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Urine Metabolomic Profiling and Machine Learning in ASD Diagnosis: Toward Precision Treatment

Background

Autism Spectrum Disorder (ASD) diagnosis traditionally relies on behavioral assessments, which can be subjective and lead to delayed identification. Recent advances in metabolomics and machine learning offer promising alternatives for more precise diagnostic approaches.

Objectives

This study aimed to investigate the potential of urine metabolomic profiling combined with machine learning techniques to differentiate between children with ASD and neurotypical controls, exploring both internal and external metabolites as potential diagnostic markers.

Methods

The study analyzed first-morning urine samples from 52 children (32 with ASD, 20 controls), aged 5.04 ± 1.87 and 5.50 ± 1.74 years, respectively. Using LC-MS, 293 polar metabolites were identified and categorized into 188 internal (endogenously produced) and 105 external (exposome-originated) metabolites. We compared the ability of different machine learning classifiers, (i.e. Random Forest, Logistic Regression, Random Tree, and Naïve Bayes), to differentiate between ASD and control groups using 10-fold cross-validation.

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Results

When using all 293 metabolites, the Random Forest classifier achieved 85% accuracy and an Area Under the Curve (AUC) of 0.9. In which classification based on 189 internal metabolites seemed to drive the effect with the Random Forest classifier achieving 85% accuracy and an AUC of 0.86. In contrast, external metabolites alone provided lower classification performance, with an accuracy of 71% and AUC of 0.72.

Conclusions

This study demonstrates the potential of urine metabolomic profiling as a complementary diagnostic tool for ASD. The independent performance of internal metabolites suggests that the body's metabolic processing may be more informative than dietary metabolites in distinguishing ASD. The high classification accuracy implies the potential for developing an assistive diagnostic method, though further research is needed to correlate metabolite profiles with specific behavioral characteristics and ASD subtypes.

Keywords

Autism Spectrum disorder(ASD), Polar Urine Metabolites, Machine Learning

Biography

Dr. Shula Shazman is a scientist and academic at The Open University of Israel, specializing in machine learning, bioinformatics, and computational biology. She earned her B.Sc. in Information Systems Engineering and Ph.D. in Biological Sciences from the Technion, followed by a postdoctoral fellowship at Columbia University. Her research focuses on complex diseases, particularly autism and Type 2 Diabetes, using AI-driven approaches. She has published widely, presented internationally, and contributed to biomarker discovery and precision nutrition. A dedicated educator, she teaches AI, data mining, and programming, and has authored textbooks used in higher education. Dr. Shazman also advises academic ML projects globally.