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Isomeric Thienothiophene Push-Pull Molecules with Tunable (Non)Linear Properties and Photoinduced *E*/*Z* Switching

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Twenty new push-pull chromophores derived from electron-donor thieno[3,2-*b*]thiophene and thieno[2,3-*b*]thiophene heterocycles (Figure 1.) were prepared through facile synthetic routes [1,2]. Tailoring of optical, electrochemical and thermal properties was achieved by alternation of acceptor units or extension of the π-linker between electron-donating and electron-withdrawing moieties. Detailed study focused on structure-property relationships elucidation was performed using UV-VIS absorption spectroscopy, cyclic voltammetry, differential scanning calorimetry, thermogravimetric analysis and investigation of second- and third harmonic generation. Gathered experimental data were also supplemented by DFT calculations to study spatial and electronic properties of all synthesized target heterocyclic compounds. Based on the structural arrangement, extended thieno[3,2-*b*]thiophene chromophores with an inserted double bond proved to be photoinducible molecular *E*/*Z* switches. The *Z* isomer can be partly obtained by Royal Blue LED irradiation, while *E* isomeric form is subsequently fully regenerated in the dark.

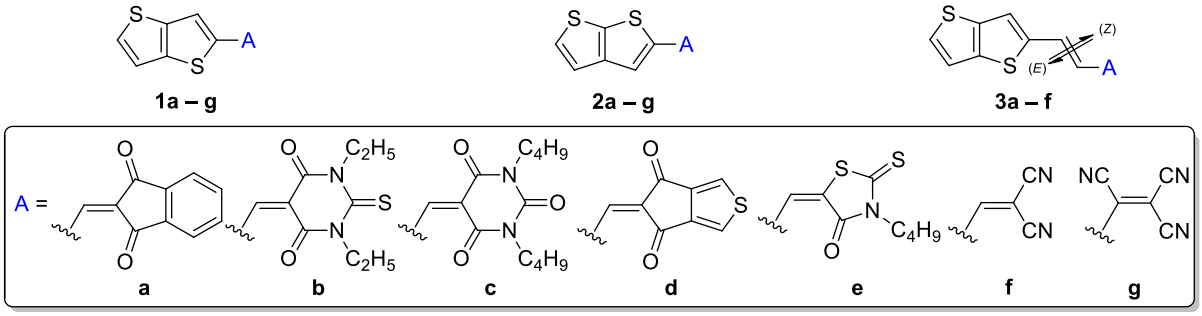

Figure 1. Synthesized thienothiophene push-pull chromophores.

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References:

[1] Podlesný, J.; Pytela, O.; Klikar, M.; Jelínková, V.; Kityk, I. V.; Ozga, K.; Jedryka, J.; Rudysh, M.; Bureš, F. Small Isomeric Push-Pull Chromophores Based on Thienothiophenes with Tunable Optical (Non)linearities. *Org. Biomol. Chem.* **2019**, *17*, 3623–3634.

[2] Podlesný, J.; Jelínková, V.; Pytela, O.; Klikar, M.; Bureš, F. Acceptor-Induced Photoisomerization in Small Thienothiophene Push-Pull Chromophores. *Dyes Pigm.* **2020,** *179*, 108398.