

**Studies on Organized Molecular Assemblies and their
Applications**

By

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Department of Chemistry

Submitted

In fulfilment of the requirements of the degree of

Doctor of Philosophy

to the



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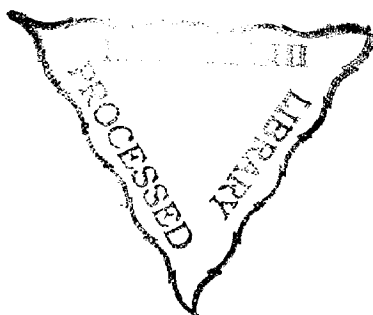
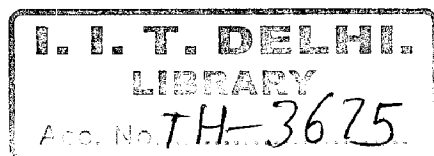
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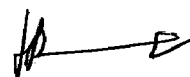
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CERTIFICATE

This is to certify that the thesis entitled “**Studies on organized molecular assemblies and their application**” being submitted by **Ms. Anjali Bishnoi** to the Department of Chemistry, Indian Institute of Technology, Delhi, for the award of degree of **Doctor of Philosophy** is a record of bonafide research work carried out by her.

Ms. Anjali Bishnoi has worked under our guidance and supervision and has fulfilled the requirements for the submission of this thesis, which to our knowledge has reached the requisite standard.

The results contained in this thesis are original and have not been submitted, in whole or in full, to any other University or Institute for the award of any other degree or diploma.



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ABSTRACT

Molecular recognition and molecular assembly are two intrinsic features of various biological processes in the living cell. For a group of molecules to assemble, they must come closer to each other through the process of molecular recognition. The complementarity of shape, size, charge and chemical functionality are some of the important requirements for molecular recognition, spontaneous construction of defined non-covalent structural arrays is required for molecular assembly. The fundamental and applied studies on synthetic receptors have led to a better understanding of design and development of molecular carriers and molecular devices for performing specific functions. The thesis titled “*Studies on organized molecular assemblies and their applications*” concerns with the development of organic molecules that can form molecular assemblies, their conversion into appropriate formulations and utilization as surface modifiers to achieve extension of shelf life of fruits and vegetables at ambient temperature. **CHAPTER I** of the thesis outlines the general features of organized molecular assemblies, methods adopted to obtain them, their characterization and typical applications. **CHAPTER II** of the thesis embodies the research work carried out to obtain molecular container compounds represented by resorcinarenes and their functionalization to obtain dansylated, diazotized, aminomethylated, esters and ether derivatives of resorcinarenes. Characterization of synthesized compounds has been accomplished by UV, IR, FAB-MS, ^1H NMR and ^{13}C NMR spectral analysis while their recognition characteristics have been determined by UV-visible spectroscopy. Since molecular entities aggregate to give molecular assemblies through non covalent interactions, resorcinarene derivatives have been examined for their aggregation in the presence and absence of surfactants and results are discussed in **CHAPTER III**. It also gives an account of experiments conducted to determine the behavior of synthesized

resorcinarenes as radical scavengers and as suitable molecule for the determination of critical micelle concentration of cetyltrimethylammonium bromide, under different experimental conditions. Since molecular aggregation can be exhibited by both synthetic and natural products, we have examined the behavior of P-104, a terpenoidal oligomer from lac by evaluation of its surface morphology and particle size through Scanning electron microscopy (SEM), Atomic force microscopy (AFM) and Transmission electron microscopy (TEM) respectively. Methods for obtaining useful formulations from P-104 and their standardization for use as surface modifiers have been delineated for preservation of fruits in **CHAPTER IV. CHAPTER V** of the thesis embodies the evaluation of formulations developed from P-104 as a surface modifier for extension of shelf life of fruits and vegetables. Three fruits (apple, sweet lime and emblic) were examined with respect to their physiological weight loss, total soluble solids, pH, color evaluation, texture analysis, microbiological quality with or without surface treatment. Sensory quality by using Hedonic scale and statistical analysis by SPSS software has been carried out to determine the efficacy of molecular assemblies obtained from P-104 as a surface modifier for fruits at ambient temperature.

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