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Japanese Garden Waterfall

Wroclaw, Poland

COMPUTATIONAL CENTER FOR MOLECULAR STRUCTURES AND INTERACTIONS

Department of Chemistry STUDENT HIGHLIGHTS

The NSF-CREST Computational Center for Molecular Structure & Interactions sends students to Wroclaw, Poland for *Research Opportunity*

On September 12, 2003, Teri Robinson, Resheemah Allen and Tomekia Simeon (all from Jackson State University), Daniel Grant (Albany State University), Christina Washington (Fort Valley State University), and Jason Ford-Green (FAMU) embarked on a European research journey to Czech Republic and Wroclaw, Poland. The students spent one week in Prague, Czech Republic. While in Czech Republic, they resided at Nove Hradky Caste, where they experienced a different view of "home". The trip served as a reward to Grant (*1st place winner*), Washington,

and Green (*both 2nd place winners*) for their outstanding poster presentations at the 2003 Summer Institute Closing Ceremony in Orange Beach, Alabama. The students attended the Modeling Interactions in Biomolecules Workshop, where they each presented their research posters. On the evening of September 20, 2003, Grant, Washington, and Green departed from Czech and returned to their home states. The students were very happy to be back at home. They described the trip as "EXCITING". However, they returned with wonderful memories of their trip.



(Pictured top to bottom) Teri Robinson, Resheemah Allen, Daniel Grant, Christina Washington, Jason Ford-Green, and Tomekia Simeon



From Czech to...

From Czech Republic, two of the six students, Robinson and Allen, continued on their journey to Poland. While in Poland, the two ladies continued their research at the Technical University of Wroclaw. When asked about the trip, the following reflections were given:

From Teri Robinson:

As a graduate student of Jackson State University, under the leadership of Dr. Jerzy Leszczynski, I was given the opportunity of a lifetime. This fall I traveled to Eastern Europe, particularly, the Czech Republic and Poland where I visited for a total of five weeks. It was a trip I had always wanted to take, yet I don't think I was actually taking a trip until I stepped off the plane into the Czech Republic. I was completely enveloped in a foreign culture. I visited four cities in two countries. It was the first time I had been outside of the United States. I neither spoke nor understood Polish or Czech. However, my fears were subdued once I left the US and arrived in the Czech Republic and Poland. I found that the airports, restaurants, and other public places had picture icons designed to make life easier for travelers. There were information booth departments that had people who spoke some form of basic English and when those sources weren't available to me I usually

Poland

I was still able to move to the next phase of my travels with ease.

My two greatest companions on my journey were my Lord and Savior Jesus Christ and my Berlitz's Polish Phrase Book. These were the two key elements and I would have had a different experience without them both. I had planned to take many pictures and film a great deal during my trip. At the trip's conclusion; I had compiled 360 minutes of video and over 272 digital photos.

During my research trip, I laid down my project's goals. I focused on two main aspects: the collection of data, the processing of which should allow me to delve into an in-depth analysis of the impact of my mini-project entitled, "Theoretical Study of Dihydrogen Bonded Complexes." The other aspect which was to focus on learning



Cesky Krumlov

from the individuals around me including those persons I was not directly working with on my project. Concerning the collection of data and processing, I acquired skills to evaluate and calculate anharmonic and harmonic frequencies. I was introduced to various programs which involve solving quantum mechanical problems particularly the Schrödinger equation. Concerning the

second aspect, I had the opportunity to converse with many of the professors in Dr. Sokalski's research group and other research groups at the university. This provided me time to focus on their research goals and receive spoonfuls of advice from them concerning my own career path while in graduate school. I thoroughly enjoyed my Eastern Europe trip. I expect so many blessings and benefits from this trip which will lead to greater things in the future. I would like to thank Dr. Jerzy Leszczynski, along with the faculty of the Computational Center for Molecular Structures and Interactions, for this wonderful opportunity to be a part of such an educational experience. I took pictures of absolutely everything. To see more pictures of my trip, see my website at <http://f1.yahoo.photos.com/tak459>.



University Emblem

Molecular Structure outside of the university



From Resheemah Allen:

My European excursion was a wonderful and enriching experience. It opened my eyes to the rich history and culture which I had only read about or heard on the news. It was a valuable pilgrimage to get a first hand exposure to how the Polish value education, family, government and career opportunities. It was a privilege to work hand-in-hand with some of the best computational chemists Poland has to offer.

I gained much knowledge about my craft for Dr. W. Andrzej Solkaski and wisdom to differentiate the numbers from Dr. Szczepan Roszak. With the guidance of Dr. Pawel Kedzierski and Borys Szeftczyki, I was able to model the tetramer urate oxidase. With the model at

hand and using the program Insight, I was able to design other possible inhibitors for the enzyme urate oxidase delicately designed around hydrogen bonding interaction. This was a wonderful experience that I truly enjoyed. I hope to repeat the experience in the near future. I would like to thank Dr. Jerzy Leszczynski and CCMSI faculty for their encouragement and support for a truly empowering experience.

Conference Participants

