

NCSU Department of Chemistry Mass Spectrometry Facility Briefing for 2006 - 2007

Personnel

Director, David C. Muddiman, Professor of Chemistry

Manager, Matthew Lyndon*

Teaching Assistant (2006-2007):

Robert B. Dixon

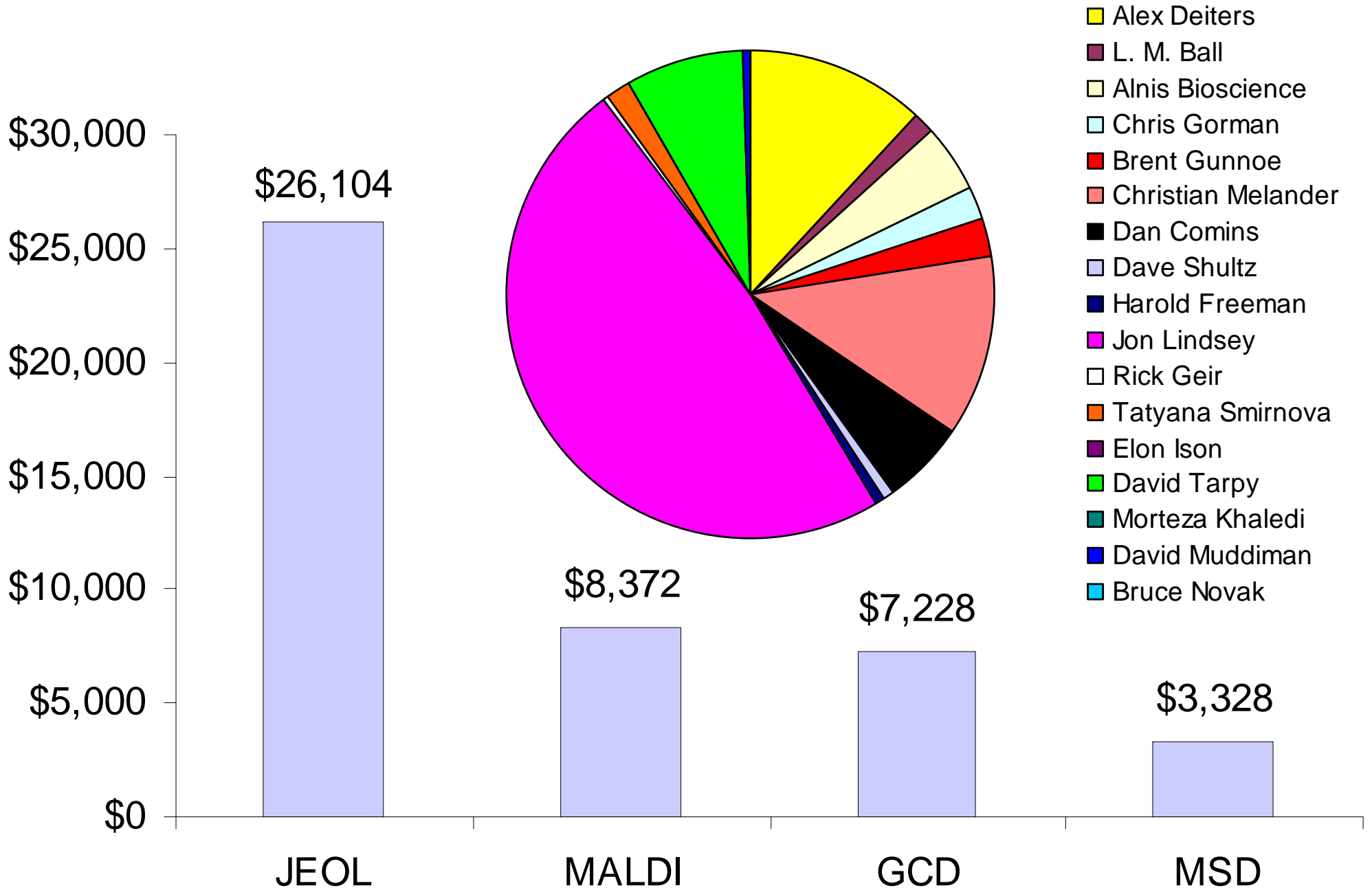
Teaching Assistant (2005-2006):

Michael S. Bereman

- Matthew Lyndon has worked very effectively over the past year with Dr. Muddiman in revamping the NCSU-Chemistry MSF and his efforts should be appropriately recognized.

Projected Financial Data

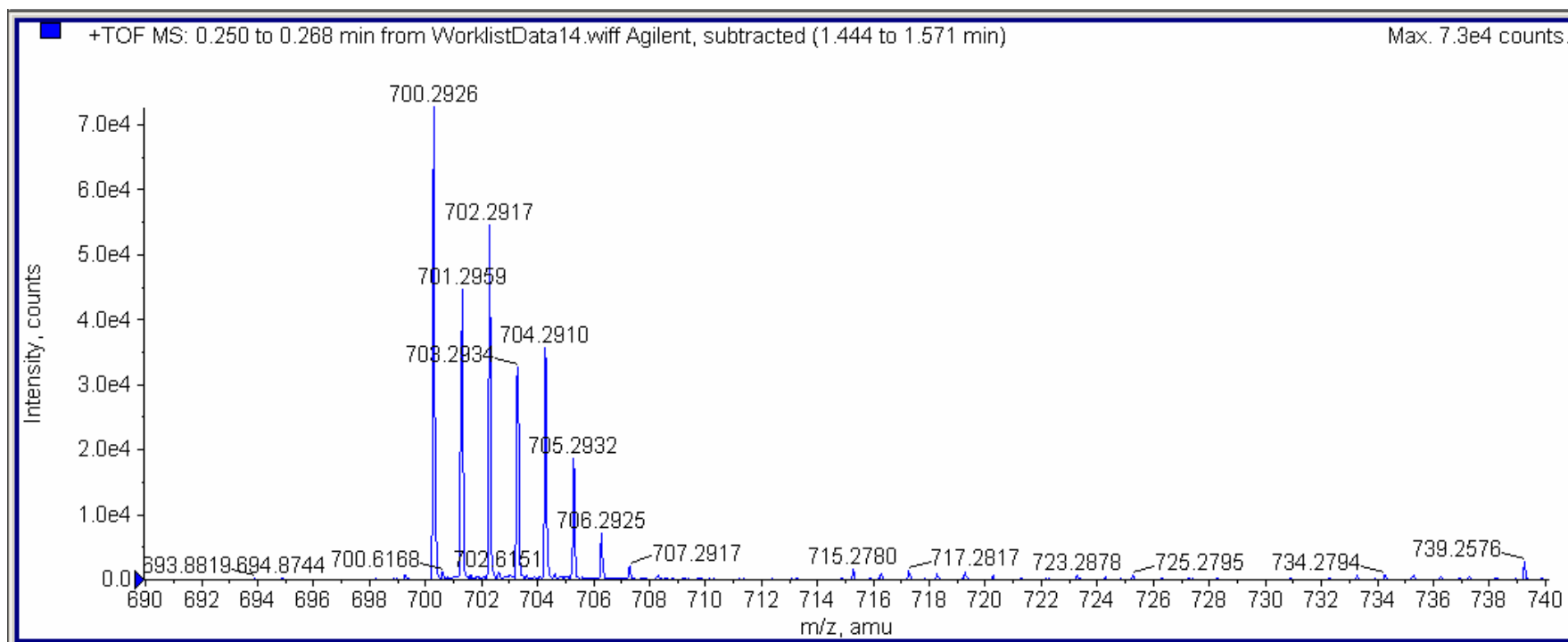
Projected 2006 - 2007 Revenue \$45,032



News

- The Mass Spectrometry Facility (MSF) relinquished its space in 1141 Burlington Nuclear Engineering Laboratories and Dabney 608. We also decommissioned the Micromass Quattro II LC/MS as well as the Hewlett Packard 5985 GC/MS.
- The MSF acquired Dabney 16B from the NMR Facility and made Dabney 16 into one large room. Renovation of Dabney 16 includes new carpet, paint, lighting, tables, and chairs. Thanks to these renovations we were able to relocate our self-use instruments: the Bruker Omniflex MALDI-TOF MS and the Agilent GCD into the same space which will allow for easier access and better oversight of these MSF instruments. We would like to thank Dr. Ken Hanck, Dr. David Muddiman and graduate student R. Brent Dixon for their help in making these renovations possible.
- Our NCBC proposal has been funded which will allow the MSF to acquire a new state of the art high resolution mass spectrometer. Currently we are evaluating several instruments, all of which will be able to drastically reduce turnaround time and be able to electronically deliver results. We plan on selecting and purchasing a new instrument within the next six months. We would like to thank Dr. David Muddiman, graduate student Michael Bereman, and all of the NCSU Department of Chemistry Faculty who provided us summaries of their research and supplied samples in order for us to obtain preliminary data which helped in writing the proposal.

- We would like to request several samples from each user of the MSF in order for us to thoroughly evaluate the instrumentation we are considering purchasing. We plan on sending these samples to each manufacturer and would like to cover the scope of samples we currently analyze using the JEOL HX110 HRMS.
- These samples will be kept confidential in regards to type, structure and application. We will only be sending ID, solubility, and molecular weight range information to help the analyst to appropriately perform their experiments.



- Agilent Technologies has agreed to set up a demo facility on Centennial Campus. This facility will help to provide Agilent, NCSU faculty and staff, as well as other academic and corporate partners a place to view and use new instrumentation and serve to create an environment conducive to collaboration. Agilent will be providing the MSF with a loaner instrument in accordance to this agreement. The loaner instrument will give the MSF a chance to diversify the problems our facility can address. We would like to thank Dr. Ken Hanck and Dr. David Muddiman for their work in making this possible.



Instrumentation

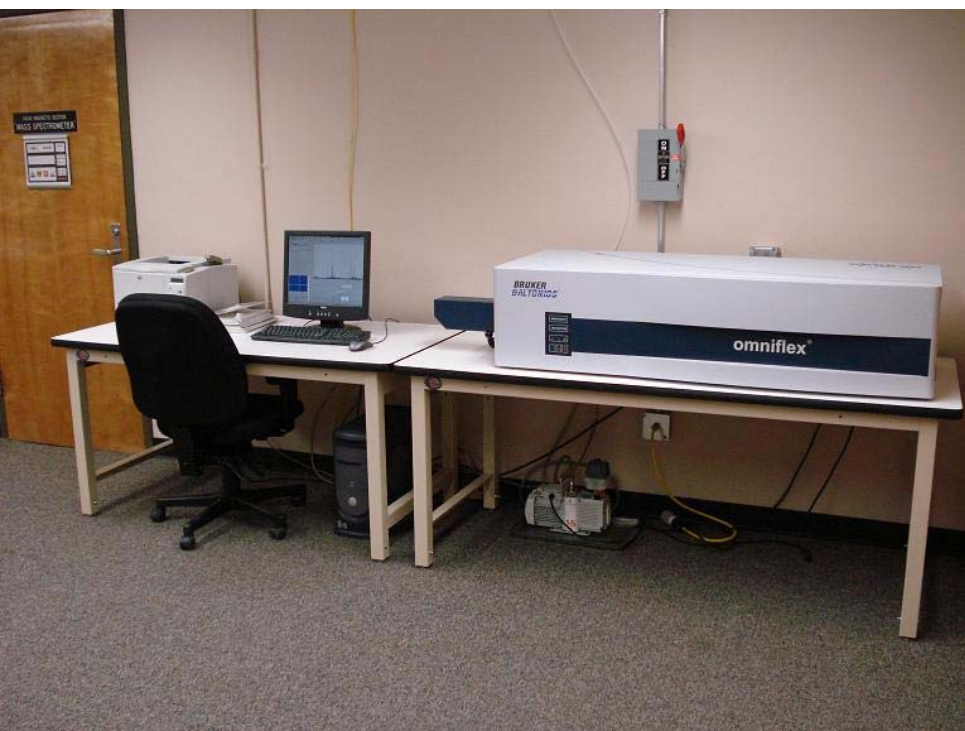
JEOL HX110 HRMS



- Exact Mass
- Elemental Composition
- Ionization Sources
FAB
EI
- *Annual Downtime: Three Weeks
- *Annual Revenue: \$26,102
- *Samples Analyzed Annually: 936

The JEOL HX110 has been in service since 1986 and has been the ‘anchor’ instrument of the MSF since that time. We are planning on replacing this instrument with a high throughput state of the art mass spectrometer via a grant from NCBC.

Bruker Omniflex MALDI-TOF



- Peptides, Proteins, Polymers, Medium to High Molecular Weight Organics/Synthetics
- Ionization Sources
MALDI
- Self-Use Available
- *Annual Downtime: Two Weeks
- *Annual Revenue: \$8,372
- *Samples Analyzed Annually: 2,704

The Omniflex has been in service since 2003 when it replaced our previous Bruker Proflex MALDI-TOF MS. This instrument sees the most self-use users and also the most samples being analyzed per year.

Agilent GCD



- Low Molecular Weight Volatile Compounds
- Online Separation and Detection
- Ionization Sources
EI
- Self-Use Available
- *Annual Downtime: One Week
- *Annual Revenue: \$7,228
- *Samples Analyzed Annually: 200

The GCD has been in service since 1996. We are not planning on replacing or decommissioning this instrument at this time. Spectral libraries are included to aid in sample identification, quantification possible via SIM/classical standard concentration methods.

Agilent LC/MSD



- Routine Analysis of Organic and Biological Molecules
- Online Separation and Detection
- Ionization Sources
ESI
APCI
- *Annual Downtime: Three Months
- *Annual Revenue: \$3,328
- *Samples Analyzed Annually: 936

The LC/MSD has been in service since 1996, and will no longer be offered as a self-use instrument due to improper usage. Over the course of the last 18 months this instrument has cost the MSF approximately \$20,000 in repairs. Projected revenue from this year comes to \$3,328 which is low due to excessive downtime for repairs, and as one can infer it will take some time for us to recover these costs. Therefore we felt it best to change over from self-use to a submission based analysis similar to the way we currently operate JEOL HRMS samples in order to minimize downtime and costs associated with repairs.

Agilent LC-TOF



- Exact Mass
- Elemental Composition
- Online Separation and Detection
- Ionization Sources
 - APCI
 - APPI
 - ESI

The Agilent LC-TOF is a loaner instrument provided to us by Agilent Technologies as part of their Demo Lab arrangement with the University. Last year we analyzed several samples given to us by faculty members in order to help prepare our grant proposal submitted to NCBC. We will be using this instrument in order to further investigate whether LC-TOF platforms are a sufficient replacement technology to Magnetic Sector Mass Spectrometers. We will not be billing any samples analyzed on this instrument over the next few months until we are confident that it can provide the requisite mass accuracy and precision.

Future Goals

- Further improve turnaround time
- Re-evaluate and better facilitate sample submission protocol
- Investigate other instrumental needs of our users; *i.e.* an MS/MS platform
- Renovation of Dabney 17 including removal of the JEOL HX-110
- Continue assessing MSF compatibility of LC-TOF technology

