1125-VP-115 **Channing S. Parker*** (parkercs@dukes.jmu.edu), **Joshua R. Abrams** (rabrams12@email.arizona.edu), **Denise J. Harness** (harnessd@etsu.edu) and **Nina E. Galanter** (galanter@grinnell.edu). *Machine Learning for the Classification of Toxicological Endpoints.* Preliminary report.

The Toxicology Reference Database (ToxRefDB), compiled by the Environmental Protection Agency (EPA) contains data on chemicals and their associated toxicological endpoints. However, this data does not contain all chemicals of interest, and further testing is resource intensive. Here we present machine learning methods used to predict whether substances will have toxic effects on rat test subjects in order to avoid further animal testing. Chemical features associated with each chemical are utilized to generate these predictions. Support Vector Machine and Decision Tree machine learning algorithms are applied to toxicology data sets provided by the Environmental Protection Agency. These methods are tested and improved through cross-validation, parameter optimization, and the committee of machines approach. Feature selection is employed to optimize the models and provide information on which chemical features are potentially relevant to toxicological effects. Methods implemented include PCA, ROC curves, and F-Scores for pre-processing, and sensitivity analysis for post-processing. Long term outcomes of this study are to support further research in reducing the amount of animal testing, as well as in developing mechanistic-based toxicological models. (Received August 01, 2016)