

# Metabolomics – from study designs to data interpretation

## Abstract

Metabolomics studies metabolism. The abundance of metabolites in nature, including in animals and humans, makes this science particularly challenging and interesting. But there are so many questions to consider! In this short course, we'll try to tackle them using topic introductions, surveys, polls, Q&A, and software demos.

- How many samples should we take? Which time points and treatments should we consider? How much does extraction matter? Does HILIC work robustly, or should we use ion pairing with RPLC? Should we focus only on pre-defined metabolites, or is it ok to embrace non-targeted analyses? Which mass spectrometer is the best? How can we process data? How confident are we when we annotate metabolites by MS/MS spectra? And finally, how can non-experts still get good statistical reports?

In this 3-hour course, we will explore each of these questions. We will demo MS-DIAL software, MassBank.us and MetaboAnalyst.ca . Test data will be available for downloads, and participants are invited to tag along (but do not have to !)

## Biography

Prof. Oliver Fiehn has pioneered developments and applications in metabolomics with over 400 publications to date, starting in 1998 as postdoctoral scholar and from 2000 onwards as group leader at the Max-Planck Institute for Molecular Plant Physiology in Potsdam, Germany. Since 2004 he is Professor at the UC Davis Genome Center, overseeing his research laboratory and the satellite core service laboratory in metabolomics research. Since 2012, he is Director of the UC Davis West Coast Metabolomics Center, supervising 40 staff operating 19 mass spectrometers. To focus on large cohort studies and translational metabolomics, he has added the ThermoFisher *Center of Excellence in Clinical Metabolomics* at the UC Davis clinical campus in Sacramento, CA.

The West Coast Metabolomics Center provides the most extensive and most in-depth analysis of metabolites available today, with a focus on informatics approaches to process and interpret LC-MS/MS data. Beside NIH research projects like *Dietary Biomarkers* as well as *Longevity Consortium* and *Acute to Chronic Pain*, his laboratory builds software and databases such as MassBank.us that hosts over 2 million public metabolite mass spectra, in addition to MS-DIAL data processing software and the BinVestigate public frontend to more than 2,800 GC-TOF MS metabolomic studies. He co-founded the Metabolomics Society in 2005 and served on its board until 2015. In 2017 he co-founded the Metabolomics Association of North America (MANA) for which he organizes a range of workshops and conferences. In further public outreach, the West Coast Metabolomics Center holds monthly public webinars, has a YouTube channel, a newsletter, hosts the MANA website including its job board, organizes three metabolomics professional courses per year and invites international scholars to research visits.