

By 2050, antibiotic resistance could cause 10 million deaths annually, making it deadlier than cancer unless researchers can develop new ways to combat it. In particular, Methicillin-resistant *Staphylococcus aureus* (MRSA) synthesizes bacillithiol, which interferes with antibiotics. Current research is working towards interfering with bacillithiol production to shut down the mechanism that MRSA use to become antibiotic resistant. To understand how bacillithiol confers antibiotic resistance and combat it, bacillithiol and its derivatives have been synthesized and analyzed.

To identify these derivatives and verify their structures, Nuclear Magnetic Resonance (NMR) chemical shift data is crucial, but interpreting the data correctly is challenging. Computational NMR predictions can help, but have not been tested on similar complex molecules. In response, this research utilized three distinct NMR prediction techniques—NMRdb, CASCADE, and Tantillo's linear model—to assign Carbon and Hydrogen NMR shifts for derivatives in the bacillithiol synthesis pathway. CASCADE was found to be the most accurate model and synthesis of these new derivatives was verified.

In addition to the assignment of the bacillithiol derivatives, a website (<https://js.munano.org/nmr/>) was coded in order to simplify the process of assigning future molecules by integrating all three computational models. The results will be beneficial to future research involving n-methyl-bacillithiol as NMR assignments help confirm successful synthesis. This will aid in understanding n-methyl-bacillithiol's role in antibiotic resistance and detoxification methods for bacteria to help reduce projected public health threats.