2.57E+08	2.55E+08	2.52E+08	2.52E+08	2.37E+08	2.04E+08	2.14E+08	2.18E+08	2.23E+08	2.03E+08	2.09E+08	2.24E+08
415	22.529	43.07719	Palmitoleic acid	1				14.5	85.7	80.4	89.1	4.69	V-C-1	40.20451:	1.01E+07	1.03E+07	1.04E+07	9517643	9336284	9336284	1.09E+07	1.15E+07	1.10E+07	1.17E+07	1.16E+07	1.24E+07	9877370	1.03E+07	1.03E+07	1.12E+07	1.14E+07	1.21E+07
329	20.675	57.09979	Octacosane	0.944	C28H58			null	85.7	82	86.3	6.49	S-C-3	40.18621:	3016100	2801388	7006898	3492307	3954991	3954991	5410277	4449266	3883869	4804593	4118696	3926027	2588146	3094314	3454700	4868846	4818977	4213186
666	28.372	69.08588	Eicosene<1->	0.944	C20H40			null	85.7	90.3	81.2	12.59	BLANK	40.17178:	1.01E+07	9830070	8534715	9485371	7363414	7363414	9643252	9773931	9896248	1.17E+07	1.25E+07	1.09E+07	6261949	7524361	8634075	1.00E+07	1.05E+07	1.09E+07
922	33.112	73.0181	Hexadienal<2E,4E->	0.611	C6H8O			null	85.7	100	68.2	122.13	QC2	41.02551:	140605.1	3579083	7.19E+09	2.81E+09	7.20E+09	7.20E+09	2.89E+09	4.27E+09	3.39E+09	8.84E+09	8.36E+09	4.49E+09	1.66E+09	1.57E+09	1.64E+09	9.14E+08	6.41E+09	6.61E+09
46	10.905	43.08125	Asparagine	1				33.2	85.5	78.3	88.9	11.18	QC2	40.21693:	2.37E+07	2.22E+07	2.20E+07	2.19E+07	2.08E+07	2.08E+07	2.49E+07	2.30E+07	2.30E+07	2.59E+07	2.52E+07	2.33E+07	2.21E+07	2.24E+07	1.98E+07	2.20E+07	2.25E+07	2.15E+07
338	20.428	174.1364	N-Alpha-AcetylLysine	0.944	C13H14N:	QJOZJXNK	COc(c3)cc	17	85.3	88.1	77.7	26.29	S-T-1	40.16743:	2.35E+08	2.39E+08	2.35E+08	2.37E+08	2.35E+08	2.35E+08	2.57E+08	2.55E+08	2.52E+08	2.52E+08	2.37E+08	2.06E+08	2.14E+08	2.18E+08	2.23E+08	2.03E+08	2.09E+08	2.24E+08
431	23.292	71.1097	Heneicosane	1	C21H44			null	84.2	79.8	86.8	9.51	BLANK	40.16713:	1565126	1433875	1273263	1774612	1188005	1188005	1511119	1645164	1633533	1847113	1708158	1937536	1705856	1305240	1513881	1438164	2051663	1674607
596	26.948	57.07468	Pentacosane	0.278	C25H52			null	83.5	76.2	88	3.61	BLANK	40.16794:	4997343	4800287	6689626	6951357	4997449	4997449	5903701	5617666	6008640	1.07E+07	9875313	3117322	5212189	5176751	4364555	5889034	6500184	6549802
361	21.892	42.09589	Octadecane	0.833	C18H38			null	83.4	78.2	85	3.03	V-C-1	40.19662:	1050225	1357057	1521299	1383741	1109739	1109739	1435884	193309.8	1219434	2048028	2591113	1416008	1233219	1033183	2242203	2580285	1623694	906690.4
22	9.789	71.11179	Citronellene<tetrahydro->	1	C10H22			null	83.1	86.2	81	5.05	QC1	41.06717:	1.03E+07	9316983	8393690	9777285	7988368	7988368	9868707	8656394	9732164	9561891	9724976	7794651	8558218	8803546	8803198	8143024	9326802	1.03E+07
410	22.9	73.06094	Hexanal, dimethyl acetal	0.889	C8H18O2			null	83	100	49	5.8	V-C-1	40.16874:	8006182	9391847	945604.1	766222.4	1680678	1680678	831440.6	297811.4	98879.42	2.45E+07	2.35E+07	2.38E+07	612525.8	1.59E+08	1.65E+08	1.10E+07	1.31E+07	1.55E+07
119	13.707	174.125	Tryptamine	1	C10H11N:	YCKHXOW	NCCc(c1)c	84.9	82.8	78.4	85.3	76.14	BLANK	40.18039:	4.99E+07	5.06E+07	4223827	4889488	4466000	4466000	6229777	5745418	5947465	4983690	4653931	4393634	9623578	9615882	9746526	6021843	6347759	6628492
51	10.915	147.0961	propane-1,3-diol	0.722	C3H8O2	YPFDHNV	OCCCO	34.1	82.7	72.9	95.9	5.69	V-T-3	41.0672:9	1.07E+07	1.02E+07	1.11E+07	1.21E+07	1.08E+07	1.08E+07	1.06E+07	1.38E+07	1.15E+07	9918820	1.10E+07	8182421	9467286	9565463	1.01E+07	8032800	212994.2	8399023
291	19.168	245.0802	Fumaric acid	0.944	C4H4O4	VZCYOOQ	OC(=O)C=	23.5	82.7	79.2	90.3	49.55	S-T-2	45.04796:	270684.5	269884.8	932423	1053192	1170194	1170194	1987785	1820873	2300592	4861596	5730759	4308759	585982.1	671822.8	625879.4	3928045	4633454	4359157
596	26.491	204.1195	Pantothenic acid	1				70.8	82.6	75.7	84.3	19.1	BLANK 1	41.06821:	5632740	4834525	2036075	2575719	2821302	2821302	3270550	3836486	4093247	6013830	6294703	6698520	3047691	2606369	2632372	5510891	6784324	8695595
85	12.195	57.10927	6-phospho-2-dehydro-D-gluconate	0.667				96.8	82	76.3	81.6	11.31	BLANK	40.20246:	1.54E+07	1.98E+07	1.57E+07	1.50E+07	1.43E+07	1.43E+07	0	1.61E+07	1.54E+07	1.86E+07	1.83E+07	1.56E+07	1.38E+07	1.35E+07	1.28E+07	1.34E+07	1.32E+07	1.33E+07
368	22.041	43.0778	Nonadecane	0.167	C19H40			null	81.4	79.7	83.2	6.79	S-T-1	40.20663:	2.32E+07	2.49E+07	1.74E+07	1.82E+07	1.81E+07	1.81E+07	1.77E+07	2.07E+07	2.06E+07	1.96E+07	2.23E+07	2.13E+07	1.93E+07	1.66E+07	2.23E+07	2.14E+07	2.22E+07	2.29E+07
706	28.993	69.07954	Hexadecanol<n->	0.944	C16H34O			null	81.3	85	75.1	8.15	BLANK	40.1854:2	1.20E+07	1.22E+07	9445426	9654818	8745383	8745383	9293482	8620203	9316369	9018375	8810381	8349695	7326462	7915071	7634210	7961013	8526843	8178884
1202	38.764	69.07813	Octadecanol<n->	0.889	C18H38O			null	80.8	75.6	83.5	3.86	BLANK 1	40.18466:	1967374	1981389	2186511	3015236	2089982	2089982	2238145	2312027	1768955	1764466	1737919	1826407	1143191	1311097	1480915	1365354	1814159	1723739
225	17.311	299.0504	2-Phosphoglycerate	0.944	C3H9O6P	AWUCVR(	OCC(O)CC	29.9	80.8	80.7	73.4	60722.29	QC2	40.19307:	2499726	10254.04	3.63E+08	5.72E+08	6.46E+08	6.46E+08	3.65E+08	4.17E+08	4.69E+08	2.16E+09	2.15E+09	1.83E+09	1.51E+08	1.55E+08	1.65E+08	3.04E+09	3.20E+09	3.35E+09
64	11.39	43.08266	Dihydro citronellol	0.667	C10H22O			null	80.2	68.1	91.4	4.87	QC1	40.21425:	1.62E+07	1.53E+07	1.12E+07	1.03E+07	1.02E+07	1.02E+07	1.59E+07	1.18E+07	1.10E+07	9921007	9818601	8011077	1.04E+07	1.07E+07	1.06E+07	9901928	1.03E+07	1.02E+07
583	26.263	175.1931	Cysteamine	0.667	C2H7NS	UFULAYFC	NCCS	15.8	79.6	74.2	81	9.33	S-T-1	41.06573:	583189.3	532410.1	522843.6	17233.98	375759.4	375759.4	682059.9	692676.8	724781.4	779859.2	765211.8	732327.5	497223.4	516756.9	440885.7	634474.9	682913.8	24960.52
634	27.776	85.12577	Hexalactone<gamma->	0.389	C6H10O2			null	79.6	80.8	67.7	6.55	V-C-2	40.18346:	7.25E+07	6.16E+07	7.30E+07	7.40E+07	6.93E+07	6.93E+07	8.91E+07	0	6.41E+07	1.10E+08	1.91E+07	1.01E+08	8.07E+07	2.41E+07	6.62E+07	0	1.82E+07	1.93E+07
44	10.884	73.07725	Hexyl acetate	0.333	C8H16O2			null	79.5	76.9	78.3	4.17	V-C-1	40.20045:	4807861	4952650	6059353	6927695	7425788	7425788	30291.2	7405269	5816145	4084869	6072597	41082.22	4924343	5252030	3257869	4397681	5212519	130079.1
482	24.355	69.07524	Octadecene<1->	0.778	C18H36			null	79	80	80.1	3.86	S-C-2	40.21493:	6377797	6505773	5695728	6040810	5299985	5299985	6132744	6191775	5843396	5854577	5905174	5950602	4091632	4490841	4636256	4816952	5199476	5181063
189	16.895	71.10254	Pentadecane	0.556	C15H32			null	78.6	69.9	81.1	35.3	QC1	40.15556:	1.74E+07	1.79E+07	1.60E+07	1.58E+07	1.78E+07	1.78E+07	2.06E+07	2.06E+07	1.78E+07	2.31E+07	2.26E+07	2.05E+07	1.85E+07	1.59E+07	1.64E+07	1.69E+07	1.72E+07	1.81E+07
585	26.735	69.07056	Nonacosane	1	C29H60			null	78.5	81.1	79.2	4.39	BLANK	41.07352:	4202581	4073350	3341419	2895081	3417375	3417375	3932489	4034704	3488775	4037554	4254064	3740992	3560035	2902198	3360900	4028727	4521076	3724056
1500	45.57	72.00406	Octanol acetate<3->	0.444	C10H20O2			null	78.4	74.8	73	29388.17	V-C-2	40.17009:	79935.3	166588.8	447902.8	1109268	1439604	1439604	4022917	2653258	1011960	488902.5	1959103	1694857	1035819	1390889	1532010	3138358	1566757	1189991
34	10.537	73.07565	Galactitol	1				98.9	78.2	69.7	82.1	28.93	BLANK 1	40.1893:2	9976716	7988461	1.93E+07	2.20E+07	2.53E+07	2.53E+07	9576085	2.23E+07	9738351	2.33E+07	8731979	7179747	6780422	6950174	6961623	9901580	1.07E+07	1.27E+07
864	31.917	45.0437	Ethyl ether	0.611	C4H10O			null	78.1	69.1	80.7	36.04	V-T-1	40.17681:	138262.5	53958.32	8.08E+07	8.55E+07	8.34E+07	8.34E+07	6.62E+07	6.36E+07	6.65E+07	1.49E+08	7873217	1.26E+08	1.40E+07	1.44E+07	1.44E+07	6.12E+07	6.40E+07	6.68E+07
972	34.239	111.1373	Cyclohexadecanolide	0.778	C16H30O2			null	78	68.4	84	3.75	BLANK 1	40.15625:	664834.1	722450.9	744906.6	924579.9	472580.8	472580.8	1008482	866620.6	744338.6	2451685	2925162	4053640	618830	716614.9	559715.6	619063.6	503212.4	547670.7
435	23.352	43.06794	Isobutyl acetate	0.444	C6H12O2			null	78	78.7	66.1	7.63	S-T-3	40.17125:	2201982	796891.4	2524868	2.61E+07	6682116	6682116	2465153	2411298	777062.3	164437.2	136311.4	142455.1	2280367	9738.801	2067489	1391577	1505156	1221463
241	18.257	147.0836	Lavandulyl acetate<tetrahydro->	0.944	C12H24O2			null	77.9	75.1	74.3	33.47	V-C-2	41.07391:	8682513	5776444	5.39E+07	5.79E+07	5.99E+07	5.99E+07	7.09E+07	7.32E+07	7.41E+07	1.44E+08	1.43E+08	1.24E+08	1.74E+07	1.84E+07	2.00E+07	5.85E+07	6.15E+07	6.39E+07
171	16.427	155.2287	Nonane<n->	0.333	C9H20			null	77.8	69.8	88.7	10.27	S-C-1	41.05875:	895183.6	1103942	1061548	935807.8	917354.5	917354.5	444762.8	1073731	1097481	598746.2	1432169	1219495	1117718	849511.3	868935.9	1102129	1082535	456627
191	16.454	147.0937	Urea	0.667	CH4N2O	XSQUKJJJF	NC(N)=O	15.6	77.7	62.8	90.3	9.52	S-T-3	40.18866:	2.71E+07	2.51E+07	358952	1.31E+07	1.37E+07	1.37E+07	2.18E+07	1.93E+07	2.33E+07	5.47E+07	5.27E+07	3.82E+07	1.99E+07	1.91E+07	1.90E+07	2.01E+07	483430.8	2.54E+07
148	15.275	57.0892	Heptadecane	0.389	C17H36			null	77.7	82.7	68.5	3.13	V-T-2	40.16578:	1.60E+07	1.52E+07	1.56E+07	1.52E+07	1.56E+07	1.56E+07	1.79E+07	1.73E+07	1.69E+07	1.87E+07	1.81E+07	1.71E+07	1.51E+07	622175.2	1.44E+07	1.58E+07	1.58E+07	1.75E+07
302	19.43	75.04804	Phosphorylcholine	1				24.1	77.1	68.8	80.2	18.31	QC2	40.18588:	1.70E+07	1.73E+07	1.62E+07	1.41E+07	1.46E+07	1.46E+07	1.81E+07	1.83E+07	1.97E+07	2.51E+07	2.70E+07	2.53E+07	1.63E+07	1.79E+07	1.81E+07	1.57E+07	1.77E+07	1.86E+07
293	19.62	43.08371	Eicosane	0.444	C20H42			null	77	74.9	80.3	4.45	V-C-3	40.1494:1	3245687	2267763	2894501	3097922	1985995	1985995	2255836	3615037	2207199	3414796	3055731	3152696	3664046	1453967	1832048	3133104	3437138	1692400
696	28.802	72.11828	Isopulegyl acetate	0.667	C12H20O2			null	76.8	94.4	49	25.24	S-C-1	40.19697:	287790	1320586	1.36E+07	2735506	2848227	2848227	4027068	3275410	2771371	3064782	3571256	3983237	925809.9	2513900	2380068	4310077	876675	3093342
351	21.625	69.06414	Untriacontane	0.889	C31H64			null	76.3	82.3	69.2	3.11	V-C-2	40.1929:2	4438847	4604586	4531163	4274624	4168853	4168853	5116117	4969200	5099899	5357396	5293996	5345644	4361361	4648117	4146156	4913496	4757755	6068877
1061	38.4	174.131	Cystamine	0.944	C4H12N2!	APQPRKL/	NCCSSCCI	55.9	75.9	64.3	88.7	68.97	V-T-3	45.05381:	75948.66	102447.4	1857571	2540263	3477069	3477069	3537266	3725581	3900416	6368901	6272402	5740635	419552.8	261072.3	262845.2	4959191	5364491	5761961
150	15.548	68.09096	Jasmolactone, extra C<Z->	1	C11H18O2			null	75.7	71.2	76	153.25	QC2	40.18653:	2.25E+07	2.19E+07	2.33E+07	2.34E+07	2.27E+07	2.27E+07	2.61E+07	2.50E+07	2.63E+07	2.66E+07	2.60E+07	2.32E+07	2.31E+07	2.33E+07	2.34E+07	2.56E+07	2.66E+07	2.71E+07
33	10.311	73.07027	Cysteinylglycine	1	C5H10N2(	ZUKPVRW	OC(=O)CN	91.2	75.7	73.9	73.9	22.2	BLANK 1	43.07549:	3.49E+07	3.47E+07	7549320	8341526	5901898	5901898	9812908	7706437	9622272	6778080	6269376	6826967	1.23E+07	1.40E+07	1.42E+07	8725921	8010067	9541772
3	9.139	73.07539	Geranyl-PP	0.889				89.6	75.7	85.5	59.5	42.72	S-T-1	40.19016:	5.68E+07	5.79E+07	4.72E+07	6.54E+07	5.70E+07	5.70E+07	1.15E+08	6.10E+07	6.41E+07	8.99E+07	5.71E+07	4.75E+07	5.39E+07	5.68E+07	3.77E+07	3.94E+07	5.93E+07	6.29E+07
1282	40.72	159.1259	Calamenene<cis->	0.278	C15H22			null	75.5	87	65	4.77	BLANK 1	40.18729:	1.90E+07	1.78E+07	1.63E+07	1.72E+07	1.46E+07	1.46E+07	1.85E+07	2.10E+07	2.07E+07	2.56E+07	2.40E+07	2.10E+07	1.75E+07	1.82E+07	1.87E+07	1.99E+07	2.13E+07	2.27E+07
114	13.425	100.0653	5,6-Dihydrouracil	1	C4H6N2O	OIVLITBTE	O=C(C1)N	23.1	75.4	71.7	68.7	5.95	S-C-2	40.18925:	226198.5	23289.09	564134.5	533575.9	415200.6	415200.6	554796.9	626882.9	312454.4	2124715	5474600	3983528	194476.1	225544.2	262200.6	1239323	574698.6	450953.3
693	28.77	73.03434	Dodecadien-1-al<2Z,6E->	0.944	C12H20O			null	75.3	64.5	79.2	100.08	S-T-1	40.18942:	1.94E+09	1.97E+09	4.63E+09	2.42E+09	3.15E+09	3.15E+09	4.83E+09	2.30E+09	2.35E+09	4.97E+09	4.94E+09	1.74E+09	1.98E+09	1.90E+09	1.92E+09	2.00E+09	2.06E+09	1.88E+09
664	28.311	71.0983	Tricosane	1	C23H48			null	74.8	77.1	74.7	9.38	S-C-2	40.16622:	4838089	5304968	7452480	3462031	3631846	3631846	4207907	4298437	5023841	7689187	6383122	4236775	5693211	4589004	4581491	4547288	3785668	4158194
689	28.762	73.00526	Camphenilone	0.833	C9H14O			null	74.8	79.1	60.2	263.96	V-C-2	40.16314:	1.94E+09	1.97E+09	4.62E+09	3.07E+09	2.35E+09	2.35E+09	4.83E+09	3.41E+09	3.38E+09	4.97E+09	4.94E+09	2.75E+09	4.27E+09	2.57E+09	1.92E+09	2.00E+09	2.99E+09	3.33E+09
54	11.12	73.05946	UDP-N-acetylglucosamine	0.944	C17H27N:	LFTYTUAZ	CC(O)=N[(	45.7	74.8	84.4	52.2	16.16	V-T-2	40.17606:	5.68E+07	6.04E+07	1.28E+08	1.83E+07	3.19E+07	3.19E+07	7.00E+07	9.96E+07	7.59E+07	4.51E+08	5.51E+08	5.28E+08	9.15E+07	7.75E+07	8.72E+07	1.86E+08	2.00E+08	1.96E+08
280	18.901	73.0577	Gluconolactone	0.611	C6H12O7	RGHNJXZE	OC[C@@I	26.1	74.7	78.7	63.1	7.25	V-T-3	44.0661:1	4901067	0	4.95E+07	5.10E+07	5.27E+07	5.27E+07	6.32E+07	6.37E+07	6.23E+07	6.98E+07	7.06E+07	5.54E+07	2.51E+07	2.58E+07	2.55E+07	7.24E+07	7.49E+07	7.72E+07
258	18.709	134.0641	Karahanaenone	0.889	C10H16O			null	74.5	89.3	41.3	7.11	V-C-2	40.175:65	31770.38	41999.53	55102.62	63441.85	85340.33	85340.33	31989.03	38346.17	39945.03	61385.97	41479.99	65682.65	27092.78	6.18E+08	63690.11	9515.846	10554.06	58926.65
37	10.556	43.08191	Tridecane	1	C13H28			null	74.3	63	83	3.33	S-C-2	41.07705:	2516778	3374144	3978525	3839110	4548271	4548271	5617947	3596266	3373851	4614934	4806034	4116013	2243479	3978396	3414531	3608916	3778203	3605601
33	10.502	73.05753	N-Acetyl-D-glucosamine	0.833	C8H15NO	OVRNDRC	OC[C@@I	25	74.1	71.2	73.5	30.26	V-T-3	40.18496:	1.40E+07	1.29E+07	1.92E+07	2.20E+07	6384145	6384145	2.08E+07	2.22E+07	2.23E+07	2.32E+07	3.27E+07	2.34E+07	6823813	1.85E+07	1.82E+07	2.05E+07	2.06E+07	1.90E+07
866	32.975	291.2278	Cysteine	0.833	C3H7NO2	XUJNEKJL	N[C@@H]	99	73.9	87.4	41.5	40.72	V-C-1	41.07666:	12312.06	7396.396	27624.86	37947.79	36005.65	36005.65	23110.84	36542.92	17635.96	33065.25	11030.39	23728.32	4452.58	0	12836.44	16231.45	10404.74	0
196	16.555	179.074	Benzoic acid	0.833	C7H6O2	WPYMKLE	OC(=O)c(c	17.4	73.6	58.2	97.2	7.72	QC2	40.17675:	0	724083.5	506878.4	895324	853395.8	853395.8	1305969	1159790	879464.8	758943.5	1830655	1800792	1555527	709368.1	1414381	788694.8	352459.2	634720.8
79	11.644	116.1149	Phenylephrine	0.889	C9H13NO	SONNWYI	CNC[C@H	68.1	73.6	65.5	86.8	10.21	V-C-3	45.03687:	2201005	2393476	321813.3	629592.4	1038017	1038017	1617236	1860354	1850783	4131784	2484537	1787706	2106587	2195802	2063607	1745574	2212831	1654821
526	25.318	147.0862	Trimethyl benzaldehyde<2,3,6->	1	C10H12O			null	73.6	61.8	78	17.2	S-C-2	40.19051:	7347579	7327325	6815531	6765573	6393139	6393139	8500204	8245625	8100145	8637233	8270803	8180516	7386855	7303289	7583634	8281865	8440606	9062080
951	33.666	57.09142	Tritriacontane	1	C33H68			null	73.6	77.2	76.8	5.3	QC2	40.14482:	4901353	5718715	4761399	4603514	4107278	4107278	5566402	5141362	5188466	4905076	353375.9	1323950	5149444	4943735	5203710	5494183	5874328	5970128
58	11.145	147.0828	oxamic acid	0.222	C2H3NO3	SOWBFZR	NC(=O)C(	55	73.4	78.2	67.4	6.72	V-C-3	40.19287:	6.35E+07	5.46E+07	1.12E+08	8.17E+07	1.08E+08	1.08E+08	1.04E+08	1.08E+08	1.12E+08	5.51E+08	4.97E+08	5.48E+08	5.56E+07	4.35E+07	8.14E+07	1.42E+08	1.79E+08	2.09E+08
914	33.033	43.07652	Heptanone<5-methyl-3->	0.778	C8H16O			null	73.3	91.5	60.2	21.34	V-C-2	40.16465:	1.15E+08	1.13E+08	9.16E+07	9.24E+07	9.67E+07	9.67E+07	1.09E+08	1.12E+08	1.09E+08	1.25E+08	1.18E+08	9041254	9.31E+07	9.28E+07	9.35E+07	1.10E+08	1.14E+08	1.16E+08
68	11.288	221.1058	lactic acid	0.833	C3H6O3	JVTAAEKC	CC(O)C(O]	31.1	73.3	82.2	54.3	13.32	V-T-1	40.1789:3	869340.6	805286.5	1950726	2798467	1746614	1746614	2025020	2292171	1699904	3777216	2645312	2437547	871718.4	847521.8	894036.2	2181580	2602231	2602583
413	22.976	41.06836	Heptan-2-ol<6-methyl-	0.5	C8H18O			null	73.2	61.4	82.7	12.9	S-C-1	40.20737:	4946029	4427358	9102591	9318198	9901968	9901968	1.18E+07	1.16E+07	1.18E+07	1.25E+07	1.27E+07	1.10E+07	6591050	2000185	1219808	1.09E+07	1.18E+07	1.13E+07
866	31.953	43.05616	Penten-3-ol<1->	0.556	C5H10O			null	73.1	71.7	76.9	11.27	S-T-3	40.18434:	3493344	4147139	2.29E+07	2.28E+07	2.10E+07	2.10E+07	2.09E+07	2.05E+07	2.01E+07	1.55E+07	1.41E+07	1.29E+07	3686644	3604609	3743076	2.00E+07	2.05E+07	2.12E+07
92	12.423	147.0918	Succinic acid	0.889	C4H6O4	KDYFGRW	OC(=O)CC	24.2	72.9	83.1	49.9	22.53	V-T-2	40.19677:	1.31E+08	1.34E+08	9.16E+07	7.87E+07	1.01E+08	1.01E+08	8.20E+07	9.67E+07	9.60E+07	9.43E+07	1.02E+08	1.06E+08	1.12E+08	1.12E+08	1.20E+08	1.07E+08	1.17E+08	1.20E+08
34	10.314	73.05958	2-Oxoglutaric acid	0.611	C5H6O5	KPGXRSRI	OC(=O)CC	79.8	72.8	63.3	75.1	8.99	S-C-3	40.18467:	3.49E+07	3.49E+07	7549320	8341526	5933355	5933355	9812908	7706437	9622272	1.19E+07	6664392	9433536	1.30E+07	1.40E+07	1.42E+07	8761357	8039872	9884913
1571	47.314	69.08158	Farnesol <2E, 6Z->	0.889	C15H26O			null	72.5	67.1	79.2	8.36	BLANK	40.18662:	3998871	5051217	6466613	834114.9	4480690	4480690	3.49E+07	3.64E+07	2.97E+07	2.94E+07	3.04E+07	3.10E+07	7851436	8569149	7006741	9466032	9361015	9845160
838	31.285	205.1011	Cedranone<5->	0.556	C15H24O			null	72.5	72.4	75.1	9.13	V-T-3	40.19054:	1607955	1662465	63561.25	941905.3	877791.7	877791.7	1099001	1146266	1267822	1802468	2094076	2018616	1016081	1422334	1136619	1579560	1097562	1636238
552	26.123	73.05536	Encecalin	0.944	C14H16O3			null	72.5	64.4	75	7.85	BLANK 1	40.17484:	1.25E+07	8857188	1.99E+07	2.26E+07	2.33E+07	2.33E+07	2.24E+07	2.24E+07	2.32E+07	5.37E+07	5.89E+07	4.76E+07	9845161	9895598	1.01E+07	3.58E+07	4.01E+07	4.30E+07
615	27.371	279.1833	Musk ketone	1	C14H18N2O5			null	72.5	70.2	70.1	134.91	V-C-3	41.07576:	2550571	2448724	1792696	1826284	2351960	2351960	2624498	3092401	3106549	4435672	4541798	2701062	2145971	2348433	2435546	3550036	4191127	4277269
908	32.47	147.0526	Maltotriose	0.556	C18H32O:	FYGDTML	OCC(O1)C	13.8	72.5	75	59.7	12522.56	QC2	40.27504:	1479256	991723.3	2.43E+09	2.49E+09	2.47E+09	2.47E+09	0	2.43E+09	2.45E+09	3.88E+09	3.84E+09	3.30E+09	8.31E+07	8.60E+07	8.86E+07	2.95E+09	3.07E+09	3.19E+09
1572	47.317	69.08734	Sesquilavandulol<E->	0.944	C15H26O			null	72.3	71.7	76.6	9.94	V-C-2	41.04871:	3093942	2616240	6466613	5200196	4480690	4480690	3.99E+07	3.28E+07	2.97E+07	2.94E+07	3.04E+07	3.10E+07	7851436	6514325	7143373	9466032	9361015	9918340
716	29.146	140.0544	Ethyl menthone<2->	0.722	C12H22O			null	72.3	71.2	72.1	28.44	V-C-1	40.21317:	2198069	1788715	4640565	2394938	2303216	2303216	8968482	3855358	6407111	1.07E+07	9329976	0	3114867	5114314	4407466	1867375	5346410	8002811
207	17.302	299.0623	D-Ribose 5-phosphate	0.889	C5H11O8I	KTVPXOY/	OC(O1)[C(	54.3	72	74.2	58.6	37.57	V-T-3	42.0731:1	14688.79	10254.04	12980.57	5.86E+08	6.47E+08	6.47E+08	3.67E+08	4.19E+08	4.69E+08	2.16E+09	2.16E+09	1.83E+09	1.51E+08	1.56E+08	1.65E+08	3.04E+09	3.20E+09	3.36E+09
74	11.729	147.0759	Senecioic acid	1				38.6	71.9	70.3	65.3	8.6	V-T-3	44.04787:	3066330	2765163	3642661	4715599	4904479	4904479	4033340	5981329	5606611	8726032	1.10E+07	1.10E+07	4489962	4265662	4521975	8371424	8205504	8629636
888	32.312	205.0865	Nootkatinol	1	C15H22O3			null	71.8	73.2	66.7	118.75	BLANK 1	45.07209:	5685285	5910041	7.65E+07	8.73E+07	8.71E+07	8.71E+07	6.87E+07	6.93E+07	7.25E+07	3.19E+08	3.14E+08	2.79E+08	3.20E+07	3.38E+07	3.50E+07	7.37E+07	7.85E+07	8.25E+07
235	18.145	207.1314	Laciniata furanone H	0.389	C15H22O3			null	71.8	70.2	62.6	17.94	S-T-1	41.0684:1	2.19E+07	2.21E+07	6.28E+07	1.51E+07	4.23E+07	4.23E+07	1.86E+07	1.85E+07	1.76E+07	1.78E+07	1.94E+07	6.06E+07	1.74E+07	1.73E+07	1.68E+07	1.61E+07	1.57E+07	1.51E+07
1284	40.768	71.09708	Octen-3-ol butanoate<1->	0.333	C12H22O2			null	71.6	82.7	47.2	5.64	V-C-3	40.17059:	3771945	3484334	4312841	8286369	7655538	7655538	1.05E+07	1.06E+07	1.00E+07	1.28E+07	8413759	7656535	3789649	7112214	3273441	4195308	4122864	4355950
461	23.367	267.0791	4-Hydroxybenzoic acid	0.722	C7H6O3	FJKROLUG	Oc(c1)ccc(	14.8	71.5	66.7	66.8	168.52	V-T-1	43.06947:	15830.53	25150.68	1.49E+07	1.64E+07	1.57E+07	1.57E+07	3.11E+07	3.10E+07	3.26E+07	9872664	9700504	8335503	288211	10826.33	159211.8	4.19E+07	4.48E+07	4.79E+07
475	23.665	156.0868	Glutamine	0.833	C5H10N2(	ZDXPYRJP	NC(=O)CC	19.1	71.5	69.4	62.2	8538.47	S-C-3	40.18658:	0	31123.43	2.06E+08	1.94E+08	2.47E+08	2.47E+08	9.47E+08	1.04E+09	1.15E+09	6.59E+08	6.38E+08	5.39E+08	9543.14	2.35E+07	38887.05	7.54E+08	8.35E+08	8.70E+08
122	13.62	110.0402	glycolic acid	1	C2H4O3	AEMRFAC	OCC(O)=C	14.5	71.4	59.4	89.2	9.32	QC3	40.18431:	2372759	2153085	975084.9	1194847	813380.4	813380.4	1483017	1272564	1844599	1135345	1447511	1086676	1925849	2014201	1973366	1316362	1394924	1592417
43	10.876	112.1572	Isopentyl butanoate	1	C9H18O2			null	71.3	55.8	87.2	9.08	QC1	40.19565:	1780106	1732678	768304.3	1844426	886743.3	886743.3	1730257	918450.5	858315.9	1914066	1882558	1642099	1637633	1422491	1596159	1634592	1679152	1850331
525	25.291	119.05	Tumerol<ar->	0.778	C15H22O			null	71.3	63.1	79.1	6.15	S-T-2	40.16644:	5932585	5994859	5589077	5683449	48189.29	48189.29	35752.15	6523067	6817726	7886878	7608676	7248892	5652918	6028283	5843153	44086.74	7164677	7174185
330	20.713	57.09616	Docosane	0.722	C22H46			null	71.3	66.5	78.1	3.21	V-C-1	40.18549:	3016100	4423636	5664226	6642664	3954991	3954991	7111930	2104950	3883869	2560598	2417582	2168407	2588146	3094314	3454700	0	4024722	4332900
234	18.135	169.2128	Dotriacontane	1	C32H66			null	71.3	66.4	75.1	29.47	S-C-3	40.21466:	3737294	6320827	9683775	3426165	3223139	3223139	6920490	3568688	3669097	3996215	3990511	6528118	3499643	5295317	3490083	3573932	3610268	3695062
746	29.684	73.03237	Linalool<tetrahydro->	0.889	C10H22O			null	71.2	53.2	85.7	13.49	S-C-1	40.17194:	224985.7	186924.6	4.32E+07	4.43E+07	4.38E+07	4.38E+07	1.91E+07	1.97E+07	3.85E+07	1.40E+08	1.35E+08	1.31E+08	7890093	7587851	8020239	4.12E+07	4.46E+07	4.31E+07
143	15.118	71.14721	Phytol	0.167	C20H40O			null	71.2	77.9	56.4	3.14	S-T-2	40.16507:	553644.4	390392.6	311759.8	188548.8	142832.1	142832.1	254696.7	151161.7	188351.1	229175.9	102384.6	187187.8	0	0	174991.9	218866.9	0	49585.51
231	18.101	73.05315	Hexenoic acid<2E->	0.833	C6H10O2			null	71	54.1	81.8	106.74	V-C-3	40.18736:	1.23E+09	1.23E+09	6109562	1.17E+09	1.08E+09	1.08E+09	1.20E+09	1.20E+09	1.22E+09	1.25E+09	1.23E+09	1.10E+09	1.08E+09	1.08E+09	1.11E+09	1.11E+09	1.20E+09	1.21E+09
375	21.705	243.09	DethioBiotin	0.667	C10H18N:	AUTOLBM	OC(=O)CC	27	71	63.5	75.1	55.95	V-T-1	42.08928:	3241829	3556884	12295.76	9652.517	12202	12202	688928.4	958385.7	879193.2	1362670	1627716	3127253	1634699	2307144	2660995	3734478	4074749	4024026
124	13.638	197.1519	tranexamic acid	0.722	C8H15NO	GYDJEQRT	NCC1CCC(	70.3	70.9	50.6	87	5.8	BLANK 1	40.17924:	470119.9	471545.1	497416.3	477977.4	539333.6	539333.6	511313.6	480986.5	499268.6	594958.8	476456.6	544238.1	480711.5	420840	436154.4	427730.4	424338.7	589046.8
716	28.812	216.4012	Raffinose	0.333	C18H32O:	QWIZNVH	OC[C@H]:	16	70.9	67	63.9	41.15	QC3	41.07196:	84780.47	40591.21	176533.8	434798.8	569656.2	569656.2	354529.7	1672223	382363.8	733610.1	391599.2	604244.6	436469.2	58169.41	455751.6	208901.6	354017.3	385295.5
8	9.376	117.1079	Ornithine	1				86.4	70.8	70.6	64.7	9.25	S-C-2	44.08364:	2495503	2514437	4330849	5534079	4497576	4497576	4178011	4033410	4190754	6618002	6388903	5311590	3782552	3361290	3593822	4291309	4165157	4429492
40	10.528	123.0316	pyruvic acid	0.944	C3H4O3	LCTONWC	CC(=O)C(	37.3	70.7	64.6	82	27.45	BLANK	46.015:97	1880104	2500259	1972300	1849981	1703309	1703309	2235349	2003371	1933661	1625187	1891970	1557385	1815920	1784563	1805908	1785108	1824183	1774217
930	33.219	73.0119	Octane<n->	0.722	C8H18			null	70.6	63.9	68.7	111.71	QC2	41.01729:	600360.7	737025.2	9.89E+08	9.60E+08	9.31E+08	9.31E+08	1.08E+09	1.10E+09	1.15E+09	6.62E+08	1.17E+09	0	9944405	3.51E+07	1.15E+07	8.17E+08	7.64E+08	7.60E+08
459	23.815	57.0784	Tetracosane	0.333	C24H50			null	70.6	87.5	54.3	3.77	V-C-3	40.19899:	1.17E+08	1.21E+08	1.25E+08	1.11E+08	1.17E+08	1.17E+08	1.43E+08	1.43E+08	1.29E+08	1.62E+08	1.59E+08	1.45E+08	1.28E+08	1.27E+08	1.15E+08	1.45E+08	1.48E+08	1.52E+08
686	28.706	85.09742	Tagetone<dihydro->	0.444	C10H18O			null	70.5	80.4	69	9.53	V-C-3	40.22885:	1.76E+07	1.99E+07	6.89E+07	1.90E+07	7.09E+07	7.09E+07	9.00E+07	8.75E+07	8.92E+07	2.08E+07	2.25E+07	1.53E+07	1.07E+08	2.61E+07	2.24E+07	8.34E+07	2.02E+07	9.26E+07
111	13.23	174.1382	putrescine	0.833	C4H12N2	KIDHWZJL	NCCCCN	39.2	70.3	61.5	81.6	8.75	BLANK	40.17702:	922990.6	996798.9	8626.191	22039.41	5527.818	5527.818	65169.4	81822.91	227849	260091.3	280177.8	332841.8	365659.5	209217.8	345899.9	373947.8	360215.3	353741.1
91	12.494	73.05812	Leaf alcohol<ethyl acetal->	0.722	C10H20O2			null	70.3	82.1	66	12.52	V-C-1	40.1717:1	1.06E+09	1.21E+09	1.18E+09	1.18E+09	1.17E+09	1.17E+09	1.29E+09	1.26E+09	1.26E+09	1.14E+09	9.70E+08	7.68E+08	9.63E+08	9.76E+08	9.73E+08	7.47E+08	7.74E+08	8.45E+08
107	13.41	174.1096	Aspartate	0.944	C4H5NO4	CKLJMWT	NC(CC([O-	60.3	69.9	75.4	54.1	8.81	S-T-2	40.13517:	190768.9	216462.4	361964.6	393118.6	565729.9	565729.9	538390.4	618323.9	580217.7	761493.4	694062.6	493127.1	340931.2	325987.8	320170.9	593397.9	723860.1	838797.2
203	17.093	147.0937	2-Coumaric acid	0.833	C9H8O3	PMOWTIH	OC(=O)C=	18	69.8	77.7	51.8	16.22	QC1	45.0358:0	1.75E+07	1.66E+07	7364567	5943602	5358330	5358330	1.10E+07	1.62E+07	1.45E+07	1.46E+07	7684892	5442841	322545.3	1.30E+07	1.58E+07	7900928	8424306	1.53E+07
109	13.431	100.0583	Taurine	1	C2H7NO3	XOAAWQ;	NCCS(O)(=	96	69.5	82.4	46.3	6.77	V-C-3	41.06807:	226198.5	75052.2	785366.4	373887.1	426897.5	426897.5	554796.9	626882.9	290993.6	5379825	5714396	4510160	745060.5	225544.2	273748.3	1357976	1749277	1852453
32	10.482	207.0471	2'-Deoxyadenosine	0.889	C10H13N!	OLXZPDW	OC[C@@I	76.5	69.3	64.8	62.6	47.61	V-C-2	40.1655:1	1.41E+07	1.31E+07	1.88E+07	2.28E+07	2.69E+07	2.69E+07	2.17E+07	2.22E+07	2.26E+07	2.35E+07	3.15E+07	1.99E+07	2.40E+07	1.85E+07	1.87E+07	1.99E+07	2.02E+07	1.69E+07
341	21.709	243.0924	Harmaline	0.778	C13H14N:	QJOZJXNK	COc(c3)cc	99.8	69.2	52	83	48.56	V-C-2	44.03472:	3242018	3693056	12295.76	8284.016	490727.4	490727.4	291528.9	579697.8	912787.1	1380112	1627716	3127253	1634699	2332903	2721721	3688504	4268811	4161098
118	13.639	197.1403	Serotonin	0.944	C5H14N2	VHRGRCV	NCCCCCN	70.3	68.4	54.3	82.8	6.3	BLANK 1	40.17924:	470119.9	471545.1	497416.3	477977.4	475585.4	475585.4	511002	480986.5	499268.6	498285.9	476456.6	544238.1	480711.5	420840	436154.4	429615.3	423585.3	474246.1
28	10.312	73.05958	Urocanic acid	0.944	C6H5N2O	MOSFIJXA	OC(=O)C=	22.3	68.4	69.6	59.2	7.3	S-C-3	40.18467:	3.49E+07	3.44E+07	7580742	8341526	5933355	5933355	9812908	7694068	9622272	6767499	6323750	9433536	1.21E+07	1.40E+07	1.42E+07	8761357	8039872	9541772
113	13.502	100.0414	5-Aminolevulinic acid	0.611	C5H9NO3	ZGXJTSGN	NCC(=O)C	72.6	68.2	64.1	71.7	4.83	S-C-1	41.06688:	5.53E+07	5.55E+07	2.76E+07	1.98E+07	2.01E+07	2.01E+07	2.56E+07	2.71E+07	3.13E+07	4.89E+07	5.21E+07	6046076	4.54E+07	4.70E+07	4.50E+07	6.60E+07	6.51E+07	2432720
65	11.287	221.104	N-Formylkynurenine	0.722				91.7	68.1	87.2	31.1	13.81	V-T-1	40.1789:3	869340.6	805286.5	1950726	2798467	1746614	1746614	2025020	2292171	1778719	3777216	5157720	2437547	871718.4	847521.8	894036.2	2181580	2602231	2602583
111	13.484	73.0613	3-Nitro-L-Tyrosine	0.889	C9H11NO	OUYCCCA	N[C@@H]	28.8	67.7	77.3	37.3	77.87	V-T-1	40.16267:	3.51E+08	3.51E+08	6.28E+07	2466430	6271364	6271364	2064417	680926.8	1.73E+08	2.75E+08	2.19E+07	3.82E+08	2.48E+08	2.49E+08	2.54E+08	4.10E+08	4.26E+08	4.30E+08
1030	37.455	174.1232	Trehalose	0.833	C12H22O:	HDTRYLNI	OC[C@@I	15.9	67.2	60.6	62.8	76.41	S-T-3	41.06916:	54727.31	59072.47	2783786	3149083	5741096	5741096	5374433	5952847	6394508	1.25E+07	1.22E+07	1.11E+07	382506.5	474047.5	436009.7	9971309	1.07E+07	1.13E+07
292	19.711	219.1415	Ribose	0.778	C5H10O5	HMFHBZS	OC[C@@I	14.4	66.7	62.1	62.9	4.79	V-T-2	40.19256:	92454.92	70492.57	324058.9	369985.3	357148.5	357148.5	320746.9	320085.7	365169.5	733738.9	719853	646228.1	250477.6	275588.8	249524.5	416770.9	448142.9	457143.9
605	27.536	217.1167	Tyrosine	0.889	C9H11NO	OUYCCCA	OC(=O)C(I	14.5	65.7	45.3	79.1	13.55	V-T-2	40.17235:	7971251	5535431	7641440	8638336	9184377	9184377	8281894	8527771	8707037	1.63E+07	1.57E+07	1.43E+07	6535039	6392858	6479584	3.38E+07	3.90E+07	4.45E+07
232	18.022	75.04422	Stearic acid	0.722	C18H36O:	QIQXTHQI	CCCCCCC(	69.3	65.6	52.4	69.2	8.1	V-C-2	40.18391:	3.86E+08	6737515	5528412	5151795	4255347	4255347	3626190	7391850	6311072	7793854	6841949	7116703	2132905	4706736	5008596	5286304	6218768	6409230
137	14.418	147.0827	Gallic acid	1	C7H6O5	LNTHITQV	OC(=O)c(c	15.6	65.1	66.3	53.4	30.85	S-C-3	42.07726:	2513382	2724540	7023673	7760735	8108657	8108657	9425955	9556424	1.05E+07	6895380	7581409	9346918	6339309	6100725	6429424	6559377	7216443	7098806
166	16.175	147.0929	cis-Aconitic acid	0.444	C6H6O6	GTZCVFV(	OC(=O)CC	15.7	64.9	88.6	31	4.52	S-T-1	40.21589:	0	2.29E+08	1.63E+08	1.81E+08	1.81E+08	1.81E+08	2.06E+08	2.01E+08	0	2.16E+08	0	2.00E+08	2.01E+08	0	0	2.05E+08	2.15E+08	2.24E+08
72	11.642	116.1112	Epinephrine	0.833	C9H13NO	UCTWMZ(	CNC[C@H	65.4	63.8	43.7	82.1	10.44	V-T-2	45.03685:	2201005	2393476	350307.2	629592.4	1038017	1038017	1617236	1860354	1850783	4131784	2484537	1787706	2106587	2195802	2063607	1745574	2263044	1654821
175	16.431	278.0987	Homocystine	0.778	C8H16N2(	ZTVZLYBC	NC(CCSSC	100	63.8	71	49.6	5.63	V-C-2	46.06123:	1.78E+07	1.73E+07	6379504	8144462	8735748	8735748	1.40E+07	1.38E+07	1.44E+07	1.75E+07	1.48E+07	1.22E+07	1.18E+07	1.13E+07	1.07E+07	1.29E+07	1.40E+07	1.77E+07
213	17.426	299.083	D-Ribulose 1,5-diphosphate	0.611	C5H12O1:	YAHZABJC	OC(COP(C	28	63.7	86.4	33.7	8.77	QC1	45.03891:	730609.3	589220.1	3.57E+08	5.99E+08	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	10.616	218.1512	Methylmalonic acid	0.278	C4H6O4	ZIYVHBGG	OC(=O)C((	50.4	63.6	61.4	67.9	3.47	BLANK	45.04496:	260402.1	253348.9	213916.8	280027.4	234481.1	234481.1	548727.2	319633.8	268564.8	266658.4	276850.1	221137.3	227447.5	212147.7	211036.8	240894.3	292445.7	289348.2
94	12.496	73.05856	beta-Alanine	1	C3H7NO2	UCMIRNV	NCCC(O)=	30.7	63.6	59.8	51.2	400.6	S-T-2	40.18689:	1.06E+09	1.08E+09	1.18E+09	1.18E+09	1.17E+09	1.17E+09	1.28E+09	1.26E+09	1.25E+09	1.13E+09	9.71E+08	7.69E+08	9.63E+08	9.76E+08	9.73E+08	7.38E+08	7.75E+08	8.45E+08
206	17.266	147.0825	octadecylglycerol	0.667	C21H44O:	OGBUMN	CCCCCCC(	21	63.5	67.7	60.7	5.65	V-C-1	43.08238:	139356	127259.7	1.33E+08	191242	1.62E+08	1.62E+08	56515.33	191479.2	167877.5	4.06E+08	4.00E+08	3.42E+08	6.27E+07	157672.4	6.90E+07	2.60E+08	2.81E+08	2.93E+08
23	9.872	103.0623	Xylose	0.5	C5H10O5	SRBFZHD(	O[C@@H]	76.1	63.4	63.7	63.3	10.52	V-C-2	45.04617:	1643954	908816.8	2060859	5411937	1458370	1458370	905789.1	1340164	5610861	1364653	5880403	4679470	2568937	1496776	1385103	4971305	2120067	3985086
316	20.596	261.1078	Xylulose	0.944	C5H10O5	LQXVFWR	OCC(O)(O	17.9	63.3	55.2	71.9	13.46	S-T-2	40.22295:	14056.37	17486.61	373118.6	379310	311455.3	311455.3	195700.6	289831.8	4001.08	625680.2	567720.6	549443.7	5828.885	13556.02	8510.371	753192.6	738168.9	803872.3
50	10.941	234.1306	DL-Homocysteine	1	C4H9NO2	FFFHZYDV	SCCC(N)C(	97	63.3	70.3	49.2	202.61	QC2	46.04885:	2694724	2614955	2297728	3041803	2914435	2914435	2530944	2488795	2636792	2326890	2725483	2028377	2616009	2719650	2918138	2206241	2360587	2045045
306	20.407	128.1336	S-Adenosyl-L-methionine	0.944	C15H22N(	MEFKEPW	[O-1]C(=O	73.8	63.1	81.1	36.4	31.05	QC3	40.30941:	1443805	1458116	1591713	1664811	1571300	1571300	1855756	1834539	1887744	1467882	1377170	1228936	1467674	1607472	1444221	1231840	1227893	1251569
164	16.106	147.0826	Quinolinic acid	1	C7H5NO4	GJAWHXH	OC(=O)c(c	36.2	62.8	58.1	54.5	322.33	S-C-1	40.18188:	2.28E+08	2.27E+08	1.59E+08	1.76E+08	1.76E+08	1.76E+08	2.01E+08	1.99E+08	2.06E+08	2.13E+08	2.12E+08	2.00E+08	1.99E+08	2.03E+08	2.08E+08	2.04E+08	2.13E+08	2.21E+08
9	9.379	66.05894	Pyridoxine	0.333	C8H11NO	LXNHXLLT	OCc(c1)c((	51.2	62.5	62.5	52.4	4.88	V-T-3	40.20747:	617905.1	473408.3	822486.5	942220.8	814272.1	814272.1	832347.8	1103045	810890.5	1246248	1365085	870795.9	659136.4	701557.6	591975.6	763275.5	736707	654347.8
75	11.78	73.07889	Melibiose	0.833	C12H22O:	DLRVVLD;	OC[C@@I	39.1	62.5	63.3	50.9	7.8	S-C-2	40.22112:	57830.61	736183.9	4674079	7430295	6340386	6340386	7903780	8861630	7963670	1.20E+07	1.44E+07	8239245	185743.9	64531.95	103559.1	47614.18	149623.8	1.18E+07
179	16.479	154.0681	L-Histidine	1	C6H8N3O	MOSFIJXA	OC(=O)C(I	88.8	62.1	69.1	61.9	102.23	S-C-2	41.04909:	9261395	1.01E+07	8939917	8422524	8175497	8175497	9919483	9719185	9786562	1.03E+07	1.05E+07	9009661	8955255	8852819	8846043	9226567	9881703	1.03E+07
227	17.837	117.0948	palatinitol	0.889	C12H24O:	SERLAGPL	OC[C@@I	47.4	62.1	58	57.4	8.5	S-T-2	41.06858:	298946.6	196597.7	9293198	7856644	7307278	7307278	5875224	4186735	4101958	1.80E+07	1.37E+07	1.58E+07	7987162	7924658	8212036	4434904	4806230	4831567
156	15.575	281.069	Catechin	0.944	Like tag cc	Like tag cc	Like tag cc	69.1	61.8	62.4	58.5	25.63	V-C-3	44.04878:	2473027	2388557	2444807	3775488	4664485	4664485	41938.05	3361019	3552113	3643312	5141909	3296466	3736396	3244026	3347420	3733856	3742035	2966064
7	9.328	235.1146	Malonic acid	1	C3H4O4	OFOBLEOI	OC(=O)CC	98.5	61.6	60	70.7	8.19	S-T-3	44.07641:	131363	111708.1	102664.2	140707.9	160566.7	160566.7	135587.6	175124.5	167148.4	155270.7	215540.4	127895.5	142643.4	131340.4	146440.5	186735.5	213473.7	176107
26	10.277	162.1114	Ureidopropionate	0.833	C4H8N2O	JSJWCHRY	OC(=O)CC	44.5	61.1	72.8	44.7	37.28	V-T-3	40.18648:	5043169	5010046	14074.06	71966.45	31992.61	31992.61	38040.65	409045.1	454374.6	359533.3	490882.3	218062.2	1151150	1153278	1181289	265933.8	312824.7	397184.3
176	16.434	73.06393	DL-Homocystine	1	C8H16N2(	ZTVZLYBC	OC(=O)C(I	83.3	61	62	47.9	14.18	QC2	40.17695:	6.24E+07	6.04E+07	2.90E+07	3.31E+07	3.50E+07	3.50E+07	5.12E+07	5.06E+07	5.50E+07	7.21E+07	6.91E+07	6.00E+07	4.30E+07	4.13E+07	4.11E+07	4.99E+07	5.23E+07	6.42E+07
123	13.843	86.06218	Spermidine	1	C8H16N2(	VEYYWZR'	NCCCCC(N	76.6	60.9	73.2	26.9	178.78	BLANK 1	41.06353:	0	8.47E+07	7.34E+07	7.54E+07	7.85E+07	7.85E+07	8.53E+07	8.88E+07	8.82E+07	8.98E+07	9.35E+07	8.36E+07	8.78E+07	8.55E+07	8.78E+07	8.56E+07	9.08E+07	9.39E+07
905	33.802	57.08467	Nonadecanoic acid methyl ester	1	C20H40O:	BDXAHSJL	CCCCCCC(	28.2	60.6	70.2	36.1	5.49	BLANK 1	40.19583:	1.16E+07	1.15E+07	1.20E+07	1.23E+07	1.08E+07	1.08E+07	1.36E+07	1.24E+07	1.25E+07	1.97E+07	3.00E+07	8.94E+07	1.04E+07	1.05E+07	1.17E+07	1.30E+07	1.37E+07	1.48E+07
88	12.268	73.06743	Maltose	0.778	C12H22O:	GUBGYTA	OCC(O1)C	24	60.5	73.6	35.4	3.97	BLANK	46.05747:	1755794	1821209	101475.8	39100.14	1955538	1955538	36682.14	274726.6	1275378	3097925	2264346	1898244	905767.6	622831.7	1886090	1081210	1843611	2033646
17	9.657	281.0737	3-Hydroxyphenylacetic acid	1	C8H8O3	FVMDYYG	OC(=O)Cc	57.4	60.2	74.8	33.9	10.99	V-C-2	48.05137:	734116.9	861243.1	530507.4	751098.8	644414.4	644414.4	767194.9	783449.2	931841.2	828259.6	910895.6	572950.8	997483	852868.1	799263.4	851705.6	814302.7	844089.9



Alignment	Quant ma	Metabolite nan	MSFIDNER ID	Average Rt(mir	Fill %	S/N averag	Spectrum	EI spectrur	BLANK	BLANK_1	QC1	QC2	QC3	QC4	S-C-1	S-C-2	S-C-3	S-T-1	S-T-2	S-T-3	V-C-1	V-C-2	V-C-3	V-T-1	V-T-2	V-T-3
2	77.0491	Unknown	6''-O-p-Coumaroyltrifolin	9.119	0.833	467.01	BLANK	40.18069:	0.00417	0.00422	0.00146	0.00205	0.00192	0.00192	0.00247	0.00183	0.00199	0.00167	0.00146	0.00144	0.00291	0.00244	0.00248	0.00178	0.00176	0.00163
38	207.05	Unknown	Nothramicin	10.484	1	64.96	BLANK	44.07312:	0.00077	0.00087	0.00025	0.00029	0.00035	0.00035	0.00031	0.00031	0.00031	0.00019	0.00025	0.00019	0.00074	0.00051	0.00051	0.00026	0.00025	0.00021
32	162.111	Unknown	Landomycin D	10.277	0.833	37.23	BLANK	41.07087:	0.00016	0.0002	2.7E-07	6.1E-07	4E-07	4E-07	3.5E-06	4.2E-06	4.6E-06	2.2E-06	2.3E-06	1.7E-06	2.5E-05	2.3E-05	2.4E-05	2.1E-06	2.9E-06	3.5E-06
54	207.051	Unknown	Naringin	11.015	0.944	34.1	BLANK	45.03836:	0.00045	0.0006	0.00021	0.00027	0.00026	0.00026	0.00021	0.00021	0.00018	0.00011	0.00012	0.0001	0.00038	0.0003	0.0003	0.00016	0.00015	0.00012
31	126.066	Unknown	CE(14:0)	10.245	1	31.99	BLANK	40.20779:	0.00015	0.00017	3.5E-05	3.7E-05	3.4E-05	3.4E-05	4.2E-05	4E-05	3.6E-05	2.4E-05	2.2E-05	2E-05	7.2E-05	6.4E-05	6.6E-05	3.2E-05	3.2E-05	3E-05
56	191.117	Unknown	Cyl-2	11.227	0.944	24.21	BLANK	45.03757:	0.00042	0.00032	0.0004	0.00046	0.00038	0.00038	0.00027	0.00032	0.0003	0.00111	0.00114	0.00112	0.00035	0.00035	0.00036	0.00044	0.00044	0.00046
828	174.05	Unknown	5'-hydroxystreptomycin	30.842	0.611	17.89	BLANK	46.08522:	5.9E-06	5.4E-06	6.4E-07	5E-05	3.3E-06	3.3E-06	5.5E-05	3.2E-07	3.5E-06	2.5E-06	2.7E-06	3.7E-05	6.9E-06	3.2E-06	2.4E-06	1.8E-06	5.3E-05	1.8E-06
824	41.0731	Unknown	Ouabain	30.789	1	17.62	BLANK	40.19583:	0.00041	0.00051	0.00011	0.00011	0.00011	0.00011	0.00016	0.00016	0.00016	8.7E-06	1.1E-05	0.00014	3.3E-05	0.00024	0.00026	0.00014	0.00015	0.00017
829	292.146	Unknown	Eriocitrin	30.858	0.5	15.88	QC1	40.19519:	3.8E-07	9.9E-07	3.7E-06	4.7E-06	4.4E-06	4.4E-06	2.7E-06	2.2E-06	2.9E-06	1E-05	9.5E-06	1E-05	1E-06	8.5E-07	1.2E-06	5.5E-06	5.5E-06	6E-06
838	71.1076	Unknown	DG(16:0/18:0/0:0)	31.027	0.833	13.61	QC1	40.19006:	9.6E-05	0.00012	1.3E-05	1.2E-05	3.8E-06	3.8E-06	2.8E-05	2.7E-05	2.8E-05	5.1E-06	9.2E-06	1.1E-05	2.9E-05	2E-05	2.5E-05	2.4E-05	1.1E-05	1.2E-05
101	145.137	Unknown	1-[(2S,3R)-2-[(1,3-benzodioxol-5-ylmethyl(meth	12.523	0.667	13.44	BLANK	93.03789:	4.1E-05	5.6E-05	5.5E-06	8.1E-06	1.8E-05	1.8E-05	2E-05	4.7E-05	1.9E-05	8.3E-06	1.5E-05	2E-05	2.8E-05	5.9E-05	3.4E-05	2.9E-05	8E-07	1.4E-05
1	58.0475	Unknown	Nummularine B	9.078	0.5	12.3	BLANK	40.18113:	0.00065	0.00022	9.6E-05	0.0001	0.0001	0.0001	0.0002	0.00011	7.1E-06	0.0001	9.6E-05	1.1E-05	0.00034	0.00026	0.00029	7.6E-06	0.00017	0.00013
18	281.074	Unknown	Crassostreaxanthin A	9.657	1	10.95	BLANK	40.17297:	4.1E-05	4.4E-05	1.5E-05	2.3E-05	1.9E-05	1.9E-05	1.9E-05	2.1E-05	2.2E-05	1.7E-05	1.7E-05	1.5E-05	3.9E-05	3.3E-05	3.1E-05	2.1E-05	1.9E-05	1.9E-05
108	155.054	Unknown	Deserpidine	12.913	1	9.57	BLANK	41.04411:	3.4E-05	3.6E-05	3.6E-06	3.9E-06	4.3E-06	4.3E-06	5.6E-06	5.5E-06	6.4E-06	4.1E-06	4.9E-06	4.1E-06	1.7E-05	1.3E-05	1.5E-05	9.4E-06	8.9E-06	8.1E-06
818	57.0777	Unknown	dihydro-alpha-ergocryptine	30.665	0.778	9.38	BLANK_1	41.07564:	0.00045	0.00054	0.00015	0.00014	0.00013	0.00013	0.00018	0.00018	0.00016	0.00018	0.00017	0.00018	0.00027	0.00024	0.00025	0.00022	0.00023	0.00023
27	58.065	Unknown	N-[(3R,9S,10R)-12-[(2R)-1-hydroxypropan-2-yl]-	9.832	0.833	8.51	BLANK	42.09188:	5.1E-05	3.4E-05	0	1.2E-05	1.1E-05	1.1E-05	1.2E-05	1.7E-05	1.2E-05	9.4E-06	5E-06	1.5E-05	2.2E-05	1.8E-05	3.2E-05	1.2E-05	1.7E-05	6.1E-06
99	245.095	Unknown	D-Urobilinogen	12.987	1	8.12	BLANK	40.17538:	3.3E-06	1.7E-06	5.8E-06	6.3E-06	6.1E-06	6.1E-06	5E-06	3.6E-06	4.2E-06	7.6E-06	8E-06	6.8E-06	4.4E-06	4.2E-06	3.8E-06	9.7E-06	6.5E-06	7.7E-06
830	58.0433	Unknown	Geniposide pentaacetate	31.173	0.944	7.79	BLANK	47.01701:	8.7E-06	4.3E-06	7.1E-06	5.2E-06	3.7E-06	3.7E-06	4E-06	3.4E-06	3.9E-06	5.8E-06	5.7E-06	1.3E-05	8.2E-06	6.6E-06	5.6E-06	3.3E-06	3.5E-06	4.3E-06
24	58.065	Unknown	8-Hydroxyergotamine	9.829	0.889	7.77	BLANK	42.09188:	5.4E-05	3E-05	0	2.9E-05	2.7E-05	2.7E-05	2.1E-05	3.2E-05	2.3E-05	2.4E-05	1.6E-05	4.2E-05	3.2E-05	2.7E-05	4.7E-05	2E-05	3.4E-05	1.2E-05
88	71.1008	Unknown	Irinotecan	12.004	0.944	6.35	BLANK_1	41.07904:	0.0029	0.00348	0.00062	0.00061	0.00059	0.00059	0.00074	0.00072	0.00068	0.00051	0.00046	0.00046	0.00135	0.00117	0.00119	0.00061	0.00063	0.00064
51	73.0268	Unknown	Amikacin	11.136	0.167	5.79	S-T-2	49.05967:	0.0031	0.00286	0.00285	0.00249	0.00279	0.00279	0.00236	0.00261	0.0025	0.00962	0.00574	0.01153	0.00307	0.00275	0.00272	0.00387	0.00386	0.00384
25	43.0897	Unknown	DG(14:1(9Z)/20:3(8Z,11Z,14Z)/0:0)	9.787	1	5.57	BLANK	40.19815:	0.00027	0.00037	7.7E-05	7E-05	6.3E-05	6.3E-05	8.6E-05	7.9E-05	7.7E-05	4.9E-05	4.9E-05	4.8E-05	0.00016	0.00014	0.00015	6.7E-05	7E-05	6.5E-05
46	73.0527	Unknown	Zizyphine F	10.92	0.722	5.4	BLANK	45.03973:	0.00019	0.00019	0.00012	0.00015	0.00014	0.00014	0.0001	0.00013	0.0001	7.5E-05	8.5E-05	8.5E-05	0.00014	0.00014	0.00013	1.4E-06	0.00025	7.2E-05
82	127.112	Unknown	L-Urobilinogen	11.803	0.556	5.11	BLANK_1	47.01791:	0.0001	0.00012	2.6E-05	2.4E-05	1.5E-06	1.5E-06	1.4E-06	2.6E-05	2.4E-05	1.8E-05	1.9E-05	1.8E-05	4.9E-05	4E-05	4E-05	2.5E-05	2.2E-05	2.5E-05
9	147.096	Unknown	Jurubine	9.327	0.556	4.9	BLANK	40.19248:	4.6E-05	4.2E-05	1.1E-05	9.3E-06	2.9E-05	2.9E-05	1.4E-05	2.9E-05	1.5E-05	2.5E-05	2.6E-05	9.3E-06	2.6E-05	4.8E-05	2.4E-05	1.5E-05	1.7E-05	1.4E-05
5	127.047	Unknown	10-Acetoxyoleuropein	9.199	0.389	4.87	BLANK	40.19949:	2.4E-05	2.7E-05	7E-06	6.7E-06	4.4E-06	4.4E-06	5.6E-06	4.2E-06	4.9E-06	3.9E-06	2.9E-06	4.4E-06	6E-06	7.2E-06	1E-05	2.8E-06	3.9E-06	3.8E-06
94	188.161	Unknown	Quercetin 3-lathyroside	12.252	1	4.73	BLANK	46.05409:	1.7E-05	7E-06	3.8E-06	8.9E-07	1.5E-06	1.5E-06	4.2E-06	4.6E-06	9.4E-07	2.8E-06	2.6E-06	6.3E-07	8.5E-06	8.1E-06	7.6E-06	9.3E-07	3.8E-06	4.4E-06
70	52.0739	Unknown	cis-Livariamicin IV	11.341	0.278	4.47	BLANK	51.07204:	3E-05	5.7E-05	1.3E-05	3.2E-05	2.8E-06	2.8E-06	2.8E-05	2.9E-05	1.1E-05	5.6E-05	1.1E-05	2.1E-06	1.5E-05	1.2E-05	2E-05	4.2E-06	6.3E-06	8.7E-06
10	79.0619	Unknown	Ergostine	9.336	0.111	4.31	BLANK_1	40.17038:	5.4E-05	7E-05	1.6E-05	1.4E-05	1.3E-05	1.3E-05	7.1E-06	1.4E-05	6.3E-06	1E-05	9.4E-06	6.8E-06	2E-05	2.1E-05	1.2E-05	1.1E-05	1.4E-05	8.1E-06
11	79.0728	Unknown	Astaxanthin	9.366	0.389	4.15	BLANK	41.08023:	3E-05	4.5E-05	1.2E-05	8.9E-06	1.6E-05	1.6E-05	1.3E-05	1.4E-05	1.3E-05	1.1E-05	7E-06	6.8E-06	2E-05	2E-05	2.2E-05	1.1E-05	1.6E-05	1.2E-05
55	173.167	Unknown	Cevadine	11.094	0.833	4.13	BLANK	40.16422:	6.3E-06	1E-05	1.8E-06	1.9E-06	1.8E-06	1.8E-06	1.9E-06	1.8E-06	2.2E-06	1.5E-06	1.9E-06	1.5E-06	3.9E-06	3.9E-06	3.2E-06	1.9E-06	2E-06	2E-06
16	58.0707	Unknown	L-Urobilin	9.489	0.5	4.05	BLANK	46.07729:	4.4E-05	7.9E-05	2.8E-05	1.8E-05	9.8E-06	9.8E-06	1.2E-05	1.3E-05	7.9E-06	7.9E-06	6.4E-06	1.3E-05	3.4E-05	2.6E-05	4E-05	8.5E-06	1.5E-05	9.5E-06
22	248.99	Unknown	Mytiloxanthin	9.671	0.222	3.96	BLANK	41.08401:	5.3E-06	5.2E-06	9.6E-07	1E-06	1.3E-06	1.3E-06	1.3E-06	1.5E-06	1.4E-06	1.1E-06	7.7E-07	5.1E-07	3.4E-06	2.5E-07	2.5E-06	1.5E-06	1.3E-06	1.1E-06
14	43.0949	Unknown	Cer(d18:0/20:0)	9.419	0.778	3.79	BLANK	40.21151:	0.00026	0.00033	6.4E-05	5.3E-05	5.2E-05	5.2E-05	5.9E-05	5E-05	5.3E-05	3.1E-05	3E-05	2.9E-05	9.8E-05	7.8E-05	8.6E-05	3.2E-05	3.3E-05	3.1E-05
141	52.0786	Unknown	Idoxanthin	14.245	0.333	3.66	BLANK	48.08081:	3.2E-05	3.9E-05	1.1E-05	1E-05	8.4E-06	8.4E-06	1.3E-05	5.6E-06	7.5E-06	5.5E-06	4.6E-06	6.7E-06	1.9E-05	1.5E-05	1.6E-05	7E-06	8E-06	9.1E-06
60	148.097	Unknown	Pipercyclobutanamide B	11.179	0.833	3.58	BLANK	41.08801:	0.00033	0.00034	0.00012	0.00013	0.00013	0.00013	0.00016	0.00014	0.00012	0.00053	0.00033	0.00037	0.00021	0.00021	0.00024	0.00019	0.00019	0.0002
20	79.0573	Unknown	Azinomycin A;Carzinophilin B	9.611	0.111	3.34	BLANK	44.05146:	6E-05	5.7E-05	1.8E-05	1.8E-05	1.6E-05	1.6E-05	1.8E-05	1.1E-05	1.8E-05	9.2E-06	8E-06	9.1E-06	3.3E-05	2.4E-05	2.5E-05	1.3E-05	1.7E-05	1.1E-05
6	111.162	Unknown	Isowertin 2''-rhamnoside	9.264	0.667	3.33	BLANK	40.1954:2	2.9E-05	3.4E-05	7.6E-06	6.4E-06	6E-06	6E-06	8.7E-06	7.2E-06	7.4E-06	5.8E-06	4.8E-06	3.5E-06	1.3E-05	1.3E-05	1.1E-05	5.2E-06	5.4E-06	6E-06
4	79.0737	Unknown	(+)-Discodermolide	9.293	0.056	3.31	V-C-3	41.07309:	5.8E-05	5.4E-05	3.8E-05	2.5E-05	3.5E-05	3.5E-05	2.1E-05	2.3E-05	1E-05	1.3E-05	1.1E-05	1.7E-05	2.1E-05	3.1E-05	1.5E-05	1.5E-05	2.6E-05	2.4E-05
7	41.0799	Unknown	[(19S)-19-ethyl-19-hydroxy-14,18-dioxo-8-prop-	9.268	0.111	3.2	V-C-2	40.20058:	2.6E-05	3.9E-05	8.8E-06	8.3E-06	7.7E-06	7.7E-06	1.1E-05	9E-06	1.1E-05	7.4E-06	6.1E-06	2.4E-06	2.5E-05	1.9E-05	1.3E-05	1E-05	7.7E-06	7E-06
0	281.08	Unknown	DG(16:0/18:1(9Z)/0:0)	9.045	0.611	3.1	BLANK_1	52.08683:	1E-05	1.4E-05	5E-06	4.7E-06	4.1E-06	4.1E-06	5E-06	4.5E-06	3.5E-06	1.9E-06	1.9E-06	1.4E-06	4.9E-06	4.4E-06	6E-06	2.5E-06	3.1E-06	1.9E-06

	S-C-1	S-C-2	S-C-3	S-T-1	S-T-2	S-T-3	V-C-1	V-C-2	V-C-3	V-T-1	V-T-2	V-T-3
Label	SC	SC	SC	ST	ST	ST	VC	VC	VC	VT	VT	VT
Manool ox	0.294	0.25736	0.31746	1.19237	2.21073	4.25848	0.35804	0.32529	0.32616	0.27385	0.31118	0.32419
Hexacosar	1.18887	1.1995	1.12921	1.10586	1.13878	1.17371	1.20412	1.1909	1.20878	1.17582	1.18744	1.16479
Manool ox	0.5888	0.88456	0.83961	0.6063	0.8804	1.44491	0.6261	0.63466	0	0.76572	0.80846	0.3264
Decane<n-	1.01564	1.02045	0.97234	0.9267	0.99561	1.13133	1.03459	1.05383	1.08709	0.94714	1.01131	0.90618
2-Hydroxy	1.54756	1.70207	1.61045	1.64453	1.79543	1.77441	1.5789	1.55573	1.55138	1.87602	1.89871	1.77478
Cytidine	1.91686	1.97202	2.06128	1.71969	2.0927	2.11225	2.42725	2.4256	2.44205	2.27129	2.2595	2.08077
Tetradecer	1.47815	1.49982	1.46458	1.39493	1.45043	1.43521	1.4721	1.45795	1.47232	1.38834	1.39393	1.34435
Hexadecer	1.19167	1.22597	1.18828	1.24781	1.29067	1.33006	1.2464	1.23309	1.2262	1.20809	1.22139	1.19063
Hexadecar	1.69275	1.7626	1.7232	0	1.93769	1.89952	1.74363	1.73491	1.73654	1.87957	1.89414	1.82241
Hydroxyla	2.13273	2.32376	2.24826	2.05182	2.22178	2.34597	2.60982	2.60436	2.64915	2.37404	2.4469	2.33879
Cedroxyde	1.09111	1.09795	1.07706	1.41424	0	3.66506	0	0	0	0.7696	1.17865	1.11804
Sorbate	2.14834	2.24159	2.18613	2.02353	2.15762	2.15899	2.40458	2.37724	2.38985	2.21835	2.23513	2.16428
Undecane	0.63102	0.69376	0.71269	0.59866	0.65265	0.59457	0.71159	0.68301	0.66185	0.57908	0.6097	0.55347
Heptacosa	1.12977	1.15907	1.16244	1.04552	1.07373	0	1.19307	1.15368	1.16478	1.09849	1.13256	1.09462
Hexadienc	0.90621	0.98542	0.95841	7.07595	7.43175	5.70648	1.286	1.2976	1.35619	0.46746	0.42556	0.48071
Gly-Gly	3.12876	3.21042	3.10679	2.8845	2.95241	2.90896	3.2385	3.2326	3.25697	2.93894	2.95222	2.88774
Palmitolei	1.09111	1.14274	1.0939	1.03673	1.07997	1.14376	1.16168	1.16863	1.16858	1.11883	1.11961	1.09162
Octacosan	0.86391	0.83268	0.77315	0.77059	0.76474	0.77955	0.74336	0.78269	0.81192	0.84756	0.84027	0.76797
Eicosene<:	1.04746	1.08244	1.05601	1.03673	1.10721	1.09564	0.99795	1.0525	1.10184	1.07736	1.08934	1.05427
Hexadiena	7.00961	8.21343	7.38887	9.44251	9.68269	8.15223	6.41074	6.24261	6.33374	4.85298	9.24101	8.92366
Asparagin	1.43701	1.43976	1.3988	1.35115	1.39871	1.41139	1.51939	1.51408	1.45301	1.4012	1.40441	1.32217
N-Alpha-A	3.12876	3.21042	3.10679	2.8845	2.95241	2.91844	3.2385	3.2326	3.25697	2.93894	2.95222	2.88774
Heneicosa	0.56471	0.59766	0.57928	0.56032	0.5703	0.61604	0.64692	0.58699	0.6167	0.56445	0.63212	0.56465
Pentacosa	0.88941	0.89998	0.8942	1.00631	1.02355	0.72186	0.93874	0.92915	0.87773	0.90304	0.92841	0.88965
Octadecar	0.55518	0.29273	0.52549	0.57994	0.65527	0.5549	0.58061	0.54299	0.70297	0.68588	0.5847	0.46022
Citronellyl	1.05556	1.03951	1.05014	0.96929	1.01833	0.97978	1.10747	1.10905	1.10899	1.00605	1.04716	1.03456
Hexanal, d	0.46274	0.33809	0.22745	1.32635	1.36652	1.42141	0.45981	2.90981	2.94583	1.11213	1.17271	1.18555
Tryptamin	0.90549	0.90675	0.89116	0.78005	0.79653	0.80935	1.15164	1.14217	1.14726	0.90978	0.9211	0.8932
propane-1	1.08101	1.21434	1.11022	0.9812	1.06102	0.99576	1.14537	1.14017	1.16097	1.00149	0.29709	0.96654
Fumaric ac	0.61875	0.61822	0.64932	0.77362	0.85375	0.8041	0.45307	0.47042	0.45942	0.78901	0.82934	0.77674
Pantothen	0.73047	0.79255	0.78681	0.83046	0.88088	0.93151	0.78499	0.73917	0.74159	0.88328	0.94175	0.97778
6-phosphc	0	1.27837	1.22373	1.20997	1.25722	1.23472	1.29867	1.27892	1.25636	1.18776	1.17569	1.12657
Nonadeca	1.28249	1.39008	1.34834	1.23128	1.34285	1.36979	1.4523	1.37015	1.51175	1.38834	1.39814	1.35027
Hexadecar	1.03464	1.03806	1.03497	0.95056	0.98535	1.0025	1.05157	1.07041	1.05755	0.9985	1.01632	0.95802
Octadecar	0.64371	0.66944	0.59486	0.55183	0.57359	0.60403	0.56612	0.58787	0.61219	0.55476	0.60672	0.57012
2-Phosphc	3.51689	3.78234	3.82152	5.90321	6.15753	6.04428	2.88313	2.88521	2.94583	7.24409	7.33078	7.11471
Dihydro ci	1.23745	1.15259	1.0939	0.98127	1.02159	0.98876	1.18182	1.18357	1.17982	1.07382	1.08238	1.0312
Cysteamin	0.43318	0.44795	0.44182	0.42035	0.43637	0.44541	0.42893	0.43102	0.40878	0.4297	0.43808	0.13896
Hexalactor	2.19796	0	1.96848	2.1881	1.27528	2.30127	2.33972	1.55145	2.17269	0	1.30855	1.27544
Hexyl acet	0.1534	0.9868	0.88455	0.73001	0.8704	0.17051	0.92113	0.93363	0.7962	0.81928	0.86255	0.24092
Octadecen	0.90077	0.92965	0.88593	0.82307	0.86233	0.89546	0.86597	0.88615	0.89557	0.84453	0.86183	0.82278
Pentadeca	1.34902	1.38784	1.28426	1.30059	1.34885	1.35242	1.43195	1.35062	1.36456	1.28328	1.28413	1.24844
Nonacosar	0.77675	0.80597	0.746	0.72718	0.77303	0.76711	0.82672	0.76614	0.80451	0.7957	0.82258	0.73702
Octanol ac	0.78266	0.70088	0.49382	0.35976	0.59696	0.58917	0.54781	0.59956	0.61916	0.73214	0.57779	0.50388
Galactitol	1.04502	1.42501	1.05036	1.30433	0.99304	0.9033	1.02476	1.02502	1.02553	1.07381	1.09621	1.10937
Ethyl ethe	1.99074	2.02085	1.99275	2.42102	0.9491	2.47733	1.30491	1.30673	1.30667	1.97065	1.98988	1.92931
Cyclohexa	0.4935	0.48268	0.44576	0.61578	0.6823	0.78791	0.46138	0.48065	0.44262	0.42619	0.39569	0.38903
Isobutyl ac	0.66478	0.67889	0.4522	0.25019	0.24553	0.25808	0.71265	0.1147	0.68422	0.55829	0.57011	0.50828
Lavanduly	2.03678	2.1178	2.06594	2.39363	2.49482	2.46416	1.40299	1.41799	1.45788	1.94123	1.96362	1.90097
Nonane<n	0.37564	0.51842	0.50735	0.3849	0.53776	0.52794	0.56189	0.50869	0.51252	0.51654	0.5108	0.36615
Urea	1.37472	1.358	1.40485	1.73354	1.78867	1.66424	1.4672	1.43574	1.43317	1.35964	0.39043	1.39772
Heptadeca	1.2873	1.30938	1.26224	1.21213	1.25262	1.27309	1.33823	0.45853	1.30667	1.25481	1.2483	1.23449
Phosphory	1.29207	1.33413	1.32842	1.33709	1.43125	1.45067	1.37278	1.40502	1.41017	1.25216	1.29646	1.25983
Eicosane	0.6454	0.777	0.64041	0.68769	0.69231	0.72458	0.83469	0.60849	0.65719	0.73173	0.75076	0.56664
Isopulegyl	0.78293	0.75186	0.69089	0.66334	0.72923	0.78332	0.52769	0.73032	0.71709	0.81381	0.47612	0.69282
Untriacont	0.84796	0.86393	0.84664	0.79908	0.83149	0.86403	0.8846	0.89638	0.86283	0.85014	0.8367	0.86732
Cystamine	0.74981	0.78484	0.77425	0.8465	0.87984	0.88481	0.40532	0.34328	0.34404	0.85277	0.87085	0.85244
Jasmolacto	1.45974	1.48034	1.46273	1.36321	1.41336	1.40937	1.54197	1.53409	1.53621	1.4738	1.485	1.42823
Cysteinylg	1.05356	1	1.04617	0.86425	0.8797	0.93743	1.2498	1.29452	1.30059	1.02951	0.99536	1.00852
Geranyl-Pl	2.3931	1.99293	1.96848	2.04577	1.83713	1.78961	2.0452	2.06466	1.80091	1.7016	1.93993	1.891
Calamenei	1.30152	1.39676	1.35052	1.34591	1.37614	1.36333	1.40567	1.41283	1.42558	1.35512	1.37899	1.34633
5,6-Dihydr	0.40436	0.43329	0.33376	0.58709	0.84084	0.78334	0.31369	0.32695	0.34376	0.53714	0.4136	0.36463
Dodecadie	8.31847	6.68279	6.53935	7.79332	8.12524	5.94353	6.79872	6.65249	6.67543	6.30042	6.32979	5.86852
Tricosane	0.79448	0.82316	0.84241	0.90136	0.88499	0.7996	0.96677	0.89256	0.89203	0.82847	0.77532	0.76462
Campheni	8.31847	7.62021	7.3816	7.79332	8.12524	6.92317	8.78378	7.35717	6.67543	6.30042	7.16678	7.10052
UDP-N-acc	2.02812	2.34676	2.08253	3.5021	3.91121	3.99398	2.43975	2.28999	2.38169	2.8545	2.90922	2.76203
Gluconola	1.9602	2.02191	1.94988	1.88028	1.9718	1.88378	1.58525	1.58711	1.58086	2.0842	2.09698	2.02464
Karahanae	0.15622	0.17072	0.16814	0.18015	0.16515	0.19938	0.16261	4.57505	0.21449	0.10597	0.10912	0.18503
Tridecane	0.87482	0.77565	0.73771	0.76031	0.80511	0.79193	0.70878	0.85108	0.80877	0.76704	0.77481	0.72912
N-Acetyl-D	1.35337	1.42287	1.38446	1.30247	1.52561	1.4134	1.02695	1.42055	1.41276	1.3686	1.36371	1.2688
Cysteine	0.14017	0.168	0.12803	0.14658	0.1062	0.142	0.08907	0	0.12576	0.12661	0.1086	0
Benzoic ac	0.5379	0.53191	0.47125	0.41656	0.58362	0.6012	0.62733	0.47902	0.60289	0.46202	0.3514	0.40864
Phenylegh	0.57763	0.62265	0.6039	0.7328	0.64616	0.59974	0.69406	0.69812	0.68379	0.6021	0.64826	0.56242
Trimethyl	1.00432	1.0228	0.98782	0.93698	0.96481	0.99568	1.05445	1.04209	1.05521	1.01174	1.01288	0.99133
Tritriacont	0.87214	0.87379	0.85151	0.77592	0.33729	0.54261	0.93496	0.91499	0.93072	0.88239	0.89761	0.86259
oxamic aci	2.31423	2.41096	2.37092	3.74387	3.77902	4.04378	2.06648	1.88899	2.32767	2.60889	2.80361	2.82179
Heptanon	2.35073	2.44037	2.34956	2.28336	2.34003	1.02945	2.45389	2.43173	2.43771	2.39602	2.41214	2.31897
lactic acid	0.62259	0.66752	0.58702	0.7112	0.65981	0.66504	0.51721	0.5083	0.51741	0.64856	0.68425	0.65405
Heptan-2-	1.12035	1.14604	1.1198	1.05984	1.11309	1.09899	1.01513	0.67674	0.57386	1.10875	1.13256	1.06701
Penten-3-o	1.35553	1.38559	1.33735	1.13863	1.15257	1.15893	0.8364	0.82354	0.83392	1.35738	1.3615	1.316
Succinic ac	2.13796	2.32376	2.25217	2.07862	2.22909	2.33864	2.60982	2.58904	2.64915	2.37404	2.43311	2.34532
2-Oxoglut	1.05356	1	1.04617	1.0426	0.8978	1.04413	1.27307	1.29452	1.30059	1.0309	0.99659	1.02047
Farnesol <	1.60819	1.67784	1.52322	1.40946	1.48897	1.55232	1.07611	1.09912	1.02774	1.05783	1.04843	1.0191
Cedranone	0.50784	0.52984	0.53235	0.55577	0.61037	0.62452	0.54431	0.60404	0.56051	0.58238	0.51315	0.56031
Encecalin	1.38722	1.42713	1.40284	1.72291	1.85623	1.79087	1.16041	1.15314	1.16097	1.64811	1.70274	1.66583
Musk keto	0.6788	0.73759	0.71769	0.75034	0.79008	0.68819	0.69836	0.71394	0.72262	0.76285	0.80207	0.77185
Maltotrios	0	6.8064	6.63082	7.17597	7.47086	7.35697	2.36268	2.37082	2.39436	7.17189	7.23013	6.99959
Sesquilava	1.68159	1.62059	1.52322	1.40946	1.48897	1.55232	1.07611	1.00313	1.03438	1.05783	1.04843	1.02162
Ethyl meni	1.02243	0.79385	0.91355	1.00631	1.00436	0	0.79071	0.9254	0.88059	0.6158	0.86987	0.95109
D-Ribose 5	3.5233	3.78838	3.82152	5.90321	6.16706	6.04428	2.88313	2.8914	2.94583	7.24409	7.33078	7.12178
Senecioic /	0.78334	0.919	0.8738	0.94018	1.06102	1.09899	0.89321	0.87109	0.88815	1.01537	1.00339	0.9753
Nootkatin	2.01549	2.0795	2.05096	3.12033	3.24268	3.22896	1.71892	1.73662	1.75685	2.0966	2.13005	2.06995
Laciniata f	1.30386	1.33898	1.27943	1.19237	1.28192	1.94097	1.40299	1.38915	1.37557	1.2627	1.24566	1.17526
Octen-3-o	1.0776	1.11212	1.05969	1.06825	0.97034	0.97395	0.84412	1.03292	0.79747	0.80652	0.79769	0.77655
4-Hydroxy	1.54756	1.59039	1.57127	0.97967	1.01748	1.00193	0.35764	0.11882	0.2911	1.73686	1.76682	1.72685
Glutamine	4.83257	5.12932	5.15321	3.97404	4.10709	4.02152	0.11484	1.53847	0.18196	4.55145	4.68449	4.53923
glycolic ac	0.56119	0.54862	0.60322	0.47641	0.53968	0.50804	0.67362	0.67832	0.67367	0.54805	0.55584	0.55526
Isopentyl l	0.59079	0.49212	0.46744	0.56701	0.58908	0.58299	0.63818	0.60406	0.62768	0.58906	0.59128	0.58375
Tumerol<a	0.16212	0.94595	0.93266	0.90902	0.93835	0.95635	0.96449	0.97753	0.96737	0.17666	0.95903	0.91706
Docosane	0.94636	0.64883	0.77315	0.62477	0.64031	0.6396	0.74336	0.78269	0.81192	0	0.79131	0.77518
Dotriacont	0.93779	0.77366	0.75863	0.72469	0.75672	0.92354	0.82202	0.93619	0.81469	0.76455	0.76316	0.73511
Linalool<tr	1.31544	1.36732	1.66086	2.37126	2.4474	2.50968	1.07787	1.05545	1.07508	1.72713	1.76419	1.66712
Phytol	0.31194	0.26969	0.28195	0.27946	0.22319	0.28267	0	0	0.30041	0.30136	0	0.17469
Hexenoic a	5.22944	5.37992	5.25571	4.91934	5.11166	5.10104	5.55495	5.51071	5.56101	5.17766	5.28641	5.06684
DethioBio	0.43463	0.49915	0.4712	0.50629	0.5612	0.72263	0.6378	0.70973	0.74426	0.77583	0.79457	0.7563
tranexami	0.39351	0.39667	0.3902	0.38409	0.37262	0.40345	0.42413	0.40251	0.40731	0.37678	0.37383	0.39859
Raffinose	0.34829	0.60092	0.357	0.41187	0.34904	0.41776	0.4107	0.20811	0.41332	0.29672	0.35192	0.346
Ornithine	0.79259	0.80588	0.793	0.85739	0.88526	0.86219	0.84359	0.80458	0.82268	0.81262	0.80041	0.7809
pyruvic aci	0.64344	0.63822	0.61278	0.53691	0.59006	0.57279	0.66055	0.65149	0.65405	0.60662	0.60784	0.57563
Octane<n-	5.04897	5.22612	5.15321	3.98006	4.02716	0	1.1643	1.75861	1.2123	4.67484	4.54776	4.33924
Tetracosar	2.5734	2.64745	2.48528	2.48948	2.5846	2.59607	2.72861	2.69982	2.61183	2.62713	2.6314	2.5376
Tagetone<	2.20534	2.2476	2.19769	1.25591	1.34686	1.22676	2.5704	1.59323	1.51401	2.18482	1.35483	2.15119
putrescine	0.19804	0.21979	0.30042	0.2915	0.31218	0.34246	0.38717	0.31886	0.37702	0.36027	0.35396	0.33628
Leaf alcoh	5.35704	5.46813	5.31254	4.77059	4.72263	4.52531	5.34664	5.32782	5.3221	4.53732	4.56752	4.49533
Aspartate	0.40034	0.43131	0.41024	0.41702	0.4224	0.3904	0.37823	0.36966	0.36743	0.42022	0.44667	0.44843
2-Coumari	1.09444	1.28101	1.19941	1.11615	0.94147	0.86923	0.37131	1.26293	1.34772	0.99598	1.01223	1.18043
Taurine	0.40436	0.43329	0.32594	0.80019	0.85294	0.81644	0.49084	0.32695	0.34874	0.55376	0.5994	0.58397
2'-Deoxyar	1.37261	1.42287	1.39064	1.30806	1.50671	1.3391	1.56174	1.42055	1.42048	1.35512	1.35483	1.22022
Harmaline	0.3263	0.42213	0.47713	0.50844	0.5612	0.72263	0.6378	0.71236	0.74988	0.77264	0.80699	0.76479
Serotonin	0.39343	0.39667	0.3902	0.36205	0.37262	0.40345	0.42413	0.40251	0.40731	0.37733	0.37361	0.3708
Urocanic a	1.05356	0.99946	1.04617	0.8638	0.88224	1.04413	1.24299	1.29452	1.30059	1.0309	0.99659	1.00852
5-Aminole	1.45036	1.52068	1.5501	1.66996	1.78186	0.90023	1.93148	1.93835	1.91037	2.02088	2.00121	0.6395
N-Formylk	0.62259	0.66752	0.59596	0.7112	0.82429	0.66504	0.51721	0.5083	0.51741	0.64856	0.68425	0.65405
3-Nitro-L-T	0.6266	0.4454	2.74069	2.96971	1.33478	3.58549	3.40165	3.37909	3.40139	3.71496	3.74314	3.58893
Trehalose	0.862	0.91754	0.91295	1.05984	1.09828	1.10231	0.39302	0.4188	0.40727	1.07632	1.09621	1.06701
Ribose	0.33686	0.34631	0.35157	0.41189	0.42757	0.42722	0.34129	0.34953	0.33813	0.37353	0.38069	0.36629
Tyrosine	0.99564	1.03433	1.01189	1.15789	1.19461	1.19942	1.01225	0.99685	1.00129	1.61683	1.68703	1.68498
Stearic aci	0.75604	0.9862	0.90896	0.90543	0.90571	0.9505	0.69694	0.90013	0.91893	0.87112	0.91482	0.88324
Gallic acid	1.03953	1.07435	1.07706	0.86921	0.93722	1.04092	1.00204	0.98143	0.9987	0.93608	0.96133	0.91384
cis-Aconiti	2.90637	2.96561	0	2.74003	0	2.88982	3.17154	0	0	2.94856	2.98021	2.88774
Epinephrir	0.57763	0.62265	0.6039	0.7328	0.64616	0.59974	0.69406	0.69812	0.68379	0.6021	0.65313	0.56242
Homocysti	1.18605	1.21434	1.19665	1.18563	1.17133	1.13758	1.23263	1.20529	1.18351	1.1728	1.19897	1.23918
Methylma	0.40288	0.34615	0.31734	0.29394	0.31094	0.29882	0.3305	0.32034	0.31977	0.31115	0.3302	0.3145
beta-Alani	5.34316	5.46813	5.29844	4.7566	4.72426	4.52727	5.34664	5.32782	5.3221	4.51903	4.56949	4.49533
octadecylg	0.18885	0.2918	0.27134	0.38152	0.51518	3.4557	2.15094	0.29017	2.2029	3.19166	3.25838	3.15814
Xylose	0.47614	0.55817	0.87402	0.50654	0.86112	0.82653	0.74152	0.6144	0.5987	0.85346	0.63907	0.75386
Xylulose	0.28571	0.33504	0.07809	0.39059	0.39504	0.40473	0.09744	0.12807	0.10966	0.45498	0.44959	0.44212
DL-Homoc	0.67064	0.68609	0.67952	0.60515	0.66641	0.62552	0.74602	0.74973	0.7675	0.65099	0.66238	0.60355
S-Adenosy	0.60474	0.61976	0.60789	0.519	0.53079	0.5293	0.61529	0.62919	0.6071	0.53606	0.53271	0.51242
Quinolinic	2.88266	2.95574	2.90492	2.72728	2.84472	2.88982	3.16099	3.15669	3.18224	2.94376	2.97094	2.87479
Pyridoxine	0.46291	0.52309	0.45867	0.49144	0.52923	0.47188	0.47119	0.47726	0.45097	0.457	0.4493	0.41281
Melibiose	0.98026	1.04766	0.98224	1.04552	1.16069	0.99806	0.30892	0.21544	0.25222	0.18125	0.2641	1.08252
L-Histidine	1.05736	1.08042	1.0521	0.99361	1.0447	1.02825	1.12434	1.11112	1.11078	1.04883	1.06752	1.03456
palatinitol	0.88798	0.81597	0.78736	1.19682	1.14156	1.23998	1.08227	1.07084	1.08358	0.82159	0.83953	0.80384
Catechin	0.17097	0.75835	0.75048	0.7027	0.82345	0.73543	0.84015	0.79511	0.80343	0.77579	0.77233	0.68318
Malonic ac	0.25281	0.28325	0.27094	0.24545	0.28605	0.24897	0.28289	0.27302	0.2831	0.28583	0.29731	0.26652
Ureidopro	0.1655	0.37581	0.37814	0.32473	0.37635	0.29743	0.56743	0.56326	0.56776	0.32158	0.3377	0.34952
DL-Homoc	1.82733	1.87255	1.87054	1.90071	1.95773	1.93454	1.89683	1.85659	1.8535	1.84102	1.86038	1.90394
Spermidin	2.16626	2.25867	2.18945	2.04501	2.16536	2.16071	2.40641	2.36622	2.38714	2.20386	2.23595	2.16121
Nonadeca	1.17465	1.17181	1.14152	1.23337	1.48241	2.20957	1.18182	1.17615	1.21929	1.17582	1.19035	1.16743
Maltose	0.16351	0.32912	0.53341	0.66572	0.62648	0.61185	0.52385	0.45869	0.66359	0.51325	0.60999	0.60242
3-Hydroxy	0.4505	0.46672	0.48043	0.42887	0.46247	0.41042	0.54097	0.50936	0.49844	0.47401	0.46455	0.44937

Label	FC (ST/SC)	P-val	FC(VT/VC)	P-Val
Cedroxyde	1.555144	0.601424	NA	0.001312
Glutamine	0.800699	0.000806	7.505785	0.001032
4-Hydroxybenzoic acid	0.636854	4.23E-06	6.814534	3.27E-05
Xylulose	1.703348	0.106242	4.018021	4.01E-06
Octane<n->	0.583811	0.234953	3.279601	0.000126
Maltotriose	1.637527	0.271719	3.002524	2.78E-07
Trehalose	1.210936	0.001066	2.657351	4.9E-07
2-Phosphoglycerate	1.628039	4.26E-05	2.489004	3.26E-07
D-Ribose 5-phosphate	1.627075	4.35E-05	2.488047	2.82E-07
Cystamine	1.130905	0.003164	2.357627	2.09E-05
Fumaric acid	1.289026	0.002053	1.731929	3.52E-05
Tyrosine	1.167677	0.000596	1.657203	9.62E-06
Penten-3-ol<1->	0.845937	0.000165	1.617926	4.4E-06
Linalool<tetrahydro->	1.68715	0.000974	1.607791	2.39E-05
Ethyl ether	0.973872	0.921798	1.503155	3.27E-06
Taurine	2.122362	0.000258	1.489165	0.023131
Encecalin	1.273362	0.000669	1.443852	6.01E-06
Lavandulyl acetate<tetrahyd	1.181993	0.000589	1.356864	3.21E-05
oxamic acid	1.630002	0.000112	1.310539	0.010809
Gluconolactone	0.966937	0.155744	1.305606	2.69E-05
N-Formylkynurenine	1.166728	0.112587	1.287737	0.00021
lactic acid	1.08466	0.136042	1.287737	0.00021
Pantothenic acid	1.144181	0.034563	1.23704	0.004624
Nootkatinol	1.560696	1.16E-05	1.208006	6.14E-05
UDP-N-acetylglucosamine	1.766541	0.000805	1.19888	0.001528
2-Hydroxypyridine	1.0729	0.143891	1.184269	0.001804
Aspartate	0.990288	0.780084	1.179316	0.002349
Senecioic acid	1.203424	0.04865	1.128792	0.001122
Musk ketone	1.04429	0.410419	1.094543	0.008235
Ribose	1.224158	0.000327	1.08898	0.004729
3-Nitro-L-Tyrosine	2.069397	0.244472	1.084944	0.003867
Hexadecane	0.740984	0.523252	1.073065	0.004509
Galactitol	0.920369	0.609216	1.06636	0.002806
Hexacosane	0.971793	0.323053	0.978982	0.040459
Calamenene<cis->	1.009035	0.694358	0.961439	0.008641
Trimethyl benzaldehyde<2,3	0.961041	0.118297	0.956913	0.005236
Palmitoleic acid	0.97978	0.559902	0.951749	0.004053
Jasmolactone, extra C<Z->	0.950742	0.014006	0.951166	0.012792
Tritriacontane	0.637481	0.068711	0.950342	0.017618
Heptacosane	0.614047	0.277407	0.947067	0.021124
Isopentyl butanoate	1.121738	0.175391	0.943406	0.026934
Gallic acid	0.892322	0.089642	0.942686	0.019693
L-Histidine	0.961339	0.077301	0.941628	0.003485
Tetradecene<1->	0.963539	0.05024	0.937364	0.00496
Hexadecanol<n->	0.945539	0.02115	0.934993	0.019075
Hexenoic acid<2E->	0.953796	0.03479	0.934097	0.005023
Citronellene<tetrahydro->	0.943466	0.01927	0.928509	0.002869
Quinolinic acid	0.967804	0.151677	0.925217	0.001338
Sorbate	0.964124	0.208197	0.922764	0.001262
Spermidine	0.963217	0.16753	0.92196	0.001622
Pentadecane	0.995214	0.861646	0.920119	0.016369
Asparagine	0.97326	0.1671	0.92005	0.025231
Dodecadien-1-al<2Z,6E->	1.014924	0.909642	0.919116	0.025317
Succinic acid	0.989939	0.820182	0.911374	0.001768
Hydroxylamine	0.987296	0.794051	0.91052	0.002531
pyruvic acid	0.897237	0.023862	0.910481	0.005717
6-phospho-2-dehydro-D-glu	1.479521	0.392383	0.910291	0.006838
Phosphorylcholine	1.066855	0.078314	0.909377	0.002155
Serotonin	0.964261	0.325596	0.909064	0.005392
Cytidine	0.995711	0.952595	0.906327	0.021162
N-Alpha-AcetylLysine	0.926886	0.00344	0.902431	0.000113
Gly-Gly	0.925883	0.003315	0.902431	0.000113
Decane<n->	1.015028	0.819994	0.902097	0.038843
Dihydro citronellol	0.85869	0.019517	0.899074	0.001676
3-Hydroxyphenylacetic acid	0.9314	0.14216	0.89615	0.021512
Laciniata furanone H	1.12569	0.52567	0.88385	0.004446
Epinephrine	1.096724	0.230081	0.875566	0.031753
Cyclohexadecanolide	1.467007	0.013221	0.874517	0.021716
Phenylephrine	1.096724	0.230081	0.873222	0.02522
Tricosane	1.051175	0.290516	0.86081	0.015805
S-Adenosyl-L-methionine	0.861766	0.000137	0.853966	0.000777
Leaf alcohol<ethyl acetal->	0.868682	0.001317	0.850193	3.56E-06
beta-Alanine	0.869544	0.001339	0.849172	4.05E-06
Undecane<n->	0.905967	0.108229	0.847214	0.008513
DL-Homocysteine	0.931657	0.06681	0.846974	0.00385
glycolic acid	0.889718	0.062784	0.819086	2.04E-06
Tryptamine	0.882561	0.000425	0.791636	9.76E-06
Urocanic acid	0.900284	0.159703	0.791019	0.000214
Cysteinylglycine	0.865033	0.007471	0.788935	0.000137
2-Oxoglutaric acid	0.962833	0.496004	0.787955	3.16E-05
palatinitol	1.436335	0.000932	0.761566	2.03E-05
Benzoic acid	1.039129	0.76411	0.714972	0.043952
Ureidopropionate	1.085971	0.740421	0.59395	9.76E-06
Hexadienol butanoate<2E,4I	7.092602	0.000389	0.348679	6.23E-06
cis-Aconitic acid	0.958765	0.955412	2.77988	0.149807
octadecylglycerol	13.76668	3.53E-07	2.068942	0.058342
Melibiose	1.064485	0.29013	1.967444	0.434924
Phytol	0.909392	0.320781	1.584644	0.6823
Manool oxide	1.267463	0.477555	1.507491	0.459022
Heptan-2-ol<6-methyl-	0.96625	0.103491	1.46015	0.061282
5,6-Dihydrouracil	1.887682	0.013571	1.336224	0.10143
Hexadienal<2E,4E->	1.20633	0.058745	1.212279	0.395715
Heptadecane	0.968628	0.147336	1.204344	0.503907
Xylose	1.149792	0.596026	1.149272	0.273519
Harmaline	1.462407	0.072759	1.116371	0.08281
DethioBiotin	1.274129	0.130197	1.112306	0.078069
Cysteine	0.905016	0.471883	1.094907	0.906584
Isobutyl acetate	0.419742	0.009095	1.082776	0.841632
2-Coumaric acid	0.81873	0.076597	1.06931	0.838993
Stearic acid	1.041654	0.623266	1.060877	0.518802
Octacosane	0.937296	0.128106	1.050395	0.290153
Maltose	1.855744	0.053786	1.04831	0.716356
N-Acetyl-D-glucosamine	1.019414	0.710263	1.036488	0.743582
Octanol acetate<3->	0.781794	0.282574	1.026761	0.834152
Eicosene<1->	1.016848	0.501258	1.021786	0.510406
Malonic acid	0.967118	0.603417	1.012695	0.729694
Sesquilavandulol<E->	0.922358	0.113922	1.004582	0.851121
Isopulegyl acetate	0.97763	0.72508	1.003864	0.9839
Tagetone<dihydro->	0.575814	1.82E-05	1.002324	0.992411
DL-Homocystine	1.039955	0.028673	0.999719	0.983039
Homocystine	0.971504	0.106592	0.997103	0.891074
Pentacosane	1.025387	0.827889	0.991073	0.730252
Nonadecanoic acid methyl e	1.412094	0.177393	0.987794	0.389704
Methylmalonic acid	0.847449	0.101847	0.9848	0.511323
Nonacosane	0.973632	0.414811	0.982456	0.672984
Octadecanol<n->	0.906417	0.088851	0.980424	0.601627
Hexadecene<1->	1.072831	0.030287	0.976904	0.05603
Farnesol <2E, 6Z->	0.925456	0.121163	0.97577	0.342662
Eicosane	1.020248	0.778166	0.975605	0.859092
Heptanone<5-methyl-3->	0.79164	0.311796	0.973207	0.090907
putrescine	1.3173	0.09231	0.969964	0.654461
Tetracosane	0.995332	0.845735	0.969638	0.155512
Cedranone<5->	1.140522	0.030244	0.968966	0.549915
Ornithine	1.089214	0.001803	0.968866	0.15334
Untriacontane	0.97501	0.337046	0.966087	0.0868
Raffinose	0.90236	0.645738	0.963666	0.867298
Tridecane	0.987089	0.82277	0.958774	0.504904
Octadecene<1->	0.950119	0.139616	0.95522	0.050437
Nonadecane	0.980854	0.651858	0.954443	0.20541
Heneicosane	1.002878	0.936243	0.951699	0.353352
Octadecane	1.303418	0.190769	0.947567	0.71421
Pyridoxine	1.033145	0.582999	0.942608	0.164988
Ethyl menthone<2->	0.736553	0.521455	0.938405	0.648824
Geranyl-PP	0.892675	0.224903	0.936008	0.322211
tranexamic acid	0.982871	0.503915	0.931314	0.050291
Catechin	1.346329	0.382418	0.914959	0.106646
Camphenilone	0.979479	0.743844	0.901445	0.332636
Manool oxide<13-epi->	8.818388	0.065991	0.900672	0.145757
2'-Deoxyadenosine	0.992294	0.873603	0.892656	0.07267
Octen-3-ol butanoate<1->	0.927106	0.090541	0.890164	0.248322
Nonane<n->	1.035107	0.819738	0.880229	0.291795
Dotriacontane	0.973632	0.809284	0.879483	0.063119
5-Aminolevulinic acid	0.9626	0.849595	0.806477	0.460623
Cysteamine	0.984264	0.459529	0.793505	0.425798
Urea	1.253499	0.000817	0.725948	0.295963
Hexyl acetate	0.874634	0.814917	0.725303	0.302207
Tumerol<ar->	1.373882	0.382469	0.70556	0.324023
Docosane	0.804221	0.148235	0.670018	0.381699
propane-1,3-diol	0.89206	0.06074	0.657223	0.161019
Hexanal, dimethyl acetal	4.001149	0.00015	0.549508	0.313397
Hexalactone<gamma->	1.383591	0.526812	0.42613	0.078282
Karahanaenone	1.100179	0.202835	0.080797	0.358093

Names	total	Metabolites
Up ST/SC Up VT/VC	9	D-Ribose 5-phosphate
		Trehalose
		Encecalin
		2-Phosphoglycerate
		Fumaric acid
		Linalool<tetrahydro->
		oxamic acid
		Nootkatinol
		Taurine
Down VT/VC Up ST/SC	2	palatinitol
		Hexadienol butanoate<2E,4E->
Down ST/SC Up VT/VC	1	4-Hydroxybenzoic acid
Up ST/SC	8	Ribose
		octadecylglycerol
		Senecioic acid
		UDP-N-acetylglucosamine
		Urea
		5,6-Dihydrouracil
		Hexanal, dimethyl acetal
		Cyclohexadecanolide
Down ST/SC	2	Isobutyl acetate
		Tagetone<dihydro->
Up VT/VC	14	Pantothenic acid
		Gluconolactone
		lactic acid
		Tyrosine
		Glutamine
		Ethyl ether
		Penten-3-ol<1->
		Maltotriose
		Lavandulyl acetate<tetrahydro->
		Octane<n->
		Cedroxyde
		N-Formylkynurenine
		Xylulose
		Cystamine
Down VT/VC	6	Ureidopropionate
		Urocanic acid
		Cysteinylglycine
		Benzoic acid
		Tryptamine
		2-Oxoglutaric acid

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9	PC10	PC11	PC12
Manool ox	0.14306	0.25218	0.00067	0.18485	0.24389	-0.12218	-0.10008	0.13794	-0.27673	-0.15324	-0.03962	0.23956
Hexacosar	-0.0044	-0.00145	-0.00459	0.0044	0.00054	0.00078	-0.00056	-0.00138	-0.02145	0.00975	-0.00953	0.31133
Manool ox	0.03815	0.01336	0.01569	0.05115	0.11877	-0.02053	-0.04734	-0.07308	-0.07673	-0.18547	-0.19565	-0.12183
Decanen-	-0.00522	0.01082	-0.00343	0.00853	0.01643	-0.00242	-0.00144	0.01036	-0.03034	0.01011	-0.0478	0.19445
2-Hydroxy	0.02222	-0.01239	-0.01813	-0.00368	-0.00491	-0.00503	-0.01169	-0.00485	-0.04647	-0.01018	-0.04086	0.06203
Cytidine	-0.02604	0.00829	-0.05838	-0.0321	-0.00356	0.00927	-0.01978	0.01992	-0.08847	-0.05908	-0.06429	0.09129
Tetradece	-0.00619	0.00297	0.00945	0.00097	0.00925	0.00797	-0.00822	0.00204	-0.01343	0.00206	-0.02336	-0.19171
Hexadecer	0.00353	0.01054	-0.00067	0.00308	0.00492	0.00133	-0.00391	-0.00482	-0.01619	-0.00324	-0.01239	-0.32511
Hexadecar	-0.02282	-0.04551	-0.05538	-0.00673	0.07933	-0.03266	-0.06677	0.18281	-0.45434	-0.21127	-0.01644	-0.07749
Hydroxyfa	-0.02412	0.0083	-0.04925	-0.02094	0.00681	0.02525	0.00888	-0.00138	-0.07207	-0.00055	-0.03956	0.25908
Cedroxyde	0.11937	0.03122	-0.03507	0.33061	0.32572	-0.12052	0.09185	0.07069	0.15076	0.11658	-0.11254	-0.07645
Sorbate	-0.01902	0.00293	-0.01916	-0.0127	0.00293	0.01917	-0.00315	-0.00391	-0.04538	-0.00826	-0.02662	-0.16599
Undecane	-0.00728	0.00189	0.00786	-0.00767	0.00939	0.01802	-0.00181	-0.00202	-0.00514	-0.01854	-0.02328	0.01492
Heptacosa	-0.03074	-0.04989	0.02725	-0.08548	-0.10044	0.04927	0.01411	-0.03389	0.03979	0.00363	0.00867	0.00343
Hexadienc	0.33063	0.62076	0.35411	-0.06303	-0.11912	-0.03527	-0.1931	-0.176	0.16276	0.01105	0.03395	0.03173
Gly-Gly	-0.03008	0.0013	0.00858	-0.00871	0.01515	0.02764	-0.00469	-0.00597	-0.02769	0.0188	-0.03213	-0.12429
Palmitolei	-0.00551	0.00163	-0.00781	0.00021	0.00864	0.00361	-0.00242	-0.00236	-0.02138	0.00427	-0.01233	-0.03526
Octacosan	-0.00086	-0.00712	0.00097	0.00458	0.00145	-0.01152	-0.00799	0.00231	-0.00609	0.02491	-0.03181	0.01168
Eicosene1	0.00278	0.00047	-0.00065	-0.0051	0.00442	-0.00511	-0.00448	0.01332	-0.01685	0.01924	-0.01579	-0.04349
Hexadiena	0.22301	0.06536	0.21876	-0.03326	-0.09855	0.1636	0.77726	0.07405	-0.22559	0.09395	-0.03526	-0.00434
Asparagin	-0.00996	0.00454	-0.00109	0.00024	0.0041	0.00313	-0.00668	-0.01488	-0.01862	-0.0146	-0.03313	0.05949
N-Alpha-A	-0.02988	0.00171	0.00833	-0.00796	0.01608	0.02732	-0.00479	-0.00565	-0.02811	0.0187	-0.03235	0.11094
Heneicosa	-0.00193	0.00214	-0.00496	0.00365	0.00174	0.01107	0.00567	0.001	-0.0109	-0.00407	-0.02708	0.00362
Pentacosa	0.00064	-0.00089	0.01106	-0.02221	-0.02974	0.00884	0.00225	-0.02241	0.00945	-0.01276	-0.00658	-0.02142
Octadecar	-0.0004	0.01318	-0.01386	-0.00999	-0.03394	-0.019	-0.0384	0.04009	0.0227	-0.02021	-0.05112	0.05026
Citronellel	-0.00921	-0.0005	-0.00262	-0.00568	-0.00278	0.00452	0.00745	0.00476	-0.01223	-0.00691	-0.00409	0.04353
Hexanal, d	-0.04586	0.14361	-0.14255	-0.21745	-0.03269	0.26712	0.08433	0.04588	-0.05713	0.48575	-0.00979	0.0117
Tryptamin	-0.02575	0.00373	-0.02045	-0.0116	-0.00697	0.01416	0.00655	-0.0084	-0.01725	-0.00061	-0.01016	-0.02982
propane-1	-0.02342	0.02	0.03213	-0.00604	0.04053	0.02639	-0.08869	-0.01749	0.0071	0.0343	0.25474	-0.04932
Fumaric ac	0.03137	-0.0068	0.00084	0.00297	-0.00811	-0.02266	-0.00319	0.01215	-0.00794	-0.0164	-0.01489	-0.01808
Pantothen	0.01537	-0.00353	-0.01448	0.00396	-0.00294	-0.00086	0.01344	0.00518	-0.02032	-0.0156	0.02097	-0.03447
6-phosphc	0.0186	0.03066	-0.06341	-0.10479	0.06066	0.13769	0.00202	-0.07471	-0.01171	-0.00383	-0.00347	0.01964
Nonadeca	-0.00698	0.00095	-0.01596	-0.00559	0.0032	0.02232	-0.00858	0.01812	-0.03491	0.0127	-0.02036	0.0115
Hexadecar	-0.00716	2.39E-05	-0.0003	-0.00148	0.00699	0.00138	-0.00185	0.00137	-0.00971	-0.00319	-0.02531	0.0447
Octadecar	-0.0023	-0.00309	0.0057	0.00519	0.00878	-5.08E-05	0.00484	0.00488	-0.01668	0.02079	-0.01787	0.03081
2-Phosphc	0.34731	-0.12584	-0.2272	0.00498	-0.23922	-0.25294	0.00103	0.01915	-0.07634	-0.07204	0.02937	-0.17695
Dihydro ci	-0.01714	-0.00627	0.00503	0.00414	-0.00357	-0.00822	-0.00028	-0.00051	-0.01838	0.00596	-0.02298	0.05489
Cysteamin	-0.00292	0.00665	0.00979	0.00013	0.01113	0.00209	-0.02996	-0.01199	0.00322	-0.00791	-0.12587	0.01618
Hexalactor	-0.04714	0.16054	0.02505	0.14586	-0.05434	-0.00523	0.24606	0.30208	0.35203	-0.27266	-0.05551	-0.01236
Hexyl acet	-0.01327	-0.00554	0.00067	-0.11654	-0.00225	0.10993	-0.04354	-0.10004	0.00179	-0.02412	-0.23292	-0.04766
Octadecen	-0.00331	3.25E-05	0.00423	0.00262	0.01154	0.00108	-0.00266	0.00385	-0.01482	0.00971	-0.01903	-0.00236
Pentadeca	-0.00609	0.00756	0.00445	0.00671	0.00183	0.01429	-0.00835	-0.01228	-0.02519	0.00117	-0.01517	0.07454
Nonacosar	-0.00253	-0.00158	-0.00351	0.00239	-0.00351	0.00844	-0.00569	-0.00199	-0.02014	0.00192	-0.0338	-0.01471
Octanol ac	-0.00818	-0.01285	0.00371	0.01428	0.00346	-0.02906	-0.04727	0.00568	-0.07434	0.02587	-0.03424	0.03717
Galactitol	0.00514	-0.01541	0.01733	-0.00158	0.00604	0.03695	0.01679	-0.07052	0.02789	0.10542	0.00447	0.0796
Ethyl ethe	0.04769	-0.03636	-0.00521	0.10471	-0.03729	0.04481	-0.04771	0.26713	0.15128	-0.06664	0.01856	
Cyclohexa	0.01224	0.02846	0.01358	0.01426	0.01837	-0.01205	-0.01704	-0.0042	-0.01649	-0.00648	-0.00723	0.01878
Isobutyl ac	-0.01669	-0.03483	-0.00562	0.0427	-0.03217	0.07461	-0.02448	0.0486	-0.03596	0.06383	-0.03201	0.02695
Lavanduly	0.07053	0.01078	0.06866	0.0326	0.03578	-0.02824	-0.03356	0.02778	0.00698	0.01327	-0.03331	0.1248
Nonanen-	-0.00198	0.00497	-0.00688	-0.00982	0.01328	0.01949	-0.02129	-0.00202	-0.03265	-0.02528	-0.05745	-0.01484
Urea	0.00337	0.0653	0.04712	-0.00247	0.02504	0.00648	-0.12001	-0.02193	0.05195	0.00492	0.39268	-0.00239
Heptadeca	0.01748	-0.01385	0.0105	0.05936	-0.03106	0.10163	-0.04945	0.10313	-0.00716	0.04153	-0.01699	-0.01406
Phosphory	-0.00156	0.01829	0.00228	-0.00498	0.01182	0.00372	-0.00026	0.00591	-0.02212	-0.002	-0.01683	-0.00161
Eicosane	0.00101	0.00122	-0.00237	0.01295	-0.00231	0.03376	-0.02	-0.0267	-0.02098	-0.01059	-0.07254	0.01357
Isopulegyl	0.00066	0.00118	0.00931	0.00123	0.02329	-0.03643	-0.04959	0.00696	-0.00608	0.04541	0.07728	0.01872
Untriacont	-0.0036	3.94E-05	-0.0039	0.00049	0.00558	-0.00034	0.00112	-0.0032	-0.01282	-0.00632	0.01276	0.02959
Cystamine	0.04188	-0.02201	0.01791	0.02317	0.00656	-0.01747	-0.00886	0.01458	0.00172	-0.01488	-0.0046	-0.00418
Jasmolact	-0.01009	-0.00254	-0.00743	-0.00483	0.00064	0.00655	-0.00213	-0.00091	-0.01686	-0.00409	-0.02253	-0.07972
Cysteinylg	-0.02977	0.00396	-0.02108	-0.01165	0.00063	0.00485	0.00257	0.00411	-0.0087	-9.25E-05	0.00276	0.05094
Geranyl-PI	-0.018	-0.00743	0.04263	0.03495	-0.01917	-0.02897	0.05408	-0.0344	0.0327	-0.03341	-0.01936	0.06873
Calamenei	-0.00289	0.00375	-0.00512	-0.00868	0.00278	0.01078	0.00164	-0.00575	-0.01395	0.00916	-0.01229	-0.08082
5,6-Dihydr	0.0288	0.02642	0.01304	0.00539	0.00308	-0.02241	-0.05044	0.00187	-0.05166	-0.00331	-0.01911	0.03046
Dodecadie	-0.01255	0.05704	0.25359	0.00214	-0.24859	-0.09664	-0.10104	-0.02828	0.05077	-0.00816	-0.17722	-0.20574
Tricosane	-0.00552	0.01108	0.00178	-0.00901	0.00877	0.01891	-0.01247	-0.01664	0.01258	-0.01439	-0.00261	0.01862
Campheni	-0.03589	0.04349	0.17381	0.09322	-0.14322	0.14844	0.11851	-0.16705	0.09594	-0.42374	0.02675	-0.00411
UDP-N-acı	0.11861	0.11691	-0.02282	0.01256	-0.02939	-0.02955	-0.04979	-0.0329	-0.11968	-0.01725	-0.03675	-0.09226
Gluconola	0.0302	-0.03873	0.01297	0.01078	0.00144	-0.01929	-0.01096	0.01254	-0.01788	0.00074	-0.02485	0.09817
Karahanae	-0.12548	0.08574	-0.05485	-0.29237	0.19121	-0.48675	0.24047	-0.54748	-0.05077	-0.21055	0.08251	0.0269
Tridecane	-0.00318	0.00265	0.00646	-2.44E-05	0.00025	-0.02789	-0.00215	0.00289	-0.01371	0.01864	-0.02106	0.02975
N-Acetyl-D	0.00777	0.00182	0.01392	-0.02953	0.02565	-0.04301	-0.01533	0.03148	-0.03667	0.05826	-0.04505	0.01134
Cysteine	0.0026	-2.33E-05	0.00829	0.01009	0.00432	0.01232	-0.02045	0.00766	0.00919	0.02469	-0.05019	0.00351
Benzoic ac	-0.0072	0.01553	0.00578	0.01167	0.00688	0.01758	-0.03274	0.01614	-0.0405	-0.00342	0.01798	0.00896
Phenyleph	-0.00268	0.00957	-0.0006	-0.00987	-0.00902	0.01014	0.00542	-0.02151	0.01732	0.0094	-0.03304	0.03074
Trimethyl	-0.006	-0.00088	-0.00601	0.00067	0.00212	0.00187	-0.00163	-0.00057	-0.01485	0.0033	-0.00918	0.02858
Tritriacont	-0.02496	-0.02916	-0.02277	0.00798	-0.00563	0.01523	0.02751	-0.03003	0.07389	0.04924	-0.0188	-0.05287
oxamic aci	0.13364	0.10265	0.02851	0.05221	-0.00369	-0.03256	-0.01384	0.06229	0.00051	0.06741	0.00425	0.1301
Heptanon	-0.03557	-0.05871	0.02805	-0.10643	-0.12526	0.05645	0.00792	-0.05563	0.03114	0.02104	-0.00703	0.13343
lactic acid	0.01367	-0.00508	0.00592	0.00789	-0.00253	-0.00383	0.00322	-0.00833	0.00225	0.01947	-0.01113	0.02011
Heptan-2-	0.02632	-0.02515	0.02348	0.03948	0.00314	0.02012	-0.01425	-0.01858	-0.00933	-0.09242	-0.0186	0.04454
Penten-3-(	0.02713	-0.051	0.02279	0.02501	0.01748	-0.01864	-0.00914	0.02383	0.00167	0.00721	-0.02056	0.05381
Succinic ac	-0.02335	0.00867	-0.04721	-0.02057	0.00427	0.02724	0.00765	-0.00133	-0.06542	0.00228	-0.03156	-0.08758
2-Oxoglut	-0.02376	0.01394	-0.01947	-0.0032	0.00024	0.00669	0.00699	-0.0108	0.02431	0.01217	0.00517	-0.02547
Farnesol 2	0.01313	0.00547	0.0836	0.03886	0.07161	0.00088	-0.02839	0.00542	-0.01066	0.01364	-0.032	0.02136
Cedranone	0.00224	0.0077	-0.00417	-0.0053	0.00573	-0.00841	-0.00973	-0.004	-0.00991	-0.00495	0.01957	-0.007
Encecalin	0.05464	8.19E-07	0.00456	0.00953	-0.01324	-0.03093	-0.00676	0.01226	-0.02336	-0.01358	-0.00483	0.11101
Musk keto	0.00528	-0.00373	-0.00251	-0.01163	-0.00965	0.00243	0.00466	-0.00149	-0.00825	0.00407	-0.00759	0.04864
Maltotrios	0.52773	-0.1073	-0.14064	-0.349	0.3912	0.44191	-0.04639	-0.15533	0.06568	0.00238	0.00291	-0.03029
Sesquilava	0.01428	0.00416	0.08655	0.0511	0.05984	-0.0007	-0.03376	0.02863	-0.00288	0.00953	-0.03301	0.0104
Ethyl mem	-0.01681	-0.02531	0.04919	-0.07059	-0.09816	0.00517	0.06667	-0.00074	0.05331	0.00521	0.05365	0.03706
D-Ribose 5	0.34731	-0.12595	-0.22646	0.00452	-0.23947	-0.25386	0.00152	0.01872	-0.0789	-0.07213	0.03254	0.03854
Senecioic (	0.01596	0.00687	-0.01335	-0.003	0.00519	0.00195	-0.01137	-4.49E-05	-0.0338	-0.0076	-0.00718	-0.03765
Nootkaton	0.10127	0.09091	0.06241	0.02599	0.01313	-0.0408	-0.04213	-0.00045	0.00655	-0.00087	-0.02564	-0.14578
Laciniata f	0.00109	0.0346	-0.01751	0.04917	0.07242	-0.01283	-0.01978	0.01499	-0.05747	-0.01244	-0.04526	-0.01246
Octen-3-o	-0.00132	0.00467	0.04096	0.00294	0.03561	-0.01345	0.00081	-0.03588	0.02796	0.00345	-0.01594	-0.02809
4-Hydroxy	0.07269	-0.14965	0.03215	0.06538	0.01582	-0.02924	-0.01235	0.0875	0.00857	-0.00667	-0.01373	0.03051
Glutamine	0.26363	-0.32703	0.26932	0.11142	0.2615	-0.3207	0.0053	0.07759	0.10128	-0.06423	-0.07066	-0.03515
glycolic ac	-0.01267	0.00174	-0.00688	-0.01029	-2.14E-05	0.00709	0.00264	0.00699	-0.00923	-0.01646	0.00042	0.02158
Isopentyl l	-0.00278	0.00684	-0.0092	0.00434	-0.01927	-0.00807	-0.00077	-0.00181	-0.01392	-0.00067	-0.00029	-0.03546
Tumerolar	0.00545	0.04152	-0.01259	-0.05831	0.05133	0.11215	0.15441	-0.00321	-0.03963	-0.00376	-0.00503	-0.04907
Docosane	-0.02003	0.01245	0.03238	0.01683	-0.00094	0.00338	0.15358	0.07156	-0.02372	-0.01259	-0.00816	0.01001
Dotriacont	-0.00902	0.00825	0.00068	0.01734	0.01441	-0.0333	-0.00021	-0.00295	-0.01984	-0.01064	-0.01616	-0.04107
Linalooltet	0.1061	0.05324	0.02863	0.01572	0.01485	-0.03961	-0.03334	0.03482	0.0509	-0.06509	-0.03543	0.0262
Phytol	0.00713	-0.00136	0.01833	0.01215	0.01509	-0.00651	-0.05656	0.0496	0.03705	0.08359	0.05204	0.00675
Hexenoic a	-0.03807	0.00068	-0.01672	-0.01711	0.01218	0.03845	-0.00019	-0.00204	-0.0708	0.00308	-0.09032	0.29176
DethioBio	0.0024	0.00141	-0.04854	-0.00883	-0.00723	-0.01465	0.00757	0.00439	-0.03706	0.0144	-0.00982	-0.01914
tranexami	-0.00219	0.00155	-0.00128	0.00294	0.00194	0.00383	0.0019	-0.00094	-0.00078	-0.0005	0.00942	0.01419
Raffinose	0.00289	-0.00123	0.0109	0.0164	0.01295	0.04852	0.00024	-0.00495	-0.01885	0.06255	-0.00814	0.00382
Ornithine	0.00274	0.00824	0.00179	-0.00013	-0.00303	0.00487	-0.00825	-0.00319	-0.00507	-0.00381	-0.0073	0.00079
pyruvic ac	-0.00748	-0.00194	-0.00017	-0.00073	0.00085	0.00298	-0.00399	0.00098	-0.01569	-0.00229	-0.01348	0.03765
Octanen-	0.13472	-0.42881	0.3887	-0.24249	-0.2395	-0.06026	-0.08529	0.02027	0.11494	-0.05175	0.00231	0.15918
Tetracosar	-0.00822	0.00219	-0.01048	0.00131	0.00496	-0.0072	-0.03314	-0.04986	-0.01072	-0.03296	-0.155	
Tagetoned	-0.04757	-0.0893	0.01219	0.06052	0.00145	0.12074	-0.09973	-0.05045	-0.00752	-0.18843	0.32987	-0.04486
putrescine	0.00033	0.00551	-0.01911	-0.0064	-0.00651	0.01067	-0.00316	0.00888	0.00105	-0.01766	-0.00455	-0.01554
Leaf alcoh	-0.07266	-0.002	0.07027	-0.01122	0.04897	0.07413	-0.00295	-0.01989	0.01124	0.04199	-0.05187	-0.15436
Aspartate	0.0043	-0.00544	0.00105	-0.00077	-0.00259	0.00168	0.00523	-0.00128	-0.00331	0.00092	0.00287	-0.01084
2-Coumari	-0.00279	-0.02133	0.01933	-0.06194	0.0457	-0.06894	0.04107	0.05067	0.04773	0.2341	0.04677	-0.053
Taurine	0.03547	0.02583	0.00123	0.01559	-0.0263	-0.00116	-0.00583	-0.02092	-0.02463	-0.0163	0.00403	0.0493
2'-Deoxya	-0.00864	0.00907	0.00802	-0.00816	-0.00548	0.02707	-0.02435	-0.00881	-0.03897	-0.0421	-0.0507	-0.01491
Harmaline	0.0047	0.0054	-0.05812	-0.01862	-0.00818	-0.00979	0.01211	0.00898	-0.0271	0.00024	-0.00925	0.0358
Serotonin	-0.003	0.00167	-0.00104	0.00282	0.00366	0.00168	-0.00183	0.00028	-0.00514	-0.00314	-0.00214	-0.01959
Urocanic a	-0.02728	0.00844	-0.02381	-0.00381	0.01118	0.00024	0.00128	0.00843	-0.01377	-0.00041	-0.00022	0.05222
5-Aminole	-0.03367	0.00278	-0.00604	-0.10261	-0.0929	0.03275	-0.12572	-0.09488	0.03386	-0.03027	-0.53543	-0.00307
N-Formylk	0.0174	-0.00059	0.01363	-0.0032	-0.01014	-0.00392	-0.00506	0.00026	-0.02316	0.00162	-0.00721	0.00768
3-Nitro-L-1	0.01862	0.06754	-0.42791	-0.066	-0.02423	-0.01458	0.13193	0.05694	0.47377	-0.28877	-0.03901	0.07523
Trehalose	0.05787	-0.0264	0.01658	0.02045	0.00711	-0.0363	-0.00921	0.01985	0.00456	-0.00374	-0.00748	0.0026
Ribose	0.00636	0.00504	0.00019	-0.00046	-0.00018	-0.00351	-0.00154	-0.00137	-0.00173	-0.00445	-0.00473	-0.01506
Tyrosine	0.03642	-0.04014	-0.06098	-0.00366	-0.04908	-0.03344	0.02504	0.00232	-0.03209	-0.01214	0.02255	-0.01431
Stearic aci	0.00828	0.00038	-0.00073	-0.01848	0.0274	-0.00286	0.00806	0.00414	-0.00715	0.05771	-0.01706	-0.0368
Gallic acid	-0.00619	-0.00315	0.00665	0.00947	0.02726	-0.00828	-0.00458	0.01656	-0.01695	-0.00761	-0.02577	-0.00585
cis-Aconiti	0.08898	-0.14646	-0.10277	0.59339	-0.15438	0.13823	0.04795	-0.57354	-0.02231	0.15932	-0.00698	0.06164
Epinephrir	-0.00261	0.00944	-0.00075	-0.00989	-0.0092	0.01012	0.00598	-0.02143	0.01709	0.00928	-0.03492	-0.00169
Homocysti	-0.0023	-0.00383	-0.00052	-0.00198	-0.00398	0.00838	0.01112	-0.00748	-0.00109	-0.00524	0.01911	0.02788
Methylma	-0.00313	-0.00383	0.00516	0.00651	-0.00296	-0.00447	0.00108	0.00211	-0.00832	0.00114	-0.00697	-0.00763
beta-Alani	-0.0727	-0.00112	0.06955	-0.01163	0.04945	0.07543	0.00043	-0.01984	0.00457	0.04256	-0.05214	-0.01765
octadecylg	0.22129	0.13892	-0.2606	0.03063	-0.36776	0.08394	-0.07564	0.10163	-0.08395	0.05081	0.04062	-0.00388
Xylose	0.01155	0.00128	-0.01839	-0.01721	0.02241	0.01585	-0.04678	0.04264	-0.0245	-0.12128	0.05181	0.03621
Xylulose	0.02731	-0.01037	-0.00594	0.01566	-0.01924	-0.02926	-0.00274	-0.02588	-0.03759	0.04317	0.00453	0.04037
DL-Homoc	-0.01013	0.00321	-0.00174	-0.00827	0.00048	0.00769	-0.0045	0.00215	-0.01382	-0.00028	-0.02449	0.0189
5-Adenosy	-0.00899	0.00083	0.00463	-0.00179	0.00848	0.00551	-0.00196	-0.00309	-0.00326	-0.00083	-0.01055	-0.01753
Quinolinic	-0.02439	0.00503	-0.02464	-0.01305	0.00387	0.01686	-0.00126	-0.00159	-0.04531	-0.00063	-0.03851	-0.0065
Pyridoxine	0.00106	0.00335	0.00787	-0.00359	0.00242	0.00459	-0.00765	-0.01259	-0.0111	0.00311	-0.01416	0.01443
Melibiose	0.04524	0.0063	0.10955	0.04226	0.05116	0.01738	0.05751	0.05941	-0.003	0.00936	0.32222	-0.02453
L-Histidine	-0.00696	8.98E-05	-0.00334	-0.00335	0.00013	0.00661	9.72E-05	-0.00191	-0.01724	-0.00343	-0.01254	0.04062
palatinitol	0.0028	0.05233	0.00044	0.00673	-0.00767	-0.00395	-0.00458	-0.01982	0.00343	0.0099	-0.01703	0.0185
Catechin	0.00684	0.01478	-0.03359	-0.05552	0.01984	0.0678	-0.00863	-0.02988	-0.02252	-0.01865	-0.02554	0.00908
Malonic ac	-0.00048	-0.00181	-0.00188	-0.00444	-0.00197	0.00422	-0.00181	0.00054	-0.00961	-0.00188	-0.01101	0.01002
Ureidopro	-0.01472	0.01404	-0.01785	-0.0326	0.00144	0.03648	0.00799	-0.01489	-0.01313	-0.0045	0.00925	-0.02189
DL-Homoc	0.005	0.00698	0.00142	-0.00118	0.00112	0.00805	0.00359	0.00044	-0.01233	-0.01385	0.0201	-0.07685
Spermidin	-0.01858	0.00319	-0.01566	-0.01062	0.00222	0.02116	-0.00115	-0.00477	-0.04372	-0.00458	-0.02857	-0.15661
Nonadeca	0.02893	0.05669	-0.01468	0.06097	0.07813	-0.03461	-0.02446	0.04592	-0.08831	-0.02168	-0.02591	-0.04508
Maltose	0.01496	0.02108	-0.02912	-0.03042	-0.01146	0.03155	0.01694	0.0316	0.03282	0.00261	0.00122	0.02161
3-Hydroxy	-0.00579	-0.00049	-0.00282	-0.00652	-0.00381	0.00922	-0.0031	-0.00427	-0.00458	-0.01441	-0.00406	-0.00755

	Comp. 1	Comp. 2	Comp. 3
3-Nitro-L-T	4.8282	4.6674	4.5504
2-Phospho	4.4903	4.3812	4.3389
D-Ribose 5	4.4863	4.3772	4.3358
octadecylg	4.1974	4.0581	4.0218
Hexadienc	4.1658	4.0384	4.1768
Glutamine	2.8748	3.065	2.9808
Dodecadie	2.1854	2.1462	2.1976
Octanen-	2.107	2.0525	2.1597
Hexanal, d	1.9171	1.9108	1.8722
Maltotrios	1.8144	2.6105	2.5411
Campheni	1.6667	1.6468	1.6726
Hexadiena	1.4232	1.392	1.7463
Melibiose	1.3833	1.3503	1.315
Manool ox	1.3141	1.3973	1.365
Sesquilava	1.2938	1.2613	1.2287
cis-Aconiti	1.2828	1.2876	1.2515
Farnesol 2	1.2675	1.2357	1.204
Cedroxyde	1.1427	1.4353	1.5681
Leaf alcoh	1.1338	1.1009	1.0844
beta-Alani	1.1246	1.0923	1.0757
Tyrosine	1.0663	1.0312	1.0087
Hexalactor	0.89504	0.87841	0.8571
Lavanduly	0.86881	0.8793	0.85663
Karahanae	0.82953	1.0521	1.0632
Nootkatin	0.7903	0.80158	0.80837
Urea	0.76858	0.74302	0.72288
Harmaline	0.73733	0.71316	0.6932
Cytidine	0.67497	0.66096	0.64392
6-phospho	0.62292	0.60628	0.59506
DethioBiol	0.6171	0.59699	0.58029
propane-1	0.60623	0.5862	0.57546
Octen-3-o	0.59238	0.57393	0.55843
Manool ox	0.58514	0.61996	0.61944
Hexadecar	0.52932	0.51169	0.51683
Hydroxyla	0.52491	0.51419	0.50284
Succinic ac	0.50654	0.49656	0.48533
Ethyl ethe	0.45729	0.60416	0.67828
Geranyl-Pl	0.44824	0.4394	0.43124
Docosane	0.39685	0.39254	0.38448
UDP-N-acı	0.38415	0.40903	0.51698
oxamic aci	0.37608	0.48561	0.52791
5-Aminole	0.37215	0.41148	0.40681
Maltose	0.37043	0.35834	0.34879
Catechin	0.36854	0.35656	0.34757
Linalooltet	0.33713	0.43754	0.44959
Phytol	0.3315	0.33096	0.3296
Heptanon	0.32796	0.41444	0.46509
2-Hydroxy	0.30985	0.30381	0.29721
Cyclohexa	0.26851	0.26287	0.25572
Tritriacont	0.25359	0.24805	0.25829
Heptan-2-	0.24947	0.26641	0.2592
Nonadeca	0.24372	0.28545	0.29619
Quinolinic	0.23675	0.24052	0.23849
putrescine	0.22812	0.22074	0.21463
Tryptamin	0.22479	0.23533	0.23026
Octadecan	0.22308	0.21897	0.21466
2-Coumari	0.22206	0.21779	0.21813
Pantothen	0.22171	0.21656	0.21229
Xylulose	0.219	0.21571	0.22784
Penten-3-o	0.21873	0.25955	0.25469
Raffinose	0.21757	0.21578	0.21434
Tagetoned	0.2075	0.20133	0.2623
N-Alpha-A	0.20695	0.20841	0.21368
Gly-Gly	0.20504	0.20715	0.21194
Heptacosa	0.20433	0.29165	0.33581
Gallic acid	0.20207	0.19805	0.20586
Heptadeca	0.20088	0.22804	0.23387
Cysteamin	0.1976	0.19199	0.19109
Ureidopro	0.19477	0.19896	0.19358
Cysteinylg	0.19407	0.20754	0.2082
Laciniata f	0.19387	0.21039	0.25639
Sorbate	0.19249	0.19548	0.19279
Isopulegyl	0.18706	0.18366	0.18179
Galactitol	0.17863	0.17599	0.17106
N-Acetyl-D	0.17304	0.17089	0.16611
Urocanic a	0.17272	0.18028	0.18927
Benzoic ac	0.17086	0.16534	0.16285
Tetradecei	0.1662	0.16067	0.15791
Senecioic a	0.16219	0.16141	0.15768
5,6-Dihydr	0.15997	0.16667	0.17573
Cysteine	0.15754	0.15683	0.15673
Xylose	0.15586	0.16247	0.16451
Isopentyl t	0.15536	0.15588	0.15585
Spermidin	0.15063	0.15673	0.15523
Nonadeca	0.14847	0.14393	0.14496
2-Oxoglut	0.14655	0.15861	0.16127
Cystamine	0.14427	0.20439	0.20122
Undecane	0.13584	0.13151	0.12986
4-Hydroxy	0.13433	0.39625	0.39234
Tetracosar	0.12881	0.13083	0.12743
Hexyl acet	0.11551	0.12629	0.12276
2'-Deoxya	0.10443	0.10714	0.10462
Musk keto	0.1035	0.10015	0.10283
Encecalin	0.10121	0.15699	0.19396
Octadecen	0.09956	0.09663	0.09742
Octadecan	0.0991	0.09623	0.09532
Hexenoic a	0.09903	0.13412	0.15448
S-Adenosy	0.09681	0.09429	0.09551
Fumaric ac	0.09615	0.11913	0.13166
Pentadeca	0.09467	0.09299	0.09054
Pyridoxine	0.09454	0.0914	0.08947
Phosphory	0.09448	0.09149	0.08904
Dotriacont	0.09133	0.08974	0.09007
palatinitol	0.08466	0.09004	0.10217
Taurine	0.08402	0.09008	0.15596
Trehalose	0.08052	0.20679	0.20862
Jasmolacto	0.07627	0.07861	0.07909
N-Formylk	0.07148	0.07427	0.09848
Tridecane	0.06849	0.06849	0.06814
glycolic ac	0.06837	0.07773	0.07716
Dihydro ci	0.06762	0.07991	0.07947
Decanen-	0.06228	0.06036	0.07101
Ethyl meni	0.05899	0.21086	0.32636
Isobutyl ac	0.05638	0.05451	0.09959
Octanol ac	0.05433	0.05321	0.05546
Methylma	0.05326	0.05218	0.05079
Trimethyl	0.05178	0.05185	0.05321
Calamenei	0.05103	0.05074	0.04953
Palmitolei	0.04937	0.04826	0.05354
3-Hydroxy	0.04384	0.04812	0.04678
Hexacosar	0.04364	0.04374	0.04346
Nonacosar	0.04222	0.04149	0.04068
Stearic aci	0.03858	0.0617	0.06722
Malonic ac	0.03753	0.03659	0.03568
Citronellel	0.03739	0.04937	0.04804
Cedranone	0.03534	0.03416	0.03378
Homocysti	0.03393	0.0358	0.03638
lactic acid	0.03299	0.05082	0.05463
Hexadecar	0.03287	0.03326	0.04053
L-Histidine	0.03276	0.03868	0.03834
Heneicosa	0.03274	0.03167	0.03375
Gluconola	0.03243	0.11784	0.11668
Tumerolar	0.02852	0.02772	0.02695
Epinephrir	0.0277	0.03837	0.04228
Untriacont	0.02739	0.02759	0.02856
Ornithine	0.02549	0.02464	0.02761
Phenyleph	0.02476	0.03643	0.04047
Hexadecer	0.0242	0.02456	0.02438
Asparagin	0.02377	0.03601	0.03781
Tricosane	0.02204	0.03796	0.03883
Nonanen-	0.02188	0.02338	0.04146
Pentacosa	0.02141	0.05448	0.10055
Aspartate	0.02128	0.02253	0.02542
DL-Homoc	0.01635	0.01673	0.02508
Serotonin	0.01607	0.01571	0.02054
pyruvic aci	0.0094	0.02058	0.02346
Eicosane	0.00911	0.01755	0.02582
tranexami	0.00398	0.0051	0.00933
Ribose	0.00394	0.01228	0.01959
Octacosan	0.00377	0.00628	0.01115
Eicosene1-	0.00359	0.01197	0.01215
DL-Homoc	0.00165	0.03046	0.03262

	MeanDecreaseAccuracy
octadecylg	0.0068
Glutamine	0.00667
Farnesol 2	0.0066
Lavandulyl	0.00593
Sorbate	0.00593
Sesquilava	0.00565
Pentadeca	0.0054
Hexadienc	0.00533
Ribose	0.00516
palatinitol	0.00513
Tritriacont	0.00513
2-Phosphc	0.00497
Harmaline	0.0049
Nootkatin	0.0049
3-Nitro-L-T	0.00467
DethioBiot	0.0045
Tyrosine	0.0043
Dihydro ci	0.00423
Urocanic a	0.00417
Palmitolei	0.00417
Linalooltet	0.0041
Trehalose	0.004
UDP-N-ace	0.00398
Gluconola	0.00395
S-Adenosy	0.00393
glycolic ac	0.00393
Trimethyl	0.0039
N-Alpha-A	0.0039
Hydroxyla	0.00374
Cysteinylg	0.0037
Leaf alcoh	0.00367
Tryptamin	0.00363
Gly-Gly	0.00353
5-Aminole	0.00347
Penten-3-o	0.00337
lactic acid	0.00333
Senecioic a	0.00332
Ureidopro	0.00327
N-Formylk	0.0032
Octen-3-o	0.0032
oxamic aci	0.00317
L-Histidine	0.003
Epinephrir	0.003
Pantothen	0.003
Encecalin	0.00297
2-Oxoglut	0.00297
Cystamine	0.00297
Spermidin	0.0029
Pyridoxine	0.00287
Hexadecar	0.00287
Urea	0.00285
2-Hydroxy	0.00282
Hexenoic a	0.00281
Manool ox	0.0028
4-Hydroxy	0.00267
Tetracosar	0.00263
Methylma	0.0026
Tetradecer	0.00257
Cytidine	0.0025
Gallic acid	0.00247
2'-Deoxya	0.00233
3-Hydroxy	0.00233
Succinic ac	0.0022
DL-Homoc	0.00213
Cedranone	0.002
Asparagin	0.002
Hexadecar	0.002
beta-Alani	0.00199
Octadecan	0.0019
Serotonin	0.00187
Hexacosar	0.00183
Cysteine	0.0018
Tagetoned	0.00179
pyruvic ac	0.0017
Ornithine	0.00167
Citronellel	0.00167
Cedroxyde	0.00167
Xylulose	0.00159
Geranyl-PI	0.00157
Fumaric ac	0.0015
Calamenei	0.0015
Ethyl ethe	0.0015
Taurine	0.0014
Laciniata f	0.0014
D-Ribose 5	0.0014
Heptan-2-	0.0014
Phosphory	0.0014
Cyclohexa	0.00133
Hexadecer	0.00133
Jasmolacto	0.0013
Maltose	0.0013
Tumerolar	0.0013
Phenyleph	0.0013
Heptadeca	0.00129
Nonadeca	0.0012
Isobutyl ac	0.00117
Nonadeca	0.00107
Octanen-	0.00107
Musk keto	0.00107
Docosane	0.001
5,6-Dihydr	0.001
Galactitol	0.001
propane-1	0.001
Manool ox	0.001
Quinolinic	9.00E-04
Pentacosa	9.00E-04
tranexami	0.00083
Phytol	0.00083
putrescine	0.00067
Hexanal, d	0.00067
Aspartate	0.00063
6-phosphc	0.00063
Hexadiena	6.00E-04
Catechin	0.00057
Isopentyl I	4.00E-04
Tricosane	4.00E-04
Dodecadie	4.00E-04
Heptanon	0.00033
Stearic aci	3.00E-04
Melibiose	0
Xylose	0
cis-Aconiti	0
2-Coumari	0
Maltotrios	0
Benzoic ac	0
Karahanae	0
Untriacont	0
Nonanen-	0
Decanen-	0
Raffinose	-0.00017
Octadecen	-0.00017
DL-Homoc	-0.00023
Heptacosa	-3.00E-04
Isopulegyl	-0.00033
Malonic ac	-4.00E-04
Tridecane	-4.00E-04
Campheni	-4.00E-04
Octanol ac	-4.00E-04
Hexalacto	-0.00043
N-Acetyl-D	-5.00E-04
Undecane	-5.00E-04
Dotriacont	-0.00051
Eicosane	-6.00E-04
Homocysti	-0.00063
Ethyl meni	-0.00067
Octadecan	-0.00067
Cysteamin	-0.00093
Eicosene-1	-0.001
Octacosan	-0.001
Heneicosa	-0.00117
Hexyl acet	-0.00173
Nonacosar	-0.00367

Differential olive grove management regulates the levels of primary metabolites in xylem sap

Plant and Soil Journal

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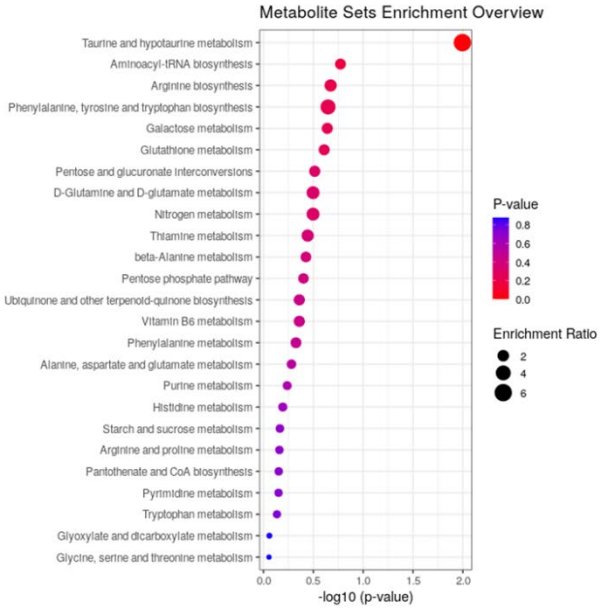
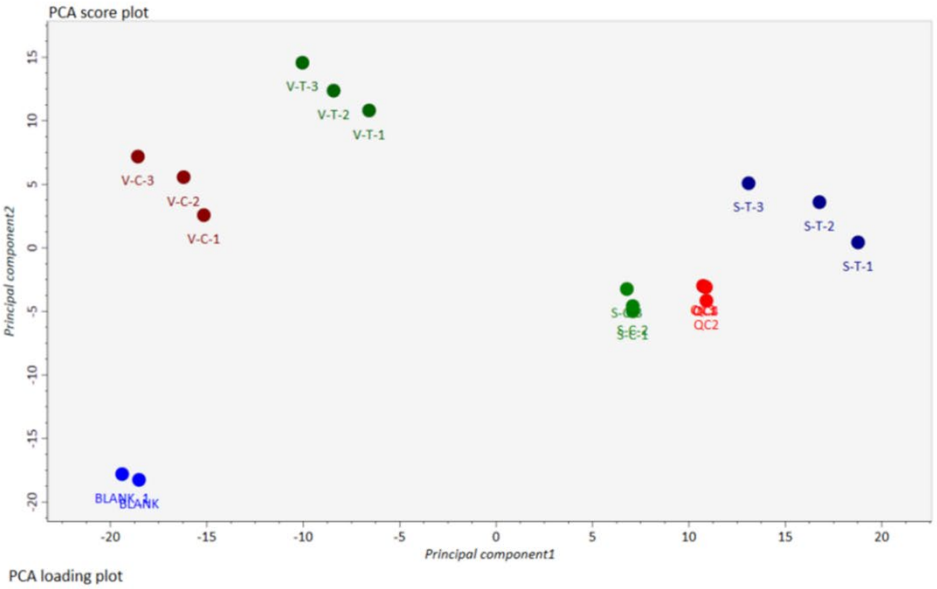
Supplementary material

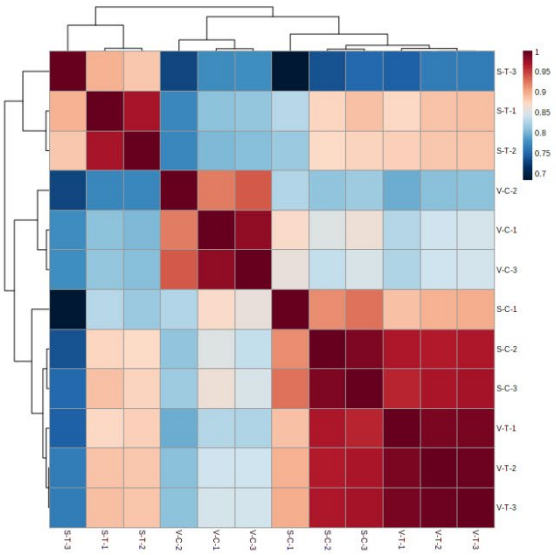
Supplementary Figure S1. Pathway enrichment analysis revealed different metabolic pathways that were enriched, but none were significantly differential (p value cut off ≤ 0.05).



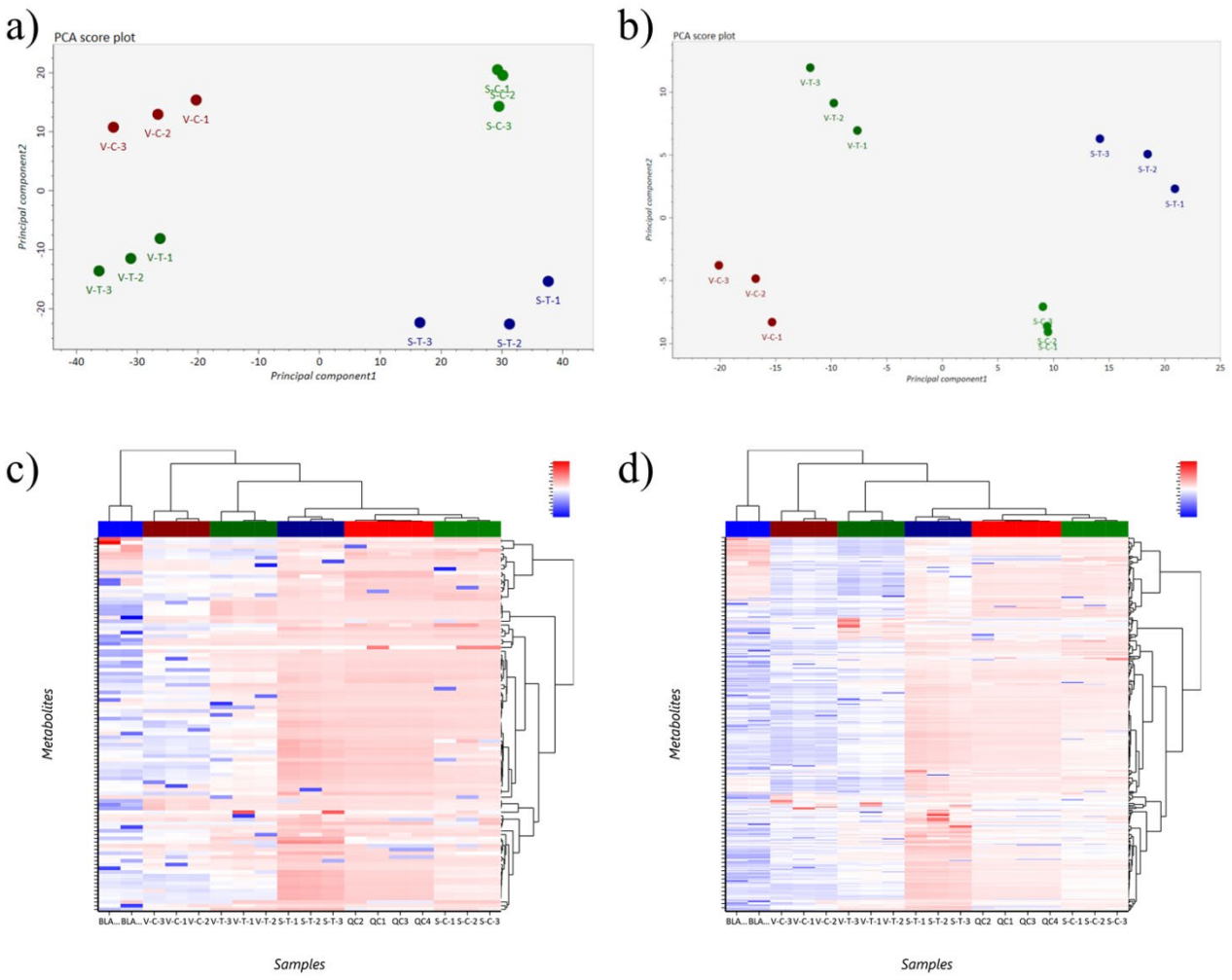
Supplementary Figure S2. A score plot for the principal component analysis (PCA) displaying the first 2 principal components (PC1, PC2) showing the good separation of blanks, QCs, and the 4 sample groups (S_{sust}, S_{ctrl}, V_{sust} V_{ctrl}) thus indicating a good quality assurance of our untargeted GC-MS based platform. Note the S_{ctrl}, S_{sust} groups located in different quadrants than V_{ctrl}, V_{sust} sample groups. (S_{ctrl} = SC, S_{sust} = ST, V_{ctrl} = VC, and V_{sust} = VT) (n =3).



Supplementary Figure S3. Pearson correlation among the samples based on the relative metabolite abundances. (S_{ctrl} = SC, S_{sust} = ST, V_{ctrl} = VC, and V_{sust} = VT) (n =3).



Supplementary Figure S4. Principal component analysis (PCA) and hierarchical clustering analysis (HCA) for the sample groups used in the study. **(a)** PCA showing PC1, PC2 based on relative abundances of all identified compounds. **(b)** PCA showing PC1, PC2 based on relative abundances of all unknown/ unassigned compounds. **(c)** HCA is shown as a heat map displaying the sample groups and QCs for all identified metabolites. **(d)** HCA is shown as a heat map displaying the sample groups and QCs for all unknown/ unassigned metabolites. (S_{ctrl} = SC, S_{sust} = ST, V_{ctrl} = VC, and V_{sust} = VT) (n =3).



Supplementary Figure S5. (a) Pearson correlation showing clustered groups of metabolites in the study samples. **(b)** Hierarchical clustering analysis (HCA) of relative normalized abundances of top 25 metabolites (selected from3-way ANOVA) displayed as a heatmap where columns are individual samples and the rows are metabolites. (S_{ctrl} = SC, S_{sust} = ST, V_{ctrl} = VC, and V_{sust} = VT) (n =3).