MS32-P17 Crystalline forms of dihydroergocornine salts

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Dihydroergocornine is a semi-synthetic ergot alkaloid, which is used in a mixture for the treatment of age-related cognitive decline and acute migraine. Due to the low solubility of dihydroergocornine in water, many pharmaceutically acceptable salts were reported, but for industrial production methansulfonate salt was chosen. Most of the reported salts have not been characterized at all. Within this study we are growing crystalline forms of dihydroergocornine salts and their solvates. The crystalline forms are characterized mainly from structural and stability points of view. Samples are prepared by solution crystallization under various conditions and analysed by X-ray diffraction techniques. Up to date two solvates of dihydroergocornine mandelate were solved from SC-XRD data. According to experience with solvated structures of dihydroergocornine mesylate, the large number of dihydroergocornine mandelate solvates is expected. We assume this solid-state behaviour in all new salts and their solvates.

Keywords: solvates, X-ray diffraction, ergot alkaloids

MS32-P18 The ISX Stage: A Novel Home-Lab Solution for Automated Screening of Crystallization Plates

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Recent developments in hardware and software are greatly increasing the capabilities of in-house diffraction systems making it more routine to obtain *de novo* structural information in the home lab. We have now introduced the D8 Venture solution for structural biology with the PHOTON II detector featuring the first CPAD for in-house X-ray crystallography. Our new microfocus source, the METALJET delivers beam intensity exceeding those of typical bending-magnet beamlines.

Very recently, we developped a fully automated solution for in situ crystal screening in plates : the ISX stage. This stage facilitates the investigation of a large number of crystals within the routine workflow of the crystallization lab. The combination of the sensitive PHOTON II detector and a high intensity X-ray source maximizes the diffraction signal from even the smallest, most weakly diffracting crystals. The ISX software provides an intuitive user environment to maximize the productivity of even occasional users.

The system can be quickly converted from the typical single crystal diffractometer to the completely motorized in situ crystal screening device leaving the KAPPA untouched and allowing you to revert just as quickly once you identified your favorite crystal on which you want to collect data. Here we present all the ISX stage features and data we collected in house.

Keywords: plate, screening, structural biology,