

# NATIONAL HIGH MAGNETIC FIELD LABORATORY

## Conducting the Quartet: synchronizing data streams in a custom-built mass spectrometer with four mass analyzers

David S. Butcher and  
Chad R. Weisbrod

January 22<sup>nd</sup>, 2025



The MagLab is closed  
for a Snow Day!



Tallahassee, FL  
1/22/25

# MagLab Overview



Headquartered at **Florida State University**, the MagLab also has branch campuses at the **University of Florida** and **Los Alamos National Laboratory**.

• **LANL**  
LOS ALAMOS, NM

• **FSU**  
TALLAHASSEE, FL

• **UF**  
GAINESVILLE, FL

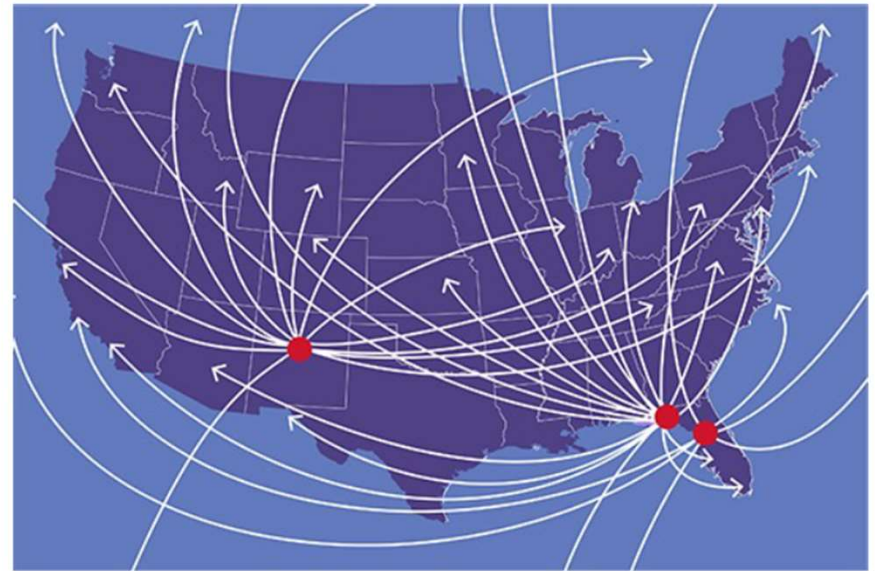


# MagLab Overview

**1 Lab. 3 Sites.**

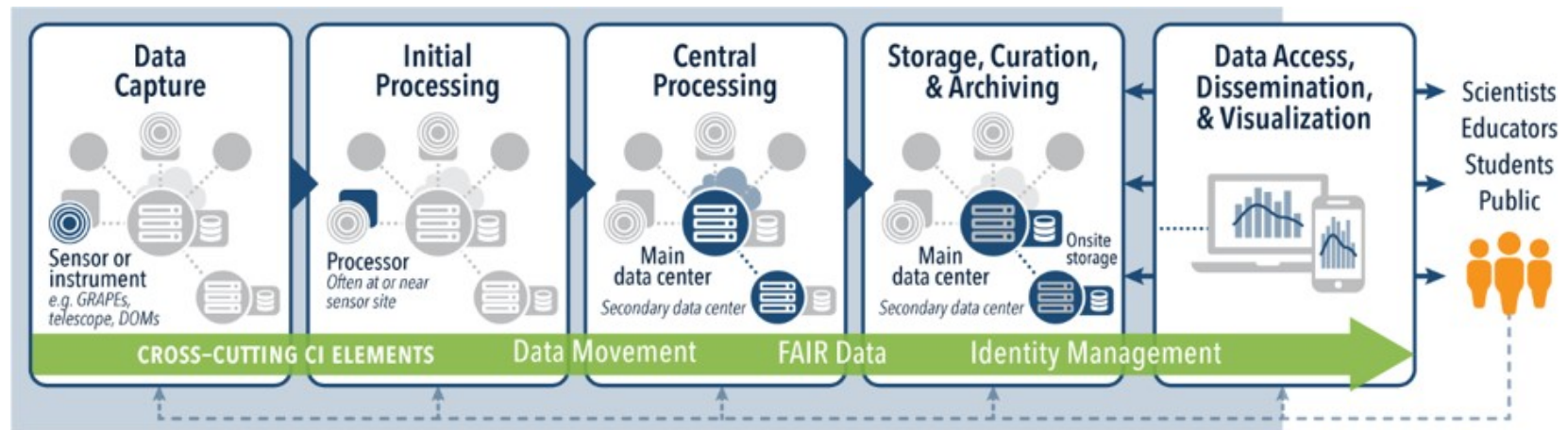
**7 User Facilities.**

- **DC Field User Facility (at Florida State University):** *continuous fields up to 45T.*
- **Electron Magnetic Resonance User Facility (at Florida State University):** *continuous and pulsed magnetic resonance techniques associated with unpaired electron spins.*
- **Nuclear Magnetic Resonance User Facility (at Florida State University):** *solution and solid state NMR and animal MRI.*
- **Ion Cyclotron Resonance User Facility (at Florida State University):** *ultra-high resolution and high mass accuracy Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry.*
- **Advanced Magnetic Resonance Imaging and Spectroscopy (AMRIS) (at the University of Florida):** *high-resolution solution and solid state NMR, in vivo imaging and spectroscopy, MRI microscopy, and diffusion.*
- **High B/T (at the University of Florida):** *magnetic fields up to 15T combined with ultra-cold electron temperatures to 0.4mK.*
- **Pulsed Field User Facility (at Los Alamos National Laboratory):** *short, ultra-powerful magnetic fields up to 100T.*

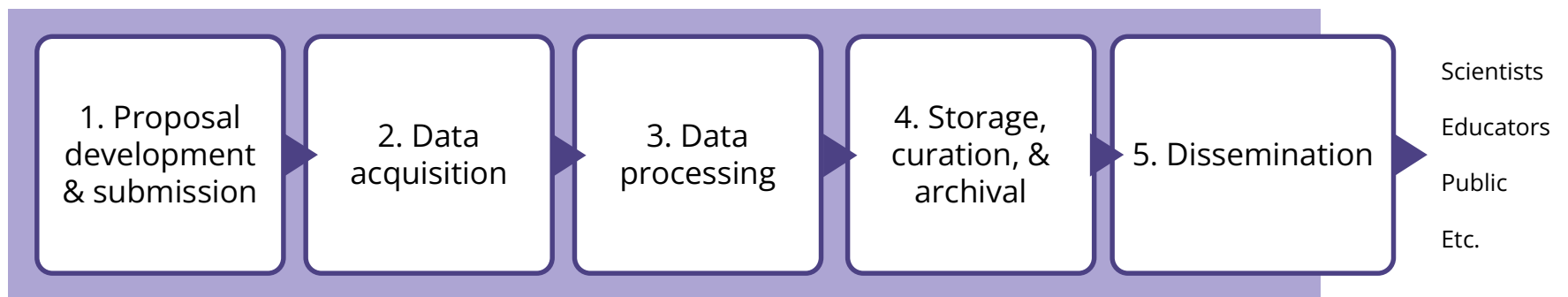


# Data Lifecycles

## CI Compass Data Lifecycle Model<sup>1</sup>



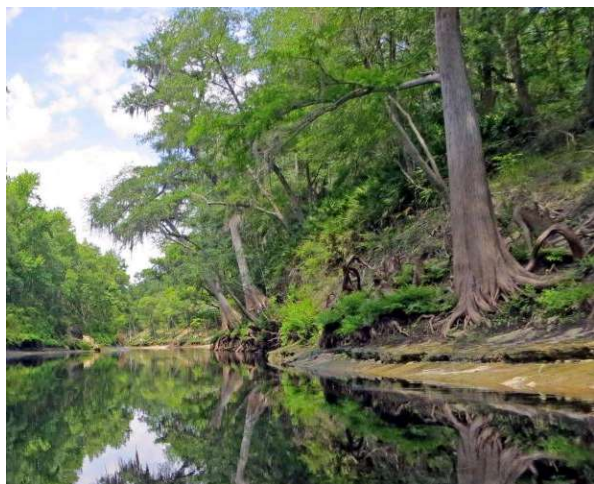
## MagLab Data Lifecycle Model



# Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

FT-ICR MS has great utility in studying...

Dissolved organic  
matter



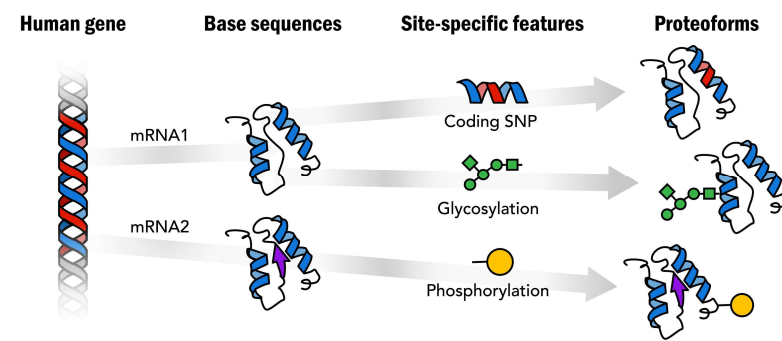
DOM in natural  
waterways

Persistent organic  
pollutants



PFAS in aqueous film-  
forming foam

Proteoforms

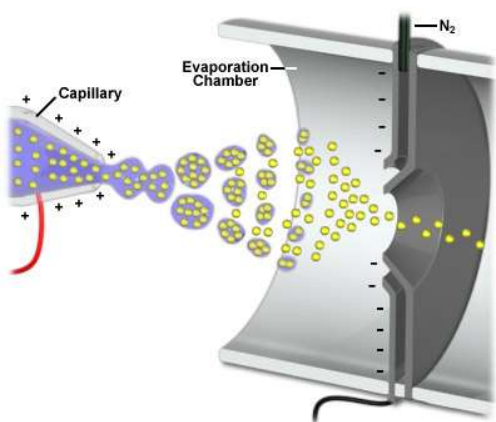


The molecularly distinct products  
of a single gene

1. Florida Department of Environmental Protection. <https://www.floridastateparks.org/parks-and-trails/suwannee-river-wilderness-trail>
2. Khatchadourian, R. Deepwater Horizon's Lasting Damage. *The New Yorker* (2011).
3. Smith, L. M.; Agar, J. N.; Chamot-Rooke, J.; Danis, P. O.; Ge, Y.; Loo, J. A.; Paša-Tolić, L.; Tsybin, Y. O.; Kelleher, N. L.; THE CONSORTIUM FOR TOP-DOWN PROTEOMICS. The Human Proteoform Project: Defining the Human Proteome. *Science Advances* **2021**, 7 (46), eabk0734. <https://doi.org/10.1126/sciadv.abk0734>.

# Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

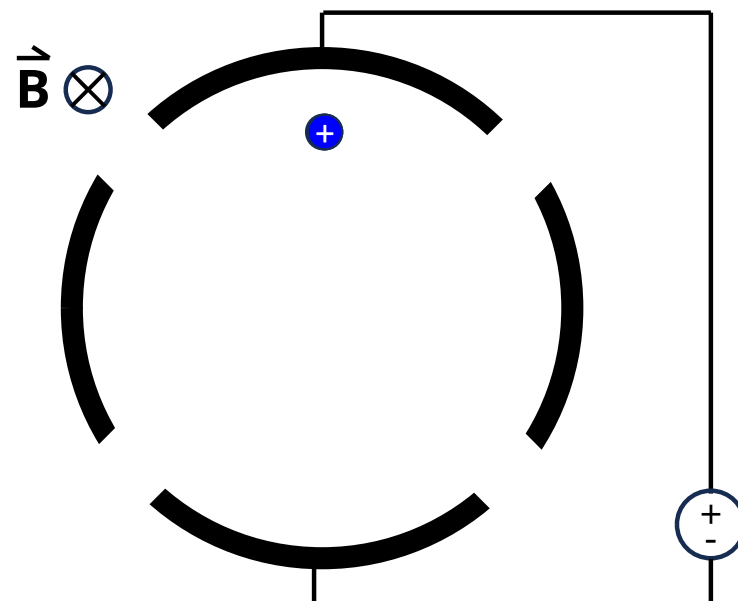
## Ionization<sup>1</sup>



## Ion Routing and Manipulation<sup>2</sup>

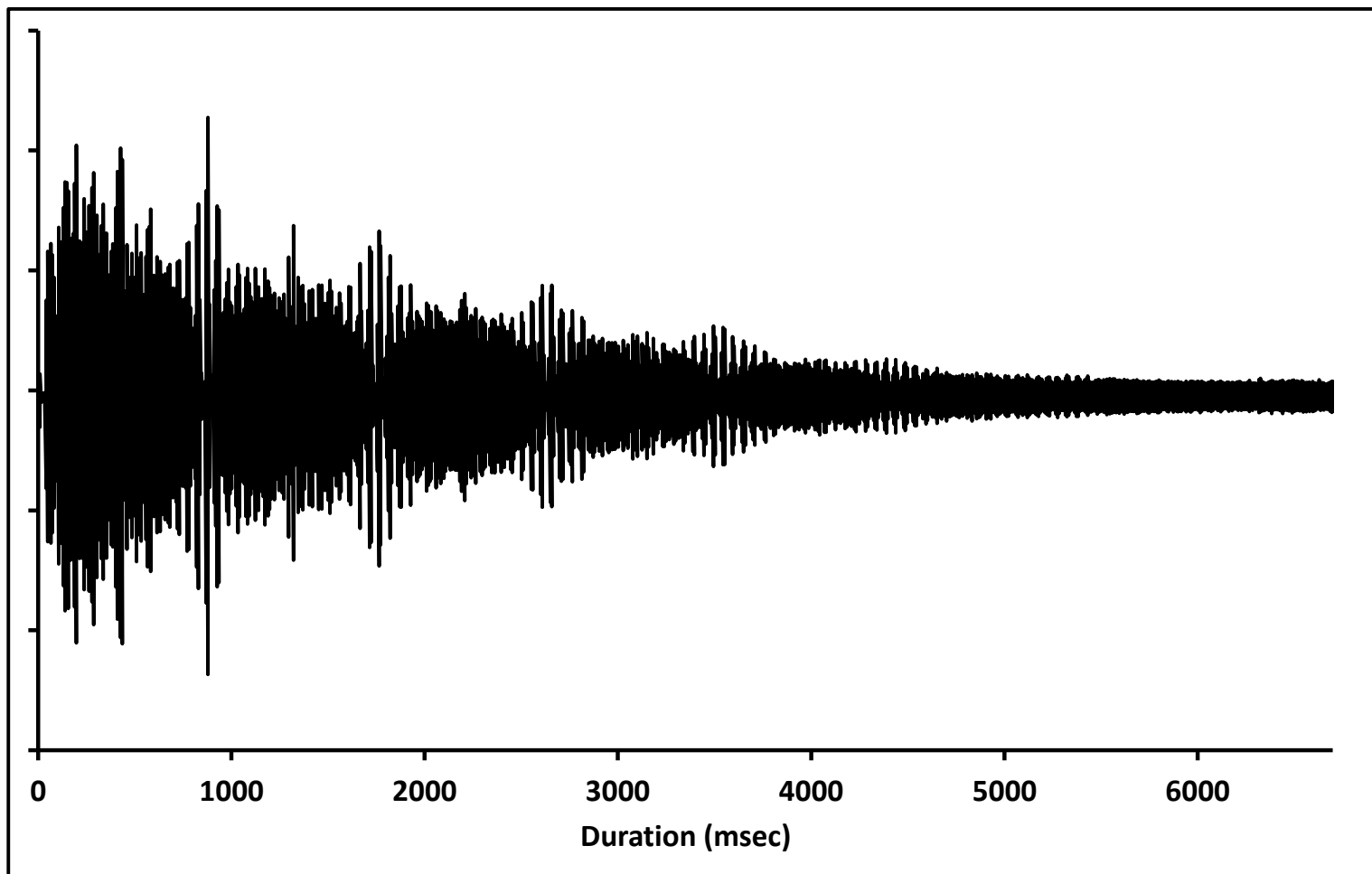


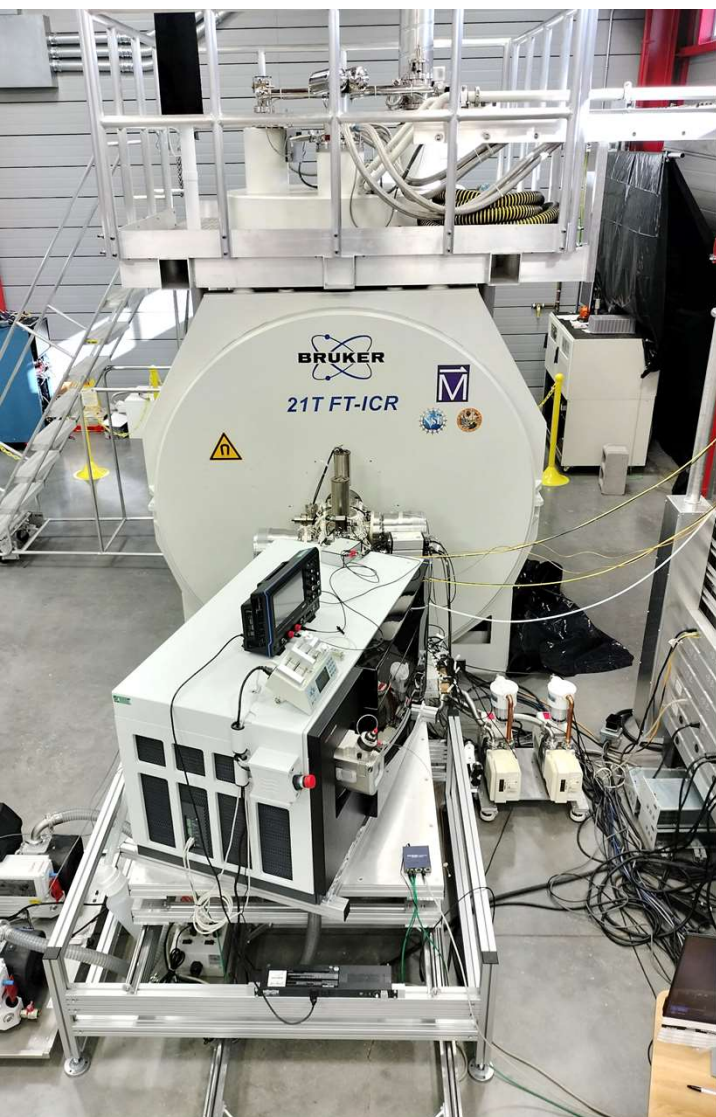
## Ion Cyclotron Resonance



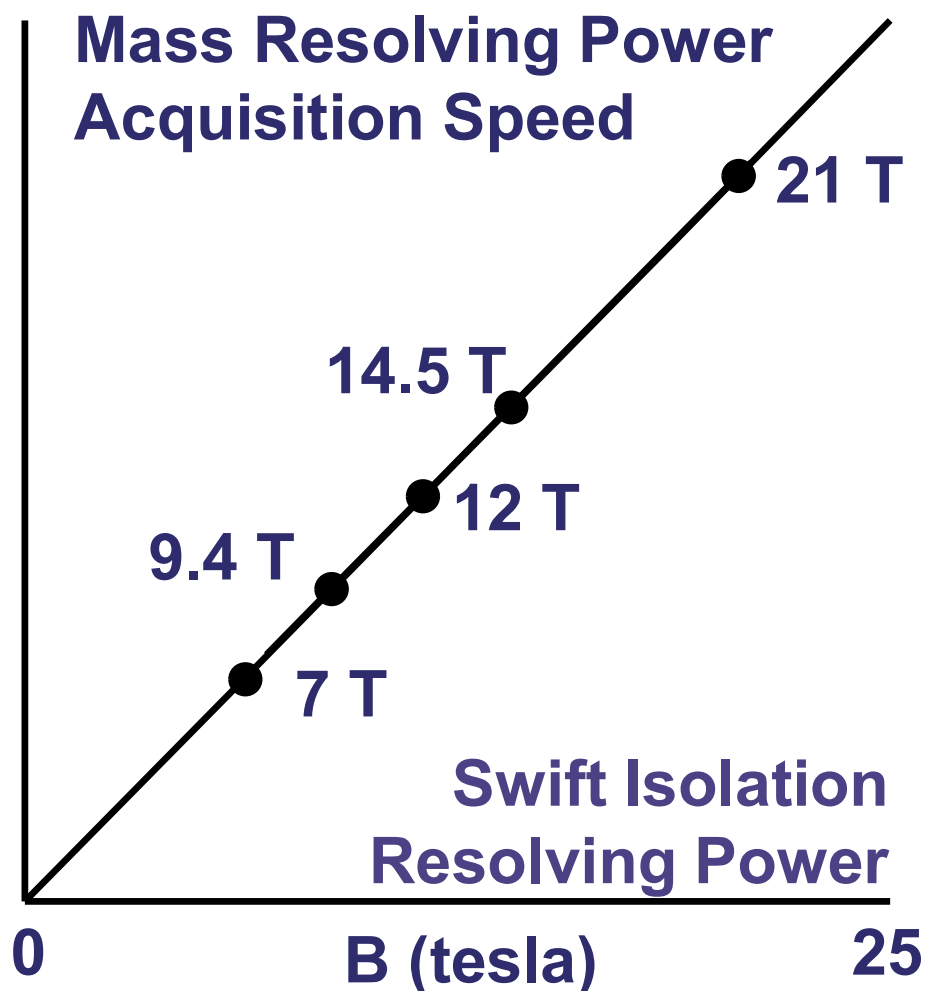
1. Electrospray Ionization. <https://nationalmaglab.org/user-facilities/icr/techniques/ionization-techniques/esi/>  
2. Fulvio314. Wikimedia Commons. [https://commons.wikimedia.org/wiki/File:Mass\\_spectrometer\\_quadrupole.JPG](https://commons.wikimedia.org/wiki/File:Mass_spectrometer_quadrupole.JPG)

## Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

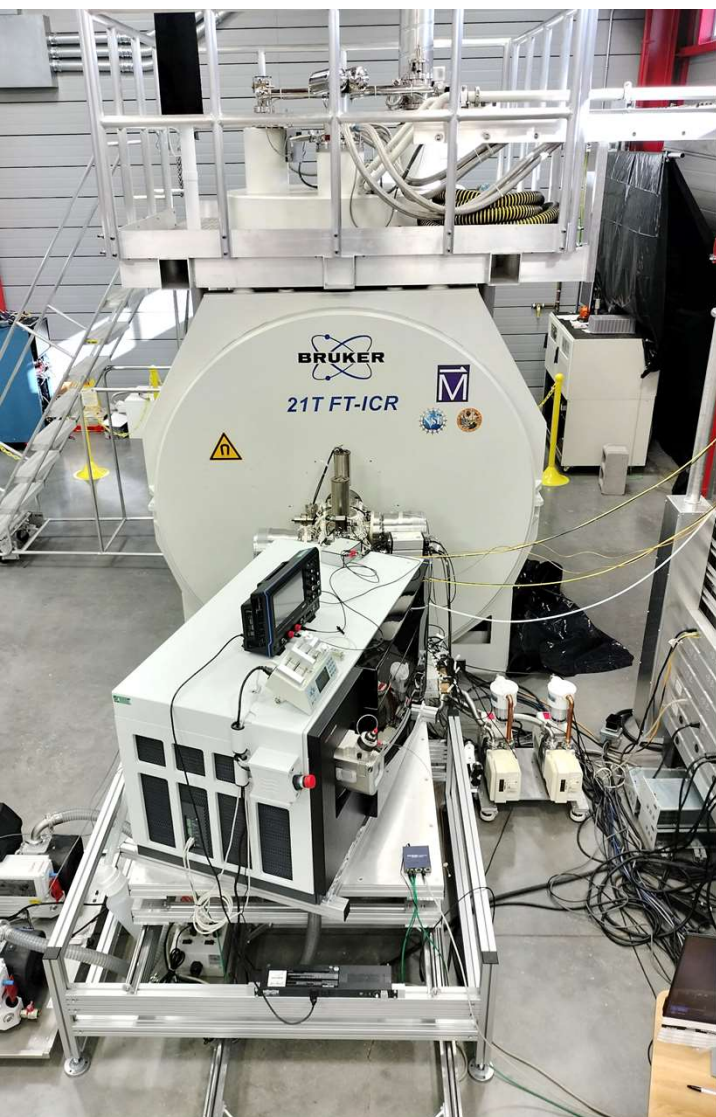




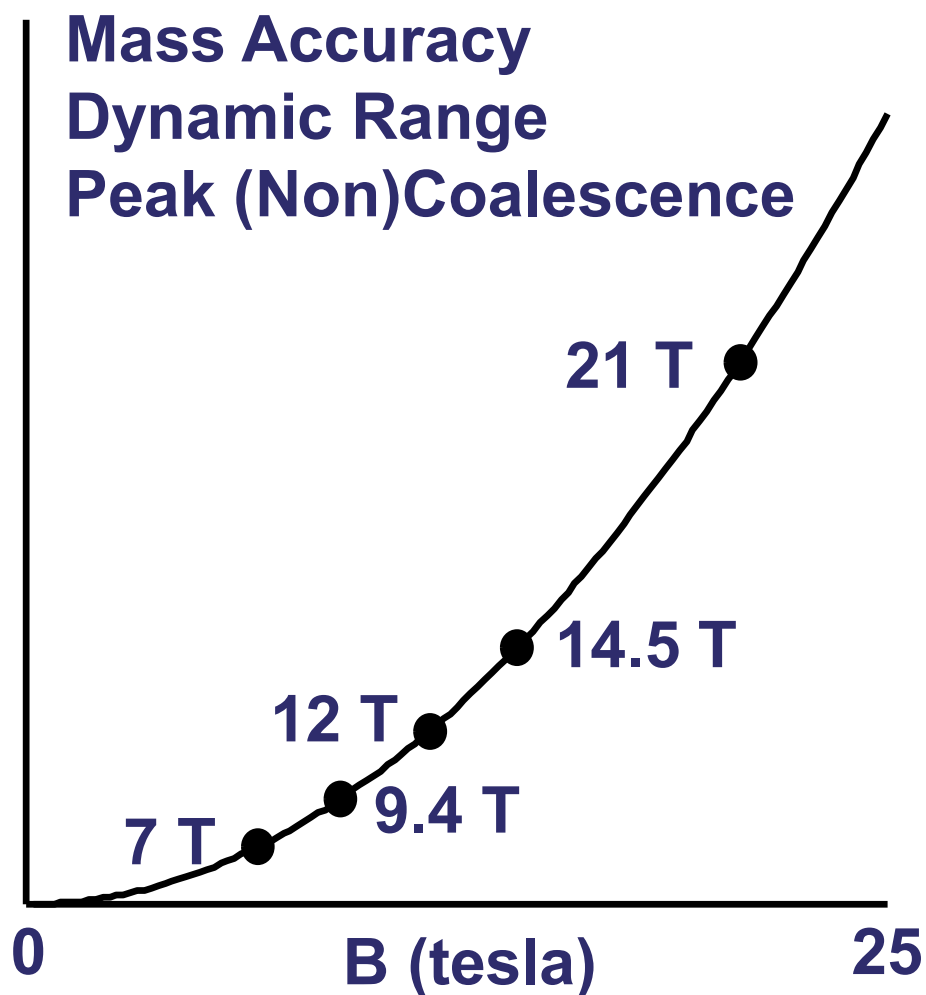
## Advantages of High Magnetic Field



Marshall and Guan, *Rapid Commun. Mass Spectrom.* 1996, 10, 1819-1823.

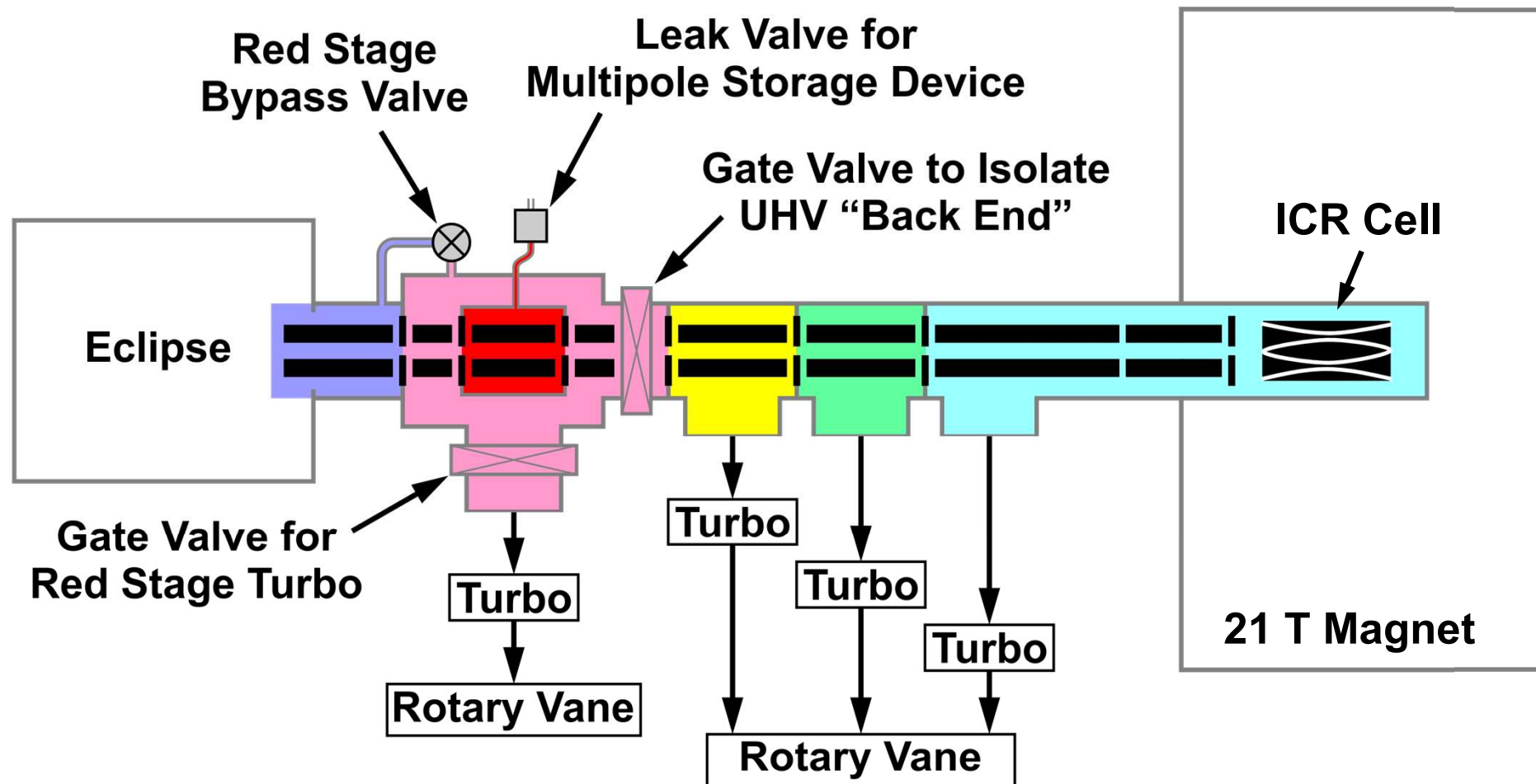


## Advantages of High Magnetic Field



Marshall and Guan, *Rapid Commun. Mass Spectrom.* 1996, 10, 1819-1823.

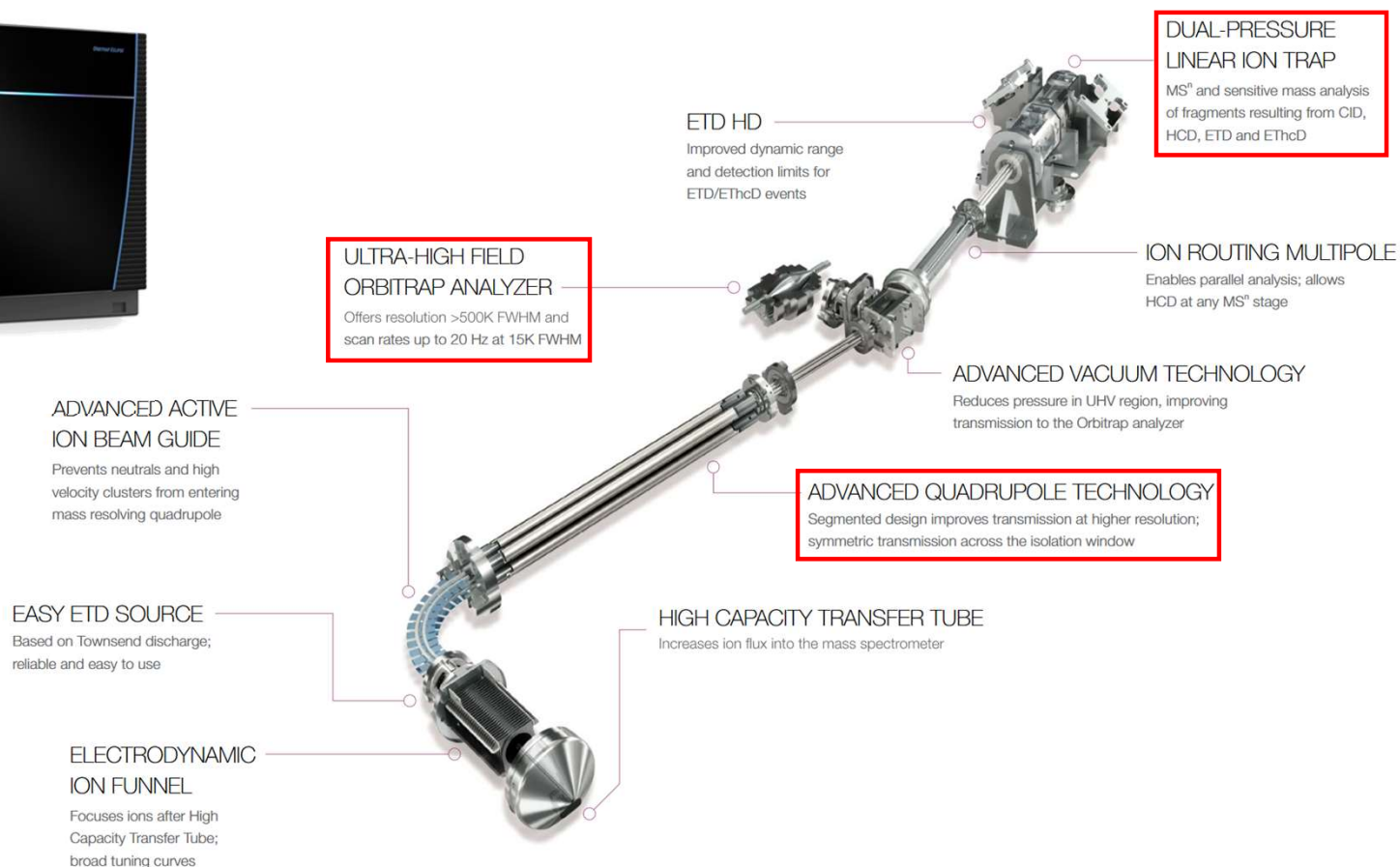
# Eclipse-21 T FT-ICR System



# Orbitrap Tribrid Architecture

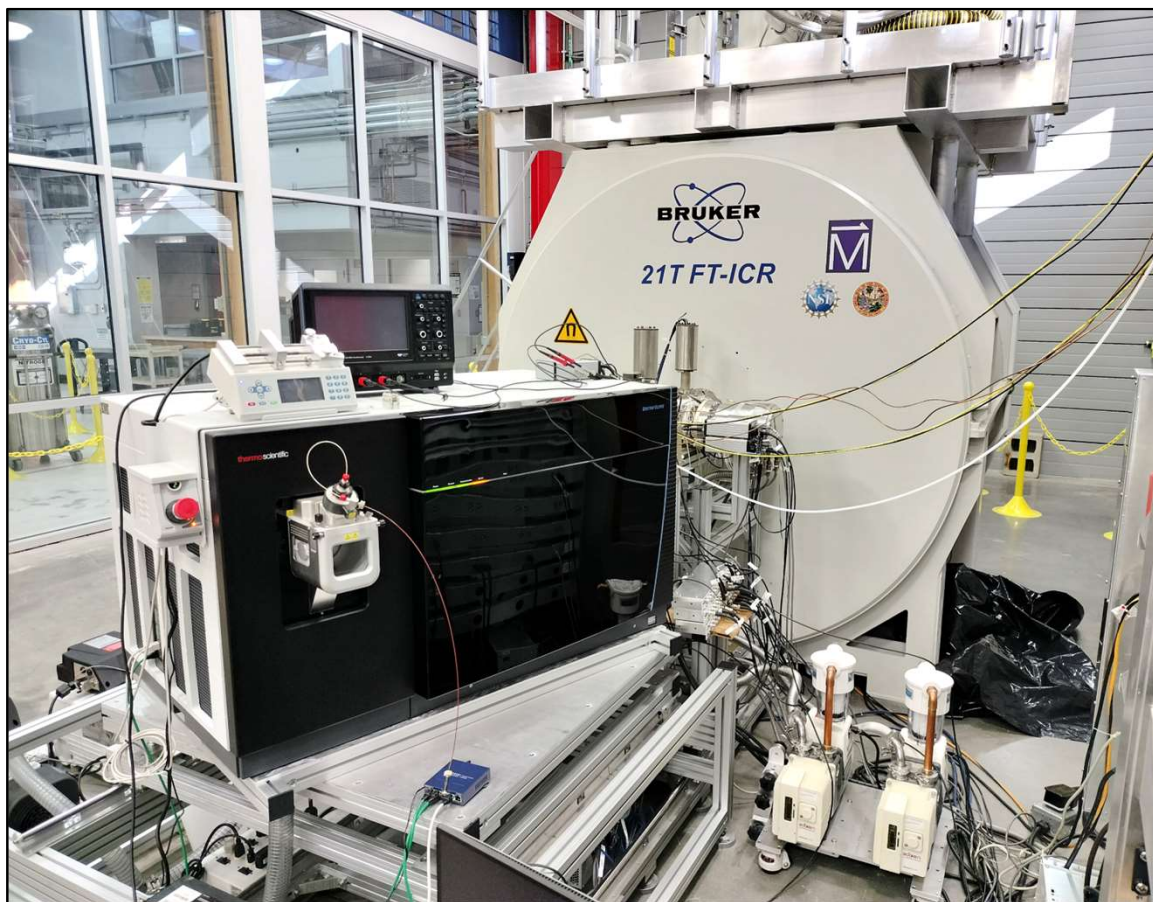


The Orbitrap Eclipse “tribrid” front end contains three mass analyzers. The ICR analyzer on the back end creates a unique “quadbrid” instrument.



1. Thermo Scientific™ Orbitrap Eclipse™ Tribrid™ Mass Spectrometer: <https://www.thermofisher.com/order/catalog/product/FSN04-10000>

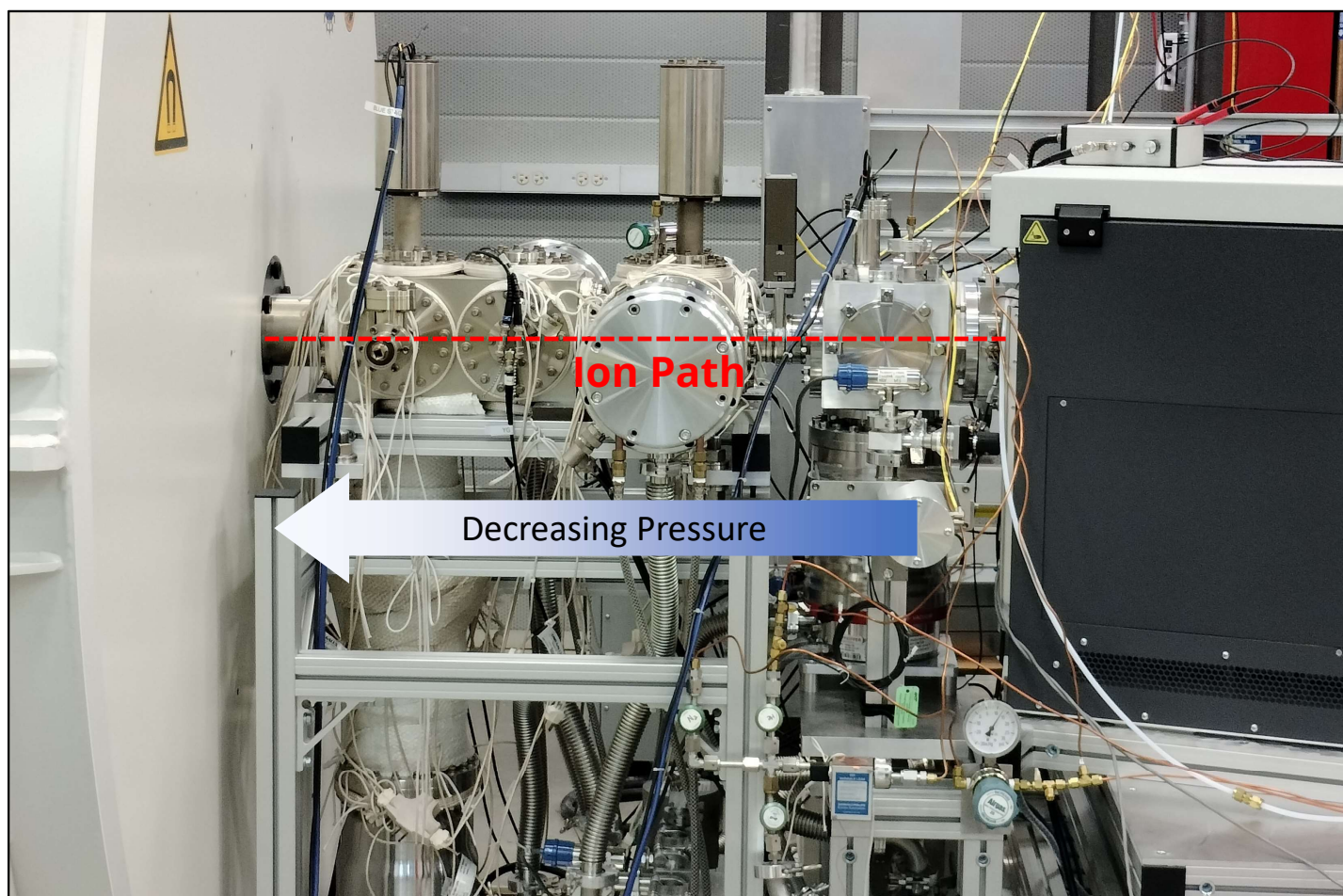
# 21 T FT-ICR System



## 21 T FT-ICR System

Ion routing quadrupoles transmit ions ~2 m into the ICR cell inside the 21 T superconducting electromagnet.

A series of pumping stages decreases pressure to the ultrahigh vacuum region ( $<10^{-11}$  Torr).



## 21 T FT-ICR System



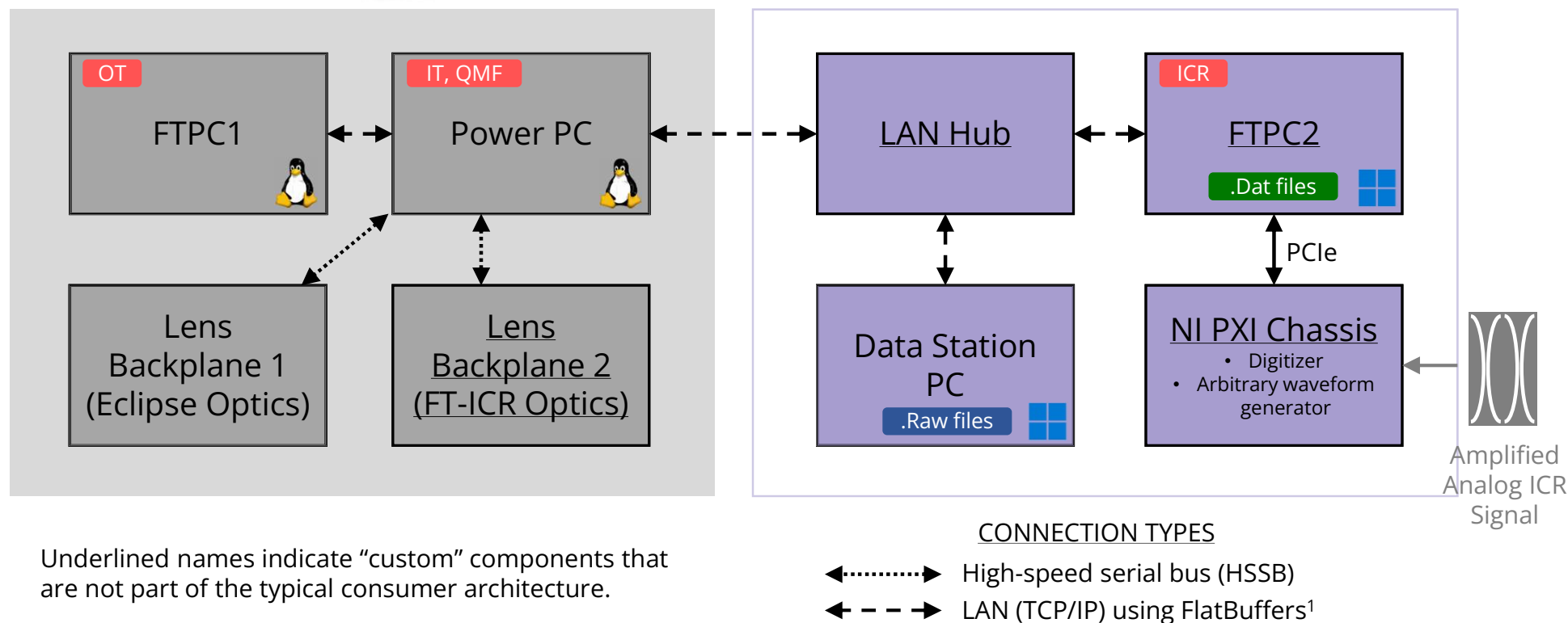
The Data Station PC – the only interface that a typical user has to the system.

# Eclipse-ICR System Architecture

Orbitrap  
Eclipse

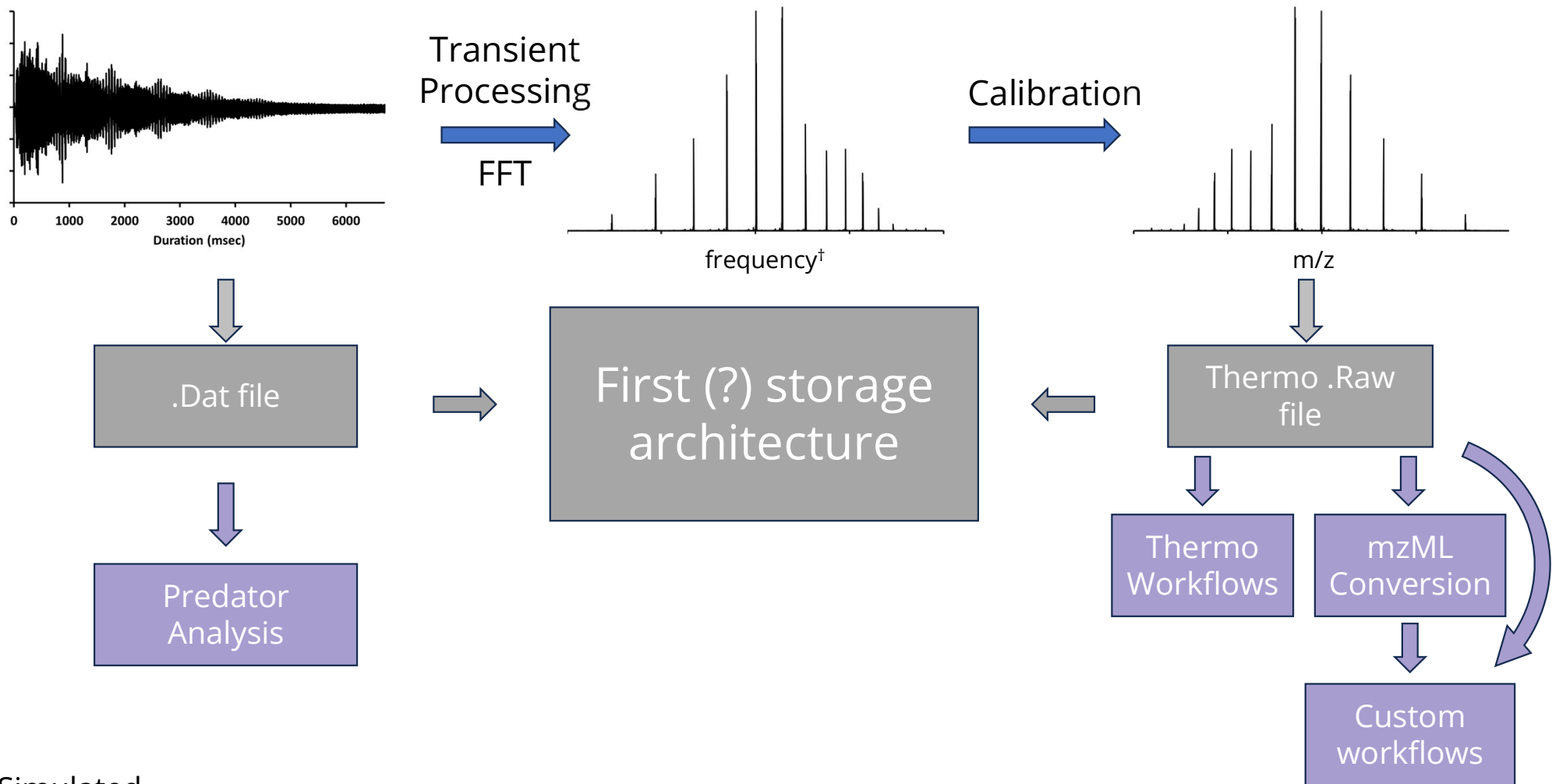


External  
Components

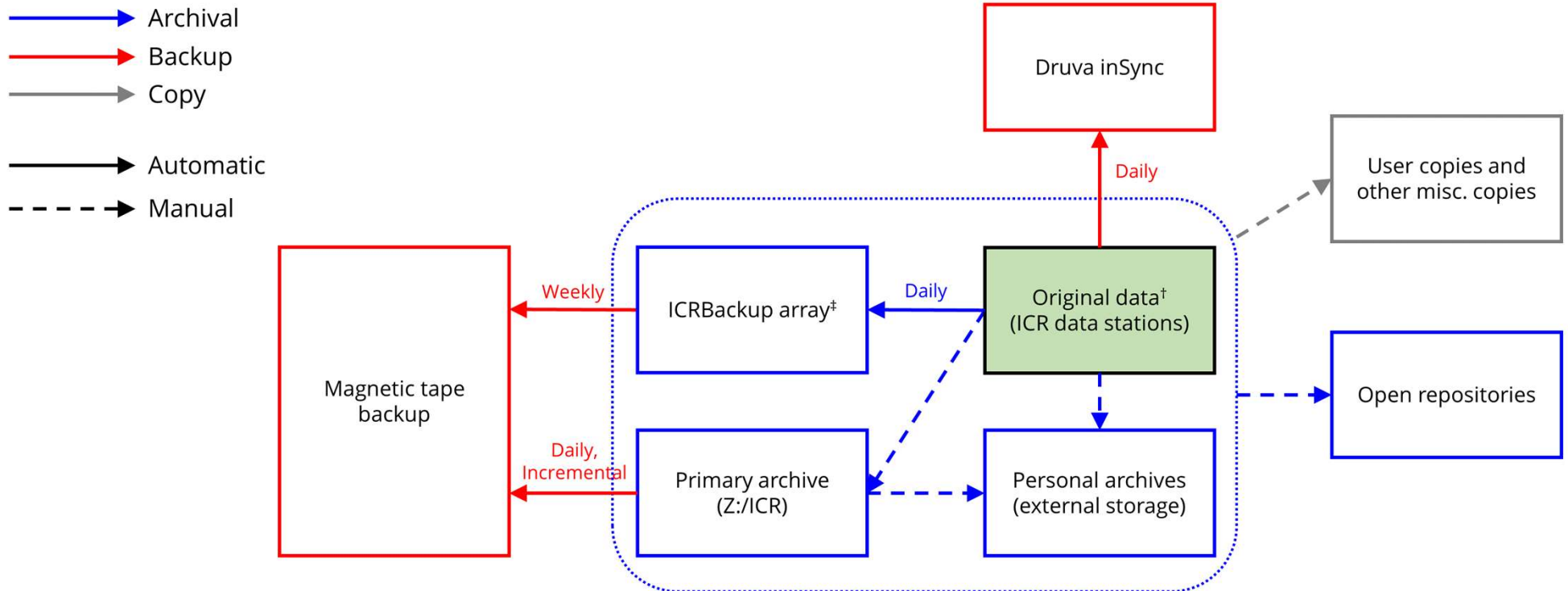


1. FlatBuffers Docs. <https://flatbuffers.dev/>

# Data Processing



# ICR Data Management Map



† : Data stations run Windows 10. Acquired data is stored in C:/Data.

‡ : Contents of C:/Data and a few other relevant folders containing instrument methods are automatically archived daily. Read-only access to ICRBackup is available to ICR faculty & staff.

## Shortcomings of the Existing Architecture

### Enabling FAIR data and metadata

- Missing metadata
- Facilitating machine actionability

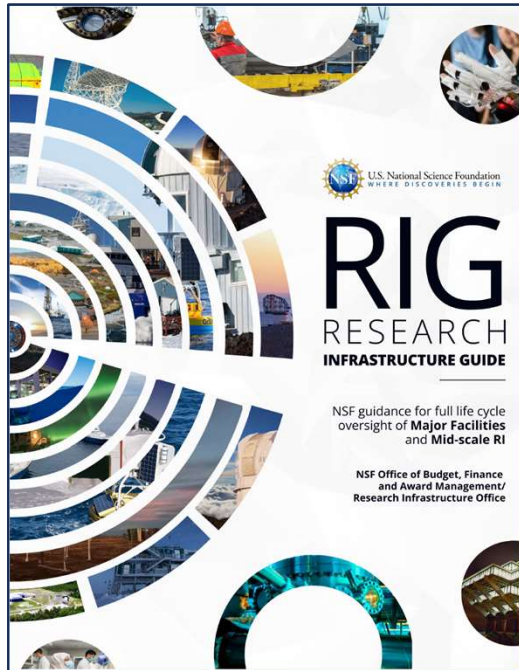
### Handling large and increasing data volumes and densities

- Exacerbated by new instrument developments
- As the amount of archived data grows, the potential for data mining increases

### Information Assurance

- New Information Assurance guidance focusing on data management and curation
- We want enable user access and facilitate ML and HPC
  - but this introduces security concerns

# Information Assurance



A draft of the revised NSF Research Infrastructure Guide was (released January 6<sup>th</sup>) outline the need for an Information Assurance (IA) program and the importance of **integrating IA with data management and curation efforts.**

All new CI for handling data generated by RI must consider IA to address the evolving threat landscape.

We believe this is particularly important for well-annotated FAIR data, which could be **easily reused by data thieves.**

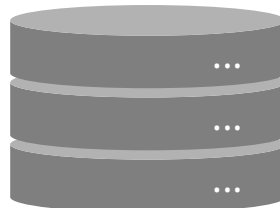
# Future Solutions

21 T FT-ICR

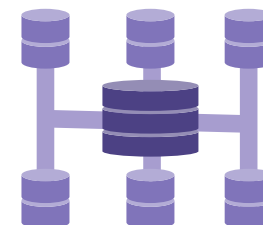


Data  
Transfer

ICR Database



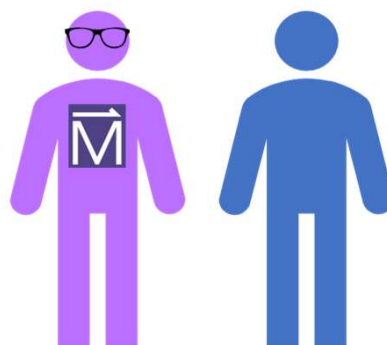
High-speed Access for  
HPC and ML Applications



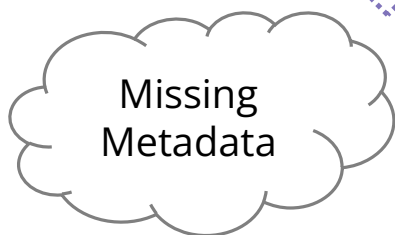
Cloud-based Analysis  
and Visualization



Access for Project  
Collaborators

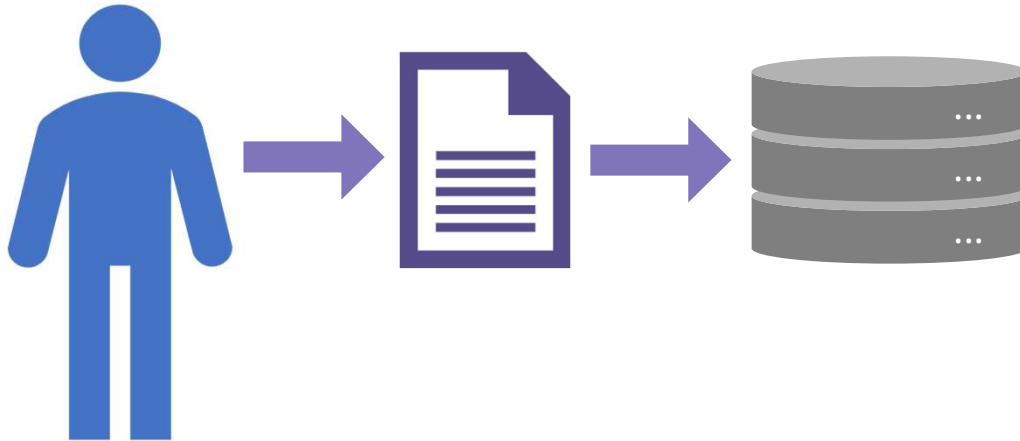
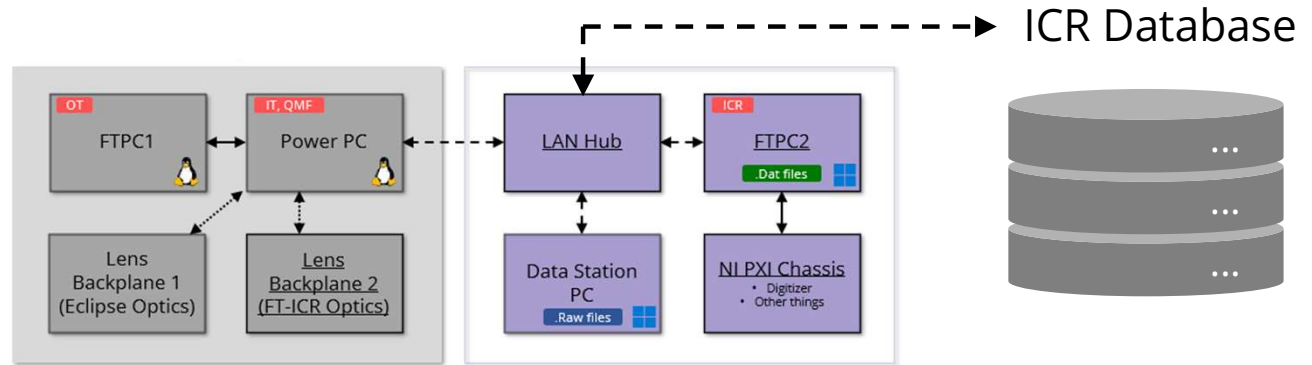


Missing  
Metadata



## Future Solutions

Additional software components on DS PC/FTPC2 could transfer data after analysis is complete or stream it in real time to ensure data is catalogued, indexed, immediately available, and has integrity.



The “missing metadata” needs to be provided by users, but a very low activation barrier is needed for compliance. A standalone GUI application or web-based form could provide ease-of-use.

# Data Ingestion Prototype

The screenshot displays a web application running on a browser at the address `localhost:3000`. The application's title is "Proteomics Experiment Metadata". A navigation bar at the top includes a "Home" link and an "Experiments" link. The main content area features a form titled "Enter Experiment Details" with the following fields:

- Experiment Name
- Description
- Creator**
  - Name
  - Role (dropdown menu with "Select a role" as the current selection)
- ORCID (pre-filled with "0000-0000-0000-0000")
- Keywords
- NHMFL Proposal Identifier
- NHMFL Experiment Identifier

# Data Ingestion Prototype

The screenshot shows a web browser window with a single tab titled 'React App' at the address 'localhost:3000'. The browser's address bar and navigation icons are visible. The main content area displays a form titled 'Creator' with the following fields and controls:

- Name:** A text input field.
- Role:** A dropdown menu with the placeholder text 'Select a role'.
- ORCID:** A text input field with the placeholder text '0000-0000-0000-0000'.
- Keywords:** A text input field.
- NHMFL Proposal Identifier:** A text input field.
- NHMFL Experiment Identifier:** A text input field.
- Date Created:** A text input field with the placeholder text 'mm/dd/yyyy' and a calendar icon on the right.
- External Repository URI:** A text input field with the placeholder text 'Any valid URI'.
- Public Accessibility:** A dropdown menu with the placeholder text 'No'.
- Upload Raw File (Max 1 GB):** A section containing a 'Choose File' button and the text 'No file chosen'.
- Submit:** A green button located at the bottom of the form.



# Thank you !

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