Protein Crystallization Setup and Workflows in the BI Structural Research Group
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The Boehringer Ingelheim Biberach Structural Research Group has integrated protein expression and purification, biophysics and protein crystallography units. Focus of the group is to elucidate, characterize and quantify the interaction between ligands and their target proteins. We apply our technologies in preclinical stages of drug discovery projects and support projects in the target assessment, lead identification and lead optimization phases. We have a state-of-the-art crystallization laboratory equipped with high-throughput instrumentation that allows for the conduction of efficient crystallization campaigns. In our poster, we show details of the setup in our lab and give some insight into the strategies and workflows that are implemented.

### Protein Expression & Purification
- baculovirus/ insect cell expression systems
- wavebag cell culture
- Techfors 10L fermentors
- Multifors 1L fermentors
- range of Äkta systems

### Biophysics
- Static Light Scattering
- Massspectrometry
- Isothermal Titration Calorimetry
- Thermofluor
- Microscale Thermophoresis
- NMR
- Circular Dichroism

### Crystallization Software: Rockmaker

### X-ray Hardware
- Rigaku Micro7 HFM
  - Varimax-HF, AFC11, Saturn944+, Actor, Cobra Cryosystem
- Varimax-HF, Mar345DTB, Cobra Cryosystem

- Incoatec Microfocus Source IµS
  - Incoatec Optics, Mar345DTB, Cobra Cryosystem

### Crystallization
- hanging drop
- sitting drop
- seeding (various methods)
- 24 well VDX plates

### Primary Screens
- hardware: Phoenix
- 12 primary screens on hand
- incubation at 2 temperatures
- +/- ligands
- various drop-mixtures
- 96 well MTP

### Finescreens
- Hardware: Formulator and Mosquito
- 96 and 24 well plates

### Crystal Production
- CRYSTALClear:
  - provide a flexible, multifaceted protein crystallization service
  - provide (high) crystallization throughput adapted to project needs
  - crystallize on demand freshly prepared protein without delay
  - give advice on crystallization options and optimization protocols

- CRYSTALClear:
  - Identify and characterize protein structures and ligand binding sites
  - validate and prioritize High Throughput Screening hits
  - support Lead Optimization process by structure-based molecular design
  - supply novel chemical matter by Fragment Based Screening

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