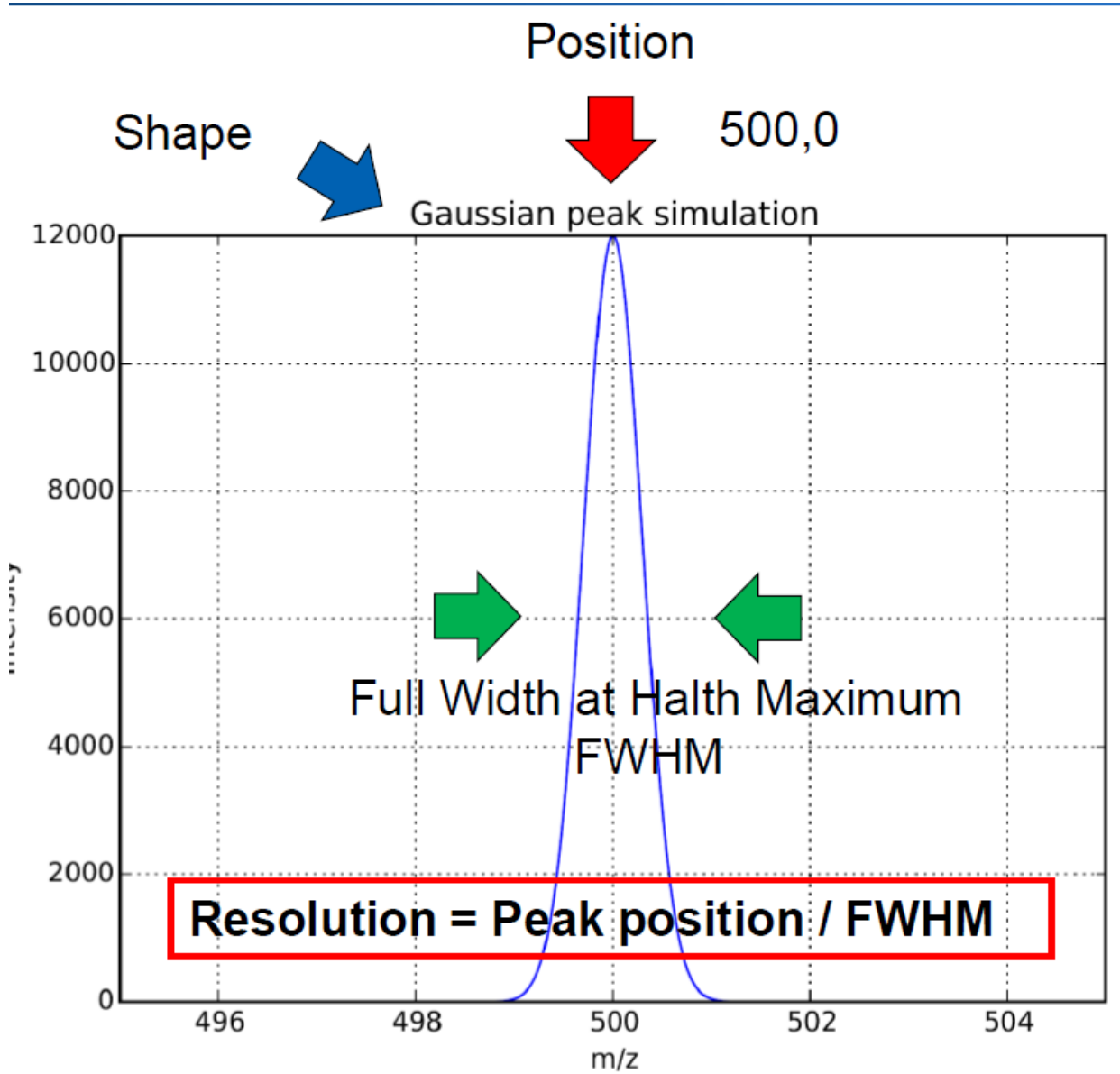
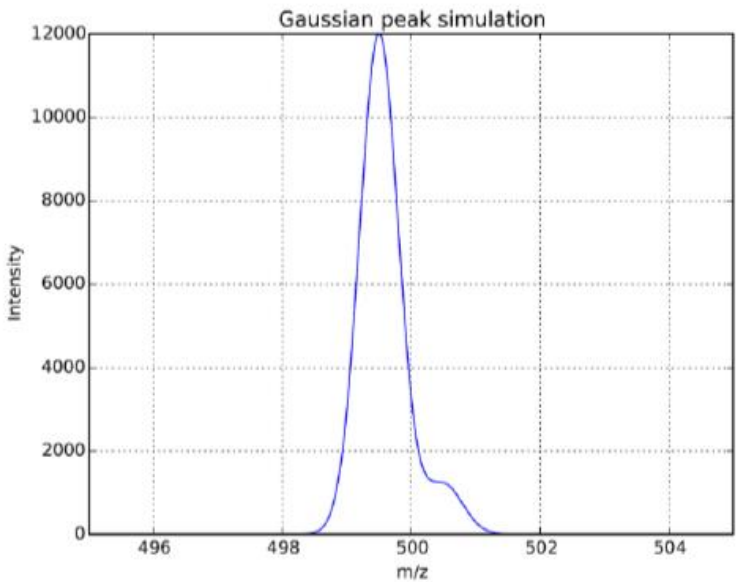
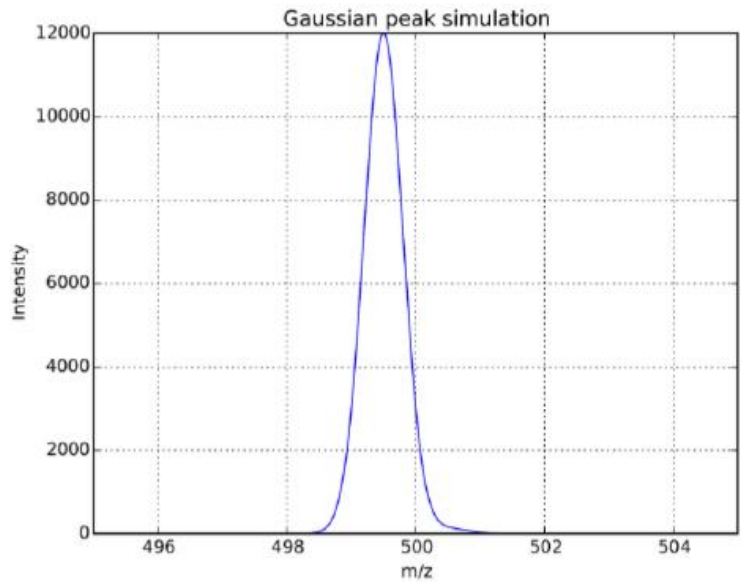
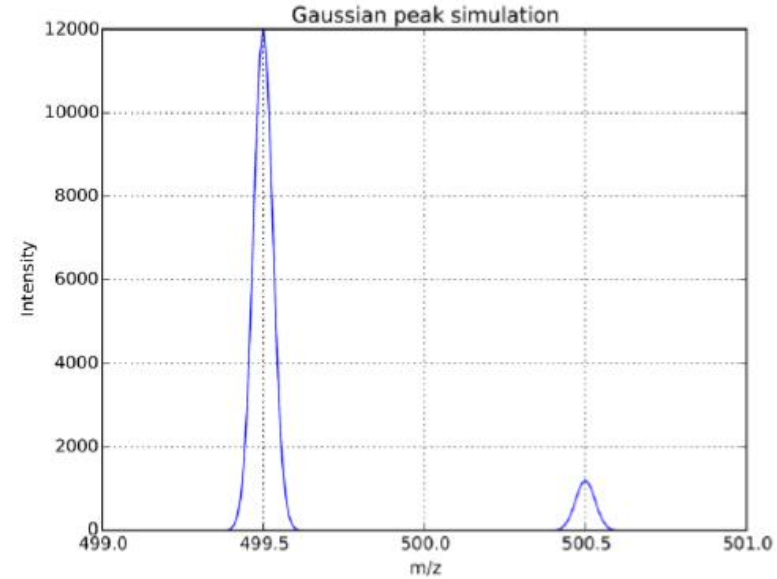
SPETTROMETRIA DI MASSA
Potere Risolutivo, Risoluzione e accuratezza di massa

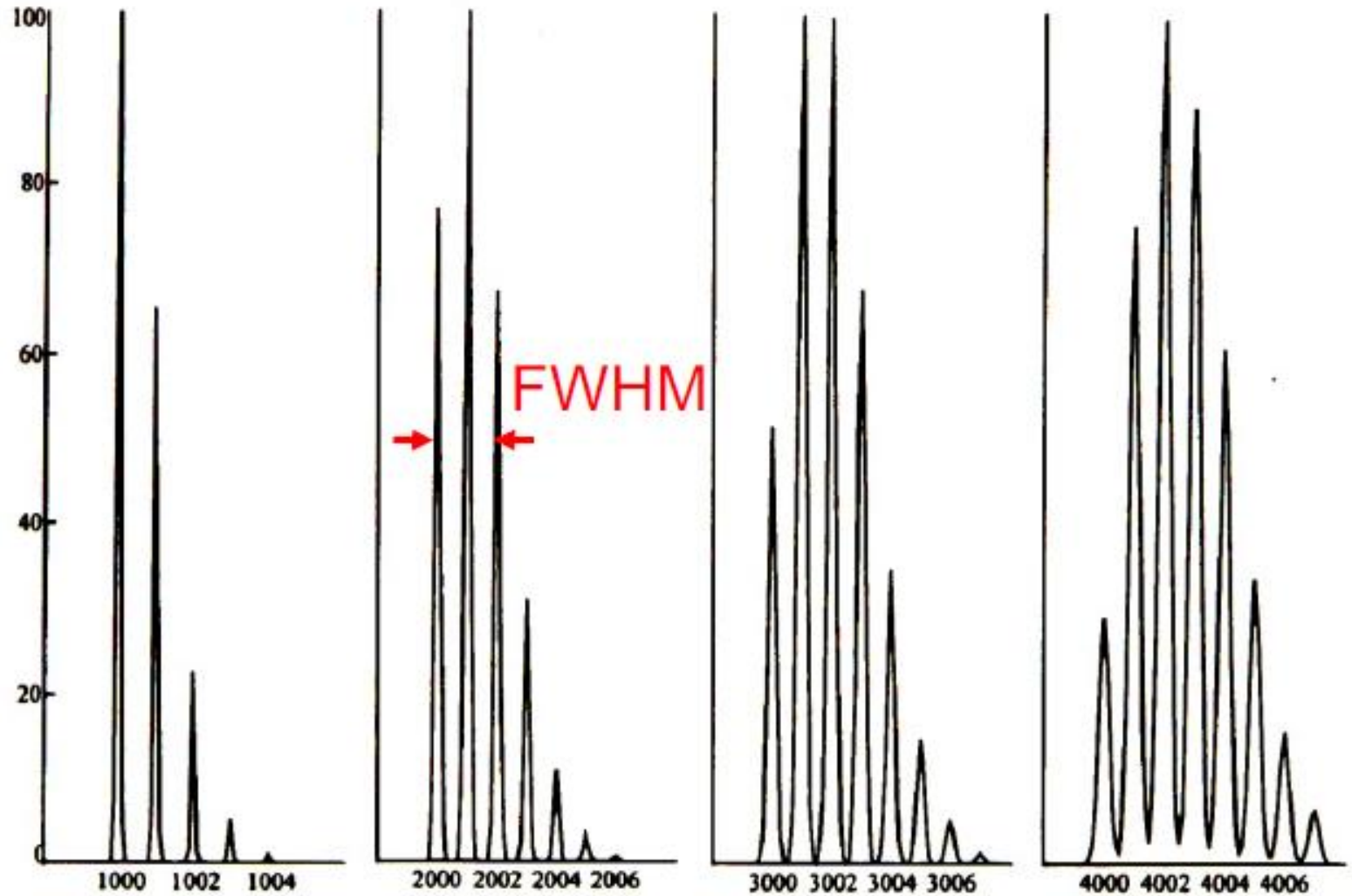

Position
Shape
500,0
Gaussian peak simulation
12000
10000
8000
6000
4000
2000
0
496
498
500
502
504
m/z
Full Width at Halth Maximum
FWHM
Resolution = Peak position / FWHM


Gaussian peak simulation
12000
10000
8000
6000
4000
2000
0
Intensity
496
498
500
502
504
m/z


Gaussian peak simulation
12000
10000
8000
6000
4000
2000
0
Intensity
496
498
500
502
504
m/z


Gaussian peak simulation
12000
10000
8000
6000
4000
2000
0
Intensity
499.0
499.5
500.0
500.5
501.0
m/z

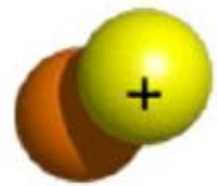
Mass Analyzer	Mass Range (u)	Mass Resolution	Mass Accuracy (ppm)
Fourier Transform Ion Cyclotron Resonance (FT ICR)	30.000	1.000.000+	< 1 (@ 400 u)
Orbitrap	50.000	500.000	< 2 (@ 100-2000)
Magnetic Sector (BE)	20.000	100.000	< 10
Time-of-Flight (TOF, RTOF)	> 1.000.000	5.000-20.000	200; 5-10
Quadrupole (Q)	4.000	2.000	100
Iontrap (IT)	6.000	4.000	100

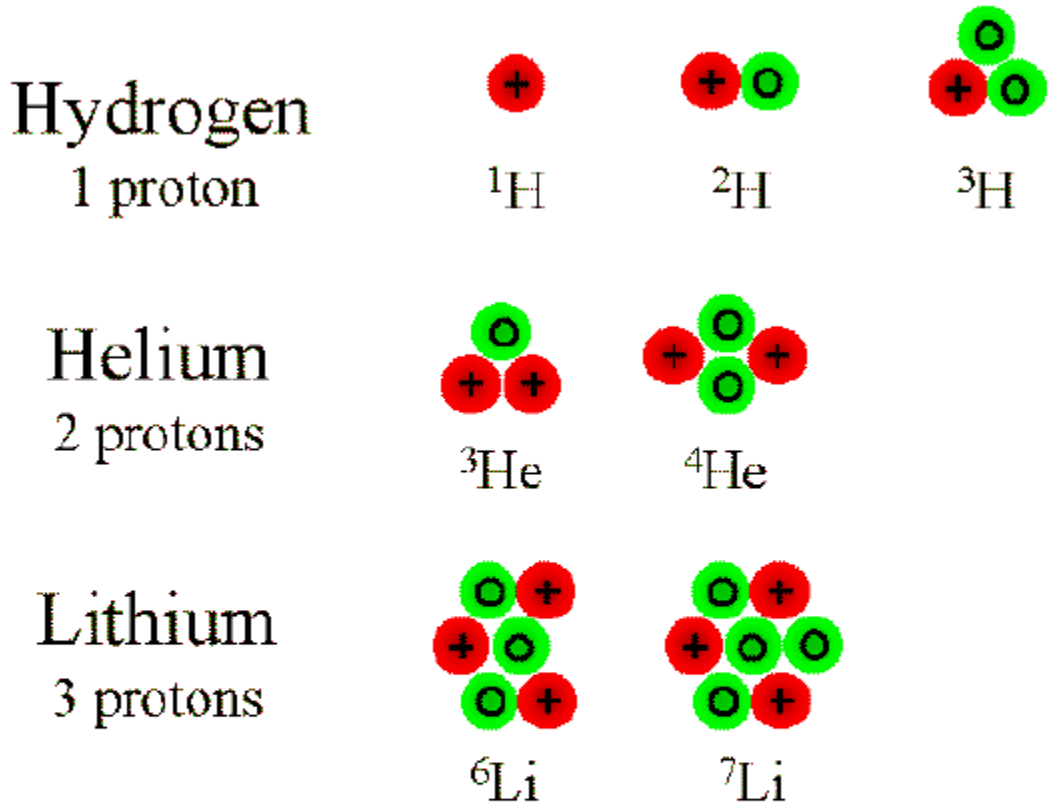


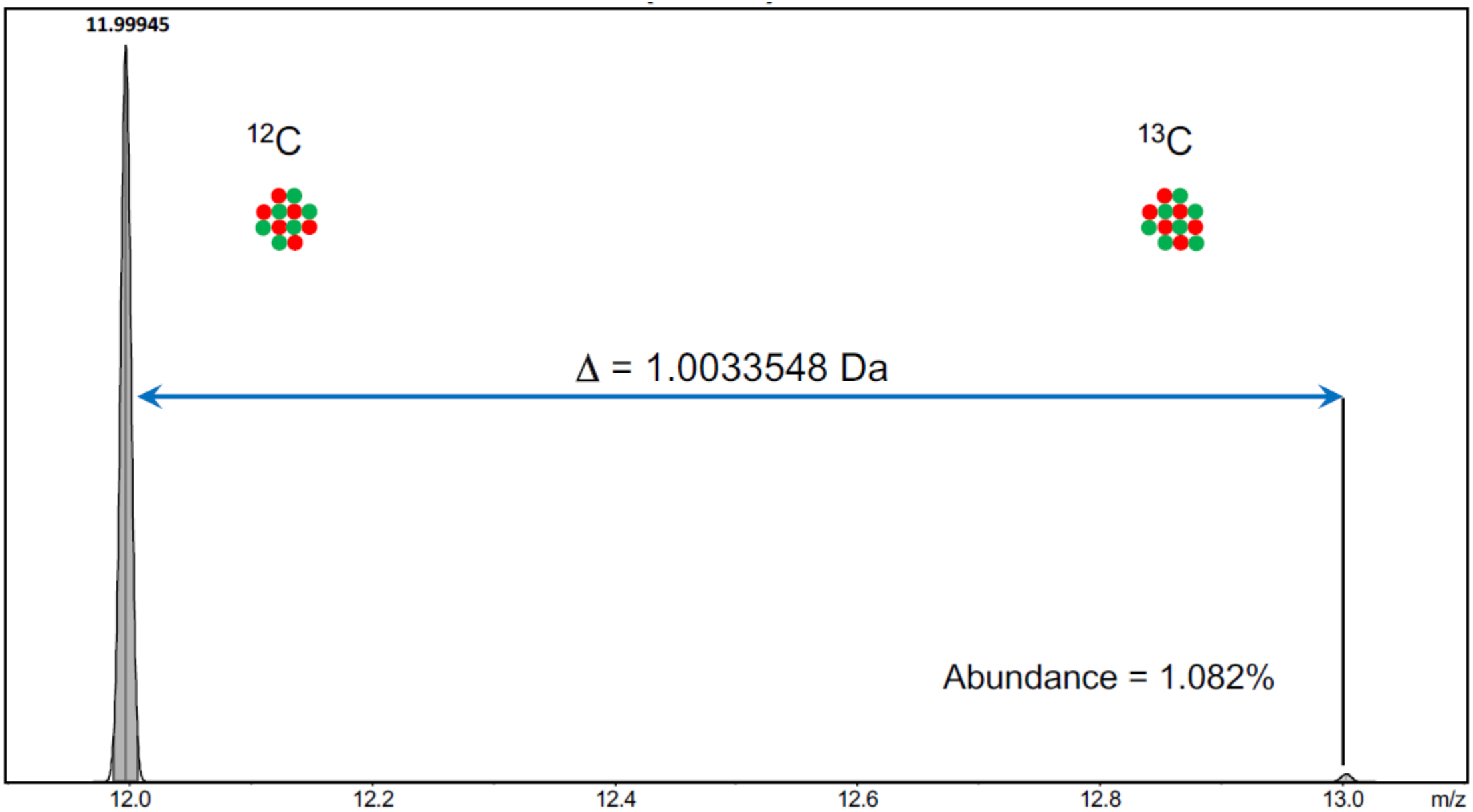
Theoretical isotope distributions of peptides of 1000, 2000, 3000 and 4000 Da.

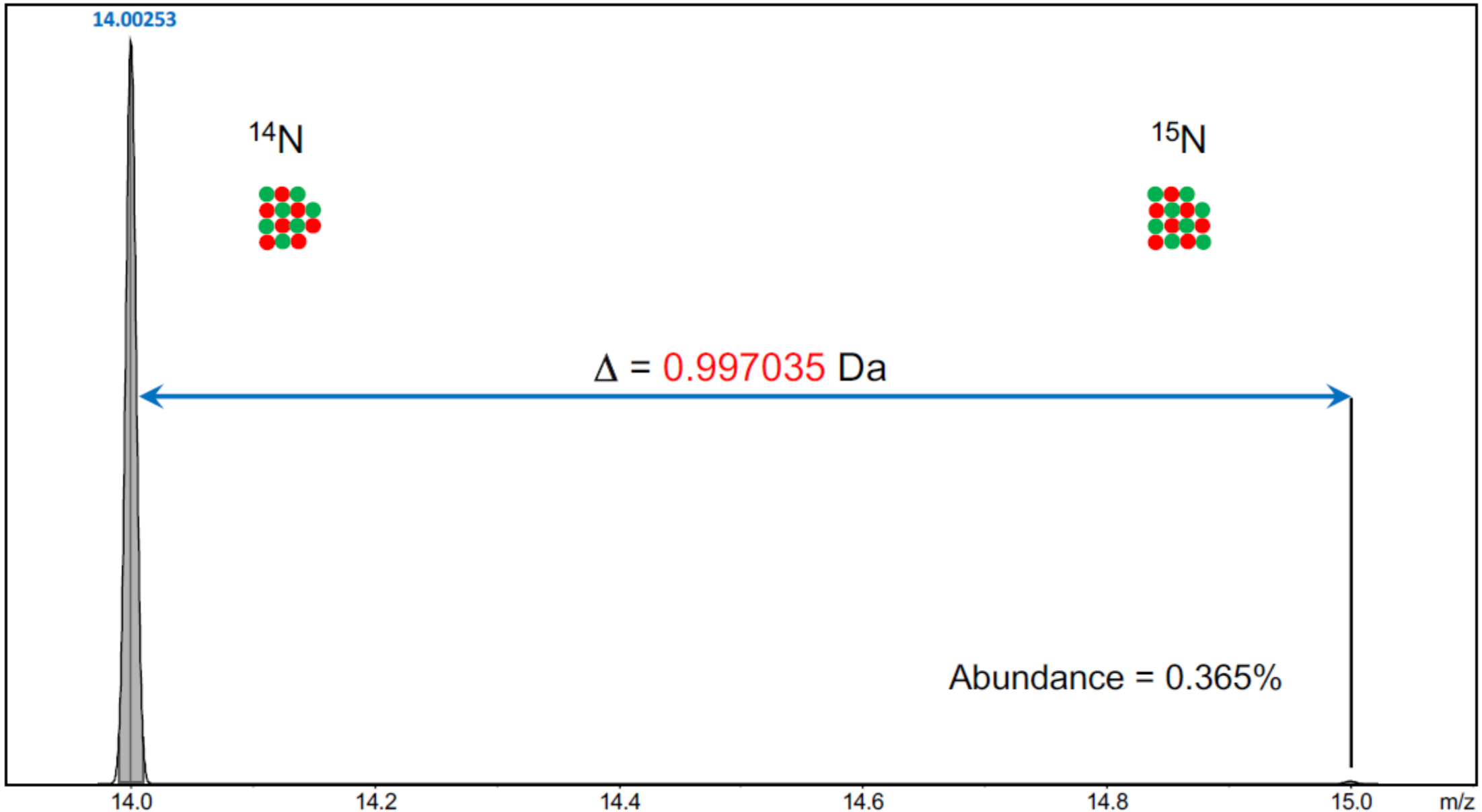
Isotope	*Mass*	*Abundance*	*Chemical mass*	*Deviation from the whole number*
^{1}H	1.00782510	99.9852%	1.00794	+0.0079
^{2}H (D)	2.01410222	0.0148%		
^{12}C	12.0(0)	98.892%	12.011	+0.011
^{13}C	13.0033544	1.108%		
^{14}N	14.00307439	99.635%	14.00674	+0.007
^{15}N	15.0001077	0.365%		
^{16}O	15.99491502	99.759%	15.9994	-0.0006
^{17}O	16.9991329	0.037%		
^{18}O	17.99916002	0.204%		
^{31}P	30.9737647	100%	30.9737647	-0.0262
^{32}S	31.9720737	95.0%	32.066	+0.066
^{33}S	32.9714619	0.76%		
^{34}S	33.9678646	4.22%		
^{36}S	35.967090	0.014%		

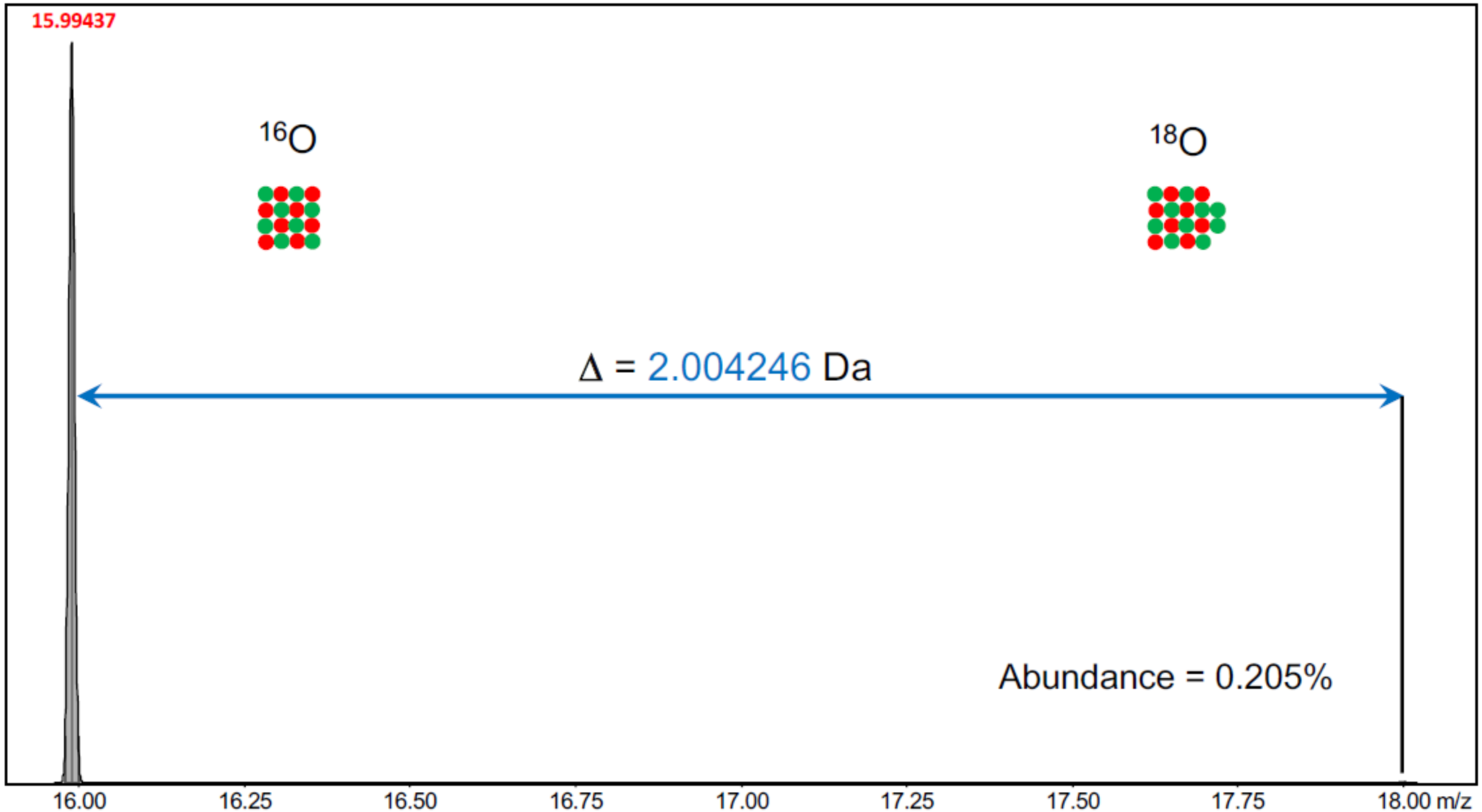
The Nuclei of the Three Isotopes of Hydrogen

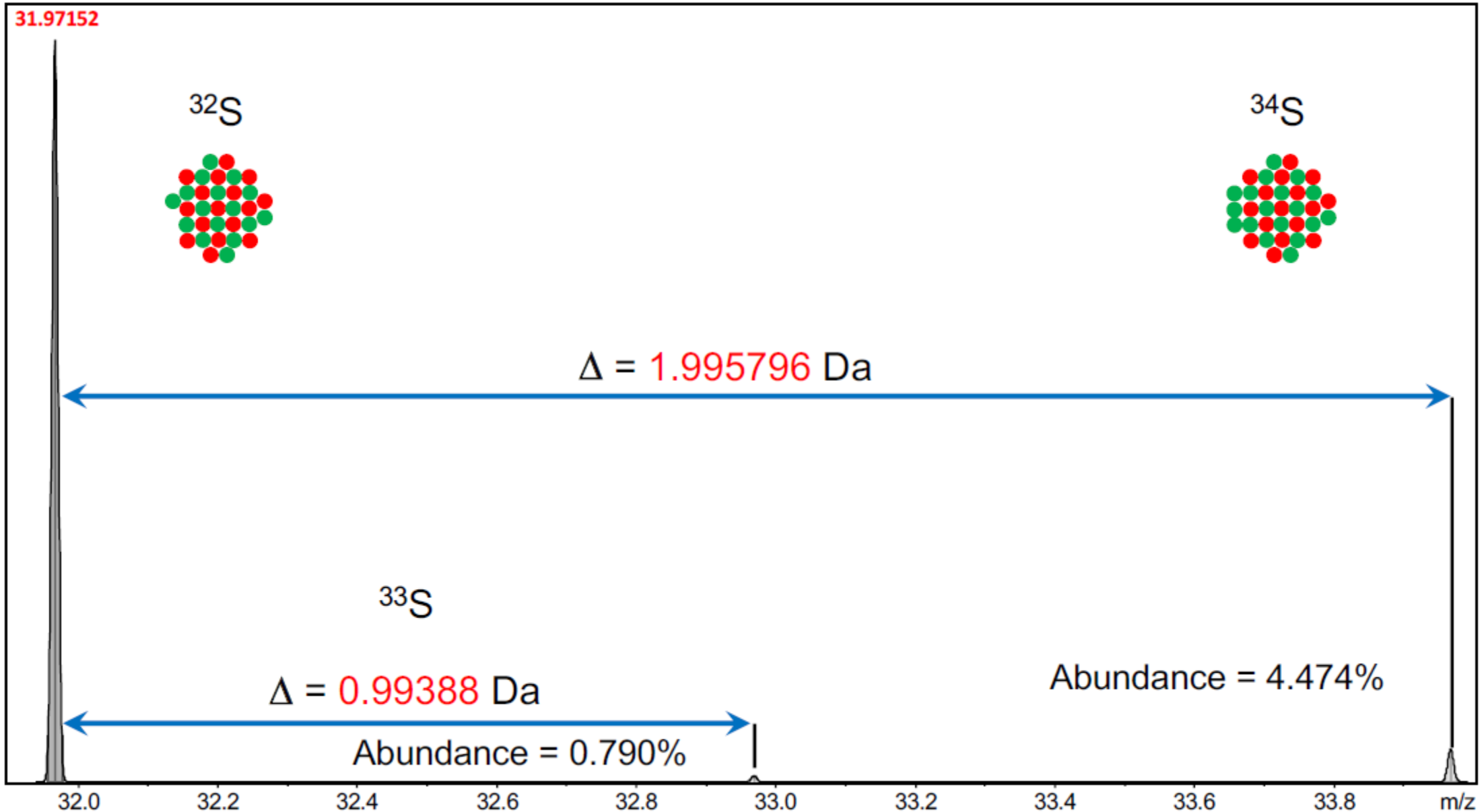
Protium	Deuterium	Tritium
		
1 proton	1 proton 1 neutron	1 proton 2 neutrons

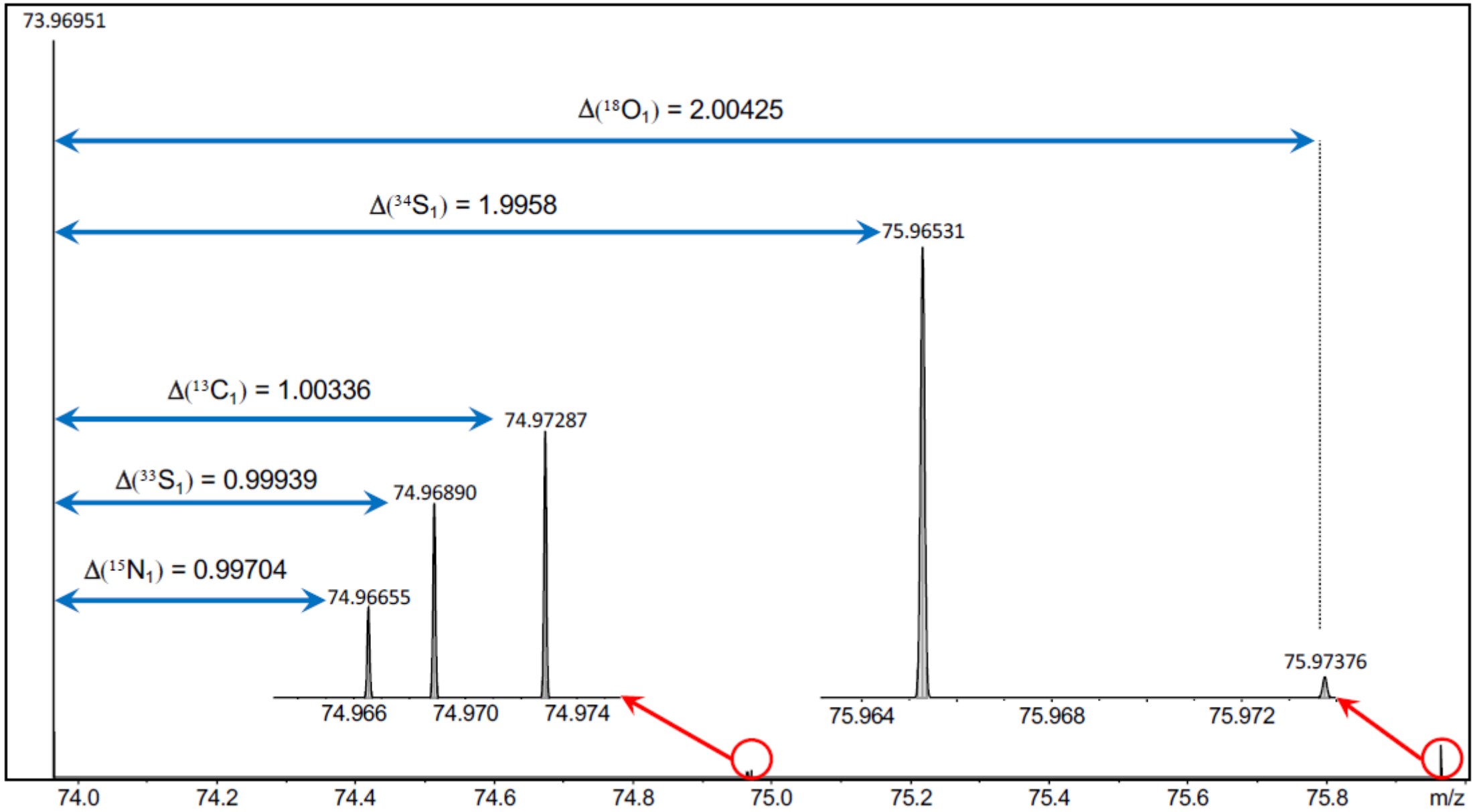

Hydrogen
1 proton
^{1}H
^{2}H
^{3}H
Helium
2 protons
^{3}He
^{4}He
Lithium
3 protons
^{6}Li
^{7}Li
Proton:
Neutron:
1.00727
1.00866


11.99945
^{12}C
^{13}C
Δ = 1.0033548 Da
Abundance = 1.082%
12.0
12.2
12.4
12.6
12.8
13.0
m/z


14.00253
^{14}N
^{15}N
Δ = 0.997035 Da
Abundance = 0.365%
14.0
14.2
14.4
14.6
14.8
15.0
m/z


15.99437
^{16}O
^{18}O
Δ = 2.004246 Da
Abundance = 0.205%
16.00
16.25
16.50
16.75
17.00
17.25
17.50
17.75
18.00 m/z

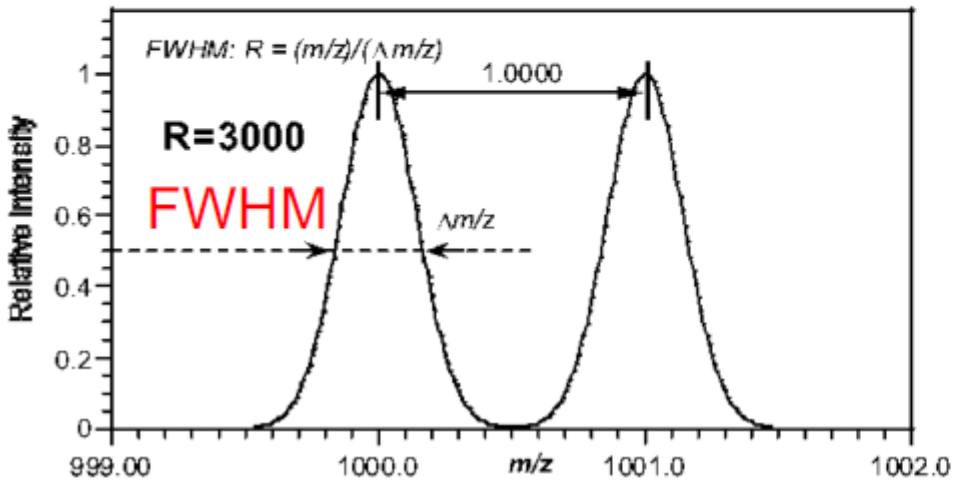

31.97152
32S
34S
Δ = 1.995796 Da
33S
Δ = 0.99388 Da
Abundance = 0.790%
Abundance = 4.474%
32.0
32.2
32.4
32.6
32.8
33.0
33.2
33.4
33.6
33.8
m/z

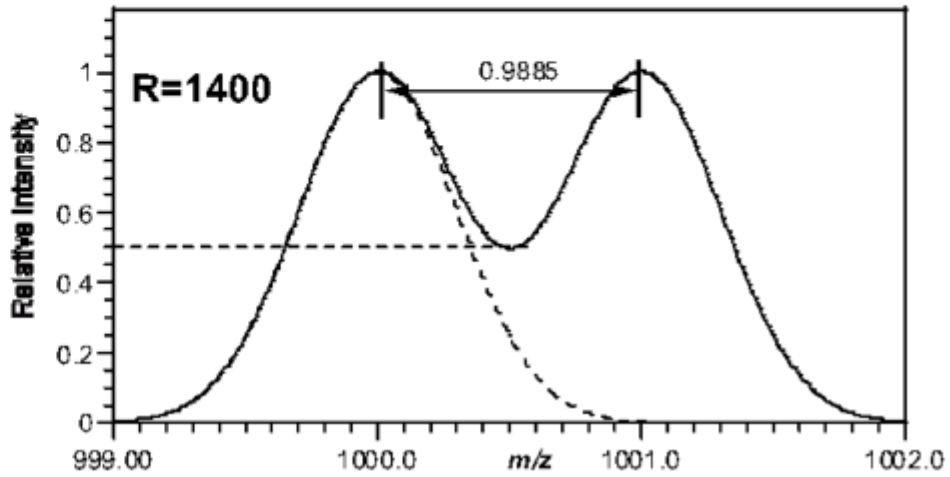

73.96951
Δ(18O1) = 2.00425
Δ(34S1) = 1.9958
75.96531
Δ(13C1) = 1.00336
74.97287
Δ(33S1) = 0.99939
74.96890
Δ(15N1) = 0.99704
74.96655
75.97376
74.966
74.970
74.974
75.964
75.968
75.972
74.0
74.2
74.4
74.6
74.8
75.0
75.2
75.4
75.6
75.8
m/z

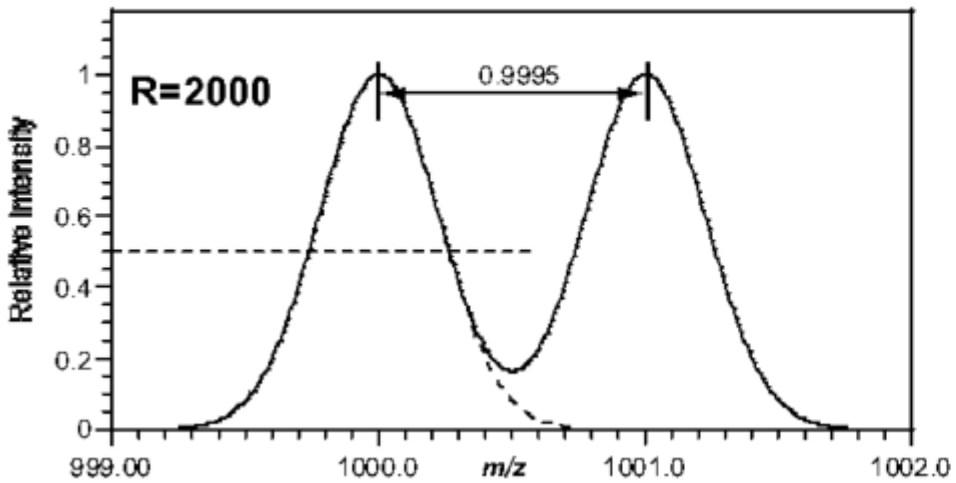
	mass	probability	^{1}H	^{2}H	^{12}C	^{13}C	^{14}N	^{15}N	^{16}O	^{17}O	^{18}O	^{32}S	^{33}S	^{34}S	^{36}S
1	5731.6075806688	0.1123023514	377	0	252	2	65	0	75	0	0	6	0	0	0
2	5732.6109355040	0.1028778936	377	0	251	3	65	0	75	0	0	6	0	0	0
3	5730.6042258336	0.0814037470	377	0	253	1	65	0	75	0	0	6	0	0	0
4	5733.6142903392	0.0704027660	377	0	250	4	65	0	75	0	0	6	0	0	0
5	5734.6176451744	0.0383896060	377	0	249	5	65	0	75	0	0	6	0	0	0
7	5733.6033765247	0.0301636876	377	0	252	2	65	0	75	0	0	5	0	1	0
6	5729.6008709984	0.0293871014	377	0	254	0	65	0	75	0	0	6	0	0	0
8	5734.6067313599	0.0276323390	377	0	251	3	65	0	75	0	0	5	0	1	0
9	5732.6046155640	0.0266824062	377	0	252	2	64	1	75	0	0	6	0	0	0

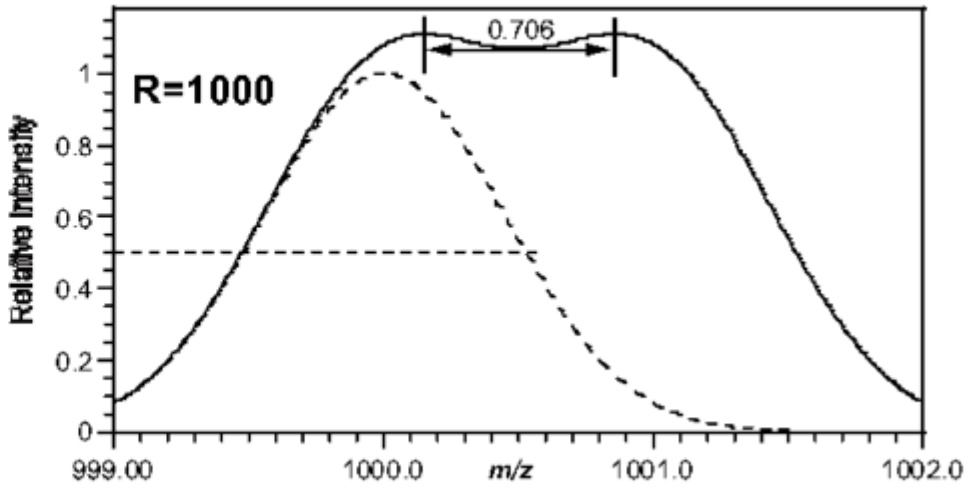
$R = (m/z)_0/FWHM(m/z)$

FWHM: **f**ull **w**idth at **h**alf **m**aximum

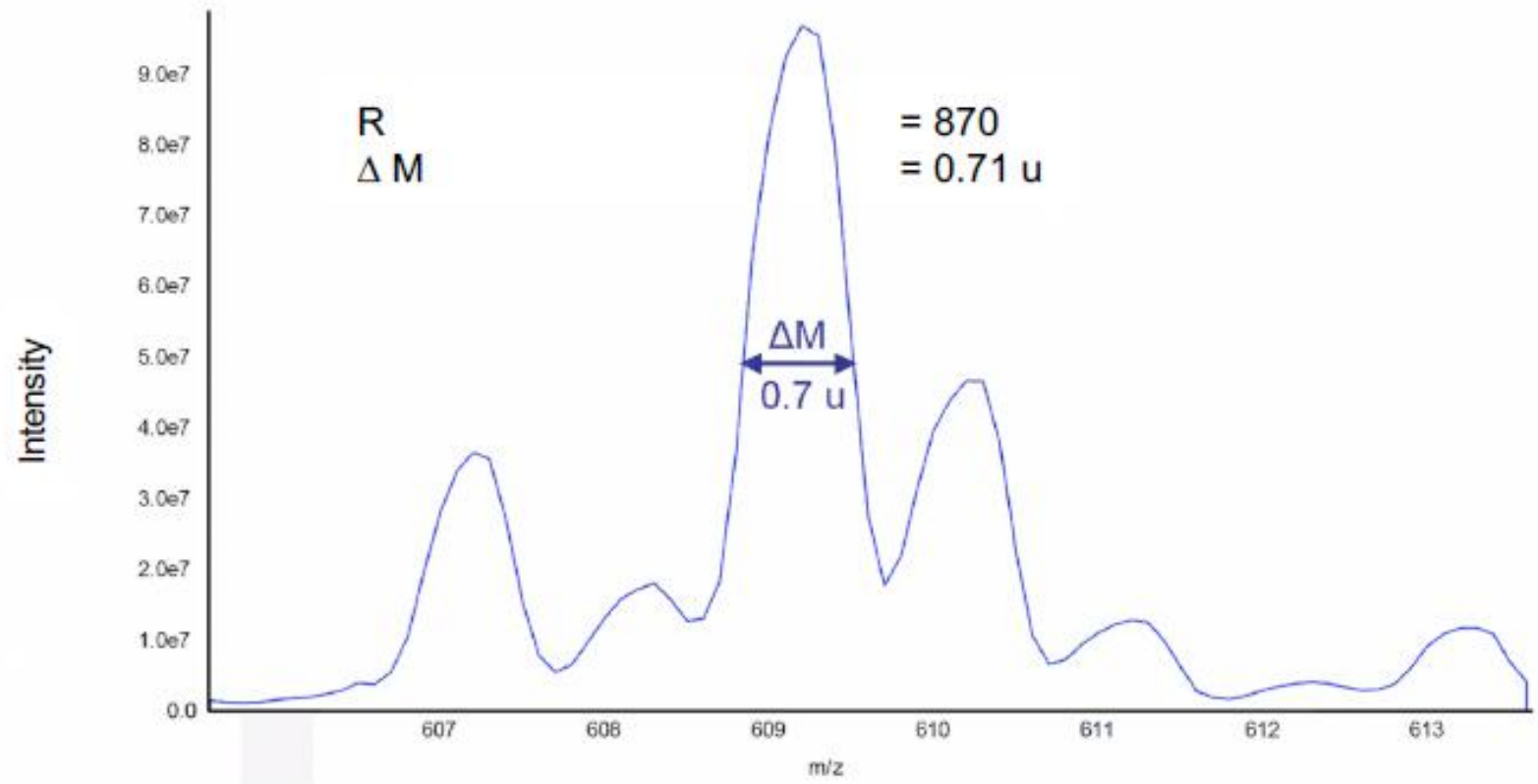




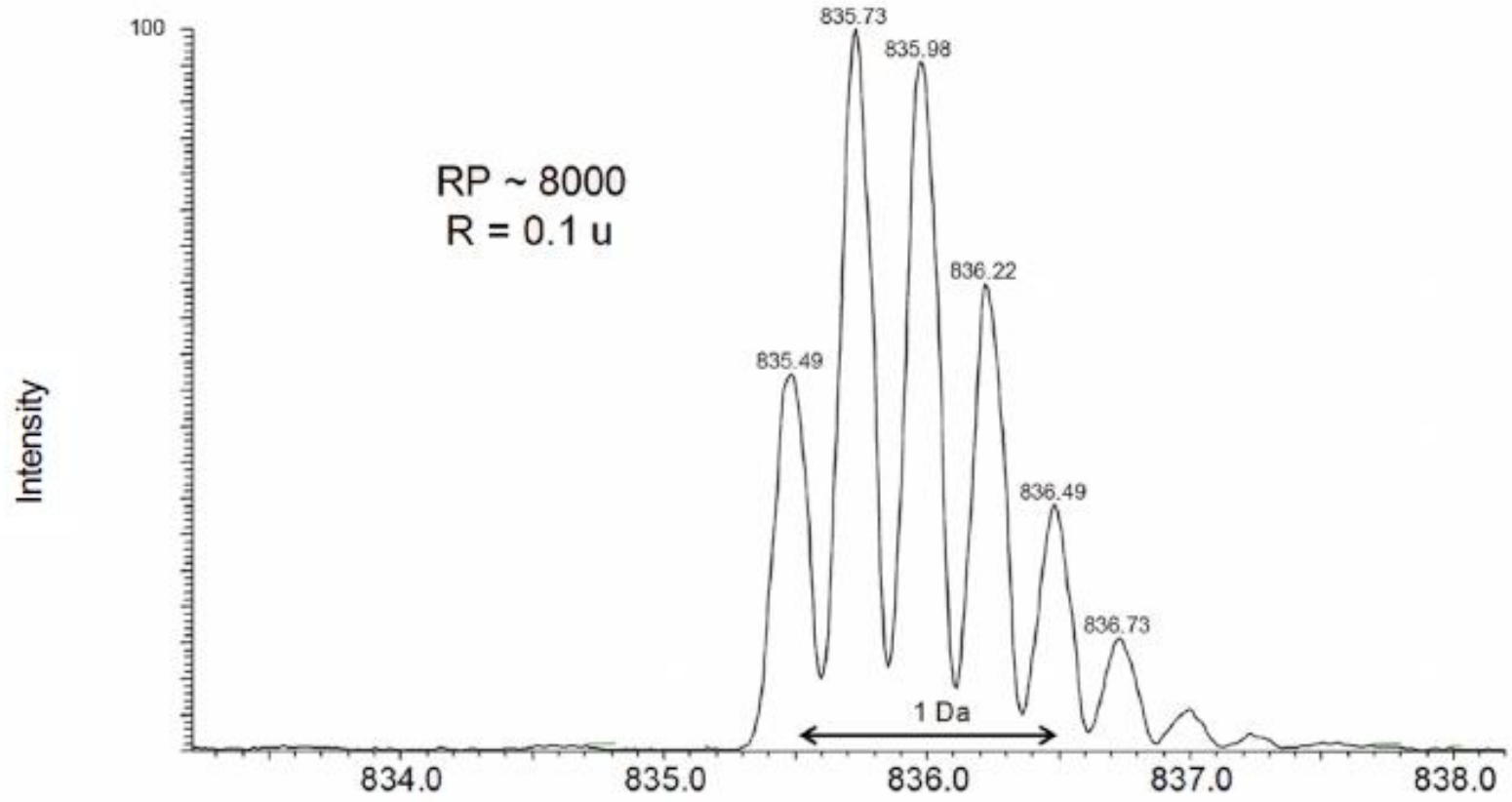




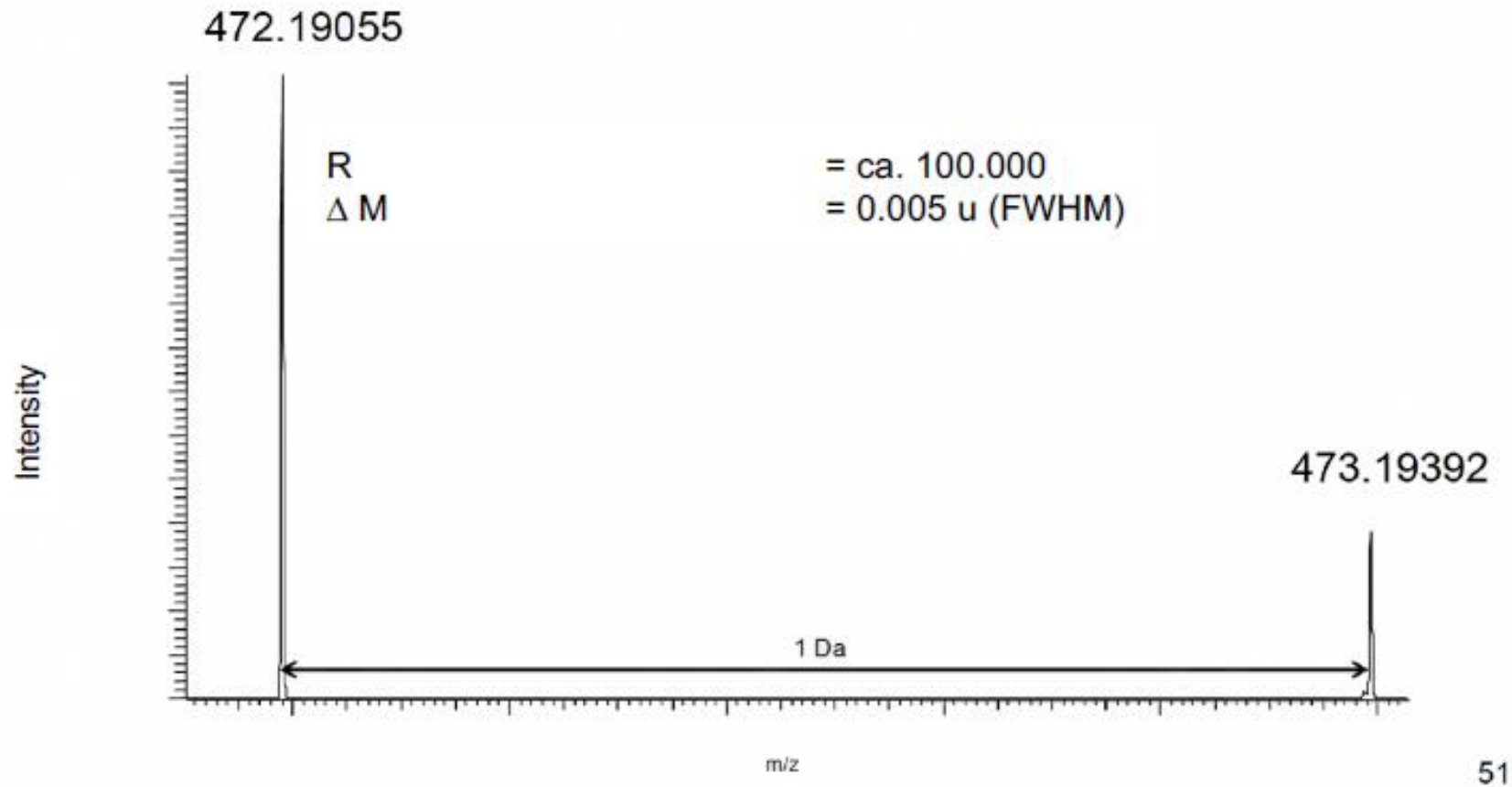
low resolution



moderate resolution



high resolution



Average Mass e.g C=12.01115

Mass of an ion or molecule weighted
for its *isotopic composition*.

Monoisotopic Mass (Exact Mass) e.g. C=12.000000

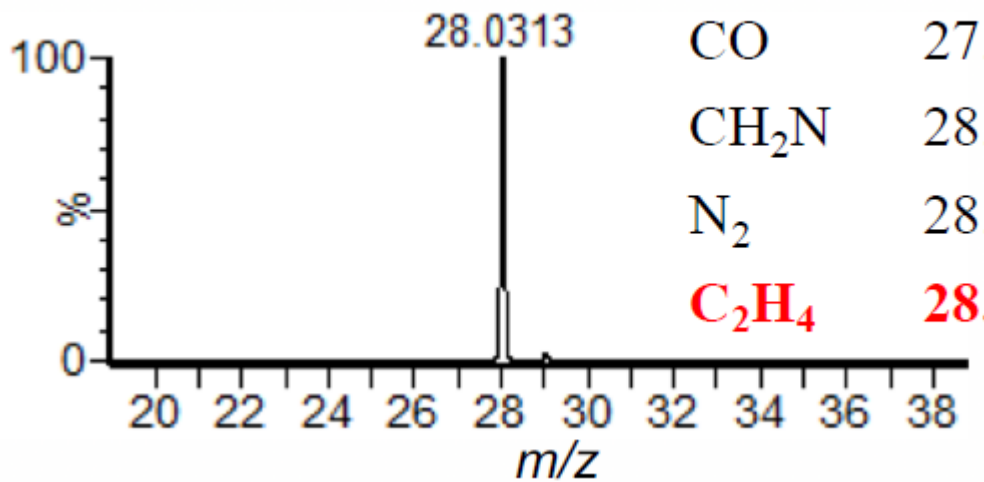
Exact mass of an ion or molecule calculated
using the *mass of the most abundant isotope*
of each element.

Nominal Mass e.g. C=12

Mass of a molecular ion or molecule calculated using
the *isotope mass of the most abundant constituent* (ignoring mass defect)
element isotope of each element rounded to the *nearest integer* value and
multiplied by the number of atoms of each element (C=12, H=1, N=14, O=16, ….)

e.g. *m/z* 28 can have 4 different elemental compositions with different exact mass values.

CO	27.9949 u	CH_2N	28.0187 u
N_2	28.0061 u	C_2H_4	28.0313 u



CO	27.9949 u
CH_2N	28.0187 u
N_2	28.0061 u
C_2H_4	**28.0313 u**

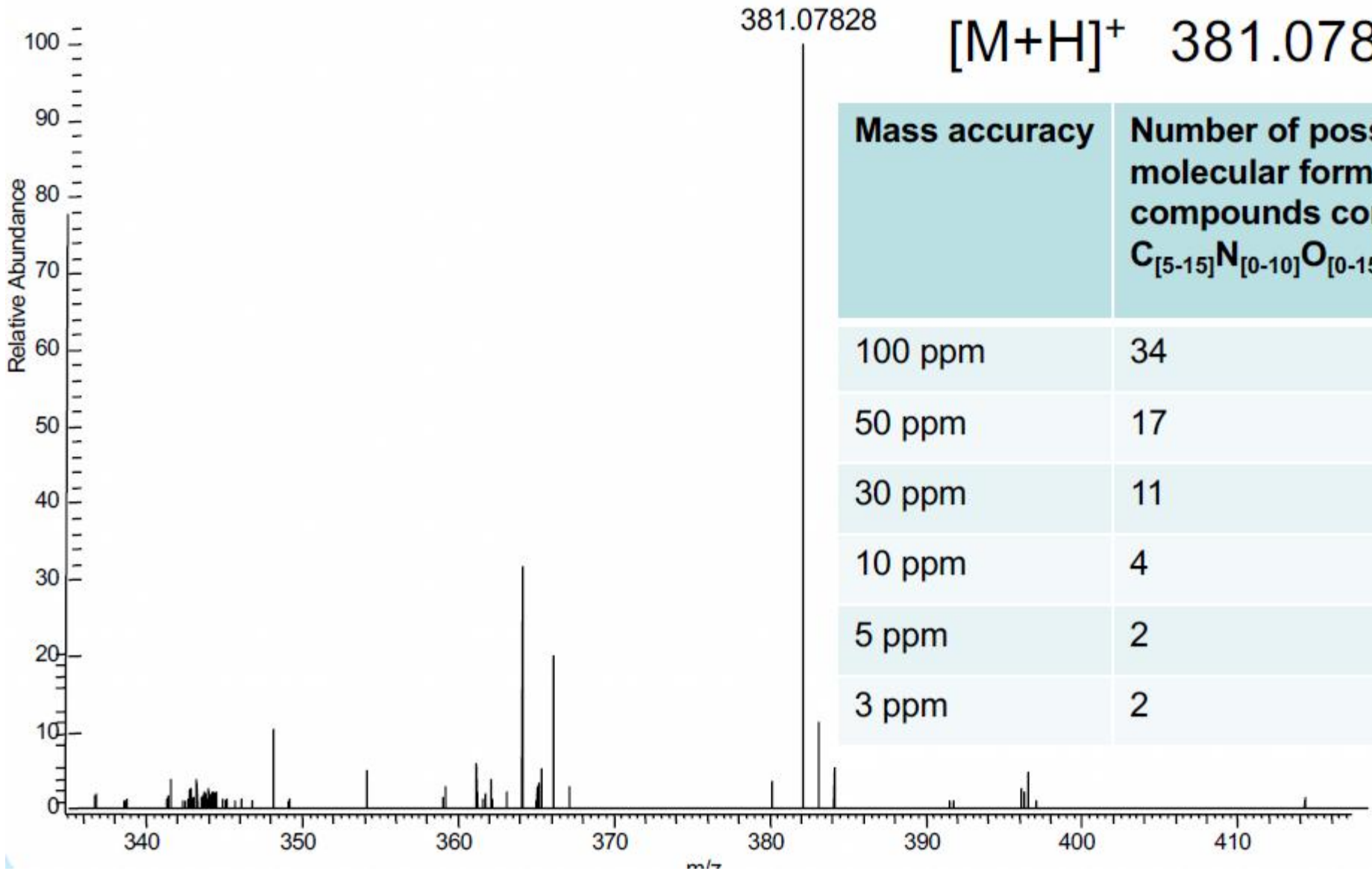
- Mass error in millimass units (mmu)

  [measured mass (u) – theoretical mass (u)] x 1000

- Mass error in parts per million (ppm)

$$\frac{[\text{measured mass (u)} - \text{theoretical mass (u)}]}{\text{theoretical mass (u)}} \times 1000000$$

Measured Mass	Theoretical Mass	Mass Difference (u)	ppm error
200.0020	200.0000	0.002	$(0.002/200)1e^6 = 10$ ppm
400.0020	400.0000	0.002	$(0.002/400)1e^6 = 5$ ppm
800.0020	800.0000	0.002	$(0.002/800)1e^6 = 2.5$ ppm
1000.0020	1000.0000	0.002	$(0.002/1000)1e^6 = 2$ ppm
		Constant with mass	Varies with mass

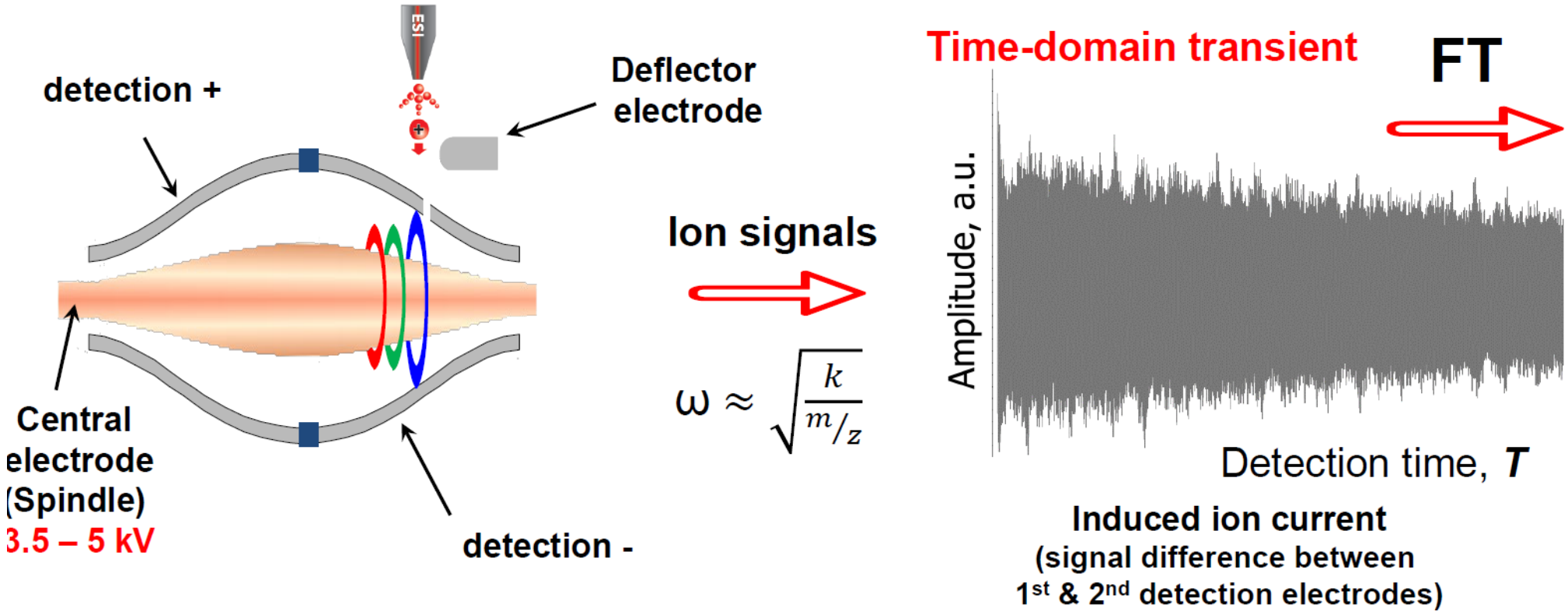


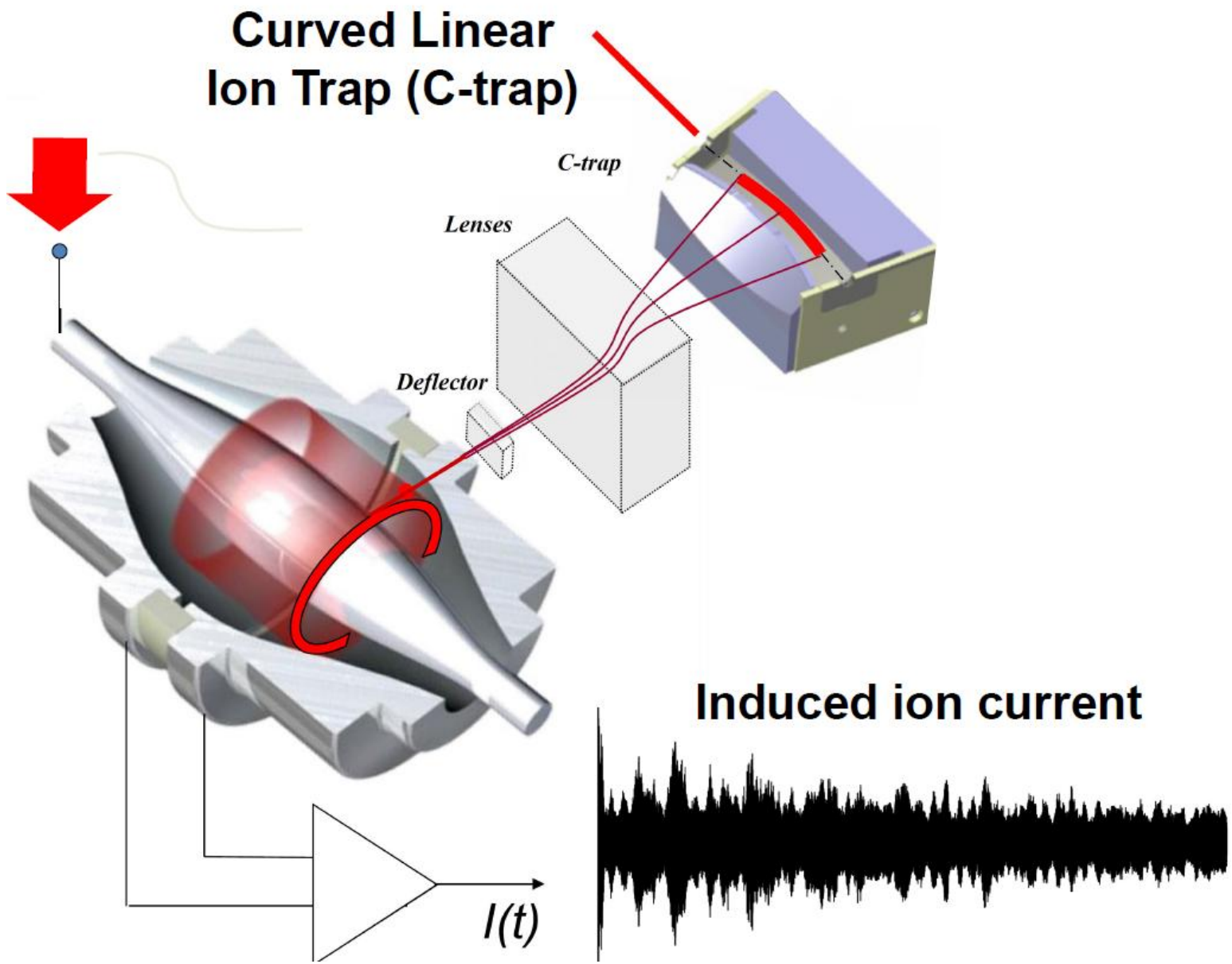
$[M+H]^+$ 381.07828

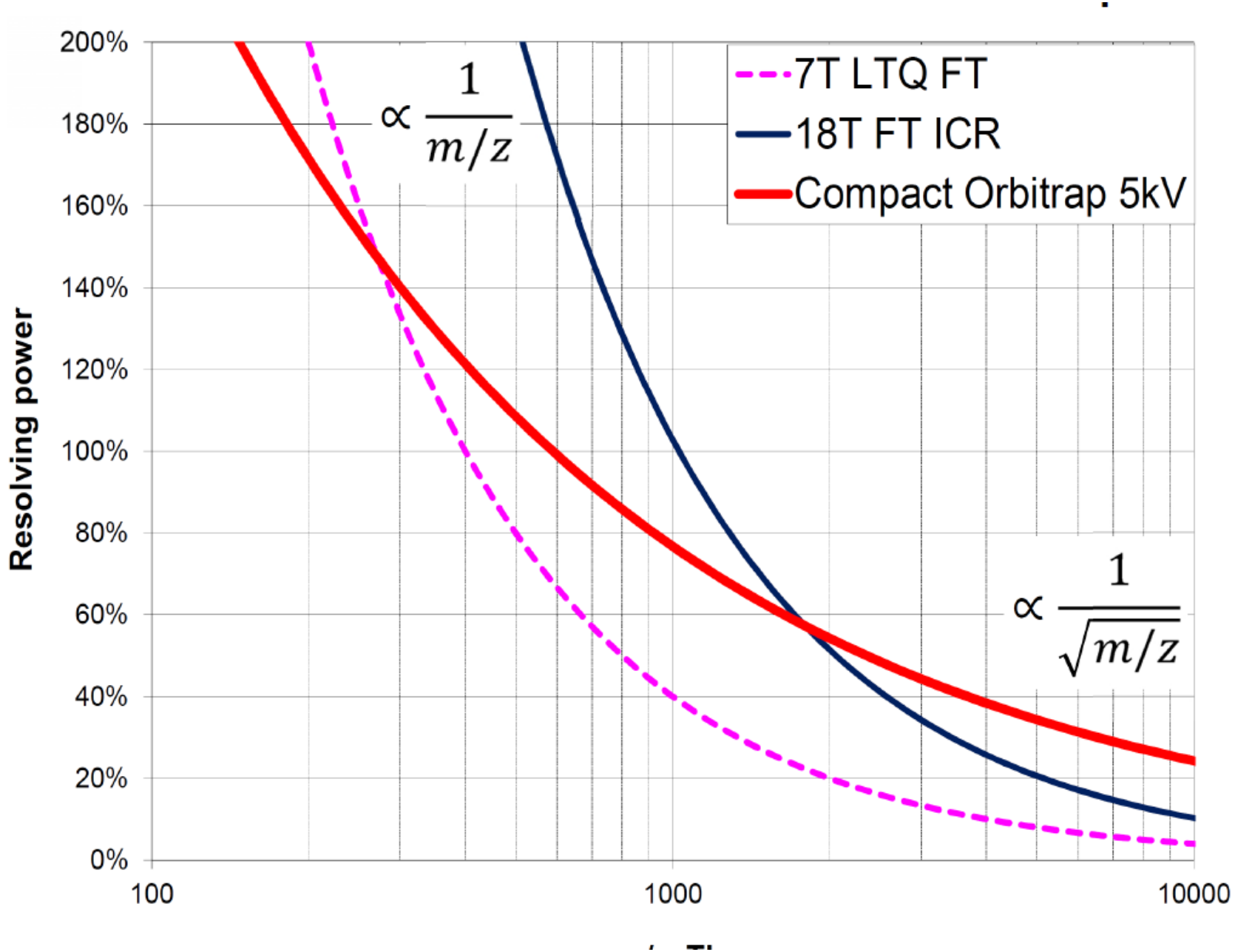
Mass accuracy	Number of possible molecular formulae for compounds containing $C_{[5-15]}N_{[0-10]}O_{[0-15]}H_{[0-40]}$
100 ppm	34
50 ppm	17
30 ppm	11
10 ppm	4
5 ppm	2
3 ppm	2

ANALIZZATORI DI MASSA AD ALTA RISOLUZIONE

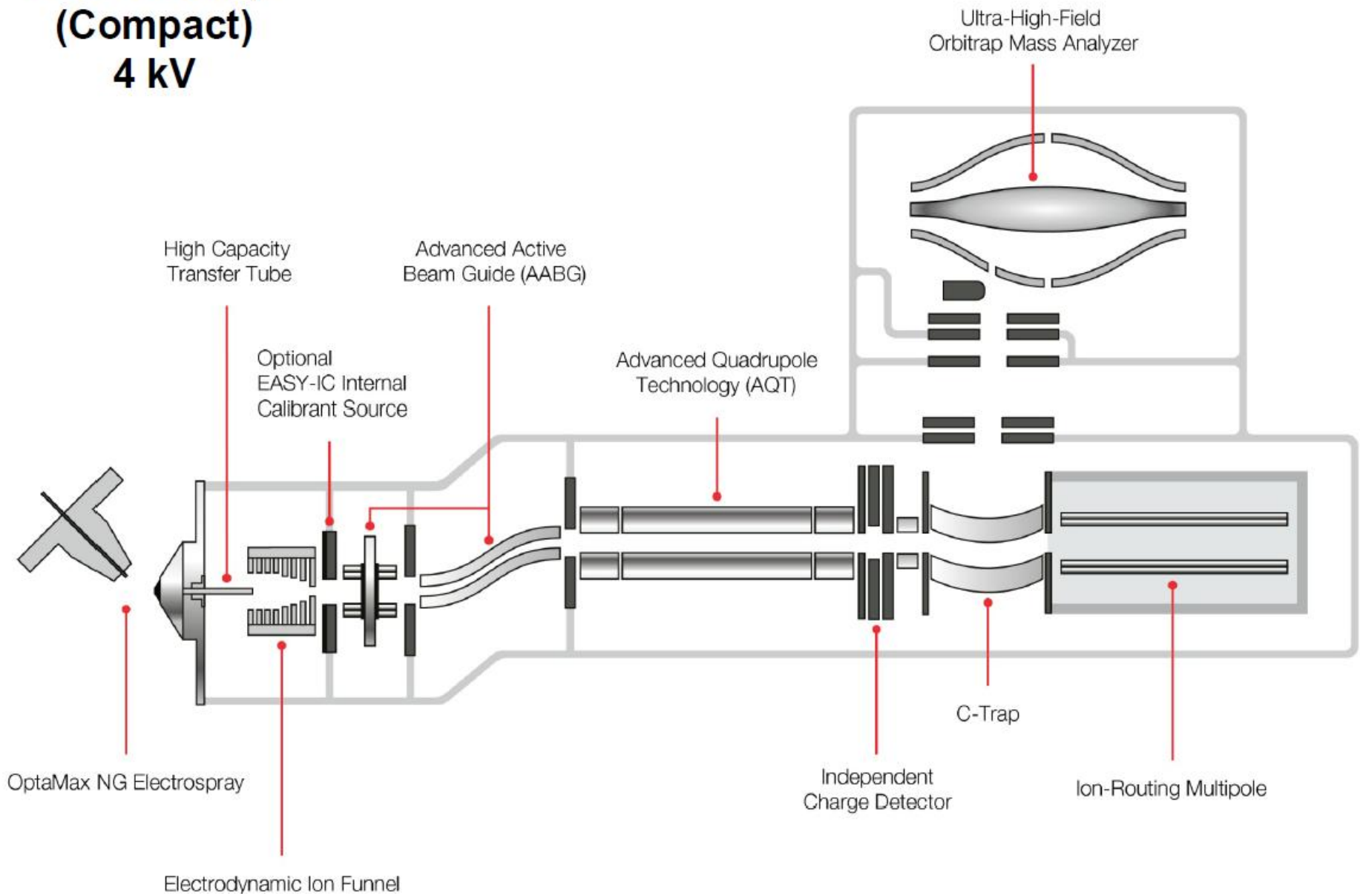
ORBITRAP

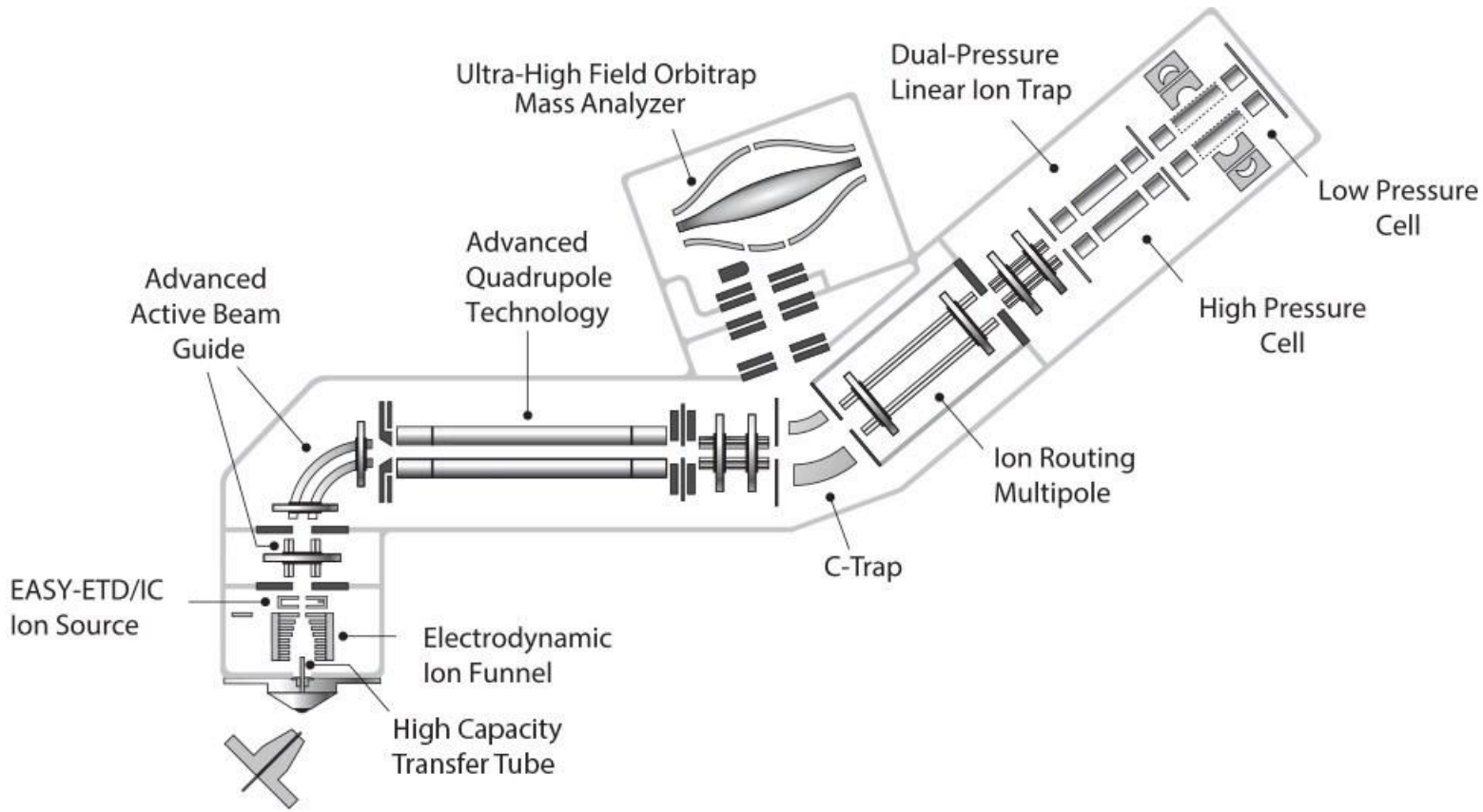

ESI
detection +
Deflector electrode
Central electrode (Spindle)
3.5 – 5 kV
detection -
Ion signals
$\omega \approx \sqrt{\frac{k}{m/z}}$
Time-domain transient
FT
Amplitude, a.u.
Detection time, T
Induced ion current
(signal difference between
1st & 2nd detection electrodes)


Curved Linear
Ion Trap (C-trap)
C-trap
Lenses
Deflector
I(t)
Induced ion current


Resolving power
200%
180%
160%
140%
120%
100%
80%
60%
40%
20%
0%
100
1000
10000
7T LTQ FT
18T FT ICR
Compact Orbitrap 5kV
$\propto \frac{1}{m/z}$
$\propto \frac{1}{\sqrt{m/z}}$

D20 Orbitrap (Compact) 4 kV




Ultra-High Field Orbitrap
Mass Analyzer
Dual-Pressure
Linear Ion Trap
Low Pressure
Cell
Advanced
Quadrupole
Technology
Advanced
Active Beam
Guide
High Pressure
Cell
Ion Routing
Multipole
C-Trap
EASY-ETD/IC
Ion Source
Electrodynamic
Ion Funnel
High Capacity
Transfer Tube

TIME OF FLIGHT

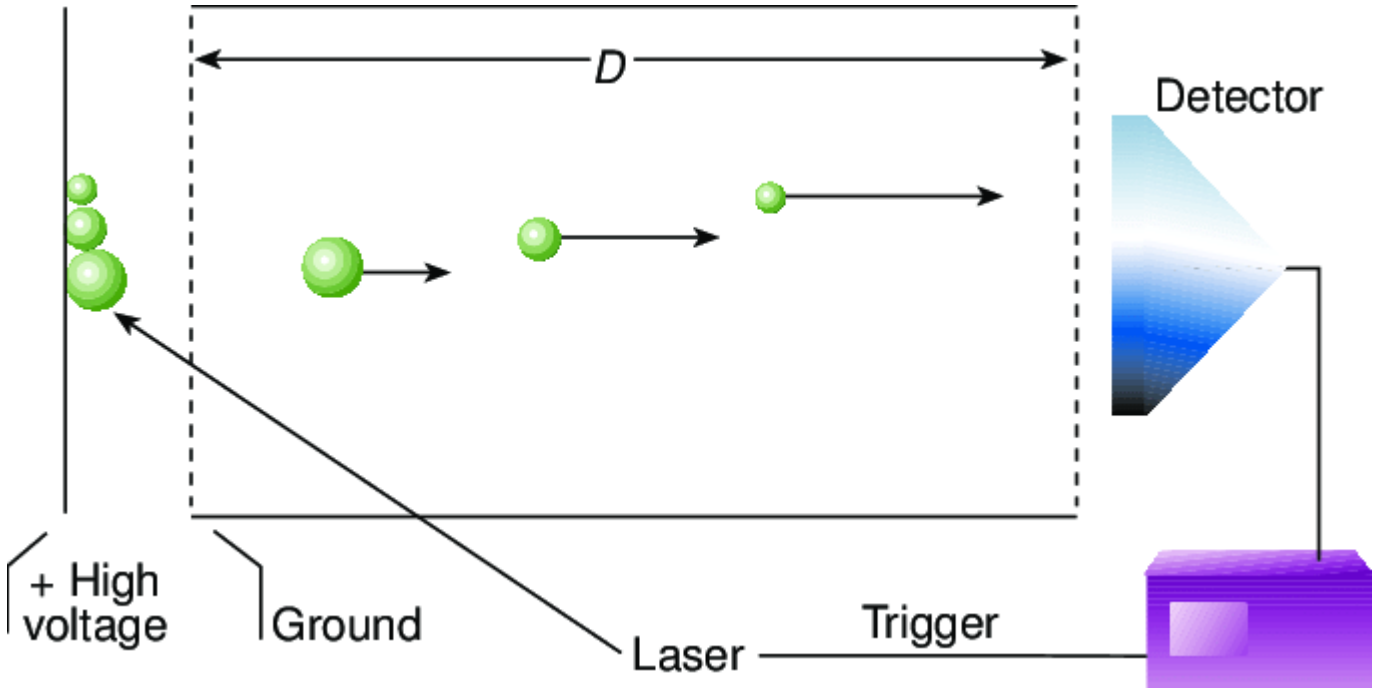
$$E_p = qU$$

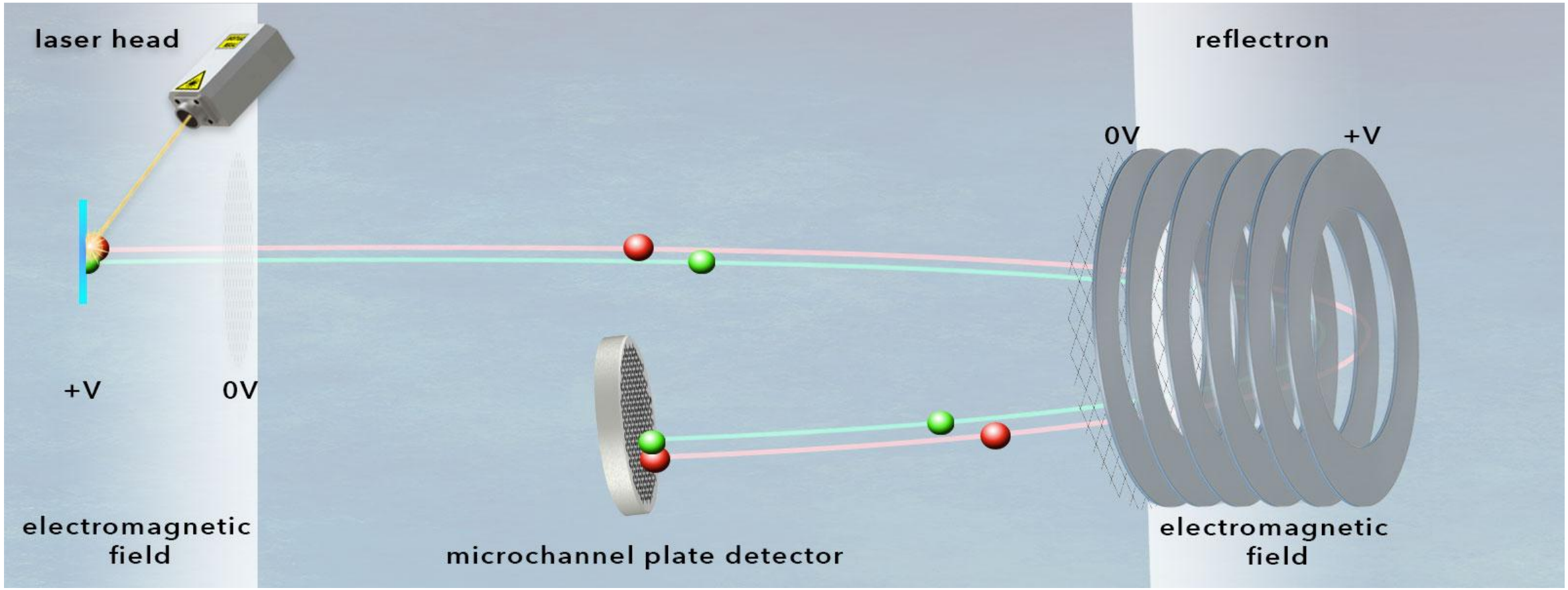
$$E_k = \frac{1}{2}mv^2$$

$$E_p = E_k$$

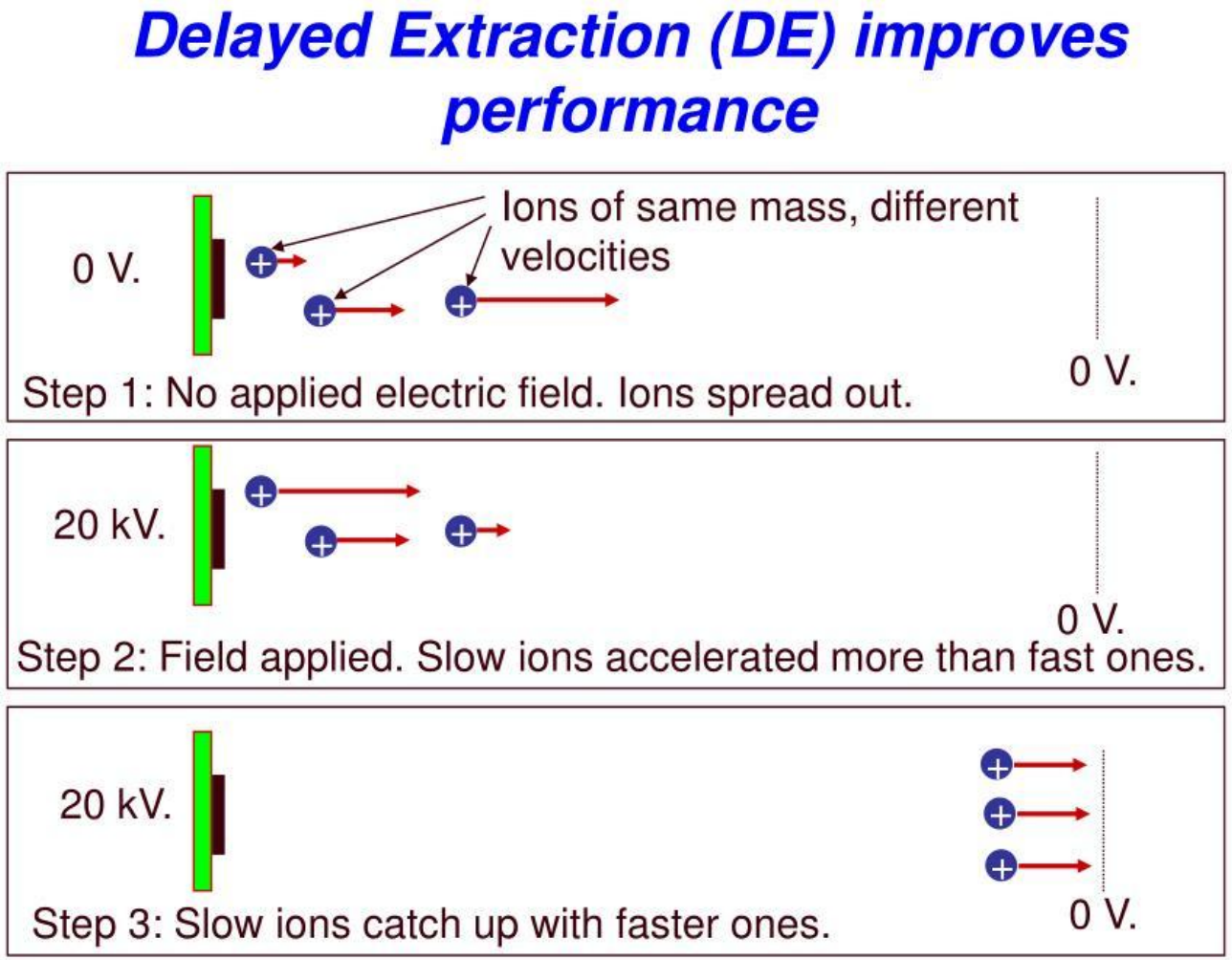
$$qU = \frac{1}{2}mv^2 \qquad v = \frac{d}{t}$$

$$t = k\sqrt{\frac{m}{q}}$$



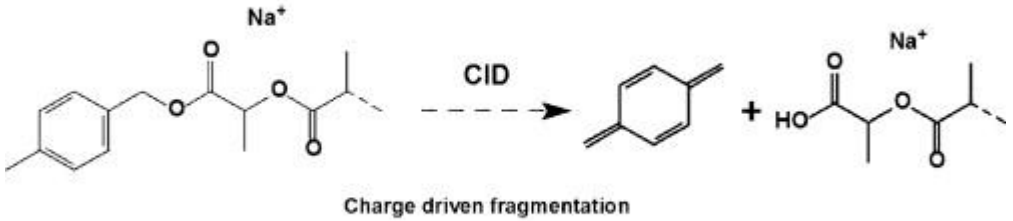

laser head
reflectron
0V
+V
+V
0V
electromagnetic field
microchannel plate detector
electromagnetic field

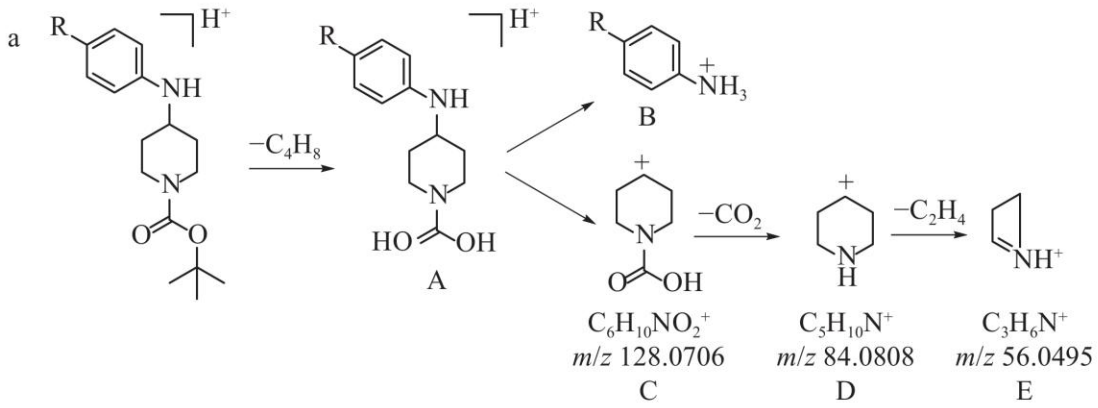
DELAYED EXTRACTION

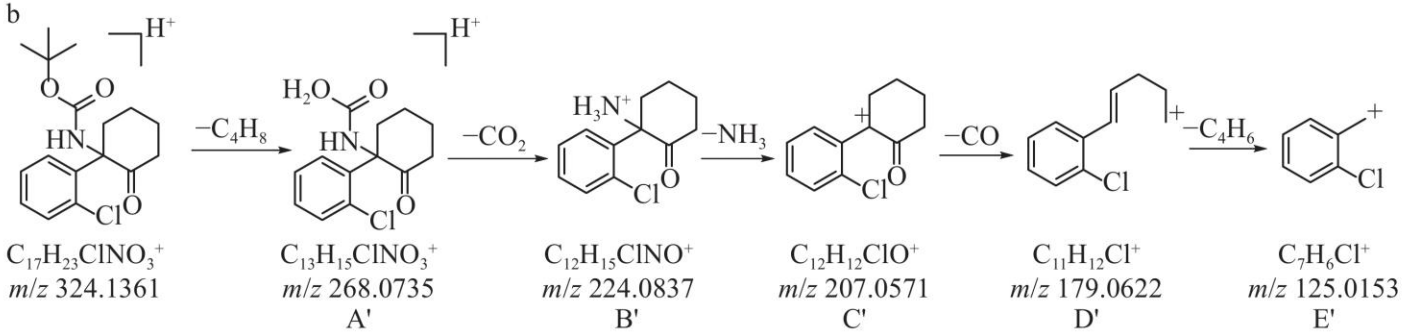


Frammentazione Collision Induced Dissociation (CID)

La CID è un processo in cui uno ione viene accelerato e fatto collidere con un gas inerte (come azoto o elio), causando la sua frammentazione in pezzi più piccoli (ioni frammento).

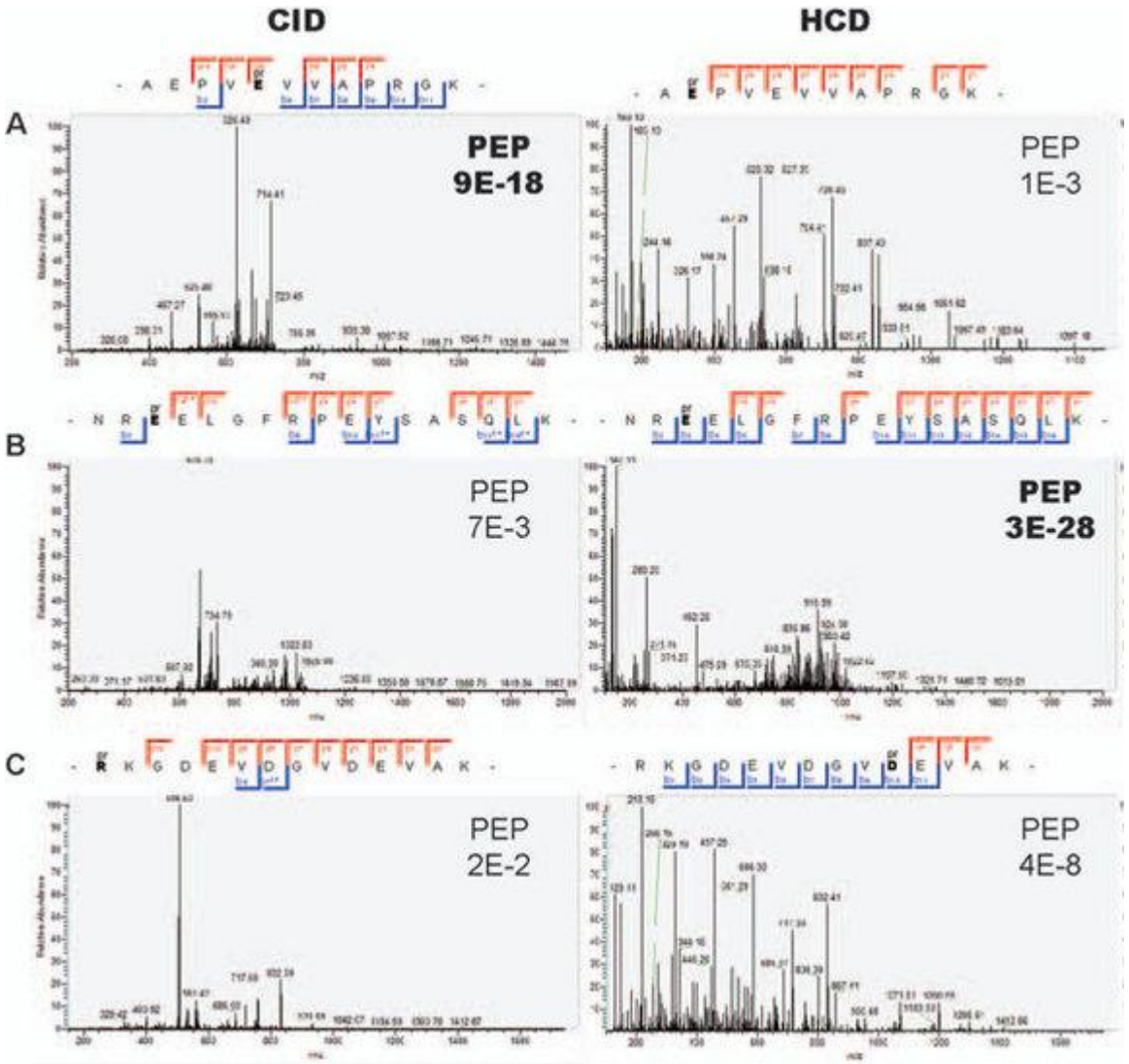






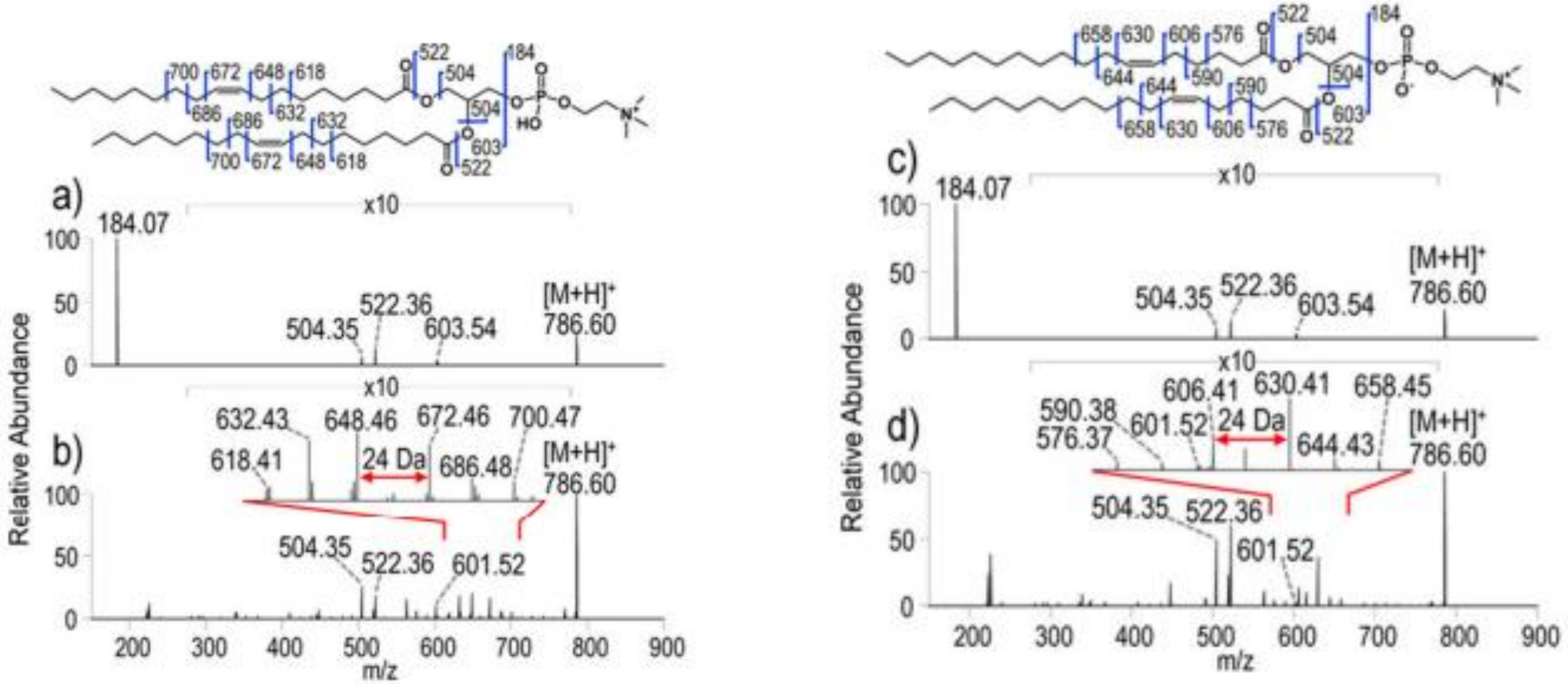
Frammentazione Higher-energy Collisional Dissociation (HCD)

HCD (Higher-energy Collisional Dissociation) è una tecnica di frammentazione usata in spettrometria di massa in cui gli ioni vengono accelerati ad alta energia e fatti collidere con un gas inerte (come azoto o argon) all'interno di una cella di collisione. Questo provoca la rottura dei legami chimici e la formazione di frammenti ionici, che vengono poi analizzati per ottenere informazioni strutturali sulla molecola originale.



Frammentazione UltraViolet PhotoDissociation (UVPD)

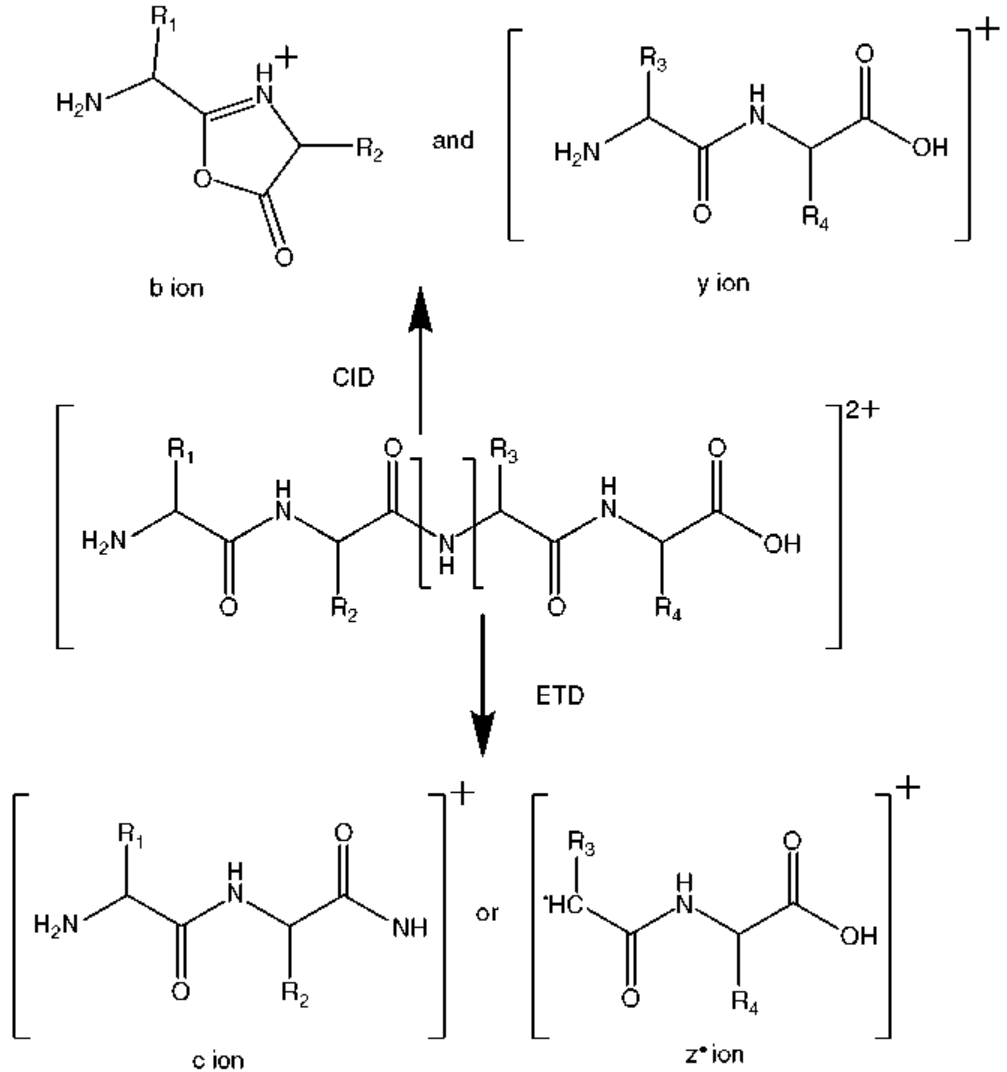
UVPD (Ultraviolet Photodissociation) è una tecnica di frammentazione in spettrometria di massa che utilizza **radiazione ultravioletta ad alta energia** per rompere le molecole ionizzate in frammenti. Gli ioni vengono irradiati con luce UV (tipicamente 193 o 213 nm), assorbono energia e si dissociano in molti frammenti, permettendo un'analisi strutturale molto dettagliata.



Frammentazione Electron Transfer Dissociation (ETD)

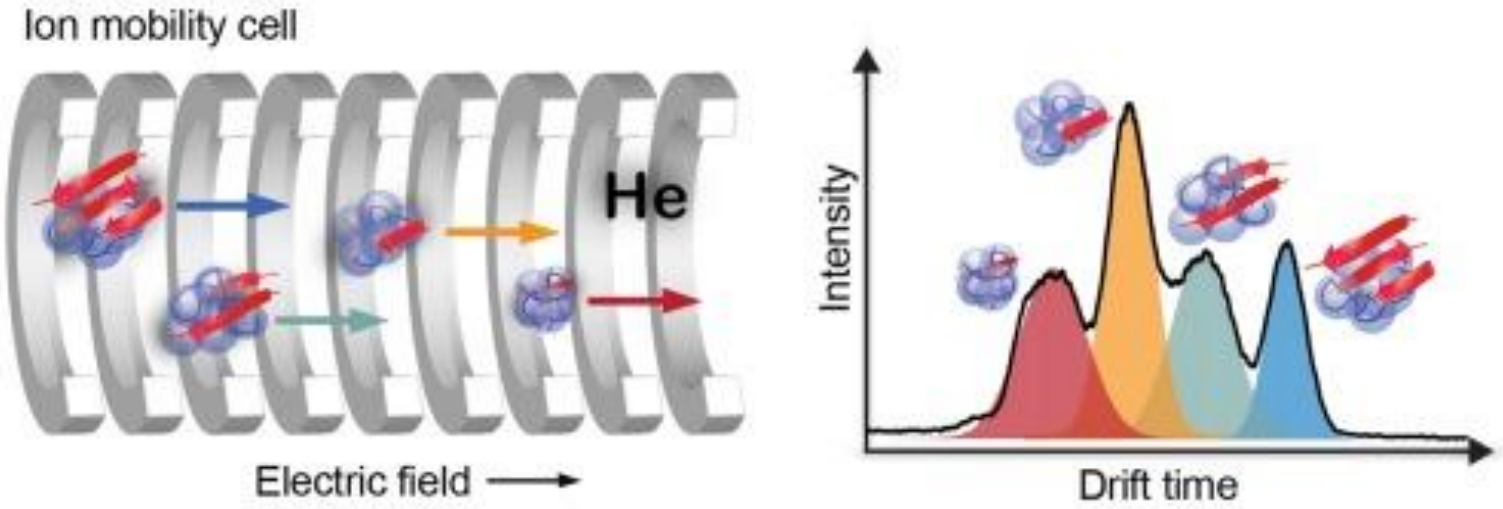
ETD (Electron Transfer Dissociation) è una tecnica di frammentazione in spettrometria di massa in cui uno ione carico positivamente riceve un **elettrone** da un anione reattivo. Questo trasferimento di elettrone causa la rottura della **catena principale (backbone)** della molecola, generando frammenti **senza rompere i legami laterali** o modificare i gruppi post-traduzionali.

1. Produce frammenti **c e z●**, tipici della rottura del backbone.
2. Usata molto in **proteomica** per lo studio di **peptidi modificati** e **proteine grosse**.
3. Funziona meglio con ioni **ad alta carica** (es. peptidi/proteine multiple cariche).
4. **Meccanismo "morbido"**: non rompe i legami labili (es. modifiche post-traduzionali come fosforilazioni, glicosilazioni).

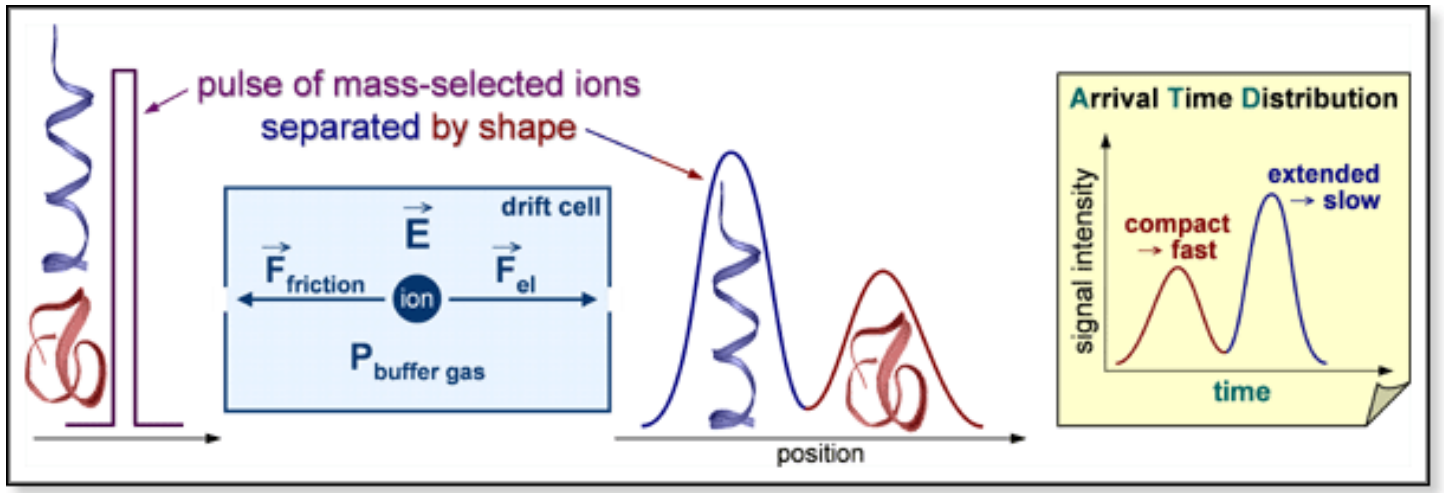


Ion mobility (IM)

Ion Mobility (mobilità ionica) è una tecnica usata in spettrometria di massa che separa gli ioni **in base alla loro forma, dimensione e carica** mentre si muovono attraverso un **gas neutro** sotto l'influenza di un **campo elettrico**.



1. Gli ioni vengono spinti da un campo elettrico attraverso una **cella piena di gas** (come azoto o elio).
2. Durante il percorso, gli ioni **collidono con le molecole del gas**.
3. Ioni **più compatti** (o con meno resistenza) si muovono **più velocemente**, quelli **più estesi** o "soffiati" si muovono **più lentamente**.
4. Questo tempo di transito viene misurato e chiamato **drift time**.



SPETTROMETRIA DI MASSA E SCIENZE OMICHE - APPLICAZIONI

SCIENTIFIC REPORTS

Corrected: Author Correction

OPEN

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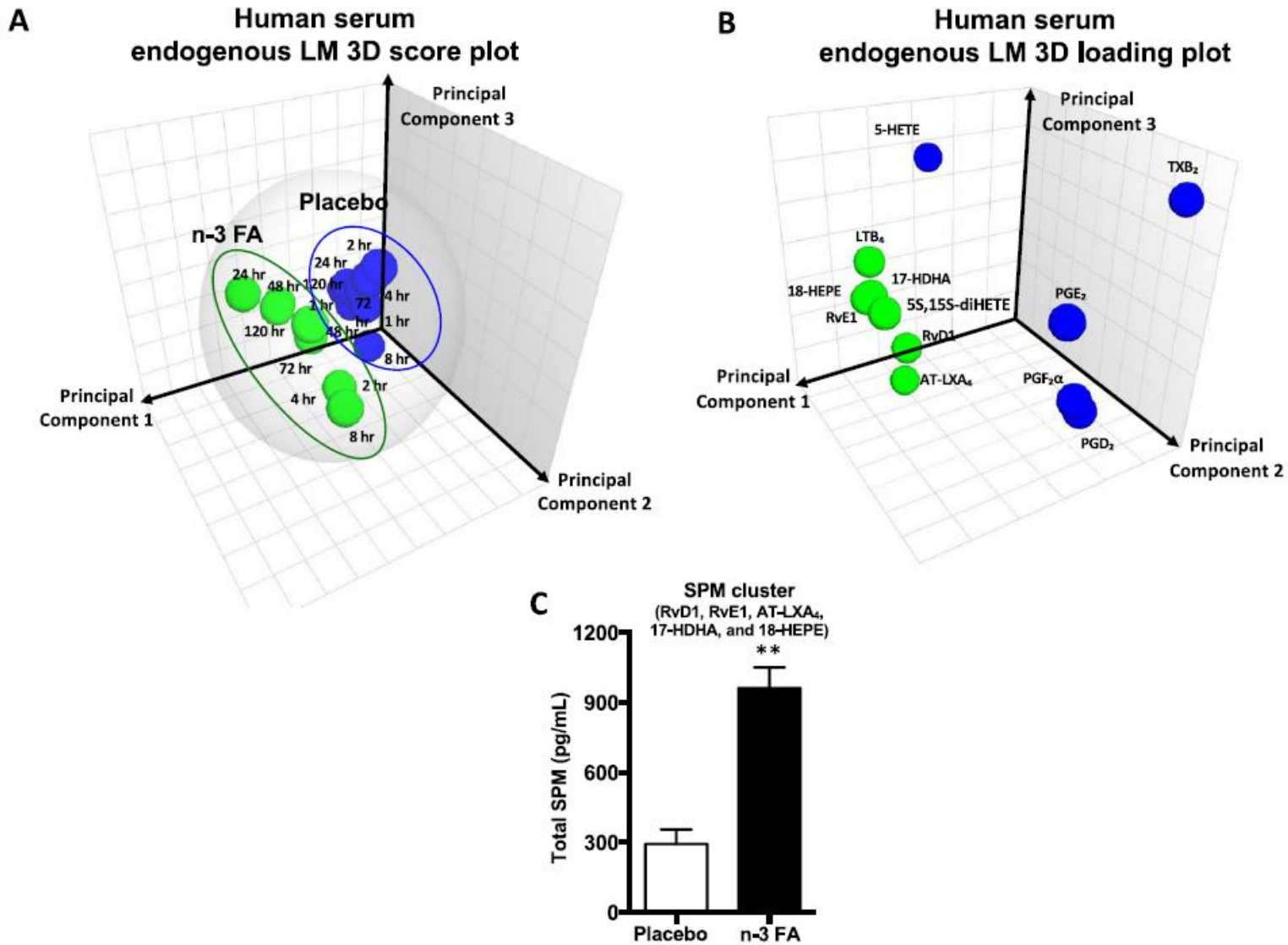
Published online: 21 December 2018

Identification of specialized pro-resolving mediator clusters from healthy adults after intravenous low-dose endotoxin and omega-3 supplementation: a methodological validation

Paul C. Norris[1], Ann C. Skulas-Ray[2], Ian Riley[1], Chesney K. Richter[2], Penny M. Kris-Etherton[3], Gordon L. Jensen[4], Charles N. Serhan[1] & Krishna Rao Maddipati[5]

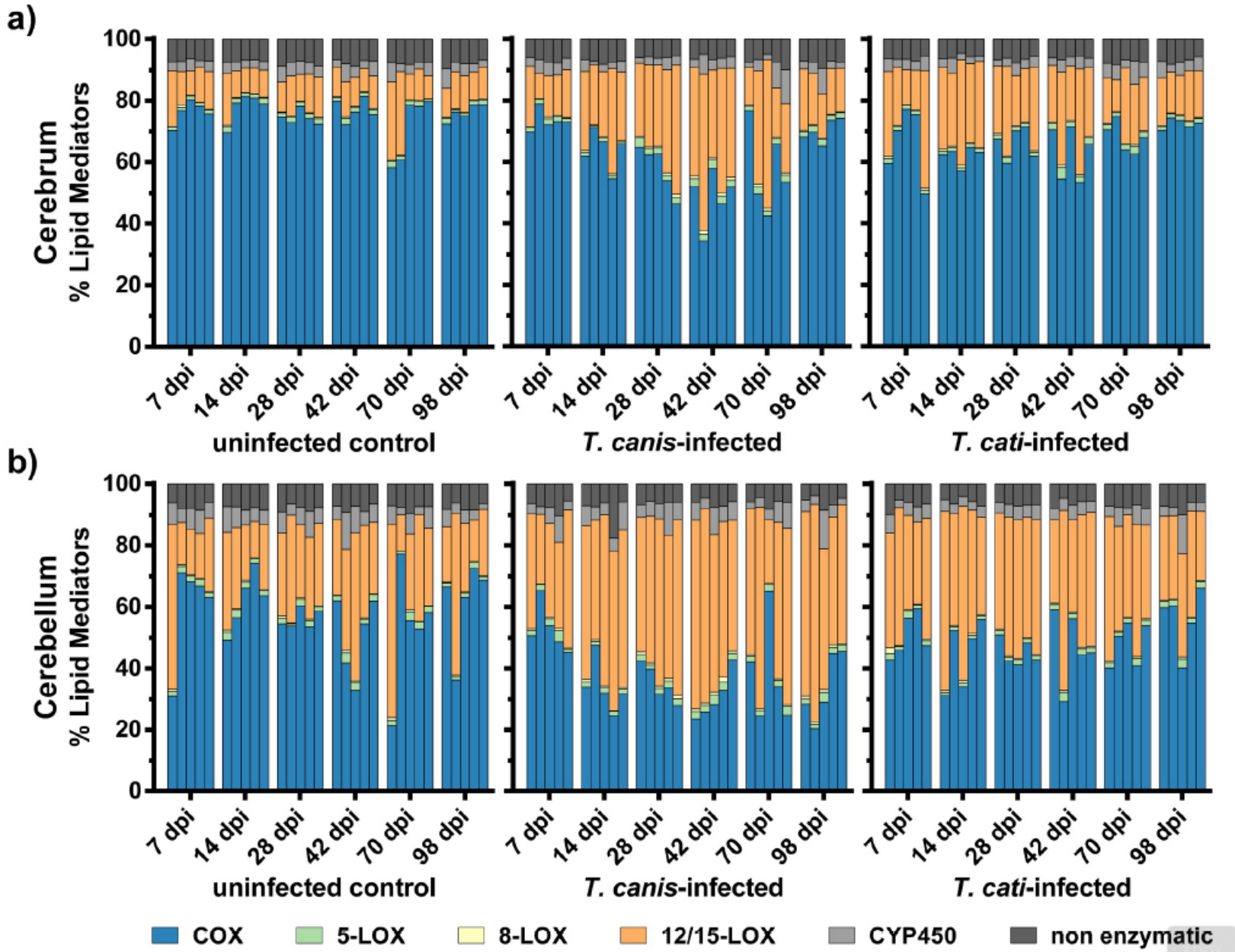

A
Human serum
endogenous LM 3D score plot
Principal
Component 3
Placebo
n-3 FA
2 hr
24 hr
24 hr
48 hr
120 hr
72
hr
4 hr
1 hr
1 hr
48 hr
120 hr
8 hr
72 hr
2 hr
4 hr
8 hr
Principal
Component 1
Principal
Component 2
B
Human serum
endogenous LM 3D loading plot
Principal
Component 3
5-HETE
TXB2
LTB4
17-HDHA
18-HEPE
5S,15S-diHETE
PGE2
RvE1
RvD1
AT-LXA4
PGF2α
PGD2
Principal
Component 1
Principal
Component 2
C
SPM cluster
(RvD1, RvE1, AT-LXA4,
17-HDHA, and 18-HEPE)
**
1200
900
600
300
0
Total SPM (pg/mL)
Placebo
n-3 FA

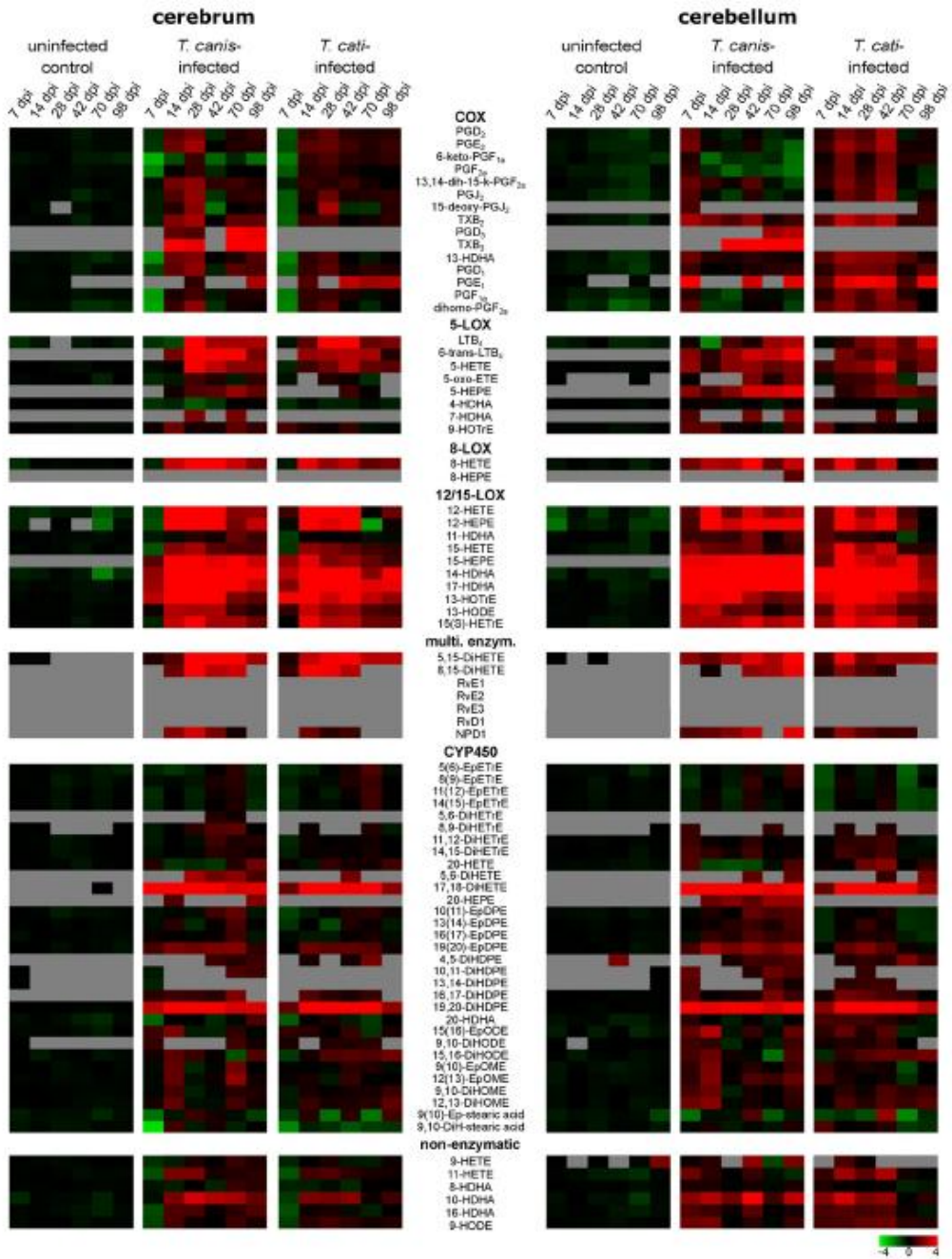
PLOS | NEGLECTED TROPICAL DISEASES

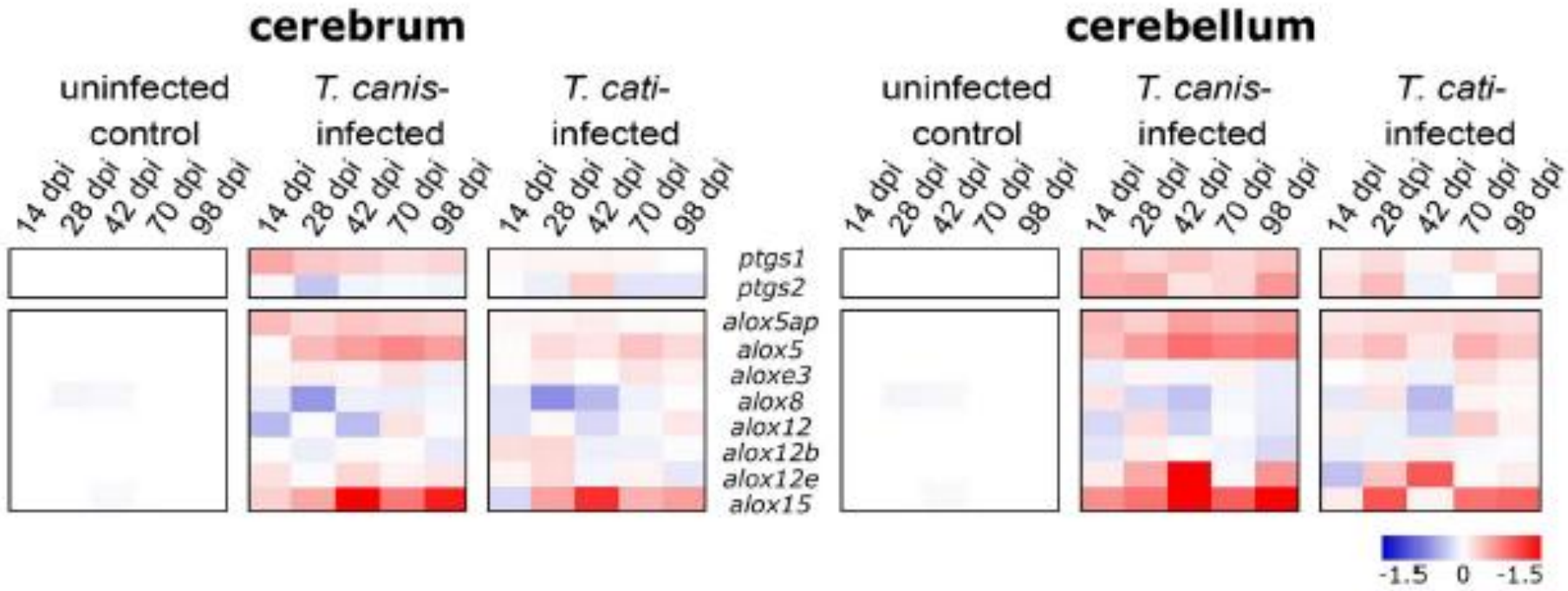
RESEARCH ARTICLE

Multiplex profiling of inflammation-related bioactive lipid mediators in *Toxocara canis*- and *Toxocara cati*-induced neurotoxocarosis

Patrick Waindok[1], Elisabeth Janecek-Erfurth[1¤a], Dimitri Lindenwald[1¤b], Esther Wilk[2], Klaus Schughart[2,3], Robert Geffers[4], Laurence Balas[5], Thierry Durand[5], Katharina Maria Rund[6,7], Nils Helge Schebb[6,7], Christina Strube[1]*


a)
Cerebrum
% Lipid Mediators
100
80
60
40
20
0
7 dpi
14 dpi
28 dpi
42 dpi
70 dpi
98 dpi
uninfected control
T. canis-infected
T. cati-infected
b)
Cerebellum
% Lipid Mediators
COX
5-LOX
8-LOX
12/15-LOX
CYP450
non enzymatic


cerebrum
cerebellum
uninfected control
T. canis-infected
T. cati-infected
7 dpi
14 dpi
28 dpi
42 dpi
70 dpi
98 dpi
COX
PGD2
PGE2
6-keto-PGF1a
PGF2a
13,14-dh-15-k-PGF2a
PGJ2
15-deoxy-PGJ2
TXB2
PGD3
TXB3
13-HDHA
PGD1
PGE1
PGF1a
dihomo-PGF2a
5-LOX
LTB4
6-trans-LTB4
5-HETE
5-oxo-ETE
5-HEPE
4-HDHA
7-HDHA
9-HOTrE
8-LOX
8-HETE
8-HEPE
12/15-LOX
12-HETE
12-HEPE
11-HDHA
15-HETE
15-HEPE
14-HDHA
17-HDHA
13-HOTrE
13-HODE
15(S)-HETrE
multi. enzym.
5,15-DiHETE
8,15-DiHETE
RvE1
RvE2
RvE3
RvD1
NPD1
CYP450
5(6)-EpETrE
8(9)-EpETrE
11(12)-EpETrE
14(15)-EpETrE
5,6-DiHETrE
8,9-DiHETrE
11,12-DiHETrE
14,15-DiHETrE
20-HETE
5,6-DiHETE
17,18-DiHETE
20-HEPE
10(11)-EpDPE
13(14)-EpDPE
16(17)-EpDPE
19(20)-EpDPE
4,5-DiHDPE
10,11-DiHDPE
13,14-DiHDPE
16,17-DiHDPE
19,20-DiHDPE
20-HDHA
15(16)-EpODE
9,10-DiHODE
15,16-DiHODE
9(10)-EpOME
12(13)-EpOME
9,10-DiHOME
12,13-DiHOME
9(10)-Ep-stearic acid
9,10-DiH-stearic acid
non-enzymatic
9-HETE
11-HETE
8-HDHA
10-HDHA
16-HDHA
9-HODE
-4
0
4


cerebrum
cerebellum
uninfected control
T. canis-infected
T. cati-infected
14 dpi
28 dpi
42 dpi
70 dpi
98 dpi
ptgs1
ptgs2
alox5ap
alox5
aloxe3
alox8
alox12
alox12b
alox12e
alox15
-1.5
0
-1.5

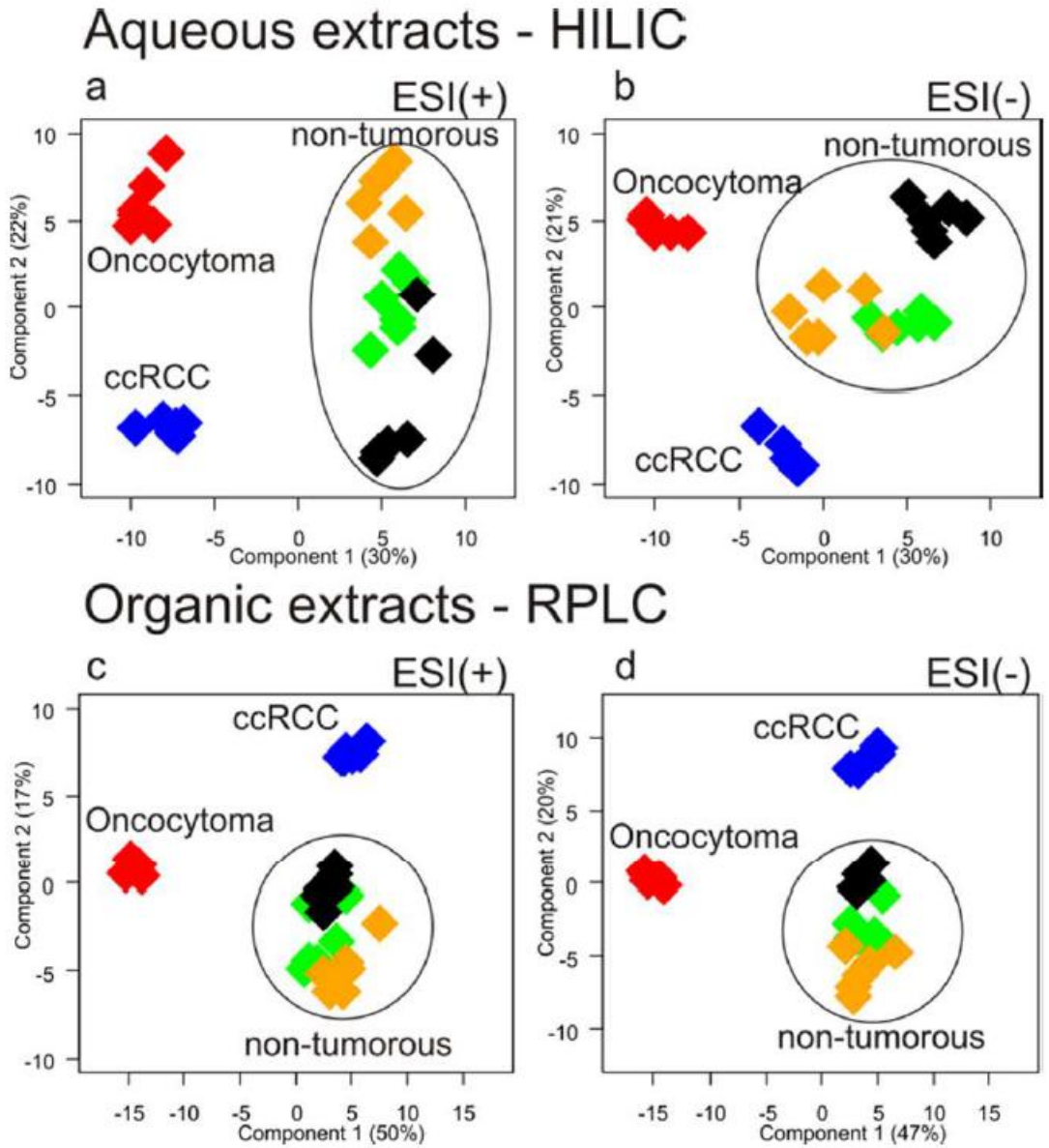
Journal of proteome research

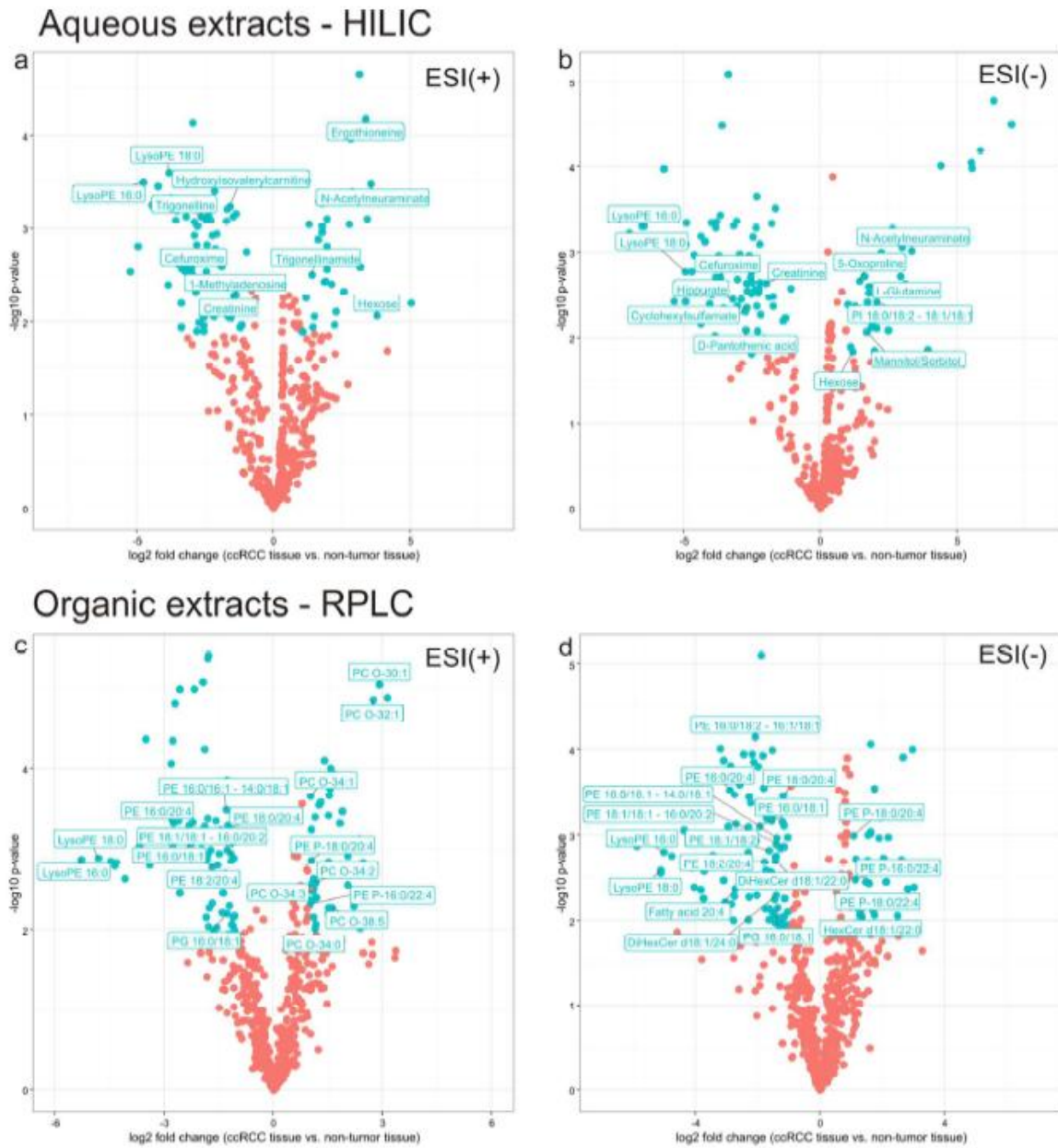
Article

Comprehensive metabolomic and lipidomic profiling of human kidney tissue: a platform comparison

Patrick Leuthold, Elke Schaeffeler, Stefan Winter, Florian Büttner, Ute Hofmann, Thomas E Mürdter, Steffen Rausch, Denise Sonntag, Judith Wahrheit, Falko Fend, Jörg Hennenlotter, Jens Bedke, Matthias Schwab, and Mathias Haag

J. Proteome Res., **Just Accepted Manuscript** • DOI: 10.1021/acs.jproteome.6b00875 • Publication Date (Web): 19 Dec 2016


Aqueous extracts - HILIC
a
ESI(+)
non-tumorous
Oncocytoma
ccRCC
Component 2 (22%)
Component 1 (30%)
b
ESI(-)
non-tumorous
Oncocytoma
ccRCC
Component 2 (21%)
Component 1 (30%)
Organic extracts - RPLC
c
ESI(+)
ccRCC
Oncocytoma
non-tumorous
Component 2 (17%)
Component 1 (50%)
d
ESI(-)
ccRCC
Oncocytoma
non-tumorous
Component 2 (20%)
Component 1 (47%)


Aqueous extracts - HILIC
a
ESI(+)
Ergothioneine
LysoPE 18:0
Hydroxyisovalerylcarnitine
LysoPE 16:0
N-Acetylneuraminate
Trigonelline
Cefuroxime
Trigonellinamide
1-Methyladenosine
Hexose
Creatinine
-log10 p-value
log2 fold change (ccRCC tissue vs. non-tumor tissue)
b
ESI(-)
LysoPE 16:0
LysoPE 18:0
N-Acetylneuraminate
Cefuroxime
Creatinine
5-Oxoproline
Hippurate
L-Glutamine
Cyclohexylsulfamate
PI 18:0/18:2 - 18:1/18:1
D-Pantothenic acid
Mannitol/Sorbitol
Hexose
-log10 p-value
log2 fold change (ccRCC tissue vs. non-tumor tissue)
Organic extracts - RPLC
c
ESI(+)
PC O-30:1
PC O-32:1
PE 16:0/16:1 - 14:0/18:1
PC O-34:1
PE 16:0/20:4
PE 18:0/20:4
PE 18:1/18:1 - 16:0/20:2
LysoPE 18:0
PE P-18:0/20:4
PE 16:0/18:1
PC O-34:2
LysoPE 16:0
PE 18:2/20:4
PC O-34:3
PE P-16:0/22:4
PC O-38:6
PG 16:0/16:1
PC O-34:0
-log10 p-value
log2 fold change (ccRCC tissue vs. non-tumor tissue)
d
ESI(-)
PE 16:0/20:4
PE 18:0/20:4
PE 16:0/16:1 - 14:0/18:1
PE 16:0/18:1
PE P-18:0/20:4
PE 18:1/18:1 - 16:0/20:2
LysoPE 16:0
PE 18:1/18:2
PE 18:2/20:4
PE P-16:0/22:4
DiHexCer d18:1/22:0
LysoPE 18:0
PE P-18:0/22:4
Fatty acid 20:4
HexCer d18:1/22:0
DiHexCer d18:1/24:0
PG 16:0/18:1
-log10 p-value
log2 fold change (ccRCC tissue vs. non-tumor tissue)

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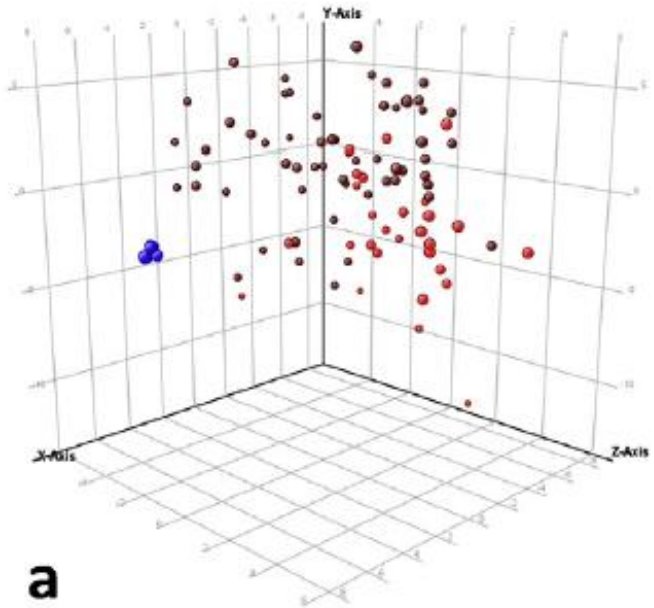
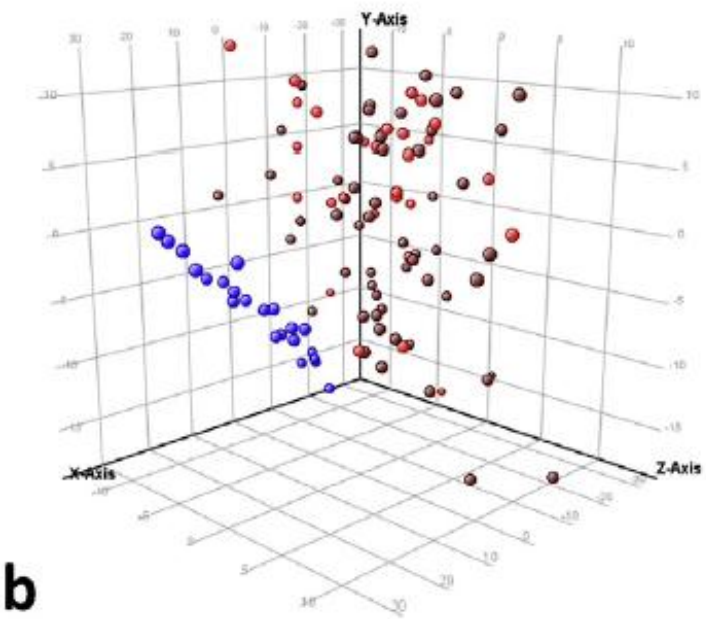
journal homepage: www.elsevier.com/locate/jpba

Urinary and plasma metabolite differences detected by HPLC-ESI-QTOF-MS in systemic sclerosis patients

Álvaro Fernández-Ochoa[a,b], Rosa Quirantes-Piné[a], Isabel Borrás-Linares[a,*], David Gemperline[c], PRECISESADS Clinical Consortium , Marta E. Alarcón Riquelme[d], Lorenzo Beretta[e,1], Antonio Segura-Carretero[a,b,1]

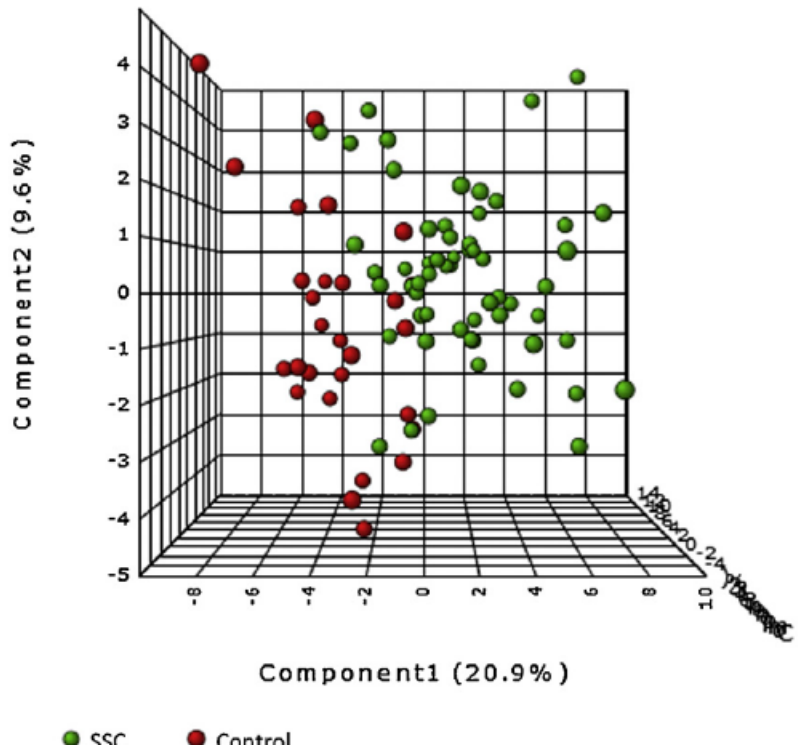


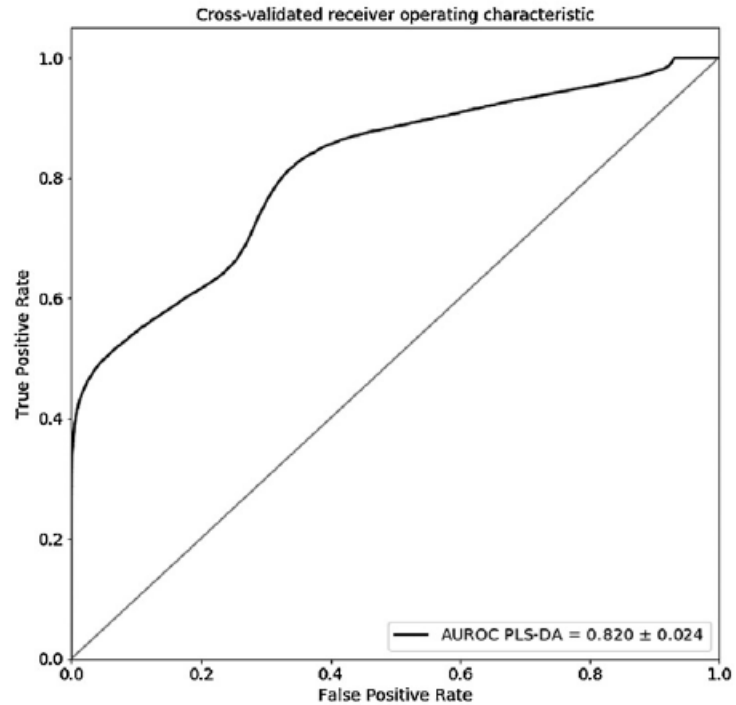
a



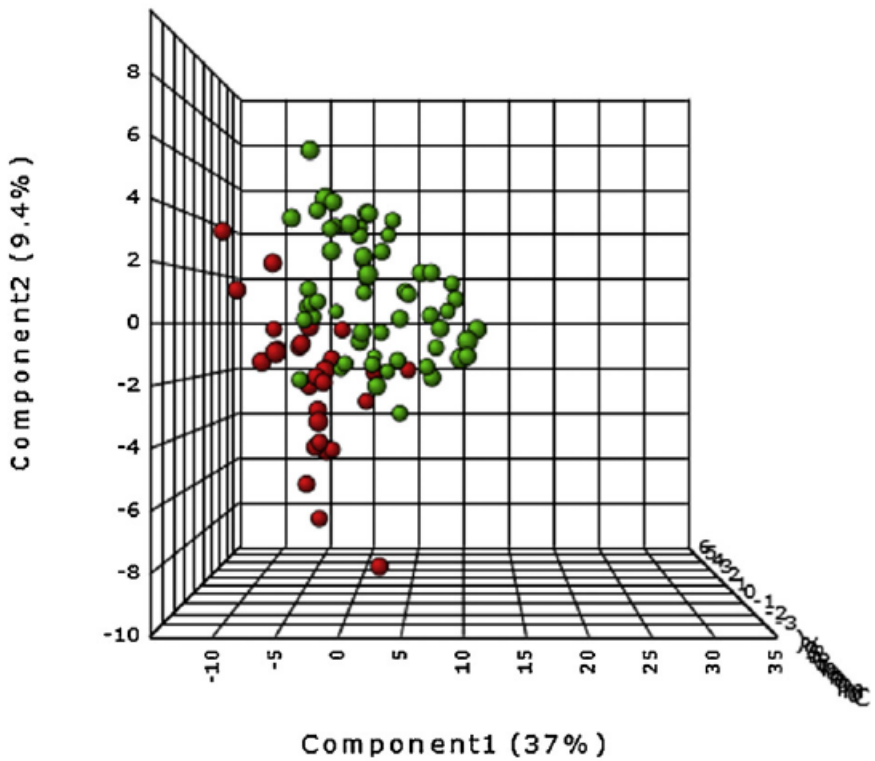
b

URINE


Component2 (9.6%)
Component1 (20.9%)
SSC
Control


Cross-validated receiver operating characteristic
True Positive Rate
False Positive Rate
AUROC PLS-DA = 0.820 ± 0.024

PLASMA


Component2 (9.4%)
Component1 (37%)
8
6
4
2
0
-2
-4
-6
-8
-10
-10
-5
0
5
10
15
20
25
30
35

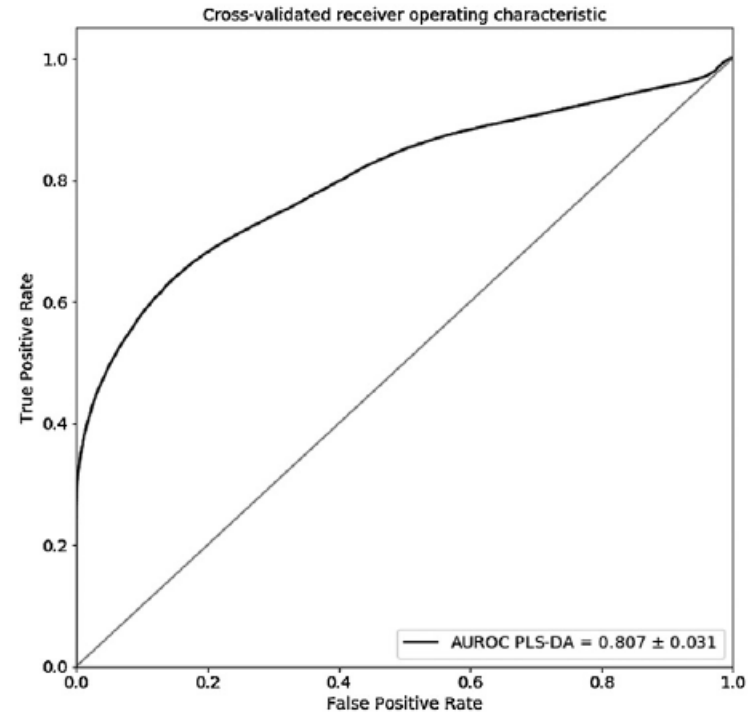

Cross-validated receiver operating characteristic
True Positive Rate
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0
AUROC PLS-DA = 0.807 ± 0.031

Table 2
Molecular and statistical details of annotated urinary metabolites that presented significant differences between SSc patients and healthy volunteers. (FC < 0, metabolites overexpressed in SSc)

RT (min)	Mass(Da)	p-value	FC	VIP-value	AUC	Molecular Formula	Score	Error (ppm)	Metabolite	MS/MS fragments
0.9	182.0788	9.02 E-4	−5.48	1.813	0.800	$C_6H_{16}O_6$	92.4	1.58	D-Sorbitol	69.0441/83.0598/183.0886
0.9	136.0617	8.37 E-3	1.52	1.148	0.700	$C_7H_8N_2O$	99.0	1.13	N-Methylnicotinamide	92.0456/94.0567/120.0550/137.0718
1.0	143.0946	7.89 E-3	2.42	1.607	0.728	$C_7H_{13}NO_2$	97.8	−2.80	Proline Betaine	42.0335/58.0652/84.0810
1.0	113.0588	7.89 E-3	1.44	1.007	0.728	$C_4H_7N_3O$	97.6	−4.09	Creatinine	43.0288/44.0495/86.0715
1.4	127.0997	0.016	−4.91	1.406	0.716	$C_7H_{13}NO$	90.1	2.06	N-cyclohexylformamide	Annotated by Formula
2.5	299.1477	0.026	−4.73	1.346	0.677	$C_{13}H_{21}N_3O_5$	98.9	3.20	Ser Pro Pro	Annotated by Formula
2.9	143.0585	0.025	2.50	1.055	0.628	$C_6H_9NO_3$	99.8	0.09	Vinylacetylglycine	41.0374/58.0283/69.0336/98.0607/144.0699
3.1	152.0583	3.75 E-4	1.56	1.227	0.812	$C_7H_8N_2O_2$	95.8	−0.44	N1-methyl-4pyridine-3-carboxamide	84.0440/108.0442/136.0389/153.0654
3.5	152.0583	1.19 E-3	1.68	1.367	0.770	$C_7H_8N_2O_2$	95.9	−2.55	N1-methyl-2-pyridine-5-carboxamide	42.0333/53.0385/78.0333/108.0441/110.0603/153.0602
3.7	325.0789	0.022	−1.75	1.095	0.661	$C_{14}H_{15}NO_8$	95.3	2.60	Dihydroxy-1H-indole glucuronide	150.055/326.085
6.6	230.1263	0.079	1.56	1.097	0.739	$C_{10}H_{18}N_2O_4$	93.5		Hydroxyprolyl-Valine	Annotated by Formula
10.2	246.1206	0.030	2.08	1.003	0.653	$C_{10}H_{18}N_2O_5$	96.4	4.68	L-beta-aspartyl-L-Leucine	74.0246/86.0966/132.1013/201.1236/247.1296
11.6	246.1372	0.011	1.99	1.745	0.678	$C_{14}H_{18}N_2O_2$	92.5	−1.62	Hypaphorine	Annotated by Formula
14.8	129.0429	0.0079	−1.52	1.038	0.695	$C_5H_7NO_3$	98.8	−1.42	Pyroglutamic acid	45.0337/58.0367/84.0447/130.0501
14.8	264.1150	0.014	−1.46	1.001	0.677	$C_{13}H_{16}N_2O_4$	92.4	−4.41	Alpha-N-Phenylacetyl – L glutamine	91.0536/101.0715/129.0662/130.0495/147.077
20.7	265.0951	0.0079	−1.62	1.326	0.710	$C_{13}H_{15}NO_5$	78.4	4.04	2-(2-Phenylacetoxy)propinylglycine	57.0339/119.0489/266.1007
34.3	285.1935	0.038	1.78	1.426	0.656	$C_{15}H_{27}NO_4$	96.8	−1.95	2-octenoyl-carnitine	55.0539/85.0284
33.8	285.1943	0.038	1.45	1.068	0.646		95.1	−0.63		
36.6	309.1921	0.027	1.41	1.036	0.669	$C_{17}H_{27}NO_4$	99.8	0.55	Decatrienoylcarnitine	85.0288/251.1297/310.2026
37.1	309.1922	0.038	1.44	1.021	0.623		86.8	5.00		
36.8	299.2078	6.29 E-3	1.70	1.292	0.739	$C_{16}H_{29}NO_4$	96.6	5.00	2-Nonenoylcarnitine	85.0218/300.2181
37.8	301.2235	9.02 E-4	1.91	1.468	0.776	$C_{16}H_{31}NO_4$	94.6	0.90	2,6-Dimethylheptanoyl carnitine	60.0804/85.0282/302.228
38.2	313.2245	0.010	1.62	1.061	0.701	$C_{17}H_{31}NO_4$	96.4	1.53	9-Decenoylcarnitine	60.0804/85.0282/157.0501/255.159
38.3	313.2218	7.89 E-3	1.73	1.160	0.701		96.6	1.27		
38.6	357.2498	0.010	1.87	1.173	0.673	$C_{19}H_{35}NO_5$	96.6	−0.67	Hydroxydodecenoylcarnitine	60.081/81.0698/85.0282/95.0856/137.1333/155.1437
39.0	327.2389	7.89 E-3	2.44	1.431	0.706	$C_{18}H_{33}NO_4$	96.1	−1.86	Undecenoyl carnitine	85.0283/328.2484

SCIENTIFIC REPORTS

OPEN

SDS-PAGE analysis of Aβ oligomers is disserving research into Alzheimer´s disease: appealing for ESI-IM-MS

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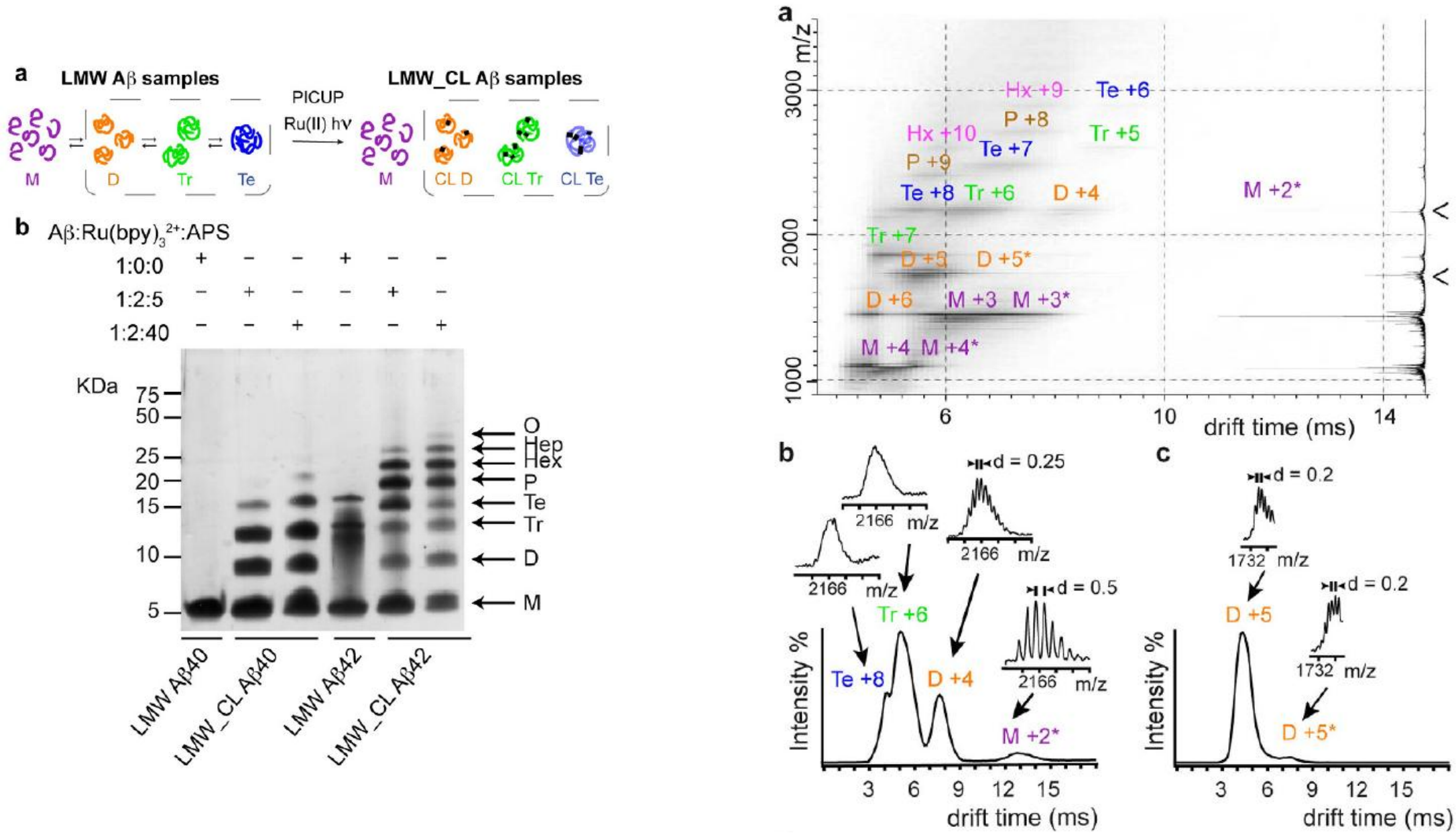
Rosa Pujol-Pina[1,*], Sílvia Vilaprinyó-Pascual[1,*], Roberta Mazzucato[1], Annalisa Arcella[2], Marta Vilaseca[3], Modesto Orozco[2,4] & Natàlia Carulla[1]


a
LMW Aβ samples
LMW_CL Aβ samples
PICUP
Ru(II) hν
M
D
Tr
Te
M
CL D
CL Tr
CL Te
b
Aβ:Ru(bpy)3 2+:APS
1:0:0
1:2:5
1:2:40
KDa
75
50
25
20
15
10
5
O
Hep
Hex
P
Te
Tr
D
M
LMW Aβ40
LMW_CL Aβ40
LMW Aβ42
LMW_CL Aβ42
a
3000 m/z
2000
1000
Hx +9
Te +6
P +8
Hx +10
Tr +5
Te +7
P +9
Te +8
Tr +6
D +4
M +2*
Tr +7
D +3
D +5*
D +6
M +3
M +3*
M +4
M +4*
6
10
14
drift time (ms)
b
d = 0.25
2166 m/z
d = 0.5
Tr +6
Te +8
D +4
M +2*
Intensity %
3
6
9
12
15
drift time (ms)
c
d = 0.2
1732 m/z
D +5
D +5*
Intensity %
drift time (ms)