**Boltzmann statistics maximum entropy of solid-state NMR dipolar recoupling and magic angle spinning data**

*J.D. Gehman,[1] M.-A. Sani[1] and A.K. Mehta,[2] [1]School of Chemistry & Bio21 Institute, University of Melbourne. Melbourne, VIC 3010, Australia and [2]Chemistry Department, Emory University, Atlanta, Georgia 30322, USA.*

We have engineered algorithms to employ maximum entropy as commonly used to derive Boltzmann's distribution for application in solid state NMR data analysis. The approach is used to characterise distributions of chemical shift tensor parameters from magic angle spinning sideband peak intensities, as well as distances from rotational-echo double-resonance (REDOR) data, in heterogenous samples. In the case of REDOR data, the method can reveal multiple distances with relatively few data points, which is of particular benefit in application to biological systems. This reverses the common practice of comparing REDOR data to dephasing curves simulated for several preconceived structural models, by providing the information necessary to construct models based on unbiased data analysis. In the case of chemical shift tensor analysis, it allows arbitrarily complex phospholipid mixtures to be analyzed for subtle perturbations, for example by association with antimicrobial peptides.

The method provides for a model-free approach to data analysis, in the sense that one need not assume the presence of any specific number of different chemical shift tensors or distances that contribute to observed signal. The strategy differs from the more common practice of including a single weighted  term in a fitting procedure, as each datum constitutes additional "information" and independently adds to or subtracts from the entropy of the distribution. A constrained optimisation problem with 100s of unknowns (the number of points used to approximate a continuous probability distribution of the desired parameter(s)) is thereby turned into an unconstrained optimisation problem with one coefficient for each data point.

The Boltzmann Statistics method also offers intriguing philosophical implications — it gives the broadest, and perhaps most  probability distribution consistent with the data, but also helps to determine which data points hold the greatest information content, such that experimental time can be focussed on gaining the best signal-to-noise where it is likely to benefit most.