From:	Lloyd Rooney
To:	David Baltensperger
Cc:	Amir M Ibrahim; Dirk Hays; Joseph M Awika; Russell W Jessup; Richard H Loeppert; Scott A Finlayson; Seth C Murray; Terry J Gentry; Scott Senseman; Bill L Rooney
Subject:	Request for Equipment PUF funds
Date:	Wednesday, November 04, 2009 3:19:10 PM
Attachments:	LC-MSpufrequestfinal.doc

I am attaching a request for PUF funds to purchase state of the art LC and GC Mass Spec equipment. Several faculty members have indicated that they will provide sufficient funds to meet a 50% Cost Sharing.

At the Dept heads meeting this week we were told that a deadline for PUF requests has not been established but it is going forward with goal of awarding by or in December. Lloyd

Texas AgriLife Research FY'10 Research Equipment Support and Facilities Upgrade

Instruments: **Ultra Performance Liquid Chromatograph/Mass Spectrometer (UPLC-MS: ACQUITY UPLC TQD, Waters Corporation) and Gas Chromatograph/Mass Spectrometer (GC-MS: Agilent)**
Principal Investigators:

Lloyd Rooney	Regents Professor, Department of Soil & Crop Sciences.
Joseph Awika	Asst. Professor, Departments of Soil & Crop Sciences/Nutrition & Food Science
Dirk Hays	Assoc. Professor, Department of Soil & Crop Sciences
Scott Senseman	Professor, Department of Soil & Crop Sciences
Scott Finlayson	Assoc. Professor, Department of Soil & Crop Sciences
William Rooney	Professor, Department of Soil & Crop Sciences
Terry Gentry	Asst Professor, Department of Soil & Crop Sciences
Amir Ibrahim	Assoc. Professor, Soil and Crop Sci. Dept.
Seth Murray	Asst. Professor, Department of Soil & Crop Sciences
Russell Jessup	Asst. Professor, Department of Soil & Crop Sciences
Richard Loeppert	Professor, Department of Soil & Crop Sciences

Administrative Approval:

David Baltensperger, Head Soil & Crop Science, TAMU

[redacted]

Equipment Description/Projected Impact of Research:

Description of UPLC-MS: Ultra performance liquid chromatograph-mass spectrometer (UPLC-MS) is a state-of-the-art technology that is used to detect and quantify compounds in various matrices. This new technology is rigorous and reliable, particularly for identifying trace-level organic compounds. This particular technology is currently not available in any academic department on campus.

This instrument separates, identifies and quantifies chemical compounds in complex matrices. It uses liquid as a carrier to move analytes through a column that separates the materials followed by quantitation and identification based on the compound's mass and fragmentation when passed through the mass spectrometer. This technology has become ***state-of-the-art in the analysis of phytochemicals, biofuels, pesticides, pharmaceuticals, metabolites, polymers, and proteins***. It is quickly ***replacing high performance liquid chromatography-mass spectrometry*** (HPLC-MS) as the preferred analysis method since it uses small column particles and very low solvent volumes, which result in higher resolution and higher throughput to detect more compounds more efficiently than HPLC-MS. The tandem quadrupole (TQD) mass detector is able to employ both ESI and APCI ionization modes in the same analysis to extend the types of compounds that can be analyzed in a single run. Other LC-MS instruments require that each mode be run separately, which requires more sample and solvent, produces more waste, and slows productivity.

Description of GC-MS: This instrument uses a gas as a carrier to move analytes through a column and into a mass spectrometer. However, only volatile organic compounds can be analyzed with this instrument. Like the LC-MS, analytes are quantified and identified based on mass and fragmentation. This instrument is used to

identify and quantify volatile organic compounds in environmental, food, and biological matrices. The sensitivity of this instrument to some volatile compounds exceeds that of the LC-MS and it is therefore complimentary to the LC-MS for the analysis of ultra low abundance molecules such as phytohormones.

Impact to research program if grant request is not funded: We expect to be more competitive for grants involving trace-level detections of organic materials in plants, microbes, cereals, legumes, oilseeds, soils, and water. The broad group of collaborators have outstanding records in grant dollar acquisition. These PIs have ongoing or newly funded projects and grants submitted or in preparation to DOE, ARP, TDA-TIE-BARD, BARD, NSF, NIH, and AFRI that are dependent on these technologies. These instruments are critical to core research in the department involving chemical and molecular characterization of plants, microbes, soils, water, grains, legumes, and grasses for bioactives, health, safety, bioenergy, and genetic properties. **We currently do not have any working mass spectroscopy equipment in the department.** Our research programs are limited to sporadic use of instruments in other departments, which is a distinct disadvantage in our plant, microbe, soil, water, and grain analysis. The lack of these instruments is a disadvantage to our programs in terms of generating quality and timely data to compete for external grants. The new UPLC-MS will reduce costs in terms of solvent and waste and is environmental friendly. With recent hiring of new faculty, the SCSC department has accumulated a critical mass of scientists who would capitalize on opportunities using this instrumentation. Students will be provided training on these instruments which will give them a distinct advantage in the business sector where similar technology is used with high regularity.

The PIs have expertise in analysis of plants, microbes, soils, water, and grains, and ***they each have federally funded collaborative projects that requires the use of LC-MS and GC-MS to complete the following objectives:***

1. Identification of phytochemicals in cereal grains and legumes for breeding of nutraceutical sorghum and other cereals/legumes (L. Rooney, J. Awika, W. Rooney, D. Hays, S. Murray). Cereals and legumes have a wide variety of phytochemicals that are comparable to fruits and vegetables. These have been reported to have anti-cancer, anti-inflammatory, and antioxidant properties. We must identify various derivatives of key flavonoids present in grains especially sorghum and cowpeas which have some unique compounds. This information will help plant breeders produce crops with maximum levels of the desired phytochemicals.
2. Identification of sorghum phytochemicals that affect the prevention of colon cancer (L. Rooney and N. Turner). There are ongoing collaborative studies with Dr. Nancy Turner (Department of Nutrition-Food Science) on the effect of sorghum phytochemicals in colon cancer is ongoing, which includes identification of absorbed and/or metabolized phytochemicals. LC/MS is the best instrument to identify those compounds.
3. A project funded by Texas AgriLife Bioenergy Initiative entitled "Systems optimization of high biomass native Texas plant species with high foliar triacylglycerol storage oils as ideal sources of high value biodiesel" will require a UPLC-MS to identify the leaf triacylglycerol chemical composition and content (Senseman, Hays, Jessup, Redmond,). Results from this study will be used to attract additional Federal, State, and Corporate funding.
4. Analysis of pesticides, herbicides, and water quality (Senseman, Gentry). From an environmental standpoint, newer chemistry for pest control tends to be highly specific, applied at low application rates, and often more water soluble. Additionally, the low application rates cause detection problems due to background noise that can be eliminated by analyzing these compounds through LC-MS^n. Water quality is also a major issue and the LC-MS instrument is vital to the thorough study of potential contaminants in soil and water.
5. Fulfilling the mandates of a new USDA-CSREES-AFRI funded project to Dirk Hays and Amir Ibrahim entitled "*Linking the Genetic Loci in Wheat that Regulate the Distinct Wax Cuticle Layers and its Variable Composition to Improved Drought Tolerance"* This is a QTL mapping project which will link the variable leaf wax layers in wheat and the variable chemical composition in each layer to improved functionality for heat and drought tolerance in wheat. This is an exciting project with a clear impact that will require a UPLC-MS to be successful (Hays, Ibrahim).
6. Both GC-MS and LC-MS are necessary to quantify phytohormones involved in the regulation of branching by phytochrome (NSF, Finlayson).