CALIFORNIA STATE SCIENCE FAIR
2010 PROJECT SUMMARY

Name(s)
Symphony Y. Yu

Project Number
S0518

Project Title
Rotational Barriers and Protein Backbones

Abstract

Objectives/Goals
The objective of my project is to explore the effects of R-groups with varying electronegativities on the structures of protein backbones through the determination of the rotational barriers of the R-groups of nicotinamide, the model protein in this experiment.

Methods/Materials
Methods in computational chemistry were implemented to find the rotational barrier. The molecule sample, prepared in a solution of deuterated nitrobenzene, is first analyzed using NMR spectroscopy, with data points collected at incremented temperatures. The raw data collected by the Bruker TOPSPIN program is then transferred to Mathematica 7.0 for nonlinear regression. A composite curve is obtained and the values of the change in enthalpy and the change in entropy and solved for, using the transition-state theory.

Results
According to the experiment, the rotational barrier of 6-CH3-nicotinamide was found to be H = 16.012 kcal/mol, the rotational barrier of 6-CF3-nicotinamide was found to be H = 12.90 kcal/mol, and the rotational barrier of 6-Cl-nicotinamide was found to be H = 12.6 kcal/mol.

Conclusions/Discussion
The results from the experiment yielded a percent error of 27.079% for 6-CH3-nicotinamide, a very large percent error, and relatively smaller percent errors for 6-CF3-nicotinamide and 6-Cl-of 0.077% and 0% respectively. Although the experimental values of the rotational barriers closely matched those of the theoretical values, some data points on the apparent rate graph had such a large percent error that these points were nulled and cut out of the data analysis in order to achieve the similarity between the calculated and experimental values of the rotational barriers. With such high percent error, even if the rotational barriers matched, the results are inconclusive. The percent error in the apparent graph was in part due to some discrepancy in the best-fit model and errors in the assumptions on which the theory that is the foundation of the project is based upon, in addition to procedural issues.

Summary Statement
I explored the effects of R-groups with varying electronegativities on the protein backbone structures by the determination of the rotational barriers of the R-groups of nicotinamide through NMR spectroscopy with computational chemistry.

Help Received
Used lab equipment at the University of California, Riverside under the supervision of Professor Leonard J. Mueller and the graduate students in his research group, Jin Feng Lai and Tian Ye; mother and father helped decorate display board