each case, XAFS would confirm or reject the random character of the solution. Athena and Artemis codes as interfaces for IFEFFIT [2] and FEFF8.4 [3] codes were employed for XAFS spectra interpretation.

γ-$Fe_{2-x}Cr_xO_3$ maghemite for x=0.75, 1 and 1.25 was investigated by XAFS in both Fe and Cr K-edges. Pre-edge decomposition and theoretical modeling of XANES transitions were performed and interatomic distances were determined. Possible distortion of oxygen octahedra around both Fe(III) and Cr(III) cations was checked for potential ferroelectricity explanation, as well as possible vacancy superstructure.

$LaFeNiTiO_3$ has been confirmed to display magnetic behavior and was studied by its Fe and Ti K-edges. Interatomic distances were modeled for preferential occupation of sites by Fe or Ti atoms and for geometry of oxygen octahedra occupied by different cations.

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Keywords: X-ray_diffraction, XANES, EXAFS

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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 not, are usually highly difficult to be precisely localized in a ^{13}C solid state NMR (ssNMR) spectrum. This is e.g. the case by comparison with liquid state ^{13}C NMR data, since no more than two signals are expected in solution for such dicarboxylic acids; whatever the salt/base stechiometry 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 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 crystal structures 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: ssNMR, structure elucidation

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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-acetylmuramic acid to form the peptidoglycan pentapeptide precursor, UDP-*N*-acetylmuramoyl-L-alanyl-γ-D-glutamyl-*meso*-diaminopimelyl-D-alanyl-D-alanine. In gram-negative bacteria, ~30-60% of the bacterial cell wall is recycled every generation in a complex process that involves ~18 proteins. LdcA catabolizes the bond between L- and D-amino acids in the degradation of the tetrapeptide L-alanyl-γ-D-glutamyl-*meso*-diaminopimelyl-D-alanine to form L-alanyl-γ-D-glutamyl-*meso*-diaminopimelate, which is the substrate for Mpl. Loss of LdcA or Mpl activity results in increased sensitivity to stationary phase lysis or antibiotic susceptibility, respectively. Crystal structures of a novel LdcA from *Novosphingobium aromaticivorans* (*Na*LdcA) and the Mpl from *Psychrobacter arcticum* (*Pa*Mpl) have been determined at 1.89 and 1.65 Å resolution, respectively. *Na*LdcA and the LdcA from *Pseudomonas aeruginosa* have similar overall structures and a conserved catalytic triad despite only a 20% sequence identity. Modeling a tetrapeptide substrate into the active site of the *Na*LdcA structure reveals residues that may be important in substrate recognition and how the catalytic triad is positioned for action. An unidentified ligand in the dimer interface might be involved in enzyme dimerization and indicates a possible site for inhibitor design. In *Pa*Mpl, ~30 residues are likely to be important for substrate recognition or may be involved in interdomain conformational changes on substrate binding. The *Pa*Mpl enzymatic activity has been characterized at different temperatures and with different peptide substrates. At 15 °C, *Pa*Mpl has almost twice the activity of Mpl from *E. coli*, consistent with *P. arcticum* adaptation at cold temperatures. These results expand the structural coverage of two important protagonists in bacterial cell wall peptidoglycan recycling and provide novel targets for anti-bacterial drug discovery.

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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