samples during SAXS measurements with an eye toward better repeatability and ease-of-use.

Keywords: Nanomaterials, SAXS, Nanotechnology

FA1-MS05-P17

Crystallization and structure of the human Co-insulin derivative – a new crystal form. Biserka Prugovečki, Adela Jurković, Dubravka Matković-Čalogović. *Laboratory of General and Inorganic Chemistry, Department of Chemistry, Faculty of Science, University of Zagreb, Croatia.*
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Insulin is synthesized in humans and other mammals within the beta cells of the islets of Langerhans in the pancreas. It is structured as a two polypeptide chains (chain A consists of 21 and chain B of 30 amino acids) linked by two sulfur bridges. Insulin is used medically in Type 1 diabetes mellitus.
As a part of our ongoing research on the crystallization and structural studies on human insulin derivatives [1], [2] in the present study the zinc ions in insulin were substituted with cobalt. Cobalt plays numerous biological roles and is essential to all animals. It is a key constituent of cobalamin-based and other enzymes.
Crystals of a new form of the human Co-insulin derivative were grown by the hanging drop vapour diffusion method using Zn-free insulin. The single crystal diffraction data were collected at the ELETTRA Synchrotron Light Laboratory, beam line XRD-1, to 1.23 Å resolution. The investigated insulin derivative belongs to the R3 space group (hexagonal setting) with cell parameters $a = b = 45.87$, $c = 116.84$ Å, $\gamma = 120°$. There are two cobalt ions in the hexamer, coordinated octahedrally by three histidines and three water molecules. The coordination is similar as in the 2Zn-insulin in the T6 form. However, the packing of the hexamers in the unit cell is quite different than in the Zn-derivative.

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Keywords: insulin, cobalt, X-ray

FA1-MS05-P18

Studies of XRD, *Profile Matching* and TEM of Poly(o-methoxyaniline) - POMA in different times of synthesis. Edgar Ap. Sanches[a], Graziella Trovati[b], Yvonne P. Mascarenhas[a]. [a]*University of São Paulo (USP), Institute of Physics of São Carlos (IFSC), São Carlos – SP, Brazil.* [b]*University of São Paulo (USP), Institute of Chemistry of São Carlos (IQSC), São Carlos – SP, Brazil.*
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Some studies have been developed to produce derivatives of Polyaniline (PANI) without compromising their electrical and electrochemical properties. The incorporation of polar functional groups or long and flexible chains in the structure of the polymer is a common technique for preparing soluble polymers in water or organic solvents [1,2]. The insolubility of PANI can be attributed to the rigidity of the main chain, which occurs due to the existence of a system of strongly conjugated π electrons. Electron donor substituents in positions 2 and 5 of the rings in the main chain make it more flexible. As a result, there is an increased solubility and decreased electrical conductivity [2,3]. Structural aspects in polymers are still a mystery and so continue to be an interesting researched topic [4,5]. Understanding of the regular arrangement of polymer materials is essential for the prediction of processing methods and thus relates the material properties. Crystalline structure determination of polymers, in special conducting polymers, using conventional XRD data and *Profile Matching* refinement is still scarce. Poly(o-methoxyaniline) – POMA – was prepared by oxidation of the monomer with ammonium persulfate in the presence of hydrochloric acid. During the synthesis, the polymer samples were collected in different times: 30 minutes, 3, 24 and 48 hours. POMA in powder form was subjected to the techniques of XRD and TEM. *Profile Matching* method [6] was successfully used to extract average microstructural properties from the analysis of broadened lines of constant wavelength diffraction patterns through a whole profile fitting approach. The freely distributed FULLPROF program [7] was used as a routine tool for the structural characterization of POMA powders, checking possible changes in cell parameters and crystallite sizes. Changes were noted in the diffraction patterns of the polymers, suggesting an increase in the percentage of crystallinity when the time of synthesis is increased and the peaks of the diffractograms become thinner and more intense with the increasing of the time of synthesis. Were also seen changes in the morphology of polymers, as evidenced by TEM.

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Keywords: Poly(o-methoxyaniline), DRX, Profile Matching

FA1-MS05-P19

SAXS Structural Analysis of Human Thrombomodulin Domains. Tsung-Wei Su, Po-Tsang Huang, Guey-Yueh Shi, Hua-Lin Wu, Kuo-Long Lou. *Institute of Biotechnology, National Taiwan University. Taipei, Taiwan.*
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Thrombomodulin (TM) is a membrane protein distributed in many different tissues with crucial functions in coagulation and fibrinolysis. Enhancement of blood coagulation function was not supposed to be through blood vessel per se, instead, possibly through pivotal mediations by molecules like thrombomodulin. With such involvement of TM participation, coagulations and immune responses may be bridging in many important aspects. The structures of TM are proposed to be responsible for its functions. The lectin-like domain of TM can be categorized as family containing C-type lectin, which is strongly involved in cell adhesion and inflammations,

especially the properties regarding its carbohydrate recognition domain structure. As a consequence, it is absolutely essential to understand the structure of TM, in order to get into more functional details of its regulation in the aforementioned properties. Thrombomodulin (TM) forms a 1:1 complex with thrombin. Whereas thrombin alone cleaves fibrinogen to make the fibrin clot, the thrombin-TM complex cleaves protein C to initiate the anticoagulant pathway. Until present, the so-far available structures, either through NMR or through X-ray analyses, can not shed lights into the decent structural-functional interpretations for TM regulations. Crystallographic investigations of the complex between thrombin and TM-EGF456 did not show any changes in the thrombin active site. Therefore, research has focused recently on how TM may provide a docking site for the protein C substrate with different Ca^{2+} concentration. Previous work, however, showed that when the thrombin active site was occupied by substrate analogues labeled with fluorophores, the fluorophores responded differently to active (TMEGF1-6) versus inactive (TMEGF56) fragments of TM.

Keywords: Thrombomodulin, Structural analysis, Calcium-induced dimerization.

FA1-MS05-P20

Crystal structure of 6- Methoxy- 4-bromomethylcoumarin. Ramakrishna Gowda[a], K.V Arjuna Gowda[b], Mahantesha Basanagouda[c], Manohar V. Kulkarni[c]. [a]*Department of Physics, Govt. College for Women, Kolar - 563 101, Karnataka, India.* [b]*Department of Physics, Govt. First Grade College, K.R. Pura, Bangalore-560 036, Karnataka, India.* [c]*Department of Chemistry, Karnatak University, Dharwad-580 003, Karnataka, India.* E-mail: arjunagowda@indiainfo.com

Coumarins are a class of naturally occurring oxygen heterocycles which have been found to exhibit wide ranging biological activities [1-3] through its innumerable derivatives. Structural studies on coumarins have been focused on their solid state photochemical dimerization [4], hydrogen bonding [5], mode of packing [6], molecular self assembling [7] and photophysical properties [8]. Introduction of bromine has resulted in formation of hydrates, intermolecular hydrogen bonding, eclipsed conformation observed in 3-bromocoumarin [9], 6-bromo-3-acetylcoumarin [10] and 3-bromoacetylcoumarin [11] respectively. 3-Bromophenyl-6-acetoxymethyl-coumarin-3-carboxylates have been found to exhibit potential anticancer and antitumour activity [12].

Crystals suitable for diffraction studies were grown by slow evaporation technique using acetic acid as a solvent. The crystals of the compound crystallize in Monoclinic with space group $P2_1/n$ having 8 molecules in the unit cell of dimensions crystal system: a = 4.3573(3), b = 9.2859(6), c = 25.2677(17) Å and β = 91.927(3) ^{0}. The three dimensional intensity data was collected using a crystal of size 0.25 × 0.15 × 0.10 mm mounted on Bruker axs kappa apex2 ccd diffractiometer with Mok_α radiation. The data was collected using ω and φ scan mode. 9957 measured reflections of which 2130 independent reflections and 1502 reflections with $I > 2\sigma(I)$. With absorption correction: multi-scan.

The structure was solved using wingx software package and the model was refined by the full-matrix least-square method. The refinement was continued till the final R = 0.0449, R_w = 0.1103.

The title compound is cyclic and planar but non-aromatic in nature due to the continuous delocalization of electrons around the coumarin ring. Skeleton is not possible. There is a significance deviation in bond angle at 01-C1-C2 (117.2(3) ° due to the electronic repulsion of oxygen (02) atom which is present at C1 carbon atom.

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Keywords: x-ray, single crystal, coumarin.