



UNIVERSITÄT GREIFSWALD
Wissen lockt. Seit 1456



Das **Institut für Biochemie** lädt gemeinsam mit dem Ortsverband
der **Gesellschaft Deutscher Chemiker** zu einem

K o l l o q u i u m d e r G D C h

Kleiner Hörsaal des Instituts für Biochemie
Felix-Hausdorff-Str. 4, Greifswald

Dienstag, 05. November 2019, 15 Uhr c.t.

Dr. Manfred Weiss

Helmholtz-Zentrum Berlin für Materialien und Energie

spricht zum Thema:

Crystallographic fragment-screening: challenges and chances

Abstract:

In recent years, crystallographic fragment screening (CFS) has become a quite popular tool for the early stages of tool compound and drug development. In such an experiment, suitable protein crystals are soaked with individual fragments (organic molecules with $M < 300$ Da) at high concentrations and the binding event is detected via X-ray crystallographic analysis. The obtained hits provide the necessary structural information to improve the compounds in a rational way. Since fragments cover a large chemical space, meaningful libraries need to encompass only about 100-1000 molecules. Recently, we have developed in collaboration with the Drug Design Group in Marburg a novel library aiming for maximal chemical diversity. This library is called the F2X-Universal Library. From this over 1000 fragment library, a compact set of maximally diverse 96 fragments was selected, called the F2X-Entry Screen. The libraries are dispensed via acoustic liquid handling and dried on ready-to-use 96-well plates, enabling easy experimental workflows. In the lecture the workflow will be discussed as well as some application examples.

Einladender
Prof. Dr. Michael Lammers

PD Dr. Heike Kahlert
Vorsitzende des Ortsverbandes der GDCh