ADVENTURES IN (MACHINE) LEARNING TO DETERMINE 3D STRUCTURE WITH NMR SPECTROSCOPY

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Interpreting NMR spectra has become somewhat of an art form in chemistry, particularly when applied to molecular structure elucidation. Skilled practitioners will often pore over several, often complex, NMR spectra for hours, days and even weeks to work out the connectivity (2D structure), stereochemistry and conformation (3D structure) of challenging new molecules. Our team develop tools that help with the steps in this process: creating new NMR experiments that provide different or more quantitative information than existing methods; applying quantum chemical calculations (usually DFT) to accurately predict the NMR properties of candidate molecular structures; developing machine learning tools that can accelerate predictions by 10,000-fold and thus potentially allow us to screen hundreds of thousands of molecular structures to find good fits to the experimental NMR spectra. The potential (and limits!) of these approaches will be illustrated by the case of the structure reassignment of natural products that have billions of potential 3D geometries and exploring how machine learning is starting to compete with DFT as a method to be used in these approaches.