J Proteomics Bioinform 2016, 9:11(Suppl)
http://dx.doi.org/10.4172/0974-276X.C1.092

Targeted lipidomics: Analytical approach for the seperation of lipids by using UPLC-ESI/MS/MS in serum samples of diabetes mellitus pateints

Smita Panchal
Indian Institue of Toxicology and Research, India

In the present study, an ionic liquid based vortex assisted surfactant-enhanced emulsification microextraction (IL-VASEME) method followed by Plackett-Burmann Design (PBD) and Central Composite Design (CCD) using liquid chromatography-electrospray mass spectrometry (LC-ESI-MS/MS) has been applied for the determination of fatty acids, triglycerides and phospholipids in serum samples of healthy and diabetic subjects. Study afforded the separation of these lipid classes in a single run with Rt of 5 min. The method was statistically optimized to reduce the extraction time. The extraction parameters further were optimized by design of experiment (DOE) approach. The ionic liquid, 1-butyl-3-methylimmidazolium hexafluorophosphate ($BMIMPF_6$) was used as an extraction solvent, while surfactant Triton X-100 was used as an emulsifying agent. Statistical method, PBD screened the most significant factors such as ionic liquid volume, surfactant strength and pH for optimizing conditions for the separation of lipids. The screened factor values were based on the CCD, which was optimized as 45 µL of ionic liquid, 7.5 pH and 1.25% of surfactant strength for extraction of lipids. The limit of detection (LOD) and limit of quantification (LOQ) were 0.012-0.034 ng/mL and 0.046-0.114 ng/mL respectively. The recovery of lipids was in the range of 90.9-114%. The intraday and interday precision in the serum sample ranged between 1.42-4.48% and 3.75-10.8% respectively. The study revealed that the IL-VASEME method was comparatively more sensitive with other conventional methods for the separation of both polar and non-polar lipids in single step.

sptina6@gmail.com

Structure based pharmacophore modeling for design of riboswitch based potent inhibitors for *Vibrio cholerae*

Somdutt Mujwar
Maulana Azad National Institute of Technology, India

Cholera pandemics are caused by facultative pathogenic *Vibrio cholerae* bacteria persisting in the countries having warmer climatic conditions as well as the presence of large water bodies with huge amount of organic matter, it is responsible for the millions of deaths annually. Presently, the available therapy for cholera is Oral Rehydration Therapy (ORT) with an antibiotic drug. Excessive utilization of life saving antibiotics drugs leads to the development of resistance by the infectious microorganism against the antibiotic drugs resulting in loss of effectiveness of these drugs. Also, many side effects are associated with the use of these antibiotic drugs. This riboswitch is explored as an alternative drug target for *Vibrio cholerae* bacteria to overcome the problem of drug resistance as well as side effects associated with the antibiotics drugs. The bacterial riboswitch is virtually screened with 24407 ligands to get possible drug candidates. The 10 ligands showing best binding with the riboswitch are selected to design a pharmacophore which can be utilized to design lead molecules by using the phenomenon of bioisosterism.

simplysom4u@gmail.com