Yale Day of Instrumentation 2020
Core facilities and instrument development at Yale

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):

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

Commercial Mass Spectrometer

Cryogenic Ion Trap

Room Temperature Ion → Cold “Tagged” Ion → IR Absorption → Evaporation of “Tag” → Photofragment Detection

Laser Vision Nd:YAG 600 - 4500 cm⁻¹
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
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.

**Hybrid spectrometer construction in the CBIC**

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Dr. Fabian Menges
What can core facilities do for instrument development at Yale?

A common research workflow:

Custom built instrument

Upgrade/Rebuild/Replace with improved capabilities

Journal Articles & Grants

Ideas for improvement
What can core facilities do for instrument development at Yale?

A possible workflow:

- Custom-built instrument prototype
- "alpha" test
- Custom-built production instrument
- "beta" test
- Commercial instrument

Individual Lab

Core Facility

Support Services

Prof. Sean Barrett
MR Imaging of solids
What can core facilities do for instrument development at Yale?

...people come first

Custom-built instrument prototype

Custom-built production instrument

Commercial instrument

The World

"Broader Impacts"