**ANNUAL REPORT**

**OF THE**

**UNIVERSITY OF CALIFORNIA, DAVIS**

**NUCLEAR MAGNETIC RESONANCE (NMR) FACILITY**

**FOR THE**

**FISCAL YEAR 2007-2008**

**PROFESSOR GARY M. SMITH, DIRECTOR**

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## I. OVERVIEW

### A. Introduction

The UCD NMR Facility is an interdepartmental, inter-college central facility operated under the auspices of the Office of Research to provide campus wide access to sophisticated NMR instrumentation and technical support for NMR research. The breadth and scope of research at the Facility is extensive, with research in several areas of NMR applications active and supported by substantial extramural funding.

Given below is a concise summary of important data concerning the Facility; further information can be found under the appropriate headings in Sections II-X.

| | |
|---|---|
| Number of UCD faculty investigators utilizing Facility in 07-08: | 74 |
| Number of UCD departments utilizing Facility in 07-08: | 26 |
| Number of publications in 07-08: | 83 |
| Value of major equipment in inventory as of June 30, 2008: | $5,332,592 |

Extramural Faculty Grants involving research conducted at the Facility:

| | |
|---|---|
| Number of Extramural Grants | 76 |
| Total costs in 07-08 | $15,135,000 |
| Overhead | $4,200,000 |

Long-term health of the Facility will continue to be dependent on receiving matching funds for major instrumentation grants and replacement of obsolete equipment as needed, along with staff salary support from general funds.

Significant developments at the Facility in FY 07-08 included:

1) The number of faculty investigators using the Facility reached an all-time high. The number of publications produced by faculty using the Facility also reached a new all-time high.

2) The NMR Facility was awarded a NSF Major Research Instrumentation grant, and a purchase order for a high-field 800 MHz NMR spectrometer was placed.

## II. RESEARCH SUMMARY

Research at the Facility in FY 07-08 covered a wide range of topics and involved 74 faculty from 26 different UCD departments in six Colleges and Schools (also see Section VI). Research results from the Facility were part of 83 peer-reviewed publications by UCD faculty users in 07-08; a complete listing of publications is given in Section X. A total of 76 extramural grants with $15,135,000 in annual costs supported this work (Section VII). The work at the Facility can be roughly grouped into several broad research areas: **biomedicine, structural biology, materials, organic molecules, inorganic complexes,** and **plants**. Brief descriptions of the recent NMR research accomplishments by UCD faculty in these areas follow. A listing of all faculty users is included in Section VI, and a breakdown of usage by College and by research area is included in the Appendix.

1) NMR applications in **Biomedicine**: This research area includes the use of both NMR spectroscopic and imaging methods applied to the fields of biology and medicine. Systems studied include intact animals, perfused organs, biofluids, tissue extracts, and model systems. These studies include work in NMR metabolomics. Faculty participants in the Biomedicine area are listed below, followed by a short synopsis of some of their recent research accomplishments using the NMR Facility.

Dr. S. Anderson (MED: Human Physiology)
Professor A. Angelastro (VET: Molecular Biosciences)
Professor R. Berman (MED: Neurological Surgery)
Professor P. Cala (MED: Human Physiology)
Professor S. Cherry (ENG: Biomed. Eng.)
Dr. Y. Chung (MED: Biological Chemistry)
Professor F. Fathallah (ENG: Biological & Ag. Engineering)
Professor D. Fhyrie (MED: Orthopedics)
Professor O. Fiehn (CBS: Genome Center)
Professor N. Glaser (MED: Pediatrics)
Professor M. Hull: (ENG: Mech. & Aero. Eng.)
Professor T. Jue (MED: Biological Chemistry)
Dr. U. Kreutzer (MED: Biological Chemistry)
Professor A. Louie (ENG: Biomed. Eng.)
Professor J. Medrano (A&ES: Animal Science)
Professor C. Neu (MED: Orthopedics)
Professor M. O'Donnell (MED: Human Physiology)
Dr. G. Pettygrove (A&ES: LAWR)
Professor K. Pinkerton (MED: Pediatrics)
Professor A. Reddi (MED: Orthopedics)
Professor R. Tjeerdema (A&ES: Env. Toxicology)

The Anderson/Cala group demonstrated that Mn-enhanced MRI (MEMRI) can be used effectively to assess increased transport via Na/Ca exchange in hypoxic myocardium.

The Cherry lab has been working on 3D mouse brain imaging in conjunction with the Berman group. They have also completed a year-and-a-half long study using MRI to track volumetric change in the murine thymus.

The Fhyrie group measured T2 values for cartilage samples that were subject to mechanical testing. The results demonstrate significant correlations between specific cartilage molecular T2's and parameters describing the mechanical behavior. They also demonstrated that changes in the specific T2's are associated with enzymatic digestion of specific cartilage molecules.

Recent work undertaken in the Fiehn lab sought to compare MS- and NMR-based metabolite profiles in the characterization of white wines including varieties Chardonnay, Viognier, Pinot gris, Riesling and Sauvignon Blanc. The ultimate goal of this work was to identify compositional differences in these wines which correlate to wine sensory properties. Additionally the work sought to compare independently-curated metabolite lists and

resulting experimental conclusions for the same sample set with the purpose of a direct comparison of the two most frequently used analytical tools in metabolomic studies.

The Glaser group uses H1 and P31 MRS to measure brain metabolites in control and DKA rats.

The Jue lab has successfully demonstrated a novel approach to image apolipoprotein and HDL in vivo and has continued to measure the impact of Mb on metabolic regulation with wild type and Mb KO mice.

Kreutzer has noted that noninvasive imaging techniques hold strong promises for the effective diagnosis, prognosis, and treatment of diseases. To realize these promises, however, requires an effective strategy to identify imaging biomarkers with selectivity, specificity, and sensitivity. Many rely on the dramatic metabolic alteration in tumors. Kreutzer's experiments have developed a strategy using $^{19}F$ labeled precursors to screen the efficacy of fluorinated candidate biomarkers to track tumor progression in cell and xenograft models of prostate cancer.

The Louie group has utilized NMR to characterize the synthesis of compounds as MRI contrast agents and have published these results in per reviewed journals. They have developed a molecular switch that responded to light and electrical potential, and shown that these changes result in a change in the MR contrast. They have also characterized the synthesis of other molecular cages for chelating metals for MRI and positron emission tomography (PET) applications.

The Neu lab has documented deformation (i.e. displacement and strain) fields and glycosaminoglycan concentrations by noninvasive MRI. Field and concentration data was quantified in three separate systems: (i) normal articular cartilage, (ii) tissue engineered articular cartilage, and (iii) degenerated invertebral disc.

The O'Donnell lab continued studies aimed at assessing the role of Na/H exchange and Na+K+2Cl cotransport in blood-brain barrier (BBB) contributions to cerebral edema and injury in stroke. Results of these experiments demonstrate that inhibition of these transporters before and up to 2 hr after middle cerebral artery occlusion in rats limits brain Na uptake. These experiments are the first using 23Na CSI and DyTTHA to assess changes in extravascular brain Na in vivo. The data are consistent with previous results showing transporter inhibition limits infarct size and increases the apparent diffusion coefficient (ADC) for water in brain. Decreased ADC is an accepted indicator of cerebral edema.

The Pinkerton lab has completed NMR studies on serum and homogenized tissues of both rhesus macaque primates and Charles River guinea pigs in order to determine the metabolite changes that occurred with exposure to environmental tobacco smoke (ETS) in adult and developing animals. Differences were noted in the spectra of plasma of adult non-human primates and were identified as lactate. Spectra of homogenized lung tissues of the guinea pigs showed multiple significant changes occurred in the animals which were exposed to both Der F and ETS.

In the Tjeerdema group NMR data (1D $^1H$ and 2D J-res) has been collected on pre-smolt Chinook salmon muscle and liver tissues. This data is now being analyzed and is in the beginning stages of becoming a paper on the effects of crude versus dispersed oil on chinook salmon using NMR based metabolomics.

2) NMR applications in **Structural Biology**: This program utilizes solution state NMR methods to determine the three dimensional structure and dynamics of biological macromolecules, principally proteins and nucleic acids. Faculty participants in this Program are listed below, followed by a short synopsis of their recent research accomplishments using the NMR Facility. Though only three faculty are listed in this area their use of the Facility is heavy, making this one of the key research areas of the Facility.

Professor J. Ames (L&S: Chemistry)
Professor G. La Mar (L&S: Chemistry)
Professor M. Wood (A&ES: Env. Toxicology)

The Ames group uses multinuclear, multi-dimensional NMR to elucidate the molecular structure, dynamics and mechanisms of calcium sensor proteins in the brain and retina that serve as important regulators in cell signaling. In the last year, they solved NMR-derived structures of four different calcium-sensor proteins in the brain and retina related to signal transduction.

2D NMR was used by the La Mar lab to characterize the two resting state, equilibrium populated, human heme oxygenase(HO)-heme complexes in the high-spin ferric aquo-complex and the low-spin ferric-hydroxide

complex. The coupling of the deprotonation of the exogenous ligand to the H-bonding network was found much stronger than in a pathogenic bacterial HO with strong sequence homology to human HO. To date, this is the most prominent functional difference between the two HOs.

The Wood laboratory works on elucidating the structure and function of proteins with NMR. Currently they are working on two proteins. The first is a protein involved in responding to oxidative stress. The second is an enzyme involved in reduction of arsenate.

3) NMR applications in **Materials** science: Applications in this area include the characterization of polymers, glasses, nanoparticles, and surface chemistry phenomena. This field also utilizes magnetic resonance imaging methods and spectroscopy to investigate mass transport phenomena and transient structure of materials such as foams and oils; an allied application is the study of the internal organization of foods and agricultural products. Dynamic processes such as creaming of emulsions, drying in porous media, sedimentation and foaming are also focal points of study in the materials area. Leading faculty participants in the Materials are listed below, followed by a short synopsis of their recent research accomplishments using the NMR Facility.

Professor S. Dungan (A&ES: Food Science & Technology)
Professor S. Kauzlarich (L&S: Chemistry)
Professor K. McCarthy (A&ES: Food Science & Technology)
Professor M. McCarthy (A&ES: Food Science & Technology)
Professor A. Navrotsky (ENG: Chemical Engineering & Materials Science)
Professor R. Phillips (ENG: Chemical Engineering & Materials Science)
Professor R. Powell (ENG: Chemical Engineering & Materials Science)
Professor S. Risbud (ENG: Chemical Engineering & Materials Science)
Professor S. Sen (ENG: Chemical Engineering & Materials Science)

The Kauzlarich group has characterized several new inorganic clathrate structures such as Ba8-xSrxAl16Si30 and K8Si46 via solid state NMR. They have also used solid state NMR to explore the bonding of dopants in nanocrystalline silicon.

The K. McCarthy group continued collaborative work with Cornell University through a USDA subcontract, using MRI to study temperature and moisture mapping of potatoes.

The M. McCarthy lab in one project focused on development of MRI based protocols to predict the quality of fresh fruit and fruit derived products. They also continued work on design, fabrication, and testing of novel NMR microcoils.

Navrotsky's group conducted 71Ga solid state NMR experiments to characterize the structure features of Ga-containing aluminosilicate zeolites. NMR data indicate that substitution of Al by Ga alters the distribution of tetrahedral, trigonal and octahedral sites. They also conducted 1H, 13C and 29Si NMR experiments for the study of mesoporous silica. The results were used to analyze the species and distribution of defects and impurities in these synthetic materials.

Powell and Phillips have measured Ostwald Ripening via proton MRI in a concentrated emulsion (~70 vol%). They have also shown that increasing micelle concentration increases the Ostwald Ripening rate.

The work of Risbud uses solid state NMR to evaluate the structure of phosphate glasses and bioceramics. They study the local coordination of P atoms in these glasses and relate the data to dissolution in simulated body fluid.

The Sen lab group has used solid state NMR spectroscopy for several research projects this year. First, they discovered the existence of "plastic crystal-like dynamics" in glass using variable temperature 31P wideline NMR. Second, they have solved the structure of Be-B-Al oxide glasses using 9Be, 27Al and 11B NMR and 3QMAS NMR. Third, the Sen group has found the first evidence of anomalous polymerization in Mg2SiO4 glass using 29Si MAS NMR. Fourth, they have recently found novel size dependence of vacancy distribution in Y-doped CeO2 and ZrO2 using 89Y MAS NMR. Fifth, they have just finished a variable temperature 13C NMR of supercooled glycerol in the bulk and confined state where they have found novel effects of confinement on molecular dynamics.

4) A number of research groups utilize the Facility to characterize the structure and identity of **organic molecules** such as natural products and synthetic organic molecules. This is done by one- and two-dimensional NMR on the Facility's liquids NMR spectrometers. Faculty investigators in this area include:

Professor P. Beal (L&S: Chemistry)
Professor X. Chen (L&S: Chemistry)
Professor S. Ebeler (A&ES: Viticulture)
Professor K. Ferrara (ENG: Biomed. Engineering)
Professor A. Franz (L&S: Chemistry)
Professor J. Gervay-Hague (L&S: Chemistry)
Professor B. Hammock (A&ES: Entomology)
Professor M. Kurth (L&S: Chemistry)
Professor C. Lagarias (BIOSCI: Molecular & Cellular Biol.)
Professor K. Lam (MED: Hemat. & Oncol.)
Professor M. Mascal (L&S: Chemistry)
Professor R. Parales (BIOSCI: Microbiology)
Professor T. Patten (L&S: Chemistry)
Professor N. Schore (L&S: Chemistry)
Professor J. Shaw (L&S: Chemistry)
Professor G. Sun (A&ES: Textiles)
Professor J. Theis (MED: Microbiology & Immunology)
Professor H. Wulff (MED: Pharmacology)

The Beal research group has recently completed two projects and submitted manuscripts on these projects where NMR was used extensively. These projects involved the synthesis and characterization of novel heterocyclic structures (purine derivatives and quinoline derivatives). 1H, 13C and 31P NMR was used for characterization of the synthetic intermediates as well and the final products of these efforts.

Chen's group uses 1D and 2D NMR to characterize oligosaccharide compounds synthesized by chemical and enzymatic methods. Over one hundred synthesized compounds have been characterized by NMR in the period July 2007 to June 2008; these results are a key component of ten publications and two manuscripts to be submitted.

Ebeler's research group used NMR to determine the structure of a compound with potential anti-fungal properties from an industrial fermentation process. They continue to employ NMR to evaluate interactions between grape tannins and aroma compounds.

The Ferrara lab has developed radioisotope (F-18 and Cu-64) labeling methods for liposomes. To achieve this goal, several lipids conjugate or chelate radio active material were synthesized and characterized by NMR. A near-infra red dye for dual imaging purposes was also synthesized and characterized by NMR.

The Franz group used NMR to characterize new synthetic molecules and the interactions of new catalysts with substrates.

The Gervay-Hague laboratory makes extensive use of 1D and 2D NMR methods for the structural characterization of complex glycoconjugates that have significant biological activities. These compounds include polysialic acids, amide-linked sugar oligomers, and glycolipids.

The Hammock group uses NMR to identify the structures of the synthetic soluble epoxide hydrolase inhibitors, fatty acid amide hydrolase inhibitors, and some environmental toxics.

The Kurth research group has recently published large libraries of novel heterocycles in various organic and medicinal chemistry journals that were characterized by NMR spectroscopy, principally 1H and 13C NMR.

In the Lagarias lab the newly synthesized biliverdin IX$\alpha$ 8- and 12- monoamides and biliverdin XIII$\alpha$ monoamide were characterized by NMR. NMR characterization of the novel reaction products, which are derived from the reaction of biliverdin amides and biliverdin reductases, is in process. These will be used to test the role of the free propionic acids in the phytochrome photocycle.

The Lam group uses proton and C13 NMR to characterize both small molecular structure and the conformation of peptides.

The Mascal group used NMR to monitor the inertness of a synthesized compound towards highly reactive reagents. They also monitored the fluoride intake of another compound using 19F-NMR.

The Meares lab works on engineering the permanent formation of a receptor-ligand complex with a number of promising applications in chemistry, biology, and medicine. Two ligands bearing thiol side chains were synthesized, characterized by NMR and other methods, and incubated with the cysteinylated antibody Fab fragment 2D12.5 G54C, with the finding that both ligands become covalently attached within a few minutes under physiological conditions.

The Patten group uses NMR to identify new compounds and determine the degree of polymerization of new polymers. They have also used NMR in the past year for protein identification.

The Schore group uses 1H and 13C NMR to characterize organic molecules synthesized in their lab. These molecules are being explored for use as solid-phase catalysts and RNA analogs, as porphyrin nanostructures, and in kinetic studies of homogeneous catalysis.

The Shaw research group notes that NMR is critical to every experiment they run. They are currently engaged in several multistep syntheses, and in each case every compound has to be characterized by NMR (1H and 13C). As a typical example, in the papers they have recently submitted results on from 10 to 30 compounds will be presented; all will have been characterized with 1H and 13C NMR data.

In the past year the research lab of G. Sun used 1D and 2D NMR in the research of chemical modification of functional polymers and textiles, and characterization of natural colorants produced by fungi and bacteria.

The Tantillo group has utilized the NMR instruments for several projects, mainly for the purpose of helping to verify the identity of synthesized products.

The Wulff laboratory has used 1H and 13C NMR spectroscopy to determine the structure of newly synthesized benzothizole, psoralens and triarylmethanes. These three compound classes are being synthesized and then tested for their effect on potassium channels or connexins (= gap junction channels).

5) Several research groups use the Facility to characterize the structure of **inorganic complexes**, either in solution or solid state, by NMR spectroscopy. Faculty in this area are:

Professor A. Balch (L&S: Chemistry)
Professor B. Gates (ENG: Chemical Engineering & Materials Science)
Professor W. Casey (L&S: Chemistry)
Professor P. Power (L&S: Chemistry)

The Balch group used 1H NMR to characterize indium porphyrin dimers in deuterated chloroform and indium porphyrin monomers in deuterated pyridine.

The Casey laboratory has continued their efforts to characterize ligand-exchange properties of nanometer-size clusters using both classical line-broadening methods and oxygen-isotope exchange reactions. They published work on 2.5 nm size Keplerate molecules and on Nb(V) and Ta(V) Lindqvist ions. These include high-pressure 17O-NMR experiments with a home-built titanium probe.

NMR spectroscopy is used almost daily by the Power group in the characterization of low valent transition metal and main group compounds. Multinuclear ($^{1}H$, $^{13}C$, $^{29}Si$, $^{119}Sn$, $^{11}B$, $^{27}Al$, $^{31}P$, $^{111}Cd$) NMR spectroscopy has been the central characterization technique for the identification of products from reactions between main group compounds and molecular hydrogen. NMR spectroscopy has also helped characterize and guide reactions with tin formates as regeneration agents in chemical hydrogen storage.

6) NMR imaging and spectroscopy are used to analyze the structure and metabolism of intact **plants** and fruits by the following campus faculty:

Professor P. Hernes (A&ES: Land, Air, and Water Resources)
Professor J. Labavitch (A&ES: Pomology)
Professor J. Thompson (ENG: Biological & Ag. Engineering)

The Hernes lab in conjunction with the the USGS uses solid state 13C CPMAS on XAD8 isolated dissolved organic matter (DOM). The 13C-NMR data provides structural information for samples collected within

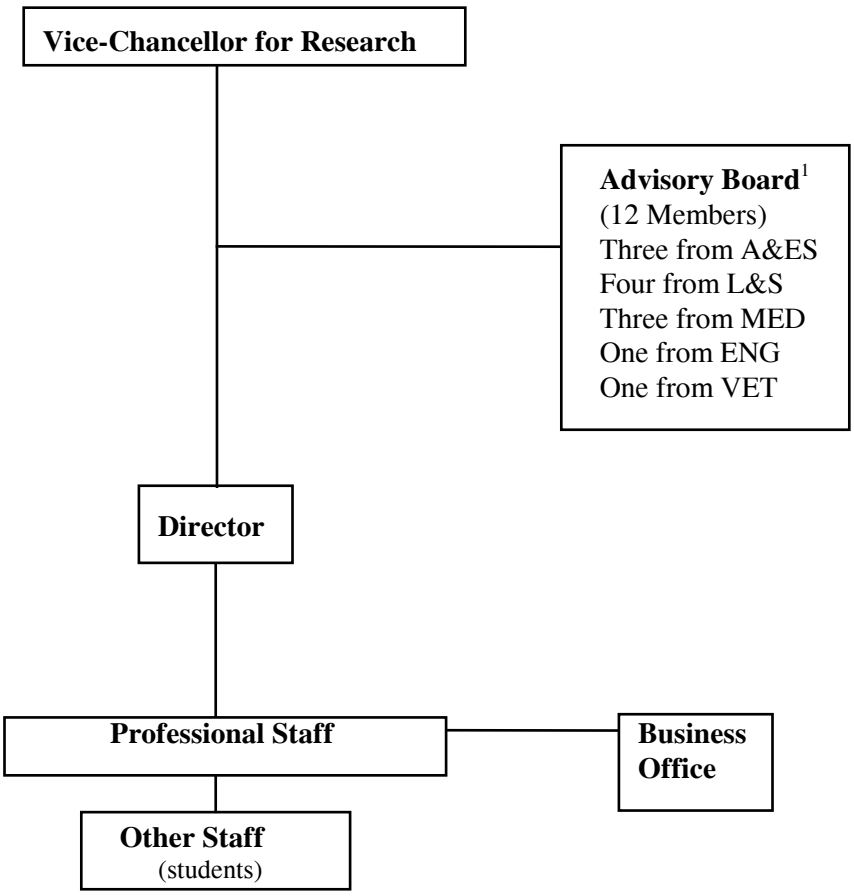
the California State Water Project. Information about how the chemical properties of DOM changes as water travels through the SWP will help determine whether dissolved organic matter (DOM) is produced, degraded and/or transformed during transport through the SWP, and to elucidate which processes are responsible for changes in DOM concentration and composition.

The Labavitch lab uses MRI to study the xylem system of grapevine stems. Grapevines that are affected by Pierce's disease (PD) have many water-conducting cells (vessels) that are plugged and non-functional because of the activities of the PD-causing bacterium that resides in the vessels. MRI is used as a non-destructive way to reveal air-filled vessels (non-functional, cavitated vessels) in stems of infected vines.

Finally, several non-UCD entities, both academic and industrial, utilized the Facility this FY. They are listed in Section VI and their percent utilization (~9%) of the Facility is reported in the Appendix.

## III. ORGANIZATION

### A. NMR Facility Organizational Chart




[1] A&ES is the College of Agriculture and Environmental Science.
L&S is the College of Letters and Science.
MED is the School of Medicine.
ENG is the College of Engineering.
VET is the School of Veterinary Medicine.

**B. NMR Facility Personnel**

Director:

Gary M. Smith, Professor, Department of Food Science & Technology

NMR Facility Professional Staff:

Jeffrey S. de Ropp, Ph.D., Research Spectroscopist, 100% time
Address: NMR Facility; jsderopp@ucdavis.edu
Jeffrey H. Walton, Ph.D., Assoc. Research Physicist, 100% time
Address: NMR Facility; jhwalton@ucdavis.edu
Ping Yu, Ph.D., Asst. Project Scientist, 100% time
Address: NMR Facility; pyu@ucdavis.edu

Advisory Board:

James Ames, Assoc. Professor, Department of Chemistry
Matt Augustine, Assoc. Professor, Department of Chemistry
Michael Buonocore, Professor, Department of Radiology (Med.)
Peter Cala (Board Chair), Professor, Department of Physiology & Membrane Biology
William Casey, Professor, Department of Chemistry
Simon Cherry, Professor, Biomedical Engineering
Thomas Jue, Professor, Department of Biochemistry & Molecular Medicine
Michael McCarthy, Professor, joint appointment Food Science & Technology; Biol. & Ag. Engineering
Robert Powell, Professor, Department of Chemical Engineering & Materials Science
Ron Tjeerdema, Professor, Department. of Environmental Toxicology
Erik Wisner, Professor, Department of Surgical & Radiological Sciences (Vet.)
Matt Wood, Assistant Professor, Department of Environmental Toxicology

NMR Facility Other Staff:

Students, Asst. III, ~50% time total

Business Office

Edson Kong, Administrative Specialist I; Ellie O'Shea Administrative Assistant III; total ~30% time
Address: Biochemistry & Molecular Medicine; Phone 2-6485

## IV. FACILITY STAFF & DUTIES

The Facility has three full-time, Ph.D professionals and a varying number of part-time employees. In FY 07-08 funding for 1.8 FTE of the Professional Staff positions and ~0.2 office personnel was provided by the Office of Research and central administration; other positions were funded by Facility recharges and grants. The Staff members are:

**Professional Staff**

| Name | Position |
|---|---|
| Dr. Jeff de Ropp | Research Spectroscopist (100%) |
| Dr. Jeff Walton | Project Scientist (100%) |
| Dr. Ping Yu | Asst. Project Scientist (100%) |

Professional Staff Duties:

The duties of the professional Staff primarily consist of four areas:

1) Research & Consultation: collaborative research and consultation with UCD faculty. The primary function of the Professional Staff is to supply research collaboration, technical NMR expertise, and consultation for the research applications of campus faculty. In this year the Professional Staff was active in supporting/collaborating with faculty in all of the campus' NMR Research Areas (Section II). The Professional Staff provides on-going expertise in developing pulse sequences, making instrument hardware modifications for specialized applications, writing software for specific faculty research projects, and providing technical consultation in the design and execution of NMR experiments. Publications involving the Professional Staff are given in Section X.

2) Instrument maintenance and repair: Providing all performance tests, regular maintenance, and (after warranty) repair of each Facility spectrometer, along with in-house modifications to enhance spectrometer performance for special campus research applications, and software support for UCD researchers. This continual support enables the Facility spectrometers to be scheduled 24 hours/day, 365 days/year. Bruker-NMR has quoted $187,000/year for a service contract for just one-half of our spectrometer inventory; the Staff provides such support at lower cost and performs many additional duties listed here.

3) Administration: supervising daily operations of the Facility including activities of non-permanent Staff; scheduling of spectrometers, budgeting, personnel, and fiscal processes, coordinating purchase and installation of Facility instrumentation, overseeing physical plant, and coordinating and writing Facility multi-user instrumentation grants (Section VII-A).

4) Education: Conducting the annual NMR Facility Training course (Section VI-C); overseeing hands-on training of all users, participating in campus courses involving NMR (Section VI-D).

**Other Staff**

Student Assistants III (50% total); Administrative Assistants (30%), misc.

Duties:

The students:

1) Handle secretarial/clerical duties.
2) Assist with cryogen fills.
3) Do PC software maintenance.

The Administrative Assistants:

1) Processes purchases in DaFIS.
2) Processes NMR recharges.
3) Handle payroll.

## V. INSTRUMENTATION

The Table below lists the major Facility instrumentation available to campus users as of the completion of FY 07-08. (The list does not include spectrometer accessories, or maintenance, test, and repair equipment used to service the spectrometers).

| **A**. | NMR Spectrometers | Purchase Price | Year Installed | Primary Uses |
|---|---|---|---|---|
| 1. | DRX-600 (600 MHz) | $873,000 | 1998 | Liquids spectroscopy |
| 2. | VNMRS-600 (600 MHz) | $893,392 | 2005 | Liquids spectroscopy |
| 3. | DRX-500 (500 MHz) | $622,000[1] | 1998 | Liquids spectroscopy |
| 4. | DRX-500 solids (500 MHz) | $1,005,000 | 2004 | Solids spectroscopy |
| 5. | DRX-400 (400 MHz) | $550,000[1] | 2001 | In vivo spectroscopy |
| 6. | Inova-400 (400 MHz) | $250,000 | 1999 | Liquids spectroscopy |
| 7. | Biospec-7T (300 MHz) | $790,000[1] | 1999 | Imaging |
| 8. | Mercury-300 (300 MHz) | $192,000 | 1999 | Liquids spectroscopy |
| 9. | Mercury Plus-300 (300 MHz) | $154,000 | 2003 | Liquids spectroscopy |
| **B.** | Data Processing Stations | | | |
| 1. | Linux box | $2,000 | 2004 | |
| 2. | Linux box | $1,200 | 2005 | |
| **Total value of instrument inventory** | | **$5,332,592** | | |

[1]Sum of original magnet cost plus upgrade cost.

## VI. USAGE & EDUCATION

### A. Faculty Users

Given below is a listing of all UCD faculty whose research groups utilized the Facility in FY 07-08, grouped by College. 74 faculty research groups from 26 departments utilized the Facility this FY. An asterisk denotes users of >200 hours of spectrometer time in the FY. The Appendix provides graphical representations of Facility usage by College and research area.

| Faculty | Department | College |
|---|---|---|
| Boulton | Viticulture & Enology | A&ES |
| Dungan | Food Science & Technology | A&ES |
| Ebeler | Viticulture & Enology | A&ES |
| Hammock | Entomology | A&ES |
| Hernes | LAWR | A&ES |
| Hsieh | Textiles & Clothing | A&ES |
| Labavitch | Pomology | A&ES |
| K. McCarthy* | Food Science & Technology | A&ES |
| M. McCarthy | Food Science & Technology | A&ES |
| Medrano | Animal Science | A&ES |
| Pettygrove | LAWR | A&ES |
| G. Sun* | Textiles & Clothing | A&ES |
| Tjeerdema* | Env. Toxicology | A&ES |
| Wood | Env. Toxicology | A&ES |
| | | |
| Cherry* | Biomed. Eng. | ENG |
| Fathallah | Biol. & Agr. Engineering | ENG |
| Ferrara | Biomed. Eng. | ENG |
| Gates | Chem. Eng. & Mtrl. Sci. | ENG |
| Hull* | Mech. & Aero. Eng. | ENG |
| Louie* | Biomed. Eng. | ENG |
| Navrotsky | Chem. Eng. & Mtrl. Sci. | ENG |
| R. Phillips | Chem. Eng. & Mtrl. Sci. | ENG |
| Powell | Chem. Eng. & Mtrl. Sci. | ENG |
| Risbud | Chem. Eng. & Mtrl. Sci. | ENG |
| Sen* | Chem. Eng. & Mtrl. Sci. | ENG |
| J. Thompson | Biol. & Agr. Engineering | ENG |
| | | |
| Ames* | Chemistry | L&S |
| Balch | Chemistry | L&S |
| Beal* | Chemistry | L&S |
| Britt | Chemistry | L&S |
| Casey* | Chemistry | L&S |
| Chen* | Chemistry | L&S |
| David* | Chemistry | L&S |
| Franz | Chemitry | L&S |
| Gervay-Hague* | Chemistry | L&S |
| Guo | Chemistry | L&S |
| Kauzlarich | Chemistry | L&S |
| Kurth* | Chemistry | L&S |
| La Mar* | Chemistry | L&S |
| Mascal* | Chemistry | L&S |

| | | |
|---|---|---|
| Meares | Chemistry | L&S |
| Nambiar | Chemistry | L&S |
| Olmstead | Chemistry | L&S |
| Patten | Chemistry | L&S |
| Power* | Chemistry | L&S |
| Schore | Chemistry | L&S |
| Shaw* | Chemistry | L&S |
| Tantillo | Chemistry | L&S |
| Toney | Chemistry | L&S |
| | | |
| Anderson | Physiology & Membrane Biol. | MED |
| Berman | Neurological Surgery | MED |
| Cala | Physiology & Membrane Biol. | MED |
| Chung | Biochemistry & Molecular Med. | MED |
| Fyhrie | Orthopedics | MED |
| Glaser* | Pediatrics | MED |
| Huser | Center for Biophotonics | MED |
| Jue* | Biochemistry & Molecular Med. | MED |
| Kaysen | Biochemistry & Molecular Med. | MED |
| Kim, K. | Neurological Surgery | MED |
| Kreutzer* | Biochemistry & Molecular Med. | MED |
| Lam, K. | Hemat. & Oncol. | MED |
| Neu | Orthopedics | MED |
| O'Donnell* | Physiology & Membrane Biol. | MED |
| Pinkerton | Pediatrics | MED |
| Reddi | Orthopedics | MED |
| Theis | Microbiology & Immunol. | MED |
| Wulff | Pharmacology | MED |
| | | |
| Fiehn | Genome Center | CBS |
| Lagarias | Molecular & Cellular Biol. | CBS |
| Parales | Microbiology | CBS |
| Tolstikov | Genome Center | CBS |
| | | |
| Angelastro | Mol. Biosciences | VET |
| North | Mol. Biosciences | VET |
| Vulliet | Mol. Biosciences | VET |

*Off-campus Users, Academic & Industrial:*
Eion Energy Corporation
UC Berkeley
UC Santa Cruz*

*Users of >200 hours spectrometer time in the FY.

**B. Non-Faculty Usage**

Most of the daily hands-on use of the Facility instrumentation is by students, post-doctorals, and staff researchers. In FY 07-08 the Facility was used by 227 such individuals. Here is a listing of hands-on users by type:

Undergraduate Students 40

| | |
|---|---|
| Graduate Students | 127 |
| Post-Doctorals | 49 |
| SRAs, staff | 5 |
| Non-Senate faculty | 4 |
| Visiting scientists | 2 |

**C. NMR Training Class**

The Facility offers an annual operator training course with lecture and laboratory covering both theory of NMR and hands-on instrument training. (The lecture portion of the course can be taken for credit as BCM 230). The course, open to all UCD students and staff, is primarily attended by graduate students. Over the last 21 years we have averaged 24 students per year in the class. The NMR Training Class of Fall 2007 had an enrollment of 24. The attendees came from 12 different departments of six Colleges and Schools of the Davis campus. All three Staff members (de Ropp, Walton, Yu) participate in teaching the class.

The students in the Fall 2007 class are listed below by department and College. Those who attended consisted of 12 graduate students, two undergraduates, seven post-doctoral scholars, two visiting scholars, and one staff member.

| Name | Department | College |
|---|---|---|
| Ai, Leo* | Biomed. Eng. | ENG |
| Arias, Angelo D.#* | Molecular Biosci. | VET |
| Chen, Jay# | Physiology & MB | MED |
| Davis, Ryan#* | Chemistry | MPS |
| Go, Joan Lorraine# | Chemistry | MPS |
| Islas-Trejo, Alma# | Animal Sciences | AES |
| Kumar, Dinesh# | Genome Center | CBS |
| Liu, Ning#* | Textiles | AES |
| Luo, Anwei# | FS&T | AES |
| Mazi, Bekir# | FS&T | AES |
| Miller, Brandon#* | Biological & Ag. Eng. | ENG |
| Musnicki, Wyatt J.#* | Chem. Eng. & Mat. Sci. | ENG |
| Oztop, Halil M.#* | FS&T | AES |
| Peng, Dungeng# | Chemistry | MPS |
| Roa, Adan E.* | NMR Facility | OR |
| Schmidt, Leigh C.* | FS&T | AES |
| Schombs, Matt# | Chemistry | MPS |
| Seo, Jay# | Biomed. Eng. | ENG |
| Sheng, Liang# | Internal Medicine | MED |
| Van Scoy, April#* | Environmental Tox. | AES |
| Villa, Eric* | Chemistry | MPS |
| Witschi, Mark# | Chemistry | MPS |
| Xiao, Wenwu# | Internal Medicine | MED |
| Zou, Wei# | Genome Center | CBS |

* Took BMM 230 for credit (11 total).
# Attended lab portion of class (20 total).

**D. NMR Facility Staff Participation in Other UCD Courses**

In addition to BCM 230, the NMR Facility Staff participate in, or assist, instruction in several other courses annually. In FY 2007-8 these were:

CHE 219, Spectroscopy of Organic Compounds, Spring 2008. Oversee two TAs in instruction of use of NMR spectrometers for first year organic chemistry graduate students. Two lab sections of 2.5 hours each, 20 total students (de Ropp).

CHE 125, Advanced Methods in Physical Chemistry, Winter and Spring 2008. Prepare undergraduate NMR lab exercises, train TAs, and assist in lab instruction. (de Ropp).

CHE 124L, Inorganic Chemistry Lab, Spring 2008. Train students in use of NMR for undergraduate inorganic chemistry lab (de Ropp)

EMS 251- Applications of Solid State Nuclear Magnetic Resonance Spectroscopy, Spring 2008 (Yu).

**E. Undergraduate Research**

UCD undergraduates have regularly participated in the NMR Training Class and in the individual research projects of the various faculty using the Facility. In FY 07-08, 40 undergraduates from various different research groups were involved in hands-on usage of the Facility instruments. The projects included NMR studies of natural products, synthesized molecules, plants, and development of methodologies for NMR imaging.

**F. Dissertations.**

Following is a list of Ph.D and M.S. dissertations completed in FY 2007-2008 that made use of the NMR Facility. There are 13 total.

Ciprian Catana, Biomedical Engineering, Ph. D., 2007. “Development of an integrated multi-slice PET-MRI scanner using fiber optically coupled LSO/PSAPD detectors”.

Cathei Condron, Chemistry, Ph. D., 2006. “Exploring light element materials for thermoelectric applications”.

Zhenming Du, Chemistry, Ph. D., 2007. “Solution $^{1}$H NMR studies of heme oxygenase from the pathogenic bacterium Corynebacterium diphtheriae”.

Mohamed El-Badri, Chemistry, Ph. D., 2007. “Synthetic and physical organic studies of stereoselective glycosylation reactions using glycosyl iodides”.

Sabyasachi Gaan, Agricultural and Environmental Chemistry, Ph. D., 2007. “A study on flame retardancy and flame retardants of textile material”.

Melissa Jeddeloh, Chemistry, Ph. D., 2007. “Diversity oriented synthesis : methods and applications”.

Yoojung Kim, Food Science, Ph. D., 2007. “Influence of [alpha]-lactalbumin on structure of surfactant self-assemblies in oil/water mixtures”.

David Lane, Chemistry, Ph. D., 2007. “Solution phase and polymer bound ruthenium carbene complexes for olefin metathesis”.

Song Liu, Agricultural and Environmental Chemistry, Ph. D., 2007. “Functional modification of textile polymers via dry-state radical grafting polymerization”.

Lori Robins, Chemistry, Ph. D., 2007. “Interfacing chemistry and biology : assay development for aldose reductase inhibitors and combinatorial synthesis of diazocinones, isoxazoles and indazolo-benzoxazines”.

Lixia Shang, Chemistry, Ph. D., 2008. “Chemical synthesis and biological applications of bilin amides”.

Diment Singh, Chemistry, Ph. D., 2006. “Formation of linker side chains for use in binding metal chelates to biological species”.

Pingping Sun, Chemical Engineering, Ph. D., 2007. “Synthesis, characterization and energetics of zeolites”.

## VII. RESEARCH SUPPORT

### A. Extramural: NMR Facility/Instrument Grants

1. Funding History: Major instrumentation grants awarded to the Facility.

| Grant | Purpose | Total Direct Costs, $ |
|---|---|---|
| NIH RR02479 | Regional Resource for *in vivo* NMR; Purchase CSI-2T | 733,707 |
| NSF PCM8417289 | Purchase Ω-7T; fund Staff | 275,021 |
| NIH RR02511 | Purchase Ω-7T | 200,000 |
| NIH 1S10 RR04795 | Purchase Ω-500 | 400,000 |
| NSF BBS88-04739 | Purchase Ω-500; SUN 3/260 | 185,000 |
| NSF DIR9016484 | Purchase Ω-300 | 205,000 |
| NIH RR08206 | Purchase AMX-400 | 262,000 |
| NIH RR11973 | Purchase DRX-600 | 400,000 |
| NSF OSTI 97-24412 | Upgrade of Ω-500 and Ω-7T to DRXs | 596,000 |
| NIH S10 RR13871 | Upgrade of AMX-400 to DRX | 434,084 |
| NSF DBI0079461 | Purchase 600 MHz cryoprobe | 150,803 |
| NSF EAR0213546 | Purchase 500 MHz solids | 505,000 |
| NSF CHE0443516 | Purchase 600 MHz | 540,080 |

2. Instrumentation grant currently active:

| | | |
|---|---|---|
| NSF DBI-0722538 | Purchase 800 MHz | 1,600,000 |
| | **Total Awarded** | **6,486,695** |

**B. Extramural: FY 07-08 Individual Faculty Research Grants**

Numerous faculty have on-going major grants devoted largely or entirely to research utilizing the NMR Facility, and many additional faculty grants have NMR as a significant component. The FY 07-08 grants are listed below (dollar amounts are rounded to the nearest thousand).

*Major Federal Grants* that rely heavily on research conducted at the NMR Facility:

| Faculty, Dept. | Grant | Total Costs per annum, $ |
|---|---|---|
| Ames, Chem. | NIH EY012347 | 309,000 |
| | NIH NS045909 | 145,000 |
| | NIH NS059969 | 225,000 |
| Casey, Chem. | NSF EAR-0515600 | 101,000 |
| La Mar, Chem. | NIH GM62830 | 216,000 |
| Louie, Biomed Eng. | NIH EB000993 | 127,000 |
| M. McCarthy, FS&T | USDA CSREES 2008-35503-18665 | 82,000 |
| O'Donnell, Human Physio. | NIH NS39953 | 76,000 |
| Powell, Chem. Eng. | NASA NNC04GA73G | 76,000 |
| | Total | **1,357,000** |

*Major Federal Grants* that utilize NMR methodology in part:

| | | |
|---|---|---|
| Balch, Chem. | NSF CHE-0716843 | 145,000 |
| Beal, Chem. | NIH GM080784 | 255,000 |
| | NIH GM061115 | 239,000 |
| Berman, Med. Neuro. Surg. | NIH 1RL1NS062411 | 787,000 |
| Casey, Chem. | DOE DE-FG02-OR34I5693 | 114,000 |
| | NASA NNX07AV56G | 74,000 |
| Chen, Chem. | NIH GM076360 | 275,000 |
| | NSF CHE-0548235 | 124,000 |
| | NIH CA128442 | 70,000 |
| | NIH 06-002909 | 50,000 |
| Cherry, Biomed. Eng. | NIH EB000993 | 179,000 |
| Dungan, FS&T | USDA 2006-02670 | 150,000 |
| Ferrara, Biomed, Eng. | NIH CA103828 | 1,100,000 |
| Gates, CE&MS | DOE DE-FG02-04ER15513 | 118,000 |
| Gervay-Hague, Chem. | NIH GM075093 | 150,000 |
| Glaser, Pediatrics | NIH NS048610 | 330,000 |
| Guo, Chem. | NSF CHE-0135132 | 77,000 |
| Hammock, Entomology | NIH ES-004699 | 665,000 |
| Kauzlarich, Chem. | DOE DE-FC36-05GO15055 | 204,000 |
| Kurth, Chem. | NSF CHE-0614756 | 150,000 |
| | NIH DK067003 | 291,000 |
| | NIH DK072517 | 445,000 |
| | NIH CA113298 | 773,000 |
| | NIGMS P41 GM076151 | 480,000 |
| Lam, Internal Med. | NIH CA097257 | 76,000 |
| | NIH CA113298 | 806,000 |
| Mascal, Chem. | NSF CHE-0448976 | 108,000 |
| | NCI CA127256 | 228,000 |
| Meares, Chem. | NCI CA016861 | 306,000 |

| | | |
|---|---|---|
| Navrotsky, CE&MS | NSF DMR-0601892 | 144,000 |
| Pan, Bio. Ag. Eng. | USDA ARS 58-5325-5-742 | 56,000 |
| Parales, Microbiology | NSF MCB-0627248 | 166,000 |
| Pinkerton, Pediatrics | NIH ES013932 | 527,000 |
| Power, Chem. | NSF CHE-0304871 | 291,000 |
| | NSF CHE-0346715 | 118,000 |
| | NSF CHE-0641020 | 165,000 |
| | DOE DE-FC36-05GO15055 | 204,000 |
| | DOE DE-FG02-07ER46475 | 165,000 |
| Sen, CE&MS | NSF DMR-0603933 | 76,000 |
| Sutcliffe, Biomed Eng. | NIH CA107792 | 250,000 |
| Tantillo, Chem. | NSF CHE-0449845 | 101,000 |
| Toney, Chem. | NIH GM054779 | 153,000 |
| Wulff, Pharmacology | NIH NS053426 | 134,000 |
| Yao, Hematology/Oncology | ARMY W81XWH-06-1-0447 | 133,000 |
| | Total | **11,452,000** |

*Other Government Grants* that utilize NMR methodology wholly or in part:

| | | |
|---|---|---|
| Hernes, LAWR | CA State Water Research Board | 1,050,000 |
| Theis, Microbiology & Immun. | CA Dept. Fish & Game | 8,000 |
| Tjeerdema, Env. Tox | CA State Wildlife Care Network | 39,000 |
| | CA State Wildlife Care Network | 37,000 |
| | Total | **1,134,000** |

*Industrial, Commodity Board or Private Grants* that utilize NMR methodology wholly or in part:

| | | |
|---|---|---|
| Angelastro, VMMB | Richard A. Freedland Fellowship | 3,000 |
| Casey, Chem. | Amer. Chem. Soc. 40412-AC2 | 27,000 |
| | Lawrence Livermore NS B553620 | 81,000 |
| Chen, Chem. | Arnold/Mabel Beckman Found. 107454 | 66,000 |
| Fiehn, Genome & Biomed. | Agilent 06-0020666 | 94,000 |
| Gervay, Chem. | Novartis 1 PO1 AI066287 | 202,000 |
| Jue, Biol. Chem. | Bayer 07-00166V | 34,000 |
| Kaysen, Biochem &Mol. Med. | Bayer 07-00166V | 34,000 |
| Kreutzer, Biochem& Mol. Med. | Bayer 07-00166V | 34,000 |
| | American Heart Assoc. 0265319Y | 20,000 |
| Kurth, Chem. | Dow AgraSciences | 40,000 |
| Mascal, Chem. | Chevron CHV1MA4 | 12,000 |
| M. McCarthy, FS&T | Cornell/USDA 434938329 | 17,000 |
| | Kraft Foods 07000908 | 14,000 |
| | University of Washington 339599 | 10,000 |
| Medrano, Animal Sci. | CDRF 05 MEJ-01-NH | 109,000 |
| Pinkerton, Pediatrics | Philip Morris USA 010759 | 227,000 |
| Tjeerdema, Env. Tox. | CA Rice Research | 38,000 |
| Wood, Env. Tox. | American Heart Assoc. 0635328N | 130,000 |
| | Total | **1,192,000** |

**Grand Total** **$ 15,135,000**

for FY 07-08

The indirect costs the Davis campus received from all listed individual faculty research grants in FY 07-08 was in excess of **$4,200,000**.

## C. Intramural: NMR Awards

The UCD Office of Research has annually made available small Awards through the Facility for campus faculty to pursue research utilizing the NMR Facility. Given below are the recipients of 07-08 NMR Awards with the amount of each Award. Publications arising from NMR Award funded research are included in Section X. The NMR Awards have proven their value in seeding the creation of extramurally funded research. The large, successful NMR research programs of Anderson/Cala, Casey, Jue, Louie, K. McCarthy, M. McCarthy, Sen, and Tjeerdema were all initially helped through NMR Awards; and several other extramurally funded programs (X. Chen, Dungan, Ebeler, Gervay-Hague, Hull, O'Donnell, among others) have been aided by NMR Awards. A separate detailed annual Report on NMR Awards is produced every year and submitted to the Office of Research; it is also available upon request. Due to the UC budget crisis there will be no NMR Award program in the next FY.

2007-08 NMR AWARDS

| Faculty | Department | Award, $ |
|---|---|---|
| Ames, J | Chemistry | 1,600 |
| Barrett, D. | Food Science & Technology | 1,000 |
| Berger, T. | Animal Science | 500 |
| Boulton, R. | Viticulture & Enology | 1,000 |
| Chen, X. | Chemistry | 800 |
| Chung, Y. | Biochem. & Mol. Medicine | 500 |
| Ebeler, S. | Viticulture & Enology | 700 |
| Gervay-Hague, J. | Chemistry | 1,000 |
| Giulivi, C. | Molecular Biosciences | 1,000 |
| Hernes, P. | Land, Air & Water Resources | 800 |
| Kauzlarich, S. | Chemistry | 1,000 |
| Kaysen, G. | Biochem. & Molecular Med. | 500 |
| Kreutzer, U. | Biochem. & Molecular Med. | 1,000 |
| Labavitch, J. | Plant Sciences | 800 |
| Lagarias, J. | Molecular & Cell. Biology | 400 |
| Lesher, C. | Geology | 700 |
| Louie, A. | Biomedical Eng. | 1,500 |
| McCarthy, K. | Food Science & Technology | 1,000 |
| Nambiar, K. | Chemistry | 400 |
| Neu, C. | Orthopedic Surgery | 1,000 |
| Sen, S. | Chem. Eng. & Mat. Science | 1,600 |
| Tolstikov, V. | Genome Center | 1,200 |

## VIII. FISCAL DATA

### A. Introduction

The NMR Facility operations (recharge) account had a 07-08 FY budget deficit of -$5,729. The cumulative balance is now -$5,282. The full statement of the FY 07-08 Operating Budget is given on the next page as Section VIII-B.

The expenses of the Facility reported here include all expenditures associated with Facility operations (save for equipment expenses). These expenditures include the salaries and benefits of the Facility Staff (see Sections VIII-B, C) and all Supplies & Expenses. Income to the Facility consists of 1) recharges for spectrometer time (FY 07-08 recharge rates are given as Section VIII-D) 2) support from the Office of Research and central administration for Professional Staff and business office salaries and benefits, and 3) grant support.

The proposed Operating Budget for FY 08-09 is Section VIII-C. The projected recharge income is based on the FY 07-08 results.

**B. Fiscal Statement for FY 07-08 Operating Budget**[1] (rounded to nearest dollar).

Expenses

| | |
|---|---|
| Salaries: | |
| 3.0 Professional Staff | 247,236 |
| Director's Stipend | 6,000 |
| 0.5 student Assts | 6,270 |
| 0.3 Business Office Staff (BMM dept.) | 18,889 |
| Benefits[2] | 30,282 |
| Leave Transfer | -6,397 |
| Subtotal Salaries & Benefits | 302,278 |
| Supplies & Expenses: | |
| Magnet cryogens | 17,853 |
| Liability | 165 |
| Books, subscriptions | 388 |
| Computer licenses & software | 9,444 |
| Repairs, service, maintenance | 19,689 |
| Fleet Services | 0 |
| Telephone & EtherNet, etc | 3,296 |
| Reprographics; mail; Illustration Services, freight | 1,685 |
| Facilities Services | 1,221 |
| Lab & office supplies | 45,202 |
| Minor equipment | 6,471 |
| Miscellaneous | 944 |
| Subtotal Supplies & Expenses | 106,359 |
| Travel | 3,464 |
| Minor Equipment | 2,625 |
| **Total Expenses** | **$414,726** |

Income

| | |
|---|---|
| Recharges | 177,238 |
| Regular Contribution from Office of Research & Colleges for Professional Staff Salaries; Dir. Stipend; Business Office | 189,919 |
| Grant support for staff | 41,840 |
| **Total Income** | **$408,997** |
| **Deficit in FY 07-08:** | **$ -5,729** |
| **Cumulative Balance** | **$-5,282** |

[1]Operating Budget does not include outlay for major equipment, if any.
[2]Non-19900 benefits only.

**C. Proposed Operating Budget for FY 08-09**[1]

| | | |
|---|---|---|
| Projected Outlay | | |
| Salaries: | | |
| 3.0 Professional Staff | | 260,000 |
| Director's Stipend | | 6,000 |
| 0.5 student Asst | | 6,000 |
| 0.3 Business Office Staff (BMM Dept.) | | 18,000 |
| Benefits[2] | | 32,000 |
| Leave Transfer | | -6,000 |
| | Subtotal Salaries & Benefits | 316,000 |
| Supplies & Expenses: | | |
| Magnet cryogens | | 35,000 |
| Liability | | 200 |
| Books, subscriptions | | 600 |
| Computer licenses & software | | 9,000 |
| Repairs, service, maintenance | | 38,000 |
| Fleet Services | | 200 |
| Telephone & EtherNet, etc | | 3,500 |
| Reprographics; mail; Illustration Services, freight | | 1,500 |
| Facilities Services | | 3,000 |
| Lab & office supplies | | 46,000 |
| Miscellaneous | | 1,000 |
| | Subtotal Supplies & Expenses | 138,000 |
| Travel | | 2,000 |
| Minor Equipment | | 3,000 |
| | **Total Outlay** | **$459,000** |
| Projected Inflow | | |
| Projected Recharges & Income | | 262,000 |
| Contribution from Office of Research for Professional Staff Salaries; Dir. Stipend; Business Office | | 160,000 |
| Grant support | | 42,000 |
| | **Total Inflow** | **$464,000** |
| | **Projected Surplus** | **$5,000** |

[1]Operating Budget does not include outlay for equipment, if any.
[2]Benefits only for non-19900 salaries.

**D. Facility FY 07-08 Recharge Rates**

Rates are set by the Office of Planning & Budget and the Vice-Chancellor for Research based on recommendations by the NMR Facility Director and Advisory Board. Rates reflect the operating costs of Facility instrumentation, and are used to fund the Operating Budget of the Facility (Section VIII-B).

Staff Run Rates - Spectra run by Facility Staff.

| | |
|---|---|
| All spectrometers, all hours | $43/hour |
| Work Stations | $43/hour |

User Rates - Spectra run by user.

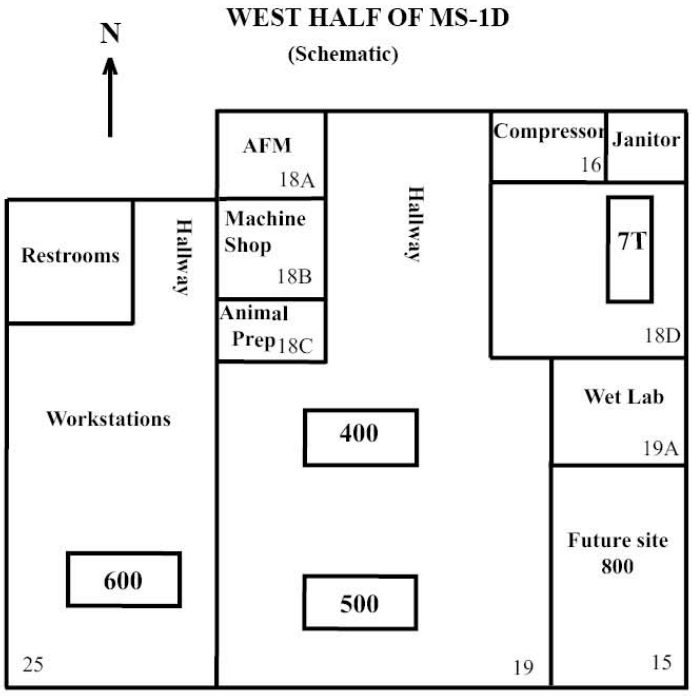
| | |
|---|---|
| All spectrometers weekdays 8 AM -5 PM (assisted rate) | $10.50/hour |
| All spectrometers weekdays 5 PM-8 AM & weekends all hours | $4/hour |
| Work Stations | $3/hour |
| Operator Training Lab (adjunct to BCM 230) | $330/student |
| Non-UC Rate – for non-UC entities utilizing Facility | Campus rates + NUD* |

*NUD= Non-University Differential, currently 29.5%.

## IX. PHYSICAL PLANT

The NMR Facility as of June 30, 2008 occupies space in three separate locations on campus. Most Facility space is in Rooms 15/18/19/25 of MS1-D, and an adjacent trailer. This building space has been supplied by the Medical School. The solids 500 MHz spectrometer is housed in Kemper Hall in space supplied by the Department of Chemical Engineering & Materials Science. Four instruments are housed in Chemistry in space supplied by that department.

The MS1-D location provides ca. 5000 square feet of space for up to seven possible spectrometers, five or more off-line computers, and two wet labs. (Room 18A is used by the Medical School for an atomic force microscope). The trailer provides ca. 1400 square feet for offices, an electronics shop, and additional computer space.



## X. LIST OF PUBLICATIONS

Listed here are publications from FY 07-08 that utilized research accomplished at the NMR Facility. The works listed are reviewed publications in recognized international journals/review series; abstracts are not included. The principal UCD faculty investigator(s) for each publication is underlined. There are 83 total publications.


Jacqueline D. Lusin, Murugendra Vanarotti, Congmin Li, Aswani Valiveti, and James B. Ames. (2008). NMR Structure of DREAM: Implications for Ca2+-Dependent DNA Binding and Protein Dimerization. *Biochemistry,* 47(8), 2252-2264.

Thomas Strahl, Inken G. Huttner, Jacqueline D. Lusin, Masanori Osawa, David King, Jeremy Thorner, and James B. Ames. (2007). Structural insights into activation of phosphatidylinositol 4-kinase (Pik1) by yeast frequenin (Frq1). *The Journal of biological chemistry*, 282(42), 30949-30959.

Medina DC, Kirkland DM, Tavazoie MF, Springer CS, Anderson SE. (2007). Na+/Ca2+-exchanger-mediated Mn2+-enhanced (H2O)-H-1 MRI in hypoxic, perfused rat myocardium. *Contrast media and molecular imaging*, 2(5), 248-257.

J.R. Giuliani, S.J. Harleya, R.S. Cartera, P.P. Power, and M.P. Augustine. (2007). Using liquid and solid state NMR and photoluminescence to study the synthesis and solubility properties of amine capped silicon nanoparticles. *Solid State Nuclear Magnetic Resonance*, 32(1), 1-10.

Daniel Rios, David M. Pham, James C. Fettinger, Marilyn M. Olmstead, and Alan L. Balch. (2008). Blue or green glowing crystals of the cation [Au{C(NHMe)(2)}(2)](+) structural effects of anions, hydrogen bonding, and solvate molecules on the luminescence of a two-coordinate gold(I) carbene complex. *Inorganic chemistry*, 47(8), 3442-3451.

Leone Spicci and William H. Casey. (2007). Synthesis of experimental models for molecular inorganicgeochemistry - A review with examples. *Geochimica et cosmochimica acta*, 71(23), 5590-5604.

Edina Balogh, Travis M. Anderson, James R. Rustad, May Nyman, and William H. Casey. (2007). Rates of oxygen-isotope exchancie between sites in the [HxTa6O19]((8-x))-(aq) lindqvist ion and aqueous solutions: Comparisons to [HxNb6O19]((8-x))-(aq). *Inorganic chemistry*, 46(17), 7032-7039.

Edina Balogh, Ana Maria Todea, Achim Müller, and William H. Casey. (2007). Rates of ligand exchange between > Fe-III-OH2 functional groups on a nanometer-sized aqueous cluster and bulk solution. *Inorganic chemistry*, 46(17), 7087-7092.

William H. Casey and James R. Rustad. (2007). Reaction dynamics, molecular clusters, and aqueous geochemistry. *Annual Review of Earth and Planetary Sciences*, 35(1), 21-46.

Mingchi Sun, Yanhong Li, Harshal A. Chokhawala, Ryan Henning and Xi Chen. (2008). N-Terminal 112 amino acid residues are not required for the sialyltransferase activity of Photobacterium damsela alpha 2,6-sialyltransferase. *Biotechnology letters*, 30(4), 671-676.

Saddam Muthana, Hai Yu, Shengshu Huang, and Xi Chen. (2007). Chemoenzymatic synthesis of size-defined polysaccharides by sialyltransferase-catalyzed block transfer of oligosaccharides. *Journal of the American Chemical Society*, 129(39), 11918-11919.

Amanda L. Lewis, Hongzhi Cao, Silpa K. Patel, Sandra Diaz, Wesley Ryan, Aaron F. Carlin, Vireak Thon, Warren G. Lewis, Ajit Varki, Xi Chen, and Victor Nizet. (2007). NeuA sialic acid O-acetylesterase activity modulates O-acetylation of capsular polysaccharide in Group B Streptococcus. *The Journal of biological chemistry*, 282(38), 27562-27571.

Harshal A. Chokhawala, Hongzhi Cao, Hai Yu, and Xi Chen. (2007). Enzymatic synthesis of fluorinated mechanistic probes for sialidases and sialyltransferases. *Journal of the American Chemical Society*, 129(35), 10630-10631.

Yanhong Li, Mingchi Sun, Shengshu Huang, Hai Yu, Harshal A. Chokhawala, Vireak Thon and Xi Chen. (2007). The Hd0053 gene of Haemophilus ducreyi encodes an alpha 2,3-sialyltransferase. *Biochemical and biophysical research communications*, 361(2), 555-560.

Huang SS, Yu H, Chen X. (2007). Carbohydrate post-glycosylational modifications. *Organic& Biomolecular Chemistry,* 5(6), 865-872.

Ciprian Catana, Daniel Procissi, Yibao Wu, Martin S. Judenhofer, Jinyi Qi, Bernd J. Pichler, Russell E. Jacobs, and Simon R. Cherry. (2008). Simultaneous in vivo positron emission tomography and magnetic resonance imaging. *Proceedings of the National Academy of Sciences of the United States of America*, 105(10), 3705-3710.

Cherry, S.R.; Louie, A.Y.; Jacobs, R.E. (2008). The integration of positron emission tomography with magnetic resonance imaging. *Proceedings of the IEEE,* 96(3), 416 -438.

Judenhofer MS, Catana C, Swann BK, Siegel SB, Jung WI, Nutt RE, Cherry SR, Claussen CD, Pichler BJ. (2007). PET/MR images acquired with a compact MR-compatiable PET detector in a 7-T magnet. *Radiology*, 244(3), 807-814.

Jun Y. Kim and Stephanie R. Dungan. (2008). Effect of -Lactalbumin on Aerosol-OT Phase Structures in Oil/Water Mixtures. *Journal of Physical Chemistry B*, 112(17), 5381-5392.

Jessica H. Wong, Marilyn M. Olmstead, James C. Fettinger and Jacquelyn Gervay-Hague. Vinyl sulfones. (2008). Acta crystallographica. Section C, *Crystal structure communications*, 64(3), o132-o136.

Yan Lu and Jacquelyn Gervay-Hague. (2007). Synthesis of C-4 and C-7 triazole analogs of zanamivir as multivalent sialic acid containing scaffolds. *Carbohydrate Research*, 342(12-13), 1636-1650.

Mohamed H. El-Badri, Dan Willenbring, Dean J. Tantillo, and Jacquelyn Gervay-Hague. (2007). Mechanistic studies on the stereoselective formation of beta-mannosides from mannosyl iodides using alpha-deuterium kinetic isotope effects. *Journal of organic chemistry*, 72(13), 4663-4672.

Wenjun Du, Suvarn S. Kulkarni and Jacquelyn Gervay-Hague. Efficient, one-pot syntheses of biologically active alpha-linked glycolipids. (2007). *Chemical communications*, (23), 2336-2338.

Christophe Morisseau, John W. Newman, Craig E. Wheelock, Thomas Hill III, Dexter Morin, Alan R. Buckpitt, and Bruce D. Hammock. (2008). Development of metabolically stable inhibitors of mammalian microsomal epoxide hydrolase. *Chemical research in toxicology*, 21(4), 951-957.

In-Hae Kim, Hsing-Ju Tsai, Kosuke Nishi, Takeo Kasagami, Christophe Morisseau, and Bruce D. Hammock. (2007). 1,3-disubstituted ureas functionalized with ether groups are potent inhibitors of the soluble epoxide hydrolase with improved pharmacokinetic properties. *Journal of medicinal chemistry*, 50(21), 5217-5226.

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## APPENDIX

## USAGE DATA

The Appendix presents graphically usage of the Facility by campus Colleges and Schools, and by the type of NMR research.

Figure One shows usage of the Facility by College (see Section VI), expressed as percent recharges from each College. The "other" category is use by non-UCD users, either academic or industrial. Total recharge income was $177,238 and total hours of recharged usage on all spectrometers was 25,219.

Figure Two shows usage of the Facility by research type as described in Section II of this Report. The "other" category is non-UCD industrial or academic users.

Figure One
Facility Usage By College

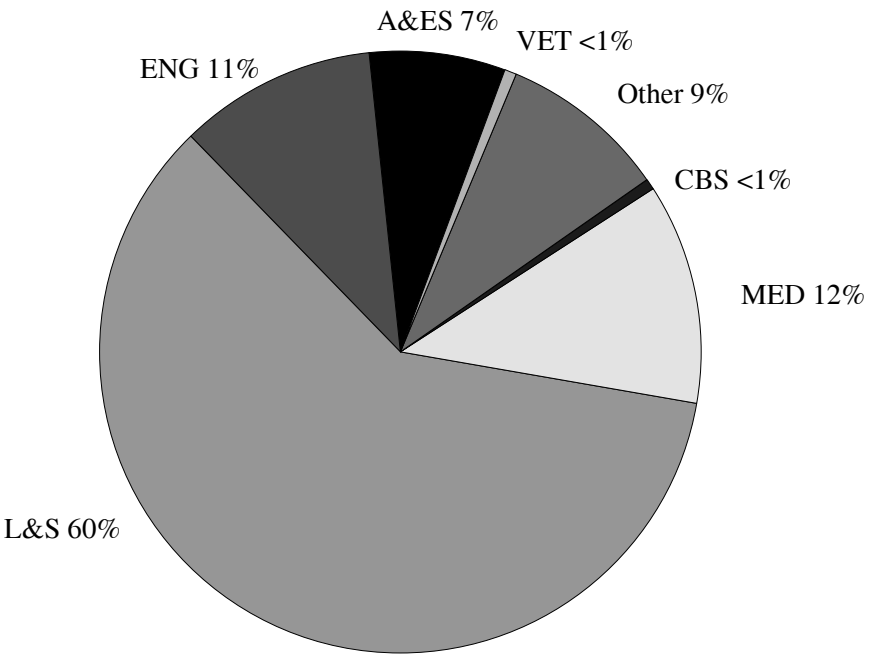

Figure Two
Facility Usage By Reseach Type