ABSTRACT **INDEX NO. 52/17/Chem./25**

Thesis Title: SYNTHESIS AND SPECTRAL CHARACTERIZATION OF TYROSINE BASED PEPTIDE NANOSTRUCTURES

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This thesis work, on "Synthesis and Spectral Characterization of Tyrosine Based Peptide Nanostructures" contains *de-novo* tyrosine based short peptides have been synthesized, their self-assembly pattern and physicochemical properties have been characterized through AFM, FE-SSEM and several vibrational spectroscopic analysis such as FT-IR, NMR, powder XRD, UV-vis and Fluorescence spectroscopy. This thesis is divided into four chapters. A brief description of each chapter is discussed below, as a snap shot.

Chapter 1

This part contains brief background on peptide based self-assembled nanostructures and their potential applications in industries and academia. Self-assembly involves low-energy especially non-covalent interactions that are combined to form well-defined and stable supramolecular architechtures. Therefore, self-recognition of peptide molecules and their applications in modern nanotechnology owing to their specific molecular recognition patterns and the feasibility to manipulate them for specific functions have been discussed here.

Chapter 2

In this chapter, a small tyrosine based dipeptide was designed and synthesized. Surprisingly, this dipeptide was able to form gel in various solvent mixture. The structural insights of these gels were characterized by FE-SEM, AFM, FT-IR analysis, and X-ray diffraction studies. The mechanical strength of these gels was investigated through rheological experiments. Moreover, the gel obtained from this dipeptide had potential application for waste water treatment by removing toxic dyes and was used as a phase selective gelator for oil-spillage recovery.

Chapter 3

This section provides detail study of assembly formation and structural intricacy of two *de-novo* tyrosine based dipeptides by NMR and vibrational spectroscopic analysis. In this work, a thorough investigation was carried out on the ability of self-assembly pattern of two benzyl protected tyrosine and different side chain protected glutamic acid residues. The small variation of the substituent groups in the peptide moieties caused significant difference in their self-assembly formation and structural alignment. This difference in morphological behaviour motivated us to study them in detail by FT-IR, NMR and Raman spectroscopic analyses. Furthermore, these spectroscopic results were verified by DFT calculation.

Chapter 4

In this chapter, efforts were made to synthesize and analyse the self-assembly pattern of di-tyrosine based dipeptide. The single crystal X-ray analysis of this peptide confirmed that this peptide exhibited in a parallel ß-sheet pattern which further self-assembled to form ß-sheet promoted helical architectures by various non-covalent interactions in the crystalline state. Hirshfeld surface analysis and DFT study also carried out for this dipeptide which concluded the same result as obtained from single crystal X-ray, AFM, FE-SEM, and CD analyses.

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