1145-05-1408 Torin Greenwood* (greenwo1@rose-hulman.edu) and Christine E Heitsch. Using Experimental Data to Deconvolve Structural Signals.

The combinatorial arrangement of RNA base pairings encodes functional information, and a sequence is typically predicted to fold to a single minimum free energy conformation. But, an increasing number of RNA molecules are now known to fold into multiple stable structures. Discrete optimization methods are commonly used to predict foldings, and adding experimental data as auxiliary information improves prediction accuracy when there is a single dominant conformation. In this talk, we describe the challenges of extending the thermodynamic prediction approaches with experimental data to multimodal structural distributions. Using a probabilistic framework, we illustrate that with significant probability, current prediction models fail to recognize the presence of multiple structures. (Received September 21, 2018)