Book of Abstracts

4th Workshop in Lipidomics

6th May 2015, University of Aveiro
Organized by the Mass Spectrometry Centre
QOPNA, Department of Chemistry
University of Aveiro
Campus Universitário de Santiago
3810-193 Aveiro, Portugal

Scientific Committee
Rosário Domingues, Pedro Domingues, Rui Vitorino, Rita Ferreira, Tânia Melo,
Rita Araújo, Eliana Alves, Felisa Rey

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Rita Araújo, Eliana Alves, Felisa Rey, Núcleo de estudantes de química

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Programme

13h45 - 14h15 | Registration
14h15 - 14h30 | Opening
14h30 - 15h30 | Marine Lipids

Rosário Domingues (UAveiro)
Marine lipidomics: from the lipid signature of marine organisms to the discovery of new bioactive compounds

Felisa Rey (UAveiro)
Unraveling polar lipids’ dynamics during embryonic development of two sympatric brachyuran crabs (*Carcinus maenas* and *Necora puber*) using lipidomics

Fernando Ricardo (UAveiro)
Traceability of collection site using fatty acid profiles of the adductor muscle of cockles (*Ceraestoderma edule*)

Elisabete Costa (UAveiro)
Deciphering the lipidomic profile of the seaweed *Codium tomentosum* toward the bioprospection of phytochemicals

16h00 - 16h30 | Instrumentation

Daniel Ettlin (Thermo Unicam)
Lower or higher resolution for quantitative and qualitative analysis in mass spectrometers: Orbitrap, TripleQuad and Linear Trap features

16h00 - 16h30 | Coffee-break and networking (posters)

16h30 - 17h45 | Lipids in health and disease

Fátima Macedo (UAveiro)
Sphingolipids as immune system modulators

Catarina Morais (UCoimbra)
Lipid-based strategies in gene therapy: from the design of gen carriers to the modulation of membrane lipids

Marta Almada (UPorto)
Lipidomic approach towards anandamide-induced cell death in rat decidual cell

Bebiana Sousa (UAveiro)
Lipid profile alteration of cardiomyocytes in acute myocardial infarction

17h45 - 18h00 | Q&A

18h00 | Closing session

Venue: Department of environment and planning
MARINE LIPIDOMICS: FROM THE LIPID SIGNATURE OF MARINE ORGANISMS TO THE DISCOVERY OF NEW BIOACTIVE COMPOUNDS

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Abstract

Lipids are major components of marine organisms, which have a unique lipid composition. However, identification of lipid profile of marine organisms in not fully elucidated and their potential is waiting to be explored. So far marine organisms (e.g. fish, seafood, macro- and microalgae) and marine-derived natural products (e.g. fish oil) are an endless source of lipids with many beneficial effects on human health. Lipids such as polyunsaturated fatty acids are valuable nutrients while others such as glycolipids are considered promising bioactive natural products with potential therapeutic applications such as anti-inflammatory, anti-proliferative, antioxidant and antimicrobial. Different marine organisms have a typical lipid profile representing the marine chemical biodiversity. Lipid composition is very sensitive to environmental conditions, and also to the nutritional support. This feature allows the manipulation of environmental conditions in order to improve the production of bioactive natural compounds, but the identification of a specific lipid signature is still a challenge. Lipidome of eukaryotes comprises thousands of lipids that are structurally and functionally diverse. In the last years, the most recent advances of mass spectrometry associated with high sensitivity, and capability of high throughput analysis have been opening new perspectives in the understanding of the role of lipids in marine organism’s biochemistry. In this lecture, the most common analytical strategies based on mass spectrometry analysis used in marine lipidomics will be briefly presented, as well as how it can be used to fully explore the potential of the sea as a source of added-value products.
UNRAVELLING POLAR LIPIDS DYNAMICS DURING EMBRYONIC DEVELOPMENT OF TWO SYMPATRIC BRACHYURAN CRABS (CARCINUS MAENAS AND NECORA PUBER) USING LIPIDOMICS

REY Felisa¹a, ALVES Eliana², MELO Tânia², DOMINGUES Pedro², QUEIROGA Henrique¹, ROSA Rui³,⁴, DOMINGUES M. Rosário M.², CALADO Ricardo¹b

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Abstract

Embryogenesis is an important stage of marine invertebrates with biphasic lifecycles, as it conditions their larval and adult life. Throughout embryogenesis, phospholipids (PL) play a key role as an energy source, as well as constituents of biological membranes. However, the dynamics of PL during embryogenesis in marine invertebrates is still poorly studied. The present work used a lipidomic approach to determine how polar lipid profiles shift during embryogenesis in two sympatric estuarine crabs, Carcinus maenas and Necora puber. The combination of thin layer chromatography (TLC), liquid chromatography – mass spectrometry (LC-MS/MS) and gas chromatography – mass spectrometry (GC-MS) allowed us to achieve an unprecedented resolution on PL classes and molecular species present on newly extruded embryos (stage 1) and those near hatching (stage 3). Embryogenesis proved to be a dynamic process, with four PL classes being recorded at stage 1 embryos (68 molecular species in total) and seven PL classes at stage 3 embryos (98 molecular species in total). The low interspecific difference recorded in the lipidomic profiles of stage 1 embryos appears to indicate the existence of a similar maternal investment. The same pattern was recorded for stage 3 embryos revealing a similar catabolism of embryonic resources during incubation for both crab species.

Acknowledgements

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TRACEABILITY OF COLLECTION SITE USING FATTY ACID PROFILES OF THE ADDUCTOR MUSCLE OF COCKLES (CERASTODERMA EDULE)

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Abstract
Geographic traceability of seafood is key for controlling its quality and safeguarding consumers’ interest. The present study assessed if the fatty acid (FA) profile of the adductor muscle (AM) of fresh cockles (Cerastoderma edule) can be used to discriminate the origin of specimens collected in different bivalve capture/production areas legally defined within a coastal lagoon. Results suggest that this biochemical approach holds the potential to trace sampling locations with a spatial resolution < 10 Km, even for areas with identical classification for bivalve production. Cockles further away from the inlet, i.e. in areas exposed to a higher saline variation, exhibited lower levels of saturated fatty acids, which are key for stabilizing the bilayer structure of cell membranes, and a higher percentage of polyunsaturated fatty acids, which enhance bilayer fluidity. Results suggest that the structural nature of the lipids present in the AM provides a stable fatty acid signature and holds potential for tracing the origin of bivalves to their capture/production areas.

Acknowledgements
This work was supported by European Funds and by National Funds through the Portuguese Science Foundation (FCT) QREN, FEDER, and COMPETE within project PEst-C/MAR/LA0017/2013, QOPNA research unit (project PEst-C/QUI/UI0062/2013; FCOMP-01-0124-FEDER-037296), and RNEM (REDE/1504/REM/2005 that concerns the Portuguese National Mass Spectrometry Network). F. Ricardo, T. Pimentel, F. Rey and A.S.P. Moreira were supported by PhD scholarships (SFRH/BD/84263/2012, SFRH/BD/51041/2010, SFRH/BD/62594/2009, SFRH/BD/80553/2011 respectively) funded by the Fundação para a Ciência e a Tecnologia (QREN-POPH-Type 4.1 – Advanced training, subsidized by the European Social Fund and national funds MEC). The present study was funded by PROMAR, a Portuguese instrument for the sectors of fisheries and aquaculture funded by the European Fisheries Fund, within the research project RASTREMAR - Use of molecular tools in the traceability of marine food products (PROMAR 31-03-05-FEP-0015).
DECIPHERING THE LIPIDOMIC PROFILE OF THE SEAWEED CODIUM TOMENTOSUM TOWARD THE BIOPROSPECTION OF PHYTOCHEMICALS

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Abstract

Biotechnological applications of marine macroalgae have gained a new interest due the added-value of their chemical constituents, as they exhibit biological activity with multiple applications in industrial and agricultural sectors, as well as in human health. This is the case of glycerolipids, phospholipids and glycolipids, high value products that display several commercial applications in the food, pharmaceutical and cosmetic industries [1]. The present study is the first to report the isolation and characterization of the polar lipids of the seaweed Codium tomentosum originating from land-based integrated multi-trophic aquaculture (IMTA) systems using a lipidomic-based approach employing hydrophilic interaction liquid chromatography – electrospray ionization mass spectrometry (HILIC-ESI-MS) [2].

The polar lipid profile of C. tomentosum revealed the presence of more than two hundred species corresponding to glycolipids (sulfoquinovosyl diacylglycerols, sulfoquinovosyl monoacylglycerols, digalactosyl and monogalactosyl diacylglycerols), glycerophospholipids (lyso- and phosphatidylycholines, phosphatidylinositolos, phosphatidic acids, lyso- and phosphatidyglycerols), and di- and monoacyl betaine lipids. Phosphatidylinositolos, sulfoquinovosyl monoacylglycerols and some species of monoacyl betaine lipids were reported for the first time in green algae. Some of these polar lipids contain polyunsaturated fatty acids (PUFAs) of the n-3 series, namely 20:5 and 22:6 species, revealing the ability of Codium tomentosum to synthesize larger PUFA.

Several of the lipids identified were already reported to have nutritional and health benefits and thus the present study unravels the potential of Codium tomentosum from IMTA [3] as an edible product with high nutritional value and bioactive compounds already known to be important for human wellbeing and prevention of disease.

References


Acknowledgements
The authors are grateful to ALGAplus- Produção e Comércio de algas e seus derivados, Lda. for providing the macroalgae samples. Thanks are due to Fundação para a Ciência e a Tecnologia (FCT, Portugal), European Union, QREN, POPH, FEDER and COMPETE for funding the QOPNA research unit (project PEst-C/QUI/UI0062/2011 and the project PTDC/QUI-BIQ/104968/2008), to RNEM (REDE/1504/REM/ 2005) for the Portuguese Mass Spectrometry Network. Elisabete da Costa (SFRH/ BD/452499/2014), Tânia Melo (SFRH/BD/84691/2012), Ana Moreira (SFRH/BD/80553/2011) and Eliana Alves (BPD/UI51/5441/2015 from RNEM/2013/UA) are grateful to FCT for their grants.
LOWER OR HIGHER RESOLUTION IMPLICATIONS FOR QUANTITATIVE AND QUALITATIVE ANALYSIS IN MASS SPECTROMETERS: ORBITRAP, TRIPLEQUAD AND LINEAR TRAP FEATURES

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Abstract
The number of users and areas of specialization in mass spectrometry has increased enormously in recent years. In the world of small molecules and Proteins, the new analytical procedures require sensitivity, selectivity and robustness within a short analysis time. Several different types of mass spectrometers are available, each one with their specific strengths and drawbacks. The decision on which one to use is usually based on the quality of the data combined to cost/time of the analysis.

Different types of “traditional” Mass Analyzers, like Triple Quads, Ion Trap, and Linear Traps will be presented. We will discuss the instrumental arrangements, its advantages, features and disadvantages in Quantitation and qualifying the molecules.

Recent publications have shown that high resolution mass spectrometry is a well-accepted and better alternative to the analysis molecules. There is a high need to add the possibility to perform data dependent MS2 experiments by making use of a resolving power of up to 140,000 FWHM. On that way, the mass analyzer Orbitrap represents one of the best alternatives currently available in the market [1]. This mass analyzer was first described in 2000 and has now reached the status of a mainstream mass spectrometry technique as it can support a wide range of applications from routine compound identification to the analysis of trace-level components in complex matrices.

This presentation will discuss the application and use of the different technologies with some examples that will show the features of the different technologies.

SPHINGOLIPIDS AS IMMUNE SYSTEM MODULATORS

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Abstract
Traditionally, proteins are considered the biomolecules with the highest capacity to induce an immune response. Tradition was challenged around 20 years ago with the discovery of T lymphocytes that are activated by the sphingolipid alpha-galactosylceramide. The most studied lipid specific T lymphocytes are the invariant Natural Killer T (iNKT) cells; these cells have the capacity to rapidly produce high amounts of cytokines having an important role in the immune response against infection and cancer.

My team is interested in identifying “new players”, both lipids and lipid binding proteins, important for the differentiation and peripheral activation of lipid specific T lymphocytes. Our strategy is to study several Sphingolipidoses that are rare, genetic diseases that arise mostly due to enzymatic defects in lysosomal hydrolases that lead to the specific accumulation of its substrates.

In this presentation, results of iNKT cell analysis in Fabry, Gaucher, GM2 gangliosidoses and Niemann Pick D diseases will be presented. In these four diseases there is accumulation of sphingolipids in the lysosome; however the alterations found seem to be dependent on the type of lipid accumulated and not merely on lysosomal dysfunction, as initially mouse models postulated. For Fabry and Niemann Pick D diseases the presence of inhibitory lipids explains the phenotype observed.

Our results suggest that iNKT cell activation is a complex process, involving both immunogenic and inhibitory lipids. The lipids accumulated in multiple lysosomal storage diseases may represent new regulators of lipid antigen presentation.
LIPIDOMIC APPROACH TOWARDS ANANDAMIDE-INDUCED CELL DEATH IN RAT DECIDUAL CELL

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Abstract

Altered phospholipid (PL) metabolism has been associated with pregnancy disorders. Moreover, lipid molecules such as endocannabinoids (eCBs) and prostaglandins (PGs) are important mediators of reproductive events. In humans, abnormal decidualization has been linked with unexplained infertility, miscarriage and endometrial pathologies. Anandamide (AEA), the major eCB, induces apoptosis in rat decidual cells. In this study, the PL profile of rat decidual cells was characterized by a Mass spectrometry (MS) based lipidomic approach. Furthermore, we analyzed a possible correlation between changes in PL of rat decidual cells' membrane and AEA-induced apoptosis. We found an increase in phosphatidylserine and a reduction of cardiolipin and phosphatidylinositol relative contents. In addition, we observed an increase in the content of alkyl(alkenyl)acylPL, plasmalogens, and of long chain fatty acids especially with high degrees of unsaturation, as well as an increase in lipid hydroperoxides in treated cells. These findings provide novel insights on deregulation of lipid metabolism by anandamide, which may display further implications in decidualization process.
LIPID-BASED STRATEGIES IN GENE THERAPY: FROM THE DESIGN OF GENE CARRIERS TO THE MODULATION OF MEMBRANE LIPIDS

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Abstract
The goal of gene therapy is to treat diseases caused by genetic disorders, which is a key feature of cancer, making this disease one of the major targets of the gene therapy field. The application of this therapeutic modality requires the delivery of nucleic acids into cells, which, depending on the strategy, will induce the expression of a missing/defective gene or block the expression of a gene excessively expressed. Therefore, identification of a therapeutic target gene is crucial to define the strategy and to maximize therapeutic efficacy while minimizing toxicity. In the cancer context, cells frequently exhibit specific alterations in their metabolic activity, namely, increased rate of lipid synthesis to generate biological membranes and support cancer cell proliferation. Specific changes of the lipid metabolism affect the diversity of lipids with structural and signalling functions with repercussions to numerous cellular processes, such as survival and death. Given the importance of lipids in cancer biology, genes involved in lipid metabolism will be discussed as novel targets for cancer gene therapy. In addition, the success of this approach implies the improvement of delivery systems to assist nucleic acids to overcome various biological barriers, such as those imposed by cellular membranes. The recognized ability of cell penetrating peptides (CPPs) to transpose membranes and condense nucleic acids, facilitating their cellular uptake, provides those molecules with a great potential as nucleic acid delivery systems. However, CPP efficacy in mediating gene regulation and safety are still main issues. In this context, the potential for nucleic acid delivery of the S413-PV CPP, a dermaseptin derived peptide fused to the nuclear localization sequence of the SV40 large T antigen, has been tentatively modulated in our laboratory through peptide acylation. In this presentation, we will discuss two important aspects where lipids have contributed to advances in the gene therapy field, i.e., as potential targets for cancer therapeutic interventions and as modulators of the efficiency of peptide-based systems for nucleic acid delivery.
LIPID PROFILE ALTERATION OF CARDIOMYOCYTES IN ACUTE MYOCARDIAL INFARCTION

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Abstract
Acute myocardial infarction (AMI) is one of the main causes of death all over the world [1]. AMI is characterized by ischemia, in response to simultaneous nutrient and oxygen deprivation, also called starvation and hypoxia respectively [2]. The cell response to this injury can be autophagy or apoptosis that are very important for the evolution and recovery of the myocardium infarction [3].

It is well known that lipids play an important role in AMI although it is not completely understood [4]. Some studies report changes in plasma lipids but studies regarding cellular and molecular changes are scarce [5]. Identification of lipid variation in cardiomyocytes at a molecular level upon AMI can be important to identify new biomarkers to aid in AMI diagnostic and prognostic. The diagnostic of AMI is still difficult even though it is essential to prevent further complications. Several enzymes have clinical significance in the cardiac muscle, such as troponin (Tn), and are released from the injured tissues but only show up hours after the cardiac event [6]. Our aim is to find possible variations in phospholipid profile of cardiomyocytes induced by starvation and ischemia conditions, using a modern lipidomic approach.

Our results revealed a tendency for a decrease in the phospholipid content both in ischemia and starvation. This may be associated with autophagy, a process of adaptation to stress that prevents cell death. The phospholipid content of each class was accessed and compared. An increase in SMs and PIs and a decrease in PCs and CLs content in cells were observed in both conditions. The increase in SM content may be related to the decrease in PC since one can be converted into the other through sphingomyelin synthase. In addition to structural functions, SM plays an important role in signaling pathways since it is located in “lipids raft”. Also PIs are important precursors of signaling molecules that modulate for instance proliferation and cell death and may therefore be increased in ischemia and starvation. On the other hand, the decrease in CL content suggests a mitochondrial dysfunction, a common feature in cardiovascular diseases. Additionally oxidative redox state in ischemia and starvation leads to cardiolipin oxidation followed by release into cytoplasm, triggering the decrease in CL content in cells [7].

We can conclude that starvation and ischemia are conditions that induce changes in the lipid homeostasis and metabolism that can be important for cardiomyocytes death or recovery.

References


LIPIDOMICS AND PROTEOMICS TO UNDERSTAND THE HEALTH BENEFITS OF MARINE FISH OIL ENRICHED DIETS

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Abstract
By using lipidomics and proteomics approaches, we highlighted the importance of specific dietary designs with EPA and DHA to potentiate their health benefits. Results showed that balanced proportions of EPA and DHA promote an anti-oxidant environment that leads to lower oxidative stress and inflammation in vivo. Eicosanoids, docosanoids and carbonylated proteins were the target of these studies. In detail, for the simultaneous quantification in plasma of a large number of lipid mediators, a robust and sensitive targeted analysis platform based on SPE-LC-ESI-IT-MS/MS was developed. Carbonylated proteins were identified by tandem mass spectrometry (LC-ESI-IT-MS/MS) after prefractionation by 2D-gels.

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LIPIOMICS STUDIES OF MESENCHYMAL STROMAL CELLS UNDER PRO-INFLAMMATORY STIMULUS

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Abstract
Mesenchymal stromal cells (MSCs) are adult stem cells that can be found in different tissues. These cells are immunomodulatory and can suppress inflammatory reactions. Thereafter MSCs have been successfully applied as biological therapy in several clinical trials regarding autoimmune and inflammatory diseases. Despite the wide use of these cells, no unique marker has been identified. Also the immunomodulatory mechanism employed by these cells is not fully understood. The aim of this work is to study MSCs’ lipidome changes depending on pro-inflammatory stimulus subjected to the cells, in order to identify markers that allow recognizing powerful immunomodulatory cells. This is the first study ever made that aims to analyse the phospholipid profile of MSCs subjected to proinflammatory stimulus.
LIPIDOMICS AS A NEW APPROACH FOR UNRAVELING THE POLAR LIPID COMPOSITION OF *CHONDRUS CRISPUS*

AZEVEDO Vítor¹,a, MELO Tânia¹, ALVES Eliana¹, DOMINGUES Pedro¹, CALADO Ricardo², ABREU Maria H.³, DOMINGUES M. Rosário M.¹,b

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Abstract

Marine macroalgae have been used for direct human consumption, as additives in food and as fertilizers in agriculture. Over the last decade, the fatty acid composition of several species of macroalgae has been extensively studied, however, the polar lipid components are insufficiently known. Herein, it is reported, for the first time, a lipidomic study of polar lipid composition of the red seaweed *Chondrus crispus* through hydrophilic interaction liquid chromatography — electrospray ionization mass spectrometry (HILIC–ESI–MS). The main polar lipid classes identified include glycolipids, glycosphingolipids, inositolphosphoceramides, glycerophospholipids and betaine lipids. A total of 354 lipid molecular species were detected. The identification of macroalgae lipidome signature is important for the valorization of macroalgae as edible products and a source of bioactive compounds.
STRUCTURAL CHARACTERIZATION OF NITRATED PHOSPHATIDYLSERINE BY MASS SPECTROMETRY

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Abstract
The nitroalkenes derivatives of unsaturated fatty acids (NO₂-FA) represent endogenously occurring products of nitroxidative stress. Although NO₂-FA can be present endogenously as free species or adducted to proteins, studies concerning the NO₂-FA esterified to phospholipids have been overlooked. The aim of this study was to develop mass spectrometry (MS)-based approaches for identification and characterization of the fragmentation pattern of nitroalkenes derivatives of POPS (1-palmitoyl-2-oleoyl-sn-glycero-3-phosphoserine). Analysis of NO₂-POPS derivatives formed after reaction with nitronium tetrafluoroborate (NO₂BF₄) was carried out in negative mode in an ESI linear ion trap mass spectrometer LXQ (ThermoFinnigan). Tandem mass spectra fingerprinting of NO₂-POPS were identified and proposed as tools for identification in biological samples.
CINNAMYLIDENEACETOPHENONES: THE PROTECTIVE ROLE TOWARDS OXIDATION OF PHOSPHATIDYLCHOLINES

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Abstract
Curcumin (CR) is a natural polyphenol. Inspired by the anti-inflammatory and antioxidant activities shown by CR, it was considered to study the ability of compounds with structural resemblance to inhibit lipid oxidation. These compounds are cinnamylideneacetophenones (CA), an important group of α,β,γ,δ-diunsaturated ketones. Biological studies concerning these compounds are scarce and refer mainly to antiviral and antibacterial evaluations. The lipid oxidation reaction was induced by the hydroxyl radical (Fenton reaction) and monitored by electrospray ionization (ESI) mass spectrometry (MS) using PC liposomes as a model of cell membrane. Compound CA4, holding a methylated hydroxyl group in the position R2, and CR showed similar effects in inhibiting lipid peroxidation. We performed other different assays to support the results obtained from MS analysis.
ALTERATIONS IN THE PHOSPHOLIPIDOME OF YEAST CELLS BEARING A MUTATED SERYL-TRNA

ARAÚJO Ana Rita D.1,2,3, SANTINHA Deolinda R.2, MELO Tânia2, MACIEL Elisabete A.2, DOMINGUES Pedro2, DOMINGUES Maria Rosário M.2, SANTOS Manuel A. S.3

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Abstract
The induction of mistranslation in yeast can trigger the environmental stress response (ESR), the unfolded protein response (UPR), among other effects. DNA microarray analyses showed alterations in lipid/fatty acid metabolism-related genes, but it is still unclear how mistranslation affects the lipidome. To clarify this question we transformed yeast cells with a seryl-tRNA bearing an anticodon that recognizes either alanine or glycine codons, but introduces serine into the nascent protein. Then, total lipid extracts of different growth phases were analysed with a lipidomic approach: fractionation by liquid and thin layer chromatography (LC and TLC, respectively) followed by characterization by ESI-MS/MS; total fatty acid (FA) content was evaluated by gas chromatography (GC). Here we show that, in both growth phases, the abundances within some lipid classes and in total FA were altered.
ESTUDO LIPIDÔMICO DE PLASMA SANGUÍNEO DA GRÁVIDA PARA DETECÇÃO DE TRISSOMIA 21 NO 1º E 2º TRIMESTRES

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Abstract
A Trissomia 21, ou Síndrome de Down, caracteriza-se pela ocorrência de 3 cópias do cromossoma 21, tendo uma maior incidência em casos de idade materna avançada, tabagismo, diabetes, entre outros. Actualmente os seus métodos de detecção visam técnicas pouco sensíveis e específicas e a sua confirmação vai de encontro a métodos de carácter invasivo para a paciente associados a risco de aborto. Este trabalho, através de uma abordagem lipidómica, procurou alterações no perfil dos lípidos de extractos lipídicos plasma sanguíneo da grávida, para o 1º e 2º trimestres da gravidez, através de MALDI-MS, para procurar um método alternativo mais sensível, específico, que auxilie ainda num diagnóstico precoce da doença.