on protein size, secondary structure and overall conformation will be presented. The characterization of the solution structure and oligomerization state of the Arabidopsis gamma subunit is novel and important contribution to studies on G-proteins providing insights also for the mammalian proteins

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Keywords: GTP-binding proteins, biophysical analysis, SAXS

FA1-MS05-P11

Structural Analysis of 1-aryl-3-isopropilamino-1-propanone hydrochlorides. Barış Anıl[a], Ertan Şahin[a], Ebru Mete[a], H. İnci Gül[b]. [a]*Department of Chemistry, Faculty of Science, Atatürk University; Erzurum 25240, Turkey*. [b]*Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Atatürk University; Erzurum 25240, Turkey.*
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Mannich bases are generally formed by the reaction between formaldehyde, a secondary amine and a compound containing reactive hydrogen atoms. They display varied biological activities such as antimicrobial [1], cytotoxic [2,3], anticancer [2], analgesic [4], anti-inflammatory [5] and anticonvulsant [6] and DNA topoisomerase I inhibiting activities [3].
In this study, it was planned to synthesize some Mannich bases having the chemical structure of 1-aryl-3-isopropilamino-1-propanone hydrochlorides, which are possible cytotoxic/ anticancer compounds. Aryl part was changed as C_6H_5, 4-$CH_3C_6H_4$, 4-ClC_6H_4, 4-BrC_6H_4, 4-HOC_6H_4. The logic behind the synthesis of the compounds was to investigate the effect of substituents having different electronic nature. The chemical structures of the compounds were determined by X-Ray diffraction, ^{1}H-NMR, ^{13}C-NMR, DEPT, gCOSY, gHMQC, GHMBC and double resonance techniques.

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Keywords: Mannich bases, X-Ray diffraction, chemical structure

FA1-MS05-P12

Experimental and DFT studies on a pyrimidine-thione derivative. Muharrem Dinçer[a], Namık Özdemir[a], İrfan Koca[b], İsmail Yıldırım[c]. [a]*Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139, Samsun, Turkey*. [b]*Department of Chemistry, Faculty of Arts and Sciences, Bozok University, 66200, Yozgat, Turkey*. [c]*Department of Chemistry, Faculty of Arts and Sciences, Erciyes University, 38039, Kayseri, Turkey.*
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In general, pyrimidines have found much interest for their widespread potential biological activities [1] and medicinal applications, thus their chemistry has been investigated extensively [2]. In particular, various analogues of pyrimidine-thiones possess effective antibacterial, antifungal, antiviral, anti-AIDS, insecticidal and miticidal activities [3].

FA1-MS05-P13

New developments in low power beam delivery systems with aspheric multilayer optics. Nicoleta Galatanu[a], Sergio Rodrigues[a], Ronan Mahé[a], Peter Hoghoj[a]. [a]*Xenocs SA, Sassenage, France.*
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Low power microfocus X-ray sources coupled to multilayer optics are increasingly used in single crystal applications benefiting from very low maintenance requirements and high brilliance x-ray beam. The performance of these systems is typically better than traditional high power rotating anode X-ray sources in particular for small crystal analysis. However the performance remains significantly lower compared to the new generation of microfocus rotating anode sources.
We will present new developments in the field of beam delivery systems made of low power sources providing increased beam brightness (photons per second per solid angle). We have indeed developed new aspheric multilayer optics with increased capture angle and focusing properties as well as a new source optic design for single crystal diffraction applications. Such new developments provide an increased intensity (photons per second per mm^2) of at least a factor two compared to previous generation of microfocus sealed tube systems.
With the collaboration of our academic partners, different crystals of various sizes have been studied with different sources optics combination and compared with rotating anode generators. We will illustrate the new developments impact for protein crystallography and single crystal diffraction applications.

Keywords: Single crystal diffraction, multilayer optics, laboratory sources

FA1-MS05-P14

SWAXS Studies on Topical Lamellar Liquid Crystal Drug Delivery Systems. Semra İde[a], Elif Hilal Soylu[b], Merve Aytekin[c], R. Neslihan Gürsoy[c], Süeda Hekimoğlu[c]. [a]*Hacettepe University, Faculty of Engineering, Department of Physics Engineering,06800 Beytepe-Ankara.* [b]*Karadeniz Technical University,*

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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].

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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.

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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.

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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