<u>4 Groups</u>
* ASD: *n* = 75
* Control: *n* = 29
* Mother: *n* = 40
* Father: *n* = 39

<u>Untargeted Molecular Profiling</u>

* HILIC-HRMS (positive mode)
* RPLC-HRMS (negative mode)

<u>Data Preprocessing</u>
* Feature detection, alignment, and filtering; batch effect correction

No. of features
HILIC: 10 173
RPLC: 8 011

Only on the significant features

<u>Data processing</u>
For each familial group
* Extract residuals after adjusting for age, sex, and batch

Familial pairs: *n* = 35
No. of mutual features
HILIC: 79
RPLC: 45

A) Physiological Analysis

<u>A1) Metabolome-wide association study</u>
For ASD and control groups
* Logistic regression

No. of significant features
HILIC: 125
RPLC: 66

<u>A2) Putative annotation</u>
* Match features to chemicals by accurate mass

No. of annotated features
HILIC: 20
RPLC: 10

B) Shared Environment Analysis

<u>B1) Correlations within household</u>
Estimate Spearman's rank correlations
* ASD-mother, ASD-father

<u>B2) Correlation patterns within household</u>
Create correlation globes
* Visualize the Spearman's rank correlations matrixes of ASD, mother, father, ASD-mother, ASD-father

<u>B3) Correlations of feature relatedness</u>
* Examine in ASD-mother, ASD-father
* Use ASD-control for comparison