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Synthesis and photovoltaic properties of copolymers based on diketopyrrolopyrrole with broad absorption and high open-circuit voltage

Songting Tan

Xiangtan University, P R China

A series of donor-acceptor (D-A) conjugated polymers based on alkylthienyl-substituted benzodithiophene (BDTT) as electron-rich unit, diketopyrrolopyrrole (DPP) and DPP based side chain (TTDPP) as electron-deficient units have been designed and synthesized by Stille-coupling reaction. Compared with the binary copolymers, the random terpolymers exhibited broader absorption range. By tuning the ratio of DPP and TTDPP, the photophysical, electrochemical properties, lamellar distance, π - π^* stacking distance and photovoltaic properties of the random terpolymers were changed dramatically. Bulk heterojunction polymer solar cells based on the as-synthesized copolymers as electron donors and (6,6)-phenyl-C61-butyric acid methyl ester (PC₆₁BM) as the acceptor were fabricated. The best power conversion efficiency (PCE) of 4.46% (a short-circuit current (J_{sc}) of 12.05 mA cm⁻², an open-circuit voltage (V_{oc}) of 0.77 V and a fill factor (FF) of 49.0%) was obtained from terpolymer P4. As well as optimization on device performance via solution vapor annealing (SVA) are investigated. The binary copolymer P2 obtained the best power conversion efficiency (PCE) of 4.74% with the J_{sc} of 10.63 mA cm⁻², a high V_{oc} of 0.88 V and a FF of 51.0%.

tanst2008@163.com

Characterization and biotransformation of racemic analogues of potent calcium channel blockers

Jaspreet Kaur, Ranju Bansal and Anupreet Kaur

Panjab University, India

1,4-dihydropyridines also popular as calcium channel blockers have been widely used in the clinical medicine as potent drug candidates in the treatment of vasodilation and other cardiac disorders. This class of drug possesses the plethora of biological activities as a result of different functional groups substitutions on the Dihydropyridine (DHP) moiety. Such molecules possessing asymmetric carbon atom at position 4 become chiral, and thus exist as two stereo-isomers. The activity of each enantiomer may differ, one being calcium antagonist of the channel and the other as agonist. In the light of the structural and chiral variations of DHP moiety, it becomes important to investigate and establish the structures of these isomers in order to prepare the title compounds in enantiomerically pure form. For this purpose, racemic mixtures of these title compounds were synthesized and structures were elucidated via NMR, IR and MS analysis. Normal phase liquid chromatographic characterizations of the racemic mixtures have been optimized with retention time below 10 minutes. Further, the transformation on the racemic mixtures has been investigated by subjecting them to enzymatic treatment at different concentrations and temperatures. It has been found that enzymatic treatment with hydrolases has led to change in the optical rotation values indicating stereo selective transformation. Further work is being done to resolve them into enantiomerically pure compounds with chiral HPLC.

jaspreet_virdi@yahoo.com