

# PROFESSIONAL DEVELOPMENT GRANT (April 2016) FINAL REPORT

## PROJECT: "A Two-Day Intensive Workshop: A Practical Introduction to Molecular Modeling"

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### **Purpose of the project:**

The purpose of this project was to participate in the workshop in order to develop necessary skills in using the molecular modeling software in a scientifically reliable way.

### **Review of the professional enhancement opportunity:**

I conduct research on design, preparation, and characterization of biologically active compounds with a potential in diagnosis and therapy. I am currently in the process of developing collaborations with specialists in the area, as this field is extremely broad and requires collaborative efforts. I have been working with UAMS faculty members interested in the molecular biology aspects of my interests. In order to progress in my scholarship, I need access to certain instrumentation which, as of now, is not available at ATU. Additionally, I needed access to molecular modeling software (Spartan). The purchase request has been reviewed and approved (4/13/2016) by ATU Office of Information Systems. Moreover, Physical Sciences Department sponsored a purchase of customized computing station, which allows me to perform complex hypothesis driven computer assisted drug design *in silico*. To maximize the depth, reliability and efficiency of using Spartan, closely tied to my research, I needed a professional training. This proposal was aimed at acquiring funds for it. The authors described the event as follows: *"two days of lectures and "hands-on" exercises covering a number of important aspects of molecular modeling and providing practical experience in the use of models to address a variety of chemical problems."*

## Summary of experiences:

The PI had a great experience participating in the workshop. Besides the copious amount of material studied, the PI also had an opportunity to network with the specialists in the area and authors of the studied software. That led to obtaining a substantial discount (45%) for purchase of two licenses of the software in question, which was completed later in 2016. The software allowed the PI to model molecules, for which he later (2017) obtained external grant from Arkansas INBRE, which covered their synthesis, characterization, testing their biological activity, collaboration with a specialist from UAMS and employment of one undergrad student.

## Conclusion:

The PI is grateful for the financial support from ATU Professional Development Grant that enabled him to participate in this valuable opportunity.



The image shows a screenshot of the Wavefunction, Inc. website. The top navigation bar includes links for HOME, PRODUCTS, EVENTS, SUPPORT, PURCHASE, and CORPORATE. The main content area features a banner for a workshop with the Wavefunction, Inc. logo and the tagline "Chemistry at Your Fingertips". The banner also displays images of software boxes for Spartan and Odyssey, and a computer monitor showing a molecular model. Below the banner, a sidebar lists various event categories: EVENTS, ACADEMIC WORKSHOPS, TRADE SHOWS, ON-SITE WORKSHOPS (highlighted with a mouse cursor), and INDUSTRIAL WORKSHOPS. The main content area contains the following text:

**A Two-Day Intensive Workshop:  
A Practical Introduction to Molecular Modeling**  
*presented by Dr. Warren Hehre, CEO, Wavefunction, Inc.  
at Wavefunction, Inc. offices, Irvine, CA*

This workshop includes two days of lectures and "hands-on" exercises covering a number of important aspects of molecular modeling and providing practical experience in the use of models to address a variety of chemical problems.

Enrollment is open to industrial and government chemists as well as university and college faculty. Registration fee is \$1,200 industrial and \$600 academic/government. For more information please contact us [here](#).

Please [contact us](#) for future workshop dates.