

GI-MS46-P17 | ADVANCED PROTEIN CRYSTALLISATION FOR NEUTRON MACROMOLECULAR CRYSTALLOGRAPHY

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The major tool to determine the 3D structure with atomic resolution of large molecules is X-ray crystallography. With X-ray data collection heavy atoms could be seen for 3D structure calculation, but the position of hydrogen atoms, which are biologically important could only be estimated due to the fact that such small atoms couldn't diffract high energy radiation and particle radiation. To locate these hydrogens the frequently used methods are 2D-NMR and Neutron Crystallography where the hydrogens are replaced with a heavier isotope → deuterium atoms that can produce cleaner neutron diffraction. With the combination of the listed methods, the complete biologically active macromolecular structure and function could be determined. In collaboration with European Spallation Source, we have developed a method to produce standard deuterated test crystals for instrument characterisation. The method can be extended to support hanging and sitting drop crystallisation experiments in deuterated environment.