In view of the increasing problems to fight infectious diseases, caused by bacteria or viruses, and the growing shortage of new and effective drugs to treat infectious diseases it is urgently required to identify and optimize new compounds, which can be applied, or optimized to treat infectious diseases in future. Structural Biology is already contributing substantial, mainly through analyses of three-dimensional, infection-relevant biomolecules, usually of enzymes, a prerequisite for structure-based development of new anti-infectives. In the terms of the presentation new methods, procedures and results of high-resolution X-ray structure analysis will be shown and discussed, particular highlighting new opportunities provided by super-intensive radiation sources of 3rd, upcoming 4th generation of synchrotron sources, in combination with pulsed XFEL radiation sources, allowing to perform time resolved experiments.

In this context first examples will be presented tracking the conventional identification and development of lead compounds, based on the hypothetically key-lock principle postulated already by the chemist Emil Fischer as early as 1894. This procedures are efficient but it is known that after identification of initial lead compounds all follow up investigations and procedures towards pre-clinical investigations require a substantial time line and are extremely cost intensive.

Therefore in recent years drug re-purposing came in favor utilizing drugs which have already marketing authorization or are licensed for human use to treat a particular health condition. Within drug re-purposing such drugs, mostly available today via compound data banks, are screened against a distinct new target molecule or organism. This procedures came more in favor along the SARS-Cov-2 pandemic. Examples of an initiative coordinated by the University Hamburg and DESY will be presented, targeting to vital enzymes of the severe acute respiratory syndrome coronavirus type 2 (SARS-Cov-2).