Nové Hrady and Institute of Microbiology

• Experimental and Modeling research
• Participation in the annual Visegrad Conference and Summer School
• Great opportunities to meet researchers from Europe

The Castle: both laboratory and residential hall
The town and Institute
Work responsibilities

• Reaction mechanism of human 3’-phosphoadenosine 5’-phosphosulfate synthase I (hPAPSSI)

• Computational Chemistry: a hybrid quantum mechanics and molecular mechanics approach (QM/MM)

• Analytical transition structure search using Schrödinger Biological Suite
A brief description of computation chemistry

- Using models of varying degrees of accuracy to predict and understand molecular behavior at pico-second to nano-second scale
Impact on the organization

- Elucidation of bona fide transition structure
- Generated a detailed application note for continuation of the same project
- Introduced a package that was rarely used at the Institute for future work (Amber molecular dynamics using QM/MM)
- Winner of Best Presentation Award at the conclusion of summer school

Interaction between ligand and critical protein residues
Visegrad Conference

- Poster presentations
- Lectures on experimental and modeling work
- Networking with scholars and researchers all over Europe and beyond
Most valuable experience: meeting people from all over the World
Traveling in Europe

Vienna

Prague

Vatican City
Impact on academics and career path

• Opened up a new way for me in the field of theoretical studies
• Reaffirmed my decision to pursue a career in medicine
• Motivated me to study biology in a more quantitative manner

Side project using skills learnt from work: peptide embedded in membrane
Acknowledgments

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