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Theoretical and experimental studies of aryl-bithiophene based push-pull  $\pi$ -conjugated heterocyclic systems bearing cyanoacetic or rhodanine-3-acetic acid acceptors for SHG nonlinear optical applications

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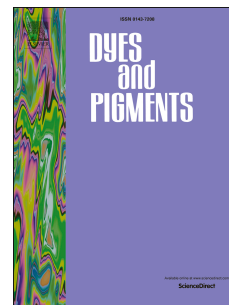
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**Theoretical and experimental studies of aryl-bithiophene based push-pull  $\pi$ -conjugated heterocyclic systems bearing cyanoacetic or rhodanine-3-acetic acid acceptors for SHG nonlinear optical applications**

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**Abstract:** A series of push-pull aryl-bithiophene based systems **2-3** were designed and synthesized in order to understand how structural modifications influence the electronic, linear and nonlinear optical properties. The push-pull conjugated chromophores **2-3** bear a bithiophene spacer conjugated with a phenyl ring functionalized with *N,N*-dialkylamino electron-donor groups together with cyanoacetic or rhodanine-3-acetic acid acceptor groups. Theoretical (DFT calculations) and experimental studies were carried out to obtain information on conformation, electronic structure, electron distribution, dipolar moment, and molecular nonlinearity response of the push-pull

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