Annals of Proteomics and Bioinformatics

Volume - 3, Issue - 1

Research Article **Published Date:-2019-12-31 00:00:00**

The importance of gestational age in first trimester, maternal urine MALDI-Tof MS screening tests for Down Syndrome

Background: The proposal that MALDI-ToF mass spectrometry could be used as a direct, rapid and affordable diagnostic tool in clinical laboratory medicine has moved from a theoretical possibility to a reality for Microbiology. Several studies have proposed the application of this technology in obstetric and gynaecological evaluation of patients. In particular, we have proposed that the adoption of MALDI-ToF mass spectrometry in examination of maternal pregnancy urine samples for the detection of Downs syndrome.

Methods: A retrospective collection of 20 Down Syndrome and 100 non-aneuploid pregnancy urines at 12 to 14 weeks gestation, collected in 2007-2008 from high risk pregnancy cohorts, were examined by MALDI-ToF mass spectrometry in the mass/charge range between 1000 and 100000 m/z. Normalisation of spectral data was defined using mass bins of 100 m/z expressed as a percentage of the total ion count of the mass spectra from 2000 to 11000 m/z. Of the ninety 100 m/z bins, forty-six were identified as m/z bins at which statistically significant differences in spectra occurred between Downs and control/non-aneuploid samples. Based on the differences and variance, for values at these bins, weighted scores of the probability of being Downs were assigned. Comparative algorithms consisting of various mass bins were tested for ability to distinguish Down syndrome from non-aneuploid pregnancy.

Results: Although various algorithms could distinguish Downs from non-aneuploid controls, it was found that gestational age was a confounding factor and that if separated into gestational age matched cohorts the ability to distinguish the groups improved dramatically e.g. whilst a 19 bins algorithm separated 100% of Downs from non-aneuploid pregnancies for a 9% false positive rate in the mixed gestational ages group; a two bin algorithm distinguished 100% of Downs for a 6% false positive rate for the 12 weeks gestational age pregnancies.

Conclusion: Normalised MALDI-ToF mass spectra, at 2000 to 11000 m/z, of maternal urine gives rise to gestational age specific screening tests algorithms for Downs's syndrome.

Research Article **Published Date:-2019-12-19 00:00:00**

Theoretical study on binding interactions of laccase-enzyme from Ganoderma weberianum with multiples ligand substrates with environmental impact

Laccase catalyzes oxidation of lignin and aromatic compound with similar structure to this one. Their low substrate specificity results on degradation of similar phenolic compounds. In this context, Molecular Docking was performed with different ligands suggesting potential bio-degradation. Binding active-sites prediction of fungal laccase (access number uniprotkb: A0A166P2X0), from Ganoderma weberianum was performed using machine learning algorithm based on Deep Convolutional Neural Networks (DeepSite-CNNs chemoinformatic tool). Herein, ligands like 2,4 - dichlorophenol, benzidine, sulfisoxazole, trimethoprim and tetracycline were analyzed and two additional reference controls which were 2,2 – azinobis 3 – ethylbenzothiazoline – 6 - sulfonic acid (ABTS) and 2,6 - dimetoxyphenol (2,6 DMP) were used in comparison with the other former mentioned ligands based on high laccase affinity. The five ligands were carried out because their potential biotechnological interest: the antibiotics sulfisoxazole, trimethoprim and tetracycline, and xenobiotics 2,4 - dichlorophenol and benzidine. Molecular docking experiments returned Gibbs free energy of binding (FEB or affinity) for laccase-ligand complexes. The best docking binding-interaction from each laccase-ligand conformation complexes suggest great ability of these ligands to interact with the laccase active-binding site. Herein, FEB values (kcal/mol) were obtained with higher affinity values for reference controls like 2,6 - dimethoxyphenol with -4.8 Kcal/mol and ABTS with -7.1 Kcal/mol. Furthermore, the FEB values were -4.7, -6.5, -6.8, -5.2 and -6.5 Kcal/mol, for 2,4 - dichlorophenol, benzidine, sulfisoxazole, tetracycline and trimethoprim respectively with high prevalence of hydrophobic interaction with functional laccase binding residues. Lastly, this study presents for first time at the bioinformatics field a molecular docking approach for the prediction of potential substrate of laccase from Ganoderma weberianum towards biotechnological application.