



**ABRF 2010**

**Metabolomics Research Group  
Presentation**



# Metabolomics Research Group

**Chris Turck:**

*MRG2010 Survey*

**Thomas M. O'Connell:**

*An Introduction to NMR-based Metabolomics*

**Pavel Aronov:**

*Mass Spectrometry Based Metabolomics*

**Vladimir Tolstikov:**

*Metabolomics Core at UC Davis: Evolution*



# Metabolomics Research Group

- established in March 2009 -

The screenshot shows the ABRF website header with navigation links: Home, ABRF Sponsors, Contact Us, Help, and Log In. The main navigation bar includes: Journal of Biomolecular Techniques, Discussion Forum, White Pages, Yellow Pages, and Join ABRF. The page title is "Metabolomics Research Group (MRG)" with sub-links for "Current Members" and "Activities".

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- Light Microscopy (LMRG)
- ▶ **Metabolomics (MRG)**
- MicroArray (MARG)
- Molecular Interactions (MIRG)
- Nucleic Acids (NARG)
- Protein Expression (PERG)
- Protein Sequencing (PSRG)
- Proteome Informatics (IPRG)
- Proteomics (PRG)
- Proteomics Standards (sPRG)
- Former Research Groups
  - Amino Acid Analysis

Welcome to the new Metabolomics Research Group of the ABRF. This RG was formed in March of 2009.

Metabolomics is the comprehensive profiling of metabolites and other small molecules. The large structural diversity of these compounds makes both comprehensive profiling and identification challenging. The major platforms are NMR and mass spectrometry, particularly LC/MS and GC/MS. There is currently a great variety of approaches, including untargeted profiling, targeted approaches, and fluxomics. Both semi-quantitative and quantitative approaches can be used. Challenges include identification of metabolites and how they change in relation to a biological perturbation (e.g. drug, diet, disease) and determining the biological significance of these changes. The Metabolomics Research Group consists of members from academic core and research laboratories, industrial analytical laboratories and providers of metabolomic services, analytical standards and instrumentation. The immediate aim of the Metabolomics Research Group is a) to educate research scientists and resource facilities in the analytical approaches and management of data resulting from comprehensive metabolite studies and b) to promote the science and standardization of metabolomic analyses for a variety of applications. Short term efforts of the group will include conducting surveys and organizing sessions at the annual ABRF meeting to explore the current state of the art in the field. Further activities will include the organization of research studies.

**Current Membership**

- [Chris W Turck](#) (Chair) - *Max Planck Institute of Psychiatry*
- [Dr. Pavel Aronov](#) - *Stanford University*
- [Dr. Nathan Dodder](#) - *NIST*
- [Dr. Brenda Kesler](#) - *Thermo Fisher Scientific*
- [Dr. Thomas M. O'Connell](#) - *University of North Carolina*
- [Dr. Vladimir V. Tolstikov](#) - *UC Davis Genome Center*
- [Dr. William R. Wikoff](#) - *The Scripps Research Institute*



# Metabolomics Research Group

## Mission

**Metabolomics is the comprehensive profiling of metabolites and other small molecules. The large structural diversity of these compounds makes both comprehensive profiling and identification challenging. The major platforms are NMR and mass spectrometry, particularly LC/MS and GC/MS. There is currently a great variety of approaches, including untargeted profiling, targeted approaches, and fluxomics. Both semi-quantitative and quantitative approaches can be used. Challenges include identification of metabolites and how they change in relation to a biological perturbation (e.g. drug, diet, disease) and determining the biological significance of these changes. The Metabolomics Research Group consists of members from academic core and research laboratories, industrial analytical laboratories and providers of metabolomic services, analytical standards and instrumentation. The immediate aim of the Metabolomics Research Group is a) to educate research scientists and resource facilities in the analytical approaches and management of data resulting from comprehensive metabolite studies and b) to promote the science and standardization of metabolomic analyses for a variety of applications. Short term efforts of the group will include conducting surveys and organizing sessions at the annual ABRF meeting to explore the current state of the art in the field. Further activities will include the organization of research studies.**



# Metabolomics Research Group

Pavel Aronov – *Stanford University*

Nathan Dodder - *NIST*

Brenda Kesler – *Thermo Fisher Scientific*

Thomas M. O'Connell - *University of North Carolina*

Vladimir V. Tolstikov - *UC Davis Genome Center*

Chris W. Turck (EB Liaison / Chair) - *Max Planck Institute*

William R. Wikoff (**Incoming Chair**) – *The Scripps Research Institute*

John Asara – *Harvard University*

David Powell – *University of Florida*

Vladimir Shulaev – *Virginia Bioinformatics Institute*

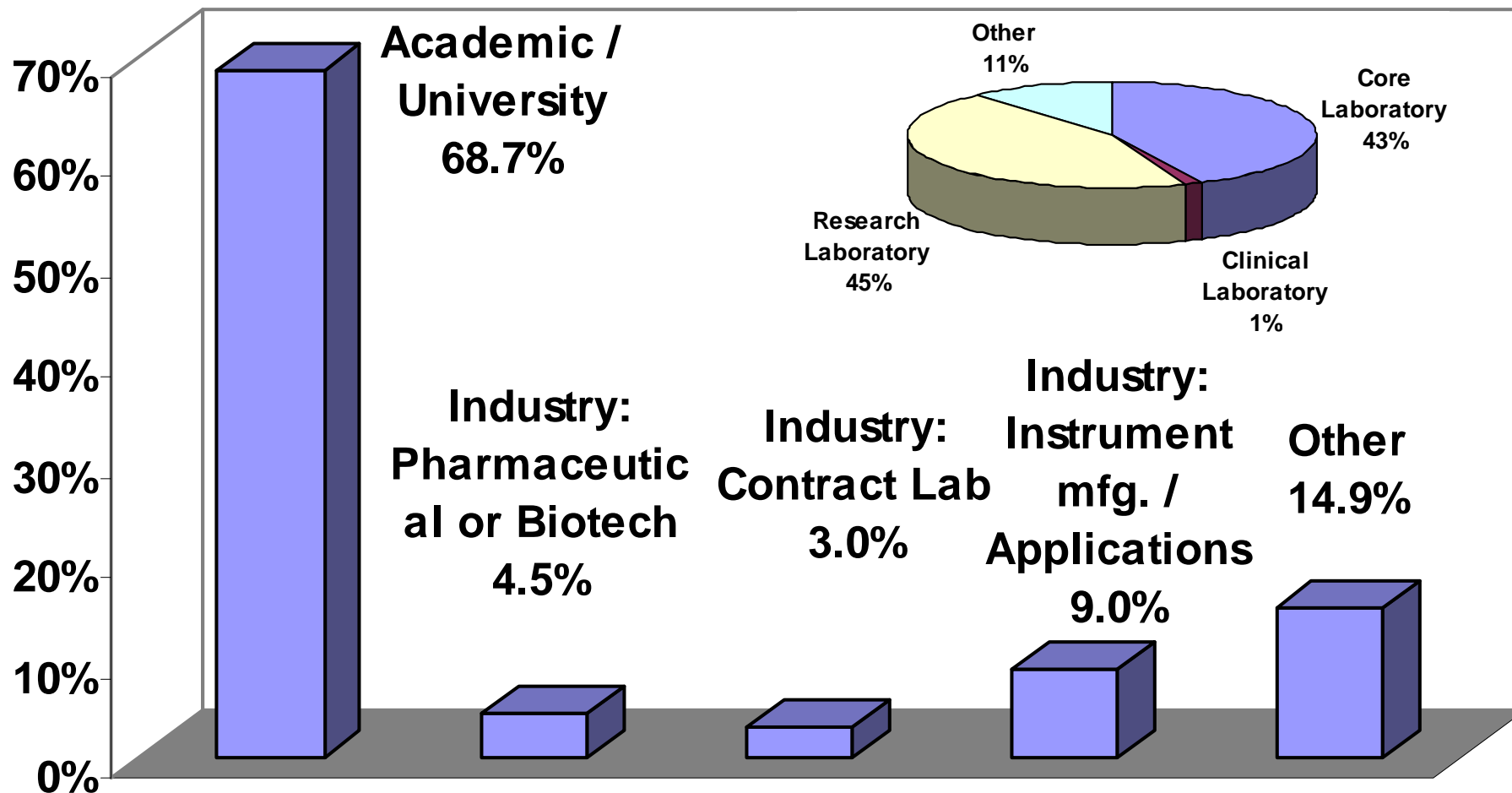


# Metabolomics Research Group

## *MRG2010 Survey*

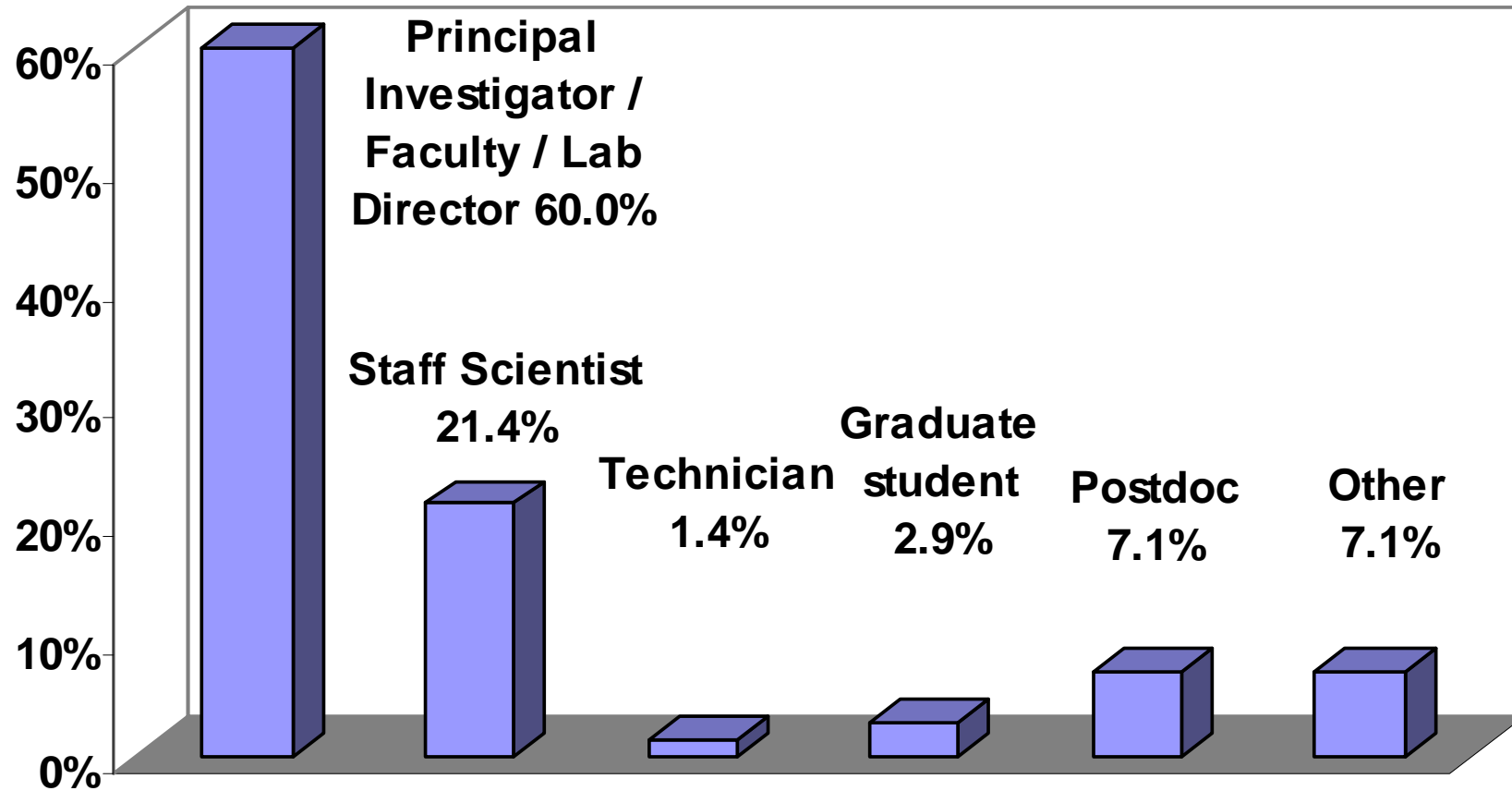


# Type of Institution / Laboratory





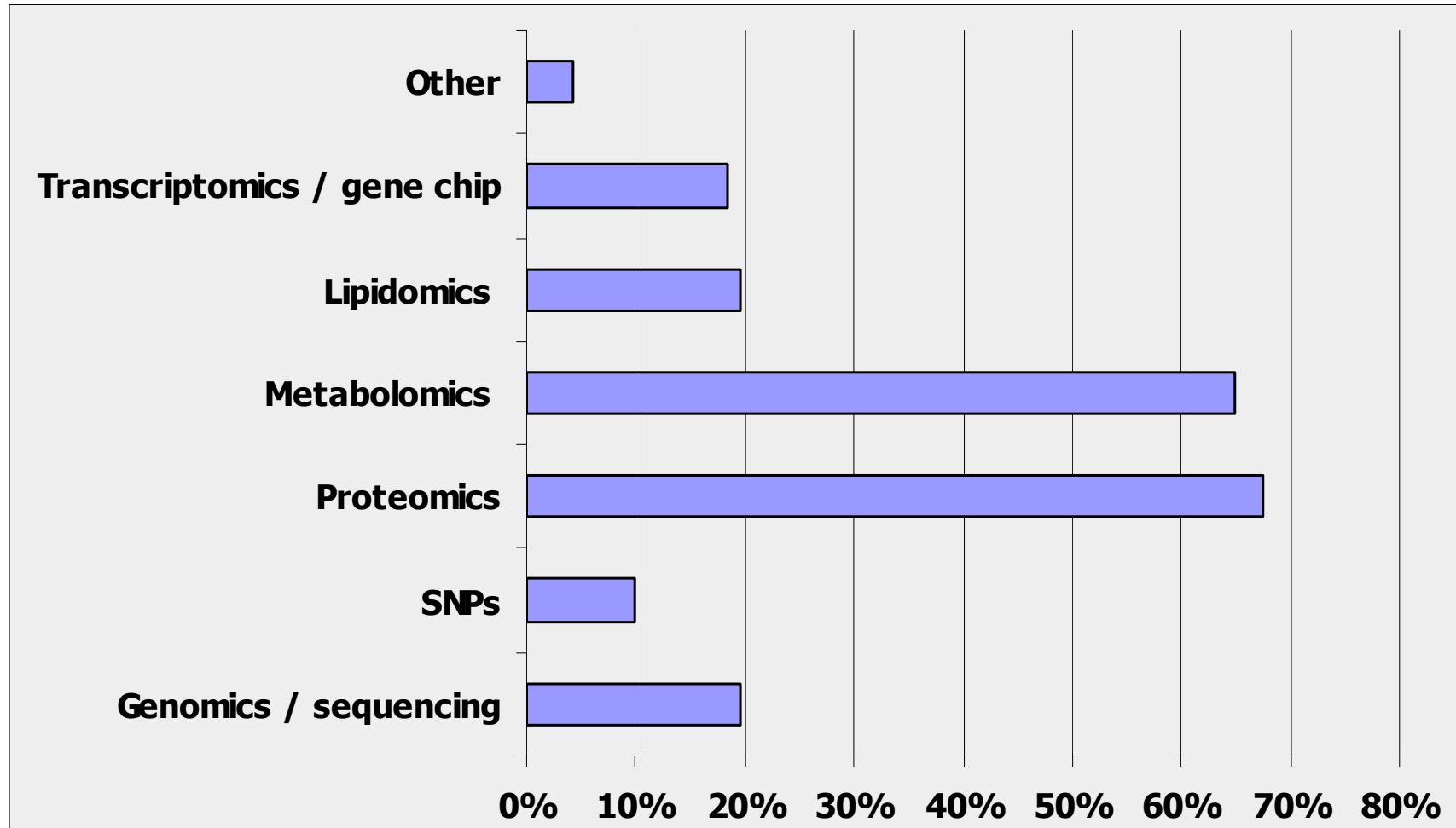
# Position





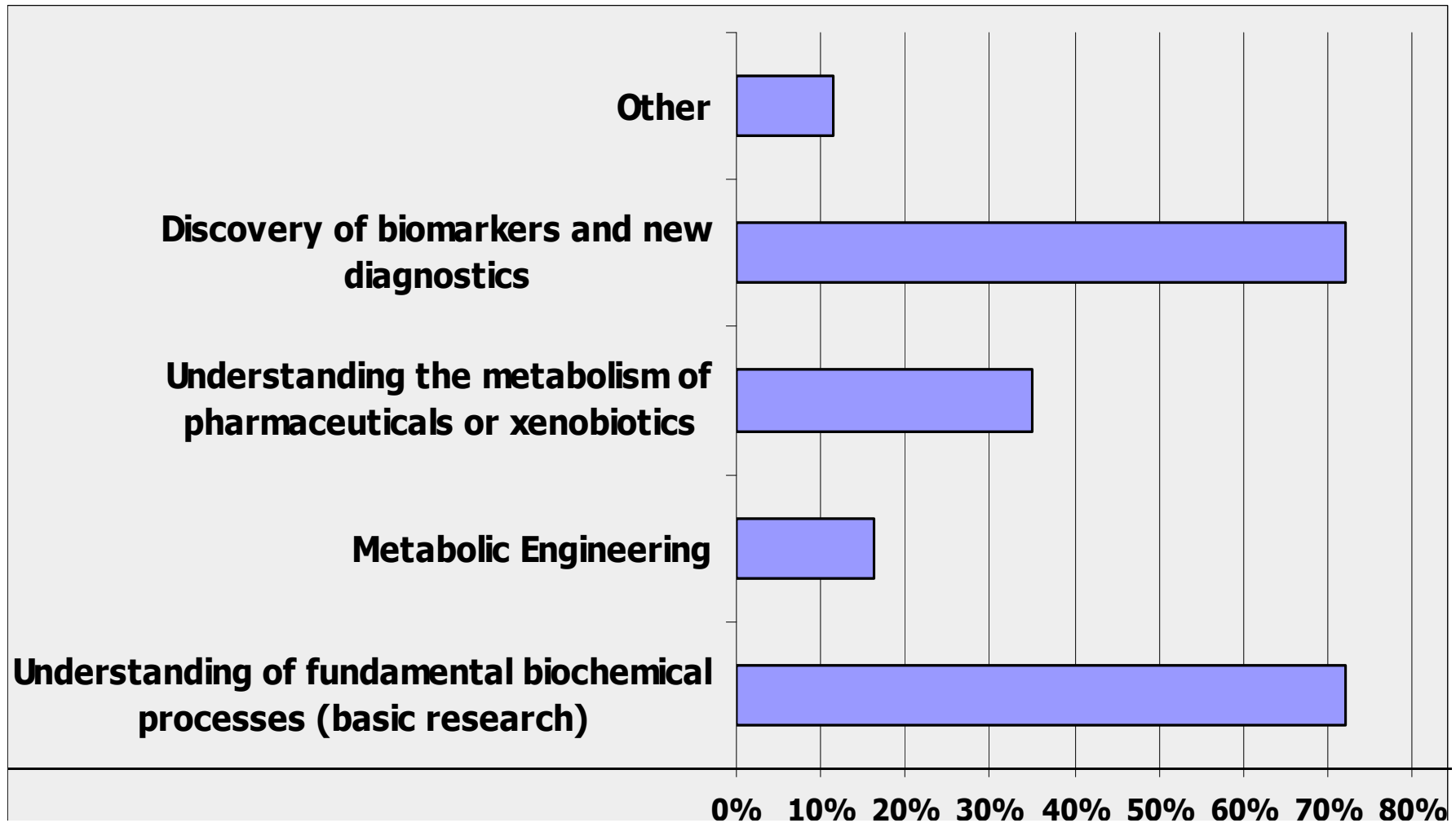


# -Omics Analysis Methods



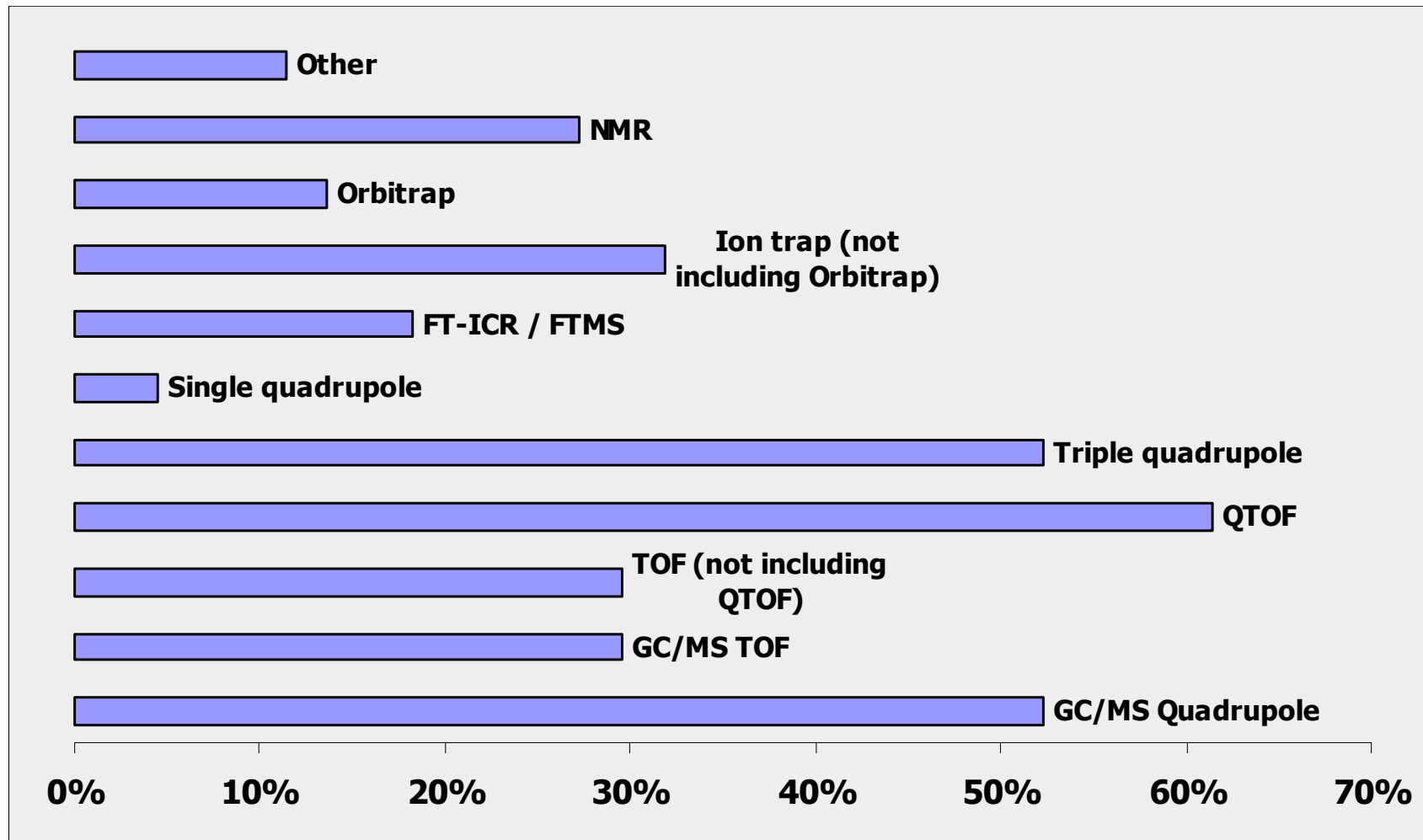


# Metabolomics Applications



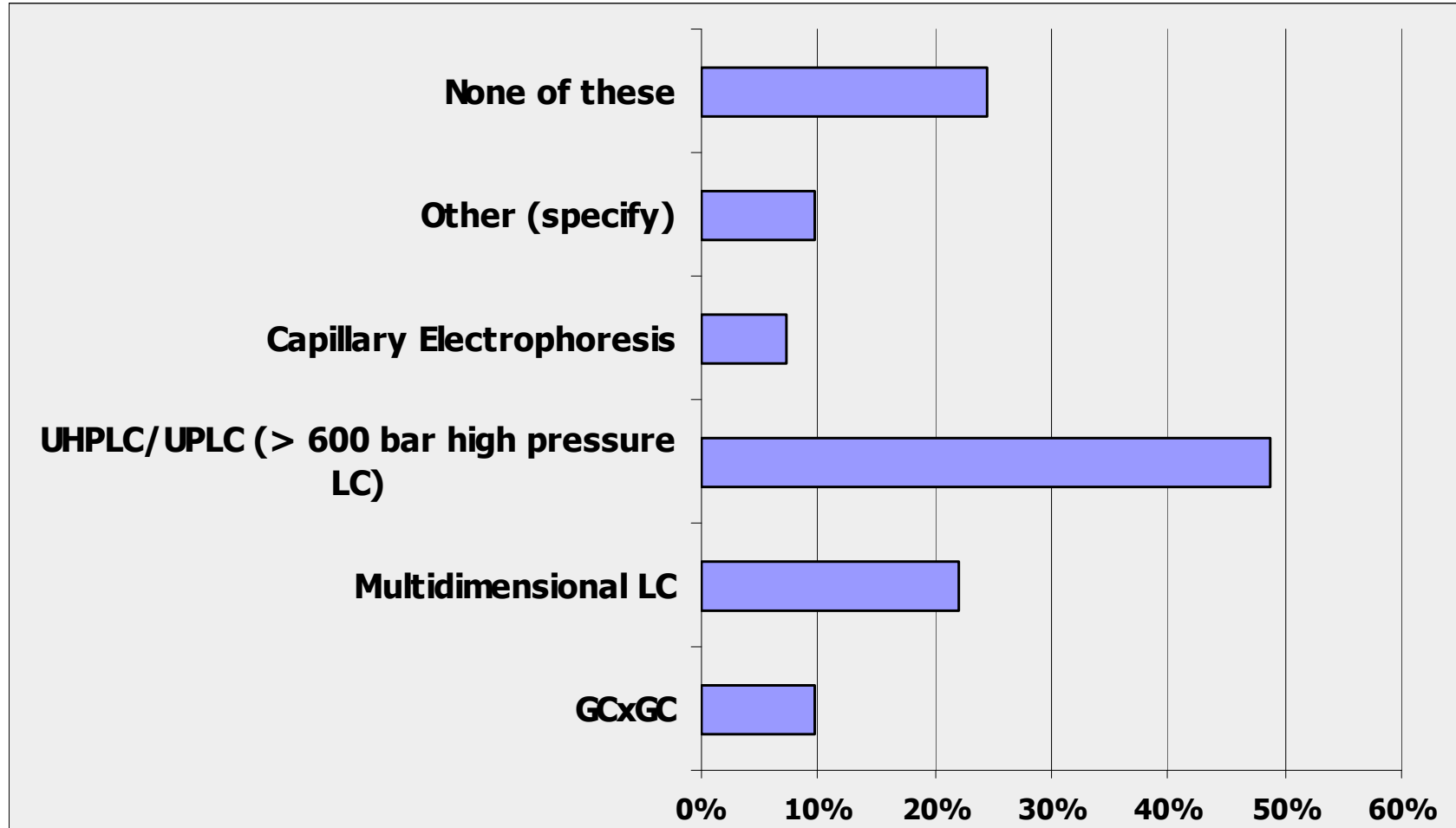


# Metabolomics Instrumentation





# Advanced Separation Techniques





## Type of Metabolomics Studies

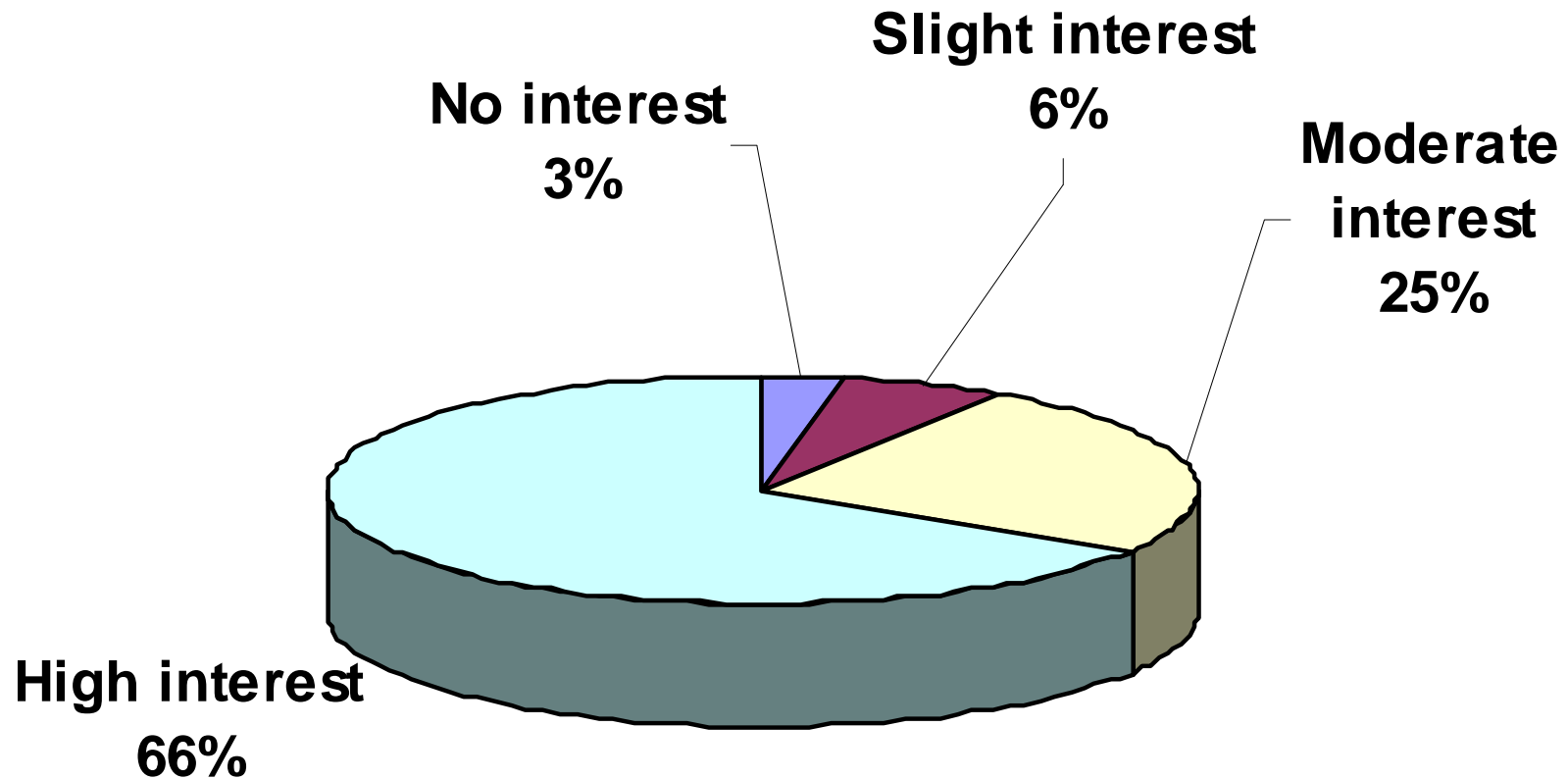
|  |              |
|--|--------------|
| <b>Untargeted 'shotgun' methods</b>                  | <b>62,2%</b> |
| <b>Targeted methods, e.g. multiple MRMs</b>          | <b>24,4%</b> |
| <b>Semi-targeted, e.g. specific compound classes</b> | <b>11,1%</b> |
| <b>Other</b>   | <b>2,2%</b>  |

## Metabolomics Bottlenecks

|                                    |              |     |
|------------------------------------|--------------|-----|
| <b>Sample preparation</b>          | <b>4.4%</b>  |     |
| <b>Chromatography</b>              | <b>2.2%</b>  |     |
| <b>Achieving Comprehensiveness</b> | <b>22.2%</b> | !   |
| <b>Metabolite quantitation</b>     | <b>6.7%</b>  |     |
| <b>Data processing/software</b>    | <b>11.1%</b> |     |
| <b>Compound identification</b>     | <b>51.1%</b> | !!! |
| <b>Other</b>                       | <b>2.2%</b>  |     |



# Level of Interest in Metabolomics





# ABRF 2010

## Metabolomics Session Attendance?

|                           |              |
|---------------------------|--------------|
| <b>No / unlikely</b>      | <b>3.4%</b>  |
| <b>Possibly/Undecided</b> | <b>15.5%</b> |
| <b>Yes/most likely</b>    | <b>81.0%</b> |

## Interest in Metabolomics Course?

|                           |              |
|---------------------------|--------------|
| <b>No / unlikely</b>      | <b>17.7%</b> |
| <b>Possibly/Undecided</b> | <b>37.1%</b> |
| <b>Yes/most likely</b>    | <b>45.2%</b> |



# ABRF 2010

**Metabolomics Scientific Session (s6)**

**Tuesday, 9:00 – 10:30 am**

**Chair: Bill Wikoff, The Scripps Research Institute**

**Oliver Fiehn, University of California Davis**

*Managing Complexity - How Many Platforms Do We  
Need for Metabolomics?*

**David Wishart, University of Alberta**

*Trends in Quantitative Metabolomics*

**Chris Beecher, University of Michigan**

*Metabolomics Techniques and Applications*