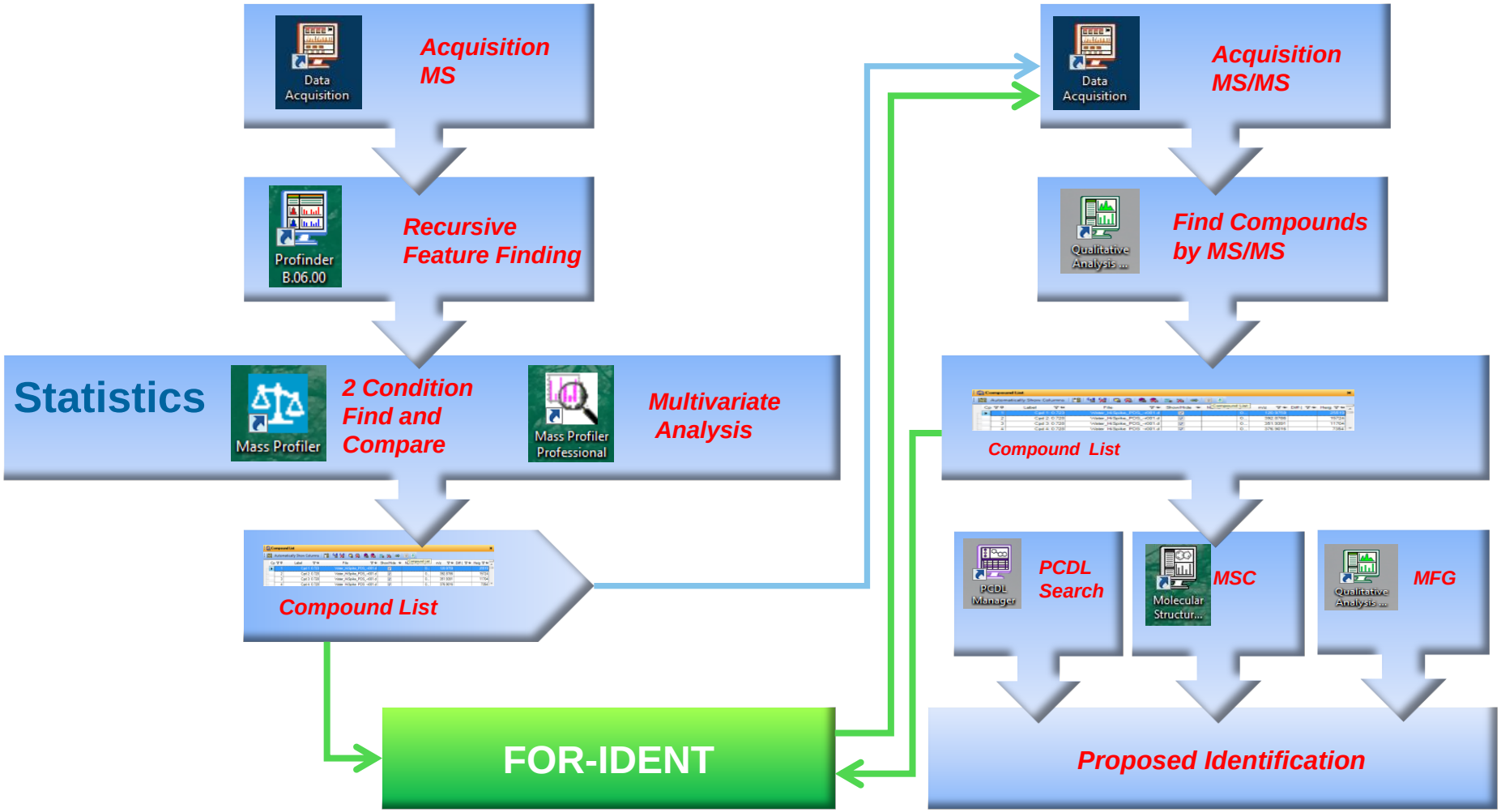
Screening strategies

Target screening	Suspect screening *„What else is in my sample?“*	Non-target screening *„De-replication“*
All Ions MS/MS Reference standard	All Ions MS/MS MS *and* target (auto) MS/MS	MS *and* target (auto) MS/MS

- Find-by-Formula (***Subset PCDL***)
- Assign fragments as Qualifiers (Qual)
- Generate Quant Method
	- Find-by-Formula (***Comprehensive PCDL***)
	- Identify compounds
	  - fragment co-elution (***PCDL***)
	  - library searching (***PCDL***)
		- Molecular Feature Extraction
		- Mass Profiler (2-sample comparison)
		- Mass Profiler Professional (Multivariate statistics)

- Batch overview - Quantitation - Identification (Accurate Mass, Isotopes, Qualifiers (fragments), RTs	- Suspect List - Identification by fragment co-elution, library searching - Tentative Identification by in-silico fragmentation (MSC)	- Differential results - Identification by MS/MS library searching (***PCDL***) - Tentative Identification by in-silico fragmentation (MSC)

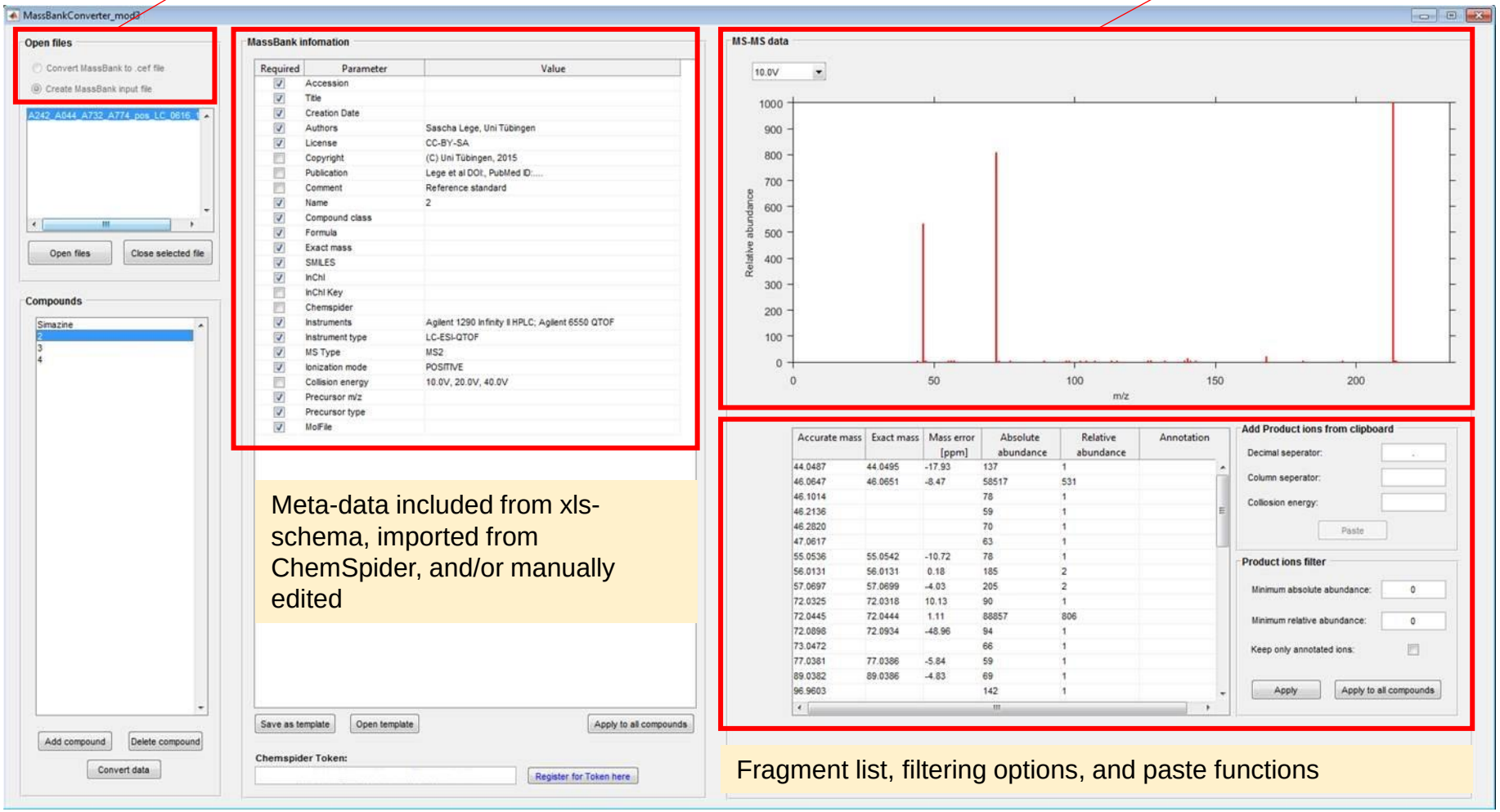
Non-target screening – statistical sample comparison



Intermediate solution - MassBank Converter GUI

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

Spectral display for single CE



Meta-data included from xls-schema, imported from ChemSpider, 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)