Universidade de Aveiro
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Dissertação apresentada à Universidade de Aveiro para cumprimento dos requisitos necessários à obtenção do grau de Mestre em Biologia Marinha Aplicada, realizada sob a orientação científica da Doutora Felisa Rey Eiras, Investigadora Júnior do Departamento de Química da Universidade de Aveiro e coorientação científica do Doutor Ricardo Calado, Investigador Principal com Agregação do Departamento de Biologia da Universidade de Aveiro.

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**o júri**

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**palavras-chave** Fosfolípidos, LC-MS, Lipidómica, Produtos de origem marinha, Rastreabilidade

**resumo**

Nas últimas décadas, o polvo comum (*Octopus vulgaris*) tem-se tornado um dos cefalópodes mais importantes nas pescarias internacionais devido ao seu elevado valor comercial e gastronómico. Na cultura Mediterrânica, o polvo é um símbolo da cozinha tradicional pelo seu requintado sabor e elevado valor nutricional, nomeadamente a sua riqueza em ácidos gordos ómega-3 polinsaturados de cadeia longa. A maioria dos consumidores considera que conhecer a proveniência dos produtos do mar é de extrema importância, encorajando ao desenvolvimento de métodos de confiança para permitir rastrear a origem geográfica destes produtos de elevado valor económico. Recentemente, o uso de ferramentas lipidómicas têm aberto novas oportunidades na rastreabilidade da origem geográfica de produtos de origem marinha. Os lípidos, como principais constituintes das membranas biológicas e das reservas energéticas, refletem a composição bioquímica dos organismos, que pela sua vez é influenciada diretamente pela sua dieta e pelas condições do habitat. Este estudo pretende determinar as impressões digitais lipidómicas no músculo de *O. vulgaris* capturado ao longo da costa Ibérica Atlântica e usar estes perfis para rastrear o seu local de origem.

As amostras biológicas de *O. vulgaris* analisadas foram adquiridas em portos comercialmente relevantes para a pesca de polvo comum na costa Atlântica da Península Ibérica (Ria de Arousa, Ria de Pontevedra, Peniche, Sesimbra e Santa Luzia). Os resultados obtidos revelaram que não existem diferenças significativas nos extratos totais de lípidos analisados. Contudo, no que diz respeito ao conteúdo de fosfolípidos, as amostras de Peniche exibiram valores significativamente inferiores. A análise do lipidoma do músculo de polvo permitiu a identificação de mais de 300 espécies moleculares lipídicas e de 13 classes diferentes destes compostos, mostrando ser uma fonte rica em fosfolípidos plasmalogénios, ceramidas e ácidos gordos de cadeia longa. As ferramentas estatísticas utilizadas permitiram discriminar com sucesso as cinco localidades de origem das amostras de polvo analisadas. A maior contribuição para esta discriminação está associada a espécies moleculares minoritárias, sendo algumas delas caracterizadas por um elevado grau de insaturação na sua composição molecular. Este estudo abre novas perspetivas para o uso das análises lipidómicas como ferramenta para a rastreabilidade de produtos de origem marinha.

**keywords** LC-MS, Lipidomics, Phospholipids, Seafood, Traceability

**abstract**

In recent decades, the common octopus (*Octopus vulgaris*) has become one of the most important cephalopods in international fisheries due to its high commercial and gastronomic value. In Mediterranean culture, the octopus is a symbol of traditional cuisine for its exquisite flavor and high nutritional value, namely its richness in long-chain polyunsaturated omega-3 fatty acids. Most consumers consider that knowing the origin of seafood is extremely important, encouraging the development of reliable methods to trace the geographical origin of these highly-value products. Recently, the use of lipidomic tools has opened new opportunities in the traceability of the geographic origin of seafood products. Lipids, as the main constituents of biological membranes and energy reserves, reflect organisms' biochemical composition, which in turn is influenced by their diet and habitat conditions. This study aimed to determine the lipidomic fingerprints in the muscle of *O. vulgaris* captured along the Iberian Atlantic coast and use these profiles to determine their origin place.

Samples of *O. vulgaris* were acquired in commercially relevant ports for fishing for common octopus on the Atlantic coast of the Iberian Peninsula (Ria de Arousa, Ria de Pontevedra, Peniche, Sesimbra and Santa Luzia). The recorded results allowed to determine that there are no significant differences in total lipid extracts. However, on what concerns phospholipid content, samples from Peniche exhibited significantly lower values. The analysis of the octopus lipidome allowed the identification of more than 300 molecular lipid species and 13 different lipid classes, evidencing that this cephalopod is a rich source of plasmalogens phospholipids, ceramides and long chain polyunsaturated fatty acids. The statistical tools employed allowed to successfully discriminate all five locations. The major contribution to this discrimination is associated to minority molecular lipid species, some of which are characterized by a high degree of unsaturation in their composition. This study opens new perspectives for the use of lipidomic analyses as a tool for the traceability of seafood products.

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| **Abbreviations** | |
|---|---|
| **AGC** | Automatic gain control |
| **ARA** | Arachidonic acid |
| **CAEP** | Ceramides aminoethylphosphonates |
| **Cer** | Ceramides |
| **$CH_2Cl_2$** | Dicloromethane |
| **CPE** | Ceramides phosphoethanolamine |
| **DHA** | Docosahexaenoic acid |
| **DW** | Dry weight |
| **EFA** | Essential fatty acids |
| **EPA** | Eicosapentaenoic acid |
| **FA** | Fatty acid |
| **HexCer** | Hexosylceramides |
| **HILIC-ESI-MS/MS** | Hydrophilic interaction liquid chromatography in electrospray ionization tandem mass spectrometry |
| **HILIC-LC-MS** | Hydrophilic interaction liquid chromatography mass spectrometry |
| **IR** | Infrared |
| **IRMS** | Isotope ratio mass spectrometry |
| **LC-MS** | Liquid chromatography – mass spectrometry |
| **LPC** | Lyso phosphatidylcholine |
| **LPE** | Lyso phosphatidylethanolamine |
| **MeOH** | Methanol |
| **MS/MS** | Tandem mass spectrometry |
| **MUFA** | Monounsaturated fatty acids |
| ***N*-CH3-CAEP** | *N*-methyl-ceramides aminoethylphosphonates |
| **NIRS** | Near infrared spectroscopy |
| **PA** | Phosphatidyl acid |
| **PC** | Phosphatidylcholine |
| **PCA** | Principal Component Analysis |
| **Pe** | Peniche |
| **PE** | Phosphatidylethanolamine |

| | |
|---|---|
| **PG** | Phosphatidylglycerol |
| **PI** | Phosphatidylinositol |
| **PS** | Phosphatidylserine |
| **PUFA** | Polyunsaturated fatty acids |
| **RAr** | Ria de Arousa |
| **RP** | Ria de Pontevedra |
| **Ses** | Sesimbra |
| **SFA** | Saturated fatty acids |
| **SL** | Santa Luzia |
| **SM** | Sphingomyelin |
| **SNP** | Single-nucleotide polymorphism |
| **TEF** | Trace elements fingerprints |
| **UHPLC** | Ultra high-performance liquid chromatography |
| **XIC** | Extracted ion chromatogram |

## Introduction

In the last decades, a growing world population[1] has contributed for an increase in the resources consumed by human population[2]. From 1961 to 2016, the annual average global food fish consumption almost doubled with population growth and, per capita, it has also increased in more than 220% (Table 1)[3]. Seafood is an important resource, being a source of quality nutrients, and its production has been trying to keep-up with the growth of human population[3]. Due to the increasing demand for seafood products, aquaculture has been growing and already accounted for 46% of the fish production in 2018, contributing almost as much as the main source of fish over the centuries, the catch of wild organisms[3,4]. However, seafood production is not homogeneous for all countries, with a small part of them being responsible for most of production. Moreover, a country that has large seafood production does not necessarily means it is also a big consumer, as many are large exporters[3]. The global seafood market has increased substantially over recent decades until the point that seafood currently leads as the main traded food in the world[5,6].

Table 1. Seafood fisheries and aquaculture, their utilization and value in the market. Source: FAO 2020[3]

| | 1986-1995 | 1996-2005 | 2006-2015 | 2016 | 2017 | 2018 |
|---|---|---|---|---|---|---|
| | Average per year | | | | | |
| | (Million tones, live weight) | | | | | |
| **Production** | | | | | | |
| Capture | 86.9 | 91.4 | 89.8 | 89.6 | 93.1 | 96.4 |
| Aquaculture | 14.9 | 34.2 | 59.7 | 76.5 | 79.5 | 82.1 |
| Total world fisheries and aquaculture | 101.8 | 125.6 | 149.6 | 166.1 | 172.7 | 178.5 |
| **Utilization** | | | | | | |
| Human consumption | 71.8 | 98.5 | 129.2 | 148.2 | 152.9 | 156.4 |
| Population (billions) | 5.4 | 6.2 | 7.0 | 7.5 | 7.5 | 7.6 |
| Per capita apparent consumption (kg) | 13.4 | 15.9 | 18.4 | 19.9 | 20.3 | 20.5 |
| **Trade** | | | | | | |
| Fish exports – in quantity | 34.9 | 46.7 | 56.7 | 59.5 | 64.9 | 67.1 |
| Fish exports – in value (USD billions) | 37.0 | 59.6 | 117.1 | 142.6 | 156.0 | 164.1 |

The increased global demand for seafood has led to market globalization due to the divergence between production versus demand and its diversity for each country.

Continuous trades of seafood should be further controlled, and a higher investment in the development and improvement of traceability tools is needed to ensure and promote food security and safety standards[7,8].

Over the years, the global seafood market has been evolving to respond to increased production, as well as consumer needs[5]. Due to some food safety scandals in the past[7,9], consumers are more interested in seafood related questions like "what, where and how"[10]. Furthermore, seafood quality is associated with regulated trade, by control of seafood capture or production[11]. These concerns led to the implementation of national and international laws to control seafood trade and provide more information to consumers. The complexity of the seafood market has led to the need of improving multiple steps of the trade chain: transport and storage between producers and consumers, in order to maintain the food quality, has been safeguarded by evolution of preservation technologies; advances in logistics not only prevented information loss but also aimed to foster a more complex and informative labelling process[4,7]. These improvements were important to assure an increase in food security and product traceability in the seafood market.

Traceability is defined by the Codex Alimentarius Commission as "the ability to follow the movement of a food through specified stage(s) of production, processing, and distribution"[12]. Seafood traceability is not only a need to increase market credibility[4], but also encompasses several indirect benefits to products in the eyes of consumer. Geographic origin is frequently associated with the quality of certain products by the consumers, which influences on the valorization of those same products[13,14]. Globalization of seafood market allowed a better distribution of products around the world, with local specific products to be available in the global market[6]. However, it has a cost by increasing the difficulty of tracking those products, which is a problem, especially when a product is contaminated or damaged[15]. An effective and validated traceability system is essential to address possible future food alerts and a breakthrough in the fight against seafood fraud due to misleading information provided by fishermen, producers and traders[7]. False reports modify species names, geographical origin, and production method[16]. Furthermore, due to the increase in consumers attention to environmental problems, more information regarding production method (wild or farmed) and how they are managed is required[7,8]. A system providing information at these levels, needs reliable traceability tools to obtain origin certification of seafood products.

Traceability tools have been in development to authenticate geographic origins from the diverse seafood products to increase food security, decrease fraud and resource sustainability[17]. These tools screen for intrinsic differences of seafood products that can be used to detect different productions method such as wild or farmed products, and differences between them[17]. Trace element fingerprints (TEF) is one of the methods that is being studied to allow the discrimination of geographical origins of seafood products[7]. Due to the influence of the surrounding environment in the growth of marine species, unique biogeochemical signatures can be associated with specific geographic origins, thus allowing to discriminate of samples from different locations[18]. Positive results have been already published using this method, with the discrimination of harvesting locations achieved by several authors with a high degree of accuracy[15,18,19]. In the blue mussel (*Mytilus edulis*), this method allowed to discriminate four harvesting locations, with two being only 6 km apart[18]. A successful discrimination of sampling locations was also been achieved for king scallops (*Pecten maximus*) using TEF[19]. In Ria de Aveiro, TEF analysis allowed to discriminate the origin of cockles (*Cerastoderma edule*) from 5 different locations within this ecosystem[15]. Another method employed for traceability of seafood origin is isotope ratio mass spectrometry (IRMS), which measures isotopic signatures to gain insights into samples origin[20]. As previously stated, environmental conditions and food availability influence marine species growth and then the isotope ratios present in their biomass[21]. Zhang et al.[20] were able to discriminate the origin and species of three different scallops (*Patinopecten yessoensis*, *Chlamys farreri* and *Argopecten irradians*) along the coastal area of China using IRMS. Croaker (*Micropogonias furnieri*) caught in two distinct regions in the Brazilian coast were also successfully discriminated using this same method[21]. A study by Carrera & Gallardo[22] successfully discriminated the geographic origin of all commercial fish species within family Merlucciidae using IRMS. Genetic analyses are also a possible method to confirm the geographic origin of seafood products[23,24], however it is more associated with species authentication rather than discriminating their origin[16,25,26]. A study using single-nucleotide polymorphism (SNP) markers was able to discriminate different European hake populations (*Merluccius merluccius*) between the Eastern Atlantic Ocean and the Mediterranean Sea[24]. Other studies have also provided positive results in the discrimination of geographic origins of marine species using SNP data[23,27]. Near infrared spectroscopy (NIRS) is a vibrational

spectroscopy technique and is capable to authenticate species and trace their local of origin[28]. This method has been growing in attention by being fast, easy, cheap, and non-destructive of major components of the products being screened[28–30]. The infrared (IR) spectra is the combination of several interactions between the IR and the molecules such as water, proteins, carbohydrate and fat, and its spectra is located between the 700-2500 nm[28–30]. This method has been successfully used to discriminate European sea bass (*Dicentrarchus labrax*) originating from different locations within the Mediterranean Sea[29], with Varrà et al.[30] using NIRS to track the origin of salt ripened anchovies, whose raw product originated from four different harvesting locations.

Fatty acid (FA) and lipid analyses have been successfully used to discriminate the geographic origin of several seafood products in recent studies[31–33]. Lipids play diverse roles in cells and can be divided in two major sub-classes: neutral lipids and polar lipids[34]. Neutral lipids, mainly triacylglycerols and sterol, play a relevant role as energy source, to maintain the integrity and fluidity of cell membranes and as precursor for several biomolecules[35,36]. Main polar lipids include phospholipids, glycolipids and sphingolipids, with these being important components of cell membranes, safeguarding their fluidity through their composition and structure[34]. Furthermore, polar lipids are also key precursors in cell signaling pathways, play a role in immunological processes and display several other key functions in cells[37]. Lipids are increasingly being used for the discrimination of seafood geographic origin due to the adaptation that these biomolecules display to different environments experienced by marine organisms[32,38,39]. Indeed, the environmental conditions prevailing in different habitats influence cell membranes, as a consequence of physiological adaptations of organism to different environments[40]. As previously stated, polar lipids play an important structural role in cell membranes, so the composition and structure of these lipids will be modified according to the different environmental conditions that the organism is exposed to[37]. In addition, FA profiles and lipid composition will also be affected by the dietary regime, which can vary with habitat and ecosystem[7,41]. These characteristics of polar lipids make them a good choice as a tool to trace the geographic origin of seafood. Ricardo et al[31] studied the FA profile of the adductor muscle of common cockles (*Cerastoderma edule*) to trace their local of origin. The study, which included organisms from eight different locations, showed that the FA profile was able to discriminate the sampling locations with 100% success. The work of Arechavala-Lopez et

al.[33] with the common octopus (*Octopus vulgaris*) represents another success in the use of FA analysis to associate samples to their respective local of origin. Regarding lipidomic analysis, the pioneering works of da Costa et al.[32] with sea lettuce (*Ulva* spp.) and Monteiro et al.[38] with sugar kelp (*Saccharina latissimi*) are good examples on how lipidomic signatures can be successfully used in the discrimination of harvesting locations of seafood products.

To date, there are already a considerable number of techniques that have successfully traced the geographic origin of seafood products. With the continuous study to improve these techniques and the discover of new methodological approaches, the traceability of seafood products will likely experience additional breakthroughs. It is important to state that, due to the complexity of present day seafood trade chains, which involve several countries over the world targeting a single species, the development of international projects will improve traceability more rapidly than local approaches[42].

The common octopus (*O. vulgaris*) is one of the most important cephalopod species worldwide due to its high commercial and gastronomic value[33]. This species occurs along the Mediterranean Sea and the Eastern Atlantic, mainly in the Iberian Peninsula and Northwest of Africa[43]. The main habitats of this species are located on the continental shelf, mainly within the first 100 m, occupying different types of ocean bottoms, such as rocks, sand, mud and seagrass[44–46]. Due to their palatability and richness in polyunsaturated *n*-3 FA, such as docosahexaenoic acid (DHA) and eicosapentaenoic acid (EPA), the common octopus has become a highly halieutic resource, with increasing market value[33]. In the Iberian Peninsula, the common octopus is one of the most important fishing resources, with thousands of people involved in its fisheries[47]. In the last decades, there was an increase in the landings of cephalopods, with the common octopus being one of the main organisms captured in the coastal waters of Galicia (Spain) and mainland Portugal (namely in its southern coast)[48]. However, in recent years, the *O. vulgaris* has also become a more limited resource with lower catches each year, which could be due to the overfishing practiced during the last decades[45]. With an increasing demand for this seafood, but a lower availability of this valuable resource, this species currently holds an even higher economic value[3]. Following its market value and high demand, a huge investment has been made to develop the aquaculture of this cephalopod species[45]. Due to the biological features of the common octopus, such as short life cycle (12-18 months),

rapid development and great food conversions, it is considered a good candidate species for aquaculture[45,49]. In Galicia (NW Spain), there has already been some level of success in the aquaculture of *O. vulgaris*, although the dependence on natural foods, or ranching of wild juveniles, still hampers its economic viability[50,51]. One of the main difficult of the aquaculture of *O. vulgaris* is associated with the high paralarvae mortality due to possibly nutritional problems and inadequate environmental conditions[52–54]. Another problem is associated with the use of natural feeds, which may represent 60% of total production cost[55]. Several studies have shown the importance of crustaceans in the diet of the common octopus, with either a mono-diet of or a mixed-diet mainly based on these marine invertebrates, being paramount to achieve suitable growth and survival rates[56–58]. However, when considering a natural diet, the fluctuation of market price and availability is a step back to make the aquaculture of this species commercially viable[59]. The development of an artificial feed which can fulfil the nutritional needs of the common octopus, holds great potential, along with the simultaneous use of discard fishery products to reduce feeding costs[55,60,61]. Further studies on these topics are crucial to develop a technically and commercially feasible aquacultures of *O. vulgaris.*

*Octopus vulgaris* is a highly versatile feeder and a generalist predator, whose diet is dependent on available preys. A wide range of species, from bivalves to crustaceans, have been identified in the diet of the common octopus, as well as finfish and polychaetes, with the occurrence of cannibalism and autophagy also being commonly recorded[62]. Factors such as seasonal and geographical differences are also influencers in its diet[63]. This versatility of common octopus' dietary regimes can be crucial to discriminate its geographic origin. In aquaculture, several diets have been administered to specimens of the common octopus and, given the fact that natural diets can change in different aquaculture stations, traceability tools might be able to discriminate wild specimens from those produced in aquaculture, as already performed for other domesticated seafood species[64–67].
The present study aimed to evaluate the potential use of lipidomic fingerprints as a biochemical tool to pinpoint the geographic origin of common octopus captured and landed along the Iberian Atlantic coast. In order to do so, the characterization of the polar lipidome of the muscle of *O. vulgaris* was performed for the first time. The development of this tool is extremely important to control the fisheries of the common octopus in the

Iberian Atlantic coast, and a further step towards the eradication of misleading information in the sale of these valuable seafood products to consumers.

## Materials and Methods

### Sampling

Samples of *O. vulgaris* were sourced from fishermen operating in five different areas along the Atlantic coast of Galicia (Spain) [Ria de Arousa (RAr) and Ria de Pontevedra (RP)] and Portugal [Sesimbra (Ses), Peniche (Pe) and Santa Luzia (SL)] (Figure 1), in the summer of 2018. A total of 10 common octopus were sourced per location, with specimens being transported in coolers to the laboratory immediately after being landed in the different fishing harbors. The fourth right arm counted from the sagittal plane, front to back, was cut (Figure 2) and stored at -80 ºC. Samples were subsequently freeze-dried and stored at -80 ºC for further analysis.

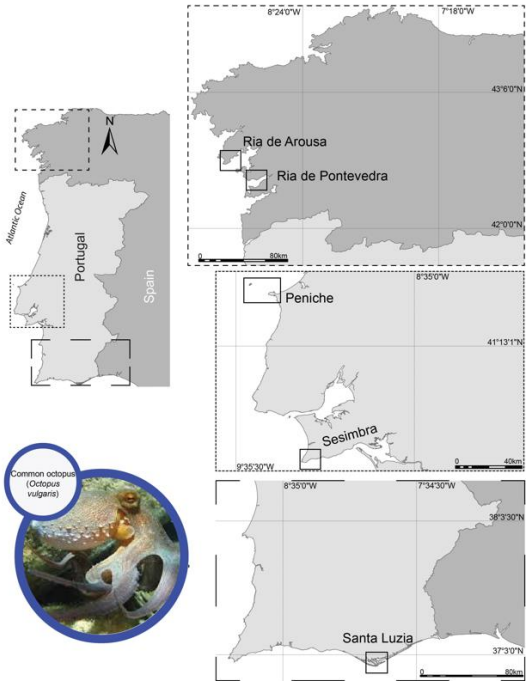



**Figure 1.** Sampling areas of *Octopus vulgaris* specimens along the Atlantic coast of the Iberian Peninsula: Ria de Arousa, Ria de Pontevedra, Peniche, Sesimbra and Santa Luzia.

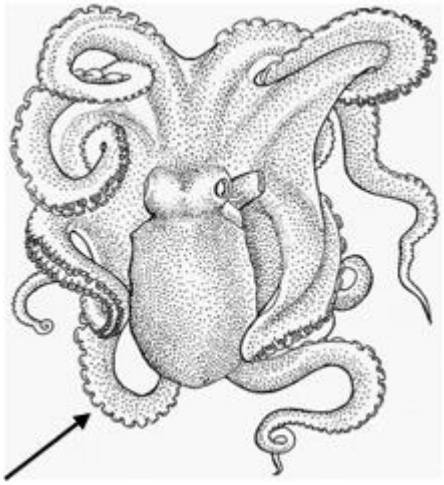


**Figure 2.** Fourth arm of *Octopus vulgaris* sampled in the present study. Source: FAO[68]

### Lipid extraction

Total lipids from *O. vulgaris* samples were extracted using the Bligh and Dyer protocol[69]. Freeze-dried samples were homogenized using a mortar grinder (RM 200,

Retsch, Hann, Germany) followed by another freeze-drying process. A biomass amount of approximately 50 mg of *O. vulgaris* was mixed with 2.5 mL of methanol (MeOH) and 1.25 mL of dichloromethane ($CH_2Cl_2$) in a glass centrifuge tube identified as tube 1, followed by homogenization through vortex and sonication for 1 min and incubation on ice on a rocking platform shaker (Stuart Scientific STR6, Bibby, UK) for 30 min. Samples were centrifugated at 2000 rpm for 10 min at room temperature (UNIVERSAL 320 R). Organic (lower) phase (3 mL) containing lipids was collected in a tube, identified as tube 2. The biomass residue (tube 1) was re-extracted with 2.5 mL of MeOH and 1.25 mL of $CH_2Cl_2$ followed by homogenization through vortex for 1 min and centrifugation at 2000 rpm for 10 min. Organic phase (3.5 mL) was collected in a tube, identified as tube 3. A volume of 1.25 mL of $CH_2Cl_2$ and 1.25 mL of Mili Q water was added to the organic phases (tube 2 and tube 3) followed by vortex and centrifugation for 10 min at 2000 rpm, promoting phase separation. The organic phase containing lipids (3.5mL) was collected in a new tube (tube 4). The aqueous (upper) phase of tube 2 was re-extracted with 1.88 mL of $CH_2Cl_2$ followed by vortex and centrifugation by 10 min at 2000 rpm, and the organic phase (1.5 mL) was transferred to tube 4. Total lipid extract (tube 4) was dried using a speed vacuum (UNIVAPO-100H coupled with UNIJET II refrigerated aspirator) and transferred to dark vials previously dried and weight by adding 0.3 mL of $CH_2Cl_2$, repeating the process twice, to recover total lipid extract. Lipid extracts were stored at -20 ºC prior to analysis by liquid chromatography – mass spectrometry (LC-MS). Total lipid content was estimated by gravimetry, with the amount of lipid by biomass dry weight (µg $mg^{-1}$ DW) also being calculated.

**Phospholipid quantification**

Quantification of phospholipids in total lipid extracts was performed through the phosphorus assay[70]. A total of 10 µL of each sample lipid extract was added to glass tubes and dried under a nitrogen stream. Then, 125 µL of 70% perchloric acid was added followed by incubation at 180 ºC for 60 min in a heating block (Block Heater SBH200D/3, Stuart, Bibby Scientific Ltd., Stone, UK). After cooling at room temperature, 825 µL of MiliQ water, 125 µL of 2.5% aqueous solution of ammonium molybdate ($NaMoO_4 \cdot H_2O$) and 125 µL of 10% ascorbic acid were added to the samples, with homogenization being performed using a vortex mixer between the addiction of each reagent. Standards were prepared using 0.1 to 2 µg of phosphate (standard solution of $NaH_2PO_4 \cdot 2H_2O$ [100 µg $mL^{-}$

[1]) to prepare a standard curve of phosphate and followed the same treatment as the samples. Both samples and standards were incubated at 100 ºC in a water bath (Precisterm, JP Selecta S.A., Barcelona, Spain) for 10 min, followed by cooling in cold water. The absorbance of samples and standards was measured at 797 nm using a microplate ultraviolet-visible spectrophotometer (Multiskan GO, Thermo Scientific, Hudson, NH, USA).

Phospholipid amount was estimated by multiplying the phosphorus amount of each sample by 25, the conversion factor between phosphorus and phospholipids.

**Hydrophilic interaction liquid chromatography mass spectrometry**

Lipid extracts were analyzed by hydrophilic interaction liquid chromatography mass spectrometry (HILIC-LC-MS) on an Ultimate 3000 Dionex ultra high-performance liquid chromatography (UHPLC) system (Thermo Fisher Scientific, Bremen, Germany) with an autosampler coupled online to a Q-Exactive mass spectrometer with Orbitrap ® technology (Thermo Fisher, Scientific, Bremen, Germany). A two-mobile phase solvent system was used to perform the analysis: a mobile phase A consisting of a mix of water, acetonitrile, and methanol (25/50/25, by volume) and a mobile phase B consisting of acetonitrile and methanol (60/40, by volume), with both phases presenting 5 mM ammonium acetate. To perform the analysis of each sample by HILIC-LC-MS, 75 µL of the starting eluent (95/5 B/A, by volume), 4 µL of each phospholipid standard (Cer – 0.04 µg, PA – 0.08 µg, PG – 0.012 µg, LPC - 0.02 µg, PE – 0.02 µg), and 5 µg of phospholipids from each sample were diluted in $CH_2Cl_2$ (1 µg $\mu L^{-1}$) and introduced into an ACE HILIC-N microbore column (100 mm x 1.0 mm x 3 µm) at a flow rate of 50 µL $min^{-1}$ and a temperature of 35 ºC. Initially, 5% of mobile phase A was held isocratically for 2 min, followed by a linear increase to 70% of mobile phase A within 11 min and a new linear increase to 90% within 7 min, maintained for a period of 30 min, and returning to the initial conditions in 5 min, being held for an additional 5 min.

The mass spectrometer employed was operated using a positive/negative switching toggles between positive (electrospray voltage 3.0 kV) and negative (electrospray voltage -2.7 kV) ion modes with a capillary temperature of 250 °C and a sheath gas flow of 15 U. In MS experiments, a high resolution of 70,000 was used, as well as an automatic gain control (AGC) target of 1 x $10^6$. In tandem mass spectrometry (MS/MS) experiments, a resolution

of 17,500 and AGC target of $1x10^5$ were used and cycles consisted of one full-scan mass spectrum and 10 data-dependent MS/MS scans were repeated continuously throughout the experiments with the dynamic exclusion of 60 s and an intensity threshold of $2 \times 10^4$. Normalized collision energy™ (CE) ranged between 25, 30 and 35 eV. Data acquisition was performed using the Xcalibur data system (V3.3, Thermo Fisher Scientific, USA). The molecular identification of lipid species was performed using LC-MS typical retention time and accurate mass measurements (≤ 5 ppm) to confirm the elemental composition. The interpretation of liquid chromatography-tandem mass spectrometry spectra was used as a confirmation method by identifying the polar head group and the fatty acyl chains of the molecular species (see Supplementary Figures S1-S11 for fragmentation interpretation). The quantification of polar lipids molecular species was performed in the bioinformatic tool MZmine 2.53[71]. The MS raw data were pre-processed by filtering and smoothing, peak detection, peak processing, and assignment against an in-house lipid database. The previous features assured the exclusion of peaks with raw intensity lower than $1.0^4$, with a mass tolerance of 5 ppm also being used. Integrated peak area values from lipid species were exported using the comma separated values (.csv) format, with data being normalized by dividing the values of each molecular species of each lipid class with that of the internal standard selected for each class. The normalization of the lipid classes phosphatidylinositol (PI) and phosphatidylglycerol (PG) was performed with the internal standard PG; lipid classes lyso phosphatidylethanolamine (LPE), sphingomyelin (SM) and lyso phosphatidylcholine (LPC) with internal standard LPC; internal standard phosphatidylethanolamine (PE) was used to normalize the lipid classes phosphatidylserine (PS), phosphatidylcholine (PC) and PE; lipid classes Ceramides (Cer) and Hexosylceramides (HexCer) by the internal standard Cer.

**Statistical Analysis**

Normalized data was resampled independently by bootstrap, increasing the 10 original samples to 30 simulated samples, with the goal to enhance data robustness, at a 95% confidence interval. Resampling data were then processed using Metaboanalyst 4.0[72]. Data filtering was performed to remove variables that evidenced a low repeatability by relative standard deviation (RSD=SD/mean) followed by glog transformation and auto scaling. Hierarchical clustering dendrogram followed by principal component analysis (PCA) were performed to assess the clustering of the five sampling locations being studied.

Hierarchical clustering heatmap was performed using Euclidean distances and the Ward clustering algorithm to better understand the significance of the variables in the separation of different landing locations. The top 25 molecular species were ranked using p-values from ANOVA tests. ANOVA were performed to compare the normalized values of the top 25 molecular species that contributed the most for the separation of common octopus' geographic origins, as well as to assess significant differences in the content of lipids (µg $mg^{-1}$ DW) and phospholipids (% of total lipids) between landing sites. Shapiro-Wilks and Bartlett's tests were performed to evaluate ANOVA assumptions of normality and homogeneity of variance, respectively. Kruskal-Wallis test were performed when ANOVA assumptions were not met. All statistical analyses were performed using the GraphPad Prism 8.0.2 software.

**Results**

Total lipid content (Table 2) of *O. vulgaris* revealed that Pe and SL were the landing locations that presented the highest and the lowest lipid contents with 45.86 ± 7.47 and 40.40 ± 7.53 µg $mg^{-1}$ DW, respectively. However, no significant differences were found between common octopus samples originating from different locations. Phospholipid quantification (Table 2), expressed as percentage of total lipids, showed significant differences between Pe and the other sites, with Pe recording the lowest value at 36.98% ± 4.59 and Ses the highest at 57.17% ± 12.21.

Table 2. Total lipid content and phospholipid amount in the muscle of *Octopus vulgaris* captured and landed in five different locations along the Iberian Atlantic coast. Abbreviations: Pe, Peniche; RAr, Ria Arousa; RP, Ria Pontevedra; Ses, Sesimbra; SL, Santa Luzia.

| Sampling sites | Lipid (µg $mg^{-1}$ DW) | Phospholipids (% of total lipids) |
|---|---|---|
| **Pe** | 45.86 ± 7.47 | 36.98 ± 4.59[a] |
| **RAr** | 41.53 ± 4.29 | 50.61 ± 10.79[b] |
| **RP** | 42.52 ± 5.64 | 54.30 ± 6.18[b] |
| **Ses** | 44.20 ± 6.57 | 57.17 ± 12.21[b] |
| **SL** | 40.40 ± 7.53 | 53.46 ± 5.34[b] |

The lipidomic profile of the muscle of *O. vulgaris* originating from five different locations analyzed by HILIC-LC-MS and MS/MS allowed to identify 13 polar lipid classes: PE, LPE, PC, LPC, ceramides aminoethylphosphonates (CAEP), PI, PS, Cer, SM, ceramides phosphoethanolamine (CPE), *N*-methyl ceramides aminoethylphosphonates (*N*-$CH_3$-CAEP), PG and HexCer. Supplementary Figure S1-11 show the hydrophilic interaction liquid chromatography in electrospray ionization tandem mass spectrometry (HILIC-ESI-MS/MS) spectra of each lipid class identified in the muscle of *O. vulgaris*. A total of 395 molecular species were identified (Supplementary Table S1), of which 105 corresponded to plasmanyl (O) and/or plasmenyl (P) species of the classes PE, LPE, PC, LPC, PI, PS and PG (Table 3.). The quantification of polar lipids was performed in 10 polar lipid classes (except CAEP, CPE and *N*-$CH_3$-CAEP) with a total of 328 molecular species. Twenty-one molecular species (twelve PC, three PE, two PI, two PS and two LPE) were not considered for statistical analysis due to the presence of odd FA in their fatty acyl composition, likely associated with common octopus' microbiome and not its muscle. The mean relative abundance of each molecular species by sampling location is represented in supplementary Table S2.

PE and PC were the lipid classes with the highest number of identified molecular species, as represented in Table 3, with the highest relative abundance recorded by the molecular species PE (O-38:6) and/or PE (P-38:5), and PC (38:6), corresponding to $[M+H]^+$ ions at *m/z* 750.5 and 806.7, respectively. LPE and LPC were also identified, although there was no dominant molecular species in LPE profile, but rather several with close relative abundances. Molecular species LPC (22:6) and LPC (20:5), corresponding to $[M+H]^+$ ions at *m/z* 568.3 and 542.3, respectively, showed the highest relative abundances. PI and PS showed the prevalence of the molecular species PI (38:5) and PS (38:5), corresponding to $[M-H]^-$ ions at *m/z* 883.5 and 808.5, respectively. Concerning PG, the molecular species PG (34:1) corresponding to $[M-H]^-$ ion at *m/z* 747.5 displayed the highest abundance in common octopus originating from all locations. SM, Cer and HexCer were also identified, with SM (d32:1), Cer (d30:1) and Cer (d32:1), and HexCer (38:2) molecular species, corresponding to $[M+H]^+$ ions at *m/z* 675.5, 482.5, 510.5 and 754.6, respectively, presenting the highest relative abundances. In the lipid classes CAEP, CPE and *N*-methyl-CAEP, all presenting a sphingoid base, were identified a total of 46 molecular species, with CAEP being the most well-represented ceramide lipid class, with 33 molecular species.

Plasmanyl and/or plasmenyl molecular species corresponded to more than 25% of the total molecular species identified. PC and PE displayed the highest number of these molecular species, but ether phospholipids were also identified in the lyso forms of these phospholipid classes (i.e. LPC and LPE) as well as in PG, PI, PS (Table 3).

The analysis of MS/MS spectra allowed to confirm the identification of the polar head group of all lipid classes and, in most cases FA composition of the different molecular lipid species was elucidated (Supplementary Table S1). Saturated FA (SFA), monounsaturated FA (MUFA) and polyunsaturated FA (PUFA) were identified in the molecular species described above. Molecular species with the highest relative abundance in the lipid classes PE and PC were characterized by the presence of DHA (22:6 *n*-3), EPA (20:5 *n*-3) and arachidonic acid (20:4 *n*-6, ARA) in their fatty acyl composition, as well as in PS and PI. Palmitic acid (16:0), stearic acid (18:0) and oleic acid (18:1) were the main SFA and MUFA identified in the most abundant molecular species within each class. SFA and MUFA were the main FA classes in the fatty acyl composition of CAEP, CPE and *N*-methyl-CAEP. Additionally, odd FA were also identified in these lipid classes.

Table 3. Lipid classes, total molecular species and specific plasmanyl and/or plasmenyl molecular species identified in the muscle of *Octopus vulgaris* captured and landed in five different locations along the Iberian Atlantic coast.

| Lipid classes | Total molecular species | Plasmanyl and/or Plasmenyl molecular species |
|---|---|---|
| **PE** | 95 | 43 |
| **LPE** | 26 | 5 |
| **PC** | 102 | 36 |
| **LPC** | 27 | 8 |
| **CAEP** | 33 | 0 |
| **PI** | 33 | 7 |
| **PS** | 31 | 5 |
| **Cer** | 15 | 0 |
| **SM** | 14 | 0 |
| **CPE** | 8 | 0 |
| ***N*-CH$_3$-CAEP** | 5 | 0 |
| **PG** | 4 | 1 |
| **HexCer** | 2 | 0 |
| **Total** | 395 | 105 |

In this study, all chromatographic peaks corresponding to the 328 identified ions were integrated, in all samples, and their confirmation was performed manually. These quantitative data, normalized by the internal standard, were used for statistical analysis.

The PCA plot was performed using the normalized extracted ion chromatograms (XIC) areas of the 328 lipid species identified (Figure 3), with the clustering of samples originating from different locations being well evidenced. The eigenvalues of the two principal components represented 61.7%. The PC1 axis explained 49.9% of variability and allows a visual separation of the locations in three distinct groups: RAr, RP/Pe and Ses/SL. Concerning PC2 axis, it explained 11.8% of the variability recorded and it allowed a clearer dissociation between Ses and SL, along with some level of separation between Pe and RP. These results are supported by the hierarchical clustering dendrogram (Supplementary Figure 12) using the normalized areas of total lipid species, showing a first separation between the samples of RAr and the samples from other sampling sites. Additionally, it also allows a second separation between Pe/RP and Ses/SL. Both groups were separated in a next level of separation. A heatmap was calculated using the top 25 lipid species that contributed the most for capture/landing site discrimination (Figure 4), identifying four PS, five PI, fourteen PC, one LPC and one PE. Table 4 displays the top 25 lipid species and their molecular composition (which was determined whenever possible), by interpretation of MS/MS spectra.

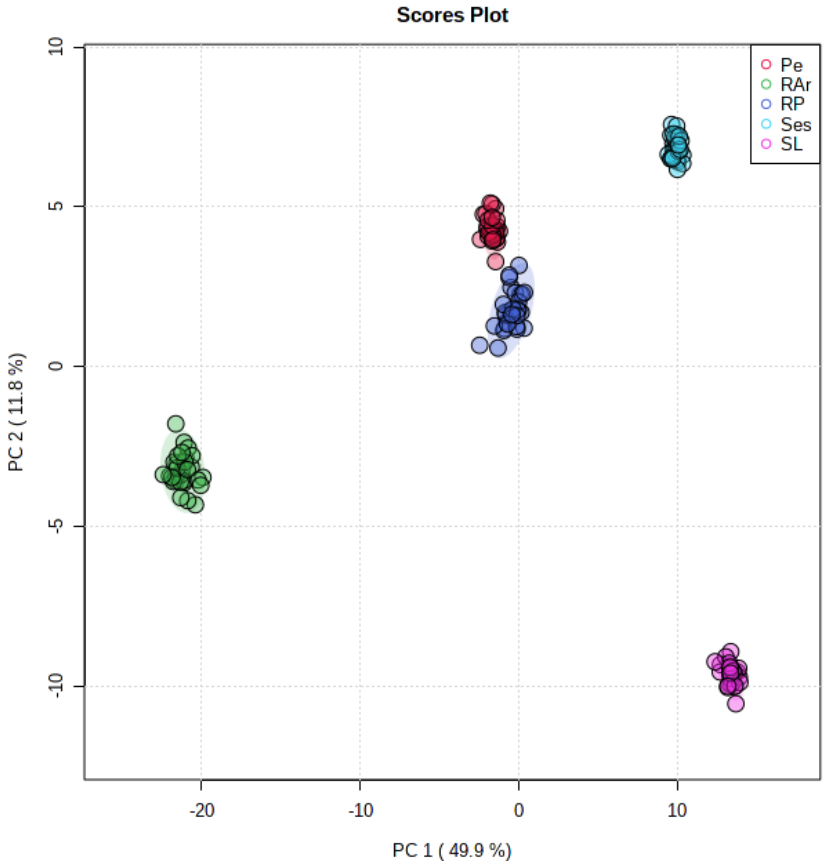



Figure 3. Principal component analyses (PCA) score plot using normalized areas from 328 lipid molecular species identified in the muscle of *Octopus vulgaris* samples captured and landed in five different locations along the Iberian Atlantic coast. Abbreviations: Pe, Peniche; RAr, Ria Arousa; RP, Ria Pontevedra; Ses, Sesimbra; SL, Santa Luzia.

Boxplots of the top 25 molecular species ranked by the lowest p-value using ANOVA test show that, in general, molecular species from RAr samples present a higher relative abundance than the other four locations, while Pe, RP, Ses and SL exhibited a closer relative abundance between them (Figure 5).

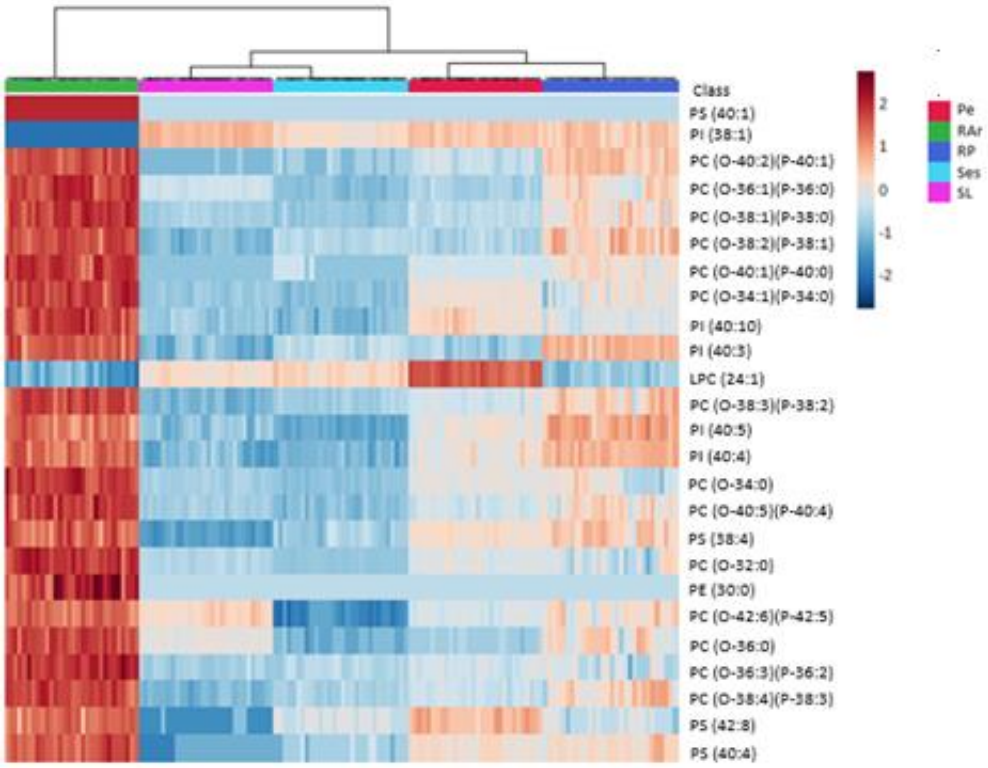



Figure 4. Hierarchical clustering heatmap of the top 25 lipid species sorted by analysis of variance test displaying the lowest p-values. The dendrogram at the top represents the clustering of the sample groups. Relative abundance levels are indicated on the colour scale, with numbers indicating fold differences from the mean. Abbreviations: Peniche (Pe), Ria de Arousa (RAr), Ria de Pontevedra (RP), Sesimbra (Ses), Santa Luzia (SL). Labels of lipid species are according to the notation: AAA (C:N), (AAA, lipid class; C, total carbon atoms; N, total double bonds of fatty acid substituents) and AAA (O-C:N)(P-C:N), correspond to O- plasmanyl and/or P- plasmenyl, respectively).

Table 4. Top 25 lipid species sorted by analysis of variance test displaying the lowest p-values. Labels of lipid species are according to the notation: AAA (C:N), (AAA, lipid class; C, total carbon atoms; N, total double bonds of fatty acid substituents) and AAA (O-C:N)(P-C:N), correspond to O- plasmanyl and/or P- plasmenyl, respectively). Molecular species identified by retention time, mass accuracy calculation and typical ion product are marked with (*) and molecular species identified only by retention time and mass accuracy calculation are marked with (**).

| ***m/z* observed** | **Ion** | **Lipid species (C:N)** | **Fatty acyl chain** |
|---|---|---|---|
| 796.62 | $[M+H]^+$ | PC(O-38:4)(P-38:3) * | |
| 838.56 | $[M-H]^-$ | PS(40:4) ** | |
| 858.53 | $[M-H]^-$ | PS(42:8) ** | |
| 770.61 | $[M+H]^+$ | PC(O-36:3) | O-16:0/20:3 |
| 776.65 | $[M+H]^+$ | PC (O-36:0) * | |
| 848.65 | $[M+H]^+$ | PC(O-42:6)(P-42:5) * | O-18:0/24:6; O-18:1/24:5; P-18:0/24:5 |
| 664.49 | $[M+H]^+$ | PE(30:0) * | |
| 720.59 | $[M+H]^+$ | PC(O-32:0) | 16:0/16:0 |
| 810.53 | $[M-H]^-$ | PS(38:4) | 18:0/20:4; 16:0/22:4 |
| 822.63 | $[M+H]^+$ | PC(O-40:5) | O-18:0/22:5 |
| 748.62 | $[M+H]^+$ | PC(O-34:0)* | |
| 911.56 | $[M-H]^-$ | PI(40:5)** | |
| 913.58 | $[M-H]^-$ | PI(40:4) | 18:0/22:4 |
| 798.63 | $[M+H]^+$ | PC(O-38:3)(P-38:2) | O-18:0/20:3; O-16:1/22:2; P-16:0/22:2; P-18:0/20:2 |
| 606.45 | $[M+H]^+$ | LPC(24:1)* | |
| 915.59 | $[M-H]^-$ | PI(40:3) | 20:2/20:1 |
| 901.49 | $[M-H]^-$ | PI(40:10) | 20:5/20:5 |
| 891.60 | $[M-H]^-$ | PI(38:1) | 18:0/20:1 |
| 844.60 | $[M-H]^-$ | PS(40:1)** | |
| 746.61 | $[M+H]^+$ | PC(O-34:1)(P-34:0) | O-16:0/18:1; P-18:0/16:0 |
| 830.70 | $[M+H]^+$ | PC(O-40:1) | O-18:0/22:1 |
| 800.65 | $[M+H]^+$ | PC(O-38:2)(P-38:1) | O-16:0/22:2; O-18:1/20:1; P-18:0/20:1 |
| 802.67 | $[M+H]^+$ | PC(O-38:1) | O-18:0/20:1 |
| 774.64 | $[M+H]^+$ | PC(O-36:1)(P-36:0) | O-16:0/20:1; O-18:0/18:1; P-18:0/18:0 |
| 828.69 | $[M+H]^+$ | PC(O-40:2) | O-18:0/22:2 |

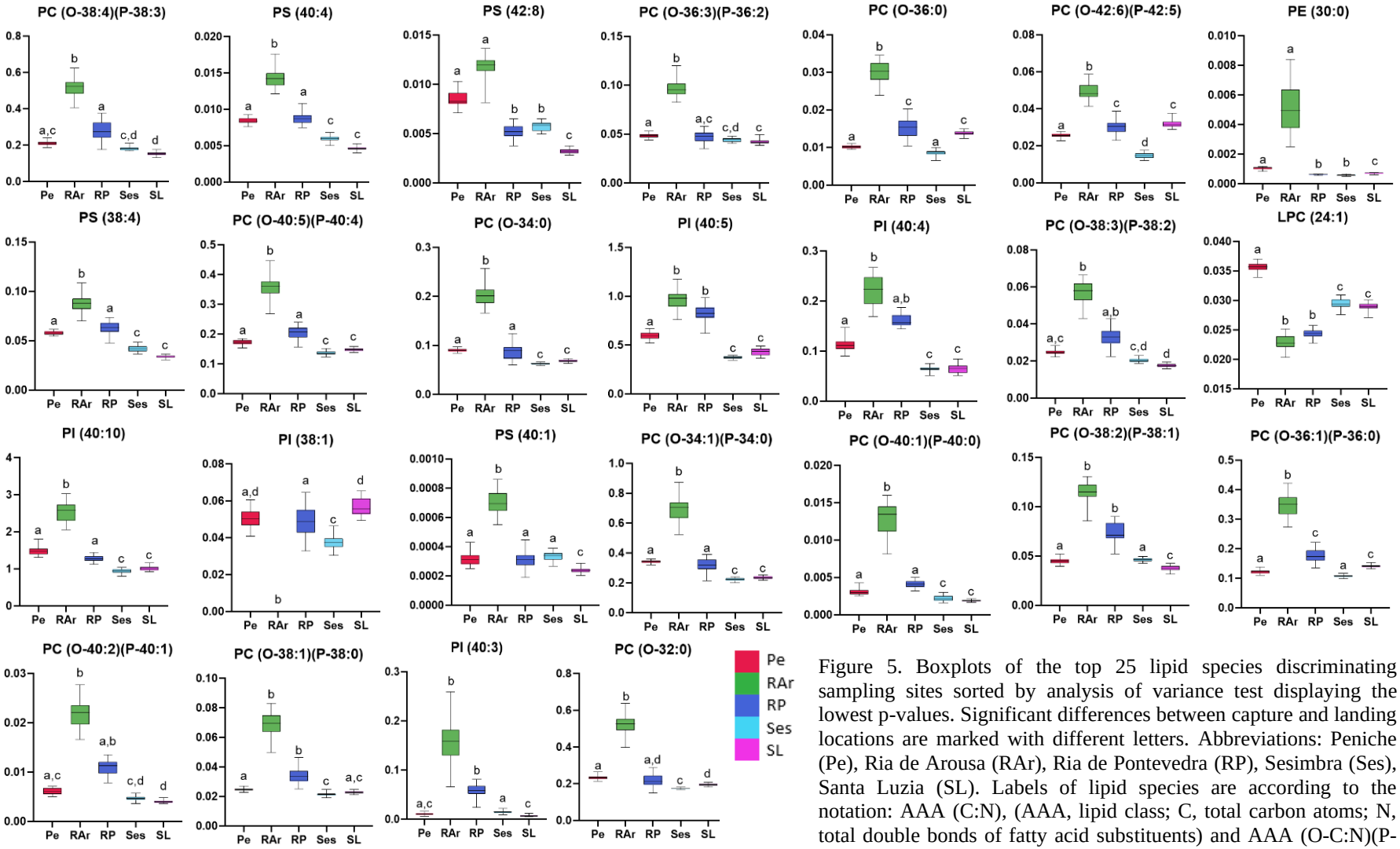



Figure 5. Boxplots of the top 25 lipid species discriminating sampling sites sorted by analysis of variance test displaying the lowest p-values. Significant differences between capture and landing locations are marked with different letters. Abbreviations: Peniche (Pe), Ria de Arousa (RAr), Ria de Pontevedra (RP), Sesimbra (Ses), Santa Luzia (SL). Labels of lipid species are according to the notation: AAA (C:N), (AAA, lipid class; C, total carbon atoms; N, total double bonds of fatty acid substituents) and AAA (O-C:N)(P-C:N) correspond to O- plasmanyl and/or P- plasmenyl, respectively).

**Discussion**

In this work, it was possible to discriminate the origin of *O. vulgaris* samples from five different capture and landing sites using lipidomic analysis together with statistical and clustering analysis. The lipid characterization of the muscle of *O. vulgaris* was the first step to evaluate the potential use of lipidomic analysis as a tool to discriminate specimens from different capture and landing locations. Concerning total lipid content, our results are in accordance with previous studies addressing the muscle[73] and mantle[74] of *O. vulgaris*. Prato et al.[56] studied the total lipid class composition of the common octopus, revealing that the amount of phospholipids in wild animals was 51.77% ± 1.10 of total lipids, which are in line with the values recorded in the present study. Differences in extrinsic factors (e.g. temperature, salinity, depth) between the five geographic locations addressed were not reflected in total lipid content in common octopus' muscle. Extrinsic factors might not have a significant influence in the total lipid content, but rather an effect on the lipid classes[75]. Differences in total lipid content are related to the abundance and/or lack of aliment, as well as other stressful conditions[74,76].

Phospholipids play relevant roles in organism biology, such as structural functions, influence in regulation of metabolism, physiology and energy production[77,78]. The lipidome of *O. vulgaris* muscle allowed the identification of four major lipid classes PE, PC, PI and PS, as already indicated by previous studies addressing in this marine invertebrate and other marine animals[77,79,80]. A higher relative abundance was identified to plasmanyl and/or plasmenyl molecular species in the lipid class PE with fatty acyl chains 22:6 and 20:5. This finding was somehow expected due to the higher abundance of DHA, EPA and ARA in marine organisms[81]. In fact, these are essential fatty acids (EFA), playing relevant roles in physiological and metabolic processes[82]. The lipid class PC also presented a higher relative abundance of molecular species containing EFA in their structural composition, in the form of diacyl molecular species. Fitahia et al.[83] studied the lipid compositions of *Octopus cyanea* and *Loligo* sp. byproducts, being PC (most abundant), LPC, PE, LPE the major lipid classes, and EPA, DHA and ARA as the major FA. Losito et al.[84] presented the analysis of PE and PC lipid classes in the common octopus, with our results being supported by their findings. The prevalence of plasmanyl and/or plasmenyl molecular species in PE, as well as of diacyl molecular species in PC, was already reported in common octopus[84] and other molluscs[85,86]. In this study, plasmanyl and plasmenyl

molecular species were considerably abundant, mainly in PE and PC lipid classes. Plasmalogens are ether phospholipids with slightly different ether bond linkages in the *sn-1* position of the glycerol backbone found in animal cells. Plasmanyls have a 1-O-alkyl fatty chain linked to the *sn-1* position while plasmenyls have a 1-O-alk-1´-enyl fatty chain[87]. The role of plasmalogens has been described as a structural component of cell membranes[88], in the response against to oxidative stress[89,90] and some studies have also suggested that these lipid molecules have an impact in signal transduction[91,92].

Lipid classes LPE and LPC, lyso forms of the phospholipid classes PE and PC, were also found in the muscle lipidome of *O. vulgaris*. The presence of lyso forms in marine organisms has been previously reported[60,79,80,84]. Phospholipid lyso forms are associated with the synthesis of other phospholipids as precursors, contributing to the regulation of intracellular signaling pathways and to the shifting of the structure and fluidity of lipid rafts[93]. These biomolecules are generally less abundant compared to other lipid classes in cephalopods[80,94].

The presence of sphingolipids in the common octopus lipidome has already been reported[79,95], as well as in other cephalopods species[83], with this lipid class being considered to play key structural and functional roles in nervous system cells[96,97]. Furthermore, our study identified CAEP as the third lipid class with more molecular species identified, followed by Cer, SM, CPE, *N*-$CH_3$-CAEP and HexCer. Although Cer and SM classes have been identified in previous works in the common octopus[79], there is little knowledge about CAEP, CPE and *N*-methyl-CAEP classes in this organism. These lipid classes have a strong C-P bond and play a role in cell membrane protection due to their ability to provide resistance to hydrolytic enzymes and the participation in metabolic pathways[98]. The presence of these lipid classes have been described in the lipidome of other marine organisms[96,98–100]. These studies have suggested that CAEP represent the main source of sphingosine found in marine invertebrates and that they develop similar biochemical functions to SM, which is the main sphingosine found in vertebrates[101,102]. The most usual sphingoid base in *O. vulgaris* samples was d16:1, followed by the odd sphingoid base d19:3. Similar results have been reported in the cephalopod species *Loligo chinensis*[103] and in the jumbo flying squid (*Dosidicus gigas*)[101]. The study performed by Komatsu et al.[101] showed that CAEP isolated from the jumbo flying squid can possibly have a bioactive effect against liver damage. The development of medicine or dietary

health supplements using this lipid class will contribute for the valorization of the jumbo flying squid. In this sense, the identification of CAEP in *O. vulgaris* samples will increase the value of this species in biomedicine, although further studies are needed to screen the biotechnological potential of this lipid class.

Our analysis allowed to clearly separate the five geographic capture and landing locations, with the most evident separation being that of RAr from the other four sampling sites. RAr is the northernmost sampling site and although it has a close proximity to RP, there are clear differences between them. RAr is the largest ria in the coast of Galicia (Spain) and it is highly influenced by upwelling events, raking it amount the most productive marine ecosystem of the world[104,105]. Furthermore, it is an area with a relevant mussel aquaculture production, representing 67% of the total Spanish mussel production and 15% of world production[106]. The practice of such level of aquaculture has an influence in the ecosystem, with negative and positive impacts[107]. An excessive biomass production can alter the local environmental, with an increase on organic loading which will increase the demand for oxygen. Furthermore, a reduction in phytoplankton biomass and an increase in nutrients can also occur[107]. Mussel aquaculture can have a relevant influence in the diet of common octopus occurring in this location, as mussel production rafts can attract possible octopus' prey, thus enhancing feeding opportunities. The influence of raft culture in the diet of other invertebrates (e.g. the harbor crab *Liocarcinus depurator*) has already been reported[108]. Feeding behavior, available food resources and environmental conditions shape the lipidome of marine organisms[109,110]. Different studies have shown that, under controlled conditions, different diets impact grow and food intake, which tune the lipid composition and the FA profile of marine organisms[56,58]. In natural habitats, dietary regimes are influenced by environment conditions, available resources, seasonal changes, and circadian rhythm[62,111,112]. Studies on the feeding behavior of *O. vulgaris* in the wild are scarce. However, studies carried out on the Portuguese coast have reported that common octopus preys a higher percentage of bivalves on southern coasts than on central and north coasts[58,62]. The differences of available preys present in the ecosystems of southern Portugal could explain the separation between SL samples from those of Pe and Ses. Outside the Iberian Atlantic coast, the diet of common octopus has been reported to be mainly derived from crustaceans (such as in the coast of Catalonia, Spain), or on multiple mollusk species (e.g., east coast of South Africa and in the Mediterranean coast of

France)[113,114]. These data support the idea of how the common octopus' diet can change according to its habitat, influencing its lipidome profile.

Environmental conditions are also an important factor when considering lipidomic analysis to discriminate samples from different geographic origins, as already shown in previous studies addressing traceability of seafood products[31,115]. The Iberian Peninsula presents a range of temperatures along its Atlantic coast, increasing from North to South[62,116]. Sea water temperature can influence marine organism lipidome in two ways. The first refers to the impact of temperature in membrane fluidity by shifting the level of FA saturation in lipid membranes[117–119]. On the other hand, differences in seawater temperature can impact the lipid composition of species by shaping their feeding behavior. These effects are registered in the diversity and abundance of the marine plankton communities, the basis for the production and the bottom of oceans food webs[120–122]. Overall, the diversity of marine plankton will influence the number and diversity of organisms from higher trophic levels[120,123–125]. Some of these effects are reflected in EFA that must be derived from dietary sources and, as such, are also mirrored in the lipidome[120]. Differences in temperature, strong upwelling events that occur in RAr and its effects on the *O. vulgaris* trophic regime might overall contribute to the discrimination recorded from the other four locations[58,62,104]. Furthermore, our results discriminated these four locations between themselves. The previous factors described above, which we use as important factors affecting the lipidome of the common octopus's muscle, are different between the geographical locations. In the south of Portugal, warmer waters[62], weaker upwelling events compared to the western coast[126] and a richer diet in bivalves[58,62] influences the discrimination from the specimens capture and landed in Pe and Ses. Additionally, environmental and dietary factors must also contribute to the discrimination of RP from Pe and Ses, as this place has colder waters and stronger upwelling events.

## Conclusion

The aims of this study were successfully achieved, with the characterization of the lipidome of the muscle of *O. vulgaris* and the discrimination of specimens from the five capture and landing sites surveyed. This work confirmed that lipidomic analysis is a powerful tool to discriminate *O. vulgaris* from different geographic origins, becoming a step in the right direction in the quest to identify analytical methodologies that can enhance seafood traceability. Furthermore, expanding the sampling locations, such as to Mediterranean and/or Moroccan coasts, and sampling over consecutive seasons and years, will allow to better understand how the environmental and trophic conditions of different ecosystems shape the polar lipidome and the biochemical phenotypes of the common octopus.

**References**


1. Leridon, H. World population outlook: Explosion or implosion? *Popul. Soc.* **573**, 1–4 (2020). doi:10.3917/popsoc.573.0001
2. Uniyal, S., Paliwal, R., Saun, B. & Sharma, R. Human overpopulation: Impact on environment. in *Megacities and Rapid Urbanization: Breakthroughs in Research and Practice* 20–30 (2020). doi:10.4018/978-1-5225-9276-1.ch002.
3. FAO. *The State of World Fisheries and Aquaculture 2020*. (2020). doi:10.4060/ca9229en.
4. El Sheikha, A. F. & Xu, J. (JP). Traceability as a key of seafood safety: Reassessment and possible applications. *Rev. Fish. Sci. Aquac.* **25**, 158–170 (2017). doi:10.1080/23308249.2016.1254158
5. Anderson, J. L., Asche, F. & Garlock, T. Globalization and commoditization: The transformation of the seafood market. *J. Commod. Mark.* **12**, 2–8 (2018). doi:10.1016/j.jcomm.2017.12.004
6. Asche, F., Bellemare, M. F., Roheim, C., Smith, M. D. & Tveteras, S. Fair enough? Food security and the international trade of seafood. *World Dev.* **67**, 151–160 (2015). doi:10.1016/j.worlddev.2014.10.013
7. Leal, M. C., Pimentel, T., Ricardo, F., Rosa, R. & Calado, R. Seafood traceability: current needs, available tools, and biotechnological challenges for origin certification. *Trends Biotechnol.* **33**, 331–336 (2015). doi:10.1016/j.tibtech.2015.03.003
8. Turchini, G. M., Quinn, G. P., Jones, P. L., Palmeri, G. & Gooley, G. Traceability and discrimination among differently farmed fish: a case study on Australian Murray Cod. *J. Agric. Food Chem.* **57**, 274–281 (2009). doi:10.1021/jf801962h

9. Zhao, X. Tracing the geographical origins of Yesso scallop (*Patinopecten yessoensis*) by using compound-specific isotope analysis: An approach for overcoming the seasonal effect. *Food Control* **102**, 38–45 (2019). doi:10.1016/j.foodcont.2019.03.016

10. Chatterjee, N. S., Chevallier, O. P., Wielogorska, E., Black, C. & Elliott, C. T. Simultaneous authentication of species identity and geographical origin of shrimps: Untargeted metabolomics to recurrent biomarker ions. *J. Chromatogr. A* **1599**, 75–84 (2019). doi:10.1016/j.chroma.2019.04.001

11. Pieniak, Z., Vanhonacker, F. & Verbeke, W. Consumer knowledge and use of information about fish and aquaculture. *Food Policy* **40**, 25–30 (2013). doi:10.1016/j.foodpol.2013.01.005

12. CAC. *Twenty-seventh Session, Centre International de Conférences de Genève, Geneva, Switzerland, 28 June - 3 July*. http://www.fao.org/tempref/codex/Meetings/CAC/cac27/al2707ae.pdf (2004).

13. El Sheikha, A. F. & Montet, D. How to determine the geographical origin of seafood? *Crit. Rev. Food Sci. Nutr.* **56**, 306–317 (2016). doi:10.1080/10408398.2012.745478

14. D'Amico, P., Armani, A., Gianfaldoni, D. & Guidi, A. New provisions for the labelling of fishery and aquaculture products: Difficulties in the implementation of Regulation (EU) n. 1379/2013. *Mar. Policy* **71**, 147–156 (2016). doi:10.1016/j.marpol.2016.05.026

15. Ricardo, F. *et al.* Trace element fingerprinting of cockle (*Cerastoderma edule*) shells can reveal harvesting location in adjacent areas. *Sci. Rep.* **5**, 11932 (2015). doi:10.1038/srep11932

16. Delpiani, G. *et al.* Are we sure we eat what we buy? Fish mislabelling in Buenos Aires province, the largest sea food market in Argentina. *Fish. Res.* **221**, 105373 (2020). doi:10.1016/j.fishres.2019.105373

17. Luykx, D. M. A. M. & van Ruth, S. M. An overview of analytical methods for determining the geographical origin of food products. *Food Chem.* **107**, 897–911 (2008). doi:10.1016/j.foodchem.2007.09.038

18. Bennion, M. *et al.* Trace element fingerprinting of blue mussel (*Mytilus edulis*) shells and soft tissues successfully reveals harvesting locations. *Sci. Total Environ.* **685**, 50–58 (2019). doi:10.1016/j.scitotenv.2019.05.233

19. Morrison, L., Bennion, M., Gill, S. & Graham, C. T. Spatio-temporal trace element fingerprinting of king scallops (*Pecten maximus*) reveals harvesting period and location. *Sci. Total Environ.* **697**, 134121 (2019). doi:10.1016/j.scitotenv.2019.134121

20. Zhang, X. *et al.* Geographical origin traceability and species identification of three scallops (*Patinopecten yessoensis, Chlamys farreri*, and *Argopecten irradians*) using stable isotope analysis. *Food Chem.* **299**, 125107 (2019). doi:10.1016/j.foodchem.2019.125107

21. Chaguri, M. P. *et al.* Different tools to trace geographic origin and seasonality of croaker (*Micropogonias furnieri*). *LWT - Food Sci. Technol.* **61**, 194–200 (2015). doi:10.1016/j.lwt.2014.11.006

22. Carrera, M. & Gallardo, J. M. Determination of the geographical origin of all commercial hake species by stable isotope ratio (SIR) Analysis. *J. Agric. Food Chem.* **65**, 1070–1077 (2017). doi:10.1021/acs.jafc.6b04972

23. Barria, A. *et al.* Population genomic structure and genome-wide linkage disequilibrium in farmed Atlantic salmon (*Salmo salar* L.) using dense SNP genotypes. *Front. Genet.* **9**, 649 (2018). doi:10.3389/fgene.2018.00649

24. Milano, I. *et al.* Outlier SNP markers reveal fine-scale genetic structuring across European hake populations (*Merluccius merluccius*). *Mol. Ecol.* **23**, 118–135 (2014). doi:10.1111/mec.12568

25. Scarano, D. & Rao, R. DNA markers for food products authentication. *Diversity* **6**, 579–596 (2014). doi:10.3390/d6030579

26. Fernandes, T. J. R., Amaral, J. S. & Mafra, I. DNA barcode markers applied to seafood authentication: an updated review. *Crit. Rev. Food Sci. Nutr.* (2020) doi:10.1080/10408398.2020.1811200.

27. Hosegood, J. *et al.* Phylogenomics and species delimitation for effective conservation of manta and devil rays. *Mol. Ecol.* **29**, 4783–4796 (2020). doi:10.1111/mec.15683

28. Power, A. & Cozzolino, D. How fishy is your fish? Authentication, provenance and traceability in fish and seafood by means of vibrational spectroscopy. *Appl. Sci.* **10**, 4150 (2020). doi:10.3390/app10124150

29. Ghidini, S. *et al.* Rapid authentication of European sea bass (*Dicentrarchus labrax* L.) according to production method, farming system, and geographical origin by near infrared spectroscopy coupled with chemometrics. *Food Chem.* **280**, 321–327 (2019). doi:10.1016/j.foodchem.2018.12.075

30. Varrà, M. O., Ghidini, S., Ianieri, A. & Zanardi, E. Near infrared spectral fingerprinting: A tool against origin-related fraud in the sector of processed anchovies. *Food Control* 107778 (2020). doi:10.1016/j.foodcont.2020.107778.

31. Ricardo, F., Maciel, E., Domingues, M. R. & Calado, R. Spatio-temporal variability in the fatty acid profile of the adductor muscle of the common cockle *Cerastoderma edule* and its relevance for tracing geographic origin. *Food Control* **81**, 173–180 (2017). doi:10.1016/j.foodcont.2017.06.005

32. da Costa, E. *et al.* Site-specific lipidomic signatures of sea lettuce (*Ulva* spp., Chlorophyta) hold the potential to trace their geographic origin. *Biomolecules* **10**, 489 (2020). doi:10.3390/biom10030489

33. Arechavala-Lopez, P. *et al.* Fatty acids and elemental composition as biomarkers of *Octopus vulgaris* populations: does origin matter? *Mar. Pollut. Bull.* **139**, 299–310 (2019). doi:10.1016/j.marpolbul.2018.12.048

34. Guschina, I. A. & Harwood, J. L. Algal lipids and effect of the environment on their biochemistry. in *Lipids in Aquatic Ecosystems* (eds. Kainz, M., Brett, M. T. & Arts, M. T.) 1–24 (Springer New York, 2009). doi:10.1007/978-0-387-89366-2_1.

35. Rod-in, W., Monmai, C., Shin, I., You, S. & Park, W. J. Neutral lipids, glycolipids, and phospholipids, isolated from sandfish (*Arctoscopus japonicus*) eggs, exhibit anti-inflammatory activity in LPS-stimulated RAW264.7 cells through NF-κB and MAPKs pathways. *Mar. Drugs* **18**, 480 (2020). doi:10.3390/md18090480

36. Zampelas & Magriplis. New insights into cholesterol functions: A friend or an enemy? *Nutrients* **11**, 1645 (2019). doi:10.3390/nu11071645

37. Ronan Lordan, Alexandros Tsoupras & Ioannis Zabetakis. Phospholipids of animal and marine origin: structure, function, and anti-inflammatory properties. *Molecules* **22**, 1964 (2017). doi:10.3390/molecules22111964

38. Monteiro, J. P. *et al.* The unique lipidomic signatures of *Saccharina latissima* can be used to pinpoint their geographic origin. *Biomolecules* **10**, 107 (2020). doi:10.3390/biom10010107

39. Sun, T., Wang, X., Cong, P., Xu, J. & Xue, C. Mass spectrometry-based lipidomics in food science and nutritional health: A comprehensive review. *Compr. Rev. Food Sci. Food Saf.* **19**, 2530–2558 (2020). doi:10.1111/1541-4337.12603

40. Koelmel, J. P. *et al.* Environmental lipidomics: understanding the response of organisms and ecosystems to a changing world. *Metabolomics* **16**, 56 (2020). doi:10.1007/s11306-020-01665-3

41. Kelly, J. & Scheibling, R. Fatty acids as dietary tracers in benthic food webs. *Mar Ecol Prog Ser* **446**, 1–22 (2012). doi:10.3354/meps09559

42. Qian, J. *et al.* Food traceability system from governmental, corporate, and consumer perspectives in the European Union and China: A comparative review. *Trends Food Sci. Technol.* **99**, 402–412 (2020). doi:10.1016/j.tifs.2020.03.025

43. Hermosilla, C., Rocha, F. & Valavanis, V. D. Assessing *Octopus vulgaris* distribution using presence-only model methods. *Hydrobiologia* **670**, 35–47 (2011). doi:10.1007/s10750-011-0671-y

44. Belcari, P., Cuccu, D., González, M., Srairi, A. & Vidoris, P. Distribution and abundance of *Octopus vulgaris* Cuvier, 1797 (Cephalopoda: Octopoda) in the Mediterranean Sea. *Sci. Mar.* **66**, 157 (2002). doi:10.3989/scimar.2002.66s2157

45. Vaz-Pires, P., Seixas, P. & Barbosa, A. Aquaculture potential of the common octopus (*Octopus vulgaris* Cuvier, 1797): a review. *Aquaculture* **238**, 221–238 (2004). doi:10.1016/j.aquaculture.2004.05.018

46. Katsanevakis, S. & Verriopoulos, G. Abundance of *Octopus vulgaris* on soft sediment. *Sci. Mar.* **68**, 553–560 (2004). doi:10.3989/scimar.2004.68n4553

47. Sonderblohm, C. P. *et al.* Participatory assessment of management measures for *Octopus vulgaris* pot and trap fishery from southern Portugal. *Mar. Policy* **75**, 133–142 (2017). doi:10.1016/j.marpol.2016.11.004

48. Bañón, R., Otero, J., Campelos-Álvarez, J. M., Garazo, A. & Alonso-Fernández, A. The traditional small-scale octopus trap fishery off the Galician coast (Northeastern Atlantic): Historical notes and current fishery dynamics. *Fish. Res.* **206**, 115–128 (2018). doi:10.1016/j.fishres.2018.05.005

49. Navarro, J. C. & Villanueva, R. The fatty acid composition of *Octopus vulgaris* paralarvae reared with live and inert food: deviation from their natural fatty acid profile. *Aquaculture* **219**, 613–631 (2003). doi:10.1016/S0044-8486(02)00311-3

50. *Cephalopod Culture*. (Springer Netherlands, 2014). doi:10.1007/978-94-017-8648-5.

51. Márquez, L., Larson, M. & Almansa, E. Effects of temperature on the rate of embryonic development of cephalopods in the light of thermal time applied to aquaculture. *Rev. Aquac.* **13**, 706–718 (2021). doi:10.1111/raq.12495

52. Casalini, A. *et al.* Evaluation of reproductive performances of the common octopus (*Octopus vulgaris*) reared in water recirculation systems and fed different diets. *Sci. Rep.* **10**, 15261 (2020). doi:10.1038/s41598-020-72151-y

53. Reis, D. B. *et al.* Effect of Artemia inherent fatty acid metabolism on the bioavailability of essential fatty acids for *Octopus vulgaris* paralarvae development. *Aquaculture* **500**, 264–271 (2019). doi:10.1016/j.aquaculture.2018.10.021

54. Reis, D. B. *et al.* Effects of feeding with different live preys on the lipid composition, growth and survival of *Octopus vulgaris* paralarvae. *Aquac. Res.* are.14873 (2020). doi:10.1111/are.14873.

55. Domingues, P., Rosas, C., Sánchez, A., Chimal, M. E. & Gallardo, P. Effect of the processing of four marine species on their in vitro digestibility of *Octopus vulgaris* adults. *Aquac. Int.* **28**, 1269–1277 (2020). doi:10.1007/s10499-020-00524-1

56. Prato, E., Portacci, G. & Biandolino, F. Effect of diet on growth performance, feed efficiency and nutritional composition of *Octopus vulgaris*. *Aquaculture* **309**, 203–211 (2010). doi:10.1016/j.aquaculture.2010.09.036

57. Garcia Garcia, B. & Cerezo Valverde, J. Optimal proportions of crabs and fish in diet for common octopus (*Octopus vulgaris*) ongrowing. *Aquaculture* 502–511 (2006). doi:10.1016/j.aquaculture.2005.04.055.

58. Giménez, F. A. & García, B. G. Growth and food intake models in *Octopus vulgaris* Cuvier (1797): Influence of body weight, temperature, sex and diet. *Aquac. Int.* **10**, 361–377 (2002). doi:10.1023/A:1023335024053

59. Cerezo Valverde, J., Hernández, M. D., Aguado-Giménez, F. & García García, B. Development of low-lipid formulated feeds with different protein/energy ratios for *Octopus vulgaris* ongrowing. *Aquac. Nutr.* **23**, 681–691 (2017). doi:10.1111/anu.12435

60. Morillo-Velarde, P. S., Cerezo Valverde, J. & García-García, B. Utilization of diets with different fish oil content in common octopus (*Octopus vulgaris* Cuvier, 1797) and resulting changes in its biochemical composition. *Aquac. Res.* **46**, 2871–2884 (2015). doi:10.1111/are.12439

61. Martínez, R. *et al.* Growth, survival and physiological condition of *Octopus maya* when fed a successful formulated diet. *Aquaculture* **426–427**, 310–317 (2014). doi:10.1016/j.aquaculture.2014.02.005

62. Rosa, R., Marques, A. M., Nunes, M. L., Bandarra, N. & Sousa Reis, C. Spatial-temporal changes in dimethyl acetal (octadecanal) levels of *Octopus vulgaris* (Mollusca, Cephalopoda): relation to feeding ecology. *Sci. Mar.* **68**, 227–236 (2004). doi:10.3989/scimar.2004.68n2227

63. Rodríguez, C., Carrasco, J. F., Arronte, J. C. & Rodríguez, M. Common octopus (*Octopus vulgaris* Cuvier, 1797) juvenile ongrowing in floating cages. *Aquaculture* **254**, 293–300 (2006). doi:10.1016/j.aquaculture.2005.10.053

64. Busetto, M. L. *et al.* Authentication of farmed and wild turbot (*Psetta maxima*) by fatty acid and isotopic analyses combined with chemometrics. *J. Agric. Food Chem.* **56**, 2742–2750 (2008). doi:10.1021/jf0734267

65. Li, L., Kokkuar, N., Han, C., Ren, W. & Dong, S. Effects of dietary shifts on the stable isotope signature of Pacific white shrimp *Litopenaeus vannamei* and implications for traceability. *Mar. Freshw. Res.* **71**, 1294 (2020). doi:10.1071/MF19214

66. Molkentin, J., Lehmann, I., Ostermeyer, U. & Rehbein, H. Traceability of organic fish – Authenticating the production origin of salmonids by chemical and isotopic analyses. *Food Control* **53**, 55–66 (2015). doi:10.1016/j.foodcont.2015.01.003

67. Axelson, D. E., Standal, I. B., Martinez, I. & Aursand, M. Classification of wild and farmed salmon using bayesian belief networks and gas chromatography-derived fatty acid distributions. *J. Agric. Food Chem.* **57**, 7634–7639 (2009). doi:10.1021/jf9013235

68. FAO Fisheries & Aquaculture - Species Fact Sheets - *Octopus vulgaris* (Lamarck, 1798). http://www.fao.org/fishery/species/3571/en.

69. Bligh, E. G. & Dyer, W. J. A rapid method of total lipid extraction and purification. *Can J Biochem Physiol* **37**, 911–917 (1959). doi:10.1139/o59-099

70. Bartlett, E. M. & Lewis, D. H. Spectrophotometric determination of phosphate esters in the presence and absence of orthophosphate. *Anal. Biochem.* **36**, 159–167 (1970). doi:10.1016/0003-2697(70)90343-X

71. Pluskal, T., Castillo, S., Villar-Briones, A. & Orešič, M. MZmine 2: Modular framework for processing, visualizing, and analyzing mass spectrometry-based molecular profile data. *BMC Bioinformatics* **11**, 395 (2010). doi:10.1186/1471-2105-11-395

72. Chong, J. *et al.* MetaboAnalyst 4.0: towards more transparent and integrative metabolomics analysis. *Nucleic Acids Res.* **46**, W486–W494 (2018). doi:10.1093/nar/gky310

73. Rosa, R., Pereira, J. & Nunes, M. L. Biochemical composition of cephalopods with different life strategies, with special reference to a giant squid, *Architeuthis* sp. *Mar. Biol.* **146**, 739–751 (2005). doi:10.1007/s00227-004-1477-5

74. García-Garrido, S., Hachero-Cruzado, I., Garrido, D., Rosas, C. & Domingues, P. Lipid composition of the mantle and digestive gland of *Octopus vulgaris* juveniles (Cuvier, 1797) exposed to prolonged starvation. *Aquac. Int.* **18**, 1223–1241 (2010). doi:10.1007/s10499-010-9335-6

75. Nemova, N. N., Fokina, N. N., Nefedova, Z. A., Ruokolainen, T. R. & Bakhmet, I. N. Modifications of gill lipid composition in littoral and cultured blue mussels *Mytilus*

*edulis* L. under the influence of ambient salinity. *Polar Rec.* **49**, 272–277 (2013). doi:10.1017/S0032247412000629

76. Ozogul, Y., Duysak, O., Ozogul, F., Özkütük, A. S. & Türeli, C. Seasonal effects in the nutritional quality of the body structural tissue of cephalopods. *Food Chem.* **108**, 847–852 (2008). doi:10.1016/j.foodchem.2007.11.048

77. Tocher, D. R., Bendiksen, E. Å., Campbell, P. J. & Bell, J. G. The role of phospholipids in nutrition and metabolism of teleost fish. *Aquaculture* **280**, 21–34 (2008). doi:10.1016/j.aquaculture.2008.04.034

78. Navarro, J. C. & Villanueva, R. Lipid and fatty acid composition of early stages of cephalopods: an approach to their lipid requirements. *Aquaculture* **183**, 161–177 (2000). doi:10.1016/S0044-8486(99)00290-2

79. Morillo-Velarde, P. S., Valverde, J. C., Serra Llinares, R. M. & García, B. G. Changes in lipid composition of different tissues of common octopus (*Octopus vulgaris*) during short-term starvation. *Aquac. Res.* **44**, 1177–1189 (2013). doi:10.1111/j.1365-2109.2012.03131.x

80. Valverde, J. C. *et al.* Lipid classes from marine species and meals intended for cephalopod feeding. *Aquac. Int.* **20**, 71–89 (2012). doi:10.1007/s10499-011-9442-z

81. Zhukova, N. V. Fatty acids of marine mollusks: impact of diet, bacterial symbiosis and biosynthetic potential. *Biomolecules* **9**, 857 (2019). doi:10.3390/biom9120857

82. Parrish, C. C. Essential fatty acids in aquatic food webs. in *Lipids in Aquatic Ecosystems* (eds. Kainz, M., Brett, M. T. & Arts, M. T.) 309–326 (Springer New York, 2009). doi:10.1007/978-0-387-89366-2_13.

83. Fitahia, E. M., Croyal, M., Raheriniaina, C. E., Ferchaud-Roucher, V. & Nazih, H. High-resolution mass spectrometry unravels a broad range of bioactive lipid species in

*Octopus cyanea* and *Loligo* sp. By-products from southwestern Madagascar. *Waste Biomass Valorization* **9**, 1787–1793 (2018). doi:10.1007/s12649-017-9933-x

84. Losito, I. *et al.* Tracing the thermal history of seafood products through lysophospholipid analysis by hydrophilic interaction liquid chromatography–electrospray ionization Fourier transform mass spectrometry. *Molecules* **23**, 2212 (2018). doi:10.3390/molecules23092212

85. Facchini, L., Losito, I., Cataldi, T. R. I. & Palmisano, F. Seasonal variations in the profile of main phospholipids in *Mytilus galloprovincialis* mussels: A study by hydrophilic interaction liquid chromatography-electrospray ionization Fourier transform mass spectrometry. *J. Mass Spectrom.* **53**, 1–20 (2018). doi:10.1002/jms.4029

86. Kraffe, E., Soudant, P. & Marty, Y. Fatty acids of serine, ethanolamine, and choline plasmalogens in some marine bivalves. *Lipids* **39**, 59–66 (2004). doi:10.1007/s11745-004-1202-x

87. Nagan, N. & Zoeller, R. A. Plasmalogens: biosynthesis and functions. *Prog. Lipid Res.* **40**, 199–229 (2001). doi:10.1016/S0163-7827(01)00003-0

88. Hanuš, L. O., Levitsky, D. O., Shkrob, I. & Dembitsky, V. M. Plasmalogens, fatty acids and alkyl glyceryl ethers of marine and freshwater clams and mussels. *Food Chem.* **116**, 491–498 (2009). doi:10.1016/j.foodchem.2009.03.004

89. Brosche, T., Brueckmann, M., Haase, K. K., Sieber, C. & Bertsch, T. Decreased plasmalogen concentration as a surrogate marker of oxidative stress in patients presenting with acute coronary syndromes or supraventricular tachycardias. *Clin. Chem. Lab. Med.* **45**, 689–691 (2007). doi:10.1515/CCLM.2007.111

90. Maeba, R., Sawada, Y., Shimasaki, H., Takahashi, I. & Ueta, N. Ethanolamine plasmalogens protect cholesterol-rich liposomal membranes from oxidation caused by

free radicals. *Chem. Phys. Lipids* **120**, 145–151 (2002). doi:10.1016/S0009-3084(02)00101-9

91. Latorre, E., Collado, M. P., Fernández, I., Aragonés, M. D. & Catalán, R. E. Signaling events mediating activation of brain ethanolamine plasmalogen hydrolysis by ceramide: Activated plasmalogen hydrolysis by ceramide. *Eur. J. Biochem.* **270**, 36–46 (2003). doi:10.1046/j.1432-1033.2003.03356.x

92. Braverman, N. E. & Moser, A. B. Functions of plasmalogen lipids in health and disease. *Biochim. Biophys. Acta BBA - Mol. Basis Dis.* **1822**, 1442–1452 (2012). doi:10.1016/j.bbadis.2012.05.008

93. Grzelczyk, A. & Gendaszewska-Darmach, E. Novel bioactive glycerol-based lysophospholipids: New data – New insight into their function. *Biochimie* **95**, 667–679 (2013). doi:10.1016/j.biochi.2012.10.009

94. Shen, Y. *et al.* Characterization of glycerophospholipid molecular species in muscles from three species of cephalopods by direct infusion-tandem mass spectrometry. *Chem. Phys. Lipids* **226**, 104848 (2020). doi:10.1016/j.chemphyslip.2019.104848

95. Reis, D. B. *et al.* Composition and metabolism of phospholipids in *Octopus vulgaris* and *Sepia officinalis* hatchlings. *Comp. Biochem. Physiol. B Biochem. Mol. Biol.* **200**, 62–68 (2016). doi:10.1016/j.cbpb.2016.06.001

96. Facchini, L., Losito, I., Cataldi, T. R. I. & Palmisano, F. Ceramide lipids in alive and thermally stressed mussels: An investigation by hydrophilic interaction liquid chromatography-electrospray ionization Fourier transform mass spectrometry. *J. Mass Spectrom.* **51**, 768–781 (2016). doi:10.1002/jms.3832

97. Colombaioni, L. & Garcia-Gil, M. Sphingolipid metabolites in neural signalling and function. *Brain Res. Rev.* **46**, 328–355 (2004). doi:10.1016/j.brainresrev.2004.07.014

98. Kariotoglou, D. M. & Mastronicolis, S. K. Phosphonolipids in the mussel *Mytilus galloprovincialis*. *Z. Für Naturforschung C* **53**, 888–896 (1998). doi:10.1515/znc-1998-9-1018

99. Sinanoglou, V. J. & Miniadis-Meimaroglou, S. Structural analysis of ceramide-amino-ethyl-phosphonate in edible Mediterranean cephalopods. *Acta Aliment.* **33**, 359–370 (2004). doi:10.1556/AAlim.33.2004.4.6

100. de Souza, L. M. *et al.* Glyco- and sphingophosphonolipids from the medusa *Phyllorhiza punctata*: NMR and ESI-MS/MS fingerprints. *Chem. Phys. Lipids* **145**, 85–96 (2007). doi:10.1016/j.chemphyslip.2006.11.001

101. Komatsu, M. *et al.* Ceramide aminoethylphosphonate from jumbo flying squid *Dosidicus gigas* attenuates the toxicity of cyanotoxin microcystin-LR. *Fish. Sci.* **79**, 313–320 (2013). doi:10.1007/s12562-012-0593-2

102. Bhat, H. B. *et al.* Evaluation of aegerolysins as novel tools to detect and visualize ceramide phosphoethanolamine, a major sphingolipid in invertebrates. *FASEB J.* **29**, 3920–3934 (2015). doi:10.1096/fj.15-272112

103. Wang, R. Identification of ceramide 2-aminoethylphosphonate molecular species from different aquatic products by NPLC/Q-Exactive-MS. *Food Chem.* **304**, 125425 (2020). doi:10.1016/j.foodchem.2019.125425

104. Outeiro, L., Byron, C. & Angelini, R. Ecosystem maturity as a proxy of mussel aquaculture carrying capacity in Ria de Arousa (NW Spain): A food web modeling perspective. *Aquaculture* **496**, 270–284 (2018). doi:10.1016/j.aquaculture.2018.06.043

105. Tenore, K. R. *et al.* Coastal upwelling in the Rías Bajas, NW Spain: Contrasting the benthic regimes of Rías de Arosa and de Muros. *J. Mar. Res.* **40**, 701–772 (1982). ISSN:0022-2402

106. Fernández-Reiriz, M.-J. *Bateeiros, mar, mejillón. Una perspectiva bioeconómica*. (2004). ISBN:84-95491-69-9

107. Duarte, P., Labarta, U. & Fernández-Reiriz, M. J. Modelling local food depletion effects in mussel rafts of Galician Rias. *Aquaculture* **274**, 300–312 (2008). doi:10.1016/j.aquaculture.2007.11.025

108. Freire, J. Feeding ecology of *Liocarcinus depurator* (Decapoda: Portunidae) in the Ria de Arousa (Galicia, north-west Spain): effects of habitat, season and life history. *Mar. Biol.* **126**, 297–311 (1996). doi:10.1007/BF00347454

109. Gilabert, A., Geraudie, P., Jaumot, J. & Porte, C. Partial characterization of the lipidome of the cold-water scallop, *Chlamys islandica*. *Environ. Sci. Pollut. Res.* **27**, 1475–1484 (2020). doi:10.1007/s11356-019-06751-1

110. Ezgeta-Balić, D., Najdek, M., Peharda, M. & Blažina, M. Seasonal fatty acid profile analysis to trace origin of food sources of four commercially important bivalves. *Aquaculture* **334–337**, 89–100 (2012). doi:10.1016/j.aquaculture.2011.12.041

111. Rosa, R. *et al.* Bioenergetics of small pelagic fishes in upwelling systems: relationship between fish condition, coastal ecosystem dynamics and fisheries. *Mar. Ecol. Prog. Ser.* **410**, 205–218 (2010). doi:10.3354/meps08635

112. Cortez, T., Castro, B. G. & Guerra, A. Feeding dynamics of *Octopus mimus* (Mollusca:Cephalopoda) in northern Chile waters. *Mar. Biol.* **123**, 497–503 (1995). doi:10.1007/BF00349228

113. Smale, M. J. & Buchan, P. R. Biology of *Octopus vulgaris* off the east coast of South Africa. *Mar. Biol.* **65**, 1–12 (1981). doi:10.1007/BF00397061

114. Ambrose, R. F. & Nelson, B. V. Predation by *Octopus vulgaris* in the Mediterranean. *Mar. Ecol.* **4**, 251–261 (1983). doi:10.1111/j.1439-0485.1983.tb00299.x

115. Gong, Y., Li, Y., Chen, X. & Chen, L. Potential use of stable isotope and fatty acid analyses for traceability of geographic origins of jumbo squid (*Dosidicus gigas*). *Rapid Commun. Mass Spectrom.* **32**, 583–589 (2018). doi:10.1002/rcm.8071

116. Santos, M. Characterizing phytoplankton biomass seasonal cycles in two NE Atlantic coastal bays. *Cont. Shelf Res.* **207**, 104200 (2020). doi:10.1016/j.csr.2020.104200

117. Hall, J. M., Parrish, C. C. & Thompson, R. J. Eicosapentaenoic Acid Regulates Scallop (*Placopecten magellanicus*) Membrane Fluidity in Response to Cold. *Biol. Bull.* **202**, 201–203 (2002). doi:10.2307/1543469

118. Velansky, P. V. & Kostetsky, E. Ya. Lipids of marine cold-water fishes. *Russ. J. Mar. Biol.* **34**, 51–56 (2008). doi:10.1134/S1063074008010070

119. Murzina, S. *et al.* Lipid status of the two high latitude fish species, *Leptoclinus maculatus* and *Lumpenus fabricii*. *Int. J. Mol. Sci.* **14**, 7048–7060 (2013). doi:10.3390/ijms14047048

120. Helenius, L., Budge, S. M., Nadeau, H. & Johnson, C. L. Ambient temperature and algal prey type affect essential fatty acid incorporation and trophic upgrading in a herbivorous marine copepod. *Philos. Trans. R. Soc. B Biol. Sci.* **375**, 20200039 (2020). doi:10.1098/rstb.2020.0039

121. Parzanini, C. *et al.* Discrimination between freshwater and marine fish using fatty acids: ecological implications and future perspectives. *Environ. Rev.* **28**, 546–559 (2020). doi:10.1139/er-2020-0031

122. Rodas, A. M. *et al.* Eukaryotic plankton communities across reef environments in Bocas del Toro Archipelago, Panamá. *Coral Reefs* **39**, 1453–1467 (2020). doi:10.1007/s00338-020-01979-7

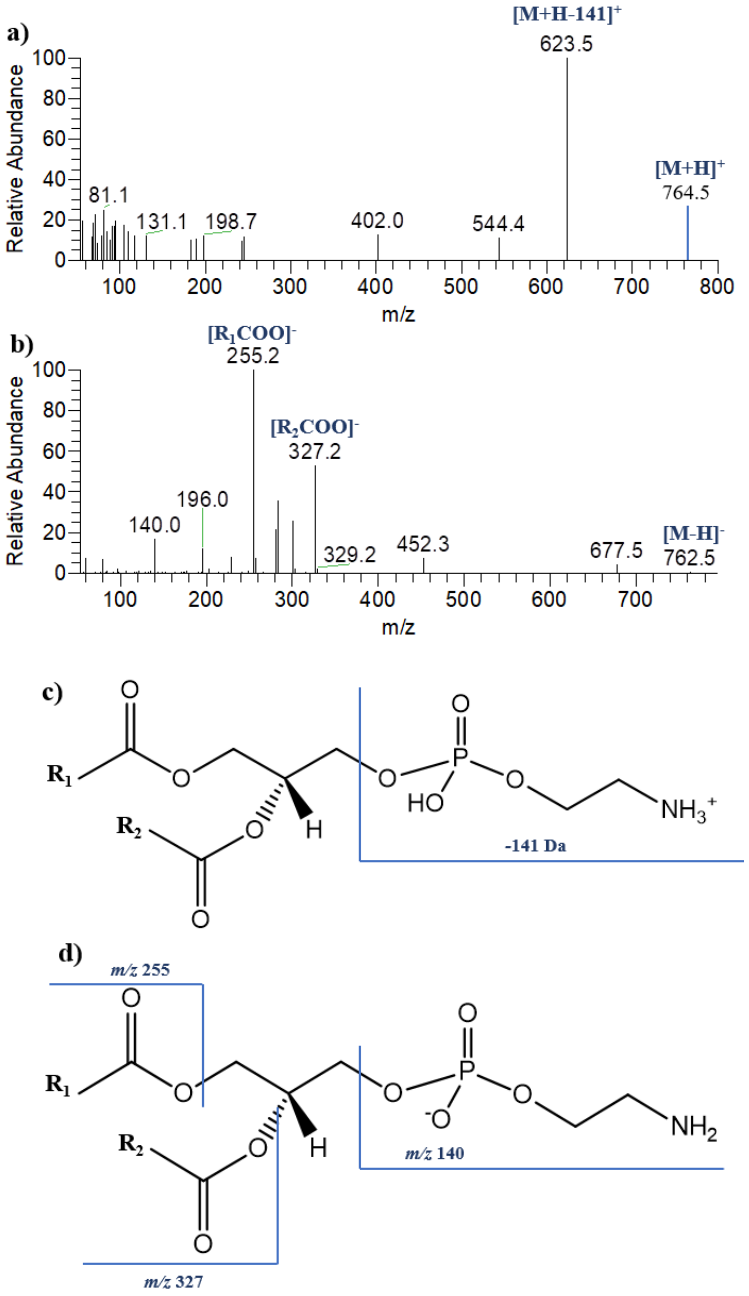
123. Bode, A., Alvarez-Ossorio, M. T., Cabanas, J. M., Miranda, A. & Varela, M. Recent trends in plankton and upwelling intensity off Galicia (NW Spain). *Prog. Oceanogr.* **83**, 342–350 (2009). doi:10.1016/j.pocean.2009.07.025

124. Benincà, E., Dakos, V., Van Nes, E. H., Huisman, J. & Scheffer, M. Resonance of Plankton Communities with Temperature Fluctuations. *Am. Nat.* **178**, E85–E95 (2011). doi:10.1086/661902

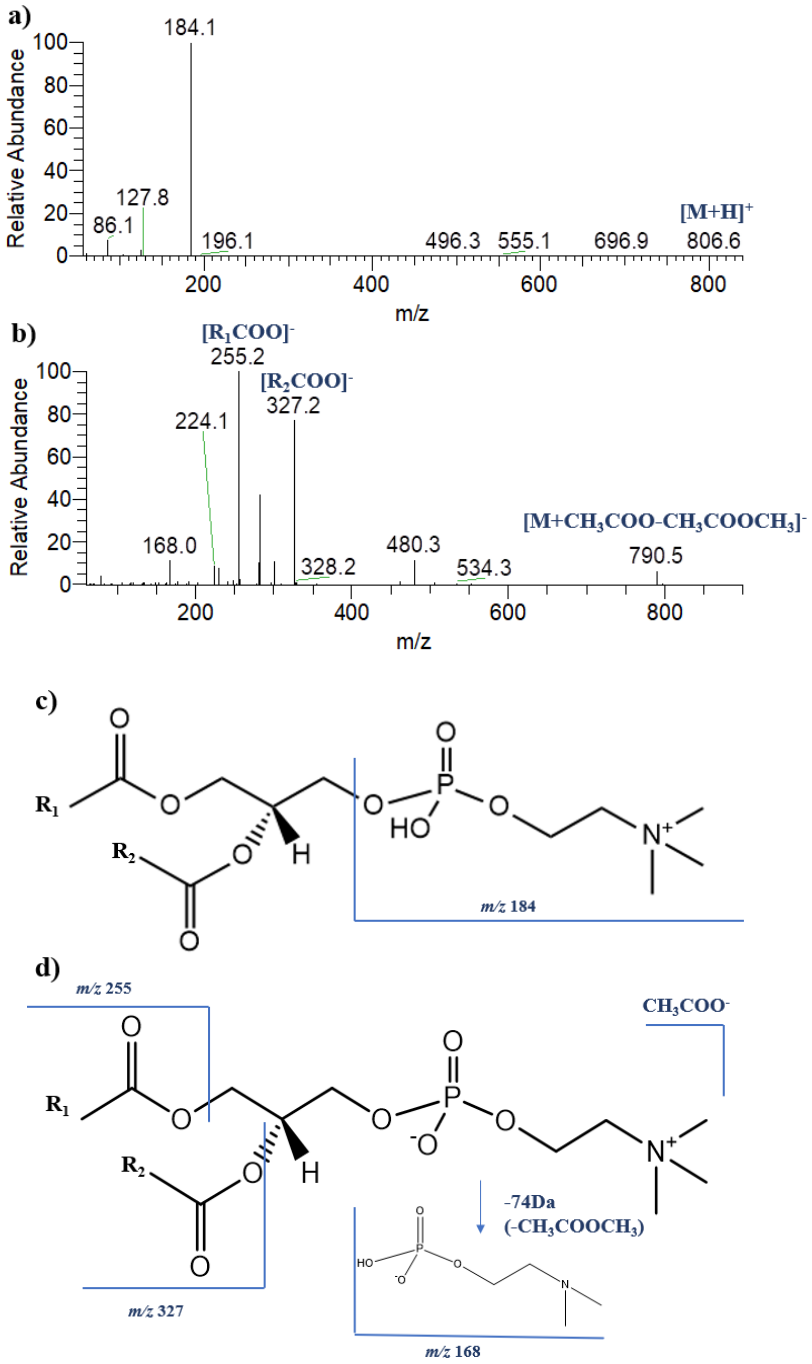
125. Huang, M. *et al.* Growth and lipidomic responses of juvenile pacific white shrimp *Litopenaeus vannamei* to low salinity. *Front. Physiol.* **10**, 1087 (2019). doi:10.3389/fphys.2019.01087

126. Relvas, P. & Barton, E. D. Mesoscale patterns in the Cape São Vicente (Iberian Peninsula) upwelling region. *J. Geophys. Res. Oceans* **107**, 28-1-28–23 (2002). doi:10.1029/2000JC000456

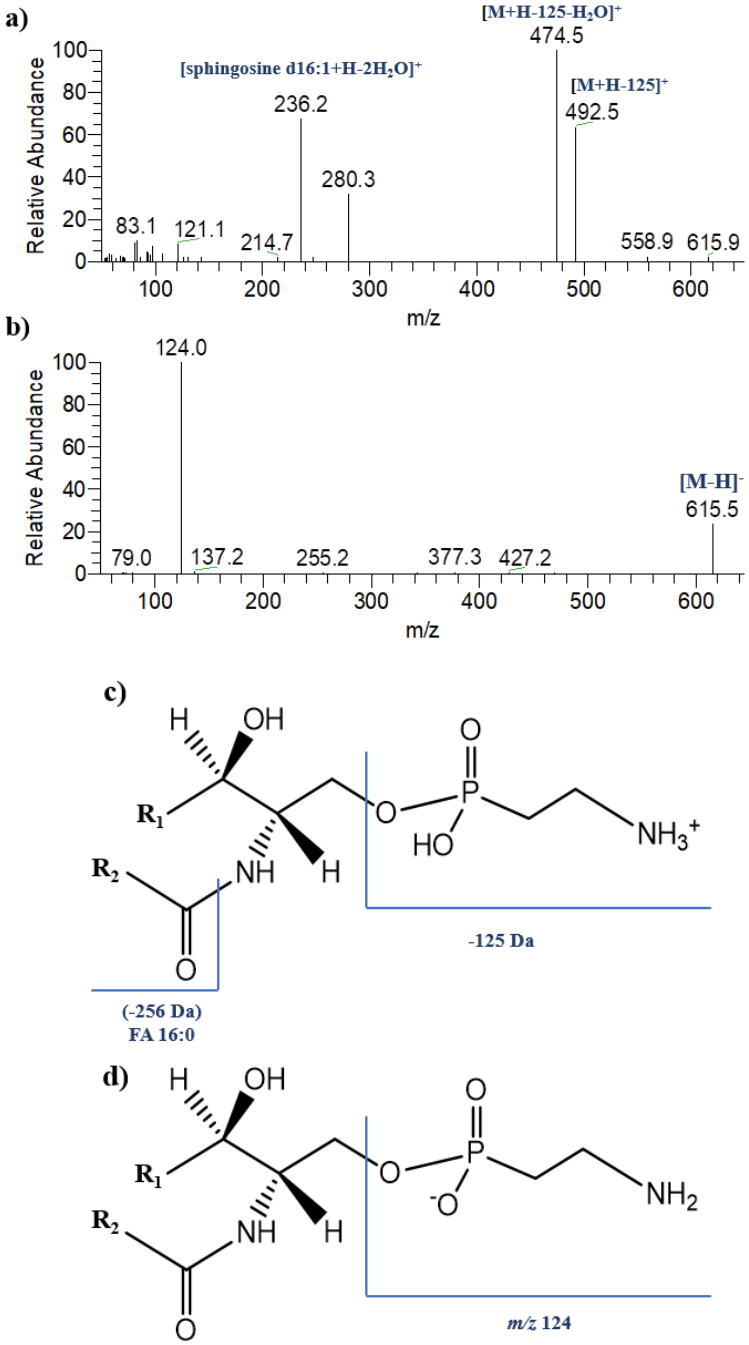
## Supplementary data



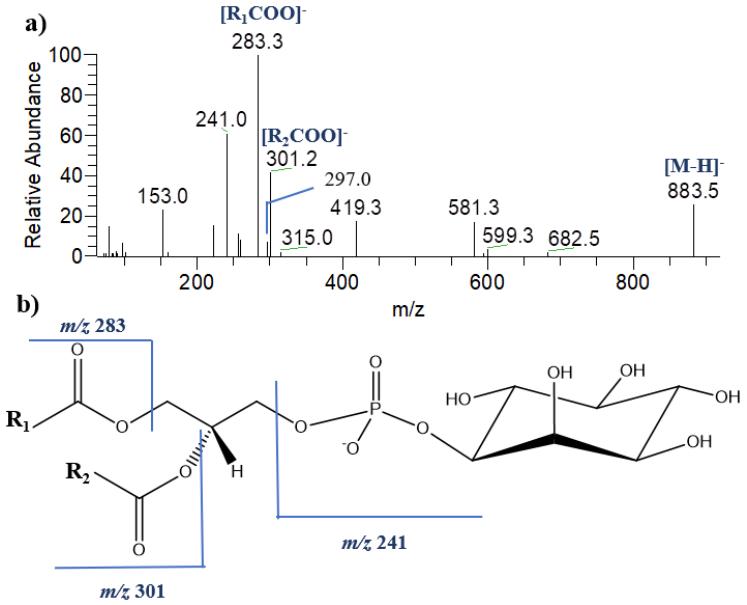

**Supplementary Figure S1 Phosphatidylethanolamine (PE) identification. a)** HILIC-ESI-MS/MS spectrum of PE (38:6; 16:0/22:6) corresponding to $[M+H]^+$ ion at *m/z* 764.5. b) HILIC-ESI-MS/MS spectrum of PE (38:6; 16:0/22:6) as $[M-H]^-$ ion at *m/z* 762.5. c) Phospholipid class was confirmed through the identification of phosphoethanolamine head group as the neutral loss of -141 Da, in the positive mode. d) Molecular species composition was confirmed by the identification of product ions corresponding to the fatty acyl chains as carboxylate anions $[RCOO]^-$ seen at *m/z* 255.2 (16:0) and *m/z* 327.2 (22:6). LysoPE (LPE) class was confirmed following the same identification process, but only one product ion corresponding to fatty acyl chain was identified.



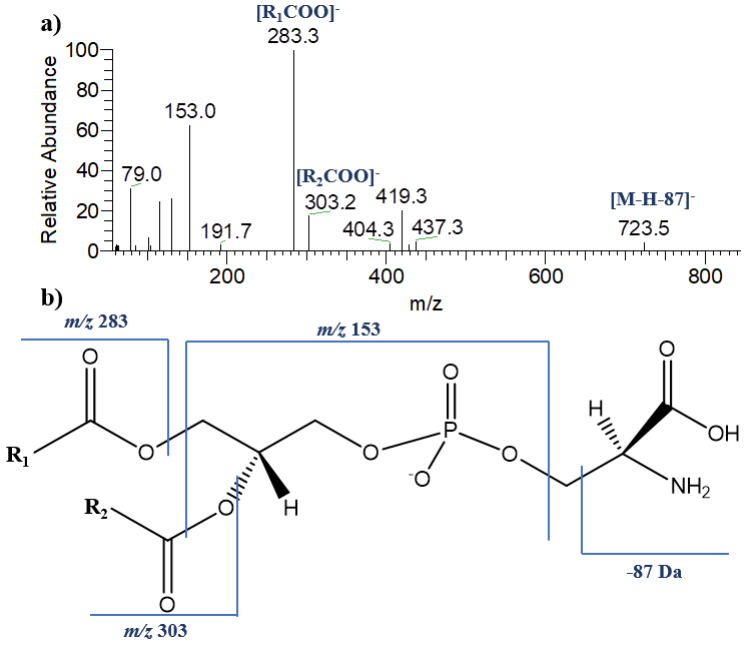

**Supplementary Figure S2 Phosphatidylcholine (PC) identification.** a) HILIC-ESI-MS/MS spectrum of PC (38:6; 16:0/22:6) corresponding to $[M+H]^+$ ion at *m/z* 806.5. b) HILIC-ESI-MS/MS spectrum of PC (38:6; 16:0/22:6) as $[M+CH_3COO]^-$ ion at *m/z* 864.5. c) Phospholipid class was confirmed through the identification of phosphocholine cation, at m/z 184, typical product of the polar head, in the positive mode. d) Molecular species composition was confirmed by the identification of product ions corresponding to the fatty acyl chains as carboxylate anions $[RCOO]^-$ seen at *m/z* 255.2 (16:0) and *m/z* 327.2 (22:6). In the negative mode, phospholipid class was confirmed through the identification the typical anion $[C_4H_{11}O_4NP]^-$, at m/z 168. LysoPC (LPC) class was confirmed following the same identification process, but only one product ion corresponding to fatty acyl chain was identified.



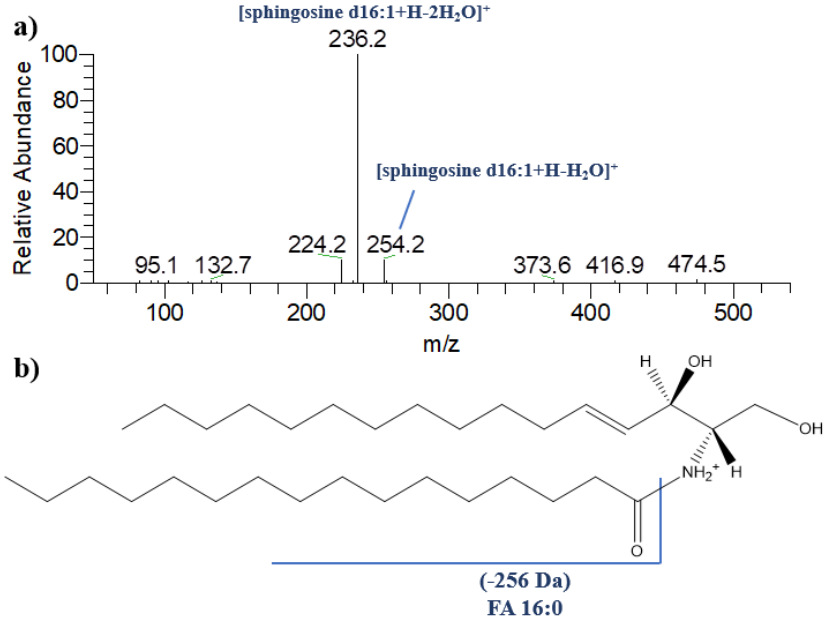

**Supplementary Figure S3 ceramides aminoethylphosphonates (CAEP) identification.** A) HILIC-ESI-MS/MS spectrum of CAEP (d32:1; d16:1/16:0) corresponding to $[M+H]^+$ ion at *m/z* 617.5. B) HILIC-ESI-MS/MS spectrum of CAEP (d32:1; d16:1/16:0) ion as $[M-H]^-$ at *m/z* 615.5. C) CAEP molecular species were confirmed through the identification of the headgroup aminoethylphosphonate as a neutral loss of -125 Da in positive mode. Molecular species composition was confirmed by the identification of the sphingoid base $[d16:1+H-2H_2O]^+$ seen at *m/z* 236.2 and the fatty acyl chain confirmed as a neutral loss between the ion $[M+H-125]^+$ at *m/z* 492.5 and the sphingosine $[d16:1+H-2H_2O]^+$. D) The aminoethylphosphonate anion, headgroup of CAEP, was confirmed in negative HILIC-ESI-MS/MS spectrum as *m/z* 124.



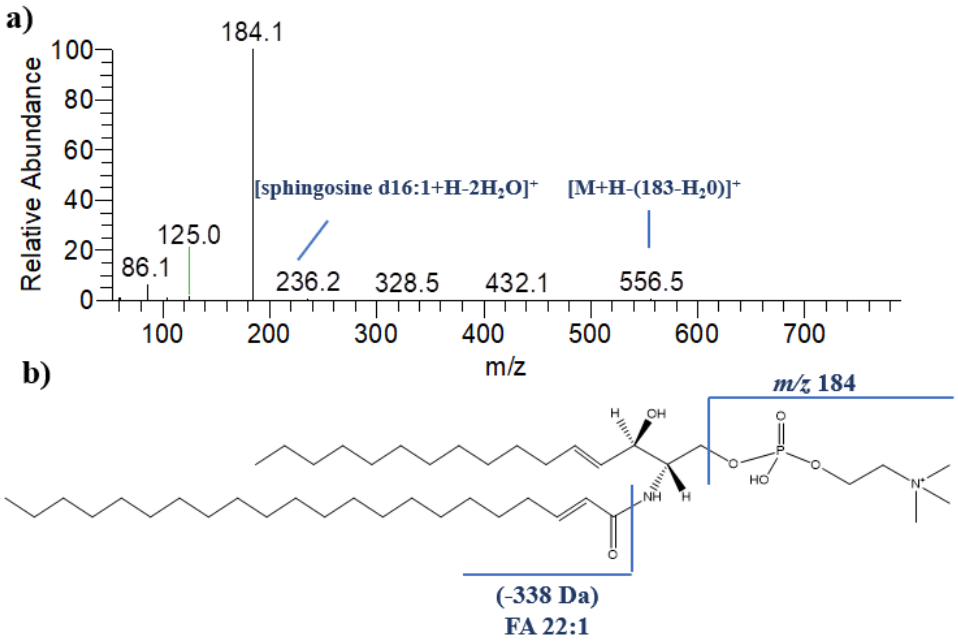

**Supplementary Figure S4 Phosphatidylinositol (PI) identification.** A) HILIC-ESI-MS/MS spectrum of PI (38:5; 18:0 /20:5) corresponding to $[M-H]^-$ ion at *m/z* 883.5. B) Phospholipid class was confirmed through the identification of the inositol head group by the product ions at *m/z* 223, *m/z* 241, *m/z* 297 and *m/z* 315. Molecular species composition was confirmed by the identification of product ions corresponding to the fatty acyl chains as carboxylate anions $[RCOO]^-$ seen at *m/z* 283.2 (18:0) and *m/z* 301.2 (20:5).



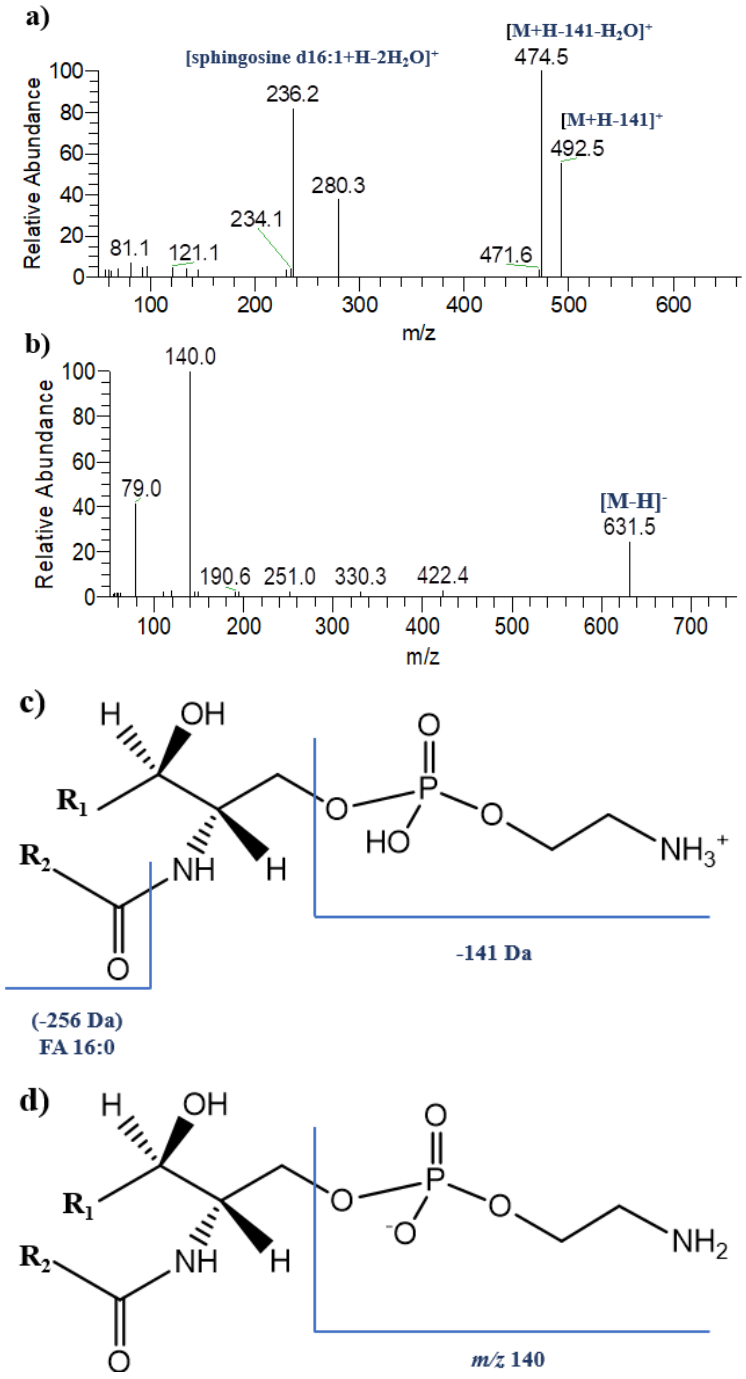

**Supplementary Figure S5 Phosphatidylserine (PS) identification.** A) HILIC-ESI-MS/MS spectrum of PS (38:4; 18:0/20:4) corresponding to $[M-H]^-$ ion at *m/z* 810.5. B) Phospholipid class was confirmed through the identification of glycerol phosphate anion $-H_2O$, ion at *m/z* 153, and the loss of -87 Da, corresponding to the serine moiety. Molecular species composition was confirmed by the identification of product ions corresponding to the fatty acyl chains as carboxylate anions $[RCOO]^-$ seen at *m/z* 283.3(18:0) and *m/z* 303.2 (20:4).



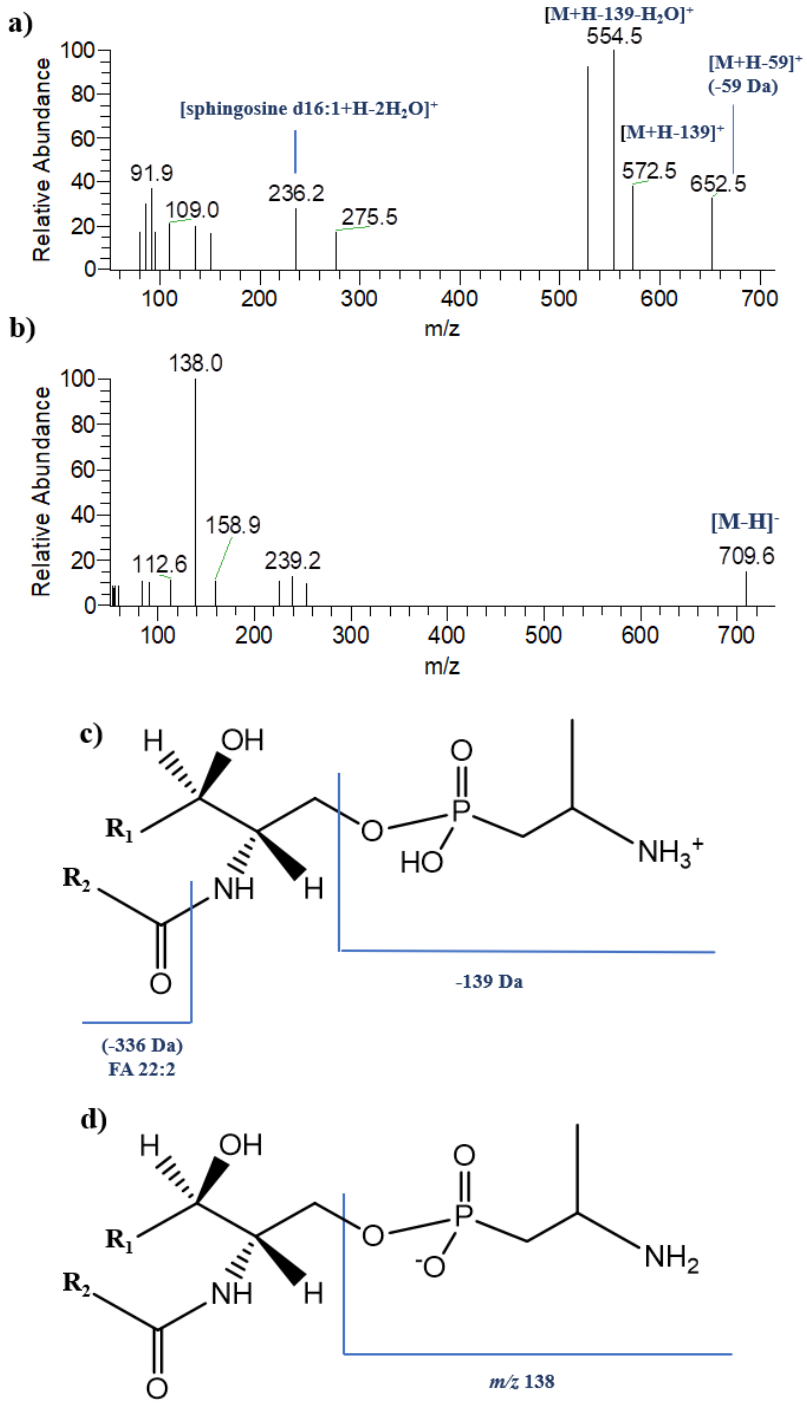

**Supplementary Figure S6 Ceramide (Cer) identification.** A) HILIC-ESI-MS/MS spectrum of Cer (d32:1; d16:1/16:0) corresponding to $[M+H]^+$ ion at *m/z* 510.5. B) Molecular species composition was confirmed by the identification of the sphingoid base $[d16:1+H-2H_2O]^+$ seen at *m/z* 236.2 and the fatty acyl chain confirmed as neutral loss between the ion $[M+H]^+$ at *m/z* 510.5 and the sphingosine base $[d16:1 +H-H_2O]^+$.



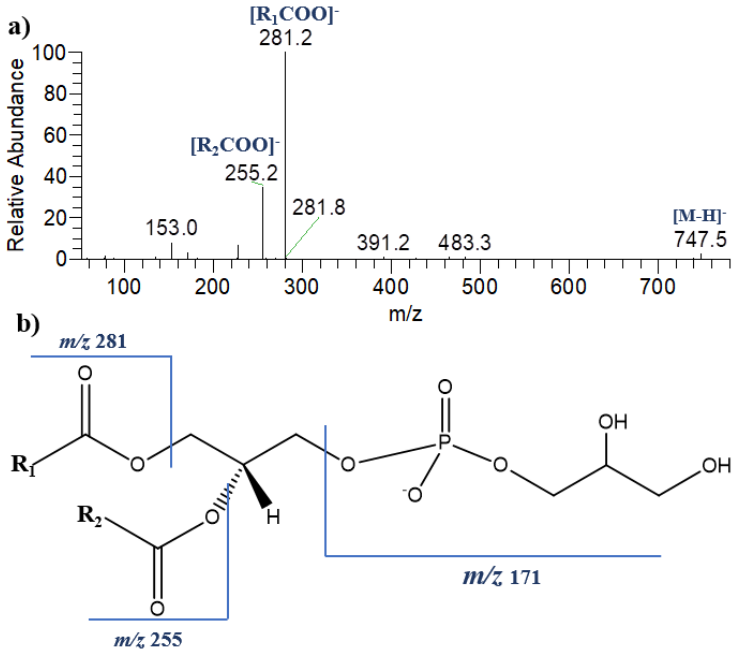

**Supplementary Figure S7 sphingomyelin (SM) identification.** A) HILIC-ESI-MS/MS spectrum of SM (d38:2; d16:1/22:1) corresponding to $[M+H]^+$ ion at *m/z* 757.6. B) SM were confirmed through the identification of phosphocholine head group, at *m/z* 184.1. Molecular species composition was confirmed by the identification of the sphingoid base $[d16:1 -2H_2O+H]^+$ seen at *m/z* 236.2 and the fatty acyl chain confirmed as a neutral loss between the ion $[M+H-(183-H_2O)]^+$ at *m/z* 556.6 and the sphingosine $[d16:1+H-H_2O]^+$.



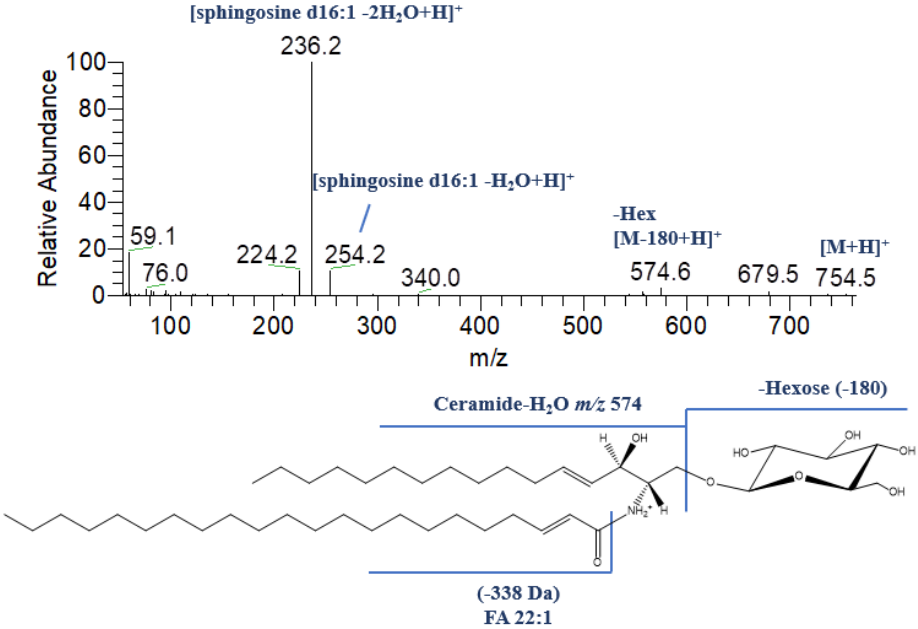

**Supplementary Figure S8 ceramides phosphoethanolamines (CPE) identification.** A) HILIC-ESI-MS/MS spectrum of CPE (d32:1; d16:1/16:0) corresponding to $[M+H]^+$ ion at *m/z* 633.5. B) HILIC-ESI-MS/MS spectrum of CPE (d32:1; d16:1/16:0) ion as $[M-H]^-$ at *m/z* 631.5. C) CPE molecular species were confirmed through the identification of the headgroup phosphoethanolamine as a neutral loss of -141 Da. Molecular species composition was confirmed by the identification of the sphingoid base $[d16:1+H-2H_2O]^+$ seen at *m/z* 236.2 and the fatty acyl chain confirmed as a neutral loss between the ion $[M+H-141]^+$ at *m/z* 492.5 and the sphingosine $[d16:1+H-2H_2O]^+$. D) The phosphoethanolamine anion, headgroup of CPE, was confirmed in negative HILIC-ESI-MS/MS spectrum as *m/z* 140.



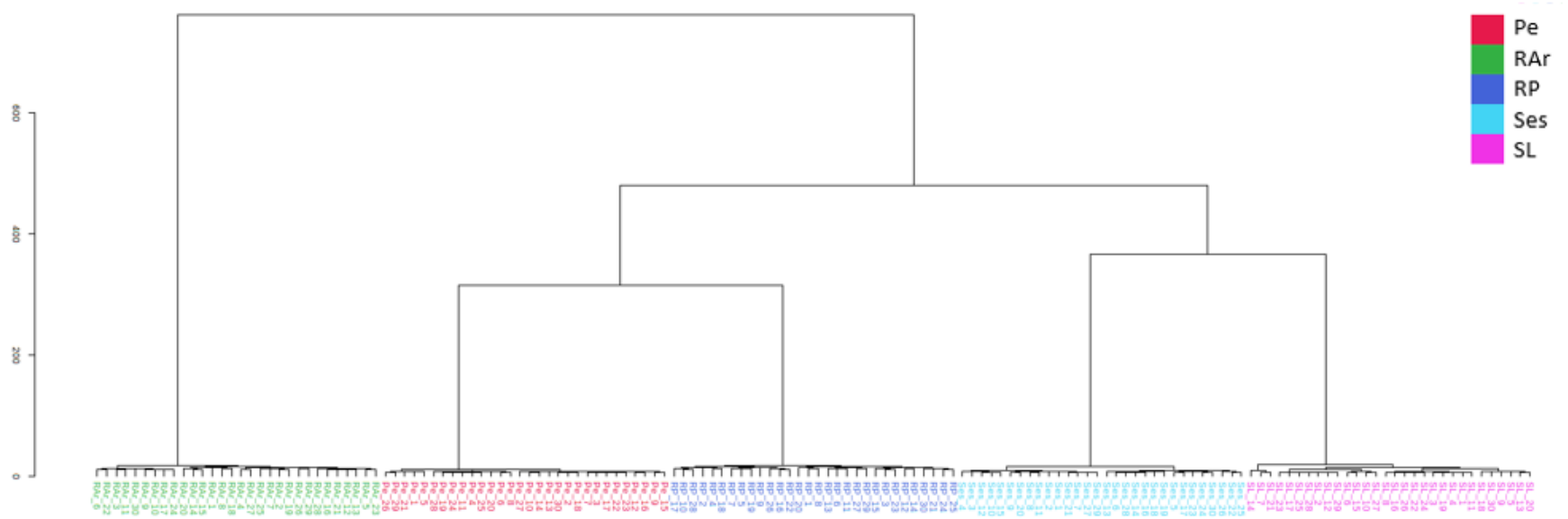

**Supplementary Figure S9 *N*-methyl ceramides aminoethylphosphonates (*N*-$CH_3$-CAEP) identification.** A) HILIC-ESI-MS/MS spectrum of *N*-$CH_3$-CAEP (d38:3; d16:1/22:2) corresponding to $[M+H]^+$ ion at *m/z* 711.6. B) HILIC-ESI-MS/MS spectrum of *N*-$CH_3$-CAEP (d38:3; d16:1/22:2) ion as $[M-H]^-$ at *m/z* 709.6. C) *N*-$CH_3$-CAEP molecular species were confirmed through the identification of the headgroup *N*-methyl aminoethylphosphonate as a neutral loss of -139 Da. Molecular species composition was confirmed by the identification of the sphingoid base $[d16:1+H-2H_2O]^+$ seen at *m/z* 236.2 and the fatty acyl chain confirmed as a neutral loss between the ion $[M+H-139]^+$ at *m/z* 572.5 and the sphingosine $[d16:1+H-2H_2O]^+$. D) The *N*-methyl phosphonoethylamine anion, headgroup of *N*-$CH_3$-CAEP, was confirmed in negative HILIC-ESI-MS/MS spectrum as *m/z* 138.




**Supplementary Figure S10 Phosphatidylglycerol (PG) identification.** A) HILIC-ESI-MS/MS spectrum of PG (34:1; 16:0 /18:1) corresponding to $[M-H]^-$ ion at *m/z* 747.5. B) Phospholipid class was confirmed through the identification of the polar head ions at *m/z* 153, *m/z* 171 and *m/z* 227, corresponding to glycerol phosphate anion $-H_2O$, glycerol phosphate anion and glycerolphosphate glycerol anion $-H_2O$, respectively. Molecular species composition was confirmed by the identification of product ions corresponding to the fatty acyl chains as carboxylate anions $[RCOO]^-$ seen at *m/z* 255.2 (16:0) and *m/z* 281.2 (18:1).




**Supplementary Figure S11 HexosylCeramide (HexCer) identification.** A) HILIC-ESI-MS/MS spectrum of HexCer (d38:2; d16:1/22:1) corresponding to $[M+H]^+$ ion at *m/z* 754.6. B) HexCer were confirmed through the identification of the neutral loss the hexose moiety (-180 Da). Molecular species composition was confirmed by the identification of the sphingoid base $[d16:1+H-2H_2O]^+$ seen at *m/z* 236.2 and the fatty acyl chain confirmed as a neutral loss between the ion $[M+H-180]^+$and the sphingosine $[d16:1+H-2H_2O]^+$.




**Supplementary Figure S12**. Hierarchical clustering using normalized areas from all lipid species identified in *Octopus vulgaris* samples. Abbreviations: Pe, Peniche; RAr, Ria Arousa; RP, Ria Pontevedra; Ses, Sesimbra; SL, Santa Luzia.

**Table S1.** Total molecular species of the different lipid classes identified by LC-MS and MS/MS in *Octopus vulgaris* specimens captured and landed along the Atlantic coast of the Iberian Peninsula. Labels of lipid species are according to the notation: AAA (C:N), (AAA, lipid class; C, total carbon atoms; N, total double bonds of fatty acid substituents) and AAA (O-C:N)(P-C:N) correspond to O- plasmanyl; P-plasmenyl, respectively). Molecular species identified by retention time, mass accuracy calculation and typical ion product are marked with (*) and molecular species identified only by retention time and mass accuracy calculation are marked with (**). Bold lipid species were not considered in the statistical analysis for discrimination between locations.

| Lipid species (C:N) | Library *m/z* | Observed *m/z* | Fatty acyl chains | Error (ppm) |
|---|---|---|---|---|
| **[M-H]$^-$** | | | | |
| PG(O-34:4)(P-34:3)** | 727.4914 | 727.4932 | | 2.474 |
| PG(34:1) | 747.5176 | 747.521 | 16:0/18:1 | 4.548 |
| PG(36:5) | 767.4863 | 767.489 | 16:0/20:5 | 3.518 |
| PG(40:6)** | 821.5333 | 821.5344 | | 1.881 |
| **[M-H]$^-$** | | | | |
| PI(34:4)** | 829.4867 | 829.4858 | | -1.085 |
| PI(34:2)** | 833.518 | 833.5164 | | -1.920 |
| PI(O-36:5) | 841.5231 | 841.5266 | O-16:0/20:5 | 4.159 |
| PI(O-36:4)(P-36:3)** | 843.5388 | 843.5373 | | -1.778 |
| PI(O-36:3)(P-36:2)* | 845.5544 | 845.5505 | | -4.612 |
| PI(36:5) | 855.5024 | 855.5063 | 16:0/20:5 | 4.559 |
| PI(36:4) | 857.518 | 857.5157 | 16:0/20:4; 18:2/18:2 | -2.682 |
| PI(36:3) | 859.5337 | 859.5326 | 16:0:20:3 | -1.280 |
| PI(36:2) | 861.5493 | 861.5507 | 16:0/20:2 | 1.625 |
| **PI (37:5)** | 869.5186 | 869.5196 | 17:0/20:5 | 1,150 |
| PI(O-38:5)(P-38:4) | 869.5544 | 869.5585 | O-18:0/20:5; P-18:0/20:4; | 4.715 |
| PI(O-38:4) | 871.5701 | 871.5707 | O-18:0/20:4 | 0.688 |
| PI(O-38:3) | 873.5857 | 873.5822 | O-18:0/20:3 | -4.006 |
| PI(38:6) | 881.518 | 881.5217 | 18:1/20:5; 16:0/22:6 | 4.197 |
| PI(38:5) | 883.5337 | 883.5378 | 18:0/20:5; 18:1/20:4; 16:0/22:5 | 4.640 |
| PI(38:4) | 885.5493 | 885.5473 | 18:0/20:4 | -2.258 |
| PI(38:3) | 887.565 | 887.5619 | 18:0/20:3 | -3.493 |
| PI(38:2) | 889.5806 | 889.5819 | 18:0/20:2 | 1.461 |
| PI(38:1) | 891.5963 | 891.5968 | 18:0/20:1 | 0.561 |

| | | | | |
|---|---|---|---|---|
| **PI (39:5)** | 897.5499 | 869.5426 | 19:0/20:5 | 0,891 |
| PI(O-40:5)(P-40:4)* | 897.5857 | 897.583 | | -3.008 |
| PI(40:10) | 901.4867 | 901.4908 | 20:5/20:5 | 4.548 |
| PI(40:9) | 903.5024 | 903.5034 | 20:4/20:5 | 1.107 |
| PI(40:8) | 905.518 | 905.5199 | 20:3/20:5 | 2.098 |
| PI(40:7) | 907.5337 | 907.5363 | 20:2/20:5; 18:1/22:6 | 2.865 |
| PI(40:6) | 909.5493 | 909.5531 | 20:5/20:1 | 4.178 |
| PI(40:5)** | 911.565 | 911.5638 | | -1.316 |
| PI(40:4) | 913.5806 | 913.5799 | 18:0/22:4; 20:1/20:3 | -0.766 |
| PI(40:3) | 915.5963 | 915.5946 | 20:1/20:2 | -1.857 |
| PI(42:10) | 929.518 | 929.5204 | 20:5/22:5 | 2.582 |
| PI(42:9) | 931.5337 | 931.5382 | 20:4/22:5; 20:5/22:4 | 4.831 |
| PI(42:8)** | 933.5493 | 933.5511 | | 1.928 |
| PI(42:7) | 935.565 | 935.5695 | 22:2/20:5; 20:1/22:6 | 4.810 |
| **$[M-H]^-$** | | | | |
| PS(34:1) | 760.5129 | 760.5142 | 16:0/18:1 | 1.709 |
| PS(36:6)** | 778.4659 | 778.4687 | | 3.597 |
| PS(36:4) | 782.4972 | 782.4998 | 16:0/20:4 | 3.323 |
| PS(36:3)** | 784.5129 | 784.5139 | | 1.275 |
| PS(36:2)** | 786.5285 | 786.5327 | | 5.340 |
| PS(36:1) | 788.5442 | 788.5484 | 18:0/18:1 | 5.326 |
| PS(O-38:6)(P-38:5) | 792.518 | 792,5220 | O-16:0/22:6; P-18:0/20:5 | 5,047 |
| PS(O-38:5)(P-38:4)** | 794.5336 | 794.5369 | | 4.153 |
| **PS(37:4)** | 796.5134 | 796.5156 | 17:0/20:4 | 2.762 |
| PS(O-38:4) | 796.5493 | 796.5498 | O-18:0/20:4 | 0.628 |
| PS(38:5) | 808.5129 | 808.5166 | 18:0/20:5; 16:0/22:5 | 4.576 |
| PS(38:4) | 810.5285 | 810.531 | 18:0/20:4; 16:0/22:4 | 3.084 |
| PS(38:3)** | 812.5442 | 812.5401 | | -5.046 |
| PS(38:1)** | 816.5755 | 816.5796 | | 5.021 |
| PS(O-40:6) | 820.5493 | 820.5528 | O-18:0/22:6 | 4.265 |
| **PS(39:5)** | 822.5291 | 822.5292 | 17:0/22:5 | 0.122 |
| PS(O-40:5) | 822.5649 | 822.5642 | O-18:0/22:5 | -0.851 |
| PS(40:9)** | 828.4816 | 828.4846 | | 3.621 |
| PS(40:8)** | 830.4972 | 830.5005 | | 3.974 |
| PS(40:5)** | 836.5442 | 836.5421 | | -2.510 |
| PS(40:4)** | 838.5598 | 838.5596 | | -0.239 |
| PS(40:3)** | 840.5755 | 840.5753 | | -0.238 |
| PS(40:2)** | 842.5911 | 842.5952 | | 4.866 |
| PS(40:1)** | 844.6068 | 844.6039 | | -3.434 |

| | | | | |
|---|---|---|---|---|
| PS(42:11) | 852.4816 | 852.4858 | 20:5/22:6 | 4.927 |
| PS(42:10)** | 854.4972 | 854.4992 | | 2.341 |
| PS(42:9) | 856.5129 | 856.5162 | 20:3/22:6 | 3.853 |
| PS(42:8)** | 858.5285 | 858.5314 | | 3.378 |
| PS(42:7) | 860.5442 | 860.5484 | 20:1/22:6 | 4.881 |
| PS(42:6)** | 862.5598 | 862.5596 | | -0.232 |
| PS(44:10)** | 882.5285 | 882.5323 | | 4.306 |
| **$[M+H]^+$** | | | | |
| PC(28:0) | 678.5074 | 678.5094 | 14:0/14:0 | 2.9742 |
| PC(O-30:2)(P-30:1)** | 688.5281 | 688.5247 | | -4.9628 |
| PC(O-30:1)(P-30:0)* | 690.5438 | 690.5455 | | 2.5096 |
| **PC(29:0)** | 692.5225 | 692.5256 | 14:0/15:0 | 4.4764 |
| PC(O-30:0) | 692.5594 | 692.5605 | O-14:0/16:0 | 1.5652 |
| PC(30:1) | 704.5230 | 704.5248 | 16:0/14:1 | 2.5095 |
| PC(30:0) | 706.5387 | 706.5406 | 14:0/16:0 | 2.7146 |
| PC(O-32:2)(P-32:1)* | 716.5594 | 716.559 | | -0.5806 |
| PC(O-32:1)(P-32:0) | 718.5751 | 718.5767 | O-16:1/16:0; P-16:0/16:0 | 2.2726 |
| PC(O-32:0) | 720.5907 | 720.5912 | O-16:0/16:0 | 0.6703 |
| PC(32:2)* | 730.5387 | 730.5406 | | 2.6255 |
| PC(32:1) | 732.5543 | 732.5564 | 16:0/16:1; 14:0/18:1 | 2.8244 |
| PC(32:0) | 734.5700 | 734.5709 | 16:0/16:0; 14:0/18:0 | 1.2497 |
| PC(O-34:5)(P-34:4)* | 738.5438 | 738.5454 | | 2.2111 |
| PC(O-34:4)(P-34:3)* | 740.5599 | 740.5578 | | -2.8924 |
| PC(O-34:3)(P-34:2)* | 742.5751 | 742.574 | | -1.4369 |
| PC(O-34:2)(P-34:1) | 744.5907 | 744.5919 | O-16:1/18:1; O-18:2/16:0; P-16:0/18:1; P-18:1/16:0 | 1.5888 |
| PC(O-34:1)(P-34:0) | 746.6064 | 746.6081 | O-16:0/18:1; P-18:0/16:0 | 2.3212 |
| **PC(33:0)** | 748.5851 | 748.5862 | 16:0/17:0 | 1.4694 |
| PC(O-34:0)* | 748.6220 | 748.6215 | | -0.6893 |
| PC(34:6) | 750.5074 | 750.5093 | 12:0/22:6 | 2.5556 |
| PC(34:5) | 752.5230 | 752.5252 | 14:0/20:5 | 2.8810 |
| PC(34:4) | 754.5387 | 754.5387 | 14:0/20:4 | 0.0239 |
| PC(34:3) | 756.5543 | 756.5553 | 16:0/18:3 | 1.2808 |
| PC(34:2) | 758.5700 | 758.5721 | 16:0/18:2 | 2.7921 |

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|---|---|---|---|---|
| PC(34:1) | 760.5856 | 760.5877 | 16:0/18:1 | 2.7190 |
| PC(O-36:6)(P-36:5) | 764.5594 | 764.5612 | O-14:0/22:6; O-16:1/20:5; P-16:0/20:5 | 2.3321 |
| PC(O-36:5)(P-36:4) | 766.5751 | 766.5763 | O-16:0/20:5; O-14:0/22:5; P-16:0/20:4 | 1.6085 |
| PC(O-36:4)(P-36:3)* | 768.5907 | 768.589 | | -2.2340 |
| PC(O-36:3) | 770.6064 | 770.6051 | O-16:0/20:3 | -1.6442 |
| PC(O-36:2)(P-36:1) | 772.6220 | 772.6229 | O-18:1/18:1; O-16:0/20:2; P- 18:0/18:1 | 1.1442 |
| PC(36:8) * | 774.5074 | 774.5076 | | 0.2815 |
| PC(O-36:1)(P-36:0) | 774.6377 | 774.6395 | O-16:0/20:1; O-18:0/18:1; P-18:0/18:0 | 2.3663 |
| PC(O-36:0)* | 776.6533 | 776.6496 | | -4.7640 |
| PC(36:6) | 778.5387 | 778.541 | 14:0/22:6 | 2.9774 |
| PC(36:5) | 780.5543 | 780.5563 | 16:0/20:5 | 2.5226 |
| PC(36:4) | 782.5700 | 782.5681 | 16:0/20:4 | -2.4049 |
| PC(36:3) | 784.5856 | 784.5831 | 18:1/18:2; 16:0/20:3 | -3.2272 |
| PC(36:2) | 786.6013 | 786.6029 | 18:1/18:1; 16:0/20:2 | 2.0570 |
| PC(36:1) | 788.6169 | 788.6187 | 16:0/20:1 | 2.2419 |
| PC(O-38:7)(P-38:6) | 790.5751 | 790.5768 | O-16:1/22:6; P-16:0/22:6 | 2.1921 |
| PC(36:0) | 790.6326 | 790.6295 | 16:0/20:0 | -3.9209 |
| PC(O-38:6)(P-38:5) | 792.5907 | 792.5925 | O-16:0/22:6; P-18:0/20:5 | 2.2496 |
| **PC(37:5)** | 794.5694 | 794.5702 | 17:0/20:5 | 1.0068 |
| PC(O-38:5)(P-38:4) | 794.6064 | 794.6045 | O-18:1/20:4; P-18:0/20:4 | -2.3496 |
| PC(O-38:4)(P-38:3)* | 796.6220 | 796.6205 | | -1.9030 |
| **PC(37:3)** | 798.6007 | 798.6001 | 17:0/20:3 | -0.7513 |
| PC(O-38:3)(P-38:2) | 798.6377 | 798.6340 | O-18:0/20:3; O-16:0/22:3; P-16:0/22:2; P-18:0/20:2 | -4.5916 |
| PC(38:9)* | 800.5230 | 800.5234 | | 0.4597 |
| **PC(37:2)** | 800.6164 | 800.6186 | 17:1/20:1; 18:1/19:1 | 2.7479 |
| PC(O-38:2)(P-38:1) | 800.6533 | 800.6543 | O-16:0/22:2; O-18:1/20:1; P-18:0/20:1 | 1.2277 |
| PC(38:8)* | 802.5387 | 802.5382 | | -0.6006 |
| **PC(37:1)** | 802.6320 | 802.6337 | 17:0/20:1; 18:0/19:1 | 2.1180 |
| PC(O-38:1) | 802.669 | 802.6694 | O-18:0/20:1 | 0.4983 |
| PC(38:7) | 804.5543 | 804.556 | 16:1/22:6 | 2.0744 |
| PC(38:6) | 806.5700 | 806.5722 | 16:0/22:6 | 2.7499 |

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|---|---|---|---|---|
| PC(38:5) | 808.5856 | 808.583 | 16:0/22:5 | -3.2551 |
| PC(38:4)* | 810.6013 | 810.6003 | | -1.2114 |
| PC(38:3) | 812.6169 | 812.6164 | 18:1/20:2; 16:0/22:3 | -0.6547 |
| PC(38:2) | 814.6326 | 814.634 | 18:1/20:1 | 1.7407 |
| PC(38:1) | 816.6482 | 816.6477 | 16:0/22:1 | -0.6514 |
| **PC(39:7)** | 818.5694 | 818.5703 | 17:1/22:6 | 1.0995 |
| PC(O-40:7)(P-40:6) | 818.6064 | 818.6079 | O-18:1/22:6; P-18:0/22:6; P-18:1/22:5 | 1.8727 |
| **PC(39:6)** | 820.5851 | 820.5871 | 17:0/22:6 | 2.4314 |
| PC(O-40:6) | 820.6220 | 820.6226 | O-18:0/22:6 | 0.7117 |
| **PC(39:5)** | 822.6007 | 822.6014 | 19:1/20:4; 17:0/22:5; 19:0/20:5 | 0.8510 |
| PC(O-40:5) | 822.6377 | 822,6336 | O-18:0/22:5; | -4,9439 |
| PC(O-40:4)(P-40:3)* | 824.6533 | 824.6524 | | -1.1120 |
| PC(40:10) | 826.5387 | 826.5399 | 20:5/20:5 | 1.4736 |
| PC(40:9)* | 828.5543 | 828.5537 | | -0.7616 |
| PC(O-40:2) | 828.6846 | 828.6853 | O-18:0/22:2 | 0.8447 |
| PC(40:8) | 830.5699 | 830.5696 | 18:2/22:6; 20:4/20:4; 20:3/20:5 | -0.3997 |
| PC(O-40:1) | 830.7003 | 830.7024 | O-18:0/22:1 | 2.5280 |
| PC(40:7) | 832.5856 | 832.5874 | 18:1/22:6; 20:2/20:5 | 2.1235 |
| PC(40:6) | 834.6013 | 834.6028 | 20:1/20:5; 18:0/22:6; 18:1/22:5 | 1.8188 |
| PC(40:5) | 836.6169 | 836.6145 | 20:1/20:4; 18:0/22:5 | -2.9069 |
| PC(40:4) | 838.6326 | 838.6283 | 18:0/22:4 | -5.1059 |
| PC(40:3) | 840.6482 | 840.6467 | 20:1/20:2 | -1.8224 |
| PC(40:2) | 842.6639 | 842.6656 | 20:1/20:1; 18:1/22:1 | 2.0388 |
| PC(40:1)* | 844.6795 | 844.676 | | -4.1815 |
| **PC(41:7)** | 846.6007 | 846.6023 | 19:1/22:6 | 1.8899 |
| PC(O-42:7)(P-42:6)* | 846.6377 | 846.6396 | | 2.2831 |
| **PC(41:6)** | 848.6164 | 848.6189 | 19:0/22:6 | 2.9460 |
| PC(O-42:6)(P-42:5) | 848.6533 | 848.6527 | O-18:0/24:6; O-18:1/24:5; P-18:0/24:5 | -0.7270 |
| PC(O-42:5)(P-42:4)* | 850.6690 | 850.6656 | | -3.9581 |
| PC(42:11) | 852.5543 | 852.5564 | 20:5/22:6 | 2.4268 |
| PC(42:10) | 854.5700 | 854.5685 | | -1.7342 |
| PC(42:9) | 856.5856 | 856.5859 | 20:3/22:6; 20:5/22:4 | 0.3129 |
| PC(42:8) | 858.6013 | 858.6019 | 20:2/22:6; 20:3/22:5 | 0.7198 |
| PC(42:7) | 860.6169 | 860.6189 | 20:1/22:6; 20:2/22:5 | 2.2867 |

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|---|---|---|---|---|
| PC(42:6) | 862.6326 | 862.6288 | 20:1/22:5; 20:2/22:4; 18:1/24:5 | -4.3843 |
| PC(42:5) | 864.6482 | 864.649 | 20:1/22:4; 20:4/22:1 | 0.8882 |
| **PC(43:7)** | **874.6320** | **874.6339** | **21:1/22:6** | **2.1723** |
| PC(O-44:7)(P-44:6)* | 874.6690 | 874.6715 | | 2.8960 |
| PC(44:12)* | 878.5700 | 878.5721 | | 2.4107 |
| PC(44:11) | 880.5856 | 880.585 | 22:5/22:6 | -0.7177 |
| PC(44:10)* | 882.6013 | 882.6007 | | -0.6594 |
| PC(44:9) | 884.6169 | 884.6144 | 22:3/22:6; 20:3/24:6 | -2.8623 |
| PC(44:8) | 886.6326 | 886.6357 | 22:2/22:6 | 3.5167 |
| PC(44:7) | 888.6482 | 888.6504 | 22:1/22:6; 20:1/24:6 | 2.4397 |
| PC(44:6) | 890.6639 | 890.6602 | 20:1/24:5 | -4.1340 |
| PC(46:12) | 906.6013 | 906.6038 | 22:6/24:6 | 2.7774 |
| **$[M+H]^+$** | | | | |
| LPC(O-14:1)(P-14:0)* | 452.3141 | 452.315 | | 1.9853 |
| LPC(O-14:0)* | 454.3298 | 454.3304 | | 1.4263 |
| LPC(14:1)* | 466.2934 | 466.2942 | | 1.7864 |
| LPC(14:0) | 468.3090 | 468.3101 | 14:0 | 2.3126 |
| LPC(O-16:1)(P-16:0)* | 480.3454 | 480.3459 | | 1.0368 |
| LPC(O-16:0)* | 482.3611 | 482.3617 | | 1.3434 |
| LPC(16:1) | 494.3247 | 494.3254 | 16:1 | 1.4828 |
| LPC(16:0) | 496.3403 | 496.3412 | 16:0 | 1.7810 |
| LPC(O-18:2)(P-18:1) * | 506.3611 | 506.3616 | | 1.0822 |
| LPC(O-18:1)(P-18:0)* | 508.3767 | 508.3777 | | 1.9631 |
| LPC(O-18:0)* | 510.3924 | 510.3924 | | 0.0940 |
| LPC(18:4)* | 516.3090 | 516.3092 | | 0.3544 |
| LPC(18:3)* | 518.3247 | 518.3234 | | -2.4444 |
| LPC(18:2) | 520.3403 | 520.3413 | 18:2 | 1.8911 |
| LPC(18:1) | 522.3560 | 522.3573 | 18:1 | 2.5519 |
| LPC(18:0) | 524.3716 | 524.3725 | 18:0 | 1.6839 |
| LPC(O-20:1)(P-20:0)* | 536.4080 | 536.4093 | | 2.4198 |
| LPC(20:5) | 542.3247 | 542.326 | 20:5 | 2.4579 |
| LPC(20:4) | 544.3403 | 544.3384 | 20:4 | -3.5199 |
| LPC(20:3) | 546.3560 | 546.3571 | 20:3 | 2.0737 |
| LPC(20:2) | 548.3716 | 548.3731 | 20:2 | 2.7044 |
| LPC(20:1) | 550.3873 | 550.3885 | 20:1 | 2.2402 |

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|---|---|---|---|---|
| LPC(22:6) | 568.3403 | 568.3418 | 22:6 | 2.6111 |
| LPC(22:5) | 570.3560 | 570.3566 | 22:5 | 1.1098 |
| LPC(22:4) | 572.3716 | 572.3715 | 22:4 | -0.2044 |
| LPC(22:1) | 578.4186 | 578.4199 | 22:1 | 2.3063 |
| LPC(24:1)* | 606.4487 | 606.4488 | | 0.2144 |
| **$[M+H]^+$** | | | | |
| PE(30:3)* | 658.4448 | 658.4439 | | -1,3395 |
| PE(30:0)* | 664.4917 | 664.4925 | | 1,1558 |
| PE(O-32:1)(P-32:0) | 676.5281 | 676.5288 | O-16:0/16:1; O-16:1/16:0; P-16:0/16:0 | 1,0096 |
| PE(32:1) | 690.5074 | 690.5082 | 16:0/16:1 | 1,1846 |
| PE(32:0) | 692.5230 | 692.5217 | 16:0/16:0 | -1,9234 |
| PE(O-34:6)(P-34:5) | 694.4812 | 694.4824 | O-14:1/20:5; P- 14:0/20:5 | 1,7769 |
| PE(O-34:5)(P-34:4)* | 696.4968 | 696.4942 | | -3,7574 |
| PE(O-34:4)(P-34:3)* | 698.5125 | 698.5127 | | 0,3336 |
| PE(O-34:1)(P-34:0) | 704.5594 | 704.5597 | O-18:0/16:1; O-16:0/18:1; P-18:0/16:0 | 0,4031 |
| PE(34:5) | 710.4761 | 710.4778 | 14:0/20:5 | 2,4181 |
| PE(34:4)** | 712.4917 | 712.4915 | | -0,3256 |
| PE(34:3) | 714.5074 | 714.5086 | 16:0/18:3 | 1,7047 |
| PE(34:2) | 716.5230 | 716.5249 | 16:0/18:2 | 2,6070 |
| PE(34:1) | 718.5387 | 718.5403 | 16:0/18:1 | 2,2518 |
| PE(O-36:7)(P-36:6) | 720.4968 | 720.4981 | O-14:1/22:6; P-16:1/20:5; P-14:0/22:6 | 1,7807 |
| PE(34:0)* | 720.5543 | 720.5517 | | -3,6514 |
| PE(O-36:6)(P-36:5) | 722.5125 | 722.514 | O-16:1/20:5; P-16:0/20:5 | 2,1218 |
| PE(O-36:5)(P-36:4) | 724.5281 | 724.5291 | O-16:0/20:5; O-16:1/20:4; P-16:0/20:4 | 1,3567 |
| PE(O-36:4) | 726.5438 | 726.5411 | O-16:0/20:4 | -3,6708 |
| PE(O-36:3)(P-36:2)* | 728.5594 | 728.5566 | | -3,8652 |
| PE(O-36:2)(P-36:1) | 730.5751 | 730.5767 | O-18:1/18:1; O-16:1/20:1; P-18:0/18:1; P-16:0/20:1 | 2,2352 |
| PE(36:8)* | 732.4604 | 732.4596 | | -1,1359 |
| PE(O-36:1)(P-36:0) | 732.5907 | 732.5917 | O-18:0/18:1; O-16:0/20:1; P-18:0/18:0 | 1,3418 |
| PE(36:7) | 734.4761 | 734.4731 | 16:2/20:5; 14:1/22:6 | -4,0600 |
| PE(36:6) | 736.4917 | 736.4935 | 16:1/20:5 | 2,4440 |

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|---|---|---|---|---|
| PE(36:5) | 738.5074 | 738.5095 | 16:0/20:5 | 2,8436 |
| PE(36:4) | 740.5230 | 740.5204 | 16:0/20:4 | -3,5542 |
| PE(36:3) | 742.5387 | 742.5384 | 16:0/20:3 | -0,4040 |
| PE(O-38:9)(P-38:8)* | 744.4968 | 744.4963 | | -0,6716 |
| PE(36:2) | 744.5543 | 744.5549 | 18:1/18:1; 16:0/20:2 | 0,8059 |
| PE(O-38:8)(P-38:7)* | 746.5125 | 746.5123 | | -0,2237 |
| PE(36:1) | 746.5670 | 746.5697 | 18:0/18:1; 16:0/20:1 | -0,3777 |
| PE(O-38:7)(P-38:6) | 748.5281 | 748.5298 | O-16:1/22:6; P-18:1/20:5; P-16:0/22:6 | 2,2711 |
| PE(O-38:6)(P-38:5) | 750.5438 | 750.5453 | O-18:1/20:5; P-18:0/20:5 | 2,0425 |
| PE(O-38:5)(P-38:4) | 752.5594 | 752.5593 | O-18:1/20:4; P-18:0/20:4 | -0,1541 |
| PE(O-38:4) | 754.5751 | 754.572 | O-18:0/20:4 | -4,1083 |
| **PE(37:3)** | 756.5538 | 756.5521 | 17:0/20:3 | -2.2470 |
| PE(O-38:3)(P-38:2) | 756.5907 | 756.5885 | O-18:0/20:3; P-18:0/20:2 | -2,9078 |
| PE(38:9)* | 758.4761 | 758.4749 | | -1,5584 |
| PE(O-38:2)(P-38:1) | 758.6064 | 758.6078 | O-16:0/22:2; P-18:0/20:1 | 1,8890 |
| PE(38:8)* | 760.4917 | 760.4911 | | -0,8310 |
| PE(O-38:1) | 760.6220 | 760.6225 | O-16:0/22:1 | 0,6363 |
| PE(38:7) | 762.5074 | 762.5046 | 16:1/22:6; 18:2/20:5 | -3,6721 |
| PE(38:6) | 764.5230 | 764.5247 | 16:0/22:6; 18:1/20:5 | 2,1818 |
| PE(38:5) | 766.5387 | 766.54 | 18:0/20:5 | 1,7194 |
| PE(O-40:11)(P-40:10)* | 768.4968 | 768.4948 | | -2,6025 |
| PE(38:4) | 768.5543 | 768.5526 | 18:0/20:4 | -2,2523 |
| PE(O-40:10)(P-40:9)* | 770.5125 | 770.5123 | | -0,2167 |
| PE(38:3)* | 770.5700 | 770.5702 | 18:0/20:3; 18:1/20:2 | 0,2829 |
| PE(O-40:9)(P-40:8)* | 772.5281 | 772.5275 | | -0,7987 |
| PE(38:2) | 772.5856 | 772.5836 | 16:0/22:2; 18:1/20:1 | -2,6301 |
| PE(P-40:7) | 774.5438 | 774.5436 | P-18:1/22:6 | -0,2156 |
| PE(38:1) | 774.6012 | 774.5992 | 18:0/20:1 | -2,6878 |
| PE(O-40:7)(P-40:6) | 776.5594 | 776.561 | O-18:1/22:6; P- 18:0/22:6 | 2,0604 |
| **PE(39:6)** | 778.5381 | 778.5402 | 17:0/22:6 | 2.6974 |
| PE(O-40:6)(P- | 778.5751 | 778.5752 | O-18:0/22:6; P- 18:0/22:5 | 0,1708 |

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|---|---|---|---|---|
| 40:5) | | | | |
| PE(O-40:5)(P-40:4) | 780.5907 | 780.5896 | O-18:0/22:5; O-18:1/22:4; P-18:0/22:4; | -1,4310 |
| PE(O-40:4) | 782.606367 | 782.6086 | O-18:0/22:4 | 2,8533 |
| PE(40:10) | 784.491732 | 784.491 | 20:5/20:5 | -0,9331 |
| PE(O-40:3)(P-40:2) | 784.622016 | 784.6225 | O-18:1/22:2; P-18:0/22:2 | 0,6169 |
| PE(40:9)* | 786.507382 | 786.5071 | | -0,3585 |
| PE(O-40:2)(P-40:1) | 786.637667 | 786.6377 | O-18:0/22:2; P-18:0/22:1 | 0,0420 |
| PE(40:8) | 788.523032 | 788.523 | 18:2/22:6; 20:4/20:4; 20:3/20:5 | -0,0406 |
| PE(O-40:1) | 788.653317 | 788.6509 | O-18:0/22:1 | -3,0647 |
| PE(40:7) | 790.538682 | 790.5395 | 18:1/22:6; 20:2/20:5 | 1,0347 |
| PE(40:6) | 792.554331 | 792.5559 | 20:1/20:5; 18:0/22:6 | 1,9797 |
| PE(O-42:12)(P-42:11)* | 794.512467 | 794.51 | | -3,1050 |
| PE(40:5) | 794.569982 | 794.5661 | 20:1/20:4; 20:5/20:0 | -4,8857 |
| PE(O-42:11)(P-42:10)* | 796.5281 | 796.5249 | | -4,0174 |
| PE(40:4) | 796.5856 | 796.5872 | 18:0/22:4 | 1,9684 |
| PE(O-42:10)(P-42:9)* | 798.5438 | 798.543 | | -0,9605 |
| PE(40:3)* | 798.6013 | 798.6027 | 18:0/22:3 | 1,7756 |
| PE(O-42:9)(P-42:8)* | 800.559 | 800.5578 | | -1,4990 |
| PE(40:2)* | 800.6169 | 800.6169 | | -0,0400 |
| PE(O-42:8)(P-42:7)* | 802.5751 | 802.5758 | | 0,8722 |
| PE(O-42:7)(P-42:6)* | 804.5907 | 804.5913 | | 0,7122 |
| **PE(41:6)** | 806.5694 | 806.5710 | 19:0/22:6 | 1.9837 |
| PE(O-42:6)(P-42:5) | 806.6064 | 806.6077 | O-18:0/24:6; O-18:1/24:5; P-18:0/24:5 | 1,6117 |
| PE(42:11) | 810.5074 | 810.5071 | 20:5/22:6 | -0,3479 |
| PE(42:10) | 812.5230 | 812.5208 | 20:4/22:6; 20:5/22:5 | -2,7470 |
| PE(42:9) | 814.5387 | 814.5384 | 20:3/22:6 | -0,3462 |
| PE(42:8) | 816.5543 | 816.5536 | 20:2/22:6 | -0,8952 |
| PE(42:7) | 818.5700 | 818.5717 | 20:1/22:6; 20:2/22:5; 22:2/20:5 | 2,0988 |
| PE(O-44:13)(P-44:12)* | 820.5281 | 820.5255 | | -3,1687 |

| | | | | |
|---|---|---|---|---|
| PE(42:6) | 820.5856 | 820.5828 | 22:1/20:5; 20:1/22:5 | -3,4512 |
| PE(O-44:12)(P-44:11)* | 822.5438 | 822.5409 | | -3,4855 |
| PE(42:5) | 822.6013 | 822.6038 | 20:1/22:4 | 3,0610 |
| PE(O-44:11)(P-44:10)* | 824.5594 | 824.5576 | | -2.2024 |
| PE(O-44:10)(P-44:9)* | 826.5751 | 826.5722 | | -3,5085 |
| PE(44:12) | 836.523 | 836.5229 | 22:6/22:6 | -0,1195 |
| PE(44:11)* | 838.5387 | 838.5371 | | -1.8866 |
| PE(44:10)* | 840.5543 | 840.5535 | | -0,9886 |
| PE(44:9)* | 842.5670 | 842.5662 | | -4,4886 |
| PE(44:8) | 844.5856 | 844.5854 | 22:6/22:2 | -0.2747 |
| PE(44:7)** | 846.6013 | 846.6031 | | 2,1474 |
| **$[M+H]^+$** | | | | |
| LPE(14:0) | 426.2621 | 426.2624 | 14:0 | 0.7812 |
| LPE(O-16:1)(P-16:0)* | 438.2985 | 438.2992 | | 1.7066 |
| LPE(O-16:0)* | 440.3141 | 440.3148 | | 1.5852 |
| LPE(16:1) | 452.2777 | 452.2788 | 16:1 | 2.3945 |
| LPE(16:0) | 454.2934 | 454.2942 | 16:0 | 1.8336 |
| **LPE(17:1)** | 466.2928 | 466.2945 | 17:1 | 3.6458 |
| LPE(O-18:1)(P-18:0)* | 466.3298 | 466.3308 | | 2.2473 |
| **LPE(17:0)** | 468.3085 | 468.3101 | 17:0 | 3.4166 |
| LPE(O-18:0) * | 468.3454 | 468.3462 | | 1.7039 |
| LPE(18:3)** | 476.2777 | 476.2763 | | -2.9752 |
| LPE(18:2) | 478.2934 | 478.2949 | 18:2 | 3.2051 |
| LPE(18:1) | 480.3090 | 480.31 | 18:1 | 2.0466 |
| LPE(18:0) | 482.3247 | 482.3256 | 18:0 | 1.9344 |
| LPE(P-20:0) * | 494.3611 | 494.362 | | 1.9176 |
| LPE(20:5) | 500.2777 | 500.2789 | 20:5 | 2.3647 |
| LPE(20:4) | 502.2934 | 502.2949 | 20:4 | 3.0520 |
| LPE(20:3) | 504.3090 | 504.3087 | 20:3 | -0.6286 |
| LPE(20:2) | 506.3247 | 506.3271 | 20:2 | 4.8052 |
| LPE(20:1) | 508.3403 | 508.3415 | 20:1 | 2.3291 |
| LPE(20:0)* | 510.3560 | 510.3565 | | 1.0463 |
| LPE(22:6) | 526.2934 | 526.2945 | 22:6 | 2.1528 |
| LPE(22:5)** | 528.3090 | 528.3096 | | 1.1035 |
| LPE(22:4) | 530.3247 | 530.3238 | 22:4 | -1.6348 |
| LPE(22:2)** | 534.3560 | 534.3573 | | 2.4946 |
| LPE(22:1)** | 536.3716 | 536.3733 | | 3.1377 |

| | | | | |
|---|---|---|---|---|
| LPE(24:6)** | 554.3247 | 554.3261 | | 2.5851 |
| **[M+H]$^+$** | | | | |
| Cer(d30:1) | 482.4573 | 482.4579 | d18:1/12:0 | 1.2043 |
| Cer(d32:3) | 506.4573 | 506.4559 | | -2.8018 |
| Cer(d32:1) | 510.4886 | 510.4893 | d16:1/16:0 | 1.3360 |
| Cer(d34:2) | 536.5043 | 536.5054 | d18:2/16:0 | 2.1081 |
| Cer(d34:1) | 538.5200 | 538.521 | d18:1/16:0 | 2.0074 |
| Cer(d36:3) | 562.5200 | 562.5213 | | 2.4550 |
| Cer(d36:2) | 564.5356 | 564.5366 | | 1.8263 |
| Cer(d36:1) | 566.5512 | 566.5523 | d18:1/18:0 | 1.9080 |
| Cer(d38:3) | 590.5512 | 590.5525 | d16:1/22:2 | 2.1692 |
| Cer(d38:2) | 592.5669 | 592.5679 | d16:1/22:1 | 1.7399 |
| Cer(d38:1) | 594.5825 | 594.5839 | d16:1/22:0 | 2.3226 |
| Cer(d40:2) | 620.5982 | 620.5991 | d16:1/24:1; d18:1/22:1 | 1.5002 |
| Cer(d40:1) | 622.6138 | 622.6141 | | 0.4513 |
| Cer(d42:2) | 648.6295 | 648.629 | | -0.7231 |
| Cer(d42:1) | 650.6451 | 650.6446 | | -0.7977 |
| **[M+H]$^+$** | | | | |
| SM(d30:1) | 647.5128 | 647.5147 | | 2.9328 |
| SM(d30:0)* | 649.528 | 649.5265 | | -3.0037 |
| SM(d32:2) | 673.5285 | 673.5297 | d16:1/16:1 | 1.8544 |
| SM(d32:1)* | 675.5441 | 675.546 | | 2.8111 |
| SM(d34:1) | 703.5754 | 703.5766 | d16:1/18:0 | 1.7042 |
| SM(d34:0)* | 705.5911 | 705.5909 | | -0.2140 |
| SM(d35:1) | 717.5911 | 717.5915 | d16:1/19:0 | 0.6257 |
| SM(d36:3) | 727.5754 | 727.5767 | d16:1/20:2; d18:1/18:2 | 1.7854 |
| SM(d36:2) | 729.5911 | 729.5924 | d16:1/20:1 | 1.8490 |
| SM(d36:1)* | 731.6067 | 731.6083 | | 2.1856 |
| SM(d38:3) | 755.6067 | 755.6086 | d18:1/20:2 | 2.5132 |
| SM(d38:2) | 757.6224 | 757.6239 | d16:1/22:1 | 2.0446 |
| SM(d40:2)* | 785.6537 | 785.6554 | | 2.2262 |
| SM(d42:2)** | 813.6850 | 813.6865 | | 1.9037 |
| **[M+H]$^+$** | | | | |
| HexCer(38:2) | 754.6197 | 754.6213 | d16:1/22:1 | 2.1282 |
| HexCer(d40:1) | 784.6667 | 784.6653 | | -1.7128 |
| **[M+H]$^+$** | | | | |
| **CPE(d32:1)** | 633.4972 | 633.4992 | d16:1/16:0 | 3.1571 |
| **CPE(d33:1)** | 647.5128 | 647.5150 | d16:1/17:0 | 3.3976 |
| **CPE(d34:1)** | 661.5285 | 661.5299 | d18:1/16:0; d16:1/18:0 | 2.1163 |
| **CPE(d35:3)** | 671.5128 | 671.5148 | d19:3/16:0 | 2.9783 |
| **CPE(d36:3)** | 685.5285 | 685.5301 | d14:0/22:3; d19:3/17:0 | 2.3340 |

| | | | | |
|---|---|---|---|---|
| **CPE(d36:2)*** | 687.5441 | 687.5431 | | -1.4545 |
| **CPE(d38:2)** | 715.5754 | 715.5775 | d16:1/22:1 | 2.9347 |
| **CPE(d40:2)** | 743.6067 | 743.6078 | d16:1/24:1 | 1.4793 |
| **$[M+H]^+$** | | | | |
| **CAEP(d30:1)** | 589.4709 | 589.4729 | d14:1/16:0 | 3.3929 |
| **CAEP(d31:1)** | 603.4866 | 603.4882 | d16:1/15:0; d15:1/16:0; d14:1/17:0 | 2.6513 |
| **CAEP(d32:1)** | 617.5022 | 617.5039 | d16:1/16:0 | 2.7530 |
| **CAEP(d33:1)** | 631.5179 | 631.5194 | d16:1/17:0 | 2.3752 |
| **CAEP(d34:2)** | 643.5179 | 643.52 | d18:2/16:0 | 3.2633 |
| **CAEP(d34:1)** | 645.5335 | 645.5351 | d18:1/16:0 | 2.4786 |
| **CAEP(d35:3)** | 655.5179 | 655.5195 | d19:3/16:0 | 2.4408 |
| **CAEP(d35:1)** | 659.5492 | 659.5508 | d19:1/16:0 | 2.4259 |
| **CAEP(d35:0)** | 661.5648 | 661.5667 | d19:0/16:0 | 2.8720 |
| **CAEP(d36:3)** | 669.5335 | 669.5351 | d19:3/17:0 | 2.3897 |
| **CAEP(d36:2)** | 671.5492 | 671.5506 | d16:1/20:1 | 2.0847 |
| **CAEP(d36:1)** | 673.5648 | 673.5665 | d16:1/20:0; d18:1/18:0; | 2.5239 |
| **CAEP(d37:3)** | 683.5492 | 683.551 | d19:3/18:0 | 2.6333 |
| **CAEP(d37:1)** | 687.5805 | 687.5821 | d16:1/21:0; d18:1/19:0 | 2.3270 |
| **CAEP(d38:4)** | 695.5492 | 695.5503 | d16:1/22:3 | 1.5815 |
| **CAEP(d38:3)** | 697.5648 | 697.5661 | d16:1/22:2 | 1.8636 |
| **CAEP(d38:2)** | 699.5805 | 699.5822 | d16:1/22:1 | 2.4300 |
| **CAEP(d39:4)** | 709.5648 | 709.5657 | d19:3/20:1 | 1.2684 |
| **CAEP(d39:3)** | 711.5805 | 711.5818 | d16:1/23:2 | 1.8269 |
| **CAEP(d39:2)** | 713.5961 | 713.5976 | d16:1/23:1 | 2.1020 |
| **CAEP(d40:5)** | 721.5648 | 721.564 | d16:1/24:4 | -1.1087 |
| **CAEP(d40:4)*** | 723.5805 | 723.5804 | | -0.1382 |
| **CAEP(d40:3)** | 725.5961 | 725.5978 | d18:2/22:1 | 2.3429 |
| **CAEP(d40:2)** | 727.6118 | 727.6133 | d18:1/22:1, d16:1/24:1 | 2.0615 |
| **CAEP(d41:4)** | 737.5961 | 737.5964 | d19:3/22:1 | 0.4067 |
| **CAEP(d41:3)** | 739.6118 | 739.6118 | d19:2/22:1 | 0.0000 |
| **CAEP(d41:2)** | 741.6274 | 741.6288 | d17:1/24:1 | 1.8877 |
| **CAEP(d41:1)** | 743.6431 | 743.64 | d16:1/25:0 | -4.1687 |
| **CAEP(d42:6)** | 747.5805 | 747.5813 | d16:1/26:5 | 1.0701 |
| **CAEP(d42:3)** | 753.6274 | 753.6288 | d18:2/24:1 | 1.8577 |
| **CAEP(d43:5)*** | 763.6117 | 763.6138 | | 2.7501 |
| **CAEP(d43:4)** | 765.6274 | 765.6296 | d19:3/24:1 | 2.8735 |
| **CAEP(d44:6)** | 775.6118 | 775.6135 | d16:1/28:5 | 2.1918 |
| **$[M+H]^+$** | | | | |
| **N-methyl-CAEP(d35:3)** | 669.5335 | 669.5351 | d19:3/16:0 | 2.3897 |
| **N-methyl-** | 711.5805 | 711.5823 | d16:1/22:2 | 2.5296 |

| | | | | |
|---|---|---|---|---|
| **CAEP(d38:3)** | | | | |
| **N-methyl-CAEP(d38:2)** | 713.5961 | 713.5979 | d16:1/22:1 | 2.5224 |
| **N-methyl-CAEP(d39:2)** | 727.6118 | 727.6138 | d16:1/23:1; d18:1/21:1 | 2.7487 |
| **N-methyl-CAEP(d39:1)** | 729.6274 | 729.6298 | d16:1/23:0 | 3.2894 |

**Table S2.** Relative abundance of lipid molecular species identified by LC-MS in *Octopus vulgaris* specimens captured and landed along the Atlantic coast of the Iberian Peninsula. Labels of lipid species are according to the notation: AAA (C:N), (AAA, lipid class; C, total carbon atoms; N, total double bonds of fatty acid substituents) and AAA (O-C:N)(P-C:N) correspond to O- plasmanyl; P- plasmenyl, respectively). Values are mean ± SD of thirty samples (n = 30).

| **Lipid specie** | **Pe** | | **Rar** | | **RP** | | **Ses** | | **SL** | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Avg | SD | Avg | SD | Avg | SD | Avg | SD | Avg | SD |
| **PG(O-34:4)(P-34:3)** | 5.36 | 0.62 | 4.53 | 1.13 | 6.18 | 0.98 | 4.43 | 0.42 | 5.46 | 0.71 |
| **PG(34:1)** | 79.33 | 1.29 | 54.18 | 9.12 | 79.52 | 1.87 | 81.35 | 0.97 | 79.03 | 1.11 |
| **PG(36:5)** | 7.01 | 0.57 | 33.96 | 10.66 | 5.46 | 1.10 | 3.73 | 0.35 | 4.87 | 0.62 |
| **PG(40:6)** | 8.30 | 0.49 | 7.33 | 1.34 | 8.84 | 0.60 | 10.49 | 0.60 | 10.64 | 0.56 |
| **PI(34:4)** | 0.02 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.02 | 0.00 | 0.04 | 0.01 |
| **PI(34:2)** | 0.02 | 0.00 | 0.02 | 0.01 | 0.04 | 0.01 | 0.04 | 0.00 | 0.04 | 0.00 |
| **PI(O-36:5)(P-36:4)** | 0.28 | 0.04 | 0.17 | 0.02 | 0.25 | 0.05 | 0.38 | 0.03 | 0.55 | 0.05 |
| **PI(O-36:4)(P-36:3)** | 0.11 | 0.01 | 0.11 | 0.02 | 0.14 | 0.01 | 0.18 | 0.01 | 0.17 | 0.01 |
| **PI(O-36:3)(P-36:2)** | 0.07 | 0.00 | 0.03 | 0.01 | 0.07 | 0.02 | 0.08 | 0.01 | 0.06 | 0.00 |
| **PI(36:5)** | 12.12 | 1.18 | 8.30 | 0.72 | 9.57 | 1.48 | 15.02 | 0.76 | 16.84 | 0.70 |
| **PI(36:4)** | 3.75 | 0.30 | 2.83 | 0.24 | 3.23 | 0.46 | 3.85 | 0.19 | 4.06 | 0.26 |
| **PI(36:3)** | 0.40 | 0.03 | 0.27 | 0.03 | 0.33 | 0.04 | 0.42 | 0.03 | 0.33 | 0.04 |
| **PI(36:2)** | 0.09 | 0.01 | 0.07 | 0.01 | 0.08 | 0.01 | 0.14 | 0.02 | 0.18 | 0.01 |
| **PI(O-38:5)(P-38:4)** | 0.50 | 0.04 | 0.48 | 0.04 | 0.57 | 0.09 | 0.90 | 0.07 | 1.18 | 0.07 |
| **PI(O-38:4)(P-38:3)** | 0.32 | 0.03 | 0.46 | 0.05 | 0.44 | 0.05 | 0.59 | 0.05 | 0.51 | 0.03 |
| **PI(O-38:3)(P-38:2)** | 0.03 | 0.00 | 0.06 | 0.01 | 0.05 | 0.01 | 0.06 | 0.00 | 0.04 | 0.01 |
| **PI(38:6)** | 5.42 | 0.44 | 4.09 | 0.20 | 4.97 | 0.54 | 4.17 | 0.26 | 4.17 | 0.20 |
| **PI(38:5)** | 46.21 | 1.71 | 45.29 | 1.89 | 43.83 | 2.00 | 45.24 | 1.35 | 44.81 | 1.06 |
| **PI(38:4)** | 14.62 | 1.12 | 16.12 | 1.35 | 15.87 | 1.04 | 13.41 | 0.64 | 11.78 | 0.57 |
| **PI(38:3)** | 1.34 | 0.12 | 1.53 | 0.19 | 1.47 | 0.16 | 1.50 | 0.09 | 1.18 | 0.12 |
| **PI(38:2)** | 0.14 | 0.02 | 0.54 | 0.12 | 0.33 | 0.07 | 0.23 | 0.02 | 0.23 | 0.02 |
| **PI(38:1)** | 0.13 | 0.02 | 0.00 | 0.00 | 0.16 | 0.03 | 0.14 | 0.01 | 0.19 | 0.02 |
| **PI(O-40:5)(P-40:4)** | 0.02 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 0.03 | 0.00 | 0.02 | 0.00 |
| **PI(40:10)** | 3.91 | 0.32 | 6.33 | 0.64 | 4.19 | 0.34 | 3.61 | 0.25 | 3.48 | 0.21 |
| **PI(40:9)** | 1.89 | 0.19 | 2.57 | 0.26 | 2.36 | 0.23 | 1.71 | 0.13 | 1.60 | 0.17 |
| **PI(40:8)** | 1.22 | 0.12 | 1.73 | 0.23 | 1.13 | 0.11 | 1.25 | 0.12 | 0.92 | 0.08 |
| **PI(40:7)** | 0.85 | 0.06 | 1.04 | 0.12 | 0.82 | 0.05 | 0.96 | 0.10 | 0.70 | 0.05 |
| **PI(40:6)** | 4.43 | 0.34 | 4.31 | 0.21 | 6.33 | 0.51 | 4.12 | 0.19 | 4.97 | 0.30 |
| **PI(40:5)** | 1.57 | 0.07 | 2.40 | 0.24 | 2.72 | 0.26 | 1.43 | 0.06 | 1.48 | 0.13 |
| **PI(40:4)** | 0.29 | 0.03 | 0.56 | 0.07 | 0.53 | 0.04 | 0.24 | 0.02 | 0.22 | 0.03 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **PI(40:3)** | 0.03 | 0.01 | 0.39 | 0.11 | 0.19 | 0.04 | 0.06 | 0.01 | 0.02 | 0.01 |
| **PI(42:10)** | 0.12 | 0.01 | 0.12 | 0.01 | 0.13 | 0.01 | 0.09 | 0.00 | 0.10 | 0.01 |
| **PI(42:9)** | 0.05 | 0.00 | 0.06 | 0.01 | 0.04 | 0.01 | 0.04 | 0.00 | 0.02 | 0.00 |
| **PI(42:8)** | 0.01 | 0.00 | 0.02 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| **PI(42:7)** | 0.06 | 0.01 | 0.08 | 0.01 | 0.10 | 0.01 | 0.08 | 0.01 | 0.07 | 0.01 |
| **PS(34:1)** | 1.42 | 0.09 | 1.22 | 0.11 | 1.52 | 0.19 | 1.38 | 0.09 | 2.04 | 0.13 |
| **PS(36:6)** | 0.07 | 0.01 | 0.04 | 0.00 | 0.06 | 0.01 | 0.07 | 0.01 | 0.10 | 0.01 |
| **PS(36:4)** | 1.39 | 0.04 | 1.42 | 0.15 | 1.38 | 0.20 | 1.25 | 0.10 | 1.20 | 0.08 |
| **PS(36:3)** | 0.19 | 0.01 | 0.20 | 0.02 | 0.16 | 0.03 | 0.19 | 0.01 | 0.23 | 0.01 |
| **PS(36:2)** | 0.53 | 0.02 | 0.51 | 0.05 | 0.53 | 0.08 | 0.55 | 0.04 | 0.60 | 0.03 |
| **PS(36:1)** | 1.80 | 0.09 | 1.76 | 0.14 | 1.80 | 0.24 | 1.77 | 0.10 | 2.21 | 0.12 |
| **PS(O-38:6)(P-38:5)** | 8.84 | 0.38 | 7.50 | 0.81 | 9.72 | 1.02 | 9.68 | 0.44 | 11.78 | 0.54 |
| **PS(O-38:5)(P-38:4)** | 5.60 | 0.26 | 6.62 | 0.58 | 7.41 | 0.87 | 7.96 | 0.26 | 7.44 | 0.39 |
| **PS(O-38:4)(P-38:3)** | 4.09 | 0.36 | 6.05 | 0.94 | 6.61 | 0.55 | 6.88 | 0.44 | 5.30 | 0.28 |
| **PS(38:5)** | 19.00 | 0.56 | 17.79 | 1.35 | 17.78 | 1.43 | 18.08 | 0.79 | 18.34 | 1.06 |
| **PS(38:4)** | 9.87 | 0.33 | 11.49 | 1.10 | 10.67 | 0.90 | 9.09 | 0.61 | 7.43 | 0.28 |
| **PS(38:3)** | 1.28 | 0.05 | 1.48 | 0.17 | 1.34 | 0.13 | 1.19 | 0.09 | 0.97 | 0.07 |
| **PS(38:1)** | 0.67 | 0.03 | 0.81 | 0.09 | 0.59 | 0.07 | 0.63 | 0.04 | 0.69 | 0.04 |
| **PS(O-40:6)(P-40:5)** | 15.47 | 0.73 | 13.29 | 1.48 | 13.53 | 1.17 | 12.40 | 0.59 | 17.04 | 0.42 |
| **PS(O-40:5)(P-40:4)** | 2.88 | 0.12 | 2.80 | 0.30 | 2.97 | 0.35 | 2.85 | 0.10 | 3.34 | 0.11 |
| **PS(40:9)** | 0.75 | 0.02 | 0.51 | 0.06 | 0.54 | 0.05 | 0.67 | 0.03 | 0.63 | 0.03 |
| **PS(40:8)** | 0.66 | 0.03 | 0.62 | 0.06 | 0.53 | 0.05 | 0.69 | 0.06 | 0.61 | 0.05 |
| **PS(40:5)** | 8.70 | 0.27 | 9.33 | 0.75 | 7.96 | 0.73 | 9.00 | 0.55 | 8.04 | 0.34 |
| **PS(40:4)** | 1.43 | 0.07 | 1.85 | 0.17 | 1.48 | 0.16 | 1.30 | 0.09 | 1.02 | 0.05 |
| **PS(40:3)** | 0.20 | 0.01 | 0.30 | 0.02 | 0.21 | 0.03 | 0.19 | 0.02 | 0.12 | 0.01 |
| **PS(40:2)** | 0.71 | 0.04 | 0.92 | 0.09 | 0.76 | 0.09 | 0.88 | 0.05 | 0.76 | 0.04 |
| **PS(40:1)** | 0.05 | 0.01 | 0.09 | 0.01 | 0.05 | 0.01 | 0.07 | 0.01 | 0.05 | 0.00 |
| **PS(42:11)** | 0.60 | 0.04 | 0.46 | 0.07 | 0.30 | 0.04 | 0.49 | 0.05 | 0.25 | 0.03 |
| **PS(42:10)** | 0.35 | 0.02 | 0.30 | 0.04 | 0.24 | 0.04 | 0.29 | 0.02 | 0.16 | 0.02 |
| **PS(42:9)** | 2.17 | 0.18 | 2.29 | 0.25 | 1.52 | 0.16 | 2.33 | 0.20 | 1.56 | 0.11 |
| **PS(42:8)** | 1.47 | 0.14 | 1.53 | 0.17 | 0.89 | 0.10 | 1.25 | 0.10 | 0.71 | 0.05 |
| **PS(42:7)** | 7.42 | 0.40 | 6.63 | 1.19 | 7.08 | 0.53 | 6.81 | 0.47 | 5.64 | 0.41 |
| **PS(42:6)** | 2.16 | 0.08 | 2.01 | 0.24 | 2.18 | 0.19 | 1.88 | 0.11 | 1.59 | 0.10 |
| **PS(44:10)** | 0.22 | 0.02 | 0.19 | 0.02 | 0.19 | 0.02 | 0.18 | 0.01 | 0.12 | 0.01 |
| **Cer(d30:1)** | 21.95 | 1.94 | 24.97 | 1.55 | 29.94 | 3.40 | 28.69 | 1.99 | 24.48 | 0.88 |
| **Cer(d32:3)** | 0.21 | 0.02 | 0.40 | 0.03 | 0.30 | 0.03 | 0.25 | 0.03 | 0.21 | 0.01 |
| **Cer(d32:1)** | 29.68 | 1.75 | 21.75 | 1.34 | 23.17 | 2.23 | 23.12 | 1.33 | 29.05 | 1.04 |
| **Cer(d34:2)** | 2.26 | 0.12 | 2.32 | 0.23 | 2.58 | 0.31 | 2.66 | 0.30 | 2.40 | 0.13 |
| **Cer(d34:1)** | 6.50 | 0.48 | 6.60 | 0.36 | 4.92 | 0.51 | 5.61 | 0.58 | 6.34 | 0.27 |
| **Cer(d36:3)** | 1.98 | 0.12 | 1.99 | 0.26 | 2.12 | 0.22 | 2.47 | 0.26 | 1.69 | 0.10 |

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|---|---|---|---|---|---|---|---|---|---|---|
| **Cer(d36:2)** | 2.02 | 0.14 | 1.87 | 0.13 | 1.89 | 0.14 | 1.91 | 0.32 | 1.90 | 0.06 |
| **Cer(d36:1)** | 1.26 | 0.15 | 1.55 | 0.10 | 1.13 | 0.11 | 1.34 | 0.13 | 1.66 | 0.06 |
| **Cer(d38:3)** | 2.13 | 0.21 | 2.51 | 0.40 | 1.52 | 0.19 | 2.12 | 0.22 | 1.35 | 0.09 |
| **Cer(d38:2)** | 17.08 | 1.83 | 16.63 | 1.24 | 16.84 | 1.25 | 16.21 | 1.12 | 15.58 | 0.70 |
| **Cer(d38:1)** | 2.67 | 0.28 | 3.41 | 0.36 | 2.73 | 0.34 | 2.96 | 0.28 | 3.24 | 0.16 |
| **Cer(d40:2)** | 7.26 | 0.75 | 9.11 | 0.99 | 7.73 | 1.03 | 6.62 | 0.73 | 6.01 | 0.32 |
| **Cer(d40:1)** | 1.33 | 0.15 | 1.65 | 0.19 | 1.20 | 0.13 | 1.67 | 0.19 | 1.44 | 0.06 |
| **Cer(d42:2)** | 0.61 | 0.07 | 1.06 | 0.11 | 0.52 | 0.10 | 0.68 | 0.09 | 0.61 | 0.04 |
| **Cer(d42:1)** | 0.06 | 0.01 | 0.11 | 0.03 | 0.03 | 0.01 | 0.11 | 0.04 | 0.10 | 0.02 |
| **HexCer(38:2)** | 2.53 | 0.37 | 3.28 | 0.33 | 2.95 | 0.28 | 2.98 | 0.20 | 3.39 | 0.16 |
| **HexCer(d40:1)** | 0.48 | 0.07 | 0.80 | 0.11 | 0.44 | 0.06 | 0.58 | 0.05 | 0.54 | 0.02 |
| **LPC(O-14:1)(P-14:0)** | 0.09 | 0.02 | 0.11 | 0.04 | 0.05 | 0.01 | 0.04 | 0.01 | 0.03 | 0.00 |
| **LPC(O-14:0)** | 0.14 | 0.03 | 0.29 | 0.09 | 0.20 | 0.04 | 0.16 | 0.02 | 0.20 | 0.02 |
| **LPC(14:1)** | 0.05 | 0.01 | 0.02 | 0.01 | 0.05 | 0.01 | 0.05 | 0.01 | 0.07 | 0.01 |
| **LPC(14:0)** | 1.27 | 0.12 | 0.88 | 0.12 | 1.11 | 0.18 | 1.23 | 0.17 | 1.72 | 0.16 |
| **LPC(O-16:1)(P-16:0)** | 0.64 | 0.08 | 0.90 | 0.23 | 0.45 | 0.06 | 0.41 | 0.03 | 0.47 | 0.04 |
| **LPC(O-16:0)** | 3.17 | 0.28 | 7.68 | 1.12 | 3.62 | 0.37 | 3.02 | 0.19 | 2.81 | 0.20 |
| **LPC(16:1)** | 1.02 | 0.07 | 0.84 | 0.09 | 1.00 | 0.11 | 1.01 | 0.11 | 1.05 | 0.08 |
| **LPC(16:0)** | 16.87 | 0.92 | 14.87 | 1.66 | 14.55 | 1.49 | 16.30 | 1.33 | 16.66 | 0.98 |
| **LPC(O-18:2)(P-18:1)** | 0.06 | 0.01 | 0.12 | 0.03 | 0.04 | 0.01 | 0.05 | 0.00 | 0.06 | 0.01 |
| **LPC(O-18:1)(P-18:0)** | 0.85 | 0.08 | 1.67 | 0.36 | 0.74 | 0.10 | 0.55 | 0.03 | 0.52 | 0.03 |
| **LPC(O-18:0)** | 1.09 | 0.11 | 3.07 | 0.47 | 1.30 | 0.17 | 1.03 | 0.07 | 1.09 | 0.05 |
| **LPC(18:4)** | 0.13 | 0.01 | 0.12 | 0.02 | 0.11 | 0.01 | 0.13 | 0.01 | 0.27 | 0.02 |
| **LPC(18:3)** | 1.64 | 0.14 | 1.62 | 0.22 | 1.28 | 0.14 | 1.61 | 0.13 | 1.69 | 0.11 |
| **LPC(18:2)** | 0.52 | 0.04 | 0.68 | 0.09 | 0.40 | 0.05 | 0.66 | 0.09 | 0.58 | 0.04 |
| **LPC(18:1)** | 4.58 | 0.36 | 4.59 | 0.55 | 5.00 | 0.76 | 4.60 | 0.40 | 5.65 | 0.41 |
| **LPC(18:0)** | 2.07 | 0.22 | 2.21 | 0.18 | 2.17 | 0.27 | 2.29 | 0.24 | 2.41 | 0.20 |
| **LPC(O-20:1)(P-20:0)** | 0.14 | 0.01 | 0.52 | 0.11 | 0.19 | 0.02 | 0.11 | 0.01 | 0.13 | 0.01 |
| **LPC(20:5)** | 22.99 | 1.26 | 19.31 | 3.18 | 23.50 | 2.62 | 23.07 | 1.65 | 24.58 | 1.24 |
| **LPC(20:4)** | 3.36 | 0.37 | 3.93 | 0.88 | 3.61 | 0.47 | 3.16 | 0.23 | 3.06 | 0.32 |
| **LPC(20:3)** | 0.87 | 0.06 | 1.16 | 0.16 | 0.71 | 0.09 | 0.97 | 0.09 | 0.72 | 0.05 |
| **LPC(20:2)** | 0.48 | 0.04 | 0.67 | 0.09 | 0.53 | 0.06 | 0.64 | 0.06 | 0.50 | 0.04 |
| **LPC(20:1)** | 3.15 | 0.26 | 2.88 | 0.35 | 4.29 | 0.59 | 3.16 | 0.26 | 3.95 | 0.32 |
| **LPC(22:6)** | 31.65 | 1.25 | 27.63 | 3.10 | 31.40 | 2.55 | 32.71 | 2.53 | 28.86 | 1.83 |
| **LPC(22:5)** | 2.14 | 0.18 | 3.02 | 0.43 | 2.51 | 0.40 | 2.11 | 0.20 | 2.01 | 0.23 |
| **LPC(22:4)** | 0.76 | 0.06 | 0.93 | 0.11 | 0.88 | 0.15 | 0.64 | 0.05 | 0.64 | 0.06 |
| **LPC(22:1)** | 0.12 | 0.01 | 0.16 | 0.02 | 0.17 | 0.02 | 0.14 | 0.01 | 0.19 | 0.01 |
| **LPC(24:1)** | 0.13 | 0.01 | 0.12 | 0.01 | 0.12 | 0.01 | 0.14 | 0.01 | 0.10 | 0.00 |
| **LPE(14:0)** | 0.13 | 0.01 | 0.08 | 0.01 | 0.13 | 0.01 | 0.16 | 0.02 | 0.21 | 0.02 |
| **LPE(O-16:1)(P-** | 2.43 | 0.17 | 3.04 | 0.80 | 1.85 | 0.26 | 1.97 | 0.17 | 3.01 | 0.22 |

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|---|---|---|---|---|---|---|---|---|---|---|
| **16:0)** | | | | | | | | | | |
| **LPE(O-16:0)** | 2.01 | 0.12 | 2.51 | 0.58 | 2.19 | 0.36 | 2.17 | 0.15 | 2.99 | 0.24 |
| **LPE(16:1)** | 0.17 | 0.01 | 0.10 | 0.01 | 0.16 | 0.03 | 0.14 | 0.01 | 0.17 | 0.02 |
| **LPE(16:0)** | 14.32 | 1.20 | 8.05 | 1.39 | 12.55 | 1.78 | 15.08 | 0.80 | 15.57 | 0.81 |
| **LPE(O-18:1)(P-18:0)** | 14.78 | 0.66 | 30.50 | 4.61 | 17.92 | 1.63 | 15.89 | 0.97 | 13.90 | 0.78 |
| **LPE(O-18:0)** | 3.30 | 0.23 | 5.16 | 1.21 | 3.28 | 0.51 | 3.23 | 0.21 | 3.72 | 0.22 |
| **LPE(18:3)** | 1.34 | 0.11 | 1.00 | 0.26 | 1.36 | 0.19 | 1.54 | 0.13 | 1.62 | 0.15 |
| **LPE(18:2)** | 0.32 | 0.02 | 0.21 | 0.05 | 0.26 | 0.06 | 0.36 | 0.04 | 0.31 | 0.02 |
| **LPE(18:1)** | 4.38 | 0.33 | 2.36 | 0.42 | 4.57 | 0.85 | 3.69 | 0.20 | 3.91 | 0.30 |
| **LPE(18:0)** | 15.22 | 1.21 | 11.27 | 1.49 | 14.69 | 2.37 | 15.81 | 1.20 | 16.44 | 1.38 |
| **LPE(O-20:1)(P-20:0)** | 0.40 | 0.02 | 0.68 | 0.19 | 0.53 | 0.08 | 0.37 | 0.03 | 0.44 | 0.03 |
| **LPE(20:5)** | 12.87 | 1.09 | 10.60 | 1.47 | 12.64 | 1.66 | 13.27 | 0.83 | 13.31 | 0.73 |
| **LPE(20:4)** | 2.69 | 0.24 | 2.78 | 0.28 | 2.77 | 0.42 | 2.33 | 0.13 | 2.04 | 0.29 |
| **LPE(20:3)** | 3.52 | 0.19 | 3.41 | 0.53 | 2.96 | 0.33 | 3.54 | 0.23 | 2.77 | 0.19 |
| **LPE(20:2)** | 0.89 | 0.06 | 0.77 | 0.16 | 0.76 | 0.13 | 0.97 | 0.12 | 0.63 | 0.05 |
| **LPE(20:1)** | 9.80 | 0.70 | 6.27 | 1.48 | 12.19 | 1.44 | 8.53 | 0.57 | 9.34 | 1.00 |
| **LPE(20:0)** | 0.11 | 0.01 | 0.06 | 0.02 | 0.13 | 0.03 | 0.08 | 0.01 | 0.10 | 0.01 |
| **LPE(22:6)** | 9.16 | 0.59 | 8.83 | 1.49 | 6.66 | 0.93 | 8.98 | 0.60 | 7.65 | 0.47 |
| **LPE(22:5)** | 0.60 | 0.05 | 0.80 | 0.08 | 0.59 | 0.12 | 0.59 | 0.05 | 0.52 | 0.07 |
| **LPE(22:4)** | 1.37 | 0.10 | 1.32 | 0.22 | 1.66 | 0.26 | 1.15 | 0.06 | 1.22 | 0.10 |
| **LPE(22:2)** | 0.04 | 0.00 | 0.09 | 0.03 | 0.05 | 0.01 | 0.05 | 0.01 | 0.03 | 0.01 |
| **LPE(22:1)** | 0.03 | 0.00 | 0.01 | 0.01 | 0.04 | 0.01 | 0.02 | 0.00 | 0.05 | 0.01 |
| **LPE(24:6)** | 0.11 | 0.01 | 0.09 | 0.02 | 0.06 | 0.01 | 0.08 | 0.01 | 0.05 | 0.01 |
| **PC(28:0)** | 0.07 | 0.01 | 0.05 | 0.01 | 0.05 | 0.01 | 0.06 | 0.01 | 0.12 | 0.01 |
| **PC(O-30:2)(P-30:1)** | 0.02 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 |
| **PC(O-30:1)(P-30:0)** | 0.24 | 0.02 | 0.20 | 0.04 | 0.19 | 0.03 | 0.16 | 0.02 | 0.16 | 0.01 |
| **PC(O-30:0)** | 0.22 | 0.01 | 0.37 | 0.05 | 0.29 | 0.05 | 0.23 | 0.01 | 0.32 | 0.01 |
| **PC(30:1)** | 0.11 | 0.01 | 0.08 | 0.01 | 0.11 | 0.02 | 0.11 | 0.01 | 0.14 | 0.01 |
| **PC(30:0)** | 0.28 | 0.03 | 0.29 | 0.03 | 0.22 | 0.03 | 0.27 | 0.03 | 0.42 | 0.03 |
| **PC(O-32:2)(P-32:1)** | 0.12 | 0.01 | 0.11 | 0.03 | 0.09 | 0.01 | 0.09 | 0.01 | 0.08 | 0.00 |
| **PC(O-32:1)(P-32:0)** | 0.91 | 0.02 | 1.10 | 0.16 | 0.81 | 0.10 | 0.70 | 0.04 | 0.70 | 0.02 |
| **PC(O-32:0)** | 0.51 | 0.02 | 0.91 | 0.10 | 0.54 | 0.08 | 0.47 | 0.01 | 0.55 | 0.02 |
| **PC(32:2)** | 0.09 | 0.01 | 0.09 | 0.01 | 0.08 | 0.01 | 0.11 | 0.01 | 0.12 | 0.01 |
| **PC(32:1)** | 1.28 | 0.08 | 1.26 | 0.10 | 1.34 | 0.22 | 1.37 | 0.11 | 1.64 | 0.08 |
| **PC(32:0)** | 0.59 | 0.05 | 0.65 | 0.07 | 0.47 | 0.07 | 0.55 | 0.05 | 0.67 | 0.03 |
| **PC(O-34:5)(P-34:4)** | 0.11 | 0.02 | 0.12 | 0.02 | 0.16 | 0.03 | 0.14 | 0.01 | 0.18 | 0.01 |
| **PC(O-34:4)(P-34:3)** | 0.13 | 0.01 | 0.14 | 0.02 | 0.14 | 0.02 | 0.12 | 0.01 | 0.13 | 0.00 |
| **PC(O-34:3)(P-** | 0.09 | 0.00 | 0.13 | 0.01 | 0.09 | 0.02 | 0.09 | 0.00 | 0.10 | 0.00 |

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|---|---|---|---|---|---|---|---|---|---|---|
| **34:2)** | | | | | | | | | | |
| **PC(O-34:2)(P-34:1)** | 0.17 | 0.01 | 0.23 | 0.04 | 0.17 | 0.03 | 0.16 | 0.01 | 0.16 | 0.01 |
| **PC(O-34:1)(P-34:0)** | 0.75 | 0.02 | 1.21 | 0.13 | 0.79 | 0.10 | 0.61 | 0.03 | 0.66 | 0.03 |
| **PC(O-34:0)** | 0.20 | 0.01 | 0.35 | 0.04 | 0.21 | 0.03 | 0.17 | 0.01 | 0.19 | 0.01 |
| **PC(34:6)** | 0.03 | 0.00 | 0.02 | 0.00 | 0.03 | 0.00 | 0.04 | 0.00 | 0.04 | 0.00 |
| **PC(34:5)** | 0.71 | 0.04 | 0.72 | 0.07 | 0.76 | 0.11 | 0.89 | 0.06 | 1.03 | 0.07 |
| **PC(34:4)** | 0.36 | 0.01 | 0.41 | 0.03 | 0.42 | 0.07 | 0.46 | 0.04 | 0.57 | 0.04 |
| **PC(34:3)** | 0.20 | 0.01 | 0.24 | 0.03 | 0.18 | 0.03 | 0.25 | 0.02 | 0.30 | 0.02 |
| **PC(34:2)** | 0.67 | 0.04 | 0.84 | 0.07 | 0.62 | 0.10 | 0.84 | 0.08 | 0.86 | 0.05 |
| **PC(34:1)** | 2.76 | 0.14 | 3.38 | 0.37 | 3.34 | 0.63 | 3.10 | 0.19 | 4.19 | 0.19 |
| **PC(O-36:6)(P-36:5)** | 0.89 | 0.06 | 0.76 | 0.10 | 0.97 | 0.19 | 0.82 | 0.07 | 0.89 | 0.03 |
| **PC(O-36:5)(P-36:4)** | 1.95 | 0.09 | 2.81 | 0.31 | 2.30 | 0.30 | 1.98 | 0.10 | 1.97 | 0.12 |
| **PC(O-36:4)(P-36:3)** | 0.62 | 0.03 | 1.08 | 0.15 | 0.88 | 0.11 | 0.66 | 0.04 | 0.59 | 0.04 |
| **PC(O-36:3)(P-36:2)** | 0.11 | 0.00 | 0.17 | 0.01 | 0.12 | 0.01 | 0.12 | 0.01 | 0.12 | 0.01 |
| **PC(O-36:2)(P-36:1)** | 0.14 | 0.00 | 0.20 | 0.02 | 0.16 | 0.02 | 0.12 | 0.01 | 0.14 | 0.01 |
| **PC(36:8)** | 0.05 | 0.00 | 0.05 | 0.00 | 0.06 | 0.01 | 0.08 | 0.01 | 0.08 | 0.01 |
| **PC(O-36:1)(P-36:0)** | 0.27 | 0.01 | 0.61 | 0.07 | 0.43 | 0.06 | 0.29 | 0.01 | 0.40 | 0.01 |
| **PC(O-36:0)** | 0.02 | 0.00 | 0.05 | 0.01 | 0.04 | 0.01 | 0.02 | 0.00 | 0.04 | 0.00 |
| **PC(36:6)** | 2.03 | 0.12 | 1.60 | 0.11 | 1.98 | 0.22 | 2.25 | 0.14 | 2.28 | 0.14 |
| **PC(36:5)** | 10.05 | 0.33 | 9.41 | 0.69 | 9.06 | 0.90 | 9.91 | 0.43 | 9.95 | 0.68 |
| **PC(36:4)** | 2.91 | 0.08 | 3.34 | 0.33 | 3.03 | 0.43 | 3.16 | 0.14 | 3.10 | 0.25 |
| **PC(36:3)** | 0.41 | 0.01 | 0.52 | 0.06 | 0.40 | 0.05 | 0.51 | 0.03 | 0.47 | 0.03 |
| **PC(36:2)** | 0.53 | 0.03 | 0.68 | 0.09 | 0.80 | 0.12 | 0.67 | 0.03 | 0.78 | 0.04 |
| **PC(36:1)** | 0.75 | 0.04 | 1.02 | 0.12 | 0.91 | 0.13 | 0.89 | 0.06 | 1.08 | 0.05 |
| **PC(O-38:7)(P-38:6)** | 1.80 | 0.17 | 1.09 | 0.19 | 1.38 | 0.13 | 1.32 | 0.11 | 1.32 | 0.04 |
| **PC(36:0)** | 0.07 | 0.01 | 0.09 | 0.01 | 0.08 | 0.01 | 0.09 | 0.01 | 0.10 | 0.01 |
| **PC(O-38:6)(P-38:5)** | 7.28 | 0.33 | 8.42 | 1.01 | 8.49 | 0.82 | 7.47 | 0.27 | 6.80 | 0.26 |
| **PC(O-38:5)(P-38:4)** | 1.87 | 0.09 | 2.67 | 0.28 | 2.34 | 0.29 | 1.85 | 0.07 | 1.83 | 0.08 |
| **PC(O-38:4)(P-38:3)** | 0.46 | 0.03 | 0.91 | 0.09 | 0.70 | 0.13 | 0.50 | 0.03 | 0.43 | 0.03 |
| **PC(O-38:3)(P-38:2)** | 0.05 | 0.00 | 0.10 | 0.01 | 0.08 | 0.01 | 0.06 | 0.00 | 0.05 | 0.00 |
| **PC(38:9)** | 0.14 | 0.01 | 0.09 | 0.01 | 0.14 | 0.01 | 0.16 | 0.01 | 0.16 | 0.01 |
| **PC(O-38:2)(P-38:1)** | 0.10 | 0.01 | 0.20 | 0.02 | 0.18 | 0.02 | 0.13 | 0.01 | 0.11 | 0.01 |
| **PC(38:8)** | 0.69 | 0.03 | 0.64 | 0.05 | 0.66 | 0.07 | 0.83 | 0.03 | 0.80 | 0.05 |

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|---|---|---|---|---|---|---|---|---|---|---|
| **PC(O-38:1)(P-38:0)** | 0.05 | 0.00 | 0.12 | 0.01 | 0.08 | 0.01 | 0.06 | 0.00 | 0.06 | 0.00 |
| **PC(38:7)** | 1.04 | 0.05 | 0.87 | 0.06 | 0.95 | 0.10 | 1.12 | 0.05 | 0.90 | 0.06 |
| **PC(38:6)** | 22.93 | 0.60 | 18.95 | 1.25 | 19.95 | 1.70 | 21.82 | 0.47 | 20.17 | 0.77 |
| **PC(38:5)** | 5.53 | 0.14 | 5.25 | 0.41 | 5.48 | 0.75 | 5.84 | 0.29 | 5.66 | 0.29 |
| **PC(38:4)** | 1.17 | 0.03 | 1.49 | 0.18 | 1.36 | 0.16 | 1.26 | 0.03 | 1.17 | 0.07 |
| **PC(38:3)** | 0.20 | 0.01 | 0.25 | 0.03 | 0.25 | 0.04 | 0.24 | 0.01 | 0.23 | 0.01 |
| **PC(38:2)** | 0.33 | 0.02 | 0.39 | 0.03 | 0.56 | 0.09 | 0.39 | 0.02 | 0.52 | 0.04 |
| **PC(38:1)** | 0.09 | 0.00 | 0.10 | 0.01 | 0.13 | 0.02 | 0.10 | 0.01 | 0.13 | 0.01 |
| **PC(O-40:7)(P-40:6)** | 2.15 | 0.09 | 1.57 | 0.18 | 1.77 | 0.24 | 1.49 | 0.04 | 1.51 | 0.05 |
| **PC(O-40:6)(P-40:5)** | 2.37 | 0.13 | 2.93 | 0.24 | 2.69 | 0.32 | 2.25 | 0.11 | 2.52 | 0.06 |
| **PC(O-40:5)(P-40:4)** | 0.38 | 0.02 | 0.63 | 0.06 | 0.50 | 0.06 | 0.37 | 0.02 | 0.42 | 0.02 |
| **PC(O-40:4)(P-40:3)** | 0.01 | 0.00 | 0.05 | 0.01 | 0.03 | 0.01 | 0.01 | 0.00 | 0.01 | 0.00 |
| **PC(40:10)** | 0.43 | 0.03 | 0.41 | 0.03 | 0.27 | 0.04 | 0.39 | 0.03 | 0.34 | 0.02 |
| **PC(40:9)** | 1.63 | 0.06 | 1.33 | 0.13 | 1.51 | 0.15 | 1.72 | 0.05 | 1.57 | 0.07 |
| **PC(O-40:2)(P-40:1)** | 0.01 | 0.00 | 0.04 | 0.00 | 0.03 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 |
| **PC(40:8)** | 0.94 | 0.05 | 1.05 | 0.08 | 0.82 | 0.09 | 1.11 | 0.07 | 0.85 | 0.06 |
| **PC(O-40:1)(P-40:0)** | 0.01 | 0.00 | 0.02 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 |
| **PC(40:7)** | 3.20 | 0.09 | 2.74 | 0.22 | 3.07 | 0.39 | 3.14 | 0.17 | 2.82 | 0.10 |
| **PC(40:6)** | 4.42 | 0.16 | 3.76 | 0.21 | 4.83 | 0.46 | 4.66 | 0.22 | 5.38 | 0.20 |
| **PC(40:5)** | 0.93 | 0.03 | 0.94 | 0.09 | 1.21 | 0.16 | 1.04 | 0.04 | 1.06 | 0.07 |
| **PC(40:4)** | 0.12 | 0.00 | 0.15 | 0.01 | 0.15 | 0.03 | 0.12 | 0.01 | 0.12 | 0.01 |
| **PC(40:3)** | 0.01 | 0.00 | 0.02 | 0.00 | 0.02 | 0.01 | 0.01 | 0.00 | 0.01 | 0.00 |
| **PC(40:2)** | 0.04 | 0.00 | 0.04 | 0.00 | 0.06 | 0.01 | 0.04 | 0.00 | 0.07 | 0.00 |
| **PC(40:1)** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| **PC(P-42:6)** | 0.28 | 0.02 | 0.41 | 0.05 | 0.40 | 0.05 | 0.26 | 0.01 | 0.33 | 0.02 |
| **PC(O-42:6)(P-42:5)** | 0.06 | 0.00 | 0.09 | 0.01 | 0.07 | 0.01 | 0.04 | 0.00 | 0.09 | 0.01 |
| **PC(O-42:5)(P-42:4)** | 0.05 | 0.00 | 0.07 | 0.01 | 0.07 | 0.01 | 0.04 | 0.00 | 0.05 | 0.00 |
| **PC(42:11)** | 1.11 | 0.07 | 0.96 | 0.12 | 0.61 | 0.08 | 0.90 | 0.05 | 0.68 | 0.03 |
| **PC(42:10)** | 0.54 | 0.02 | 0.50 | 0.04 | 0.44 | 0.06 | 0.54 | 0.03 | 0.43 | 0.02 |
| **PC(42:9)** | 0.94 | 0.06 | 1.05 | 0.08 | 0.80 | 0.09 | 1.03 | 0.05 | 0.78 | 0.04 |
| **PC(42:8)** | 0.52 | 0.03 | 0.59 | 0.05 | 0.47 | 0.05 | 0.64 | 0.05 | 0.48 | 0.02 |
| **PC(42:7)** | 2.31 | 0.12 | 1.88 | 0.18 | 2.90 | 0.35 | 2.39 | 0.11 | 2.84 | 0.18 |
| **PC(42:6)** | 0.64 | 0.03 | 0.54 | 0.05 | 0.71 | 0.10 | 0.51 | 0.02 | 0.63 | 0.04 |
| **PC(42:5)** | 0.19 | 0.01 | 0.18 | 0.02 | 0.21 | 0.02 | 0.19 | 0.01 | 0.17 | 0.02 |
| **PC(P-44:6)** | 0.02 | 0.00 | 0.01 | 0.00 | 0.02 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 |
| **PC(44:12)** | 0.54 | 0.02 | 0.42 | 0.05 | 0.31 | 0.04 | 0.43 | 0.02 | 0.31 | 0.01 |
| **PC(44:11)** | 0.33 | 0.02 | 0.27 | 0.02 | 0.21 | 0.03 | 0.29 | 0.02 | 0.18 | 0.01 |

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|---|---|---|---|---|---|---|---|---|---|---|
| **PC(44:10)** | 0.28 | 0.01 | 0.22 | 0.02 | 0.31 | 0.03 | 0.28 | 0.01 | 0.28 | 0.01 |
| **PC(44:9)** | 0.09 | 0.00 | 0.06 | 0.00 | 0.09 | 0.01 | 0.07 | 0.00 | 0.07 | 0.00 |
| **PC(44:8)** | 0.04 | 0.00 | 0.03 | 0.00 | 0.05 | 0.00 | 0.05 | 0.00 | 0.04 | 0.00 |
| **PC(44:7)** | 0.08 | 0.00 | 0.06 | 0.00 | 0.11 | 0.01 | 0.10 | 0.01 | 0.13 | 0.01 |
| **PC(44:6)** | 0.03 | 0.00 | 0.04 | 0.00 | 0.05 | 0.01 | 0.04 | 0.00 | 0.05 | 0.00 |
| **PC(46:12)** | 0.13 | 0.01 | 0.09 | 0.02 | 0.08 | 0.01 | 0.11 | 0.01 | 0.05 | 0.00 |
| **PE(30:3)** | 0.58 | 0.02 | 0.53 | 0.03 | 0.67 | 0.04 | 0.75 | 0.02 | 0.80 | 0.02 |
| **PE(30:0)** | 0.00 | 0.00 | 0.02 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| **PE(O-32:1)(P-32:0)** | 0.02 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 |
| **PE(32:1)** | 0.06 | 0.00 | 0.24 | 0.09 | 0.05 | 0.01 | 0.04 | 0.00 | 0.04 | 0.00 |
| **PE(32:0)** | 0.01 | 0.00 | 0.02 | 0.01 | 0.01 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 |
| **PE(P-34:5)** | 0.02 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.03 | 0.00 | 0.07 | 0.01 |
| **PE(O-34:5)(P-34:4)** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 |
| **PE(O-34:4)(P-34:3)** | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 |
| **PE(O-34:1)(P-34:0)** | 0.02 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 0.04 | 0.00 |
| **PE(34:5)** | 0.05 | 0.00 | 0.07 | 0.01 | 0.06 | 0.01 | 0.07 | 0.01 | 0.09 | 0.00 |
| **PE(34:4)** | 0.03 | 0.00 | 0.06 | 0.02 | 0.03 | 0.00 | 0.03 | 0.00 | 0.04 | 0.00 |
| **PE(34:3)** | 0.02 | 0.00 | 0.03 | 0.01 | 0.01 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 |
| **PE(34:2)** | 0.05 | 0.00 | 0.09 | 0.02 | 0.04 | 0.01 | 0.06 | 0.01 | 0.05 | 0.00 |
| **PE(34:1)** | 0.12 | 0.01 | 0.12 | 0.02 | 0.13 | 0.02 | 0.11 | 0.01 | 0.18 | 0.01 |
| **PE(P-36:6)** | 0.05 | 0.00 | 0.02 | 0.01 | 0.03 | 0.01 | 0.06 | 0.01 | 0.14 | 0.02 |
| **PE(34:0)** | 0.01 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.02 | 0.00 |
| **PE(O-36:6)(P-36:5)** | 2.33 | 0.11 | 1.39 | 0.15 | 1.61 | 0.22 | 1.95 | 0.11 | 3.16 | 0.26 |
| **PE(O-36:5)(P-36:4)** | 2.37 | 0.06 | 2.04 | 0.15 | 2.17 | 0.22 | 2.10 | 0.13 | 2.71 | 0.10 |
| **PE(O-36:4)(P-36:3)** | 0.53 | 0.03 | 0.53 | 0.05 | 0.56 | 0.07 | 0.50 | 0.03 | 0.51 | 0.03 |
| **PE(O-36:3)(P-36:2)** | 0.04 | 0.00 | 0.05 | 0.00 | 0.05 | 0.01 | 0.04 | 0.00 | 0.05 | 0.00 |
| **PE(O-36:2)(P-36:1)** | 0.03 | 0.00 | 0.04 | 0.00 | 0.03 | 0.00 | 0.04 | 0.00 | 0.06 | 0.00 |
| **PE(36:8)** | 0.02 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 0.03 | 0.00 |
| **PE(O-36:1)(P-36:0)** | 0.05 | 0.01 | 0.05 | 0.00 | 0.05 | 0.01 | 0.06 | 0.01 | 0.11 | 0.01 |
| **PE(36:7)** | 0.01 | 0.00 | 0.01 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 |
| **PE(36:6)** | 0.10 | 0.01 | 0.10 | 0.02 | 0.10 | 0.01 | 0.12 | 0.01 | 0.14 | 0.01 |
| **PE(36:5)** | 6.10 | 0.18 | 5.14 | 0.43 | 5.13 | 0.43 | 5.85 | 0.30 | 5.97 | 0.21 |
| **PE(36:4)** | 1.48 | 0.05 | 1.30 | 0.11 | 1.31 | 0.14 | 1.41 | 0.07 | 1.38 | 0.09 |
| **PE(36:3)** | 0.16 | 0.01 | 0.16 | 0.02 | 0.14 | 0.02 | 0.18 | 0.01 | 0.19 | 0.01 |
| **PE(O-38:9)(P-38:8)** | 0.25 | 0.01 | 0.16 | 0.02 | 0.22 | 0.04 | 0.19 | 0.01 | 0.31 | 0.03 |

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|---|---|---|---|---|---|---|---|---|---|---|
| **PE(36:2)** | 0.09 | 0.00 | 0.10 | 0.01 | 0.09 | 0.01 | 0.10 | 0.01 | 0.10 | 0.00 |
| **PE(O-38:8)(P-38:7)** | 0.59 | 0.02 | 0.51 | 0.05 | 0.63 | 0.12 | 0.49 | 0.03 | 0.62 | 0.04 |
| **PE(36:1)** | 0.10 | 0.00 | 0.08 | 0.01 | 0.11 | 0.01 | 0.10 | 0.01 | 0.14 | 0.00 |
| **PE(O-38:7)(P-38:6)** | 2.68 | 0.11 | 2.05 | 0.25 | 2.33 | 0.32 | 2.56 | 0.16 | 3.45 | 0.17 |
| **PE(O-38:6)(P-38:5)** | 18.21 | 0.51 | 17.65 | 1.10 | 20.29 | 2.03 | 19.34 | 0.55 | 19.70 | 0.43 |
| **PE(O-38:5)(P-38:4)** | 11.07 | 0.30 | 14.09 | 1.04 | 12.85 | 1.22 | 11.98 | 0.38 | 10.51 | 0.44 |
| **PE(O-38:4)(P-38:3)** | 2.05 | 0.15 | 2.48 | 0.23 | 2.21 | 0.21 | 2.06 | 0.10 | 1.77 | 0.15 |
| **PE(O-38:3)(P-38:2)** | 0.16 | 0.01 | 0.20 | 0.02 | 0.17 | 0.02 | 0.15 | 0.01 | 0.16 | 0.01 |
| **PE(38:9)** | 0.03 | 0.00 | 0.02 | 0.00 | 0.03 | 0.01 | 0.02 | 0.00 | 0.03 | 0.00 |
| **PE(O-38:2)(P-38:1)** | 0.09 | 0.01 | 0.12 | 0.01 | 0.13 | 0.02 | 0.13 | 0.01 | 0.17 | 0.01 |
| **PE(38:8)** | 1.66 | 0.09 | 1.30 | 0.16 | 1.50 | 0.24 | 1.31 | 0.08 | 1.27 | 0.10 |
| **PE(O-38:1)(P-38:0)** | 0.04 | 0.00 | 0.05 | 0.00 | 0.04 | 0.01 | 0.05 | 0.00 | 0.10 | 0.00 |
| **PE(38:7)** | 0.49 | 0.03 | 0.45 | 0.05 | 0.48 | 0.08 | 0.42 | 0.02 | 0.39 | 0.03 |
| **PE(38:6)** | 6.01 | 0.23 | 4.37 | 0.32 | 4.37 | 0.41 | 5.24 | 0.20 | 5.03 | 0.21 |
| **PE(38:5)** | 6.41 | 0.16 | 6.31 | 0.54 | 5.48 | 0.52 | 6.32 | 0.21 | 6.24 | 0.20 |
| **PE(O-40:11)(P-40:10)** | 0.09 | 0.01 | 0.06 | 0.01 | 0.09 | 0.02 | 0.05 | 0.01 | 0.07 | 0.01 |
| **PE(38:4)** | 2.04 | 0.07 | 2.20 | 0.20 | 1.96 | 0.19 | 2.03 | 0.09 | 1.78 | 0.12 |
| **PE(O-40:10)(P-40:9)** | 0.24 | 0.01 | 0.20 | 0.02 | 0.23 | 0.04 | 0.21 | 0.02 | 0.29 | 0.02 |
| **PE(38:3)** | 0.44 | 0.03 | 0.43 | 0.04 | 0.34 | 0.03 | 0.46 | 0.02 | 0.44 | 0.01 |
| **PE(O-40:9)(P-40:8)** | 1.75 | 0.05 | 1.79 | 0.19 | 2.08 | 0.27 | 1.79 | 0.08 | 1.81 | 0.08 |
| **PE(38:2)** | 0.22 | 0.02 | 0.20 | 0.02 | 0.18 | 0.02 | 0.20 | 0.02 | 0.19 | 0.01 |
| **PE(O-40:8)(P-40:7)** | 1.80 | 0.03 | 2.10 | 0.15 | 2.17 | 0.34 | 1.79 | 0.07 | 1.67 | 0.07 |
| **PE(38:1)** | 0.03 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 0.03 | 0.00 |
| **PE(O-40:7)(P-40:6)** | 7.11 | 0.24 | 7.90 | 0.62 | 8.19 | 0.70 | 8.13 | 0.33 | 7.61 | 0.25 |
| **PE(O-40:6)(P-40:5)** | 3.90 | 0.10 | 4.41 | 0.39 | 4.20 | 0.51 | 4.22 | 0.16 | 4.44 | 0.15 |
| **PE(O-40:5)(P-40:4)** | 1.00 | 0.04 | 1.32 | 0.10 | 1.11 | 0.09 | 1.08 | 0.05 | 1.02 | 0.04 |
| **PE(O-40:4)(P-40:3)** | 0.27 | 0.01 | 0.36 | 0.03 | 0.28 | 0.04 | 0.28 | 0.01 | 0.24 | 0.02 |
| **PE(40:10)** | 0.15 | 0.01 | 0.13 | 0.01 | 0.12 | 0.02 | 0.12 | 0.01 | 0.11 | 0.01 |
| **PE(O-40:3)(P-40:2)** | 0.08 | 0.00 | 0.12 | 0.01 | 0.11 | 0.01 | 0.11 | 0.00 | 0.11 | 0.01 |
| **PE(40:9)** | 0.92 | 0.05 | 0.76 | 0.12 | 0.81 | 0.16 | 0.75 | 0.03 | 0.69 | 0.04 |

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|---|---|---|---|---|---|---|---|---|---|---|
| **PE(O-40:2)(P-40:1)** | 0.08 | 0.00 | 0.13 | 0.01 | 0.14 | 0.02 | 0.12 | 0.00 | 0.13 | 0.00 |
| **PE(40:8)** | 1.57 | 0.09 | 1.74 | 0.14 | 1.40 | 0.22 | 1.50 | 0.08 | 1.18 | 0.08 |
| **PE(O-40:1)(P-40:0)** | 0.00 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 | 0.02 | 0.00 |
| **PE(40:7)** | 1.28 | 0.03 | 1.27 | 0.13 | 1.15 | 0.13 | 1.23 | 0.07 | 1.02 | 0.05 |
| **PE(40:6)** | 4.17 | 0.15 | 3.82 | 0.34 | 3.74 | 0.36 | 3.83 | 0.12 | 4.17 | 0.19 |
| **PE(P-42:11)** | 0.21 | 0.02 | 0.17 | 0.01 | 0.24 | 0.06 | 0.16 | 0.01 | 0.18 | 0.02 |
| **PE(40:5)** | 1.22 | 0.04 | 1.22 | 0.11 | 1.15 | 0.14 | 1.00 | 0.04 | 0.99 | 0.05 |
| **PE(O-42:11)(P-42:10)** | 0.19 | 0.01 | 0.21 | 0.02 | 0.23 | 0.04 | 0.15 | 0.01 | 0.15 | 0.01 |
| **PE(40:4)** | 0.18 | 0.01 | 0.18 | 0.02 | 0.16 | 0.02 | 0.18 | 0.02 | 0.13 | 0.01 |
| **PE(O-42:10)(P-42:9)** | 0.53 | 0.01 | 0.68 | 0.05 | 0.67 | 0.08 | 0.62 | 0.02 | 0.57 | 0.03 |
| **PE(40:3)** | 0.55 | 0.04 | 0.41 | 0.04 | 0.36 | 0.04 | 0.48 | 0.05 | 0.39 | 0.02 |
| **PE(O-42:9)(P-42:8)** | 0.40 | 0.01 | 0.49 | 0.05 | 0.45 | 0.06 | 0.43 | 0.02 | 0.41 | 0.02 |
| **PE(40:2)** | 0.17 | 0.01 | 0.15 | 0.02 | 0.12 | 0.01 | 0.15 | 0.02 | 0.14 | 0.01 |
| **PE(O-42:8)(P-42:7)** | 0.46 | 0.02 | 0.61 | 0.04 | 0.74 | 0.07 | 0.61 | 0.05 | 0.50 | 0.03 |
| **PE(O-42:7)(P-42:6)** | 0.36 | 0.01 | 0.41 | 0.03 | 0.49 | 0.06 | 0.41 | 0.03 | 0.42 | 0.01 |
| **PE(O-42:6)(P-42:5)** | 0.12 | 0.00 | 0.13 | 0.01 | 0.15 | 0.01 | 0.12 | 0.00 | 0.13 | 0.01 |
| **PE(42:11)** | 0.53 | 0.04 | 0.56 | 0.08 | 0.40 | 0.08 | 0.48 | 0.03 | 0.33 | 0.02 |
| **PE(42:10)** | 0.22 | 0.01 | 0.24 | 0.03 | 0.20 | 0.03 | 0.20 | 0.01 | 0.15 | 0.01 |
| **PE(42:9)** | 0.76 | 0.05 | 0.82 | 0.09 | 0.59 | 0.09 | 0.68 | 0.04 | 0.54 | 0.03 |
| **PE(42:8)** | 0.35 | 0.02 | 0.38 | 0.04 | 0.28 | 0.04 | 0.34 | 0.03 | 0.24 | 0.01 |
| **PE(42:7)** | 1.20 | 0.04 | 1.04 | 0.11 | 1.22 | 0.12 | 1.05 | 0.05 | 1.09 | 0.05 |
| **PE(O-44:13)(P-44:12)** | 0.04 | 0.00 | 0.05 | 0.00 | 0.05 | 0.01 | 0.04 | 0.00 | 0.04 | 0.00 |
| **PE(42:6)** | 0.37 | 0.02 | 0.33 | 0.02 | 0.36 | 0.04 | 0.32 | 0.01 | 0.31 | 0.01 |
| **PE(O-44:12)(P-44:11)** | 0.03 | 0.00 | 0.04 | 0.00 | 0.04 | 0.01 | 0.03 | 0.00 | 0.03 | 0.00 |
| **PE(42:5)** | 0.09 | 0.01 | 0.08 | 0.01 | 0.07 | 0.01 | 0.07 | 0.00 | 0.05 | 0.00 |
| **PE(O-44:11)(P-44:10)** | 0.03 | 0.00 | 0.05 | 0.00 | 0.06 | 0.01 | 0.04 | 0.00 | 0.03 | 0.00 |
| **PE(O-44:10)(P-44:9)** | 0.02 | 0.00 | 0.02 | 0.00 | 0.03 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 |
| **PE(44:12)** | 0.37 | 0.04 | 0.41 | 0.05 | 0.20 | 0.03 | 0.32 | 0.04 | 0.16 | 0.01 |
| **PE(44:11)** | 0.10 | 0.01 | 0.12 | 0.01 | 0.06 | 0.01 | 0.09 | 0.01 | 0.04 | 0.00 |
| **PE(44:10)** | 0.10 | 0.00 | 0.10 | 0.01 | 0.10 | 0.01 | 0.08 | 0.00 | 0.07 | 0.01 |
| **PE(44:9)** | 0.04 | 0.00 | 0.03 | 0.00 | 0.03 | 0.01 | 0.03 | 0.00 | 0.02 | 0.00 |
| **PE(44:8)** | 0.03 | 0.00 | 0.03 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 | 0.02 | 0.00 |
| **PE(44:7)** | 0.02 | 0.00 | 0.01 | 0.00 | 0.02 | 0.00 | 0.01 | 0.00 | 0.01 | 0.00 |
| **SM(d30:1)** | 0.95 | 0.07 | 0.68 | 0.07 | 0.94 | 0.12 | 0.59 | 0.07 | 0.88 | 0.07 |

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|---|---|---|---|---|---|---|---|---|---|---|
| **SM(d30:0)** | 0.25 | 0.03 | 0.40 | 0.09 | 0.33 | 0.03 | 0.41 | 0.07 | 0.28 | 0.05 |
| **SM(d32:2)** | 0.70 | 0.05 | 0.85 | 0.08 | 0.86 | 0.09 | 0.65 | 0.04 | 0.55 | 0.03 |
| **SM(d32:1)** | 43.68 | 1.00 | 40.63 | 1.61 | 45.11 | 1.65 | 46.02 | 1.87 | 52.07 | 1.82 |
| **SM(d34:1)** | 16.73 | 0.89 | 14.31 | 1.12 | 11.62 | 1.20 | 13.32 | 0.76 | 11.60 | 0.65 |
| **SM(d34:0)** | 0.91 | 0.09 | 0.73 | 0.08 | 0.76 | 0.08 | 1.05 | 0.08 | 0.90 | 0.10 |
| **SM(d35:1)** | 3.19 | 0.24 | 3.12 | 0.42 | 3.92 | 0.19 | 4.13 | 0.30 | 2.78 | 0.23 |
| **SM(d36:3)** | 1.41 | 0.06 | 1.05 | 0.13 | 1.49 | 0.12 | 1.93 | 0.21 | 1.40 | 0.10 |
| **SM(d36:2)** | 2.89 | 0.13 | 3.08 | 0.24 | 3.68 | 0.26 | 2.92 | 0.18 | 2.61 | 0.15 |
| **SM(d36:1)** | 2.25 | 0.10 | 3.03 | 0.34 | 2.39 | 0.20 | 2.71 | 0.15 | 2.49 | 0.14 |
| **SM(d38:3)** | 2.64 | 0.16 | 3.38 | 0.22 | 2.05 | 0.18 | 2.86 | 0.28 | 1.65 | 0.08 |
| **SM(d38:2)** | 18.67 | 0.63 | 21.31 | 1.49 | 21.27 | 1.42 | 18.29 | 0.92 | 18.15 | 1.16 |
| **SM(d40:2)** | 5.38 | 0.32 | 7.00 | 0.66 | 5.32 | 0.31 | 4.84 | 0.31 | 4.43 | 0.33 |
| **SM(d42:2)** | 0.36 | 0.03 | 0.44 | 0.08 | 0.26 | 0.02 | 0.29 | 0.03 | 0.21 | 0.02 |