1077-92-673 Charles (Chip) E Lawrence* (Charles_Lawrence@brown.edu), 182 George Street, Providence, RI 02912, and Donglai Wei and Lauren Alpert (Lauren_Alpert@brown.edu), 182 George Street, Box M, Providence, RI 02912. RNAG: A New Gibbs Sampler for Predicting RNA Secondary Structural Ensembles of Unaligned Sequences.

RNA secondary structures play an important role in the function of many RNAs, and structural features are often crucial to their interaction with other cellular components. We present a new algorithm, RNAG, to predict consensus secondary structures for unaligned sequences using the blocked Gibbs sampler, which has theoretical advantage in convergence time (Liu JASA, 1994). This algorithm iteratively samples from the conditional probability distributions P(Structure – Alignment) and P(Alignment – Structure) using efficient recursive sampling algorithms for each of these conditional distributions. We used hierarchical clustering to characterize the expected complex posterior space of these structural ensembles, gamma-centroid estimator to generate predictions, and credibility limits to characterize their uncertainty. An analysis of 17 RNA families shows substantially improved structural prediction based on PPV-SEN curves comparisons, compactness of sampled structures around their ensemble centroids, and at least eleven families with well separated clusters. (Received September 09, 2011)