



**M.Sc. Defense - Tuesday December 23, 2014  
2:00 p.m. Food Science Building, RM. 128**

**DREF C. DE MOURA**

**Biophysics Interdepartmental Graduate Program  
Department of Food Science**

**“*IN SILICO* INSIGHTS INTO PROTEIN-PROTEIN INTERACTIONS AND FOLDING DYNAMICS  
OF THE SAPOSIN-LIKE DOMAIN OF *SOLANUM TUBEROSUM* ASPARTIC PROTEASE”**

**ABSTRACT:**

The plant-specific insert (PSI) domain from plant aspartic proteases is a member of the saposin-like protein (SAPLIP) family. The crystal structure of potato (*Solanum tuberosum*) PSI has been shown to exist in an open conformation that oligomerizes to form homodimers. There also exists a closed conformation observed in other SAPLIPs including barley (*Hordeum vulgare* L.) PSI. The present study investigates the mechanisms of tertiary and quaternary conformation changes of potato PSI in silico as a function of pH. Molecular dynamics simulations revealed that increasing pH of the system to physiological levels reduced the free energy barrier to dissociation of the homodimer. Principal component analysis revealed conformational changes at acidic and neutral pH, suggesting that monomeric PSI adopts a tertiary structure similar to the closed saposin-fold, presenting a potential new structural motif among SAPLIPs. This second PSI structure presents the first example of an alternative saposin-fold motif for any SAPLIP member.

**EXAMINATION COMMITTEE:**

Dr. Hermann Eberl, CHAIR (Department of Mathematics & Statistics)

Dr. Rickey Yada, ADVISOR (Department of Food Science)

Dr. George Harauz, EXAMINATION COMMITTEE MEMBER (Dept. of Molecular and Cellular Biology)