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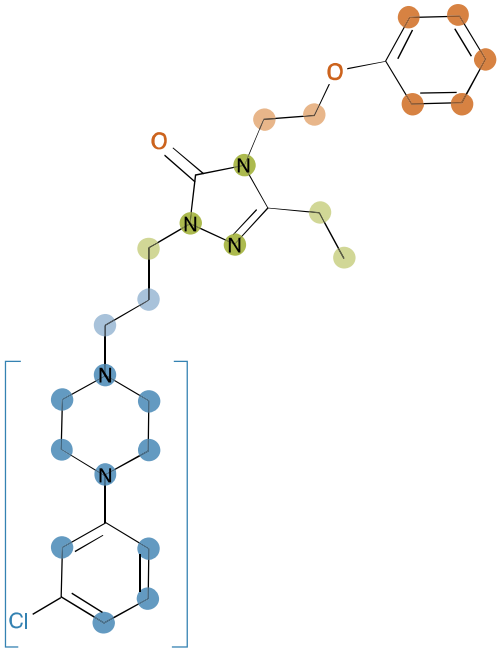
UNIFI Solution

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

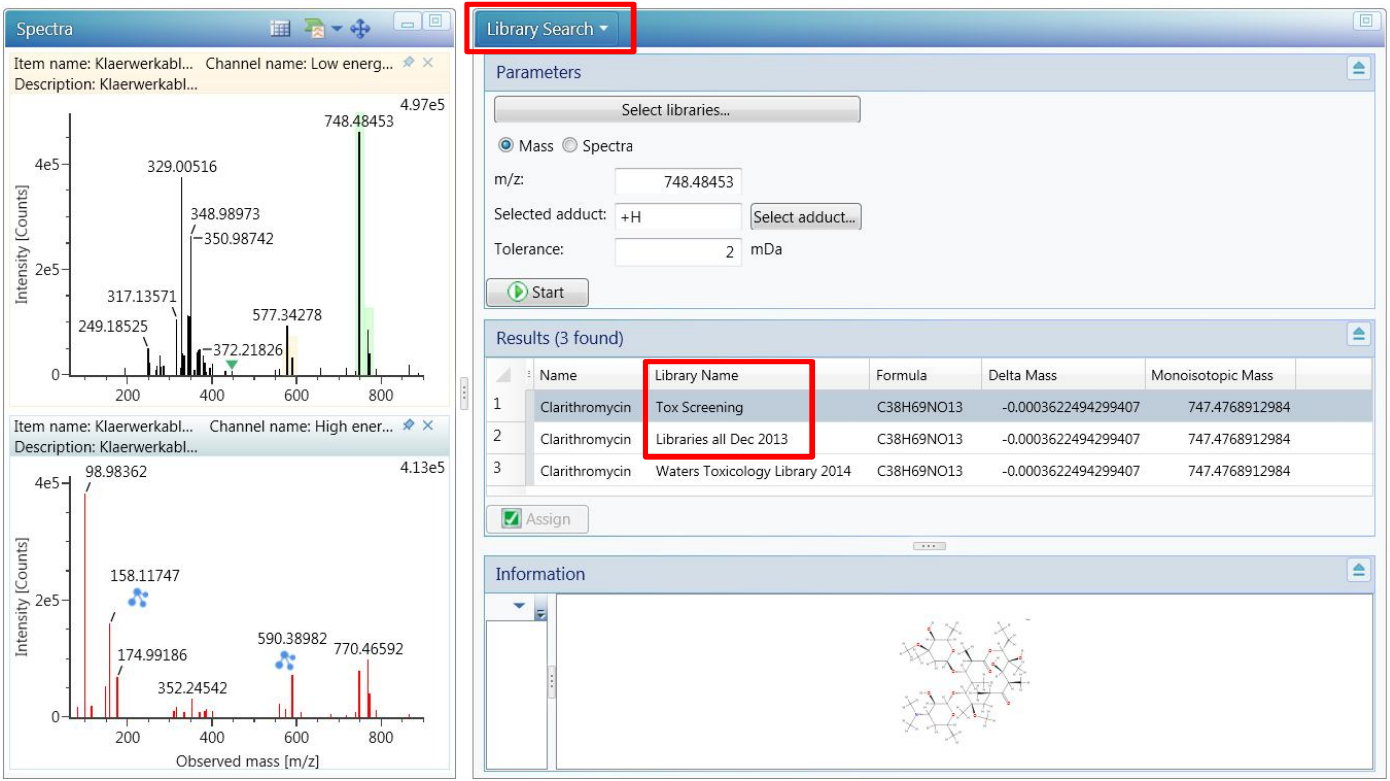


Library Search Options

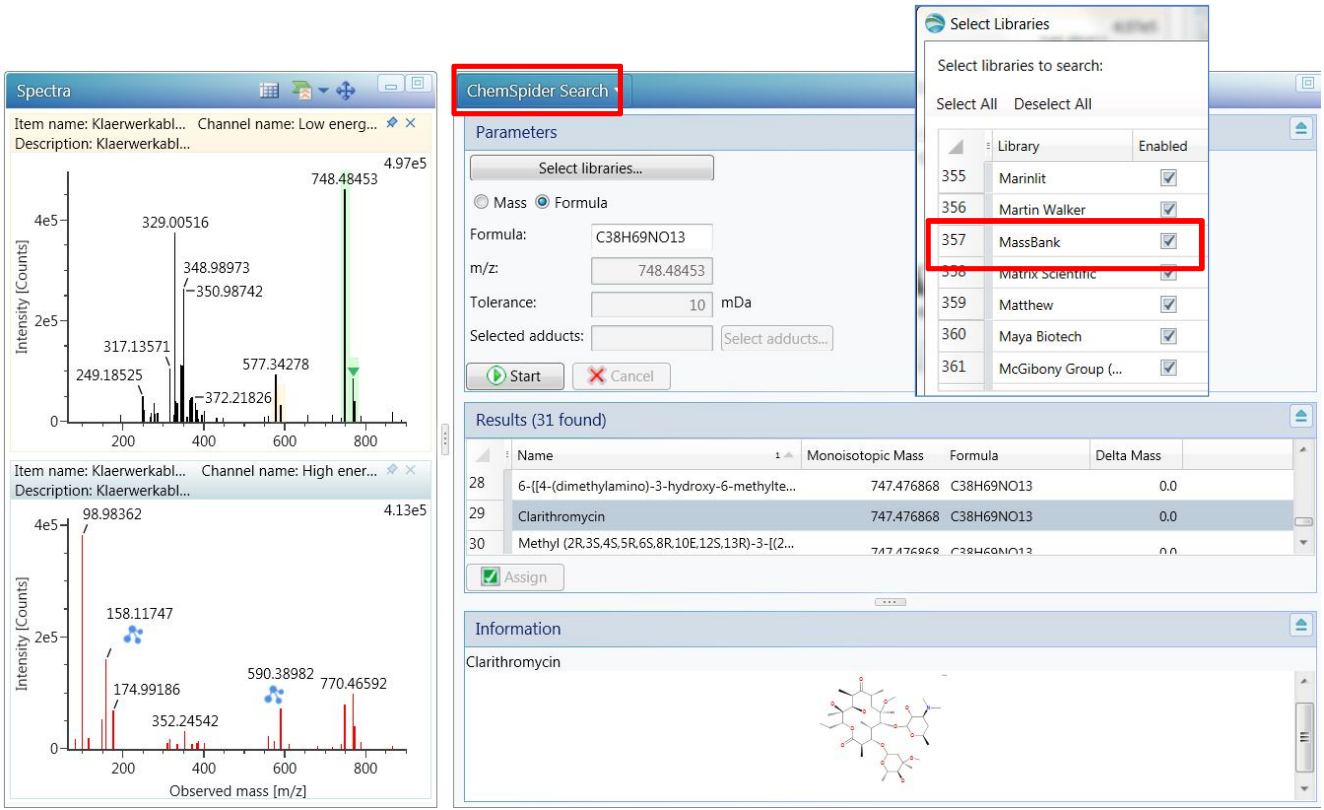
- **UNIFI Library**
  - search in internal libraries

- **UNIFI to ChemSpider**
  - direct link to Chemspider
  - up to almost 600 libraries

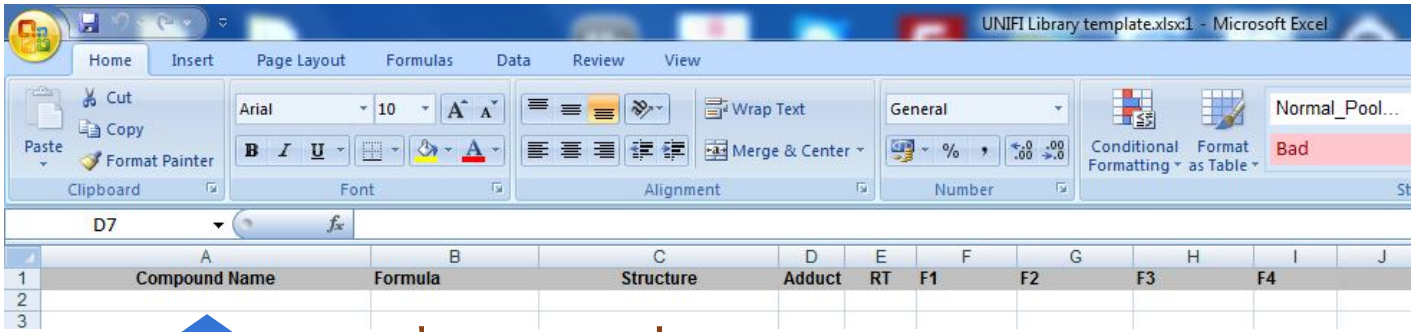
UNIFI Library



UNIFI to Chemspider

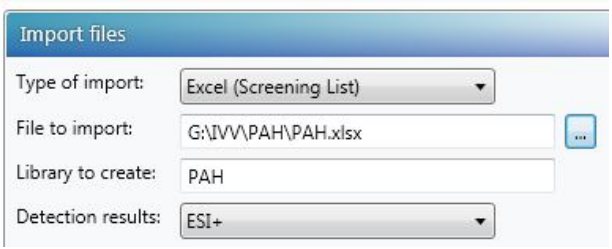


Import (your own Library to Unifi)



Entry name in Lib

Either Elemental Comp or Structure Mol File



Limit Checks and Custom Calculations

Component Limit Checks

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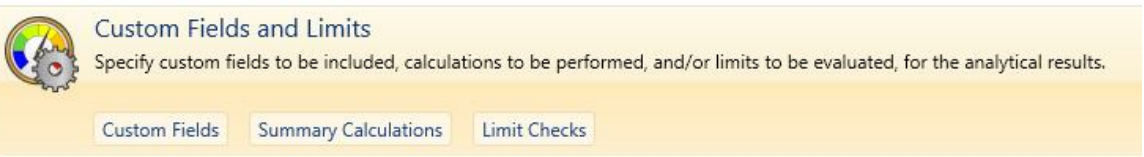


Selected fields and limits checking

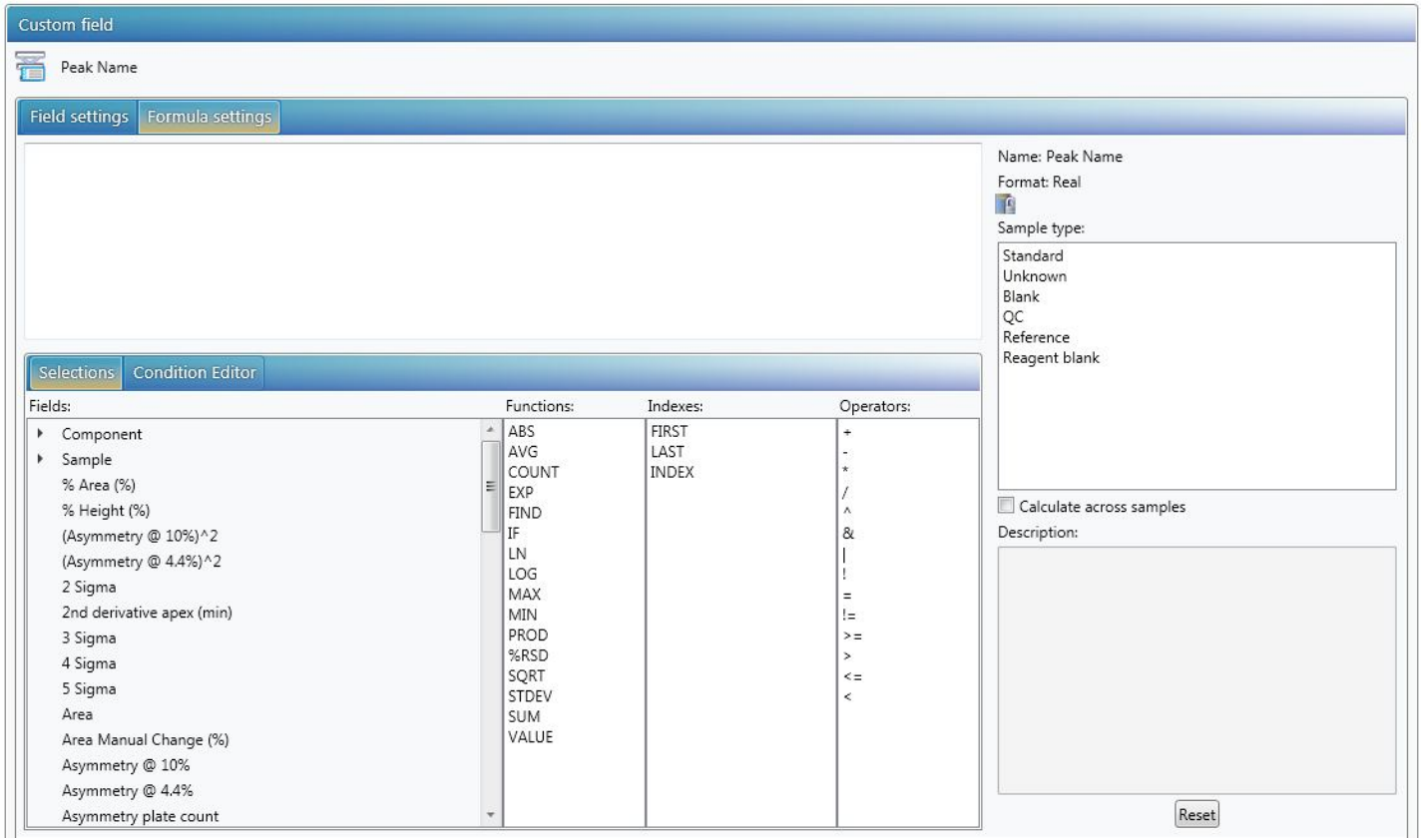
	Node	Field name	Sample type	Level	Error minimum	Warning minimum	Target value	Warning maximum	Error maximum
1	Component	Identified High Energy Fragments	All	All		0	1		
2	Component	Isotope Match Mz RMS PPM	All	All			0	5	10
3	Component	Retention Time Error (min)	All	All	-0.15	-0.1	0	0.1	0.15
4	Component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



Reporting in UNIFI

Enhanced Reporting – Template Editor

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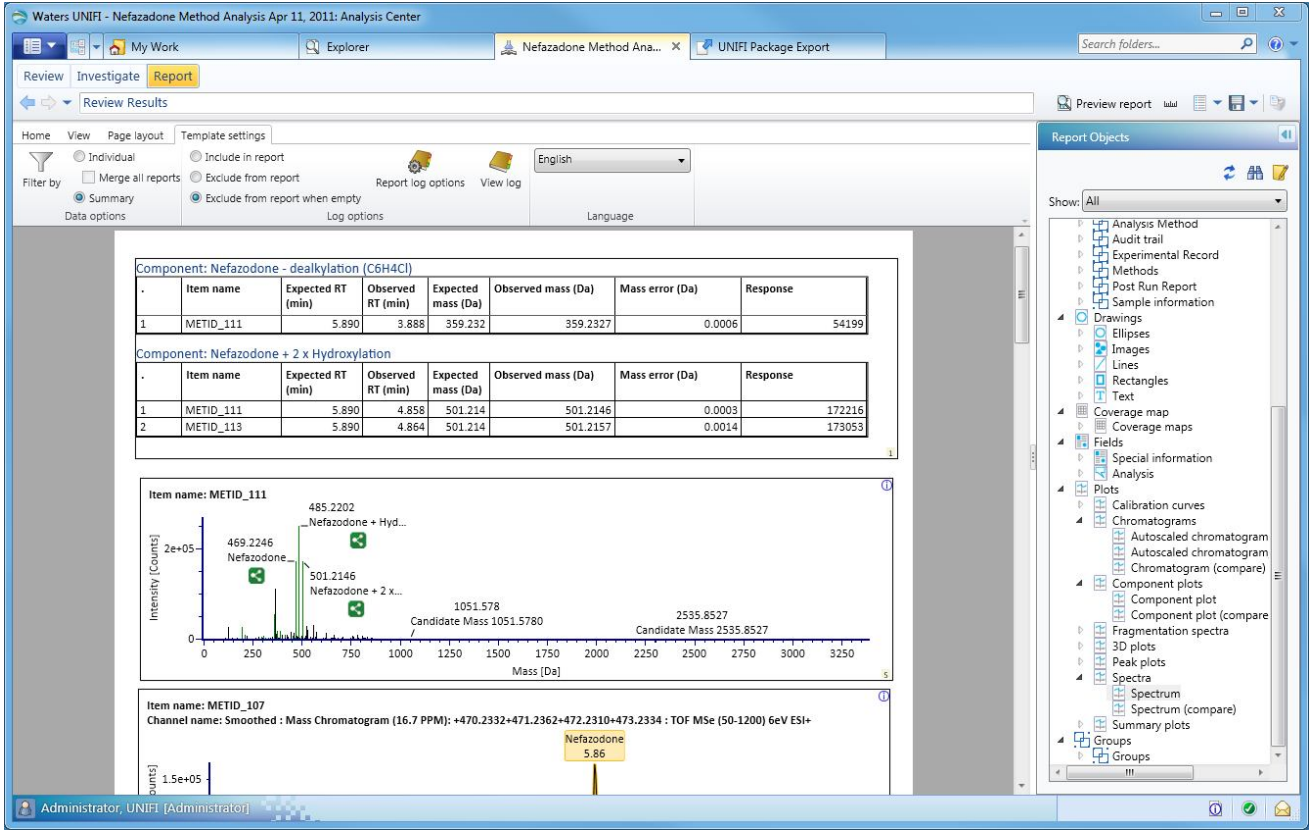
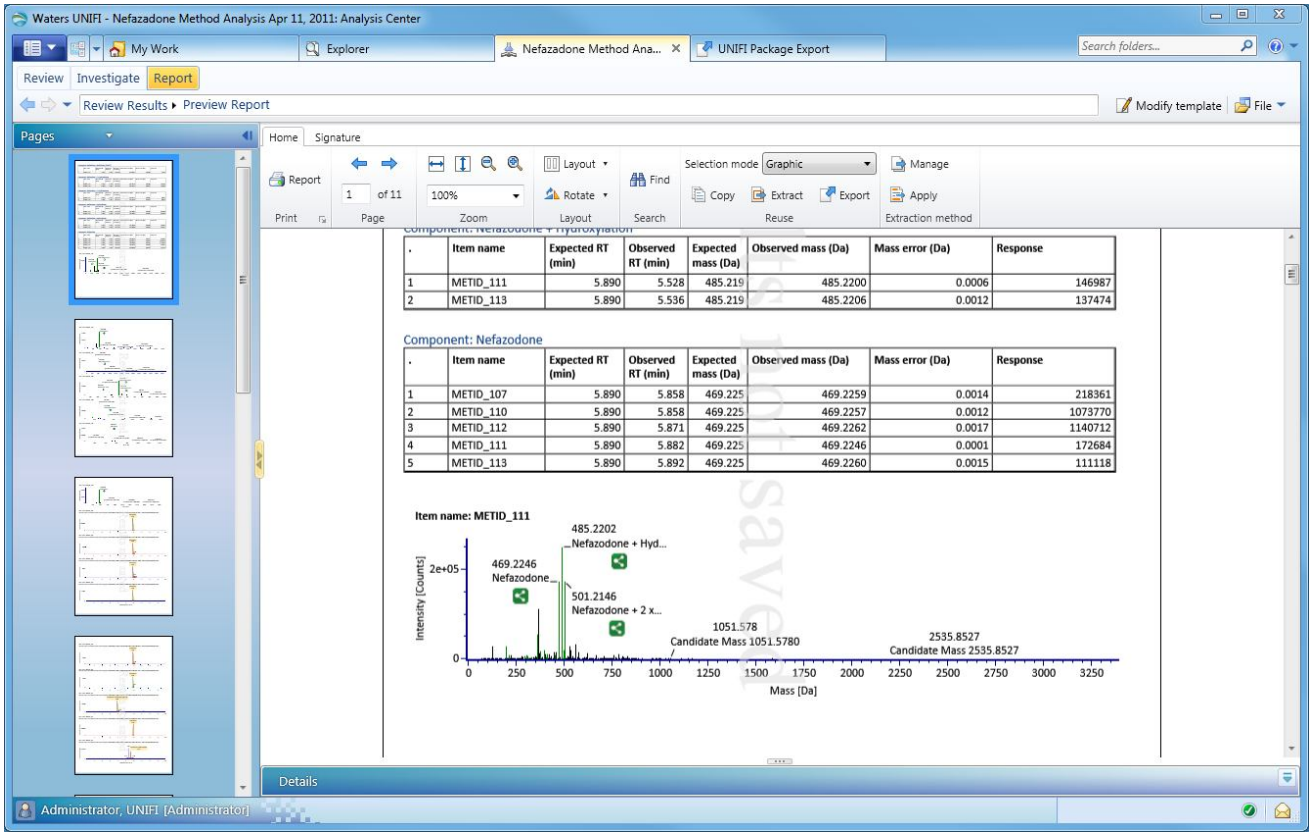


Enhanced Reporting – View and Print Reports



UNIFI CCS

Three dimensions of resolution

Representative
analytical measurement

Property of molecule

rt → K_D

Tof → accurate mass

dt → CCS
Size/Shape

Mehr Information
...SELEKTIVITÄT (and SPEZIFITÄT)

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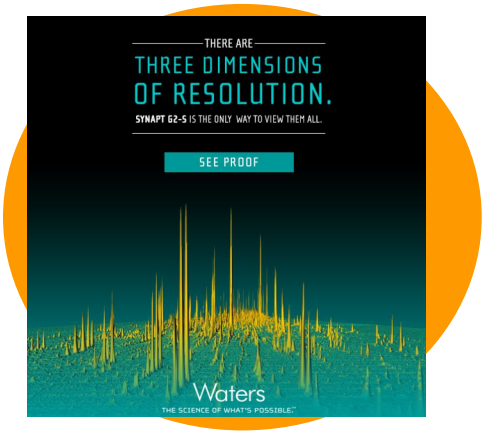
T-WAVE ION MOBILITY POWERED

X

=



UPLC **T-Wave IMS** QuanTof LC/HDMS

3 orthogonal separation techniques

Intellistart - Routine

Ergebnis

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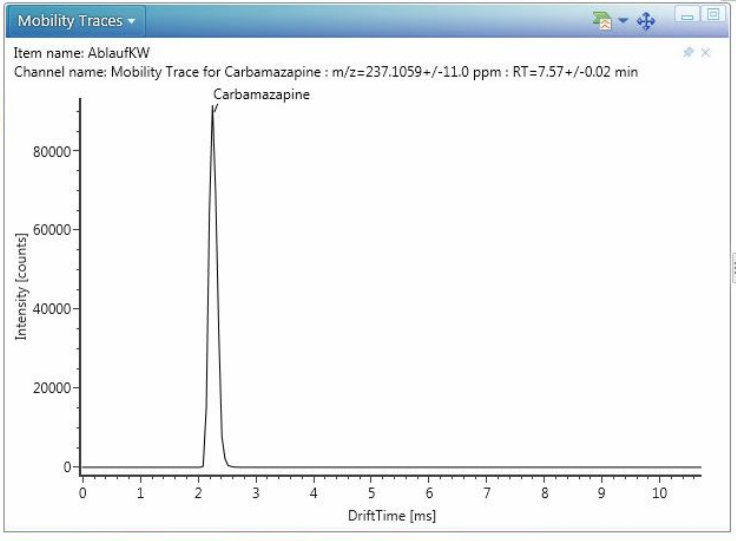
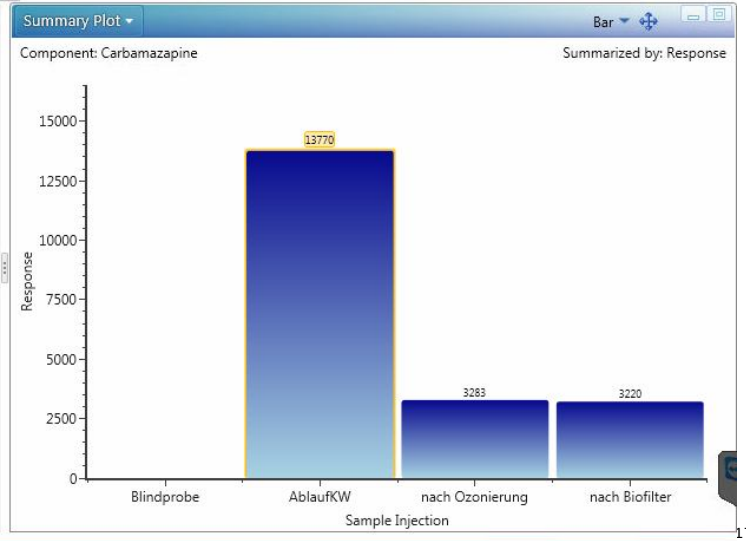
3D: Rt CCS Acc Mass

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	Carbamazapine	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	Bezafibrat	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.

http://www.waters.com/webassets/cms/library/docs/720004720en.pdf

Ciprofloxacin protomers

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http://www.waters.com/webassets/cms/library/docs/720004720en.pdf

MS^E spectra ciprofloxacin Protomers - different daughter ions

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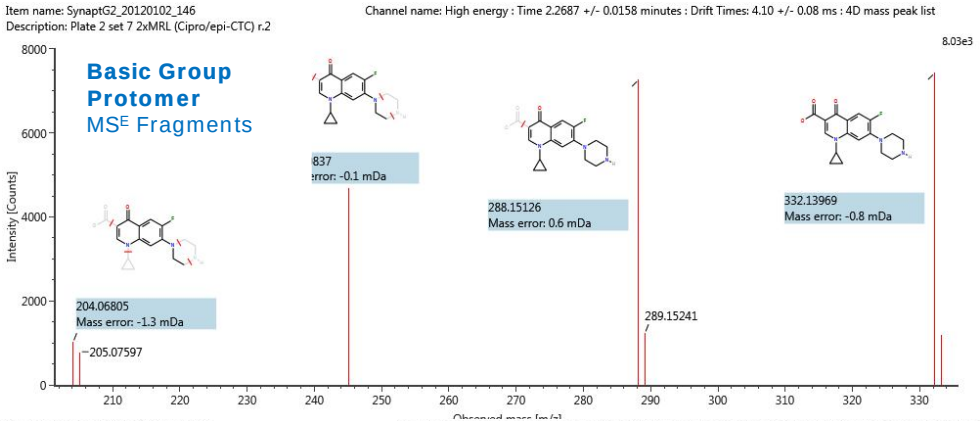

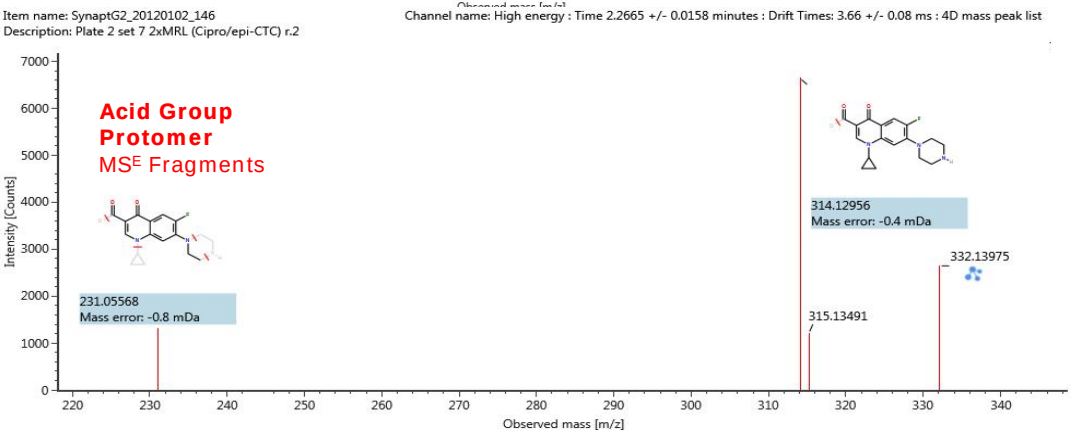

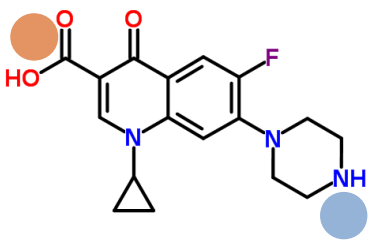

http://www.waters.com/webassets/cms/library/docs/720004720en.pdf

Danke ...

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

... Ihre Aufmerksamkeit!