Poster Sessions

MS57.P01  
Crystal structures of an enzyme duo involved in bacterial cell wall recycling

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Peptidoglycan in bacterial cell walls is synthesized by bacteria-specific enzymes by sequential addition of amino acids to UDP-N-acetyluramuramic acid to form the peptidoglycan pentapeptide precursor, UDP-N-acetyluramahexaamino acid to form the peptidoglycan pentapeptide precursor.

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NMR Crystallography applied to dicarboxylic acids

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A large number of active pharmaceutical ingredients (API) are developed as salts, generally for solubility reasons. Beside the common inorganic hydrochloride acid (by far the most represented) and sulphuric acid, others carbon-containing acids are widely used as counterions, e.g. fumaric and succinic acids. These organic dicarboxylic acids, having their carbon skeletons that differ only by an inner bond saturated or unsaturated, are usually highly difficult to be precisely localized in a °C solid state NMR (ssNMR) spectrum. This is e.g. the case by comparison with liquid state °C NMR data, since no more than two signals are expected in solution for such dicarboxylic acids; whatever the salt/base stoechiometry may be (for instance, salts of mono-, hemi- or sesqui-fumaric acid could be found in the Cambridge Structural Database). The NMR chemical shifts of the carbons belonging to the base may also vary in the liquid and solid state; which represent an additional difficulty for salt identification. However, using NMR crystallography, we were able to find the peak positions of fumaric and succinic acids mono or di-sodium complexed to a given API, notwithstanding the large number of carbons (35) displayed in their respective cross polarized magic angle spinning (CPMAS) spectrum. Crystallographic studies have been carried out for both salts; they crystallize in triclinic non centrosymmetrical structures, without organic solvent or water. The two crystalstructures are remarkably isomorphous; this similarity even somewhat extends to the counterions, where the inner single bond for succinic acid is shorter than expected (both at room and low temperature). In contrast indeed to solution NMR data, four distinct signals are found by ssNMR both with fumaric and succinic salts, a consequence of salt bridges established in each case by only one carboxylic acid. Furthermore, this study allows the attribution without ambiguities of the carbons peak positions of each salt; they could readily be deduced from comparison of the two CPMAS spectra, since the chemical shifts characteristic of the base are found at same positions.

Keywords: X-ray diffraction, XANES, EXAFS

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Structure Determination of HP0902, a Putative Secretory Protein from H. pylori

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As a structural genomics approach to the HP0902, a putative candidate for virulence factor of Helicobacter pylori, crystal structures were obtained from two different constructs and validated by nuclear