



# Yale Keck MS & Proteomics Resource: Supporting research through mass spectrometry

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**Mission** to provides efficient and cost effective proteomics and small molecule mass spectrometry based services.

**Introduction** The Mass Spectrometry (MS) & Proteomics Resource at Yale has its roots in 1980 in the Department of Molecular Biophysics and Biochemistry and has a history of providing investigators with access to the most advanced protein and small molecule profiling technologies.

## Mass Spectrometers (MS)

**For Protein ID**

Thermo Fisher Scientific nano-UPLC ESI **LTQ-Orbitrap ELITE** MS systems

**For Protein PTM, Profiling, & Quantitation**

Thermo Fisher Scientific nano-UPLC ESI **Q-Exactive Plus** MS systems

**For Open Access Usage**

Thermo Fisher Scientific nano-UPLC ESI **LTQ-Velos** MS systems

**For Metabolism Separation & Quantitation**

PE UPLC AB Sciex **4000 QTRAP** MS system

**New Instrumentation**

Waters H-Class **UPLC**

**Q-Exactive HF-X** mass spectrometer with **ACQUITY UPLC C-M-Class**

## MS Capabilities

**Resolution**

**Mass Accuracy**

**Fragmentation Capabilities**

**Quantitation**

**Facile loss of H<sub>3</sub>PO<sub>4</sub>, X-cleavage preferred**

**Retention of m+H<sup>+</sup>**

**Retention of label modifications**

**No X-P cleavage**

## Instrument Funding

(4000 QTRAP) NIH CTSA, UL1 RR024139 (Orbitrap ELITE) NIH SIG, RR031795 (Orbitrap Fusion and Q-Exactive Plus) [1S10OD018034-01 & YSM] (UPLC H-Class) [1S10OD019967-01 & YSM] (Q-Exactive HF-X Mass Spectrometry system) [S10OD023651-01A1 & YSM]

## Services

- Protein Identification**
- (1) Basic Protein ID
  - (2) Protein Post Translational Modifications:
    - Phosphorylation
    - Ubiquitinylation
    - Acetylation
    - Methylation
- Protein Profiling and Quantitation**
- (1) Label Free Quantitation:
    - Protein Level
    - Peptide Level
    - PTM Level
  - (2) TMT (multiplexed isobaric tagging; 6- or 10-plex)
  - (3) Stable-Isotopic Labeling of Amino acid in Cell culture (SILAC).
  - (4) Targeted Protein Quantitation (PRM).
  - (5) Untargeted Protein Quantitation (DIA).

## Small Molecule Analyses

- (1) Exact/Accurate Mass Determinations
- (2) Structural Elucidation
- (3) Small Molecule Quantitation: Targeted Compound Specific (e.g.: drug, hormones, lipids, etc.)

## Basic Protein ID of 1D or 2D\* gel bands or spots

Just want to know what protein that band or spot in your gel is? Then this is the service for you!

### Samples need to be...

- In a Coomassie blue stained gel band (additional charge applies for silver stained gel bands)
- Place in an Eppendorf tube without buffer (\*\*Do not use color tubes)
- Gel volumes (lane width x gel thickness x band height) less than 50mm<sup>3</sup>, (additional charges applies if gel bands are larger than this).
- Simple protein mixtures (e.g.< than 30 proteins in the band)
- Submitted in YPED (The Yale Protein Expression Database, <http://yepd.med.yale.edu>)

### Samples will be...

- Digested with trypsin
- Analyzed by LC MS/MS on a LTQ Orbitrap Elite
- Database searched against the NCBItr or SwissProt databases (any taxonomy in these databases)
- Results will be posted online in YPED
- All with a quick turn-around

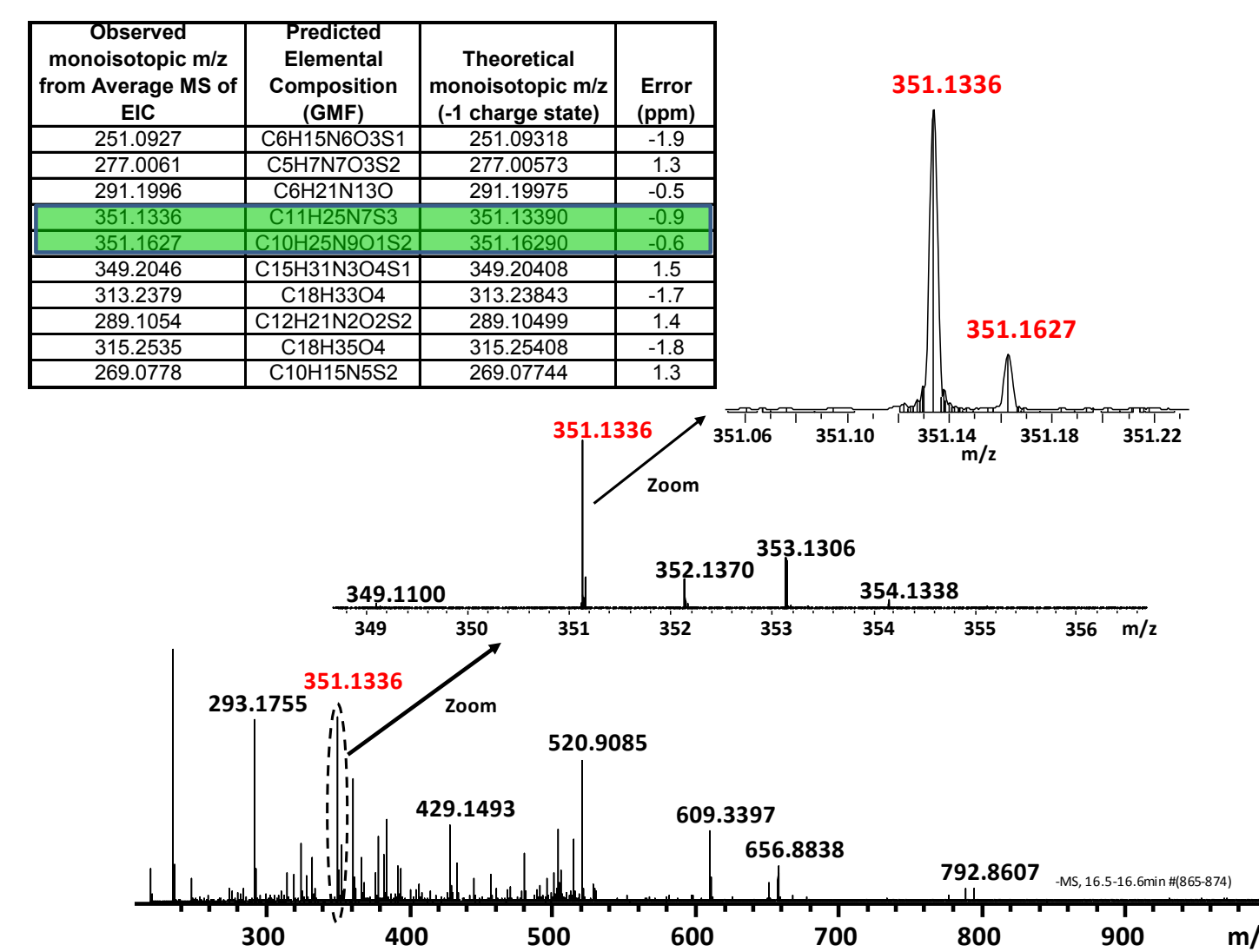
**Cost:** \$114 per sample/gel band (Yale) \$137 per sample/gel band (Non-Profit)\*\*

**Sample Submission:**

- 1) Drop off at Yale's MS & Proteomics Resource located at 300 George St, Rm G001 (ground level)
- 2) Ship to: Attn: Basic Protein ID MS & Proteomics Resource 300 George Street Suite G001 New Haven, CT 06510

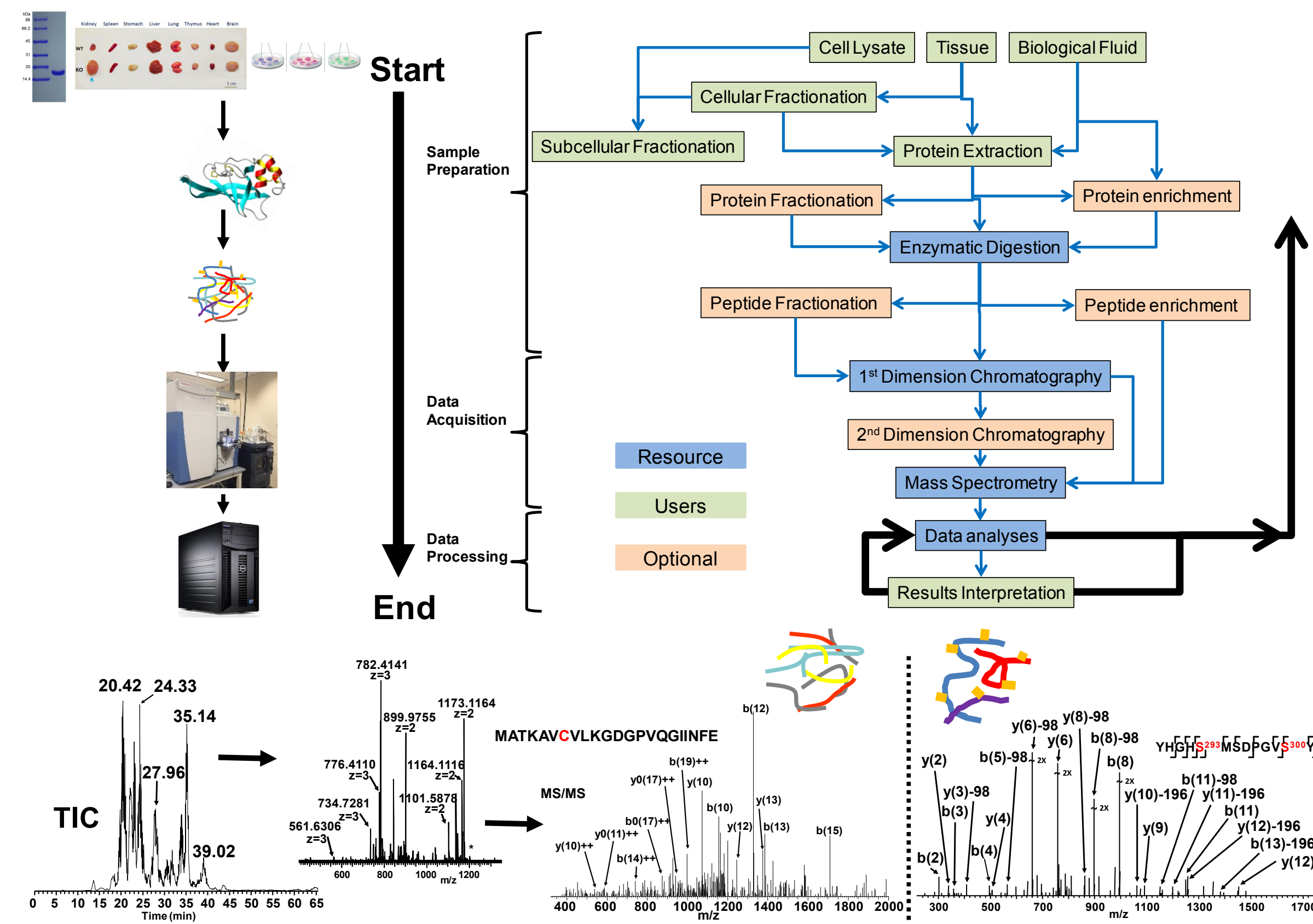
\*Volume discount available for 20+ spots per submission.

## Small Molecule: Exact Mass Determination

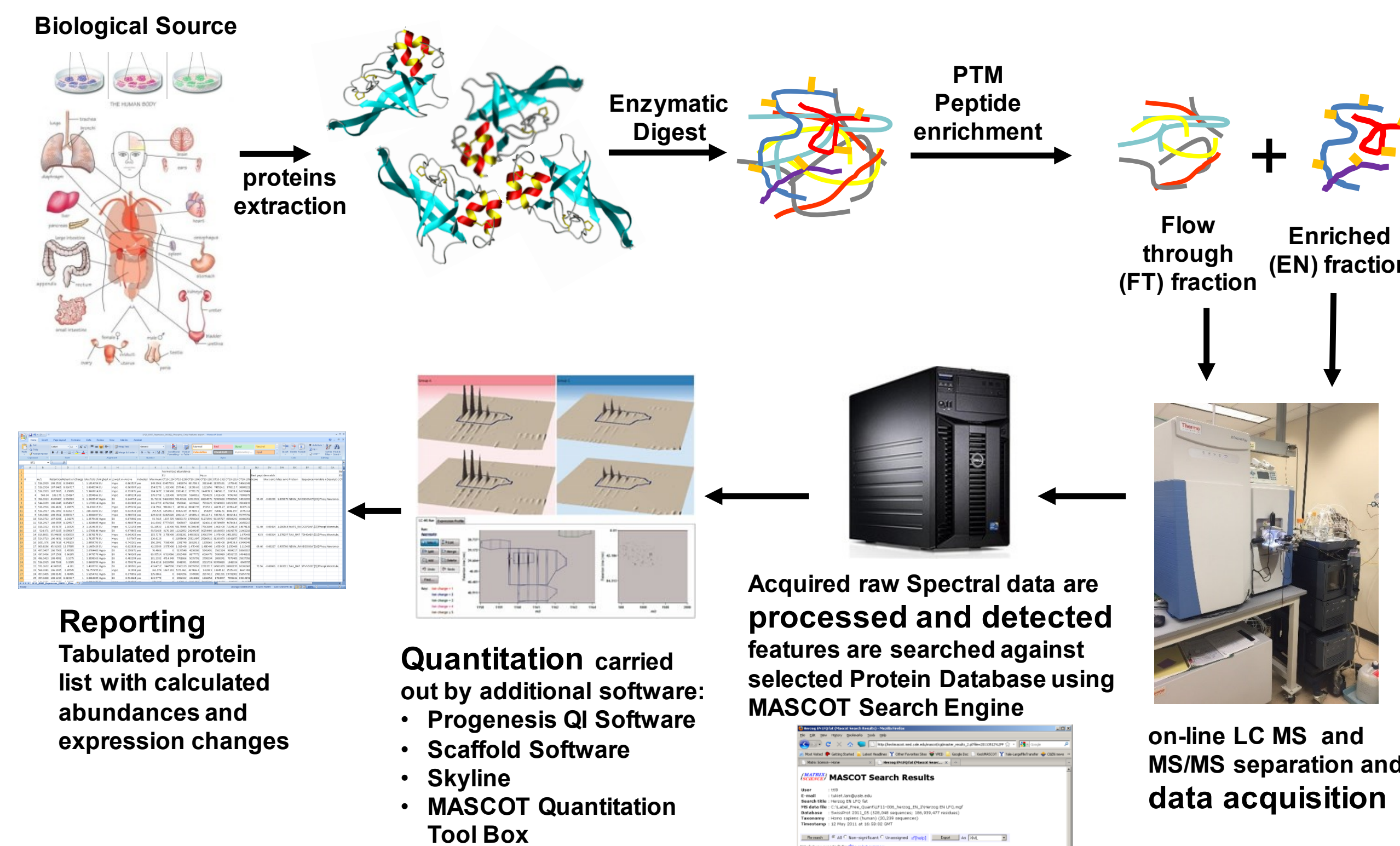


## Workflows

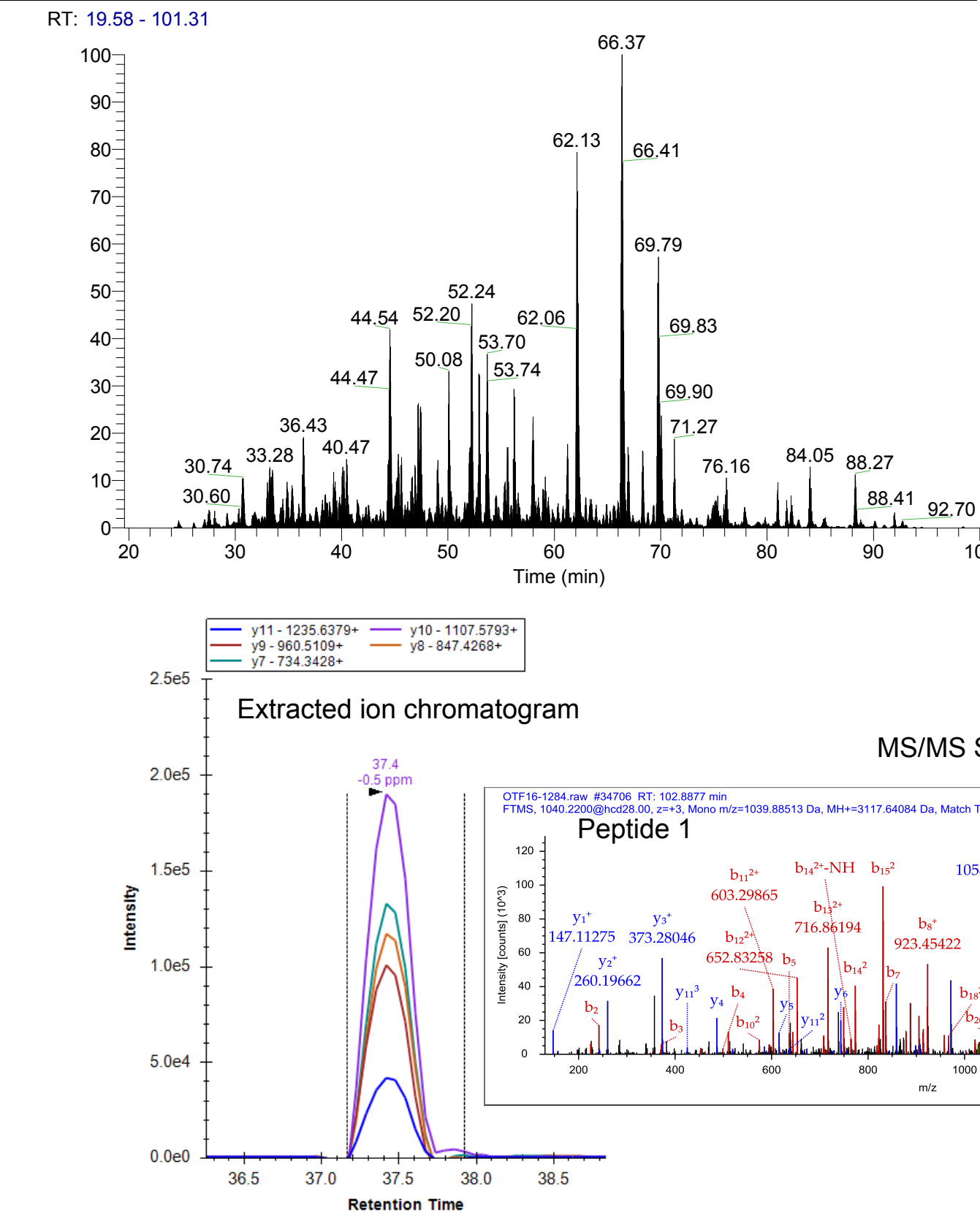
### Identification of Protein and Protein Posttranslational Modification (PTM)



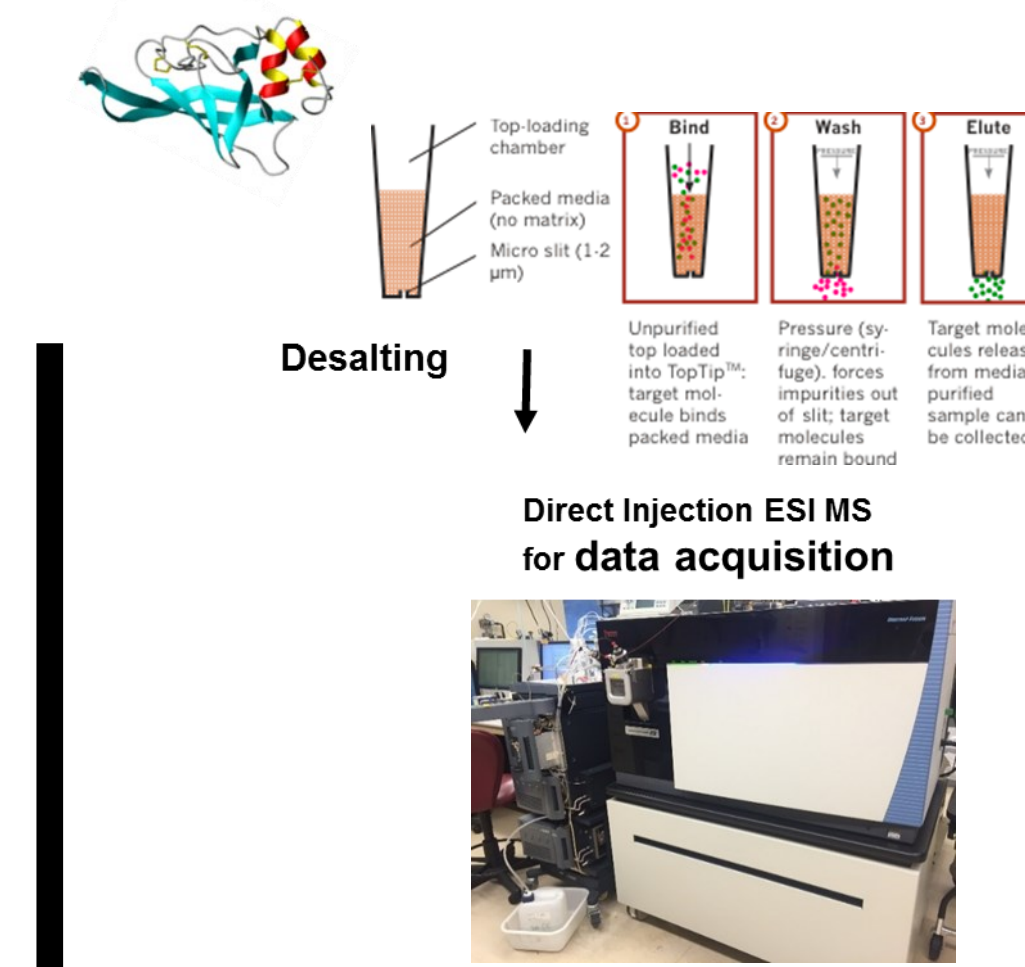
## Quantitative Proteomics



## Parallel Reaction Monitoring (PRM)



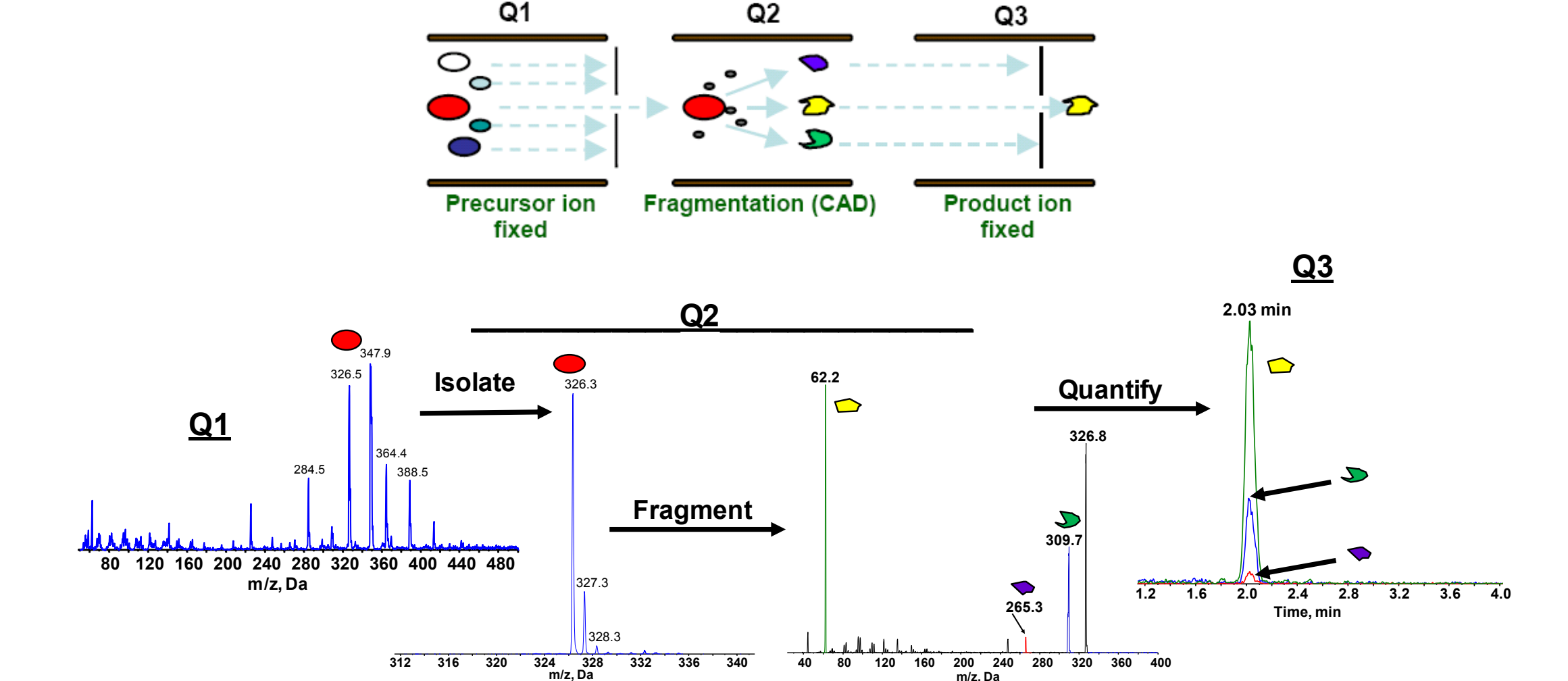
## Intact protein analysis



**Sample:** Single purified protein of molecular weight up to 50 kDa that is either lyophilized or dissolved in water. **No salts, detergents, or chemicals.** We currently require at least 100 micrograms of protein; and is working to improve on this to hopefully only requiring 10 µg or less.

- Steps**
- Samples will be analyzed by direct infusion method on Orbitrap-Fusion mass spectrometer (ThermoFisher Scientific).
  - Standard Pressure Mode (8 mTorr) or Intact Protein Mode (3 mTorr and 1 mTorr) pressure will be tested to get best results.
  - Data will be analyzed with Protein Deconvolution 4.0 software.

## Small Molecule Quantitation (Targeted)



## Recent Publications

**proteome**

**Cell Reports**

**SCIENTIFIC REPORTS**

**PLOS ONE**

**bioRxiv**

## Contacts

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