Supplementary Materials

Table S1. Details of the TD-DFT reveal the following, electron density isocontour plots for energy levels above and below the band gap edge and the orbitals involved in the strongest transitions seen in the simulated optical absorptions spectrum. Energy of optical absorption (eV), wavelength of optical absorption (nm), Oscillator strength (*f*), orbital involved and coefficient representing the contribution of the respective excitation to the wave function expansion.

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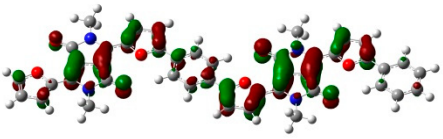
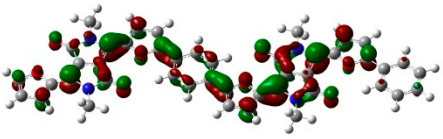
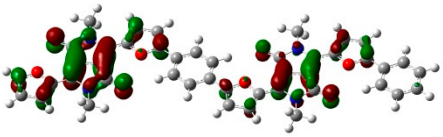
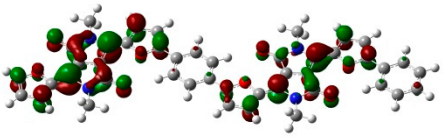
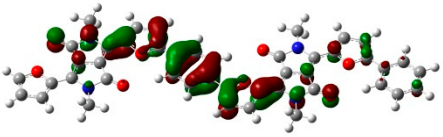
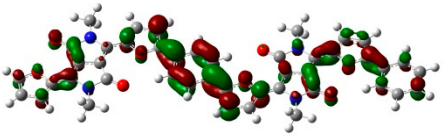
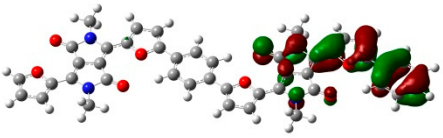
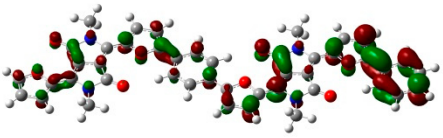
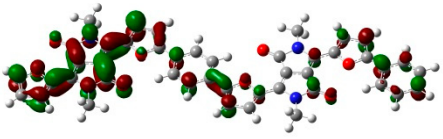
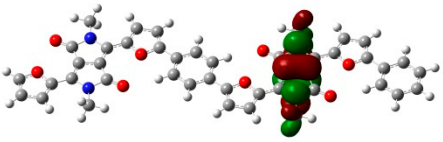
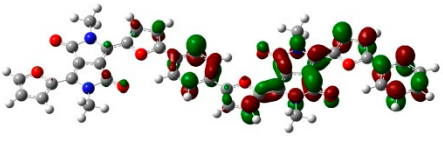
HOMO (H)		LUMO (L)	
H − 1		L + 1	
H − 2		L + 2	
H − 3		L + 3	
H − 4		L + 4	
H − 5		L + 5	

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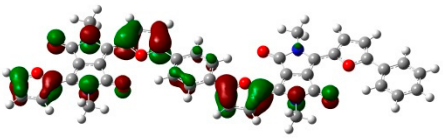
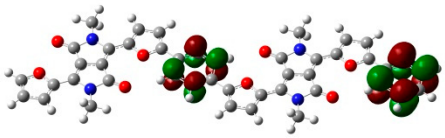
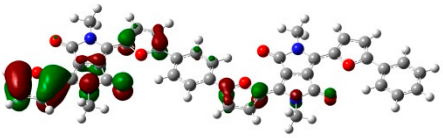
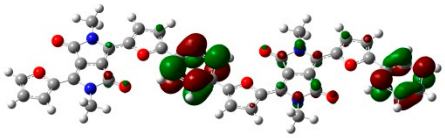
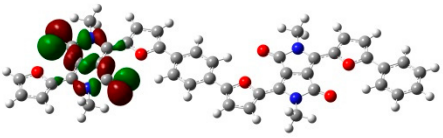
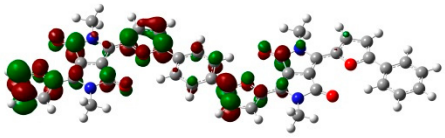
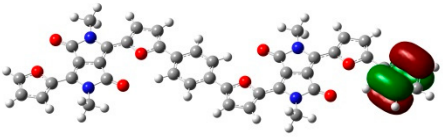
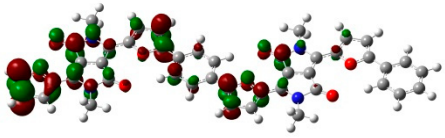
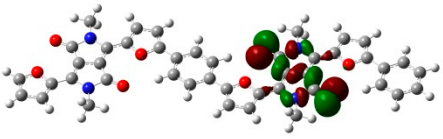
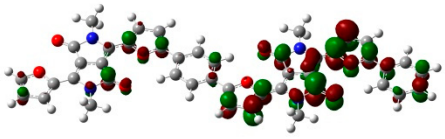
H − 6		L + 6	
H − 7		L + 7	
H − 8		L + 8	
H − 9		L + 9	
H − 10		L + 10	
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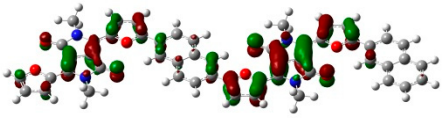
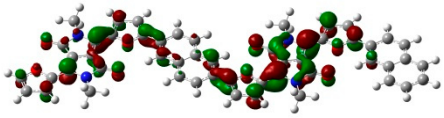
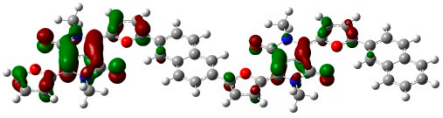
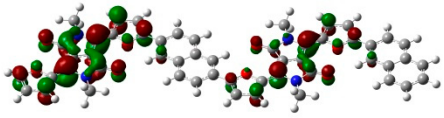
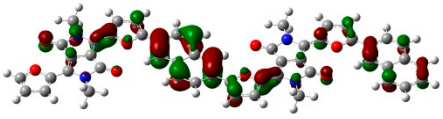
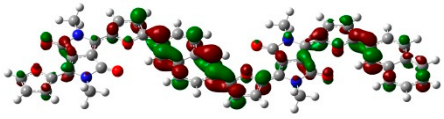
HOMO (H)		LUMO (L)	
H − 1		L + 1	
H − 2		L + 2	

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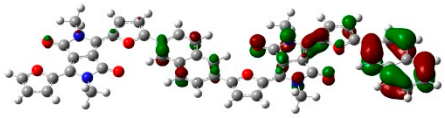
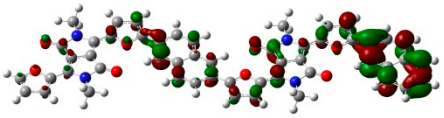
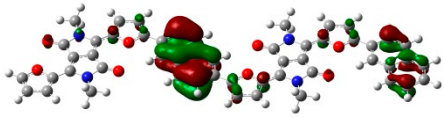
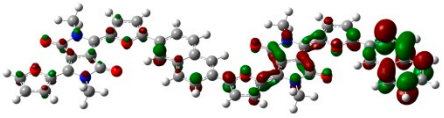
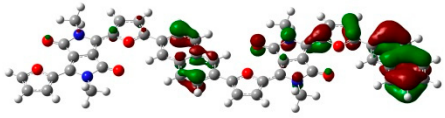
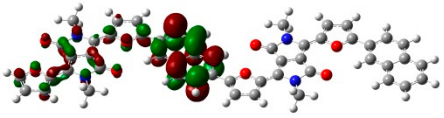
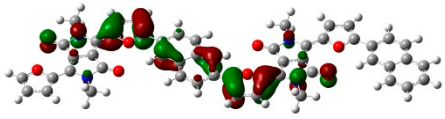
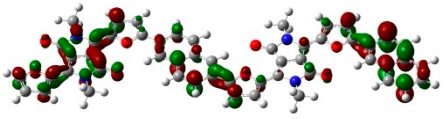
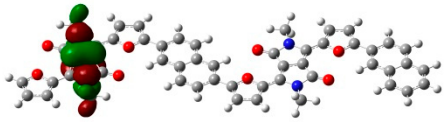
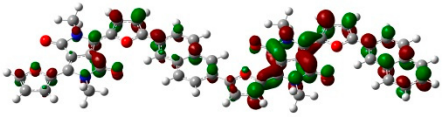
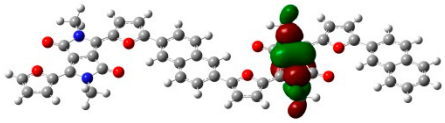
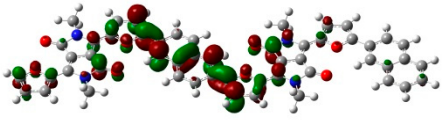
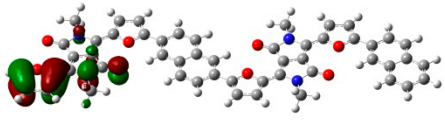
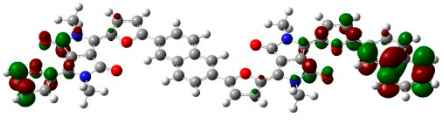
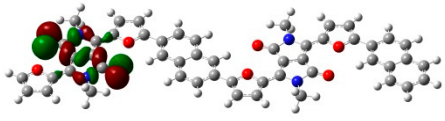
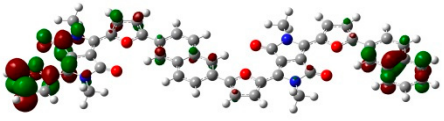
H – 3		L + 3	
H – 4		L + 4	
H – 5		L + 5	
H – 6		L + 6	
H – 7		L + 7	
H – 8		L + 8	
H – 9		L + 9	
H – 10		L + 10	

Table S1. *Cont.*

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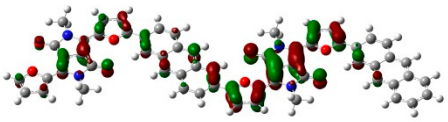
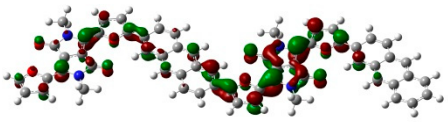
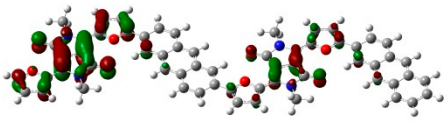
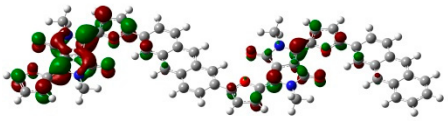
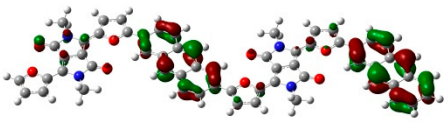
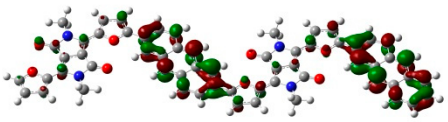
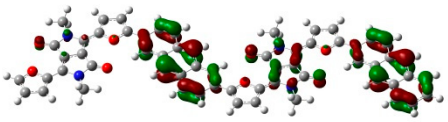
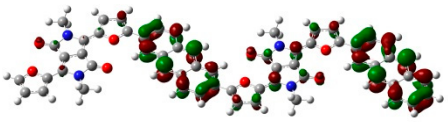
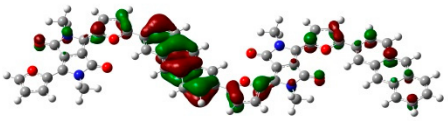
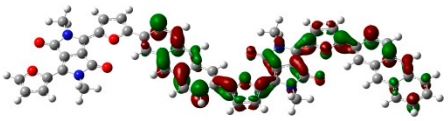
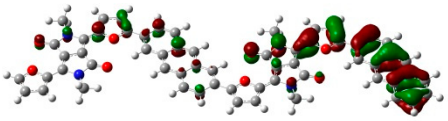
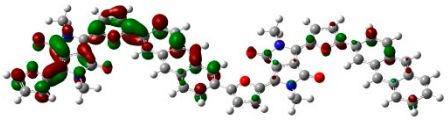
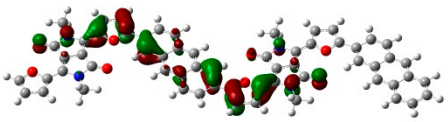
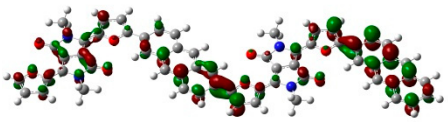
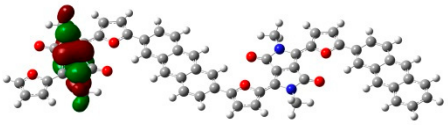
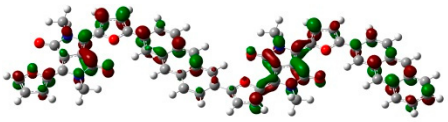
HOMO (H)		LUMO (L)	
H − 1		L + 1	
H − 2		L + 2	
H − 3		L + 3	
H − 4		L + 4	
H − 5		L + 5	
H − 6		L + 6	
H − 7		L + 7	

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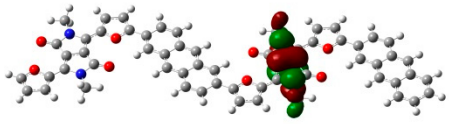
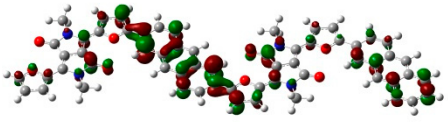
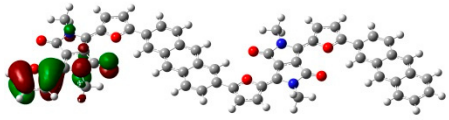
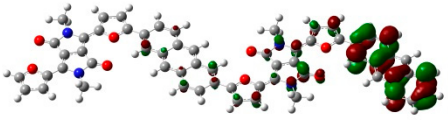
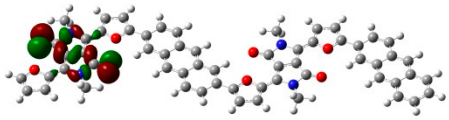
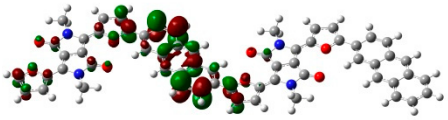
H − 8		L + 8	
H − 9		L + 9	
H − 10		L + 10	
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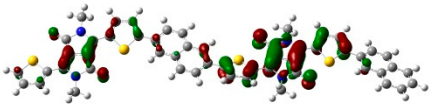
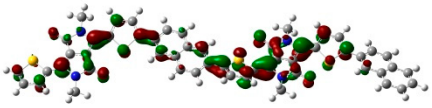
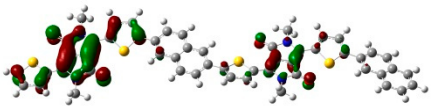
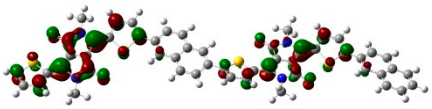
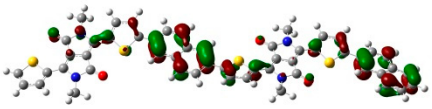
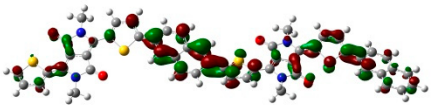
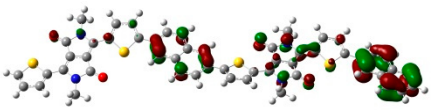
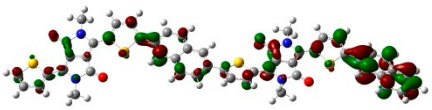
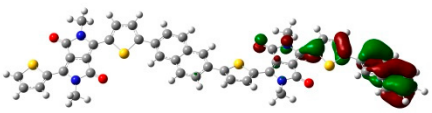
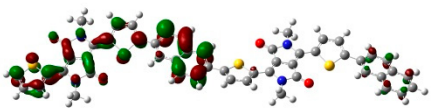
HOMO (H)		LUMO (L)	
H – 1		L + 1	
H – 2		L + 2	
H – 3		L + 3	
H – 4		L + 4	

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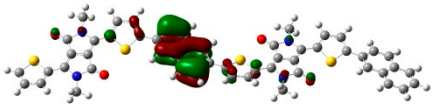
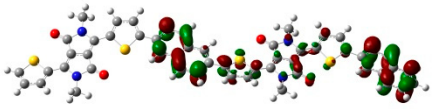
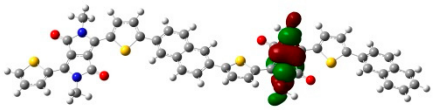
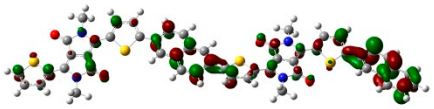
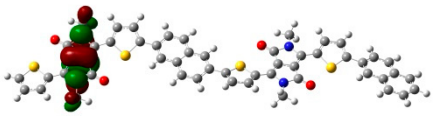
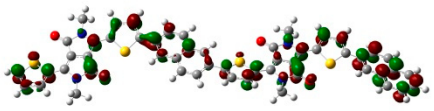
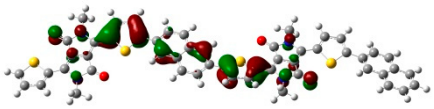
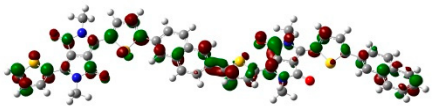
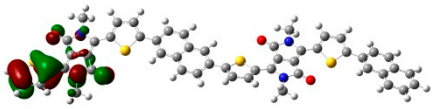
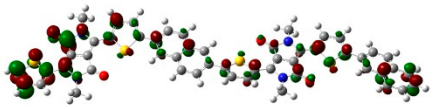
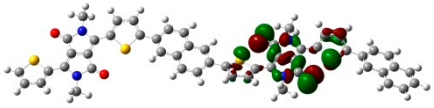
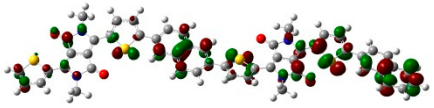
H – 5		L + 5	
H – 6		L + 6	
H – 7		L + 7	
H – 8		L + 8	
H – 9		L + 9	
H – 10		L + 10	

Table S2. Energy of optical absorption, wavelength of optical absorption, oscillator strength (*f*), orbitals involved and coefficient representing the contribution of the respective excitation to the wave function expansion.

DPP-FPF		
1.8897 eV	656.11 nm	f = 1.2969
HOMO	LUMO	0.70763
2.4353 eV	509.11 nm	f = 0.3406
HOMO − 1	LUMO	0.13446
HOMO − 1	LUMO + 1	0.66145
HOMO	LUMO + 1	0.16964
3.0827 eV	402.20 nm	f = 0.2475

Table S2. *Cont.*

HOMO − 3	LUMO	0.35214
HOMO − 2	LUMO	0.2098
HOMO − 2	LUMO + 1	0.28284
HOMO − 1	LUMO + 2	−0.32876
HOMO	LUMO + 2	0.26248
3.1650 eV	391.74 nm	f = 0.1916
HOMO − 3	LUMO	−0.22659
HOMO − 3	LUMO + 1	0.10742
HOMO − 2	LUMO	−0.20902
HOMO − 2	LUMO + 1	0.37869
HOMO − 1	LUMO + 2	−0.34253
3.5701 eV	347.28 nm	f = 0.1976
HOMO − 7	LUMO	−0.17183
HOMO − 3	LUMO + 1	−0.41578
HOMO − 2	LUMO + 1	0.11131
HOMO − 1	LUMO + 3	0.13116
HOMO	LUMO + 3	0.46861
HOMO	LUMO + 4	−0.12929
4.0058 eV	309.51 nm	f = 0.1954
HOMO − 9	LUMO	0.10351
HOMO − 7	LUMO	0.48913
HOMO − 7	LUMO + 1	−0.16316
HOMO − 6	LUMO + 1	−0.18302
HOMO	LUMO + 4	−0.37922
4.0940 eV	302.84 nm	f = 0.1460
HOMO − 7	LUMO	0.16201
HOMO − 6	LUMO	−0.19355
HOMO − 6	LUMO + 1	0.35101
HOMO − 2	LUMO + 2	0.31564
HOMO − 1	LUMO + 4	−0.32399
HOMO	LUMO + 5	0.25356
DPP-FNF		
1.8992 eV	652.83 nm	f = 1.2325
HOMO	LUMO	0.70497
2.3706 eV	523.01 nm	f = 0.3327
HOMO − 1	LUMO	−0.14487
HOMO − 1	LUMO + 1	0.65783
HOMO	LUMO + 1	0.17556
2.8514 eV	434.82 nm	f = 0.1243
HOMO − 3	LUMO	0.59056
HOMO − 3	LUMO + 1	0.13625
HOMO − 2	LUMO + 1	0.22451
HOMO − 1	LUMO + 2	0.15533
HOMO	LUMO + 3	0.19881

Table S2. *Cont.*

3.2531 eV	381.13 nm	f = 0.1996
HOMO − 5	LUMO	−0.26877
HOMO − 4	LUMO	0.55956
HOMO − 3	LUMO + 1	0.11574
HOMO	LUMO + 2	0.10786
HOMO	LUMO + 5	0.1806
3.3783 eV	367.00 nm	f = 0.2836
HOMO − 5	LUMO	0.45593
HOMO − 5	LUMO+ 1	0.16772
HOMO − 4	LUMO	0.21159
HOMO − 3	LUMO + 1	0.10948
HOMO − 1	LUMO + 4	−0.10657
HOMO	LUMO + 3	−0.35055
HOMO	LUMO + 4	0.14335
3.9173 eV	316.50 nm	f = 0.1747
HOMO − 9	LUMO	-0.25896
HOMO − 9	LUMO + 1	0.12111
HOMO − 6	LUMO + 1	0.24399
HOMO − 2	LUMO + 2	0.54119
3.9173 eV	316.50 nm	f = 0.1747
HOMO − 9	LUMO	-0.25896
HOMO − 9	LUMO + 1	0.12111
HOMO − 6	LUMO + 1	0.24399
HOMO − 2	LUMO + 2	0.54119
3.9335 eV	315.20 nm	f = 0.1429
HOMO − 8	LUMO + 1	-0.13755
HOMO − 6	LUMO	0.11722
HOMO − 3	LUMO+ 2	0.13696
HOMO − 1	LUMO+4	0.33792
HOMO − 1	LUMO+6	-0.18371
HOMO	LUMO+5	0.13222
HOMO	LUMO+6	0.45705
HOMO	LUMO+7	-0.11387
	DPP-FAF	
1.8370 eV	674.95 nm	f = 1.2488
HOMO	LUMO	0.70187
2.2897 eV	541.48 nm	f = 0.2585
HOMO − 3	LUMO	0.11214
HOMO − 2	LUMO	−0.2093
HOMO − 1	LUMO + 1	0.64503
2.8199 eV	439.68 nm	f = 0.2328
HOMO − 3	LUMO	−0.1814
HOMO − 3	LUMO + 1	0.15127
HOMO − 2	LUMO + 1	0.15769
HOMO	LUMO + 3	0.61742

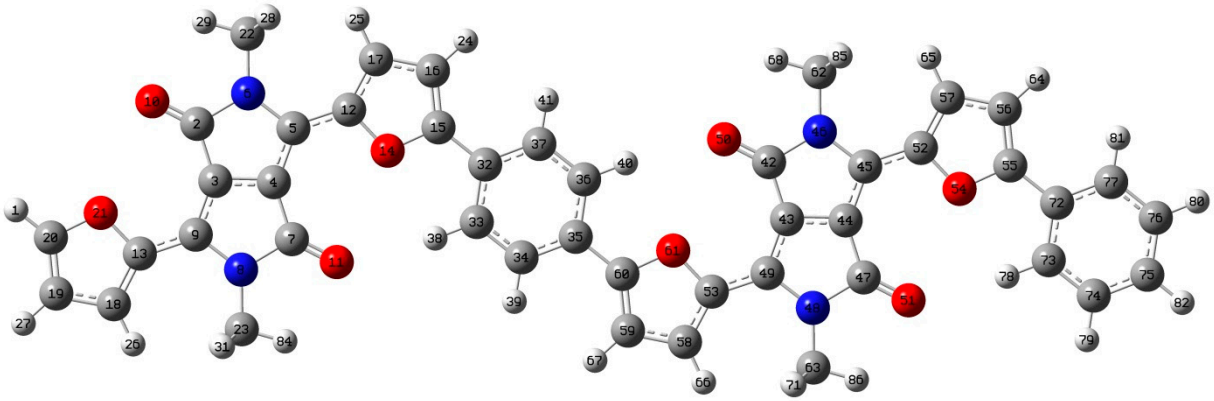
Table S2. *Cont.*

3.2013 eV	387.29 nm	f = 0.2946
HOMO − 8	LUMO	−0.11718
HOMO − 5	LUMO	0.47574
HOMO − 5	LUMO + 1	−0.11222
HOMO − 4	LUMO + 1	0.15448
HOMO − 2	LUMO + 2	−0.31581
HOMO − 1	LUMO + 4	0.14478
HOMO	LUMO + 4	0.15445
HOMO	LUMO + 5	0.18787
3.5261 eV	351.62 nm	f = 0.5316
HOMO − 6	LUMO + 1	-0.24882
HOMO − 5	LUMO	0.2459
HOMO − 5	LUMO + 1	0.368
HOMO − 3	LUMO + 3	−0.15318
HOMO − 2	LUMO + 4	0.11356
HOMO − 1	LUMO + 4	−0.15725
HOMO − 1	LUMO + 5	−0.1214
HOMO	LUMO + 5	−0.31984
HOMO	LUMO + 6	0.1177
4.0414 eV	306.79 nm	f = 0.1273
HOMO − 9	LUMO	−0.17423
HOMO − 6	LUMO + 2	0.19378
HOMO − 3	LUMO + 5	−0.18321
HOMO − 2	LUMO + 4	0.23448
HOMO − 2	LUMO + 5	0.2287
HOMO − 2	LUMO + 6	0.10754
HOMO − 1	LUMO + 6	0.27751
HOMO − 1	LUMO + 7	0.1555
HOMO	LUMO + 7	0.32172
DPP-TNT		
1.9243 eV	644.30 nm	f = 1.6251
HOMO	LUMO	0.70428
2.3443 eV	528.86 nm	f = 0.4020
HOMO − 1	LUMO	−0.12455
HOMO − 1	LUMO + 1	0.67192
HOMO − 1	LUMO + 1	0.15641
2.8733 eV	431.51 nm	f = 0.2056
HOMO − 3	LUMO	0.53497
HOMO − 2	LUMO + 1	0.26751
HOMO − 1	LUMO + 2	0.25186
HOMO	LUMO + 2	−0.11072
HOMO	LUMO + 3	−0.11072

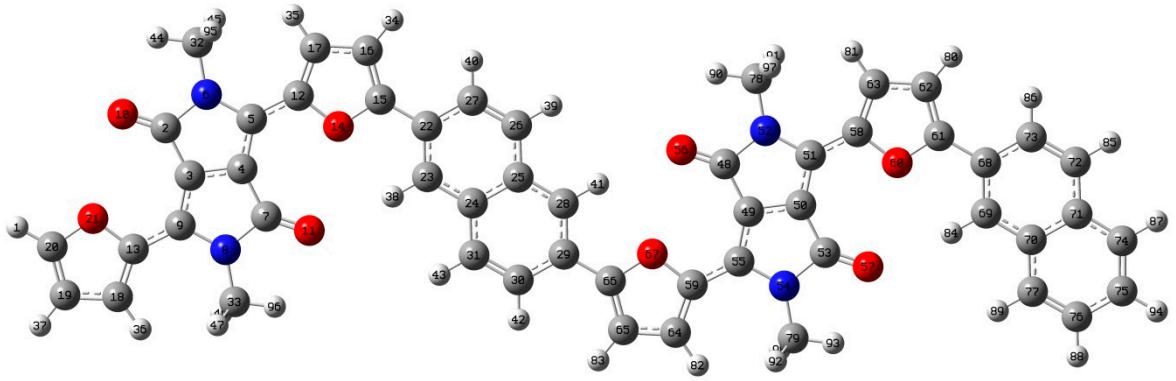
Table S2. *Cont.*

2.9849 eV	415.37 nm	f = 0.1212
HOMO − 3	LUMO	−0.15762
HOMO − 3	LUMO + 1	−0.166
HOMO − 2	LUMO	0.27695
HOMO − 2	LUMO + 1	0.28991
HOMO − 1	LUMO + 2	0.33613
HOMO − 1	LUMO + 3	0.10874
HOMO	LUMO + 2	0.36993
3.3647 eV	368.48 nm	f = 0.1857
HOMO − 10	LUMO	0.25314
HOMO – 10	LUMO + 1	0.15559
HOMO − 5	LUMO	−0.12402
HOMO − 4	LUMO	0.47092
HOMO − 4	LUMO + 1	0.21933
HOMO − 1	LUMO + 3	−0.11915
HOMO	LUMO + 3	−0.20658
HOMO	LUMO + 5	−0.10067
3.8733 eV	320.10 nm	f = 0.1539
HOMO − 9	LUMO	−0.11564
HOMO − 8	LUMO	−0.11283
HOMO − 8	LUMO + 1	−0.15158
HOMO − 7	LUMO	0.25639
HOMO − 7	LUMO + 1	0.27157
HOMO − 6	LUMO	0.16778
HOMO − 6	LUMO + 1	−0.28683
HOMO − 1	LUMO + 5	−0.11649
HOMO − 1	LUMO + 6	−0.10707
HOMO	LUMO + 6	0.34125

C44H30N4O8														
D(3,9,13,21)	0.0087	D(6,5,12,17)	-0.0072	D(16,15,32,37)	0.0114	D(36,35,60,61)	0.0081	D(43,49,53,61)	-0.0115	D(46,45,52,57)	-0.0250	D(56,55,72,77)	0.0174
D(8,9,13,18)	0.0100	D(4,5,12,14)	-0.0029	D(14,15,32,33)	0.0098	D(34,35,60,59)	0.0081	D(48,49,53,58)	-0.0082	D(44,45,52,54)	-0.0217	D(54,55,72,73)	0.0186

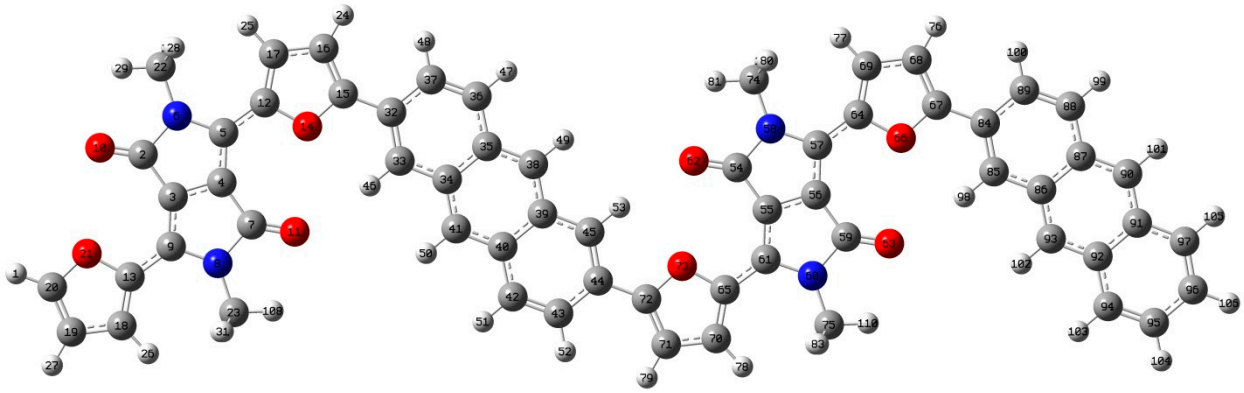


C52H34N4O8														
D(3,9,13,21)	-0.0076	D(6,5,12,17)	-0.0028	D(16,15,22,27)	0.0028	D(28,29,66,67)	-0.0063	D(49,55,59,67)	0.0000	D(52,51,58,63)	-0.0073	D(62,61,68,73)	0.0014
D(8,9,13,18)	-0.0079	D(4,5,12,14)	-0.0017	D(14,15,22,23)	0.0011	D(30,29,66,65)	-0.0079	D(54,55,59,64)	0.0018	D(50,51,58,60)	-0.0083	D(60,61,68,69)	0.0016

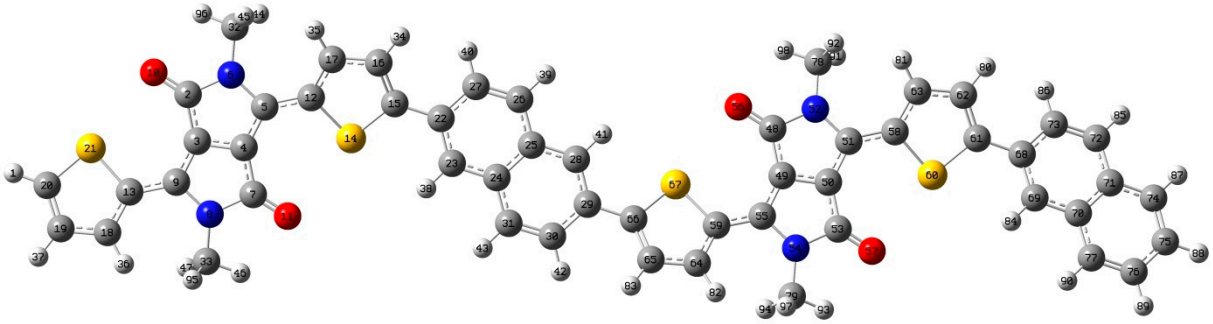


Scheme S1. *Cont.*

C60H38N4O8														
D(3,9,13,21)	0.0049	D(6,5,12,17)	0.0003	D(16,15,32,37)	-0.0063	D(45,44,72,73)	0.0063	D(55,61,65,73)	-0.0117	D(58,57,64,69)	-0.0093	D(68,67,84,89)	0.0088
D(8,9,13,18)	0.0053	D(4,5,12,14)	0.0032	D(14,15,32,33)	-0.0046	D(43,44,72,71)	0.0070	D(60,61,65,70)	-0.0179	D(56,57,64,66)	-0.0061	D(66,67,84,85)	0.0071



C52H34N4O4S4 (-4114.71010312)														
D(3,9,13,21)	-9.9538	D(6,5,12,17)	-12.0788	D(16,15,22,27)	21.2857	D(28,29,66,67)	-22.1440	D(49,55,59,67)	3.2358	D(52,51,58,63)	-8.1389	D(60,61,68,69)	22.6283
D(8,9,13,18)	-10.2236	D(4,5,12,14)	-11.9722	D(14,15,22,23)	20.7067	D(30,29,66,65)	-22.3107	D(54,55,59,64)	3.2130	D(50,51,58,60)	-8.0012	D(62,61,68,73)	22.9294



Scheme S1. Planarity information of the dimer analogues for the investigated polymers according to G09 geometry optimization for the four dimers (side chains: –CH3). Dihedral angles in degrees.