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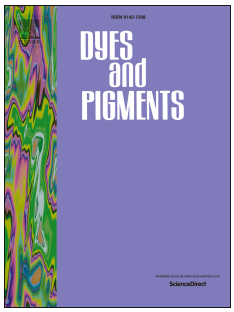

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The possible tautomerism of the potential rotary switch 2-(2-(2-Hydroxy-4-nitrophenyl)hydrazono)-1-phenylbutane-1,3-dione

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Abstract:

The title compound is potentially tautomeric and its tautomerism was studied by means of molecular spectroscopy (^{1}H and ^{13}C NMR and UV-Vis) in DMSO as well as by quantum chemical calculations (M06-2X/TZVP). The detailed assignment of the NMR signals supported by the theoretical calculations clearly shows that the previous interpretation, available in the literature, about the coexistence of two tautomeric forms is not correct. The compound exists as major and minor isomer of a single tautomeric form. In addition, a 2-methoxy derivative (the OH group replaced by a methoxy group) is also investigated and show similar trends.

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