Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

Photovoltaic and field effect transistor performance of selenophene and thiophene diketopyrrolopyrole co-polymers with dithienothiophene

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Supporting Information.

DFT calculations for the different isomers of the DTT-DPP trimer.

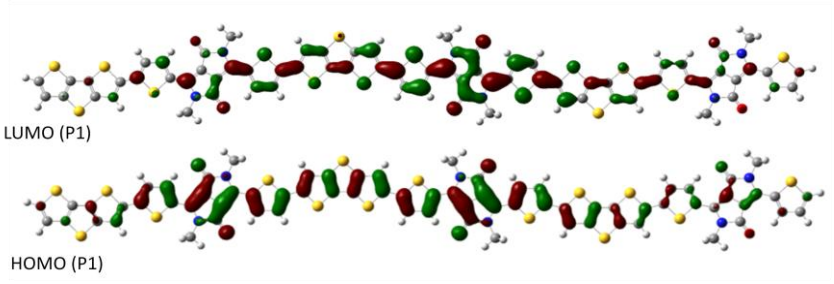

Figure S1. Energy-minimised structure of a methyl-substituted trimers of **P1** with all anti conformations (Heteroatom pointing towards N lactam)

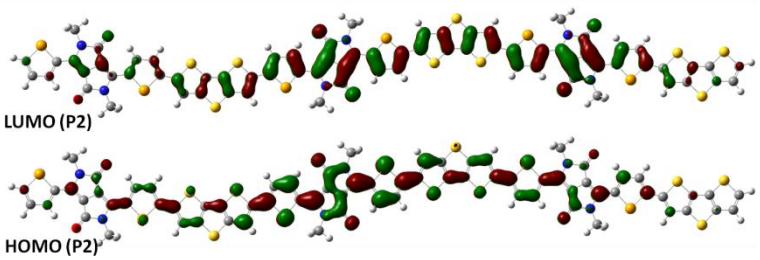

Figure S2. Energy-minimised structure of a methyl-substituted trimers of **P2** with all anti conformations (Heteroatom pointing towards N lactam)

Table S1. Calculated HOMO – LUMO for polymers with anti conformations

	HOMO (eV)	LUMO (eV)
P1; S towards N-CH_3	-4.71	-3.04
P2; Se towards N-CH_3	-4.69	-3.07

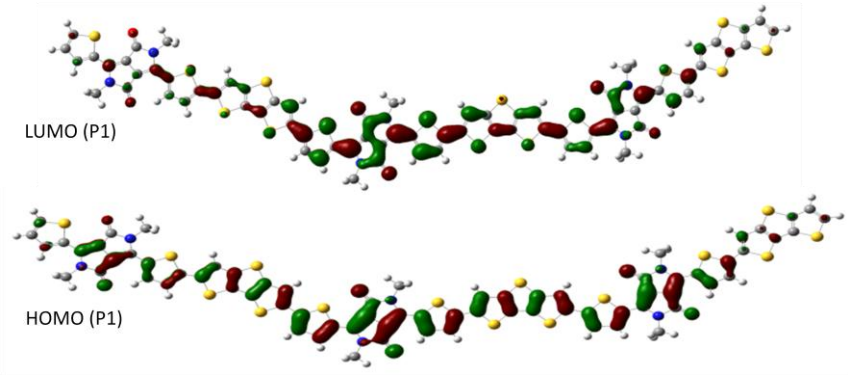

Figure S3. Energy-minimised structure of a methyl-substituted trimers of **P1** with with one syn and one anti conformation per DPP unit.

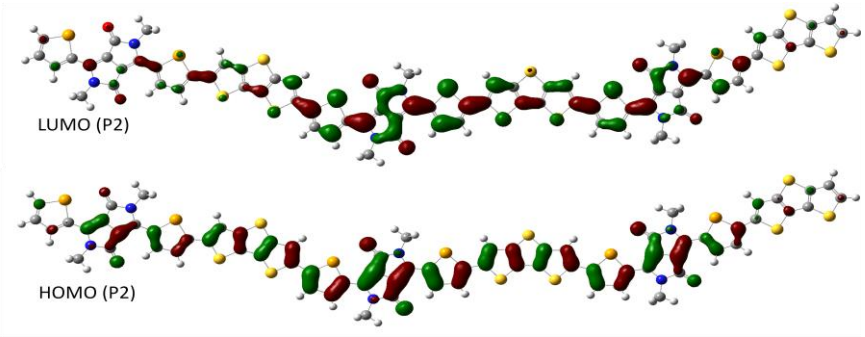

Figure S4. Energy-minimised structure of a methyl-substituted trimers of **P2** with with one syn and one anti conformation per DPP unit.

Table S2. Calculated HOMO – LUMO values for polymers with one syn and one anti conformation

	HOMO (eV)	LUMO (eV)
P1; Alternate S towards O and N (syn)	-4.71	-3.00
P2; Alternate Se towards O and N (syn)	-4.69	-3.04