Enabling Routine Isotopic Fine Structure Analysis

2ω-MRMS with Quadrupolar Detection

Jochen Friedrich
Global Product Manager MRMS

Agenda

- **Part 1:** Mass measurement and **I**sotopic **F**ine **S**tructure (**IFS**)
- **Part 2:** Mass Spectrometry techniques and MRMS evolution
- **Part 3:** 1ω and 2ω spectra – harmonics detection
- **Part 4:** Applications

Mass measurement

Macroscopic:

Scales

e.g.
Weight 88.8 kg
Resolution 0.1 kg
Accuracy ± 0.3 kg (0.1%-range)

Single mass value but no information on weight distribution (muscles/fat/brain)

Any assignment is guesswork (or wishful thinking)

Microscopic:

Mass Spectrometer

e.g.
Weight 800.630 amu
Resolution 0.01 amu
Accuracy ± 2 ppm

Single mass value but (often) no information on weight distribution (Carbon/Oxygen/Nitrogen)

Any assignment is guesswork, consequently:

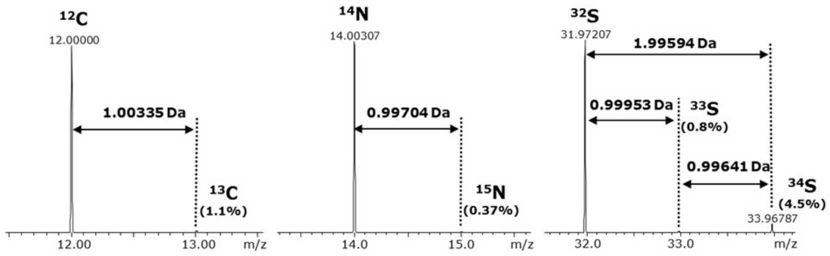
EVERY DAY AROUND THE WORLD

SMART MS SCIENTISTS MAKE INCORRECT FORMULA ASSIGNMENTS

Isotopic Fine Structure (IFS)
Basics: Mass Defect

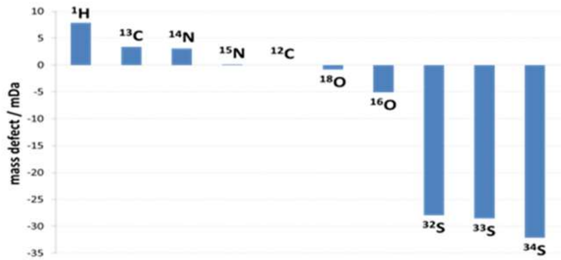
Nature offers a way to avoid wrong formula assignments:

- Chemical elements consist of isotopes with different abundance. E.g. carbon consists mainly of ^{12}C with 1.1% heavier ^{13}C



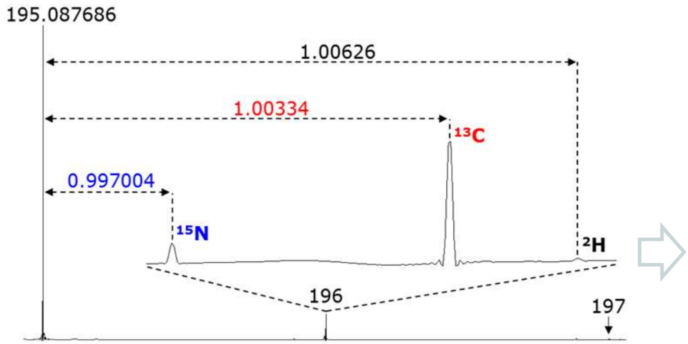
- Due to the mass defect, the mass difference between these isotopes are non integer values, e.g. $\Delta(^{12}C;^{13}C)$ = 1.00335 Da

- The mass difference between different isotopes are different



- ***Example:*** IFS of caffeine (measured with 7T 2xR)

  IFS yields information on the elemental composition of the analyte



molecule contains N, C and H

Required resolving power for IFS

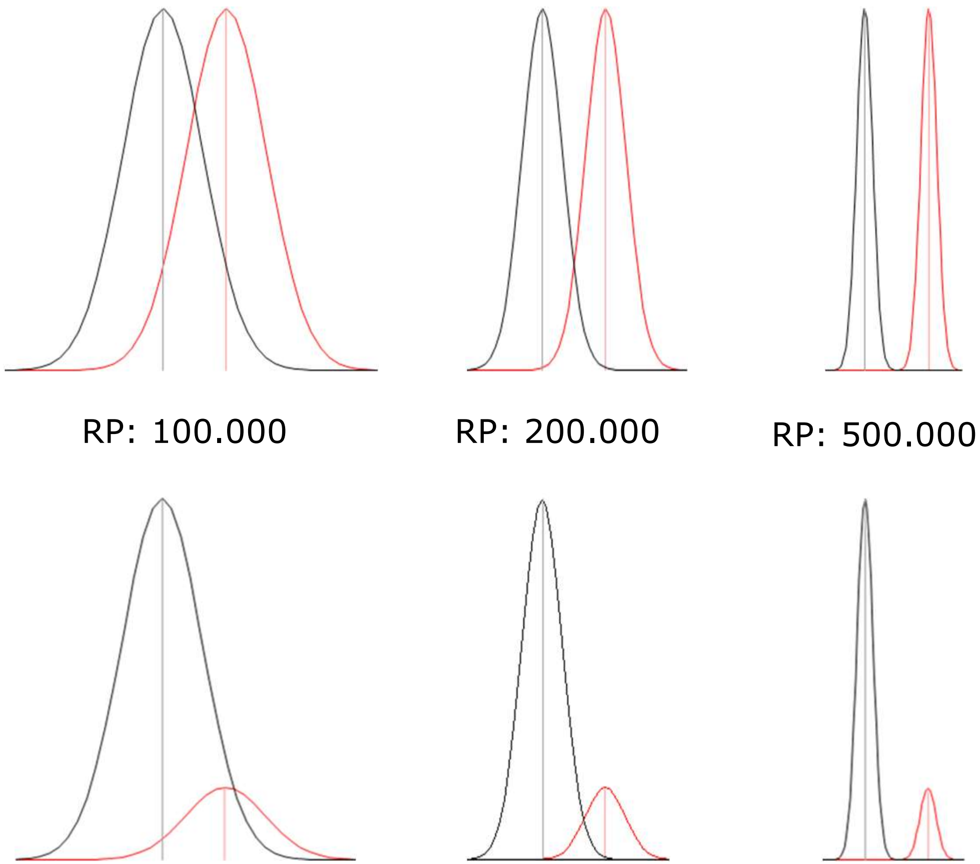
Example: detection of sulfur compounds in crude oil, simulated peak width

C_3 vs. SH_4 3.4 mDa split

Intensity ratio 1:1

– $C_{37}H_{56}$, M+ ,500.43765
– $C_{34}H_{60}S$, M+ ,500.44102

Intensity ratio 1:5

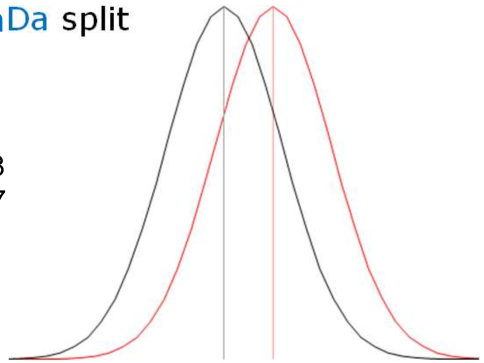


Required resolving power for IFS

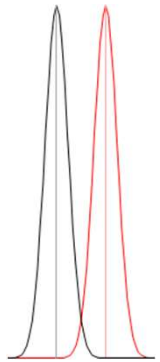
Example: detection of compounds in crude oil, simulated peak width

H_4NO_3 vs. $C_2{}^{13}CHN_2$ 1.8 mDa split

– $C_{32}{}^{13}CH_{41}N_3$, M+nH ,481.34068
– $C_{30}H_{44}N_2O_3$, M+nH ,481.34247



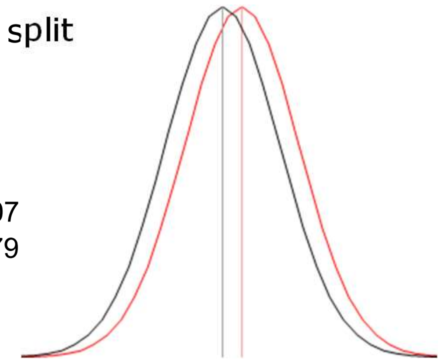
RP: 100.000



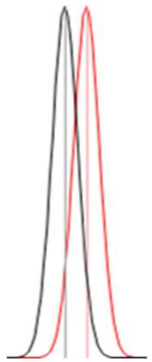
RP: 480.000

$^{13}CNO_2$ vs. C_2SH_3 0.7 mDa split

– $C_{30}{}^{13}CH_{40}N_2O_2$, M+nH, 473.31107
– $C_{32}H_{43}NS$, M+nH, 473,31179



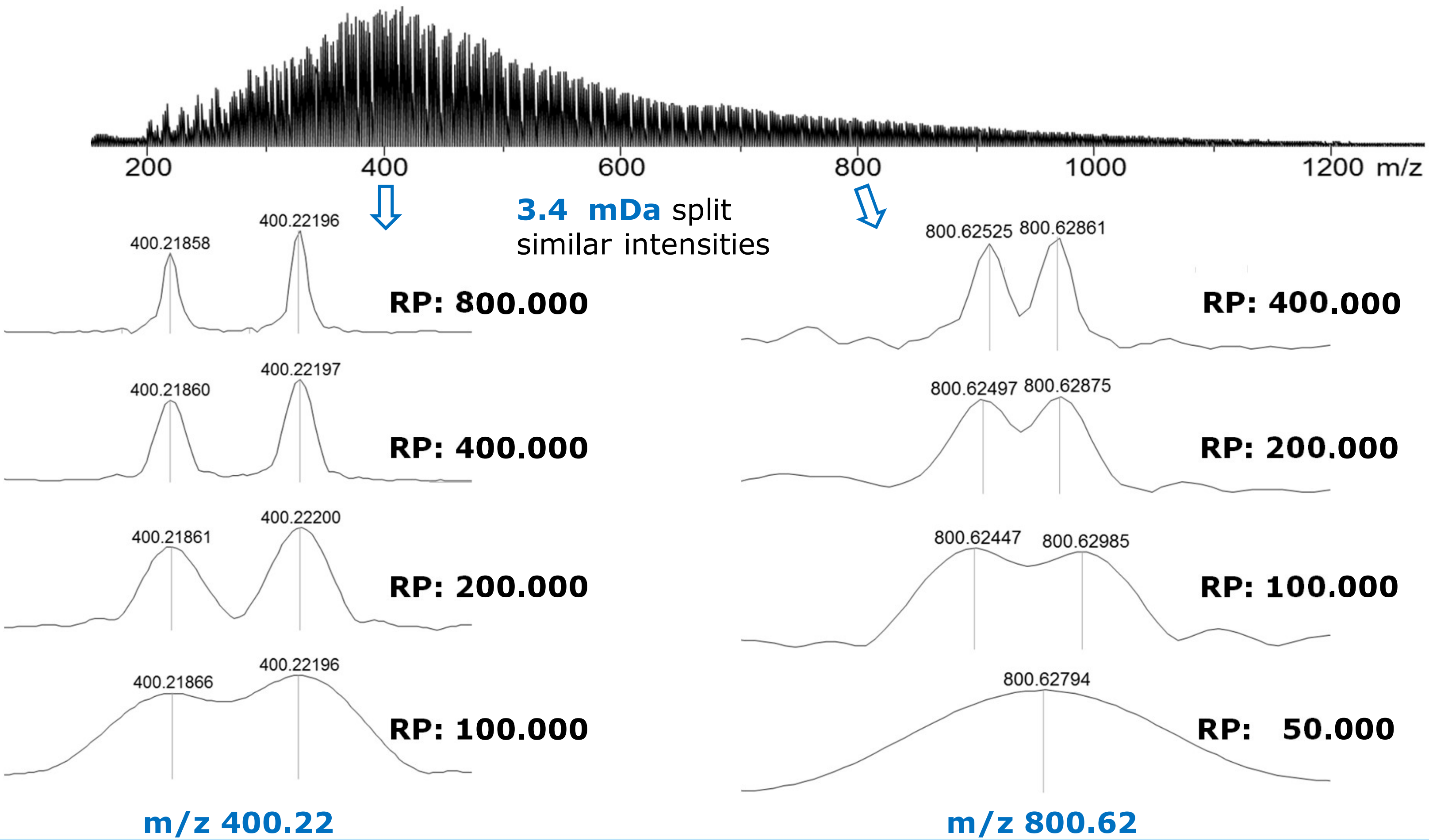
RP: 100.000



RP: 480.000

Required resolving power for IFS

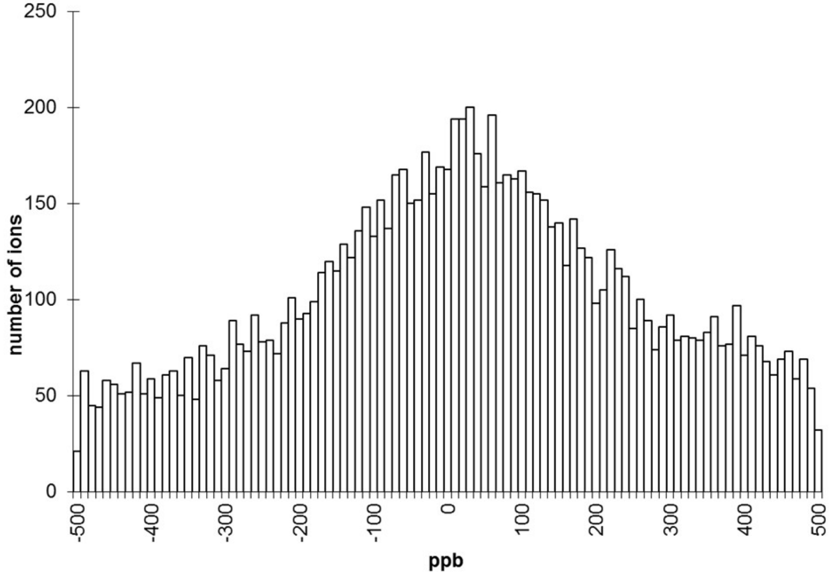
Example: detection of sulfur compounds in crude oil, experimental peak width



Required resolving power

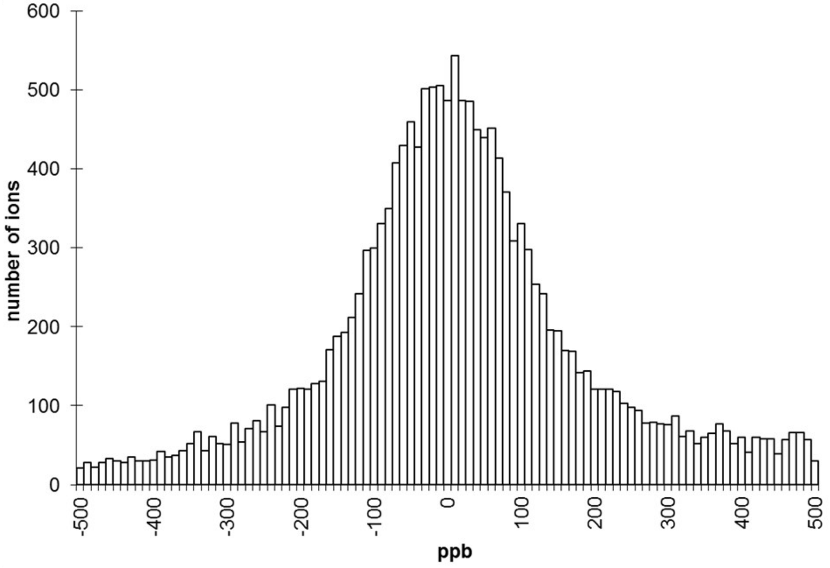
Example: detection of compounds in crude oil, mass error plots

18 ± **236 ppb**
10107 ions



RP: 200.000 (at m/z 400)

7 ± **169 ppb**
15752 ions



RP: 800.000 (at m/z 400)

Confident Assignment of sum formulae...

... Is enabled by access to

Isotopic Fine Structure

information.

This requires

- High resolving power: **> 500.000** over a **broad mass range**
- Very good mass accuracy: **sub-ppm**

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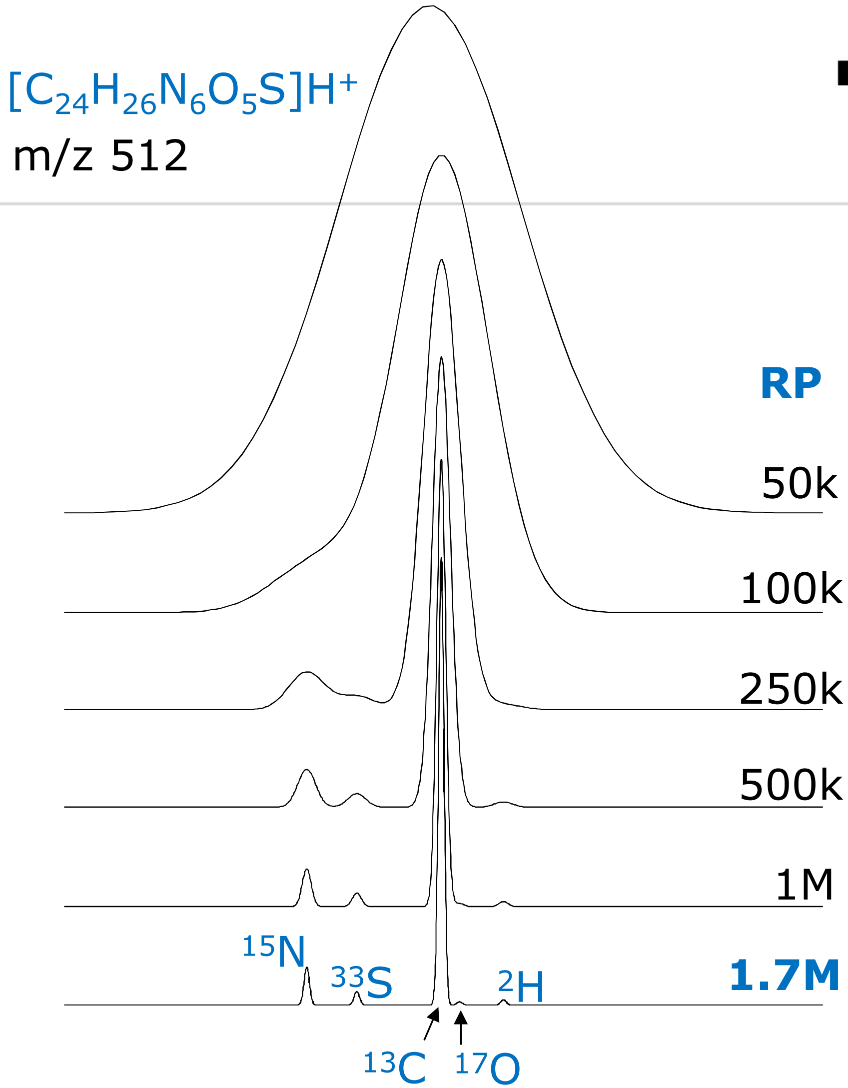
MS Detection Methods

What are the options?

Low Resolution

- **Electron Multiplier** – for ion signal detection
- **Microchannel Plates** – for ion signal detection
- Image charge detection in **Electrostatic field**
- **MRMS** – Image charge detection in **Magnetic field**

eXtreme Resolution



The **MRMS detector** distinguishes solariX and scimaX from other MS

MS Detection Methods
MRMS

ParaCell detector

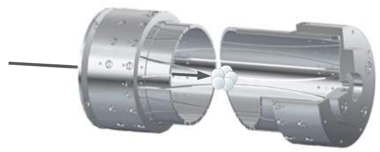
- Dynamically harmonized ICR cell (DHC): Harmonic, parabolic potential for all cyclotron orbits
- Maximum resolution > 20M already at 7T 2xR
- Detector cell for the **solariX XR** and **scimaX** series
- Detector cell for the NHMFL 21T instrument based on DHC concept

I. A. Boldin, E. N. Nikolaev, *Rapid Commun. Mass Spectrom.*, **25**, 122, (2011)
E. N. Nikolaev, I. A. Boldin, R. Jertz, G. Baykut, *J. Am. Soc. Mass Spectrom.*, **22**, 1125, (2011)

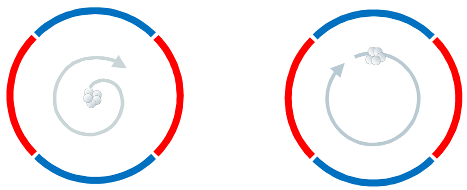
Making an MR Mass Spectrum

Key Detection Technology

- The analyte ions enter our ParaCell Detector located in a **M**agnetic field.

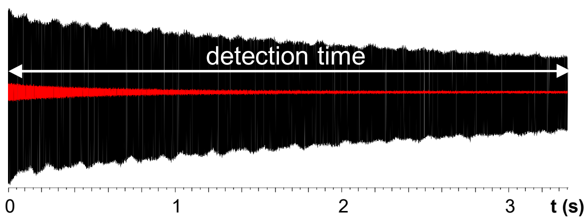


- Ions get **R**esonantly excited for detection:



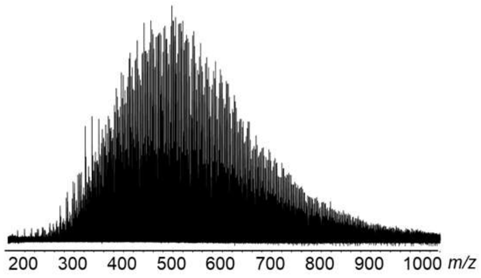
ParaCell stabilizes also low abundant ion motion

The analytes rotation in the detector is recorded for some detection time



Recorded ion motion („transient", „FID")

- After calibration a **M**ass **S**pectrum is created



FID: I(t)

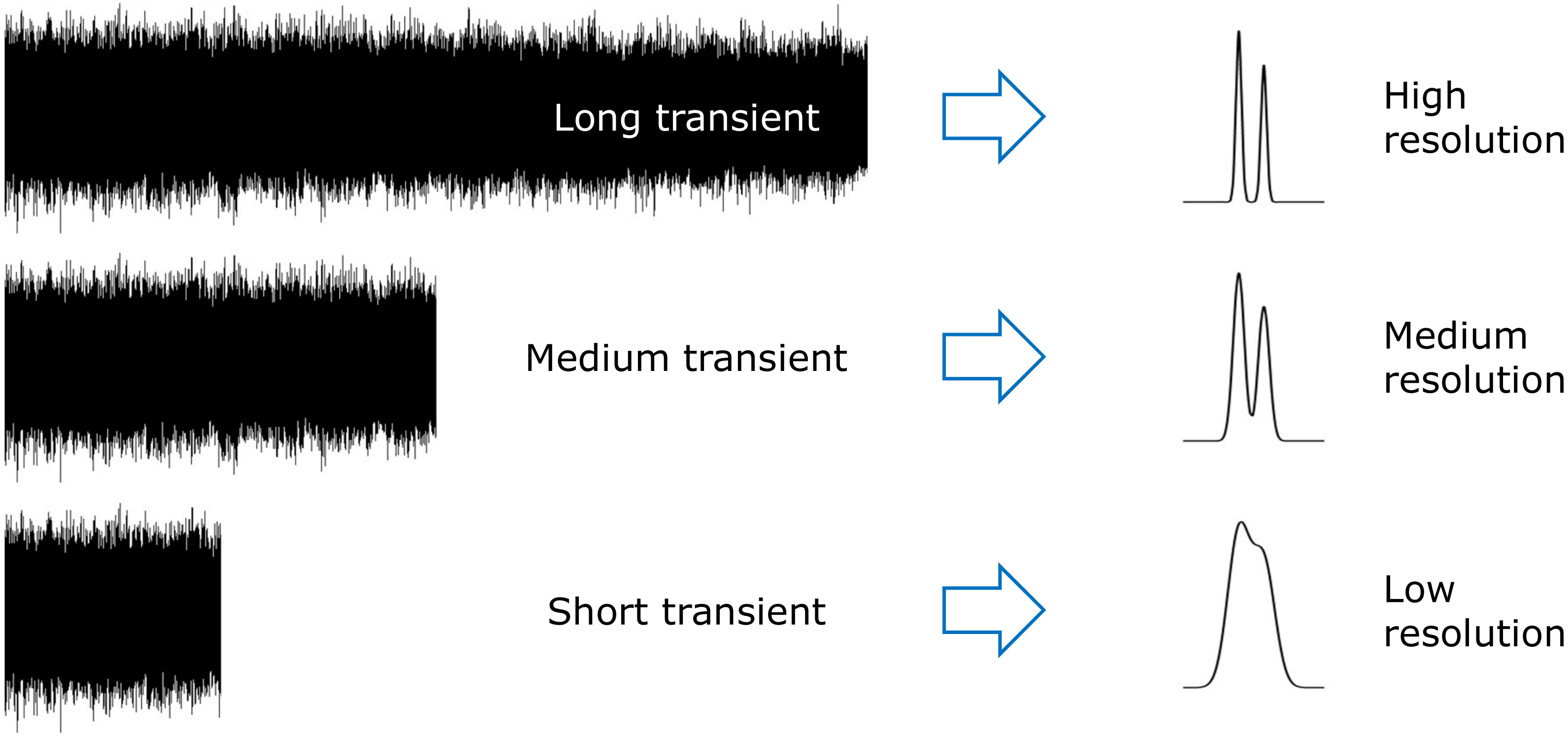
FT

I (ω)

calibration

I (m/z)

MRMS Basics:
Transient Length and Resolution



MRMS can trade resolution for speed or speed for resolution

MRMS
Not your parent's FT-ICR MS

Magnetic **R**esonance **M**ass **S**pectrometry

1973 › 1983 › 2009 › 2013 › 2016 › 2018

- Fourier transform ion cyclotron resonance mass spectrometry *FT-ICR MS* is a technique invented in **1973**.
- Commercially marketed as **FTMS** by Bruker starting in the **mid 80s**.
- Introduction of solariX in **2009**.
- The **ParaCell™** was introduced in **2013** with solariX XR and several generations later, the modern FT-ICR MS was nothing like the ones from 40 years ago.
- Introduction of solariX 2xR in **2016** with **quadrupolar detection**.
- Introduction of **scimaX** in **2018** with **Maxwell magnet technology**.
- Today **MRMS** defines the next generation of FTMS instrumentation.

Bruker's Magnet Technology

NMR, MRI & MRMS: A long history of magnet innovations

Refrigerated Magnet

- 7T, 12T & 15T magnets
- Compact design
- Small stray field
- **No** Liquid Nitrogen
- Extended liquid Helium hold time (290 L Helium once a year)
- Biennial cold-head exchange
- Quench duct required

solarix

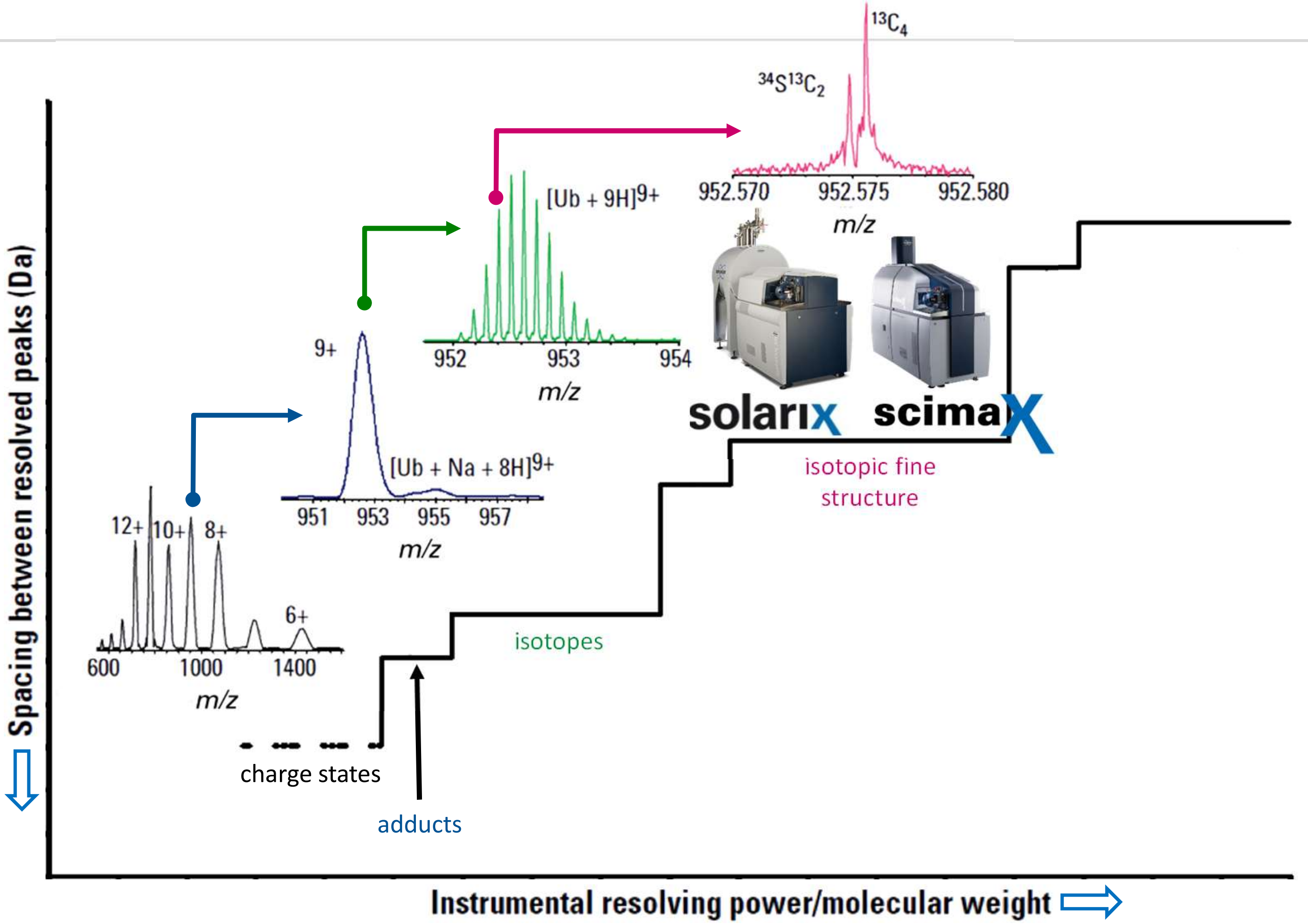
Maxwell Magnet

- 7T magnet
- Very compact design
- Small stray field
- **No** Liquid Nitrogen
- **No** Liquid Helium fill needed

- Biennial cold-head exchange
- **No** Quench duct required

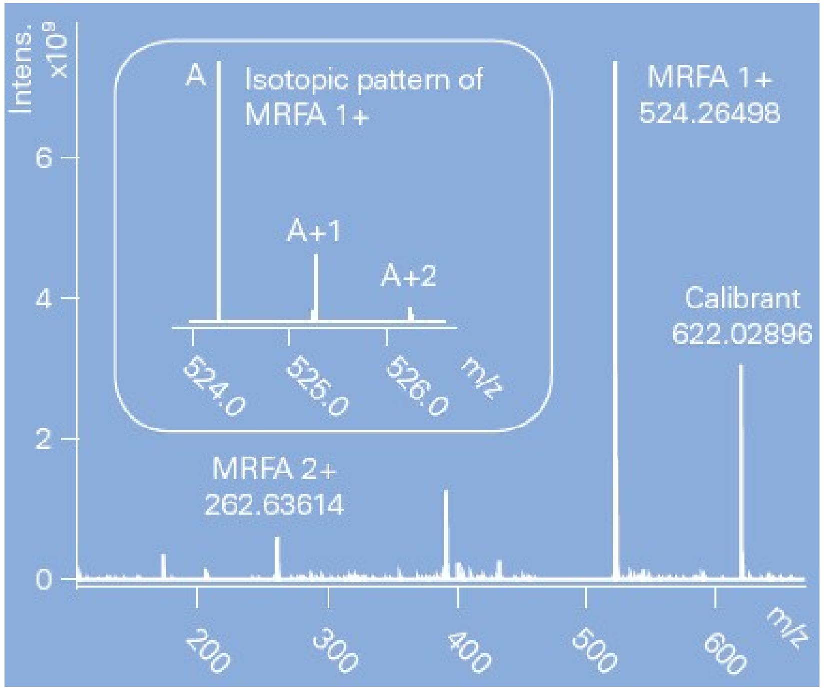
scimaX

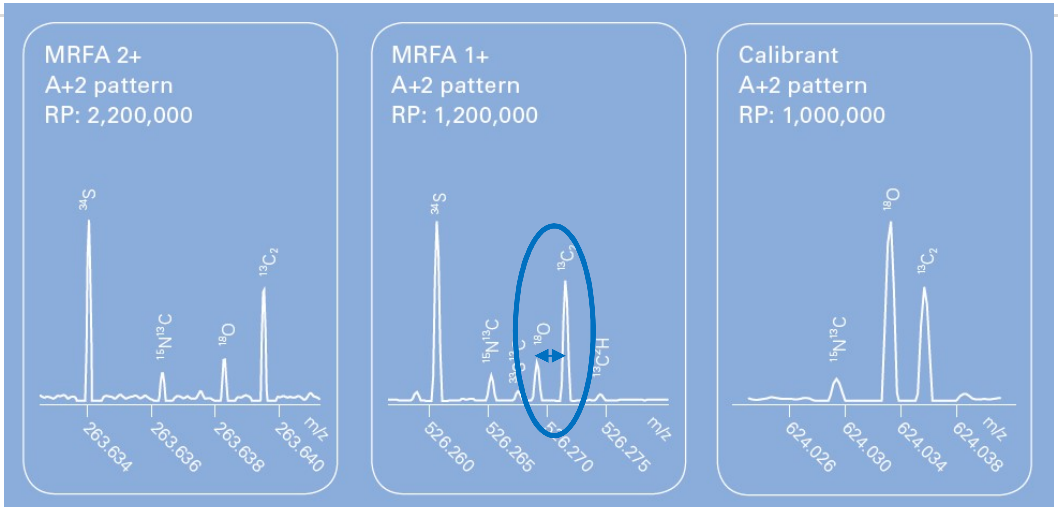
Evolutionary steps towards Isotopic Fine Structure



Marshall, A.G.; Hendrickson, C.L.; Shi, S.D-H. *Scaling MS Plateaus with FTICR MS,* Anal. Chem., 2002, 74, 252A-259A.

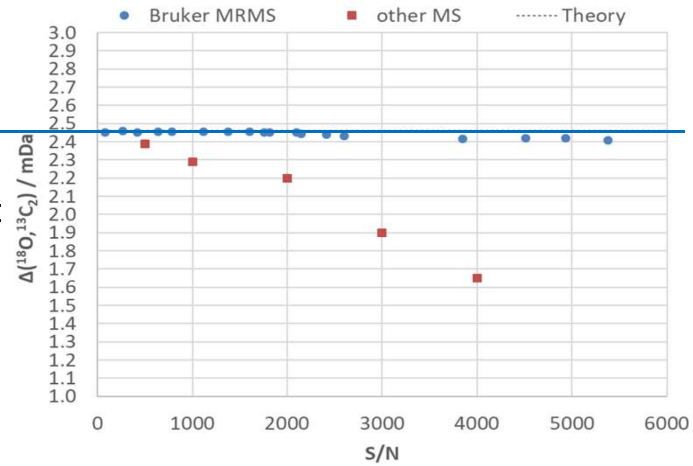
scimaX - routine Isotopic Fine Structure





Narrow peak distances stay constant with MRMS.

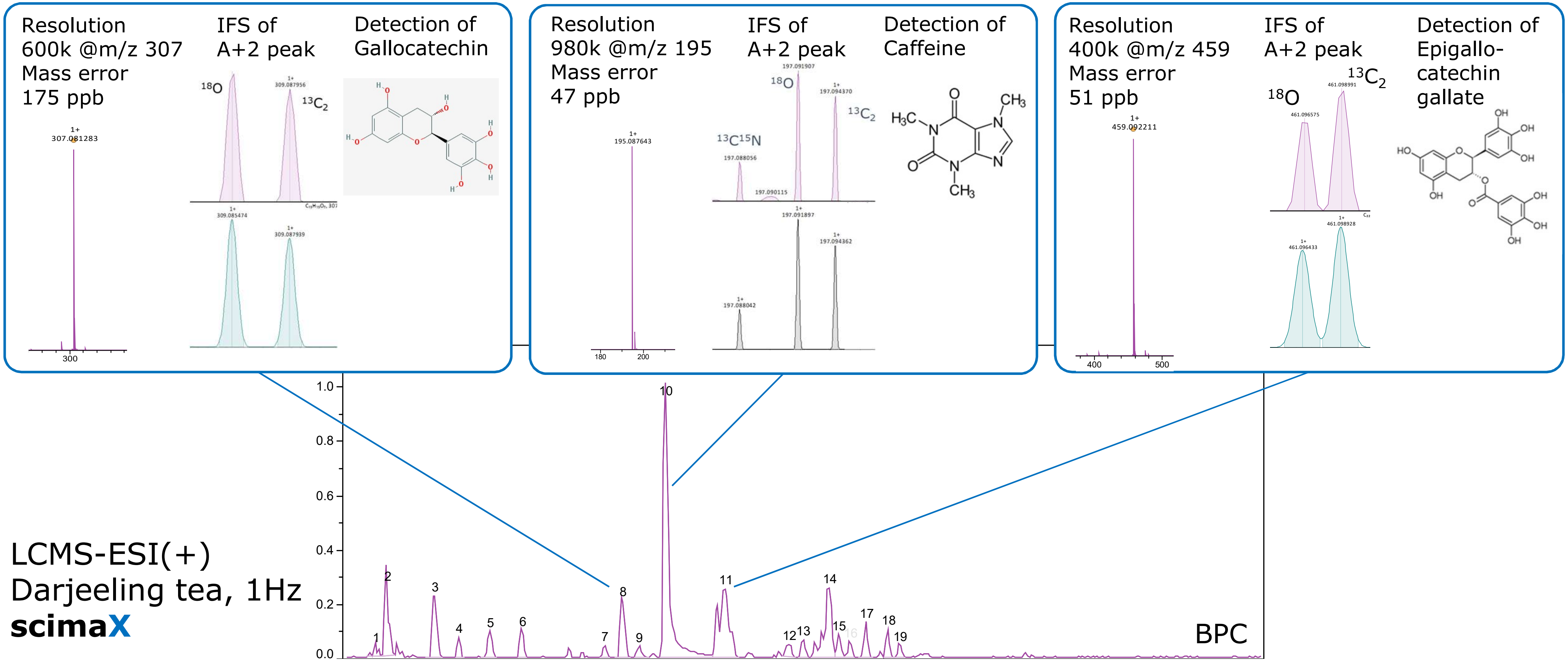
Other technologies cannot provide reliable IFS information as peaks coalesce with increasing S/N.



Routine **I**sotopic **F**ine **Structure** (**IFS**)

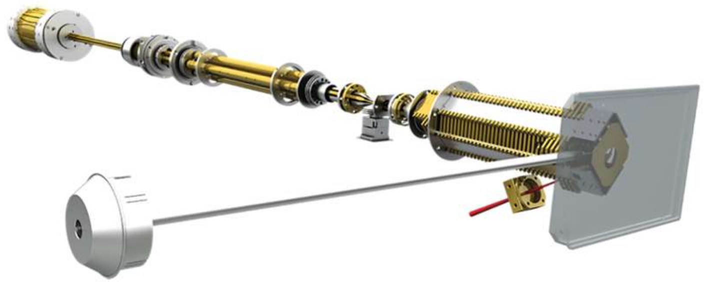
- 1M resolving power also above m/z 200
- Broad band Isotopic Fine Structure
- Precise IFS also at higher ion loads

scimaX - routine Isotopic Fine Structure



LCMS-ESI(+)
Darjeeling tea, 1Hz
scimaX

Instrumentation



scimaX

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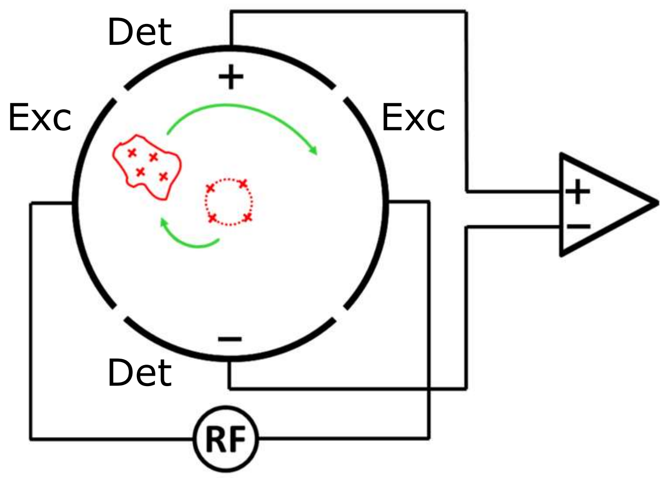
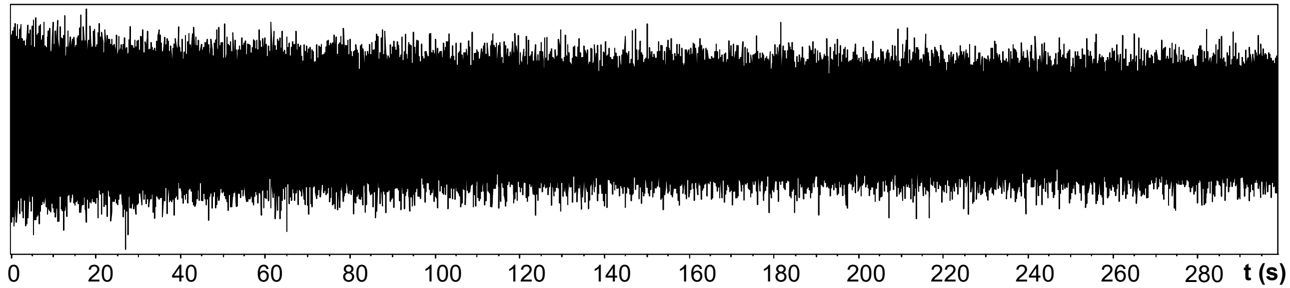
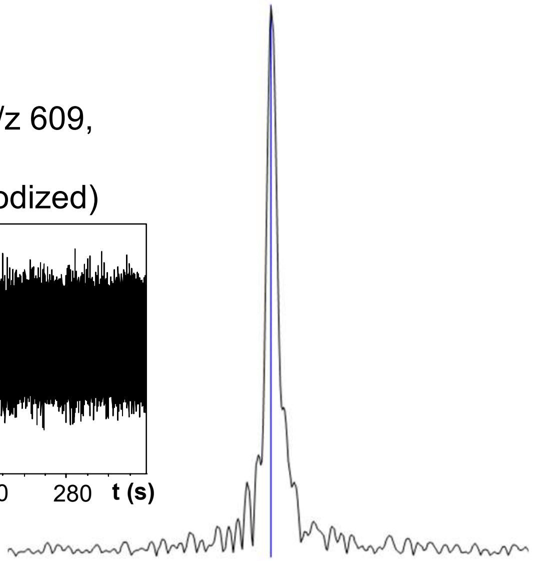
Dipole **1ω** detection scheme



- Alternating 90° Excitation, 90° Detection segments
- Dipolar rf exciation
- Dipolar detection of cyclotron frequency ω_c (ideal case)

Reserpine, m/z 609,
7T ParaCell
R = 39 M (apodized)





Dipolar 1ω detection: harmonics – simulated spectra

a) Centered cyclotron, no magnetron motion: only uneven harmonics

b) Off center cyclotron, no magnetron motion: also even harmonics

c) Centered magnetron motion: some sidebands

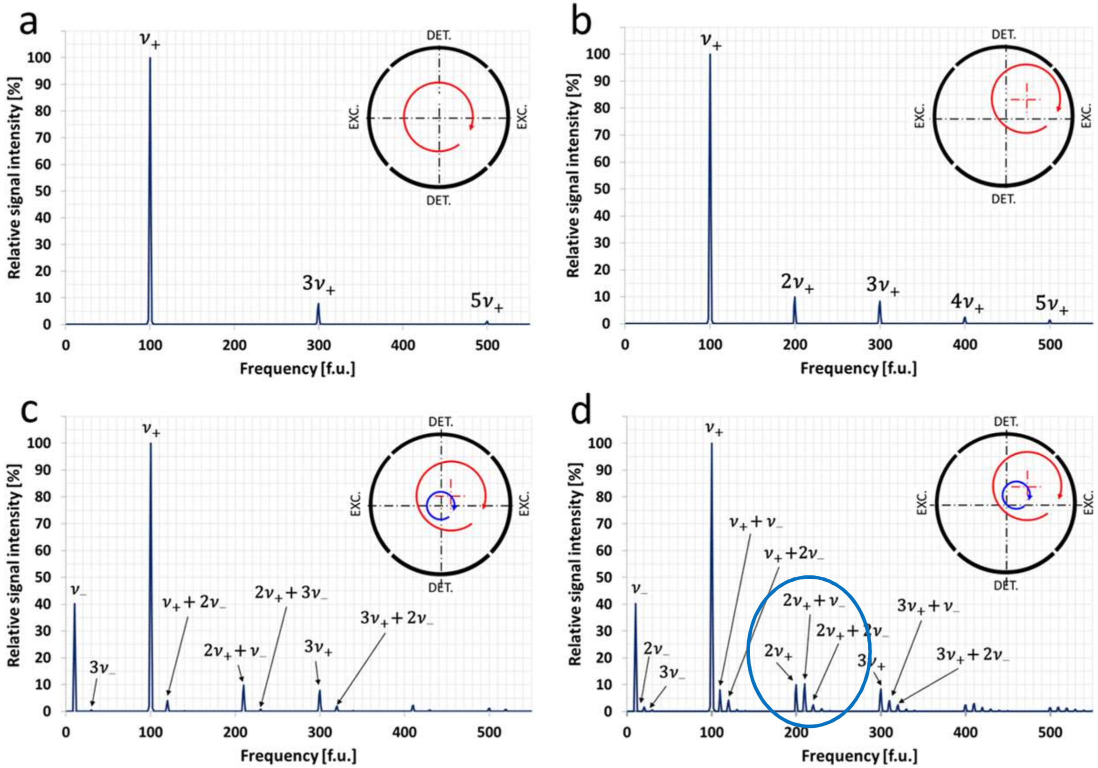
d) Off center magnetron motion: several sidebands

Goal: simple spectra

→ Control ion position in cell

→ (i) Understand magnetron motion

(ii) control & reduce magnetron motion

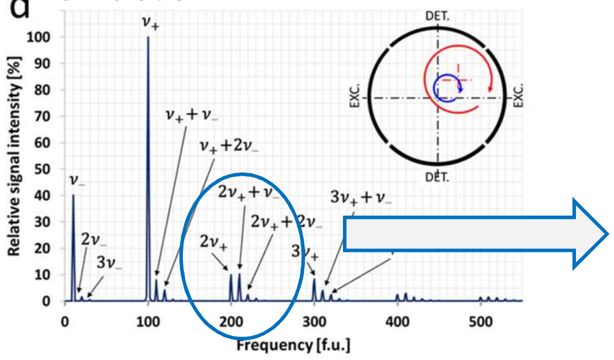


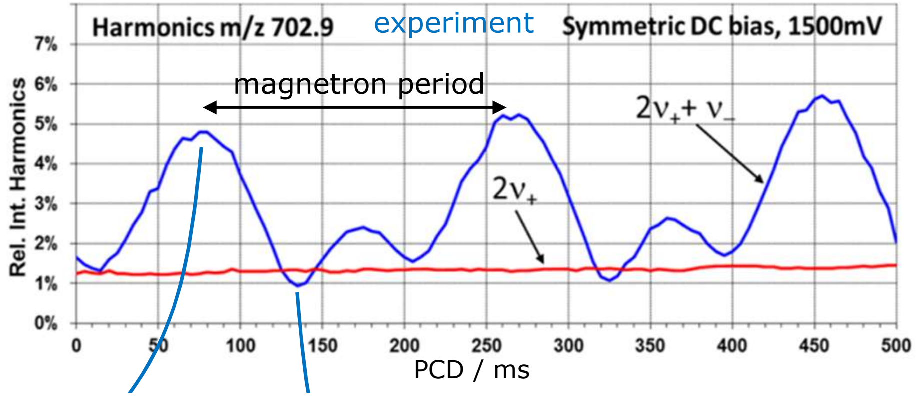
R. Jertz, J. Friedrich, C. Kriete, E. N. Nikolaev, G. Baykut, J. Am. Soc. Mass Spectrom., 26, 1349, (2015)

Step 1: Understand Magnetron motion

Observe 2ν harmonics

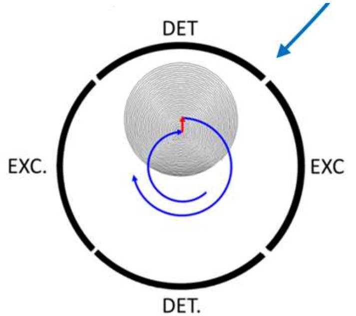
- 2nd harmonic $2\nu_+$ is steady
- Magnetron sideband of 2nd harmonic $2\nu_+ + \nu_-$ oscillates depending on post capture delay (PCD)



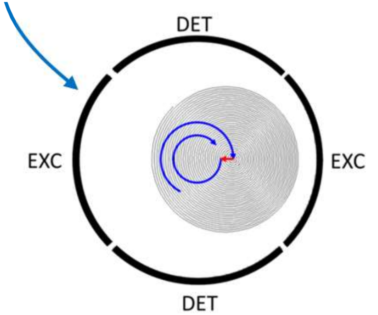


- Oscillation of $2\nu_+ + \nu_-$ due to ion position dependant magnetron excitation/relaxation

Simulation:

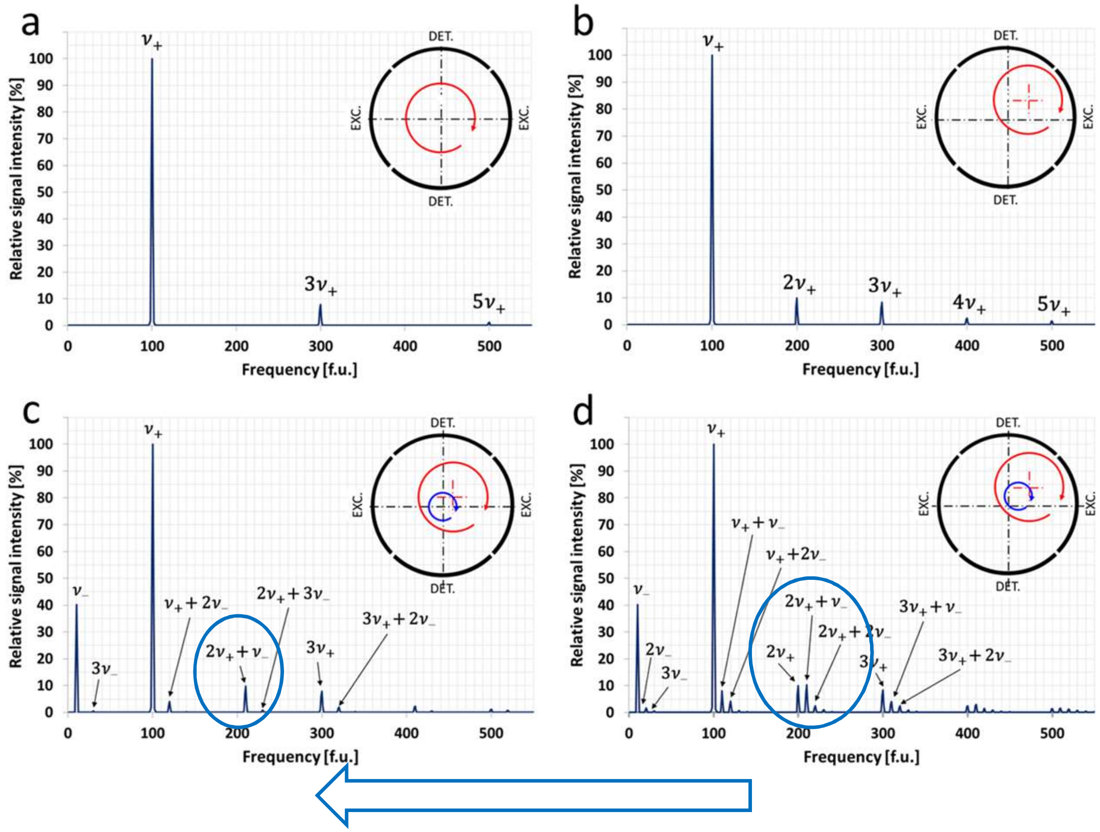


Ion cloud close to detection segment
→ Magnetron excitation



Ion cloud close to excitation segment
→ Magnetron relaxation

Dipolar **1ω** detection:
harmonics – simulated spectra



Goal: simple spectra

→ Control ion position in cell

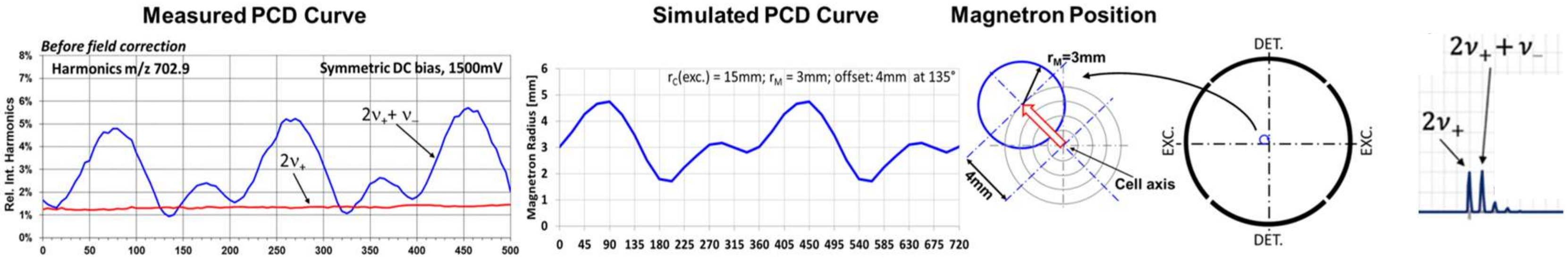
→ (i) Understand magnetron motion

(ii) control & reduce magnetron motion

R. Jertz, J. Friedrich, C. Kriete, E. N. Nikolaev, G. Baykut, J. Am. Soc. Mass Spectrom., 26, 1349, (2015)

Step 2: Control and reduce Magnetron motion

Shim the cell (dc)

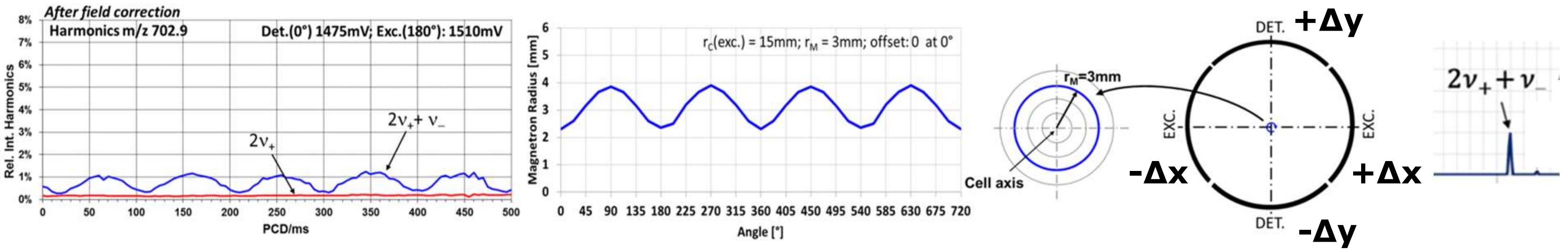


Magnetron motion: rotation around electrical axis of the cell

- Ensure that the electrical axis matches with the cell axis.
- Shim cell via small dc offset on ParaCell bias voltages (20 mV range)

→ minimize $2\nu_+$ peak

→ axialize magnetron motion



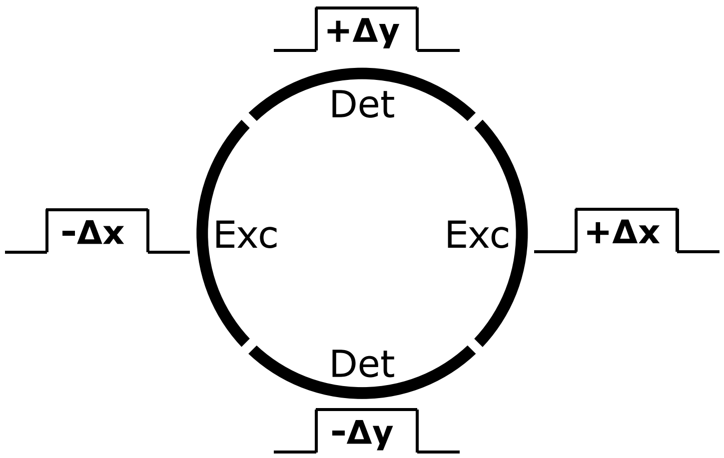
Step 2: Control and reduce magnetron motion

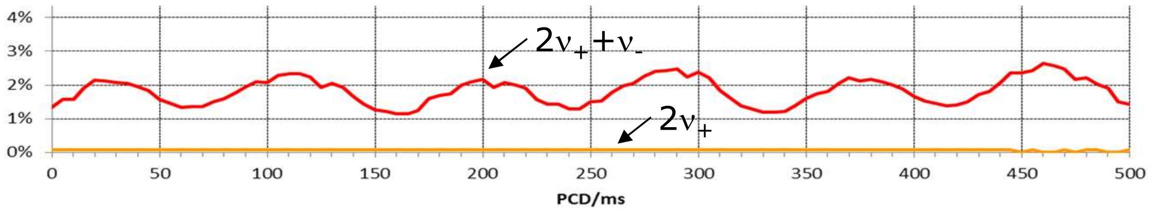
Apply gated injection

- Ensure that the magnetron motion is not/minimal excited
- Apply gated injection voltages during ion capture

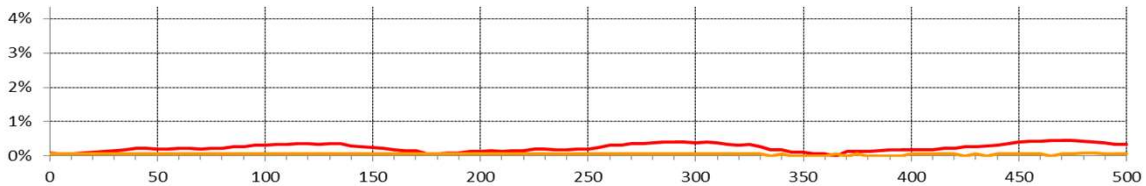
→ minimize $2\nu_+ + \nu_-$ peak

→ minimize magnetron motion

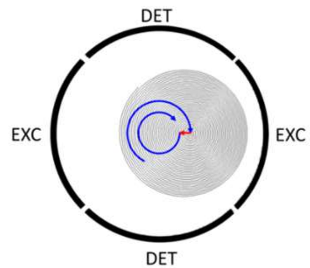




Shimmed (dc)

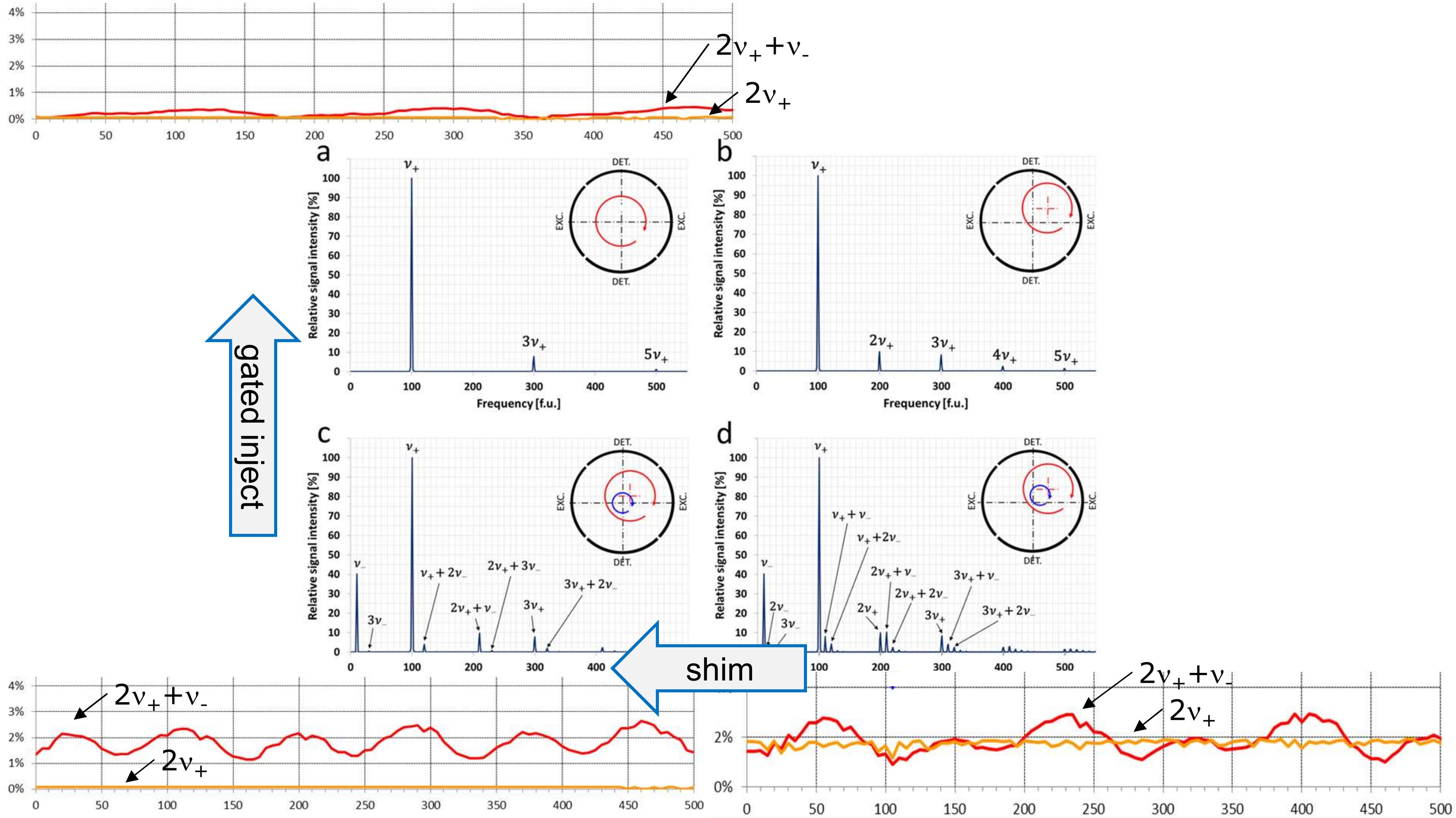


Shimmed (dc) and gated injection



Step 2: Control and reduce Magnetron motion

Minimized spectra complexity by minimized magnetron motion



So far:

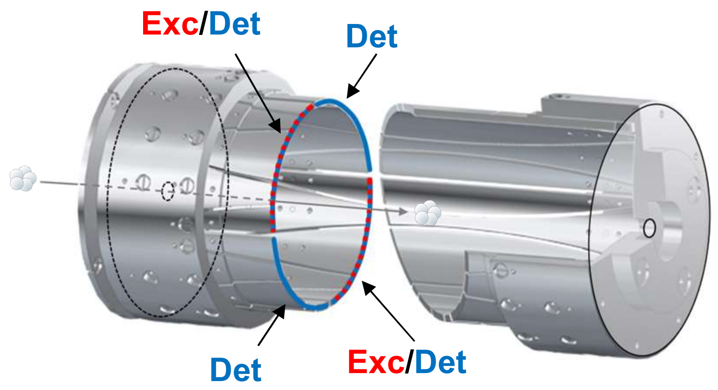
Standard 1ω detection methods

Now:

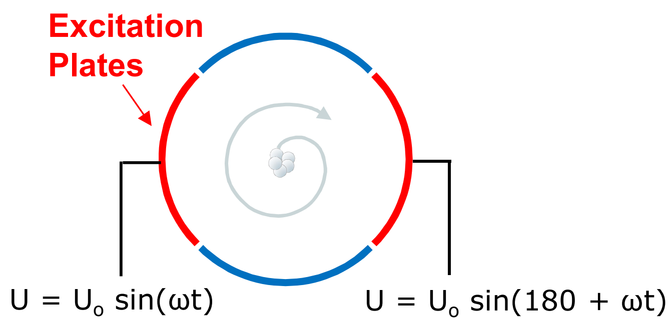
Switch to 2ω detection and its implementation

Signal Generation: Quadrupolar Detection

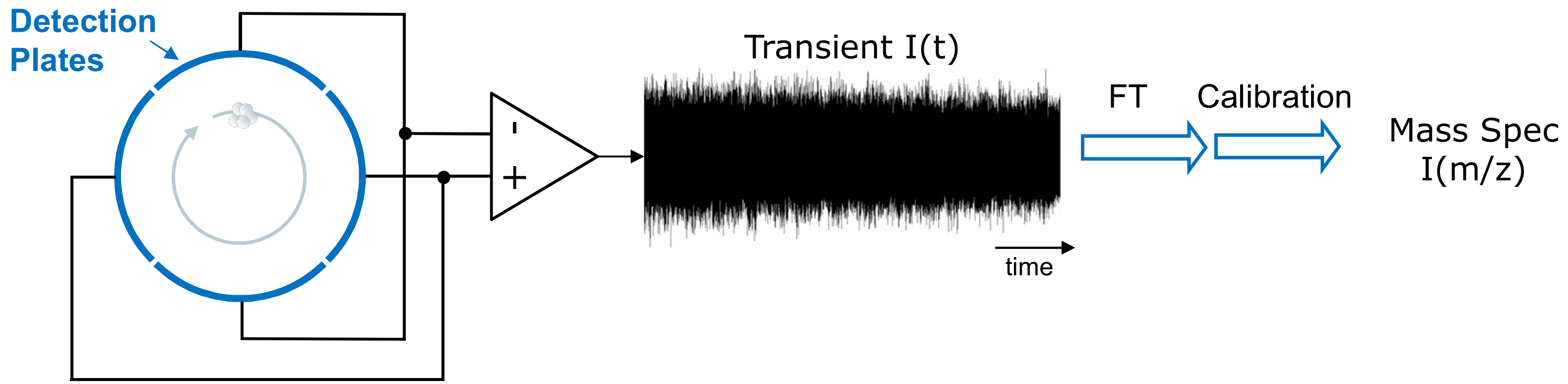
1) Trap Ions



2) Excitaton

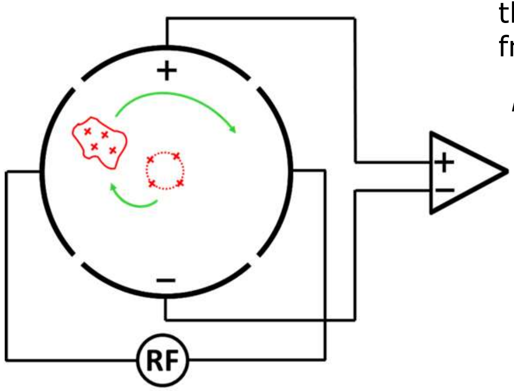


3) Quadrupolar Detection



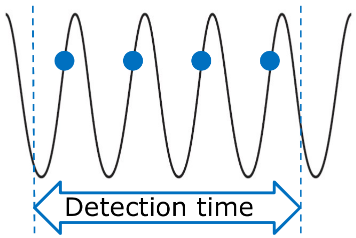
FT-ICR 1ω vs. 2ω Detection

Standard 1ω Dipole Detection



Direct detection of the cyclotron frequency ω_+

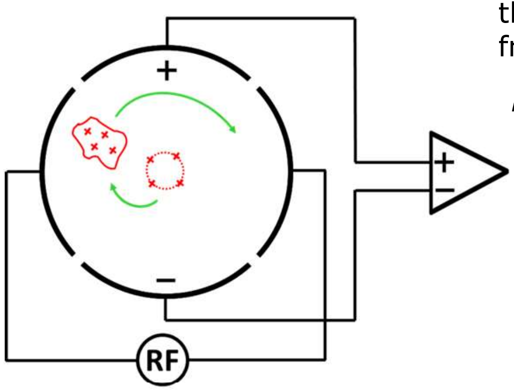
$$R_{Dipole} = \nu \cdot T$$



information

FT-ICR 1ω vs. 2ω Detection

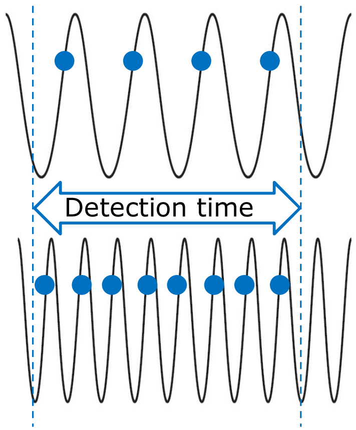
Standard 1ω Dipole Detection



Direct detection of the cyclotron frequency ω_+

$$R_{Dipole} = \nu \cdot T$$

xR detection

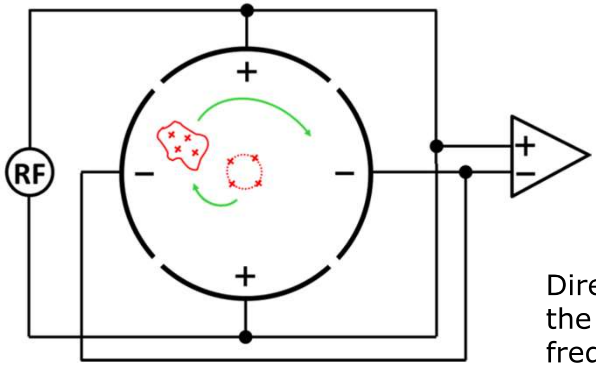


⇨ information

⇨ **double** information

double resolution
or
double detection speed

2ω Quadrupolar Detection (QPD)



Direct detection of the **double** cyclotron frequency $2\omega_+$

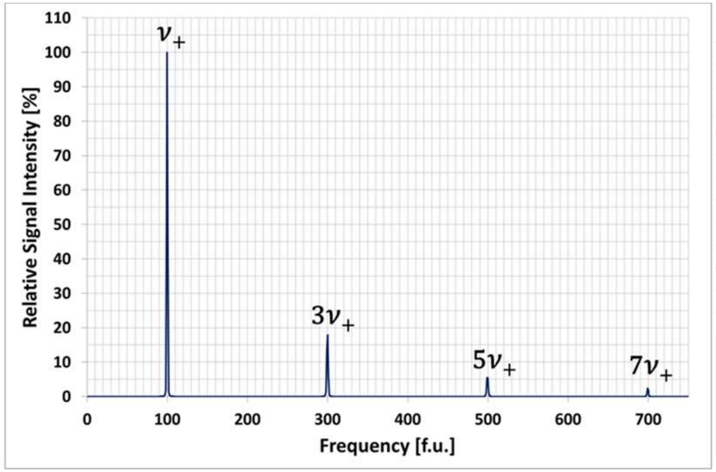
$$R_{QPD} = 2 \cdot \nu \cdot T = 2 \cdot R_{Dipole}$$

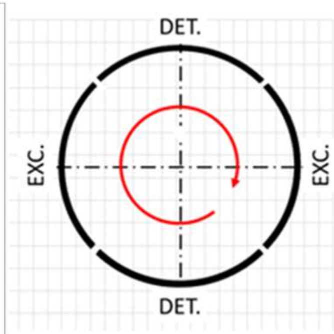
2xR

Ion cyclotron resonance signal-detection at multiples of the cyclotron frequency
E. N. Nikolaev, M. V. Gorshkov, A. V. Mordehai, V. L. Talrose
Soviet Union patent 1985, published 1990
Quadrupole-Detection FT-ICR Mass Spectrometry
L- Schweickhard, M. Lindinger, H.-J. Kluge, published 1990

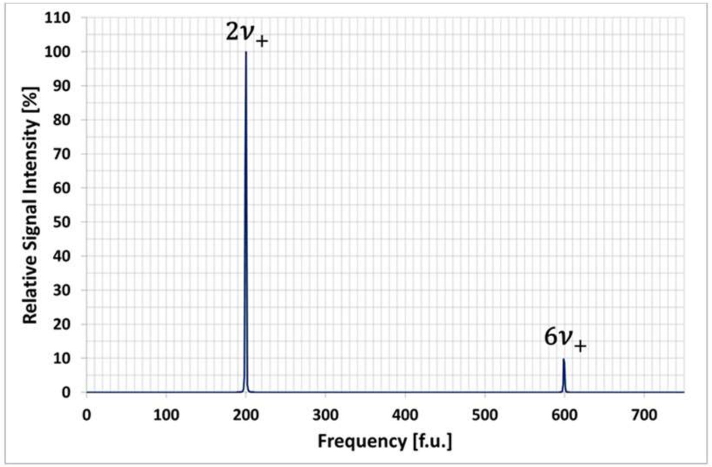
2ω Detection:
Harmonics – simulated spectra

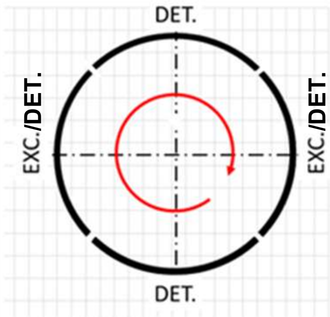
1ω Dipolar Detection





2ω Quadrupolar Detection





Pure cycloton motion
→ less harmonics $6\nu_+$ with good separation from main $2\nu_+$ signal

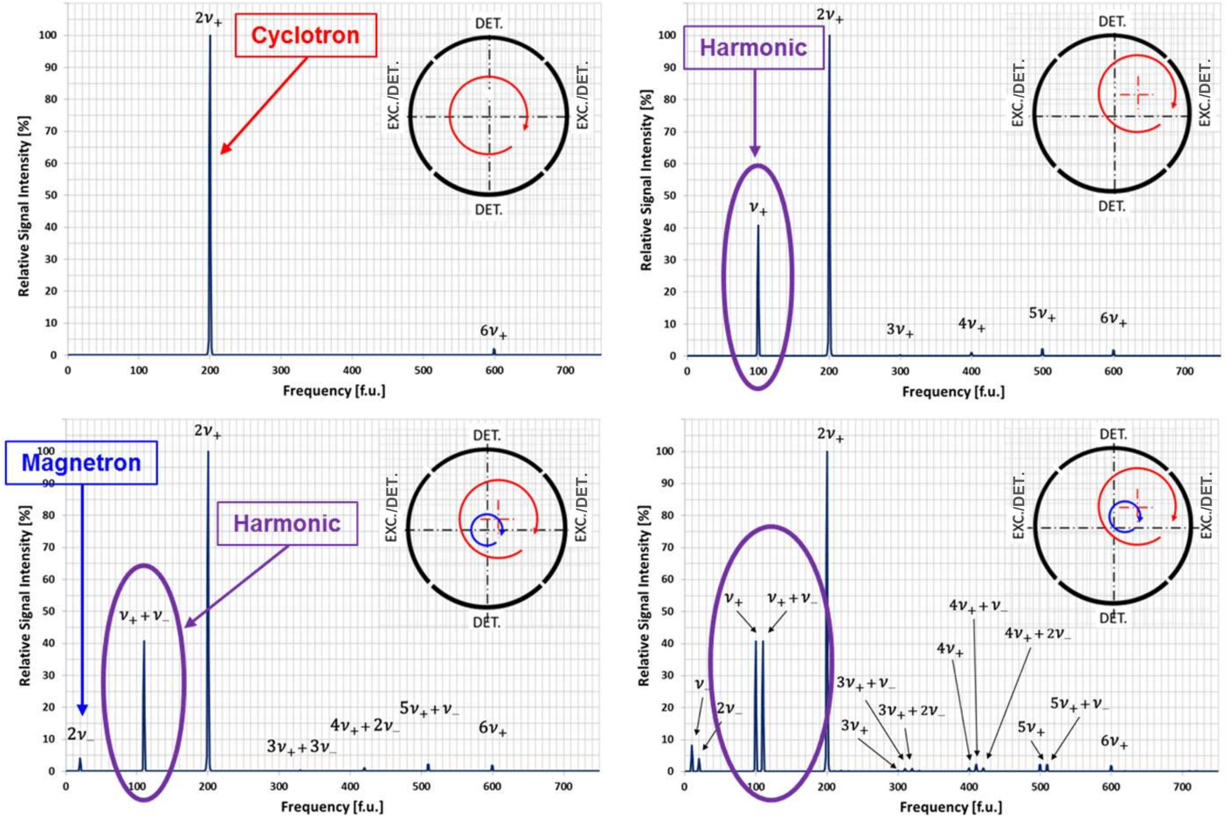
2ω Detection:
Harmonics – simulated spectra

→ Excessive **1ν harmonics** due to magnetron motion or off-center cyclotron motion.

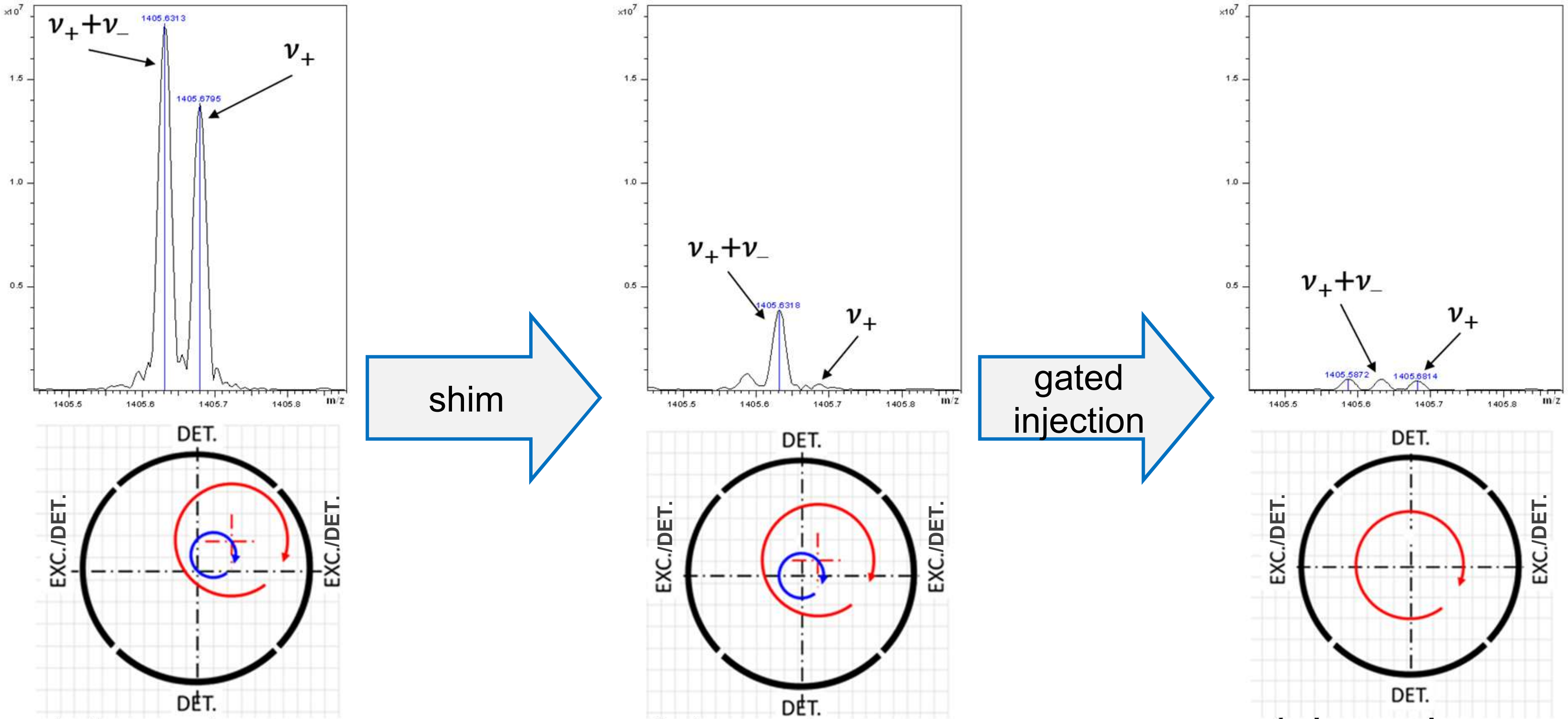
Goal: simple spectra

→ Control ion position in cell

→ control & reduce magnetron motion



2ω Detection:
Experimental minimization of harmonics



1ν harmonic group
14% / 11%
of $2\nu_+$ signal

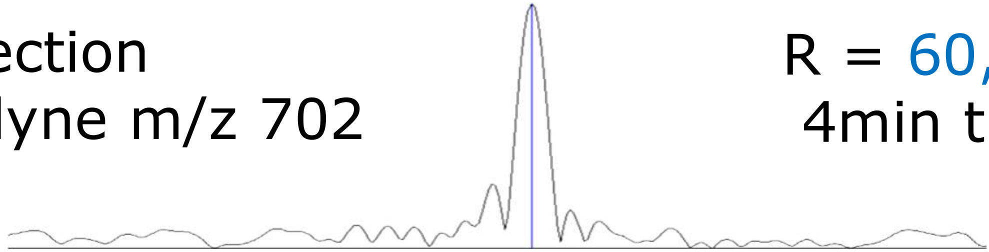
1ν harmonic group
3% / 0.2%
of $2\nu_+$ signal

1ν harmonic group
0.35% / 0.3%
of $2\nu_+$ signal

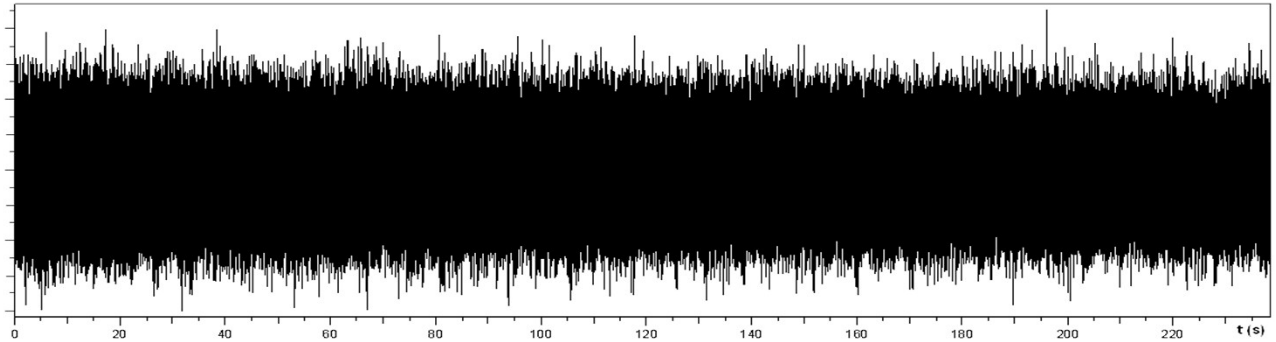
1ν harmonics group minimized → **2ω detection is now feasible** → **2xR ParaCell detector** → solarix 2xR scimaX

2xR Maximum Resolution – example (no spec)

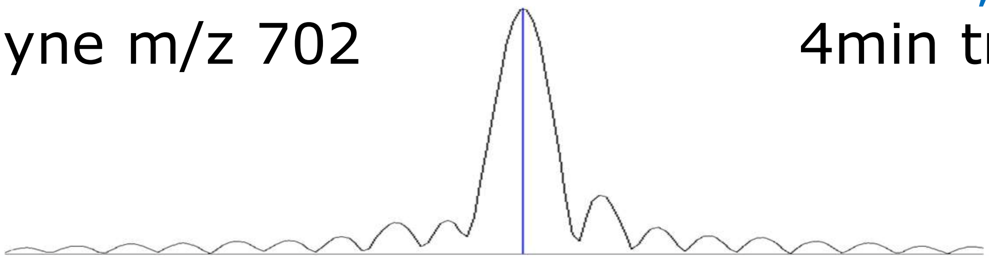
2ω detection
heterodyne m/z 702



R = 60,000,000
4min transient



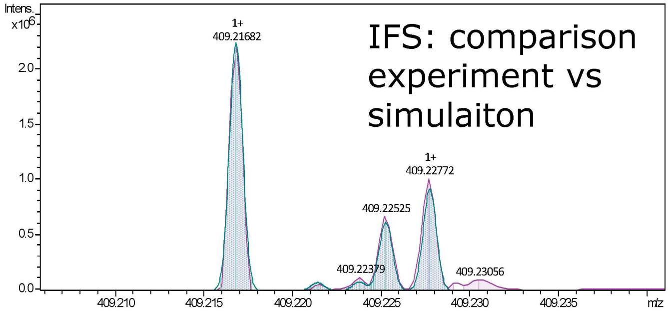
1ω detection
heterodyne m/z 702

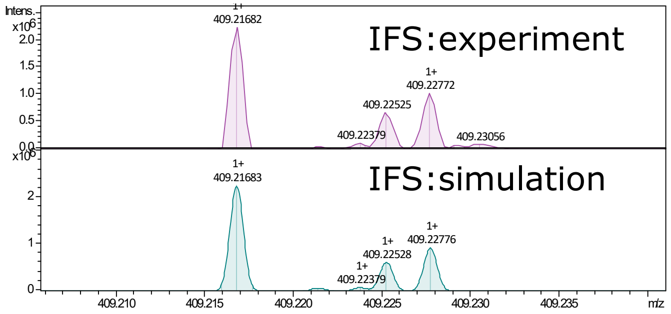


R = 30,000,000
4min transient

2xR Resolution per time – examples (no specs)

- Lincomycin – **1,03Hz** – Resolution 7T solariX **2xR** with AMP **470.000**





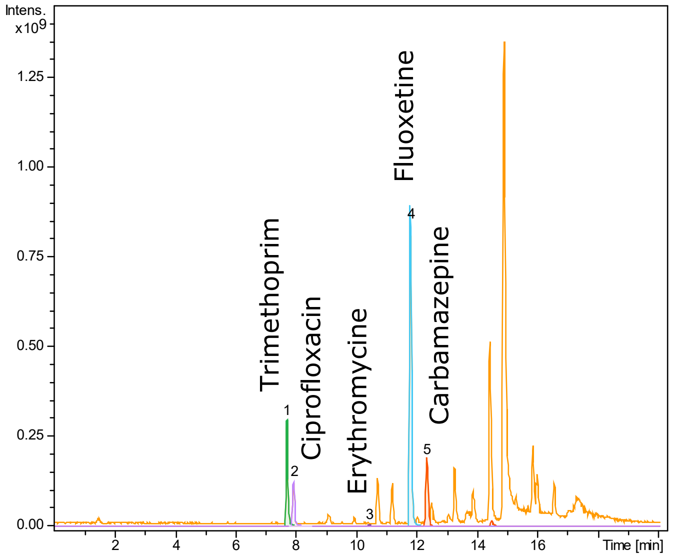
- Pesticide mix – **1Hz** – Resolution 7T solariX **2xR** with AMP **247.000** (m/z 746) **– 922.000** (m/z 200)

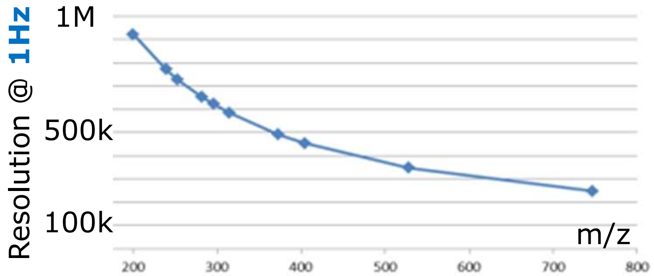
m/z [detected ion POS]	sum formula	name	resolution
200.1182239	C12H13N3	Pyrimethanil	922675
239.1502523	C11H18N4O2	Pirimicarb	772362
253.0309212	C10H9ClN4S	Thiacloprid	728045
282.1448326	C13H19N3O4	Pendimethalin	652673
296.116031	C14H18ClN3O2	Triadimenol I	622587
314.072275	C12H16N3O3PS	Triazophos	585518
372.9424183	C11H15BrClO3PS	Profenophos	492171
404.1240971	C22H17N3O5	Azoxystrobin	453690
528.0779887	C22H17ClF3N3O7	Indoxacarb	348608
746.4837738	C42H67NO10	Spinosad D	247808

LC/MS of pharma Mix

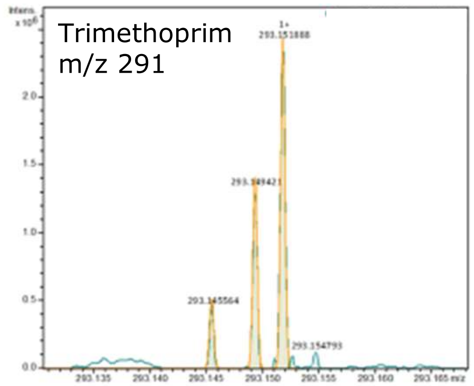
solarix 2xR measurement, 1 Hz, AMP

Multi step gradient H_2O/ACN with 0.1% formic acid, 300 µl/min,
Acquity UPLC HSS T3 2.1 x 150mm, 1.8 µm, 40° C

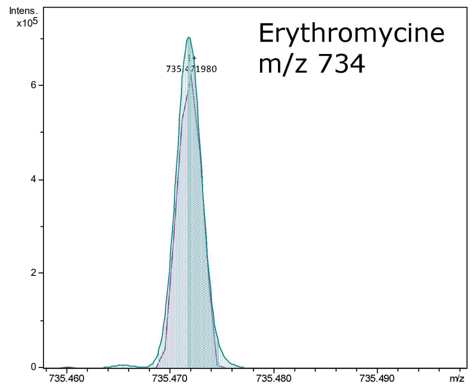




	Meas. m/z	Ion Formula	err [ppm]	mSigma	resolution
Carbamazpine	237.102262	C15H13N2O	-0.094	3.5	772383
Trimethoprim	291.145175	C14H19N4O3	-0.024	1.03	640949
Fluoxetine	310.141501	C17H19F3NO	-0.558	2.33	590874
Ciprofloxacin	332.140499	C17H19FN3O3	-0.003	7.13	568237
Erythromycine	734.46862	C37H68NO13	-0.182	25.8	258162



Good isotopic ratio if IFS resolved



Reduced isotopic fidelity if IFS not resolved

→ solarix 2xR enables **450k Resolution** at **1 Hz** (m/z 400)

→ Good isotopic ratios if **IFS** is resolved

Agenda

- **Part 1:** Mass measurement and **I**sotopic **F**ine **S**tructure (**IFS**)
- **Part 2:** Mass Spectrometry techniques and MRMS evolution
- **Part 3:** 1ω and 2ω spectra – harmonics detection
- **Part 4:** Applications

MRMS- The Solutions

Metabolomics & Phenomics

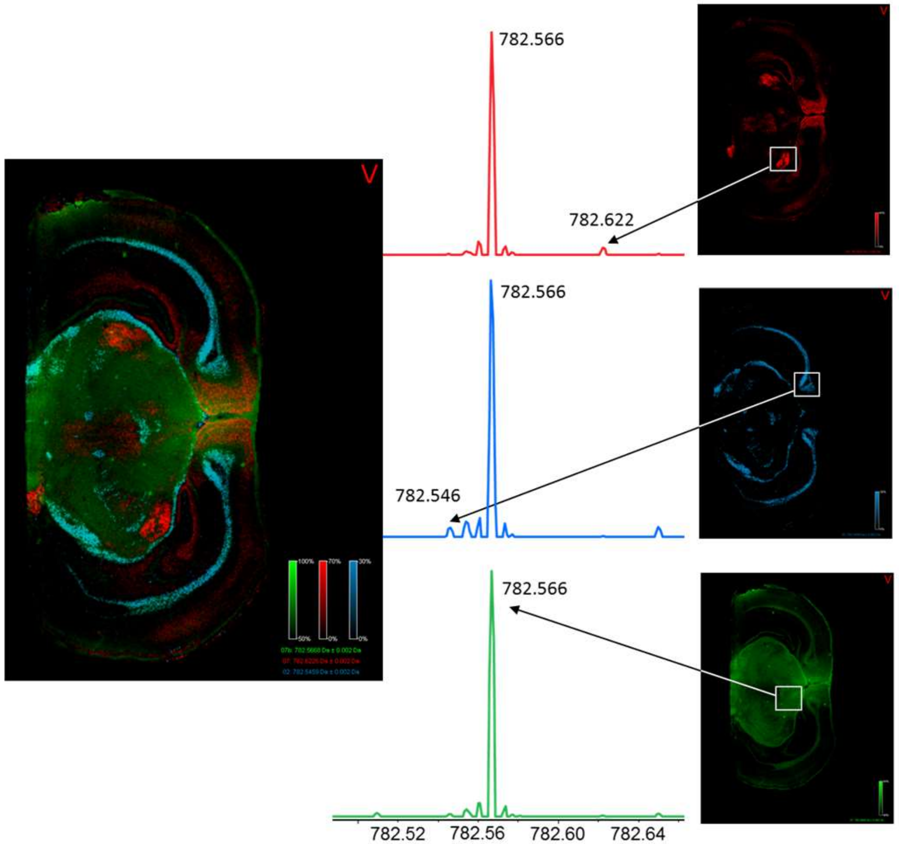
MALDI Imaging

Petroleomics

Protein Analysis

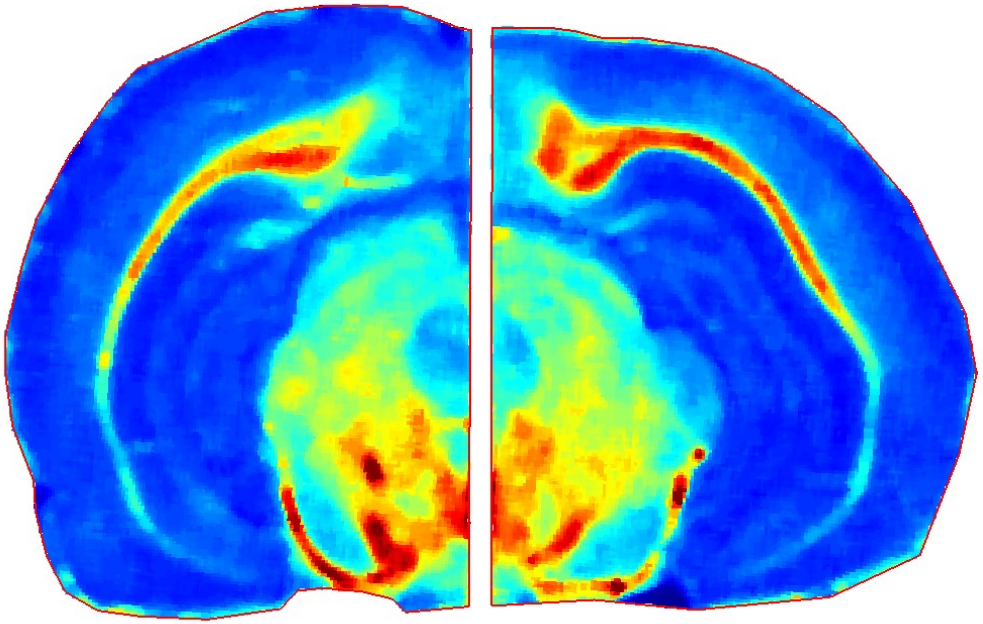
MALDI imaging
solarix 2xR measurement, 1 Hz, Mouse Brain

- 56,000-pixel MALDI imaging
- mouse brain sample raster width 30µm
- CASI or m/z 760 with a 120 Da window
- Acquired in 15h with a scan speed of ~1Hz.
- resolving power 300,000 at *m/z* 800



Imaging of rat brain

2xR detector
50 µm lateral resolution
RP 820.000 @ m/z 273
22123 pixel
6 h 40 min min
> 0.9 Hz



m/z 788.616 (PC 36:1 H^+)

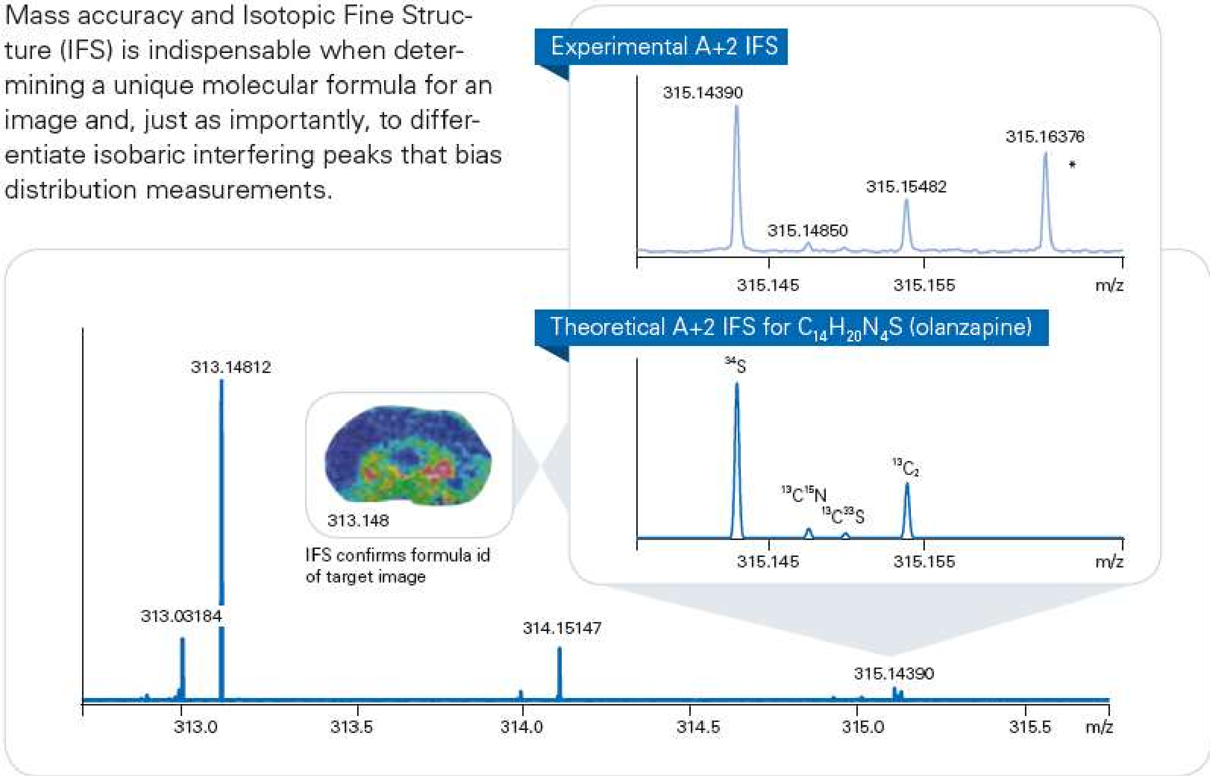
XR detector
50 µm lateral resolution
RP 790.000 @ m/z 273
21039 pixel
10 h 40 min
> 0.5Hz

scimaX MALDI imaging

scimaX is the ultimate MALDI imaging system for analyzing small to medium molecules, m/z 100-1500

- unrivaled eXtreme Resolution capability
- sub-ppm mass accuracy over a wide mass range
- can differentiate images that are only mDa apart
- prerequisite for IFS analysis and formula confirmation

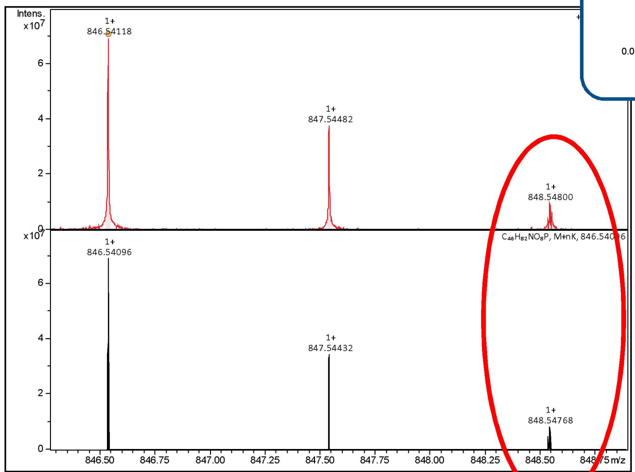
Mass accuracy and Isotopic Fine Structure (IFS) is indispensable when determining a unique molecular formula for an image and, just as importantly, to differentiate isobaric interfering peaks that bias distribution measurements.

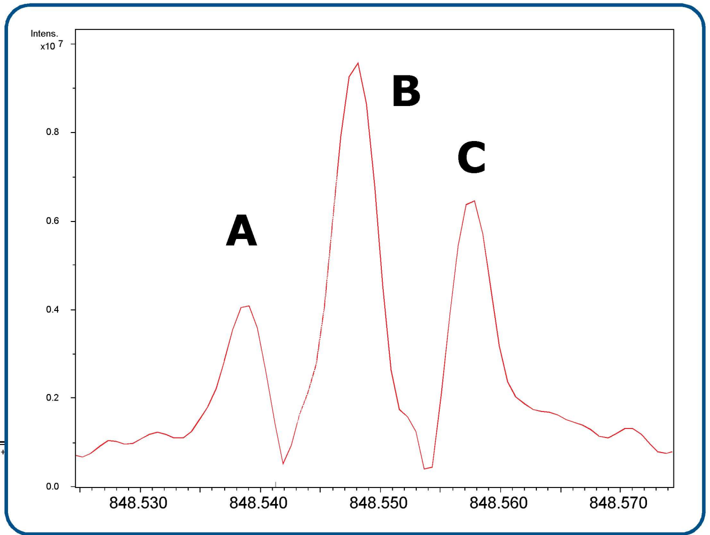


* Interfering ion

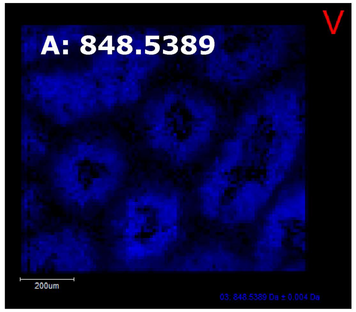
scimaX - The power …

… to find the needle in the haystack

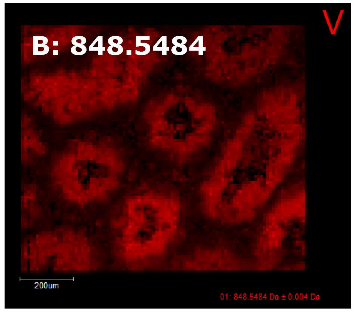




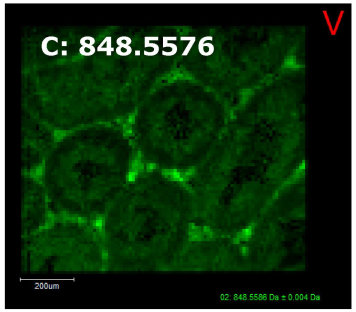
RP ~200k
@ m/z 850
@ imaging speed



PC(38:5) $^{13}C_2$ + $^{39}K^+$



PC(38:5) + $^{41}K^+$



PC(38:4) + $^{39}K^+$

scimaX - The best system…

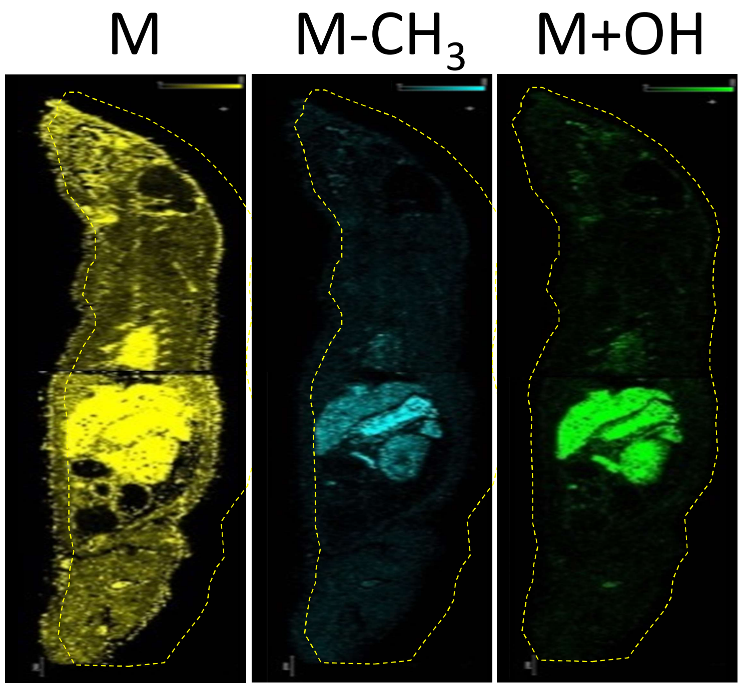
BRUKER

… for small molecule imaging

- Bridge the gap between LC-MS and radiolabeling for drug ADME/T
- Reveal greater insight into metabolic pathways
- Unravel PK and discover new markers

Steve Castellino, Head of US Ex Vivo Imaging and Senior GSK Fellow

"MALDI-MS Imaging fills an analytical void by permitting us to discretely examine the distribution of parent drug and metabolites in tissues. We have been able to achieve the spatial and spectral resolution required to examine sub-compartment tissue distributions and correlate them with histology in the preclinical setting. This ability to link chemistry and biology is permitting us to more closely examine the basis of drug toxicity and pharmacology as well as refine our understanding of pharmacokinetics and drug transport."

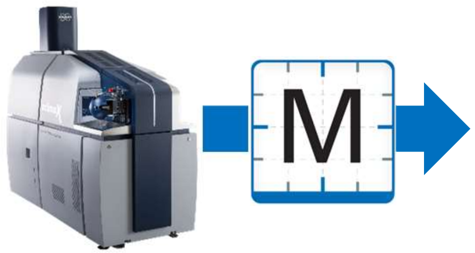


Locate, identify & quantify in a single measurement

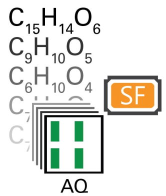
MRMS aXelerate

scimaX

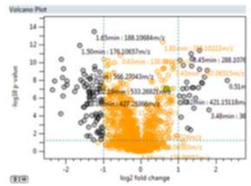
High throughput Phenomics research for everyone…



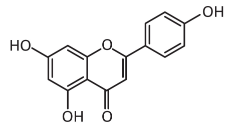
T-ReX 2D
Feature extraction



Smart Formula



Statistical Analysis



Putative Structure
Annotations

- **Accelerate** throughput (> 200 samples/day)
- **Complementary to** established **NMR** based solutions.
- **Simultaneous analysis** of known and unknown metabolites
- **Access compounds** not readily detectable by LC-MS analysis
- **3-tiered confidence** in identification

*"**MRMS** eXtreme Resolution enables us to address next generation metabotyping, i.e. simultaneous rapid description of **hundreds of known and thousands of new metabolites** relevant for dynamic biological/chemical processes."*

Prof. Philippe Schmitt-Kopplin
Analytical BioGeoChemistry,
Helmholtz Zentrum München, Germany

MRMS aXelerate

scimaX

MRMS aXelerate

High information content across a wide dynamic range

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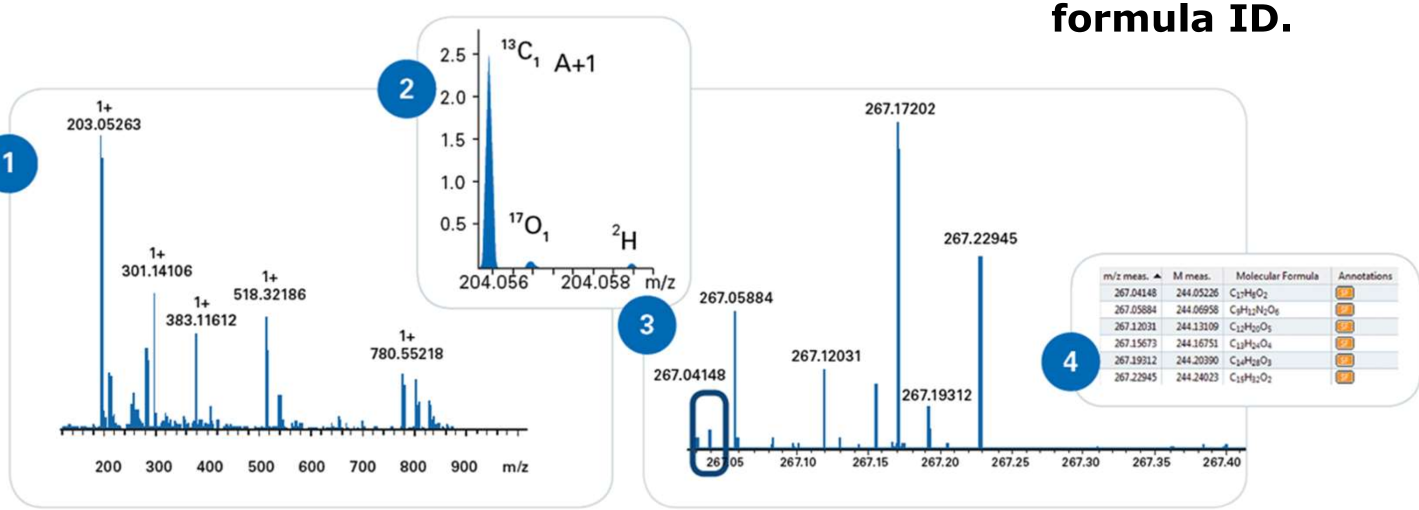
1 **Compound confidently annotated** as: $C_6H_{12}O_6Na$
mass accuracy: 0.09 ppm
RP: 1,500,000

Note: Such hexose sugars are not well retained on reversed phase LC-MS and difficult to detect.

2 Expanded A+1 region of $C_6H_{12}O_6Na$ reveals Isotopic Fine Structure **substantiating formula ID.**



m/z meas.	M meas.	Molecular Formula	Annotations
267.04148	244.05226	$C_{17}H_8O_2$	
267.05884	244.06958	$C_9H_{12}N_2O_6$	
267.12031	244.13109	$C_{12}H_{20}O_5$	
267.15673	244.16751	$C_{13}H_{24}O_4$	
267.19312	244.20390	$C_{14}H_{28}O_3$	
267.22945	244.24023	$C_{15}H_{32}O_2$	

Example of information derived from a **single** spectrum
obtained by FIA-MRMS of human plasma extract

3 Low intensity Ion vs. highest abundant peak demonstrates > 3 order dynamic range.

4 Mass zoom: **0.40 Da mass region** shows the richness of information in FIA-MRMS data: **6 species annotated**.

MRMS aXelerate

MRMS aXelerate

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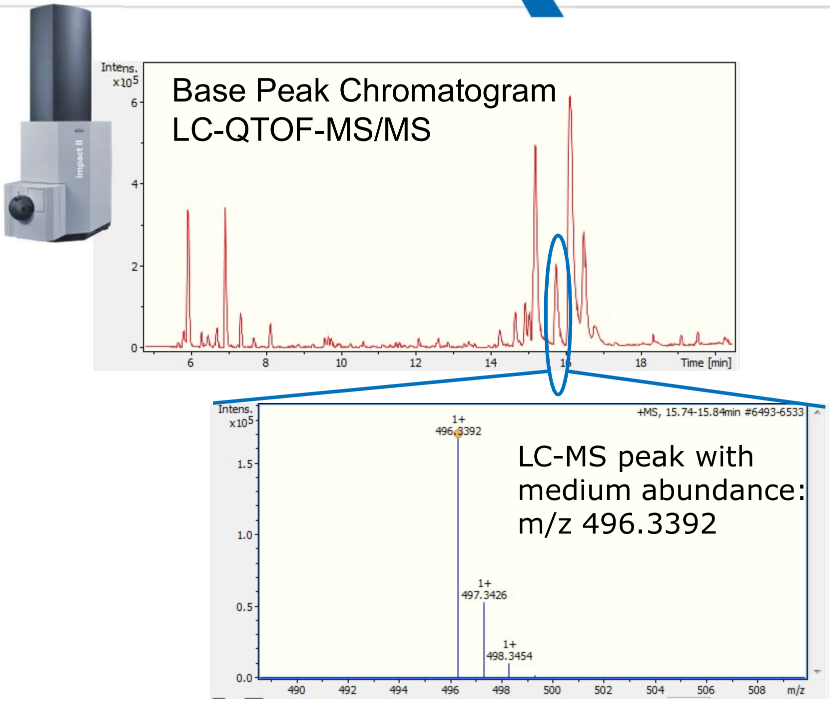
Metabolomics: LC-QTOF-MS vs. FIA-MRMS - example

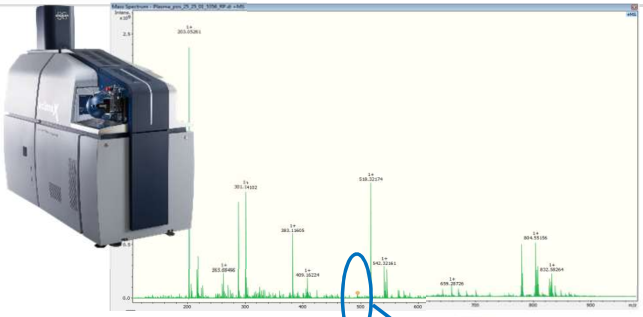
commercially available Plasma Extract (Sigma Aldrich)

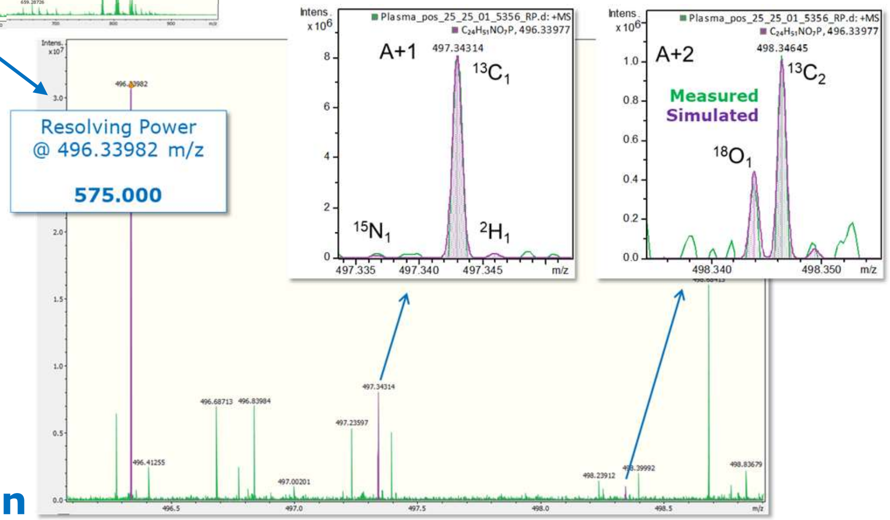


Measured m/z 496.3392 Tolerance: 2 ppm Charge: 1

Meas. m/z	#	Ion Formula	m/z	err [ppm]	err [mDa]	mSigma	# mSigma	Score	rdb	e⁻ Conf
496.3392	1	$C_{28}H_{53}NP_3$	496.3385	-1.4	-0.7	7.8	1	93.58	5.0	even
496.3392	2	$C_{24}H_{51}NO_7P$	496.3398	1.1	0.5	22.9	2	100.00	1.0	even

LC-QTOF-MS: ~25 min turnover time





unambiguous formula generation for unknowns

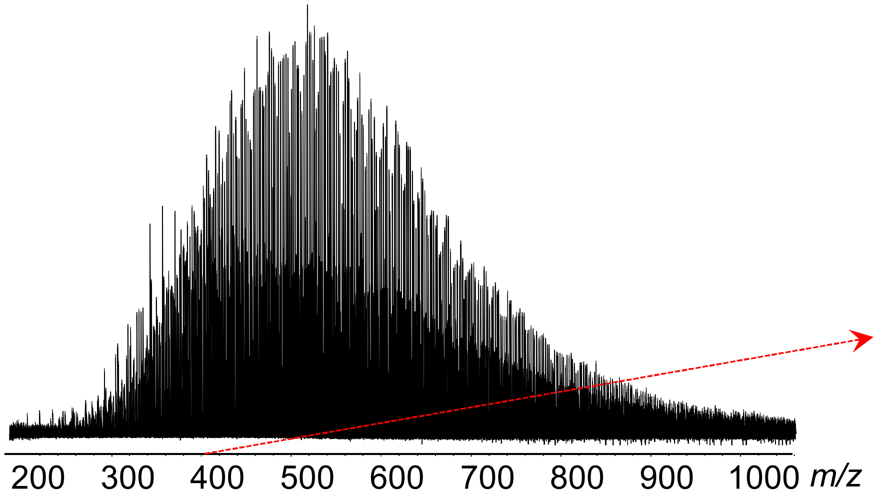
Measured m/z 496.33982 Tolerance: 0.3 ppm Charge: 1

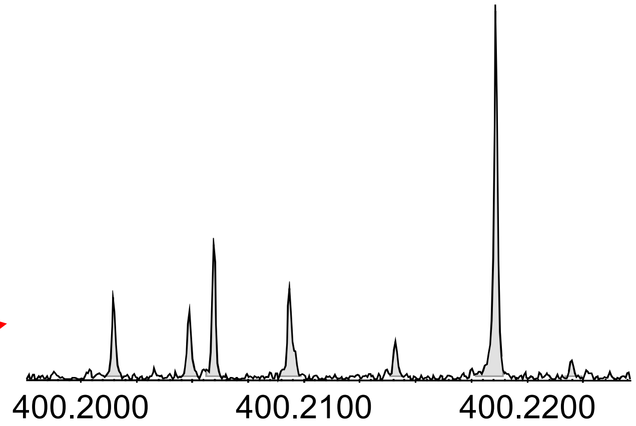
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
496.33982	1	$C_{24}H_{51}NO_7P$	100.00	496.33977	-0.10	-0.03	6.6	1.0	even	ok

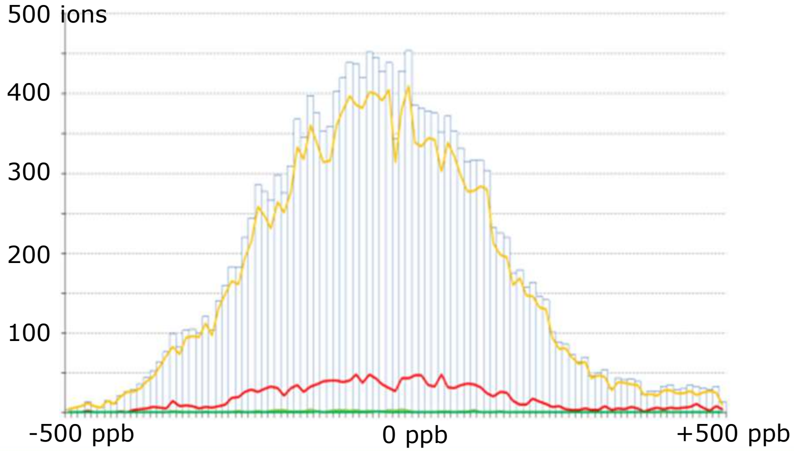
FIA-MRMS (single spectrum): ~2.5 min turnover time

Petroleomics

solarix 2xR, 7T, AMP, APPI, Oil Residue, m/z 250-800







Resolution (m/z 400): **1,950,000**

Mass accuracy: **-20 ± 168 ppb**

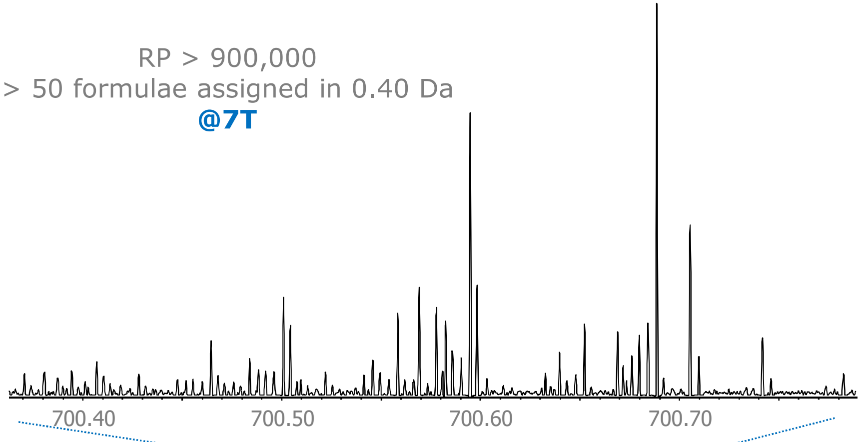
Ions: **18200**

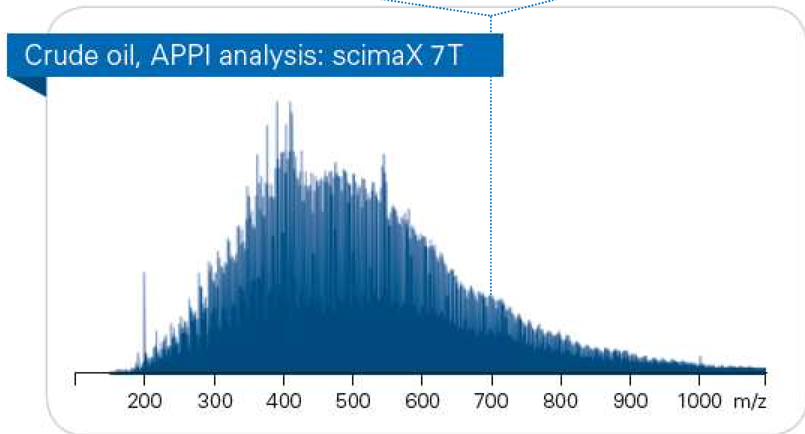
m/z	Calc. Res.
300	2368970
400	1950080
500	1600250
600	1313480
700	1083770
800	905120
900	771530
1000	677000

scimaX The industrial standard for Petroleomics

Molecular management

- Prediction of bulk properties (TAN, corrosion, fouling) requires seeing the complete chemical space of a sample
- powered by 2xR technology, scimaX matches the resolving power of many conventional high field MRMS
- high field systems are no longer mandatory for crude oils, bio-fuels, DOM, or any complex mixture



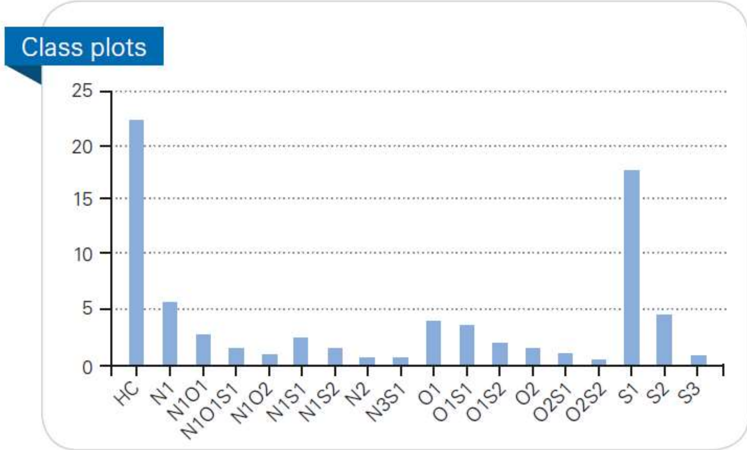


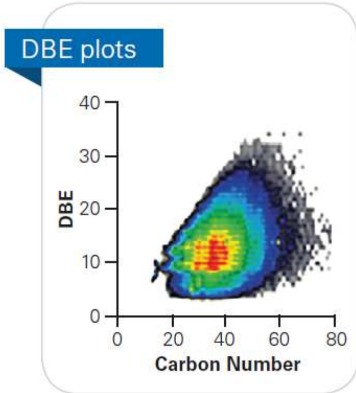
C2MC – Complex Matrices Molecular Characterization, Joint Laboratory
Carlos Afonso, University of Rouen
Pierre Giusti, TOTAL

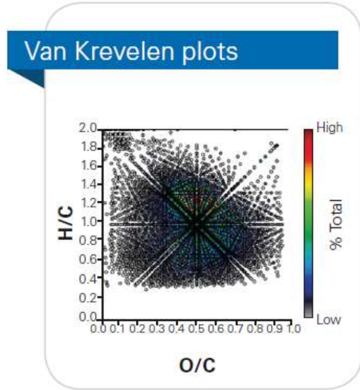
"With our Bruker MRMS in Rouen the analysis of highly Complex Mixtures has been pushed further than ever and could also be made on a routine basis in the framework of the C2MC joint lab".

Versatile and Complete Solution

- scima**X** data can be imported to Petroleomics software (PetroOrg/Composer)
- The software generates reliable elemental composition assignment, classic Petroleomic diagrams, automated report construction, and much more based on accurate mass measurement.
- scimaX provides the widest array of compatible ionization sources to access different molecule species:
  - ESI for basic and acidic compounds;
  - LDI and optional APCI, APPI to access polar and non-polar compounds





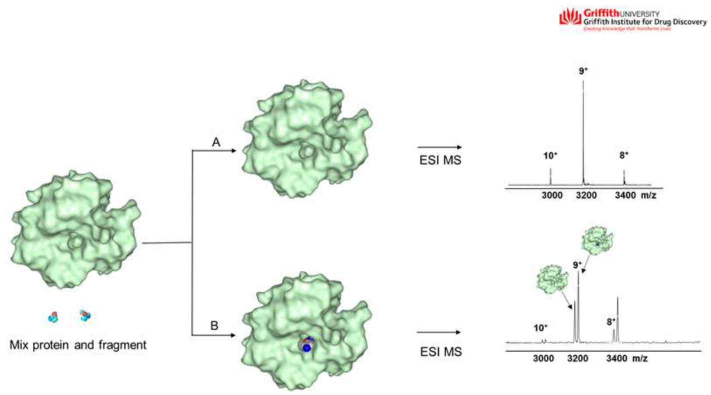


scimaX Protein Analysis

Scientific literature states that Bruker MRMS is a “bona-fide” platform for native protein work.

It is unmatched for top-down native protein MS analysis and for preserving complex biomolecular interactions at ultra high resolution

- Only instrument to offer high resolution from 100 – 10,000 m/z
- Easily interfaces to a wide variety of commercial and custom ion sources
- Bruker MRMS ion source leaves most fragile non-covalent interactions intact
- The ultimate companion for FBDD – eliminate your false positives



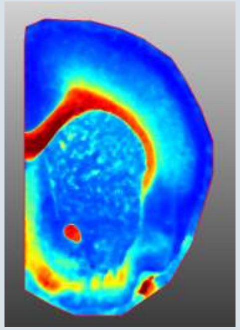
Weak binding (Kd>10 uM) interactions typical in fragment based drug design (FBDD) are routinely preserved and observed by MRMS.

MRMS

Confidence and Power for Applications

- **Provides** unmatched e**X**treme **R**esolution and mass accuracy
- **Enables** routine **I**sotopic **F**ine **S**tructure (**IFS**) analysis for a broad mass range
- **Results** in unmatched confidence for compound identification

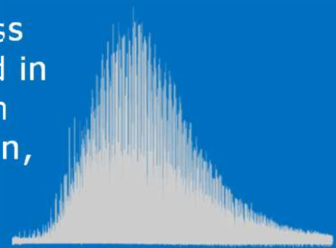
MALDI Imaging



Label-free MALDI imaging maps the localization of drugs and metabolites, providing spatial correlation with ‘omics studies

Petroleomics

Exact chemical class information can aid in solving problems in petroleum collection, processing, and transport

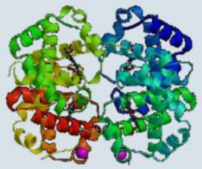


Small Molecules

Flow Injection Analysis (FIA) MRMS workflows accelerate sample throughput and increase data depth in Phenomics research

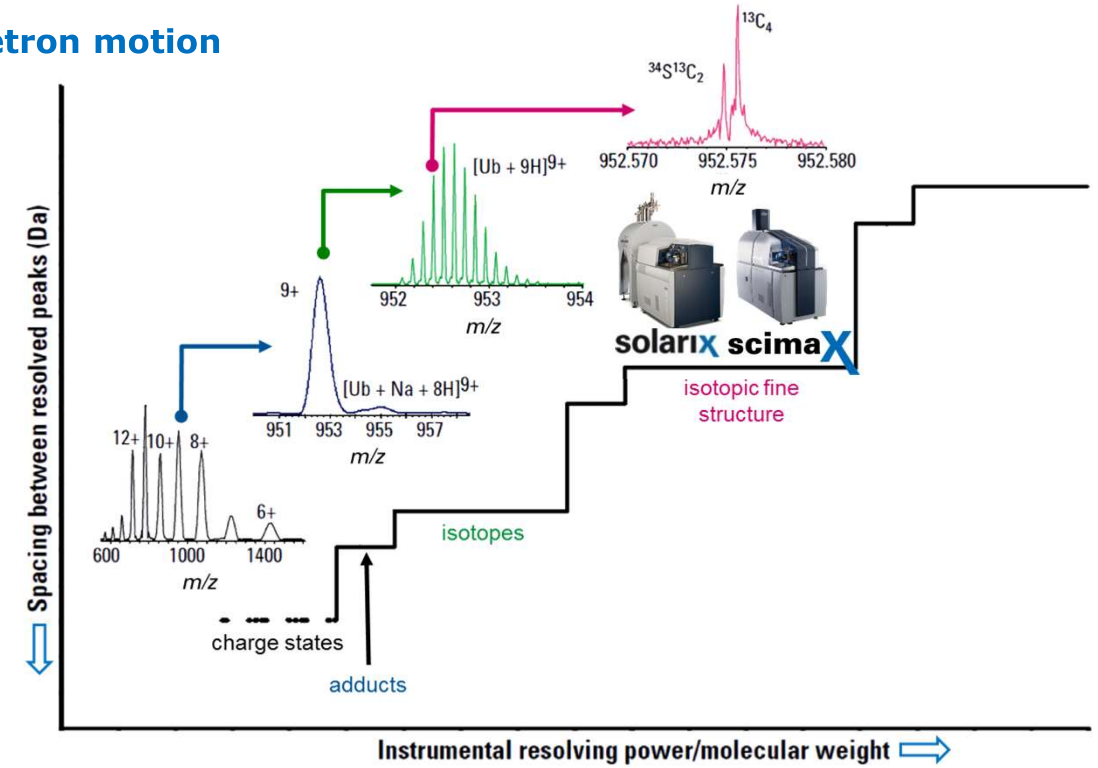
Intact Biomolecules

Large intact biomolecules can be analyzed for applications in proteomics, biopharmaceutical analysis, and protein science



Summary

- **Isotopic Fine Structure** reveals detailed information on the analytes composition and enables **confident results**
- **IFS** analyses requires **MRMS**: resolving power **> 500.000** over a broad mass range and **sub-ppm** mass accuracy
- Routine high resolution analyses require **understanding** and **control** of **magnetron motion**
- Shimming and gated injection **minimize magnetron motion**
- Mass spec evolution step to **routine IFS analysis** was already done
- Application to **2ω detection** allows for further increase in **resolving power** or **speed**
- **2ω detection** capability enhances **MALDI imaging, LC/MS** and **Petroleomics** applications



2xR enables

fast AND confident results

Thanks

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