TD-DFT Simulation and Experimental Studies of a Mirrorless Lasing of Poly[(9,9-Dioctylfluorenyl-2,7-diyl)-co-(1,4-Diphenylene-Vinylene-2-Methoxy-5-{2-Ethylhexyloxy}-Benzene)]

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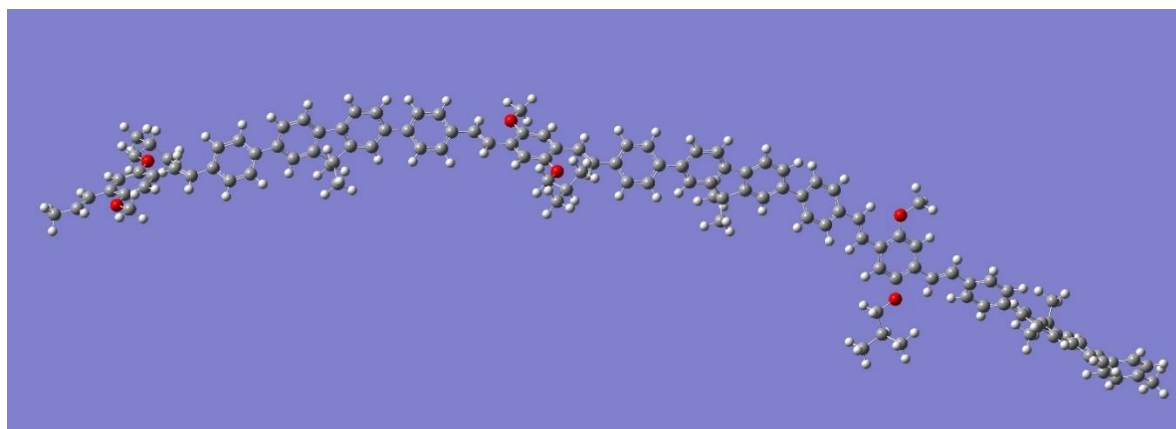*****   Correspondence: malsalhi@ksu.edu.sa; Tel.: +966-50-510-4815.

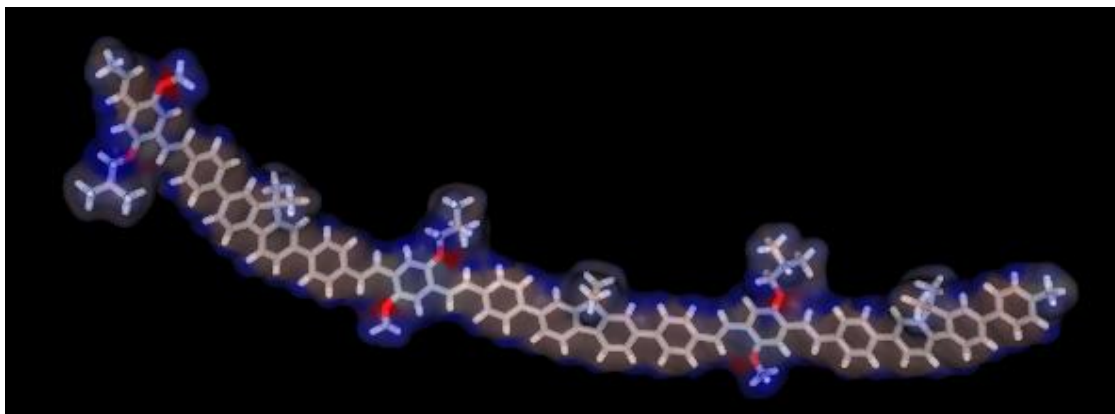Figure S1 Optimized structure of the copolymer PFO-co-PPV-MEHB Using DFT calculations.

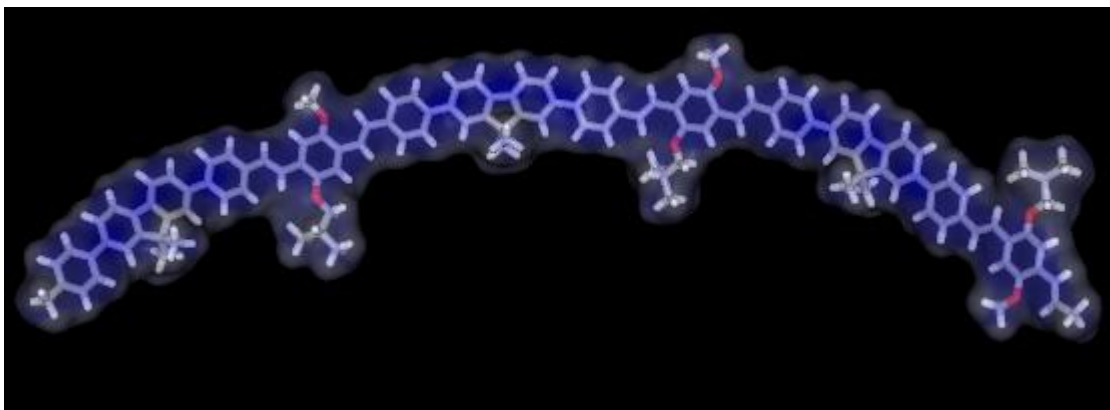Figure S2 a. Charge distribution of PFO-co-PPV-MEHB (tail-truncated and n= 3 model)

Figure S2 b. Polarizability of PFO-co-PPV-MEHB is 229.15 $Å^3$ (tail-truncated and n= 3 model)
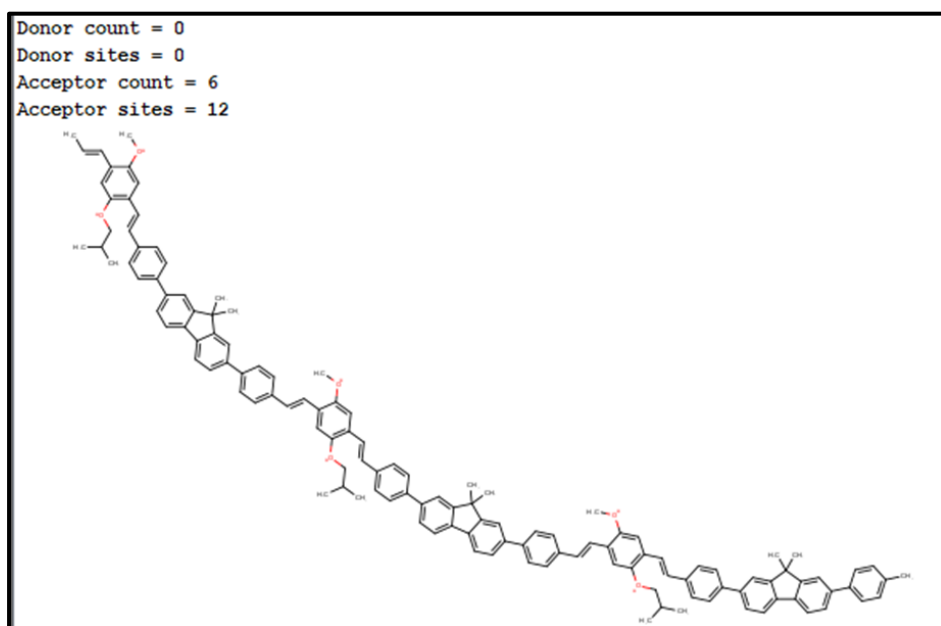

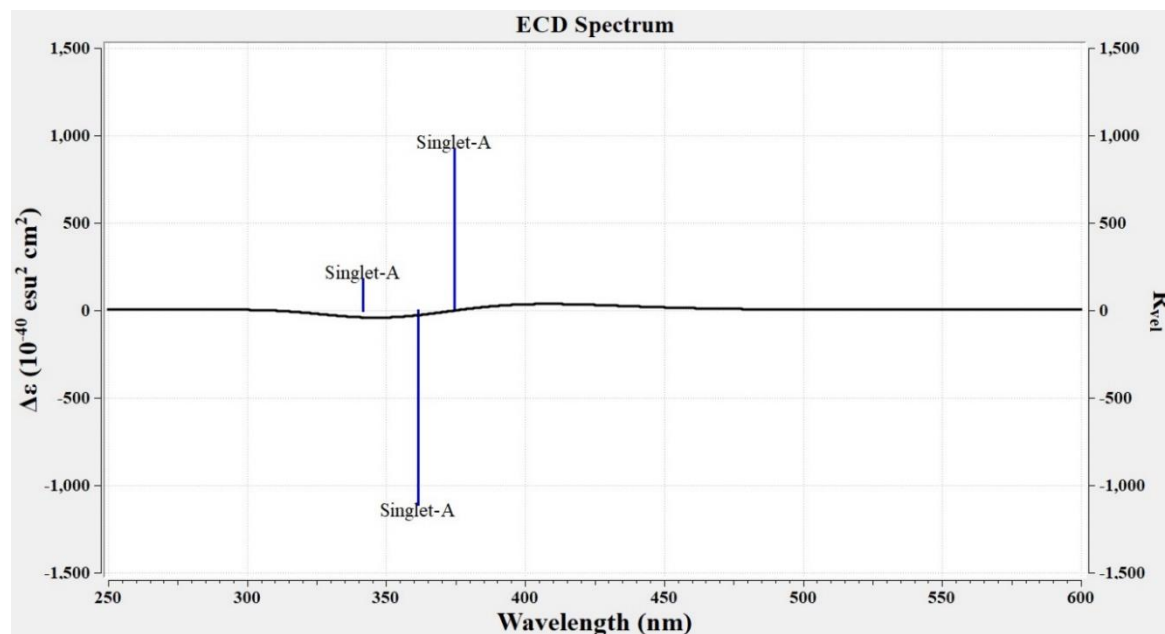Figure S2 c. H bond donor acceptor of PFO-co-PPV-MEHB (tail-truncated and n= 3 model).

Figure S3. Electronic circular dichroism (ECD) of PFO-co-PPV-MEHB (tail-truncated and n= 3 model) calculated using the CAM-B3LYP/6-31G(d,p) basis set.
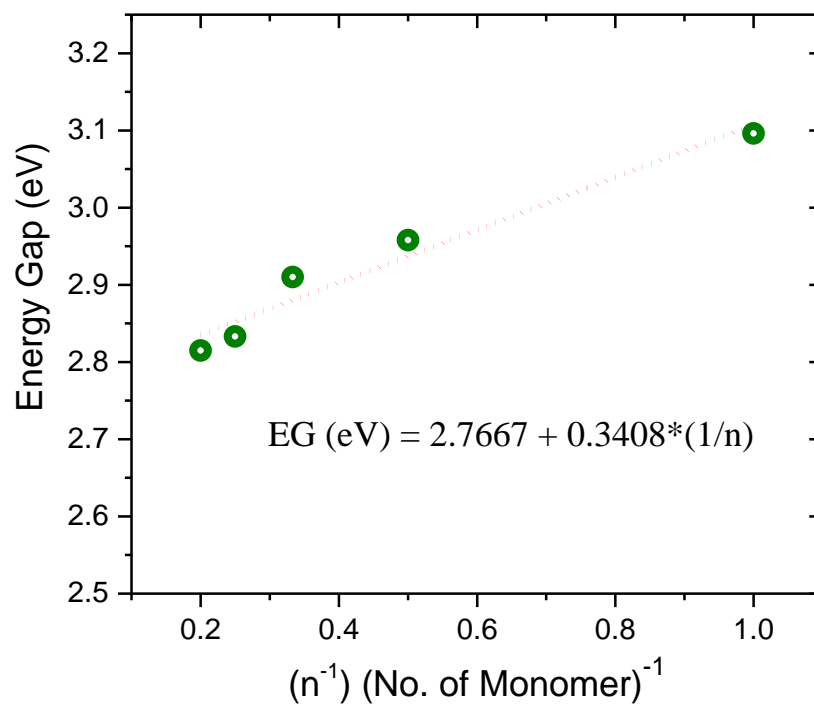

$$EG\ (eV) = 2.7667 + 0.3408*(1/n)$$

Figure S4 Estimation of HOMO−LUMO gaps for PFO-co-PPV-MEHB using bandgap extrapolation of oligomers (n =1 to 5).