การตอบสนองทางเมแทบอลิซึมของ *Aspergillus niger* ES4 ต่อความเครียดจากเอทานอล

นางสาววิมลสิริ กองไชย

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรมหาบัณฑิต
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METABOLIC RESPONSES OF *Aspergillus niger* ES4 TO ETHANOL STRESS

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วิมลสิริ กองไชย : การตอบสนองทางเมแทบอลิซึมของ *Aspergillus niger* ES4 ต่อความเครียดจากเอทานอล (METABOLIC RESPONSES OF *Aspergillus niger* ES4 TO ETHANOL STRESS) อ.ที่ปรึกษาวิทยานิพนธ์หลัก: ผศ. ดร. นวพร วินยเวคิน, อ.ที่ปรึกษาวิทยานิพนธ์ร่วม: ผศ. ดร. วรินทร ชวศิริ, 89 หน้า.

Aspergillus niger ES4 เป็นราที่แยกมาจากผนังด้านบนของถังเก็บเอทานอลของบริษัท ปตท. จำกัด (มหาชน) เนื่องจากโดยปกติจุลินทรีย์จะไม่สามารถทนต่อเอทานอลในปริมาณสูงได้ การโตของ *A. niger* ES4 บนถังเก็บเอทานอล จึงบ่งชี้ถึงคุณสมบัติพิเศษของราสายพันธุ์นี้ในการตอบสนองต่อเอทานอล งานวิจัยนี้จึงสนใจศึกษาผลของเอทานอลต่อการผลิตสารเมแทบอไลต์ของ *A. niger* ES4 โดยการวิเคราะห์เมตาโบโลมิกส์ทั้งแบบไม่มีเป้าหมายและแบบมีเป้าหมาย เมื่อเลี้ยง *A. niger* ES4 ในอาหารเลี้ยงเชื้อ minimal media ที่มีเอทานอลเข้มข้น 4% เป็นเวลา 3 วัน *A. niger* ES4 มีการตอบสนองต่อเอทานอล โดยการผลิตสารเมแทบอไลต์ที่เปลี่ยนแปลงไป เมื่อเทียบกับภาวะที่ไม่มีเอทานอล สำหรับการวิเคราะห์เมตาโบโลมิกส์แบบไม่มีเป้าหมาย เราพบจำนวนไอออนสุดท้ายจากโหมดไอออนลบ คือ 18 และ 53 ไอออน มีปริมาณเพิ่มขึ้น และพบ 35 และ 69 ไอออน มีปริมาณลดลง จากตัวอย่างในภาวะที่มีเอทานอลของส่วนอาหารเลี้ยงเชื้อและเส้นใย ตามลำดับ สำหรับโหมดไอออนบวก พบ 177 และ 474 ไอออน มีปริมาณเพิ่มขึ้น และพบ 18 และ 90 ไอออน มีปริมาณลดลงจากตัวอย่างในภาวะที่มีเอทานอลของส่วนอาหารเลี้ยงเชื้อและเส้นใย ตามลำดับ สำหรับการวิเคราะห์สารเมแทบอไลต์แบบมีเป้าหมายในเส้นใย พบว่า ไขมัน 2 ชนิด ได้แก่ ไดเอซิลกลีเซอรอล และไตรเอซิลกลีเซอรอล มีปริมาณเพิ่มขึ้นอย่างมีนัยสำคัญทางสถิติ เมื่อเทียบกับภาวะที่ไม่มีเอทานอล ในขณะที่ไขมันอื่นๆ ได้แก่ กรดไขมัน กรดฟอสฟาติดิก ฟอสฟาติดิลเอทาโนลามีน ฟอสฟาติดิลเซอรีน ฟอสฟาติดิลกลีเซอรอล และฟอสฟาติดิลอินโนซิทอล มีปริมาณเปลี่ยนแปลงเพียงเล็กน้อยหรือไม่เปลี่ยนแปลง สารเหล่านี้อาจเกี่ยวข้องกับการทนทานเอทานอลของ *A. niger* ES4 ซึ่งอาจนำไปสู่การใช้ประโยชน์ในอุตสาหกรรมที่เกี่ยวข้องกับเอทานอล หรือเป็นวิธีใหม่ในการกำจัดราต่อไป

ภาควิชา	เคมี	ลายมือชื่อนิสิต	....
สาขาวิชา	เคมี	ลายมือชื่อ อ.ที่ปรึกษาหลัก	....
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WIMONSIRI KONGCHAI: METABOLIC RESPONSES OF *Aspergillus niger* ES4 TO ETHANOL STRESS. ADVISOR: ASST. PROF. NAWAPORN VINAYAVEKHIN, Ph.D., CO-ADVISOR: ASST. PROF. WARINTHORN CHAVASIRI, Ph.D., 89 pp.

Aspergillus niger ES4 is a fungus isolated from the top wall of an ethanol tank of the PTT public company limited. Because normally, microorganism cannot tolerate high amount of ethanol, the growth of *A. niger* ES4 on the ethanol tank indicates the special properties of this fungal strain in response to ethanol. This research was therefore aimed at studying the effects of ethanol on the metabolites production of *A. niger* ES4 by using both untargeted and targeted metabolomics. When *A. niger* ES4 cultures were grown in minimal media containing 4% of ethanol for 3 days, *A. niger* ES4 responded to ethanol stress by changing contents of metabolite production, when compared with no ethanol conditions. For untargeted metabolomics, we found the final ion lists from the negative ion modes with 18 and 53 ions with increasing levels and 35 and 69 ions with decreasing levels in ethanol-treated samples in media and mycelium, respectively. For the positive ion modes, we found 177 and 474 ions with increasing levels and 18 and 90 ions with decreasing levels in ethanol-treated samples in media and mycelium, respectively. For targeted metabolomics in mycelium, two lipids, diacylglycerol and triacylglycerol, were statistically-significantly elevated when compared with no ethanol conditions, while other lipids, such as fatty acid, phosphatidic acid, phosphatidylethanolamine, phosphatidylserine, phosphatidyl-glycerol, and phosphatidylinositol, remained unaltered. These metabolites might be related to the tolerance of *A. niger* ES4, potentially benefiting ethanol-related industries or leading to discovery of the novel methods to eliminate mold.

Department:	Chemistry	Student's Signature	....
Field of Study:	Chemistry	Advisor's Signature	....
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LIST OF ABBREVIATIONS

Abbreviation	Full name
mL	millilitre
µL	microlitre
mm	millimetre
µm	micrometre
mM	millimolar
v/v	volume/volume
g	gram
min	minute
°C	degree Celsius
Da	dalton
V	volt

CHAPTER I

INTRODUCTION

1.1 Background and rationales

Molds are a type of microorganism, which are eukaryotic cells in the kingdom Fungi and have cell walls. The main components of cell membranes are chitin and ergosterol. Fungus can be reproduced both sexually and asexually [1]. We usually observe the contamination of fungi in foods or in soil and indoor environment [2]. From the previous experiments, many fungal strains were isolated in the laboratory of Asst. Prof. Dr. Jittra Piapukiew in the Department of Botany, Faculty of Science, Chulalongkorn University from the top wall of the tanks of an ethanol or gasohol of the PTT Public Company Limited (Figure 1.1), which included *Aspergillus niger* ES4, *Aspergillus carneus* EN1, and *Curvularia lunata* ES3 from the top wall of an ethanol tank, and *Penicillium polonicum* GP3, *Aspergillus neoniger* GP5, and *Curvularia lunata* GP6 from the top wall of a gasohol tank. Because normally, microorganism cannot tolerate high amount of ethanol, the growth of these fungi on the ethanol tank indicates some special properties of these fungal strains for survival or ethanol response.

Figure 1.1 Fungal strains on the top wall of an ethanol and gasohol tanks of the PTT Public Company Limited.

From the isolation of these fungal strains, we selected *A. niger* ES4 for studying in this work, because *A. niger* was used in many industries for the production of citric acid [3] and gluconic acid [4], as well as for water treatment [3]. In addition, *A. niger* is used in the production of prolyl endoprotease for using in the treatment of intestinal inflammation (celiac disease) [5].

Microorganisms are coming sources of a various number of natural products, which have the benefit for agriculture and food development, as well as be used as precursors of the new bioactive compounds [6]. Metabolite in microorganisms consist of two types, primary and secondary metabolites. Primary metabolites are products that directly involved in general processes in microbe cells, such as growth, physiological expression, and reproduction. The examples of primary metabolites include amino acids, nucleotides, organic acids and vitamins. Normally, microorganisms will produce primary metabolites during active cell in log growth phase [7]. Secondary metabolites, in contrast with primary metabolites are created for survival or response to environment. These metabolites are usually produced in the early stationary growth phase and may be used for signalers, activators, or inhibitors in cells [8]. Bioactive compounds are mainly secondary metabolites, such as the anticancer compounds nigerasperone from *A. niger* [9] and penicillenols from *Penicillium* sp. [10], and the antifungal compounds cryptocandin A [11] and cryptocin [12] from *Cryptosporiopsis quercina* and clavatol from *A. clavatonanicus* [13].

The extreme environment tends to affect the adaptation of microorganisms. The organic solvent stress is one of the harsh environmental conditions that are highly toxic to microorganisms [14]. Microorganisms then have the adaptive mechanism for survival [15]. For example, the activity of ATPase is inhibited resulting in reduced energy dissipation in the cells, ATP is thus higher in level allowing the repairment of damaged cells [16]. In addition, the efflux pump, which is proteins inserted in the cell membranes, played a role in helping to drive toxic solvents out of cytoplasm [17]. The changed in composition of cell membranes, including the conversion of *cis* isomer of unsaturated fatty acids to *trans* isomer in *Pseudomonas putida*, affect the arrangement of fat, making it more difficult for solvents to enter the cells [18]. Thus, the mechanism of these responses of microorganisms may involve changing in some metabolite production.

Because the importance of metabolites to these organisms in the previous report demonstrated that organic-solvent stress response of microorganism affected metabolite productions within cells of many microorganisms, including energy generation and transport [7], we are interested in studying the effect of ethanol stress on metabolites production both in the cells and outside the cells of *A. niger* ES4, which may be involved in ethanol tolerance of *A. niger* ES4 or its interaction with the other fungi that were found on the top wall of ethanol or gasohol tanks. These metabolites may benefit many industries that are related to ethanol processes or, in the future, may be used as a new method for mold elimination.

1.2 Theory and literature review

1.2.1 *Aspergillus niger*

Aspergillus niger is a dark colored fungus that produces black conidial head and white septate hypha, which is abundantly branched [3] (Figure 1.2). We usually find the contamination of *A. niger* on fruits and vegetable such as grapes, apricots, onions, and peanuts [19] (Figure 1.3), as well as in soil and indoor environment [2]. This fungal species can be grown under different temperature such as 6-8 °C (minimum), 45-47 °C (maximum), and 35-37 °C (optimum) [20].

Figure 1.2 Features of *Aspergillus niger* [21].

Figure 1.3 The contamination of *A. niger* on onions, grapes, and peanuts [22-24].

A. niger has many benefits in biotechnology and many industries, especially in the production of citric acid, gluconic acid, and oxalic acid, as well as various enzymes such as amylase, lipase, pectinase and amyloglucosidase [25]. Many of its industrial applications have been given GRAS (generally regarded as safe) status [2]. In addition, *A. niger* is used in the production of prolyl endoprotease for the treatment of intestinal inflammation (celiac disease) [5]. Moreover, *A. niger* could be produced bioactive compounds as an anticancer agents, such as asnipyrone A, nigerapyrone B, nigerapyrone D, and nigerapyrone E [26].

1.2.2 Metabolites in microorganisms

Microorganisms are very important to environment and necessary to life systems. Microbes are basic sources of nutrients, as well as are first recyclers in environment. These organisms are used in the preparation of many foods [6]. Normally, microorganisms will produce both primary and secondary metabolites in metabolic processes for their living. The details are explained as follow:

1.2.2.1 Primary metabolites are a key for suitable growth of microorganisms, including nucleotides, amino acids, vitamins, and the fermentation of final products, such as ethanol and organic acids [27].

Amino acids are builders of protein molecules and are used in nutritive, meal supplements, and pharmaceutical industries as additives and drugs [28]. Many microorganisms can produce various amino acid. For example, glutamate are obtained from a lot of microorganisms of the genus *Brevibacterium*, *Corynebacterium*, *Micrococcus* and *Microbacterium* [7]. In addition, some microbes can produced amino acids by fermentation. For example, *C. glutamicum* produced L-valine [29] and L-tryptophan [30], and L-arginine from *Serratia marcescens* [29].

Vitamins are necessary micronutrients, which are required in small amount and cannot be synthesized by mammals. Therefore, nutritive supplements from external sources are essential for controlling the metabolism in all living systems [31]. Microorganisms produced vitamins during normal metabolism. These vitamins are universally used as food additive, meal supplements, and therapeutic agents [32]. For example, riboflavin was produced from *Eremothecium ashbyii*, *Ashbya gossypii*, *Bacillus subtilis* and *Corynebacterium ammoniagenes* [33]. Moreover, cyanocobalamin (vitamins B_{12}) are synthesized from *Propionibacterium shermanii* and *Pseudomonas denitrificans* [34].

Organic acids are used as various ingredients, such as in food, drinks, pharmaceuticals, solvents, petrochemicals, rubber, perfumes, plastics, and dyes [27]. In addition, microorganisms are used in the production of many organic acids for commerce, such as acetic acid, lactic acid, gluconic acid, and citric acid [35]. The examples of microbes that are used in various industries are *Candida catenula*, *C. guilliermondii*, *C. tropicalis* and *Yarrowia lipolytica*, and *Aspergillus* sp. The fungus *Aspergillus* sp. are used for citric acid production in food industries, as citric acid serves as flavoring agents, preservatives, and emulsifiers [6]. Other genus of microorganisms, such as *Ustilago*, *Candida*, and *Rhodotorula*, can be used to produce itaconic acid, which is used mainly in the production of resins and plastics [36]. *Aspergillus terreus* is preferred because it produces higher yield of itaconic acid [37].

Alcohol (or ethanol) is widely used as biofuel and also as raw materials for several chemical industries, such as waxes, oils, explosives, dyes, cosmetics, laboratories, as well as antibiotic agents [6]. It has been reported in the previous studies that the maximal production of total ethanol (about 90-95%) could be achieved the process of microbial fermentation [38]. The recombinant strains of *E. coli*, *Klebsiella oxytoca*, and *Clostridium thermocellum* strains, under different carbon sources also allow the production of ethanol [39].

Lipids are one of primary metabolites, which are important energy sources for microorganism [7], and can act as signaling messengers between cells once secreted [40]. Fatty acids are the basic carboxylic acids with long aliphatic chains of all kinds of lipids. Fatty acid composition is changed affect transformation of membrane properties and functions in cells [41].

In this work, we focused on studying the production of lipid metabolites in the cells of *A. niger* ES4 under ethanol stress. For example of lipids in this work, including diacylglycerol (DAG, 16:0/18:1), triacylglycerol (TAG, 16:0/16:0/18:1), free fatty acid (FFA, C18:0), phosphatidic acid (PA, 16:0/18:1), phosphatidylethanolamine (PE, 16:0/18:1), phosphatidylserine (PS, 16:0/18:1), phosphatidylglycerol (PG, 16:0/18:1), phosphatidylinositol (PI, 16:0/18:1) (Figure 1.4).

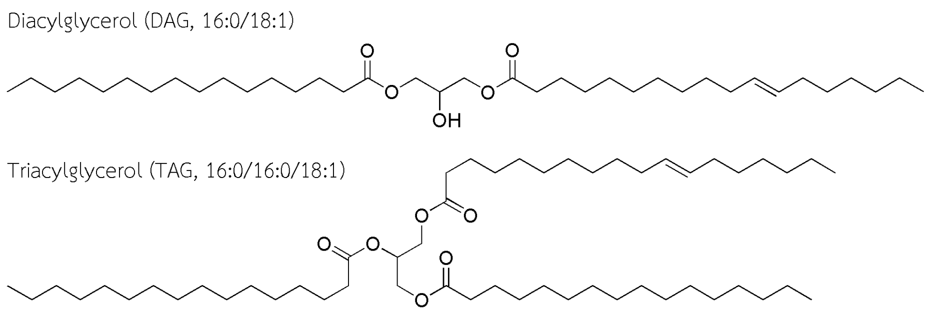

Figure 1.4 Examples of lipids

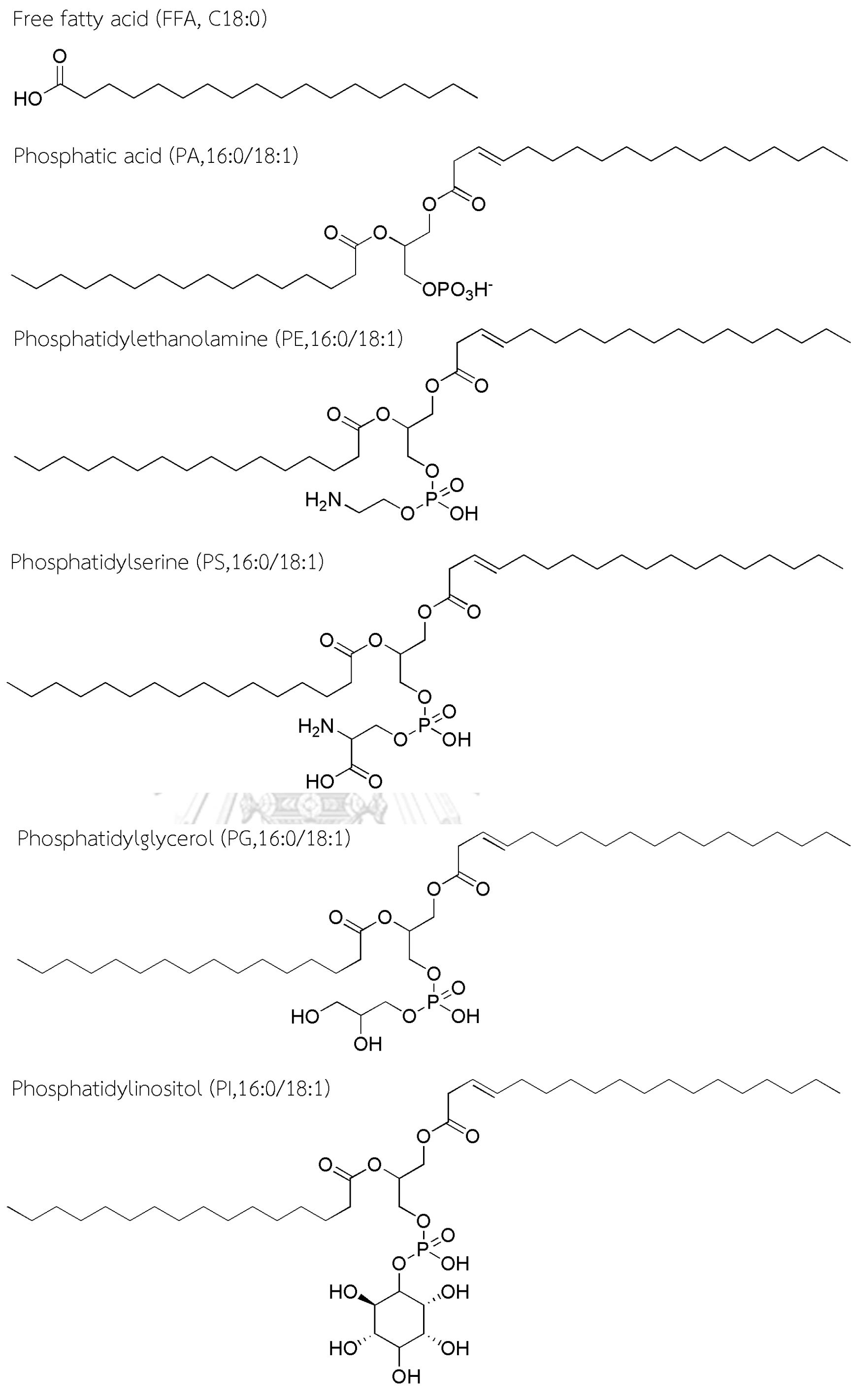

Figure 1.4 Examples of lipids (continued).

The important properties that differentiate all types of lipids in living systems are carbon chain length, saturation, and substitution. The main source for production of lipids in industries are yeasts and fungi, and the minor is bacteria. Fungal species, such as *Cryptococcus curvatus*, *Rhodosporidium*, *Rhodotorula*, and *Lipomyces* can produce 60% to 70% of lipids per biomass weight [42].

1.2.2.2 Secondary metabolites organic compounds that are produced in the growth processes of the near or end of stationary phases, and are not essential for growth and reproduction of microorganisms [43]. Secondary metabolites have been reported that used as plant growth motives, herbicides, insecticides, antibiotics, and antifungal agents. They are also used as active drug ingredients in medicine [44], including in anesthetics, anti-inflammatory agents, anti-coagulants, vasodilatories hypocholesterolemics, and hemolytics, as well as used as antitumor compounds, such as adriamycin, bleomycin, daunomycin, and mithramycin [6]. The examples of secondary metabolites that are obtained from many microorganisms are as follow:

The beginning compound of antibiotics for commercial production are penicillin from the fungal *Penicillin notatum* in 1929 [45]. Next, the discovery of antibiotics are increased from fungi and actinomycetes for the development of higher effective pharmacological properties [46]. For example, streptothricin is obtained from *Streptomyces* sp. [47], and pestacin and isopestacin are produced by *Penicillium microspore*. The other fungus *Aspergillus* sp. produces brefeldin A for using as antibiotics [9].

From the data of *A. niger* above, we explained about the benefits of its metabolites for using in many industrial applications. In this section, we will explain more about known metabolites that *A. niger* usually produces. One of the interesting applications of known metabolites from *A. niger* is for making biopolymers, such as chitin and chitosan and their derivatives such as glucosamine (Figure 1.5) [3]. Moreover, *A. niger* is also found in the production of the important secondary metabolites for using in the food, feed, and biotechnological industries [48], such as asperic acid [49], aspernigrin A [50], nigragillin [48], kotanin [51], funalenone [52], and atromentin [53] (Figure 1.6).

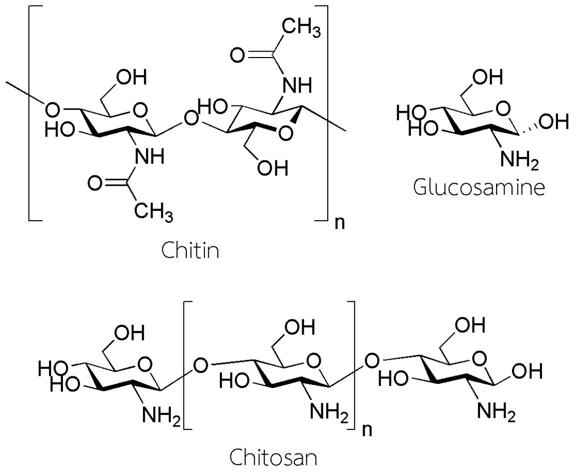

Figure 1.5 Structures of chitin, chitosan, and glucosamine [3].

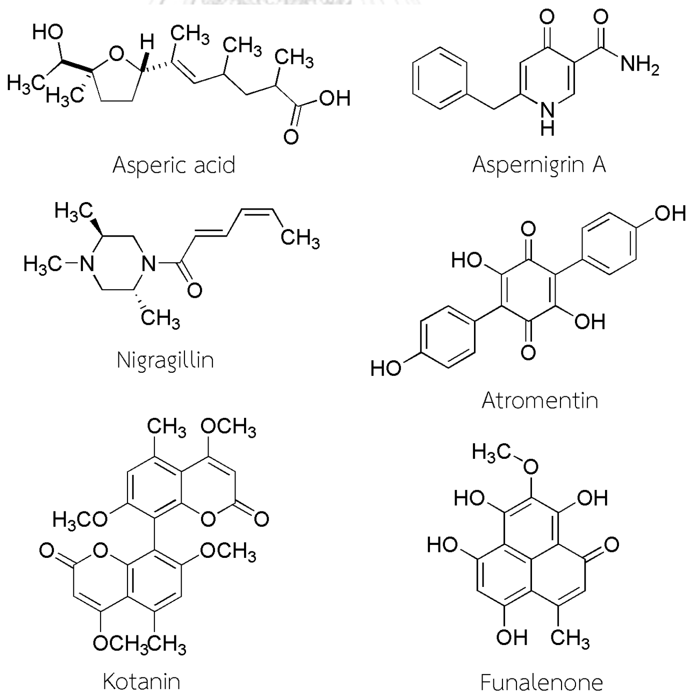

Figure 1.6 Structures of secondary metabolites from *A. niger* [48].

However, *A. niger* has the potentials to produce two groups of carcinogenic mycotoxins, which are fumonisins, such as fumonisin B2, fumonisin B4, and fumonisin B6 [2] (Figure 1.7), and ochratoxins, such as ochratoxin A and B [48] (Figure 1.8).

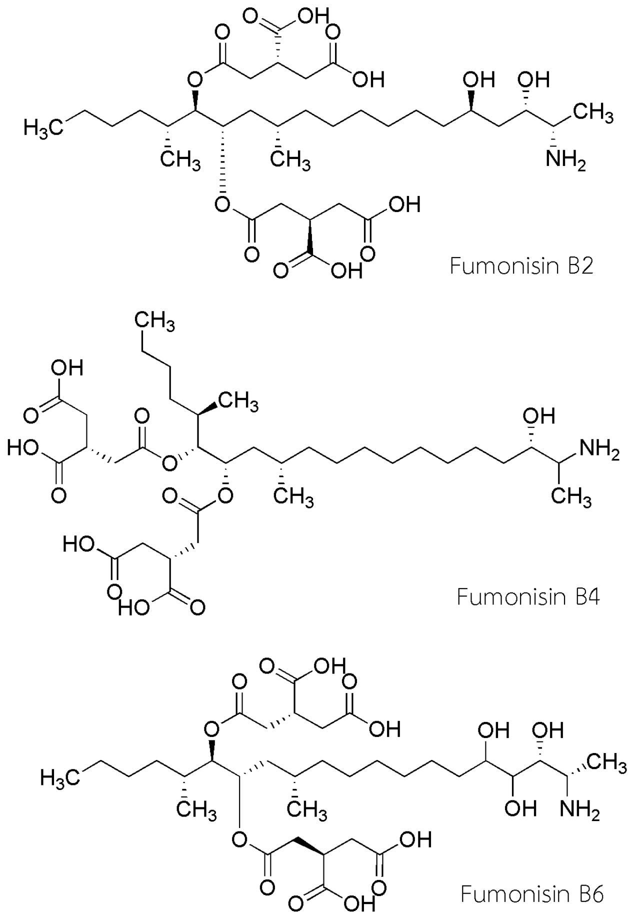

Figure 1.7 Structures of fumonisins from *A. niger* [2].

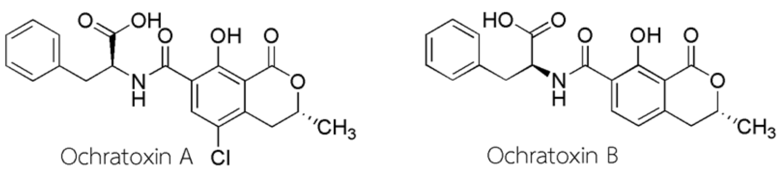

Figure 1.8 Structures of ochratoxins from *A. niger* [48].

1.2.3 Effect of organic solvents on microorganisms

Organic solvents, such as alcohols, phenols, or aromatics, are classified as toxics. Microorganisms then have the mechanisms of adaptation for survival [54]. Several previous studies demonstrated that toxic solvents influence numerous responses of cells, such as abnormal DNA and RNA unfolding, as well as damaged structures of membrane lipids by oxidation reaction [55]. These effects may induce severe stress responses or cell death [15]. In addition, toxic solvents affect to biophysical changes in cell membranes, including energy generation and transport [56].

Mechanistic details of cellular responses or adaptation of micro-organism to toxic solvents are provided as follow:

1.2.3.1 Effects on cell membranes

Cell membranes consist of phospholipid bilayer and proteins. They play roles in maintaining membrane structures and in controlling a signaler for transmission and energy productions from going in and out of cells [15].

The effects of solvent explained above lead to the change in rate of biosynthesis of phospholipid components. For instance, *Pseudomonas putida* changes isomers from *cis*- to *trans*- unsaturated fatty acids, increases the ratio of unsaturated to saturated fatty acids [57], and changes the composition of phospholipid head groups [15] (Figure 1.9).

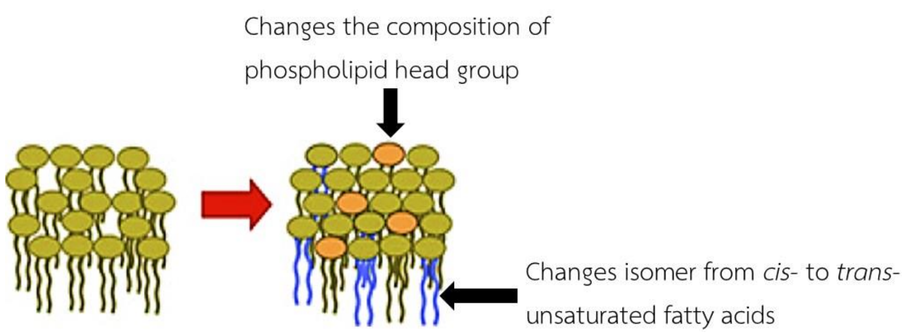

Figure 1.9 Changes in membrane composition and biophysics [15].

Moreover, the carbon chain length of solvent also affects responses of cells. For example, short-chain (C2-C4) alkanols increased the synthesis of unsaturated fatty acids in *Escherichia coli*, while long-chain (C5-C9) alkanols affect increase its saturated fatty acid contents [58].

Ethanol response processes in microorganisms have been abundantly reported in *E. coli* [59] and *Saccharomyces cerevisiae* [60]. The concentration of unsaturated fatty acids in lipid composition was increased in these organisms. The synthesis of oleic acid (C18:1) and palmitoleic acid (C16:1) in *S. cerevisiae* was increased [61]. Other organisms, such as *Bacillus subtilis* [62] and *Clostridium acetobutylicum* [63], on the other hand, increased the production of saturated fatty acids. *Vibrio parahaemolyticus* increased the production of vaccenic acid (C18:1), while decreasing the production of palmitic acid (C16:0) and ratio of saturated fatty acid to unsaturated fatty acids. In *Mucor rouxii*, the ratio of unsaturated fatty acids to saturated fatty acids was decreased [64]. Moreover, in *Schizosaccharomyces pombe*, the production of trehalose [65], lanosterol, and unsaturated fatty acids was increased [66].

From the reports above, the changes in the cell membranes involved the changed production of many metabolites in microbes. In this work, we are therefore interested in studying the changes in production of metabolites in the presence of ethanol.

1.2.3.2 Effects on efflux pumps

Efflux pumps are proteins on cell membranes, which usually help keep toxic solvents or contamination out of cytoplasm [17]. Efflux pumps comprise three parts: an inner membrane protein (IMP), a membrane fusion protein (MFP), and an outer membrane protein (OMP), which simplifies for outflow from the cell (Figure 1.10) [15].

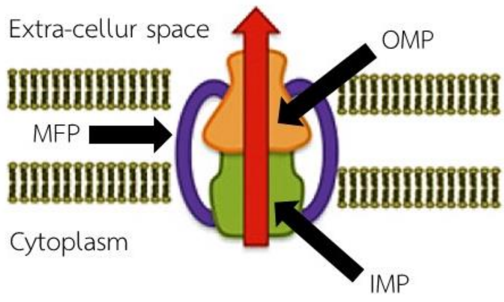

Figure 1.10 Features of efflux pumps in microorganism cell membranes [15].

For example, *E. coli* strain K-12 showed higher cyclohexane tolerance by overexpression of *marA*, *robA*, and *soxS* genes, which increased the activity of efflux pumps by incresing the production of outer membrane proteins AcrA and TolC [67].

1.2.3.3 Effects on heat-shock proteins (HSPs)

Heat-shock proteins (HSPs) is one of chaperone proteins. They are protein complexes, consisting of many proteins subunits. They protected the cells from abnormal polypeptide chains folding, and played a role in the transportation, and decomposition of proteins. Effects of solvent stress leads to overexpression of HSPs for higher survivability [15].

HSPs stress has been most widely studied in *E. coli*. The mechanism of HSPs under solvent stress can be explained through GroEL and GroES (Figure 1.11). GroEL and GroES are the types of HSPs. GroEL will build an empty bucket for protein refolding under solvent stress. At the same time, GroES cap is opened for building a convenient environment for processing ATP hydrolysis [68].

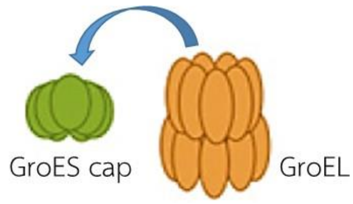

Figure 1.11 HSPs refolding under solvent stress [15].

For example, the overexpression of *groESL* in *C. acetobutylicum* could increase its growth under butanol stress by up to 85% [69]. *groESL* overexpression leads to increased expression of several other HSP genes such as *dnaKJ*, *hsp18*, *hsp90* [70]. Moreover, HSP overexpression was also described in other organisms with more solvent tolerance, including *Lactococcus lactis*, *Lactobacillus paracasei* NFBC 338 [71], *Lactobacillus plantarum* [72] and *S. cerevisiae* [73]. In addition, it was shown that *hsp70* overexpression was involved in ethanol tolerance of *S. cerevisiae* [74]. Thus, these studies explained that responses of HSPs under solvent stress resulted in cell damage protection and allow microbes to have higher tolerance to toxic solvent by refolding proteins, which are importance for cell survival [15].

1.2.3.4 Effects on energy metabolism

Generating energy is an important process for various living systems, including microorganisms. Energy plays a necessary role in management of toxic solvents, such as the activity of efflux pumps and HSP proteins as explained above. Moreover, macromolecules in the cells of organism are damaged when they are under solvent stress. However, energy is essential for cell repairing or synthesis of the important molecules in the presence of stress conditions [15].

For instance, it has been previously reported that the sugar transportation and catabolism of glucose and citric acid cycle was activated, when *P. putida* was under toluene stress effects, to generate high energy for survival, especially for ATP processes in efflux pumps [75]. Other studies of *P. putida* showed that *P. putida* increased the ATP synthase production under toluene stress [75]. In *S. cerevisiae*, the proton and potassium transportations in membrane was stopped when treated with toluene [76]. Also, studies of *C. acetobutylicum* under butanol stress demonstrated that cells must spend more energy for biosynthesis to control the toxicity of butanol [77].

It has been reported that organic solvent stress, such as ethanol, could damage mitochondria DNA and some enzyme types, such as hexokinase and dehydrogenase, causing equilibrium changes in metabolism processes in cells of microbes [78]. Different ethanol concentrations could affect growth of microorganisms as follow:

In 1981, Brown et al. [79] studied different ethanol concentrations on the growth of two yeast strains (*S. cerevisiae* 5D-cyc and NCYC 479) in yeast extract with supplements (YES) medium. The results showed that trends of growth rates (μ, h^{-1}) of both 5D-cyc and NCYC 479 went in the same direction (Table 1.1). At below 1% w/v ethanol, growth was not changed, but growth continued to decrease from ethanol concentrations of 2% w/v to 10% w/v, and growth was completely inhibited under 12% w/v ethanol.

In 1998, Walters et al. [80] studied the growth of *Pyrenophora avenae* that was isolated from plant diseases by weighing *P. avenae*, which were cultured in potato dextrose broth (PDB) under 1%, 3%, and 6 % ethanol conditions, compared to no ethanol conditions. The researchers found that biomass of *P. avenae* in the present of 1%, 3%, and 6% ethanol were 18.0, 9.8, and 1.1 g, respectively. The results showed that the values of all these biomass continued to decrease with higher ethanol concentrations, when compared with normal conditions of 22.3 g (Table 1.2).

Table 1.1 The growth rates (μ, h^{-1}) of NCYC 479 and 5D-cyc under different ethanol concentrations in YES medium [79].

Ethanol (w/v%)	NCYC 479		5D-cyc	
	Growth rate	Percent of control	Growth rate	Percent of control
0	0.280	100	0.258	100
1	0.280	100	0.258	100
2	0.251	89.6	0.239	92.6
3	0.220	78.5	0.213	82.5
4	0.200	71.4	0.180	69.7
5	0.164	58.5	0.156	60.4
6	0.139	49.6	0.135	52.3
7	0.110	39.3	0.109	42.2
8	0.081	28.9	0.081	31.4
9	0.052	18.6	0.056	21.7
10	0.024	8.6	0.027	10.4

Table 1.2 Biomass of *P. avenae* grown under various ethanol concentrations in PDB [80].

Treatment	Biomass (g f.wt)		
	1 day	2 days	3 days
Control	4.1 ± 0.21	19.4 ± 1.20	22.3 ± 1.77
1% Ethanol	4.5 ± 0.56	14.4 ± 0.94*	18.0 ± 1.14
3% Ethanol	1.8 ± 0.12*	4.8 ± 0.29*	9.8 ± 0.63*
6% Ethanol	0.8 ± 0.05*	1.0 ± 0.03*	1.1 ± 0.06*

Results are the means of four replicates.
*Significantly different at $P < 0.001$.

In 2009, Yoshikawa et al. [81] studied the growth behavior of *S. cerevisiae* in single gene deletion strains under 8% ethanol conditions compared with in the absence of ethanol in yeast extract peptone dextrose (YPD). They found average specific growth rate of *S. cerevisiae* in 8% ethanol condition as 0.178 h^{-1} while normal condition as 0.452 h^{-1}. Therefore, the average specific growth rate decreased about 2.5-

fold in the presence of ethanol, compared to no ethanol conditions (Table 1.3).

Table 1.3 The average specific growth rate of single gene deletion strains derived from *S. cerevisiae* under 8% ethanol concentration [81].

Condition	Average specific growth rate (h^{-1})	SD (h^{-1})	Threshold for sensitive strains (h^{-1})*	Threshold for tolerant strains (h^{-1})*
Control	0.452	4.4×10^{-3}	0.437	0.466
8% Ethanol	0.178	5.6×10^{-3}	0.160	0.196

*Thresholds were defined as average specific growth rate ± 3.3 SDs.

In addition, the toxicity of ethanol also affects the production of primary metabolites in microorganisms for adaptation to survive. One of the mechanism in response to ethanol is the change in lipid contents on cell membranes, as found in several of the following reports:

In 1982, Beaven et al. [60] found that *S. cerevisiae* NCYC 431 produced fatty-acyl residues that changed when it was grown under supplementation with ethanol concentrations of 0, 0.5, 1.0, and 1.5 M for 8 h. All three ethanol concentrations increased the ratio of monounsaturated residues, especially in $C_{18:1}$ residues, while decreased the ratio of saturated residues (Table 1.4).

Table 1.4 The adaptation of fatty-acyl composition in *S. cerevisiae* NCYC 431 under supplementation with various ethanol concentrations [60].

Fatty-acyl residue	Fatty-acyl composition (% of total) of phospholipids in organisms from cultures supplemented with ethanol at:			
	0 M	0.5 M	1.0 M	1.5 M
$C_{14:0}$	1.7	1.5	0.4	1.0
$C_{14:1}$	0.4	0.3	0.2	0.4
$C_{16:0}$	42.4	39.0	28.8	21.3

Fatty-acyl residue	Fatty-acyl composition (% of total) of phospholipids in organisms from cultures supplemented with ethanol at:			
	0 M	0.5 M	1.0 M	1.5 M
$C_{16:1}$	29.1	27.9	33.5	37.1
$C_{18:0}$	9.9	11.8	13.4	6.9
$C_{18:1}$	16.7	19.6	23.7	33.5

In 2001, Sakaki et al. [82] studied the production of glycolipid compounds from various fungal species under ethanol stress. *Pichia pastoris* GS115 grown in YPD has sterol glycoside (SG) accumulated when supplemented with 3% or 6% ethanol for 4 h, while cerebroside (Cer) was decreased as shown on thin-layer chromatography in Figure 1.12.

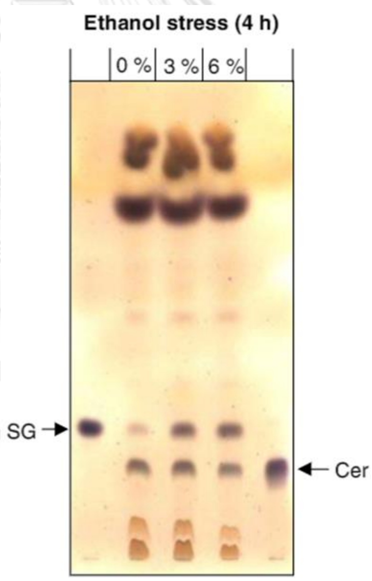

Figure 1.12 Thin-layer chromatography of SG and Cer from *P.pastoris* GS115 in the present of ethanol stress for 4 h [82].

In 2003, You et al. [83] reported that ethanol stress affects unsaturated fatty acids composition in cell membrane of *S. cerevisiae* (*Tni*NPVE trans-formant strain) when cultured in YPD under 5% ethanol conditions. They found that oleic acid ($\triangle^{9}$Z-$C_{18:1}$) content was statistically-significantly elevated, when compared with no ethanol conditions, while other fatty acids, such as, palmitic ($C_{16:0}$), stearic ($C_{18:0}$), and palmitoleic acid ($\triangle^{9}Z\text{-}C_{16:1}$), were decreased (Figure 1.13).

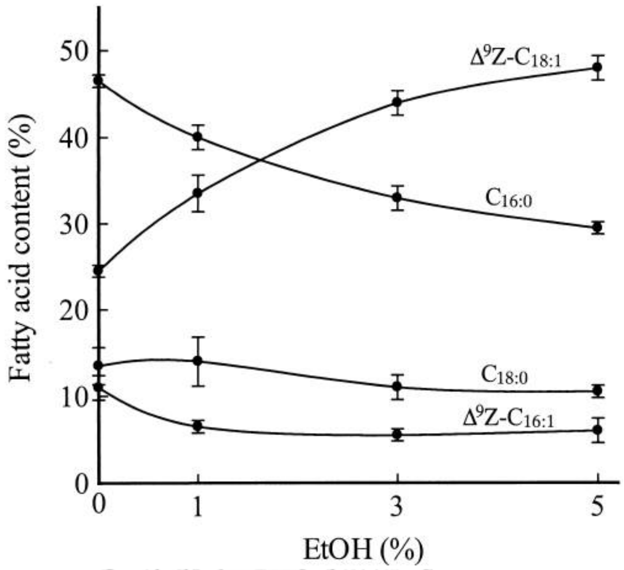

Figure 1.13 Effects of different ethanol concentrations on fatty acid contents of *Tni*NPVE transformant strain [83].

The effect of ethanol stress in the previous reports above, can be explained in terms of lipid metabolites groups. In addition, organic solvents stress also affects other primary metabolites and secondary metabolites, as follow:

In 2000, Chen et al. [84] studied the effect of dimethyl sulfoxide (DMSO) on the production of secondary metabolites in antibiotics group, including chloramphenicol, thiostrepton and tetracenomycin, of various *Streptomyces* strains. The results showed that chloramphenicol from *S. venezuelae* in GNY medium, tetracenomycin C from *S. glaucescens* in TSB medium, and thiostreptone from *S. azureus* in R5 medium were increased over two-fold under 3% DMSO conditions when compared with control conditions. In contrast to 5% DMSO, the yield of chloramphenicol was decreased but there was no effect on tetracenomycin C, while the production of thiostrepton was increased.

In 2015, Zhang et al. [85] studied the primary metabolites production in cyanobacterium *Synechocystis* sp. PCC6803 both in the wild type and the △*slr0982* mutant strains in the presence of 1.5% ethanol at 24, 48, and 72 h. The wild type strain at 24 h showed elevated levels of the key metabolites in various important pathways, including AcCOA, NADPH, NADP, NADH, NAD, ADP-GCS, ATP, ADP, G6P, F6P, and R5P under the ethanol stress conditions, while at 48 and 72 h, these metabolites, including AcCOA, ADP-GCS, ATP, ADP, G6P, F6P, and R5P, were enhanced in the △*slr0982* mutant strain.

1.2.4 Metabolomics

Metabolomics is a technology involved in studying of the metabolites in all living or biological systems [86]. Metabolomics or metabolite profiling is one of omics technologies. It focuses on a study of small biomolecules (below 1.5 kDa) [87], such as nucleic acids, nucleotides, small chain of peptides, fatty acids, lipids, sugars, vitamins, as well as the other organic compounds, such as phenolic and aromatic hydrocarbons [88]. The objective of metabolomics are to compile both types and contents of metabolomes from within the cells or outside the cells through metabolic processes [89].

In the beginning, metabolomics is used for the research in medical sciences, such as studying the relationship between biological fluids, like blood, urine, and saliva obtained from patients, with types of pathology [79]. In the present, this technology is applied for using in agriculture, food science and nutrition [90], including in microorganisms with yeast metabolism to study its responses to different stress conditions [91].

Metabolite analysis will be used for high-throughput chemical techniques, such as nuclear magnetic resonance (NMR) spectroscopy [87] and mass spectrometry (MS). These two techniques are used together with separation techniques, such as gas chromatography–mass spectrometry (GC–

MS), or especially, liquid chromatography–mass spectrometry (LC–MS) [92]. The data analysis can be divided into two types: targeted and untargeted studies [88]. The targeted metabolomics analysis aims to study predefined metabolites, which were carried in reference databases. It provides more sensitivity and accuracy of known metabolites. The untargeted metabolomics is used for unknown metabolites analysis [93]. The metabolomics workflow is shown in Figure 1.14.

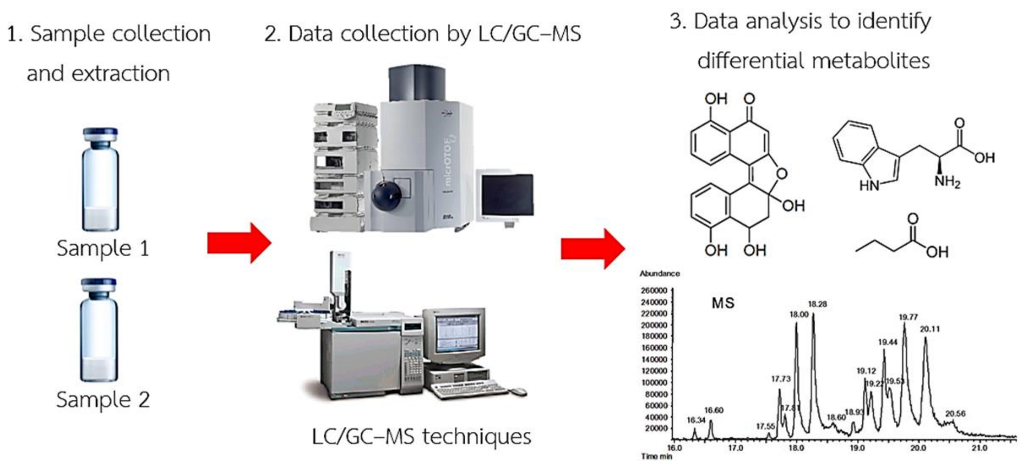

Figure 1.14 The metabolomics workflow.

Many metabolites are analyzed by using metabolomics methods. LC–MS technique is the main technique used for metabolomics analysis, because it is a high-throughput chemical analysis [94], which provides rich mass spectra data of many metabolites in living system for evaluating sample category and biomarker detection [88]. In this work, we are interested in using LC–MS techniques for studying production of many metabolites external and internal of fungal cells under ethanol stress. The examples of metabolomics studies under solvent stress by using LC or LC-MS techniques are shown as follow:

In 1995, Sajbidor et al. [95] analyzed amount of total lipids, ergosterol, squalene, and fatty acids, such as palmitic acid, palmitoleic acid, stearic acid, and oleic acid, in the distillery strain *S. cerevisiae* LH 02/2 grown in basic medium with different ethanol concentrations of 5%, 10% and 15% for three time points (3, 48 and 120 h) by using high performance liquid chromatography (HPLC) and GC techniques. The results showed that higher ethanol concentrations caused more collection of total lipids, and ergosterol, palmitoleic acid, and oleic acid, while palmitic acid and stearic acid were decreased.

In 2015, Vinayavekhin et al. [96] studied untargeted metabolomics analysis of *Bacillus subtilis* under 1-butanol stress by using LC–MS techniques. The researchers found that the production of lipid metabolites of *B. subtilis* changed a lot in Spizizen's minimal media under 1-butanol concentration of 1% with three lipids, including phosphatidylethanolamine (PE), phosphatidyl-serine (PS), and diglucosyldiacylglycerol (DGDAG) being elevated, while other lipids, diacylglycerol (DAG) and lysylphosphatidylglycerol (LysylPG) were decreased (Figure 1.15).

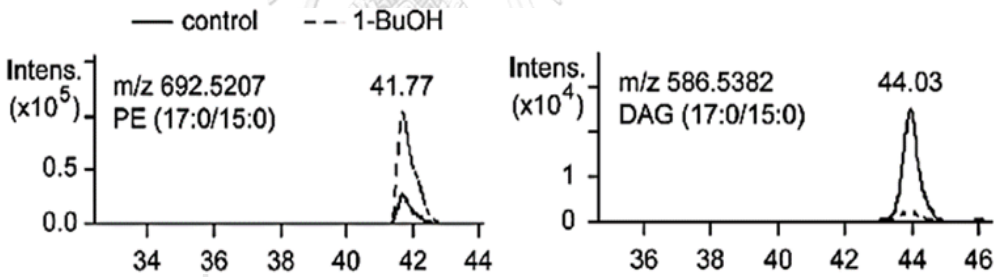

Figure 1.15 Extracted ion chromatograms of some lipids, such as PE and DAG of *B. subtilis* under 1-butanol stress [96].

In the literature review above, it was demonstrated that many microorganisms responded to ethanol stress by using different processes, such as changing the contents of fatty acids and lipids on cell membrane, and effect on the production of other metabolites. Thus, we were interested in studying the effect of ethanol on the production of many metabolites in *A. niger* ES4 both outside and inside cells by using LC–MS techniques, which were divided into two parts for untargeted and targeted analysis.

1.3 The objectives of this research

1.3.1 To study the suitable growth condition of *A. niger* ES4 in MM under ethanol stress for metabolomics analysis.

1.3.2 To study the effects of ethanol on the production of metabolites both in the cells and out of the cells of *A. niger* ES4 by using untargeted metabolomics technique.

1.3.3 To study the effects of ethanol on the production of lipid metabolites in the cells of *A. niger* ES4 by using targeted metabolomics technique.

1.4 Expected beneficial outcomes

1.4.1 Know the suitable growth condition of *A. niger* ES4 in MM under ethanol stress for metabolomics analysis.

1.4.2 Know the change of metabolites production both in the cells and out of the cells of *A. niger* ES4 under ethanol stress for confirming that *A. niger* ES4 shows response to ethanol stress. These metabolites might be used to study the genes or metabolism that were involved in the changed production of these metabolite contents.

1.4.3 Know the change of lipid metabolites production in the cells of *A. niger* ES4 under ethanol stress. These metabolites might relate to the tolerance of *A. niger* ES4, potentially benefiting ethanol-related industries or leading to discovery of the novel methods to eliminate mold in the future.

CHAPTER II
EXPERIMENTAL

2.1 Fungal strain and material

1. *A. niger* strain ES4 was isolated from the top wall of an ethanol tank of the PTT Public Company Limited in the laboratory of Asst. Prof. Dr. Jittra Piapukiew in the Department of Botany, Faculty of Science, Chulalongkorn University

2. Fresh potato for preparation of potato dextrose agar (PDA)

2.2 Chemicals

1. Potato dextrose broth (PDB), Analytical grade; Himedia Laboratories
2. Agar power, Analytical grade; Himedia Laboratories
3. Sodium nitrate ($NaNO_3$), Analytical grade; Ajax Finechem
4. Potassium chloride (KCl), Analytical grade; Ajax Finechem
5. Potassium dihydrogen phosphate (KH_2PO_4), Analytical grade; Ajax Finechem
6. Magnesium sulfate heptahydrate ($MgSO_4 \cdot 7H_2O$), Analytical grade; Ajax Finechem
7. Iron(II) sulfate heptahydrate ($FeSO_4 \cdot 7H_2O$), Analytical grade; Ajax Finechem
8. Ethylenediaminetetraacetic acid disodium salt dihydrate (EDTA; $C_{10}H_{14}N_2Na_2O_8 \cdot 2H_2O$), Analytical grade; Ajax Finechem
9. Zinc sulfate heptahydrate ($ZnSO_4 \cdot 7H_2O$), Analytical grade; Ajax Finechem
10. Boric acid (H_3BO_3), Analytical grade; Ajax Finechem
11. Manganese(II) chloride ($MnCl_2 \cdot 4H_2O$), Analytical grade; Ajax Finechem
12. Cobalt(II) chloride hexahydrate ($CoCl_2 \cdot 6H_2O$), Analytical grade; Ajax Finechem
13. Copper(II) sulfate pentahydrate ($CuSO_4 \cdot 5H_2O$), Analytical grade; Ajax Finechem
14. Ammonium molybdate tetrahydrate ($(NH_4)Mo_7O_{24} \cdot 4H_2O$), Analytical grade; Ajax Finechem

15. Streptomycin sulfate ($C_{42}H_{84}N_{14}O_{36}S_3$), Analytical grade; Sigma-Aldrich
16. Potassium hydroxide (KOH), Analytical grade; Merck KGaA
17. D-glucose anhydrous ($C_6H_{12}O_6$), Analytical grade; Ajax Finechem
18. Ethanol (C_2H_6O), ACS grade; Merck KGaA
19. Methanol (CH_4O), ACS grade; Merck KGaA
20. Methanol (CH_4O), HPLC grade; Honeywell
21. Trichloromethane ($CHCl_3$), AR grade; RCI Labscan
22. Water (H_2O), LiChrosolv grade; Merck KGaA
23. Distillated water (H_2O)
24. Isopropyl alcohol, HPLC grade; Honeywell
25. Ammonium hydroxide (NH_4OH), RPE for analysis grade; CARLO ERBA Reagents
26. Formic acid (CH_2O_2), ACS grade; Merck KGaA
27. Ammonium formate (CH_5O_2N), ≥ 99.995% trace metals basis; Sigma-Aldrich
28. Acetonitrile (CH_3CN), LiChrosolv grade; Merck KGaA

2.3 Instruments

1. Shaker, 120 rpm
2. High pressure steam autoclaves TC-459
3. Hot air oven UF110
4. Centrifuges C2 series
5. Electronic balance ATX224 (for dry weight of mycelium)
6. Electronic balance AL204 (for chemicals)
7. Suction filtration
8. Laminar airflow 212/2
9. pH meter S220
10. Microwave R-240
11. Freezer SF-C997
12. Stirring hot plate SAFE-T SHP9
13. Ultrasonic baths DT 100
14. Bruker MicrOTOF Q-II MS

15. Ultimate DGP 3600SD LC

2.4 Fungal strain and growth condition

A. niger strain ES4 was isolated from the top wall of an ethanol tank of the Petroleum Authority of Thailand (PTT). *A. niger* ES4 was grown on potato dextrose agar (PDA) (Appendix, A1) for 7 days at room temperature (30-33 ^{o}C), before cutting three small pieces by cork borer (~ 0.7 cm) for using as a starting culture, and put in 20 mL of PDB (Appendix, A2). The cultures in PDB were shook continuously at room temperature for 3 days.

2.5 Screening for suitable growth conditions under ethanol stress for metabolomics

In the previous experiment, we obtained the starting cultures of *A. niger* ES4. Then, 1 mL of starting PDB was transferred into 20 mL of minimal medium (MM) [97] (Appendix, A3) in 60-mL bottles under the absence of ethanol (0%; controls) or various ethanol concentrations, including 2%, 3%, 4%, and 5%. After that culture broth was collected at day 0 and every day until day 6 by separating the mycelium from media using suction filtration method using 110 mm Whatman filter paper No. 1 (dry with stable weight). The mycelium from three bottles were combined to constitute a data point. These mycelium were washed with 5 mL of distillated water (4 times) and washed again with 20 mL of distillated water (2 times). Then, incubated the mycelium on the filter paper were dried at 70 ^{o}C for 2-3 days until the weight recorded the dry weight did not change. Each ethanol concentration were three replicates. Plotted graph of the relation between average dry weight (g) and time (days) for the selection of the most suitable condition.

For metabolomics, we cultured *A. niger* ES4 alongside those for metabolomics and took samples of *A. niger* ES4 in MM under the absence of ethanol or 4% ethanol for 3 days using the same method as the section above. After that, we obtained the dry weight from three replicates and calculated the mean of dry weight both in the absence and in the presence of ethanol for normalization of the LC–MS data.

2.6 Metabolites extraction

A. niger was cultured in MM under the absence of ethanol or 4% ethanol for 3 days as section 2.4 and 2.5. Then, mycelium and media were separated by filtration through cotton. The mycelium was washed with 10 mL of distillated water and soaked in the mixture solution with 3 mL of chloroform and 1.5 mL of methanol in a 12-mL vial for 1 day. After that, 1.5 mL of MM (without D-glucose) were added, and shook. Samples were then centrifuged at 1500g for 3 min at room temperature. Then, chloroform layers were separated into 4-mL vial, and solvent was evaporated under nitrogen gas. The collected culture broth was divided equally into two parts. Each part was added into a 22-mL vial and extracted with the mixture solution with 5 mL of chloroform and 2.5 mL of methanol. Then, it was centrifuged at 1500g for 3 min at room temperature. After that, chloroform layers from both parts were separated and combined in a 12-mL vial, and solvent was evaporated under nitrogen gas. Crude extract was then dissolved in 1 mL of chloroform, put into a 4-mL vial, and washed again with 500 µL of chloroform (2 times). Then, solvent was evaporated under nitrogen gas again. Kept all of crude extracts at -20 °C before dissolving in 200 µL of chloroform for analysis by LC–MS or liquid chromatography–tandem mass spectrometry (LC–MS/MS).

2.7 LC–MS analysis of metabolomes

Metabolites from crude extracts of both media and mycelium of *A. niger* ES4 were analyzed by using LC–MS methods in the positive and negative ion modes as described by Vinayavekhin et al. [98], except this work used Ultimate DGP 3600SD LC joined to Bruker MicrOTOF Q-II MS instead. For the positive ion mode of LC analysis, Luna C5 column (5 µm, 4.6 mm x 50 mm), and two mobile phases, mobile phases A (95/5 water/methanol) and mobile phase B (60/35/5 isopropanol/methanol/water) were used. 0.1% (v/v) of formic acid and 5 mM of ammonium formate were added into these two mobile phases. For metabolites analysis, a 60-min gradient was used, starting from 100% A for 5 min at 0.1 mL min^{-1}. It was then changed to 80% A, increased linearly to 0% A for 45 min at 0.4 mL min^{-1}, maintained at 0% A for 8 min at 0.5 mL min^{-1}, and equilibrated at 100% A for 7 min at 0.5 mL min^{-1}. For the negative ion mode of LC analysis, Gemini C18 column (5 µm, 4.6 mm x 50 mm) was used. Mobile phases was the same as in the positive ion mode, but 0.1% (v/v) ammonium hydroxide was added instead of 0.1% (v/v) of formic acid and 5 mM of ammonium formate. The gradient was the same as in the positive ion mode. Electrospray ionization source was used for MS analysis, the parameters were specified as follow: end plate offset at -500 V, capillary voltage at 4000 V, nebulizer pressure at 3 bar, dry gas at 8 L/min, dry temperature at 200 ^{o}C, and collision RF at 150 Vpp. Data was compiled in a mass range of 100-1500 Da. Each running of samples were calibrated by using 10 mM sodium formate solution and each of samples (40 µL) were injected for metabolites analysis.

2.8 Untargeted data analysis

All of the ion chromatograms from LC–MS analysis were obtained for the two groups of samples: control (0% ethanol) and 4% ethanol. The data analysis was processed as follows. In the first step, the ion chromatogram files were converted from the .d to the mzXML format using CompassXport software. Then, XCMS program was used to output information for each ion in Excel file in term of average mass-to-charge ratio (*m/z*), average retention time, and integrated mass ion intensity (peak area) for each ion chromatogram. In the next step, each peak area was normalized by dividing the data by average dry weight of mycelium in controls (0% ethanol) or 4% ethanol, and then multiplied by the average dry weight of both groups to give averaged normalized peak areas of each group (*i.e.*, control groups). After that, the metabolite content were analyzed using the following criterion: the ratio of control/ethanol or ethanol/control of more than or equal to four, statistical significance (t-test; *p*) of less than 0.05, and the mean of peak areas (not normalized) in the increased samples of more than or equal to 5000. Isotopic peaks and false positives were cut out by using Data Analysis 4.0 program for observation of each peak.

2.9 Targeted data analysis

Targeted metabolomics of lipids were analyzed for free fatty acid (FFA), phosphatidic acid (PA), phosphatidylethanolamine (PE), phosphatidylserine (PS), phosphatidylglycerol (PG), phosphatidylinositol (PI), diacylglycerol (DAG), and triacylglycerol (TAG) by calculating peak areas of interesting metabolites in each chromatogram. These peak areas were normalized by dividing the data by the dry weight of mycelium from controls (0% ethanol) or 4% ethanol samples. After that, the mean of peak areas after normalization was calculated for each groups (*i.e.*, control groups). The difference of all of these mean was tested by t-test method with specified significance value at 0.05. Lastly, the ratios of these peak areas of both controls and 4% ethanol samples were compared.

2.10 LC–MS/MS analysis

The MS/MS analysis was operated on the final list of all changing ion using an Ultimate DGP 3600SD LC joined to Bruker MicrOTOF Q-II MS, which were adapted from Vinayavekhin et al. [98]. The MS/MS analysis was operated in auto MS/MS mode with the set list of interesting ions. The collision energies was set at 30 V for *m/z* 500, 45 V for *m/z* 1000, and 60 V for *m/z* 1500. The MS/MS data were compiled in the profile modes using a mass range of 100-1500 Da. Each of samples were calibrated by using 10 mM sodium formate solution and each running of samples (40 µL) were injected for metabolites analysis as section 2.7.

CHAPTER III

RESULTS AND DISCUSSION

3.1 Growth of *A. niger* ES4 in MM under various ethanol concentrations.

A. niger ES4 was grown in MM in the presence of the following ethanol concentrations: 0%, 2%, 3%, 4%, and 5%. The dry weight of mycelium was collected daily since day 0 until day 6 of each ethanol concentration. The results showed that the average dry weight of *A. niger* ES4 continued to decrease with higher ethanol concentrations (Figure 3.1 and Table 3.1). We found that the fungus at days 1 and 2 was rapidly growing in every ethanol concentration. The growth of *A. niger* ES4 started stationary phase at day 3. We observed that after day 3, the growth continuously had decreasing trend, and no growth was observed at day 6. From the trend of growth curves, we selected the suitable condition for metabolomics by considering two things. First, we selected the ethanol concentration that the growth of *A. niger* ES4 was half that of no ethanol condition, because the half growth of this fungal strain suggests that the production of metabolites will be changed, when compared with no ethanol condition. If the growth is more than half, it is more likely that the production of metabolites might not be different from that of control condition. If the growth is less than half, this fungal strain might be dying. Second, we selected the time for collecting of *A. niger* ES4 in the range of early stationary growth phase, because normally, microorganisms will produce many metabolites in this growth phase. We found that dry weight at day 3 of *A. niger* ES4 at the ethanol concentration of 2%, 3%, 4%, and 5% was 0.97, 1.45, 1.90, and 2.77 times of that of control, respectively. Therefore, we found that culturing *A. niger* ES4 in MM under 4% ethanol for 3 days was the most suitable condition for metabolomics because the growth of *A. niger* ES4 decreased about 1.9-fold from that of control condition, and the growth was in early stationary phase.

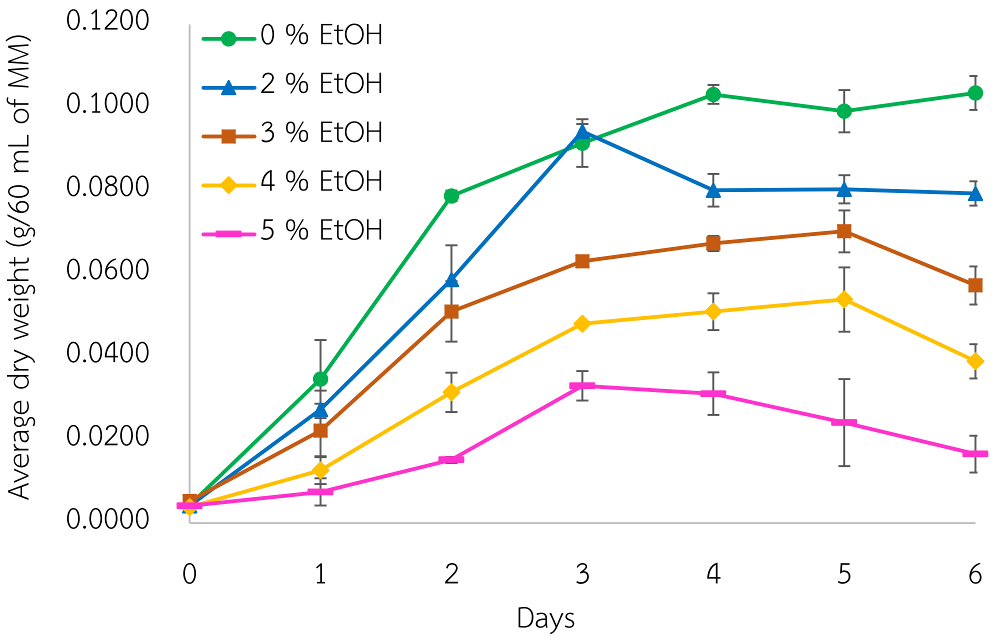

Figure 3.1 Growth curve of *A. niger* ES4 in MM supplemented with various ethanol concentrations from day 0 to day 6.

Table 3.1 The average dry weight of mycelium (g/60 mL of MM) of *A. niger* ES4 in MM supplemented with various ethanol concentrations.

Day	Average dry weight of mycelium (g/60 mL of MM)				
	0 % EtOH	2 % EtOH	3 % EtOH	4 % EtOH	5 % EtOH
0	0.0043 ± 0.001	0.0041 ± 0.001	0.0053 ± 0.001	0.0039 ± 0.001	0.0041 ± 0.001
1	0.0346 ± 0.009	0.0274 ± 0.005	0.0223 ± 0.006	0.0127 ± 0.003	0.0075 ± 0.003
2	0.0787 ± 0.001	0.0586 ± 0.008	0.0509 ± 0.007	0.0315 ± 0.005	0.0152 ± 0.001
3	0.0914 ± 0.006	0.0942 ± 0.002	0.0630 ± 0.001	0.0480 ± 0.000	0.0330 ± 0.004
4	0.1031 ± 0.002	0.0801 ± 0.004	0.0673 ± 0.002	0.0509 ± 0.004	0.0311 ± 0.005
5	0.0991 ± 0.005	0.0803 ± 0.003	0.0702 ± 0.005	0.0538 ± 0.008	0.0242 ± 0.011
6	0.1035 ± 0.004	0.0793 ± 0.003	0.0572 ± 0.005	0.0389 ± 0.004	0.0166 ± 0.004

3.2 Untargeted metabolomics of *A. niger* ES4 under ethanol stress

From the experiment of the most suitable growth condition of *A. niger* ES4 for metabolomics, *A. niger* ES4 was grown in MM in the absence of ethanol or 4% ethanol alongside those for metabolomics and samples were taken at day 3. We found that the average dry weight of mycelium in control was 0.0897 ± 0.0026 g/60 mL of MM and in the presence of 4% ethanol was 0.0374 ± 0.0007 g/60 mL of MM. The growth of *A. niger* ES4 under ethanol stress therefore had a 2.4-fold decrease from in the absence of ethanol. These average dry weight was used for metabolomics analysis.

Untargeted metabolomics was performed on *A. niger* ES4 cells cultured in MM under 4% ethanol for 3 days, together with in the absence of ethanol as controls. The metabolites were extracted from supernatant by using $CHCl_3$/MeOH/media (5 mL/2.5 mL/10 mL) and from the cells by soaking in the $CHCl_3$/MeOH (3 mL/1.5 mL) mixture. The extracts from chloroform layers of both parts were then concentrated. Metabolites from crude extracts of both media and mycelium of *A. niger* ES4 were analyzed by using LC–MS methods in the positive and negative ion modes.

XCMS is one of the software programs that used for metabolite profiles analysis, including LC–MS raw data processing and peak alignment [99]. We used XCMS program for outputting the following information for each ions into an Excel file: average mass-to-charge ratio (*m/z*), average retention time, and integrated mass ion intensity (peak area) for each of ion chromatograms. We compared the metabolite profiles of the samples treated in the presence of ethanol together with in the absence of ethanol. Each peak area of controls and ethanol groups was normalized by dividing the data by average dry weight of controls or 4% ethanol and then was multiplied by the average dry weight of both groups to obtain average normalized peak areas of each groups. The metabolite content were analyzed using the same criterion as experiment section 2.8. Isotopic peaks and false positives were cut out by using Data Analysis 4.0 program.

We obtained the final ion lists from the comparison of all these samples for both the negative and positive ion modes. For the negative ion modes, we found 29 and 77 ions with increasing contents and obtained 64 and 76 ions with decreasing contents in the ethanol-treated samples in the media and mycelium, respectively. For the positive ion modes, we obtained 196 and 539 ions with increasing contents and found 33 and 111 ions with decreasing contents in the ethanol-treated samples in the media and mycelium, respectively. We repeated this experiment again, kept only the overlapped ions from the two repeats, and obtained the final ion lists from the negative ion modes with 18 and 53 ions with increasing contents and obtained 35 and 69 ions with decreasing contents in the ethanol-treated samples in the media and mycelium, respectively. For the positive ion modes, we obtained 177 and 474 ions with increasing contents and found 18 and 90 ions with decreasing contents in the ethanol-treated samples in the media and mycelium, respectively. (Appendix, Tables A1-A4).

For untargeted metabolomics, the results showed so many metabolites, especially metabolite ions obtained from the cells in the positive ion mode with increasing contents. All these metabolites were not yet identified. However, the changes of the production of these metabolites from *A. niger* ES4 could be evidences that this fungal strain showed the response to ethanol stress, which might include, for example, inhibiting or activating some enzymes on the biosynthesis of these metabolites. These metabolites might be used to study the genes or metabolism that were involved in the changed production of these metabolite contents. Therefore, in the beginning, we were interested in studying the targeted lipid metabolites of *A. niger* ES4 under ethanol stress from untargeted metabolomics data, because ethanol solvent affects changed in cell membrane composition directly [15], and lipid is one of the important component of cell membranes in organisms.

3.3 Targeted metabolomics of *A. niger* ES4 under ethanol stress

We used the same data from untargeted metabolomics for targeted metabolomics analysis. We selected to analyze the carbon chains C16:0, C18:0, C18:1, and C18:2, because free fatty acids (FFA) with these carbon chains showed the highest peak areas in chromatograms (Figure 3.2), when compared with other numbers of carbon atoms and double bonds of other FFAs. Because microorganisms used FFA as the precursor for the synthesis of other lipids, such as diacylglycerol (DAG), triacylglycerol (TAG), and phosphatidic acid (PA), we may also find many of these carbon chains in other targeted lipids.

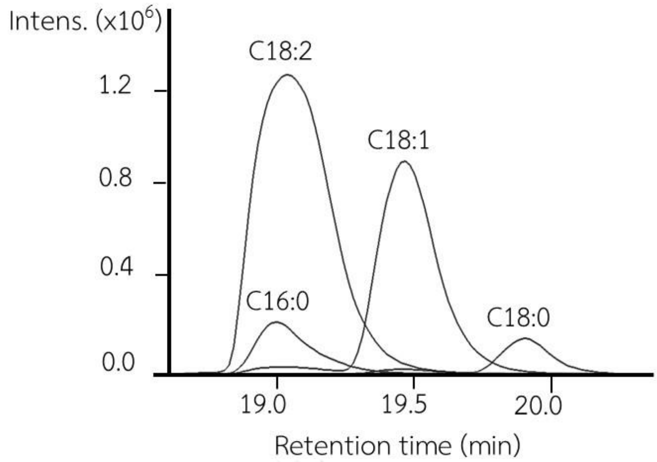

Figure 3.2 Extracted ion chromatogram of free fatty acids C16:0, C18:0, C18:1, and C18:2 with the highest peak area.

The important things that made the various lipids in organism systems have the different properties are the number of carbon atoms, saturation, and substitution in chain. The most common fatty acids in fungi are the fatty acids with chain lengths of 16 or 18 carbons, and the main unsaturated fatty acids are oleic acid (C18:1) and linoleic acid (C18:2) [100]. For *A. niger*, the saturated and unsaturated fatty acids are also found with carbon chain lengths of 16 to 18 carbons, but the major fatty acids are linoleic acid (C18:2) and palmitic acid (C16:0) and the minor are stearic acid (C18:0) and linolenic acid (C18:3) [101]. In this research, we also found the most abundant chain lengths of fatty acids and many lipids in the cells of *A. niger* ES4 to be C16:0, C18:0, C18:1, and C18:2, which was related to the report above.

From the previous experiment, we found the contents of DAG and TAG in 4% ethanol-treated samples to have 8-15-fold and 4-9-fold increases from without ethanol conditions, respectively. In addition, other lipids, such as FFA, PA, PE, PS, PG, and PI remained a little altered or unaltered (Table 3.2 and Figure 3.3).

Table 3.2 The amount of various lipids in the cells of *A. niger* ES4 grown in MM under 4% ethanol compared with in the absence of ethanol.

Lipid class	Ion	m/z	RT (min)	Ethanol/Control[a,b]
Increased lipids in 4% ethanol stress				
Diacylglycerol (DAG)				
16:0/18:1	$[M + NH_4]^+$	612.5	44.6	8.0*
16:0/18:2	$[M + NH_4]^+$	610.5	44.0	7.0***
18:2/18:2	$[M + NH_4]^+$	634.5	43.7	12.7***
18:2/18:1	$[M + NH_4]^+$	636.5	44.3	14.7***
Triacylglycerol (TAG)				
16:0/16:0/18:1	$[M + NH_4]^+$	850.7	48.5	4.4***
18:2/18:2/18:2	$[M + NH_4]^+$	896.7	48.0	8.4***
18:2/18:2/18:1	$[M + NH_4]^+$	898.7	48.3	8.8***
18:1/18:1/18:1	$[M + NH_4]^+$	902.8	48.7	9.1***
Other lipids (Ethanol/Control < 4 or p > 0.05)				
Free fatty acid (FFA)				
16:0	$[M - H]^-$	255.2	19.0	1.3**
18:2	$[M - H]^-$	279.2	19.1	0.7**
18:1	$[M - H]^-$	281.2	19.4	1.0**
18:0	$[M - H]^-$	283.2	19.9	0.5*
Phosphatidic acid (PA)				
16:0/18:1	$[M - H]^-$	673.4	32.4	2.5***
16:0/18:2	$[M - H]^-$	671.4	31.2	2.2***
18:2/18:2	$[M - H]^-$	695.4	30.6	3.0***
18:2/18:1	$[M - H]^-$	697.4	31.8	3.6***
Phosphatidylethanolamine (PE)				
16:0/18:1	$[M - H]^-$	716.5	42.4	1.9***
16:0/18:2	$[M - H]^-$	714.5	41.4	1.3**
18:2/18:2	$[M - H]^-$	738.5	40.7	2.2***
18:2/18:1	$[M - H]^-$	740.5	41.8	2.5***
Phosphatidylserine (PS)				
16:0/18:1	$[M - H]^-$	760.5	34.9	2.2***
16:0/18:2	$[M - H]^-$	758.4	33.8	2.0***
18:2/18:2	$[M - H]^-$	782.4	33.1	1.2*
18:2/18:1	$[M - H]^-$	784.5	34.2	2.4***
Phosphatidylglycerol (PG)				
16:0/18:1	$[M - H]^-$	747.5	37.5	0.9
16:0/18:2	$[M - H]^-$	745.4	36.6	1.0
Phosphatidylinositol (PI)				
16:0/18:1	$[M - H]^-$	835.5	37.2	1.6**
16:0/18:2	$[M - H]^-$	833.5	36.2	1.7***
18:2/18:2	$[M - H]^-$	857.5	35.6	1.8*
18:2/18:1	$[M - H]^-$	859.5	36.6	2.2***

[a]Ethanol/Control is the ratio of the normalized average peak area of metabolite ions in sample under 4% ethanol stress compared with the absence of ethanol.

[b]Student's *t* test: *p < 0.05; ** p < 0.01; ***p < 0.005; N = 3

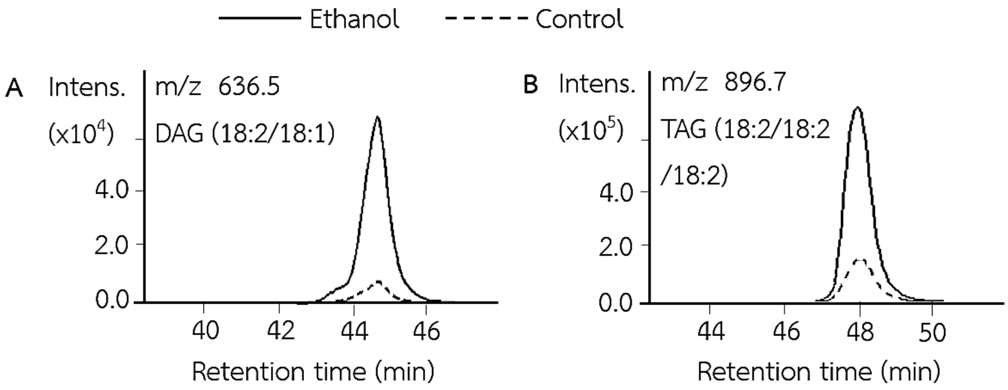

Figure 3.3 Example of extracted ion chromatogram of (A) DAG (18:2/18:1) and (B) TAG (18:2/18:2/18:2) in the cells of *A. niger* ES4 grown in MM under 4% ethanol (thick line) compared with in the absence of ethanol (dash line).

TAG is an important lipid in microorganism cells. It is an energy source of cells [100], and it amounts up to 50% of all lipids [102]. The biosynthesis of TAG in yeasts and high levels of living systems started from PA. PA is converted to DAG by using PA phosphatase as a catalyst. DAG acts as the composition of cell membranes and is the lipid second messenger for controlling the synthesis of protein. Then, DAG will be used as a precursor for the synthesis of TAG and other lipids, such as PE and phosphatidylcholine (PC). In addition, PA is also used as a precursor in the production of PI and PG via CDP-diacylglycerol [100, 102] (Figure 3.4).

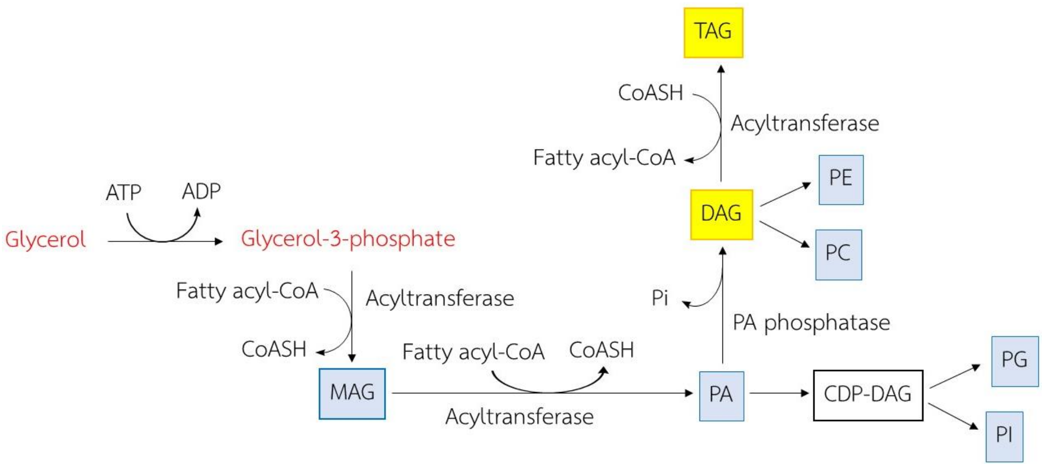

Figure 3.4 Biosynthesis of TAG in yeasts and high levels of living systems [100, 102].

From the biosynthesis of lipid as shown in Figure 3.4, we could be observed that the production of lipids in microbe cells was related to the glycerol metabolism. Glycerol is one of precursors in the synthesis of DAG and TAG [98]. In the past report, Hayashi and co-worker (2003) [103] studied *Escherichia coli* strain OST3410 with high resistance to organic solvents, such as hexane, and found that genes in glycerol metabolism, including *glpB*, *glpC*, *glpF*, and *glpQ* had statistically-significantly higher expression levels in strain OST3410 than the parent strain JA300. Moreover, Shimizu and co-worker (2005) [104] also found more expression of *glpC* gene in other *E. coli* strains with high tolerance to other organic solvents, such as xylene and cyclohexane. These reports then indicated that the collection of glycerol within microorganism cells might be related to response and tolerance of microbes to organic solvents. Glycerol might help protect cells from osmotic stress caused by organic solvents and result in higher solvent tolerance [15]. This increase in glycerol level may cause other lipids, such as DAG and TAG, to also increase as shown in this work. However, other genes in the biosynthesis of lipid may be involved, because we found the only increased contents of DAG and TAG, while other lipids, which were product of glycerol metabolism, remained unaltered.

The changes in rate of biosynthesis of phospholipid components might be related to increasing contents of DAG and TAG in the cells of *A. niger* ES4 under ethanol stress, because microorganisms also used fatty acids as the precursor for the synthesis of lipids. For example, Loffeld and co-work (1996) [57] found the changes isomers from *cis*- to *trans*- unsaturated fatty acids in *P. putida* under 10% ethanol for 2 h at 30 ^{o}C, and Beaven and co-work (1982) [60] found the changes of fatty-acyl residues in *S. cerevisiae* NCYC 431 under 1.5 M ethanol for 8 h that increased the ratio of unsaturated residues were C18:1 and C16:1, respectively, while decreased the ratio of saturated residues was C16:0. From these previous report, in this work, we assumed that DAG and TAG with increasing contents might be related to the changes isomers from *cis*- to *trans*- unsaturated fatty acids by considering two reasons. First, normally, *cis*-unsaturated fatty acids are the most in double bonds in microorganism, including yeasts. *A. niger* ES4 is also eukaryotic cells like yeasts, which might be indicated the same mechanism of adaptation for ethanol stress by changing configuration from *cis*-

to *trans*- isomer in structure of unsaturated fatty acids. Second, we did not found increased the ratio of unsaturated residues in the cells of *A. niger* ES4 under ethanol stress, because this fungal strain might be showed special properties for ethanol response, for example, inhibiting or activating some enzyme on the biosynthesis of fatty acids. However, we expected that ethanol might be one of carbon source in the cells of *A. niger* ES4 that affected increased contents of DAG and TAG. At present, there is still no report on the increases of DAG or TAG under ethanol stress, including in *A. niger* ES4. This research was the first report that showed the increased contents of DAG and TAG in response to organic solvents, which whether they are related to ethanol tolerance or not still needs further proof.

CHAPTER IV
CONCLUSION

4.1 Conclusion

From studying *A. niger* ES4 that was isolated from the top wall of an ethanol tank of the PTT Public Company Limited using untargeted and targeted metabolomics, we found that growing *A. niger* ES4 in MM under 4% ethanol for 3 days was the most suitable condition for metabolomics, because the growth of *A. niger* ES4 has about 1.9-fold decrease from control conditions, and the growth was in early stationary phase.

For metabolomics, we obtained the average dry weight of *A. niger* ES4 under ethanol stress and found a 2.4-fold decrease from in the absence of ethanol. These average dry weight were used for normalization in metabolomics analysis.

For untargeted metabolomics, we obtained the final ion lists from the negative ion modes with 18 and 53 ions with increasing levels and obtained 35 and 69 ions with decreasing levels in the ethanol-treated samples in the media and mycelium, respectively. For the positive ion modes, we obtained 177 and 474 ions with increasing levels and found 18 and 90 ions with decreasing levels in the ethanol-treated samples in the media and mycelium, respectively. These untargeted metabolomics data could be used for the analysis of other targeted metabolites.

For targeted metabolomics, we analyzed lipids that had carbon chain of C16:0, C18:0, C18:1, and C18:2. We found that *A. niger* ES4 responded to 4% ethanol stress in MM for 3 days with increasing levels of DAG and TAG in the cells when compared with the absence of ethanol, while other lipids, such as FFA, PA, PE, PS, PG, and PI remained unaltered. These metabolites might be related to the tolerance of *A. niger* ES4, potentially benefiting ethanol-related industries or leading to discovery of the novel methods to eliminate mold in the future.

4.2 Future work

4.2.1 We will analyze data from untargeted metabolomics to identify other metabolites changes of *A. niger* ES4 under ethanol stress.

4.2.2 *A. niger* ES4 responded to ethanol stress with increasing levels of DAG and TAG. Therefore, we can test the ethanol tolerance of *A. niger* ES4 by culturing these two lipids together with *A. niger* ES4 under ethanol stress. The test should affect higher ethanol tolerance of *A. niger* ES4. These metabolites may be used in ethanol-related industries. On the other hand, if we can decrease the production of DAG and TAG in *A. niger*, such as by modifying the genes that were involved in the production of these two lipids or adding the inhibitor of some enzymes in the biosynthesis pathway of these two lipids, *A. niger* should have decreased tolerant toward ethanol and could constitute new methods to eliminate mold.

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APPENDIX

A1 Preparation of potato dextrose agar (PDA)

1. Fresh potato is washed and peeled, and then weighed (about 200 g).

2. Cut fresh potato like dices and boil in 1 L of distilled water for 20 min.

3. Filter through white cheesecloth for saving liquid part and mix with 20 g of D-glucose and 15 g of agar. Stir until the solution is homogeneous.

4. Pour 250 mL of solution into each 500 mL Erlenmeyer flask (4 flasks) and autoclave for 15 min at 121°C. Wait until PDA is warm, and keep it at room temperature in closed cabinet.

Note: Before using PDA, dissolve agar by using microwave and wait until the solution is warm. Then, add 80 µL of 100 mg/mL streptomycin into solution before pouring into sterile petri dishes (in lamina flow).

A2 Preparation of potato dextrose broth (PDB)

Weigh 2.4 g of PDB and dissolve in 100 mL of distillated water. Autoclave for 15 min at 121°C. Wait until PDB is warm, and keep it at room temperature in closed cabinet.

A3 Preparation of minimal medium (MM)

1. Solution A: $NaNO_3$ 6 g, KCl 0.52 g, $MgSO_4.7H_2O$ 0.52 g, KH_2PO_4 1.52 g, glucose 10 g and dissolve in 1 L of distillated water. Then, adjust pH 6.8 by KOH pellets.

2. Solution B: $ZnSO_4.7H_2O$ 2.2 g, H_3BO_3 1.1 g, $MnCl_2.4H_2O$ 0.5 g, $FeSO_4.7H_2O$ 0.5 g, $CoCl_2.6H_2O$ 0.16 g, $CuSO_4.5H_2O$ 0.16 g, $(NH_4)Mo_7O_{24}.4H_2O$ 0.11 g, and EDTA 5 g, and dissolve in 100 mL of distillated water. Then, adjust pH 6.8 by KOH pellets.

3. Mix the solution A (1 L) and B (2 mL) to obtain MM. 20 mL of MM is divided into each 60 mL volume bottle for culturing *A. niger* ES4.

4. Autoclave for 15 min at 121°C. Wait until MM is warm, and keep it at room temperature in closed cabinet.

Table A1 Negative-mode ions in media of the ethanol-treated samples, compared with the control samples.

A1.1 Integrated mass ion intensity (MSII) of negative-mode ions in media with increased levels under 4% ethanol stress.

No.	*m/z*	RT	Integrated mass ion intensity (MSII)							
		(min)	EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	113.0608	10.2	6.2E+03	6.6E+03	6.5E+03	6.4E+03	1.1E+03	9.9E+02	1.0E+03	1.0E+03
2	129.0915	9.9	6.3E+03	5.9E+03	5.8E+03	6.0E+03	3.9E+02	3.3E+02	3.4E+02	3.6E+02
3	161.0452	13.1	2.6E+04	3.9E+04	2.6E+04	3.0E+04	2.1E+03	1.8E+03	7.0E+03	1.5E+03
4	257.1762	12.3	5.2E+03	5.8E+03	6.6E+03	5.9E+03	1.2E+03	6.8E+02	1.1E+03	1.0E+03
5	271.2281	16.5	6.2E+04	5.2E+04	4.6E+04	5.3E+04	7.2E+03	5.9E+03	5.8E+03	6.3E+03
6	339.2536	14.5	9.4E+03	1.0E+04	8.9E+03	9.7E+03	6.1E+02	8.3E+02	4.3E+02	6.2E+02
7	355.2492	12.9	1.1E+04	1.2E+04	1.0E+04	1.1E+04	1.0E+03	1.4E+03	1.0E+03	1.2E+03
8	359.1256	9.4	1.6E+04	1.4E+04	1.5E+04	1.5E+04	2.5E+03	1.8E+03	2.7E+03	2.3E+03
9	383.2443	10.3	4.3E+04	3.4E+04	2.0E+04	3.2E+04	6.4E+03	2.8E+04	2.3E+03	1.2E+03
10	383.2441	9.7	2.8E+04	2.3E+04	1.2E+04	2.1E+04	2.0E+03	4.8E+03	6.9E+02	2.5E+03
11	413.1974	24.8	5.2E+03	5.3E+03	6.8E+03	5.8E+03	9.2E+02	1.8E+03	1.2E+03	1.3E+03
12	439.2370	17.8	6.8E+03	6.4E+03	3.3E+03	5.5E+03	1.2E+03	1.2E+03	8.8E+02	1.1E+03
13	489.2713	21.2	8.3E+03	8.3E+03	6.7E+03	7.8E+03	2.5E+03	3.0E+03	7.2E+03	4.2E+03
14	501.2841	14.7	1.4E+04	1.1E+04	7.2E+03	1.0E+04	4.3E+03	6.1E+03	3.4E+03	4.6E+03
15	519.3685	24.3	2.7E+04	2.6E+04	2.7E+04	2.7E+04	2.4E+03	2.9E+03	2.1E+03	2.5E+03
16	537.2710	13.1	1.0E+04	1.6E+04	1.1E+04	1.2E+04	9.2E+02	7.0E+02	3.6E+02	6.6E+02
17	705.4164	18.1	1.1E+04	7.1E+03	6.5E+03	8.3E+03	3.3E+03	3.5E+03	3.0E+03	3.3E+03
18	827.3986	24.8	6.3E+03	5.2E+03	8.4E+03	6.6E+03	7.0E+02	1.1E+03	8.3E+02	9.0E+02

A1.2 Normalized integrated mass ion intensity (nMSII) of negative-mode ions in media with increased levels under 4% ethanol stress.

No.	*m/z*	RT	Normalized integrated mass ion intensity (nMSII)							
		(min)	EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	113.0608	10.2	1.0E+04	1.1E+04	1.1E+04	1.1E+04	8.2E+02	7.0E+02	7.4E+02	7.5E+02
2	129.0915	9.9	1.0E+04	1.0E+04	9.9E+03	1.0E+04	2.8E+02	2.3E+02	2.4E+02	2.5E+02
3	161.0452	13.1	4.4E+04	6.7E+04	4.4E+04	5.2E+04	1.5E+03	1.2E+03	5.0E+02	1.0E+03
4	257.1762	12.3	8.8E+03	9.9E+03	1.1E+04	1.0E+04	8.9E+02	4.8E+02	7.8E+02	7.2E+02
5	271.2281	16.5	1.0E+05	8.8E+04	7.9E+04	9.1E+04	5.1E+03	4.1E+03	4.1E+03	4.4E+03
6	339.2536	14.5	1.6E+04	1.8E+04	1.5E+04	1.6E+04	4.3E+02	5.9E+02	3.0E+02	4.2E+02
7	355.2492	12.9	2.0E+04	2.1E+04	1.7E+04	1.9E+04	7.6E+02	1.0E+03	7.4E+02	8.5E+02
8	359.1256	9.4	2.7E+04	2.5E+04	2.5E+04	2.6E+04	1.8E+03	1.3E+03	1.9E+03	1.6E+03
9	383.2443	10.3	7.4E+04	5.8E+04	3.4E+04	5.5E+04	4.5E+03	2.0E+04	1.6E+03	8.7E+03
10	383.2441	9.7	4.8E+04	4.0E+04	2.1E+04	3.6E+04	1.4E+03	3.4E+03	4.9E+02	1.7E+03
11	413.1974	24.8	8.9E+03	9.1E+03	1.1E+04	9.9E+03	6.5E+02	1.3E+03	8.8E+02	9.5E+02
12	439.2370	17.8	1.1E+04	1.0E+04	5.7E+03	9.4E+03	8.5E+02	8.7E+02	6.3E+02	7.8E+02
13	489.2713	21.2	1.4E+04	1.4E+04	1.1E+04	1.3E+04	1.7E+03	2.1E+03	5.1E+03	3.0E+03
14	501.2841	14.7	2.4E+04	1.9E+04	1.2E+04	1.8E+04	3.0E+03	4.3E+03	2.4E+03	3.3E+03
15	519.3685	24.3	4.7E+04	4.5E+04	4.6E+04	4.6E+04	1.7E+03	2.1E+03	1.5E+03	1.7E+03
16	537.2710	13.1	1.7E+04	2.7E+04	1.9E+04	2.1E+04	6.5E+02	5.2E+02	2.5E+02	4.7E+02
17	705.4164	18.1	1.9E+04	1.1E+04	1.1E+04	1.4E+04	2.3E+03	2.5E+03	2.1E+03	2.3E+03
18	827.3986	24.8	1.0E+04	8.9E+03	1.4E+04	1.1E+04	4.9E+02	8.2E+02	5.9E+02	6.3E+02

A1.3 Integrated mass ion intensity (MSII) of negative-mode ions in media with decreased levels under 4% ethanol stress.

No.	*m/z*	RT	Integrated mass ion intensity (MSII)							
		(min)	EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	111.0450	9.8	2.2E+03	2.3E+03	1.1E+03	1.9E+03	2.1E+04	1.4E+04	2.5E+04	2.0E+04
2	138.0318	22.7	3.4E+02	4.8E+02	4.3E+02	4.3E+02	2.6E+04	2.0E+04	2.7E+04	2.5E+04
3	138.0323	9.8	1.3E+03	1.8E+03	7.8E+02	1.3E+03	1.8E+04	1.4E+04	2.4E+04	1.9E+04
4	188.0837	25.4	2.4E+03	4.0E+03	3.1E+03	3.2E+03	3.7E+04	4.4E+04	6.6E+04	4.9E+04
5	271.1703	11.1	1.6E+03	1.9E+03	1.3E+03	1.6E+03	2.4E+04	1.6E+04	2.1E+04	2.0E+04
6	289.1807	11.1	5.5E+02	1.1E+03	7.8E+02	8.2E+02	1.6E+04	1.0E+04	1.6E+04	1.4E+04
7	315.1597	10.5	4.5E+02	4.0E+02	4.4E+02	4.3E+02	1.6E+04	1.1E+04	1.3E+04	1.3E+04
8	317.1748	10.2	1.8E+03	5.1E+02	4.1E+02	9.2E+02	2.5E+04	1.2E+04	1.5E+04	1.8E+04
9	331.1917	15.0	1.0E+03	1.1E+03	7.6E+02	9.8E+02	3.3E+04	1.7E+04	3.3E+04	2.7E+04
10	343.2269	23.3	4.9E+02	1.7E+03	8.0E+02	1.0E+03	6.4E+04	6.2E+04	8.2E+04	6.9E+04
11	345.2070	13.7	2.8E+02	2.7E+02	1.9E+02	2.5E+02	5.7E+03	4.3E+03	6.2E+03	5.5E+03
12	359.2215	22.7	6.8E+02	1.3E+03	5.3E+03	8.5E+02	2.7E+04	2.0E+04	2.7E+04	2.5E+04
13	388.2482	19.3	2.5E+02	2.8E+02	4.7E+02	3.3E+02	5.7E+04	7.1E+04	4.5E+04	5.8E+04
14	390.2286	12.5	1.0E+02	3.8E+01	4.9E+01	6.4E+01	7.9E+03	5.8E+03	6.6E+03	6.8E+03
15	390.2632	18.0	9.6E+02	1.0E+03	1.0E+03	1.0E+03	5.4E+04	5.8E+04	3.5E+04	4.9E+04
16	404.2434	18.8	7.4E+02	4.1E+02	8.1E+02	6.6E+02	4.7E+04	6.2E+04	4.6E+04	5.2E+04
17	404.2449	13.8	8.9E+02	8.8E+02	1.0E+03	9.4E+02	8.7E+04	7.9E+04	7.7E+04	8.1E+04
18	404.2438	15.3	3.6E+02	3.0E+02	3.4E+02	3.3E+02	1.9E+04	2.2E+04	1.6E+04	1.9E+04
19	406.2602	17.9	1.8E+03	1.3E+03	1.8E+03	1.6E+03	4.9E+04	5.6E+04	3.9E+04	4.8E+04
20	406.2603	14.1	1.2E+03	1.3E+03	1.3E+03	1.3E+03	8.7E+04	5.8E+04	7.3E+04	7.3E+04
21	406.2603	15.9	1.1E+03	1.1E+03	1.3E+03	1.1E+03	3.0E+04	4.5E+04	3.4E+04	3.6E+04
22	422.2552	14.0	1.1E+03	1.1E+03	8.5E+02	1.0E+03	3.0E+04	1.6E+04	2.2E+04	2.3E+04
23	422.2559	15.7	6.7E+02	5.6E+02	6.9E+02	6.4E+02	8.8E+03	1.0E+04	9.5E+03	9.7E+03
24	430.2601	17.4	3.1E+02	3.1E+02	3.7E+02	3.3E+02	1.0E+04	1.2E+04	9.7E+03	1.0E+04
25	430.2605	16.3	8.0E+02	6.9E+02	5.3E+02	6.7E+02	2.4E+04	2.4E+04	2.0E+04	2.3E+04
26	432.2759	17.0	1.3E+04	1.1E+04	1.5E+04	1.3E+04	2.2E+05	2.9E+05	2.2E+05	2.4E+05
27	434.2908	19.6	3.9E+02	5.5E+02	6.1E+02	5.2E+02	2.3E+04	2.4E+04	2.7E+04	2.5E+04
28	446.2549	16.2	2.1E+02	2.6E+02	2.7E+02	2.5E+02	1.0E+04	1.0E+04	8.8E+03	9.7E+03
29	448.2712	16.9	7.0E+03	5.7E+03	6.6E+03	6.4E+03	8.5E+04	9.6E+04	8.1E+04	8.7E+04
30	448.2712	15.0	2.0E+03	1.3E+03	1.7E+03	1.7E+03	3.6E+04	5.4E+04	3.6E+04	4.2E+04
31	450.2870	18.1	6.1E+02	6.8E+02	5.0E+02	6.0E+02	1.0E+04	1.0E+04	1.0E+04	1.0E+04
32	450.2869	16.1	4.4E+02	3.9E+02	4.6E+02	4.3E+02	9.5E+03	1.2E+04	1.0E+04	1.0E+04
33	537.2859	15.3	4.5E+02	9.6E+02	4.1E+02	6.1E+02	5.9E+03	1.2E+04	8.3E+03	8.7E+03
34	833.4482	22.7	7.8E+02	6.7E+02	4.9E+02	6.4E+02	1.7E+04	1.2E+04	1.4E+04	1.4E+04
35	841.4822	22.7	4.1E+01	8.6E+01	9.0E+01	7.2E+01	8.5E+03	7.9E+03	1.0E+04	8.8E+03

A1.4 Normalized integrated mass ion intensity (nMSII) of negative-mode ions in media with decreased levels under 4% ethanol stress.

No.	*m/z*	RT	Normalized integrated mass ion intensity (nMSII)							
		(min)	EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	111.0450	9.8	3.7E+03	3.9E+03	2.0E+03	3.2E+03	1.5E+04	1.0E+04	1.8E+04	1.4E+04
2	138.0318	22.7	6.5E+02	8.2E+02	7.4E+02	7.4E+02	1.8E+04	1.4E+04	1.9E+04	1.7E+04
3	138.0323	9.8	2.3E+03	3.1E+03	1.3E+02	2.2E+03	1.3E+04	1.0E+04	1.7E+04	1.3E+04
4	188.0837	25.4	4.2E+03	6.9E+03	5.2E+03	5.4E+03	2.6E+04	3.1E+04	4.6E+04	3.5E+04
5	271.1703	11.1	2.8E+03	3.2E+03	2.3E+03	2.8E+03	1.7E+04	1.1E+04	1.5E+04	1.4E+04
6	289.1807	11.1	9.4E+02	1.9E+03	1.3E+03	1.4E+03	1.1E+04	7.5E+03	1.1E+04	1.0E+04
7	315.1597	10.5	7.7E+02	6.9E+02	7.5E+02	7.4E+02	1.1E+04	8.3E+03	9.2E+03	9.8E+03
8	317.1748	10.2	3.1E+03	8.7E+02	6.9E+02	1.5E+03	1.8E+04	8.8E+03	1.1E+04	1.2E+04
9	331.1917	15.0	1.7E+03	1.9E+03	1.2E+03	1.6E+03	2.3E+04	1.2E+04	2.3E+04	1.9E+04
10	343.2269	23.3	8.5E+02	2.9E+03	1.3E+03	1.7E+03	4.5E+04	4.4E+04	5.8E+04	4.9E+04

No.	*m/z*	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
11	345.2070	13.7	4.8E+02	4.6E+02	3.3E+02	4.2E+02	4.0E+03	3.0E+03	4.4E+03	3.8E+03
12	359.2215	22.7	1.1E+03	2.2E+03	9.0E+02	1.4E+03	1.9E+04	1.4E+04	1.9E+04	1.7E+04
13	388.2482	19.3	4.3E+02	4.8E+02	8.0E+02	5.7E+02	4.0E+04	5.0E+04	3.2E+04	4.1E+04
14	390.2286	12.5	1.7E+02	6.5E+01	8.4E+01	1.0E+02	5.6E+03	4.1E+03	4.7E+03	4.8E+03
15	390.2632	18.0	1.6E+03	1.7E+03	1.7E+03	1.7E+03	3.8E+04	4.1E+04	2.4E+04	3.4E+04
16	404.2434	18.8	1.2E+03	7.0E+02	1.3E+03	1.1E+03	3.3E+04	4.4E+04	3.3E+04	3.7E+04
17	404.2449	13.8	1.5E+03	1.5E+03	1.7E+03	1.6E+03	6.1E+04	5.6E+04	5.5E+04	5.7E+04
18	404.2438	15.3	6.1E+02	5.1E+02	5.7E+02	5.7E+02	1.3E+04	1.6E+04	1.1E+04	1.3E+04
19	406.2602	17.9	3.1E+03	2.2E+03	3.2E+03	2.8E+03	3.4E+04	3.9E+04	2.7E+04	3.4E+04
20	406.2603	14.1	2.1E+03	2.2E+03	2.2E+03	2.2E+03	6.2E+04	4.1E+04	5.1E+04	5.1E+04
21	406.2603	15.9	1.9E+03	1.9E+03	2.2E+03	2.0E+03	2.1E+04	3.2E+04	2.4E+04	2.6E+04
22	422.2552	14.0	1.9E+03	1.9E+03	1.4E+03	1.8E+03	2.1E+04	1.1E+04	1.5E+04	1.6E+04
23	422.2559	15.7	1.1E+03	9.6E+02	1.1E+03	1.0E+03	6.2E+03	7.7E+03	6.7E+03	6.9E+03
24	430.2601	17.4	5.3E+02	5.2E+02	6.3E+02	5.6E+02	7.6E+03	8.7E+03	6.9E+03	7.7E+04
25	430.2605	16.3	1.3E+03	1.1E+03	9.0E+02	1.1E+03	1.7E+04	1.7E+04	1.4E+04	1.6E+04
26	432.2759	17.0	2.2E+04	1.9E+04	2.6E+04	2.2E+04	1.6E+05	2.0E+05	1.5E+05	1.7E+05
27	434.2908	19.6	6.6E+02	9.4E+02	1.0E+03	8.8E+02	1.6E+04	1.7E+04	1.9E+04	1.7E+04
28	446.2549	16.2	3.7E+02	4.5E+02	4.6E+02	4.2E+02	7.3E+03	7.1E+03	6.2E+03	6.9E+03
29	448.2712	16.9	1.2E+04	9.0E+03	1.1E+04	1.1E+04	6.0E+04	6.8E+04	5.7E+04	6.2E+04
30	448.2712	15.0	3.4E+03	2.3E+03	3.0E+03	2.9E+03	2.6E+04	3.8E+04	2.5E+04	3.0E+04
31	450.2870	18.1	1.0E+03	1.1E+03	8.5E+02	1.0E+03	7.2E+03	7.7E+03	7.6E+03	7.5E+03
32	450.2869	16.1	7.5E+02	6.6E+02	7.8E+02	7.3E+02	6.7E+03	8.5E+03	7.1E+03	7.4E+03
33	537.2859	15.3	7.6E+02	1.6E+03	6.9E+02	1.0E+03	4.2E+03	8.5E+03	5.9E+03	6.2E+03
34	833.4482	22.7	1.3E+03	1.1E+03	8.4E+02	1.1E+03	1.2E+04	8.9E+03	1.0E+04	1.0E+04
35	841.4822	22.7	7.0E+01	1.4E+02	1.5E+02	1.2E+02	6.0E+03	5.6E+03	7.1E+04	6.2E+03

Table A2 Negative-mode ions in mycelium of the ethanol-treated samples, compared with the control samples.

A2.1 Integrated mass ion intensity (MSII) of negative-mode ions in mycelium with increased levels under 4% ethanol stress.

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	159.0836	45.0	4.9E+04	7.0E+04	6.1E+04	6.0E+04	1.3E+04	1.8E+04	8.5E+03	1.3E+04
2	227.2001	47.4	1.2E+04	8.2E+03	7.8E+03	9.3E+03	5.3E+03	4.4E+03	5.8E+03	5.2E+03
3	241.2144	48.1	4.1E+04	5.8E+04	5.1E+04	5.0E+04	2.3E+04	1.4E+04	1.9E+04	1.9E+04
4	301.1656	46.6	6.3E+03	8.1E+03	7.0E+03	7.1E+03	1.5E+03	1.6E+03	8.1E+02	1.3E+03
5	355.2805	49.1	1.3E+04	1.2E+04	1.0E+04	1.2E+04	1.3E+03	7.0E+02	1.5E+03	1.2E+03
6	359.1504	41.2	7.4E+03	9.4E+03	9.6E+03	8.8E+03	1.9E+03	4.7E+03	3.3E+03	3.3E+03
7	408.3795	45.7	2.6E+04	1.4E+04	1.8E+04	1.9E+04	3.0E+03	3.8E+03	6.5E+03	4.5E+03
8	413.2353	48.3	9.4E+03	7.3E+03	6.1E+03	7.6E+03	1.3E+03	1.1E+03	1.7E+03	1.4E+03
9	422.4226	46.5	5.5E+03	6.3E+03	5.7E+03	5.8E+03	2.6E+02	4.0E+02	5.0E+01	2.4E+02
10	424.3747	45.0	3.0E+04	2.3E+04	2.7E+04	2.7E+04	5.6E+03	6.3E+03	9.5E+03	7.1E+03
11	427.2136	41.2	5.3E+03	7.9E+03	7.0E+03	6.7E+03	1.5E+03	3.6E+03	2.1E+03	2.4E+03
12	443.2454	41.2	2.1E+04	3.0E+04	2.8E+04	2.6E+04	5.8E+03	1.4E+04	8.3E+03	9.5E+03
13	483.2458	37.0	6.0E+03	4.8E+03	4.6E+03	5.1E+03	2.3E+03	2.5E+03	2.8E+03	2.5E+03
14	485.2614	38.9	5.5E+03	4.4E+03	5.4E+03	5.1E+03	2.0E+03	2.1E+03	2.6E+03	2.2E+03
15	559.4112	46.7	1.4E+05	1.0E+05	9.1E+04	1.1E+05	1.1E+04	1.1E+04	1.6E+04	1.3E+04
16	562.5165	47.5	2.9E+04	2.2E+04	2.2E+04	2.5E+04	4.0E+03	3.6E+03	4.2E+03	3.9E+03
17	585.3244	45.0	2.6E+04	3.3E+04	3.1E+04	3.0E+04	8.3E+03	1.1E+04	6.8E+03	8.6E+03
18	592.3627	36.0	1.9E+04	1.3E+04	1.4E+04	1.5E+04	2.8E+03	2.6E+03	4.0E+03	3.1E+03
19	593.3705	36.8	2.9E+04	2.2E+04	2.2E+04	2.4E+04	3.9E+03	3.6E+03	6.7E+03	4.7E+03
20	594.3768	37.5	1.6E+04	1.3E+04	1.3E+04	1.4E+04	2.0E+03	1.7E+03	4.0E+03	2.6E+03

No.	m/z	RT (min)	Integrated mass ion intensity (MSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
21	627.4754	48.4	1.8E+04	1.7E+04	1.6E+04	1.7E+04	3.0E+03	1.4E+03	2.8E+03	2.4E+03
22	639.4967	48.6	6.5E+03	5.3E+03	5.8E+03	5.8E+03	1.0E+03	7.5E+02	1.2E+03	1.0E+03
23	695.5339	49.9	3.3E+05	2.8E+05	2.7E+05	2.9E+05	2.8E+04	9.7E+03	4.0E+04	2.6E+04
24	708.6829	51.9	1.6E+05	8.9E+04	1.3E+05	1.3E+05	2.3E+04	2.6E+03	5.8E+03	1.0E+04
25	712.4829	43.8	1.4E+04	1.2E+04	1.2E+04	1.3E+04	2.0E+03	2.6E+03	6.2E+03	3.6E+03
26	751.5218	38.5	1.5E+05	1.3E+05	1.1E+05	1.3E+05	2.1E+04	1.9E+04	2.1E+04	2.0E+04
27	752.5137	41.5	1.2E+04	1.3E+04	1.1E+04	1.2E+04	2.7E+03	2.2E+03	2.7E+03	2.5E+03
28	753.5371	39.4	2.3E+05	1.8E+05	1.5E+05	1.9E+05	2.2E+04	2.2E+04	2.2E+04	2.2E+04
29	754.6819	50.9	1.9E+04	1.8E+04	1.6E+04	1.8E+04	7.0E+03	6.1E+02	2.3E+03	3.3E+03
30	766.5275	38.2	3.6E+04	4.0E+04	3.9E+04	3.8E+04	6.2E+03	5.4E+03	7.4E+03	6.3E+03
31	768.5454	39.2	4.0E+04	3.9E+04	4.2E+04	4.0E+04	5.0E+03	3.2E+03	5.3E+03	4.5E+03
32	774.5414	46.1	3.0E+04	2.8E+04	3.1E+04	2.9E+04	8.6E+03	1.6E+04	1.4E+04	1.3E+04
33	779.4424	46.5	8.9E+03	7.8E+03	8.0E+03	8.2E+03	1.6E+03	2.8E+03	2.2E+03	2.2E+03
34	796.5244	46.1	5.5E+03	4.4E+03	5.6E+03	5.2E+03	9.1E+02	1.9E+03	1.7E+03	1.5E+03
35	811.6130	43.2	3.3E+04	2.4E+04	2.0E+04	2.5E+04	6.7E+03	6.3E+03	1.5E+04	9.5E+03
36	813.6287	43.8	2.6E+04	1.8E+04	1.8E+04	2.1E+04	2.8E+03	2.2E+03	5.5E+03	3.5E+03
37	829.9175	39.4	4.7E+03	5.8E+03	5.9E+03	5.5E+03	1.4E+03	2.4E+03	2.1E+03	2.0E+03
38	870.5783	47.4	1.9E+04	1.6E+04	1.5E+04	1.7E+04	4.8E+03	5.6E+03	5.5E+03	5.3E+03
39	897.7355	48.6	5.5E+03	4.9E+03	4.7E+03	5.0E+03	0.0E+00	1.8E+01	0.0E+00	6.0E+00
40	1021.7114	45.6	1.8E+04	2.0E+04	1.1E+04	1.7E+04	4.9E+03	1.0E+04	9.9E+03	8.4E+03
41	1210.0098	48.3	1.0E+04	7.1E+03	6.6E+03	8.0E+03	1.6E+03	2.0E+02	6.1E+02	8.0E+02
42	1214.0352	49.1	9.1E+03	5.7E+03	4.9E+03	6.6E+03	2.5E+02	1.4E+02	6.4E+02	3.4E+02
43	1236.0226	48.7	9.1E+03	5.8E+03	4.7E+03	6.5E+03	7.4E+01	1.1E+01	2.5E+02	1.1E+02
44	1366.2633	49.7	1.1E+04	1.2E+04	6.8E+03	9.9E+03	4.4E+03	1.3E+03	1.8E+03	2.5E+03
45	1401.0796	48.0	7.0E+03	7.0E+03	6.6E+03	6.9E+03	1.5E+03	1.3E+03	2.5E+03	1.8E+03
46	1425.9648	43.8	7.4E+03	5.0E+03	5.6E+03	6.0E+03	5.6E+02	6.3E+02	1.6E+03	9.3E+02
47	1427.9812	44.3	8.9E+03	6.8E+03	6.9E+03	7.5E+03	1.1E+03	9.0E+02	2.7E+03	1.6E+03
48	1447.9456	42.9	8.6E+03	6.4E+03	7.7E+03	7.6E+03	8.1E+02	7.1E+02	2.7E+03	1.4E+03
49	1449.9660	43.4	3.4E+04	2.6E+04	2.4E+04	2.8E+04	4.2E+03	3.6E+03	1.0E+04	6.0E+03
50	1452.0135	38.1	1.2E+05	9.3E+04	8.1E+04	9.9E+04	2.4E+04	2.2E+04	2.5E+04	2.4E+04
51	1451.9796	44.0	2.7E+04	1.9E+04	2.3E+04	2.3E+04	2.3E+03	2.2E+03	6.7E+03	3.7E+03
52	1471.9489	43.5	8.0E+03	6.6E+03	7.2E+03	7.3E+03	8.7E+02	7.8E+02	2.2E+03	1.3E+03
53	1473.9581	44.0	6.3E+03	4.8E+03	6.0E+03	5.7E+03	4.8E+02	4.9E+02	1.2E+03	7.4E+02

A2.2 Normalized integrated mass ion intensity (nMSII) of negative-mode ions in mycelium with increased levels under 4% ethanol stress.

No.	m/z	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	159.0836	45.0	8.4E+04	1.2E+05	1.0E+05	1.0E+05	9.0E+03	1.3E+04	6.0E+03	9.3E+03
2	227.2001	47.4	2.0E+04	1.4E+04	1.3E+04	1.6E+04	3.8E+03	3.1E+03	4.1E+03	3.7E+03
3	241.2144	48.1	7.0E+04	9.8E+04	8.7E+04	8.5E+04	1.7E+04	1.0E+04	1.3E+04	1.3E+04
4	301.1656	46.6	1.1E+04	1.4E+04	1.2E+04	1.2E+04	1.1E+03	1.1E+03	5.7E+02	9.3E+02
5	355.2805	49.1	2.1E+04	2.0E+04	1.7E+04	2.0E+04	9.4E+02	4.9E+02	1.1E+03	8.4E+02
6	359.1504	41.2	1.3E+04	1.6E+04	1.6E+04	1.5E+04	1.4E+03	3.4E+03	2.3E+03	2.4E+03
7	408.3795	45.7	4.5E+04	2.3E+04	3.0E+04	3.3E+04	2.1E+03	2.7E+03	4.6E+03	3.2E+03
8	413.2353	48.3	1.6E+04	1.2E+04	1.0E+04	1.3E+04	9.3E+02	7.7E+02	1.2E+03	9.8E+02
9	422.4226	46.5	9.4E+03	1.1E+04	9.6E+03	9.9E+03	1.8E+02	2.8E+02	3.6E+01	1.7E+02
10	424.3747	45.0	5.1E+04	3.9E+04	4.5E+04	4.5E+04	4.0E+03	4.5E+03	6.7E+03	5.1E+03
11	427.2136	41.2	8.9E+03	1.3E+04	1.2E+04	1.1E+04	1.0E+03	2.6E+03	1.5E+03	1.7E+03
12	443.2454	41.2	3.6E+04	5.1E+04	4.7E+04	4.4E+04	4.1E+03	1.0E+04	5.9E+03	6.7E+03
13	483.2458	37.0	1.0E+04	8.2E+03	7.8E+03	8.7E+03	1.7E+03	1.8E+03	2.0E+03	1.8E+03
14	485.2614	38.9	9.4E+03	7.5E+03	9.2E+03	8.7E+03	1.4E+03	1.5E+03	1.8E+03	1.6E+03
15	559.4112	46.7	2.4E+05	1.7E+05	1.5E+05	1.9E+05	8.1E+03	8.1E+03	1.1E+04	9.2E+03
16	562.5165	47.5	5.0E+04	3.8E+04	3.8E+04	4.2E+04	2.8E+03	2.5E+03	2.9E+03	2.8E+03
17	585.3244	45.0	4.4E+04	5.5E+04	5.2E+04	5.1E+04	5.9E+03	7.6E+03	4.8E+03	6.1E+03

No.	m/z	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
18	592.3627	36.0	3.1E+04	2.3E+04	2.4E+04	2.6E+04	2.0E+03	1.8E+03	2.8E+03	2.2E+03
19	593.3705	36.8	4.9E+04	3.7E+04	3.7E+04	4.1E+04	2.8E+03	2.5E+03	4.7E+03	3.3E+03
20	594.3768	37.5	2.7E+04	2.2E+04	2.3E+04	2.4E+04	1.4E+03	1.2E+03	2.8E+03	1.8E+03
21	627.4754	48.4	3.1E+04	2.9E+04	2.7E+04	2.9E+04	2.2E+03	9.7E+02	2.0E+03	1.7E+03
22	639.4967	48.6	1.1E+04	8.9E+03	9.8E+03	9.9E+03	7.3E+02	5.3E+02	8.6E+02	7.1E+02
23	695.5339	49.9	5.6E+05	4.8E+05	4.5E+05	5.0E+05	2.0E+04	6.9E+03	2.9E+04	1.9E+04
24	708.6829	51.9	2.7E+05	1.5E+05	2.3E+05	2.2E+05	1.6E+04	1.9E+03	4.1E+03	7.3E+03
25	712.4829	43.8	2.3E+04	2.0E+04	2.1E+04	2.1E+04	1.4E+03	1.8E+03	4.4E+03	2.5E+03
26	751.5218	38.5	2.6E+05	2.2E+05	1.8E+05	2.2E+05	1.5E+04	1.3E+04	1.5E+04	1.4E+04
27	752.5137	41.5	2.0E+04	2.2E+04	1.9E+04	2.0E+04	1.9E+03	1.5E+03	1.9E+03	1.8E+03
28	753.5371	39.4	3.9E+05	3.1E+05	2.6E+05	3.2E+05	1.6E+04	1.6E+04	1.6E+04	1.6E+04
29	754.6819	50.9	3.2E+04	3.1E+04	2.7E+04	3.0E+04	4.9E+03	4.3E+02	1.6E+03	2.3E+03
30	766.5275	38.2	6.0E+04	6.8E+04	6.6E+04	6.5E+04	4.4E+03	3.8E+03	5.3E+03	4.5E+03
31	768.5454	39.2	6.8E+04	6.7E+04	7.1E+04	6.9E+04	3.5E+03	2.3E+03	3.8E+03	3.2E+03
32	774.5414	46.1	5.1E+04	4.7E+04	5.2E+04	5.0E+04	6.1E+03	1.1E+04	9.9E+03	9.1E+03
33	779.4424	46.5	1.5E+04	1.3E+04	1.4E+04	1.4E+04	1.1E+03	2.0E+03	1.6E+03	1.6E+03
34	796.5244	46.1	9.4E+03	7.5E+03	9.6E+03	8.8E+03	6.5E+02	1.3E+03	1.2E+03	1.1E+03
35	811.6130	43.2	5.6E+04	4.0E+04	3.4E+04	4.3E+04	4.8E+03	4.5E+03	1.1E+04	6.7E+03
36	813.6287	43.8	4.4E+04	3.0E+04	3.0E+04	3.5E+04	2.0E+03	1.5E+03	3.9E+03	2.5E+03
37	829.9175	39.4	8.1E+03	9.9E+03	1.0E+04	9.3E+03	1.0E+03	1.7E+03	1.5E+03	1.4E+03
38	870.5783	47.4	3.2E+04	2.8E+04	2.5E+04	2.8E+04	3.4E+03	4.0E+03	3.9E+03	3.8E+03
39	897.7355	48.6	9.4E+03	8.3E+03	8.0E+03	8.6E+03	0.0E+00	1.3E+01	0.0E+00	4.3E+00
40	1021.7114	45.6	3.1E+04	3.4E+04	1.9E+04	2.8E+04	3.5E+03	7.3E+03	7.0E+03	5.9E+03
41	1210.0098	48.3	1.8E+04	1.2E+04	1.1E+04	1.4E+04	1.1E+03	1.4E+02	4.3E+02	5.6E+02
42	1214.0352	49.1	1.5E+04	9.7E+03	8.4E+03	1.1E+04	1.8E+02	9.7E+01	4.5E+02	2.4E+02
43	1236.0226	48.7	1.5E+04	9.8E+03	8.0E+03	1.1E+04	5.2E+01	7.8E+00	1.8E+02	7.9E+01
44	1366.2633	49.7	1.8E+04	2.1E+04	1.1E+04	1.7E+04	3.1E+03	9.1E+02	1.3E+03	1.8E+03
45	1401.0796	48.0	1.2E+04	1.2E+04	1.1E+04	1.2E+04	1.1E+03	9.4E+02	1.7E+03	1.3E+03
46	1425.9648	43.8	1.3E+04	8.5E+03	9.6E+03	1.0E+04	4.0E+02	4.5E+02	1.1E+03	6.6E+02
47	1427.9812	44.3	1.5E+04	1.2E+04	1.2E+04	1.3E+04	7.7E+02	6.4E+02	1.9E+03	1.1E+03
48	1447.9456	42.9	1.5E+04	1.1E+04	1.3E+04	1.3E+04	5.8E+02	5.0E+02	1.9E+03	1.0E+03
49	1449.9660	43.4	5.8E+04	4.4E+04	4.2E+04	4.8E+04	2.9E+03	2.6E+03	7.2E+03	4.2E+03
50	1452.0135	38.1	2.1E+05	1.6E+05	1.4E+05	1.7E+05	1.7E+04	1.6E+04	1.8E+04	1.7E+04
51	1451.9796	44.0	4.6E+04	3.3E+04	3.9E+04	3.9E+04	1.7E+03	1.6E+03	4.7E+03	2.6E+03
52	1471.9489	43.5	1.4E+04	1.1E+04	1.2E+04	1.2E+04	6.2E+02	5.5E+02	1.5E+03	9.0E+02
53	1473.9581	44.0	1.1E+04	8.1E+03	1.0E+04	9.7E+03	3.4E+02	3.5E+02	8.7E+02	5.2E+02

A2.3 Integrated mass ion intensity (MSII) of negative-mode ions in mycelium with decreased levels under 4% ethanol stress.

No.	m/z	RT (min)	Integrated mass ion intensity (MSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	147.0816	15.3	3.4E+02	3.0E+02	6.4E+02	4.3E+02	1.7E+04	1.0E+04	1.7E+04	1.5E+04
2	233.2270	18.8	2.4E+01	9.1E+01	5.1E+01	5.5E+01	7.0E+03	4.2E+03	5.4E+03	5.6E+03
3	251.2016	18.2	7.1E+02	5.8E+02	4.3E+02	5.7E+02	1.9E+04	1.1E+04	1.4E+04	1.5E+04
4	265.2172	18.7	4.9E+03	4.4E+03	3.8E+03	4.4E+03	9.8E+04	6.7E+04	8.5E+04	8.3E+04
5	277.2177	18.8	2.7E+04	2.5E+04	2.4E+04	2.6E+04	1.9E+06	1.1E+06	1.5E+06	1.5E+06
6	295.2274	16.3	3.4E+02	6.1E+02	4.5E+02	4.7E+02	7.9E+03	5.0E+03	6.0E+03	6.3E+03
7	325.2750	13.3	7.2E+02	9.4E+02	1.5E+03	1.1E+03	1.3E+04	7.5E+03	1.4E+04	1.2E+04
8	341.3034	27.9	1.3E+03	1.7E+03	2.3E+03	1.7E+03	2.5E+04	1.7E+04	2.3E+04	2.2E+04
9	369.2652	13.3	8.7E+02	2.1E+03	2.1E+03	1.7E+03	2.0E+04	1.2E+04	2.2E+04	1.8E+04
10	390.2649	18.1	4.5E+02	1.0E+03	9.4E+02	8.0E+02	2.5E+04	1.4E+04	1.8E+04	1.9E+04
11	404.2452	18.6	3.8E+02	5.1E+02	1.5E+02	3.5E+02	1.1E+04	7.0E+03	9.5E+03	9.1E+03
12	404.2788	27.4	5.6E+01	1.5E+02	1.6E+02	1.2E+02	8.8E+03	3.9E+03	6.2E+03	6.3E+03
13	405.3127	29.5	2.7E+02	2.7E+02	1.7E+02	2.4E+02	4.0E+03	5.4E+03	6.1E+03	5.2E+03
14	406.2598	18.0	5.1E+02	8.9E+02	4.8E+02	6.3E+02	1.3E+04	7.5E+03	1.0E+04	1.0E+04

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII) EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
15	412.2477	24.3	9.5E+01	1.1E+02	2.3E+02	1.5E+02	7.9E+03	4.8E+03	6.9E+03	6.5E+03
16	416.2806	18.4	9.1E+02	1.0E+03	1.0E+03	9.9E+02	2.7E+04	1.4E+04	2.0E+04	2.0E+04
17	426.2998	27.7	3.4E+02	2.4E+02	5.4E+02	3.7E+02	9.4E+03	4.7E+03	7.5E+03	7.2E+03
18	432.2749	18.4	4.3E+02	5.8E+02	3.1E+02	4.4E+02	8.2E+03	4.8E+03	7.4E+03	6.8E+03
19	432.2752	17.0	2.3E+03	3.4E+03	2.5E+03	2.7E+03	3.8E+04	2.7E+04	3.6E+04	3.4E+04
20	434.2905	18.1	4.6E+02	6.2E+02	6.4E+02	5.8E+02	1.9E+04	1.2E+04	1.8E+04	1.6E+04
21	448.2711	16.9	5.6E+02	8.7E+02	5.7E+02	6.6E+02	7.7E+03	5.7E+03	8.3E+03	7.2E+03
22	449.2991	16.8	5.3E+02	5.4E+02	7.3E+02	6.0E+02	7.6E+03	4.5E+03	7.8E+03	6.6E+03
23	463.2880	14.1	3.5E+02	4.2E+02	6.4E+02	4.7E+02	7.0E+03	5.5E+03	8.5E+03	7.0E+03
24	463.3193	29.7	2.4E+03	1.8E+03	1.5E+03	1.9E+03	3.9E+04	4.5E+04	4.7E+04	4.3E+04
25	477.2961	24.7	3.6E+01	2.9E+01	1.3E+02	6.6E+01	5.6E+03	5.3E+03	8.2E+03	6.4E+03
26	493.2963	15.3	2.7E+03	3.2E+03	4.7E+03	3.5E+03	6.2E+04	4.5E+04	6.5E+04	5.8E+04
27	524.7914	29.1	1.5E+02	4.8E+01	2.6E+02	1.5E+02	2.2E+04	2.2E+04	2.1E+04	2.2E+04
28	532.7888	28.5	2.6E+02	1.2E+03	7.0E+02	7.1E+02	5.9E+04	6.8E+04	5.4E+04	6.0E+04
29	537.2863	13.6	1.9E+03	2.1E+03	3.2E+03	2.4E+03	4.7E+04	3.6E+04	5.8E+04	4.7E+04
30	537.2865	15.3	6.1E+03	7.1E+03	1.1E+04	8.0E+03	1.4E+05	1.0E+05	1.5E+05	1.3E+05
31	540.7861	27.6	2.9E+02	5.3E+01	1.1E+02	1.5E+02	5.4E+03	6.7E+03	6.0E+03	6.0E+03
32	550.5514	48.7	1.8E+02	3.7E+02	3.0E+02	2.8E+02	1.1E+04	6.9E+03	1.1E+04	9.6E+03
33	556.3598	27.2	2.0E+02	3.2E+02	3.1E+02	2.8E+02	6.2E+03	6.0E+03	9.2E+03	7.1E+03
34	559.2682	15.3	1.1E+03	1.0E+03	1.7E+03	1.3E+03	1.4E+04	1.2E+04	1.5E+04	1.4E+04
35	559.2690	13.6	5.8E+02	5.9E+02	6.7E+02	6.1E+02	8.1E+03	6.1E+03	9.8E+03	8.0E+03
36	568.5273	47.4	3.6E+02	6.7E+02	6.3E+02	5.6E+02	9.2E+03	7.7E+03	8.1E+03	8.3E+03
37	574.8332	20.5	8.1E+01	4.8E+02	1.2E+02	2.3E+02	1.3E+04	7.2E+03	7.3E+03	9.0E+03
38	574.8346	33.0	5.6E+02	7.0E+02	6.9E+02	6.5E+02	2.3E+04	2.2E+04	1.7E+04	2.1E+04
39	575.8271	31.7	1.3E+02	4.6E+02	3.0E+02	3.0E+02	5.8E+03	5.6E+03	4.4E+03	5.3E+03
40	575.8285	20.4	1.3E+02	2.5E+02	2.6E+02	2.1E+02	7.3E+03	5.6E+03	4.3E+03	5.7E+03
41	580.8531	35.4	5.7E+01	1.4E+01	1.4E+01	2.8E+01	8.4E+03	7.7E+03	5.2E+03	7.1E+03
42	582.5424	47.9	1.2E+04	1.3E+04	1.3E+04	1.3E+04	2.3E+05	1.9E+05	1.8E+05	2.0E+05
43	582.8315	20.4	4.9E+03	1.0E+04	6.3E+03	7.1E+03	2.1E+05	1.3E+05	1.2E+05	1.5E+05
44	582.8325	32.5	1.1E+04	2.2E+04	1.4E+04	1.6E+04	2.8E+05	2.8E+05	2.0E+05	2.5E+05
45	589.8420	20.5	8.3E+02	2.9E+03	1.7E+03	1.8E+03	2.3E+04	1.7E+04	1.5E+04	1.8E+04
46	594.5422	47.7	3.0E+03	3.8E+03	4.0E+03	3.6E+03	5.4E+04	4.1E+04	4.1E+04	4.6E+04
47	612.5540	48.2	6.9E+02	7.6E+02	5.3E+02	6.6E+02	8.0E+03	5.5E+03	5.7E+03	6.4E+03
48	691.4307	28.7	1.4E+03	8.6E+02	1.3E+03	1.2E+03	2.2E+04	1.5E+04	1.2E+04	1.6E+04
49	778.5322	45.7	1.2E+04	1.2E+04	1.2E+04	1.2E+04	1.6E+05	1.0E+05	1.2E+05	1.2E+05
50	780.4773	32.2	4.0E+03	4.2E+03	3.6E+03	3.9E+03	4.7E+04	4.5E+04	4.8E+04	4.7E+04
51	803.5431	37.8	1.0E+02	8.2E+02	1.1E+03	6.7E+02	1.1E+04	1.0E+04	9.8E+03	1.0E+04
52	808.5648	36.9	0.0E+00	0.0E+00	0.0E+00	0.0E+00	7.5E+04	6.7E+04	7.1E+04	7.1E+04
53	824.5601	36.4	9.7E+01	2.7E+01	2.6E+01	5.0E+01	2.3E+04	2.0E+04	2.1E+04	2.2E+04
54	836.5932	38.5	0.0E+00	0.0E+00	0.0E+00	0.0E+00	2.5E+04	1.7E+04	1.9E+04	2.0E+04
55	854.5463	45.7	7.0E+02	7.6E+02	6.5E+02	7.0E+02	1.5E+04	8.0E+03	1.0E+04	1.1E+04
56	855.4958	34.7	3.7E+03	3.7E+03	6.4E+03	4.6E+03	4.7E+04	5.5E+04	5.7E+04	5.3E+04
57	885.5392	38.8	4.1E+02	1.0E+03	1.0E+03	8.2E+02	7.8E+03	9.0E+03	8.1E+03	8.3E+03
58	908.6498	40.7	9.8E+02	2.4E+03	1.1E+03	1.5E+03	2.8E+04	2.0E+04	1.9E+04	2.2E+04
59	920.6856	42.7	3.9E+01	4.4E+01	1.1E+01	3.1E+01	3.4E+04	2.0E+04	2.0E+04	2.5E+04
60	1050.5841	29.1	4.9E+01	0.0E+00	1.9E+02	7.9E+01	1.4E+04	1.3E+04	1.3E+04	1.3E+04
61	1066.5772	28.5	2.9E+02	1.9E+02	3.4E+02	2.7E+02	2.6E+04	3.0E+04	2.4E+04	2.7E+04
62	1088.5506	19.8	2.2E+02	3.3E+02	2.6E+02	2.7E+02	7.5E+03	4.5E+03	4.1E+03	5.4E+03
63	1088.5574	28.5	0.0E+00	1.9E+02	2.6E+02	1.5E+02	6.1E+03	6.2E+03	4.8E+03	5.7E+03
64	1150.6680	33.0	8.4E+01	5.8E+01	2.1E+02	1.2E+02	7.2E+03	7.6E+03	5.6E+03	6.8E+03
65	1166.6613	20.4	1.7E+03	3.5E+03	2.2E+03	2.5E+03	6.3E+04	4.3E+04	4.1E+04	4.9E+04
66	1166.6663	32.5	3.5E+03	6.9E+03	3.9E+03	4.8E+03	8.1E+04	7.9E+04	5.6E+04	7.2E+04
67	1188.6435	20.4	1.9E+02	4.8E+02	6.6E+02	4.4E+02	6.0E+03	6.6E+03	7.1E+03	6.6E+03
68	1188.6465	32.6	6.8E+02	1.4E+03	8.4E+02	9.7E+02	1.2E+04	1.2E+04	9.4E+03	1.1E+04
69	1387.8938	29.6	3.8E+02	3.9E+02	2.8E+02	3.5E+02	7.0E+03	6.3E+03	4.7E+03	6.0E+03

A2.4 Normalized integrated mass ion intensity (nMSII) of negative-mode ions in mycelium with decreased levels under 4% ethanol stress.

No.	*m/z*	RT	Normalized integrated mass ion intensity (nMSII)							
		(min)	EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	147.0816	15.3	5.8E+02	5.1E+02	1.1E+03	7.2E+02	1.2E+04	7.1E+03	1.2E+04	1.0E+04
2	233.2270	18.8	4.1E+01	1.6E+02	8.7E+01	9.4E+01	5.0E+03	3.0E+03	3.8E+03	3.9E+03
3	251.2016	18.2	1.2E+03	9.9E+02	7.3E+02	9.7E+02	1.3E+04	8.0E+03	1.0E+04	1.0E+04
4	265.2172	18.7	8.3E+03	7.5E+03	6.5E+03	7.4E+03	6.9E+04	4.8E+04	6.0E+04	5.9E+04
5	277.2177	18.8	4.6E+04	4.3E+04	4.1E+04	4.3E+04	1.4E+06	7.9E+05	1.1E+06	1.1E+06
6	295.2274	16.3	5.7E+02	1.0E+03	7.7E+02	7.9E+02	5.6E+03	3.5E+03	4.2E+03	4.4E+03
7	325.2750	13.3	1.2E+03	1.6E+03	2.6E+03	1.8E+03	9.3E+03	5.3E+03	1.0E+04	8.2E+03
8	341.3034	27.9	2.2E+03	2.9E+03	3.9E+03	3.0E+03	1.8E+04	1.2E+04	1.6E+04	1.5E+04
9	369.2652	13.3	1.5E+03	3.5E+03	3.6E+03	2.9E+03	1.4E+04	8.2E+03	1.6E+04	1.3E+04
10	390.2649	18.1	7.7E+02	1.7E+03	1.6E+03	1.4E+03	1.7E+04	1.0E+04	1.2E+04	1.3E+04
11	404.2452	18.6	6.4E+02	8.7E+02	2.6E+02	5.9E+02	7.6E+03	5.0E+03	6.7E+03	6.4E+03
12	404.2788	27.4	9.5E+01	2.5E+02	2.8E+02	2.1E+02	6.2E+03	2.8E+03	4.4E+03	4.5E+03
13	405.3127	29.5	4.6E+02	4.6E+02	3.0E+02	4.0E+02	2.8E+03	3.8E+03	4.3E+03	3.7E+03
14	406.2598	18.0	8.7E+02	1.5E+03	8.2E+02	1.1E+03	9.1E+03	5.3E+03	7.1E+03	7.1E+03
15	412.2477	24.3	1.6E+02	1.9E+02	3.9E+02	2.5E+02	5.6E+03	3.4E+03	4.9E+03	4.6E+03
16	416.2806	18.4	1.6E+03	1.7E+03	1.8E+03	1.7E+03	1.9E+04	1.0E+04	1.4E+04	1.5E+04
17	426.2998	27.7	5.8E+02	4.0E+02	9.1E+02	6.3E+02	6.6E+03	3.3E+03	5.3E+03	5.1E+03
18	432.2749	18.4	7.4E+02	9.9E+02	5.3E+02	7.5E+02	5.8E+03	3.4E+03	5.3E+03	4.8E+03
19	432.2752	17.0	3.9E+03	5.8E+03	4.3E+03	4.6E+03	2.7E+04	1.9E+04	2.6E+04	2.4E+04
20	434.2905	18.1	7.9E+02	1.1E+03	1.1E+03	9.8E+02	1.3E+04	8.7E+03	1.3E+04	1.2E+04
21	448.2711	16.9	9.4E+02	1.5E+03	9.7E+02	1.1E+03	5.5E+03	4.0E+03	5.9E+03	5.1E+03
22	449.2991	16.8	9.0E+02	9.2E+02	1.2E+03	1.0E+03	5.4E+03	3.2E+03	5.5E+03	4.7E+03
23	463.2880	14.1	6.0E+02	7.2E+02	1.1E+03	8.0E+02	5.0E+03	3.9E+03	6.0E+03	5.0E+03
24	463.3193	29.7	4.0E+03	3.0E+03	2.5E+03	3.2E+03	2.7E+04	3.2E+04	3.3E+04	3.1E+04
25	477.2961	24.7	6.1E+01	5.0E+01	2.2E+02	1.1E+02	4.0E+03	3.8E+03	5.8E+03	4.5E+03
26	493.2963	15.3	4.5E+03	5.4E+03	8.0E+03	6.0E+03	4.4E+04	3.2E+04	4.6E+04	4.1E+04
27	524.7914	29.1	2.5E+02	8.2E+01	4.5E+02	2.6E+02	1.6E+04	1.6E+04	1.5E+04	1.5E+04
28	532.7888	28.5	4.5E+02	2.0E+03	1.2E+03	1.2E+03	4.2E+04	4.8E+04	3.8E+04	4.3E+04
29	537.2863	13.6	3.2E+03	3.5E+03	5.4E+03	4.0E+03	3.3E+04	2.6E+04	4.1E+04	3.3E+04
30	537.2865	15.3	1.0E+04	1.2E+04	1.8E+04	1.4E+04	9.7E+04	7.4E+04	1.0E+05	9.1E+04
31	540.7861	27.6	4.9E+02	8.9E+01	1.9E+02	2.6E+02	3.8E+03	4.8E+03	4.2E+03	4.3E+03
32	550.5514	48.7	3.1E+02	6.3E+02	5.1E+02	4.8E+02	7.8E+03	4.9E+03	7.8E+03	6.8E+03
33	556.3598	27.2	3.4E+02	5.4E+02	5.2E+02	4.7E+02	4.4E+03	4.3E+03	6.5E+03	5.1E+03
34	559.2682	15.3	1.8E+03	1.7E+03	2.9E+03	2.1E+03	9.8E+03	8.5E+03	1.0E+04	9.6E+03
35	559.2690	13.6	9.8E+02	1.0E+03	1.1E+03	1.0E+03	5.7E+03	4.3E+03	7.0E+03	5.7E+03
36	568.5273	47.4	6.2E+02	1.1E+03	1.1E+03	9.4E+02	6.5E+03	5.5E+03	5.7E+03	5.9E+03
37	574.8332	20.5	1.4E+02	8.1E+02	2.0E+02	3.8E+02	9.0E+03	5.1E+03	5.1E+03	6.4E+03
38	574.8346	33.0	9.5E+02	1.2E+03	1.2E+03	1.1E+03	1.7E+04	1.6E+04	1.2E+04	1.5E+04
39	575.8271	31.7	2.3E+02	7.8E+02	5.0E+02	5.0E+02	4.1E+03	4.0E+03	3.1E+03	3.7E+03
40	575.8285	20.4	2.2E+02	4.2E+02	4.4E+02	3.6E+02	5.2E+03	4.0E+03	3.1E+03	4.1E+03
41	580.8531	35.4	9.7E+01	2.4E+01	2.5E+01	4.8E+01	5.9E+03	5.5E+03	3.7E+03	5.0E+03
42	582.5424	47.9	2.0E+04	2.2E+04	2.3E+04	2.2E+04	1.6E+05	1.4E+05	1.3E+05	1.4E+05
43	582.8315	20.4	8.3E+03	1.7E+04	1.1E+04	1.2E+04	1.5E+05	9.0E+04	8.7E+04	1.1E+05
44	582.8325	32.5	1.9E+04	3.7E+04	2.4E+04	2.7E+04	2.0E+05	2.0E+05	1.4E+05	1.8E+05
45	589.8420	20.5	1.4E+03	5.0E+03	3.0E+03	3.1E+03	1.6E+04	1.2E+04	1.1E+04	1.3E+04
46	594.5422	47.7	5.2E+03	6.5E+03	6.8E+03	6.2E+03	3.9E+04	2.9E+04	2.9E+04	3.2E+04
47	612.5540	48.2	1.2E+03	1.3E+03	9.0E+02	1.1E+03	5.7E+03	3.9E+03	4.0E+03	4.5E+03
48	691.4307	28.7	2.4E+03	1.5E+03	2.3E+03	2.0E+03	1.6E+04	1.0E+04	8.5E+03	1.2E+04
49	778.5322	45.7	2.1E+04	2.0E+04	2.1E+04	2.0E+04	1.1E+05	7.3E+04	8.2E+04	8.8E+04
50	780.4773	32.2	6.8E+03	7.1E+03	6.1E+03	6.6E+03	3.3E+04	3.2E+04	3.4E+04	3.3E+04
51	803.5431	37.8	1.7E+02	1.4E+03	1.8E+03	1.1E+03	7.8E+03	7.2E+03	6.9E+03	7.3E+03
52	808.5648	36.9	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.3E+04	4.7E+04	5.0E+04	5.0E+04
53	824.5601	36.4	1.7E+02	4.6E+01	4.3E+01	8.5E+01	1.6E+04	1.4E+04	1.5E+04	1.5E+04
54	836.5932	38.5	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.8E+04	1.2E+04	1.4E+04	1.5E+04

No.	m/z	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
55	854.5463	45.7	1.2E+03	1.3E+03	1.1E+03	1.2E+03	1.1E+04	5.7E+03	7.1E+03	7.8E+03
56	855.4958	34.7	6.2E+03	6.2E+03	1.1E+04	7.8E+03	3.3E+04	3.9E+04	4.0E+04	3.7E+04
57	885.5392	38.8	7.1E+02	1.7E+03	1.8E+03	1.4E+03	5.5E+03	6.4E+03	5.7E+03	5.9E+03
58	908.6498	40.7	1.7E+03	4.0E+03	1.9E+03	2.5E+03	2.0E+04	1.4E+04	1.4E+04	1.6E+04
59	920.6856	42.7	6.5E+01	7.5E+01	1.9E+01	5.3E+01	2.4E+04	1.5E+04	1.4E+04	1.8E+04
60	1050.5841	29.1	8.3E+01	0.0E+00	3.2E+02	1.3E+02	9.7E+03	9.3E+03	9.2E+03	9.4E+03
61	1066.5772	28.5	4.9E+02	3.3E+02	5.7E+02	4.6E+02	1.9E+04	2.1E+04	1.7E+04	1.9E+04
62	1088.5506	19.8	3.7E+02	5.7E+02	4.4E+02	4.6E+02	5.3E+03	3.2E+03	2.9E+03	3.8E+03
63	1088.5574	28.5	0.0E+00	3.3E+02	4.3E+02	2.5E+02	4.3E+03	4.4E+03	3.4E+03	4.0E+03
64	1150.6680	33.0	1.4E+02	9.9E+01	3.7E+02	2.0E+02	5.1E+03	5.4E+03	4.0E+03	4.8E+03
65	1166.6613	20.4	2.9E+03	5.9E+03	3.7E+03	4.2E+03	4.5E+04	3.1E+04	2.9E+04	3.5E+04
66	1166.6663	32.5	6.0E+03	1.2E+04	6.7E+03	8.1E+03	5.7E+04	5.6E+04	4.0E+04	5.1E+04
67	1188.6435	20.4	3.2E+02	8.1E+02	1.1E+03	7.5E+02	4.3E+03	4.6E+03	5.0E+03	4.6E+03
68	1188.6465	32.6	1.2E+03	2.3E+03	1.4E+03	1.6E+03	8.2E+03	8.7E+03	6.6E+03	7.8E+03
69	1387.8938	29.6	6.4E+02	6.7E+02	4.7E+02	6.0E+02	5.0E+03	4.5E+03	3.3E+03	4.3E+03

Table A3 Positive-mode ions in media of the ethanol-treated samples, compared with the control samples.

A3.1 Integrated mass ion intensity (MSII) of positive-mode ions in media with increased levels under 4% ethanol stress.

No.	m/z	RT (min)	Integrated mass ion intensity (MSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	105.0691	21.1	1.6E+06	1.2E+06	1.4E+06	1.4E+06	1.0E+05	1.6E+05	9.8E+04	1.2E+05
2	117.0698	23.8	9.9E+03	8.8E+03	1.1E+04	9.8E+03	5.8E+03	6.2E+03	4.3E+03	5.4E+03
3	118.0892	5.9	6.7E+03	5.4E+03	4.3E+03	5.4E+03	1.2E+03	2.4E+03	1.9E+03	1.9E+03
4	127.0419	23.8	3.2E+04	3.0E+04	4.3E+04	3.5E+04	1.6E+04	1.6E+04	1.4E+04	1.5E+04
5	129.0528	21.1	6.1E+04	3.2E+04	5.9E+04	5.1E+04	1.0E+04	4.6E+03	9.5E+03	8.1E+03
6	144.1010	20.5	1.7E+05	2.3E+05	1.8E+05	1.9E+05	5.8E+03	5.8E+03	6.8E+03	6.1E+03
7	144.1007	12.4	3.0E+04	3.4E+04	3.1E+04	3.2E+04	1.0E+03	9.7E+02	8.9E+02	9.6E+02
8	144.1014	10.7	5.3E+04	6.1E+04	5.4E+04	5.6E+04	8.9E+02	8.2E+02	6.1E+02	7.7E+02
9	147.0653	23.8	8.6E+04	8.2E+04	1.1E+05	9.3E+04	4.3E+04	4.8E+04	3.4E+04	4.2E+04
10	153.0550	12.8	9.2E+04	1.1E+05	1.1E+05	1.0E+05	2.1E+04	1.9E+04	2.0E+04	2.0E+04
11	158.0787	9.8	7.6E+03	1.4E+04	7.6E+03	9.6E+03	1.0E+03	0.0E+00	0.0E+00	3.3E+02
12	160.1323	14.3	3.1E+04	3.5E+04	2.9E+04	3.2E+04	1.4E+03	1.2E+03	1.0E+03	1.2E+03
13	160.1322	9.9	9.1E+04	1.1E+05	5.7E+04	8.7E+04	1.3E+03	1.7E+03	1.1E+03	1.4E+03
14	163.1453	20.2	7.7E+04	7.4E+04	7.3E+04	7.5E+04	1.5E+04	1.5E+04	1.3E+04	1.5E+04
15	190.0527	14.5	2.8E+04	3.3E+04	2.8E+04	3.0E+04	7.1E+02	7.8E+02	5.6E+02	6.8E+02
16	194.1169	14.3	1.6E+04	2.1E+04	1.6E+04	1.7E+04	8.8E+02	8.8E+02	7.7E+02	8.4E+02
17	194.1164	10.1	8.8E+04	1.2E+05	5.7E+04	8.7E+04	2.2E+03	2.0E+03	2.1E+03	2.1E+03
18	201.1048	16.7	1.7E+04	1.8E+04	1.4E+04	1.6E+04	2.6E+03	2.0E+03	2.2E+03	2.3E+03
19	207.1341	11.7	1.4E+04	1.5E+04	1.5E+04	1.4E+04	5.3E+03	4.9E+03	4.5E+03	4.9E+03
20	207.6383	24.4	1.4E+04	9.6E+03	1.1E+04	1.1E+04	1.3E+03	9.3E+02	6.8E+02	9.7E+02
21	209.1490	20.2	6.7E+04	6.5E+04	7.0E+04	6.7E+04	1.7E+04	1.5E+04	1.3E+04	1.5E+04
22	216.1003	14.9	3.2E+04	3.7E+04	3.4E+04	3.5E+04	6.9E+02	9.1E+02	8.5E+02	8.2E+02
23	217.1531	20.6	2.7E+04	2.8E+04	3.0E+04	2.8E+04	1.5E+04	1.1E+04	1.1E+04	1.2E+04
24	219.1672	20.2	4.3E+04	5.5E+04	4.4E+04	4.7E+04	8.0E+03	9.3E+03	9.4E+03	8.9E+03
25	223.1702	21.3	8.8E+05	9.7E+05	9.2E+05	9.2E+05	7.2E+05	4.2E+05	2.6E+05	4.7E+05
26	225.1422	11.7	1.5E+04	1.8E+04	1.6E+04	1.6E+04	7.7E+03	6.7E+03	6.9E+03	7.1E+03
27	235.1636	20.6	7.5E+04	8.2E+04	8.0E+04	7.9E+04	2.6E+04	2.3E+04	2.1E+04	2.3E+04
28	237.1680	20.6	3.8E+04	3.8E+04	3.2E+04	3.6E+04	1.8E+04	1.3E+04	1.4E+04	1.5E+04
29	243.1004	15.1	6.9E+03	8.6E+03	8.7E+03	8.1E+03	1.3E+03	1.0E+03	7.0E+02	9.9E+02
30	247.0946	12.8	1.8E+04	2.1E+04	1.6E+04	1.8E+04	6.6E+03	4.1E+03	4.6E+03	5.1E+03

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII) EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
31	249.1099	13.1	1.3E+04	1.7E+04	1.1E+04	1.4E+04	3.4E+03	0.0E+00	0.0E+00	1.1E+03
32	251.6658	24.4	2.5E+04	1.6E+04	1.8E+04	1.9E+04	1.6E+03	9.0E+02	1.2E+03	1.2E+03
33	252.1474	17.6	1.9E+04	1.4E+04	1.6E+04	1.6E+04	9.4E+03	6.7E+03	4.5E+03	6.9E+03
34	253.1736	20.6	3.5E+04	3.3E+04	3.3E+04	3.4E+04	1.7E+04	1.2E+04	1.2E+04	1.4E+04
35	256.0684	10.4	7.4E+03	7.1E+03	7.9E+03	7.4E+03	4.1E+03	3.0E+03	5.9E+03	4.3E+03
36	263.1332	23.8	1.3E+04	1.2E+04	1.8E+04	1.5E+04	5.6E+03	7.4E+03	5.1E+03	6.0E+03
37	263.0933	21.2	2.2E+04	1.6E+04	1.9E+04	1.9E+04	2.3E+02	2.3E+02	2.1E+02	2.2E+02
38	265.1407	15.4	1.3E+04	1.1E+04	9.2E+03	1.1E+04	5.7E+03	2.5E+03	2.4E+03	3.5E+03
39	265.1729	20.2	2.0E+05	2.3E+05	2.1E+05	2.1E+05	6.0E+04	5.4E+04	4.4E+04	5.3E+04
40	270.2413	12.9	3.0E+04	3.4E+04	2.8E+04	3.1E+04	0.0E+00	0.0E+00	0.0E+00	0.0E+00
41	272.2566	18.8	5.4E+03	7.0E+03	5.1E+03	5.8E+03	2.7E+03	1.3E+03	4.3E+02	1.5E+03
42	272.2547	18.1	8.7E+03	8.9E+03	5.3E+03	7.6E+03	0.0E+00	0.0E+00	3.8E+01	1.3E+01
43	288.2519	12.9	1.9E+04	1.8E+04	1.7E+04	1.8E+04	1.3E+01	0.0E+00	0.0E+00	4.4E+00
44	297.1658	18.1	1.2E+05	1.1E+05	8.4E+04	1.1E+05	2.4E+04	1.2E+04	7.3E+03	1.4E+04
45	297.1663	16.4	4.2E+04	3.9E+04	2.8E+04	3.6E+04	4.4E+03	2.2E+03	2.1E+03	2.9E+03
46	301.1507	27.7	1.2E+05	9.2E+04	1.0E+05	1.1E+05	2.8E+04	9.0E+04	6.1E+04	6.0E+04
47	305.1558	20.3	1.7E+05	1.4E+05	1.6E+05	1.6E+05	7.6E+04	6.9E+04	5.7E+04	6.7E+04
48	307.1863	18.0	6.9E+04	8.4E+04	6.6E+04	7.3E+04	1.1E+04	9.4E+03	7.8E+03	9.4E+03
49	311.2127	17.6	2.8E+04	2.9E+04	3.5E+04	3.0E+04	6.7E+03	5.1E+03	4.4E+03	5.4E+03
50	313.2413	37.3	6.2E+04	6.1E+04	5.7E+04	6.0E+04	2.6E+04	2.9E+04	2.1E+04	2.5E+04
51	313.2333	16.5	4.2E+04	4.8E+04	5.2E+04	4.7E+04	2.3E+03	1.6E+03	1.6E+03	1.8E+03
52	316.1150	16.9	6.6E+03	8.9E+03	4.9E+03	6.8E+03	9.1E+02	2.7E+02	5.3E+02	5.7E+02
53	317.2675	22.7	1.7E+05	1.8E+05	1.9E+05	1.8E+05	8.8E+03	8.8E+03	7.5E+03	8.3E+03
54	317.2670	23.4	9.5E+04	4.5E+04	8.7E+04	7.6E+04	9.8E+03	1.7E+03	2.1E+03	4.5E+03
55	319.1503	18.1	1.0E+04	1.1E+04	1.2E+04	1.1E+04	2.6E+03	1.8E+03	1.7E+03	2.0E+03
56	321.1334	13.2	1.8E+04	1.9E+04	1.7E+04	1.8E+04	6.9E+03	5.3E+03	5.0E+03	5.7E+03
57	321.1764	20.5	5.1E+04	6.0E+04	5.6E+04	5.5E+04	1.5E+04	1.2E+04	9.9E+03	1.2E+04
58	326.7237	24.4	1.1E+04	9.0E+03	6.7E+03	9.0E+03	4.9E+02	2.7E+02	4.6E+02	4.1E+02
59	340.2097	24.4	3.0E+04	2.1E+04	2.4E+04	2.5E+04	3.9E+03	2.2E+03	1.9E+03	2.6E+03
60	343.1409	17.5	1.5E+04	1.2E+04	8.9E+03	1.2E+04	2.8E+03	4.6E+03	9.3E+02	2.8E+03
61	345.1427	14.3	1.0E+04	1.3E+04	1.2E+04	1.2E+04	1.9E+02	0.0E+00	0.0E+00	6.4E+01
62	345.2993	26.3	3.0E+05	2.4E+05	2.6E+05	2.7E+05	2.0E+04	1.6E+04	1.3E+04	1.6E+04
63	347.2522	25.4	1.2E+05	1.4E+05	1.2E+05	1.3E+05	4.2E+04	1.3E+04	7.5E+03	2.1E+04
64	348.7348	24.5	1.3E+04	8.4E+03	8.7E+03	9.9E+03	3.7E+02	1.6E+02	7.5E+01	2.0E+02
65	354.1424	14.9	2.5E+04	3.2E+04	2.9E+04	2.8E+04	1.0E+02	1.9E+01	2.1E+02	1.1E+02
66	355.2466	21.3	3.1E+04	2.7E+04	3.4E+04	3.1E+04	3.5E+03	2.5E+03	2.8E+03	2.9E+03
67	355.1731	20.5	1.4E+04	1.6E+04	1.1E+04	1.4E+04	4.8E+03	3.4E+03	3.0E+03	3.7E+03
68	363.2102	20.6	8.7E+04	6.6E+04	8.1E+04	7.8E+04	4.0E+04	2.6E+04	2.0E+04	2.9E+04
69	369.1748	21.2	3.7E+04	2.8E+04	3.4E+04	3.3E+04	7.4E+03	5.1E+03	5.5E+03	6.0E+03
70	370.7431	24.3	9.9E+03	5.7E+03	7.9E+03	7.9E+03	1.1E+03	3.0E+02	2.9E+02	5.5E+02
71	373.1535	16.3	2.8E+04	2.4E+04	2.3E+04	2.5E+04	8.6E+03	7.5E+03	6.8E+03	7.6E+03
72	379.3030	22.5	8.9E+04	9.4E+04	5.8E+04	8.0E+04	7.8E+03	7.3E+03	4.1E+03	6.4E+03
73	387.1800	21.2	1.6E+06	1.1E+06	1.5E+06	1.4E+06	9.7E+04	1.9E+05	8.6E+04	1.2E+05
74	388.3395	18.3	8.4E+03	1.1E+04	8.7E+03	9.4E+03	9.9E+01	1.1E+01	1.9E+01	4.3E+01
75	389.3254	26.1	8.8E+05	6.9E+05	8.1E+05	7.9E+05	5.8E+04	4.4E+04	4.1E+04	4.8E+04
76	404.2061	21.2	8.2E+05	5.2E+05	7.8E+05	7.1E+05	6.2E+04	1.2E+05	5.2E+04	7.9E+04
77	405.3201	22.9	5.4E+05	6.2E+05	4.5E+05	5.4E+05	2.6E+04	1.9E+04	1.4E+04	2.0E+04
78	409.1618	21.1	1.8E+05	1.3E+05	1.8E+05	1.6E+05	9.2E+03	1.4E+04	9.6E+03	1.1E+04
79	423.3296	21.7	1.7E+05	2.4E+05	1.2E+05	1.8E+05	3.5E+03	1.9E+04	5.0E+03	9.3E+03
80	433.3515	25.8	8.9E+05	6.7E+05	7.9E+05	7.8E+05	1.2E+03	1.6E+04	1.4E+04	1.1E+04
81	436.3398	18.1	1.6E+04	2.2E+04	1.8E+04	1.9E+04	2.6E+02	3.1E+02	2.6E+02	2.8E+02
82	440.3554	22.5	1.1E+05	9.9E+04	8.3E+04	9.9E+04	2.4E+04	1.6E+04	1.6E+04	1.9E+04
83	445.8240	24.4	6.7E+04	4.3E+04	4.5E+04	5.2E+04	2.9E+03	1.4E+03	9.2E+02	1.7E+03
84	449.3463	22.8	3.7E+05	3.8E+05	2.9E+05	3.5E+05	1.8E+04	1.4E+04	8.5E+03	1.4E+04
85	449.3457	22.2	2.3E+05	1.3E+05	1.9E+05	1.8E+05	1.2E+04	8.3E+03	8.1E+03	9.3E+03
86	451.3366	26.6	1.3E+04	1.4E+04	1.3E+04	1.3E+04	5.2E+03	4.3E+03	3.7E+03	4.4E+03
87	455.2298	20.6	5.0E+04	4.4E+04	4.1E+04	4.5E+04	2.1E+04	2.5E+04	2.6E+04	2.4E+04
88	459.8407	26.9	5.2E+03	6.3E+03	5.0E+03	5.5E+03	1.3E+03	4.7E+02	2.7E+02	6.7E+02
89	467.3551	22.1	1.7E+05	2.6E+05	1.2E+05	1.8E+05	0.0E+00	4.3E+02	0.0E+00	1.4E+02

No.	*m/z*	RT	Integrated mass ion intensity (MSII)							
		(min)	EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
90	467.8376	24.3	7.0E+04	4.7E+04	4.9E+04	5.5E+04	2.9E+03	1.5E+03	1.0E+03	1.8E+03
91	468.8771	45.9	9.9E+03	7.4E+03	8.6E+03	8.6E+03	3.6E+03	4.9E+03	1.8E+03	3.5E+03
92	475.8337	21.2	8.2E+03	9.5E+03	1.1E+04	9.5E+03	8.4E+02	7.6E+02	1.6E+02	5.8E+02
93	477.3764	25.6	5.9E+05	4.2E+05	5.1E+05	5.1E+05	4.2E+04	2.7E+04	2.6E+04	3.2E+04
94	481.8525	26.8	9.3E+03	1.2E+04	8.6E+03	1.0E+04	2.4E+03	1.2E+03	7.7E+02	1.4E+03
95	484.3815	21.9	5.0E+05	2.8E+05	3.6E+05	3.8E+05	6.2E+04	3.2E+04	3.2E+04	4.2E+04
96	485.3630	23.2	1.1E+05	1.1E+05	1.1E+05	1.1E+05	1.0E+04	1.2E+04	8.1E+03	9.9E+03
97	489.8509	24.2	6.0E+04	4.1E+04	4.5E+04	4.9E+04	2.6E+03	9.9E+02	1.1E+03	1.6E+03
98	493.3714	22.6	1.9E+05	1.9E+05	1.6E+05	1.8E+05	1.0E+04	8.0E+03	4.3E+03	7.5E+03
99	495.3882	25.6	3.4E+05	2.5E+05	2.9E+05	2.9E+05	2.4E+04	1.6E+04	1.6E+04	1.8E+04
100	501.3518	22.4	1.3E+04	1.3E+04	1.2E+04	1.2E+04	4.5E+03	4.2E+03	2.6E+03	3.8E+03
101	503.8663	26.7	1.4E+04	1.8E+04	1.2E+04	1.5E+04	1.7E+03	0.0E+00	0.0E+00	5.7E+02
102	511.3794	22.6	8.9E+04	5.2E+04	7.0E+04	7.0E+04	2.0E+04	2.6E+04	0.0E+00	1.5E+04
103	511.8644	24.1	4.7E+04	3.2E+04	3.3E+04	3.7E+04	1.6E+03	7.1E+02	9.4E+02	1.1E+03
104	512.4148	25.6	5.9E+05	4.1E+05	4.2E+05	4.8E+05	5.8E+04	4.4E+04	3.5E+04	4.6E+04
105	515.3658	21.8	1.7E+04	8.8E+03	1.7E+04	1.4E+04	4.3E+03	6.5E+03	2.1E+03	4.3E+03
106	521.4031	25.5	3.0E+05	2.2E+05	2.7E+05	2.6E+05	2.0E+04	1.3E+04	1.3E+04	1.5E+04
107	525.8799	26.6	1.5E+04	1.9E+04	1.2E+04	1.6E+04	2.4E+03	1.3E+03	9.6E+02	1.6E+03
108	528.4089	22.5	8.1E+05	4.2E+05	4.9E+05	5.7E+05	6.7E+04	7.1E+04	4.7E+03	4.8E+04
109	529.3494	24.4	9.2E+04	1.0E+05	9.3E+04	9.7E+04	4.4E+04	5.4E+04	2.1E+04	4.0E+04
110	533.8779	24.1	2.8E+04	1.9E+04	2.2E+04	2.3E+04	1.0E+03	6.5E+02	5.6E+02	7.5E+02
111	537.3984	22.5	7.7E+04	7.4E+04	6.4E+04	7.2E+04	4.4E+03	3.7E+03	2.7E+03	3.6E+03
112	539.4141	25.5	2.1E+05	1.5E+05	1.9E+05	1.9E+05	1.5E+04	1.0E+04	8.7E+03	1.1E+04
113	541.3461	22.4	2.4E+04	2.1E+04	2.6E+04	2.4E+04	6.2E+03	4.6E+03	4.4E+03	5.0E+03
114	543.3600	23.2	2.4E+05	2.3E+05	2.5E+05	2.4E+05	1.6E+04	1.8E+04	1.1E+04	1.5E+04
115	547.8933	26.5	1.6E+04	1.9E+04	1.5E+04	1.7E+04	2.7E+03	1.2E+03	7.3E+02	1.6E+03
116	554.4240	24.6	4.4E+04	3.7E+04	3.6E+04	3.9E+04	6.9E+03	5.6E+03	3.8E+03	5.5E+03
117	555.8912	24.0	1.6E+04	1.2E+04	1.3E+04	1.3E+04	8.9E+02	4.2E+02	3.3E+02	5.4E+02
118	556.4413	25.4	9.4E+05	6.7E+05	7.6E+05	7.9E+05	7.6E+04	5.2E+04	4.1E+04	5.6E+04
119	557.1464	20.6	2.7E+04	2.3E+04	2.6E+04	2.5E+04	1.2E+04	1.5E+04	1.4E+04	1.4E+04
120	559.3353	23.2	1.9E+04	1.9E+04	2.2E+04	2.0E+04	3.6E+03	3.2E+03	2.9E+03	3.2E+03
121	565.4298	25.3	1.4E+05	1.0E+05	1.2E+05	1.2E+05	1.0E+04	7.2E+03	5.5E+03	7.7E+03
122	571.1590	21.5	4.0E+04	5.1E+04	4.9E+04	4.6E+04	1.5E+04	2.1E+04	2.9E+04	2.2E+04
123	573.9111	24.0	8.7E+03	6.3E+03	5.4E+03	6.8E+03	6.1E+02	3.3E+02	1.3E+02	3.5E+02
124	581.4230	22.3	3.1E+04	2.2E+04	2.7E+04	2.7E+04	1.8E+03	1.4E+03	7.4E+02	1.3E+03
125	583.4399	25.3	1.2E+05	8.5E+04	1.0E+05	1.0E+05	7.7E+03	6.2E+03	5.0E+03	6.3E+03
126	587.4219	26.4	1.4E+04	1.7E+04	1.1E+04	1.4E+04	2.3E+03	1.4E+04	3.2E+02	5.5E+03
127	591.9183	26.3	1.2E+04	1.2E+04	8.9E+03	1.1E+04	1.8E+03	7.4E+02	6.3E+02	1.1E+03
128	600.4676	25.3	1.1E+06	7.9E+05	9.0E+05	9.3E+05	7.2E+04	5.6E+04	4.2E+04	5.7E+04
129	609.4546	25.2	5.7E+04	4.1E+04	5.2E+04	5.0E+04	0.0E+00	4.6E+02	4.0E+02	2.9E+02
130	609.4359	26.3	1.9E+04	2.2E+04	1.6E+04	1.9E+04	4.5E+03	2.0E+03	1.4E+03	2.7E+03
131	611.1149	20.0	5.9E+04	7.3E+04	4.3E+04	5.8E+04	1.8E+04	1.2E+04	1.0E+04	1.4E+04
132	613.9332	26.2	7.6E+03	7.6E+03	6.6E+03	7.2E+03	1.1E+03	7.9E+02	3.6E+02	7.6E+02
133	616.1794	29.6	5.7E+03	6.2E+03	5.4E+03	5.8E+03	1.5E+03	1.9E+03	1.3E+03	1.6E+03
134	616.4620	22.3	3.4E+05	4.4E+05	2.4E+05	3.4E+05	2.3E+04	1.9E+04	1.0E+04	1.7E+04
135	621.4813	40.0	6.1E+04	5.1E+04	5.0E+04	5.4E+04	3.2E+03	2.7E+03	5.0E+03	3.6E+03
136	629.9914	46.0	1.7E+04	1.0E+04	1.5E+04	1.4E+04	5.2E+03	5.4E+03	1.2E+03	3.9E+03
137	644.4936	25.1	1.1E+06	7.4E+05	8.7E+05	8.9E+05	6.5E+04	4.6E+04	3.8E+04	5.0E+04
138	653.4600	26.1	2.2E+04	2.5E+04	1.5E+04	2.1E+04	1.6E+02	2.2E+02	0.0E+00	1.3E+02
139	660.4874	22.2	2.5E+05	3.0E+05	1.8E+05	2.4E+05	1.4E+04	1.2E+04	7.2E+03	1.1E+04
140	671.4915	25.0	3.1E+04	2.3E+04	2.6E+04	2.7E+04	4.6E+03	1.6E+03	8.6E+02	2.3E+03
141	688.5205	25.0	9.2E+05	6.3E+05	7.4E+05	7.6E+05	5.4E+04	3.6E+04	2.9E+04	4.0E+04
142	697.4861	25.9	1.9E+04	1.8E+04	1.0E+04	1.6E+04	3.5E+03	1.8E+03	3.7E+02	1.9E+03
143	704.5132	21.6	1.6E+05	2.0E+05	2.4E+05	2.0E+05	1.9E+04	1.6E+04	1.1E+04	1.5E+04
144	732.5459	24.9	7.1E+05	5.1E+05	5.7E+05	6.0E+05	4.1E+04	2.7E+04	2.1E+04	2.9E+04
145	748.5396	22.0	9.5E+04	1.3E+05	1.6E+05	1.3E+05	1.2E+04	9.5E+03	7.1E+03	9.5E+03
146	776.5712	24.8	5.0E+05	3.5E+05	3.9E+05	4.1E+05	2.6E+04	1.7E+04	1.4E+04	1.9E+04
147	792.5649	21.9	4.8E+04	6.3E+04	3.6E+04	4.9E+04	3.0E+03	2.1E+03	1.4E+03	2.2E+03
148	820.5980	24.6	2.8E+05	2.1E+05	2.4E+05	2.5E+05	1.7E+04	9.2E+03	8.1E+03	1.1E+04

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
149	836.5912	21.9	2.6E+04	2.0E+04	2.0E+04	2.2E+04	2.3E+03	1.5E+03	9.9E+02	1.6E+03
150	846.4411	23.8	8.9E+03	6.3E+03	1.2E+04	9.1E+03	3.2E+03	3.8E+03	1.9E+03	3.0E+03
151	851.3977	23.8	1.4E+04	9.5E+03	1.7E+04	1.3E+04	5.4E+03	6.8E+03	3.2E+03	5.1E+03
152	854.4285	23.8	7.0E+03	5.2E+03	7.7E+03	6.6E+03	3.2E+03	3.2E+03	1.5E+03	2.6E+03
153	864.6233	24.5	1.7E+05	1.2E+05	1.3E+05	1.4E+05	9.2E+03	4.9E+03	4.5E+03	6.2E+03
154	908.6494	24.4	9.0E+04	6.9E+04	7.2E+04	7.7E+04	6.5E+03	3.4E+03	2.7E+03	4.2E+03
155	1051.6301	23.0	7.7E+03	7.9E+03	7.5E+03	7.7E+03	8.1E+02	5.0E+02	2.8E+02	5.3E+02
156	1063.7393	23.2	2.7E+04	2.1E+04	1.8E+04	2.2E+04	5.2E+02	3.6E+02	3.6E+02	4.1E+02
157	1213.9861	47.7	1.4E+05	1.0E+05	1.4E+05	1.3E+05	4.2E+04	4.9E+04	9.9E+03	3.4E+04
158	1227.9682	46.8	2.1E+05	1.3E+05	1.8E+05	1.7E+05	5.5E+04	6.8E+04	9.3E+03	4.4E+04
159	1231.0136	47.7	8.3E+04	5.6E+04	7.5E+04	7.1E+04	2.2E+04	2.9E+04	4.8E+03	1.9E+04
160	1242.0157	48.0	5.5E+04	3.8E+04	5.5E+04	4.9E+04	1.7E+04	2.0E+04	5.0E+03	1.4E+04
161	1241.9467	46.0	1.0E+05	6.4E+04	9.4E+04	8.7E+04	3.2E+04	3.7E+04	7.4E+03	2.5E+04
162	1244.9931	46.9	2.5E+05	1.6E+05	2.3E+05	2.1E+05	6.2E+04	7.6E+04	9.8E+03	4.9E+04
163	1248.9323	45.6	2.7E+04	3.5E+04	2.9E+04	3.0E+04	1.4E+04	1.0E+04	7.7E+03	1.1E+04
164	1253.9149	45.6	1.3E+04	1.3E+04	1.2E+04	1.3E+04	6.2E+03	1.9E+03	2.0E+03	3.3E+03
165	1253.9593	46.6	2.4E+04	2.1E+04	2.0E+04	2.2E+04	1.2E+04	1.3E+04	7.7E+03	1.1E+04
166	1258.9741	46.0	2.8E+05	1.7E+05	2.5E+05	2.3E+05	7.2E+04	8.0E+04	9.6E+03	5.4E+04
167	1259.0420	48.0	3.5E+04	2.7E+04	3.7E+04	3.3E+04	1.2E+04	1.5E+04	3.9E+03	1.0E+04
168	1263.9508	45.9	1.6E+05	1.1E+05	1.4E+05	1.4E+05	4.9E+04	6.0E+04	2.7E+04	4.5E+04
169	1263.9656	46.7	7.2E+04	5.0E+04	7.7E+04	6.6E+04	3.0E+04	2.5E+04	1.6E+04	2.4E+04
170	1267.9451	46.9	1.7E+04	9.1E+03	1.0E+04	1.2E+04	5.0E+03	0.0E+00	1.2E+03	2.1E+03
171	1269.9725	45.8	6.9E+04	6.9E+04	8.6E+04	7.4E+04	3.5E+04	4.2E+04	8.2E+03	2.8E+04
172	1272.9494	44.9	5.0E+04	3.2E+04	5.1E+04	4.5E+04	1.3E+04	1.9E+04	5.0E+03	1.2E+04
173	1281.9348	46.1	2.4E+04	2.1E+04	1.8E+04	2.1E+04	1.4E+04	3.8E+03	4.1E+03	7.2E+03
174	1283.9562	44.6	7.1E+04	6.0E+04	8.1E+04	7.1E+04	3.0E+04	4.0E+04	7.6E+03	2.6E+04
175	1297.9352	43.2	3.3E+04	3.0E+04	4.3E+04	3.5E+04	1.5E+04	2.2E+04	3.5E+03	1.3E+04
176	1309.9357	44.7	2.8E+04	3.3E+04	3.1E+04	3.1E+04	1.4E+04	2.0E+02	7.7E+03	7.3E+03
177	1323.9745	45.4	3.5E+04	2.0E+04	2.9E+04	2.8E+04	5.3E+03	1.4E+04	3.1E+03	7.6E+03

A3.2 Normalized integrated mass ion intensity (nMSII) of positive-mode ions in media with increased levels under 4% ethanol stress.

No.	*m/z*	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	105.0691	21.1	2.7E+06	2.0E+06	2.4E+06	2.4E+06	7.4E+04	1.2E+05	6.9E+04	8.6E+04
2	117.0698	23.8	1.7E+04	1.5E+04	1.8E+04	1.7E+04	4.1E+03	4.4E+03	3.0E+03	3.8E+03
3	118.0892	5.9	1.1E+04	9.1E+03	7.3E+03	9.3E+03	8.5E+02	1.7E+03	1.4E+03	1.3E+03
4	127.0419	23.8	5.4E+04	5.1E+04	7.4E+04	6.0E+04	1.1E+04	1.2E+04	9.8E+03	1.1E+04
5	129.0528	21.1	1.0E+05	5.4E+04	1.0E+05	8.6E+04	7.1E+03	3.3E+03	6.8E+03	5.7E+03
6	144.1010	20.5	2.8E+05	3.8E+05	3.0E+05	3.2E+05	4.1E+03	4.1E+03	4.8E+03	4.3E+03
7	144.1007	12.4	5.1E+04	5.8E+04	5.2E+04	5.4E+04	7.2E+02	6.9E+02	6.3E+02	6.8E+02
8	144.1014	10.7	8.9E+04	1.0E+05	9.2E+04	9.5E+04	6.3E+02	5.8E+02	4.3E+02	5.5E+02
9	147.0653	23.8	1.5E+05	1.4E+05	1.9E+05	1.6E+05	3.0E+04	3.4E+04	2.4E+04	3.0E+04
10	153.0550	12.8	1.6E+05	1.8E+05	1.9E+05	1.8E+05	1.5E+04	1.3E+04	1.4E+04	1.4E+04
11	158.0787	9.8	1.3E+04	2.3E+04	1.3E+04	1.6E+04	7.1E+02	0.0E+00	0.0E+00	2.4E+02
12	160.1323	14.3	5.3E+04	6.0E+04	4.9E+04	5.4E+04	9.9E+02	8.6E+02	7.3E+02	8.6E+02
13	160.1322	9.9	1.6E+05	1.9E+05	9.6E+04	1.5E+05	8.9E+02	1.2E+03	7.7E+02	9.7E+02
14	163.1453	20.2	1.3E+05	1.3E+05	1.2E+05	1.3E+05	1.1E+04	1.1E+04	9.3E+03	1.0E+04
15	190.0527	14.5	4.7E+04	5.6E+04	4.8E+04	5.0E+04	5.0E+02	5.5E+02	3.9E+02	4.8E+02
16	194.1169	14.3	2.7E+04	3.5E+04	2.7E+04	3.0E+04	6.3E+02	6.2E+02	5.4E+02	6.0E+02
17	194.1164	10.1	1.5E+05	2.0E+05	9.7E+04	1.5E+05	1.6E+03	1.4E+03	1.5E+03	1.5E+03
18	201.1048	16.7	2.9E+04	3.0E+04	2.5E+04	2.8E+04	1.8E+03	1.4E+03	1.5E+03	1.6E+03
19	207.1341	11.7	2.4E+04	2.5E+04	2.5E+04	2.5E+04	3.8E+03	3.5E+03	3.2E+03	3.5E+03
20	207.6383	24.4	2.3E+04	1.6E+04	1.9E+04	1.9E+04	9.3E+02	6.6E+02	4.8E+02	6.9E+02
21	209.1490	20.2	1.1E+05	1.1E+05	1.2E+05	1.1E+05	1.2E+04	1.1E+04	9.1E+03	1.1E+04

No.	*m/z*	RT (min)	Normalized integrated mass ion intensity (nMSII) EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
22	216.1003	14.9	5.4E+04	6.4E+04	5.9E+04	5.9E+04	4.9E+02	6.4E+02	6.1E+02	5.8E+02
23	217.1531	20.6	4.6E+04	4.7E+04	5.1E+04	4.8E+04	1.0E+04	7.7E+03	7.9E+03	8.6E+03
24	219.1672	20.2	7.2E+04	9.3E+04	7.5E+04	8.0E+04	5.6E+03	6.6E+03	6.6E+03	6.3E+03
25	223.1702	21.3	1.5E+06	1.6E+06	1.6E+06	1.6E+06	5.1E+05	3.0E+05	1.9E+05	3.3E+05
26	225.1422	11.7	2.5E+04	3.0E+04	2.8E+04	2.8E+04	5.4E+03	4.7E+03	4.9E+03	5.0E+03
27	235.1636	20.6	1.3E+05	1.4E+05	1.4E+05	1.3E+05	1.8E+04	1.6E+04	1.5E+04	1.6E+04
28	237.1680	20.6	6.5E+04	6.5E+04	5.5E+04	6.2E+04	1.3E+04	9.0E+03	9.9E+03	1.0E+04
29	243.1004	15.1	1.2E+04	1.5E+04	1.5E+04	1.4E+04	9.1E+02	7.1E+02	5.0E+02	7.0E+02
30	247.0946	12.8	3.0E+04	3.6E+04	2.7E+04	3.1E+04	4.7E+03	2.9E+03	3.3E+03	3.6E+03
31	249.1099	13.1	2.3E+04	2.9E+04	1.9E+04	2.4E+04	2.4E+03	0.0E+00	0.0E+00	8.0E+02
32	251.6658	24.4	4.3E+04	2.6E+04	3.0E+04	3.3E+04	1.1E+03	6.4E+02	8.5E+02	8.7E+02
33	252.1474	17.6	3.3E+04	2.3E+04	2.7E+04	2.8E+04	6.6E+03	4.7E+03	3.2E+03	4.9E+03
34	253.1736	20.6	6.0E+04	5.6E+04	5.7E+04	5.8E+04	1.2E+04	8.5E+03	8.5E+03	9.8E+03
35	256.0684	10.4	1.2E+04	1.2E+04	1.3E+04	1.3E+04	2.9E+03	2.1E+03	4.2E+03	3.0E+03
36	263.1332	23.8	2.2E+04	2.1E+04	3.1E+04	2.5E+04	4.0E+03	5.2E+03	3.6E+03	4.3E+03
37	263.0933	21.2	3.7E+04	2.8E+04	3.2E+04	3.2E+04	1.6E+02	1.6E+02	1.5E+02	1.6E+02
38	265.1407	15.4	2.2E+04	1.9E+04	1.6E+04	1.9E+04	4.1E+03	1.8E+03	1.7E+03	2.5E+03
39	265.1729	20.2	3.5E+05	3.9E+05	3.5E+05	3.6E+05	4.3E+04	3.8E+04	3.1E+04	3.7E+04
40	270.2413	12.9	5.1E+04	5.8E+04	4.8E+04	5.2E+04	0.0E+00	0.0E+00	0.0E+00	0.0E+00
41	272.2566	18.8	9.2E+03	1.2E+04	8.6E+03	9.9E+03	1.9E+03	9.1E+02	3.1E+02	1.0E+03
42	272.2547	18.1	1.5E+04	1.5E+04	9.1E+03	1.3E+04	0.0E+00	0.0E+00	2.7E+01	8.9E+00
43	288.2519	12.9	3.2E+04	3.0E+04	3.0E+04	3.1E+04	9.2E+00	0.0E+00	0.0E+00	3.1E+00
44	297.1658	18.1	2.1E+05	1.9E+05	1.4E+05	1.8E+05	1.7E+04	8.4E+03	5.2E+03	1.0E+04
45	297.1663	16.4	7.1E+04	6.7E+04	4.8E+04	6.2E+04	3.1E+03	1.6E+03	1.5E+03	2.1E+03
46	301.1507	27.7	2.1E+05	1.6E+05	1.7E+05	1.8E+05	2.0E+04	6.4E+04	4.4E+04	4.3E+04
47	305.1558	20.3	2.9E+05	2.4E+05	2.6E+05	2.6E+05	5.4E+04	4.9E+04	4.0E+04	4.8E+04
48	307.1863	18.0	1.2E+05	1.4E+05	1.1E+05	1.2E+05	7.9E+03	6.7E+03	5.5E+03	6.7E+03
49	311.2127	17.6	4.7E+04	4.9E+04	5.9E+04	5.2E+04	4.7E+03	3.6E+03	3.1E+03	3.8E+03
50	313.2413	37.3	1.0E+05	1.0E+05	9.7E+04	1.0E+05	1.8E+04	2.1E+04	1.5E+04	1.8E+04
51	313.2333	16.5	7.2E+04	8.1E+04	8.8E+04	8.0E+04	1.7E+03	1.1E+03	1.1E+03	1.3E+03
52	316.1150	16.9	1.1E+04	1.5E+04	8.3E+03	1.2E+04	6.5E+02	1.9E+02	3.8E+02	4.1E+02
53	317.2675	22.7	2.9E+05	3.1E+05	3.3E+05	3.1E+05	6.2E+03	6.2E+03	5.3E+03	5.9E+03
54	317.2670	23.4	1.6E+05	7.6E+04	1.5E+05	1.3E+05	6.9E+03	1.2E+03	1.5E+03	3.2E+03
55	319.1503	18.1	1.7E+04	1.9E+04	2.0E+04	1.9E+04	1.8E+03	1.3E+03	1.2E+03	1.4E+03
56	321.1334	13.2	3.1E+04	3.2E+04	2.8E+04	3.0E+04	4.9E+03	3.8E+03	3.5E+03	4.1E+03
57	321.1764	20.5	8.6E+04	1.0E+05	9.5E+04	9.4E+04	1.1E+04	8.2E+03	7.0E+03	8.6E+03
58	326.7237	24.4	1.9E+04	1.5E+04	1.1E+04	1.5E+04	3.5E+02	1.9E+02	3.3E+02	2.9E+02
59	340.2097	24.4	5.0E+04	3.5E+04	4.1E+04	4.2E+04	2.7E+03	1.5E+03	1.4E+03	1.9E+03
60	343.1409	17.5	2.6E+04	2.0E+04	1.5E+04	2.0E+04	2.0E+03	3.3E+03	6.6E+02	2.0E+03
61	345.1427	14.3	1.8E+04	2.2E+04	2.0E+04	2.0E+04	1.4E+02	0.0E+00	0.0E+00	4.5E+01
62	345.2993	26.3	5.1E+05	4.1E+05	4.5E+05	4.5E+05	1.5E+04	1.1E+04	9.3E+03	1.2E+04
63	347.2522	25.4	2.1E+05	2.3E+05	2.1E+05	2.2E+05	2.9E+04	9.0E+03	5.3E+03	1.5E+04
64	348.7348	24.5	2.1E+04	1.4E+04	1.5E+04	1.7E+04	2.6E+02	1.1E+02	5.3E+01	1.4E+02
65	354.1424	14.9	4.2E+04	5.4E+04	4.9E+04	4.8E+04	7.3E+01	1.4E+01	1.5E+02	7.8E+01
66	355.2466	21.3	5.3E+04	4.5E+04	5.8E+04	5.2E+04	2.5E+03	1.8E+03	2.0E+03	2.1E+03
67	355.1731	20.5	2.4E+04	2.7E+04	1.9E+04	2.3E+04	3.4E+03	2.4E+03	2.1E+03	2.6E+03
68	363.2102	20.6	1.5E+05	1.1E+05	1.4E+05	1.3E+05	2.8E+04	1.9E+04	1.4E+04	2.0E+04
69	369.1748	21.2	6.3E+04	4.8E+04	5.8E+04	5.6E+04	5.3E+03	3.6E+03	3.9E+03	4.2E+03
70	370.7431	24.3	1.7E+04	9.8E+03	1.4E+04	1.3E+04	7.5E+02	2.1E+02	2.1E+02	3.9E+02
71	373.1535	16.3	4.7E+04	4.1E+04	3.8E+04	4.2E+04	6.1E+03	5.3E+03	4.8E+03	5.4E+03
72	379.3030	22.5	1.5E+05	1.6E+05	9.9E+04	1.4E+05	5.5E+03	5.2E+03	2.9E+03	4.5E+03
73	387.1800	21.2	2.7E+06	2.0E+06	2.6E+06	2.4E+06	6.9E+04	1.3E+05	6.1E+04	8.7E+04
74	388.3395	18.3	1.4E+04	1.9E+04	1.5E+04	1.6E+04	7.0E+01	7.9E+00	1.4E+01	3.1E+01
75	389.3254	26.1	1.5E+06	1.2E+06	1.4E+06	1.3E+06	4.1E+04	3.1E+04	2.9E+04	3.4E+04
76	404.2061	21.2	1.4E+06	8.8E+05	1.3E+06	1.2E+06	4.4E+04	8.7E+04	3.7E+04	5.6E+04
77	405.3201	22.9	9.2E+05	1.1E+06	7.6E+05	9.1E+05	1.9E+04	1.3E+04	1.0E+04	1.4E+04
78	409.1618	21.1	3.1E+05	2.2E+05	3.1E+05	2.8E+05	6.5E+03	1.0E+04	6.8E+03	7.9E+03
79	423.3296	21.7	2.8E+05	4.1E+05	2.1E+05	3.0E+05	2.5E+03	1.4E+04	3.5E+03	6.6E+03
80	433.3515	25.8	1.5E+06	1.1E+06	1.3E+06	1.3E+06	8.5E+02	1.2E+04	1.0E+04	7.5E+03

No.	m/z	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
81	436.3398	18.1	2.8E+04	3.7E+04	3.1E+04	3.2E+04	1.8E+02	2.2E+02	1.8E+02	2.0E+02
82	440.3554	22.5	1.9E+05	1.7E+05	1.4E+05	1.7E+05	1.7E+04	1.2E+04	1.1E+04	1.3E+04
83	445.8240	24.4	1.1E+05	7.3E+04	7.7E+04	8.8E+04	2.0E+03	9.6E+02	6.5E+02	1.2E+03
84	449.3463	22.8	6.3E+05	6.4E+05	5.0E+05	5.9E+05	1.3E+04	9.9E+03	6.0E+03	9.6E+03
85	449.3457	22.2	3.9E+05	2.3E+05	3.2E+05	3.1E+05	8.2E+03	5.9E+03	5.8E+03	6.6E+03
86	451.3366	26.6	2.2E+04	2.4E+04	2.2E+04	2.2E+04	3.7E+03	3.0E+03	2.6E+03	3.1E+03
87	455.2298	20.6	8.5E+04	7.5E+04	7.1E+04	7.7E+04	1.5E+04	1.7E+04	1.8E+04	1.7E+04
88	459.8407	26.9	8.8E+03	1.1E+04	8.5E+03	9.4E+03	9.0E+02	3.3E+02	1.9E+02	4.7E+02
89	467.3551	22.1	2.8E+05	4.4E+05	2.0E+05	3.1E+05	0.0E+00	3.0E+02	0.0E+00	1.0E+02
90	467.8376	24.3	1.2E+05	8.0E+04	8.3E+04	9.4E+04	2.1E+03	1.1E+03	7.3E+02	1.3E+03
91	468.8771	45.9	1.7E+04	1.3E+04	1.5E+04	1.5E+04	2.6E+03	3.5E+03	1.3E+03	2.4E+03
92	475.8337	21.2	1.4E+04	1.6E+04	1.8E+04	1.6E+04	5.9E+02	5.4E+02	1.1E+02	4.1E+02
93	477.3764	25.6	1.0E+06	7.2E+05	8.6E+05	8.6E+05	3.0E+04	1.9E+04	1.9E+04	2.3E+04
94	481.8525	26.8	1.6E+04	2.1E+04	1.5E+04	1.7E+04	1.7E+03	8.3E+02	5.4E+02	1.0E+03
95	484.3815	21.9	8.6E+05	4.8E+05	6.1E+05	6.5E+05	4.4E+04	2.3E+04	2.3E+04	3.0E+04
96	485.3630	23.2	1.9E+05	1.9E+05	1.9E+05	1.9E+05	7.1E+03	8.2E+03	5.7E+03	7.0E+03
97	489.8509	24.2	1.0E+05	7.1E+04	7.7E+04	8.3E+04	1.8E+03	7.0E+02	7.8E+02	1.1E+03
98	493.3714	22.6	3.1E+05	3.2E+05	2.7E+05	3.0E+05	7.1E+03	5.6E+03	3.1E+03	5.3E+03
99	495.3882	25.6	5.8E+05	4.2E+05	4.9E+05	5.0E+05	1.7E+04	1.1E+04	1.1E+04	1.3E+04
100	501.3518	22.4	2.2E+04	2.2E+04	2.0E+04	2.1E+04	3.2E+03	3.0E+03	1.8E+03	2.7E+03
101	503.8663	26.7	2.4E+04	3.1E+04	2.1E+04	2.5E+04	1.2E+03	0.0E+00	0.0E+00	4.0E+02
102	511.3794	22.6	1.5E+05	8.9E+04	1.2E+05	1.2E+05	1.4E+04	1.9E+04	0.0E+00	1.1E+04
103	511.8644	24.1	7.9E+04	5.4E+04	5.6E+04	6.3E+04	1.2E+03	5.0E+02	6.7E+02	7.7E+02
104	512.4148	25.6	1.0E+06	7.0E+05	7.2E+05	8.1E+05	4.1E+04	3.1E+04	2.5E+04	3.2E+04
105	515.3658	21.8	2.9E+04	1.5E+04	2.8E+04	2.4E+04	3.1E+03	4.6E+03	1.5E+03	3.0E+03
106	521.4031	25.5	5.1E+05	3.7E+05	4.6E+05	4.5E+05	1.4E+04	8.9E+03	9.0E+03	1.1E+04
107	525.8799	26.6	2.6E+04	3.3E+04	2.1E+04	2.7E+04	1.7E+03	9.3E+02	6.8E+02	1.1E+03
108	528.4089	22.5	1.4E+06	7.2E+05	8.3E+05	9.7E+05	4.8E+04	5.0E+04	3.3E+03	3.4E+04
109	529.3494	24.4	1.6E+05	1.8E+05	1.6E+05	1.6E+05	3.1E+04	3.8E+04	1.5E+04	2.8E+04
110	533.8779	24.1	4.8E+04	3.3E+04	3.7E+04	3.9E+04	7.3E+02	4.6E+02	3.9E+02	5.3E+02
111	537.3984	22.5	1.3E+05	1.3E+05	1.1E+05	1.2E+05	3.1E+03	2.6E+03	1.9E+03	2.6E+03
112	539.4141	25.5	3.6E+05	2.6E+05	3.2E+05	3.1E+05	1.0E+04	7.2E+03	6.1E+03	7.9E+03
113	541.3461	22.4	4.1E+04	3.6E+04	4.4E+04	4.0E+04	4.4E+03	3.2E+03	3.1E+03	3.6E+03
114	543.3600	23.2	4.0E+05	4.0E+05	4.3E+05	4.1E+05	1.1E+04	1.3E+04	8.1E+03	1.1E+04
115	547.8933	26.5	2.7E+04	3.3E+04	2.5E+04	2.8E+04	1.9E+03	8.8E+02	5.2E+02	1.1E+03
116	554.4240	24.6	7.4E+04	6.2E+04	6.2E+04	6.6E+04	4.9E+03	4.0E+03	2.7E+03	3.9E+03
117	555.8912	24.0	2.7E+04	2.0E+04	2.1E+04	2.3E+04	6.3E+02	2.9E+02	2.3E+02	3.9E+02
118	556.4413	25.4	1.6E+06	1.1E+06	1.3E+06	1.3E+06	5.4E+04	3.7E+04	2.9E+04	4.0E+04
119	557.1464	20.6	4.5E+04	3.8E+04	4.4E+04	4.2E+04	8.6E+03	1.1E+04	9.9E+03	9.7E+03
120	559.3353	23.2	3.2E+04	3.2E+04	3.7E+04	3.3E+04	2.5E+03	2.2E+03	2.1E+03	2.3E+03
121	565.4298	25.3	2.4E+05	1.7E+05	2.0E+05	2.0E+05	7.3E+03	5.1E+03	3.9E+03	5.4E+03
122	571.1590	21.5	6.7E+04	8.6E+04	8.3E+04	7.9E+04	1.1E+04	1.5E+04	2.1E+04	1.5E+04
123	573.9111	24.0	1.5E+04	1.1E+04	9.1E+03	1.2E+04	4.3E+02	2.3E+02	8.9E+01	2.5E+02
124	581.4230	22.3	5.2E+04	3.8E+04	4.6E+04	4.5E+04	1.3E+03	9.9E+02	5.2E+02	9.3E+02
125	583.4399	25.3	2.0E+05	1.4E+05	1.7E+05	1.7E+05	5.4E+03	4.4E+03	3.5E+03	4.4E+03
126	587.4219	26.4	2.4E+04	2.9E+04	1.9E+04	2.4E+04	1.6E+03	9.9E+03	2.3E+02	3.9E+03
127	591.9183	26.3	2.0E+04	2.1E+04	1.5E+04	1.9E+04	1.3E+03	5.3E+02	4.5E+02	7.5E+02
128	600.4676	25.3	1.9E+06	1.3E+06	1.5E+06	1.6E+06	5.1E+04	4.0E+04	3.0E+04	4.0E+04
129	609.4546	25.2	9.6E+04	7.0E+04	8.8E+04	8.5E+04	0.0E+00	3.2E+02	2.8E+02	2.0E+02
130	609.4359	26.3	3.3E+04	3.8E+04	2.7E+04	3.3E+04	3.2E+03	1.4E+03	1.0E+03	1.9E+03
131	611.1149	20.0	1.0E+05	1.2E+05	7.2E+04	9.9E+04	1.3E+04	8.5E+03	7.3E+03	9.6E+03
132	613.9332	26.2	1.3E+04	1.3E+04	1.1E+04	1.2E+04	7.9E+02	5.6E+02	2.5E+02	5.4E+02
133	616.1794	29.6	9.6E+03	1.1E+04	9.2E+03	9.8E+03	1.1E+03	1.3E+03	9.1E+02	1.1E+03
134	616.4620	22.3	5.8E+05	7.5E+05	4.1E+05	5.8E+05	1.6E+04	1.4E+04	7.3E+03	1.2E+04
135	621.4813	40.0	1.0E+05	8.6E+04	8.6E+04	9.2E+04	2.2E+03	1.9E+03	3.6E+03	2.6E+03
136	629.9914	46.0	2.8E+04	1.7E+04	2.6E+04	2.4E+04	3.7E+03	3.8E+03	8.3E+02	2.8E+03
137	644.4936	25.1	1.8E+06	1.3E+06	1.5E+06	1.5E+06	4.6E+04	3.3E+04	2.7E+04	3.5E+04
138	653.4600	26.1	3.7E+04	4.2E+04	2.6E+04	3.5E+04	1.1E+02	1.5E+02	0.0E+00	8.9E+01
139	660.4874	22.2	4.2E+05	5.1E+05	3.0E+05	4.1E+05	1.0E+04	8.4E+03	5.1E+03	7.8E+03

No.	*m/z*	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
140	671.4915	25.0	5.3E+04	3.9E+04	4.5E+04	4.6E+04	3.3E+03	1.1E+03	6.1E+02	1.7E+03
141	688.5205	25.0	1.6E+06	1.1E+06	1.3E+06	1.3E+06	3.9E+04	2.5E+04	2.1E+04	2.8E+04
142	697.4861	25.9	3.2E+04	3.1E+04	1.8E+04	2.7E+04	2.5E+03	1.3E+03	2.6E+02	1.3E+03
143	704.5132	21.6	2.8E+05	3.4E+05	4.1E+05	3.4E+05	1.4E+04	1.1E+04	7.7E+03	1.1E+04
144	732.5459	24.9	1.2E+06	8.6E+05	9.8E+05	1.0E+06	2.9E+04	1.9E+04	1.5E+04	2.1E+04
145	748.5396	22.0	1.6E+05	2.1E+05	2.7E+05	2.2E+05	8.5E+03	6.7E+03	5.0E+03	6.8E+03
146	776.5712	24.8	8.5E+05	6.0E+05	6.6E+05	7.0E+05	1.8E+04	1.2E+04	9.7E+03	1.3E+04
147	792.5649	21.9	8.2E+04	1.1E+05	6.2E+04	8.4E+04	2.1E+03	1.5E+03	9.7E+02	1.5E+03
148	820.5980	24.6	4.8E+05	3.6E+05	4.1E+05	4.2E+05	1.2E+04	6.5E+03	5.7E+03	8.1E+03
149	836.5912	21.9	4.5E+04	3.4E+04	3.3E+04	3.7E+04	1.6E+03	1.1E+03	7.0E+02	1.1E+03
150	846.4411	23.8	1.5E+04	1.1E+04	2.1E+04	1.6E+04	2.3E+03	2.7E+03	1.3E+03	2.1E+03
151	851.3977	23.8	2.3E+04	1.6E+04	2.8E+04	2.2E+04	3.8E+03	4.8E+03	2.3E+03	3.6E+03
152	854.4285	23.8	1.2E+04	8.8E+03	1.3E+04	1.1E+04	2.3E+03	2.3E+03	1.0E+03	1.9E+03
153	864.6233	24.5	2.8E+05	2.0E+05	2.3E+05	2.4E+05	6.5E+03	3.4E+03	3.2E+03	4.4E+03
154	908.6494	24.4	1.5E+05	1.2E+05	1.2E+05	1.3E+05	4.6E+03	2.4E+03	1.9E+03	3.0E+03
155	1051.6301	23.0	1.3E+04	1.3E+04	1.3E+04	1.3E+04	5.8E+02	3.5E+02	2.0E+02	3.8E+02
156	1063.7393	23.2	4.5E+04	3.7E+04	3.1E+04	3.8E+04	3.7E+02	2.6E+02	2.5E+02	2.9E+02
157	1213.9861	47.7	2.4E+05	1.8E+05	2.4E+05	2.2E+05	3.0E+04	3.5E+04	7.0E+03	2.4E+04
158	1227.9682	46.8	3.5E+05	2.2E+05	3.1E+05	2.9E+05	3.9E+04	4.8E+04	6.6E+03	3.1E+04
159	1231.0136	47.7	1.4E+05	9.6E+04	1.3E+05	1.2E+05	1.6E+04	2.0E+04	3.4E+03	1.3E+04
160	1242.0157	48.0	9.3E+04	6.5E+04	9.3E+04	8.4E+04	1.2E+04	1.4E+04	3.6E+03	1.0E+04
161	1241.9467	46.0	1.8E+05	1.1E+05	1.6E+05	1.5E+05	2.2E+04	2.6E+04	5.2E+03	1.8E+04
162	1244.9931	46.9	4.3E+05	2.7E+05	3.9E+05	3.6E+05	4.4E+04	5.4E+04	6.9E+03	3.5E+04
163	1248.9323	45.6	4.6E+04	6.0E+04	4.9E+04	5.2E+04	1.0E+04	7.1E+03	5.4E+03	7.5E+03
164	1253.9149	45.6	2.2E+04	2.2E+04	2.1E+04	2.2E+04	4.4E+03	1.3E+03	1.4E+03	2.4E+03
165	1253.9593	46.6	4.1E+04	3.5E+04	3.4E+04	3.7E+04	8.2E+03	9.5E+03	5.5E+03	7.7E+03
166	1258.9741	46.0	4.7E+05	2.9E+05	4.2E+05	3.9E+05	5.1E+04	5.7E+04	6.8E+03	3.8E+04
167	1259.0420	48.0	6.0E+04	4.5E+04	6.2E+04	5.6E+04	8.6E+03	1.0E+04	2.8E+03	7.2E+03
168	1263.9508	45.9	2.7E+05	1.9E+05	2.3E+05	2.3E+05	3.5E+04	4.3E+04	1.9E+04	3.2E+04
169	1263.9656	46.7	1.2E+05	8.4E+04	1.3E+05	1.1E+05	2.1E+04	1.8E+04	1.2E+04	1.7E+04
170	1267.9451	46.9	2.9E+04	1.6E+04	1.7E+04	2.1E+04	3.6E+03	0.0E+00	8.5E+02	1.5E+03
171	1269.9725	45.8	1.2E+05	1.2E+05	1.5E+05	1.3E+05	2.5E+04	3.0E+04	5.8E+03	2.0E+04
172	1272.9494	44.9	8.5E+04	5.5E+04	8.7E+04	7.6E+04	9.2E+03	1.4E+04	3.5E+03	8.8E+03
173	1281.9348	46.1	4.1E+04	3.6E+04	3.1E+04	3.6E+04	9.7E+03	2.7E+03	2.9E+03	5.1E+03
174	1283.9562	44.6	1.2E+05	1.0E+05	1.4E+05	1.2E+05	2.1E+04	2.9E+04	5.4E+03	1.8E+04
175	1297.9352	43.2	5.7E+04	5.1E+04	7.3E+04	6.0E+04	1.1E+04	1.5E+04	2.4E+03	9.5E+03
176	1309.9357	44.7	4.8E+04	5.6E+04	5.3E+04	5.2E+04	1.0E+04	1.4E+02	5.5E+03	5.2E+03
177	1323.9745	45.4	5.9E+04	3.5E+04	5.0E+04	4.8E+04	3.8E+03	1.0E+04	2.2E+03	5.4E+03

A3.3 Integrated mass ion intensity (MSII) of positive-mode ions in media with decreased levels under 4% ethanol stress.

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	120.0440	28.7	7.5E+02	8.5E+01	7.8E+02	5.4E+02	4.3E+04	4.5E+04	3.7E+04	4.2E+04
2	123.1161	24.9	2.2E+04	2.1E+04	2.2E+04	2.2E+04	5.8E+05	5.9E+05	5.5E+05	5.7E+05
3	158.0601	5.7	0.0E+00	1.4E+01	2.6E+01	1.3E+01	6.7E+03	8.7E+03	9.9E+03	8.4E+03
4	233.1881	24.9	7.3E+03	6.2E+03	5.7E+03	6.4E+03	1.1E+05	1.1E+05	9.8E+04	1.1E+05
5	251.1993	24.9	1.8E+04	1.7E+04	1.8E+04	1.8E+04	5.5E+05	5.1E+05	4.8E+05	5.2E+05
6	333.2032	24.9	5.7E+03	5.9E+03	4.1E+03	5.2E+03	8.9E+04	8.7E+04	7.8E+04	8.4E+04
7	343.2253	24.6	7.8E+03	1.1E+04	7.9E+03	9.0E+03	9.6E+04	9.7E+04	1.5E+05	1.1E+05
8	355.2942	29.3	1.0E+04	1.7E+04	1.2E+04	1.3E+04	1.9E+05	1.4E+05	1.4E+05	1.6E+05
9	385.2346	22.9	7.7E+04	1.8E+05	1.0E+05	1.2E+05	1.3E+06	1.2E+06	1.6E+06	1.3E+06
10	387.2485	22.7	1.3E+04	1.6E+04	1.4E+04	1.4E+04	3.8E+05	3.5E+05	4.5E+05	3.9E+05
11	399.2130	23.1	1.5E+04	2.9E+04	1.9E+04	2.1E+04	2.4E+05	2.5E+05	3.8E+05	2.9E+05
12	401.2173	23.1	4.0E+02	1.6E+04	3.6E+03	6.6E+03	1.0E+05	1.0E+05	1.1E+05	1.1E+05

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII) EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
13	405.2599	18.9	2.2E+03	3.5E+03	2.1E+03	2.6E+03	4.0E+04	4.6E+04	3.5E+04	4.0E+04
14	456.2720	28.7	7.6E+03	6.1E+03	6.2E+03	6.6E+03	1.4E+05	1.4E+05	9.4E+04	1.2E+05
15	489.2318	20.7	8.7E+02	3.0E+02	4.3E+02	5.3E+02	5.8E+03	7.2E+03	6.4E+03	6.5E+03
16	531.2861	26.8	3.5E+03	7.5E+03	3.6E+03	4.9E+03	7.6E+04	6.0E+04	4.1E+04	5.9E+04
17	533.2362	18.3	9.3E+02	7.2E+02	6.8E+02	7.8E+02	1.2E+04	1.0E+04	7.2E+03	9.7E+03
18	545.2701	20.0	3.5E+03	3.3E+03	3.9E+03	3.6E+03	3.4E+05	2.0E+05	3.0E+05	2.8E+05

A3.4 Normalized integrated mass ion intensity (nMSII) of positive-mode ions in media with decreased levels under 4% ethanol stress.

No.	*m/z*	RT (min)	Normalized integrated mass ion intensity (nMSII) EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	120.0440	28.7	1.3E+03	1.4E+02	1.3E+03	9.2E+02	3.1E+04	3.2E+04	2.7E+04	3.0E+04
2	123.1161	24.9	3.8E+04	3.6E+04	3.7E+04	3.7E+04	4.1E+05	4.1E+05	3.9E+05	4.0E+05
3	158.0601	5.7	0.0E+00	2.4E+01	4.4E+01	2.3E+01	4.7E+03	6.2E+03	7.0E+03	6.0E+03
4	233.1881	24.9	1.2E+04	1.0E+04	9.6E+03	1.1E+04	8.1E+04	7.7E+04	7.0E+04	7.6E+04
5	251.1993	24.9	3.1E+04	2.9E+04	3.1E+04	3.1E+04	3.9E+05	3.6E+05	3.4E+05	3.7E+05
6	333.2032	24.9	9.6E+03	1.0E+04	6.9E+03	8.9E+03	6.3E+04	6.2E+04	5.5E+04	6.0E+04
7	343.2253	24.6	1.3E+04	1.9E+04	1.3E+04	1.5E+04	6.8E+04	6.9E+04	1.1E+05	8.1E+04
8	355.2942	29.3	1.8E+04	3.0E+04	2.0E+04	2.2E+04	1.3E+05	1.0E+05	1.0E+05	1.1E+05
9	385.2346	22.9	1.3E+05	3.0E+05	1.7E+05	2.0E+05	8.9E+05	8.6E+05	1.1E+06	9.5E+05
10	387.2485	22.7	2.3E+04	2.8E+04	2.3E+04	2.5E+04	2.7E+05	2.5E+05	3.2E+05	2.8E+05
11	399.2130	23.1	2.6E+04	4.9E+04	3.1E+04	3.6E+04	1.7E+05	1.8E+05	2.7E+05	2.1E+05
12	401.2173	23.1	6.7E+02	2.7E+04	6.1E+03	1.1E+04	7.4E+04	7.1E+04	7.8E+04	7.4E+04
13	405.2599	18.9	3.7E+03	5.9E+03	3.6E+03	4.4E+03	2.9E+04	3.2E+04	2.5E+04	2.9E+04
14	456.2720	28.7	1.3E+04	1.0E+04	1.0E+04	1.1E+04	9.7E+04	9.6E+04	6.6E+04	8.6E+04
15	489.2318	20.7	1.5E+03	5.2E+02	7.3E+02	9.1E+02	4.1E+03	5.1E+03	4.5E+03	4.6E+03
16	531.2861	26.8	5.9E+03	1.3E+04	6.2E+03	8.3E+03	5.4E+04	4.2E+04	2.9E+04	4.2E+04
17	533.2362	18.3	1.6E+03	1.2E+03	1.2E+03	1.3E+03	8.5E+03	7.2E+03	5.1E+03	6.9E+03
18	545.2701	20.0	6.0E+03	5.6E+03	6.7E+03	6.1E+03	2.4E+05	1.4E+05	2.1E+05	2.0E+05

Table A4 Positive-mode ions in mycelium of the ethanol-treated samples, compared with the control samples.

A4.1 Integrated mass ion intensity (MSII) of positive-mode ions in mycelium with increased levels under 4% ethanol stress.

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII) EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	109.1004	47.3	9.3E+04	9.8E+04	9.8E+04	9.7E+04	4.1E+04	3.0E+04	7.4E+04	4.8E+04
2	109.1003	46.4	7.4E+04	8.0E+04	7.4E+04	7.6E+04	2.2E+04	1.8E+04	1.9E+04	2.0E+04
3	111.1099	39.9	6.6E+04	6.9E+04	7.6E+04	7.0E+04	2.6E+04	2.6E+04	2.6E+04	2.6E+04
4	118.0866	5.9	5.6E+03	8.4E+03	7.1E+03	7.0E+03	9.8E+02	9.1E+02	1.4E+03	1.1E+03
5	121.1008	39.9	1.4E+05	1.6E+05	1.5E+05	1.5E+05	6.6E+04	6.3E+04	6.2E+04	6.4E+04
6	123.1155	47.3	7.0E+04	7.9E+04	7.7E+04	7.5E+04	3.8E+04	2.6E+04	5.9E+04	4.1E+04
7	123.1156	46.4	6.9E+04	7.3E+04	7.1E+04	7.1E+04	2.5E+04	2.0E+04	2.2E+04	2.2E+04
8	123.1151	38.8	1.6E+05	1.8E+05	1.7E+05	1.7E+05	1.0E+05	9.1E+04	9.3E+04	9.5E+04
9	125.1314	33.5	1.3E+05	1.3E+05	1.3E+05	1.3E+05	6.3E+04	5.5E+04	4.7E+04	5.5E+04
10	135.1152	47.3	7.9E+04	8.4E+04	8.4E+04	8.2E+04	3.8E+04	2.6E+04	6.0E+04	4.2E+04
11	135.1157	39.9	2.0E+05	2.2E+05	2.1E+05	2.1E+05	7.5E+04	6.3E+04	6.9E+04	6.9E+04
12	137.1312	47.3	5.0E+04	5.3E+04	5.4E+04	5.2E+04	2.6E+04	1.7E+04	4.0E+04	2.8E+04

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII) EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
13	137.1309	46.4	5.1E+04	5.5E+04	5.2E+04	5.3E+04	1.8E+04	1.4E+04	1.4E+04	1.5E+04
14	143.1069	39.9	3.4E+04	4.0E+04	3.8E+04	3.7E+04	1.3E+04	1.2E+04	1.4E+04	1.3E+04
15	144.1013	20.7	1.1E+04	1.4E+04	1.2E+04	1.3E+04	4.0E+03	2.0E+03	1.7E+03	2.6E+03
16	145.1005	33.5	7.2E+04	7.8E+04	7.4E+04	7.5E+04	2.7E+04	2.4E+04	2.4E+04	2.5E+04
17	145.1007	40.4	4.5E+04	7.3E+04	6.0E+04	5.9E+04	1.5E+04	1.5E+04	1.7E+04	1.6E+04
18	153.1291	39.9	5.0E+04	5.5E+04	6.1E+04	5.5E+04	1.8E+04	1.8E+04	1.9E+04	1.8E+04
19	155.1054	41.1	3.2E+04	3.1E+04	3.0E+04	3.1E+04	1.5E+04	1.7E+04	1.8E+04	1.6E+04
20	160.1320	9.9	1.9E+04	1.8E+04	2.1E+04	1.9E+04	3.9E+03	3.3E+03	4.4E+03	3.8E+03
21	163.1464	47.3	7.8E+04	8.7E+04	9.0E+04	8.5E+04	3.5E+04	2.2E+04	6.3E+04	4.0E+04
22	163.1463	46.4	7.8E+04	7.7E+04	7.6E+04	7.7E+04	2.1E+04	1.3E+04	1.4E+04	1.6E+04
23	163.1466	39.9	1.3E+05	1.4E+05	1.3E+05	1.3E+05	5.0E+04	4.2E+04	4.6E+04	4.6E+04
24	170.0572	41.6	5.9E+04	6.7E+04	6.6E+04	6.4E+04	7.2E+03	6.7E+03	7.9E+03	7.3E+03
25	170.0569	42.3	2.3E+04	2.7E+04	2.8E+04	2.6E+04	4.2E+03	3.2E+03	4.0E+03	3.8E+03
26	173.1293	47.3	2.2E+04	2.6E+04	2.6E+04	2.5E+04	1.4E+04	1.1E+04	1.8E+04	1.4E+04
27	175.1442	47.3	4.1E+04	4.4E+04	4.5E+04	4.3E+04	2.1E+04	1.7E+04	3.1E+04	2.3E+04
28	177.1612	47.3	8.4E+04	9.6E+04	1.0E+05	9.4E+04	3.2E+04	2.4E+04	7.1E+04	4.2E+04
29	177.1429	38.1	4.8E+04	5.6E+04	5.8E+04	5.4E+04	2.8E+04	3.1E+04	2.3E+04	2.7E+04
30	177.1612	46.4	6.1E+04	6.5E+04	6.7E+04	6.4E+04	1.3E+04	3.6E+03	9.9E+03	8.7E+03
31	177.1617	39.9	9.2E+04	1.1E+05	1.0E+05	1.0E+05	3.7E+04	3.5E+04	3.5E+04	3.6E+04
32	181.0887	47.3	2.5E+04	2.6E+04	2.7E+04	2.6E+04	7.6E+03	6.5E+03	1.9E+04	1.1E+04
33	181.1613	39.9	3.9E+04	4.6E+04	4.3E+04	4.3E+04	1.5E+04	1.2E+04	1.4E+04	1.4E+04
34	189.1614	47.3	4.6E+04	4.9E+04	5.1E+04	4.9E+04	1.8E+04	1.4E+04	3.4E+04	2.2E+04
35	189.1616	46.4	4.1E+04	4.2E+04	4.0E+04	4.1E+04	9.9E+03	4.8E+03	7.3E+03	7.3E+03
36	191.1776	47.3	6.7E+04	8.1E+04	8.3E+04	7.7E+04	3.2E+04	2.2E+04	5.7E+04	3.7E+04
37	191.1776	39.9	7.4E+04	9.4E+04	8.5E+04	8.5E+04	3.5E+04	2.9E+04	3.2E+04	3.2E+04
38	194.1160	10.1	1.1E+04	1.5E+04	1.6E+04	1.4E+04	1.9E+03	2.7E+03	1.8E+03	2.1E+03
39	197.1547	41.1	9.2E+03	7.3E+03	6.7E+03	7.8E+03	3.1E+03	4.8E+03	5.3E+03	4.4E+03
40	197.0802	46.4	3.8E+05	3.9E+05	3.8E+05	3.8E+05	1.5E+04	1.2E+04	2.9E+04	1.9E+04
41	198.9398	4.8	1.5E+04	8.8E+03	8.8E+03	1.1E+04	2.1E+03	3.9E+03	2.0E+03	2.7E+03
42	199.1592	38.8	4.3E+04	5.3E+04	5.3E+04	5.0E+04	1.8E+04	2.3E+04	1.9E+04	2.0E+04
43	200.9684	4.8	6.9E+03	4.9E+03	4.0E+03	5.3E+03	1.8E+03	1.8E+03	1.0E+03	1.5E+03
44	201.1598	33.5	2.5E+04	2.8E+04	2.7E+04	2.7E+04	8.4E+03	7.7E+03	5.8E+03	7.3E+03
45	201.1224	9.7	9.1E+03	9.5E+03	8.3E+03	9.0E+03	1.5E+03	1.0E+03	9.6E+02	1.1E+03
46	202.1061	28.4	5.3E+03	7.9E+03	4.6E+03	5.9E+03	1.5E+03	1.3E+03	1.2E+03	1.4E+03
47	203.1760	47.3	6.2E+04	7.2E+04	7.9E+04	7.1E+04	2.5E+04	1.6E+04	5.2E+04	3.1E+04
48	203.1763	46.4	4.9E+04	5.5E+04	5.3E+04	5.2E+04	2.9E+03	0.0E+00	0.0E+00	9.8E+02
49	205.1911	38.0	1.2E+05	1.6E+05	1.6E+05	1.5E+05	6.9E+04	6.4E+04	5.3E+04	6.2E+04
50	205.1932	47.3	4.3E+04	4.9E+04	5.0E+04	4.7E+04	1.7E+04	1.2E+04	3.6E+04	2.2E+04
51	205.1928	46.4	3.3E+04	3.2E+04	3.4E+04	3.3E+04	8.1E+03	6.4E+03	7.6E+03	7.4E+03
52	207.1694	38.7	4.3E+04	5.0E+04	5.1E+04	4.8E+04	2.1E+04	2.3E+04	1.8E+04	2.1E+04
53	209.1864	39.9	2.8E+04	3.2E+04	3.2E+04	3.1E+04	9.6E+03	8.7E+03	9.3E+03	9.2E+03
54	211.1537	41.1	6.0E+03	6.1E+03	6.6E+03	6.2E+03	1.9E+03	3.1E+03	4.0E+03	3.0E+03
55	213.1783	36.9	9.4E+04	1.1E+05	1.2E+05	1.1E+05	1.1E+04	2.1E+04	1.6E+04	1.6E+04
56	214.9171	4.8	7.5E+03	6.2E+03	5.7E+03	6.4E+03	1.6E+03	2.6E+03	1.2E+03	1.8E+03
57	216.9494	4.8	9.2E+03	4.5E+03	6.2E+03	6.6E+03	1.0E+03	7.9E+02	1.2E+03	1.0E+03
58	217.1924	38.0	1.8E+05	2.2E+05	2.4E+05	2.1E+05	8.0E+04	9.1E+04	7.1E+04	8.1E+04
59	217.1933	46.4	5.9E+04	6.0E+04	6.2E+04	6.0E+04	1.7E+04	1.2E+04	1.1E+04	1.4E+04
60	221.1190	47.3	1.5E+04	1.7E+04	1.9E+04	1.7E+04	7.5E+03	5.5E+03	1.3E+04	8.7E+03
61	221.2200	38.8	5.2E+04	6.4E+04	5.6E+04	5.8E+04	3.7E+04	2.8E+04	3.6E+04	3.4E+04
62	231.2083	47.3	4.9E+04	5.2E+04	5.2E+04	5.1E+04	2.1E+04	1.4E+04	3.8E+04	2.4E+04
63	231.2055	38.0	9.8E+04	1.2E+05	1.4E+05	1.2E+05	6.0E+04	5.7E+04	5.0E+04	5.6E+04
64	231.2078	46.4	3.3E+04	3.3E+04	3.0E+04	3.2E+04	8.0E+03	6.0E+03	7.2E+03	7.1E+03
65	233.1572	38.0	3.3E+04	3.8E+04	3.8E+04	3.6E+04	1.7E+04	1.8E+04	1.6E+04	1.7E+04
66	234.9606	4.8	1.2E+04	7.6E+03	9.1E+03	9.5E+03	2.3E+03	3.3E+03	1.7E+03	2.4E+03
67	243.2090	43.8	2.9E+04	2.4E+04	2.7E+04	2.7E+04	6.2E+03	5.7E+03	1.0E+04	7.5E+03
68	247.2410	39.9	8.2E+05	9.2E+05	9.6E+05	9.0E+05	2.1E+05	1.9E+05	2.3E+05	2.1E+05
69	249.1250	47.3	7.7E+03	8.8E+03	8.2E+03	8.2E+03	8.5E+02	0.0E+00	6.2E+03	2.3E+03
70	251.1279	47.3	5.9E+04	6.8E+04	6.9E+04	6.5E+04	2.0E+04	1.4E+04	4.8E+04	2.7E+04
71	251.1289	46.4	1.8E+04	1.8E+04	1.8E+04	1.8E+04	1.7E+03	2.6E+03	1.1E+02	1.5E+03

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII) EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
72	253.1928	33.5	1.0E+05	1.1E+05	1.1E+05	1.1E+05	3.0E+04	2.7E+04	2.5E+04	2.7E+04
73	253.1941	40.4	5.8E+04	1.0E+05	8.5E+04	8.1E+04	1.7E+04	1.9E+04	1.9E+04	1.8E+04
74	261.1715	37.9	2.9E+05	3.2E+05	3.2E+05	3.1E+05	1.2E+05	1.2E+05	1.1E+05	1.2E+05
75	261.2182	43.8	1.5E+05	1.2E+05	1.3E+05	1.3E+05	2.2E+04	1.9E+04	4.7E+04	2.9E+04
76	263.1278	47.3	8.4E+04	9.5E+04	9.5E+04	9.1E+04	3.2E+04	2.3E+04	7.1E+04	4.2E+04
77	263.2362	44.0	8.5E+05	6.9E+05	7.1E+05	7.5E+05	1.8E+05	1.7E+05	2.9E+05	2.1E+05
78	265.2516	39.9	8.4E+05	9.2E+05	9.2E+05	9.0E+05	2.2E+05	1.9E+05	2.3E+05	2.1E+05
79	271.2388	46.4	2.3E+04	2.6E+04	2.4E+04	2.4E+04	6.7E+03	5.8E+03	6.2E+03	6.2E+03
80	273.1842	38.1	2.3E+05	2.6E+05	2.7E+05	2.5E+05	5.8E+04	5.1E+04	1.7E+04	4.2E+04
81	284.2928	35.8	2.5E+05	2.4E+05	3.7E+05	2.8E+05	9.7E+04	2.8E+05	9.6E+04	1.6E+05
82	285.2749	40.9	6.5E+04	8.7E+04	9.0E+04	8.1E+04	1.1E+04	1.2E+04	2.0E+04	1.4E+04
83	287.2686	47.3	1.3E+04	1.6E+04	1.5E+04	1.5E+04	3.6E+03	2.1E+03	9.3E+03	5.0E+03
84	287.2671	46.4	8.4E+03	8.7E+03	9.0E+03	8.7E+03	3.9E+02	0.0E+00	2.7E+02	2.2E+02
85	289.1809	37.4	3.3E+04	3.7E+04	4.0E+04	3.7E+04	1.2E+04	1.3E+04	9.6E+03	1.2E+04
86	290.2679	13.9	1.9E+04	3.1E+04	2.6E+04	2.5E+04	1.5E+02	2.3E+01	1.6E+01	6.3E+01
87	290.2681	12.9	5.0E+04	8.5E+04	7.2E+04	6.9E+04	9.7E+01	1.3E+02	1.3E+01	8.0E+01
88	299.2568	43.5	1.4E+05	1.3E+05	1.3E+05	1.3E+05	6.4E+04	5.7E+04	7.4E+04	6.5E+04
89	299.2571	44.2	1.1E+05	8.9E+04	8.4E+04	9.4E+04	4.7E+04	4.3E+04	4.8E+04	4.6E+04
90	307.2543	39.6	1.3E+04	1.6E+04	1.6E+04	1.5E+04	0.0E+00	0.0E+00	9.0E+03	3.0E+03
91	309.2549	40.4	4.3E+04	7.2E+04	6.1E+04	5.9E+04	2.0E+03	5.5E+03	2.7E+03	3.4E+03
92	310.1740	9.7	2.2E+04	2.3E+04	2.3E+04	2.3E+04	2.1E+03	1.2E+03	1.1E+03	1.5E+03
93	311.2928	39.9	5.2E+05	5.9E+05	6.2E+05	5.8E+05	1.4E+05	1.2E+05	1.4E+05	1.4E+05
94	313.2391	38.1	9.8E+04	1.3E+05	1.2E+05	1.2E+05	4.9E+04	4.7E+04	3.6E+04	4.4E+04
95	313.2732	44.0	3.6E+06	5.1E+06	5.0E+06	4.6E+06	1.4E+06	1.3E+06	2.2E+06	1.6E+06
96	318.9373	4.8	6.9E+03	5.2E+03	4.5E+03	5.6E+03	2.2E+03	2.8E+03	1.8E+03	2.3E+03
97	319.1930	47.3	1.8E+04	2.3E+04	2.3E+04	2.1E+04	5.5E+03	2.1E+03	1.7E+04	8.3E+03
98	331.2789	44.0	1.7E+05	1.3E+05	1.3E+05	1.4E+05	2.9E+04	3.0E+04	6.6E+04	4.2E+04
99	331.2532	38.6	1.2E+05	1.2E+05	1.1E+05	1.2E+05	2.8E+04	2.8E+04	2.1E+04	2.6E+04
100	333.2750	40.0	2.6E+05	2.8E+05	2.5E+05	2.7E+05	5.1E+04	5.9E+04	7.2E+04	6.1E+04
101	335.2572	43.7	1.9E+05	1.6E+05	1.7E+05	1.7E+05	5.1E+04	5.0E+04	1.3E+05	7.7E+04
102	336.1984	9.6	2.7E+04	2.6E+04	2.0E+04	2.4E+04	1.7E+03	1.6E+03	1.6E+03	1.7E+03
103	337.2740	44.0	8.7E+06	6.7E+06	7.0E+06	7.4E+06	1.2E+06	1.1E+06	2.2E+06	1.5E+06
104	338.2033	10.0	2.5E+04	2.3E+04	2.3E+04	2.4E+04	1.7E+03	1.6E+03	1.5E+03	1.6E+03
105	339.2896	44.6	9.4E+06	8.0E+06	8.2E+06	8.5E+06	1.2E+06	9.6E+05	1.9E+06	1.3E+06
106	340.1834	9.8	2.6E+04	2.4E+04	2.4E+04	2.5E+04	3.3E+03	2.7E+03	2.5E+03	2.8E+03
107	341.1962	35.3	2.5E+04	1.7E+04	2.0E+04	2.1E+04	1.0E+04	1.1E+04	9.8E+03	1.0E+04
108	343.2565	38.0	4.1E+04	4.4E+04	5.1E+04	4.5E+04	1.0E+04	5.6E+03	0.0E+00	5.2E+03
109	344.1586	9.9	1.4E+04	2.0E+04	1.7E+04	1.7E+04	1.3E+03	1.1E+03	1.1E+03	1.2E+03
110	345.2090	47.3	1.3E+04	1.4E+04	1.4E+04	1.4E+04	5.9E+03	4.2E+03	1.0E+04	6.8E+03
111	352.2195	12.4	2.2E+04	3.0E+04	2.6E+04	2.6E+04	1.5E+03	1.3E+03	1.1E+03	1.3E+03
112	352.2193	10.6	2.9E+04	2.6E+04	2.4E+04	2.7E+04	1.3E+03	1.2E+03	1.1E+03	1.2E+03
113	354.1970	10.2	1.4E+04	1.6E+04	1.4E+04	1.5E+04	1.9E+03	1.1E+03	1.3E+03	1.4E+03
114	355.2631	38.0	2.6E+05	3.0E+05	3.2E+05	2.9E+05	1.1E+05	1.1E+05	9.6E+04	1.0E+05
115	355.2321	32.8	4.4E+04	5.8E+04	3.3E+04	4.5E+04	2.2E+04	2.7E+04	1.2E+04	2.0E+04
116	355.2352	47.3	1.9E+04	2.1E+04	2.2E+04	2.1E+04	0.0E+00	0.0E+00	1.4E+04	4.7E+03
117	357.2972	44.4	5.7E+04	5.2E+04	5.5E+04	5.5E+04	8.0E+03	7.3E+03	1.2E+04	9.0E+03
118	358.3439	47.5	1.1E+04	1.2E+04	1.2E+04	1.2E+04	1.0E+03	1.3E+03	1.4E+03	1.3E+03
119	367.3565	43.1	1.6E+04	1.6E+04	1.9E+04	1.7E+04	1.1E+03	1.5E+03	1.5E+03	1.4E+03
120	368.2130	9.8	1.7E+04	1.8E+04	1.7E+04	1.7E+04	1.7E+03	1.6E+03	1.7E+03	1.7E+03
121	368.2135	12.2	1.4E+04	1.3E+04	1.3E+04	1.4E+04	1.8E+03	1.9E+03	1.4E+03	1.7E+03
122	369.2783	38.0	1.2E+05	1.4E+05	1.7E+05	1.4E+05	5.8E+04	5.8E+04	5.0E+04	5.5E+04
123	370.1783	10.2	1.3E+04	1.6E+04	1.7E+04	1.5E+04	1.1E+03	7.7E+02	6.9E+02	8.5E+02
124	373.2364	47.3	3.5E+04	3.8E+04	4.1E+04	3.8E+04	1.3E+04	9.5E+03	2.8E+04	1.7E+04
125	375.3030	47.5	1.3E+05	1.5E+05	1.6E+05	1.5E+05	2.5E+04	1.5E+04	2.8E+04	2.3E+04
126	376.2219	24.1	1.1E+04	1.6E+04	1.8E+04	1.5E+04	6.6E+03	6.9E+03	1.1E+04	8.0E+03
127	379.3349	33.5	1.6E+06	1.7E+06	1.6E+06	1.6E+06	3.1E+05	2.7E+05	3.0E+05	2.9E+05
128	379.3356	40.4	1.0E+06	1.8E+06	1.5E+06	1.5E+06	1.8E+05	2.0E+05	2.1E+05	2.0E+05
129	382.2294	10.4	1.4E+04	1.3E+04	1.1E+04	1.3E+04	1.5E+03	9.1E+02	1.1E+03	1.2E+03
130	386.2031	11.1	2.0E+04	2.7E+04	2.6E+04	2.4E+04	4.5E+03	3.8E+03	3.7E+03	4.0E+03

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
131	387.2561	47.3	2.0E+04	2.2E+04	2.3E+04	2.2E+04	8.7E+03	7.1E+03	1.7E+04	1.1E+04
132	393.3644	41.1	1.9E+04	1.6E+04	1.7E+04	1.7E+04	7.1E+03	8.2E+03	9.4E+03	8.2E+03
133	395.3547	47.3	2.4E+04	2.0E+04	3.0E+04	2.5E+04	5.2E+03	2.9E+03	2.5E+04	1.1E+04
134	395.3548	46.4	2.9E+04	2.2E+04	2.5E+04	2.5E+04	0.0E+00	0.0E+00	0.0E+00	0.0E+00
135	395.3284	37.5	1.3E+05	1.5E+05	1.6E+05	1.5E+05	6.9E+04	6.3E+04	4.5E+04	5.9E+04
136	397.3975	45.1	1.7E+05	1.7E+05	1.6E+05	1.7E+05	2.2E+04	2.2E+04	1.9E+04	2.1E+04
137	399.2535	47.3	3.7E+04	4.0E+04	4.2E+04	4.0E+04	1.3E+04	9.8E+03	3.2E+04	1.8E+04
138	400.2165	12.0	8.2E+03	7.8E+03	6.6E+03	7.5E+03	9.1E+02	6.8E+02	6.9E+02	7.6E+02
139	402.1985	10.1	1.5E+04	1.9E+04	1.8E+04	1.7E+04	5.6E+02	2.9E+02	6.1E+02	4.9E+02
140	407.3377	38.1	4.9E+05	5.6E+05	6.1E+05	5.5E+05	2.3E+05	2.3E+05	1.8E+05	2.1E+05
141	411.3605	38.7	2.6E+05	2.4E+05	2.6E+05	2.5E+05	6.9E+04	7.1E+04	6.2E+04	6.7E+04
142	411.3809	41.1	6.9E+04	6.8E+04	6.3E+04	6.7E+04	2.9E+04	3.6E+04	3.9E+04	3.5E+04
143	417.2392	41.6	4.3E+04	3.7E+04	3.8E+04	3.9E+04	2.1E+04	2.8E+04	1.9E+04	2.3E+04
144	425.4262	45.9	4.2E+04	3.9E+04	3.8E+04	4.0E+04	0.0E+00	0.0E+00	0.0E+00	0.0E+00
145	428.4057	41.1	5.7E+04	5.3E+04	5.3E+04	5.4E+04	2.1E+04	2.7E+04	2.8E+04	2.5E+04
146	438.4614	43.9	7.0E+03	6.3E+03	8.6E+03	7.3E+03	2.0E+03	2.0E+03	3.4E+02	1.4E+03
147	442.3868	45.8	6.6E+04	7.1E+04	7.3E+04	7.0E+04	3.9E+04	3.8E+04	3.4E+04	3.7E+04
148	444.2447	13.6	6.6E+03	6.8E+03	6.7E+03	6.7E+03	3.5E+02	3.6E+02	3.0E+02	3.3E+02
149	445.2707	42.6	4.8E+04	4.2E+04	4.0E+04	4.3E+04	1.4E+04	1.9E+04	1.7E+04	1.7E+04
150	445.2706	41.9	5.9E+04	4.3E+04	4.2E+04	4.8E+04	1.2E+04	1.5E+04	1.1E+04	1.3E+04
151	446.2258	10.7	5.8E+03	5.5E+03	5.0E+03	5.4E+03	5.6E+02	2.9E+02	5.5E+02	4.6E+02
152	451.3598	38.2	5.6E+04	5.9E+04	6.4E+04	6.0E+04	3.6E+04	3.0E+04	2.7E+04	3.1E+04
153	452.4779	43.6	7.4E+03	9.3E+03	9.0E+03	8.6E+03	1.2E+02	0.0E+00	2.1E+01	4.7E+01
154	453.3720	38.7	1.9E+06	1.8E+06	2.0E+06	1.9E+06	4.4E+05	4.4E+05	4.1E+05	4.3E+05
155	455.3473	37.2	3.0E+05	3.5E+05	3.9E+05	3.4E+05	8.2E+04	7.7E+04	6.0E+04	7.3E+04
156	455.3190	47.3	3.6E+04	3.9E+04	4.0E+04	3.9E+04	1.9E+04	1.6E+04	2.9E+04	2.1E+04
157	464.2145	12.1	4.7E+03	6.6E+03	5.0E+03	5.5E+03	3.7E+02	2.5E+02	3.0E+02	3.1E+02
158	469.3657	38.2	4.0E+04	4.5E+04	4.6E+04	4.4E+04	1.8E+04	1.6E+04	1.2E+04	1.5E+04
159	469.3291	40.4	3.4E+04	4.0E+04	2.5E+04	3.3E+04	9.9E+03	1.9E+04	1.8E+04	1.6E+04
160	471.3803	38.6	2.0E+05	1.7E+05	2.1E+05	1.9E+05	3.2E+04	3.2E+04	3.1E+04	3.2E+04
161	472.3766	37.5	5.8E+04	7.6E+04	9.8E+04	7.8E+04	7.4E+03	6.4E+03	5.9E+03	6.6E+03
162	476.3486	33.5	8.8E+05	8.8E+05	8.9E+05	8.8E+05	9.8E+04	1.1E+05	1.4E+05	1.2E+05
163	477.3330	37.0	3.6E+05	4.2E+05	4.8E+05	4.2E+05	1.1E+05	1.0E+05	8.6E+04	9.9E+04
164	483.3618	34.1	1.6E+04	2.2E+04	2.6E+04	2.1E+04	1.1E+04	1.3E+04	6.7E+03	1.0E+04
165	488.4072	38.6	2.1E+05	1.7E+05	2.1E+05	2.0E+05	1.9E+04	2.2E+04	2.0E+04	2.0E+04
166	490.3269	29.2	1.1E+04	1.5E+04	1.3E+04	1.3E+04	3.6E+03	4.0E+03	4.1E+03	3.9E+03
167	491.2821	29.4	2.2E+04	2.3E+04	2.5E+04	2.3E+04	6.0E+03	5.1E+03	4.7E+03	5.3E+03
168	492.3408	31.8	1.4E+04	1.6E+04	1.3E+04	1.4E+04	3.2E+03	2.2E+03	3.5E+03	3.0E+03
169	493.3617	38.9	1.1E+06	1.2E+06	1.3E+06	1.2E+06	3.2E+05	4.0E+05	2.7E+05	3.3E+05
170	496.5021	43.6	6.3E+03	7.4E+03	7.1E+03	6.9E+03	1.3E+03	1.7E+03	1.3E+03	1.4E+03
171	497.2684	32.8	1.1E+05	1.4E+05	8.4E+04	1.1E+05	4.4E+04	6.7E+04	4.0E+04	5.0E+04
172	499.3866	38.6	1.5E+04	2.1E+04	1.9E+04	1.8E+04	4.5E+03	4.9E+03	3.7E+03	4.4E+03
173	503.4586	46.4	4.9E+03	6.7E+03	6.2E+03	5.9E+03	4.7E+03	2.6E+03	1.4E+03	2.9E+03
174	505.3885	43.8	3.2E+04	2.8E+04	2.8E+04	2.9E+04	5.3E+03	6.4E+03	9.9E+03	7.2E+03
175	506.3105	9.7	1.6E+04	1.1E+04	9.2E+03	1.2E+04	3.2E+02	3.0E+02	1.7E+02	2.6E+02
176	506.3243	30.8	9.9E+03	2.0E+04	1.8E+04	1.6E+04	3.3E+03	2.4E+03	4.2E+03	3.3E+03
177	507.3440	34.1	3.2E+04	3.5E+04	3.6E+04	3.4E+04	1.5E+04	1.3E+04	1.1E+04	1.3E+04
178	508.3386	32.2	1.1E+04	1.9E+04	1.6E+04	1.5E+04	5.3E+03	3.2E+03	4.0E+03	4.2E+03
179	517.4716	46.4	7.6E+03	8.5E+03	9.2E+03	8.4E+03	1.3E+03	4.2E+02	6.6E+01	6.0E+02
180	519.4118	43.7	2.1E+04	1.8E+04	1.9E+04	1.9E+04	4.5E+03	4.7E+03	6.2E+03	5.1E+03
181	523.3744	47.3	2.4E+04	2.4E+04	2.6E+04	2.5E+04	5.3E+03	4.8E+03	1.8E+04	9.2E+03
182	531.4891	46.4	2.6E+04	2.7E+04	2.6E+04	2.6E+04	1.8E+03	4.2E+02	1.6E+03	1.3E+03
183	538.3124	28.3	1.3E+05	1.8E+05	1.0E+05	1.4E+05	7.8E+03	1.2E+04	8.0E+03	9.2E+03
184	538.3814	33.1	7.7E+03	1.2E+04	7.1E+03	8.9E+03	2.2E+03	3.0E+03	2.6E+03	2.6E+03
185	543.4135	40.4	2.5E+04	4.8E+04	4.4E+04	3.9E+04	4.4E+03	4.8E+03	5.8E+03	5.0E+03
186	545.5066	49.5	7.3E+04	8.0E+04	7.0E+04	7.4E+04	5.4E+01	6.2E+03	0.0E+00	2.1E+03
187	545.5020	45.4	5.3E+04	5.1E+04	4.8E+04	5.1E+04	5.5E+03	4.7E+03	2.7E+03	4.3E+03
188	561.4869	41.7	1.5E+05	1.2E+05	1.0E+05	1.2E+05	6.5E+04	7.5E+04	6.1E+04	6.7E+04
189	562.5322	49.5	5.9E+04	6.0E+04	6.1E+04	6.0E+04	2.1E+03	6.2E+03	1.6E+03	3.3E+03

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
190	563.5011	44.2	1.1E+05	8.4E+04	8.0E+04	9.0E+04	3.3E+04	2.7E+04	4.0E+04	3.3E+04
191	575.5035	44.1	2.9E+06	2.3E+06	2.3E+06	2.5E+06	6.1E+05	6.3E+05	1.1E+06	7.9E+05
192	577.5185	44.6	2.9E+06	2.5E+06	2.5E+06	2.7E+06	6.5E+05	5.8E+05	1.0E+06	7.6E+05
193	583.2547	23.6	8.0E+03	4.8E+03	7.4E+03	6.7E+03	1.2E+03	1.1E+03	2.0E+03	1.4E+03
194	585.4968	45.4	3.2E+04	3.3E+04	3.1E+04	3.2E+04	4.3E+03	4.6E+03	4.0E+03	4.3E+03
195	587.5051	44.0	7.0E+04	5.7E+04	5.9E+04	6.2E+04	1.7E+04	1.7E+04	2.2E+04	1.9E+04
196	589.5150	44.5	1.1E+05	9.8E+04	9.7E+04	1.0E+05	3.3E+04	2.9E+04	4.7E+04	3.6E+04
197	591.5287	45.1	6.8E+04	6.3E+04	6.1E+04	6.4E+04	2.8E+04	2.5E+04	3.2E+04	2.8E+04
198	593.5154	44.1	2.9E+05	2.4E+05	2.3E+05	2.6E+05	6.9E+04	6.4E+04	1.2E+05	8.4E+04
199	594.5439	40.6	8.5E+04	9.0E+04	8.6E+04	8.7E+04	3.4E+04	5.5E+04	5.2E+04	4.7E+04
200	595.5281	44.6	2.6E+05	2.2E+05	2.1E+05	2.3E+05	5.7E+04	4.8E+04	8.5E+04	6.3E+04
201	599.5044	41.8	5.4E+06	4.0E+06	3.7E+06	4.4E+06	1.6E+06	1.9E+06	1.7E+06	1.7E+06
202	599.5026	43.8	1.3E+06	1.0E+06	1.0E+06	1.1E+06	1.7E+05	1.8E+05	3.1E+05	2.2E+05
203	601.5186	44.4	3.1E+06	2.7E+06	2.7E+06	2.8E+06	3.5E+05	3.5E+05	6.1E+05	4.4E+05
204	603.5360	43.3	9.8E+06	8.2E+06	7.9E+06	8.7E+06	2.4E+06	2.8E+06	2.8E+06	2.7E+06
205	603.5334	44.9	2.1E+06	1.8E+06	1.9E+06	1.9E+06	2.9E+05	2.8E+05	4.8E+05	3.5E+05
206	605.5484	44.0	1.3E+06	1.0E+06	1.0E+06	1.1E+06	3.2E+05	8.3E+04	4.3E+05	2.8E+05
207	610.5394	44.0	1.0E+06	8.0E+05	8.1E+05	8.8E+05	2.4E+05	2.2E+05	4.3E+05	3.0E+05
208	610.5635	46.7	3.2E+04	3.1E+04	3.2E+04	3.2E+04	1.6E+04	1.5E+04	1.4E+04	1.5E+04
209	613.5668	46.5	1.7E+05	1.8E+05	1.7E+05	1.8E+05	0.0E+00	1.7E+02	0.0E+00	5.6E+01
210	617.5133	43.7	2.9E+06	2.3E+06	2.3E+06	2.5E+06	3.4E+05	3.5E+05	6.8E+05	4.6E+05
211	617.5101	44.7	6.7E+05	5.8E+05	5.6E+05	6.0E+05	2.3E+05	2.4E+05	3.6E+05	2.8E+05
212	618.3002	29.2	1.8E+04	2.4E+04	1.4E+04	1.8E+04	5.5E+03	1.2E+04	8.4E+03	8.8E+03
213	619.5266	44.4	1.5E+06	1.3E+06	1.4E+06	1.4E+06	2.6E+05	2.5E+05	4.3E+05	3.2E+05
214	621.5416	44.9	3.7E+05	3.4E+05	4.2E+05	3.8E+05	8.0E+04	7.4E+04	1.1E+05	8.8E+04
215	627.4336	35.0	6.8E+04	6.5E+04	5.6E+04	6.3E+04	1.9E+04	2.3E+04	2.2E+04	2.2E+04
216	627.5333	43.0	1.7E+05	1.4E+05	1.3E+05	1.5E+05	2.2E+04	2.7E+04	2.5E+04	2.5E+04
217	629.5477	43.5	4.6E+05	3.7E+05	3.3E+05	3.9E+05	6.0E+04	6.8E+04	5.9E+04	6.2E+04
218	630.5951	50.2	9.5E+04	1.1E+05	1.1E+05	1.1E+05	3.1E+03	9.5E+03	4.4E+03	5.7E+03
219	630.5941	46.5	1.7E+05	1.8E+05	1.7E+05	1.7E+05	5.9E+02	1.6E+03	1.1E+02	7.6E+02
220	631.5539	44.2	2.7E+05	2.5E+05	2.2E+05	2.4E+05	3.7E+04	4.0E+04	4.3E+04	4.0E+04
221	633.5441	44.6	4.2E+04	3.7E+04	3.4E+04	3.8E+04	1.6E+04	1.5E+04	2.2E+04	1.7E+04
222	634.5394	43.8	1.4E+06	1.2E+06	1.2E+06	1.3E+06	1.7E+05	1.8E+05	3.6E+05	2.4E+05
223	636.5550	44.4	1.8E+06	1.5E+06	1.6E+06	1.6E+06	2.2E+05	2.0E+05	3.8E+05	2.6E+05
224	638.5700	44.9	1.1E+06	9.1E+05	9.9E+05	1.0E+06	1.8E+05	1.5E+05	2.8E+05	2.0E+05
225	639.4951	43.8	1.2E+06	1.2E+06	1.2E+06	1.2E+06	1.3E+05	1.6E+05	3.9E+05	2.3E+05
226	640.5815	45.3	2.3E+05	2.0E+05	2.2E+05	2.2E+05	5.6E+04	5.0E+04	6.9E+04	5.9E+04
227	641.5108	44.3	1.8E+06	1.7E+06	1.8E+06	1.8E+06	2.3E+05	2.7E+05	5.6E+05	3.5E+05
228	643.5256	44.9	1.0E+06	9.5E+05	1.0E+06	1.0E+06	2.3E+05	2.0E+05	4.1E+05	2.8E+05
229	645.5386	45.4	2.1E+05	1.9E+05	2.3E+05	2.1E+05	7.3E+04	6.1E+04	1.3E+05	8.7E+04
230	645.4906	47.3	3.6E+04	4.2E+04	4.5E+04	4.1E+04	1.6E+04	1.3E+04	3.1E+04	2.0E+04
231	647.4636	47.3	1.2E+06	1.4E+06	1.6E+06	1.4E+06	2.4E+04	3.4E+04	1.8E+04	2.5E+04
232	648.6029	46.5	1.0E+05	1.2E+05	1.1E+05	1.1E+05	1.8E+04	1.7E+04	1.5E+04	1.6E+04
233	652.5492	45.0	2.8E+04	3.0E+04	3.0E+04	2.9E+04	2.2E+02	4.5E+02	2.4E+02	3.0E+02
234	655.4700	43.7	4.0E+04	3.9E+04	3.7E+04	3.9E+04	6.6E+03	7.2E+03	1.5E+04	9.5E+03
235	657.4889	44.3	5.8E+04	6.7E+04	6.6E+04	6.4E+04	1.3E+04	1.5E+04	2.3E+04	1.7E+04
236	659.5072	47.3	2.2E+04	2.5E+04	2.5E+04	2.4E+04	8.2E+03	5.5E+03	1.8E+04	1.1E+04
237	659.5346	44.9	6.9E+04	6.8E+04	6.7E+04	6.8E+04	1.0E+04	1.6E+04	2.6E+04	1.8E+04
238	661.5837	47.6	1.3E+04	1.4E+04	1.4E+04	1.4E+04	3.7E+03	3.0E+03	1.6E+03	2.8E+03
239	661.5884	45.4	4.1E+04	4.1E+04	3.8E+04	4.0E+04	1.3E+04	1.6E+04	1.6E+04	1.5E+04
240	662.5667	44.6	4.0E+04	3.8E+04	3.4E+04	3.7E+04	4.9E+03	5.0E+03	6.1E+03	5.3E+03
241	663.5715	47.5	2.9E+04	2.8E+04	3.3E+04	3.0E+04	9.2E+03	8.0E+03	8.7E+03	8.6E+03
242	664.6204	45.1	4.4E+04	3.9E+04	3.8E+04	4.1E+04	1.6E+04	1.1E+04	1.4E+03	9.5E+03
243	667.5271	44.6	3.7E+04	4.0E+04	3.7E+04	3.8E+04	5.6E+03	5.9E+03	1.1E+04	7.6E+03
244	669.5434	46.4	1.6E+04	1.6E+04	2.0E+04	1.8E+04	2.9E+03	2.7E+03	2.3E+03	2.6E+03
245	671.5034	47.3	2.1E+04	2.4E+04	2.5E+04	2.3E+04	8.5E+03	6.0E+03	1.7E+04	1.1E+04
246	673.5917	45.4	3.8E+04	4.0E+04	3.5E+04	3.8E+04	2.3E+03	5.2E+03	4.5E+03	4.0E+03
247	676.5484	44.7	8.9E+04	9.8E+04	9.5E+04	9.4E+04	5.8E+03	5.3E+03	7.0E+03	6.0E+03
248	678.5655	45.2	9.2E+04	9.8E+04	1.1E+05	1.0E+05	0.0E+00	2.6E+03	3.6E+03	2.1E+03

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII) EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
249	678.6161	47.6	8.7E+04	9.8E+04	8.7E+04	9.0E+04	9.4E+03	9.4E+03	9.2E+03	9.3E+03
250	679.4350	46.8	3.2E+04	3.7E+04	3.3E+04	3.4E+04	1.4E+04	1.2E+04	1.0E+04	1.2E+04
251	685.4368	45.8	6.6E+04	9.4E+04	9.0E+04	8.3E+04	4.6E+04	4.7E+04	3.8E+04	4.4E+04
252	687.4948	41.7	1.1E+04	8.0E+03	7.5E+03	8.6E+03	4.2E+03	4.8E+03	3.5E+03	4.2E+03
253	687.6256	45.7	1.7E+05	1.6E+05	1.4E+05	1.6E+05	6.4E+04	8.0E+04	1.0E+05	8.1E+04
254	687.5702	47.4	5.6E+04	5.5E+04	6.6E+04	5.9E+04	1.1E+04	7.7E+03	1.7E+04	1.2E+04
255	689.6393	46.0	1.7E+05	1.6E+05	1.5E+05	1.6E+05	3.9E+04	5.7E+04	6.7E+04	5.4E+04
256	689.5876	47.7	4.2E+04	4.5E+04	5.1E+04	4.6E+04	9.2E+03	6.8E+03	1.5E+04	1.0E+04
257	696.5843	45.3	1.1E+04	1.0E+04	1.0E+04	1.1E+04	3.3E+03	3.1E+03	3.6E+03	3.4E+03
258	696.6845	46.1	6.7E+05	6.1E+05	7.4E+05	6.7E+05	1.5E+05	1.1E+05	1.4E+05	1.3E+05
259	701.6339	46.0	2.9E+04	2.9E+04	2.3E+04	2.7E+04	0.0E+00	0.0E+00	2.1E+03	7.1E+02
260	703.6533	46.3	2.7E+04	2.6E+04	2.5E+04	2.6E+04	5.9E+03	7.7E+03	9.9E+03	7.8E+03
261	710.6588	45.1	9.2E+03	1.0E+04	9.0E+03	9.6E+03	8.1E+03	6.1E+03	2.5E+03	5.6E+03
262	710.6975	46.4	1.1E+05	1.0E+05	1.2E+05	1.1E+05	2.1E+04	1.4E+04	1.2E+04	1.5E+04
263	713.5111	42.2	1.7E+04	1.5E+04	1.3E+04	1.5E+04	7.1E+03	8.5E+03	7.1E+03	7.6E+03
264	717.6623	46.5	2.1E+04	1.9E+04	1.7E+04	1.9E+04	0.0E+00	0.0E+00	2.1E+03	6.9E+02
265	718.6616	46.1	7.7E+04	7.2E+04	8.9E+04	7.9E+04	1.8E+04	0.0E+00	1.1E+04	9.8E+03
266	721.6047	47.6	2.5E+04	2.7E+04	2.9E+04	2.7E+04	5.3E+03	2.4E+03	9.6E+03	5.8E+03
267	725.5111	41.9	9.1E+05	6.8E+05	6.4E+05	7.4E+05	2.0E+05	2.5E+05	2.1E+05	2.2E+05
268	729.5412	43.3	1.0E+06	8.2E+05	8.1E+05	8.8E+05	2.0E+05	2.4E+05	2.5E+05	2.3E+05
269	731.5549	44.0	9.8E+04	7.4E+04	7.2E+04	8.1E+04	1.8E+04	2.8E+04	2.9E+04	2.5E+04
270	732.6927	46.4	1.7E+04	2.5E+04	1.9E+04	2.0E+04	1.7E+04	9.9E+03	5.1E+03	1.1E+04
271	736.6246	47.4	8.6E+04	9.5E+04	1.1E+05	9.6E+04	9.1E+03	5.8E+03	3.0E+04	1.5E+04
272	744.5527	41.8	4.0E+05	4.2E+05	4.3E+05	4.2E+05	8.0E+04	8.1E+04	7.8E+04	8.0E+04
273	748.5812	44.0	1.8E+05	1.3E+05	1.3E+05	1.5E+05	4.7E+04	4.9E+04	5.5E+04	5.0E+04
274	749.5139	42.7	5.1E+04	5.1E+04	6.0E+04	5.4E+04	2.1E+04	2.6E+04	3.0E+04	2.6E+04
275	753.5381	43.0	4.6E+04	4.8E+04	4.1E+04	4.5E+04	1.0E+04	1.2E+04	1.5E+04	1.2E+04
276	755.5577	43.6	8.2E+04	6.8E+04	5.8E+04	6.9E+04	9.0E+03	1.2E+04	1.2E+04	1.1E+04
277	756.5522	42.3	6.1E+04	7.0E+04	6.6E+04	6.5E+04	2.0E+04	1.8E+04	1.8E+04	1.9E+04
278	763.5884	47.3	2.4E+04	2.6E+04	2.7E+04	2.6E+04	1.1E+04	7.3E+03	1.9E+04	1.2E+04
279	768.5534	41.5	6.8E+05	7.1E+05	6.9E+05	6.9E+05	5.5E+04	5.3E+04	3.4E+04	4.7E+04
280	770.5688	42.3	5.0E+05	4.9E+05	4.8E+05	4.9E+05	6.7E+04	5.8E+04	6.0E+04	6.2E+04
281	772.5838	43.0	3.3E+05	3.5E+05	3.3E+05	3.4E+05	9.7E+04	7.9E+04	8.3E+04	8.7E+04
282	772.5834	43.8	2.1E+05	2.0E+05	1.6E+05	1.9E+05	4.3E+04	3.9E+04	4.1E+04	4.1E+04
283	777.6176	47.3	4.8E+04	5.7E+04	5.9E+04	5.5E+04	2.0E+04	1.3E+04	4.3E+04	2.5E+04
284	780.2305	9.3	9.2E+03	8.1E+03	7.6E+03	8.3E+03	3.5E+03	4.7E+03	4.1E+03	4.1E+03
285	798.5985	43.2	5.8E+04	6.1E+04	5.7E+04	5.9E+04	2.8E+04	2.2E+04	2.1E+04	2.3E+04
286	806.5016	40.7	2.9E+04	2.9E+04	2.7E+04	2.8E+04	1.3E+04	1.2E+04	1.6E+04	1.4E+04
287	812.6535	47.3	3.8E+05	4.6E+05	4.9E+05	4.4E+05	1.3E+05	8.7E+04	3.2E+05	1.8E+05
288	816.7036	47.6	8.4E+04	9.9E+04	1.0E+05	9.5E+04	3.4E+04	1.8E+04	2.5E+04	2.6E+04
289	818.7699	49.5	1.6E+04	1.6E+04	1.6E+04	1.6E+04	5.0E+02	6.7E+02	3.8E+02	5.2E+02
290	830.5968	41.0	3.0E+04	3.4E+04	1.7E+04	2.7E+04	7.6E+03	2.2E+04	1.6E+04	1.5E+04
291	830.6578	43.3	1.6E+04	1.4E+04	1.5E+04	1.5E+04	0.0E+00	0.0E+00	0.0E+00	0.0E+00
292	832.6678	45.9	3.1E+04	3.2E+04	2.8E+04	3.0E+04	1.5E+04	1.4E+04	1.8E+04	1.6E+04
293	833.5881	47.3	1.6E+04	1.8E+04	1.9E+04	1.7E+04	6.7E+03	6.4E+03	1.3E+04	8.9E+03
294	840.6949	47.4	3.9E+04	4.3E+04	4.8E+04	4.3E+04	1.1E+04	8.8E+03	2.0E+04	1.3E+04
295	841.7007	46.3	1.4E+04	1.6E+04	1.4E+04	1.5E+04	6.8E+03	5.7E+03	6.6E+03	6.3E+03
296	842.7186	47.7	1.3E+05	1.5E+05	1.6E+05	1.4E+05	2.6E+04	2.3E+04	3.9E+04	2.9E+04
297	842.7713	49.4	8.1E+04	8.1E+04	7.4E+04	7.9E+04	9.3E+02	7.3E+03	1.5E+02	2.8E+03
298	844.7360	47.8	8.3E+05	9.0E+05	9.3E+05	8.9E+05	1.7E+05	1.3E+05	2.4E+05	1.8E+05
299	844.7843	49.5	6.1E+04	6.7E+04	6.2E+04	6.3E+04	2.1E+03	5.9E+03	1.0E+03	3.0E+03
300	853.7255	46.4	5.2E+04	6.8E+04	5.9E+04	6.0E+04	1.3E+04	1.2E+04	1.6E+04	1.4E+04
301	854.7055	47.3	2.6E+04	2.9E+04	3.3E+04	2.9E+04	1.1E+04	8.5E+03	2.3E+04	1.4E+04
302	855.7380	46.6	8.3E+04	1.1E+05	1.1E+05	1.0E+05	1.3E+04	1.2E+04	1.8E+04	1.4E+04
303	856.5921	33.5	2.3E+05	2.3E+05	2.1E+05	2.2E+05	5.9E+04	6.0E+04	6.2E+04	6.0E+04
304	856.7357	47.8	1.1E+05	1.2E+05	1.2E+05	1.2E+05	3.5E+04	6.2E+04	7.5E+04	5.7E+04
305	857.7513	46.8	6.5E+04	8.6E+04	8.7E+04	7.9E+04	8.9E+03	7.2E+03	1.5E+04	1.1E+04
306	858.7521	48.0	6.8E+05	7.4E+05	7.3E+05	7.1E+05	1.7E+05	1.6E+05	2.3E+05	1.9E+05
307	860.7302	46.6	2.0E+04	2.5E+04	2.1E+04	2.2E+04	7.0E+03	6.5E+03	8.1E+03	7.2E+03

No.	*m/z*	RT	Integrated mass ion intensity (MSII)							
		(min)	EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
308	862.7455	46.9	6.0E+04	7.8E+04	8.1E+04	7.3E+04	1.3E+04	1.0E+04	2.3E+04	1.5E+04
309	864.7565	47.2	9.6E+04	1.2E+05	1.3E+05	1.1E+05	2.4E+04	2.1E+04	9.2E+03	1.8E+04
310	865.4917	40.3	8.3E+03	1.0E+04	8.4E+03	9.0E+03	3.8E+03	5.2E+03	4.5E+03	4.5E+03
311	868.7438	47.6	4.2E+05	4.4E+05	4.8E+05	4.5E+05	1.0E+05	1.3E+05	1.4E+05	1.3E+05
312	870.7528	47.9	1.6E+06	1.6E+06	1.7E+06	1.6E+06	4.1E+05	3.8E+05	6.5E+05	4.8E+05
313	873.7264	47.6	4.1E+04	6.3E+04	3.8E+04	4.7E+04	1.8E+04	2.4E+04	2.1E+04	2.1E+04
314	877.7317	46.3	5.2E+04	7.3E+04	5.6E+04	6.1E+04	1.2E+04	9.5E+03	1.5E+04	1.2E+04
315	879.7409	46.5	1.4E+05	1.9E+05	1.6E+05	1.6E+05	1.3E+04	1.7E+04	2.1E+04	1.7E+04
316	882.7522	47.9	3.2E+05	3.2E+05	3.3E+05	3.2E+05	8.8E+04	8.2E+04	1.4E+05	1.0E+05
317	883.5179	32.9	4.0E+04	5.1E+04	2.6E+04	3.9E+04	9.1E+03	1.6E+04	9.1E+03	1.1E+04
318	883.7685	47.0	1.5E+05	2.0E+05	2.0E+05	1.8E+05	1.8E+04	2.1E+04	2.9E+04	2.3E+04
319	884.7700	47.0	8.5E+04	1.1E+05	1.1E+05	1.0E+05	7.2E+03	6.0E+03	1.4E+04	9.0E+03
320	885.7775	47.1	6.3E+04	8.9E+04	9.0E+04	8.1E+04	0.0E+00	0.0E+00	8.9E+03	3.0E+03
321	886.6647	34.0	4.9E+04	7.3E+04	7.4E+04	6.6E+04	1.8E+04	1.5E+04	3.0E+04	2.1E+04
322	888.7606	47.1	3.2E+05	4.2E+05	4.3E+05	3.9E+05	2.7E+04	2.7E+04	6.0E+04	3.8E+04
323	890.7736	47.3	3.1E+05	4.2E+05	4.1E+05	3.8E+05	3.0E+04	2.7E+04	6.2E+04	4.0E+04
324	892.7468	47.6	4.3E+05	4.0E+05	5.3E+05	4.5E+05	1.2E+05	1.5E+05	2.6E+05	1.8E+05
325	894.7602	47.8	3.0E+06	2.9E+06	3.3E+06	3.1E+06	7.9E+05	8.5E+05	1.6E+06	1.1E+06
326	895.7413	46.8	1.2E+05	2.1E+05	1.3E+05	1.5E+05	4.6E+03	3.0E+03	0.0E+00	2.5E+03
327	896.5901	40.9	7.3E+03	6.4E+03	6.3E+03	6.7E+03	2.9E+03	3.4E+03	4.2E+03	3.5E+03
328	903.4975	40.6	1.5E+04	1.6E+04	1.6E+04	1.6E+04	3.0E+03	4.3E+03	3.7E+03	3.7E+03
329	904.8319	49.0	1.1E+07	1.2E+07	1.2E+07	1.2E+07	2.2E+06	2.7E+06	3.7E+06	2.9E+06
330	906.8451	49.1	4.4E+06	4.9E+06	5.1E+06	4.8E+06	9.6E+05	1.2E+06	1.7E+06	1.3E+06
331	907.7274	33.5	1.4E+06	1.5E+06	1.5E+06	1.4E+06	3.8E+04	3.2E+04	3.3E+04	3.4E+04
332	910.8335	50.0	2.1E+05	2.3E+05	2.0E+05	2.1E+05	9.5E+03	2.2E+04	1.1E+04	1.4E+04
333	911.7346	45.9	2.0E+04	2.7E+04	2.3E+04	2.3E+04	7.4E+03	4.7E+03	5.9E+03	6.0E+03
334	912.7626	46.9	2.0E+05	2.7E+05	2.4E+05	2.4E+05	2.5E+04	3.0E+04	3.3E+04	2.9E+04
335	912.8479	50.3	1.8E+05	2.1E+05	2.0E+05	2.0E+05	4.8E+03	1.6E+04	5.8E+03	8.8E+03
336	914.7771	47.2	3.2E+05	4.5E+05	4.2E+05	4.0E+05	3.6E+04	4.1E+04	4.6E+04	4.1E+04
337	914.8605	50.5	1.4E+05	1.7E+05	1.7E+05	1.6E+05	0.0E+00	1.2E+04	6.9E+03	6.3E+03
338	916.7907	46.7	2.3E+05	3.0E+05	3.0E+05	2.8E+05	1.8E+04	2.0E+04	3.0E+04	2.3E+04
339	916.7929	47.5	2.8E+05	4.3E+05	3.8E+05	3.6E+05	1.8E+04	2.3E+04	3.2E+04	2.4E+04
340	918.8068	47.7	1.4E+05	2.0E+05	1.8E+05	1.8E+05	1.5E+04	1.5E+04	2.2E+04	1.7E+04
341	918.8057	46.9	2.6E+05	3.3E+05	3.5E+05	3.1E+05	2.0E+04	1.8E+04	3.7E+04	2.5E+04
342	920.8140	47.1	1.6E+05	2.2E+05	2.3E+05	2.1E+05	2.2E+04	2.4E+04	3.4E+04	2.7E+04
343	921.7798	46.6	1.7E+05	2.1E+05	2.2E+05	2.0E+05	2.4E+04	2.5E+04	3.4E+04	2.8E+04
344	924.6702	33.4	1.8E+04	2.0E+04	1.9E+04	1.9E+04	7.7E+03	1.3E+04	5.7E+03	8.7E+03
345	924.7992	48.4	2.2E+05	2.4E+05	2.2E+05	2.2E+05	8.8E+04	1.1E+05	1.4E+05	1.1E+05
346	925.7758	47.1	6.5E+04	8.0E+04	8.5E+04	7.7E+04	1.1E+04	1.1E+04	1.9E+04	1.4E+04
347	926.8112	48.6	3.7E+05	3.6E+05	3.4E+05	3.6E+05	9.5E+04	1.3E+05	1.6E+05	1.3E+05
348	928.7549	46.3	9.5E+04	1.6E+05	9.6E+04	1.2E+05	0.0E+00	0.0E+00	0.0E+00	0.0E+00
349	929.7093	33.5	2.6E+06	2.6E+06	2.6E+06	2.6E+06	1.4E+05	1.5E+05	1.9E+05	1.6E+05
350	930.8448	49.1	9.0E+05	9.8E+05	9.5E+05	9.4E+05	1.9E+05	2.2E+05	3.0E+05	2.4E+05
351	930.8694	51.1	3.1E+04	3.6E+04	4.8E+04	3.8E+04	1.8E+02	4.5E+03	1.4E+03	2.0E+03
352	932.7856	46.9	7.5E+04	1.3E+05	9.4E+04	1.0E+05	7.9E+03	1.2E+04	1.2E+04	1.0E+04
353	932.8611	49.3	1.2E+06	1.4E+06	1.4E+06	1.3E+06	3.0E+05	3.2E+05	4.6E+05	3.6E+05
354	933.6921	37.5	1.1E+05	1.4E+05	1.7E+05	1.4E+05	2.3E+04	1.8E+04	2.0E+04	2.0E+04
355	934.8749	49.5	8.5E+05	1.1E+06	1.1E+06	1.0E+06	2.4E+05	2.5E+05	3.2E+05	2.7E+05
356	938.8041	48.0	8.7E+04	8.3E+04	8.5E+04	8.5E+04	3.9E+04	4.1E+04	5.3E+04	4.4E+04
357	946.7617	45.9	3.7E+04	5.3E+04	3.0E+04	4.0E+04	0.0E+00	2.0E+04	2.4E+03	7.4E+03
358	947.7817	48.0	3.4E+04	3.4E+04	2.9E+04	3.2E+04	1.1E+04	1.1E+04	1.3E+04	1.2E+04
359	949.7226	38.3	1.5E+05	1.8E+05	1.9E+05	1.7E+05	5.1E+04	4.9E+04	3.9E+04	4.6E+04
360	953.8235	48.8	3.2E+04	3.1E+04	2.5E+04	2.9E+04	1.2E+04	1.2E+04	1.2E+04	1.2E+04
361	954.8396	49.0	7.4E+04	7.1E+04	6.9E+04	7.1E+04	3.0E+04	2.9E+04	4.4E+04	3.5E+04
362	956.8622	49.2	6.7E+05	7.1E+05	6.8E+05	6.9E+05	2.1E+05	2.2E+05	3.4E+05	2.6E+05
363	958.8768	49.4	1.4E+06	1.6E+06	1.6E+06	1.5E+06	3.1E+05	3.4E+05	5.5E+05	4.0E+05
364	963.7386	38.8	2.6E+05	3.0E+05	3.2E+05	2.9E+05	3.4E+04	3.8E+04	2.2E+04	3.1E+04
365	968.8537	48.3	2.0E+04	1.9E+04	1.3E+04	1.7E+04	0.0E+00	0.0E+00	0.0E+00	0.0E+00
366	970.8761	49.4	4.0E+05	4.5E+05	4.3E+05	4.3E+05	9.6E+04	1.1E+05	1.3E+05	1.1E+05

No.	m/z	RT (min)	Integrated mass ion intensity (MSII) EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
367	972.8919	49.6	8.2E+05	9.4E+05	9.0E+05	8.9E+05	1.9E+05	2.0E+05	2.4E+05	2.1E+05
368	974.9076	49.8	9.8E+05	1.1E+06	1.2E+06	1.1E+06	2.4E+05	2.7E+05	3.0E+05	2.7E+05
369	976.9215	50.0	6.5E+05	8.3E+05	8.3E+05	7.7E+05	1.8E+05	2.0E+05	2.0E+05	1.9E+05
370	982.8686	48.3	2.8E+04	2.9E+04	2.7E+04	2.8E+04	0.0E+00	4.7E+02	6.7E+03	2.4E+03
371	984.7103	44.2	5.7E+04	6.6E+04	5.5E+04	5.9E+04	2.9E+04	2.9E+04	2.3E+04	2.7E+04
372	996.8861	49.4	2.3E+04	1.9E+04	2.1E+04	2.1E+04	1.1E+04	1.1E+04	1.4E+04	1.2E+04
373	998.9078	49.7	5.3E+05	5.8E+05	5.7E+05	5.6E+05	1.3E+05	1.7E+05	1.8E+05	1.6E+05
374	998.9545	52.1	4.3E+04	3.9E+04	4.9E+04	4.4E+04	4.1E+02	6.2E+03	7.7E+03	4.8E+03
375	1000.9229	49.9	9.0E+05	1.0E+06	1.0E+06	9.7E+05	1.5E+05	2.0E+05	2.0E+05	1.8E+05
376	1002.9375	50.2	8.7E+05	1.0E+06	1.1E+06	9.9E+05	1.4E+05	1.8E+05	1.7E+05	1.6E+05
377	1004.9508	50.4	4.2E+05	5.1E+05	5.4E+05	4.9E+05	7.5E+04	9.4E+04	9.6E+04	8.8E+04
378	1018.9654	50.5	3.5E+05	4.6E+05	5.1E+05	4.4E+05	1.3E+05	1.4E+05	2.4E+05	1.7E+05
379	1022.8612	47.5	1.9E+04	2.1E+04	1.0E+04	1.7E+04	0.0E+00	0.0E+00	0.0E+00	0.0E+00
380	1030.9590	49.8	8.7E+04	1.4E+05	1.3E+05	1.2E+05	2.8E+04	3.2E+04	4.0E+04	3.3E+04
381	1033.7943	45.0	2.3E+04	2.4E+04	2.4E+04	2.4E+04	1.0E+04	1.0E+04	1.3E+04	1.1E+04
382	1034.9607	50.2	2.7E+04	3.2E+04	3.0E+04	3.0E+04	2.7E+03	2.6E+03	1.1E+04	5.4E+03
383	1037.9163	49.7	1.4E+04	1.5E+04	1.4E+04	1.4E+04	5.2E+03	5.0E+03	7.0E+03	5.8E+03
384	1039.9283	49.9	1.4E+04	1.6E+04	1.6E+04	1.5E+04	5.8E+03	5.4E+03	7.2E+03	6.2E+03
385	1040.9507	50.2	2.6E+04	3.0E+04	3.0E+04	2.8E+04	1.2E+04	1.1E+04	1.6E+04	1.3E+04
386	1048.8810	47.6	2.2E+04	2.7E+04	2.2E+04	2.4E+04	8.3E+03	1.0E+04	8.5E+03	9.1E+03
387	1050.8917	47.7	1.2E+04	1.4E+04	8.8E+03	1.1E+04	5.1E+03	3.3E+03	4.8E+03	4.4E+03
388	1058.9915	50.0	2.3E+04	2.4E+04	2.3E+04	2.3E+04	6.6E+03	6.6E+03	8.7E+03	7.3E+03
389	1061.0158	51.2	3.8E+04	4.9E+04	5.8E+04	4.9E+04	1.7E+04	2.0E+04	2.6E+04	2.1E+04
390	1068.9836	49.5	1.3E+04	1.6E+04	1.6E+04	1.5E+04	6.5E+03	5.4E+03	9.5E+03	7.2E+03
391	1070.9948	49.7	2.1E+04	2.6E+04	2.6E+04	2.4E+04	7.0E+03	7.2E+03	9.9E+03	8.0E+03
392	1089.0457	51.6	4.2E+04	5.5E+04	6.1E+04	5.3E+04	2.0E+04	2.5E+04	3.1E+04	2.5E+04
393	1093.5439	24.6	7.6E+03	1.1E+04	1.1E+04	1.0E+04	4.8E+03	2.9E+03	2.6E+03	3.4E+03
394	1106.8801	38.8	1.5E+04	1.8E+04	1.8E+04	1.7E+04	1.7E+02	6.8E+01	8.7E+01	1.1E+02
395	1153.0069	49.4	9.4E+03	1.1E+04	1.1E+04	1.0E+04	2.1E+03	1.7E+03	2.1E+03	2.0E+03
396	1155.0211	49.6	1.3E+04	1.6E+04	1.6E+04	1.5E+04	3.8E+03	2.9E+03	3.7E+03	3.5E+03
397	1157.0344	49.9	1.4E+04	1.8E+04	1.8E+04	1.7E+04	3.8E+03	4.2E+03	3.3E+03	3.8E+03
398	1158.2668	38.7	5.9E+04	4.7E+04	5.5E+04	5.4E+04	8.4E+03	1.1E+04	1.4E+04	1.1E+04
399	1181.0317	49.7	1.3E+04	1.5E+04	1.6E+04	1.5E+04	4.6E+03	5.3E+03	3.9E+03	4.6E+03
400	1183.0476	49.9	1.5E+04	1.7E+04	1.7E+04	1.6E+04	5.4E+03	5.5E+03	5.2E+03	5.4E+03
401	1185.0651	50.2	1.3E+04	1.5E+04	1.5E+04	1.4E+04	5.7E+03	5.0E+03	5.6E+03	5.4E+03
402	1205.0317	43.5	1.0E+04	8.6E+03	1.1E+04	9.9E+03	1.1E+03	2.3E+03	4.2E+03	2.5E+03
403	1208.0048	44.0	7.7E+04	6.6E+04	6.5E+04	6.9E+04	2.1E+04	2.5E+04	5.4E+04	3.3E+04
404	1212.0287	44.7	1.9E+05	1.4E+05	1.6E+05	1.6E+05	4.3E+04	4.8E+04	9.6E+04	6.2E+04
405	1224.0229	44.6	1.3E+04	1.2E+04	1.1E+04	1.2E+04	5.2E+03	4.7E+03	8.5E+03	6.1E+03
406	1228.6712	39.6	9.8E+03	7.0E+03	8.4E+03	8.4E+03	8.2E+02	1.7E+03	2.1E+03	1.6E+03
407	1231.9962	43.8	5.2E+04	5.4E+04	5.3E+04	5.3E+04	5.0E+03	5.8E+03	1.9E+04	1.0E+04
408	1234.0106	44.1	8.9E+04	9.4E+04	9.4E+04	9.2E+04	1.4E+04	1.5E+04	3.6E+04	2.2E+04
409	1236.0261	44.3	1.3E+05	1.3E+05	1.4E+05	1.3E+05	1.9E+04	2.1E+04	4.9E+04	3.0E+04
410	1238.0424	44.8	1.8E+05	1.6E+05	1.8E+05	1.7E+05	2.7E+04	2.5E+04	6.1E+04	3.7E+04
411	1242.0644	45.3	4.1E+04	2.9E+04	4.9E+04	4.0E+04	1.6E+04	1.5E+04	2.6E+04	1.9E+04
412	1252.0519	45.0	1.2E+04	8.9E+03	1.1E+04	1.0E+04	3.4E+03	2.8E+03	5.1E+03	3.8E+03
413	1255.9951	43.7	3.9E+04	3.5E+04	3.2E+04	3.5E+04	2.9E+03	3.5E+03	7.7E+03	4.7E+03
414	1260.0226	44.3	8.0E+04	7.4E+04	7.6E+04	7.7E+04	5.8E+03	8.8E+03	1.7E+04	1.0E+04
415	1264.0575	45.0	1.3E+05	1.0E+05	1.1E+05	1.1E+05	1.2E+04	4.1E+03	2.4E+04	1.4E+04
416	1266.3738	40.0	5.0E+03	6.4E+03	6.6E+03	6.0E+03	1.1E+02	3.7E+02	1.9E+02	2.2E+02
417	1268.0776	45.4	2.7E+04	2.1E+04	2.6E+04	2.5E+04	2.4E+03	1.2E+03	1.3E+04	5.6E+03
418	1270.0929	45.6	1.8E+04	1.6E+04	1.7E+04	1.7E+04	3.1E+03	4.3E+03	1.2E+04	6.5E+03
419	1290.0624	45.1	7.1E+03	6.1E+03	6.4E+03	6.5E+03	2.7E+03	1.8E+03	2.5E+03	2.3E+03
420	1308.8166	43.6	1.0E+04	1.1E+04	1.0E+04	1.0E+04	4.4E+03	3.6E+03	2.0E+03	3.3E+03
421	1310.0108	45.8	1.8E+04	2.1E+04	2.0E+04	1.9E+04	6.7E+03	1.4E+04	7.5E+03	9.2E+03
422	1313.1763	45.5	1.2E+04	7.6E+03	1.1E+04	1.0E+04	4.8E+03	3.2E+03	6.5E+03	4.8E+03
423	1325.9027	45.8	1.5E+04	1.9E+04	1.8E+04	1.7E+04	5.8E+03	7.3E+03	5.9E+03	6.3E+03
424	1327.1596	45.2	1.6E+04	1.5E+04	1.6E+04	1.6E+04	7.9E+03	4.5E+03	8.2E+03	6.9E+03
425	1329.1735	45.3	1.5E+04	1.4E+04	1.5E+04	1.5E+04	9.1E+03	6.0E+03	1.1E+04	8.6E+03

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
426	1333.2595	54.6	4.2E+04	5.9E+04	6.4E+04	5.5E+04	1.9E+03	2.9E+03	2.0E+03	2.2E+03
427	1335.2722	55.3	5.2E+04	6.5E+04	7.9E+04	6.5E+04	2.5E+03	4.5E+03	4.5E+03	3.8E+03
428	1340.7524	39.0	7.5E+03	8.0E+03	7.5E+03	7.7E+03	1.5E+03	1.4E+03	1.8E+03	1.6E+03
429	1341.4247	39.0	2.1E+04	1.9E+04	1.9E+04	2.0E+04	1.5E+03	1.3E+03	2.6E+03	1.8E+03
430	1342.0085	43.5	8.0E+03	7.9E+03	8.6E+03	8.2E+03	2.4E+03	3.2E+03	4.7E+03	3.4E+03
431	1342.0888	39.0	1.2E+04	1.2E+04	1.3E+04	1.2E+04	2.1E+02	3.3E+02	1.5E+03	6.9E+02
432	1342.9225	45.8	2.4E+05	2.8E+05	2.9E+05	2.7E+05	6.1E+04	6.7E+04	4.9E+04	5.9E+04
433	1344.0244	43.6	1.1E+04	1.3E+04	1.4E+04	1.3E+04	3.0E+03	3.9E+03	7.6E+03	4.8E+03
434	1368.0255	43.5	3.7E+04	3.5E+04	3.6E+04	3.6E+04	4.2E+03	4.7E+03	9.8E+03	6.2E+03
435	1369.9486	41.8	1.4E+04	1.0E+04	1.2E+04	1.2E+04	5.8E+03	7.8E+03	3.8E+03	5.8E+03
436	1371.9645	42.2	2.0E+04	1.4E+04	1.5E+04	1.6E+04	7.5E+03	1.1E+04	8.3E+03	8.9E+03
437	1375.1170	45.8	9.3E+03	9.2E+03	9.9E+03	9.5E+03	3.4E+03	2.3E+03	3.2E+03	3.0E+03
438	1378.0096	42.9	2.4E+04	2.1E+04	2.2E+04	2.2E+04	1.1E+04	1.4E+04	1.3E+04	1.3E+04
439	1383.0704	33.5	1.4E+05	1.4E+05	1.5E+05	1.4E+05	6.0E+03	5.7E+03	7.7E+03	6.5E+03
440	1389.7816	39.7	1.0E+04	1.1E+04	1.2E+04	1.1E+04	1.1E+03	1.1E+03	1.5E+03	1.2E+03
441	1390.4462	39.7	2.8E+04	3.1E+04	3.1E+04	3.0E+04	2.0E+03	1.7E+03	2.7E+03	2.1E+03
442	1391.1129	39.7	1.9E+04	2.0E+04	2.0E+04	2.0E+04	4.0E+02	1.3E+03	1.5E+03	1.1E+03
443	1391.7875	39.7	6.6E+03	6.0E+03	6.6E+03	6.4E+03	1.2E+03	8.1E+02	1.4E+03	1.2E+03
444	1393.9483	41.5	3.6E+04	2.7E+04	2.7E+04	3.0E+04	3.7E+03	1.4E+04	6.0E+03	7.9E+03
445	1397.1113	45.8	6.2E+03	7.7E+03	7.7E+03	7.2E+03	3.5E+03	2.5E+03	2.7E+03	2.9E+03
446	1397.9810	41.9	1.1E+05	7.9E+04	7.8E+04	8.9E+04	2.3E+04	3.1E+04	2.3E+04	2.6E+04
447	1402.0094	42.4	2.0E+05	1.4E+05	1.5E+05	1.7E+05	4.6E+04	7.1E+04	5.4E+04	5.7E+04
448	1404.0240	43.1	1.1E+05	9.5E+04	1.0E+05	1.0E+05	2.5E+04	3.8E+04	3.6E+04	3.3E+04
449	1406.0409	43.0	2.0E+05	1.4E+05	1.5E+05	1.6E+05	3.8E+04	6.1E+04	5.6E+04	5.2E+04
450	1426.0107	42.3	1.6E+05	1.0E+05	9.9E+04	1.2E+05	1.8E+04	3.0E+04	2.2E+04	2.4E+04
451	1428.0265	42.5	2.5E+05	1.5E+05	1.5E+05	1.8E+05	2.7E+04	4.5E+04	2.9E+04	3.3E+04
452	1428.0231	43.1	7.7E+04	6.3E+04	6.0E+04	6.7E+04	1.6E+04	2.7E+04	3.0E+04	2.5E+04
453	1430.0408	43.0	4.0E+05	2.8E+05	2.9E+05	3.3E+05	4.8E+04	7.5E+04	6.8E+04	6.4E+04
454	1432.0543	43.2	3.9E+05	2.7E+05	2.9E+05	3.2E+05	4.6E+04	6.5E+04	6.1E+04	5.7E+04
455	1441.0230	41.9	7.5E+05	6.3E+05	5.8E+05	6.6E+05	2.7E+05	3.2E+05	2.4E+05	2.8E+05
456	1445.0153	50.5	2.4E+05	2.0E+05	1.9E+05	2.1E+05	5.5E+04	7.9E+04	1.3E+05	8.7E+04
457	1445.0552	42.6	8.2E+05	6.8E+05	6.3E+05	7.1E+05	2.7E+05	3.1E+05	2.8E+05	2.9E+05
458	1449.9774	50.2	2.4E+05	1.9E+05	1.8E+05	2.1E+05	7.4E+04	9.7E+04	1.6E+05	1.1E+05
459	1451.9893	50.3	5.1E+05	4.0E+05	3.9E+05	4.4E+05	1.1E+05	1.6E+05	2.4E+05	1.7E+05
460	1454.0007	50.6	4.8E+05	4.0E+05	3.7E+05	4.2E+05	7.9E+04	1.3E+05	1.9E+05	1.3E+05
461	1456.0536	43.2	2.0E+05	1.5E+05	1.6E+05	1.7E+05	2.2E+04	3.2E+04	2.7E+04	2.7E+04
462	1458.0727	43.3	1.0E+06	6.7E+05	6.6E+05	7.8E+05	6.2E+04	7.8E+04	7.8E+04	7.3E+04
463	1467.0395	41.8	2.6E+05	1.8E+05	1.6E+05	2.0E+05	4.4E+04	4.7E+04	4.9E+04	4.7E+04
464	1467.0005	50.1	4.1E+05	3.2E+05	2.9E+05	3.4E+05	1.2E+05	1.6E+05	2.6E+05	1.8E+05
465	1469.0144	50.4	9.4E+05	7.5E+05	7.0E+05	8.0E+05	2.0E+05	2.9E+05	4.5E+05	3.1E+05
466	1469.0525	42.5	1.9E+05	1.3E+05	1.2E+05	1.5E+05	3.7E+04	3.8E+04	2.5E+04	3.4E+04
467	1469.0524	41.6	1.6E+05	1.2E+05	1.2E+05	1.3E+05	6.1E+04	6.8E+04	4.7E+04	5.8E+04
468	1471.0279	50.6	9.3E+05	7.7E+05	7.5E+05	8.2E+05	1.5E+05	2.5E+05	3.7E+05	2.6E+05
469	1471.0664	42.8	4.4E+05	3.2E+05	3.0E+05	3.5E+05	7.8E+04	8.5E+04	8.7E+04	8.3E+04
470	1473.0813	43.2	2.6E+05	2.2E+05	1.9E+05	2.2E+05	5.5E+04	5.4E+04	5.3E+04	5.4E+04
471	1475.0984	43.3	2.7E+05	2.0E+05	1.9E+05	2.2E+05	5.3E+04	5.6E+04	6.2E+04	5.7E+04
472	1480.0584	43.3	1.9E+05	1.6E+05	1.6E+05	1.7E+05	2.8E+04	3.7E+04	3.8E+04	3.4E+04
473	1499.0961	43.2	5.4E+04	5.5E+04	5.1E+04	5.4E+04	1.3E+04	1.2E+04	1.2E+04	1.2E+04
474	1500.0352	41.4	3.8E+04	4.4E+04	3.8E+04	4.0E+04	1.5E+04	1.4E+04	2.3E+04	1.7E+04

A4.2 Normalized integrated mass ion intensity (nMSII) of positive-mode ions in mycelium with increased levels under 4% ethanol stress.

No.	*m/z*	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	109.1004	47.3	1.6E+05	1.7E+05	1.7E+05	1.6E+05	2.9E+04	2.1E+04	5.3E+04	3.4E+04
2	109.1003	46.4	1.3E+05	1.4E+05	1.3E+05	1.3E+05	1.6E+04	1.3E+04	1.3E+04	1.4E+04
3	111.1099	39.9	1.1E+05	1.2E+05	1.3E+05	1.2E+05	1.9E+04	1.8E+04	1.9E+04	1.8E+04
4	118.0866	5.9	9.4E+03	1.4E+04	1.2E+04	1.2E+04	6.9E+02	6.5E+02	1.0E+03	7.8E+02
5	121.1008	39.9	2.5E+05	2.7E+05	2.6E+05	2.6E+05	4.7E+04	4.5E+04	4.4E+04	4.5E+04
6	123.1155	47.3	1.2E+05	1.3E+05	1.3E+05	1.3E+05	2.7E+04	1.9E+04	4.2E+04	2.9E+04
7	123.1156	46.4	1.2E+05	1.2E+05	1.2E+05	1.2E+05	1.8E+04	1.4E+04	1.5E+04	1.6E+04
8	123.1151	38.8	2.7E+05	3.0E+05	3.0E+05	2.9E+05	7.2E+04	6.4E+04	6.6E+04	6.7E+04
9	125.1314	33.5	2.2E+05	2.3E+05	2.1E+05	2.2E+05	4.5E+04	3.9E+04	3.4E+04	3.9E+04
10	135.1152	47.3	1.3E+05	1.4E+05	1.4E+05	1.4E+05	2.7E+04	1.9E+04	4.3E+04	2.9E+04
11	135.1157	39.9	3.5E+05	3.7E+05	3.6E+05	3.6E+05	5.3E+04	4.5E+04	4.9E+04	4.9E+04
12	137.1312	47.3	8.4E+04	9.0E+04	9.2E+04	8.9E+04	1.9E+04	1.2E+04	2.8E+04	2.0E+04
13	137.1309	46.4	8.6E+04	9.3E+04	8.9E+04	8.9E+04	1.2E+04	9.8E+03	9.7E+03	1.1E+04
14	143.1069	39.9	5.8E+04	6.8E+04	6.5E+04	6.4E+04	9.6E+03	8.7E+03	9.8E+03	9.4E+03
15	144.1013	20.7	1.9E+04	2.4E+04	2.1E+04	2.1E+04	2.9E+03	1.4E+03	1.2E+03	1.8E+03
16	145.1005	33.5	1.2E+05	1.3E+05	1.3E+05	1.3E+05	1.9E+04	1.7E+04	1.7E+04	1.8E+04
17	145.1007	40.4	7.6E+04	1.2E+05	1.0E+05	1.0E+05	1.1E+04	1.1E+04	1.2E+04	1.1E+04
18	153.1291	39.9	8.6E+04	9.3E+04	1.0E+05	9.4E+04	1.3E+04	1.3E+04	1.3E+04	1.3E+04
19	155.1054	41.1	5.4E+04	5.3E+04	5.1E+04	5.3E+04	1.0E+04	1.2E+04	1.2E+04	1.2E+04
20	160.1320	9.9	3.2E+04	3.1E+04	3.5E+04	3.3E+04	2.7E+03	2.3E+03	3.1E+03	2.7E+03
21	163.1464	47.3	1.3E+05	1.5E+05	1.5E+05	1.4E+05	2.5E+04	1.6E+04	4.4E+04	2.8E+04
22	163.1463	46.4	1.3E+05	1.3E+05	1.3E+05	1.3E+05	1.5E+04	9.2E+03	1.0E+04	1.1E+04
23	163.1466	39.9	2.2E+05	2.3E+05	2.3E+05	2.3E+05	3.5E+04	3.0E+04	3.3E+04	3.3E+04
24	170.0572	41.6	1.0E+05	1.1E+05	1.1E+05	1.1E+05	5.1E+03	4.7E+03	5.6E+03	5.1E+03
25	170.0569	42.3	3.9E+04	4.6E+04	4.8E+04	4.4E+04	3.0E+03	2.2E+03	2.8E+03	2.7E+03
26	173.1293	47.3	3.8E+04	4.4E+04	4.5E+04	4.2E+04	1.0E+04	7.7E+03	1.3E+04	1.0E+04
27	175.1442	47.3	7.0E+04	7.5E+04	7.6E+04	7.4E+04	1.5E+04	1.2E+04	2.2E+04	1.6E+04
28	177.1612	47.3	1.4E+05	1.6E+05	1.7E+05	1.6E+05	2.3E+04	1.7E+04	5.0E+04	3.0E+04
29	177.1429	38.1	8.2E+04	9.4E+04	9.9E+04	9.2E+04	2.0E+04	2.2E+04	1.7E+04	1.9E+04
30	177.1612	46.4	1.0E+05	1.1E+05	1.1E+05	1.1E+05	8.9E+03	2.6E+03	7.0E+03	6.1E+03
31	177.1617	39.9	1.6E+05	1.8E+05	1.8E+05	1.7E+05	2.6E+04	2.5E+04	2.5E+04	2.5E+04
32	181.0887	47.3	4.2E+04	4.4E+04	4.6E+04	4.4E+04	5.4E+03	4.6E+03	1.4E+04	7.8E+03
33	181.1613	39.9	6.7E+04	7.8E+04	7.4E+04	7.3E+04	1.0E+04	8.4E+03	1.0E+04	9.6E+03
34	189.1614	47.3	7.8E+04	8.4E+04	8.6E+04	8.3E+04	1.2E+04	1.0E+04	2.4E+04	1.6E+04
35	189.1616	46.4	6.9E+04	7.1E+04	6.9E+04	7.0E+04	7.0E+03	3.4E+03	5.2E+03	5.2E+03
36	191.1776	47.3	1.1E+05	1.4E+05	1.4E+05	1.3E+05	2.3E+04	1.6E+04	4.0E+04	2.6E+04
37	191.1776	39.9	1.3E+05	1.6E+05	1.5E+05	1.4E+05	2.5E+04	2.1E+04	2.3E+04	2.3E+04
38	194.1160	10.1	1.9E+04	2.6E+04	2.7E+04	2.4E+04	1.4E+03	1.9E+03	1.3E+03	1.5E+03
39	197.1547	41.1	1.6E+04	1.2E+04	1.1E+04	1.3E+04	2.2E+03	3.4E+03	3.7E+03	3.1E+03
40	197.0802	46.4	6.4E+05	6.6E+05	6.5E+05	6.5E+05	1.1E+04	8.7E+03	2.1E+04	1.3E+04
41	198.9398	4.8	2.5E+04	1.5E+04	1.5E+04	1.8E+04	1.5E+03	2.8E+03	1.4E+03	1.9E+03
42	199.1592	38.8	7.3E+04	9.0E+04	8.9E+04	8.4E+04	1.3E+04	1.6E+04	1.4E+04	1.4E+04
43	200.9684	4.8	1.2E+04	8.4E+03	6.9E+03	9.0E+03	1.3E+03	1.3E+03	7.4E+02	1.1E+03
44	201.1598	33.5	4.3E+04	4.8E+04	4.6E+04	4.6E+04	6.0E+03	5.4E+03	4.1E+03	5.2E+03
45	201.1224	9.7	1.6E+04	1.6E+04	1.4E+04	1.5E+04	1.0E+03	7.0E+02	6.8E+02	8.1E+02
46	202.1061	28.4	8.9E+03	1.3E+04	7.8E+03	1.0E+04	1.1E+03	9.5E+02	8.7E+02	9.6E+02
47	203.1760	47.3	1.0E+05	1.2E+05	1.4E+05	1.2E+05	1.8E+04	1.1E+04	3.7E+04	2.2E+04
48	203.1763	46.4	8.4E+04	9.3E+04	9.1E+04	8.9E+04	2.1E+03	0.0E+00	0.0E+00	6.9E+02
49	205.1911	38.0	2.0E+05	2.6E+05	2.8E+05	2.5E+05	4.9E+04	4.5E+04	3.7E+04	4.4E+04
50	205.1932	47.3	7.3E+04	8.3E+04	8.6E+04	8.1E+04	1.2E+04	8.8E+03	2.5E+04	1.5E+04
51	205.1928	46.4	5.5E+04	5.4E+04	5.8E+04	5.6E+04	5.8E+03	4.5E+03	5.4E+03	5.2E+03
52	207.1694	38.7	7.2E+04	8.5E+04	8.7E+04	8.1E+04	1.5E+04	1.6E+04	1.3E+04	1.5E+04
53	209.1864	39.9	4.8E+04	5.4E+04	5.4E+04	5.2E+04	6.8E+03	6.2E+03	6.6E+03	6.5E+03
54	211.1537	41.1	1.0E+04	1.0E+04	1.1E+04	1.1E+04	1.4E+03	2.2E+03	2.8E+03	2.1E+03

No.	*m/z*	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
55	213.1783	36.9	1.6E+05	2.0E+05	2.0E+05	1.9E+05	7.9E+03	1.5E+04	1.1E+04	1.1E+04
56	214.9171	4.8	1.3E+04	1.0E+04	9.7E+03	1.1E+04	1.1E+03	1.8E+03	8.6E+02	1.3E+03
57	216.9494	4.8	1.6E+04	7.7E+03	1.0E+04	1.1E+04	7.3E+02	5.6E+02	8.5E+02	7.1E+02
58	217.1924	38.0	3.0E+05	3.8E+05	4.0E+05	3.6E+05	5.7E+04	6.5E+04	5.0E+04	5.7E+04
59	217.1933	46.4	1.0E+05	1.0E+05	1.0E+05	1.0E+05	1.2E+04	8.6E+03	8.0E+03	9.6E+03
60	221.1190	47.3	2.6E+04	3.0E+04	3.2E+04	2.9E+04	5.3E+03	3.9E+03	9.3E+03	6.2E+03
61	221.2200	38.8	8.9E+04	1.1E+05	9.5E+04	9.8E+04	2.6E+04	2.0E+04	2.5E+04	2.4E+04
62	231.2083	47.3	8.4E+04	8.8E+04	8.9E+04	8.7E+04	1.5E+04	9.8E+03	2.7E+04	1.7E+04
63	231.2055	38.0	1.7E+05	2.0E+05	2.3E+05	2.0E+05	4.2E+04	4.0E+04	3.6E+04	3.9E+04
64	231.2078	46.4	5.6E+04	5.6E+04	5.1E+04	5.5E+04	5.7E+03	4.2E+03	5.1E+03	5.0E+03
65	233.1572	38.0	5.6E+04	6.5E+04	6.4E+04	6.2E+04	1.2E+04	1.3E+04	1.1E+04	1.2E+04
66	234.9606	4.8	2.0E+04	1.3E+04	1.5E+04	1.6E+04	1.6E+03	2.3E+03	1.2E+03	1.7E+03
67	243.2090	43.8	4.9E+04	4.1E+04	4.6E+04	4.5E+04	4.4E+03	4.1E+03	7.4E+03	5.3E+03
68	247.2410	39.9	1.4E+06	1.6E+06	1.6E+06	1.5E+06	1.5E+05	1.4E+05	1.6E+05	1.5E+05
69	249.1250	47.3	1.3E+04	1.5E+04	1.4E+04	1.4E+04	6.0E+02	0.0E+00	4.4E+03	1.7E+03
70	251.1279	47.3	9.9E+04	1.2E+05	1.2E+05	1.1E+05	1.4E+04	1.0E+04	3.4E+04	1.9E+04
71	251.1289	46.4	3.0E+04	3.0E+04	3.1E+04	3.0E+04	1.2E+03	1.9E+03	7.9E+01	1.1E+03
72	253.1928	33.5	1.8E+05	1.9E+05	1.8E+05	1.8E+05	2.1E+04	1.9E+04	1.8E+04	1.9E+04
73	253.1941	40.4	9.8E+04	1.7E+05	1.4E+05	1.4E+05	1.2E+04	1.3E+04	1.3E+04	1.3E+04
74	261.1715	37.9	4.9E+05	5.5E+05	5.5E+05	5.3E+05	8.8E+04	8.7E+04	7.7E+04	8.4E+04
75	261.2182	43.8	2.6E+05	2.0E+05	2.2E+05	2.3E+05	1.5E+04	1.4E+04	3.3E+04	2.1E+04
76	263.1278	47.3	1.4E+05	1.6E+05	1.6E+05	1.6E+05	2.2E+04	1.6E+04	5.1E+04	3.0E+04
77	263.2362	44.0	1.4E+06	1.2E+06	1.2E+06	1.3E+06	1.3E+05	1.2E+05	2.1E+05	1.5E+05
78	265.2516	39.9	1.4E+06	1.6E+06	1.6E+06	1.5E+06	1.6E+05	1.4E+05	1.6E+05	1.5E+05
79	271.2388	46.4	4.0E+04	4.5E+04	4.0E+04	4.2E+04	4.8E+03	4.1E+03	4.4E+03	4.4E+03
80	273.1842	38.1	3.9E+05	4.4E+05	4.5E+05	4.3E+05	4.1E+04	3.6E+04	1.2E+04	3.0E+04
81	284.2928	35.8	4.2E+05	4.0E+05	6.3E+05	4.8E+05	6.9E+04	2.0E+05	6.8E+04	1.1E+05
82	285.2749	40.9	1.1E+05	1.5E+05	1.5E+05	1.4E+05	7.7E+03	8.6E+03	1.4E+04	1.0E+04
83	287.2686	47.3	2.3E+04	2.7E+04	2.6E+04	2.5E+04	2.6E+03	1.5E+03	6.6E+03	3.6E+03
84	287.2671	46.4	1.4E+04	1.5E+04	1.5E+04	1.5E+04	2.8E+02	0.0E+00	1.9E+02	1.6E+02
85	289.1809	37.4	5.6E+04	6.3E+04	6.9E+04	6.3E+04	8.8E+03	9.0E+03	6.8E+03	8.2E+03
86	290.2679	13.9	3.2E+04	5.2E+04	4.5E+04	4.3E+04	1.1E+02	1.6E+01	1.1E+01	4.4E+01
87	290.2681	12.9	8.5E+04	1.4E+05	1.2E+05	1.2E+05	6.9E+01	9.2E+01	9.2E+00	5.6E+01
88	299.2568	43.5	2.4E+05	2.1E+05	2.2E+05	2.2E+05	4.5E+04	4.0E+04	5.2E+04	4.6E+04
89	299.2571	44.2	1.8E+05	1.5E+05	1.4E+05	1.6E+05	3.3E+04	3.1E+04	3.4E+04	3.3E+04
90	307.2543	39.6	2.2E+04	2.7E+04	2.7E+04	2.5E+04	0.0E+00	0.0E+00	6.3E+03	2.1E+03
91	309.2549	40.4	7.4E+04	1.2E+05	1.0E+05	1.0E+05	1.4E+03	3.9E+03	1.9E+03	2.4E+03
92	310.1740	9.7	3.7E+04	3.9E+04	3.9E+04	3.8E+04	1.5E+03	8.4E+02	7.9E+02	1.0E+03
93	311.2928	39.9	8.9E+05	1.0E+06	1.1E+06	9.8E+05	9.9E+04	8.6E+04	1.0E+05	9.6E+04
94	313.2391	38.1	1.7E+05	2.2E+05	2.1E+05	2.0E+05	3.5E+04	3.4E+04	2.6E+04	3.1E+04
95	313.2732	44.0	6.2E+06	8.8E+06	8.6E+06	7.8E+06	9.9E+05	8.9E+05	1.6E+06	1.2E+06
96	318.9373	4.8	1.2E+04	8.9E+03	7.7E+03	9.5E+03	1.6E+03	2.0E+03	1.3E+03	1.6E+03
97	319.1930	47.3	3.1E+04	3.9E+04	3.9E+04	3.6E+04	3.9E+03	1.5E+03	1.2E+04	5.9E+03
98	331.2789	44.0	2.8E+05	2.3E+05	2.2E+05	2.4E+05	2.1E+04	2.1E+04	4.7E+04	3.0E+04
99	331.2532	38.6	2.1E+05	2.1E+05	1.9E+05	2.0E+05	2.0E+04	2.0E+04	1.5E+04	1.8E+04
100	333.2750	40.0	4.4E+05	4.8E+05	4.3E+05	4.5E+05	3.6E+04	4.2E+04	5.1E+04	4.3E+04
101	335.2572	43.7	3.2E+05	2.7E+05	2.9E+05	2.9E+05	3.6E+04	3.5E+04	9.1E+04	5.4E+04
102	336.1984	9.6	4.6E+04	4.4E+04	3.4E+04	4.1E+04	1.2E+03	1.1E+03	1.2E+03	1.2E+03
103	337.2740	44.0	1.5E+07	1.1E+07	1.2E+07	1.3E+07	8.6E+05	7.9E+05	1.5E+06	1.1E+06
104	338.2033	10.0	4.2E+04	4.0E+04	3.9E+04	4.1E+04	1.2E+03	1.1E+03	1.1E+03	1.1E+03
105	339.2896	44.6	1.6E+07	1.4E+07	1.4E+07	1.4E+07	8.3E+05	6.8E+05	1.3E+06	9.4E+05
106	340.1834	9.8	4.5E+04	4.2E+04	4.0E+04	4.2E+04	2.3E+03	1.9E+03	1.8E+03	2.0E+03
107	341.1962	35.3	4.3E+04	2.9E+04	3.4E+04	3.5E+04	7.3E+03	7.9E+03	6.9E+03	7.4E+03
108	343.2565	38.0	7.0E+04	7.5E+04	8.7E+04	7.7E+04	7.1E+03	4.0E+03	0.0E+00	3.7E+03
109	344.1586	9.9	2.4E+04	3.3E+04	2.9E+04	2.9E+04	9.5E+02	8.0E+02	7.6E+02	8.3E+02
110	345.2090	47.3	2.3E+04	2.4E+04	2.4E+04	2.3E+04	4.2E+03	3.0E+03	7.3E+03	4.8E+03
111	352.2195	12.4	3.8E+04	5.0E+04	4.5E+04	4.4E+04	1.0E+03	9.0E+02	7.8E+02	9.1E+02
112	352.2193	10.6	5.0E+04	4.4E+04	4.1E+04	4.5E+04	9.1E+02	8.6E+02	7.9E+02	8.5E+02
113	354.1970	10.2	2.4E+04	2.7E+04	2.4E+04	2.5E+04	1.4E+03	7.6E+02	9.0E+02	1.0E+03

No.	*m/z*	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
114	355.2631	38.0	4.4E+05	5.1E+05	5.5E+05	5.0E+05	7.7E+04	7.6E+04	6.8E+04	7.4E+04
115	355.2321	32.8	7.4E+04	9.9E+04	5.7E+04	7.6E+04	1.6E+04	1.9E+04	8.5E+03	1.4E+04
116	355.2352	47.3	3.2E+04	3.5E+04	3.8E+04	3.5E+04	0.0E+00	0.0E+00	9.9E+03	3.3E+03
117	357.2972	44.4	9.7E+04	8.9E+04	9.4E+04	9.3E+04	5.7E+03	5.1E+03	8.4E+03	6.4E+03
118	358.3439	47.5	1.8E+04	2.0E+04	2.0E+04	2.0E+04	7.3E+02	9.4E+02	1.0E+03	8.9E+02
119	367.3565	43.1	2.7E+04	2.7E+04	3.1E+04	2.8E+04	8.1E+02	1.1E+03	1.1E+03	9.9E+02
120	368.2130	9.8	2.8E+04	3.1E+04	2.9E+04	2.9E+04	1.2E+03	1.1E+03	1.2E+03	1.2E+03
121	368.2135	12.2	2.3E+04	2.3E+04	2.3E+04	2.3E+04	1.3E+03	1.4E+03	9.9E+02	1.2E+03
122	369.2783	38.0	2.0E+05	2.4E+05	2.8E+05	2.4E+05	4.1E+04	4.1E+04	3.5E+04	3.9E+04
123	370.1783	10.2	2.2E+04	2.7E+04	2.8E+04	2.6E+04	7.8E+02	5.4E+02	4.9E+02	6.0E+02
124	373.2364	47.3	6.0E+04	6.5E+04	7.0E+04	6.5E+04	9.3E+03	6.7E+03	2.0E+04	1.2E+04
125	375.3030	47.5	2.3E+05	2.5E+05	2.7E+05	2.5E+05	1.8E+04	1.1E+04	2.0E+04	1.6E+04
126	376.2219	24.1	1.9E+04	2.8E+04	3.1E+04	2.6E+04	4.7E+03	4.9E+03	7.4E+03	5.7E+03
127	379.3349	33.5	2.7E+06	3.0E+06	2.7E+06	2.8E+06	2.2E+05	1.9E+05	2.2E+05	2.1E+05
128	379.3356	40.4	1.7E+06	3.1E+06	2.6E+06	2.5E+06	1.3E+05	1.4E+05	1.5E+05	1.4E+05
129	382.2294	10.4	2.4E+04	2.2E+04	1.9E+04	2.2E+04	1.1E+03	6.5E+02	8.1E+02	8.4E+02
130	386.2031	11.1	3.3E+04	4.7E+04	4.4E+04	4.1E+04	3.2E+03	2.7E+03	2.6E+03	2.8E+03
131	387.2561	47.3	3.3E+04	3.8E+04	4.0E+04	3.7E+04	6.2E+03	5.0E+03	1.2E+04	7.8E+03
132	393.3644	41.1	3.2E+04	2.7E+04	2.9E+04	2.9E+04	5.0E+03	5.8E+03	6.7E+03	5.8E+03
133	395.3547	47.3	4.2E+04	3.4E+04	5.2E+04	4.3E+04	3.7E+03	2.1E+03	1.8E+04	7.8E+03
134	395.3548	46.4	4.9E+04	3.8E+04	4.2E+04	4.3E+04	0.0E+00	0.0E+00	0.0E+00	0.0E+00
135	395.3284	37.5	2.2E+05	2.5E+05	2.8E+05	2.5E+05	4.9E+04	4.4E+04	3.2E+04	4.2E+04
136	397.3975	45.1	2.9E+05	2.9E+05	2.8E+05	2.9E+05	1.5E+04	1.6E+04	1.3E+04	1.5E+04
137	399.2535	47.3	6.2E+04	6.9E+04	7.1E+04	6.7E+04	9.1E+03	6.9E+03	2.3E+04	1.3E+04
138	400.2165	12.0	1.4E+04	1.3E+04	1.1E+04	1.3E+04	6.4E+02	4.8E+02	4.9E+02	5.4E+02
139	402.1985	10.1	2.5E+04	3.2E+04	3.0E+04	2.9E+04	4.0E+02	2.1E+02	4.3E+02	3.4E+02
140	407.3377	38.1	8.3E+05	9.5E+05	1.0E+06	9.4E+05	1.7E+05	1.6E+05	1.3E+05	1.5E+05
141	411.3605	38.7	4.4E+05	4.0E+05	4.5E+05	4.3E+05	4.9E+04	5.0E+04	4.4E+04	4.8E+04
142	411.3809	41.1	1.2E+05	1.2E+05	1.1E+05	1.1E+05	2.1E+04	2.5E+04	2.7E+04	2.5E+04
143	417.2392	41.6	7.3E+04	6.2E+04	6.4E+04	6.7E+04	1.5E+04	2.0E+04	1.4E+04	1.6E+04
144	425.4262	45.9	7.1E+04	6.6E+04	6.5E+04	6.7E+04	0.0E+00	0.0E+00	0.0E+00	0.0E+00
145	428.4057	41.1	9.7E+04	9.1E+04	8.9E+04	9.2E+04	1.5E+04	1.9E+04	2.0E+04	1.8E+04
146	438.4614	43.9	1.2E+04	1.1E+04	1.5E+04	1.2E+04	1.4E+03	1.4E+03	2.4E+02	1.0E+03
147	442.3868	45.8	1.1E+05	1.2E+05	1.2E+05	1.2E+05	2.8E+04	2.7E+04	2.4E+04	2.6E+04
148	444.2447	13.6	1.1E+04	1.2E+04	1.1E+04	1.1E+04	2.5E+02	2.5E+02	2.1E+02	2.4E+02
149	445.2707	42.6	8.2E+04	7.1E+04	6.8E+04	7.4E+04	1.0E+04	1.4E+04	1.2E+04	1.2E+04
150	445.2706	41.9	1.0E+05	7.4E+04	7.1E+04	8.2E+04	8.5E+03	1.1E+04	7.9E+03	9.1E+03
151	446.2258	10.7	9.9E+03	9.3E+03	8.5E+03	9.2E+03	4.0E+02	2.0E+02	3.9E+02	3.3E+02
152	451.3598	38.2	9.6E+04	1.0E+05	1.1E+05	1.0E+05	2.5E+04	2.2E+04	1.9E+04	2.2E+04
153	452.4779	43.6	1.3E+04	1.6E+04	1.5E+04	1.5E+04	8.4E+01	0.0E+00	1.5E+01	3.3E+01
154	453.3720	38.7	3.3E+06	3.0E+06	3.3E+06	3.2E+06	3.1E+05	3.1E+05	2.9E+05	3.0E+05
155	455.3473	37.2	5.1E+05	6.0E+05	6.5E+05	5.9E+05	5.8E+04	5.5E+04	4.3E+04	5.2E+04
156	455.3190	47.3	6.2E+04	6.7E+04	6.8E+04	6.6E+04	1.3E+04	1.2E+04	2.1E+04	1.5E+04
157	464.2145	12.1	8.1E+03	1.1E+04	8.5E+03	9.3E+03	2.6E+02	1.8E+02	2.1E+02	2.2E+02
158	469.3657	38.2	6.8E+04	7.6E+04	7.8E+04	7.4E+04	1.3E+04	1.1E+04	8.4E+03	1.1E+04
159	469.3291	40.4	5.8E+04	6.8E+04	4.2E+04	5.6E+04	7.0E+03	1.4E+04	1.3E+04	1.1E+04
160	471.3803	38.6	3.5E+05	3.0E+05	3.5E+05	3.3E+05	2.2E+04	2.3E+04	2.2E+04	2.2E+04
161	472.3766	37.5	9.9E+04	1.3E+05	1.7E+05	1.3E+05	5.3E+03	4.6E+03	4.2E+03	4.7E+03
162	476.3486	33.5	1.5E+06	1.5E+06	1.5E+06	1.5E+06	6.9E+04	7.8E+04	1.0E+05	8.3E+04
163	477.3330	37.0	6.2E+05	7.1E+05	8.2E+05	7.2E+05	7.8E+04	7.1E+04	6.1E+04	7.0E+04
164	483.3618	34.1	2.7E+04	3.7E+04	4.5E+04	3.6E+04	7.9E+03	9.5E+03	4.7E+03	7.4E+03
165	488.4072	38.6	3.6E+05	2.8E+05	3.5E+05	3.3E+05	1.3E+04	1.6E+04	1.4E+04	1.4E+04
166	490.3269	29.2	1.9E+04	2.5E+04	2.1E+04	2.2E+04	2.6E+03	2.8E+03	2.9E+03	2.8E+03
167	491.2821	29.4	3.7E+04	3.9E+04	4.2E+04	3.9E+04	4.2E+03	3.6E+03	3.4E+03	3.7E+03
168	492.3408	31.8	2.3E+04	2.7E+04	2.3E+04	2.4E+04	2.3E+03	1.5E+03	2.5E+03	2.1E+03
169	493.3617	38.9	1.8E+06	2.1E+06	2.3E+06	2.0E+06	2.3E+05	2.8E+05	1.9E+05	2.3E+05
170	496.5021	43.6	1.1E+04	1.3E+04	1.2E+04	1.2E+04	9.5E+02	1.2E+03	8.9E+02	1.0E+03
171	497.2684	32.8	1.8E+05	2.4E+05	1.4E+05	1.9E+05	3.1E+04	4.7E+04	2.8E+04	3.6E+04
172	499.3866	38.6	2.6E+04	3.5E+04	3.2E+04	3.1E+04	3.2E+03	3.5E+03	2.6E+03	3.1E+03

No.	*m/z*	RT (min)	Normalized integrated mass ion intensity (nMSII) EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
173	503.4586	46.4	8.4E+03	1.1E+04	1.0E+04	1.0E+04	3.3E+03	1.9E+03	9.8E+02	2.1E+03
174	505.3885	43.8	5.5E+04	4.8E+04	4.7E+04	5.0E+04	3.8E+03	4.5E+03	7.0E+03	5.1E+03
175	506.3105	9.7	2.7E+04	1.8E+04	1.6E+04	2.0E+04	2.2E+02	2.1E+02	1.2E+02	1.8E+02
176	506.3243	30.8	1.7E+04	3.3E+04	3.0E+04	2.7E+04	2.3E+03	1.7E+03	3.0E+03	2.3E+03
177	507.3440	34.1	5.5E+04	6.0E+04	6.1E+04	5.9E+04	1.0E+04	9.1E+03	7.5E+03	9.0E+03
178	508.3386	32.2	1.9E+04	3.2E+04	2.7E+04	2.6E+04	3.7E+03	2.3E+03	2.9E+03	3.0E+03
179	517.4716	46.4	1.3E+04	1.4E+04	1.6E+04	1.4E+04	9.4E+02	3.0E+02	4.7E+01	4.3E+02
180	519.4118	43.7	3.5E+04	3.0E+04	3.2E+04	3.3E+04	3.2E+03	3.4E+03	4.4E+03	3.6E+03
181	523.3744	47.3	4.0E+04	4.2E+04	4.4E+04	4.2E+04	3.7E+03	3.4E+03	1.2E+04	6.5E+03
182	531.4891	46.4	4.4E+04	4.6E+04	4.4E+04	4.5E+04	1.3E+03	3.0E+02	1.2E+03	9.1E+02
183	538.3124	28.3	2.2E+05	3.0E+05	1.7E+05	2.3E+05	5.6E+03	8.3E+03	5.7E+03	6.5E+03
184	538.3814	33.1	1.3E+04	2.0E+04	1.2E+04	1.5E+04	1.5E+03	2.1E+03	1.8E+03	1.8E+03
185	543.4135	40.4	4.2E+04	8.1E+04	7.5E+04	6.6E+04	3.1E+03	3.4E+03	4.1E+03	3.5E+03
186	545.5066	49.5	1.2E+05	1.4E+05	1.2E+05	1.3E+05	3.8E+01	4.4E+03	0.0E+00	1.5E+03
187	545.5020	45.4	9.0E+04	8.7E+04	8.1E+04	8.6E+04	3.9E+03	3.4E+03	1.9E+03	3.1E+03
188	561.4869	41.7	2.5E+05	2.0E+05	1.8E+05	2.1E+05	4.6E+04	5.3E+04	4.4E+04	4.8E+04
189	562.5322	49.5	1.0E+05	1.0E+05	1.0E+05	1.0E+05	1.5E+03	4.4E+03	1.1E+03	2.3E+03
190	563.5011	44.2	1.8E+05	1.4E+05	1.4E+05	1.5E+05	2.4E+04	1.9E+04	2.8E+04	2.4E+04
191	575.5035	44.1	4.9E+06	4.0E+06	3.9E+06	4.2E+06	4.3E+05	4.4E+05	8.0E+05	5.6E+05
192	577.5185	44.6	5.0E+06	4.3E+06	4.3E+06	4.5E+06	4.6E+05	4.1E+05	7.3E+05	5.4E+05
193	583.2547	23.6	1.4E+04	8.1E+03	1.3E+04	1.1E+04	8.3E+02	7.7E+02	1.4E+03	1.0E+03
194	585.4968	45.4	5.5E+04	5.6E+04	5.3E+04	5.5E+04	3.0E+03	3.3E+03	2.9E+03	3.1E+03
195	587.5051	44.0	1.2E+05	9.6E+04	1.0E+05	1.1E+05	1.2E+04	1.2E+04	1.6E+04	1.3E+04
196	589.5150	44.5	1.9E+05	1.7E+05	1.7E+05	1.7E+05	2.3E+04	2.1E+04	3.3E+04	2.6E+04
197	591.5287	45.1	1.1E+05	1.1E+05	1.0E+05	1.1E+05	2.0E+04	1.7E+04	2.2E+04	2.0E+04
198	593.5154	44.1	5.0E+05	4.1E+05	3.9E+05	4.4E+05	4.9E+04	4.5E+04	8.3E+04	5.9E+04
199	594.5439	40.6	1.5E+05	1.5E+05	1.5E+05	1.5E+05	2.4E+04	3.9E+04	3.7E+04	3.3E+04
200	595.5281	44.6	4.4E+05	3.7E+05	3.5E+05	3.9E+05	4.0E+04	3.4E+04	6.1E+04	4.5E+04
201	599.5044	41.8	9.2E+06	6.8E+06	6.3E+06	7.4E+06	1.2E+06	1.4E+06	1.2E+06	1.2E+06
202	599.5026	43.8	2.2E+06	1.8E+06	1.7E+06	1.9E+06	1.2E+05	1.3E+05	2.2E+05	1.6E+05
203	601.5186	44.4	5.2E+06	4.6E+06	4.6E+06	4.8E+06	2.5E+05	2.5E+05	4.3E+05	3.1E+05
204	603.5360	43.3	1.7E+07	1.4E+07	1.3E+07	1.5E+07	1.7E+06	2.0E+06	2.0E+06	1.9E+06
205	603.5334	44.9	3.5E+06	3.1E+06	3.2E+06	3.3E+06	2.0E+05	2.0E+05	3.4E+05	2.5E+05
206	605.5484	44.0	2.2E+06	1.7E+06	1.7E+06	1.9E+06	2.3E+05	5.9E+04	3.0E+05	2.0E+05
207	610.5394	44.0	1.7E+06	1.4E+06	1.4E+06	1.5E+06	1.7E+05	1.6E+05	3.0E+05	2.1E+05
208	610.5635	46.7	5.4E+04	5.3E+04	5.5E+04	5.4E+04	1.1E+04	1.0E+04	9.6E+03	1.0E+04
209	613.5668	46.5	3.0E+05	3.1E+05	2.8E+05	3.0E+05	0.0E+00	1.2E+02	0.0E+00	4.0E+01
210	617.5133	43.7	4.9E+06	4.0E+06	3.9E+06	4.3E+06	2.4E+05	2.4E+05	4.8E+05	3.2E+05
211	617.5101	44.7	1.1E+06	9.8E+05	9.5E+05	1.0E+06	1.6E+05	1.7E+05	2.6E+05	2.0E+05
212	618.3002	29.2	3.0E+04	4.0E+04	2.4E+04	3.1E+04	3.9E+03	8.8E+03	5.9E+03	6.2E+03
213	619.5266	44.4	2.6E+06	2.2E+06	2.3E+06	2.4E+06	1.9E+05	1.8E+05	3.1E+05	2.2E+05
214	621.5416	44.9	6.3E+05	5.8E+05	7.2E+05	6.4E+05	5.7E+04	5.2E+04	7.8E+04	6.2E+04
215	627.4336	35.0	1.2E+05	1.1E+05	9.5E+04	1.1E+05	1.4E+04	1.7E+04	1.6E+04	1.5E+04
216	627.5333	43.0	2.9E+05	2.4E+05	2.2E+05	2.5E+05	1.6E+04	1.9E+04	1.8E+04	1.8E+04
217	629.5477	43.5	7.9E+05	6.2E+05	5.5E+05	6.5E+05	4.2E+04	4.8E+04	4.2E+04	4.4E+04
218	630.5951	50.2	1.6E+05	1.9E+05	1.9E+05	1.8E+05	2.2E+03	6.7E+03	3.1E+03	4.0E+03
219	630.5941	46.5	2.9E+05	3.0E+05	2.9E+05	2.9E+05	4.2E+02	1.1E+03	7.8E+01	5.4E+02
220	631.5539	44.2	4.5E+05	4.2E+05	3.7E+05	4.1E+05	2.6E+04	2.9E+04	3.1E+04	2.8E+04
221	633.5441	44.6	7.2E+04	6.2E+04	5.8E+04	6.4E+04	1.1E+04	1.0E+04	1.6E+04	1.2E+04
222	634.5394	43.8	2.4E+06	2.0E+06	2.0E+06	2.1E+06	1.2E+05	1.3E+05	2.5E+05	1.7E+05
223	636.5550	44.4	3.0E+06	2.6E+06	2.7E+06	2.8E+06	1.6E+05	1.4E+05	2.7E+05	1.9E+05
224	638.5700	44.9	1.9E+06	1.5E+06	1.7E+06	1.7E+06	1.3E+05	1.1E+05	2.0E+05	1.4E+05
225	639.4951	43.8	2.1E+06	2.1E+06	2.0E+06	2.1E+06	9.5E+04	1.1E+05	2.8E+05	1.6E+05
226	640.5815	45.3	3.9E+05	3.4E+05	3.7E+05	3.7E+05	4.0E+04	3.6E+04	4.9E+04	4.2E+04
227	641.5108	44.3	3.0E+06	2.9E+06	3.1E+06	3.0E+06	1.6E+05	1.9E+05	3.9E+05	2.5E+05
228	643.5256	44.9	1.7E+06	1.6E+06	1.7E+06	1.7E+06	1.6E+05	1.4E+05	2.9E+05	2.0E+05
229	645.5386	45.4	3.5E+05	3.2E+05	3.9E+05	3.5E+05	5.1E+04	4.3E+04	9.1E+04	6.2E+04
230	645.4906	47.3	6.2E+04	7.2E+04	7.7E+04	7.0E+04	1.2E+04	9.4E+03	2.2E+04	1.4E+04
231	647.4636	47.3	2.0E+06	2.4E+06	2.8E+06	2.4E+06	1.7E+04	2.4E+04	1.3E+04	1.8E+04

No.	m/z	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
232	648.6029	46.5	1.8E+05	2.0E+05	1.8E+05	1.8E+05	1.3E+04	1.2E+04	1.0E+04	1.2E+04
233	652.5492	45.0	4.8E+04	5.1E+04	5.2E+04	5.0E+04	1.6E+02	3.2E+02	1.7E+02	2.2E+02
234	655.4700	43.7	6.7E+04	6.6E+04	6.3E+04	6.5E+04	4.6E+03	5.1E+03	1.0E+04	6.7E+03
235	657.4889	44.3	9.8E+04	1.1E+05	1.1E+05	1.1E+05	9.2E+03	1.1E+04	1.6E+04	1.2E+04
236	659.5072	47.3	3.7E+04	4.3E+04	4.3E+04	4.1E+04	5.8E+03	3.9E+03	1.3E+04	7.5E+03
237	659.5346	44.9	1.2E+05	1.2E+05	1.1E+05	1.2E+05	7.4E+03	1.2E+04	1.8E+04	1.2E+04
238	661.5837	47.6	2.3E+04	2.4E+04	2.3E+04	2.3E+04	2.6E+03	2.1E+03	1.1E+03	2.0E+03
239	661.5884	45.4	6.9E+04	7.0E+04	6.4E+04	6.8E+04	9.3E+03	1.1E+04	1.1E+04	1.1E+04
240	662.5667	44.6	6.8E+04	6.4E+04	5.8E+04	6.4E+04	3.4E+03	3.6E+03	4.3E+03	3.8E+03
241	663.5715	47.5	4.9E+04	4.7E+04	5.6E+04	5.1E+04	6.5E+03	5.7E+03	6.1E+03	6.1E+03
242	664.6204	45.1	7.5E+04	6.7E+04	6.5E+04	6.9E+04	1.1E+04	7.8E+03	1.0E+03	6.7E+03
243	667.5271	44.6	6.3E+04	6.8E+04	6.2E+04	6.4E+04	4.0E+03	4.2E+03	7.9E+03	5.4E+03
244	669.5434	46.4	2.8E+04	2.8E+04	3.4E+04	3.0E+04	2.0E+03	1.9E+03	1.7E+03	1.9E+03
245	671.5034	47.3	3.6E+04	4.1E+04	4.2E+04	4.0E+04	6.0E+03	4.2E+03	1.2E+04	7.5E+03
246	673.5917	45.4	6.4E+04	6.8E+04	5.9E+04	6.4E+04	1.6E+03	3.7E+03	3.2E+03	2.8E+03
247	676.5484	44.7	1.5E+05	1.7E+05	1.6E+05	1.6E+05	4.1E+03	3.8E+03	5.0E+03	4.3E+03
248	678.5655	45.2	1.6E+05	1.7E+05	1.8E+05	1.7E+05	0.0E+00	1.8E+03	2.6E+03	1.5E+03
249	678.6161	47.6	1.5E+05	1.7E+05	1.5E+05	1.5E+05	6.6E+03	6.6E+03	6.5E+03	6.6E+03
250	679.4350	46.8	5.5E+04	6.3E+04	5.5E+04	5.8E+04	9.6E+03	8.5E+03	7.3E+03	8.5E+03
251	685.4368	45.8	1.1E+05	1.6E+05	1.5E+05	1.4E+05	3.3E+04	3.3E+04	2.7E+04	3.1E+04
252	687.4948	41.7	1.8E+04	1.4E+04	1.3E+04	1.5E+04	3.0E+03	3.4E+03	2.5E+03	3.0E+03
253	687.6256	45.7	2.9E+05	2.6E+05	2.4E+05	2.6E+05	4.6E+04	5.6E+04	7.1E+04	5.8E+04
254	687.5702	47.4	9.5E+04	9.3E+04	1.1E+05	1.0E+05	7.4E+03	5.4E+03	1.2E+04	8.4E+03
255	689.6393	46.0	2.9E+05	2.8E+05	2.6E+05	2.7E+05	2.7E+04	4.0E+04	4.7E+04	3.8E+04
256	689.5876	47.7	7.1E+04	7.6E+04	8.7E+04	7.8E+04	6.5E+03	4.8E+03	1.1E+04	7.4E+03
257	696.5843	45.3	1.9E+04	1.7E+04	1.7E+04	1.8E+04	2.3E+03	2.2E+03	2.6E+03	2.4E+03
258	696.6845	46.1	1.1E+06	1.0E+06	1.3E+06	1.1E+06	1.1E+05	7.7E+04	9.8E+04	9.4E+04
259	701.6339	46.0	5.0E+04	4.9E+04	4.0E+04	4.6E+04	0.0E+00	0.0E+00	1.5E+03	5.0E+02
260	703.6533	46.3	4.7E+04	4.5E+04	4.2E+04	4.5E+04	4.2E+03	5.5E+03	7.0E+03	5.5E+03
261	710.6588	45.1	1.6E+04	1.8E+04	1.5E+04	1.6E+04	5.8E+03	4.3E+03	1.8E+03	4.0E+03
262	710.6975	46.4	1.9E+05	1.7E+05	2.0E+05	1.9E+05	1.5E+04	1.0E+04	8.2E+03	1.1E+04
263	713.5111	42.2	3.0E+04	2.5E+04	2.2E+04	2.6E+04	5.0E+03	6.0E+03	5.0E+03	5.4E+03
264	717.6623	46.5	3.6E+04	3.2E+04	2.9E+04	3.2E+04	0.0E+00	0.0E+00	1.5E+03	4.9E+02
265	718.6616	46.1	1.3E+05	1.2E+05	1.5E+05	1.3E+05	1.3E+04	0.0E+00	7.8E+03	6.9E+03
266	721.6047	47.6	4.2E+04	4.5E+04	5.0E+04	4.6E+04	3.7E+03	1.7E+03	6.8E+03	4.1E+03
267	725.5111	41.9	1.5E+06	1.2E+06	1.1E+06	1.3E+06	1.4E+05	1.7E+05	1.5E+05	1.6E+05
268	729.5412	43.3	1.7E+06	1.4E+06	1.4E+06	1.5E+06	1.4E+05	1.7E+05	1.8E+05	1.6E+05
269	731.5549	44.0	1.7E+05	1.3E+05	1.2E+05	1.4E+05	1.3E+04	2.0E+04	2.1E+04	1.8E+04
270	732.6927	46.4	2.8E+04	4.3E+04	3.2E+04	3.4E+04	1.2E+04	7.0E+03	3.6E+03	7.6E+03
271	736.6246	47.4	1.5E+05	1.6E+05	1.8E+05	1.6E+05	6.4E+03	4.1E+03	2.1E+04	1.1E+04
272	744.5527	41.8	6.8E+05	7.2E+05	7.3E+05	7.1E+05	5.7E+04	5.8E+04	5.5E+04	5.7E+04
273	748.5812	44.0	3.0E+05	2.2E+05	2.2E+05	2.5E+05	3.3E+04	3.5E+04	3.9E+04	3.6E+04
274	749.5139	42.7	8.6E+04	8.6E+04	1.0E+05	9.2E+04	1.5E+04	1.9E+04	2.2E+04	1.8E+04
275	753.5381	43.0	7.8E+04	8.1E+04	7.1E+04	7.7E+04	7.3E+03	8.6E+03	1.0E+04	8.8E+03
276	755.5577	43.6	1.4E+05	1.1E+05	9.9E+04	1.2E+05	6.4E+03	8.5E+03	8.2E+03	7.7E+03
277	756.5522	42.3	1.0E+05	1.2E+05	1.1E+05	1.1E+05	1.4E+04	1.3E+04	1.3E+04	1.3E+04
278	763.5884	47.3	4.0E+04	4.5E+04	4.6E+04	4.4E+04	7.7E+03	5.2E+03	1.3E+04	8.7E+03
279	768.5534	41.5	1.2E+06	1.2E+06	1.2E+06	1.2E+06	3.9E+04	3.7E+04	2.4E+04	3.3E+04
280	770.5688	42.3	8.5E+05	8.4E+05	8.2E+05	8.4E+05	4.8E+04	4.1E+04	4.2E+04	4.4E+04
281	772.5838	43.0	5.7E+05	5.9E+05	5.6E+05	5.7E+05	6.9E+04	5.6E+04	5.9E+04	6.1E+04
282	772.5834	43.8	3.5E+05	3.4E+05	2.6E+05	3.2E+05	3.0E+04	2.7E+04	2.9E+04	2.9E+04
283	777.6176	47.3	8.2E+04	9.7E+04	1.0E+05	9.3E+04	1.4E+04	9.4E+03	3.0E+04	1.8E+04
284	780.2305	9.3	1.6E+04	1.4E+04	1.3E+04	1.4E+04	2.5E+03	3.3E+03	2.9E+03	2.9E+03
285	798.5985	43.2	9.8E+04	1.0E+05	9.7E+04	1.0E+05	2.0E+04	1.5E+04	1.5E+04	1.7E+04
286	806.5016	40.7	4.9E+04	4.9E+04	4.7E+04	4.8E+04	9.2E+03	8.8E+03	1.1E+04	9.8E+03
287	812.6535	47.3	6.5E+05	7.8E+05	8.3E+05	7.5E+05	9.3E+04	6.2E+04	2.3E+05	1.3E+05
288	816.7036	47.6	1.4E+05	1.7E+05	1.8E+05	1.6E+05	2.4E+04	1.3E+04	1.8E+04	1.8E+04
289	818.7699	49.5	2.7E+04	2.7E+04	2.7E+04	2.7E+04	3.5E+02	4.7E+02	2.7E+02	3.7E+02
290	830.5968	41.0	5.1E+04	5.7E+04	2.9E+04	4.6E+04	5.4E+03	1.6E+04	1.1E+04	1.1E+04

No.	*m/z*	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
291	830.6578	43.3	2.7E+04	2.3E+04	2.6E+04	2.5E+04	0.0E+00	0.0E+00	0.0E+00	0.0E+00
292	832.6678	45.9	5.3E+04	5.4E+04	4.7E+04	5.2E+04	1.1E+04	1.0E+04	1.3E+04	1.1E+04
293	833.5881	47.3	2.7E+04	3.0E+04	3.2E+04	2.9E+04	4.7E+03	4.5E+03	9.5E+03	6.3E+03
294	840.6949	47.4	6.6E+04	7.3E+04	8.2E+04	7.4E+04	8.0E+03	6.3E+03	1.4E+04	9.4E+03
295	841.7007	46.3	2.4E+04	2.7E+04	2.4E+04	2.5E+04	4.8E+03	4.0E+03	4.6E+03	4.5E+03
296	842.7186	47.7	2.1E+05	2.5E+05	2.8E+05	2.5E+05	1.9E+04	1.6E+04	2.8E+04	2.1E+04
297	842.7713	49.4	1.4E+05	1.4E+05	1.3E+05	1.3E+05	6.6E+02	5.2E+03	1.0E+02	2.0E+03
298	844.7360	47.8	1.4E+06	1.5E+06	1.6E+06	1.5E+06	1.2E+05	9.4E+04	1.7E+05	1.3E+05
299	844.7843	49.5	1.0E+05	1.1E+05	1.1E+05	1.1E+05	1.5E+03	4.2E+03	7.4E+02	2.1E+03
300	853.7255	46.4	8.9E+04	1.2E+05	1.0E+05	1.0E+05	8.9E+03	8.7E+03	1.2E+04	9.7E+03
301	854.7055	47.3	4.4E+04	5.0E+04	5.7E+04	5.0E+04	7.9E+03	6.0E+03	1.6E+04	1.0E+04
302	855.7380	46.6	1.4E+05	1.9E+05	1.8E+05	1.7E+05	8.9E+03	8.7E+03	1.3E+04	1.0E+04
303	856.5921	33.5	3.9E+05	4.0E+05	3.6E+05	3.8E+05	4.2E+04	4.3E+04	4.4E+04	4.3E+04
304	856.7357	47.8	1.9E+05	2.0E+05	2.1E+05	2.0E+05	2.5E+04	4.4E+04	5.3E+04	4.1E+04
305	857.7513	46.8	1.1E+05	1.5E+05	1.5E+05	1.3E+05	6.3E+03	5.1E+03	1.1E+04	7.5E+03
306	858.7521	48.0	1.1E+06	1.3E+06	1.2E+06	1.2E+06	1.2E+05	1.1E+05	1.6E+05	1.3E+05
307	860.7302	46.6	3.3E+04	4.3E+04	3.6E+04	3.7E+04	4.9E+03	4.6E+03	5.7E+03	5.1E+03
308	862.7455	46.9	1.0E+05	1.3E+05	1.4E+05	1.2E+05	9.4E+03	7.2E+03	1.6E+04	1.1E+04
309	864.7565	47.2	1.6E+05	2.0E+05	2.1E+05	1.9E+05	1.7E+04	1.5E+04	6.5E+03	1.3E+04
310	865.4917	40.3	1.4E+04	1.7E+04	1.4E+04	1.5E+04	2.7E+03	3.7E+03	3.2E+03	3.2E+03
311	868.7438	47.6	7.1E+05	7.6E+05	8.1E+05	7.6E+05	7.3E+04	9.1E+04	1.0E+05	8.9E+04
312	870.7528	47.9	2.7E+06	2.8E+06	2.9E+06	2.8E+06	2.9E+05	2.7E+05	4.6E+05	3.4E+05
313	873.7264	47.6	7.0E+04	1.1E+05	6.5E+04	8.0E+04	1.3E+04	1.7E+04	1.5E+04	1.5E+04
314	877.7317	46.3	8.9E+04	1.2E+05	9.6E+04	1.0E+05	8.5E+03	6.7E+03	1.1E+04	8.6E+03
315	879.7409	46.5	2.3E+05	3.2E+05	2.7E+05	2.7E+05	9.4E+03	1.2E+04	1.5E+04	1.2E+04
316	882.7522	47.9	5.4E+05	5.4E+05	5.5E+05	5.5E+05	6.3E+04	5.8E+04	1.0E+05	7.4E+04
317	883.5179	32.9	6.8E+04	8.7E+04	4.5E+04	6.7E+04	6.5E+03	1.1E+04	6.4E+03	8.0E+03
318	883.7685	47.0	2.6E+05	3.4E+05	3.5E+05	3.1E+05	1.3E+04	1.5E+04	2.1E+04	1.6E+04
319	884.7700	47.0	1.4E+05	1.9E+05	1.9E+05	1.7E+05	5.1E+03	4.2E+03	9.8E+03	6.4E+03
320	885.7775	47.1	1.1E+05	1.5E+05	1.5E+05	1.4E+05	0.0E+00	0.0E+00	6.3E+03	2.1E+03
321	886.6647	34.0	8.4E+04	1.2E+05	1.3E+05	1.1E+05	1.3E+04	1.1E+04	2.1E+04	1.5E+04
322	888.7606	47.1	5.4E+05	7.1E+05	7.3E+05	6.6E+05	1.9E+04	1.9E+04	4.2E+04	2.7E+04
323	890.7736	47.3	5.3E+05	7.2E+05	7.0E+05	6.5E+05	2.1E+04	1.9E+04	4.4E+04	2.8E+04
324	892.7468	47.6	7.2E+05	6.9E+05	9.0E+05	7.7E+05	8.7E+04	1.1E+05	1.8E+05	1.3E+05
325	894.7602	47.8	5.1E+06	4.9E+06	5.6E+06	5.2E+06	5.6E+05	6.1E+05	1.1E+06	7.6E+05
326	895.7413	46.8	2.0E+05	3.6E+05	2.2E+05	2.6E+05	3.2E+03	2.1E+03	0.0E+00	1.8E+03
327	896.5901	40.9	1.2E+04	1.1E+04	1.1E+04	1.1E+04	2.1E+03	2.4E+03	3.0E+03	2.5E+03
328	903.4975	40.6	2.6E+04	2.7E+04	2.7E+04	2.7E+04	2.1E+03	3.0E+03	2.6E+03	2.6E+03
329	904.8319	49.0	1.9E+07	2.1E+07	2.0E+07	2.0E+07	1.5E+06	1.9E+06	2.6E+06	2.0E+06
330	906.8451	49.1	7.5E+06	8.4E+06	8.7E+06	8.2E+06	6.8E+05	8.4E+05	1.2E+06	9.1E+05
331	907.7274	33.5	2.3E+06	2.5E+06	2.5E+06	2.4E+06	2.7E+04	2.2E+04	2.4E+04	2.4E+04
332	910.8335	50.0	3.6E+05	3.9E+05	3.5E+05	3.6E+05	6.7E+03	1.6E+04	7.6E+03	1.0E+04
333	911.7346	45.9	3.3E+04	4.6E+04	3.9E+04	3.9E+04	5.2E+03	3.3E+03	4.2E+03	4.2E+03
334	912.7626	46.9	3.5E+05	4.6E+05	4.0E+05	4.0E+05	1.7E+04	2.2E+04	2.3E+04	2.1E+04
335	912.8479	50.3	3.0E+05	3.7E+05	3.3E+05	3.3E+05	3.4E+03	1.1E+04	4.1E+03	6.2E+03
336	914.7771	47.2	5.5E+05	7.7E+05	7.1E+05	6.8E+05	2.5E+04	2.9E+04	3.2E+04	2.9E+04
337	914.8605	50.5	2.3E+05	2.9E+05	2.9E+05	2.7E+05	0.0E+00	8.6E+03	4.9E+03	4.5E+03
338	916.7907	46.7	4.0E+05	5.0E+05	5.1E+05	4.7E+05	1.3E+04	1.4E+04	2.1E+04	1.6E+04
339	916.7929	47.5	4.8E+05	7.2E+05	6.5E+05	6.2E+05	1.3E+04	1.6E+04	2.3E+04	1.7E+04
340	918.8068	47.7	2.5E+05	3.5E+05	3.0E+05	3.0E+05	1.0E+04	1.0E+04	1.6E+04	1.2E+04
341	918.8057	46.9	4.4E+05	5.6E+05	5.9E+05	5.3E+05	1.4E+04	1.3E+04	2.7E+04	1.8E+04
342	920.8140	47.1	2.7E+05	3.8E+05	3.9E+05	3.5E+05	1.5E+04	1.7E+04	2.4E+04	1.9E+04
343	921.7798	46.6	2.9E+05	3.6E+05	3.8E+05	3.4E+05	1.7E+04	1.8E+04	2.4E+04	2.0E+04
344	924.6702	33.4	3.1E+04	3.4E+04	3.3E+04	3.3E+04	5.4E+03	8.9E+03	4.1E+03	6.1E+03
345	924.7992	48.4	3.7E+05	4.0E+05	3.7E+05	3.8E+05	6.2E+04	8.1E+04	9.7E+04	8.0E+04
346	925.7758	47.1	1.1E+05	1.4E+05	1.4E+05	1.3E+05	7.5E+03	8.1E+03	1.4E+04	9.7E+03
347	926.8112	48.6	6.2E+05	6.2E+05	5.8E+05	6.1E+05	6.8E+04	9.2E+04	1.1E+05	9.0E+04
348	928.7549	46.3	1.6E+05	2.7E+05	1.6E+05	2.0E+05	0.0E+00	0.0E+00	0.0E+00	0.0E+00
349	929.7093	33.5	4.4E+06	4.5E+06	4.4E+06	4.4E+06	9.8E+04	1.0E+05	1.4E+05	1.1E+05

No.	*m/z*	RT	Normalized integrated mass ion intensity (nMSII)							
		(min)	EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
350	930.8448	49.1	1.5E+06	1.7E+06	1.6E+06	1.6E+06	1.3E+05	1.6E+05	2.1E+05	1.7E+05
351	930.8694	51.1	5.3E+04	6.1E+04	8.1E+04	6.5E+04	1.3E+02	3.2E+03	9.9E+02	1.4E+03
352	932.7856	46.9	1.3E+05	2.3E+05	1.6E+05	1.7E+05	5.6E+03	8.2E+03	8.2E+03	7.3E+03
353	932.8611	49.3	2.0E+06	2.3E+06	2.4E+06	2.2E+06	2.1E+05	2.3E+05	3.3E+05	2.6E+05
354	933.6921	37.5	1.9E+05	2.3E+05	2.9E+05	2.4E+05	1.6E+04	1.3E+04	1.4E+04	1.4E+04
355	934.8749	49.5	1.4E+06	1.8E+06	1.8E+06	1.7E+06	1.7E+05	1.8E+05	2.3E+05	1.9E+05
356	938.8041	48.0	1.5E+05	1.4E+05	1.5E+05	1.5E+05	2.8E+04	2.9E+04	3.7E+04	3.1E+04
357	946.7617	45.9	6.3E+04	9.0E+04	5.2E+04	6.8E+04	0.0E+00	1.4E+04	1.7E+03	5.3E+03
358	947.7817	48.0	5.7E+04	5.8E+04	5.0E+04	5.5E+04	8.0E+03	7.9E+03	9.1E+03	8.3E+03
359	949.7226	38.3	2.5E+05	3.1E+05	3.2E+05	2.9E+05	3.6E+04	3.5E+04	2.7E+04	3.3E+04
360	953.8235	48.8	5.5E+04	5.3E+04	4.3E+04	5.0E+04	8.4E+03	8.8E+03	8.7E+03	8.6E+03
361	954.8396	49.0	1.3E+05	1.2E+05	1.2E+05	1.2E+05	2.2E+04	2.1E+04	3.1E+04	2.4E+04
362	956.8622	49.2	1.1E+06	1.2E+06	1.2E+06	1.2E+06	1.5E+05	1.6E+05	2.4E+05	1.8E+05
363	958.8768	49.4	2.3E+06	2.7E+06	2.7E+06	2.5E+06	2.2E+05	2.4E+05	3.9E+05	2.8E+05
364	963.7386	38.8	4.4E+05	5.1E+05	5.4E+05	5.0E+05	2.4E+04	2.7E+04	1.5E+04	2.2E+04
365	968.8537	48.3	3.3E+04	3.2E+04	2.3E+04	2.9E+04	0.0E+00	0.0E+00	0.0E+00	0.0E+00
366	970.8761	49.4	6.9E+05	7.7E+05	7.3E+05	7.3E+05	6.8E+04	7.9E+04	9.1E+04	7.9E+04
367	972.8919	49.6	1.4E+06	1.6E+06	1.5E+06	1.5E+06	1.3E+05	1.4E+05	1.7E+05	1.5E+05
368	974.9076	49.8	1.7E+06	1.9E+06	2.0E+06	1.9E+06	1.7E+05	1.9E+05	2.1E+05	1.9E+05
369	976.9215	50.0	1.1E+06	1.4E+06	1.4E+06	1.3E+06	1.2E+05	1.4E+05	1.4E+05	1.3E+05
370	982.8686	48.3	4.8E+04	5.0E+04	4.6E+04	4.8E+04	0.0E+00	3.3E+02	4.8E+03	1.7E+03
371	984.7103	44.2	9.7E+04	1.1E+05	9.4E+04	1.0E+05	2.0E+04	2.1E+04	1.6E+04	1.9E+04
372	996.8861	49.4	4.0E+04	3.2E+04	3.6E+04	3.6E+04	7.6E+03	7.6E+03	9.6E+03	8.3E+03
373	998.9078	49.7	9.1E+05	9.9E+05	9.6E+05	9.5E+05	9.5E+04	1.2E+05	1.3E+05	1.1E+05
374	998.9545	52.1	7.3E+04	6.7E+04	8.3E+04	7.4E+04	2.9E+02	4.4E+03	5.5E+03	3.4E+03
375	1000.9229	49.9	1.5E+06	1.7E+06	1.7E+06	1.7E+06	1.1E+05	1.4E+05	1.4E+05	1.3E+05
376	1002.9375	50.2	1.5E+06	1.8E+06	1.8E+06	1.7E+06	9.9E+04	1.3E+05	1.2E+05	1.2E+05
377	1004.9508	50.4	7.2E+05	8.7E+05	9.2E+05	8.4E+05	5.3E+04	6.7E+04	6.8E+04	6.3E+04
378	1018.9654	50.5	6.0E+05	7.8E+05	8.6E+05	7.5E+05	9.1E+04	1.0E+05	1.7E+05	1.2E+05
379	1022.8612	47.5	3.2E+04	3.6E+04	1.7E+04	2.8E+04	0.0E+00	0.0E+00	0.0E+00	0.0E+00
380	1030.9590	49.8	1.5E+05	2.4E+05	2.3E+05	2.0E+05	2.0E+04	2.3E+04	2.8E+04	2.3E+04
381	1033.7943	45.0	3.9E+04	4.1E+04	4.1E+04	4.0E+04	7.2E+03	7.1E+03	9.4E+03	7.9E+03
382	1034.9607	50.2	4.5E+04	5.5E+04	5.2E+04	5.1E+04	1.9E+03	1.8E+03	7.8E+03	3.8E+03
383	1037.9163	49.7	2.3E+04	2.6E+04	2.5E+04	2.5E+04	3.7E+03	3.6E+03	5.0E+03	4.1E+03
384	1039.9283	49.9	2.3E+04	2.7E+04	2.7E+04	2.6E+04	4.1E+03	3.9E+03	5.1E+03	4.4E+03
385	1040.9507	50.2	4.4E+04	5.1E+04	5.1E+04	4.8E+04	8.8E+03	8.0E+03	1.2E+04	9.5E+03
386	1048.8810	47.6	3.8E+04	4.6E+04	3.8E+04	4.1E+04	5.9E+03	7.3E+03	6.0E+03	6.4E+03
387	1050.8917	47.7	2.0E+04	2.4E+04	1.5E+04	2.0E+04	3.6E+03	2.3E+03	3.4E+03	3.1E+03
388	1058.9915	50.0	3.8E+04	4.1E+04	3.9E+04	3.9E+04	4.7E+03	4.7E+03	6.2E+03	5.2E+03
389	1061.0158	51.2	6.5E+04	8.4E+04	9.8E+04	8.3E+04	1.2E+04	1.4E+04	1.9E+04	1.5E+04
390	1068.9836	49.5	2.3E+04	2.6E+04	2.7E+04	2.5E+04	4.6E+03	3.8E+03	6.7E+03	5.1E+03
391	1070.9948	49.7	3.6E+04	4.5E+04	4.4E+04	4.2E+04	5.0E+03	5.1E+03	7.0E+03	5.7E+03
392	1089.0457	51.6	7.2E+04	9.4E+04	1.0E+05	9.0E+04	1.4E+04	1.7E+04	2.2E+04	1.8E+04
393	1093.5439	24.6	1.3E+04	1.9E+04	1.9E+04	1.7E+04	3.4E+03	2.1E+03	1.8E+03	2.4E+03
394	1106.8801	38.8	2.6E+04	3.1E+04	3.0E+04	2.9E+04	1.2E+02	4.8E+01	6.2E+01	7.8E+01
395	1153.0069	49.4	1.6E+04	1.8E+04	1.8E+04	1.7E+04	1.5E+03	1.2E+03	1.5E+03	1.4E+03
396	1155.0211	49.6	2.3E+04	2.8E+04	2.8E+04	2.6E+04	2.7E+03	2.1E+03	2.6E+03	2.5E+03
397	1157.0344	49.9	2.4E+04	3.1E+04	3.1E+04	2.8E+04	2.7E+03	3.0E+03	2.3E+03	2.7E+03
398	1158.2668	38.7	1.0E+05	8.1E+04	9.3E+04	9.2E+04	6.0E+03	7.9E+03	9.6E+03	7.8E+03
399	1181.0317	49.7	2.2E+04	2.6E+04	2.8E+04	2.5E+04	3.3E+03	3.7E+03	2.8E+03	3.3E+03
400	1183.0476	49.9	2.5E+04	2.8E+04	2.8E+04	2.7E+04	3.8E+03	3.9E+03	3.7E+03	3.8E+03
401	1185.0651	50.2	2.2E+04	2.6E+04	2.6E+04	2.5E+04	4.0E+03	3.6E+03	3.9E+03	3.8E+03
402	1205.0317	43.5	1.8E+04	1.5E+04	1.8E+04	1.7E+04	8.1E+02	1.6E+03	3.0E+03	1.8E+03
403	1208.0048	44.0	1.3E+05	1.1E+05	1.1E+05	1.2E+05	1.5E+04	1.8E+04	3.8E+04	2.4E+04
404	1212.0287	44.7	3.3E+05	2.5E+05	2.7E+05	2.8E+05	3.1E+04	3.4E+04	6.8E+04	4.4E+04
405	1224.0229	44.6	2.2E+04	2.0E+04	1.9E+04	2.0E+04	3.7E+03	3.3E+03	6.0E+03	4.3E+03
406	1228.6712	39.6	1.7E+04	1.2E+04	1.4E+04	1.4E+04	5.8E+02	1.2E+03	1.5E+03	1.1E+03
407	1231.9962	43.8	8.9E+04	9.2E+04	9.0E+04	9.0E+04	3.5E+03	4.1E+03	1.4E+04	7.1E+03
408	1234.0106	44.1	1.5E+05	1.6E+05	1.6E+05	1.6E+05	1.0E+04	1.1E+04	2.6E+04	1.6E+04

No.	*m/z*	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
409	1236.0261	44.3	2.2E+05	2.2E+05	2.3E+05	2.3E+05	1.3E+04	1.5E+04	3.5E+04	2.1E+04
410	1238.0424	44.8	3.1E+05	2.7E+05	3.0E+05	2.9E+05	1.9E+04	1.7E+04	4.3E+04	2.6E+04
411	1242.0644	45.3	7.0E+04	5.0E+04	8.3E+04	6.8E+04	1.1E+04	1.0E+04	1.8E+04	1.3E+04
412	1252.0519	45.0	2.0E+04	1.5E+04	1.8E+04	1.8E+04	2.4E+03	2.0E+03	3.6E+03	2.7E+03
413	1255.9951	43.7	6.6E+04	5.9E+04	5.4E+04	6.0E+04	2.1E+03	2.5E+03	5.4E+03	3.3E+03
414	1260.0226	44.3	1.4E+05	1.3E+05	1.3E+05	1.3E+05	4.1E+03	6.3E+03	1.2E+04	7.4E+03
415	1264.0575	45.0	2.2E+05	1.7E+05	1.9E+05	1.9E+05	8.7E+03	2.9E+03	1.7E+04	9.6E+03
416	1266.3738	40.0	8.5E+03	1.1E+04	1.1E+04	1.0E+04	8.1E+01	2.6E+02	1.3E+02	1.6E+02
417	1268.0776	45.4	4.6E+04	3.6E+04	4.5E+04	4.2E+04	1.7E+03	8.7E+02	9.3E+03	3.9E+03
418	1270.0929	45.6	3.0E+04	2.7E+04	3.0E+04	2.9E+04	2.2E+03	3.0E+03	8.5E+03	4.6E+03
419	1290.0624	45.1	1.2E+04	1.0E+04	1.1E+04	1.1E+04	1.9E+03	1.3E+03	1.8E+03	1.6E+03
420	1308.8166	43.6	1.7E+04	1.9E+04	1.7E+04	1.8E+04	3.2E+03	2.5E+03	1.4E+03	2.4E+03
421	1310.0108	45.8	3.0E+04	3.5E+04	3.3E+04	3.3E+04	4.7E+03	9.6E+03	5.3E+03	6.5E+03
422	1313.1763	45.5	2.0E+04	1.3E+04	1.9E+04	1.7E+04	3.4E+03	2.3E+03	4.6E+03	3.4E+03
423	1325.9027	45.8	2.5E+04	3.2E+04	3.0E+04	2.9E+04	4.1E+03	5.2E+03	4.2E+03	4.5E+03
424	1327.1596	45.2	2.7E+04	2.6E+04	2.8E+04	2.7E+04	5.6E+03	3.2E+03	5.8E+03	4.9E+03
425	1329.1735	45.3	2.5E+04	2.4E+04	2.6E+04	2.5E+04	6.4E+03	4.2E+03	7.5E+03	6.1E+03
426	1333.2595	54.6	7.1E+04	1.0E+05	1.1E+05	9.3E+04	1.3E+03	2.0E+03	1.4E+03	1.6E+03
427	1335.2722	55.3	8.8E+04	1.1E+05	1.3E+05	1.1E+05	1.7E+03	3.2E+03	3.2E+03	2.7E+03
428	1340.7524	39.0	1.3E+04	1.4E+04	1.3E+04	1.3E+04	1.1E+03	9.9E+02	1.3E+03	1.1E+03
429	1341.4247	39.0	3.5E+04	3.2E+04	3.3E+04	3.3E+04	1.0E+03	9.5E+02	1.8E+03	1.3E+03
430	1342.0085	43.5	1.4E+04	1.3E+04	1.5E+04	1.4E+04	1.7E+03	2.2E+03	3.3E+03	2.4E+03
431	1342.0888	39.0	2.0E+04	2.0E+04	2.2E+04	2.1E+04	1.5E+02	2.4E+02	1.1E+03	4.9E+02
432	1342.9225	45.8	4.0E+05	4.8E+05	5.0E+05	4.6E+05	4.3E+04	4.7E+04	3.4E+04	4.2E+04
433	1344.0244	43.6	1.8E+04	2.3E+04	2.3E+04	2.1E+04	2.1E+03	2.7E+03	5.4E+03	3.4E+03
434	1368.0255	43.5	6.3E+04	5.9E+04	6.1E+04	6.1E+04	3.0E+03	3.3E+03	7.0E+03	4.4E+03
435	1369.9486	41.8	2.4E+04	1.7E+04	2.1E+04	2.0E+04	4.1E+03	5.5E+03	2.7E+03	4.1E+03
436	1371.9645	42.2	3.5E+04	2.3E+04	2.5E+04	2.8E+04	5.3E+03	7.8E+03	5.9E+03	6.3E+03
437	1375.1170	45.8	1.6E+04	1.6E+04	1.7E+04	1.6E+04	2.4E+03	1.6E+03	2.3E+03	2.1E+03
438	1378.0096	42.9	4.1E+04	3.5E+04	3.8E+04	3.8E+04	7.6E+03	1.0E+04	9.4E+03	9.0E+03
439	1383.0704	33.5	2.4E+05	2.4E+05	2.5E+05	2.4E+05	4.2E+03	4.0E+03	5.4E+03	4.6E+03
440	1389.7816	39.7	1.8E+04	1.8E+04	2.0E+04	1.9E+04	7.5E+02	7.9E+02	1.1E+03	8.7E+02
441	1390.4462	39.7	4.8E+04	5.2E+04	5.2E+04	5.1E+04	1.4E+03	1.2E+03	1.9E+03	1.5E+03
442	1391.1129	39.7	3.3E+04	3.4E+04	3.4E+04	3.3E+04	2.8E+02	9.0E+02	1.1E+03	7.5E+02
443	1391.7875	39.7	1.1E+04	1.0E+04	1.1E+04	1.1E+04	8.8E+02	5.8E+02	9.9E+02	8.2E+02
444	1393.9483	41.5	6.1E+04	4.6E+04	4.6E+04	5.1E+04	2.6E+03	9.9E+03	4.3E+03	5.6E+03
445	1397.1113	45.8	1.1E+04	1.3E+04	1.3E+04	1.2E+04	2.5E+03	1.8E+03	1.9E+03	2.1E+03
446	1397.9810	41.9	1.9E+05	1.3E+05	1.3E+05	1.5E+05	1.6E+04	2.2E+04	1.6E+04	1.8E+04
447	1402.0094	42.4	3.5E+05	2.5E+05	2.5E+05	2.8E+05	3.3E+04	5.0E+04	3.8E+04	4.0E+04
448	1404.0240	43.1	1.9E+05	1.6E+05	1.7E+05	1.8E+05	1.8E+04	2.7E+04	2.6E+04	2.4E+04
449	1406.0409	43.0	3.4E+05	2.4E+05	2.6E+05	2.8E+05	2.7E+04	4.3E+04	4.0E+04	3.7E+04
450	1426.0107	42.3	2.8E+05	1.7E+05	1.7E+05	2.1E+05	1.3E+04	2.2E+04	1.6E+04	1.7E+04
451	1428.0265	42.5	4.3E+05	2.5E+05	2.6E+05	3.1E+05	1.9E+04	3.2E+04	2.1E+04	2.4E+04
452	1428.0231	43.1	1.3E+05	1.1E+05	1.0E+05	1.1E+05	1.2E+04	1.9E+04	2.2E+04	1.7E+04
453	1430.0408	43.0	6.9E+05	4.7E+05	5.0E+05	5.5E+05	3.4E+04	5.3E+04	4.8E+04	4.5E+04
454	1432.0543	43.2	6.6E+05	4.7E+05	5.0E+05	5.4E+05	3.3E+04	4.6E+04	4.3E+04	4.1E+04
455	1441.0230	41.9	1.3E+06	1.1E+06	9.9E+05	1.1E+06	1.9E+05	2.3E+05	1.7E+05	2.0E+05
456	1445.0153	50.5	4.0E+05	3.4E+05	3.2E+05	3.5E+05	3.9E+04	5.6E+04	9.1E+04	6.2E+04
457	1445.0552	42.6	1.4E+06	1.2E+06	1.1E+06	1.2E+06	1.9E+05	2.2E+05	2.0E+05	2.0E+05
458	1449.9774	50.2	4.2E+05	3.2E+05	3.1E+05	3.5E+05	5.2E+04	6.9E+04	1.1E+05	7.8E+04
459	1451.9893	50.3	8.7E+05	6.9E+05	6.7E+05	7.4E+05	7.8E+04	1.1E+05	1.7E+05	1.2E+05
460	1454.0007	50.6	8.2E+05	6.8E+05	6.3E+05	7.1E+05	5.6E+04	9.2E+04	1.3E+05	9.4E+04
461	1456.0536	43.2	3.3E+05	2.6E+05	2.8E+05	2.9E+05	1.6E+04	2.3E+04	1.9E+04	1.9E+04
462	1458.0727	43.3	1.7E+06	1.1E+06	1.1E+06	1.3E+06	4.4E+04	5.6E+04	5.5E+04	5.2E+04
463	1467.0395	41.8	4.4E+05	3.0E+05	2.8E+05	3.4E+05	3.1E+04	3.3E+04	3.4E+04	3.3E+04
464	1467.0005	50.1	6.9E+05	5.4E+05	5.0E+05	5.7E+05	8.3E+04	1.2E+05	1.9E+05	1.3E+05
465	1469.0144	50.4	1.6E+06	1.3E+06	1.2E+06	1.4E+06	1.4E+05	2.0E+05	3.2E+05	2.2E+05
466	1469.0525	42.5	3.3E+05	2.2E+05	2.0E+05	2.5E+05	2.7E+04	2.7E+04	1.8E+04	2.4E+04
467	1469.0524	41.6	2.7E+05	2.1E+05	2.0E+05	2.3E+05	4.3E+04	4.8E+04	3.3E+04	4.1E+04

No.	*m/z*	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
468	1471.0279	50.6	1.6E+06	1.3E+06	1.3E+06	1.4E+06	1.1E+05	1.8E+05	2.6E+05	1.8E+05
469	1471.0664	42.8	7.4E+05	5.5E+05	5.1E+05	6.0E+05	5.5E+04	6.0E+04	6.1E+04	5.9E+04
470	1473.0813	43.2	4.4E+05	3.8E+05	3.2E+05	3.8E+05	3.9E+04	3.8E+04	3.7E+04	3.8E+04
471	1475.0984	43.3	4.5E+05	3.4E+05	3.3E+05	3.8E+05	3.8E+04	4.0E+04	4.4E+04	4.0E+04
472	1480.0584	43.3	3.3E+05	2.8E+05	2.7E+05	2.9E+05	2.0E+04	2.6E+04	2.7E+04	2.4E+04
473	1499.0961	43.2	9.3E+04	9.4E+04	8.7E+04	9.1E+04	8.9E+03	8.5E+03	8.7E+03	8.7E+03
474	1500.0352	41.4	6.5E+04	7.4E+04	6.4E+04	6.8E+04	1.1E+04	9.7E+03	1.6E+04	1.2E+04

A4.3 Integrated mass ion intensity (MSII) of positive-mode ions in mycelium with decreased levels under 4% ethanol stress.

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	120.0445	38.6	0.0E+00	6.4E+01	6.5E+01	4.3E+01	1.2E+05	6.3E+04	7.4E+04	8.4E+04
2	123.1162	24.8	5.6E+03	4.1E+03	4.7E+03	4.8E+03	7.9E+04	6.9E+04	6.1E+04	7.0E+04
3	134.0448	35.2	8.6E+03	9.1E+03	9.1E+03	8.9E+03	1.0E+05	9.9E+04	7.8E+04	9.3E+04
4	136.0397	36.5	0.0E+00	4.6E+02	9.3E+02	4.6E+02	3.0E+04	1.4E+04	2.2E+04	2.2E+04
5	136.0418	35.2	8.0E+01	1.3E+02	1.6E+03	6.0E+02	1.2E+04	7.6E+03	7.9E+03	9.2E+03
6	151.0755	35.0	6.1E+04	5.8E+04	1.0E+05	7.4E+04	9.8E+05	8.7E+05	1.5E+06	1.1E+06
7	177.0947	35.0	3.1E+03	5.3E+03	1.9E+03	3.5E+03	4.1E+04	3.5E+04	5.8E+04	4.4E+04
8	191.1062	35.0	1.4E+04	1.5E+04	2.4E+04	1.7E+04	1.9E+05	1.6E+05	2.6E+05	2.0E+05
9	205.1232	34.9	7.0E+03	5.6E+03	1.5E+04	9.1E+03	1.0E+05	8.6E+04	1.5E+05	1.1E+05
10	207.1997	35.9	8.5E+02	2.8E+02	0.0E+00	3.8E+02	8.7E+03	1.2E+04	1.0E+04	1.0E+04
11	251.1987	24.8	4.3E+03	3.2E+03	3.3E+03	3.6E+03	6.8E+04	5.6E+04	5.0E+04	5.8E+04
12	268.2991	29.5	3.3E+03	3.2E+03	3.7E+03	3.4E+03	1.6E+05	1.6E+05	1.2E+05	1.5E+05
13	286.3101	29.5	5.6E+03	6.2E+03	6.8E+03	6.2E+03	3.6E+05	3.0E+05	2.6E+05	3.1E+05
14	296.3299	31.9	4.2E+03	4.1E+03	4.4E+03	4.2E+03	7.8E+04	6.0E+04	6.2E+04	6.6E+04
15	308.2913	29.5	2.1E+03	2.1E+03	1.7E+03	2.0E+03	4.3E+04	6.2E+04	5.2E+04	5.2E+04
16	314.3045	29.1	1.1E+03	7.8E+01	3.6E+01	3.9E+02	6.0E+04	8.3E+04	6.6E+04	7.0E+04
17	314.3405	31.8	2.4E+04	2.8E+04	2.9E+04	2.7E+04	2.9E+05	2.9E+05	2.7E+05	2.8E+05
18	323.1986	34.1	6.8E+03	7.3E+03	8.4E+03	7.5E+03	1.0E+05	9.0E+04	1.1E+05	9.9E+04
19	323.2435	35.8	2.4E+03	1.6E+03	4.1E+02	1.5E+03	4.4E+04	3.6E+04	4.2E+04	4.1E+04
20	342.3707	32.9	6.4E+02	1.1E+03	2.8E+02	6.9E+02	1.7E+04	2.0E+04	1.4E+04	1.7E+04
21	342.3349	31.4	8.1E+03	6.7E+03	9.5E+03	8.1E+03	9.7E+04	1.2E+05	9.1E+04	1.0E+05
22	355.2922	29.3	5.0E+03	5.1E+03	4.0E+03	4.7E+03	8.9E+04	9.6E+04	9.7E+04	9.4E+04
23	365.2449	35.0	1.2E+04	7.9E+03	1.6E+04	1.2E+04	1.3E+05	1.2E+05	2.0E+05	1.5E+05
24	381.2437	33.0	2.0E+03	3.7E+03	5.9E+03	3.9E+03	3.7E+04	4.1E+04	5.1E+04	4.3E+04
25	425.3398	34.9	1.5E+04	3.1E+04	4.2E+04	3.0E+04	4.7E+05	3.4E+05	3.1E+05	3.8E+05
26	443.3479	35.9	5.0E+04	5.3E+04	5.8E+04	5.4E+04	6.8E+05	5.7E+05	6.2E+05	6.2E+05
27	447.3250	35.1	1.9E+04	2.4E+04	2.4E+04	2.2E+04	2.7E+05	2.0E+05	1.9E+05	2.2E+05
28	460.3765	36.4	1.0E+04	1.3E+04	1.3E+04	1.2E+04	3.5E+05	2.7E+05	3.5E+05	3.2E+05
29	461.2705	28.7	2.6E+03	3.4E+03	3.4E+03	3.1E+03	3.4E+04	2.5E+04	3.2E+04	3.0E+04
30	465.3328	36.6	1.9E+05	1.9E+05	2.2E+05	2.0E+05	2.6E+06	2.1E+06	2.3E+06	2.3E+06
31	471.2695	28.7	5.7E+03	5.5E+03	7.1E+03	6.1E+03	7.1E+04	5.2E+04	6.1E+04	6.1E+04
32	475.2858	28.7	3.9E+03	5.0E+03	7.7E+03	5.5E+03	8.5E+04	7.1E+04	8.1E+04	7.9E+04
33	489.2640	28.7	2.2E+03	3.0E+03	4.5E+03	3.2E+03	5.3E+04	4.3E+04	5.2E+04	5.0E+04
34	491.2777	26.9	1.5E+03	1.7E+03	2.4E+03	1.9E+03	2.3E+04	1.9E+04	2.2E+04	2.1E+04
35	503.2773	28.7	3.6E+03	5.1E+03	6.1E+03	4.9E+03	6.1E+04	4.8E+04	5.8E+04	5.6E+04
36	514.3858	35.2	5.9E+03	6.6E+03	6.5E+03	6.4E+03	6.8E+04	6.7E+04	5.5E+04	6.3E+04
37	521.2904	28.7	5.3E+03	5.9E+03	6.3E+03	5.8E+03	1.1E+05	8.2E+04	1.0E+05	9.7E+04
38	526.3807	35.3	0.0E+00	0.0E+00	0.0E+00	0.0E+00	6.0E+04	6.5E+04	5.9E+04	6.1E+04
39	528.3997	35.3	1.0E+03	2.9E+03	3.6E+03	2.5E+03	4.3E+04	4.0E+04	3.2E+04	3.8E+04
40	582.5755	44.2	2.8E+02	0.0E+00	1.0E+03	4.4E+02	2.5E+04	1.6E+04	1.8E+04	2.0E+04
41	584.5599	43.2	3.7E+03	2.3E+03	3.7E+03	3.3E+03	1.6E+05	1.5E+05	1.4E+05	1.5E+05
42	590.4399	36.0	5.4E+03	8.7E+03	7.9E+03	7.4E+03	9.0E+04	6.6E+04	7.6E+04	7.7E+04
43	597.4095	36.7	0.0E+00	0.0E+00	2.5E+03	8.4E+02	2.8E+04	2.6E+04	2.6E+04	2.7E+04

No.	*m/z*	RT (min)	Integrated mass ion intensity (MSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
44	605.2457	28.7	1.5E+02	1.0E+02	1.5E+03	5.7E+02	1.1E+04	1.4E+04	1.7E+04	1.4E+04
45	627.1731	31.2	1.2E+02	0.0E+00	1.0E+03	3.8E+02	9.5E+03	9.8E+03	1.2E+04	1.0E+04
46	678.6712	44.7	0.0E+00	0.0E+00	2.3E+03	7.7E+02	1.1E+05	8.3E+04	6.1E+04	8.5E+04
47	695.4767	37.1	8.4E+03	5.4E+03	6.1E+03	6.6E+03	2.0E+05	1.2E+05	2.5E+05	1.9E+05
48	702.6650	46.6	0.0E+00	0.0E+00	0.0E+00	0.0E+00	2.0E+04	1.3E+04	2.4E+04	1.9E+04
49	742.5368	40.4	1.7E+04	2.1E+04	2.0E+04	1.9E+04	3.3E+05	1.9E+05	2.0E+05	2.4E+05
50	742.4472	37.0	0.0E+00	0.0E+00	0.0E+00	0.0E+00	8.2E+04	8.6E+04	3.9E+04	6.9E+04
51	751.5206	34.0	1.8E+03	2.6E+03	1.4E+03	1.9E+03	2.4E+04	1.8E+04	1.6E+04	1.9E+04
52	758.4426	35.4	0.0E+00	0.0E+00	0.0E+00	0.0E+00	4.6E+04	6.5E+04	3.0E+04	4.7E+04
53	772.6429	31.9	2.5E+03	2.0E+03	4.0E+03	2.8E+03	7.7E+04	1.0E+05	7.0E+04	8.4E+04
54	780.5542	40.6	1.1E+06	1.1E+06	1.2E+06	1.1E+06	1.9E+07	1.3E+07	1.5E+07	1.5E+07
55	818.5364	37.3	2.5E+03	2.6E+03	3.0E+03	2.7E+03	3.4E+04	2.9E+04	2.1E+04	2.8E+04
56	822.5573	38.2	3.5E+03	2.2E+03	1.4E+03	2.4E+03	3.9E+04	3.0E+04	2.9E+04	3.3E+04
57	846.4964	38.4	4.3E+02	8.3E+02	1.8E+03	1.0E+03	2.1E+05	1.6E+05	1.2E+05	1.6E+05
58	861.6343	34.0	1.8E+04	2.6E+04	3.7E+04	2.7E+04	4.6E+05	3.2E+05	2.7E+05	3.5E+05
59	868.4827	38.3	0.0E+00	1.2E+02	2.0E+02	1.1E+02	2.2E+04	1.4E+04	1.4E+04	1.7E+04
60	872.6414	45.0	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.8E+03	5.7E+03	4.3E+03	5.3E+03
61	874.5369	40.1	1.5E+03	6.0E+02	1.8E+03	1.3E+03	3.1E+04	3.4E+04	2.7E+04	3.1E+04
62	877.6628	36.7	1.3E+03	3.9E+03	2.8E+03	2.7E+03	7.5E+04	6.0E+04	5.5E+04	6.3E+04
63	879.6455	33.9	1.7E+04	1.7E+04	3.2E+04	2.2E+04	6.8E+05	5.5E+05	3.3E+05	5.2E+05
64	893.6606	36.1	1.3E+04	2.1E+04	3.7E+04	2.4E+04	6.5E+05	4.2E+05	5.3E+05	5.3E+05
65	899.6257	43.2	1.6E+03	2.1E+03	1.6E+03	1.8E+03	1.7E+05	1.4E+05	1.6E+05	1.6E+05
66	901.6417	43.8	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.2E+05	1.1E+05	1.2E+05	1.2E+05
67	902.7173	36.4	3.1E+03	2.5E+03	2.8E+03	2.8E+03	3.7E+04	3.0E+04	3.1E+04	3.3E+04
68	907.6764	36.5	1.3E+04	1.5E+04	1.8E+04	1.5E+04	7.6E+05	5.3E+05	5.8E+05	6.2E+05
69	910.6728	44.1	1.1E+04	1.0E+04	1.4E+04	1.2E+04	1.3E+05	1.2E+05	1.2E+05	1.2E+05
70	923.6660	36.5	4.2E+03	5.1E+03	5.2E+03	4.8E+03	6.9E+04	5.5E+04	5.5E+04	6.0E+04
71	923.6296	42.9	0.0E+00	0.0E+00	6.3E+01	2.1E+01	4.1E+04	6.3E+04	3.2E+04	4.5E+04
72	961.8363	49.1	8.3E+02	0.0E+00	0.0E+00	2.8E+02	1.3E+04	1.0E+04	1.2E+04	1.2E+04
73	1051.7535	35.1	0.0E+00	0.0E+00	0.0E+00	0.0E+00	3.6E+04	2.0E+04	3.8E+04	3.1E+04
74	1084.7278	45.2	3.1E+03	4.4E+03	5.9E+03	4.5E+03	8.2E+04	9.5E+04	6.2E+04	8.0E+04
75	1084.7757	35.4	4.4E+02	2.8E+02	4.0E+02	3.7E+02	5.3E+04	3.7E+04	2.8E+04	3.9E+04
76	1125.5214	30.7	1.5E+03	1.2E+03	2.6E+03	1.7E+03	3.5E+04	2.6E+04	3.1E+04	3.0E+04
77	1136.1273	43.8	4.5E+02	1.8E+02	1.7E+02	2.7E+02	5.9E+03	6.2E+03	4.8E+03	5.6E+03
78	1187.4361	31.1	5.9E+02	3.9E+02	6.6E+02	5.4E+02	8.9E+03	8.8E+03	1.2E+04	9.8E+03
79	1287.0745	43.1	8.7E+02	5.4E+02	1.1E+03	8.5E+02	8.3E+03	9.3E+03	7.8E+03	8.5E+03
80	1305.9555	35.4	0.0E+00	3.6E+02	5.2E+02	2.9E+02	1.7E+04	1.4E+04	1.8E+04	1.6E+04
81	1321.9857	36.0	7.4E+02	2.3E+03	4.0E+03	2.4E+03	6.6E+04	3.6E+04	6.1E+04	5.4E+04
82	1327.7481	39.4	9.4E+02	5.0E+02	1.4E+03	9.6E+02	1.4E+04	1.1E+04	7.1E+03	1.1E+04
83	1336.0015	36.3	4.9E+02	9.6E+02	6.2E+02	6.9E+02	4.2E+04	2.7E+04	3.4E+04	3.4E+04
84	1350.0176	36.5	3.8E+02	5.7E+02	5.2E+02	4.9E+02	5.1E+04	3.2E+04	3.7E+04	4.0E+04
85	1365.9287	47.1	1.0E+03	2.3E+03	2.9E+03	2.1E+03	1.9E+04	3.1E+04	2.1E+04	2.3E+04
86	1389.9382	46.9	6.3E+02	1.8E+02	1.1E+03	6.5E+02	1.2E+04	2.2E+04	1.7E+04	1.7E+04
87	1424.9914	40.7	1.3E+03	1.1E+03	7.6E+02	1.1E+03	1.8E+04	1.4E+04	9.8E+03	1.4E+04
88	1451.0055	40.6	3.2E+03	3.5E+03	2.6E+03	3.1E+03	6.6E+04	4.3E+04	3.5E+04	4.8E+04
89	1468.0340	40.6	3.0E+03	2.8E+03	3.0E+03	2.9E+03	4.0E+04	2.9E+04	3.2E+04	3.4E+04
90	1477.0198	40.8	6.4E+03	5.4E+03	5.6E+03	5.8E+03	8.5E+04	5.8E+04	5.2E+04	6.5E+04

A4.4 Normalized integrated mass ion intensity (nMSII) of positive-mode ions in mycelium with decreased levels under 4% ethanol stress.

No.	*m/z*	RT (min)	Normalized integrated mass ion intensity (nMSII)							
			EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
1	120.0445	38.6	0.0E+00	1.1E+02	1.1E+02	7.3E+01	8.2E+04	4.5E+04	5.2E+04	6.0E+04
2	123.1162	24.8	9.5E+03	7.0E+03	8.0E+03	8.2E+03	5.6E+04	4.9E+04	4.3E+04	4.9E+04
3	134.0448	35.2	1.5E+04	1.6E+04	1.6E+04	1.5E+04	7.1E+04	7.0E+04	5.6E+04	6.6E+04
4	136.0397	36.5	0.0E+00	7.8E+02	1.6E+03	7.9E+02	2.2E+04	1.0E+04	1.6E+04	1.6E+04
5	136.0418	35.2	1.4E+02	2.2E+02	2.7E+03	1.0E+03	8.5E+03	5.4E+03	5.6E+03	6.5E+03
6	151.0755	35.0	1.0E+05	9.9E+04	1.7E+05	1.3E+05	6.9E+05	6.2E+05	1.1E+06	8.0E+05
7	177.0947	35.0	5.4E+03	9.0E+03	3.3E+03	5.9E+03	2.9E+04	2.5E+04	4.1E+04	3.1E+04
8	191.1062	35.0	2.3E+04	2.5E+04	4.0E+04	3.0E+04	1.4E+05	1.1E+05	1.9E+05	1.4E+05
9	205.1232	34.9	1.2E+04	9.5E+03	2.5E+04	1.6E+04	7.3E+04	6.1E+04	1.1E+05	8.0E+04
10	207.1997	35.9	1.4E+03	4.8E+02	0.0E+00	6.4E+02	6.1E+03	8.2E+03	7.4E+03	7.3E+03
11	251.1987	24.8	7.4E+03	5.5E+03	5.6E+03	6.2E+03	4.8E+04	4.0E+04	3.5E+04	4.1E+04
12	268.2991	29.5	5.7E+03	5.5E+03	6.3E+03	5.8E+03	1.1E+05	1.1E+05	8.5E+04	1.0E+05
13	286.3101	29.5	9.5E+03	1.1E+04	1.2E+04	1.1E+04	2.5E+05	2.2E+05	1.8E+05	2.2E+05
14	296.3299	31.9	7.1E+03	6.9E+03	7.5E+03	7.2E+03	5.5E+04	4.2E+04	4.4E+04	4.7E+04
15	308.2913	29.5	3.6E+03	3.5E+03	2.9E+03	3.4E+03	3.0E+04	4.4E+04	3.7E+04	3.7E+04
16	314.3045	29.1	1.8E+03	1.3E+02	6.1E+01	6.6E+02	4.3E+04	5.9E+04	4.6E+04	4.9E+04
17	314.3405	31.8	4.1E+04	4.8E+04	4.9E+04	4.6E+04	2.1E+05	2.1E+05	1.9E+05	2.0E+05
18	323.1986	34.1	1.2E+04	1.2E+04	1.4E+04	1.3E+04	7.1E+04	6.4E+04	7.5E+04	7.0E+04
19	323.2435	35.8	4.1E+03	2.7E+03	7.0E+02	2.5E+03	3.1E+04	2.5E+04	3.0E+04	2.9E+04
20	342.3707	32.9	1.1E+03	2.0E+03	4.7E+02	1.2E+03	1.2E+04	1.4E+04	1.0E+04	1.2E+04
21	342.3349	31.4	1.4E+04	1.1E+04	1.6E+04	1.4E+04	6.9E+04	8.6E+04	6.4E+04	7.3E+04
22	355.2922	29.3	8.5E+03	8.7E+03	6.7E+03	8.0E+03	6.3E+04	6.8E+04	6.9E+04	6.7E+04
23	365.2449	35.0	2.1E+04	1.4E+04	2.7E+04	2.0E+04	9.6E+04	8.5E+04	1.4E+05	1.1E+05
24	381.2437	33.0	3.4E+03	6.4E+03	9.9E+03	6.6E+03	2.7E+04	2.9E+04	3.6E+04	3.1E+04
25	425.3398	34.9	2.6E+04	5.3E+04	7.2E+04	5.0E+04	3.4E+05	2.4E+05	2.2E+05	2.7E+05
26	443.3479	35.9	8.4E+04	9.1E+04	9.9E+04	9.1E+04	4.8E+05	4.1E+05	4.4E+05	4.4E+05
27	447.3250	35.1	3.2E+04	4.1E+04	4.1E+04	3.8E+04	1.9E+05	1.4E+05	1.4E+05	1.6E+05
28	460.3765	36.4	1.8E+04	2.1E+04	2.2E+04	2.0E+04	2.5E+05	1.9E+05	2.5E+05	2.3E+05
29	461.2705	28.7	4.4E+03	5.8E+03	5.9E+03	5.3E+03	2.4E+04	1.8E+04	2.2E+04	2.1E+04
30	465.3328	36.6	3.2E+05	3.2E+05	3.8E+05	3.4E+05	1.8E+06	1.5E+06	1.6E+06	1.6E+06
31	471.2695	28.7	9.7E+03	9.4E+03	1.2E+04	1.0E+04	5.0E+04	3.7E+04	4.3E+04	4.4E+04
32	475.2858	28.7	6.6E+03	8.5E+03	1.3E+04	9.4E+03	6.0E+04	5.0E+04	5.7E+04	5.6E+04
33	489.2640	28.7	3.7E+03	5.1E+03	7.6E+03	5.5E+03	3.8E+04	3.1E+04	3.7E+04	3.5E+04
34	491.2777	26.9	2.5E+03	2.9E+03	4.1E+03	3.2E+03	1.6E+04	1.3E+04	1.5E+04	1.5E+04
35	503.2773	28.7	6.1E+03	8.6E+03	1.0E+04	8.4E+03	4.4E+04	3.4E+04	4.1E+04	3.9E+04
36	514.3858	35.2	1.0E+04	1.1E+04	1.1E+04	1.1E+04	4.8E+04	4.8E+04	3.9E+04	4.5E+04
37	521.2904	28.7	8.9E+03	1.0E+04	1.1E+04	9.9E+03	7.6E+04	5.8E+04	7.1E+04	6.9E+04
38	526.3807	35.3	0.0E+00	0.0E+00	0.0E+00	0.0E+00	4.2E+04	4.6E+04	4.2E+04	4.3E+04
39	528.3997	35.3	1.8E+03	4.9E+03	6.1E+03	4.3E+03	3.1E+04	2.8E+04	2.3E+04	2.7E+04
40	582.5755	44.2	4.8E+02	0.0E+00	1.8E+03	7.5E+02	1.7E+04	1.2E+04	1.3E+04	1.4E+04
41	584.5599	43.2	6.4E+03	4.0E+03	6.3E+03	5.6E+03	1.1E+05	1.1E+05	1.0E+05	1.1E+05
42	590.4399	36.0	9.3E+03	1.5E+04	1.3E+04	1.3E+04	6.4E+04	4.7E+04	5.4E+04	5.5E+04
43	597.4095	36.7	0.0E+00	0.0E+00	4.3E+03	1.4E+03	2.0E+04	1.9E+04	1.9E+04	1.9E+04
44	605.2457	28.7	2.5E+02	1.7E+02	2.5E+03	9.8E+02	8.1E+03	9.6E+03	1.2E+04	9.9E+03
45	627.1731	31.2	2.1E+02	0.0E+00	1.7E+03	6.5E+02	6.7E+03	7.0E+03	8.4E+03	7.4E+03
46	678.6712	44.7	0.0E+00	0.0E+00	3.9E+03	1.3E+03	7.8E+04	5.9E+04	4.3E+04	6.0E+04
47	695.4767	37.1	1.4E+04	9.2E+03	1.0E+04	1.1E+04	1.4E+05	8.7E+04	1.8E+05	1.3E+05
48	702.6650	46.6	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.4E+04	8.9E+03	1.7E+04	1.3E+04
49	742.5368	40.4	2.8E+04	3.5E+04	3.3E+04	3.2E+04	2.3E+05	1.3E+05	1.4E+05	1.7E+05
50	742.4472	37.0	0.0E+00	0.0E+00	0.0E+00	0.0E+00	5.8E+04	6.1E+04	2.8E+04	4.9E+04
51	751.5206	34.0	3.1E+03	4.4E+03	2.3E+03	3.3E+03	1.7E+04	1.3E+04	1.1E+04	1.4E+04
52	758.4426	35.4	0.0E+00	0.0E+00	0.0E+00	0.0E+00	3.3E+04	4.6E+04	2.1E+04	3.3E+04
53	772.6429	31.9	4.3E+03	3.3E+03	6.8E+03	4.8E+03	5.5E+04	7.4E+04	4.9E+04	5.9E+04
54	780.5542	40.6	1.9E+06	1.8E+06	2.0E+06	1.9E+06	1.3E+07	9.3E+06	1.0E+07	1.1E+07

No.	m/z	RT	Normalized integrated mass ion intensity (nMSII)							
		(min)	EtOH-1	EtOH-2	EtOH-3	EtOH-avg	Con-1	Con-2	Con-3	Con-avg
55	818.5364	37.3	4.3E+03	4.5E+03	5.0E+03	4.6E+03	2.4E+04	2.1E+04	1.5E+04	2.0E+04
56	822.5573	38.2	6.0E+03	3.7E+03	2.4E+03	4.0E+03	2.8E+04	2.1E+04	2.0E+04	2.3E+04
57	846.4964	38.4	7.3E+02	1.4E+03	3.1E+03	1.7E+03	1.5E+05	1.1E+05	8.3E+04	1.1E+05
58	861.6343	34.0	3.1E+04	4.5E+04	6.3E+04	4.6E+04	3.2E+05	2.3E+05	1.9E+05	2.5E+05
59	868.4827	38.3	0.0E+00	2.1E+02	3.5E+02	1.9E+02	1.5E+04	1.0E+04	9.9E+03	1.2E+04
60	872.6414	45.0	0.0E+00	0.0E+00	0.0E+00	0.0E+00	4.1E+03	4.0E+03	3.1E+03	3.7E+03
61	874.5369	40.1	2.5E+03	1.0E+03	3.1E+03	2.2E+03	2.2E+04	2.4E+04	1.9E+04	2.2E+04
62	877.6628	36.7	2.3E+03	6.7E+03	4.8E+03	4.6E+03	5.3E+04	4.3E+04	3.9E+04	4.5E+04
63	879.6455	33.9	2.9E+04	2.8E+04	5.4E+04	3.7E+04	4.8E+05	3.9E+05	2.4E+05	3.7E+05
64	893.6606	36.1	2.2E+04	3.6E+04	6.2E+04	4.0E+04	4.6E+05	3.0E+05	3.7E+05	3.8E+05
65	899.6257	43.2	2.8E+03	3.6E+03	2.8E+03	3.1E+03	1.2E+05	9.8E+04	1.1E+05	1.1E+05
66	901.6417	43.8	0.0E+00	0.0E+00	0.0E+00	0.0E+00	8.7E+04	7.4E+04	8.5E+04	8.2E+04
67	902.7173	36.4	5.3E+03	4.3E+03	4.7E+03	4.8E+03	2.6E+04	2.1E+04	2.2E+04	2.3E+04
68	907.6764	36.5	2.1E+04	2.5E+04	3.0E+04	2.6E+04	5.4E+05	3.7E+05	4.1E+05	4.4E+05
69	910.6728	44.1	1.9E+04	1.8E+04	2.4E+04	2.0E+04	9.2E+04	8.8E+04	8.2E+04	8.7E+04
70	923.6660	36.5	7.1E+03	8.6E+03	8.8E+03	8.2E+03	4.9E+04	3.9E+04	3.9E+04	4.2E+04
71	923.6296	42.9	0.0E+00	0.0E+00	1.1E+02	3.6E+01	2.9E+04	4.5E+04	2.3E+04	3.2E+04
72	961.8363	49.1	1.4E+03	0.0E+00	0.0E+00	4.7E+02	9.1E+03	7.4E+03	8.6E+03	8.4E+03
73	1051.7535	35.1	0.0E+00	0.0E+00	0.0E+00	0.0E+00	2.5E+04	1.4E+04	2.7E+04	2.2E+04
74	1084.7278	45.2	5.2E+03	7.5E+03	1.0E+04	7.6E+03	5.8E+04	6.7E+04	4.4E+04	5.6E+04
75	1084.7757	35.4	7.5E+02	4.8E+02	6.9E+02	6.4E+02	3.8E+04	2.6E+04	2.0E+04	2.8E+04
76	1125.5214	30.7	2.5E+03	2.1E+03	4.3E+03	3.0E+03	2.4E+04	1.8E+04	2.2E+04	2.1E+04
77	1136.1273	43.8	7.7E+02	3.1E+02	2.9E+02	4.5E+02	4.2E+03	4.4E+03	3.4E+03	4.0E+03
78	1187.4361	31.1	1.0E+03	6.6E+02	1.1E+03	9.3E+02	6.3E+03	6.2E+03	8.4E+03	7.0E+03
79	1287.0745	43.1	1.5E+03	9.1E+02	1.9E+03	1.4E+03	5.9E+03	6.6E+03	5.5E+03	6.0E+03
80	1305.9555	35.4	0.0E+00	6.1E+02	8.9E+02	5.0E+02	1.2E+04	1.0E+04	1.3E+04	1.2E+04
81	1321.9857	36.0	1.3E+03	3.9E+03	6.8E+03	4.0E+03	4.7E+04	2.6E+04	4.3E+04	3.9E+04
82	1327.7481	39.4	1.6E+03	8.6E+02	2.5E+03	1.6E+03	1.0E+04	7.6E+03	5.0E+03	7.6E+03
83	1336.0015	36.3	8.4E+02	1.6E+03	1.0E+03	1.2E+03	3.0E+04	1.9E+04	2.4E+04	2.4E+04
84	1350.0176	36.5	6.4E+02	9.7E+02	8.8E+02	8.3E+02	3.6E+04	2.3E+04	2.6E+04	2.8E+04
85	1365.9287	47.1	1.7E+03	4.0E+03	5.0E+03	3.6E+03	1.3E+04	2.2E+04	1.5E+04	1.7E+04
86	1389.9382	46.9	1.1E+03	3.1E+02	2.0E+03	1.1E+03	8.3E+03	1.6E+04	1.2E+04	1.2E+04
87	1424.9914	40.7	2.2E+03	1.9E+03	1.3E+03	1.8E+03	1.2E+04	1.0E+04	6.9E+03	9.8E+03
88	1451.0055	40.6	5.5E+03	5.9E+03	4.4E+03	5.2E+03	4.7E+04	3.0E+04	2.5E+04	3.4E+04
89	1468.0340	40.6	5.0E+03	4.8E+03	5.0E+03	4.9E+03	2.9E+04	2.0E+04	2.3E+04	2.4E+04
90	1477.0198	40.8	1.1E+04	9.3E+03	9.6E+03	9.9E+03	6.0E+04	4.1E+04	3.7E+04	4.6E+04

VITA

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