On PCBM look-alikes showing unexpected properties

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Methanofullerene 'Phenyl-C61-butyric acid methyl ester' (PCBM)is presently used as the standard molecular acceptor material in donor-acceptor bulk-heterojunction composites. Up to now, blends of PCBM and conjugated polymers show the highest solar energy conversion efficiency in 'plastic' PV devices. The present record is close to 3a PCBM:MDMO-PPV 4:1 mixture. We now report on the synthesis, characterization, and functional properties of a number of structural analogs of PCBM. Several series of compounds were prepared. First, a series in which the ester was changed from methyl to an increasingly larger substituent. Second, a series in which parts of the addend in PCBM were removed. Third, a series of PCBM look-alikes in which the phenyl group was substituted at various positions. While the first two series of compounds mainly showed large variations in solubility and miscibility, the latter group of compounds showed quite interesting differences in the first reduction potential. These differences are somewhat unexpected in the framework of previously published data and hypotheses. A new working hypothesis explaining these differences will be presented. Since the open circuit voltage of the PV devices is directly infuenced by the position of the first reduction potential of the acceptor, the above mentioned structural variations may lead to more efficient bulk-heterojunction materials.