

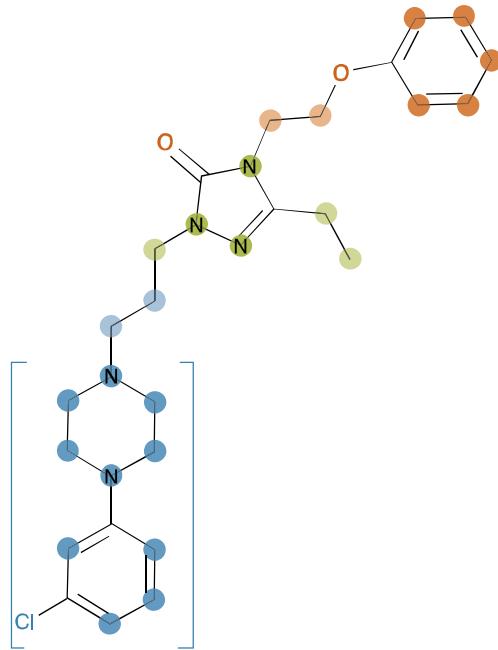
# UNIFI Solution

Dr. Mathias Hofmann

Fachtagung "Fortschritte in der Suspected- und Non-Target-Analytik"  
28. März 2014 – LfU Augsburg

# Agenda

- Library search
- Limit Checks and Custom Calculations
- Reporting
- CCS Screening



# Library Search Options

Waters

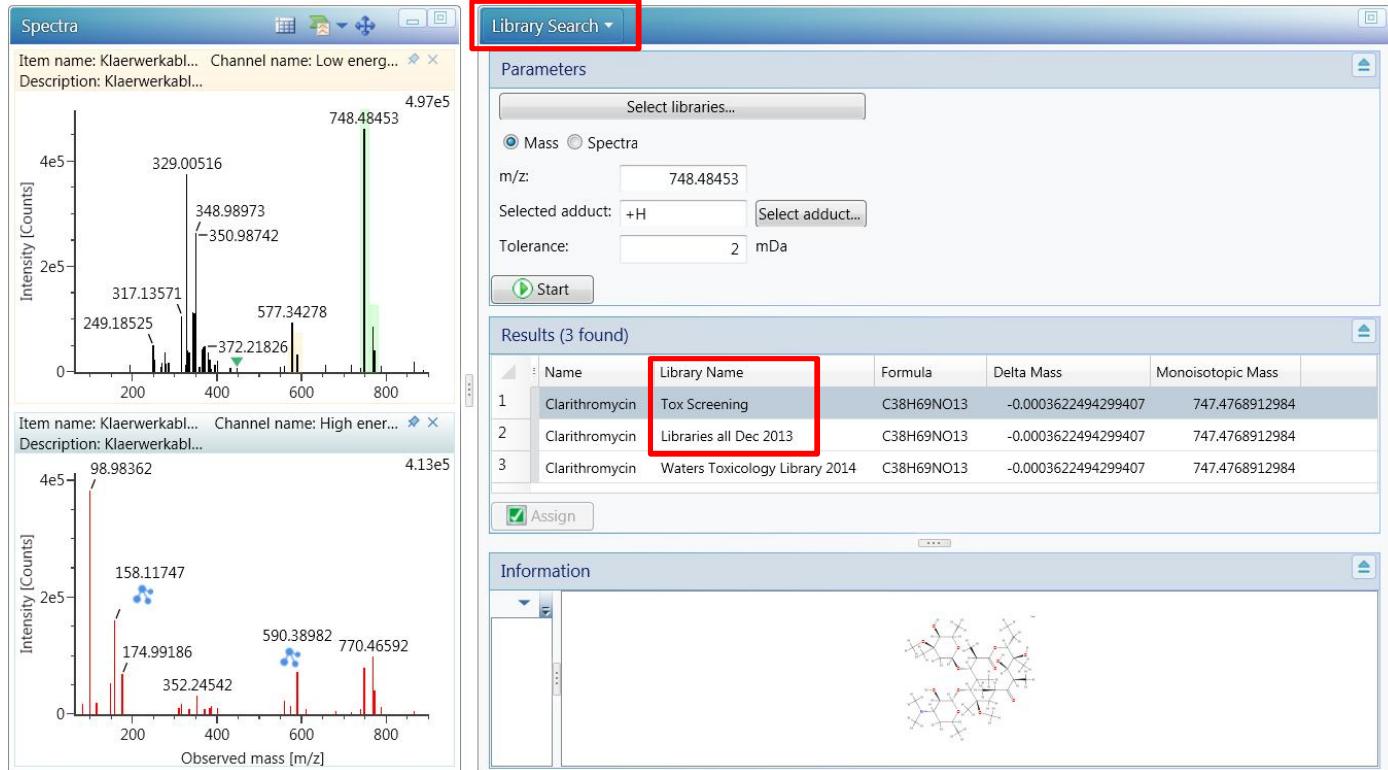
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## ■ UNIFI Library

- search in internal libraries

## ■ UNIFI to ChemSpider

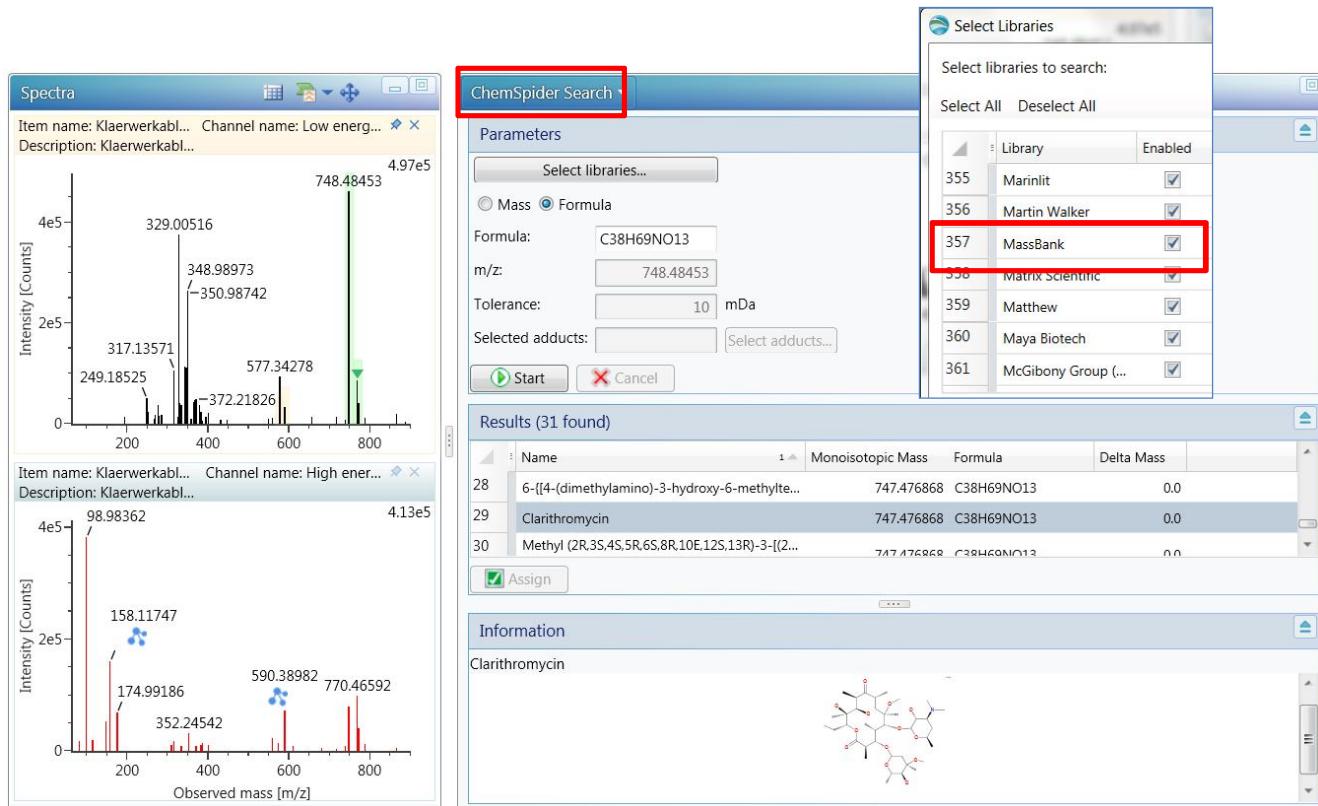
- direct link to Chemspider
- up to almost 600 libraries



# UNIFI to ChemSpider

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# Import (your own Library to Unifi)

Waters

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	A	B	C	D	E	F	G	H	I	J
1	Compound Name	Formula	Structure	Adduct	RT	F1	F2	F3	F4	
2										
3										

Entry name in Lib

Either Elemental Comp  
or Structure Mol File

Name	Type	Date modified	Size
PAH.xlsx	Microsoft Office E...	19.03.2014 15:04	35 KB
Phenanthren.mol	MDL Molfiles	19.03.2014 14:51	2 KB
Anthracen.mol	MDL Molfiles	19.03.2014 14:58	2 KB

Import files

Type of import: Excel (Screening List)

File to import: G:\IVV\PAH\PAH.xlsx

Library to create: PAH

Detection results: ESI+

## Limit Checks and Custom Calculations

# Component Limit Checks

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## Custom Fields and Limits

Specify custom fields to be included, calculations to be performed, and/or limits to be evaluated, for the analytical results.

Custom Fields

Summary Calculations

Limit Checks

### Selected fields and limits checking

	Node	Field name	Sample type	Level	Error minimum	Warning minimum	Target value	Warning maximum	Error maximum
1	Component	Identified High Energy Fragments	All	All	0	1			
2	Component	Isotope Match Mz RMS PPM	All	All		0	5	10	
3	Component	Retention Time Error (min)	All	All	-0.15	-0.1	0	0.1	0.15
4	Component	Mass error (ppm)	All	All		0	5	10	

### Selected limit graphic representation:



### Component Summary

View: Screening Summary View

	Component name	m/z	Mass error (ppm)	Expected RT (min)	Retention Time	Error (min)	Observed RT (min)	Label	Identified High Energy Fragments	Isotope Match Mz RMS PPM	Response	C
1	6-MAM	328.1541	-0.67	2.10		-0.03	2.07		1	0.96	46256	
2	7-aminoclonazepam	286.0743	0.51	3.47		-0.05	3.42		1	2.34	4641	
3	7-aminoflunitrazepam	284.1196	0.68	4.29		-0.06	4.23		0	1.53	27295	
4	7-aminonitazepam	252.1136	1.75	2.01		-0.17	1.84		1	1.75	11232	
5	Alprazolam	309.0915	4.40	8.47		-0.03	8.44		0	5.00	1352	

# No more Excel

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Custom field

Peak Name

Peak Name

Field settings  Formula settings

Selections  Condition Editor

Fields:	Functions:	Indexes:	Operators:
Component	ABS	FIRST	+
Sample	AVG	LAST	-
% Area (%)	COUNT	INDEX	*
% Height (%)	EXP		/
(Asymmetry @ 10%)^2	FIND		^
(Asymmetry @ 4.4%)^2	IF		&
2 Sigma	LN		
2nd derivative apex (min)	LOG		:
3 Sigma	MAX		=
4 Sigma	MIN		!=
5 Sigma	PROD		>=
Area	%RSD		>
Area Manual Change (%)	SQRT		<=
Asymmetry @ 10%	STDEV		<
Asymmetry @ 4.4%	SUM		
Asymmetry plate count	VALUE		

Name: Peak Name  
Format: Real  
 Sample type:  
Standard  
Unknown  
Blank  
QC  
Reference  
Reagent blank

Calculate across samples

Description:

# Reporting in UNIFI

# Enhanced Reporting – Template Editor

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Waters UNIFI - Nefazadone Method Analysis Apr 11, 2011: Analysis Center

Review Investigate Report

Review Results

Home View Page layout Template settings

Filter by: Individual, Merge all reports, Exclude from report, Summary, Exclude from report when empty.

Data options: Report log options, View log, English Language

Report Objects

Show: All

- Analysis Method
- Audit trail
- Experimental Record
- Methods
- Post Run Report
- Sample information
- Drawings
  - Ellipses
  - Images
  - Lines
  - Rectangles
  - Text
- Coverage map
- Coverage maps
- Fields
  - Special information
  - Analysis
- Plots
  - Calibration curves
  - Chromatograms
    - Autoscaled chromatogram
    - Autoscaled chromatogram
    - Chromatogram (compare)
  - Component plots
    - Component plot
    - Component plot (compare)
  - 3D plots
  - Peak plots
- Spectra
  - Spectrum
  - Spectrum (compare)
- Groups
  - Groups

Component: Nefazadone - dealkylation (C6H4Cl)

	Item name	Expected RT (min)	Observed RT (min)	Expected mass (Da)	Observed mass (Da)	Mass error (Da)	Response
1	METID_111	5.890	3.888	359.232	359.2327	0.0006	54199

Component: Nefazadone + 2 x Hydroxylation

	Item name	Expected RT (min)	Observed RT (min)	Expected mass (Da)	Observed mass (Da)	Mass error (Da)	Response
1	METID_111	5.890	4.858	501.214	501.2146	0.0003	172216
2	METID_113	5.890	4.864	501.214	501.2157	0.0014	173053

Item name: METID\_111

Intensity [Counts]

Mass [Da]

Item name: METID\_107

Channel name: Smoothed : Mass Chromatogram (16.7 PPM): +470.2332+471.2362+472.2310+473.2334 : TOF MSe (50-1200) 6eV ESI+

Nefazadone  
5.86

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# Enhanced Reporting – View and Print Reports

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Waters UNIFI - Nefazadone Method Analysis Apr 11, 2011: Analysis Center

Review Investigate Report

Review Results > Preview Report

Pages

Home Signature

Report 1 of 11 100% Find Copy Extract Export Apply Reuse Extraction method

Print Page Zoom Layout Selection mode Graphic Manage

Component: Nefazadone

.	Item name	Expected RT (min)	Observed RT (min)	Expected mass (Da)	Observed mass (Da)	Mass error (Da)	Response
1	METID_111	5.890	5.528	485.219	485.2200	0.0006	146987
2	METID_113	5.890	5.536	485.219	485.2206	0.0012	137474

Component: Nefazadone

.	Item name	Expected RT (min)	Observed RT (min)	Expected mass (Da)	Observed mass (Da)	Mass error (Da)	Response
1	METID_107	5.890	5.858	469.225	469.2259	0.0014	218361
2	METID_110	5.890	5.858	469.225	469.2257	0.0012	1073770
3	METID_112	5.890	5.871	469.225	469.2262	0.0017	1140712
4	METID_111	5.890	5.882	469.225	469.2246	0.0001	172684
5	METID_113	5.890	5.892	469.225	469.2260	0.0015	111118

Item name: METID\_111

Intensity [Counts]

Mass [Da]

Administrator, UNIFI [Administrator]



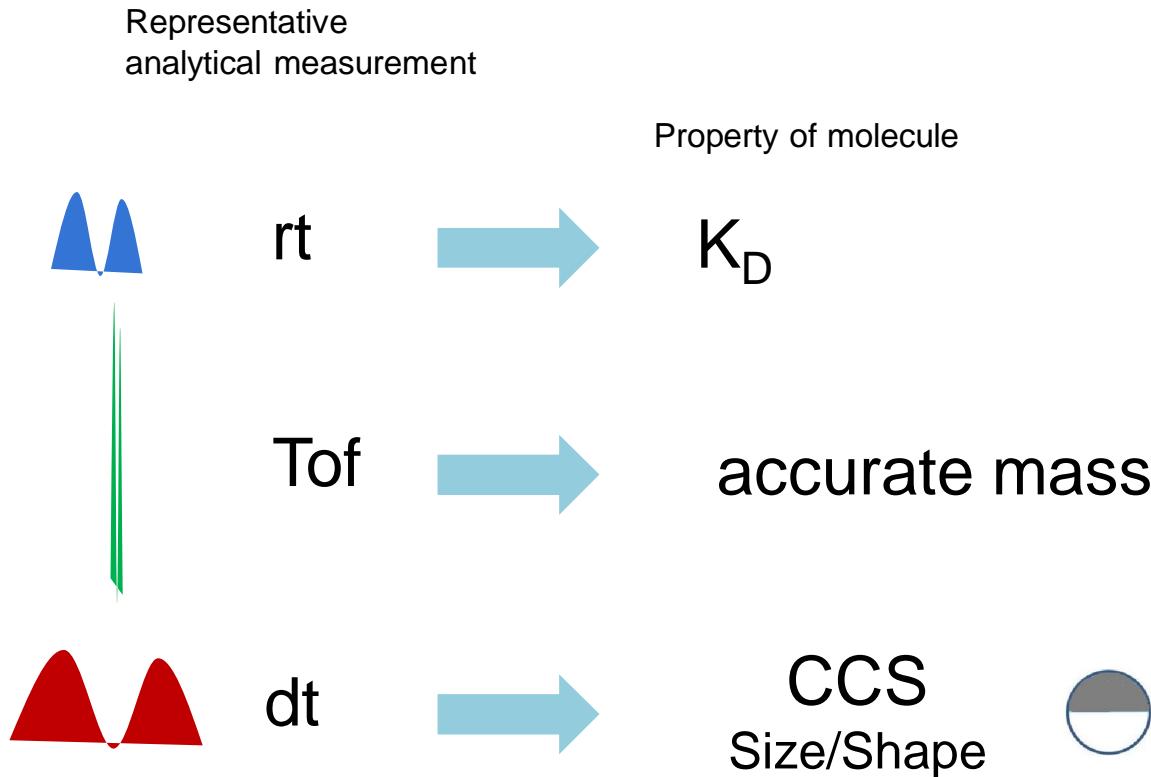
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# UNIFI CCS

# Three dimensions of resolution

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# Mehr Information ...SELEKTIVITÄT (and SPEZIFITÄT)

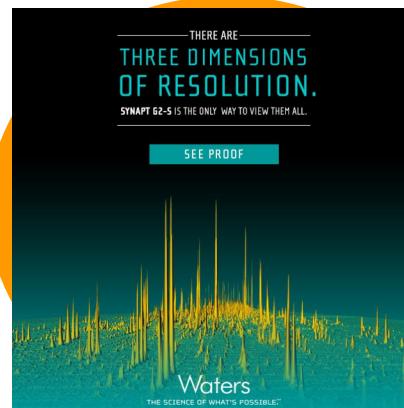
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X



=



UPLC

T-Wave IMS

QuanTof

LC/HDMS

3 orthogonal separation techniques

# Intellistart - Routine

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IntelliStart

## Instrument Configuration



Create Calibration



Create CCS Calibration



Resolution Optimization



Stop Flow



Resolve



Start



Standby



Operate



Tune

# Ergebnis

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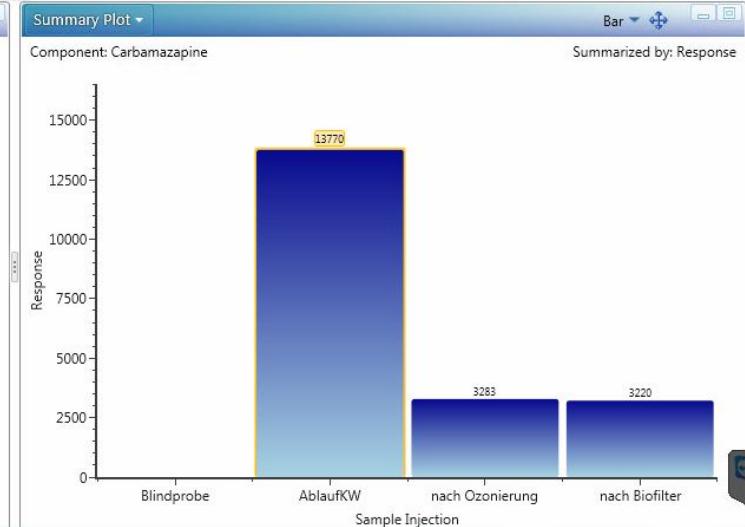
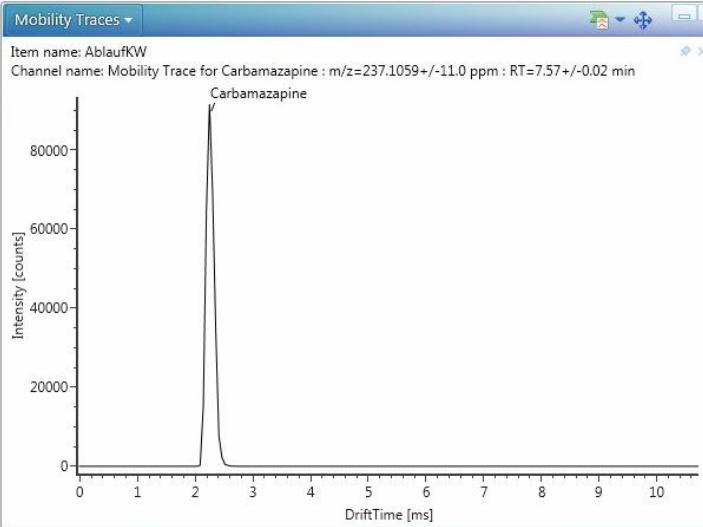
3D:

Rt

CCS

Acc Mass

Component Summary										View: *Accurate Mass Screening IMS		
Component name	Identification status	Observed RT (min)	Observed collision cross sectio...	Observed neutral mass...	Response	Observed drift time (ms)	Expected RT (min)	Expected neutral mass (Da)	m/z			
1 Benzotriazole	Identified	4.09	133.5	119.0503	1848		1.37		119.0483	120.0		
2 Aminoantipyrine	Identified	5.09	150.7	203.1088	4858		2.03	6.00	203.1059	204.1		
3 Carbamazepine	Identified	7.57	156.9	236.0986	13770		2.25	6.50	236.0950	237.1		
4 Metoprolol	Identified	5.47	176.7	267.1879	39028		2.88	5.47	267.1834	268.1		
5 Bezafibrate	Identified	7.82	184.1	361.1135	1110		3.17	7.83	361.1081	362.1		



# Screening with CCS

## Example: EU proficiency test pesticides

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	MS	HDMs
m/z error (+/-)	5 ppm	10 ppm
rt error (+/-)	2.5%	2.5%
CCS error (+/-)	-	2%
Correct ID's	7/8	8/8
False Negatives	1	0
False Positives	3	0

Screening for known Pesticides with CCS in a small scale proficiency test. Using CCS values as an additional filter for molecular identification **enables false positive identifications to be reduced**, improving **confidence** and **efficiency** of the analysis.

# Ciprofloxacin protomers

Waters UNIFI - SYANPT G2 IMS FQ5 NO FRAGMENTS: Analysis Center

My Work    Welcome to UNIFI    SYANPT G2 IMS FQ5 NO F...    Search folders...

Review    Investigate    Report    Review Results    Limits    Process    Edit    Tools    File    Filters

Injections and Components

Tray: 2:25    SynaptG2\_20120102\_334 [1]    Ciprofloxacin

Component Summary

	Component name	m/z	Mass error (ppm)	Collision cross section error (%)	Observed collision cross section ( $\text{\AA}^2$ )	Expected collision cross section ( $\text{\AA}^2$ )	Expected RT (min)
1	Ciprofloxacin	332.1398	-2.01	-1.70	116.98	119.00	2.22
2	Ciprofloxacin_1	332.1398	-1.99	-0.67	107.98	108.70	2.22

Mobility Traces

Item name: SynaptG2\_20120102\_334  
Channel name: Mobility Trace for Ciprofloxacin : m/z=332.1398+-27.8 ppm ; RT=...

Spectra

Item name: SynaptG2\_20120102\_334    Channel name: Low energy : Time 2.252...  
Description: Plate 2 set 7 2xMRL (Cipro...

Item name: SynaptG2\_20120102\_334    Channel name: High energy : Time 2.25...  
Description: Plate 2 set 7 2xMRL (Cipro...

Components (SynaptG2)

Status Name

1		Ciprofloxacin
2		Ciprofloxaci...

Administrator, UNIFI [Administrator]

# MS<sup>E</sup> spectra ciprofloxacin Protomers - different daughter ions

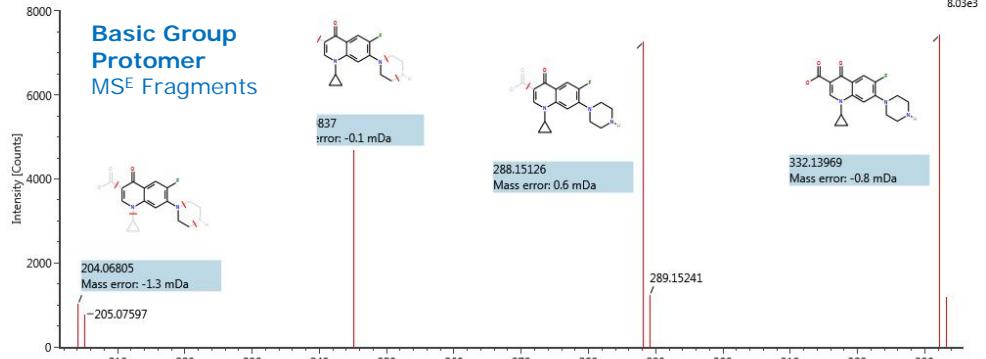
Waters

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Item name: SynaptG2\_20120102\_146  
Description: Plate 2 set 7 2xMRL (Cipro/epi-CTC) r.2

Channel name: High energy : Time 2.2687 +/- 0.0158 minutes : Drift Times: 4.10 +/- 0.08 ms : 4D mass peak list

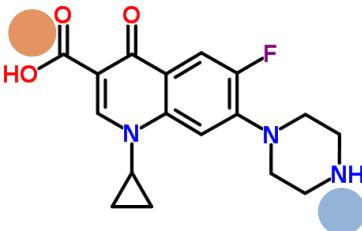
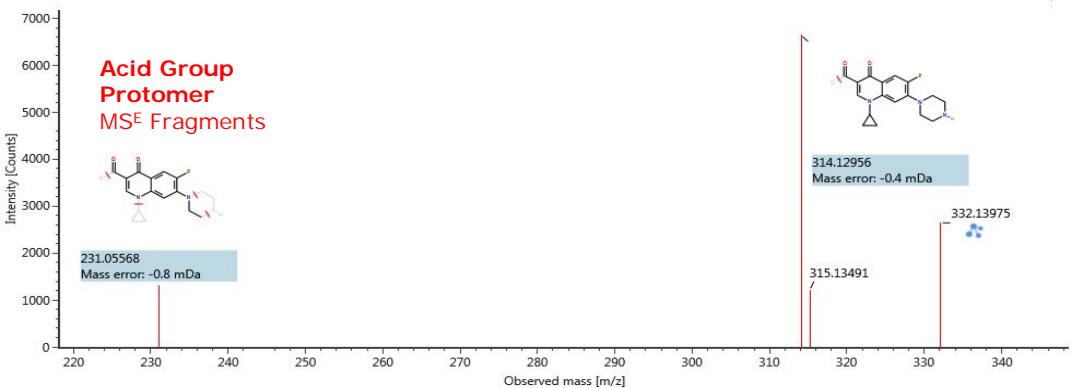
## Basic Group Protomer MS<sup>E</sup> Fragments



Item name: SynaptG2\_20120102\_146  
Description: Plate 2 set 7 2xMRL (Cipro/epi-CTC) r.2

Channel name: High energy : Time 2.2665 +/- 0.0158 minutes : Drift Times: 3.66 +/- 0.08 ms : 4D mass peak list

## Acid Group Protomer MS<sup>E</sup> Fragments



Danke ...

- Frau Dr. Seiwert für die Arbeit (Datenaufnahme)
- Herrn Dr. Dünnbier für die Einladung und die Proben.

... Ihre Aufmerksamkeit!