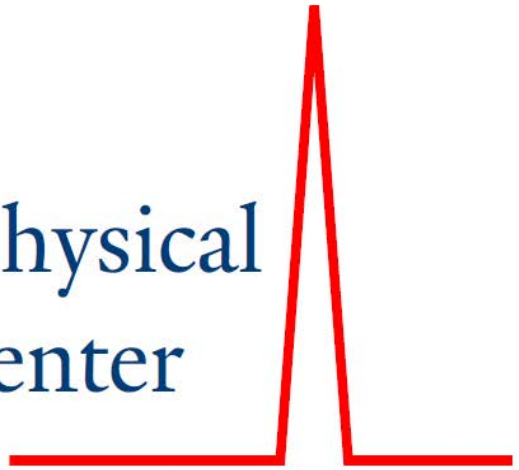
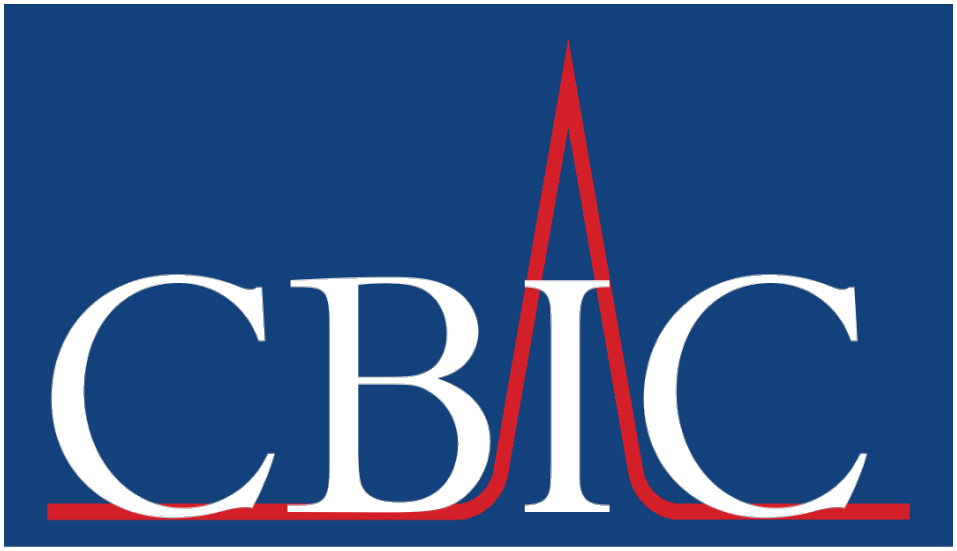
Yale

Chemical and Biophysical Instrumentation Center



Yale Day of Instrumentation 2020

Core facilities and instrument development at Yale



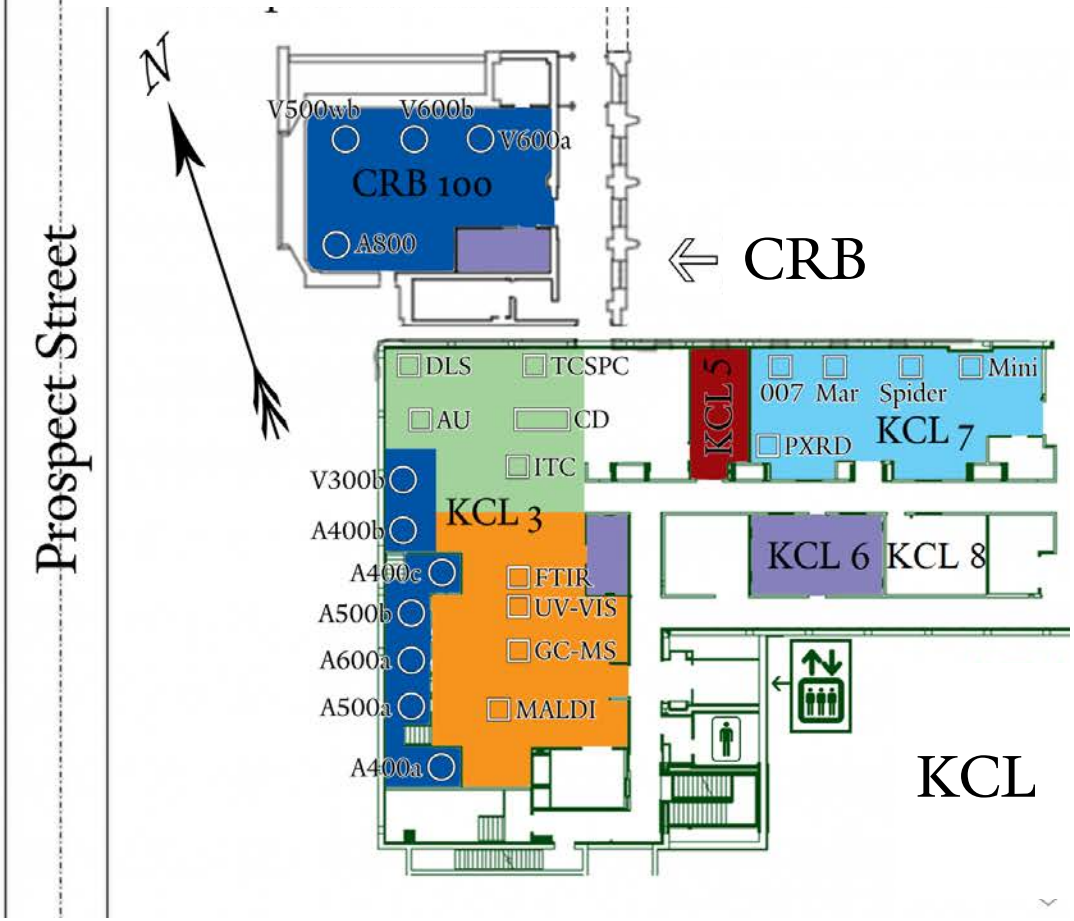
Yale Chemical and Biophysical Instrumentation Center

Who are we?

How can we fit into instrument development?

http://cbic.yale.edu

The Yale CBIC is a core instrumentation facility located in the chemistry department.



Three key areas of expertise:

NMR Spectroscopy

Mass Spectrometry

X-ray Diffraction

Also:
optical spectroscopy, calorimetry, etc.

We have many instruments, however…

People in the CBIC

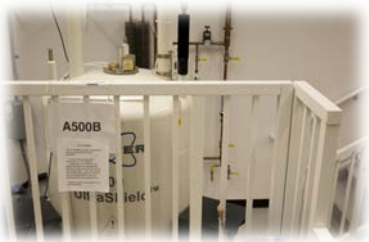
- Eric Paulson, Ph.D.
  - Director, NMR Spectroscopist
- Xiaoling Wu, Ph.D.
  - NMR Spectroscopist
- Brandon Mercado, Ph. D.
  - X-ray crystallographer
- Fabian Menges, Ph. D.
  - Mass Spectrometrist
- David Keller
  - X-ray & BIC instrument support

…people come first.

NMR Spectroscopy

12 NMR Spectrometers:

- 300 MHz
- 3x 400 MHz
- 2x 500 MHz
- 500 MHz wide-bore
- 3x 600 MHz
- 700 MHz
- 800 MHz

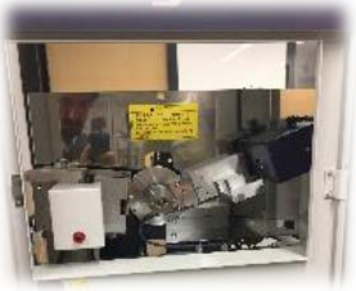


Mass Spectrometry

8 Mass Spectrometers:

- GCMS Quad
- GCMS Triple Quad
- LCMS Quad
- LCMS Triple Quad
- 2x LCMS Q-TOF
- MALDI-TOF
- LCMS Orbitrap

X-Ray Instrumentation



7 X-Ray Diffractometers

- Powder XRD
- 2x sealed tube
- 3x rotating-anode
- SAXS/WAXS

X-Ray MicroCT

Other Instrumentation

- Analytical Ultracentrifuge
- CD Spectrometer
- Dynamic Light Scattering
- Fluorimeter
- Isothermal Titration Calorimetry
- UV-Vis-NIR Spectrometer
- FTIR Spectrometer
- Polarimeter
- EPR Spectrometer

What can the CBIC do for instrument development at Yale?

People:

- User base of 200+ researchers
  - “customers”
  - seminars, events
- Professional Staff
  - operation, oversight
  - maintenance, repair
  - training
- Community
  - outreach, education

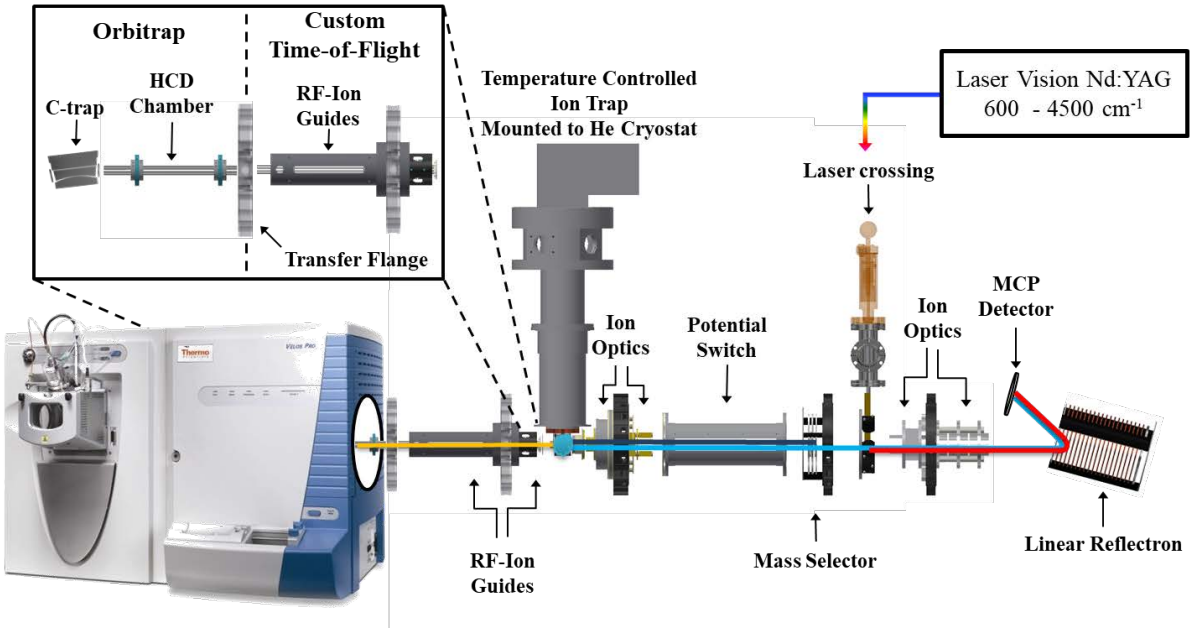
What can the CBIC do for instrument development at Yale?

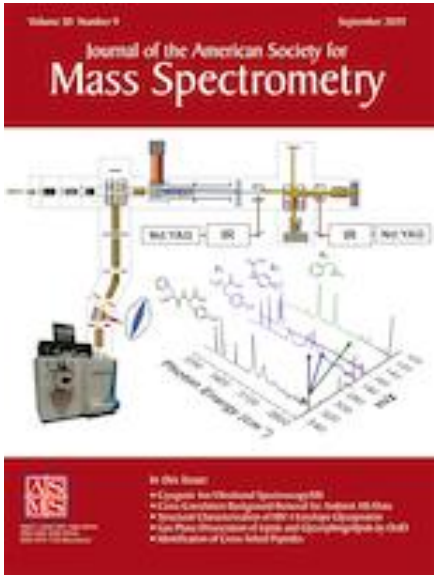
A Case Study (in progress):

© American Society for Mass Spectrometry, 2019
J. Am. Soc. Mass Spectrom. (2019) 30:1551-1557
DOI: 10.1007/s13361-019-02238-y
RESEARCH ARTICLE

Integration of High-Resolution Mass Spectrometry with Cryogenic Ion Vibrational Spectroscopy

Fabian S. Menges, Evan H. Perez, Sean C. Edington, Chinh H. Duong, Nan Yang, Mark A. Johnson
Department of Chemistry, Yale University, New Haven, CT 06520, USA

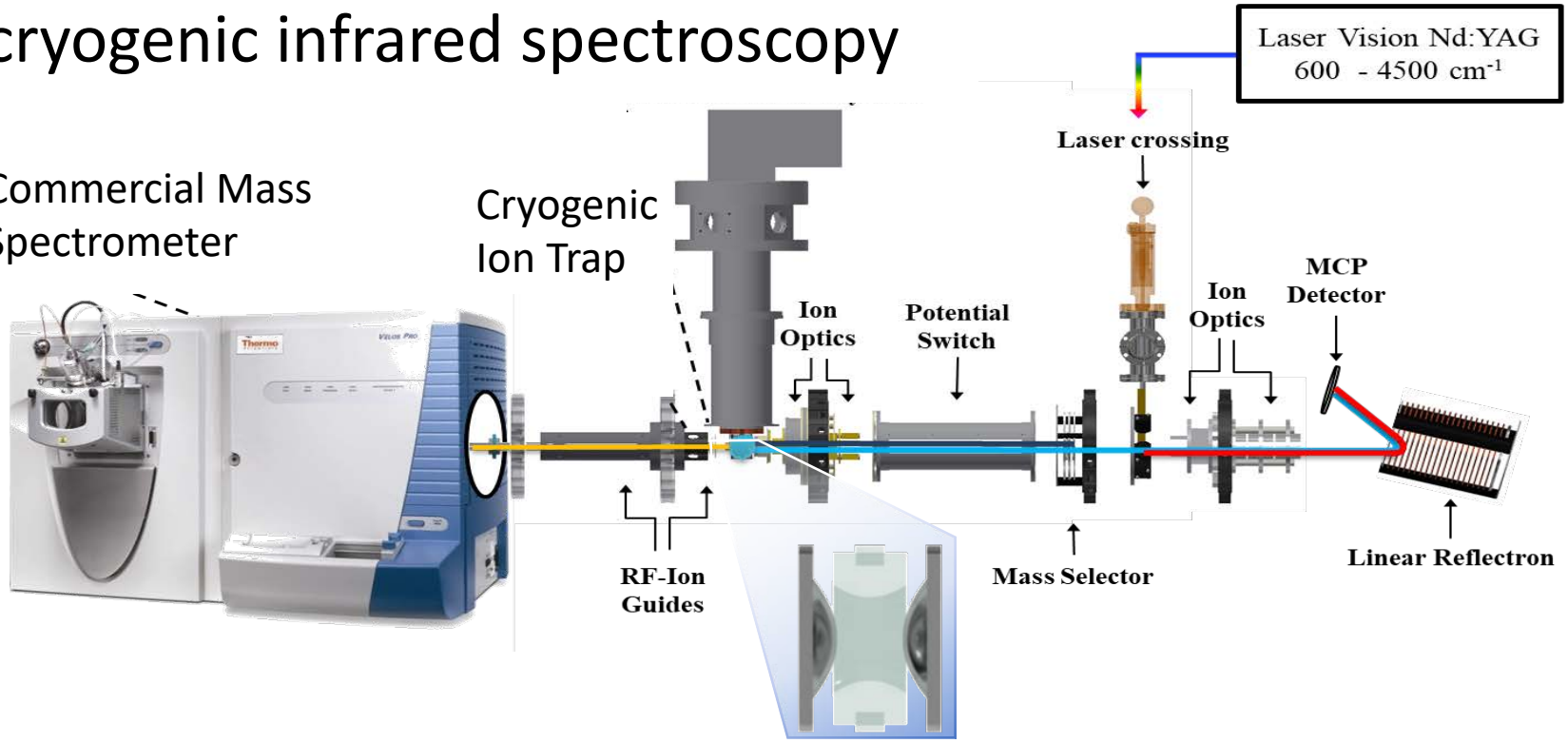


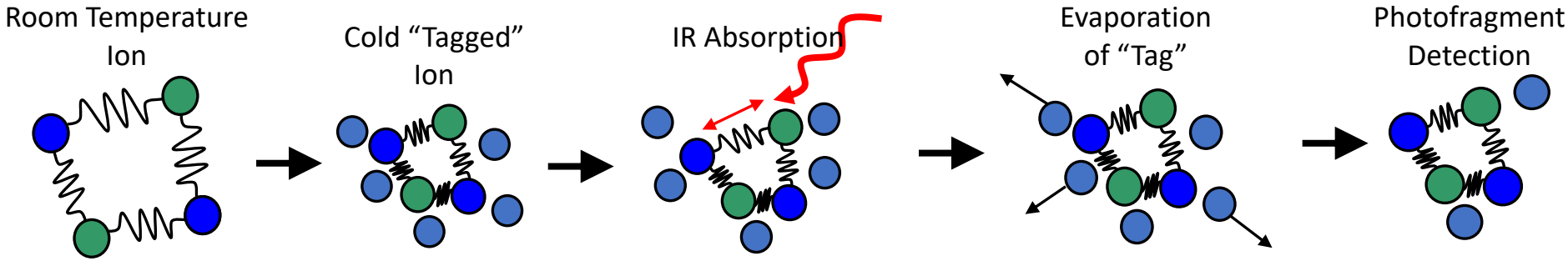


Hybrid Spectroscopy Instrument Developed in Prof. Mark Johnson's Lab –

Coming soon to a core facility near you!

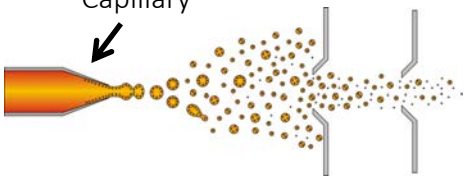
High resolution mass spectrometry integrated with cryogenic infrared spectroscopy





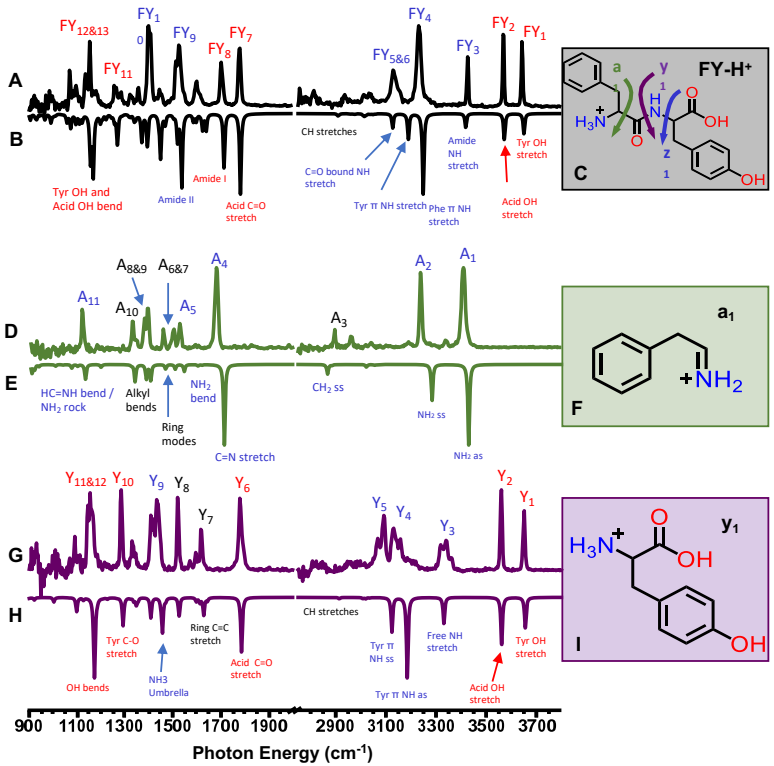
The promise of Hybrid MS/IR: Provide the **selectivity** and **sensitivity** of Mass Spectrometry and detailed **structural information** via cryogenic gas-phase IR Spectroscopy

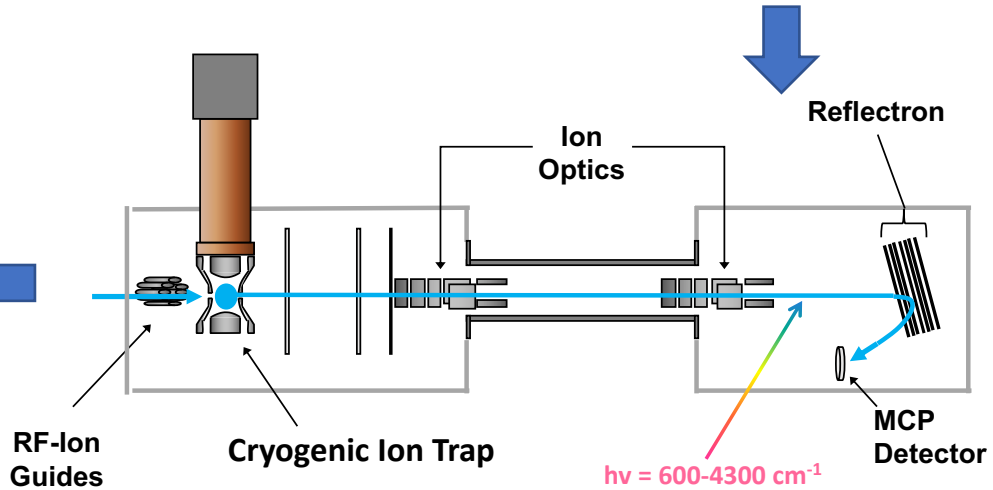
Molecule(s) of Interest



Electrospray Ionization

Mass Spectrometry

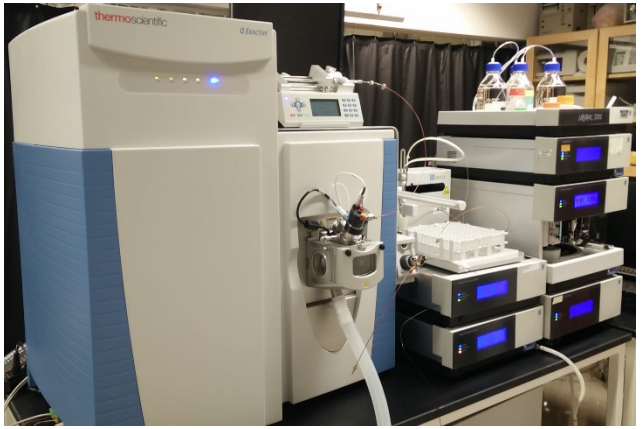




Cryogenic Gas-Phase IR Spectrometer

Hybrid spectrometer construction in the CBIC

- We successfully applied for an **NSF MRI development grant** in 2018
- Design is based on existing instrument in Johnson Lab
  - Thermo Fisher **QExactive Orbitrap** installed and running
  - Added LC-MS front end: **Dionex Ultimate 3000 UHPLC**
  - Currently building parts for the **cryo-IR extension**
- We plan to offer vibrational analysis as an “add on” to our existing high-resolution mass spectrometry service
- Initially will target samples/problems where structural information is crucial
- Eventually we hope to develop a streamlined workflow to offer the technique as a more “routine” analysis
- **Inert sample introduction** planned for air and moisture sensitive samples also planned

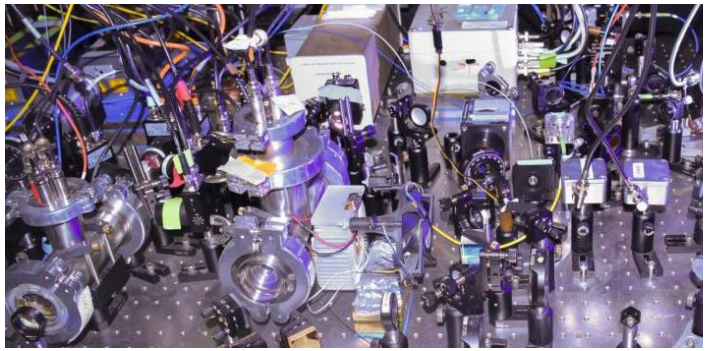


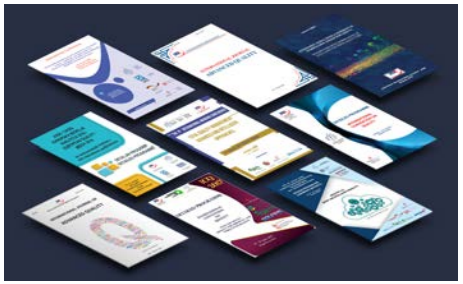
Dr. Fabian Menges

What can core facilities do for instrument development at Yale?

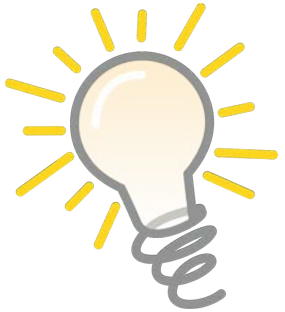
A common research workflow:

Custom built instrument





Journal Articles & Grants



Ideas for improvement

Upgrade/Rebuild/Replace with improved capabilities

What can core facilities do for instrument development at Yale?

A possible workflow:

Individual Lab

"alpha" test

Custom-built instrument prototype

Core Facility

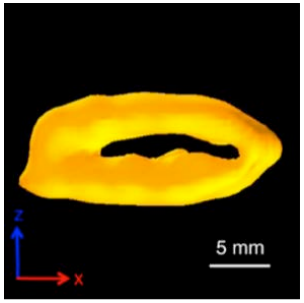
Support Services

Core Facility

"beta" test

Custom-built production instrument

Commercial instrument



Prof. Sean Barrett
MR Imaging of solids

What can core facilities do for instrument development at Yale?

…people come first