



Executive Summary

MS Orchestra

- Mass spectrometry has a data analysis problem
- MSO is AI to unlock untapped goldmines in mass spec data
- B2B SaaS for analytical chemists
- Assemble & operationalize scattered knowledge to make MS fly
- Accelerate biomedical research, environmental chem, and other fields
- Market is organized, accessible, hungry for new tools

Medical diagnostics overcost and underperform

**WW clinical diagnostic spend in
2024 = \$84B**



<https://www.mordorintelligence.com/industry-reports/clinical-diagnostic-market>

but

**795,000 Americans a year die
or are permanently disabled
after being misdiagnosed**



[Misdiagnosis kills, disables an alarming number of Americans each year \(usatoday.com\)](https://www.usatoday.com/story/news/health/2023/03/28/misdiagnosis-kills-disables-795000-americans-a-year/7000000000/)

and

**We all know someone who was
misdiagnosed. And misdiagnosed.
And misdiagnosed again.**



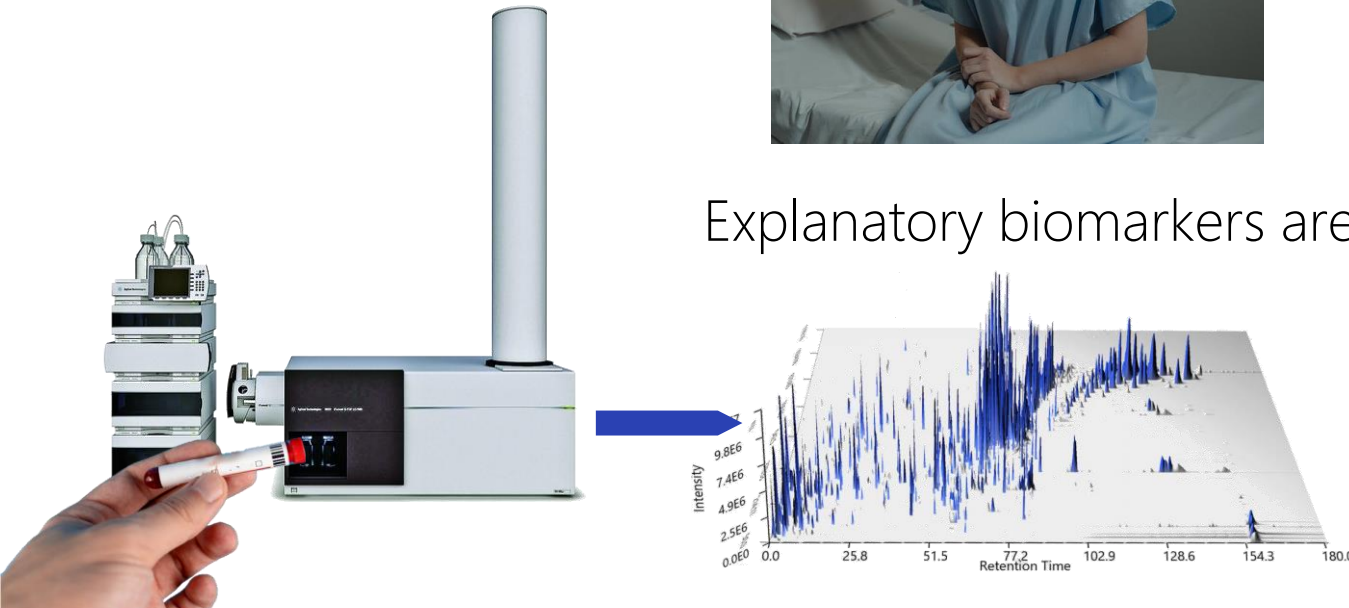
Mass spectrometry offers untapped green field of **granular** new diagnostics



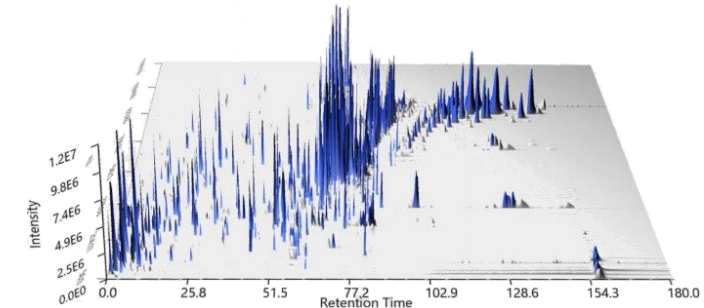
Vs.



Explanatory biomarkers are in these complex molecular patterns.



Vs.



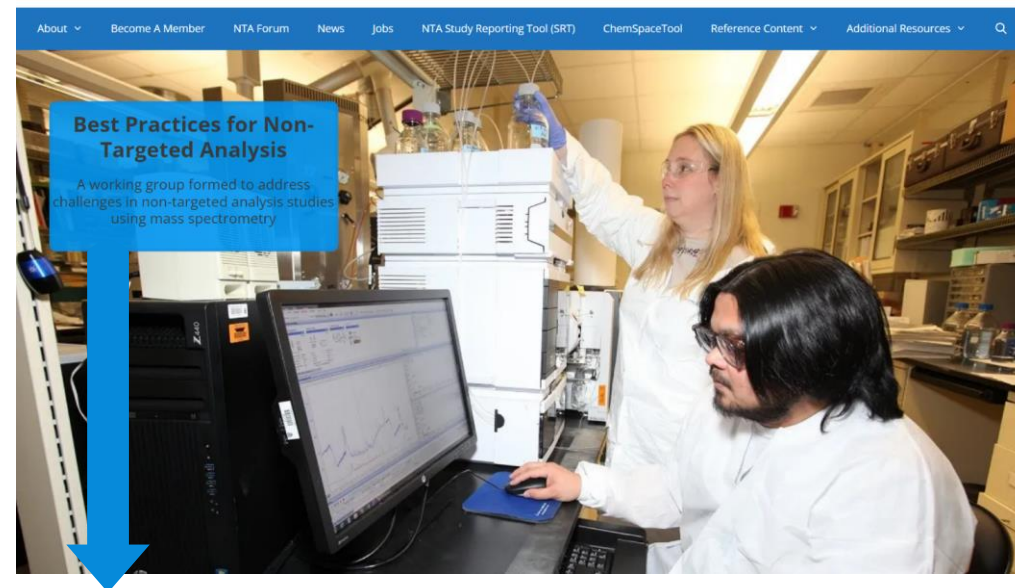
Overt frustration

ASMS Task Force: Perspectives on Data Analysis in Metabolomics



ASMS Special Task Force

- ① “The ability to process and interpret data is still severely limited.”
- ② “The informatic burden can require days, weeks, or months...”
- ③ “Even after extensive data analysis, there may be large numbers of “unknowns” that cannot be characterized.”
- ④ “These obstacles are preventing the full potential of metabolomics from being realized.”



Top line

”A working group **formed to address challenges** in non-targeted analysis studies using mass spectrometry”

Metabolomics is the fastest-growing segment in mass spectrometry, but...



GRAND VIEW RESEARCH

“Metabolomics is projected to be the fastest-growing segment over the forecast period due to the wide range of applications of mass spectrometry in cancer screening and diagnosis. The technique can be used to study a vast number of compounds in a single sample which enables the analysis of multiple sample constituents in a single run. As metabolomics is gaining traction as an important omics technology for diagnostic and prognostic applications in several chronic and infectious diseases, the segment is expected to witness significant growth.

...The requirement of skilled labor for operating and maintaining such complex systems represents a key operational constraint faced by users. Such factors may limit the industry's growth over the forecast period.”

[Mass Spectrometry Market Size, Share, Growth Report, 2030 \(grandviewresearch.com\)](https://www.grandviewresearch.com/industry-analysis/mass-spectrometry-market)

“Metabolomics”

Google Books Ngram Viewer

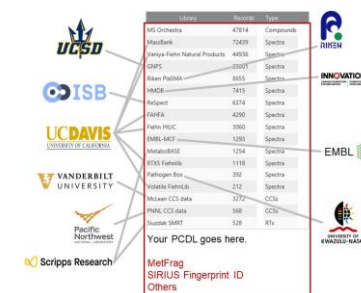
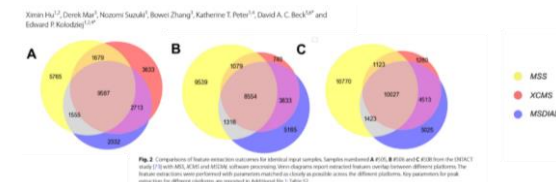
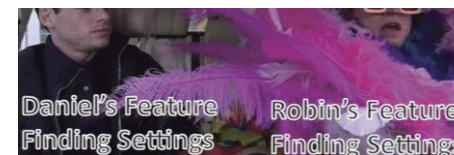
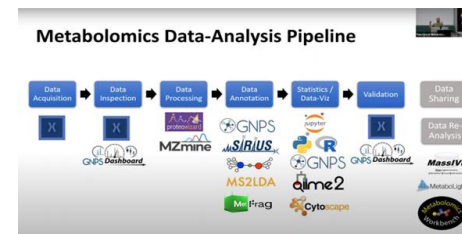


1820 1840 1860 1880 1900 1920 1940 1960 1980 2000

Problems

Current software:

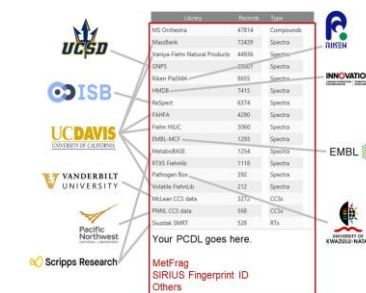
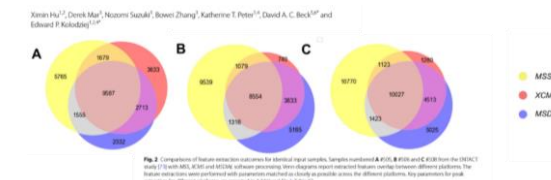
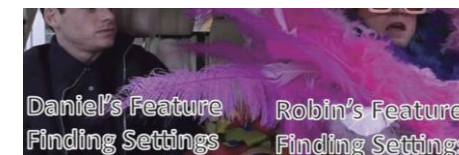
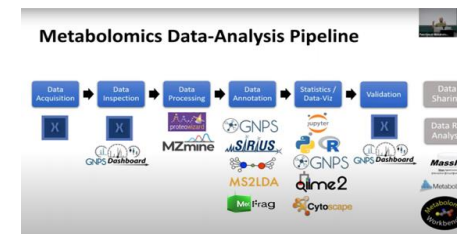
- Too many tools, transformations, and contortions to perform essential operations.
- Requires ill-informed, stress-inducing guesswork.
- Results are frighteningly irreproducible.
- Reference databases are splintered, incomplete, and lacking essential search capability.



What did we notice?

Those are all “dis-integration” problems

- It's now possible to integrate these.
- True integration allows math here.
- It's now possible to integrate these.
- It's now possible to integrate these, and FINALLY all the dimensions within them!!



Introducing



- One platform to integrate all the others, like an MS Orchestra.
- All data formats are embraced and unified.
You can forget formats and/or export any format any time.
- AI assistant to model/calculate those “wild-guess” user inputs mathematically, defensibly.
- Integrate multiple open-source tools to see discordant results, compare, and reconcile.
- Biggest, cleanest compendium of ref libraries in one place.
- First true integration of acquired *and* in-silico reference library search.
- Powerful graph DB with state-of-the-art ML search/match capabilities.
- Lab notebook integration
- Social medium integration to phone a friend or consult historical resolutions.

Winning playbook

MS Orchestra : Mass Spectrometry

Salesforce : CRM

= \$282.3B

Monday.com : Project Mgmt

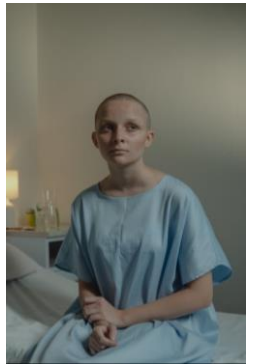
= \$11.4B

*Transform messy solitary tools into capable cloud coordination platforms.
ADD CAPABILITIES that become possible in a cloud/graph computing platform.
Remove friction from the work of cutting-edge science with specialized B2B SAAS.*

Work worth doing

Biomedical Metabolomic Applications:

- **Biomarker Discovery:** Identifying specific molecules (biomarkers) associated with diseases.
- **Drug Discovery:** Using metabolomics to understand drug effects and interactions.
- **Toxicology Testing:** Assessing the impact of toxins on metabolic pathways.
- **Nutrigenomics:** Studying how nutrients affect gene expression and metabolism.
- **Functional Genomics:** Investigating gene function through metabolite profiles.
- **Personalized Medicine:** Tailoring treatments based on individual metabolic profiles.



MSO Also Supports:

- **Environmental Chemistry:** Identifying pollutants and their sources.
- **Food Safety:** Assess, identify, measure contaminants in consumable products.
- **Forensics:** Identifying chemicals that reveal historical events, causes of harm.
- **Petrochemicals & fuels:** Support analysis of fuels, geologic formations.



Voice of the customer

SME comments after MSO software overview:

"This has blown me away."

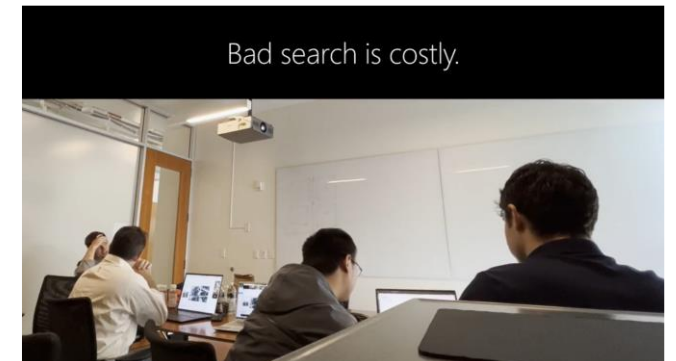
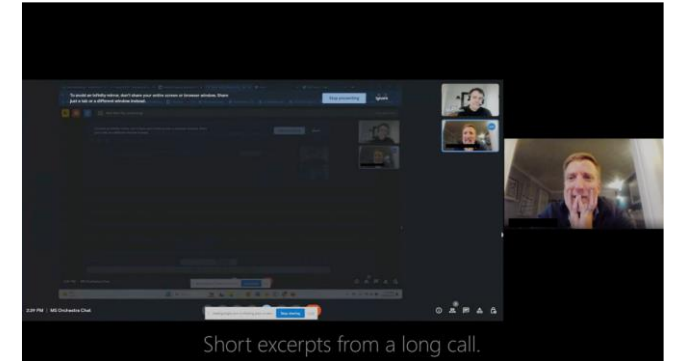
"This is way more radical than I was expecting."

"This is not another niche, me too product."

"80% of our effort is in data analysis."

"If we *could* search [like this], absolutely we would."

See 1-minute SME videos at <https://orchestra.ms/friends>



Customers

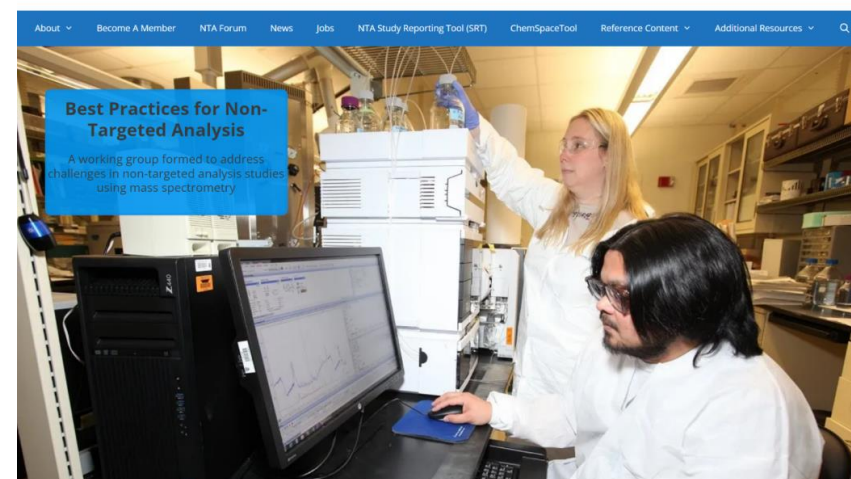
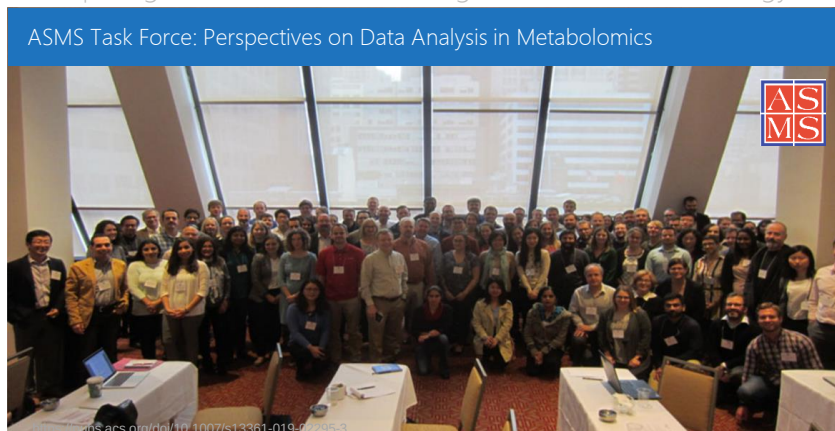
Customer profile is clear:

- High-res mass spec users for small molecules
- Well funded laboratories - academic and corporate
- Practitioners of “nontargeted analysis”
- FUD up, frustrated with current tools
- They know they have a problem

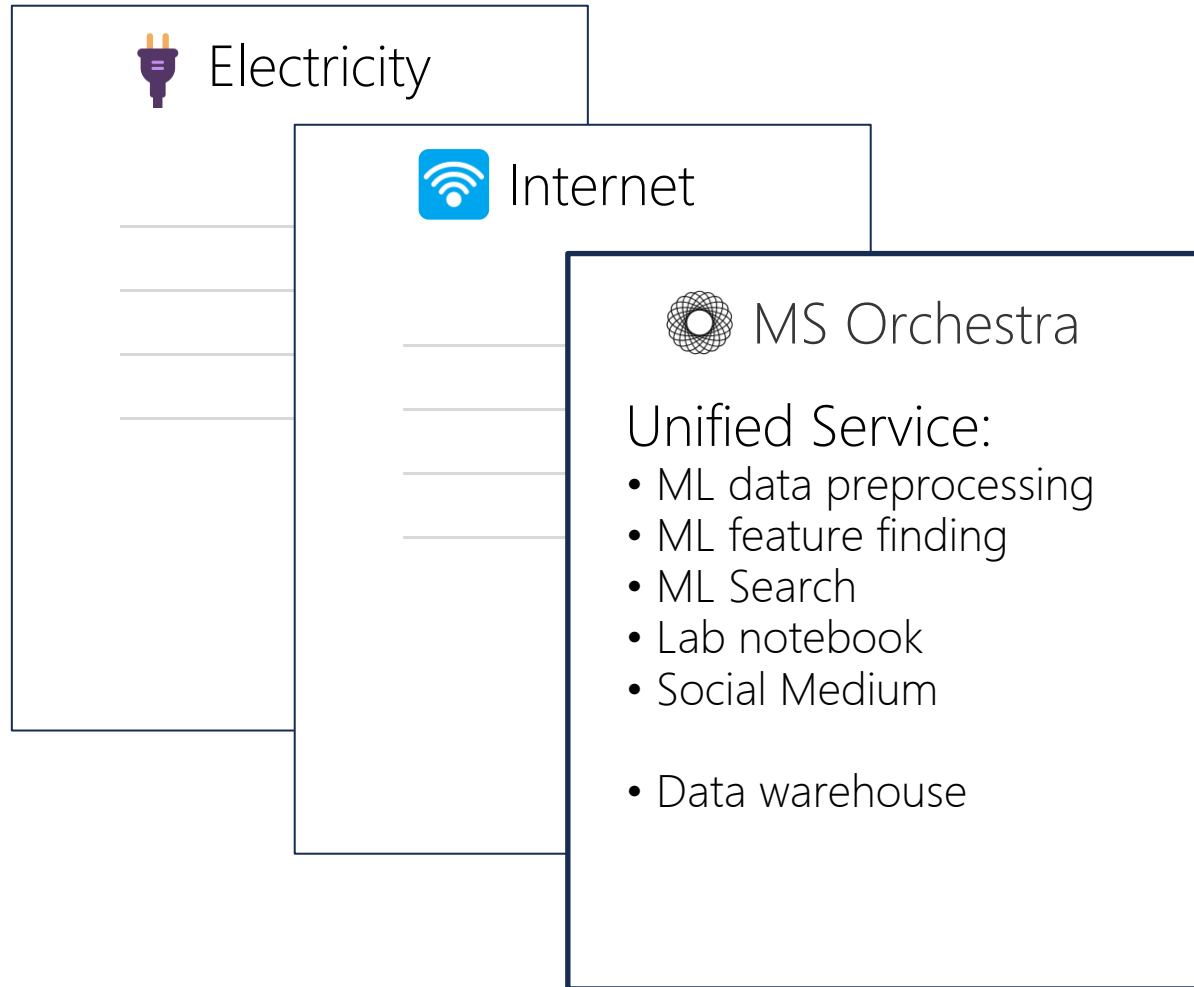
Urgency:

Hair on fire

Groups organized to discuss challenges with current technology.



Business model (business essentials)



Phase 1

Subscription utility

Tiered services to maximize inclusion, scale

Mission critical informatics, notebook, social media

Price points \$3-4 digits per user

Phase 2

Add data warehouse

Support regulatory compliance

Price points \$5-6 digits per lab

Go to market

Provide a differentiated product to actively shopping market

Speak to groups ORGANIZED TO DISCUSS these topics

Offer subset of invaluable Search utilities for free to generate awareness & engagement

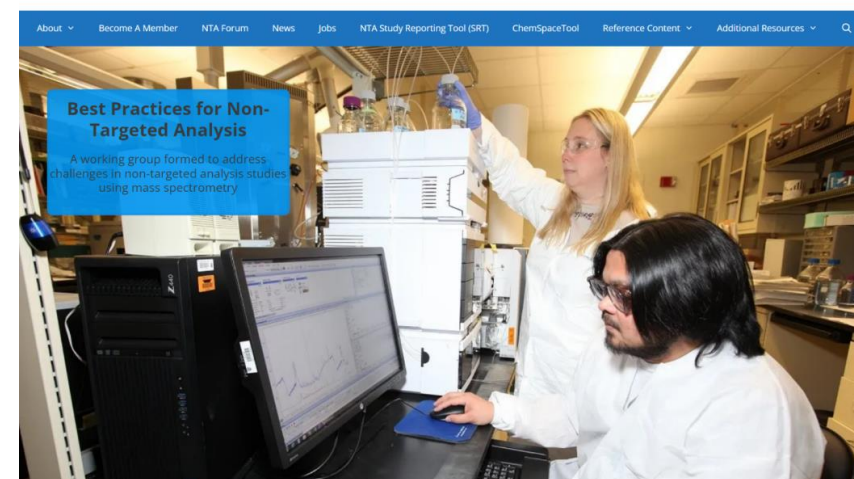
Insert MSO software into community TRAINING

Collaborate with thought leaders to gain traction, publications, influential support

Host must-see conversations in OUR social media platform

Groups organized to discuss challenges with current technology.

ASMS Task Force: Perspectives on Data Analysis in Metabolomics



Addressable Market

Mass spec market is \$6B with 8.2 CAGR
~100K target customers in phase 1 (estimate)

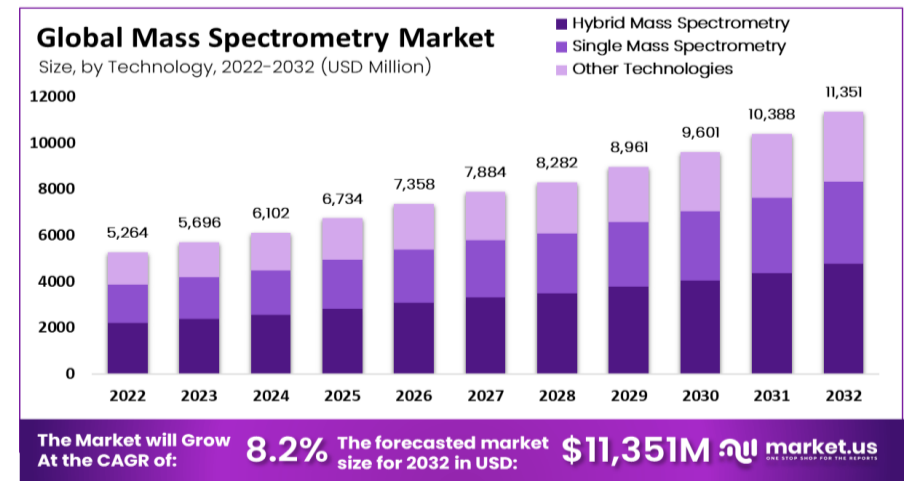
Public reports:

- 7K members of ASMS (2022)
- 10K members of GNPS (2017)
- 18K downloads/yr of open-source MZmine (2018-22)

- 
- Targeting 10,000 MSO subscriptions by EO year 2
 - Then self-sustaining R&D/growth
 - Minimal dilution for early partners
 - Adjacent markets are lined up like dominoes

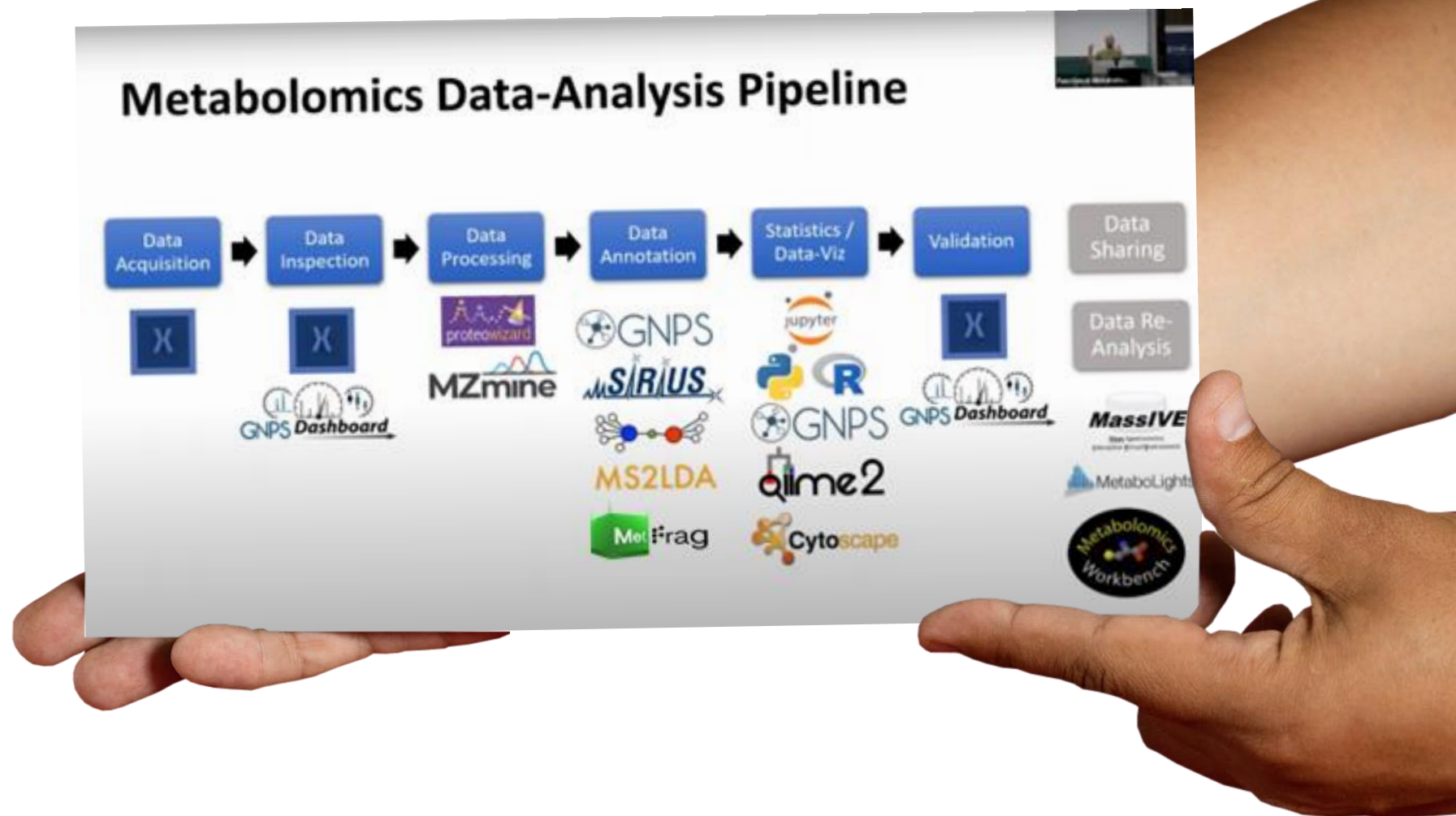
Groups organized to discuss challenges with current technology.

ASMS Task Force: Perspectives on Data Analysis in Metabolomics



Competition

Individually sophisticated.
Collectively incoherent.
This is the problem.



MS Orchestra Team



Matt Rain. PhD molecular genetics, 17 years at global mass spec vendor.



Quinn Rain. Applied math & biochemistry, "I marry those 2 things in code."



Mike Meadway. Computer scientist, IOT, inventor of our proprietary graph database.



Priya Dwivedi. Deep learning/AI expert, founder Deep Learning Analytics.

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- Accelerate biomedical research, environmental chem, and other fields
- Market is organized, accessible, hungry for new tools

The state of the art in mass spectrometry is...



...ready for a revolution

Contact Matt at matt.rain@orchestra.ms

"The challenge of interpreting results has created major obstacles that are preventing the full potential of metabolomics from being realized."

ASMS task force report



Appendix

Hey Chat GPT... what do you think?

Appendix

“Hey Chat GPT, what are some success stories that demonstrate the ability of metabolomics to reveal new biomedical insights?”

Metabolomics is a rapidly growing field that has the potential to revolutionize healthcare by providing personalized insights into an individual's health status. Here are some success stories that demonstrate the ability of metabolomics to reveal new health insights:

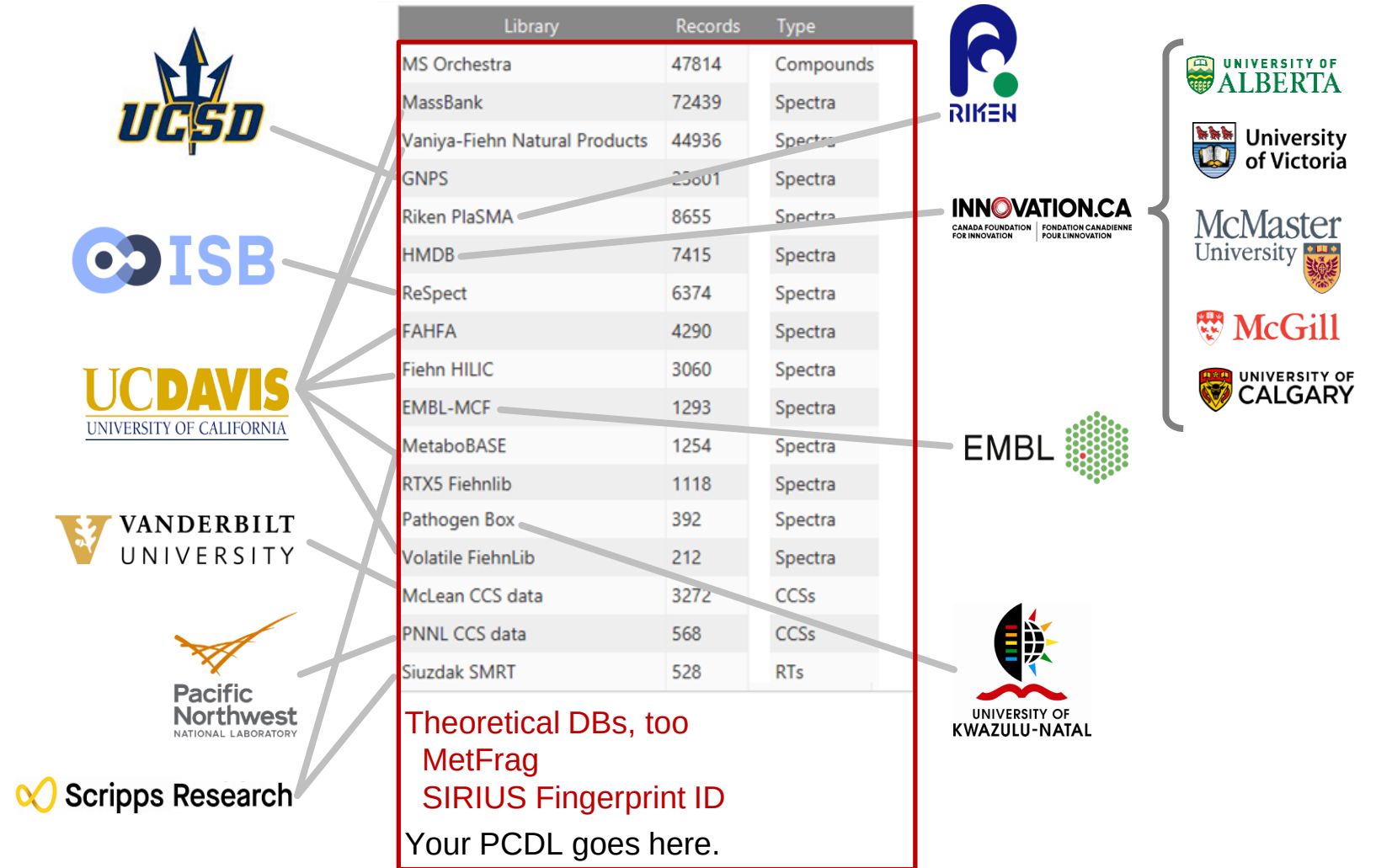
- 1.Precision Health:** Metabolomics is shifting the conversation around human health towards a personalized approach that is based on the activity of the small molecule metabolites in the body. [This approach is improving clinical trial design and efficacy to bring more life-saving drugs to the market faster¹.](#)
- 2.Drug Discovery:** Metabolomics is helping researchers unravel complex interactions between biological processes and the environment. [This is leading to the discovery of new biomarkers and drug targets, which can be used to develop more effective treatments².](#)
- 3.Disease Diagnostics:** Metabolomics is being used to identify new biomarkers for various diseases, including cancer, diabetes, and Alzheimer's disease. [This is helping doctors diagnose these diseases earlier and with greater accuracy³.](#)
- 4.Nutritional Quality of Crops:** Metabolomics is being used to improve the nutritional quality of crops and accelerate plant-derived bioactive leads discovery through disease diagnostics. [This has the potential to preserve human health by increasing the therapeutic efficacy of drugs via a more personalized approach⁴.](#)

These are just a few examples of how metabolomics is transforming healthcare. With continued research and development, metabolomics has the potential to provide even more personalized insights into an individual's health status and revolutionize the way we approach healthcare.

Ready, set, go

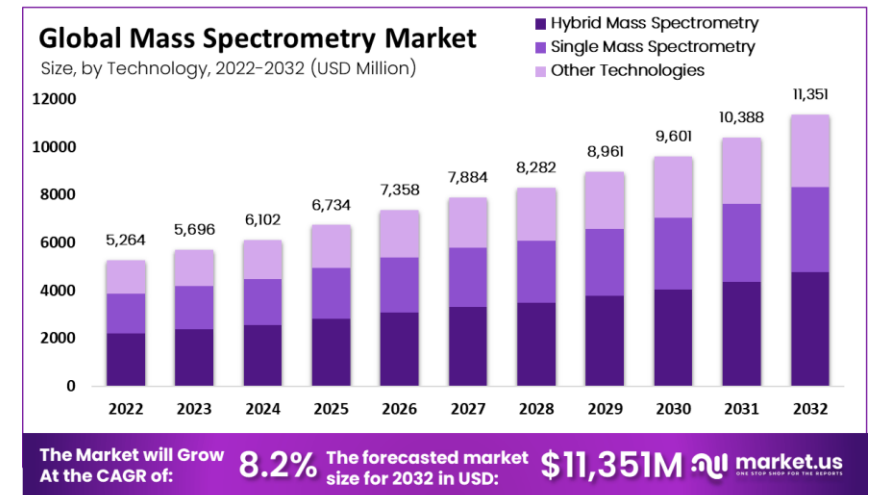
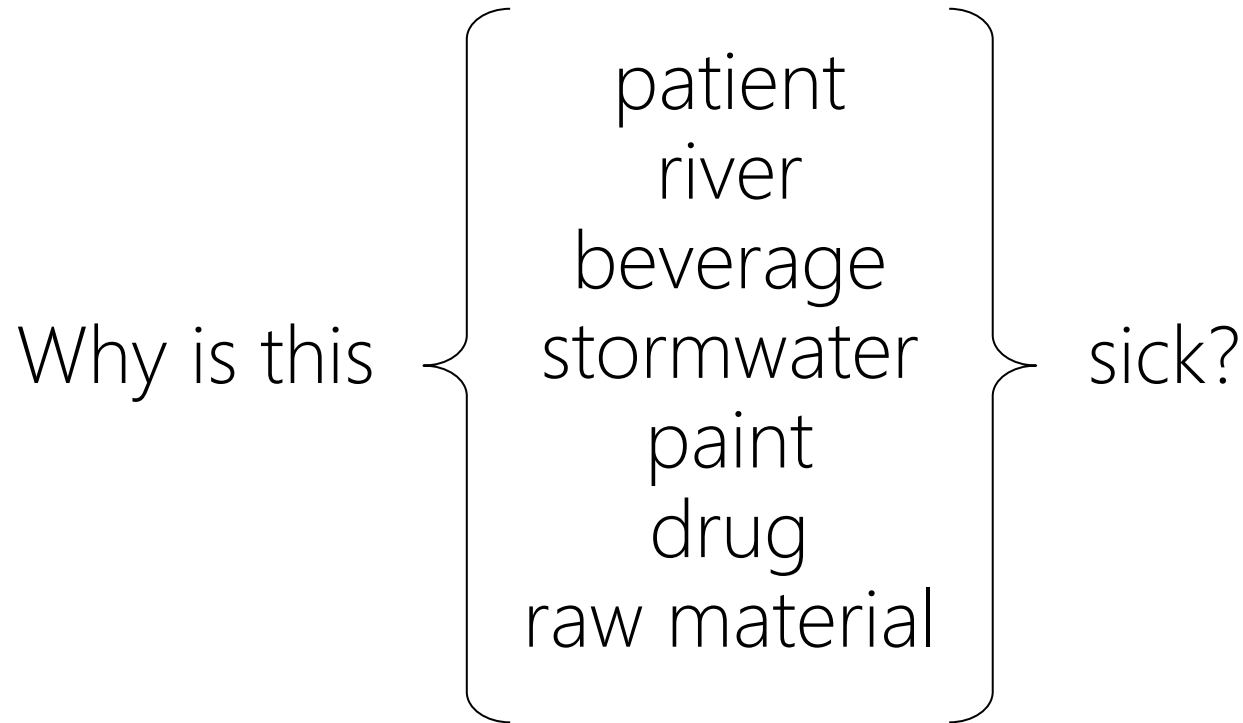
On day 1 we'll deploy worldwide reference libraries:

- Unified
- Cleaned up
- Combined across classes(!)
- More searchable



Appendix

By the way, everything is “molecular diagnostics.”



Jersey City, New Jersey, Nov 10, 2021 (GLOBE NEWSWIRE) – Verified Market Research recently published a report, “Mass Spectrometry Market” by Platform and by Application (Pharmaceutical & Biotechnology, Food & Beverage Testing, Environmental Testing)

Following My Own Path

Sitting Down With... Koen Sandra, CEO and Co-owner, RIC group;
Visiting Professor, Ghent University, Belgium

Markella Loi, Rich Whitworth | 11/10/2023



Koen Sandra, RIC

"Our field has to follow the artificial intelligence route... But I think people are still trying to understand what it can do for chromatography. To be honest, it's not entirely clear to me either!"

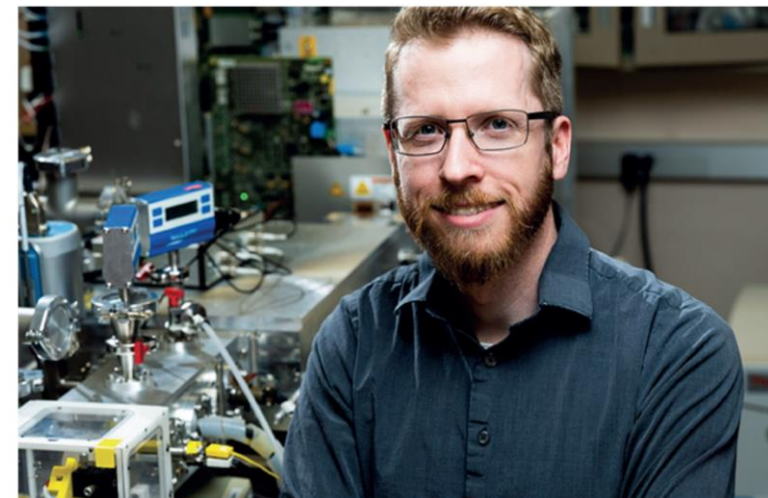
<https://theanalyticalscientist.com/fields-applications/following-my-own-path>



Exploring the Deep Sea of Unknown Compounds

How high-resolution ion mobility-mass spectrometry holds the answer to unraveling the structures of the many molecules we know must exist

Adam Hollerbach | 10/12/2023



Adam Hollerbach, PNNL

"we're hoping to use the SLIM-Orbitrap to fully identify unknown compounds that challenge other researchers. And though we aren't yet sure on the role of AI, computational models are sure to play a big role in decoding the data acquired from the SLIM-Orbitrap."

Exploring the Deep Sea of Unknown Compounds
<https://theanalyticalscientist.com/techniques-tools/exploring-the-deep-sea-of-unknown-compounds>

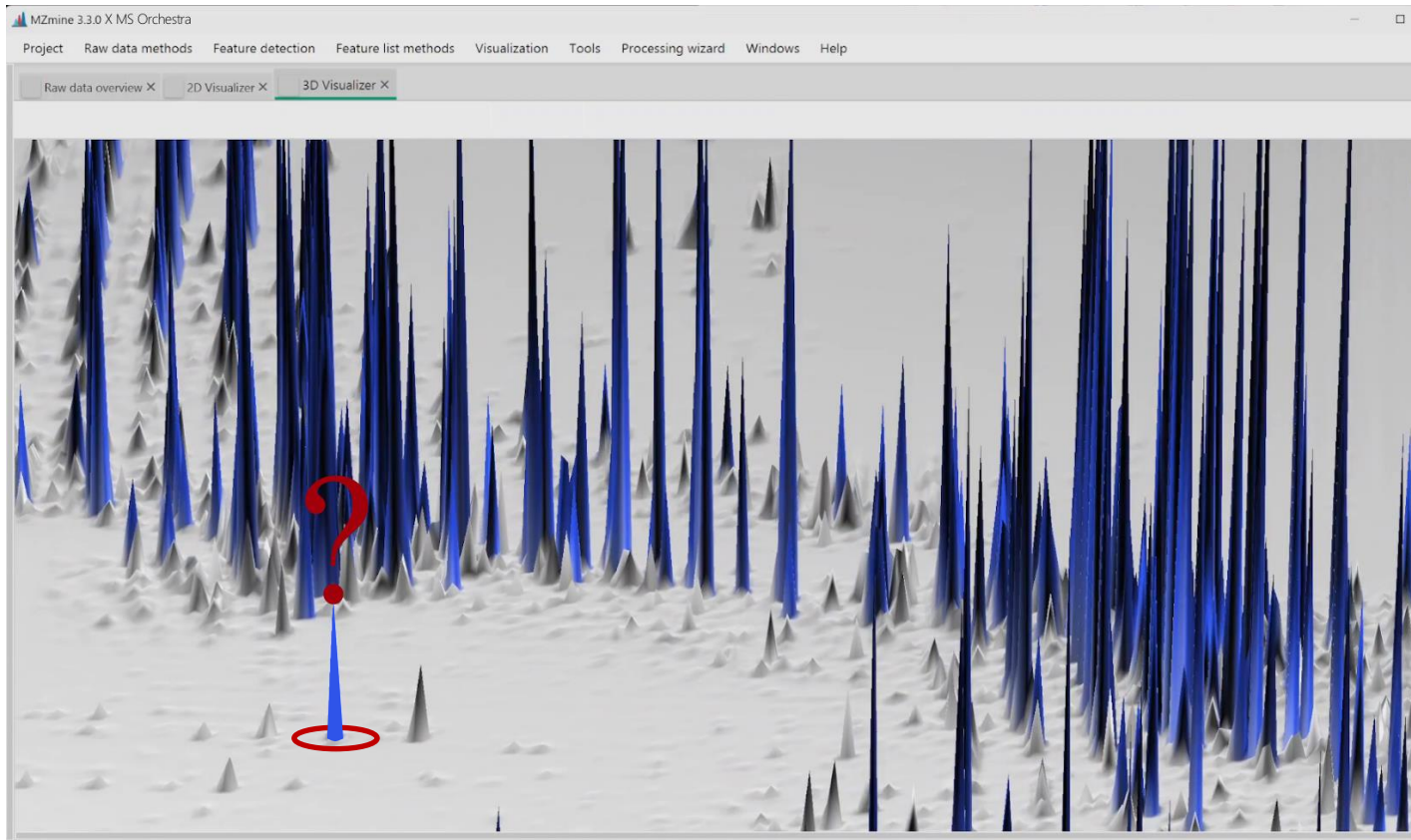
What *should* we do with AI?



- Predict retention times?
- Predict fragmentation?
- Match spectra to compound names?
- New similarity scoring techniques?

Search

Appendix

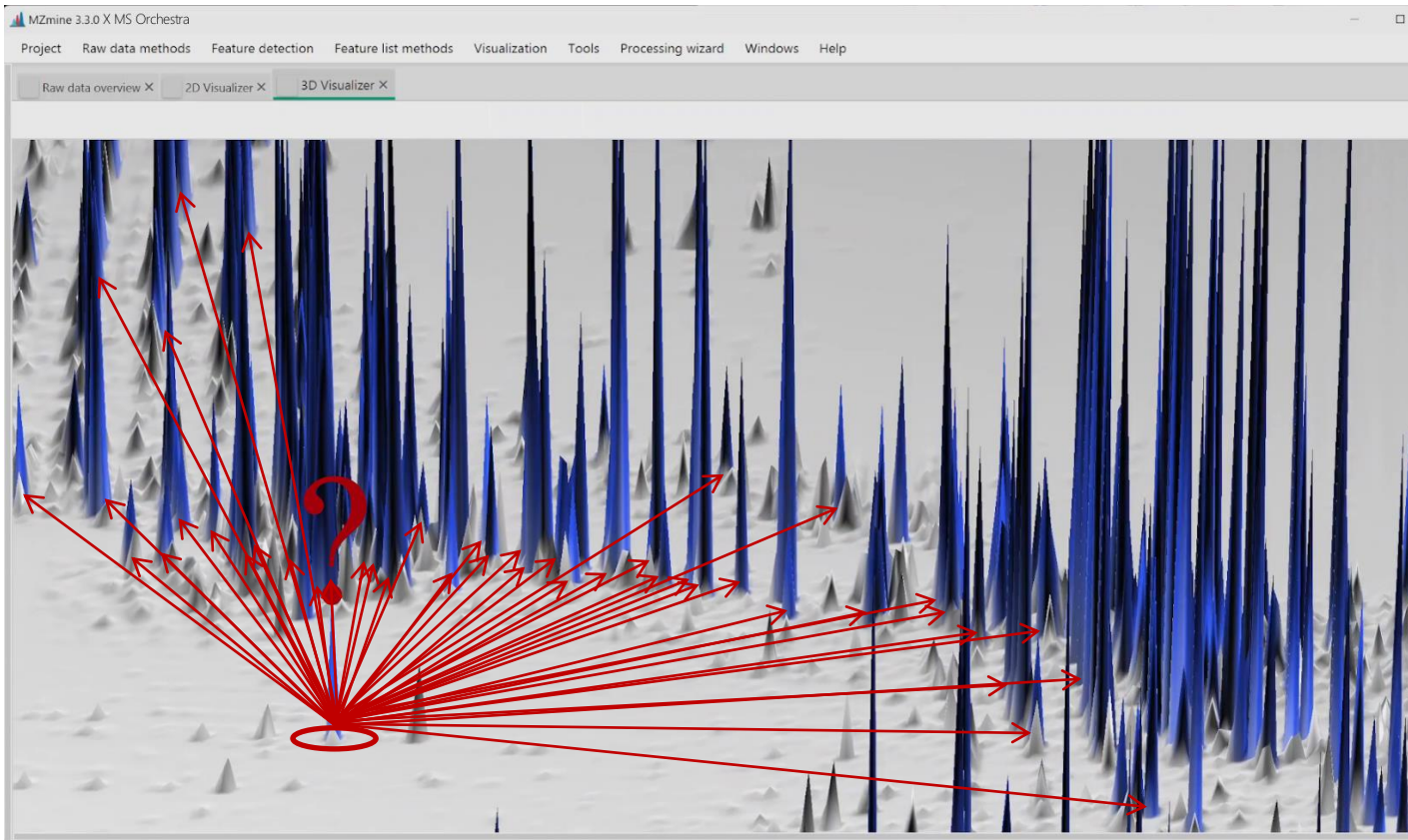


Isolate compound of interest.
Preserve PEAK's properties.
Discard all contextual info.

Search for similars to this
ONE object

Search

Appendix



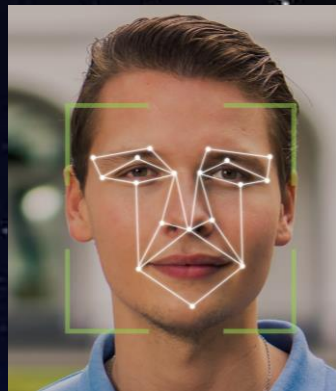
What properties *do we have*?

- Intact mass
- Fragments
- Isotopes
- Chromatographic address Extrinsic
- CCS

A “which is which” problem: Go find Betelgeuse.

Appendix

Cheat sheet 1 (intrinsic)



		Distance (ly)	Spectral type
		0.0	G2 V
	α CMa	8.6	A0mA1 Va, DA2
	α Car	310	A9 II
	α Cen	4.34	G2 V, K1 V
	α Boo	37	K0 III
	α Lyr	25	A0 Va
	α Aur	43	K0 III, G1 III
	β Ori	860	B8 Ia
Procyon	α CMi	11	F5 IV-V
Achernar	α Eri	139	B3 Vpe
Betelgeuse	α Ori	550	M1-M2 Ia-ab
Hadar	β Cen	390	B1 III
Altair	α Aql	17	A7 V
Acrux	α Cru	320	B0.5 IV, B1 V
Aldebaran	α Tau	65	K5 III
Antares	α Sco	550	M1.5 Ia-b, B2.5 V
Spica	α Vir	250	B1 III-IV, B2 V
Pollux	β Gem	34	K0 III
Fomalhaut	α PsA	25	A3 V
Deneb	α Cyg	2,600	A2 Ia

Cheat sheet 2 (intrinsic)



Cheat sheet 3 (extrinsic)

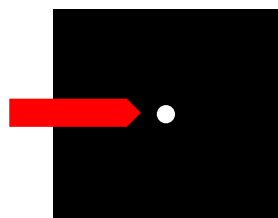


Can we agree this is Betelgeuse?

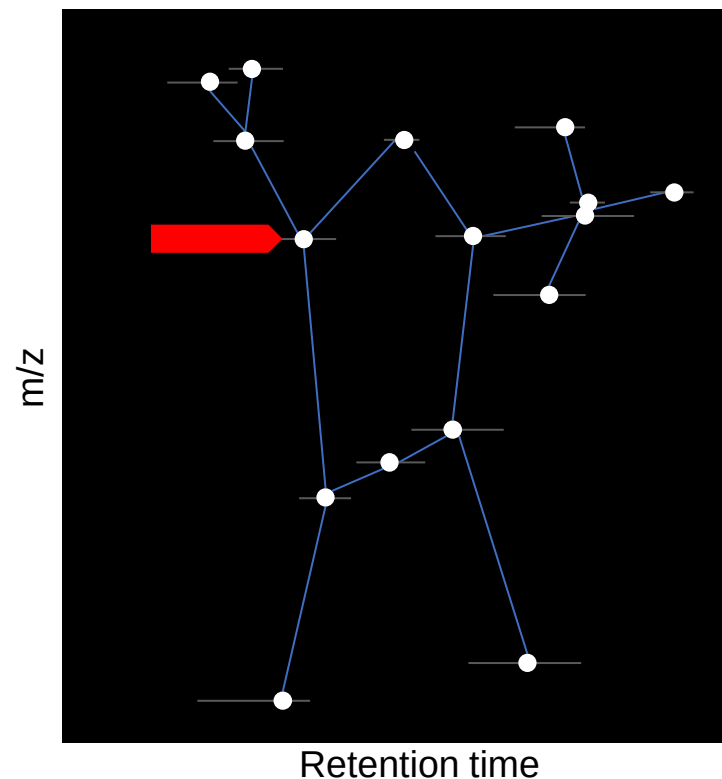
Appendix

MS Orchestra is using ML to invent new ways to ORGANIZE and search MS data.

Before MSO



In MSO



We turn this problem into solutions

Appendix

Mass-Suite: a novel open-source python package for high-resolution mass spectrometry data analysis

Ximin Hu^{1,2}, Derek Mar³, Nozomi Suzuki³, Bowei Zhang³, Katherine T. Peter^{1,4}, David A. C. Beck^{5,6*} and Edward P. Kolodziej^{1,2,4*}

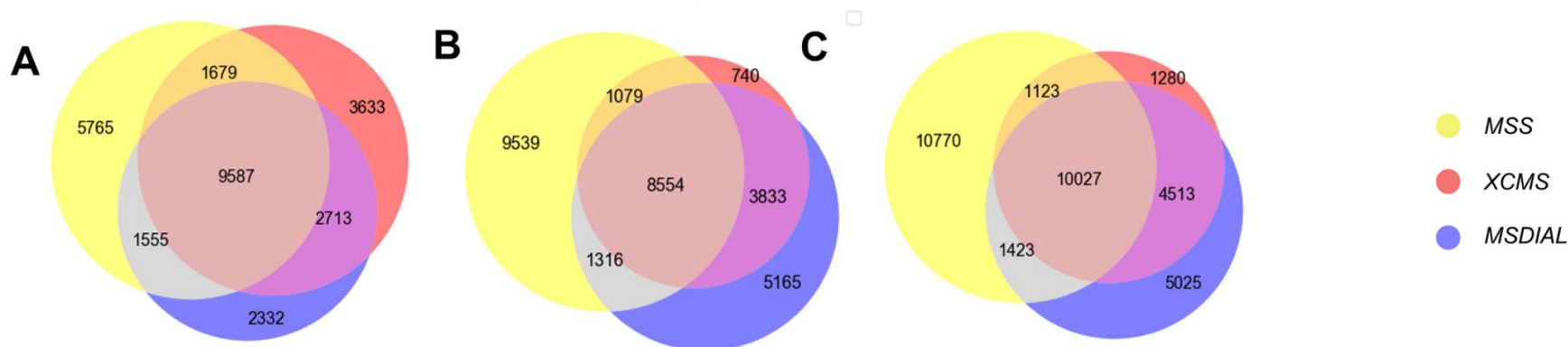


Fig. 2 Comparisons of feature extraction outcomes for identical input samples. Samples numbered **A** #505, **B** #506 and **C** #508 from the ENTACT study [73] with MSS, XCMS and MSDIAL software processing. Venn diagrams report extracted features overlap between different platforms. The feature extractions were performed with parameters matched as closely as possible across the different platforms. Key parameters for peak extraction for different platforms are reported in Additional file 1: Table S2

This is a reproducibility problem.
A statistical power problem.



Do it like Google Photos

Appendix

We found 437 individuals
in your collection of 23,657
photos.

Make your photos searchable.
Click one to add a name!



Do you know this person?

(appears in 33 pictures)

Appendix



[Add a name](#)

Find them fast by name with search

Fri, Oct 8, 2021



Tue, Jun 24, 2008



Mon, Dec 24, 2007



Fri, Feb 23, 2007



Sat, Aug 21, 2004



Tue, Nov 25, 2003



Tue, Nov 26, 2002



Sat, Dec 22, 2001



Sun, Apr 1, 2001



Sun, Nov 19, 2000



Thu, Jul 13, 2000



Tue, Feb 9, 1999



Thu, Feb 4, 1999



More fundamental integration

Appendix

Every datum lives in information-rich relationship to others.

