restricted Hartree Fock closed- shell wave function. The minimizations were terminated at r. m. s. gradient of less than 0.01 KJ-mol^{-1} Å^{-1}. The optimized geometry of the structure displays significant change in the orientation of thiophene rings thereby resulting participation of such rings in the C-H…O and C-H… π interactions. The Semi-empirical Quantum Chemical C alculations were also performed on the analogous structure that has the substitution of two thiophene rings at position 2 to pentadiene moiety and these results will be compared with the present one and their detailed analysis will be presented later.

Keywords: bis-chalcones, hydrogen bond interactions and MOPAC 2009

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Characterization of some di-block copolymers and investigation of their temperature-dependent structural behaviors

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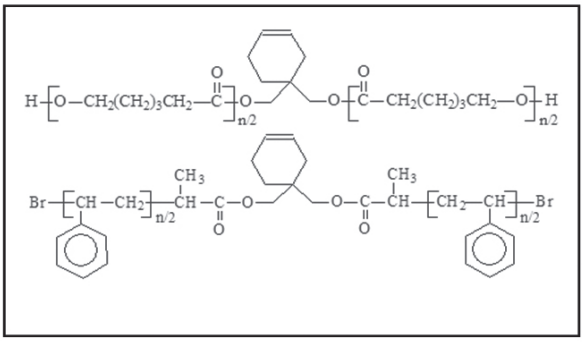
The synthesis and characterization of novel polymeric materials is crucially important for new scientific researches and technological applications. The present research is focused on Cyclohexene Mid-Chain polymers containing polystyrene (PS) and [Poly(ε- Caprolactone)] (PCL) functional groups. These polymers, because of their easily crystallization feature, can make some blends with other polymers, that have a wide technological utilization field [1]. The usage of an apolar aliphatic polyester [Poly(ε- Caprolactone)] and polystyrene which has a low melting point can cause radical polymerization controlling with light and cationic polymerization. Thus, molecular weight of the polymer and end-groups of the polymer chains can be also controlled. So, the physical properties of the polymers can be changed by adding different functional end groups (such as PS and PCL) to the Cyclohexene Mid-Chain.

In the present work, X-Ray diffraction (XRD) and X-Ray scattering methods (SAXS and WAXS) have been used to characterize these type polymeric structures (Figure 1.) in solid and solution forms. On the other hand, because of their big importance in living radical polymerization, thermo response behaviors of the novel synthesized polymers (in solution form) have been also examined.



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A SAXS Study of an enzyme-reponsive self-assembling polymer/ peptide conjugate

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Enzyme-responsive biopolymer systems are attracting considerable interest for applications in biocatalysis, drug delivery, tissue scaffolding and other applications. Recent work in our group led to the development of an enzyme-responsive nanocontainer delivery and release system [1].

The micelles are formed by PEG/peptide conjugates comprising a core of amyloid peptide βAβAKLVFF. This peptide has been the subject of recent investigation by our group, having interesting self-assembly properties [2] and the potential to develop amyloid inhibition systems with therapeutic applications [3]. In the PEG/peptide construct, the polymer-peptide linkage is selectively cleaved using the model enzyme α-chymotrypsin which cleaves between phenylalanine (F) residues. This produces products βAβAKLVF and F-PEG3000 (PEG with molar mass of 3 kDa). Remarkably, the product βAβAKLVF was found not to aggregate into amyloid fibrils, in contrast to the parent peptide βAβAKLVFF, pointing to the importance of aromatic interactions and the presence of two phenylalanine residues in driving self-assembly. The relase of unassociated non-amyloid peptide may be useful in applications.

The release of the peptide from the PEGylated nanocontainer delivery system upon enzymatic cleavage was studied by mass spectrometry, circular dichroism, SAXS, TEM (including cryo-TEM) and FTIR spectroscopy. These materials are under further study as bio-responsive self-assembling systems, with potential applications in detection and delivery.

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Keywords: peptide, enzyme, SAXS

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Characterization by SAXS of lignin from modified straw and bagasse sugarcane

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A biorefinery deals with process of converting biomass like bagasse and straw sugarcane into a variety of products [1]. Different useful products derived from sugarcane bagasse and straw can be obtained via separation process of hemicellulose, cellulose and lignin matrix [2]. Separation processes consists of a pretreatment that removes hemicellulose and the remaining product is submitted to a delignification procedure leading to a final product composed of pure lignin. Lignin can be modified for generation of a variety of novel and useful chemical agents and substances.

A standardized lignin for industrial applications is required to minimize the costs of reagents and processing power. In this work the effects of different pretreatment and delignification processes