



# Manipulation of the electronic and photovoltaic properties of materials based on small push–pull molecules by substitution of the arylamine donor block by aliphatic groups

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## ABSTRACT

Push–pull molecules with an arylamine donor block connected to a dicyanovinyl acceptor *via* a thienyl  $\pi$ -conjugating spacer have been synthesized in order to analyze the effects of replacing an outer phenyl ring of the triphenylamine (TPA) block of a reference compound by methyl, hexyl, heptafluoropentyl and dioxaocetyl groups. Optical, electrochemical and X-ray diffraction data show that these substitutions have minor influence on the energy levels of the molecule but exert a considerable effect on the structure, optical, electrical and photovoltaic properties of the resulting materials.

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## 1. Introduction

Owing to a combination of electron-donor properties, high hole-mobility and resistance to crystallization, triarylamines (TAAs) have become a major class of key building blocks for the design of active materials for light-emitting diodes [1,2], metal-free chromophores for dye-sensitized solar cells [3–5] and donor materials for organic photovoltaics (OPV) [6–16]. Using the triphenylamine (TPA)-based compound **1** [14] (Fig. 1) as a reference, we have shown that rigidification of the molecular structure, modulation of the internal charge-transfer, or introduction of hole-transporting groups, represent interesting synthetic approaches for the optimization of PV parameters such as light-harvesting properties, charge-mobility, open-circuit voltage and fill factor [14–16]. These analyses aim at developing active OPV materials that combine simple, cost-effective, clean and scalable syntheses [11,17,18]. In a recent analysis of the effects of replacing the outer phenyl rings of compound **1** by naphthyl groups we have shown that the introduction of a single  $\beta$ -naphthyl group leads to a five-fold increase of the hole-

mobility and to a significant improvement of PV conversion efficiency [19]. In the continuation of this systematic approach, we report here on a series of molecules in which a phenyl ring of compound **1** is replaced by methyl (**2**), *n*-Hexyl (**3**), heptafluoropentyl (**4**) and dioxaocetyl (**5**) groups (Fig. 1). Preliminary results on compounds **2** and **5** were recently reported [20,21], however, it was nevertheless interesting to resituate them in the more general context of the introduction of aliphatic groups in TPA-based D–A systems. The synthesis and characterization of the compounds are described and the relationships between their chemical structure, the electronic properties of the molecules and resulting materials and the characteristics of simple bi-layer solar cells based on these materials are discussed.

## 2. Results and discussion

Compounds **1**, **2** and **5** were synthesized according to the already reported procedures [14,20,21]. The synthesis of compounds **3** and **4** is depicted in Fig. 2. Buchwald–Hartwig amination of *N*-hexylaniline (**6**) with 1-bromo-4-iodobenzene (**7**) in the presence of *t*-BuOH and tris(dibenzylideneacetone)-dipalladium(0) in toluene at 50–60 °C gave bromide (**8**) in 33% yield. A Stille cross-

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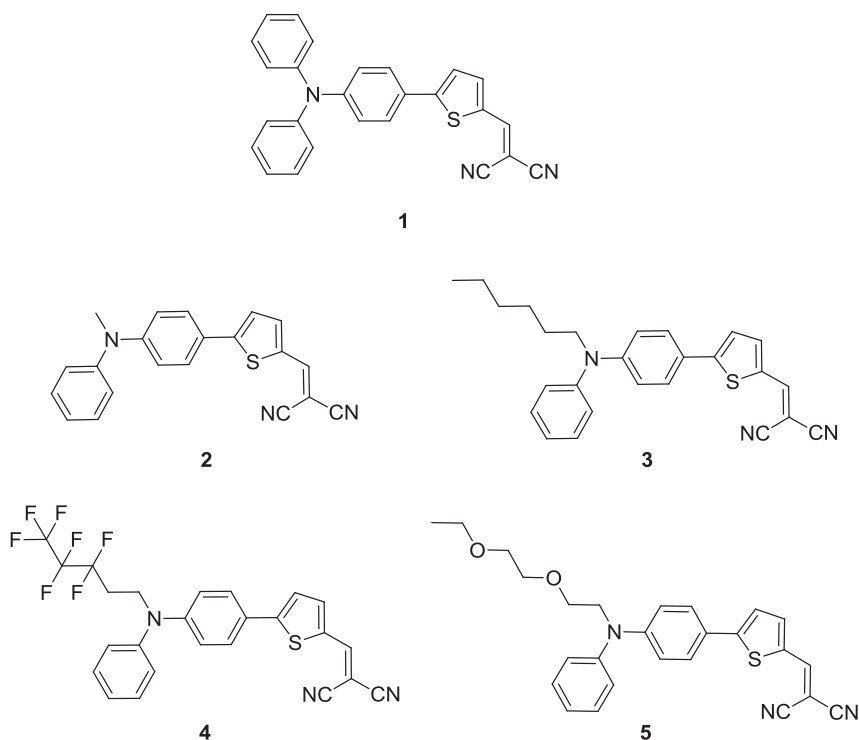


Fig. 1. Chemical structures of the target compounds.

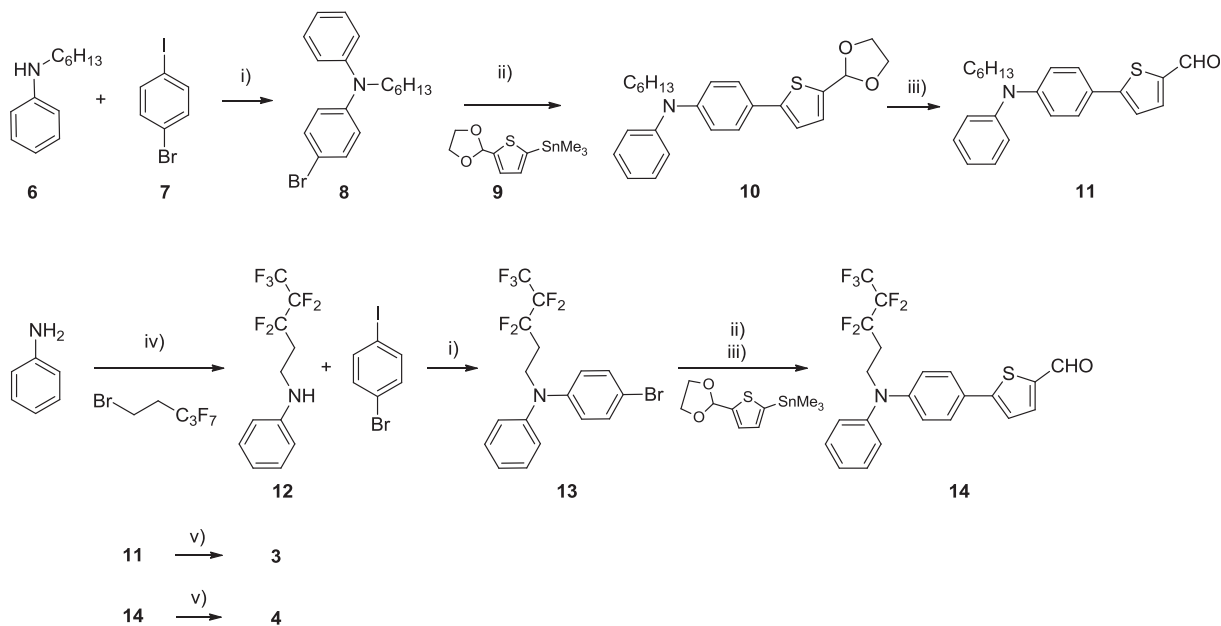


Fig. 2. Synthesis of the target compounds. i) *t*-BuOH, Tris(dibenzylideneacetone) dipalladium(0), Tris-*t*-butylphosphine, toluene, 55–120 °C; ii) Tetrakis(triphenylphosphine) palladium(0), toluene, 96–120 °C; iii) 1M HCl, acetone, room temp; iv) 140 °C, 12 h; v) malononitrile, Et<sub>3</sub>N, chloroform.

coupling reaction between bromide **8** and (5-(1,3-dioxolan-2-yl)thiophen-2-yl)trimethylstannane (**9**) in toluene at 120 °C led to compound **10** which was subsequently hydrolyzed with 1M HCl to give the aldehyde **11** in 30% yield. *N*-alkylation of aniline with 5-Bromo-1,1,1,2,2,3,3-heptafluoropentane at 140 °C, gave the secondary amine **12** in 94% yield. A Buchwald–Hartwig amination of **12** with **7** afforded the bromophenyl compound **13** in 24% yield. A Stille cross-coupling reaction of **13** with **9** in toluene at 96 °C and

hydrolysis with 1M HCl gave compound **14** in 21% yield. The final compounds **3** and **4** were obtained in 58 and 56% yield respectively by Knoevenagel condensation of aldehydes **11** and **14** with malononitrile in the presence of triethylamine in chloroform at room temperature.

The thermal properties and stability of compounds **1–5** have been investigated by differential scanning calorimetry (DSC) and thermal gravimetry (TGA). As a general trend, the replacement of

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