1135-VN-3114 **Ryan M. Evans*** (ryan.evans@nist.gov), NIST, 100 Bureau Drive, Gaithersburg, MD 20899, **Anthony J. Kearsley**, NIST, 100 Bureau Drive, Gaithersburg, PA 20899, **Robert G. Brinson**, IBBR, 9600 Gudelsky Drive, Rockville, MD 20850, **Luke W. Arbogast**, IBBR, 9600 Gudelsky Drive, Rockville, MD 20850, and **Frank Delaglio**, IBBR, 9600 Gudelsky Drive, Rockville, MD 20850. *Classifying Nuclear Magnetic Resonance Spectra of Biologics.*

The term *biologics* refers to a class of medicines derived from living organisms, such as insulin, penicillin, or any vaccine. A very important type of biologic that has recently garnered attention is monoclonal antibodies—these are therapeutic proteins used to treat a wide variety of diseases from rheumatoid arthritis to certain cancers. Recent patent expiration of many name-brand biologics has created the opportunity for pharmaceutical companies to develop less expensive alternatives known as biosimilars. The popularity of biosimilars has created a need for novel analytic techniques to characterize the structure of monoclonal antibodies. Although Nuclear Magnetic Spectroscopy (NMR) has been shown an excellent tool for this task, current analysis of NMR spectra relies on a combination of visual inspection and Principle Component Analysis (PCA). The use of the first Wasserstein metric for comparing spectra will be presented and it will be shown that the pairing of this metric with an appropriate unsupervised learning algorithm enables superior grouping of spectra according to chemical structure. (Received September 26, 2017)