Dr. Marc Nicklaus earned his Ph.D. in applied physics at the University Tübingen, Germany, with a minor in computer science. This computational track led him to enter the field of molecular modeling in his postdoctoral work at the Molecular Modeling group in the Laboratory of Medicinal Chemistry, National Cancer Institute (NCI), National Institutes of Health (NIH) in late 1989. Expanding the scope of his work to all aspects of chemical information, he started the Computer-Aided Drug Design (CADD) Group at the NCI in the early 2000s. He conducted research to increase understanding of drugs' and potential drug molecules' properties and interactions with biomacromolecules at the basic science level; to improve the chemoinformatics "infrastructure" for the drug discovery and development process at NCI and worldwide; and to contribute CADD resources in collaborative projects involving specific molecular targets relevant for the fight against cancer, HIV/AIDS, and other diseases. He has also done computational work in the field of tautomerism, including in the context of further development of InChI. Nicklaus initiated, and led, the Synthetically Accessible Virtual Inventory (SAVI) project. SAVI is an international collaborative project, generating billion-size libraries of compounds that are easily synthesizable from commercially available building blocks. The SAVI project has been utilizing, and enlarging, a set of transforms based on the CHMTRN/PATRAN programming languages, which can describe detailed chemical synthesis logic derived from expert knowledge in a LHASA-type way. Marc Nicklaus joined the startup company Actyon Discovery, Inc., first as a Founding Advisor, and after his retirement from NCI in 2025, as the Chief Scientific Officer. He has authored or co-authored over 160 refereed journal articles and book chapters.