



# Evolution


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Core

Director

UC Davis Metabolomics

Core

<http://metabolomics-core.ucdavis.edu/>



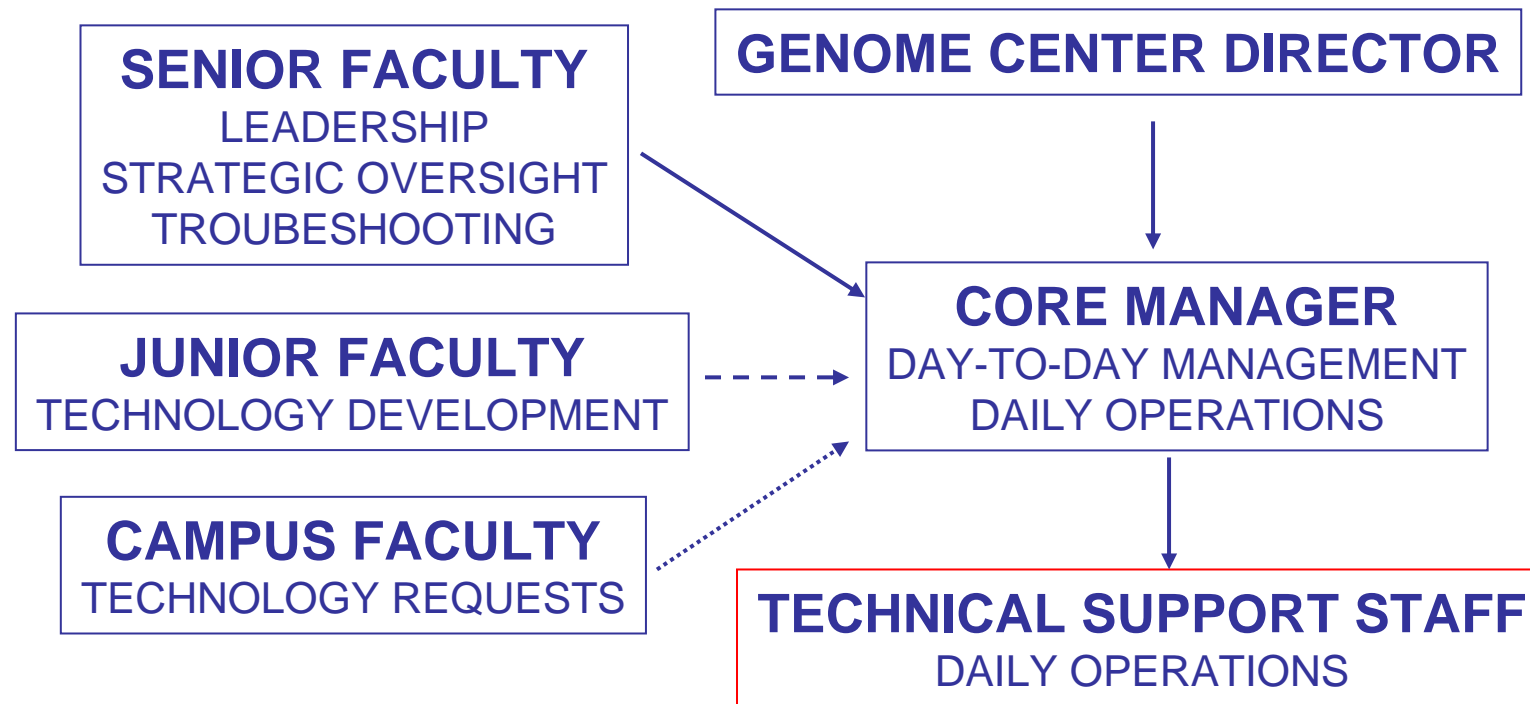
.....process in which something passes by degrees to a different stage (especially a more advanced or mature stage).....

## The Mission

- **Our goal is to apply efficiently our skills and knowledge for providing quality services in a timely, convenient, and cost-effective manner.**
- **The services offered by the Metabolomics Core Facility at Genome Center complement other UC Davis Core Facilities.**

# ORGANIZATIONAL STRUCTURE FOR SERVICE CORES

DNA TECHNOLOGIES, EXPRESSION ANALYSIS,  
PROTEOMICS, METABOLOMICS, BIOINFORMATICS

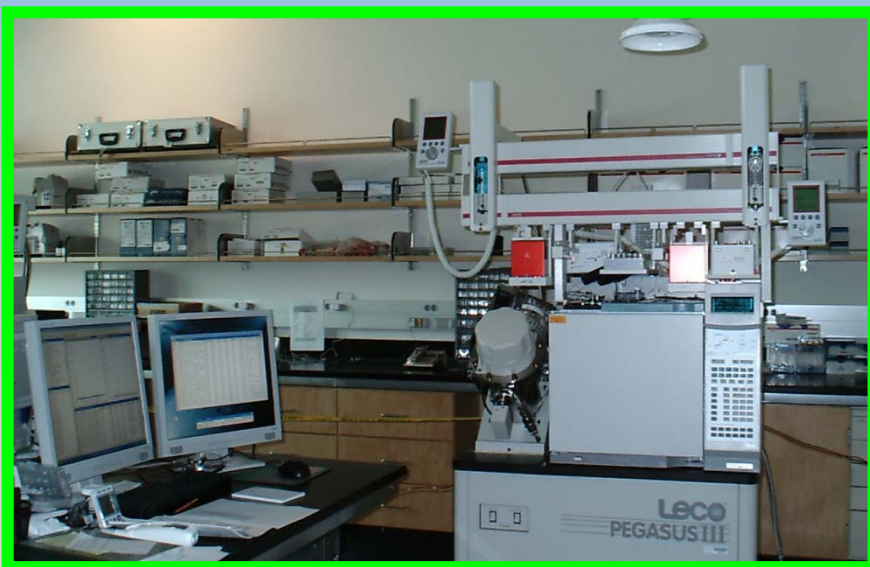


Extensions of research labs, available on an as needed, at cost basis  
Recharges based on costs of consumables, labor, and service contract  
minimal equipment and administrative overhead.  
State-of-the-art equipment and experienced staff.  
Economies of scale and institutional learning curves.

**UC Davis Metabolomics Core  
Facility started in 2005**

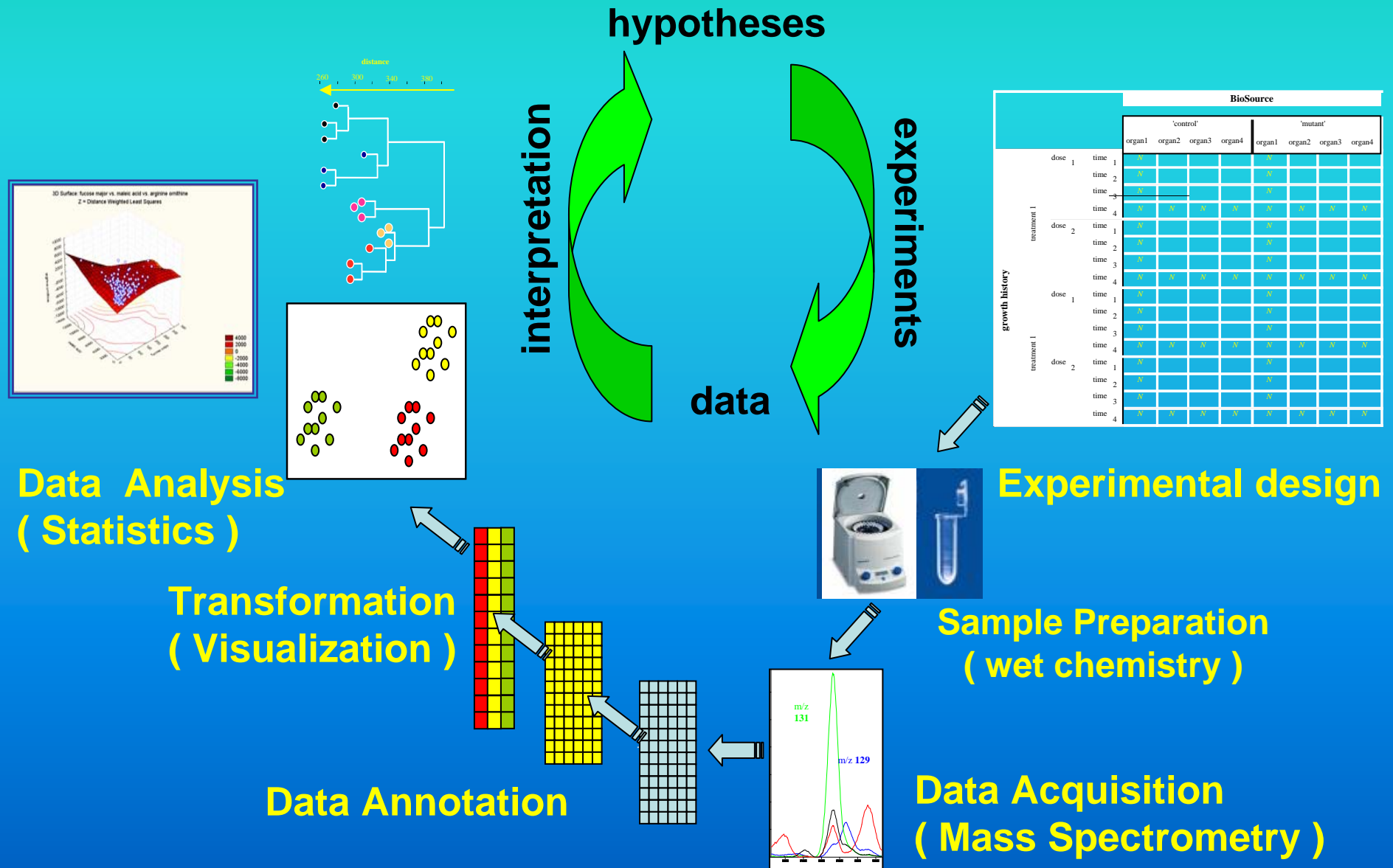


# Metabolomics Services



	Samples per year	Metabolites detected	% RSD	dynamic range	DB and QC
GC-TOF-MS	7,000	1-800	10-20	$10^3 - 10^4$	full integration
UPLC-MS	10,000	1-1500	10-30	$10^3 - 10^4$	flexible

# Metabolomics workflow



		BioSource											
		'control'				'mutant'							
growth history	treatment 1	dose 1	time 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	
			time 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
			time 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
			time 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
		dose 2	time 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
			time 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
			time 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
			time 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
	treatment 2	dose 1	time 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
			time 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
			time 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
			time 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
		dose 2	time 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
			time 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
			time 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
			time 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓

Data Analysis  
( Statistics )

Transformation  
( Visualization )

Data Annotation

Experimental design

Sample Preparation  
( wet chemistry )

Data Acquisition  
( Mass Spectrometry )

interpretation

experiments

hypotheses

data

# Small Molecule Biomarkers Workflow

Primary Metabolites

Secondary Metabolites

GC-MS

Gas Chromatography

RP-LC-MS

Reversed Phase LC-MS

HILIC-LC-MS

Hydrophilic Interaction LC-MS

Component Detection and Peak Alignment  
(mzmine and xcms)

Feature Selection of Important Components  
(Statistica Dataminer)

Univariate and Multivariate Statistics and Machine Learning  
(ANOVA, PCA, PLS, CART)

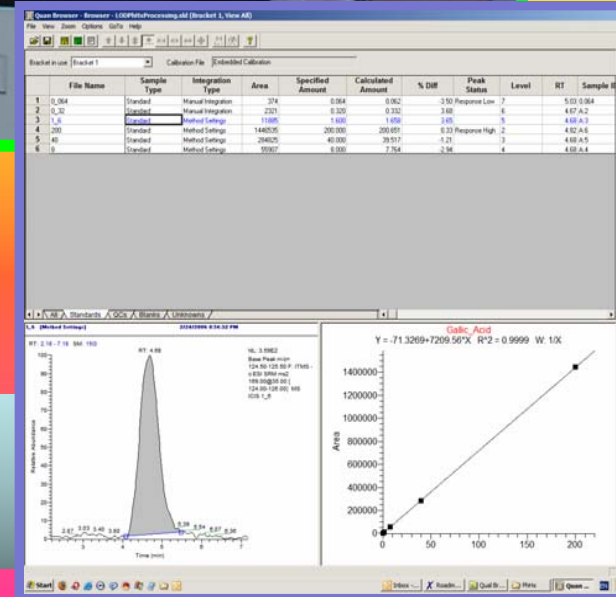
**Fast Line**

Direct Deployment of Classification Models  
Pattern Recognition

**Slow Line**

Biomarker Structure Elucidation  
Isolation, HR-MS/MS, NMR

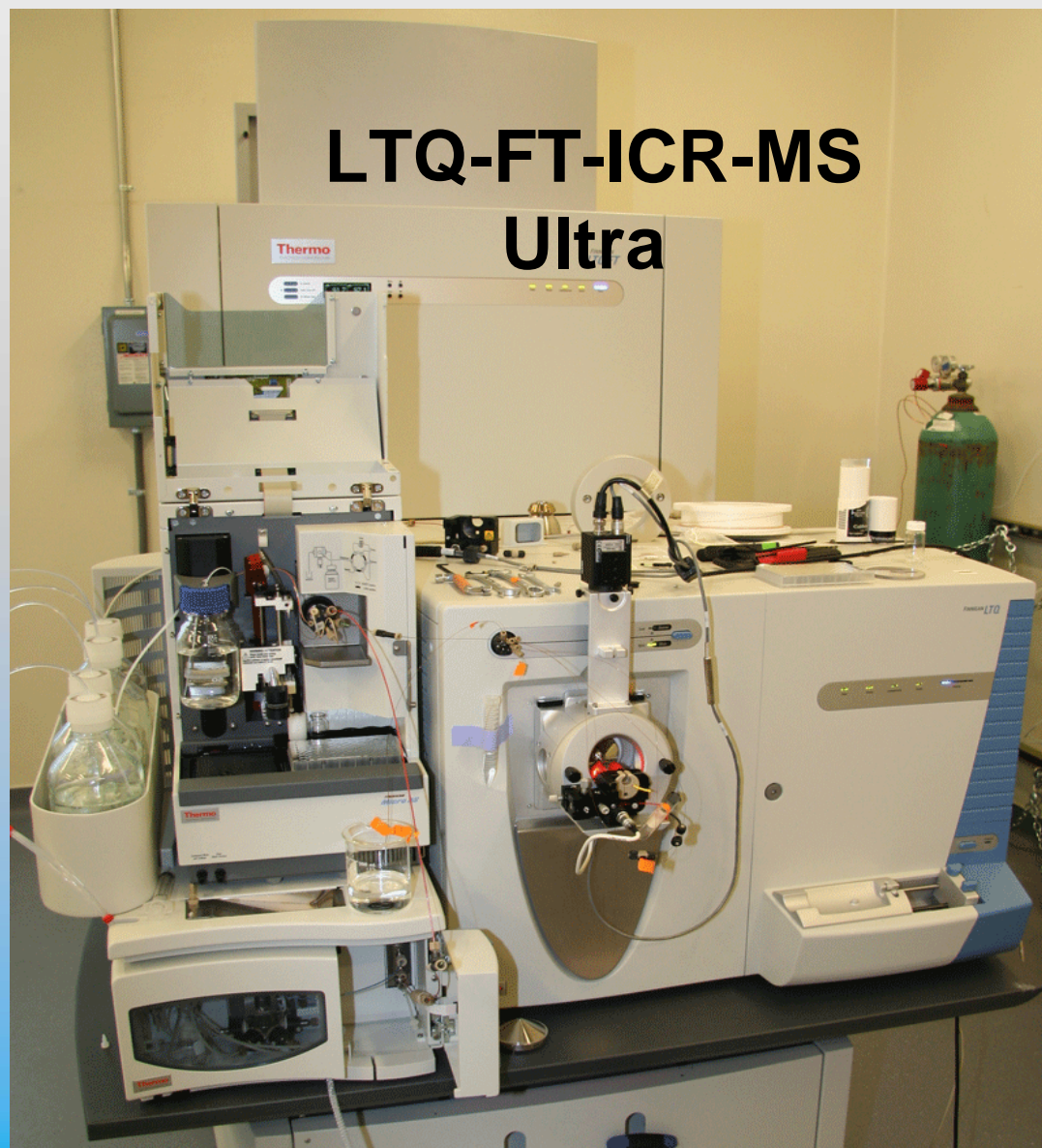
# GC-TOF-MS and LC-MS/MS Target Analysis



Identification and calibration are performed with authentic standards.



# Structure elucidation



Highest resolution:  
1000000

High mass accuracy

Hybrid IT-FT-ICR

API ion sources

Elemental composition  
assignment

Biomarkers  
identification

Instrument is  
share with  
Proteomics Core

**30%**

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## Services at the Metabolomics Core



- Consulting on the design of metabolomics experiments
- GC-TOF-MS and LC-IT-MS metabolic profiling
- LC-MS small molecule target analysis
- Metabolic Biomarkers Discovery Project
- Mass Spectrometry Based Structure Elucidation Project
- [Exploratory Project](#)
- [Basic multivariate analysis on obtained results](#)

### [Advising on the extraction protocols](#)

...It has been said that the foundation of all chromatographic research can be found in the sample preparation.

An assay can be doomed before it starts if not prepared properly.....



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## Sample Submission & Rates

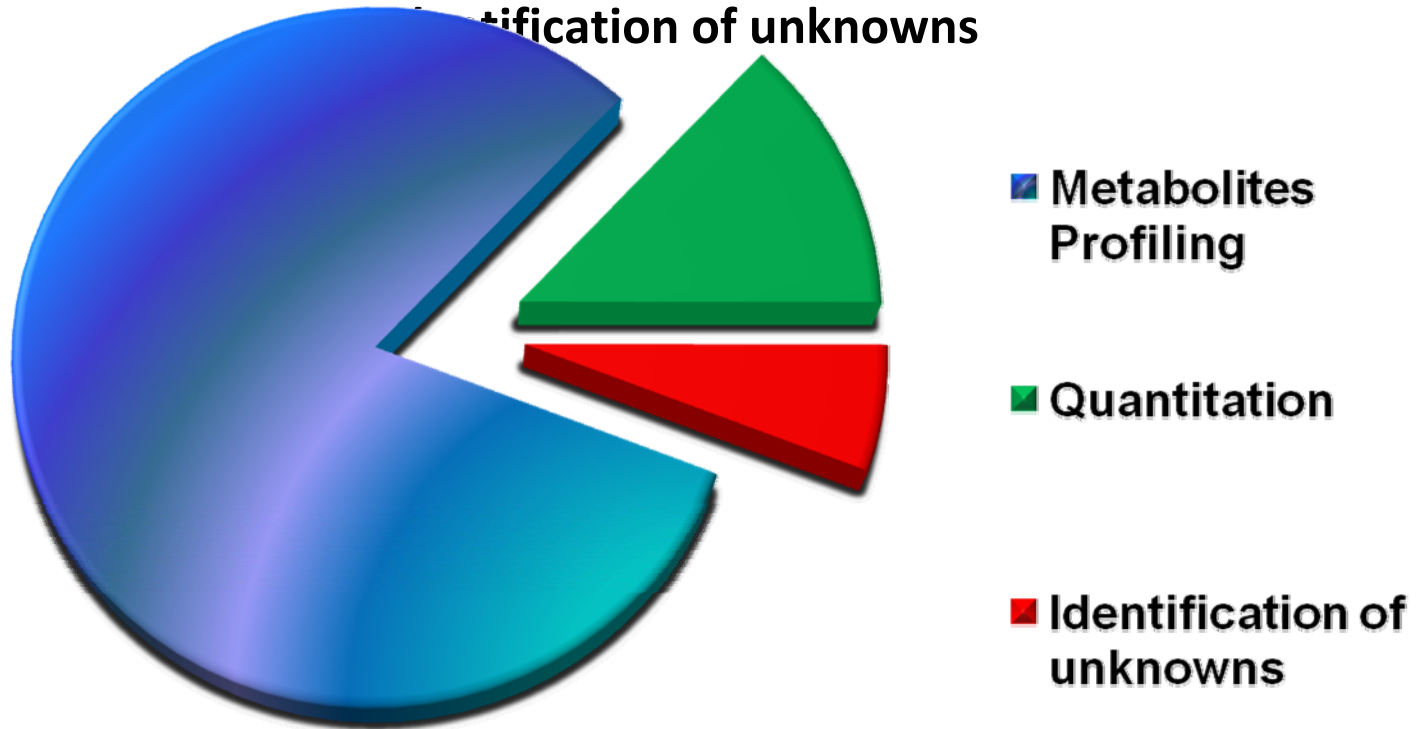


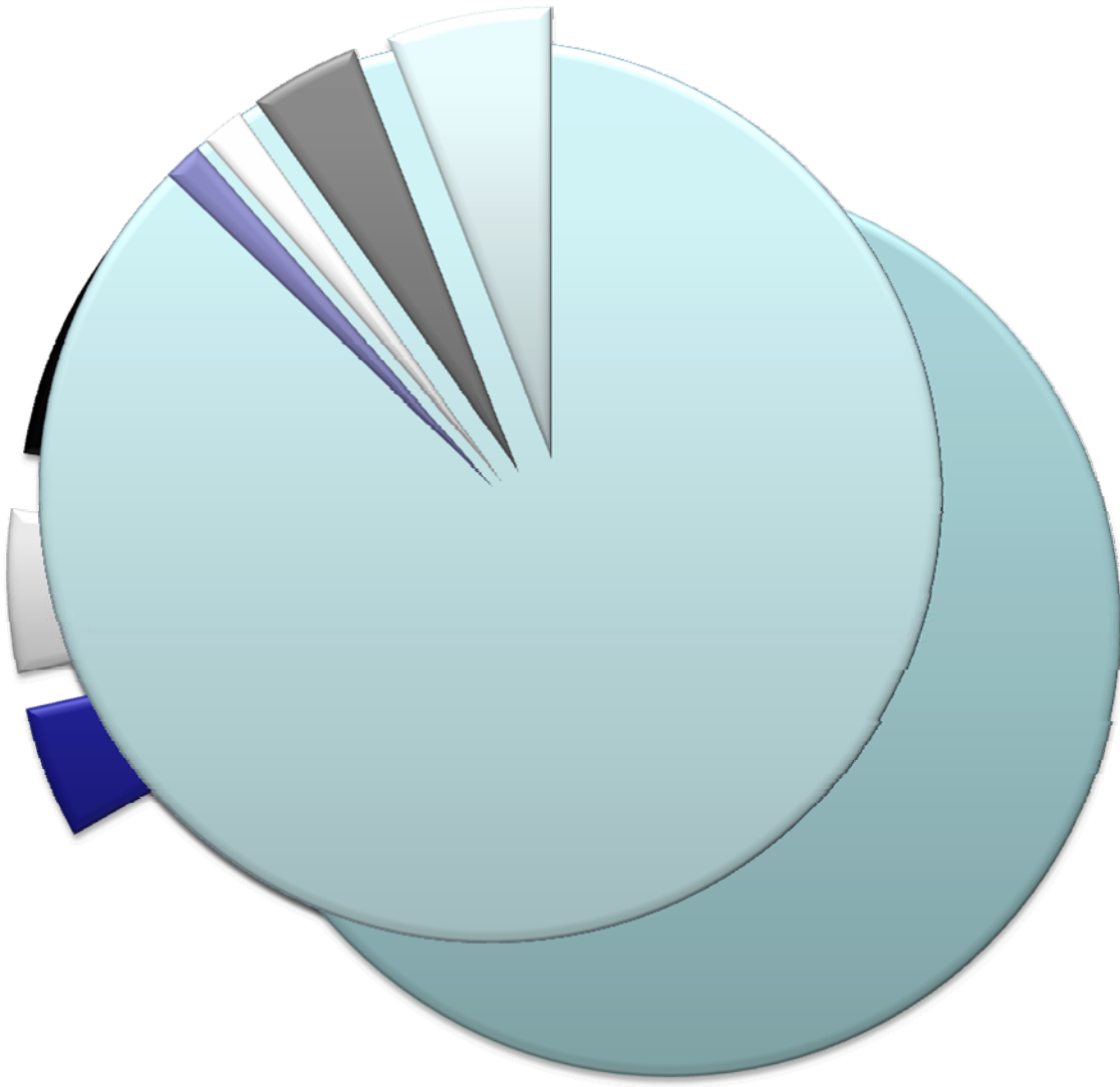
### Rates/Fee:

<u>Description</u>		<u>Item Code</u>	<u>UC Rate</u>	<u>Item Code</u>	<u>Non-Profit Rate</u>	<u>Item Code</u>	<u>Industry Rate</u>
Sample Preparation Labor	P/H	R61	\$79	M01	\$120	M11	\$143
Data Processing Presentation	P/H	R63	\$78	M03	\$119	M13	\$142
GC-TOF-MS Analysis	P/S	R64	\$51	M04	\$77	M14	\$93
Bioinformatics Statistics	P/H	R65	\$85	M05	\$129	M15	\$154
Nominal Mass, MS n	P/S	R66	\$44	M06	\$67	M16	\$80
Low Resolution LC-MS	P/S	R67	\$52	M07	\$79	M17	\$94
Accurate mass MS n	P/S	R68	\$44	M08	\$67	M18	\$80
HighRes LCMS	P/S	R69	\$61	M09	\$93	M19	\$111

# Services on campus

General Metabolic Profiling  
Quantitation (LC-MS/MS)  
Identification of unknowns





- Dept Plant Sciences
- Dept Evolution & Ecology
- Genome Center
- Cancer Center
- Dept Chemistry
- Dept Internal Medicine
- Dept Entomology
- USDA
- UCSF
- Off State Universities
- Industry

# Building Clientele 2005



Traffic More... Map Satellite Terrain



# Building Clientele 2010



# 2010 Building Clientele





# Contributions to Metabolomics and Small Molecules Analysis methodology delivered by UCD Metabolomics Core this year:

1. H. Yasuor, W. Zou, V. Tolstikov, R. S. Tjeerdema, A. J. Fischer: Differential oxidative metabolism and 5-ketoclozazone accumulation are involved in *Echinochloa phyllopogon* resistance to clozazone: *Plant Physiology*, **2010**, May, v.153, pp 1-8.
2. Y. Duan, X. Ma, W. Zou, C. Wang, I.S. Behbahan, T.P. Ahuja, V. Tolstikov, M.Zern: Differentiation and Characterization of Metabolically Functioning Hepatocytes from Human Embryonic Stem Cells: *Stem Cells*, **2010**,
3. S. Urayama, W. Zou, K. Brooks, V. Tolstikov: Comprehensive Mass Spectrometry Based Metabolic Profiling of Blood Plasma Reveals Potent Discriminatory Classifiers of Pancreatic Cancer: *Rapid Commun. Mass Spectrometry*, **2010**, 24, 613-620.

# Acknowledgments

UC Davis Genome  
Center



Metabolomics  
Fiehn Lab

