Faculty of Science & Literatur, Department of Physics 61080, Trabzon, Turkey. [c]*Hacettepe University Faculty of Pharmacy, Department of Pharmaceutical Technology, 06100 Ankara – Turkey.*
E-mail: side@hacettepe.edu.tr

Lamellar liquid crystals are promising systems for topical drug delivery [1]. They are transition states, possessing both the crystalline characteristics of solids and flow properties of liquids [2]. They are composed of oil, surfactant, water, and generally co-surfactant, and they have the advantage of being easily produced, increasing solubility of poorly water-soluble compounds, delivering fragile substances, and controlling release of drugs [3, 4].
In this work, SWAXS analysis of some Lyotropic Liquid Crystal Formulations was carried out to characterize nano aggregations in the structure. In the preparation of the samples, liquid paraffin, non-ionic surfactants (Brij 72 and Brij 721P) and/or ultrapure water have been used. Small and wide angle X-ray scattering (SWAXS) experiments were simultaneously performed with a Kratky compact Hecus (Hecus X-ray systems, Graz, Austria) system equipped with a linear collimation system and X-ray tube Cu target (λ= 1.54 Å).
Various models for the form factor were considered for fitting the SAXS patterns. Lamellar stackings in distorted spherulite forms have been observed in the structures. While the microscopic sizes of these spherulites were measured in the range of 20.33 - 99.15 µm, the range of the lamellar distances occurring inside of the spherulite aggregations was measured as 6.21- 6.47 nm. Briefly, SWAXS analysis has indicated that the polyethylene fibrils themselves were build up bundles of crystalline lamellae separated by layers of disordered material, with a period length of approximately 6 nm such as measured in the previous studies [5, 6].

[1] M. Aytekin, R. N. Gürsoy, S. Hekimoğlu, 35th Annual Meeting and Exposition of the Controlled Release Society (CRS Meeting), New York, USA, (2008). [2] S. Savic Colloid Polym Sci. 283: 439 – 445 (2005). [3] G. Burducea I. Specific structures Rom Rep Phys. 56(1): 66 – 73 (2004). [4] G. Burducea II. Structural polymorphism Rom Rep Phys. 56(1): 87 – 93 (2004). [5] A.Owen, A. Bergmann, Polmer International Vol. 53, No 1. 2004 pp 12-14 (3). [6] Y. Nozue, Y. Shinohara,Y.Ogaawa, Photon Factory Activity Report, 2004,22 Part B 4A

Keywords: SAXS, WAXS, Lamellar Liquid Crystals, LLC

FA1-MS05-P15

Small-Angle X-Ray Scattering Analysis of the Ectodomains of VEGFR-3 and the VEGF-C Ligand Complex.

Kuo-Long Lou[a]*, Po-Tsang Huang[a], U-Ser Jeng[b], Yu-Shan Huang[b], Tsung-wei Su[a], San-Tai Shen[c]*. [a]*Institute of Biochemistry and Molecular Biology; and Graduate Institute of Oral Biology, Medical College, National Taiwan University, Taipei 10051, Taiwan.* [b]*National Synchrotron Radiation Research Center, Hsinchu 30067, Taiwan.* [c]*Institute of Molecular Biology, Academia Sinica, Taipei 11529, Taiwan.*
E-mail: kllou@ntu.edu.tw

The Vascular Endothelial Growth Factor receptors (VEGF-Rs) play a significant role in tumor development and tumor angiogenesis and are therefore interesting targets in cancer therapy. Targeting the VEGF-R is of special importance as the feed of the tumor has to be reduced. Receptor tyrosine kinases are activated upon ligand-induced dimerization. Here we show that the monomeric extracellular domain of vascular endothelial growth factor C (VEGF-C) receptor-3 (VEGFR-3) has a flexible structure. Binding of VEGF to membrane-distal immunoglobulin-like domains causes receptor dimerization and promotes further interaction between receptor monomers through the membrane-proximal immunoglobulinlike. By this mechanism, ligand-induced dimerization of VEGFR-2 can be communicated across the membrane, activating the intracellular tyrosine kinase domains.
VEGF-C stimulates lymphangiogenesis and contributes to pathological angiogenesis via VEGFR-3. Here we present the SAXS analysis of VEGF-C bound to the VEGFR-3 h This structure reveals a symmetrical 2:2 complex, in which left-handed twisted receptor domains wrap around the 2-fold axis of VEGF-C. In the VEGFs, receptor specificity is determined by an N-terminal alpha helix and three peptide loops.
Our structure shows that two of these loops in VEGF-C bind toVEGFR-3 subdomains D2 and D3, while one interacts primarily with D3. Additionally, the N-terminal helix of VEGF-C interacts with D2, and the groove separating the two VEGF-C monomers binds to the D2/D3 linker. VEGF-C, unlike VEGF-A, does not bind VEGFR-1. We therefore docked VEGF-A, VEGF-C to VEGFR-1, VEGFR-2. This molecular simulation analysis, together with our structural data, defined VEGFR-3 residues critical for the binding of VEGF-C. Our results provide significant insights into the structural features that the Dimmer Complex of VEGFR3 inducing upon VEGF-C binding in solution.

Keywords: Small angle X-ray scattering (SAXS), VEGF-C, VEGFR3

FA1-MS05-P16

Investigation of alternative methods of holding samples for X-ray solution scattering.

P. U. Pennartz, M. Degen, L. Fan, N. Grupido, S. Bendle. *Rigaku Innovative Technologies, Auburn Hills, Michigan, USA.*
E-mail: paul.pennartz@rigaku.com

Small Angle X-ray Scattering (SAXS) is a powerful technique used to analyze liquid samples, such as proteins in solution, particles in solution, melts, foams, etc. The availability of bright x-ray sources coupled to state-of-the-art x-ray optics combined with beam conditioning hardware and photon counting detectors allows collection of SAXS data in the home lab without the need to travel to a synchrotron. Home labs typically utilize Cu-Ka radiation which requires evacuation of the beam path and therefore necessitates containment of liquid samples in a "cell" or capillary. While quartz or glass capillaries are the traditional choice, they are not without their limitations, being fragile, non-uniform and producing non-negligible background scattering. Cells have a metal super-structure with two transparent x-ray windows and o-ring seals. Kapton™ and mica are two of the usual choices for the windows. In order to extract structural information of the particles in solution the background scattering from the buffer or solvent and the container should be subtracted properly. It is particularly critical for solution scattering. Ideally, the exact same container at the exact same position should be used for both the background and the sample data collections. This presentation will discuss alternative methods of holding liquid

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.*
E-mail: biserka@chem.pmf.hr

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.

[1] Prugovečki B., Dodson E.J., Dodson G.G., Matković-Čalogović D. *Croat. Chem. Acta*, 2009, 82 (2), 433-438. [2] Prugovečki, B.; PhD Thesis, University of Zagreb, 2005.

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.*
E-mail: edgar.sanches@ifsc.usp.br

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.

[1] Hwang G.W., Wu K.Y., Hua, M.Y., Lee H.T., Chen S.A., *Synth. Met.,* 1998, 92 ,39. [2] Mattoso L.H.C., Macdiarmid A.G., Epstein A.J., *Synth. Met.*, 1994, 68, 1. [3] Gonçalves D., Mattoso L.H.C., Bulhões L.O.S., *Elecrrochim. Acta,* 1994, 39, 2271. [4] Pouget J.P., Józefowics M.E., Epstein A.J., Tang X., MacDiarmid A.G., *Macromolecules*, 1991, 24, 779. [5] Epstein A.J., MacDiarmid A.G., Synth. Met.., 1991, 601, 41. [6] Le Bail A., Duroy H., Fourquet J.L. *Mat Res Bull*, 1988, 23, 447.[7] Rodríguez-Carvajal, J. FullProf Program: Rietveld, Profile Matching and Integrated Intensities Refinement of X-ray and/or Neutron Data (powder and/or single-crystal). Laboratoire Leon Brillouin (CEA-CNRS), version September 2007.

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.*
E-mail: darren0615@msn.com

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,