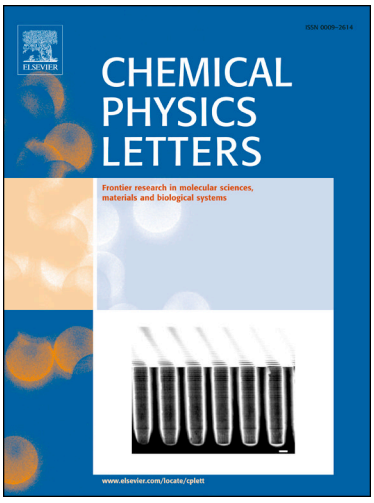

Research paper

Photo-physics Study of a Styrylquinoline as Inhibitor of Pim-1 Kinase: Solvent and Concentration Effects

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Photo-physics Study of a Styrylquinoline as Inhibitor of Pim-1 Kinase: Solvent and Concentration Effects

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Abstract

7-Nicotinoyl-styrylquinoline (MB96) displays an antiviral activity on HIV-1 infected CEM cell lines and is a promising inhibitor of the serine/threonine-protein Pim-1 kinase. By means of UV-vis spectroscopy supported by theoretical calculations this styrylquinoline is shown to exist in different conformations: the s-trans planar conformation along with other twisted ones with respect to the torsion around the single bond between the quinoline and the phenylethenyl appendage. Hydrogen bonding interactions with the solvent shift the skeleton of the MB96 towards the planar form, enhancing conjugation of π-electrons between the quinoline and the catechol parts, while self-association process seems furthering this planar conformation.