Processing node 33: Select Spectra

1. 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: 0
- Highest Charge State: 0
- Min. Precursor Mass: 0 Da
- Max. Precursor Mass: 5000 Da
- Total Intensity Threshold: 0
- Minimum Peak Count: 1

2. Scan Event Filters:
- Mass Analyzer: (not specified)
- MS Order: Any
- Activation Type: (not specified)
- Min. Collision Energy: 0
- Max. Collision Energy: 1000
- Scan Type: Any
- Polarity Mode: Is +

3. Peak Filters:
- S/N Threshold (FT): 1.5

4. Replacements for Unrecognized Properties:
- Unrecognized Charge Replacements: 1
- Unrecognized Mass Analyzer Replacements: ITMS
- Unrecognized MS Order Replacements: MS2
- Unrecognized Activation Type Replacements: CID
- Unrecognized Polarity Replacements: +
- Unrecognized MS Resolution@200 Replacements: 60000
- Unrecognized MSn Resolution@200 Replacements: 30000

5. General Settings:
- Precursor Selection: Use MS(n - 1) Precursor
- Use Isotope Pattern in Precursor Reevaluation: True
- Provide Profile Spectra: Automatic
- Store Chromatograms: False

Processing node 26: Align Retention Times

1. General Settings:
- Alignment Model: Adaptive curve
- Alignment Fallback: None
- Maximum Shift [min]: 2
- Shift Reference File: True
- Mass Tolerance: 5 ppm
- Remove Outlier: True

Processing node 9: Detect Compounds

1. General Settings:
- Mass Tolerance [ppm]: 5 ppm
- Intensity Tolerance [%]: 30
- S/N Threshold: 3
- Min. Peak Intensity: 10000
- Ions:
  
  \[2\text{M+ACN+H}^+]_1
  [2\text{M+ACN+Na}^+]_1
  [2\text{M+H}^+]_1
  [2\text{M+K}^+]_1
  [2\text{M+Na}^+]_1
  [2\text{M+NH}_4^+]_1
  [\text{M+2H}^+]_2
  [\text{M+3H}^+]_3
  [\text{M+ACN+2H}^+]_2
  [\text{M+ACN+H}^+]_1
  [\text{M+ACN+Na}^+]_1
  [\text{M+DMSO+H}^+]_1
  [\text{M+H}^+]_1
  [\text{M+H+K}^+]_2
  [\text{M+H+MeOH}^+]_1
  [\text{M+H+Na}^+]_2
  [\text{M+H+NH}_4^+]_2
  [\text{M+H-H}_2\text{O}^+]_1
  [\text{M+H-NH}_3^+]_1
  [\text{M+K}^+]_1
  [\text{M+Na}^+]_1
  [\text{M+NH}_4^+]_1

- Base Ions:  \([\text{M+H}^+]_1; [\text{M-H}]-1\)
- Min. Element Counts:  C H
- Max. Element Counts:  C90 H190 Br3 Cl4 K2 N10 Na2 O15 P3 S5

2. Peak Detection:
   - Filter Peaks:  True
   - Max. Peak Width [min]:  0.5
   - Remove Songlets:  True
   - Min. # Scans per Peak:  5
   - Min. # Isotopes:  1

3. Isotope Grouping:
   - Min. Spectral Distance Score:  0
   - Remove Potentially False Positive Isotopes:  True

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Processing node 31: Group Compounds
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1. Compound Consolidation:
   - Mass Tolerance:  5 ppm
   - RT Tolerance [min]:  0.5

2. Fragment Data Selection:
   - Preferred Ions:  \([\text{M+H}^+]_1\)

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Processing node 43: Mark Background Compounds
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1. General Settings:
   - Max. Sample/Blank:  5
- Max. Blank/Sample: 0
- Hide Background: False

Processing node 23: Search ChemSpider

1. Search Settings:
   - Database(s): BioCyc; ChEBI; Human Metabolome Database; KEGG
   - Search Mode: By Formula or Mass
   - Mass Tolerance: 5 ppm
   - Max. # of results per compound: 100
   - Max. # of Predicted Compositions to be searched per Compound: 3
   - Result Order (for Max. # of results per compound): Order By Reference Count (DESC)

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

Processing node 35: Apply mzLogic

1. Search Settings:
   - FT Fragment Mass Tolerance: 10 ppm
   - IT Fragment Mass Tolerance: 0.4 Da
   - Max. # Compounds: 0
   - Max. # mzCloud Similarity Results to consider per Compound: 10
   - Match Factor Threshold: 30

Processing node 34: Map to Metabolika Pathways

1. Search Mode: By Formula or Mass

2. By Mass Search Settings:
   - Mass Tolerance: 5 ppm

3. By Formula Search Settings:
   - Max. # of Predicted Compositions to be searched per Compound: 3

4. Display Settings:
   - Max. # Pathways in 'Pathways' column: 20

Processing node 40: Search Mass Lists

1. Search Settings:
   - Mass Lists: 061921_InHouseMassList_C18_pos_438Compounds.massList
   - Mass Tolerance: 5 ppm
   - Use Retention Time: True
   - RT Tolerance [min]: 0.5

Processing node 29: Predict Compositions
1. Prediction Settings:
- Mass Tolerance: 5 ppm
- Min. Element Counts: C H
- Max. Element Counts: C90 H190 Br3 Cl4 N10 O18 P3 S5
- Min. RDBE: 0
- Max. RDBE: 40
- Min. H/C: 0.1
- Max. H/C: 4
- Max. # Candidates: 10
- Max. # Internal Candidates: 200

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

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

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Processing node 25: Assign Compound Annotations
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1. General Settings:
- Mass Tolerance: 5 ppm

2. Data Sources:
- Data Source #1: MassList Search
- Data Source #2: mzCloud Search
- Data Source #3: Predicted Compositions
- Data Source #4: ChemSpider Search
- Data Source #5: Metabolika Search
- Data Source #6: (not specified)
- Data Source #7: (not specified)

3. Scoring Rules:
- Use mzLogic: True
- Use Spectral Distance: True
- SFit Threshold: 20
- SFit Range: 20

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Processing node 38: Search mzCloud
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1. General Settings:
- Compound Classes: All
- Precursor Mass Tolerance: 10 ppm
- FT Fragment Mass Tolerance: 10 ppm
- IT Fragment Mass Tolerance: 0.4 Da
- Library: Autoprocessed; Reference
- Post Processing: Recalibrated
- Max. # Results: 10
- Annotate Matching Fragments: True

2. DDA Search:
   - Identity Search: Cosine
   - Match Activation Type: True
   - Match Activation Energy: Match with Tolerance
   - Activation Energy Tolerance: 20
   - Apply Intensity Threshold: True
   - Similarity Search: None
   - Match Factor Threshold: 60

3. DIA Search:
   - Use DIA Scans for Search: False
   - Max. Isolation Width [Da]: 500
   - Match Activation Type: False
   - Match Activation Energy: Any
   - Activation Energy Tolerance: 100
   - Apply Intensity Threshold: False
   - Match Factor Threshold: 20

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Processing node 42: Scripting Node
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Executable and Parameters:
- Path to Executable: C:\Program Files\R\R-4.0.4\bin\Rscript.exe
- Command Line Arguments: C:\Rscripts\CompoundsMZ_OriginalRowNum\CompoundsMZ_OriginalRowNum.R %NODEARGS%
- Requested Tables and Columns:
  Compounds: Calc MW
  Compounds per File: Area
  Features: mz, Ion, Area
- Use R-Friendly Columns: True
- Archive Datafiles: False