



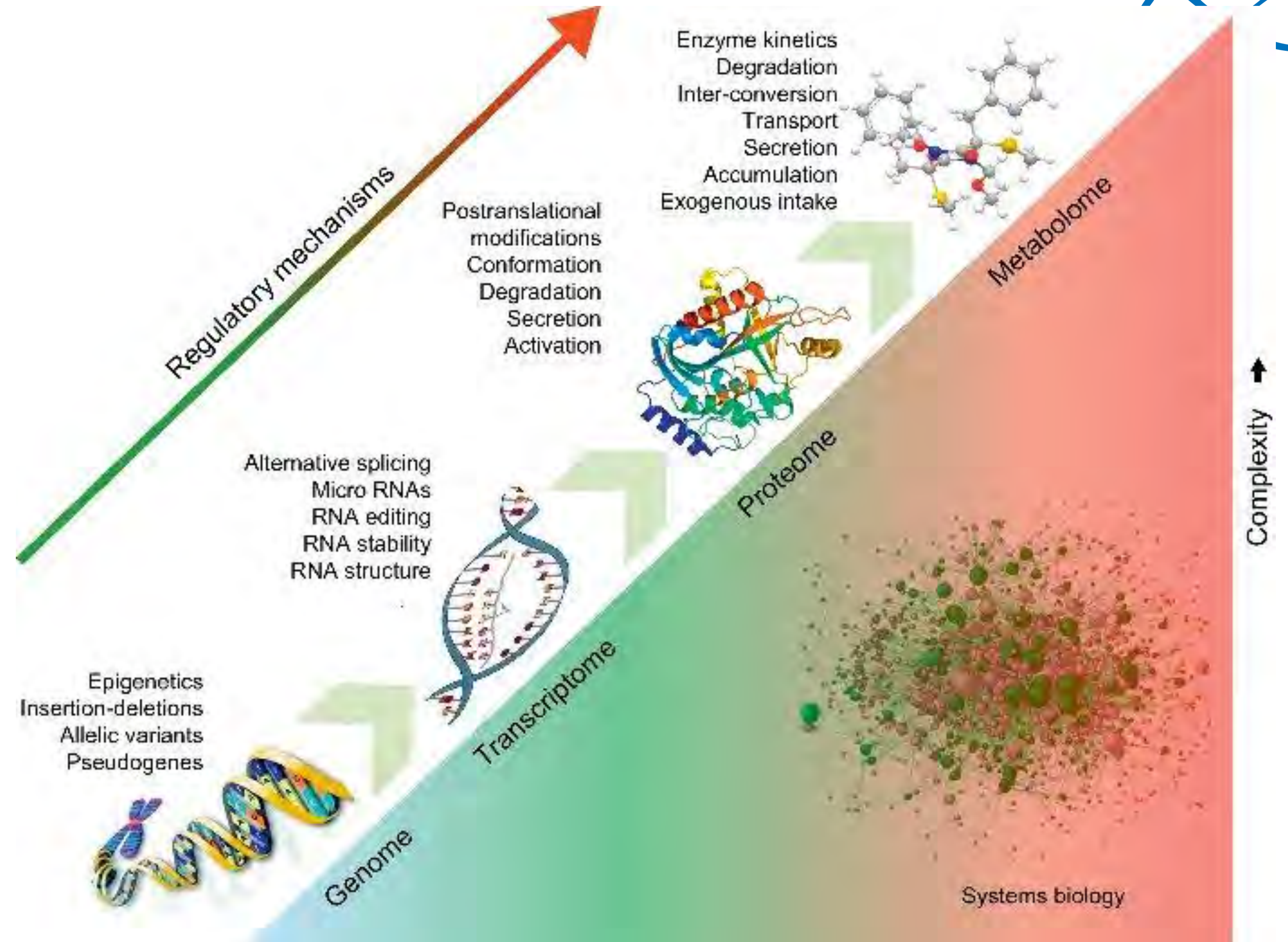
# The “MRMS aXelerate workflow”

Matthias Witt, Bruker Daltonics GmbH & Co. KG, MRMS Solutions, Bremen, Germany



# What is Metabolomics?

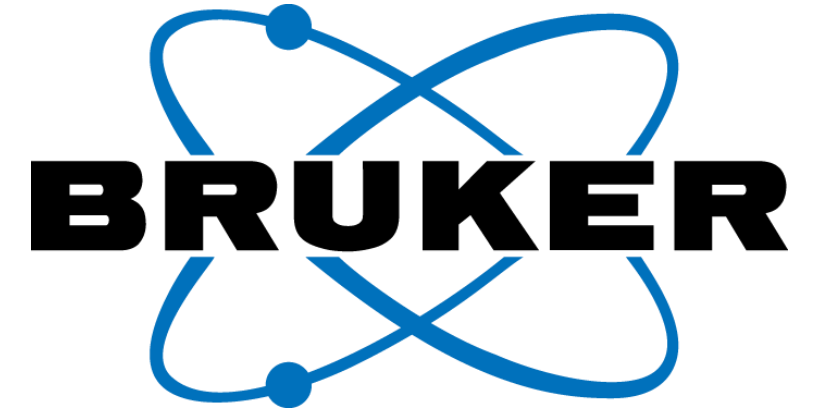
- Metabolomics is the systematic study of the small molecular metabolites in a cell, tissue, biofluid, or cell culture media that are the tangible result of cellular processes or responses to an environmental stress. The metabolome is the total complement of metabolites present in a biological sample under given genetic, nutritional or environmental conditions. Metabolomics technologies yield many insights into basic biological research in areas such as systems biology and metabolic modelling, pharmaceutical research, nutrition and toxicology.
- Applications of metabolomics are found within the pharmaceutical, healthcare, and agricultural industries, among others. There are two main approaches used in metabolomic studies: untargeted (global) and targeted (specific).
- Nuclear magnetic resonance* (NMR) and *mass spectrometry* (MS) are two of the most commonly used analytical methods in metabolomic studies. Careful planning and design of experiments is of paramount importance in metabolomic studies.





# MRMS – Breakthrough Innovations

Not your father's FT-ICR MS



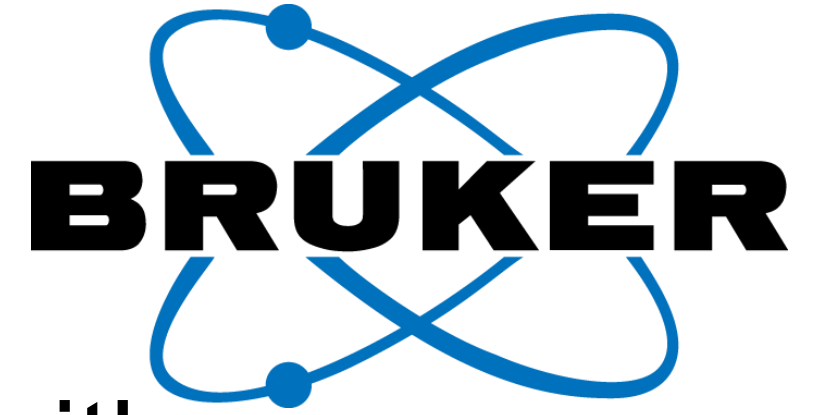
## Magnetic Resonance Mass Spectrometry



- 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.



# scimaX Versatility, performance and accuracy all in one platform



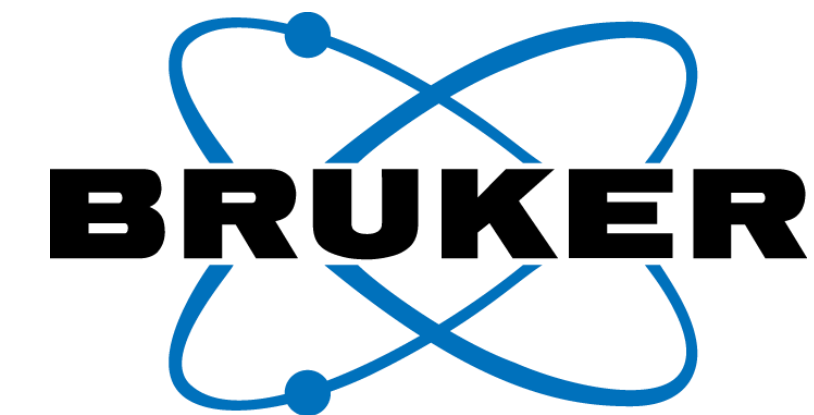
scimaX delivers unmatched versatility and unparalleled performance to provide answers with confidence for your most challenging applications

- Molecular imaging of tissues
- In-depth analysis of petroleum products
- In-depth analysis of complex environmental samples
- **Comprehensive metabolomics and other life science studies**
- Intact protein analysis
- Glycan analysis



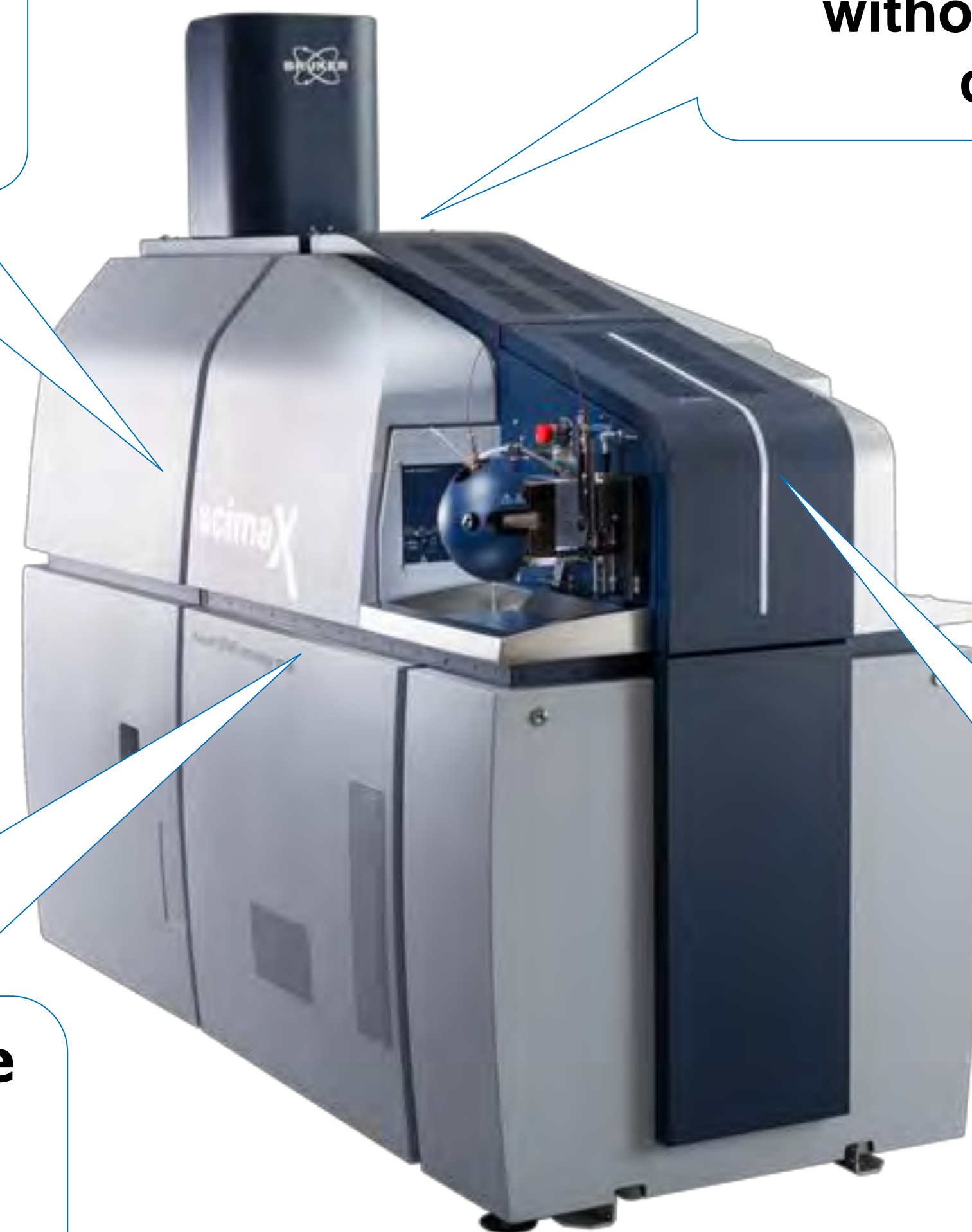


# scimaX Versatility, performance and accuracy all in one platform



**ParaCell™**  
for 20M  
resolution

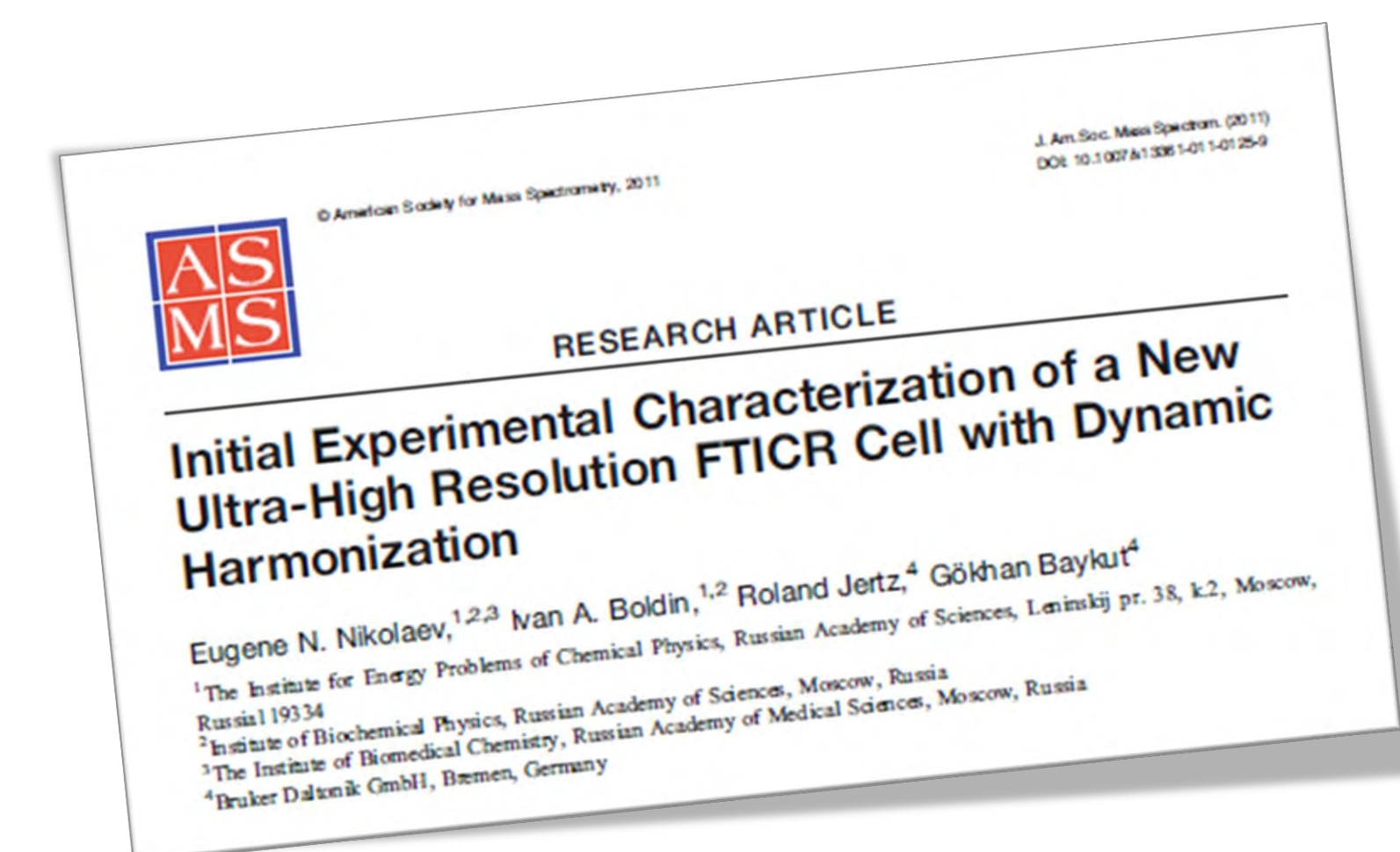
**High field magnet**  
without the need of  
cryogenics



**Front-end quadrupole  
CASI for enhanced  
sensitivity**

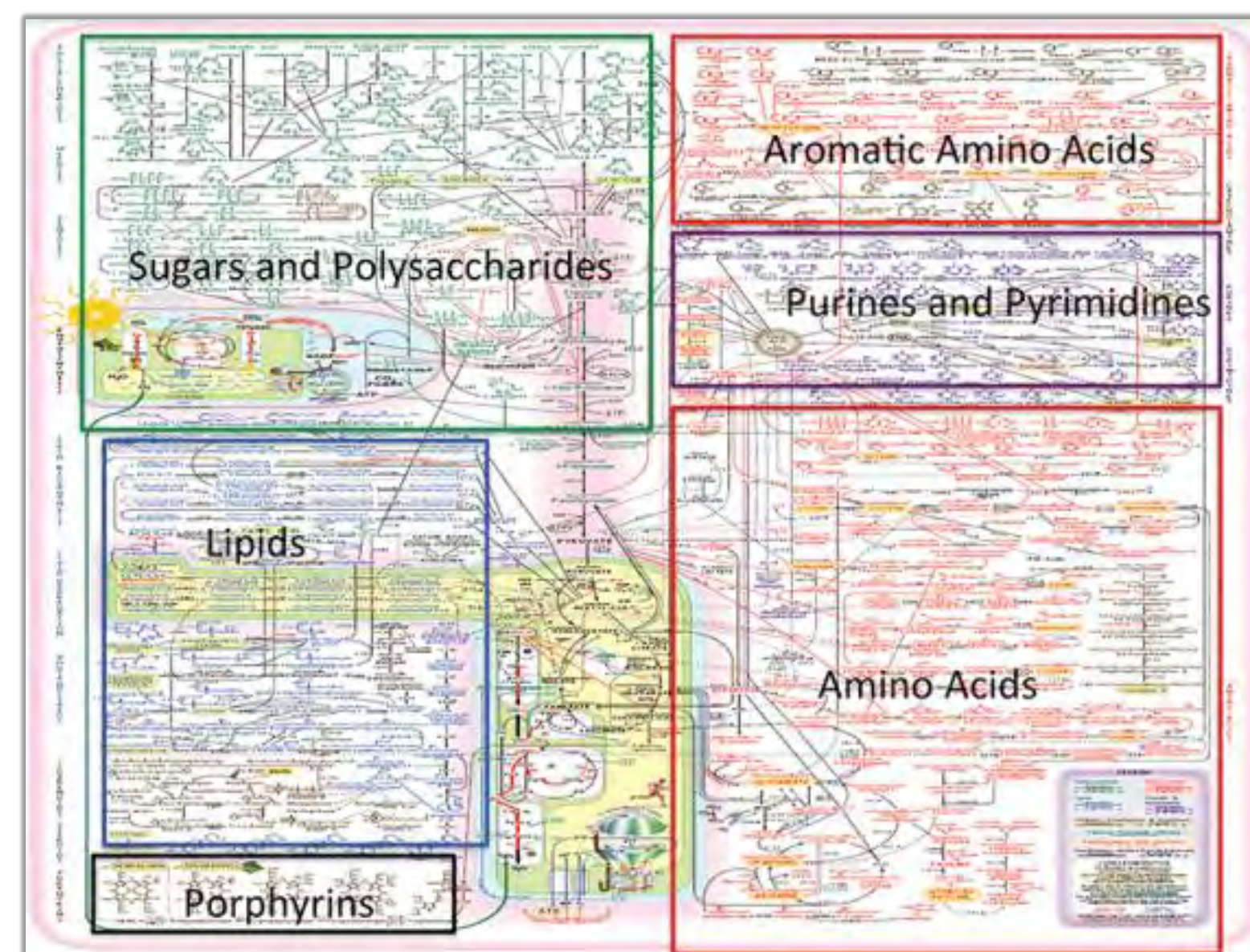
**ESI/MALDI  
dual ion  
source:  
2kHz  
smartbeam  
II MALDI  
laser**

- Extremely high mass resolution  
(**access to isotopic fine structure**)
- Ultimate mass accuracy for  
confident results  
(**ppb range**)
- Continuous Accumulation of  
Selected Ions (CASI) for enhanced  
sensitivity and enhanced dynamic
- **2 $\omega$  detection** enabling **doubled  
acquisition speed**





# MS-based OMICs solutions



<https://fornacelab.georgetown.edu/Metabolomics>  
(Lab of Prof. A. J. Fornace Jr., U. Georgetown, Washington D.C.)

The "dark metabolome"

## QTOF technology

- QTOF: workhorse for routine metabolomics projects



## TIMS technology

- Advancing research by 4D-Lipidomics and 4D-Metabolomics



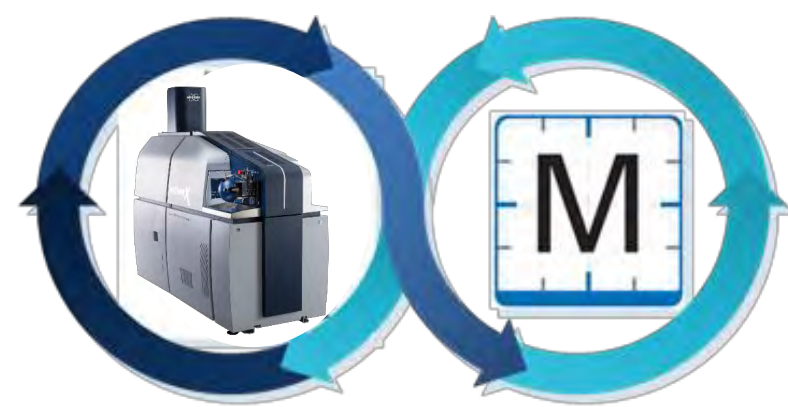
## MRMS solutions

- skip time-consuming chromatography
- complementary MALDI data
- Pinpoint formulae with isotopic fine structures

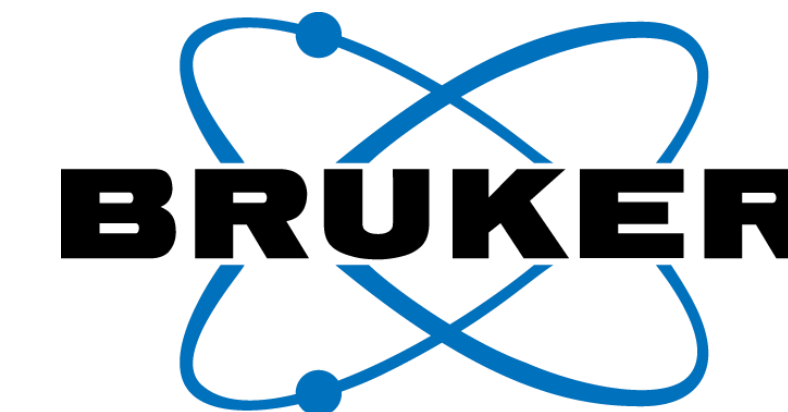


A novel method, **FIA-MRMS** provides **high sample throughput** for complex samples (e.g. urine, plasma, tissue extracts, fecal extracts) in **phenomics** research with **~250 samples/day**.





# MRMS metabolomics workflow



Hardware

+

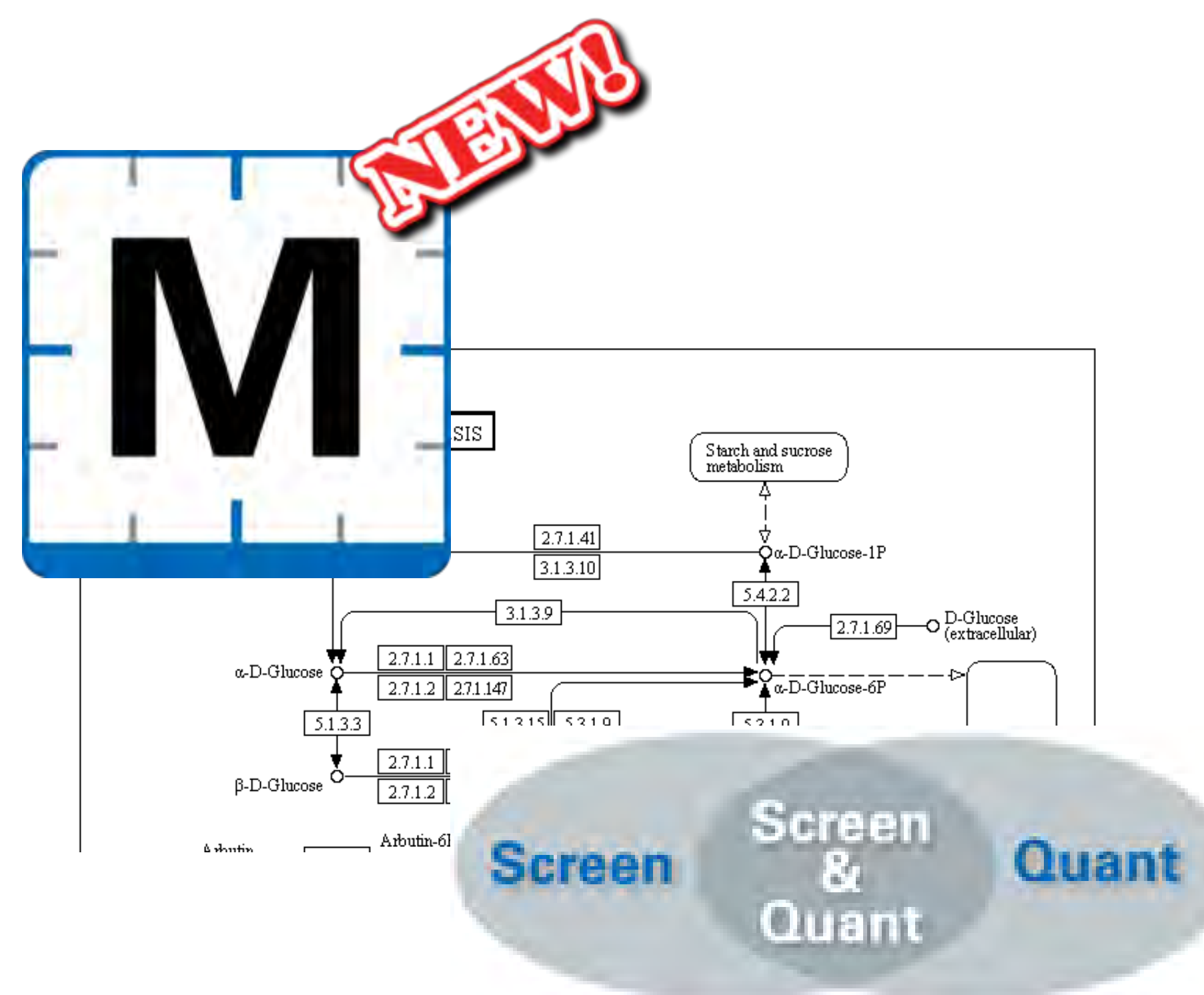
Software

+

Content



scimaX



MetaboScape + TASQ



HMDB Metabolite Library



MetaboBASE Personal Library

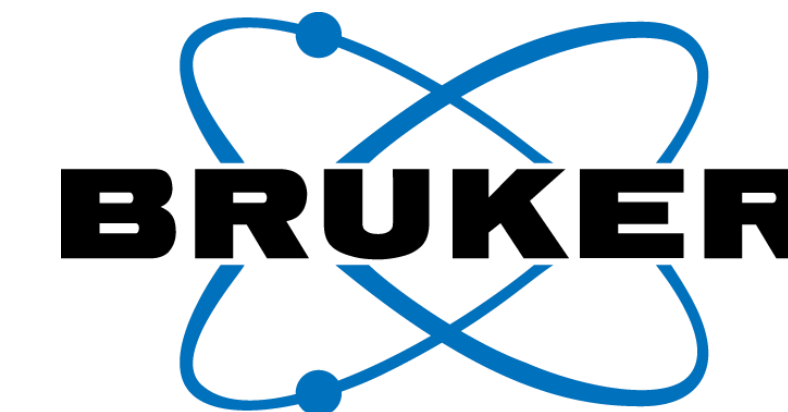


MetaboBASE Plant Library

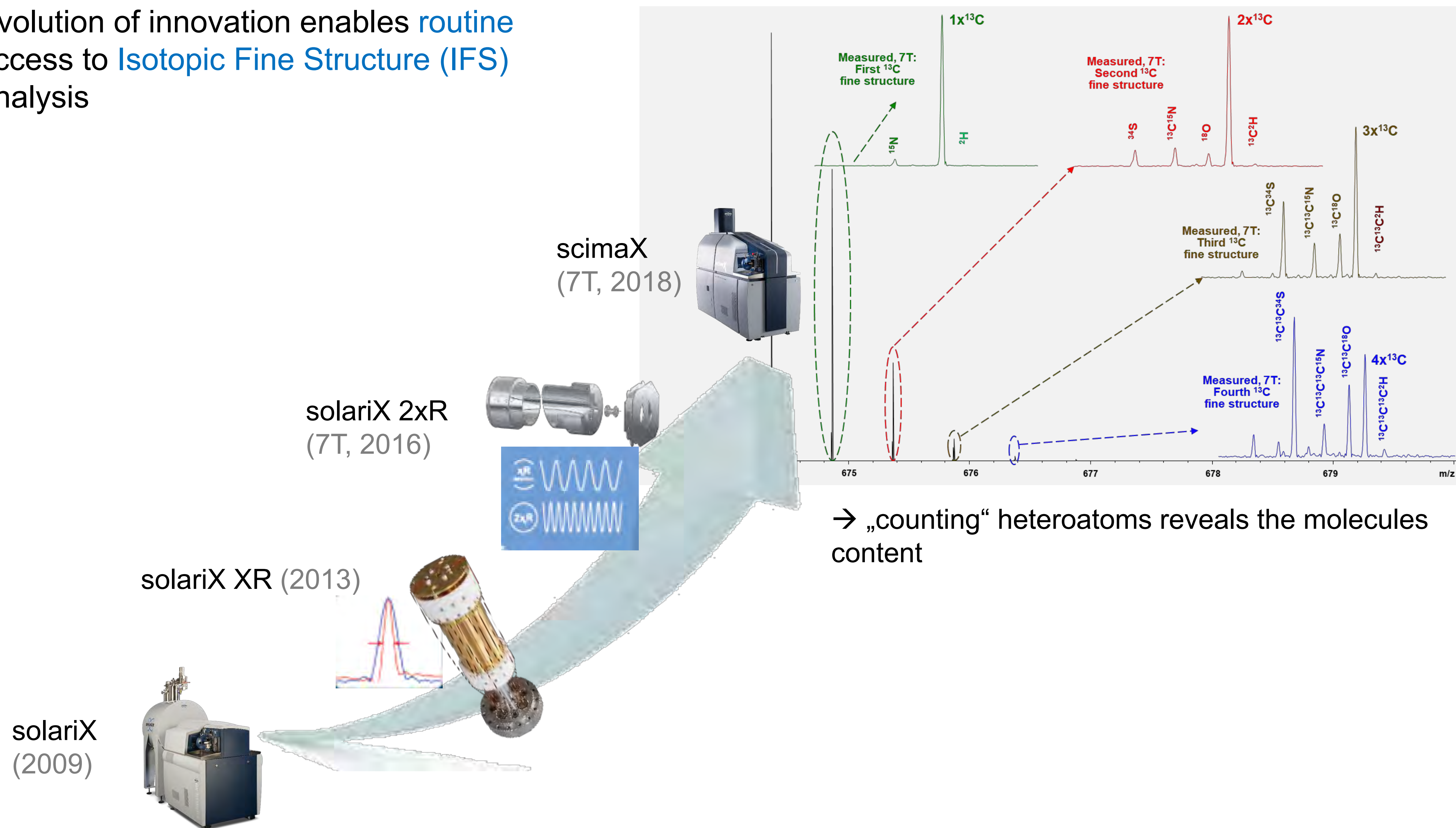




# MRMS Technical innovations

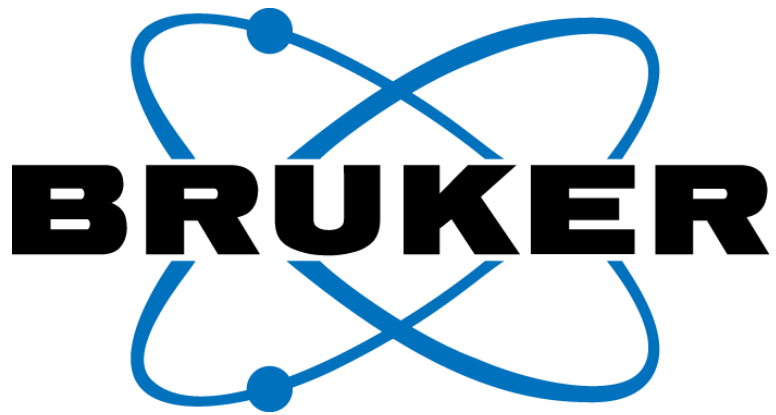


Evolution of innovation enables routine access to **Isotopic Fine Structure (IFS)** analysis



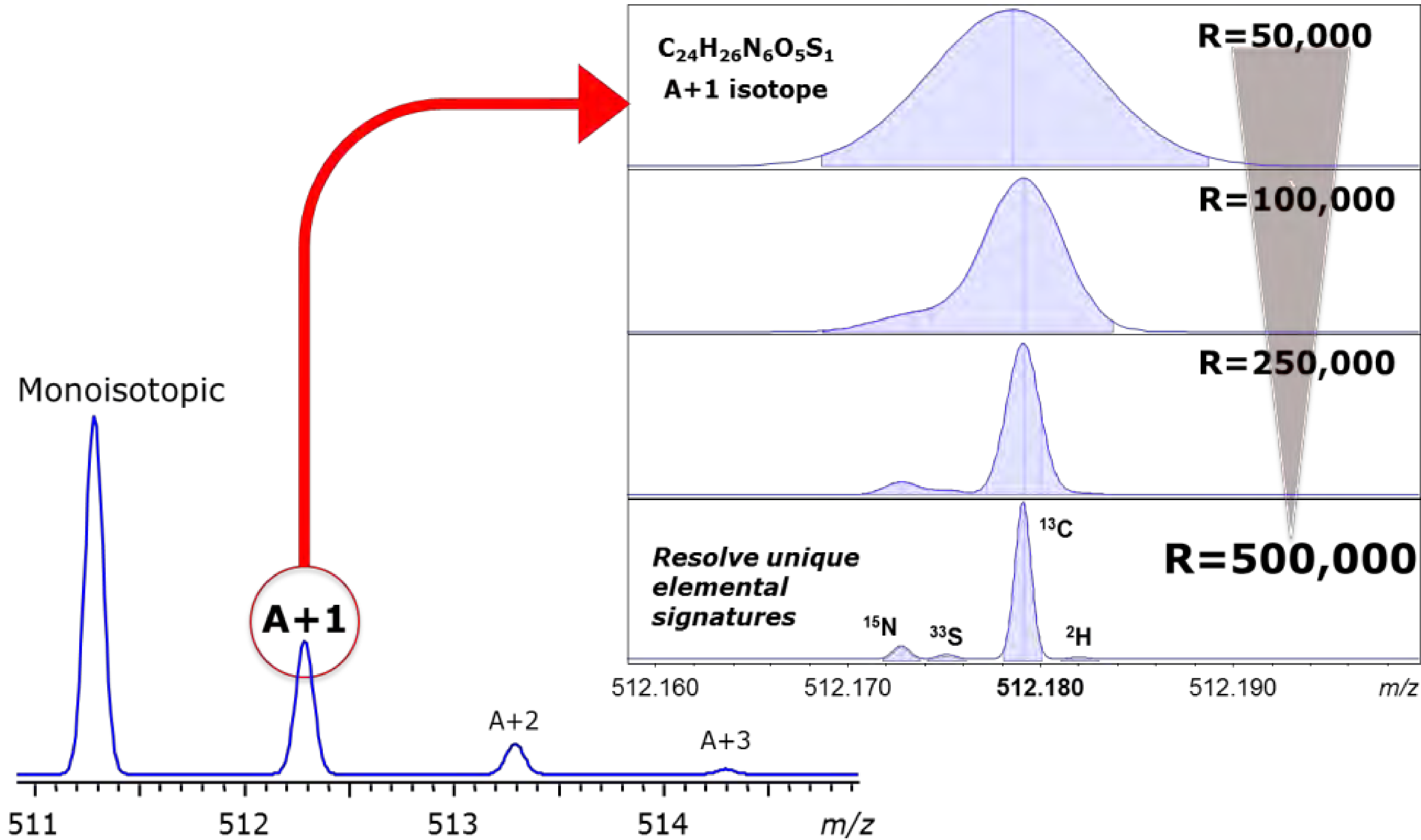


# FIA-MRMS provides Isotopic Fine Structure

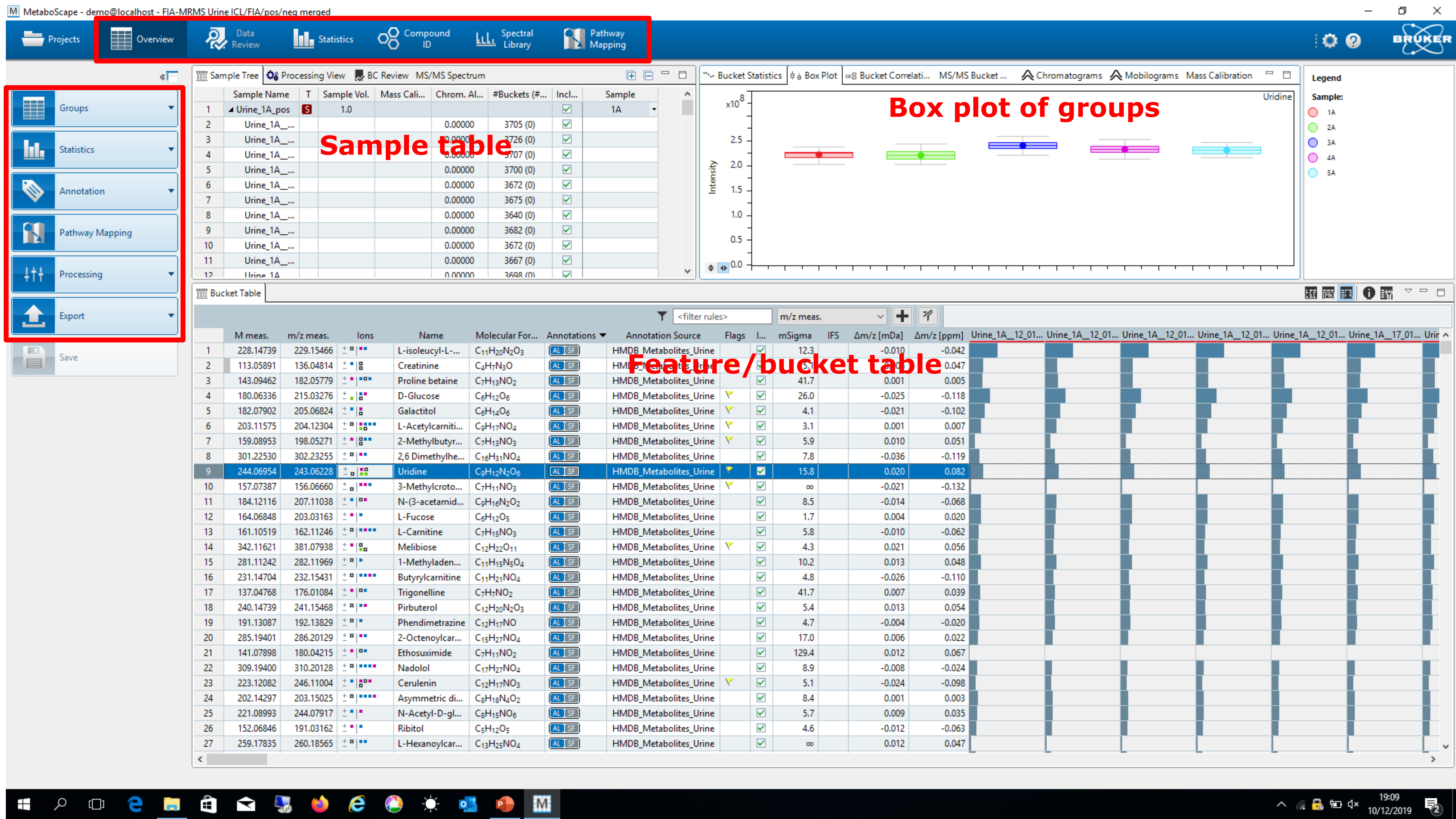


eXtreme Resolution enables confident results

Example:



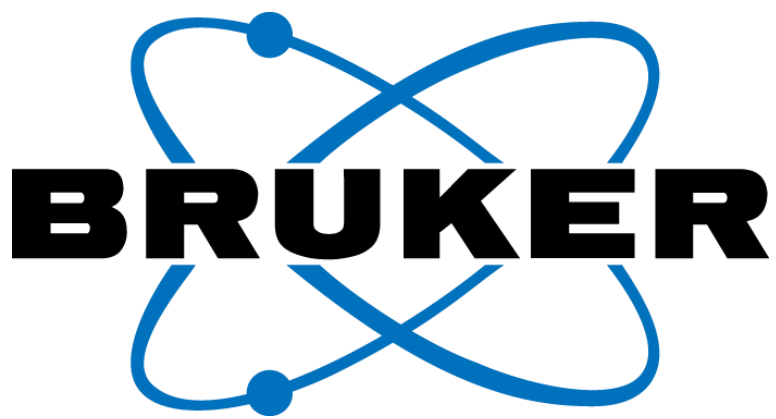




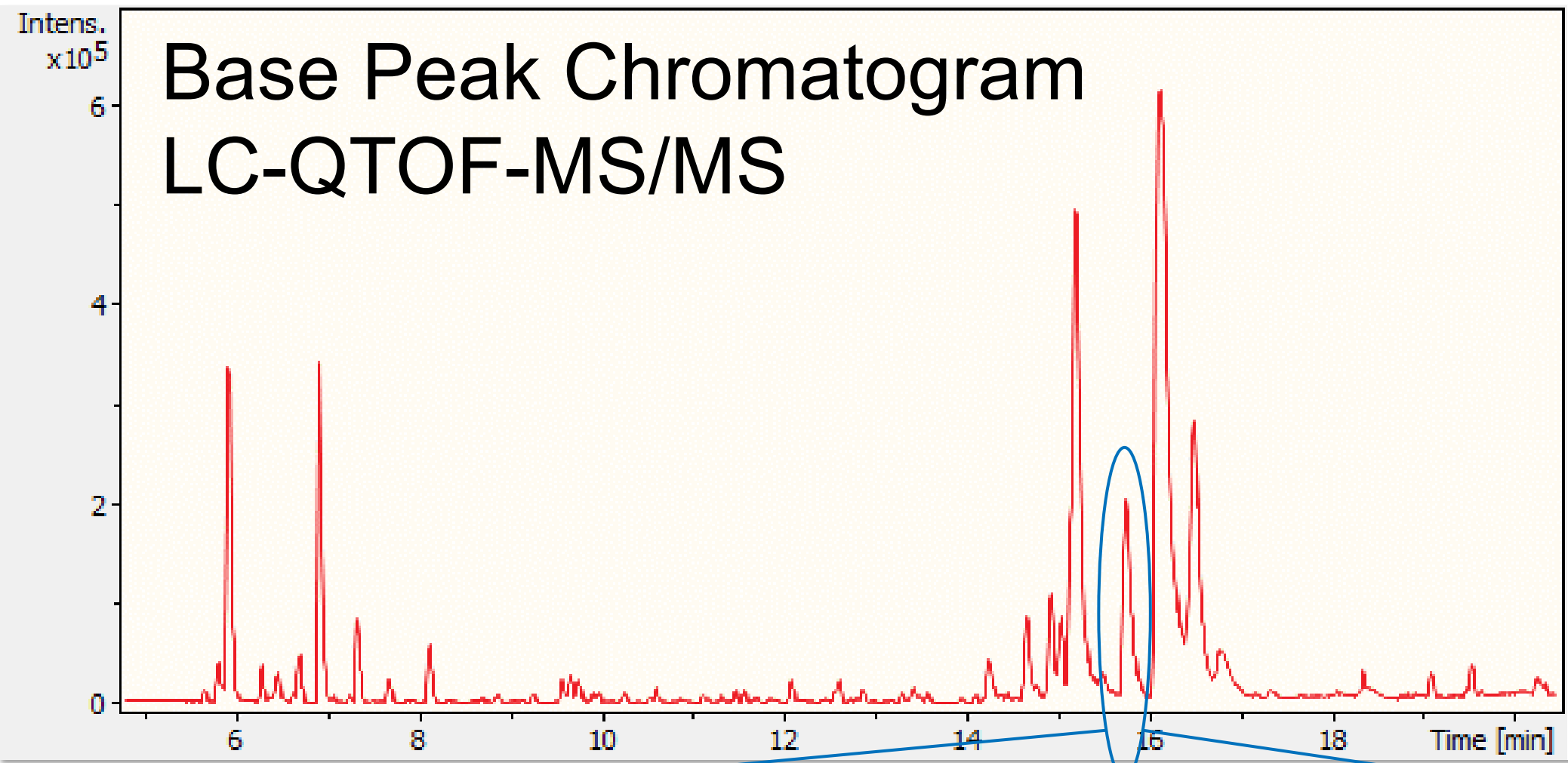


# FIA-MRMS solution

Can MRMS support the ID of unknowns in Phenomics research by generating unique molecular formulae?

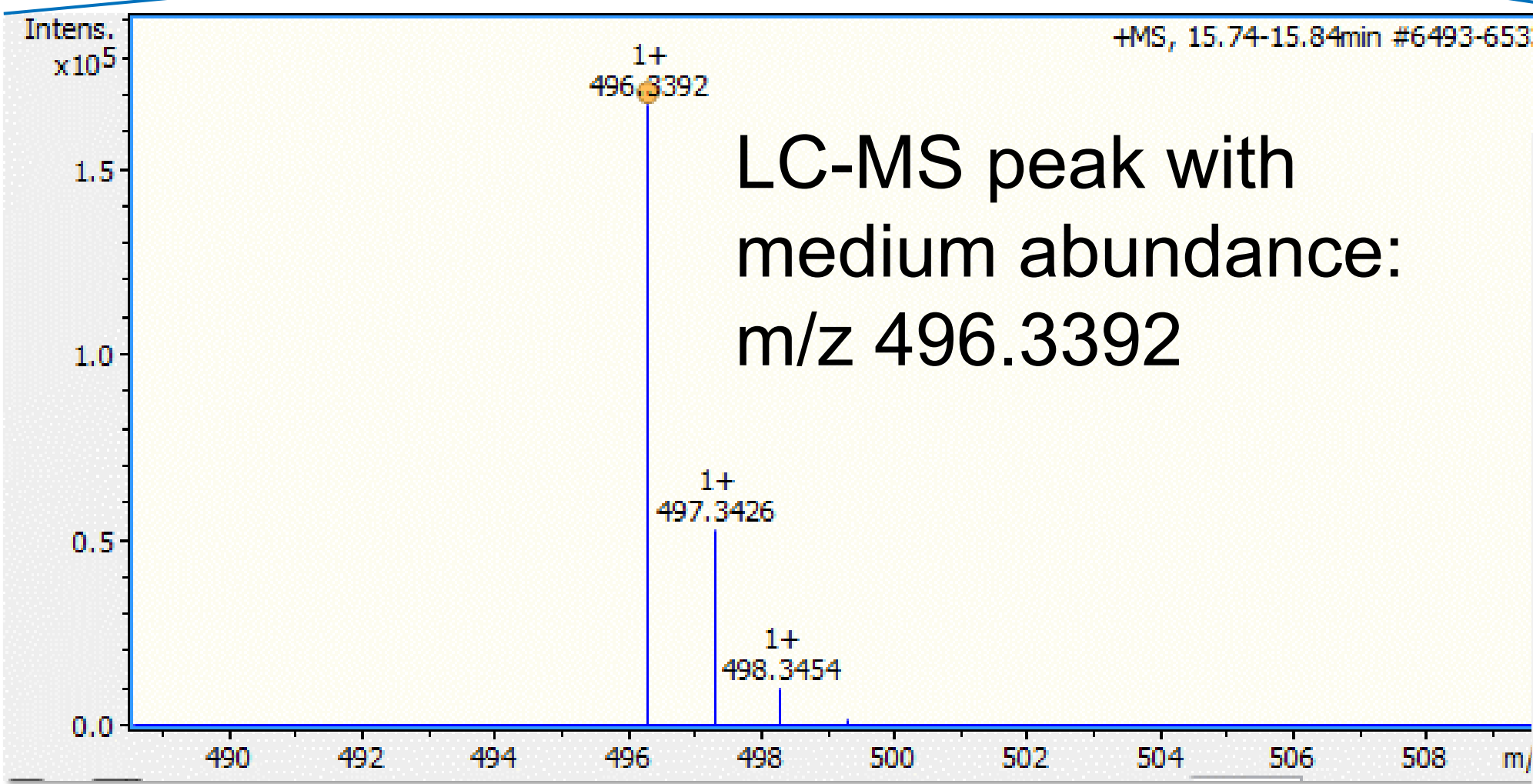
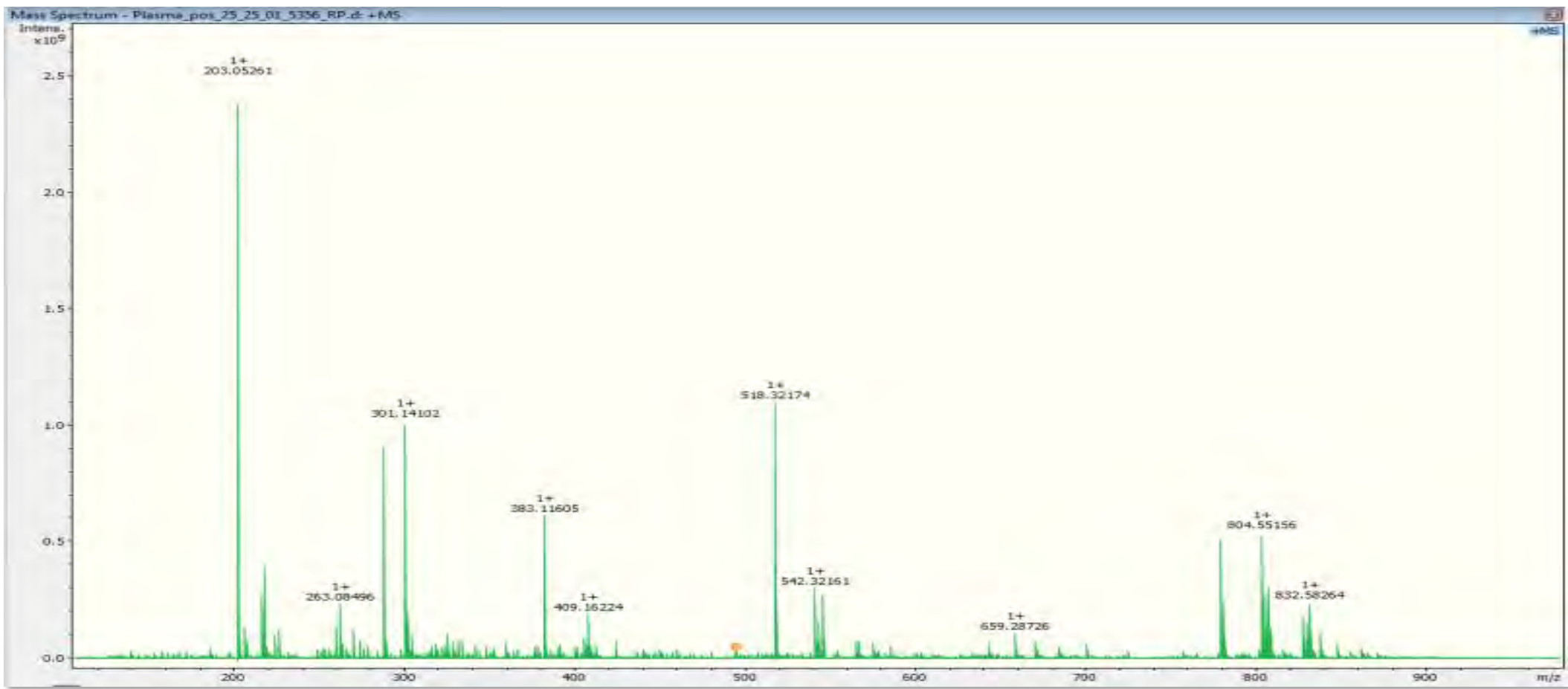


LC-QTOF-MS (~25 min turnover time)



A human Plasma extract analyzed by  
<- LC-QTOF-MS/MS (impact II)  
and FIA-MRMS (solarix XR 7T)  
->

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



Lower formula: C<sub>22</sub>P<sub>1</sub>

Upper formula:

C 22-n, P 1-n

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos. M+H

Adducts, neg. M-H

Measured m/z 496.3392

Tolerance: 2 ppm

Charge: 1

Generate

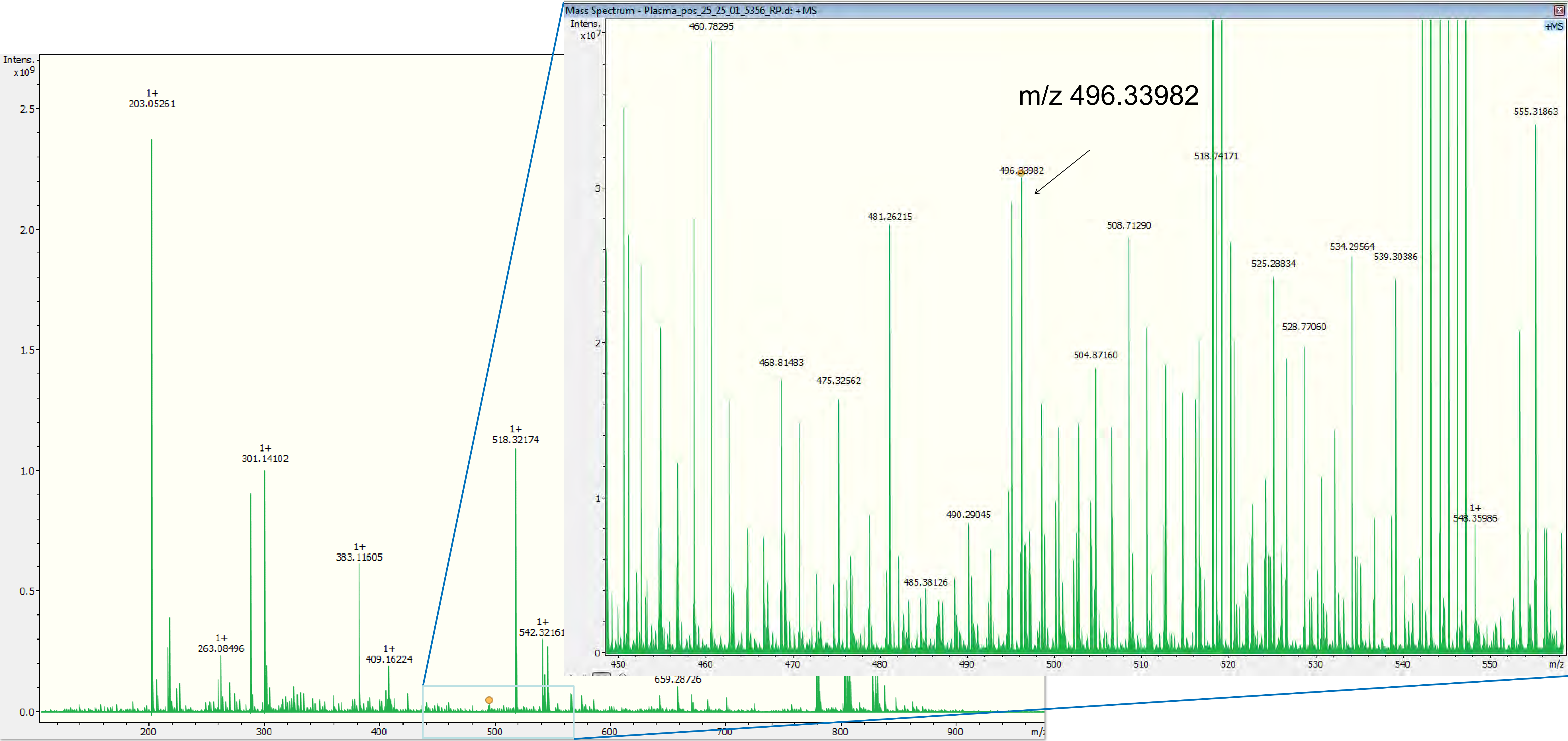
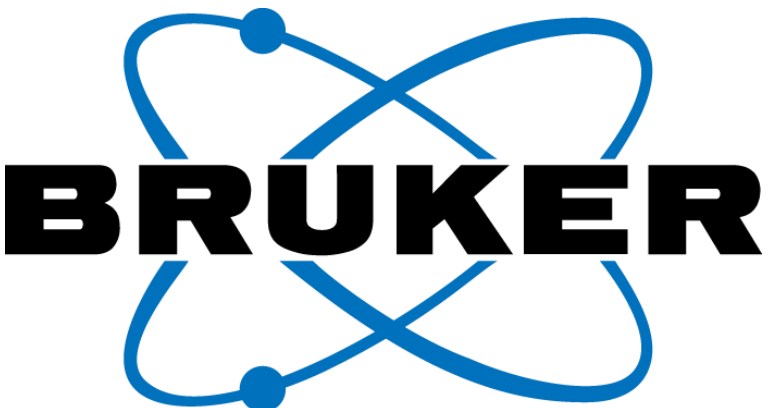
Help

Meas. m/z	#	Ion Formula	m/z	err [ppm]	err [mDa]	mSigma	# mSigma	Score	rdb	e <sup>-</sup> Conf
496.3392	1	C <sub>28</sub> H <sub>53</sub> NP <sub>3</sub>	496.3385	-1.4	-0.7	7.8	1	93.58	5.0	even
496.3392	2	C <sub>24</sub> H <sub>51</sub> NO <sub>7</sub> P	496.3398	1.1	0.5	22.9	2	100.00	1.0	even



# FIA-MRMS single spectra analysis

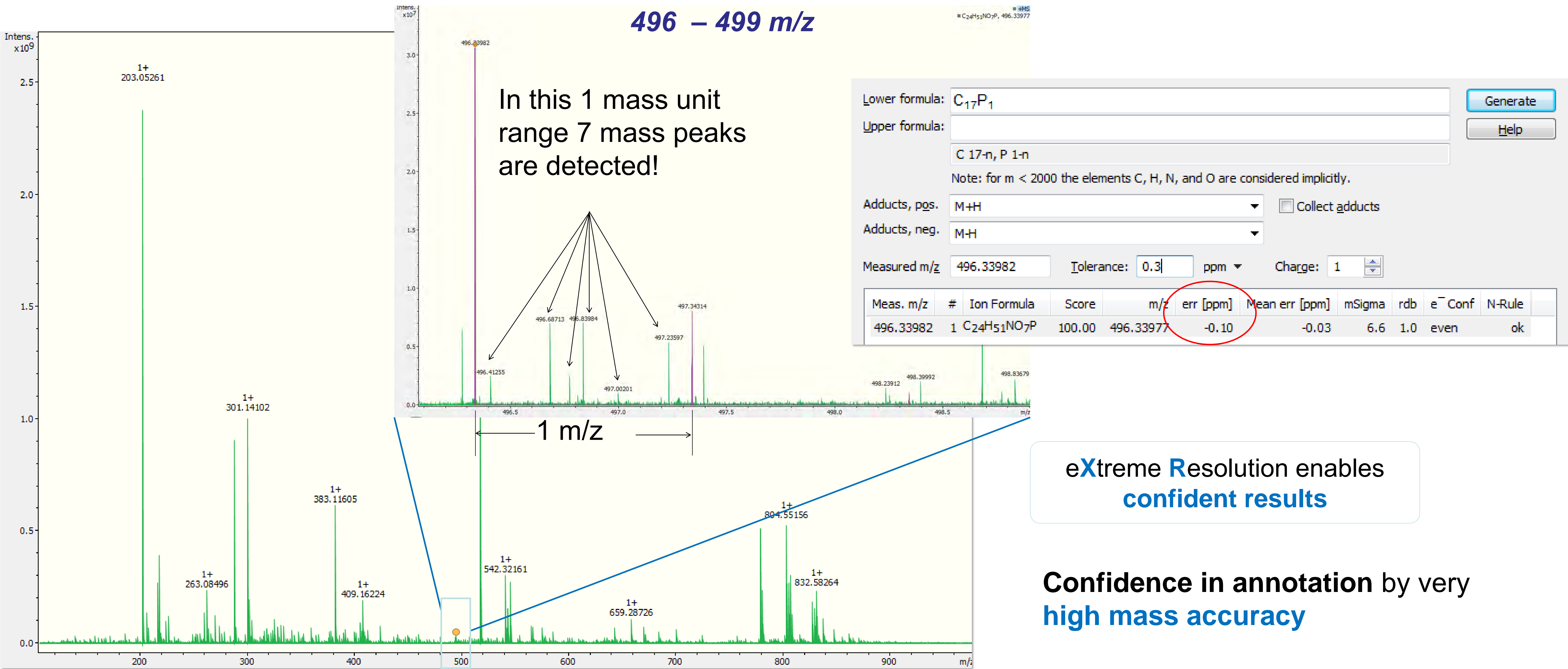
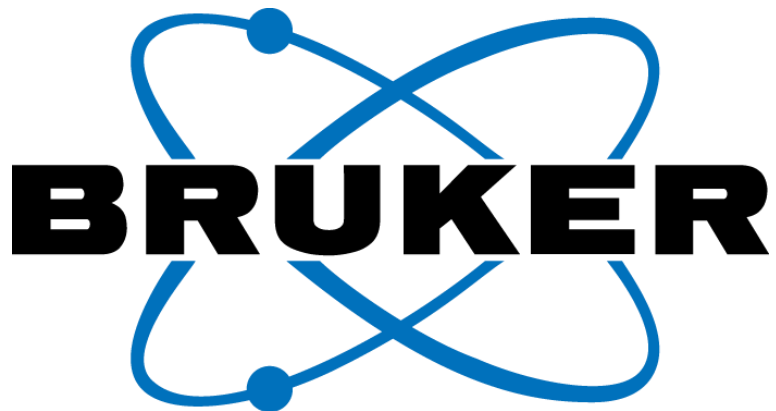
Zoom-in reveals data richness





# FIA-MRMS single spectra analysis

Example: target mass 496.3392 m/z



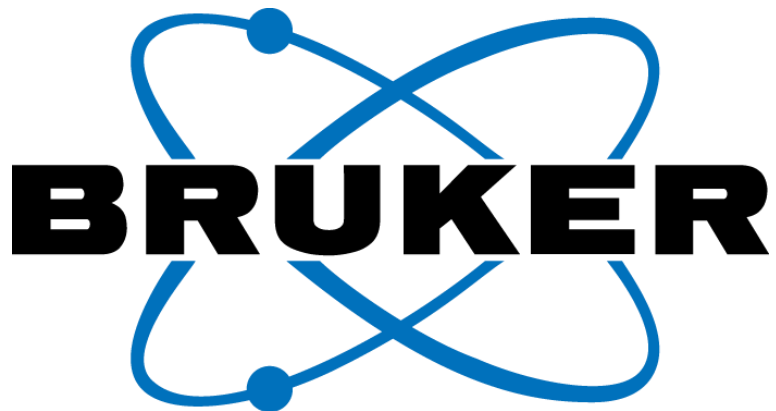
eXtreme Resolution enables confident results

Confidence in annotation by very high mass accuracy



# FIA-MRMS single spectra analysis

Example: target mass 496.3392 m/z



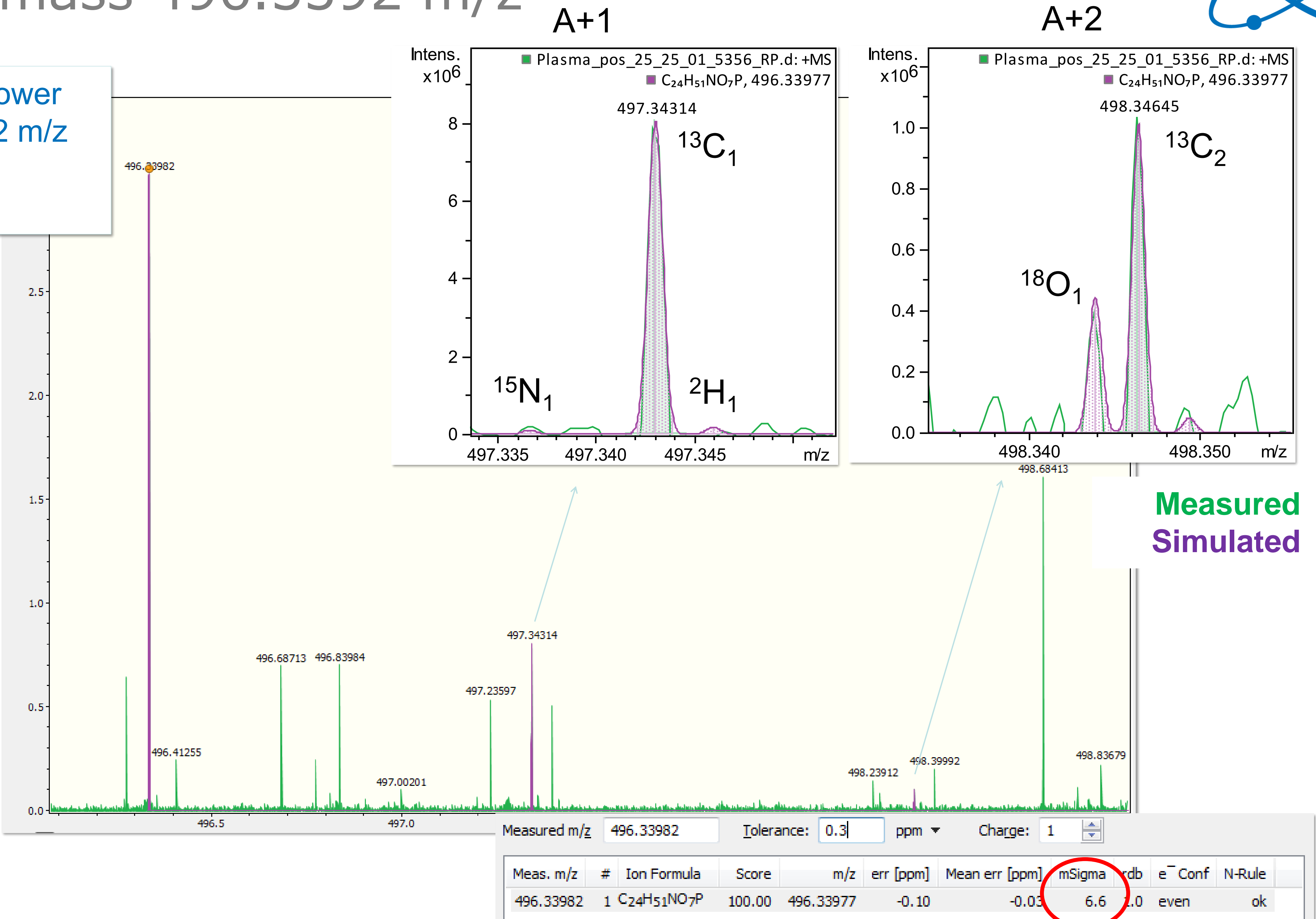
Resolving Power  
@ 496.33982 m/z

575.000

eXtreme Resolution enables  
confident results

Isotopic Fine Structure  
information allows  
elemental **formula** to be  
**READ** directly from  
extreme resolution mass  
spectra.

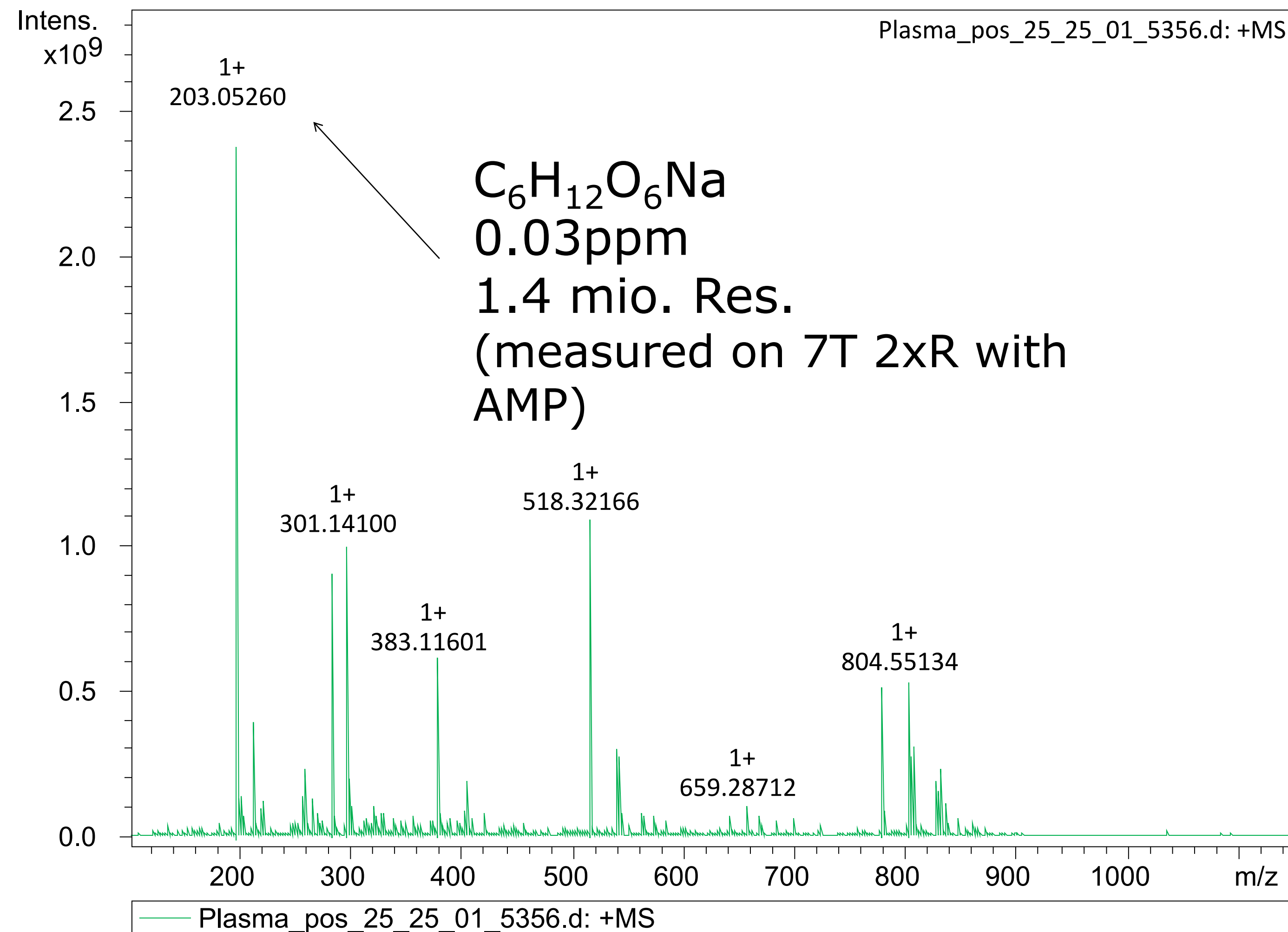
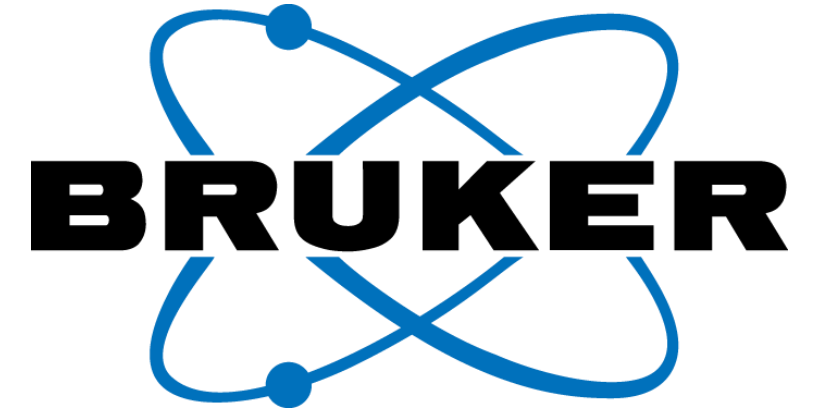
**mSigma value:**  
Expresses the matching of  
measured and theoretical  
isotopic pattern in a  
numerical value – the lower  
value the better the fit  
(Scale 0-1000).





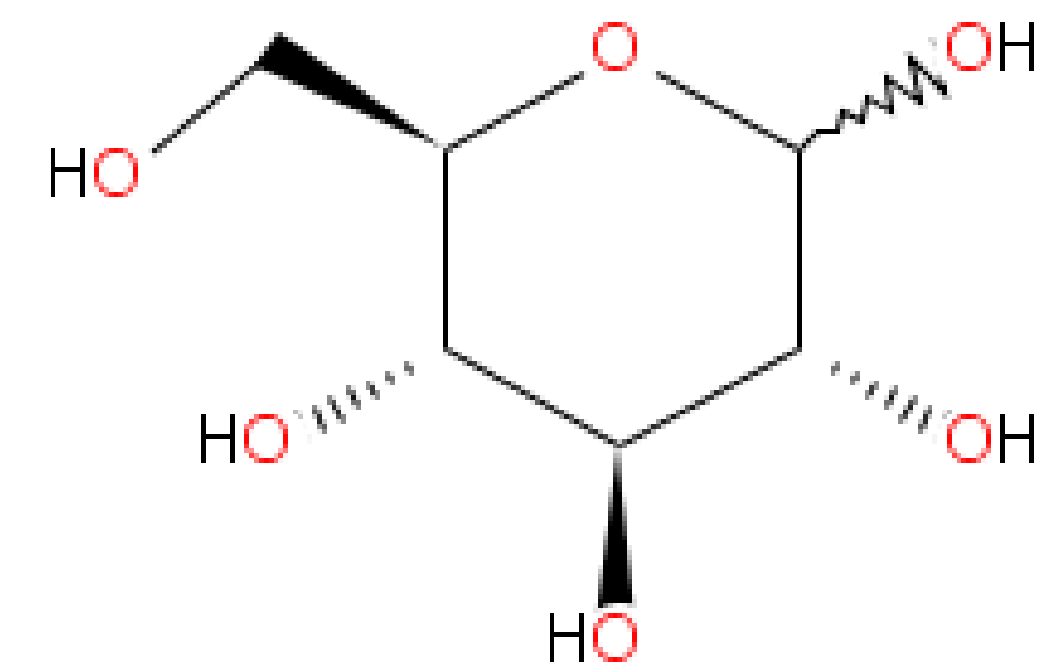
# FIA-MRMS high-throughput solution

Access compounds not readily detectable by LC-MS analysis:



- Like  $C_6H_{12}O_6Na$  = *hexose sugars* in plasma extract
- Hexose sugars are not well retained on reversed phase LC-MS and therefore typically not detected!

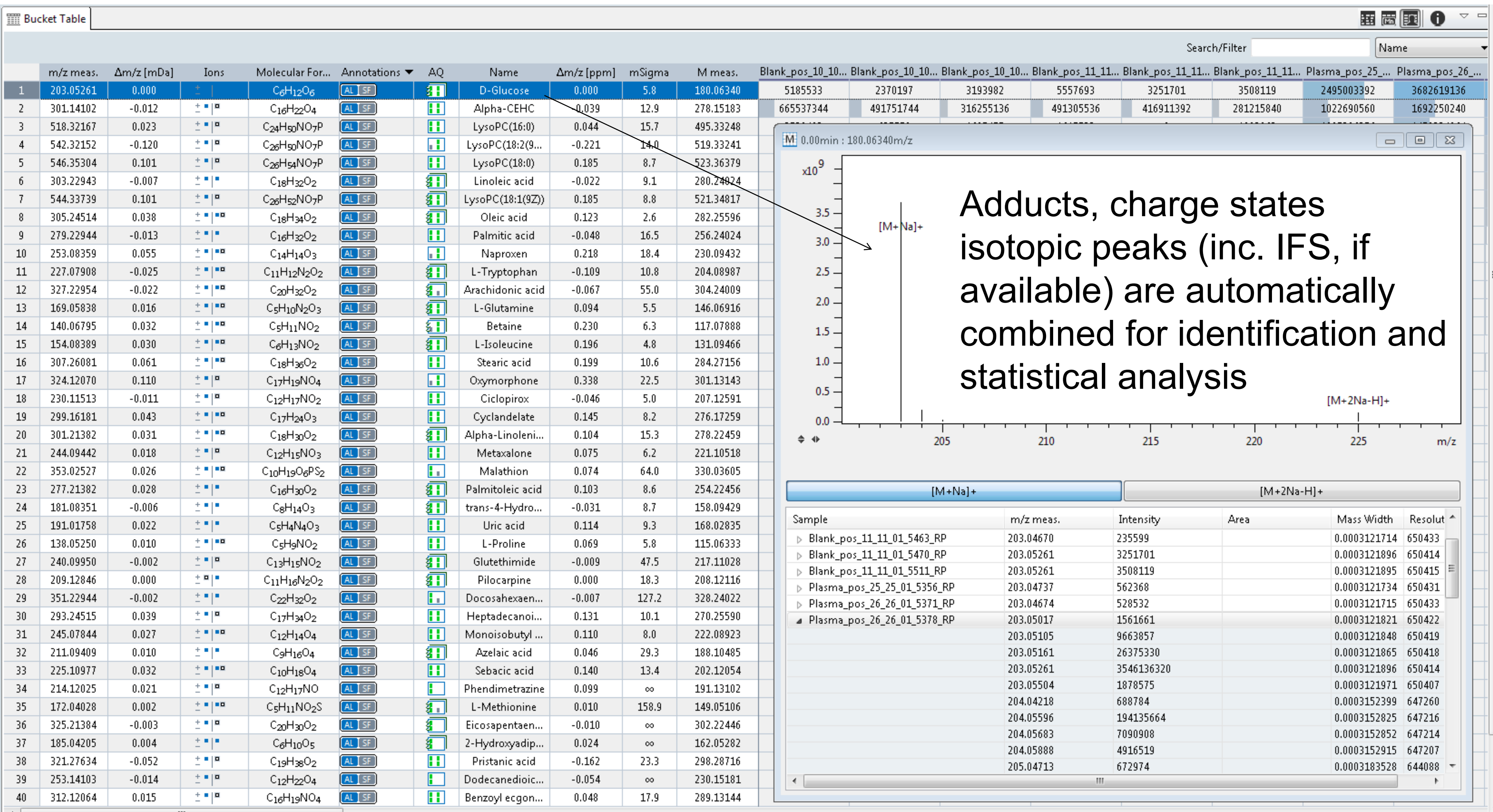
- Glucose a hexose sugar



- **Glucose is the typical biomarker in diabetes**



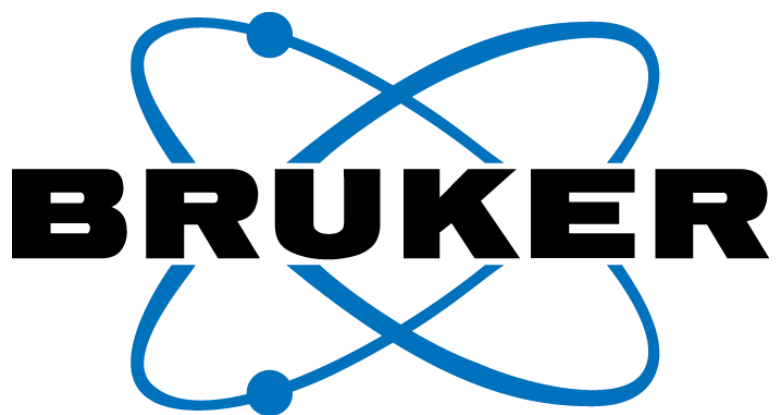
Automatic declustering & deisotoping *Simplifies* the data for statistical analysis



- Here, 3963 reproducibly extracted buckets were deisotoped and declustered from the FIA-MRMS data of the plasma extract by T-ReX 2D.



# MetaboScape - Automatic Annotation



Analyte List: >4,500 Human plasma metabolites from HMDB ([www.hmdb.ca/](http://www.hmdb.ca/))

Bucket Table

	m/z meas.	Δm/z [mDa]	Ions	Molecular For...	Annotations	AQ	Name	Δm/z [ppm]	mSigma	M meas.	Blank_pos_10_10...	Blank_pos_10_10...	Blank_pos_10_10...	Blank_pos_11_11...	Blank_pos_11_11...	Blank_pos_11_11...	Plasma_pos_25
1	203.05261	0.000	+	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	AL SF		D-Glucose	0.000	5.8	180.06340	5185533	2370197	3193982	5557693	3251701	3508119	2495003392
2	301.14102	-0.012	+	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	AL SF		Alpha-CEHC	-0.039	12.9	278.15183							
3	518.32167	0.023	+	C <sub>24</sub> H <sub>50</sub> NO <sub>7</sub> P	AL SF		LysoPC(16:0)	0.044	15.7	495.33248							
4	542.32152	-0.120	+	C <sub>26</sub> H <sub>50</sub> NO <sub>7</sub> P	AL SF		LysoPC(18:2(9...	-0.221	14.0	519.33241							
5	546.35304	0.101	+	C <sub>26</sub> H <sub>54</sub> NO <sub>7</sub> P	AL SF		LysoPC(18:0)	0.185	8.7	523.36379							
6	303.22943	-0.007	+	C <sub>18</sub> H <sub>32</sub> O <sub>2</sub>	AL SF		Linoleic acid	-0.022	9.1	280.24024							
7	544.33739	0.101	+	C <sub>26</sub> H <sub>52</sub> NO <sub>7</sub> P	AL SF		LysoPC(18:1(9Z))	0.185	8.8	521.34817							
8	305.24514	0.038	+	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	AL SF		Oleic acid	0.123	2.6	282.25596							
9	279.22944	-0.013	+	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	AL SF		Palmitic acid	-0.048	16.5	256.24024							
10	253.08359	0.055	+	C <sub>14</sub> H <sub>14</sub> O <sub>3</sub>	AL SF		Naproxen	0.218	18.4	230.09432							
11	227.07908	-0.025	+	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	AL SF		L-Tryptophan	-0.109	10.8	204.08987							
12	327.22954	-0.022	+	C <sub>20</sub> H <sub>32</sub> O <sub>2</sub>	AL SF		Arachidonic acid	-0.067	55.0	304.24009							
13	169.05838	0.016	+	C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	AL SF		L-Glutamine	0.094	5.5	146.06916							
14	140.06795	0.032	+	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	AL SF		Betaine	0.230	6.3	117.07888							
15	154.08389	0.030	+	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>	AL SF		L-Isoleucine	0.196	4.8	131.09466							
16	307.26081	0.061	+	C <sub>18</sub> H <sub>36</sub> O <sub>2</sub>	AL SF		Stearic acid	0.199	10.6	284.27156							
17	324.12070	0.110	+	C <sub>17</sub> H <sub>19</sub> NO <sub>4</sub>	AL SF		Oxymorphone	0.338	22.5	301.13143							
18	230.11513	-0.011	+	C <sub>12</sub> H <sub>17</sub> NO <sub>2</sub>	AL SF		Ciclopirox	-0.046	5.0	207.12591							
19	299.16181	0.043	+	C <sub>17</sub> H <sub>24</sub> O <sub>3</sub>	AL SF		Cyclandelate	0.145	8.2	276.17259							
20	301.21382	0.031	+	C <sub>18</sub> H <sub>30</sub> O <sub>2</sub>	AL SF		Alpha-Linoleni...	0.104	15.3	278.22459							
21	244.09442	0.018	+	C <sub>12</sub> H <sub>15</sub> NO <sub>3</sub>	AL SF		Metaxalone	0.075	6.2	221.10518							
22	353.02527	0.026	+	C <sub>10</sub> H <sub>19</sub> O <sub>6</sub> PS <sub>2</sub>	AL SF		Malathion	0.074	64.0	330.03605							
23	277.21382	0.028	+	C <sub>16</sub> H <sub>30</sub> O <sub>2</sub>	AL SF		Palmitoleic acid	0.103	8.6	254.22456							
24	181.08351	-0.006	+	C <sub>8</sub> H <sub>14</sub> O <sub>3</sub>	AL SF		trans-4-Hydro...	-0.031	8.7	158.09429							
25	191.01758	0.022	+	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>	AL SF		Uric acid	0.114	9.3	168.02835							
26	138.05250	0.010	+	C <sub>9</sub> H <sub>9</sub> NO <sub>2</sub>	AL SF		L-Proline	0.069	5.8	115.06333							
27	240.09950	-0.002	+	C <sub>13</sub> H <sub>15</sub> NO <sub>2</sub>	AL SF		Glutethimide	-0.009	47.5	217.11028							
28	209.12846	0.000	+	C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>	AL SF		Pilocarpine	0.000	18.3	208.12116							
29	351.22944	-0.002	+	C <sub>22</sub> H <sub>32</sub> O <sub>2</sub>	AL SF		Docosahexaen...	-0.007	127.2	328.24022							
30	293.24515	0.039	+	C <sub>17</sub> H <sub>34</sub> O <sub>2</sub>	AL SF		Heptadecanoi...	0.131	10.1	270.25590							
31	245.07844	0.027	+	C <sub>12</sub> H <sub>14</sub> O <sub>4</sub>	AL SF		Monoisobutyl ...	0.110	8.0	222.08923							
32	211.09409	0.010	+	C <sub>9</sub> H <sub>16</sub> O <sub>4</sub>	AL SF		Azelaic acid	0.046	29.3	188.10485							
33	225.10977	0.032	+	C <sub>10</sub> H <sub>18</sub> O <sub>4</sub>	AL SF		Sebacic acid	0.140	13.4	202.12054							
34	214.12025	0.021	+	C <sub>12</sub> H <sub>17</sub> NO	AL SF		Phendimetrazine	0.099	∞	191.13102							
35	172.04028	0.002	+	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> S	AL SF		L-Methionine	0.010	158.9	149.05106							
36	325.21384	-0.003	+	C <sub>20</sub> H <sub>30</sub> O <sub>2</sub>	AL SF		Eicosapentaen...	-0.010	∞	302.22446							
37	185.04205	0.004	+	C <sub>6</sub> H <sub>10</sub> O <sub>5</sub>	AL SF		2-Hydroxyadip...	0.024	∞	162.05282							

Search/Filter

Manage Analyte List

Edit or import Analyte List and optionally connect to Spectral Library.

Select Analyte List: 

HMDB\_plasma\_from web\_4546\_MpHp\_MmHm

ExportDelete

Import from file: ImportGet Template

Automatically assign Analyte entries to compounds from MS/MS library: 

MoNA-export-LipidBlast.msp

Assign

#	Name	Molecular Formula	Neutral Ma...	RT [min]	Library Compound
4527	N-Desalkyl flurazepam	C <sub>15</sub> H <sub>10</sub> ClFN <sub>2</sub> O	288.04657	0.00	Click to assign MS/MS lib...
4528	N-Mononitrosopiperazine	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O	114.07931	0.00	Click to assign MS/MS lib...
4529	N-Nitroso-3-hydroxypyrrolidine	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	116.05858	0.00	Click to assign MS/MS lib...
4530	N-Trifluoroacetyladiamycin	C <sub>29</sub> H <sub>28</sub> F <sub>3</sub> NO <sub>12</sub>	639.15636	0.00	Click to assign MS/MS lib...
4531	N,N-Didemethyl orphenadrine	C <sub>16</sub> H <sub>19</sub> NO	241.14666	0.00	Click to assign MS/MS lib...
4532	N,N,O-Didesmethylvenlafaxine	C <sub>17</sub> H <sub>27</sub> NO <sub>2</sub>	277.20418	0.00	Click to assign MS/MS lib...
4533	N,O-Didesmethylvenlafaxine glucur	C <sub>21</sub> H <sub>31</sub> NO <sub>8</sub>	425.20497	0.00	Click to assign MS/MS lib...
4534	N2-Monodes-methylinazidine	C <sub>11</sub> H <sub>19</sub> N <sub>5</sub> O <sub>2</sub> S <sub>2</sub>	317.09802	0.00	Click to assign MS/MS lib...
4535	nor-Levomethadyl acetate	C <sub>22</sub> H <sub>29</sub> NO <sub>2</sub>	339.21983	0.00	Click to assign MS/MS lib...
4536	Norfluoxetine glucuronide	C <sub>22</sub> H <sub>24</sub> F <sub>3</sub> NO <sub>8</sub>	487.14540	0.00	Click to assign MS/MS lib...
4537	O-Desmethylvenlafaxine glucuronid	C <sub>20</sub> H <sub>29</sub> NO <sub>8</sub>	411.18932	0.00	Click to assign MS/MS lib...
4538	p-Chlorobenzenesulfonamide	C <sub>6</sub> H <sub>6</sub> ClNO <sub>2</sub> S	190.98078	0.00	Click to assign MS/MS lib...
4539	p-Hydroxyl-ethotoin	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>	220.08479	0.00	Click to assign MS/MS lib...
4540	p-Hydroxynordiazepam	C <sub>15</sub> H <sub>11</sub> ClN <sub>2</sub> O <sub>2</sub>	286.05091	0.00	Click to assign MS/MS lib...
4541	Phenylacetic acid-N-isopropylnoctr	C <sub>27</sub> H <sub>34</sub> BrNO <sub>4</sub>	515.16712	0.00	Click to assign MS/MS lib...
4542	Pyridine N-oxide glucuronide	C <sub>11</sub> H <sub>14</sub> NO <sub>7</sub>	272.07703	0.00	Click to assign MS/MS lib...
4543	Trandolapril-d5 Diketopiperazine	C <sub>24</sub> H <sub>32</sub> N <sub>2</sub> O <sub>4</sub>	412.23621	0.00	Click to assign MS/MS lib...
4544	Trilecan glucuronide	C <sub>24</sub> H <sub>24</sub> Cl <sub>2</sub> O <sub>8</sub>	462.08225	0.00	Click to assign MS/MS lib...

Type to filter. Delete selected Analyte

< BackNext >FinishCancel

226

697.58955

0.149

+

C<sub>47</sub>H<sub>78</sub>O<sub>2</sub>

AL SF

CE(20:3(8Z,11Z...

0.213

∞

674.600

227

278.09186

0.053

+

C<sub>13</sub>H<sub>18</sub>ClNO<sub>2</sub>

AL

Hydroxybupro...

0.191

185.3

255.102

228

198.08490

-0.009

+

C<sub>6</sub>H<sub>13</sub>N<sub>3</sub>O<sub>3</sub>

AL

Citrulline

-0.043

241.1

175.095

229

140.90356

-0.066

+

CHCl<sub>3</sub>

AL

Chloroform

-0.469

∞

117.914

230

229.03190

0.028

+

C<sub>7</sub>H<sub>10</sub>O<sub>7</sub>

AL

2-Methylcitric ...

0.124

394.6

206.042

231

148.00391

0.015

+

C<sub>2</sub>H<sub>7</sub>NO<sub>3</sub>S

AL

Taurine

0.102

∞

125.014

Target list derived from Human Metabolome Data Base (HMDB)

Annotation Quality Scoring

231 automatic annotations

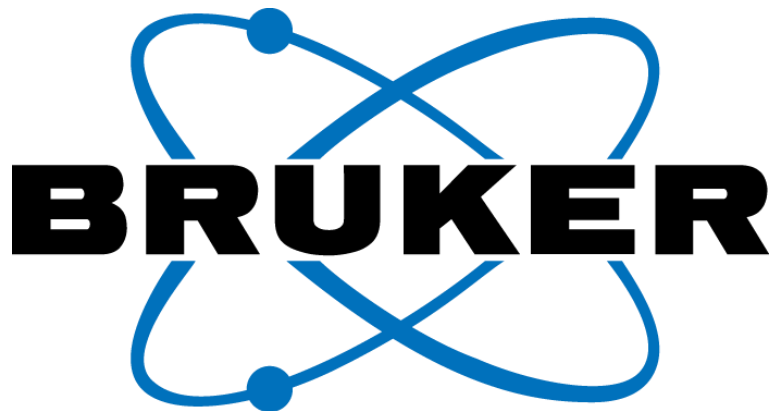
196 within 0.2 ppm mass accuracy

Mass accuracy

Isotopic pattern quality



# MetaboScape - Automatic Annotation



SmartFormula: Mass Accuracy, True Isotopic Pattern & Isotopic Fine Structure

Bucket Table

	m/z meas.	$\Delta m/z$ [mDa]	Ions	Molecular For...	Annotations	AQ	Name	$\Delta m/z$ [ppm]	mSigma	M meas.
2450	954.44852	0.013	$^{+1}$	C <sub>50</sub> H <sub>61</sub> N <sub>9</sub> O <sub>9</sub>	SF			0.013	∞	931.45930
2451	925.72484	-0.055	$^{+1}$	C <sub>51</sub> H <sub>102</sub> N <sub>2</sub> O <sub>8</sub> S	SF			-0.059	∞	902.73562
2452	379.20921	0.072	$^{+1}$	C <sub>19</sub> H <sub>32</sub> O <sub>6</sub>	SF			0.189	∞	356.21999
2453	1130.40994	-0.002	$^{+1}$	C <sub>37</sub> H <sub>77</sub> N <sub>3</sub> O <sub>32</sub> S	SF			-0.002	∞	1107.42072
2454	531.51116	-0.108	$^{+1}$	C <sub>34</sub> H <sub>68</sub> O <sub>2</sub>	SF			-0.204	∞	508.52194
2455	447.41727	-0.011	$^{+1}$	C <sub>28</sub> H <sub>58</sub> O <sub>2</sub>	SF			-0.023	∞	424.42805
2456	697.63219	-0.218	$^{+1}$	C <sub>34</sub> H <sub>66</sub> N <sub>6</sub> O <sub>4</sub> S	SF			-0.312	∞	674.64296
2457	869.69911	0.028	$^{+1}$	C <sub>41</sub> H <sub>96</sub> N <sub>8</sub> O <sub>5</sub> S <sub>2</sub>	SF			0.033	∞	846.70989
2458	856.02576	0.005	$^{+1}$	C <sub>24</sub> H <sub>51</sub> NO <sub>6</sub> S <sub>12</sub>	SF			0.005	∞	833.03654
2459	769.49608	0.057	$^{+1}$	C <sub>36</sub> H <sub>79</sub> N <sub>2</sub> O <sub>7</sub> PS <sub>2</sub>	SF			0.074	∞	746.50686
2460	856.54354	-0.068	$^{+1}$	C <sub>41</sub> H <sub>87</sub> NO <sub>9</sub> S <sub>3</sub>	SF			-0.079	∞	833.55432
2461	801.69422	-0.078	$^{+1}$	C <sub>42</sub> H <sub>102</sub> N <sub>2</sub> O <sub>3</sub> S <sub>3</sub>	SF			-0.097	101.4	778.70500
2462	667.95641	-0.007	$^{+1}$	C <sub>29</sub> H <sub>111</sub> NO <sub>13</sub> S <sub>2</sub>	SF			-0.010	∞	644.96719
2463	440.87823	0.149	$^{+1}$	C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> S <sub>7</sub>	SF			0.338	∞	417.88901
2464	884.57486	-0.004	$^{+1}$	C <sub>36</sub> H <sub>99</sub> N <sub>3</sub> O <sub>6</sub> S <sub>6</sub>	SF			-0.005	∞	861.58564
2465	911.11830	-0.001	$^{+1}$	C <sub>36</sub> H <sub>34</sub> N <sub>4</sub> O <sub>19</sub> P <sub>2</sub>	SF			-0.001	∞	888.12908
2466	633.50629	-0.016	$^{+1}$	C <sub>37</sub> H <sub>70</sub> O <sub>6</sub>	SF			-0.025	∞	610.51707
2467	382.95951	-0.075	$^{+1}$	C <sub>8</sub> H <sub>8</sub> N <sub>8</sub> O <sub>4</sub>	SF			-0.196	∞	359.97029
2468	306.07448	0.121	$^{+1}$	C <sub>9</sub> H <sub>13</sub> N <sub>7</sub> O <sub>2</sub> S	SF			0.396	∞	283.08526
2469	874.57090	-0.012	$^{+1}$	C <sub>45</sub> H <sub>83</sub> N <sub>5</sub> O <sub>6</sub> P <sub>2</sub>	SF			-0.014	∞	851.58168
2470	327.01737	-0.118	$^{+1}$	C <sub>10</sub> H <sub>13</sub> N <sub>2</sub> O <sub>5</sub> PS	SF			-0.361	∞	304.02815
2471	872.61837	0.008	$^{+1}$	C <sub>27</sub> H <sub>79</sub> N <sub>25</sub> O <sub>2</sub> S <sub>2</sub>	SF			0.009	∞	849.62915
2472	912.55360	0.009	$^{+1}$	C <sub>36</sub> H <sub>81</sub> N <sub>11</sub> O <sub>10</sub> P <sub>2</sub>	SF			0.009	∞	889.56438
2473	345.15206	0.075	$^{+1}$	C <sub>14</sub> H <sub>26</sub> O <sub>8</sub>	SF			0.218	∞	322.16284
2474	657.50649	0.082	$^{+1}$	C <sub>24</sub> H <sub>74</sub> N <sub>8</sub> O <sub>6</sub> S <sub>2</sub>	SF			0.125	∞	634.51727
2475	686.93227	0.007	$^{+1}$	C <sub>23</sub> H <sub>13</sub> N <sub>4</sub> O <sub>12</sub> PS <sub>3</sub>	SF			0.010	∞	663.94305
2476	321.04563	0.012	$^{+1}$	C <sub>8</sub> H <sub>15</sub> N <sub>2</sub> O <sub>8</sub> P	SF			0.037	∞	298.05641
2477	645.44673	-0.045	$^{+1}$	C <sub>29</sub> H <sub>58</sub> N <sub>12</sub> OS	SF			-0.070	∞	622.45750
2478	900.46213	-0.067	$^{+1}$	C <sub>49</sub> H <sub>71</sub> N <sub>3</sub> O <sub>7</sub> S <sub>2</sub>	SF			-0.074	83.0	877.47291
2479	649.60430	0.107	$^{+1}$	C <sub>39</sub> H <sub>82</sub> N <sub>2</sub> OS	SF			0.165	∞	626.61508
2480	972.50865	-0.016	$^{+1}$	C <sub>49</sub> H <sub>76</sub> N <sub>9</sub> O <sub>4</sub> PS <sub>2</sub>	SF			-0.017	∞	949.51943
2481	303.14146	0.047	$^{+1}$	C <sub>12</sub> H <sub>24</sub> O <sub>7</sub>	SF			0.154	∞	280.15224
2482	706.60542	0.192	$^{+1}$	C <sub>33</sub> H <sub>64</sub> N <sub>5</sub> O <sub>6</sub> P	SF			0.274	∞	677.61620
2483	316.11305	-0.030	$^{+1}$							
2484	213.02654		$^{+1}$							
2485	261.01123		$^{+1}$							
2486	328.99869		$^{+1}$							
2487	318.96983		$^{+1}$							
2488	217.95629		$^{+1}$							194.96706
2489	320.96692		$^{+1}$							297.97771

Annotate with SmartFormula

Annotate with SmartFormula

Configure SmartFormula to annotate the Bucket Table.

Tolerances and Scoring

Narrow

Wide

Unit

m/z: 0.2 0.5 ppm

mSigma: 50 200

Composition

Elements: CHNOPS

Lower formula: Estimate carbon number

Upper formula: Auto upper formula

C 0-∞, H 0-∞, N 0-∞, O 0-∞, P 0-∞, S 0-∞

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Element Ratios

☒ Apply element ratio filters

Element ratio presets: Common Extended Extreme

H/C 0.2 - 3.1 P/C 0.0 - 0.3 F/C 0.0 - 1.5

N/C 0.0 - 1.3 P/O 0.0 - 0.34 Cl/C 0.0 - 0.8

O/C 0.0 - 1.2 S/C 0.0 - 0.8 Br/C 0.0 - 0.8

Si/C 0.0 - 0.5

Filters

Electron configuration: Even (Senior and Lewis)

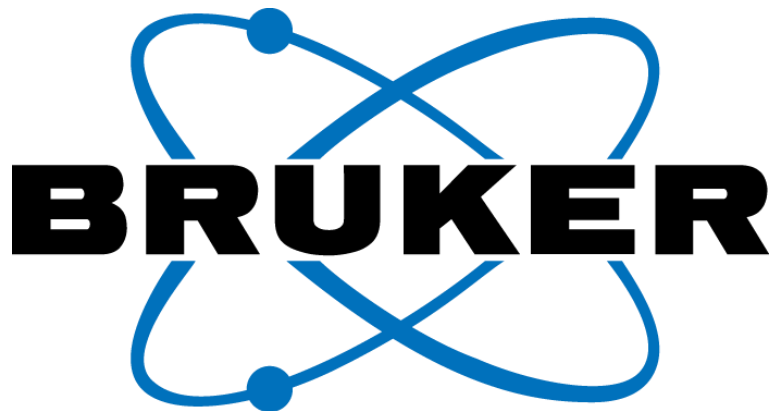
☒ Apply heuristic element count probability check.

OK Cancel

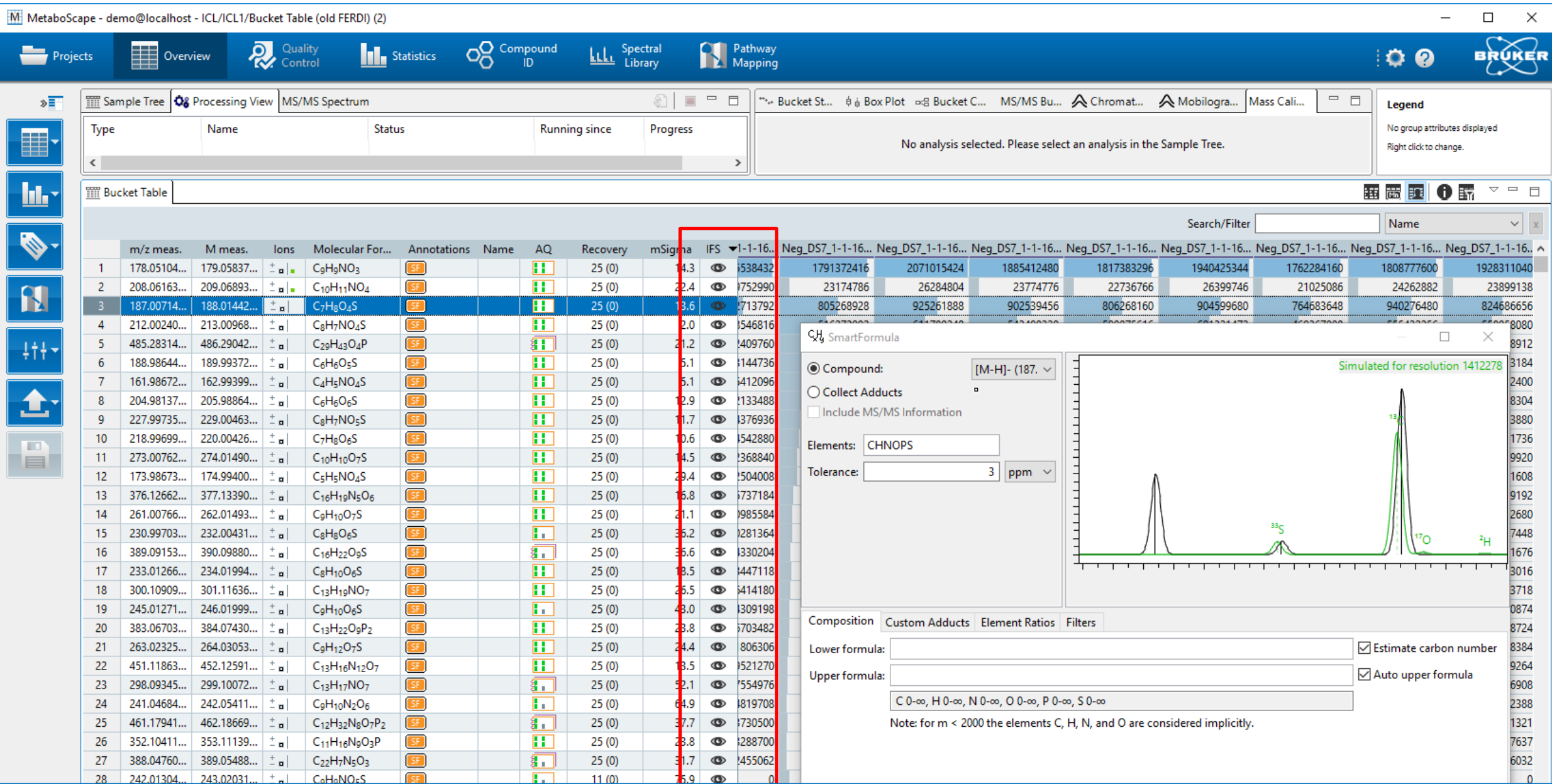
Molecular formulae automatically generated for 2,483 out of 3,963 reproducibly extracted buckets



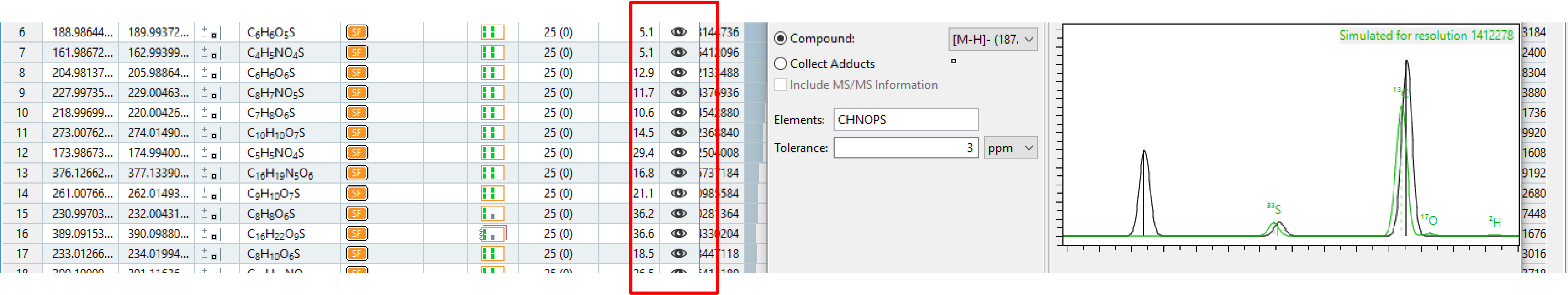
# MetaboScape - Automatic Annotation



SmartFormula: Mass Accuracy, True Isotopic Pattern & Isotopic Fine Structure



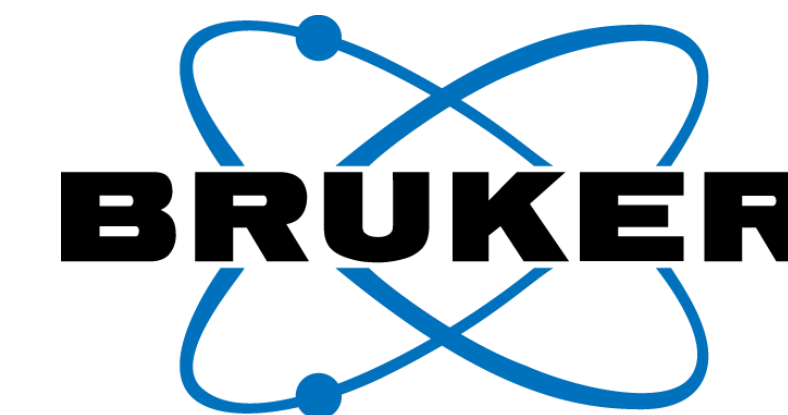
- MetaboScape can use the Isotopic Fine Structure and flag the compounds identified on the basis of IFS (only for high abundant peaks)





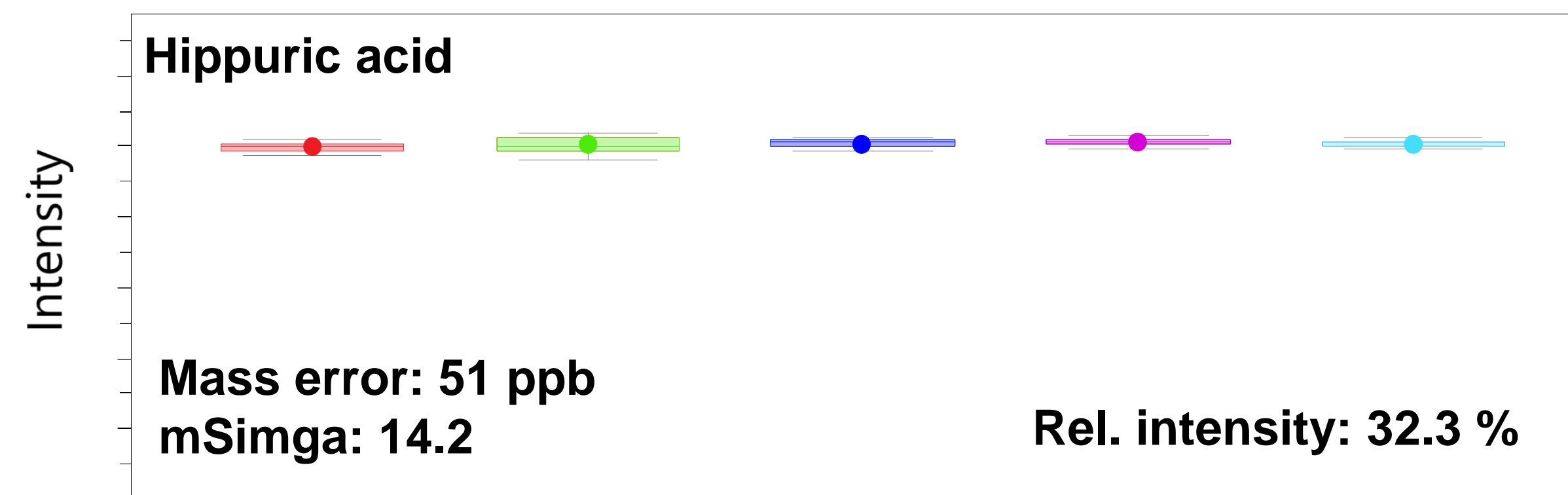
# FIA-MRMS of urine samples

## Reproducibility



Sample:

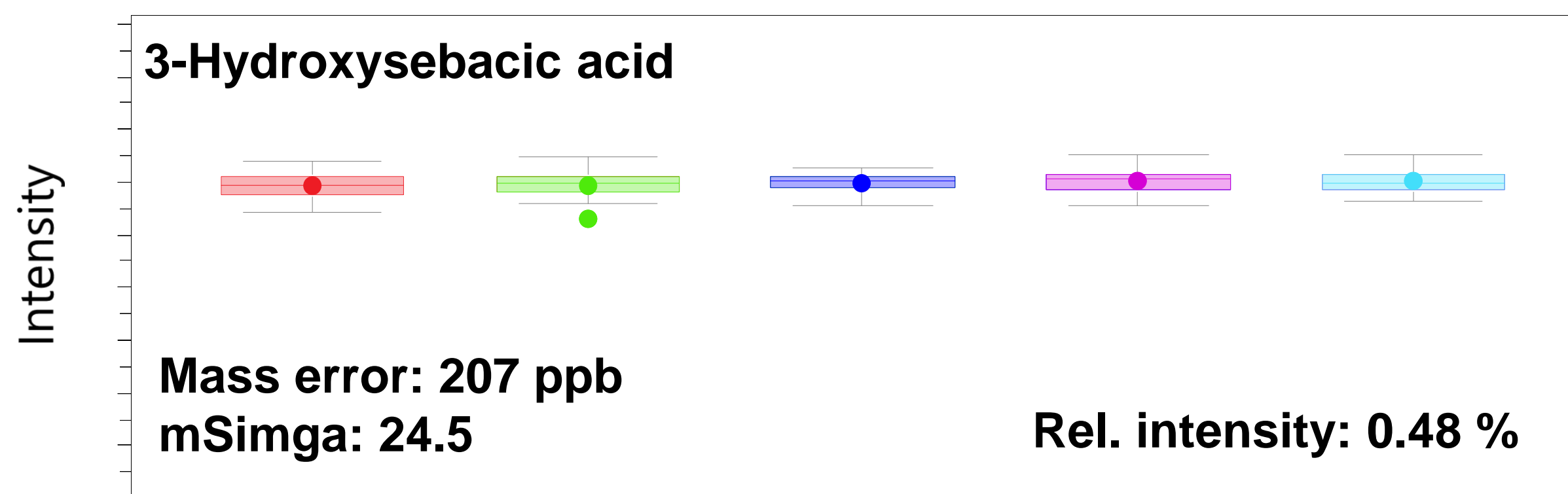
- 1A
- 2A
- 3A
- 4A
- 5A



**Standard deviation:**  
Average each vial 1.2 %  
All injections: 1.4 %

Sample:

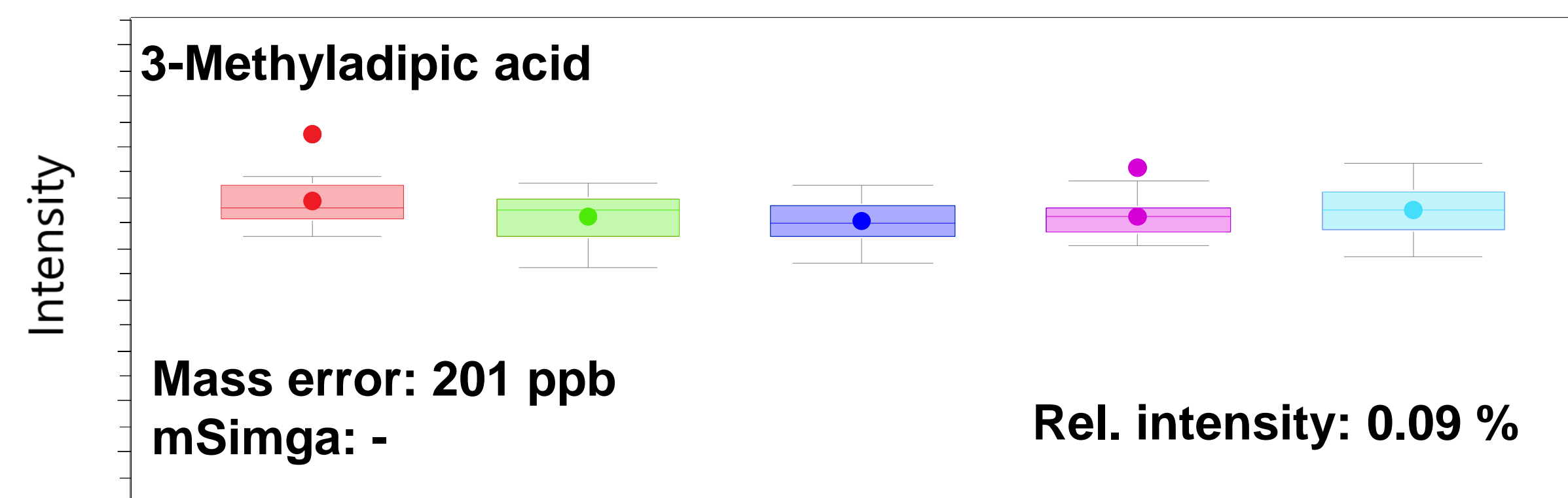
- 1A
- 2A
- 3A
- 4A
- 5A



**Standard deviation:**  
Average each vial 3.8 %  
All injections: 3.8 %

Sample:

- 1A
- 2A
- 3A
- 4A
- 5A



**Standard deviation:**  
Average each vial 7.7 %  
All injections: 8.0 %



# FIA-MRMS of urine samples



- Desalted urine samples have been measured in 125 replicates for each mode (ESI(+)) and ESI(-)) using FIA-MRMS and MetaboScape

Measurement	Features	Analytes with HMDB urine list	Mol. Formula with SF calc.
FIA-MRMS(+)	4502	203	2838
FIA-MRMS(-)	1738	221	1176
FIA-MRMS(+) and FIA-MRMS(-) combined	6055	<b>363</b>	3748

Mass tolerance for HMDB search and SF calculation: 0.5 ppm

- Pooled desalted urine samples have been measured in multiple replicates\* for

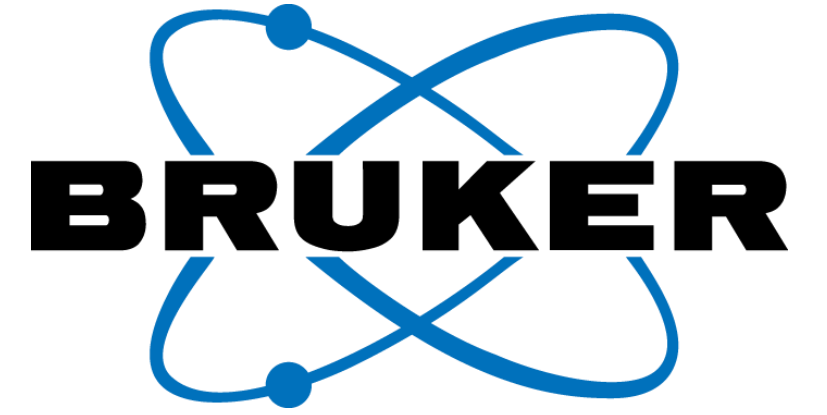
Measurement	Features	Analytes with HMDB urine list	Mol. Formula with SF calc.
LC-MRMS(+)	1374	202	1212
LC-MRMS(-)	1448	203	1126
LC-MRMS(+) and LC-MRMS(-) combined	2585	<b>304</b>	2113

Mass tolerance for HMDB search and SF calculation: 0.5 ppm

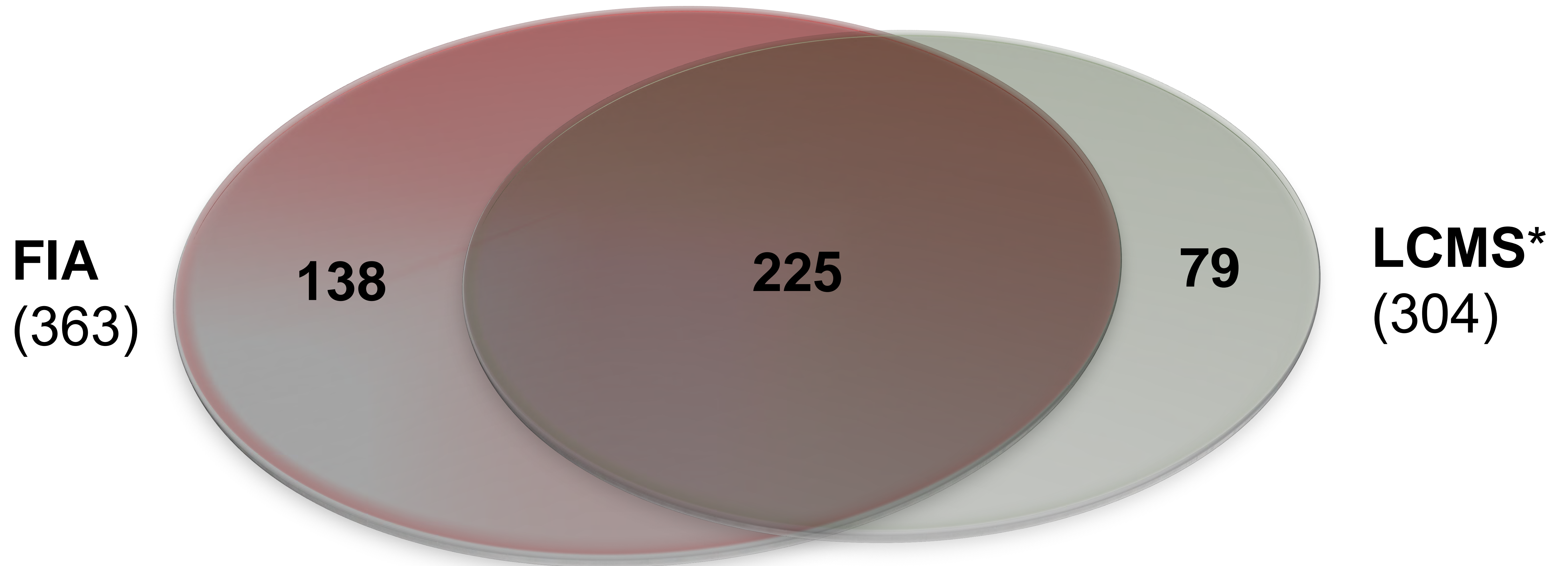
\* Pooled urine sample was measure in 12 replicates    \*\* column: Waters Acquity BEH C18 1.7 um (2.1 x 50 mm), flow 0.6 ml/min



# FIA-MRMS of urine samples

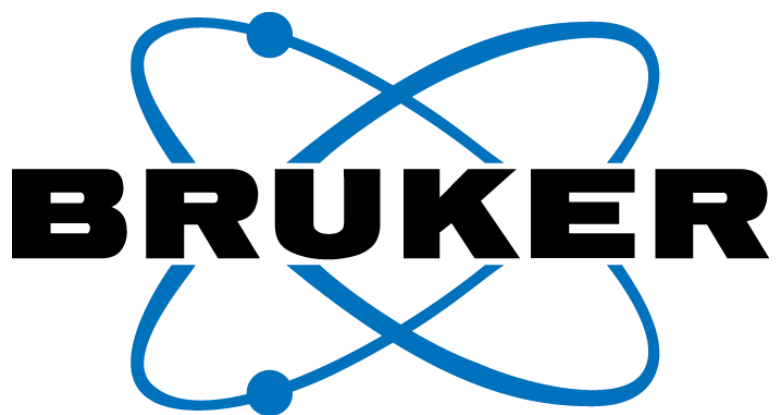


Comparison of FIA and LCMS results (ESI(+)) and ESI(-) were merged)

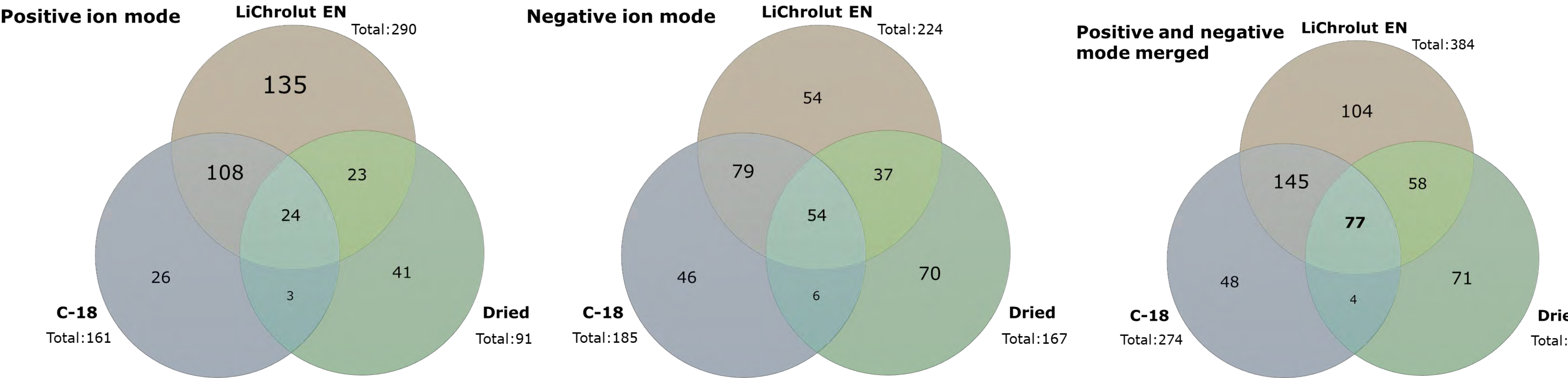
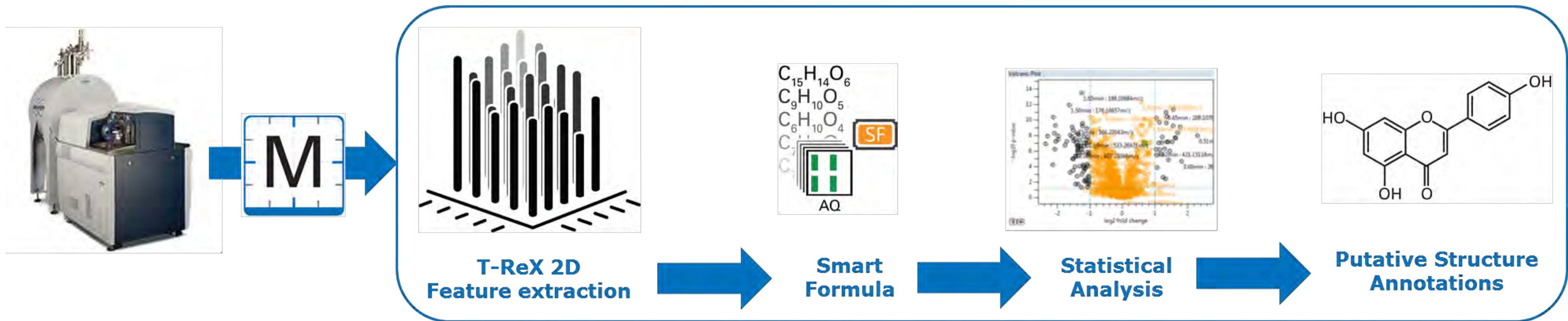




# FIA-MRMS of urine samples

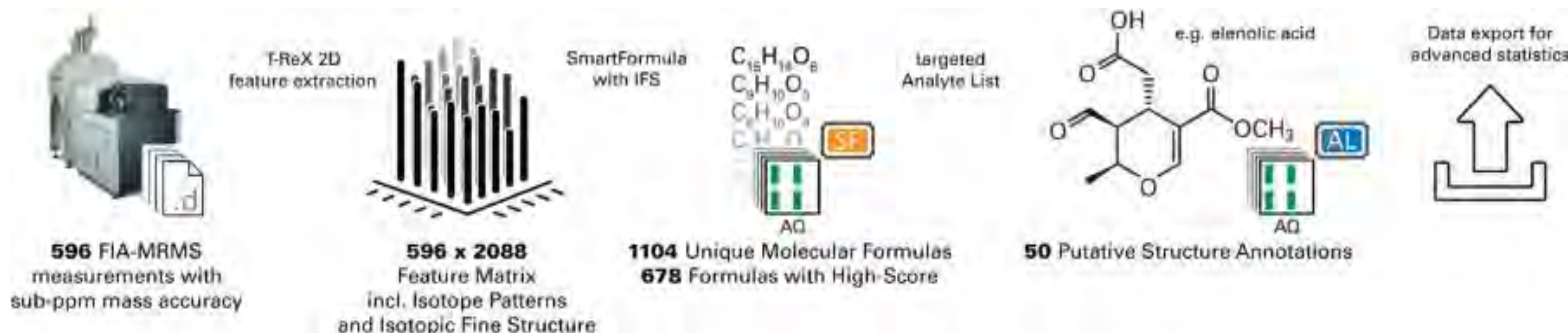


Comparison of sample preparation of urine





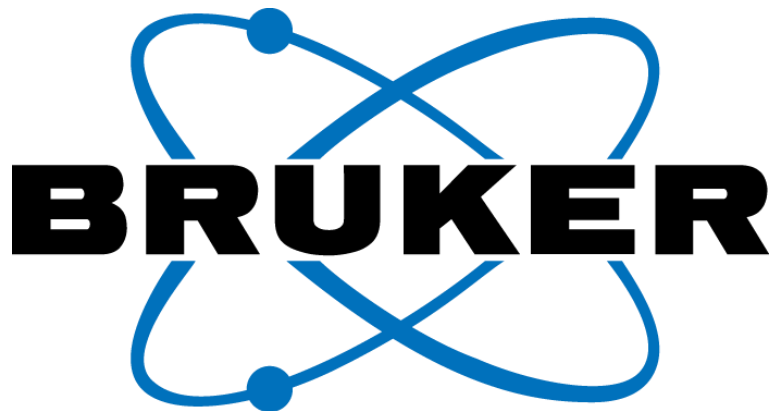
# FIA-MRMS of EEVO samples and polyphenols



- **Samples collection:** Samples were collected from the main Greek olive oil producing regions and stored at room temperature, in darkness, under nitrogen.
- **Sample Preparation:** Stock solutions were prepared by dissolving 10uL of samples in 500 mL MeOH. The stock solutions were then diluted 1:20 in 50% MeOH + 10 mM Ammonium Acetate.
- **MS analysis:** EVOO (extra virgin olive oil) samples and their biophenolic extracts were analyzed using a Bruker solarix-XR 7T mass spectrometer using ESI (-) mode by FIA.

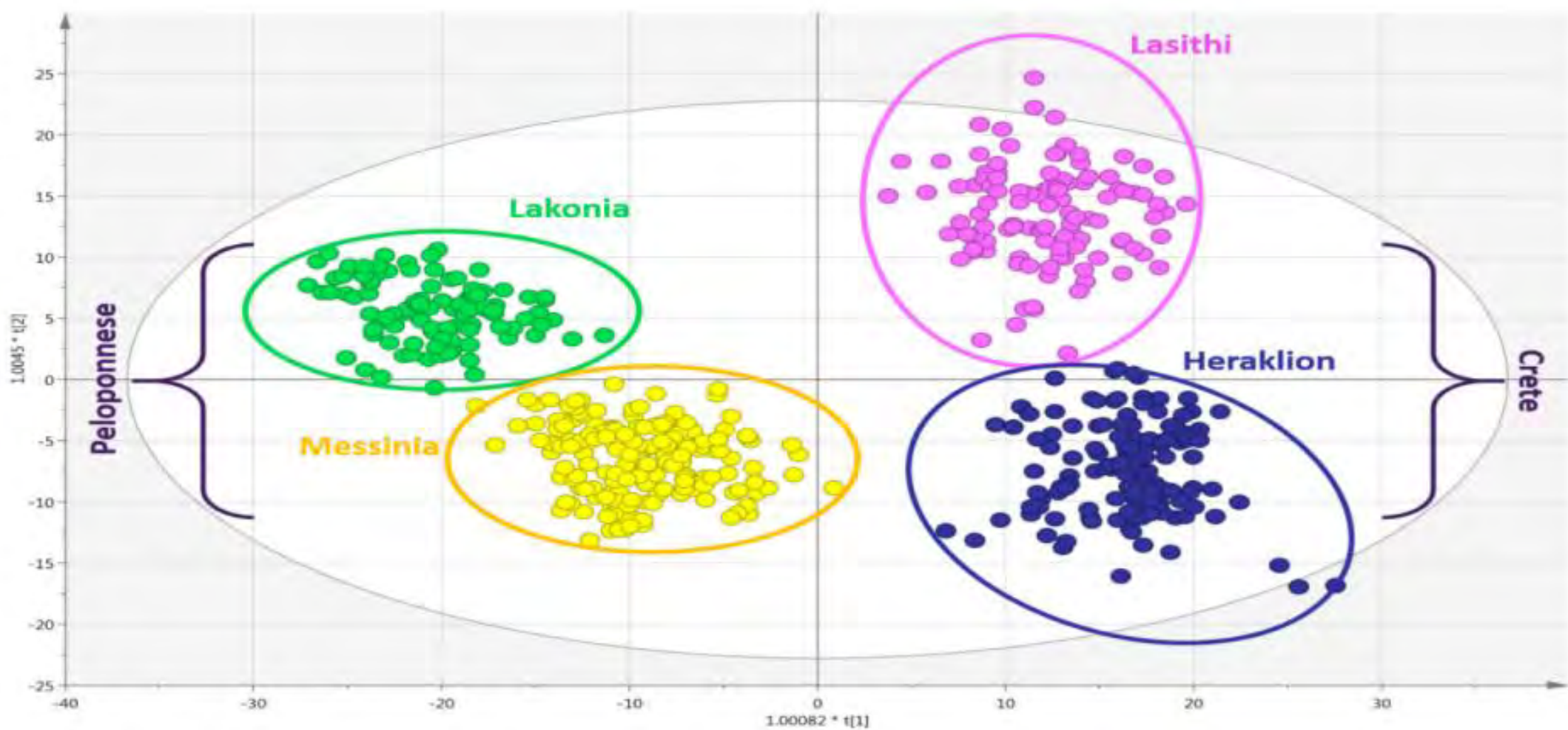


# FIA-MRMS of EEVO samples and polyphenols

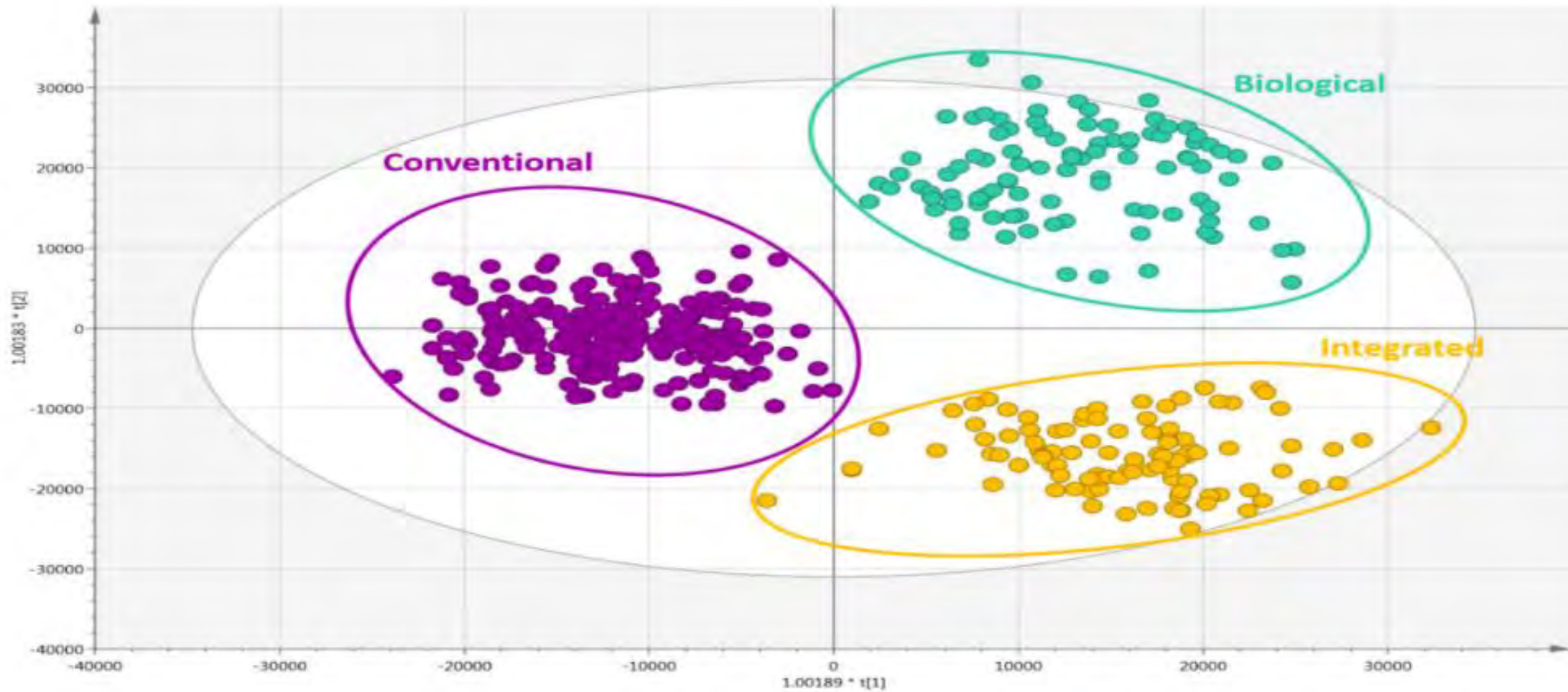


Geographical origin

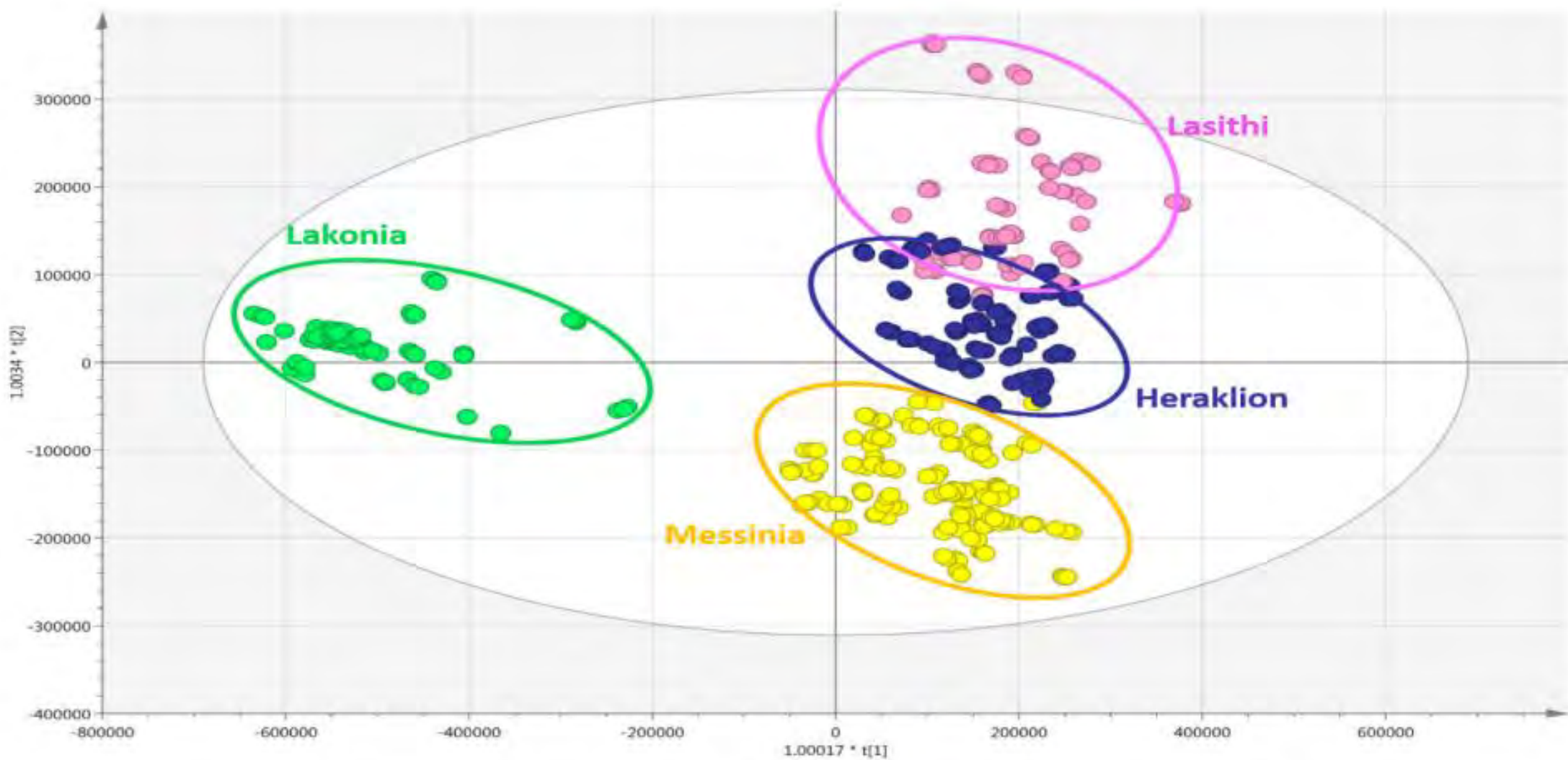
Geographical origin-EVOO



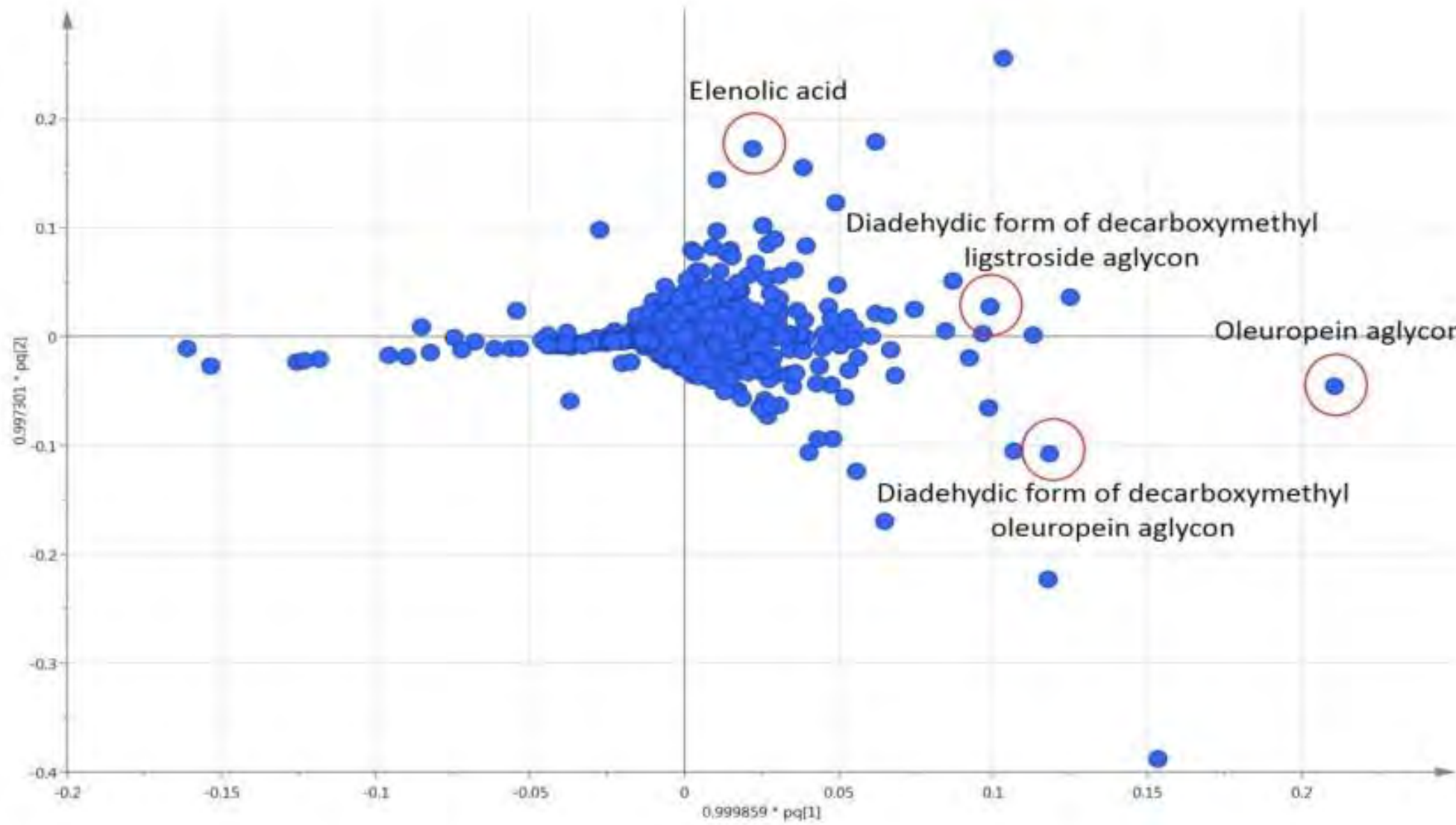
Cultivation practice-EVOO



Geographical origin- Biophenols

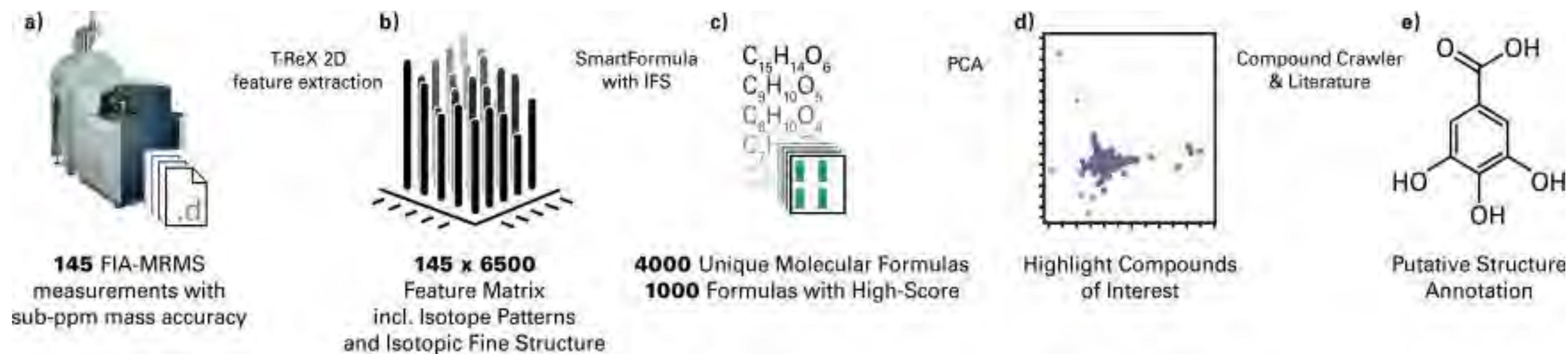


loading plot





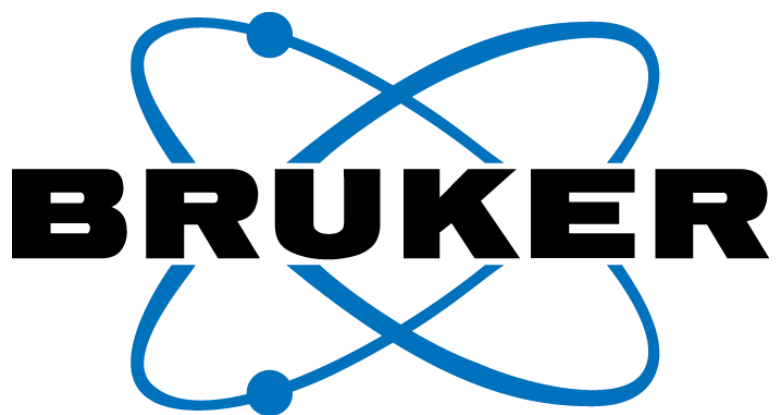
# FIA-MRMS of wine samples



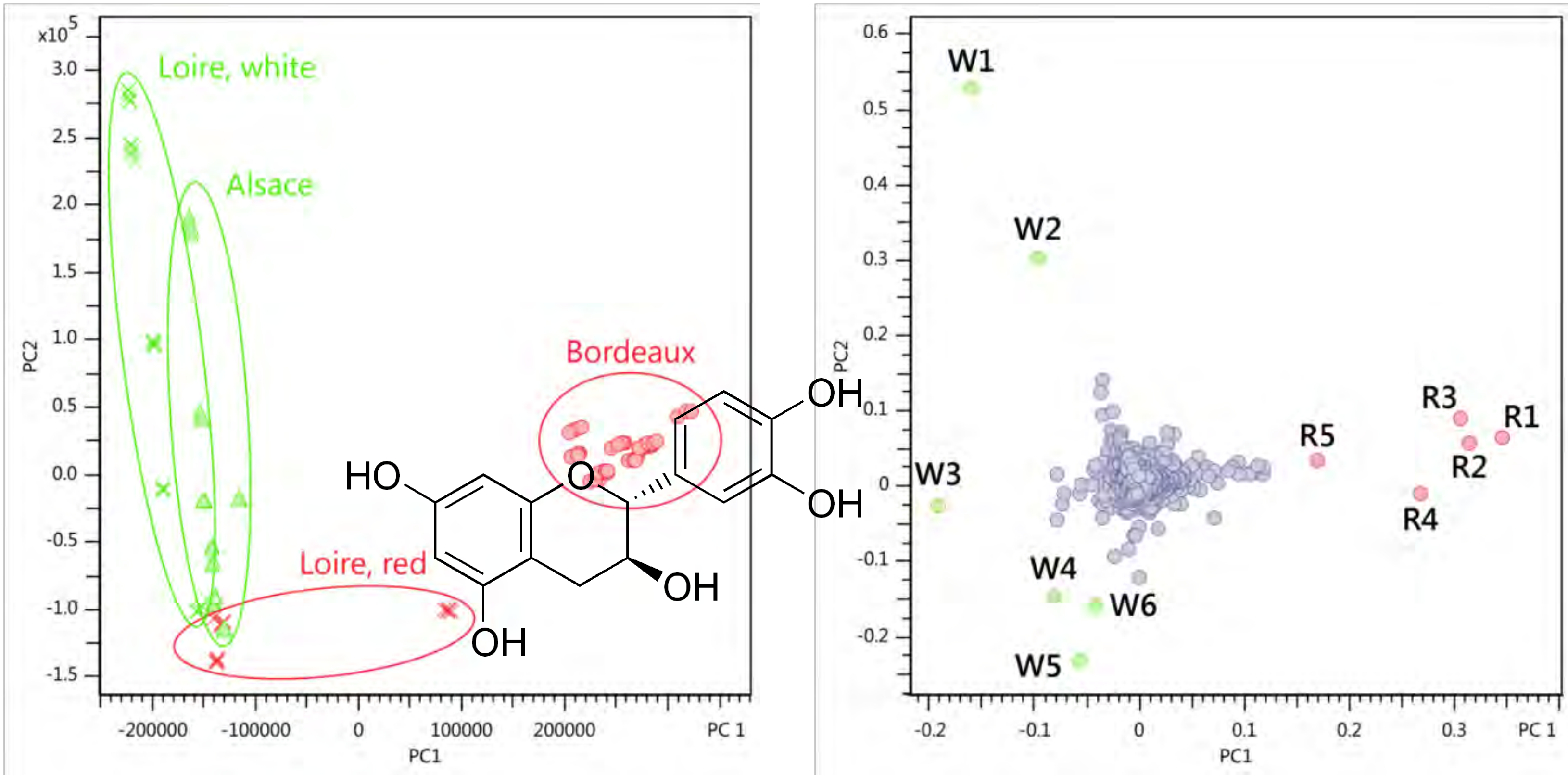
- **Sample preparation:** Solid phase extraction (SPE)
- **MS Analysis:** Bruker solarix XR 7T mass spectrometer using ESI (-) with a resolving power of 300,000 at m/z 400.
- **Data Processing:** Deisotoping and adduct collation in MetaboScape.
- **Statistical analysis:** PCA as well as molecular formula calculation based on accurate mass, IFS and filtering based on elemental composition in MetaboScape. Annotated features were investigated using filters for mass defects and DBE.



# FIA-MRMS of wine samples



PCA plots



High abundance in white wine

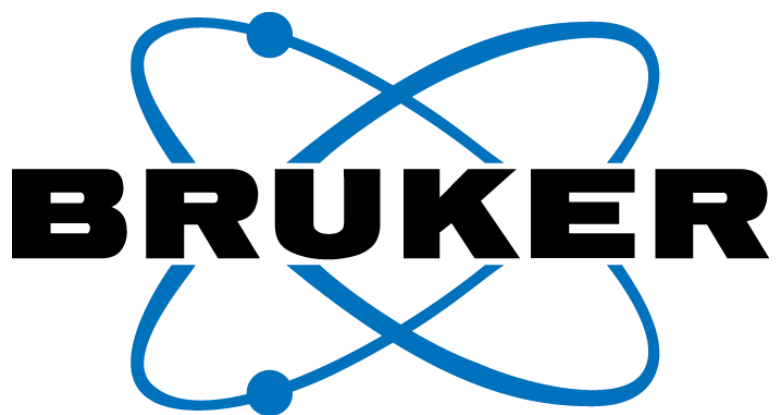
Compound	Molecular formula	Name
W1	C <sub>15</sub> H <sub>18</sub> O <sub>6</sub>	Methoxycoumarin
W2	C <sub>14</sub> H <sub>16</sub> O <sub>3</sub>	-
W3	C <sub>6</sub> H <sub>10</sub> O <sub>5</sub>	3-Hydroxy-3-methyl-glutaric acid
W4	C <sub>6</sub> H <sub>8</sub> O <sub>2</sub>	Sorbic acid
W5	C <sub>13</sub> H <sub>12</sub> O <sub>9</sub>	Caftaric acid
W6	C <sub>14</sub> H <sub>14</sub> O <sub>9</sub>	Fertaric acid

High abundance in red wine

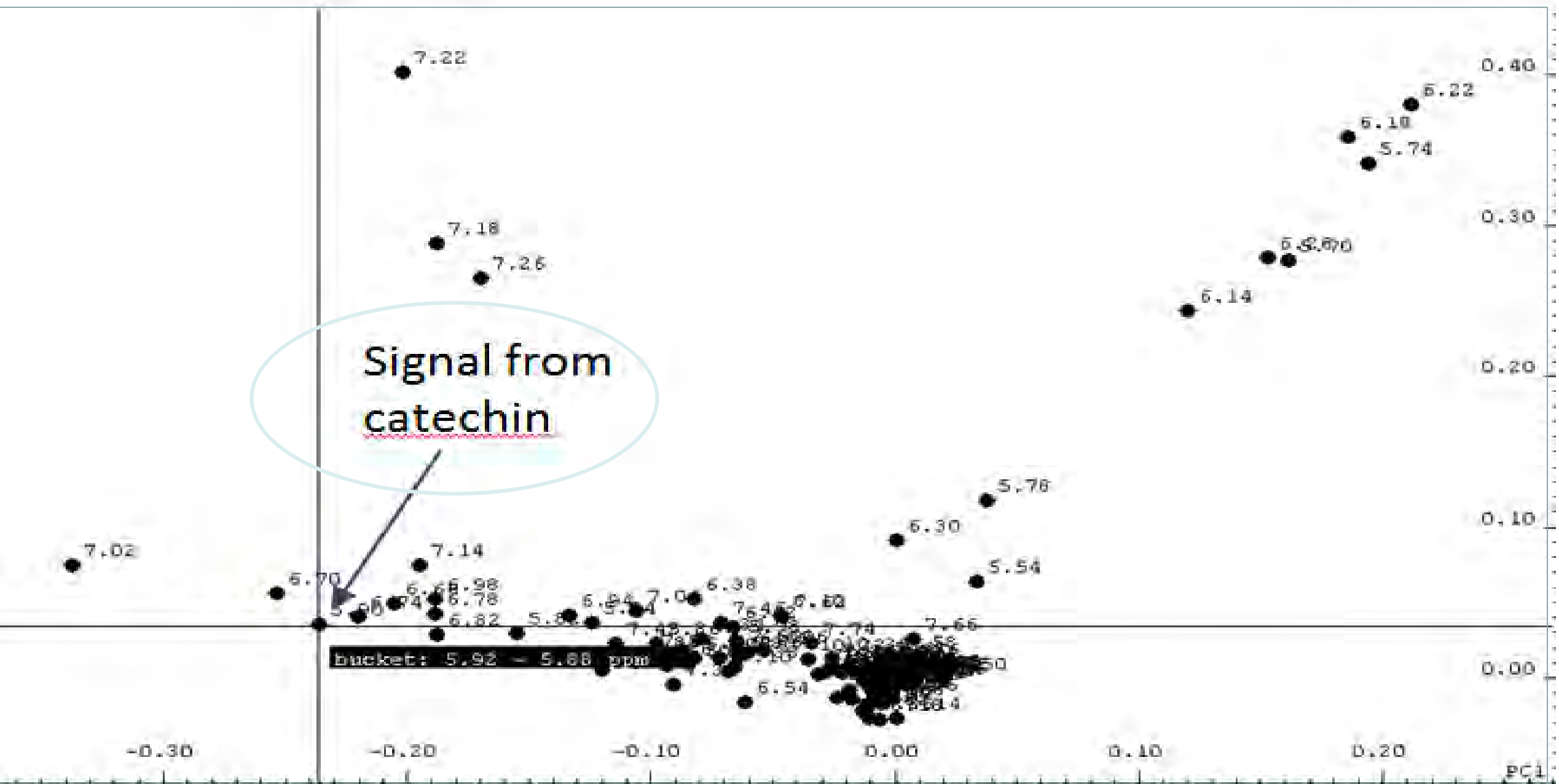
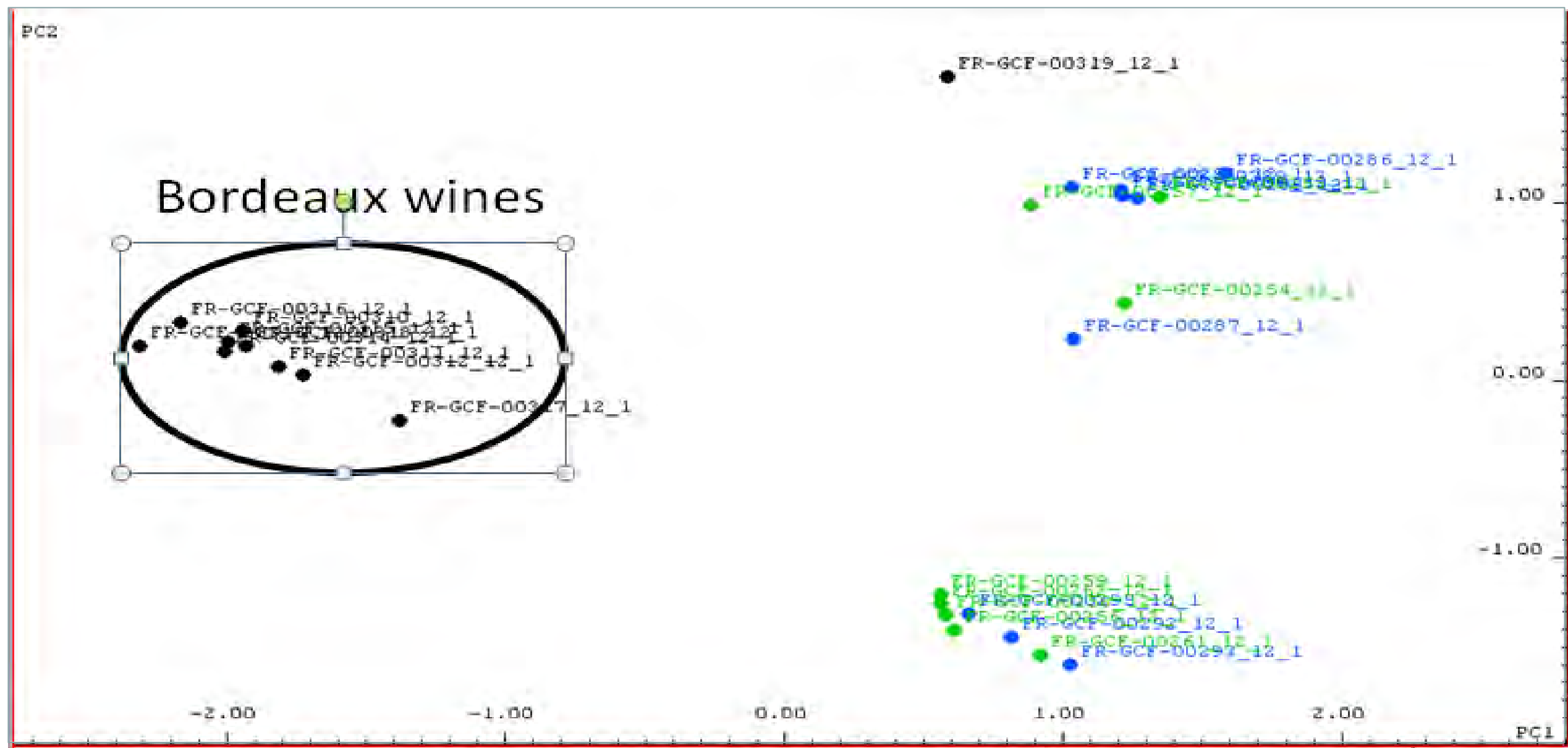
Compound	Molecular formula	Name
R1	C <sub>15</sub> H <sub>14</sub> O <sub>6</sub>	Catechin
R2	C <sub>9</sub> H <sub>10</sub> O <sub>5</sub>	Syringic acid
R3	C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>	Adipic acid / 3-Methyl glutamic acid
R4	C <sub>7</sub> H <sub>12</sub> O <sub>5</sub>	Diacetin
R5	C <sub>7</sub> H <sub>6</sub> O <sub>5</sub>	Gallic acid



# FIA-MRMS of wine samples

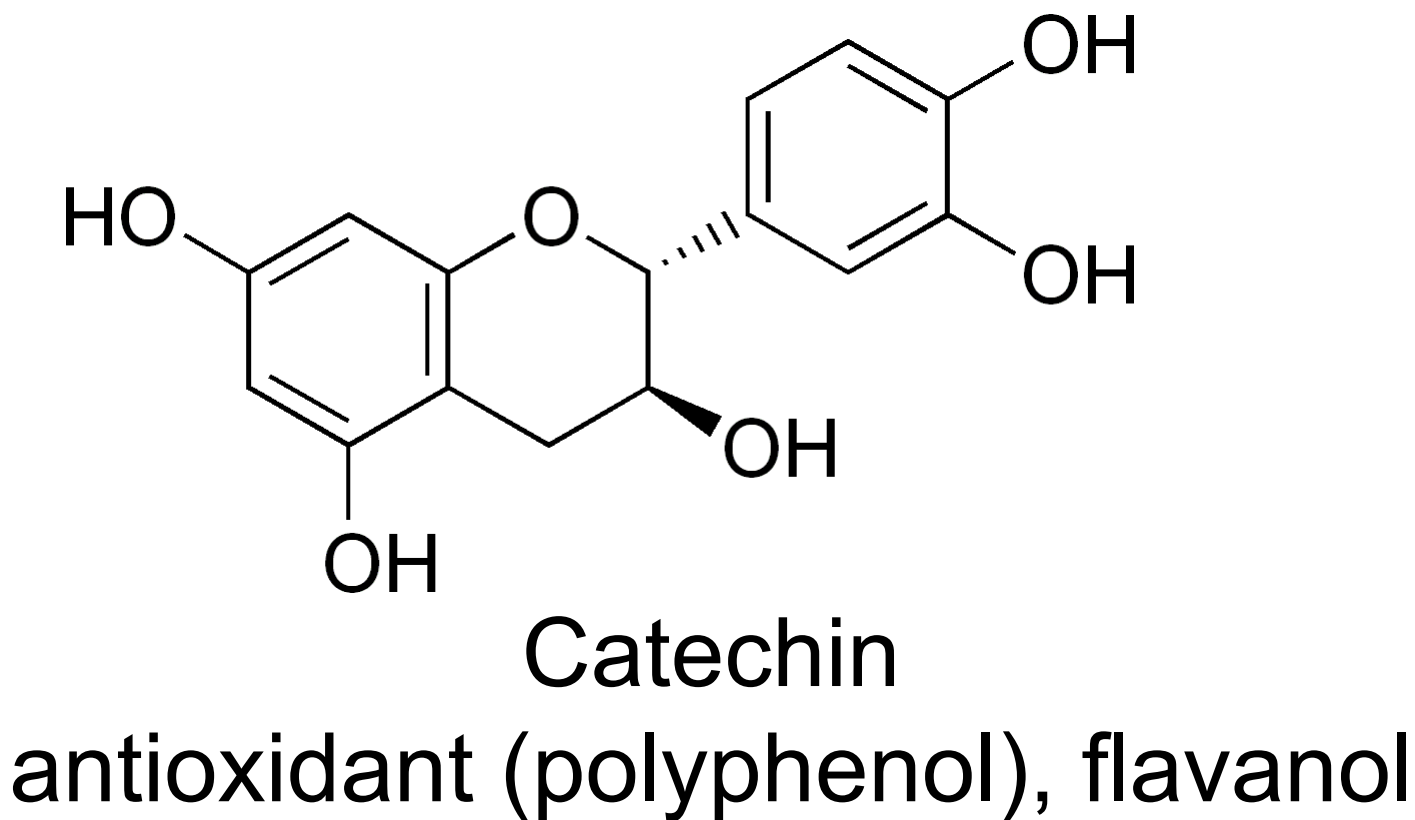


## <sup>1</sup>H-NMR analysis



Compound	Molecular formula	Name
R1	C <sub>15</sub> H <sub>14</sub> O <sub>6</sub>	Catechin
R2	C <sub>9</sub> H <sub>10</sub> O <sub>5</sub>	Syringic acid
R3	C <sub>6</sub> H <sub>10</sub> O <sub>4</sub>	Adipic acid / 3-Methyl glutamic acid
R4	C <sub>7</sub> H <sub>12</sub> O <sub>5</sub>	Diacetin
R5	C <sub>7</sub> H <sub>6</sub> O <sub>5</sub>	Gallic acid

- MRMS and 1H-NMR analyses results in same grouping of wines.
- Catechin is mainly responsible to separate white wine and red wine in PCA plot.





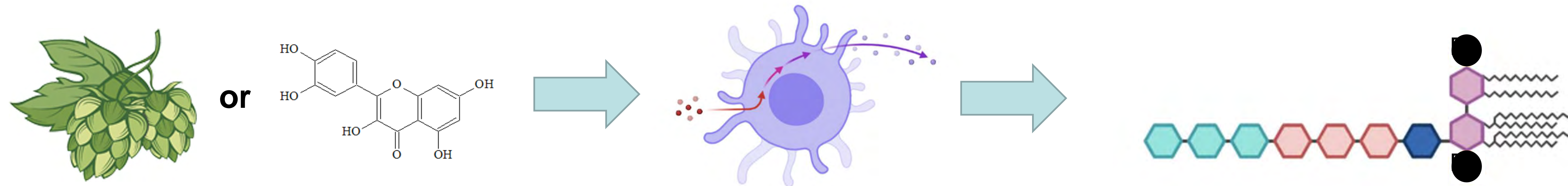
# Detection of intermediates

## Anti-inflammatory Effects of Hop bitter acids in Dendritic cells

### *Stimulation of dendritic cells (DCs) and sample preparation protocol for extraction of metabolites.*

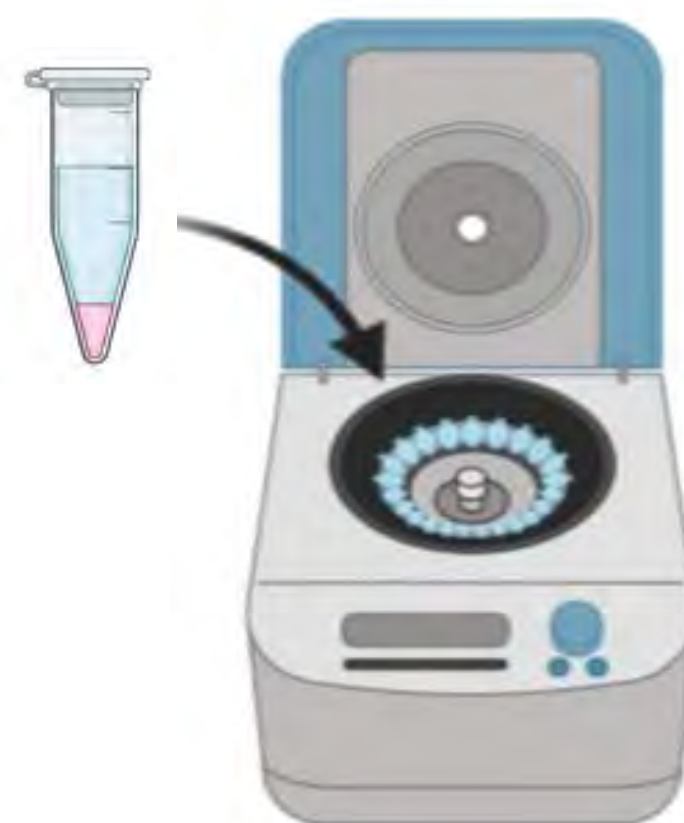
DCs from murine bone marrow (BMDCs) from six- to eight-week-old mice.

24 h later LPS stimulation (1  $\mu$ L/mL)



On day 10. Hop fractions (A, B, C) 25  $\mu$ g/mL or quercetin 25  $\mu$ M administration

14680 rpm, 10 min, 4°C.



Sonicate 6 min, 25 °C  
+ vortex for 30 sec



Pelleted cells thawed on ice

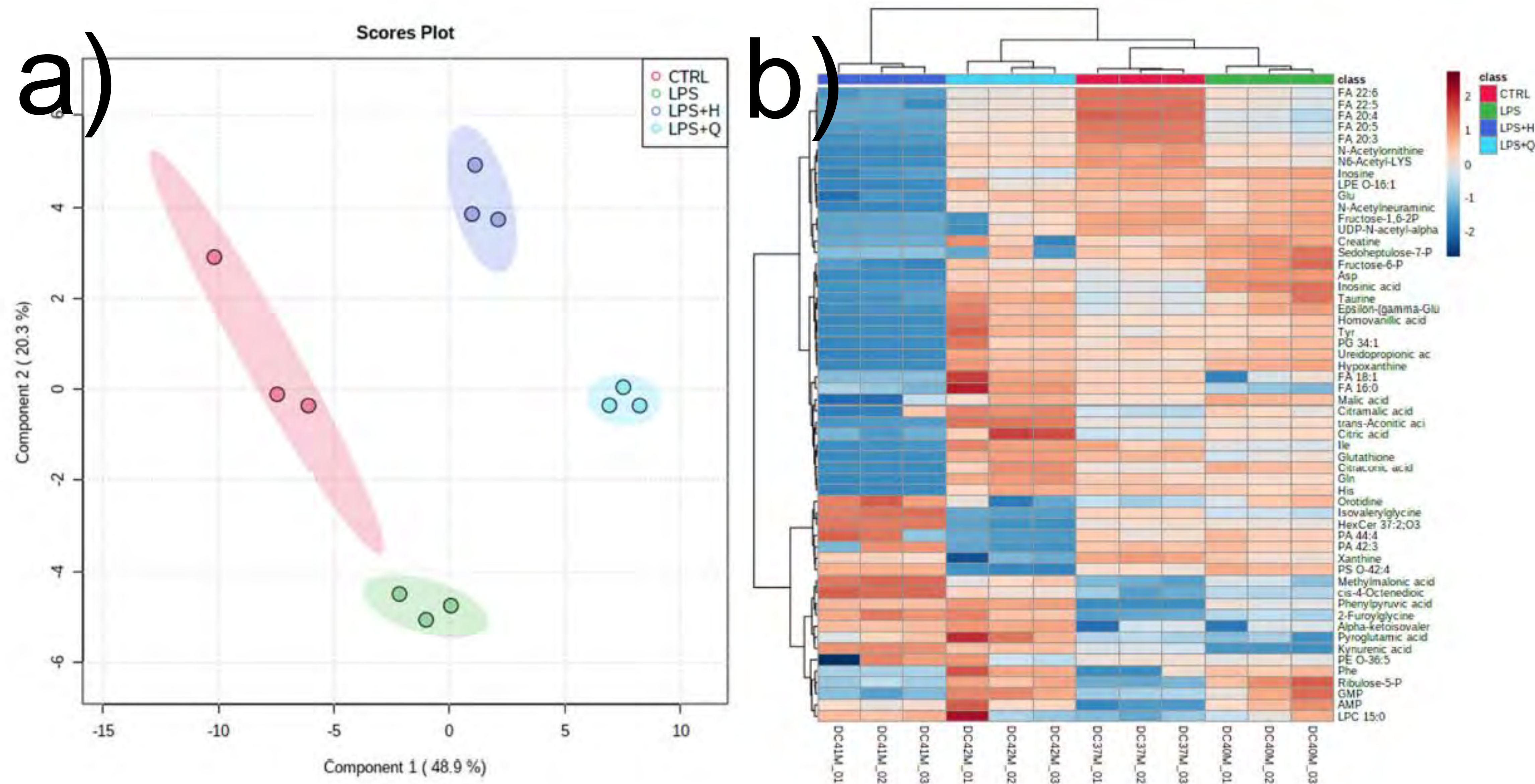


100  $\mu$ L of ice-cold  
MeOH/H<sub>2</sub>O (80:20  
v/v).



# Detection of intermediates

Anti-inflammatory Effects of Hop bitter acids in Dendritic cells

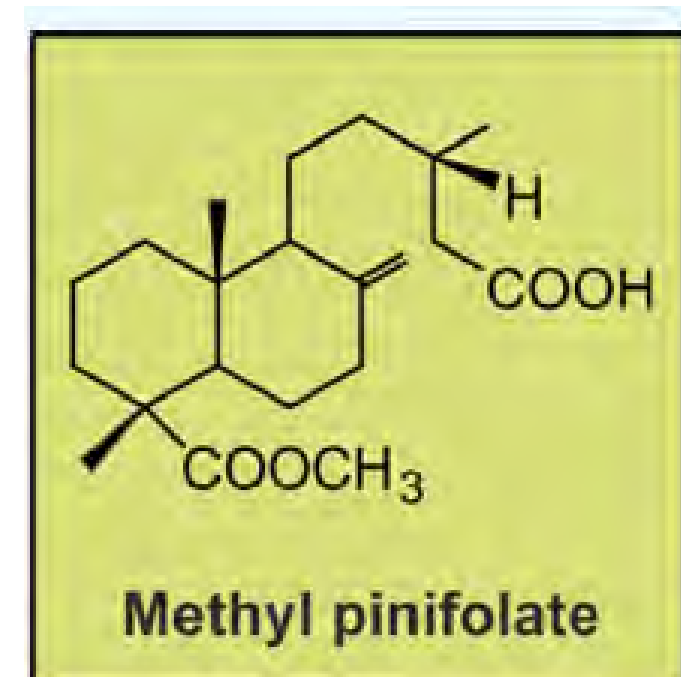
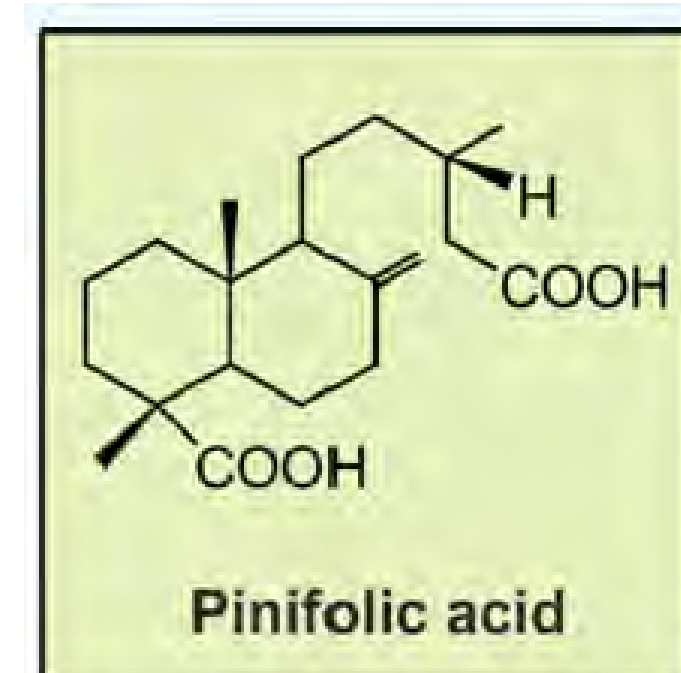


PLS-DA score plot (A) and heat map (B) of statistically relevant (ANOVA,  $p < 0.05$ ) DC metabolites modulated by LPS, HOP C, and quercetin. Color changes reflect the normalized intensity.

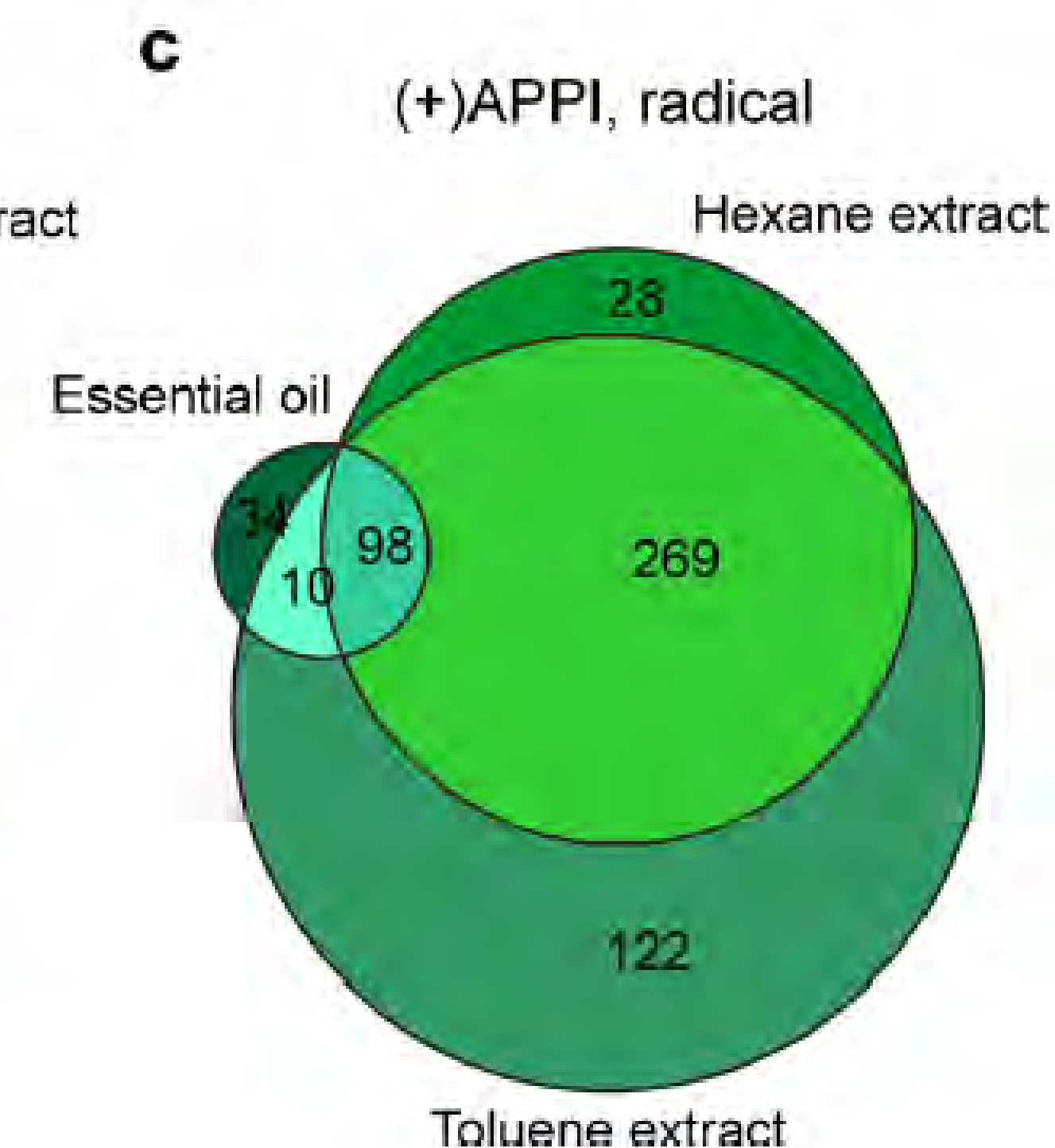
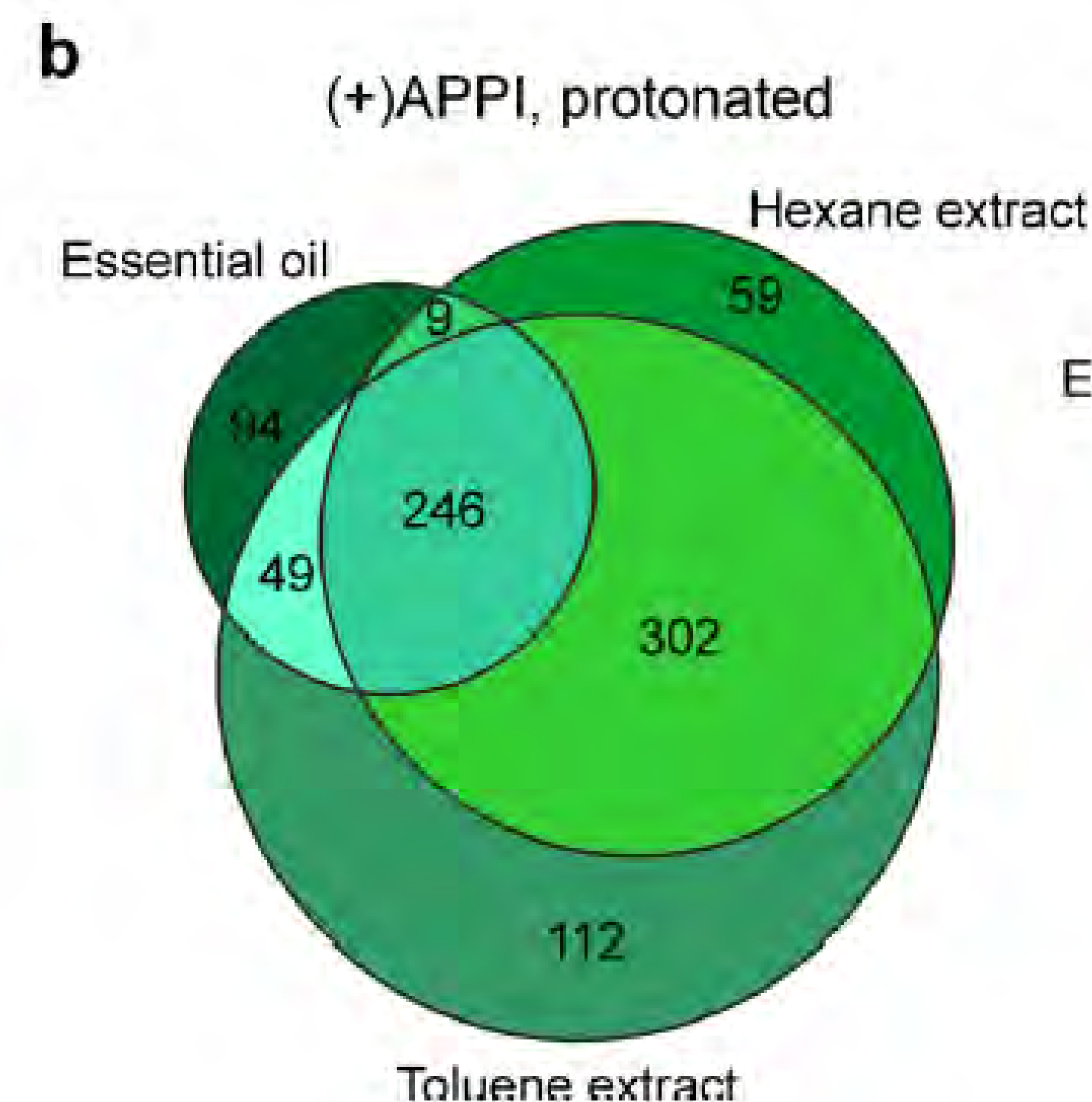
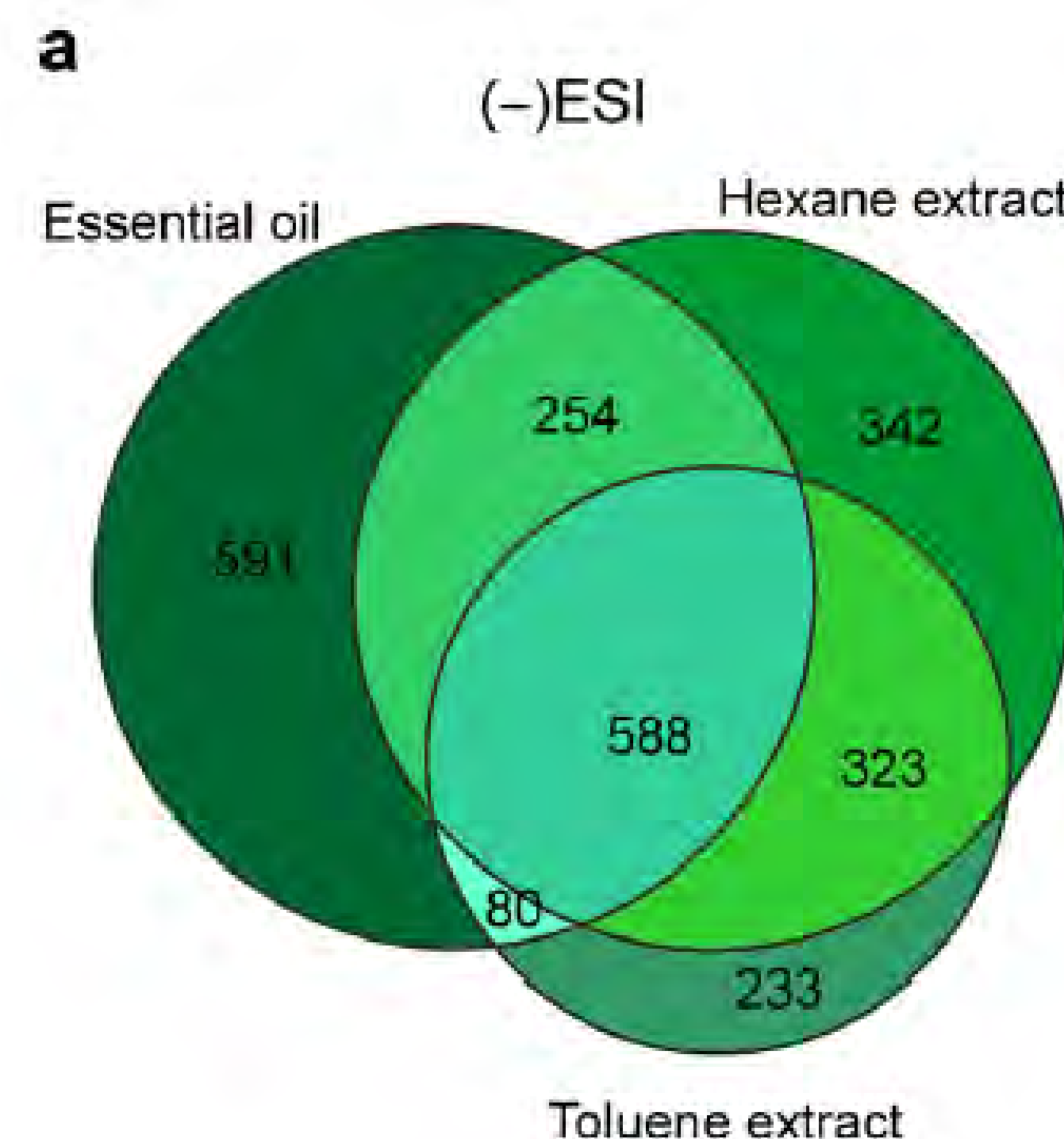


# Fingerprinting of Plant extracts

## Detection of compounds in Conifer Needle Essential Oils



Venn diagrams showing distribution of compounds between pine needle essential oil and two solvent extracts: (a) (–)ESI, (b) (+)APPI (protonated molecules), (c) (+)APPI (radical cations)



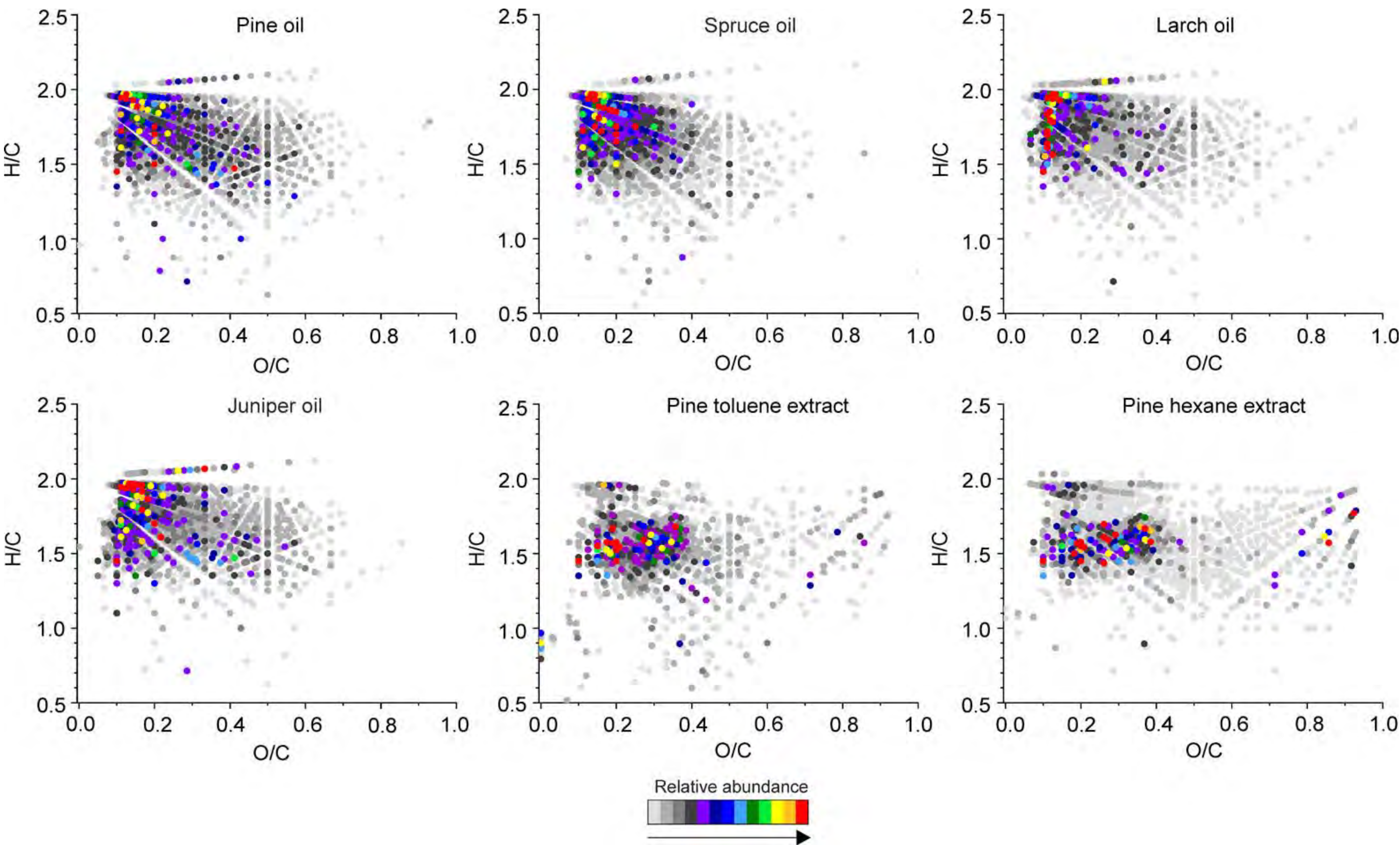


# Fingerprinting of Plant extracts

## Detection of compounds in Conifer Needle Essential Oils



O. O. Mofikoya et al., ACS Omega 2020, 5, 18, 10543–10552.

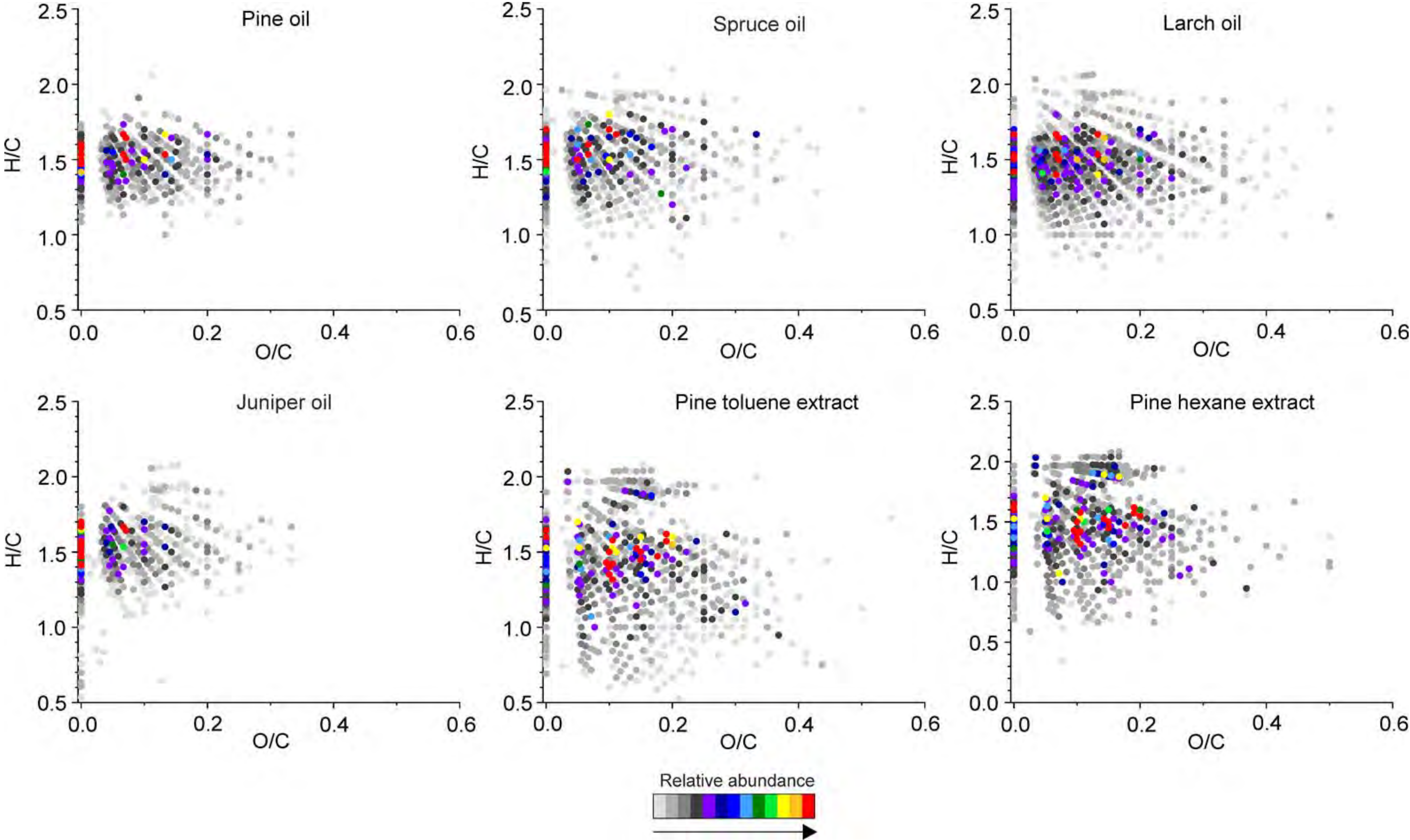
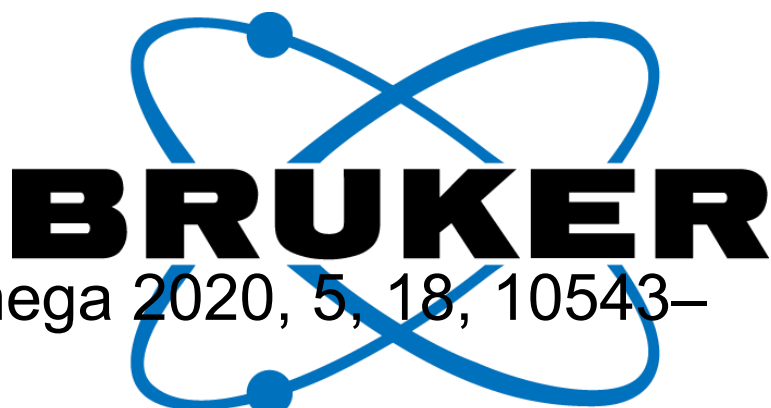


Van Krevelen diagrams of the compounds detected in the conifer needle essential oils and solvent extracts by (–)ESI FT-ICR MS.



# Fingerprinting of Plant extracts

## Detection of compounds in Conifer Needle Essential Oils

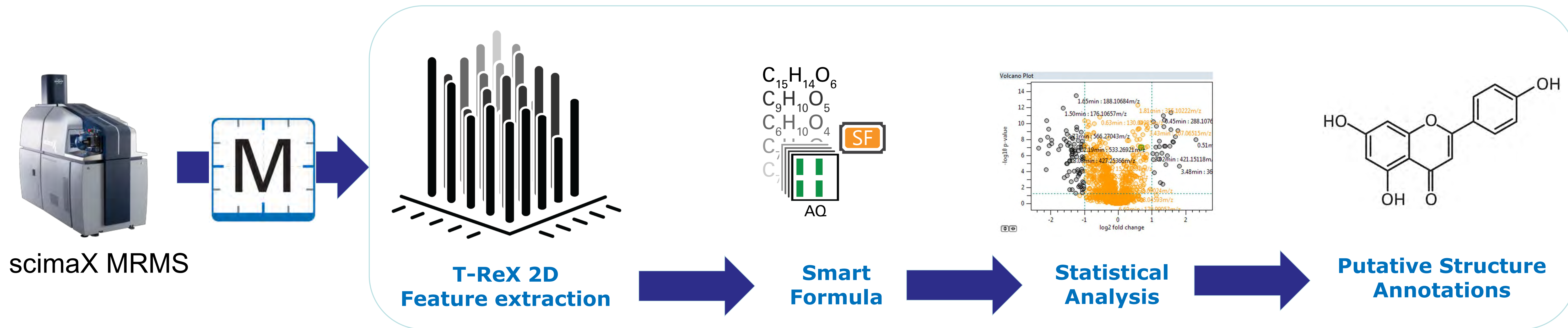
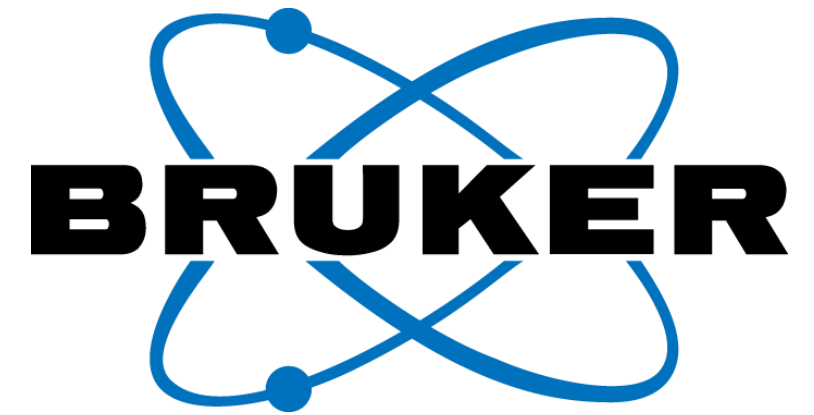


Van Krevelen diagrams of the compounds detected in the conifer needle essential oils and solvent extracts by (+)APPI FT-ICR MS.



# MRMS aXelerate

Now everyone can achieve high sample throughput on Phenomics research...



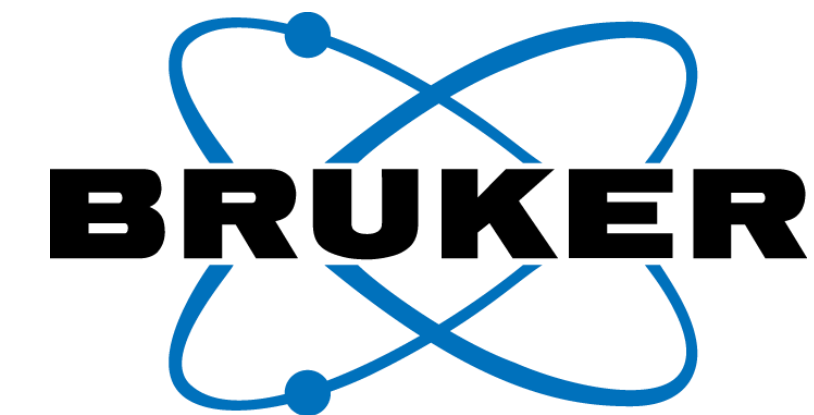
- Extreme resolving power of **scimaX MRMS** system enables chromatography-free FIA or MALDI data acquisition for >200 samples / day
- Powerful data extraction in **MetaboScape: T-ReX 2D** for evaluating > 1000 samples
- Automatic ID with 3 tier confidence:
  - *Routinely <0.2ppm mass accuracy*
  - *True Isotopic Pattern*
  - *Mass resolution >1 million, boosts Isotopic Fine Structure fidelity*







MetaboScape  
*Key advantages*



**T-ReX (Time aligned Region complete eXtraction)** feature extraction technology for processing data from **complementary systems**:

### **T-ReX 2D** for FIA-MRMS

High-throughput phenomics by MRMS  
~5 min/sample, 3-tier confidence in formula, complementary to LC-MS

### **T-ReX 3D** for LC-QTOF-MS/MS

Deep metabolome profiling by different LC methods and integrated processing of positive / negative mode data  
>1000 LC-MS runs from Phenomics Workhorse can be evaluated

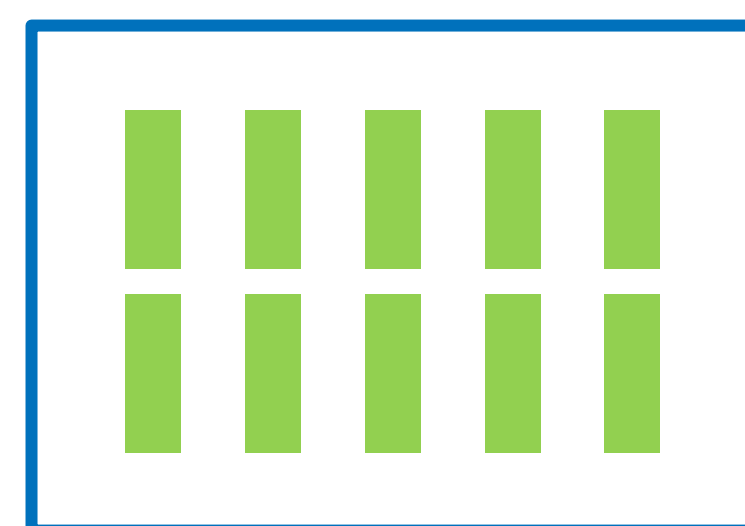
### **T-ReX 4D** for LC-TIMS-QTOF-MS/MS

For metabolomics methods development with 4D separations, robust CCS raised to next level with TIMS  
Accurate Collisional Cross Sections (CCS) from **TIMS**

### **Intuitive Annotation Quality scoring** for high confidence ID

Rates all annotations with up to five quality factors  
New: CCS matching for timsTOF and timsTOF Pro

### **AQ score**



**A B C D E**

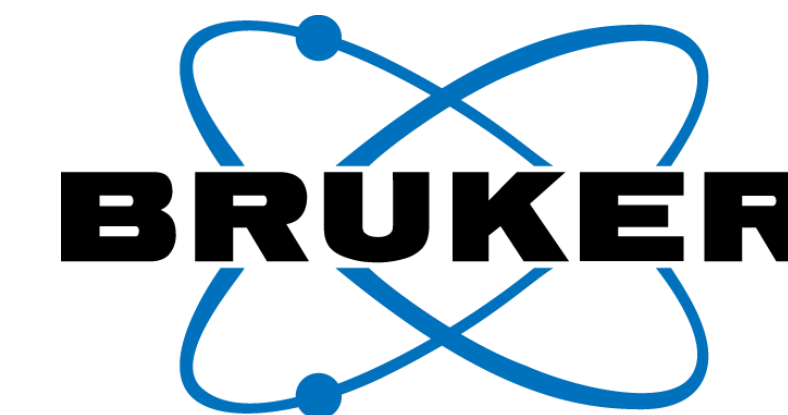
- A** Precursor mass accuracy
- B** Retention time
- C** Isotopic pattern
- D** MS/MS fragment spectra
- E** CCS values



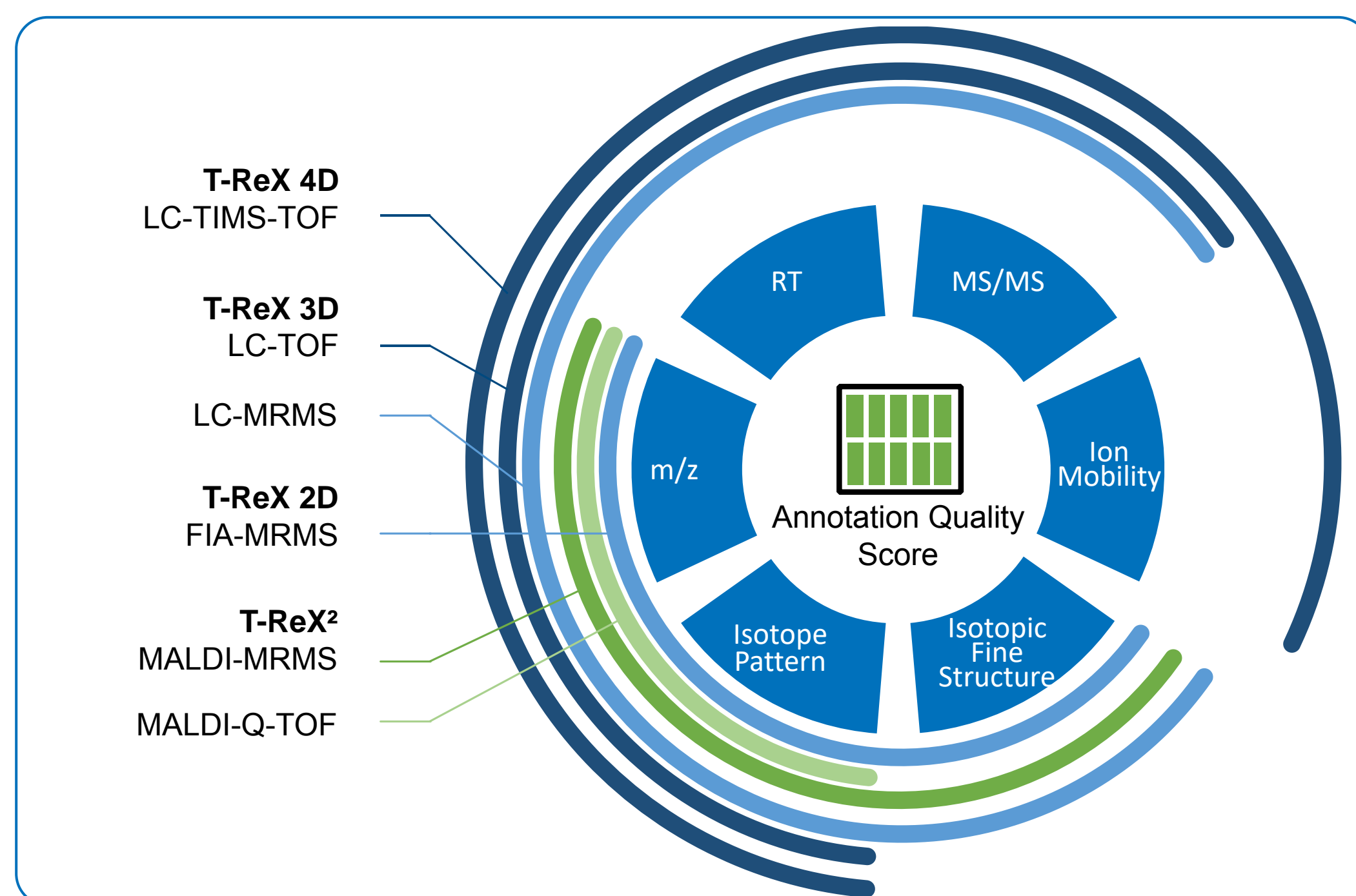


# MetaboScape

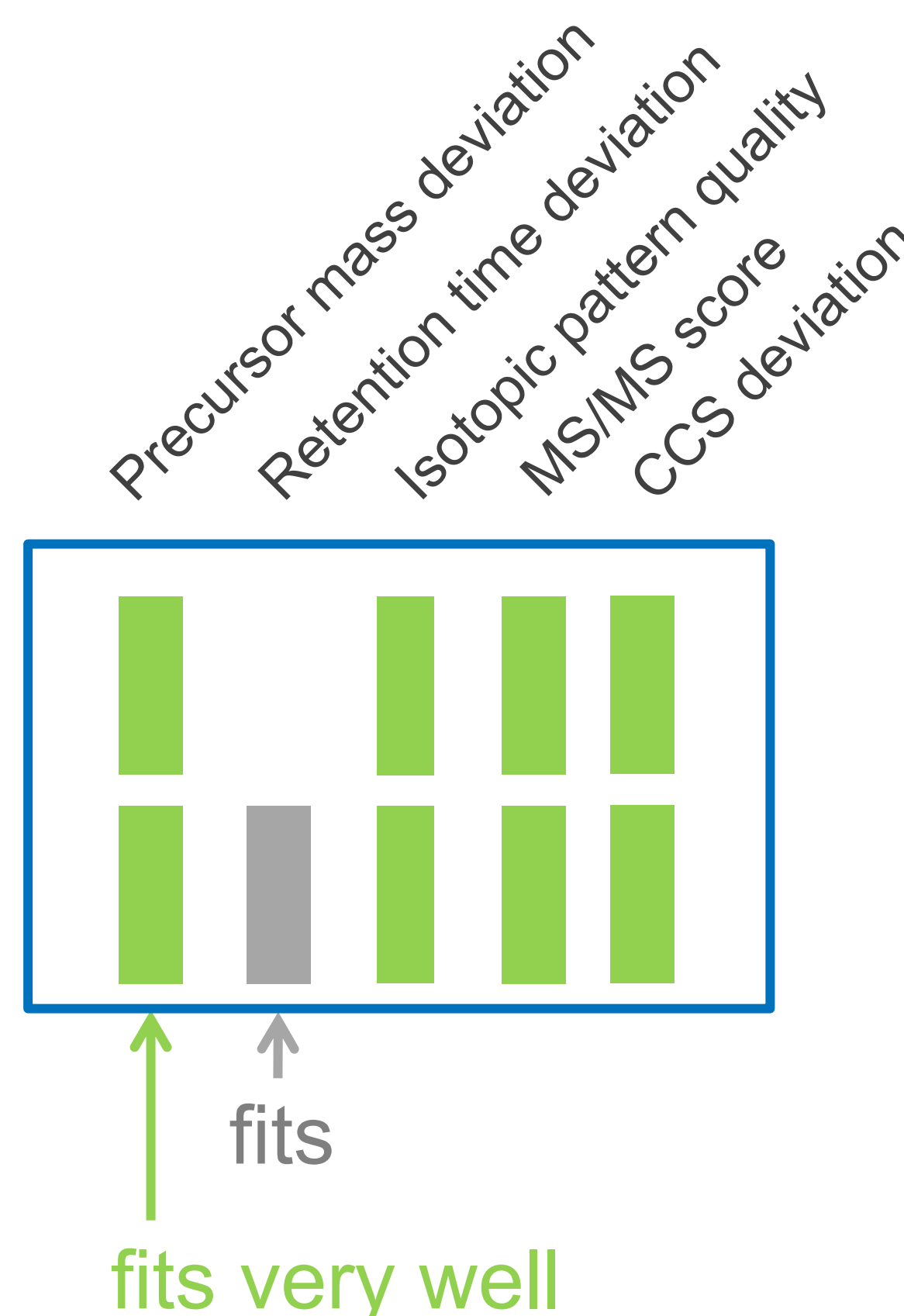
Identification / Dereplication



The Goodness of annotation is indicated by the **annotation quality** symbol



MetaboScape and T-ReX support different instrument types, exploiting the respective strengths of each: For the sake of separation, annotation quality, or throughput.



User-definable **confidence levels** can be set for the **annotation quality**.

	Narrow	Wide	Unit
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Retention time:	<input type="text" value="0.15"/>	<input type="text" value="0.4"/>	[T] minutes
mSigma:	<input type="text" value="15"/>	<input type="text" value="50"/>	[T]
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CCS:	<input type="text" value="1"/>	<input type="text" value="2"/>	[T] %



# Acknowledgements

## **Australian National Phenome Center, Perth, Australia**

- Jeremy Nicholson



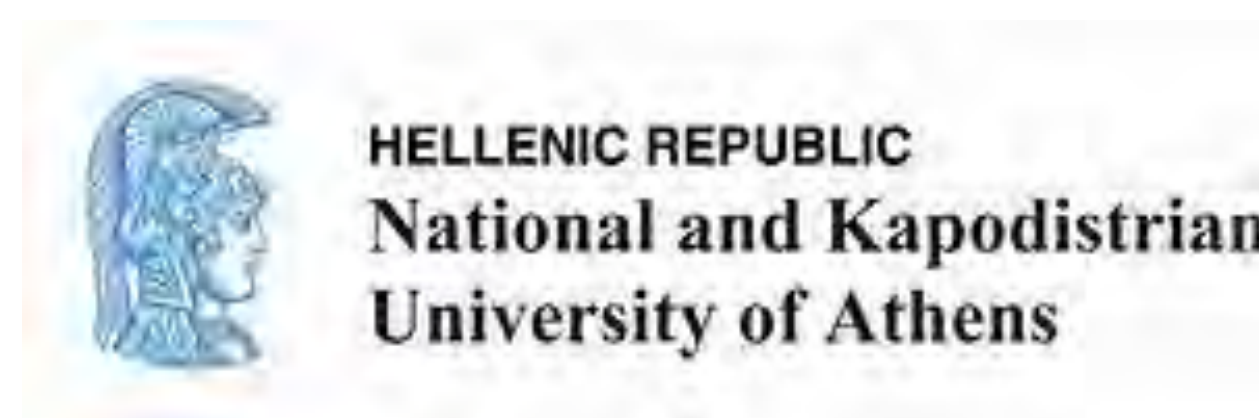
## **Imperial College London, UK**

- Matt Lewis



## **University of Athens, Greece**

- Theodora Nikou
- Maria Halabalaki



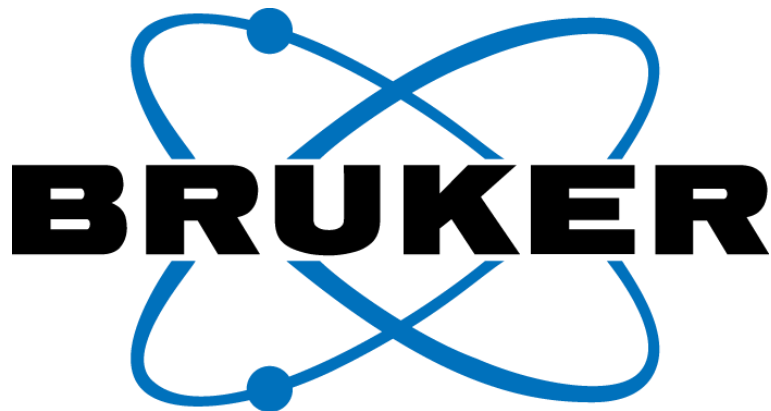
## **Bruker Daltonics GmbH & Co. KG Bremen**

- Aiko Barsch
- Sven Meyer
- Ulrike Schweiger-Hufnagel





# Bruker MRMS Metabolomics Application Notes



## Unambiguous Natural product ID

- **Comparison of CID and EID Mass Spectrum of Glycosides from solarix XR**

Tandem mass spectrometry (MS/MS) is an important tool for structural determination and molecular identification. Collision-induced dissociation (CID) is the most commonly used ion activation method; however, it only gives limited fragments for some classes of compounds. Electron-induced dissociation (EID) provides an alternative ion activation mechanism for fragment generation, which can gain more wealthy information. Here, CID and EID were applied to potatoes glycoalkaloids and flavonoid glycosides for comparison.

Mass spectrometry is now an indispensable analytical technique for molecular characterization because of its high sensitivity and precision. Tandem mass spectrometry (MS/MS) breaks down molecular ions into fragment pieces which allows in-depth structural determination and elucidation. Collision-induced dissociation (CID) is the most commonly used ion activation method for MS/MS. In conventional CID, precursor ion is vibrationally activated through collisions with inert gas atoms/molecules. Bond cleavage occurs preferentially at weak linkages and hence, gives limited structural information. Electron-induced dissociation (EID) is an alternative ion activation approach that is based on electron-ion interaction. Different from CID, EID activates precursor ions by impacting them with high energy electrons. EID produces more cleavages and provides important structural information that cannot be obtained from the traditional CID techniques. In addition, EID can be applied on both singly and multiple charged ions. In this study, two types of glycoconjugates, potatoes glycoalkaloids and flavonoid glycosides, have been analyzed by both CID and EID for comparison.

**Keywords:**  
Tandem mass spectrometry, glycosides, collision-induced dissociation (CID), electron-induced dissociation (EID), structural elucidation.

**Authors:** Yi. Zhao Wang<sup>1</sup>, H. S. Wang<sup>2</sup> and T. H. Dennis Chua<sup>1\*</sup>  
<sup>1</sup> Department of Chemistry, The Chinese University of Hong Kong, HKSAR  
<sup>2</sup> Bruker Scientific Instruments Hong Kong Co., Limited

MRMS-60

## Biomarker Identification in sample cohorts

- **Automated MALDI Magnetic Resonance Mass Spectrometry (MRMS) for biomarker identification in large clinical sample sets**

The selection of a MALDI MS approach in conjunction with the high mass accuracy and resolving power of the MRMS platform has enabled increased sample throughput and the direct interrogation of complex clinical biofluids such as serum and urine without the need for any advanced sample preparation or purification after collection

In conjunction with advanced automated acquisition strategies, data has been acquired in a fraction of the time previously required to facilitate high quality data with the high sample throughput required for large clinical sample sets.

**Introduction**

Mass spectrometry has increasingly been applied in the clinical setting due to the high and specific information content provided to researchers that enables a positive effect on patient outcomes. The foundation of this application is the high sensitivity, mass resolving power, and mass accuracy in combination with the multiplex detection advantage of MRMS when compared to other analytical approaches. A major drawback through is the additional sample preparation required for biofluids prior to LC-MS or direction infusion ESI-MS. An alternative to the approach that eliminates the majority of sample preparation is MALDI-MS. Beyond mixing with a suitable ionization matrix, small amounts of sample (1–1 µL) can be analyzed with no prior preparation or purification after clinical collection and in a high throughput fashion via MALDI

**Keywords:**  
Biomarkers, Clinical MS/MS, MRMS

**Author:** Franklin G. Lench III, University of Georgia, Athens, GA

MRMS-61

## Micropollutants and plant response metabolites

- **MRMS aXelerate – rapidly detected micropollutants and plant response metabolites in poplar leaves**

MRMS aXelerate is demonstrated to be a new and powerful workflow to rapidly profile plant extracts in a context of environmental pollution. This technique enables increased sample throughput by chromatography-free flow injection analysis (FIA) in combination with extreme mass resolution provided by the scimaX MRMS system complementary to deep profiling by LC-MS.

MRMS aXelerate incorporates a 3-tier confidence engine provided by MetaboScape 4.0 allowing confident assignments of molecular formulae: a combination of ultra-high mass accuracy, True Isotopic Pattern and Isotopic Fine Structure to ensure confident assignments at any level. Here it enabled the annotation of plant metabolites from several classes. Additionally, micropollutants (drugs and pesticides) which accumulated in poplar leaves could be detected. This accumulation reflected the growth conditions of the analysed plants, either near polluted water or using only rain water. This study shows the straightforward workflow from plant crude extracts to detect drugs and pesticides using MRMS aXelerate.

**Keywords:**  
Plant metabolites, drugs, pesticides, MS, aXelerate, screening, metabolite profiling, metabolomics

**Author:** Chate Mitter, Matthias Wink, Abu Baraki, Oliver Heiser<sup>1</sup>  
<sup>1</sup> Institut de Biologie Moléculaire des Plantes (IBMP), CNRS, Université de Strasbourg, France; <sup>2</sup> Bruker Daltonik GmbH, Bremen, Germany

MRMS-62

## Metabolic changes in murine hair follicles

- **Analysis of metabolic changes in murine hair follicles treated with Procyanidin-B2 rich nutraceuticals by DI-MRMS**

Known for anti-inflammatory and antioxidant properties, nutraceuticals enriched in Procyanidin-B2 promote hair growth both in vitro and in vivo. However, the metabolic changes associated with the treatment have not been elucidated.

**Abstract**

In this study, direct infusion magnetic resonance mass spectrometry (DI-MRMS) was employed to understand the metabolic shift produced by treatment with Procyanidin-B2 nutraceuticals (Annurca apple extract) in murine models. DI-MRMS allowed the identification of several metabolites using ultra-high mass accuracy and fast analysis time, glutaminylation, peroxide phosphate pathway, glutathione, citrulline and nucleotide synthesis derived metabolites were detected. The metabolic profile revealed that the treatment with Procyanidin-B2 results in the early exit of hair follicles from telogen phase and increased keratin biosynthesis.

**Keywords:**  
Metabolomics, Metabolic, DI-MRMS, MRMS, aXelerate

**Authors:** Giovanni Somerski<sup>1</sup>, Giovanni Sestini<sup>1</sup>, Matthias Wink<sup>2</sup>, Christopher Pissinatti<sup>1</sup>, Peter Caviglioli<sup>1</sup>  
<sup>1</sup> Università degli Studi di Salerno, Fisciano, Campania, Italy; <sup>2</sup> Bruker Daltonik GmbH, Bremen, Germany; <sup>3</sup> Bruker Scientific LLC, Billerica, MA, USA

MRMS-63

## Isotopic fine structure to reveal potential biomarkers

- **A strategy using isotopic fine structure to reveal potential biomarkers showing the effects of traditional Chinese medicines on Alzheimer disease in rats**

Alzheimer disease (AD) is a progressive, unremitting, neurodegenerative disease characterized by progressive memory decline and subsequent loss of broader cognitive functions.

**Introduction**

As the pathogenesis and progression of AD remain unclear, no curative treatment is currently available to slow down or stop the degenerative effects of AD until now, *Rhodiola crenulata* has been widely served as antifatigue, antidepressant and health food for many years in China. Recently, researches showed that not only the *Rhodiola crenulata* extract (RCE) but also its major component, salidroside, has ameliorative effects on the learning and memory deficits in the treatment of AD. However, the therapeutic mechanisms underlying the protective effects of RCE against AD are still unclear. In this study, a metabolomic strategy based on accurate mass and isotopic fine structure (IFS) by Magnetic Resonance Mass Spectrometry (MRMS, traditionally known as FT-ICR MS), was established to explore the effects of *Rhodiola crenulata* extract (RCE) on Alzheimer disease (AD) in rats.

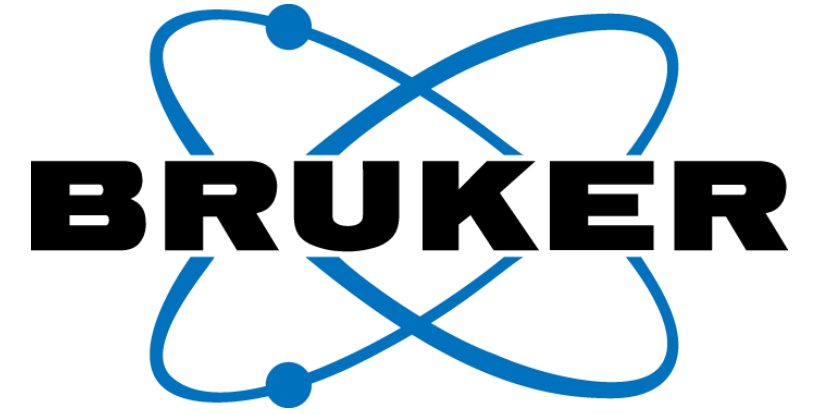
**Keywords:**  
MRMS, traditional Chinese medicine, Rhodiola crenulata, metabolomics, study, degenerative disease, isotopic fine structure

**Authors:** Xiaohua Zhang<sup>1</sup>, Xian Jiang<sup>1</sup>, Jiao Wang<sup>1</sup>, Weiqiang Chen<sup>1</sup>, Jiaojiao Bai<sup>1</sup>, Chen Chen<sup>1</sup>, Ben Huo<sup>1</sup>, De Han<sup>1</sup>  
<sup>1</sup> School of Pharmacy, Shenyang Pharmaceutical University, 101220 Xuhua Road, Shenyang District, Shenyang, 11016, China; <sup>2</sup> School of Medical Devices, Shenyang Pharmaceutical University, 101220 Xuhua Road, Shenyang District, Shenyang, 11016, China; <sup>3</sup> Key Laboratory of Ministry of Education for TCM Modernization Theory and Application, Liaoning University of Traditional Chinese Medicine, 79 Changchun Street Road, Hangege District, Shenyang, 110002, China

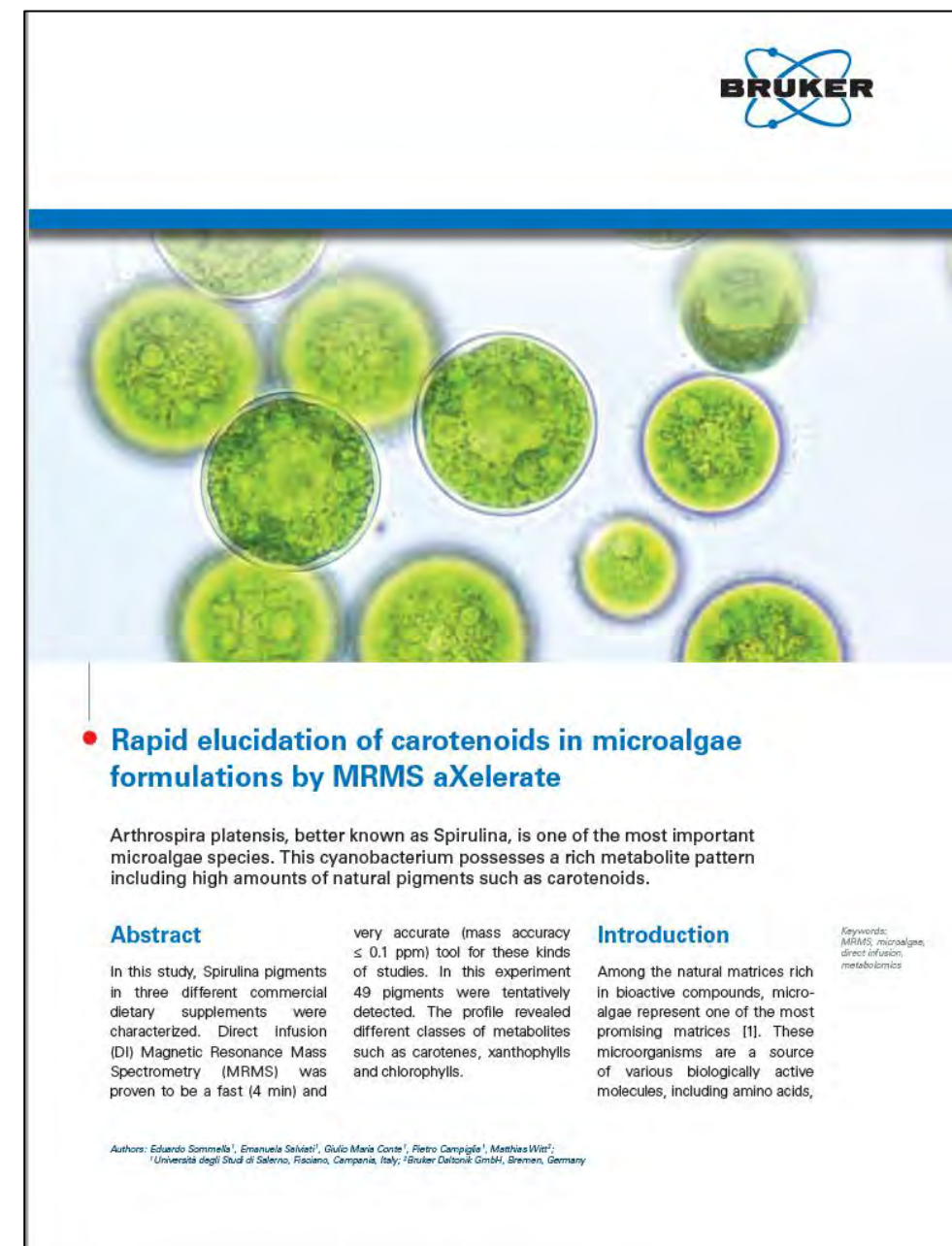
MRMS-65



# Bruker MRMS Metabolomics Application Notes

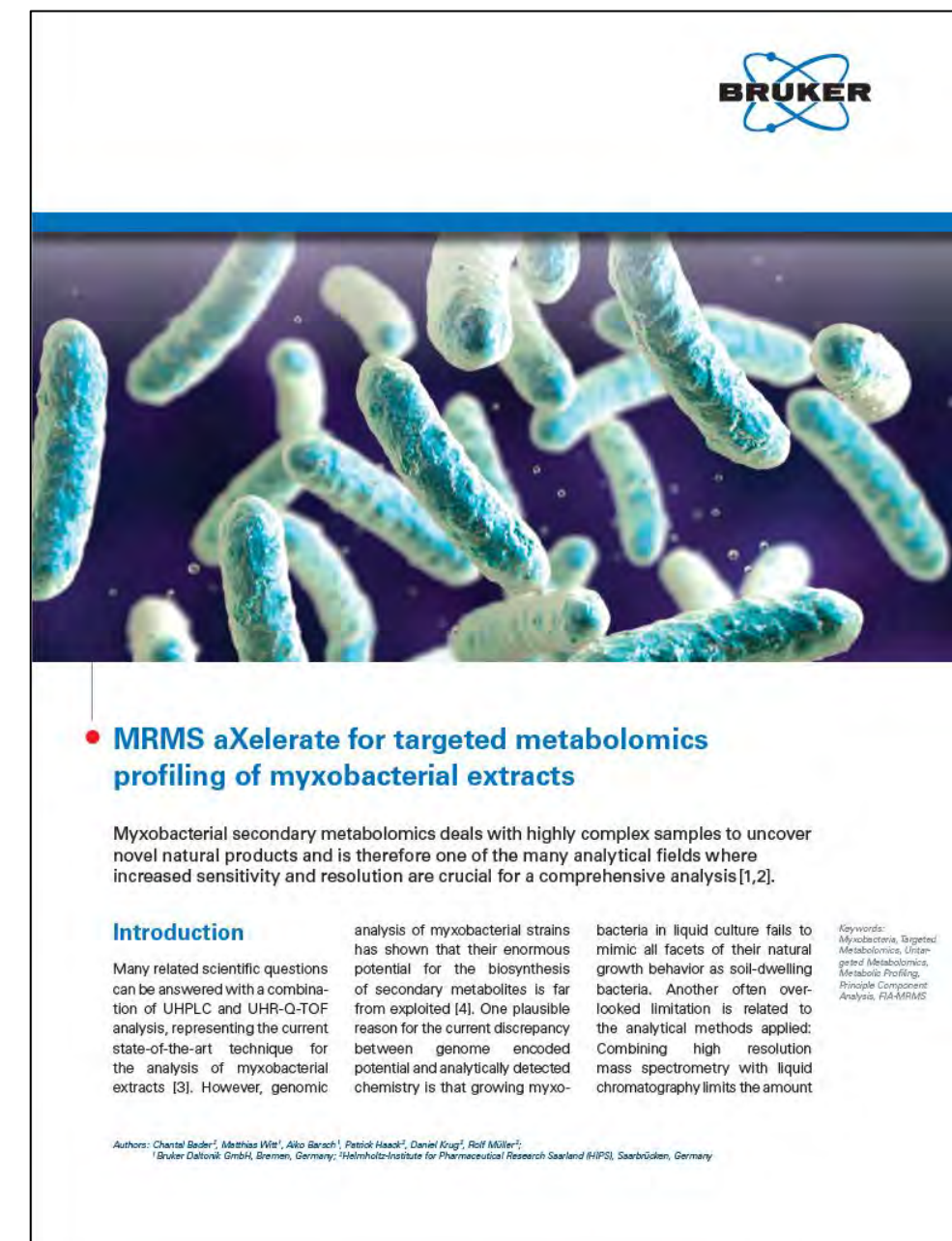


## Carotenoids in microalgae formulations



MRMS-66

## Profiling of myxobacterial extracts



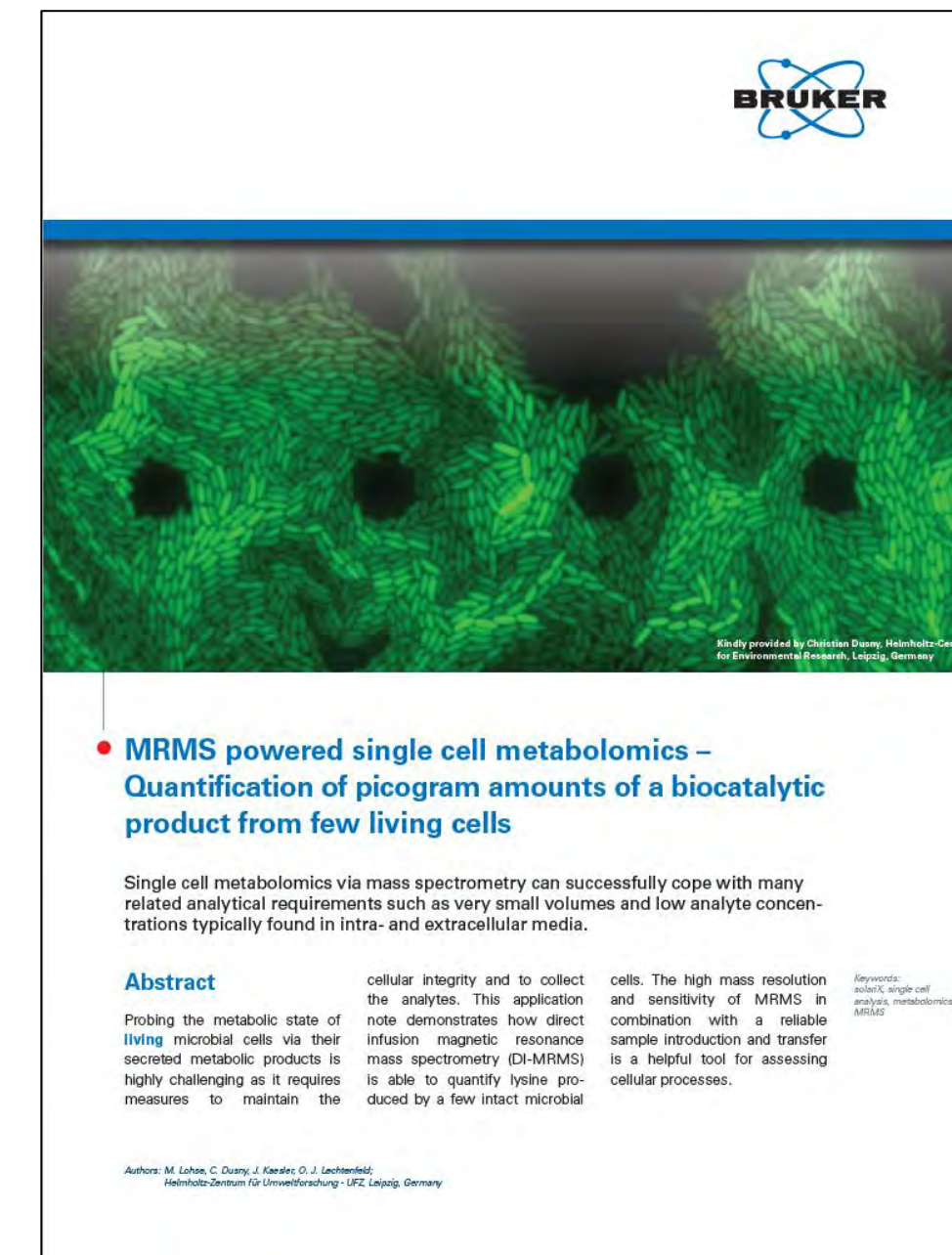
MRMS-67

# Fast profiling of sphingolipids



MRMS-68

## Single cell metabolomics



MRMS-70

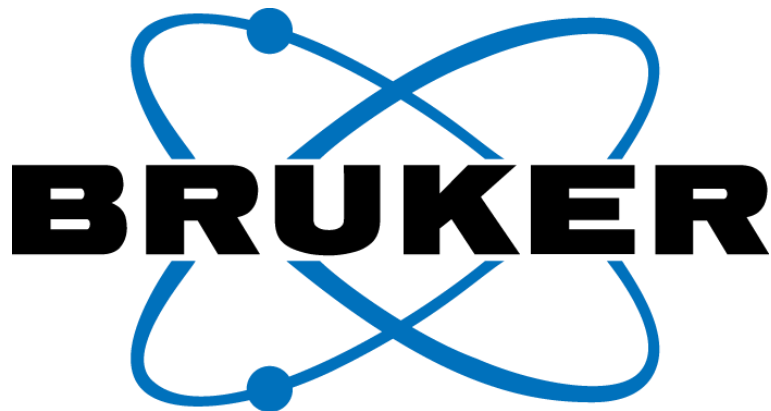
## Fast profiling of sphingolipids



MRMS-71



# Bruker MRMS Metabolomics Application Notes



## Elucidation of metabolic changes

**Elucidation of metabolic changes in HFD-ApoE<sup>-/-</sup> model by SP6 peptide: A flow injection analysis magnetic resonance mass spectrometry (FIA-MRMS) study**

Natural peptides have emerged as an attractive option for the treatment of cardiovascular diseases. A novel peptide from *Spirulina Platensis* (SP6) was evaluated for its potential anti-atherosclerotic effect in a high fat diet ApoE<sup>-/-</sup> mice model using a metabolomics approach.

**Abstract**

employed to evaluate its potential anti-atherosclerotic effect in high fat diet ApoE<sup>-/-</sup> mice model. Untargeted metabolomics and lipidomics was performed by a Flow Injection Analysis Magnetic Resonance Mass Spectrometry (FIA-MRMS) approach, resulting in high mass resolution and mass accuracy as well as repeatability and fast analysis time. Results showed a distinct metabolic switch, with the positive modulation of several key markers of atherosclerosis progression, such as sphingolipids and glycerophospholipids, amino acids and tricarboxylic acid (TCA) cycle intermediates.

**Keywords:** Metabolomics, lipidomics, FIA-MRMS, ApoE<sup>-/-</sup> mice model, SP6 peptide

**Authors:** Eduardo Gonzalez<sup>1</sup>, Anaïs Galt<sup>2</sup>, Fabrice Mercier<sup>3</sup>, Adrien Ouchetto<sup>4</sup>, Marine Del<sup>5</sup>, Pierre Camilleri<sup>6</sup>,  
<sup>1</sup>Department of Pharmacy, University of Salerno, Italy; <sup>2</sup>INSERM U1055, University of Salerno, Italy; <sup>3</sup>INSERM U1055, University of Salerno, Italy; <sup>4</sup>INSERM U1055, University of Salerno, Italy; <sup>5</sup>INSERM U1055, University of Salerno, Italy; <sup>6</sup>INSERM U1055, University of Salerno, Italy

MRMS-73

## Discrimination of yeast mutants by metabolomics

**Magnetic Resonance Mass Spectrometry (MRMS) discriminates yeast mutants through metabolomics**

An untargeted metabolomics approach based on the MRMS aXelerate® workflow was employed to examine changes in methylglyoxal catabolism using *Saccharomyces cerevisiae* as a model system. This approach allowed for subtle changes in cell metabolism to be revealed and phenotypically identical single-gene deletion mutants of isogenic yeast strains to be accurately distinguished.

**Abstract**

An eukaryote model of *Saccharomyces cerevisiae* was used to study the methylglyoxal pathway by Magnetic resonance mass spectrometry (MRMS). It was discovered that glutathione plays a major role in driving metabolic differences between different strains. It is expected that metabolomics-based discrimination of microorganisms surpass other molecular biotyping methods.

**Introduction**

*Saccharomyces cerevisiae* is a model eukaryote with around 6000 genes, most of which can be deleted without compromising cell viability. A vast induced dissociation (EID) is complementary to collision induced dissociation (CID). In this work, CID and EID have been examined. We demonstrate the effectiveness of EID for better characterization of degradation products of pesticides.

**Abstract**

In some cases, differentiation of isomers is challenging. It has been shown that electron induced dissociation (EID) is the most commonly used ion activation method for MS/MS. In conventional CID, precursor ion is vibrationally activated through collisions with inert gas atoms/molecules. Bond cleavage occurs preferentially at weak linkages and hence, gives limited structural information. Electron-induced dissociation (EID) is an alternative ion activation approach that is based on electron-ion interaction. Different from CID, EID activates precursor ions by impacting them with high energy electrons. EID produces more cleavages and provides important structural information that cannot be obtained from the traditional CID techniques. In addition, EID can be applied on both singly and multiply charged ions. In this study, two types of glycoconjugates, potassium glycoalkaloids and flavonoid glycosides, have been analyzed by both CID and EID for comparison.

**Keywords:** Metabolomics, MRMS, aXelerate®, yeast mutants, methylglyoxal catabolism

**Authors:** Maria Druze-Ribe, João Lúcio, Ana Sofia Pereira, Carlos Cordeiro, FICOM and Structural Mass Spectrometry Laboratory, MRE - Marine and Environmental Sciences Centre, Faculdade de Ciências, Universidade de Lisboa, Portugal

MRMS-75

## Structural characterization of pesticide products

**Electron-Induced Dissociation (EID) as a complementary tool to collision induced dissociation (CID) for structural characterization of pesticides photo-oxidation products**

High resolution mass spectrometry (HR-MS) and tandem mass spectrometry (MS/MS) are essential tools for structural elucidation of unknown compounds such as pollutant degradation compounds.

**Abstract**

In some cases, differentiation of isomers is challenging. It has been shown that electron induced dissociation (EID) is the most commonly used ion activation method for MS/MS. In conventional CID, precursor ion is vibrationally activated through collisions with inert gas atoms/molecules. Bond cleavage occurs preferentially at weak linkages and hence, gives limited structural information. Electron-induced dissociation (EID) is an alternative ion activation approach that is based on electron-ion interaction. Different from CID, EID activates precursor ions by impacting them with high energy electrons. EID produces more cleavages and provides important structural information that cannot be obtained from the traditional CID techniques. In addition, EID can be applied on both singly and multiply charged ions. In this study, two types of glycoconjugates, potassium glycoalkaloids and flavonoid glycosides, have been analyzed by both CID and EID for comparison.

**Keywords:** Tandem mass spectrometry, pesticides, photo-oxidation products, EID, CID, structural characterization

**Authors:** Béatrice Nivet, Sophie Bourcier, LCM, CNRS, Ecole Polytechnique, Institut de polytechnique de Paris, Route de Saclay, 91128 Palaiseau, France

MRMS-76

## CID and EID of Glycosides

**Comparison of CID and EID Mass Spectrum of Glycosides from solarix XR**

Tandem mass spectrometry (MS/MS) is an important tool for structural determination and molecular identification. Collision-induced dissociation (CID) is the most commonly used ion activation method; however, it only gives limited fragments for some classes of compounds. Electron-induced dissociation (EID) provides an alternative ion activation mechanism for fragment generation, which can gain more wealthy information. Here, CID and EID were applied to potatoes glycoalkaloids and flavonoid glycosides for comparison.

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**Keywords:** Tandem mass spectrometry, glycosides, CID, EID, structural elucidation

**Authors:** Li, Bao-Ming<sup>1</sup>, H. J. Wang<sup>2</sup> and T. H. Chen<sup>3</sup> et al.  
<sup>1</sup> Department of Chemistry, The Chinese University of Hong Kong, HK SAR  
<sup>2</sup> Bruker Scientific Instruments Hong Kong Co. Limited

FTMS-57

## EID of isomeric metabolites

**Electron Induced Dissociation for the Differentiation of Isomeric Metabolites of Diclofenac**

Electron induced dissociation (EID) is applied for the differentiation of structural isomers of diclofenac metabolites. EID showed superior capability over collision induced dissociation (CID) by providing detailed structural information to locate the hydroxyl groups on different rings.

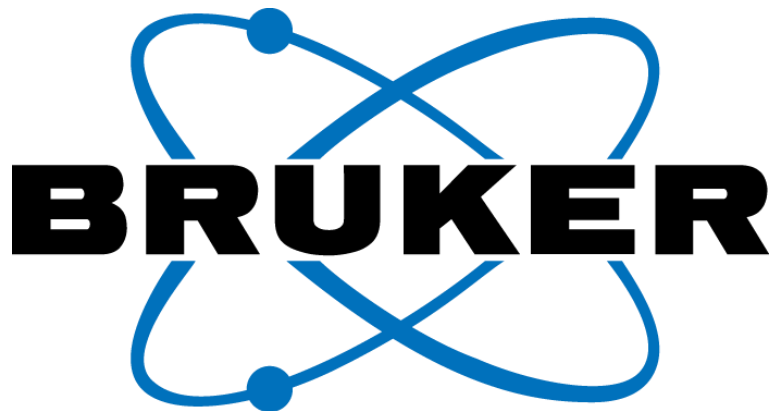
In the human body, metabolism of drugs is a detoxification process. In some cases, the metabolites formed are chemically or pharmacologically active and may play an important role in observed pharmacology and/or toxicology in humans. Diclofenac is a non-steroidal anti-inflammatory drug (NSAID) commonly used to reduce inflammation and pain. A major metabolic pathway for diclofenac is phenyl hydroxylation, resulting in two major metabolites, 4'-OH-diclofenac (4'-OHD) and 5-OH-diclofenac (5-OHD), catalyzed by cytochrome CYP2C9 and 2C19, respectively<sup>1</sup>. Determining the structures of these metabolites is critical for understanding the underlying biological activities and safety risk. NMR is well-established as a powerful structural elucidation technique<sup>2</sup>; however, it requires a relatively large amount of purified material that requires labor-intensive and time-consuming purification steps. Alternatively, low energy CID, one of the most commonly used MS/MS techniques, provides detailed structural information for molecules of interest. Unfortunately, low energy CID is unable to differentiate the structural isomers due to the lack of specific bond cleavages.

**Keywords:** EID, NMR, Metabolism

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# Bruker MRMS Metabolomics Application Notes



## Mapping of olive oil

- Mapping of Greek olive oil using magnetic resonance mass spectrometry flow injection analysis and multivariate data analysis

In this study, LC free magnetic resonance mass spectrometry (MRMS) analysis was employed for mapping and quality control assessment of Greek extra virgin olive oil (EVOO) using a new and intuitive software workflow.

**Introduction**

The increasing popularity of EVOO over the last decade has provided the need for quality and authenticity control<sup>(1)</sup>. Its chemical complexity impedes the

transaction of the typical analytical methodologies<sup>(2)</sup>. In this study, a holistic approach to map Greek EVOO is presented. The workflow takes advantage of the rapid, LC free, flow injection analysis (FIA) based data acquisition by

ultra-high resolution MRMS. The obtained mass spectra were evaluated using the new MetaboScape<sup>®</sup> 3.0 software for deconvoluting, as well as for identifying the most significant metabolites.

Keywords: MetaboScape 3.0, Magnetic Resonance Mass Spectrometry (MRMS), Flow Injection Analysis, Authenticity Assessment

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## Profiling of wine

- Profiling of Wine using ultra-high resolution Flow Injection Magnetic Resonance Mass Spectrometry (MRMS) and <sup>1</sup>H-NMR Spectroscopy

The complexity of organic compounds in food products such as wine can be analyzed by LC free magnetic resonance mass spectrometry.

**Introduction**

Beside GC/MS and LC/MS, wine can be analyzed on the molecular level by Flow Injection Analysis (FIA) after solid phase extraction

(SPE) when combined with ultra-high resolution magnetic resonance mass spectrometry (MRMS). The mass spectra are a fingerprint of these complex mixtures of organic compounds.

Multivariate statistical analysis of FIA-MRMS and <sup>1</sup>H-NMR spectroscopy resulted in similar results.

Keywords: MetaboScape 3.0, Magnetic Resonance Mass Spectrometry (MRMS), <sup>1</sup>H-NMR Spectroscopy, Flow Injection Analysis

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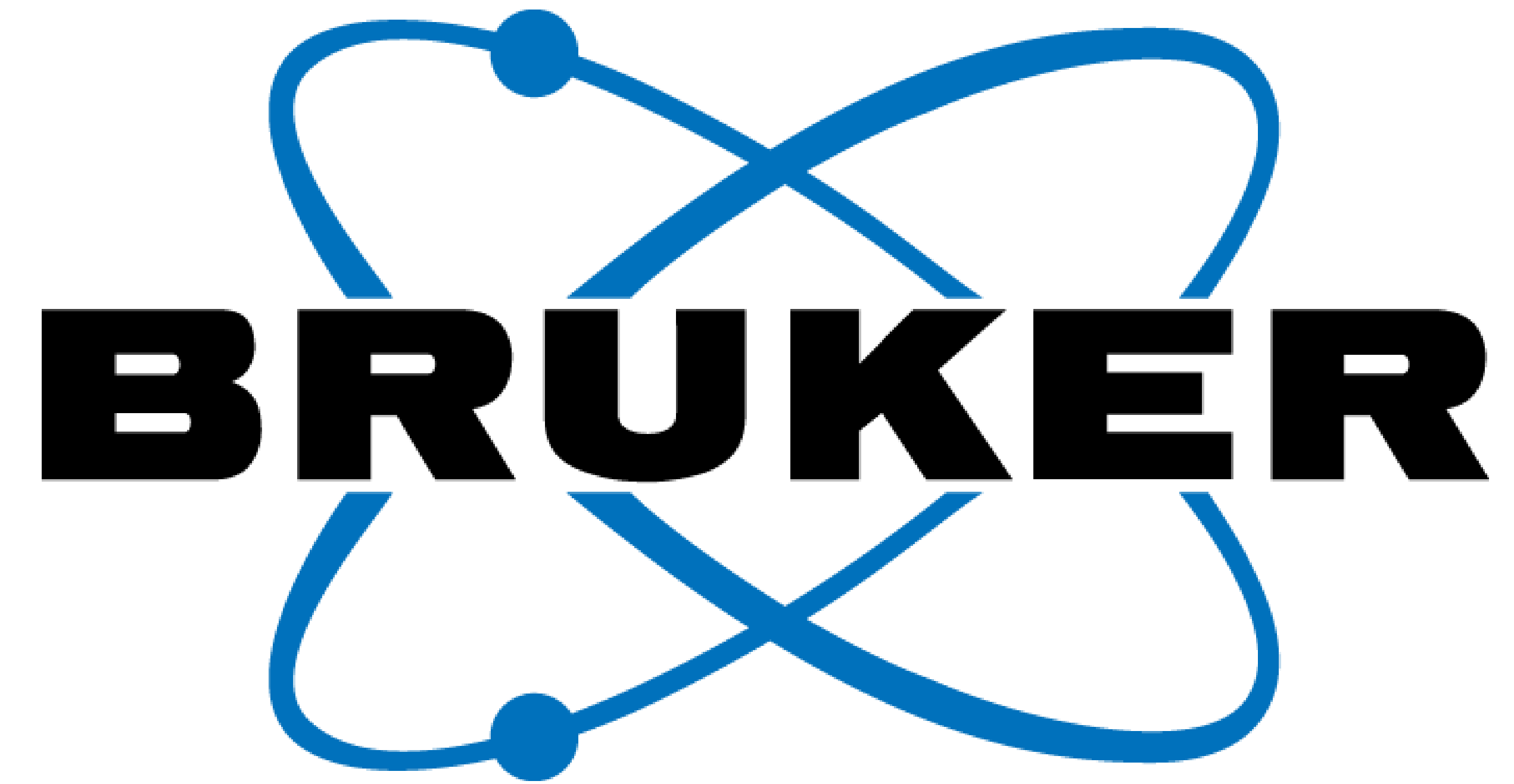






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