J Material Sci Eng 2016, 5:8 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.050

International Conference on
Applied Crystallography
October 17-19, 2016 Houston, USA

From art to science in protein crystallography by LB nanotechnology

Eugenia Pechkova and **Claudio Nicolini**
Genova University, Italy

Protein X-ray crystallography will remain the most powerful method to obtain the protein 3D atomic structures in foreseeable future. An impressive progress has been done in the last decades both in terms of instrumentation (X-ray sources of new generation, robotic systems and automatization) and data collection strategy and data reduction software, program and packaging, which permits to collect the data and solve the structure in the fast and optimal way. However, the crystal itself remains still the challenge for crystallographers. It particularly concerns the big protein such as membrane protein and protein complexes. In the post-genomic era, the structural and functional proteomics come to the forefront and this requires the fast and routinely successful structure determination of the huge number of proteins of the various nature and families, as well as their complexes with ligands, drugs or other protein, in order to understand protein-protein interaction, lying in the base of our understanding of all life processes and the major challenges of the century- cancer and the degenerative diseases. The new generation of synchrotrons and microfocus beamlines, as well as X-ray free lasers could accelerate the resolution of new protein structures of high industrial, pharmaceutical and fundamental life science interest. The routine production of the protein crystal of high quality (order, intensity of diffraction and radiation stability) is therefore very important. We hereby present the method capable to produce high quality protein crystal based on the LB (Langmur-Blodgett) nanotechnology, applicable to the any protein (high molecular weight and membrane proteins). In comparison to the standard crystallization protocols, the obtained crystals are more ordered and radiation stable. The process can be controlled AFM, QCM and by micro- and nano GISAX, giving the insight to the described phenomena which lead to trigger and accelerate protein crystallization by LB nano template. Moreover, highly ordered LB protein templates approach has the potential to solve the crystallization problem, also with the recent progress in X-ray free electron lasers.

eugenia.pechkova@gmail.com

Triclinic polymorphs of ethyl-6-methyl-4-(3-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate: Study of intermolecular interactions from crystal structure and Hirshfeld surface analysis

Mukesh M Jotani
Bhavan's Sheth R. A. College Science, India

The important pharmacological properties of dihydropyrimidines are the motivations for the extensive research in this class of compunds. As three dimensional structure and the crystal packnig interactions are pre-requisite for the bilogical action of a molecule, the attempts have been made to study the crystal packing interactions in the structures of two triclinic polymorphs of title tetrahydropyrimidine molecule through the crystal structure and Hirshfeld surface analysis.The polymorphs I and II of title molecule crystallize into same triclinic crystal system, but in different crystallographic environments with Z = 2 and Z = 4 respectively. The conformational flexibility due to the rotation of ester group and ary ring in the structure has resulted different conformations of the tetrahydropyrimidine ring in I and II.The intermolecular N-H...O, N-H...S, C-H...O and π-π stacking interactions have their influence on the the crystal packing of polymorph I, whereas in polymorph II, the interactions are of intra and inter molecular N-H...S and intermolecular C-H...O type. The Hirshfeld surface analysis for both the polymorphs were carried out using a computer program *Crystal Explorer*. The intermolecular interactions can be easily visualized from the Hirshfeld surfaces mapped over dnorm, de, curvedness, shape-index and electrostatic potential. The electrostatic potentials were calculated using TONTO integrated with *Crystal Explorer*. Further, the electrostatic potentials were mapped on Hirshfeld surfaces using STO-3G basis set at Hartree-Fock theory over a range from ± 0.15 au. The summary of various intermolecular contacts in the crystal is obtained from two dimensional fingerprint plot based on the Hirshfeld surface analysis. The close relationship between molecular conformation and the intermolecular interactions for polymorphs I and II using the Hirshfeld surface analysis and their comparative studies will be discussed in the presentation.

mmjotani@rediffmail.com