Search name:
20190718_Autism_UNPaired_v2.6_NoNorm_noGF_7sc_allAdd_mzClO_DBs_RT_0.1min_1E5_0.1min_DBS
Search description: Untargeted Metabolomics workflow: Retention time alignment, Component Detection, Grouping, Elemental Composition Prediction, Gap Filling, Hide chemical Background (using blanks), ID using mzCloud (needs MS/MS) and ChemSpider (using Formula); KEGG Pathway Mapping and Differential Analysis (ANOVA, adjusted p-values, fold change, CV, etc.)
Search date: 18-07-2019 18:15:51
Created with Discoverer version: 2.1.0.401

[Input Files (6)]
-->Select Spectra (7)

[Select Spectra (7)]
-->Align Retention Times (10)
-->Create Mass Trace (28)

[Align Retention Times (10)]
-->Detect Unknown Compounds (9)

[Detect Unknown Compounds (9)]
-->Group Unknown Compounds (8)

[Group Unknown Compounds (8)]
-->Search mzCloud (22)
-->Predict Compositions (16)
-->Search ChemSpider (23)
-->Search Mass Lists (27)
-->Mark Background Compounds (20)

[Predict Compositions (16)]
-->Search ChemSpider (23)

[Search mzCloud (22)]

[Search ChemSpider (23)]

[Search Mass Lists (27)]

[Mark Background Compounds (20)]

[Create Mass Trace (28)]

[Differential Analysis (17)]

[Descriptive Statistics (24)]

[Assign Compound Annotations (29)]

Processing node 6: Input Files

Input Data:
- File Name(s) (Hidden):

Processing node 7: Select Spectra
---
1. General Settings:
- Precursor Selection: Use MS(n - 1) Precursor
- Use New Precursor Reevaluation: True
- Use Isotope Pattern in Precursor Reevaluation: True
- Store Chromatograms: False

2. Spectrum Properties Filter:
- Lower RT Limit: 0
- Upper RT Limit: 15
- First Scan: 0
- Last Scan: 0
- Ignore Specified Scans: (not specified)
- Lowest Charge State: 1
- Highest Charge State: 3
- Min. Precursor Mass: 70 Da
- Max. Precursor Mass: 1050 Da
- Total Intensity Threshold: 500000
- Minimum Peak Count: 1

3. Scan Event Filters:
- Mass Analyzer: Is FTMS
- MS Order: Any
- Activation Type: Is HCD
- Min. Collision Energy: 0
- Max. Collision Energy: 1000
- Scan Type: Any
- Polarity Mode: Is +

4. Peak Filters:
- S/N Threshold (FT-only): 3

5. Replacements for Unrecognized Properties:
- Unrecognized Charge Replacements: 1
- Unrecognized Mass Analyzer Replacements: FTMS
- Unrecognized MS Order Replacements: MS2
- Unrecognized Activation Type Replacements: HCD
- Unrecognized Polarity Replacements: +
- Unrecognized MS Resolution@200 Replacements: 75000
- Unrecognized MSn Resolution@200 Replacements: 17500

Processing node 10: Align Retention Times
---
1. General Settings:
- Alignment Model: Adaptive curve
- Alignment Fallback: Use Linear Model
- Maximum Shift [min]: 0.1
- Shift Reference File: True
- Mass Tolerance: 5 ppm
- Remove Outlier: True

Processing node 9: Detect Unknown Compounds
---
1. General Settings:
- Mass Tolerance [ppm]: 5 ppm
- Intensity Tolerance [%]: 30
- S/N Threshold: 2
- Min. Peak Intensity: 100000
- Ions:
  [2M+ACN+H]+1
  [2M+ACN+Na]+1
  [2M+FA-H]-1
  [2M+H]+1
  [2M+K]+1
  [2M+Na]+1
  [2M+NH4]+1
  [2M-H]-1
  [2M-H+HAc]-1
  [M+2H]+2
  [M+3H]+3
  [M+ACN+2H]+2
  [M+ACN+H]+1
  [M+ACN+Na]+1
  [M+Cl]-1
  [M+DMSO+H]+1
  [M+FA-H]-1
  [M+H]+1
  [M+H+K]+2
  [M+H+MeOH]+1
  [M+H+Na]+2
  [M+H+NH4]+2
  [M+H-H2O]+1
  [M+H-NH3]+1
  [M+K]+1
  [M+Na]+1
  [M+NH4]+1
  [M-2H]-2
  [M-2H+K]-1
  [M-H]-1
  [M-H+HAc]-1
  [M-H+TFA]-1
  [M-H-H2O]-1
- Base Ions: [M+H]+1; [M-H]-1
- Min. Element Counts: C H
- Max. Element Counts: C90 H190 Br3 Cl4 K2 N10 Na2 O15 P2 S5

2. Peak Detection:
- Filter Peaks: True
- Max. Peak Width [min]: 0.5
- Remove Singlets: True
- Min. # Scans per Peak: 7
- Min. # Isotopes: 2

Processing node 8: Group Unknown Compounds
---
1. Compound Consolidation:
- Mass Tolerance: 5 ppm
- RT Tolerance [min]: 0.1

2. Fragment Data Selection:
- Preferred Ions: [M+H]+1; [M-H]-1

Processing node 22: Search mzCloud
---
1. Search Settings:
- Compound Classes: All
- Match Ion Activation Type: True
- Match Ion Activation Energy: Any
- Ion Activation Energy Tolerance: 100
- Apply Intensity Threshold: False
- Precursor Mass Tolerance: 5 ppm
- FT Fragment Mass Tolerance: 10 ppm
- IT Fragment Mass Tolerance: 0.1 Da
- Identity Search: HighChem HighRes
- Similarity Search: Similarity Forward
- Library: Reference
- Post Processing: Recalibrated
- Match Factor Threshold: 0
- Max. # Results: 20

Processing node 16: Predict Compositions
---
1. Prediction Settings:
- Mass Tolerance: 5 ppm
- Min. Element Counts: C H
- Max. Element Counts: C90 H190 Br3 Cl4 N10 O15 P2 S5
- Min. RDBE: -1
- Max. RDBE: 40
- Min. H/C: 0.1
- Max. H/C: 3
- Max. # Candidates: 10
- Max. # Internal Candidates: 500

2. Pattern Matching:
- Intensity Tolerance [%]: 30
- Intensity Threshold [%]: 0.1
- S/N Threshold: 3
- Min. Spectral Fit [%]: 10
- Min. Pattern Cov. [%]: 90
- Use Dynamic Recalibration: True

3. Fragments Matching:
- Use Fragments Matching: True
- Mass Tolerance: 5 ppm
- S/N Threshold: 3

Processing node 23: Search ChemSpider
---
1. Search Settings:
- Mass Tolerance: 5 ppm
- Database(s):
    BioCyc
    Cayman Chemical
    ChEBI
    FDA UNII - NLM
    Human Metabolome Database
    KEGG
    LipidMAPS
    MCISB
    SMPDB Small Molecule Pathway Database
- Max. # of results per compound: 100
- Max. # of Predicted Compositions to be searched per Compound: 5
- Result Order (for Max. # of results per compound): Order By Reference Count (DESC)

2. Predicted Composition Annotation:
- Check All Predicted Compositions: False

Processing node 27: Search Mass Lists
---
1. Search Settings:
- Input file(s): IEM_4400_AAAC_database_V2.0.csv
- Mass Tolerance: 5 ppm
- Show extra Fields as Columns: True
- Consider Retention Time: True
- RT Tolerance : 1

Processing node 20: Mark Background Compounds
---
1. General Settings:
- Max. Sample/Blank: 5
- Max. Blank/Sample: 0
- Hide Background: True

Processing node 28: Create Mass Trace
---
1. General Settings:
- Trace Type: TIC
- MS Order: MS1
- Polarity: +
- Custom Label: (not specified)

2. XIC Settings:
- Mass [Da]: 0
- Mass Tolerance: 5 ppm

Processing node 17: Differential Analysis
---
1. General Settings:
- Log10 Transform Values: True

Processing node 24: Descriptive Statistics

No parameters

Processing node 29: Assign Compound Annotations
---
1. General Settings:
- Mass Tolerance: 5 ppm

2. Data Sources:
- Data Source #1: mzCloud Search
- Data Source #2: (not specified)
- Data Source #3: (not specified)
- Data Source #4: (not specified)