

UNIFI Screening Workflow - HRMS

Instrument Set Up

- IntelliStart for "Instrument Setup"
 - Mass calibration
 - LockSpray Setup

Analysis Method

- Instrument, processing and reporting methods
- Selection of analytes from **UNIFI Scientific Library** for target- and suspect screening

Data Acquisition

- Data acquisition of **accurate parent masses** and **fragment ions** (MSE) in one single injection
- **3D peak list generation** (Apex 3D)

Data Review

- **Customized workflow** for data review (Target- and Suspect Screening)

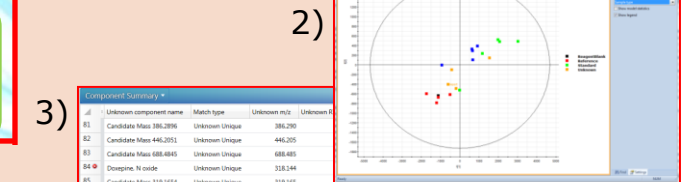
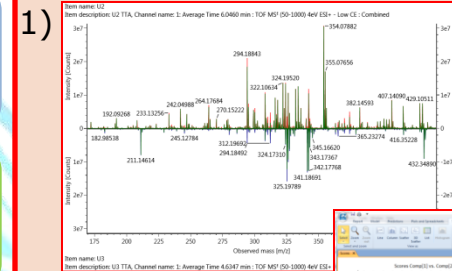
Non-Target Screening

What else is in my sample?

- 1) Binary Compare
- 2) Statistics
- 3) Unknow Unique List
- 4) Elemental Composition
- 5) ChemSpider/Library Search
- 6) Fragment Match

Reporting

- Flexible report generation



3)

Component	Unknown component name	Match type	Unknown m/z	Unknown
81	Candidate Mass 386.2896	Unknown Unique	386.290	
82	Candidate Mass 446.2051	Unknown Unique	446.205	
83	Candidate Mass 688.6845	Unknown Unique	688.685	
84	Dioxepine, N oxide	Unknown Unique	318.144	
85	Candidate Mass 319.1654	Unknown Unique	319.165	
86	4-Methylpyridopyridine (P...	Unknown Unique	386.337	2.22
87	Candidate Mass 328.1905	Unknown Unique	328.190	4.31
88	Paripropazine	Unknown Unique	384.082	6.32
89	Candidate Mass 385.1979	Unknown Unique	385.198	3.76
90	Candidate Mass 544.1247	Unknown Unique	544.125	9.10
91	Candidate Mass 430.1839	Unknown Unique	430.184	4.09
92	Candidate Mass 335.2195	Unknown Unique	335.219	11.54
93	Candidate Mass 470.2175	Unknown Unique	470.217	5.21
94	Candidate Mass 338.1758	Unknown Unique	338.176	7.75
95	Candidate Mass 240.1905	Unknown Unique	240.190	3.37

Automatic batch processing of unknowns from unknown unique list

Additional tools:

- Halogen Match
- Neutral Loss
- Common Fragment Search