

Controlling How Fast a Chameleon Changes its Color: Emergence of Persistent Isomers in Triazine Containing Macrocycles



COLLEGE OF
SCIENCE & ENGINEERING



Alexander Menke, Camryn Gloor, Liam Claton, and Eric E. Simanek*
Department of Chemistry & Biochemistry, Texas Christian University

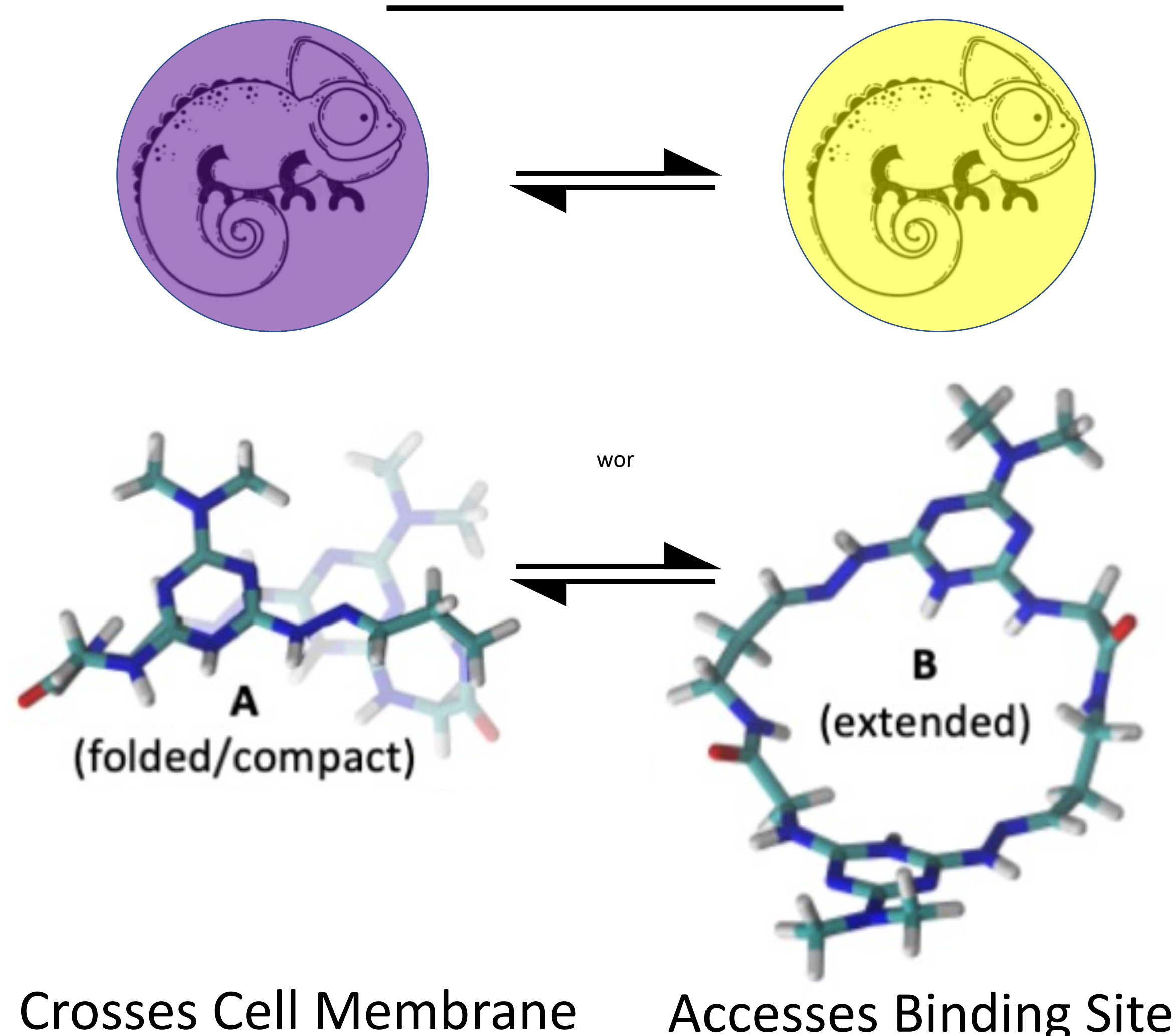
THIS PROJECT

The impact of β -branching is assessed by synthesizing macrocycles incorporating valine, threonine and isoleucine which are synthesized at near quantitative yields. Valine and threonine macrocycles exist as one species while isoleucine exists as two isomers in a 6:4 ratio. All isomers adopt the same rotamer state and a folded 'taco' conformation. The minor isomer of the isoleucine macrocycle persists even at high temperatures (60°C).

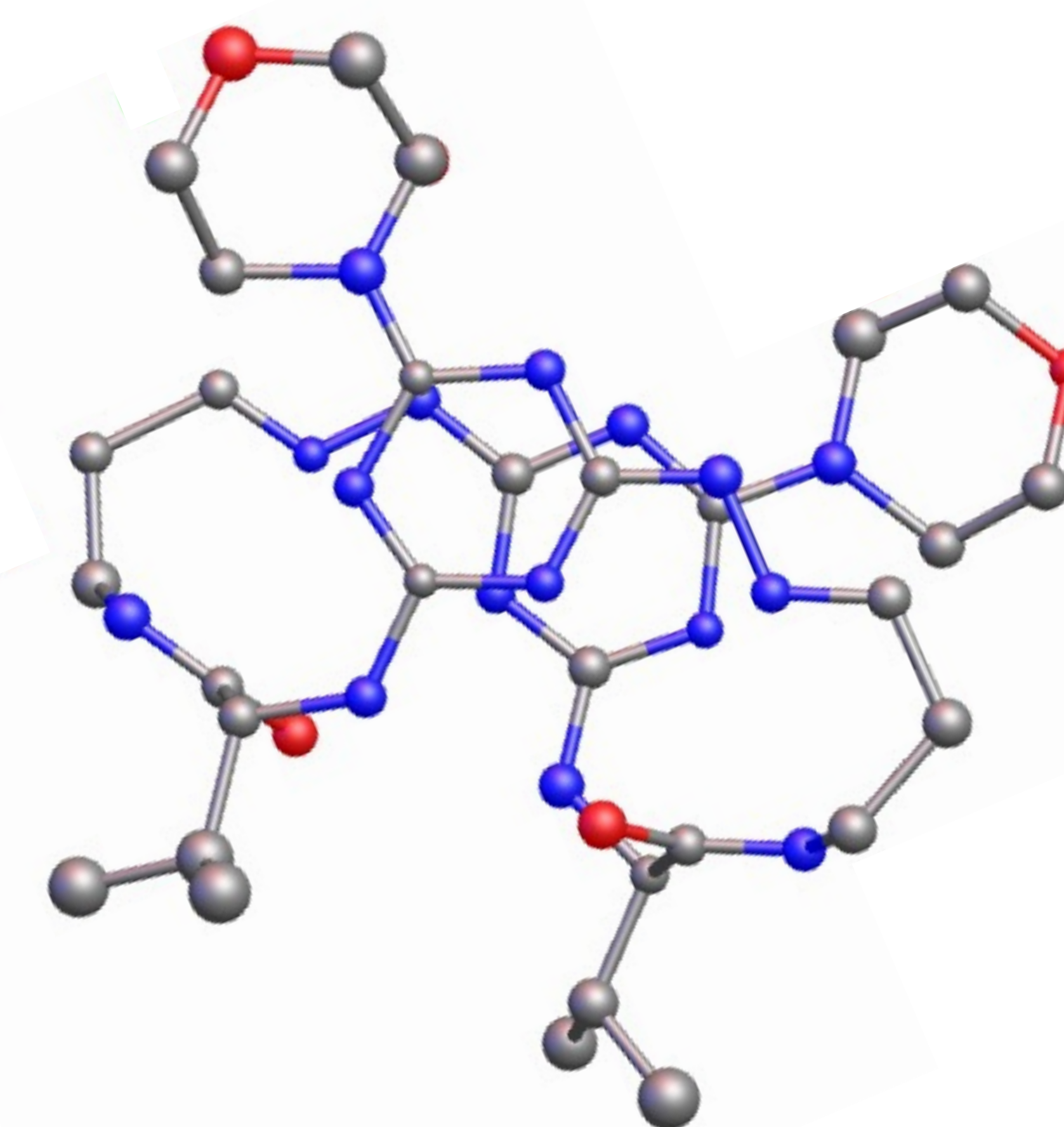
LONG-TERM GOAL

- Develop an efficient strategy to produce new drugs for various diseases.
- Mimic drugs found in nature such as Cyclosporin instead of small molecules like ibuprofen.

CHAMELEONICITY OF MACROCYCLIC COMPOUNDS



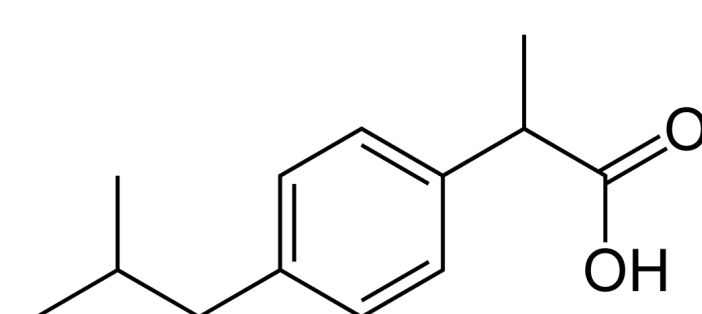
XRD Structure of V-V



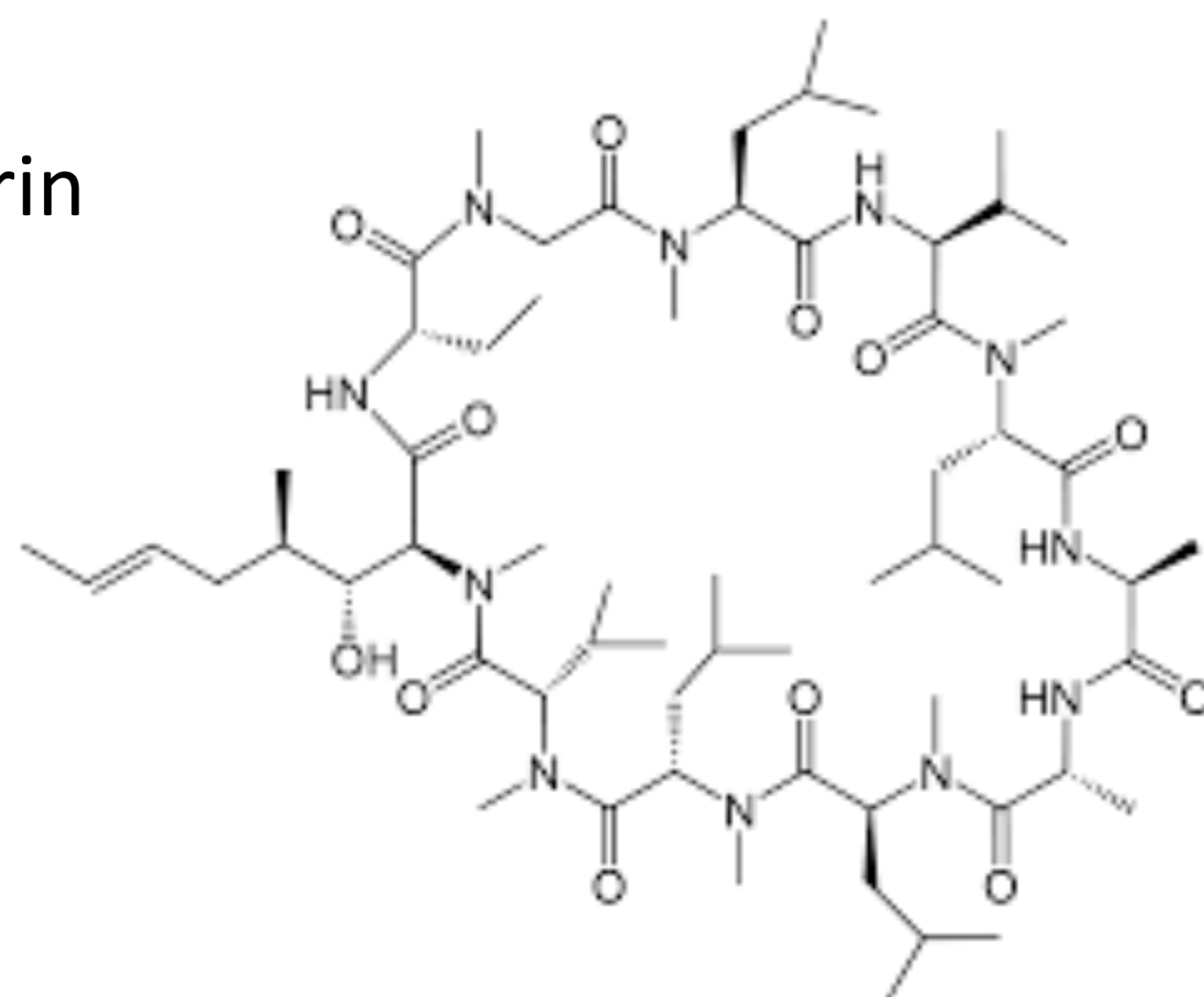
- Crystal structure resembles folded structure A

INSPIRATION: DRUGS FROM PHARMA AND NATURE

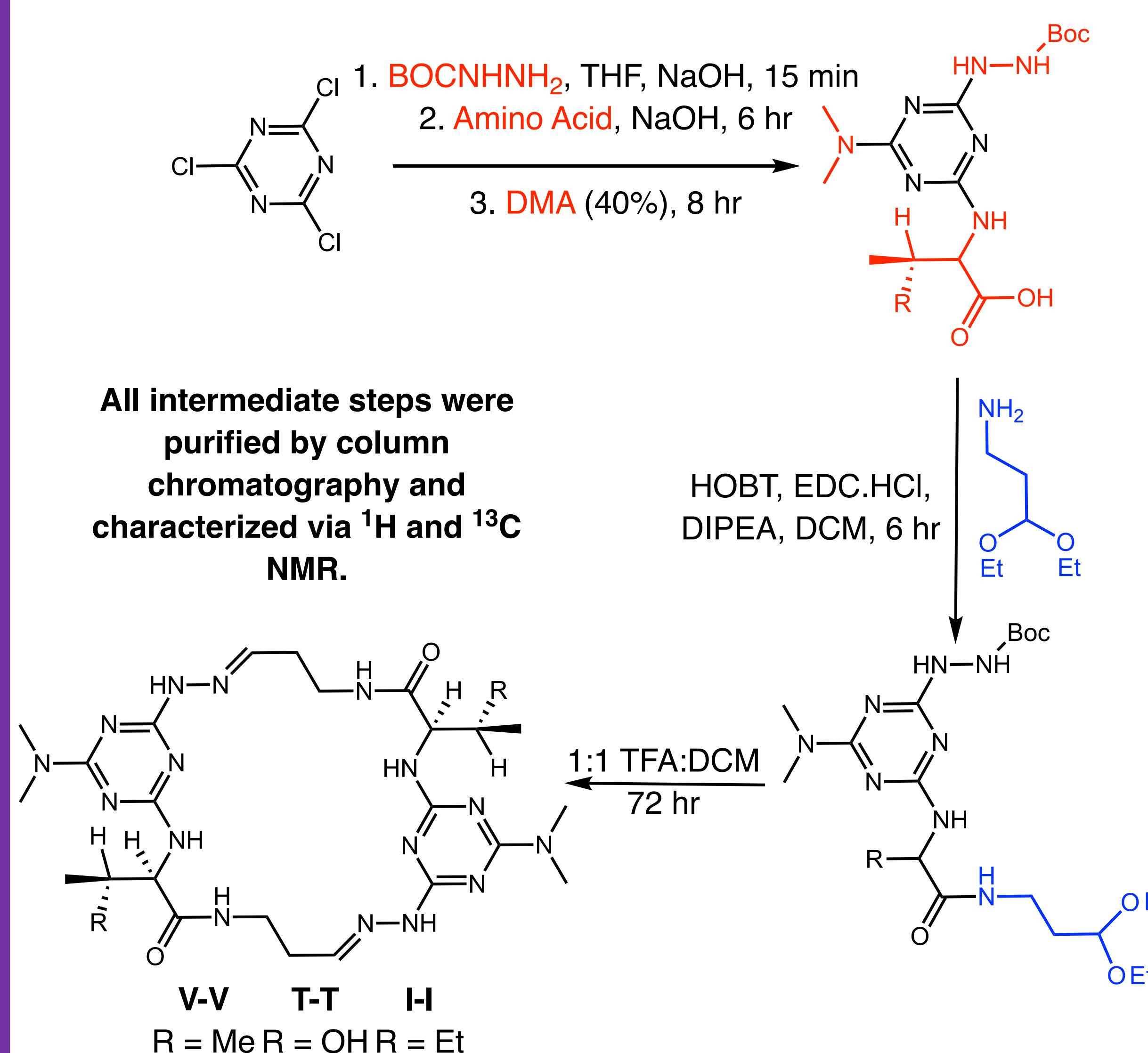
Ibuprofen



Cyclosporin



SYNTHETIC SCHEME



CONCLUSION

1. β -branched amino acids can be incorporated into macrocycles.
2. Larger side chains lead to persistent isomers.

FUTURE WORK

1. Make changes to the macrocycles to allow for conversion to happen in different environments like acidic/basic, different solvents, etc.
2. Begin targeting various cancer lines by docking macrocycles into binding pockets

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Contact: alexander.menke@tcu.edu; e.simanek@tcu.edu; TCU Box 298860, Fort Worth TX 76129