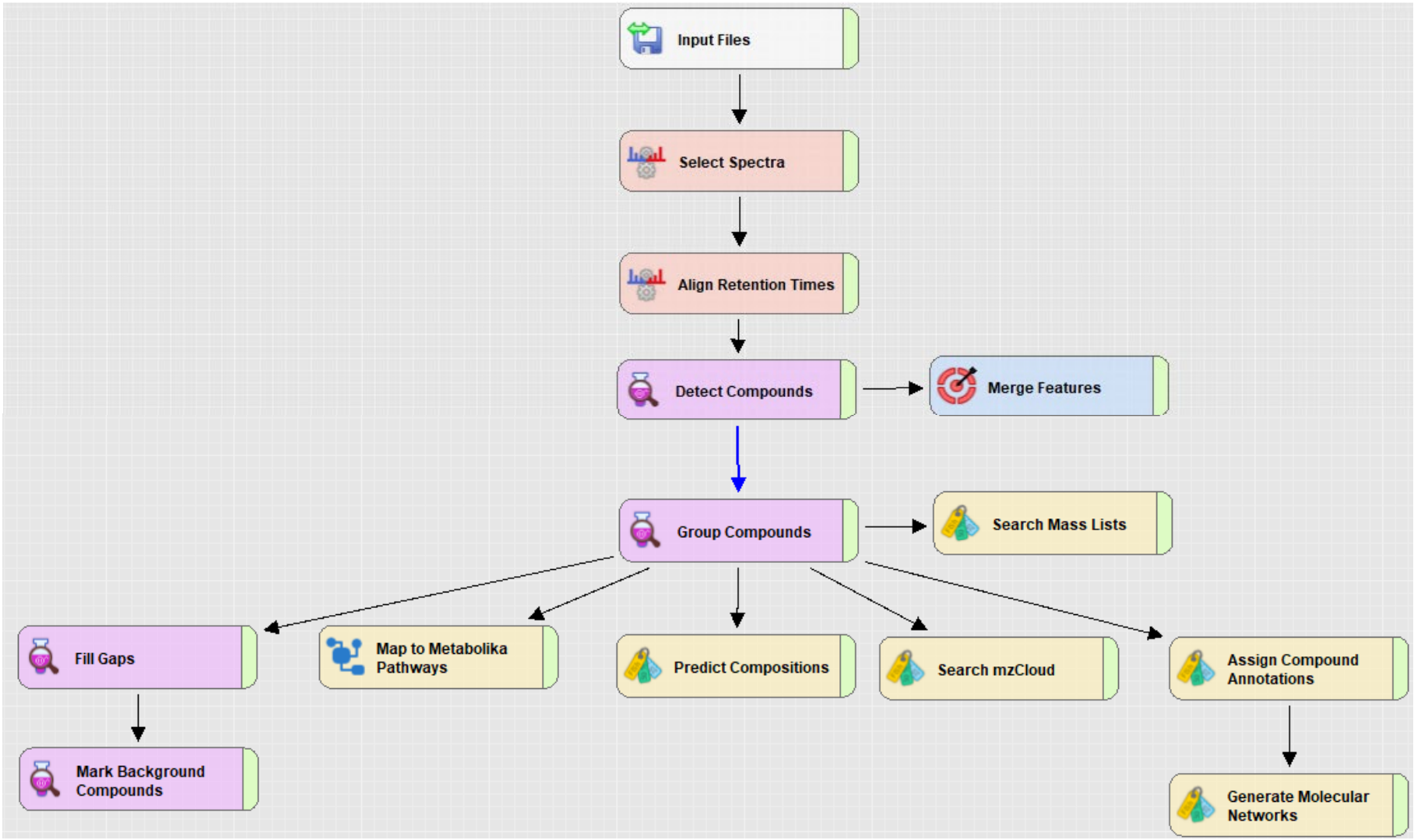
Workflow scheme in Compound Discoverer



Processing node 6: Input Files

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

Processing node 33: Select Spectra
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1. Spectrum Properties Filter:
- Lower RT Limit: 0.25
- Upper RT Limit: 0
- 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 +
- MS1 Mass Range: (not specified)
- FAIMS CV: (not specified)
3. Peak Filters:
- S/N Threshold (FT-only): 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

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

Processing node 45: Detect Compounds

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1. General Settings:
- Mass Tolerance [ppm]: 5 ppm
- Min. Peak Intensity: 10000
- Min. # Scans per Peak: 5
- Use Most Intense Isotope Only: True

2. Trace Detection:
- Max. Number of Gaps to Correct: 2
- Min. Number of Adjacent Non-Zeros: 2

3. Peak Detection:
- Chromatographic S/N Threshold: 1.5
- Remove Baseline: False
- Gap Ratio Threshold: 0.35
- Max. Peak Width [min]: 1
- Min. Relative Valley Depth: 0.1

4. Isotope Pattern Detection:
- Group Isotopes for: Br; Cl
- Use Peak Quality for Isotope Grouping: True
- Filter out Features with Bad Peaks Only: True
- Zig-Zag Index Threshold: 0.2
- Jaggedness Threshold: 0.4
- Modality Threshold: 0.9
- Remove Potentially False Positive Isotopes: True

5. Compound Detection:
- Ions: [M+H]+1; [M+K]+1; [M+Na]+1
- Base Ions: [M+H]+1; [M-H]-1
- Remove Singlets: True

6. AcquireX Settings:
- Detect Persistent Background Ions: False

Processing node 31: Group Compounds
---
1. General Settings:
- Mass Tolerance: 5 ppm
- RT Tolerance [min]: 0.2
- Align Peaks: False
- Preferred Ions: (not specified)
- Area Integration: Most Common Ion
2. Peak Rating Contributions:
- Area Contribution: 3
- CV Contribution: 10
- FWHM to Base Contribution: 5
- Jaggedness Contribution: 5
- Modality Contribution: 5
- Zig-Zag Index Contribution: 5
3. Peak Rating Filter:
- Peak Rating Threshold: 0
- Number of Files: 0

Processing node 44: Map to KEGG Pathways
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1. Search Settings:
- 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 23: Search ChemSpider
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1. Search Settings:
- Database(s): BioCyc; 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 25: Assign Compound Annotations
---
1. General Settings:
- Mass Tolerance: 5 ppm
2. Data Sources:
- Data Source #1: mzCloud Search
- Data Source #2: Predicted Compositions
- Data Source #3: MassList Search
- 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
4. Reprocessing:
- Clear Names: False

Processing node 40: Generate Molecular Networks
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1. Spectral Similarity:
- Use Full MSn Tree: True
- Match Mass Shift: True
- Match Transformations: True
- Variate Transformations: False
- S/N Threshold: 3
- Mass Tolerance: 2.5 mmu
- Min. Fragment m/z: 50
2. Transformations:
- Phase I: (not specified)
- Phase II: (not specified)
- Others: (not specified)
- Max. # Phase II: 1
- Max. # All Steps: 3
3. Applied View Filters:
- Require Transformation: True
- Require MSn: True
- Min. MSn Score: 50
- Min. MSn Coverage: 70
- Min. Fragments: 3
4. Applied Thresholds:
- Require Transformation: False
- Require MSn: False
- Min. MSn Score: 20
- Min. MSn Coverage: 20
- Min. Fragments: 0

Processing node 34: Map to Metabolika Pathways

- 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 42: Search Mass Lists
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1. Search Settings:
- Mass Lists: Endogenous Metabolites database 4400 compounds.masslist|LipidMaps Structure Database 2021-09-13.massList|Natural Products Atlas 2020_06.masslist|Exposome_Biomarkers.massList|HMDB_metabolites_masslist.massList

- Mass Tolerance: 5 ppm
- Use Retention Time: True
- RT Tolerance [min]: 2

Processing node 38: Search mzCloud
---
1. General Settings:
- Compound Classes: Endogenous Metabolites
- 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
- Search MSn Tree: False
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

Processing node 29: Predict Compositions
---
1. Prediction Settings:
- Mass Tolerance: 5 ppm
- Min. Element Counts: C H
- Max. Element Counts: C90 H190 Cl4 N10 O18 P4 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

Processing node 32: Fill Gaps
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1. General Settings:
- Mass Tolerance: 5 ppm
- S/N Threshold: 1.5
- Use Real Peak Detection: True

Processing node 41: Apply QC Correction
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1. General Settings:
- Regression Model: Linear
- Min. QC Coverage [%]: 50
- Max. QC Area RSD [%]: 30
- Max. Corrected QC Area RSD [%]: 25
- Max. # Files Between QC Files: 15

Processing node 28: Mark Background Compounds
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1. General Settings:
- Max. Sample/Blank: 5
- Max. Blank/Sample: 0
- Hide Background: True

Processing node 17: Differential Analysis
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1. General Settings:
- Log10 Transform Values: True
2. Peak Rating Contributions: