Habilitation

Fachbereich Mathematik und Informatik

E I N L A D U N G

zum Habilitationsvortrag

Im Rahmen seines Habilitationsverfahrens wird

Herr Dr. Thilo Muth

am **Dienstag**, d. **05. Juli 2022** um **14:00 Uhr**

im gr. Hörsaal der Informatik
(Takustr. 9, 14195 Berlin)

einen Vortrag über das Thema:

Computational techniques for identifying and classifying metabolites using untargeted mass spectrometry

halten.

Der Vortrag wird ca. 45 Minuten dauern (Zusammenfassung s.u.).

Die Universitätsöffentlichkeit ist dazu herzlich eingeladen.

gez. Prof. Dr. K. Reinert
Dekan des FB Mathematik und Informatik

Abstract: In metabolomics, thousands of molecular compounds can be identified from a biological sample using untargeted mass spectrometry. Despite much progress in instrumentation and advances in computational tools, many challenges remain in the field. The identification of compounds is typically performed using reference spectral libraries: however, these are of limited size in many cases while they are typically obtained from only commercially available compounds. In case a compound is unknown, the comparison of experimental spectra to spectral databases will result in incorrect or even no identifications at all. Besides determining the molecular formula of the compounds, another issue concerns the structural elucidation which refers to the identification of the whole molecular structure including stereochemical properties. Even for much larger structure databases, not all molecular structures are covered for unknown sample compositions. In this presentation, novel bioinformatic methods of spectral prediction and compound classification are presented that aim to overcome some of the mentioned issues.