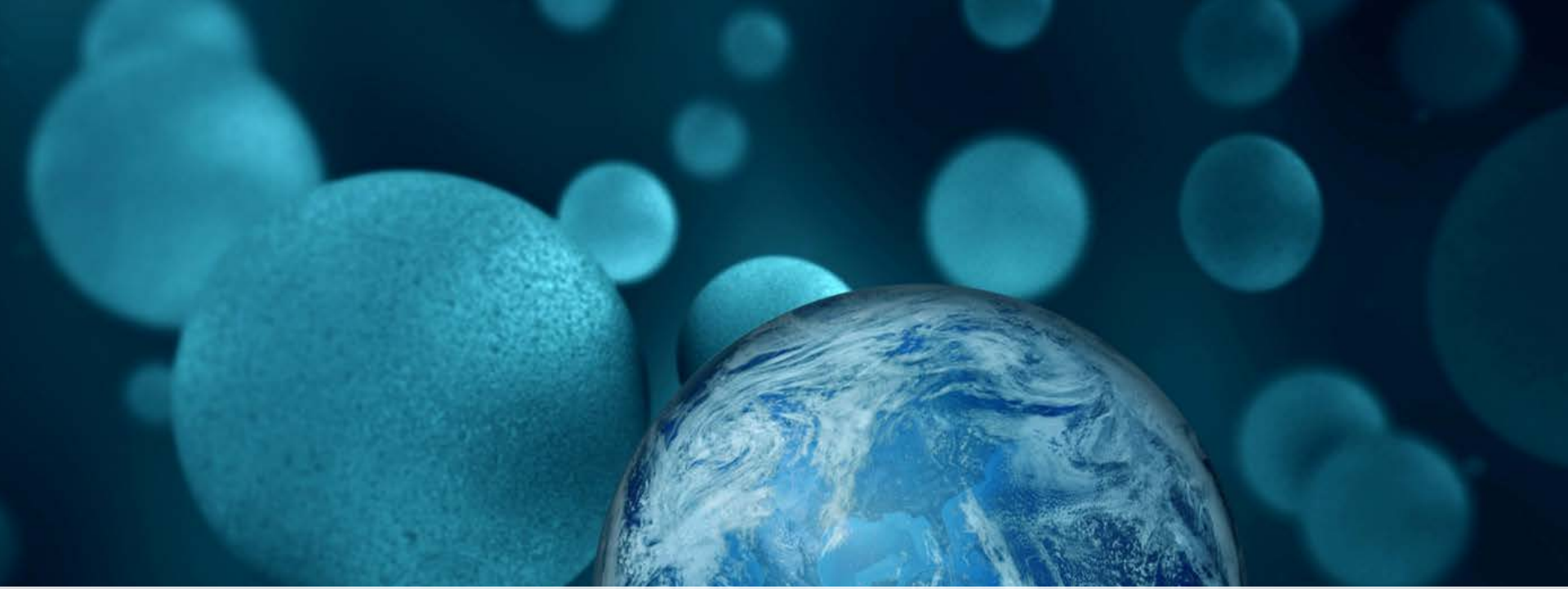

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Orbitrap-based HRAM Workflows for Next Generation Contaminants Screening

GOH Lin-Tang, PhD

Senior Manager (SEA), Mass Spectrometry

Introduction

- **Food Safety**

  Ensuring that food is free from microbiological or chemical contaminants/residues that might cause harm to human health

- **Food Security**

  Ensuring a plentiful supply of safe food, energy and nutritional needs are met, at the global, national and household level

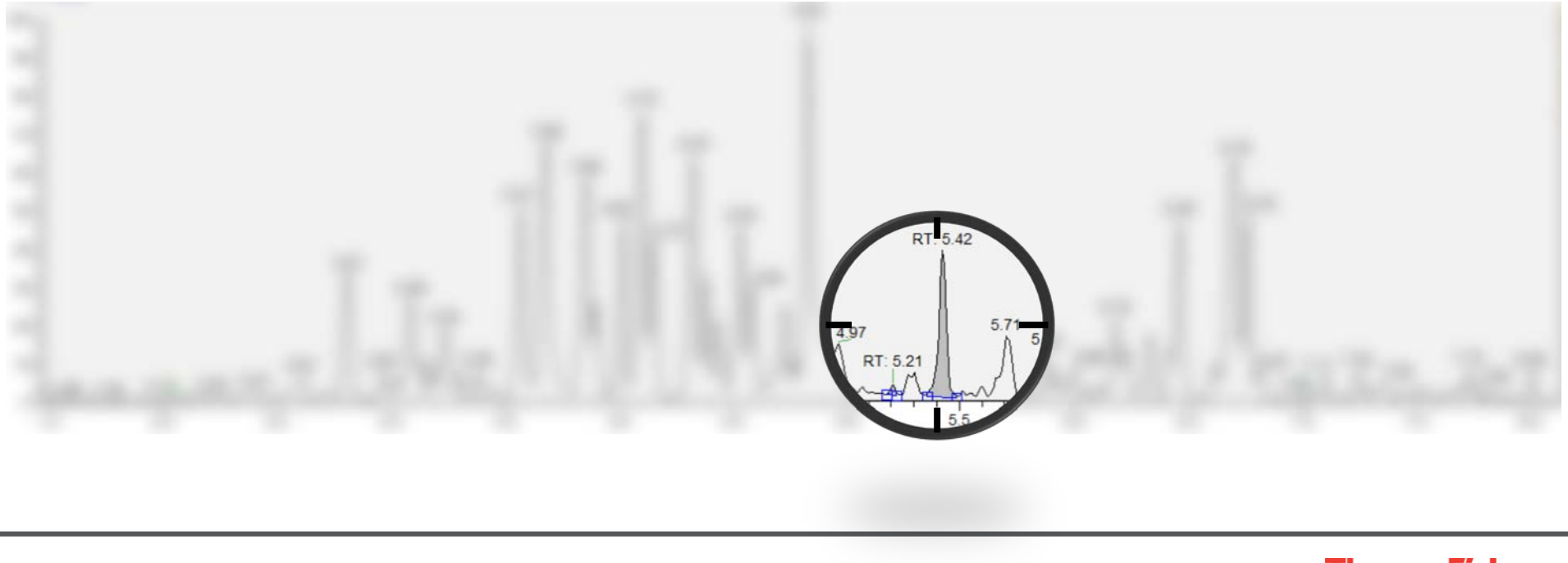
- **Food Fraud**

  Deliberate adulteration of food to deceive consumers usually for financial gain. Such act may not have food safety implications however most adulteration cases invariably involve addition of illegal substances to foods.

Screening Contaminants

Target screening is an excellent tool

- **+ High throughput, high sensitivity**
- **+ Easy to use**



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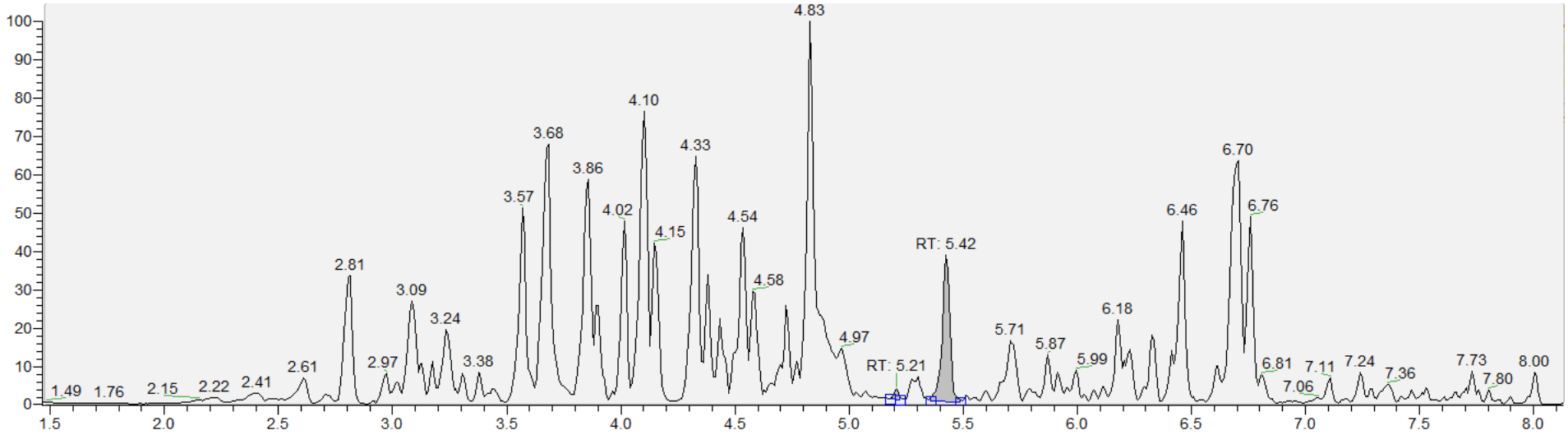
What about Everything Else?

Targeted analysis has its limits… its targeted

How do we detect all the other contaminants in a sample?

Which mass spectrometry platform technology to use?



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Benefits of HRAM Screening

- Capable of global analysis of sample
- Multiple target contaminants can be included and screened at high specificity
- Other compounds within specified mass range can be screened
- Detected masses can be identified via HRAM libraries, without standards – providing putative IDs
- Detected compounds can be quantified accurately

Current Thermo Scientific Product Portfolio

LTQ Velos Pro

LTQ XL

Ion Trap

TSQ Quantiva

TSQ Endura

Triple Quadrupole

Tribrid Orbitrap

Orbitrap Fusion

Orbitrap Fusion Lumos

Orbitrap Elite

QE Focus, QE
QE Plus, QE HF

LTQ Orbitrap XL

Hybrid Orbitrap

Exactive Plus
(EMR version)

Exactive Portfolio

2000: The Principle of Orbitrap Mass Analyzer

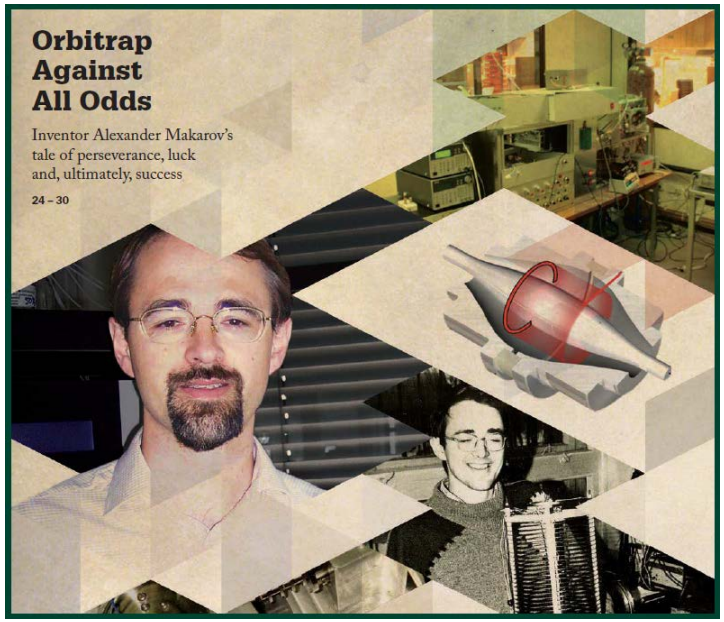
Anal. Chem. **2000,** *72,* 1156−1162

Electrostatic Axially Harmonic Orbital Trapping: A High-Performance Technique of Mass Analysis

Alexander Makarov*

HD Technologies Ltd., Atlas House, Simonsway, Manchester, M22 5PP, U.K.

This work describes a new type of mass analyzer which employs trapping in an electrostatic field. The potential distribution of the field can be represented as a combination of quadrupole and logarithmic potentials. In the absence of any magnetic or rf fields, ion stability is achieved only due to ions orbiting around an axial electrode. Orbiting ions also perform harmonic oscillations along the electrode with frequency proportional to $(m/z)^{-1/2}$. These oscillations are detected using image current detection and are transformed into mass spectra using fast FT, similarly to FT ICR. Practical aspects of the trap design are presented. High-mass resolution up to 150 000 for ions produced by laser ablation has been demonstrated, along with high-energy acceptance and wide mass range.



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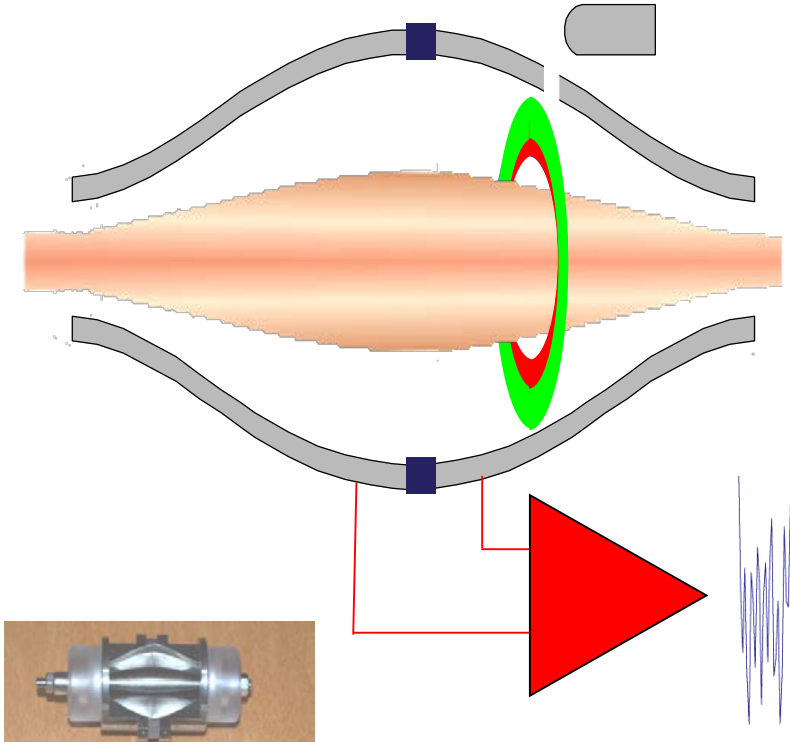
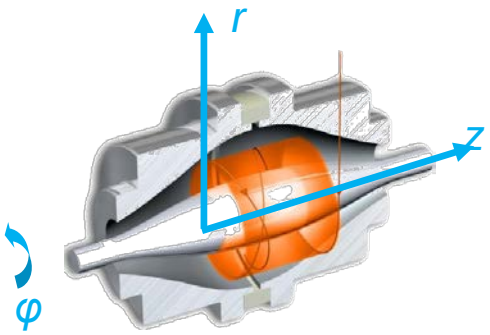
Orbitrap Mass Analyzer: Principle of Operation



$$\omega_z = \sqrt{\frac{k}{m/q}}$$



Hyper-logarithmic potential distribution: "ideal Kingdon trap"

$$U(r,z) = \frac{k}{2} \cdot \left\{ z^2 - r^2/2 + R_m^2 \cdot \ln(r/R_m) \right\}$$

- Characteristic frequencies:
  - Frequency of rotation ω_φ
  - Frequency of radial oscillations ω_r
  - Frequency of axial oscillations ω_z

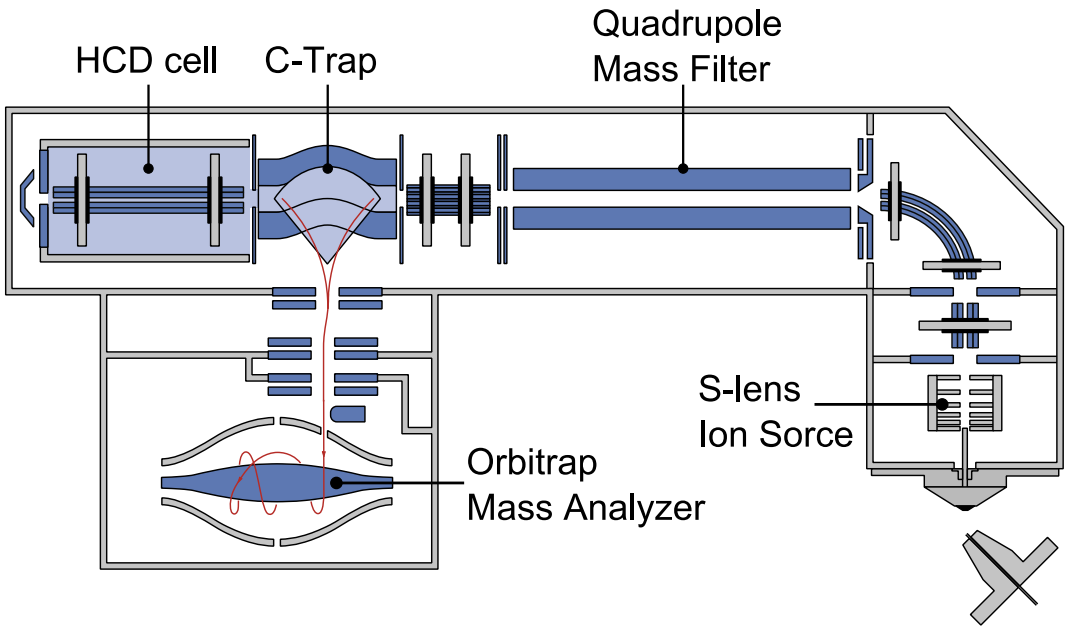
CONCLUSIONS

These results show that the orbitrap is a new and effective mass spectrometer which could potentially find its own unique niche. With mass resolution surpassed only by FT ICR, the orbitrap has the advantage of a much simpler and compact design.

To become useful for the main stream of mass spectrometric analysis, the orbitrap requires external collisional cooling and possibly external ion accumulation. These goals become the main priorities of further development work.

Makarov A. *Anal. Chem.* 2000, *72*, 1156-1162.

Schematic of Quadrupole-Orbitrap HRAM System



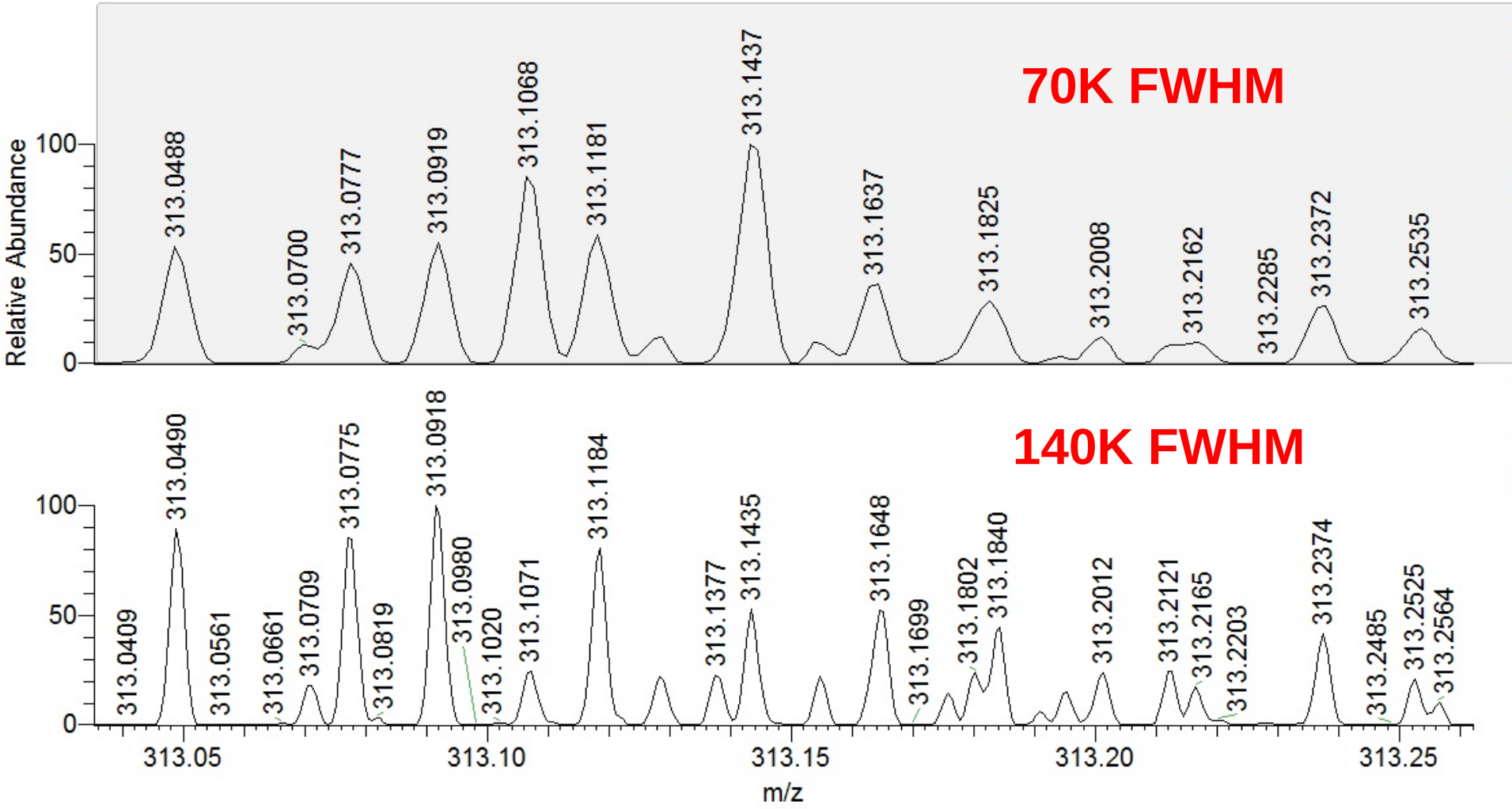
J.-P. Hauschild; U. Froehlich; O. Lange; A. Makarov; E. Damoc; S. Kanngiesser; F. Czemper; C. Crone; Y. Xuan; M. Kellmann; A. Wieghaus. „Performance Investigation of an Orbitrap Mass Analyzer Combined with a Quadrupole Mass Filter", Proc. 59th Conf. Amer. Soc. Mass Spectrom., Denver June 5-9, 2011.

HCD

- Quad-(C-Trap)-Orbitrap platform
- HCD cell enables MS/MS
- Predictive automatic gain control (pAGC) and parallel filling & detection
- Improved targeted MSMS duty cycle by spectrum multiplexing
- High mass resolution measurements (up to 240K FWHM) leads to sub-ppm mass accuracy

Mass Resolution: The Most Direct Approach to Deal with Complexity

Protonated AFB1: $C_{17}H_{13}O_6$; m/z = 313.071215



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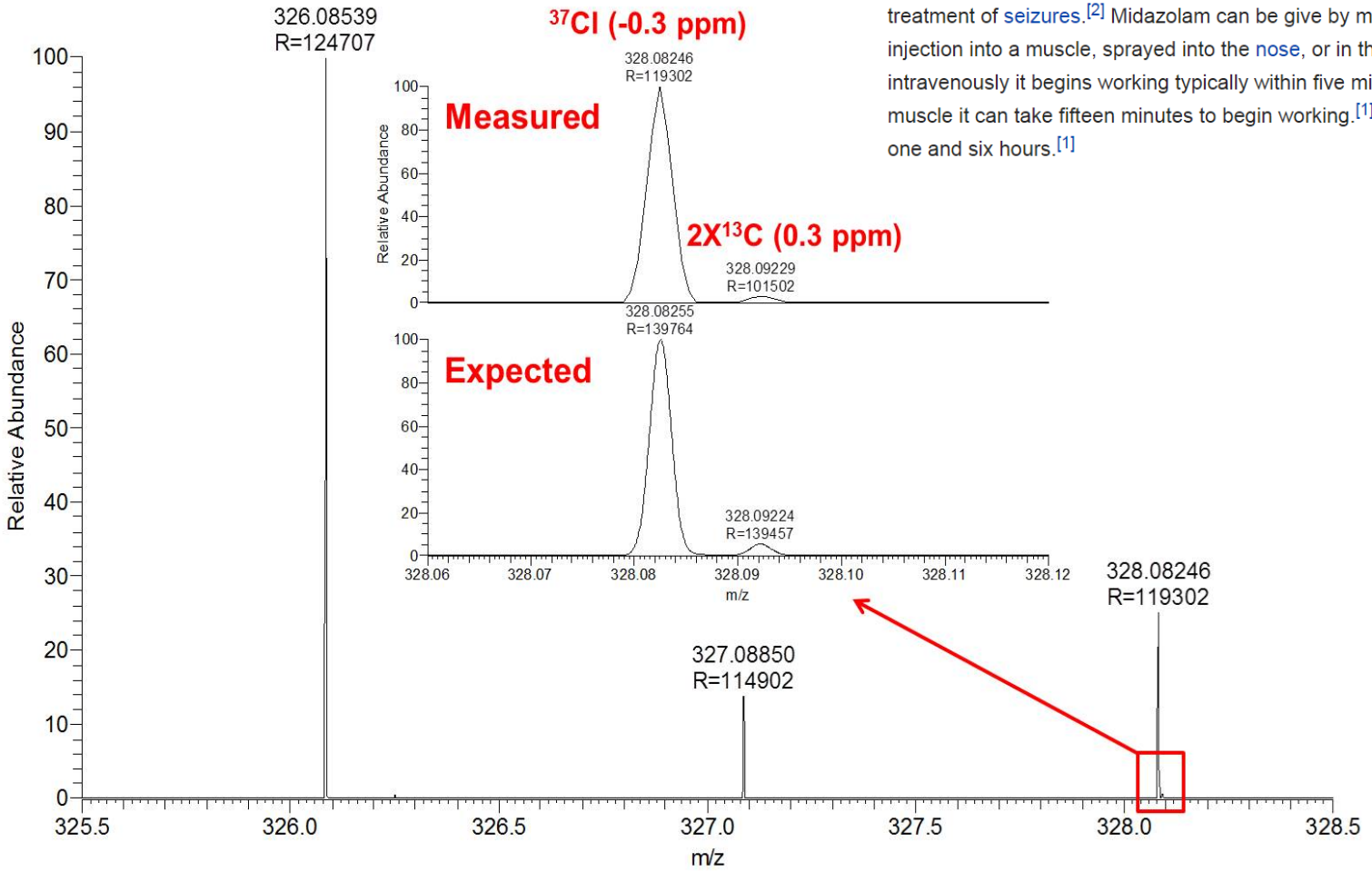
Unparallel Discriminating Power: Midazolam Mystery

Midazolam, marketed under the trade names **Versed** among others, is a medication used for anesthesia, procedural sedation, trouble sleeping, and severe agitation.[1] It works by making people sleepy, decreasing anxiety, and causing a loss of ability to create new memories.[1] It is also useful for the treatment of seizures.[2] Midazolam can be give by mouth, intravenously, by injection into a muscle, sprayed into the nose, or in the cheek.[1][2] When given intravenously it begins working typically within five minutes, when injected into a muscle it can take fifteen minutes to begin working.[1] Effects last for between one and six hours.[1]



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2014: Recent HRMS Comparison Study by US FDA

J. Am. Soc. Mass Spectrom. (2014) 25:1285–1294
DOI: 10.1007/s13361-014-0880-5

RESEARCH ARTICLE

Mass Accuracy and Isotopic Abundance Measurements for HR-MS Instrumentation: Capabilities for Non-Targeted Analyses

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U.S. Department of Health and Human Services

U.S. Food and Drug Administration
Protecting and Promoting *Your* Health

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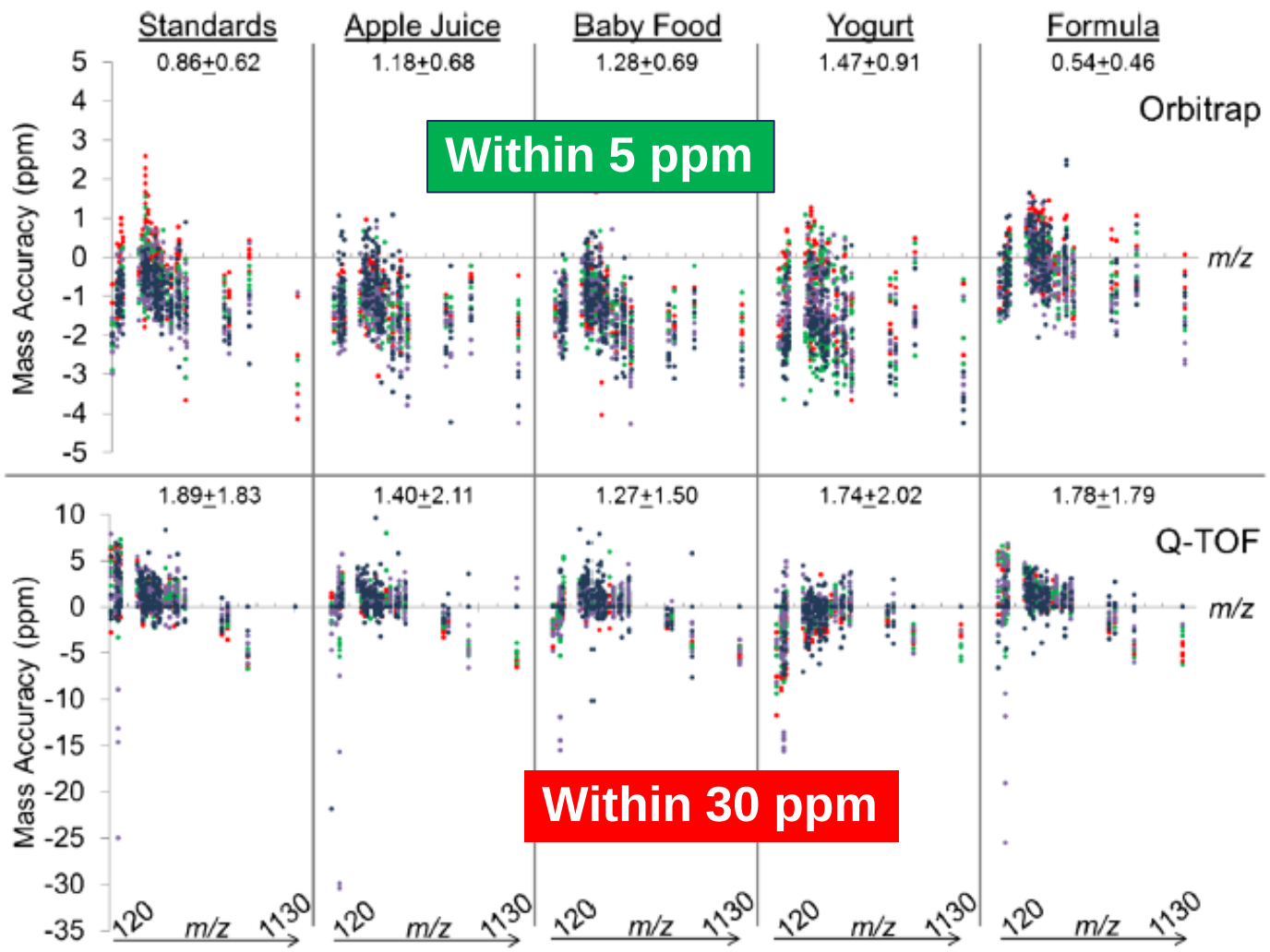
Critical Parameter #1: Mass Accuracy



Detection of 48 compounds (antibiotics, toxins, pesticides, drugs etc) in various food matrices.

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Critical Parameter #2: Isotopic Abundance/Pattern

Table 1. Average Absolute Isotope Ratio Deviation Values

pg on column	Standards	Apple juice	Baby food	Yogurt	Formula
A + 1					
Q-Exactive, Overall: 1.69 ± 2.30					
10	1.95 ± 2.26	3.17 ± 3.27	3.67 ± 3.33	3.21 ± 2.83	2.18 ± 1.69
100	2.61 ± 4.81	1.95 ± 1.98	1.91 ± 2.19	1.95 ± 1.87	2.10 ± 2.08
500	0.86 ± 0.96	1.07 ± 1.05	1.07 ± 1.18	1.26 ± 1.47	1.18 ± 1.36
2000	1.02 ± 1.79	0.75 ± 0.96	0.89 ± 1.34	0.74 ± 0.97	0.66 ± 0.89
MaXis, Overall: 5.01 ± 7.53					
10	9.20 ± 7.07	13.47 ± 9.06	15.30 ± 11.03	11.78 ± 7.62	11.49 ± 9.44
100	4.85 ± 6.66	7.78 ± 13.99	6.79 ± 7.02	6.94 ± 7.91	5.99 ± 6.25
500	3.05 ± 6.45	5.22 ± 9.58	3.30 ± 3.85	3.23 ± 3.79	3.33 ± 4.34
2000	1.77 ± 2.36	2.79 ± 6.28	2.13 ± 3.13	1.88 ± 2.56	2.03 ± 2.62
A + 2					
Q-Exactive, Overall: 1.59 ± 4.33					
10	5.31 ± 18.09	3.36 ± 5.42	4.38 ± 9.08	5.15 ± 6.56	6.44 ± 5.03
100	1.75 ± 3.01	1.93 ± 2.91	2.24 ± 4.60	1.70 ± 2.37	1.57 ± 1.86
500	1.03 ± 1.26	0.91 ± 0.62	0.86 ± 0.59	1.05 ± 0.81	1.22 ± 1.94
2000	0.81 ± 1.05	0.86 ± 1.20	0.73 ± 0.56	0.82 ± 0.57	0.74 ± 0.53
MaXis, Overall: 3.67 ± 6.47					
10	10.96 ± 9.71	12.89 ± 6.70	19.43 ± 38.22	11.21 ± 5.68	14.92 ± 7.62
100	3.55 ± 4.75	6.09 ± 6.85	6.73 ± 7.02	4.67 ± 4.46	5.22 ± 5.24
500	2.13 ± 3.14	4.02 ± 7.02	3.02 ± 3.17	3.01 ± 4.27	2.78 ± 3.38
2000	1.24 ± 2.06	2.23 ± 4.56	1.69 ± 2.36	1.68 ± 2.57	1.94 ± 3.21

Values listed are the average ± standard deviation for the calculated absolute isotope ratio deviation for all compounds for A + 1 and A + 2.

Superior HRAM Attributes in Complex Matrix Analysis

Analytica Chimica Acta 853 (2015) 415–424

Contents lists available at ScienceDirect

Analytica Chimica Acta

journal homepage: www.elsevier.com/locate/aca

Quantitative performance of liquid chromatography coupled to Q-Exactive high resolution mass spectrometry (HRMS) for the analysis of tetracyclines in a complex matrix

Morgan Solliec, Audrey Roy-Lachapelle, Sébastien Sauvé *

Department of Chemistry, Université de Montréal, Montréal, QC, Canada

Impeccable Mass Stability at High Mass Accuracy

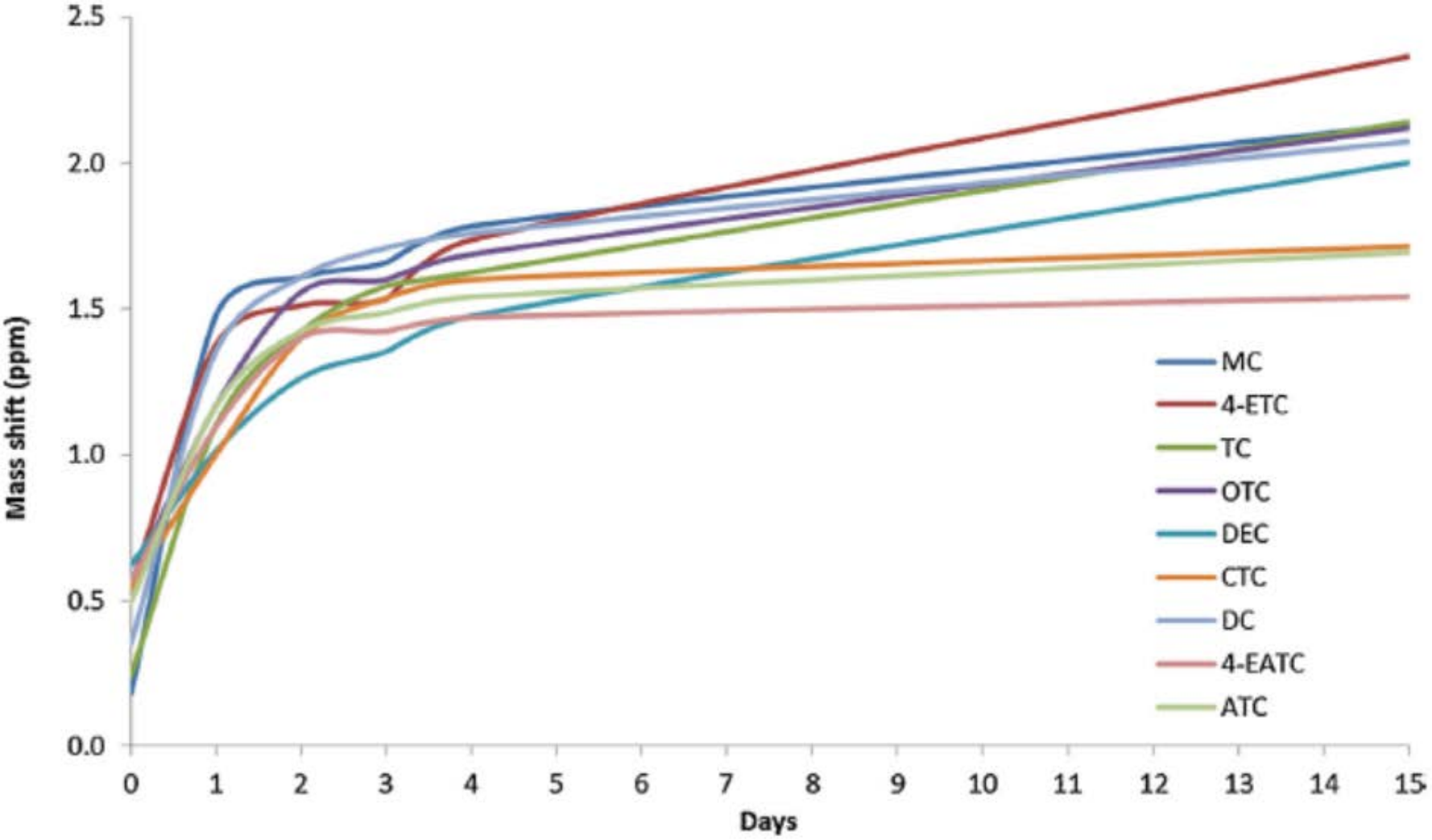

Fig. 4. Mass accuracy stability of TCs measured in FS without lock mass (250 $\mu g L^{-1}$; $n=3$).

ThermoFisher SCIENTIFIC

Animal Feed Matrix Challenge: Orbitrap *vs* TOF MS

Food Additives & Contaminants: Part A, 2015
http://dx.doi.org/10.1080/19440049.2015.1023742

Taylor & Francis
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Analysis of veterinary drug and pesticide residues in animal feed by high-resolution mass spectrometry: comparison between time-of-flight and Orbitrap

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Research Group "Analytical Chemistry of Contaminants", Department of Chemistry and Physics, Research Centre for Agricultural and Food Biotechnology (BITAL), University of Almería, Agrifood Campus of International Excellence, Almería, Spain

(*Received 22 December 2014; accepted 24 February 2015*)

The use of medium–high-resolution mass spectrometers (M–HRMS) provides many advantages in multi-residue analysis. A comparison between two mass spectrometers, medium-resolution (MRMS) time-of-flight (TOF) and high-resolution (HRMS) Orbitrap, has been carried out for the analysis of toxic compounds in animal feed. More than 300 compounds belonging to several classes of veterinary drugs (VDs) and pesticides have been determined in different animal feed samples using a generic extraction method. The use of a clean-up procedure has been evaluated in both instruments, and several validation parameters have been established, such as the matrix effect, linearity, recovery and sensitivity. Finally, both instruments have been used during the analysis of 18 different feed samples (including chicken, hen, rabbit and horse). Some VDs (sulfadiazine, trimethoprim, robenidine and monensin sodium) and one pesticide (chlorpyrifos) have been identified. In general, better results were obtained using the Orbitrap, such as sensitivity (1–12.5 μg kg^{-1}) and recovery values (60–125%). Moreover, this analyser had several software tools, which reduced the time for data processing and were easy to use, performing quick screening for more than 450 compounds in less than 5 min. However, some disadvantages such as the high cost and a decrease in the number of detected compounds at low concentrations must be taken into account.

Keywords: animal feed; pesticide; veterinary drug; TOF; Orbitrap

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Quantitative Comparative Study: Orbitrap MS *vs* QqQ

Food Additives and Contaminants
Vol. 28, No. 10, October 2011, 1424–1437

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Quantitative analysis of mycotoxins in cereal foods by collision cell fragmentation-high-resolution mass spectrometry: performance and comparison with triple-stage quadrupole detection

V.M.T. Lattanzio[a]*, S. Della Gatta[a], M. Godula[b] and A. Visconti[a]

[a]*National Research Council of Italy, Institute of Sciences of Food Production, Via Amendola, 122/O, 70126 Bari, Italy;*
[b]*Thermo Fisher Scientific Praha, Slunečná 27 Praha 10, CZ-100 00, Czech Republic*

(*Received 29 March 2011; final version received 30 May 2011*)

A liquid chromatography-high-resolution mass spectrometry (LC-HRMS) method for the simultaneous determination of aflatoxins (B_1, B_2, G_1, G_2), ochratoxin A, deoxynivalenol, zearalenone, T-2 and HT-2 toxins in wheat flour, barley flour and crisp bread was developed. Mycotoxin fragmentation patterns obtained by high-energy collision dissociation (HCD) were investigated to obtain quantitative and confirmatory information (two characteristic masses per mycotoxin) using Orbitrap™-based high-resolution mass spectrometry. LC-HRMS (full-scan) detection carried out by HCD allows the monitoring of the pseudo-molecular ion and an additional characteristic fragment (for each mycotoxin) with mass accuracy in the range 0.1–3.9 ppm, meeting current European regulatory requirements for LC-MS confirmatory analysis. A sample preparation procedure based on polymeric solid-phase extraction cartridges was applied, allowing recoveries higher than 74% for nine mycotoxins, with a relative standard deviation lower than 13%. Detection limits in the range 0.5–3.4 $\mu g\,kg^{-1}$ were obtained for three cereal matrices. A critical comparison between the proposed method and a validated method based on triple quadrupole mass spectrometry showed similar performance in terms of detection limits, recoveries and repeatability, and matrix effects. Based on an efficient sample extraction and clean-up, the LC-HCD-HRMS method reported here represents a reliable and robust alternative tool for mycotoxin analysis in food matrices as compared with well-established triple quadrupole-based approaches.

Keywords: LC/MS; in-house validation; mycotoxins; *Fusarium*; aflatoxins; ochratoxin A; zearalenone; bakery products; cereals

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Quantitative Comparative Study: Orbitrap MS *vs* QqQ

Table 3. Mass accuracy of quantifier and qualifier ions for each mycotoxin, measured in LC-HCD-HRMS chromatograms of standard solutions and cereal food extracts after SPE clean-up.

Mycotoxin	Calculated mass	Mass accuracy (ppm)[b]				
		Standard solution	Wheat flour	Barley flour	Crisp bread (wheat based)	Crisp bread (rye based)
DON	297.13381	2.2	0.2	0.6	2.1	3.9
	231.10157[a]	1.0	0.4	0.3	1.5	1.9
AFG_2	331.08123	0.9	0.3	1.7	0.3	0.8
	245.30808[a]	0.5	0.6	1.1	0.6	1.5
AFG_1	329.06558	1.2	0.2	1.5	1.5	1.8
	243.06518[a]	1.2	0.5	1.3	0.8	1.3
AFB_2	315.08631	1.2	0.2	1.6	2.2	0.9
	287.09140[a]	1.1	0.4	1.7	3.3	1.5
AFB_1	313.07066	1.1	0.1	1.3	0.4	2.6
	241.04953[a]	1.0	0.3	1.2	0.4	1.2
HT-2	442.24409	1.2	0.2	0.3	1.7	1.6
	245.11722[a]	1.2	0.6	1.2	1.5	1.6
T-2	484.25460[a]	0.7	0.4	1.7	1.6	1.9
	215.10660	0.4	0.1	0.5	0.1	1.6
ZEN	319.15450[a]	1.0	0.1	0.6	1.5	2.2
	283.13287	0.9	0.4	2.1	1.9	1.5
OTA	404.08950[a]	0.8	0.1	0.5	2.9	1.6
	358.08406	1.0	0.3	0.8	2.5	1.5

Notes: [a]Quantifier ion.
[b]Absolute value, average of triplicate injections of 1 ng toxin (relevant to 40 mg matrix for wheat and barley flour and wheat-based crisp bread, and to 100 mg matrix for rye-based crisp bread).

Quantitative Comparative Study: Orbitrap MS *vs* QqQ

Table 5. Comparison of recovery and repeatability values obtained in durum wheat flour, wheat- and rye-based crisp bread by using LC-HRMS and LC-MRM methodologies after SPE clean up.

		Recoveries, % (RSDr, %)								
		DON	AFG_2	AFG_1	AFB_2	AFB_1	HT-2	T-2	ZEN	OTA
Spiking level ($\mu g\,kg^{-1}$):		300	0.4	1.2	0.4	2	20	20	30	1.2
Wheat flour	MRM	95 (2)	n.d.	82 (4)	84 (6)	89 (4)	95 (4)	92 (4)	95 (9)	74 (7)
	HRMS	102 (5)	90 (8)	89 (0)	95 (2)	81 (6)	104 (4)	98 (6)	76 (6)	97 (9)
Wheat crisp bread	MRM	100 (0)	n.d.	106 (5)	85 (10)	102 (6)	107 (2)	108 (6)	84 (5)	101 (3)
	HRMS	104 (0)	102 (5)	104 (4)	80 (2)	102 (2)	105 (1)	103 (1)	85 (1)	93 (2)
Rye crisp bread	MRM	95 (3)	91 (7)	79 (2)	85 (7)	77 (3)	97 (2)	91 (3)	96 (7)	82 (2)
	HRMS	105 (1)	93 (2)	95 (6)	93 (8)	87 (4)	100 (3)	95 (3)	101 (9)	74 (13)

Table 6. Comparison of detection limits in durum wheat flour, barley flour and wheat- and rye-based crisp bread by using LC-HRMS, with and without HCD, and LC-MRM methodologies after SPE clean-up.

	Detection limits ($\mu g\,kg^{-1}$)											
	Wheat flour			Barley flour			Crisp bread (wheat based)			Crisp bread (rye based)		
	HRMS	HCD-HRMS	MRM	HRMS	HCD-HRMS	MRM	HRMS	HCD-HRMS	MRM	HRMS	HCD-HRMS	MRM
DON	0.2	1.6	3.9	0.2	1.8	10.3	0.3	3.4	29.0	0.5	2.3	59.2
AFG_2	0.1	1.5	0.1	0.1	0.5	0.2	0.1	0.2	0.4	0.1	0.5	1.9
AFG_1	0.1	0.6	0.2	0.1	1.1	0.7	0.2	0.1	0.7	0.3	1.2	2.6
AFB_2	0.1	0.7	0.3	0.1	0.5	0.3	0.1	0.2	0.4	0.1	0.5	1.1
AFB_1	0.1	1.0	0.3	0.1	1.0	0.5	0.1	0.4	0.5	0.1	1.6	1.1
HT-2	0.3	1.7	0.3	0.2	2.5	1.1	0.3	1.0	0.5	0.4	1.7	1.7
T-2	0.2	1.0	0.2	0.2	0.5	0.5	0.3	2.9	0.5	0.5	1.6	0.9
ZEN	0.8	1.0	2.8	0.3	1.4	4.0	0.4	1.0	2.2	1.6	2.3	5.8
OTA	0.2	1.4	0.1	0.6	1.9	0.3	0.5	0.4	0.1	0.5	2.9	0.4

2015: Quadrupole-Orbitrap MS Quantifies like a QqQ

Analytica Chimica Acta 856 (2015) 54–67

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Analytica Chimica Acta

journal homepage: www.elsevier.com/locate/aca

Reliability of veterinary drug residue confirmation: High resolution mass spectrometry versus tandem mass spectrometry

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ABSTRACT

Confirmation of suspected residues has been a long time domain of tandem triple quadrupole mass spectrometry (QqQ). The currently most widely used confirmation strategy relies on the use of two selected reaction monitoring signals (SRM). The details of this confirmation procedure are described in detail in the Commission Decision 93/256/EC (CD). On the other hand, high resolution mass spectrometry (HRMS) is nowadays increasingly used for trace analysis. Yet its utility for confirmatory purposes has not been well explored and utilized, since established confirmation strategies like the CD do not yet include rules for modern HRMS technologies.

It is the focus of this paper to evaluate the likelihood of false positive and false negative confirmation results, when using a variety of HRMS based measurement modes as compared to conventional QqQ mass spectrometry. The experimental strategy relies on the chromatographic separation of a complex blank sample (bovine liver extract) and the subsequent monitoring of a number of dummy transitions respectively dummy accurate masses. The term "dummy" refers to precursor and derived product ions (based on a realistic neutral loss) whose elemental compositions ($C_xH_yN_zO_dCl_e$) were produced by a random number generator. Monitoring a large number of such hypothetical SRM's, or accurate masses inevitably produces a number of mass traces containing chromatographic peaks (false detects) which are caused by eluting matrix compounds. The number and intensity of these peaks were recorded and standardized to permit a comparison among the two employed MS technologies. QqQ performance (compounds which happen to produce a response in two SRM traces at identical retention time) was compared with a number of different HRMS[1] and HRMS[2] detection based modes. A HRMS confirmation criterion based on two full scans (an unfragmented and an all ion fragmented) was proposed. Compared to the CD criteria, a significantly lower probability of false positive and false negative findings is obtained by utilizing this criterion.

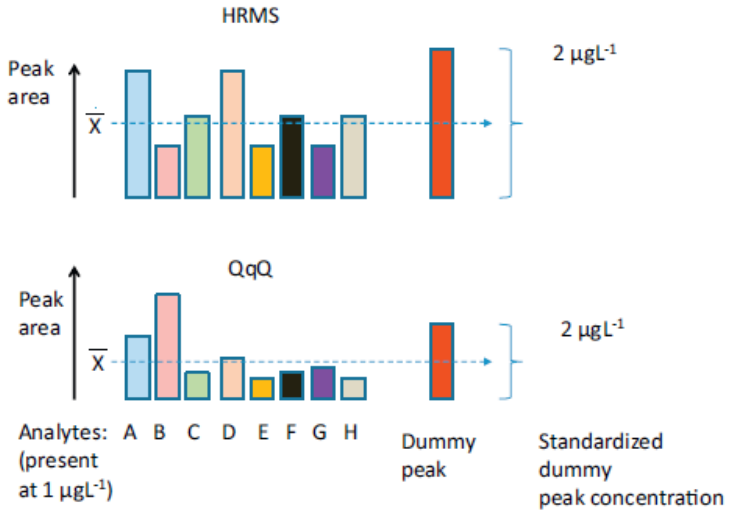

Fig. 1. The standardization process used to make QqQ and HRMS peak areas comparable. The dummy peak area is divided by the average response produced by eight veterinary drugs present at 1 µg L^{-1} in mixed standard solution.

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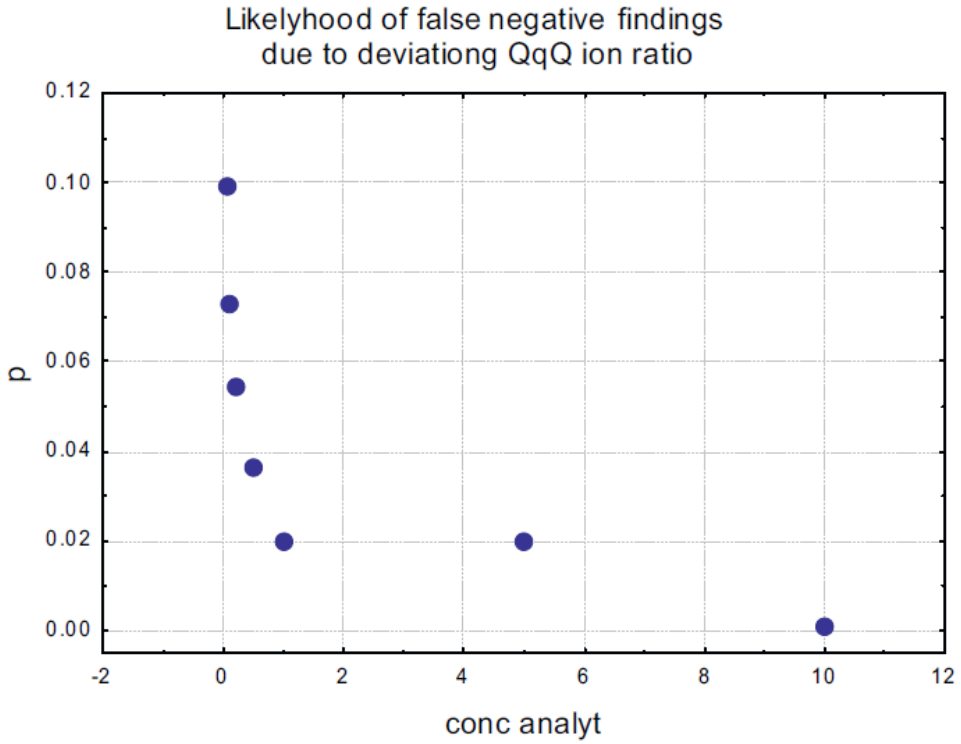
Assessment of False Negative Detection by QqQ and Q-Orbi

Table 8
Number of false negative findings obtained when analyzing a liver extract spiked with different concentrations of a total of 42 vet. drugs. HRMS data was confirmed by the proposed criterion, while QqQ data was evaluated according to the CD

Conc. $\mu g\,L^{-1}$	QqQ (CD)	HRMS
1	19	9
5	9	4
50	0	0

An important conclusion from this work is the fact that QqQ instrument based SRM sensitivity has tremendously increased over the last decade, while the selectivity of detection has remained virtually unchanged. Yet it makes less and less sense to proceed further in this direction. This has been realized by a number of instrument vendors which are actively promoting selectivity enhancing devices (e.g., ion mobility). An alternative, less tuning intensive strategy, is the use of HRMS. In the future, HRMS technology is not only expected to be produce more sensitivity but also more selectivity by the availability of even higher mass resolving instrumentations.

The HRMS confirmation criteria proposed in this paper does not rely on ion ratio and permits the monitoring of additional product ions which may finally lead to the acceptance or rejection of the confirmation hypothesis. The obtained data permits the conclusion that the use of a precursor ion and a single product ion can be sufficient for a successful confirmation. This is certainly an advantage over current unit mass resolving MS/MS instrumentation, since confirmation of poorly fragmenting analytes becomes more feasible.



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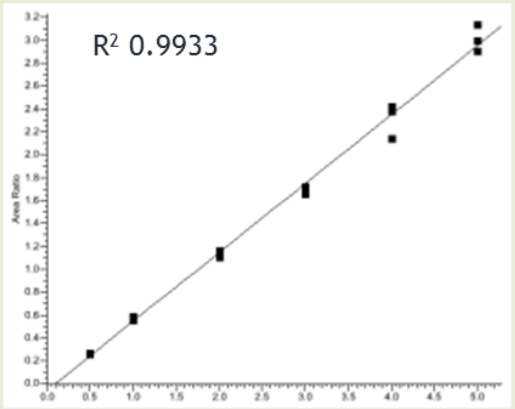
HRAM Quantitative Comparative Study by FERA (UK)

Quinolones - Sarafloxicin

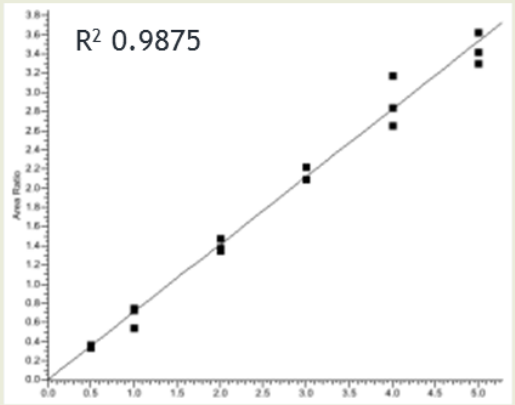
Target RL = 30 µg/kg		15 µg/kg spike level			30 µg/kg spike limit			45 µg/kg spike limit			60 µg/kg spike limit		
		QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ	QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ	QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ	QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ
Sarafloxacin	Average Concn (n =7)	15.4	15.2	15.0	31.2	30.8	30.6	45.8	45.9	43.3	62.3	61.5	59.5
	RSD	5%	6%	3%	4%	6%	1%	5%	4%	3%	3%	5%	3%

- Mass accuracy was < 2 ppm in QE Focus both acquisition modes

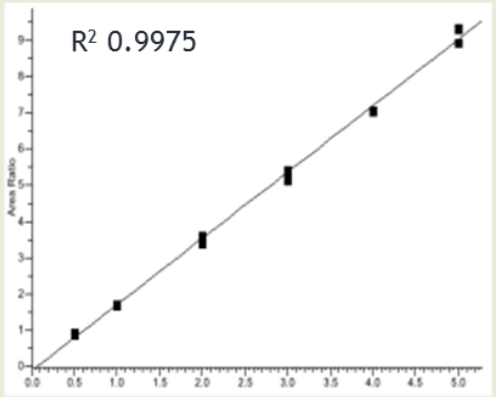
vDIA calibration graph



dd-MS2 calibration graph



QQQ calibration graph



This material was presented by Dr Stuart Adams (FERA)

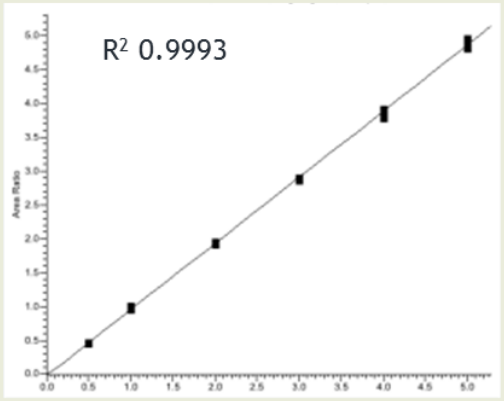
HRAM Quantitative Comparative Study by FERA (UK)

NSAIDs - Flunixin

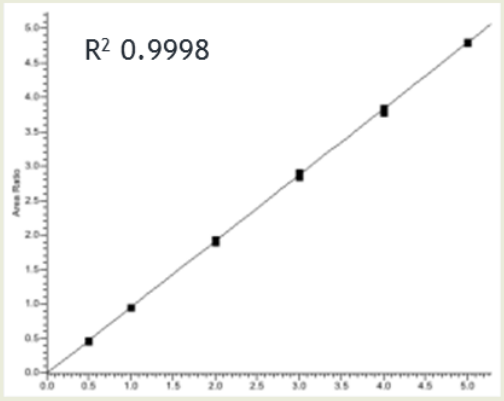
Target RL = 20 µg/kg		10 µg/kg spike level			20 µg/kg spike level			30 µg/kg spike level			40 µg/kg spike level		
		QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ	QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ	QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ	QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ
Flunixin	Average Concn (n =7)	10.3	10.4	10.0	20.1	20.5	20.1	30.1	30.4	30.4	40.2	40.7	40.4
	RSD	1%	1%	2%	2%	1%	1%	2%	1%	2%	2%	1%	1%

- Mass accuracy was < 2 ppm in both QE Focus acquisition modes

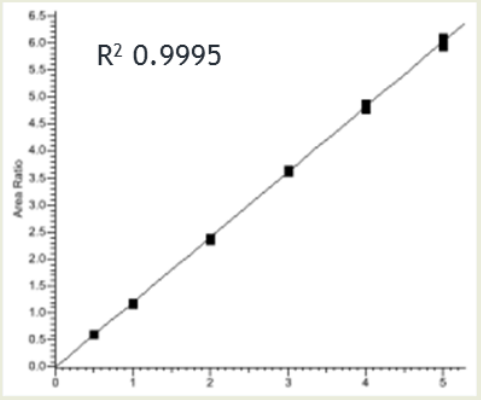
vDIA calibration graph



dd-MS2 calibration graph



QQQ calibration graph



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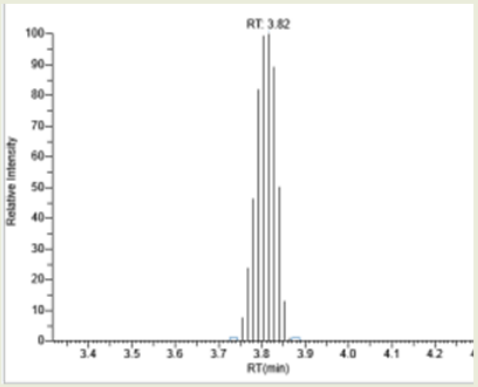
HRAM Quantitative Comparative Study by FERA (UK)

Nitroimidazoles - Ronidazole

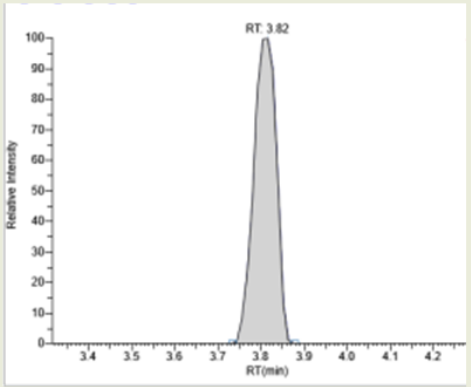
Target RL = 3 µg/kg		1.5 µg/kg spike level			3 µg/kg spike level			4.5 µg/kg spike level			6 µg/kg spike level		
		QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ	QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ	QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ	QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ
Ronidazole	Average Concn (n =7)	1.5	1.6	1.6	3.2	3.1	3.2	4.7	4.5	4.5	6.3	5.9	6.0
	RSD	10%	7%	2%	5%	4%	4%	7%	4%	3%	4%	4%	2%

- Mass accuracy was < 2 ppm in both QE Focus acquisition modes

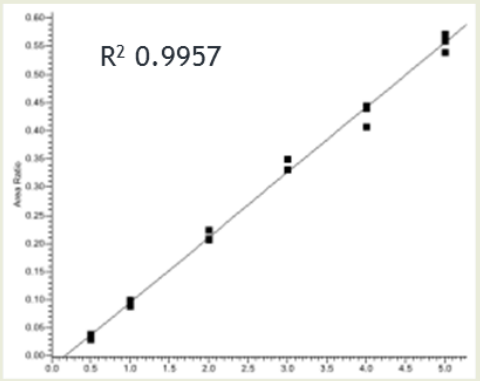
vDIA 10 µg/kg extracted matrix calib



vDIA 10 µg/kg extracted matrix calib



vDIA calibration graph



This material was presented by Dr Stuart Adams (FERA)

HRAM Quantitative Comparative Study by FERA (UK)

Tetracyclines - Doxycycline

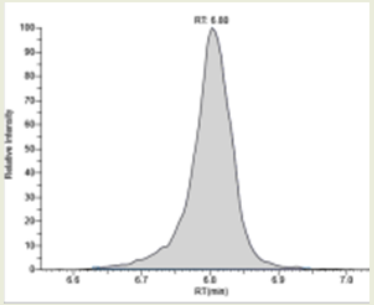
Target RL = 100 µg/kg		50 µg/kg spike level			100 µg/kg spike level			150 µg/kg spike level			200 µg/kg spike level		
		QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ	QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ	QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ	QE Focus vDIA	QE Focus dd-MS2	Quantiva QQQ
Doxycycline	Average Concn (n =7)	56.4	44.5	49.0	91.3	97.8	98.7	130.1	161.3	147.0	210.8	238.3	207.5
	RSD	5%	9%	7%	7%	8%	4%	5%	15%	5%	21%	13%	6%

- Mass accuracy was < 2 ppm in both acquisition modes
- Ion ratio checks passed using LC-MS/MS approach (Quantiva)
- Data sets comparable between 3 acquisition strategies

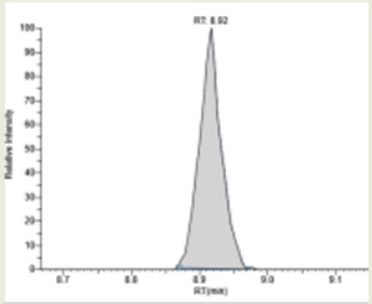
This material was presented by Dr Stuart Adams (FERA)

HRAM Quantitative Comparative Study by FERA (UK)

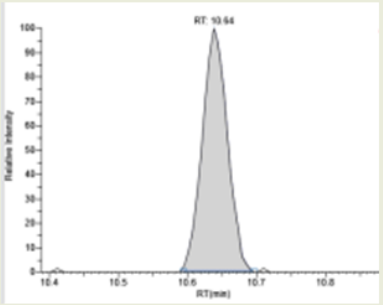
dd-MS2 Sensitivity



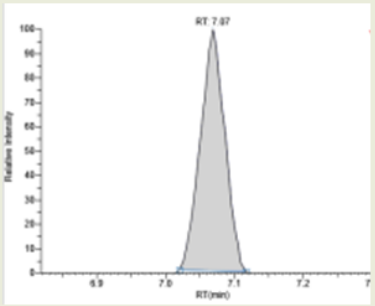
Lincomycin (lincosamide), 50µg/kg extracted matrix calib



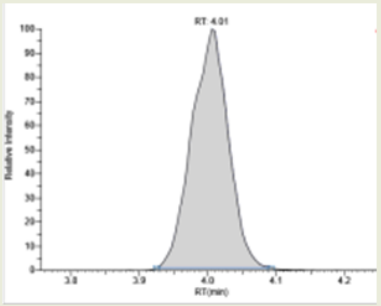
Ceftiofur (cefalosporin), 10µg/kg extracted matrix calib



Penicillin-V (penicillin), 12.5µg/kg extracted matrix calib



Clorsulon (anthelmintic), 17.5µg/kg extracted matrix calib



Sulfadiazine (sulfa), 50µg/kg extracted matrix calib

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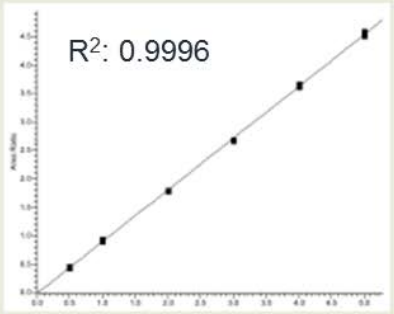
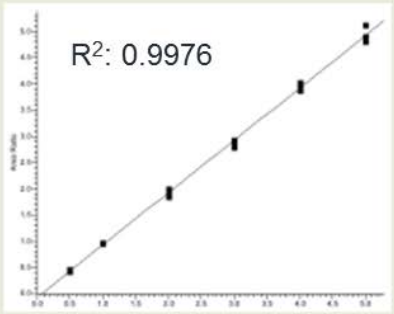
HRAM Quantitative Comparative Study by FERA (UK)

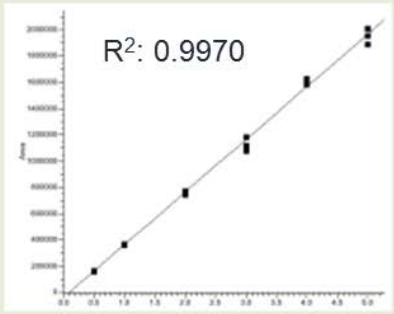
dd-MS2 calibrations



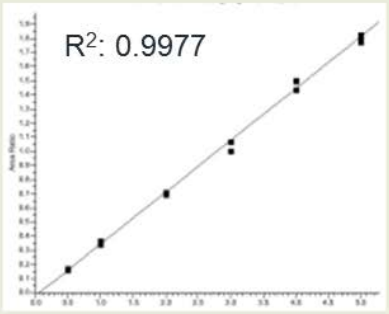
Lincomycin (lincosamide)



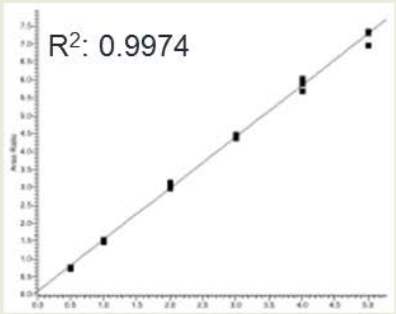
Ceftiofur (cefalosporin)



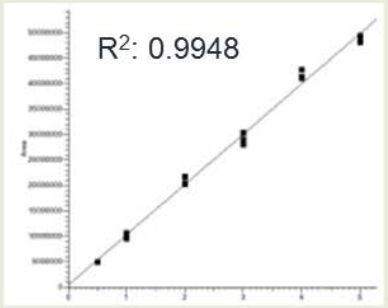
Penicillin-V (penicillin)



Clorsulon
(anthelmintic)



Sulfadiazine (sulfa),
Internally standardised

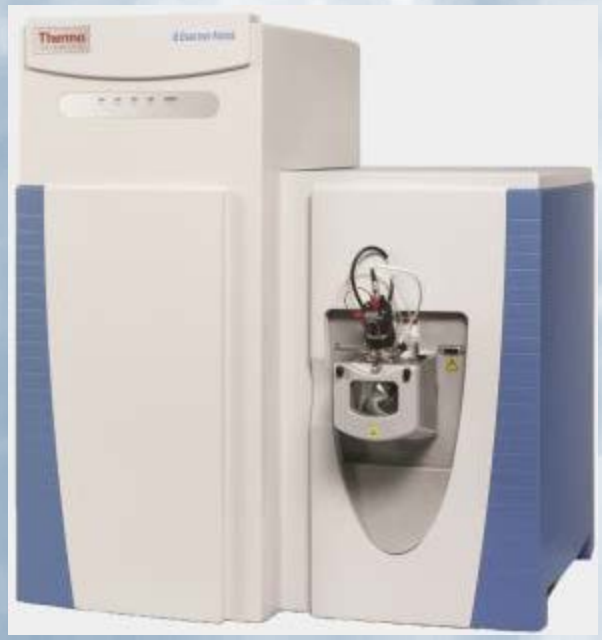


Sulfadiazine (sulfa),
Externally standardised

This material was presented by Dr Stuart Adams (FERA)

Targeted and “Unknown” Screening in TraceFinder

Full MS / Discovery dd-MS^2
Full MS / AIF/DIA



Tools:
Fragment ion matching
MS/MS library matching
Isotope pattern
Retention Time
Exact mass (MEW)
Screening View
Unknown Screening View

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Screening View-Oxacillon in Cattle Muscle Extract

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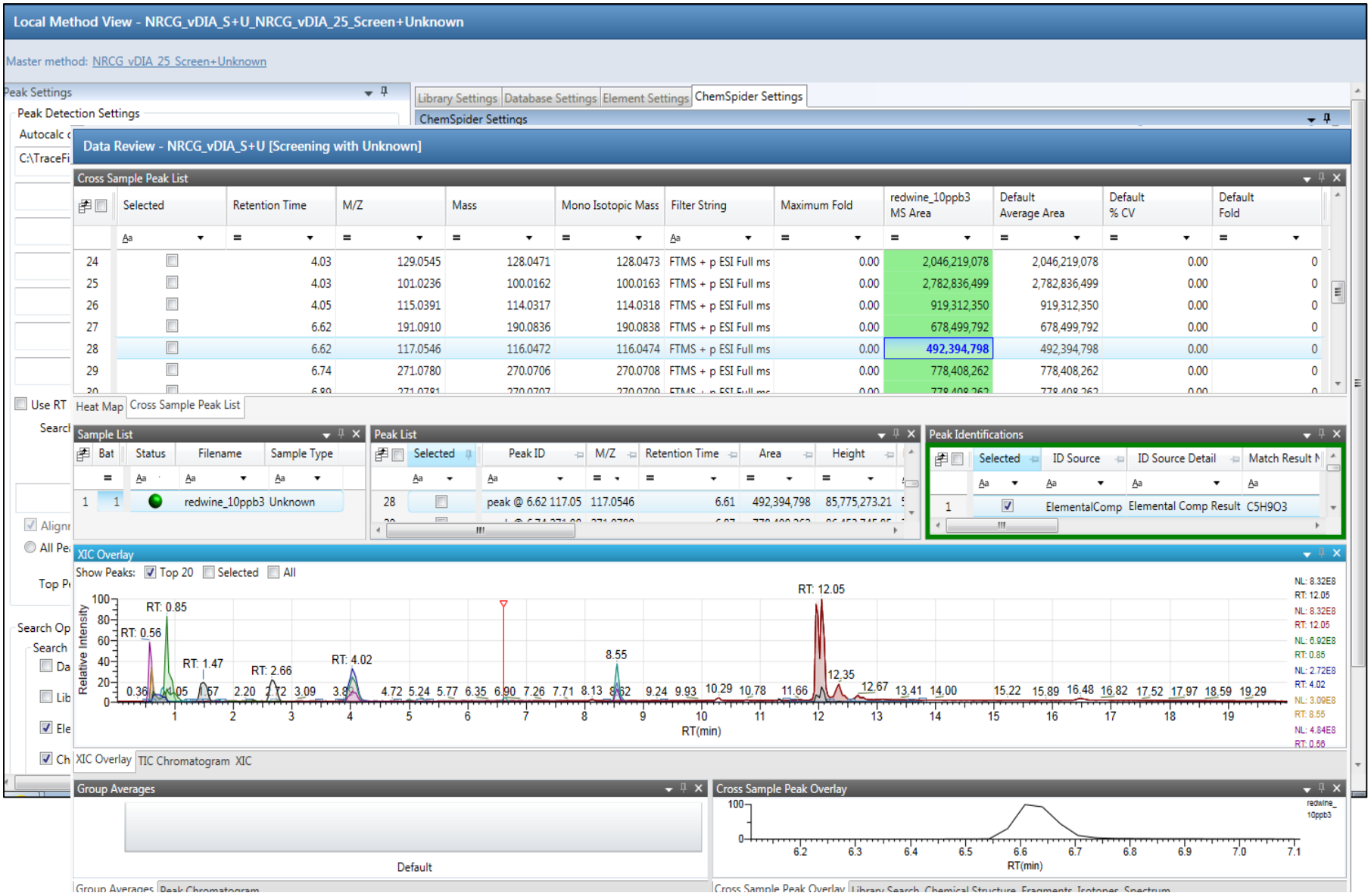
Unknown Views



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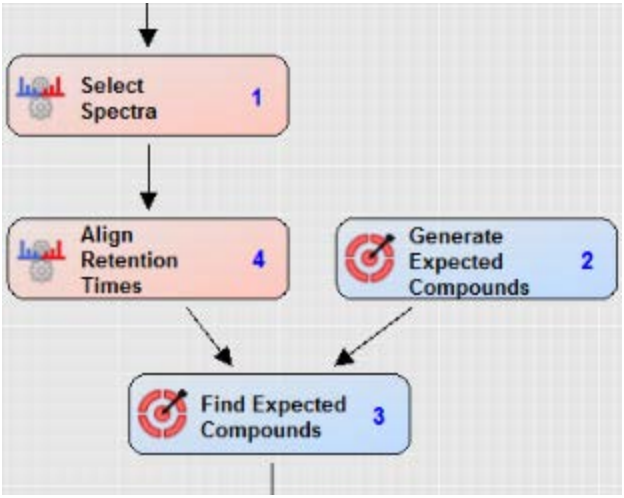
Compound Discoverer 2.0 – Flexible Small Molecule Processing

Compound Discoverer

- Customizable
- Easy
- Flexible
- Powerful



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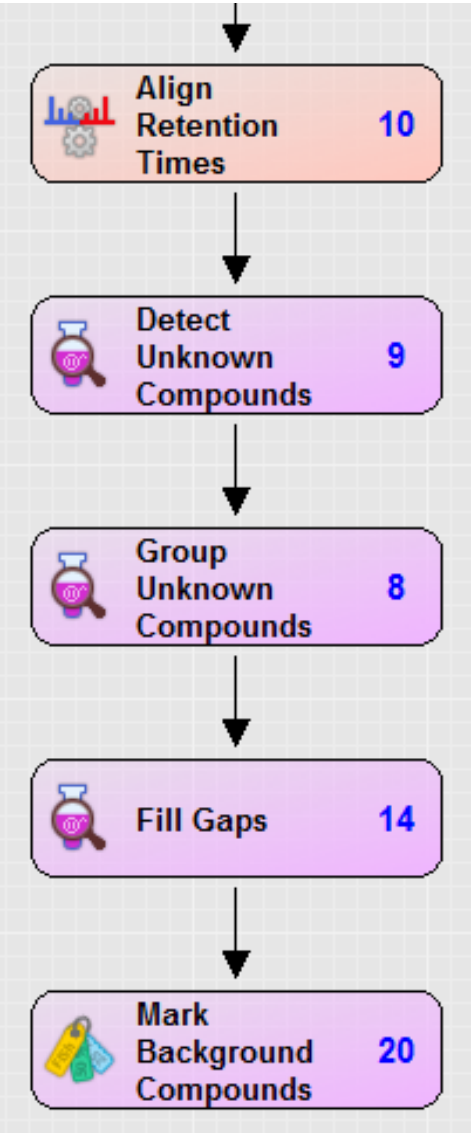
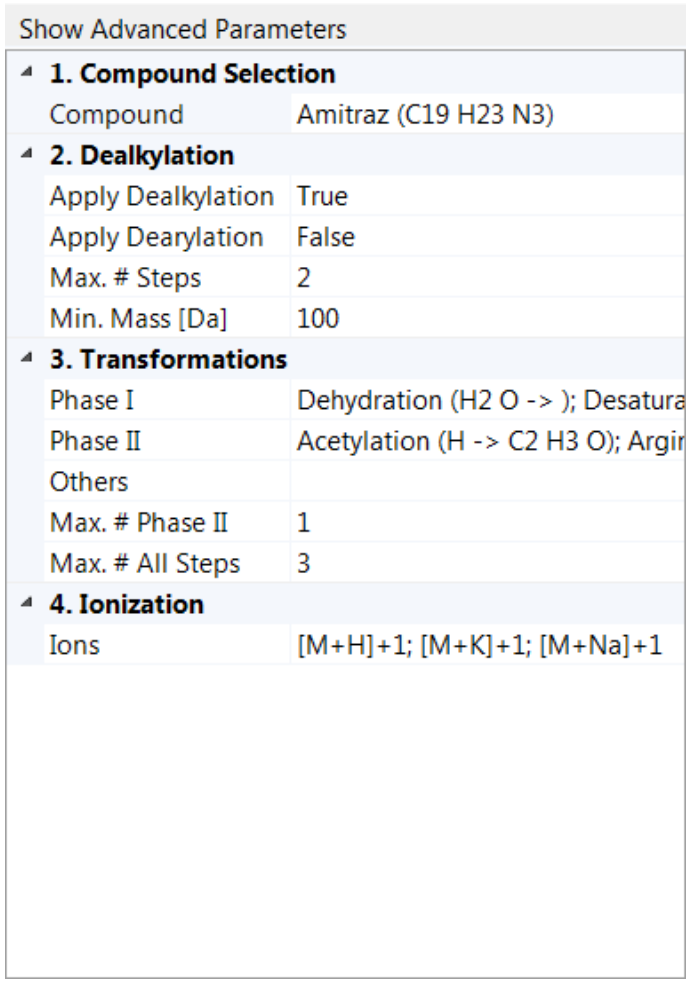
Deeper Dive: Unknown Tools in Compound Discoverer



Simple Workflow Creation

- **Unknown peak detection**
- **Cross sample grouping and comparison**
- **Automatic background determination**

Known Parent – Automatic Metabolite List Generation



- Combinatorial Approach
  - Calculate as may transformations as possible
- Built-in “Phase I” and “Phase II” Transformations
  - Completely customizable lists
- Biologically Relevant Dealkylation Prediction

Library Searching for Unknowns – mzCloud™

m/z CLOUD

Advanced Mass Spectral Database

Server location : US

search for compounds... Search

Home About Features App Database Partners Contact

mzCloud is a state of the art mass spectral database that assists analysts in identifying compounds in areas such as life sciences, metabolomics, pharmaceutical research, toxicology, forensic investigations, environmental analysis, food control and various industrial applications. mzCloud™ features a freely searchable collection of high resolution/accurate mass spectra using a new third generation spectra correlation algorithm.

Online access to the database is free of charge and no registration is required.

read more...

Enter Database

Google play New mzCloud App!

Your current browser is not supported. To enter the database use a different browser.

Search for Compounds by Name or ID

Search

6,585	10,294	2,045,858	7,896,557	700,998	view more statistics
compounds	trees	spectra	annotations	QM models	

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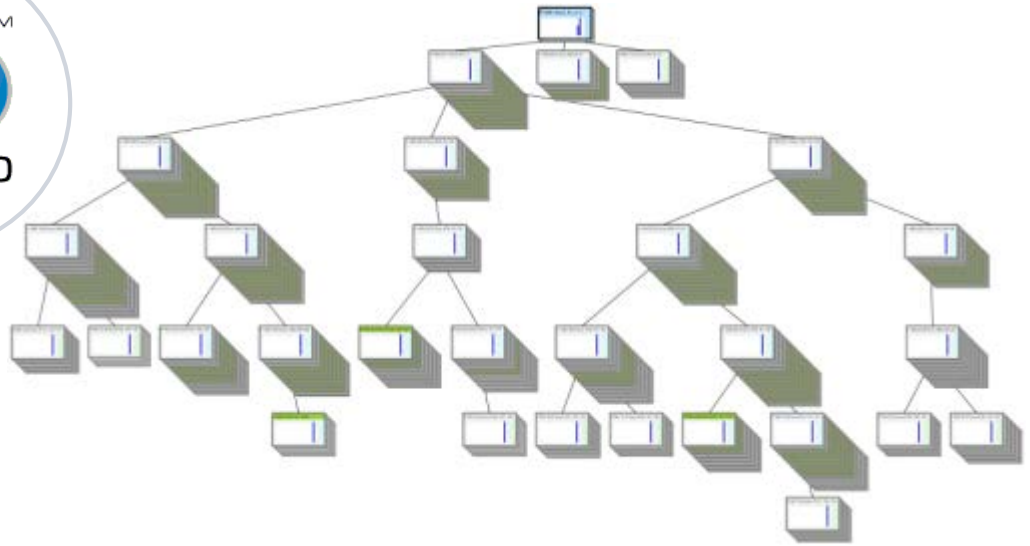
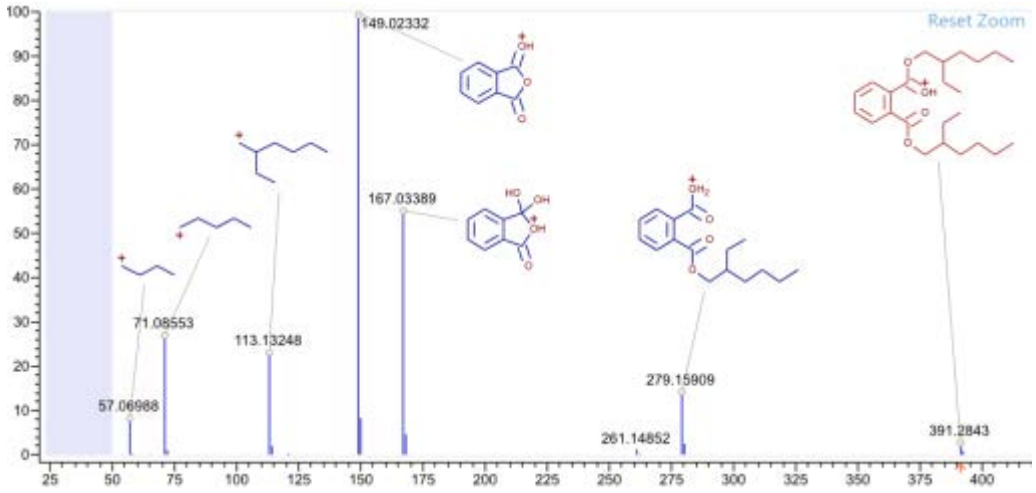
A Diverse Library

mzCloud™

- Extensive MS/MS and MS^n data
- Highly curated
- Annotated with formulas and structures
- New compounds every day





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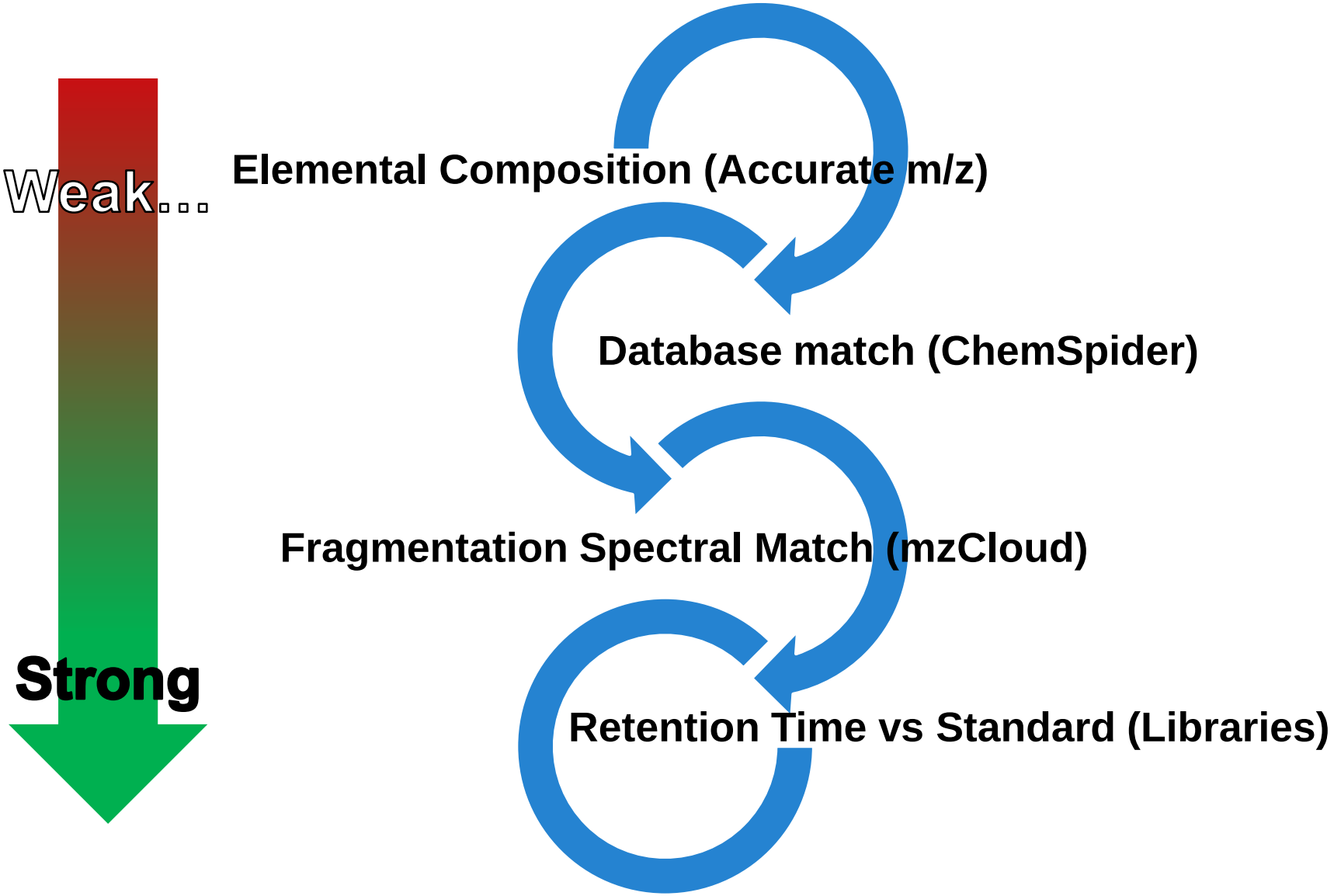
Compound Identification via HRAM Analysis



Thank You!

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Acknowledgment:

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Thomas Moerhing