

Structural Study of N-(1-Benzoyl-3-pyrrolidinyl) Benzamide

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Oxazolidinones show potent activity against vancomycin-resistant *Staphylococcus aureus* (VRSA) species, and are currently under active development. We present NMR spectroscopy and molecular dynamics calculation studies on N-(1-benzoyl-3-pyrrolidinyl) benzamide, an oxazolidinone derivative with substitution at the amine group of 3-pyrrolidinamine. The ^1H -NMR and ^{13}C -NMR spectra exhibited two sets of peaks, one major and one minor, giving rise to the existence of isomers at room temperature. In order to deduce the nature of its isomeric distribution, a series of derivatives were synthesized and analyzed using NMR spectroscopy and computer-aided molecular modeling (CAMM) simulations. The results suggest that rotation of the benzoyl group attached to the secondary amine in N-(1-benzoyl-3-pyrrolidinyl) benzamide is responsible for conformational heterogeneity.