

STUDIES ON INTRAMOLECULAR HYDROGEN BONDING IN SMALL PEPTIDES

by

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to the



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Certificate

This is to certify that the thesis entitled "**Studies On Intramolecular Hydrogen Bonding in Small Peptides**" being submitted by **Abhishek Upadhyay** to the Indian Institute of Technology, Delhi for the award of **Doctor of Philosophy** is a record of bonafide research work carried out by him.

Abhishek Upadhyay has worked under my guidance and supervision and has fulfilled the requirements for the submission of this thesis which to my knowledge has reached the requisite standards.

The results contained in this thesis have not been submitted in part or full to any other university institute for the award of any degree / diploma.



24/3/22

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Acknowledgments

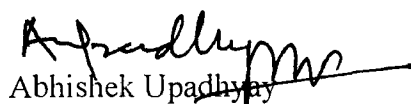
By the way of this document I wish to record my grateful thanks to all those who directly or indirectly helped me in the completion of this work. The first set of names that comes to my mind is of my parents, it is because of their careful rearing that I am able to see this day in my life.

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Abstract:

**STUDIES ON INTRAMOLECULAR HYDROGEN BONDING IN
SMALL PEPTIDES**

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This work deals with the rational design, synthesis and characterisation of a turn in short peptides. Chain reversal has been achieved by manipulating the side chains of the constituent amino acids, with a special focus on their chirality.

Similar attempts in the past have been successful but they rely on a covalently constrained geometry of the constituent groups to facilitate the turn.

Five different simple, linear tripeptides were synthesised to achieve the chain reversal and study the effect of the changes so made. To bias the condition for the setting up of an intramolecular H bond array, the N terminal of all these peptides was capped with an unnatural amino acid N', N' Dimethyl Glycine. A butyl amine was added to the C terminal so as to make the peptides soluble in a weakly polar solvent, chloroform.

The conformation of the peptides were studied with the help of simple and steady state NOESY . These results were compared on a relative scale with the HYPERCHEM™ software derived distances. The existence of any H bond was studied with the help of Variable Temperature NMR and FT-IR dilution studies.

Finally we could establish that the stereochemistry of the constituent amino acids affected the conformation of short linear peptides in an apolar solvent. With the help of suitable controls, the FT-IR spectroscopy could be used in a qualitative way to predict the conformation of short peptides.

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