Association of Biomolecular Resource Facilities
Metabolomics Research Group
http://www.abrf.org/mrg

Metabolomics Research Group Study 2013

Sample Information
The study samples are supplied in six vials (labeled "**A1, A2, A3**" and "**B1, B2, B3**") and consist of lyophilized plasma samples. These should be either frozen upon receipt or resuspended and extracted immediately upon receipt for maximum stability. After sample analysis, participants are asked to provide a copy of their standard report (such as you would send to a collaborator or client).

Reconstitution of Samples
Add 100 microliters of ultrapure water to each sample. Vortex thoroughly. All material should resuspend. If a bath sonicator is available, sonication will aid in the resuspension process. Do not centrifuge. Either proceed to extraction and analysis immediately or freeze sample at -80^{o}C.

Sample Analysis
The purpose of the study is to identify the significant differences between groups A and B. Each group has three samples (n=3) for a total of six. Samples should be analyzed using the technique or combination of techniques normally used (e.g. LC/MS, GC/MS, NMR) in the individual laboratory. There are multiple small molecule differences to be found and identified between groups A and B.

You can decide if you want to perform the analysis:
A) untargeted only
B) targeted only
C) first untargeted and then targeted
In case you want to carry out a targeted analysis please send an e-mail to … and we will provide you with the IDs of the metabolites to be compared.

Returning Results
Deadline for retuning results is November 30, 2013
The summary of your methods and results should be combined into one document. Please indicate any qualitative differences between samples A and B that were observed and provide supporting information, along with compound identification. Use your 6-digit identification number as the file name, and in place of your name, and save the file in MS Word or pdf format. Please remove any identifying information from the report so that it remains anonymous; it will be posted along with the study results.

Please submit a **standard report summarizing the results** that you would normally provide to the client or collaborator. **List the compounds that you identified as changing significantly** between the different test samples and **give an estimation of the intensity difference between the samples as a ratio**.

Your summary report should also contain the following information:

- Type of analysis performed on the test samples (GC-MS, LC-MS, NMR, other).
- Analysis run conditions (i.e., LC-MS in profiling mode, etc.) and instrument vendor info.
- Quality controls that were used.
- Methods used to quantitatively determine difference peaks between the test samples such as biostatistical profiling, ratio analysis, etc.
- Number of peaks significantly changed in intensity across the test samples in either direction.
- Variability/reproducibility between the biological replicates.
- Percentage of the peaks that changed and led to an identification.
- Peaks (metabolites) that showed the most dramatic changes in either direction.
- Number of times the analysis was performed.
- Reproducibility between replicates.

Also, please indicate:

- whether the time and sample size was enough for the study.
- level of difficulty of the study from 1-5 with 1 being easy and 5 being very difficult.

Information and any updates about the study will be posted on the ABRF MRG website: http://www.abrf.org/MRG

Questions? Please email … for completely anonymous communications.

The ABRF Metabolomics Research Group
John Asara – Harvard University
Amrita Cheema – Georgetown University
Thomas Neubert – New York University
Chris Turck – Max Planck Institute of Psychiatry