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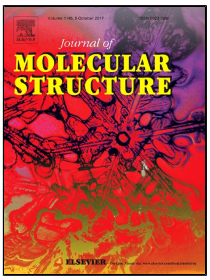

Synthesis and structural analysis of 3-phenylethyl-2,4(1*H*,3*H*)-quinazolinediones

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Synthesis and structural analysis of 3-phenylethyl-2,4(1*H*,3*H*)-quinazolinediones

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Abstract

This article presents the unexpected synthesis of 3-phenylethyl-2,4(1H,3H)-quinazolinediones by means of oxidative expansion of the 3-phenylethylimino-2-indolinone ring promoted by sodium borohydride. The ^{1}H-NMR spectroscopic patterns showed the presence of two conformational isomers in equilibrium, the first was a staggered conformation and the second was a gauche structure. The crystal structure of 3-phenylethyl-2,4(1*H*,3*H*)-quinazolinedione revealed a staggered conformation with the quinazoline fragment and the phenyl ring in *anti*-arrangement. The molecules of quinazolinedione are associated in centrosymmetric dimers through two N-H···O hydrogen bonds between the NH moieties and the adjacent carbonyl groups.

Keywords

Ring expansion
Oxidative cleavage
Isatin
Quinazolinedione
Schiff base