

Research Opportunities in the Poutsma Group

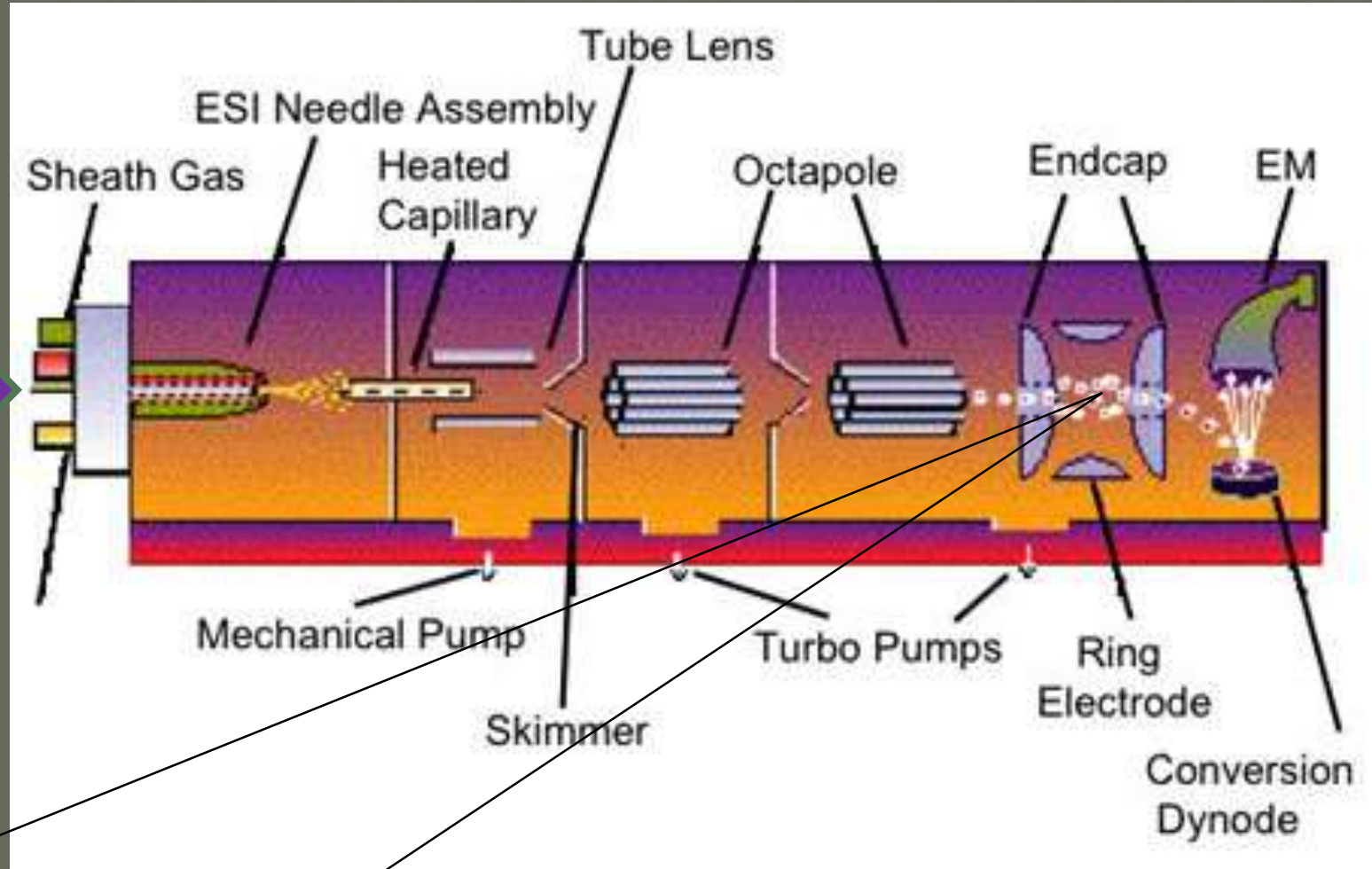
IONS

are
the
new **BLACK**

On-going Projects

- **Gas-phase biophysical chemistry**
 - effects of systematic substitutions on amino acid thermochemistry
 - thermochemistry of small peptides
- **Gas-phase ion structure**
 - H/D exchange
 - Infrared multiphoton dissociation (IRMPD)
- **Gas-phase proteomics research**
 - custom solid-phase synthesis of peptides
 - mass spectrometer fragmentation studies
 - collaborative studies with Biology Dept.

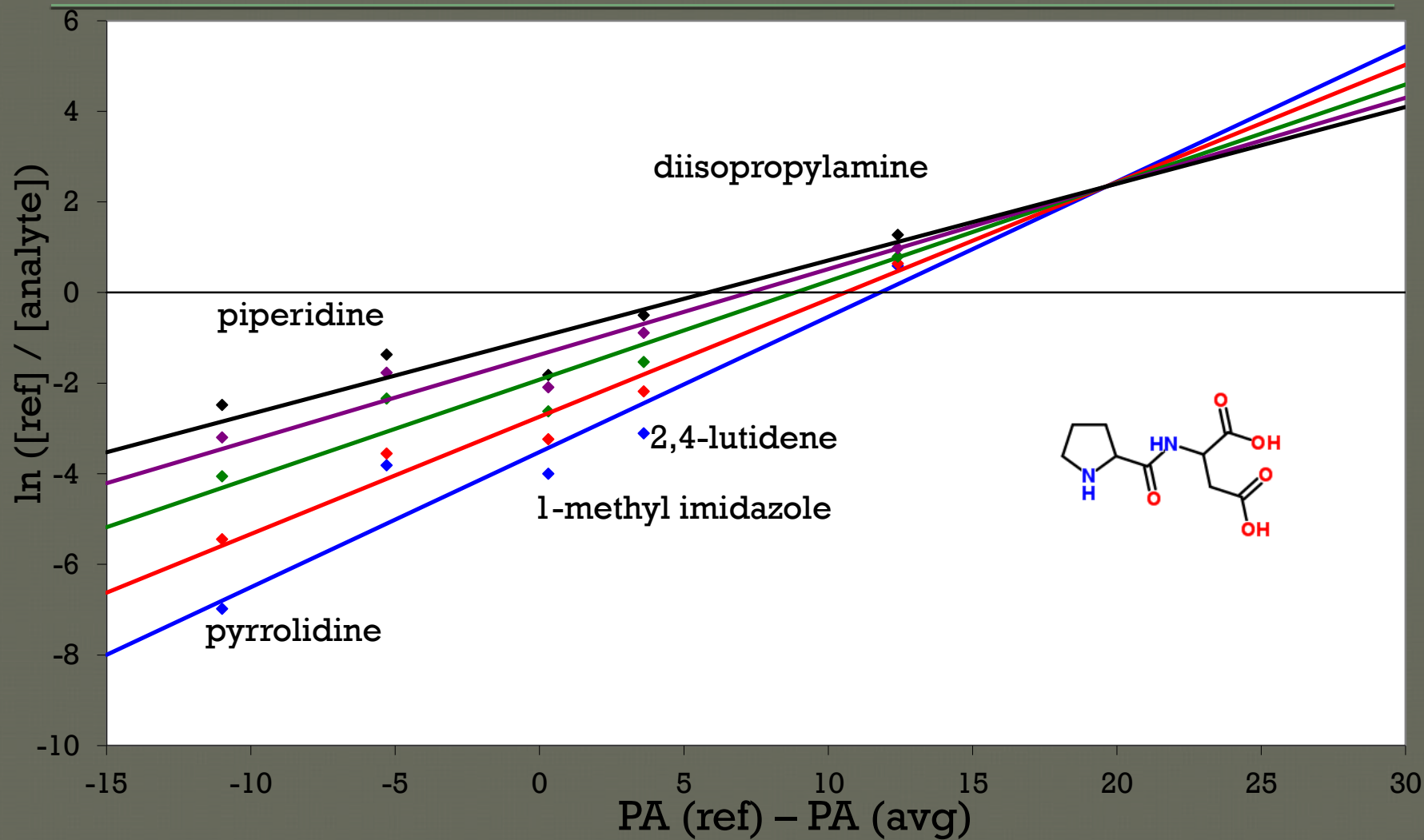
ESI-ion trap instrument kinetic method studies



sample



Pro-Asp: kinetic method plot



New instruments are here!!!

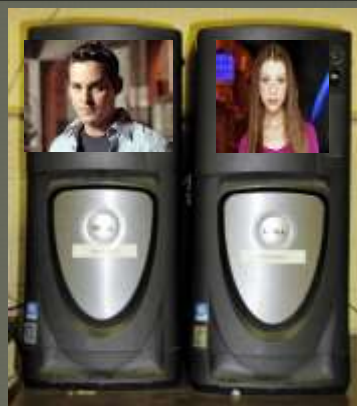
Electrospray ionization
triple quadrupole



UPLC-nanospray
linear ion trap
with ETD



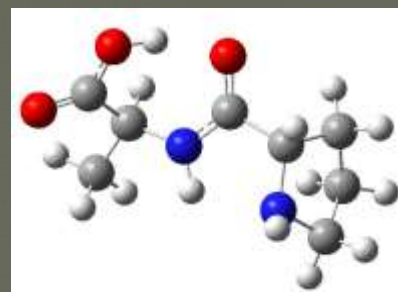
Computational Studies



- We use computational chemistry to support and guide our experimental work.
- Collaborator: Prof. Jennifer Poutsma (ODU)



Pro-Gly



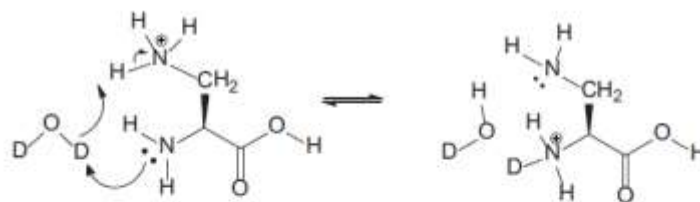
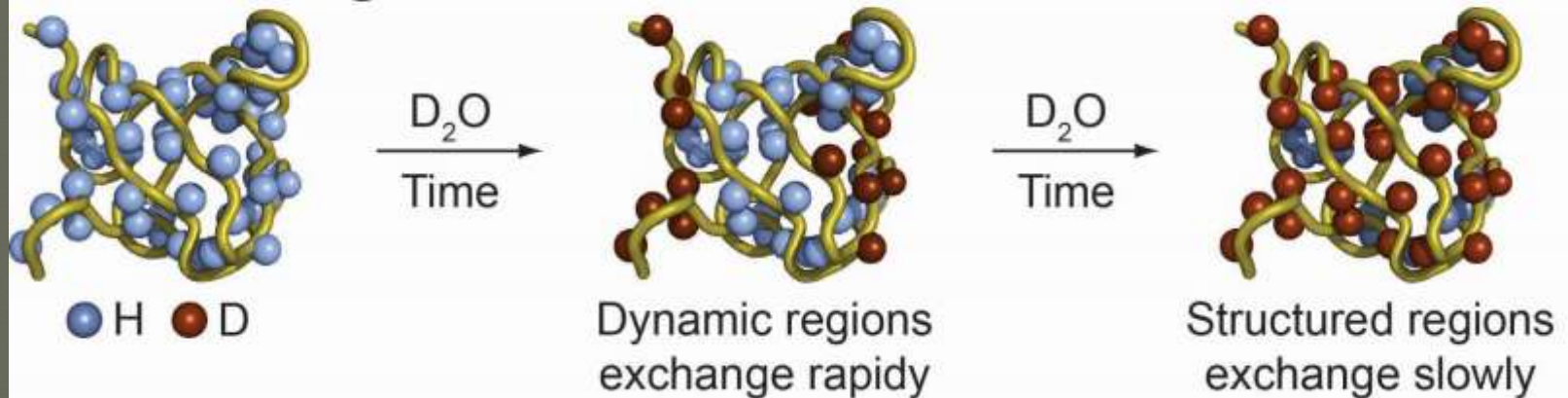
Pro-Ala

On-going Projects

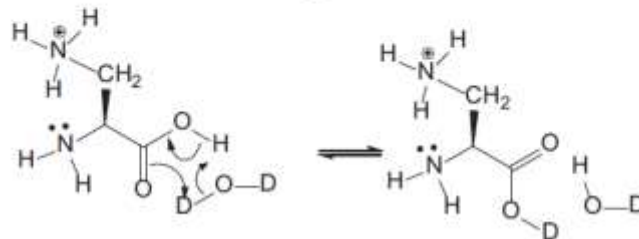
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Hydrogen-deuterium exchange

H/D Exchange



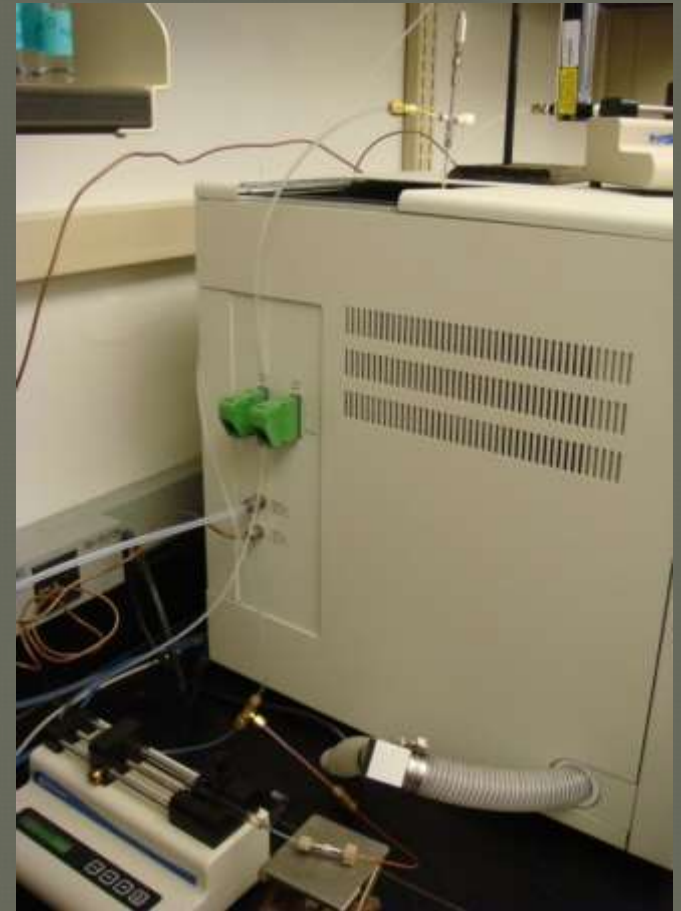
Relay Mechanism



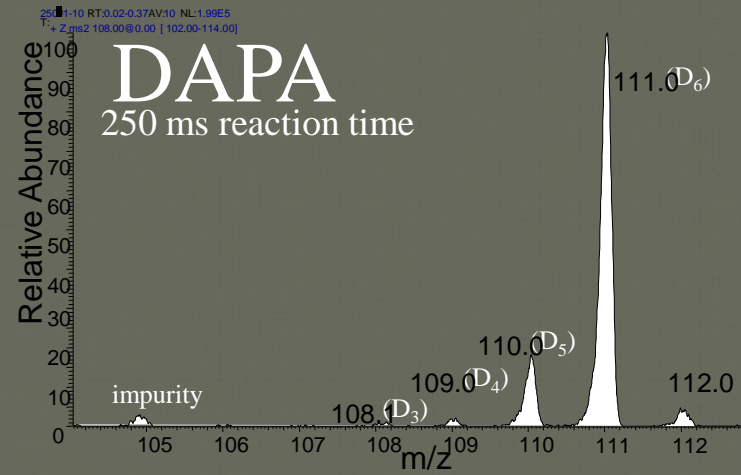
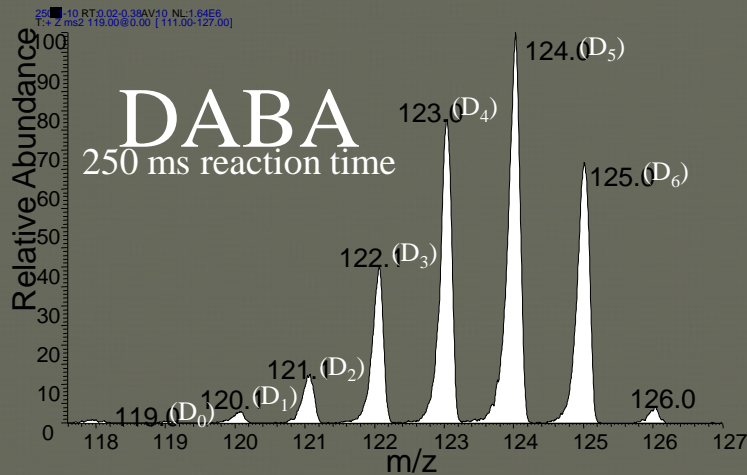
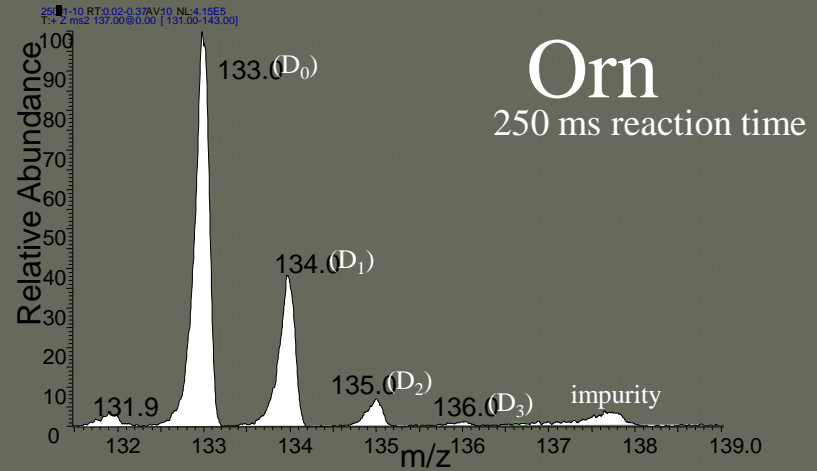
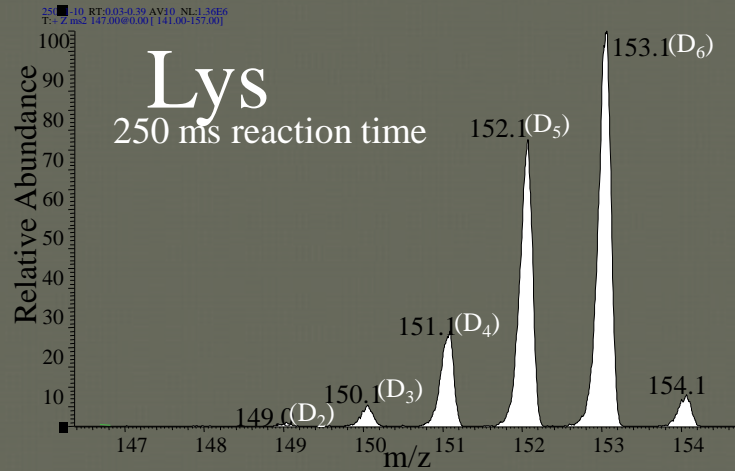
Flip-Flop Mechanism

H/D-exchange - instrumentation

- A syringe pump is used to pump D₂O reagent gas into the helium line of the mass spectrometer
- The helium line is then connected to a needle valve for finer control of pressure inside the ion trap
- The D₂O pressure in the trap is obtained by measuring the rate of H/D exchange for betaine, which has a known rate coefficient of $1 \times 10^{12} \text{ cm}^3/\text{molec s}$

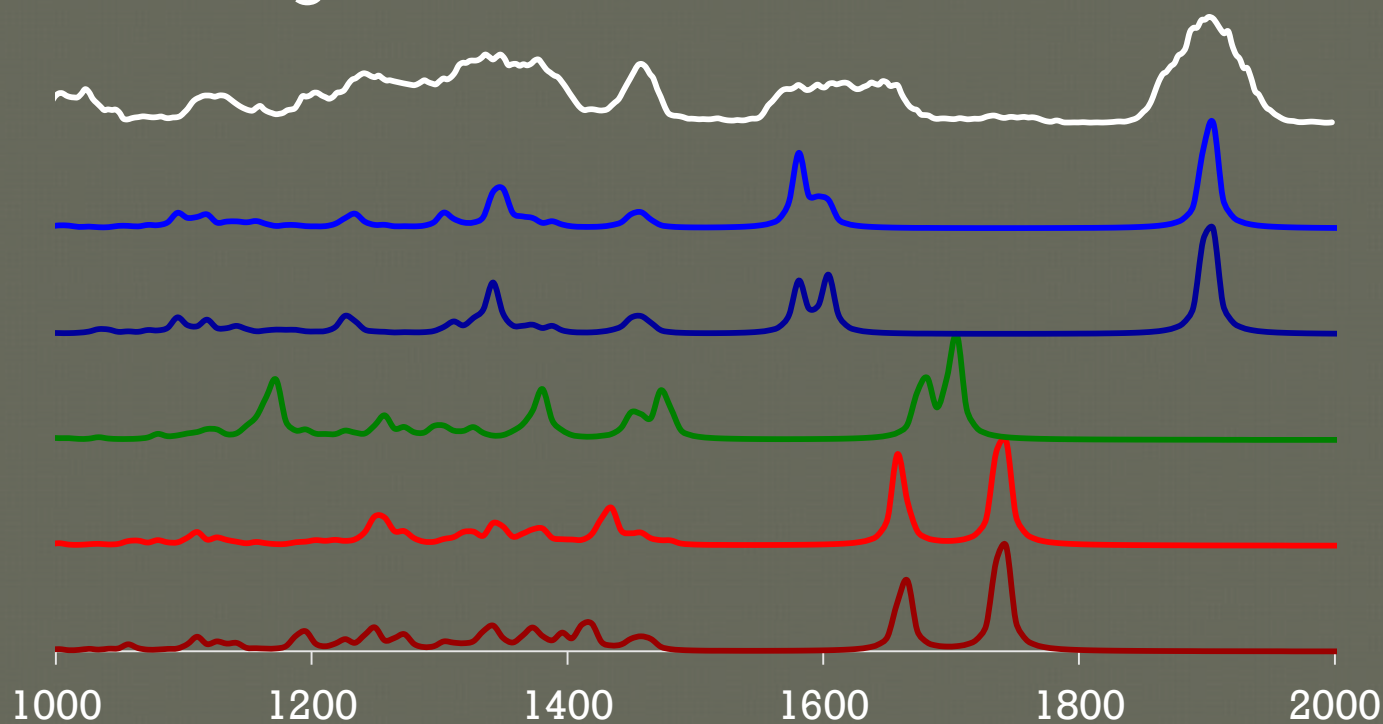


H/D-exchange – data acquisition



IRMPD studies of vibrational spectroscopy

- CLIO (Orsay) and FELIX (Nijmegen) FEL's
- infrared action spectroscopy of ions
- 1-2 week trips to France and Netherlands during the summer



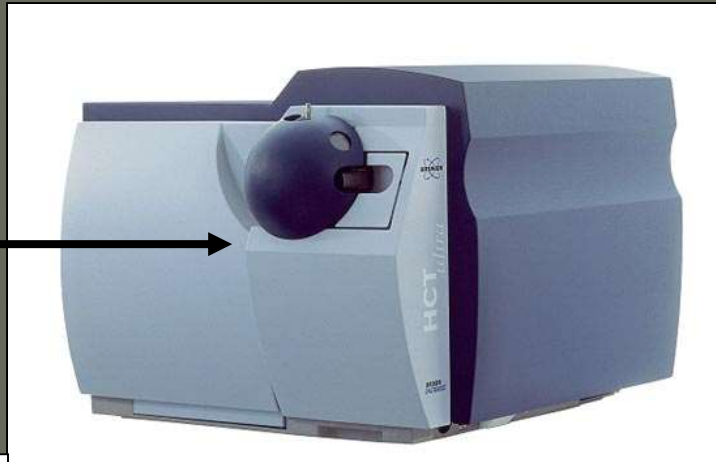
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Proteomics – mass spectrometry approach

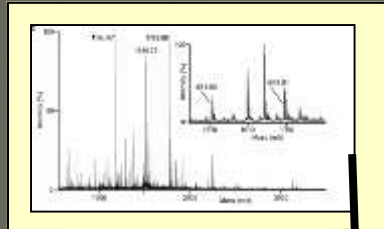


Peptide

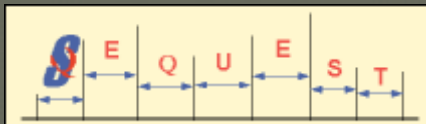


Tandem Mass Spectrometer

Collision-Induced Dissociation (CID)



Mass Spectrum



Mascot

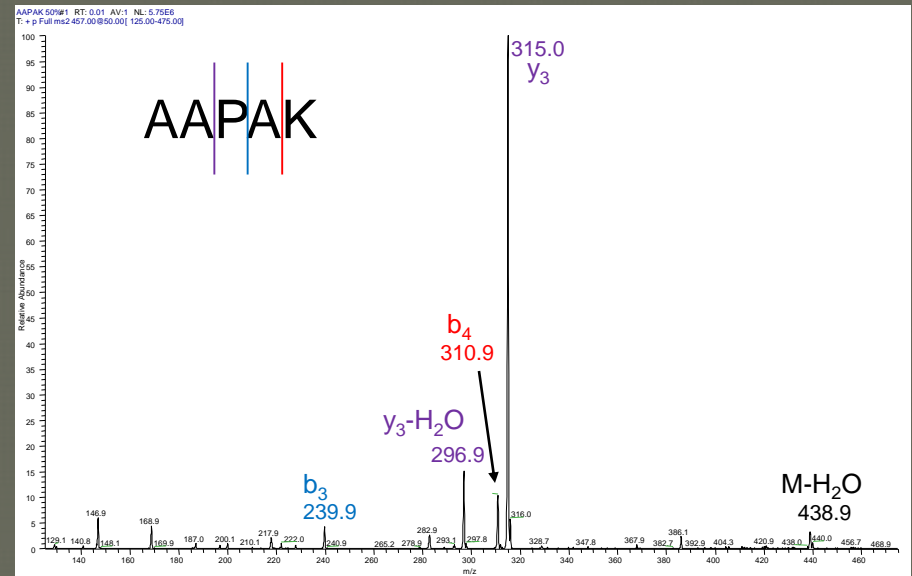
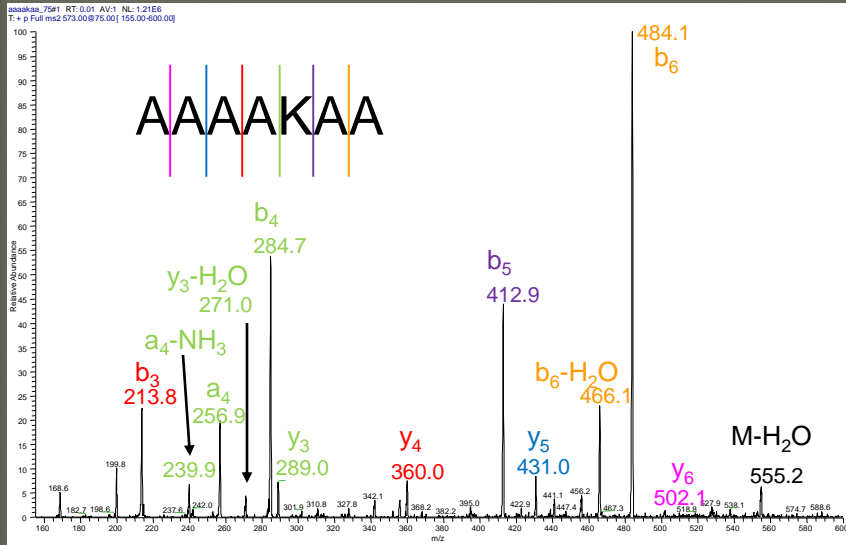
MATRIX SCIENCE

PeptideSearch

Peak Mass (Da)	Sequence
1871.9	1-18 acetyl-GEEDVQALVVDNGSGNVK
928.45	19-28 AGVAGDDAPR
1186.67	29-39 SVFPSIVGRPK
2522.16	40-62 NPGIMVGMEEKDAFVGDEAQTKR
800.53	62-68 RGILTLK
1946.91	69-84 YPIEHGIVTNWDDMEK
1515.73	85-95 WHHTFYNELR
1926.03	96-113 AAPEEHPVLLTEAPLNPK
3169.49	148-177 TTGIVLDSGDGVSHIVPIYEGYALPHAMR
644.4	178-183 LDLAGR
1012.5	184-191 DLTEYLMK
667.4	192-196 ILHER
1046.51	197-206 GYGFSTSAEK
1129.65	207-215 EIVRDIKEK
1645.72	216-228 LCYALNFDEEMK
1776.88	239-254 SYELPDGNITVGNER
1796.92	255-269 FRCPEALFQPSFLGK
1617.83	270-284 EAAGIHTTFFNSIKK
1033.56	284-291 KCDVDIRK
2245.08	292-312 DLYGNVLSGGTTMYEGIGER
1177.61	316-326 DITTLAPSTMK
1136.72	327-336 IKVAPPERRK
1517.68	360-372 EYDESGPSIVHR

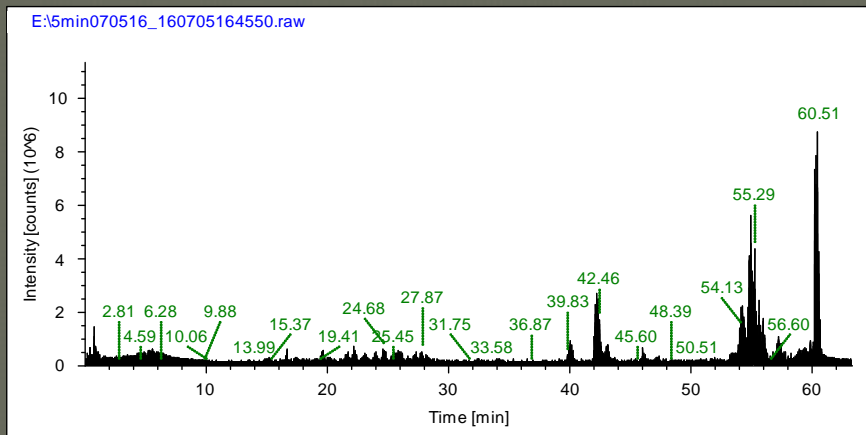
“Fingerprint”

Selective Cleavages

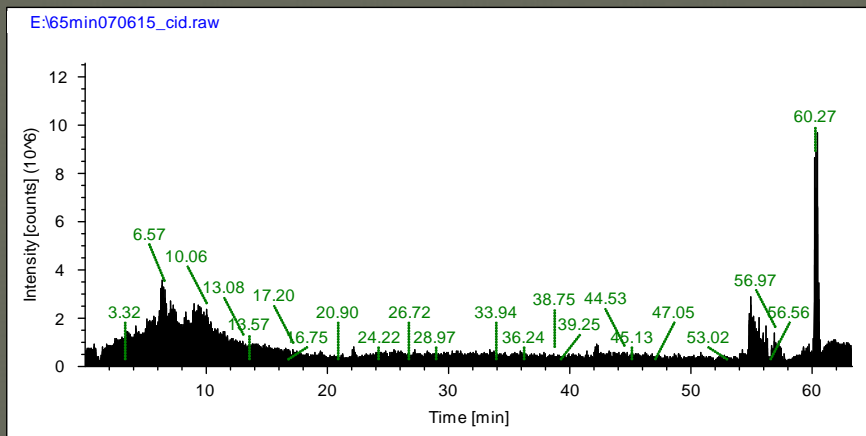


Actual real-life samples

- We are collaborating with Professors Allison, Forsyth, and Williamson on bacterial and viral samples



44 e. coli protein groups
1 T7 protein group



5 e. coli protein groups
6 T7 protein groups

Needs

- I have NSF and NIH funding that can be spent on students. Looking for honor students!
- We have plenty of peptides to synthesize and fragment and analyze.
- I have two returning Juniors
- I would like to pick up 1-2 additional 320 students and 1-2 Freshman in the Spring.