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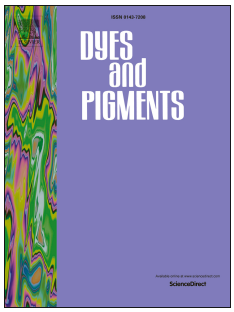

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PII: S0143-7208(17)31802-8

DOI: 10.1016/j.dyepig.2017.10.001

Reference: DYPI 6299

To appear in: *Dyes and Pigments*

Received Date: 24 August 2017

Revised Date: 27 September 2017

Accepted Date: 1 October 2017

Please cite this article as: Fernandes SSM, Herbivo C, Aires-de-Sousa Joã, Comel A, Belsley M, Raposo MMM, Theoretical and experimental studies of aryl-bithiophene based push-pull π-conjugated heterocyclic systems bearing cyanoacetic or rhodanine-3-acetic acid acceptors for SHG nonlinear optical applications, *Dyes and Pigments* (2017), doi: 10.1016/j.dyepig.2017.10.001.

Theoretical and experimental studies of aryl-bithiophene based push-pull π-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