BEGIN Compound_Identification_Process

3.1 Database Matching

INPUT: Unknown compound arguments (RF-value, RGB values, ...)

STEP 1: Select paired databases

- Pair 1: AN and AV
- Pair 2: BN and BV

STEP 2: For each pair:

a. Search AN (or BN) with unknown arguments → return candidate list1

b. Search AV (or BV) with unknown arguments → return candidate list2

c. Compute INTERSECTION of list1 and list2 → matched_candidates

STEP 3: Combine results from both pairs

OUTPUT: Final list of possible compounds after database matching

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3.2 Spectra Overlay

INPUT: Unknown compound spectrum (CSV file)

Spectra of candidate compounds (CSV files)

STEP 1: Load spectra data from CSV files

STEP 2: Plot all spectra:

- Overlay unknown compound spectrum

- Overlay candidate spectra

STEP 3: Diagnosis Cases

CASE A: If no candidate spectra are similar to unknown:

→ OUTPUT: "No match found. Confirmation ends."

CASE B: If exactly 1 candidate spectrum matches:

→ OUTPUT: "Single match found. Confirmation ends."

CASE C: If multiple candidate spectra match:

FOR each candidate spectrum:

- Compute upper_bound = spectrum * 1.25
- Compute lower_bound = spectrum * 0.75
- Check if UNKNOWN spectrum lies completely within bounds

IF yes:

OUTPUT: "Confirmed compound = this candidate"

STOP

IF no complete containment:

- For each candidate:

Calculate percentage overlap =

(# of points of UNKNOWN within bounds) /

(total # of points in UNKNOWN)

- Select candidate with highest overlap

OUTPUT: "Most likely compound = candidate with highest overlap"

END Compound_Identification_Process