

## VARIABLE-TEMPERATURE $^1\text{H-NMR}$ STUDIES ON THE CONFORMATIONS OF N'-PALMITOYL-RIFABUTIN IN SOLUTION

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In addition to structural demands, it is well known that geometry of the entire molecule is important for the expression of biological activity. Accordingly, elucidation of conformational properties of compounds could be interesting.

We noticed the broadening of some peaks in the  $^1\text{H-NMR}$  spectra of a series of recently developed Rifabutin (RFB) derivatives.<sup>1</sup> This fact let us to suspect the existence of a dynamic conformational equilibrium of these in solution.

Although a standard protocol for NMR structure determination provides a static picture of the molecule, additional NMR experiments can provide information on the frequencies of the rate processes that mediate transitions between discrete states of the molecule within the conformation space spanned by the static bundle of NMR-conformers.<sup>2,3,4,5</sup>

Having chosen the derivative with the longer side chain of that series – N'-palmitoyl-RFB – the most prone of the series of producing the highest steric constrain to RFB's backbone, a  $^1\text{H-NMR}$  study over a range of temperatures was undertaken. The results of this study are herein presented.

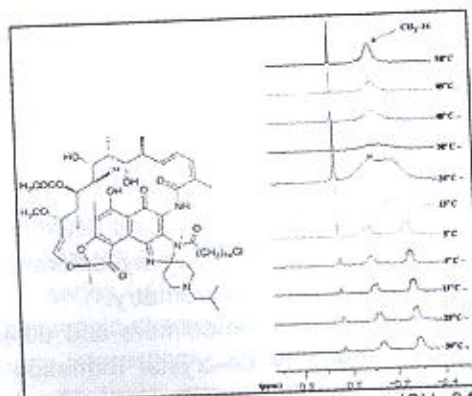


Figure 1: High-field region of  $^1\text{H-NMR}$  at different temperatures ( $\text{CH}_3\text{-34}$  peak variation)

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