

## Channing Microbiome Seminar

June 9 (Friday), 2023, 9AM (ET)

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## Large-scale reconstruction of the microbiome highlights widespread drug-metabolising capacities

The human microbiome influences the efficacy and safety of a wide variety of commonly prescribed drugs, yet comprehensive systems-level approaches to interrogate drug-microbiome interactions are lacking. Here, I will present a computational resource of human microbial genome-scale reconstructions, deemed AGORA2, which accounts for 7,302 strains, includes microbial drug degradation and biotransformation, and was extensively curated based on comparative genomics and literature searches. AGORA2 follows the quality standards developed by the systems biology research community and is fully compatible with generic and organ-resolved, sex-specific, whole-body human metabolic reconstructions. I will illustrate how AGORA2 enables the prediction of microbial drug metabolism using 616 personalised microbiomes. This analysis revealed that some drug activation capabilities are present in only a subset of individuals, moreover, drug conversion potential correlates with clinical parameters. Taken together, the AGORA2 reconstructions can be used independently or together for investigating microbial metabolism and host-microbiota co-metabolism *in silico*.

Bio: **Professor Ines Thiele** is the principal investigator of the Molecular Systems Physiology group at the University of Galway, Ireland. Her research aims to improve the understanding of how diet influences human health. Therefore, she uses a computational modeling approach, termed constraint-based modeling, which has gained increasing importance in systems biology. Her group builds comprehensive models of human cells and human-associated microbes; then employs them together with experimental data to investigate how nutrition and genetic predisposition can affect one's health. In particular, she is interested in applying her

computational modeling approach for better understanding of inherited and neurodegenerative diseases. Ines Thiele has been pioneering models and methods allowing large-scale computational modeling of the human gut microbiome and its metabolic effect on human metabolism. Ines Thiele earned her PhD in bioinformatics from the University of California, San Diego, in 2009. Ines Thiele was an Assistant and Associate Professor at the University of Iceland (2009 - 2013), and Associate Professor at the University of Luxembourg (2013-2019). In 2013, Ines Thiele received the ATTRACT fellowship from the Fonds National de la Recherche (Luxembourg). In 2015, she was elected as EMBO Young Investigator. In 2017, she was awarded the prestigious ERC starting grant. In 2020, Ines Thiele was named a highly cited researcher by Clarivate, and received the NUI Galway President's award in research excellence. She is an author of over 100 international scientific papers and reviewer for multiple journals and funding agencies.

