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Combining Alphafold and MHz nanoSFX to unravel the structural basis of the specific activity of bacterial insecticides.

Bacterial insecticides are important in green agricultural pest control and the combat against arboviruses. They act very specific on target organisms, thus neither harming other insects, nor vertebrates (including humans). Their occurrence as native nanocrystals and lack of structural homologues prevent current structure determination efforts to understand their mode of action. Alphafold v2.0 (AF2) –employing neural network based artificial intelligence –is the most advanced tool for protein structure prediction and the first one coming close to experimental methods. While it will not render experimental structural biology (crystallography, cryoEM, NMR) superfluous, it has many advantages for structural biologists, from better starting models for MD-simulations and molecular replacement phasing to producing place holders for structures that are not yet amenable for experimental determination. Combining Alphafold structure prediction with nanofocus serial femtosecond crystallography (nanoSFX) data collection under near physiological, radiation damage free conditions allowed the de novo structure determination of two, so far unknown protein structures from *Lysinibacillus sphaericus* from native nano crystals. In another case, we used Alphafold to generate a structure from an insecticidal protein for which no experimental model was available for subsequent docking studies with a novel structure to asses the structural basis of combined mode of action.

Primary author: OBERTHUER, Dominik (FS-CFEL-1 (Forschung mit Photonen Experimente 1))

Co-authors: Prof. BERRY, Colin; Prof. CHAPMAN, Henry N; Ms WILLIAMSON, Lainey; Dr BEAN, Richard; Dr MANCUSO, Adrian; Dr YEFANOV, Oleksandr; Ms GALCHENKOVA, Marina

Presenter: OBERTHUER, Dominik (FS-CFEL-1 (Forschung mit Photonen Experimente 1))

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