TUMI Introduction to Microbiome, Metabolomics, and Data Science Course

Hosted via Zoom April 12-16, 2021
Course will run from 9AM-1PM, Monday-Friday
Recorded for on-demand access after the course
Afternoon office hours available every day after lectures and data workshops

PRE-COURSE SOFTWARE INSTALL (Thursday April 8th and Friday April 9th, 2021):

1. Students will be asked to pre-install software required for the course the week prior to the course begins.
2. Students can sign up for a time during which one of the course instructors will guide them through the download and installation process for all software.
3. If students are able to install on their own, there is no need to sign up.

DAY 1 (Monday, April 12th, 2021):

1. Gnotobiotic Mice: From Generation to Experimentation

    9:00 AM - 9:15 AM Casey Hoffman, Brett Moreau
    - Introduction to the course
    - Summary of published paper (contains the original 16S rRNA and datasets that will be used for hands on sessions throughout the course)

    9:15 AM - 11:00 AM Kumari Andarawewa
    - History of gnotobiotic mice
    - How to generate/maintain gnotobiotic mice
    - Novel surgery techniques for generation of gnotobiotic mice

    11:10 AM - 12:00 PM Carrie Cowardin
    - Designing gnotobiotic mouse experiments
    - How many mice/humans/samples do you need for meaningful study?
    - Colonizing mice with single species or FMT
    - Sample preparation, handling, storage, and quality control

2. An Introduction to 16S rRNA Sequencing

    12:10 AM - 1:00PM Carrie Cowardin, Greg Medlock, Maureen Carey
    - What is 16S Sequencing?
    - 16S vs metagenomics: What are the pros and cons? What can you measure?
    - Experimental Design (talk to your bioinformatician before starting)

DAY 2 (Tuesday, April 13th, 2021):

3. 16S Sequencing Data analysis

9:00AM - 10:00AM Pankaj Kumar, Ph.D., Maureen Carey, Ph.D., and Greg Medlock, Ph.D.

- Introduction to 16S rRNA data analysis
- General how-to, what programs are important and can be used

10:10AM - 1:00PM Pankaj Kumar, Ph.D., Maureen Carey, Ph.D., and Greg Medlock, Ph.D.

- Workshop component (students will be provided with a data set, raw 16S data from Day 1 manuscript)
    - Information about the samples and metadata
    - Accessing data
    - Hands on data analysis using pre-installed software

1:00PM – 5:00PM

- Course instructors available for one-on-one consultation about content introduced today.

DAY 3 (Wednesday, April 14th, 2021):

4. Metabolomics and LC-MS/MS

Metabolomics and LC-MS/MS 9:00AM - 11:00AM Nishikant Wase, Ph.D.

- Theory behind and history LC-MS/MS for metabolomics
- Sample prep, understanding targeted vs untargeted and polar/nonpolar analysis, sample handling do's and don'ts
- Best practices for consistency among samples (reproducibility)
- New methods developed at UVA - Bile Acids, SCFAs, metabolite library, etc.

11:00AM - 12:20PM Nishikant Wase, Ph.D.

- Workshop Component:
    - Analysis of untargeted mass spec data (open-source programs - mzMine, xcms or MS-DIAL)
    - Analysis of targeted mass spec data (open-source program - Skyline)
    - Generation of standard curves, stable isotope labelling experiment etc

12:30PM - 1:00PM Greg Medlock, Ph.D., and Maureen Carey, Ph.D.

- Planning metabolomics experiments

1:00PM – 5:00PM

- Course instructors available for one-on-one consultation about content introduced today.

DAY 4 (Thursday, April 15th, 2021):

5. LC-MS/MS Metabolomics Data Analysis

9:00AM - 10:00AM Greg Medlock, Ph.D., and Maureen Carey, Ph.D.

- Introduction to metabolomics data analysis
- General how-to, what programs are important and can be used

10:10AM – 1:00PM Greg Medlock, Ph.D., and Maureen Carey, Ph.D.

- Workshop component (students will be provided with a data set, metabolomics data from the Day 1 manuscript)
    - Information about the samples and metadata
    - Accessing data
    - Hands on data analysis using pre-installed software

DAY 5 (Friday, April 16th, 2021):

6. Metabolomics and NMR

9:00AM – 10:00AM Jeff Ellena, Ph.D.

- Aspects of NMR theory which are important for metabolomics
    - Magnetic nuclei
    - Spin states, boltzman distribution, magnetic resonance expression for a single spin
    - Nuclear precession about a magnetic field
    - Pulse NMR
    - Pulse sequence diagram
    - Spin relaxation
    - Chemical shifts
- Quantitative NMR
    - Chemical shift standard
    - Eretic
- Peak assignment 1
    - Chemical shifts, Spin Spin (J) coupling, peak intensities
- Peak Assignment 2
    - Crowding in 1D NMR
    - 2 Dimensional NMR

11:15AM – 12:00PM Jeff Ellena, Ph.D.

- Demonstration of Mestrenova software
    - Analysis of NMR data sets using open-source software
    - Students can participate using software and dataset, but this is not meant to be a hands-on workshop. Additional training can be offered in afternoon consultations.
- Commentary on
    - NMR metabolomics workflow
        - Experimental protocol (importance of uniformity, simplicity, and planning)
        - Targeted or untargeted
    - Use of NMR and MS for metabolomics
        - Relative strengths and weaknesses
        - Advantages of combining NMR and MS

12:05PM - 1:00PM Gregory Medlock, Ph.D.

- The pros and cons of NMR, comparison to vs LC-MS/MS
- Decision tree for MS vs NMR
- Statistical analysis of NMR Data (could be workshop?

1:00PM – 5:00PM

- Course instructors available for one-on-one consultation about content introduced today

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SPECIALTY SESSIONS (1-2 hour seminars to be offered throughout the year)

1. Spectral Flow Cytometry - **Stacey Burgess, Mike Solga**
2. Higher order analyses of OMICs Data - Big Data/Data Science analysis - **Greg Medlock, Maureen Carey, Jason Papin**
3. Bile Acid and SCFA Metabolism - **Jhansi Leslie**
4. From Stool to Microbial Libraries (sequencing clones) - **Carrie Cowardin**
5. Circadian dynamics of microbiome and metabolome studies/the clock - **Sean Moore**
6. Studying mouse behavior associated with the microbiome - **Alban Gaultier, John Lukens**

General info:

1. Will be offered to TUMI associated investigators and scientists - should we cap the course limit?
2. Training Grants to include: ID, Cancer?, others? Future Microbiome training grant?
3. After inaugural course,
    a. Will be offered to ICDDR,B
    b. Will be offered to Aga Khan University
    c. Time differential may make courses hard - will pre record and then students can watch on their own time.
    d. Data workshop will be hosted at times when all groups could participate (suggested 8AM Cville, 4PM Pakistan?)