

# Screening strategies

## Target screening

All Ions MS/MS  
Reference standard

- Find-by-Formula (**Subset PCDL**)
- Assign fragments as Qualifiers (Qual)
- Generate Quant Method

- Batch overview
- Quantitation
- Identification (Accurate Mass, Isotopes, Qualifiers (fragments), RTs)

## Suspect screening

„What else is in my sample?“

All Ions MS/MS  
MS and target (auto) MS/MS

- Find-by-Formula (**Comprehensive PCDL**)
- Identify compounds
  - fragment co-elution (**PCDL**)
  - library searching (**PCDL**)

- Suspect List
- Identification by fragment co-elution, library searching
- Tentative Identification by in-silico fragmentation (MSC)

## Non-target screening

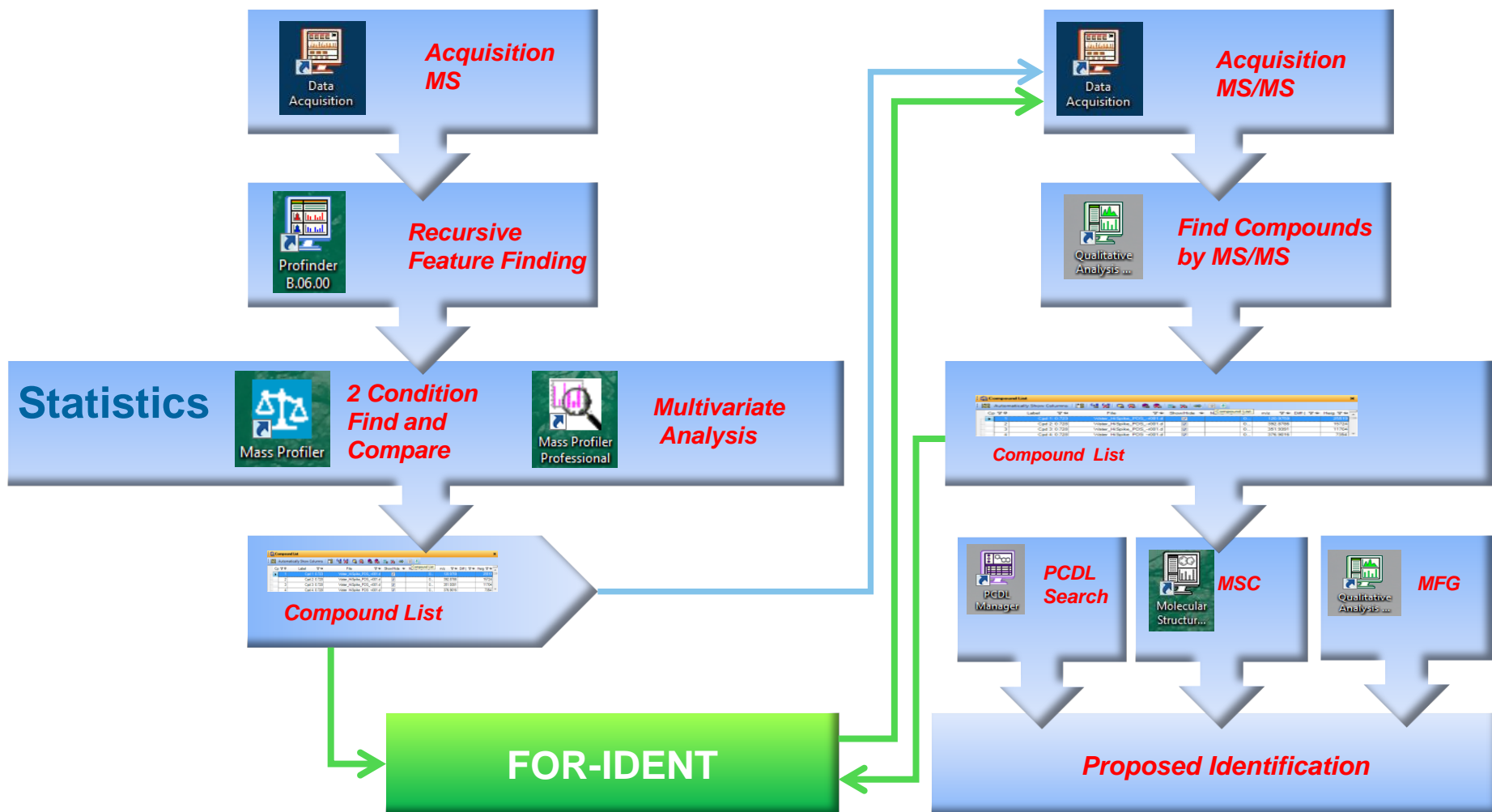
„De-replication“

MS and target (auto) MS/MS

- Molecular Feature Extraction
- Mass Profiler (2-sample comparison)
- Mass Profiler Professional (Multivariate statistics)

- Differential results
- Identification by MS/MS library searching (**PCDL**)
- Tentative Identification by in-silico fragmentation (MSC)

# Non-target screening – statistical sample comparison



# Intermediate solution - MassBank Converter GUI

Works in both directions (.cef → MassBank; MassBank → .cef)

Spectral display for single CE

The screenshot displays the MassBank Converter GUI with several key components highlighted by red boxes:

- Open files:** Contains radio buttons for "Convert MassBank to .cef file" and "Create MassBank input file", a file list, and "Open files" and "Close selected file" buttons.
- MassBank information:** A table with columns "Required", "Parameter", and "Value". It lists various metadata fields such as Accession, Title, Creation Date, Authors, License, Copyright, Publication, Comment, Name, Compound class, Formula, Exact mass, SMILES, InChI, InChI Key, ChempSpider, Instruments, Instrument type, MS Type, Ionization mode, Collision energy, Precursor m/z, Precursor type, and MoFile.
- MS-MS data:** A mass spectrum plot showing relative abundance versus m/z. The x-axis ranges from 0 to 200, and the y-axis ranges from 0 to 1000. A dropdown menu at the top left is set to "10.0V".
- Fragment list and filtering:** A table with columns: Accurate mass, Exact mass, Mass error [ppm], Absolute abundance, Relative abundance, and Annotation. Below the table are controls for "Add Product ions from clipboard" (Decimal separator, Column separator, Collision energy, Paste), "Product ions filter" (Minimum absolute abundance, Minimum relative abundance, Keep only annotated ions), and "Apply" and "Apply to all compounds" buttons.

Meta-data included from xls-schema, imported from ChempSpider, and/or manually edited

Fragment list, filtering options, and paste functions

# Intermediate solution - MassBank Converter GUI

Individual data files for each CE are generated

```
AG000442 - Notepad
File Edit Format View Help
ACCESSION: AG000441, AG000442, AG000443
RECORD_TITLE: Chlorotoluron, QTOF, CE=10,20,40V
DATE: 20150820
AUTHORS: Sascha Lege, Uni Tübingen
LICENSE: CC-BY-SA
COPYRIGHT: (C) Uni Tübingen, 2015
PUBLICATION: Lege et al DOI:, PubMed ID:....
COMMENT: Reference standard
CH$NAME: chlortoluron
CH$COMPOUND_CLASS: Pesticide
CH$FORMULA: C10H13ClN2O
CH$EXACT_MASS: 212.07164
CH$SMILES: Cc1ccc(cc1Cl)/N=C(\N(C)C)/O
CH$IUPAC: InChI=1/C10H13ClN2O/c1-7-4-5-8(6-9(7)11)12-10(14)13(2)3/h4-6H,1-3H3,(H,12,14)
CH$LINK: INCHIKEY JXCGFZXSOMJFOA-UHFFFAOYAE
CH$LINK: CHEMSPIDER 25472
AC$INSTRUMENT: Agilent 1290 Infinity II HPLC; Agilent 6550 QTOF
AC$INSTRUMENT_TYPE: LC-ESI-QTOF
AC$MASS_SPECTROMETRY: MS_TYPE MS2
AC$MASS_SPECTROMETRY: ION_MODE POSITIVE
AC$MASS_SPECTROMETRY: COLLISION_ENERGY 20.0V
MS$FOCUSED_ION: PRECURSOR_M/Z 213.0789
MS$FOCUSED_ION: PRECURSOR_TYPE [M+H]+
MS$DATA_PROCESSING: IGNORE_PEAK abs.int. < 5
PK$NUM_PEAK: 29
PK$PEAK: m/z int. rel.int.
42.0332 139 1
44.0493 1153 7
46.0648 81039 509
47.0684 126 1
55.0543 135 1
55.9338 122 1
56.0131 414 3
57.0702 111 1
72.0446 159015 999
72.3325 113 1
72.3945 100 1
72.4326 113 1
72.9377 99 1
73.0480 181 1
77.0387 437 3
96.9601 404 3
101.9389 131 1
104.0494 656 4
105.0574 85 1
109.9647 85 1
113.0148 396 2
125.0144 795 5
132.0433 305 2
133.0515 368 2
137.9637 84 1
140.0260 9355 59
140.0898 112 1
168.0206 3628 23
213.0784 3833 24
//
```

Generate customized output format from MassHunter to FOR-IDENT; use same format to generate import file (.cef)