QUICK START

Input Data Requirements

- Upload Excel file
- Row 1 = column headers only (no numerical values)
- Each row = one feature
- ID columns: annotation or *m/z* + RT (metabolomics)
- Numeric columns = values for correlation analysis
- Optional: user-defined cluster column

Filtering Parameters

- Set: *Minimum area to consider + Number of replicates*
- Feature is retained if:
  area ≥ threshold in ≥ N samples (N = replicates)
- Purpose: remove noise / low-quality features
- Correlation filtering: significance level (α)
- Typical values: 0.05 / 0.01 / 0.1
- Optional: Bonferroni correction

Data Reduction (Ion Grouping – metabolomics only)

- Requires *m/z* + RT (metabolomic data)
- Set:
  - RT shift (min) → allowed shift between runs (instrument variability)
  - *m/z* error (Da) → mass deviation tolerance
- RT - groups ions from same metabolite
- *m/z* error used for isotopes + pseudomolecular ions
- Result: multiple ions → single metabolite node (network simplification)

Clustering

- Layout changes per *Create network* run (iterations affect visualisation)
- Set clustering strength: **weak / normal / strong**
  - strong = clearer cluster separation
  - increases distance of negative correlations
  - compresses positive correlations
- If no user-defined clusters:
  - DBSCAN automatically detects clusters
  - clusters are auto-colored
  - ε (epsilon) is automatically optimised
- Re-cluster option:
  - re-run DBSCAN
  - ε can be adjusted manually
  - lower ε → more clusters
  - higher ε → less clusters

The software also provides tooltip help for each parameter when hovering the mouse over it.