

# Unconventional Approach to Drug Design: Synthesis of Aspartic Acid-Containing Macrocycle

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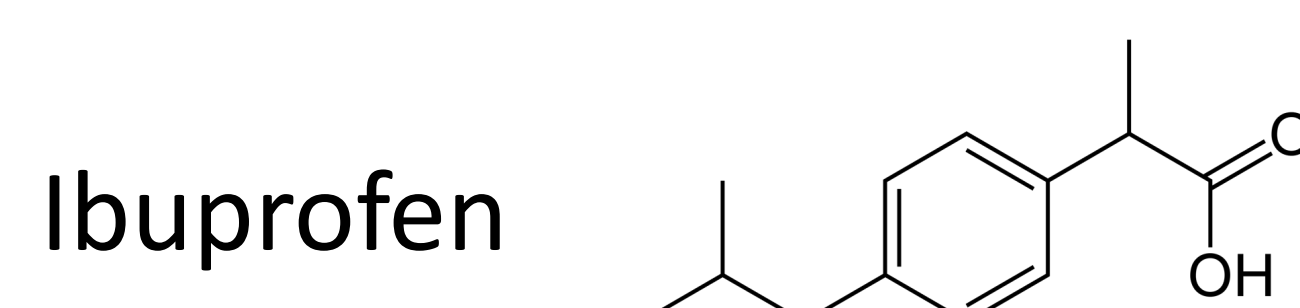
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## LONG TERM GOAL

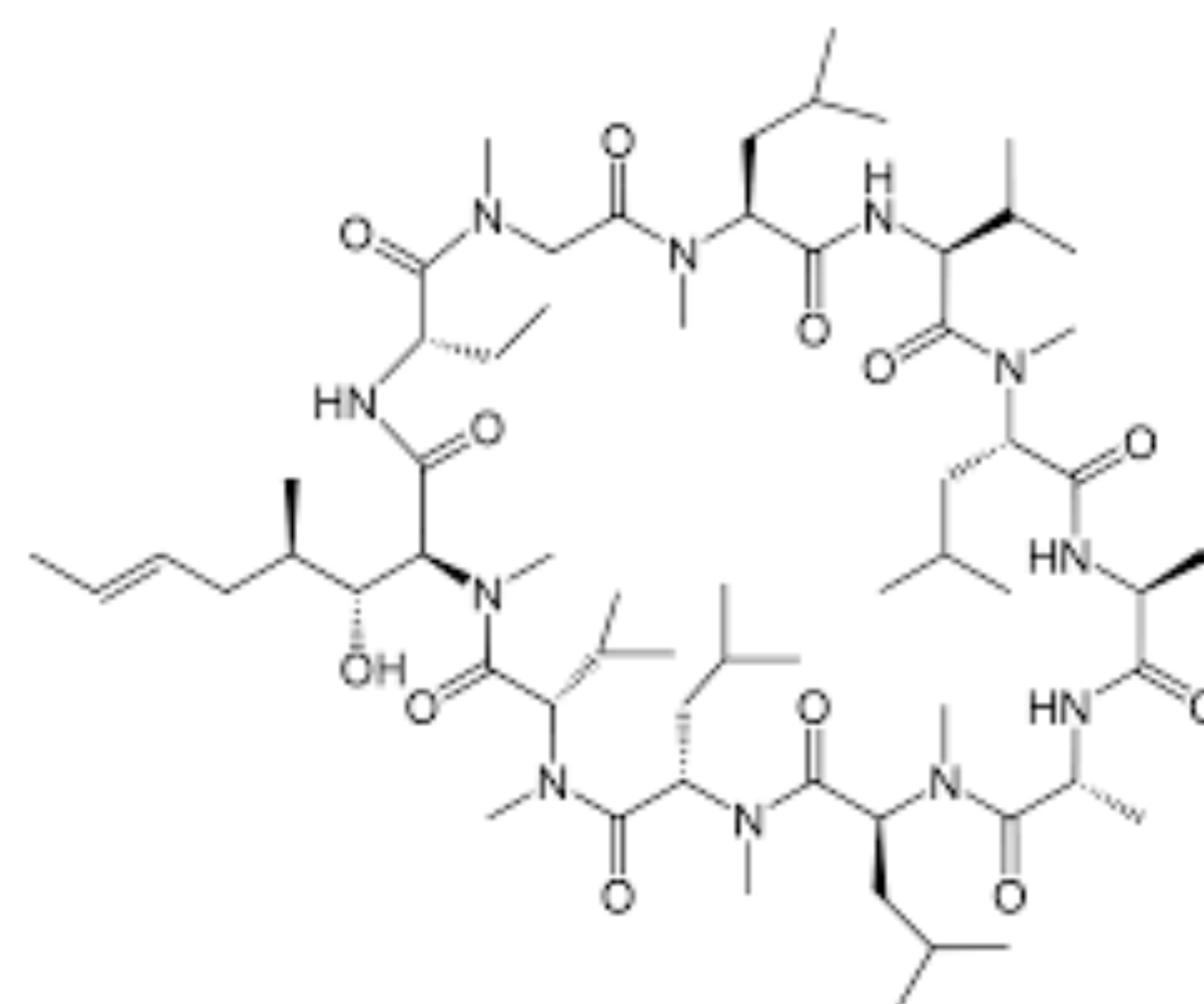
The long-term idea of developing macrocycles is to be able to produce possible biological drugs that can interfere with certain protein-protein interactions within cells. This could have the potential to alter the effects of certain diseases caused by abnormalities within protein-protein interactions. The macrocycles were synthesized via a five-step process.

Most drugs are developed from a small number of atoms in a straight manner. Here, we are examining strategies to arrange large numbers of atoms in a ring. The first strategy is most common because these molecules are easy to make (like ibuprofen). Nature has given us very useful drugs where the atoms are arranged in a ring (like cyclosporin).

## DRUGS FROM PHARMA AND NATURE

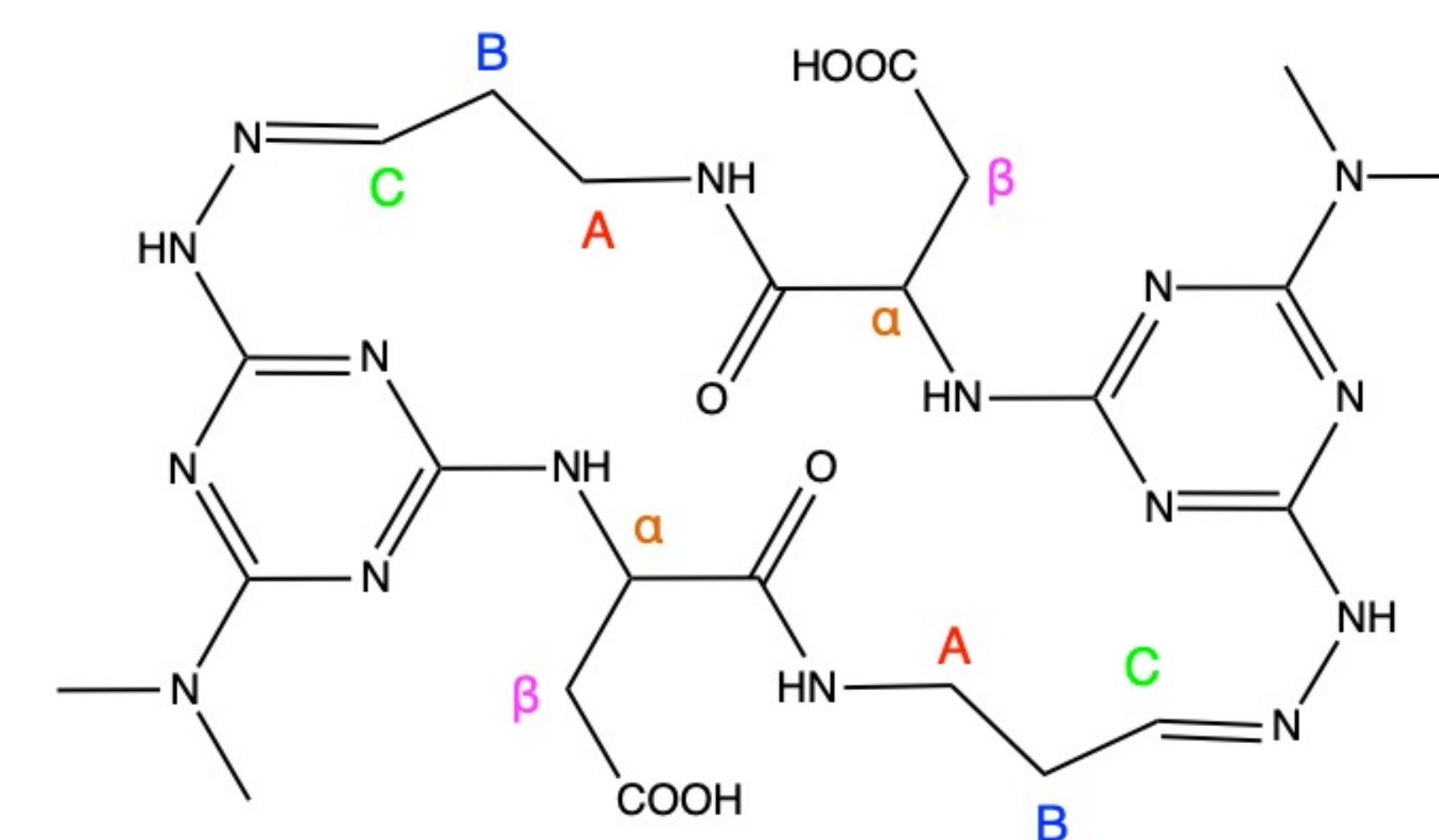


Cyclosporin

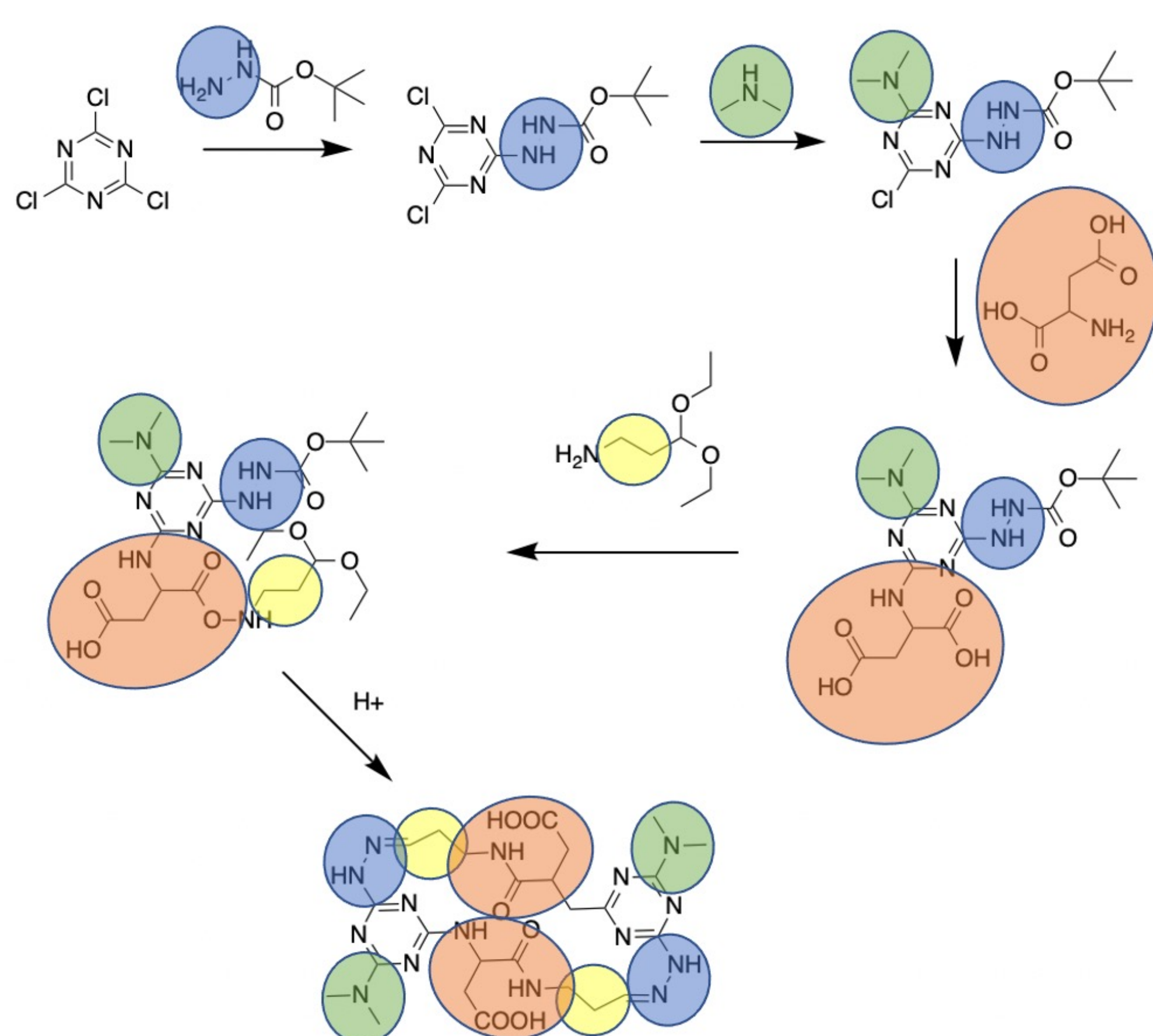


## THIS PROJECT

Development of a macrocycle containing aspartate. This amino acid is particularly interesting due to the acidic hydrogen on the side chain. These macrocyclic molecules exhibit dynamic behavior allowing for possible biological activity

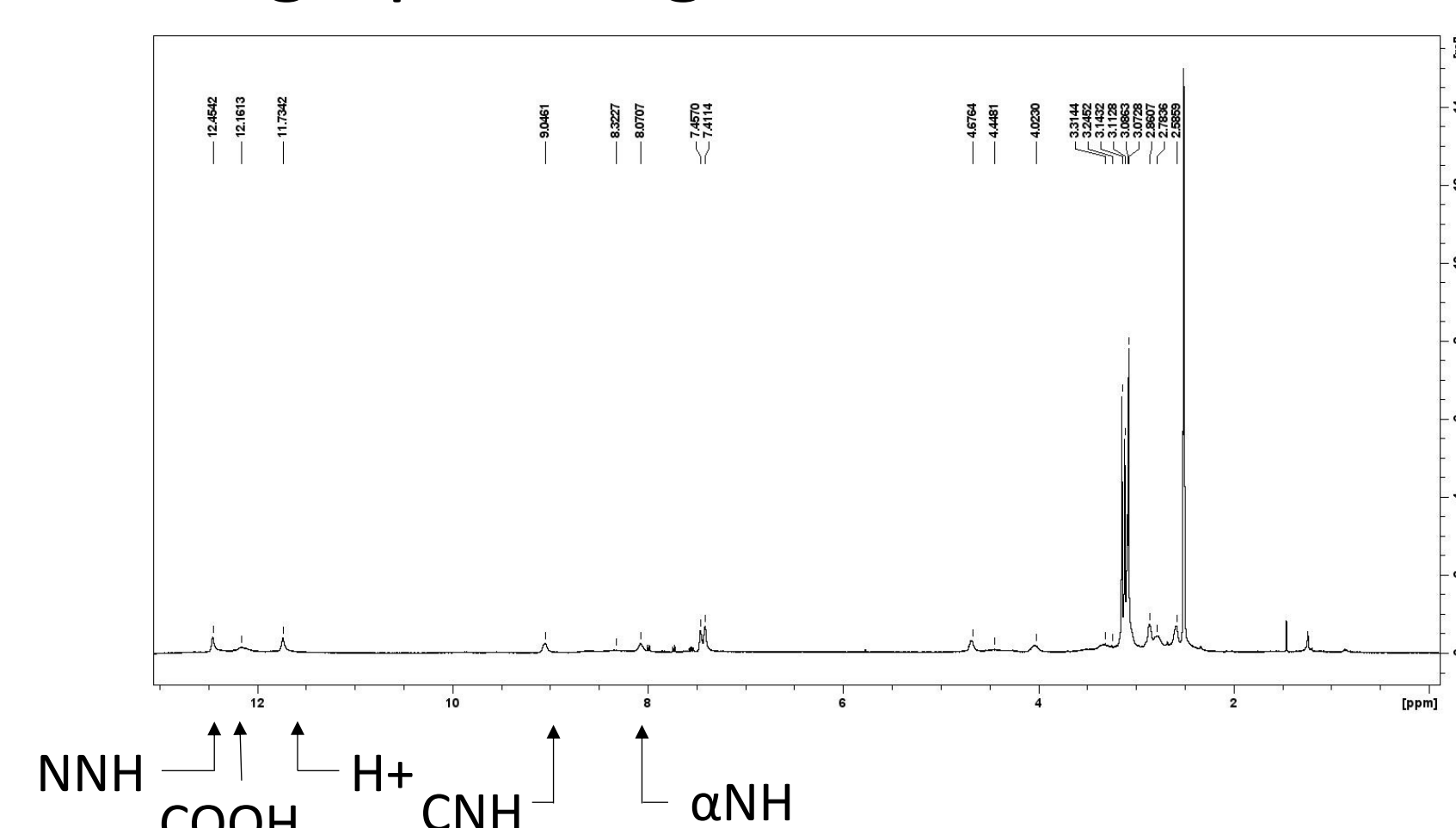


## THE APPROACH



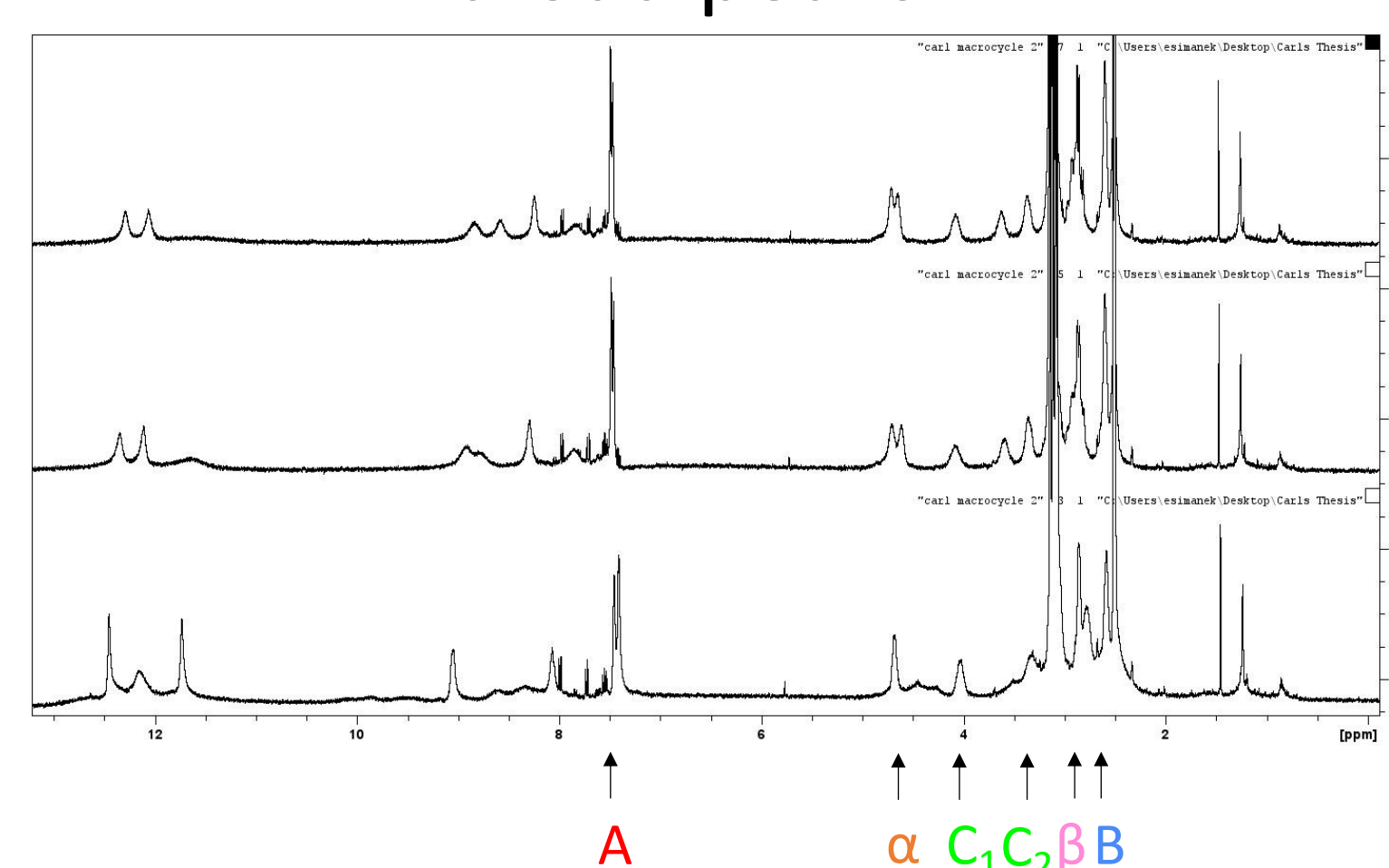
## IMPORTANT RESULTS

Fingerprint region confirms structure:



Upfield region shows dynamic behavior:

broad peaks:



## CONCLUSION & FUTURE WORK

- 1) Characterization techniques indicate completed synthesis
- 2) Further characterizations including LogP values
- 3) Biological assays to determine biological activity

## ACKNOWLEDGMENT

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