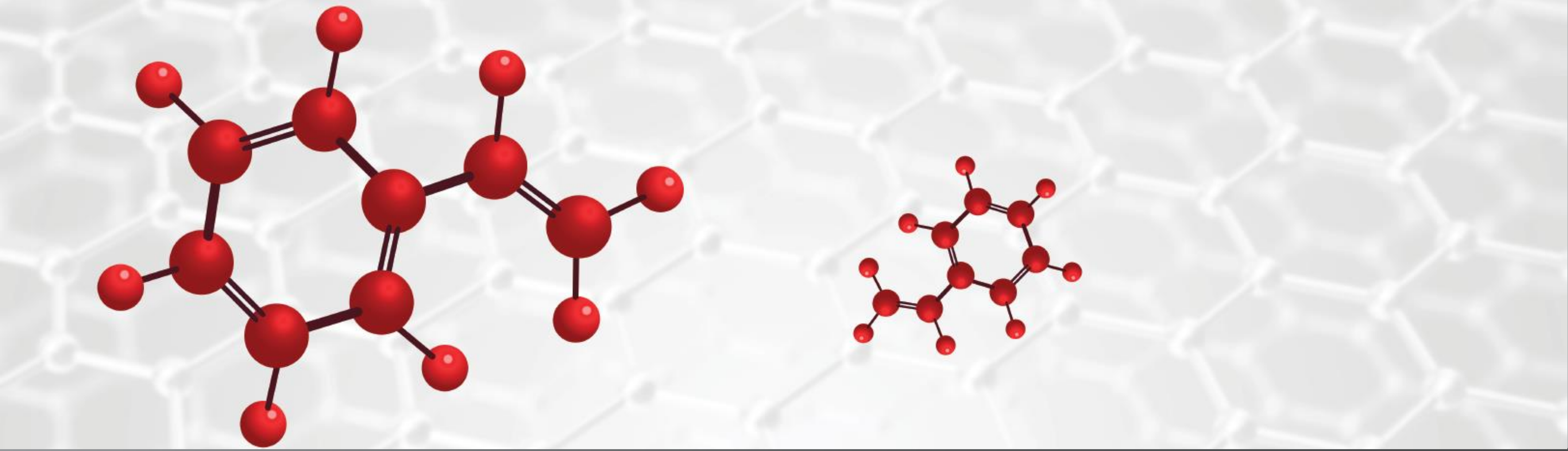
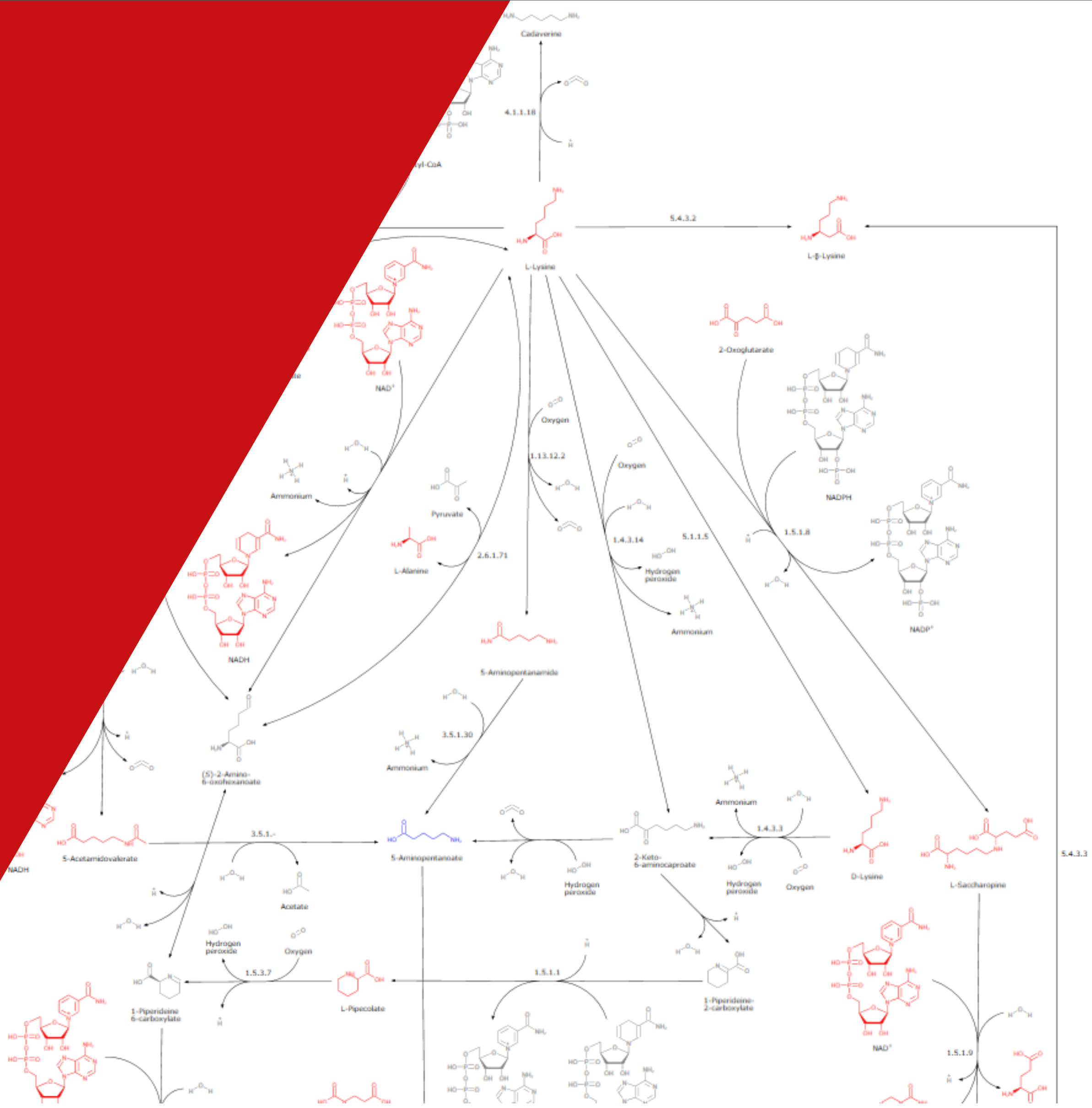


Escape the Metabolomics Identity Crisis with Intelligence Driven Mass Spectrometry

Amanda Souza
Metabolomics Program Manager
Thermo Fisher Scientific

The Identity Crisis in Untargeted Metabolomics


Cadaverine
4.1.1.18
L-Lysine
5.4.3.2
L-β-Lysine
NAD⁺
2-Oxoglutarate
NADPH
Oxygen
1.13.12.2
Ammonium
Pyruvate
L-Alanine
2.6.1.71
1.4.3.14
5.1.1.5
1.5.1.8
Hydrogen peroxide
NADH
NADP⁺
5-Aminopentanamide
(S)-2-Amino-6-oxohexanoate
3.5.1.30
5-Acetamidovalerate
3.5.1.-
5-Aminopentanoate
2-Keto-6-aminocaproate
1.4.3.3
D-Lysine
L-Saccharopine
5.4.3.3
Acetate
1.5.3.7
L-Pipecolate
1.5.1.1
1-Piperideine-6-carboxylate
1-Piperideine-2-carboxylate
1.5.1.9

Identity Crisis | Unknown Annotation in Metabolomics

> “An important aspect underlying most if not all the methods for the analysis of metabolomics data that we will address…is to properly identify the metabolites”
>
> - Rosato et al. 2018 Metabolomics;14(4):37.

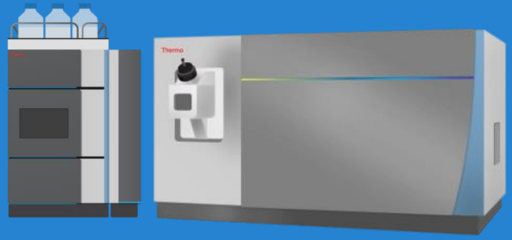
> “Metabolite identification is a major bottleneck in untargeted metabolomics
>
> In order to convert LC-MS data into biological information, metabolites need to be annotated”
>
> - Chaleckis et al. 2019 Curr Opin Biotech;55:44.

Untargeted Metabolomics Bottleneck: Confident Compound Annotation

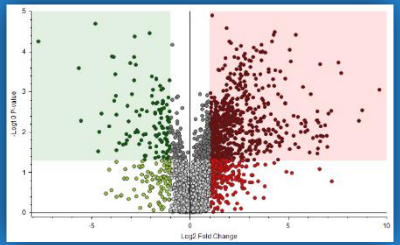
Untargeted Metabolomics Workflow

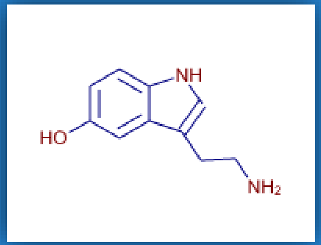
Sample Collection → Data Acquisition → Data Analysis → Compound Annotation → Pathway Analysis

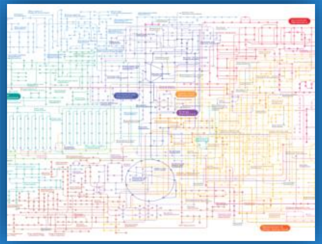
Healthy
Disease



Orbitrap ID-X MS with AcquireX

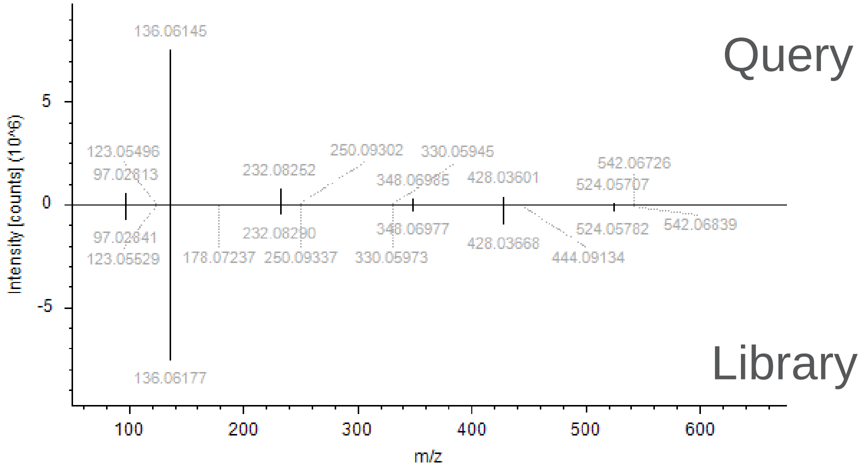




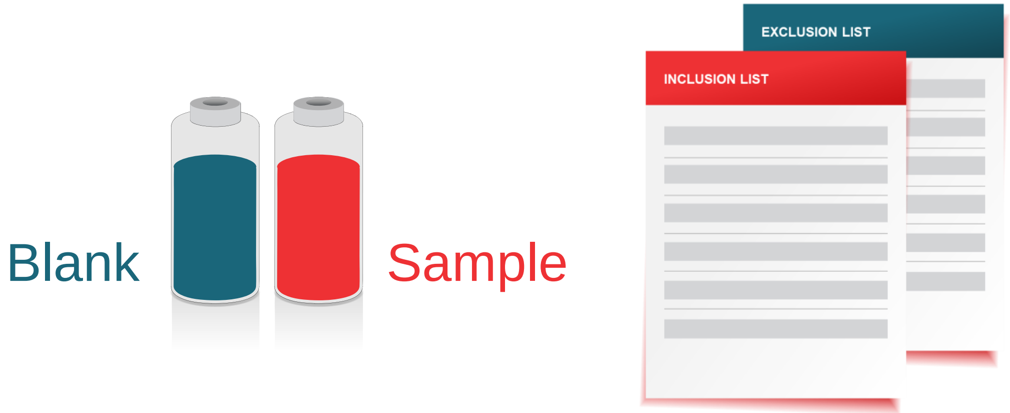


Addressing the Identity Crisis

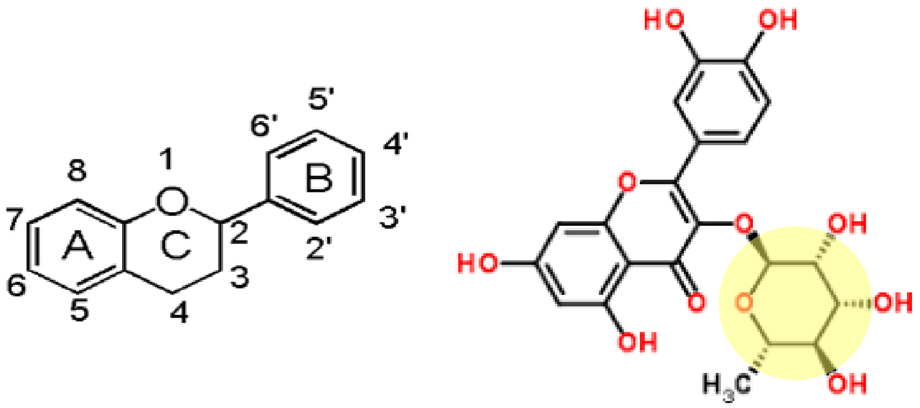
Fragmentation Spectra to Increase Confidence



Prioritize Sample Relevant Ions

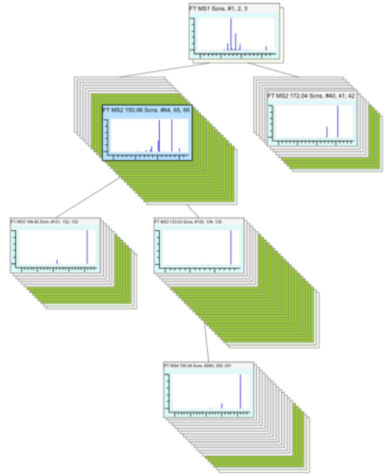

Blank
Sample
EXCLUSION LIST
INCLUSION LIST

Structure-Based Acquisition


A
B
C
1
2
3
4
5
6
7
8
2'
3'
4'
5'
6'
HO
OH
O
OH
HO
OH
O
O
OH
OH
OH
H_3C

Ultra High-Quality Spectral Library

m/z™ CLOUD



Thermo Scientific™ Obitrap ID-X™ Tribrid™ Mass Spectrometer

thermo scientific
ORBITRAP ID-X

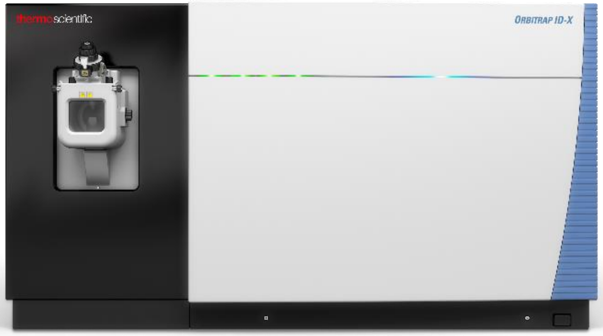
Small Molecule Tribrid Mass Spectrometer

Thermo Scientific™
Orbitrap ID-X™
Tribrid™ MS

Dedicated Instrumentation

Features include streamlined calibrations, pre-defined templates for small molecule applications and MS^n library method for custom libraries

Optimized for Small Molecules



Multi-Stage Fragmentation

More structural information for chemical characterization and elucidation to know more unknowns

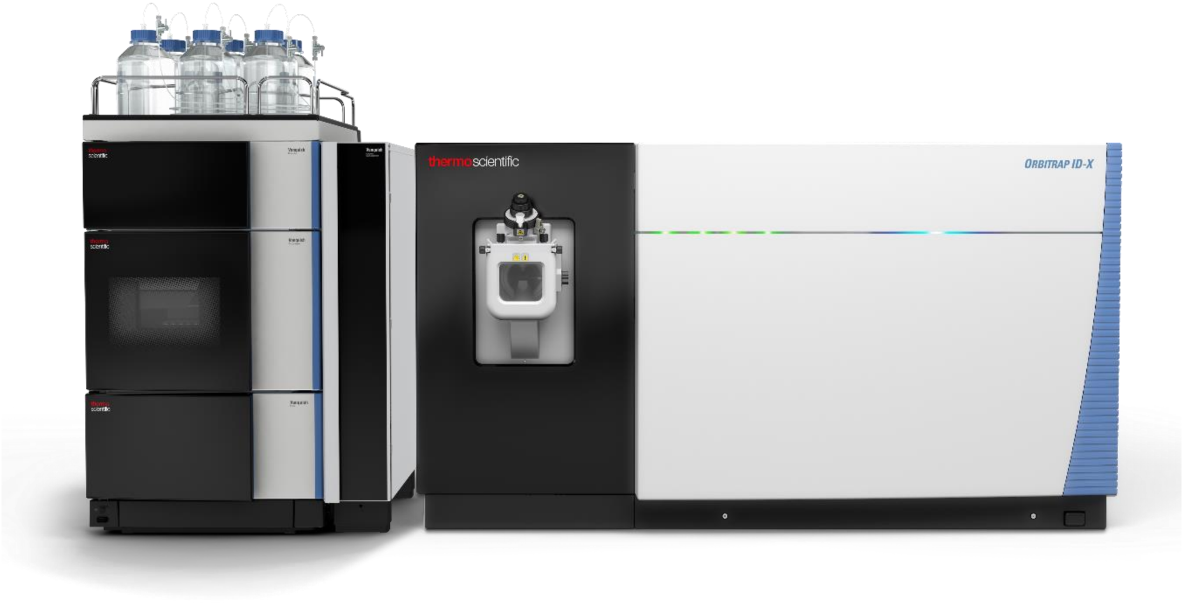
MS/MS and MS^n

Novel Data Acquisition

AcquireX™

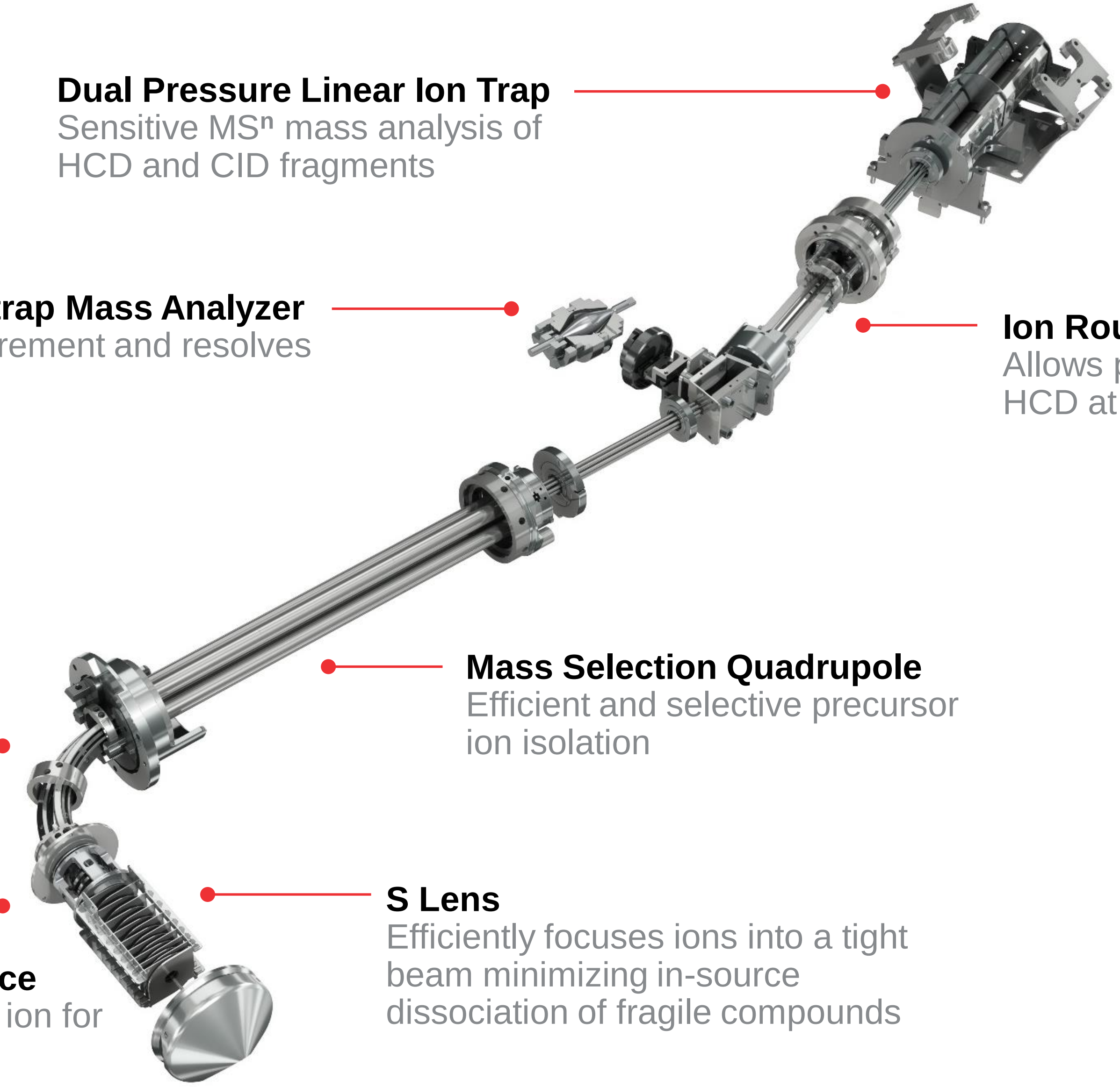
Automated data dependent acquisition iterative injections to generate more fragmentation spectra of unique precursor ions

Orbitrap ID-X Tribrid Mass Spectrometer


thermoscientific
ORBITRAP ID-X

Max Resolution	500,000 at m/z 200
Scan Rate OTMS^2	30 Hz
Scan Rate ITMS^2	40 Hz
Quad Mass Selection	Precursor isolation to 0.4 amu
Ion Trap MS^n	Up to MS^{10}
Mass Accuracy	3 ppm external, 1ppm internal
Dissociation	CID, HCD

Transforming Small Molecule Identification and Characterization



Dual Pressure Linear Ion Trap
Sensitive MSⁿ mass analysis of
HCD and CID fragments

Ultra High Field Orbitrap Mass Analyzer
Accurate mass measurement and resolves
isobaric species

Ion Routing Multipole
Allows parallel analysis
HCD at any fragmentation level

Mass Selection Quadrupole
Efficient and selective precursor
ion isolation

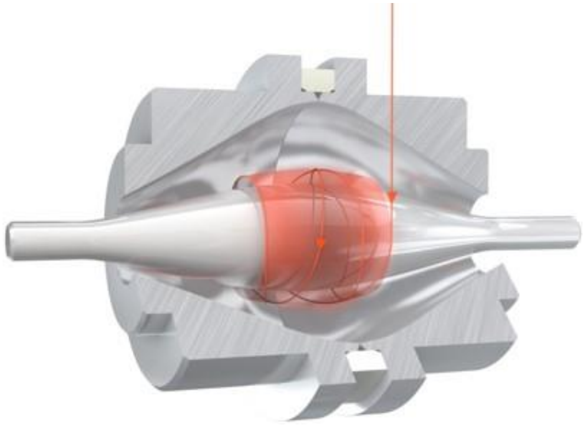
Active Beam Guide
Prevents neutrals and
high velocity clusters from
entering mass selecting
quadrupole

S Lens
Efficiently focuses ions into a tight
beam minimizing in-source
dissociation of fragile compounds

Optional Easy-IC Ion Source
Generates internal calibrant ion for
real-time mass calibration

Built on Orbitrap Technology

High Quality Data for High Quality Results



High Resolution

- Complex matrix
- Differentiate similar masses
- Isobaric species
- Fine isotopic pattern

Mass Accuracy

- Identification of unknowns
- Narrow mass tolerance
- Mass stability from peak-to-peak and run-to-run

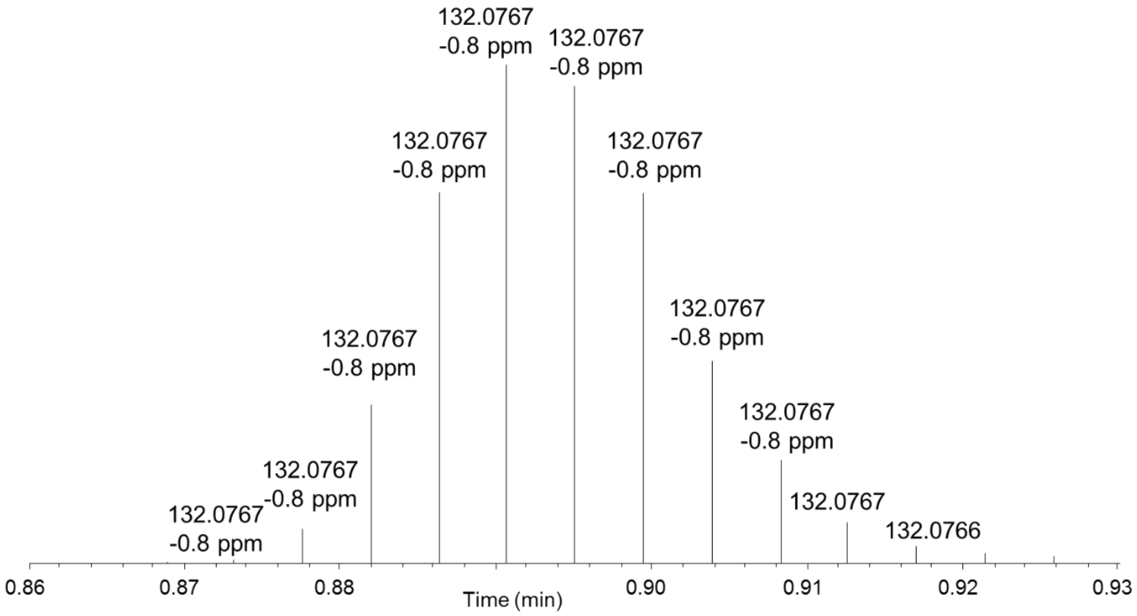
Instrument Performance

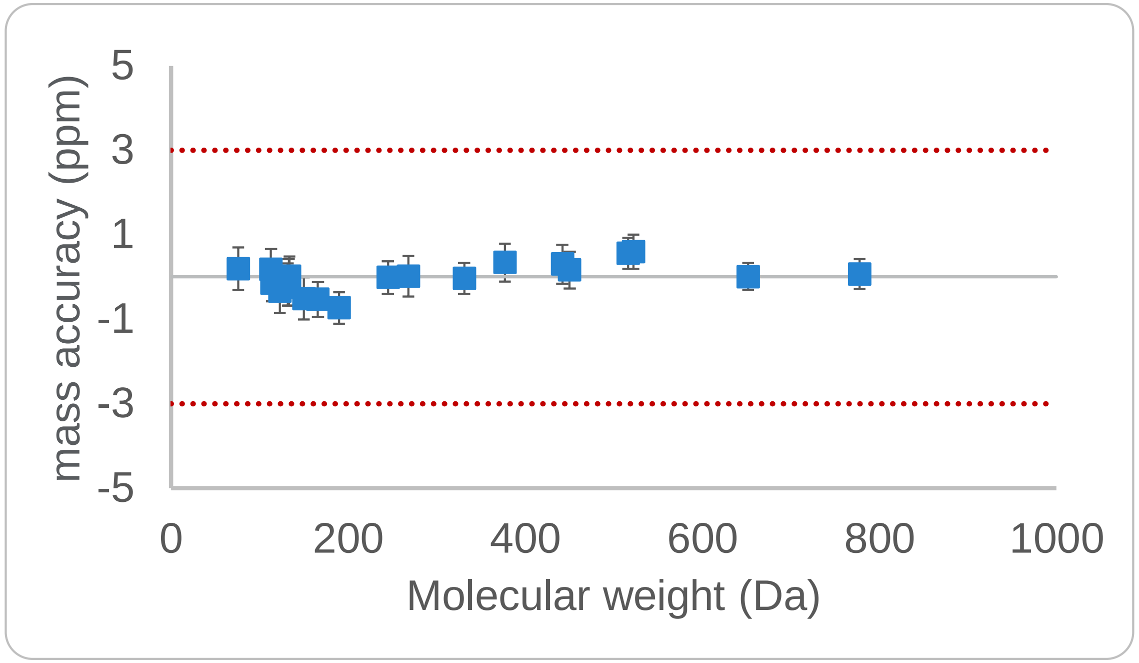
- Scan-to-scan consistency
- Injection-to-injection reproducibility
- Robustness over extended time periods

Robust Mass Accuracy from Run to Run Across the MW Range

excellent mass stability from scan-to-scan across the peak

excellent mass accuracy for all metabolites from run-to-run (during a 72h experiment)

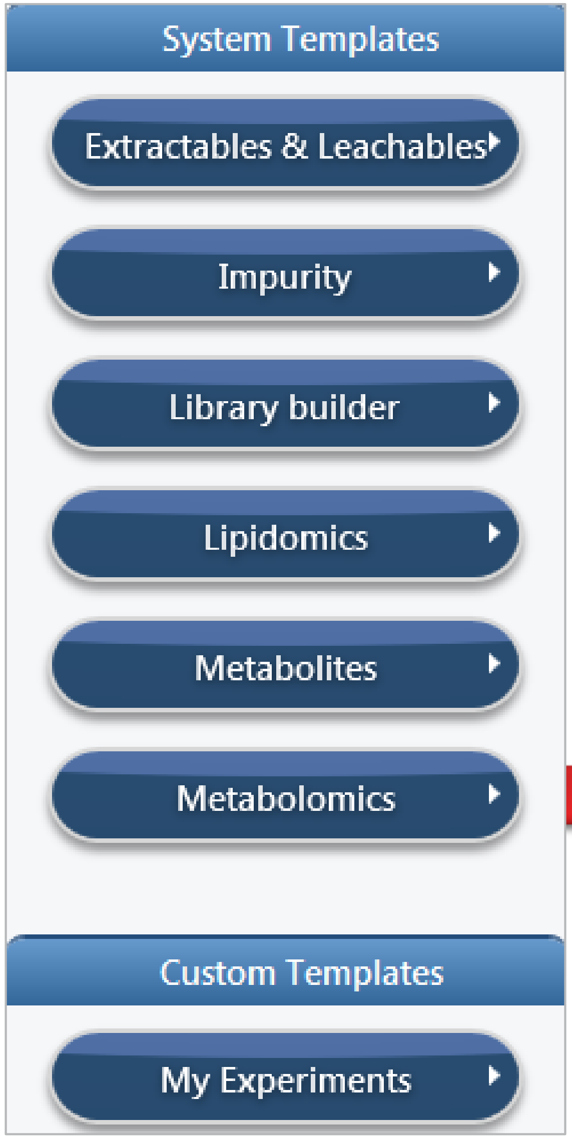


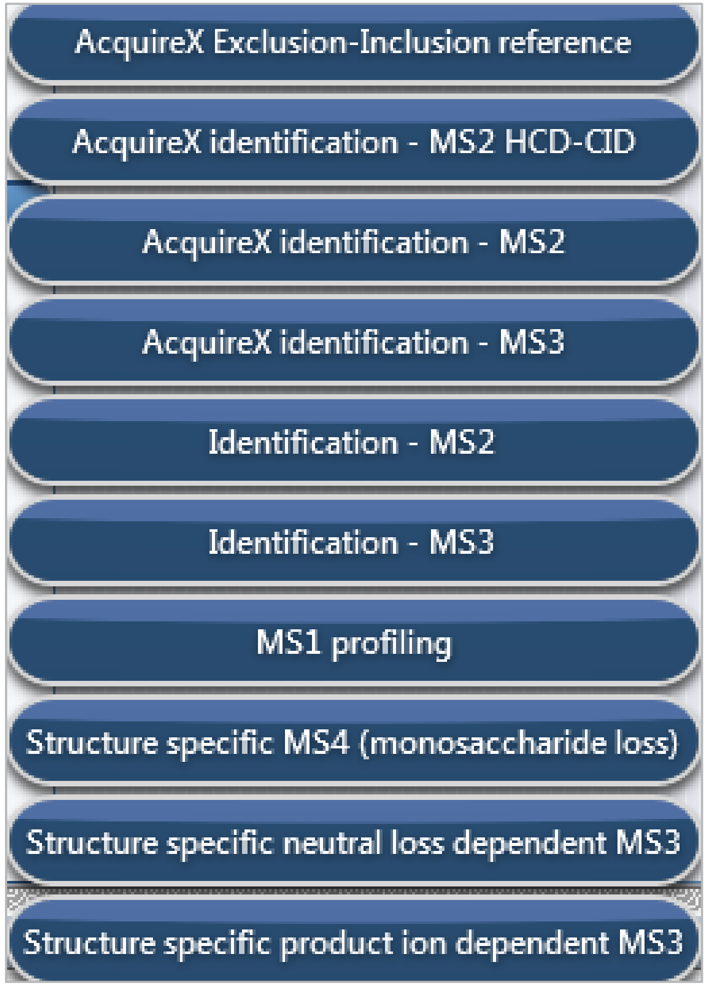


Endogenous creatine (theoretical M+H$^+$ 132.0768 Da) detected in human plasma (NIST SRM1950)

Injections of a mixture of 24 small molecule standards conducted over 72 hours

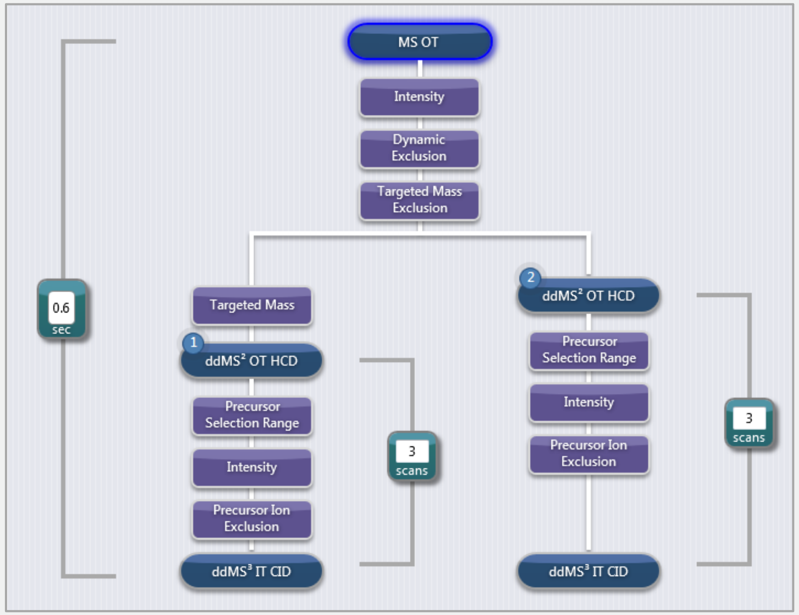
Pre-Defined Method Templates for Getting Started


System Templates
Extractables & Leachables
Impurity
Library builder
Lipidomics
Metabolites
Metabolomics
Custom Templates
My Experiments

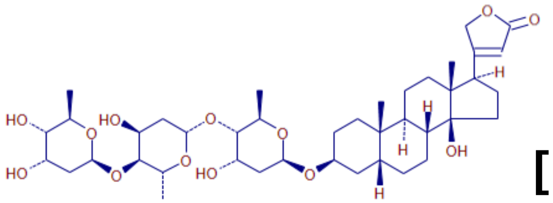

AcquireX Exclusion-Inclusion reference
AcquireX identification - MS2 HCD-CID
AcquireX identification - MS2
AcquireX identification - MS3
Identification - MS2
Identification - MS3
MS1 profiling
Structure specific MS4 (monosaccharide loss)
Structure specific neutral loss dependent MS3
Structure specific product ion dependent MS3

One-Click Method Set-Up

- Expansive collection of application specific method templates
- Easy-to-use methods covering advanced workflows for small molecule profiling, identification and characterization


MS OT
Intensity
Dynamic Exclusion
Targeted Mass Exclusion
0.6 sec
Targeted Mass
1
ddMS^2 OT HCD
Precursor Selection Range
Intensity
Precursor Ion Exclusion
ddMS^3 IT CID
3 scans
2
ddMS^2 OT HCD
Precursor Selection Range
Intensity
Precursor Ion Exclusion
ddMS^3 IT CID
3 scans

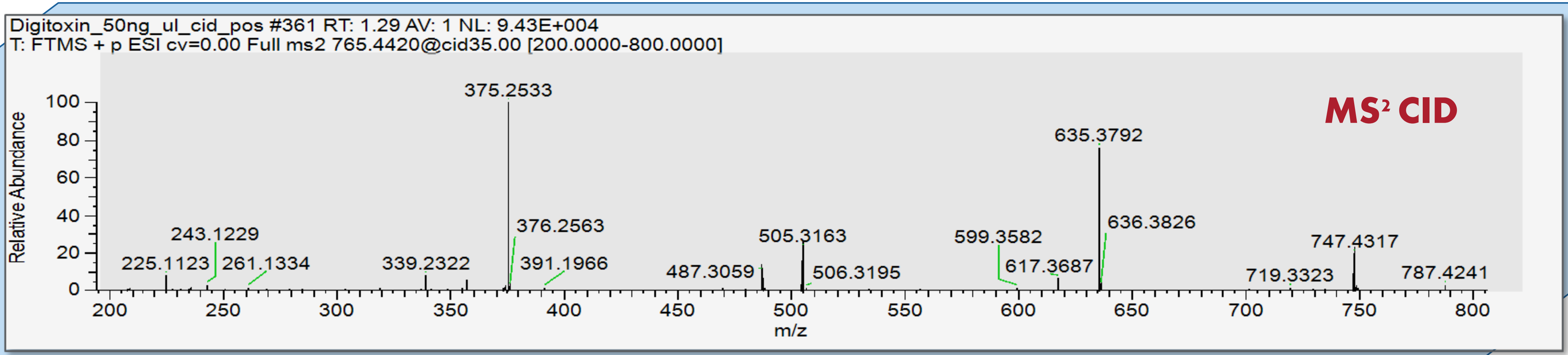
Multiple Dissociation for Complementary Knowledge



Digitoxin

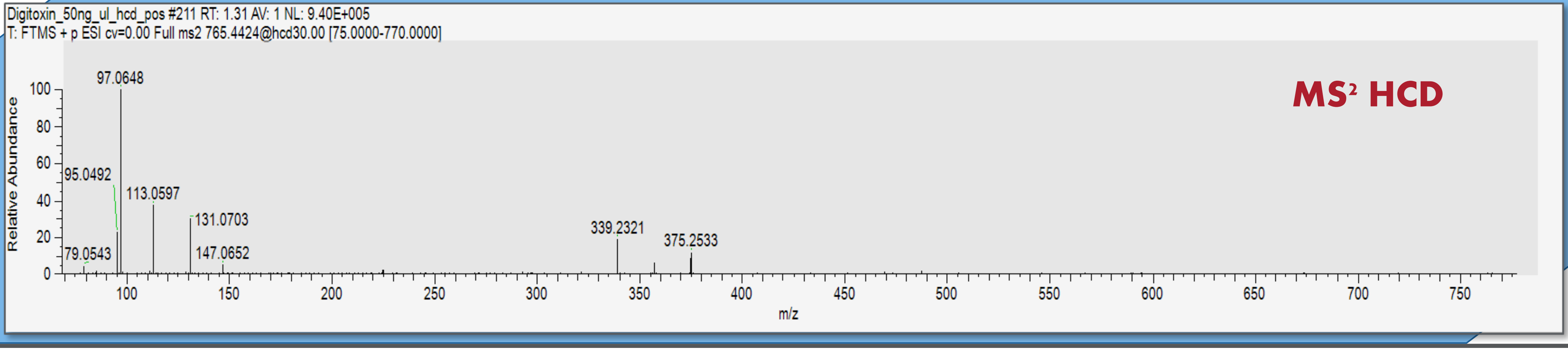
$C_{41}H_{64}O_{13}$

$[M+H]^+ = 765.4420$



Digitoxin_50ng_ul_cid_pos #361 RT: 1.29 AV: 1 NL: 9.43E+004
T: FTMS + p ESI cv=0.00 Full ms2 765.4420@cid35.00 [200.0000-800.0000]

MS² CID



Digitoxin_50ng_ul_hcd_pos #211 RT: 1.31 AV: 1 NL: 9.40E+005
T: FTMS + p ESI cv=0.00 Full ms2 765.4424@hcd30.00 [75.0000-770.0000]

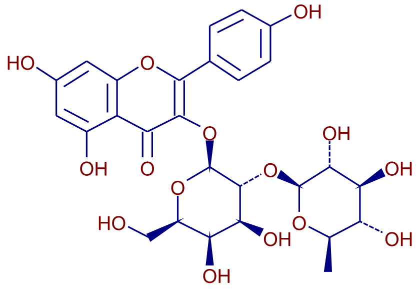
MS² HCD

MS^n to Distinguish Flavonoid Isomers

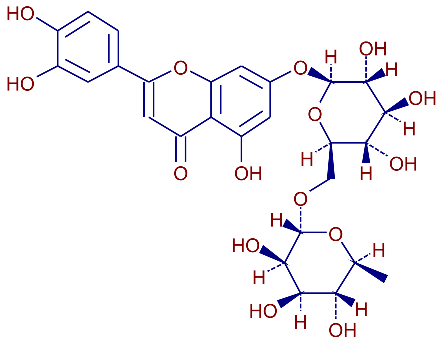
Indistinguishable by MS^2

Distinguishable by MS^3

Kaempferol 3-O-ß -rutinoside

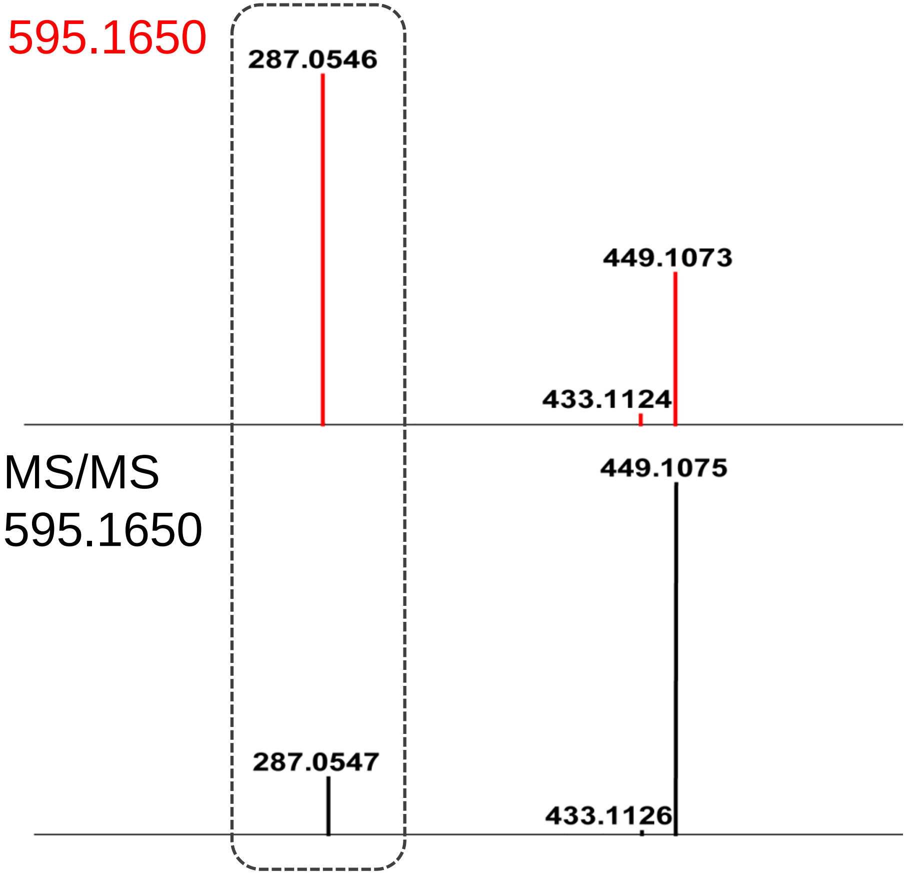

OH
HO
O
O
OH
O
OH
O
OH
O
HO
OH
O
OH
OH

Luteolin 7-rutinoside

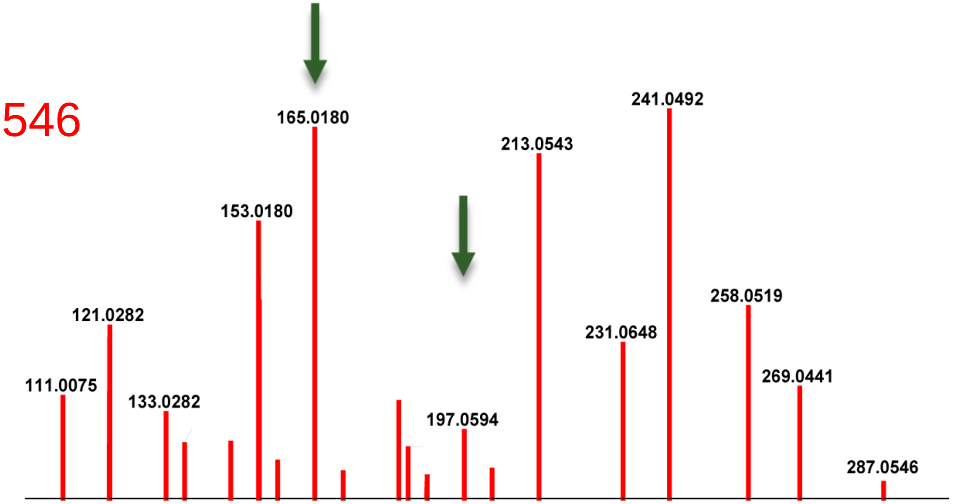

HO
HO
O
O
OH
O
OH
H
H
OH
O
H
OH
H
H
O
H
O
HO
H
H
HO
H
OH
H

MS/MS
595.1650

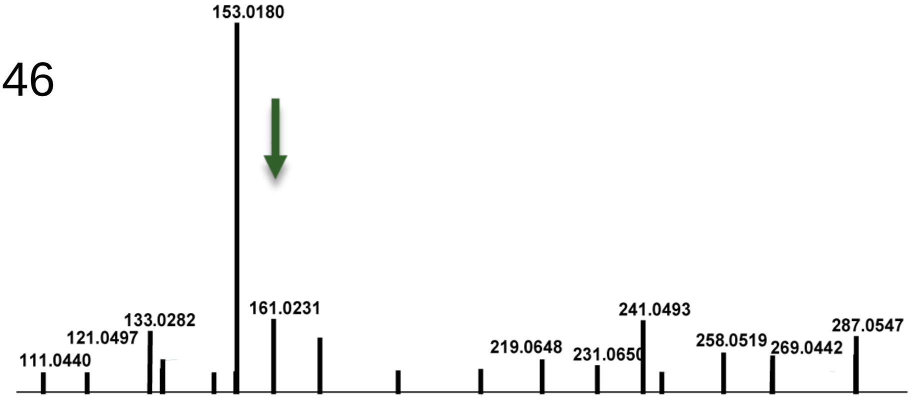
MS/MS
595.1650



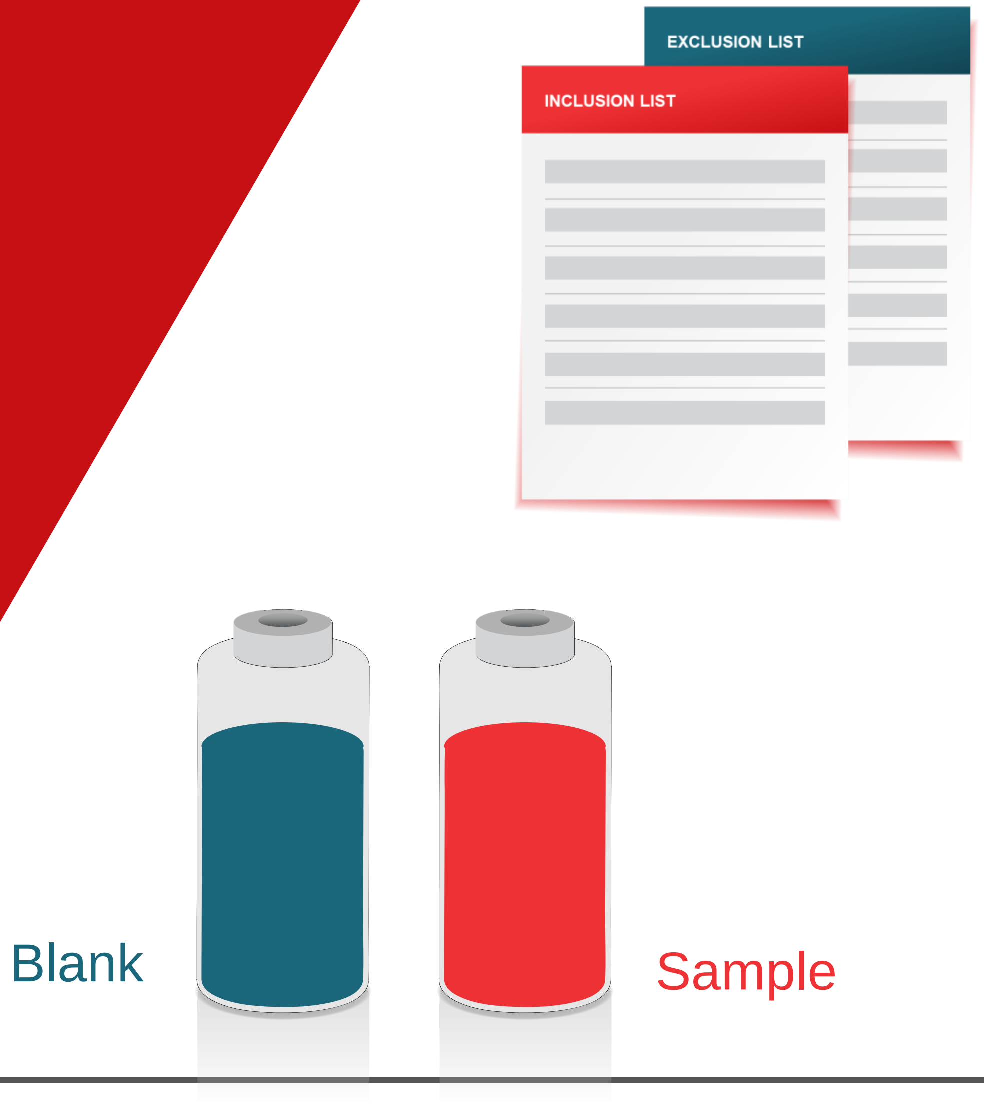
MS^3
287.0546



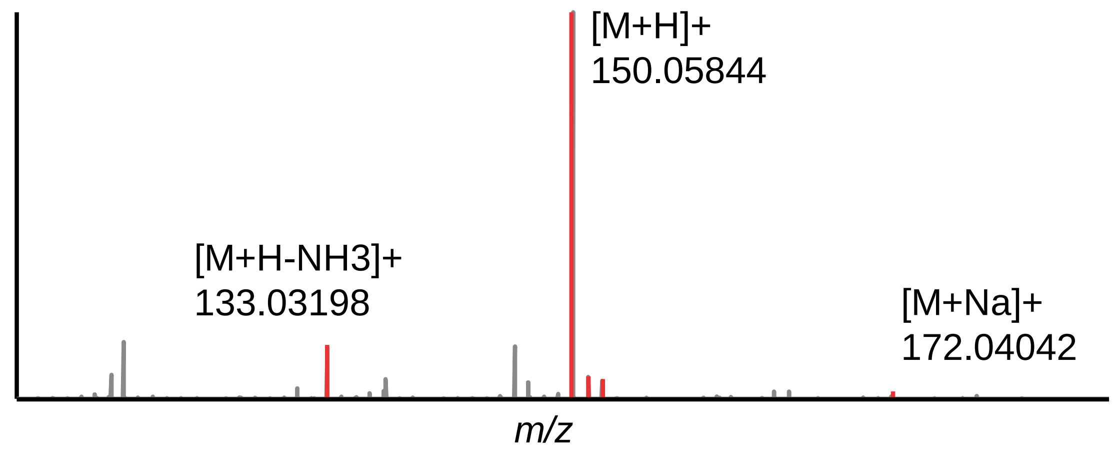
MS^3
287.0546



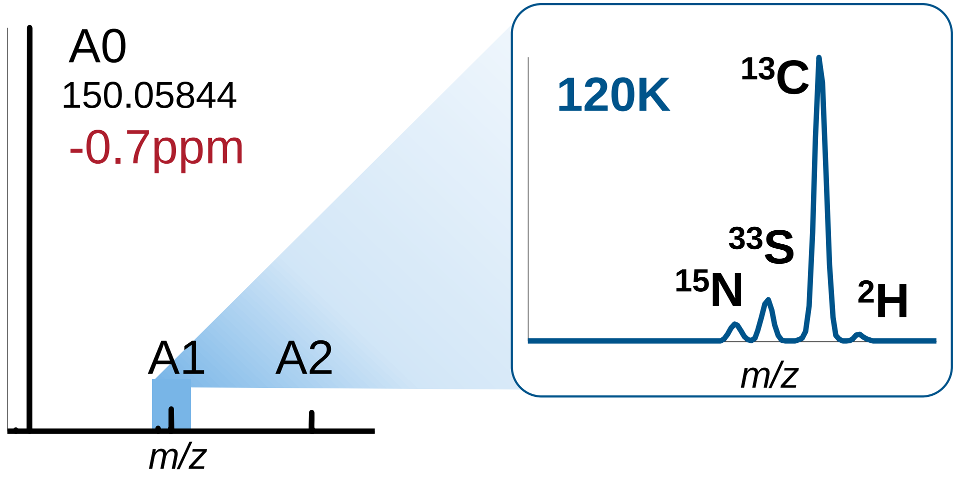
AcquireX Intelligent Acquisition


EXCLUSION LIST
INCLUSION LIST
Blank
Sample

Confident Identification



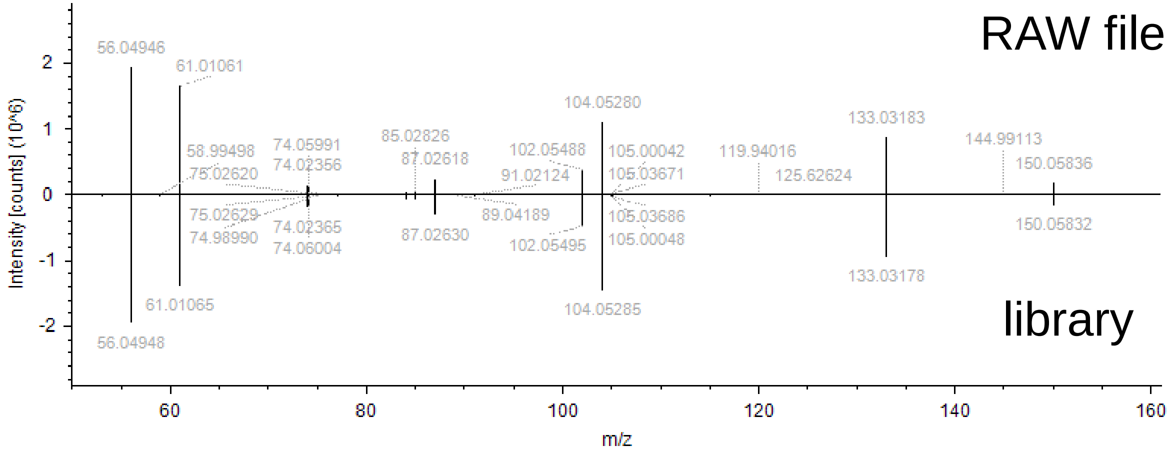
Data reduction



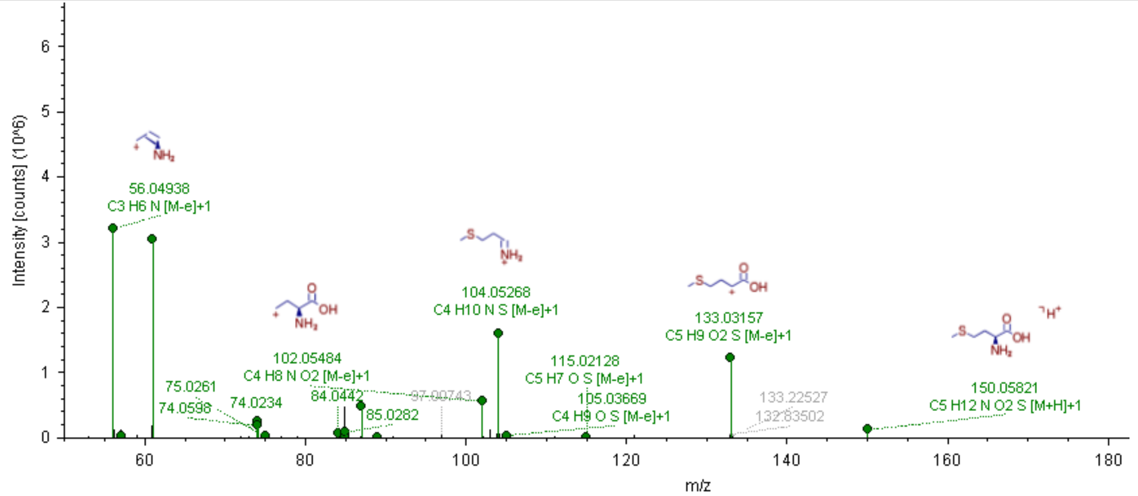
$C_5H_{11}NO_2S$

2 ChemSpider candidates

Elemental Composition / Database Search

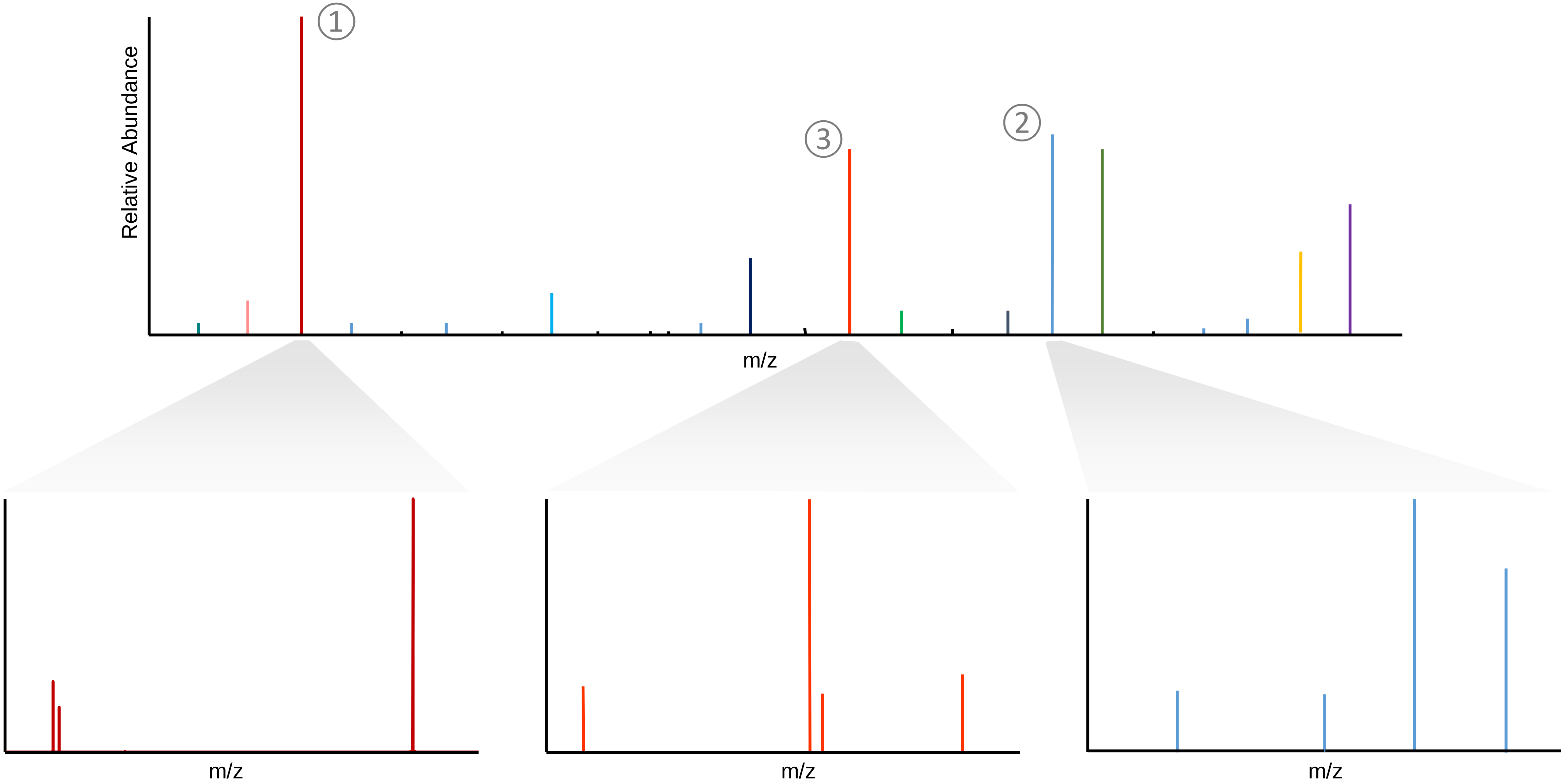


Fragmentation Spectral Match

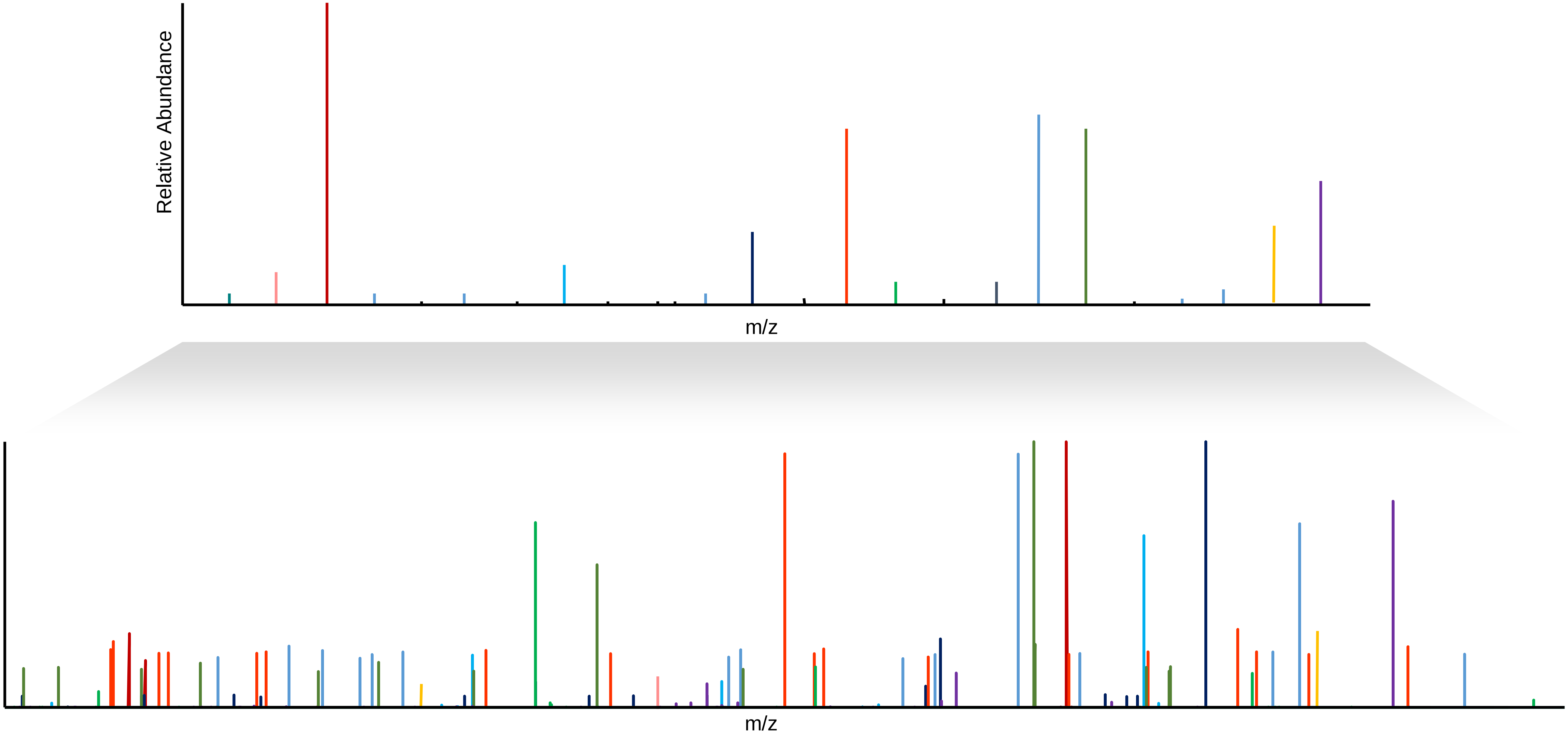


Structure Annotation of Spectrum

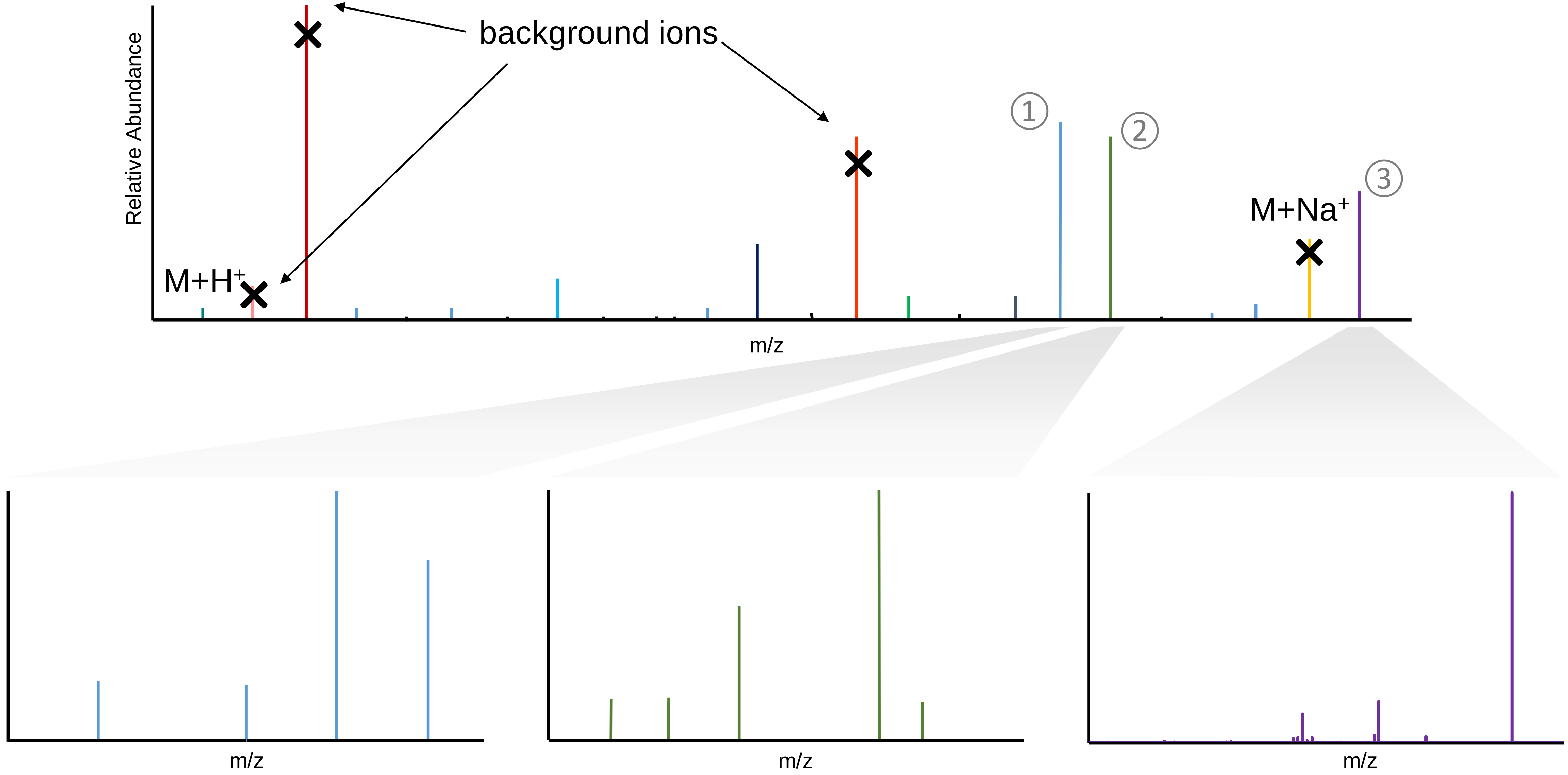
Data-Dependent Acquisition (DDA)


Relative Abundance
①
③
②
m/z
m/z
m/z
m/z

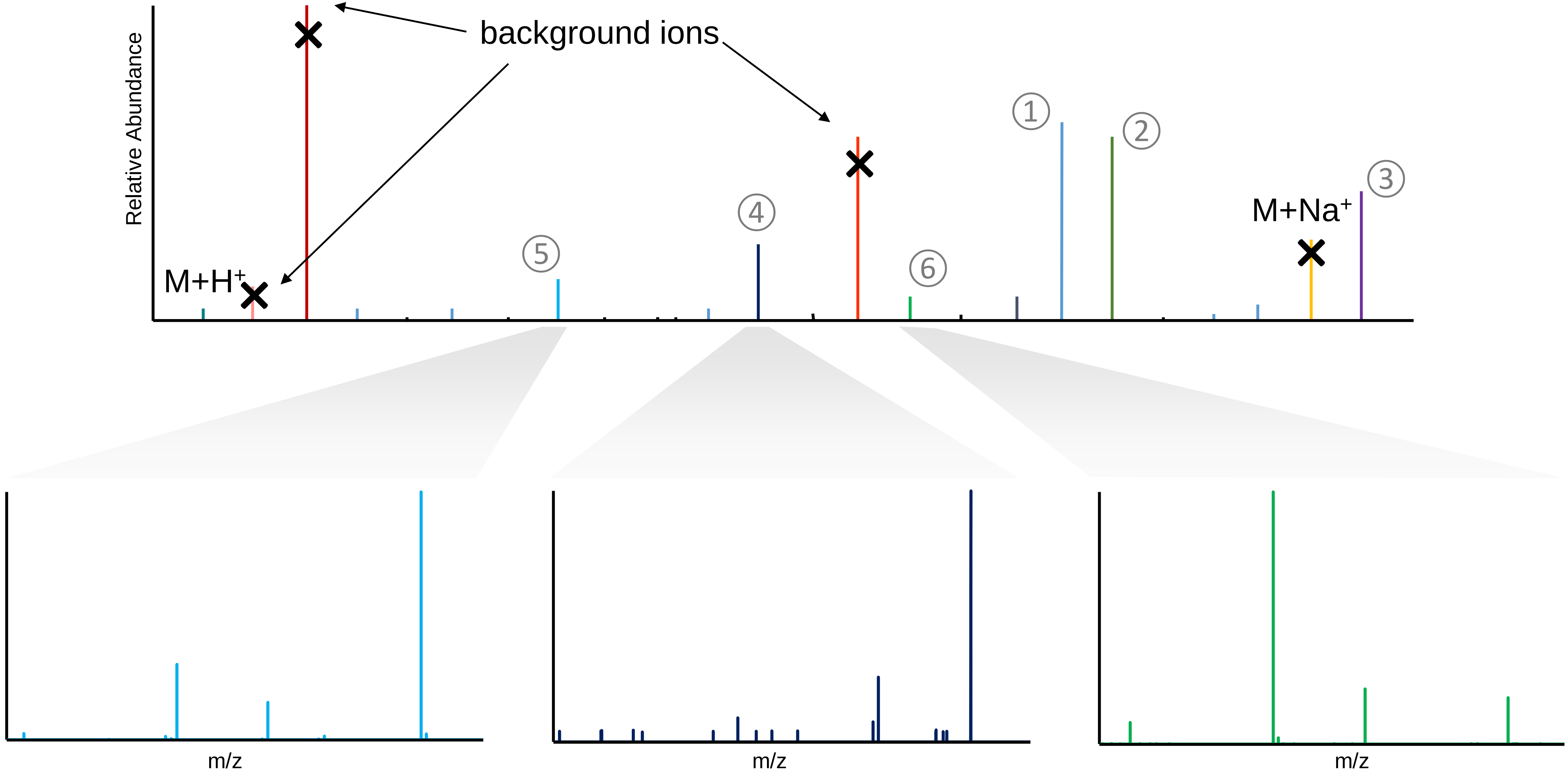
Data Independent Acquisition (DIA)



Intelligent Data-Dependent Acquisition

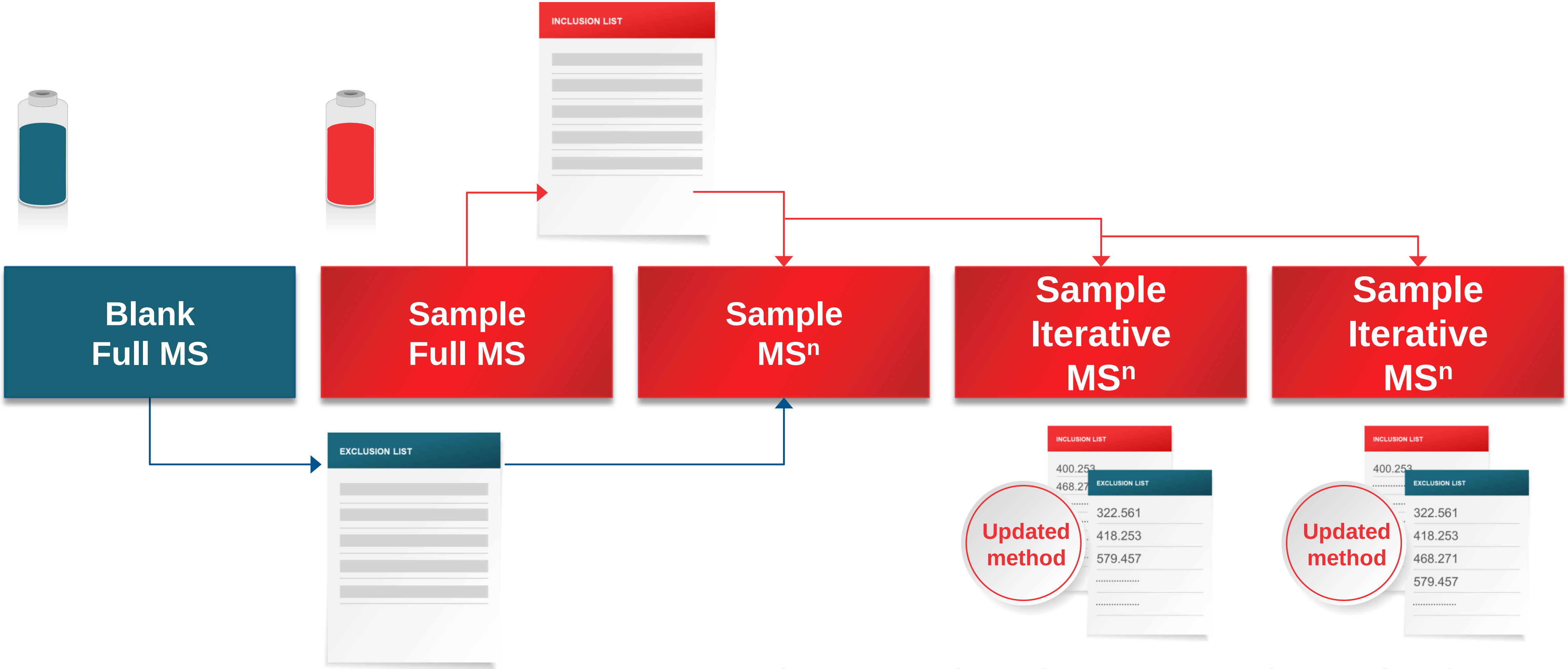

Relative Abundance
background ions
M+H⁺
M+Na⁺
①
②
③
m/z
m/z
m/z
m/z

Intelligent Data-Dependent Acquisition


Relative Abundance
background ions
M+H⁺
M+Na⁺
①
②
③
④
⑤
⑥
m/z
m/z
m/z

AcquireX – A New Acquisition Paradigm

Collect more meaningful data, not just more data


INCLUSION LIST
EXCLUSION LIST
INCLUSION LIST
400.253
468.27
EXCLUSION LIST
322.561
418.253
579.457
INCLUSION LIST
400.253
EXCLUSION LIST
322.561
418.253
468.271
579.457

Blank Full MS

Sample Full MS

Sample MS^n

Sample Iterative MS^n

Sample Iterative MS^n

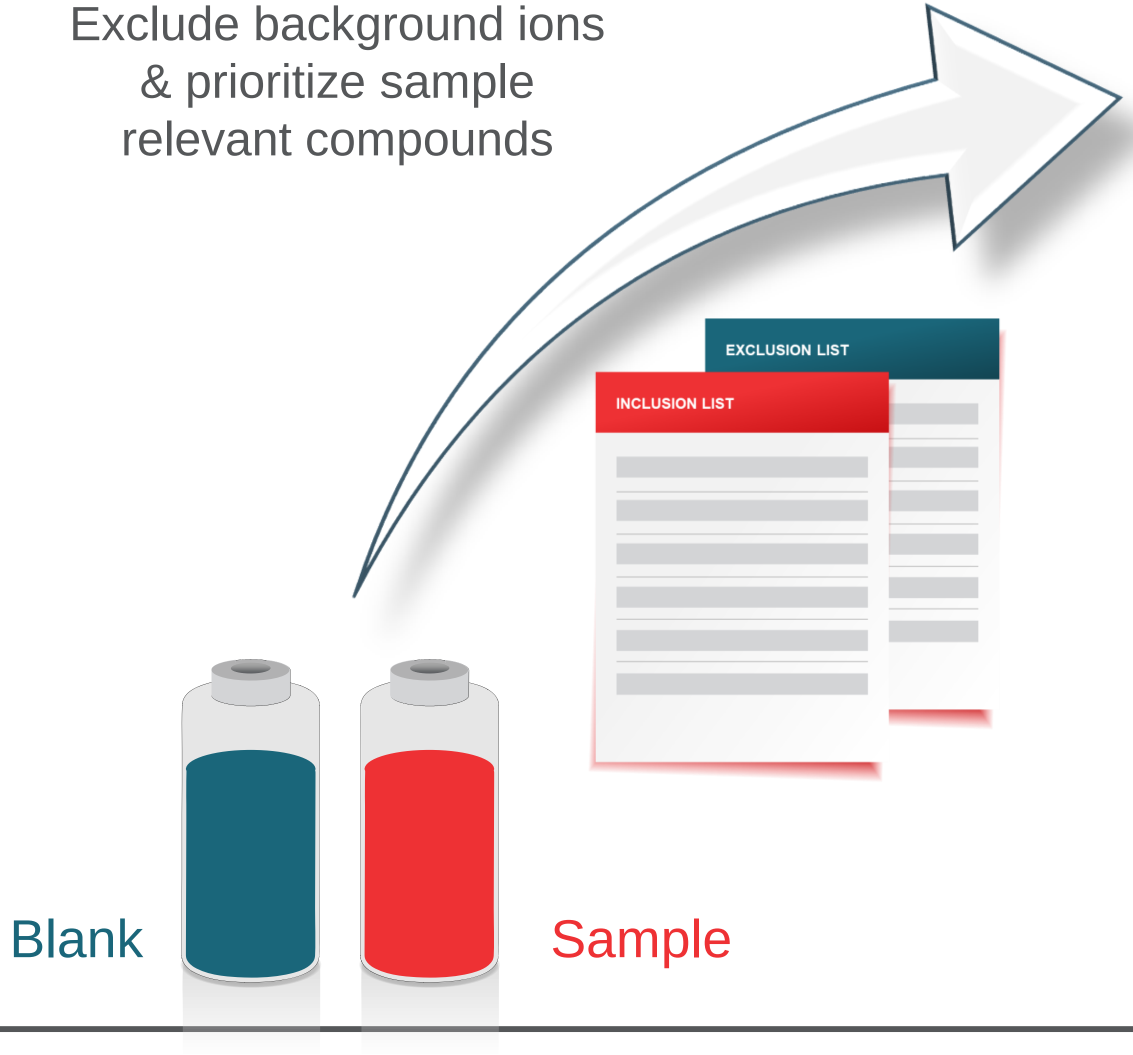
Updated method

Updated method

Automatically updated run-to-run inclusion/exclusion

Collect More Meaningful Data

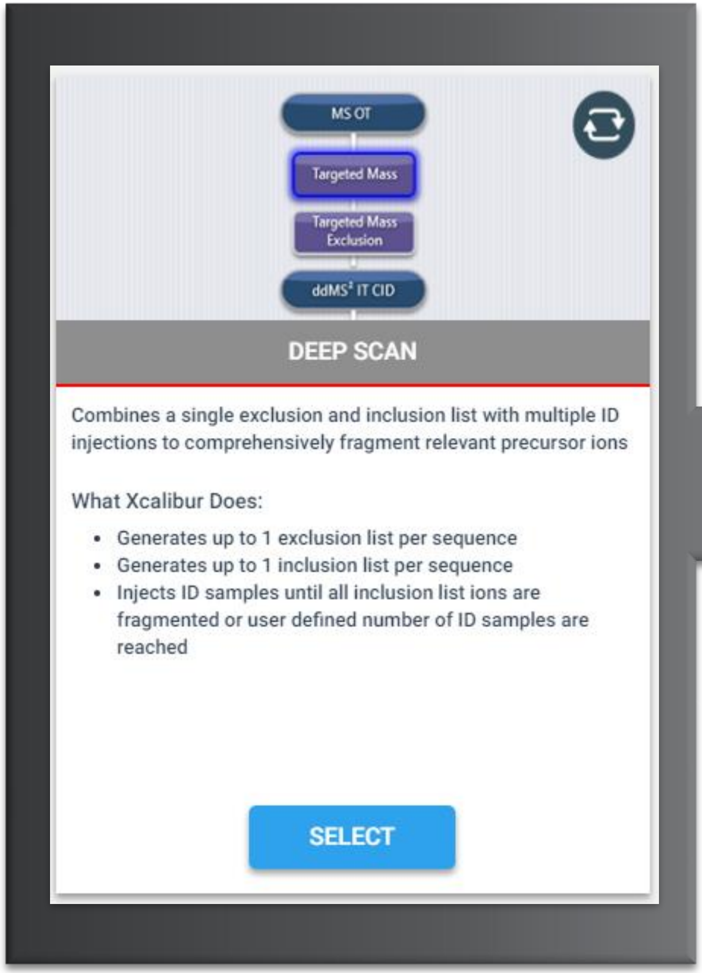
MS/MS & MS^n
Exclude background ions
& prioritize sample
relevant compounds


EXCLUSION LIST
INCLUSION LIST
Blank
Sample

AcquireX
Intelligent Data-Dependent Acquisition

- Fully automated to save time
- Avoid unrelated background ions and remove redundancy
- Fragment more sample relevant compounds
- Go deeper by fragmenting low abundant ions

Intuitive Sequence Builder for Automated Processing


MS OT
Targeted Mass
Targeted Mass Exclusion
ddMS² IT CID

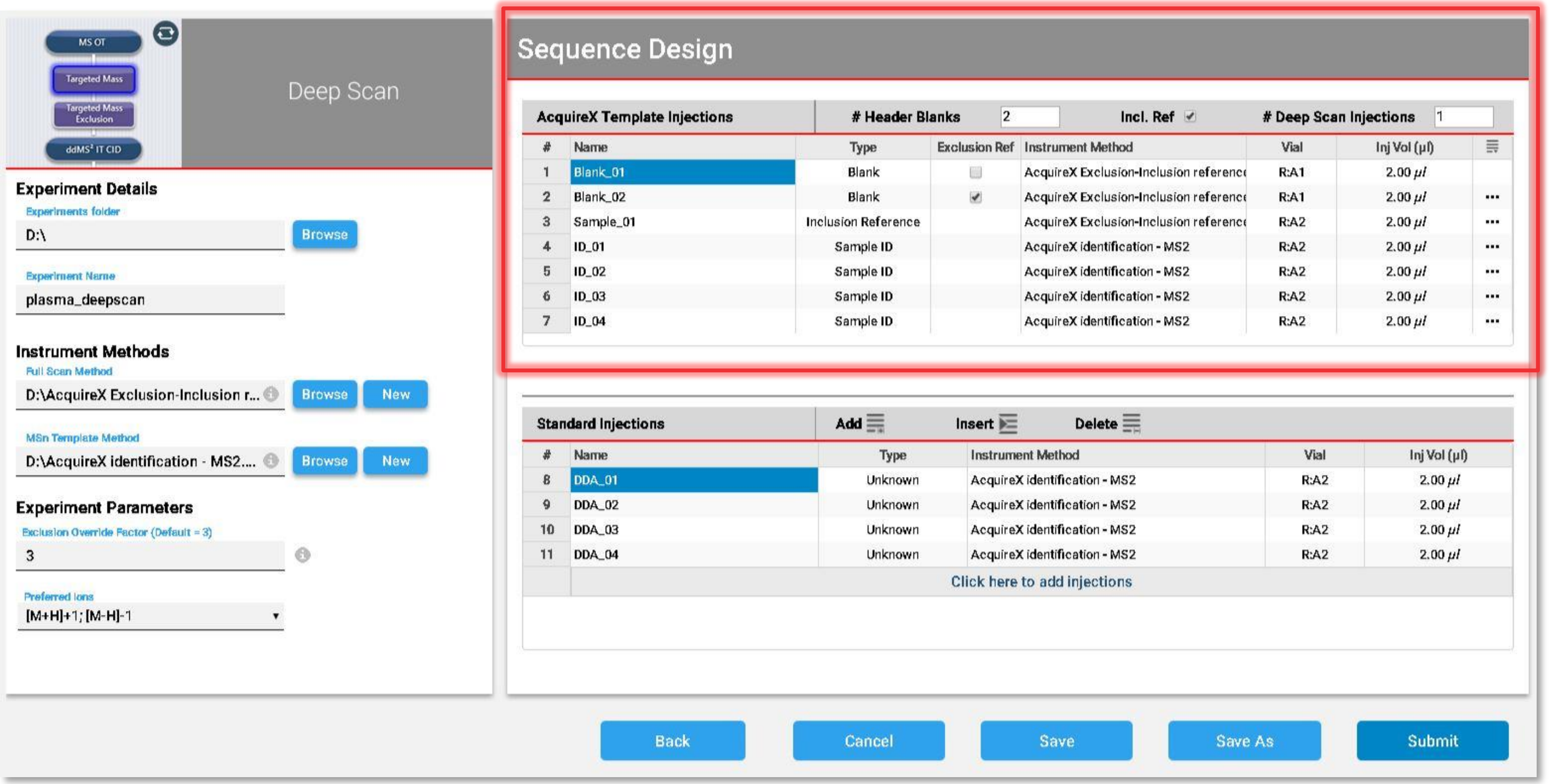
DEEP SCAN

Combines a single exclusion and inclusion list with multiple ID injections to comprehensively fragment relevant precursor ions

What Xcalibur Does:

- Generates up to 1 exclusion list per sequence
- Generates up to 1 inclusion list per sequence
- Injects ID samples until all inclusion list ions are fragmented or user defined number of ID samples are reached

AcquireX Deep Scan Template Setup


MS OT
Targeted Mass
Targeted Mass Exclusion
ddMS² IT CID
Deep Scan

Experiment Details

Experiments folder: D:\

Experiment Name: plasma_deepscan

Instrument Methods

Full Scan Method: D:\AcquireX Exclusion-Inclusion r...

MSn Template Method: D:\AcquireX identification - MS2....

Experiment Parameters

Exclusion Override Factor (Default = 3): 3

Preferred Ions: [M+H]+1; [M-H]-1

Browse
Browse
New
Browse
New

Sequence Design

AcquireX Template Injections — **# Header Blanks** 2 — **Incl. Ref** ☑ — **# Deep Scan Injections** 1

#	Name	Type	Exclusion Ref	Instrument Method	Vial	Inj Vol (µl)
1	Blank_01	Blank	☐	AcquireX Exclusion-Inclusion reference	R:A1	2.00 µl
2	Blank_02	Blank	☑	AcquireX Exclusion-Inclusion reference	R:A1	2.00 µl
3	Sample_01	Inclusion Reference		AcquireX Exclusion-Inclusion reference	R:A2	2.00 µl
4	ID_01	Sample ID		AcquireX identification - MS2	R:A2	2.00 µl
5	ID_02	Sample ID		AcquireX identification - MS2	R:A2	2.00 µl
6	ID_03	Sample ID		AcquireX identification - MS2	R:A2	2.00 µl
7	ID_04	Sample ID		AcquireX identification - MS2	R:A2	2.00 µl

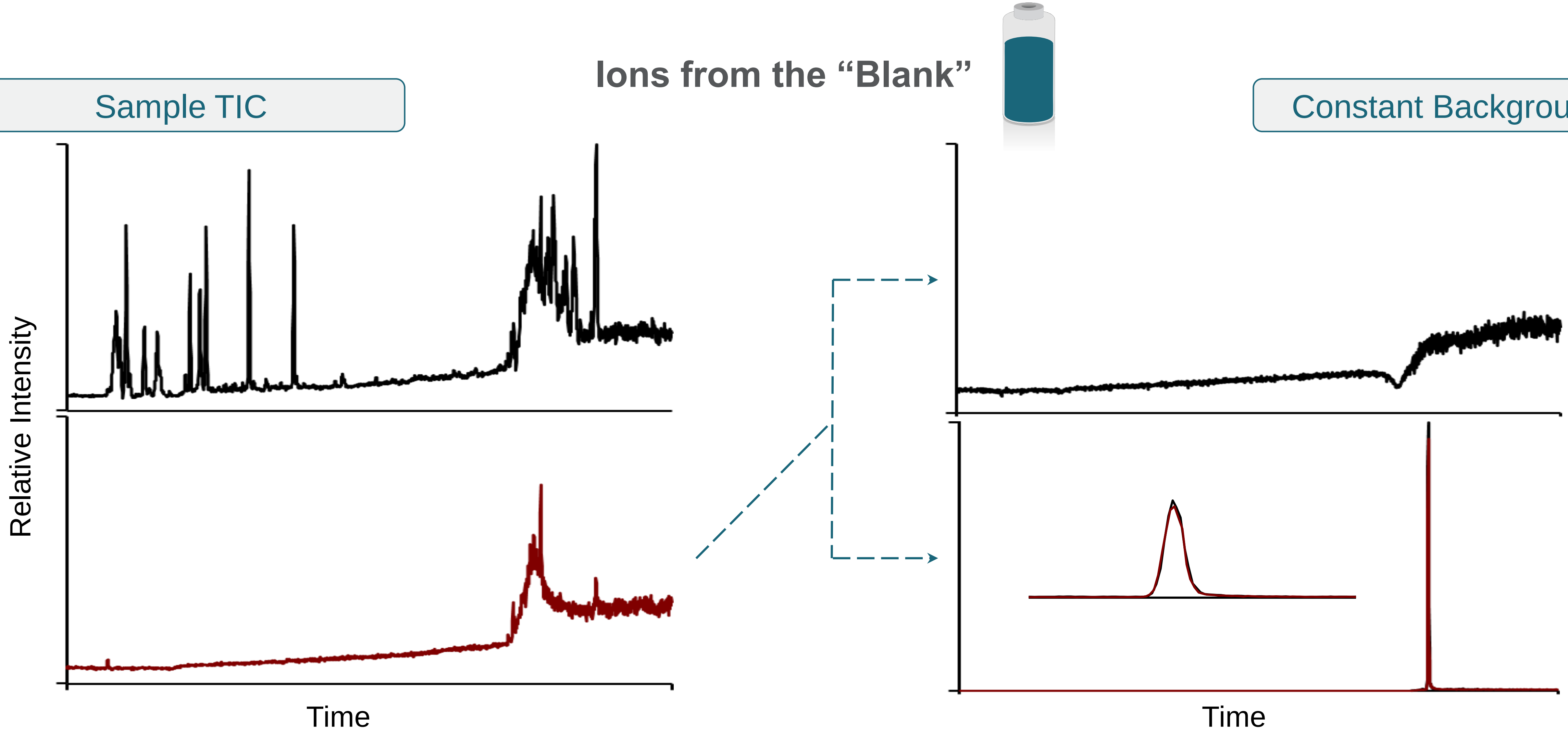
Standard Injections — Add — Insert — Delete

#	Name	Type	Instrument Method	Vial	Inj Vol (µl)
8	DDA_01	Unknown	AcquireX identification - MS2	R:A2	2.00 µl
9	DDA_02	Unknown	AcquireX identification - MS2	R:A2	2.00 µl
10	DDA_03	Unknown	AcquireX identification - MS2	R:A2	2.00 µl
11	DDA_04	Unknown	AcquireX identification - MS2	R:A2	2.00 µl

Click here to add injections

Back
Cancel
Save
Save As
Submit

Avoid Useless Data and Wasted Time



Ions from the “Blank”

Sample TIC

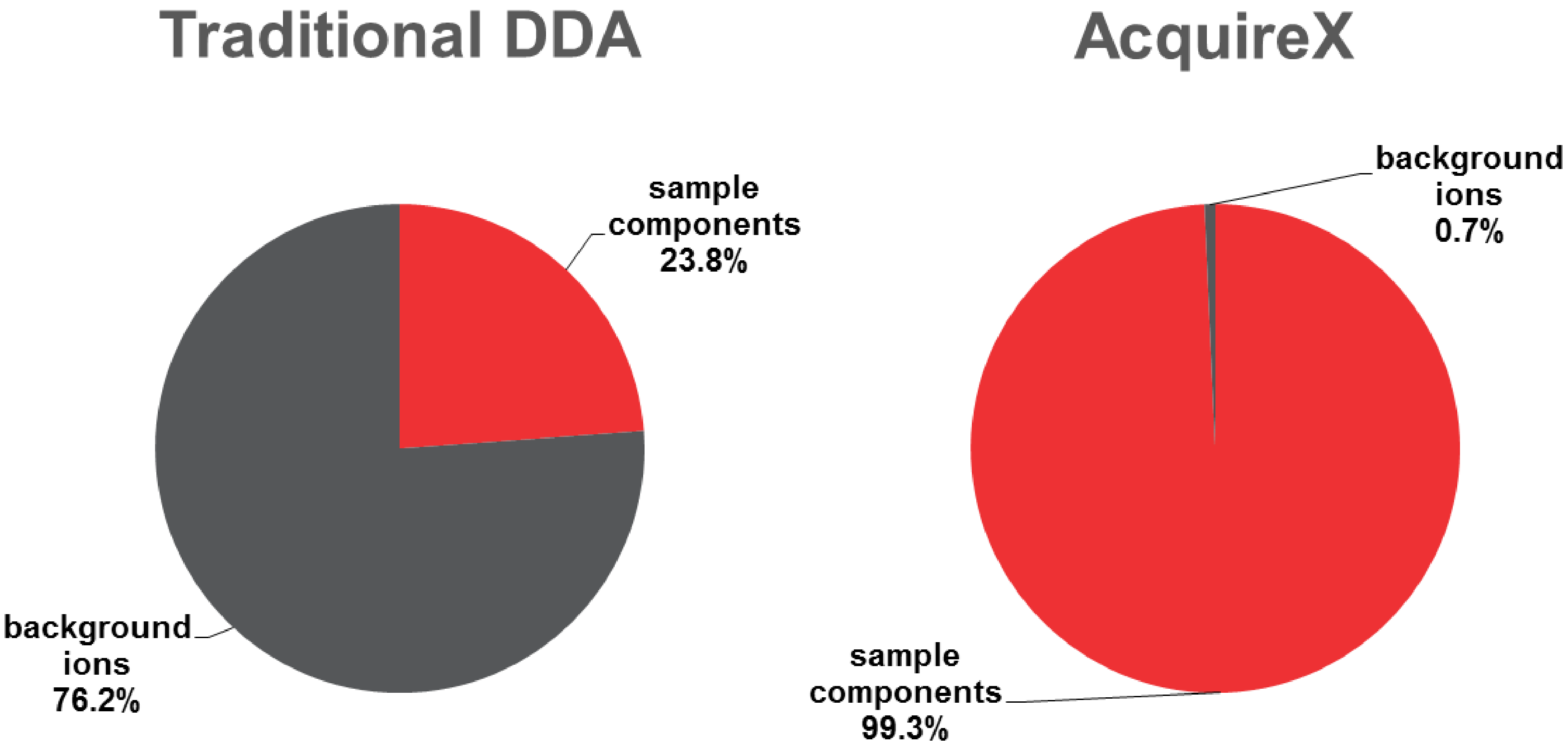
Constant Background Ion

Solvent Blank TIC

Peak-shape Background Ion

Confidently Ignore Background Ions

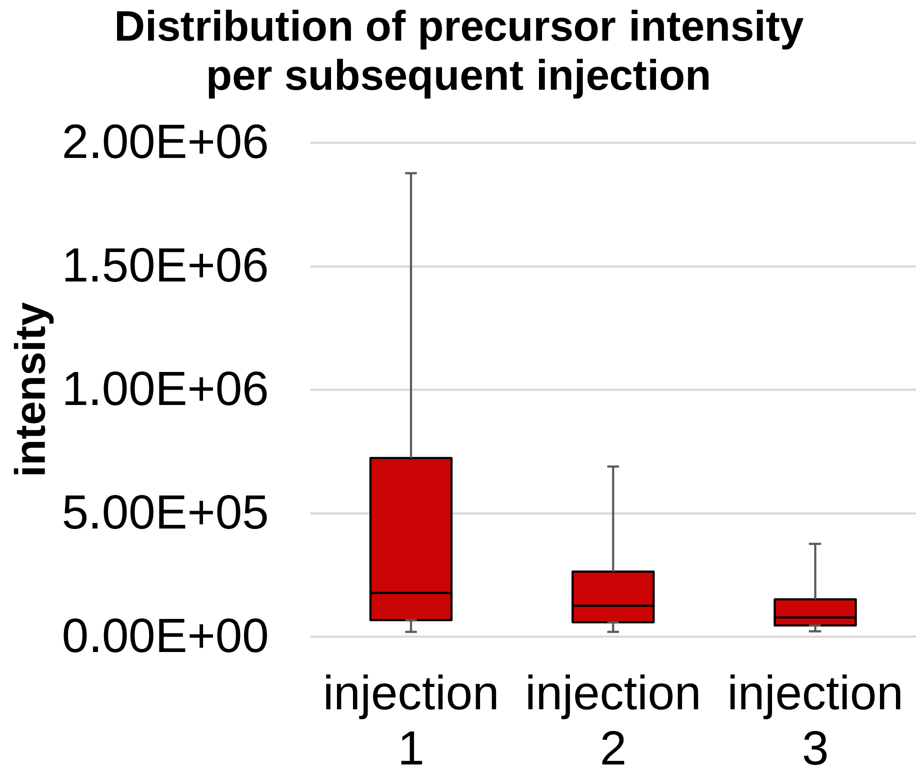
Fragment more true sample components



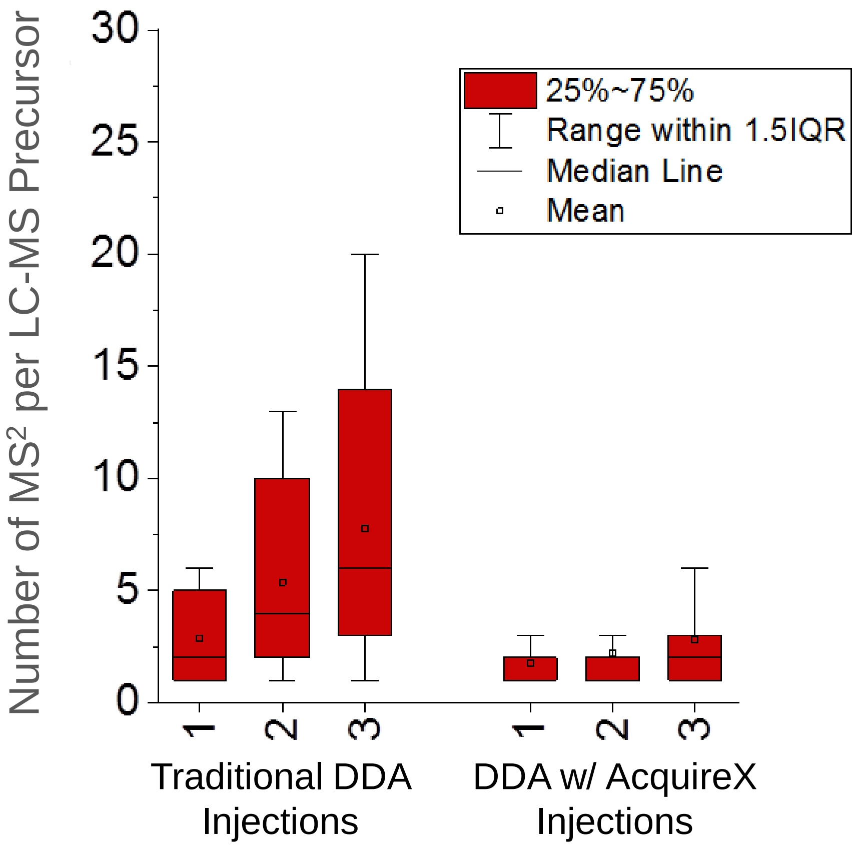
Human plasma (NIST SRM1950), C18, 15min gradient

AcquireX: Deeper Interrogation of Sample

Access precursors of lower abundance…

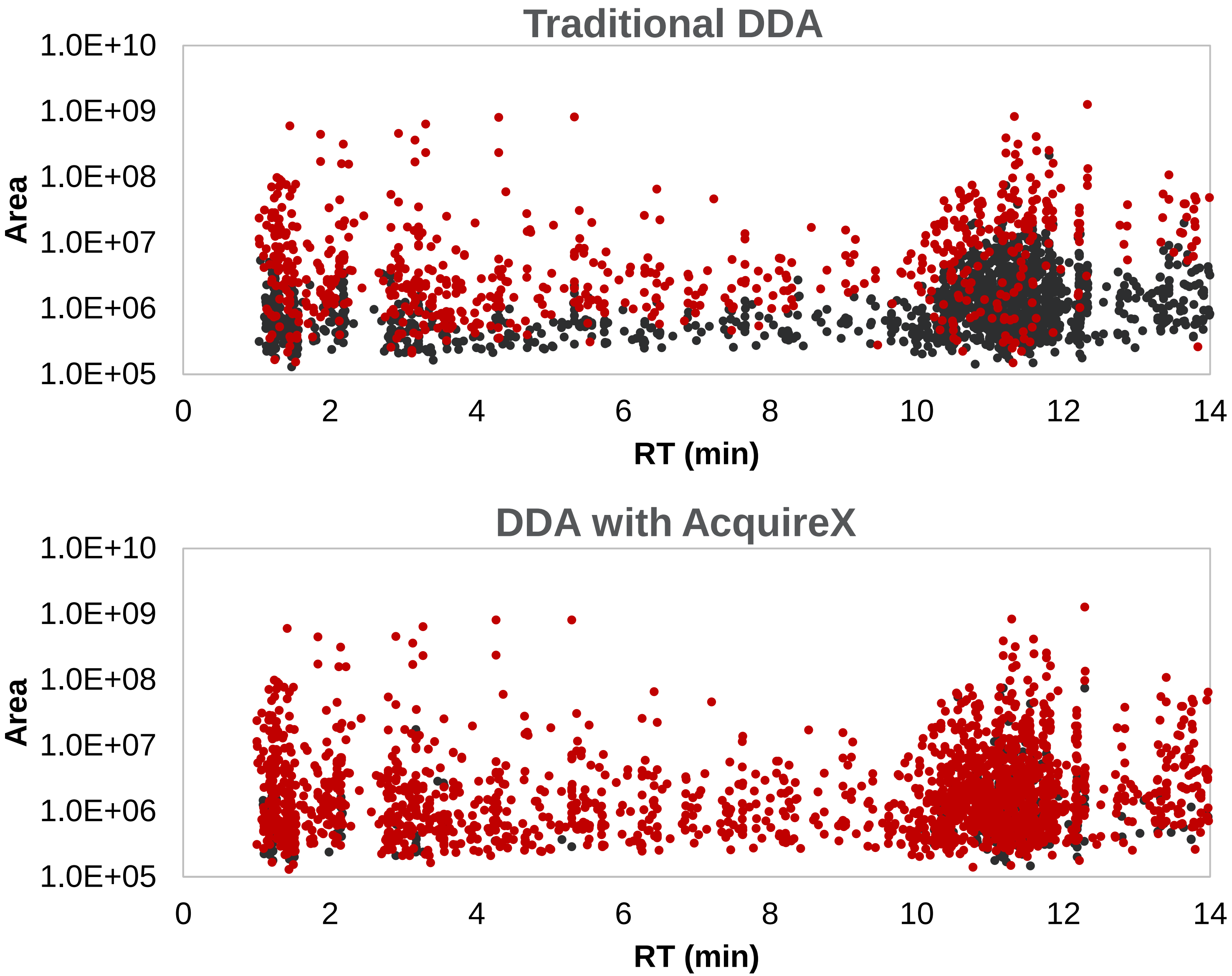


…With Less Redundancy



Human plasma (NIST SRM1950), C18, 15min gradient

Fragment Lower Abundant Peaks



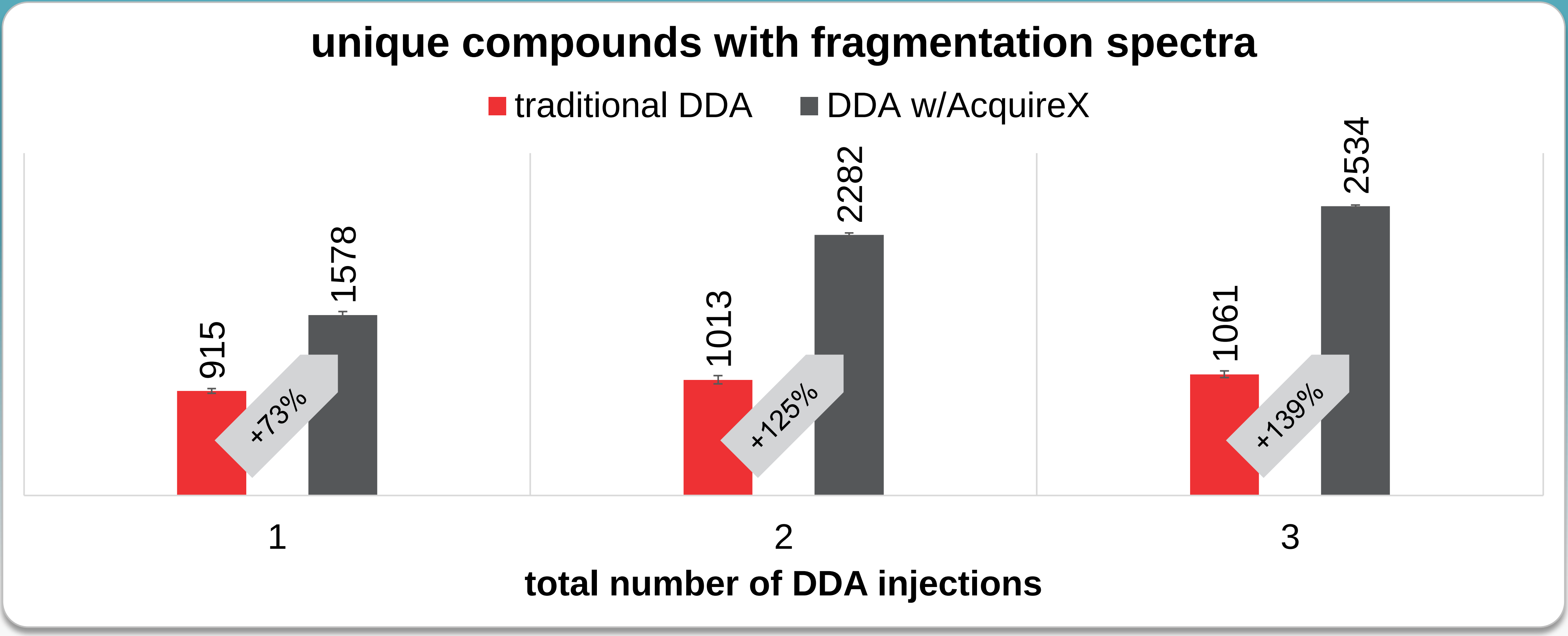
Increased Precursor Sampling Depth

Comparison of traditional DDA and AcquireX shows increased coverage with the AcquireX acquisitions (compounds triggered for MS/MS in red)

Human plasma (NIST SRM1950), C18, 15min gradient

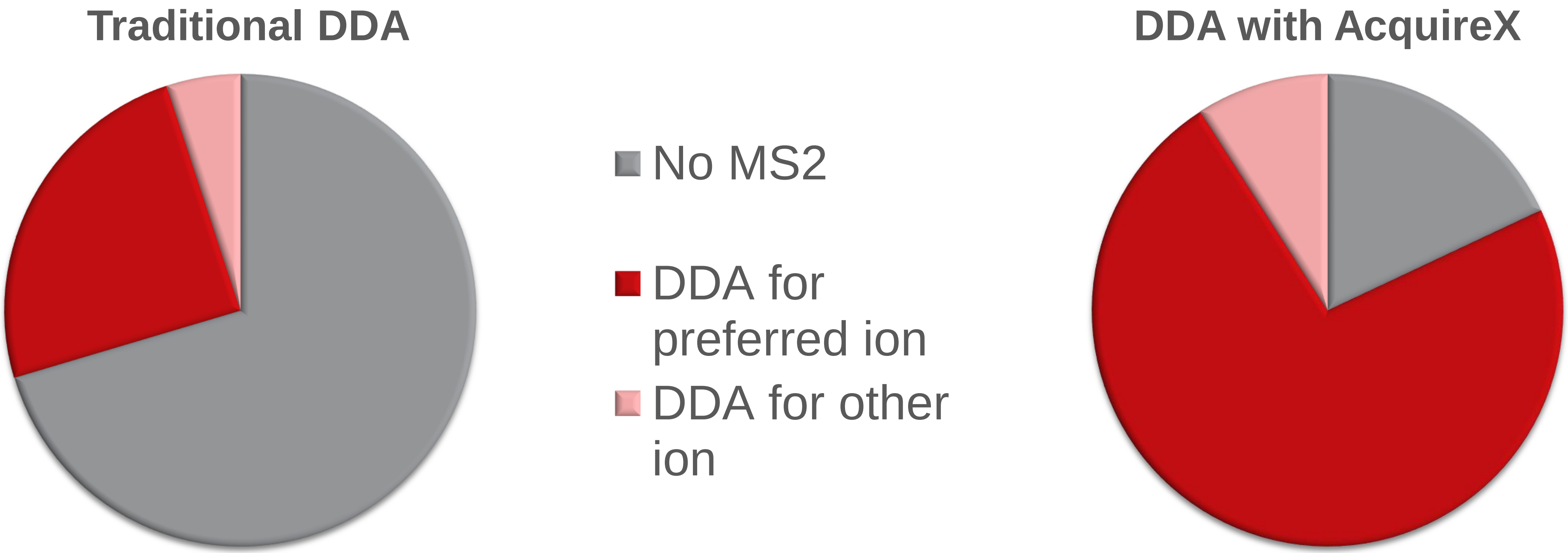
AcquireX – A New Acquisition Paradigm

Collect more meaningful data, not just more data



Human plasma (NIST SRM1950), C18, 15min gradient

Fragmentation Spectra for Sample Relevant Compounds

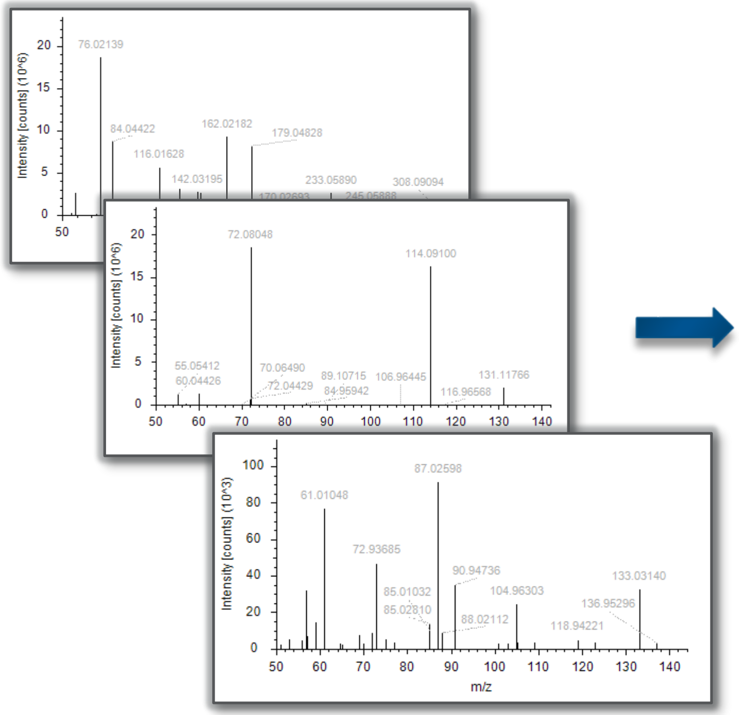


Human plasma (NIST SRM1950), C18, 15min gradient

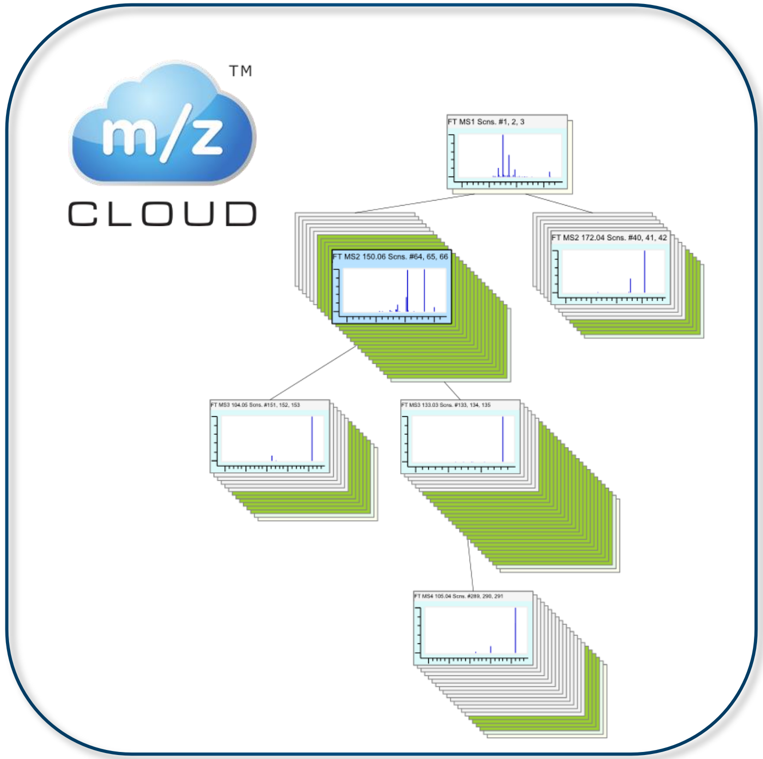
Importance of Fragmentation Spectra and Spectral Libraries

Increase Annotation Confidence

Information-Rich MS/MS & MS^n Spectra



Open-Source & In-House Spectral Libraries



m/z CLOUD™
FT MS1 Scns. #1, 2, 3
FT MS2 150.06 Scns. #64, 65, 66
FT MS2 172.04 Scns. #40, 41, 42
FT MS3 104.05 Scns. #151, 152, 153
FT MS3 133.03 Scns. #133, 134, 135
FT MS4 105.04 Scns. #289, 290, 291

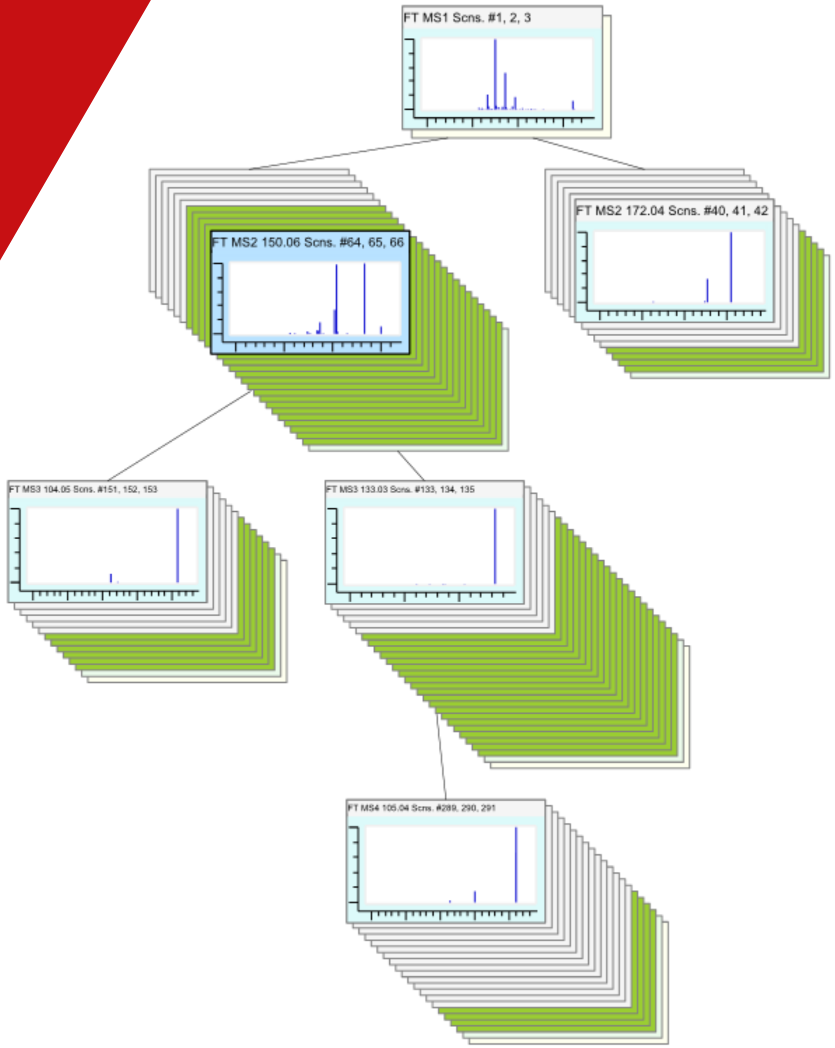
High Quality Untargeted Metabolomics Data

Confirm Targeted Knowns

Annotate Known Unknowns

Annotate Novel Unknown Unknowns

mzCloud™ Spectral Library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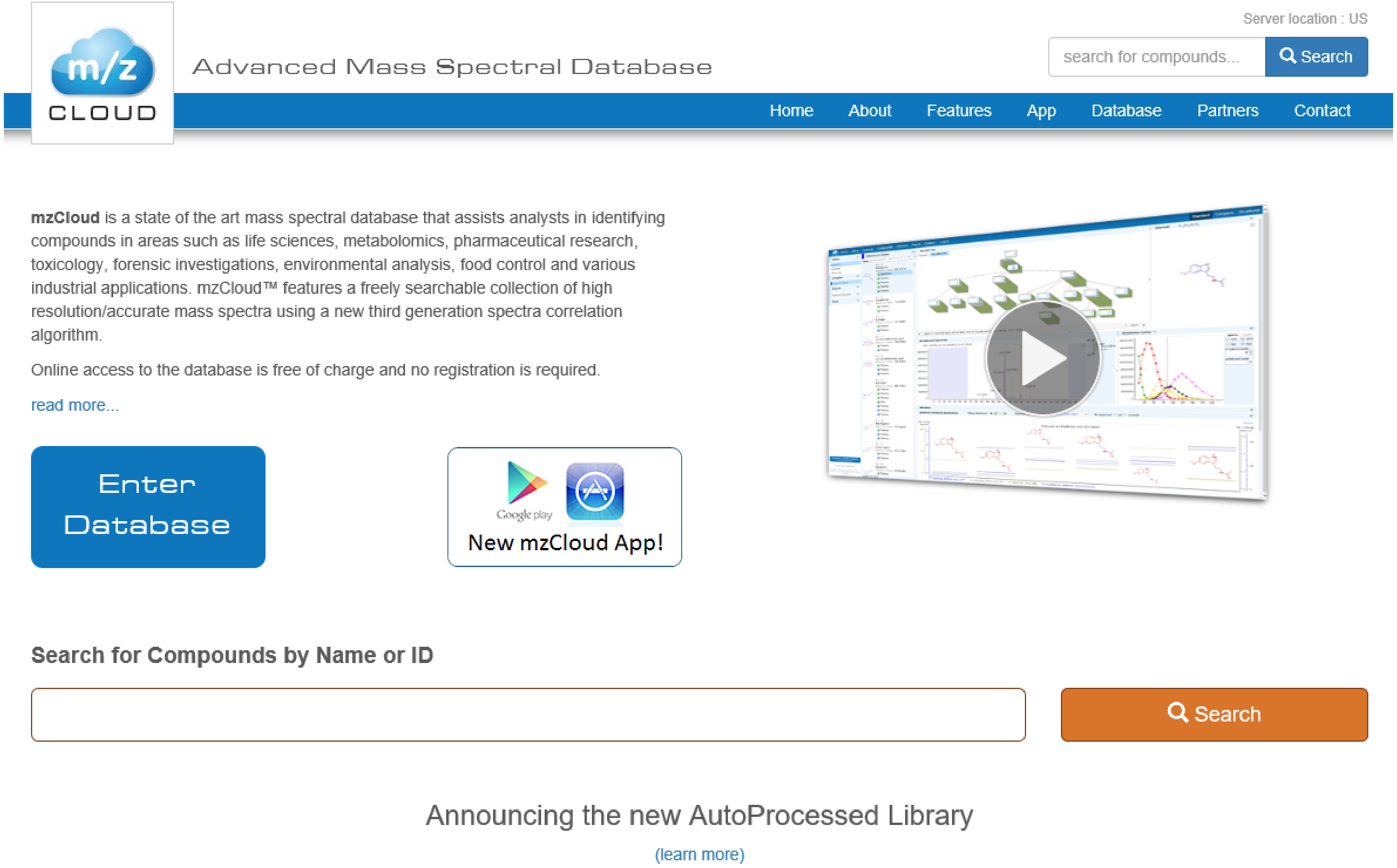
FT MS3 133.03 Scns. #133, 134, 135
FT MS4 105.04 Scns. #289, 290, 291

mzCloud™ Spectral Library


m/z CLOUD
Advanced Mass Spectral Database
Server location : US
search for compounds...
Search
Home
About
Features
App
Database
Partners
Contact
Enter Database
Google play
New mzCloud App!

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

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

read more...

Search for Compounds by Name or ID

Announcing the new AutoProcessed Library

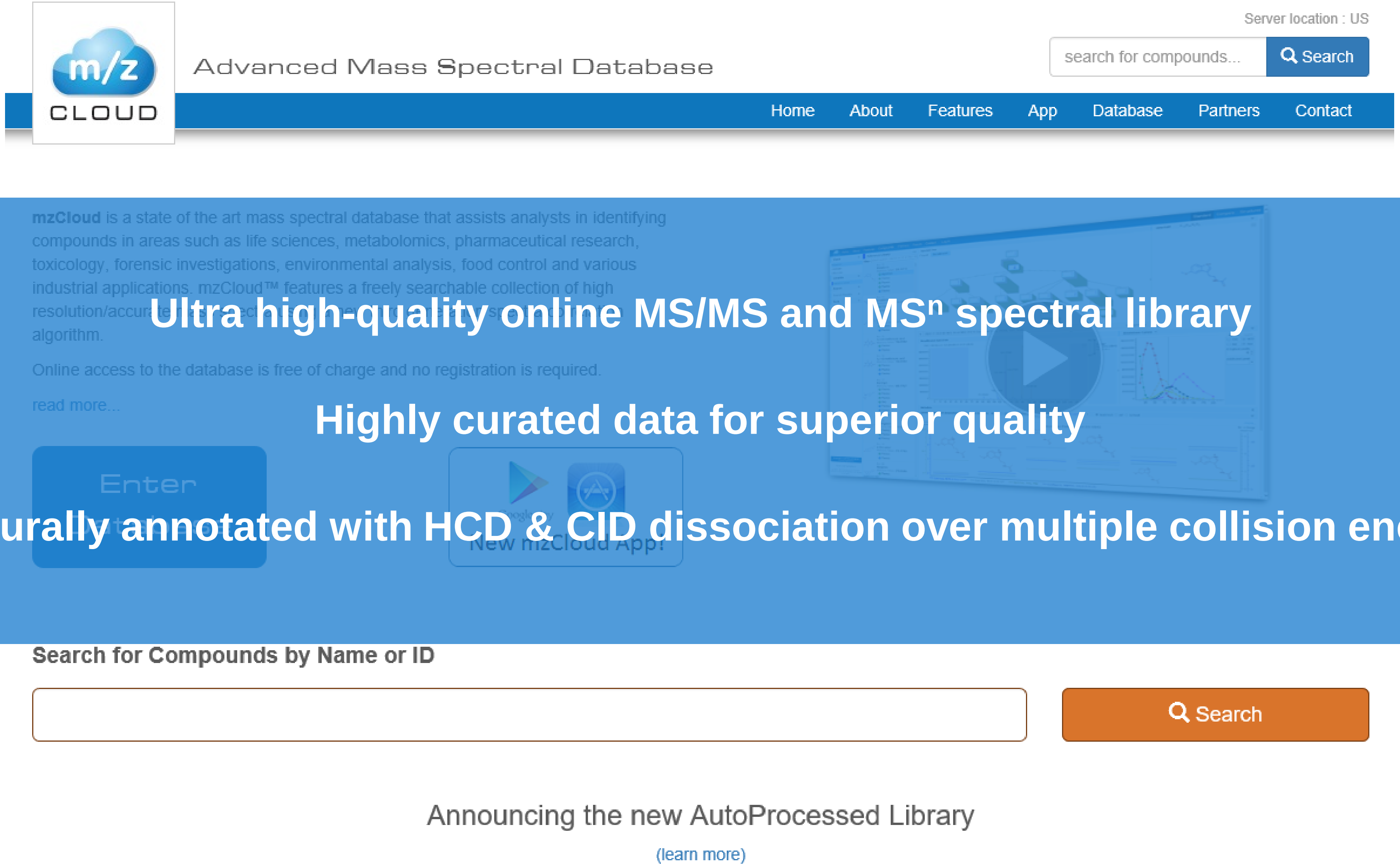
(learn more)

mzCloud™ Spectral Library

Ultra high-quality online MS/MS and MS^n spectral library

Highly curated data for superior quality

Structurally annotated with HCD & CID dissociation over multiple collision energies


m/z CLOUD
Advanced Mass Spectral Database
Server location : US
search for compounds...
Search
Home
About
Features
App
Database
Partners
Contact

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

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

read more...

Enter
New mzCloud App!

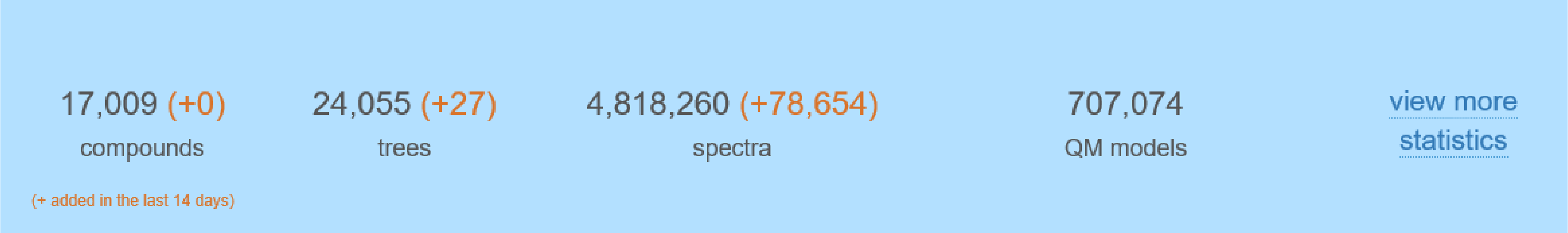
Search for Compounds by Name or ID

Announcing the new AutoProcessed Library

(learn more)

ThermoFisher SCIENTIFIC

mzCloud™ Spectral Library



17,009 (+0)
compounds

24,055 (+27)
trees

4,818,260 (+78,654)
spectra

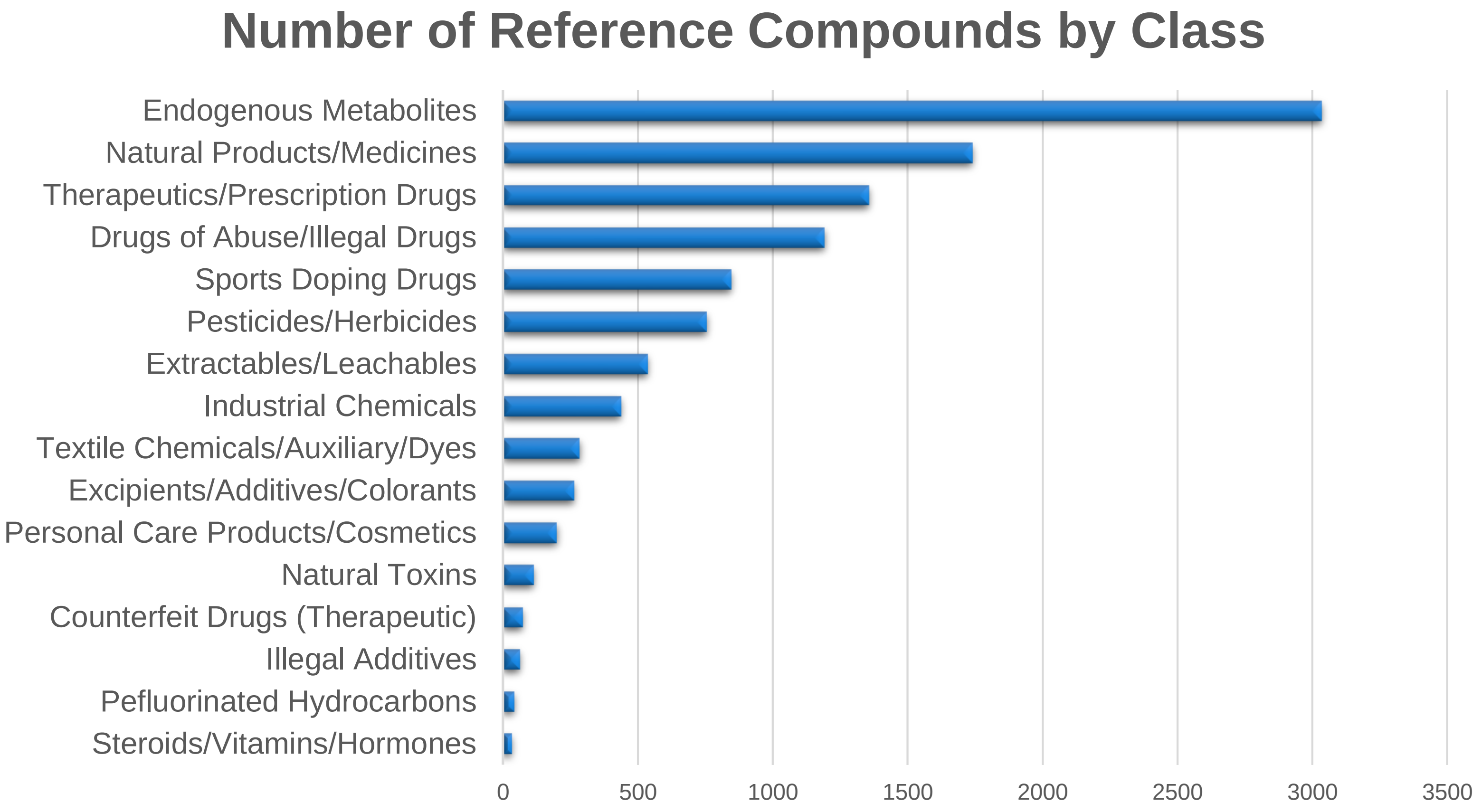
707,074
QM models

view more statistics

(+ added in the last 14 days)

Taken from mzCloud.org on 5/11/2019

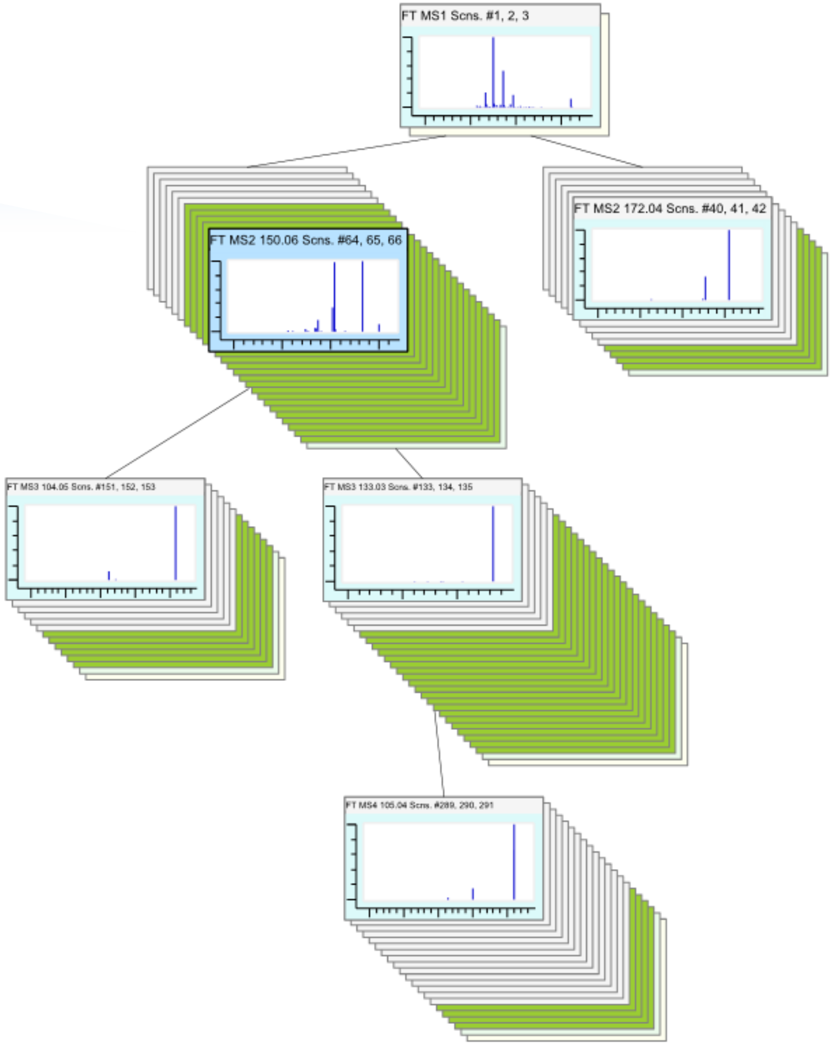
mzCloud™ Spectral Library | Chemical Diversity



Taken from mzCloud.org on 5/11/2019

mzCloud™ Spectral Library | More Structural Information

Professionally Curated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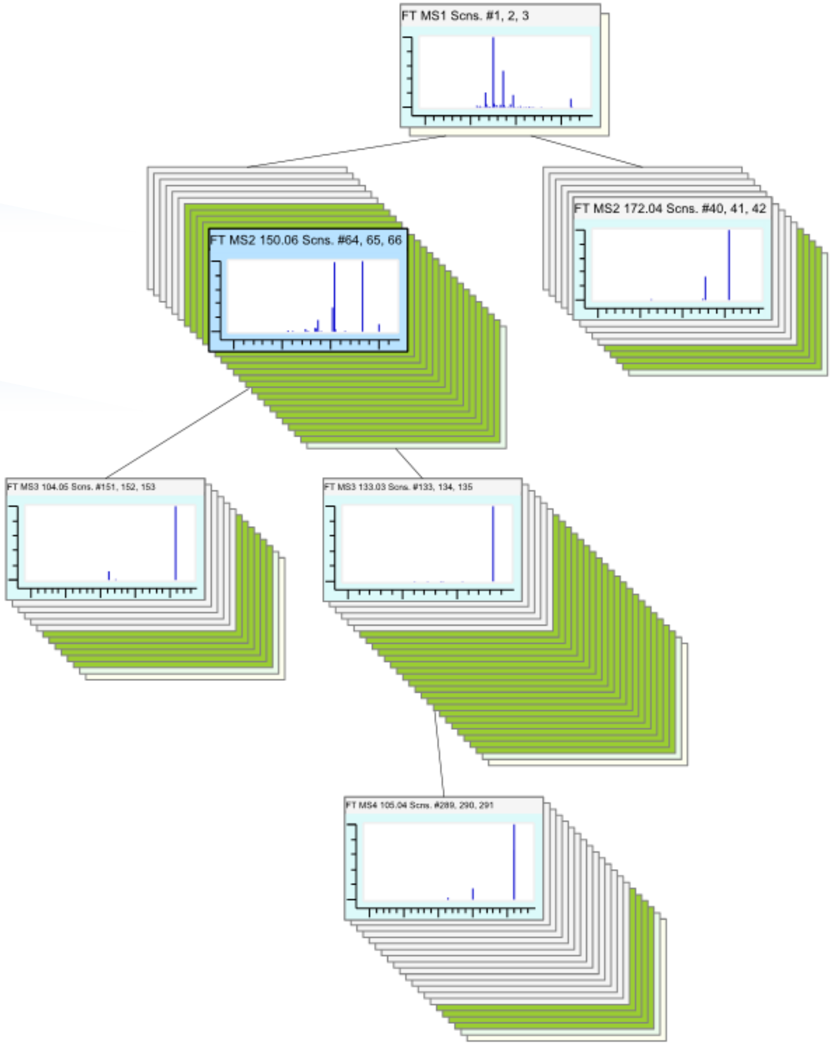
FT MS3 133.03 Scns. #133, 134, 135
FT MS4 105.04 Scns. #289, 290, 291

mzCloud™ Spectral Library | More Structural Information

Professionally Curated

Multi-Stage Fragmentation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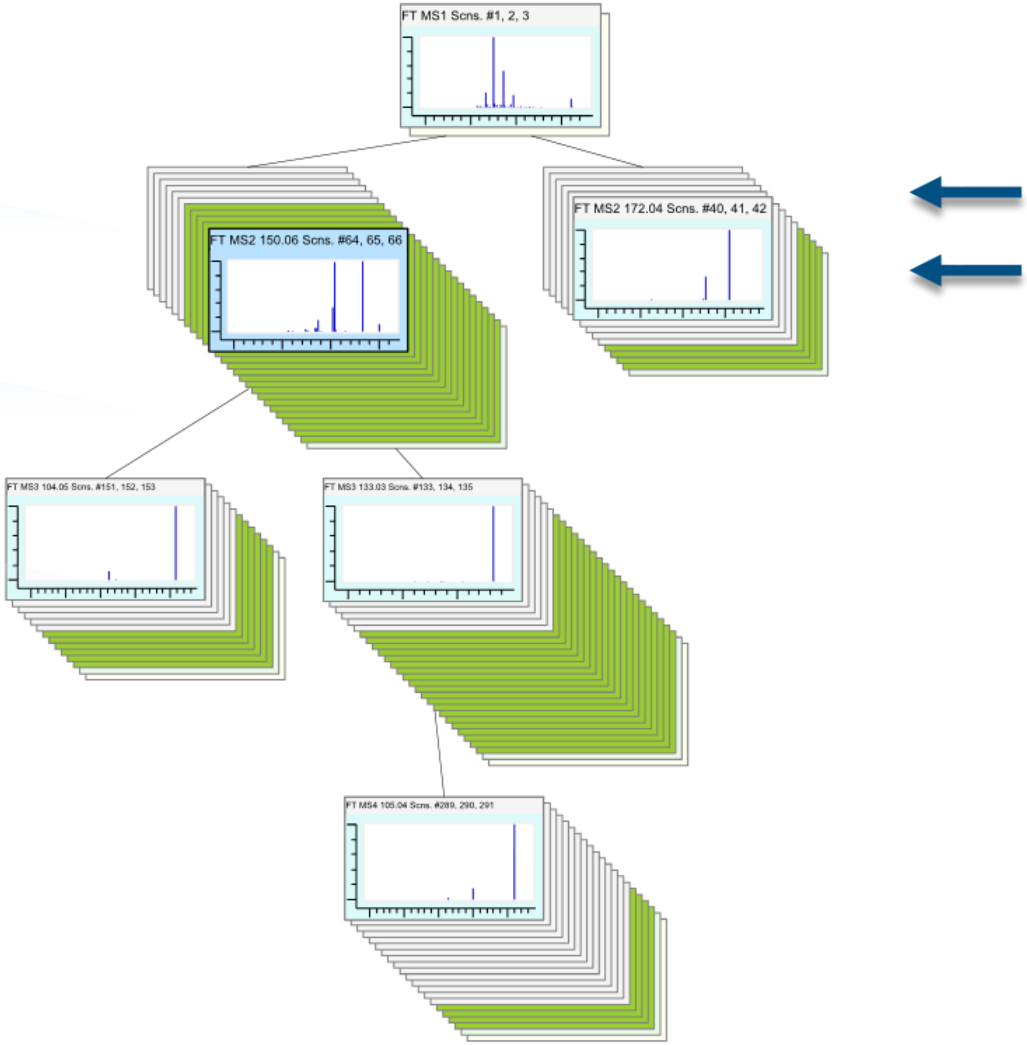
FT MS3 133.03 Scns. #133, 134, 135
FT MS4 105.04 Scns. #289, 290, 291

mzCloud™ Spectral Library | More Structural Information

Professionally Curated

Multi-Stage Fragmentation

HCD/CID Dissociation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FT MS2 150.06 Scns. #64, 65, 66
FT MS2 172.04 Scns. #40, 41, 42
FT MS3 104.05 Scns. #151, 152, 153
FT MS3 133.03 Scns. #133, 134, 135
FT MS4 105.04 Scns. #289, 290, 291

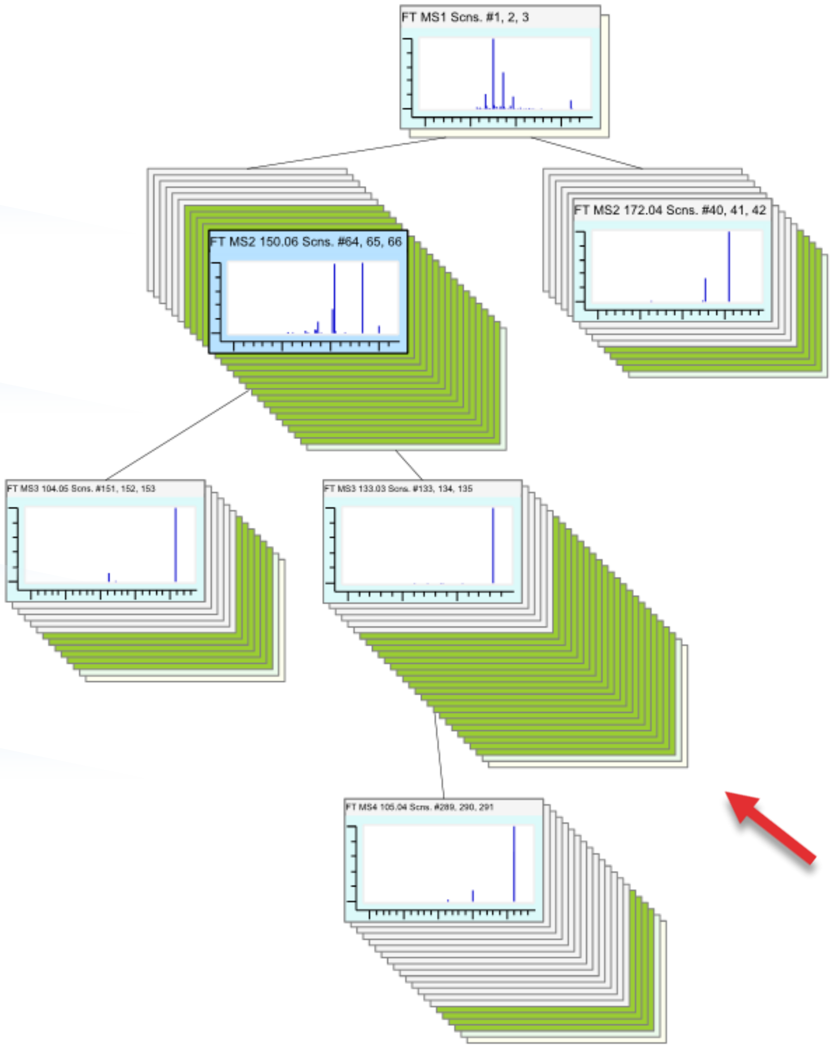
mzCloud™ Spectral Library | More Structural Information

Professionally Curated

Multi-Stage Fragmentation

HCD/CID Dissociation

Multiple Collision Energies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FT MS2 172.04 Scns. #40, 41, 42
FT MS3 104.05 Scns. #151, 152, 153
FT MS3 133.03 Scns. #133, 134, 135
FT MS4 105.04 Scns. #289, 290, 291

mzCloud™ Spectral Library | More Structural Information

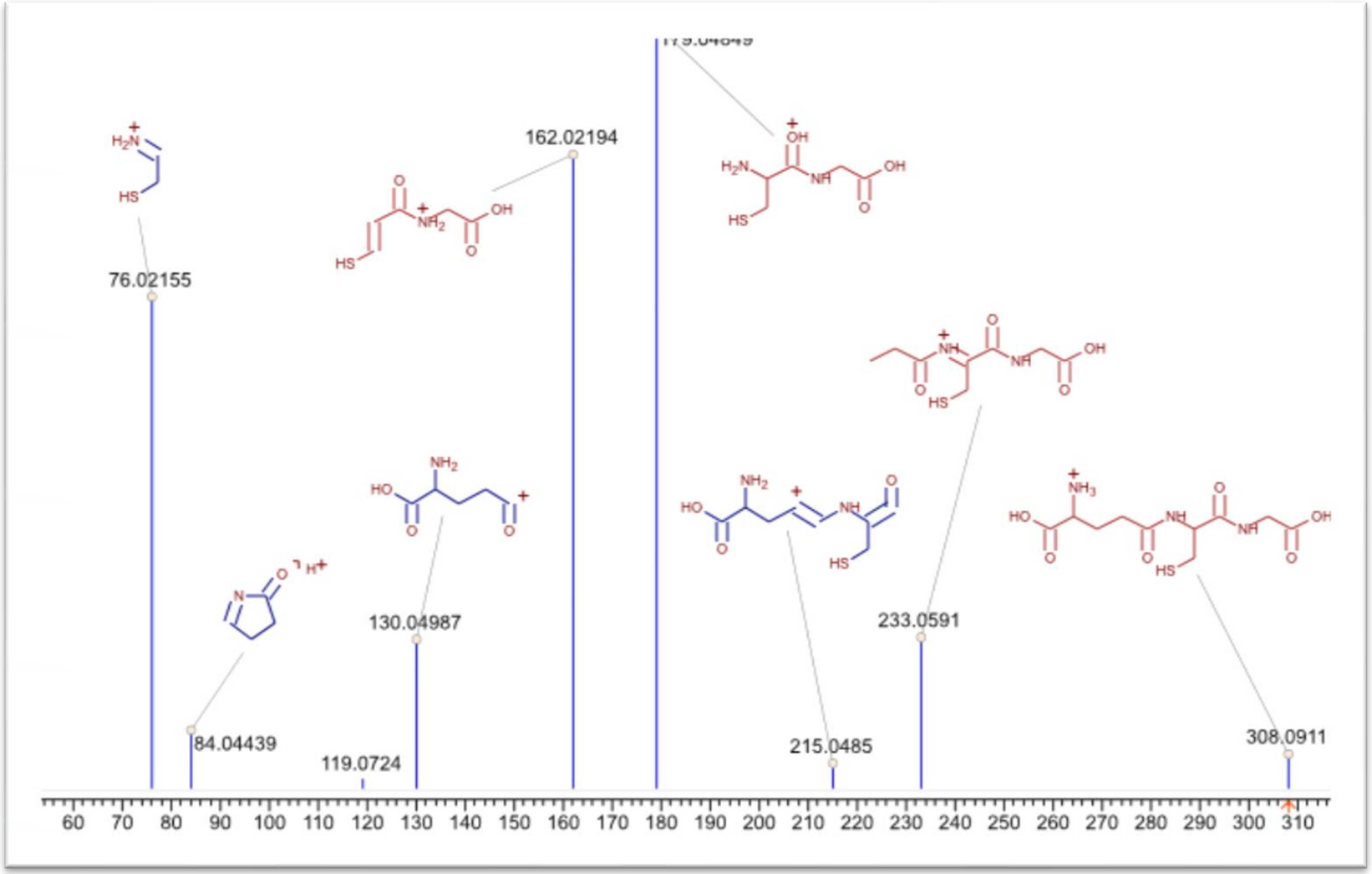
Professionally Curated

Multi-Stage Fragmentation

HCD/CID Dissociation

Multiple Collision Energies

Structural Annotations

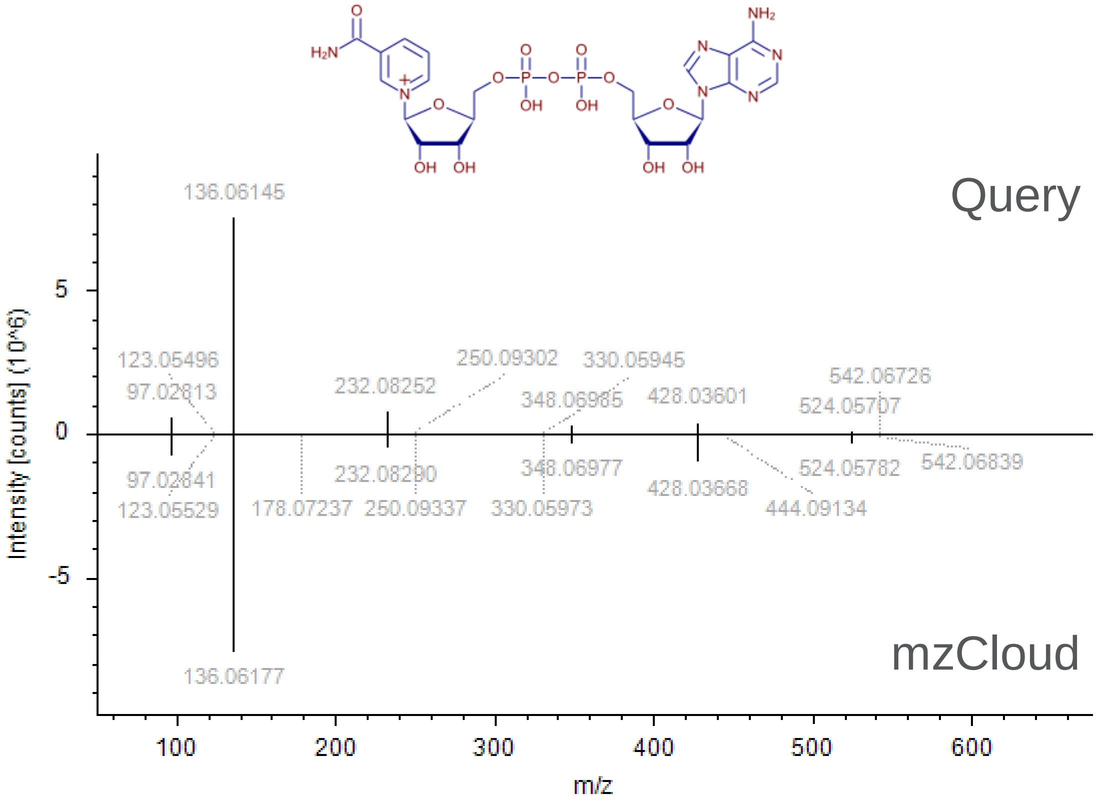


ThermoFisher SCIENTIFIC

Beyond the Identity Match

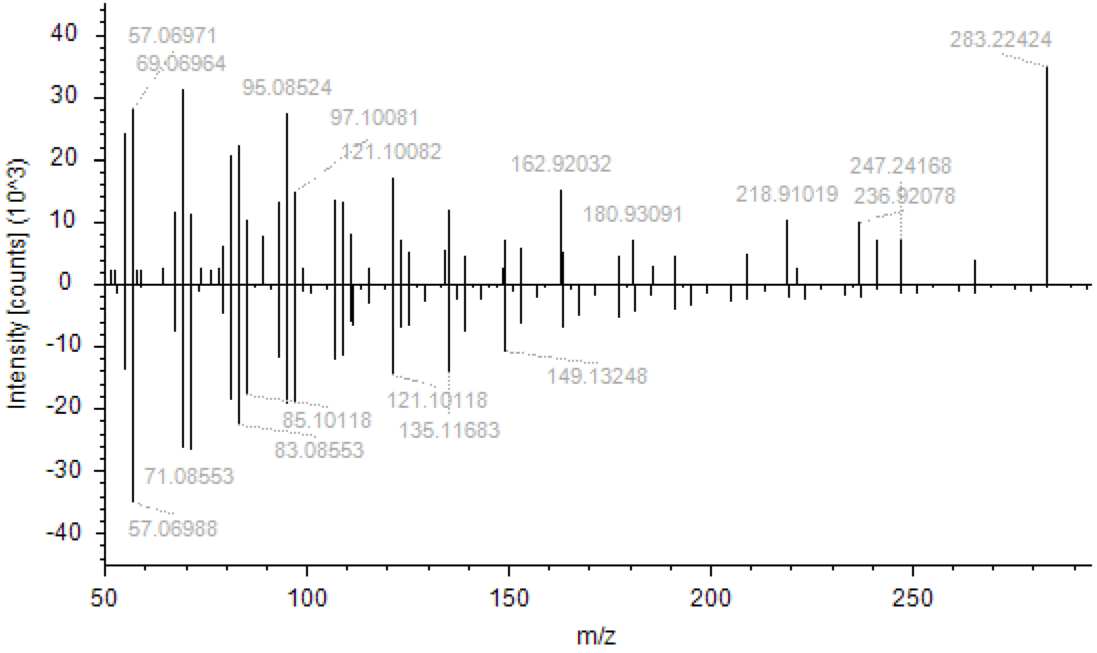
Spectral Similarity to Annotate Structurally Related Compounds

Identity Match for NAD+



Similar to Nervonic Acid

Δ Mass 98.2 Daltons

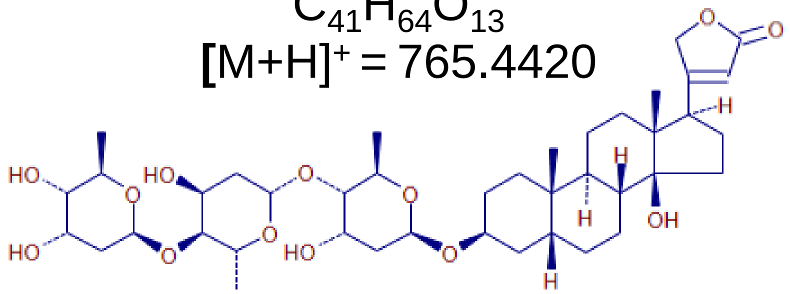


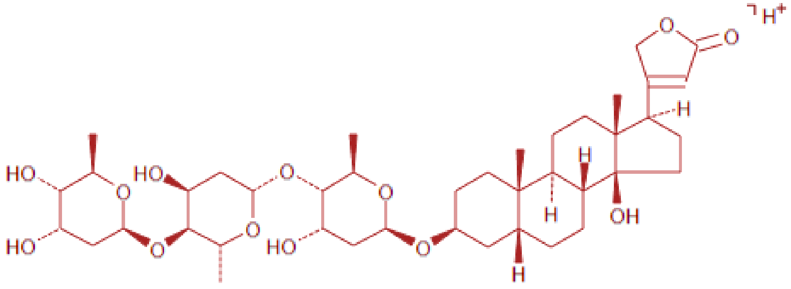
MS^n for More Structural Information

Digitoxin

$C_{41}H_{64}O_{13}$

$[M+H]^+ = 765.4420$

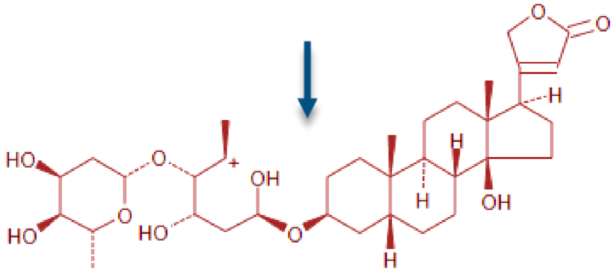




m/z 765.44197

MS

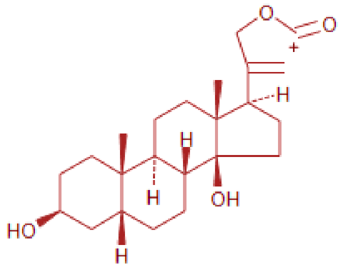
C I D



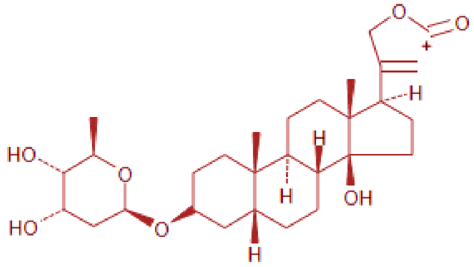
m/z 635.37897

MS^2

C I D



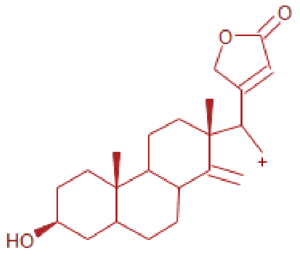
m/z 375.25299



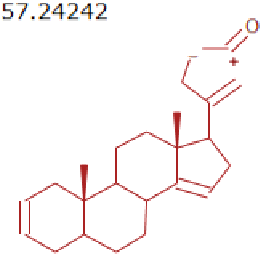
m/z 505.31598

MS^3

C I D



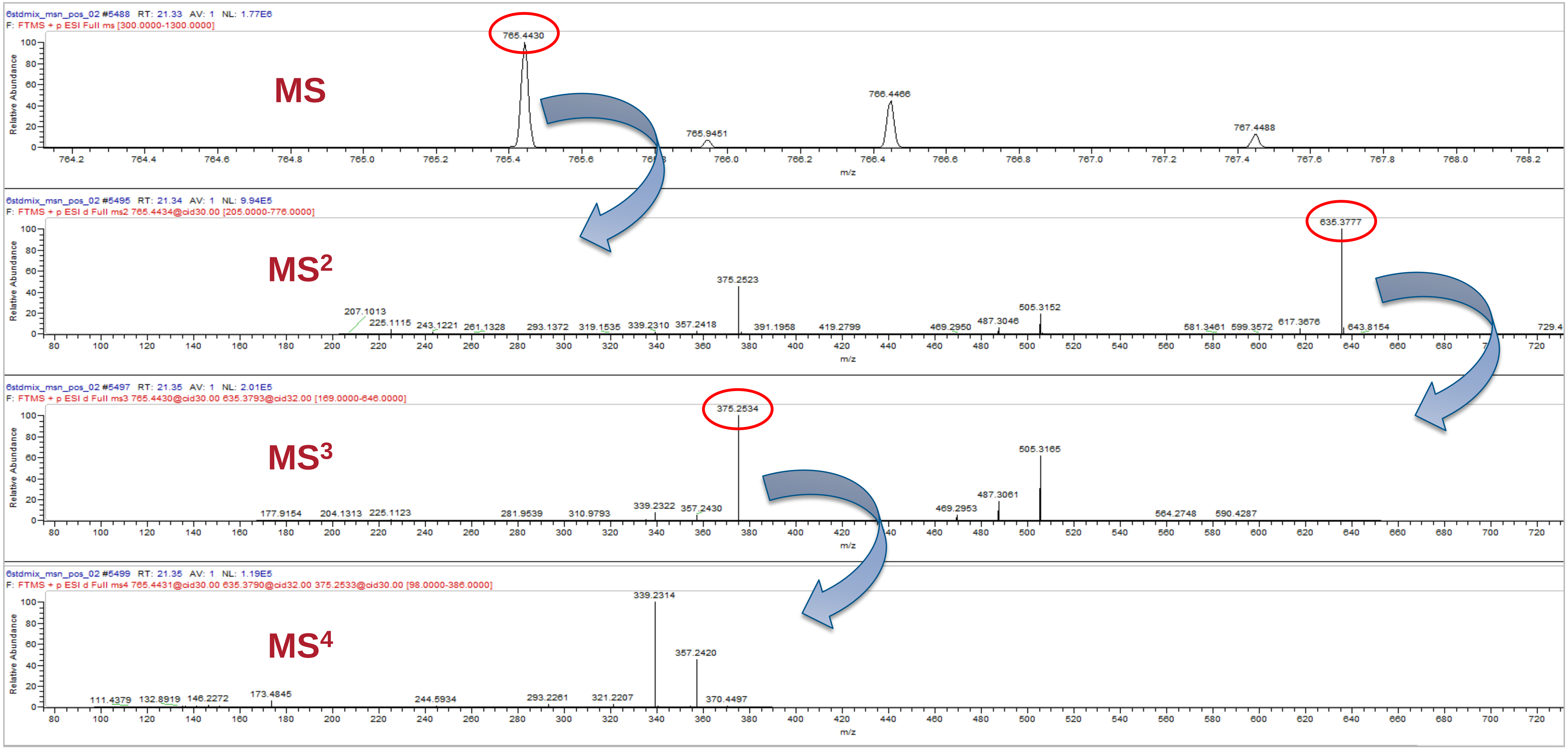
m/z 357.24242



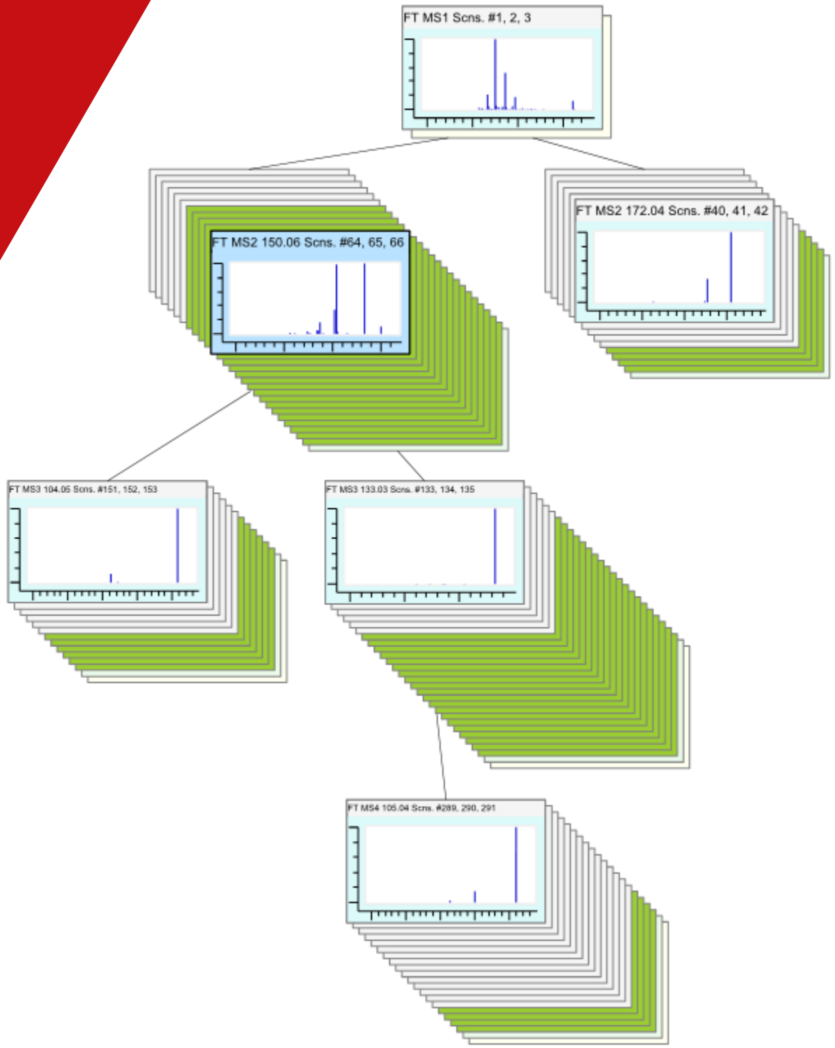
m/z 339.23186

MS^4

MS^n Data Acquisition for Sub-Structure Information



MS^n for Structure-Based Annotation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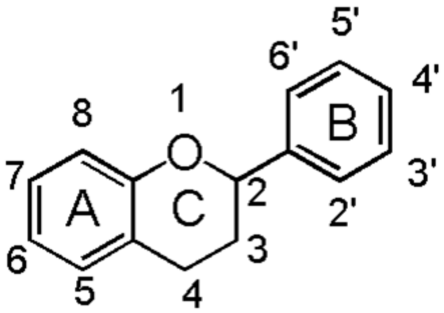
FT MS3 104.05 Scns. #151, 152, 153
FT MS3 133.03 Scns. #133, 134, 135
FT MS4 105.04 Scns. #289, 290, 291

The Chemical Complexity of Flavonoids

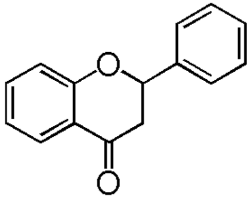
Challenge
Annotate flavonoids with limited available standards & reference spectra


5'
6'
4'
8
1
B
7
O
3'
A
C
2
2'
6
3
5
4

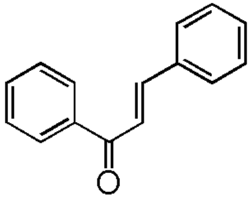
Core Structure

Hydroxylation
Methylation
Acylation
Prenylation
O- and C- Glycolsylation

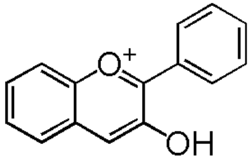
Chemical Modifications



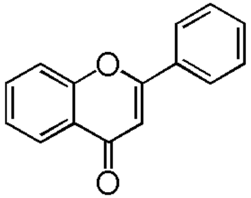
Flavanone



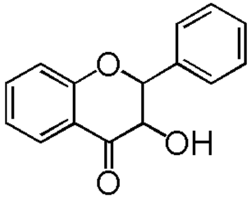
Chalcone



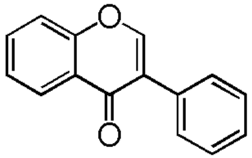
Anthocyanidin



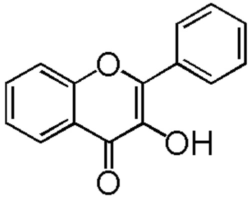
Flavone



Dihydroflavonol



Isoflavone



Flavonol

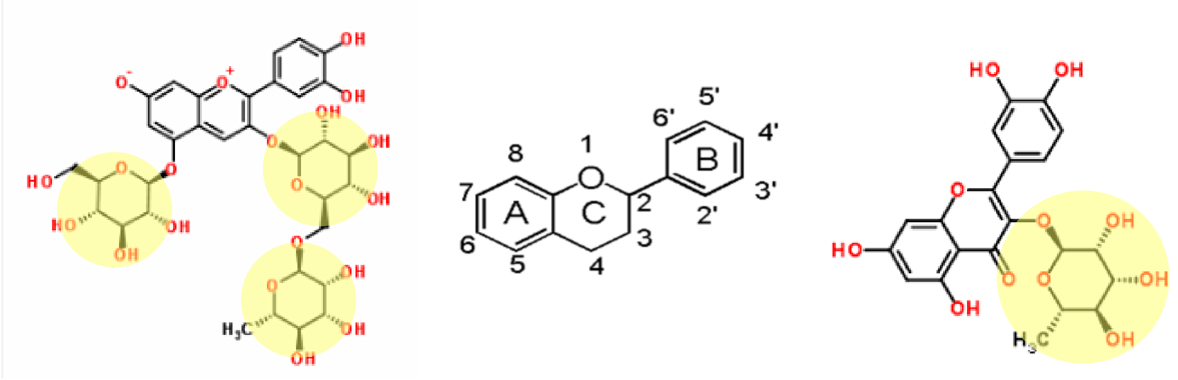
Sub-Classes

>10,000 Flavonoid Species Reported

Class-Informed Approach to Annotate More

Structure-Based Acquisition

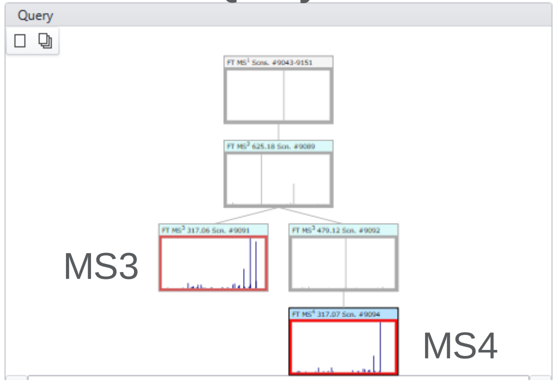
MS^n fragmentation dependent on neutral loss of monosacharide


A
B
C
1
2
3
4
5
6
7
8
2'
3'
4'
5'
6'
HO
OH
H_3C

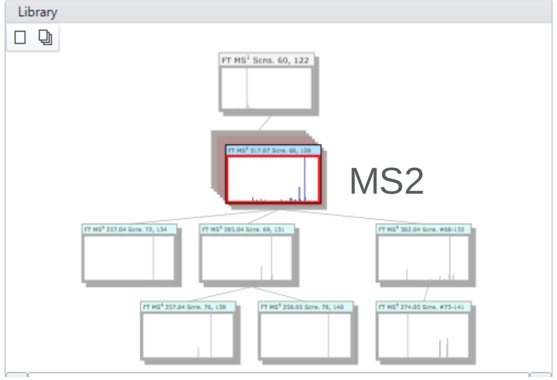
Full & Sub-Structure Search

Detect compounds with flavonoid scaffold

Query

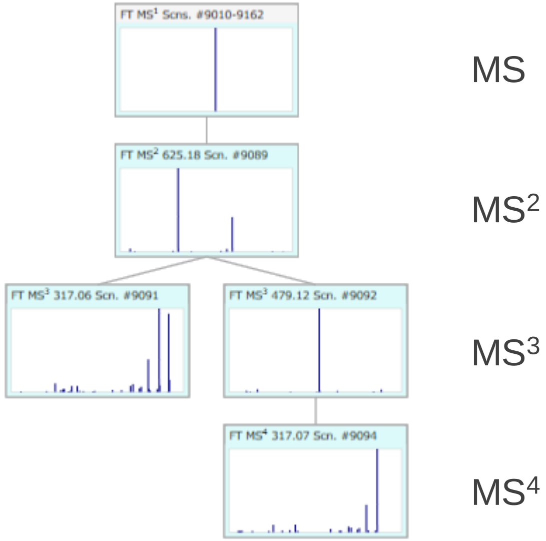

Query
FT MS¹ Scns. #9043-9151
FT MS² 625.18 Scn. #9089
FT MS³ 317.06 Scn. #9091
FT MS³ 479.12 Scn. #9092
FT MS⁴ 317.07 Scn. #9094
MS3
MS4

mzCloud/Custom Library


Library
FT MS¹ Scns. 60, 122
FT MS² 317.07 Scns. 66, 128
MS2

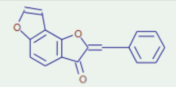
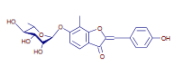
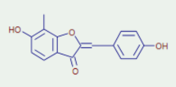
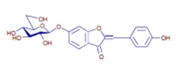
MS^n Spectral Trees

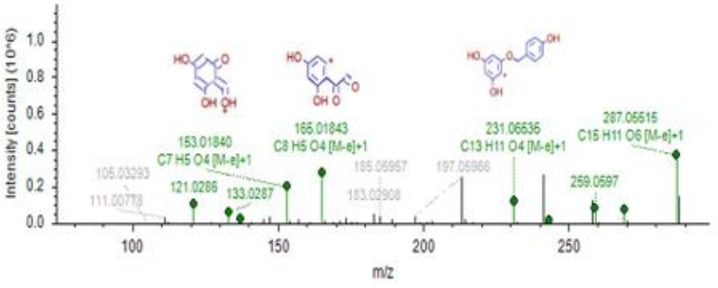
Generate more spectral information to detect related compounds


FT MS¹ Scns. #9010-9162
FT MS² 625.18 Scn. #9089
FT MS³ 317.06 Scn. #9091
FT MS³ 479.12 Scn. #9092
FT MS⁴ 317.07 Scn. #9094
MS
MS²
MS³
MS⁴

Compound Annotation

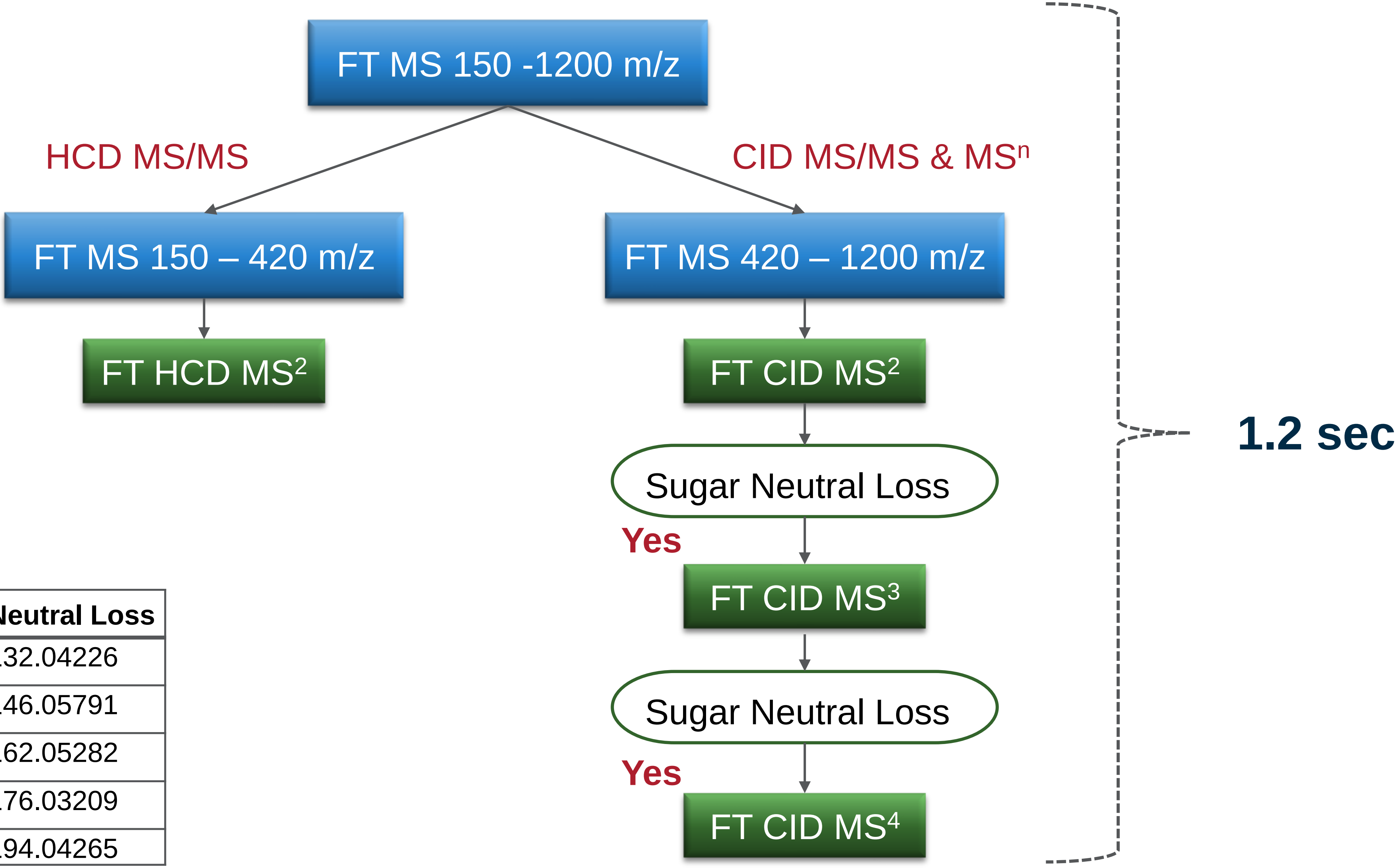
Structure database and structure ranking tools

	Furano [2",3":6,7] aurone
	6,4'-Dihydroxy-7-methylaurone 6-rhamnoside
	FL1A1AGM0001_a
	Hispidol 6-glucoside



Class Informed Data Acquisition

Neutral Loss Dependent MS^n


FT MS 150 -1200 m/z

HCD MS/MS

CID MS/MS & MS^n

FT MS 150 – 420 m/z

FT MS 420 – 1200 m/z

FT HCD MS^2

FT CID MS^2

Sugar Neutral Loss

Yes

FT CID MS^3

Sugar Neutral Loss

Yes

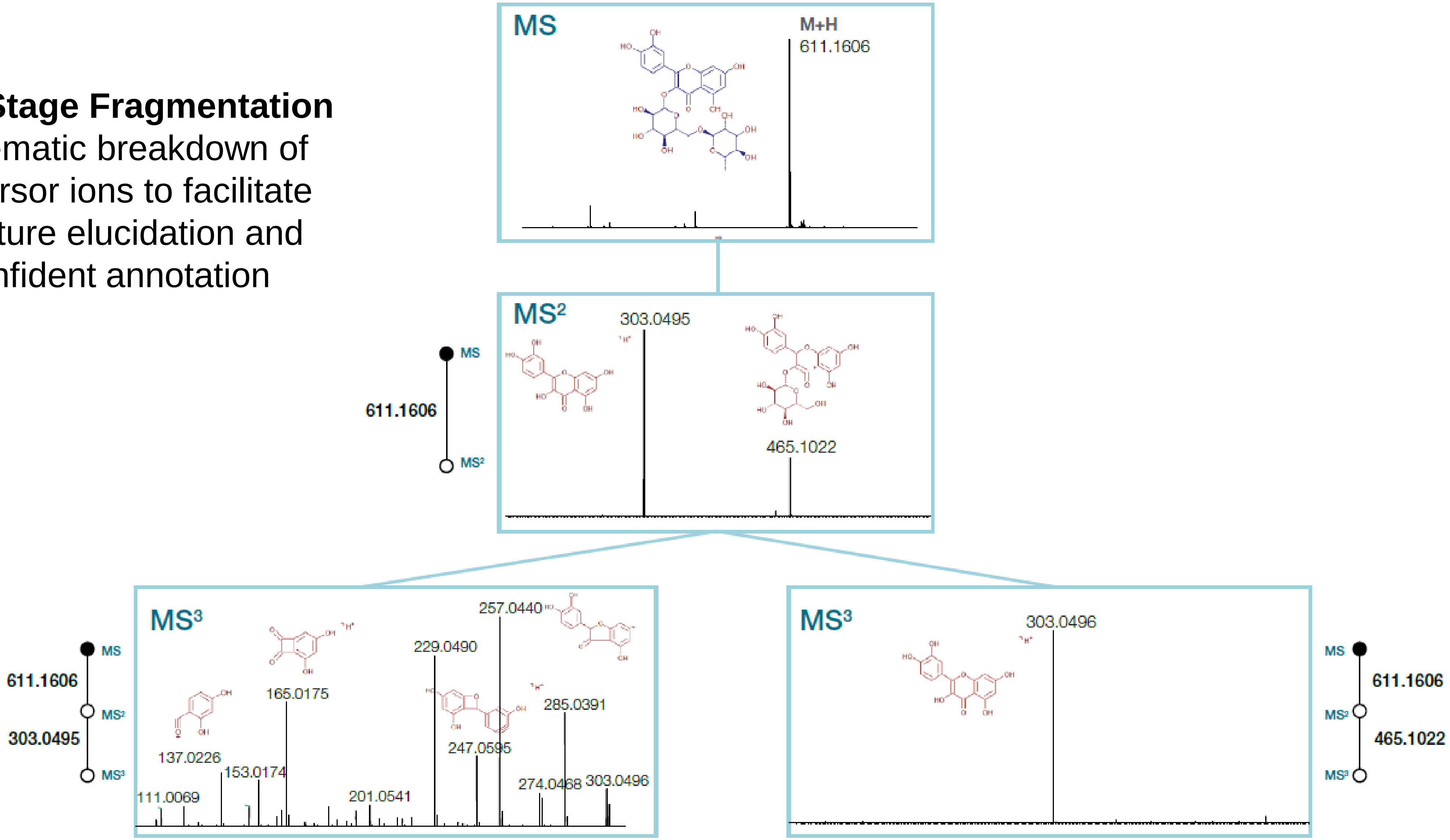
FT CID MS^4

1.2 sec

Saccharide	**Neutral Loss**
Pentose (xylose, arabinose)	132.04226
Deoxyhexose (rhamnose)	146.05791
Hexose (glucose, galactose)	162.05282
Glucuronide	176.03209
Glucuronic acid	194.04265

Flavonoid-Based MS^n Spectral Tree

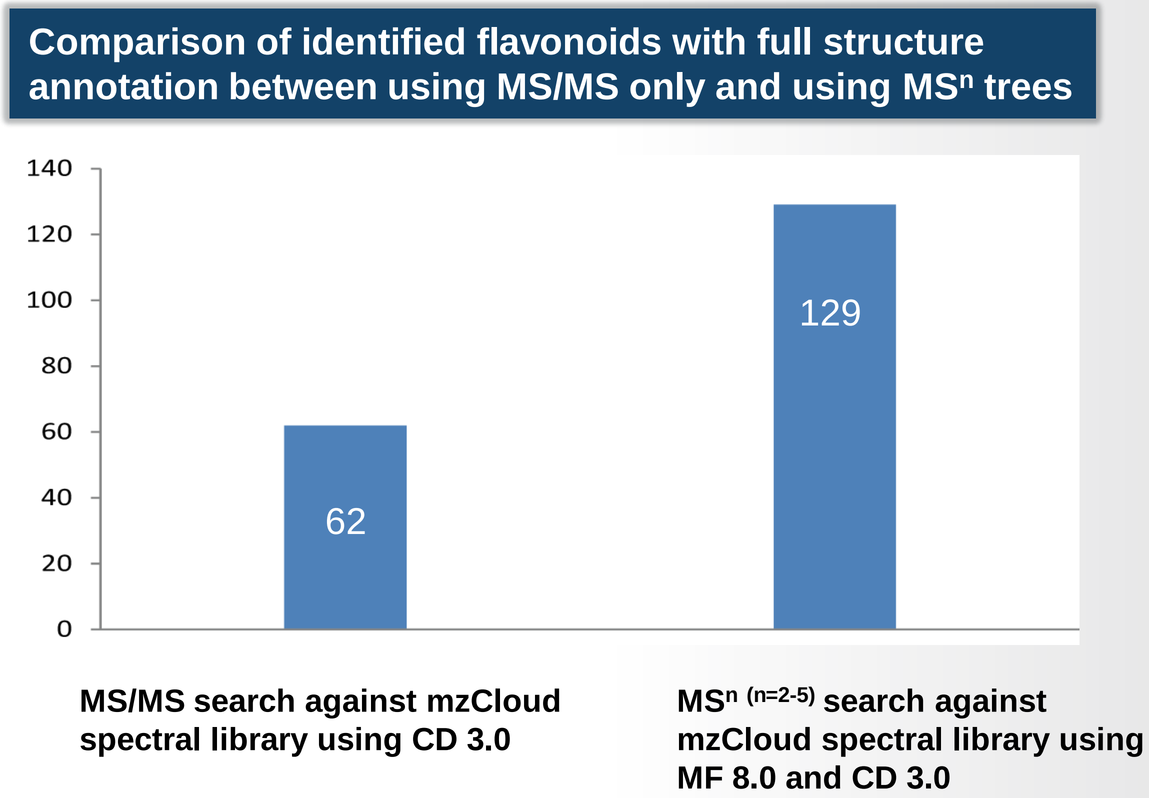
Multi-Stage Fragmentation
Systematic breakdown of precursor ions to facilitate structure elucidation and confident annotation



Flavonoid Annotation in Juice Samples

kale blazer
Naked
red rhapsody
odwalla
berries gomega
odwalla

- Three fruit juices purchased from Safeway store
- Samples filtered, methanol diluted, injected as duplicate on Orbitrap ID-X Tribrid
- Two times more flavonoids are confidently annotated using MS^n than MS/MS only

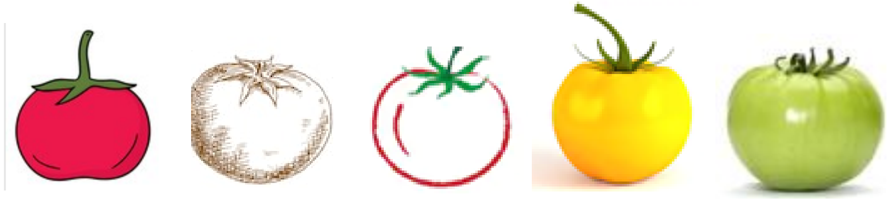

Comparison of identified flavonoids with full structure annotation between using MS/MS only and using MS^n trees

Flavonoid Annotation for Tomato Research

Q: Do flavonoids impact tomato produce?

Dr. Sheng Zhang
Dr. Jocelyn Rose

Flavonoid-Based MS^n Acquisition on Tomato Peel & Cuticle Tissues

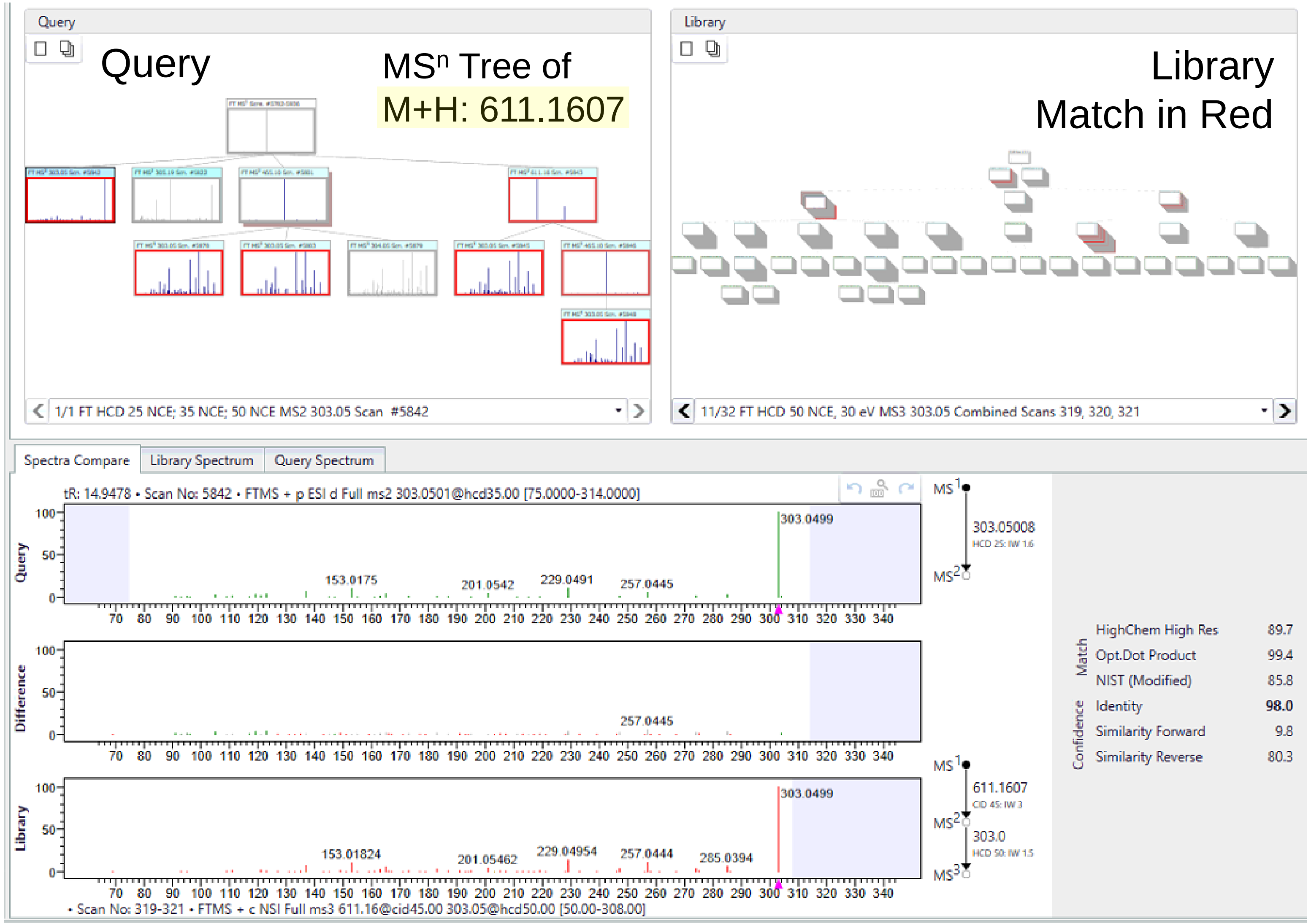


Orbitrap ID-X Tribrid MS

More Flavonoid Annotations to Drive Biology

- 562 flavonoid compounds annotated (487 known structures)
- 75 novel “unknown unknown” compounds
- 13 novel compounds manually annotated for structure using MS^n will be purified for confirmation by NMR
- Profiling shows concentration of most flavonoids ↑ in peel yet some novel flavonoids are ↑ in cuticle
- Flavonoids with additional sugar moieties exclusively in peel

Exact MS^n Tree Match for Rutin



Query

MS^n Tree of M+H: 611.1607

Library Match in Red

1/1 FT HCD 25 NCE; 35 NCE; 50 NCE MS2 303.05 Scan #5842

11/32 FT HCD 50 NCE, 30 eV MS3 303.05 Combined Scans 319, 320, 321

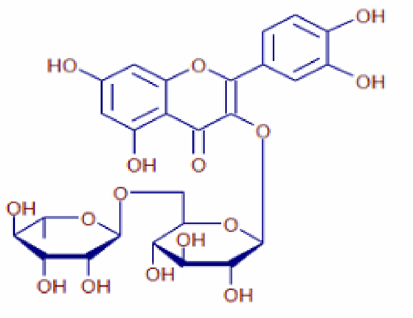
tR: 14.9478 • Scan No: 5842 • FTMS + p ESI d Full ms2 303.0501@hcd35.00 [75.0000-314.0000]

• Scan No: 319-321 • FTMS + c NSI Full ms3 611.16@cid45.00 303.05@hcd50.00 [50.00-308.00]

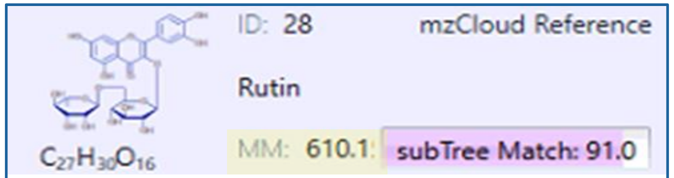
Match	HighChem High Res	89.7
	Opt.Dot Product	99.4
	NIST (Modified)	85.8
Confidence	Identity	**98.0**
	Similarity Forward	9.8
	Similarity Reverse	80.3

Query
Library
Spectra Compare
Library Spectrum
Query Spectrum
Query
Difference
Library
100
50
0
303.0499
153.0175
201.0542
229.0491
257.0445
257.0445
303.0499
153.01824
201.05462
229.04954
257.0444
285.0394
70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340
MS1
303.05008
HCD 25: IW 1.6
MS2
MS1
611.1607
CID 45: IW 3
MS2
303.0
HCD 50: IW 1.5
MS3

Full structure match of query compound M+H: 611.1607



HO
OH
OH
O
OH
O
O
OH
O
OH
O
OH OH
OH
OH
O
OH



ID: 28

mzCloud Reference

Rutin

$C_{27}H_{30}O_{16}$

MM: 610.1

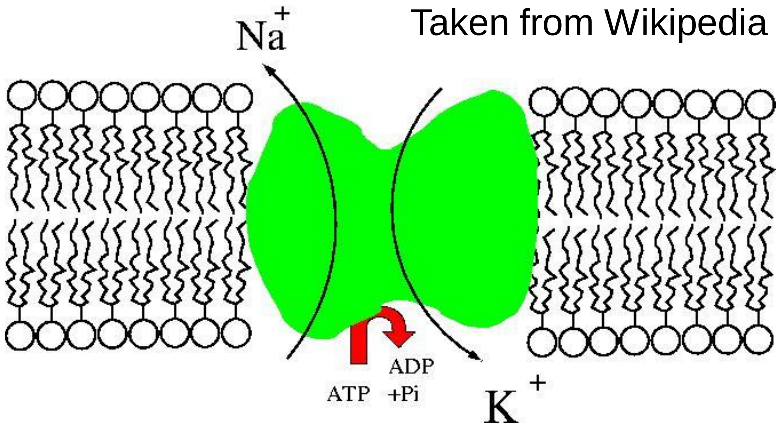
subTree Match: 91.0

Structure of library reference

Class Informed MS^n for Endogenous Cardiac Steroids

Cerebral spinal fluid

Endogenous cardiac steroids as inhibitors of the sodium-potassium ATPase pump



Na^+
ADP
ATP +Pi
K^+

Taken from Wikipedia

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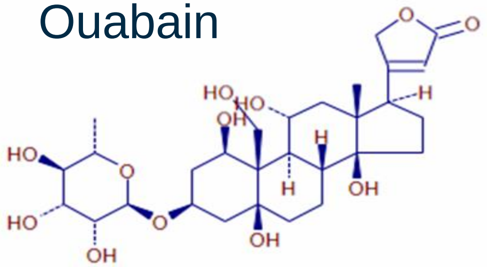
Dr. Michael G. Harrington
Dr. Alfred N. Fonteh

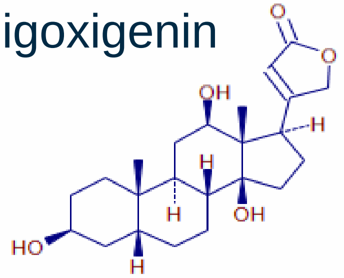
L|E|C|O|M
LAKE ERIE COLLEGE OF OSTEOPATHIC MEDICINE

Dr. Roger G. Biringer

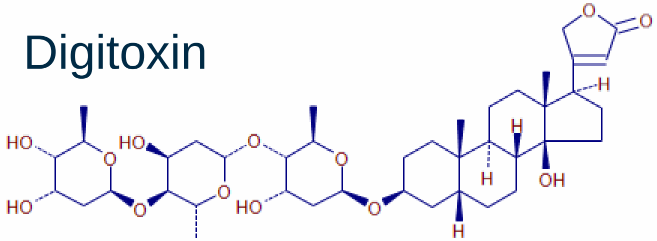
Ouabain

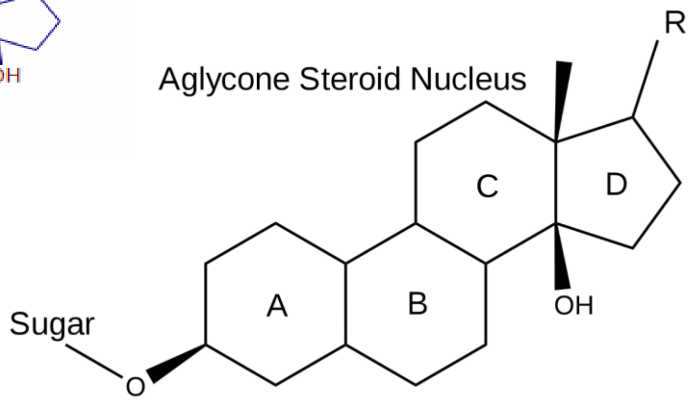


Digoxigenin



Digitoxin

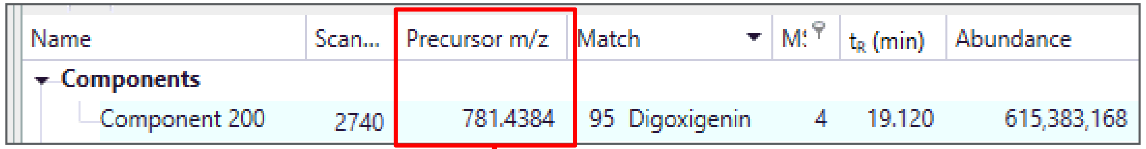




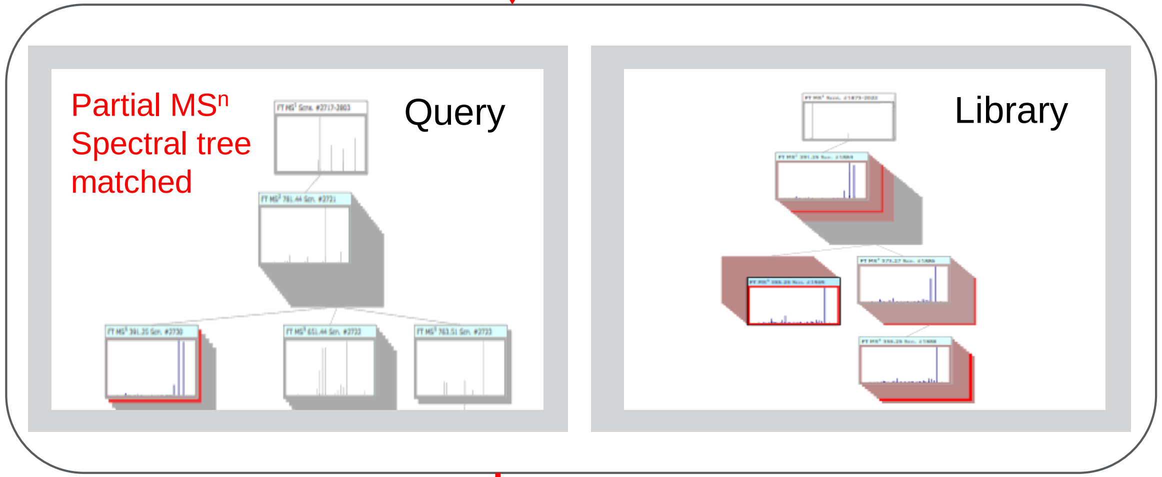
Aglycone Steroid Nucleus
R
A
B
C
D
OH
Sugar
O

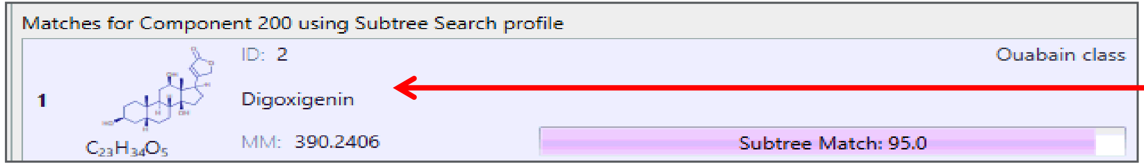
Orbitrap ID-X Tribrid MS

Sub-Structure Annotation for Cardiac Steroids



Name	Scan...	Precursor m/z	Match	M!	t_R (min)	Abundance
Components						
Component 200	2740	781.4384	95 Digoxigenin	4	19.120	615,383,168


Partial MS^n Spectral tree matched
Query
Library



Matches for Component 200 using Subtree Search profile

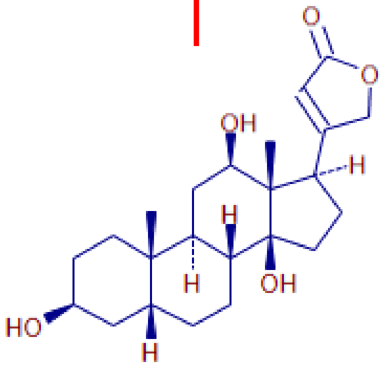
1 ID: 2 Ouabain class

Digoxigenin

$C_{23}H_{34}O_5$ MM: 390.2406

Subtree Match: 95.0

Sub-structure of query compound
M+H: 781.4384


O
O
OH
H
H
H
OH
HO
H

Structure of library reference
M+H: 391.2479

Delivering An Unprecedented Workflow

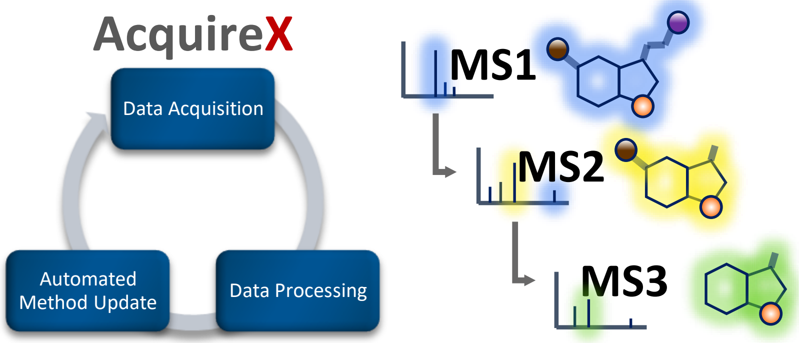
Addressing the Identification Crisis

Instrumentation Optimized for Small Molecules

thermoscientific
ORBITRAP ID-X

Orbitrap ID-X Tribrid MS for characterization and elucidation of small molecules

Acquisition Strategies to Produce Meaningful Data


AcquireX
Data Acquisition
Automated Method Update
Data Processing
MS1
MS2
MS3

AcquireX
Efficient acquisition to target what's truly relevant, even low-level compounds

MS^n
To build molecular structure from fragmentation information

Powerful Processing Software for Confident Identification

Compound Discoverer Software
mzCloud Advanced Spectral Library
Mass Frontier Software
LipidSearch Software

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