

3D structure syn/anti isomers of a valin hydrazone

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Acyl hydrazone (R-CO-NH-N=CH-R) is a versatile scaffold for the synthesis of several molecules with a huge potential as anti-viral, anti-bacterial and anti-fungal drugs [1]. The stereochemistry of this scaffold is very interesting, infact it may present a double bond configuration in the imine part with a E/Z configuration and also be present as amide in syn/anti periplanar configuration which may give place to at least four possible stable products of synthesis. Herein we conducted several NMR experiments with the intent to clarify the representative set of scaffold stereochemistry of the products obtained and their 3D structure in solution. Further work in our lab is ongoing to confirm our NMR structures by use of crystallographic techniques [2].

[1] Sugiura, M. & Kobayashi, S. (2005). Angew. Chem. Int. Ed. 19;44(33), 5176-86

[2] Bain, A. D. (2003). Prog. in Nucl. Mag. Res. Spectr. 43(3-4), 63-103.

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